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The structural variation of Ca-carbonate grown in the presence of mono-L-glutamic and mono-L-aspartic acid

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Declaration

To the best of my knowledge and belief this thesis contains no material previously published by any other person except where due acknowledgment has been made.

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university.

Signature: .....

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Abstract

Over the past four decades, the interest in biomineralisation has rapidly increased, helped along by an enormous improvement in analytical instrument capabilities. The main driving forces came initially from the field of medical and biochemical research, but the extraordinary characteristics of biologically produced materials (nano-composites) have also encouraged the involvement of scientists from other disciplines, in particular material scientists, who hope that the next industrial revolution will be driven by nano-technology, either through bio-mimicking or bio-inspired new materials

This research will focus on providing evidence to clarify an uncertainty in relation to Ca-carbonate biomineralisation. A lot is known about the effect of organic substances on the polymorph and morphology of Ca-carbonate grown in their presence, but it is not clear if only the organic template and/or soluble molecules (be they natural or synthetic) direct the growth through simple structural similarity (i.e. epitaxially) or if other phenomena are involved. The production of thick amorphous layers of Ca-carbonate and the discovery of a liquid amorphous precursor has added some uncertainty about the role of the organic component. This role will be investigated using different amino-acids and varying a number of physical and chemical factors.

The influence of two amino-acids commonly found in biomineralisation systems, namely L-glutamic acid (GLU) and L-aspartic acid (ASP) on the phase, abundance and morphology of $CaCO_3$ as a function of concentration, sequence and duration of addition, and harvesting time was investigated. Ninety-six independent samples were produced, covering a wide range of organic additive concentration, harvesting time, and reactant solution as summarized in the table below.

ASPARTIC and GLUTAMIC ACID Sample Production Matrix									
Concentration of the acid	Method A			Method C			Method D		
	Harvesting time			Harvesting time			Harvesting time		
	1 hour	1 day	1 week	1 hour	1 day	1 week	1 hour	1 day	1 week
1000 mg/L	x	x	x	x	x	x	x	x	x
100 mg/L	x	x	x	x	x	x	x	x	x
10 mg/L	x	x	x	x	x	x	x	x	x
Concentration of the acid	Method B			Method E			Method F		
	Harvesting time			Harvesting time			Harvesting time		
	1 hour	1 day	1 week	1 hour	1 day	1 week	1 hour	1 day	1 week
1000 mg/L	x	x	x	x	x	x	x	x	x
100 mg/L	x	x	x						
10 mg/L	x	x	x	x	x	x	x	x	x

The methods indicated in the table represent pairs of experiments, with methods A, C, D indicating that the precipitation experiment itself was carried out over a very short time interval of about 5 min., while the corresponding methods B, E, F use the same parameters, except for the duration of the precipitation experiment, which was slower at about 20-25 min.

For method A and B all reagents were added simultaneously to a solution containing just the organic acid at the required concentration.
For method C and E the Ca was already present in solution with the organic acid at the required concentration and the remainder was added to it.
For method D and F the CO_3^{2-} was already in solution with the organic acid and the remainder was added to it.

The precipitates produced were vacuum filtered and air dried and the samples were subsequently analysed by means of Synchrotron Radiation Diffraction (SXRPD), Neutron Diffraction (NPD), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM) and other techniques.

The main phases of $CaCO_3$ produced were calcite and vaterite, and their abundance was found to be strongly dependent on the concentration of the organic additive. At the highest concentration of the additives (1000 mg/L), vaterite was produced almost

exclusively with only traces of calcite present in 73% of the samples, independent of the harvesting time. Harvesting time played a crucial role in samples produced at the lowest concentration (10 mg/L), where initially produced vaterite was completely transformed to calcite after a day in all samples analysed. It also played a significant role in samples produced at intermediate concentration (100 mg/L) of any of the organic additives, where vaterite in all samples but one was transformed fully into calcite after a week.

The sequence of addition and the duration of addition impacts phase abundance, crystallite size and strain. The influence, however, is strongly dependent on the concentration of the amino acid; at the lowest concentration of 10 mg/L it is the duration of addition which has the strongest impact, at 100 mg/L it is a combination of sequence of addition and duration, with the former more influential. At a concentration of 1000 mg/L of amino acid, it is the amino acid that drives phase selection, crystallite size and strain. The main influence of the sequence of addition and duration of addition is on the crystallite size and strain present in the polymorphs, with higher concentrations of the organic additives resulting in smaller crystallites. Harvesting time influenced average crystallite size and strain for initially produced polymorphs, with size increasing and strain decreasing for most samples over time as expected. The results show variability related to the concentration of the amino acid, with concentrations of 1000 mg/L showing an increase in strain and decrease in crystallite size for about 30% of the samples harvested after one day when compared to samples harvested after one hour. Samples harvested after one week showed the opposite trend, with crystallite size increasing and strain decreasing.

The simple amino acids used in this study of Ca-carbonate phase selection and morphology, using varying concentration, addition sequences and harvesting times will help in developing a better understanding of the impact these factors have on the crystallisation of $CaCO_3$, a point raised in the comprehensive review presented by Sommerdijk and de With (2008), where it is stressed that the kinetics of the precipitation methods used strongly influence the outcome. The study presented here clearly shows that kinetics are only one factor, while the concentration and

availability of CO_2, of Ca and of the amino acid have an important role to play, particularly at lower amino acid concentrations.

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List of abbreviations

2D	Two dimensional
3D	Three dimensional
AA	Amino acid
ACC	Amorphous Ca-carbonate
ANSTO	Australian Nuclear Science and Technology Organisation
APS	Advanced Photon Source
ASP	Mono-L-aspartic acid
CaCl	Ca-chloride
CIF	Crystallographic information file or framework
CSIRO	Commonwealth Scientific and Industrial Research Organisation
D	Day
DNA	Deoxyribonucleic acid
esd	Estimated standard deviation
EXAFS	Extended X-ray absorption fine structure
FIZ	Fachinformationszentrum Karlsruhe
FTIR	Fourier transform infra-red
FWHM	Full width at half maximum
GLU	Mono-L-glutamic acid
GRETEP	Grenoble Thermal Ellipsoids Plot Program
H	Hour
HRPD	High resolution powder diffraction
ICSD	Inorganic Crystal Structure Database
IR	Infra-red
keV	Kilo electron Volt
LB	Langmuir-Blodgett
LBF	Langmuir-Blodgett film
MDI	Materials Data, Inc.
NaHCO	Sodium-bicarbonate
NPD	Neutron powder diffraction
NIST	National Institute of Standards and Technology
PILP	Polymer-induced liquid precursor
PVII	Pearson VII function
REE	Rare earth element
SAM	Self-assembled monolayer
SEM	Scanning electron microscope
SRM	Standard Reference Material
SXRPD	Synchrotron X-ray powder diffraction
W	Week
XRD	X-ray powder diffraction

1 INTRODUCTION

Interest in biomineralisation has increased strongly over the last forty years (Smith, 2000, Levi-Kalisman et al., 2001). Initially it was medical and biochemical research, but the extraordinary characteristics of biologically produced materials (nano-composites) have drawn in scientists from other disciplines, in particular material scientists, in the hope that the next industrial revolution will come through bio-mimicking or bio-inspired new materials (Heuer et al., 1992, Fendler, 1996, Manne and Aksay, 1997, Mann and Weiner, 1999, Feng et al., 2000a, Naka and Chujo, 2001, Vincent, 2009).

Among the more than sixty known biomaterials produced by living organisms, only a few materials are common place (Dauphin, 2002b). Amorphous silicon dioxide is the main constituent of diatoms and radiolarian shells, as well as being produced by some other organisms and plants (Jahren et al., 1998, Parkinson and Gordon, 1999, Sahai and Tossell, 2001). Iron oxides and hydroxides are produced by many bacteria (Heuer et al., 1992, Fendler, 1997, Yamashita, 2001). Ca-oxalate is mainly found in plants and for example in human kidney stones (Bouropoulos et al., 2001, Lyons Ryall et al., 2001). Hydroxyapatite is the main hard surface layer in teeth and, in a carbonated form, is the main constituent of vertebrate bones and is also found in the shells and bones of some marine life and some other organisms (Hunter, 1996, Fincham et al., 1999, Peters et al., 2000). But the most ubiquitous biomineral is Ca-carbonate, which occurs in a variety of distinct phases (calcite, aragonite, vaterite, Ca-carbonate hexahydrate and monohydrate and amorphous Ca-carbonate), of which only calcite is thermodynamically stable under ambient conditions (Kanakis and Dalas, 2000, Kirschvink and Hagedorn, 2000).

Due to the widespread occurrence of Ca-carbonate based biomaterials and biologically induced and/or produced Ca-carbonate in the environment, ranging from shells, spines and skeletons of marine organisms over bacterially produced sediments and patinas to shells and skeletons of terrestrial animals and mammalian otoconia, Ca-carbonate has been the focus of extensive biomineralisation research (Bolivar and Sanchez-Castillo, 1997, Alonso-Zarza et al., 1998, Beniash et al., 1999, Loisy et al., 1999, Lins et al., 2000, Rivadeneyra et al., 2000, Soledad Fernandez et al., 2001,

Westin and Rasmuson, 2005, Sommerdijk and de With, 2008, Zhang et al., 2010). The ease with which Ca-carbonate is crystallized also added to this strong focus (Teng et al., 1998).

Research in the area of Ca-carbonate biomaterials has covered the whole spectrum, starting with natural systems. Extensive research, for example, has gone into characterizing the soluble and insoluble organic matrix found in marine organisms and its influence on the growth morphology and phase selection of Ca-carbonate (Halloran and Donachy, 1995, Durholtz et al., 1999, Dauphin and Denis, 2000, Zhang et al., 2010). A special effort, using *in vivo* and *in vitro* techniques, has been made to understand the way in which nacre is produced by organisms, driven by its extraordinary properties, like an improvement in strength by a factor of 3000 compared to the pure crystalline Ca-carbonate phase, aragonite, while only incorporating a maximum of 5% w/w of organic material (Zaremba et al., 1996, Belcher et al., 1998, Almqvist et al., 1999, Samata et al., 1999, Dauphin and Denis, 2000, Feng et al., 2000a, Estroff and Hamilton, 2001, Levi-Kalisman et al., 2001, Naka and Chujo, 2001, Heinemann et al., 2011, Meyers et al., 2011a). Some attempts have been made towards using the knowledge gained to mimic this increase in strength in composite materials (Almqvist et al., 1999, Feng et al., 2000a, Hardy and Scheibel, 2010, Luz and Mano, 2010, Maruyama et al., 2011). Also, the sea urchin spine was studied extensively, because the pattern is that of a single crystal in diffraction studies, but it does not show the rhombohedral cleavage one would expect, instead showing a conchoidal cleavage typical for amorphous materials (Beniash et al., 1999, Mann and Weiner, 1999, Ameye et al., 2000, Urry et al., 2000, Weiner et al., 2000, Ameye et al., 2001, Peled-Kamar et al., 2002). It also shows improved mechanical properties when compared to a single crystal. More recent studies have focussed on the sea urchin teeth, as they also express greatly improved mechanical strength when compared to the inorganically produced material (Ma and Qi, 2010). The insoluble and soluble organic matrices from these organisms were extracted, analysed, purified and decoded to ascertain which sequences and features are responsible for driving and controlling the biomineralisation (Halloran and Donachy, 1995, Rivadeneyra et al., 1998, Durholtz et al., 1999, Duvail et al., 1999, Samata et al., 1999, Xu and Evans, 1999, Marxen and Becker, 2000, Moura et al., 2000, Rivadeneyra et al., 2000, Weiss et al., 2000, Zhang et al., 2000, Ameye et al.,

2001, Peled-Kamar et al., 2002, Chien et al., 2008b, Takeuchi et al., 2008, Heinemann et al., 2011). It was discovered, that a silk fibroin-like template with β-sheet conformation and acidic matrix and glycoproteins are in widespread use in organisms as a template (Falini et al., 1998, Levi et al., 1998, Levi-Kalisman et al., 2001, Naka and Chujo, 2001, Murphy and Mooney, 2002). Identified organic macromolecules from the soluble and insoluble organic matrix have subsequently been used in laboratory experiments, where they behave similarly, providing a substrate and solution pair which preferentially grows a specific Ca-carbonate polymorph (Heuer et al., 1992, Manne and Aksay, 1997, Belcher et al., 1998, Xu et al., 1998, Feng et al., 2000b, Levi-Kalisman et al., 2000). Also, the soluble organic matrix was shown to be able to drive phase and morphological selectivity, even when used without a specific template. Some results from these studies, however, can be attributed predominantly to the chemical and kinetic regime in which the Ca-carbonate was grown. Aragonite, for example, grows as the preferred polymorph if the temperature is elevated above 40-45 ºC or when Mg ions are present at elevated concentration (Küther et al., 1998a, Kuther and Tremel, 1998, Lee et al., 2001).

A next step was taken with the introduction of synthetic and/or natural organic additives and templates, extraneous to the biomineralisation system being examined, that were also able to influence the polymorph and morphology of Ca-carbonate (Xu et al., 1998, Naka and Chujo, 2001, Westin and Rasmuson, 2005, Xie et al., 2005b, Meldrum and Cölfen, 2008, Zhang et al., 2010, Ren et al., 2011, Song and Kim, 2011). The additives were mainly acidic organic macromolecules similar to the ones found in natural systems, with Ca binding or complex forming groups in a specific orientation. These were interpreted as acting like a template for epitaxial growth of the Ca-carbonate phase, possessing Ca binding groups at distances similar to the Ca-Ca distance on certain crystal faces and thus being able to provide a localized super-saturation to form a critical nucleus for the subsequent growth of the specific phase with a specific orientation (Heuer et al., 1992, Hunter, 1996, Lochhead et al., 1997, Kaplan, 1998, Xu et al., 1998, Estroff and Hamilton, 2001, Lee et al., 2001, Levi-Kalisman et al., 2001). A number of studies looked at molecules either compressed as Langmuir-Blodgett films or uncompressed as self-assembled-monolayers (SAM), which have exposed, charged and evenly spaced head groups (often carboxylic) at distances that match the lattice of a Ca-carbonate polymorph and can therefore act as

a template for subsequent growth (Heuer et al., 1992, Lahiri et al., 1997, Kato et al., 1998, Kuther and Tremel, 1998, Xu et al., 1998, DiMasi et al., 2001, Estroff and Hamilton, 2001, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008). Even patterned growth was achieved in this way, as were multilayer composites (Aizenberg, 2000, Kato, 2000).

The above studies focused on growth from a 2D surface and the systems used have, indeed, only allowed for a limited control over the growth direction perpendicular to the surface and the orientation of the crystallites once the thickness of the layer increased. Some experiments have made use of inhibitors to create thin, contiguous layers and thus effectively controlling the growth in the third dimension (Xu et al., 1998). Experiments which use 3D templates to promote and control 3D aggregates have been carried out using SAMs around gold particles, microemulsions (e.g. water in oil in water, micelles), dendrimers and sol-gel (Küther et al., 1998b, Walsh et al., 1999, Estroff and Hamilton, 2001, Lee et al., 2001, Naka and Chujo, 2001, Donners et al., 2002, Qi et al., 2002, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008).

It is an accepted fact in the interpretation of all experiments, that the morphology and phase of the Ca-carbonate produced depend on the adsorption kinetics, structural state and surface selectivity of the organic additives (Xu et al., 1998, Smith et al., 2000, Njegić-Džakula et al., 2010). What is not as clear or accepted is the proposed function of the organic (or, in some cases inorganic) template used (DiMasi et al., 2001, Naka and Chujo, 2001). There are two accepted interpretations. First, the majority of authors focus on the distance of active Ca binding groups presented to the solution as the sole driving force determining the Ca-carbonate polymorph, and propose a simple substrate driven epitaxy, a process which is very likely to happen, due to the small mismatch in the Ca-Ca distance of the template and a specific Ca-carbonate face (Addadi and Weiner, 1986, Heuer et al., 1992, Hunter, 1996, Lahiri et al., 1997, Lochhead et al., 1997, Falini et al., 1998, Kaplan, 1998, Küther et al., 1998a, Xu et al., 1998, Levi-Kalisman et al., 2001, Naka and Chujo, 2001). Another group of authors has questioned this interpretation, because their experiments produced an amorphous precursor of considerable size, which in some cases behaved like a liquid (named by one group as Polymer-induced liquid precursor, PILP,

reaching a size almost visible with the eye), and in others formed a meta-stable amorphous layer up to 28 nm thick (Lochhead et al., 1997, Xu et al., 1998, Gower and Odom, 2000, Mann et al., 2000, Naka and Chujo, 2001, Donners et al., 2002, Chien et al., 2008a, Sommerdijk and de With, 2008). The orientation and spacing of Ca binding groups on the surface of the substrate can no longer be seen as the driving force affecting the structure or orientation of the amorphous or subsequently formed crystalline phase at these thicknesses.

Only a few experiments have focused on the atomistic fine structure of this amorphous phase, with one group reporting that the basic inter-atomic distances (short range order, small domains) for the crystalline phase formed later (e.g. aragonite) are already present in the amorphous phase, even though the phase itself is amorphous, from diffraction studies (Hasse et al., 2000, Levi-Kalisman et al., 2000). This hypothesis, however, needs some thorough testing, as there are only a few possibilities in which Ca and carbonate ions can align to form a three dimensional structure, assuming that the CO_3^{2-} groups continue to be planar.

1.1 Overview of aims and objectives

This research will focus on providing evidence to clarify an uncertainty in relation to Ca-carbonate biomineralisation. A lot is known about the effect of organic substances on the polymorph and morphology of Ca-carbonate grown in their presence, but it is not clear if only the organic template and/or soluble molecules (be they natural or synthetic) direct the growth through simple structural similarity (i.e. epitaxially) or if other phenomena are involved. The production of thick amorphous layers of Ca-carbonate in the presence of organic compounds and the discovery of a liquid amorphous precursor in a number of organisms indicates that the role the organic matrix and soluble molecules play in the crystallisation of biominerals is more complex than previously thought, and some newer studies have focussed specifically on the kinetics involved. A study by Njegić-Džakula et al (2010), has shown the importance of reaction kinetics and super-saturation levels in the crystallisation of Ca-carbonate and the impact on phase selection and phase stability exercised by the presence of organic additives. According to their study, vaterite is produced at lower super-saturation conditions, while a mixture of vaterite and calcite

is produced at higher super-saturation conditions. They further investigated the influence of poly-AAs at varying concentrations on crystal growth inhibition for seed crystals of vaterite and calcite and found that inhibition is stronger for calcite than for vaterite, resulting in samples only growing vaterite at higher concentrations of the poly-AAs.

When examining the facts it becomes apparent that biomineralisation, even in simple systems, is quite complex, depending on numerous factors.

Part of this complexity will be investigated using different amino-acids and varying a number of physical and chemical factors.

Objective

The main objective of this research is to delineate the level of influence some amino-acids have on the growth process of Ca-carbonate. Amino acids, and in particular aspartic and glutamic acid were chose because of the important role they play in biomineralising systems (Meyers et al., 2011a, Ren et al., 2011, Wehrmeister et al., 2011).

As part of this study a number of other potentially influencing factors were investigated with the aim of determining the following:

- The concentration at which the effect of the amino-acid on the morphology and type of Ca-carbonate produced dominates.
- The long-term stability of meta-stable Ca-carbonate in solution with the amino-acid present.
- Morphological and structural changes due to variations in reaction speed driven by changes in the recipient solution and rate of addition of the reactants.

To limit the variables to some degree, only two amino-acids, glutamic and aspartic acid, were chosen to investigate the influence on the phase, abundance and morphology of $CaCO_3$ as a function of concentration, sequence and duration of addition and harvesting time. The effects were investigated by means of synchrotron X-ray powder diffraction (SXRPD), neutron powder diffraction (NPD and to a limited extent by Fourier-transform infra-red (FTIR) spectroscopy and scanning electron microscope (SEM) analysis.

A number of factors were varied in the experiments to determine which one had the main impact on variability in terms of phase composition, crystallite size and structure as well as stability.

Variables were the sequence of addition, the speed of addition, the residence time in solution as well as the concentration of the amino-acids.

1.1.1 Principal experimental design

The experiment set-up was developed to limit the experimental influence of external factors and to allow for controlled variation of the chosen parameters. The experiment style chosen was simple addition, mixing, precipitation, filtration and analysis.

Variables used were amino-acid concentration, rate of addition, mixture present in the reaction vessel and residence time in solution.

This set-up resulted in 96 independent samples being produced for the principle investigation.

1.2 Significance

This research will provide scientific evidence to sustain or eliminate the assumption made in the interpretation of Ca-carbonate biomineralisation processes, that the mineral polymorph and morphology are determined solely by the type of organic molecule present. It will provide a starting point for future research by eliminating doubts with regard to the interfacial processes that drive phase selection and growth of Ca-carbonate in organic/inorganic systems.

1.3 Research method

To determine what exactly drives the crystallisation of Ca-carbonate in the presence of organic molecules and how its type and morphology are impacted by these molecules, it was necessary to cover all relevant aspects of the resultant inorganic

biomineral. It was therefore necessary to select and perform growth experiments delivering sufficient material for further investigation.

Experiment-Sample production

A variety of Ca-carbonate samples were produced, based on systems already mentioned in some of the literature, which are known to produce metastable Ca-carbonate. The main one used here is Ca-carbonate crystals grown in the presence of aspartic and glutamic acid (Tong et al., 2004). These samples, together with a control set without organic additives, will provide an insight into the influence of a variety of factors on the phase and stability of Ca-carbonate biominerals. The resultant Ca-carbonate samples will be examined to establish the extent to which the amino acid molecules have influenced the phase, morphology and growth, and also if the organic molecules have been intercalated or occluded in the crystal structure.

Experiment-Analytical techniques

To examine the impact of the organic molecules on the Ca-carbonate phase, and also the type of the Ca-carbonate phase, it is essential to use techniques which are able to analyse small particles and their arrangement as well as provide structural and morphological information. The techniques used to achieve this in this study were:

Synchrotron X-ray powder diffraction (SXRPD), X-ray powder diffraction (XRD) and/or neutron powder diffraction (NPD)

This was crucial to determine the crystallographic phase(s) and quantities of the bulk Ca-carbonate material produced and also allowed for structure investigation. In this case synchrotron X-ray powder diffraction and neutron powder diffraction were preferred because they allowed for much more detailed studies of crystallite size and strain, and the ability to use a selectable monochromatic wavelength allowed for an extended d-spacing range.

Scanning electron microscope (SEM) analysis

Electron microscopy was used to provide detailed data of the morphology, grain-size and intergrowth of the Ca-carbonate product.

Fourier-transform infra-red (FTIR) spectroscopy

Vibrational spectroscopy like FTIR is particularly useful to determine co-ordination states and local environment of atoms. FTIR can elucidate the presence of organic molecules and different Ca-carbonate phases, even amorphous and/or hydrated ones. They can also give an insight into the binding mode between the organic molecules and the Ca-carbonate phase.

2 BIOMINERALISATION

2.1 Overview

First a definition of biomineralisation:
Biomineralisation is the process by which organisms induce and/or control crystallisation of inorganic or composite organic-inorganic materials. Two main streams are discerned (Connett et al., 1983)

a) Biologically mediated biomineralisation, a process in which the organism precipitates a biomineral that does not fulfil any specific physiological function.

b) Biologically controlled biomineralisation, a process involving the provision of a crystallisation space, a generally organic template and a super-saturated solution containing dissolved organic polymers that control the crystallisation in terms of mineral species, phase, morphology and orientation.

The way in which the organisms crystallize the biominerals, and the shape, type and size of the biominerals are as varied as the organisms themselves.

History and context
To understand the interest in biomineralisation, one has to look at the field of nanotechnology and its implications. The driving forces come from fields as far apart as miniaturisation of electronics and the increased understanding of the human body, including the now complete map of the human DNA. Increased knowledge in both fields has forced a re-think of current strategies employed in the development of novel materials, and the capacity of organisms to produce biominerals of almost any size and shape has been pursued as a possible avenue for future applications, for example as cell specific drug-delivery systems, to be used as micro-patterning tools and as optical components (Aizenberg, 2000, Aizenberg, 2004, Cusack and Freer, 2008, Luz and Mano, 2010, Meldrum and Cölfen, 2008, Parkinson and Gordon, 1999, Sommerdijk and de With, 2008, Vincent, 2009, Walsh et al., 1999) Complex biomineralisation by organisms can be traced back to the early Cambrian, around 540 to 525 million years ago, from when the first fossil records of Ca-carbonate shells

exist. During this period a real explosion in the number of Ca-carbonate biomineralising organisms occurred. Fossil records of Radiolarians exist from about the same period, ~ 550 million years ago. Magnetite (Fe_3O_4) biomineralisation is believed to date back even further, probably around 900 to 600 million years ago (Kirschvink and Hagedorn, 2000). There is also some evidence that cyanobacteria could be classified as the first organisms to produce biominerals (Kazmierczak et al., 2009), in this case Ca-carbonate. Another important question which has recently received more attention is the homochirality of macromolecules and the apparent preference for L-amino acids in biomineral producing systems (Cintas, 2002).

While a scientific interest in the processes that control biomineralisation has been present for centuries, a true effort in studying them was not possible until significant advances in chemistry, biology and, most importantly, analytical technology were made. This did not happen until the middle of the last century. In the early days of scientific study, the 1960's and 1970's, biomineralisation was mainly a field for biochemical and (bio)-medical research. This can be understood easily, if one considers the fact that biomineralisation is ubiquitous in the human body, all vertebrate animals and quite a large number of invertebrates, even bacteria, too. The main focus for this group has been to understand the biomineralisation processes occurring in living organisms, specifically humans, and also the development of methods to either aid the formation of mineralised tissue (bone, teeth) or prevent the pathologic formation of minerals in the body (iron overload disease, kidney stones), as well as producing tailored drug delivery systems.

Since then, interest in biomineralisation has increased rapidly, aided by an enormous improvement in analytical instrument capabilities (Levi-Kalisman et al., 2001, Smith, 2000, Meyers et al., 2011b). Characteristics like improved strength, flexibility and biocompatibility of biologically produced materials (specifically the nano composites) have encouraged scientists from other disciplines, in particular material scientists, to join in the studies. It is hoped that the next industrial revolution will be nanotechnology driven, either through bio-mimicking or bio-inspired new materials (Feng et al., 2000a, Mann and Weiner, 1999, Manne and Aksay, 1997, Heuer et al., 1992, Naka and Chujo, 2001, Fendler, 1996, Chien et al., 2008a, Fan et al., 2006,

Sommerdijk and de With, 2008, Vincent, 2009, Maruyama et al., 2011, Meyers et al., 2011a).

More than sixty biomaterials are produced by living organisms, but only a few are common place (Dauphin, 2002b, Meldrum and Cölfen, 2008). They are:

1) Amorphous silicon dioxide, frequently hydrated, the main constituent of diatoms and radiolarian shells, and which is also present in some other organisms and plants. This is the second most common biomineral by mass (Parkinson and Gordon, 1999, Sahai and Tossell, 2001, Jahren et al., 1998, Brutchey and Morse, 2008, Hildebrand, 2008, Bauer et al., 2011b).

2) Iron oxides and hydroxides, mainly ferrihydrate and magnetite, produced by many bacteria and also some higher organisms (Heuer et al., 1992, Fendler, 1997, Yamashita, 2001, Faivre and Schüler, 2008).

3) Ca-oxalate, produced by plants and in the human kidney (Bouropoulos et al., 2001, Lyons Ryall et al., 2001).

4) Hydroxyapatite, the main hard surface layer in teeth and, in a carbonated form, the main constituent of vertebrate bones, while also found in the shells and bones of some marine life and some other organisms (Hunter, 1996, Fincham et al., 1999, Peters et al., 2000, Omelon and Grynpas, 2008, Fan et al., 2006, Luz and Mano, 2010, Meyers et al., 2011a).

5) Ca-carbonate, present in the form of shells, spines and skeletons of marine organisms, in bacterially produced sediments and patinas, in shells and skeletons of terrestrial animals and in mammalian otoconia (Beniash et al., 1999, Rivadeneyra et al., 2000, Loisy et al., 1999, Alonso-Zarza et al., 1998, Bolivar and Sanchez-Castillo, 1997, Soledad Fernandez et al., 2001, Lins et al., 2000, Bauer et al., 2011a, Cusack and Freer, 2008, Dupraz et al., 2009, Wehrmeister et al., 2011).

2.2 Non-Ca-carbonate biomineralisation systems

Since this study is not focussing on other biomineralisation systems besides Ca-carbonate, only a short overview will be given here. There are numerous studies investigating some of the other minerals produced by biomineralisation.

The most intensively studied is, for obvious reasons, apatite in any of its modifications (hydroxy-, carbonate-, fluor-) found in the human body as main constituent of bones and teeth and also as pathological component in arteriosclerosis, for example. Study of the apatite biomineralisation started out with structural analysis of the mineralised tissue (i.e. bone and teeth) but has recently moved more and more towards extraction and functional analysis of the proteins and protein matrices involved in the mineralisation as well as the creation of new biodegradable composites, often by bio-mimicking and testing the usefulness of other biomineral producing systems for their use in human treatments (Fincham et al., 1999, Maas and Dumont, 1999, Moradian-Oldak et al., 2002, Zhao et al., 2002, Schmitt et al., 2002, Silve et al., 1992, Green et al., 2002, Boskey and Roy, 2008, Saygin et al., 2000, Omelon and Grynpas, 2008, Fan et al., 2006, Tay and Pashley, 2008).

Another widespread biomineral is (hydrated) amorphous silicon dioxide. As mentioned before, the organisms mainly responsible for producing (hydrated) amorphous silicon dioxide are radiolaria and diatoms, unicellular organisms inhabiting oceans in areas with specific salt content. Production of the silica occurs intra-cellular, mediated by phosphoproteins (silaffins) and unusually long-chain polyamines (Weiner et al., 2000, Coradin and Livage, 2001, Coradin et al., 2004, Parkinson and Gordon, 1999, Kroger et al., 1996, Sullivan, 1986, Sumper and Kröger, 2004, Vrieling et al., 1999, Zaremba and Stucky, 1996, Hildebrand, 2008, Bauer et al., 2011b).

The last group of the biomineral producing systems I will mention here is that of iron oxide and/or hydroxide. These systems are encountered in flora and fauna, but the main group responsible are bacteria. A very interesting system which also has received some attention is that of mineralised chiton teeth. These produce an iron oxide layer to impart hardness and wear resistance instead of the enamel usually

employed. Also, the presence of iron oxide particles in the human brain deserves a mention here (Farina et al., 1999, Grunberg et al., 2001, Kawaguchi et al., 1995, Kim et al., 1986, Kirschvink, 1989, Kirschvink et al., 1992, Matsunaga and Sakaguchi, 2000, Schuler and Baeuerlein, 1998, Schuler and Frankel, 1999, Wajnberg et al., 2001, Bazylinski et al., 1994).

2.3 Areas of research in the field of biomineralisation

Due to the nature of this research, the majority of citations in this chapter will be based on Ca biomineralisation with a strong focus on Ca-carbonate biomineralisation.

Because biomineralisation is a complex field, a number of different approaches have been developed to tackle the question of 'how do organisms do it', each with its advantages and disadvantages, and each with either an application specific focus, or representative of the knowledge base of the researchers involved. At the extreme end are technology based investigations, looking at the usefulness and adaptability of a specific analytical technique to study biomineralisation processes, or the biominerals themselves. There the focus is on the technique and not the system. Furthermore there are also the molecular modelling based approaches, which focus almost exclusively on a theoretical description of the interaction of the mineralising solution, including organic macromolecules, with crystal surfaces. At the other end is experimentally based research, focussing almost exclusively on testing organic molecules to discover their influence on the biomineralisation process and specifically the phase, morphology and size of the biominerals produced. Predictive investigations are rare, and have only been used in the context of previous experiments, i.e. predicting which organic molecules will have what effect on phase selectivity and morphology (Wilt, 2005b). Nonetheless, if we take the biomineralisation itself as criteria, most of the research activities can be grouped into major streams, even though the streams frequently overlap.

A very large group is involved in the study of natural systems *in vivo* and *in vitro*. The majority, by far, is studying the human biomineralisation systems with strong

focus on teeth and bone, as a better understanding of the biomineralisation process of these is very likely to have immediate benefits in the treatment of, for example osteoporosis and tooth decay.

A second, also very large, group is involved in the development of new biomaterials, either by biomimetic approaches or through the development of novel systems. This group is significantly more diverse and includes a wide range of scientists from all areas. However, a few major sub streams exist. These include a stream that I would call the '2D-monolayer-template' stream, which encompasses the study of biomineralisation under compressed organic monolayers (Langmuir-Blodgett films, LBFs), self-assembled monolayers (SAMs), both usually on a water based sub-phase, but also on solid substrates, mostly glass or silicon, by either transfer of the monolayer to the substrate, or functionalization of the substrate (Archibald et al., 1996, Volkmer et al., 2005, Wilt, 2005b, Evans, 2008, Chien et al., 2008a).

A second sub stream that noted here as the '3D-template' stream, focuses on producing a three dimensional template or crystallisation space for the biomineral to form in. The approaches are varied, but the most common ones are based on micro-emulsion micelles (normal, inverse, double), bubbles and micro-reactors in case of emulsion based experiments, double-block-copolymers and dendrimers in the case of self-assembling templates and surface treated nano-particles, all aimed at restricting the shape and size of the biomineral formed, which is usually a hollow sphere or coated particle once the organics are removed. There are also quite a few experiments, especially in the area of implant research, which have focussed on the testing of porous 3-dimensional templates. (Antipov et al., 2003, Aquilano et al., 2003, Donners et al., 2000, Luz and Mano, 2010, Oliveira et al., 2009, Qi, 2010, Walsh et al., 1999)

2.3.1 Natural systems

Natural systems can be characterized by the way in which the organism crystallizes the biominerals, i.e. the mechanisms and level of control employed by it. There are only two main groups of naturally produced biominerals. One where the organism has no immediate control over the size or morphology, and sometimes even the phase of the produced biominerals, classified as biologically induced biomineralisation, and the other where the organism has full control over every aspect of the process, classified as biologically controlled biomineralisation.

Biologically induced biomineralisation has been of great importance in our history and current examples include some parts of the formation of patinas on buildings and detoxification of soils, but it is neither the dominant nor the most interesting type of biomineralisation.

Biologically controlled biomineralisation however is far more common among the natural systems studied. Most organisms, where an organism refers to all simple and complex organisms from both fauna and flora, employ an approach which combines a physically structured and restricted space with an organic template (matrix) and a soluble organic component to produce the biomineral. This space is either intra-cellular or extra-cellular, often lined with an organic template and crystallisation occurs in conjunction with soluble organic compounds, whose concentration is such that the desired phase is crystallized with the desired morphology.

Fairly common is also the use of solution chemistry and kinetics to control the growth of biominerals in non-confined spaces. Due to the nature of the crystallising systems, intra- and extra-cellular spaces in living organisms, it has been difficult to study them *in vivo*. One of the few examples has been the study of nacre producing abalone, driven by its extraordinary properties, like an improvement in strength by a factor of 3000 compared to the pure crystalline Ca-carbonate phase, aragonite, while only incorporating a maximum of 5% w/w of organic material (Dauphin and Denis, 2000, Levi-Kalisman et al., 2001, Feng et al., 2000a, Samata et al., 1999, Almqvist et al., 1999, Zaremba et al., 1996, Graham and Sarikaya, 2000, Estroff and Hamilton, 2001, Naka and Chujo, 2001, Belcher et al., 1998, Rousseau et al., 2005, Evans,

2008, Chien et al., 2008a, Luz and Mano, 2010). But even there the study is limited to observations at separate points in time, as an object has to be inserted into the crystallisation space in the shell and needs to be removed from it at a later stage in order to ascertain the growth without being able to observe the changes in situ (Zaremba et al., 1996).

Due to this difficulty, the research into natural systems has principally focussed on two approaches: Firstly the (predominantly structural) analysis of the biominerals 'as extracted' from the organism at different stages with more and more sophisticated techniques, trying to determine changes and similarities as a function of time and also, as mentioned before, the introduction of foreign bodies and natural or forced changes in the environment with subsequent analysis to achieve the same goal; secondly the extraction of the matrix (insoluble) and soluble proteins from naturally occurring systems, which are subsequently studied under 'natural' conditions *in vitro*.

Structural investigations

Structural studies have been conducted especially in the area of bone and teeth, as these are the hard mineralised tissues 'closest to home', being biominerals we use and abuse in our daily lives, and also due to their importance in our genetic heritage and our understanding of illnesses and their possible cure. These illnesses (osteoporosis, tumours, tooth decay, etc.) also have a significant impact on our health system, and understanding, for example, how the structure of a healthy bone is different from bone weakened by osteoporosis or a tumour could result in better preventative measures (Peters et al., 2000, Cui et al., 2000, Weiner et al., 1999a, Wenk and Heidelbach, 1999, Weiner et al., 1999b, Maas and Dumont, 1999, Green et al., 2002, Saygin et al., 2000, Meldrum and Cölfen, 2008, Wilt, 2005a, Omelon and Grynpas, 2008, Fan et al., 2006, Tay and Pashley, 2008, Gebauer and Cölfen, 2011).

Also extensively studied are the structures, including the ultra-structures of the mineralised parts of marine and land organisms, be it their shells, spicula, otoconia or others. Here the focus has been the relationship between the organic matrix and the biominerals (Wang et al., 2003, Lins et al., 2000, Levi-Kalisman et al., 2001,

Hallworth et al., 1995, Hall et al., 2002, Wealthall et al., 2005, Wilt, 2005b, Meyers et al., 2011b, Gebauer and Cölfen, 2011).

Investigations of the matrix proteins

Extensive research has gone into characterizing the soluble and insoluble organic matrix found in teeth and bone and their influence over the crystallisation from nano to macro scale as well as genetic implications, not only in tooth and bone formation but in the body as a whole (Uemura et al., 1997, Giachelli and Steitz, 2000, Paine et al., 2001, Moradian-Oldak, 2001, Zeichner-David, 2001, Fincham et al., 1999, Wilt, 2005b, Marin and Luquet, 2005, Martina et al., 2005, Raabe et al., 2005, Rousseau et al., 2005, Gebauer and Cölfen, 2011, Bauer et al., 2011a, Chien et al., 2008b, Xie et al., 2005a, Ma and Qi, 2010, Chien et al., 2008a, Wilt, 2005a, Xie et al., 2005b).

The same can be said with regard to marine organisms, where the influence of the matrix proteins on the growth morphology and phase selection of Ca-carbonate has also been thoroughly investigated (Halloran and Donachy, 1995, Durholtz et al., 1999, Dauphin and Denis, 2000, Moura et al., 2000, Marin and Luquet, 2005, Rousseau et al., 2005, Cusack and Freer, 2008, Njegic-Dzakula et al., 2010, Takeuchi et al., 2008, Ma and Qi, 2010, Heinemann et al., 2011, Wehrmeister et al., 2011).

Another example is the sea urchin spine, in which the organic molecules influence the crystal growth in such a way that the spine in X-ray diffraction studies still shows the diffraction pattern of a single crystal, but when fractured does not show the rhombohedral cleavage one would expect, instead showing a conchoidal cleavage. This is achieved by subtle rotations of the crystallites during growth (Peled-Kamar et al., 2002, Urry et al., 2000, Ameye et al., 2000, Mann and Weiner, 1999, Beniash et al., 1999, Ameye et al., 2001, Weiner et al., 2000).

The insoluble and soluble organic matrices from a number of marine and land organisms were extracted, analysed, purified and their protein and amino acid components were genetically decoded to ascertain which sequences and features are responsible for driving and controlling the biomineralisation process (Peled-Kamar et al., 2002, Ameye et al., 2001, Zhang et al., 2000, Marxen and Becker, 2000,

Rivadeneyra et al., 2000, Moura et al., 2000, Weiss et al., 2000, Samata et al., 1999, Durholtz et al., 1999, Xu and Evans, 1999, Duvail et al., 1999, Rivadeneyra et al., 1998, Halloran and Donachy, 1995, Chien et al., 2008b, Takeuchi et al., 2008, Heinemann et al., 2011). Through these analyses it was discovered that silk fibroin-like templates with β-sheet conformation and acidic matrix as well as glycoproteins are in widespread occurrence in biomineral producing marine and land organisms (Levi-Kalisman et al., 2001, Naka and Chujo, 2001, Levi et al., 1998, Falini et al., 1998, Murphy and Mooney, 2002, Hardy and Scheibel, 2010).

Identified organic macromolecules from the soluble and insoluble organic matrices have subsequently been used in laboratory experiments, where they were shown to exact similar control of the biomineralisation process, providing a substrate and solution pair which preferentially grows a specific Ca-carbonate polymorph (Levi-Kalisman et al., 2001, Feng et al., 2000b, Belcher et al., 1998, Manne and Aksay, 1997, Heuer et al., 1992, Xu et al., 1998). Also, the soluble organic matrix was shown to be able to drive phase and morphological selectivity, even when used without a specific template. Some results from these studies, however, need to be considered in the context of the chemical and kinetic regime in which the Ca-carbonate was grown.

2.3.2 Synthetic systems

Discoveries from the studies on natural systems, especially the focus on the impact specific sections and head groups of the proteins involved have on the crystallisation, led to the introduction of synthetic and natural but extraneous organic additives and templates that are able to influence the polymorph and morphology of the biomineral (Xu et al., 1998, Naka and Chujo, 2001, Green et al., 2002, Moradian-Oldak et al., 1992, Meldrum and Cölfen, 2008, Zhang et al., 2010, Ren et al., 2011, Song and Kim, 2011). The additives are mainly acidic organic macromolecules, similar to the ones found in natural systems, with Ca binding or complex forming groups in specific orientations. It was proposed that the macromolecules act like a template for epitaxial growth of the Ca-carbonate phase, possessing Ca binding groups at distances similar to the Ca-Ca distance on certain crystal faces, thus being able to provide a localized super-saturation to form a critical nucleus for the subsequent growth of the specific phase with the specific orientation (Estroff and Hamilton, 2001, Lee et al., 2001, Xu et al., 1998, Heuer et al., 1992, Hunter, 1996, Lochhead et al., 1997, Kaplan, 1998, Levi-Kalisman et al., 2001, Antonietti et al., 1998).

2-dimensional studies

Numerous studies have investigated organic chain molecules with hydrophobic and hydrophilic head groups, for example fatty acids, compressed or uncompressed as LB films or as SAMs, with the hydrophilic head groups immersed in a water based solution. Most of these monolayers have exposed, charged and evenly spaced head groups (often carboxylic) at distances that almost match the Ca-Ca distance in the lattice of a Ca phase and therefore could act as a template for subsequent growth (Kuther and Tremel, 1998, Kato et al., 1998, Heuer et al., 1992, Xu et al., 1998, Estroff and Hamilton, 2001, DiMasi et al., 2001, Lahiri et al., 1997, Ma et al., 1997, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008). Even patterned growth was achieved in this way, as were multilayer composites (Aizenberg, 2000, Kato, 2000, Vincent, 2009, Hardy and Scheibel, 2010, Luz and Mano, 2010), but there have also been reports of unstructured monolayers which nonetheless still lead to crystallisation with preferred orientation (Volkmer et al., 2002, Lee et al., 2007) and also where a structured monolayer does not seem to influence the polymorph selection directly (Wada et al., 2004, Chien et al., 2008a).

The systems used in the above studies have only allowed for limited growth control in the direction perpendicular to the surface and the orientation of the crystallites once the thickness of the layer increased. Some experiments have made use of inhibitors to create thin, contiguous layers, effectively controlling the growth in the third dimension (Xu et al., 1998, Wilt, 2005b, Meldrum and Cölfen, 2008, Xie et al., 2005a, Ren et al., 2011).

Lastly, the usability of LB monolayer films and SAMs has extended to the production of nano-structured materials (Fendler, 1996, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008, Xie et al., 2005a, Ren et al., 2011).

3-dimensional studies

Experiments which use 3-dimensional templates to promote and control 3-dimensional growth of biominerals and nano-composites have been carried out using SAMs around nano-particles or by lipid self-assembly, micro emulsions (e.g. water in oil in water, micelles), dendrimers, surfactants and sol-gel approaches (Lee et al., 2001, Walsh et al., 1999, Qi et al., 2002, Naka and Chujo, 2001, Donnors et al., 2002, Küther et al., 1998b, Estroff and Hamilton, 2001, Yang et al., 2003, Grassmann and Lobmann, 2004, Antipov et al., 2003, Collier and Messersmith, 2001, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008) and also using polymer matrices (Schwarz and Epple, 1998, Antonietti et al., 1998, Du et al., 2000, Murphy et al., 2000, Grassmann and Lobmann, 2004, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008).

2.4 The organic-inorganic interface

Overview

The organic-inorganic interface has been studied extensively, and quite a few of the examples have already been covered. But the interface and its importance have attracted the interest of other study groups, aiming primarily at understanding the kinetics involved, but also groups involved in molecular modelling of the interactions.

There are two types of organic-inorganic interfaces of interest that have been studied, and they need to be distinguished. One is the structured organic interface. By structured I am referring to either a 2-dimensional or 3-dimensional arrangement of a surface that can act as the crystallisation initiator and also phase and morphology selector by providing structurally defined nucleation sites, trapping positively or negatively charged ions from solution and thus initiating crystal growth. The other is a soluble, possibly complex forming molecule that could form loosely bound complexes with ions in solution, around nuclei, and preferentially attach to specific crystal growth steps or faces and force a specific polymorph or morphology. In most biomineralisation systems these two occur in conjunction, but in vitro studies have shown that either one by itself can exert control over the crystallisation. Both cases were discussed before and are said to occur frequently in conjunction (Almeida et al., 2000, Dauphin, 2002a, Durholtz et al., 1999, Marxen and Becker, 1997, Pereira-Mouriès et al., 2002, Roque et al., 2004, Sud et al., 2001, Wheeler et al., 1987).

With regard to natural systems, ambivalent statements have been made with regard to the dominance of the soluble or insoluble matrix in determining the phase and morphology of the biomineral produced. More recent studies seem to confirm that the structured template (insoluble organic matrix) and the soluble organics both have important roles to play, even though their importance may vary between organisms (Cuif et al., 2012, Weiner and Dove, 2003).

The main role of the insoluble organic matrix seems to be in controlling the macroscopic texture of the biomineral and in some cases the initial supersaturation required for the formation of a critical nucleus, while the soluble organic matrix

seems to be more responsible for phase selection and growth control. It is noteworthy that most of the soluble organic matrices are, in effect, growth inhibitors of varying strength, allowing for a controlled development of the biomineral, and in some cases also its controlled dissolution.

It has been proposed that the speciation and development of the biomineral is driven by the structured matrix through epitaxy, which may well be true in a limited number of cases were the binding sites for cations on the surface of the organic matrix are at a compatible distance to the structural distances of the cations in the biomineral produced.

2.5 The template as an interface

Phase and morphology of the biominerals produced depend on the adsorption kinetics, structural state and surface selectivity of the organic macromolecules used, and to some degree on the organic (or, in some cases inorganic) template used (Xu et al., 1998, Smith et al., 2000, Naka and Chujo, 2001, DiMasi et al., 2001, Sommerdijk and de With, 2008, Zhang et al., 2010, Heinemann et al., 2011, Ren et al., 2011, Song and Kim, 2011, Cuif et al., 2012, Weiner and Dove, 2003).

There are quite a few arguments in favour of epitaxy, which I will analyse in more detail. But first a general definition of epitaxy: Epitaxy is the oriented growth of one phase (the epitaxial phase) on the surface of another phase (the substrate). This process is likely to occur when there is a close match in the structural arrangement of negatively and positively charged atoms on the surface of the substrate and the position of the atoms in the growth plane of the epitaxial phase and where bonding between the two is possible. Epitaxy is therefore a likely process in a lot of natural systems, because there often is only a small mismatch between the Ca binding groups (and therefore the Ca-Ca distance) of the template and a specific Ca-carbonate phase face (Falini et al., 1998, Küther et al., 1998a, Lahiri et al., 1997, Addadi and Weiner, 1986, Lochhead et al., 1997, Estroff and Hamilton, 2001, Xu et al., 1998, Naka and Chujo, 2001, Heuer et al., 1992, Hunter, 1996, Kaplan, 1998, Levi-Kalisman et al., 2001).

However, the explanation of crystallisation driven by epitaxy has recently been questioned (Olszta et al., 2003). Studies have revealed that amorphous Ca-carbonate (ACC) is far more common than previously believed. Experiments have produced an amorphous precursor (behaving like a liquid and given the name of Polymer-induced liquid precursor, PILP) reaching a size almost visible with the eye (Gower and Odom, 2000). Others experiments formed a meta-stable amorphous layer up to 28 nm thick (Naka and Chujo, 2001, Lochhead et al., 1997, Donnors et al., 2002, Gower and Odom, 2000, Xu et al., 1998, Mann et al., 2000, Chien et al., 2008a, Sommerdijk and de With, 2008). These results indicate that the orientation and spacing of Ca binding groups on the surface of the substrate are not the driving forces affecting the structure or orientation of the phase.

There have also been numerous investigations of amorphous phases, in particular ACC, produced by natural organisms which have led to a significant re-evaluation of the role ACC plays in biomineralisation (Addadi et al., 2003, Wilt, 2005b, Aizenberg et al., 2002, Hasse et al., 2000, Raz et al., 2003, Beniash et al., 1999, Cusack and Freer, 2008, Xu et al., 2008, Ma and Qi, 2010, Wehrmeister et al., 2011). According to these studies, ACC exists in various forms and two distinct classes. One class has been described as transient ACC, usually hydrated and mostly containing one molecule of water per molecule of $CaCO_3$, in some cases more. The other class has been described as stable ACC, usually anhydrous, but sometimes also anhydrous, which in some cases maintained its amorphous state even after extraction from the organism. Distinct forms of ACC exist, as far as is currently known, only in transient ACC, and EXAFS and IR studies have revealed that the structure of the final phase (calcite or aragonite) is short-range ordered, characteristic of the transient ACC by characteristic short range ordering (Hasse et al., 2000, Levi-Kalisman et al., 2002, Chien et al., 2008a). Assignment of fractional dimensional order to the different forms may allow for classification.

One of the most important results of the studies into amorphous ACC has been the discovery that in all forms and classes elevated levels of Mg-ions are present, and possibly also P ions (Addadi et al., 2003, Ma and Qi, 2010). This indicates that structural disorder, induced by the presence of other cations, is energetically

beneficial in the formation and stabilisation of amorphous Ca-carbonate (Radha et al., 2012).

2.6 Molecular modelling

Molecular modelling is a vast and rapidly growing field. A major effort is being made in the field of predictive modelling of macro molecules, in particular in conformational states and changes, either by themselves or in contact with other molecules or solutions. Another effort is being made in the examination of the surface of solids in contact with solutions, either with or without solubilised ions and/or organic molecules. Furthermore there is focus on modelling crystal structures. This section focusses on the molecular modelling research directly related to Ca-carbonate, inorganic-organic interfaces or biomineralisation systems.

To be able to use molecular modelling successfully, a very accurate mathematical description of the atoms is required, including their orbitals and their interatomic potentials. Due to the number of atoms involved in a normal system and the number of independent parameters that need to be determined, assumptions and boundary conditions have to be used to simplify the system. Nonetheless, the large amount of computational power required for the *ab initio* quantum mechanical calculations usually limits the number of atoms in a system to about 10000 atoms. The study of complex multiphase systems has, as a consequence, been quite limited, with most studies focussing on the surface of solids or structured monolayers in contact with a solution. The term surface in this field encompasses only a few layers of atoms, often not more than four or five. The bulk of the crystal underneath is approximated by a description as a fixed structure with clearly defined potentials, and all calculations are carried out with regard to the few surface layers only. A second approach is to describe clusters consisting of only a few atoms.

There have been numerous computational studies of the minerals involved in biomineralisation such as silica (Hench and West, 1995) and hydroxyapatite (Wierzbicki and Cheung, 2000), but studies of $CaCO_3$ and its modifications are by far the most numerous. In particular $CaCO_3$ surfaces in air or aqueous media, either with or without additives, have received a lot of attention (Cooper and de Leeuw,

2002b, de Leeuw and Parker, 1998b, de Leeuw and Parker, 1998a, Pradip and Rao, 2002, de Leeuw and Parker, 1997, de Leeuw, 2002, Felmy et al., 1998, Cooper and de Leeuw, 2002a, Ojo et al., 2002, Rohl, 2003, Ruuska et al., 1999), but computational studies of bulk $CaCO_3$ also exist (Cygan et al., 2002, Bearchell and Heyes, 2002, Mukkamala et al., 2006, Ouhenia et al., 2008). Among these studies of silica, hydroxyapatite and Ca-carbonate two major directions can be discerned, one approaching the system from a cluster perspective, e.g. (Ruuska et al., 1999), others by calculations of their surface structure in water and in the presence of organic molecules, but the overall complexity of the systems has thus far impeded the study of a complete system.

3 CALCIUM-CARBONATE

3.1 Ca-carbonate polymorphs

Ca-carbonate forms a number of anhydrous and hydrated polymorphs and constitutes about 4% of the earth's crust (Dickinson et al., 2002). Calcite, aragonite and vaterite are the crystalline forms of anhydrous Ca-carbonate, with only calcite and aragonite occurring in significant quantities in nature. Of the hydrated forms, the hexahydrate (ikaite) and monohydrate (monohydrocalcite) occur sparingly in nature and a trihydrate has also been reported (Rösler, 1984). Amorphous Ca-carbonate is, as mentioned in chapter 2, quite widespread in biomineralisation systems, either hydrous or anhydrous, with the most common hydrous form averaging one H_2O molecule per $CaCO_3$ molecule (Addadi et al., 2003, Wilt, 2005b).

3.2 Structures

The difference between the anhydrous crystalline polymorphs is in the arrangement of the CO_3^{2-} groups and Ca^{2+} ions within the structures, resulting in slightly different packing densities, nearest neighbour distances and orientation vectors. The hydrated forms show lower symmetry. All this leads to differences in their crystallographic lattice:

Calcite crystallizes in the trigonal space group *R*-3c

Aragonite crystallizes in the orthorhombic space group *P*mcn

Vaterite has been described as crystallising in two distinct space groups. One is the hexagonal space group $P6_3/mmc$, the other is the orthorhombic space group *P*bnm, a setting of the space group *P*nma

Ikaite crystallizes in the monoclinic space group *C*2/c

Monohydrocalcite or Ca-carbonate monohydrate crystallizes in the trigonal space group $P3_1$

Table 3.1 shows the variation in the crystallographic cell parameters for the different phases.

Crystallographic Parameters										
Phase	**Database**	**Number**	**Space group**	**Space group number**	**a (Å)**	**b (Å)**	**c (Å)**	**alpha (°)**	**beta (°)**	**gamma (°)**
Calcite	ICSD	20179	$R\bar{3}c$ H	167	4.994(2)	4.994(2)	17.081(5)	90	90	120
		73446			4.991(2)	4.991(2)	17.062(2)			
		80869			4.988(2)	4.988(2)	17.068(2)			
Aragonite	ICSD	34308	*P* mcn	62	4.9598(5)	7.9641(9)	5.7379(6)	90	90	90
		15198			4.9616(2)	7.9705(6)	5.7394(4)			
	ICDD	41-1475			4.9623(3)	7.968(1)	5.7439(3)			
Vaterite	ICSD	27827	*P* bnm	62	4.13	7.15	8.48	90	90	90
	ICDD	01-1033	*P* 6_3/mmc	194	4.128	4.128	8.573			120
	ICSD	18127			7.148(8)	7.148(8)	16.949(36)			
Ikaite	ICSD	16070	*C* 2/c	15	8.87(1)	8.23(1)	11.02(1)	90	110.2(2)	90
		31305			8.792(2)	8.310(2)	11.021(2)		110.53(5)	
Monohydro-calcite	ICSD	100847	*P* 3_1	144	10.5536(16)	10.5536(16)	7.5446(18)	90	90	120
		200820	*P* 3_121	152	6.0931(9)	6.0931(9)	7.5446(18)			

Table 3.1: Range of structural parameters for the Ca-carbonate phases found in nature. The structures chosen represent published values of smallest and largest unit cell and an intermediate sized one. Uncertainties are provided in brackets.

Figures 3.1 – 3.5 show some representations of the crystal structures, plotted using the Grenoble Thermal Ellipsoids Plot Program (GRETEP) (Laugier and Bochu, 2003) and Crystallographic information files (CIFs) obtained from the Inorganic Crystal Structure Database (ICSD) (FIZ, 2002). Ca ions are represented in blue, oxygen ions in green, carbon ions in grey and hydrogen ions in red. Obscured atoms are not shown in any of the plots. All representations are such that a Ca ion was chosen as the central ion. The projection is always towards the origin.

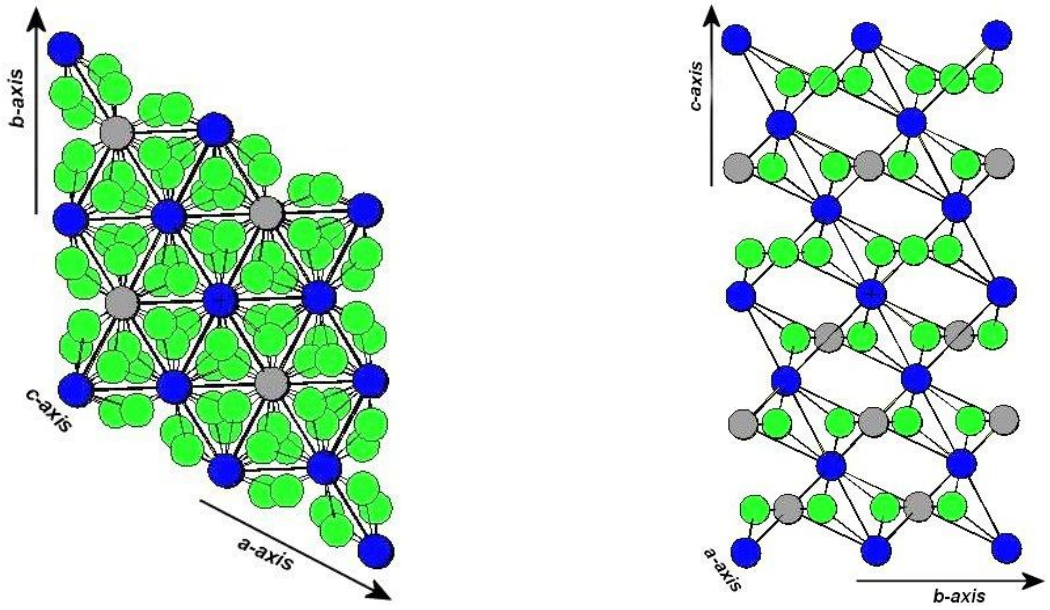

Figure 3.1: **Calcite**. ICSD Structure number 73446 with hexagonal axis. Structural parameters: a = b = 4.9910 Å, c = 17.0620 Å, α = β = 90º, γ = 120º; plot size is 2a*2b*c.

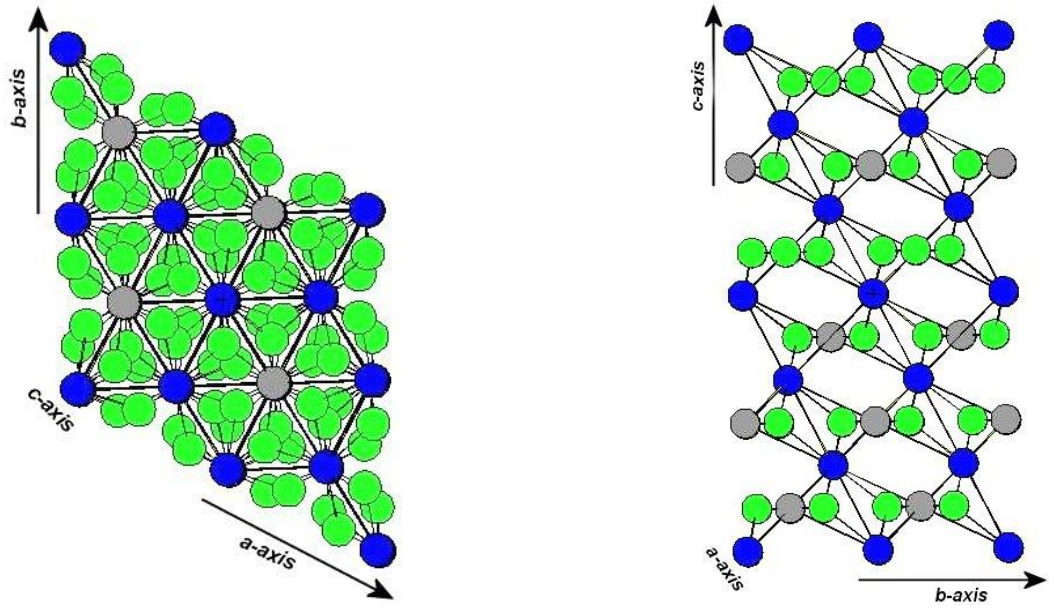

Figure 3.2: **Calcite**. ICSD Structure number 73446 with hexagonal axis. Structural parameters: a = b = 4.9910 Å, c = 17.0620 Å, α = β = 90º, γ = 120º; plot size is 2a*2b*c.

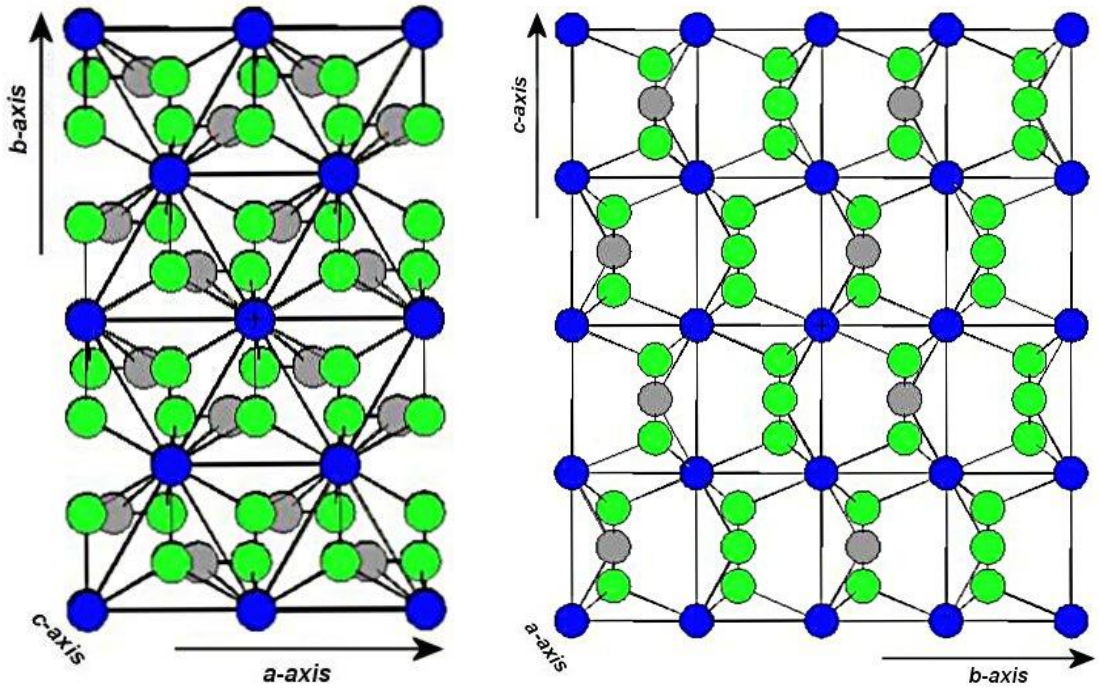

Figure 3.3: **Vaterite**. ICSD structure number 27827. Structural parameters: a = 4.13 Å, b = 7.15 Å, c = 8.48 Å, α = β = γ = 90º; plot size is 2a*2b*2c.

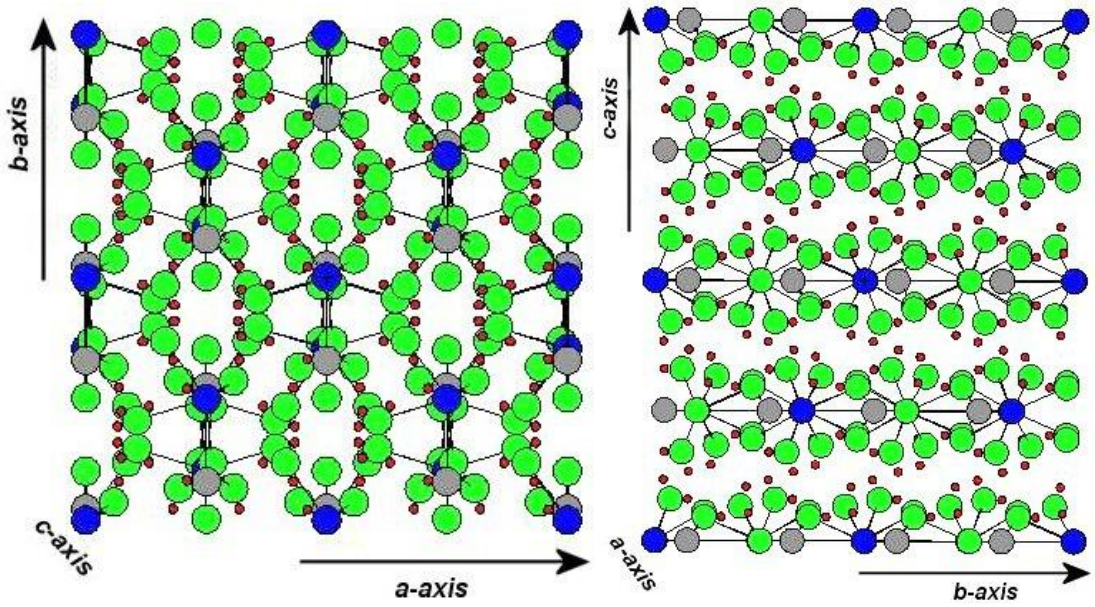

Figure 3.4: **Ikaite**. ICSD structure number 31305. Structural parameters: a = 8.7920 Å, b = 8.3100 Å, c = 11.0210 Å, α = β = 90º, γ = 110.530º; plot size is 2a*2b*2c, Ca ion shown at centre.

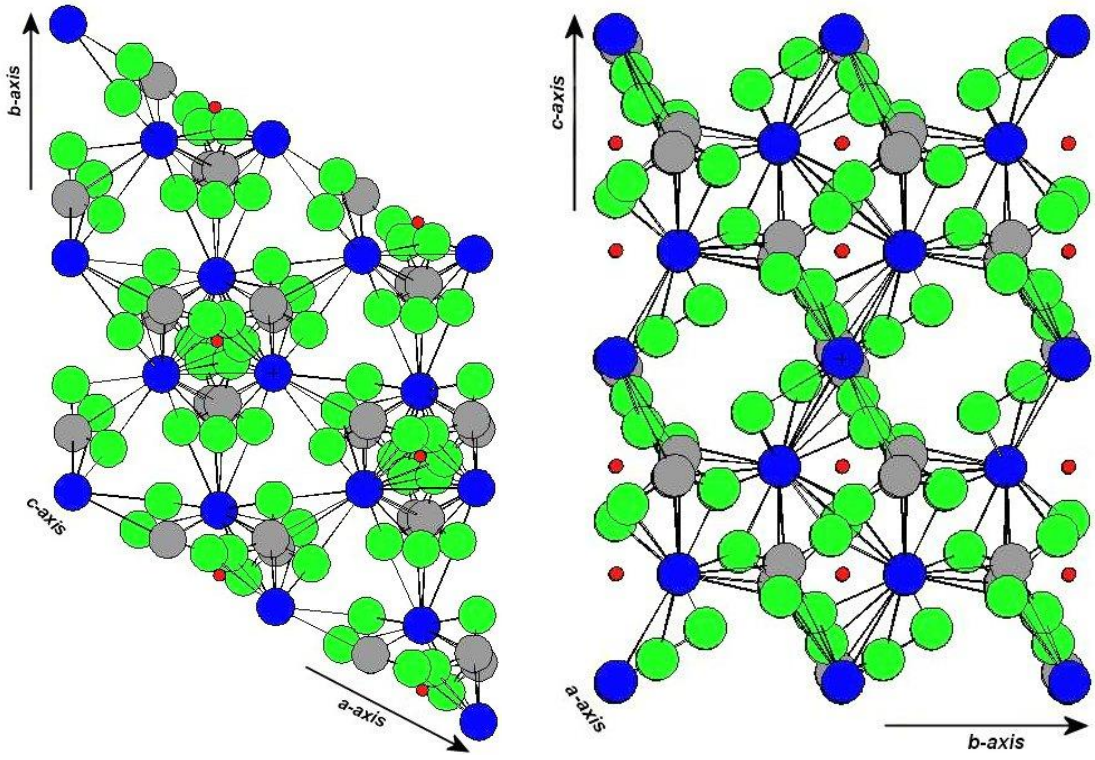

Figure 3.5: **Monohydrocalcite**. ICSD structure number 200820. Structural parameters: a = b = 6.0931 Å, c = 7.5446 Å, α = β = 90º, γ = 120º; plot size is 2a*2b*2c; Ca ion shown at centre, hydrogen position is uncertain.

3.3 Distribution, abundance and stability

The stability of the different Ca-carbonate polymorphs in nature, and thus their distribution and abundance, is strongly dependent on their origin and the environment in which they crystallise. So, to understand their presence in a specific environment, their origin has to be examined. As mentioned in chapter 2, there are two sources of crystalline Ca-carbonate minerals in nature; one is biogenic, the other inorganic. Calcite is the most common crystalline phase from both, organic and inorganic, sources. But there is a major difference in the abundance of the thermodynamically less stable polymorphs when their origin is taken into account, with aragonite and vaterite more abundant in organically produced Ca-carbonate. Table 3.2 illustrates how common each of the polymorphs is as a function of its origin, based on occurrences and abundance. The information in table 3.2 addresses only current mineralogy and does not reflect the original mineralogy that might have been present, particularly for the inorganically formed Ca-carbonate, as the metastable Ca-carbonate polymorphs will transform into the stable calcite over time (Wolf and Günther, 2001, Hull and Turnbull, 1973, Garvie, 2003, Sanchez-Moral et al., 2003, Bischoff et al., 1993, Buchardt et al., 2001, Greinert and Derkachev, 2004, Omelon et al., 2001, Marland, 1975, Lennie and Tang, 2003, Swainson and Hammond, 2001, Burt et al., 1997, Giralt et al., 2001, Grasby, 2003, Lowenstam and Abbott, 1975, Sweeting et al., 2004, Watabe, 1974).

	Biologically formed	***Inorganically formed***
Calcite	Most abundant	Most abundant
Aragonite	Very common	Common
Vaterite	Common	Extremely rare
Monohydrocalcite	Rare	Very Rare
Ikaite	Very rare	Rare
Amorphous $CaCO_3$	Common but transient	Not encountered

Table 3.2: Comparison of the relative commonality of the different Ca-carbonate polymorphs as a function of the origin.

Organisms have probably, in one way or another, contributed to the formation of most calcareous sedimentary rocks since the early Precambrian, and they certainly play an important role in maintaining the Ca-carbonate balance in our oceans (Arp et al., 2001, Ridgwell and Zeebe, 2005). However, diagenetic processes and erosion have eliminated many of the initial characteristics of the crystallites constituting these rocks and any biological matter, if initially present, has been destroyed by the same processes. Differentiation of organic and inorganic Ca-carbonate is further complicated by the fact that inorganic and biogenic precipitation of Ca-carbonate occurred often simultaneously, especially in shallow marine and lacustrine environments. It is possible to deduce biogenic influences on the formation of these rocks from traces of other chemical elements, characteristic fossilised forms or even from textural and structural indicators, but concomitant inorganic precipitation can often not be excluded and may in fact have contributed to the supersaturation of Ca-carbonate, aiding in the formation of biogenic Ca-carbonate. The differentiation between organic and inorganic Ca-carbonate in 'contemporary' Ca-carbonate deposits is simpler, where 'contemporary' means from a few years to a few 10,000 years. Here inorganically produced Ca-carbonate, either naturally formed by precipitation, for example through supersaturation in lakes and lagoons, or deposited through volcanic activity, or through dissolution/re-crystallisation in karst environments can clearly be distinguished from biogenic Ca-carbonate in the form of vertebrate and invertebrate skeletons, microbial patinas and even faecal concretions. This is simply because the latter has unusual characteristics not found in the former.

Occurrence and distribution of biogenic Ca-carbonate has been discussed in chapter 2, and a similar effort needs to be made for the inorganic Ca-carbonate to complete the picture and to understand the differences between them. Section 3.3.1 will therefore focus on inorganic Ca-carbonate.

3.3.1 Inorganic Ca-carbonate

The most common and widespread inorganic Ca-carbonate today is calcite, because it is the only thermodynamically stable Ca-carbonate polymorph. All other polymorphs will transform into calcite upon heating, and most will also do so at ambient temperatures over longer time periods. This is the reason why calcite is the most commonly found Ca-carbonate phase among sedimentary rocks and in soils,

sometimes forming pseudomorphs after aragonite, vaterite and ikaite. The second most common is aragonite. It forms preferentially at ambient pressure and temperatures from 60 ºC to 90 ºC, in the presence of Mg^{2+} and in high pressure low temperature metamorphic environments. It is meta-stable over extended periods under ambient conditions, especially when it occurs in larger aggregates or crystals (Kirschvink and Hagedorn, 2000, Kanakis and Dalas, 2000). It is believed that throughout the earth's history the relative proportions of calcite and aragonite have varied (Ridgwell and Zeebe, 2005), and that high pressure and low temperature alteration (blueschist to eclogite facies) may have produced significant amounts of aragonite which subsequently transformed to calcite, either on exhumation or through subsequent alteration (Brady et al., 2004). Inorganic formation of the other Ca-carbonate minerals, anhydrous and hydrous, is very isolated. Occurrences of vaterite (Grasby, 2003), of ikaite (Buchardt et al., 2001) and monohydrocalcite (mostly as a secondary mineral in some mines) have been reported.

The conditions of formation for these rarer minerals shall not be discussed in detail, but I will give a quick summary of the genesis of calcite and aragonite (Rösler, 1984).

Magmatic: There are numerous occurrences of magmatic calcite. It constitutes a large proportion of most carbonatites, which themselves are associated with intrusive igneous rocks and often with Rare Earth Element (REE) minerals.

Post-magmatic and hydrothermal: Calcite is ubiquitously associated with ore forming hydrothermal fluids, where aragonite is also sometimes present. In these, the variety of crystal habits is extensive and has often been used as an indicator for the ore environment. Calcite is also found filling voids of basaltic rocks and occurs jointly with aragonite in deposits around hot springs.

Sedimentary: Calcite slurries form by supersaturation and subsequent precipitation in shallow marine and lacustrine environments, for example in the Persian Gulf and on the Bahamas. Aragonite can also form in marine environments, especially where a higher concentration of Mg ions is present. A second form of sedimentary calcite and aragonite is present in karst environments, where water dissolves Ca-carbonate as it

passes through cracks in limestone and redeposits it as speleothems (deposit in caves).

Metamorphic: Metamorphic transformation can lead to an increase in crystal size (e.g. limestone to marble), without major changes to the composition of the rock. But it can also result in significant changes in the crystal chemistry and structure. Subduction, for examples, can result in the formation of aragonite from dolomite as a study by Shirasaka et al. (Shirasaka et al., 2002) has shown. The formation of calcite or aragonite within the metamorphic regime depends on the pressure/temperature (P/T) relationship, with aragonite being more stable at high P and low T while for calcite the opposite is true.

Secondary mineral formation: Aragonite and calcite can form when Ca bearing rocks or minerals decompose. This can either be through the inflow of alteration fluids rich in CO_2 or through joint alteration of other CO_2-rich minerals.

The kinetic stability of inorganic Ca-carbonate polymorphs has been the subject of many studies, mainly examining the rate of reaction for phase transformations (White, 1997, Peric et al., 1996, Kralj and Brecevic, 1997, Wolf and Günther, 2001), precipitation or dissolution under variable conditions of pH, temperature, super-saturation (Dickinson et al., 2002, Xyla et al., 1991, Kawano et al., 2002, Spanos and Koutsoukos, 1998, Kralj and Brecevic, 1990, Kralj et al., 1994, Tai and Chen, 1998, Musvoto et al., 2000, Cubillas et al., 2005, Elfil and Roques, 2004, Elfil and Roques, 2001) and in the presence of inorganic growth modifiers (Tracy et al., 1998b, Tracy et al., 1998a). All these studies conclude, that the only stable polymorph at ambient conditions is calcite, despite aragonite having lower bulk lattice energy (de Leeuw and Parker, 1998b). Aragonite becomes stable at elevated pressures and can, due to its slow transformation to calcite, persist over a geological time span (White, 1997), while inorganic vaterite only occurs under extreme conditions and is not stable once exposed to ambient conditions (Grasby, 2003). Figure 3.6a, adapted from (Madon and Gillet, 1984), and figure 3.6b, adapted from (White, 1997) show the experimental stability relationship of calcite and aragonite as a function of pressure (P) and temperature (T), based on phase transformation data. The hatched area in

figure 3.6a corresponds to variations in parameters such as grain size and impurities. For references quoted in figure 3.6b see (White, 1997).

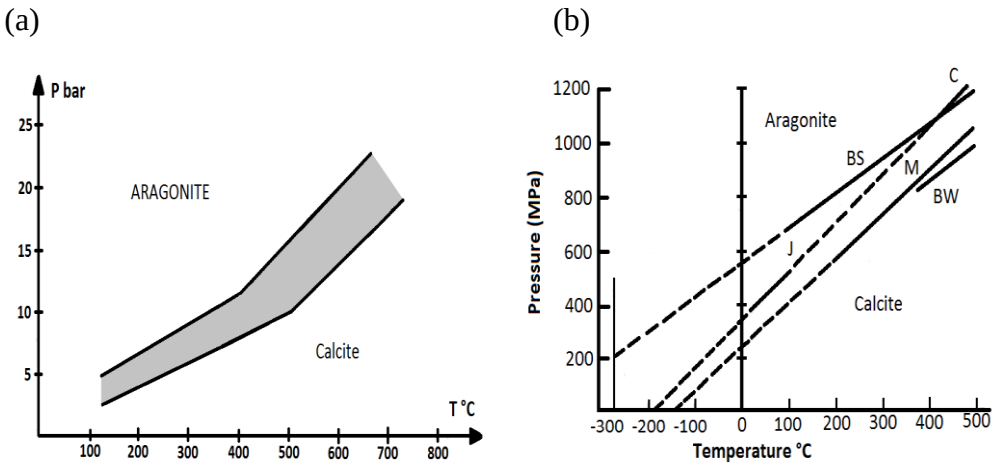

Figure 3.6: Phase stability of aragonite and calcite in the temperature-pressure field. After Madon and White. *BS*: Simmons and Bell (1963); *J*: Jamieson (1953); *M*: MacDonald (1956); *BW*: Boettcher and Wyllie (1968); *C*: Clark (1957). Adapted from Rösler (Rösler, 1984).

The relative stability of all the Ca-carbonate polymorphs, whether hydrated or not, has been considered alongside their solubility products. Table 3.3, after (Elfil and Roques, 2001) provides an overview of the logarithmic thermodynamic solubility products. Calculated logarithmic solubility products (p*K*s) for the different Ca-carbonate phases at room temperature (23 ºC), given in table 3.4, clearly indicate that aragonite and calcite have similar solubility products and as such are close in their stability, while vaterite lags behind and the hydrated phases, including Amorphous Ca-carbonate (ACC) are extremely unstable under normal conditions without organic growth modifiers.

	Equations of p*Ks* (*T* in *K* and *t* in °C)	
Calcite	$171.9065 + 0.077993T - 2839.319/T - 71.595 \log(T)$	$0 < t < 90°C$
Aragonite	$171.9773 + 0.077993T - 2903.293/T - 71.595 \log(T)$	$0 < t < 90°C$
Vaterite	$172.1295 + 0.077996T - 3074.688/T - 71.595 \log(T)$	$0 < t < 90°C$
ACC	$6.1987 + 0.0053369t + 0.0001096t^2$	$10 < t < 55°C$
$CaCO_3$ H_2O	$7.05 + 0.000159t^2$	$10 < t < 55°C$
$CaCO_3$ $6H_2O$	$2011.1/T - 0.1598$	$0 < t < 25°C$

Table 3.3: Logarithmic thermodynamic solubility products for Ca-carbonate (Elfil and Roques, 2001).

	p*Ks* calculated for 23 °C
Calcite	8.47
Aragonite	8.32
Vaterite	7.90
ACC	6.38
$CaCO_3 \cdot H_2O$	7.13
$CaCO_3 \cdot 6H_2O$	6.63

Table 3.4: Solubility products for Ca-carbonate at 23 ºC, showing the stability of each Ca-carbonate polymorph. Higher values indicate high stability.

3.4 Morphology

Not only does the presence and abundance of the Ca-carbonate polymorphs vary with the conditions under which they are formed, but their 'morphology' also varies. The 'morphology' of the different Ca-carbonate polymorphs has been used extensively in the attempt to discern between them. But the word 'morphology' itself has, unfortunately, a rather broad meaning that needs classification and which has to be used carefully and in context; while many authors have tried to be specific, a number have not. The most common example of the inappropriate use of morphology is to describe vaterite particles and calcite crystals without being specific. I will, to avoid this, use the term *crystal morphology* to describe a single crystal or an apparent expression thereof, and use *particle morphology* for clusters of

crystals where the individual crystal shape cannot be discerned with any degree of certainty or where the shape of the cluster differs greatly from the single crystal morphology. A rather important factor in this context is the size of the crystal that is produced, and therein lays the most significant difference between biogenic and inorganically produced Ca-carbonate. Single crystals produced by organisms are generally microscopic, but can be macroscopic, like in the case of the sea urchin spine; the crystallite size, however, is limited to the nanometre to micrometre range. Inorganic calcite crystals in contrast range from micrometre to metre scale, with the largest being in excess of 6 x 6 x 2 m^3 (Rösler, 1984). Here I will give an overview of the common morphologies exhibited by the Ca-carbonate polymorphs to illustrate the link between the growth environment and the size of the crystals formed. Hundreds of crystal morphologies have been reported for calcite, making it the mineral with the most crystal morphologies. Figure 3.7, adapted from Rösler (1984), shows idealised drawings of the most common inorganic calcite crystal morphologies in nature, and figure 3.8 also adapted from Rösler (1984) shows how these crystal morphologies vary in ore forming environments as a function of concentration and temperature.

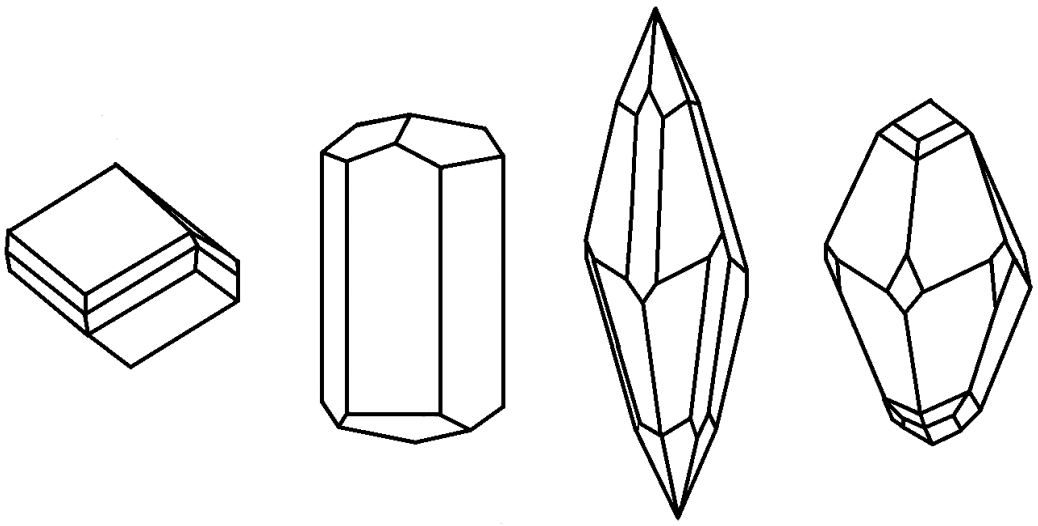

Figure 3.7: The most common crystal forms of calcite, listed in order. 1) Rhombohedron, 2) Prismatic 3) Pyramidal, 4) Scalenohedron. Adapted from Rösler (1984).

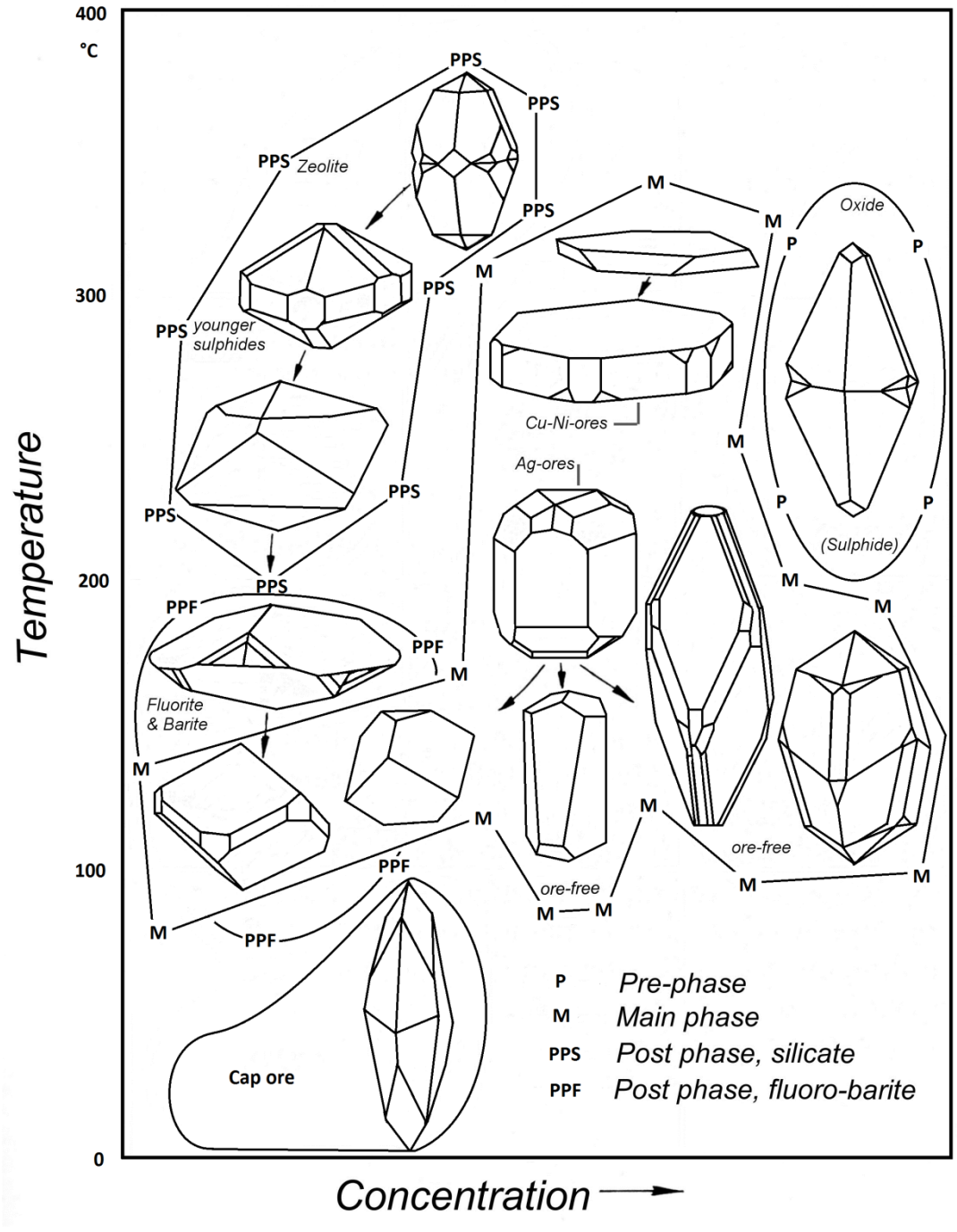

Figure 3.8: Change in crystal morphology of calcite as a function of ionic concentration and temperature in ore forming environments from the West Harz Vein Ore deposits. Adapted from Rösler (1984).

The most common crystal morphology of inorganic calcite found in nature is the scalenohedron, followed by the rhombohedron. The scalenohedron is not the energetically most favourable crystal morphology according to de Leeuw and Parker, (1998b), which found that the rhombohedron is the energetically most favourable crystal morphology when the calcite crystal is grown in water, based on the surface

energies of hydrated and un-hydrated planes. Figure 3.9 comes from their work and shows the equilibrium morphologies for calcite.

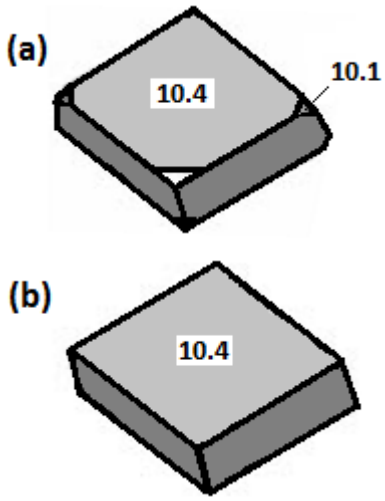

Figure 3.9: (a) Equilibrium morphology of unhydrated calcite and (b) growth morphology and equilibrium morphology of hydrated calcite crystal. Numbers represent crystal faces indexed in the hexagonal system. Adapted from (de Leeuw and Parker, 1998b).

It is not surprising that the scalenohedron is the most common inorganic crystal morphology in nature, as it is unlikely to have pure water and ambient conditions as growth environment for calcite in nature, and time might also be an issue. Their atomic modelling study (de Leeuw and Parker, 1998b) also ignores the presence of crystal faults and dislocations.

Calcite crystal morphologies produced by precipitation experiments in the laboratory are usually rhombohedral, and the presence of organic and inorganic growth modifiers at lower concentrations, and some at higher, often produce rhombohedral calcite crystals, even though these are sometimes slightly deformed (DeOliveira and Laursen, 1997, Feng et al., 2000b, Keum et al., 2003, Wei et al., 2003, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008, Zhang et al., 2010) while at higher concentrations of organic additives, or in the presence of some specific organic additives the crystal morphology can change completely (Feng et al., 2000b, Tong et al., 2004, Keum et al., 2003, Seo et al., 2004, DeOliveira and Laursen, 1997, Wei et al., 2003, Meldrum and Cölfen, 2008, Sommerdijk and de With, 2008, Zhang et al., 2010).

In addition to the effect that organic and inorganic growth modifiers have on the crystal morphology of calcite, magnetic and electrical influences have also been tested, and in some cases were found to influence the crystal morphology, leading to rhombohedral or scalenohedral crystals (Garcia Carmona et al., 2003). To further complicate things, the process route also has an impact on the crystal morphology, as have the reagents used, and scalenohedral calcite was formed without additives by bubbling CO_2 through a suspension of $Ca(OH)_2$ (Garcia Carmona et al., 2003).

Aragonite crystal morphology is also variable, but to a lesser degree than calcite crystal morphology. Figure 3.10 (Rösler, 1984) shows representations of some of the more common inorganic aragonite crystal morphologies.

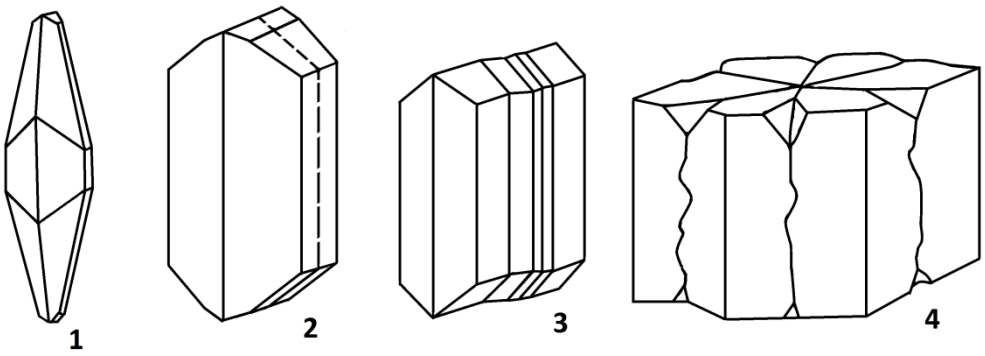

Figure 3.10: Common aragonite crystal morphologies. 1) needle, 2) platy, 3) polysynthetic twinned, 4) intergrowth (cyclic) twins. Adapted from Rosler (1984).

Most well-known are the cyclic twins, but needle like crystals and massive vein fillings, dendritic growth formations, powdery coatings and oolitic concretions are more common. The size ranges are similar to the ones for calcite, with biogenic aragonite being restricted mostly to either needle like or platy morphologies in the order of a few nanometres to a couple of tens of micrometres across in the case of the largest platelets. For the inorganic crystals the size ranges from micrometres to about a decimetre, but the larger crystals are usually cyclic twins, resembling hexagonal prisms. Figure 3.11 (de Leeuw and Parker, 1998b) shows the equilibrium morphologies of aragonite as determined through modelling of the surface energies of the most common terminal planes in both the hydrated and un-hydrated state.

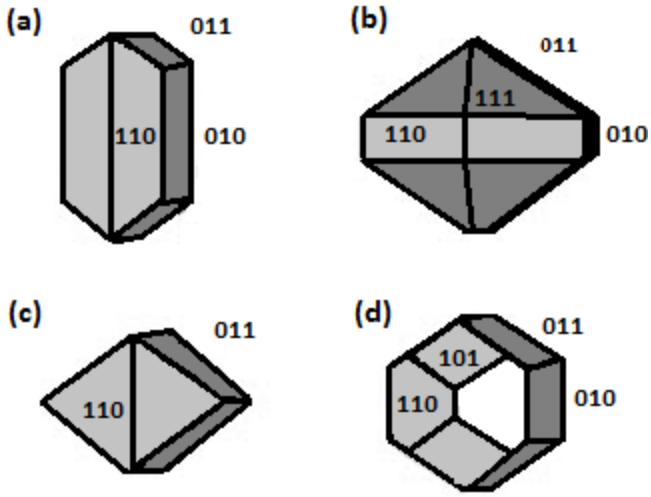

Figure 3.11: Equilibrium morphologies of aragonite (de Leeuw and Parker, 1998b) (a) Experimental morphology of aragonite, (b) equilibrium and (c) growth morphology of un-hydrated aragonite, and (d) equilibrium morphology of hydrated aragonite.

Inorganic aragonite crystals in nature often show an elongation in the direction of the crystallographic c-axis, while their organically produced counterparts are mostly shortened in this direction, leading to the well know platelets that make up the aragonitic layer of nacre and other molluscs (Chateigner et al., 2000, Feng et al., 2000a, Checa and Rodríguez-Navarro, 2001, Rousseau et al., 2005, Meldrum and Cölfen, 2008, Luz and Mano, 2010). Films with completely irregular crystal morphology, resembling spherical growth, have also been produced (Wada et al., 2004).

No reliable data exist for the crystal morphology of naturally occurring inorganic vaterite, but it is assumed that the crystals are flat and almost disc shaped. This would roughly correspond to the equilibrium morphologies determined by de Leeuw and Parker (1998b) and adapted here as figure 3.12.

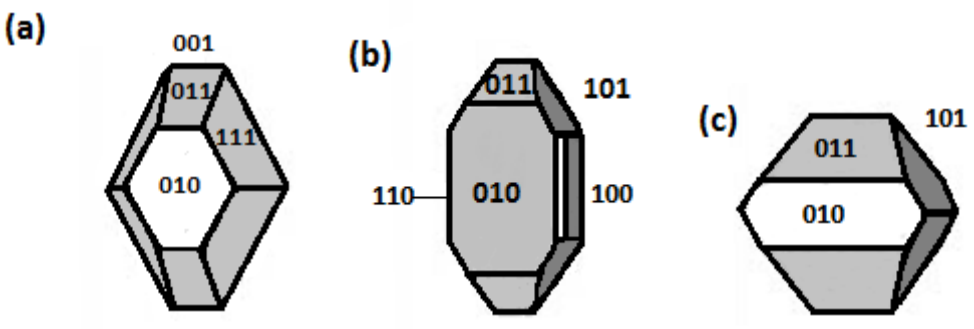

Figure 3.12: Vaterite equilibrium morphologies (de Leeuw and Parker, 1998b) (a) Equilibrium morphology of un-hydrated vaterite, (b) growth morphology, and (c) equilibrium morphology of hydrated vaterite.

Particle morphology of vaterite is very different; it almost exclusively occurs in spheres.

No significant data on the crystal morphology of the other Ca-carbonate phases exist, but their crystal morphologies have been vaguely described. Ikaite has rarely been observed in nature, and the most reliable information about its crystal morphology has been deduced from experiments and the possible pseudomorphs of calcite after ikaite called glendonites (Swainson and Hammond, 2001). It is described as forming elongated crystals with square prismatic, pyramidal and sigmoidal crystal morphology, albeit being monoclinic. Monohydrocalcite does not appear to have a dominant of well-defined crystal morphology, instead when described from natural sources it is said to be botryoidal and cryptocrystalline, and even from biogenic sources it has only been described as coatings (Garvie, 2003).

4 EXPERIMENTAL

4.1 Sample production precipitation experiment

Rationale

The experiments undertaken in this study were planned as part of an ongoing study of the factors controlling biomineralisation. A previous investigation into the influence of the organic acids mono-L-Glutamic (GLU) and mono-L-Aspartic (ASP) on the crystallisation (Guha, 2002) had produced some interesting but contradictory results. Analysis of the samples produced during that study indicates that the organic acids had an effect at higher concentrations (500 mg/L and 1000 mg/L) and also at some very low concentrations, but not in between. Since no process parameters had been recorded during the previous precipitation experiment, it could not be determined if the resultant phases and morphologies reflect an intrinsic property of the system or are a result of the kinetics. The suite of experiments which forms the basis of this thesis was therefore designed to elucidate the influence of the precipitation environment on the Ca-carbonate phases and morphologies produced.

Experiment design

Four main variables were chosen to limit the number of samples that needed to be produced, with the total number of samples reaching 96.

The main variables chosen for the experiments were the concentration of the organic acid (3), time to harvest (3), sequence of addition of the reactants (3) and speed of addition (2), each of these for two different organic acids. In detail:

Organic acids: GLU and ASP

Time to harvest: 1 hour, 1 day and 1 week

Concentration: 10 mg/L, 100 mg/L and 1000 mg/L

Sequence of addition and speed of addition are described in more detail in the next section.

Sample production methodology

A quantity of stock solution of ASP (Sigma BioUltra ≥ 99.5%) or GLU (Sigma ReagentPlus ≥ 99%) was placed in a beaker and diluted to the desired concentration for the experiment while being magnetically stirred. Burettes containing 1 M $CaCl_2$ (50 ml) (FLUKA puriss. p.a. ACS reagent ≥ 99%) and $NaHCO_3$ (90 ml) (Sigma-Aldrich ReagentPlus ≥ 99.5% crystalline) solutions, as well as burettes containing the organic acid solution at double the required concentration with a total volume equalling the combined volume of the Ca chloride and sodium bicarbonate solutions were placed above the beaker. Three different concentrations of the organic acids were selected, 1000 mg/L, 100 mg/L and 10 mg/L. Three different methods of addition were selected, each with two different addition times and three different harvesting times, resulting in eighteen independent experiments for each organic acid at each of the three different concentrations, as detailed below. This would have resulted in a total of 104 samples, but the total number of experiments was only 96, as methods E and F were not used on the samples with 100 mg/L organic acid concentration. All solutions were covered after 20 minutes, or as soon as the addition was complete for the samples with slow addition. The experimental set-up is illustrated in figure 4.1.

Figure 4.1: Crystal growth experimental setup. One experiment is under way on the left, while a second one is being prepared on the right.

Method A

Ca chloride, sodium bicarbonate and organic acid solution were added at the same time while stirring the solution. Addition was over a short time interval, around 3 to 5 minutes.

Method B
This is the same as method A, except for the time of addition which was longer, taking around 20 to 25 minutes.

Method C
Ca chloride solution was added to the recipient prior to commencement of the experiment. To ensure the organic acid concentration was kept the same, the same volume of organic acid solution, but at double the concentration was also added prior to the experiment while the solution was magnetically stirred. After an interval of 5 minutes +/- 10 s the sodium bicarbonate solution was added together with the same volume of organic acid solution at double the concentration, again to maintain the concentration of the organic acid the same, while continuing to stir the solution. Addition was over a short interval, around 3 to 5 minutes.

Method D
Sodium bicarbonate solution was added to the recipient prior to commencement of the experiment. To ensure the organic acid concentration was kept the same, the same volume of organic acid solution, but at double the concentration was also added prior to the experiment while the solution was magnetically stirred. After an interval of 5 minutes +/- 10 s the Ca chloride solution was added together with the same amount of organic acid solution at double the concentration while continuing to stir the solution. Addition was over a short time interval, around 3 to 5 minutes.

Method E
This is the same as method C, except for the time of addition which was longer, at around 20 to 25 minutes.

Method F
This is the same as method D, except for the time of addition which was longer, at around 20 to 25 minutes.

The pH and also the temperature of the solutions during each experiment were recorded to monitor and evaluate changes and similarities.

The solutions were vacuum filtered once the set time for each experiment had passed and the mother liquor was used to wash the crystalline matter onto the filter. No deionised water was used to wash the sample powder. The samples were subsequently transferred from the filter paper into a washed 50 ml labelled vial with the lid loosely covering the opening to allow the sample to dry in air. Once the sample powder was completely dry, usually after about 1 day, which was determined by examining a minute quantity admixed to silica gel, the cap was fully closed.

4.2 Morphological analysis of the samples

Two main techniques were used in the morphological analysis of the precipitated powders produced by the experiments. One was a preliminary examination with an optical microscope, the other a more detailed analysis using the scanning electron microscope, both available at the Physics Department at Curtin University.

Optical analysis

Early experiments indicated that the examination of the precipitate while it was still moist had an adverse impact on the sample. The remnants of solution still present, in conjunction with the high heat generated from the microscope lamp, forced re-crystallisation of parts of the sample during the examination. It was therefore decided to transfer a small portion of the precipitate onto the glass slide and let it dry on the slide at ambient conditions, and examine it once dry. The binocular microscope was then used to obtain an estimate of grain sizes and morphologies, and no transformation was visible during the examination.

Scanning electron microscopy (SEM) analysis

A small amount of the dry sample was transferred onto carbon tape positioned on a microscopy glass slide for SEM analysis, using a Philips XL30 Electron Microscope. The carbon tape was applied lengthwise and across, resulting in a total of 8 cross-over points on the slide. This layout was chosen to increase throughput, allowing 8 samples to be placed at the cross-over points while at the same time clearly distinguishing the sample and eliminate cross-contamination. The slide was then

placed in a gold coater and coated. Since chemical analysis was not an objective of the examinations, it was decided to use a slightly thicker gold coating to reduce some of the charging effects during the analysis. Images in the SEM were taken at a normal working distance of 20 mm, but also at distances of 10 mm and 5 mm, using a low-kV anode.

4.3 Structural analysis of the samples

A number of techniques were used in the structural characterisation of the samples. Samples were analysed first using X-ray powder diffraction (XRD), using a Siemens D500 diffractometer at Curtin University and also a PANalytical X'Pert MPD system at the CSIRO, Waterford. These initial examinations were used to establish if the concentrations of additives chosen to be used in the experiments were covering a sufficient range in additive concentration, i.e. if the samples contained more than one phase, and preferably did change from one phase dominating at the lower end of additive concentration to another phase dominating at the higher additive concentrations.

From these initial experiments it was clear that laboratory based XRD would not have the resolution or sensitivity to be able to examine the direct impact the additives were having on the structures of the phases produced, and that other techniques would be required. In particular, two areas could not be directly evaluated with the instruments at our disposal; one being the amount of amorphous material present in the samples and the other related to structural properties of the produced crystals themselves, i.e. the average crystallite sizes and the stress/strain present in the phases.

The main technique available that can deliver the resolution, speed and level of detail required is synchrotron radiation powder diffraction (SXRPD). It has a number of advantages; the main ones relevant to our experiments are tuneable wavelength, monochromatic radiation and high flux, eliminating the shortcomings of laboratory XRD.

A number of proposals were submitted to obtain access to the Advanced Photon Source (APS) in Argonne, Michigan, USA, and we were fortunate enough to be given multiple time slots to perform most of the experiments proposed and required to cover the samples produced in the precipitation experiments. Two of the most interesting experiments, however, were only possible during the last visit, and the time frame given for the experiments meant that we had to limit the number of samples analysed. A more detailed overview of the experiments, the preparation required and the set-up involved follows in section 4.3.1.

A set of samples was also produced for high resolution neutron powder diffraction analysis, (NPD), chiefly to assess the amount of amorphous material present and to possibly elucidate the structure of vaterite. The main reason for running the NPD experiments was to obtain better sampling statistics and a smaller error related to the addition of an internal standard, as the amount of material analysed by NPD is quite substantial. As a consequence, the amount of sample required for these experiments was quite high, and three precipitation experiments of the same kind were run in parallel to produce enough sample. This, combined with the time required for NPD analysis meant that only a few samples could be produced and run, and the sample selection was limited to samples produced in the presence of 1000 mg/L ASP or GLU, as these were most likely to contain some amorphous material and also a significant amount of vaterite. Of the samples produced, only a handful were analysed due to time constraints and the need to run the same sample multiple times for the different levels of internal standard added.

4.3.1 SXRPD analysis

4.3.1.1 'Reflection' mode

The primary experiments carried out at the APS were SXRPD experiments on Beamline 1BM. The set-up required the construction of specific sample holders and a spinner mechanism to use the instrument in theta-2theta (θ-2θ) mode, where the sample is located on the diffractometer axis and moved around the axis at a speed of x degrees per minute, while the detector is located on the parafocussing circle and rotated in the same direction, but at a speed of 2x (Bragg-Brentano parafocussing

geometry). The main aim of spinning the sample was to improve particle statistics by analysing the largest possible volume. Two versions of the sample holder and spinner assembly were constructed; one for the first experiment, which suffered from some problems with the spinning mechanism and also with sample height alignment, and a second version which was used for all subsequent experiments.

The sample holders were made as two-part holders in which the front part has a hole in which the powder is pressed from the back on a flat surface, while the back part is a solid piece that latches to the back of the front part; this allowed back-filling, thus maximising the packing density while minimising preferred orientation.

Figure 4.2 and 4.3 show the second version of the sample spinner mounted on the four circle goniometer with a sample in place. The sample spinner allows for exact positioning of the sample in the centre of the goniometer rotation axis and centre of the beam.

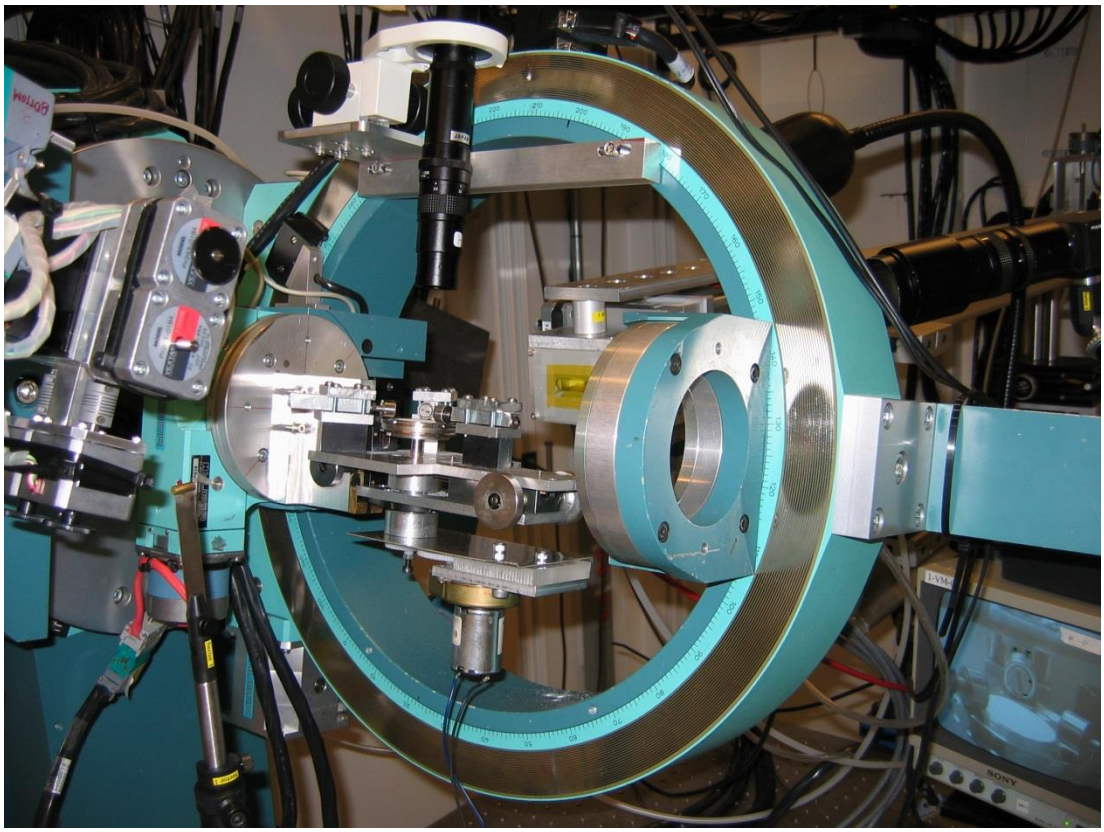

Figure 4.2: SXRPD arrangement at APS. Sample spinner mounted on the four-circle goniometer. Detector and slit assembly are on the left, the beam comes in from the right in the background. The alignment microscope

is mounted vertically to the sample surface, and the spinner is in the centre, with a sample mounted.

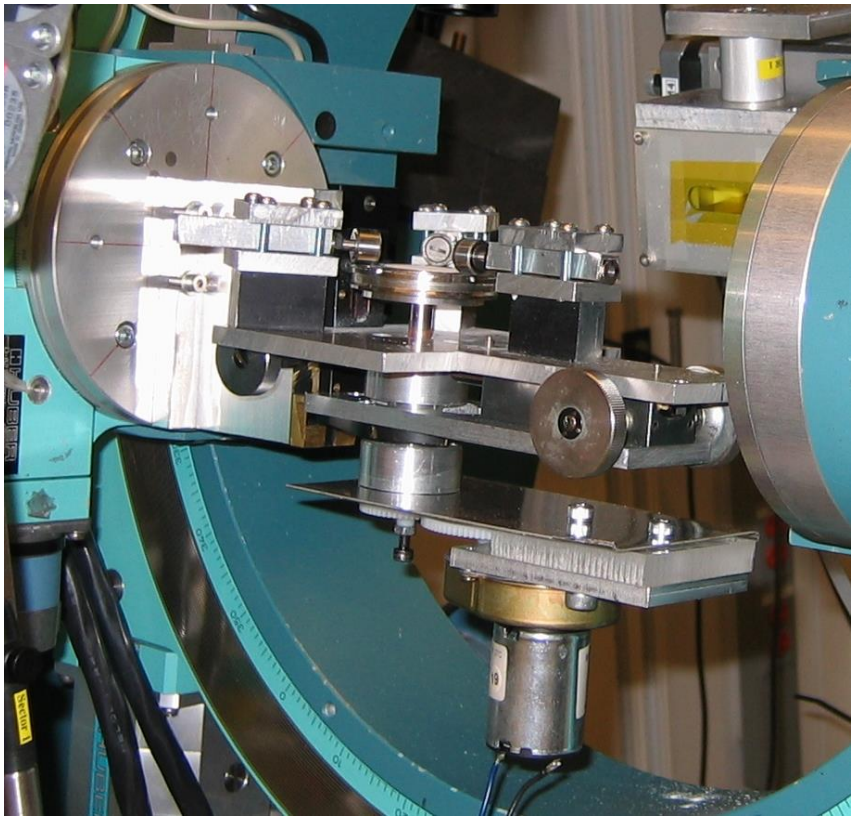

Figure 4.3: Enlarged portion of figure 4.2, showing the sample spinner assembly. The three roller bearings visible serve as reference height for the sample, making sure that the sample surface was always at the right height during each measurement and that wobble was kept to a minimum.

Initial trials were undertaken to establish the best running conditions for the samples. It was found that all samples precipitated in the presence of 1000 mg/L of amino-acid contained predominantly vaterite, regardless of the residence time, while samples precipitated in the presence of 100 mg/L of amino-acid were generally calcite were residence times in excess of 1 hour were used, and that samples precipitated in the presence of 10 mg/L of amino-acid were predominantly calcite, even after the shortest residence times. The crystallite sizes of the two Ca-carbonate phases differ significantly, as do their peak shapes and widths. Vaterite has fairly small crystallites, while calcite showed relatively large crystallites. The step size and measurement times required to adequately resolve all the peaks with sufficient

intensity at each step, with the aim of collecting data for crystallite size and stress/strain calculations, changes as a function of the phases present in each sample. Samples that contain only vaterite required scans with a lower resolution, but increased measurement times, while samples that contained exclusively calcite required relatively high resolution and slightly shorter measurement times. The main problem faced was the relatively long time for the goniometer to move and settle after each step, which often was as long as or longer than the measurement time. For samples containing both Ca-carbonate phases this would have resulted in prohibitively long measurements for a full scan. To overcome this, a lower resolution scan, using a stepsize of 0.002º 2θ for samples where calcite was present or assumed to be present and 0.005º 2θ for samples without calcite was used to capture a full pattern for the vaterite. Subsequent high resolution scans with a stepsize of 0.001º 2θ were run only over the relevant calcite peaks in those samples. For samples that contained only calcite, which were most of the samples produced at an amino acid concentration of 10 mg/L with harvesting times greater than one hour, high resolution scans were run over the calcite peaks, ensuring that peak tails were not cut off prematurely on either side. Through this approach we were able to adapt the running conditions to maximise throughput without compromising data quality. All samples produced by the experiments were run in the θ-2θ configuration at the APS beamline 1BM, using a beam at 20 keV, which corresponds to a wavelength of approximately 0.619 Å. The exact wavelength was determined using Si (NIST 660c) and LaB_6 (NIST 660a) standard reference materials. The standard reference materials were run at the beginning and at the end of each experiment, and monitoring data from the synchrotron ring itself was collected alongside the experimental data for the purpose of normalising the data collected over the extended time that each experimental sample run took. The data were collected with a SiLi and a Ge solid state detector (Canberra).

4.3.1.2 Transmission mode

Powder diffraction experiments on the Ca-carbonate produced in the experiments in transmission mode had been one of the aims when first applying for experiment time. The principle idea was to add a certain percentage of an inert standard of similar mass absorption to the samples at two different concentrations, to quantify the

amount of amorphous material present, if any. Corundum was chosen because it represented the best choice with respect to particle size, crystallite size and cost. Since mixing of the sample with the internal standard usually involves lightly grinding both together in a mortar and pestle, which may change the crystallinity of the phases being 'mixed' or even the amount of the phases present, physical force during the mixing was minimised. To achieve this goal, while still achieving sufficient random mixing, a relatively large volume of sample was used. This was possible by using an intense beam and mounting the sample in a transmission holder and oscillating the sample on an elliptical path through the beam. It also required a stationary detector, in order to eliminate time dependence of the movement of the sample through the beam. We achieved this by using beamline 1ID at the APS and running the experiment using an energy setting of approximately 80 keV, equivalent to a wavelength of 0.155 Å. Data were collected using a MAR3450 CCD area detector which collects the complete diffraction cone and extracted using Fit2D (Hammersley, 1998) and subsequently transformed into 2θ/I data for import into other programs. Time limitations meant that we could only run a small number of samples; of these a selection was run twice, with two different concentrations of internal standard, to improve the accuracy of the results for the amorphous phase content.

Since the experiment ran in transmission mode, polyimide film was chosen as a "window" material, as previous tests indicated that it generated only a small background contribution at approximately 20 keV. An initial test run confirmed the contribution from polyimide to the pattern at approximately 80 keV to be negligible. The sample holder had to be a three piece holder to protect the windows on both sides during handling and running as well as allowing for easy packing of the powder in the centre piece. Figure 4.4 shows one of the sample holders with a sample loaded in it.

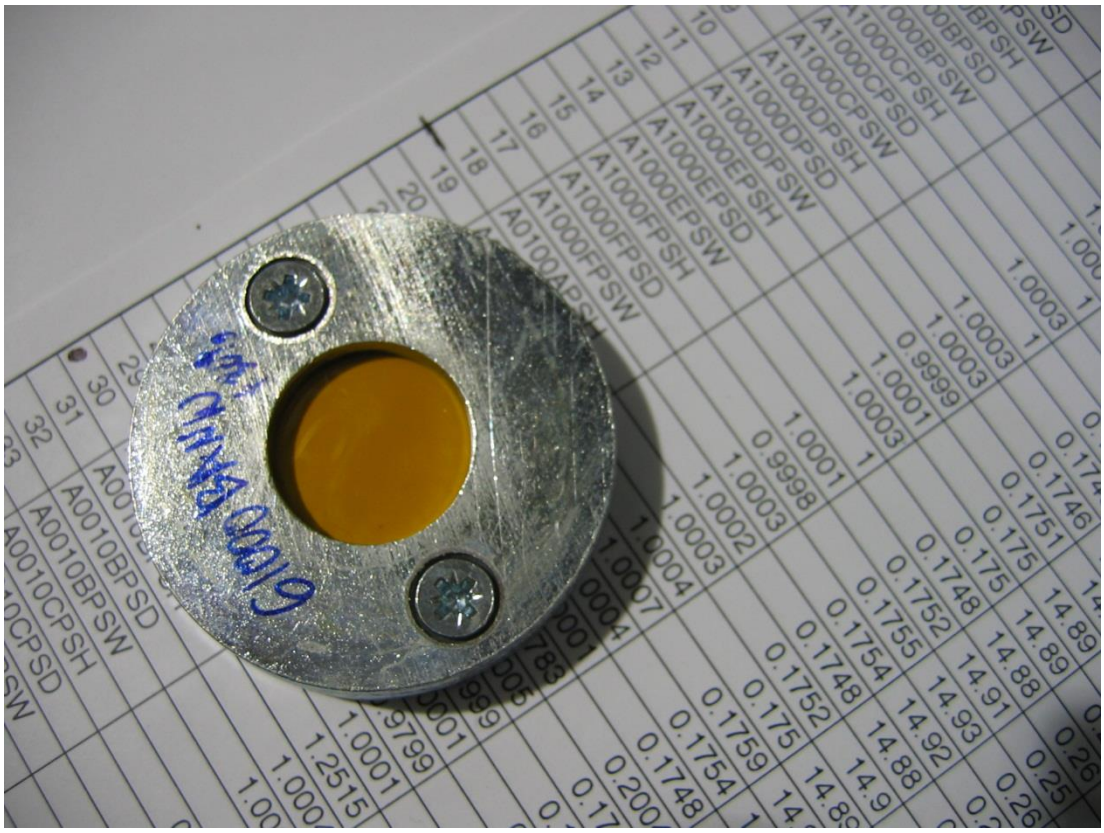

Figure 4.4: Sample holder for the transmission experiment with sample loaded.

4.3.1.3 Peak fitting

Raw data collected in 'reflection' and transmission mode were subsequently used to extract Gaussian and Lorentzian β values using single peak fitting employing a Voigt function. This was done by transforming the data into a format readable by the MDI program Shadow (Materials Data) and fitting each peak manually, extracting the values and their respective esds and entering them into a spreadsheet for calculation of (hkl) dependent coherent scattering domain sizes and micro-strain.

The same approach was used for the standards and for all samples, which consisted of:

a) Collection of data at the 1BM beamline at the APS in the native POW file format, using flat plate geometry and spinning the sample
b) Calibration and transformation of the data by using the monitor counts simultaneously measured, to account for any variation in the photon flux during data collection

c) Modification of the data into a format readable by SHADOW (Materials Data)
d) Single peak fitting of all peaks using SHADOW (Materials Data) using the Voigt function
e) Extraction of all Gaussian and Lorentzian β-values (integral breadth) and their estimated standard deviations (esd)
f) Using Gaussian and Lorentzian β-values and esd to calculate size and strain, while excluding all statistically questionable data points, i.e. The ones for which the value of 3 esd exceeds the value of the data point itself.

4.3.2 Neutron powder diffraction (NPD) analysis

NPD experiments were carried out at ANSTO on the high resolution powder diffractometer at the HIFAR, using vanadium cans to hold the sample as vanadium has a very low coherent neutron scattering cross section. A wide scanning range was chosen, and data were collected from 0.023º 2θ to 150.073º 2θ at a step size of 0.05º and to a count rate of 28000 monitor counts at every step. The wavelength was determined using the Al_2O_3 from NIST, standard reference material 676, to be 1.4929(1) Å. The pattern for the standard reference material 676 was also used to establish instrument constants.

4.4 Fourier-transform infrared (FTIR) analysis

An opportunity arose to analyse some of the samples using FTIR instruments at the ANSTO Lucas Heights facility, a BioRad FTS-40 from Spectrotec with sample heating. Two samples of the ones used in the NPD experiments were chosen, because sufficient undiluted sample material was available. The two samples were both produced in the presence of GLU at a concentration of 1000 mg/L, both using slow addition, and both were harvested after one week. The two corresponding methods were ‘B’ and ‘F’. The samples were dispersed prior to analysis by admixing KBr to obtain a concentration of about 7.8% of sample in the final mass.

The background was measured using single beam mode and the airflow was set at about 20 mL/min and monitored throughout the experiment. Background scaling was established as 1.4.

5 RESULTS – SAMPLE PRODUCTION, MORPHOLOGY AND STRUCTURE

The results reported in this chapter do not encompass all samples produced during the experimental stage, and neither all of the methods used for analysis, as some samples were only analysed by one analytical technique. Some sample groups did not show any difference, and examples have been used to indicate trends.

5.1 Sample production

96 samples were initially produced, according to the sample production methodology outlined in chapter 4, summarised in table 5.1. The methods denominated as A to F are described in chapter 4, and are summarised below. For ease of understanding, the reactants are abbreviated such:

Ca chloride – CaCl

Sodium bicarbonate – NaHCO

Amino acid - AA

Method A
CaCl, NaHCO and AA added at the same time, addition completed in 3 to 5 minutes.

Method B
CaCl, NaHCO and AA added at the same time, addition completed in 20 to 25 minutes.

Method C
CaCl and AA in receptacle, NaHCO and AA added over 3 to 5 minutes.

Method D
NaHCO and AA in receptacle, CaCl and AA added over 3 to 5 minutes.

Method E
Same as C, except for slower addition, completed between 20 and 25 minutes.

Method F
Same as D, except for slower addition, completed between 20 and 25 minutes.

ASPARTIC and GLUTAMIC ACID Sample Production Matrix									
Concentration of the acid	Method A Harvesting time			Method C Harvesting time			Method D Harvesting time		
	1 hour	1 day	1 week	1 hour	1 day	1 week	1 hour	1 day	1 week
1000 mg/L	x	x	x	x	x	x	x	x	x
100 mg/L	x	x	x	x	x	x	x	x	x
10 mg/L	x	x	x	x	x	x	x	x	x
Concentration of the acid	Method B Harvesting time			Method E Harvesting time			Method F Harvesting time		
	1 hour	1 day	1 week	1 hour	1 day	1 week	1 hour	1 day	1 week
1000 mg/L	x	x	x	x	x	x	x	x	x
100 mg/L	x	x	x						
10 mg/L	x	x	x	x	x	x	x	x	x

Table 5.1: Overview of the different samples produced for the experiments

There were some deviations from the scheduled harvesting times during the experiment, especially for the samples harvested after 1 day and 1 week. Tables A1 and A2 in the appendix provide an overview of the actual harvesting times for all samples and the respective deviations.

During the sample production stage, pH values were also recorded for all types of samples. There were some problems with the probe during the recording of about half the samples, with pH values not being consistent and data being recorded outside the possible range. Some general comments can still be made.

There is no statistically measureable difference between the samples grown in the presence of GLU and ASP in terms of the final pH.

The presence of the AAs has an effect on the solutions; this is notable in the solutions containing only 10 mg/L of AA. In these the pH oscillates within a range of +/- 0.2, while it is restricted to a variation in the order of +/- 0.1 in samples grown in solutions of 100 mg/L and 1000 mg/L. The variations are probably due to small variations in the rate of addition of the reactants, and the fact that they are more limited in samples grown at higher concentrations seems to confirm this, and is most likely due to the buffering effect stemming from the AAs.

The pH curves follow a general trend, depending on the method applied, and there is little difference between the samples grown at slower addition speeds and at higher addition speeds. Fig. 5.1 shows the change of pH with time for the principle methods (A, C, D); for the slower addition methods (B, E, F), the curves are practically the same, but they extend over the whole time interval with asymptotic approximation to a pH of about 6.5 only towards the 20 minute mark.

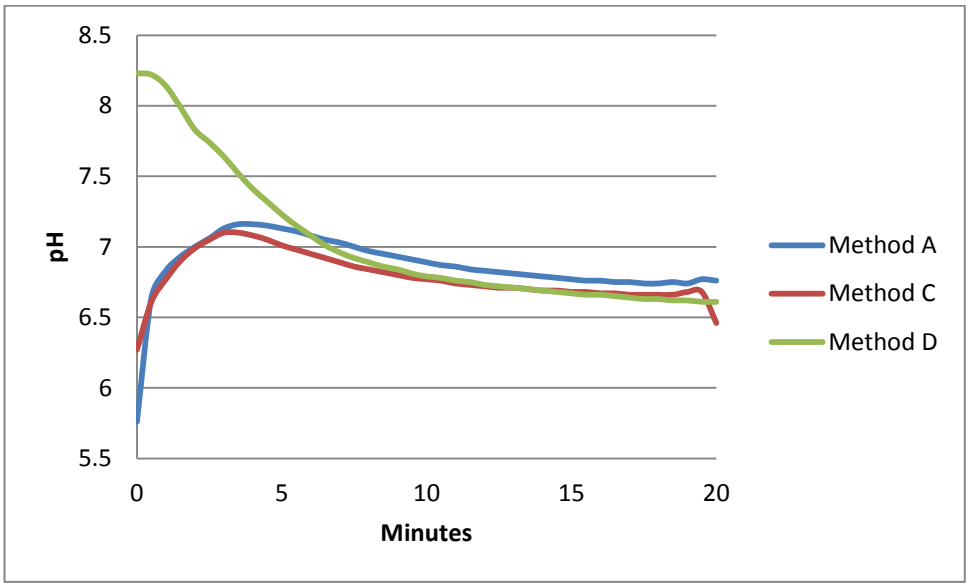

Figure 5.1: Representative pH curves for the different methods employed in the production of the samples. High starting pH for method D is due to the presence of sodium bicarbonate in the initial solution.

5.2 Morphological analysis

5.2.1 Optical microscopy

No tangible results were obtained from examinations under the optical microscope, with the information gathered in regard to particle sizes, agglomeration and transformation used to plan examination by SEM.

5.2.2 Scanning electron microscopy (SEM) analysis

The main purpose of carrying out SEM analysis of the samples was to investigate the morphologies present, and to ascertain if there are differences in the morphologies for samples produced by the different methods, concentrations and harvesting times.
It has been generally assumed that the morphology of the Ca-carbonates can be used as an indication of the phases present, with vaterite generally forming flat or lozenge shaped, rounded to pseudo-hexagonal porous aggregates, which can be intergrown, or more commonly assembled into hollow spheres. Calcite, on the other hand is generally seen as forming pristine to heavily deformed rhombohedral crystals, mostly compact with some well-defined edges. This, however, will have to be revised based on observations made in this thesis.

Vaterite morphology does not vary with any factor for samples harvested at the same time, not even when comparing ASP to GLU. One thing that does change is the porosity and the amount of vaterite that occurs in hollow spheres or 'pancake' shaped aggregates. The main changes in morphology occur with changes in harvesting time, with aggregates becoming denser and with more intergrowth resembling twinning present. At lower concentrations the transformation from vaterite to calcite, based on morphology, seems to be progressing rapidly in all samples grown in the presence of 10 mg/L of ASP or GLU after a day, and is complete after a week. It is also almost complete in samples with an additive concentration of 100 mg/L after a week. Vaterite dominates in all samples grown in the presence of 1000 mg/L, even after a week.

Calcite in these samples, grown in the presence of 100 mg/L or 1000 mg/L of AA, shows highly distorted morphologies. While the crystals formed can be quite large, the crystallites seems to be fairly small, and in some crystals the different smaller crystallites that make up the larger crystal can be seen; growth bands are also visible in a number of crystals from different samples.

The majority of samples grown in the presence of 1000 mg/L of AA, particularly for samples harvested after one week (and to a lesser extent one day) have some crystalline floats at the air/solution interface. They form morphologies that are

different, characteristic of vaterite rather than calcite. They deserve a special mention, as they form fairly massive aggregates, which still float at sizes of more than 10 mm in diameter. These aggregates also were the only crystals that were transparent or translucent, indicating only few defects; this is extremely surprising, as the morphology of the crystals is very different from the usually rhombohedral crystals. Their density coupled with surface tension appears to be a significant difference between floats and non-floats, with the former apparently less dense.

Figures 5.2 to 5.16 are representative of the different morphologies observed. It should be noted that the magnification value on the information bar on the SEM images should be ignored. Magnification should be determined from the scale bar.

The morphologies of vaterite and calcite presented in these SEM images are quite distinct, if one assumes that they truly represent one or the other. Based on laboratory XRD and SXRPD results, we can be confident that the vast majority of crystals present in samples grown in the presence of 1000 mg/L of AA are vaterite, while essentially all of the crystals present in samples grown in the presence of 10 mg/L of amino acid harvested after 1 week are calcite. Based on this information, we can assume that the vast majority of the hollow and compact spheres, the pancake and lozenge shaped crystals, the pseudo-hexagonal and disc shaped crystals, as well as their oriented intergrowth represents vaterite. Rhombohedral crystals, either well developed when fairly small, at low concentrations when harvested after extended periods of time, with significant deformations, and most often with pitted surfaces, are calcite.

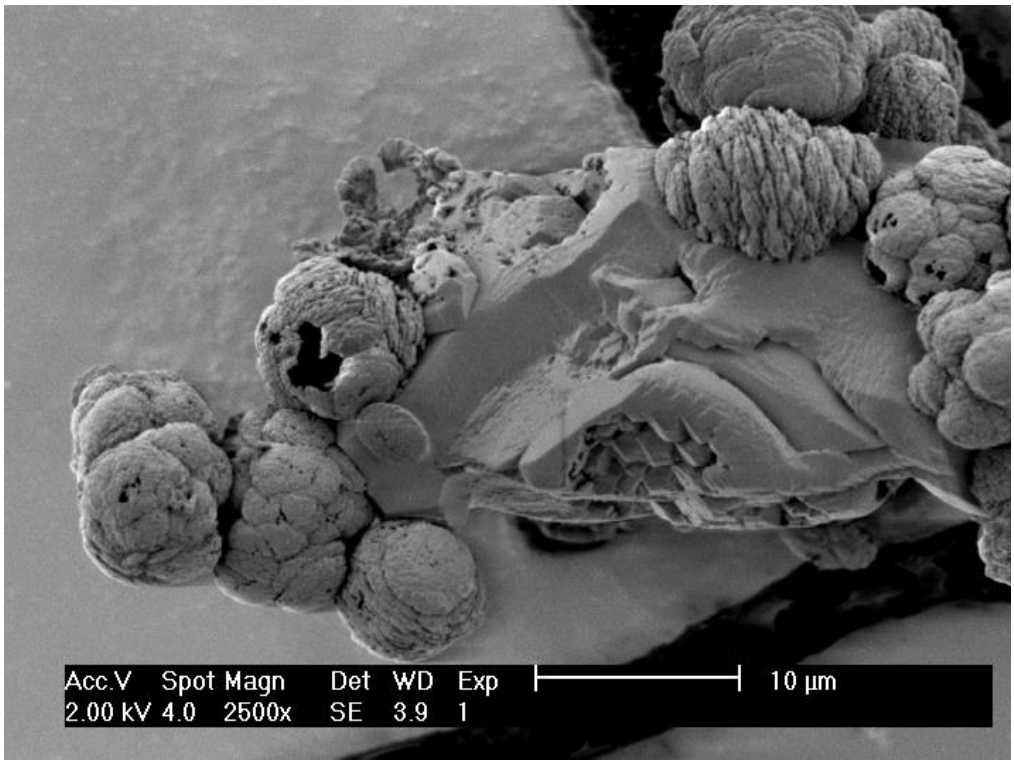

Figure 5.2: SEM image of sample produced from 100 mg/L ASP, method A, harvested after 1 hour, containing highly deformed calcite crystal with hollow vaterite spherules.

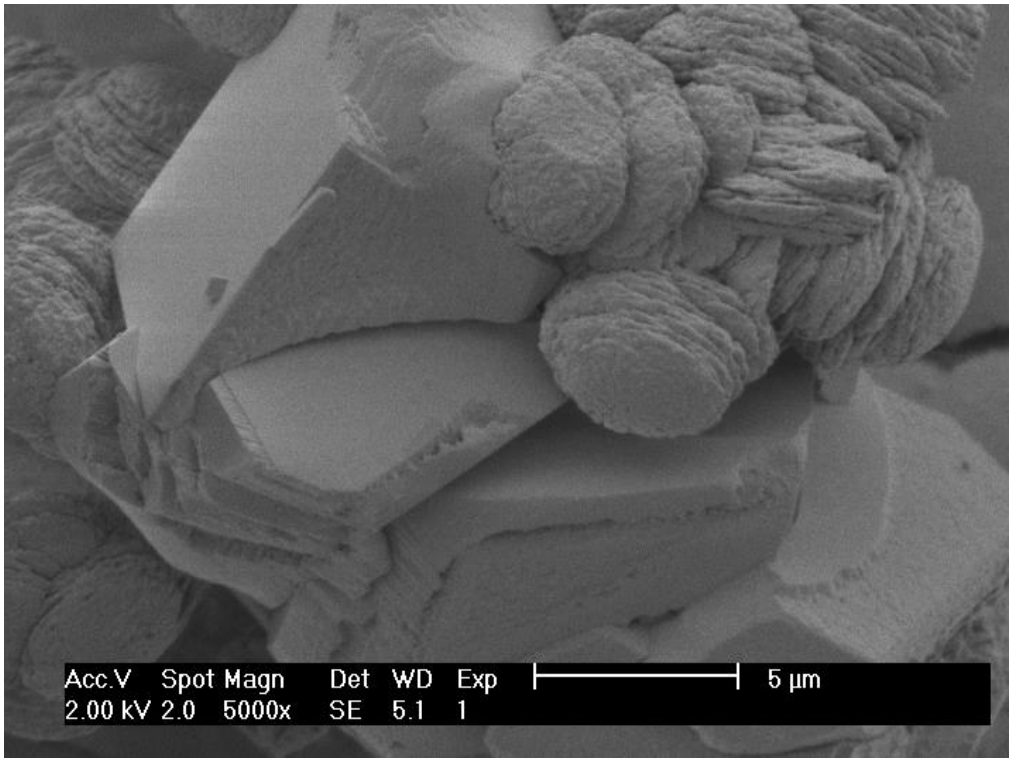

Figure 5.3: SEM image of sample produced from 100 mg/L ASP, method C, harvested after 1 day containing slightly deformed calcite crystals with intergrown vaterite.

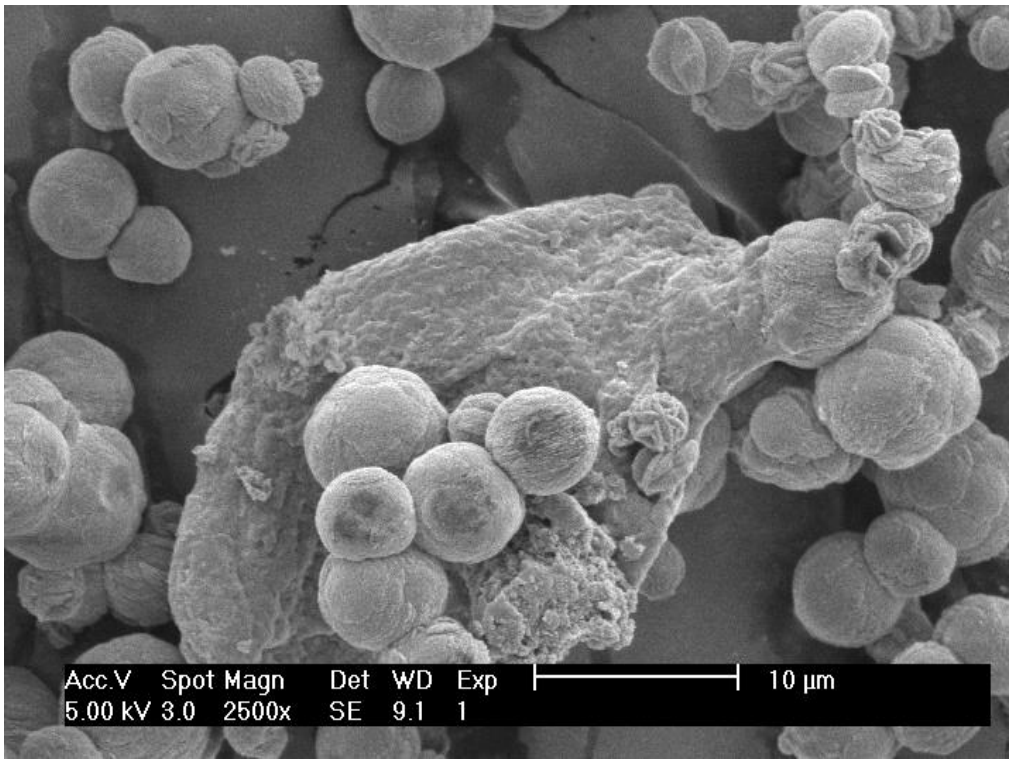

Figure 5.4: SEM image of sample produced from 1000 mg/L ASP, method D, harvested after 1 hour, containing three different vaterite morphologies with spheres, disc/lozenge shaped and oriented intergrowth, possibly on highly deformed calcite.

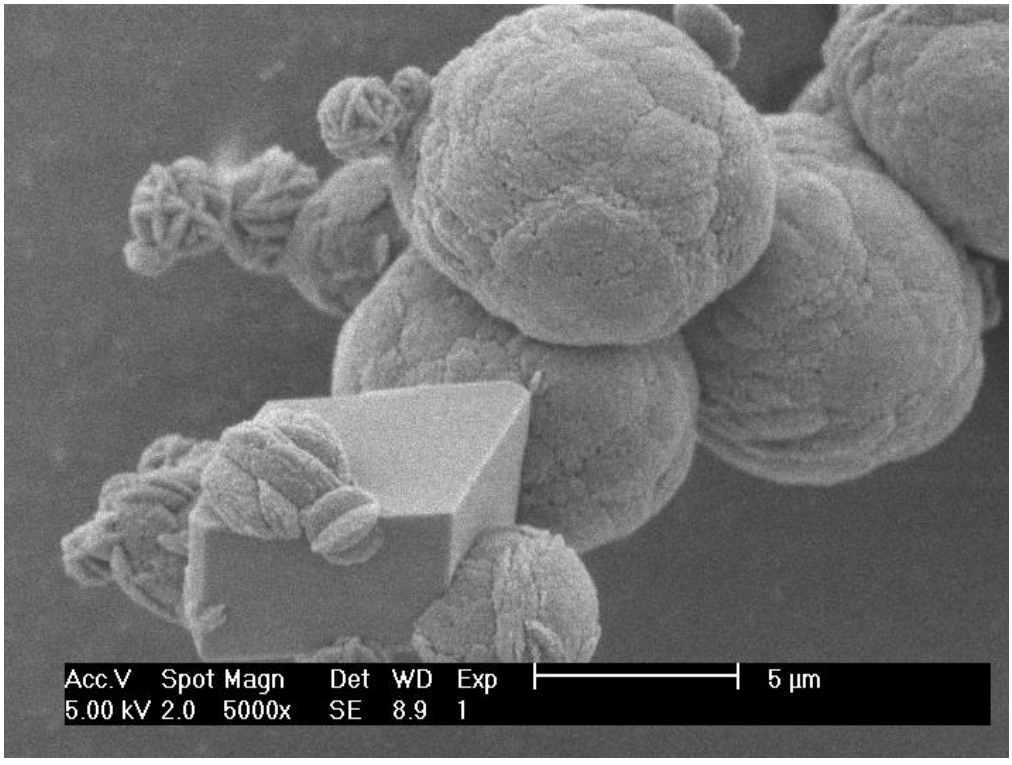

Figure 5.5: SEM image of sample produced from 1000 mg/L ASP, method D, harvested after 1 hour, containing relatively well developed calcite crystal with vaterite intergrowth.

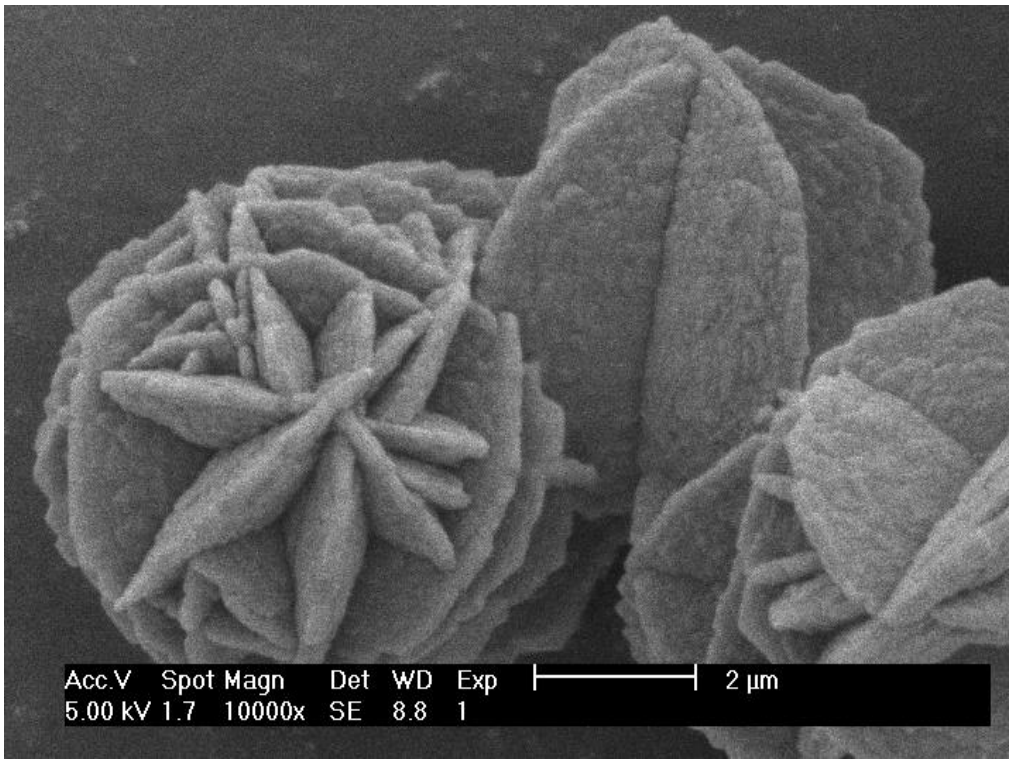

Figure 5.6: SEM image of sample produced from 1000 mg/L ASP, method E, harvested after 1 week, containing coarser and denser vaterite discs with pseudo-hexagonal shape and oriented intergrowth.

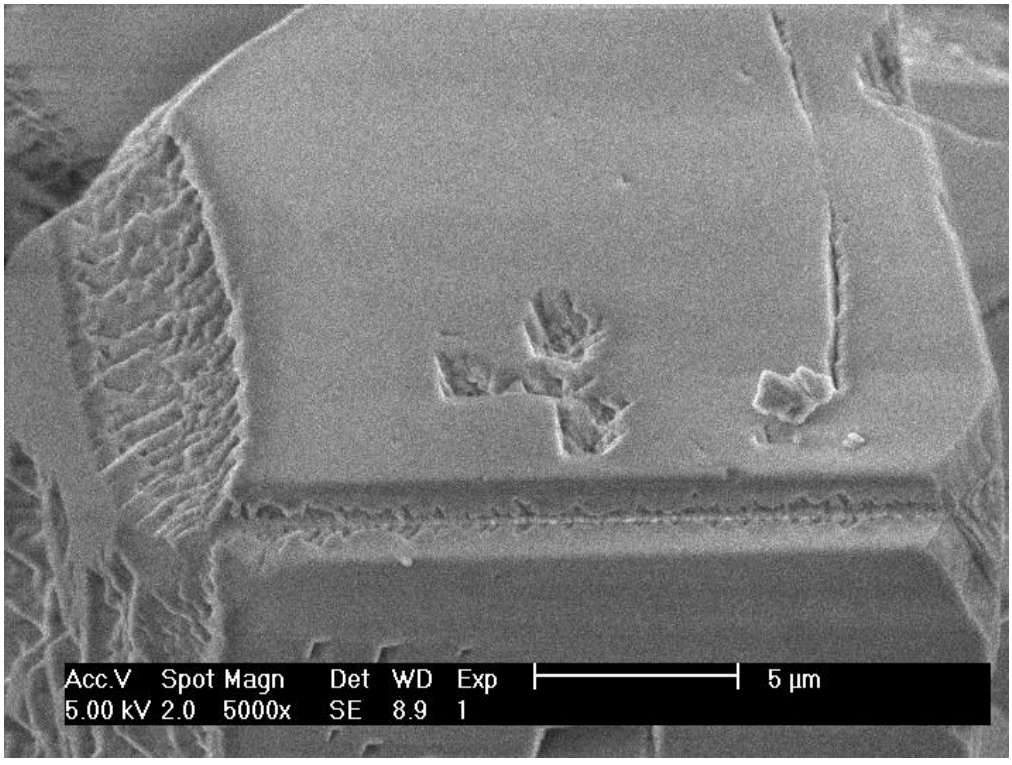

Figure 5.7: SEM image of sample produced from 10 mg/L GLU, method A, harvested after 1 hour, containing calcite crystal showing signs of growth inhibition and smaller crystallites.

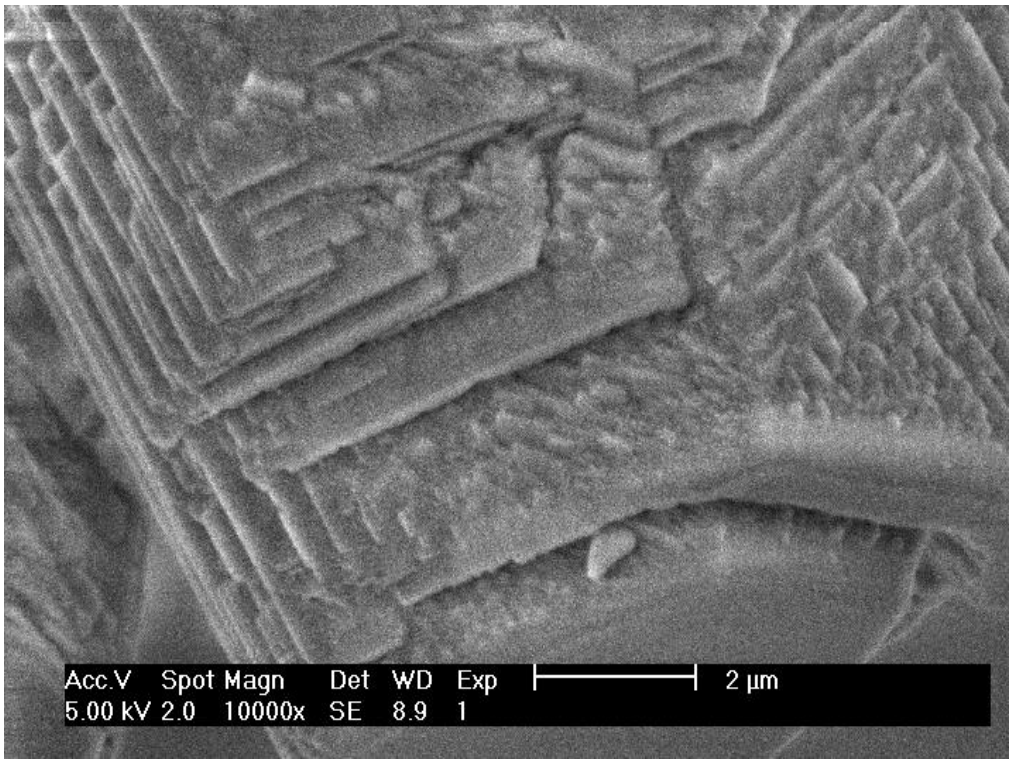

Figure 5.8: SEM image of sample produced from 10 mg/L GLU, method A, harvested after one hour. Detail of larger calcite crystal showing growth steps and possibly smaller crystallites.

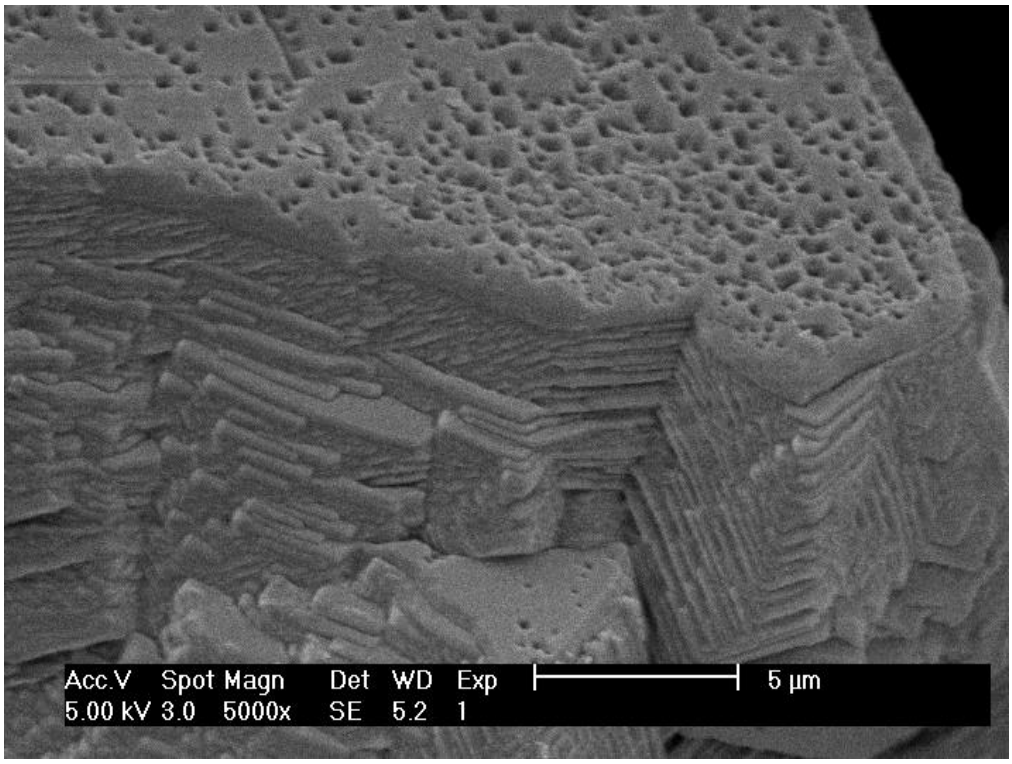

Figure 5.9: SEM image of sample produced from 10 mg/L GLU, method C, harvested after 1 week, containing calcite crystal with growth step and variable orientations.

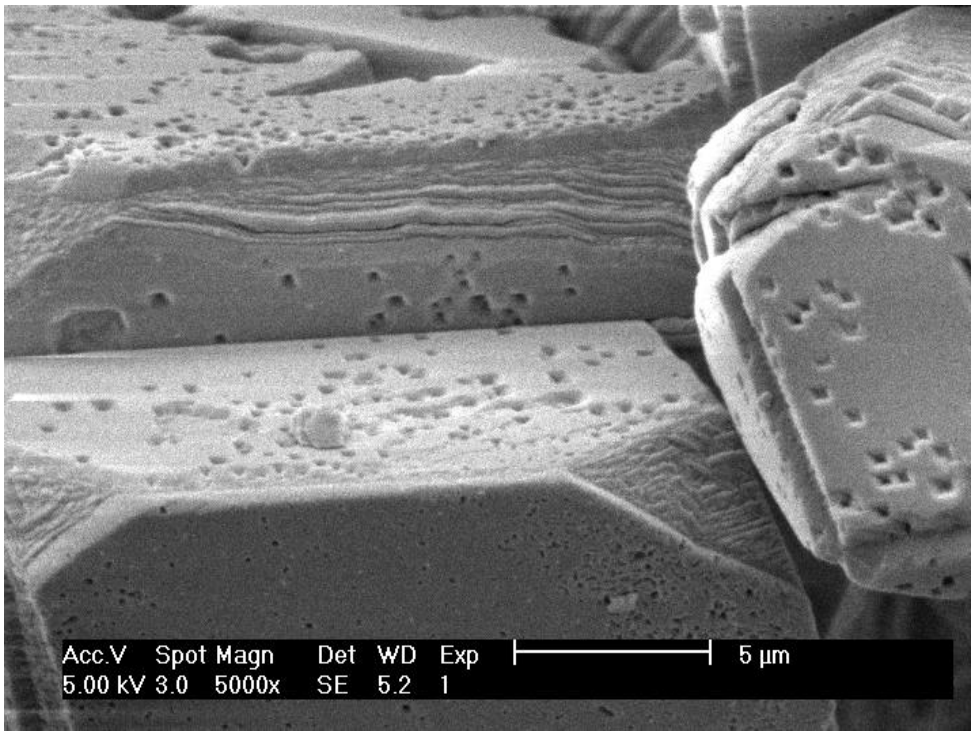

Figure 5.10: SEM image of sample produced from 10 mg/L GLU, method C, harvested after 1 week, showing growth layers in crystals and typical distortions at the edges and the pitting on the surface.

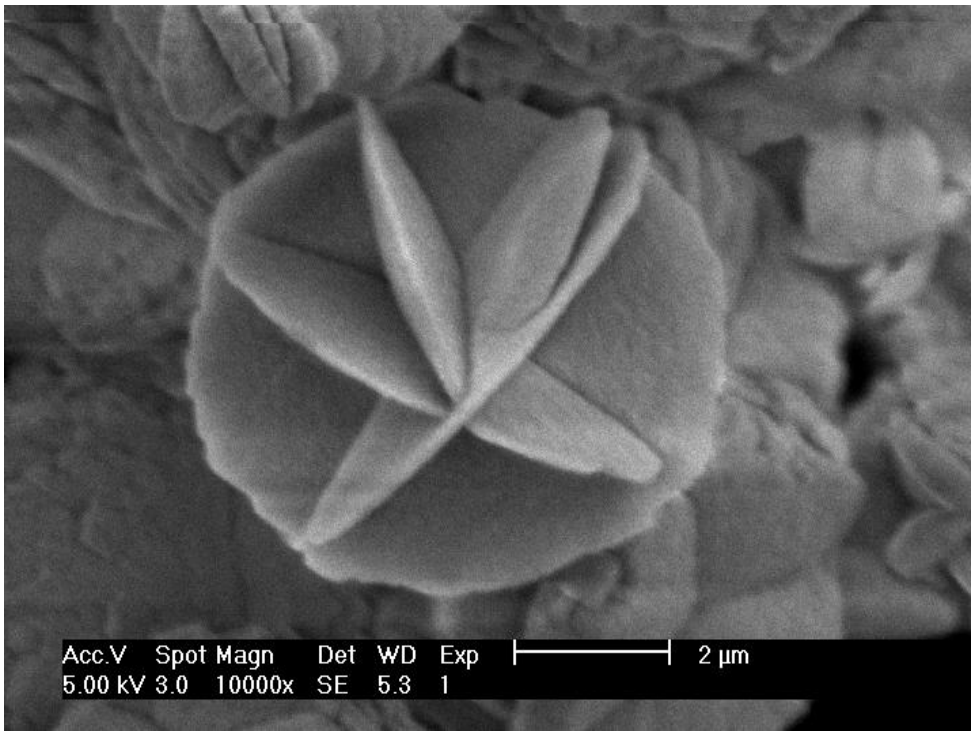

Figure 5.11: SEM image of sample produced from 1000 mg/L GLU, method E, harvested after 1 week with a crystal showing pseudo-hexagonal shape and the oriented intergrowth; most likely vaterite.

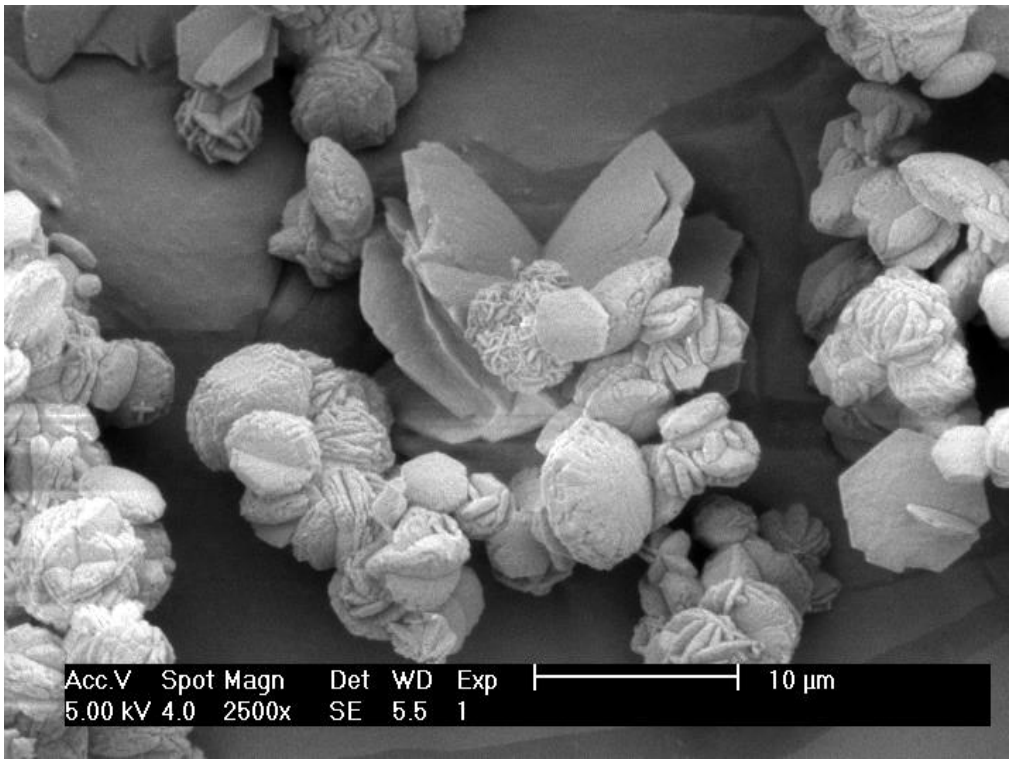

Figure 5.12: SEM image of sample produced from 1000 mg/L GLU, method F, harvested after 1 hour, showing a variety of morphologies, mostly vaterite. The pseudo-hexagonal crystals are possibly calcite.

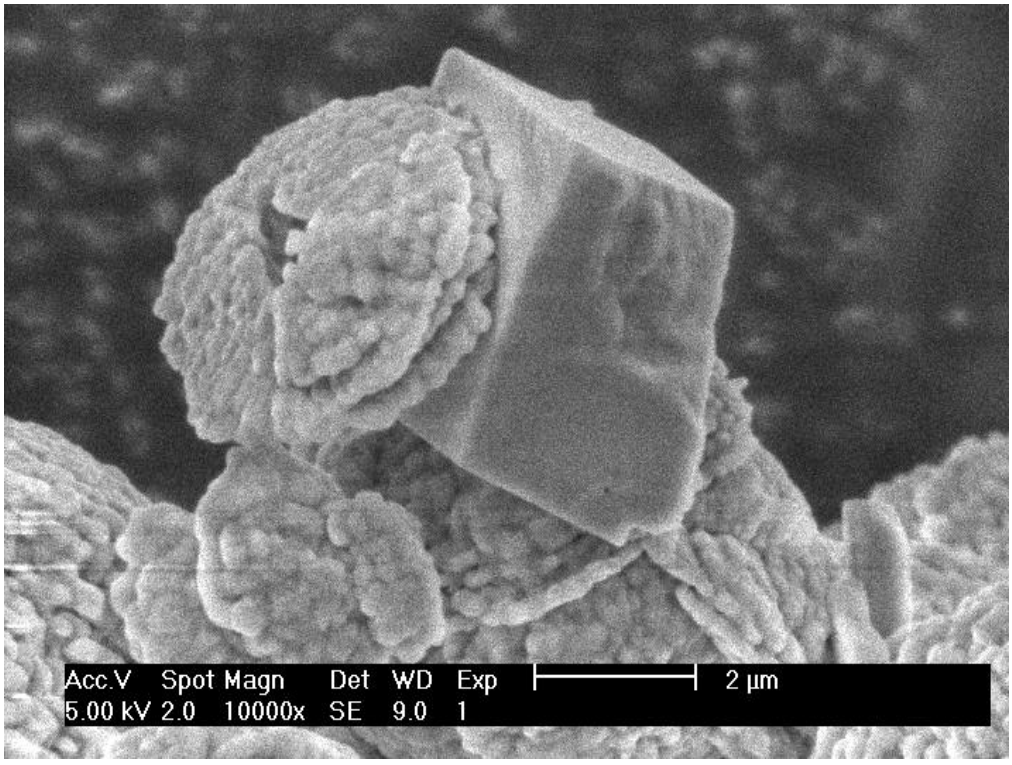

Figure 5.13: SEM image of sample produced from 10 mg/L GLU, method A, harvested after 1 day, containing 'pancake' shaped hollow crystals, most likely vaterite, in close association with calcite.

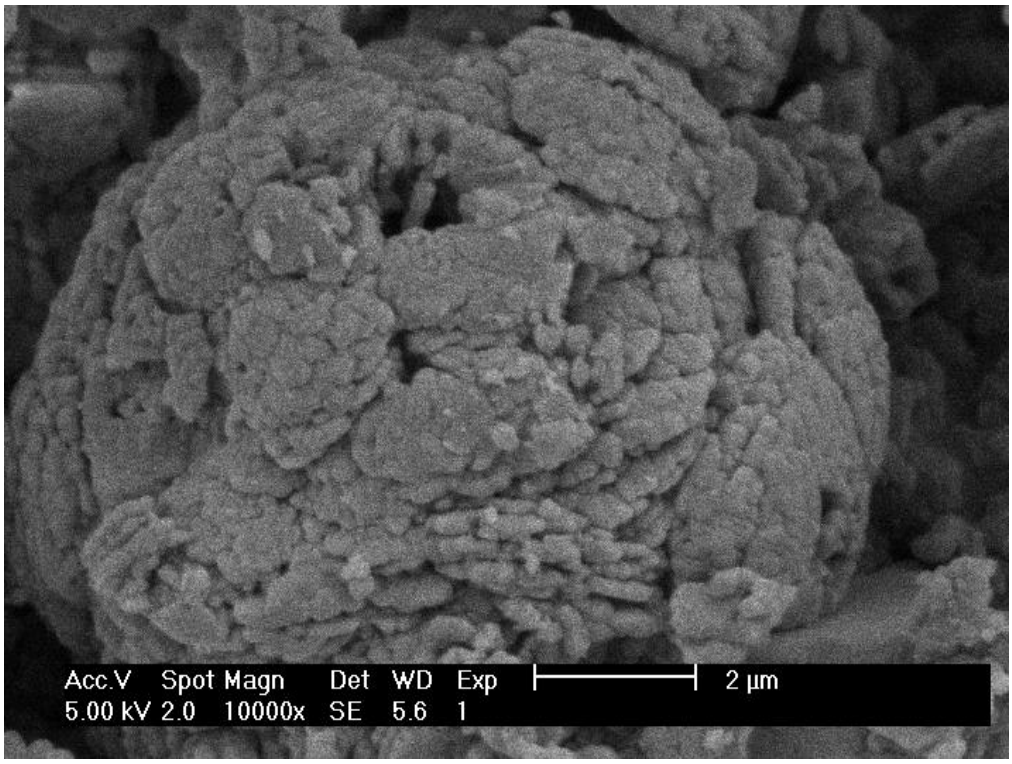

Figure 5.14: SEM image of sample produced from 100 mg/L GLU, method C, harvested after 1 day, showing a large hollow vaterite sphere.

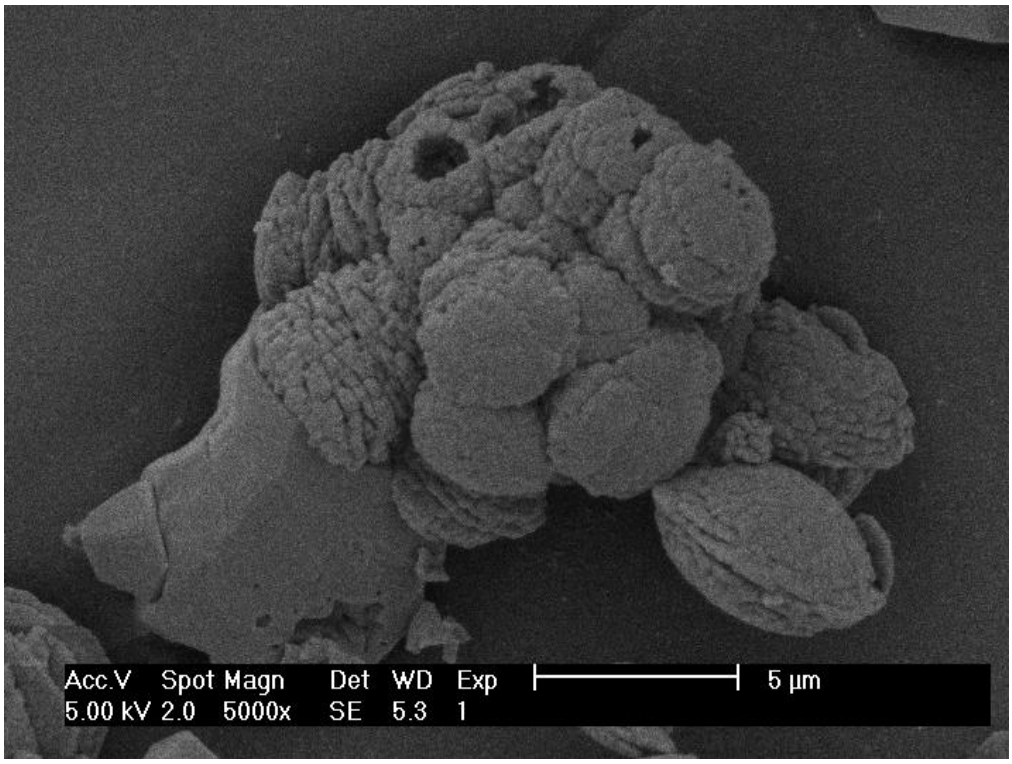

Figure 5.15: SEM image of sample produced from 100 mg/L GLU, method C, harvested after 1 hour, containing a highly deformed calcite crystal intergrown with vaterite, present as hollow spheres and pancake shaped crystals.

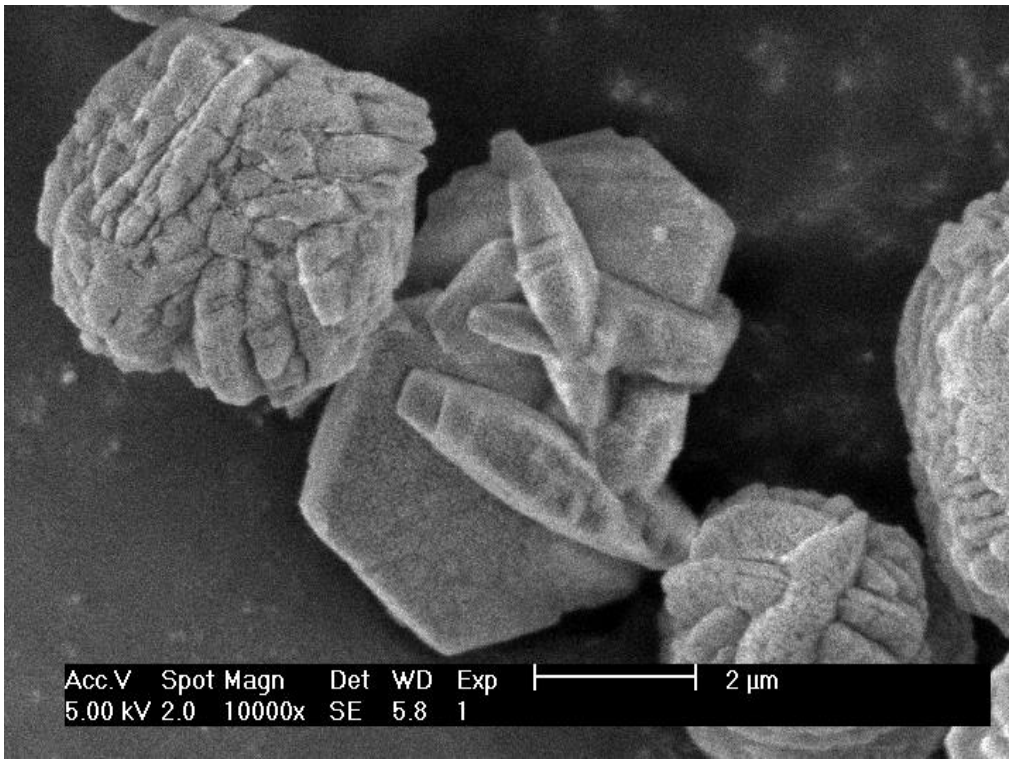

Figure 5.16: SEM image of sample produced from 1000 mg/L GLU, method B, harvested after 1 week, containing pseudo-hexagonal shaped intergrown crystals of vaterite. The increase in size and compactness of the crystals is clearly visible.

The ‘floats’ are very different from the general morphologies observed, resembling more vaterite-typical morphologies with some crystals showing highly deformed calcite-typical morphologies growing on top. They are easily recognisable, because of the immediate termination on one side, providing a flat surface. This surface represents the air-solution interface, from which the crystals grew into the solution. The appearance of the crystals is more solid and more uniform than one would expect from vaterite crystals, and the form is more rounded and disc shaped. The size of the crystals is also atypical of vaterite crystals found in the samples, with most of them significantly larger. XRD of separated floats shows that they are almost exclusively made up of calcite, which means that the two very different morphologies are both calcite morphologies. Figures 5.17 – 5.19 are some representative images.

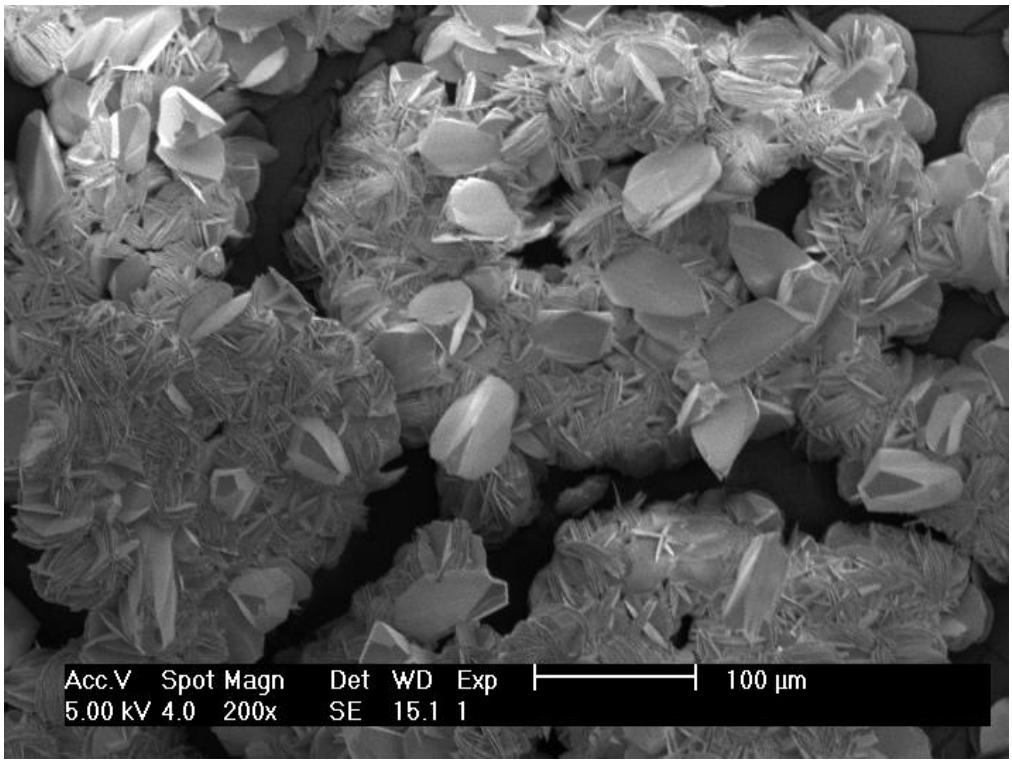

Figure 5.17: SEM image of sample produced from 1000 mg/L GLU, method B, harvested after 1 week, depicting large aggregates of 'floats', with the two distinct types of calcite.

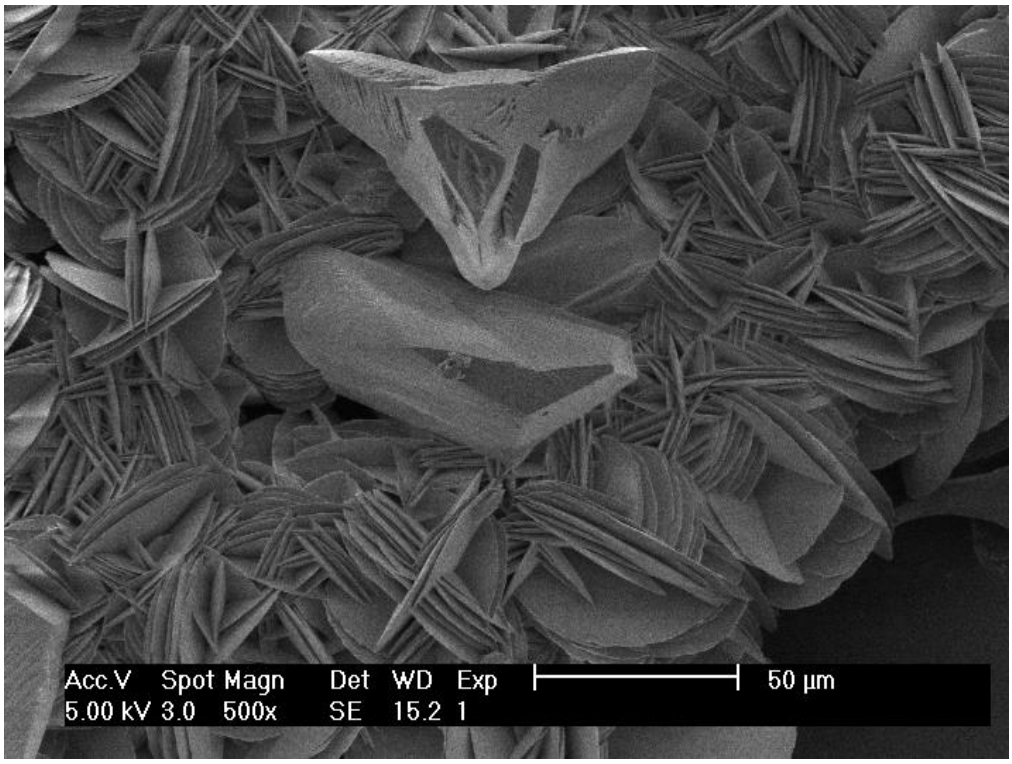

Figure 5.18: SEM image of sample produced from 1000 mg/L GLU, method F, harvested after 1 week, showing a large aggregate of 'floats', with the two distinct types of calcite.

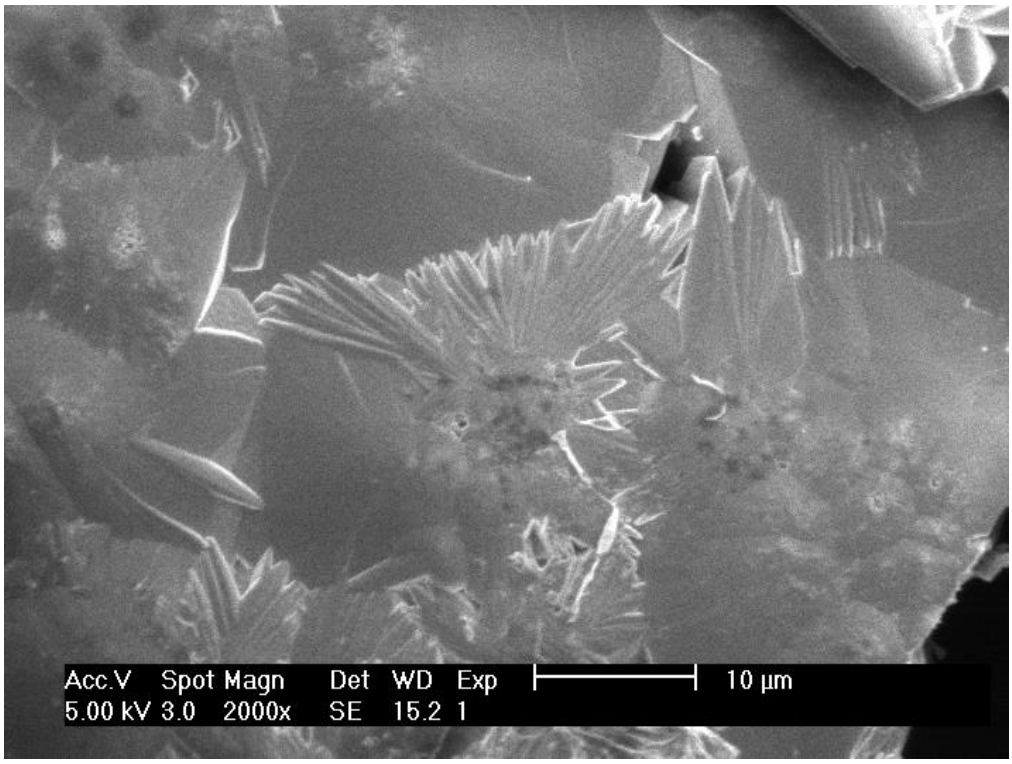

Figure 5.19: SEM image of sample produced from 1000 mg/L GLU, method B, harvested after 1 week, showing a 'float' from the side that would have been presented to the air. The flatness and competitive intergrowth of the crystals are clearly visible.

The slight changes in contrast present in Fig. 5.19 indicate that a less dense material might have provided the original nuclei and probably the first crystallites, but that has been replaced since. Crystal outlines indicate that the main growth was competitive, primarily on the surface, but also perpendicular to it. There are some indications that the growth was not solely from the interface into the solution, but that growth from the solution towards the interface has contributed to the final arrangement, where growth has been halted by spatial restrictions.

5.3 Structural analysis

5.3.1 Synchrotron X-ray Radiation Powder Diffraction (SXRPD)

This section contains the results derived from data collected at the Advanced Photon Source (APS). Two different approaches were taken to extract as much information as possible from the collected data.

The first was to use the collected patterns directly; this was employed to compare peak shapes, positions and intensities within methods, between methods and between the AAs used. It generated some very interesting results, as some minor differences that had not been apparent in the pH traces now presented themselves more clearly. Changes in peak intensities and peak positions, and phase trends between slow and fast addition were observed. Some differences between the two AAs used in the experiments also became noticeable, while the harvesting time mainly affected crystallinity and phase content.

The second was to use coherent scattering domain sizes and micro-strain values derived from single peak fits to ascertain if there are noticeable differences between the methods, harvesting times and crystallographic planes. The calculations had resulted in a very large dataset, but a relevance check (calculated values greater than 3 standard deviations) meant that a large number of the values had to be discarded because they were judged to be statistically invalid. The relevance criteria of 3 esds was chosen because of reliability and reproducibility; multiple fits of the same peak, always starting from the raw data, had revealed that 2 esds allowed for too much variation in the results, making it very difficult to identify relationships and in some cases even trends. Exclusion of data with calculated values smaller than 3 esds meant that datasets were small, but inclusion of data with values greater than 2 esds would not have aided in discerning relationships or trends.

The next two sections deal with SXRPD on samples grown in the presence of GLU and ASP. Not all possible combinations and relationships are presented, but a

representative section of samples for which data of equivalent quality and resolution are available for both AAs for direct comparison.

Two types of legends are present in the figures presented in this chapter, and any other chapter where they are used. The nine character legends, like A0010DPSH are coded such that:

A = the type of AA used, i.e. either A (for ASP) or G (for GLU).
0010 = four-digit concentration, i.e. 0010 means 10 mg/L of the specific amino acid.
D = method used, i.e. anything from A to F.
PS = Sample produced primarily for XRPD or SXRPD analysis, AN = sample produced primarily for NPD (larger volume required).
H = harvesting time, i.e. H = 1 hour, D = 1 day, W = 1 week.

The four letter legends in the figures included in this section, as in all other sections, are simply the second part of the above coding, specifying the method, the primary purpose and the harvesting time.

5.3.1.1 SXRPD on samples grown in the presence of GLU

Comparison of patterns of samples produced using different concentrations, methods and harvesting times revealed a high level of variability in terms of crystallinity and phase composition in samples grown in the presence of 10 mg/L GLU. In samples grown at this concentration some variation is noticeable between the different methods for the same harvesting time, predominantly between slow and fast addition, but the main variation is clearly associated with the harvesting time. Samples grown in the presence of 100 mg/L of GLU show similarities with the samples grown in the presence of only 10 mg/L for samples harvested after one hour, but they start to differ substantially for samples harvested after one day and one week, with the vaterite stabilising effect of the amino acid more noticeable. Samples grown in the presence of 1000 mg/L GLU show only limited variation with harvesting times, and a slight reversing trend is observable; some of the calcite that was initially formed is partially dissolved and re-crystallised as vaterite over time. The only difference that

is observable between the samples grown in the presence of 1000 mg/L of GLU is the change in crystallinity over time, and within reason the difference between the slow and the fast addition methods, with slightly less calcite formed at slower addition rates.

Figure 5.20 demonstrates that for all quick addition methods the amount of calcite, based on the intensity of the (012) peak of calcite, is higher than for the equivalent slow addition method. Also, all three quick addition methods (A, C, D) seem to produce more calcite than any of the the slow addition methods. The only method which falls within the region of uncertainty is method C. The shifts observed in the pattern are within a single step and therefore within instrumental error.

The wavelength used in all the plots in this section is equivalent to 20 keV, approximately 0.619 Å, as determined from NIST LaB_6.

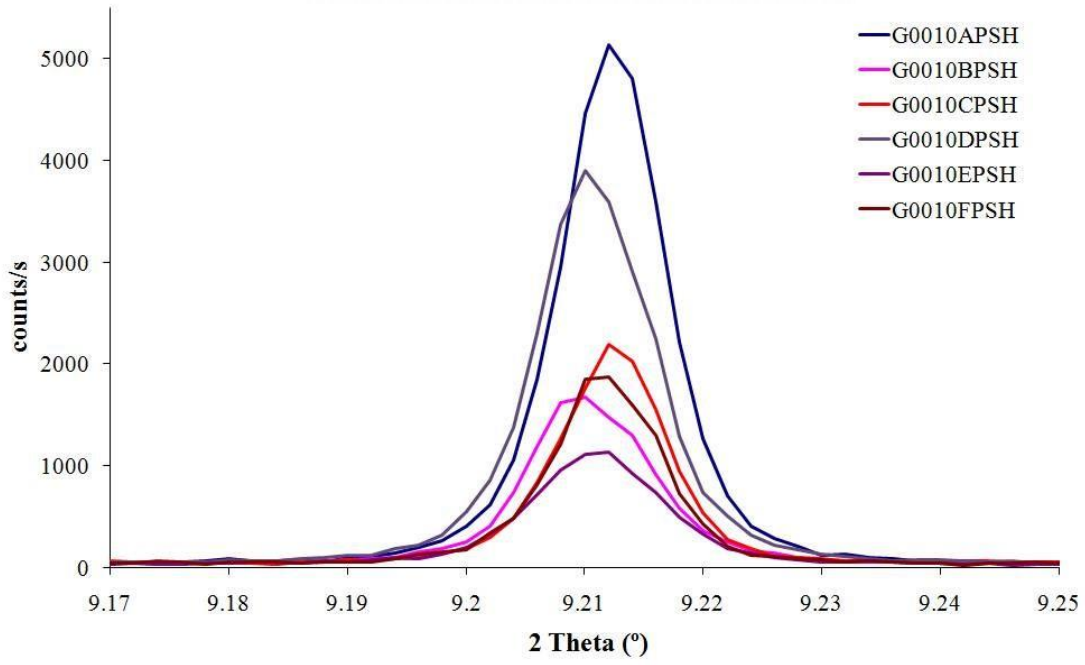

Figure 5.20: Calcite (012) peaks from samples prodcued using different methods at 10 mg/L GLU addition.

Figure 5.21 shows that the amount of calcite produced by quick addition methods is similar or lower than in samples produced in the presence of only 10 mg/L GLU, but that the amount of calcite produced by slow addition method B is significantly lower than in samples produced using 10 mg/L GLU..

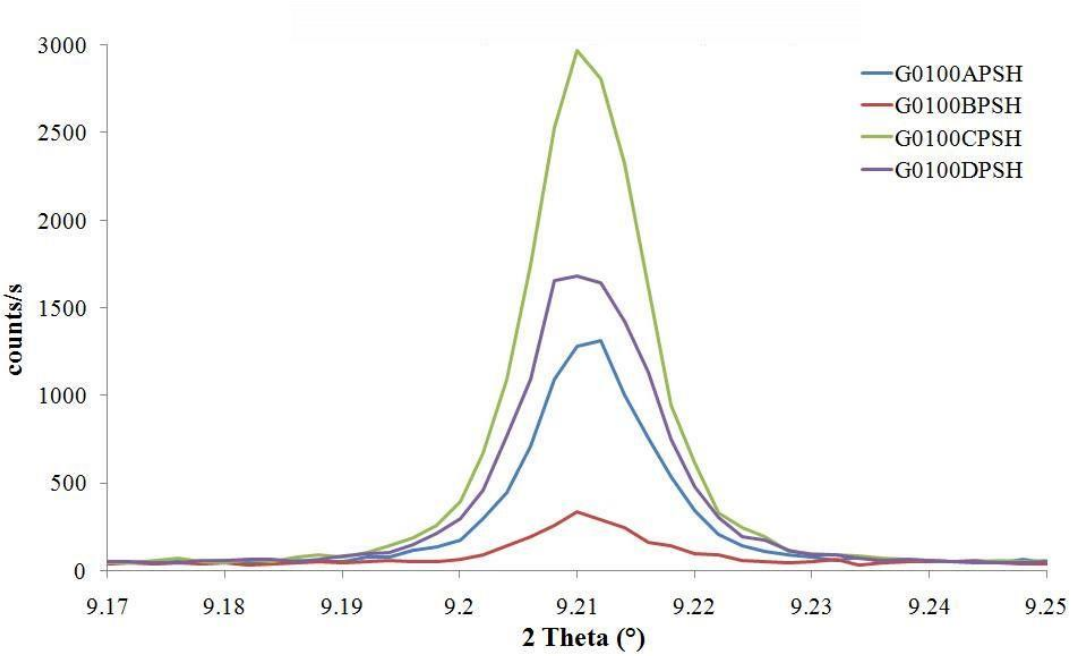

Figure 5.21: Calcite (012) peaks from samples produced using different methods at 100 mg/L GLU addition.

Figure 5.22 clearly demonstrates that at 1000 mg/L of GLU almost no calcite is produced. Only the sample produced by method A contains a significant amount of calcite. Figure 5.28 depicts the increase in the amount of calcite in the sample harvested after 1 week, suggesting that this is not due to experimental variation.

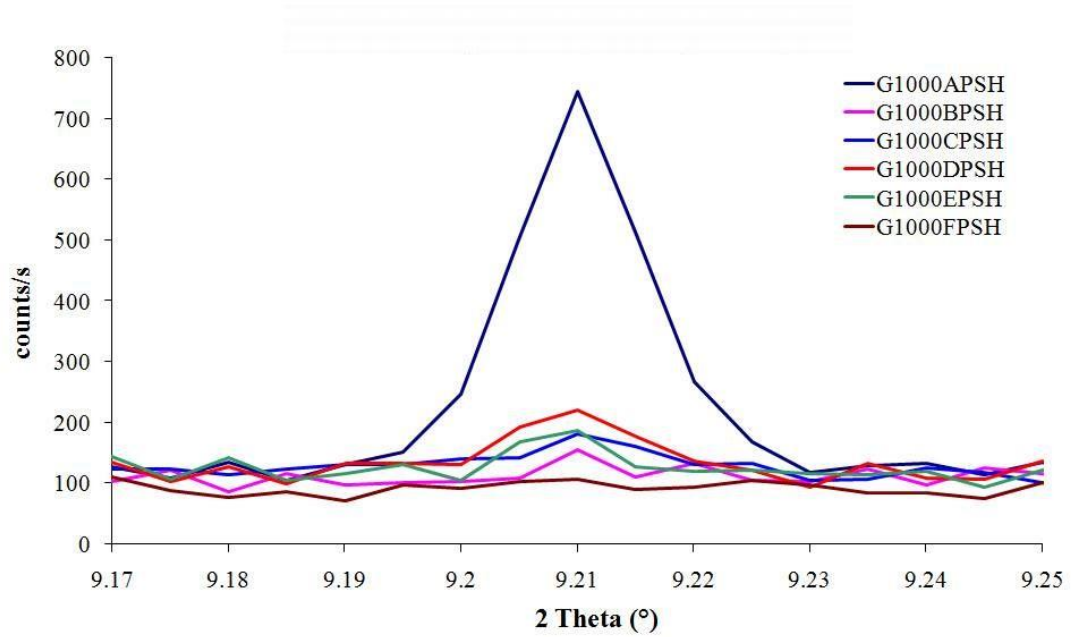

Figure 5.22: Calcite (012) peaks from samples produced using different methods at 1000 mg/L GLU addition.

Figure 5.23 shows that there is not much difference in the amount of vaterite produced by the different methods for samples grown in the presence of 10 mg/L of GLU and harvested after 1 hour. The only two samples which seem to contain less are samples grown by quick addition methods.

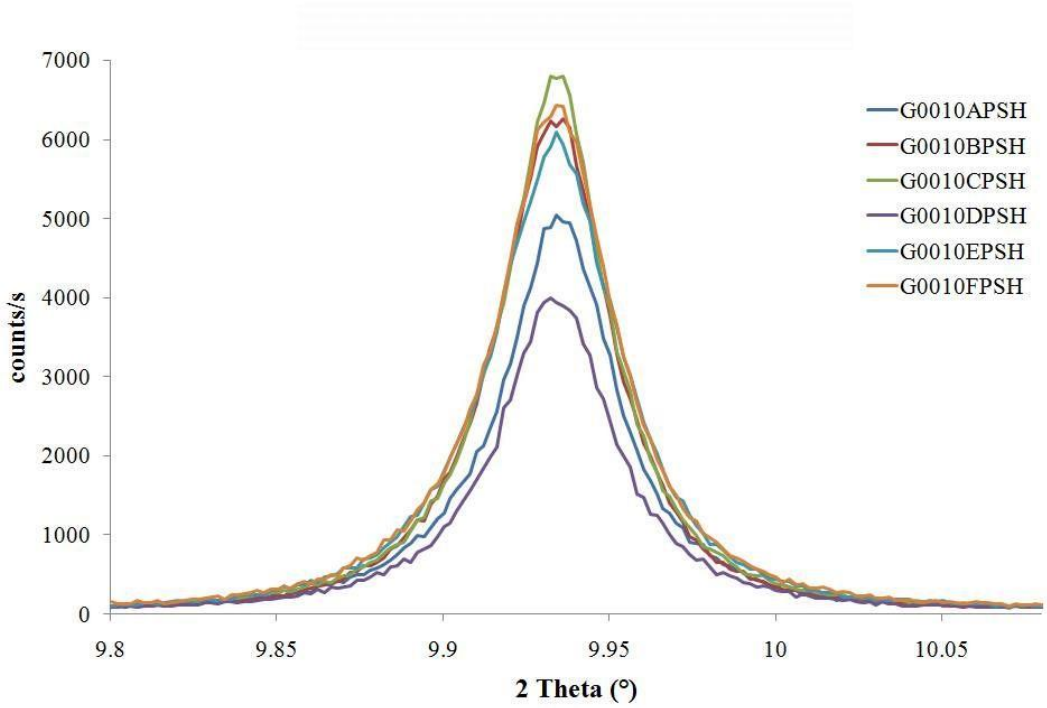

Figure 5.23: Vaterite (110) peaks from samples produced using different methods at 10 mg/L GLU addition.

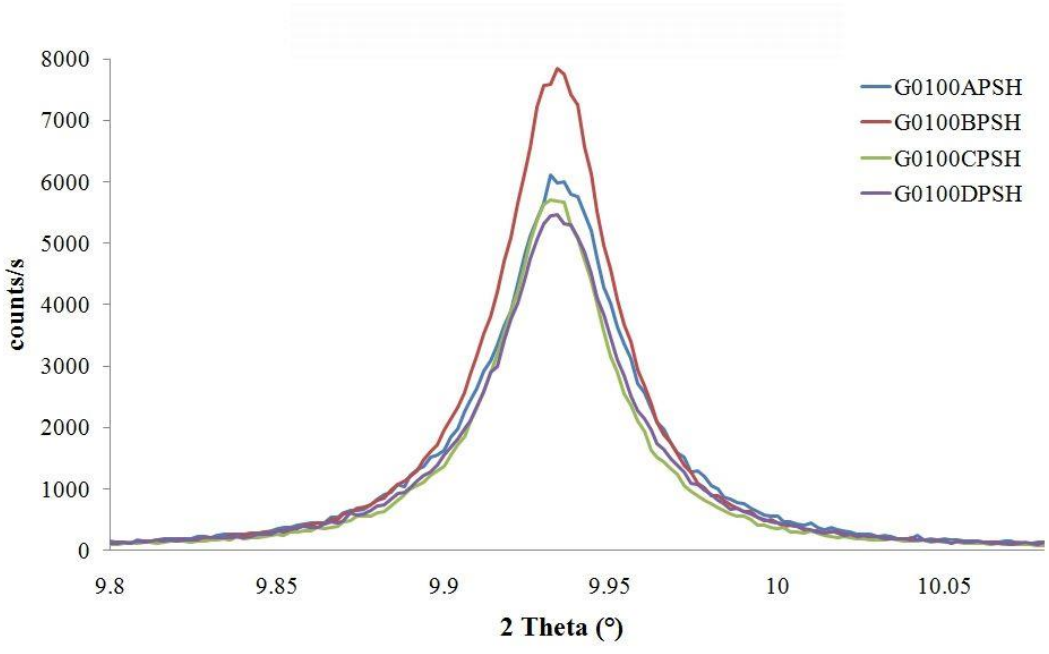

Figure 5.24: Vaterite (110) peaks from samples produced using different methods at 100 mg/L GLU addition.

Figure 5.24, depicting the same vaterite peak for samples grown in the presence of 100 mg/L GLU and harvested after 1 hour shows a similar trend as observed in figure 5.23; the sample grown by slow addition contains more vaterite.

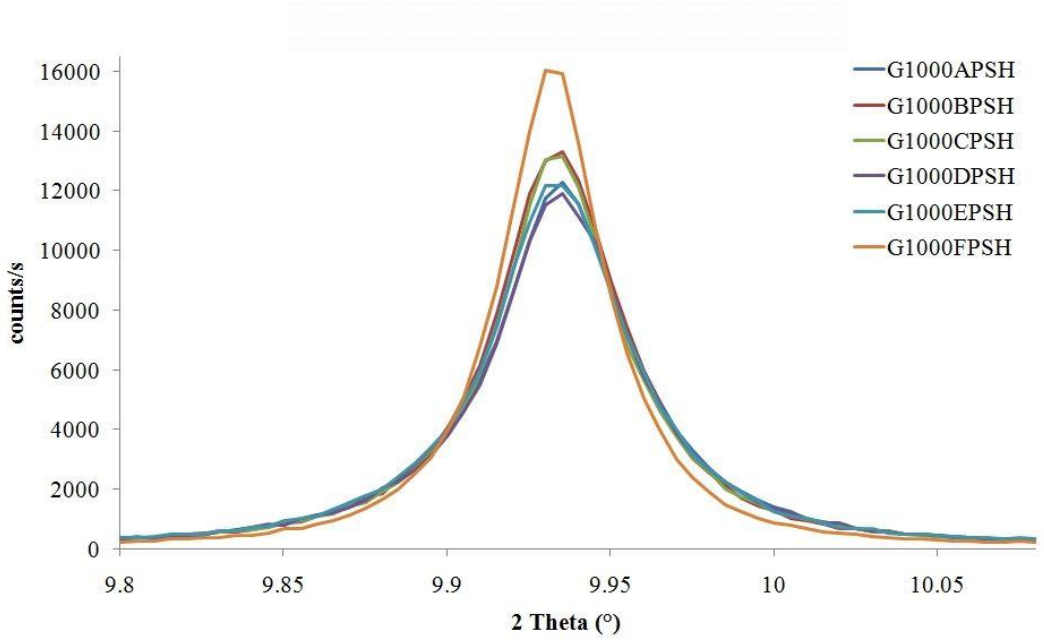

Figure 5.25: Vaterite (110) peaks from samples produced using different methods at 1000 mg/L GLU addition.

Figure 5.25 illustrates that there is very little difference between slow and fast addition methods for samples grown in the presence of 1000 mg/L GLU and harvested after 1 hour.

Overall, figures 5.20 to 5.25 illustrate the changes with concentration of the AA. From the integrated intensities presented in table 5.2 it can be seen that there is a small difference in the amount of vaterite and calcite produced between the samples grown in the presence of 10 mg/L and 100 mg/L GLU for samples harvested after one hour.

It is also apparent that slow addition of the reactants leads to increased vaterite peak intensities and decreased calcite peak intensities for samples harvested after 1 hour. That the amount of calcite produced is significantly smaller can be seen in figures 5.20 & 5.21, where the peak intensity of the (012) calcite peak for samples grown by

methods that represent slower addition is significantly lower than the one for samples grown by fast addition.

Figures 5.26 - 5.31, show some comparisons for different harvesting times and methods.

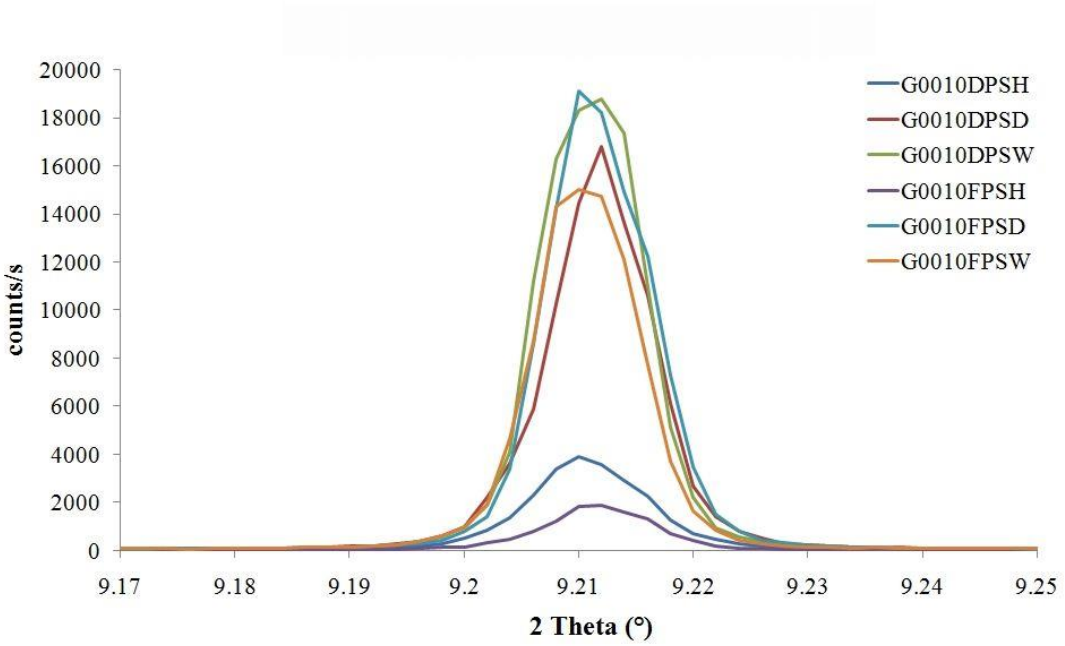

Figure 5.26: Calcite (012) peaks from samples produced using methods D and F at harvesting times of 1 hour, 1 day and 1 week, all at 10 mg/L GLU addition.

Figure 5.26 illustrates that the main change in calcite quantity, based on the scattering intensities for the (012) peak, occurs between 1 hour and 1 day, with only small changes in calcite scattering intensity after that. For the samples produced using method F, there is a small but apparent decrease in peak intensity when comparing the sample harvested after 1 day with the one harvested after 1 week, while for the samples produced using method C there is a slight increase when comparing the same samples.

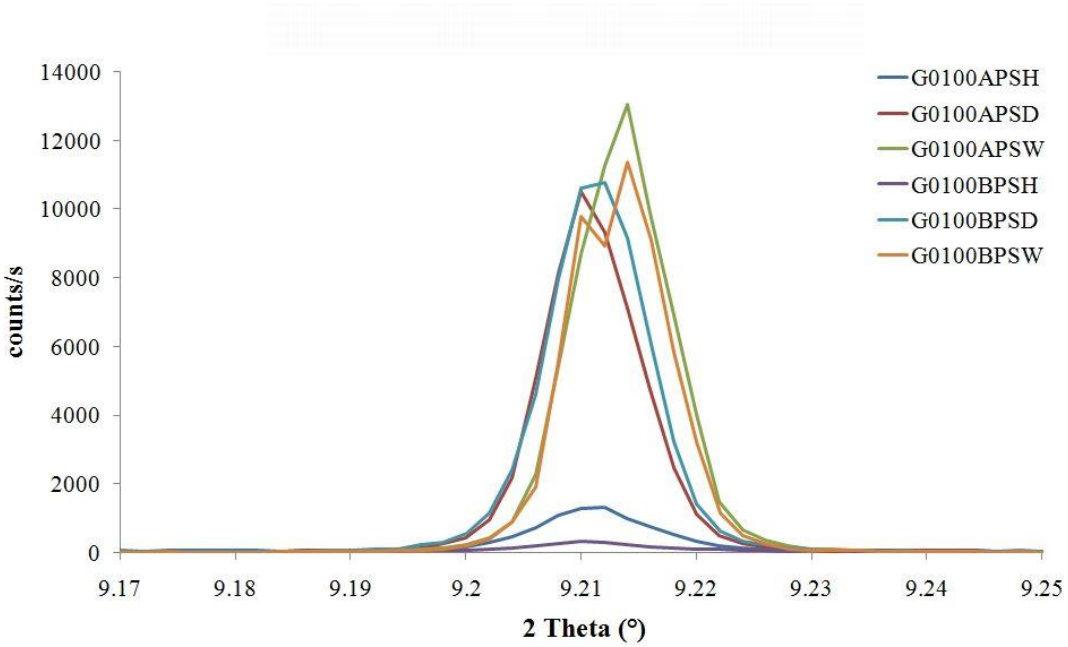

Figure 5.27: Calcite (012) peaks from samples produced using methods A and B at harvesting times of 1 hour, 1 day and 1 week, all at 100 mg/L GLU addition.

Figure 5.27 shows that the amount of calcite for samples grown in the presence of 100 mg/L GLU increases dramatically from samples harvested after 1 hour to samples harvested after 1 day with little subsequent variation. The shift in the calcite (012) peak between samples harvested after 1 day and 1 week are within experimental error (one step).

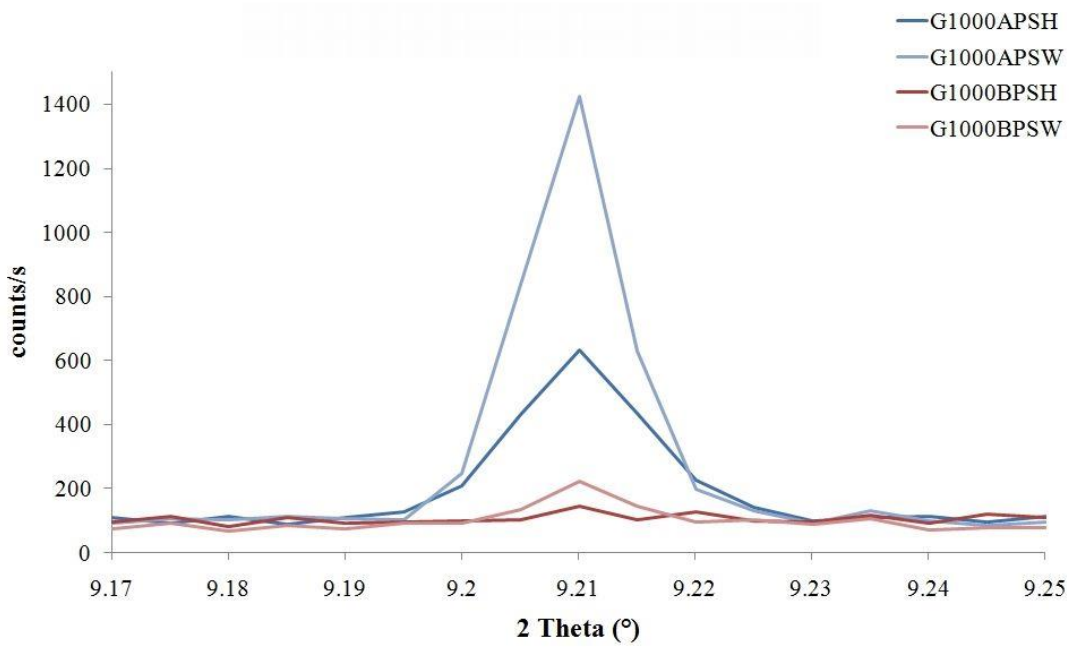

Figure 5.28: Calcite (012) peaks from samples produced using methods A and B at harvesting times of 1 hour and 1 week, all at 1000 mg/L GLU addition.

What can be seen in figure 5.28 is the change in overall coherent scattering from calcite between slow and fast addition in samples produced in the presence of 1000 mg/L GLU at harvesting times of 1 hour and 1 week. It demonstrates that slow addition of the reactants results in less initial calcite, and that the overall amount decreases when the harvesting time is increased from 1 hour to 1 week for samples grown by slow addition, but increases for the sample grown by fast addition. The pattern shapes are due to the stepsize of 0.05 º2θ, which is large for the well crystalline calcite. Only five datapoints are present across the main peak.

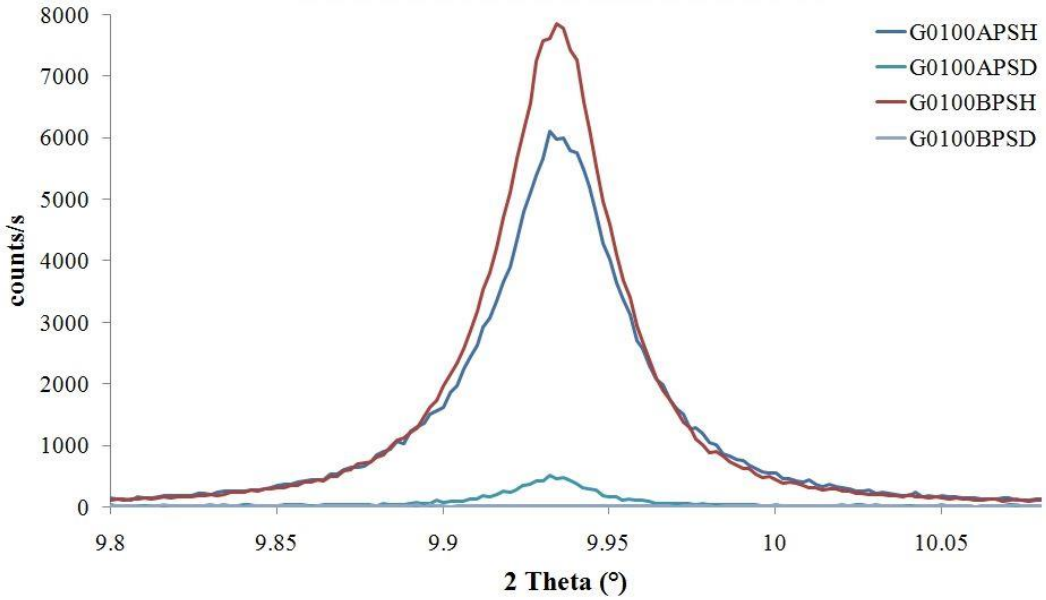

Figure 5.29: Vaterite (110) peaks from samples produced using methods A and B at harvesting times of 1 hour and 1 day, all at 100 mg/L GLU addition.

Figure 5.29 shows that 100 mg/L of GLU is not sufficient to stabilise vaterite, with the (110) vaterite peak almost disappearing between the harvesting times of 1 hour and 1 day for method A and completely disappearing for method B. If the fact that vaterite is still present in the sample produced by method A after 1 day is due to a larger initial quantity or due to the method is unclear. Figure 5.29 needs to be viewed in conjunction with figure 5.27; while the amount of vaterite present decreases dramatically with harvesting time at this concentration of GLU, the amount of calcite increases, indicating rapid and almost complete transformation of vaterite into calcite.

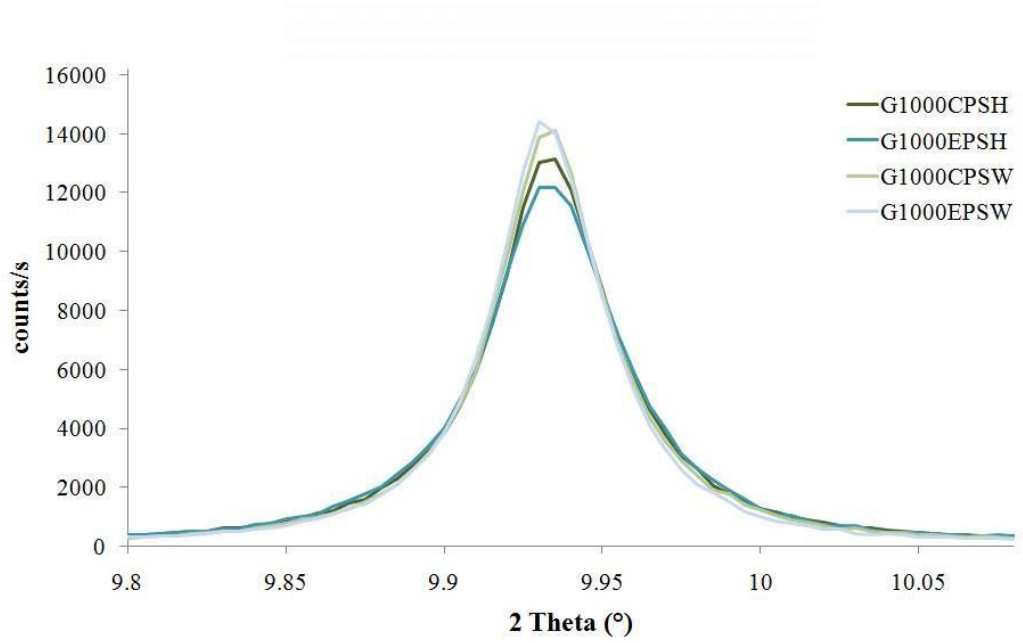

Figure 5.30: Vaterite (110) peaks from samples produced using methods C and E at harvesting times of 1 hour and 1 week, all at 1000 mg/L GLU addition.

Figure 5.30 shows that there is very little difference between samples harvested after 1 hour and 1 week, and even between slow and fast addition for the method where all Ca is present in the reaction vessel prior to addition of the other reactants; the variation in intensity of the vaterite peaks is within statistical error.

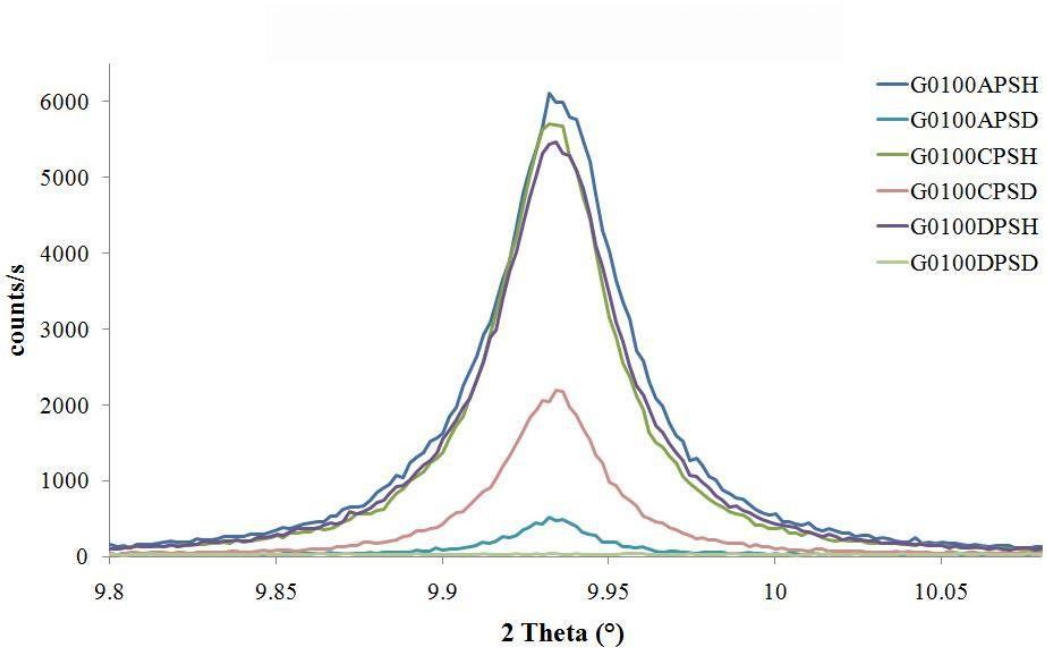

Figure 5.31: Vaterite (110) peaks from samples produced using methods A, C and D at harvesting times of 1 hour and 1 week, all at 100 mg/L GLU addition.

Figure 5.31 illustrates the rapid transformation of vaterite into calcite, epxressed throught the significant reduction in vaterite peak intensity in samples harvested after 1 day compared to samples harvested after 1 hour. For clarity only samples produced by fast addition are compared.

The following table (5.2) summarises basic peak data for the patterns used in the plots relating to samples produced in the presence of GLU.

GLU												
Concentration and method	Calcite peak 9.21° 2Θ 1 Hour		Vaterite peak 9.93° 2Θ 1 Hour		Calcite peak 9.21° 2Θ 1 Day		Vaterite peak 9.93° 2Θ 1 Day		Calcite peak 9.21° 2Θ 1 Week		Vaterite peak 9.93° 2Θ 1 Week	
	Area	2σ	Area	2σ	Area	2σ	Area	2σ	Area	2σ	Area	2σ
10 mg/L - A	124.2	8.4	544.2	36.0	171.0	8.6	0.0	0.0	131.9	6.6	0.0	0.0
10 mg/L - B	44.4	3.7	662.8	19.4	236.7	11.8	0.0	0.0	222.6	11.2	0.0	0.0
10 mg/L - C	52.1	3.5	713.7	33.2	274.0	13.8	0.0	0.0	201.0	10.0	0.0	0.0
10 mg/L - D	104.4	4.8	466.1	33.2	190.5	9.6	0.0	0.0	225.5	11.2	0.0	0.0
10 mg/L - E	33.2	3.0	720.1	24.6	187.9	9.4	0.0	0.0	207.5	10.4	0.0	0.0
10 mg/L - F	44.7	4.1	735.2	35.8	218.9	11.0	0.0	0.0	180.5	9.0	0.0	0.0
100 mg/L - A	34.8	2.5	744.8	37.2	311.0	6.0	34.7	17.1	501.0	12.6	0.0	0.0
100 mg/L - B	7.4	3.0	832.6	28.0	244.6	5.0	0.0	0.0	443.7	20.2	0.0	0.0
100 mg/L - C	78.4	8.2	614.6	40.0	198.3	4.4	200.4	13.2	498.2	11.8	0.0	0.0
100 mg/L - D	50.6	3.5	650.9	25.0	293.9	7.2	0.0	0.0	337.8	9.0	0.0	0.0
1000 mg/L - A	1.8	0.4	833.6	38.0	1.7	1.2	670.1	29.6	8.3	2.4	846.1	37.8
1000 mg/L - B	0.3	0.2	854.9	47.6	1.1	0.6	636.0	25.4	1.4	0.7	1134.9	42.2
1000 mg/L - C	3.0	0.7	854.8	41.8	1.7	0.8	640.1	34.2	2.4	3.4	843.0	47.8
1000 mg/L - D	1.0	0.2	824.4	41.8	2.7	2.0	629.5	28.6	4.6	3.2	866.5	52.2
1000 mg/L - E	0.0	0.0	856.1	42.0	0.0	0.0	0.0	0.0	0.0	0.0	837.5	31.2
1000 mg/L - F	0.0	0.0	854.4	27.6	0.0	0.0	616.0	23.0	1.4	0.6	829.2	30.2

Table 5.2: Peak area and uncertainty data for the samples produced in the presence of glutamic acid.

5.3.1.2 SXRPD on samples grown in the presence of ASP

As for the samples grown in the presence of GLU, the samples grown in the presence of ASP also show a high level of variability in terms of crystallinity and phase composition in samples grown in the presence of 10 mg/L ASP. Some variation is apparent when comparing the different methods in relation to the same harvesting time, but the main variation is related to the different harvesting times. Samples grown in the presence of 100 mg/L ASP and harvested after 1 hour show that ASP favours vaterite precipitation and growth more than GLU, with all vaterite peak areas in the samples grown in the presence of ASP higher than those from samples grown in the presence of GLU. In the samples harvested after 1 hour these differences are subtle, but they become more pronounced in samples harvested after 1 day, with the stabilising effect of ASP on vaterite more noticeable. Samples grown in the presence of 1000 mg/L ASP showed little variation with harvesting times, with the main

difference being that vaterite peak intensities decrease for samples harvested after 1 day compared to samples harvested after 1 hour, but then show a marked increase in samples harvested after 1 week, similar to samples produced using GLU.

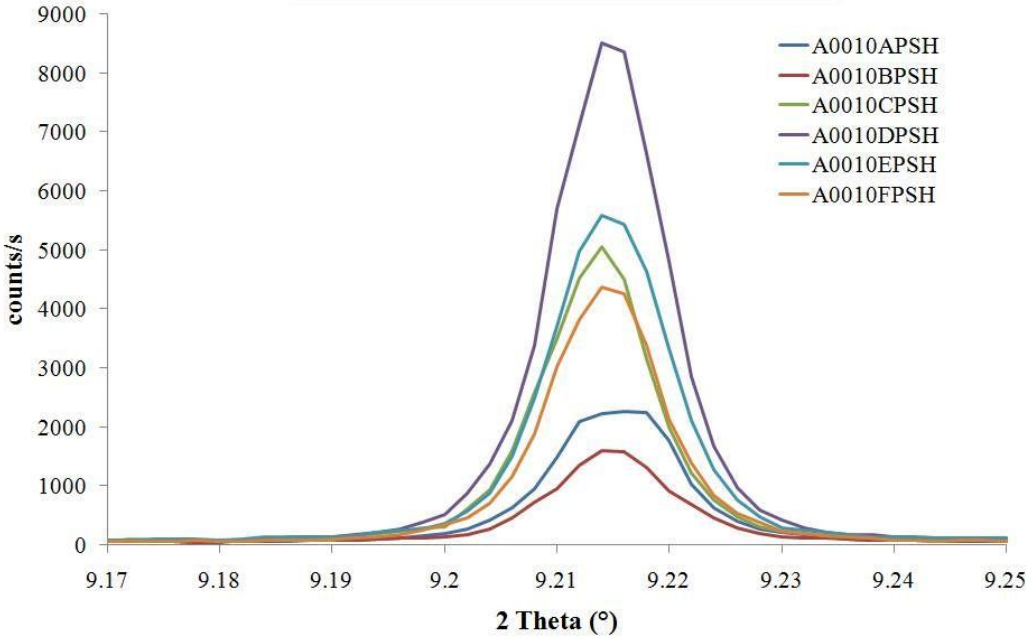

Figure 5.32: Calcite (012) peaks from samples produced using the different methods at 10 mg/L ASP addition.

Figure 5.32 does not show the same trend observed for GLU for the same methods (Fig. 5.20). While the amount of calcite, based on the peak intensity, is smaller for slow addition methods B and F when compared to their respective fast additon methods A and D, it is the same within uncertainty for method C and its slow addition equivalent E.

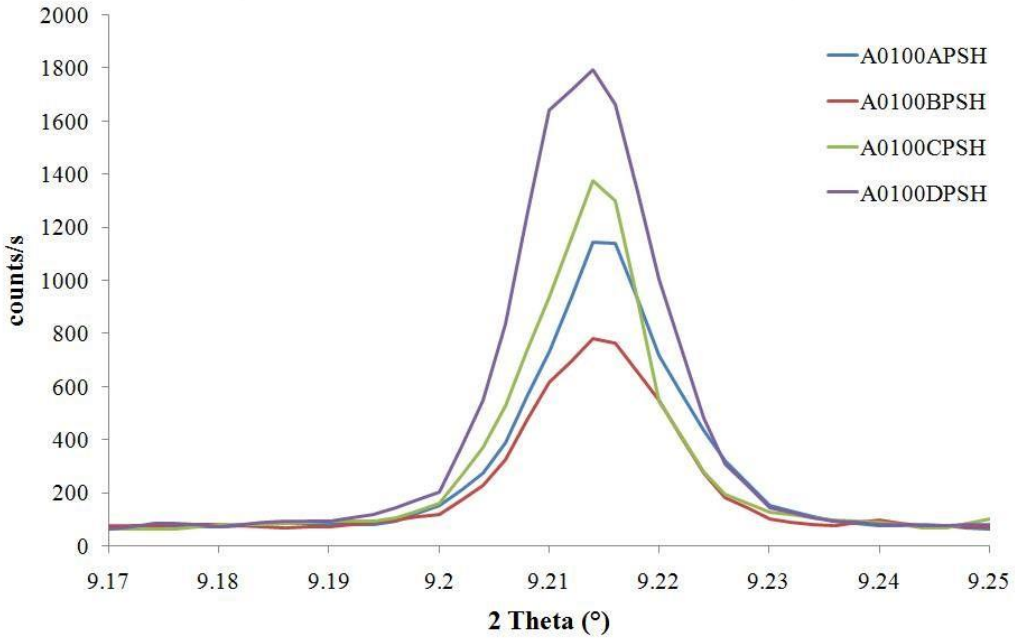

Figure 5.33: Calcite (012) peaks from samples produced using the different methods at 100 mg/L ASP addition.

Figure 5.33 shows that the amount of calcite produced in the presence of 100 mg/L ASP is lower than that in samples produced in the presence of only 10 mg/L ASP, and that the amount produced by slow addition (method B) is lower than that produced by any of the fast addition methods.

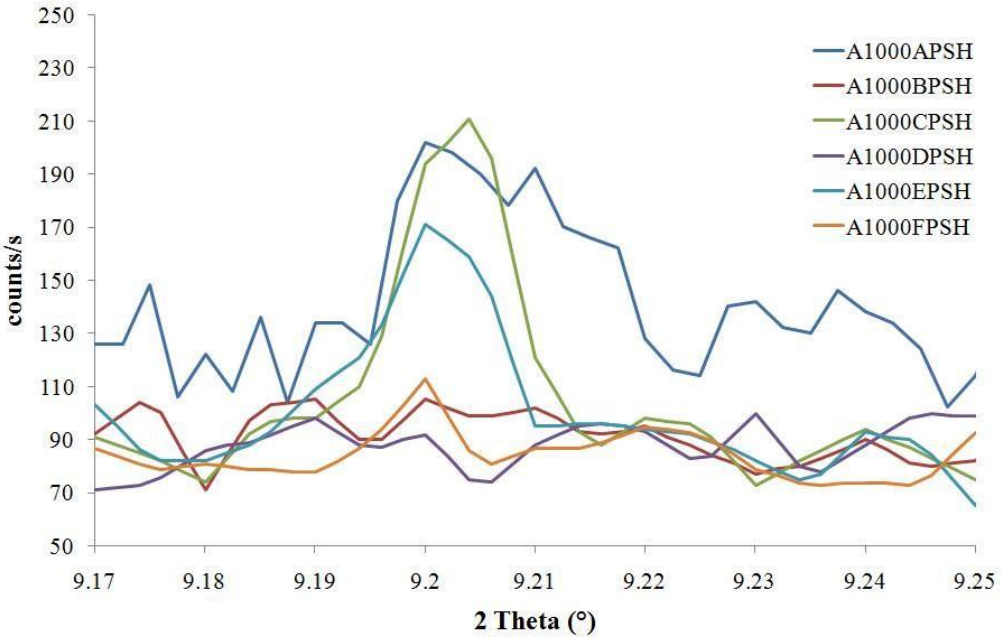

Figure 5.34: Calcite (012) peaks from samples produced using the different methods at 1000 mg/L ASP addition.

Figure 5.34 demonstrates that at 1000 mg/L of ASP almost no calcite is produced. With the exception of slow addition method B and F, where no calcite was observed, all values are statistically indistinguishable.

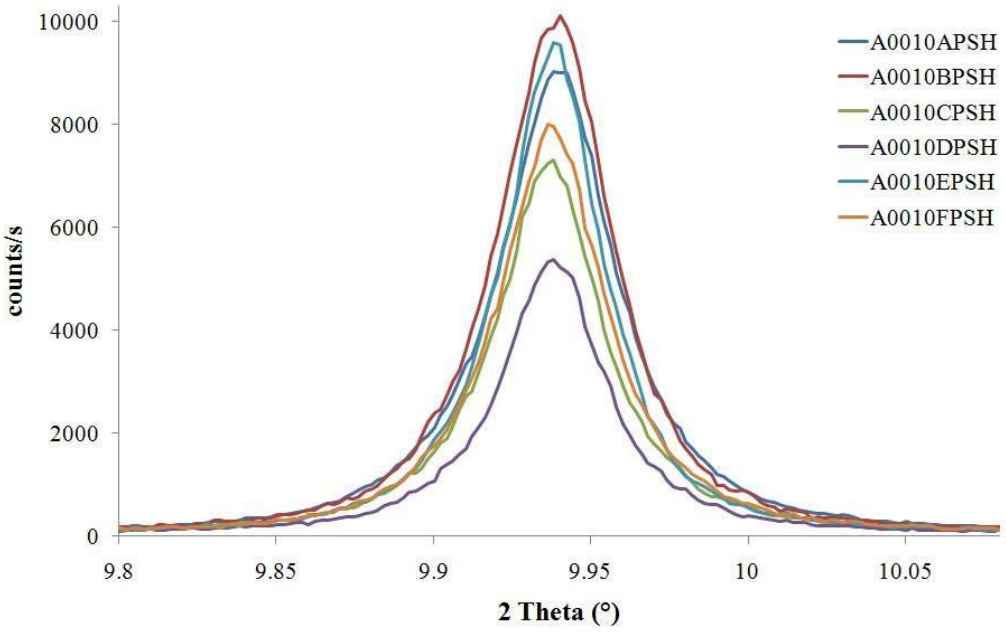

Figure 5.35: Vaterite (110) peaks from samples produced using the different methods at 10 mg/L ASP addition.

Figure 5.35 shows, that there is some difference in the amount of vaterite produced by the different methods for samples grown in the presence of 10 mg/L of ASP and harvested after 1 hour. As in samples grown in the presence of GLU, the one produced by method D shows the lowest amount.

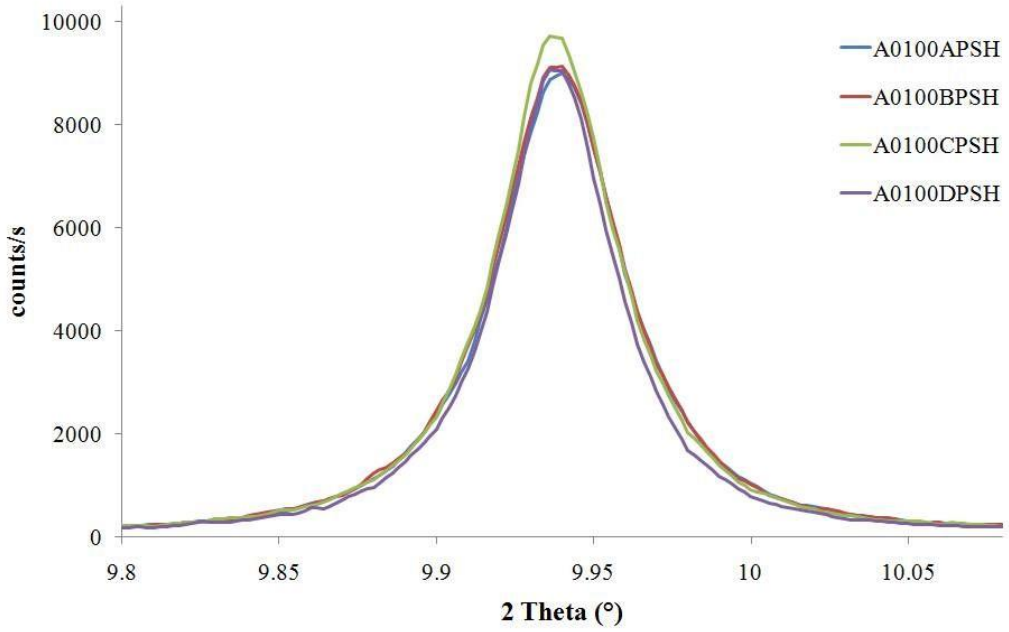

Figure 5.36: Vaterite (110) peaks from samples produced using the different methods at 100 mg/L ASP addition.

Figure 5.36, depicting the same vaterite peak for samples grown in the presence of 100 mg/L ASP and harvested after 1 hour, shows that there is little difference in the amount of vaterite present; the slightly more intense peak for the sample grown by method C is within experimental error.

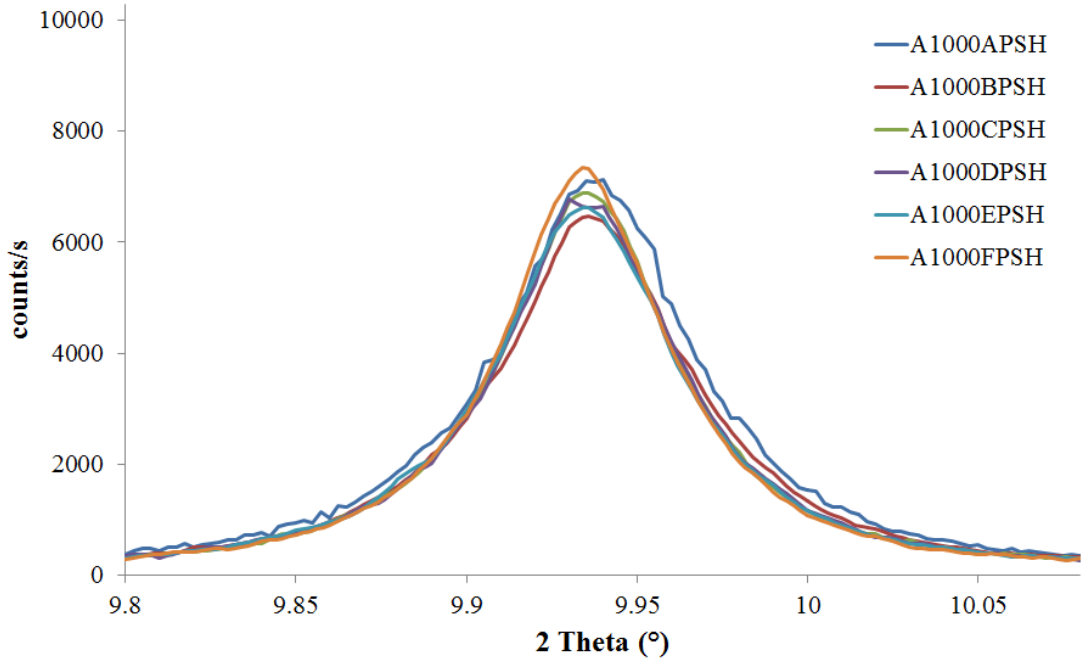

Figure 5.37: Difference in vaterite (110) peak from samples produced using the different methods at 1000 mg/L GLU addition.

Figure 5.37 illustrates that there is very little difference between slow and fast addition methods for samples grown in the presence of 1000 mg/L ASP and harvested after 1 hour. The pattern for the sample produced by method A has been rescaled, because it was run under different conditions (counting time and step size).

Figures 5.32 to 5.37 illustrate the changes with changing concentration of the AA. At concentrations of 10 mg/L and 100 mg/L of AA the samples produced in the presence of ASP show more vaterite in all but two samples when compared to samples produced in the presence of GLU by the same method and at the same concentration.

The speed of addition has an impact on the amount of calcite present in all samples produced in the presence of GLU at the lowest concentration (10 mg/L) and harvested after 1 hour and in two of the three sample pairs produced in the presence of ASP (A-B and D-F).

The amount of calcite produced is smaller and the amount vaterite produced is higher when comparing samples produced in the presence of 100 mg/L and 10 mg/L of AA produced by methods A to D in the presence of ASP, with the exception of one

sample, produced by method B, where the difference in vaterite is within the statistical error. The same applies to samples produced in the presence of GLU, but the difference, especially for vaterite, is smaller. And the only sample where more calcite is present in the sample with 100 mg/L of GLU compared to 10 mg/L is one produced by method C.

Figures 5.38 to 5.42 show some comparisons for different harvesting times and methods.

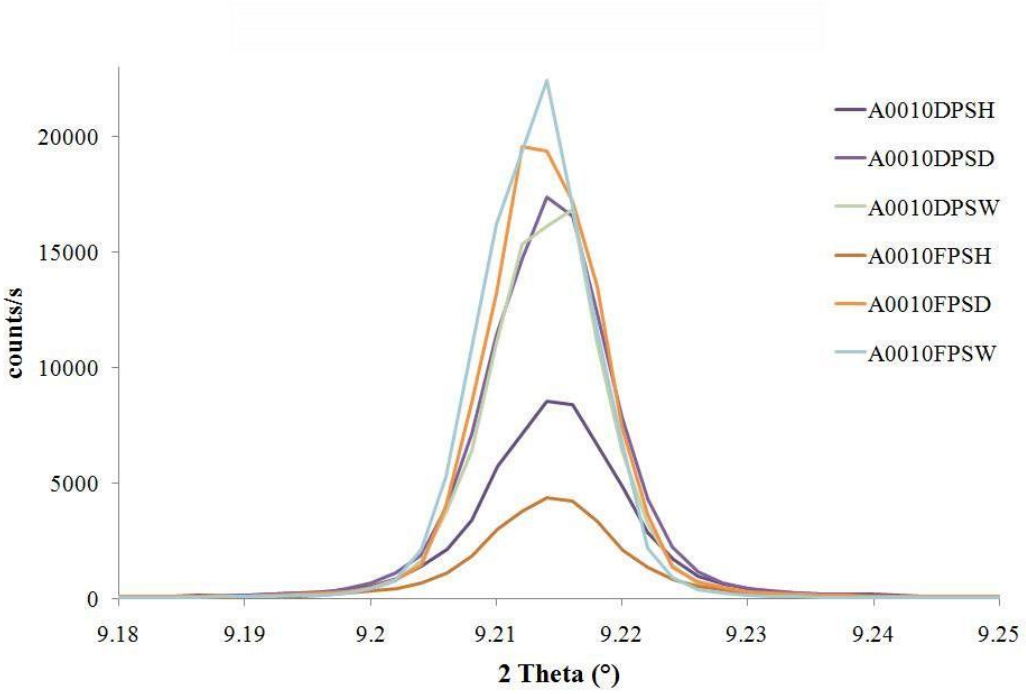

Figure 5.38: Calcite (012) peaks from samples produced using methods D and F at harvesting times of 1 hour, 1 day and 1 week, all at 10 mg/L ASP addition.

Figure 5.38 illustrates that the main change in calcite quantity, based on the scattering intensities, occurs between 1 hour and 1 day, with only small changes in calcite scattering intensity after that. The slight variations between 1 day and 1 week are not statistically valid, because the peak shapes and peak width indicate that step size and to some extent resolution of the instrument were limiting factors. The number of steps across the peak is too small to be sure that enough data points are present to adequately describe the peak shape. The step size chosen for the calcite peak measurements always meant that the number of steps might be too small; this

was, however, unavoidable given the time constraints and the instrument limitation. The goniometer and sample set-up itself has a physical resolution of half the chosen minimum stepsize of 0.001º. What can be seen is that while the amount of calcite present in the samples harvested after 1 hour is lower for the slow additon method F, this trend is reversed for the samples harvested after 1 day and 1 week.

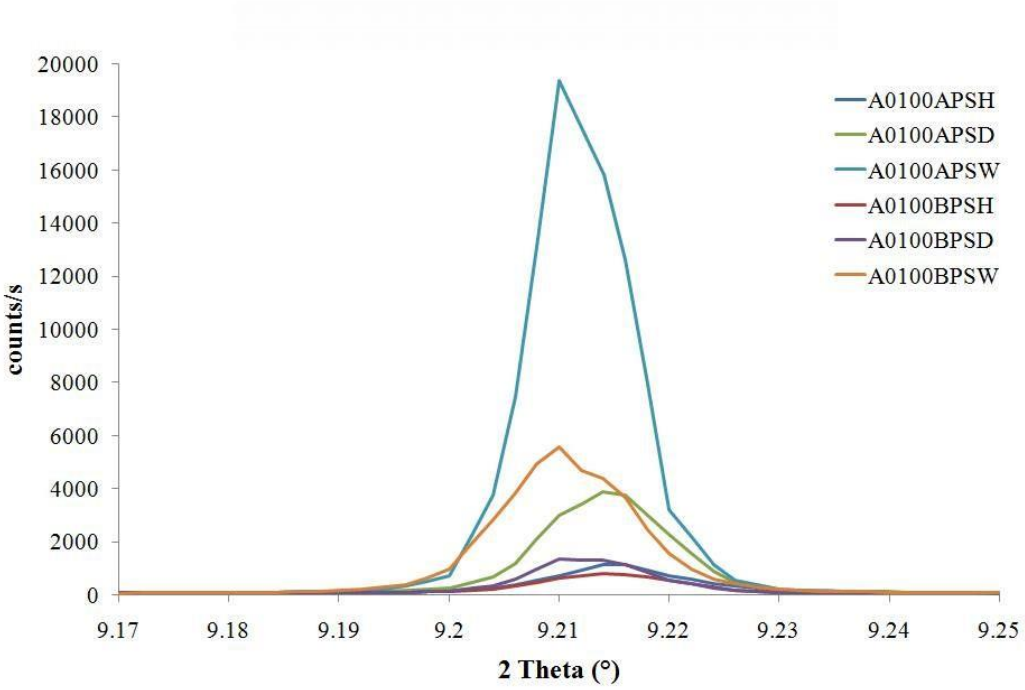

Figure 5.39: Calcite (012) peaks from samples produced using methods A and B at harvesting times of 1 hour, 1 day and 1 week, all at 100 mg/L ASP addition.

Figure 5.39 shows that the amount of calcite for samples grown in the presence of 100 mg/L ASP increases from samples harvested after 1 hour to samples harvested after 1 week, with the most dramatic increase in the time interval from 1 day to 1 week.

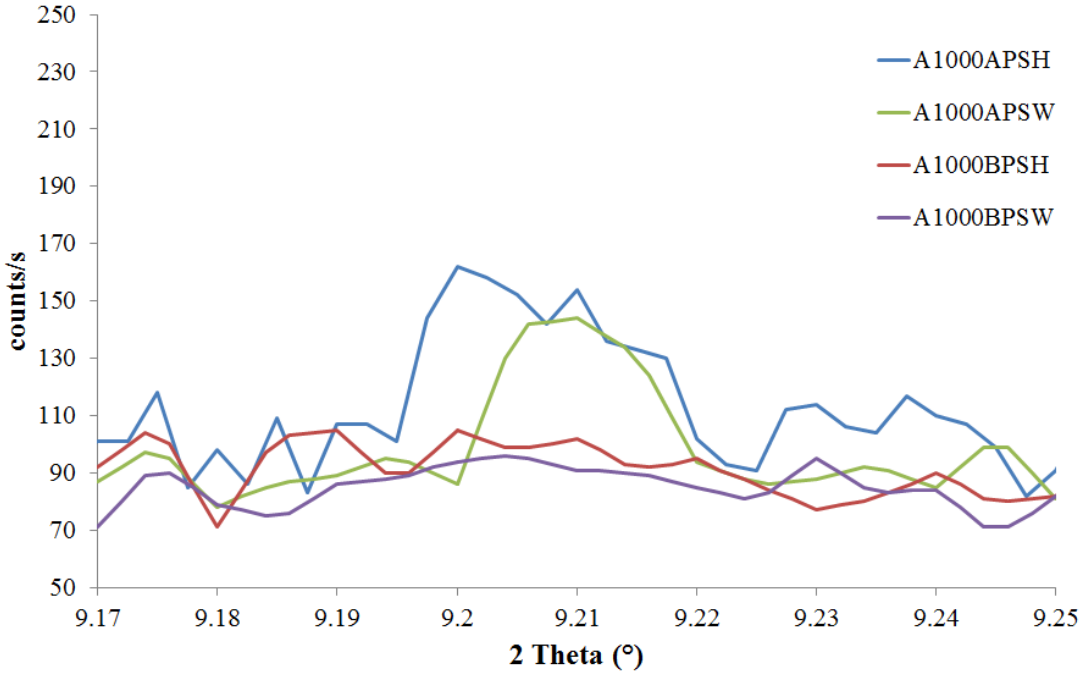

Figure 5.40: Calcite (012) peaks from samples produced using methods A and B at harvesting times of 1 hour and 1 week, all at 1000 mg/L ASP addition.

What can be seen in figure 5.40 is the change in overall coherent scattering from calcite between slow and fast addition and also for harvesting times of 1 hour and 1 week. It demonstrates that slow addition of the reactants results in less initial calcite. The peak fit data show no statistical variation between the amount of calcite present in samples harveste after 1 hour compared to samples harvested after 1 week for the same method.

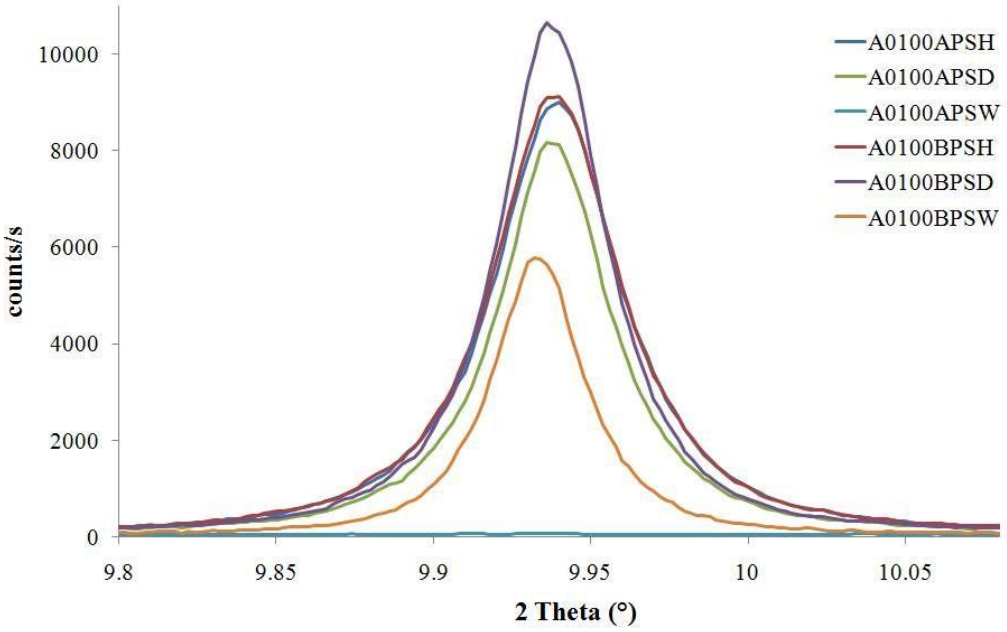

Figure 5.41: Vaterite (110) peaks from samples produced using methods A and B at harvesting times of 1 hour, 1 day and 1 week, all at 100 mg/L ASP addition.

Figure 5.41 indicates that 100 mg/L of ASP is not sufficient to stabilise vaterite if fast addition is used (method A), with the (110) vaterite peak almost completely disappearing between the harvesting times of 1 day and 1 week for the sample produced by method A, while it still lingers in the sample produced by slow addition method B; when compared to samples grown in the presence of the same amount of GLU, it highlights the stronger stabilising effect of ASP over GLU. The graph also suggests that the vaterite produced by slow addition is more stable, in contrast to the result observed in the samples grown in the presence of the same amount of GLU. This graph needs to be viewed in conjunction with figure 5.39 to complete the picture; the amount of vaterite present almost completely disappears in the sample produced by fast addition, while over the same time the amount of calcite increases dramatically, indicating almost complete transformation of vaterite into calcite.

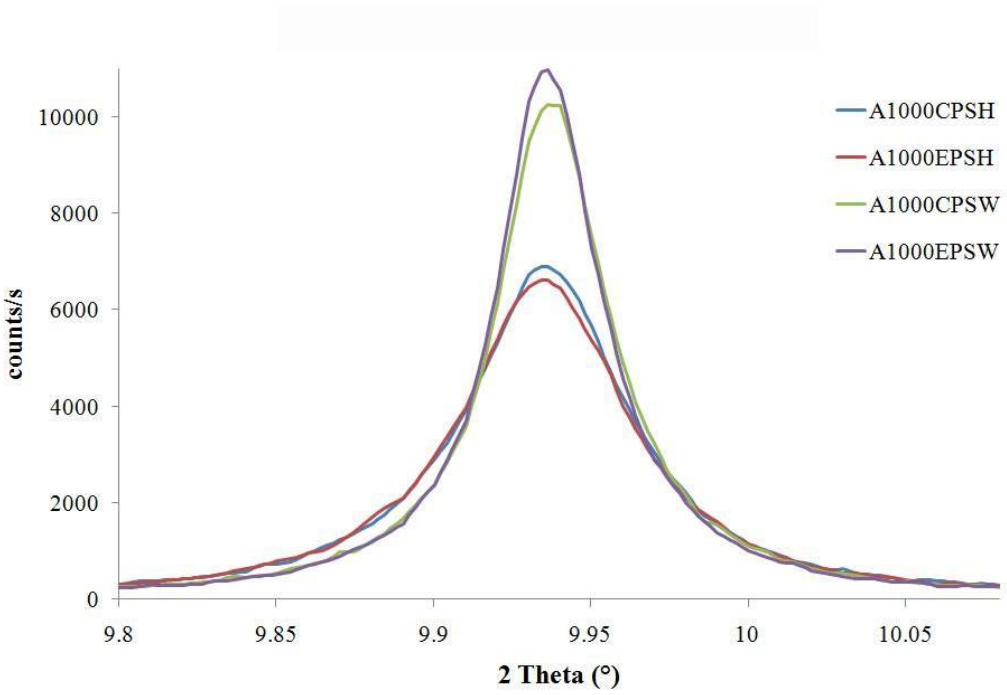

Figure 5.42: Vaterite (110) peaks from samples produced using methods C and E at harvesting times of 1 hour and 1 week, all at 1000 mg/L ASP addition.

Figure 5.42 shows that there is a big difference between samples harvested after 1 hour and 1 week for sample produced in the presence of 1000 mg/L ASP, but not so much between slow and fast addition for the method where all Ca is present in the reaction vessel prior to addition of the other reactants; the pattern suggests a significant increase in the amount of vaterite present and also in its crystallinity.

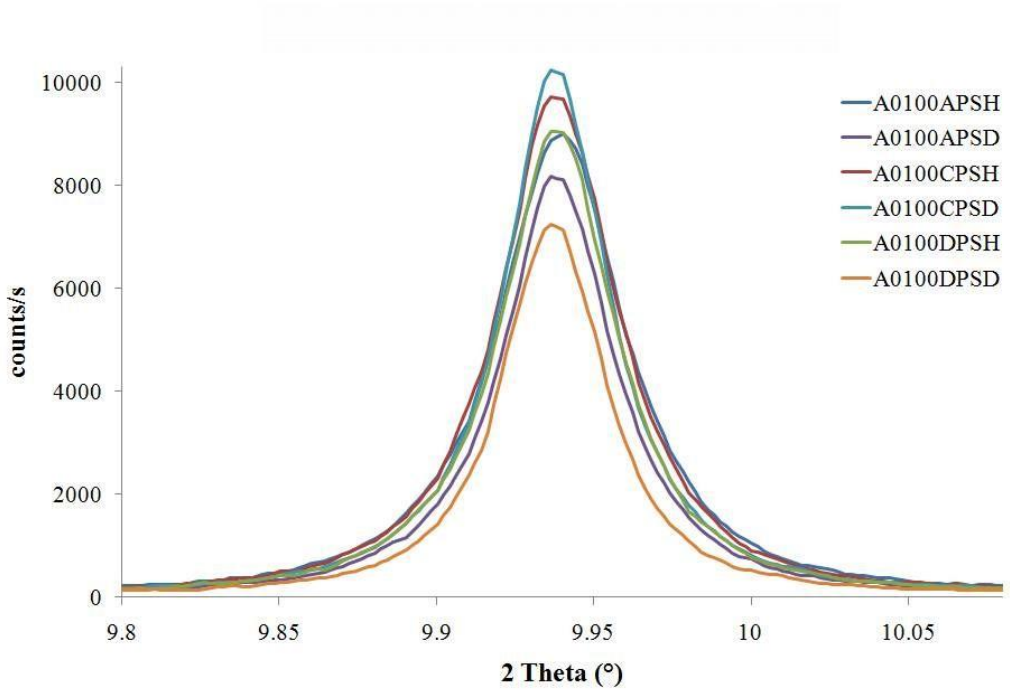

Figure 5.43: Vaterite (110) peaks from samples produced using methods A, C and D at harvesting times of 1 hour and 1 week, all at 100 mg/L ASP addition.

Figure 5.43 illustrates the rapid stabilising effect of ASP. There is no clear trend, but only an indication of a slight reduction in vaterite peak intensity in samples harvested after 1 day compared to samples harvested after 1 hour. For clarity only samples produced by fast addition are compared.

Table 5.3 summarises relevant peak data for the patterns used in the plots relating to samples produced in the presence of ASP.

ASP												
Concentration and method	Calcite peak 9.21° 2Θ 1 Hour		Vaterite peak 9.93° 2Θ 1 Hour		Calcite peak 9.21° 2Θ 1 Day		Vaterite peak 9.93° 2Θ 1 Day		Calcite peak 9.21° 2Θ 1 Week		Vaterite peak 9.93° 2Θ 1 Week	
	Area	2σ	Area	2σ	Area	2σ	Area	2σ	Area	2σ	Area	2σ
10 mg/L - A	67.2	5.1	1033.7	36.4	342.8	13.4	0.0	0.0	N/A	N/A	N/A	N/A
10 mg/L - B	44.9	6.2	1106.9	36.6	295.7	8.6	5.0	3.2	439.3	11.6	0.0	0.0
10 mg/L - C	127.0	9.1	754.6	46.8	404.8	6.8	0.0	0.0	384.4	10.4	0.0	0.0
10 mg/L - D	220.9	9.9	543.0	34.6	411.1	11.0	0.0	0.0	390.8	10.4	0.0	0.0
10 mg/L - E	124.7	7.4	742.8	28.0	386.1	12.6	0.0	0.0	511.6	13.6	0.0	0.0
10 mg/L - F	113.8	7.0	829.2	78.2	430.1	16.4	4.0	3.2	481.5	11.6	0.0	0.0
100 mg/L - A	32.7	5.0	1178.1	61.3	106.8	9.4	903.5	56.6	409.8	11.0	1.2	0.6
100 mg/L - B	22.7	3.2	1187.2	74.0	35.6	5.0	1126.3	40.0	253.6	8.4	510.6	30.2
100 mg/L - C	35.0	7.3	1192.0	99.3	31.6	5.0	1087.6	58.2	108.9	11.5	4.9	2.2
100 mg/L - D	54.7	2.1	1037.2	89.2	145.2	10.0	733.3	46.4	327.9	8.6	0.0	0.0
1000 mg/L - A	1.3	0.7	518.3	40.6	2.0	0.6	564.1	29.8	2.2	0.6	849.2	77.8
1000 mg/L - B	0.0	0.0	584.9	41.4	0.0	27.0	604.3	29.0	0.0	0.0	811.0	52.8
1000 mg/L - C	0.9	1.1	592.4	24.6	1.5	1.0	584.9	28.2	1.2	2.0	1201.5	79.6
1000 mg/L - D	0.6	0.3	579.7	29.4	0.0	0.0	502.6	32.6	2.1	418.6	1199.7	106.6
1000 mg/L - E	1.4	0.7	580.7	30.4	0.0	0.0	692.5	37.8	0.0	0.0	1219.6	104.0
1000 mg/L - F	0.0	0.0	602.5	30.2	5.2	1.2	511.7	35.2	1.7	1.2	1207.3	73.0

Table 5.3: Peak area and uncertainty data for the samples produced in the presence of ASP.

6 RESULTS – CRYSTALLITE SIZE, STRAIN, HEATING AND INFRARED ANALYSIS

6.1 Crystallite size and strain calculations

For the crystallite size and strain calculations it was necessary to determine the instrument function. This was achieved by analysing a standard material with known lattice parameters, known crystallite size and strain under the same conditions as the remainder of the samples. We chose LaB_6 (NIST standard 660a) and Si (NIST standard 640c), with LaB_6 being the main standard, certified to have a crystallite size of 2 μm and to be strain free, while the Si standard is certified to have a crystallite size of 1.4 μm and some micro-strain, determined using a laboratory instrument with Cu Kα radiation. This, according to the certificate for the standard, contributes to peak broadening of 0.02° for the (533) peak of silicon at 136.8789° 2θ. LaB_6 660a was primarily used, with Si 640c only used to compare results and to establish confidence intervals.

A number of mathematical functions were used to fit the collected peak profiles and also to calculate the micro-strain and crystallite or apparent coherent scattering domain size. The main function used was the Voigt function, as applied in X-ray diffraction (Sommerdijk and de With, 2008, Gower, 2008). This is a convolution of a Gaussian and a Lorentzian function, and the two functions used were the ones defined in SHADOW (Materials Data), where they are described as:

$$Gaussian: \qquad I_0 e^{(-kx^2)}; k = \frac{0.6931}{\left(\frac{H_k}{2}\right)^2}; H_k = FWHM$$

Equation 6.1: The Gaussian part of the Voigt line profile function. The value of 0.6931 was used as the numerical approximation for ln2.

$$Lorentzian: \qquad \frac{I_0}{(1+kx^2)}; k = \frac{1}{(\frac{H_k}{2})^2};\ H_k = FWHM$$

Equation 6.2: The Lorentzian part of the line profile function.

FWHM stands for full width at half maximum; I_0 is the inverse of the integral breadth 1/β; *x* represents the distance from the Bragg angle for the reflection caused by the wavelength.

The standards, in particular LaB_6, were used to determine the 2θ-dependent instrument function by fitting linear and polynomial functions to a regression line or curve through the plotted integral breadth values obtained from manual fits using SHADOW. Linear functions were trialled but the fit was unsatisfactory, particularly at low and high angles, resulting in correlation coefficients of 0.95 to 0.97. A simple second order polynomial was used instead, and its fit gave correlation coefficients of 0.98 to 0.99. Figure 6.1a and figure 6.1b show the comparison of linear and quadratic fitted functions.

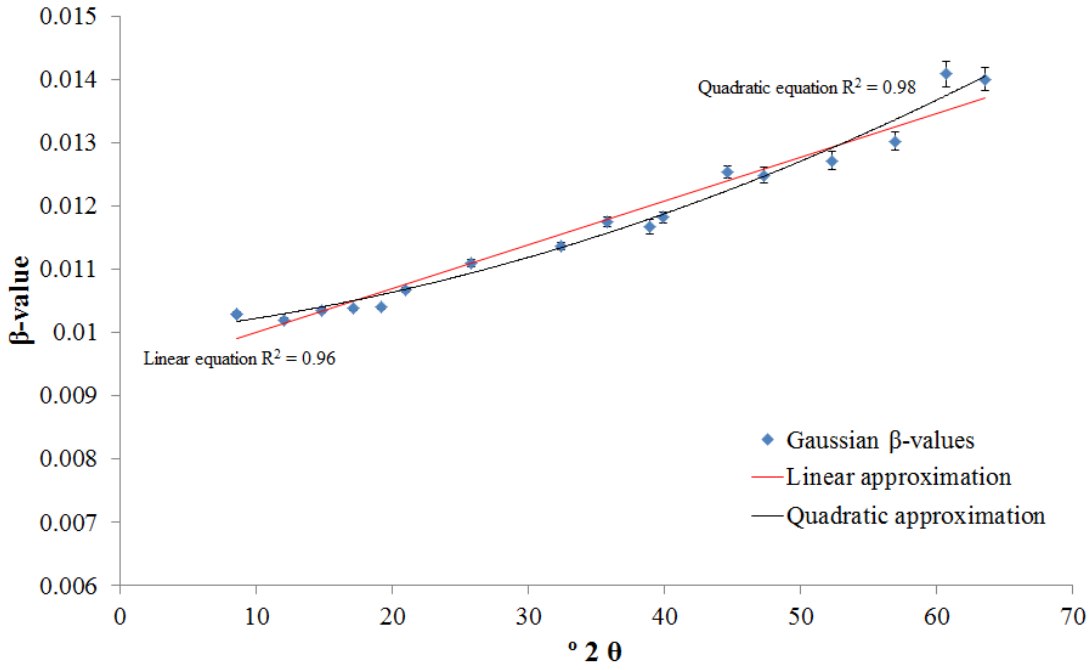

Figure 6.1a: Comparison of linear (R^2 = 0.95) and quadratic (R^2 = 0.99) fits to the plotted Lorentzian β-values for LaB_6

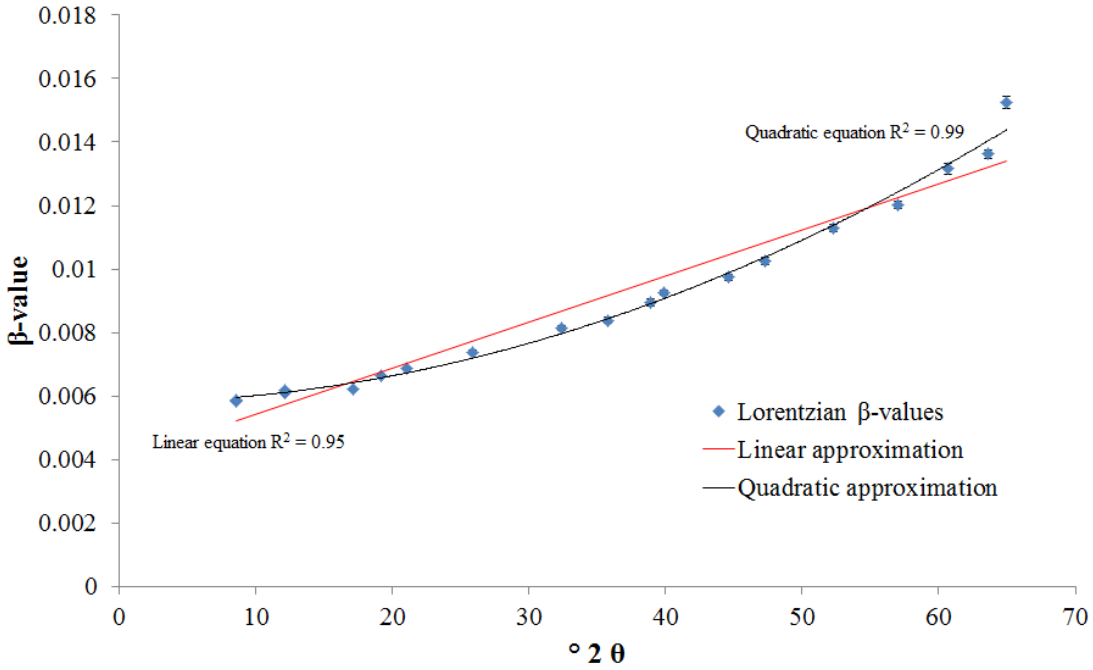

Figure 6.1b: Comparison of linear (R^2 = 0.96) and quadratic (R^2 = 0.98) fits to the plotted Gaussian β-values for LaB_6

The functions derived from the fitting were then used to subtract the instrument contribution from the integral breadth values for all the calcite and vaterite peaks. Separate calculations were made for the maximum and minimum integral breadth values to confirm the equations for the R^2 values. These are not constant over the 2θ range analysed either, and separate second order polynomial functions were fitted to plots containing all integral breadth values with the esd values subtracted and to plots with all integral breadth values with the esd values added. These functions were then used to calculate the instrument contribution at all peak positions derived from fits of peaks in the samples. To establish the largest possible error for any given single value, the integral breadth values were calculated using the function derived from fitting the minimum values of the standard for both Gaussian and Lorentzian, while for the sample peaks the maximum value for each fitted peak, obtained by adding the esd of the Gaussian and Lorentzian β-values from the fit itself was used, thus comparing the instrument value with esd added with the sample values with esd subtracted. The values obtained were compared with the coherent scattering domain size and the micro strain values calculated from the sample peak fits without adding or subtracting esd or instrument contribution. The difference was then used as a new esd value for that peak, and the statistical relevance tested by establishing if 3*esd

was still smaller than the values determined by the direct calculation. Only if this proved to be true was the peak flagged as being valid. A total of about 16,000 peaks were fitted. Of these only around 5,400 had statistically meaningful results for either Lorentzian- or Gaussian-β values based on the conservative criterion that the value needed to be larger than 3*esd. All these values were then used as input for the calculation of micro-strain and crystallite or apparent coherent scattering domain size calculations. Applying the same conservative criterion, only 3,141 micro-strain values and 3,524 size values fulfilled the criteria, some of which were repeat fits to the same data to ascertain program reproducibility, and some were for the same type of sample, but for different production times and/or analysis cycles. The majority of peaks that fulfilled the criteria were vaterite peaks particularly with regard to the size values. Due to this, only limited comparisons are possible.

The LaB_6 data were also used to determine accurately the wavelength. The data for the standard were collected at least once during each visit to the APS. Some additional runs were carried out during longer experiments and/or when changes to the experimental set-up or the beam line set-up occurred. The wavelength changes were usually small, and we have used an averaged wavelength from the different patterns acquired during each visit for all samples analysed during that visit. For comparison all peaks of the LaB_6 standard were fitted at least twice, using the simple Voigt function as well as the Pearson VII function.

The Pearson VII function used was also the one used in SHADOW, where it is described as:

$$Pearson\,VII: \qquad \frac{I_0}{(1+kx^2)^m}; k = \frac{(2^{(1/m)}-1)}{{H_k}^2};\ H_k = FWHM$$

Equation 6.3: *m* is the exponential factor of the function and *FWHM*, I_0 and *x* the same as defined in equations 6.1 and 6.2

Figure 6.2a, 6.2b and 6.2c show the calculated λ values determined by using the different functions, plotted over 2θ.

As can be seen from the plots, the wavelength range is small. The PVII in the plots indicates the values obtained by fitting a Pearson VII function to the peak. The Pearson VII function produced greatly improved peak fits, particularly at lower angles, while the peak shapes at higher angles are almost equally well fitted by a simple Voigt function.

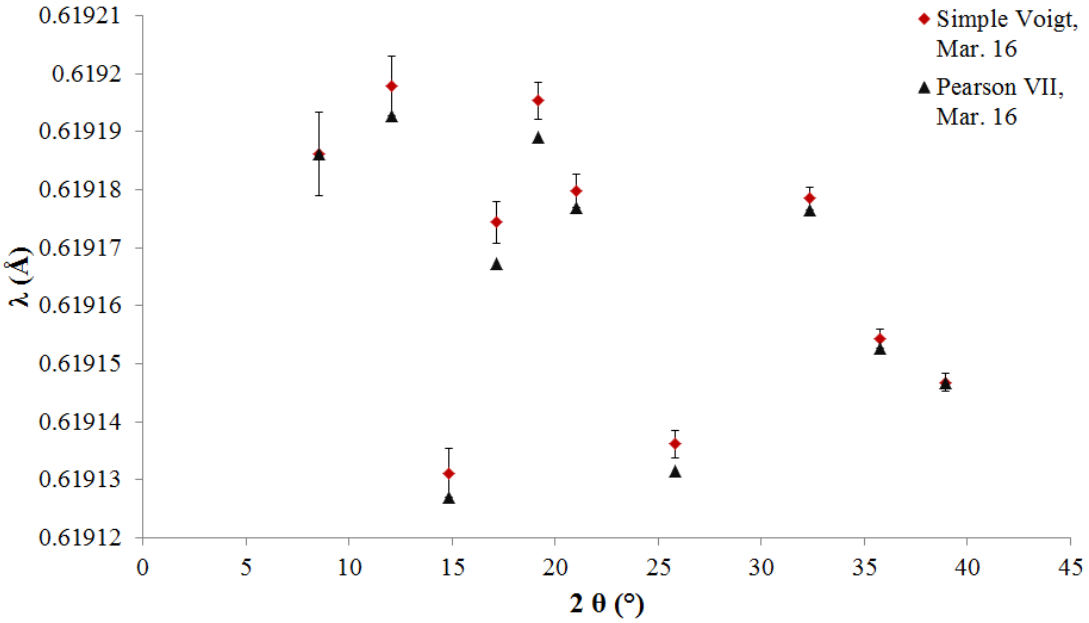

Figure 6.2a: Calculated wavelength for the experiments carried out during the first visit to the APS

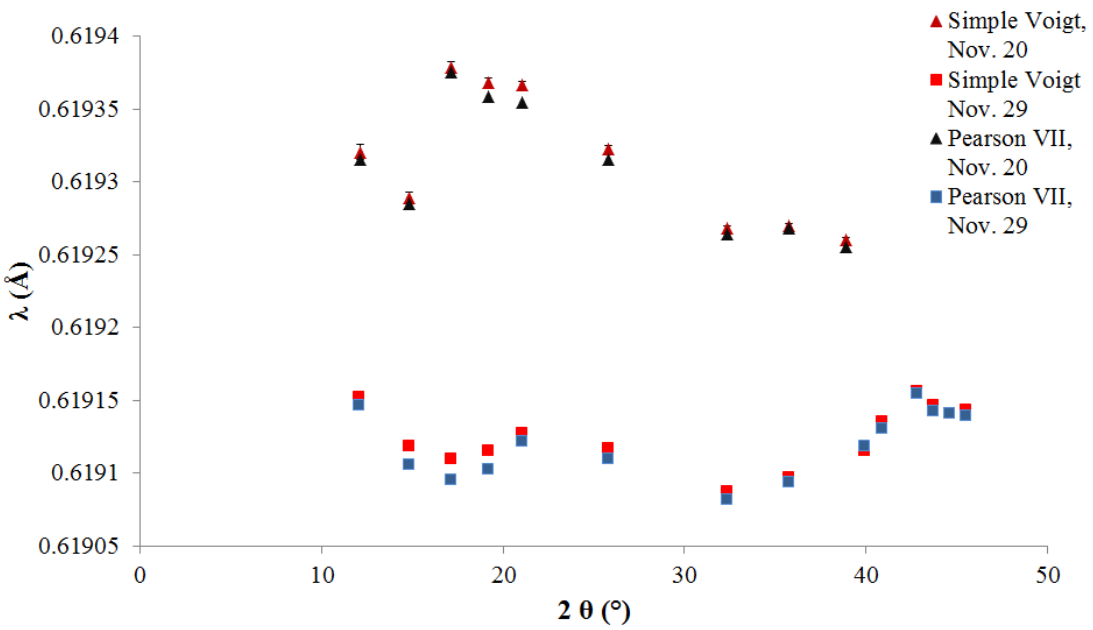

Figure 6.2b: Calculated wavelength for the experiments carried out during the second visit to the APS

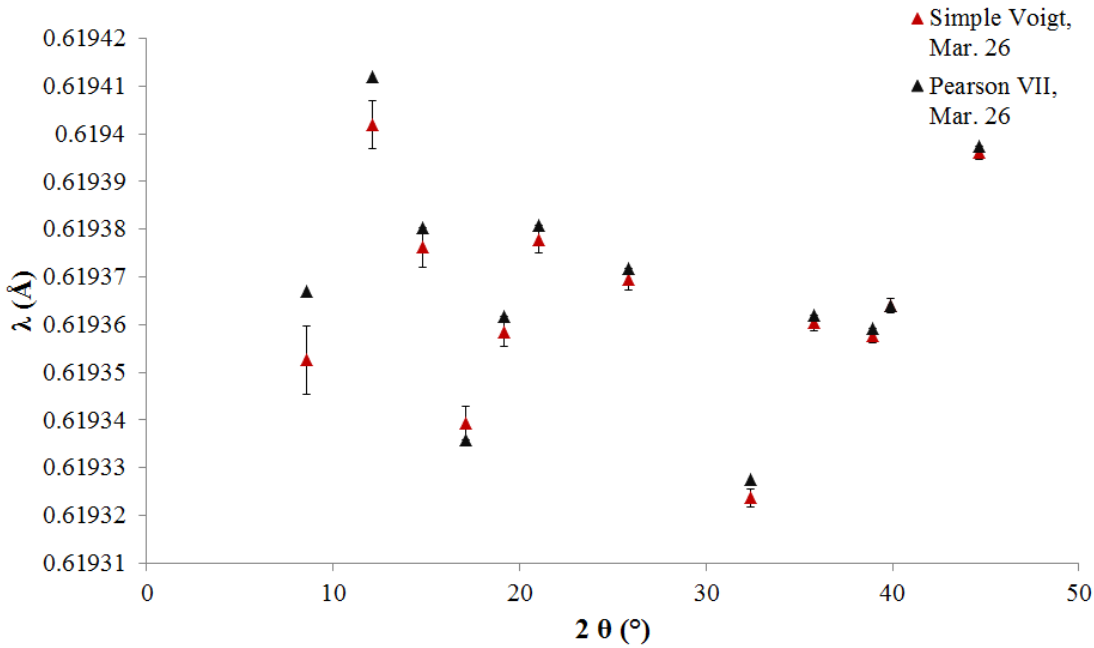

Figure 6.2c: Calculated wavelength for the experiments carried out during the third visit to the APS

Crystallite size and micro-strain calculations are quite complex and given the size of the dataset it was decided to investigate if a single wavelength value could be used in these calculations to reduce the complexity. To this effect the LaB_6 peaks from all

different runs during each visit were used to obtain an averaged λ for each visit to the APS, as well as an average λ for all experiments across the three visits. The determined values were then used to calculate the crystallite or apparent coherent scattering domain sizes for the samples run at each visit. A random selection was used to compare these values to the crystallite size values determined by using the λ determined for individual measurements. The largest error introduced by using the average wavelength for all experiments was 0.35%, which was found to be well within the esds derived from the calculation, and for simplification an average λ of 0.061922 nm was used.

Micro-strain and crystallite or apparent coherent scattering domain size were determined by using the Scherrer equation (Wang and Nancollas, 2008, Scherrer, 1918) to obtain the volume averaged crystallite size, assuming that the size contribution is exclusively Lorentzian, and using the Stokes and Wilson (Arias and Fernández, 2008, Stokes and Wilson, 1944) equation for strain, assuming that the strain contribution is exclusively Gaussian. The equations used are:

$$Scherrer: \qquad D_v = \frac{K\lambda}{\beta \cos\theta};\ 0.87 \leq K \leq 1;\ \beta = integral\ breadth\ (rad\ 2\theta)$$

Equation 6.4: D_v is the volume averaged crystallite size. K was set to one, as it is an arbitrary constant, and β was obtained from the Lorentz function.

$$Stokes\ and\ Wilson: \qquad \varepsilon_{str} = \frac{\beta}{4 \tan\theta};\ \beta = integral\ breadth\ (rad\ 2\theta)$$

Equation 6.5: ε_{str} is the weighted average strain and for β the Gaussian β was used.

The simplification and strict separation were applied because the main aim was not to obtain absolute values, but to highlight trends and to compare the effect of the two different AAs and methods and also to compare the main two phases formed, vaterite and calcite. As reported in literature (Le Bail, A. , 2008), the use of integral breadth methods should be to assess qualitative differences. As such, the information gained from the calculation of crystallite- or apparent coherent scattering domain size and from the calculation of micro-strain has provided some very useful indications of the effect that the experimental variables have had on the minerals formed.

The following plots are a based on a selection of data that are representative of the overall trends. They were chosen according to completeness of data, with samples that had the largest number of valid data points for size and strain chosen preferentially, as these provide a more complete and reliable information set. Some partially complete sets were also included, where they despite being incomplete provide evidence of some trends.

The large number of graphs is necessary because of the large number of variables that are covered by the experiments, and also the fact that calcite and vaterite needed to be treated separately, as the results are quite different for both, apparent crystallite or coherent scattering domain size and also micro strain. In the remainder of this chapter I will use the term crystallite size to represent 'crystallite or coherent scattering domain size' to simplify the explanations and the axes descriptions on the graphs should be read as representing the inclusive description.

Crystallite size and micro-strain are given without units in the charts to indicate that the results are based on the simplified assumption that micro-strain and crystallite size can be calculated independently from the Lorentzian and Gaussian β-values for integral breadth. The values derived should still be intrinsically consistent; however, the absolute values are probably not accurate. The intrinsic validity was confirmed through the fitting and calculation of micro-strain and crystallite size values from samples spiked with corundum. These had been produced for NPD experiments at the Australian Nuclear Science and Technology Organisation (ANSTO) Research Reactor at Lucas Heights and were subsequently taken to the APS for synchrotron diffraction experiments. The corundum used in all spiked samples was the same, and the corundum itself served therefore as a sample independent standard. More than 500 corundum peaks were fitted, of which 304 produced valid results for size and 273 produced valid results for micro-strain. Of all peaks fitted around 94% were within two esd of the average over all size values, suggesting an isotropic and fairly uniform shape for the crystallites. The micro-strain showed some structural dependence, and a peak-by-peak approach was used for averaging. Around 91% of all micro-strain values were within two esd of the average strain value on the peak-by-peak basis.

As such, the calculated values for crystallite size and strain should be comparable and the trends visible can be interpreted.

All graphs produced and displayed on the following pages show error bars representing 2 esd. Some of the plots were cut off to highlight details that would otherwise become obscured; this has led to the presence of some error bars in some charts without the associated data point and also the cut-off of some of the error bars. In particular the negative error bars were cut off at 0, as there is no physical meaning in negative micro-strain or negative crystallite sizes. The points and error bars in question that are no longer fully or even partially visible were not omitted from the plots to ensure data clarity.

Shortened series descriptors were used to minimise the space of the legend in the graphs, with AA and concentration information solely presented in the figure descriptions.

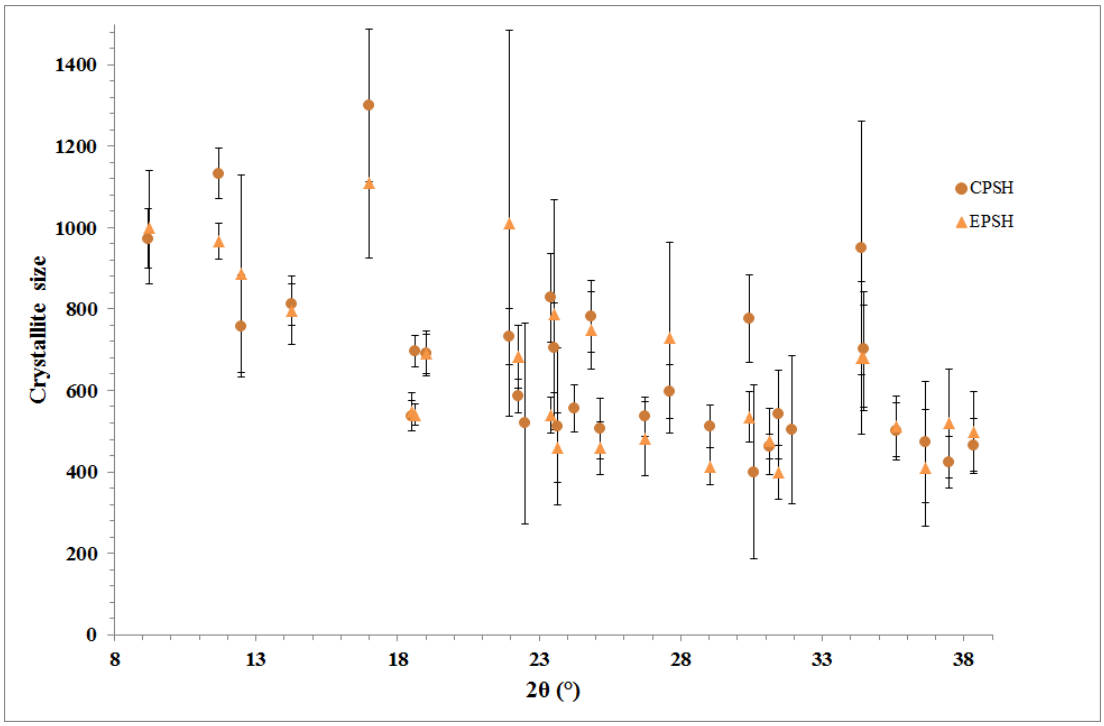

Figure 6.3a: Comparison of crystallite sizes of samples produced from slow and fast addition methods with Ca in solution and their effect on calcite crystallite size. Method C and E with an ASP concentration of 10 mg/L.

Figure 6.3a shows that there is relatively little difference between the slow and fast addition method at low concentrations of ASP, but the few peaks where some difference can be observed suggest that fast addition leads to larger crystallite sizes. It should be mentioned that the higher values are close to instrument resolution and have therefore fairly large errors associated with them.

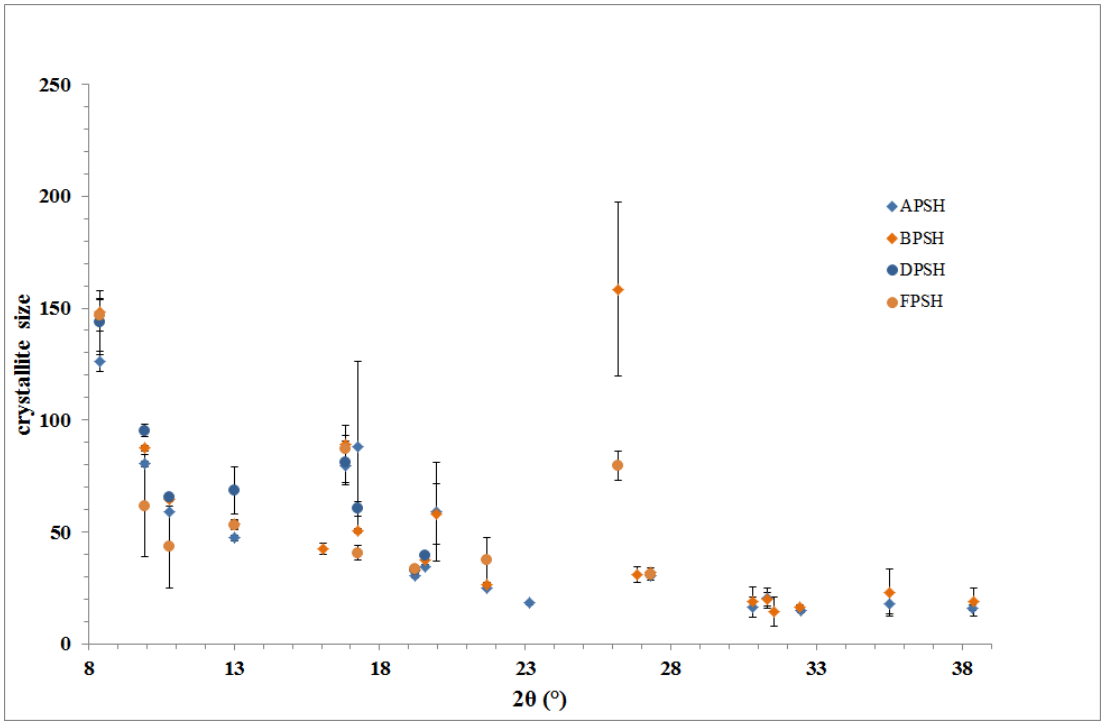

Figure 6.3b: Comparison of crystallite sizes of samples produced from slow and fast addition methods and their impact on vaterite crystallites. The methods compared are A, B, D and F at ASP concentration of 10 mg/L.

Comparison of figure 6.3a and b show clearly that the vaterite crystallite size is significantly smaller than the calcite crystallite size. At this low AA concentration it is not possible to distinguish other features, except for some indication that slow addition does not necessarily lead to larger crystallites.

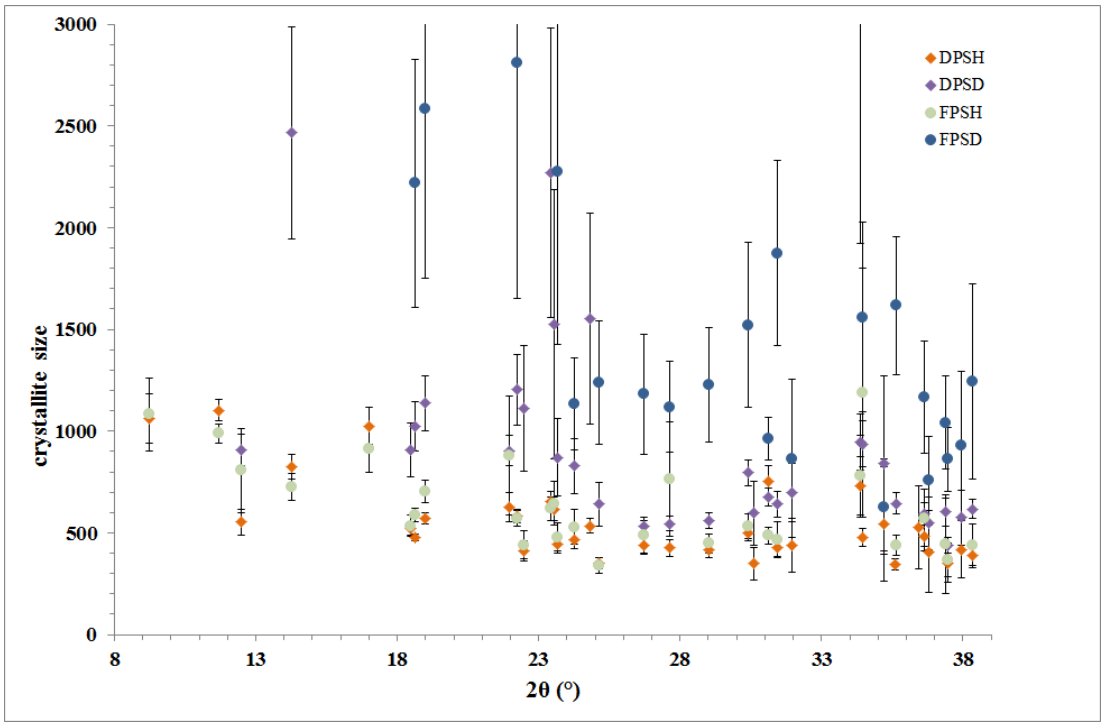

Figure 6.3c: Comparison of crystallite sizes of samples produced from slow and fast addition methods and the impact on calcite crystallite sizes with time. Values greater than 2000 are questionable as they approach the maximum values meaningfully extractable with the Standard Reference Material (SRM) used, which has a certified crystallite size of 2000 nm. The methods compared are D and F, harvested after 1 hour and 1day, grown in the presence of 10 mg/L ASP.

The most interesting fact to note in figure 6.3c is the difference between the slow and fast addition and the apparent difference for the two methods as a function of time, with the slow addition resulting in larger crystallite sizes after one hour.

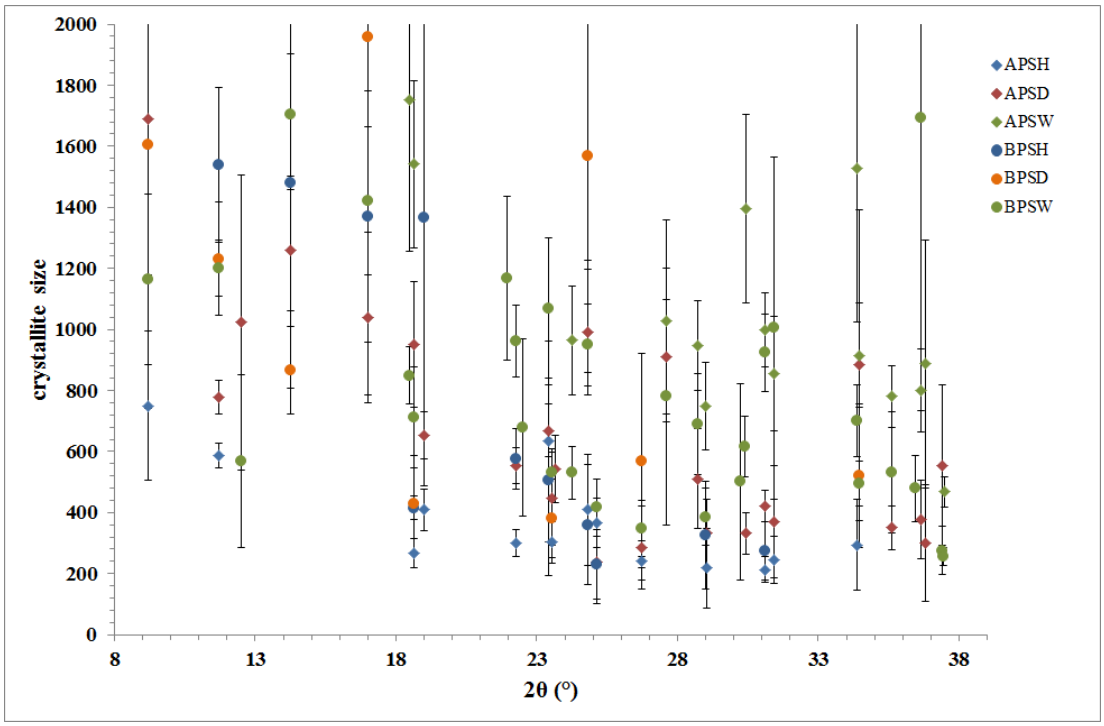

Figure 6.3d: Comparison of crystallite sizes of samples produced by slow and fast addition methods A and B and their effect on calcite crystallite size over time. Sample grown at an ASP concentration of 100 mg/L.

There seems to be a difference between these samples and the samples grown in the presence of only 10 mg/L AA. For the fast addition the expected behaviour seems to occur; the crystallite size increases over time. But for the slow addition some changes, particularly for a few selected orientations, occur, with the crystallite size first increasing between an hour and a day, but then apparently decreasing from a day to a week. As the results represent average crystallite sizes, this indicates that a number of small calcite crystallites are formed, which is consistent with the disappearance of vaterite when comparing samples harvested after 1 day and 1 week.

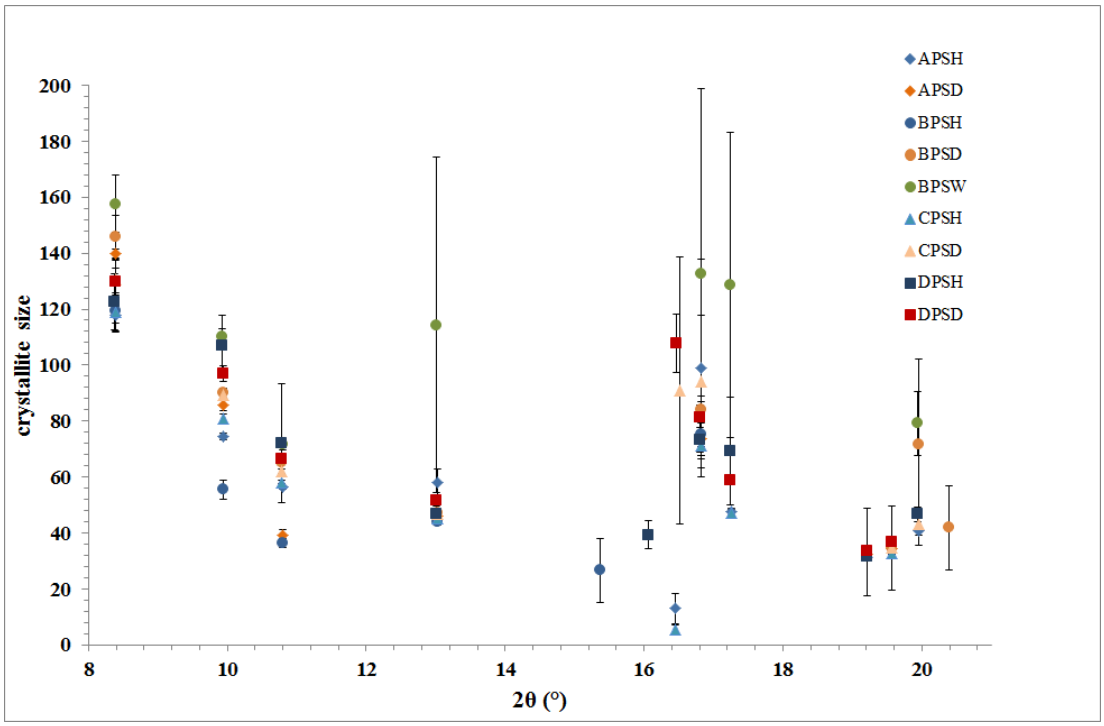

Figure 6.3e: Comparison of crystallite sizes of samples produced by methods A, B, C and D and the effect of harvesting time on the vaterite crystallite size at ASP concentration of 100 mg/L. Vaterite was only found in one sample harvested after 1 week, the sample produced by slow addition method B.

Figure 6.3e shows that the changes in crystallite size over time are relatively small but significant. Crystallite sizes differ as a function of the lattice, showing that the impact of the AA at a concentration of 100 mg/L on the development and growth of vaterite is non-uniform and most likely stronger than the influence it has on calcite growth.

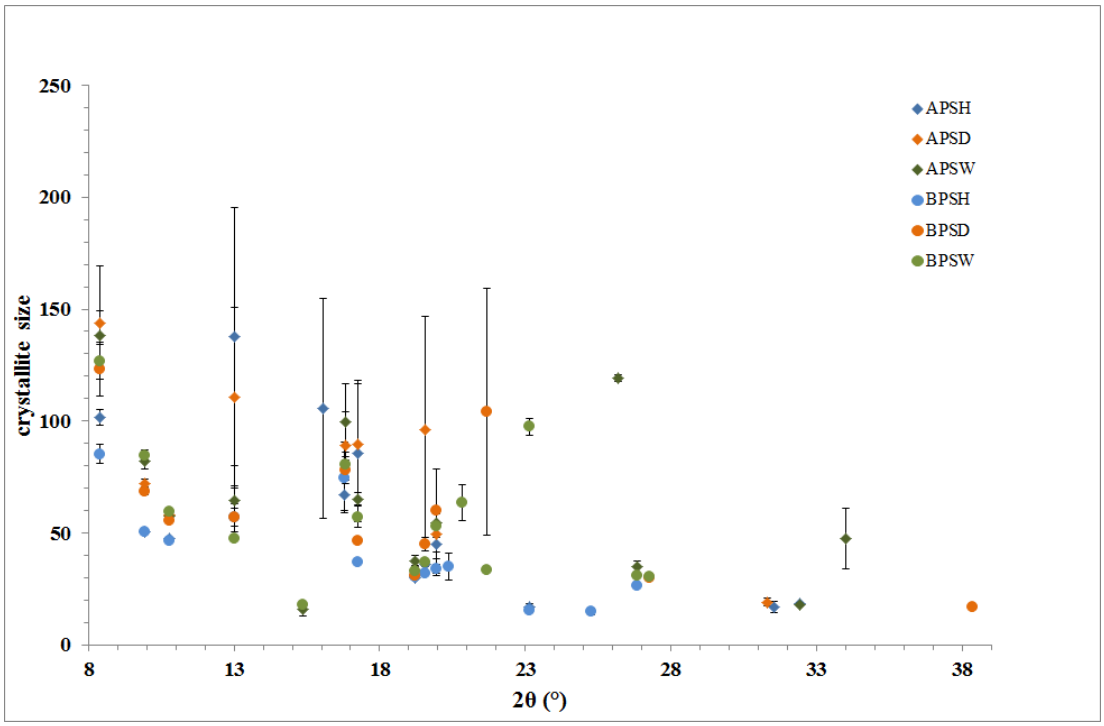

Figure 6.3f: Comparison of crystallite sizes for samples produced by slow and fast addition methods A and B and the effect of harvesting time on vaterite crystallite size at 1000 mg/L ASP concentration. The crystallite size increases over time.

Figure 6.3f shows that for 1000 mg/L the AA seems to be the controlling factor, with vaterite crystallite sizes generally increasing over time, while still maintaining some differences depending on the crystallographic direction; the size increases are not linear across the crystallographic orientations.

No sensible plot could be produced for calcite, because there is virtually no calcite present in the samples grown in the presence of 1000 mg/L ASP. The few values obtained suggest that the crystallite size for calcite is generally smaller than the one observed for the other concentrations, and that it decreases over time.

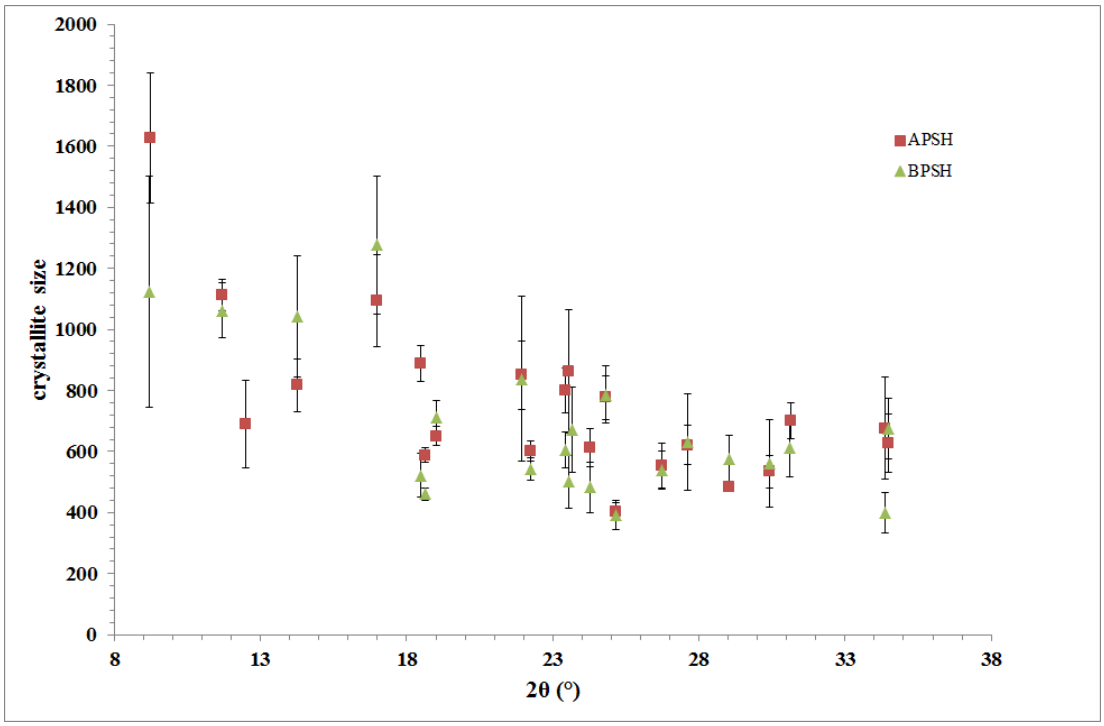

Figure 6.3g: Comparison of crystallite sizes for samples produced from fast and slow addition methods A and B and their effect on calcite crystallite size at GLU concentration of 10 mg/L. Most results are the same within 2 esd and show little difference across the angular range.

Figure 6.3g shows the opposing information present when the samples are grown in the presence of low concentrations of AA. For some lattice directions it seems that slow addition produces smaller crystallites, for others it seems that fast addition leads to smaller crystallites. Overall the values are statistically indistinguishable and the trends observed are therefore questionable. The sizes are also comparable with sizes determined for samples grown in the presence of 10 mg/L ASP, again supporting the idea that at these low concentrations the AA has only a limited influence over the growth of calcite.

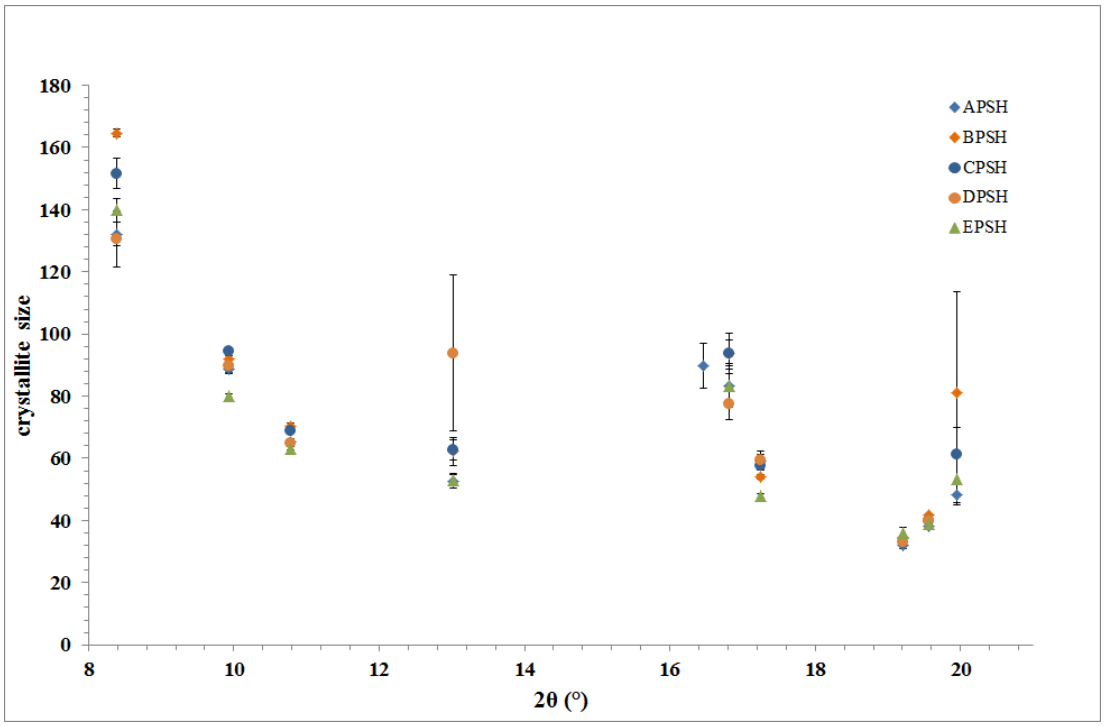

Figure 6.3h: Comparison of crystallite sizes for samples produced by methods A to E in the presence of 10 mg/L GLU and their effect on vaterite crystallite sizes. Only the hourly samples showed peaks that could be used.

Figure 6.3h is particularly interesting because it shows that the vaterite crystallite size is smaller for samples grown by slow addition method E compared to C, and for some data points the same distinctly holds true for slow addition method B when compared to method A.

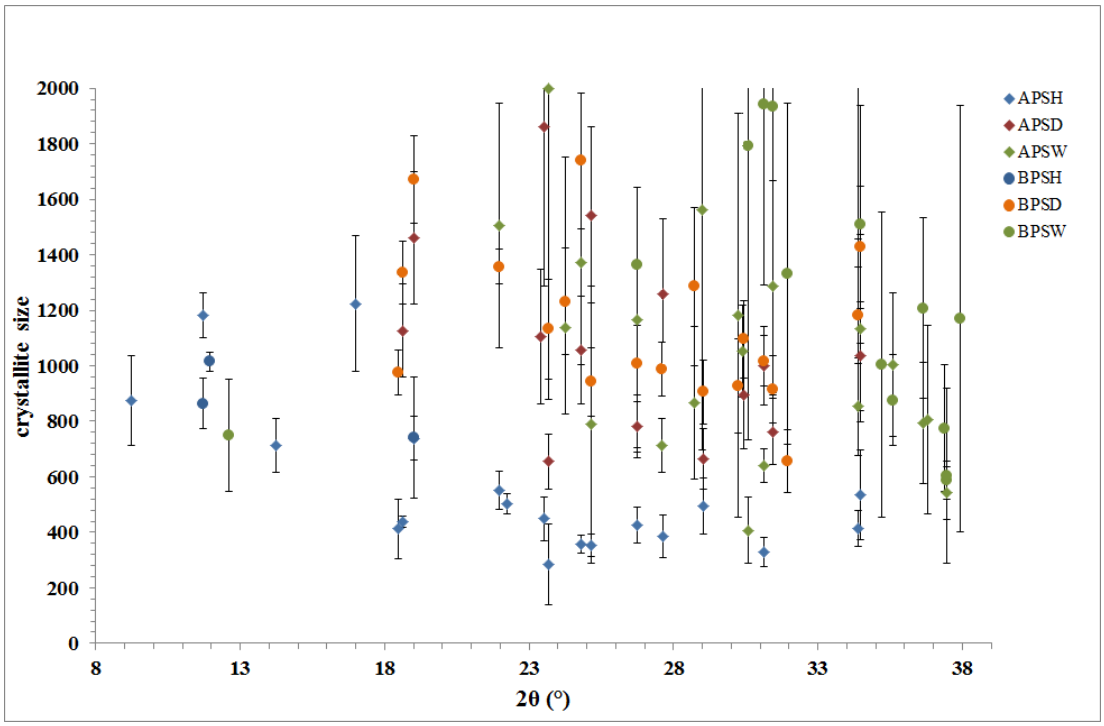

Figure 6.3i: Comparison of calcite crystallite sizes from samples produced by slow and fast addition methods A and B in the presence of 100 mg/L GLU and the changes in calcite crystallite size at harvesting times of 1 hour, 1 day and 1 week.

The errors shown are relatively large in figure 6.3i, and any trends observed are limited to statistically meaningful values reported. Similarly to the samples grown in the presence of 100 mg/L ASP, the crystallite size increases over time, but the increase is larger as are the starting values. This can be observed for the calcite (210) peak at 26.72º 2θ. For specific lattice orientations a reversing trend can be observed, particularly for the calcite (128) and (134) peak, where the crystallite size increases nearly threefold from harvesting times of 1 hour to 1 day, but then decreases from 1 day to 1 week. Vaterite has structural features that are very close to these d-spacing and the change is likely related to vaterite recrystallization and transformation.

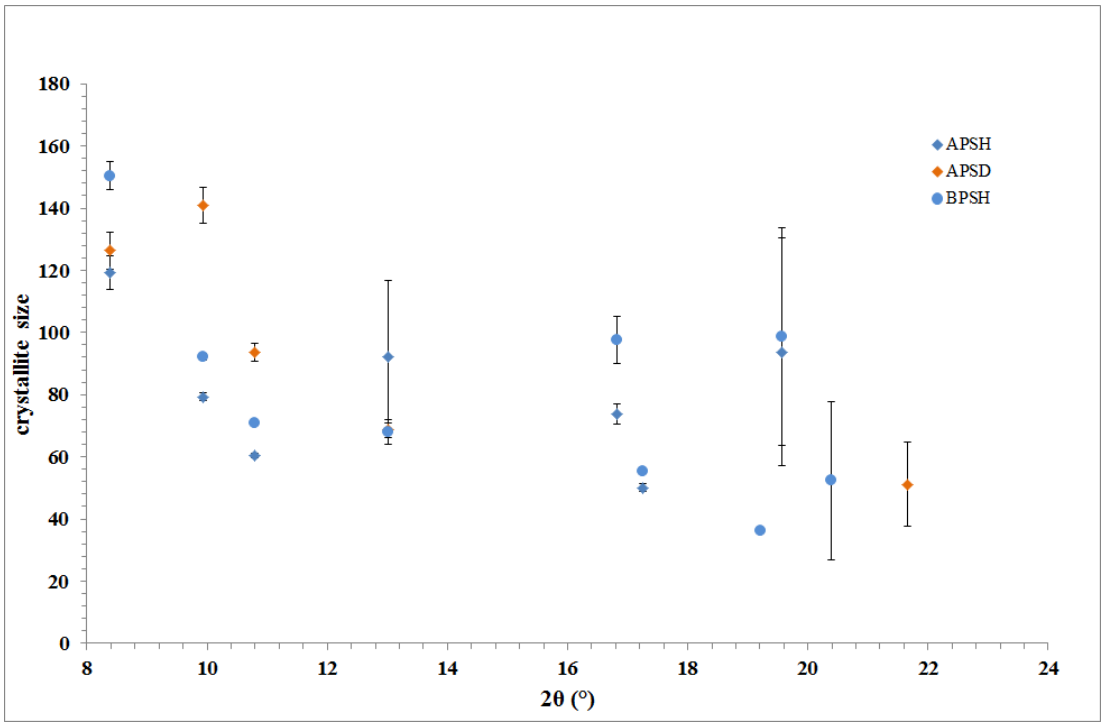

Figure 6.3j: Comparison of crystallite sizes from samples produced by methods A and B in the presence of 100 mg/L GLU, illustrating the effect of addition speed and harvesting time on vaterite crystallite size. No statistically meaningful data were obtained from the sample produced by slow addition and harvested after 1 day.

Figure 6.3j shows crystallite sizes for vaterite; for the slow addition method, when harvested after the same time, they are slightly larger, with little variation across the range. The comparison of the fast addition method as a function of time reveals that the crystallite size increases from 1 hour to 1 day.

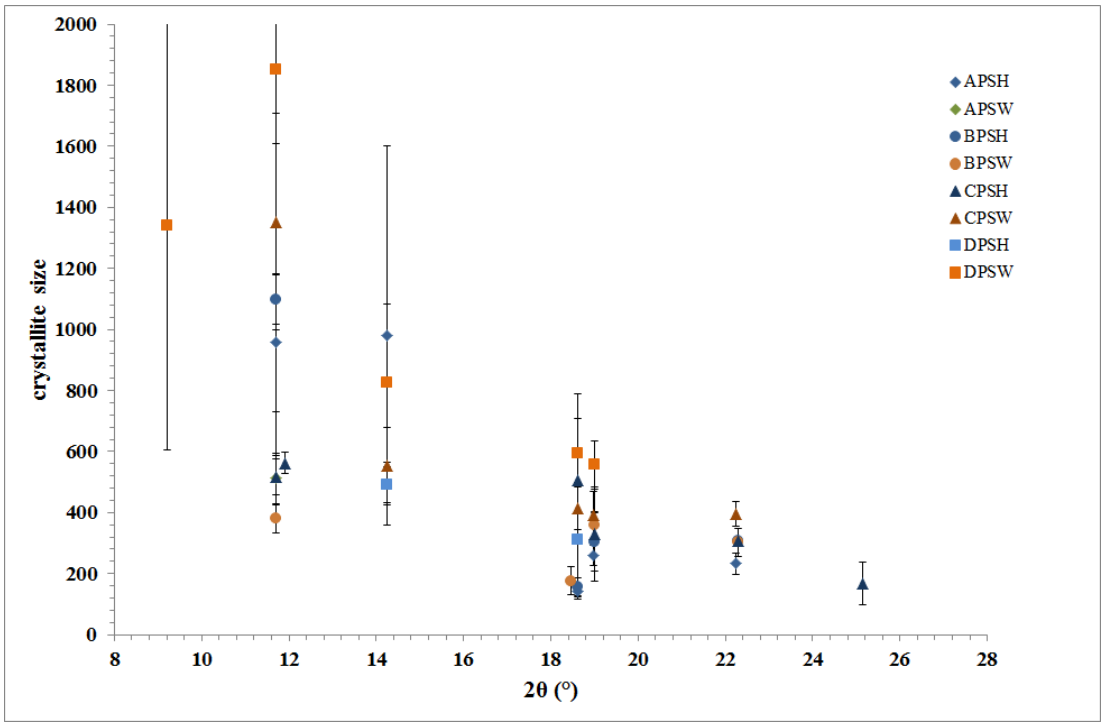

Figure 6.3k: Comparison of calcite crystallite sizes from samples produced by slow and fast addition methods A, B, C and D, grown in the presence of 1000 mg/L GLU and harvested after 1 hour and 1 week.

Figure 6.3k shows all methods for which hourly and weekly data points were available. Changes with harvesting time and with method are within statistical error of the method used. Limiting the uncertainty to one esd as a matter of evaluating trends shows that the size of the crystallites increases with harvesting time, except for method B where the size derived from the calcite (104) peak at 11.7° 2θ is smaller for the sample harvested after 1 week than for the sample harvested after 1 day. The relatively large uncertainty in the values determined for these samples is due to the small amount of calcite present in the samples, resulting in very small and poorly defined peaks with large uncertainties during peak fitting and parameter extraction.

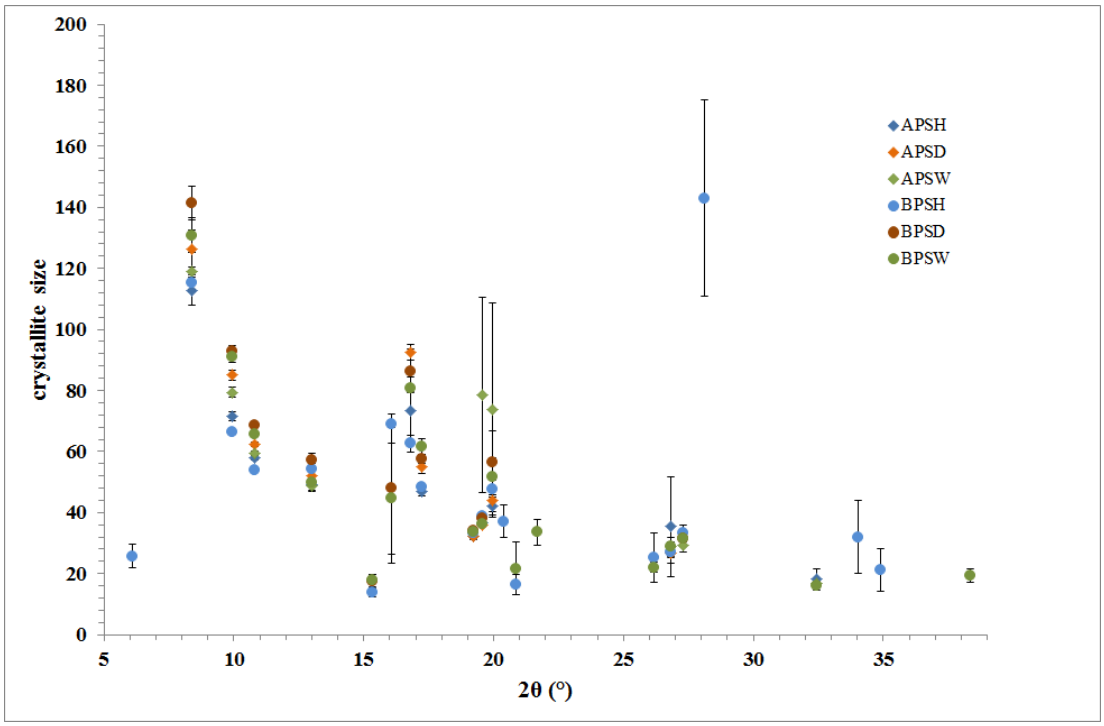

Figure 6.3l: Comparison of crystallite sizes from samples produced by methods A and B in the presence of 1000 mg/L GLU, illustrating the effect of addition speed and harvesting time on vaterite crystallite size. Harvesting times of 1 hour, 1 day and 1 week are presented. The graph shows a crystallite size increase with time, but also some dependence of crystallite size on crystallographic direction.

Figure 6.3l, particularly for the slow addition method B, shows that, depending on the reflection in question, the crystallite size does not change with harvesting time for peaks at 19.2º 2θ and 19.5º 2θ and possibly even decreases, but this is within the statistical uncertainty.

Micro-strain

The micro-strain charts are reported using the same representative approach as the size charts for comparison of the changes in the samples.

The micro-strain charts show that the micro-strain for calcite is significantly lower than that for vaterite, the inverse of the crystallite sizes where calcite crystallite size is larger.

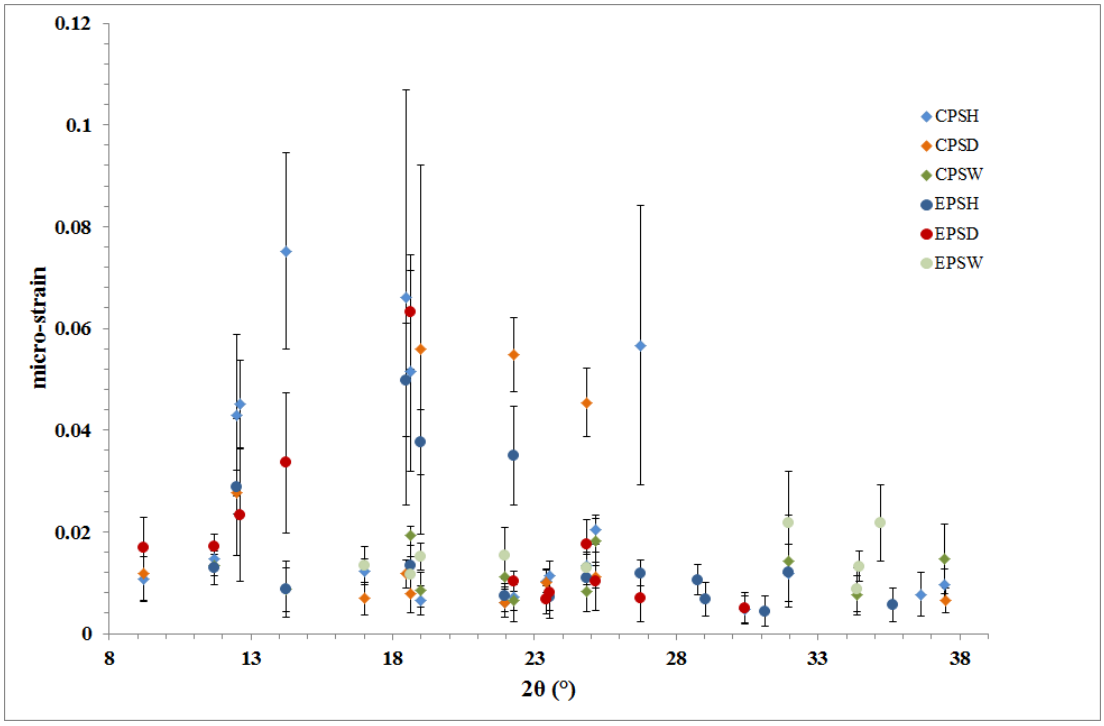

Figure 6.4a: Comparison of micro-strain from samples produced using slow and fast addition methods C and E in the presence of 10 mg/L ASP, demonstrating the effect of harvesting times of 1 hour, 1 day and 1 week on the micro-strain.

Figure 6.4a shows a mixed result for calcite micro-strain in samples grown in the presence of 10 mg/L ASP. In general, the micro-strain present in calcite diminishes with time, consistent with re-crystallisation of the most strained portions of crystallites and/or the crystallisation of substantial amounts of calcite with less strain. There is little difference in micro-strain of calcite produced by the slow and fast addition methods.

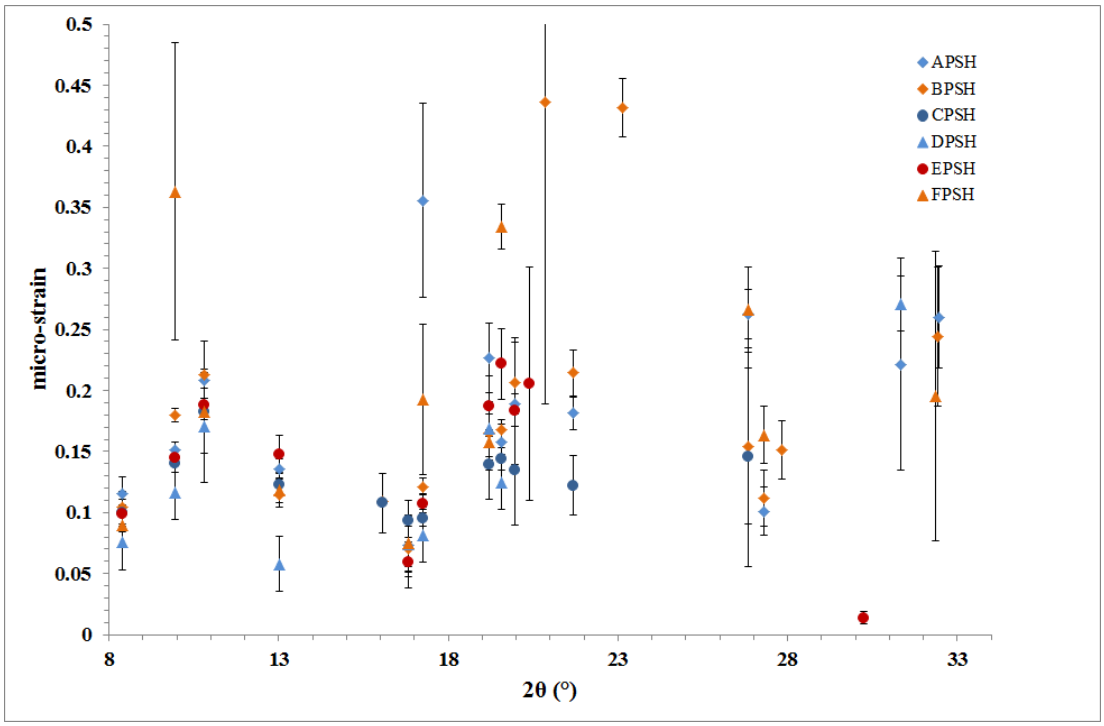

Figure 6.4b: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods in the presence of 10 mg/L ASP. Data for all methods are presented.

As with the crystallite size, only samples harvested after one hour contained enough vaterite for micro-strain determination at these low concentrations of AA. Figure 6.4b shows that the strain determined for vaterite is substantially higher than that determined for calcite and that the results are not uniform. Between methods A and B (slow and fast addition), the micro-strain is higher in the method using slow addition, while between methods C and E (slow and fast addition) the micro-strain is lower in the sample with slow addition, and for the last pairing, method D and F a mixed result is obtained. The overall uncertainty is higher for the micro-strain compared to the crystallite size determinations, when the determinations for corundum are taken as an indication, as described in the lead-in to the graphs of this section. Despite this, the results strongly indicate that for vaterite the preparation method is of importance.

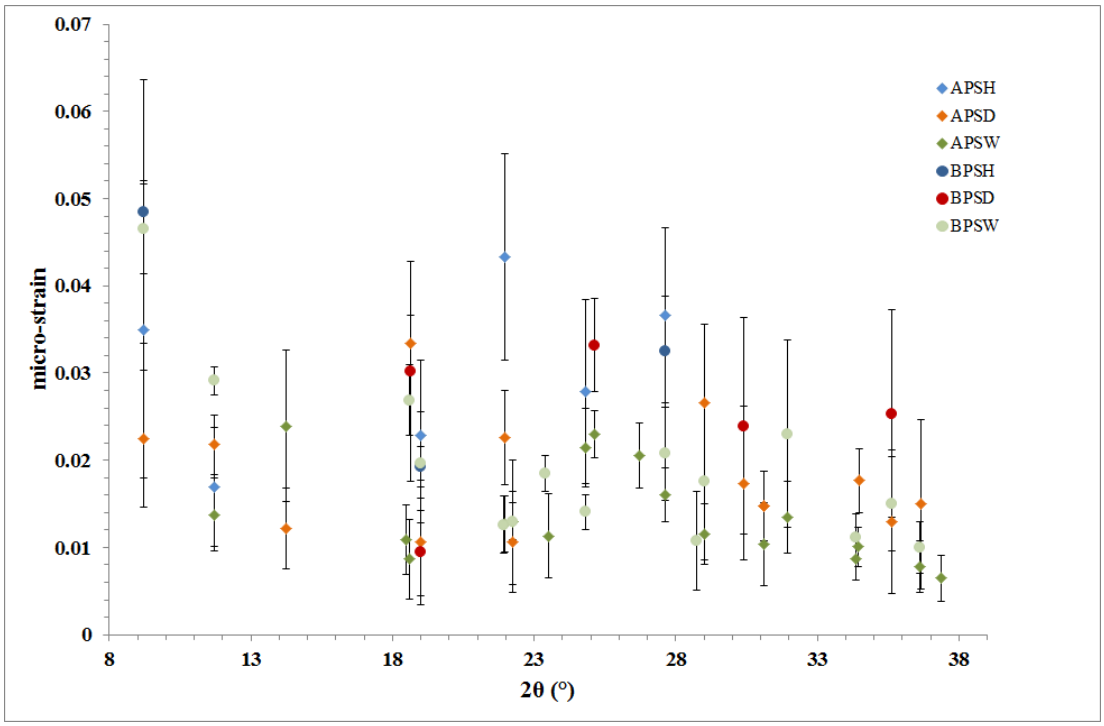

Figure 6.4c: Comparison of calcite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 100 mg/L ASP. Presented are data for harvesting times of 1 hour, 1 day and 1 week.

Similarly to the crystallite size results for samples grown in the presence of 100 mg/L ASP: the micro-strain results for fast addition method A generally show the inversed trend compared to crystallite size results, with strain decreasing over time, except for a data point at about 14.25º 2θ, the (110) peak of calcite, where it clearly increases between harvesting times of one day and one week (figure 6.4c).

The slow addition method B shows a similar behaviour, with only a single data point at 18.99º 2θ, the (116) peak of calcite, showing a decrease in strain from one hour to one day, and a subsequent increase between one day and one week.

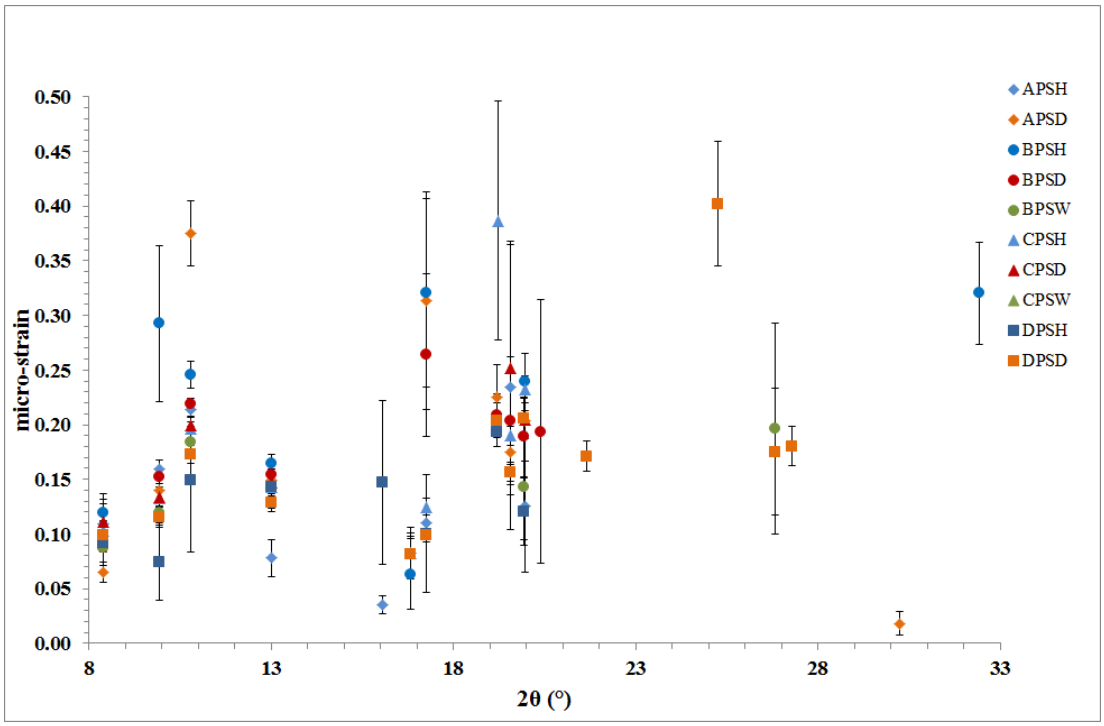

Figure 6.4d: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 100 mg/L ASP, all valid data are included, encompassing samples harvested after 1 hour, 1 day and 1 week.

Figure 6.4d of the vaterite micro-strain for samples grown in the presence of 100 mg/L ASP has been truncated at a micro-strain value of 0.5. Some values were significantly higher than those shown in figure 6.4d. Noteworthy in the micro-strain graph is that the majority of micro-strain values for most methods and harvesting times are within a certain range with only a few outliers and for one peak at 17.25º 2θ a separation into two groups. There are no clear relationships present between methods and harvesting times for the micro-strain. Given time, the micro-strain should decrease as crystals recrystallise and lower their defect density. For method D this is not the case for more than one point, with the micro-strain value actually increasing between samples harvested after 1 hour and 1 day. For method B (slow addition) the situation is different; all micro-strain values decrease with time.

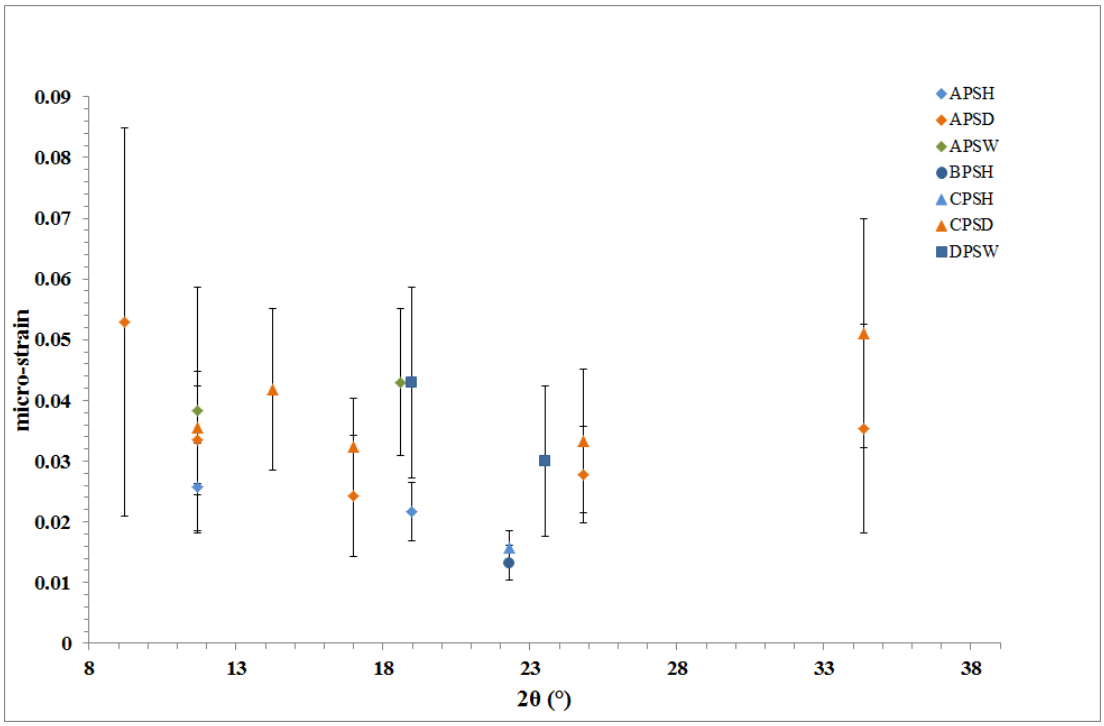

Figure 6.4e: Comparison of calcite micro-strain from samples produced using slow and fast addition methods in the presence of 1000 mg/L ASP. All statistically valid data were used, including methods and harvesting times for A (1 hour, 1 day, 1 week), B (1 hour), C (1 hour and 1 day) and D (1 week).

Only a few data points for calcite were available, and all of them have been used in figure 6.4e. The micro-strain is relatively low, and no discernible trend could be established. All values fall within the same range of statistical uncertainty, demonstrating that for 1000 mg/L ASP the calcite micro-strain is undistinguishable between methods and harvesting times.

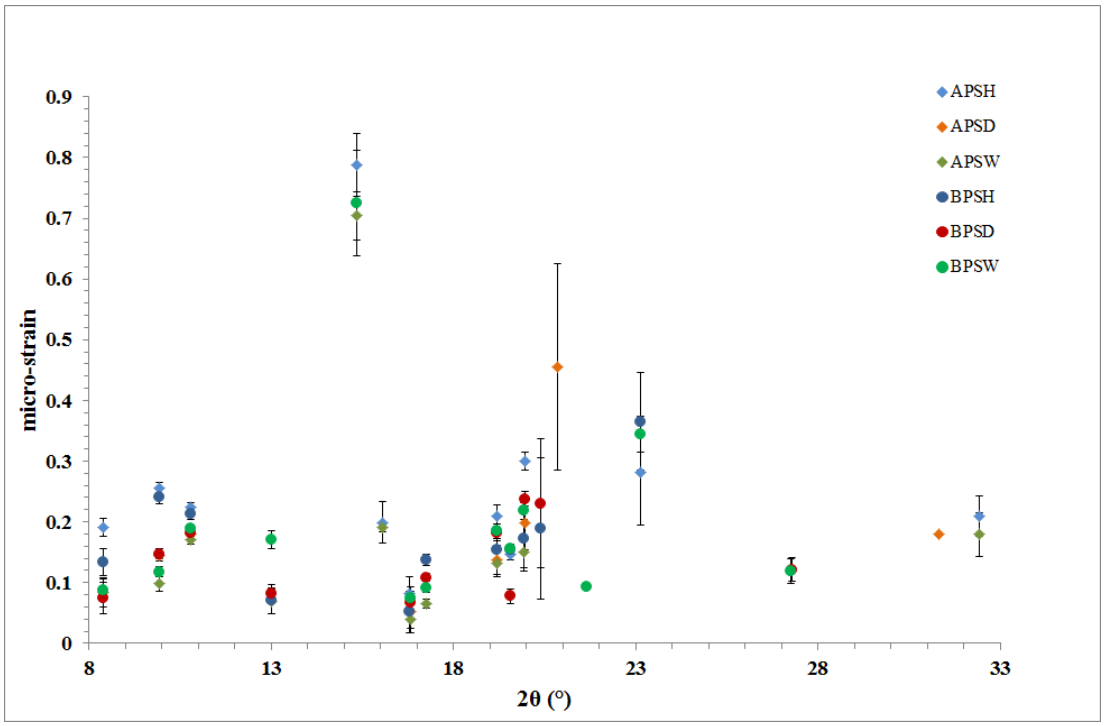

Figure 6.4f: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 1000 mg/L ASP by slow and fast addition methods A and B, with harvesting times of 1 hour, 1 day and 1 week.

Figure 6.4f shows that there is little difference in the strain values themselves between the two methods. The micro-strain generally decreases over time, but there are some crystallographic planes for which the micro-strain value increases over time, particularly for the samples grown by slow addition (method B). Slow addition would have allowed the AA present to exert a greater influence on the initial nucleation and growth process, making it more likely that a greater number of crystallites are directly influenced and that there are less crystallites present. During subsequent growth this would result in a larger overall micro-strain, particularly on growth planes directly affected by the AA.

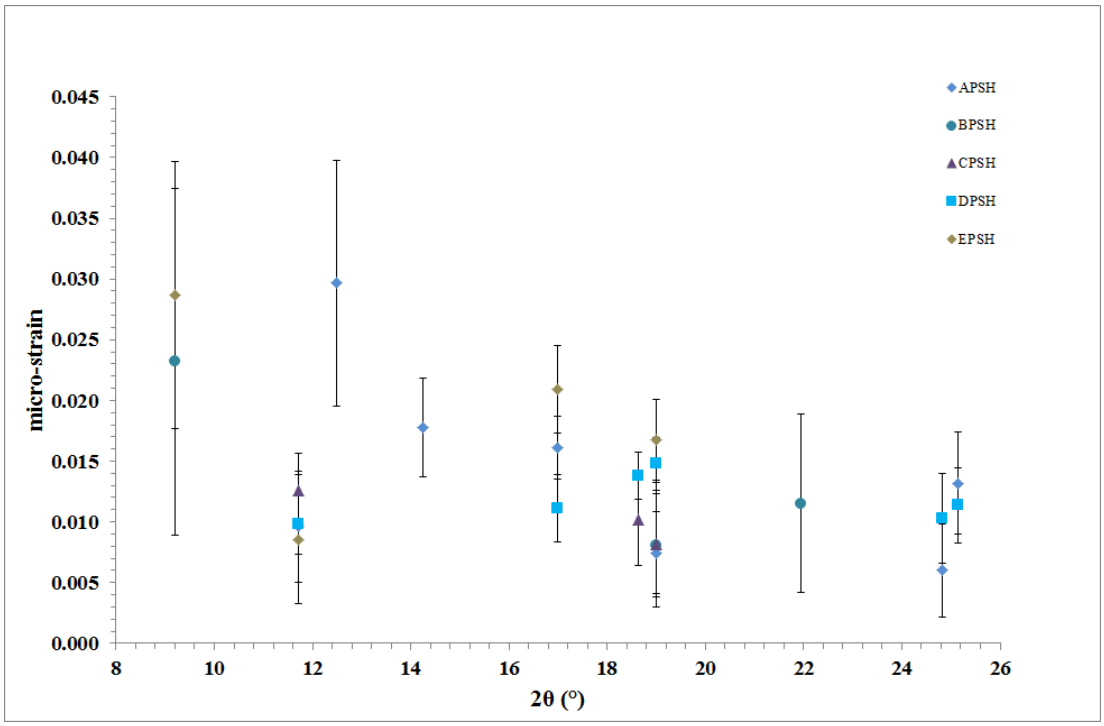

Figure 6.4g: Comparison of calcite micro-strain from samples produced using slow and fast addition methods in the presence of 10 mg/L GLU and harvested after 1 hour. Methods A to E are presented.

As can be seen in figure 6.4g there is very little difference in the calcite micro-strain values for the different methods, not even between slow and fast addition, suggesting that this AA at this concentration does not have a large impact on the growth of calcite.

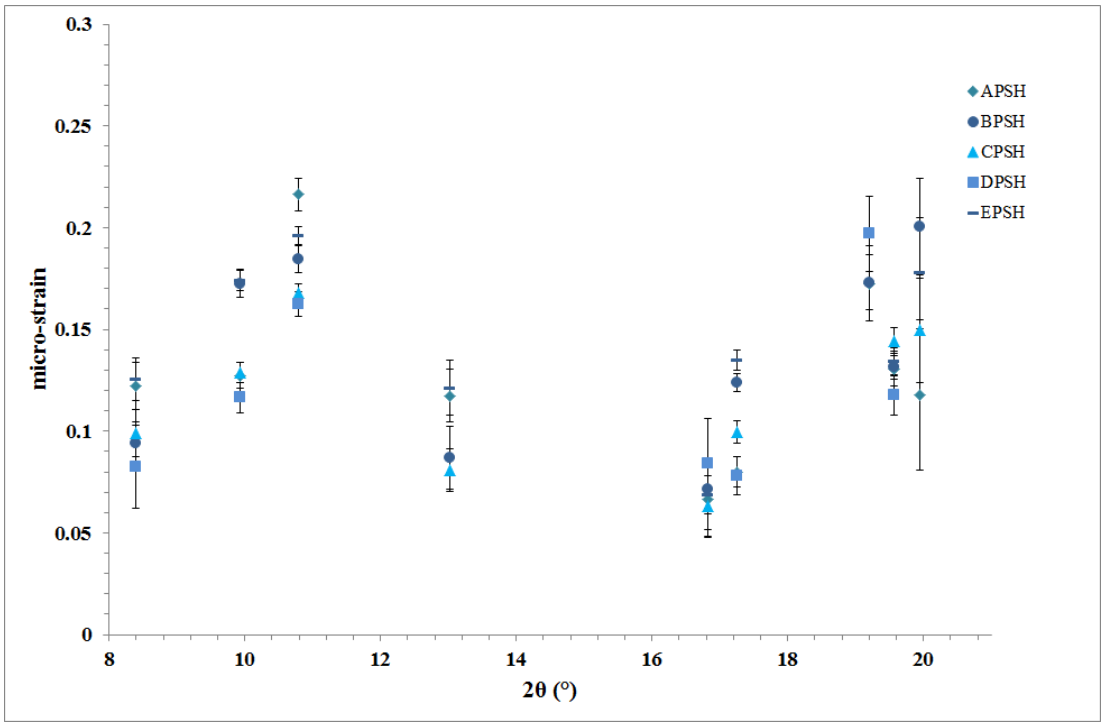

Figure 6.4h: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 10 mg/L GLU, harvested after 1 hour. Data for methods A to E are presented.

As for the calcite, there is very little difference between the different methods in terms of micro-strain (figure 6.4h). The micro-strain of the vaterite is nonetheless substantially higher than that of calcite, indicating that the AA has a greater influence on vaterite crystallisation than it has on calcite crystallisation.

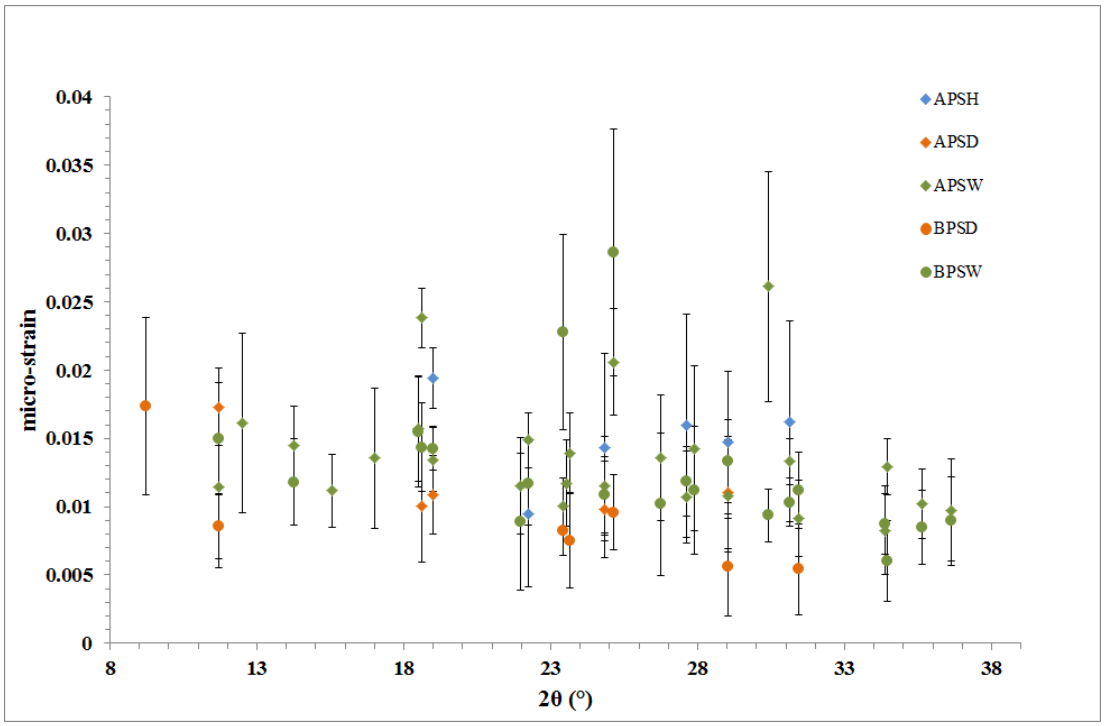

Figure 6.4i: Comparison of calcite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 100 mg/L GLU, with harvesting times of 1 hour, 1 day and 1 week. Data for method B, harvesting time of 1 hour, were not statistically valid.

Figure 6.4i shows the changes in calcite micro-strain and contains some indications that, when seen in the context of what happens in the sample, make sense. For the fast addition method A the situation is split. For most crystallographic orientations the micro-strain decreases between samples harvested after 1 hour and 1 day, but then increases for samples harvested after one week. For slow addition method B we do not have any relevant data for the samples harvested after 1 hour, and as such are only observing the changes between samples harvested after 1 day and 1 week, and for these the situation is clear. The micro-strain increases when moving from one day to one week. An explanation for this maybe that almost all remaining vaterite is transformed during this period, most likely resulting in calcite with a slightly increased micro-strain.

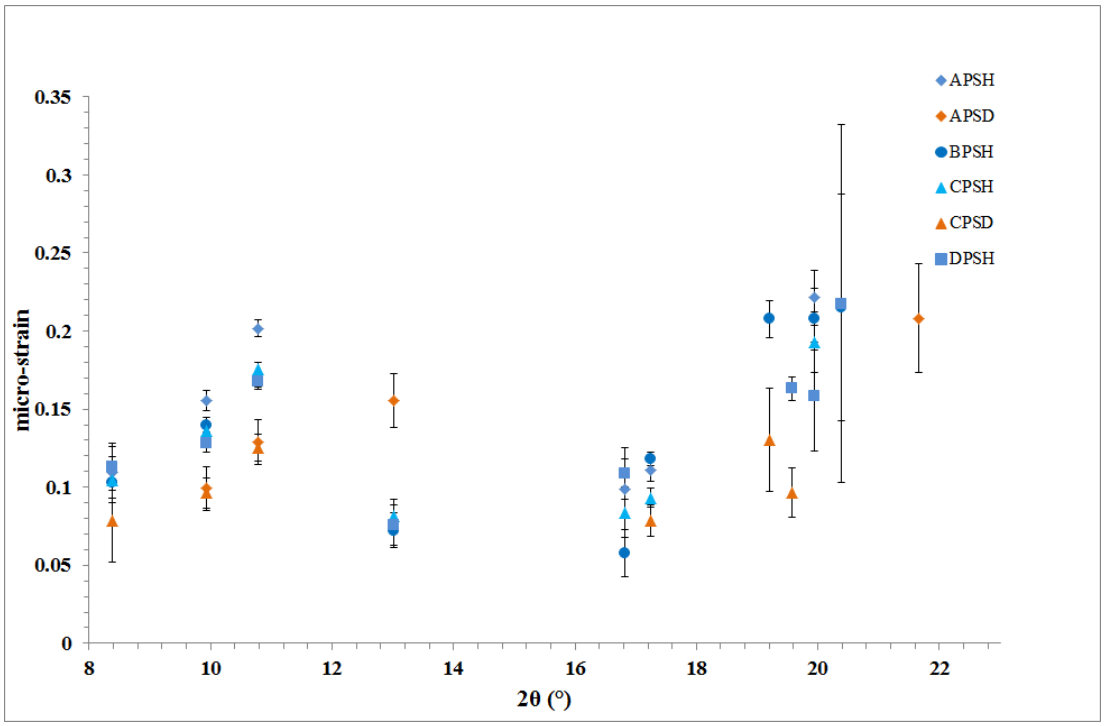

Figure 6.4j: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 100 mg/L GLU. All statistically valid data points were used, comprising methods A (1 hour and 1 day), B (1 hour), C (1 hour and 1 day) and D (1 hour).

Figure 6.4j shows the micro-strain present in vaterite samples grown in the presence of 100 mg/L GLU. There is a strong dependence of the micro-strain with crystallographic orientation. The micro-strain values are, on average, slightly higher than the ones calculated for the same orientations in the samples grown in the presence of 10 mg/L GLU. Both are lower than their respective counterparts from the series grown in the presence of ASP, indicating that GLU does not have as strong an influence on the growth of the Ca-carbonate as ASP. When comparing data for samples harvested after 1 hour, 1 day, and even 1 week, the micro-strain decreases with time, suggesting that either re-crystallisation occurs, eliminating defects, or, more likely, that the crystallites with the highest micro-strain are effectively transformed into calcite.

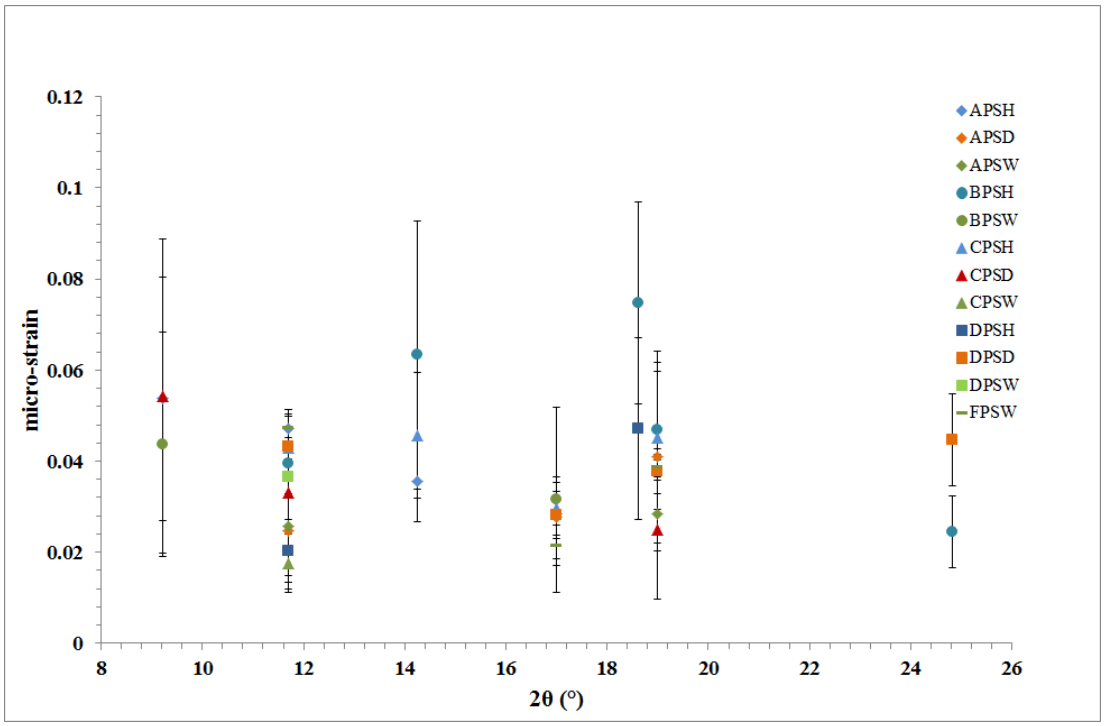

Figure 6.4k: Comparison of calcite micro-strain from samples produced using slow and fast addition methods in the presence of 1000 mg/L GLU. All statistically valid data points were used, and data for harvesting times of 1 hour, 1 day and 1 week are presented for methods A, C and D. For method B only the samples with harvesting times of 1 hour and 1 week had statistically valid data and for method F only the sample with harvesting time of 1 week.

As with previous results for calcite grown in the presence of 1000 mg/L of AA, in the case of GLU vaterite was the major product at high concentrations. From figure 6.4k it is apparent that the micro-strain is relatively low, indicating that any calcite formed is mostly free of defects and/or that any calcite with a higher micro-strain has been dissolved and re-crystallised as either calcite, or, more likely in most cases, as vaterite. The few orientations for which data exist for the same method and more than one harvesting time indicate that the micro-strain is decreasing over time.

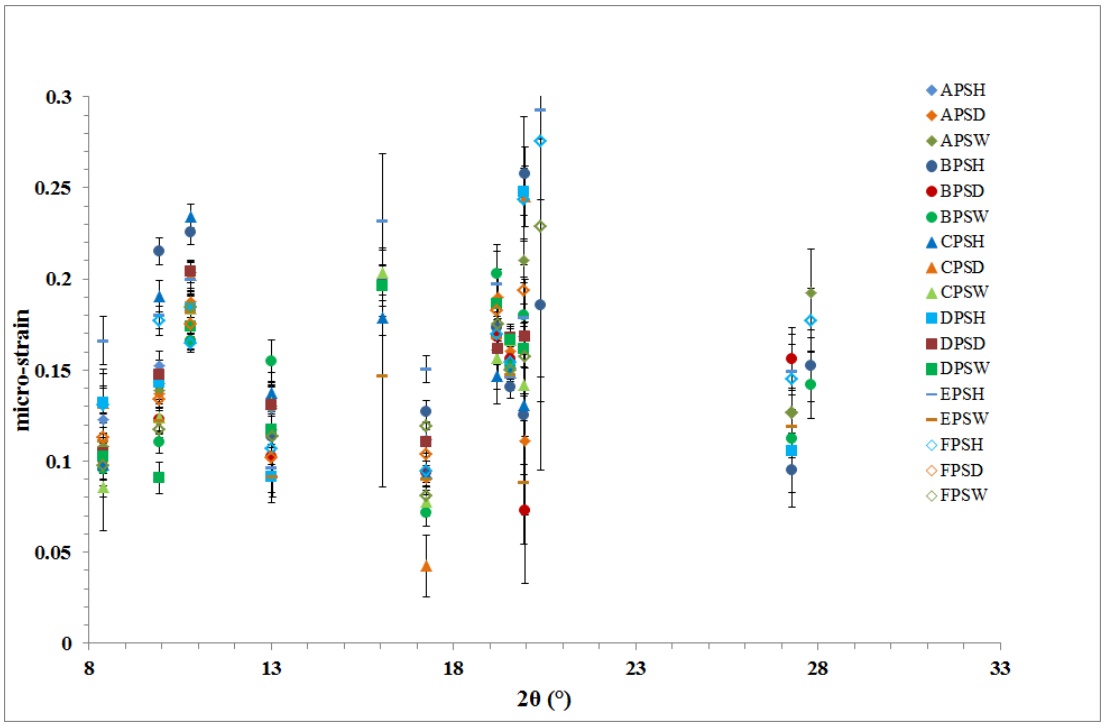

Figure 6.4l: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods in the presence of 1000 mg/L GLU. With the exception of one sample for method E, the one harvested after 1 day, all methods and harvesting times are presented. The plot shows the strong orientation dependence of the micro-strain.

Figure 6.4l shows that there is little difference in the strain values themselves between the methods, but there is some difference between crystallographic orientations. This is particularly noticeable for the two peaks at 10.78º 2θ (112 peak) and 13.02º 2θ (114 peak), with the former showing statistically significant greater micro-strain.

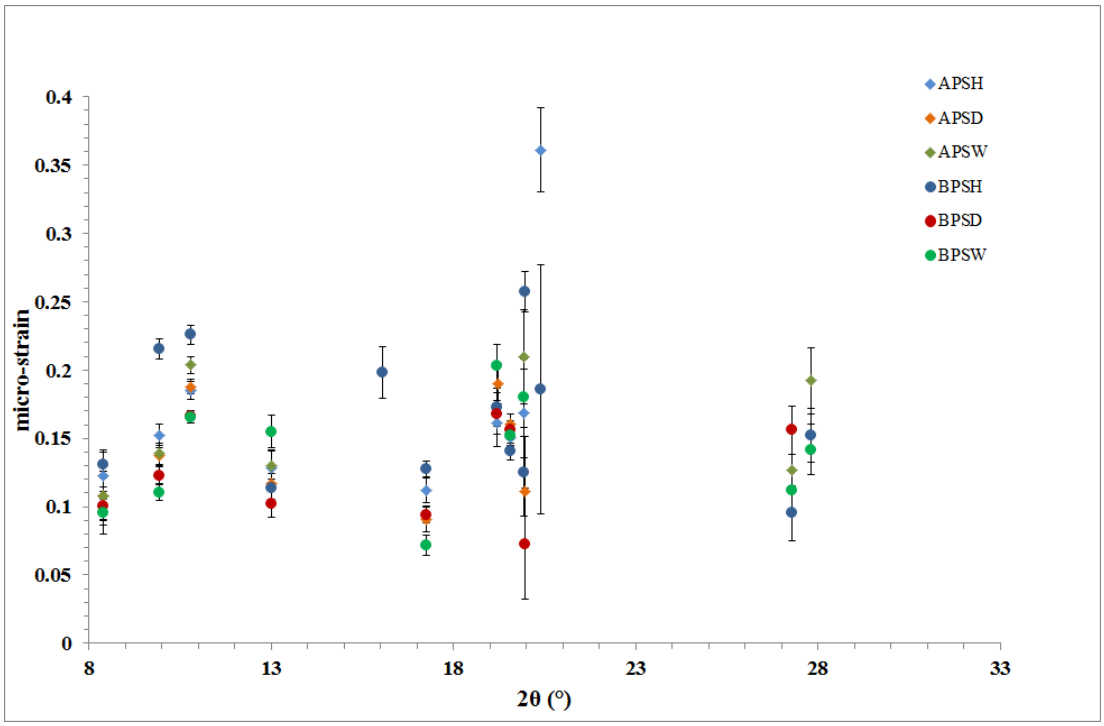

Figure 6.4m: Comparison of vaterite micro-strain from samples produced using slow and fast addition methods A and B in the presence of 1000 mg/L GLU. Data for harvesting times of 1 hour, 1 day and 1 week are reported.

The data for method B show some variation, of the micro-strain with crystallographic orientation. For the peak at 13.02º 2θ, which corresponds to (111) in hexagonal setting and (112) in orthorhombic setting, it increases from 1 hour to 1 week, while for the peak at 10.78º 2θ, which corresponds to (112) in hexagonal setting and (114) in orthorhombic setting, it decreases from 1 hour to 1 week. This indicates that the process of crystallisation at this high concentration of GLU shows some crystallographic dependence.

6.2 Transmission experiments

Two different transmission experiments were carried out. The first was a SXRPD experiment in which all available samples were analysed with an internal standard to enable quantification of the mineral phases present, particularly for samples containing calcite and vaterite.

The second was an in-situ SXRPD experiment where samples were heated to induce vaterite-calcite transformation. A few samples grown in the presence of 1000 mg/L of GLU or ASP were selected for this experiment.

6.2.1 SXRPD transmission experiment

The main problem with the data was that the original purpose, to quantify the amount of vaterite and calcite present in the samples was not achievable, due to the fact that the vaterite structure could not be solved (see section 6.2.3 for further details). The graphs produced from data extracted during the experiment were so similar to the ones derived from the SXRPD experiments that no further work was done on them.

6.2.2 In-situ heating experiments

The heating experiment was performed using a heating coil under a sample contained in a kapton capillary and with a thermocouple inside the sample measuring the temperature. Some attempts were made before it was discovered that the thermocouple was faulty, after which the first experiments had to be discarded. Once the thermocouple had been exchanged, there was still sufficient time to record a number of patterns. These were also recorded using the MAR3450 CCD detector and extracted in the same way as the data from the SXRPD transmission experiment, using the same wavelength used for the transmission experiments of 0.155 Å. Subsequently some x-y-z contour plots were created using SigmaPlot (Various, 2001), producing a projected plot of stacked patterns recorded at increasing temperatures over °2θ with the intensities along 2θ represented as coloured contours. Only a number of colours are available to represent the different intensities at the various points and the intensities have therefore been truncated at higher intensities to differentiate the smaller peaks and variations. There is little difference between the two different AAs and between the different methods, but there are some indications that the temperature of transformation is slightly different. The samples that were grown in the presence of 100 mg/L ASP were the last samples to run, after the thermocouple had been exchanged and calibrated and have therefore most likely the most accurate temperature values recorded. Of the samples grown in the presence of 1000 mg/L ASP only the sample grown using method F was part of that run, as it

was repeated with a new aliquot of sample due to the difficulties with the thermocouple. Taking the two different concentrations and using the sample produced by method F in the presence of 1000 mg/L ASP as indicative of the correct transformation temperature for samples produced in the presence of 1000 mg/L it appears that lower AA concentrations result in lower transformation temperatures. When comparing the sample produced by method F at a concentration of 1000 mg/L to samples produced in the presence of GLU at a concentration of 1000 mg/L it appears to the transformation temperature for the sample produced in the presence of 1000 mg/L ASP transforms at a higher temperature than the sample produced in the presence of 1000 mg/L GLU. Further experiments are needed to confirm this. The plots for samples grown in the presence of 1000 mg/L ASP using method A, B and C should be taken as indicative of how the transformation occurs and not precisely at what temperature. What can also be seen in the plots is the fact that the phase transition might be a combination of first and second order, with the majority of peaks showing a well defined change or 'jump' in the peak position when reaching a certain temperature, which would indicate a first order phase transition, while the vaterite peak at 2.63 Å (300) at around 4.28° 2θ in the plots is shifting gradually with temperature. It cannot be established by the measurements if the transition is continuous or if there is still a clear jump in the peak position. The experiment setup using the MAR3450 CCD detector meant that patterns could only be recorded at intervals, with readout of the detector taking slightly more than 2 minutes.

The plots on the following pages are two dimensional projections of three dimensional data. The legend in each one the plots indicates the colour corrsponding to a certain number of counts in the traces. A low and high intensity cut-off was used to allow for a better definition of the peaks in the plots. The values were chosen so that all measurable peaks are visible in the pattern plots. Where the plots show undefined colours, particularly white, which are not represented in the colour legend, these represent intensity values outside the plot scale.

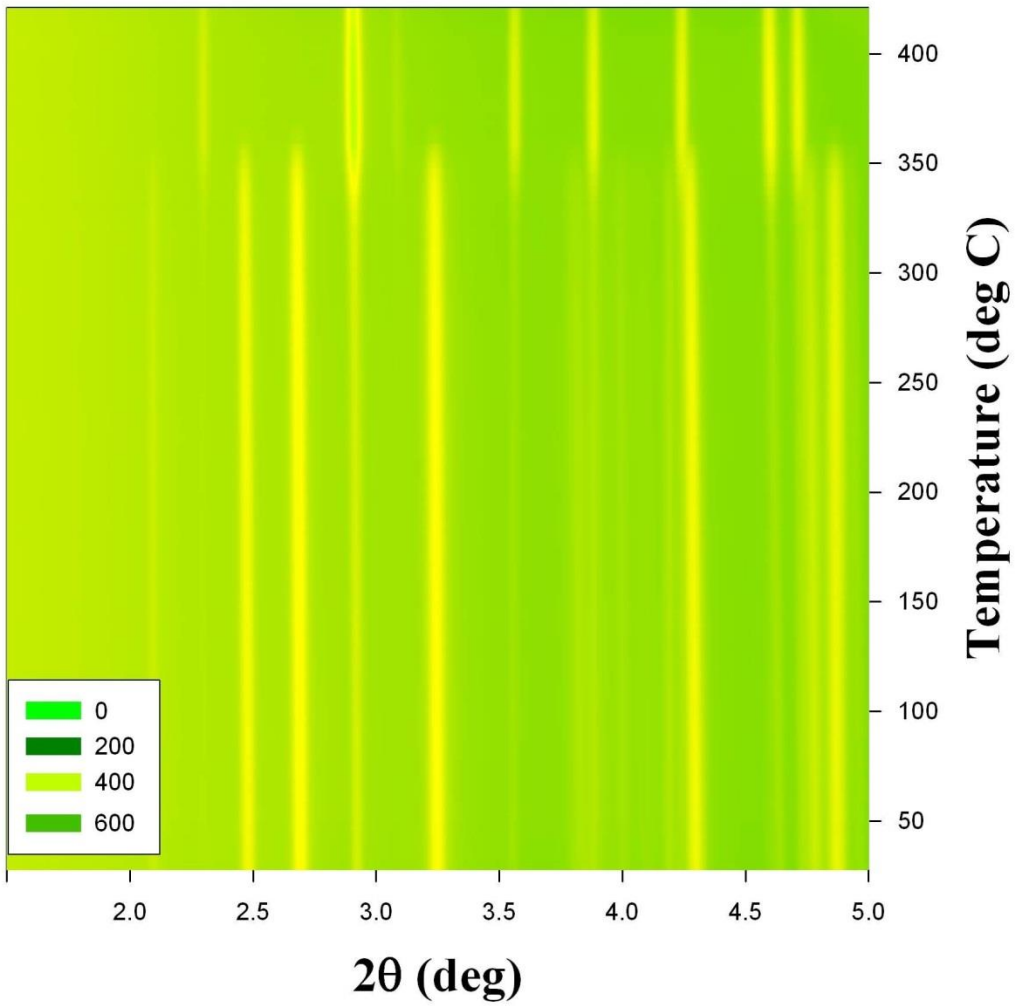

Figure 6.5a: Temperature dependent in-situ data for a sample grown in the presence of 100 mg/L ASP, using the fast addition method A, harvested after 1 hour. Vaterite to calcite transformation occurs around 350 °C.

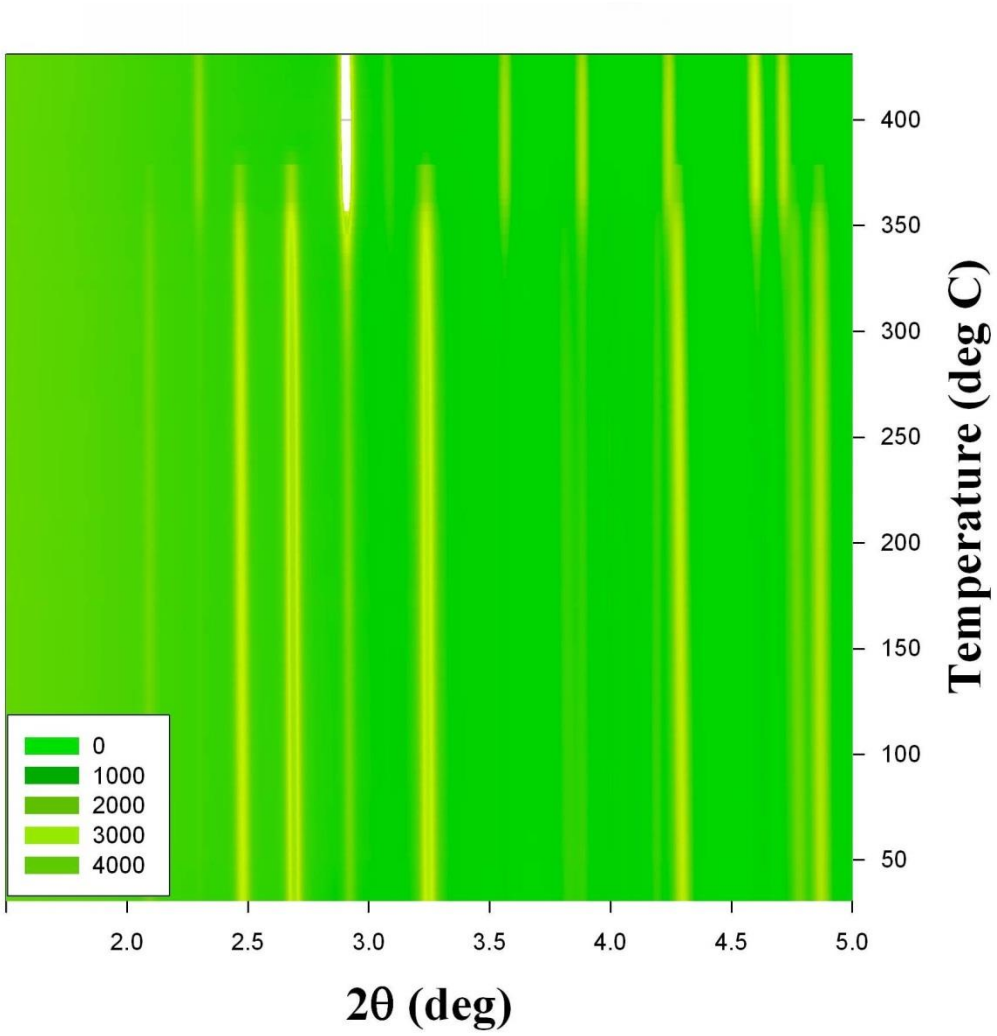

Figure 6.5b: Temperature dependent in-situ data for a sample grown in the presence of 100 mg/L ASP, using the slow addition method B, harvested after 1 hour. Vaterite to calcite transformation occurs around 350 °C.

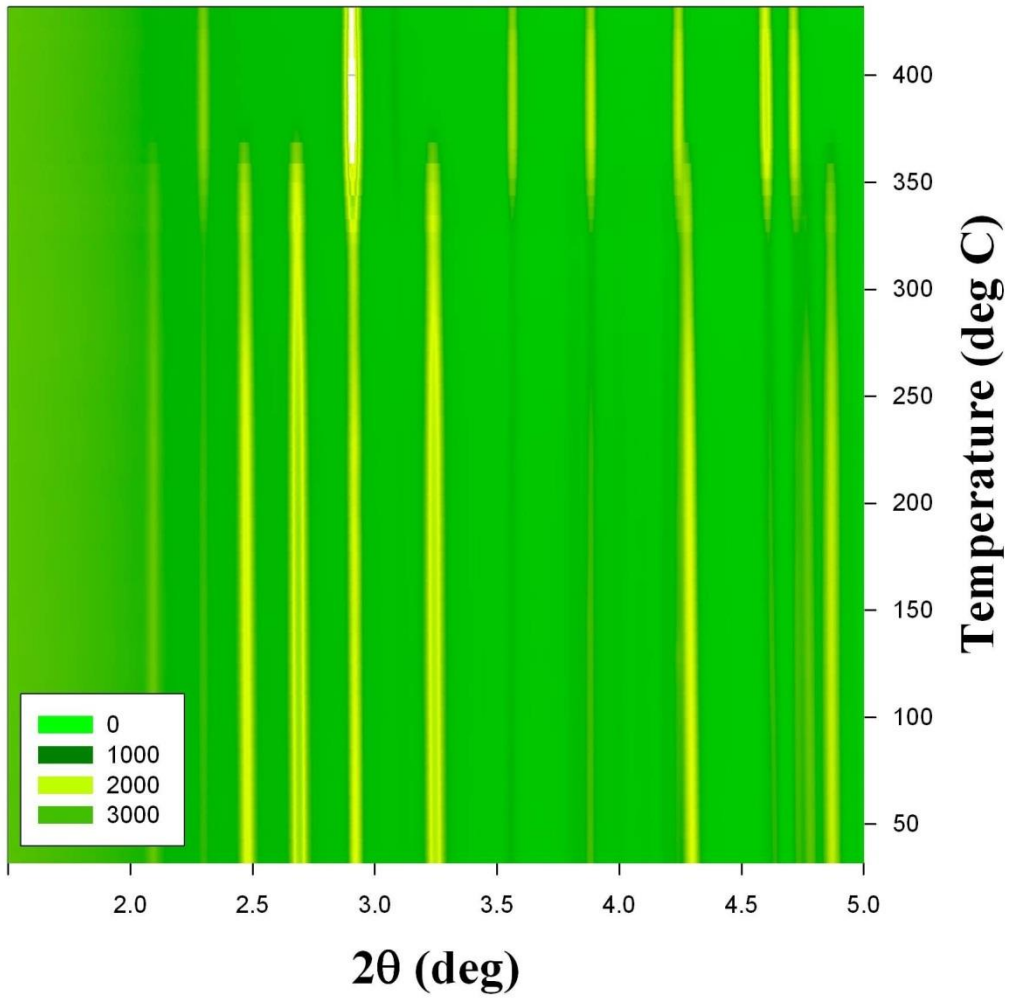

Figure 6.5c: Temperature dependent in-situ data for a sample grown in the presence of 100 mg/L ASP, using the fast addition method D, harvested after 1 hour. Vaterite to calcite transformation occurs around 350 °C.

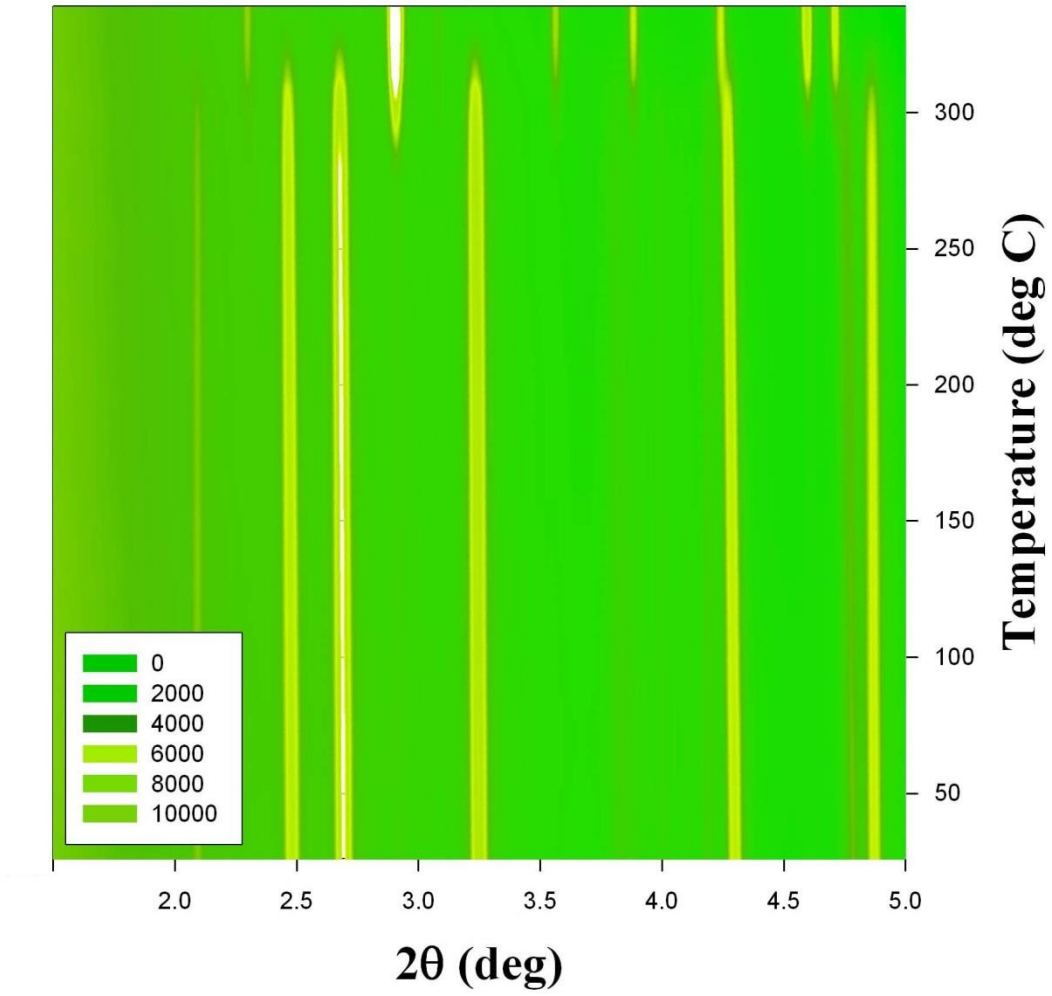

Figure 6.5d: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L ASP, using the fast addition method A, harvested after 1 hour. Vaterite to calcite transformation occurs around 300 °C.

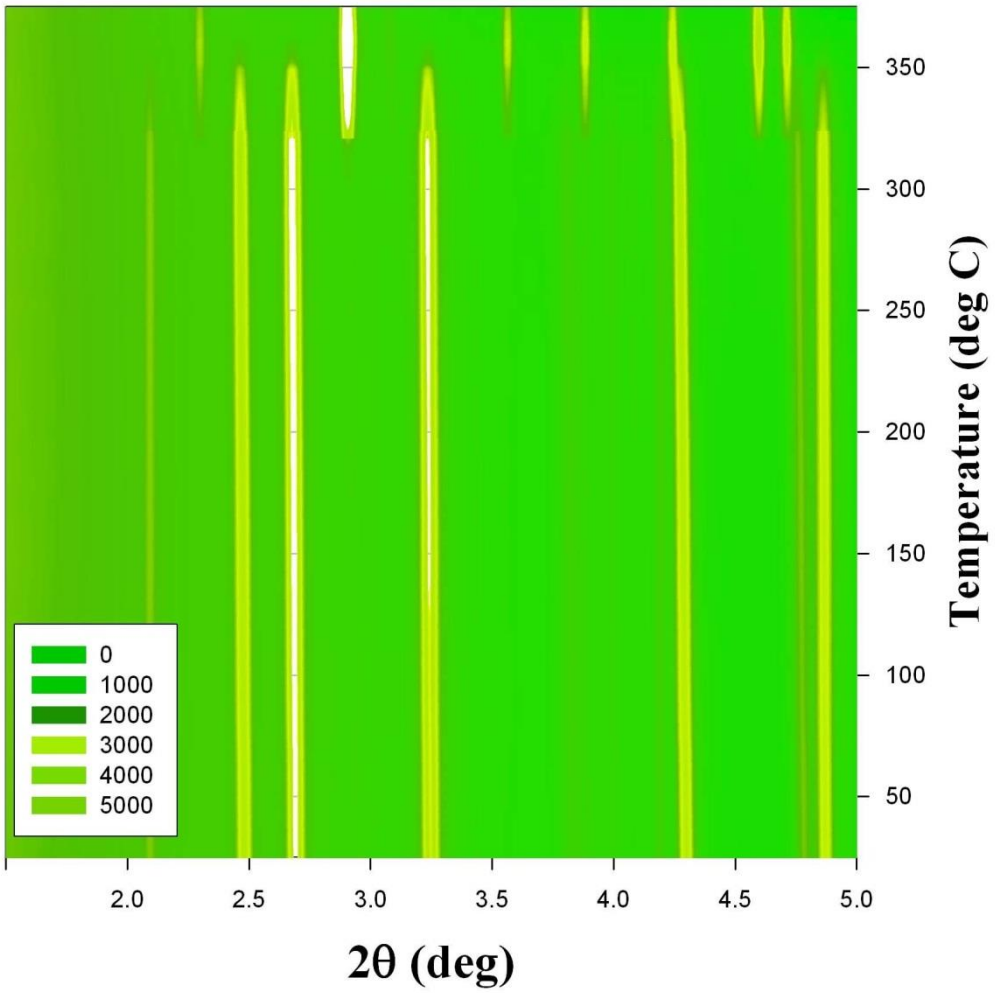

Figure 6.5e: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L ASP, using the slow addition method B, harvested after 1 hour. Vaterite to calcite transformation occurs around 300 °C.

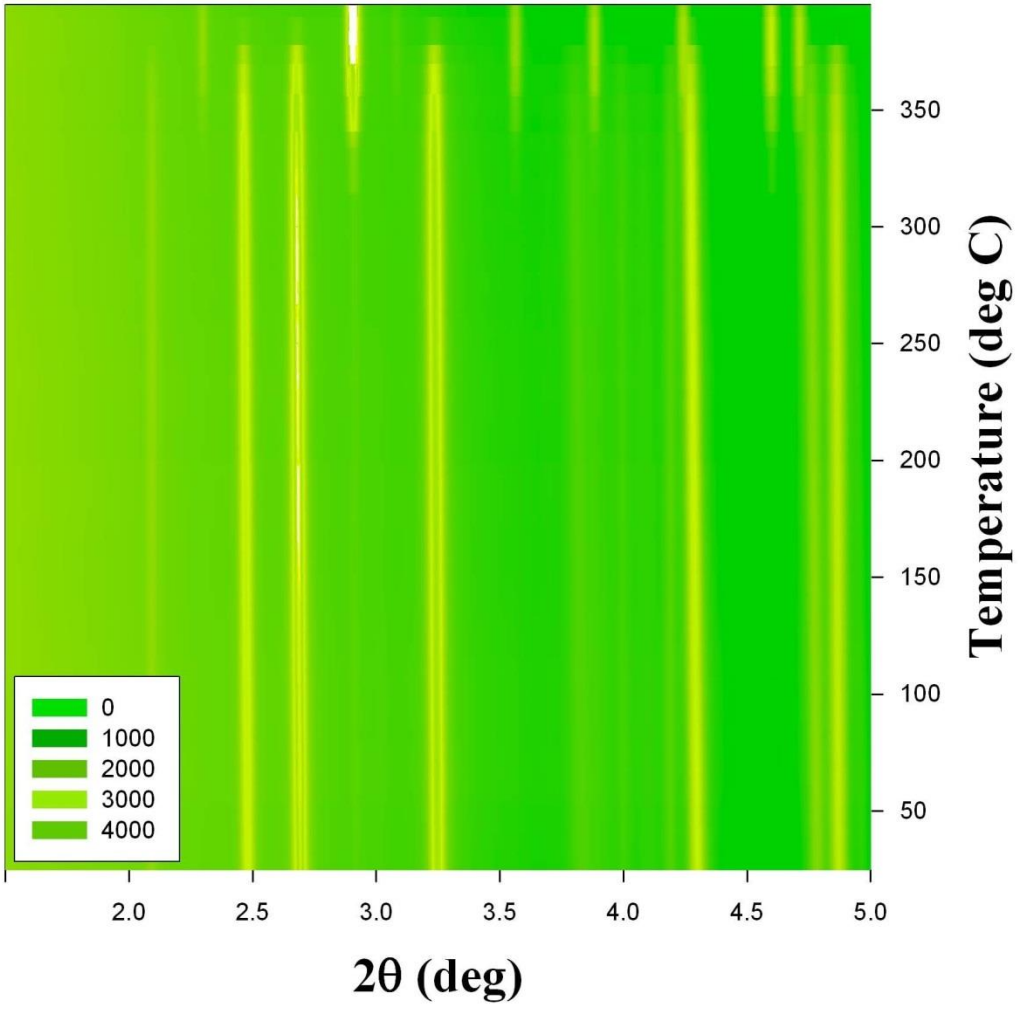

Figure 6.5f: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L ASP, using the fast addition method C, harvested after 1 hour. Vaterite to calcite transformation occurs around 350 to 360 °C.

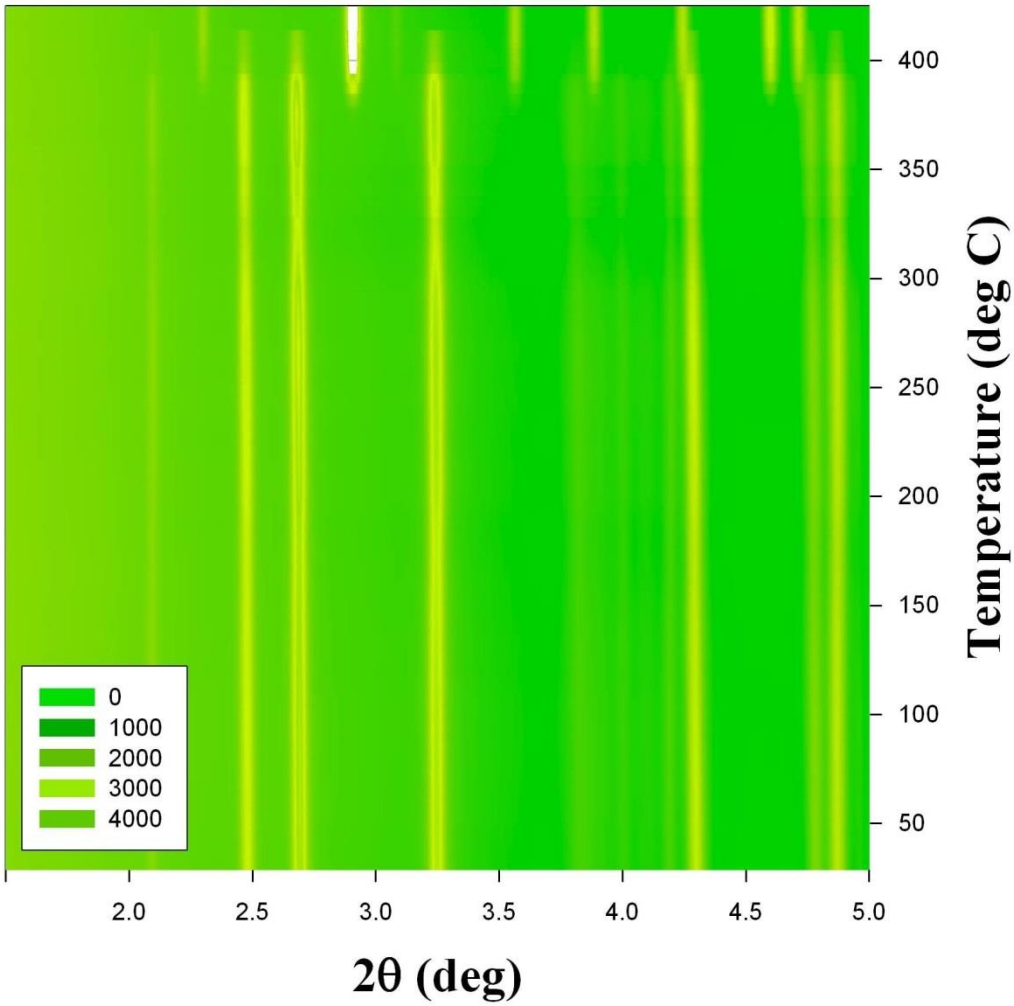

Figure 6.5g: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L ASP, using the slow addition method F, harvested after 1 hour. Vaterite to calcite transformation occurs around 380 °C.

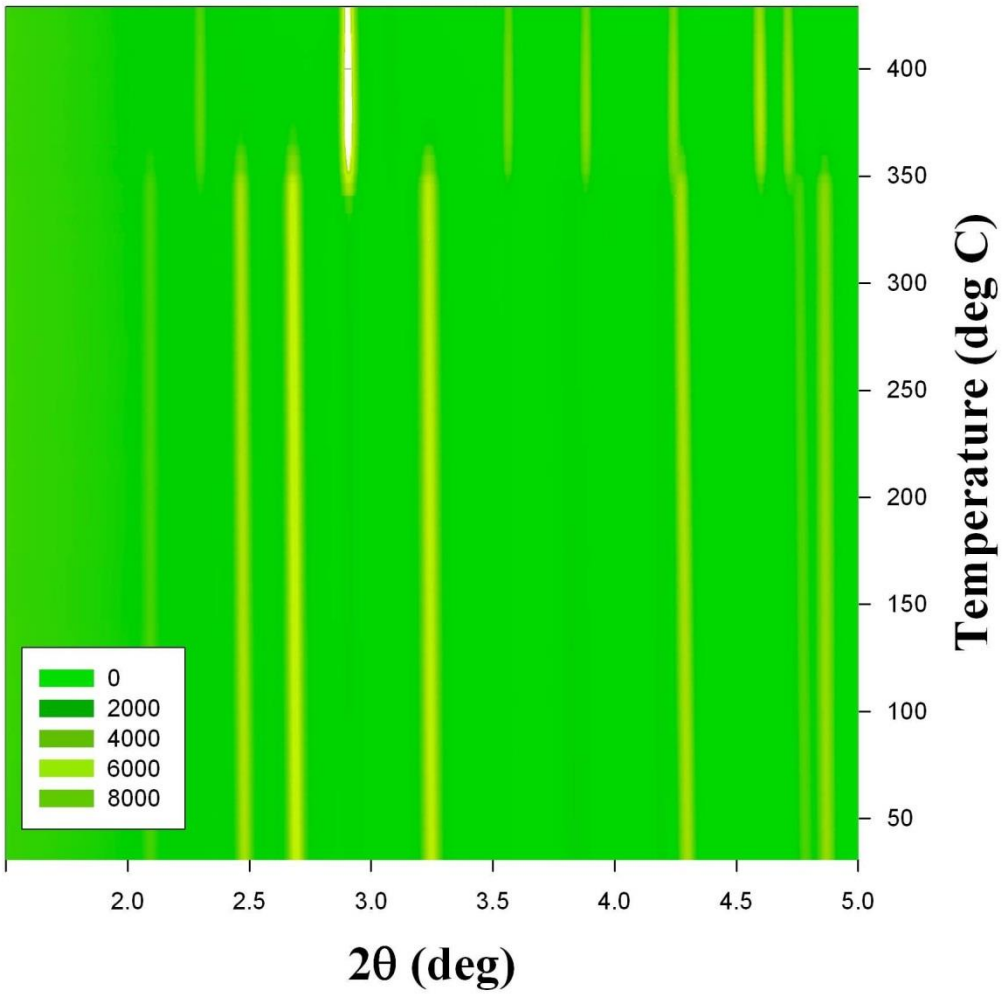

Figure 6.5h: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L GLU, using the slow addition method B, harvested after 1 hour. Vaterite to calcite transformation occurs around 350 °C.

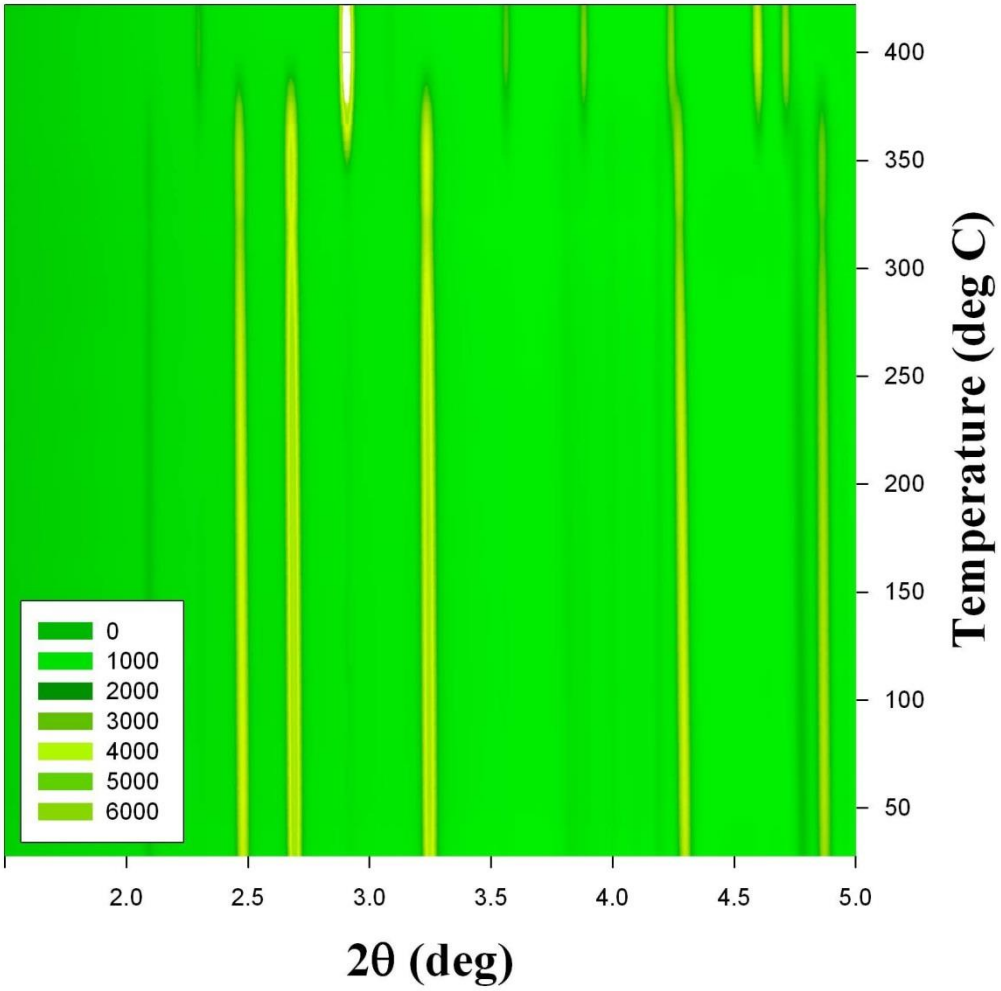

Figure 6.5i: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L GLU, using the slow addition method B, harvested after 1 week. Vaterite to calcite transformation occurs around slightly higher than 350 °C.

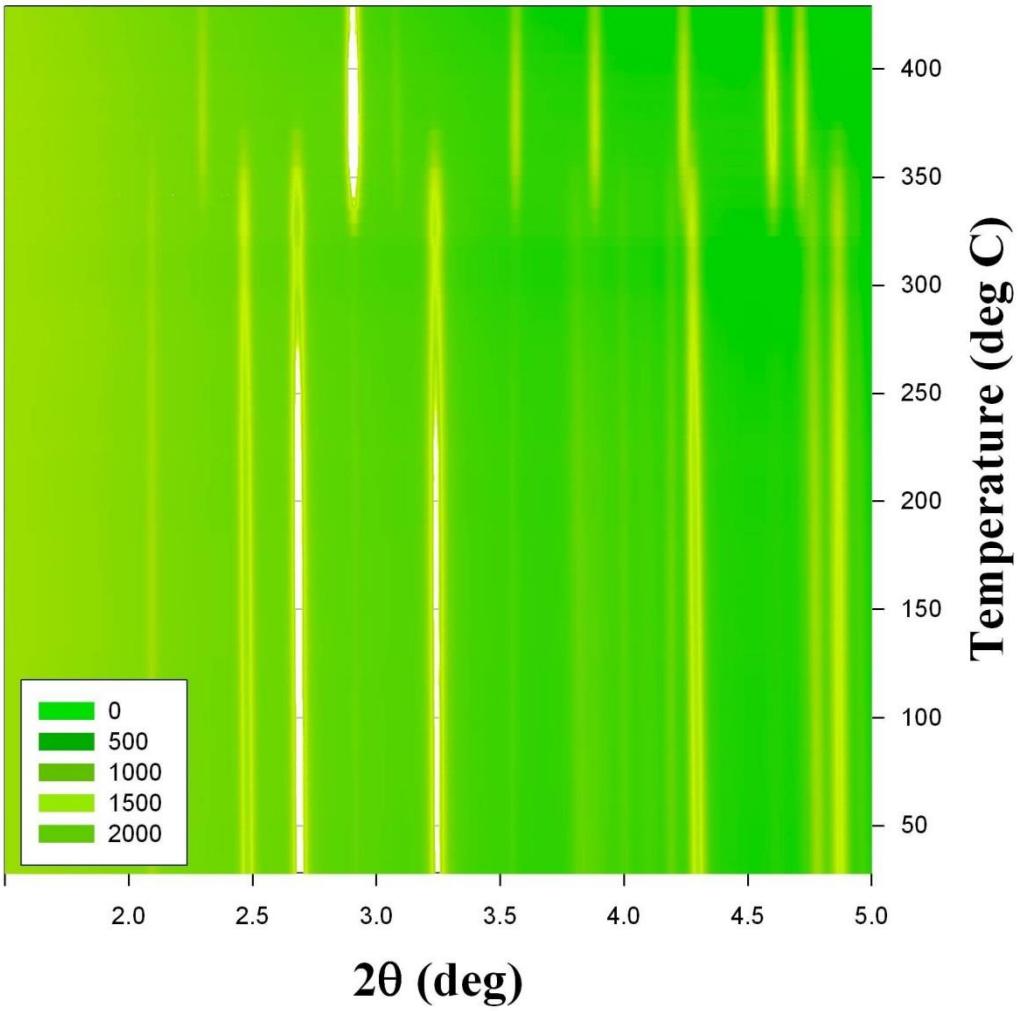

Figure 6.5j: Temperature dependent in-situ data for a sample grown in the presence of 1000 mg/L GLU, using the slow addition method F, harvested after 1 week. Vaterite to calcite transformation occurs around 350 °C.

6.2.3 Neutron Powder Diffraction (NPD) experiments

As mentioned in section 4.3, some samples were specifically prepared for NPD experiments at the Lucas Heights facility. The samples were spiked with corundum and high resolution diffraction experiments carried out. The idea was the same as for the spiked samples run at the APS, to quantify, if possible the amount of vaterite and calcite present in the samples. The data generated in the experiments were exported and used in structure refinements with a number of Rietveld packages, primarily Rietica (Hunter, 1997). This was done because the vaterite pattern reported in literature did not match the one observed in the experiments. A major problem

existed with the two main structures used, which report vaterite as hexagonal. The one produced by the experiments was not exclusively hexagonal and an attempt was made to use an orthorhombic structure transformed from the hexagonal cell as a starting point for the structure refinement. Joint refinements with measurements from the APS were also attempted. The vaterite produced in the experiments exhibited differences in the positions of the CO_3 group. Even 'ab initio' structure determination, which involves the collection of high quality diffraction data, complete indexing to determine unit cell and space group symmetry, structure factor extraction, Fourier and Patterson methods for structure definition and structure refinement by the Rietveld method did not resolve the issue. Symmetry reduction and a superstructure approach did not lead to a viable structure model either. Difference Fourier maps were generated, based on the orthorhombic structure, which seemed more likely because of two low angle peaks were observed in patterns collected at the APS, which are forbidden by the hexagonal space group usually assigned to vaterite. But even the difference Fourier maps were unclear. In the end it was decided to desist, as the most likely cause for the uncertainties lies in the fact that either vaterite is present in more than one crystallographic structure, or that some of the AA might be occluded in the crystals, creating a non-isotropic distortion in the lattice with some short range order but almost no long range order. One solution that was investigated was the use of deuterium tagged AAs in further growth experiments to be able to detect if some of it is truly occluded. This was discarded due to cost constraints, but might be something to consider in future.

6.4 Infrared experiments

While at ANSTO it was decided to investigate the vaterite-calcite transformation with an Infrared spectrometer. Time and availability restricted the use of the instrument to one afternoon, but the results were quite intriguing.

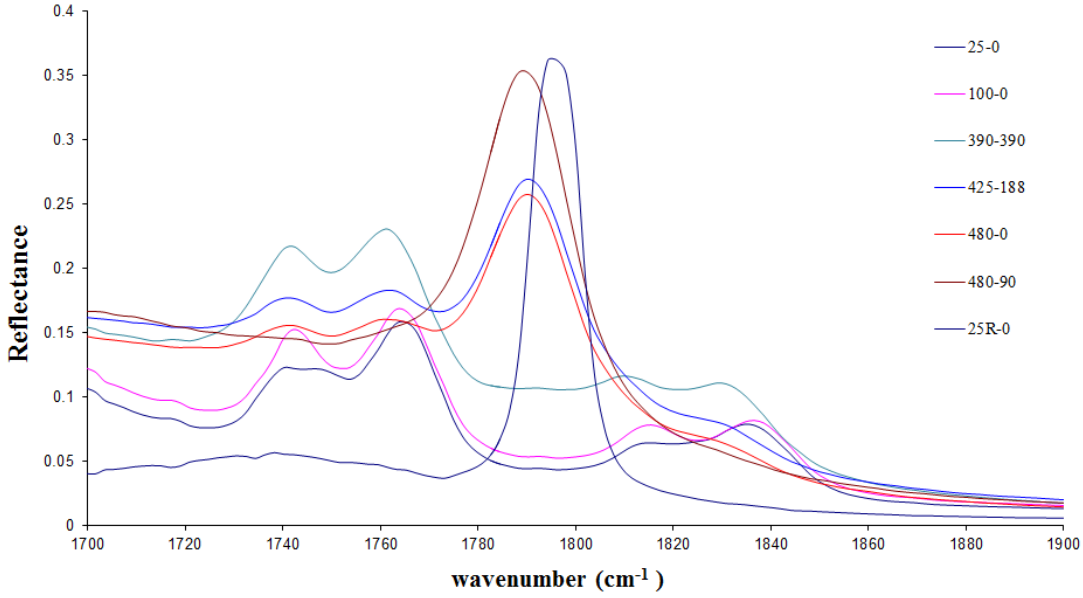

Figure 6.6: Plot of reflectance versus wavenumber for a sample grown in the presence of GLU at a concentration of 1000 mg/L using method B, harvested after 1 hour. The legend consists of two parts. The first number indicates the temperature at which the measurement was taken, the second number the amount of time that had passed before the pattern was collected in seconds (s). The 'R' attached to the last second '25' in the legend indicates that that measurement was taken after the sample had cooled completely back down to room temperature. The plot clearly shows the vaterite – calcite transformation.

A number of vibrational modes are visible for vaterite, namely the features at around 1740-1743, 1761-1763, 1809-1815 and 1830-1837 cm^{-1}. The wavenumbers representing vaterite were determined form the sample initially analysed at room temperature, knowing that it consisted almost entirely of vaterite. Calcite vibrational modes were defined by using a pure calcite sample. The main calcite mode present in the displayed range is around 1788 cm^{-1} in the hot sample and 1796 cm^{-1} in the cooled sample.

The transformation temperatures seemed to be higher than those recorded at the APS, and some of the vibrational modes indicative of the presence of calcite appeared gradually, again supporting the idea that a combined first and second order phase transformation is likely; even more so, as the calcite vibrational modes observed

disappeared again when the sample was cooled rapidly back to room temperature leaving just the vaterite vibrational modes and the slight indications of the calcite modes that had already been present in the original sample. This suggests that the driving force in the phase transformation from vaterite to calcite is of second order, allowing for a return to the initial state if the transition is not complete. Only one plot of reflectance versus wavenumber is included here and an area where the disappearance of the vaterite vibrational modes and the establishment of the calcite vibrational modes can easily be seen.

7 Discussion and outlook

Both AAs investigated in this research are crystal growth inhibitors. All the results obtained in this thesis clearly show the important role they play in the morphological, phase composition and weight recovery changes with increasing concentration. At the lowest concentration used, the impact is the small with mainly calcite produced for both types of AA. Also, the recovered weight of the solids is the highest for samples grown at the lowest concentration of AA, indicating that crystallisation is occurring at almost a regular rate. At the lowest concentration used the AAs are also not able to stabilise metastable vaterite in solution for any significant length of time, with all vaterite completely transformed after 1 day. The largest variability can be observed at intermediate concentration of AAs, with method, time of addition and harvesting time all playing a role. However, the concentration of AA at 100 mg/L is still not enough to stabilise vaterite for a week in solution in all cases except for slow addition method B grown in the presence of ASP. At 1000 mg/L, the highest concentration of AAs used, the amino acid drives phase selection and is able to stabilise vaterite over a week and even longer, with two test samples harvested after 1 year still showing vaterite. For this concentration there is again not much difference between the methods used, instead the difference is mainly between the AAs used and to some extent between slow and fast addition, with slow addition allowing the AAs a better control over phase selection and crystallisation. The growth inhibition is also noticeable in the amount of solids recovered from solution in comparison to the amount of salts present. For samples grown in the presence of 10 mg/L AAs or 100 mg/L AAs this ranges between 75 and 90% w/w, while in

samples grown in the presence of 1000 mg/L this is between 55 and 70% w/w. (Appendix A3 and A4).

7.1 Morphological analysis

7.1.1 Optical microscopy

Optical microscopy was used to study the dried product, and all information gathered in this way was employed to plan detailed examination by SEM. A few interesting observations were made when portions of the precipitating solution were examined in real time while the crystallisation was occurring. During these examinations it became quite obvious that the AAs only worked at limited super-saturation levels, furthermore relying on mobility in solution to control crystallisation, and that upon drying the crystallisation proceded at an accelerated rate, as all remaining Ca-carbonate was precipitated. There was also a noted change in the crystal shapes observable under the microscope, with the crystals growing at a late stage more angular in nature and showing distinct rhombohedral crystal shapes, and which are therefore most likely calcite. This is similar to observations made by Njegić-Džakula et al, (2010), who found that vaterite is precipitated at lower super-saturation conditions, and a mixture of vaterite and calcite at higher super-saturation conditions without organic additives, and that crystal growth is delayed in solutions with organic additives.

7.1.2 Scanning Electron Microscopy (SEM) analysis

The main purpose of carrying out SEM analysis of the samples was to investigate the morphologies present, and to ascertain if there are differences in the morphologies for samples produced by the different methods, concentrations and harvesting times. It has generally been assumed that the morphology of the Ca-carbonates can be used as an indication of the phases present, with vaterite forming flat or lozenge shaped, rounded to pseudo-hexagonal porous aggregates, which can be intergrown, or more commonly assembled into hollow spheres. Calcite, on the other hand is generally seen as forming pristine to heavily deformed rhombohedral crystals, mostly compact with well-defined edges. Over the recent years there have been a lot more

morphological studies and some very unusual morphologies have been reported, not only for the $CaCO_3$ polymorphs, but also for a number of other carbonates, silica, Fe-oxide and a range of elements and chemical phases not usually encountered in nature (Meldrum and Cölfen, 2008).

Vaterite morphology does not vary a great deal between the different samples harvested at the same time, not even when comparing samples grown in the presence of the different AAs, ASP and GLU. One thing that does change is the visually apparent porosity and the amount of vaterite that occurs as hollow spheres or 'pancake' shaped aggregates. The main changes in morphology are related to changes in harvesting time, with aggregates becoming denser over time and with more intergrowth resembling twinning present. These particular morphologies are most likely linked to the initial nucleation, and it is now very much accepted that the hollow spheres form initially as nuclei around bubbles (Evans, 2008, Meldrum and Cölfen, 2008). At lower concentrations the transformation from vaterite to calcite, apparent in the change in crystal morphology, seems to be progressing rapidly in all samples grown in the presence of 10 mg/L of ASP or GLU after a day, and is complete after a week. It is also almost complete in samples with an additive concentration of 100 mg/L after a week. What is not quite clear is how the transformation occurs. A couple of trial samples, that had been vacuum filtered but not completely dried and then enclosed in a vial converted from vaterite to calcite over a very short timeframe; however, samples that were vacuum filtered and allowed to air dry before being put into a vial and sealed showed that there were no transformations occurring, even after substantial amounts of time. This suggests that moisture is definitely an aid in the transformation from vaterite to calcite, aiding in the dissolution and re-crystallisation of the Ca-carbonate. Considering that calcite is the preferred mineral formed during the latest stages of crystallisation, it is postulated here that calcite will form and vaterite preferentially transform into calcite at increasing levels of super-saturation.

Vaterite is the dominant phase present in all samples grown in the presence of 1000 mg/L. Moisture is no longer an issue at these concentration levels; two solutions, with the precipitate still inside were kept air tight over a year, and analysis of the precipitate after this time showed that the majority of the precipitate was still

vaterite, even though the AA in the solution would have broken down over this time. This leads to the question posed by various scientists: How much of the AA is incorporated into the crystal structure? The amount that can be incorporated into the crystal lattice without destabilising it is dependent on the size of the molecule and its location in the lattice. For large organic molecules the strain introduced by its presence would result in a significant increase in contained crystal energy and the distance between these distortions would have to be large in order to prevent the breakdown of the crystal into smaller domains or its transformation into an energetically more favourable structure arrangement. At higher concentrations these molecules are therefore most likely encapsulated and occluded in the crystal rather than forming an integral part of it. However, for small molecules the situation is quite different and given the size of the ASP and GLU molecules, they might be incorporated along growth steps at a relatively high density.

The majority of samples grown in the presence of 1000 mg/L of AA had some crystalline floats at the air/solution interface in samples harvested after one day and especially one week. The morphologies in these were indicative of vaterite, as can be seen in figures 5.17-5.19. They deserve a special mention, as they form fairly massive aggregates, which still float at sizes of more than 10 mm in diameter, apparently due to surface tension, because as soon as they are disturbed they sink. XRD analysis was carried out on these floats from a number of different samples to determine the polymorph or polymorphs present, and the analysis revealed that they are entirely made up of calcite, suggesting that morphology alone should not be used to identify the phase present, and that instead a more thorough approach is required. This that has also been reported in some morphological studies (Meldrum and Cölfen, 2008, Zhang et al., 2010).

Using crystal morphology as an indicator, and postulating that the more angular crystals are calcite and the more rounded crystals are vaterite, the intergrowth of the two can give an indication of crystallisation sequence. For samples grown in the presence of 10 mg/L of AA both vaterite and calcite co-precipitate, particularly for samples produced by fast addition methods, while vaterite precipitates first and calcite is a late stage product in samples grown at higher concentrations of AAs. This is supported by the fact that most of the calcite crystals found in samples grown at

concentrations of 100 mg/L and 1000 mg/L of AA seem to have grown around and through vaterite crystals and aggregates.

The formation of the floats remains an area of interest, as the exact reason for their presence could not be determined. It is proposed, based on the growth structures, that they most likely formed from nucleation on dust particles that settled on the surface of the solution before it was covered, or by association with gas bubbles containing CO_2, whereby increased CO_2 pressure (present in the air pocket over the sample after enclosing the solution) provides the impetus for the formation of the large aggregates.

The clear and fully transparent appearance of the floats suggests that the defect density is low, even though the microscopic appearance of the crystals suggests otherwise. Some of the calcite crystals found in the floats are quite peculiar, in particular the ones displayed in figures 5.17 and 5.18. These have platy crystals growing in only a few preferred directions, suggesting that the growth of crystals from the surface into the solution is controlled by other mechanisms besides the AA used and its concentration. If competitive growth from initial nuclei or changes in kinetics and reagent concentrations at or near the air-solution interface have the greater influence on the crystallisation of these unusual calcite crystals is unclear.

7.2.1 Structural analysis from synchrotron X-ray powder diffraction (SXRPD)

While morphology analysis using SEM indicated little difference in the calcite and vaterite that was formed in the presence of 10 mg/L and 100 mg/L of AAs, there are significant differences found using SXRPD. Coherent scattering domain sizes indicate that calcite crystals, which appear to be large but deformed when examined with the SEM (e.g. figure 5.7) have smaller coherently scattering domains, indicating a high defect density even at the low AA concentrations.

The influence of the AAs at concentrations of 100 mg/L and 1000 mg/L is far more pronounced, and at concentrations of 100 mg/L the first differences between the two AAs start to appear, with ASP (Krammer et al., 2002) apparently with a stronger inhibiting influence than GLU, evidenced by the fact that vaterite is stabilised for longer periods of time.

The difference is visible in direct comparison when looking at the SXRPD data, as illustrated by figures 5.27 and 5.39 for the samples grown in the presence of 100 mg/L GLU and figures 5.29 and 5.40 for samples grown in the presence of 1000 mg/L. The calcite peaks for the same methods and harvesting times are more intense in all samples produced in the presence of 100 mg/L GLU when compared with ASP for samples harvested after 1 day and 1 week, while at 10 mg/L AA concentration very little difference is visible.

What also becomes clear by just plotting the diffraction scan data is that both AAs are very effective in stabilising vaterite at concentrations of 1000 mg/L. No statistically significant change in calcite peak intensity is observed for samples produced by methods A to D for ASP and methods C and E for GLU. For samples produced by methods B, D and F in the presence of GLU there is only a relatively small but statistically significant increase in calcite peak intensity present in the samples harvested after 1 week and only for method A is the increase noteworthy, but also only for the sample harvested after 1 week. For samples produced using method E in the presence of ASP the calcite peak is only visible in the sample harvested after 1 hour. For samples produced using method F in the presence of ASP the change is significant; no calcite is observed in the sample harvested after 1 hour and very little in the sample harvested after 1 week, while the sample harvested after 1 day shows the third largest amount of all samples produced in the presence of either of the AAs at 1000 mg/L. This shows that ASP is more effective in inhibiting the growth of calcite when compared to GLU, but that GLU is more effective in inhibiting calcite growth when Ca is added to the solution prior to the experiment (no calcite found for fast and slow addition, methods C and E). The results demonstrate further that ASP is more effective at stabilising vaterite over time (method F) and can potentially induce recrystallization of calcite as vaterite (method E), while GLU

shows that the amount calcite increases with time for 4 of the 6 methods (A, B, D and F).

That crystallinity of the vaterite increases over time, either by re-crystallisation of some of the less crystalline material or by controlled growth is illustrated in figure 6.3f.

The complexity of the system becomes clear when examining the calculated apparent crystallite or coherent scattering domain size and micro-strain values. Again, for consistency, I will use the term ‘crystallite size’ to mean ‘apparent crystallite or coherent scattering domain size’ throughout the remainder of this chapter.

Calcite crystallite size is, on average at least an order of magnitude larger than vaterite crystallite size, and in a number of cases even two orders of magnitude. The crystallite size determined by the calculations is, however, an apparent size, meaning that it represents a weighted quantity. Due to this, smaller crystals seen in the SEM images do not influence the overall size determined by the calculation very much, because the amount of smaller crystallites make up a much smaller volume and therefore contribute only little to the overall scattering when compared to the larger crystallites. Calcite also forms large crystals and crystal aggregates, with the largest represented by the floats.

For micro-strain we have the opposite result, with vaterite showing higher strain, in most cases for samples grown in the presence of the same amount of AA also by about an order of magnitude, and in some cases significantly higher. The results reported in chapter 5 point to significant differences in the effect the amino acids have on the two polymorphs. The effect that the AAs have on calcite is on external deformations, expressed in morphology rather than in changes in structure. This picture appears reversed for vaterite. All crystallite sizes are very small, indicating that the AAs directly influence crystallisation as otherwise the crystals would grow larger, as is apparent for the calcite crystallites. The fact that no commensurate structure could be determined for vaterite, even when combining neutron and synchrotron diffraction data is a further indication that the AAs most likely operate on a local structural level, causing small aberrations in the structure that show no

long range ordering. The diffraction patterns collected at the synchrotron support the idea of a mixed or alternating structure, with some peaks indicative of an orthorhombic structure present in the same pattern where peaks indicative of a hexagonal structure are apparent.

Even though the AAs used were mono acids and not the poly acids usually found in nature, they still exerted a similarly strong influence on the crystallisation of Ca-carbonate. This might also explain the apparent favouring of vaterite; being a metastable phase with higher crystal energy, it seems that its structure is more easily controlled and that the resultant crystallites require less energy for remobilisation by dissolution when new Ca-carbonate structures need to be formed or existent ones modified. This is also expressed by the fact that vaterite is generally the first crystalline phase to form from amorphous Ca-carbonate (Gago-Duport et al., 2008). The combination of high micro-strain, small crystallite size and porous morphology predestines the mineral as a temporary storage solution, because the energy differential between crystallisation and dissolution is small, and it furthermore is easily stabilised by simple organic acid molecules.

The effect of the AAs at a concentration of 10 mg/L is limited. While they favour the formation of vaterite initially, they do not inhibit the formation of calcite, and over time all vaterite is transformed into calcite. At these lower concentrations, the differences in preparation are more pronounced, with slow addition methods producing smaller calcite crystallites for samples harvested after one hour than the ones using the fast addition, as demonstrated by figures 6.3a and 6.3g. For vaterite grown under the same conditions the situation is more complex than for samples grown in the presence of ASP; the crystallite sizes produced by the different methods are similar, including by slow and fast addition, and for some orientations the crystallite size for the slow addition methods seems to be smaller, while for other orientations it seems to be larger. For GLU the trend is clearer, with slow addition methods producing smaller crystallites, as shown in figure 6.3h. This might be an expression of the impact the AAs have on the structural properties, because at very small crystallite sizes any defect or change in growth speed can already cause a noticeable change in the crystallite size calculated for that orientation, and the fact that some of the AA molecules are very likely occluded in the vaterite crystals might

certainly cause a significant change. At the speed at which the reactants are introduced during the fast addition experiments nucleation might occur too rapidly for the AA to inhibit the crystal growth from initially formed nuclei, leading to slightly larger crystallite sizes, while the slow addition methods permit the AA to disassemble freshly formed nuclei.

At a concentration of 100 mg/L the AAs exert a greater influence on the crystallographic properties of vaterite and calcite as well as the amount of each that is formed then it is the case for samples produced at concentration of 10 mg/L of AAs. For calcite crystallite size the difference between slow and fast addition and between the different methods is ambiguous, with indication that slow addition leads to slightly larger crystallite sizes (fig. 6.3d and fig. 6.3i) for some orientations. At this concentration the inhibitory effect of the AA is more pronounced than at 10 mg/L and crystal growth is controlled by the AA for short harvesting times. What is noticeable is that the crystallite size for calcite increases with time within the limits of statistical uncertainty. When just the values are considered the size seems to increase first from samples harvested after 1 hour to samples harvested after 1 day, but then decreases for samples harvested after 1 week. If this apparent discrepancy is a real feature, there is one possible explanation: the transformation of vaterite into calcite, which progresses rapidly with harvesting time in these samples. If the change in vaterite crystallite size, which shows a strong increase, is an indication (fig. 6.3e and 6.3j), then the calcite crystallites produced would have to grow significantly to reach the same size as calcite crystallites precipitated during the initial stages of the experiment. Because this is unlikely given the limited amount of Ca and CO_3 present, the recrystallization of very small vaterite crystallites would lead to the production of relatively small calcite crystallites and a reduction in the average crystallite size for calcite, i.e. the crystallites grow substantially over the first day, but then the growth slows and the transformation of vaterite to calcite produces small crystallites.

Vaterite produced in the presence of 100 mg/L AA shows a significant impact of the AA on crystallite size, but also demonstrates that the method has a strong influence. The differences between the methods are noticeable, but the main changes are

associated with the development of orientation-dependent size distributions. This trend continues for the samples grown in the presence of 1000 mg/L AA. For these no calcite data were plotted for the samples grown in the presence of ASP, because there were too few, and only a few data points were available for samples grown in the presence of GLU. These data points indicate that the presence of 1000 mg/L of GLU has a strong inhibiting effect even on calcite, with some differences between the different orientations visible.

The micro-strain, as mentioned before, is very low for all calcite in all samples produced at all AA concentrations. Some trends are observable: The average micro-strain increases with increasing AA concentration and the micro-strain in calcite decreases over time in samples grown in the presence of the lowest concentration and also in samples grown in the presence of 100 mg/L of AA; in these, however we observe a similar trend as the one seen for crystallite sizes, with the strain value at least in one case (fig. 6.4i, method B) increasing between the sample harvested after one day and one week. This can be explained in the same way as for the crystallite size value: It is probably related to the transformation of vaterite into calcite, with the conditions not conducive to a micro-strain free transformation. This might indicate that the recrystallization mechanism is a mixture of dissolution-recrystallization and phase transformation, which maintains some of the defects and disorder present in the vaterite in the calcite that is formed.

In vaterite, the micro-strain at the lowest AA concentration of 10 mg/L is highly variable and shows strong variations with crystallographic orientation and less with method or harvesting time. Figure 6.4b illustrates this, with vaterite grown by slow addition methods or fast addition methods showing the higher micro-strain values for specific crystallographic orientations. The AA at this concentration has a stronger control over the crystal growth, but the observed variations indicate that growth inhibition is limited. Micro-strain values for the different methods but for the same crystallographic orientation are generally close, while the differences between the orientations become very noticeable. The change in micro-strain with time is variable; for most methods the micro-strain decreases with time, suggesting re-crystallisation or organised growth.

In samples grown in the presence of 100 mg/L of AA the situation reflects what had been reported for the crystallite sizes and this is visible in the plots. The micro-strain for some methods, and more importantly for some orientations, increases over time while for most methods and orientations it decreases (fig. 6.4c).

In samples grown in the presence of 1000 mg/L of AA the acid concentration itself becomes the most influential factor. Figure 6.4f illustrates this quite distinctively; the micro-strain for some orientations is by a factor of 4 to 6 higher than for others e.g. peak at 15.356º 2θ, 2.136 Å, a (00l)-peak for both the orthorhombic (004) and hexagonal (008) setting, probably indicating where the amino acids exercise the strongest growth inhibition and where they might be occluded, while the variation by method is smaller but still important, with slow addition resulting in smaller micro-strain. The orientation also seems to drive the change in micro-strain over time. For some orientations the micro-strain increases with time, like it does for the main peak at 13.015º 2θ, 2.731 Å (which corresponds to the (102) peak for the orthorhombic structure and the (104) peak for the hexagonal setting), while for others it decreases, suggesting that the AAs have some preferred attachment sites.

7.2.2 In-situ heating experiments

Regardless of the phase transformation experiment performed, the samples produced in these experiments show transformation temperatures far below the expected ones of around 500° C for the vaterite to calcite transformation and about 700° C for the calcite to CaO transformation (Nassrallah-Aboukais, N. et al., , 2008). Unfortunately we could only analyse a few samples in the capillary experiments at the APS. The data recorded after the exchange and calibration of the instrument showed some very interesting features. In particular the gradual change in the peak position of one of the vaterite peaks and the apparently continuous change into a calcite peak could provide some vital clues for the structure determination of the vaterite structure. What can be seen is, that the transformation temperatures are located between 350 °C and 400 °C, with samples produced in the presence of 1000 mg/L of ASP showing higher transformation temperatures and samples produced in the presence of 100 mg/L ASP showing lower transformation temperatures.

There are a number of factors that influence the transformation temperature; the main ones to consider are crystallite size and defect density, both influencing the crystal energy. Higher defect density and smaller crystallites both increase the crystal energy, lowering the energy required to modify the structure. For all samples produced during the experiments, the relatively small crystallite size and significant micro-strain would strongly influence the energy input required to trigger a phase transformation. Within the range of lower temperatures expected for the phase transformation the AAs can influence the transformation temperature of the vaterite by acting as a stabilising influence. Phase transformation temperatures might also have been influenced by the presence of calcite in the starting samples, especially for samples produced in the presence of 100 mg/L AA, where the intergrown calcite crystallites might acts as a 'catalyst' in the transformation.

This idea that the AA might be influencing phase stability is substantiated by the few samples analysed by FTIR, which also showed significantly lower transformation temperatures, but also indicated that some of the vibrational features change more gradually and continually, suggesting that both first (discontinuous change of thermodynamic or structural parameter) and second order (continuous change of thermodynamic or structural parameter) phase transformations might be involved.

7.3 Summary and outlook

This work has focussed on simple amino acids that are among the three most common and important ones associated with biomineralisation (Ren et al., 2011). Overall the systems analysed are quite complex, revealing that a number of factors contribute to the final product. Being relatively small molecules, their impact is limited at lower concentrations, but increases with increasing concentration, and it seems that part of the impact is due to the interaction with Ca ions, both during the nucleation process and also during the crystal growth and dissolution (Tong et al., 2004, Yoshino et al., 2010).

This work demonstrates that at low AA concentrations the impact of the method used is strong, while the impact the AA has, particularly over time, is limited.

At the intermediate concentration the impact of the AA used can be quite strong, while the method used is less critical, except in some particular circumstances, which are not conclusive. The type of AA used has a strong impact at this concentration level, with ASP showing a stronger influence over the crystal growth and phase composition than GLU, especially over time.

At the highest concentration the type of AA is the driving force, determining the phase composition and the development over time. The method used has only a limited influence over the way in which the precipitates are produced. The influence of the AAs is highly variable in regard to the vaterite, but much less so in regard to the calcite, which might explain the occurrence of vaterite in natural biomineralisation systems, as it is easier to manipulate, and therefore less energy intensive. This would also be the reason behind the use of amorphous Ca-carbonate by a large number of organisms to store, distribute and mobilise $CaCO_3$ with ease (Meldrum and Cölfen, 2008, Chien et al., 2008a, Addadi et al., 2003, Weiner et al., 2003).

The simple amino acids used in this study of Ca-carbonate phase selection and morphology, using varying concentration, addition sequences and harvesting times will help in developing a better understanding of the impact these factors have on the crystallisation of $CaCO_3$, a point raised in the comprehensive review presented by (Sommerdijk and de With), where it is stressed that the kinetics of the precipitation methods used strongly influence the outcome.

The work presented here shows that the factors over which the AAs exert a control or influence vary with the AA concentration; at the highest concentration the AAs determine phase, morphology and phase stability with little difference between the two AAs used. The intermediate concentration of AAs is the most varied, with the impact the AAs are having on the Ca-carbonate produced varying with experimental methods, harvesting times and super-saturation driven by the speed of reactant addition. At the lowest concentration the effect of the AAs is very limited. Only samples harvested after 1 hour and to a lesser extent after 1 day showed the impact of the AAs on phase selection and stability, with sample production method and speed of reactant addition far less important than at higher concentrations. The work

presented here will aid researches in developing novel approaches for controlling the phase selection and stability of Ca-carbonate polymorphs by tailoring the parameters of the crystallisation environment, with medium-level concentration of AAs (100 mg/L) offering the highest degree of flexibility; at similar concentration of AA it should be possible to select the other parameters (rate of addition of reactants, sequence of addition and harvesting time) to successfully produce a specific polymorph with desired characteristics (crystallite size, shape, micro-strain).

7.4 Future work

A number of areas for future work have been established:

1) The use of deuterium tagged simple AAs like the ones used in this study to identify where they are placed inside the precipitated phases.

2) The study of the phase transformation of vaterite and possibly also of aragonite and amorphous Ca-carbonate into calcite upon heating, thus hopefully creating an indicator for the stabilising influence specific organic additives have on metastable $CaCO_3$ phases.

3) Include temperature and pH as controlled variables in the system to establish the order of importance of the different factors influencing the crystallisation.

4) Study of the floats to see if they are a phenomenon due to surface contamination, related to energetic changes at the air-solution interface or driven by gas concentration and/or pressure, hopefully establishing the main reason for the unusual morphology.

5) TEM work to contribute to resolving the vaterite structure.

6) FTIR studies of the vaterite – calcite transition and also of amorphous calcium carbonate (ACC) crystallisation to determine the exact transformation temperatures and which vibrational modes change or disappear for first and second order phase transition.

7) Single crystal studies of the larger calcite crystals produced to establish the misalignment (if any) of the crystallites constituting the larger deformed crystals.

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APPENDIX

Additional experimental data

Amino Acid used	Concentration mg/L	Method	Expected Harvesting Time	Harvested after Days	Hours	Minutes	% error in time
GLU	10	A	1 hour	0	1	0	0.0
GLU	10	A	1 day	1	0	17	1.2
GLU	10	A	1 week	7	2	10	1.3
GLU	10	B	1 hour	0	1	0	0.0
GLU	10	B	1 day	0	23	45	-1.0
GLU	10	B	1 week	7	0	35	0.3
GLU	10	C	1 hour	0	1	2	3.3
GLU	10	C	1 day	1	1	35	6.6
GLU	10	C	1 week	7	2	25	1.4
GLU	10	D	1 hour	0	1	0	0.0
GLU	10	D	1 day	1	0	52	3.6
GLU	10	D	1 week	7	1	29	0.9
GLU	10	E	1 hour	0	1	0	0.0
GLU	10	E	1 day	1	0	14	1.0
GLU	10	E	1 week	7	4	55	2.9
GLU	10	F	1 hour	0	1	0	0.0
GLU	10	F	1 day	1	0	0	0.0
GLU	10	F	1 week	7	3	59	2.4
GLU	100	A	1 hour	0	1	0	0.0
GLU	100	A	1 day	1	0	31	2.2
GLU	100	A	1 week	7	2	36	1.5
GLU	100	B	1 hour	0	1	0	0.0
GLU	100	B	1 day	0	23	45	-1.0
GLU	100	B	1 week	7	1	10	0.7
GLU	100	C	1 hour	0	1	5	8.3
GLU	100	C	1 day	1	1	37	6.7
GLU	100	C	1 week	7	2	50	1.7
GLU	100	D	1 hour	0	1	0	0.0
GLU	100	D	1 day	1	1	2	4.3
GLU	100	D	1 week	7	1	55	1.1
GLU	1000	A	1 hour	0	1	0	0.0
GLU	1000	A	1 day	1	0	43	3.0
GLU	1000	A	1 week	7	3	11	1.9
GLU	1000	B	1 hour	0	1	0	0.0
GLU	1000	B	1 day	1	0	17	1.2
GLU	1000	B	1 week	7	1	35	0.9
GLU	1000	C	1 hour	0	1	0	0.0
GLU	1000	C	1 day	1	2	6	8.8
GLU	1000	C	1 week	7	0	12	0.1
GLU	1000	D	1 hour	0	1	0	0.0
GLU	1000	D	1 day	1	1	2	4.3
GLU	1000	D	1 week	7	2	12	1.3
GLU	1000	E	1 hour	0	1	0	0.0
GLU	1000	E	1 day	1	0	43	3.0
GLU	1000	E	1 week	7	5	27	3.2
GLU	1000	F	1 hour	0	1	0	0.0
GLU	1000	F	1 day	1	0	0	0.0
GLU	1000	F	1 week	7	4	29	2.7

Table A1: Harvesting times for samples produced in the presence of GLU

Amino Acid used	Concentration mg/L	Method	Expected Harvesting Time	Harvested after			% error in time
				Days	Hours	Minutes	
ASP	10	A	1 hour	0	1	0	0.0
ASP	10	A	1 day	1	0	30	2.1
ASP	10	A	1 week	6	23	36	-0.2
ASP	10	B	1 hour	0	1	0	0.0
ASP	10	B	1 day	1	5	6	21.3
ASP	10	B	1 week	6	22	52	-0.7
ASP	10	C	1 hour	0	1	0	0.0
ASP	10	C	1 day	1	4	17	17.8
ASP	10	C	1 week	6	22	10	-1.1
ASP	10	D	1 hour	0	1	0	0.0
ASP	10	D	1 day	1	3	22	14.0
ASP	10	D	1 week	6	21	26	-1.5
ASP	10	E	1 hour	0	1	0	0.0
ASP	10	E	1 day	1	2	54	12.1
ASP	10	E	1 week	6	20	58	-1.8
ASP	10	F	1 hour	0	1	0	0.0
ASP	10	F	1 day	1	2	17	9.5
ASP	10	F	1 week	6	20	33	-2.1
ASP	100	A	1 hour	0	1	0	0.0
ASP	100	A	1 day	1	0	36	2.5
ASP	100	A	1 week	7	0	0	0.0
ASP	100	B	1 hour	0	1	0	0.0
ASP	100	B	1 day	1	5	45	24.0
ASP	100	B	1 week	6	23	47	-0.1
ASP	100	C	1 hour	0	1	0	0.0
ASP	100	C	1 day	1	4	25	18.4
ASP	100	C	1 week	6	22	19	-1.0
ASP	100	D	1 hour	0	1	0	0.0
ASP	100	D	1 day	1	3	40	15.3
ASP	100	D	1 week	6	21	38	-1.4
ASP	1000	A	1 hour	0	1	0	0.0
ASP	1000	A	1 day	1	0	42	2.9
ASP	1000	A	1 week	7	0	14	0.1
ASP	1000	B	1 hour	0	1	0	0.0
ASP	1000	B	1 day	1	0	25	1.7
ASP	1000	B	1 week	6	23	30	-0.3
ASP	1000	C	1 hour	0	1	0	0.0
ASP	1000	C	1 day	1	4	47	19.9
ASP	1000	C	1 week	6	22	24	-1.0
ASP	1000	D	1 hour	0	1	0	0.0
ASP	1000	D	1 day	1	4	0	16.7
ASP	1000	D	1 week	6	21	57	-1.2
ASP	1000	E	1 hour	0	1	0	0.0
ASP	1000	E	1 day	1	3	9	13.1
ASP	1000	E	1 week	6	21	13	-1.7
ASP	1000	F	1 hour	0	1	0	0.0
ASP	1000	F	1 day	1	2	31	10.5
ASP	1000	F	1 week	6	20	42	-2.0

Table A2: Harvesting times for samples produced in the presence of ASP. Note that some of the samples harvested after one day show a significant deviation from the planned time.

Amino Acid used	Concentration mg/L	Method	Harvesting Time	Sample mass (g)		Water Content (g)
				Moist	Dry	
GLU	10	A	H	4.00	3.06	0.94
GLU	10	A	D	4.43	3.45	0.98
GLU	10	A	W	4.60	3.77	0.83
GLU	10	B	H	4.46	3.05	1.41
GLU	10	B	D	3.97	3.32	0.65
GLU	10	B	W	4.36	3.77	0.59
GLU	10	C	H	4.30	3.29	1.01
GLU	10	C	D	4.25	3.24	1.01
GLU	10	C	W	4.47	3.74	0.73
GLU	10	D	H	4.00	3.06	0.94
GLU	10	D	D	4.19	3.38	0.81
GLU	10	D	W	4.45	3.78	0.67
GLU	10	E	H	4.29	2.98	1.31
GLU	10	E	D	4.10	3.42	0.68
GLU	10	E	W	4.43	3.72	0.71
GLU	10	F	H	3.40	2.62	0.78
GLU	10	F	D	4.14	3.42	0.72
GLU	10	F	W	4.58	3.85	0.74
GLU	100	A	H	3.89	2.97	0.92
GLU	100	A	D	4.20	3.23	0.97
GLU	100	A	W	4.66	3.61	1.05
GLU	100	B	H	3.98	2.89	1.09
GLU	100	B	D	4.12	3.36	0.76
GLU	100	B	W	4.46	3.70	0.76
GLU	100	C	H	4.26	3.29	0.97
GLU	100	C	D	4.40	3.47	0.93
GLU	100	C	W	4.75	3.70	1.05
GLU	100	D	H	3.86	3.03	0.83
GLU	100	D	D	4.33	3.27	1.06
GLU	100	D	W	4.68	3.75	0.93
GLU	1000	A	H	3.42	2.50	0.92
GLU	1000	A	D	3.67	2.87	0.80
GLU	1000	A	W	4.30	3.34	0.96
GLU	1000	B	H	3.68	2.64	1.04
GLU	1000	B	D	4.03	2.86	1.17
GLU	1000	B	W	4.64	3.29	1.35
GLU	1000	C	H	3.73	2.85	0.88
GLU	1000	C	D	3.84	2.89	0.95
GLU	1000	C	W	4.49	3.28	1.21
GLU	1000	D	H	3.43	2.57	0.86
GLU	1000	D	D	3.95	2.96	0.99
GLU	1000	D	W	4.14	3.22	0.92
GLU	1000	E	H	3.38	2.53	0.85
GLU	1000	E	D	3.91	2.79	1.12
GLU	1000	E	W	4.18	3.17	1.01
GLU	1000	F	H	2.97	2.18	0.79
GLU	1000	F	D	4.06	2.83	1.23
GLU	1000	F	W	4.28	3.19	1.09

Table A3: Sample mass for samples produced in the presence of GLU. The mass was measured after vacuum filtration and again after air-drying.

Amino Acid used	Concentration mg/L	Method	Harvesting Time	Sample mass (g)		Water Content (g)
				Moist	Dry	
ASP	10	A	H	2.96	2.42	0.54
ASP	10	A	D	3.60	2.83	0.77
ASP	10	A	W	4.35	3.33	1.02
ASP	10	B	H	3.60	2.60	1.00
ASP	10	B	D	3.42	3.01	0.41
ASP	10	B	W	4.21	3.40	0.81
ASP	10	C	H	3.88	2.75	1.14
ASP	10	C	D	3.69	3.09	0.60
ASP	10	C	W	4.12	3.39	0.73
ASP	10	D	H	3.71	2.71	1.00
ASP	10	D	D	3.52	3.18	0.34
ASP	10	D	W	4.08	3.36	0.72
ASP	10	E	H	3.88	2.74	1.14
ASP	10	E	D	3.54	3.19	0.35
ASP	10	E	W	4.11	3.41	0.70
ASP	10	F	H	3.57	2.63	0.94
ASP	10	F	D	3.48	3.15	0.34
ASP	10	F	W	4.14	3.38	0.76
ASP	100	A	H	3.50	2.50	1.00
ASP	100	A	D	3.73	2.76	0.97
ASP	100	A	W	4.07	3.14	0.93
ASP	100	B	H	3.25	2.44	0.81
ASP	100	B	D	3.64	2.82	0.82
ASP	100	B	W	4.48	3.12	1.36
ASP	100	C	H	3.19	2.47	0.72
ASP	100	C	D	3.37	2.81	0.56
ASP	100	C	W	3.94	3.08	0.86
ASP	100	D	H	3.31	2.49	0.82
ASP	100	D	D	4.02	2.98	1.04
ASP	100	D	W	4.03	3.22	0.81
ASP	1000	A	H	2.40	1.73	0.67
ASP	1000	A	D	3.10	2.21	0.89
ASP	1000	A	W	3.73	2.72	1.01
ASP	1000	B	H	2.42	1.72	0.71
ASP	1000	B	D	2.84	2.13	0.71
ASP	1000	B	W	4.13	2.75	1.38
ASP	1000	C	H	2.53	1.83	0.70
ASP	1000	C	D	3.07	2.26	0.81
ASP	1000	C	W	3.67	2.75	0.93
ASP	1000	D	H	2.64	1.86	0.78
ASP	1000	D	D	2.84	2.31	0.53
ASP	1000	D	W	3.65	2.79	0.86
ASP	1000	E	H	2.65	1.80	0.85
ASP	1000	E	D	3.16	2.35	0.81
ASP	1000	E	W	3.42	2.73	0.69
ASP	1000	F	H	2.56	1.79	0.77
ASP	1000	F	D	3.25	2.42	0.83
ASP	1000	F	W	3.60	2.70	0.90

Table A4: Sample mass for samples produced in the presence of ASP. The mass was measured after vacuum filtration and again after air-drying.

Table A5: Data for all peak-fitting that falls within 2 esds for either Lorentzian or Gaussian β-values. The scheme follows the general sample production outline, with ASP samples presented first, sorted by method, concentration, harvesting time and 2θ values, followed by the same order for all GLU samples.
Duplicate fits have been removed, and the values with the highest confidence were chosen.

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	A	H	177.42	7.97	8.3907	0.0004	4.2321	0.0002	0.03418	0.00096	0.02191	0.00210
ASP	10	A	H	64.18	2.55	9.2152	0.0002	3.8542	0.0001	0.00937	0.00092	0.01151	0.00080
ASP	10	A	H	1033.73	18.16	9.9387	0.0002	3.5742	0.0001	0.05026	0.00060	0.03191	0.00118
ASP	10	A	H	1788.40	26.11	10.7901	0.0002	3.2929	0.0001	0.06639	0.00064	0.04616	0.00136
ASP	10	A	H	899.81	15.85	11.7072	0.0000	3.0358	<0.0001	0.00971	0.00022	0.01010	0.00030
ASP	10	A	H	15.74	3.97	12.4997	0.0004	2.8440	0.0001	0.01090	0.00180	0.00601	0.00362
ASP	10	A	H	1902.98	45.81	13.02	0.0002	2.7308	<0.0001	0.08172	0.00194	0.03696	0.00214
ASP	10	A	H	77.92	4.00	14.2574	0.0002	2.4949	<0.0001	0.01218	0.00040	0.00925	0.00098
ASP	10	A	H	173.62	8.06	15.5747	0.0002	2.285	<0.0001	0.01300	0.00062	0.01097	0.00106
ASP	10	A	H	209.55	18.85	15.6224	0.0410	2.2781	0.0060	0.00000	0.00000	0.54173	0.08576
ASP	10	A	H	143.01	17.28	16.8237	0.0008	2.1164	0.0001	0.05142	0.00458	0.02679	0.00784
ASP	10	A	H	227.57	5.36	17.0012	0.0002	2.0945	<0.0001	0.00764	0.00054	0.01024	0.00042
ASP	10	A	H	315.53	81.72	17.2501	0.0028	2.0645	0.0003	0.00000	0.00000	0.12406	0.02746
ASP	10	A	H	943.09	396.44	17.2544	0.0008	2.0640	0.0001	0.04720	0.02234	0.00000	0.00000
ASP	10	A	H	94.75	10.47	18.4852	0.0002	1.9277	<0.0001	0.01086	0.00082	0.00627	0.00156
ASP	10	A	H	286.28	10.94	18.6296	0.0002	1.9128	<0.0001	0.01248	0.00034	0.01001	0.00074
ASP	10	A	H	179.89	9.20	19.004	0.0002	1.8755	<0.0001	0.01341	0.00064	0.01145	0.00118
ASP	10	A	H	493.79	26.48	19.2096	0.0012	1.8556	0.0001	0.12545	0.00392	0.08863	0.01092
ASP	10	A	H	1206.45	44.06	19.5714	0.0006	1.8216	0.0001	0.11063	0.00260	0.06339	0.00540
ASP	10	A	H	67.10	8.13	19.9495	0.0028	1.7874	0.0002	0.06772	0.02772	0.07701	0.01994
ASP	10	A	H	38.18	2.15	21.2315	0.0098	1.6806	0.0008	0.00000	0.00000	0.29413	0.02718
ASP	10	A	H	617.10	18.14	21.6732	0.0006	1.6468	<0.0001	0.15188	0.00316	0.08023	0.00572
ASP	10	A	H	25.76	2.14	21.9556	0.0004	1.6259	<0.0001	0.01365	0.00136	0.01166	0.00208
ASP	10	A	H	97.78	3.55	22.2556	0.0002	1.6042	<0.0001	0.01496	0.00032	0.01057	0.00082
ASP	10	A	H	17.50	2.98	22.496	0.0004	1.5873	<0.0001	0.01515	0.00162	0.00858	0.00350
ASP	10	A	H	141.66	10.74	23.1534	0.0026	1.5428	0.0002	0.20497	0.00904	0.14095	0.02554
ASP	10	A	H	82.81	5.09	23.4209	0.0002	1.5254	<0.0001	0.01083	0.00040	0.00654	0.00090
ASP	10	A	H	28.72	2.23	23.536	0.0002	1.5181	<0.0001	0.00974	0.00340	0.01233	0.00198
ASP	10	A	H	35.66	5.21	23.6683	0.0004	1.5097	<0.0001	0.01727	0.00116	0.01042	0.00368
ASP	10	A	H	155.06	10.50	24.2025	0.0030	1.4769	0.0002	0.19034	0.00610	0.12705	0.01994
ASP	10	A	H	12.48	1.99	24.2621	0.0006	1.4733	<0.0001	0.00000	0.00000	0.01647	0.00514
ASP	10	A	H	46.87	2.16	24.8236	0.0002	1.4405	<0.0001	0.01355	0.00134	0.01465	0.00132
ASP	10	A	H	29.30	7.51	25.1521	0.0004	1.422	<0.0001	0.01812	0.00294	0.00907	0.00582
ASP	10	A	H	11.35	1.45	26.3786	0.0006	1.3569	<0.0001	0.01095	0.00670	0.01410	0.00384
ASP	10	A	H	21.92	2.72	26.4899	0.0032	1.3513	0.0002	0.00000	0.00000	0.09463	0.02610
ASP	10	A	H	18.70	2.70	26.7347	0.0006	1.3392	<0.0001	0.01907	0.00252	0.01435	0.00474
ASP	10	A	H	37.40	1.68	26.8363	0.0042	1.3342	0.0002	0.00000	0.00000	0.14372	0.01102
ASP	10	A	H	223.35	16.79	27.2901	0.0010	1.3124	<0.0001	0.12752	0.00892	0.05721	0.01084
ASP	10	A	H	35.79	2.53	27.6233	0.0004	1.2969	<0.0001	0.01841	0.00184	0.01625	0.00248
ASP	10	A	H	11.02	2.40	28.74	0.0006	1.2475	<0.0001	0.01577	0.00194	0.00929	0.00482
ASP	10	A	H	22.52	2.79	29.0267	0.0004	1.2354	<0.0001	0.01833	0.00114	0.01199	0.00344
ASP	10	A	H	33.59	4.80	29.3501	0.0520	1.2221	0.0021	0.00000	0.00000	0.44977	0.11536
ASP	10	A	H	4.26	1.50	30.2413	0.0012	1.1869	<0.0001	0.01398	0.00774	0.00000	0.00000
ASP	10	A	H	44.82	10.00	30.4231	0.0002	1.18	<0.0001	0.01506	0.00374	0.00582	0.00340
ASP	10	A	H	93.13	31.78	30.8127	0.0052	1.1654	0.0002	0.23251	0.07558	0.00000	0.00000
ASP	10	A	H	35.68	4.89	31.1291	0.0004	1.1539	<0.0001	0.01950	0.00128	0.01137	0.00380
ASP	10	A	H	100.82	16.99	31.3226	0.0064	1.1469	0.0002	0.18889	0.04630	0.14270	0.05580
ASP	10	A	H	172.76	11.79	32.4438	0.0026	1.1083	0.0001	0.25893	0.01218	0.17366	0.02780
ASP	10	A	H	7.48	1.78	33.912	0.0010	1.0616	<0.0001	0.01688	0.00822	0.01561	0.00838
ASP	10	A	H	30.05	2.64	34.3875	0.0002	1.0474	<0.0001	0.01410	0.00078	0.01011	0.00198
ASP	10	A	H	19.99	2.11	34.4696	0.0004	1.045	<0.0001	0.01565	0.00248	0.01384	0.00318
ASP	10	A	H	25.91	9.90	34.7971	0.0008	1.0354	<0.0001	0.02350	0.00868	0.00000	0.00000
ASP	10	A	H	15.09	4.94	34.9113	0.0102	1.0321	0.0003	0.00000	0.00000	0.14294	0.09476
ASP	10	A	H	4.33	0.85	35.2251	0.0012	1.0232	<0.0001	0.00000	0.00000	0.01676	0.00660
ASP	10	A	H	109.29	40.08	35.5151	0.0070	1.0151	0.0002	0.21440	0.05996	0.00000	0.00000
ASP	10	A	H	33.21	4.09	35.6277	0.0004	1.012	<0.0001	0.01857	0.00120	0.01233	0.00358
ASP	10	A	H	17.29	4.65	36.6456	0.0006	0.9849	<0.0001	0.01939	0.00308	0.00000	0.00000
ASP	10	A	H	3.80	0.98	37.9541	0.0008	0.9521	<0.0001	0.00000	0.00000	0.01111	0.00614
ASP	10	A	H	89.05	9.49	38.3703	0.0052	0.9421	0.0001	0.24211	0.01556	0.15909	0.03752
ASP	10	A	H	14.44	3.06	38.552	0.0006	0.9379	<0.0001	0.01768	0.00178	0.01101	0.00556

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	A	D	427.00	6.73	9.2141	0.0000	3.8546	<0.0001	0.00496	0.00036	0.00996	0.00022
ASP	10	A	D	3283.42	93.44	11.7052	0.0002	3.0363	0.0001	0.00501	0.00038	0.00733	0.00040
ASP	10	A	D	883.59	90.88	11.7118	0.0004	3.0346	0.0001	0.00491	0.00056	0.00465	0.00086
ASP	10	A	D	60.70	22.39	12.5015	0.0010	2.8436	0.0002	0.00611	0.00294	0.00767	0.00238
ASP	10	A	D	6.32	1.73	12.6040	0.0010	2.8206	0.0002	0.01597	0.00232	0.01069	0.00668
ASP	10	A	D	402.85	112.30	14.2558	0.0012	2.4952	0.0002	0.00606	0.00064	0.00989	0.00114
ASP	10	A	D	693.35	23.01	15.574	0.0002	2.2851	<0.0001	0.00765	0.00046	0.01118	0.00028
ASP	10	A	D	479.60	44.42	17.0028	0.0010	2.0943	0.0001	0.00635	0.00074	0.00988	0.00150
ASP	10	A	D	157.35	13.65	18.4871	0.0004	1.9275	<0.0001	0.00803	0.00084	0.00720	0.00128
ASP	10	A	D	244.12	62.37	18.6269	0.0002	1.9131	<0.0001	0.00000	0.00000	0.00452	0.00166
ASP	10	A	D	849.20	69.82	18.6298	0.0006	1.9128	0.0001	0.00963	0.00094	0.01042	0.00036
ASP	10	A	D	165.47	69.97	18.9994	0.0062	1.8759	0.0006	0.00000	0.00000	0.01470	0.00490
ASP	10	A	D	532.98	72.17	19.0019	0.0004	1.8757	<0.0001	0.00639	0.00058	0.00551	0.00114
ASP	10	A	D	569.99	68.28	19.0082	0.0004	1.8751	<0.0001	0.00669	0.00052	0.00691	0.00112
ASP	10	A	D	434.74	60.99	22.2556	0.0006	1.6042	<0.0001	0.01499	0.00310	0.00892	0.00108
ASP	10	A	D	44.96	4.09	22.4971	0.0004	1.5872	<0.0001	0.01109	0.00110	0.00997	0.00178
ASP	10	A	D	167.27	7.66	23.5372	0.0002	1.518	<0.0001	0.00761	0.00048	0.00750	0.00072
ASP	10	A	D	112.37	25.16	23.6688	0.0008	1.5097	0.0001	0.01158	0.00114	0.01300	0.00258
ASP	10	A	D	72.46	26.76	24.2664	0.0008	1.473	<0.0001	0.00644	0.00184	0.00000	0.00000
ASP	10	A	D	199.52	23.37	24.8204	0.0010	1.4407	0.0001	0.00789	0.00116	0.00522	0.00074
ASP	10	A	D	81.81	15.95	24.8317	0.0010	1.4400	0.0001	0.00530	0.00142	0.00309	0.00086
ASP	10	A	D	80.97	3.76	26.3782	0.0002	1.357	<0.0001	0.00945	0.00052	0.00890	0.00078
ASP	10	A	D	96.09	18.39	26.7347	0.0010	1.3392	<0.0001	0.01289	0.00470	0.01868	0.00282
ASP	10	A	D	21.63	4.05	26.7373	0.0008	1.3391	<0.0001	0.00000	0.00000	0.00490	0.00150
ASP	10	A	D	37.82	2.12	27.8831	0.0002	1.2851	<0.0001	0.01057	0.00066	0.00955	0.00106
ASP	10	A	D	64.98	11.96	28.7379	0.0020	1.2476	0.0001	0.01226	0.00250	0.01389	0.00370
ASP	10	A	D	54.85	6.53	29.0221	0.0002	1.2356	<0.0001	0.00584	0.00086	0.00463	0.00112
ASP	10	A	D	104.36	14.31	29.0294	0.0002	1.2353	<0.0001	0.00712	0.00076	0.00409	0.00136
ASP	10	A	D	31.15	4.64	30.2398	0.0008	1.187	<0.0001	0.00792	0.00110	0.00697	0.00188
ASP	10	A	D	38.14	11.68	30.4184	0.0002	1.1802	<0.0001	0.00000	0.00000	0.00508	0.00194
ASP	10	A	D	148.91	7.79	30.4231	0.0004	1.18	<0.0001	0.01147	0.00040	0.01053	0.00070
ASP	10	A	D	4.87	1.68	30.5975	0.0008	1.1734	<0.0001	0.00580	0.00242	0.00000	0.00000
ASP	10	A	D	11.67	1.85	30.6044	0.0008	1.1732	<0.0001	0.00000	0.00000	0.01486	0.00488
ASP	10	A	D	18.22	2.40	30.6067	0.0004	1.1731	<0.0001	0.00900	0.00128	0.00728	0.00212
ASP	10	A	D	235.31	13.13	31.132	0.0002	1.1538	<0.0001	0.00997	0.00070	0.00921	0.00088
ASP	10	A	D	64.95	4.90	31.4427	0.0004	1.1426	<0.0001	0.00787	0.00078	0.00659	0.00098
ASP	10	A	D	21.25	1.20	31.9559	0.0012	1.1248	<0.0001	0.00549	0.00048	0.00105	0.00000
ASP	10	A	D	44.06	21.25	33.9095	0.0004	1.0617	<0.0001	0.00732	0.00284	0.00000	0.00000
ASP	10	A	D	38.45	3.84	33.9115	0.0006	1.0616	<0.0001	0.00471	0.00002	0.00103	0.00018
ASP	10	A	D	83.81	20.61	34.3841	0.0002	1.0475	<0.0001	0.00455	0.00108	0.00866	0.00192
ASP	10	A	D	172.49	4.84	34.3874	0.0002	1.0474	<0.0001	0.01044	0.00056	0.00995	0.00052
ASP	10	A	D	107.27	11.21	34.3891	0.0010	1.0473	<0.0001	0.01139	0.00240	0.01506	0.00182
ASP	10	A	D	82.17	34.10	34.4703	0.0036	1.0449	0.0001	0.00000	0.00000	0.02000	0.00388
ASP	10	A	D	83.86	11.63	35.6214	0.0002	1.0122	<0.0001	0.00538	0.00048	0.00394	0.00122
ASP	10	A	D	251.72	105.93	35.6282	0.0002	1.012	<0.0001	0.00449	0.00216	0.00000	0.00000
ASP	10	A	D	15.54	5.23	36.4542	0.0010	0.9899	<0.0001	0.01086	0.00292	0.00000	0.00000
ASP	10	A	D	31.45	5.60	37.3942	0.0006	0.9658	<0.0001	0.01003	0.00130	0.00606	0.00254
ASP	10	A	D	55.54	7.36	38.3271	0.0002	0.9432	<0.0001	0.00670	0.00068	0.00362	0.00110
ASP	10	B	H	191.65	8.72	8.3908	0.0004	4.2321	0.0002	0.02993	0.00082	0.02027	0.00194
ASP	10	B	H	42.66	3.09	9.2149	0.0002	3.8543	0.0001	0.01058	0.00100	0.01226	0.00128
ASP	10	B	H	1072.09	15.51	9.9379	0.0002	3.5745	0.0001	0.04674	0.00050	0.03730	0.00104
ASP	10	B	H	1867.71	21.14	10.7895	0.0002	3.2931	0.0001	0.06140	0.00048	0.04715	0.00104
ASP	10	B	H	488.99	8.05	11.7072	0.0000	3.0358	<0.0001	0.01073	0.00024	0.01128	0.00032
ASP	10	B	H	10.58	2.04	12.4998	0.0008	2.8440	0.0002	0.01284	0.00456	0.01318	0.00522
ASP	10	B	H	2027.10	64.79	13.0197	0.0002	2.7309	<0.0001	0.07305	0.00244	0.03160	0.00250
ASP	10	B	H	87.96	4.48	14.2572	0.0002	2.4949	<0.0001	0.01067	0.00048	0.00918	0.00092
ASP	10	B	H	141.03	9.13	15.574	0.0002	2.2851	<0.0001	0.01236	0.00046	0.00892	0.00126
ASP	10	B	H	92.30	2.39	16.0626	0.0028	2.2160	0.0004	0.09102	0.00504	0.03682	0.00044
ASP	10	B	H	159.26	17.03	16.8250	0.0008	2.1163	0.0001	0.04670	0.00300	0.02394	0.00620
ASP	10	B	H	80.84	3.65	17.0014	0.0002	2.0945	<0.0001	0.00866	0.00160	0.01221	0.00100
ASP	10	B	H	1349.19	33.01	17.2523	0.0004	2.0643	<0.0001	0.07731	0.00138	0.04344	0.00238
ASP	10	B	H	94.61	10.08	18.6296	0.0002	1.9128	<0.0001	0.01462	0.00118	0.00806	0.00198
ASP	10	B	H	137.06	5.46	19.0042	0.0002	1.8755	<0.0001	0.01157	0.00072	0.01154	0.00088
ASP	10	B	H	549.01	29.53	19.2080	0.0010	1.8558	0.0001	0.11538	0.00400	0.06478	0.00832
ASP	10	B	H	1240.95	28.64	19.572	0.0004	1.8216	<0.0001	0.10302	0.00128	0.06702	0.00342
ASP	10	B	H	69.66	5.90	19.9480	0.0020	1.7876	0.0002	0.06863	0.01636	0.08395	0.01454
ASP	10	B	H	18.89	5.36	20.8635	0.0136	1.7099	0.0011	0.00000	0.00000	0.18420	0.10410
ASP	10	B	H	41.64	4.30	21.2211	0.0188	1.6815	0.0015	0.00000	0.00000	0.31197	0.05340
ASP	10	B	H	595.18	22.81	21.6719	0.0010	1.6469	0.0001	0.14354	0.00278	0.09463	0.00826
ASP	10	B	H	22.15	2.74	21.956	0.0004	1.6258	<0.0001	0.01045	0.00218	0.01096	0.00272
ASP	10	B	H	72.44	3.71	22.256	0.0002	1.6042	<0.0001	0.01337	0.00086	0.01383	0.00132
ASP	10	B	H	94.16	15.17	23.1365	0.0074	1.5439	0.0005	0.00000	0.00000	0.16101	0.04444
ASP	10	B	H	104.08	3.87	23.1459	0.0044	1.5433	0.0003	0.00000	0.00000	0.20281	0.01118
ASP	10	B	H	32.18	3.43	23.4216	0.0004	1.5254	<0.0001	0.01025	0.00316	0.01130	0.00246
ASP	10	B	H	16.53	4.33	23.5356	0.0008	1.5181	0.0001	0.01356	0.00262	0.00970	0.00586
ASP	10	B	H	26.39	4.53	23.6472	0.0114	1.5110	0.0007	0.00000	0.00000	0.13834	0.02932
ASP	10	B	H	11.02	2.96	23.6689	0.0010	1.5097	0.0001	0.00000	0.00000	0.01521	0.00864
ASP	10	B	H	115.46	3.53	24.2022	0.0032	1.4769	0.0002	0.16360	0.01830	0.18216	0.00718

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	B	H	7.57	1.36	24.2625	0.0016	1.4733	0.0001	0.00000	0.00000	0.01191	0.00382
ASP	10	B	H	33.62	4.04	24.8245	0.0004	1.4404	<0.0001	0.01183	0.00086	0.01235	0.00192
ASP	10	B	H	20.70	4.69	25.1516	0.0006	1.422	<0.0001	0.01287	0.00156	0.00871	0.00448
ASP	10	B	H	34.94	2.97	25.2940	0.0124	1.4141	0.0007	0.00000	0.00000	0.22456	0.03106
ASP	10	B	H	97.71	15.36	26.2027	0.0076	1.3659	0.0004	0.03022	0.00628	0.00264	0.00002
ASP	10	B	H	7.86	0.80	26.3792	0.0008	1.3569	<0.0001	0.00000	0.00000	0.01352	0.00194
ASP	10	B	H	25.89	1.90	26.4893	0.0042	1.3514	0.0002	0.00000	0.00000	0.10348	0.01130
ASP	10	B	H	51.54	8.77	26.8306	0.0046	1.3345	0.0002	0.12570	0.01452	0.08514	0.03446
ASP	10	B	H	223.87	18.43	27.2917	0.0014	1.3124	0.0001	0.12253	0.00758	0.06323	0.01276
ASP	10	B	H	17.00	3.14	27.6243	0.0008	1.2969	<0.0001	0.01539	0.00256	0.01386	0.00550
ASP	10	B	H	378.58	24.35	27.8309	0.0014	1.2874	0.0001	0.17010	0.00818	0.08662	0.01366
ASP	10	B	H	5.16	1.36	28.7388	0.0010	1.2476	<0.0001	0.00000	0.00000	0.01262	0.00718
ASP	10	B	H	20.15	5.49	29.0283	0.0004	1.2354	<0.0001	0.01294	0.00276	0.00000	0.00000
ASP	10	B	H	66.92	33.46	30.1161	0.0038	1.1917	0.0001	0.11702	0.06210	0.00000	0.00000
ASP	10	B	H	82.87	39.43	30.8137	0.0060	1.1654	0.0002	0.20373	0.08752	0.00000	0.00000
ASP	10	B	H	29.02	4.20	31.1291	0.0004	1.1539	<0.0001	0.01614	0.00158	0.01170	0.00388
ASP	10	B	H	102.08	29.34	31.3207	0.0106	1.1470	0.0004	0.19194	0.03070	0.00000	0.00000
ASP	10	B	H	239.35	115.67	31.5276	0.0178	1.1396	0.0006	0.26107	0.14684	0.00000	0.00000
ASP	10	B	H	166.55	16.60	32.4402	0.0034	1.1084	0.0001	0.23613	0.01798	0.16321	0.03780
ASP	10	B	H	5.02	0.60	33.9128	0.0010	1.0616	<0.0001	0.00000	0.00000	0.01348	0.00228
ASP	10	B	H	24.16	2.34	34.389	0.0004	1.0473	<0.0001	0.01118	0.00178	0.01051	0.00212
ASP	10	B	H	20.19	2.55	34.4693	0.0004	1.045	<0.0001	0.01364	0.00260	0.01225	0.00334
ASP	10	B	H	17.10	4.07	34.9167	0.0140	1.0320	0.0004	0.00000	0.00000	0.14615	0.04464
ASP	10	B	H	12.91	2.27	35.6268	0.0006	1.0121	<0.0001	0.00000	0.00000	0.01470	0.00556
ASP	10	B	H	13.54	3.19	37.4737	0.0010	0.9639	<0.0001	0.00000	0.00000	0.01806	0.00936
ASP	10	B	H	105.35	36.89	38.3801	0.0074	0.9419	0.0002	0.21002	0.07766	0.00000	0.00000
ASP	10	B	H	6.61	2.63	38.5518	0.0014	0.9379	<0.0001	0.01734	0.00680	0.00000	0.00000
ASP	10	B	D	387.57	3.45	9.214	0.0000	3.8547	<0.0001	0.00582	0.00018	0.00990	0.00012
ASP	10	B	D	8.06	3.64	9.2194	0.0006	3.8524	0.0003	0.00000	0.00000	0.00392	0.00236
ASP	10	B	D	2657.77	339.28	11.7041	0.0006	3.0366	0.0002	0.00488	0.00042	0.00584	0.00076
ASP	10	B	D	4561.73	28.75	11.7068	0.0000	3.0359	<0.0001	0.00538	0.00014	0.00988	0.00008
ASP	10	B	D	2345.13	310.10	11.7089	0.0010	3.0353	0.0003	0.00426	0.00068	0.00684	0.00110
ASP	10	B	D	98.85	2.38	12.4975	0.0002	2.8445	<0.0001	0.00794	0.00080	0.01079	0.00040
ASP	10	B	D	4.22	1.38	12.6040	0.0012	2.8206	0.0003	0.01265	0.00568	0.00000	0.00000
ASP	10	B	D	514.51	8.85	14.2558	0.0002	2.4952	<0.0001	0.00549	0.00046	0.01078	0.00026
ASP	10	B	D	876.86	10.83	15.5726	0.0000	2.2853	<0.0001	0.00726	0.00022	0.01051	0.00020
ASP	10	B	D	839.22	16.83	16.9993	0.0002	2.0947	<0.0001	0.00569	0.00024	0.01077	0.00022
ASP	10	B	D	411.22	8.41	18.4827	0.0002	1.9279	<0.0001	0.00775	0.00044	0.01086	0.00036
ASP	10	B	D	917.16	25.43	18.6287	0.0002	1.9129	<0.0001	0.00865	0.00028	0.01126	0.00026
ASP	10	B	D	931.48	12.90	19.0025	0.0000	1.8756	<0.0001	0.00767	0.00028	0.01081	0.00024
ASP	10	B	D	172.85	3.58	21.9527	0.0000	1.6261	<0.0001	0.00757	0.00052	0.01055	0.00038
ASP	10	B	D	558.68	11.73	22.2536	0.0002	1.6044	<0.0001	0.00732	0.00050	0.01137	0.00036
ASP	10	B	D	58.95	1.72	22.4931	0.0002	1.5875	<0.0001	0.00747	0.00080	0.01031	0.00058
ASP	10	B	D	184.79	8.06	23.416	0.0004	1.5257	<0.0001	0.00646	0.00104	0.00967	0.00082
ASP	10	B	D	336.99	6.28	23.4183	0.0000	1.5256	<0.0001	0.00691	0.00048	0.01116	0.00032
ASP	10	B	D	50.63	19.22	23.4231	0.0004	1.5253	<0.0001	0.00605	0.00188	0.00000	0.00000
ASP	10	B	D	106.76	3.64	23.5337	0.0002	1.5182	<0.0001	0.00662	0.00100	0.01310	0.00072
ASP	10	B	D	161.71	4.77	23.667	0.0002	1.5098	<0.0001	0.00795	0.00086	0.01194	0.00058
ASP	10	B	D	33.64	7.09	23.6714	0.0008	1.5095	0.0001	0.00548	0.00182	0.00600	0.00202
ASP	10	B	D	167.78	3.81	24.2592	0.0002	1.4735	<0.0001	0.00848	0.00046	0.01081	0.00040
ASP	10	B	D	362.92	10.81	24.8201	0.0002	1.4407	<0.0001	0.00778	0.00072	0.01121	0.00054
ASP	10	B	D	140.30	8.94	25.1476	0.0004	1.4222	<0.0001	0.00897	0.00194	0.01242	0.00138
ASP	10	B	D	65.21	2.31	26.3759	0.0002	1.3571	<0.0001	0.01044	0.00052	0.01221	0.00068
ASP	10	B	D	107.95	4.99	26.7319	0.0002	1.3393	<0.0001	0.01087	0.00102	0.01433	0.00084
ASP	10	B	D	104.15	41.79	26.7335	0.0020	1.3392	0.0001	0.00822	0.00270	0.00855	0.00112
ASP	10	B	D	160.06	4.67	27.62	0.0002	1.2971	<0.0001	0.01085	0.00054	0.01167	0.00062
ASP	10	B	D	47.99	2.32	27.8813	0.0002	1.2851	<0.0001	0.01022	0.00106	0.01157	0.00102
ASP	10	B	D	75.30	8.00	28.7347	0.0004	1.2477	<0.0001	0.00964	0.00084	0.01082	0.00088
ASP	10	B	D	111.55	4.78	29.0243	0.0002	1.2355	<0.0001	0.01116	0.00056	0.01198	0.00076
ASP	10	B	D	30.21	3.87	30.2405	0.0004	1.1869	<0.0001	0.01196	0.00134	0.01199	0.00198
ASP	10	B	D	64.32	13.75	30.4189	0.0006	1.1801	<0.0001	0.00770	0.00106	0.00461	0.00168
ASP	10	B	D	126.04	5.55	30.4223	0.0002	1.18	<0.0001	0.01077	0.00072	0.01103	0.00070
ASP	10	B	D	16.77	3.37	30.6025	0.0008	1.1732	<0.0001	0.01235	0.00354	0.01165	0.00354
ASP	10	B	D	211.67	6.65	31.127	0.0002	1.1539	<0.0001	0.01030	0.00062	0.01164	0.00064
ASP	10	B	D	126.45	4.29	31.446	0.0002	1.1425	<0.0001	0.00922	0.00070	0.01122	0.00070
ASP	10	B	D	31.73	3.09	31.9513	0.0004	1.1249	<0.0001	0.00850	0.00370	0.01215	0.00224
ASP	10	B	D	57.80	3.79	33.9107	0.0004	1.0617	<0.0001	0.00992	0.00252	0.01362	0.00164
ASP	10	B	D	31.76	4.44	33.9144	0.0004	1.0616	<0.0001	0.00750	0.00078	0.00550	0.00174
ASP	10	B	D	156.45	4.97	34.3865	0.0002	1.0474	<0.0001	0.00734	0.00134	0.01285	0.00068
ASP	10	B	D	160.22	5.80	34.4682	0.0002	1.045	<0.0001	0.01066	0.00096	0.01325	0.00086
ASP	10	B	D	60.05	6.37	34.7957	0.0004	1.0355	<0.0001	0.01503	0.00100	0.01102	0.00246
ASP	10	B	D	10.13	2.85	35.2261	0.0012	1.0232	<0.0001	0.01168	0.00768	0.01227	0.00720
ASP	10	B	D	128.39	5.92	35.6264	0.0002	1.0121	<0.0001	0.01274	0.00094	0.01318	0.00112
ASP	10	B	D	17.79	3.27	36.4529	0.0006	0.9899	<0.0001	0.01259	0.00242	0.01063	0.00416
ASP	10	B	D	64.13	5.98	36.6443	0.0004	0.9849	<0.0001	0.01351	0.00080	0.01007	0.00198
ASP	10	B	D	14.38	3.70	36.8007	0.0010	0.9809	<0.0001	0.01470	0.00342	0.01180	0.00666
ASP	10	B	D	46.34	4.24	36.9541	0.0004	0.9769	<0.0001	0.01381	0.00196	0.01354	0.00246
ASP	10	B	D	56.05	4.00	37.3966	0.0004	0.9658	<0.0001	0.00860	0.00102	0.01173	0.00158
ASP	10	B	D	10.18	4.73	37.4044	0.0006	0.9656	<0.0001	0.00580	0.00182	0.00000	0.00000

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	B	D	107.97	5.40	37.4716	0.0002	0.9639	<0.0001	0.01068	0.00076	0.01062	0.00100
ASP	10	B	D	18.27	3.42	37.775	0.0006	0.9564	<0.0001	0.01226	0.00284	0.01081	0.00428
ASP	10	B	D	8.69	3.22	37.9526	0.0010	0.9521	<0.0001	0.01184	0.00350	0.00000	0.00000
ASP	10	B	D	72.41	4.35	38.3302	0.0002	0.9431	<0.0001	0.01128	0.00146	0.01267	0.00142
ASP	10	B	D	36.22	3.38	38.5512	0.0004	0.9379	<0.0001	0.00991	0.00320	0.01286	0.00230
ASP	10	B	W	200.71	2.19	9.2129	0.0000	3.8551	<0.0001	0.00471	0.00028	0.01013	0.00016
ASP	10	B	W	2029.81	27.32	11.7075	0.0000	3.0357	<0.0001	0.00468	0.00036	0.01080	0.00020
ASP	10	B	W	47.90	1.31	12.4983	0.0002	2.8443	<0.0001	0.00698	0.00034	0.00949	0.00032
ASP	10	B	W	4.76	0.53	12.6050	0.0004	2.8203	0.0001	0.01082	0.00176	0.01007	0.00230
ASP	10	B	W	306.30	3.52	14.2574	0.0000	2.4949	<0.0001	0.00543	0.00030	0.01073	0.00018
ASP	10	B	W	578.37	4.56	15.5763	0.0000	2.2848	<0.0001	0.00591	0.00018	0.01066	0.00012
ASP	10	B	W	426.83	6.81	17.002	0.0000	2.0944	<0.0001	0.00449	0.00048	0.01053	0.00024
ASP	10	B	W	168.71	3.43	18.4863	0.0002	1.9275	<0.0001	0.00741	0.00052	0.01133	0.00036
ASP	10	B	W	501.18	5.16	18.6319	0.0000	1.9126	<0.0001	0.00710	0.00020	0.01072	0.00016
ASP	10	B	W	496.80	5.13	19.0055	0.0000	1.8753	<0.0001	0.00692	0.00022	0.01094	0.00016
ASP	10	B	W	137.43	1.80	21.958	0.0000	1.6257	<0.0001	0.00711	0.00032	0.01094	0.00024
ASP	10	B	W	277.62	5.71	22.2575	0.0002	1.6041	<0.0001	0.00707	0.00050	0.01129	0.00036
ASP	10	B	W	38.28	1.62	22.4995	0.0004	1.587	<0.0001	0.00000	0.00000	0.01118	0.00072
ASP	10	B	W	174.28	2.53	23.4227	0.0000	1.5253	<0.0001	0.00693	0.00032	0.01058	0.00024
ASP	10	B	W	75.26	1.93	23.5396	0.0002	1.5178	<0.0001	0.00701	0.00070	0.01096	0.00046
ASP	10	B	W	74.77	1.96	23.6728	0.0002	1.5094	<0.0001	0.00884	0.00056	0.01126	0.00050
ASP	10	B	W	80.28	2.03	24.2638	0.0002	1.4732	<0.0001	0.00808	0.00052	0.01057	0.00044
ASP	10	B	W	187.09	4.80	24.8274	0.0002	1.4403	<0.0001	0.00758	0.00056	0.01086	0.00044
ASP	10	B	W	25.52	5.41	24.8288	0.0006	1.4402	<0.0001	0.00000	0.00000	0.00627	0.00160
ASP	10	B	W	123.04	4.66	25.1536	0.0002	1.4219	<0.0001	0.00724	0.00080	0.01013	0.00062
ASP	10	B	W	37.19	1.14	26.3805	0.0002	1.3568	<0.0001	0.00629	0.00136	0.01209	0.00060
ASP	10	B	W	56.92	1.69	26.7384	0.0002	1.339	<0.0001	0.00861	0.00048	0.00978	0.00050
ASP	10	B	W	102.31	3.42	27.6288	0.0002	1.2966	<0.0001	0.00881	0.00096	0.01251	0.00068
ASP	10	B	W	21.83	0.75	27.8877	0.0002	1.2848	<0.0001	0.00865	0.00092	0.01122	0.00070
ASP	10	B	W	64.35	2.03	28.7445	0.0002	1.2473	<0.0001	0.00720	0.00082	0.01093	0.00058
ASP	10	B	W	77.81	2.48	29.0305	0.0002	1.2353	<0.0001	0.00862	0.00076	0.01131	0.00064
ASP	10	B	W	21.12	0.85	30.2453	0.0002	1.1868	<0.0001	0.00775	0.00140	0.01159	0.00082
ASP	10	B	W	84.92	1.63	30.4258	0.0000	1.1799	<0.0001	0.00979	0.00036	0.01143	0.00038
ASP	10	B	W	60.92	15.05	30.4263	0.0006	1.1799	<0.0001	0.01161	0.00248	0.01301	0.00148
ASP	10	B	W	8.58	0.82	30.6111	0.0004	1.1729	<0.0001	0.01197	0.00328	0.01356	0.00264
ASP	10	B	W	155.37	2.48	31.1329	0.0000	1.1537	<0.0001	0.01034	0.00026	0.01127	0.00030
ASP	10	B	W	82.34	1.34	31.4515	0.0000	1.1423	<0.0001	0.00945	0.00032	0.01116	0.00032
ASP	10	B	W	0.70	0.25	31.7836	0.0020	1.1307	0.0001	0.00000	0.00000	0.01076	0.00482
ASP	10	B	W	15.49	1.00	31.9586	0.0002	1.1247	<0.0001	0.00983	0.00138	0.01080	0.00132
ASP	10	B	W	27.37	1.22	33.9173	0.0002	1.0615	<0.0001	0.00965	0.00160	0.01338	0.00108
ASP	10	B	W	90.39	1.95	34.3942	0.0002	1.0472	<0.0001	0.00902	0.00054	0.01214	0.00044
ASP	10	B	W	96.45	2.15	34.4751	0.0002	1.0448	<0.0001	0.00986	0.00046	0.01206	0.00048
ASP	10	B	W	41.44	1.35	34.8044	0.0002	1.0352	<0.0001	0.01092	0.00266	0.02042	0.00116
ASP	10	B	W	9.01	0.87	35.2327	0.0004	1.023	<0.0001	0.00911	0.00262	0.01220	0.00230
ASP	10	B	W	89.50	1.80	35.6352	0.0000	1.0118	<0.0001	0.01174	0.00032	0.01171	0.00042
ASP	10	B	W	13.22	1.20	36.4622	0.0002	0.9896	<0.0001	0.01175	0.00060	0.00825	0.00162
ASP	10	B	W	53.30	1.56	36.6542	0.0002	0.9846	<0.0001	0.01110	0.00044	0.01102	0.00060
ASP	10	B	W	13.99	1.72	36.8086	0.0002	0.9806	<0.0001	0.01210	0.00092	0.00735	0.00204
ASP	10	B	W	31.30	1.81	36.9625	0.0002	0.9767	<0.0001	0.01261	0.00040	0.00867	0.00108
ASP	10	B	W	33.18	1.76	37.4043	0.0002	0.9656	<0.0001	0.01059	0.00056	0.00927	0.00096
ASP	10	B	W	4.05	0.90	37.4053	0.0004	0.9655	<0.0001	0.00000	0.00000	0.00506	0.00156
ASP	10	B	W	53.62	2.06	37.4797	0.0002	0.9637	<0.0001	0.01340	0.00056	0.01218	0.00090
ASP	10	B	W	19.07	1.16	37.7833	0.0002	0.9562	<0.0001	0.01013	0.00148	0.01160	0.00132
ASP	10	B	W	5.87	0.69	37.9625	0.0006	0.9519	<0.0001	0.01000	0.00520	0.01427	0.00320
ASP	10	B	W	59.27	1.81	38.3379	0.0002	0.9429	<0.0001	0.01031	0.00054	0.01113	0.00060
ASP	10	B	W	25.47	1.32	38.561	0.0002	0.9377	<0.0001	0.01122	0.00130	0.01271	0.00124
ASP	10	C	H	138.20	14.68	8.3891	0.0004	4.2329	0.0002	0.02912	0.00312	0.01324	0.00342
ASP	10	C	H	125.93	4.10	9.2136	0.0002	3.8548	0.0001	0.01014	0.00034	0.00983	0.00056
ASP	10	C	H	748.76	16.30	9.9363	0.0002	3.5751	0.0001	0.04571	0.00066	0.02971	0.00134
ASP	10	C	H	1305.72	20.84	10.7878	0.0002	3.2936	0.0001	0.06180	0.00064	0.04073	0.00134
ASP	10	C	H	1775.72	13.01	11.7051	0.0000	3.0363	<0.0001	0.00947	0.00010	0.01043	0.00012
ASP	10	C	H	43.51	4.54	12.4964	0.0002	2.8447	<0.0001	0.01090	0.00068	0.00724	0.00162
ASP	10	C	H	1400.66	93.04	13.0174	0.0004	2.7314	0.0001	0.06452	0.00508	0.02293	0.00396
ASP	10	C	H	173.10	5.10	14.2555	0.0002	2.4952	<0.0001	0.01133	0.00036	0.01056	0.00056
ASP	10	C	H	390.26	8.38	15.572	0.0000	2.2854	<0.0001	0.01079	0.00036	0.01091	0.00042
ASP	10	C	H	57.63	5.73	16.0623	0.0032	2.2161	0.0004	0.08606	0.00036	0.03636	0.00754
ASP	10	C	H	100.84	9.96	16.8226	0.0008	2.1166	0.0001	0.04952	0.00266	0.03032	0.00694
ASP	10	C	H	297.13	5.91	16.9981	0.0000	2.0949	<0.0001	0.00944	0.00040	0.01130	0.00038
ASP	10	C	H	910.58	29.81	17.2493	0.0004	2.0646	<0.0001	0.07150	0.00182	0.03801	0.00290
ASP	10	C	H	117.99	5.21	18.4821	0.0002	1.928	<0.0001	0.01321	0.00038	0.01013	0.00090
ASP	10	C	H	469.10	7.03	18.6262	0.0000	1.9132	<0.0001	0.01169	0.00020	0.01136	0.00030
ASP	10	C	H	386.74	6.91	19.001	0.0000	1.8758	<0.0001	0.01200	0.00022	0.01078	0.00036
ASP	10	C	H	376.71	29.81	19.2051	0.0010	1.8560	0.0001	0.11119	0.00700	0.05493	0.01082
ASP	10	C	H	863.38	23.42	19.5688	0.0004	1.8219	<0.0001	0.10257	0.00188	0.05785	0.00366
ASP	10	C	H	54.68	7.80	19.9455	0.0022	1.7878	0.0002	0.07760	0.00708	0.05551	0.01818
ASP	10	C	H	73.33	3.02	21.9518	0.0002	1.6261	<0.0001	0.01117	0.00092	0.01230	0.00096
ASP	10	C	H	170.02	4.36	22.2522	0.0002	1.6045	<0.0001	0.01300	0.00034	0.01199	0.00058
ASP	10	C	H	20.93	3.00	22.4911	0.0004	1.5876	<0.0001	0.01472	0.00120	0.01030	0.00330

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	C	H	131.93	4.73	23.4179	0.0002	1.5256	<0.0001	0.01157	0.00036	0.00972	0.00068
ASP	10	C	H	49.38	4.00	23.5318	0.0002	1.5183	<0.0001	0.01215	0.00072	0.00933	0.00162
ASP	10	C	H	52.83	4.95	23.6647	0.0004	1.5099	<0.0001	0.01468	0.00222	0.01265	0.00260
ASP	10	C	H	39.67	3.51	24.2584	0.0004	1.4735	<0.0001	0.01278	0.00226	0.01285	0.00238
ASP	10	C	H	148.23	4.12	24.8201	0.0002	1.4407	<0.0001	0.01199	0.00042	0.01164	0.00060
ASP	10	C	H	83.51	3.88	25.1464	0.0002	1.4223	<0.0001	0.01430	0.00102	0.01390	0.00128
ASP	10	C	H	28.08	2.06	26.3738	0.0004	1.3572	<0.0001	0.00000	0.00000	0.01455	0.00202
ASP	10	C	H	26.48	10.67	26.4806	0.0054	1.3518	0.0003	0.10246	0.01816	0.00000	0.00000
ASP	10	C	H	54.06	3.16	26.7303	0.0002	1.3394	<0.0001	0.01391	0.00166	0.01442	0.00168
ASP	10	C	H	35.94	8.87	26.8267	0.0054	1.3347	0.0003	0.12442	0.00040	0.08019	0.04860
ASP	10	C	H	155.88	44.11	27.2865	0.0016	1.3126	0.0001	0.09739	0.03306	0.00000	0.00000
ASP	10	C	H	64.78	3.06	27.6192	0.0002	1.2971	<0.0001	0.01262	0.00168	0.01463	0.00134
ASP	10	C	H	30.15	2.73	28.7359	0.0004	1.2477	<0.0001	0.01333	0.00076	0.01060	0.00198
ASP	10	C	H	55.45	3.64	29.0218	0.0002	1.2357	<0.0001	0.01472	0.00064	0.01099	0.00152
ASP	10	C	H	2.21	0.85	29.4226	0.0112	1.2192	0.0005	0.00000	0.00000	0.04990	0.02888
ASP	10	C	H	10.54	1.60	30.2368	0.0006	1.1871	<0.0001	0.01076	0.00658	0.01337	0.00422
ASP	10	C	H	59.30	4.99	30.4178	0.0002	1.1802	<0.0001	0.01555	0.00080	0.00946	0.00180
ASP	10	C	H	6.55	2.88	30.5975	0.0014	1.1734	0.0001	0.01699	0.00610	0.00000	0.00000
ASP	10	C	H	95.59	4.70	31.1242	0.0002	1.154	<0.0001	0.01528	0.00050	0.01156	0.00120
ASP	10	C	H	43.87	5.32	31.4424	0.0004	1.1427	<0.0001	0.01497	0.00102	0.01028	0.00290
ASP	10	C	H	9.80	1.60	31.9479	0.0008	1.125	<0.0001	0.01523	0.00308	0.01461	0.00496
ASP	10	C	H	15.91	1.94	33.9058	0.0006	1.0618	<0.0001	0.01489	0.00574	0.01810	0.00448
ASP	10	C	H	101.81	42.00	34.3841	0.0002	1.0475	<0.0001	0.00557	0.00298	0.00000	0.00000
ASP	10	C	H	58.46	3.00	34.4646	0.0002	1.0451	<0.0001	0.01275	0.00136	0.01372	0.00136
ASP	10	C	H	35.75	3.68	34.7921	0.0006	1.0356	<0.0001	0.02142	0.00466	0.02068	0.00456
ASP	10	C	H	4.39	0.61	35.2203	0.0012	1.0234	<0.0001	0.00000	0.00000	0.01414	0.00276
ASP	10	C	H	61.95	3.78	35.6211	0.0002	1.0122	<0.0001	0.01597	0.00090	0.01476	0.00188
ASP	10	C	H	5.55	0.80	36.451	0.0016	0.9899	<0.0001	0.00000	0.00000	0.01899	0.00408
ASP	10	C	H	23.88	2.59	36.6416	0.0006	0.985	<0.0001	0.01646	0.00276	0.01511	0.00348
ASP	10	C	H	8.27	2.89	36.7977	0.0014	0.9809	<0.0001	0.01679	0.00852	0.00000	0.00000
ASP	10	C	H	24.34	3.80	36.9489	0.0006	0.9771	<0.0001	0.01603	0.00268	0.01543	0.00532
ASP	10	C	H	20.48	3.32	37.3941	0.0006	0.9658	<0.0001	0.01317	0.00802	0.01439	0.00516
ASP	10	C	H	43.82	5.28	37.4677	0.0004	0.964	<0.0001	0.01753	0.00124	0.01208	0.00336
ASP	10	C	H	10.57	3.92	37.7686	0.0014	0.9566	<0.0001	0.02352	0.00486	0.00000	0.00000
ASP	10	C	H	40.05	5.74	38.327	0.0004	0.9432	<0.0001	0.01692	0.00112	0.01073	0.00364
ASP	10	C	H	17.72	2.89	38.5468	0.0006	0.938	<0.0001	0.01657	0.00234	0.01283	0.00466
ASP	10	C	D	402.26	3.36	9.2141	0.0000	3.8546	<0.0001	0.00592	0.00018	0.01039	0.00012
ASP	10	C	D	3944.07	25.49	11.7063	0.0000	3.036	<0.0001	0.00599	0.00014	0.01085	0.00010
ASP	10	C	D	98.18	2.57	12.4985	0.0002	2.8443	<0.0001	0.00682	0.00052	0.00955	0.00040
ASP	10	C	D	5.46	0.43	12.6035	0.0008	2.8207	0.0002	0.00000	0.00000	0.01540	0.00162
ASP	10	C	D	680.64	8.24	14.2564	0.0000	2.495	<0.0001	0.00648	0.00026	0.01067	0.00018
ASP	10	C	D	978.55	14.60	15.5732	0.0000	2.2852	<0.0001	0.00667	0.00034	0.01111	0.00024
ASP	10	C	D	979.45	14.83	16.9996	0.0000	2.0947	<0.0001	0.00557	0.00042	0.01132	0.00024
ASP	10	C	D	352.34	10.97	18.4832	0.0002	1.9279	<0.0001	0.00823	0.00066	0.01080	0.00056
ASP	10	C	D	1020.96	17.59	18.6289	0.0000	1.9129	<0.0001	0.00858	0.00030	0.01084	0.00030
ASP	10	C	D	1133.21	13.64	19.0031	0.0000	1.8756	<0.0001	0.00807	0.00022	0.01088	0.00020
ASP	10	C	D	235.48	3.75	21.9536	0.0000	1.626	<0.0001	0.00816	0.00034	0.01108	0.00028
ASP	10	C	D	577.03	8.93	22.2536	0.0000	1.6044	<0.0001	0.00905	0.00026	0.01111	0.00028
ASP	10	C	D	54.08	2.27	22.4947	0.0002	1.5874	<0.0001	0.00604	0.00202	0.01202	0.00086
ASP	10	C	D	128.86	31.20	23.4167	0.0006	1.5257	<0.0001	0.00000	0.00000	0.00625	0.00204
ASP	10	C	D	326.60	6.38	23.4194	0.0002	1.5255	<0.0001	0.00739	0.00056	0.01186	0.00036
ASP	10	C	D	92.65	27.52	23.4228	0.0008	1.5253	0.0001	0.00000	0.00000	0.00697	0.00330
ASP	10	C	D	152.44	3.11	23.5347	0.0002	1.5182	<0.0001	0.00704	0.00068	0.01189	0.00038
ASP	10	C	D	120.60	3.24	23.6678	0.0002	1.5097	<0.0001	0.00959	0.00080	0.01274	0.00050
ASP	10	C	D	131.13	4.01	24.2598	0.0002	1.4734	<0.0001	0.00868	0.00080	0.01182	0.00062
ASP	10	C	D	138.83	56.34	24.8181	0.0012	1.4408	0.0001	0.00000	0.00000	0.00706	0.00226
ASP	10	C	D	592.00	16.57	24.8213	0.0002	1.4406	<0.0001	0.00667	0.00098	0.01280	0.00052
ASP	10	C	D	251.14	7.92	25.1509	0.0002	1.422	<0.0001	0.00968	0.00070	0.01217	0.00064
ASP	10	C	D	89.13	1.99	26.3765	0.0002	1.357	<0.0001	0.00872	0.00050	0.01113	0.00042
ASP	10	C	D	128.63	4.21	26.7333	0.0002	1.3393	<0.0001	0.00994	0.00066	0.01155	0.00066
ASP	10	C	D	198.30	5.50	27.6216	0.0002	1.297	<0.0001	0.01106	0.00052	0.01206	0.00058
ASP	10	C	D	43.25	1.95	27.8812	0.0002	1.2851	<0.0001	0.01079	0.00070	0.01059	0.00092
ASP	10	C	D	113.77	2.92	28.737	0.0002	1.2476	<0.0001	0.01002	0.00038	0.01057	0.00048
ASP	10	C	D	143.05	3.34	29.0249	0.0002	1.2355	<0.0001	0.01111	0.00036	0.01141	0.00048
ASP	10	C	D	30.31	1.51	30.2379	0.0002	1.187	<0.0001	0.00779	0.00240	0.01235	0.00118
ASP	10	C	D	153.00	2.66	30.4205	0.0000	1.1801	<0.0001	0.00922	0.00042	0.01161	0.00036
ASP	10	C	D	13.94	1.16	30.6014	0.0004	1.1733	<0.0001	0.00000	0.00000	0.01508	0.00246
ASP	10	C	D	29.50	5.89	31.1217	0.0006	1.1541	<0.0001	0.00000	0.00000	0.00639	0.00156
ASP	10	C	D	336.86	6.81	31.1249	0.0000	1.154	<0.0001	0.01052	0.00026	0.01031	0.00038
ASP	10	C	D	112.03	3.61	31.4437	0.0002	1.1426	<0.0001	0.01036	0.00076	0.01216	0.00070
ASP	10	C	D	25.34	1.98	31.9505	0.0004	1.1249	<0.0001	0.00792	0.00476	0.01375	0.00202
ASP	10	C	D	40.35	2.41	33.9079	0.0002	1.0618	<0.0001	0.01245	0.00114	0.01206	0.00144
ASP	10	C	D	170.14	3.17	34.3855	0.0000	1.0474	<0.0001	0.01008	0.00034	0.01113	0.00038
ASP	10	C	D	169.99	3.31	34.4659	0.0000	1.0451	<0.0001	0.01105	0.00032	0.01151	0.00040
ASP	10	C	D	72.92	3.47	34.7949	0.0002	1.0355	<0.0001	0.01731	0.00078	0.01472	0.00142
ASP	10	C	D	11.48	1.54	35.2233	0.0006	1.0233	<0.0001	0.01024	0.00394	0.01257	0.00346
ASP	10	C	D	145.61	4.19	35.6242	0.0002	1.0121	<0.0001	0.01281	0.00030	0.01168	0.00060
ASP	10	C	D	73.38	2.54	36.6425	0.0002	0.9849	<0.0001	0.01182	0.00066	0.01188	0.00078
ASP	10	C	D	14.44	1.44	36.7973	0.0004	0.9809	<0.0001	0.01157	0.00254	0.01278	0.00258

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	C	D	52.45	2.13	36.952	0.0002	0.977	<0.0001	0.01128	0.00108	0.01281	0.00100
ASP	10	C	D	50.81	2.18	37.3948	0.0002	0.9658	<0.0001	0.01202	0.00076	0.01159	0.00098
ASP	10	C	D	68.01	2.96	37.4699	0.0002	0.9639	<0.0001	0.01582	0.00074	0.01390	0.00124
ASP	10	C	D	22.01	2.87	37.7741	0.0004	0.9565	<0.0001	0.01329	0.00096	0.00844	0.00250
ASP	10	C	D	10.30	1.66	37.9511	0.0006	0.9522	<0.0001	0.01290	0.00252	0.01105	0.00388
ASP	10	C	D	87.62	2.55	38.3281	0.0002	0.9431	<0.0001	0.01164	0.00066	0.01272	0.00068
ASP	10	C	D	36.35	1.79	38.5493	0.0002	0.9379	<0.0001	0.01120	0.00190	0.01430	0.00136
ASP	10	C	W	190.55	2.54	9.2127	0.0000	3.8552	<0.0001	0.00418	0.00040	0.01043	0.00018
ASP	10	C	W	1753.90	18.60	11.7078	0.0000	3.0356	<0.0001	0.00455	0.00026	0.01031	0.00014
ASP	10	C	W	50.22	1.54	12.499	0.0002	2.8442	<0.0001	0.00554	0.00084	0.01245	0.00058
ASP	10	C	W	3.44	0.43	12.6054	0.0004	2.8202	0.0001	0.00798	0.00448	0.01090	0.00264
ASP	10	C	W	340.82	4.58	14.2571	0.0000	2.4949	<0.0001	0.00432	0.00038	0.00997	0.00018
ASP	10	C	W	523.96	7.01	15.5763	0.0000	2.2848	<0.0001	0.00481	0.00036	0.01055	0.00020
ASP	10	C	W	557.96	7.53	17.0025	0.0000	2.0944	<0.0001	0.00419	0.00042	0.01048	0.00020
ASP	10	C	W	163.42	3.05	18.4863	0.0000	1.9275	<0.0001	0.00721	0.00050	0.01144	0.00034
ASP	10	C	W	586.28	5.27	18.6317	0.0000	1.9126	<0.0001	0.00630	0.00018	0.01044	0.00014
ASP	10	C	W	631.91	6.05	19.0059	0.0000	1.8753	<0.0001	0.00556	0.00024	0.01070	0.00014
ASP	10	C	W	111.70	1.52	21.9576	0.0000	1.6257	<0.0001	0.00670	0.00040	0.01106	0.00024
ASP	10	C	W	216.43	4.34	22.2574	0.0002	1.6041	<0.0001	0.00667	0.00054	0.01150	0.00036
ASP	10	C	W	22.31	1.04	22.4988	0.0002	1.5871	<0.0001	0.00893	0.00070	0.01047	0.00084
ASP	10	C	W	30.17	3.49	23.4195	0.0004	1.5255	<0.0001	0.00000	0.00000	0.00601	0.00090
ASP	10	C	W	172.51	3.97	23.4224	0.0002	1.5253	<0.0001	0.00658	0.00060	0.01151	0.00040
ASP	10	C	W	66.78	3.59	23.5393	0.0004	1.5179	<0.0001	0.00667	0.00082	0.01093	0.00058
ASP	10	C	W	5.76	2.41	23.5423	0.0004	1.5177	<0.0001	0.00000	0.00000	0.00377	0.00244
ASP	10	C	W	111.97	3.66	23.6728	0.0002	1.5094	<0.0001	0.00620	0.00104	0.01153	0.00056
ASP	10	C	W	66.06	1.84	24.2644	0.0002	1.4732	<0.0001	0.00620	0.00088	0.01083	0.00048
ASP	10	C	W	159.41	2.94	24.8272	0.0000	1.4403	<0.0001	0.00581	0.00060	0.01108	0.00028
ASP	10	C	W	100.49	3.85	25.1547	0.0002	1.4218	<0.0001	0.00873	0.00074	0.01084	0.00070
ASP	10	C	W	52.34	1.38	26.3808	0.0002	1.3568	<0.0001	0.00612	0.00078	0.01040	0.00044
ASP	10	C	W	66.08	1.89	26.7387	0.0002	1.339	<0.0001	0.00870	0.00050	0.01027	0.00050
ASP	10	C	W	105.83	3.39	27.6285	0.0002	1.2967	<0.0001	0.00756	0.00102	0.01207	0.00058
ASP	10	C	W	25.27	1.08	27.8869	0.0002	1.2849	<0.0001	0.00855	0.00110	0.01102	0.00084
ASP	10	C	W	57.88	1.88	28.7437	0.0002	1.2474	<0.0001	0.00753	0.00086	0.01112	0.00062
ASP	10	C	W	52.35	2.08	29.0305	0.0002	1.2353	<0.0001	0.00904	0.00066	0.01048	0.00076
ASP	10	C	W	22.18	0.89	30.2461	0.0002	1.1867	<0.0001	0.00813	0.00102	0.01054	0.00076
ASP	10	C	W	89.26	1.69	30.4257	0.0000	1.1799	<0.0001	0.00887	0.00030	0.01003	0.00032
ASP	10	C	W	5.65	0.79	30.6092	0.0004	1.173	<0.0001	0.01308	0.00146	0.01003	0.00312
ASP	10	C	W	143.95	2.29	31.133	0.0000	1.1537	<0.0001	0.00942	0.00028	0.01128	0.00030
ASP	10	C	W	66.17	1.66	31.4513	0.0002	1.1423	<0.0001	0.00893	0.00046	0.01055	0.00046
ASP	10	C	W	14.53	1.03	31.9583	0.0002	1.1247	<0.0001	0.00987	0.00148	0.01070	0.00146
ASP	10	C	W	33.99	1.73	33.9173	0.0002	1.0615	<0.0001	0.00868	0.00060	0.00854	0.00082
ASP	10	C	W	82.53	2.19	34.3945	0.0002	1.0472	<0.0001	0.00885	0.00066	0.01152	0.00052
ASP	10	C	W	79.29	2.22	34.4753	0.0002	1.0448	<0.0001	0.00970	0.00062	0.01167	0.00058
ASP	10	C	W	56.55	1.86	34.8034	0.0002	1.0352	<0.0001	0.01141	0.00144	0.01652	0.00094
ASP	10	C	W	8.42	1.51	35.2334	0.0008	1.023	<0.0001	0.00738	0.00194	0.01024	0.00196
ASP	10	C	W	108.31	2.97	35.6345	0.0002	1.0119	<0.0001	0.01003	0.00028	0.00923	0.00046
ASP	10	C	W	14.76	1.57	36.4622	0.0004	0.9896	<0.0001	0.01242	0.00074	0.00855	0.00198
ASP	10	C	W	63.16	1.76	36.6543	0.0002	0.9846	<0.0001	0.01008	0.00042	0.01041	0.00052
ASP	10	C	W	8.72	1.24	36.8079	0.0004	0.9807	<0.0001	0.01166	0.00114	0.00879	0.00272
ASP	10	C	W	34.41	1.36	36.9622	0.0002	0.9767	<0.0001	0.01169	0.00058	0.01051	0.00082
ASP	10	C	W	33.70	1.52	37.4047	0.0002	0.9656	<0.0001	0.00983	0.00074	0.01023	0.00086
ASP	10	C	W	13.21	3.12	37.4742	0.0004	0.9638	<0.0001	0.00558	0.00100	0.00394	0.00172
ASP	10	C	W	58.88	1.76	37.4797	0.0002	0.9637	<0.0001	0.01067	0.00074	0.01274	0.00068
ASP	10	C	W	46.74	3.29	37.4813	0.0006	0.9637	<0.0001	0.01058	0.00076	0.01001	0.00152
ASP	10	C	W	11.39	1.30	37.7834	0.0004	0.9562	<0.0001	0.01230	0.00076	0.00830	0.00208
ASP	10	C	W	11.36	1.81	37.9622	0.0004	0.9519	<0.0001	0.01006	0.00092	0.00635	0.00228
ASP	10	C	W	45.16	4.23	38.3359	0.0006	0.943	<0.0001	0.00811	0.00092	0.00747	0.00126
ASP	10	C	W	70.63	1.83	38.3382	0.0002	0.9429	<0.0001	0.00877	0.00054	0.01079	0.00048
ASP	10	C	W	44.61	1.56	38.5613	0.0002	0.9377	<0.0001	0.00925	0.00084	0.01137	0.00072
ASP	10	D	H	93.81	9.62	8.3906	0.0006	4.2322	0.0003	0.03073	0.00254	0.01631	0.00388
ASP	10	D	H	220.44	4.94	9.2146	0.0002	3.8544	0.0001	0.00934	0.00034	0.01045	0.00040
ASP	10	D	H	543.06	17.30	9.9374	0.0002	3.5747	0.0001	0.04342	0.00102	0.02536	0.00178
ASP	10	D	H	934.31	19.43	10.7890	0.0002	3.2933	0.0001	0.06043	0.00084	0.03836	0.00168
ASP	10	D	H	2850.39	16.11	11.706	0.0000	3.0361	<0.0001	0.00933	0.00008	0.01076	0.00010
ASP	10	D	H	59.12	3.83	12.4973	0.0002	2.8445	<0.0001	0.01259	0.00072	0.01072	0.00138
ASP	10	D	H	1008.04	117.01	13.0189	0.0004	2.7310	0.0001	0.05814	0.00860	0.01828	0.00570
ASP	10	D	H	359.10	6.83	14.2572	0.0000	2.4949	<0.0001	0.01056	0.00024	0.01068	0.00036
ASP	10	D	H	603.50	10.68	15.5737	0.0000	2.2851	<0.0001	0.01117	0.00020	0.01014	0.00034
ASP	10	D	H	75.99	12.06	16.8234	0.0012	2.1165	0.0002	0.05074	0.00564	0.02725	0.01044
ASP	10	D	H	461.88	7.64	17.0006	0.0000	2.0946	<0.0001	0.00991	0.00024	0.01051	0.00030
ASP	10	D	H	671.94	33.94	17.2516	0.0004	2.0643	<0.0001	0.06577	0.00320	0.03031	0.00372
ASP	10	D	H	204.75	7.60	18.4839	0.0002	1.9278	<0.0001	0.01343	0.00032	0.00989	0.00074
ASP	10	D	H	677.30	10.22	18.6278	0.0000	1.913	<0.0001	0.01405	0.00020	0.01282	0.00034
ASP	10	D	H	627.38	10.73	19.0029	0.0000	1.8756	<0.0001	0.01286	0.00020	0.01109	0.00036
ASP	10	D	H	270.42	20.78	19.2072	0.0012	1.8558	0.0001	0.11620	0.00500	0.06620	0.01220
ASP	10	D	H	628.45	29.73	19.5707	0.0006	1.8217	0.0001	0.09830	0.00374	0.05046	0.00576
ASP	10	D	H	49.96	7.59	20.8868	0.0248	1.7081	0.0020	0.02836	0.00156	0.00085	0.00024
ASP	10	D	H	122.21	4.78	21.9544	0.0002	1.6259	<0.0001	0.01257	0.00060	0.01182	0.00088
ASP	10	D	H	318.35	7.52	22.2548	0.0002	1.6043	<0.0001	0.01303	0.00026	0.01115	0.00050
ASP	10	D	H	36.03	4.41	22.4936	0.0004	1.5875	<0.0001	0.01563	0.00106	0.01051	0.00284

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	D	H	187.94	6.23	23.4198	0.0002	1.5255	<0.0001	0.01249	0.00034	0.01048	0.00068
ASP	10	D	H	103.43	5.05	23.5333	0.0002	1.5182	<0.0001	0.01283	0.00048	0.01029	0.00102
ASP	10	D	H	112.50	8.24	23.667	0.0002	1.5098	<0.0001	0.01508	0.00074	0.00884	0.00144
ASP	10	D	H	77.45	7.15	24.2606	0.0002	1.4734	<0.0001	0.01476	0.00074	0.01012	0.00210
ASP	10	D	H	188.56	6.12	24.8232	0.0002	1.4405	<0.0001	0.01388	0.00036	0.01168	0.00072
ASP	10	D	H	122.02	5.87	25.1474	0.0002	1.4222	<0.0001	0.01744	0.00072	0.01435	0.00140
ASP	10	D	H	45.60	4.23	26.3764	0.0004	1.357	<0.0001	0.01438	0.00132	0.01181	0.00232
ASP	10	D	H	88.36	7.38	26.7324	0.0002	1.3393	<0.0001	0.01560	0.00072	0.01000	0.00186
ASP	10	D	H	105.33	5.46	27.6218	0.0002	1.297	<0.0001	0.01595	0.00072	0.01320	0.00140
ASP	10	D	H	28.12	8.08	27.882	0.0006	1.2851	<0.0001	0.01461	0.00196	0.00000	0.00000
ASP	10	D	H	55.32	4.24	28.7391	0.0004	1.2475	<0.0001	0.01519	0.00076	0.01135	0.00180
ASP	10	D	H	101.04	6.81	29.0236	0.0002	1.2356	<0.0001	0.01635	0.00070	0.01030	0.00150
ASP	10	D	H	16.36	2.44	30.24	0.0006	1.187	<0.0001	0.01401	0.00304	0.01256	0.00402
ASP	10	D	H	109.40	4.73	30.4208	0.0002	1.1801	<0.0001	0.01506	0.00046	0.01189	0.00104
ASP	10	D	H	12.61	3.22	30.6002	0.0010	1.1733	<0.0001	0.01829	0.00260	0.01263	0.00744
ASP	10	D	H	242.11	10.50	31.1274	0.0002	1.1539	<0.0001	0.01269	0.00040	0.00725	0.00070
ASP	10	D	H	40.39	3.06	31.3197	0.0078	1.1470	0.0003	0.00000	0.00000	0.17448	0.02172
ASP	10	D	H	85.29	8.30	31.4455	0.0002	1.1425	<0.0001	0.01641	0.00078	0.01001	0.00228
ASP	10	D	H	19.66	2.52	31.9508	0.0006	1.1249	<0.0001	0.01630	0.00284	0.01464	0.00400
ASP	10	D	H	38.99	4.26	33.9082	0.0004	1.0617	<0.0001	0.01819	0.00112	0.01268	0.00308
ASP	10	D	H	98.66	4.46	34.3873	0.0002	1.0474	<0.0001	0.01333	0.00096	0.01266	0.00116
ASP	10	D	H	113.39	6.17	34.4673	0.0002	1.045	<0.0001	0.01600	0.00058	0.01190	0.00140
ASP	10	D	H	8.24	2.31	35.2234	0.0010	1.0233	<0.0001	0.01518	0.00458	0.01243	0.00776
ASP	10	D	H	102.11	6.95	35.624	0.0002	1.0121	<0.0001	0.01921	0.00070	0.01299	0.00198
ASP	10	D	H	18.50	5.14	35.9125	0.0712	1.0043	0.0019	0.00000	0.00000	0.29013	0.10174
ASP	10	D	H	10.52	4.67	36.4555	0.0010	0.9898	<0.0001	0.01563	0.00328	0.00000	0.00000
ASP	10	D	H	46.45	5.49	36.644	0.0004	0.9849	<0.0001	0.01630	0.00110	0.00975	0.00266
ASP	10	D	H	10.43	3.03	36.7994	0.0012	0.9809	<0.0001	0.01776	0.00584	0.00000	0.00000
ASP	10	D	H	43.21	6.12	36.9515	0.0004	0.977	<0.0001	0.01882	0.00140	0.01269	0.00418
ASP	10	D	H	28.51	3.66	37.3969	0.0004	0.9658	<0.0001	0.01239	0.00650	0.01415	0.00394
ASP	10	D	H	49.33	5.16	37.4711	0.0004	0.9639	<0.0001	0.01930	0.00312	0.01635	0.00380
ASP	10	D	H	18.94	7.50	37.7718	0.0008	0.9565	<0.0001	0.01761	0.00652	0.00000	0.00000
ASP	10	D	H	8.36	2.67	37.9538	0.0012	0.9521	<0.0001	0.01771	0.00344	0.00000	0.00000
ASP	10	D	H	65.37	8.44	38.3304	0.0004	0.9431	<0.0001	0.01841	0.00124	0.01071	0.00330
ASP	10	D	H	36.48	5.17	38.5493	0.0006	0.9379	<0.0001	0.01970	0.00144	0.01214	0.00400
ASP	10	D	D	400.56	5.51	9.2142	0.0000	3.8546	<0.0001	0.00655	0.00032	0.01104	0.00022
ASP	10	D	D	4000.37	62.42	11.7068	0.0000	3.0359	<0.0001	0.00604	0.00038	0.01130	0.00024
ASP	10	D	D	91.91	2.58	12.4986	0.0002	2.8443	<0.0001	0.01007	0.00028	0.00909	0.00048
ASP	10	D	D	685.38	10.02	14.2567	0.0000	2.495	<0.0001	0.00768	0.00026	0.01049	0.00024
ASP	10	D	D	1011.02	14.12	15.5736	0.0000	2.2852	<0.0001	0.00803	0.00030	0.01174	0.00024
ASP	10	D	D	786.91	12.98	17.0001	0.0000	2.0946	<0.0001	0.00702	0.00038	0.01119	0.00028
ASP	10	D	D	334.65	9.66	18.4838	0.0002	1.9278	<0.0001	0.01048	0.00054	0.01169	0.00058
ASP	10	D	D	1032.77	21.47	18.6292	0.0002	1.9129	<0.0001	0.01004	0.00034	0.01143	0.00040
ASP	10	D	D	1208.04	19.84	19.0033	0.0000	1.8756	<0.0001	0.00972	0.00030	0.01187	0.00032
ASP	10	D	D	210.61	3.59	21.9539	0.0000	1.626	<0.0001	0.01081	0.00024	0.01110	0.00034
ASP	10	D	D	722.33	16.01	22.2546	0.0002	1.6043	<0.0001	0.00984	0.00036	0.01130	0.00042
ASP	10	D	D	47.66	1.67	22.4955	0.0002	1.5873	<0.0001	0.01011	0.00094	0.01226	0.00078
ASP	10	D	D	409.64	9.59	23.4194	0.0002	1.5255	<0.0001	0.00854	0.00048	0.01118	0.00042
ASP	10	D	D	127.73	5.92	23.5348	0.0002	1.5182	<0.0001	0.00933	0.00120	0.01211	0.00096
ASP	10	D	D	154.40	7.20	23.668	0.0002	1.5097	<0.0001	0.01113	0.00090	0.01259	0.00106
ASP	10	D	D	97.64	2.73	24.2603	0.0002	1.4734	<0.0001	0.01140	0.00066	0.01324	0.00052
ASP	10	D	D	33.28	4.26	24.2605	0.0008	1.4734	<0.0001	0.00000	0.00000	0.03403	0.00316
ASP	10	D	D	316.43	13.35	24.8223	0.0004	1.4405	<0.0001	0.00942	0.00082	0.01283	0.00054
ASP	10	D	D	161.83	8.37	25.1501	0.0002	1.4221	<0.0001	0.01279	0.00092	0.01281	0.00122
ASP	10	D	D	66.32	2.31	26.3766	0.0002	1.357	<0.0001	0.01079	0.00078	0.01226	0.00078
ASP	10	D	D	113.16	3.47	26.7335	0.0002	1.3392	<0.0001	0.01413	0.00026	0.01018	0.00064
ASP	10	D	D	220.55	6.30	27.6215	0.0002	1.297	<0.0001	0.01408	0.00032	0.01160	0.00064
ASP	10	D	D	41.62	2.21	27.8815	0.0004	1.2851	<0.0001	0.01169	0.00066	0.01132	0.00094
ASP	10	D	D	3.62	0.77	28.7332	0.0004	1.2478	<0.0001	0.00000	0.00000	0.00403	0.00118
ASP	10	D	D	69.84	2.73	28.7376	0.0002	1.2476	<0.0001	0.01272	0.00050	0.01205	0.00076
ASP	10	D	D	115.86	3.50	29.0256	0.0002	1.2355	<0.0001	0.01407	0.00032	0.01152	0.00068
ASP	10	D	D	71.33	27.35	29.0271	0.0036	1.2354	0.0002	0.01261	0.00312	0.01217	0.00322
ASP	10	D	D	30.07	1.96	30.2395	0.0002	1.187	<0.0001	0.01268	0.00074	0.01027	0.00142
ASP	10	D	D	156.57	3.45	30.4213	0.0000	1.1801	<0.0001	0.01234	0.00024	0.01064	0.00044
ASP	10	D	D	18.08	1.64	30.6028	0.0004	1.1732	<0.0001	0.01446	0.00144	0.01252	0.00244
ASP	10	D	D	348.97	8.95	31.1264	0.0002	1.154	<0.0001	0.01326	0.00024	0.01021	0.00052
ASP	10	D	D	123.89	5.68	31.4451	0.0002	1.1426	<0.0001	0.01360	0.00048	0.01097	0.00102
ASP	10	D	D	28.94	3.80	31.9518	0.0004	1.1249	<0.0001	0.01327	0.00094	0.00832	0.00250
ASP	10	D	D	30.44	3.09	33.9099	0.0004	1.0617	<0.0001	0.01341	0.00100	0.01074	0.00232
ASP	10	D	D	150.00	3.85	34.3864	0.0002	1.0474	<0.0001	0.01217	0.00046	0.01241	0.00060
ASP	10	D	D	192.06	4.32	34.4671	0.0002	1.045	<0.0001	0.01221	0.00034	0.01172	0.00050
ASP	10	D	D	15.76	2.09	34.7915	0.0006	1.0356	<0.0001	0.00000	0.00000	0.00939	0.00170
ASP	10	D	D	75.36	5.65	34.7947	0.0002	1.0355	<0.0001	0.01764	0.00084	0.01100	0.00184
ASP	10	D	D	19.44	5.02	35.2241	0.0004	1.0233	<0.0001	0.01278	0.00290	0.00669	0.00420
ASP	10	D	D	147.45	5.62	35.6255	0.0002	1.0121	<0.0001	0.01419	0.00034	0.01028	0.00080
ASP	10	D	D	71.19	3.05	36.6433	0.0002	0.9849	<0.0001	0.01487	0.00046	0.01176	0.00104
ASP	10	D	D	14.76	2.80	36.7993	0.0004	0.9809	<0.0001	0.01542	0.00170	0.00888	0.00400
ASP	10	D	D	46.51	2.96	36.953	0.0002	0.9769	<0.0001	0.01575	0.00060	0.01137	0.00156
ASP	10	D	D	58.68	2.92	37.3958	0.0002	0.9658	<0.0001	0.01490	0.00060	0.01202	0.00124

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	D	D	95.23	5.42	37.4716	0.0002	0.9639	<0.0001	0.01725	0.00064	0.01017	0.00132
ASP	10	D	D	23.79	3.18	37.7753	0.0004	0.9564	<0.0001	0.01751	0.00128	0.01081	0.00334
ASP	10	D	D	13.20	2.60	37.9523	0.0006	0.9521	<0.0001	0.01529	0.00156	0.00959	0.00442
ASP	10	D	D	115.26	4.21	38.3296	0.0002	0.9431	<0.0001	0.01490	0.00032	0.01044	0.00080
ASP	10	D	D	48.03	2.59	38.5501	0.0002	0.9379	<0.0001	0.01440	0.00074	0.01203	0.00134
ASP	10	D	W	192.15	2.58	9.214	0.0000	3.8547	<0.0001	0.00504	0.00036	0.01054	0.00020
ASP	10	D	W	1741.78	18.50	11.7077	0.0000	3.0357	<0.0001	0.00502	0.00028	0.01095	0.00016
ASP	10	D	W	87.66	1.72	12.4995	0.0000	2.844	<0.0001	0.00571	0.00044	0.00945	0.00028
ASP	10	D	W	2.97	0.42	12.6051	0.0006	2.8203	0.0001	0.00000	0.00000	0.01153	0.00304
ASP	10	D	W	386.52	5.47	14.257	0.0000	2.4949	<0.0001	0.00555	0.00036	0.01115	0.00022
ASP	10	D	W	472.62	6.54	15.5766	0.0000	2.2847	<0.0001	0.00619	0.00034	0.01115	0.00022
ASP	10	D	W	585.98	7.99	17.0021	0.0000	2.0944	<0.0001	0.00523	0.00038	0.01072	0.00016
ASP	10	D	W	169.29	6.20	18.4864	0.0002	1.9275	<0.0001	0.00665	0.00126	0.01180	0.00068
ASP	10	D	W	527.50	10.73	18.6324	0.0002	1.9126	<0.0001	0.00756	0.00046	0.01149	0.00036
ASP	10	D	W	607.85	7.45	19.0061	0.0000	1.8753	<0.0001	0.00687	0.00032	0.01196	0.00022
ASP	10	D	W	105.08	2.10	21.958	0.0000	1.6257	<0.0001	0.00844	0.00038	0.01073	0.00036
ASP	10	D	W	276.31	4.72	22.2573	0.0000	1.6041	<0.0001	0.00772	0.00040	0.01148	0.00030
ASP	10	D	W	30.86	1.52	22.4989	0.0002	1.5871	<0.0001	0.01047	0.00072	0.01037	0.00096
ASP	10	D	W	192.57	2.92	23.4226	0.0000	1.5253	<0.0001	0.00752	0.00032	0.01063	0.00026
ASP	10	D	W	69.00	2.19	23.5396	0.0002	1.5178	<0.0001	0.00761	0.00070	0.01044	0.00056
ASP	10	D	W	69.14	2.30	23.6728	0.0002	1.5094	<0.0001	0.00953	0.00078	0.01208	0.00068
ASP	10	D	W	73.20	2.66	24.2642	0.0002	1.4732	<0.0001	0.00957	0.00058	0.01041	0.00066
ASP	10	D	W	207.90	4.16	24.8269	0.0002	1.4403	<0.0001	0.00904	0.00042	0.01186	0.00038
ASP	10	D	W	69.16	2.80	25.1543	0.0002	1.4218	<0.0001	0.01112	0.00080	0.01225	0.00088
ASP	10	D	W	43.26	1.48	26.3809	0.0002	1.3568	<0.0001	0.00773	0.00116	0.01216	0.00070
ASP	10	D	W	71.56	1.87	26.7389	0.0002	1.339	<0.0001	0.01033	0.00050	0.01162	0.00054
ASP	10	D	W	76.02	3.75	27.628	0.0002	1.2967	<0.0001	0.01014	0.00114	0.01231	0.00104
ASP	10	D	W	23.52	1.31	27.8874	0.0002	1.2849	<0.0001	0.00989	0.00086	0.01091	0.00116
ASP	10	D	W	187.05	6.59	28.7294	0.0002	1.248	<0.0001	0.00721	0.00122	0.01187	0.00068
ASP	10	D	W	60.23	2.14	28.7439	0.0002	1.2473	<0.0001	0.00943	0.00066	0.01102	0.00072
ASP	10	D	W	89.44	7.42	29.0144	0.0004	1.236	<0.0001	0.01350	0.00130	0.01217	0.00198
ASP	10	D	W	57.06	2.57	29.0301	0.0002	1.2353	<0.0001	0.01243	0.00048	0.01085	0.00096
ASP	10	D	W	29.70	2.04	30.2327	0.0002	1.1872	<0.0001	0.01162	0.00162	0.01205	0.00168
ASP	10	D	W	21.71	1.02	30.2454	0.0002	1.1868	<0.0001	0.00964	0.00116	0.01109	0.00098
ASP	10	D	W	113.21	2.84	30.4115	0.0002	1.1804	<0.0001	0.01144	0.00074	0.01392	0.00064
ASP	10	D	W	91.90	1.84	30.427	0.0000	1.1798	<0.0001	0.01072	0.00032	0.01114	0.00040
ASP	10	D	W	9.18	1.07	30.5886	0.0008	1.1738	<0.0001	0.00000	0.00000	0.01818	0.00350
ASP	10	D	W	10.28	2.36	30.6096	0.0004	1.173	<0.0001	0.01267	0.00268	0.00603	0.00340
ASP	10	D	W	211.97	5.14	31.1198	0.0002	1.1542	<0.0001	0.01448	0.00048	0.01434	0.00064
ASP	10	D	W	121.83	2.19	31.1329	0.0000	1.1537	<0.0001	0.01226	0.00022	0.01119	0.00038
ASP	10	D	W	142.07	4.07	31.4376	0.0002	1.1428	<0.0001	0.01131	0.00058	0.01224	0.00064
ASP	10	D	W	69.72	1.89	31.4506	0.0002	1.1424	<0.0001	0.01059	0.00032	0.00984	0.00050
ASP	10	D	W	0.83	0.19	31.7841	0.0020	1.1307	0.0001	0.00000	0.00000	0.01430	0.00476
ASP	10	D	W	27.76	2.89	31.9417	0.0004	1.1252	<0.0001	0.01251	0.00128	0.01039	0.00228
ASP	10	D	W	19.67	1.16	31.9593	0.0002	1.1246	<0.0001	0.01244	0.00072	0.01074	0.00128
ASP	10	D	W	21.32	3.01	33.8976	0.0008	1.0621	<0.0001	0.00000	0.00000	0.01784	0.00508
ASP	10	D	W	46.44	1.68	33.9169	0.0002	1.0615	<0.0001	0.01196	0.00050	0.01114	0.00076
ASP	10	D	W	200.69	6.58	34.3776	0.0002	1.0477	<0.0001	0.01065	0.00060	0.01148	0.00068
ASP	10	D	W	91.70	2.08	34.3932	0.0002	1.0472	<0.0001	0.01075	0.00034	0.01099	0.00044
ASP	10	D	W	128.70	6.74	34.4583	0.0002	1.0453	<0.0001	0.01509	0.00078	0.01323	0.00138
ASP	10	D	W	110.55	2.10	34.4749	0.0000	1.0448	<0.0001	0.01067	0.00036	0.01209	0.00040
ASP	10	D	W	109.27	7.69	34.78	0.0002	1.0359	<0.0001	0.01358	0.00058	0.00964	0.00142
ASP	10	D	W	46.76	2.27	34.8028	0.0002	1.0353	<0.0001	0.01607	0.00074	0.01391	0.00134
ASP	10	D	W	9.54	1.18	35.2313	0.0004	1.0231	<0.0001	0.01237	0.00114	0.00956	0.00256
ASP	10	D	W	110.16	6.57	35.6132	0.0002	1.0124	<0.0001	0.01481	0.00070	0.01221	0.00146
ASP	10	D	W	117.04	2.77	35.6343	0.0002	1.0119	<0.0001	0.01175	0.00036	0.01177	0.00050
ASP	10	D	W	11.89	0.94	36.4622	0.0004	0.9896	<0.0001	0.01200	0.00162	0.01184	0.00188
ASP	10	D	W	74.41	3.42	36.6361	0.0002	0.9851	<0.0001	0.01468	0.00122	0.01596	0.00142
ASP	10	D	W	28.06	10.87	36.6522	0.0006	0.9847	<0.0001	0.00965	0.00394	0.00654	0.00430
ASP	10	D	W	45.56	1.58	36.6537	0.0002	0.9846	<0.0001	0.01221	0.00046	0.01102	0.00074
ASP	10	D	W	17.03	5.24	36.7916	0.0006	0.9811	<0.0001	0.01172	0.00280	0.00000	0.00000
ASP	10	D	W	11.13	1.07	36.8081	0.0004	0.9807	<0.0001	0.01341	0.00112	0.01116	0.00224
ASP	10	D	W	46.45	2.56	36.9408	0.0004	0.9773	<0.0001	0.01293	0.00324	0.01808	0.00190
ASP	10	D	W	34.47	1.46	36.961	0.0002	0.9767	<0.0001	0.01404	0.00044	0.01125	0.00096
ASP	10	D	W	53.56	3.29	37.3889	0.0002	0.966	<0.0001	0.01417	0.00148	0.01392	0.00172
ASP	10	D	W	31.26	1.52	37.4034	0.0002	0.9656	<0.0001	0.01242	0.00056	0.01054	0.00104
ASP	10	D	W	111.19	4.17	37.4623	0.0002	0.9641	<0.0001	0.01530	0.00088	0.01501	0.00110
ASP	10	D	W	56.61	2.08	37.4793	0.0002	0.9637	<0.0001	0.01464	0.00038	0.01161	0.00086
ASP	10	D	W	20.72	1.62	37.784	0.0002	0.9562	<0.0001	0.01346	0.00060	0.00941	0.00158
ASP	10	D	W	13.60	2.44	37.9434	0.0008	0.9524	<0.0001	0.01710	0.00450	0.01550	0.00602
ASP	10	D	W	8.43	1.03	37.9613	0.0004	0.9519	<0.0001	0.01351	0.00166	0.01145	0.00298
ASP	10	D	W	3.68	0.82	38.3204	0.0004	0.9433	<0.0001	0.00000	0.00000	0.00356	0.00122
ASP	10	D	W	61.42	4.63	38.3225	0.0004	0.9433	<0.0001	0.01852	0.00088	0.01358	0.00172
ASP	10	D	W	72.88	1.80	38.3374	0.0002	0.9429	<0.0001	0.01207	0.00028	0.01064	0.00050
ASP	10	D	W	33.37	2.53	38.5383	0.0004	0.9382	<0.0001	0.01924	0.00100	0.01461	0.00240
ASP	10	D	W	48.16	1.64	38.5601	0.0002	0.9377	<0.0001	0.01048	0.00042	0.00984	0.00064
ASP	10	E	H	150.60	7.84	8.3906	0.0004	4.2322	0.0002	0.02892	0.00088	0.01954	0.00216
ASP	10	E	H	124.08	3.52	9.2147	0.0002	3.8544	0.0001	0.00954	0.00046	0.01078	0.00052
ASP	10	E	H	739.83	13.95	9.9373	0.0002	3.5747	0.0001	0.04257	0.00052	0.03063	0.00116
ASP	10	E	H	1272.14	17.84	10.7887	0.0002	3.2934	0.0001	0.05770	0.00052	0.04194	0.00116

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	E	H	1374.78	12.05	11.7069	0.0000	3.0359	<0.0001	0.00978	0.00010	0.01025	0.00014
ASP	10	E	H	37.83	2.66	12.4981	0.0002	2.8444	<0.0001	0.01036	0.00104	0.01001	0.00138
ASP	10	E	H	1197.85	55.98	13.0173	0.0006	2.7314	0.0001	0.07311	0.00184	0.04006	0.00384
ASP	10	E	H	164.52	4.72	14.2571	0.0002	2.4949	<0.0001	0.01072	0.00042	0.01105	0.00056
ASP	10	E	H	320.15	7.52	15.5738	0.0000	2.2851	<0.0001	0.01117	0.00036	0.01049	0.00048
ASP	10	E	H	62.79	23.24	16.0616	0.0028	2.2162	0.0004	0.08943	0.03022	0.00000	0.00000
ASP	10	E	H	107.79	12.38	16.8247	0.0006	2.1163	0.0001	0.04303	0.00376	0.02185	0.00606
ASP	10	E	H	210.53	4.65	17.0007	0.0002	2.0946	<0.0001	0.00964	0.00050	0.01191	0.00046
ASP	10	E	H	844.33	23.86	17.2511	0.0004	2.0644	<0.0001	0.06873	0.00144	0.03886	0.00246
ASP	10	E	H	105.90	4.73	18.4839	0.0002	1.9278	<0.0001	0.01319	0.00044	0.01072	0.00096
ASP	10	E	H	351.95	7.11	18.628	0.0000	1.913	<0.0001	0.01318	0.00024	0.01175	0.00044
ASP	10	E	H	342.31	6.67	19.0029	0.0000	1.8756	<0.0001	0.01177	0.00034	0.01260	0.00042
ASP	10	E	H	328.84	17.99	19.2054	0.0020	1.8560	0.0002	0.11161	0.00434	0.07330	0.00938
ASP	10	E	H	521.77	68.97	19.5693	0.0016	1.8218	0.0001	0.10965	0.00114	0.08827	0.01124
ASP	10	E	H	37.02	1.91	19.9457	0.0022	1.7878	0.0002	0.06136	0.01512	0.07486	0.00518
ASP	10	E	H	15.47	3.30	20.3843	0.0056	1.7497	0.0005	0.00000	0.00000	0.08543	0.03910
ASP	10	E	H	49.96	2.74	21.954	0.0002	1.626	<0.0001	0.01038	0.00208	0.01380	0.00142
ASP	10	E	H	153.23	4.49	22.2546	0.0002	1.6043	<0.0001	0.01213	0.00052	0.01248	0.00066
ASP	10	E	H	19.33	2.09	22.4943	0.0006	1.5874	<0.0001	0.01248	0.00294	0.01327	0.00286
ASP	10	E	H	111.90	5.72	23.4196	0.0002	1.5255	<0.0001	0.01367	0.00046	0.01035	0.00110
ASP	10	E	H	52.07	4.00	23.5344	0.0002	1.5182	<0.0001	0.01162	0.00182	0.01145	0.00184
ASP	10	E	H	70.01	5.78	23.6674	0.0002	1.5098	<0.0001	0.01507	0.00122	0.01191	0.00216
ASP	10	E	H	40.56	3.64	24.2604	0.0004	1.4734	<0.0001	0.01315	0.00302	0.01496	0.00276
ASP	10	E	H	163.82	4.43	24.8219	0.0002	1.4406	<0.0001	0.01194	0.00054	0.01303	0.00062
ASP	10	E	H	90.72	7.06	25.1494	0.0002	1.4221	<0.0001	0.01529	0.00064	0.01030	0.00176
ASP	10	E	H	28.06	2.42	26.3763	0.0004	1.357	<0.0001	0.00894	0.00580	0.01395	0.00240
ASP	10	E	H	34.08	7.88	26.4848	0.0038	1.3516	0.0002	0.08714	0.02574	0.06464	0.03556
ASP	10	E	H	61.69	4.10	26.7323	0.0002	1.3393	<0.0001	0.01486	0.00148	0.01363	0.00188
ASP	10	E	H	79.84	3.60	27.6217	0.0002	1.297	<0.0001	0.01239	0.00178	0.01524	0.00132
ASP	10	E	H	31.60	3.32	28.738	0.0004	1.2476	<0.0001	0.01323	0.00098	0.01012	0.00228
ASP	10	E	H	56.55	4.34	29.0245	0.0004	1.2355	<0.0001	0.01641	0.00088	0.01277	0.00208
ASP	10	E	H	54.09	22.85	30.1140	0.0034	1.1918	0.0001	0.05215	0.02866	0.00000	0.00000
ASP	10	E	H	12.76	1.15	30.2398	0.0008	1.187	<0.0001	0.00913	0.00112	0.01399	0.00186
ASP	10	E	H	73.99	5.52	30.4205	0.0002	1.1801	<0.0001	0.01460	0.00062	0.00962	0.00156
ASP	10	E	H	7.30	1.91	30.6005	0.0014	1.1733	0.0001	0.00000	0.00000	0.01618	0.00912
ASP	10	E	H	89.42	4.64	31.1269	0.0002	1.1539	<0.0001	0.01555	0.00130	0.01556	0.00160
ASP	10	E	H	55.99	7.58	31.4454	0.0004	1.1425	<0.0001	0.01760	0.00148	0.01228	0.00384
ASP	10	E	H	10.94	1.67	31.9507	0.0008	1.1249	<0.0001	0.00000	0.00000	0.01605	0.00484
ASP	10	E	H	126.12	58.96	32.4691	0.0216	1.1075	0.0007	0.05485	0.02838	0.00000	0.00000
ASP	10	E	H	24.64	4.23	33.9083	0.0006	1.0617	<0.0001	0.01562	0.00144	0.01061	0.00414
ASP	10	E	H	55.25	4.06	34.0261	0.0034	1.0582	0.0001	0.04400	0.00018	0.00770	0.00098
ASP	10	E	H	54.30	3.44	34.386	0.0004	1.0474	<0.0001	0.01370	0.00160	0.01396	0.00176
ASP	10	E	H	70.60	4.42	34.4673	0.0002	1.045	<0.0001	0.01457	0.00064	0.01199	0.00154
ASP	10	E	H	49.72	4.53	34.7931	0.0006	1.0355	<0.0001	0.02026	0.00350	0.01913	0.00376
ASP	10	E	H	5.12	0.78	35.2241	0.0016	1.0233	<0.0001	0.00000	0.00000	0.01838	0.00396
ASP	10	E	H	75.52	5.67	35.6246	0.0002	1.0121	<0.0001	0.01592	0.00088	0.01215	0.00200
ASP	10	E	H	7.17	1.31	36.4535	0.0012	0.9899	<0.0001	0.00000	0.00000	0.01610	0.00482
ASP	10	E	H	23.74	3.20	36.6436	0.0006	0.9849	<0.0001	0.01767	0.00370	0.01604	0.00468
ASP	10	E	H	8.47	2.08	36.7982	0.0014	0.9809	<0.0001	0.00000	0.00000	0.02046	0.01058
ASP	10	E	H	34.28	4.44	36.9525	0.0006	0.977	<0.0001	0.01468	0.00598	0.01565	0.00444
ASP	10	E	H	19.36	3.43	37.3961	0.0006	0.9658	<0.0001	0.00000	0.00000	0.01750	0.00656
ASP	10	E	H	36.13	5.72	37.4713	0.0004	0.9639	<0.0001	0.01592	0.00194	0.01152	0.00424
ASP	10	E	H	18.29	3.47	37.7725	0.0008	0.9565	<0.0001	0.01739	0.00196	0.01238	0.00530
ASP	10	E	H	5.35	2.51	37.9501	0.0018	0.9522	<0.0001	0.01607	0.00730	0.00000	0.00000
ASP	10	E	H	45.15	6.67	38.3291	0.0004	0.9431	<0.0001	0.01635	0.00136	0.01129	0.00388
ASP	10	E	H	22.03	3.26	38.5495	0.0006	0.9379	<0.0001	0.01680	0.00350	0.01476	0.00476
ASP	10	E	D	380.88	6.34	9.2148	0.0000	3.8543	<0.0001	0.00555	0.00036	0.00994	0.00024
ASP	10	E	D	4355.05	71.21	11.706	0.0000	3.0361	<0.0001	0.00485	0.00042	0.01067	0.00024
ASP	10	E	D	180.63	7.84	12.4987	0.0002	2.8442	<0.0001	0.00521	0.00090	0.00871	0.00058
ASP	10	E	D	3.44	0.86	12.6040	0.0010	2.8206	0.0002	0.00000	0.00000	0.01239	0.00650
ASP	10	E	D	690.61	10.33	14.2564	0.0000	2.495	<0.0001	0.00559	0.00034	0.01025	0.00022
ASP	10	E	D	1115.01	10.96	15.5734	0.0000	2.2852	<0.0001	0.00634	0.00020	0.01027	0.00014
ASP	10	E	D	926.13	8.34	16.9997	0.0000	2.0947	<0.0001	0.00537	0.00022	0.01043	0.00014
ASP	10	E	D	76.39	17.80	18.4832	0.0008	1.9279	0.0001	0.00000	0.00000	0.02138	0.00360
ASP	10	E	D	247.02	14.47	18.4839	0.0002	1.9278	<0.0001	0.00000	0.00000	0.01012	0.00090
ASP	10	E	D	937.56	21.28	18.629	0.0002	1.9129	<0.0001	0.00756	0.00044	0.01077	0.00038
ASP	10	E	D	1061.36	16.62	19.0029	0.0000	1.8756	<0.0001	0.00758	0.00026	0.01033	0.00024
ASP	10	E	D	205.75	4.27	21.9533	0.0002	1.626	<0.0001	0.00811	0.00048	0.01124	0.00038
ASP	10	E	D	614.08	10.01	22.2541	0.0000	1.6043	<0.0001	0.00786	0.00034	0.01136	0.00028
ASP	10	E	D	59.70	3.85	22.4948	0.0004	1.5874	<0.0001	0.00900	0.00164	0.01147	0.00132
ASP	10	E	D	419.32	7.13	23.4187	0.0000	1.5256	<0.0001	0.00715	0.00034	0.01100	0.00028
ASP	10	E	D	41.81	17.96	23.5302	0.0004	1.5184	<0.0001	0.00669	0.00146	0.00000	0.00000
ASP	10	E	D	144.33	4.74	23.534	0.0002	1.5182	<0.0001	0.00756	0.00092	0.01136	0.00062
ASP	10	E	D	154.43	4.99	23.6671	0.0002	1.5098	<0.0001	0.00817	0.00090	0.01182	0.00064
ASP	10	E	D	155.86	5.32	24.2595	0.0002	1.4734	<0.0001	0.00896	0.00054	0.01007	0.00060
ASP	10	E	D	367.30	11.21	24.8213	0.0002	1.4406	<0.0001	0.00787	0.00084	0.01220	0.00058
ASP	10	E	D	213.39	7.99	25.1487	0.0002	1.4221	<0.0001	0.00987	0.00062	0.01099	0.00072
ASP	10	E	D	77.57	2.26	26.3764	0.0002	1.357	<0.0001	0.00868	0.00072	0.01134	0.00058
ASP	10	E	D	56.17	9.96	26.7295	0.0006	1.3394	<0.0001	0.00000	0.00000	0.00848	0.00248

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	E	D	146.43	4.42	26.7327	0.0002	1.3393	<0.0001	0.00938	0.00084	0.01276	0.00064
ASP	10	E	D	66.58	15.25	26.7364	0.0006	1.3391	<0.0001	0.00771	0.00110	0.00465	0.00224
ASP	10	E	D	232.33	10.99	27.6209	0.0002	1.297	<0.0001	0.00992	0.00068	0.01054	0.00088
ASP	10	E	D	39.12	1.43	27.881	0.0002	1.2851	<0.0001	0.00897	0.00118	0.01217	0.00082
ASP	10	E	D	89.91	3.34	28.737	0.0002	1.2476	<0.0001	0.00781	0.00094	0.01273	0.00080
ASP	10	E	D	115.65	3.38	29.0247	0.0002	1.2355	<0.0001	0.01078	0.00058	0.01181	0.00062
ASP	10	E	D	32.71	1.67	30.2385	0.0002	1.187	<0.0001	0.00739	0.00222	0.01167	0.00112
ASP	10	E	D	118.66	2.87	30.421	0.0002	1.1801	<0.0001	0.00977	0.00044	0.01070	0.00048
ASP	10	E	D	14.49	1.45	30.6022	0.0004	1.1732	<0.0001	0.00907	0.00354	0.01127	0.00228
ASP	10	E	D	303.20	5.89	31.1259	0.0000	1.154	<0.0001	0.01133	0.00030	0.01161	0.00040
ASP	10	E	D	110.64	3.60	31.4445	0.0002	1.1426	<0.0001	0.01084	0.00044	0.01042	0.00064
ASP	10	E	D	25.49	2.10	31.951	0.0004	1.1249	<0.0001	0.00751	0.00372	0.01377	0.00216
ASP	10	E	D	50.03	3.82	33.9086	0.0004	1.0617	<0.0001	0.01132	0.00150	0.01145	0.00172
ASP	10	E	D	195.98	5.27	34.3865	0.0002	1.0474	<0.0001	0.00982	0.00042	0.01137	0.00054
ASP	10	E	D	197.18	5.59	34.4664	0.0002	1.0451	<0.0001	0.00993	0.00054	0.01121	0.00056
ASP	10	E	D	103.80	5.29	34.7947	0.0002	1.0355	<0.0001	0.01465	0.00078	0.01290	0.00130
ASP	10	E	D	15.99	1.98	35.2245	0.0004	1.0233	<0.0001	0.01452	0.00190	0.01214	0.00322
ASP	10	E	D	146.99	5.07	35.625	0.0002	1.0121	<0.0001	0.01119	0.00070	0.01229	0.00076
ASP	10	E	D	91.31	3.50	36.6434	0.0002	0.9849	<0.0001	0.01164	0.00074	0.01202	0.00086
ASP	10	E	D	17.73	2.84	36.7982	0.0004	0.9809	<0.0001	0.01209	0.00126	0.00890	0.00314
ASP	10	E	D	60.32	3.26	36.952	0.0002	0.977	<0.0001	0.01222	0.00084	0.01140	0.00122
ASP	10	E	D	46.44	4.27	37.3932	0.0004	0.9659	<0.0001	0.00929	0.00072	0.01225	0.00094
ASP	10	E	D	96.09	5.03	37.4703	0.0002	0.9639	<0.0001	0.01428	0.00046	0.01143	0.00104
ASP	10	E	D	33.27	3.14	37.7734	0.0004	0.9565	<0.0001	0.01376	0.00112	0.01105	0.00222
ASP	10	E	D	15.84	1.75	37.9516	0.0004	0.9522	<0.0001	0.01303	0.00176	0.01139	0.00270
ASP	10	E	D	103.49	3.85	38.329	0.0002	0.9431	<0.0001	0.01183	0.00058	0.01133	0.00080
ASP	10	E	D	50.69	2.96	38.5501	0.0002	0.9379	<0.0001	0.01284	0.00144	0.01331	0.00152
ASP	10	E	W	254.73	3.39	9.2137	0.0000	3.8548	<0.0001	0.00441	0.00036	0.01029	0.00018
ASP	10	E	W	49.50	11.95	9.2158	0.0004	3.8539	0.0002	0.00000	0.00000	0.00671	0.00110
ASP	10	E	W	2805.51	40.57	11.7078	0.0000	3.0356	<0.0001	0.00388	0.00044	0.01105	0.00016
ASP	10	E	W	335.46	56.63	11.7110	0.0004	3.0348	0.0001	0.00000	0.00000	0.00587	0.00092
ASP	10	E	W	50.39	0.93	12.4987	0.0000	2.8442	<0.0001	0.00638	0.00046	0.01012	0.00030
ASP	10	E	W	3.90	0.20	12.6046	0.0004	2.8204	0.0001	0.00000	0.00000	0.01182	0.00086
ASP	10	E	W	328.86	5.18	14.2571	0.0000	2.4949	<0.0001	0.00480	0.00044	0.01038	0.00022
ASP	10	E	W	591.00	7.37	15.576	0.0000	2.2848	<0.0001	0.00483	0.00036	0.01091	0.00018
ASP	10	E	W	594.10	7.62	17.0022	0.0000	2.0944	<0.0001	0.00413	0.00036	0.01012	0.00018
ASP	10	E	W	197.21	4.13	18.4864	0.0000	1.9275	<0.0001	0.00594	0.00048	0.00981	0.00032
ASP	10	E	W	457.03	7.03	18.6323	0.0000	1.9126	<0.0001	0.00617	0.00038	0.01092	0.00024
ASP	10	E	W	495.06	5.25	19.0057	0.0000	1.8753	<0.0001	0.00674	0.00024	0.01105	0.00018
ASP	10	E	W	120.04	2.03	21.9578	0.0000	1.6257	<0.0001	0.00656	0.00042	0.01059	0.00028
ASP	10	E	W	295.04	4.85	22.2577	0.0000	1.6041	<0.0001	0.00615	0.00048	0.01171	0.00028
ASP	10	E	W	35.81	0.86	22.4983	0.0002	1.5871	<0.0001	0.00749	0.00070	0.01112	0.00046
ASP	10	E	W	150.11	2.94	23.4227	0.0002	1.5253	<0.0001	0.00547	0.00068	0.01127	0.00032
ASP	10	E	W	85.72	1.96	23.5391	0.0002	1.5179	<0.0001	0.00653	0.00076	0.01134	0.00042
ASP	10	E	W	101.48	2.60	23.6729	0.0002	1.5094	<0.0001	0.00615	0.00086	0.01147	0.00046
ASP	10	E	W	6.43	2.30	24.2587	0.0004	1.4735	<0.0001	0.00000	0.00000	0.00422	0.00208
ASP	10	E	W	84.84	1.98	24.2634	0.0002	1.4732	<0.0001	0.00733	0.00060	0.01111	0.00042
ASP	10	E	W	230.33	5.85	24.8271	0.0002	1.4403	<0.0001	0.00621	0.00080	0.01181	0.00044
ASP	10	E	W	82.82	4.21	25.1535	0.0002	1.4219	<0.0001	0.00931	0.00130	0.01120	0.00094
ASP	10	E	W	54.34	1.34	26.3809	0.0002	1.3568	<0.0001	0.00485	0.00106	0.01090	0.00042
ASP	10	E	W	66.05	2.00	26.7388	0.0002	1.339	<0.0001	0.00840	0.00068	0.01107	0.00056
ASP	10	E	W	81.38	2.46	27.6288	0.0002	1.2966	<0.0001	0.00000	0.00000	0.01107	0.00046
ASP	10	E	W	22.15	0.99	27.8863	0.0004	1.2849	<0.0001	0.00861	0.00098	0.01070	0.00078
ASP	10	E	W	41.62	2.02	28.7437	0.0002	1.2474	<0.0001	0.00867	0.00094	0.01062	0.00096
ASP	10	E	W	61.95	2.23	29.0305	0.0002	1.2353	<0.0001	0.00978	0.00066	0.01116	0.00072
ASP	10	E	W	19.12	0.90	30.2453	0.0002	1.1868	<0.0001	0.00694	0.00130	0.00991	0.00084
ASP	10	E	W	64.95	1.52	30.4266	0.0002	1.1799	<0.0001	0.00920	0.00052	0.01163	0.00046
ASP	10	E	W	7.50	0.58	30.6099	0.0004	1.173	<0.0001	0.00000	0.00000	0.01336	0.00196
ASP	10	E	W	136.62	2.46	31.1332	0.0000	1.1537	<0.0001	0.00985	0.00028	0.01089	0.00034
ASP	10	E	W	69.59	2.15	31.4511	0.0002	1.1423	<0.0001	0.01102	0.00034	0.01006	0.00058
ASP	10	E	W	0.90	0.19	31.7847	0.0022	1.1307	0.0001	0.00000	0.00000	0.01762	0.00538
ASP	10	E	W	18.39	1.29	31.9588	0.0002	1.1247	<0.0001	0.01202	0.00100	0.01091	0.00152
ASP	10	E	W	20.57	1.30	33.916	0.0002	1.0615	<0.0001	0.00974	0.00056	0.00826	0.00104
ASP	10	E	W	108.78	2.85	34.3937	0.0002	1.0472	<0.0001	0.00863	0.00058	0.01119	0.00050
ASP	10	E	W	10.02	4.37	34.4018	0.0056	1.0470	0.0002	0.00000	0.00000	0.01255	0.00666
ASP	10	E	W	109.36	2.04	34.4751	0.0000	1.0448	<0.0001	0.00975	0.00032	0.01098	0.00036
ASP	10	E	W	60.60	2.72	34.8028	0.0002	1.0353	<0.0001	0.01022	0.00060	0.01470	0.00124
ASP	10	E	W	18.42	2.31	34.8121	0.0014	1.035	<0.0001	0.01150	0.00300	0.01312	0.00348
ASP	10	E	W	10.37	1.17	35.2309	0.0004	1.0231	<0.0001	0.01124	0.00088	0.00859	0.00206
ASP	10	E	W	25.92	6.10	35.6318	0.0010	1.0119	<0.0001	0.00000	0.00000	0.00988	0.00158
ASP	10	E	W	103.33	2.84	35.6339	0.0002	1.0119	<0.0001	0.00962	0.00054	0.01152	0.00054
ASP	10	E	W	77.80	10.21	35.6348	0.0006	1.0118	<0.0001	0.01117	0.00122	0.01214	0.00114
ASP	10	E	W	10.58	0.76	36.4622	0.0002	0.9896	<0.0001	0.00785	0.00212	0.01040	0.00140
ASP	10	E	W	38.84	1.32	36.6543	0.0002	0.9846	<0.0001	0.01108	0.00064	0.01156	0.00072
ASP	10	E	W	8.26	0.60	36.8086	0.0002	0.9806	<0.0001	0.01012	0.00236	0.01206	0.00174
ASP	10	E	W	25.65	1.31	36.9617	0.0002	0.9767	<0.0001	0.01091	0.00066	0.00986	0.00100
ASP	10	E	W	31.09	1.85	37.4036	0.0002	0.9656	<0.0001	0.01025	0.00098	0.01042	0.00118
ASP	10	E	W	96.81	2.62	37.4801	0.0002	0.9637	<0.0001	0.01049	0.00056	0.01212	0.00058
ASP	10	E	W	3.54	1.06	37.4946	0.0006	0.9633	<0.0001	0.00508	0.00280	0.00455	0.00298

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	E	W	20.11	1.32	37.7829	0.0002	0.9562	<0.0001	0.01161	0.00068	0.00980	0.00130
ASP	10	E	W	9.23	1.93	37.9621	0.0004	0.9519	<0.0001	0.01244	0.00188	0.00672	0.00334
ASP	10	E	W	56.80	2.19	38.3373	0.0002	0.9429	<0.0001	0.00996	0.00068	0.01099	0.00076
ASP	10	E	W	37.42	1.34	38.5605	0.0002	0.9377	<0.0001	0.01047	0.00078	0.01178	0.00078
ASP	10	F	H	150.25	8.65	8.3896	0.0004	4.2327	0.0002	0.03018	0.00116	0.01821	0.00232
ASP	10	F	H	111.80	3.52	9.2144	0.0002	3.8545	0.0001	0.00927	0.00052	0.01039	0.00056
ASP	10	F	H	381.28	186.46	9.9366	0.0010	3.5750	0.0004	0.06382	0.02612	0.07302	0.02400
ASP	10	F	H	913.12	190.77	10.7884	0.0004	3.2935	0.0001	0.04508	0.02910	0.04084	0.01218
ASP	10	F	H	1575.69	17.74	11.7061	0.0000	3.0361	<0.0001	0.00970	0.00010	0.01028	0.00024
ASP	10	F	H	37.14	2.85	12.4972	0.0002	2.8446	<0.0001	0.01055	0.00122	0.01032	0.00156
ASP	10	F	H	1529.75	49.63	13.0185	0.0004	2.7311	0.0001	0.07338	0.00240	0.03259	0.00260
ASP	10	F	H	165.96	4.95	14.2568	0.0002	2.495	<0.0001	0.01116	0.00038	0.01070	0.00058
ASP	10	F	H	320.75	8.49	15.5734	0.0002	2.2852	<0.0001	0.01211	0.00038	0.01085	0.00058
ASP	10	F	H	118.98	11.19	16.8225	0.0008	2.1166	0.0001	0.04756	0.00276	0.02740	0.00606
ASP	10	F	H	230.84	5.49	16.9999	0.0002	2.0947	<0.0001	0.01034	0.00044	0.01145	0.00048
ASP	10	F	H	772.27	372.93	17.2505	0.0016	2.0645	0.0002	0.09468	0.00712	0.06778	0.02120
ASP	10	F	H	101.47	7.23	18.4833	0.0002	1.9278	<0.0001	0.01326	0.00060	0.00814	0.00128
ASP	10	F	H	336.10	7.21	18.6275	0.0002	1.9131	<0.0001	0.01267	0.00026	0.01143	0.00046
ASP	10	F	H	367.79	7.12	19.0025	0.0000	1.8756	<0.0001	0.01167	0.00034	0.01208	0.00042
ASP	10	F	H	425.76	25.35	19.2069	0.0010	1.8559	0.0001	0.11428	0.00442	0.06204	0.00892
ASP	10	F	H	263.00	16.92	19.5707	0.0028	1.8217	0.0003	0.00000	0.00000	0.13260	0.00726
ASP	10	F	H	536.28	118.93	21.6692	0.0010	1.6471	0.0001	0.10306	0.02924	0.03094	0.01862
ASP	10	F	H	60.66	3.31	21.954	0.0002	1.626	<0.0001	0.01092	0.00154	0.01270	0.00132
ASP	10	F	H	169.10	6.09	22.2544	0.0002	1.6043	<0.0001	0.01319	0.00034	0.01062	0.00076
ASP	10	F	H	28.03	4.24	22.4939	0.0004	1.5874	<0.0001	0.01507	0.00126	0.00984	0.00334
ASP	10	F	H	102.37	5.57	23.4194	0.0002	1.5255	<0.0001	0.01280	0.00046	0.00966	0.00108
ASP	10	F	H	45.13	4.91	23.5332	0.0004	1.5183	<0.0001	0.01257	0.00090	0.00922	0.00222
ASP	10	F	H	59.20	8.38	23.6664	0.0004	1.5098	<0.0001	0.01452	0.00106	0.00861	0.00290
ASP	10	F	H	47.10	6.37	24.2601	0.0004	1.4734	<0.0001	0.01388	0.00108	0.00960	0.00298
ASP	10	F	H	126.60	4.19	24.8225	0.0002	1.4405	<0.0001	0.01217	0.00062	0.01267	0.00076
ASP	10	F	H	50.01	5.49	25.1478	0.0004	1.4222	<0.0001	0.01789	0.00120	0.01270	0.00312
ASP	10	F	H	31.76	2.83	25.2916	0.0138	1.4142	0.0008	0.00000	0.00000	0.22504	0.03412
ASP	10	F	H	144.61	11.68	26.1935	0.0048	1.3664	0.0002	0.05296	0.00372	0.00627	0.00108
ASP	10	F	H	27.09	3.08	26.3768	0.0004	1.357	<0.0001	0.01226	0.00304	0.01250	0.00298
ASP	10	F	H	25.47	6.74	26.4936	0.0058	1.3511	0.0003	0.09283	0.05106	0.08472	0.05228
ASP	10	F	H	44.27	4.98	26.732	0.0004	1.3393	<0.0001	0.01471	0.00134	0.01111	0.00274
ASP	10	F	H	35.03	2.69	26.8303	0.0076	1.3345	0.0004	0.00000	0.00000	0.14575	0.01910
ASP	10	F	H	162.39	10.27	27.2883	0.0018	1.3125	0.0001	0.12544	0.00500	0.09167	0.01298
ASP	10	F	H	60.89	3.50	27.6214	0.0002	1.297	<0.0001	0.01215	0.00202	0.01440	0.00160
ASP	10	F	H	29.96	2.90	28.7383	0.0004	1.2476	<0.0001	0.01366	0.00158	0.01228	0.00242
ASP	10	F	H	61.89	4.69	29.0236	0.0004	1.2356	<0.0001	0.01572	0.00074	0.01142	0.00182
ASP	10	F	H	30.09	1.70	30.1155	0.0038	1.1918	0.0001	0.00000	0.00000	0.11689	0.00966
ASP	10	F	H	12.84	2.00	30.2397	0.0006	1.187	<0.0001	0.01307	0.00478	0.01353	0.00450
ASP	10	F	H	64.63	3.60	30.4199	0.0002	1.1801	<0.0001	0.01464	0.00070	0.01206	0.00138
ASP	10	F	H	7.31	1.91	30.6003	0.0012	1.1733	<0.0001	0.01393	0.00876	0.01414	0.00808
ASP	10	F	H	89.41	5.33	31.127	0.0002	1.1539	<0.0001	0.01535	0.00052	0.01066	0.00138
ASP	10	F	H	53.77	4.98	31.4445	0.0004	1.1426	<0.0001	0.01574	0.00148	0.01252	0.00260
ASP	10	F	H	10.75	1.56	31.9504	0.0008	1.1249	<0.0001	0.00000	0.00000	0.01819	0.00536
ASP	10	F	H	25.89	10.87	32.3703	0.0294	1.1107	0.0010	0.00000	0.00000	0.13030	0.07872
ASP	10	F	H	18.13	2.33	33.9079	0.0006	1.0618	<0.0001	0.01477	0.00428	0.01506	0.00410
ASP	10	F	H	55.82	3.10	34.3863	0.0002	1.0474	<0.0001	0.01301	0.00128	0.01301	0.00146
ASP	10	F	H	59.84	2.75	34.4668	0.0002	1.045	<0.0001	0.01138	0.00202	0.01485	0.00130
ASP	10	F	H	38.76	4.98	34.7934	0.0006	1.0355	<0.0001	0.02226	0.00150	0.01509	0.00448
ASP	10	F	H	4.26	0.67	35.2233	0.0018	1.0233	0.0001	0.00000	0.00000	0.01957	0.00448
ASP	10	F	H	55.43	5.57	35.6241	0.0004	1.0121	<0.0001	0.01690	0.00086	0.01111	0.00254
ASP	10	F	H	6.22	1.89	36.4544	0.0012	0.9898	<0.0001	0.00000	0.00000	0.01681	0.00744
ASP	10	F	H	23.75	2.92	36.6436	0.0004	0.9849	<0.0001	0.01510	0.00166	0.01207	0.00324
ASP	10	F	H	19.84	5.91	36.9524	0.0006	0.977	<0.0001	0.01601	0.00210	0.00000	0.00000
ASP	10	F	H	15.84	5.74	37.3961	0.0008	0.9658	<0.0001	0.01715	0.00624	0.00000	0.00000
ASP	10	F	H	37.49	8.37	37.4713	0.0006	0.9639	<0.0001	0.01891	0.00248	0.01010	0.00556
ASP	10	F	H	28.53	5.00	38.3296	0.0006	0.9431	<0.0001	0.01740	0.00220	0.01244	0.00508
ASP	10	F	H	18.40	8.80	38.5499	0.0006	0.9379	<0.0001	0.01456	0.00694	0.00000	0.00000
ASP	10	F	D	425.19	5.56	9.2139	0.0000	3.8547	<0.0001	0.00510	0.00032	0.01026	0.00018
ASP	10	F	D	4600.45	67.14	11.7062	0.0000	3.036	<0.0001	0.00500	0.00034	0.01047	0.00020
ASP	10	F	D	100.06	3.85	12.4985	0.0002	2.8443	<0.0001	0.00585	0.00088	0.00929	0.00056
ASP	10	F	D	3.49	0.61	12.6033	0.0008	2.8207	0.0002	0.00000	0.00000	0.01750	0.00516
ASP	10	F	D	699.24	15.28	14.2566	0.0002	2.495	<0.0001	0.00576	0.00042	0.00966	0.00030
ASP	10	F	D	265.42	46.38	15.5708	0.0004	2.2856	0.0001	0.00000	0.00000	0.00496	0.00128
ASP	10	F	D	1094.55	27.31	15.5731	0.0002	2.2852	<0.0001	0.00561	0.00062	0.01067	0.00038
ASP	10	F	D	1242.60	38.21	16.9989	0.0002	2.0948	<0.0001	0.00498	0.00074	0.01011	0.00044
ASP	10	F	D	345.38	12.44	18.4828	0.0002	1.9279	<0.0001	0.00639	0.00126	0.01202	0.00066
ASP	10	F	D	891.31	21.29	18.6284	0.0002	1.913	<0.0001	0.00815	0.00042	0.01063	0.00040
ASP	10	F	D	894.65	18.00	19.0025	0.0002	1.8756	<0.0001	0.00772	0.00040	0.01134	0.00028
ASP	10	F	D	269.71	12.20	21.9534	0.0002	1.626	<0.0001	0.00741	0.00076	0.00976	0.00070
ASP	10	F	D	682.03	19.35	22.2537	0.0002	1.6043	<0.0001	0.00812	0.00056	0.01121	0.00050
ASP	10	F	D	49.61	2.73	22.4943	0.0002	1.5874	<0.0001	0.00837	0.00186	0.01224	0.00120
ASP	10	F	D	322.51	6.70	23.4186	0.0002	1.5256	<0.0001	0.00698	0.00062	0.01195	0.00038
ASP	10	F	D	111.04	4.82	23.5345	0.0002	1.5182	<0.0001	0.00857	0.00104	0.01124	0.00084
ASP	10	F	D	155.39	5.81	23.6674	0.0002	1.5098	<0.0001	0.00856	0.00062	0.01005	0.00064

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	F	D	134.77	5.85	24.2592	0.0002	1.4735	<0.0001	0.01023	0.00060	0.01047	0.00082
ASP	10	F	D	394.06	13.88	24.8221	0.0002	1.4406	<0.0001	0.00782	0.00086	0.01152	0.00064
ASP	10	F	D	130.68	13.24	25.1488	0.0004	1.4221	<0.0001	0.01005	0.00070	0.00772	0.00154
ASP	10	F	D	74.86	6.21	26.376	0.0004	1.3571	<0.0001	0.00956	0.00154	0.01084	0.00162
ASP	10	F	D	168.44	8.16	26.7325	0.0002	1.3393	<0.0001	0.01037	0.00076	0.01093	0.00094
ASP	10	F	D	186.34	9.53	27.6211	0.0002	1.297	<0.0001	0.01065	0.00060	0.01015	0.00094
ASP	10	F	D	48.57	2.87	27.8803	0.0002	1.2852	<0.0001	0.00823	0.00218	0.01238	0.00128
ASP	10	F	D	89.30	4.99	28.737	0.0002	1.2476	<0.0001	0.01105	0.00108	0.01200	0.00122
ASP	10	F	D	147.45	6.17	29.0246	0.0002	1.2355	<0.0001	0.01053	0.00064	0.01089	0.00082
ASP	10	F	D	26.68	2.23	30.2389	0.0004	1.187	<0.0001	0.00000	0.00000	0.01246	0.00196
ASP	10	F	D	129.32	4.70	30.4204	0.0002	1.1801	<0.0001	0.01013	0.00060	0.01069	0.00072
ASP	10	F	D	12.85	1.64	30.602	0.0008	1.1733	<0.0001	0.00000	0.00000	0.01530	0.00364
ASP	10	F	D	270.80	8.21	31.1262	0.0002	1.154	<0.0001	0.01163	0.00030	0.01006	0.00058
ASP	10	F	D	111.74	7.44	31.4437	0.0002	1.1426	<0.0001	0.00981	0.00040	0.00665	0.00092
ASP	10	F	D	0.99	0.43	31.7770	0.0034	1.1309	0.0001	0.00000	0.00000	0.01267	0.00822
ASP	10	F	D	25.13	2.24	31.9518	0.0004	1.1249	<0.0001	0.01230	0.00144	0.01118	0.00206
ASP	10	F	D	43.05	4.49	33.9091	0.0004	1.0617	<0.0001	0.01284	0.00142	0.01117	0.00240
ASP	10	F	D	145.27	5.90	34.3857	0.0002	1.0474	<0.0001	0.00915	0.00050	0.01179	0.00072
ASP	10	F	D	159.99	5.88	34.4666	0.0002	1.0451	<0.0001	0.01063	0.00068	0.01151	0.00076
ASP	10	F	D	91.00	10.48	34.7939	0.0004	1.0355	<0.0001	0.01430	0.00122	0.00792	0.00210
ASP	10	F	D	13.24	4.54	35.2235	0.0010	1.0233	<0.0001	0.01428	0.00256	0.00000	0.00000
ASP	10	F	D	241.83	6.18	35.6235	0.0002	1.0122	<0.0001	0.00953	0.00030	0.00849	0.00042
ASP	10	F	D	69.94	4.02	36.6427	0.0002	0.9849	<0.0001	0.01177	0.00070	0.01040	0.00118
ASP	10	F	D	18.55	3.52	36.7994	0.0006	0.9809	<0.0001	0.01353	0.00150	0.00960	0.00404
ASP	10	F	D	53.47	3.93	36.9523	0.0004	0.977	<0.0001	0.01344	0.00096	0.01154	0.00172
ASP	10	F	D	47.21	4.88	37.3951	0.0002	0.9658	<0.0001	0.01227	0.00072	0.00839	0.00188
ASP	10	F	D	91.84	4.66	37.4706	0.0002	0.9639	<0.0001	0.01304	0.00070	0.01152	0.00116
ASP	10	F	D	24.30	4.78	37.774	0.0004	0.9565	<0.0001	0.01217	0.00144	0.00717	0.00326
ASP	10	F	D	13.47	3.31	37.9512	0.0006	0.9522	<0.0001	0.01280	0.00180	0.00905	0.00504
ASP	10	F	D	78.30	3.61	38.3287	0.0002	0.9431	<0.0001	0.01184	0.00126	0.01350	0.00116
ASP	10	F	D	44.86	2.81	38.5501	0.0004	0.9379	<0.0001	0.01380	0.00098	0.01479	0.00174
ASP	10	F	W	21.31	9.78	9.2081	0.0006	3.8571	0.0003	0.00548	0.00122	0.00000	0.00000
ASP	10	F	W	235.77	2.86	9.2132	0.0000	3.855	<0.0001	0.00451	0.00032	0.01015	0.00016
ASP	10	F	W	215.04	5.63	9.2136	0.0002	3.8548	0.0001	0.00396	0.00062	0.00968	0.00038
ASP	10	F	W	602.73	181.16	11.7041	0.0014	3.0366	0.0004	0.00469	0.00122	0.00783	0.00126
ASP	10	F	W	2029.69	22.55	11.7078	0.0000	3.0356	<0.0001	0.00420	0.00034	0.01125	0.00016
ASP	10	F	W	1433.12	177.14	11.7094	0.0012	3.0352	0.0003	0.00382	0.00074	0.00978	0.00112
ASP	10	F	W	40.03	0.86	12.4991	0.0002	2.8441	<0.0001	0.00468	0.00104	0.01135	0.00038
ASP	10	F	W	3.55	0.25	12.6055	0.0006	2.8202	0.0001	0.00000	0.00000	0.01352	0.00134
ASP	10	F	W	379.52	4.39	14.2563	0.0000	2.4951	<0.0001	0.00463	0.00030	0.01004	0.00016
ASP	10	F	W	634.31	27.19	15.5758	0.0002	2.2848	<0.0001	0.00529	0.00126	0.01130	0.00028
ASP	10	F	W	673.63	11.23	15.576	0.0000	2.2848	<0.0001	0.00515	0.00046	0.01109	0.00026
ASP	10	F	W	415.73	5.92	17.0025	0.0000	2.0944	<0.0001	0.00442	0.00050	0.01115	0.00022
ASP	10	F	W	227.42	6.81	18.4857	0.0002	1.9276	<0.0001	0.00499	0.00120	0.01155	0.00050
ASP	10	F	W	655.90	10.95	18.6335	0.0000	1.9124	<0.0001	0.00552	0.00054	0.01197	0.00028
ASP	10	F	W	90.51	14.90	19.005	0.0004	1.8754	<0.0001	0.01704	0.00222	0.01971	0.00258
ASP	10	F	W	575.60	5.93	19.0059	0.0000	1.8753	<0.0001	0.00655	0.00024	0.01104	0.00016
ASP	10	F	W	483.41	7.83	19.006	0.0000	1.8753	<0.0001	0.00000	0.00000	0.01124	0.00020
ASP	10	F	W	0.71	0.27	21.9249	0.0032	1.6281	0.0002	0.00000	0.00000	0.01486	0.00850
ASP	10	F	W	127.81	1.90	21.9576	0.0000	1.6257	<0.0001	0.00638	0.00046	0.01106	0.00026
ASP	10	F	W	322.78	5.14	22.2574	0.0000	1.6041	<0.0001	0.00602	0.00046	0.01164	0.00028
ASP	10	F	W	24.45	1.15	22.4975	0.0002	1.5872	<0.0001	0.00918	0.00098	0.01058	0.00092
ASP	10	F	W	185.96	2.25	23.4224	0.0000	1.5253	<0.0001	0.00687	0.00026	0.01058	0.00020
ASP	10	F	W	65.87	1.54	23.5394	0.0000	1.5179	<0.0001	0.00728	0.00048	0.00995	0.00038
ASP	10	F	W	27.56	12.09	23.6694	0.0022	1.5096	0.0001	0.00814	0.00108	0.00720	0.00288
ASP	10	F	W	64.61	1.64	23.6729	0.0002	1.5094	<0.0001	0.00879	0.00068	0.01201	0.00052
ASP	10	F	W	82.52	2.00	24.2635	0.0002	1.4732	<0.0001	0.00670	0.00072	0.01113	0.00044
ASP	10	F	W	130.81	3.66	24.8268	0.0002	1.4403	<0.0001	0.00640	0.00090	0.01222	0.00044
ASP	10	F	W	167.52	3.54	25.1532	0.0002	1.4219	<0.0001	0.00613	0.00062	0.01117	0.00036
ASP	10	F	W	52.69	1.37	26.3799	0.0002	1.3569	<0.0001	0.00616	0.00086	0.01084	0.00046
ASP	10	F	W	78.39	1.98	26.7385	0.0002	1.339	<0.0001	0.00750	0.00066	0.01115	0.00046
ASP	10	F	W	89.08	2.83	27.629	0.0002	1.2966	<0.0001	0.00689	0.00112	0.01210	0.00052
ASP	10	F	W	31.85	0.84	27.8873	0.0002	1.2849	<0.0001	0.00535	0.00130	0.01177	0.00050
ASP	10	F	W	41.13	1.81	28.7443	0.0002	1.2473	<0.0001	0.00910	0.00104	0.01149	0.00092
ASP	10	F	W	66.08	3.55	29.0298	0.0002	1.2353	<0.0001	0.01063	0.00036	0.00899	0.00096
ASP	10	F	W	17.35	0.66	30.2458	0.0002	1.1867	<0.0001	0.00962	0.00086	0.01085	0.00078
ASP	10	F	W	78.46	1.81	30.4261	0.0002	1.1799	<0.0001	0.00869	0.00038	0.01009	0.00040
ASP	10	F	W	7.90	1.29	30.6095	0.0004	1.173	<0.0001	0.01308	0.00120	0.00919	0.00332
ASP	10	F	W	180.98	3.89	31.1328	0.0000	1.1537	<0.0001	0.00961	0.00032	0.01050	0.00038
ASP	10	F	W	68.12	2.38	31.4503	0.0002	1.1424	<0.0001	0.00992	0.00088	0.01245	0.00074
ASP	10	F	W	16.89	0.90	31.9594	0.0002	1.1246	<0.0001	0.00000	0.00000	0.01474	0.00116
ASP	10	F	W	34.78	1.79	33.9167	0.0002	1.0615	<0.0001	0.00981	0.00080	0.01008	0.00096
ASP	10	F	W	87.68	2.22	34.3929	0.0002	1.0472	<0.0001	0.00790	0.00050	0.01023	0.00044
ASP	10	F	W	135.06	2.54	34.475	0.0002	1.0448	<0.0001	0.00866	0.00054	0.01274	0.00040
ASP	10	F	W	40.78	1.85	34.8032	0.0004	1.0353	<0.0001	0.01483	0.00206	0.01865	0.00156
ASP	10	F	W	11.91	1.11	35.2314	0.0002	1.0231	<0.0001	0.01097	0.00068	0.00823	0.00162
ASP	10	F	W	99.34	2.82	35.6346	0.0002	1.0119	<0.0001	0.01190	0.00048	0.01220	0.00062
ASP	10	F	W	13.57	1.09	36.4616	0.0002	0.9897	<0.0001	0.01070	0.00084	0.00894	0.00148
ASP	10	F	W	12.11	4.79	36.6486	0.0008	0.9848	<0.0001	0.00792	0.00136	0.00494	0.00314
ASP	10	F	W	45.98	1.25	36.6537	0.0002	0.9846	<0.0001	0.01017	0.00082	0.01319	0.00064

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	10	F	W	12.84	0.72	36.8081	0.0002	0.9807	<0.0001	0.01126	0.00176	0.01324	0.00146
ASP	10	F	W	39.12	1.48	36.9621	0.0002	0.9767	<0.0001	0.01072	0.00036	0.00916	0.00068
ASP	10	F	W	28.38	1.34	37.4042	0.0002	0.9656	<0.0001	0.01060	0.00088	0.01100	0.00098
ASP	10	F	W	79.00	2.01	37.4797	0.0002	0.9637	<0.0001	0.01034	0.00032	0.00993	0.00046
ASP	10	F	W	18.38	1.26	37.7831	0.0002	0.9562	<0.0001	0.01134	0.00084	0.01000	0.00138
ASP	10	F	W	7.74	0.92	37.9607	0.0004	0.9519	<0.0001	0.01107	0.00192	0.01032	0.00254
ASP	10	F	W	57.81	1.74	38.3381	0.0002	0.9429	<0.0001	0.01109	0.00042	0.01085	0.00060
ASP	10	F	W	31.62	1.38	38.5617	0.0002	0.9376	<0.0001	0.01104	0.00080	0.01144	0.00094
ASP	100	A	H	195.34	11.39	8.3901	0.0004	4.2324	0.0002	0.03616	0.00150	0.02104	0.00274
ASP	100	A	H	31.95	2.52	9.2151	0.0004	3.8542	0.0002	0.01073	0.00178	0.01207	0.00178
ASP	100	A	H	1132.93	22.81	9.9393	0.0002	3.5740	0.0001	0.05383	0.00076	0.03344	0.00142
ASP	100	A	H	1965.60	25.99	10.7905	0.0002	3.2928	0.0001	0.06934	0.00060	0.04735	0.00128
ASP	100	A	H	266.82	7.37	11.7066	0.0002	3.0359	0.0001	0.01217	0.00034	0.01103	0.00058
ASP	100	A	H	12.27	1.99	12.4985	0.0006	2.8443	0.0001	0.00000	0.00000	0.01194	0.00386
ASP	100	A	H	2099.96	135.46	13.0191	0.0004	2.7310	0.0001	0.06769	0.00538	0.02286	0.00392
ASP	100	A	H	77.11	8.78	15.5736	0.0004	2.2852	0.0001	0.01507	0.00088	0.01006	0.00262
ASP	100	A	H	218.39	18.28	15.6442	0.0362	2.2749	0.0052	0.00000	0.00000	0.54549	0.08524
ASP	100	A	H	109.27	7.55	16.0607	0.0032	2.2163	0.0004	0.06694	0.00044	0.01553	0.00200
ASP	100	A	H	165.18	56.04	16.8203	0.0008	2.1169	0.0001	0.04260	0.01756	0.00000	0.00000
ASP	100	A	H	87.15	3.69	16.9989	0.0002	2.0948	<0.0001	0.00760	0.00194	0.01249	0.00096
ASP	100	A	H	1424.67	45.97	17.2531	0.0004	2.0642	<0.0001	0.08212	0.00238	0.03978	0.00306
ASP	100	A	H	57.85	9.44	18.6273	0.0006	1.9131	0.0001	0.02004	0.00254	0.01051	0.00410
ASP	100	A	H	71.74	5.38	19.0015	0.0004	1.8757	<0.0001	0.01536	0.00148	0.01374	0.00216
ASP	100	A	H	91.86	17.57	19.9489	0.0024	1.7875	0.0002	0.09503	0.01148	0.05190	0.02434
ASP	100	A	H	7.72	1.14	21.9528	0.0020	1.6261	0.0001	0.00000	0.00000	0.02203	0.00462
ASP	100	A	H	43.73	7.31	22.2536	0.0006	1.6044	<0.0001	0.01886	0.00176	0.01128	0.00440
ASP	100	A	H	42.42	12.95	23.419	0.0004	1.5256	<0.0001	0.01267	0.00394	0.00000	0.00000
ASP	100	A	H	19.15	6.07	23.5320	0.0010	1.5183	0.0001	0.01895	0.00292	0.00000	0.00000
ASP	100	A	H	23.70	2.82	24.8217	0.0008	1.4406	<0.0001	0.01597	0.00496	0.01779	0.00430
ASP	100	A	H	41.63	8.46	25.1456	0.0006	1.4223	<0.0001	0.01702	0.00236	0.00939	0.00458
ASP	100	A	H	2.95	0.73	26.3742	0.0022	1.3572	0.0001	0.00000	0.00000	0.01515	0.00556
ASP	100	A	H	11.96	4.41	26.7293	0.0014	1.3394	0.0001	0.02237	0.00452	0.00000	0.00000
ASP	100	A	H	6.76	1.19	27.6204	0.0024	1.2970	0.0001	0.00000	0.00000	0.02357	0.00604
ASP	100	A	H	12.58	4.70	29.0235	0.0014	1.2356	0.0001	0.02559	0.00536	0.00000	0.00000
ASP	100	A	H	16.58	4.68	31.1249	0.0012	1.154	<0.0001	0.02509	0.00364	0.00000	0.00000
ASP	100	A	H	18.16	7.95	31.4431	0.0014	1.1426	0.0001	0.02286	0.00546	0.00000	0.00000
ASP	100	A	H	1.78	0.76	31.9544	0.0064	1.1248	0.0002	0.00000	0.00000	0.02649	0.01586
ASP	100	A	H	16.31	4.68	35.622	0.0014	1.0122	<0.0001	0.00000	0.00000	0.02511	0.01602
ASP	100	A	H	34.26	5.36	36.3786	0.0140	0.9918	0.0004	0.10220	0.00086	0.02632	0.00792
ASP	100	A	H	37.07	1.70	37.4668	0.0006	0.964	<0.0001	0.00000	0.00000	0.02588	0.00162
ASP	100	A	D	165.91	6.88	8.3895	0.0006	4.2327	0.0003	0.03142	0.00028	0.01493	0.00112
ASP	100	A	D	104.74	3.06	9.2143	0.0002	3.8545	0.0001	0.00809	0.00068	0.01101	0.00054
ASP	100	A	D	897.84	28.31	9.9382	0.0004	3.5744	0.0001	0.04751	0.00104	0.02974	0.00200
ASP	100	A	D	960.15	102.58	10.7908	0.0006	3.2927	0.0002	0.09739	0.00526	0.08188	0.00636
ASP	100	A	D	471.38	7.36	11.7063	0.0000	3.036	<0.0001	0.01067	0.00026	0.01149	0.00032
ASP	100	A	D	17.43	2.35	12.4965	0.0004	2.8447	0.0001	0.00962	0.00208	0.00928	0.00258
ASP	100	A	D	1648.32	41.61	13.0186	0.0004	2.7311	0.0001	0.08353	0.00198	0.04047	0.00242
ASP	100	A	D	217.31	4.69	14.2552	0.0002	2.4953	<0.0001	0.00907	0.00040	0.01095	0.00040
ASP	100	A	D	258.81	5.97	15.5727	0.0002	2.2853	<0.0001	0.00922	0.00064	0.01154	0.00048
ASP	100	A	D	193.36	14.09	15.5939	0.0324	2.2822	0.0047	0.00000	0.00000	0.53075	0.06140
ASP	100	A	D	82.18	3.49	16.4606	0.0072	2.1628	0.0009	0.00000	0.00000	0.29324	0.01892
ASP	100	A	D	134.16	14.05	16.8210	0.0008	2.1168	0.0001	0.05513	0.00404	0.02971	0.00752
ASP	100	A	D	137.40	4.15	16.9998	0.0002	2.0947	<0.0001	0.00986	0.00098	0.01310	0.00070
ASP	100	A	D	267.78	99.41	17.2522	0.0022	2.0643	0.0003	0.00000	0.00000	0.10939	0.03454
ASP	100	A	D	128.77	46.75	18.4837	0.0018	1.9278	0.0002	0.00784	0.00220	0.00000	0.00000
ASP	100	A	D	207.87	6.62	18.6276	0.0002	1.913	<0.0001	0.01031	0.00082	0.01641	0.00088
ASP	100	A	D	88.87	9.43	18.6330	0.0006	1.9125	0.0001	0.00863	0.00094	0.00785	0.00142
ASP	100	A	D	242.16	10.00	19.0013	0.0002	1.8758	<0.0001	0.01206	0.00060	0.01135	0.00090
ASP	100	A	D	421.06	24.54	19.2070	0.0014	1.8559	0.0001	0.11827	0.00472	0.08784	0.01156
ASP	100	A	D	1032.18	25.83	19.5679	0.0006	1.8219	0.0001	0.11186	0.00152	0.07011	0.00398
ASP	100	A	D	55.60	4.77	19.9482	0.0022	1.7876	0.0002	0.00000	0.00000	0.08295	0.01478
ASP	100	A	D	70.45	2.91	21.953	0.0002	1.626	<0.0001	0.00757	0.00264	0.01457	0.00108
ASP	100	A	D	95.91	4.53	22.2535	0.0002	1.6044	<0.0001	0.01336	0.00064	0.01177	0.00110
ASP	100	A	D	8.72	2.77	22.4934	0.0018	1.5875	0.0001	0.00000	0.00000	0.01803	0.00504
ASP	100	A	D	89.43	4.65	23.4186	0.0002	1.5256	<0.0001	0.01236	0.00064	0.01061	0.00112
ASP	100	A	D	20.01	4.37	23.5331	0.0006	1.5183	<0.0001	0.01509	0.00328	0.01167	0.00582
ASP	100	A	D	67.61	6.62	23.6635	0.0002	1.51	<0.0001	0.01365	0.00074	0.00943	0.00208
ASP	100	A	D	141.34	4.46	24.822	0.0002	1.4406	<0.0001	0.01087	0.00046	0.01085	0.00062
ASP	100	A	D	16.50	4.84	25.1465	0.0020	1.4223	0.0001	0.00000	0.00000	0.02427	0.01542
ASP	100	A	D	56.39	5.86	25.2890	0.0154	1.4144	0.0008	0.03985	0.00256	0.00235	0.00046
ASP	100	A	D	69.59	31.59	26.1810	0.1370	1.3670	0.0071	0.00000	0.00000	0.67928	0.17688
ASP	100	A	D	13.27	1.70	26.3751	0.0008	1.3571	<0.0001	0.00000	0.00000	0.01633	0.00412
ASP	100	A	D	24.47	5.16	26.4877	0.0042	1.3514	0.0002	0.00000	0.00000	0.08230	0.03946
ASP	100	A	D	20.30	6.24	26.7312	0.0014	1.3394	0.0001	0.02012	0.00798	0.00000	0.00000
ASP	100	A	D	69.92	8.78	27.6213	0.0004	1.297	<0.0001	0.01140	0.00080	0.00767	0.00210
ASP	100	A	D	12.77	1.20	27.8786	0.0006	1.2853	<0.0001	0.00000	0.00000	0.01263	0.00174
ASP	100	A	D	15.40	2.20	28.7368	0.0006	1.2476	<0.0001	0.01492	0.00236	0.01273	0.00388
ASP	100	A	D	19.43	2.14	29.0223	0.0006	1.2356	<0.0001	0.01855	0.00420	0.01932	0.00438
ASP	100	A	D	36.22	2.47	30.1052	0.0054	1.1922	0.0002	0.00000	0.00000	0.14690	0.01280

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	A	D	15.97	2.33	30.2377	0.0006	1.1871	<0.0001	0.00000	0.00000	0.01591	0.00486
ASP	100	A	D	27.62	3.27	30.4195	0.0006	1.1801	<0.0001	0.01881	0.00238	0.01559	0.00398
ASP	100	A	D	74.94	3.97	31.1263	0.0002	1.154	<0.0001	0.01656	0.00100	0.01468	0.00160
ASP	100	A	D	29.56	10.33	31.4429	0.0006	1.1426	<0.0001	0.01806	0.00474	0.00000	0.00000
ASP	100	A	D	4.74	1.28	31.9452	0.0018	1.1251	0.0001	0.00000	0.00000	0.02007	0.01120
ASP	100	A	D	126.98	11.93	32.4616	0.0170	1.1077	0.0006	0.05972	0.00034	0.00626	0.00062
ASP	100	A	D	13.40	1.46	33.9033	0.0012	1.0619	<0.0001	0.00000	0.00000	0.02558	0.00442
ASP	100	A	D	45.66	2.58	34.4657	0.0004	1.0451	<0.0001	0.01245	0.00324	0.01702	0.00188
ASP	100	A	D	11.28	2.34	34.792	0.0016	1.0356	<0.0001	0.00000	0.00000	0.02783	0.01218
ASP	100	A	D	34.41	4.14	35.6215	0.0006	1.0122	<0.0001	0.01906	0.00228	0.01491	0.00404
ASP	100	A	D	17.97	2.73	36.6409	0.0008	0.985	<0.0001	0.01851	0.00394	0.01625	0.00540
ASP	100	A	D	8.91	1.16	36.9491	0.0022	0.9770	0.0001	0.00000	0.00000	0.02961	0.00578
ASP	100	A	D	23.31	5.66	38.3277	0.0006	0.9432	<0.0001	0.01771	0.00194	0.01129	0.00658
ASP	100	A	D	11.23	4.17	38.5481	0.0012	0.938	<0.0001	0.02150	0.00390	0.00000	0.00000
ASP	100	A	W	407.74	6.20	9.2122	0.0000	3.8554	<0.0001	0.00507	0.00040	0.01024	0.00022
ASP	100	A	W	3262.11	98.56	11.7032	0.0002	3.0368	0.0001	0.00495	0.00090	0.01078	0.00026
ASP	100	A	W	3430.72	62.59	11.7034	0.0000	3.0368	<0.0001	0.00492	0.00046	0.01070	0.00026
ASP	100	A	W	122.82	5.84	12.4926	0.0002	2.8456	<0.0001	0.00564	0.00124	0.00992	0.00074
ASP	100	A	W	489.87	9.85	14.2542	0.0002	2.4954	<0.0001	0.00649	0.00048	0.01078	0.00032
ASP	100	A	W	1007.07	14.31	15.5701	0.0000	2.2857	<0.0001	0.00675	0.00028	0.01059	0.00022
ASP	100	A	W	778.79	17.48	16.9971	0.0002	2.095	<0.0001	0.00570	0.00060	0.01073	0.00034
ASP	100	A	W	332.33	8.85	18.4798	0.0002	1.9282	<0.0001	0.00857	0.00058	0.01132	0.00050
ASP	100	A	W	666.44	20.98	18.6221	0.0002	1.9136	<0.0001	0.00886	0.00036	0.01106	0.00050
ASP	100	A	W	873.04	18.16	18.9983	0.0000	1.8761	<0.0001	0.00752	0.00036	0.01021	0.00034
ASP	100	A	W	261.83	7.35	21.9507	0.0002	1.6262	<0.0001	0.00717	0.00080	0.01151	0.00052
ASP	100	A	W	254.68	78.24	22.247	0.0002	1.6048	<0.0001	0.00376	0.00160	0.00285	0.00152
ASP	100	A	W	1043.62	33.92	22.2502	0.0002	1.6046	<0.0001	0.00651	0.00076	0.01088	0.00052
ASP	100	A	W	27.04	1.39	22.4869	0.0002	1.5879	<0.0001	0.00816	0.00248	0.01310	0.00124
ASP	100	A	W	634.59	13.24	23.4153	0.0002	1.5258	<0.0001	0.00601	0.00054	0.01097	0.00034
ASP	100	A	W	127.05	6.84	23.5275	0.0002	1.5186	<0.0001	0.00630	0.00226	0.01209	0.00104
ASP	100	A	W	202.33	8.09	23.6612	0.0002	1.5102	<0.0001	0.00592	0.00190	0.01311	0.00082
ASP	100	A	W	104.03	3.11	24.2552	0.0002	1.4737	<0.0001	0.01079	0.00066	0.01230	0.00066
ASP	100	A	W	380.65	14.54	24.8177	0.0002	1.4408	<0.0001	0.00831	0.00090	0.01173	0.00072
ASP	100	A	W	193.92	9.69	25.1436	0.0010	1.4224	0.0001	0.00000	0.00000	0.01603	0.00098
ASP	100	A	W	138.96	5.09	26.3713	0.0002	1.3573	<0.0001	0.00620	0.00128	0.01138	0.00066
ASP	100	A	W	107.46	5.70	26.7261	0.0004	1.3396	<0.0001	0.00912	0.00288	0.01567	0.00140
ASP	100	A	W	172.58	7.44	27.6143	0.0002	1.2973	<0.0001	0.01094	0.00124	0.01428	0.00104
ASP	100	A	W	51.37	2.12	27.876	0.0006	1.2854	<0.0001	0.00993	0.00204	0.01382	0.00072
ASP	100	A	W	70.36	3.33	28.7329	0.0002	1.2478	<0.0001	0.01138	0.00052	0.01003	0.00092
ASP	100	A	W	76.00	3.17	29.0156	0.0002	1.2359	<0.0001	0.01243	0.00090	0.01307	0.00104
ASP	100	A	W	48.32	3.07	30.2368	0.0002	1.1871	<0.0001	0.00811	0.00152	0.01010	0.00118
ASP	100	A	W	132.09	5.26	30.414	0.0002	1.1803	<0.0001	0.01035	0.00052	0.01022	0.00074
ASP	100	A	W	12.93	2.71	30.5918	0.0014	1.1736	0.0001	0.00000	0.00000	0.01761	0.00356
ASP	100	A	W	297.59	7.43	31.1209	0.0002	1.1542	<0.0001	0.01149	0.00034	0.01131	0.00050
ASP	100	A	W	102.02	5.49	31.4401	0.0004	1.1427	<0.0001	0.01215	0.00092	0.01328	0.00072
ASP	100	A	W	41.66	2.65	31.9434	0.0004	1.1252	<0.0001	0.00792	0.00352	0.01435	0.00162
ASP	100	A	W	44.23	3.04	33.8985	0.0004	1.062	<0.0001	0.00992	0.00472	0.01714	0.00216
ASP	100	A	W	181.08	5.63	34.3827	0.0002	1.0475	<0.0001	0.01067	0.00080	0.01301	0.00072
ASP	100	A	W	195.55	6.08	34.4588	0.0002	1.0453	<0.0001	0.01231	0.00068	0.01354	0.00076
ASP	100	A	W	89.99	4.71	34.7821	0.0004	1.0359	<0.0001	0.01662	0.00146	0.01709	0.00170
ASP	100	A	W	11.79	2.74	35.2142	0.0010	1.0235	<0.0001	0.01424	0.00578	0.01371	0.00676
ASP	100	A	W	178.17	6.46	35.6151	0.0002	1.0124	<0.0001	0.01319	0.00050	0.01215	0.00082
ASP	100	A	W	101.29	3.97	36.6388	0.0002	0.985	<0.0001	0.01323	0.00070	0.01304	0.00096
ASP	100	A	W	19.62	1.65	36.7923	0.0004	0.9811	<0.0001	0.01431	0.00162	0.01310	0.00228
ASP	100	A	W	31.91	4.86	36.9435	0.0004	0.9772	<0.0001	0.01674	0.00158	0.01012	0.00352
ASP	100	A	W	111.33	3.67	37.3907	0.0002	0.9659	<0.0001	0.01033	0.00084	0.01272	0.00074
ASP	100	A	W	89.78	4.88	37.4643	0.0002	0.9641	<0.0001	0.01669	0.00072	0.01366	0.00152
ASP	100	A	W	16.85	2.33	37.7614	0.0006	0.9568	<0.0001	0.01916	0.00144	0.01312	0.00410
ASP	100	A	W	24.52	1.80	37.9465	0.0004	0.9523	<0.0001	0.00000	0.00000	0.01517	0.00206
ASP	100	A	W	135.53	4.04	38.3249	0.0002	0.9432	<0.0001	0.01299	0.00040	0.01281	0.00058
ASP	100	A	W	41.58	2.48	38.5422	0.0004	0.9381	<0.0001	0.01464	0.00270	0.01598	0.00178
ASP	100	B	H	207.03	10.78	8.3891	0.0004	4.2329	0.0002	0.03574	0.00106	0.02258	0.00260
ASP	100	B	H	24.86	1.91	8.5619	0.0424	4.1476	0.0206	0.02610	0.00030	0.00077	0.00002
ASP	100	B	H	20.71	1.61	9.2145	0.0004	3.8545	0.0002	0.00000	0.00000	0.01357	0.00188
ASP	100	B	H	823.89	333.70	9.9385	0.0006	3.5743	0.0002	0.07026	0.00396	0.05922	0.01400
ASP	100	B	H	1158.74	81.60	10.7901	0.0006	3.2929	0.0002	0.10411	0.00434	0.05418	0.00256
ASP	100	B	H	273.43	5.52	11.7057	0.0000	3.0362	<0.0001	0.00841	0.00034	0.00987	0.00034
ASP	100	B	H	2093.45	44.00	13.0187	0.0004	2.7311	0.0001	0.08766	0.00158	0.04421	0.00216
ASP	100	B	H	31.01	2.54	14.2562	0.0002	2.4951	<0.0001	0.00865	0.00134	0.00902	0.00144
ASP	100	B	H	237.14	10.67	15.3627	0.0048	2.3163	0.0007	0.14110	0.07400	0.25259	0.02082
ASP	100	B	H	90.34	15.86	15.5718	0.0002	2.2854	<0.0001	0.01008	0.00142	0.00509	0.00218
ASP	100	B	H	115.52	17.16	16.4598	0.0064	2.1629	0.0008	0.00000	0.00000	0.30028	0.11026
ASP	100	B	H	178.28	29.08	16.8200	0.0008	2.1169	0.0001	0.05415	0.00808	0.02388	0.01000
ASP	100	B	H	73.21	3.94	16.9991	0.0002	2.0948	<0.0001	0.00903	0.00084	0.00920	0.00096
ASP	100	B	H	448.94	139.58	17.2527	0.0018	2.0642	0.0002	0.00000	0.00000	0.11205	0.02980
ASP	100	B	H	63.89	5.17	18.6267	0.0004	1.9131	<0.0001	0.01520	0.00074	0.01080	0.00186
ASP	100	B	H	59.28	3.40	19.0014	0.0002	1.8757	<0.0001	0.00919	0.00240	0.01290	0.00142
ASP	100	B	H	64.66	3.80	19.9496	0.0022	1.7874	0.0002	0.00000	0.00000	0.09703	0.01058
ASP	100	B	H	29.93	3.73	21.2136	0.0232	1.6820	0.0018	0.00000	0.00000	0.27737	0.05822

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	B	H	7.58	1.30	21.9538	0.0010	1.6260	0.0001	0.00000	0.00000	0.01333	0.00380
ASP	100	B	H	40.36	3.75	22.2547	0.0004	1.6043	<0.0001	0.01313	0.00108	0.01075	0.00208
ASP	100	B	H	14.21	3.90	23.4168	0.0008	1.5257	0.0001	0.01409	0.00626	0.01204	0.00748
ASP	100	B	H	9.37	2.41	24.8213	0.0014	1.4406	0.0001	0.01716	0.00738	0.01589	0.00890
ASP	100	B	H	10.50	1.18	27.6186	0.0012	1.2971	0.0001	0.00000	0.00000	0.02137	0.00306
ASP	100	B	H	9.61	2.27	29.0174	0.0012	1.2358	0.0001	0.01953	0.00802	0.01749	0.00916
ASP	100	B	H	12.61	3.66	31.1258	0.0012	1.154	<0.0001	0.02131	0.00448	0.01614	0.01060
ASP	100	B	H	147.20	9.84	32.4382	0.0038	1.1085	0.0001	0.18793	0.05750	0.21378	0.03084
ASP	100	B	H	3.10	0.89	33.9012	0.0060	1.0620	0.0002	0.00000	0.00000	0.03619	0.01568
ASP	100	B	H	6.00	1.07	36.9457	0.0024	0.9771	0.0001	0.00000	0.00000	0.02427	0.00658
ASP	100	B	H	33.26	10.27	37.3800	0.0502	0.9662	0.0013	0.00000	0.00000	0.21808	0.08250
ASP	100	B	D	209.86	12.17	8.3899	0.0004	4.2325	0.0002	0.03035	0.00124	0.01787	0.00228
ASP	100	B	D	34.62	2.50	9.2129	0.0002	3.8551	0.0001	0.00820	0.00156	0.01018	0.00132
ASP	100	B	D	1114.96	20.01	9.9377	0.0002	3.5746	0.0001	0.04555	0.00054	0.03211	0.00116
ASP	100	B	D	1921.97	22.24	10.7891	0.0002	3.2932	0.0001	0.06059	0.00050	0.04850	0.00106
ASP	100	B	D	252.90	6.22	11.7055	0.0002	3.0362	0.0001	0.00899	0.00040	0.01032	0.00044
ASP	100	B	D	2082.26	48.36	13.0184	0.0004	2.7311	0.0001	0.08155	0.00164	0.04163	0.00226
ASP	100	B	D	51.98	4.26	14.2553	0.0002	2.4952	<0.0001	0.01036	0.00066	0.00825	0.00136
ASP	100	B	D	49.96	6.47	15.5724	0.0004	2.2853	0.0001	0.01061	0.00290	0.00993	0.00282
ASP	100	B	D	159.63	13.88	16.8214	0.0008	2.1167	0.0001	0.04898	0.00238	0.02966	0.00596
ASP	100	B	D	80.73	4.08	16.9994	0.0002	2.0947	<0.0001	0.00824	0.00148	0.01108	0.00104
ASP	100	B	D	504.33	163.83	17.2528	0.0020	2.0642	0.0002	0.00000	0.00000	0.09234	0.02574
ASP	100	B	D	32.50	3.64	18.6263	0.0006	1.9132	0.0001	0.01491	0.00372	0.01551	0.00358
ASP	100	B	D	106.69	4.23	19.0009	0.0002	1.8758	<0.0001	0.00761	0.00136	0.01120	0.00080
ASP	100	B	D	534.40	21.24	19.2067	0.0010	1.8559	0.0001	0.11743	0.00256	0.08165	0.00732
ASP	100	B	D	1163.83	392.53	19.5680	0.0022	1.8219	0.0002	0.10966	0.00822	0.08111	0.02282
ASP	100	B	D	71.65	6.43	19.9464	0.0020	1.7877	0.0002	0.05677	0.02684	0.07681	0.01444
ASP	100	B	D	27.61	7.39	20.3874	0.0060	1.7494	0.0005	0.09281	0.03738	0.08057	0.04938
ASP	100	B	D	12.19	2.27	21.9520	0.0008	1.6261	0.0001	0.00000	0.00000	0.01253	0.00470
ASP	100	B	D	14.68	6.47	23.5322	0.0012	1.5183	0.0001	0.01643	0.00372	0.00000	0.00000
ASP	100	B	D	39.40	3.27	24.8217	0.0002	1.4406	<0.0001	0.00940	0.00124	0.00939	0.00150
ASP	100	B	D	16.40	1.42	25.1454	0.0010	1.4223	0.0001	0.00000	0.00000	0.02016	0.00226
ASP	100	B	D	6.03	0.86	26.3721	0.0012	1.3573	0.0001	0.00000	0.00000	0.01542	0.00334
ASP	100	B	D	14.40	2.10	27.6144	0.0004	1.2973	<0.0001	0.00758	0.00154	0.00654	0.00208
ASP	100	B	D	3.95	1.75	28.7331	0.0016	1.2478	0.0001	0.01361	0.00848	0.00000	0.00000
ASP	100	B	D	9.05	1.99	29.0198	0.0010	1.2357	<0.0001	0.01617	0.00920	0.01655	0.00800
ASP	100	B	D	58.02	5.57	29.3890	0.0548	1.2205	0.0022	0.00000	0.00000	0.62672	0.08264
ASP	100	B	D	60.24	17.50	30.1102	0.0028	1.1920	0.0001	0.10614	0.02704	0.00000	0.00000
ASP	100	B	D	3.37	0.76	30.4175	0.0026	1.1802	0.0001	0.00000	0.00000	0.01866	0.00636
ASP	100	B	D	58.50	2.36	30.8157	0.0054	1.1653	0.0002	0.00000	0.00000	0.23745	0.01416
ASP	100	B	D	33.98	16.07	31.1258	0.0002	1.154	<0.0001	0.00859	0.00484	0.00000	0.00000
ASP	100	B	D	12.15	4.50	34.4637	0.0008	1.0451	<0.0001	0.01550	0.00334	0.00000	0.00000
ASP	100	B	D	4.04	0.92	35.6190	0.0028	1.0123	0.0001	0.00000	0.00000	0.02196	0.00760
ASP	100	B	D	14.09	5.69	38.3263	0.0014	0.9432	<0.0001	0.02208	0.00874	0.00000	0.00000
ASP	100	B	W	97.45	7.97	8.3877	0.0006	4.2336	0.0003	0.02852	0.00146	0.01795	0.00318
ASP	100	B	W	154.38	4.23	9.2107	0.0002	3.8561	0.0001	0.00904	0.00076	0.01333	0.00058
ASP	100	B	W	171.26	4.72	9.2114	0.0002	3.8558	0.0001	0.00862	0.00076	0.01166	0.00052
ASP	100	B	W	509.16	15.06	9.9333	0.0002	3.5762	0.0001	0.03833	0.00072	0.02581	0.00156
ASP	100	B	W	893.39	90.34	10.7846	0.0004	3.2946	0.0001	0.03692	0.00446	0.01286	0.00340
ASP	100	B	W	844.31	29.97	10.7945	0.0006	3.2916	0.0002	0.05575	0.00122	0.04113	0.00296
ASP	100	B	W	1451.18	12.23	11.7006	0.0000	3.0375	<0.0001	0.00906	0.00016	0.01235	0.00016
ASP	100	B	W	8.38	2.58	12.4943	0.0010	2.8452	0.0002	0.01241	0.00410	0.00000	0.00000
ASP	100	B	W	7.58	2.13	12.6013	0.0014	2.8212	0.0003	0.00000	0.00000	0.01425	0.00832
ASP	100	B	W	957.70	409.98	13.0142	0.0004	2.7320	0.0001	0.03738	0.02210	0.00000	0.00000
ASP	100	B	W	691.62	9.49	14.2522	0.0000	2.4958	<0.0001	0.00833	0.00018	0.00981	0.00022
ASP	100	B	W	345.72	8.88	15.569	0.0002	2.2858	<0.0001	0.01133	0.00056	0.01222	0.00058
ASP	100	B	W	78.41	35.65	16.8195	0.0010	2.1170	0.0001	0.03345	0.01790	0.00000	0.00000
ASP	100	B	W	433.58	7.59	16.9944	0.0000	2.0953	<0.0001	0.00893	0.00038	0.01167	0.00034
ASP	100	B	W	624.53	203.21	17.245	0.0004	2.0651	<0.0001	0.03434	0.01490	0.00000	0.00000
ASP	100	B	W	224.28	6.75	18.4774	0.0002	1.9285	<0.0001	0.01075	0.00040	0.01071	0.00058
ASP	100	B	W	115.15	4.49	18.6208	0.0002	1.9137	<0.0001	0.01158	0.00124	0.01462	0.00102
ASP	100	B	W	368.10	6.67	18.9953	0.0002	1.8763	<0.0001	0.00834	0.00058	0.01299	0.00038
ASP	100	B	W	35.19	5.69	19.9388	0.0024	1.7884	0.0002	0.05214	0.00704	0.05870	0.01936
ASP	100	B	W	178.37	5.45	21.9475	0.0002	1.6265	<0.0001	0.00990	0.00070	0.01211	0.00064
ASP	100	B	W	380.04	7.53	22.2487	0.0002	1.6047	<0.0001	0.01059	0.00038	0.01224	0.00040
ASP	100	B	W	20.32	2.97	22.4845	0.0006	1.5881	<0.0001	0.01218	0.00280	0.01161	0.00348
ASP	100	B	W	241.97	5.86	23.4121	0.0002	1.526	<0.0001	0.01033	0.00070	0.01391	0.00056
ASP	100	B	W	57.33	4.91	23.5244	0.0004	1.5188	<0.0001	0.01379	0.00096	0.01128	0.00198
ASP	100	B	W	42.06	21.02	23.6566	0.0006	1.5104	<0.0001	0.01500	0.00856	0.00000	0.00000
ASP	100	B	W	56.35	6.51	24.2524	0.0004	1.4739	<0.0001	0.01386	0.00110	0.01027	0.00262
ASP	100	B	W	304.57	6.62	24.8158	0.0002	1.4409	<0.0001	0.01091	0.00046	0.01300	0.00048
ASP	100	B	W	18.85	4.56	25.139	0.0008	1.4227	<0.0001	0.01585	0.00214	0.01090	0.00598
ASP	100	B	W	26.05	1.44	26.3679	0.0006	1.3575	<0.0001	0.00000	0.00000	0.01812	0.00128
ASP	100	B	W	30.02	4.67	26.7229	0.0006	1.3398	<0.0001	0.01774	0.00308	0.01474	0.00496
ASP	100	B	W	16.74	3.90	26.8246	0.0086	1.3348	0.0004	0.00000	0.00000	0.10782	0.05254
ASP	100	B	W	50.87	3.63	27.6134	0.0004	1.2974	<0.0001	0.01206	0.00332	0.01609	0.00218
ASP	100	B	W	57.29	3.92	28.73	0.0004	1.2479	<0.0001	0.01282	0.00132	0.01278	0.00168
ASP	100	B	W	34.17	4.10	29.0143	0.0006	1.236	<0.0001	0.01703	0.00252	0.01524	0.00380
ASP	100	B	W	13.12	2.45	30.2303	0.0010	1.1873	<0.0001	0.01503	0.00678	0.01567	0.00618

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	B	W	62.75	3.86	30.4103	0.0002	1.1805	<0.0001	0.01367	0.00090	0.01214	0.00148
ASP	100	B	W	200.55	10.68	31.1155	0.0002	1.1544	<0.0001	0.01179	0.00044	0.00707	0.00084
ASP	100	B	W	110.11	4.80	31.4355	0.0002	1.1429	<0.0001	0.01151	0.00270	0.01643	0.00140
ASP	100	B	W	11.14	1.75	31.9385	0.0010	1.1254	<0.0001	0.00000	0.00000	0.01887	0.00580
ASP	100	B	W	12.49	2.17	33.8934	0.0010	1.0622	<0.0001	0.00000	0.00000	0.01739	0.00624
ASP	100	B	W	122.80	4.56	34.3755	0.0002	1.0477	<0.0001	0.01354	0.00082	0.01394	0.00098
ASP	100	B	W	56.28	4.69	34.4572	0.0004	1.0453	<0.0001	0.01575	0.00106	0.01259	0.00220
ASP	100	B	W	52.31	3.95	34.7766	0.0004	1.036	<0.0001	0.01546	0.00418	0.01834	0.00282
ASP	100	B	W	1.98	0.80	35.2127	0.0048	1.0236	0.0001	0.00000	0.00000	0.02130	0.01200
ASP	100	B	W	49.18	4.12	35.6122	0.0004	1.0125	<0.0001	0.01543	0.00306	0.01599	0.00278
ASP	100	B	W	25.45	5.51	36.444	0.0006	0.9901	<0.0001	0.01633	0.00182	0.01715	0.00670
ASP	100	B	W	88.21	4.00	36.6325	0.0002	0.9852	<0.0001	0.01077	0.00158	0.01388	0.00114
ASP	100	B	W	31.85	9.77	37.3845	0.0008	0.9661	<0.0001	0.02226	0.00436	0.00000	0.00000
ASP	100	B	W	54.40	7.27	37.4604	0.0006	0.9642	<0.0001	0.02333	0.00158	0.01513	0.00462
ASP	100	B	W	51.38	6.50	38.3212	0.0006	0.9433	<0.0001	0.01887	0.00284	0.01539	0.00432
ASP	100	B	W	10.07	1.78	38.5394	0.0014	0.9382	<0.0001	0.00000	0.00000	0.02093	0.00660
ASP	100	C	H	198.42	11.79	8.3894	0.0004	4.2328	0.0002	0.03587	0.00164	0.02014	0.00272
ASP	100	C	H	35.33	3.67	9.2137	0.0002	3.8548	0.0001	0.01024	0.00064	0.00712	0.00154
ASP	100	C	H	1168.57	25.62	9.9382	0.0002	3.5744	0.0001	0.05006	0.00086	0.02839	0.00138
ASP	100	C	H	1985.10	26.21	10.7892	0.0002	3.2932	0.0001	0.06733	0.00060	0.04384	0.00120
ASP	100	C	H	218.11	5.82	11.7048	0.0002	3.0364	0.0001	0.01191	0.00048	0.01216	0.00060
ASP	100	C	H	14.86	2.38	12.4949	0.0006	2.8451	0.0001	0.01099	0.00352	0.01107	0.00370
ASP	100	C	H	2088.93	58.99	13.0182	0.0004	2.7312	0.0001	0.08491	0.00238	0.03885	0.00268
ASP	100	C	H	46.77	3.49	14.2561	0.0002	2.4951	<0.0001	0.01135	0.00090	0.01004	0.00150
ASP	100	C	H	75.63	8.23	15.5723	0.0004	2.2853	0.0001	0.01401	0.00188	0.01308	0.00198
ASP	100	C	H	242.34	19.52	15.6175	0.0384	2.2788	0.0056	0.00000	0.00000	0.56484	0.07940
ASP	100	C	H	129.12	4.45	16.4507	0.0064	2.1641	0.0008	0.00000	0.00000	0.33468	0.01792
ASP	100	C	H	159.63	3.26	16.8193	0.0012	2.1170	0.0002	0.05670	0.00248	0.02977	0.00026
ASP	100	C	H	43.06	3.06	16.9991	0.0004	2.0948	<0.0001	0.00919	0.00282	0.01386	0.00172
ASP	100	C	H	1402.64	33.84	17.2517	0.0004	2.0643	<0.0001	0.08227	0.00154	0.04471	0.00250
ASP	100	C	H	90.99	4.11	18.6257	0.0002	1.9132	<0.0001	0.01617	0.00074	0.01487	0.00130
ASP	100	C	H	71.73	4.46	19.0004	0.0002	1.8758	<0.0001	0.01523	0.00098	0.01266	0.00166
ASP	100	C	H	303.13	90.79	19.2081	0.0022	1.8557	0.0002	0.11560	0.06776	0.15038	0.04246
ASP	100	C	H	1303.62	26.62	19.568	0.0004	1.8219	<0.0001	0.11650	0.00124	0.07580	0.00336
ASP	100	C	H	96.21	13.71	19.9483	0.0016	1.7875	0.0001	0.08975	0.00834	0.04779	0.01676
ASP	100	C	H	41.62	4.53	21.2082	0.0236	1.6825	0.0019	0.00000	0.00000	0.38127	0.07426
ASP	100	C	H	43.61	4.07	21.2148	0.0188	1.6819	0.0015	0.00000	0.00000	0.35356	0.05788
ASP	100	C	H	11.54	2.09	21.9520	0.0008	1.6261	0.0001	0.01433	0.00214	0.01415	0.00534
ASP	100	C	H	33.24	3.31	22.2526	0.0004	1.6044	<0.0001	0.01654	0.00202	0.01546	0.00300
ASP	100	C	H	31.34	5.37	23.4176	0.0004	1.5256	<0.0001	0.01303	0.00118	0.00787	0.00318
ASP	100	C	H	9.50	3.47	23.5312	0.0010	1.5184	0.0001	0.01434	0.00816	0.01584	0.00254
ASP	100	C	H	7.61	1.49	24.2549	0.0028	1.4737	0.0002	0.00000	0.00000	0.02584	0.00774
ASP	100	C	H	26.01	3.15	24.8201	0.0006	1.4407	<0.0001	0.01689	0.00154	0.01523	0.00312
ASP	100	C	H	41.04	14.26	25.1458	0.0014	1.4223	0.0001	0.02198	0.00400	0.02242	0.00328
ASP	100	C	H	2.48	0.79	26.3763	0.0034	1.3570	0.0002	0.00000	0.00000	0.01730	0.00820
ASP	100	C	H	12.40	2.41	26.7274	0.0012	1.3395	0.0001	0.00000	0.00000	0.02232	0.00934
ASP	100	C	H	14.94	2.45	27.6188	0.0008	1.2971	<0.0001	0.00000	0.00000	0.01895	0.00516
ASP	100	C	H	2.18	0.75	30.2341	0.0042	1.1872	0.0002	0.00000	0.00000	0.02177	0.01130
ASP	100	C	H	23.72	2.69	31.1228	0.0008	1.1541	<0.0001	0.00000	0.00000	0.02201	0.00508
ASP	100	C	H	7.75	2.10	34.3846	0.0014	1.0475	<0.0001	0.00000	0.00000	0.01686	0.01006
ASP	100	C	H	5.83	1.30	36.9480	0.0032	0.9771	0.0001	0.00000	0.00000	0.02705	0.00928
ASP	100	C	H	167.30	8.02	36.9710	0.0064	0.9765	0.0002	0.05659	0.00312	0.00406	0.00032
ASP	100	C	H	9.70	1.13	38.3276	0.0016	0.9432	<0.0001	0.00000	0.00000	0.02554	0.00448
ASP	100	C	D	185.00	12.49	8.3897	0.0006	4.2326	0.0003	0.03320	0.00140	0.02132	0.00308
ASP	100	C	D	317.69	10.30	9.2124	0.0002	3.8553	0.0001	0.00515	0.00090	0.01051	0.00048
ASP	100	C	D	92.44	12.60	9.2155	0.0002	3.8540	0.0001	0.00451	0.00050	0.00313	0.00076
ASP	100	C	D	1081.91	29.10	9.9377	0.0002	3.5746	0.0001	0.04582	0.00086	0.02855	0.00164
ASP	100	C	D	1876.34	31.96	10.7892	0.0004	3.2932	0.0001	0.06335	0.00068	0.04443	0.00152
ASP	100	C	D	2062.07	53.55	11.7032	0.0002	3.0368	0.0001	0.00825	0.00042	0.01131	0.00040
ASP	100	C	D	52.46	4.95	11.9373	0.0312	2.9775	0.0078	0.00000	0.00000	0.50621	0.07214
ASP	100	C	D	79.01	4.07	12.4944	0.0004	2.8452	0.0001	0.00000	0.00000	0.01136	0.00064
ASP	100	C	D	5.42	0.54	12.6039	0.0010	2.8206	0.0002	0.00000	0.00000	0.01546	0.00206
ASP	100	C	D	1981.89	66.07	13.0181	0.0004	2.7312	0.0001	0.08255	0.00254	0.03983	0.00312
ASP	100	C	D	424.18	10.97	14.2532	0.0002	2.4956	<0.0001	0.00570	0.00088	0.01190	0.00044
ASP	100	C	D	87.77	3.87	14.2553	0.0002	2.4952	<0.0001	0.00866	0.00102	0.01082	0.00086
ASP	100	C	D	776.68	14.97	15.5693	0.0000	2.2858	<0.0001	0.00667	0.00040	0.01060	0.00030
ASP	100	C	D	119.31	2.91	15.5723	0.0002	2.2853	<0.0001	0.00000	0.00000	0.01509	0.00048
ASP	100	C	D	152.20	30.28	16.8205	0.0008	2.1168	0.0001	0.04445	0.00894	0.01868	0.00952
ASP	100	C	D	650.23	28.99	16.9942	0.0002	2.0954	<0.0001	0.00536	0.00086	0.00894	0.00060
ASP	100	C	D	129.85	4.94	17.0001	0.0002	2.0946	<0.0001	0.00777	0.00052	0.00818	0.00056
ASP	100	C	D	197.44	7.97	18.4788	0.0002	1.9283	<0.0001	0.00776	0.00112	0.01166	0.00076
ASP	100	C	D	359.48	10.29	18.6218	0.0002	1.9136	<0.0001	0.00895	0.00082	0.01329	0.00060
ASP	100	C	D	57.34	7.38	18.6253	0.0004	1.9133	<0.0001	0.01556	0.00130	0.00911	0.00268
ASP	100	C	D	520.55	9.42	18.9974	0.0002	1.8761	<0.0001	0.00748	0.00050	0.01221	0.00034
ASP	100	C	D	170.14	69.07	19.2375	0.0080	1.8529	0.0008	0.02467	0.00802	0.00000	0.00000
ASP	100	C	D	59.74	5.67	19.9477	0.0026	1.7876	0.0002	0.00000	0.00000	0.08312	0.01516
ASP	100	C	D	168.90	7.07	21.9493	0.0002	1.6263	<0.0001	0.00810	0.00126	0.01256	0.00086
ASP	100	C	D	9.68	1.18	21.9518	0.0012	1.6261	0.0001	0.00000	0.00000	0.01618	0.00272
ASP	100	C	D	278.40	92.74	22.2418	0.0008	1.6052	0.0001	0.00540	0.00044	0.00367	0.00146

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	C	D	897.59	29.90	22.2476	0.0002	1.6048	<0.0001	0.00763	0.00080	0.01212	0.00060
ASP	100	C	D	86.18	2.96	22.2532	0.0002	1.6044	<0.0001	0.00879	0.00006	0.01231	0.00062
ASP	100	C	D	45.78	15.49	23.4159	0.0004	1.5258	<0.0001	0.01018	0.00324	0.00000	0.00000
ASP	100	C	D	129.43	4.48	24.1864	0.0064	1.4778	0.0004	0.04886	0.00244	0.00676	0.00014
ASP	100	C	D	20.27	3.65	24.8213	0.0006	1.4406	<0.0001	0.01477	0.00226	0.01238	0.00440
ASP	100	C	D	6.13	1.06	26.3736	0.0016	1.3572	0.0001	0.00000	0.00000	0.01630	0.00400
ASP	100	C	D	18.87	4.10	26.7232	0.0004	1.3397	<0.0001	0.00992	0.00096	0.00678	0.00344
ASP	100	C	D	27.38	5.89	27.6184	0.0004	1.2971	<0.0001	0.01389	0.00200	0.01345	0.00370
ASP	100	C	D	8.83	3.83	28.7343	0.0010	1.2478	<0.0001	0.01202	0.00240	0.01311	0.00620
ASP	100	C	D	16.32	2.61	29.0204	0.0010	1.2357	<0.0001	0.01551	0.00794	0.01801	0.00592
ASP	100	C	D	62.59	25.10	30.1087	0.0048	1.1920	0.0002	0.12044	0.04050	0.00000	0.00000
ASP	100	C	D	14.33	1.92	30.4161	0.0022	1.1803	0.0001	0.01812	0.00016	0.00383	0.00084
ASP	100	C	D	71.90	3.96	31.1246	0.0002	1.154	<0.0001	0.01376	0.00140	0.01369	0.00152
ASP	100	C	D	22.27	6.93	34.3814	0.0004	1.0476	<0.0001	0.00969	0.00232	0.00000	0.00000
ASP	100	C	D	18.04	3.91	34.4627	0.0008	1.0452	<0.0001	0.01633	0.00288	0.01423	0.00490
ASP	100	C	D	38.24	5.73	34.9059	0.0110	1.0323	0.0003	0.02751	0.00016	0.00179	0.00048
ASP	100	C	D	5.32	1.02	35.6185	0.0016	1.0123	<0.0001	0.00000	0.00000	0.01464	0.00406
ASP	100	C	D	16.43	3.04	36.6405	0.0008	0.985	<0.0001	0.01709	0.00448	0.01493	0.00612
ASP	100	C	D	155.37	60.22	36.9700	0.0064	0.9765	0.0002	0.27372	0.10378	0.00000	0.00000
ASP	100	C	W	20.74	1.78	22.4862	0.0004	1.588	<0.0001	0.00000	0.00000	0.01274	0.00194
ASP	100	C	W	447.72	11.15	23.4131	0.0002	1.5259	<0.0001	0.00666	0.00074	0.01176	0.00044
ASP	100	C	W	55.22	2.45	23.5269	0.0002	1.5187	<0.0001	0.00890	0.00136	0.01215	0.00096
ASP	100	C	W	99.33	8.12	23.6597	0.0004	1.5102	<0.0001	0.01008	0.00112	0.01523	0.00228
ASP	100	C	W	138.02	7.02	24.2527	0.0002	1.4739	<0.0001	0.01047	0.00094	0.01162	0.00104
ASP	100	C	W	255.94	8.01	24.8159	0.0002	1.4409	<0.0001	0.01005	0.00074	0.01284	0.00066
ASP	100	C	W	172.48	18.85	25.1389	0.0006	1.4227	<0.0001	0.00887	0.00210	0.01119	0.00204
ASP	100	C	W	49.44	2.20	26.3683	0.0002	1.3575	<0.0001	0.00774	0.00278	0.01430	0.00110
ASP	100	C	W	20.13	4.95	26.7219	0.0016	1.3398	0.0001	0.00000	0.00000	0.02012	0.00342
ASP	100	C	W	74.28	12.22	26.7248	0.0008	1.3397	<0.0001	0.00814	0.00364	0.01018	0.00294
ASP	100	C	W	121.46	5.73	27.6119	0.0002	1.2974	<0.0001	0.01152	0.00078	0.01175	0.00102
ASP	100	C	W	1.19	0.46	27.8696	0.0006	1.2857	<0.0001	0.00000	0.00000	0.00357	0.00218
ASP	100	C	W	21.33	1.52	27.8727	0.0004	1.2855	<0.0001	0.01142	0.00146	0.01249	0.00142
ASP	100	C	W	82.92	5.92	28.7295	0.0004	1.248	<0.0001	0.01081	0.00212	0.01362	0.00174
ASP	100	C	W	107.71	6.01	29.0149	0.0004	1.2359	<0.0001	0.00778	0.00348	0.01496	0.00144
ASP	100	C	W	22.44	3.36	30.2313	0.0006	1.1873	<0.0001	0.01140	0.00384	0.01120	0.00340
ASP	100	C	W	14.85	2.56	30.2338	0.0016	1.1872	0.0001	0.00000	0.00000	0.01612	0.00404
ASP	100	C	W	92.30	4.85	30.4131	0.0002	1.1804	<0.0001	0.01121	0.00144	0.01335	0.00128
ASP	100	C	W	15.60	3.69	30.5876	0.0008	1.1738	<0.0001	0.01184	0.00268	0.00967	0.00490
ASP	100	C	W	414.74	11.97	31.1178	0.0002	1.1543	<0.0001	0.01073	0.00044	0.01141	0.00056
ASP	100	C	W	112.75	6.56	31.4361	0.0004	1.1429	<0.0001	0.01106	0.00154	0.01336	0.00140
ASP	100	C	W	23.73	4.22	31.9396	0.0006	1.1253	<0.0001	0.01077	0.00372	0.01111	0.00398
ASP	100	C	W	4.59	1.88	31.9455	0.0044	1.1251	0.0002	0.00000	0.00000	0.01060	0.00662
ASP	100	C	W	31.83	5.53	33.8964	0.0008	1.0621	<0.0001	0.01221	0.00434	0.01272	0.00444
ASP	100	C	W	169.24	8.36	34.378	0.0002	1.0477	<0.0001	0.00919	0.00132	0.01217	0.00104
ASP	100	C	W	155.39	8.43	34.4575	0.0004	1.0453	<0.0001	0.01103	0.00162	0.01378	0.00132
ASP	100	C	W	112.64	7.71	34.7784	0.0004	1.036	<0.0001	0.01334	0.00238	0.01625	0.00202
ASP	100	C	W	18.11	3.60	35.2111	0.0008	1.0236	<0.0001	0.00000	0.00000	0.01108	0.00420
ASP	100	C	W	158.11	8.89	35.6129	0.0004	1.0125	<0.0001	0.01162	0.00146	0.01391	0.00140
ASP	100	C	W	14.58	0.85	36.4474	0.0018	0.99	<0.0001	0.00000	0.00000	0.01896	0.00142
ASP	100	C	W	83.39	7.09	36.635	0.0004	0.9851	<0.0001	0.01139	0.00182	0.01214	0.00196
ASP	100	C	W	9.68	3.56	36.7882	0.0026	0.9812	0.0001	0.01666	0.00852	0.02456	0.01036
ASP	100	C	W	41.49	6.69	36.9416	0.0008	0.9772	<0.0001	0.01531	0.00084	0.01251	0.00412
ASP	100	C	W	78.36	6.88	37.3885	0.0004	0.966	<0.0001	0.00991	0.00188	0.01099	0.00180
ASP	100	C	W	71.93	8.50	37.4595	0.0006	0.9642	<0.0001	0.01501	0.00168	0.01302	0.00312
ASP	100	C	W	17.10	5.11	37.7625	0.0042	0.9567	0.0001	0.01890	0.00554	0.01966	0.00732
ASP	100	C	W	19.47	2.35	37.9425	0.0004	0.9524	<0.0001	0.01101	0.00466	0.01437	0.00276
ASP	100	C	W	115.65	6.79	38.3204	0.0004	0.9433	<0.0001	0.01100	0.00282	0.01660	0.00170
ASP	100	C	W	68.42	6.82	38.5377	0.0006	0.9382	<0.0001	0.01280	0.00246	0.01394	0.00264
ASP	100	D	H	126.59	10.84	8.3828	0.0006	4.2361	0.0003	0.03493	0.00240	0.01846	0.00368
ASP	100	D	H	30.23	2.16	9.2079	0.0004	3.8572	0.0002	0.01027	0.00176	0.01213	0.00158
ASP	100	D	H	570.87	84.85	9.932	0.0004	3.5766	0.0001	0.03925	0.00342	0.01791	0.00572
ASP	100	D	H	875.91	283.59	10.7828	0.0006	3.2952	0.0002	0.05549	0.01708	0.03391	0.01368
ASP	100	D	H	417.24	4.46	11.6992	0.0000	3.0378	0	0.00973	0.00020	0.01135	0.00020
ASP	100	D	H	1269.32	66.50	13.0119	0.0006	2.7325	0.0001	0.08219	0.00414	0.03880	0.00488
ASP	100	D	H	63.63	3.77	14.2505	0.0002	2.4961	<0.0001	0.01169	0.00062	0.01010	0.00116
ASP	100	D	H	108.27	3.30	15.5689	0.0002	2.2858	<0.0001	0.01251	0.00038	0.01055	0.00066
ASP	100	D	H	54.38	10.46	16.0549	0.0018	2.2171	0.0002	0.09736	0.01240	0.04859	0.02372
ASP	100	D	H	97.64	7.14	16.8105	0.0006	2.1181	0.0001	0.05535	0.00282	0.02963	0.00524
ASP	100	D	H	64.48	2.18	16.9931	0.0002	2.0955	<0.0001	0.01130	0.00048	0.01036	0.00070
ASP	100	D	H	450.60	134.87	17.2482	0.0004	2.0647	<0.0001	0.05821	0.01650	0.03643	0.01806
ASP	100	D	H	26.62	6.29	18.4792	0.0004	1.9283	<0.0001	0.01436	0.00356	0.00587	0.00356
ASP	100	D	H	81.60	2.22	18.6217	0.0002	1.9136	<0.0001	0.01619	0.00060	0.01549	0.00082
ASP	100	D	H	131.83	2.57	18.9949	0.0002	1.8764	<0.0001	0.01306	0.00048	0.01384	0.00052
ASP	100	D	H	343.02	10.47	19.2044	0.0006	1.8561	0.0001	0.12120	0.00174	0.07588	0.00546
ASP	100	D	H	55.24	5.58	19.9425	0.0014	1.7881	0.0001	0.08385	0.00436	0.04962	0.01206
ASP	100	D	H	16.83	1.06	21.9469	0.0004	1.6265	<0.0001	0.00864	0.00520	0.01590	0.00196
ASP	100	D	H	65.21	2.03	22.2492	0.0002	1.6047	<0.0001	0.01395	0.00050	0.01275	0.00078
ASP	100	D	H	48.14	2.40	23.4143	0.0002	1.5259	<0.0001	0.01370	0.00052	0.01091	0.00112
ASP	100	D	H	15.99	1.93	23.5274	0.0004	1.5186	<0.0001	0.01519	0.00288	0.01319	0.00352

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	D	H	37.58	1.71	24.8143	0.0002	1.441	<0.0001	0.01457	0.00070	0.01276	0.00116
ASP	100	D	H	22.29	1.48	25.1416	0.0004	1.4225	<0.0001	0.01664	0.00704	0.02414	0.00330
ASP	100	D	H	15.80	0.86	26.483	0.0030	1.3517	0.0002	0.00000	0.00000	0.09788	0.00778
ASP	100	D	H	21.08	1.55	27.6154	0.0004	1.2973	<0.0001	0.01631	0.00394	0.01882	0.00288
ASP	100	D	H	12.79	1.69	29.0153	0.0008	1.2359	<0.0001	0.02749	0.00316	0.02105	0.00628
ASP	100	D	H	19.79	2.10	30.4125	0.0006	1.1804	<0.0001	0.02329	0.00130	0.01543	0.00376
ASP	100	D	H	33.31	1.89	31.1199	0.0004	1.1542	<0.0001	0.01885	0.00146	0.01685	0.00202
ASP	100	D	H	16.18	4.48	31.4384	0.0006	1.1428	<0.0001	0.02105	0.00296	0.00000	0.00000
ASP	100	D	H	13.99	1.80	34.3799	0.0004	1.0476	<0.0001	0.01719	0.00122	0.01195	0.00350
ASP	100	D	H	21.73	1.47	34.4608	0.0004	1.0452	<0.0001	0.01631	0.00254	0.01684	0.00238
ASP	100	D	H	14.57	2.70	34.7809	0.0012	1.0359	<0.0001	0.03274	0.01456	0.02996	0.01264
ASP	100	D	D	131.19	11.65	8.3895	0.0006	4.2327	0.0003	0.03243	0.00210	0.01829	0.00368
ASP	100	D	D	144.88	5.04	9.2138	0.0002	3.8548	0.0001	0.01005	0.00056	0.01104	0.00066
ASP	100	D	D	739.59	23.19	9.9369	0.0002	3.5749	0.0001	0.04272	0.00096	0.02520	0.00172
ASP	100	D	D	1284.36	25.81	10.7882	0.0002	3.2935	0.0001	0.05975	0.00080	0.03877	0.00164
ASP	100	D	D	1818.62	15.64	11.705	0.0000	3.0364	<0.0001	0.00949	0.00014	0.01117	0.00016
ASP	100	D	D	64.68	4.51	12.4967	0.0002	2.8447	<0.0001	0.00910	0.00070	0.00821	0.00112
ASP	100	D	D	1352.70	67.43	13.0173	0.0004	2.7314	0.0001	0.07275	0.00380	0.03079	0.00380
ASP	100	D	D	237.91	6.74	14.2556	0.0002	2.4952	<0.0001	0.01080	0.00042	0.01119	0.00056
ASP	100	D	D	415.90	11.81	15.5721	0.0002	2.2854	<0.0001	0.01263	0.00036	0.01093	0.00062
ASP	100	D	D	114.86	8.71	16.4577	0.0106	2.1632	0.0014	0.03964	0.00328	0.00207	0.00028
ASP	100	D	D	102.71	15.87	16.8209	0.0012	2.1168	0.0002	0.04940	0.00554	0.02595	0.00976
ASP	100	D	D	347.17	7.71	16.9988	0.0002	2.0948	<0.0001	0.01023	0.00044	0.01188	0.00046
ASP	100	D	D	914.44	55.11	17.25	0.0004	2.0645	<0.0001	0.06029	0.00370	0.02602	0.00388
ASP	100	D	D	147.21	7.85	18.4819	0.0002	1.928	<0.0001	0.01472	0.00052	0.01122	0.00122
ASP	100	D	D	343.70	10.11	18.6259	0.0002	1.9132	<0.0001	0.01412	0.00032	0.01165	0.00066
ASP	100	D	D	414.67	11.02	19.0002	0.0002	1.8759	<0.0001	0.01274	0.00030	0.01104	0.00056
ASP	100	D	D	41.64	2.69	19.9461	0.0028	1.7877	0.0002	0.00000	0.00000	0.08362	0.00726
ASP	100	D	D	440.32	10.58	21.6686	0.0014	1.6471	0.0001	0.04629	0.00058	0.00668	0.00026
ASP	100	D	D	103.41	4.76	21.9531	0.0002	1.626	<0.0001	0.01094	0.00142	0.01356	0.00114
ASP	100	D	D	243.02	7.35	22.2529	0.0002	1.6044	<0.0001	0.01280	0.00052	0.01274	0.00070
ASP	100	D	D	13.87	2.58	22.4914	0.0010	1.5876	0.0001	0.00000	0.00000	0.01533	0.00582
ASP	100	D	D	148.34	4.90	23.4177	0.0002	1.5256	<0.0001	0.01336	0.00068	0.01312	0.00084
ASP	100	D	D	45.06	4.34	23.5314	0.0004	1.5184	<0.0001	0.01493	0.00106	0.01172	0.00248
ASP	100	D	D	54.28	6.35	23.664	0.0004	1.51	<0.0001	0.01732	0.00098	0.01093	0.00296
ASP	100	D	D	53.98	5.66	24.2584	0.0004	1.4735	<0.0001	0.01444	0.00302	0.01437	0.00230
ASP	100	D	D	207.80	4.88	24.8203	0.0002	1.4407	<0.0001	0.01303	0.00040	0.01301	0.00056
ASP	100	D	D	59.65	5.17	25.1465	0.0004	1.4223	<0.0001	0.02020	0.00098	0.01388	0.00266
ASP	100	D	D	37.34	2.44	26.3741	0.0004	1.3572	<0.0001	0.01000	0.00348	0.01448	0.00184
ASP	100	D	D	51.81	4.27	26.7283	0.0004	1.3395	<0.0001	0.01556	0.00092	0.01182	0.00212
ASP	100	D	D	89.84	4.13	27.6189	0.0002	1.2971	<0.0001	0.01344	0.00074	0.01216	0.00112
ASP	100	D	D	34.85	2.24	28.7356	0.0004	1.2477	<0.0001	0.01346	0.00306	0.01734	0.00212
ASP	100	D	D	42.87	3.69	29.0206	0.0004	1.2357	<0.0001	0.01952	0.00128	0.01523	0.00280
ASP	100	D	D	53.65	5.43	30.4175	0.0004	1.1802	<0.0001	0.01826	0.00112	0.01118	0.00256
ASP	100	D	D	5.23	1.27	30.5973	0.0030	1.1734	0.0001	0.00000	0.00000	0.02801	0.00632
ASP	100	D	D	108.42	7.65	31.1242	0.0002	1.154	<0.0001	0.01770	0.00076	0.01084	0.00172
ASP	100	D	D	47.52	4.06	31.443	0.0004	1.1426	<0.0001	0.01616	0.00170	0.01612	0.00288
ASP	100	D	D	9.12	1.60	31.9481	0.0012	1.125	<0.0001	0.01504	0.00962	0.01944	0.00692
ASP	100	D	D	11.32	2.49	33.9052	0.0012	1.0618	<0.0001	0.01806	0.01012	0.01842	0.00886
ASP	100	D	D	82.71	4.81	34.3841	0.0002	1.0475	<0.0001	0.01453	0.00062	0.01146	0.00138
ASP	100	D	D	82.88	3.30	34.4637	0.0002	1.0451	<0.0001	0.01177	0.00212	0.01683	0.00124
ASP	100	D	D	31.59	3.46	34.7875	0.0010	1.0357	<0.0001	0.02537	0.01084	0.03025	0.00706
ASP	100	D	D	1.97	0.66	35.2229	0.0040	1.0233	0.0001	0.00000	0.00000	0.02005	0.00988
ASP	100	D	D	57.87	4.91	35.62	0.0004	1.0123	<0.0001	0.01923	0.00190	0.01604	0.00296
ASP	100	D	D	11.47	4.18	36.4509	0.0012	0.9899	<0.0001	0.01829	0.00346	0.00000	0.00000
ASP	100	D	D	43.52	4.01	36.6406	0.0004	0.985	<0.0001	0.01416	0.00088	0.01043	0.00206
ASP	100	D	D	11.58	1.74	36.796	0.0012	0.981	<0.0001	0.00000	0.00000	0.02251	0.00674
ASP	100	D	D	16.75	5.68	36.9475	0.0014	0.9771	<0.0001	0.02402	0.01364	0.00000	0.00000
ASP	100	D	D	29.41	4.30	37.3929	0.0006	0.9659	<0.0001	0.01824	0.00756	0.01660	0.00532
ASP	100	D	D	52.73	25.32	37.467	0.0006	0.964	<0.0001	0.01707	0.00984	0.00000	0.00000
ASP	100	D	D	12.70	2.72	37.7678	0.0016	0.9566	<0.0001	0.02447	0.00852	0.02354	0.01008
ASP	100	D	D	4.19	0.72	37.9509	0.0024	0.9522	0.0001	0.00000	0.00000	0.02257	0.00552
ASP	100	D	D	43.02	6.05	38.3271	0.0004	0.9432	<0.0001	0.01929	0.00152	0.01349	0.00436
ASP	100	D	D	18.27	6.08	38.5455	0.0008	0.938	<0.0001	0.01777	0.00428	0.00000	0.00000
ASP	100	D	W	324.47	4.60	9.2119	0.0000	3.8556	<0.0001	0.00575	0.00034	0.01046	0.00022
ASP	100	D	W	3655.95	57.95	11.7032	0.0000	3.0368	<0.0001	0.00484	0.00042	0.01057	0.00022
ASP	100	D	W	65.92	2.53	12.4929	0.0002	2.8455	<0.0001	0.00729	0.00056	0.00857	0.00058
ASP	100	D	W	5.31	0.68	12.6016	0.0006	2.8211	0.0001	0.01010	0.00558	0.01265	0.00336
ASP	100	D	W	874.96	17.80	14.2538	0.0002	2.4955	<0.0001	0.00506	0.00048	0.00999	0.00028
ASP	100	D	W	1578.69	28.02	15.5693	0.0002	2.2858	<0.0001	0.00540	0.00050	0.01128	0.00020
ASP	100	D	W	649.92	8.96	16.9958	0.0000	2.0952	<0.0001	0.00672	0.00034	0.01134	0.00024
ASP	100	D	W	270.37	12.54	18.4789	0.0002	1.9283	<0.0001	0.00976	0.00078	0.01100	0.00088
ASP	100	D	W	148.43	29.73	18.6157	0.0006	1.9143	0.0001	0.00612	0.00084	0.00507	0.00166
ASP	100	D	W	736.07	17.18	18.6216	0.0002	1.9137	<0.0001	0.00825	0.00056	0.01197	0.00044
ASP	100	D	W	880.70	13.85	18.9975	0.0000	1.8761	<0.0001	0.00892	0.00030	0.01139	0.00028
ASP	100	D	W	454.11	15.01	21.9487	0.0002	1.6264	<0.0001	0.00707	0.00064	0.01026	0.00052
ASP	100	D	W	635.14	13.13	22.2493	0.0002	1.6047	<0.0001	0.00830	0.00058	0.01306	0.00042
ASP	100	D	W	31.82	1.31	22.4864	0.0002	1.588	<0.0001	0.01001	0.00094	0.01127	0.00088
ASP	100	D	W	339.88	6.93	23.4138	0.0002	1.5259	<0.0001	0.00825	0.00052	0.01219	0.00040

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	100	D	W	170.91	4.52	23.5268	0.0002	1.5187	<0.0001	0.00567	0.00142	0.01329	0.00054
ASP	100	D	W	67.17	4.35	23.6598	0.0004	1.5102	<0.0001	0.01135	0.00134	0.01224	0.00148
ASP	100	D	W	205.40	4.72	24.2535	0.0002	1.4738	<0.0001	0.00882	0.00066	0.01295	0.00048
ASP	100	D	W	259.41	7.77	24.8175	0.0002	1.4408	<0.0001	0.00979	0.00094	0.01404	0.00070
ASP	100	D	W	158.18	16.78	25.1397	0.0006	1.4226	<0.0001	0.00840	0.00252	0.01134	0.00202
ASP	100	D	W	81.69	2.18	26.3697	0.0002	1.3574	<0.0001	0.00914	0.00086	0.01303	0.00060
ASP	100	D	W	78.07	4.64	26.7231	0.0004	1.3398	<0.0001	0.01319	0.00128	0.01376	0.00152
ASP	100	D	W	338.18	16.36	27.6126	0.0002	1.2974	<0.0001	0.00859	0.00148	0.01337	0.00102
ASP	100	D	W	38.43	1.72	27.8738	0.0002	1.2855	<0.0001	0.01159	0.00090	0.01198	0.00104
ASP	100	D	W	65.27	2.83	28.7324	0.0002	1.2478	<0.0001	0.01217	0.00128	0.01434	0.00114
ASP	100	D	W	83.09	3.25	29.0139	0.0002	1.236	<0.0001	0.01251	0.00082	0.01311	0.00094
ASP	1000	A	H	65.97	5.19	8.3811	0.0006	4.237	0.0003	0.03983	0.00250	0.02108	0.00384
ASP	1000	A	H	133.04	4.68	8.3813	0.0004	4.2369	0.0002	0.04094	0.00118	0.03360	0.00238
ASP	1000	A	H	150.50	14.01	8.3814	0.0004	4.2368	0.0002	0.03913	0.00358	0.01777	0.00404
ASP	1000	A	H	1.78	0.51	9.2039	0.0010	3.8589	0.0004	0.01219	0.00296	0.00945	0.00614
ASP	1000	A	H	12.75	0.82	9.2101	0.0002	3.8563	0.0001	0.00935	0.00044	0.00737	0.00098
ASP	1000	A	H	2.30	0.45	9.2105	0.0004	3.8561	0.0002	0.00762	0.00146	0.00623	0.00266
ASP	1000	A	H	795.04	14.52	9.9372	0.0004	3.5748	0.0001	0.07628	0.00086	0.05180	0.00196
ASP	1000	A	H	368.79	9.70	9.9375	0.0004	3.5747	0.0001	0.07467	0.00140	0.04389	0.00254
ASP	1000	A	H	497.29	80.77	9.9382	0.0004	3.5744	0.0001	0.05460	0.02924	0.05071	0.01310
ASP	1000	A	H	1408.06	21.91	10.7881	0.0002	3.2936	0.0001	0.08103	0.00088	0.04945	0.00166
ASP	1000	A	H	1037.35	315.92	10.789	0.0006	3.2933	0.0002	0.06822	0.01140	0.03651	0.01526
ASP	1000	A	H	18.52	1.20	11.6872	0.0004	3.041	0.0001	0.01008	0.00112	0.00919	0.00122
ASP	1000	A	H	33.43	2.29	11.6898	0.0002	3.0403	0.0001	0.00998	0.00122	0.01035	0.00138
ASP	1000	A	H	38.43	2.31	11.6967	0.0004	3.0385	0.0001	0.01291	0.00058	0.01193	0.00086
ASP	1000	A	H	18.80	4.94	11.6973	0.0004	3.0383	0.0001	0.00643	0.00188	0.00642	0.00238
ASP	1000	A	H	16.62	4.84	11.6981	0.0008	3.0381	0.0002	0.00000	0.00000	0.01299	0.00238
ASP	1000	A	H	1532.73	458.57	13.0141	0.0004	2.732	0.0001	0.03208	0.01358	0.00000	0.00000
ASP	1000	A	H	2.83	0.92	14.2485	0.0006	2.4964	0.0001	0.01118	0.00224	0.00000	0.00000
ASP	1000	A	H	3.18	1.02	14.2544	0.0008	2.4954	0.0001	0.01562	0.00270	0.00000	0.00000
ASP	1000	A	H	84.61	4.03	15.3418	0.0052	2.3195	0.0008	0.00000	0.00000	0.24339	0.01588
ASP	1000	A	H	8.27	0.90	15.5614	0.0004	2.2869	0.0001	0.00948	0.00436	0.01235	0.00284
ASP	1000	A	H	208.74	7.39	15.5626	0.0194	2.2868	0.0028	0.00000	0.00000	0.65911	0.02894
ASP	1000	A	H	16.52	1.84	15.571	0.0002	2.2855	<0.0001	0.01299	0.00076	0.00826	0.00216
ASP	1000	A	H	18.70	1.87	16.057	0.0032	2.2168	0.0004	0.04033	0.02058	0.05219	0.01152
ASP	1000	A	H	21.57	1.70	16.0595	0.0014	2.2165	0.0002	0.00000	0.00000	0.06525	0.01106
ASP	1000	A	H	117.80	14.28	16.804	0.0008	2.1189	0.0001	0.06010	0.00580	0.02959	0.00888
ASP	1000	A	H	123.16	16.25	16.8041	0.0008	2.1189	0.0001	0.05794	0.00736	0.02494	0.00842
ASP	1000	A	H	1032.51	313.63	17.2533	0.0004	2.0641	<0.0001	0.03861	0.01620	0.00000	0.00000
ASP	1000	A	H	1015.25	305.17	17.2534	0.0004	2.0641	<0.0001	0.04848	0.02000	0.00000	0.00000
ASP	1000	A	H	6.50	1.64	18.6068	0.0004	1.9152	<0.0001	0.01314	0.00268	0.00645	0.00406
ASP	1000	A	H	5.17	0.39	18.9721	0.0012	1.8786	0.0001	0.00981	0.00300	0.01437	0.00182
ASP	1000	A	H	4.16	0.40	18.9733	0.0014	1.8785	0.0001	0.00990	0.00344	0.01308	0.00220
ASP	1000	A	H	26.11	1.09	18.9908	0.0002	1.8768	<0.0001	0.00903	0.00180	0.01290	0.00104
ASP	1000	A	H	25.43	1.26	18.9909	0.0002	1.8768	<0.0001	0.00873	0.00188	0.01346	0.00110
ASP	1000	A	H	378.42	14.16	19.2074	0.0008	1.8558	0.0001	0.12621	0.00224	0.08199	0.00716
ASP	1000	A	H	412.39	24.28	19.2081	0.0010	1.8557	0.0001	0.12451	0.00588	0.06161	0.00898
ASP	1000	A	H	952.35	309.62	19.5582	0.0004	1.8228	<0.0001	0.03554	0.01626	0.00000	0.00000
ASP	1000	A	H	913.73	24.73	19.5584	0.0004	1.8228	<0.0001	0.10689	0.00198	0.05895	0.00376
ASP	1000	A	H	52.63	4.79	19.948	0.0026	1.7876	0.0002	0.08707	0.02974	0.10241	0.02024
ASP	1000	A	H	47.61	1.74	19.9503	0.0026	1.7874	0.0002	0.00000	0.00000	0.12141	0.00626
ASP	1000	A	H	2.84	0.78	22.2405	0.0014	1.6053	0.0001	0.01528	0.00458	0.01222	0.00762
ASP	1000	A	H	8.12	0.96	22.2498	0.0004	1.6046	<0.0001	0.01451	0.00112	0.01061	0.00286
ASP	1000	A	H	94.03	12.15	23.1449	0.0072	1.5434	0.0005	0.21865	0.01732	0.13279	0.04126
ASP	1000	A	H	19.08	1.14	26.4991	0.0046	1.3509	0.0002	0.00000	0.00000	0.13233	0.01172
ASP	1000	A	H	232.61	5.33	27.8285	0.0016	1.2875	0.0001	0.04822	0.00130	0.00651	0.00026
ASP	1000	A	H	126.89	20.41	31.5331	0.0050	1.1395	0.0002	0.22634	0.03476	0.09915	0.04152
ASP	1000	A	H	107.99	7.24	32.4343	0.0026	1.1086	0.0001	0.21061	0.00732	0.13965	0.02210
ASP	1000	A	H	97.74	0.26	34.811	0.0186	1.035	0.0005	0.02283	0.00006	0.00036	0.00000
ASP	1000	A	D	96.35	13.37	8.3836	0.0004	4.2357	0.0002	0.03066	0.00468	0.01251	0.00440
ASP	1000	A	D	1.55	0.34	9.2081	0.0018	3.8571	0.0008	0.00000	0.00000	0.01412	0.00432
ASP	1000	A	D	551.47	14.86	9.9359	0.0002	3.5752	0.0001	0.05532	0.00118	0.03074	0.00186
ASP	1000	A	D	987.71	17.13	10.7876	0.0002	3.2937	0.0001	0.06742	0.00086	0.04034	0.00152
ASP	1000	A	D	36.47	1.93	11.6925	0.0002	3.0396	0.0001	0.01060	0.00154	0.01294	0.00128
ASP	1000	A	D	1084.30	293.30	13.0155	0.0004	2.7318	0.0001	0.03847	0.01438	0.00000	0.00000
ASP	1000	A	D	4.46	1.59	14.2510	0.0010	2.4960	0.0002	0.01330	0.00332	0.00000	0.00000
ASP	1000	A	D	84.25	13.91	16.8140	0.0008	2.1177	0.0001	0.04675	0.00744	0.02072	0.00868
ASP	1000	A	D	4.91	0.58	16.9941	0.0010	2.0954	0.0001	0.00000	0.00000	0.01339	0.00220
ASP	1000	A	D	750.73	168.37	17.2497	0.0004	2.0646	<0.0001	0.04652	0.01422	0.01119	0.00692
ASP	1000	A	D	301.04	20.49	19.2049	0.0010	1.8561	0.0001	0.11356	0.00664	0.05453	0.00918
ASP	1000	A	D	715.19	315.57	19.5640	0.0006	1.8223	0.0001	0.04407	0.02686	0.00000	0.00000
ASP	1000	A	D	41.21	4.08	19.9475	0.0024	1.7876	0.0002	0.07977	0.01826	0.08052	0.01734
ASP	1000	A	D	8.39	1.99	20.8395	0.0204	1.7119	0.0017	0.00000	0.00000	0.19193	0.07150
ASP	1000	A	D	2.53	0.32	24.8168	0.0014	1.4409	0.0001	0.00000	0.00000	0.01771	0.00318
ASP	1000	A	D	23.88	3.52	25.2829	0.0096	1.4147	0.0005	0.00000	0.00000	0.25468	0.08384
ASP	1000	A	D	23.31	10.43	26.4841	0.0046	1.3516	0.0002	0.11629	0.03754	0.00000	0.00000
ASP	1000	A	D	22.82	2.41	26.8241	0.0042	1.3348	0.0002	0.00000	0.00000	0.15097	0.03454
ASP	1000	A	D	33.83	11.27	30.1118	0.0036	1.1919	0.0001	0.12643	0.04010	0.00000	0.00000
ASP	1000	A	D	46.54	3.05	30.8131	0.0054	1.1654	0.0002	0.20557	0.00118	0.08575	0.01158

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	1000	A	D	63.34	1.27	31.3144	0.0058	1.1472	0.0002	0.20057	0.01802	0.11580	0.00038
ASP	1000	A	D	2.15	0.51	34.3763	0.0030	1.0477	0.0001	0.00000	0.00000	0.02758	0.01118
ASP	1000	A	D	55.90	2.29	38.3587	0.0046	0.9424	0.0001	0.05494	0.00034	0.00523	0.00034
ASP	1000	A	W	209.15	23.59	8.3873	0.0004	4.2338	0.0002	0.03131	0.00372	0.01332	0.00376
ASP	1000	A	W	1173.90	46.00	9.9391	0.0002	3.5741	0.0001	0.04940	0.00196	0.02204	0.00210
ASP	1000	A	W	2054.69	36.56	10.7901	0.0002	3.2929	0.0001	0.06822	0.00092	0.03833	0.00152
ASP	1000	A	W	30.00	3.45	11.6936	0.0006	3.0393	0.0002	0.01483	0.00260	0.01367	0.00330
ASP	1000	A	W	2139.70	784.06	13.0170	0.0004	2.7314	0.0001	0.03712	0.01846	0.00000	0.00000
ASP	1000	A	W	72.26	22.81	13.2780	0.0366	2.6780	0.0074	0.00965	0.00366	0.00000	0.00000
ASP	1000	A	W	240.45	22.10	15.3542	0.0062	2.3176	0.0009	0.23151	0.04868	0.19696	0.03434
ASP	1000	A	W	169.09	33.22	16.8150	0.0008	2.1175	0.0001	0.04666	0.00962	0.01882	0.00958
ASP	1000	A	W	213.64	6.95	26.1862	0.0026	1.3667	0.0001	0.03779	0.00032	0.00314	0.00018
ASP	1000	B	H	90.84	5.67	8.3809	0.0006	4.2371	0.0003	0.04769	0.00206	0.02783	0.00392
ASP	1000	B	H	504.72	10.99	9.9368	0.0004	3.5749	0.0001	0.07685	0.00106	0.04913	0.00228
ASP	1000	B	H	177.15	5.20	10.2075	0.0002	3.4803	0.0001	0.01707	0.00032	0.01270	0.00076
ASP	1000	B	H	903.39	275.98	10.7884	0.0002	3.2935	0.0001	0.03727	0.01574	0.00000	0.00000
ASP	1000	B	H	8.78	4.01	11.6918	0.0010	3.0398	0.0003	0.01853	0.00684	0.00000	0.00000
ASP	1000	B	H	964.78	348.18	13.0152	0.0004	2.7318	0.0001	0.03620	0.01818	0.00000	0.00000
ASP	1000	B	H	305.26	6.89	13.9421	0.0002	2.551	<0.0001	0.01778	0.00026	0.01257	0.00058
ASP	1000	B	H	1.06	0.43	14.2484	0.0048	2.4964	0.0008	0.00000	0.00000	0.02124	0.01304
ASP	1000	B	H	123.26	4.83	14.9528	0.0002	2.3795	<0.0001	0.01759	0.00042	0.01231	0.00100
ASP	1000	B	H	57.74	3.59	16.0570	0.0036	2.2168	0.0005	0.03631	0.00018	0.00392	0.00044
ASP	1000	B	H	354.94	8.08	17.0757	0.0002	2.0854	<0.0001	0.01774	0.00024	0.01279	0.00060
ASP	1000	B	H	267.73	21.98	19.2080	0.0012	1.8558	0.0001	0.12731	0.00890	0.05978	0.01234
ASP	1000	B	H	604.87	18.15	19.5622	0.0006	1.8225	0.0001	0.11927	0.00216	0.06869	0.00484
ASP	1000	B	H	43.90	17.05	19.9497	0.0034	1.7874	0.0003	0.10597	0.04244	0.00000	0.00000
ASP	1000	B	H	176.11	6.42	20.4982	0.0002	1.7401	<0.0001	0.01886	0.00040	0.01265	0.00100
ASP	1000	B	H	372.02	8.33	22.2942	0.0002	1.6015	<0.0001	0.01859	0.00026	0.01230	0.00058
ASP	1000	B	H	146.98	4.34	25.4691	0.0002	1.4045	<0.0001	0.01895	0.00032	0.01307	0.00082
ASP	1000	B	H	225.75	5.96	26.0513	0.0002	1.3737	<0.0001	0.01896	0.00028	0.01245	0.00072
ASP	1000	B	H	5.65	1.28	28.0986	0.0010	1.2754	<0.0001	0.01775	0.00324	0.01484	0.00746
ASP	1000	B	H	70.42	3.33	28.9426	0.0002	1.239	<0.0001	0.01918	0.00052	0.01289	0.00130
ASP	1000	B	H	36.37	3.15	29.0595	0.0004	1.2341	<0.0001	0.01909	0.00088	0.01194	0.00232
ASP	1000	B	H	28.31	6.38	30.1697	0.0004	1.1897	<0.0001	0.01909	0.00376	0.00868	0.00498
ASP	1000	B	H	21.55	9.20	31.3154	0.0006	1.1472	<0.0001	0.02057	0.00280	0.00000	0.00000
ASP	1000	B	H	15.57	3.85	31.9296	0.0006	1.1257	<0.0001	0.01958	0.00342	0.01010	0.00614
ASP	1000	B	H	10.83	2.11	31.9762	0.0008	1.1241	<0.0001	0.01911	0.00212	0.01331	0.00604
ASP	1000	B	H	31.56	2.96	32.7287	0.0004	1.0989	<0.0001	0.01979	0.00104	0.01235	0.00264
ASP	1000	B	H	5.17	1.47	33.2367	0.0010	1.0826	<0.0001	0.00000	0.00000	0.02029	0.01132
ASP	1000	B	H	33.39	2.88	33.3755	0.0004	1.0782	<0.0001	0.02025	0.00116	0.01455	0.00280
ASP	1000	B	H	67.41	4.16	34.5487	0.0002	1.0426	<0.0001	0.02026	0.00066	0.01278	0.00178
ASP	1000	B	H	7.59	2.45	35.4267	0.0012	1.0176	<0.0001	0.01967	0.00780	0.00000	0.00000
ASP	1000	B	H	45.57	3.03	36.1602	0.0002	0.9976	<0.0001	0.01999	0.00094	0.01488	0.00218
ASP	1000	B	H	7.76	2.83	36.7561	0.0010	0.982	<0.0001	0.01989	0.00432	0.00000	0.00000
ASP	1000	B	H	7.94	1.60	39.0124	0.0370	0.9272	0.0008	0.00840	0.00284	0.00013	0.00004
ASP	1000	B	H	6.07	0.97	39.419	0.0010	0.918	<0.0001	0.01552	0.00884	0.01966	0.00650
ASP	1000	B	H	31.08	1.80	39.8864	0.0004	0.9077	<0.0001	0.01842	0.00212	0.01861	0.00220
ASP	1000	B	D	99.34	6.19	8.3830	0.0004	4.2360	0.0002	0.03651	0.00186	0.01921	0.00278
ASP	1000	B	D	589.12	12.61	9.9359	0.0002	3.5752	0.0001	0.05875	0.00098	0.03293	0.00158
ASP	1000	B	D	1046.55	14.77	10.7874	0.0002	3.2938	0.0001	0.07052	0.00072	0.04167	0.00128
ASP	1000	B	D	1107.21	59.02	13.0153	0.0002	2.7318	<0.0001	0.06902	0.00450	0.02375	0.00334
ASP	1000	B	D	83.74	7.16	16.8142	0.0006	2.1176	0.0001	0.05233	0.00372	0.02516	0.00534
ASP	1000	B	D	748.87	16.24	17.2496	0.0002	2.0646	<0.0001	0.08353	0.00172	0.03923	0.00204
ASP	1000	B	D	295.54	8.94	19.2057	0.0006	1.8560	0.0001	0.12208	0.00208	0.07148	0.00512
ASP	1000	B	D	719.32	35.73	19.5642	0.0004	1.8223	<0.0001	0.08668	0.00536	0.03238	0.00424
ASP	1000	B	D	32.76	1.17	19.9470	0.0020	1.7877	0.0002	0.06683	0.02190	0.09639	0.00480
ASP	1000	B	D	12.67	2.59	20.3856	0.0056	1.7496	0.0005	0.00000	0.00000	0.09556	0.04334
ASP	1000	B	D	29.15	1.32	21.2176	0.0186	1.6817	0.0015	0.03998	0.00512	0.00206	0.00002
ASP	1000	B	D	360.05	153.99	21.6707	0.0006	1.647	<0.0001	0.04148	0.02486	0.00000	0.00000
ASP	1000	B	D	85.32	1.30	24.1904	0.0024	1.4776	0.0001	0.05121	0.00118	0.00667	0.00002
ASP	1000	B	D	7.91	1.71	25.2166	0.0318	1.4184	0.0018	0.00000	0.00000	0.17897	0.05990
ASP	1000	B	D	15.65	1.96	26.4874	0.0036	1.3515	0.0002	0.00000	0.00000	0.12038	0.03278
ASP	1000	B	D	113.48	7.03	27.2778	0.0012	1.3130	0.0001	0.12840	0.00560	0.06841	0.01032
ASP	1000	B	D	11.33	1.89	34.1412	0.0534	1.0547	0.0016	0.00000	0.00000	0.36702	0.08262
ASP	1000	B	D	18.61	7.25	36.3831	0.0068	0.9917	0.0002	0.18321	0.04888	0.00000	0.00000
ASP	1000	B	D	46.37	4.99	38.3613	0.0034	0.9424	0.0001	0.22988	0.01176	0.13644	0.03590
ASP	1000	B	D	7.63	2.37	38.9786	0.0194	0.9280	0.0004	0.00000	0.00000	0.29000	0.15020
ASP	1000	B	D	15.17	0.89	39.7564	0.0086	0.9106	0.0002	0.00000	0.00000	0.28472	0.02588
ASP	1000	B	W	205.57	11.08	8.3887	0.0004	4.2331	0.0002	0.03444	0.00124	0.02101	0.00250
ASP	1000	B	W	1210.59	31.71	9.9373	0.0002	3.5747	0.0001	0.04803	0.00104	0.02556	0.00152
ASP	1000	B	W	2116.21	30.04	10.7889	0.0002	3.2933	0.0001	0.06594	0.00062	0.04226	0.00126
ASP	1000	B	W	2210.11	82.49	13.0169	0.0004	2.7315	0.0001	0.07546	0.00306	0.03099	0.00290
ASP	1000	B	W	267.80	15.42	15.3556	0.0076	2.3174	0.0011	0.20900	0.01094	0.22428	0.02668
ASP	1000	B	W	67.06	23.87	16.5391	0.0706	2.1526	0.0092	0.07286	0.02268	0.00815	0.00006
ASP	1000	B	W	169.78	18.46	16.8178	0.0006	2.1172	0.0001	0.05054	0.00402	0.02596	0.00694
ASP	1000	B	W	1488.46	286.94	17.2496	0.0004	2.0646	<0.0001	0.04151	0.01098	0.01002	0.00534
ASP	1000	B	W	54.38	3.18	18.3941	0.0360	1.9371	0.0038	0.01177	0.00140	0.00011	0.00000
ASP	1000	B	W	1394.59	440.76	19.5647	0.0004	1.8222	<0.0001	0.04514	0.01932	0.00000	0.00000
ASP	1000	B	W	79.46	7.35	19.9452	0.0018	1.7878	0.0002	0.07154	0.01158	0.08853	0.00564

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	1000	B	W	197.51	2.62	23.1453	0.0040	1.5433	0.0003	0.04408	0.00132	0.00338	0.00002
ASP	1000	B	W	30.23	9.43	25.3326	0.0188	1.4120	0.0010	0.02397	0.00572	0.00159	0.00104
ASP	1000	B	W	7.73	1.94	33.0160	0.0386	1.0896	0.0012	0.00000	0.00000	0.26700	0.10162
ASP	1000	C	H	85.54	3.91	8.3808	0.0006	4.2371	0.0003	0.04498	0.00122	0.03180	0.00306
ASP	1000	C	H	513.26	11.57	9.9368	0.0004	3.5749	0.0001	0.07541	0.00118	0.04489	0.00222
ASP	1000	C	H	182.40	5.36	10.2074	0.0002	3.4804	0.0001	0.01691	0.00030	0.01156	0.00070
ASP	1000	C	H	897.70	15.17	10.7882	0.0002	3.2935	0.0001	0.08248	0.00102	0.04807	0.00180
ASP	1000	C	H	10.45	1.91	11.6911	0.0006	3.0399	0.0002	0.01674	0.00224	0.01262	0.00516
ASP	1000	C	H	953.34	50.74	13.0150	0.0004	2.7319	0.0001	0.07974	0.00492	0.02883	0.00400
ASP	1000	C	H	305.48	6.21	13.9419	0.0002	2.551	<0.0001	0.01783	0.00022	0.01265	0.00052
ASP	1000	C	H	123.49	4.23	14.9528	0.0002	2.3795	<0.0001	0.01760	0.00038	0.01292	0.00090
ASP	1000	C	H	74.72	4.14	16.4516	0.0070	2.1640	0.0009	0.11398	0.00046	0.01837	0.00184
ASP	1000	C	H	75.06	8.41	16.8100	0.0010	2.1182	0.0001	0.06543	0.00500	0.03491	0.00952
ASP	1000	C	H	357.76	7.46	17.0757	0.0000	2.0854	<0.0001	0.01775	0.00022	0.01269	0.00054
ASP	1000	C	H	1.55	0.63	18.9811	0.0060	1.8777	0.0006	0.00000	0.00000	0.02497	0.01510
ASP	1000	C	H	17.22	6.66	19.1663	0.0262	1.8598	0.0025	0.00000	0.00000	0.14118	0.05272
ASP	1000	C	H	623.41	276.85	19.5627	0.0006	1.8224	0.0001	0.03605	0.02228	0.00000	0.00000
ASP	1000	C	H	178.49	6.08	20.4985	0.0002	1.7401	<0.0001	0.01901	0.00038	0.01262	0.00092
ASP	1000	C	H	372.73	7.94	22.2945	0.0000	1.6014	<0.0001	0.01850	0.00026	0.01215	0.00054
ASP	1000	C	H	13.69	5.13	23.5892	0.0008	1.5147	0.0001	0.01996	0.00618	0.00000	0.00000
ASP	1000	C	H	0.68	0.34	24.8169	0.0050	1.4409	0.0003	0.00000	0.00000	0.01530	0.00978
ASP	1000	C	H	146.04	4.01	25.4696	0.0002	1.4045	<0.0001	0.01897	0.00030	0.01310	0.00076
ASP	1000	C	H	223.86	5.59	26.052	0.0002	1.3736	<0.0001	0.01878	0.00026	0.01258	0.00068
ASP	1000	C	H	17.78	3.34	26.8333	0.0082	1.3344	0.0004	0.00000	0.00000	0.14957	0.05236
ASP	1000	C	H	5.85	1.51	28.0996	0.0010	1.2753	<0.0001	0.01926	0.00332	0.02040	0.00872
ASP	1000	C	H	69.29	2.71	28.9435	0.0002	1.2389	<0.0001	0.01917	0.00046	0.01385	0.00114
ASP	1000	C	H	36.80	2.49	29.0607	0.0002	1.234	<0.0001	0.01901	0.00070	0.01278	0.00192
ASP	1000	C	H	29.59	11.13	30.1708	0.0004	1.1896	<0.0001	0.01580	0.00704	0.00000	0.00000
ASP	1000	C	H	17.38	3.01	31.316	0.0004	1.1472	<0.0001	0.01695	0.00400	0.01360	0.00542
ASP	1000	C	H	14.13	1.99	31.9307	0.0006	1.1256	<0.0001	0.01894	0.00160	0.01353	0.00438
ASP	1000	C	H	11.03	2.60	31.9774	0.0006	1.124	<0.0001	0.01887	0.00268	0.01051	0.00606
ASP	1000	C	H	30.86	2.29	32.7299	0.0004	1.0989	<0.0001	0.01999	0.00082	0.01355	0.00222
ASP	1000	C	H	8.01	3.53	33.2374	0.0008	1.0825	<0.0001	0.01753	0.00756	0.00000	0.00000
ASP	1000	C	H	33.12	2.15	33.3763	0.0004	1.0782	<0.0001	0.02011	0.00074	0.01411	0.00198
ASP	1000	C	H	62.74	2.60	34.5499	0.0002	1.0426	<0.0001	0.01994	0.00070	0.01594	0.00138
ASP	1000	C	H	46.75	3.33	36.1617	0.0002	0.9976	<0.0001	0.01997	0.00074	0.01256	0.00204
ASP	1000	C	H	12.53	1.35	36.3972	0.0130	0.9913	0.0003	0.00000	0.00000	0.23360	0.03844
ASP	1000	C	H	28.66	5.52	38.3619	0.0070	0.9423	0.0002	0.17310	0.00060	0.14007	0.04552
ASP	1000	C	H	12.06	2.48	38.6921	0.0006	0.9346	<0.0001	0.02058	0.00244	0.01164	0.00574
ASP	1000	C	H	8.27	2.19	39.4206	0.0010	0.918	<0.0001	0.02217	0.00394	0.01213	0.00774
ASP	1000	C	H	29.10	1.41	39.8881	0.0004	0.9077	<0.0001	0.01708	0.00212	0.01927	0.00184
ASP	1000	C	D	99.21	8.53	8.3830	0.0004	4.2360	0.0002	0.03051	0.00260	0.01387	0.00292
ASP	1000	C	D	1.38	0.26	9.2051	0.0014	3.8584	0.0006	0.00000	0.00000	0.01226	0.00318
ASP	1000	C	D	577.61	12.97	9.9354	0.0002	3.5754	0.0001	0.05190	0.00094	0.02814	0.00142
ASP	1000	C	D	1017.43	14.06	10.7870	0.0002	3.2939	0.0001	0.06482	0.00066	0.03870	0.00116
ASP	1000	C	D	32.46	1.88	11.6929	0.0004	3.0395	0.0001	0.01290	0.00120	0.01325	0.00138
ASP	1000	C	D	1096.29	250.24	13.0147	0.0002	2.7319	<0.0001	0.03996	0.01258	0.00820	0.00522
ASP	1000	C	D	3.36	1.13	14.2520	0.0014	2.4958	0.0002	0.01526	0.00672	0.01586	0.00294
ASP	1000	C	D	69.39	11.56	15.3464	0.0042	2.3188	0.0006	0.00000	0.00000	0.21443	0.06424
ASP	1000	C	D	9.32	4.62	15.5653	0.0010	2.2864	0.0001	0.01773	0.00632	0.00000	0.00000
ASP	1000	C	D	177.43	11.83	15.5788	0.0404	2.2844	0.0059	0.00000	0.00000	0.72572	0.04752
ASP	1000	C	D	70.68	2.32	16.4500	0.0070	2.1642	0.0009	0.00000	0.00000	0.38455	0.02102
ASP	1000	C	D	4.99	0.47	16.9932	0.0008	2.0955	0.0001	0.00000	0.00000	0.01526	0.00200
ASP	1000	C	D	761.95	263.31	17.2488	0.0002	2.0647	<0.0001	0.02802	0.01360	0.00000	0.00000
ASP	1000	C	D	7.91	2.51	18.5982	0.0010	1.9160	0.0001	0.02325	0.00446	0.00000	0.00000
ASP	1000	C	D	8.54	1.41	18.9838	0.0008	1.8775	0.0001	0.01748	0.00400	0.01503	0.00554
ASP	1000	C	D	294.28	9.55	19.2046	0.0006	1.8561	0.0001	0.11609	0.00194	0.07017	0.00540
ASP	1000	C	D	732.28	198.51	19.5638	0.0004	1.8223	<0.0001	0.02661	0.01004	0.00000	0.00000
ASP	1000	C	D	35.80	1.14	19.9476	0.0018	1.7876	0.0002	0.00000	0.00000	0.09626	0.00428
ASP	1000	C	D	17.51	8.71	20.3805	0.0050	1.7500	0.0004	0.10190	0.03856	0.00000	0.00000
ASP	1000	C	D	349.52	163.79	21.6697	0.0006	1.647	<0.0001	0.03727	0.02444	0.00000	0.00000
ASP	1000	C	D	1.62	0.28	24.8167	0.0020	1.4409	0.0001	0.00000	0.00000	0.02002	0.00504
ASP	1000	C	D	122.43	4.31	26.1823	0.0026	1.3669	0.0001	0.04287	0.00176	0.00361	0.00024
ASP	1000	C	D	33.42	4.85	30.1116	0.0024	1.1919	0.0001	0.13171	0.00982	0.07328	0.02658
ASP	1000	C	D	1.43	0.49	31.1114	0.0052	1.1545	0.0002	0.00000	0.00000	0.03460	0.02146
ASP	1000	C	D	1.58	0.34	34.3740	0.0048	1.0478	0.0001	0.00000	0.00000	0.03801	0.01278
ASP	1000	C	D	47.78	2.66	35.9398	0.0088	1.0035	0.0002	0.09190	0.00048	0.00917	0.00098
ASP	1000	C	W	205.50	15.22	8.3881	0.0004	4.2334	0.0002	0.03025	0.00192	0.01541	0.00268
ASP	1000	C	W	1.12	0.46	9.2095	0.0026	3.8566	0.0011	0.00000	0.00000	0.01056	0.00618
ASP	1000	C	W	1198.96	35.67	9.9378	0.0002	3.5746	0.0001	0.04596	0.00124	0.02286	0.00160
ASP	1000	C	W	2092.41	30.40	10.7891	0.0002	3.2932	0.0001	0.06534	0.00064	0.04105	0.00126
ASP	1000	C	W	19.08	4.47	11.6948	0.0006	3.0390	0.0002	0.01353	0.00168	0.00865	0.00466
ASP	1000	C	W	1969.93	70.40	13.0158	0.0004	2.7317	0.0001	0.08123	0.00124	0.04602	0.00384
ASP	1000	C	W	159.42	58.92	15.3404	0.0114	2.3197	0.0017	0.00000	0.00000	0.18605	0.09168
ASP	1000	C	W	177.78	77.13	15.6852	0.1812	2.2690	0.0264	0.00000	0.00000	0.54573	0.35540
ASP	1000	C	W	148.29	6.44	16.4515	0.0096	2.1640	0.0013	0.00000	0.00000	0.39902	0.02848
ASP	1000	C	W	179.06	61.71	16.8158	0.0008	2.1174	0.0001	0.03748	0.01584	0.00000	0.00000
ASP	1000	C	W	1497.69	553.04	17.2497	0.0004	2.0646	<0.0001	0.03131	0.01606	0.00000	0.00000
ASP	1000	C	W	562.23	17.92	19.2046	0.0008	1.8561	0.0001	0.11604	0.00222	0.08380	0.00602

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	1000	C	W	1435.81	540.08	19.5636	0.0004	1.8223	<0.0001	0.03742	0.01950	0.00000	0.00000
ASP	1000	C	W	70.71	2.78	19.9479	0.0022	1.7876	0.0002	0.05183	0.03162	0.09510	0.00516
ASP	1000	C	W	31.59	1.77	26.4849	0.0034	1.3516	0.0002	0.08928	0.02396	0.10646	0.00868
ASP	1000	C	W	60.34	29.05	26.8252	0.0038	1.3347	0.0002	0.10911	0.05426	0.00000	0.00000
ASP	1000	C	W	239.35	16.36	27.2767	0.0014	1.3131	0.0001	0.13179	0.00496	0.07265	0.01198
ASP	1000	C	W	403.22	24.69	27.8238	0.0012	1.2877	0.0001	0.16067	0.00852	0.07785	0.01180
ASP	1000	C	W	64.75	18.60	30.1072	0.0030	1.1921	0.0001	0.11217	0.02770	0.00000	0.00000
ASP	1000	C	W	86.13	23.43	30.8039	0.0056	1.1657	0.0002	0.22011	0.03538	0.00000	0.00000
ASP	1000	C	W	204.61	29.08	31.5252	0.0078	1.1397	0.0003	0.26604	0.03082	0.13423	0.04750
ASP	1000	C	W	175.08	14.58	32.4341	0.0032	1.1086	0.0001	0.23424	0.00892	0.14630	0.02920
ASP	1000	D	D	112.65	6.14	8.3828	0.0004	4.2361	0.0002	0.03477	0.00150	0.01892	0.00236
ASP	1000	D	D	650.07	12.57	9.9349	0.0002	3.5756	0.0001	0.05347	0.00078	0.03070	0.00130
ASP	1000	D	D	1144.96	15.12	10.7865	0.0002	3.2940	0.0001	0.06636	0.00062	0.03981	0.00114
ASP	1000	D	D	1205.99	79.31	13.0144	0.0002	2.732	<0.0001	0.06254	0.00518	0.01999	0.00352
ASP	1000	D	D	76.81	3.55	15.3432	0.0046	2.3193	0.0007	0.00000	0.00000	0.21920	0.01380
ASP	1000	D	D	175.89	8.88	15.5927	0.0256	2.2824	0.0037	0.00000	0.00000	0.69212	0.04374
ASP	1000	D	D	74.49	2.81	16.4475	0.0080	2.1645	0.0010	0.00000	0.00000	0.39220	0.02480
ASP	1000	D	D	94.66	16.36	16.8143	0.0008	2.1176	0.0001	0.04716	0.00852	0.01889	0.00846
ASP	1000	D	D	813.06	31.72	17.2485	0.0004	2.0647	<0.0001	0.07264	0.00296	0.03049	0.00298
ASP	1000	D	D	315.26	11.60	19.2045	0.0008	1.8561	0.0001	0.11707	0.00236	0.06962	0.00600
ASP	1000	D	D	767.36	268.04	19.5634	0.0004	1.8224	<0.0001	0.03104	0.01538	0.00000	0.00000
ASP	1000	D	D	14.51	1.08	20.3862	0.0050	1.7495	0.0004	0.00000	0.00000	0.12422	0.01388
ASP	1000	D	D	40.58	1.73	21.2186	0.0238	1.6817	0.0019	0.06107	0.00820	0.00368	0.00002
ASP	1000	D	D	15.77	1.49	29.5783	0.0450	1.2129	0.0018	0.03677	0.00880	0.00167	0.00000
ASP	1000	D	D	16.70	2.32	34.1611	0.0604	1.0541	0.0018	0.00000	0.00000	0.53242	0.10410
ASP	1000	D	D	20.32	6.22	34.9052	0.0084	1.0323	0.0002	0.05120	0.01732	0.00000	0.00000
ASP	1000	D	D	16.16	1.00	36.3866	0.0082	0.9916	0.0002	0.00000	0.00000	0.22947	0.02222
ASP	1000	D	D	49.35	3.21	37.4087	0.0088	0.9655	0.0002	0.16701	0.00098	0.04079	0.00476
ASP	1000	D	W	188.62	8.38	8.3878	0.0004	4.2336	0.0002	0.03156	0.00086	0.02244	0.00208
ASP	1000	D	W	1190.61	39.97	9.9370	0.0002	3.5748	0.0001	0.04212	0.00136	0.01995	0.00160
ASP	1000	D	W	2066.71	31.17	10.7886	0.0002	3.2934	0.0001	0.06221	0.00066	0.03785	0.00122
ASP	1000	D	W	141.85	14.69	11.6978	0.0010	3.0382	0.0003	0.00566	0.00212	0.00966	0.00106
ASP	1000	D	W	62.61	4.51	11.9306	0.0324	2.9791	0.0081	0.00000	0.00000	0.68862	0.07370
ASP	1000	D	W	58.14	5.40	11.9512	0.0434	2.9740	0.0108	0.00000	0.00000	0.65133	0.09164
ASP	1000	D	W	2132.11	144.41	13.0161	0.0004	2.7316	0.0001	0.06524	0.00520	0.02326	0.00412
ASP	1000	D	W	258.23	21.44	15.3510	0.0142	2.3181	0.0021	0.23021	0.10374	0.24542	0.04040
ASP	1000	D	W	95.35	28.15	15.6156	0.0260	2.2791	0.0038	0.00000	0.00000	0.25744	0.14132
ASP	1000	D	W	160.55	30.65	16.8168	0.0006	2.1173	0.0001	0.04002	0.00816	0.01614	0.00798
ASP	1000	D	W	1463.95	64.41	17.2491	0.0004	2.0646	<0.0001	0.06264	0.00296	0.02605	0.00288
ASP	1000	D	W	5.64	1.02	18.9853	0.0022	1.8773	0.0002	0.00000	0.00000	0.01954	0.00514
ASP	1000	D	W	561.09	20.34	19.2049	0.0008	1.8561	0.0001	0.11420	0.00210	0.07145	0.00596
ASP	1000	D	W	1302.04	28.40	19.5641	0.0004	1.8223	<0.0001	0.10270	0.00140	0.06050	0.00300
ASP	1000	D	W	82.36	8.66	19.9442	0.0018	1.7879	0.0002	0.07349	0.00736	0.06028	0.01418
ASP	1000	D	W	12.04	2.38	20.8561	0.0168	1.7105	0.0014	0.00000	0.00000	0.15004	0.04586
ASP	1000	D	W	4.97	0.91	23.5142	0.0020	1.5195	0.0001	0.00000	0.00000	0.01794	0.00482
ASP	1000	D	W	27.80	4.70	26.4830	0.0042	1.3517	0.0002	0.00000	0.00000	0.08679	0.03156
ASP	1000	D	W	33.91	1.87	26.8250	0.0038	1.3348	0.0002	0.00000	0.00000	0.11373	0.00886
ASP	1000	D	W	3.01	0.66	27.6012	0.0020	1.2979	0.0001	0.00000	0.00000	0.01537	0.00498
ASP	1000	D	W	62.43	3.85	29.4408	0.0234	1.2184	0.0009	0.00000	0.00000	0.69230	0.06760
ASP	1000	D	W	88.26	12.58	32.4277	0.0088	1.1088	0.0003	0.00000	0.00000	0.20795	0.01848
ASP	1000	D	W	51.22	1.46	34.0066	0.0030	1.0588	0.0001	0.05443	0.00414	0.01258	0.00006
ASP	1000	D	W	32.75	5.22	34.2525	0.0696	1.0514	0.0021	0.00000	0.00000	0.53473	0.16082
ASP	1000	D	W	32.04	3.73	34.6726	0.0160	1.0390	0.0005	0.00000	0.00000	0.24023	0.04814
ASP	1000	D	W	77.40	18.00	37.3983	0.0064	0.9657	0.0002	0.22548	0.03376	0.11734	0.06888
ASP	1000	E	D	106.63	3.70	8.3831	0.0004	4.2359	0.0002	0.03569	0.00074	0.02502	0.00182
ASP	1000	E	D	661.05	14.24	9.9353	0.0002	3.5755	0.0001	0.05356	0.00100	0.02779	0.00138
ASP	1000	E	D	1156.59	16.40	10.7870	0.0002	3.2939	0.0001	0.06699	0.00076	0.03564	0.00114
ASP	1000	E	D	59.80	2.28	11.9187	0.0202	2.9821	0.0050	0.00000	0.00000	0.91852	0.05420
ASP	1000	E	D	1203.16	127.77	13.0148	0.0002	2.7319	<0.0001	0.05247	0.00742	0.01368	0.00400
ASP	1000	E	D	72.05	2.37	15.3413	0.0038	2.3195	0.0006	0.24153	0.02416	0.21119	0.01060
ASP	1000	E	D	91.45	8.62	16.8150	0.0006	2.1175	0.0001	0.05064	0.00408	0.02430	0.00566
ASP	1000	E	D	815.63	192.71	17.2487	0.0002	2.0647	<0.0001	0.03704	0.01218	0.00708	0.00466
ASP	1000	E	D	347.86	160.12	19.2052	0.0006	1.8560	0.0001	0.03892	0.02510	0.00000	0.00000
ASP	1000	E	D	370.41	141.28	19.5648	0.0014	1.8222	0.0001	0.11554	0.02630	0.09779	0.03118
ASP	1000	E	D	380.15	169.29	21.6693	0.0008	1.6471	0.0001	0.04043	0.02498	0.00000	0.00000
ASP	1000	E	D	23.07	7.37	26.4863	0.0030	1.3515	0.0002	0.10354	0.02636	0.00000	0.00000
ASP	1000	E	D	29.53	4.06	26.8249	0.0030	1.3348	0.0001	0.13810	0.00894	0.08698	0.00066
ASP	1000	E	D	224.44	21.15	27.8279	0.0014	1.2876	0.0001	0.15835	0.01386	0.05884	0.01264
ASP	1000	E	D	33.94	5.21	30.1102	0.0024	1.1920	0.0001	0.13664	0.01020	0.07577	0.02918
ASP	1000	E	D	45.03	6.61	30.8095	0.0038	1.1655	0.0001	0.22398	0.01200	0.13459	0.04974
ASP	1000	E	D	76.38	1.75	31.3153	0.0054	1.1472	0.0002	0.09344	0.00482	0.01742	0.00016
ASP	1000	E	D	44.87	5.19	35.9439	0.0134	1.0034	0.0004	0.05834	0.00524	0.00409	0.00098
ASP	1000	E	D	11.28	1.38	38.9819	0.0138	0.9279	0.0003	0.04465	0.00018	0.00343	0.00070
ASP	1000	E	W	193.75	10.42	8.3878	0.0004	4.2336	0.0002	0.03126	0.00116	0.01824	0.00218
ASP	1000	E	W	1207.75	39.49	9.9367	0.0002	3.5750	0.0001	0.04178	0.00134	0.01929	0.00152
ASP	1000	E	W	2101.20	32.08	10.7883	0.0002	3.2935	0.0001	0.06175	0.00070	0.03605	0.00120
ASP	1000	E	W	2014.08	78.41	13.0152	0.0004	2.7318	0.0001	0.07567	0.00210	0.03656	0.00354
ASP	1000	E	W	220.29	39.72	15.3407	0.0062	2.3196	0.0009	0.22424	0.02942	0.19168	0.03448
ASP	1000	E	W	252.48	25.83	15.5713	0.0642	2.2855	0.0094	0.00000	0.00000	0.56061	0.10580

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
ASP	1000	E	W	152.47	6.21	16.4486	0.0100	2.1644	0.0013	0.00000	0.00000	0.42596	0.03110
ASP	1000	E	W	167.54	72.47	16.8170	0.0006	2.1173	0.0001	0.03227	0.01746	0.00000	0.00000
ASP	1000	E	W	1480.34	62.64	17.249	0.0004	2.0646	<0.0001	0.06264	0.00280	0.02611	0.00278
ASP	1000	E	W	579.98	23.14	19.2048	0.0008	1.8561	0.0001	0.11294	0.00262	0.06753	0.00626
ASP	1000	E	W	1318.28	28.43	19.5637	0.0004	1.8223	<0.0001	0.10188	0.00126	0.06341	0.00306
ASP	1000	E	W	96.10	19.38	19.9421	0.0016	1.7881	0.0001	0.07365	0.01242	0.08140	0.01166
ASP	1000	E	W	19.52	1.93	20.3815	0.0050	1.7499	0.0004	0.00000	0.00000	0.08705	0.01264
ASP	1000	E	W	169.70	18.15	24.1875	0.0026	1.4778	0.0002	0.17888	0.02358	0.11043	0.02808
ASP	1000	E	W	240.47	7.14	26.1814	0.0030	1.3670	0.0002	0.05411	0.00038	0.00563	0.00026
ASP	1000	E	W	34.20	6.26	26.4824	0.0036	1.3517	0.0002	0.08032	0.02110	0.07303	0.03040
ASP	1000	E	W	56.25	9.36	26.8244	0.0042	1.3348	0.0002	0.12840	0.02168	0.09445	0.03698
ASP	1000	E	W	239.70	25.22	27.2774	0.0014	1.3130	0.0001	0.12294	0.01466	0.06238	0.01634
ASP	1000	E	W	65.22	17.10	30.1052	0.0034	1.1922	0.0001	0.11220	0.01880	0.05807	0.03828
ASP	1000	E	W	64.17	3.56	35.9340	0.0118	1.0037	0.0003	0.00000	0.00000	0.37023	0.03498
ASP	1000	E	W	33.58	7.00	37.3925	0.0108	0.9659	0.0003	0.00000	0.00000	0.17825	0.04166
ASP	1000	F	D	111.85	4.35	8.3829	0.0002	4.2360	0.0001	0.03372	0.00082	0.02144	0.00180
ASP	1000	F	D	5.21	0.60	9.2072	0.0004	3.8575	0.0002	0.00000	0.00000	0.01085	0.00228
ASP	1000	F	D	683.04	14.42	9.9352	0.0002	3.5755	0.0001	0.05043	0.00092	0.02594	0.00126
ASP	1000	F	D	1175.64	17.22	10.7867	0.0002	3.2940	0.0001	0.06259	0.00076	0.03390	0.00112
ASP	1000	F	D	1149.86	46.06	13.0137	0.0002	2.7321	<0.0001	0.07240	0.00266	0.03142	0.00320
ASP	1000	F	D	66.38	2.47	15.3465	0.0036	2.3188	0.0005	0.00000	0.00000	0.20184	0.01088
ASP	1000	F	D	214.26	6.26	15.5586	0.0140	2.2873	0.0020	0.00000	0.00000	0.74921	0.02820
ASP	1000	F	D	179.51	16.16	15.5805	0.0518	2.2842	0.0076	0.00000	0.00000	0.68151	0.06364
ASP	1000	F	D	60.90	3.28	16.0591	0.0020	2.2165	0.0003	0.05926	0.00286	0.01474	0.00154
ASP	1000	F	D	84.06	2.40	16.4513	0.0064	2.1640	0.0008	0.00000	0.00000	0.39697	0.01890
ASP	1000	F	D	95.59	22.64	16.8135	0.0008	2.1177	0.0001	0.04093	0.01102	0.01497	0.00932
ASP	1000	F	D	842.31	248.68	17.2481	0.0002	2.0648	<0.0001	0.03650	0.01498	0.00000	0.00000
ASP	1000	F	D	8.00	1.32	18.6024	0.0008	1.9156	0.0001	0.01620	0.00346	0.01400	0.00506
ASP	1000	F	D	320.82	11.56	19.2048	0.0006	1.8561	0.0001	0.11263	0.00270	0.06210	0.00534
ASP	1000	F	D	750.80	16.00	19.5636	0.0004	1.8223	<0.0001	0.10010	0.00154	0.05479	0.00272
ASP	1000	F	D	48.30	4.44	19.9443	0.0016	1.7879	0.0001	0.08640	0.00486	0.09186	0.00498
ASP	1000	F	D	17.09	3.66	20.3810	0.0046	1.7500	0.0004	0.10489	0.03604	0.10513	0.01524
ASP	1000	F	D	383.21	165.92	21.6691	0.0008	1.6471	0.0001	0.03966	0.02432	0.00000	0.00000
ASP	1000	F	D	26.32	2.14	25.2892	0.0074	1.4144	0.0004	0.05851	0.00124	0.00728	0.00102
ASP	1000	F	D	21.79	3.87	26.4852	0.0036	1.3516	0.0002	0.10313	0.02192	0.08980	0.03440
ASP	1000	F	D	124.88	8.98	27.2766	0.0012	1.3131	0.0001	0.12054	0.00592	0.06460	0.01120
ASP	1000	F	D	36.23	11.16	30.1097	0.0024	1.1920	0.0001	0.10450	0.03358	0.00000	0.00000
ASP	1000	F	D	43.66	7.94	30.8100	0.0054	1.1655	0.0002	0.21264	0.00488	0.14128	0.04878
ASP	1000	F	D	116.84	1.81	31.5292	0.0054	1.1396	0.0002	0.05522	0.00172	0.00495	0.00002
ASP	1000	F	D	13.39	2.68	34.1626	0.0736	1.0541	0.0022	0.00000	0.00000	0.42054	0.11022
ASP	1000	F	W	197.84	10.96	8.3877	0.0004	4.2336	0.0002	0.03151	0.00118	0.01876	0.00230
ASP	1000	F	W	1.68	0.59	9.2100	0.0034	3.8563	0.0014	0.00000	0.00000	0.01571	0.00780
ASP	1000	F	W	1203.18	32.42	9.9367	0.0002	3.5750	0.0001	0.04460	0.00104	0.02312	0.00142
ASP	1000	F	W	2107.25	31.65	10.7882	0.0002	3.2935	0.0001	0.06394	0.00064	0.04045	0.00128
ASP	1000	F	W	49.85	4.18	11.9244	0.0320	2.9807	0.0080	0.00000	0.00000	0.61741	0.07864
ASP	1000	F	W	1998.87	85.67	13.0151	0.0004	2.7318	0.0001	0.07894	0.00148	0.04221	0.00380
ASP	1000	F	W	130.75	5.79	15.3429	0.0044	2.3193	0.0007	0.00000	0.00000	0.20259	0.01318
ASP	1000	F	W	359.88	13.23	15.5598	0.0182	2.2872	0.0027	0.00000	0.00000	0.71155	0.03366
ASP	1000	F	W	317.83	16.80	15.5728	0.0292	2.2853	0.0043	0.00000	0.00000	0.65963	0.04292
ASP	1000	F	W	116.08	7.71	16.0573	0.0026	2.2168	0.0004	0.08540	0.00056	0.02914	0.00384
ASP	1000	F	W	149.64	5.56	16.4474	0.0082	2.1645	0.0011	0.00000	0.00000	0.39985	0.02484
ASP	1000	F	W	172.70	25.45	16.8166	0.0008	2.1173	0.0001	0.04694	0.00608	0.02205	0.00814
ASP	1000	F	W	1520.53	630.41	17.2486	0.0004	2.0647	<0.0001	0.02997	0.01710	0.00000	0.00000
ASP	1000	F	W	573.16	22.87	19.2031	0.0010	1.8562	0.0001	0.11359	0.00242	0.08222	0.00620
ASP	1000	F	W	1422.55	546.10	19.5636	0.0004	1.8223	<0.0001	0.02671	0.01438	0.00000	0.00000
ASP	1000	F	W	84.50	7.93	19.9448	0.0018	1.7879	0.0002	0.07161	0.00838	0.08623	0.01422
ASP	1000	F	W	23.81	2.52	20.3813	0.0060	1.7500	0.0005	0.00000	0.00000	0.10146	0.01594
ASP	1000	F	W	33.57	4.46	21.1947	0.0238	1.6835	0.0019	0.00000	0.00000	0.30052	0.06858
ASP	1000	F	W	31.11	5.64	26.4820	0.0054	1.3517	0.0003	0.00000	0.00000	0.08580	0.03304
ASP	1000	F	W	3.81	1.25	26.7006	0.0028	1.3409	0.0001	0.00000	0.00000	0.01834	0.01102
ASP	1000	F	W	135.79	35.27	31.4754	0.0706	1.1415	0.0025	0.00000	0.00000	0.43984	0.08242
ASP	1000	F	W	19.01	3.07	34.9070	0.0108	1.0323	0.0003	0.00000	0.00000	0.13766	0.03488
GLU	10	A	H	92.67	3.38	8.387	0.0004	4.234	0.0002	0.03287	0.00072	0.01919	0.00134
GLU	10	A	H	126.97	2.15	9.2122	0.0002	3.8554	0.0001	0.00817	0.00024	0.00955	0.00026
GLU	10	A	H	565.24	11.21	9.9343	0.0002	3.5758	0.0001	0.04613	0.00066	0.02733	0.00116
GLU	10	A	H	891.68	16.35	10.7856	0.0004	3.2943	0.0001	0.06060	0.00080	0.04791	0.00170
GLU	10	A	H	1041.24	7.15	11.7038	0.0000	3.0367	0	0.00930	0.00008	0.01020	0.00012
GLU	10	A	H	30.10	1.81	12.497	0.0002	2.8446	<0.0001	0.01130	0.00112	0.01124	0.00132
GLU	10	A	H	975.34	39.00	13.0151	0.0004	2.7318	0.0001	0.07398	0.00306	0.03240	0.00318
GLU	10	A	H	114.72	2.65	14.2542	0.0002	2.4954	<0.0001	0.01061	0.00040	0.01156	0.00048
GLU	10	A	H	236.57	4.41	15.5729	0.0000	2.2853	0	0.01124	0.00022	0.00985	0.00036
GLU	10	A	H	88.94	6.37	16.4588	0.0056	2.163	0.0007	0.04629	0.00324	0.00277	0.00044
GLU	10	A	H	78.46	7.40	16.8175	0.0006	2.1172	0.0001	0.04941	0.00366	0.02481	0.00574
GLU	10	A	H	150.10	2.58	16.9972	0.0000	2.095	0	0.00969	0.00040	0.01186	0.00036
GLU	10	A	H	681.28	22.41	17.2508	0.0002	2.0644	<0.0001	0.06705	0.00220	0.02967	0.00242
GLU	10	A	H	146.08	3.37	18.484	0.0000	1.9278	0	0.01056	0.00018	0.00845	0.00038
GLU	10	A	H	271.33	4.31	18.6274	0.0000	1.9131	0	0.01265	0.00016	0.01051	0.00032
GLU	10	A	H	284.92	4.17	19	0.0000	1.8759	0	0.01209	0.00018	0.01097	0.00030
GLU	10	A	H	276.10	11.86	19.2058	0.0008	1.856	0.0001	0.11946	0.00300	0.06775	0.00700

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	10	A	H	637.80	16.69	19.5684	0.0004	1.8219	<0.0001	0.10091	0.00206	0.05270	0.00330
GLU	10	A	H	41.84	5.22	19.9456	0.0016	1.7878	0.0001	0.08132	0.00536	0.04866	0.01454
GLU	10	A	H	26.83	2.79	20.8579	0.0120	1.7104	0.001	0.03942	0.00010	0.00254	0.00048
GLU	10	A	H	62.38	2.14	21.9511	0.0002	1.6262	<0.0001	0.01106	0.00050	0.01050	0.00070
GLU	10	A	H	120.38	3.10	22.253	0.0002	1.6044	<0.0001	0.01285	0.00024	0.01036	0.00052
GLU	10	A	H	24.45	3.68	22.4951	0.0002	1.5873	<0.0001	0.01125	0.00150	0.00557	0.00202
GLU	10	A	H	103.86	2.57	23.4189	0.0002	1.5256	<0.0001	0.01147	0.00032	0.01070	0.00050
GLU	10	A	H	41.74	4.33	23.5343	0.0002	1.5182	<0.0001	0.01116	0.00100	0.00559	0.00138
GLU	10	A	H	51.91	16.03	23.6659	0.0002	1.5099	<0.0001	0.01114	0.00428	0.00000	0.00000
GLU	10	A	H	41.92	3.38	24.2585	0.0002	1.4735	<0.0001	0.01295	0.00054	0.00875	0.00160
GLU	10	A	H	102.24	2.44	24.8189	0.0002	1.4407	<0.0001	0.01176	0.00034	0.01130	0.00050
GLU	10	A	H	62.98	2.68	25.1483	0.0002	1.4222	<0.0001	0.01612	0.00054	0.01282	0.00112
GLU	10	A	H	16.28	1.43	26.3756	0.0004	1.3571	<0.0001	0.01297	0.00172	0.01184	0.00220
GLU	10	A	H	33.31	1.91	26.73	0.0002	1.3394	<0.0001	0.01389	0.00082	0.01155	0.00140
GLU	10	A	H	54.62	2.06	27.6208	0.0002	1.297	<0.0001	0.01327	0.00052	0.01153	0.00088
GLU	10	A	H	19.00	2.48	27.8794	0.0004	1.2852	<0.0001	0.01302	0.00260	0.01110	0.00330
GLU	10	A	H	17.13	2.65	28.7359	0.0004	1.2477	<0.0001	0.01708	0.00188	0.00921	0.00340
GLU	10	A	H	41.82	1.77	29.0216	0.0002	1.2357	<0.0001	0.01513	0.00004	0.01275	0.00108
GLU	10	A	H	40.16	2.76	30.4205	0.0002	1.1801	<0.0001	0.01460	0.00060	0.00901	0.00138
GLU	10	A	H	82.72	3.53	31.126	0.0002	1.154	<0.0001	0.01305	0.00032	0.00856	0.00080
GLU	10	A	H	24.97	1.62	33.9069	0.0002	1.0618	<0.0001	0.01381	0.00138	0.01287	0.00174
GLU	10	A	H	34.64	1.59	34.3861	0.0002	1.0474	<0.0001	0.01374	0.00140	0.01465	0.00134
GLU	10	A	H	39.06	1.95	34.4667	0.0002	1.045	<0.0001	0.01417	0.00082	0.01228	0.00126
GLU	10	A	H	27.32	2.72	34.7931	0.0004	1.0355	<0.0001	0.02194	0.00150	0.01583	0.00360
GLU	10	B	H	122.15	4.66	8.3865	0.0004	4.2342	0.0002	0.02756	0.00010	0.01883	0.00146
GLU	10	B	H	45.08	2.59	9.2105	0.0002	3.8561	0.0001	0.00915	0.00122	0.01106	0.00110
GLU	10	B	H	671.80	13.03	9.9328	0.0002	3.5763	0.0001	0.04472	0.00064	0.03584	0.00132
GLU	10	B	H	1144.19	19.09	10.7844	0.0002	3.2947	0.0001	0.05678	0.00062	0.04117	0.00136
GLU	10	B	H	551.36	8.72	11.7033	0.0000	3.0368	0	0.00945	0.00022	0.01022	0.00028
GLU	10	B	H	29.75	1.99	11.9704	0.0248	2.9693	0.0061	0.03672	0.00488	0.00174	0.00002
GLU	10	B	H	16.52	2.07	12.4966	0.0006	2.8447	0.0001	0.00897	0.00380	0.01132	0.00272
GLU	10	B	H	1250.16	72.49	13.0142	0.0004	2.732	0.0001	0.06357	0.00424	0.02498	0.00368
GLU	10	B	H	87.33	3.98	14.2537	0.0002	2.4955	<0.0001	0.00966	0.00064	0.01000	0.00082
GLU	10	B	H	118.60	3.96	15.5721	0.0002	2.2854	<0.0001	0.01185	0.00034	0.00948	0.00066
GLU	10	B	H	96.46	5.82	16.8177	0.0004	2.1172	0.0001	0.04461	0.00164	0.02631	0.00370
GLU	10	B	H	94.40	2.27	16.9961	0.0000	2.0951	0	0.00922	0.00046	0.01054	0.00046
GLU	10	B	H	797.20	12.16	17.2493	0.0002	2.0646	<0.0001	0.07294	0.00076	0.04430	0.00148
GLU	10	B	H	42.82	3.93	18.4819	0.0002	1.928	<0.0001	0.01340	0.00094	0.00718	0.00154
GLU	10	B	H	118.39	3.41	18.6272	0.0002	1.9131	<0.0001	0.01434	0.00028	0.01085	0.00062
GLU	10	B	H	148.61	3.15	18.9994	0.0000	1.8759	0	0.01161	0.00030	0.01103	0.00044
GLU	10	B	H	323.69	10.55	19.2053	0.0006	1.856	0.0001	0.11096	0.00188	0.06794	0.00514
GLU	10	B	H	762.96	14.84	19.5683	0.0004	1.8219	<0.0001	0.09316	0.00122	0.05316	0.00238
GLU	10	B	H	43.09	2.43	19.9438	0.0014	1.7879	0.0001	0.05105	0.02204	0.08145	0.00942
GLU	10	B	H	30.67	3.18	21.205	0.0142	1.6827	0.0011	0.03490	0.00362	0.00169	0.00032
GLU	10	B	H	23.25	1.48	21.9502	0.0002	1.6263	<0.0001	0.01112	0.00156	0.01189	0.00150
GLU	10	B	H	64.65	2.70	22.2523	0.0002	1.6044	<0.0001	0.01349	0.00036	0.01022	0.00086
GLU	10	B	H	38.27	2.32	23.4185	0.0002	1.5256	<0.0001	0.01293	0.00050	0.00964	0.00124
GLU	10	B	H	17.52	2.93	23.5341	0.0004	1.5182	<0.0001	0.01418	0.00126	0.00838	0.00332
GLU	10	B	H	27.27	2.63	23.6674	0.0002	1.5098	<0.0001	0.01237	0.00114	0.00963	0.00208
GLU	10	B	H	21.53	3.82	24.259	0.0004	1.4735	<0.0001	0.01454	0.00130	0.00851	0.00364
GLU	10	B	H	49.94	2.01	24.8179	0.0002	1.4408	<0.0001	0.01170	0.00046	0.01023	0.00080
GLU	10	B	H	27.21	2.35	25.1484	0.0004	1.4222	<0.0001	0.01638	0.00106	0.01234	0.00232
GLU	10	B	H	27.35	2.24	26.7312	0.0002	1.3394	<0.0001	0.01405	0.00070	0.00996	0.00182
GLU	10	B	H	24.38	2.09	26.8302	0.0038	1.3345	0.0002	0.00000	0.00000	0.12822	0.02296
GLU	10	B	H	24.40	1.55	27.621	0.0002	1.297	<0.0001	0.01317	0.00154	0.01282	0.00170
GLU	10	B	H	30.45	1.63	29.024	0.0002	1.2356	<0.0001	0.01390	0.00076	0.01196	0.00130
GLU	10	B	H	21.22	4.06	29.3221	0.0290	1.2233	0.0012	0.05278	0.01380	0.00327	0.00124
GLU	10	B	H	24.04	3.45	30.4204	0.0002	1.1801	<0.0001	0.01426	0.00176	0.00700	0.00244
GLU	10	B	H	33.06	1.81	31.1244	0.0002	1.154	<0.0001	0.01383	0.00086	0.01206	0.00138
GLU	10	B	H	17.34	1.07	34.1933	0.0324	1.0532	0.001	0.03815	0.00824	0.00194	0.00000
GLU	10	B	H	12.71	2.16	34.3857	0.0006	1.0474	<0.0001	0.01756	0.00152	0.01078	0.00432
GLU	10	B	H	24.33	1.85	34.4678	0.0002	1.045	<0.0001	0.01376	0.00072	0.01033	0.00172
GLU	10	B	H	16.04	2.61	34.7921	0.0006	1.0356	<0.0001	0.02088	0.00206	0.01420	0.00542
GLU	10	C	H	128.52	5.05	8.3874	0.0002	4.2338	0.0001	0.02942	0.00070	0.01953	0.00164
GLU	10	C	H	51.47	1.72	9.2123	0.0002	3.8554	0.0001	0.00836	0.00054	0.00968	0.00056
GLU	10	C	H	713.85	10.63	9.9332	0.0002	3.5762	0.0001	0.04375	0.00046	0.02762	0.00086
GLU	10	C	H	1211.11	13.79	10.7848	0.0002	3.2946	0.0001	0.05791	0.00044	0.03777	0.00090
GLU	10	C	H	619.95	5.34	11.7032	0.0000	3.0368	0	0.00906	0.00014	0.01070	0.00016
GLU	10	C	H	40.16	3.21	11.9371	0.0164	2.9775	0.0041	0.04453	0.00010	0.00207	0.00028
GLU	10	C	H	23.48	1.48	12.4969	0.0002	2.8446	<0.0001	0.00873	0.00118	0.00955	0.00114
GLU	10	C	H	1311.01	53.04	13.0144	0.0002	2.732	<0.0001	0.06322	0.00300	0.02350	0.00246
GLU	10	C	H	87.08	2.37	14.2539	0.0002	2.4955	<0.0001	0.00914	0.00040	0.00980	0.00048
GLU	10	C	H	88.94	5.10	15.5719	0.0002	2.2854	<0.0001	0.01279	0.00040	0.00863	0.00110
GLU	10	C	H	99.47	7.96	16.8183	0.0006	2.1171	0.0001	0.04467	0.00260	0.02386	0.00456
GLU	10	C	H	95.79	2.64	16.9965	0.0000	2.0951	0	0.00808	0.00038	0.00863	0.00044
GLU	10	C	H	844.45	18.38	17.2494	0.0002	2.0646	<0.0001	0.06876	0.00122	0.03620	0.00182
GLU	10	C	H	63.14	3.30	18.4839	0.0002	1.9278	<0.0001	0.01067	0.00034	0.00742	0.00082
GLU	10	C	H	143.10	3.20	18.6268	0.0002	1.9131	<0.0001	0.01139	0.00032	0.01125	0.00046
GLU	10	C	H	116.44	3.16	18.9996	0.0002	1.8759	<0.0001	0.01117	0.00044	0.01104	0.00056

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	10	C	H	798.67	15.82	19.569	0.0004	1.8218	<0.0001	0.09687	0.00120	0.05792	0.00260
GLU	10	C	H	45.85	3.51	19.944	0.0014	1.7879	0.0001	0.06540	0.00870	0.06125	0.01016
GLU	10	C	H	33.63	1.71	21.9509	0.0002	1.6262	<0.0001	0.00902	0.00140	0.01114	0.00106
GLU	10	C	H	50.96	2.94	22.2519	0.0002	1.6045	<0.0001	0.01355	0.00048	0.00982	0.00118
GLU	10	C	H	47.60	2.55	23.4186	0.0002	1.5256	<0.0001	0.01117	0.00048	0.00909	0.00100
GLU	10	C	H	18.01	5.76	23.5332	0.0004	1.5183	<0.0001	0.01324	0.00390	0.00000	0.00000
GLU	10	C	H	16.63	2.51	23.6662	0.0004	1.5098	<0.0001	0.01262	0.00698	0.01363	0.00448
GLU	10	C	H	16.74	4.47	24.2589	0.0006	1.4735	<0.0001	0.01552	0.00218	0.00892	0.00584
GLU	10	C	H	38.65	2.04	24.8184	0.0002	1.4408	<0.0001	0.01182	0.00066	0.01059	0.00110
GLU	10	C	H	59.80	2.75	25.1482	0.0002	1.4222	<0.0001	0.01472	0.00040	0.01042	0.00104
GLU	10	C	H	23.03	1.04	27.6207	0.0002	1.297	<0.0001	0.00000	0.00000	0.01574	0.00122
GLU	10	C	H	16.16	1.84	29.0227	0.0004	1.2356	<0.0001	0.01640	0.00108	0.01149	0.00298
GLU	10	C	H	40.81	1.86	31.1251	0.0002	1.154	<0.0001	0.01321	0.00068	0.01154	0.00108
GLU	10	C	H	15.77	2.71	34.121	0.0476	1.0553	0.0014	0.00000	0.00000	0.36896	0.07576
GLU	10	C	H	22.87	2.69	34.3853	0.0002	1.0474	<0.0001	0.01248	0.00088	0.00740	0.00202
GLU	10	C	H	21.57	2.26	34.4671	0.0004	1.045	<0.0001	0.01513	0.00088	0.01045	0.00246
GLU	10	C	H	18.33	1.87	34.7911	0.0006	1.0356	<0.0001	0.01690	0.00584	0.01846	0.00408
GLU	10	D	H	84.01	5.82	8.3861	0.0004	4.2344	0.0002	0.03320	0.00190	0.01720	0.00278
GLU	10	D	H	103.23	2.28	9.2108	0.0000	3.856	0	0.00967	0.00030	0.01025	0.00040
GLU	10	D	H	461.51	10.98	9.9334	0.0002	3.5761	0.0001	0.04568	0.00086	0.02535	0.00134
GLU	10	D	H	776.99	12.12	10.7846	0.0002	3.2946	0.0001	0.06103	0.00068	0.03662	0.00122
GLU	10	D	H	1572.88	8.00	11.7022	0.0000	3.0371	0	0.00935	0.00006	0.01054	0.00008
GLU	10	D	H	17.98	1.54	12.0239	0.0204	2.9561	0.005	0.00000	0.00000	0.39154	0.05352
GLU	10	D	H	45.56	2.20	12.4952	0.0002	2.845	<0.0001	0.01190	0.00046	0.00980	0.00094
GLU	10	D	H	831.90	162.83	13.0145	0.0002	2.732	<0.0001	0.04423	0.01166	0.01039	0.00562
GLU	10	D	H	273.07	3.52	14.2545	0.0000	2.4954	0	0.00890	0.00018	0.00996	0.00022
GLU	10	D	H	281.90	5.27	15.5715	0.0000	2.2855	0	0.01220	0.00022	0.01041	0.00038
GLU	10	D	H	60.88	5.96	16.8171	0.0008	2.1173	0.0001	0.05273	0.00306	0.03036	0.00704
GLU	10	D	H	245.18	3.46	16.9969	0.0000	2.095	0	0.00968	0.00026	0.01117	0.00028
GLU	10	D	H	548.62	23.03	17.2502	0.0004	2.0645	<0.0001	0.06674	0.00282	0.02905	0.00302
GLU	10	D	H	88.79	3.31	18.4824	0.0002	1.9279	<0.0001	0.01461	0.00032	0.01016	0.00080
GLU	10	D	H	434.98	5.17	18.6261	0.0000	1.9132	0	0.01407	0.00014	0.01178	0.00026
GLU	10	D	H	316.29	4.56	18.9994	0.0000	1.8759	0	0.01408	0.00018	0.01201	0.00034
GLU	10	D	H	208.72	8.31	19.2062	0.0008	1.8559	0.0001	0.11555	0.00220	0.07709	0.00714
GLU	10	D	H	516.76	16.58	19.568	0.0004	1.8219	<0.0001	0.09687	0.00266	0.04771	0.00372
GLU	10	D	H	76.19	2.55	21.9505	0.0002	1.6262	<0.0001	0.01276	0.00034	0.01041	0.00070
GLU	10	D	H	141.75	4.16	22.2525	0.0002	1.6044	<0.0001	0.01533	0.00028	0.01020	0.00064
GLU	10	D	H	28.98	3.21	22.4932	0.0004	1.5875	<0.0001	0.01650	0.00134	0.00895	0.00232
GLU	10	D	H	92.00	3.21	23.4182	0.0002	1.5256	<0.0001	0.01424	0.00030	0.01019	0.00074
GLU	10	D	H	48.13	4.30	23.533	0.0002	1.5183	<0.0001	0.01402	0.00102	0.00732	0.00154
GLU	10	D	H	66.70	12.04	23.665	0.0002	1.5099	<0.0001	0.01255	0.00266	0.00454	0.00212
GLU	10	D	H	43.08	2.99	24.2583	0.0002	1.4735	<0.0001	0.01560	0.00090	0.01186	0.00182
GLU	10	D	H	96.92	3.10	24.8184	0.0002	1.4408	<0.0001	0.01637	0.00032	0.01206	0.00078
GLU	10	D	H	133.07	3.62	25.146	0.0002	1.4223	<0.0001	0.01686	0.00028	0.01236	0.00070
GLU	10	D	H	28.22	2.03	26.376	0.0002	1.3571	<0.0001	0.01373	0.00072	0.01043	0.00164
GLU	10	D	H	46.90	3.32	26.73	0.0002	1.3394	<0.0001	0.01733	0.00070	0.01074	0.00172
GLU	10	D	H	47.64	2.91	27.6205	0.0002	1.297	<0.0001	0.01788	0.00060	0.01196	0.00162
GLU	10	D	H	32.34	1.71	28.7361	0.0002	1.2477	<0.0001	0.01381	0.00064	0.01140	0.00124
GLU	10	D	H	42.90	2.55	29.0215	0.0002	1.2357	<0.0001	0.02007	0.00066	0.01320	0.00174
GLU	10	D	H	63.78	3.30	30.4197	0.0002	1.1801	<0.0001	0.01567	0.00054	0.00920	0.00106
GLU	10	D	H	95.07	3.28	31.1247	0.0002	1.154	<0.0001	0.01879	0.00038	0.01314	0.00098
GLU	10	D	H	44.13	4.47	31.4443	0.0002	1.1426	<0.0001	0.01668	0.00096	0.00936	0.00228
GLU	10	D	H	19.91	1.65	33.9042	0.0004	1.0619	<0.0001	0.01879	0.00174	0.01580	0.00282
GLU	10	D	H	64.36	2.17	34.3856	0.0002	1.0474	<0.0001	0.01302	0.00044	0.01122	0.00076
GLU	10	D	H	58.19	2.48	34.4666	0.0002	1.0451	<0.0001	0.01628	0.00046	0.01227	0.00110
GLU	10	D	H	48.47	2.60	34.7909	0.0002	1.0356	<0.0001	0.02266	0.00112	0.01798	0.00210
GLU	10	E	H	141.77	4.56	8.3859	0.0002	4.2345	0.0001	0.03140	0.00066	0.02344	0.00156
GLU	10	E	H	32.46	1.49	9.211	0.0002	3.8559	0.0001	0.01029	0.00092	0.01149	0.00096
GLU	10	E	H	716.71	9.45	9.9333	0.0002	3.5762	0.0001	0.05052	0.00044	0.03611	0.00094
GLU	10	E	H	1225.70	12.53	10.7847	0.0002	3.2946	0.0001	0.06245	0.00040	0.04364	0.00090
GLU	10	E	H	351.97	4.45	11.7028	0.0000	3.0369	0	0.01001	0.00018	0.01048	0.00022
GLU	10	E	H	18.67	1.67	12.4966	0.0002	2.8447	<0.0001	0.01019	0.00102	0.00884	0.00162
GLU	10	E	H	1317.07	52.97	13.0141	0.0002	2.732	<0.0001	0.07344	0.00218	0.03334	0.00332
GLU	10	E	H	33.07	10.54	13.1475	0.1032	2.7044	0.0213	0.00000	0.00000	0.33962	0.13210
GLU	10	E	H	57.81	2.03	14.254	0.0002	2.4955	<0.0001	0.01047	0.00056	0.01069	0.00070
GLU	10	E	H	89.27	3.02	15.3418	0.0034	2.3195	0.0005	0.00000	0.00000	0.21863	0.01086
GLU	10	E	H	93.85	2.98	15.5715	0.0002	2.2855	<0.0001	0.01155	0.00056	0.01090	0.00070
GLU	10	E	H	182.67	5.50	15.5921	0.0144	2.2825	0.0021	0.00000	0.00000	0.61925	0.02402
GLU	10	E	H	114.87	9.57	16.8166	0.0004	2.1173	0.0001	0.04945	0.00284	0.02545	0.00522
GLU	10	E	H	60.98	1.76	16.9966	0.0002	2.0951	<0.0001	0.00872	0.00112	0.01271	0.00066
GLU	10	E	H	842.36	13.20	17.25	0.0002	2.0645	<0.0001	0.08140	0.00086	0.04808	0.00168
GLU	10	E	H	157.25	3.14	18.6277	0.0000	1.913	0	0.01041	0.00018	0.00916	0.00034
GLU	10	E	H	108.20	2.80	18.9996	0.0002	1.8759	<0.0001	0.01223	0.00056	0.01239	0.00062
GLU	10	E	H	63.87	13.55	19.1936	0.0082	1.8571	0.0008	0.00000	0.00000	0.19476	0.02904
GLU	10	E	H	273.82	24.60	19.2063	0.0012	1.8559	0.0001	0.10663	0.00536	0.06169	0.01110
GLU	10	E	H	873.69	17.65	19.5677	0.0004	1.822	<0.0001	0.09926	0.00140	0.05408	0.00258
GLU	10	E	H	45.98	3.16	19.9443	0.0014	1.7879	0.0001	0.07398	0.01062	0.07240	0.01084
GLU	10	E	H	13.24	1.50	21.9503	0.0004	1.6262	<0.0001	0.01167	0.00144	0.00984	0.00240
GLU	10	E	H	36.94	2.87	22.2521	0.0002	1.6045	<0.0001	0.01466	0.00070	0.00905	0.00158

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	10	E	H	27.00	3.42	23.4181	0.0002	1.5256	<0.0001	0.01339	0.00126	0.00721	0.00216
GLU	10	E	H	30.53	1.62	24.8179	0.0002	1.4408	<0.0001	0.01175	0.00066	0.01035	0.00108
GLU	10	E	H	36.97	3.40	25.1494	0.0002	1.4221	<0.0001	0.01204	0.00070	0.00698	0.00148
GLU	10	E	H	20.66	1.71	27.6214	0.0004	1.297	<0.0001	0.01250	0.00156	0.01143	0.00200
GLU	10	E	H	17.11	2.59	29.0225	0.0004	1.2356	<0.0001	0.01457	0.00138	0.00838	0.00298
GLU	10	E	H	24.36	0.48	30.4202	0.0004	1.1801	<0.0001	0.01390	0.00052	0.00703	0.00002
GLU	10	E	H	27.94	1.75	31.1244	0.0002	1.154	<0.0001	0.01372	0.00176	0.01388	0.00180
GLU	10	E	H	138.62	20.00	31.5224	0.0118	1.1398	0.0004	0.29585	0.03518	0.15389	0.05436
GLU	10	E	H	18.62	1.21	34.385	0.0004	1.0475	<0.0001	0.01177	0.00226	0.01410	0.00184
GLU	10	F	H	44.74	2.07	9.2117	0.0002	3.85698	<0.0001	0.00905	0.00056	0.00916	0.00076
GLU	10	F	H	735.19	17.91	9.9334	0.0002	3.57742	<0.0001	0.04740	0.00088	0.02721	0.00144
GLU	10	F	H	1243.10	18.05	10.7848	0.0002	3.29572	<0.0001	0.06165	0.00062	0.03833	0.00118
GLU	10	F	H	426.03	4.86	11.7023	0.0000	3.03812	<0.0001	0.00859	0.00018	0.00991	0.00020
GLU	10	F	H	10.43	1.51	12.4958	0.0004	2.84588	0.0001	0.01044	0.00200	0.00933	0.00284
GLU	10	F	H	1360.08	111.74	13.0145	0.0002	2.73292	<0.0001	0.05587	0.00592	0.01670	0.00372
GLU	10	F	H	51.60	2.84	14.2539	0.0002	2.49636	<0.0001	0.01054	0.00034	0.00742	0.00086
GLU	10	F	H	62.94	4.71	15.5719	0.0002	2.28621	<0.0001	0.01112	0.00046	0.00706	0.00120
GLU	10	F	H	103.56	10.79	16.8163	0.0006	2.11811	<0.0001	0.04761	0.00432	0.02290	0.00590
GLU	10	F	H	44.84	1.76	16.9968	0.0002	2.09579	<0.0001	0.00762	0.00166	0.01200	0.00086
GLU	10	F	H	888.01	24.30	17.25	0.0002	2.06526	<0.0001	0.07259	0.00188	0.03410	0.00224
GLU	10	F	H	48.73	13.40	18.4823	0.0002	1.92863	<0.0001	0.00889	0.00304	0.00295	0.00216
GLU	10	F	H	73.07	3.65	18.6275	0.0002	1.91374	<0.0001	0.01351	0.00042	0.00857	0.00092
GLU	10	F	H	123.47	3.16	18.9992	0.0002	1.87662	<0.0001	0.01121	0.00034	0.01044	0.00052
GLU	10	F	H	376.45	22.09	19.2059	0.0006	1.85661	<0.0001	0.11051	0.00622	0.04949	0.00736
GLU	10	F	H	827.30	13.53	19.5678	0.0004	1.82261	<0.0001	0.10125	0.00110	0.05837	0.00208
GLU	10	F	H	52.70	0.79	19.9435	0.0014	1.78861	0.0001	0.07997	0.00470	0.06342	0.00020
GLU	10	F	H	36.55	4.03	21.2056	0.0160	1.68326	0.0006	0.04818	0.00016	0.00291	0.00062
GLU	10	F	H	15.01	1.32	21.9494	0.0004	1.62689	<0.0001	0.00975	0.00284	0.01186	0.00210
GLU	10	F	H	33.31	2.18	22.2517	0.0002	1.60506	<0.0001	0.01397	0.00068	0.01102	0.00150
GLU	10	F	H	114.22	1.56	23.1501	0.0030	1.54357	0.0001	0.04524	0.00098	0.00393	0.00002
GLU	10	F	H	32.59	4.08	23.4188	0.0002	1.5261	<0.0001	0.00931	0.00092	0.00481	0.00144
GLU	10	F	H	20.06	1.87	23.5333	0.0002	1.51878	<0.0001	0.01054	0.00168	0.00972	0.00192
GLU	10	F	H	92.80	4.06	24.1831	0.0036	1.47855	0.0001	0.04876	0.00012	0.00670	0.00052
GLU	10	F	H	26.11	1.41	24.8192	0.0002	1.44123	<0.0001	0.01120	0.00128	0.01202	0.00124
GLU	10	F	H	9.37	2.81	25.148	0.0008	1.42268	<0.0001	0.01686	0.00238	0.00945	0.00688
GLU	10	F	H	4.32	0.86	26.374	0.0010	1.35765	<0.0001	0.00010	0.02166	0.01487	0.00602
GLU	10	F	H	9.92	2.36	26.7299	0.0006	1.33989	<0.0001	0.01467	0.00170	0.00945	0.00530
GLU	10	F	H	20.89	1.60	27.6209	0.0004	1.29747	<0.0001	0.01120	0.00202	0.01212	0.00190
GLU	10	F	H	262.25	3.91	27.8287	0.0012	1.28797	<0.0001	0.04741	0.00014	0.00536	0.00012
GLU	10	F	H	6.03	0.79	28.7363	0.0006	1.24811	<0.0001	0.01172	0.00572	0.01419	0.00384
GLU	10	F	H	16.62	1.55	29.022	0.0002	1.23608	<0.0001	0.01300	0.00078	0.00952	0.00194
GLU	10	F	H	19.55	6.12	30.4203	0.0002	1.18051	<0.0001	0.01015	0.00360	0.00380	0.00310
GLU	10	F	H	1.57	0.29	30.6011	0.0016	1.1737	<0.0001	0.00010	1.27092	0.01454	0.00390
GLU	10	F	H	19.51	3.14	31.1245	0.0004	1.15444	<0.0001	0.01628	0.00174	0.00876	0.00340
GLU	10	F	H	12.95	2.88	31.4436	0.0006	1.14302	<0.0001	0.01564	0.00176	0.01022	0.00546
GLU	10	F	H	1.14	0.29	31.9474	0.0024	1.12545	<0.0001	0.00010	2.13688	0.01595	0.00588
GLU	10	F	H	1.67	1.37	33.9075	0.0016	1.06214	<0.0001	0.01250	0.00476	0.00778	0.01552
GLU	10	F	H	13.71	1.32	34.3863	0.0004	1.04779	<0.0001	0.01290	0.00126	0.01071	0.00224
GLU	10	F	H	20.45	1.28	34.4678	0.0002	1.04538	<0.0001	0.01125	0.00128	0.01110	0.00144
GLU	10	F	H	8.34	1.89	34.7943	0.0008	1.03587	<0.0001	0.01945	0.00770	0.01649	0.00862
GLU	100	A	H	132.20	6.86	8.3867	0.0004	4.2341	0.0002	0.03578	0.00132	0.02101	0.00240
GLU	100	A	H	34.40	1.89	9.2112	0.0002	3.8558	0.0001	0.01005	0.00076	0.00996	0.00102
GLU	100	A	H	727.75	12.81	9.9345	0.0002	3.5757	0.0001	0.05090	0.00060	0.03264	0.00120
GLU	100	A	H	1237.00	15.00	10.7859	0.0002	3.2942	0.0001	0.06506	0.00052	0.04485	0.00110
GLU	100	A	H	529.79	5.99	11.7034	0.0000	3.0368	0	0.00911	0.00014	0.00994	0.00018
GLU	100	A	H	1334.40	256.19	13.0153	0.0002	2.7318	<0.0001	0.04486	0.01176	0.01037	0.00550
GLU	100	A	H	49.74	2.55	14.2536	0.0002	2.4955	<0.0001	0.01124	0.00064	0.01022	0.00102
GLU	100	A	H	113.95	6.69	15.5722	0.0002	2.2854	<0.0001	0.01202	0.00038	0.00767	0.00102
GLU	100	A	H	95.30	7.26	16.8156	0.0008	2.1175	0.0001	0.05504	0.00216	0.03505	0.00616
GLU	100	A	H	86.00	3.09	16.9966	0.0002	2.0951	<0.0001	0.00934	0.00056	0.00962	0.00064
GLU	100	A	H	867.29	23.16	17.2511	0.0004	2.0644	<0.0001	0.07808	0.00178	0.03995	0.00248
GLU	100	A	H	34.79	5.90	18.4817	0.0004	1.928	<0.0001	0.01523	0.00248	0.00688	0.00290
GLU	100	A	H	108.27	3.67	18.6259	0.0002	1.9132	<0.0001	0.01473	0.00030	0.01083	0.00076
GLU	100	A	H	156.82	3.00	18.9989	0.0000	1.876	0	0.01143	0.00046	0.01294	0.00044
GLU	100	A	H	827.93	245.00	19.5674	0.0004	1.822	<0.0001	0.04501	0.01854	0.00000	0.00000
GLU	100	A	H	39.51	1.75	19.9471	0.0016	1.7877	0.0001	0.00000	0.00000	0.08980	0.00710
GLU	100	A	H	23.59	2.42	21.9502	0.0004	1.6263	<0.0001	0.01335	0.00076	0.00931	0.00212
GLU	100	A	H	66.39	2.61	22.2527	0.0002	1.6044	<0.0001	0.01403	0.00046	0.01157	0.00092
GLU	100	A	H	13.88	2.75	23.533	0.0004	1.5183	<0.0001	0.01501	0.00144	0.00939	0.00440
GLU	100	A	H	13.57	3.00	23.6644	0.0008	1.51	0.0001	0.01976	0.00874	0.01699	0.00842
GLU	100	A	H	30.93	2.23	24.8175	0.0004	1.4408	<0.0001	0.01723	0.00084	0.01307	0.00198
GLU	100	A	H	21.29	2.88	25.1483	0.0004	1.4222	<0.0001	0.01738	0.00114	0.01132	0.00358
GLU	100	A	H	13.43	2.26	26.7281	0.0004	1.3395	<0.0001	0.01585	0.00130	0.01038	0.00404
GLU	100	A	H	20.76	2.01	27.6199	0.0004	1.2971	<0.0001	0.01688	0.00196	0.01423	0.00302
GLU	100	A	H	20.78	1.38	29.0183	0.0004	1.2358	<0.0001	0.01494	0.00154	0.01414	0.00192
GLU	100	A	H	20.27	1.94	31.1242	0.0004	1.154	<0.0001	0.01900	0.00182	0.01530	0.00326
GLU	100	A	H	18.18	2.00	34.3847	0.0004	1.0475	<0.0001	0.01721	0.00136	0.01271	0.00316
GLU	100	A	H	18.88	3.55	34.4661	0.0004	1.0451	<0.0001	0.01520	0.00232	0.00752	0.00348
GLU	100	A	H	70.67	3.95	34.8551	0.0190	1.0338	0.0005	0.00000	0.00000	0.53426	0.05924

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	A	D	311.94	3.76	9.212	0.0000	3.8555	0	0.00530	0.00022	0.00913	0.00016
GLU	100	A	D	34.42	1.79	9.9314	0.0004	3.5769	0.0001	0.03127	0.00098	0.02224	0.00244
GLU	100	A	D	58.06	2.59	10.783	0.0004	3.2951	0.0001	0.04414	0.00112	0.02967	0.00288
GLU	100	A	D	0.63	0.19	10.9063	0.0028	3.258	0.0008	0.00000	0.00000	0.01638	0.00698
GLU	100	A	D	779.44	4.12	11.7029	0.0002	3.0369	0.0001	0.00513	0.00010	0.00964	0.00006
GLU	100	A	D	16.15	0.80	12.4945	0.0002	2.8452	<0.0001	0.00701	0.00076	0.00896	0.00074
GLU	100	A	D	51.25	2.45	13.013	0.0008	2.7323	0.0002	0.05818	0.00168	0.04199	0.00436
GLU	100	A	D	106.27	1.80	14.2547	0.0000	2.4953	0	0.00626	0.00022	0.00857	0.00022
GLU	100	A	D	116.93	1.85	15.5724	0.0000	2.2853	0	0.00698	0.00026	0.01011	0.00024
GLU	100	A	D	150.30	2.10	16.9964	0.0000	2.0951	0	0.00654	0.00022	0.00956	0.00020
GLU	100	A	D	50.67	1.46	18.4816	0.0002	1.928	<0.0001	0.00818	0.00038	0.00945	0.00046
GLU	100	A	D	61.58	1.61	18.6245	0.0002	1.9134	<0.0001	0.00972	0.00042	0.01123	0.00050
GLU	100	A	D	92.64	1.81	18.9976	0.0002	1.8761	<0.0001	0.00902	0.00034	0.01138	0.00036
GLU	100	A	D	13.09	1.05	21.6569	0.0052	1.648	0.0004	0.07752	0.02150	0.09187	0.01524
GLU	100	A	D	184.88	2.25	21.9499	0.0002	1.6263	<0.0001	0.00710	0.00030	0.01089	0.00020
GLU	100	A	D	144.53	2.07	22.253	0.0000	1.6044	0	0.00662	0.00026	0.01013	0.00022
GLU	100	A	D	26.24	1.16	23.4176	0.0002	1.5256	<0.0001	0.01022	0.00070	0.01115	0.00086
GLU	100	A	D	23.85	1.15	23.5324	0.0002	1.5183	<0.0001	0.00890	0.00060	0.00942	0.00078
GLU	100	A	D	14.68	1.12	23.6636	0.0004	1.51	<0.0001	0.01250	0.00080	0.01065	0.00156
GLU	100	A	D	29.73	1.32	24.2571	0.0002	1.4736	<0.0001	0.00847	0.00040	0.00810	0.00064
GLU	100	A	D	38.52	1.35	24.8181	0.0002	1.4408	<0.0001	0.01052	0.00058	0.01195	0.00070
GLU	100	A	D	59.95	1.57	25.1419	0.0002	1.4225	<0.0001	0.00947	0.00042	0.01128	0.00048
GLU	100	A	D	13.89	1.00	26.3733	0.0002	1.3572	<0.0001	0.00928	0.00070	0.00849	0.00112
GLU	100	A	D	18.35	1.42	26.728	0.0002	1.3395	<0.0001	0.01194	0.00060	0.00894	0.00138
GLU	100	A	D	31.26	1.33	27.6184	0.0002	1.2971	<0.0001	0.01028	0.00056	0.01033	0.00076
GLU	100	A	D	25.30	1.17	28.7352	0.0002	1.2477	<0.0001	0.00887	0.00060	0.00952	0.00076
GLU	100	A	D	22.44	1.18	29.0184	0.0002	1.2358	<0.0001	0.01305	0.00086	0.01291	0.00122
GLU	100	A	D	19.08	1.12	30.4173	0.0002	1.1802	<0.0001	0.01182	0.00086	0.01162	0.00124
GLU	100	A	D	37.85	1.69	31.1237	0.0002	1.1541	<0.0001	0.01149	0.00042	0.00973	0.00082
GLU	100	A	D	18.76	1.62	31.4432	0.0002	1.1426	<0.0001	0.01268	0.00068	0.00874	0.00156
GLU	100	A	D	41.86	1.38	34.3842	0.0002	1.0475	<0.0001	0.00974	0.00062	0.01166	0.00064
GLU	100	A	D	28.04	1.41	34.4653	0.0002	1.0451	<0.0001	0.01184	0.00060	0.01099	0.00102
GLU	100	A	D	11.21	0.65	34.7877	0.0006	1.0357	<0.0001	0.00000	0.00000	0.02311	0.00196
GLU	100	A	W	501.04	6.30	9.2135	0.0000	3.8549	<0.0001	0.00474	0.00030	0.00986	0.00018
GLU	100	A	W	4687.27	112.99	11.7049	0.0002	3.0364	0.0001	0.00504	0.00056	0.01063	0.00034
GLU	100	A	W	930.97	153.14	11.7082	0.0002	3.0355	0.0001	0.00000	0.00000	0.00607	0.00070
GLU	100	A	W	60.15	1.95	12.4947	0.0002	2.8451	<0.0001	0.00647	0.00110	0.01108	0.00060
GLU	100	A	W	16.15	1.53	12.6026	0.0002	2.8209	<0.0001	0.00790	0.00144	0.00830	0.00154
GLU	100	A	W	621.30	11.58	14.2564	0.0002	2.495	<0.0001	0.00635	0.00042	0.01118	0.00026
GLU	100	A	W	1103.76	16.31	15.5719	0.0000	2.2854	<0.0001	0.00590	0.00036	0.01101	0.00022
GLU	100	A	W	906.74	79.27	16.9979	0.0002	2.0949	<0.0001	0.00535	0.00204	0.01148	0.00070
GLU	100	A	W	593.72	21.38	18.4811	0.0002	1.9281	<0.0001	0.00788	0.00088	0.01208	0.00066
GLU	100	A	W	1044.22	25.40	18.623	0.0002	1.9135	<0.0001	0.00717	0.00082	0.01385	0.00048
GLU	100	A	W	927.09	17.95	18.9999	0.0002	1.8759	<0.0001	0.00727	0.00048	0.01178	0.00034
GLU	100	A	W	203.10	6.63	21.9517	0.0002	1.6261	<0.0001	0.00921	0.00072	0.01189	0.00064
GLU	100	A	W	694.07	15.00	22.252	0.0002	1.6045	<0.0001	0.00756	0.00062	0.01267	0.00042
GLU	100	A	W	43.18	2.48	22.4891	0.0002	1.5878	<0.0001	0.00756	0.00184	0.01112	0.00114
GLU	100	A	W	54.76	19.52	23.4123	0.0004	1.526	<0.0001	0.00000	0.00000	0.00496	0.00252
GLU	100	A	W	368.98	6.72	23.4172	0.0000	1.5257	<0.0001	0.00705	0.00052	0.01182	0.00032
GLU	100	A	W	129.10	4.20	23.5285	0.0002	1.5186	<0.0001	0.00621	0.00138	0.01218	0.00064
GLU	100	A	W	139.40	4.63	23.6613	0.0002	1.5101	<0.0001	0.00827	0.00114	0.01272	0.00070
GLU	100	A	W	105.93	3.43	24.2569	0.0002	1.4736	<0.0001	0.01021	0.00090	0.01311	0.00074
GLU	100	A	W	436.29	15.65	24.8197	0.0002	1.4407	<0.0001	0.00973	0.00070	0.01200	0.00070
GLU	100	A	W	242.16	21.69	25.1362	0.0018	1.4228	0.0001	0.00000	0.00000	0.01515	0.00134
GLU	100	A	W	114.13	11.15	25.1418	0.0006	1.4225	<0.0001	0.00652	0.00172	0.01691	0.00286
GLU	100	A	W	78.10	2.88	26.3715	0.0002	1.3573	<0.0001	0.00812	0.00140	0.01309	0.00080
GLU	100	A	W	102.56	6.04	26.7263	0.0004	1.3396	<0.0001	0.01041	0.00148	0.01281	0.00132
GLU	100	A	W	158.68	5.91	27.6162	0.0002	1.2972	<0.0001	0.01251	0.00062	0.01258	0.00086
GLU	100	A	W	40.63	3.27	27.8774	0.0004	1.2853	<0.0001	0.01217	0.00232	0.01372	0.00208
GLU	100	A	W	55.82	5.33	28.7345	0.0004	1.2477	<0.0001	0.01174	0.00146	0.01095	0.00208
GLU	100	A	W	104.58	5.44	29.0156	0.0002	1.2359	<0.0001	0.00989	0.00166	0.01284	0.00120
GLU	100	A	W	25.99	2.45	30.2363	0.0004	1.1871	<0.0001	0.01080	0.00262	0.01375	0.00196
GLU	100	A	W	120.34	4.79	30.4138	0.0002	1.1803	<0.0001	0.01121	0.00046	0.01006	0.00076
GLU	100	A	W	10.58	3.60	30.5917	0.0012	1.1736	<0.0001	0.01677	0.00298	0.00000	0.00000
GLU	100	A	W	292.84	6.47	31.1227	0.0002	1.1541	<0.0001	0.01355	0.00044	0.01410	0.00056
GLU	100	A	W	119.05	4.07	31.4409	0.0002	1.1427	<0.0001	0.01071	0.00086	0.01273	0.00078
GLU	100	A	W	20.15	2.29	31.9451	0.0004	1.1251	<0.0001	0.00966	0.00438	0.01270	0.00284
GLU	100	A	W	49.02	3.54	33.9002	0.0004	1.062	<0.0001	0.01048	0.00334	0.01476	0.00202
GLU	100	A	W	150.57	6.27	34.3817	0.0002	1.0476	<0.0001	0.01259	0.00084	0.01288	0.00100
GLU	100	A	W	190.74	6.06	34.4624	0.0002	1.0452	<0.0001	0.01152	0.00098	0.01469	0.00082
GLU	100	A	W	57.56	3.82	34.7864	0.0006	1.0357	<0.0001	0.01383	0.00614	0.02323	0.00288
GLU	100	A	W	8.48	2.18	35.2157	0.0016	1.0235	<0.0001	0.00000	0.00000	0.01895	0.00982
GLU	100	A	W	151.34	5.74	35.6167	0.0002	1.0123	<0.0001	0.01213	0.00094	0.01380	0.00094
GLU	100	A	W	67.01	3.74	36.6397	0.0002	0.985	<0.0001	0.01327	0.00132	0.01379	0.00148
GLU	100	A	W	24.21	2.98	36.7927	0.0006	0.9811	<0.0001	0.01323	0.00232	0.01213	0.00310
GLU	100	A	W	50.29	3.35	36.9444	0.0004	0.9772	<0.0001	0.01378	0.00192	0.01484	0.00192
GLU	100	A	W	43.89	2.99	37.392	0.0004	0.9659	<0.0001	0.01214	0.00342	0.01628	0.00214
GLU	100	A	W	92.74	4.56	37.466	0.0002	0.964	<0.0001	0.01561	0.00116	0.01534	0.00148
GLU	100	A	W	17.77	2.77	37.7635	0.0006	0.9567	<0.0001	0.01429	0.00332	0.01310	0.00432

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	A	W	14.28	2.32	37.9468	0.0008	0.9523	<0.0001	0.01231	0.00484	0.01309	0.00438
GLU	100	A	W	118.30	4.52	38.325	0.0002	0.9432	<0.0001	0.01231	0.00074	0.01271	0.00090
GLU	100	A	W	44.60	2.88	38.5427	0.0004	0.9381	<0.0001	0.01243	0.00316	0.01667	0.00206
GLU	100	B	H	144.81	5.04	8.3866	0.0002	4.2342	0.0001	0.02960	0.00064	0.02008	0.00146
GLU	100	B	H	834.67	11.39	9.9333	0.0002	3.5762	0.0001	0.04462	0.00040	0.02969	0.00084
GLU	100	B	H	1396.49	14.57	10.7848	0.0002	3.2946	0.0001	0.05641	0.00040	0.03782	0.00080
GLU	100	B	H	88.32	2.64	11.7032	0.0002	3.0368	0.0001	0.01022	0.00038	0.00991	0.00056
GLU	100	B	H	33.83	0.15	11.9449	0.0136	2.9756	0.0034	0.00962	0.00004	0.00012	0.00000
GLU	100	B	H	1474.32	65.89	13.014	0.0002	2.7321	<0.0001	0.05870	0.00304	0.02154	0.00252
GLU	100	B	H	108.94	9.28	16.8166	0.0006	2.1173	0.0001	0.04316	0.00290	0.02218	0.00456
GLU	100	B	H	955.78	15.63	17.2496	0.0002	2.0646	<0.0001	0.07139	0.00082	0.04240	0.00152
GLU	100	B	H	22.95	1.98	18.999	0.0004	1.876	<0.0001	0.01141	0.00158	0.01078	0.00194
GLU	100	B	H	359.68	9.24	19.205	0.0006	1.856	0.0001	0.10616	0.00196	0.08123	0.00454
GLU	100	B	H	914.27	244.66	19.5677	0.0004	1.822	<0.0001	0.04308	0.01568	0.00000	0.00000
GLU	100	B	H	46.79	2.83	19.9445	0.0014	1.7879	0.0001	0.00000	0.00000	0.08436	0.00782
GLU	100	B	H	18.87	2.87	20.3839	0.0040	1.7497	0.0003	0.07560	0.04436	0.08917	0.02970
GLU	100	B	H	15.92	4.26	20.8488	0.0102	1.7111	0.0008	0.00000	0.00000	0.15265	0.09366
GLU	100	B	H	17.29	0.82	29.3536	0.0258	1.222	0.0011	0.04558	0.00598	0.00310	0.00000
GLU	100	B	D	242.83	2.85	9.2114	0.0002	3.8558	0.0001	0.00579	0.00024	0.00983	0.00016
GLU	100	B	D	2246.38	8.44	11.7019	0.0002	3.0372	0.0001	0.00660	0.00006	0.01048	0.00006
GLU	100	B	D	32.22	3.59	12.4945	0.0010	2.8452	0.0002	0.00567	0.00340	0.01020	0.00122
GLU	100	B	D	474.92	4.00	14.2544	0.0000	2.4954	0	0.00628	0.00016	0.01028	0.00012
GLU	100	B	D	659.28	4.93	15.5715	0.0000	2.2855	0	0.00710	0.00012	0.01024	0.00012
GLU	100	B	D	640.23	4.71	16.9961	0.0000	2.0951	0	0.00669	0.00014	0.01031	0.00012
GLU	100	B	D	175.87	3.53	18.4809	0.0000	1.9281	0	0.01020	0.00022	0.00989	0.00036
GLU	100	B	D	558.33	5.25	18.6229	0.0000	1.9135	0	0.00922	0.00014	0.01051	0.00016
GLU	100	B	D	734.74	5.67	18.9968	0.0000	1.8762	0	0.00871	0.00012	0.01068	0.00014
GLU	100	B	D	149.39	0.92	21.9501	0.0000	1.6263	0	0.00947	0.00002	0.01070	0.00002
GLU	100	B	D	487.27	4.62	22.2518	0.0000	1.6045	0	0.00858	0.00016	0.01088	0.00016
GLU	100	B	D	32.56	1.81	22.4893	0.0002	1.5878	<0.0001	0.01019	0.00070	0.00960	0.00102
GLU	100	B	D	274.78	3.34	23.4175	0.0000	1.5256	0	0.00794	0.00026	0.01150	0.00022
GLU	100	B	D	112.05	2.31	23.5311	0.0000	1.5184	0	0.00778	0.00048	0.01088	0.00036
GLU	100	B	D	98.98	2.50	23.662	0.0002	1.5101	<0.0001	0.01017	0.00044	0.01141	0.00050
GLU	100	B	D	98.38	2.56	24.2567	0.0002	1.4736	<0.0001	0.00997	0.00038	0.01051	0.00048
GLU	100	B	D	305.93	3.89	24.8179	0.0000	1.4408	0	0.00917	0.00020	0.01087	0.00022
GLU	100	B	D	106.73	2.64	25.142	0.0002	1.4225	<0.0001	0.01097	0.00042	0.01195	0.00052
GLU	100	B	D	62.77	2.02	26.3733	0.0002	1.3572	<0.0001	0.00926	0.00056	0.01051	0.00060
GLU	100	B	D	77.74	2.53	26.7262	0.0002	1.3396	<0.0001	0.01090	0.00040	0.01034	0.00062
GLU	100	B	D	152.02	3.37	27.618	0.0000	1.2971	0	0.01108	0.00026	0.01058	0.00042
GLU	100	B	D	26.07	1.82	27.8759	0.0002	1.2854	<0.0001	0.01175	0.00082	0.01022	0.00142
GLU	100	B	D	65.68	2.14	28.7349	0.0002	1.2477	<0.0001	0.01036	0.00058	0.01137	0.00066
GLU	100	B	D	96.55	2.70	29.017	0.0002	1.2359	<0.0001	0.01159	0.00042	0.01161	0.00058
GLU	100	B	D	25.18	2.04	30.2371	0.0002	1.1871	<0.0001	0.01166	0.00066	0.00907	0.00152
GLU	100	B	D	105.62	3.00	30.4165	0.0002	1.1802	<0.0001	0.01107	0.00032	0.01026	0.00054
GLU	100	B	D	284.91	4.40	31.1247	0.0000	1.154	0	0.01142	0.00020	0.01115	0.00030
GLU	100	B	D	99.41	2.78	31.4431	0.0002	1.1426	<0.0001	0.01187	0.00042	0.01181	0.00060
GLU	100	B	D	22.58	2.54	31.9443	0.0004	1.1252	<0.0001	0.01353	0.00090	0.00872	0.00216
GLU	100	B	D	49.67	2.88	33.8983	0.0002	1.062	<0.0001	0.01393	0.00050	0.01011	0.00122
GLU	100	B	D	127.15	3.16	34.3846	0.0002	1.0475	<0.0001	0.01138	0.00034	0.01104	0.00050
GLU	100	B	D	169.06	3.43	34.4647	0.0000	1.0451	0	0.01085	0.00028	0.01107	0.00040
GLU	100	B	D	52.85	15.16	34.7875	0.0010	1.0357	<0.0001	0.01867	0.00524	0.00000	0.00000
GLU	100	B	W	443.66	10.06	9.2133	0.0002	3.8550	0.0001	0.00416	0.00064	0.00999	0.00030
GLU	100	B	W	2947.15	119.63	11.7043	0.0004	3.0365	0.0001	0.00464	0.00056	0.01087	0.00028
GLU	100	B	W	56.18	1.56	12.495	0.0002	2.8451	<0.0001	0.00544	0.00082	0.00943	0.00044
GLU	100	B	W	7.88	1.37	12.6019	0.0006	2.8210	0.0001	0.01090	0.00140	0.00845	0.00316
GLU	100	B	W	558.29	8.37	14.2553	0.0000	2.4952	<0.0001	0.00549	0.00040	0.01092	0.00024
GLU	100	B	W	213.21	95.99	15.5681	0.0010	2.2860	0.0001	0.00516	0.00288	0.00451	0.00128
GLU	100	B	W	1192.03	24.28	15.5713	0.0002	2.2855	<0.0001	0.00565	0.00046	0.01055	0.00030
GLU	100	B	W	987.08	17.01	16.9978	0.0000	2.0949	<0.0001	0.00461	0.00050	0.01048	0.00024
GLU	100	B	W	410.84	15.66	18.4819	0.0002	1.928	<0.0001	0.00513	0.00160	0.01204	0.00070
GLU	100	B	W	653.90	19.42	18.6243	0.0002	1.9134	<0.0001	0.00600	0.00096	0.01187	0.00052
GLU	100	B	W	960.06	11.54	18.9996	0.0000	1.8759	<0.0001	0.00702	0.00030	0.01192	0.00022
GLU	100	B	W	1.07	0.38	21.9182	0.0016	1.6286	0.0001	0.00000	0.00000	0.00795	0.00430
GLU	100	B	W	208.99	4.13	21.9516	0.0002	1.6262	<0.0001	0.00803	0.00044	0.01104	0.00036
GLU	100	B	W	473.79	14.58	22.2521	0.0002	1.6045	<0.0001	0.00741	0.00084	0.01197	0.00056
GLU	100	B	W	50.49	2.84	22.4898	0.0002	1.5877	<0.0001	0.00781	0.00144	0.01043	0.00104
GLU	100	B	W	366.74	17.46	23.4172	0.0002	1.5257	<0.0001	0.00741	0.00106	0.01105	0.00082
GLU	100	B	W	160.94	12.32	23.5293	0.0004	1.5185	<0.0001	0.00752	0.00194	0.01105	0.00136
GLU	100	B	W	134.01	12.51	23.6601	0.0004	1.5102	<0.0001	0.00807	0.00158	0.00961	0.00154
GLU	100	B	W	81.45	2.56	24.2571	0.0002	1.4736	<0.0001	0.00807	0.00118	0.01282	0.00068
GLU	100	B	W	427.73	13.26	24.8193	0.0002	1.4407	<0.0001	0.00773	0.00084	0.01219	0.00058
GLU	100	B	W	204.04	10.99	25.1419	0.0002	1.4225	<0.0001	0.00701	0.00114	0.01554	0.00140
GLU	100	B	W	63.50	2.32	26.3717	0.0002	1.3573	<0.0001	0.00555	0.00260	0.01318	0.00084
GLU	100	B	W	88.11	5.16	26.7275	0.0002	1.3395	<0.0001	0.00996	0.00158	0.01231	0.00132
GLU	100	B	W	131.33	4.00	27.6173	0.0002	1.2972	<0.0001	0.00908	0.00100	0.01290	0.00068
GLU	100	B	W	39.21	2.22	27.8773	0.0004	1.2853	<0.0001	0.00814	0.00258	0.01277	0.00134
GLU	100	B	W	96.47	5.42	28.7343	0.0002	1.2478	<0.0001	0.00941	0.00140	0.01159	0.00118
GLU	100	B	W	110.03	4.78	29.017	0.0002	1.2359	<0.0001	0.00770	0.00212	0.01365	0.00100
GLU	100	B	W	29.53	1.92	30.2359	0.0002	1.1871	<0.0001	0.00762	0.00344	0.01280	0.00156

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	B	W	154.61	3.37	30.4149	0.0002	1.1803	<0.0001	0.00863	0.00070	0.01264	0.00046
GLU	100	B	W	16.51	2.26	30.5928	0.0004	1.1736	<0.0001	0.00979	0.00158	0.00860	0.00248
GLU	100	B	W	247.64	5.32	31.1233	0.0002	1.1541	<0.0001	0.00970	0.00062	0.01305	0.00048
GLU	100	B	W	98.81	3.72	31.4412	0.0002	1.1427	<0.0001	0.00975	0.00126	0.01339	0.00090
GLU	100	B	W	35.15	3.11	31.947	0.0004	1.1251	<0.0001	0.01068	0.00152	0.00709	0.00172
GLU	100	B	W	55.40	3.06	33.9012	0.0002	1.062	<0.0001	0.00835	0.00142	0.01062	0.00108
GLU	100	B	W	150.04	4.37	34.3828	0.0002	1.0475	<0.0001	0.00950	0.00092	0.01304	0.00066
GLU	100	B	W	155.69	4.76	34.4636	0.0002	1.0451	<0.0001	0.01071	0.00066	0.01226	0.00068
GLU	100	B	W	127.27	10.08	34.4651	0.0008	1.0451	<0.0001	0.00919	0.00122	0.00908	0.00090
GLU	100	B	W	54.35	3.57	34.7862	0.0004	1.0357	<0.0001	0.01757	0.00310	0.02023	0.00260
GLU	100	B	W	13.63	4.45	35.217	0.0008	1.0235	<0.0001	0.01206	0.00264	0.01012	0.00362
GLU	100	B	W	132.54	4.73	35.6166	0.0002	1.0123	<0.0001	0.01267	0.00072	0.01314	0.00086
GLU	100	B	W	80.35	3.79	36.6412	0.0002	0.985	<0.0001	0.01099	0.00146	0.01121	0.00114
GLU	100	B	W	24.28	2.80	36.7907	0.0006	0.9811	<0.0001	0.00867	0.00104	0.01028	0.00198
GLU	100	B	W	36.51	2.92	36.9456	0.0002	0.9771	<0.0001	0.01349	0.00060	0.00910	0.00160
GLU	100	B	W	41.01	4.03	37.392	0.0004	0.9659	<0.0001	0.01351	0.00150	0.01176	0.00242
GLU	100	B	W	8.62	3.72	37.3987	0.0008	0.9657	<0.0001	0.00724	0.00206	0.00000	0.00000
GLU	100	B	W	108.67	5.89	37.4672	0.0002	0.964	<0.0001	0.01507	0.00064	0.01219	0.00134
GLU	100	B	W	21.70	2.72	37.9487	0.0006	0.9522	<0.0001	0.01197	0.00296	0.01224	0.00312
GLU	100	B	W	112.14	4.21	38.3273	0.0002	0.9432	<0.0001	0.01055	0.00080	0.01194	0.00080
GLU	100	B	W	59.57	3.34	38.542	0.0002	0.9381	<0.0001	0.01123	0.00152	0.01292	0.00134
GLU	100	C	H	107.85	5.12	8.3865	0.0004	4.2342	0.0002	0.03242	0.00092	0.02033	0.00212
GLU	100	C	H	78.12	0.75	9.2107	0.0002	3.8561	0.0001	0.00941	0.00034	0.01026	0.00002
GLU	100	C	H	611.51	7.87	9.933	0.0002	3.5763	0.0001	0.04466	0.00026	0.02893	0.00078
GLU	100	C	H	1027.58	12.15	10.7845	0.0002	3.2946	0.0001	0.05827	0.00046	0.03935	0.00094
GLU	100	C	H	1069.53	6.68	11.7026	0.0000	3.037	0	0.00860	0.00010	0.01031	0.00010
GLU	100	C	H	15.84	1.13	12.4959	0.0004	2.8449	0.0001	0.00761	0.00458	0.01391	0.00186
GLU	100	C	H	1095.09	46.01	13.0141	0.0002	2.732	<0.0001	0.06304	0.00302	0.02363	0.00254
GLU	100	C	H	108.50	2.62	14.2533	0.0002	2.4956	<0.0001	0.01032	0.00036	0.01077	0.00046
GLU	100	C	H	196.99	5.49	15.5718	0.0000	2.2854	0	0.01192	0.00024	0.00912	0.00052
GLU	100	C	H	79.21	5.92	16.8167	0.0006	2.1173	0.0001	0.04923	0.00202	0.03029	0.00522
GLU	100	C	H	163.47	2.85	16.996	0.0000	2.0951	0	0.00870	0.00046	0.01180	0.00034
GLU	100	C	H	723.11	18.19	17.2492	0.0002	2.0646	<0.0001	0.06710	0.00148	0.03403	0.00202
GLU	100	C	H	58.49	3.18	18.4819	0.0002	1.928	<0.0001	0.01412	0.00046	0.01018	0.00116
GLU	100	C	H	210.39	3.75	18.6267	0.0000	1.9131	0	0.01282	0.00030	0.01289	0.00042
GLU	100	C	H	223.48	3.78	18.9986	0.0000	1.876	0	0.01179	0.00032	0.01252	0.00038
GLU	100	C	H	294.13	4.90	19.2052	0.0008	1.856	0.0001	0.04280	0.00084	0.00753	0.00020
GLU	100	C	H	32.82	1.78	19.9435	0.0016	1.788	0.0001	0.00000	0.00000	0.07840	0.00780
GLU	100	C	H	43.64	1.92	21.9501	0.0002	1.6263	<0.0001	0.01091	0.00124	0.01279	0.00106
GLU	100	C	H	103.86	3.03	22.2519	0.0002	1.6045	<0.0001	0.01306	0.00040	0.01184	0.00066
GLU	100	C	H	64.40	3.06	23.4179	0.0002	1.5256	<0.0001	0.01284	0.00040	0.00976	0.00096
GLU	100	C	H	38.62	3.16	23.5337	0.0002	1.5182	<0.0001	0.01264	0.00056	0.00859	0.00154
GLU	100	C	H	34.52	4.42	23.6651	0.0004	1.5099	<0.0001	0.01550	0.00096	0.01000	0.00298
GLU	100	C	H	71.18	2.38	24.8174	0.0002	1.4408	<0.0001	0.01334	0.00062	0.01320	0.00082
GLU	100	C	H	34.63	2.55	25.1476	0.0004	1.4222	<0.0001	0.01825	0.00128	0.01496	0.00234
GLU	100	C	H	15.50	1.82	26.3748	0.0004	1.3571	<0.0001	0.01298	0.00236	0.01191	0.00296
GLU	100	C	H	24.39	2.25	26.7293	0.0004	1.3394	<0.0001	0.01731	0.00230	0.01535	0.00304
GLU	100	C	H	35.56	2.23	27.6201	0.0002	1.297	<0.0001	0.01421	0.00134	0.01339	0.00172
GLU	100	C	H	16.01	1.99	28.7348	0.0004	1.2477	<0.0001	0.01200	0.00084	0.00835	0.00226
GLU	100	C	H	31.32	1.80	29.0214	0.0002	1.2357	<0.0001	0.01743	0.00078	0.01380	0.00166
GLU	100	C	H	37.03	3.22	30.4198	0.0002	1.1801	<0.0001	0.01571	0.00100	0.00859	0.00176
GLU	100	C	H	64.49	2.96	31.1242	0.0002	1.154	<0.0001	0.01475	0.00038	0.01005	0.00100
GLU	100	C	H	29.15	6.59	31.444	0.0004	1.1426	<0.0001	0.01596	0.00328	0.00719	0.00420
GLU	100	C	H	28.32	1.71	34.3849	0.0002	1.0475	<0.0001	0.01500	0.00082	0.01231	0.00156
GLU	100	C	H	35.30	2.40	34.4661	0.0002	1.0451	<0.0001	0.01606	0.00060	0.01078	0.00162
GLU	100	C	H	23.12	2.85	34.7913	0.0006	1.0356	<0.0001	0.02466	0.00176	0.01478	0.00426
GLU	100	C	D	37.27	3.52	8.3871	0.0006	4.2339	0.0003	0.02952	0.00202	0.01666	0.00360
GLU	100	C	D	199.05	2.60	9.2109	0.0000	3.856	0	0.00754	0.00024	0.01046	0.00022
GLU	100	C	D	201.92	7.06	9.9329	0.0002	3.5763	0.0001	0.03786	0.00098	0.02173	0.00168
GLU	100	C	D	346.53	9.27	10.7842	0.0002	3.2947	0.0001	0.05076	0.00104	0.02892	0.00172
GLU	100	C	D	1696.82	7.46	11.7021	0.0000	3.0371	0	0.00845	0.00006	0.01096	0.00008
GLU	100	C	D	368.24	73.74	13.0139	0.0004	2.7321	0.0001	0.04517	0.01192	0.01229	0.00672
GLU	100	C	D	685.31	4.64	14.2547	0.0000	2.4953	0	0.00724	0.00012	0.01035	0.00010
GLU	100	C	D	448.34	4.39	15.5712	0.0000	2.2855	0	0.00941	0.00016	0.01120	0.00018
GLU	100	C	D	428.02	3.79	16.9959	0.0000	2.0952	0	0.00788	0.00022	0.01175	0.00016
GLU	100	C	D	239.49	11.28	17.2485	0.0004	2.0647	<0.0001	0.05795	0.00230	0.02922	0.00330
GLU	100	C	D	136.88	2.88	18.4807	0.0002	1.9281	<0.0001	0.01233	0.00034	0.01245	0.00048
GLU	100	C	D	245.80	3.64	18.6237	0.0000	1.9134	0	0.01203	0.00024	0.01241	0.00032
GLU	100	C	D	525.26	4.63	18.9983	0.0000	1.876	0	0.01025	0.00018	0.01246	0.00018
GLU	100	C	D	100.47	9.96	19.2053	0.0012	1.856	0.0001	0.10074	0.00754	0.05166	0.01262
GLU	100	C	D	231.29	14.47	19.5683	0.0006	1.8219	0.0001	0.08440	0.00478	0.03958	0.00612
GLU	100	C	D	144.14	2.84	21.9502	0.0000	1.6263	0	0.01074	0.00032	0.01141	0.00040
GLU	100	C	D	284.28	3.85	22.2517	0.0000	1.6045	0	0.01195	0.00022	0.01238	0.00030
GLU	100	C	D	221.16	3.06	23.418	0.0000	1.5256	0	0.00993	0.00030	0.01235	0.00028
GLU	100	C	D	102.16	2.32	23.5305	0.0002	1.5184	<0.0001	0.00949	0.00040	0.01080	0.00044
GLU	100	C	D	61.15	2.80	23.6636	0.0002	1.51	<0.0001	0.01325	0.00038	0.00983	0.00092
GLU	100	C	D	67.39	3.01	24.2568	0.0002	1.4736	<0.0001	0.01240	0.00064	0.01073	0.00098
GLU	100	C	D	273.23	3.58	24.8182	0.0000	1.4408	0	0.01157	0.00022	0.01267	0.00028
GLU	100	C	D	36.59	1.97	25.1447	0.0002	1.4224	<0.0001	0.01547	0.00090	0.01379	0.00148

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	C	D	37.71	1.50	26.3732	0.0002	1.3572	<0.0001	0.01123	0.00098	0.01236	0.00094
GLU	100	C	D	60.61	1.95	26.7261	0.0002	1.3396	<0.0001	0.01299	0.00062	0.01274	0.00080
GLU	100	C	D	76.36	2.07	27.6181	0.0002	1.2971	<0.0001	0.01390	0.00058	0.01399	0.00072
GLU	100	C	D	21.24	4.86	27.8757	0.0004	1.2854	<0.0001	0.01737	0.00242	0.00917	0.00522
GLU	100	C	D	75.64	2.45	28.7342	0.0002	1.2478	<0.0001	0.01083	0.00024	0.00838	0.00054
GLU	100	C	D	33.34	1.48	29.0168	0.0002	1.2359	<0.0001	0.01511	0.00126	0.01577	0.00136
GLU	100	C	D	21.67	1.24	30.2362	0.0002	1.1871	<0.0001	0.01168	0.00156	0.01292	0.00144
GLU	100	C	D	47.51	2.68	30.4168	0.0002	1.1802	<0.0001	0.01522	0.00050	0.00989	0.00122
GLU	100	C	D	188.24	3.43	31.1231	0.0000	1.1541	0	0.01442	0.00022	0.01219	0.00042
GLU	100	C	D	58.69	2.91	31.443	0.0002	1.1426	<0.0001	0.01441	0.00054	0.01094	0.00118
GLU	100	C	D	22.60	1.53	31.9445	0.0002	1.1252	<0.0001	0.01482	0.00094	0.01233	0.00172
GLU	100	C	D	22.64	3.19	33.9007	0.0004	1.062	<0.0001	0.01762	0.00156	0.00999	0.00330
GLU	100	C	D	94.20	2.77	34.3847	0.0002	1.0475	<0.0001	0.01282	0.00044	0.01186	0.00066
GLU	100	C	D	87.50	2.69	34.464	0.0002	1.0451	<0.0001	0.01273	0.00048	0.01190	0.00070
GLU	100	C	D	19.55	1.66	34.7863	0.0008	1.0357	<0.0001	0.02244	0.00638	0.02626	0.00462
GLU	100	C	W	498.24	5.89	9.2129	0.0000	3.8551	<0.0001	0.00488	0.00028	0.00997	0.00016
GLU	100	C	W	3195.49	33.42	11.7038	0.0000	3.0367	<0.0001	0.00513	0.00024	0.01070	0.00016
GLU	100	C	W	31.87	7.54	12.4906	0.0018	2.8461	0.0004	0.00000	0.00000	0.00802	0.00184
GLU	100	C	W	65.74	1.71	12.4934	0.0002	2.8454	<0.0001	0.00599	0.00080	0.01047	0.00044
GLU	100	C	W	27.40	7.80	12.4971	0.0014	2.8446	0.0003	0.00639	0.00114	0.00518	0.00298
GLU	100	C	W	12.62	0.91	12.6025	0.0002	2.8209	<0.0001	0.00944	0.00128	0.00972	0.00138
GLU	100	C	W	734.75	9.77	14.2556	0.0000	2.4952	<0.0001	0.00575	0.00028	0.01019	0.00020
GLU	100	C	W	931.04	13.07	15.5717	0.0002	2.2854	<0.0001	0.00623	0.00022	0.01078	0.00012
GLU	100	C	W	1051.85	12.05	16.9982	0.0000	2.0949	<0.0001	0.00474	0.00034	0.01082	0.00018
GLU	100	C	W	397.54	11.21	18.4807	0.0002	1.9281	<0.0001	0.00554	0.00112	0.01179	0.00050
GLU	100	C	W	956.83	17.69	18.6234	0.0000	1.9135	<0.0001	0.00678	0.00044	0.01114	0.00030
GLU	100	C	W	908.30	11.79	18.9996	0.0000	1.8759	<0.0001	0.00807	0.00024	0.01104	0.00022
GLU	100	C	W	238.34	6.11	21.9515	0.0002	1.6262	<0.0001	0.00794	0.00058	0.01114	0.00046
GLU	100	C	W	541.79	12.87	22.2523	0.0002	1.6044	<0.0001	0.00799	0.00036	0.01189	0.00032
GLU	100	C	W	39.86	1.23	22.4897	0.0002	1.5877	<0.0001	0.00692	0.00142	0.01231	0.00066
GLU	100	C	W	333.16	5.40	23.4172	0.0000	1.5257	<0.0001	0.00712	0.00042	0.01150	0.00028
GLU	100	C	W	82.21	3.36	23.5301	0.0002	1.5184	<0.0001	0.00813	0.00096	0.01075	0.00076
GLU	100	C	W	72.87	32.63	23.6582	0.0014	1.5103	0.0001	0.00681	0.00150	0.00773	0.00234
GLU	100	C	W	157.22	3.96	23.6612	0.0002	1.5102	<0.0001	0.00734	0.00084	0.01225	0.00050
GLU	100	C	W	164.95	4.30	24.2573	0.0002	1.4736	<0.0001	0.00951	0.00050	0.01133	0.00050
GLU	100	C	W	431.43	10.05	24.8199	0.0002	1.4407	<0.0001	0.00758	0.00072	0.01280	0.00046
GLU	100	C	W	321.89	11.18	24.8204	0.0002	1.4407	<0.0001	0.00000	0.00000	0.01162	0.00056
GLU	100	C	W	102.53	3.24	25.1414	0.0002	1.4226	<0.0001	0.00998	0.00096	0.01345	0.00074
GLU	100	C	W	8.86	1.44	26.3668	0.0004	1.3575	<0.0001	0.00000	0.00000	0.00553	0.00112
GLU	100	C	W	72.40	2.93	26.3724	0.0004	1.3572	<0.0001	0.00905	0.00058	0.01228	0.00064
GLU	100	C	W	94.20	3.76	26.7276	0.0002	1.3395	<0.0001	0.01026	0.00074	0.01133	0.00082
GLU	100	C	W	181.15	5.46	27.6169	0.0002	1.2972	<0.0001	0.00901	0.00090	0.01301	0.00064
GLU	100	C	W	41.02	2.43	27.8771	0.0002	1.2853	<0.0001	0.01070	0.00088	0.01038	0.00120
GLU	100	C	W	71.07	2.51	28.7354	0.0002	1.2477	<0.0001	0.00670	0.00238	0.01413	0.00084
GLU	100	C	W	156.68	3.25	29.0192	0.0002	1.2358	<0.0001	0.00568	0.00150	0.01533	0.00050
GLU	100	C	W	34.34	2.18	30.2363	0.0002	1.1871	<0.0001	0.01188	0.00064	0.00972	0.00126
GLU	100	C	W	126.89	3.24	30.415	0.0002	1.1803	<0.0001	0.01054	0.00040	0.01235	0.00040
GLU	100	C	W	14.08	1.31	30.5934	0.0004	1.1736	<0.0001	0.01267	0.00140	0.01112	0.00218
GLU	100	C	W	346.21	5.32	31.1235	0.0000	1.1541	<0.0001	0.00965	0.00042	0.01351	0.00034
GLU	100	C	W	163.07	24.35	31.1274	0.0008	1.1539	<0.0001	0.00893	0.00046	0.00715	0.00142
GLU	100	C	W	129.49	3.80	31.4404	0.0002	1.1427	<0.0001	0.00983	0.00064	0.01180	0.00060
GLU	100	C	W	27.46	2.02	31.9449	0.0004	1.1251	<0.0001	0.01160	0.00128	0.01125	0.00166
GLU	100	C	W	44.33	2.87	33.9007	0.0002	1.062	<0.0001	0.01219	0.00116	0.01177	0.00150
GLU	100	C	W	164.98	3.88	34.3827	0.0002	1.0475	<0.0001	0.00787	0.00042	0.01175	0.00048
GLU	100	C	W	51.95	8.48	34.3879	0.0006	1.0474	<0.0001	0.00773	0.00088	0.00486	0.00172
GLU	100	C	W	172.56	8.43	34.4628	0.0004	1.0452	<0.0001	0.01099	0.00052	0.01265	0.00048
GLU	100	C	W	54.77	3.12	34.786	0.0004	1.0357	<0.0001	0.01955	0.00210	0.02030	0.00226
GLU	100	C	W	15.68	2.05	35.2162	0.0006	1.0235	<0.0001	0.01285	0.00328	0.01307	0.00352
GLU	100	C	W	181.46	3.21	35.6181	0.0000	1.0123	<0.0001	0.01180	0.00034	0.01281	0.00040
GLU	100	C	W	103.37	3.62	36.6393	0.0002	0.985	<0.0001	0.01156	0.00094	0.01352	0.00086
GLU	100	C	W	14.02	1.97	36.7935	0.0008	0.981	<0.0001	0.01240	0.00652	0.01551	0.00442
GLU	100	C	W	36.31	4.84	36.9456	0.0004	0.9771	<0.0001	0.01488	0.00128	0.01190	0.00240
GLU	100	C	W	62.13	3.01	37.3922	0.0002	0.9659	<0.0001	0.01003	0.00080	0.01340	0.00122
GLU	100	C	W	142.59	4.77	37.4664	0.0002	0.964	<0.0001	0.01215	0.00046	0.01146	0.00072
GLU	100	C	W	16.92	2.45	37.765	0.0008	0.9567	<0.0001	0.01608	0.00340	0.01482	0.00448
GLU	100	C	W	19.75	2.77	37.948	0.0004	0.9522	<0.0001	0.01293	0.00144	0.01024	0.00306
GLU	100	C	W	144.20	4.08	38.3262	0.0002	0.9432	<0.0001	0.01139	0.00060	0.01287	0.00064
GLU	100	C	W	54.88	2.91	38.5436	0.0002	0.9381	<0.0001	0.01230	0.00134	0.01354	0.00134
GLU	100	D	H	111.69	5.26	8.3858	0.0004	4.2346	0.0002	0.03491	0.00102	0.02154	0.00224
GLU	100	D	H	50.58	1.74	9.211	0.0002	3.8559	0.0001	0.01046	0.00062	0.01142	0.00070
GLU	100	D	H	650.93	12.53	9.9338	0.0002	3.576	0.0001	0.04809	0.00070	0.02756	0.00116
GLU	100	D	H	1100.88	14.64	10.7852	0.0002	3.2944	0.0001	0.06206	0.00058	0.03767	0.00106
GLU	100	D	H	718.31	5.65	11.7025	0.0000	3.037	0	0.00989	0.00012	0.01139	0.00014
GLU	100	D	H	16.95	1.22	12.4965	0.0004	2.8447	0.0001	0.00956	0.00352	0.01412	0.00194
GLU	100	D	H	1173.35	60.44	13.0146	0.0002	2.7319	<0.0001	0.06415	0.00400	0.02227	0.00300
GLU	100	D	H	122.94	2.64	14.2538	0.0000	2.4955	0	0.00935	0.00032	0.01023	0.00038
GLU	100	D	H	200.81	5.49	15.5718	0.0000	2.2854	0	0.01233	0.00022	0.00934	0.00054
GLU	100	D	H	81.04	5.04	16.8153	0.0008	2.1175	0.0001	0.05416	0.00192	0.03828	0.00534
GLU	100	D	H	120.04	2.58	16.9963	0.0002	2.0951	<0.0001	0.00870	0.00062	0.01187	0.00044

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	D	H	767.84	198.07	17.2505	0.0002	2.0645	<0.0001	0.03749	0.01304	0.00000	0.00000
GLU	100	D	H	48.05	2.52	18.4822	0.0002	1.928	<0.0001	0.01436	0.00064	0.01179	0.00126
GLU	100	D	H	232.78	3.63	18.6259	0.0000	1.9132	0	0.01299	0.00034	0.01433	0.00040
GLU	100	D	H	165.67	3.34	18.9986	0.0002	1.876	<0.0001	0.01271	0.00050	0.01402	0.00052
GLU	100	D	H	322.96	5.12	19.206	0.0008	1.8559	0.0001	0.05262	0.00098	0.01029	0.00028
GLU	100	D	H	693.41	13.96	19.567	0.0004	1.822	<0.0001	0.10438	0.00120	0.06540	0.00296
GLU	100	D	H	41.69	3.98	19.9453	0.0018	1.7878	0.0002	0.07742	0.00886	0.06462	0.01380
GLU	100	D	H	16.98	3.82	20.3868	0.0056	1.7495	0.0005	0.11203	0.02810	0.09028	0.04698
GLU	100	D	H	19.79	2.59	20.852	0.0112	1.7109	0.0009	0.02021	0.00006	0.00092	0.00022
GLU	100	D	H	379.75	5.61	21.6701	0.0008	1.647	0.0001	0.04124	0.00072	0.00497	0.00012
GLU	100	D	H	40.52	2.18	21.9497	0.0002	1.6263	<0.0001	0.01263	0.00092	0.01181	0.00126
GLU	100	D	H	83.11	3.60	22.2521	0.0002	1.6045	<0.0001	0.01541	0.00040	0.01093	0.00098
GLU	100	D	H	62.41	4.03	23.4176	0.0002	1.5256	<0.0001	0.01283	0.00048	0.00811	0.00118
GLU	100	D	H	14.66	2.31	23.532	0.0006	1.5183	<0.0001	0.01590	0.00460	0.01410	0.00498
GLU	100	D	H	16.12	1.87	24.2581	0.0006	1.4735	<0.0001	0.00000	0.00000	0.01660	0.00402
GLU	100	D	H	73.01	3.30	24.8178	0.0002	1.4408	<0.0001	0.01411	0.00038	0.00995	0.00094
GLU	100	D	H	31.61	3.27	25.1476	0.0004	1.4222	<0.0001	0.01941	0.00126	0.01084	0.00266
GLU	100	D	H	11.79	1.19	26.3746	0.0004	1.3571	<0.0001	0.01297	0.00378	0.01400	0.00298
GLU	100	D	H	17.81	3.13	26.729	0.0004	1.3395	<0.0001	0.01818	0.00202	0.00976	0.00418
GLU	100	D	H	26.22	2.35	27.6207	0.0004	1.297	<0.0001	0.01827	0.00004	0.01251	0.00262
GLU	100	D	H	21.13	1.99	29.0213	0.0004	1.2357	<0.0001	0.02122	0.00126	0.01537	0.00322
GLU	100	D	H	37.60	3.19	30.419	0.0002	1.1801	<0.0001	0.01796	0.00104	0.01021	0.00200
GLU	100	D	H	52.90	2.85	31.1237	0.0002	1.1541	<0.0001	0.01929	0.00062	0.01387	0.00162
GLU	100	D	H	29.57	3.79	31.4432	0.0004	1.1426	<0.0001	0.01754	0.00132	0.01188	0.00358
GLU	100	D	H	12.27	2.73	33.9053	0.0008	1.0618	<0.0001	0.02283	0.00288	0.01277	0.00692
GLU	100	D	H	27.19	1.56	34.3852	0.0002	1.0474	<0.0001	0.01487	0.00118	0.01344	0.00160
GLU	100	D	H	34.37	1.77	34.4655	0.0002	1.0451	<0.0001	0.01521	0.00080	0.01297	0.00138
GLU	100	D	H	26.83	2.86	34.7896	0.0006	1.0356	<0.0001	0.02695	0.00150	0.01827	0.00458
GLU	100	D	D	294.74	4.12	9.211	0.0002	3.8559	0.0001	0.01032	0.00012	0.00937	0.00024
GLU	100	D	D	740.78	9.43	11.7016	0.0000	3.0372	0	0.00877	0.00014	0.00951	0.00020
GLU	100	D	D	46.78	2.40	12.4938	0.0002	2.8453	<0.0001	0.01249	0.00040	0.00911	0.00096
GLU	100	D	D	585.76	5.81	14.2543	0.0000	2.4954	0	0.01082	0.00010	0.00978	0.00018
GLU	100	D	D	709.36	7.56	15.5715	0.0000	2.2855	0	0.01248	0.00010	0.00961	0.00020
GLU	100	D	D	671.04	6.63	16.9964	0.0000	2.0951	0	0.01160	0.00008	0.00988	0.00018
GLU	100	D	D	247.89	7.40	18.4812	0.0000	1.9281	0	0.01395	0.00030	0.00804	0.00054
GLU	100	D	D	529.13	9.20	18.6231	0.0000	1.9135	0	0.01429	0.00018	0.00883	0.00032
GLU	100	D	D	711.34	9.31	18.9973	0.0000	1.8761	0	0.01465	0.00012	0.00970	0.00026
GLU	100	D	D	185.91	4.46	21.9503	0.0000	1.6262	0	0.01406	0.00022	0.01022	0.00050
GLU	100	D	D	475.66	7.00	22.252	0.0000	1.6045	0	0.01481	0.00014	0.01052	0.00030
GLU	100	D	D	260.83	4.84	23.4176	0.0000	1.5256	0	0.01360	0.00016	0.01055	0.00038
GLU	100	D	D	137.55	3.04	23.532	0.0000	1.5183	0	0.01151	0.00028	0.01083	0.00044
GLU	100	D	D	78.77	4.00	23.6619	0.0002	1.5101	<0.0001	0.01634	0.00052	0.01027	0.00114
GLU	100	D	D	106.41	3.66	24.2572	0.0002	1.4736	<0.0001	0.01560	0.00034	0.01116	0.00078
GLU	100	D	D	332.72	5.98	24.8177	0.0000	1.4408	0	0.01494	0.00018	0.01069	0.00038
GLU	100	D	D	100.33	3.66	25.1408	0.0002	1.4226	<0.0001	0.01804	0.00040	0.01287	0.00096
GLU	100	D	D	54.66	2.92	26.3728	0.0002	1.3572	<0.0001	0.01536	0.00048	0.01055	0.00120
GLU	100	D	D	79.52	4.00	26.7255	0.0002	1.3396	<0.0001	0.01940	0.00062	0.01208	0.00134
GLU	100	D	D	116.81	8.34	27.6171	0.0002	1.2972	<0.0001	0.01700	0.00116	0.00799	0.00138
GLU	100	D	D	78.83	3.72	28.7348	0.0002	1.2477	<0.0001	0.01537	0.00044	0.00994	0.00100
GLU	100	D	D	85.46	4.87	29.016	0.0002	1.2359	<0.0001	0.01767	0.00074	0.01003	0.00130
GLU	100	D	D	97.42	4.71	30.4162	0.0002	1.1803	<0.0001	0.01721	0.00056	0.01028	0.00110
GLU	100	D	D	278.44	7.88	31.124	0.0002	1.1541	<0.0001	0.01823	0.00038	0.01049	0.00066
GLU	100	D	D	121.21	3.96	31.4433	0.0002	1.1426	<0.0001	0.01677	0.00034	0.01179	0.00080
GLU	100	D	D	35.83	3.82	33.8988	0.0004	1.062	<0.0001	0.01956	0.00152	0.01080	0.00268
GLU	100	D	D	176.25	5.54	34.3847	0.0002	1.0475	<0.0001	0.01478	0.00030	0.00946	0.00064
GLU	100	D	D	144.91	4.56	34.4646	0.0002	1.0451	<0.0001	0.01737	0.00032	0.01232	0.00082
GLU	100	D	W	321.39	9.85	9.2123	0.0002	3.8554	0.0001	0.00553	0.00062	0.01021	0.00022
GLU	100	D	W	337.84	4.47	9.2125	0.0000	3.8553	<0.0001	0.00530	0.00032	0.01028	0.00020
GLU	100	D	W	3906.03	64.24	11.7037	0.0000	3.0367	<0.0001	0.00491	0.00038	0.01018	0.00022
GLU	100	D	W	992.27	239.14	11.7079	0.0008	3.0356	0.0002	0.00455	0.00078	0.00553	0.00118
GLU	100	D	W	125.37	5.60	12.4939	0.0002	2.8453	<0.0001	0.00445	0.00116	0.00888	0.00060
GLU	100	D	W	7.68	0.84	12.6014	0.0006	2.8211	0.0001	0.00000	0.00000	0.01219	0.00248
GLU	100	D	W	666.19	8.58	14.2543	0.0000	2.4954	<0.0001	0.00571	0.00034	0.01095	0.00020
GLU	100	D	W	1163.64	16.77	15.5705	0.0000	2.2856	<0.0001	0.00608	0.00036	0.01131	0.00024
GLU	100	D	W	1049.52	23.23	16.9982	0.0002	2.0949	<0.0001	0.00517	0.00056	0.01052	0.00032
GLU	100	D	W	216.46	13.30	18.4802	0.0004	1.9282	<0.0001	0.00852	0.00180	0.01224	0.00126
GLU	100	D	W	659.39	214.48	18.6199	0.0022	1.9138	0.0002	0.00738	0.00324	0.00938	0.00206
GLU	100	D	W	1326.87	26.25	18.6229	0.0002	1.9135	<0.0001	0.00679	0.00048	0.01160	0.00034
GLU	100	D	W	803.61	11.81	18.9987	0.0000	1.876	<0.0001	0.00851	0.00028	0.01139	0.00026
GLU	100	D	W	730.35	27.42	18.9991	0.0002	1.876	<0.0001	0.00893	0.00052	0.01184	0.00032
GLU	100	D	W	1.15	0.32	21.9179	0.0022	1.6286	0.0002	0.00000	0.00000	0.01320	0.00578
GLU	100	D	W	219.48	7.11	21.9506	0.0002	1.6262	<0.0001	0.00850	0.00058	0.01053	0.00056
GLU	100	D	W	45.34	18.80	22.2485	0.0020	1.6047	0.0001	0.00000	0.00000	0.00440	0.00252
GLU	100	D	W	616.34	26.65	22.2521	0.0002	1.6045	<0.0001	0.00891	0.00058	0.01170	0.00044
GLU	100	D	W	29.09	1.54	22.489	0.0002	1.5878	<0.0001	0.00770	0.00292	0.01365	0.00130
GLU	100	D	W	459.59	7.63	23.4163	0.0000	1.5257	<0.0001	0.00733	0.00032	0.01044	0.00026
GLU	100	D	W	123.25	4.15	23.5297	0.0002	1.5185	<0.0001	0.00717	0.00102	0.01275	0.00070
GLU	100	D	W	152.17	14.70	23.6620	0.0012	1.5101	0.0001	0.00910	0.00088	0.01224	0.00064
GLU	100	D	W	55.27	22.38	24.2548	0.0010	1.4737	0.0001	0.00000	0.00000	0.00537	0.00336

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	100	D	W	137.55	4.30	24.2573	0.0002	1.4736	<0.0001	0.00864	0.00078	0.01166	0.00062
GLU	100	D	W	348.81	8.83	24.8196	0.0002	1.4407	<0.0001	0.00855	0.00066	0.01231	0.00050
GLU	100	D	W	77.30	3.88	25.1414	0.0002	1.4226	<0.0001	0.00985	0.00066	0.00966	0.00090
GLU	100	D	W	123.69	3.29	26.3715	0.0002	1.3573	<0.0001	0.00795	0.00070	0.01144	0.00050
GLU	100	D	W	149.91	5.60	26.7251	0.0002	1.3397	<0.0001	0.00801	0.00148	0.01377	0.00082
GLU	100	D	W	170.53	9.87	27.6151	0.0002	1.2973	<0.0001	0.01023	0.00084	0.01053	0.00108
GLU	100	D	W	54.21	2.22	27.8772	0.0002	1.2853	<0.0001	0.00818	0.00144	0.01217	0.00088
GLU	100	D	W	73.04	2.78	28.7358	0.0002	1.2477	<0.0001	0.01188	0.00066	0.01010	0.00070
GLU	100	D	W	82.45	2.84	29.0178	0.0002	1.2358	<0.0001	0.01284	0.00062	0.01273	0.00082
GLU	100	D	W	40.08	1.98	30.2362	0.0002	1.1871	<0.0001	0.00874	0.00166	0.01323	0.00118
GLU	100	D	W	144.09	3.48	30.4139	0.0002	1.1803	<0.0001	0.01027	0.00054	0.01234	0.00052
GLU	100	D	W	7.42	0.48	30.5918	0.0006	1.1736	<0.0001	0.00962	0.00360	0.01566	0.00140
GLU	100	D	W	76.32	6.77	31.1207	0.0002	1.1542	<0.0001	0.00755	0.00176	0.00711	0.00056
GLU	100	D	W	388.10	7.32	31.122	0.0000	1.1541	<0.0001	0.01117	0.00024	0.01219	0.00034
GLU	100	D	W	1.30	0.39	31.1920	0.0028	1.1516	0.0001	0.00000	0.00000	0.01531	0.00682
GLU	100	D	W	78.59	14.32	31.438	0.0006	1.1428	<0.0001	0.00800	0.00154	0.00559	0.00188
GLU	100	D	W	176.35	4.62	31.4404	0.0002	1.1427	<0.0001	0.01060	0.00056	0.01223	0.00056
GLU	100	D	W	2.62	1.02	31.7869	0.0326	1.1306	0.0011	0.00000	0.00000	0.14645	0.08772
GLU	100	D	W	23.65	2.09	31.9445	0.0004	1.1252	<0.0001	0.01612	0.00106	0.01242	0.00238
GLU	100	D	W	27.02	3.16	33.9004	0.0004	1.062	<0.0001	0.01506	0.00096	0.01479	0.00214
GLU	100	D	W	389.15	7.27	34.383	0.0000	1.0475	<0.0001	0.00815	0.00034	0.01052	0.00032
GLU	100	D	W	241.61	6.05	34.463	0.0002	1.0452	<0.0001	0.00998	0.00066	0.01301	0.00056
GLU	100	D	W	27.53	11.42	34.4682	0.0018	1.0450	0.0001	0.00000	0.00000	0.00581	0.00236
GLU	100	D	W	76.66	6.23	34.7828	0.0004	1.0358	<0.0001	0.01559	0.00078	0.01223	0.00196
GLU	100	D	W	74.95	3.91	34.7872	0.0004	1.0357	<0.0001	0.01419	0.00350	0.02108	0.00202
GLU	100	D	W	14.68	1.64	35.2162	0.0004	1.0235	<0.0001	0.01254	0.00254	0.01366	0.00290
GLU	100	D	W	149.54	5.99	35.6158	0.0002	1.0124	<0.0001	0.01207	0.00062	0.01185	0.00088
GLU	100	D	W	203.44	5.83	35.6179	0.0002	1.0123	<0.0001	0.01129	0.00064	0.01298	0.00064
GLU	100	D	W	26.27	1.90	36.4502	0.0006	0.99	<0.0001	0.00984	0.00348	0.01449	0.00198
GLU	100	D	W	95.43	3.49	36.6399	0.0002	0.985	<0.0001	0.01324	0.00062	0.01272	0.00088
GLU	100	D	W	20.96	3.20	36.7928	0.0006	0.9811	<0.0001	0.01538	0.00154	0.01930	0.00638
GLU	100	D	W	60.78	2.83	36.9447	0.0002	0.9772	<0.0001	0.01627	0.00108	0.01318	0.00118
GLU	100	D	W	47.29	3.37	37.3918	0.0002	0.9659	<0.0001	0.01418	0.00082	0.01139	0.00170
GLU	100	D	W	60.01	3.39	37.3931	0.0002	0.9659	<0.0001	0.01375	0.00124	0.01343	0.00150
GLU	100	D	W	122.10	4.86	37.4659	0.0002	0.964	<0.0001	0.01785	0.00052	0.01420	0.00114
GLU	100	D	W	23.53	2.56	37.762	0.0006	0.9568	<0.0001	0.01825	0.00192	0.01506	0.00350
GLU	100	D	W	21.76	2.30	37.9493	0.0004	0.9522	<0.0001	0.01344	0.00136	0.01114	0.00248
GLU	100	D	W	146.17	3.71	38.3261	0.0002	0.9432	<0.0001	0.01489	0.00050	0.01360	0.00062
GLU	100	D	W	47.03	2.86	38.5425	0.0002	0.9381	<0.0001	0.01498	0.00106	0.01719	0.00136
GLU	1000	A	H	147.27	7.59	8.3844	0.0004	4.2353	0.0002	0.03755	0.00126	0.02298	0.00258
GLU	1000	A	H	1.76	0.22	9.2094	0.0008	3.8566	0.0003	0.01037	0.00600	0.01423	0.00360
GLU	1000	A	H	833.59	19.04	9.9351	0.0002	3.5755	0.0001	0.05581	0.00098	0.03197	0.00160
GLU	1000	A	H	1418.74	22.00	10.7861	0.0002	3.2942	0.0001	0.06772	0.00074	0.04137	0.00138
GLU	1000	A	H	108.80	3.18	11.6958	0.0002	3.0387	0.0001	0.00982	0.00092	0.01323	0.00068
GLU	1000	A	H	1477.57	53.03	13.0136	0.0004	2.7321	0.0001	0.07906	0.00270	0.03521	0.00312
GLU	1000	A	H	6.03	0.39	14.2548	0.0004	2.4953	0.0001	0.00988	0.00330	0.01457	0.00180
GLU	1000	A	H	102.70	13.79	15.3443	0.0066	2.3191	0.001	0.00000	0.00000	0.22446	0.04958
GLU	1000	A	H	204.13	36.79	15.5776	0.0626	2.2846	0.0092	0.01621	0.00172	0.73365	0.10596
GLU	1000	A	H	121.36	18.33	16.8102	0.0008	2.1181	0.0001	0.05519	0.00776	0.02482	0.00948
GLU	1000	A	H	1004.69	31.49	17.2509	0.0004	2.0644	<0.0001	0.08274	0.00236	0.04021	0.00302
GLU	1000	A	H	4.60	1.22	18.6067	0.0016	1.9152	0.0002	0.03203	0.00456	0.01903	0.01210
GLU	1000	A	H	6.33	1.06	18.987	0.0008	1.8772	0.0001	0.02046	0.00186	0.01402	0.00544
GLU	1000	A	H	409.15	16.94	19.2065	0.0006	1.8559	0.0001	0.11863	0.00334	0.06335	0.00636
GLU	1000	A	H	922.31	17.99	19.563	0.0004	1.8224	<0.0001	0.10528	0.00132	0.06058	0.00274
GLU	1000	A	H	60.93	5.04	19.9453	0.0016	1.7878	0.0001	0.09220	0.00578	0.06873	0.01296
GLU	1000	A	H	21.06	1.22	20.3851	0.0050	1.7496	0.0004	0.00000	0.00000	0.14922	0.01264
GLU	1000	A	H	4.12	0.85	22.2535	0.0010	1.6044	0.0001	0.02234	0.00236	0.01473	0.00704
GLU	1000	A	H	28.51	1.72	25.2833	0.0074	1.4147	0.0004	0.00000	0.00000	0.22946	0.02264
GLU	1000	A	H	35.00	3.90	26.8272	0.0044	1.3346	0.0002	0.11051	0.06212	0.13495	0.03360
GLU	1000	A	H	123.53	22.83	32.4361	0.0030	1.1085	0.0001	0.21209	0.04298	0.08234	0.04012
GLU	1000	A	D	117.13	1.51	8.3860	0.0004	4.2345	0.0002	0.03425	0.00030	0.02120	0.00032
GLU	1000	A	D	667.02	12.64	9.9361	0.0002	3.5752	0.0001	0.04803	0.00062	0.03003	0.00120
GLU	1000	A	D	1158.47	15.01	10.7878	0.0002	3.2936	0.0001	0.06317	0.00054	0.04188	0.00112
GLU	1000	A	D	37.20	2.06	11.6976	0.0002	3.0383	0.0001	0.01101	0.00114	0.01166	0.00122
GLU	1000	A	D	1215.47	43.73	13.0169	0.0004	2.7315	0.0001	0.07490	0.00280	0.03228	0.00286
GLU	1000	A	D	65.64	3.18	15.3410	0.0046	2.3196	0.0007	0.00000	0.00000	0.19352	0.01384
GLU	1000	A	D	212.75	7.13	15.5524	0.0140	2.2883	0.0020	0.00000	0.00000	0.66076	0.02654
GLU	1000	A	D	82.56	2.56	16.4542	0.0058	2.1636	0.0008	0.00000	0.00000	0.34311	0.01628
GLU	1000	A	D	102.29	1.66	16.8209	0.0008	2.1168	0.0001	0.04517	0.00106	0.01676	0.00016
GLU	1000	A	D	6.28	0.68	16.9998	0.0008	2.0947	0.0001	0.00000	0.00000	0.01413	0.00210
GLU	1000	A	D	818.12	30.95	17.2508	0.0004	2.0644	<0.0001	0.07158	0.00260	0.03319	0.00306
GLU	1000	A	D	5.06	1.65	18.6105	0.0016	1.9148	0.0002	0.02221	0.00548	0.02324	0.01408
GLU	1000	A	D	5.41	0.89	18.9952	0.0010	1.8764	0.0001	0.00000	0.00000	0.01894	0.00614
GLU	1000	A	D	317.54	10.56	19.2080	0.0006	1.8558	0.0001	0.11883	0.00196	0.07450	0.00574
GLU	1000	A	D	752.53	13.99	19.5699	0.0004	1.8218	<0.0001	0.10718	0.00118	0.06431	0.00272
GLU	1000	A	D	52.54	7.72	19.9468	0.0020	1.7877	0.0002	0.08863	0.00734	0.04590	0.01582
GLU	1000	A	D	28.23	2.14	21.2227	0.0138	1.6813	0.0011	0.00000	0.00000	0.33905	0.04242
GLU	1000	A	D	25.04	1.01	23.6419	0.0058	1.5114	0.0004	0.07294	0.00750	0.01574	0.00008
GLU	1000	A	D	25.01	1.30	25.2868	0.0078	1.4145	0.0004	0.25906	0.03002	0.25893	0.02078

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	A	D	24.79	10.51	26.4895	0.0034	1.3514	0.0002	0.09526	0.03528	0.00000	0.00000
GLU	1000	A	D	31.71	4.73	26.8320	0.0040	1.3344	0.0002	0.14311	0.01930	0.14553	0.04120
GLU	1000	A	D	44.46	2.32	29.4293	0.0260	1.2189	0.0011	0.00000	0.00000	0.81365	0.06774
GLU	1000	A	D	1.03	0.34	34.4629	0.0044	1.0452	0.0001	0.00000	0.00000	0.02256	0.01132
GLU	1000	A	D	13.60	2.90	34.9165	0.0088	1.0320	0.0003	0.02722	0.00008	0.00242	0.00096
GLU	1000	A	D	15.88	1.27	39.0071	0.0180	0.9274	0.0004	0.00000	0.00000	0.38542	0.04758
GLU	1000	A	W	149.51	8.68	8.3854	0.0004	4.2348	0.0002	0.03583	0.00150	0.02080	0.00268
GLU	1000	A	W	846.13	18.91	9.9334	0.0002	3.5761	0.0001	0.05087	0.00086	0.02950	0.00144
GLU	1000	A	W	1424.91	18.90	10.7849	0.0002	3.2945	0.0001	0.06600	0.00056	0.04523	0.00122
GLU	1000	A	W	39.03	2.85	11.6958	0.0004	3.0387	0.0001	0.01305	0.00114	0.01193	0.00174
GLU	1000	A	W	1525.30	45.06	13.014	0.0004	2.7321	0.0001	0.07965	0.00234	0.03561	0.00258
GLU	1000	A	W	19.77	6.44	15.5709	0.0006	2.2856	0.0001	0.01338	0.00256	0.00000	0.00000
GLU	1000	A	W	23.99	1.90	18.9912	0.0004	1.8767	<0.0001	0.00000	0.00000	0.01519	0.00224
GLU	1000	A	W	972.18	318.24	19.5647	0.0004	1.8222	<0.0001	0.05253	0.02344	0.00000	0.00000
GLU	1000	A	W	52.67	4.11	19.945	0.0020	1.7878	0.0002	0.05556	0.03054	0.08530	0.01378
GLU	1000	A	W	23.23	3.93	23.6425	0.0082	1.5113	0.0005	0.00000	0.00000	0.14422	0.05236
GLU	1000	A	W	38.22	9.23	26.8239	0.0050	1.3348	0.0002	0.13379	0.01424	0.08567	0.05032
GLU	1000	A	W	165.71	15.71	27.2802	0.0018	1.3129	0.0001	0.13283	0.00840	0.07117	0.01646
GLU	1000	A	W	270.06	14.62	27.8259	0.0018	1.2876	0.0001	0.17610	0.00510	0.10964	0.01376
GLU	1000	A	W	115.83	9.07	32.4358	0.0042	1.1086	0.0001	0.22975	0.01352	0.17385	0.03068
GLU	1000	B	H	6.12	1.62	6.0703	0.0052	5.8474	0.0050	0.19524	0.03978	0.00000	0.00000
GLU	1000	B	H	3.73	1.28	6.0875	0.0064	5.8309	0.0061	0.14395	0.02148	0.00000	0.00000
GLU	1000	B	H	104.31	4.92	8.3838	0.0004	4.2356	0.0002	0.04048	0.00114	0.02239	0.00218
GLU	1000	B	H	212.98	2.75	8.3870	0.0004	4.2340	0.0002	0.03524	0.00064	0.01922	0.00018
GLU	1000	B	H	4.34	1.39	9.2113	0.0014	3.8558	0.0006	0.00000	0.00000	0.01371	0.00798
GLU	1000	B	H	580.56	9.39	9.9364	0.0002	3.5751	0.0001	0.05962	0.00062	0.04409	0.00142
GLU	1000	B	H	177.94	5.18	10.2074	0.0002	3.4804	0.0001	0.01706	0.00032	0.01388	0.00074
GLU	1000	B	H	2076.16	27.09	10.7874	0.0002	3.2938	0.0001	0.06411	0.00056	0.04083	0.00112
GLU	1000	B	H	35.95	1.67	11.7001	0.0002	3.0376	0.0001	0.00934	0.00190	0.01386	0.00116
GLU	1000	B	H	2106.96	96.79	13.0152	0.0004	2.7318	0.0001	0.07671	0.00394	0.03031	0.00352
GLU	1000	B	H	301.62	5.92	13.942	0.0002	2.551	<0.0001	0.01780	0.00024	0.01369	0.00052
GLU	1000	B	H	9.44	2.23	14.2543	0.0006	2.4954	0.0001	0.00852	0.00286	0.02091	0.00746
GLU	1000	B	H	124.90	4.91	14.9527	0.0002	2.3795	<0.0001	0.01785	0.00042	0.01237	0.00102
GLU	1000	B	H	121.98	5.12	15.3386	0.0044	2.3200	0.0007	0.00000	0.00000	0.20172	0.01282
GLU	1000	B	H	244.40	15.00	15.3492	0.0076	2.3184	0.0011	0.15583	0.06944	0.23621	0.02684
GLU	1000	B	H	360.47	9.26	15.5549	0.0130	2.2879	0.0019	0.00000	0.00000	0.66311	0.02226
GLU	1000	B	H	50.72	3.09	16.0611	0.0030	2.2162	0.0004	0.05839	0.00054	0.01249	0.00138
GLU	1000	B	H	146.95	4.87	16.4491	0.0068	2.1643	0.0009	0.00000	0.00000	0.37575	0.02026
GLU	1000	B	H	84.40	5.84	16.8173	0.0010	2.1172	0.0001	0.06374	0.00266	0.04609	0.00716
GLU	1000	B	H	4.36	0.65	16.9988	0.0010	2.0948	0.0001	0.00000	0.00000	0.01081	0.00224
GLU	1000	B	H	353.39	7.38	17.0757	0.0002	2.0854	<0.0001	0.01785	0.00024	0.01334	0.00056
GLU	1000	B	H	1444.35	36.72	17.2487	0.0004	2.0647	<0.0001	0.08151	0.00140	0.04407	0.00254
GLU	1000	B	H	774.26	311.28	17.2515	0.0004	2.0643	<0.0001	0.03671	0.02048	0.00000	0.00000
GLU	1000	B	H	4.63	2.05	18.1385	0.0016	1.9642	0.0002	0.01958	0.00438	0.00000	0.00000
GLU	1000	B	H	10.03	2.51	18.6112	0.0016	1.9147	0.0002	0.02944	0.00468	0.02998	0.00784
GLU	1000	B	H	7.80	2.46	18.9956	0.0012	1.8763	0.0001	0.01840	0.00436	0.02084	0.00584
GLU	1000	B	H	299.12	13.07	19.2066	0.0010	1.8559	0.0001	0.12728	0.00268	0.09256	0.00640
GLU	1000	B	H	1349.33	29.36	19.5643	0.0004	1.8223	<0.0001	0.10561	0.00132	0.06478	0.00318
GLU	1000	B	H	90.28	10.47	19.9442	0.0022	1.7879	0.0002	0.09180	0.00668	0.09803	0.00606
GLU	1000	B	H	35.58	1.16	19.9503	0.0020	1.7874	0.0002	0.00000	0.00000	0.10499	0.00480
GLU	1000	B	H	17.58	4.60	20.8602	0.0154	1.7102	0.0013	0.00000	0.00000	0.22812	0.14270
GLU	1000	B	H	20.02	2.05	21.2172	0.0164	1.6818	0.0013	0.00000	0.00000	0.29103	0.04710
GLU	1000	B	H	382.89	173.00	21.6740	0.0008	1.6467	0.0001	0.04083	0.02562	0.00000	0.00000
GLU	1000	B	H	3.98	1.92	22.2550	0.0018	1.6043	0.0001	0.02162	0.00508	0.00000	0.00000
GLU	1000	B	H	14.42	7.07	23.5885	0.0008	1.5147	0.0001	0.01724	0.00798	0.00000	0.00000
GLU	1000	B	H	37.47	7.67	23.6505	0.0004	1.5108	<0.0001	0.01876	0.00400	0.00764	0.00406
GLU	1000	B	H	75.29	8.94	24.1928	0.0024	1.4774	0.0001	0.16695	0.01510	0.16892	0.03360
GLU	1000	B	H	5.08	0.69	24.8196	0.0014	1.4407	0.0001	0.00000	0.00000	0.01664	0.00314
GLU	1000	B	H	40.12	2.35	25.2766	0.0088	1.4151	0.0005	0.00000	0.00000	0.25276	0.02148
GLU	1000	B	H	20.61	2.79	25.2835	0.0098	1.4147	0.0005	0.18398	0.08736	0.24255	0.03286
GLU	1000	B	H	21.23	0.97	25.2839	0.0070	1.4147	0.0004	0.00000	0.00000	0.25864	0.01696
GLU	1000	B	H	146.88	4.15	25.4693	0.0002	1.4045	<0.0001	0.01914	0.00032	0.01313	0.00078
GLU	1000	B	H	224.19	5.45	26.0515	0.0002	1.3737	<0.0001	0.01872	0.00026	0.01240	0.00066
GLU	1000	B	H	28.88	1.78	26.4873	0.0038	1.3515	0.0002	0.00000	0.00000	0.10797	0.00980
GLU	1000	B	H	14.67	0.82	26.5002	0.0040	1.3508	0.0002	0.00000	0.00000	0.12635	0.01040
GLU	1000	B	H	24.49	0.91	26.8312	0.0038	1.3345	0.0002	0.00000	0.00000	0.17495	0.00934
GLU	1000	B	H	400.02	9.15	27.8264	0.0020	1.2876	0.0001	0.04765	0.00036	0.00531	0.00018
GLU	1000	B	H	4.45	0.48	28.0982	0.0012	1.2754	0.0001	0.03301	0.00632	0.01944	0.00292
GLU	1000	B	H	70.73	2.64	28.9428	0.0002	1.239	<0.0001	0.01967	0.00042	0.01395	0.00110
GLU	1000	B	H	37.78	0.51	29.0601	0.0002	1.2341	<0.0001	0.01986	0.00062	0.01324	0.00008
GLU	1000	B	H	49.59	3.46	29.4395	0.0254	1.2185	0.0010	0.00000	0.00000	0.60377	0.06636
GLU	1000	B	H	67.04	10.96	30.1077	0.0036	1.1921	0.0001	0.14263	0.01030	0.09205	0.03654
GLU	1000	B	H	24.42	3.26	30.1703	0.0004	1.1896	<0.0001	0.01857	0.00116	0.01193	0.00376
GLU	1000	B	H	74.34	9.60	30.7995	0.0052	1.1659	0.0002	0.18295	0.07112	0.18478	0.05616
GLU	1000	B	H	4.79	0.82	31.1311	0.0010	1.1538	<0.0001	0.00000	0.00000	0.02045	0.00708
GLU	1000	B	H	10.75	1.66	31.9763	0.0006	1.1241	<0.0001	0.01965	0.00212	0.01717	0.00476
GLU	1000	B	H	30.61	1.93	32.729	0.0004	1.0989	<0.0001	0.02023	0.00082	0.01490	0.00204
GLU	1000	B	H	6.88	1.29	33.2369	0.0008	1.0826	<0.0001	0.01908	0.00216	0.01500	0.00618
GLU	1000	B	H	32.82	1.94	33.3755	0.0002	1.0782	<0.0001	0.01927	0.00068	0.01391	0.00176

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	B	H	45.47	19.31	34.0114	0.0044	1.0586	0.0001	0.12411	0.05268	0.00000	0.00000
GLU	1000	B	H	64.40	2.66	34.5487	0.0002	1.0426	<0.0001	0.02045	0.00060	0.01466	0.00130
GLU	1000	B	H	30.02	7.61	34.6814	0.0506	1.0388	0.0015	0.17412	0.00062	0.04389	0.01958
GLU	1000	B	H	37.29	10.39	34.8948	0.0144	1.0326	0.0004	0.18357	0.07050	0.15694	0.05132
GLU	1000	B	H	46.06	2.44	36.1602	0.0002	0.9976	<0.0001	0.02041	0.00068	0.01595	0.00166
GLU	1000	B	H	7.76	1.91	36.7558	0.0008	0.982	<0.0001	0.01989	0.00234	0.01530	0.00660
GLU	1000	B	H	19.18	5.66	39.7409	0.0098	0.9109	0.0002	0.05687	0.01986	0.00000	0.00000
GLU	1000	B	H	32.15	2.05	39.8862	0.0004	0.9077	<0.0001	0.02015	0.00078	0.01459	0.00200
GLU	1000	B	D	108.23	4.09	8.3852	0.0002	4.2349	0.0001	0.03113	0.00072	0.02107	0.00168
GLU	1000	B	D	628.79	9.97	9.9348	0.0002	3.5756	0.0001	0.04468	0.00048	0.02845	0.00094
GLU	1000	B	D	1097.90	12.81	10.7868	0.0002	3.2939	0.0001	0.05804	0.00044	0.03732	0.00090
GLU	1000	B	D	8.57	1.40	11.7000	0.0006	3.0376	0.0002	0.01297	0.00216	0.01168	0.00412
GLU	1000	B	D	1158.38	37.98	13.0165	0.0002	2.7315	<0.0001	0.06867	0.00238	0.02865	0.00236
GLU	1000	B	D	130.07	8.00	15.3524	0.0044	2.3179	0.0007	0.21262	0.02888	0.22443	0.02614
GLU	1000	B	D	141.71	18.94	15.6387	0.0516	2.2757	0.0075	0.00000	0.00000	0.49213	0.11130
GLU	1000	B	D	90.38	8.40	16.8214	0.0006	2.1167	0.0001	0.04781	0.00346	0.02458	0.00550
GLU	1000	B	D	1.82	0.36	17.0032	0.0012	2.0943	0.0001	0.00000	0.00000	0.01008	0.00292
GLU	1000	B	D	789.38	19.12	17.25	0.0002	2.0645	<0.0001	0.06871	0.00148	0.03437	0.00196
GLU	1000	B	D	320.20	12.23	19.2075	0.0008	1.8558	0.0001	0.11219	0.00242	0.06606	0.00590
GLU	1000	B	D	739.09	13.83	19.5704	0.0004	1.8217	<0.0001	0.10106	0.00112	0.06259	0.00262
GLU	1000	B	D	53.85	10.52	19.9476	0.0014	1.7876	0.0001	0.07058	0.01304	0.03127	0.01546
GLU	1000	B	D	22.37	1.23	25.2853	0.0078	1.4146	0.0004	0.00000	0.00000	0.23776	0.01876
GLU	1000	B	D	15.23	0.94	26.4906	0.0034	1.3513	0.0002	0.00000	0.00000	0.09336	0.00832
GLU	1000	B	D	120.39	6.20	27.2893	0.0014	1.3125	0.0001	0.12387	0.00336	0.08754	0.00964
GLU	1000	B	D	37.60	2.12	30.1161	0.0032	1.1917	0.0001	0.04722	0.00314	0.00762	0.00072
GLU	1000	B	W	204.67	14.02	8.3882	0.0004	4.2334	0.0002	0.03079	0.00186	0.01535	0.00246
GLU	1000	B	W	1.84	0.31	9.2100	0.0012	3.8563	0.0005	0.00000	0.00000	0.01301	0.00300
GLU	1000	B	W	36.34	2.68	9.2116	0.0002	3.8557	0.0001	0.00728	0.00096	0.00827	0.00088
GLU	1000	B	W	495.32	9.76	9.9349	0.0002	3.5756	0.0001	0.04788	0.00060	0.03248	0.00132
GLU	1000	B	W	1134.94	21.09	9.9356	0.0002	3.5753	0.0001	0.04527	0.00058	0.02784	0.00110
GLU	1000	B	W	854.52	11.36	10.7868	0.0002	3.2939	0.0001	0.06233	0.00054	0.04543	0.00120
GLU	1000	B	W	1973.73	27.91	10.7870	0.0002	3.2939	0.0001	0.06149	0.00056	0.04150	0.00120
GLU	1000	B	W	21.07	2.44	11.7007	0.0004	3.0375	0.0001	0.01551	0.00104	0.01100	0.00274
GLU	1000	B	W	2088.81	61.59	13.016	0.0002	2.7316	<0.0001	0.07437	0.00226	0.03213	0.00234
GLU	1000	B	W	911.65	27.47	13.0167	0.0004	2.7315	0.0001	0.07603	0.00222	0.03505	0.00254
GLU	1000	B	W	56.39	3.75	15.3410	0.0062	2.3196	0.0009	0.20314	0.07888	0.20077	0.02040
GLU	1000	B	W	219.17	31.85	15.3423	0.0042	2.3194	0.0006	0.20687	0.02396	0.10521	0.03098
GLU	1000	B	W	138.87	6.88	15.5764	0.0234	2.2848	0.0034	0.00000	0.00000	0.60333	0.03628
GLU	1000	B	W	261.45	18.94	15.6116	0.0348	2.2796	0.0051	0.00000	0.00000	0.57012	0.06570
GLU	1000	B	W	157.52	7.58	16.8180	0.0008	2.1172	0.0001	0.05085	0.00052	0.02752	0.00298
GLU	1000	B	W	70.76	7.31	16.8217	0.0008	2.1167	0.0001	0.05122	0.00316	0.02950	0.00722
GLU	1000	B	W	2.32	0.58	17.0008	0.0024	2.0946	0.0003	0.00000	0.00000	0.01524	0.00552
GLU	1000	B	W	1446.39	354.17	17.2478	0.0002	2.0648	<0.0001	0.03514	0.01194	0.00000	0.00000
GLU	1000	B	W	629.76	155.82	17.2498	0.0004	2.0645	<0.0001	0.03889	0.01298	0.00000	0.00000
GLU	1000	B	W	56.04	8.44	18.4677	0.0304	1.9295	0.0032	0.02692	0.00480	0.00063	0.00016
GLU	1000	B	W	5.66	1.77	18.6068	0.0012	1.9152	0.0001	0.00000	0.00000	0.01323	0.00868
GLU	1000	B	W	11.30	5.22	18.9899	0.0012	1.8769	0.0001	0.01660	0.00424	0.00000	0.00000
GLU	1000	B	W	4.81	1.00	18.9948	0.0010	1.8764	0.0001	0.00000	0.00000	0.01541	0.00676
GLU	1000	B	W	542.17	18.33	19.2033	0.0008	1.8562	0.0001	0.11376	0.00204	0.07940	0.00608
GLU	1000	B	W	1351.32	544.77	19.5649	0.0004	1.8222	<0.0001	0.03965	0.02218	0.00000	0.00000
GLU	1000	B	W	586.22	11.58	19.5705	0.0004	1.8217	<0.0001	0.10571	0.00116	0.06643	0.00294
GLU	1000	B	W	75.27	5.52	19.9440	0.0016	1.7879	0.0001	0.06122	0.01634	0.07323	0.01124
GLU	1000	B	W	166.83	5.42	20.4991	0.0002	1.74	<0.0001	0.01933	0.00012	0.01315	0.00084
GLU	1000	B	W	12.51	1.47	20.8502	0.0154	1.7110	0.0013	0.00000	0.00000	0.20009	0.03762
GLU	1000	B	W	19.81	1.78	21.2149	0.0174	1.6819	0.0014	0.00000	0.00000	0.33232	0.05010
GLU	1000	B	W	308.19	32.97	21.6731	0.0008	1.6468	0.0001	0.11432	0.01416	0.04112	0.01166
GLU	1000	B	W	35.16	7.50	21.949	0.0002	1.6263	<0.0001	0.00814	0.00136	0.00416	0.00218
GLU	1000	B	W	350.70	6.84	22.2952	0.0000	1.6014	<0.0001	0.01881	0.00024	0.01221	0.00050
GLU	1000	B	W	44.96	2.16	25.2843	0.0072	1.4146	0.0004	0.00000	0.00000	0.25622	0.01786
GLU	1000	B	W	138.25	3.90	25.4702	0.0002	1.4045	<0.0001	0.01897	0.00034	0.01393	0.00080
GLU	1000	B	W	175.08	32.74	26.1881	0.0040	1.3666	0.0002	0.17245	0.01298	0.09587	0.04470
GLU	1000	B	W	42.31	14.30	26.4818	0.0036	1.3517	0.0002	0.09940	0.01856	0.00000	0.00000
GLU	1000	B	W	59.13	7.53	26.8266	0.0034	1.3347	0.0002	0.13289	0.00052	0.07871	0.02468
GLU	1000	B	W	223.13	13.09	27.2810	0.0012	1.3129	0.0001	0.12886	0.00410	0.07743	0.01068
GLU	1000	B	W	98.52	4.47	27.2881	0.0012	1.3125	0.0001	0.12447	0.00414	0.09247	0.00942
GLU	1000	B	W	62.09	3.50	29.4377	0.0216	1.2186	0.0009	0.00000	0.00000	0.66866	0.05776
GLU	1000	B	W	16.93	3.41	31.3151	0.0006	1.1472	<0.0001	0.01870	0.00188	0.01490	0.00678
GLU	1000	B	W	15.14	2.20	31.9301	0.0006	1.1256	<0.0001	0.02052	0.00152	0.01345	0.00384
GLU	1000	B	W	37.65	4.54	36.3755	0.0082	0.9919	0.0002	0.09660	0.00060	0.02566	0.00562
GLU	1000	B	W	1.02	0.38	36.6255	0.0078	0.9854	0.0002	0.00000	0.00000	0.03557	0.02020
GLU	1000	B	W	84.59	7.08	38.3643	0.0044	0.9423	0.0001	0.20249	0.02228	0.22576	0.03568
GLU	1000	B	W	11.20	1.79	38.6905	0.0006	0.9346	<0.0001	0.02076	0.00168	0.01342	0.00494
GLU	1000	B	W	6.78	1.24	39.4183	0.0008	0.9181	<0.0001	0.02022	0.00316	0.02071	0.00544
GLU	1000	C	H	92.99	5.09	8.3837	0.0004	4.2356	0.0002	0.04173	0.00150	0.02575	0.00310
GLU	1000	C	H	4.33	0.86	9.2094	0.0008	3.8566	0.0003	0.01140	0.00666	0.01314	0.00532
GLU	1000	C	H	517.62	10.41	9.9360	0.0002	3.5752	0.0001	0.06062	0.00080	0.03932	0.00166
GLU	1000	C	H	175.50	5.68	10.2069	0.0002	3.4806	0.0001	0.01710	0.00038	0.01313	0.00084
GLU	1000	C	H	884.96	11.56	10.7875	0.0002	3.2937	0.0001	0.07290	0.00062	0.05176	0.00136
GLU	1000	C	H	74.49	2.49	11.6978	0.0002	3.0382	0.0001	0.01299	0.00066	0.01341	0.00082

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	C	H	949.82	29.55	13.0162	0.0004	2.7316	0.0001	0.08373	0.00260	0.03738	0.00284
GLU	1000	C	H	302.01	7.31	13.9418	0.0002	2.5511	<0.0001	0.01766	0.00028	0.01322	0.00064
GLU	1000	C	H	6.43	1.07	14.2557	0.0008	2.4952	0.0001	0.00000	0.00000	0.01532	0.00518
GLU	1000	C	H	121.85	4.55	14.9527	0.0002	2.3795	<0.0001	0.01748	0.00040	0.01216	0.00094
GLU	1000	C	H	16.88	2.27	15.5706	0.0006	2.2856	0.0001	0.01334	0.00348	0.01263	0.00372
GLU	1000	C	H	72.41	6.05	16.8171	0.0010	2.1173	0.0001	0.06264	0.00258	0.04044	0.00784
GLU	1000	C	H	10.63	1.26	16.9996	0.0006	2.0947	0.0001	0.00000	0.00000	0.01480	0.00354
GLU	1000	C	H	354.82	7.44	17.0757	0.0000	2.0854	<0.0001	0.01790	0.00024	0.01313	0.00058
GLU	1000	C	H	656.34	217.24	17.2515	0.0004	2.0643	<0.0001	0.04441	0.02006	0.00000	0.00000
GLU	1000	C	H	3.85	0.45	18.1388	0.0014	1.9641	0.0002	0.00000	0.00000	0.02040	0.00328
GLU	1000	C	H	19.23	2.09	18.6039	0.0004	1.9155	<0.0001	0.01122	0.00194	0.01006	0.00234
GLU	1000	C	H	13.66	2.16	18.6202	0.0008	1.9138	0.0001	0.01527	0.00266	0.01249	0.00434
GLU	1000	C	H	11.76	1.89	18.9942	0.0008	1.8765	0.0001	0.01752	0.00662	0.02032	0.00548
GLU	1000	C	H	251.16	12.00	19.2087	0.0010	1.8557	0.0001	0.12670	0.00286	0.07776	0.00884
GLU	1000	C	H	615.57	16.45	19.5679	0.0006	1.8219	0.0001	0.11444	0.00188	0.06544	0.00408
GLU	1000	C	H	38.16	5.97	19.9513	0.0026	1.7873	0.0002	0.09376	0.00694	0.05993	0.02218
GLU	1000	C	H	179.19	6.27	20.4985	0.0002	1.7401	<0.0001	0.01892	0.00040	0.01217	0.00092
GLU	1000	C	H	373.35	9.27	22.2945	0.0002	1.6014	<0.0001	0.01866	0.00032	0.01152	0.00062
GLU	1000	C	H	14.63	6.39	23.589	0.0006	1.5147	<0.0001	0.01857	0.00760	0.00000	0.00000
GLU	1000	C	H	41.35	10.87	23.6509	0.0004	1.5108	<0.0001	0.01839	0.00558	0.00000	0.00000
GLU	1000	C	H	2.67	0.59	24.8247	0.0012	1.4404	0.0001	0.00000	0.00000	0.01632	0.00730
GLU	1000	C	H	3.04	0.39	25.1062	0.0014	1.4245	0.0001	0.00000	0.00000	0.01678	0.00330
GLU	1000	C	H	146.74	4.10	25.4696	0.0002	1.4045	<0.0001	0.01895	0.00030	0.01317	0.00078
GLU	1000	C	H	228.43	5.98	26.0518	0.0002	1.3737	<0.0001	0.01908	0.00028	0.01206	0.00070
GLU	1000	C	H	1.51	0.39	27.6132	0.0036	1.2974	0.0002	0.00000	0.00000	0.02345	0.00886
GLU	1000	C	H	5.21	1.20	28.0986	0.0010	1.2754	<0.0001	0.01611	0.00470	0.01364	0.00702
GLU	1000	C	H	70.16	3.92	28.9433	0.0002	1.2389	<0.0001	0.01943	0.00064	0.01351	0.00162
GLU	1000	C	H	38.32	5.01	29.0606	0.0004	1.234	<0.0001	0.01890	0.00186	0.01005	0.00310
GLU	1000	C	H	30.16	13.95	30.1707	0.0006	1.1896	<0.0001	0.01718	0.00904	0.00000	0.00000
GLU	1000	C	H	2.59	0.87	30.9651	0.0026	1.1598	0.0001	0.00000	0.00000	0.02178	0.01452
GLU	1000	C	H	2.94	0.62	31.1300	0.0032	1.1538	0.0001	0.00000	0.00000	0.02732	0.00856
GLU	1000	C	H	18.07	5.20	31.3161	0.0008	1.1471	<0.0001	0.01841	0.00436	0.00000	0.00000
GLU	1000	C	H	15.40	2.84	31.9306	0.0008	1.1256	<0.0001	0.02062	0.00234	0.01462	0.00620
GLU	1000	C	H	10.05	2.03	31.977	0.0010	1.124	<0.0001	0.01848	0.00580	0.01626	0.00730
GLU	1000	C	H	30.65	2.99	32.7297	0.0004	1.0989	<0.0001	0.02084	0.00122	0.01499	0.00320
GLU	1000	C	H	7.69	2.88	33.2373	0.0012	1.0826	<0.0001	0.01967	0.00472	0.00000	0.00000
GLU	1000	C	H	34.09	3.16	33.376	0.0004	1.0782	<0.0001	0.02004	0.00104	0.01353	0.00274
GLU	1000	C	H	67.53	4.05	34.5461	0.0002	1.0427	<0.0001	0.02062	0.00068	0.01436	0.00188
GLU	1000	C	H	47.48	4.27	36.1572	0.0004	0.9977	<0.0001	0.02010	0.00102	0.01243	0.00254
GLU	1000	C	H	1.43	0.57	36.6365	0.0098	0.9851	0.0003	0.00000	0.00000	0.04093	0.02448
GLU	1000	C	H	8.61	2.36	36.7521	0.0012	0.9821	<0.0001	0.02157	0.00462	0.01595	0.01006
GLU	1000	C	H	11.35	2.81	38.6871	0.0010	0.9347	<0.0001	0.02110	0.00294	0.01255	0.00738
GLU	1000	C	H	5.55	1.00	39.4157	0.0012	0.9181	<0.0001	0.00000	0.00000	0.02054	0.00734
GLU	1000	C	H	33.87	2.99	39.883	0.0004	0.9078	<0.0001	0.02052	0.00106	0.01454	0.00280
GLU	1000	C	D	109.20	5.29	8.3857	0.0004	4.2346	0.0002	0.03628	0.00108	0.02438	0.00250
GLU	1000	C	D	1.67	0.40	9.2111	0.0026	3.8559	0.0011	0.00000	0.00000	0.01429	0.00474
GLU	1000	C	D	639.02	14.39	9.9366	0.0002	3.5750	0.0001	0.05255	0.00086	0.03112	0.00152
GLU	1000	C	D	1097.98	15.39	10.7882	0.0002	3.2935	0.0001	0.06718	0.00062	0.04518	0.00130
GLU	1000	C	D	16.04	2.09	11.6990	0.0006	3.0379	0.0002	0.01286	0.00256	0.01288	0.00274
GLU	1000	C	D	1172.05	441.79	13.0176	0.0004	2.7313	0.0001	0.01604	0.00840	0.00000	0.00000
GLU	1000	C	D	174.60	9.59	15.5720	0.0302	2.2854	0.0044	0.00000	0.00000	0.62594	0.03646
GLU	1000	C	D	77.48	2.35	16.4556	0.0058	2.1635	0.0008	0.00000	0.00000	0.34647	0.01684
GLU	1000	C	D	95.76	12.90	16.8208	0.0008	2.1168	0.0001	0.05329	0.00694	0.02346	0.00806
GLU	1000	C	D	2.79	0.49	16.9993	0.0012	2.0947	0.0001	0.00000	0.00000	0.01198	0.00296
GLU	1000	C	D	808.05	82.17	17.2517	0.0004	2.0643	<0.0001	0.05729	0.00726	0.01815	0.00494
GLU	1000	C	D	7.51	3.59	18.6128	0.0016	1.9146	0.0002	0.02574	0.00832	0.00000	0.00000
GLU	1000	C	D	2.26	0.51	18.9956	0.0020	1.8763	0.0002	0.00000	0.00000	0.01466	0.00478
GLU	1000	C	D	759.70	313.36	19.5705	0.0004	1.8217	<0.0001	0.01835	0.01042	0.00000	0.00000
GLU	1000	C	D	35.84	1.86	19.9518	0.0024	1.7872	0.0002	0.06301	0.02558	0.09947	0.00668
GLU	1000	C	D	21.59	1.90	21.2297	0.0158	1.6808	0.0012	0.00000	0.00000	0.30867	0.04462
GLU	1000	C	D	0.83	0.32	23.4218	0.0038	1.5254	0.0002	0.00000	0.00000	0.01679	0.00994
GLU	1000	C	D	15.46	1.36	23.6486	0.0058	1.5109	0.0004	0.00000	0.00000	0.14442	0.01966
GLU	1000	C	D	1.10	0.27	24.8269	0.0030	1.4403	0.0002	0.00000	0.00000	0.02125	0.00748
GLU	1000	C	D	20.90	3.70	26.4922	0.0034	1.3512	0.0002	0.10900	0.01106	0.07762	0.03272
GLU	1000	C	D	1.13	0.35	31.1320	0.0044	1.1538	0.0002	0.00000	0.00000	0.02429	0.01124
GLU	1000	C	D	22.03	8.58	34.0238	0.0032	1.0582	0.0001	0.10644	0.02558	0.08527	0.05350
GLU	1000	C	D	18.19	3.95	34.1705	0.0886	1.0538	0.0027	0.00000	0.00000	0.44699	0.09300
GLU	1000	C	D	31.42	1.65	35.9464	0.0114	1.0034	0.0003	0.00000	0.00000	0.37563	0.03376
GLU	1000	C	W	147.48	12.09	8.3861	0.0004	4.2344	0.0002	0.03392	0.00232	0.01763	0.00334
GLU	1000	C	W	842.96	23.91	9.9336	0.0002	3.5761	0.0001	0.04806	0.00108	0.02668	0.00168
GLU	1000	C	W	1419.81	23.93	10.785	0.0002	3.2945	0.0001	0.06388	0.00072	0.04109	0.00144
GLU	1000	C	W	44.73	3.07	11.6967	0.0002	3.0385	0.0001	0.01013	0.00126	0.01064	0.00140
GLU	1000	C	W	40.81	1.13	11.6971	0.0002	3.0384	0.0001	0.00873	0.00072	0.01108	0.00056
GLU	1000	C	W	1505.74	51.20	13.0138	0.0004	2.7321	0.0001	0.07919	0.00262	0.03602	0.00298
GLU	1000	C	W	7.29	1.39	14.2554	0.0004	2.4952	0.0001	0.01271	0.00162	0.00703	0.00322
GLU	1000	C	W	7.29	1.11	15.5696	0.0006	2.2857	0.0001	0.01486	0.00210	0.01162	0.00406
GLU	1000	C	W	22.91	0.82	16.053	0.0030	2.2173	0.0004	0.00000	0.00000	0.06655	0.00390
GLU	1000	C	W	110.36	9.08	16.8141	0.0006	2.1176	0.0001	0.05192	0.00286	0.02820	0.00556
GLU	1000	C	W	1022.09	35.90	17.2491	0.0002	2.0646	<0.0001	0.06800	0.00246	0.02901	0.00252

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	C	W	15.45	2.48	18.6144	0.0004	1.9144	<0.0001	0.01520	0.00148	0.00893	0.00336
GLU	1000	C	W	7.22	1.11	18.9888	0.0006	1.877	0.0001	0.01573	0.00186	0.01182	0.00414
GLU	1000	C	W	422.15	18.40	19.2041	0.0006	1.8561	0.0001	0.11669	0.00352	0.06156	0.00652
GLU	1000	C	W	921.64	16.69	19.5645	0.0004	1.8223	<0.0001	0.10605	0.00108	0.06677	0.00270
GLU	1000	C	W	64.30	5.94	19.9426	0.0016	1.7881	0.0001	0.08484	0.00406	0.05827	0.01248
GLU	1000	C	W	14.54	1.08	22.2496	0.0004	1.6046	<0.0001	0.01598	0.00086	0.01207	0.00198
GLU	1000	C	W	22.43	1.62	23.633	0.0060	1.5119	0.0004	0.00000	0.00000	0.15643	0.01812
GLU	1000	C	W	27.83	7.80	26.4867	0.0034	1.3515	0.0002	0.09898	0.01388	0.00000	0.00000
GLU	1000	C	W	38.31	5.66	26.8233	0.0036	1.3348	0.0002	0.13406	0.01416	0.09698	0.03386
GLU	1000	C	W	282.88	11.57	27.8244	0.0020	1.2877	0.0001	0.04326	0.00162	0.00481	0.00040
GLU	1000	D	H	146.31	6.96	8.384	0.0004	4.2355	0.0002	0.03908	0.00120	0.02436	0.00252
GLU	1000	D	H	824.38	20.89	9.9351	0.0002	3.5755	0.0001	0.05504	0.00110	0.03026	0.00172
GLU	1000	D	H	1406.17	22.70	10.7861	0.0002	3.2942	0.0001	0.06792	0.00078	0.04106	0.00142
GLU	1000	D	H	34.85	1.17	11.6954	0.0002	3.0388	0.0001	0.00771	0.00112	0.01133	0.00068
GLU	1000	D	H	1504.77	76.52	13.0137	0.0004	2.7321	0.0001	0.07053	0.00428	0.02604	0.00344
GLU	1000	D	H	7.83	0.93	14.2551	0.0004	2.4953	0.0001	0.01350	0.00084	0.00876	0.00242
GLU	1000	D	H	91.77	4.17	15.3416	0.0052	2.3195	0.0008	0.00000	0.00000	0.22911	0.01528
GLU	1000	D	H	124.78	15.09	16.8102	0.0008	2.1181	0.0001	0.05705	0.00614	0.02651	0.00802
GLU	1000	D	H	1023.63	295.39	17.2509	0.0004	2.0644	<0.0001	0.03487	0.01392	0.00000	0.00000
GLU	1000	D	H	5.42	0.79	18.6076	0.0010	1.9151	0.0001	0.01805	0.00982	0.02063	0.00654
GLU	1000	D	H	46.43	1.73	19.9458	0.0022	1.7878	0.0002	0.05885	0.03662	0.10041	0.00518
GLU	1000	D	H	20.37	1.88	23.6428	0.0072	1.5113	0.0005	0.00000	0.00000	0.14561	0.02162
GLU	1000	D	H	124.40	4.04	24.1865	0.0026	1.4778	0.0002	0.04058	0.00018	0.00418	0.00022
GLU	1000	D	H	136.09	2.92	26.1915	0.0034	1.3665	0.0002	0.04496	0.00016	0.00477	0.00002
GLU	1000	D	H	37.38	6.42	26.8285	0.0052	1.3346	0.0003	0.14037	0.03940	0.12138	0.04864
GLU	1000	D	H	169.08	13.86	27.2756	0.0012	1.3131	0.0001	0.12559	0.00882	0.05955	0.01222
GLU	1000	D	H	97.14	1.76	32.4366	0.0026	1.1085	0.0001	0.00000	0.00000	0.25856	0.00648
GLU	1000	D	D	108.03	6.72	8.3857	0.0004	4.2346	0.0002	0.03515	0.00158	0.02023	0.00280
GLU	1000	D	D	629.52	14.31	9.9366	0.0002	3.5750	0.0001	0.05221	0.00084	0.03112	0.00152
GLU	1000	D	D	1080.44	14.46	10.7883	0.0002	3.2935	0.0001	0.06702	0.00058	0.04536	0.00124
GLU	1000	D	D	41.67	1.85	11.7002	0.0002	3.0376	0.0001	0.00963	0.00190	0.01442	0.00114
GLU	1000	D	D	1149.74	35.69	13.0178	0.0004	2.7313	0.0001	0.08016	0.00248	0.03579	0.00272
GLU	1000	D	D	7.80	1.55	14.2572	0.0006	2.4949	0.0001	0.01245	0.00200	0.01007	0.00430
GLU	1000	D	D	108.03	3.39	15.3566	0.0040	2.3173	0.0006	0.18838	0.04738	0.24687	0.01120
GLU	1000	D	D	66.04	1.86	16.4638	0.0050	2.1624	0.0007	0.00000	0.00000	0.32111	0.01368
GLU	1000	D	D	92.33	11.33	16.8206	0.0006	2.1168	0.0001	0.05208	0.00622	0.02255	0.00704
GLU	1000	D	D	8.07	0.51	17.0020	0.0006	2.0944	0.0001	0.00000	0.00000	0.01445	0.00130
GLU	1000	D	D	782.82	18.02	17.2519	0.0002	2.0643	<0.0001	0.07987	0.00158	0.03986	0.00216
GLU	1000	D	D	8.73	2.26	18.6148	0.0010	1.9143	0.0001	0.02487	0.00324	0.01650	0.01010
GLU	1000	D	D	12.29	0.55	18.997	0.0004	1.8762	<0.0001	0.00000	0.00000	0.01833	0.00110
GLU	1000	D	D	317.22	13.29	19.2083	0.0008	1.8557	0.0001	0.12020	0.00352	0.06352	0.00642
GLU	1000	D	D	731.31	13.44	19.5702	0.0004	1.8217	<0.0001	0.11237	0.00124	0.06715	0.00284
GLU	1000	D	D	43.49	3.54	19.9491	0.0016	1.7875	0.0001	0.08476	0.00570	0.06871	0.01248
GLU	1000	D	D	22.52	1.68	21.2296	0.0130	1.6808	0.0010	0.00000	0.00000	0.29960	0.03716
GLU	1000	D	D	1.22	0.36	21.9571	0.0028	1.6257	0.0002	0.00000	0.00000	0.01614	0.00700
GLU	1000	D	D	15.71	1.77	23.4229	0.0002	1.5253	<0.0001	0.01145	0.00090	0.00853	0.00218
GLU	1000	D	D	2.48	0.32	24.8277	0.0018	1.4402	0.0001	0.00000	0.00000	0.02507	0.00458
GLU	1000	D	D	0.85	0.32	27.6186	0.0040	1.2971	0.0002	0.00000	0.00000	0.01759	0.01004
GLU	1000	D	D	1.26	0.27	28.7466	0.0030	1.2472	0.0001	0.00000	0.00000	0.02348	0.00740
GLU	1000	D	D	25.42	2.80	29.4056	0.0518	1.2199	0.0021	0.00000	0.00000	0.54121	0.12372
GLU	1000	D	D	41.67	6.39	30.1178	0.0032	1.1917	0.0001	0.09486	0.01752	0.02444	0.00938
GLU	1000	D	D	3.63	0.86	31.1199	0.0014	1.1542	0.0001	0.00000	0.00000	0.02084	0.01054
GLU	1000	D	D	2.71	0.40	31.1317	0.0020	1.1538	0.0001	0.00000	0.00000	0.02364	0.00532
GLU	1000	D	D	91.15	5.06	32.4356	0.0026	1.1086	0.0001	0.25064	0.00924	0.18187	0.02350
GLU	1000	D	D	2.52	1.10	34.3950	0.0018	1.0472	0.0001	0.01821	0.01084	0.00000	0.00000
GLU	1000	D	D	0.91	0.34	34.4648	0.0070	1.0451	0.0002	0.00000	0.00000	0.03062	0.01732
GLU	1000	D	D	4.65	1.26	34.6469	0.0172	1.0398	0.0005	0.00000	0.00000	0.10674	0.04394
GLU	1000	D	D	1.75	0.50	35.5965	0.0048	1.0129	0.0001	0.00000	0.00000	0.03247	0.01456
GLU	1000	D	D	28.29	3.09	35.9433	0.0172	1.0034	0.0005	0.00000	0.00000	0.32186	0.06874
GLU	1000	D	D	0.85	0.33	36.6436	0.0070	0.9849	0.0002	0.00000	0.00000	0.03070	0.01804
GLU	1000	D	D	50.47	7.81	38.3600	0.0040	0.9424	0.0001	0.21863	0.02338	0.11132	0.04340
GLU	1000	D	D	18.40	1.00	39.7507	0.0094	0.9107	0.0002	0.00000	0.00000	0.30069	0.02408
GLU	1000	D	W	146.33	7.83	8.3856	0.0004	4.2347	0.0002	0.03156	0.00096	0.01998	0.00234
GLU	1000	D	W	4.63	0.46	9.2104	0.0004	3.8562	0.0002	0.00864	0.00194	0.00921	0.00184
GLU	1000	D	W	866.49	26.11	9.933	0.0002	3.5763	0.0001	0.04247	0.00116	0.02079	0.00146
GLU	1000	D	W	1427.15	18.71	10.7846	0.0002	3.2946	0.0001	0.06025	0.00052	0.03894	0.00106
GLU	1000	D	W	130.96	3.15	11.6965	0.0002	3.0385	0.0001	0.00802	0.00078	0.01341	0.00054
GLU	1000	D	W	58.23	3.11	11.915	0.0238	2.983	0.0059	0.00000	0.00000	0.72444	0.05596
GLU	1000	D	W	1512.45	46.03	13.0135	0.0002	2.7322	<0.0001	0.07434	0.00228	0.03232	0.00240
GLU	1000	D	W	8.88	0.70	14.2562	0.0004	2.4951	0.0001	0.01057	0.00154	0.01050	0.00172
GLU	1000	D	W	9.92	1.15	15.5703	0.0004	2.2856	0.0001	0.01174	0.00108	0.00897	0.00238
GLU	1000	D	W	21.46	0.81	16.0561	0.0014	2.2169	0.0002	0.00000	0.00000	0.06422	0.00348
GLU	1000	D	W	112.95	10.72	16.8142	0.0008	2.1176	0.0001	0.04886	0.00312	0.02708	0.00612
GLU	1000	D	W	32.22	1.66	16.9953	0.0002	2.0952	<0.0001	0.00000	0.00000	0.01084	0.00094
GLU	1000	D	W	8.15	0.82	18.608	0.0004	1.915	<0.0001	0.01259	0.00232	0.01218	0.00262
GLU	1000	D	W	9.48	1.18	18.9897	0.0004	1.8769	<0.0001	0.01303	0.00088	0.00892	0.00254
GLU	1000	D	W	404.89	15.15	19.2038	0.0008	1.8562	0.0001	0.11521	0.00212	0.07288	0.00624
GLU	1000	D	W	909.10	15.26	19.5643	0.0004	1.8223	<0.0001	0.10257	0.00094	0.06660	0.00248
GLU	1000	D	W	56.68	3.91	19.9418	0.0014	1.7881	0.0001	0.07802	0.00516	0.06595	0.00986

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	D	W	31.52	1.29	20.3851	0.0054	1.7496	0.0005	0.03404	0.00242	0.00387	0.00004
GLU	1000	D	W	20.97	2.79	23.6412	0.0052	1.5114	0.0003	0.00000	0.00000	0.13049	0.03572
GLU	1000	D	W	36.73	6.42	25.2767	0.0068	1.4151	0.0004	0.19679	0.08938	0.17772	0.07096
GLU	1000	D	W	28.62	6.74	26.4875	0.0030	1.3515	0.0002	0.09718	0.00976	0.05832	0.03396
GLU	1000	D	W	37.19	4.89	26.8254	0.0034	1.3347	0.0002	0.13029	0.01352	0.09878	0.02994
GLU	1000	D	W	39.30	1.75	28.9973	0.0002	1.2367	<0.0001	0.00783	0.00208	0.01308	0.00104
GLU	1000	E	H	90.85	3.99	8.3843	0.0004	4.2353	0.0002	0.04097	0.00108	0.02865	0.00264
GLU	1000	E	H	199.39	6.88	8.3862	0.0004	4.2344	0.0002	0.03933	0.00090	0.02970	0.00208
GLU	1000	E	H	518.91	9.22	9.9352	0.0002	3.5755	0.0001	0.05671	0.00064	0.03826	0.00140
GLU	1000	E	H	1166.06	20.83	9.9361	0.0002	3.5752	0.0001	0.05403	0.00068	0.03247	0.00124
GLU	1000	E	H	170.56	4.74	10.2067	0.0002	3.4806	0.0001	0.01701	0.00030	0.01263	0.00070
GLU	1000	E	H	896.84	12.33	10.7867	0.0002	3.2940	0.0001	0.06834	0.00062	0.04487	0.00128
GLU	1000	E	H	2048.17	26.45	10.7872	0.0002	3.2938	0.0001	0.06727	0.00060	0.04130	0.00114
GLU	1000	E	H	10.30	1.01	11.6982	0.0008	3.0381	0.0002	0.00000	0.00000	0.01499	0.00198
GLU	1000	E	H	965.38	43.54	13.0154	0.0004	2.7318	0.0001	0.07202	0.00370	0.02716	0.00314
GLU	1000	E	H	2196.48	525.58	13.0159	0.0002	2.7317	<0.0001	0.03413	0.01122	0.00000	0.00000
GLU	1000	E	H	290.77	5.96	13.9411	0.0002	2.5512	<0.0001	0.01794	0.00024	0.01346	0.00054
GLU	1000	E	H	121.96	4.94	14.9516	0.0002	2.3796	<0.0001	0.01773	0.00046	0.01093	0.00098
GLU	1000	E	H	130.59	30.61	15.3409	0.0062	2.3196	0.0009	0.22771	0.04356	0.19621	0.06060
GLU	1000	E	H	150.22	12.52	15.5687	0.0464	2.2859	0.0068	0.00000	0.00000	0.62457	0.05854
GLU	1000	E	H	61.80	3.05	16.4518	0.0080	2.1640	0.0010	0.00000	0.00000	0.37052	0.02694
GLU	1000	E	H	165.52	11.03	16.8152	0.0008	2.1175	0.0001	0.06080	0.00210	0.03856	0.00592
GLU	1000	E	H	80.87	10.91	16.8177	0.0008	2.1172	0.0001	0.06002	0.00684	0.02859	0.00954
GLU	1000	E	H	346.71	7.73	17.0746	0.0000	2.0856	<0.0001	0.01804	0.00024	0.01225	0.00058
GLU	1000	E	H	1470.93	520.94	17.249	0.0004	2.0646	<0.0001	0.03562	0.01742	0.00000	0.00000
GLU	1000	E	H	628.48	12.90	17.2493	0.0004	2.0646	<0.0001	0.08787	0.00106	0.05339	0.00246
GLU	1000	E	H	4.02	1.39	18.1363	0.0014	1.9644	0.0002	0.01714	0.00488	0.01842	0.00834
GLU	1000	E	H	577.71	21.97	19.2050	0.0006	1.8560	0.0001	0.11791	0.00288	0.06556	0.00594
GLU	1000	E	H	251.80	9.66	19.2063	0.0008	1.8559	0.0001	0.12309	0.00244	0.07717	0.00684
GLU	1000	E	H	1360.46	29.88	19.5643	0.0004	1.8223	<0.0001	0.10451	0.00162	0.05652	0.00292
GLU	1000	E	H	612.48	14.89	19.5674	0.0004	1.822	<0.0001	0.10911	0.00168	0.06283	0.00354
GLU	1000	E	H	94.21	14.89	19.9449	0.0016	1.7878	0.0001	0.08443	0.01064	0.04182	0.01658
GLU	1000	E	H	39.44	5.33	19.9465	0.0022	1.7877	0.0002	0.09174	0.00636	0.07289	0.01678
GLU	1000	E	H	10.77	1.12	20.3806	0.0076	1.7500	0.0006	0.00000	0.00000	0.12099	0.02002
GLU	1000	E	H	169.77	5.04	20.497	0.0002	1.7402	<0.0001	0.01917	0.00034	0.01359	0.00086
GLU	1000	E	H	89.85	2.37	21.0848	0.0418	1.6922	0.0033	0.13333	0.01076	0.00701	0.00004
GLU	1000	E	H	62.65	7.75	21.2275	0.0174	1.6810	0.0014	0.04733	0.00020	0.00288	0.00070
GLU	1000	E	H	357.64	6.96	22.2929	0.0000	1.6016	<0.0001	0.01888	0.00024	0.01266	0.00050
GLU	1000	E	H	18.35	1.22	25.2805	0.0108	1.4149	0.0006	0.00000	0.00000	0.25898	0.02896
GLU	1000	E	H	138.41	4.06	25.4676	0.0002	1.4046	<0.0001	0.01874	0.00032	0.01240	0.00078
GLU	1000	E	H	79.76	6.32	26.0044	0.0394	1.3761	0.0021	0.05725	0.00026	0.00311	0.00002
GLU	1000	E	H	212.40	5.06	26.0498	0.0002	1.3738	<0.0001	0.01900	0.00026	0.01284	0.00066
GLU	1000	E	H	185.22	11.25	26.1918	0.0036	1.3664	0.0002	0.04811	0.00226	0.00543	0.00068
GLU	1000	E	H	12.16	0.77	26.4913	0.0042	1.3513	0.0002	0.09293	0.05860	0.11335	0.01074
GLU	1000	E	H	3.23	0.41	26.7997	0.0014	1.3360	0.0001	0.00000	0.00000	0.01825	0.00346
GLU	1000	E	H	64.63	3.60	26.8235	0.0036	1.3348	0.0002	0.06315	0.00080	0.01170	0.00110
GLU	1000	E	H	23.10	5.73	26.8282	0.0076	1.3346	0.0004	0.13579	0.01786	0.09286	0.04906
GLU	1000	E	H	237.66	16.77	27.2780	0.0012	1.3130	0.0001	0.13096	0.00676	0.06842	0.01176
GLU	1000	E	H	99.91	5.79	27.2829	0.0014	1.3128	0.0001	0.13662	0.00398	0.08361	0.01142
GLU	1000	E	H	4.79	0.68	28.0981	0.0010	1.2754	<0.0001	0.00000	0.00000	0.02081	0.00596
GLU	1000	E	H	67.22	2.40	28.941	0.0002	1.239	<0.0001	0.01964	0.00046	0.01494	0.00110
GLU	1000	E	H	35.70	2.42	29.0581	0.0002	1.2341	<0.0001	0.01941	0.00074	0.01253	0.00190
GLU	1000	E	H	61.31	14.84	30.1094	0.0036	1.1920	0.0001	0.13263	0.02132	0.06761	0.04144
GLU	1000	E	H	24.73	3.10	30.1684	0.0004	1.1897	<0.0001	0.02054	0.00118	0.01608	0.00422
GLU	1000	E	H	13.91	2.52	30.4219	0.0250	1.1800	0.0009	0.00000	0.00000	0.23818	0.07050
GLU	1000	E	H	77.86	12.63	30.8019	0.0052	1.1658	0.0002	0.22617	0.03494	0.16677	0.06648
GLU	1000	E	H	16.99	3.56	31.3133	0.0006	1.1472	<0.0001	0.01914	0.00350	0.01366	0.00668
GLU	1000	E	H	13.27	1.61	31.928	0.0006	1.1257	<0.0001	0.01959	0.00252	0.01580	0.00432
GLU	1000	E	H	10.46	2.26	31.9745	0.0006	1.1241	<0.0001	0.01897	0.00222	0.01105	0.00578
GLU	1000	E	H	29.02	2.07	32.727	0.0004	1.099	<0.0001	0.01989	0.00080	0.01392	0.00220
GLU	1000	E	H	6.67	1.25	33.2353	0.0008	1.0826	<0.0001	0.01899	0.00212	0.01371	0.00580
GLU	1000	E	H	30.89	1.72	33.3735	0.0004	1.0783	<0.0001	0.01990	0.00070	0.01542	0.00178
GLU	1000	E	H	69.10	2.24	34.0093	0.0048	1.0587	0.0001	0.08201	0.00454	0.01801	0.00012
GLU	1000	E	H	26.81	7.11	34.3311	0.0520	1.0491	0.0015	0.00000	0.00000	0.43113	0.25194
GLU	1000	E	H	62.57	3.19	34.547	0.0002	1.0427	<0.0001	0.02023	0.00054	0.01278	0.00148
GLU	1000	E	H	23.27	6.22	34.6696	0.0296	1.0391	0.0009	0.00000	0.00000	0.22935	0.09352
GLU	1000	E	H	8.48	4.07	35.4253	0.0008	1.0176	<0.0001	0.01880	0.00712	0.00000	0.00000
GLU	1000	E	H	43.01	2.35	36.1584	0.0002	0.9977	<0.0001	0.02012	0.00068	0.01448	0.00174
GLU	1000	E	H	1.30	0.32	36.6248	0.0042	0.9854	0.0001	0.00000	0.00000	0.02847	0.01052
GLU	1000	E	H	8.27	3.48	36.7543	0.0008	0.982	<0.0001	0.01940	0.00746	0.00000	0.00000
GLU	1000	E	H	10.34	1.31	38.689	0.0006	0.9347	<0.0001	0.01978	0.00198	0.01514	0.00430
GLU	1000	E	H	6.23	0.86	39.4165	0.0008	0.9181	<0.0001	0.01646	0.00874	0.02088	0.00542
GLU	1000	E	H	32.66	2.73	39.8849	0.0002	0.9077	<0.0001	0.02096	0.00092	0.01279	0.00250
GLU	1000	E	H	11.74	3.11	39.9992	0.0028	0.9053	0.0001	0.02087	0.00350	0.01465	0.00976
GLU	1000	E	W	4.20	0.97	5.7645	0.0200	6.1573	0.0214	0.00000	0.00000	0.15153	0.05356
GLU	1000	E	W	207.34	6.92	8.3870	0.0004	4.2340	0.0002	0.03343	0.00028	0.02123	0.00154
GLU	1000	E	W	214.19	13.72	8.3921	0.0004	4.2314	0.0002	0.03223	0.00168	0.01708	0.00252
GLU	1000	E	W	1173.91	23.56	9.9398	0.0002	3.5738	0.0001	0.04534	0.00066	0.02743	0.00118
GLU	1000	E	W	2049.00	25.70	10.7863	0.0002	3.2941	0.0001	0.06005	0.00048	0.04063	0.00104

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	E	W	2047.74	25.73	10.7913	0.0002	3.2926	0.0001	0.06002	0.00050	0.04069	0.00104
GLU	1000	E	W	34.12	3.21	11.9429	0.0228	2.9761	0.0057	0.00000	0.00000	0.40380	0.05622
GLU	1000	E	W	2164.02	400.71	13.0149	0.0002	2.7319	<0.0001	0.04269	0.01076	0.01014	0.00520
GLU	1000	E	W	2163.27	86.52	13.0199	0.0002	2.7308	<0.0001	0.06689	0.00296	0.02610	0.00266
GLU	1000	E	W	106.53	30.30	15.7996	0.0426	2.2527	0.0061	0.02545	0.00012	0.00078	0.00036
GLU	1000	E	W	172.41	17.92	16.8176	0.0008	2.1172	0.0001	0.05109	0.00400	0.02630	0.00662
GLU	1000	E	W	169.64	16.71	16.8225	0.0008	2.1166	0.0001	0.05176	0.00346	0.02834	0.00662
GLU	1000	E	W	1446.72	39.41	17.2522	0.0004	2.0643	<0.0001	0.07139	0.00158	0.03755	0.00236
GLU	1000	E	W	578.10	20.27	19.2034	0.0006	1.8562	0.0001	0.11114	0.00226	0.06600	0.00536
GLU	1000	E	W	1360.36	27.73	19.5648	0.0004	1.8222	<0.0001	0.10043	0.00130	0.05910	0.00274
GLU	1000	E	W	1367.05	27.16	19.5697	0.0004	1.8218	<0.0001	0.10073	0.00126	0.05901	0.00266
GLU	1000	E	W	91.32	13.19	19.9425	0.0014	1.7881	0.0001	0.07145	0.00748	0.03724	0.01316
GLU	1000	E	W	93.96	16.00	19.9475	0.0014	1.7876	0.0001	0.07037	0.00992	0.03381	0.01436
GLU	1000	E	W	55.26	2.19	20.8562	0.0122	1.7105	0.0010	0.20760	0.02390	0.09182	0.00110
GLU	1000	E	W	45.39	3.52	21.2221	0.0136	1.6814	0.0011	0.00000	0.00000	0.30303	0.03856
GLU	1000	E	W	4.30	0.73	22.2486	0.0018	1.6047	0.0001	0.00000	0.00000	0.01377	0.00366
GLU	1000	E	W	4.20	0.65	22.2534	0.0012	1.6044	0.0001	0.00000	0.00000	0.01336	0.00292
GLU	1000	E	W	52.42	13.97	26.0419	0.0956	1.3742	0.0050	0.00000	0.00000	0.43070	0.12378
GLU	1000	E	W	43.74	6.99	29.3685	0.0738	1.2214	0.0030	0.00000	0.00000	0.52721	0.14430
GLU	1000	E	W	53.02	11.30	30.1113	0.0034	1.1919	0.0001	0.11308	0.01518	0.07689	0.03924
GLU	1000	E	W	54.85	10.50	30.4169	0.1940	1.1802	0.0074	0.00000	0.00000	1.04429	0.34138
GLU	1000	E	W	79.12	14.53	30.4529	0.2108	1.1789	0.0080	0.00000	0.00000	1.28887	0.45184
GLU	1000	E	W	55.74	3.18	30.8146	0.0050	1.1654	0.0002	0.00000	0.00000	0.20231	0.01788
GLU	1000	E	W	178.92	13.22	32.4340	0.0028	1.1086	0.0001	0.22663	0.00804	0.14682	0.02556
GLU	1000	E	W	17.50	2.19	34.9024	0.0080	1.0324	0.0002	0.00000	0.00000	0.12819	0.02530
GLU	1000	E	W	44.59	7.90	36.3811	0.0072	0.9918	0.0002	0.03968	0.00834	0.00377	0.00150
GLU	1000	E	W	67.70	21.47	37.3944	0.0070	0.9658	0.0002	0.20861	0.04834	0.00000	0.00000
GLU	1000	E	W	72.94	6.50	38.3646	0.0042	0.9423	0.0001	0.18711	0.06368	0.17613	0.03430
GLU	1000	F	H	90.37	5.14	8.3841	0.0006	4.2354	0.0003	0.03937	0.00138	0.02521	0.00310
GLU	1000	F	H	211.25	11.07	8.3858	0.0004	4.2346	0.0002	0.03597	0.00128	0.02151	0.00250
GLU	1000	F	H	510.76	10.14	9.9355	0.0002	3.5754	0.0001	0.05535	0.00070	0.03666	0.00152
GLU	1000	F	H	1158.77	21.97	9.9367	0.0002	3.5750	0.0001	0.05354	0.00068	0.03402	0.00136
GLU	1000	F	H	173.77	4.80	10.2069	0.0002	3.4806	0.0001	0.01714	0.00034	0.01351	0.00074
GLU	1000	F	H	878.31	12.24	10.7870	0.0002	3.2939	0.0001	0.06721	0.00060	0.04669	0.00132
GLU	1000	F	H	2027.89	27.90	10.7877	0.0002	3.2937	0.0001	0.06522	0.00058	0.04249	0.00122
GLU	1000	F	H	1.65	0.49	11.6974	0.0056	3.0383	0.0015	0.00000	0.00000	0.03261	0.01418
GLU	1000	F	H	2156.08	627.15	13.0153	0.0002	2.7318	<0.0001	0.03423	0.01390	0.00000	0.00000
GLU	1000	F	H	949.59	34.59	13.0159	0.0004	2.7317	0.0001	0.07684	0.00292	0.03288	0.00296
GLU	1000	F	H	292.08	6.15	13.9413	0.0002	2.5512	<0.0001	0.01766	0.00026	0.01368	0.00056
GLU	1000	F	H	115.61	4.23	14.9521	0.0002	2.3796	<0.0001	0.01734	0.00048	0.01395	0.00100
GLU	1000	F	H	71.33	12.36	16.8175	0.0010	2.1172	0.0001	0.04884	0.00804	0.02197	0.00962
GLU	1000	F	H	335.66	7.14	17.075	0.0002	2.0855	<0.0001	0.01765	0.00028	0.01434	0.00060
GLU	1000	F	H	1462.40	296.87	17.2494	0.0004	2.0646	<0.0001	0.04555	0.01246	0.01144	0.00640
GLU	1000	F	H	637.46	219.38	17.2497	0.0004	2.0646	<0.0001	0.03847	0.01820	0.00000	0.00000
GLU	1000	F	H	2.95	0.82	18.1379	0.0024	1.9642	0.0003	0.00000	0.00000	0.01874	0.01010
GLU	1000	F	H	1.13	0.48	18.9966	0.0042	1.8762	0.0004	0.00000	0.00000	0.01678	0.01054
GLU	1000	F	H	577.68	21.94	19.2047	0.0008	1.8561	0.0001	0.11572	0.00272	0.06652	0.00596
GLU	1000	F	H	243.23	11.28	19.2079	0.0010	1.8558	0.0001	0.11926	0.00274	0.07659	0.00790
GLU	1000	F	H	1366.95	29.35	19.5633	0.0004	1.8224	<0.0001	0.10245	0.00144	0.05843	0.00290
GLU	1000	F	H	587.09	16.26	19.5674	0.0006	1.8220	0.0001	0.10781	0.00170	0.06593	0.00410
GLU	1000	F	H	29.91	2.56	19.9459	0.0028	1.7878	0.0002	0.00000	0.00000	0.10013	0.01638
GLU	1000	F	H	94.32	11.56	19.9461	0.0018	1.7877	0.0002	0.08912	0.00602	0.05194	0.01530
GLU	1000	F	H	10.05	2.26	20.3802	0.0092	1.7501	0.0008	0.00000	0.00000	0.11397	0.05294
GLU	1000	F	H	169.64	6.27	20.4975	0.0002	1.7401	<0.0001	0.01890	0.00042	0.01338	0.00102
GLU	1000	F	H	20.19	2.64	21.0928	0.0452	1.6916	0.0036	0.00000	0.00000	0.57003	0.12180
GLU	1000	F	H	1.61	0.46	24.8186	0.0020	1.4408	0.0001	0.00000	0.00000	0.01175	0.00502
GLU	1000	F	H	36.67	5.84	26.4885	0.0038	1.3514	0.0002	0.09751	0.03738	0.09454	0.03456
GLU	1000	F	H	50.66	2.47	26.8253	0.0040	1.3347	0.0002	0.10504	0.00624	0.14052	0.01102
GLU	1000	F	H	393.27	16.51	27.8247	0.0012	1.2877	0.0001	0.17585	0.00466	0.10116	0.00992
GLU	1000	F	H	58.66	1.67	34.0085	0.0038	1.0587	0.0001	0.04604	0.00276	0.00717	0.00008
GLU	1000	F	H	36.39	14.63	36.3844	0.0082	0.9917	0.0002	0.17488	0.03370	0.00000	0.00000
GLU	1000	F	H	174.35	6.52	36.9660	0.0050	0.9766	0.0001	0.05977	0.00058	0.00484	0.00032
GLU	1000	F	D	103.48	6.22	8.3850	0.0004	4.2350	0.0002	0.03293	0.00098	0.02157	0.00294
GLU	1000	F	D	9.48	1.61	8.5456	0.0546	4.1555	0.0267	0.00000	0.00000	0.33868	0.09650
GLU	1000	F	D	613.73	11.30	9.9341	0.0002	3.5759	0.0001	0.04629	0.00058	0.02919	0.00114
GLU	1000	F	D	1053.60	13.58	10.7857	0.0002	3.2943	0.0001	0.05983	0.00052	0.03949	0.00106
GLU	1000	F	D	1114.67	39.35	13.0148	0.0002	2.7319	<0.0001	0.06950	0.00268	0.02862	0.00254
GLU	1000	F	D	64.15	3.02	15.3365	0.0042	2.3203	0.0006	0.00000	0.00000	0.19727	0.01370
GLU	1000	F	D	222.20	19.85	15.5627	0.0252	2.2868	0.0037	0.57579	0.05672	0.48569	0.09310
GLU	1000	F	D	85.91	7.83	16.8185	0.0006	2.1171	0.0001	0.05028	0.00328	0.02660	0.00586
GLU	1000	F	D	1.02	0.37	16.9984	0.0028	2.0949	0.0003	0.00000	0.00000	0.01267	0.00668
GLU	1000	F	D	760.79	18.05	17.2473	0.0002	2.0648	<0.0001	0.07197	0.00142	0.03752	0.00208
GLU	1000	F	D	1.09	0.39	18.6076	0.0040	1.9151	0.0004	0.00000	0.00000	0.01922	0.01016
GLU	1000	F	D	298.38	10.46	19.2030	0.0008	1.8562	0.0001	0.11350	0.00210	0.07145	0.00572
GLU	1000	F	D	730.72	234.18	19.5667	0.0004	1.8221	<0.0001	0.04320	0.01906	0.00000	0.00000
GLU	1000	F	D	39.05	2.76	19.9443	0.0018	1.7879	0.0002	0.06920	0.01054	0.07865	0.01138
GLU	1000	F	D	28.67	3.98	25.2797	0.0058	1.4149	0.0003	0.21538	0.03460	0.21602	0.05120
GLU	1000	F	D	31.59	1.72	29.4391	0.0238	1.2185	0.0010	0.00000	0.00000	0.64590	0.05026
GLU	1000	F	D	37.07	7.14	30.1093	0.0026	1.1920	0.0001	0.12912	0.01842	0.06449	0.03180

Amino Acid	Conc. mg/L	Method	Time	Area	Area esd	° 2Θ	2 esd ° 2Θ	d-spacing	2 esd d-spacing	βL	2 esd βL	βG	2 esd βG
GLU	1000	F	D	34.07	1.05	30.8132	0.0040	1.1654	0.0001	0.00000	0.00000	0.22868	0.01048
GLU	1000	F	D	1.09	0.38	31.1272	0.0062	1.1539	0.0002	0.00000	0.00000	0.03062	0.01586
GLU	1000	F	D	96.06	21.75	36.9717	0.0046	0.9765	0.0001	0.06150	0.01868	0.00476	0.00290
GLU	1000	F	W	111.56	3.24	8.3857	0.0004	4.2346	0.0002	0.03124	0.00022	0.01958	0.00122
GLU	1000	F	W	211.33	8.64	8.3913	0.0002	4.2318	0.0001	0.03015	0.00084	0.01728	0.00160
GLU	1000	F	W	630.02	10.89	9.9346	0.0002	3.5757	0.0001	0.04401	0.00052	0.02721	0.00100
GLU	1000	F	W	1178.69	15.98	9.9396	0.0002	3.5739	0.0001	0.04328	0.00040	0.02706	0.00078
GLU	1000	F	W	1084.15	14.19	10.7864	0.0002	3.2941	0.0001	0.05803	0.00050	0.03884	0.00104
GLU	1000	F	W	2037.33	17.41	10.7910	0.0002	3.2927	0.0001	0.05849	0.00032	0.04123	0.00070
GLU	1000	F	W	9.51	3.46	11.7003	0.0006	3.0376	0.0002	0.01118	0.00380	0.00000	0.00000
GLU	1000	F	W	7.41	3.63	11.7037	0.0010	3.0367	0.0003	0.01475	0.00530	0.00000	0.00000
GLU	1000	F	W	29.36	2.67	11.9548	0.0152	2.9731	0.0038	0.03544	0.00018	0.00156	0.00024
GLU	1000	F	W	1150.62	34.35	13.0159	0.0002	2.7317	<0.0001	0.06966	0.00224	0.02908	0.00216
GLU	1000	F	W	2059.20	42.78	13.0203	0.0002	2.7307	<0.0001	0.07083	0.00150	0.03148	0.00160
GLU	1000	F	W	233.98	9.54	15.6342	0.0168	2.2764	0.0024	0.00000	0.00000	0.53688	0.04244
GLU	1000	F	W	141.47	2.98	16.4548	0.0042	2.1636	0.0005	0.00000	0.00000	0.36657	0.01220
GLU	1000	F	W	87.29	6.78	16.8209	0.0008	2.1168	0.0001	0.04944	0.00214	0.03030	0.00540
GLU	1000	F	W	174.84	1.95	16.8230	0.0004	2.1165	0.0001	0.03745	0.00058	0.01232	0.00008
GLU	1000	F	W	5.02	0.58	17.0028	0.0012	2.0943	0.0001	0.00000	0.00000	0.01799	0.00302
GLU	1000	F	W	776.48	19.70	17.2487	0.0002	2.0647	<0.0001	0.06808	0.00152	0.03398	0.00202
GLU	1000	F	W	1408.49	30.09	17.2528	0.0002	2.0642	<0.0001	0.06511	0.00136	0.03001	0.00156
GLU	1000	F	W	33.75	5.87	17.8349	0.0374	1.9973	0.0042	0.01813	0.00010	0.00027	0.00008
GLU	1000	F	W	314.01	10.52	19.2059	0.0006	1.8560	0.0001	0.11151	0.00204	0.06596	0.00520
GLU	1000	F	W	547.61	12.54	19.2085	0.0004	1.8557	<0.0001	0.10986	0.00138	0.06878	0.00358
GLU	1000	F	W	739.61	12.53	19.5693	0.0004	1.8218	<0.0001	0.10067	0.00102	0.06131	0.00234
GLU	1000	F	W	1306.49	17.91	19.5704	0.0002	1.8217	<0.0001	0.09925	0.00082	0.06015	0.00186
GLU	1000	F	W	93.88	10.99	19.9490	0.0012	1.7875	0.0001	0.07983	0.00620	0.04291	0.01228
GLU	1000	F	W	55.70	2.83	20.3890	0.0038	1.7493	0.0003	0.03475	0.00036	0.00317	0.00026
GLU	1000	F	W	12.81	2.11	20.8468	0.0136	1.7113	0.0011	0.00000	0.00000	0.16304	0.04188
GLU	1000	F	W	102.23	13.50	21.1202	0.0560	1.6894	0.0044	0.00000	0.00000	0.75466	0.20376
GLU	1000	F	W	43.05	5.77	21.2232	0.0100	1.6813	0.0008	0.00000	0.00000	0.29931	0.09172
GLU	1000	F	W	698.96	255.32	21.672	0.0006	1.6469	<0.0001	0.04523	0.02302	0.00000	0.00000
GLU	1000	F	W	2.09	0.44	21.9564	0.0010	1.6258	0.0001	0.00000	0.00000	0.00883	0.00296
GLU	1000	F	W	18.47	3.40	22.4023	0.0498	1.5938	0.0035	0.05558	0.01002	0.00269	0.00086
GLU	1000	F	W	0.90	0.32	23.4186	0.0030	1.5256	0.0002	0.00000	0.00000	0.01473	0.00788
GLU	1000	F	W	34.44	1.02	23.6430	0.0052	1.5113	0.0003	0.10012	0.03698	0.12947	0.00092
GLU	1000	F	W	33.76	7.26	25.2436	0.0126	1.4169	0.0007	0.15789	0.02562	0.15842	0.05296
GLU	1000	F	W	28.44	1.04	25.2820	0.0054	1.4148	0.0003	0.17123	0.09010	0.25975	0.01374
GLU	1000	F	W	46.59	2.52	25.9793	0.0212	1.3774	0.0011	0.03265	0.00022	0.00392	0.00002
GLU	1000	F	W	64.69	13.07	26.1262	0.0524	1.3698	0.0027	0.00000	0.00000	0.48640	0.04102
GLU	1000	F	W	80.57	20.06	26.1933	0.0022	1.3664	0.0001	0.15170	0.02610	0.14151	0.05036
GLU	1000	F	W	39.68	5.97	26.4900	0.0024	1.3513	0.0001	0.09874	0.00696	0.08584	0.02232
GLU	1000	F	W	58.52	6.27	26.8309	0.0022	1.3345	0.0001	0.12716	0.00638	0.09850	0.01946
GLU	1000	F	W	248.24	2.93	27.286	0.0010	1.3126	<0.0001	0.04897	0.00030	0.00888	0.00010
GLU	1000	F	W	406.17	4.96	27.8299	0.0008	1.2875	<0.0001	0.05107	0.00034	0.00695	0.00014
GLU	1000	F	W	36.09	2.56	29.2631	0.0342	1.2257	0.0014	0.05698	0.00040	0.00315	0.00008
GLU	1000	F	W	25.06	1.71	29.5670	0.0244	1.2134	0.0010	0.05102	0.00810	0.00385	0.00008
GLU	1000	F	W	70.55	29.93	30.1144	0.0020	1.1918	0.0001	0.09307	0.04696	0.00000	0.00000
GLU	1000	F	W	16.94	2.58	30.4148	0.0116	1.1803	0.0004	0.09622	0.00124	0.02256	0.00634
GLU	1000	F	W	102.73	41.67	30.8150	0.0038	1.1653	0.0001	0.19488	0.08984	0.00000	0.00000
GLU	1000	F	W	2.78	0.49	31.1300	0.0020	1.1538	0.0001	0.00000	0.00000	0.01948	0.00512
GLU	1000	F	W	123.09	20.41	31.3201	0.0034	1.1470	0.0001	0.17726	0.01508	0.09235	0.03894
GLU	1000	F	W	15.05	1.02	34.2260	0.0314	1.0522	0.0009	0.03907	0.00886	0.00194	0.00004
GLU	1000	F	W	47.75	1.39	38.9755	0.0122	0.9281	0.0003	0.02786	0.00168	0.39282	0.03198
GLU	1000	F	W	61.57	3.21	39.7467	0.0072	0.9108	0.0002	0.05041	0.00040	0.00351	0.00032
GLU	1000	F	W	37.44	2.12	40.3005	0.0158	0.8988	0.0003	0.00000	0.00000	0.47889	0.04486
GLU	1000	F	W	19.20	1.57	41.0134	0.0152	0.8838	0.0003	0.00000	0.00000	0.31718	0.04156
GLU	1000	F	W	15.79	6.92	41.4803	0.0100	0.8743	0.0002	0.26238	0.07314	0.33677	0.03786
GLU	1000	F	W	14.20	1.45	42.3301	0.0200	0.8575	0.0004	0.00000	0.00000	0.33209	0.05278
GLU	1000	F	W	19.15	1.80	42.9074	0.0238	0.8465	0.0004	0.00000	0.00000	0.43174	0.06410
GLU	1000	F	W	25.73	0.67	43.6086	0.0124	0.8335	0.0002	0.00000	0.00000	0.34567	0.00180
GLU	1000	F	W	32.55	2.55	45.0519	0.0388	0.8082	0.0007	0.00000	0.00000	0.93598	0.08982
GLU	1000	F	W	11.08	0.89	46.0289	0.0170	0.7919	0.0003	0.00000	0.00000	0.33091	0.04232
GLU	1000	F	W	26.70	1.41	46.5831	0.0146	0.7830	0.0002	0.00000	0.00000	0.54226	0.04644
GLU	1000	F	W	42.37	17.42	47.7090	0.0078	0.7656	0.0001	0.33433	0.14438	0.00000	0.00000
GLU	1000	F	W	8.70	1.26	50.0320	0.0362	0.7322	0.0005	0.00000	0.00000	0.45035	0.11704

The tables presented over the next few pages provide all valid crystallite size data. Duplicates have been removed and only the values with the highest confidence have been included.

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	10	A	H	8.3907	126.0	4.5	ASP	10	B	H	19.0042	717.8	108.1
ASP	10	A	H	9.2152	1050.7	267.7	ASP	10	B	H	19.2080	33.1	1.2
ASP	10	A	H	9.9387	80.5	1.2	ASP	10	B	H	19.5720	37.3	0.5
ASP	10	A	H	10.7901	59.1	0.7	ASP	10	B	H	19.9482	58.1	13.6
ASP	10	A	H	11.7072	985.9	77.3	ASP	10	B	H	21.6719	26.4	0.6
ASP	10	A	H	12.4997	748.7	246.3	ASP	10	B	H	22.2560	553.3	76.2
ASP	10	A	H	13.0200	47.3	1.2	ASP	10	B	H	23.4216	1095.9	725.4
ASP	10	A	H	14.2574	601.0	46.8	ASP	10	B	H	23.5356	548.7	188.0
ASP	10	A	H	15.5747	535.5	53.7	ASP	10	B	H	24.2026	23.2	2.6
ASP	10	A	H	16.8237	79.7	7.9	ASP	10	B	H	24.8245	765.2	142.6
ASP	10	A	H	17.0012	2914.5	1187.5	ASP	10	B	H	25.1516	670.2	294.7
ASP	10	A	H	17.2544	88.0	38.0	ASP	10	B	H	26.2027	158.4	38.7
ASP	10	A	H	18.4852	827.9	157.7	ASP	10	B	H	26.8306	30.8	3.6
ASP	10	A	H	18.6296	604.2	42.6	ASP	10	B	H	27.2917	31.7	2.1
ASP	10	A	H	19.0040	525.0	53.5	ASP	10	B	H	27.6243	588.6	388.2
ASP	10	A	H	19.2096	30.3	1.0	ASP	10	B	H	27.8309	22.5	1.1
ASP	10	A	H	19.5714	34.6	0.9	ASP	10	B	H	30.1161	33.6	14.9
ASP	10	A	H	19.9495	59.0	21.9	ASP	10	B	H	30.8137	18.8	6.9
ASP	10	A	H	21.6732	24.9	0.6	ASP	10	B	H	31.1291	441.8	82.7
ASP	10	A	H	21.9556	528.1	102.2	ASP	10	B	H	31.3207	20.0	3.1
ASP	10	A	H	22.2556	445.0	22.8	ASP	10	B	H	31.5276	14.6	6.5
ASP	10	A	H	22.4960	436.2	82.3	ASP	10	B	H	32.4402	16.2	1.2
ASP	10	A	H	23.1534	18.3	0.8	ASP	10	B	H	34.3890	1262.6	625.1
ASP	10	A	H	23.4209	932.3	115.0	ASP	10	B	H	34.4693	689.2	280.6
ASP	10	A	H	23.6683	351.9	40.9	ASP	10	B	H	35.5119	22.9	10.4
ASP	10	A	H	24.2025	19.8	0.7	ASP	10	B	H	36.9778	12.7	6.3
ASP	10	A	H	24.8236	561.7	113.7	ASP	10	B	H	37.4186	14.4	6.1
ASP	10	A	H	25.1521	330.3	80.6	ASP	10	B	H	38.3801	18.7	6.1
ASP	10	A	H	26.7347	309.4	62.4	ASP	10	B	H	38.5518	443.0	258.1
ASP	10	A	H	27.2901	30.4	2.2	ASP	10	B	D	9.2147	6056.6	3856.3
ASP	10	A	H	27.6233	331.3	54.3	ASP	10	B	D	12.4973	1974.8	771.2
ASP	10	A	H	28.7400	443.5	98.8	ASP	10	B	D	12.6040	548.2	336.1
ASP	10	A	H	29.0267	339.8	37.9	ASP	10	B	D	18.4827	2917.4	1039.7
ASP	10	A	H	29.6252	16.3	6.7	ASP	10	B	D	18.6285	1881.4	336.0
ASP	10	A	H	30.4231	500.6	209.1	ASP	10	B	D	19.0025	3235.2	935.7
ASP	10	A	H	30.8127	16.4	4.7	ASP	10	B	D	21.9524	2453.2	948.2
ASP	10	A	H	31.1291	314.9	36.1	ASP	10	B	D	22.2530	3155.6	1455.2
ASP	10	A	H	31.3226	20.4	4.6	ASP	10	B	D	23.6660	1715.8	1037.8
ASP	10	A	H	32.4438	14.7	0.7	ASP	10	B	D	24.2592	2495.2	822.4
ASP	10	A	H	33.9120	426.0	276.6	ASP	10	B	D	24.8216	3370.6	2040.9
ASP	10	A	H	34.3875	633.6	93.6	ASP	10	B	D	25.1489	1524.6	757.9
ASP	10	A	H	34.4696	502.0	151.8	ASP	10	B	D	26.3746	786.2	125.2
ASP	10	A	H	34.7971	244.5	110.1	ASP	10	B	D	26.7319	1016.9	279.6
ASP	10	A	H	35.5151	18.1	4.6	ASP	10	B	D	27.6200	1053.6	184.8
ASP	10	A	H	35.6277	367.0	46.1	ASP	10	B	D	27.8790	1301.8	454.5
ASP	10	A	H	35.9381	10.2	2.1	ASP	10	B	D	28.7347	1720.2	638.9
ASP	10	A	H	36.6456	345.2	90.0	ASP	10	B	D	29.0240	1008.2	170.7
ASP	10	A	H	36.9702	13.4	5.2	ASP	10	B	D	30.2405	861.1	254.1
ASP	10	A	H	38.3703	16.1	1.1	ASP	10	B	D	30.4223	1203.4	296.3
ASP	10	A	H	38.5520	426.0	85.0	ASP	10	B	D	30.6025	797.4	454.6
ASP	10	A	D	15.5740	2677.8	907.4	ASP	10	B	D	31.1270	1475.0	390.1
ASP	10	A	D	18.4871	2377.7	1122.6	ASP	10	B	D	31.4460	2678.3	1255.3
ASP	10	A	D	18.6298	1159.5	331.6	ASP	10	B	D	34.4682	1541.1	579.3
ASP	10	A	D	22.2551	443.4	145.7	ASP	10	B	D	34.7957	552.1	87.4
ASP	10	A	D	22.4971	854.5	213.3	ASP	10	B	D	35.6264	861.6	194.6
ASP	10	A	D	23.5372	5531.8	3440.3	ASP	10	B	D	36.4529	921.4	445.5
ASP	10	A	D	23.6688	785.9	187.8	ASP	10	B	D	36.6443	755.7	134.4
ASP	10	A	D	26.3782	1652.9	420.1	ASP	10	B	D	36.8007	611.7	277.5
ASP	10	A	D	26.7347	650.5	391.3	ASP	10	B	D	36.9541	719.5	244.4
ASP	10	A	D	27.8831	1157.7	256.8	ASP	10	B	D	37.4716	1881.9	712.5
ASP	10	A	D	28.7379	771.2	334.6	ASP	10	B	D	37.7750	1064.0	636.9
ASP	10	A	D	30.4231	979.1	130.9	ASP	10	B	D	38.3302	1527.8	762.1
ASP	10	A	D	31.1320	1700.2	552.8	ASP	10	B	W	12.4983	4212.5	1664.0
ASP	10	A	D	34.3873	1686.8	471.5	ASP	10	B	W	12.6050	812.8	286.3
ASP	10	A	D	34.8004	322.4	171.8	ASP	10	B	W	18.4862	4030.4	2065.0
ASP	10	A	D	37.7751	510.6	325.4	ASP	10	B	W	18.6319	6300.0	2586.3
ASP	10	B	H	8.3908	148.4	5.4	ASP	10	B	W	19.0055	9946.4	6047.9
ASP	10	B	H	9.2149	774.2	161.2	ASP	10	B	W	23.6728	1936.4	589.2
ASP	10	B	H	9.9379	87.4	1.2	ASP	10	B	W	24.2638	3443.3	1592.3
ASP	10	B	H	10.7895	64.4	0.6	ASP	10	B	W	24.8271	4287.8	2741.0
ASP	10	B	H	11.7072	770.7	53.8	ASP	10	B	W	26.7384	2751.2	1020.0
ASP	10	B	H	13.0197	53.4	2.0	ASP	10	B	W	27.6288	2561.2	1413.0
ASP	10	B	H	14.2572	818.4	108.7	ASP	10	B	W	27.8877	2954.9	1758.1
ASP	10	B	H	15.5740	614.5	58.8	ASP	10	B	W	29.0305	3411.6	2002.3
ASP	10	B	H	16.0626	42.3	2.5	ASP	10	B	W	30.4258	1772.0	379.8
ASP	10	B	H	16.8250	89.0	8.5	ASP	10	B	W	30.6111	869.2	500.2
ASP	10	B	H	17.0014	1593.8	870.0	ASP	10	B	W	31.1329	1452.2	212.8
ASP	10	B	H	17.2523	50.6	1.0	ASP	10	B	W	31.4515	2295.8	578.0
ASP	10	B	H	18.6296	446.0	82.1	ASP	10	B	W	31.9586	1922.2	1092.6

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	10	B	W	34.3942	4757.2	2931.5
ASP	10	B	W	34.4752	2308.2	741.3
ASP	10	B	W	35.6352	1121.2	151.3
ASP	10	B	W	36.4622	1204.0	288.6
ASP	10	B	W	36.6542	1474.9	315.0
ASP	10	B	W	36.8086	1065.0	285.4
ASP	10	B	W	36.9625	935.7	124.0
ASP	10	B	W	37.4043	1960.0	628.2
ASP	10	B	W	37.4797	795.5	114.4
ASP	10	B	W	38.3379	2525.5	977.6
ASP	10	B	W	38.5610	1591.0	757.0
ASP	10	C	H	8.3857	132.5	4.4
ASP	10	C	H	9.2105	973.1	73.9
ASP	10	C	H	9.9363	89.7	1.6
ASP	10	C	H	10.7878	63.9	0.8
ASP	10	C	H	11.7020	1133.0	61.3
ASP	10	C	H	12.4964	758.2	126.5
ASP	10	C	H	13.0134	53.1	1.6
ASP	10	C	H	14.2533	810.9	50.2
ASP	10	C	H	15.5712	780.6	47.1
ASP	10	C	H	16.0623	44.9	0.3
ASP	10	C	H	16.8160	80.5	3.4
ASP	10	C	H	16.9960	1299.2	187.6
ASP	10	C	H	17.2487	56.7	1.5
ASP	10	C	H	18.4821	537.1	36.8
ASP	10	C	H	18.6262	696.6	38.7
ASP	10	C	H	19.0010	690.2	48.1
ASP	10	C	H	19.2051	34.4	2.3
ASP	10	C	H	19.5688	37.5	0.8
ASP	10	C	H	19.9455	50.8	4.9
ASP	10	C	H	21.6661	32.0	2.4
ASP	10	C	H	21.9501	732.6	68.7
ASP	10	C	H	22.2522	586.4	41.0
ASP	10	C	H	22.4911	518.7	247.4
ASP	10	C	H	23.4179	827.9	108.0
ASP	10	C	H	23.5318	704.3	109.9
ASP	10	C	H	23.6647	512.5	192.5
ASP	10	C	H	24.2579	556.2	57.7
ASP	10	C	H	24.8201	781.6	88.2
ASP	10	C	H	25.1464	506.0	74.2
ASP	10	C	H	26.4806	38.3	6.7
ASP	10	C	H	26.7278	535.7	48.3
ASP	10	C	H	26.8267	31.1	0.1
ASP	10	C	H	27.2865	40.5	12.6
ASP	10	C	H	27.6201	597.2	65.2
ASP	10	C	H	28.7349	619.8	88.7
ASP	10	C	H	29.0218	510.8	52.2
ASP	10	C	H	30.4184	776.3	106.6
ASP	10	C	H	30.5975	399.2	213.3
ASP	10	C	H	31.1240	461.1	30.2
ASP	10	C	H	31.4424	540.7	109.9
ASP	10	C	H	31.9478	504.1	181.9
ASP	10	C	H	33.9058	552.1	336.6
ASP	10	C	H	34.3872	949.4	311.5
ASP	10	C	H	34.4666	700.8	142.1
ASP	10	C	H	34.7921	283.3	87.8
ASP	10	C	H	35.6218	499.8	71.1
ASP	10	C	H	36.6416	473.3	148.0
ASP	10	C	H	36.9495	504.1	162.3
ASP	10	C	H	37.4677	423.7	62.6
ASP	10	C	H	37.7686	253.6	73.7
ASP	10	C	H	38.3270	463.8	68.6
ASP	10	C	H	38.5468	487.2	136.6
ASP	10	C	D	9.2102	5580.2	1822.1
ASP	10	C	D	11.7024	6395.0	1195.5
ASP	10	C	D	12.4961	1501.3	354.8
ASP	10	C	D	14.2531	13282.5	3503.9
ASP	10	C	D	15.5713	5994.1	1611.4
ASP	10	C	D	16.9956	6067.6	2116.1
ASP	10	C	D	18.4819	1029.3	104.7
ASP	10	C	D	18.6266	1311.6	151.0
ASP	10	C	D	19.0031	2379.3	450.2
ASP	10	C	D	21.9536	2671.0	755.5
ASP	10	C	D	22.2516	1074.2	219.7
ASP	10	C	D	22.2536	1631.8	249.5
ASP	10	C	D	23.4175	3529.2	928.1
ASP	10	C	D	23.5328	3369.4	1252.9
ASP	10	C	D	23.6653	1366.5	214.5
ASP	10	C	D	24.2577	1616.8	320.5
ASP	10	C	D	24.8173	1893.8	288.2
ASP	10	C	D	25.1483	543.0	138.5
ASP	10	C	D	26.3747	1478.3	273.1
ASP	10	C	D	26.7297	1093.0	124.6
ASP	10	C	D	27.6216	993.5	160.6
ASP	10	C	D	27.8812	1082.2	236.2
ASP	10	C	D	28.7370	1459.8	269.9
ASP	10	C	D	29.0249	1028.0	132.8
ASP	10	C	D	30.4205	2442.1	763.6
ASP	10	C	D	31.1243	795.9	50.1
ASP	10	C	D	31.4439	798.4	118.8
ASP	10	C	D	33.9079	866.9	227.6
ASP	10	C	D	34.3846	1741.9	336.1
ASP	10	C	D	34.4659	1331.1	233.1
ASP	10	C	D	34.7949	412.5	40.8
ASP	10	C	D	35.6242	847.8	84.5
ASP	10	C	D	36.9520	1401.3	530.7
ASP	10	C	D	37.3948	1450.4	550.3
ASP	10	C	D	37.4699	525.4	63.0
ASP	10	C	D	37.7741	977.9	530.1
ASP	10	C	D	37.9511	906.8	445.2
ASP	10	C	D	38.3281	1332.5	343.4
ASP	10	C	D	38.5493	1603.3	983.7
ASP	10	C	W	12.4945	2535.8	837.8
ASP	10	C	W	15.5706	5134.3	1845.0
ASP	10	C	W	18.4863	5195.6	3122.2
ASP	10	C	W	18.6258	2603.1	1534.8
ASP	10	C	W	18.9986	2621.5	1132.3
ASP	10	C	W	22.2509	2119.4	490.8
ASP	10	C	W	22.4987	1744.8	568.9
ASP	10	C	W	24.8165	4439.3	1867.6
ASP	10	C	W	25.1464	1083.6	166.2
ASP	10	C	W	26.7387	2576.4	929.7
ASP	10	C	W	29.0305	2452.7	1028.0
ASP	10	C	W	30.4257	3183.5	1015.0
ASP	10	C	W	30.6092	745.8	295.7
ASP	10	C	W	31.1330	2278.9	525.3
ASP	10	C	W	31.4430	997.1	314.1
ASP	10	C	W	31.9583	1882.9	1103.4
ASP	10	C	W	34.4753	2563.1	1082.2
ASP	10	C	W	34.7927	476.4	98.4
ASP	10	C	W	35.6345	2309.0	555.1
ASP	10	C	W	36.4622	962.1	200.8
ASP	10	C	W	36.6543	2468.6	800.3
ASP	10	C	W	36.8079	1217.5	427.1
ASP	10	C	W	36.9622	1219.3	295.9
ASP	10	C	W	37.4047	3254.3	1843.1
ASP	10	C	W	37.4797	1892.6	707.2
ASP	10	C	W	37.7834	1052.4	243.3
ASP	10	C	W	37.9622	2895.9	1717.3
ASP	10	D	H	8.3906	143.6	14.4
ASP	10	D	H	9.2146	1060.1	121.7
ASP	10	D	H	9.9374	95.2	2.7
ASP	10	D	H	10.7890	65.5	1.1
ASP	10	D	H	11.7060	1101.6	51.5
ASP	10	D	H	12.4973	552.7	64.3
ASP	10	D	H	13.0189	68.7	10.6
ASP	10	D	H	14.2572	826.0	59.2
ASP	10	D	H	15.5737	737.2	42.1
ASP	10	D	H	16.8234	80.9	9.8
ASP	10	D	H	17.0006	1024.7	92.2
ASP	10	D	H	17.2516	60.5	3.3
ASP	10	D	H	18.4839	520.0	30.3
ASP	10	D	H	18.6278	478.0	18.4
ASP	10	D	H	19.0029	570.8	26.2
ASP	10	D	H	19.2072	32.8	1.5
ASP	10	D	H	19.5707	39.3	1.6
ASP	10	D	H	20.8868	166.7	12.3
ASP	10	D	H	21.9544	627.1	72.4
ASP	10	D	H	22.2548	583.6	33.6
ASP	10	D	H	22.4936	412.3	51.4
ASP	10	D	H	23.4198	653.3	51.0
ASP	10	D	H	23.5333	616.8	59.1
ASP	10	D	H	23.6670	446.8	44.6
ASP	10	D	H	24.2606	469.2	49.1
ASP	10	D	H	24.8232	534.4	36.2
ASP	10	D	H	25.1474	352.1	27.4
ASP	10	D	H	26.3764	510.7	93.7
ASP	10	D	H	26.7324	438.5	42.3

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	10	D	H	27.6218	426.4	40.2	ASP	10	D	W	27.6280	1325.4	495.3
ASP	10	D	H	27.8820	507.9	128.7	ASP	10	D	W	27.8874	1475.7	490.6
ASP	10	D	H	28.7391	477.0	52.3	ASP	10	D	W	28.7439	1909.5	653.0
ASP	10	D	H	29.0236	416.2	37.6	ASP	10	D	W	29.0301	750.3	88.5
ASP	10	D	H	30.2400	581.7	233.8	ASP	10	D	W	30.2327	935.4	341.9
ASP	10	D	H	30.4208	500.5	39.2	ASP	10	D	W	30.4270	1223.6	173.3
ASP	10	D	H	30.6002	348.5	80.1	ASP	10	D	W	30.6096	745.8	331.5
ASP	10	D	H	31.1274	753.6	79.1	ASP	10	D	W	31.1329	828.4	68.1
ASP	10	D	H	31.4455	430.3	44.0	ASP	10	D	W	31.4506	1342.5	208.5
ASP	10	D	H	31.9508	439.8	132.8	ASP	10	D	W	31.9593	814.7	142.0
ASP	10	D	H	33.9082	370.2	44.2	ASP	10	D	W	33.9169	1197.6	307.8
ASP	10	D	H	34.3873	729.4	144.0	ASP	10	D	W	34.3932	1710.8	424.7
ASP	10	D	H	34.4673	479.3	43.4	ASP	10	D	W	34.4583	542.9	69.5
ASP	10	D	H	35.2234	545.5	281.2	ASP	10	D	W	34.8028	478.3	52.2
ASP	10	D	H	35.6240	345.2	26.5	ASP	10	D	W	35.2313	927.8	292.1
ASP	10	D	H	36.4555	526.6	205.8	ASP	10	D	W	35.6132	582.5	73.5
ASP	10	D	H	36.6440	483.1	73.1	ASP	10	D	W	36.4622	1078.8	442.1
ASP	10	D	H	36.7994	407.6	201.1	ASP	10	D	W	36.6537	1025.6	162.2
ASP	10	D	H	36.9515	366.4	52.2	ASP	10	D	W	36.8079	775.6	182.6
ASP	10	D	H	37.4711	353.1	94.8	ASP	10	D	W	36.9610	696.9	81.6
ASP	10	D	H	37.7718	422.5	231.3	ASP	10	D	W	37.4034	1001.2	177.9
ASP	10	D	H	37.9538	419.3	140.9	ASP	10	D	W	37.4793	629.7	55.6
ASP	10	D	H	38.3304	391.7	53.8	ASP	10	D	W	37.7840	794.0	119.9
ASP	10	D	H	38.5493	346.6	48.0	ASP	10	D	W	37.9434	449.9	196.9
ASP	10	D	D	9.2142	6269.8	3199.4	ASP	10	D	W	37.9613	790.6	255.8
ASP	10	D	D	12.4986	906.5	78.6	ASP	10	D	W	38.3225	387.2	39.9
ASP	10	D	D	14.2567	2467.6	520.7	ASP	10	D	W	38.5383	361.9	38.7
ASP	10	D	D	15.5736	2085.2	420.9	ASP	10	E	H	8.3906	154.9	6.3
ASP	10	D	D	17.0001	5872.1	3261.4	ASP	10	E	H	9.2147	1000.5	138.5
ASP	10	D	D	18.4838	907.2	134.5	ASP	10	E	H	9.9373	97.4	1.6
ASP	10	D	D	18.6292	1024.0	119.4	ASP	10	E	H	10.7887	69.0	0.8
ASP	10	D	D	19.0033	1137.7	134.1	ASP	10	E	H	11.7069	967.2	44.8
ASP	10	D	D	21.9539	902.8	74.7	ASP	10	E	H	12.4981	886.2	242.6
ASP	10	D	D	22.2546	1203.0	173.4	ASP	10	E	H	13.0173	53.3	1.5
ASP	10	D	D	22.4955	1111.8	308.4	ASP	10	E	H	14.2571	796.5	84.3
ASP	10	D	D	23.4194	2269.5	708.8	ASP	10	E	H	15.5738	748.0	66.5
ASP	10	D	D	23.5348	1525.7	660.1	ASP	10	E	H	16.0616	43.1	13.3
ASP	10	D	D	23.6683	870.9	188.7	ASP	10	E	H	16.8247	97.9	9.8
ASP	10	D	D	24.2604	829.6	134.9	ASP	10	E	H	17.0007	1110.3	185.7
ASP	10	D	D	24.8221	1554.0	518.4	ASP	10	E	H	17.2511	57.6	1.4
ASP	10	D	D	25.1501	640.6	107.3	ASP	10	E	H	18.4839	547.8	47.5
ASP	10	D	D	26.3766	1028.0	232.0	ASP	10	E	H	18.6280	540.6	26.5
ASP	10	D	D	26.7335	532.7	29.0	ASP	10	E	H	19.0029	690.2	55.4
ASP	10	D	D	27.6215	545.5	35.2	ASP	10	E	H	19.2054	34.3	1.4
ASP	10	D	D	27.8815	854.5	144.1	ASP	10	E	H	19.5693	34.9	0.4
ASP	10	D	D	28.7376	703.1	80.3	ASP	10	E	H	19.9451	65.8	16.1
ASP	10	D	D	29.0256	561.7	37.6	ASP	10	E	H	21.9540	1011.5	473.8
ASP	10	D	D	30.2395	739.8	135.0	ASP	10	E	H	22.2546	682.8	76.3
ASP	10	D	D	30.4213	794.9	62.4	ASP	10	E	H	22.2546	682.8	76.3
ASP	10	D	D	30.6028	596.8	157.9	ASP	10	E	H	23.4196	538.7	43.9
ASP	10	D	D	31.1264	674.9	45.5	ASP	10	E	H	23.5344	786.9	282.1
ASP	10	D	D	31.4451	640.3	65.7	ASP	10	E	H	23.6674	458.7	84.9
ASP	10	D	D	31.9518	697.5	142.6	ASP	10	E	H	24.8219	747.8	94.6
ASP	10	D	D	33.9099	708.1	140.4	ASP	10	E	H	25.1494	458.7	64.4
ASP	10	D	D	34.3864	944.6	137.1	ASP	10	E	H	26.4848	45.6	12.7
ASP	10	D	D	34.4671	937.9	110.5	ASP	10	E	H	26.7323	481.3	92.1
ASP	10	D	D	34.7947	397.9	40.3	ASP	10	E	H	27.6217	729.6	233.4
ASP	10	D	D	35.2241	841.6	432.5	ASP	10	E	H	28.7380	640.4	113.4
ASP	10	D	D	35.6255	645.3	53.6	ASP	10	E	H	29.0245	413.4	44.7
ASP	10	D	D	36.6433	592.7	56.0	ASP	10	E	H	30.1140	82.6	40.4
ASP	10	D	D	36.7993	547.3	131.5	ASP	10	E	H	30.2398	2555.8	1555.0
ASP	10	D	D	36.9530	524.0	53.4	ASP	10	E	H	30.4205	534.7	61.4
ASP	10	D	D	37.3958	602.0	70.1	ASP	10	E	H	31.1269	475.4	80.9
ASP	10	D	D	37.4716	437.6	39.5	ASP	10	E	H	31.4454	398.6	67.2
ASP	10	D	D	37.7753	427.4	65.3	ASP	10	E	H	32.4691	78.8	36.8
ASP	10	D	D	37.9523	574.8	134.7	ASP	10	E	H	33.9083	498.0	96.2
ASP	10	D	D	38.3296	617.9	48.2	ASP	10	E	H	34.0261	103.6	1.0
ASP	10	D	D	38.5501	677.9	103.3	ASP	10	E	H	34.3860	680.0	188.3
ASP	10	D	W	11.7087	421.7	107.7	ASP	10	E	H	34.4673	680.3	130.2
ASP	10	D	W	18.6324	3488.4	1479.5	ASP	10	E	H	34.7931	310.7	82.4
ASP	10	D	W	21.9580	2213.6	573.3	ASP	10	E	H	35.6246	511.5	75.5
ASP	10	D	W	22.2573	4083.6	1817.2	ASP	10	E	H	36.6436	410.4	143.7
ASP	10	D	W	22.4989	1001.1	205.8	ASP	10	E	H	37.4713	518.8	133.4
ASP	10	D	W	23.4226	6514.7	3875.3	ASP	10	E	H	37.7725	440.4	101.2
ASP	10	D	W	23.6728	1414.9	419.5	ASP	10	E	H	38.3291	498.9	97.7
ASP	10	D	W	24.2642	1426.5	342.4	ASP	10	E	H	38.5495	473.1	177.7
ASP	10	D	W	24.8269	1856.1	447.1	ASP	10	E	D	18.6288	2126.2	759.0
ASP	10	D	W	25.1543	907.9	186.6	ASP	10	E	D	19.0029	487.3	104.6
ASP	10	D	W	26.7389	1197.4	222.3	ASP	10	E	D	21.9533	2773.4	1017.9

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	10	E	D	22.2544	390.7	120.8	ASP	10	F	H	26.7320	491.1	88.1
ASP	10	E	D	22.4948	1687.5	977.4	ASP	10	F	H	27.2883	30.9	1.3
ASP	10	E	D	23.6671	3014.3	1785.2	ASP	10	F	H	27.6214	766.4	281.7
ASP	10	E	D	24.2595	1876.0	542.5	ASP	10	F	H	28.7383	595.6	145.5
ASP	10	E	D	25.1487	1319.8	311.5	ASP	10	F	H	29.0236	448.3	45.4
ASP	10	E	D	26.3764	2539.7	1152.1	ASP	10	F	H	30.2397	683.4	428.8
ASP	10	E	D	26.7327	1739.7	650.1	ASP	10	F	H	30.4199	530.9	60.6
ASP	10	E	D	27.6209	1439.9	395.0	ASP	10	F	H	31.1270	488.0	41.0
ASP	10	E	D	27.8810	2346.5	1387.4	ASP	10	F	H	31.4445	466.8	87.0
ASP	10	E	D	29.0247	1132.9	224.7	ASP	10	F	H	33.9079	562.1	282.7
ASP	10	E	D	30.2413	2010.7	1295.5	ASP	10	F	H	34.3863	778.3	203.5
ASP	10	E	D	30.4210	1788.7	441.0	ASP	10	F	H	34.4668	1186.6	612.0
ASP	10	E	D	31.1265	1044.2	122.9	ASP	10	F	H	34.7934	266.2	29.8
ASP	10	E	D	31.4445	1259.5	269.9	ASP	10	F	H	35.6241	439.2	49.8
ASP	10	E	D	33.9086	1178.1	490.0	ASP	10	F	H	36.6436	571.8	140.2
ASP	10	E	D	34.3861	2347.8	722.5	ASP	10	F	H	36.9524	505.5	134.3
ASP	10	E	D	34.4664	2210.3	758.1	ASP	10	F	H	37.3961	442.1	242.7
ASP	10	E	D	34.7947	585.1	80.4	ASP	10	F	H	37.4713	366.5	84.1
ASP	10	E	D	35.2245	775.0	320.0	ASP	10	F	H	38.3296	437.8	106.4
ASP	10	E	D	35.6250	1342.7	360.6	ASP	10	F	D	18.6284	2218.0	607.9
ASP	10	E	D	36.6434	1215.2	311.9	ASP	10	F	D	19.0028	2584.4	834.5
ASP	10	E	D	36.7982	1067.5	361.2	ASP	10	F	D	22.2537	2812.2	1158.1
ASP	10	E	D	36.9520	1036.4	253.8	ASP	10	F	D	23.6674	2276.2	850.5
ASP	10	E	D	37.4703	592.7	59.6	ASP	10	F	D	24.2592	1132.5	227.0
ASP	10	E	D	37.7734	746.3	169.9	ASP	10	F	D	25.1488	1238.8	302.8
ASP	10	E	D	37.9516	879.2	324.6	ASP	10	F	D	26.3760	1574.2	831.6
ASP	10	E	D	38.3290	1248.4	278.0	ASP	10	F	D	26.7325	1181.6	295.8
ASP	10	E	D	38.5501	943.4	317.9	ASP	10	F	D	27.6211	1118.2	223.8
ASP	10	E	W	25.1528	1656.9	809.0	ASP	10	F	D	28.7370	1034.9	302.4
ASP	10	E	W	26.7388	3269.3	1731.0	ASP	10	F	D	29.0246	1227.8	281.3
ASP	10	E	W	27.6287	3819.7	2305.2	ASP	10	F	D	30.4204	1522.1	403.4
ASP	10	E	W	27.8862	3053.2	1931.4	ASP	10	F	D	31.1262	962.4	104.9
ASP	10	E	W	28.7437	3162.6	2000.2	ASP	10	F	D	31.4437	1874.3	454.3
ASP	10	E	W	29.0305	1640.3	494.1	ASP	10	F	D	31.9518	866.1	391.0
ASP	10	E	W	30.4266	2476.2	898.4	ASP	10	F	D	33.9091	794.5	229.1
ASP	10	E	W	31.1332	1800.0	335.9	ASP	10	F	D	34.3857	4072.7	2153.1
ASP	10	E	W	31.4511	1160.7	163.9	ASP	10	F	D	34.4666	1560.4	466.0
ASP	10	E	W	31.9588	898.0	219.5	ASP	10	F	D	34.7939	619.2	127.4
ASP	10	E	W	33.9160	2366.7	1156.3	ASP	10	F	D	35.2235	628.4	234.6
ASP	10	E	W	34.4751	2773.5	1090.8	ASP	10	F	D	35.6245	1616.4	339.5
ASP	10	E	W	34.8028	571.7	87.5	ASP	10	F	D	36.6427	1165.8	277.4
ASP	10	E	W	35.2309	1291.6	538.8	ASP	10	F	D	36.7994	756.5	218.3
ASP	10	E	W	35.6348	1353.2	542.6	ASP	10	F	D	36.9523	774.6	161.9
ASP	10	E	W	36.6543	1486.7	410.7	ASP	10	F	D	37.3951	1042.6	229.7
ASP	10	E	W	36.9617	1627.9	496.6	ASP	10	F	D	37.4706	861.0	156.5
ASP	10	E	W	37.4036	2384.0	1276.9	ASP	10	F	D	37.7740	1091.8	414.9
ASP	10	E	W	37.4801	2082.0	702.0	ASP	10	F	D	37.9512	929.3	364.8
ASP	10	E	W	37.7829	1305.1	336.8	ASP	10	F	D	38.3287	1244.2	477.6
ASP	10	E	W	37.9621	1020.8	445.5	ASP	10	F	D	38.5504	760.2	159.0
ASP	10	E	W	38.3373	3302.4	1802.6	ASP	10	F	W	19.0050	343.2	68.3
ASP	10	E	W	38.5605	2421.0	1393.7	ASP	10	F	W	22.4975	1556.9	590.6
ASP	10	F	H	8.3896	146.8	7.3	ASP	10	F	W	23.6729	1989.6	710.3
ASP	10	F	H	9.2144	1082.6	178.0	ASP	10	F	W	28.7443	2306.4	1242.7
ASP	10	F	H	9.9366	61.6	22.8	ASP	10	F	W	29.0298	1188.2	175.6
ASP	10	F	H	10.7899	43.3	18.2	ASP	10	F	W	30.2458	1907.0	1025.4
ASP	10	F	H	11.7061	988.6	46.8	ASP	10	F	W	30.4261	3771.5	1583.5
ASP	10	F	H	12.4972	808.0	206.9	ASP	10	F	W	30.6095	688.6	153.4
ASP	10	F	H	13.0185	53.1	1.9	ASP	10	F	W	31.1328	2039.2	461.6
ASP	10	F	H	14.2568	725.4	64.9	ASP	10	F	W	31.4503	1775.8	701.8
ASP	10	F	H	15.5734	617.7	47.7	ASP	10	F	W	33.9167	2265.7	1021.7
ASP	10	F	H	16.8225	87.1	5.8	ASP	10	F	W	34.8032	569.1	165.1
ASP	10	F	H	16.9999	912.6	115.2	ASP	10	F	W	35.2314	1425.1	394.5
ASP	10	F	H	17.2505	40.7	3.2	ASP	10	F	W	35.6346	1011.6	119.1
ASP	10	F	H	18.4833	533.1	52.2	ASP	10	F	W	36.4616	1727.2	651.3
ASP	10	F	H	18.6275	585.5	32.9	ASP	10	F	W	36.6537	2330.0	1095.3
ASP	10	F	H	19.0025	703.7	57.6	ASP	10	F	W	36.8081	1399.9	742.1
ASP	10	F	H	19.2069	33.4	1.4	ASP	10	F	W	36.9621	1774.7	394.6
ASP	10	F	H	21.6692	37.5	9.9	ASP	10	F	W	37.4042	1949.8	836.6
ASP	10	F	H	21.9540	878.7	293.0	ASP	10	F	W	37.4797	2271.2	587.1
ASP	10	F	H	22.2544	568.9	38.6	ASP	10	F	W	37.7831	1440.5	468.6
ASP	10	F	H	22.4939	440.4	67.7	ASP	10	F	W	37.9607	1627.1	1015.6
ASP	10	F	H	23.4194	618.7	57.5	ASP	10	F	W	38.3381	1656.7	383.7
ASP	10	F	H	23.5332	645.4	106.6	ASP	10	F	W	38.5617	1722.3	629.0
ASP	10	F	H	23.6664	480.0	69.1	ASP	100	A	H	8.3901	117.8	6.0
ASP	10	F	H	24.2601	529.4	84.8	ASP	100	A	H	9.2151	749.7	244.4
ASP	10	F	H	25.1478	337.4	38.9	ASP	100	A	H	9.9393	74.5	1.3
ASP	10	F	H	26.1935	79.6	6.4	ASP	100	A	H	10.7905	56.3	0.6
ASP	10	F	H	26.3768	726.7	348.3	ASP	100	A	H	11.7066	586.8	38.8
ASP	10	F	H	26.4936	42.6	19.6	ASP	100	A	H	13.0191	58.0	4.9

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	100	A	H	15.5736	408.9	42.7	ASP	100	A	W	37.4643	468.2	49.3
ASP	100	A	H	16.0607	59.1	0.5	ASP	100	A	W	37.7614	458.6	199.0
ASP	100	A	H	16.4511	13.0	5.5	ASP	100	A	W	38.3249	900.9	116.0
ASP	100	A	H	16.8203	99.1	38.8	ASP	100	A	W	38.5417	649.6	258.6
ASP	100	A	H	17.2531	47.4	1.5	ASP	100	B	H	8.3891	119.4	4.4
ASP	100	A	H	18.6273	266.1	47.3	ASP	100	B	H	8.5619	176.6	3.2
ASP	100	A	H	19.0015	408.7	67.2	ASP	100	B	H	9.9385	55.4	3.4
ASP	100	A	H	19.5678	855.8	81.0	ASP	100	B	H	10.7901	36.3	1.6
ASP	100	A	H	19.9489	40.8	5.0	ASP	100	B	H	11.7057	1538.9	252.9
ASP	100	A	H	21.2137	10.9	5.1	ASP	100	B	H	13.0187	43.8	0.9
ASP	100	A	H	22.2536	300.7	43.3	ASP	100	B	H	14.2562	1478.1	671.4
ASP	100	A	H	23.4190	632.7	330.6	ASP	100	B	H	15.3627	26.6	11.4
ASP	100	A	H	23.5320	302.1	67.8	ASP	100	B	H	15.5718	950.5	316.6
ASP	100	A	H	24.8217	408.7	181.6	ASP	100	B	H	16.8200	75.1	11.8
ASP	100	A	H	25.1456	367.0	81.6	ASP	100	B	H	16.9991	1368.7	412.4
ASP	100	A	H	26.7293	241.7	64.5	ASP	100	B	H	18.6267	414.6	38.1
ASP	100	A	H	29.0235	217.6	129.0	ASP	100	B	H	19.0014	1366.7	879.2
ASP	100	A	H	31.1249	213.0	42.0	ASP	100	B	H	22.2547	574.3	98.9
ASP	100	A	H	31.4431	245.4	77.2	ASP	100	B	H	23.4168	507.0	312.6
ASP	100	A	H	34.3856	293.3	148.7	ASP	100	B	H	24.8213	360.5	195.4
ASP	100	A	H	36.3786	39.9	0.4	ASP	100	B	H	25.1467	231.2	113.7
ASP	100	A	D	8.3895	139.7	1.9	ASP	100	B	H	29.0174	325.6	175.6
ASP	100	A	D	9.2143	1688.7	509.5	ASP	100	B	H	31.1258	274.5	95.4
ASP	100	A	D	9.9382	85.8	2.3	ASP	100	B	H	32.4382	20.5	5.7
ASP	100	A	D	10.7908	39.0	2.2	ASP	100	B	D	8.3899	145.8	7.6
ASP	100	A	D	11.7063	779.1	55.0	ASP	100	B	D	9.2129	1604.9	862.2
ASP	100	A	D	12.4965	1023.4	483.5	ASP	100	B	D	9.9377	90.1	1.4
ASP	100	A	D	13.0186	46.2	1.2	ASP	100	B	D	10.7891	65.3	0.7
ASP	100	A	D	14.2552	1259.4	197.0	ASP	100	B	D	11.7055	1230.9	186.5
ASP	100	A	D	15.5727	1231.7	273.3	ASP	100	B	D	13.0184	47.4	1.1
ASP	100	A	D	16.8210	73.6	6.0	ASP	100	B	D	14.2553	865.9	142.7
ASP	100	A	D	16.9998	1039.5	279.0	ASP	100	B	D	15.5724	833.3	429.7
ASP	100	A	D	18.6237	950.8	205.2	ASP	100	B	D	16.8214	84.2	4.7
ASP	100	A	D	19.0013	653.8	77.8	ASP	100	B	D	16.9994	1959.2	1175.7
ASP	100	A	D	19.2070	32.2	1.4	ASP	100	B	D	18.6263	429.0	159.1
ASP	100	A	D	19.5679	34.2	0.5	ASP	100	B	D	19.2067	32.5	0.8
ASP	100	A	D	22.2535	554.1	60.0	ASP	100	B	D	19.5680	34.9	2.7
ASP	100	A	D	23.4186	668.9	86.7	ASP	100	B	D	19.9464	71.9	30.4
ASP	100	A	D	23.5331	445.5	153.7	ASP	100	B	D	20.3874	41.8	15.0
ASP	100	A	D	23.6635	543.2	109.2	ASP	100	B	D	23.5322	382.5	128.6
ASP	100	A	D	24.8220	990.5	207.0	ASP	100	B	D	24.8217	1567.3	709.4
ASP	100	A	D	25.1468	236.0	133.1	ASP	100	B	D	26.7271	569.2	350.6
ASP	100	A	D	25.2890	111.1	8.7	ASP	100	B	D	30.1102	37.3	9.0
ASP	100	A	D	26.7312	284.1	136.3	ASP	100	B	D	34.4637	519.5	234.8
ASP	100	A	D	27.6213	909.4	188.1	ASP	100	B	D	38.3263	283.3	142.5
ASP	100	A	D	28.7368	510.9	163.5	ASP	100	B	W	8.3877	157.6	10.3
ASP	100	A	D	29.0223	333.0	109.5	ASP	100	B	W	9.2107	1164.0	277.9
ASP	100	A	D	30.4195	331.4	67.5	ASP	100	B	W	9.9333	110.2	2.7
ASP	100	A	D	31.1263	420.6	51.4	ASP	100	B	W	10.7945	71.7	1.8
ASP	100	A	D	31.4429	370.9	183.3	ASP	100	B	W	11.7006	1201.7	91.5
ASP	100	A	D	32.4616	71.4	0.7	ASP	100	B	W	12.4943	568.6	283.9
ASP	100	A	D	34.4657	884.3	509.1	ASP	100	B	W	13.0142	114.4	60.0
ASP	100	A	D	35.6215	350.0	72.0	ASP	100	B	W	14.2522	1703.2	199.9
ASP	100	A	D	36.6409	375.8	128.6	ASP	100	B	W	15.5690	713.7	86.3
ASP	100	A	D	36.7938	301.2	191.7	ASP	100	B	W	16.8195	132.6	66.2
ASP	100	A	D	37.3925	555.5	262.4	ASP	100	B	W	16.9944	1422.8	242.5
ASP	100	A	D	38.3277	422.6	89.8	ASP	100	B	W	17.2450	128.6	54.4
ASP	100	A	D	38.5481	298.4	83.1	ASP	100	B	W	18.4774	849.3	93.7
ASP	100	A	W	15.5701	8185.2	4823.8	ASP	100	B	W	18.6208	711.7	166.1
ASP	100	A	W	18.4798	1751.4	494.2	ASP	100	B	W	18.9953	2018.1	643.3
ASP	100	A	W	18.6221	1542.1	274.1	ASP	100	B	W	19.9388	79.2	11.5
ASP	100	A	W	18.9983	3738.4	1432.1	ASP	100	B	W	21.9475	1168.2	269.2
ASP	100	A	W	24.2552	963.9	179.7	ASP	100	B	W	22.2487	962.6	117.2
ASP	100	A	W	24.8177	2957.8	1730.8	ASP	100	B	W	22.4845	679.4	291.4
ASP	100	A	W	27.6143	1026.8	330.8	ASP	100	B	W	23.4121	1069.7	228.7
ASP	100	A	W	27.8748	1451.4	873.4	ASP	100	B	W	23.5244	530.1	77.0
ASP	100	A	W	28.7329	946.5	146.9	ASP	100	B	W	24.2524	530.9	86.6
ASP	100	A	W	29.0156	750.0	143.3	ASP	100	B	W	24.8158	948.9	132.8
ASP	100	A	W	30.4140	1394.6	309.5	ASP	100	B	W	25.1390	416.1	95.2
ASP	100	A	W	31.1209	998.7	122.3	ASP	100	B	W	26.7229	348.7	92.6
ASP	100	A	W	31.4401	855.8	187.9	ASP	100	B	W	27.6134	780.9	420.5
ASP	100	A	W	34.3827	1526.9	501.2	ASP	100	B	W	28.7300	689.8	165.8
ASP	100	A	W	34.4588	914.5	170.6	ASP	100	B	W	29.0143	386.3	94.8
ASP	100	A	W	34.7821	446.5	79.0	ASP	100	B	W	30.2303	500.7	320.8
ASP	100	A	W	35.6151	780.1	101.0	ASP	100	B	W	30.4103	617.2	98.9
ASP	100	A	W	36.6388	800.9	136.0	ASP	100	B	W	31.1155	923.4	125.4
ASP	100	A	W	36.7923	887.4	406.9	ASP	100	B	W	31.4355	1005.0	561.3
ASP	100	A	W	36.9435	460.1	89.3	ASP	100	B	W	34.3755	700.3	117.9
ASP	100	A	W	37.3907	2265.7	1059.8	ASP	100	B	W	34.4572	495.1	74.2

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	100	B	W	34.7766	518.7	241.0	ASP	100	D	H	9.2079	830.1	291.8
ASP	100	B	W	35.6122	531.0	198.3	ASP	100	D	H	9.9320	107.1	10.7
ASP	100	B	W	36.4440	479.2	108.2	ASP	100	D	H	10.7828	72.1	21.3
ASP	100	B	W	36.6325	1693.2	959.6	ASP	100	D	H	11.6992	980.4	71.4
ASP	100	B	W	37.3845	275.7	78.8	ASP	100	D	H	13.0119	47.0	2.5
ASP	100	B	W	37.4604	255.8	28.8	ASP	100	D	H	14.2505	654.9	79.1
ASP	100	B	W	37.7603	325.0	159.6	ASP	100	D	H	15.5689	577.8	41.8
ASP	100	B	W	38.3212	373.7	97.5	ASP	100	D	H	16.0549	39.4	5.1
ASP	100	C	H	8.3894	119.0	7.0	ASP	100	D	H	16.8105	73.3	4.2
ASP	100	C	H	9.2137	837.9	142.4	ASP	100	D	H	16.9931	733.4	80.7
ASP	100	C	H	9.9382	80.9	1.8	ASP	100	D	H	17.2482	69.3	19.1
ASP	100	C	H	10.7892	58.2	0.6	ASP	100	D	H	18.4792	458.3	173.2
ASP	100	C	H	11.7048	613.0	59.7	ASP	100	D	H	18.6217	372.1	25.8
ASP	100	C	H	12.4949	734.8	397.1	ASP	100	D	H	18.9949	553.2	46.9
ASP	100	C	H	13.0182	45.0	1.4	ASP	100	D	H	19.2044	31.4	0.5
ASP	100	C	H	14.2561	698.5	122.2	ASP	100	D	H	19.9425	46.7	2.6
ASP	100	C	H	15.5723	558.0	159.8	ASP	100	D	H	22.2492	508.1	41.6
ASP	100	C	H	16.4571	5.4	1.9	ASP	100	D	H	23.4143	536.2	47.8
ASP	100	C	H	16.8193	71.3	3.6	ASP	100	D	H	23.5274	440.0	135.2
ASP	100	C	H	17.2517	47.3	1.0	ASP	100	D	H	24.8143	485.1	50.1
ASP	100	C	H	18.6257	372.9	30.9	ASP	100	D	H	25.1416	381.6	208.4
ASP	100	C	H	19.0005	414.8	48.5	ASP	100	D	H	27.6154	409.2	151.8
ASP	100	C	H	19.2091	33.0	15.7	ASP	100	D	H	29.0153	183.7	28.0
ASP	100	C	H	19.5675	32.8	0.4	ASP	100	D	H	30.4125	236.0	20.8
ASP	100	C	H	19.9483	43.3	4.2	ASP	100	D	H	31.1199	333.4	45.0
ASP	100	C	H	22.2526	372.5	73.6	ASP	100	D	H	31.4384	279.1	58.7
ASP	100	C	H	23.4176	636.0	251.7	ASP	100	D	H	34.3799	414.8	59.2
ASP	100	C	H	23.6643	214.2	97.0	ASP	100	D	H	34.4608	460.8	132.0
ASP	100	C	H	24.8201	477.5	165.8	ASP	100	D	H	34.7809	152.1	70.4
ASP	100	C	H	25.1458	244.5	59.5	ASP	100	D	D	8.3840	129.9	4.8
ASP	100	C	H	33.9094	98.5	42.5	ASP	100	D	D	9.2093	860.2	81.0
ASP	100	C	H	36.9710	78.0	5.2	ASP	100	D	D	9.9369	97.0	2.7
ASP	100	C	D	8.3897	130.6	6.8	ASP	100	D	D	10.7882	66.4	1.1
ASP	100	C	D	9.9377	89.5	2.1	ASP	100	D	D	11.7050	1049.7	64.4
ASP	100	C	D	10.7892	62.2	0.8	ASP	100	D	D	12.4932	708.5	120.6
ASP	100	C	D	11.7030	1652.9	340.2	ASP	100	D	D	13.0111	51.5	1.3
ASP	100	C	D	13.0181	46.7	1.6	ASP	100	D	D	14.2513	741.9	42.1
ASP	100	C	D	14.2553	1472.0	622.2	ASP	100	D	D	15.5693	861.3	53.3
ASP	100	C	D	16.5128	90.8	47.7	ASP	100	D	D	16.4577	107.8	10.4
ASP	100	C	D	16.8205	94.2	23.4	ASP	100	D	D	16.8120	81.1	4.8
ASP	100	C	D	17.0001	2636.0	1138.6	ASP	100	D	D	16.9931	969.2	96.9
ASP	100	C	D	18.4788	2893.2	1899.5	ASP	100	D	D	17.2470	58.7	1.4
ASP	100	C	D	18.6253	398.1	57.1	ASP	100	D	D	18.4784	490.9	24.5
ASP	100	C	D	18.9974	3900.2	1904.8	ASP	100	D	D	18.6219	463.2	19.6
ASP	100	C	D	19.2375	198.9	72.9	ASP	100	D	D	18.9950	530.4	24.1
ASP	100	C	D	19.5694	34.7	15.0	ASP	100	D	D	19.2026	33.6	0.7
ASP	100	C	D	22.2532	1848.7	1203.1	ASP	100	D	D	19.5631	36.9	0.5
ASP	100	C	D	24.1864	86.7	5.1	ASP	100	D	D	21.6686	91.4	1.6
ASP	100	C	D	24.8213	472.5	126.5	ASP	100	D	D	21.9471	732.5	84.7
ASP	100	C	D	26.7233	1342.1	538.3	ASP	100	D	D	22.2484	528.1	29.0
ASP	100	C	D	27.6184	561.4	196.8	ASP	100	D	D	22.4886	330.8	55.1
ASP	100	C	D	29.0205	425.4	208.5	ASP	100	D	D	23.4141	589.4	43.5
ASP	100	C	D	30.1087	32.6	9.9	ASP	100	D	D	23.5286	614.7	104.1
ASP	100	C	D	30.4161	353.3	10.0	ASP	100	D	D	23.6640	350.1	35.1
ASP	100	C	D	31.1246	618.2	141.6	ASP	100	D	D	24.2540	482.2	48.3
ASP	100	C	D	34.4627	459.7	145.4	ASP	100	D	D	24.8203	610.8	50.8
ASP	100	C	D	34.9059	193.7	3.2	ASP	100	D	D	25.1465	277.8	22.4
ASP	100	C	D	36.9700	14.1	4.6	ASP	100	D	D	26.3705	748.9	282.5
ASP	100	C	W	23.5269	1862.2	1021.6	ASP	100	D	D	26.7283	440.6	52.2
ASP	100	C	W	23.6597	1164.3	384.6	ASP	100	D	D	26.8234	40.7	15.2
ASP	100	C	W	24.2527	1053.4	279.5	ASP	100	D	D	27.2788	35.4	2.9
ASP	100	C	W	24.8159	1223.8	308.4	ASP	100	D	D	27.6189	603.1	80.5
ASP	100	C	W	27.6119	882.8	174.3	ASP	100	D	D	28.7302	408.3	49.2
ASP	100	C	W	27.8727	911.9	301.4	ASP	100	D	D	29.0156	306.0	28.1
ASP	100	C	W	28.7295	1414.2	938.3	ASP	100	D	D	30.4136	396.3	27.9
ASP	100	C	W	28.7301	1109.9	564.6	ASP	100	D	D	31.1202	363.3	20.2
ASP	100	C	W	30.4131	1051.5	387.2	ASP	100	D	D	31.4393	392.2	51.6
ASP	100	C	W	30.5876	896.1	458.1	ASP	100	D	D	33.9000	295.3	81.7
ASP	100	C	W	31.1178	1257.8	227.0	ASP	100	D	D	34.3802	472.3	52.0
ASP	100	C	W	31.4361	1145.5	474.8	ASP	100	D	D	34.4605	608.8	121.7
ASP	100	C	W	34.4575	1335.3	646.1	ASP	100	D	D	34.4637	1055	515.3
ASP	100	C	W	34.7784	736.7	296.0	ASP	100	D	D	34.7875	217.7	106.1
ASP	100	C	W	35.6129	1161.9	468.8	ASP	100	D	D	35.6200	344.5	59.9
ASP	100	C	W	36.6350	1322.0	687.3	ASP	100	D	D	36.4509	382.9	120.0
ASP	100	C	W	36.9425	558.2	78.0	ASP	100	D	D	36.6406	719.3	131.5
ASP	100	C	W	37.4595	592.5	151.2	ASP	100	D	D	36.9475	242.7	150.2
ASP	100	C	W	37.7625	368.8	161.8	ASP	100	D	D	37.3927	391.7	225.5
ASP	100	C	W	38.5377	952.4	476.8	ASP	100	D	D	37.7678	238.3	103.1
ASP	100	D	H	8.3828	122.8	10.0	ASP	100	D	D	38.3271	367.6	64.7

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	100	D	D	38.5455	477.3	287.1	ASP	1000	A	W	26.1862	119.2	1.7
ASP	100	D	W	9.2076	7147.9	3214.6	ASP	1000	A	W	26.8211	34.8	2.8
ASP	100	D	W	11.6990	4768.9	2581.3	ASP	1000	A	W	32.4278	18	0.8
ASP	100	D	W	12.4929	3083.3	1330.7	ASP	1000	A	W	33.9994	47.6	13.6
ASP	100	D	W	15.5686	2456.7	701.5	ASP	1000	B	H	8.3799	93.8	4.7
ASP	100	D	W	16.9930	3478	856.7	ASP	1000	B	H	8.3809	85.2	4.2
ASP	100	D	W	18.4781	918.7	66.6	ASP	1000	B	H	9.9352	50.7	1.0
ASP	100	D	W	18.6216	2088.5	667.4	ASP	1000	B	H	9.9368	50.3	0.8
ASP	100	D	W	18.9937	1163.2	92.4	ASP	1000	B	H	10.7861	46.6	0.7
ASP	100	D	W	22.2490	1478.1	174.4	ASP	1000	B	H	10.7884	114.1	46.1
ASP	100	D	W	22.4859	603.4	158.1	ASP	1000	B	H	11.6918	286.7	124.7
ASP	100	D	W	23.4138	2772.1	1077.9	ASP	1000	B	H	13.0124	56.8	6.4
ASP	100	D	W	23.5276	1291.5	261.2	ASP	1000	B	H	13.0152	118.9	55.4
ASP	100	D	W	23.6573	994.9	130.6	ASP	1000	B	H	16.0570	119.6	1.1
ASP	100	D	W	24.2530	1056.4	130.9	ASP	1000	B	H	16.8035	74.8	15.8
ASP	100	D	W	24.8141	1495.8	204.3	ASP	1000	B	H	17.2516	37.2	0.9
ASP	100	D	W	25.1422	2132	1371.7	ASP	1000	B	H	18.5927	204.3	98.5
ASP	100	D	W	26.3697	1922.4	790.9	ASP	1000	B	H	19.2066	30.4	1.2
ASP	100	D	W	26.7231	617.3	131.1	ASP	1000	B	H	19.2080	29.8	2.1
ASP	100	D	W	27.6146	1084.7	129.2	ASP	1000	B	H	19.5585	35.6	0.7
ASP	100	D	W	27.8738	874.8	191.6	ASP	1000	B	H	19.5622	32	0.6
ASP	100	D	W	28.7305	992.6	147.2	ASP	1000	B	H	19.9464	34	2.0
ASP	100	D	W	29.0139	737.9	129.1	ASP	1000	B	H	19.9497	36.3	12.8
ASP	100	D	W	30.4129	1066.8	421.7	ASP	1000	B	H	20.3859	34.8	6.0
ASP	100	D	W	31.1196	725.3	44.4	ASP	1000	B	H	22.2942	307.7	9.5
ASP	100	D	W	31.9373	1623.8	980.0	ASP	1000	B	H	23.1393	15.3	1.2
ASP	100	D	W	33.8940	521.6	118.0	ASP	1000	B	H	25.2771	14.9	1.7
ASP	100	D	W	34.3801	843.5	93.3	ASP	1000	B	H	26.8258	26.4	0.1
ASP	100	D	W	34.4605	1293.6	647.2	ASP	1000	B	H	28.0986	420.2	222.0
ASP	100	D	W	34.7803	414.2	56.6	ASP	1000	B	H	30.1161	22.3	1.7
ASP	1000	A	H	8.3813	101.7	3.6	ASP	1000	B	H	31.3154	289.1	59.8
ASP	1000	A	H	9.2101	1056.9	148.5	ASP	1000	B	H	36.3961	73.9	35.8
ASP	1000	A	H	9.9372	50.7	0.7	ASP	1000	B	D	8.3830	123.2	12.0
ASP	1000	A	H	10.7881	47.5	0.6	ASP	1000	B	D	9.9359	68.4	1.6
ASP	1000	A	H	11.6967	523.1	47.9	ASP	1000	B	D	10.7874	55.5	0.7
ASP	1000	A	H	13.0141	137.8	57.5	ASP	1000	B	D	13.0153	56.8	4.0
ASP	1000	A	H	14.2544	380.8	98.3	ASP	1000	B	D	16.8142	78.1	6.2
ASP	1000	A	H	15.5710	536.3	63.9	ASP	1000	B	D	17.2496	46.5	1.1
ASP	1000	A	H	16.0570	105.4	49.2	ASP	1000	B	D	19.2057	31.2	0.6
ASP	1000	A	H	16.8040	66.8	6.9	ASP	1000	B	D	19.5642	45	3.0
ASP	1000	A	H	17.2534	85.3	32.9	ASP	1000	B	D	19.9470	59.8	18.5
ASP	1000	A	H	18.6068	543.7	188.6	ASP	1000	B	D	21.2176	108.6	15.8
ASP	1000	A	H	18.9908	1454.7	806.2	ASP	1000	B	D	21.6707	104.1	55.1
ASP	1000	A	H	19.2074	30.1	0.6	ASP	1000	B	D	24.1904	82.1	2.4
ASP	1000	A	H	19.5584	35.9	0.7	ASP	1000	B	D	27.2778	30.2	1.4
ASP	1000	A	H	19.9480	44.8	14.0	ASP	1000	B	D	36.3831	21.4	5.3
ASP	1000	A	H	22.2498	471	69.7	ASP	1000	B	D	38.3613	17	0.9
ASP	1000	A	H	23.1449	17.1	1.4	ASP	1000	B	W	8.3887	126.5	7.6
ASP	1000	A	H	27.8285	89.6	3.1	ASP	1000	B	W	9.9373	84.8	2.2
ASP	1000	A	H	31.5331	16.9	2.5	ASP	1000	B	W	10.7889	59.5	0.7
ASP	1000	A	H	32.4343	18.2	0.7	ASP	1000	B	W	13.0088	47.7	0.8
ASP	1000	A	H	34.8110	255.9	3.8	ASP	1000	B	W	15.3556	17.7	0.9
ASP	1000	A	D	8.3836	144	25.2	ASP	1000	B	W	16.5391	53.9	15.8
ASP	1000	A	D	9.9359	72.2	1.8	ASP	1000	B	W	16.8083	80.6	5.6
ASP	1000	A	D	10.7876	58.1	0.9	ASP	1000	B	W	17.2446	56.8	1.7
ASP	1000	A	D	11.6925	791.1	240.3	ASP	1000	B	W	18.3941	683.4	170.0
ASP	1000	A	D	13.0155	110.5	40.4	ASP	1000	B	W	19.2002	32.9	0.6
ASP	1000	A	D	14.2510	505.8	196.2	ASP	1000	B	W	19.5584	37.2	0.5
ASP	1000	A	D	16.8140	88.9	15.2	ASP	1000	B	W	19.9371	53.1	5.1
ASP	1000	A	D	17.2497	89.5	27.1	ASP	1000	B	W	20.8468	63.5	7.9
ASP	1000	A	D	19.2049	33.6	2.1	ASP	1000	B	W	21.6630	33.5	0.3
ASP	1000	A	D	19.5640	96.1	50.8	ASP	1000	B	W	23.1453	97.4	3.7
ASP	1000	A	D	19.9475	49.3	11.0	ASP	1000	B	W	24.1813	23.5	1.2
ASP	1000	A	D	26.4841	33.4	9.8	ASP	1000	B	W	25.3326	216	63.8
ASP	1000	A	D	30.1118	31.2	9.8	ASP	1000	B	W	26.8201	30.7	4.4
ASP	1000	A	D	30.8131	18.6	0.1	ASP	1000	B	W	27.2709	30.5	1.6
ASP	1000	A	D	31.3144	19.1	1.7	ASP	1000	B	W	30.7988	17.8	2.3
ASP	1000	A	D	38.3587	81.5	0.9	ASP	1000	C	H	8.3808	91.1	3.0
ASP	1000	A	W	8.3828	138.4	10.7	ASP	1000	C	H	9.9368	51.8	1.0
ASP	1000	A	W	9.9391	82.1	3.8	ASP	1000	C	H	10.7882	46.8	0.7
ASP	1000	A	W	10.7901	57.3	0.9	ASP	1000	C	H	11.6911	351.1	88.6
ASP	1000	A	W	11.6919	482.7	65.5	ASP	1000	C	H	13.0150	48.8	3.4
ASP	1000	A	W	13.0107	64.3	7.0	ASP	1000	C	H	16.4516	33.3	0.2
ASP	1000	A	W	15.3542	15.9	3.1	ASP	1000	C	H	16.8100	60.8	5.0
ASP	1000	A	W	15.5618	402.4	126.7	ASP	1000	C	H	19.5627	122.3	67.3
ASP	1000	A	W	16.8083	99.6	17.0	ASP	1000	C	H	22.2945	310.1	9.6
ASP	1000	A	W	17.2462	64.8	3.0	ASP	1000	C	H	31.3160	411.1	164.5
ASP	1000	A	W	19.1989	37.6	2.5	ASP	1000	C	H	38.3619	22.9	0.1
ASP	1000	A	W	19.9392	54.7	5.3	ASP	1000	C	D	8.3830	149.6	19.2

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
ASP	1000	C	D	9.9354	77.6	1.7
ASP	1000	C	D	10.7869	60.6	0.8
ASP	1000	C	D	11.6929	523.8	89.7
ASP	1000	C	D	13.0147	105.6	33.3
ASP	1000	C	D	15.5653	314.2	149.3
ASP	1000	C	D	17.2488	166.2	80.0
ASP	1000	C	D	18.5982	215	51.5
ASP	1000	C	D	18.9838	344.4	139.3
ASP	1000	C	D	19.2046	32.9	0.6
ASP	1000	C	D	19.5638	182.4	94.4
ASP	1000	C	D	20.3805	37.9	12.8
ASP	1000	C	D	21.6697	118.5	68.0
ASP	1000	C	D	26.1823	102.2	5.3
ASP	1000	C	D	30.1116	29.6	2.3
ASP	1000	C	D	35.9398	44.7	0.3
ASP	1000	C	W	8.3881	146.4	11.5
ASP	1000	C	W	9.9378	89.1	2.9
ASP	1000	C	W	10.7891	60.1	0.7
ASP	1000	C	W	11.6948	480.1	107.6
ASP	1000	C	W	13.0158	47.6	0.8
ASP	1000	C	W	16.8158	115.4	47.1
ASP	1000	C	W	17.2497	144.2	70.7
ASP	1000	C	W	19.2046	32.9	0.7
ASP	1000	C	W	19.5636	116.8	56.4
ASP	1000	C	W	19.9480	79.7	41.4
ASP	1000	C	W	26.4846	44.4	11.4
ASP	1000	C	W	26.8252	35.8	15.1
ASP	1000	C	W	27.2768	29.3	1.3
ASP	1000	C	W	27.8238	23.8	1.3
ASP	1000	C	W	30.1072	36.3	11.8
ASP	1000	C	W	30.8039	17.3	2.7
ASP	1000	C	W	31.5252	14.3	1.6
ASP	1000	C	W	32.4341	16.3	0.6
ASP	1000	C	W	34.6933	11.7	3.2
ASP	1000	D	D	8.3828	123.4	6.5
ASP	1000	D	D	9.9349	77	1.9
ASP	1000	D	D	10.7865	59.4	0.8
ASP	1000	D	D	11.6934	489.3	286.6
ASP	1000	D	D	13.0144	63.3	5.6
ASP	1000	D	D	16.8143	88	16.8
ASP	1000	D	D	17.2485	54.2	2.4
ASP	1000	D	D	19.2045	32.6	0.7
ASP	1000	D	D	19.5634	147.3	70.9
ASP	1000	D	D	20.3866	31.5	12.4
ASP	1000	D	D	20.8534	29.4	13.7
ASP	1000	D	D	21.2186	66.4	9.4
ASP	1000	D	D	29.5783	125.8	33.4
ASP	1000	D	D	34.9052	86.7	29.4
ASP	1000	D	D	37.4087	23.7	0.2
ASP	1000	D	W	8.3878	138.9	4.9
ASP	1000	D	W	9.9370	98.6	3.8
ASP	1000	D	W	10.7886	63.5	0.8
ASP	1000	D	W	13.0161	60.4	5.2
ASP	1000	D	W	15.3413	16	6.0
ASP	1000	D	W	16.8168	118.2	42.6
ASP	1000	D	W	17.2491	63.8	3.4
ASP	1000	D	W	19.2049	33.4	0.7
ASP	1000	D	W	19.5641	37.5	0.6
ASP	1000	D	W	19.9442	53.9	5.7
ASP	1000	D	W	20.8542	16.1	5.0
ASP	1000	D	W	34.0066	80.2	7.1
ASP	1000	D	W	34.8975	27.4	13.5
ASP	1000	D	W	37.3983	17.3	2.5
ASP	1000	E	D	8.3831	121.1	5.0
ASP	1000	E	D	9.9353	74.9	1.7
ASP	1000	E	D	10.7869	59	0.8
ASP	1000	E	D	13.0148	77.1	11.6
ASP	1000	E	D	15.3481	15.2	1.5
ASP	1000	E	D	16.0544	85.2	1.1
ASP	1000	E	D	16.8150	81.1	7.3
ASP	1000	E	D	17.2487	117.2	39.1
ASP	1000	E	D	19.2052	111.2	62.4
ASP	1000	E	D	19.5648	33	7.1
ASP	1000	E	D	21.6693	107.4	58.3
ASP	1000	E	D	25.9826	144.8	52.2
ASP	1000	E	D	26.4863	38.8	11.1
ASP	1000	E	D	26.8249	27.9	1.9
ASP	1000	E	D	27.8279	24.2	2.1
ASP	1000	E	D	30.1102	28.5	2.2
ASP	1000	E	D	30.8095	17	0.9
ASP	1000	E	D	31.3153	43	2.4
ASP	1000	E	D	35.5046	108.4	1.3
ASP	1000	E	D	35.9439	74.8	7.7
ASP	1000	E	W	8.3878	145.9	10.6
ASP	1000	E	W	9.9367	105	5.7
ASP	1000	E	W	10.7883	64.4	1.0
ASP	1000	E	W	13.0152	51.4	1.6
ASP	1000	E	W	15.3407	16.4	2.1
ASP	1000	E	W	16.0583	44.7	23.4
ASP	1000	E	W	16.8170	138.6	70.2
ASP	1000	E	W	17.2490	63.8	3.2
ASP	1000	E	W	19.2048	33.8	0.9
ASP	1000	E	W	19.5637	37.8	0.5
ASP	1000	E	W	19.9421	53.8	9.2
ASP	1000	E	W	24.1875	21.1	2.7
ASP	1000	E	W	26.1814	77.7	0.8
ASP	1000	E	W	26.4824	49.9	12.7
ASP	1000	E	W	26.8244	30.1	5.0
ASP	1000	E	W	27.2774	31.6	3.8
ASP	1000	E	W	30.1052	35.1	5.8
ASP	1000	F	D	8.3829	128.5	4.9
ASP	1000	F	D	9.9352	81.3	2.3
ASP	1000	F	D	10.7867	63.2	1.0
ASP	1000	F	D	13.0137	53.9	2.2
ASP	1000	F	D	15.5634	338.5	153.2
ASP	1000	F	D	16.0591	67.7	3.7
ASP	1000	F	D	16.8135	121.5	55.1
ASP	1000	F	D	17.2481	119.3	47.8
ASP	1000	F	D	18.6024	371.7	115.4
ASP	1000	F	D	19.2045	40.6	4.3
ASP	1000	F	D	19.2048	33.9	0.9
ASP	1000	F	D	19.5636	38.5	0.7
ASP	1000	F	D	19.9443	45.2	2.7
ASP	1000	F	D	20.3810	36.7	11.4
ASP	1000	F	D	21.6691	109.9	59.5
ASP	1000	F	D	25.2892	70.8	1.8
ASP	1000	F	D	26.4852	38	7.8
ASP	1000	F	D	27.2766	32.3	1.7
ASP	1000	F	D	30.1097	37.9	11.3
ASP	1000	F	D	30.8100	18	0.4
ASP	1000	F	D	31.5292	77.8	3.0
ASP	1000	F	W	8.3877	139.9	8.1
ASP	1000	F	W	9.9367	93.3	3.0
ASP	1000	F	W	10.7882	61.6	0.8
ASP	1000	F	W	13.0151	49.1	1.0
ASP	1000	F	W	16.0573	45.3	0.4
ASP	1000	F	W	16.8166	88.5	12.5
ASP	1000	F	W	17.2486	152.4	81.5
ASP	1000	F	W	19.2031	33.6	0.8
ASP	1000	F	W	19.5636	179.1	94.8
ASP	1000	F	W	19.9448	55.4	6.8
ASP	1000	F	W	37.3915	21	10.6

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	10	A	H	8.387	132.2	3.8	GLU	10	C	H	10.785	68.7	0.7
GLU	10	A	H	9.212	1626.9	214.6	GLU	10	C	H	11.703	1201.8	84.0
GLU	10	A	H	9.934	88.8	1.6	GLU	10	C	H	11.937	92.8	0.4
GLU	10	A	H	10.786	65.3	1.0	GLU	10	C	H	12.497	1374.1	535.5
GLU	10	A	H	11.704	1111.9	52.5	GLU	10	C	H	13.014	62.6	3.3
GLU	10	A	H	12.497	690.7	143.4	GLU	10	C	H	14.254	1229.1	188.0
GLU	10	A	H	13.015	52.7	2.4	GLU	10	C	H	15.572	552.8	39.9
GLU	10	A	H	14.254	816.5	85.1	GLU	10	C	H	16.818	93.7	6.4
GLU	10	A	H	15.573	726.7	43.7	GLU	10	C	H	16.997	2146.6	529.0
GLU	10	A	H	16.459	89.8	7.2	GLU	10	C	H	17.249	57.6	1.2
GLU	10	A	H	16.818	83.4	7.0	GLU	10	C	H	18.484	865.7	86.1
GLU	10	A	H	16.997	1093.3	151.9	GLU	10	C	H	18.627	739.6	60.5
GLU	10	A	H	17.251	59.2	2.2	GLU	10	C	H	19.000	779.9	85.7
GLU	10	A	H	18.484	889.3	58.4	GLU	10	C	H	19.569	39.9	0.6
GLU	10	A	H	18.627	587.4	23.9	GLU	10	C	H	19.944	61.3	8.5
GLU	10	A	H	19.000	650.2	31.6	GLU	10	C	H	21.951	1632.9	828.9
GLU	10	A	H	19.206	31.9	0.9	GLU	10	C	H	22.252	538.4	45.1
GLU	10	A	H	19.568	38.2	0.9	GLU	10	C	H	23.419	857.3	112.0
GLU	10	A	H	19.946	48.2	3.4	GLU	10	C	H	23.533	576.6	278.9
GLU	10	A	H	20.858	110.3	0.7	GLU	10	C	H	24.259	427.2	101.6
GLU	10	A	H	21.951	849.7	113.0	GLU	10	C	H	24.818	766.7	116.1
GLU	10	A	H	22.253	601.1	33.7	GLU	10	C	H	25.148	478.0	31.4
GLU	10	A	H	22.495	823.3	254.7	GLU	10	C	H	29.023	413.9	53.0
GLU	10	A	H	23.419	800.5	72.7	GLU	10	C	H	31.125	681.1	96.1
GLU	10	A	H	23.534	861.8	201.1	GLU	10	C	H	34.385	875.5	190.4
GLU	10	A	H	24.259	612.5	64.1	GLU	10	C	H	34.467	539.9	75.6
GLU	10	A	H	24.819	776.5	72.2	GLU	10	C	H	34.791	432.1	223.3
GLU	10	A	H	25.148	403.7	28.4	GLU	10	D	H	8.386	130.6	9.1
GLU	10	A	H	26.376	636.5	176.4	GLU	10	D	H	9.211	965.2	92.0
GLU	10	A	H	26.730	552.0	73.6	GLU	10	D	H	9.933	89.8	2.1
GLU	10	A	H	27.621	620.6	64.6	GLU	10	D	H	10.785	64.8	0.9
GLU	10	A	H	28.736	382.7	72.8	GLU	10	D	H	11.702	1094.8	44.4
GLU	10	A	H	29.022	483.1	10.8	GLU	10	D	H	12.495	618.8	55.1
GLU	10	A	H	30.421	534.0	54.3	GLU	10	D	H	13.015	93.8	25.1
GLU	10	A	H	31.126	701.9	59.1	GLU	10	D	H	14.255	1339.6	125.3
GLU	10	A	H	33.907	657.8	157.5	GLU	10	D	H	15.572	608.2	30.8
GLU	10	A	H	34.386	675.0	167.2	GLU	10	D	H	16.817	77.4	5.1
GLU	10	A	H	34.467	627.4	95.5	GLU	10	D	H	16.997	1096.6	111.3
GLU	10	A	H	34.793	272.5	31.2	GLU	10	D	H	17.250	59.5	2.8
GLU	10	B	H	8.387	164.6	1.3	GLU	10	D	H	18.482	444.2	22.2
GLU	10	B	H	9.211	1123.6	379.9	GLU	10	D	H	18.626	476.8	14.6
GLU	10	B	H	9.933	92.0	1.7	GLU	10	D	H	18.999	478.2	17.2
GLU	10	B	H	10.784	70.2	1.0	GLU	10	D	H	19.206	33.0	0.7
GLU	10	B	H	11.703	1062.2	89.4	GLU	10	D	H	19.568	39.9	1.2
GLU	10	B	H	11.970	116.5	17.4	GLU	10	D	H	21.951	607.1	43.8
GLU	10	B	H	13.014	62.2	4.5	GLU	10	D	H	22.253	425.6	18.9
GLU	10	B	H	14.254	1042.7	198.6	GLU	10	D	H	22.493	375.1	52.4
GLU	10	B	H	15.572	646.7	47.9	GLU	10	D	H	23.418	496.6	27.2
GLU	10	B	H	16.818	93.9	4.2	GLU	10	D	H	23.533	512.9	76.0
GLU	10	B	H	16.996	1276.1	227.3	GLU	10	D	H	23.665	649.3	258.3
GLU	10	B	H	17.249	54.0	0.7	GLU	10	D	H	24.258	423.2	47.3
GLU	10	B	H	18.482	522.3	73.0	GLU	10	D	H	24.818	391.1	17.9
GLU	10	B	H	18.627	460.3	21.6	GLU	10	D	H	25.146	373.0	14.9
GLU	10	B	H	18.999	712.0	53.7	GLU	10	D	H	26.376	561.9	68.5
GLU	10	B	H	19.205	34.5	0.6	GLU	10	D	H	26.730	363.0	28.6
GLU	10	B	H	19.568	41.6	0.6	GLU	10	D	H	27.621	348.0	23.3
GLU	10	B	H	19.944	81.1	32.4	GLU	10	D	H	28.736	581.4	67.1
GLU	10	B	H	21.205	128.2	15.9	GLU	10	D	H	29.022	292.6	17.9
GLU	10	B	H	21.950	837.9	271.2	GLU	10	D	H	30.420	462.1	37.8
GLU	10	B	H	22.252	543.3	36.8	GLU	10	D	H	31.125	335.2	15.5
GLU	10	B	H	23.419	605.2	58.8	GLU	10	D	H	31.444	417.1	49.0
GLU	10	B	H	23.534	501.6	86.9	GLU	10	D	H	33.904	349.3	57.2
GLU	10	B	H	23.667	671.0	139.3	GLU	10	D	H	34.386	776.6	91.0
GLU	10	B	H	24.259	482.9	83.1	GLU	10	D	H	34.467	462.6	34.2
GLU	10	B	H	24.818	786.6	92.3	GLU	10	D	H	34.791	258.8	22.0
GLU	10	B	H	25.148	392.4	46.9	GLU	10	E	H	8.386	139.8	3.9
GLU	10	B	H	26.731	538.9	61.8	GLU	10	E	H	9.211	826.3	170.1
GLU	10	B	H	27.621	631.3	158.9	GLU	10	E	H	9.933	80.0	0.9
GLU	10	B	H	29.024	576.7	75.7	GLU	10	E	H	10.785	63.2	0.5
GLU	10	B	H	29.322	81.1	21.7	GLU	10	E	H	11.703	910.4	57.4
GLU	10	B	H	30.420	561.7	142.3	GLU	10	E	H	12.497	879.7	209.5
GLU	10	B	H	31.124	611.0	93.7	GLU	10	E	H	13.014	53.1	1.8
GLU	10	B	H	34.193	124.0	30.5	GLU	10	E	H	14.254	843.4	118.7
GLU	10	B	H	34.386	398.4	65.7	GLU	10	E	H	15.572	683.7	79.4
GLU	10	B	H	34.468	674.1	99.2	GLU	10	E	H	16.817	83.3	5.5
GLU	10	B	H	34.792	295.4	47.8	GLU	10	E	H	16.997	1552.2	643.9
GLU	10	C	H	8.387	151.6	4.9	GLU	10	E	H	17.250	47.9	0.6
GLU	10	C	H	9.212	1496.9	339.8	GLU	10	E	H	18.628	926.4	63.3
GLU	10	C	H	9.933	94.4	1.3	GLU	10	E	H	19.000	634.2	69.3

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	10	E	H	19.206	36.0	1.9	GLU	100	A	W	28.735	866.0	274.2
GLU	10	E	H	19.568	38.9	0.6	GLU	100	A	W	29.016	1562.1	863.5
GLU	10	E	H	19.944	53.5	7.9	GLU	100	A	W	30.236	1182.3	726.5
GLU	10	E	H	21.950	743.1	203.8	GLU	100	A	W	30.414	1051.5	165.7
GLU	10	E	H	22.252	462.0	45.3	GLU	100	A	W	30.592	407.1	119.9
GLU	10	E	H	23.418	562.0	108.0	GLU	100	A	W	31.123	640.8	61.7
GLU	10	E	H	24.818	778.2	119.4	GLU	100	A	W	31.441	1285.7	382.6
GLU	10	E	H	25.149	738.2	113.1	GLU	100	A	W	34.382	853.3	175.1
GLU	10	E	H	27.621	713.9	202.0	GLU	100	A	W	34.462	1135.6	335.9
GLU	10	E	H	29.023	521.7	101.4	GLU	100	A	W	35.617	1002.7	258.7
GLU	10	E	H	30.420	594.4	60.0	GLU	100	A	W	36.640	794.1	216.5
GLU	10	E	H	31.124	622.4	172.3	GLU	100	A	W	36.793	805.2	340.1
GLU	10	E	H	31.522	12.8	1.5	GLU	100	A	W	36.944	723.4	243.0
GLU	10	E	H	34.385	1051.5	535.8	GLU	100	A	W	37.466	541.2	94.9
GLU	100	A	D	9.931	141.0	5.7	GLU	100	A	W	37.764	674.9	322.7
GLU	100	A	D	10.783	93.6	2.9	GLU	100	A	W	38.325	1076.4	249.3
GLU	100	A	D	12.495	4067.5	2627.1	GLU	100	A	W	38.543	1051.2	668.7
GLU	100	A	D	13.013	68.6	2.3	GLU	100	B	D	11.702	7024.5	1648.7
GLU	100	A	D	15.572	5366.0	2207.1	GLU	100	B	D	15.572	4547.8	1050.1
GLU	100	A	D	18.482	2162.5	540.0	GLU	100	B	D	16.996	12757.9	7400.6
GLU	100	A	D	18.625	1126.6	168.2	GLU	100	B	D	18.481	976.2	79.9
GLU	100	A	D	18.998	1460.9	237.6	GLU	100	B	D	18.623	1335.8	111.6
GLU	100	A	D	21.657	51.1	13.5	GLU	100	B	D	18.997	1671.3	159.7
GLU	100	A	D	23.418	1105.8	243.5	GLU	100	B	D	21.950	1356.9	62.6
GLU	100	A	D	23.532	1862.7	575.7	GLU	100	B	D	22.252	2071.0	294.0
GLU	100	A	D	23.664	655.2	99.7	GLU	100	B	D	22.489	1084.9	234.4
GLU	100	A	D	24.257	2512.1	758.7	GLU	100	B	D	23.418	3635.4	1140.6
GLU	100	A	D	24.818	1056.6	194.2	GLU	100	B	D	23.531	4388.9	2314.2
GLU	100	A	D	25.142	1543.5	316.0	GLU	100	B	D	23.662	1131.7	179.5
GLU	100	A	D	26.373	1790.5	601.6	GLU	100	B	D	24.257	1232.4	190.7
GLU	100	A	D	26.728	783.1	112.9	GLU	100	B	D	24.818	1739.7	244.7
GLU	100	A	D	27.618	1260.8	267.1	GLU	100	B	D	25.142	942.9	122.8
GLU	100	A	D	28.735	2694.8	1142.4	GLU	100	B	D	26.373	1808.3	523.3
GLU	100	A	D	29.018	665.6	110.0	GLU	100	B	D	26.726	1008.2	136.0
GLU	100	A	D	30.417	895.4	194.1	GLU	100	B	D	27.618	988.0	98.2
GLU	100	A	D	31.124	998.8	141.2	GLU	100	B	D	27.876	842.6	165.9
GLU	100	A	D	31.443	762.1	119.4	GLU	100	B	D	28.735	1285.5	285.2
GLU	100	A	D	34.384	2472.4	1014.3	GLU	100	B	D	29.017	905.8	115.7
GLU	100	A	D	34.465	1034.5	197.0	GLU	100	B	D	30.237	926.1	169.1
GLU	100	A	H	8.387	119.3	5.4	GLU	100	B	D	30.417	1095.5	140.0
GLU	100	A	H	9.211	875.0	161.8	GLU	100	B	D	31.125	1018.2	91.7
GLU	100	A	H	9.935	79.3	1.2	GLU	100	B	D	31.443	915.4	119.5
GLU	100	A	H	10.786	60.4	0.6	GLU	100	B	D	31.944	656.4	111.6
GLU	100	A	H	11.703	1181.9	81.3	GLU	100	B	D	33.898	644.0	69.1
GLU	100	A	H	13.015	92.3	24.5	GLU	100	B	D	34.385	1182.0	172.7
GLU	100	A	H	14.254	713.8	95.9	GLU	100	B	D	34.465	1428.2	220.8
GLU	100	A	H	15.572	627.4	49.2	GLU	100	B	D	34.788	358.3	147.9
GLU	100	A	H	16.816	73.7	3.3	GLU	100	B	H	8.387	150.4	4.4
GLU	100	A	H	16.997	1223.8	244.2	GLU	100	B	H	9.933	92.2	1.1
GLU	100	A	H	17.251	50.1	1.3	GLU	100	B	H	10.785	70.8	0.7
GLU	100	A	H	18.482	412.6	106.2	GLU	100	B	H	11.703	864.0	90.3
GLU	100	A	H	18.626	438.4	20.6	GLU	100	B	H	11.945	1014.7	32.8
GLU	100	A	H	18.999	738.3	79.7	GLU	100	B	H	13.014	68.0	3.9
GLU	100	A	H	19.567	93.7	36.6	GLU	100	B	H	16.817	97.6	7.6
GLU	100	A	H	21.950	552.3	68.5	GLU	100	B	H	17.250	55.2	0.8
GLU	100	A	H	22.253	502.5	38.1	GLU	100	B	H	18.999	741.4	218.4
GLU	100	A	H	23.533	449.9	79.0	GLU	100	B	H	19.205	36.1	0.7
GLU	100	A	H	23.664	283.4	145.7	GLU	100	B	H	19.568	98.7	35.1
GLU	100	A	H	24.818	358.0	32.2	GLU	100	B	H	20.384	52.3	25.5
GLU	100	A	H	25.148	354.1	40.9	GLU	100	B	H	29.354	96.5	14.4
GLU	100	A	H	26.728	425.7	65.3	GLU	100	B	W	12.602	749.6	201.3
GLU	100	A	H	27.620	384.7	76.2	GLU	100	B	W	19.000	7784.0	4669.1
GLU	100	A	H	29.018	495.5	100.7	GLU	100	B	W	21.952	2954.5	1077.7
GLU	100	A	H	31.124	328.9	53.0	GLU	100	B	W	26.728	1362.4	657.7
GLU	100	A	H	34.385	413.9	64.5	GLU	100	B	W	27.617	2151.9	1072.2
GLU	100	A	H	34.466	534.4	161.6	GLU	100	B	W	30.415	4012.7	2518.4
GLU	100	A	W	12.603	2026.0	1219.7	GLU	100	B	W	30.593	1790.6	1056.4
GLU	100	A	W	18.481	2638.7	1390.1	GLU	100	B	W	31.123	1941.1	648.5
GLU	100	A	W	19.000	5051.5	2909.2	GLU	100	B	W	31.441	1933.0	1039.4
GLU	100	A	W	21.952	1503.8	441.0	GLU	100	B	W	31.947	1331.6	615.1
GLU	100	A	W	23.662	1999.3	1120.5	GLU	100	B	W	34.383	2942.1	1757.6
GLU	100	A	W	24.257	1139.5	313.0	GLU	100	B	W	34.464	1509.4	429.2
GLU	100	A	W	24.258	2529.7	1469.1	GLU	100	B	W	34.786	400.8	119.7
GLU	100	A	W	24.820	1371.9	366.3	GLU	100	B	W	35.217	1004.9	551.1
GLU	100	A	W	24.820	2331.7	1277.8	GLU	100	B	W	35.617	875.5	164.2
GLU	100	A	W	25.142	789.4	499.1	GLU	100	B	W	36.641	1207.1	325.7
GLU	100	A	W	26.726	1166.2	475.9	GLU	100	B	W	36.946	784.1	170.9
GLU	100	A	W	27.616	712.5	96.7	GLU	100	B	W	37.392	775.0	228.3
GLU	100	A	W	27.877	768.2	314.3	GLU	100	B	W	37.467	587.1	70.0

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	100	B	W	37.468	604.1	314.8	GLU	100	C	W	21.952	3189.1	1481.5
GLU	100	B	W	37.949	1169.6	767.4	GLU	100	C	W	22.252	3128.1	1051.0
GLU	100	B	W	38.327	2172.4	954.7	GLU	100	C	W	23.530	3082.1	1929.2
GLU	100	B	W	38.542	1582.2	832.1	GLU	100	C	W	24.257	1460.6	321.2
GLU	100	C	D	8.387	150.9	12.8	GLU	100	C	W	25.141	1268.7	401.5
GLU	100	C	D	9.211	2284.8	412.2	GLU	100	C	W	25.143	856.3	384.4
GLU	100	C	D	9.933	111.8	3.6	GLU	100	C	W	26.372	2018.5	657.0
GLU	100	C	D	10.784	79.7	2.0	GLU	100	C	W	26.728	1225.1	310.3
GLU	100	C	D	11.702	1512.7	84.2	GLU	100	C	W	27.617	2244.4	1076.1
GLU	100	C	D	13.014	91.5	24.4	GLU	100	C	W	27.877	1111.7	295.4
GLU	100	C	D	14.255	3543.3	644.2	GLU	100	C	W	30.236	877.4	149.0
GLU	100	C	D	15.571	1156.1	88.2	GLU	100	C	W	30.415	1300.9	226.1
GLU	100	C	D	16.996	2438.3	464.5	GLU	100	C	W	30.593	827.7	342.5
GLU	100	C	D	17.249	69.6	3.2	GLU	100	C	W	31.124	1993.6	525.6
GLU	100	C	D	18.481	618.4	44.5	GLU	100	C	W	31.440	1855.0	610.3
GLU	100	C	D	18.624	653.5	38.6	GLU	100	C	W	31.945	1069.1	469.9
GLU	100	C	D	18.998	974.3	70.2	GLU	100	C	W	33.901	922.8	259.1
GLU	100	C	D	19.205	38.2	3.0	GLU	100	C	W	34.383	3668.6	1954.8
GLU	100	C	D	19.568	46.3	2.8	GLU	100	C	W	34.463	1355.2	297.4
GLU	100	C	D	21.950	918.8	94.3	GLU	100	C	W	34.786	330.3	60.2
GLU	100	C	D	22.252	706.8	43.7	GLU	100	C	W	35.216	828.2	458.4
GLU	100	C	D	23.418	1213.2	156.2	GLU	100	C	W	35.618	954.0	127.8
GLU	100	C	D	23.531	1429.1	261.8	GLU	100	C	W	36.639	1247.3	388.6
GLU	100	C	D	23.664	576.9	43.5	GLU	100	C	W	36.946	928.1	285.8
GLU	100	C	D	24.257	675.2	88.5	GLU	100	C	W	37.390	2768.0	1459.9
GLU	100	C	D	24.818	809.4	58.4	GLU	100	C	W	37.466	1082.3	180.5
GLU	100	C	D	25.145	435.1	49.9	GLU	100	C	W	37.765	510.4	199.6
GLU	100	C	D	26.373	914.4	222.1	GLU	100	C	W	37.948	900.2	291.7
GLU	100	C	D	26.726	639.0	78.1	GLU	100	C	W	38.326	1462.0	382.7
GLU	100	C	D	27.618	560.5	57.7	GLU	100	C	W	38.544	1090.9	393.2
GLU	100	C	D	27.876	367.1	83.3	GLU	100	D	D	9.211	820.5	35.0
GLU	100	C	D	28.734	1103.4	116.8	GLU	100	D	D	11.702	1331.9	102.8
GLU	100	C	D	29.017	484.4	81.6	GLU	100	D	D	12.494	561.4	40.6
GLU	100	C	D	30.236	921.4	323.3	GLU	100	D	D	14.254	779.1	30.3
GLU	100	C	D	30.417	489.8	39.9	GLU	100	D	D	15.572	580.6	17.2
GLU	100	C	D	31.123	556.5	29.6	GLU	100	D	D	16.996	691.0	22.2
GLU	100	C	D	31.443	561.3	55.4	GLU	100	D	D	18.481	483.6	25.0
GLU	100	C	D	31.945	533.9	77.7	GLU	100	D	D	18.623	463.2	16.1
GLU	100	C	D	33.901	392.5	65.2	GLU	100	D	D	18.997	444.5	11.7
GLU	100	C	D	34.385	810.5	98.9	GLU	100	D	D	21.950	498.2	21.9
GLU	100	C	D	34.464	829.0	109.8	GLU	100	D	D	22.252	453.3	13.8
GLU	100	C	D	34.786	262.8	98.7	GLU	100	D	D	23.418	544.3	21.7
GLU	100	C	H	8.387	134.4	4.9	GLU	100	D	D	23.532	795.5	65.5
GLU	100	C	H	9.211	1038.4	116.9	GLU	100	D	D	23.662	386.7	25.2
GLU	100	C	H	9.933	92.1	0.8	GLU	100	D	D	24.257	423.2	21.8
GLU	100	C	H	10.785	68.2	0.7	GLU	100	D	D	24.818	462.3	17.1
GLU	100	C	H	11.702	2260.6	835.2	GLU	100	D	D	25.141	332.7	15.4
GLU	100	C	H	11.703	1422.2	95.9	GLU	100	D	D	26.373	449.0	32.1
GLU	100	C	H	11.703	2397.3	707.5	GLU	100	D	D	26.726	301.0	17.9
GLU	100	C	H	13.014	62.8	3.3	GLU	100	D	D	27.617	379.9	47.6
GLU	100	C	H	14.253	874.4	89.6	GLU	100	D	D	28.735	466.0	32.7
GLU	100	C	H	15.572	638.6	36.0	GLU	100	D	D	29.016	361.9	29.9
GLU	100	C	H	16.817	83.7	4.0	GLU	100	D	D	30.416	387.2	27.5
GLU	100	C	H	16.996	1565.7	335.4	GLU	100	D	D	31.124	353.2	17.2
GLU	100	C	H	17.249	59.1	1.5	GLU	100	D	D	31.443	412.9	21.7
GLU	100	C	H	18.482	472.8	33.3	GLU	100	D	D	33.899	325.6	44.6
GLU	100	C	H	18.627	571.5	34.8	GLU	100	D	D	34.385	567.7	38.2
GLU	100	C	H	18.999	687.5	52.6	GLU	100	D	D	34.465	407.3	20.7
GLU	100	C	H	19.205	99.3	2.5	GLU	100	D	H	8.386	122.8	4.5
GLU	100	C	H	21.950	880.7	248.2	GLU	100	D	H	9.211	1344.3	356.3
GLU	100	C	H	22.252	580.8	45.4	GLU	100	D	H	9.211	794.9	113.6
GLU	100	C	H	23.418	614.5	51.0	GLU	100	D	H	9.934	84.6	1.5
GLU	100	C	H	23.534	637.4	71.1	GLU	100	D	H	10.785	63.6	0.7
GLU	100	C	H	23.665	424.8	50.2	GLU	100	D	H	11.703	939.1	47.0
GLU	100	C	H	24.817	580.5	64.5	GLU	100	D	H	13.015	61.6	4.2
GLU	100	C	H	25.148	326.5	38.5	GLU	100	D	H	14.254	1146.3	138.7
GLU	100	C	H	26.375	635.4	226.1	GLU	100	D	H	15.572	595.1	29.5
GLU	100	C	H	26.729	363.7	78.4	GLU	100	D	H	16.815	75.1	3.1
GLU	100	C	H	27.620	535.1	103.8	GLU	100	D	H	16.996	1565.7	420.0
GLU	100	C	H	28.735	815.8	159.3	GLU	100	D	H	17.251	115.5	40.3
GLU	100	C	H	29.021	370.7	32.7	GLU	100	D	H	18.482	458.4	41.0
GLU	100	C	H	30.420	459.8	61.1	GLU	100	D	H	18.626	556.4	36.2
GLU	100	C	H	31.124	530.1	38.3	GLU	100	D	H	18.999	584.7	54.0
GLU	100	C	H	31.444	454.1	158.1	GLU	100	D	H	19.206	78.1	1.8
GLU	100	C	H	34.385	549.2	73.9	GLU	100	D	H	19.567	36.8	0.5
GLU	100	C	H	34.466	475.6	43.9	GLU	100	D	H	19.945	50.9	6.1
GLU	100	C	H	34.791	227.2	25.1	GLU	100	D	H	20.387	34.2	8.1
GLU	100	C	W	12.603	1114.8	513.8	GLU	100	D	H	20.852	267.2	3.2
GLU	100	C	W	19.000	2378.9	475.7	GLU	100	D	H	21.670	104.8	2.5

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	100	D	H	21.950	620.6	100.5	GLU	1000	A	H	26.827	35.3	16.4
GLU	100	D	H	22.252	421.6	24.2	GLU	1000	A	H	32.436	18.1	3.5
GLU	100	D	H	23.418	615.5	58.8	GLU	1000	A	W	8.385	119.1	6.1
GLU	100	D	H	23.532	405.1	168.9	GLU	1000	A	W	9.933	79.4	1.6
GLU	100	D	H	24.818	516.9	35.2	GLU	1000	A	W	10.785	59.4	0.6
GLU	100	D	H	25.148	295.7	31.4	GLU	1000	A	W	11.696	512.6	82.3
GLU	100	D	H	26.375	636.5	323.5	GLU	1000	A	W	13.014	48.6	1.6
GLU	100	D	H	26.729	334.7	59.9	GLU	1000	A	W	15.571	506.7	159.8
GLU	100	D	H	27.621	335.6	5.1	GLU	1000	A	W	19.565	78.4	32.0
GLU	100	D	H	29.021	268.0	26.0	GLU	1000	A	W	19.945	73.6	35.1
GLU	100	D	H	30.419	358.8	39.0	GLU	1000	A	W	26.824	28.8	3.1
GLU	100	D	H	31.124	320.6	20.6	GLU	1000	A	W	27.280	29.1	1.9
GLU	100	D	H	31.443	380.1	53.3	GLU	1000	A	W	27.826	21.7	0.7
GLU	100	D	H	33.905	253.0	47.4	GLU	1000	A	W	32.436	16.7	1.0
GLU	100	D	H	34.385	560.0	102.4	GLU	1000	B	D	8.385	141.3	5.7
GLU	100	D	H	34.466	533.7	68.6	GLU	1000	B	D	9.935	92.9	1.7
GLU	100	D	H	34.790	199.3	17.0	GLU	1000	B	D	10.787	68.5	0.7
GLU	100	D	W	18.480	1795.2	1153.0	GLU	1000	B	D	11.700	604.7	293.2
GLU	100	D	W	18.999	1842.6	323.7	GLU	1000	B	D	13.017	57.1	2.2
GLU	100	D	W	21.951	2134.3	718.8	GLU	1000	B	D	15.345	17.4	2.3
GLU	100	D	W	22.252	1741.8	494.4	GLU	1000	B	D	16.062	47.9	24.5
GLU	100	D	W	23.420	1728.3	861.0	GLU	1000	B	D	16.821	86.4	7.2
GLU	100	D	W	23.662	1699.4	641.1	GLU	1000	B	D	17.250	57.6	1.4
GLU	100	D	W	24.257	2247.6	974.6	GLU	1000	B	D	19.208	34.1	0.8
GLU	100	D	W	24.820	2474.6	1034.6	GLU	1000	B	D	19.570	38.1	0.5
GLU	100	D	W	25.141	1329.0	330.7	GLU	1000	B	D	19.948	56.3	10.5
GLU	100	D	W	27.615	1282.8	372.2	GLU	1000	B	D	27.289	31.3	0.9
GLU	100	D	W	28.736	838.3	139.2	GLU	1000	B	D	30.116	92.9	7.4
GLU	100	D	W	29.018	692.0	91.8	GLU	1000	B	H	6.088	25.7	3.7
GLU	100	D	W	30.414	1438.2	336.8	GLU	1000	B	H	8.384	115.2	2.8
GLU	100	D	W	31.123	747.4	75.1	GLU	1000	B	H	8.384	99.2	3.4
GLU	100	D	W	31.440	1336.9	302.1	GLU	1000	B	H	9.934	76.5	1.2
GLU	100	D	W	31.945	455.5	96.7	GLU	1000	B	H	9.936	66.4	0.9
GLU	100	D	W	33.900	538.4	117.8	GLU	1000	B	H	10.787	61.4	0.7
GLU	100	D	W	34.383	1075.8	222.2	GLU	1000	B	H	10.788	54.1	0.6
GLU	100	D	W	34.463	1092.2	278.9	GLU	1000	B	H	11.700	1098.1	512.1
GLU	100	D	W	34.783	509.6	61.5	GLU	1000	B	H	13.013	54.2	2.0
GLU	100	D	W	35.616	1019.1	196.6	GLU	1000	B	H	13.016	49.2	2.1
GLU	100	D	W	36.640	799.2	123.9	GLU	1000	B	H	15.349	23.9	9.0
GLU	100	D	W	36.793	550.4	122.8	GLU	1000	B	H	15.356	13.9	1.6
GLU	100	D	W	36.944	488.3	73.5	GLU	1000	B	H	15.571	244.0	157.8
GLU	100	D	W	37.392	680.6	112.3	GLU	1000	B	H	16.060	113.8	45.8
GLU	100	D	W	37.466	408.9	29.7	GLU	1000	B	H	16.061	68.8	0.8
GLU	100	D	W	37.762	394.0	78.0	GLU	1000	B	H	16.816	71.0	4.2
GLU	100	D	W	37.948	825.0	269.0	GLU	1000	B	H	16.818	62.5	2.9
GLU	100	D	W	38.326	618.9	65.1	GLU	1000	B	H	17.249	71.5	8.8
GLU	100	D	W	38.543	613.6	112.4	GLU	1000	B	H	17.249	48.3	0.8
GLU	1000	A	D	8.386	126.3	6.1	GLU	1000	B	H	17.251	92.6	38.7
GLU	1000	A	D	9.936	85.1	1.6	GLU	1000	B	H	18.611	156.9	29.6
GLU	1000	A	D	10.788	62.4	0.7	GLU	1000	B	H	18.996	303.8	96.2
GLU	1000	A	D	11.698	754.3	198.8	GLU	1000	B	H	19.205	33.3	0.7
GLU	1000	A	D	13.017	51.9	2.1	GLU	1000	B	H	19.207	29.8	0.7
GLU	1000	A	D	15.573	417.0	174.5	GLU	1000	B	H	19.564	38.9	0.5
GLU	1000	A	D	16.821	92.5	2.7	GLU	1000	B	H	19.568	33.6	0.6
GLU	1000	A	D	17.251	55.1	2.2	GLU	1000	B	H	19.942	47.8	2.7
GLU	1000	A	D	18.611	227.8	74.1	GLU	1000	B	H	19.949	43.2	3.7
GLU	1000	A	D	19.208	32.1	0.6	GLU	1000	B	H	20.385	37.1	5.4
GLU	1000	A	D	19.570	35.8	0.5	GLU	1000	B	H	20.385	36.3	9.7
GLU	1000	A	D	19.947	43.9	3.8	GLU	1000	B	H	20.862	16.4	3.4
GLU	1000	A	D	23.642	54.9	6.0	GLU	1000	B	H	21.215	134.2	1.2
GLU	1000	A	D	25.285	14.4	1.6	GLU	1000	B	H	21.674	106.1	58.2
GLU	1000	A	D	26.490	41.4	13.9	GLU	1000	B	H	22.294	306.4	8.9
GLU	1000	A	D	26.832	26.9	3.6	GLU	1000	B	H	23.651	320.9	137.0
GLU	1000	A	D	34.917	196.7	2.5	GLU	1000	B	H	24.193	22.7	2.1
GLU	1000	A	H	8.384	112.6	4.6	GLU	1000	B	H	25.284	20.6	8.2
GLU	1000	A	H	9.935	71.5	1.5	GLU	1000	B	H	26.192	25.2	8.1
GLU	1000	A	H	10.786	57.8	0.8	GLU	1000	B	H	26.489	38.9	5.5
GLU	1000	A	H	11.696	956.7	225.3	GLU	1000	B	H	26.490	36.9	12.0
GLU	1000	A	H	13.014	49.0	1.8	GLU	1000	B	H	26.827	27.2	1.9
GLU	1000	A	H	14.255	979.8	620.5	GLU	1000	B	H	27.276	33.2	2.5
GLU	1000	A	H	15.570	361.8	60.5	GLU	1000	B	H	27.824	23.0	0.8
GLU	1000	A	H	16.810	73.5	10.9	GLU	1000	B	H	27.826	90.8	1.1
GLU	1000	A	H	17.251	47.0	1.5	GLU	1000	B	H	28.098	143.0	32.0
GLU	1000	A	H	18.607	141.0	23.6	GLU	1000	B	H	30.108	27.2	2.0
GLU	1000	A	H	18.987	258.7	34.0	GLU	1000	B	H	30.120	30.2	13.2
GLU	1000	A	H	19.207	32.1	1.0	GLU	1000	B	H	30.800	21.0	7.1
GLU	1000	A	H	19.563	36.5	0.5	GLU	1000	B	H	34.011	32.0	11.9
GLU	1000	A	H	19.945	42.1	2.8	GLU	1000	B	H	34.388	439.4	204.2
GLU	1000	A	H	22.254	233.2	34.4	GLU	1000	B	H	34.681	22.4	0.1

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)	Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	1000	B	H	34.895	21.2	7.1	GLU	1000	C	H	23.097	314.1	206.0
GLU	1000	B	H	39.741	78.9	27.3	GLU	1000	C	H	25.134	167.5	70.4
GLU	1000	B	W	8.386	127.9	6.6	GLU	1000	C	H	25.984	166.5	35.6
GLU	1000	B	W	8.386	130.9	5.7	GLU	1000	C	H	26.803	246.0	88.5
GLU	1000	B	W	9.935	85.1	1.9	GLU	1000	C	H	26.828	37.5	15.2
GLU	1000	B	W	9.936	91.0	1.8	GLU	1000	C	W	8.386	127.2	10.4
GLU	1000	B	W	10.785	65.7	0.7	GLU	1000	C	W	9.934	84.7	2.3
GLU	1000	B	W	10.787	63.3	0.7	GLU	1000	C	W	10.785	61.6	0.8
GLU	1000	B	W	11.697	1652.7	469.8	GLU	1000	C	W	11.697	1352.0	354.1
GLU	1000	B	W	11.701	379.1	50.2	GLU	1000	C	W	13.014	48.9	1.8
GLU	1000	B	W	13.013	49.9	0.8	GLU	1000	C	W	14.255	551.9	128.1
GLU	1000	B	W	13.017	51.1	1.7	GLU	1000	C	W	15.570	418.9	95.0
GLU	1000	B	W	15.342	17.8	2.0	GLU	1000	C	W	16.814	78.8	4.9
GLU	1000	B	W	16.062	44.5	18.2	GLU	1000	C	W	17.249	58.3	2.4
GLU	1000	B	W	16.818	80.7	1.1	GLU	1000	C	W	18.614	414.6	69.0
GLU	1000	B	W	16.822	80.0	5.6	GLU	1000	C	W	18.989	392.1	75.6
GLU	1000	B	W	17.249	61.7	2.6	GLU	1000	C	W	19.204	32.7	1.1
GLU	1000	B	W	17.250	111.8	42.7	GLU	1000	C	W	19.565	36.2	0.4
GLU	1000	B	W	17.881	590.0	209.8	GLU	1000	C	W	19.943	46.1	2.4
GLU	1000	B	W	18.468	176.2	37.7	GLU	1000	C	W	22.250	395.3	39.7
GLU	1000	B	W	18.990	358.2	127.2	GLU	1000	C	W	26.487	39.7	5.6
GLU	1000	B	W	19.203	33.6	0.7	GLU	1000	C	W	26.823	28.8	3.1
GLU	1000	B	W	19.207	33.1	0.8	GLU	1000	C	W	27.824	101.9	4.9
GLU	1000	B	W	19.565	37.5	0.5	GLU	1000	D	D	8.386	121.8	6.7
GLU	1000	B	W	19.571	36.3	0.5	GLU	1000	D	D	9.937	77.1	1.5
GLU	1000	B	W	19.944	66.0	17.3	GLU	1000	D	D	10.788	58.5	0.7
GLU	1000	B	W	19.948	51.8	6.1	GLU	1000	D	D	11.700	1025.5	471.3
GLU	1000	B	W	20.851	21.7	8.7	GLU	1000	D	D	13.018	48.3	1.6
GLU	1000	B	W	21.673	33.6	4.2	GLU	1000	D	D	14.257	617.6	219.5
GLU	1000	B	W	22.295	302.0	8.6	GLU	1000	D	D	15.354	19.7	4.5
GLU	1000	B	W	26.188	22.0	1.7	GLU	1000	D	D	16.821	78.5	10.1
GLU	1000	B	W	26.482	39.6	7.3	GLU	1000	D	D	17.252	48.9	1.1
GLU	1000	B	W	26.827	29.0	0.1	GLU	1000	D	D	18.615	196.0	32.7
GLU	1000	B	W	27.280	31.5	0.7	GLU	1000	D	D	19.208	31.7	1.0
GLU	1000	B	W	27.288	31.2	1.1	GLU	1000	D	D	19.570	34.1	0.4
GLU	1000	B	W	27.824	23.9	1.1	GLU	1000	D	D	19.949	46.1	3.3
GLU	1000	B	W	32.437	16.0	0.6	GLU	1000	D	D	23.423	804.1	162.2
GLU	1000	B	W	36.376	42.4	0.4	GLU	1000	D	D	30.118	42.1	7.7
GLU	1000	B	W	38.364	19.4	2.1	GLU	1000	D	D	32.436	15.2	0.6
GLU	1000	C	D	8.386	117.3	4.4	GLU	1000	D	D	38.360	17.9	1.9
GLU	1000	C	D	9.937	76.7	1.8	GLU	1000	D	H	8.384	107.4	4.0
GLU	1000	C	D	10.788	58.3	0.7	GLU	1000	D	H	9.935	72.6	1.7
GLU	1000	C	D	11.699	560.9	197.4	GLU	1000	D	H	10.786	57.6	0.8
GLU	1000	C	D	13.018	361.4	217.0	GLU	1000	D	H	11.695	2204.2	1188.9
GLU	1000	C	D	16.821	76.5	10.7	GLU	1000	D	H	13.014	55.5	3.6
GLU	1000	C	D	17.252	70.6	9.5	GLU	1000	D	H	14.255	491.9	58.7
GLU	1000	C	D	18.613	187.1	67.2	GLU	1000	D	H	16.810	70.8	8.2
GLU	1000	C	D	19.571	306.5	189.6	GLU	1000	D	H	17.251	126.2	49.9
GLU	1000	C	D	19.951	63.9	23.7	GLU	1000	D	H	18.608	312.0	187.7
GLU	1000	C	D	26.492	35.8	3.7	GLU	1000	D	H	19.946	69.0	35.9
GLU	1000	C	D	34.024	37.8	8.7	GLU	1000	D	H	24.187	108.1	0.9
GLU	1000	C	H	8.384	99.4	4.3	GLU	1000	D	H	26.192	96.5	0.7
GLU	1000	C	H	8.384	120.5	5.6	GLU	1000	D	H	26.829	27.4	7.1
GLU	1000	C	H	9.934	84.6	2.3	GLU	1000	D	H	27.276	30.9	2.3
GLU	1000	C	H	9.936	65.2	1.0	GLU	1000	D	W	8.386	138.9	5.5
GLU	1000	C	H	10.786	62.2	0.8	GLU	1000	D	W	9.210	1339.2	734.6
GLU	1000	C	H	10.788	53.3	0.5	GLU	1000	D	W	9.933	97.7	3.2
GLU	1000	C	H	11.697	584.9	182.5	GLU	1000	D	W	10.785	65.7	0.7
GLU	1000	C	H	11.698	517.8	59.2	GLU	1000	D	W	11.697	1849.8	671.5
GLU	1000	C	H	11.919	562.0	35.6	GLU	1000	D	W	13.013	52.8	2.0
GLU	1000	C	H	13.013	53.5	2.2	GLU	1000	D	W	13.014	52.4	1.8
GLU	1000	C	H	13.016	46.0	1.6	GLU	1000	D	W	14.256	824.0	259.5
GLU	1000	C	H	15.346	14.6	1.3	GLU	1000	D	W	15.570	659.8	127.9
GLU	1000	C	H	15.571	602.1	357.7	GLU	1000	D	W	16.814	84.5	6.2
GLU	1000	C	H	16.059	125.2	6.2	GLU	1000	D	W	18.608	593.0	197.0
GLU	1000	C	H	16.811	77.6	8.9	GLU	1000	D	W	18.990	555.7	77.9
GLU	1000	C	H	16.817	63.8	3.0	GLU	1000	D	W	19.204	33.1	0.7
GLU	1000	C	H	17.250	52.9	1.6	GLU	1000	D	W	19.564	37.5	0.4
GLU	1000	C	H	17.252	95.5	42.6	GLU	1000	D	W	19.942	50.5	3.6
GLU	1000	C	H	18.620	504.8	203.5	GLU	1000	D	W	20.385	131.7	11.6
GLU	1000	C	H	18.994	328.1	153.9	GLU	1000	D	W	25.277	19.2	7.3
GLU	1000	C	H	19.206	33.7	1.2	GLU	1000	D	W	26.488	40.5	4.2
GLU	1000	C	H	19.209	30.0	0.7	GLU	1000	D	W	26.825	29.7	3.1
GLU	1000	C	H	19.563	37.9	0.5	GLU	1000	E	H	8.384	101.6	3.3
GLU	1000	C	H	19.568	33.4	0.6	GLU	1000	E	H	8.386	106.6	3.0
GLU	1000	C	H	19.944	45.9	2.5	GLU	1000	E	H	9.935	70.3	1.0
GLU	1000	C	H	19.951	41.3	3.2	GLU	1000	E	H	9.936	75.4	1.6
GLU	1000	C	H	21.668	113.6	2.4	GLU	1000	E	H	10.787	57.2	0.7
GLU	1000	C	H	22.295	305.9	10.9	GLU	1000	E	H	10.787	58.4	0.7

Amino Acid	Conc mg/L	Method	Time	2Θ°	Crystallite Size (nm)	2-esd (nm)
GLU	1000	E	H	13.015	54.2	3.0
GLU	1000	E	H	13.016	127.7	42.9
GLU	1000	E	H	15.341	16.2	2.9
GLU	1000	E	H	16.058	56.5	12.2
GLU	1000	E	H	16.815	65.9	2.6
GLU	1000	E	H	16.818	66.9	8.1
GLU	1000	E	H	17.249	44.1	0.6
GLU	1000	E	H	17.250	47.6	1.1
GLU	1000	E	H	19.205	32.3	0.9
GLU	1000	E	H	19.206	30.9	0.7
GLU	1000	E	H	19.563	37.1	0.6
GLU	1000	E	H	19.567	35.1	0.6
GLU	1000	E	H	19.943	43.4	3.8
GLU	1000	E	H	19.947	42.3	3.1
GLU	1000	E	H	20.387	36.9	7.3
GLU	1000	E	H	21.085	28.5	2.3
GLU	1000	E	H	21.228	88.9	0.7
GLU	1000	E	H	22.293	300.3	8.5
GLU	1000	E	H	25.220	192.5	86.1
GLU	1000	E	H	25.282	17.9	4.8
GLU	1000	E	H	26.004	72.8	0.6
GLU	1000	E	H	26.192	89.1	5.0
GLU	1000	E	H	26.490	42.5	21.7
GLU	1000	E	H	26.828	28.4	3.7
GLU	1000	E	H	27.278	29.5	1.6
GLU	1000	E	H	27.283	28.2	0.9
GLU	1000	E	H	30.112	26.8	3.6
GLU	1000	E	H	30.802	16.8	2.5
GLU	1000	E	H	34.009	50.3	3.1
GLU	1000	E	W	8.385	123.4	5.1
GLU	1000	E	W	9.940	91.1	1.9
GLU	1000	E	W	10.791	66.0	0.7
GLU	1000	E	W	13.020	58.8	2.9
GLU	1000	E	W	15.800	187.3	2.0
GLU	1000	E	W	16.060	47.7	2.2
GLU	1000	E	W	16.813	75.4	3.2
GLU	1000	E	W	17.252	55.2	1.4
GLU	1000	E	W	19.203	34.4	0.8
GLU	1000	E	W	19.564	39.3	0.5
GLU	1000	E	W	19.943	55.6	6.1
GLU	1000	E	W	20.856	18.0	2.0
GLU	1000	E	W	25.279	16.9	4.3
GLU	1000	E	W	26.486	41.1	6.2
GLU	1000	E	W	26.822	35.2	0.2
GLU	1000	E	W	27.278	31.6	1.3
GLU	1000	E	W	30.111	34.9	4.7
GLU	1000	E	W	32.435	17.1	0.5
GLU	1000	E	W	36.381	119.9	28.8
GLU	1000	E	W	37.394	18.7	4.1
GLU	1000	E	W	38.366	21.1	6.4
GLU	1000	F	D	8.385	131.9	5.0
GLU	1000	F	D	9.934	88.7	1.5
GLU	1000	F	D	10.786	66.3	0.7
GLU	1000	F	D	13.015	56.4	2.4
GLU	1000	F	D	13.015	58.0	2.8
GLU	1000	F	D	15.563	6.3	0.6
GLU	1000	F	D	16.819	81.7	6.0
GLU	1000	F	D	17.247	54.7	1.2
GLU	1000	F	D	19.203	33.7	0.7
GLU	1000	F	D	19.567	98.4	40.8
GLU	1000	F	D	19.944	57.6	9.0
GLU	1000	F	D	25.280	17.5	2.7
GLU	1000	F	D	26.012	10.3	2.8
GLU	1000	F	D	30.109	30.3	4.3
GLU	1000	F	D	36.972	70.7	21.4
GLU	1000	F	H	8.384	107.3	4.8
GLU	1000	F	H	8.386	138.3	6.2
GLU	1000	F	H	9.932	95.6	1.8
GLU	1000	F	H	9.936	72.2	1.1
GLU	1000	F	H	10.784	70.1	0.8
GLU	1000	F	H	10.787	58.3	0.6
GLU	1000	F	H	11.695	1189.6	240.7
GLU	1000	F	H	13.013	56.1	1.9
GLU	1000	F	H	13.016	50.5	2.1
GLU	1000	F	H	16.818	84.5	14.8
GLU	1000	F	H	17.247	59.1	1.4
GLU	1000	F	H	17.250	112.0	49.7
GLU	1000	F	H	19.203	35.9	1.2
GLU	1000	F	H	19.208	31.9	0.8
GLU	1000	F	H	19.563	37.6	0.6
GLU	1000	F	H	19.565	39.2	0.5
GLU	1000	F	H	19.941	63.4	16.7
GLU	1000	F	H	19.946	43.7	3.1
GLU	1000	F	H	26.484	45.6	5.3
GLU	1000	F	H	26.489	40.4	13.9
GLU	1000	F	H	26.824	31.4	2.5
GLU	1000	F	H	26.825	37.3	2.4
GLU	1000	F	H	27.281	30.6	0.9
GLU	1000	F	H	27.825	21.7	0.6
GLU	1000	F	H	30.108	35.8	4.7
GLU	1000	F	H	31.526	18.0	3.6
GLU	1000	F	H	32.435	17.1	0.7
GLU	1000	F	H	34.009	98.0	7.3
GLU	1000	F	H	36.384	22.4	4.1
GLU	1000	F	H	36.966	73.1	1.1
GLU	1000	F	W	8.391	148.4	6.0
GLU	1000	F	W	9.935	70.5	1.4
GLU	1000	F	W	9.940	96.4	1.3
GLU	1000	F	W	10.786	57.8	0.8
GLU	1000	F	W	10.791	68.2	0.5
GLU	1000	F	W	11.697	1983.6	1219.0
GLU	1000	F	W	11.704	423.2	244.7
GLU	1000	F	W	11.948	2141.9	1159.1
GLU	1000	F	W	11.955	121.6	1.1
GLU	1000	F	W	13.014	51.0	1.7
GLU	1000	F	W	13.020	55.2	1.3
GLU	1000	F	W	14.254	835.6	279.9
GLU	1000	F	W	15.570	891.3	482.9
GLU	1000	F	W	16.058	136.8	1.6
GLU	1000	F	W	16.446	123.1	6.9
GLU	1000	F	W	16.810	72.1	6.3
GLU	1000	F	W	16.823	115.5	2.5
GLU	1000	F	W	17.253	61.2	1.5
GLU	1000	F	W	17.835	308.0	5.0
GLU	1000	F	W	18.604	352.7	44.0
GLU	1000	F	W	19.206	32.3	0.9
GLU	1000	F	W	19.209	34.8	0.5
GLU	1000	F	W	19.563	37.0	0.5
GLU	1000	F	W	19.570	38.9	0.4
GLU	1000	F	W	19.945	47.8	5.2
GLU	1000	F	W	20.387	33.7	7.6
GLU	1000	F	W	20.389	128.4	2.1
GLU	1000	F	W	21.672	117.2	59.3
GLU	1000	F	W	22.248	471.0	109.9
GLU	1000	F	W	22.253	343.2	185.2
GLU	1000	F	W	22.402	74.2	14.0
GLU	1000	F	W	23.643	38.9	12.9
GLU	1000	F	W	25.244	24.1	3.8
GLU	1000	F	W	25.979	76.7	0.8
GLU	1000	F	W	26.193	25.2	4.2
GLU	1000	F	W	26.490	39.8	3.0
GLU	1000	F	W	26.831	30.4	1.6
GLU	1000	F	W	27.286	87.7	0.9
GLU	1000	F	W	27.830	83.7	0.9
GLU	1000	F	W	29.263	74.2	0.8
GLU	1000	F	W	29.567	84.5	14.6
GLU	1000	F	W	30.114	29.0	7.9
GLU	1000	F	W	30.114	43.0	18.6
GLU	1000	F	W	30.415	41.5	0.6
GLU	1000	F	W	30.815	19.7	7.6
GLU	1000	F	W	31.320	21.7	1.9
GLU	1000	F	W	31.534	93.2	4.4
GLU	1000	F	W	34.226	120.3	30.7
GLU	1000	F	W	38.976	198.7	18.6
GLU	1000	F	W	39.747	91.2	1.3
GLU	1000	F	W	41.480	15.0	3.8
GLU	1000	F	W	42.327	13.6	2.7
GLU	1000	F	W	47.709	12.0	4.4

The tables present over the next few pages represent all valid micro-strain data determined for the samples. As with the crystallite size tables, all duplicate values have been removed and only the ones with the highest confidence have been included

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	10	A	H	8.3907	0.11543	0.01416	ASP	10	B	D	24.2584	0.01208	0.00376
ASP	10	A	H	9.2152	0.02889	0.00929	ASP	10	B	D	24.8204	0.01346	0.00303
ASP	10	A	H	9.9387	0.15169	0.00633	ASP	10	B	D	25.1486	0.01714	0.00496
ASP	10	A	H	10.7901	0.20794	0.00650	ASP	10	B	D	26.3759	0.00997	0.00309
ASP	10	A	H	13.0200	0.13569	0.00858	ASP	10	B	D	26.7319	0.01688	0.00258
ASP	10	A	H	15.6224	1.72275	0.27283	ASP	10	B	D	27.6200	0.00669	0.00356
ASP	10	A	H	16.8237	0.07273	0.02493	ASP	10	B	D	29.0240	0.00747	0.00358
ASP	10	A	H	17.2501	0.35559	0.07926	ASP	10	B	D	30.4222	0.01358	0.00603
ASP	10	A	H	19.0040	0.01135	0.00753	ASP	10	B	D	33.9107	0.01057	0.00433
ASP	10	A	H	19.2096	0.22689	0.02837	ASP	10	B	D	34.3865	0.00815	0.00239
ASP	10	A	H	19.5714	0.15810	0.01388	ASP	10	B	D	34.4682	0.00930	0.00263
ASP	10	A	H	19.9495	0.18923	0.04992	ASP	10	B	D	35.6264	0.00859	0.00330
ASP	10	A	H	21.2315	0.68428	0.06332	ASP	10	B	D	36.9541	0.00900	0.00597
ASP	10	A	H	21.6732	0.18124	0.01318	ASP	10	B	D	38.3312	0.04136	0.02734
ASP	10	A	H	23.5360	0.01239	0.00804	ASP	10	B	W	9.2134	0.01353	0.00852
ASP	10	A	H	24.2025	0.25761	0.04073	ASP	10	B	W	11.7075	0.01402	0.00335
ASP	10	A	H	24.2621	0.02514	0.01335	ASP	10	B	W	14.2574	0.00943	0.00308
ASP	10	A	H	24.8236	0.01944	0.00401	ASP	10	B	W	15.5763	0.00690	0.00265
ASP	10	A	H	26.3786	0.01648	0.01068	ASP	10	B	W	18.4863	0.01096	0.00301
ASP	10	A	H	26.4899	0.17424	0.04869	ASP	10	B	W	19.0055	0.00715	0.00226
ASP	10	A	H	26.8363	0.26209	0.02023	ASP	10	B	W	22.2575	0.00808	0.00478
ASP	10	A	H	27.2901	0.10090	0.01986	ASP	10	B	W	23.6728	0.00711	0.00387
ASP	10	A	H	27.6233	0.02115	0.00599	ASP	10	B	W	24.2647	0.04748	0.00685
ASP	10	A	H	29.3501	0.74916	0.19226	ASP	10	B	W	24.8271	0.00986	0.00342
ASP	10	A	H	31.3226	0.22140	0.08708	ASP	10	B	W	25.1550	0.02499	0.01408
ASP	10	A	H	32.4438	0.25989	0.04179	ASP	10	B	W	26.3805	0.00945	0.00290
ASP	10	A	H	38.3703	0.19896	0.04718	ASP	10	B	W	26.7370	0.05127	0.01981
ASP	10	A	D	15.5740	0.01278	0.00289	ASP	10	B	W	27.6288	0.01042	0.00279
ASP	10	A	D	18.9994	0.02658	0.01734	ASP	10	B	W	30.2440	0.04073	0.02412
ASP	10	A	D	22.2551	0.02841	0.01148	ASP	10	B	W	30.4263	0.01058	0.00465
ASP	10	A	D	23.6688	0.01499	0.00909	ASP	10	B	W	30.6105	0.01468	0.00820
ASP	10	A	D	25.1530	0.02411	0.01561	ASP	10	B	W	33.9173	0.00992	0.00313
ASP	10	A	D	26.7347	0.02773	0.00642	ASP	10	B	W	34.3942	0.00558	0.00228
ASP	10	A	D	30.4228	0.01353	0.00832	ASP	10	B	W	34.4752	0.00815	0.00193
ASP	10	A	D	34.3891	0.01375	0.00403	ASP	10	B	W	34.8044	0.02349	0.00208
ASP	10	A	D	34.4703	0.02303	0.00665	ASP	10	B	W	36.6547	0.01375	0.00525
ASP	10	B	H	8.3908	0.10429	0.01340	ASP	10	B	W	37.9625	0.01031	0.00673
ASP	10	B	H	9.2150	0.03684	0.01222	ASP	10	C	H	8.3857	0.09986	0.01137
ASP	10	B	H	9.9379	0.18003	0.00550	ASP	10	C	H	9.9363	0.14002	0.00725
ASP	10	B	H	10.7895	0.21264	0.00498	ASP	10	C	H	10.7878	0.18216	0.00646
ASP	10	B	H	11.7072	0.01971	0.00389	ASP	10	C	H	12.4953	0.03206	0.00632
ASP	10	B	H	13.0197	0.11419	0.01017	ASP	10	C	H	13.0134	0.12267	0.00930
ASP	10	B	H	16.0626	0.10917	0.00148	ASP	10	C	H	15.5720	0.01013	0.00478
ASP	10	B	H	16.8250	0.07019	0.01898	ASP	10	C	H	16.0623	0.10769	0.02430
ASP	10	B	H	17.0014	0.01920	0.00574	ASP	10	C	H	16.8160	0.09301	0.01679
ASP	10	B	H	17.2523	0.12123	0.00710	ASP	10	C	H	16.9981	0.01220	0.00331
ASP	10	B	H	19.0043	0.01278	0.00563	ASP	10	C	H	17.2487	0.09541	0.00687
ASP	10	B	H	19.2080	0.16479	0.02176	ASP	10	C	H	17.2494	0.09169	0.00907
ASP	10	B	H	19.5720	0.16740	0.00879	ASP	10	C	H	18.6262	0.01105	0.00256
ASP	10	B	H	19.9480	0.20661	0.03637	ASP	10	C	H	18.9983	0.02098	0.00320
ASP	10	B	H	20.8635	0.43582	0.24705	ASP	10	C	H	19.2051	0.13900	0.02843
ASP	10	B	H	21.2211	0.72620	0.12445	ASP	10	C	H	19.5688	0.14389	0.00945
ASP	10	B	H	21.6719	0.21433	0.01897	ASP	10	C	H	19.9455	0.13519	0.04587
ASP	10	B	H	22.2560	0.01930	0.00472	ASP	10	C	H	21.6661	0.12212	0.02422
ASP	10	B	H	23.1459	0.43153	0.02386	ASP	10	C	H	21.9518	0.01351	0.00449
ASP	10	B	H	23.6472	0.28746	0.06130	ASP	10	C	H	22.2522	0.01178	0.00313
ASP	10	B	H	24.2022	0.37006	0.01465	ASP	10	C	H	23.6647	0.01555	0.00986
ASP	10	B	H	24.8246	0.01156	0.00752	ASP	10	C	H	24.2584	0.01396	0.00847
ASP	10	B	H	25.2940	0.43615	0.06047	ASP	10	C	H	24.8201	0.00817	0.00354
ASP	10	B	H	26.3792	0.01470	0.00605	ASP	10	C	H	25.1464	0.01761	0.00420
ASP	10	B	H	26.4893	0.19075	0.02108	ASP	10	C	H	26.3743	0.01904	0.00592
ASP	10	B	H	26.8306	0.15445	0.06350	ASP	10	C	H	26.7303	0.01714	0.00480
ASP	10	B	H	27.2917	0.11190	0.02329	ASP	10	C	H	26.8267	0.14533	0.08959
ASP	10	B	H	27.8309	0.15130	0.02426	ASP	10	C	H	27.6192	0.01703	0.00373
ASP	10	B	H	32.4402	0.24421	0.05683	ASP	10	C	H	29.4226	0.08083	0.04899
ASP	10	B	H	33.9128	0.01020	0.00591	ASP	10	C	H	33.9058	0.02007	0.00813
ASP	10	B	H	34.9167	0.20214	0.06211	ASP	10	C	H	34.0138	0.11658	0.03122
ASP	10	B	D	12.4975	0.01262	0.00561	ASP	10	C	H	34.4666	0.01269	0.00263
ASP	10	B	D	14.2558	0.01010	0.00382	ASP	10	C	H	34.7921	0.02393	0.00760
ASP	10	B	D	15.5726	0.01138	0.00282	ASP	10	C	H	34.7921	0.02393	0.00760
ASP	10	B	D	16.9993	0.00700	0.00338	ASP	10	C	H	35.2203	0.01125	0.00629
ASP	10	B	D	18.4827	0.00673	0.00435	ASP	10	C	H	35.6211	0.01246	0.00415
ASP	10	B	D	18.6283	0.01030	0.00242	ASP	10	C	H	36.4510	0.01990	0.00679
ASP	10	B	D	19.0022	0.00934	0.00283	ASP	10	C	H	36.6416	0.01271	0.00691
ASP	10	B	D	21.9529	0.00711	0.00359	ASP	10	C	D	9.2141	0.01075	0.00439
ASP	10	B	D	22.2536	0.00822	0.00280	ASP	10	C	D	11.7063	0.01470	0.00199
ASP	10	B	D	23.4179	0.00788	0.00289	ASP	10	C	D	12.4987	0.04284	0.01590
ASP	10	B	D	23.5337	0.01548	0.00286	ASP	10	C	D	12.6035	0.04517	0.00864
ASP	10	B	D	23.6670	0.01050	0.00309	ASP	10	C	D	14.2560	0.07519	0.01925

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	10	C	D	15.5732	0.01214	0.00268	ASP	10	D	D	23.6680	0.01339	0.00438
ASP	10	C	D	16.9996	0.01235	0.00228	ASP	10	D	D	24.2605	0.06547	0.00681
ASP	10	C	D	18.4837	0.06602	0.04079	ASP	10	D	D	24.8220	0.05753	0.00569
ASP	10	C	D	18.6283	0.05163	0.01966	ASP	10	D	D	25.1500	0.06214	0.00576
ASP	10	C	D	19.0031	0.00650	0.00282	ASP	10	D	D	26.3766	0.01018	0.00342
ASP	10	C	D	21.9539	0.00617	0.00297	ASP	10	D	D	27.6215	0.00629	0.00381
ASP	10	C	D	22.2516	0.00713	0.00260	ASP	10	D	D	28.7373	0.00811	0.00351
ASP	10	C	D	22.4951	0.03769	0.01338	ASP	10	D	D	31.1267	0.01091	0.00715
ASP	10	C	D	23.4194	0.01027	0.00217	ASP	10	D	D	34.3865	0.00741	0.00245
ASP	10	C	D	23.5347	0.01145	0.00284	ASP	10	D	D	37.3975	0.01297	0.00521
ASP	10	C	D	23.6671	0.06203	0.00758	ASP	10	D	W	9.2140	0.01441	0.00495
ASP	10	C	D	24.2605	0.04644	0.00882	ASP	10	D	W	11.7077	0.01598	0.00255
ASP	10	C	D	24.8213	0.01335	0.00220	ASP	10	D	W	12.4988	0.05039	0.01635
ASP	10	C	D	25.1483	0.02046	0.00280	ASP	10	D	W	14.2570	0.01417	0.00256
ASP	10	C	D	26.7318	0.05669	0.02739	ASP	10	D	W	15.5766	0.01251	0.00245
ASP	10	C	D	27.6220	0.05617	0.00786	ASP	10	D	W	17.0021	0.00958	0.00246
ASP	10	C	D	30.2379	0.00839	0.00447	ASP	10	D	W	18.4864	0.01408	0.00424
ASP	10	C	D	30.4205	0.00481	0.00264	ASP	10	D	W	18.6326	0.02465	0.00554
ASP	10	C	D	30.6014	0.01606	0.00581	ASP	10	D	W	19.0061	0.01448	0.00158
ASP	10	C	D	31.4437	0.00704	0.00331	ASP	10	D	W	21.9603	0.03402	0.00904
ASP	10	C	D	31.9505	0.01191	0.00564	ASP	10	D	W	22.2573	0.00893	0.00228
ASP	10	C	D	34.7949	0.01279	0.00329	ASP	10	D	W	23.6728	0.01117	0.00337
ASP	10	C	D	36.6425	0.00774	0.00433	ASP	10	D	W	24.2647	0.03790	0.00982
ASP	10	C	D	36.9520	0.00694	0.00328	ASP	10	D	W	24.8269	0.00933	0.00223
ASP	10	C	D	37.4699	0.00967	0.00310	ASP	10	D	W	25.1523	0.06057	0.00746
ASP	10	C	D	38.3281	0.00610	0.00252	ASP	10	D	W	26.3809	0.00975	0.00321
ASP	10	C	D	38.5493	0.01013	0.00313	ASP	10	D	W	26.7389	0.00691	0.00328
ASP	10	C	W	9.2127	0.01184	0.00537	ASP	10	D	W	27.6280	0.00964	0.00421
ASP	10	C	W	12.4990	0.02778	0.00435	ASP	10	D	W	28.7307	0.01388	0.00622
ASP	10	C	W	15.5765	0.02429	0.00994	ASP	10	D	W	30.4115	0.01324	0.00195
ASP	10	C	W	16.9952	0.00688	0.00322	ASP	10	D	W	30.5886	0.02282	0.00705
ASP	10	C	W	18.4863	0.01176	0.00272	ASP	10	D	W	31.1198	0.01391	0.00183
ASP	10	C	W	18.6258	0.00788	0.00383	ASP	10	D	W	31.4376	0.00737	0.00280
ASP	10	C	W	19.0056	0.05585	0.03627	ASP	10	D	W	33.8976	0.01960	0.00924
ASP	10	C	W	21.9576	0.00599	0.00273	ASP	10	D	W	34.4595	0.01542	0.00441
ASP	10	C	W	22.2591	0.05488	0.00730	ASP	10	D	W	34.8028	0.01089	0.00343
ASP	10	C	W	23.4231	0.01011	0.00267	ASP	10	D	W	36.6361	0.01440	0.00288
ASP	10	C	W	23.6725	0.04986	0.01557	ASP	10	D	W	36.9408	0.01806	0.00335
ASP	10	C	W	24.8267	0.04538	0.00672	ASP	10	D	W	37.4623	0.01211	0.00244
ASP	10	C	W	25.1464	0.01126	0.00221	ASP	10	D	W	37.9437	0.01740	0.00701
ASP	10	C	W	27.6293	0.04325	0.00851	ASP	10	D	W	38.3225	0.00854	0.00428
ASP	10	C	W	31.4430	0.00772	0.00363	ASP	10	D	W	38.5383	0.01080	0.00498
ASP	10	C	W	34.8034	0.01651	0.00199	ASP	10	E	H	8.3906	0.09924	0.01507
ASP	10	C	W	37.4797	0.00651	0.00249	ASP	10	E	H	9.2147	0.02098	0.00852
ASP	10	D	H	8.3906	0.07584	0.02879	ASP	10	E	H	9.9373	0.14491	0.00626
ASP	10	D	H	9.9374	0.11648	0.00984	ASP	10	E	H	10.7887	0.18792	0.00559
ASP	10	D	H	10.7890	0.17080	0.00812	ASP	10	E	H	11.7062	0.04099	0.01638
ASP	10	D	H	11.7060	0.01345	0.00215	ASP	10	E	H	13.0173	0.14802	0.01523
ASP	10	D	H	13.0189	0.05766	0.02576	ASP	10	E	H	14.2571	0.01318	0.00575
ASP	10	D	H	14.2572	0.00871	0.00546	ASP	10	E	H	16.8247	0.05926	0.02072
ASP	10	D	H	16.8234	0.07421	0.03299	ASP	10	E	H	17.0007	0.01732	0.00310
ASP	10	D	H	17.2516	0.08177	0.01143	ASP	10	E	H	17.2511	0.10761	0.00740
ASP	10	D	H	18.6278	0.01929	0.00186	ASP	10	E	H	18.6280	0.01464	0.00291
ASP	10	D	H	19.0029	0.00858	0.00348	ASP	10	E	H	19.0029	0.01780	0.00227
ASP	10	D	H	19.2072	0.16851	0.03187	ASP	10	E	H	19.2054	0.18705	0.02446
ASP	10	D	H	19.5707	0.12480	0.01493	ASP	10	E	H	19.5693	0.22171	0.02866
ASP	10	D	H	21.9544	0.01113	0.00474	ASP	10	E	H	19.9457	0.18388	0.01301
ASP	10	D	H	22.2548	0.00656	0.00425	ASP	10	E	H	20.3843	0.20571	0.09552
ASP	10	D	H	24.8232	0.00839	0.00402	ASP	10	E	H	21.9540	0.01951	0.00512
ASP	10	D	H	25.1474	0.01825	0.00429	ASP	10	E	H	22.2546	0.01406	0.00308
ASP	10	D	H	27.6218	0.01283	0.00456	ASP	10	E	H	22.4943	0.01703	0.01008
ASP	10	D	H	31.3197	0.27101	0.03389	ASP	10	E	H	24.2604	0.02090	0.00797
ASP	10	D	H	31.9508	0.01416	0.00906	ASP	10	E	H	24.8219	0.01420	0.00245
ASP	10	D	H	34.3873	0.00754	0.00390	ASP	10	E	H	26.3764	0.01899	0.00704
ASP	10	D	H	35.9125	0.39032	0.13708	ASP	10	E	H	26.4848	0.11811	0.06672
ASP	10	D	H	37.4711	0.01470	0.00683	ASP	10	E	H	26.7323	0.01479	0.00575
ASP	10	D	D	9.2142	0.02289	0.00365	ASP	10	E	H	27.6217	0.01864	0.00352
ASP	10	D	D	11.7068	0.01992	0.00290	ASP	10	E	H	29.0245	0.01055	0.00672
ASP	10	D	D	14.2570	0.02922	0.00784	ASP	10	E	H	30.2398	0.01353	0.00499
ASP	10	D	D	15.5736	0.01715	0.00203	ASP	10	E	H	31.1269	0.01682	0.00373
ASP	10	D	D	17.0001	0.01130	0.00276	ASP	10	E	H	31.9507	0.01735	0.00996
ASP	10	D	D	18.4838	0.01341	0.00383	ASP	10	E	H	34.3860	0.01121	0.00437
ASP	10	D	D	18.6294	0.05565	0.00744	ASP	10	E	H	34.7931	0.02129	0.00653
ASP	10	D	D	19.0033	0.01398	0.00217	ASP	10	E	H	35.2241	0.01967	0.00693
ASP	10	D	D	21.9551	0.04753	0.01255	ASP	10	E	H	36.4535	0.01477	0.00882
ASP	10	D	D	22.2545	0.06863	0.00718	ASP	10	E	H	36.6436	0.01455	0.00857
ASP	10	D	D	22.4955	0.01288	0.00372	ASP	10	E	H	36.9525	0.01364	0.00828
ASP	10	D	D	23.4198	0.00862	0.00342	ASP	10	E	D	11.7062	0.01286	0.00333
ASP	10	D	D	23.5345	0.05136	0.01229	ASP	10	E	D	12.4980	0.02876	0.01350

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	10	E	D	14.2566	0.00872	0.00428	ASP	10	F	W	11.7078	0.01939	0.00217
ASP	10	E	D	18.4832	0.04984	0.01107	ASP	10	F	W	12.4991	0.01887	0.00396
ASP	10	E	D	18.6288	0.01339	0.00563	ASP	10	F	W	12.6055	0.03451	0.00818
ASP	10	E	D	19.0029	0.03769	0.00638	ASP	10	F	W	15.5758	0.01381	0.00272
ASP	10	E	D	21.9533	0.00750	0.00320	ASP	10	F	W	17.0025	0.01095	0.00236
ASP	10	E	D	22.2544	0.03494	0.00965	ASP	10	F	W	18.4857	0.01251	0.00356
ASP	10	E	D	23.5340	0.00727	0.00428	ASP	10	F	W	18.6335	0.01492	0.00191
ASP	10	E	D	23.6671	0.00989	0.00350	ASP	10	F	W	19.0050	0.04333	0.00799
ASP	10	E	D	24.8213	0.01092	0.00279	ASP	10	F	W	21.9576	0.00599	0.00288
ASP	10	E	D	26.7327	0.01189	0.00254	ASP	10	F	W	22.2574	0.00990	0.00200
ASP	10	E	D	27.8810	0.00892	0.00358	ASP	10	F	W	23.6729	0.01083	0.00276
ASP	10	E	D	28.7370	0.01058	0.00298	ASP	10	F	W	24.2638	0.03724	0.01123
ASP	10	E	D	29.0247	0.00666	0.00331	ASP	10	F	W	24.8272	0.05081	0.01013
ASP	10	E	D	31.1259	0.00443	0.00292	ASP	10	F	W	26.3809	0.03567	0.00752
ASP	10	E	D	31.9510	0.01196	0.00563	ASP	10	F	W	27.6275	0.04614	0.01098
ASP	10	E	D	34.7947	0.00813	0.00401	ASP	10	F	W	27.8863	0.01323	0.00333
ASP	10	E	D	35.6250	0.00566	0.00321	ASP	10	F	W	31.1343	0.02438	0.00933
ASP	10	E	W	9.2132	0.01699	0.00595	ASP	10	F	W	31.4503	0.00816	0.00292
ASP	10	E	W	11.7074	0.01719	0.00240	ASP	10	F	W	31.9594	0.01466	0.00359
ASP	10	E	W	12.6046	0.02326	0.01298	ASP	10	F	W	33.9177	0.01290	0.00817
ASP	10	E	W	14.2569	0.03364	0.01378	ASP	10	F	W	34.4750	0.00776	0.00165
ASP	10	E	W	15.5760	0.01013	0.00252	ASP	10	F	W	34.8032	0.02044	0.00288
ASP	10	E	W	18.6317	0.06324	0.01119	ASP	10	F	W	35.6346	0.00529	0.00289
ASP	10	E	W	22.2577	0.01030	0.00194	ASP	10	F	W	36.6537	0.00819	0.00207
ASP	10	E	W	23.4227	0.00670	0.00277	ASP	10	F	W	36.8081	0.00826	0.00403
ASP	10	E	W	23.5391	0.00799	0.00338	ASP	100	A	H	8.3901	0.10956	0.01860
ASP	10	E	W	23.6729	0.00790	0.00316	ASP	100	A	H	9.2151	0.03495	0.01705
ASP	10	E	W	24.8273	0.01754	0.00487	ASP	100	A	H	9.9393	0.15977	0.00756
ASP	10	E	W	25.1528	0.01035	0.00577	ASP	100	A	H	10.7905	0.21357	0.00611
ASP	10	E	W	26.7379	0.00691	0.00447	ASP	100	A	H	11.7066	0.01695	0.00685
ASP	10	E	W	27.6289	0.04153	0.00497	ASP	100	A	H	13.0191	0.07797	0.01674
ASP	10	E	W	27.8878	0.01786	0.00472	ASP	100	A	H	15.6442	1.73226	0.27079
ASP	10	E	W	30.2456	0.01964	0.01089	ASP	100	A	H	16.0607	0.03551	0.00834
ASP	10	E	W	30.4266	0.00493	0.00307	ASP	100	A	H	16.9989	0.01975	0.00524
ASP	10	E	W	30.6099	0.01131	0.00633	ASP	100	A	H	17.2531	0.11035	0.00917
ASP	10	E	W	31.4527	0.03129	0.00534	ASP	100	A	H	19.0015	0.02282	0.00861
ASP	10	E	W	36.9610	0.01803	0.00894	ASP	100	A	H	19.5688	0.23443	0.13084
ASP	10	E	W	38.3388	0.01814	0.00584	ASP	100	A	H	19.9489	0.12603	0.06148
ASP	10	F	H	8.3896	0.08986	0.01660	ASP	100	A	H	21.9528	0.04328	0.01183
ASP	10	F	H	9.9366	0.36290	0.12152	ASP	100	A	H	24.8217	0.02790	0.01058
ASP	10	F	H	10.7884	0.18267	0.05795	ASP	100	A	H	27.6205	0.03658	0.01003
ASP	10	F	H	13.0185	0.11820	0.01053	ASP	100	A	H	36.3786	0.03136	0.01163
ASP	10	F	H	16.8225	0.07469	0.01927	ASP	100	A	H	37.4668	0.02971	0.00243
ASP	10	F	H	16.9999	0.01334	0.00375	ASP	100	A	D	8.3895	0.06502	0.00922
ASP	10	F	H	17.2505	0.19261	0.06165	ASP	100	A	D	9.2143	0.02246	0.00785
ASP	10	F	H	18.6275	0.01155	0.00348	ASP	100	A	D	9.9382	0.14015	0.01076
ASP	10	F	H	19.0025	0.01515	0.00255	ASP	100	A	D	10.7908	0.37530	0.02964
ASP	10	F	H	19.2069	0.15764	0.02335	ASP	100	A	D	11.7063	0.02180	0.00342
ASP	10	F	H	19.5707	0.33439	0.01844	ASP	100	A	D	13.0186	0.14963	0.00962
ASP	10	F	H	21.9540	0.01527	0.00551	ASP	100	A	D	14.2552	0.01213	0.00464
ASP	10	F	H	24.8225	0.01285	0.00313	ASP	100	A	D	15.5939	1.69094	0.19569
ASP	10	F	H	25.2916	0.43713	0.06644	ASP	100	A	D	16.4606	0.88403	0.05712
ASP	10	F	H	26.4936	0.15570	0.09755	ASP	100	A	D	16.8210	0.08203	0.02360
ASP	10	F	H	26.8303	0.26587	0.03505	ASP	100	A	D	16.9998	0.02287	0.00360
ASP	10	F	H	27.2883	0.16358	0.02351	ASP	100	A	D	17.2522	0.31318	0.09976
ASP	10	F	H	27.6214	0.01640	0.00448	ASP	100	A	D	18.6276	0.03339	0.00319
ASP	10	F	H	30.1155	0.18871	0.01576	ASP	100	A	D	19.0013	0.01064	0.00625
ASP	10	F	H	31.9504	0.02171	0.01017	ASP	100	A	D	19.2070	0.22487	0.03004
ASP	10	F	H	32.3703	0.19514	0.11870	ASP	100	A	D	19.5679	0.17535	0.01021
ASP	10	F	H	33.9079	0.01401	0.00857	ASP	100	A	D	19.9482	0.20411	0.03697
ASP	10	F	H	34.3863	0.00864	0.00434	ASP	100	A	D	21.9530	0.02259	0.00543
ASP	10	F	H	34.4668	0.01325	0.00303	ASP	100	A	D	22.2535	0.01063	0.00578
ASP	10	F	H	35.2233	0.02173	0.00755	ASP	100	A	D	22.4934	0.03174	0.01346
ASP	10	F	D	11.7062	0.00833	0.00507	ASP	100	A	D	26.1810	1.27446	0.33194
ASP	10	F	D	12.6033	0.05585	0.02457	ASP	100	A	D	26.3751	0.02339	0.00674
ASP	10	F	D	15.5733	0.02280	0.00705	ASP	100	A	D	26.4877	0.15121	0.07371
ASP	10	F	D	18.6283	0.03538	0.01875	ASP	100	A	D	27.8786	0.01072	0.00606
ASP	10	F	D	19.0028	0.01057	0.00243	ASP	100	A	D	29.0223	0.02662	0.00894
ASP	10	F	D	22.2537	0.00705	0.00404	ASP	100	A	D	30.1052	0.23765	0.02084
ASP	10	F	D	22.4943	0.01279	0.00544	ASP	100	A	D	30.2377	0.01824	0.01057
ASP	10	F	D	23.4186	0.01072	0.00219	ASP	100	A	D	30.4195	0.01738	0.00886
ASP	10	F	D	24.8213	0.04834	0.01238	ASP	100	A	D	31.1263	0.01476	0.00398
ASP	10	F	D	26.3759	0.03563	0.01020	ASP	100	A	D	31.1263	0.01476	0.00398
ASP	10	F	D	27.8803	0.00977	0.00491	ASP	100	A	D	33.9033	0.03275	0.00710
ASP	10	F	D	30.4199	0.04061	0.01295	ASP	100	A	D	34.4657	0.01767	0.00368
ASP	10	F	D	30.6020	0.01658	0.00824	ASP	100	A	D	34.7920	0.03465	0.01921
ASP	10	F	D	31.1276	0.02176	0.01219	ASP	100	A	D	35.6215	0.01292	0.00825
ASP	10	F	D	38.3287	0.00833	0.00311	ASP	100	A	D	36.6409	0.01495	0.00969
ASP	10	F	D	38.5501	0.01117	0.00367	ASP	100	A	D	36.9491	0.03555	0.00823

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	100	A	W	11.7032	0.01374	0.00417	ASP	100	B	W	24.8158	0.01409	0.00199
ASP	100	A	W	14.2547	0.02391	0.00866	ASP	100	B	W	26.3679	0.02686	0.00311
ASP	100	A	W	16.9974	0.02510	0.00671	ASP	100	B	W	26.8246	0.19626	0.09656
ASP	100	A	W	18.4798	0.01089	0.00394	ASP	100	B	W	27.6134	0.02077	0.00535
ASP	100	A	W	18.6221	0.00864	0.00462	ASP	100	B	W	28.7300	0.01076	0.00560
ASP	100	A	W	21.9510	0.01271	0.00320	ASP	100	B	W	29.0143	0.01756	0.00902
ASP	100	A	W	22.2508	0.01289	0.00717	ASP	100	B	W	31.4355	0.01852	0.00311
ASP	100	A	W	22.4869	0.01639	0.00481	ASP	100	B	W	31.9385	0.02303	0.01079
ASP	100	A	W	23.5275	0.01132	0.00485	ASP	100	B	W	33.8934	0.01875	0.01138
ASP	100	A	W	23.6612	0.01541	0.00319	ASP	100	B	W	34.3755	0.01117	0.00262
ASP	100	A	W	24.2552	0.01174	0.00306	ASP	100	B	W	34.7766	0.01990	0.00508
ASP	100	A	W	24.8188	0.02143	0.00447	ASP	100	B	W	35.6122	0.01501	0.00543
ASP	100	A	W	25.1436	0.02299	0.00275	ASP	100	B	W	36.6325	0.00998	0.00292
ASP	100	A	W	26.7261	0.02051	0.00371	ASP	100	B	W	38.3212	0.01247	0.00797
ASP	100	A	W	27.6143	0.01607	0.00306	ASP	100	B	W	38.5394	0.02160	0.00979
ASP	100	A	W	27.8760	0.01457	0.00231	ASP	100	C	H	8.3894	0.10300	0.01981
ASP	100	A	W	29.0156	0.01156	0.00347	ASP	100	C	H	9.9382	0.13243	0.00794
ASP	100	A	W	30.5918	0.02165	0.00730	ASP	100	C	H	10.7892	0.19695	0.00576
ASP	100	A	W	31.1238	0.01037	0.00476	ASP	100	C	H	11.7048	0.02761	0.00530
ASP	100	A	W	31.4401	0.01086	0.00234	ASP	100	C	H	13.0182	0.14322	0.01068
ASP	100	A	W	31.9434	0.01346	0.00408	ASP	100	C	H	15.6175	1.79684	0.25267
ASP	100	A	W	33.8985	0.01827	0.00422	ASP	100	C	H	16.4507	1.00973	0.05412
ASP	100	A	W	34.3827	0.00865	0.00240	ASP	100	C	H	16.8193	0.08223	0.00090
ASP	100	A	W	34.4588	0.01010	0.00225	ASP	100	C	H	16.9991	0.02642	0.00762
ASP	100	A	W	34.7821	0.01761	0.00331	ASP	100	C	H	17.2517	0.12500	0.00744
ASP	100	A	W	36.6388	0.00777	0.00298	ASP	100	C	H	18.6257	0.02782	0.00500
ASP	100	A	W	37.3907	0.00648	0.00267	ASP	100	C	H	19.0004	0.01809	0.00765
ASP	100	A	W	37.4643	0.00909	0.00383	ASP	100	C	H	19.2081	0.38681	0.10974
ASP	100	A	W	37.9465	0.01221	0.00417	ASP	100	C	H	19.5675	0.18991	0.00861
ASP	100	A	W	38.3251	0.00715	0.00235	ASP	100	C	H	19.9479	0.23216	0.01211
ASP	100	A	W	38.5422	0.01349	0.00340	ASP	100	C	H	21.2148	0.82337	0.13491
ASP	100	B	H	8.3891	0.11994	0.01735	ASP	100	C	H	22.2526	0.02465	0.00907
ASP	100	B	H	9.2145	0.04847	0.01511	ASP	100	C	H	23.5314	0.02378	0.01307
ASP	100	B	H	9.9385	0.29272	0.07125	ASP	100	C	H	24.2549	0.04761	0.01716
ASP	100	B	H	10.7898	0.24581	0.01209	ASP	100	C	H	24.8201	0.02112	0.00862
ASP	100	B	H	13.0187	0.16438	0.00854	ASP	100	C	H	25.1455	0.03833	0.00737
ASP	100	B	H	15.3627	0.81646	0.06742	ASP	100	C	H	26.7274	0.03568	0.01928
ASP	100	B	H	16.4598	0.90533	0.33281	ASP	100	C	H	27.6188	0.02733	0.01106
ASP	100	B	H	16.8200	0.06331	0.03228	ASP	100	C	H	31.1228	0.02963	0.00920
ASP	100	B	H	17.2527	0.32085	0.08606	ASP	100	C	H	36.9480	0.02928	0.01248
ASP	100	B	H	19.0014	0.01920	0.00641	ASP	100	C	H	38.3276	0.02743	0.00628
ASP	100	B	H	19.9496	0.23928	0.02642	ASP	100	C	D	8.3897	0.11147	0.02079
ASP	100	B	H	21.2136	0.64579	0.13575	ASP	100	C	D	9.2118	0.02878	0.00806
ASP	100	B	H	27.6186	0.03248	0.00638	ASP	100	C	D	9.9377	0.13378	0.00890
ASP	100	B	H	32.4382	0.32022	0.04633	ASP	100	C	D	10.7892	0.19975	0.00727
ASP	100	B	H	33.9012	0.04915	0.02349	ASP	100	C	D	11.7032	0.02003	0.00441
ASP	100	B	H	36.9457	0.02781	0.00973	ASP	100	C	D	11.9373	2.11217	0.30113
ASP	100	B	H	37.3800	0.28088	0.10655	ASP	100	C	D	12.4944	0.01897	0.00617
ASP	100	B	D	8.3899	0.08741	0.01645	ASP	100	C	D	12.6039	0.04548	0.01085
ASP	100	B	D	9.9377	0.15277	0.00622	ASP	100	C	D	13.0181	0.14710	0.01240
ASP	100	B	D	10.7891	0.21903	0.00506	ASP	100	C	D	14.2532	0.02029	0.00342
ASP	100	B	D	13.0184	0.15422	0.00897	ASP	100	C	D	15.5723	0.03477	0.00308
ASP	100	B	D	16.8214	0.08187	0.01875	ASP	100	C	D	16.9958	0.01673	0.01081
ASP	100	B	D	17.2528	0.26386	0.07448	ASP	100	C	D	18.4788	0.01323	0.00488
ASP	100	B	D	18.6263	0.03019	0.01263	ASP	100	C	D	18.6218	0.02143	0.00283
ASP	100	B	D	19.0009	0.00950	0.00612	ASP	100	C	D	18.9974	0.01585	0.00207
ASP	100	B	D	19.2067	0.20878	0.01906	ASP	100	C	D	19.5694	0.25158	0.11618
ASP	100	B	D	19.5680	0.20347	0.05820	ASP	100	C	D	19.9477	0.20454	0.03792
ASP	100	B	D	19.9464	0.18876	0.03617	ASP	100	C	D	21.9493	0.01467	0.00386
ASP	100	B	D	20.3874	0.19379	0.12065	ASP	100	C	D	22.2476	0.01242	0.00310
ASP	100	B	D	25.1454	0.03317	0.00532	ASP	100	C	D	26.3736	0.02245	0.00980
ASP	100	B	D	26.3721	0.02018	0.00861	ASP	100	C	D	29.0204	0.02387	0.01231
ASP	100	B	D	29.3890	1.04260	0.13752	ASP	100	C	D	31.1246	0.01220	0.00423
ASP	100	B	D	30.4175	0.02394	0.01240	ASP	100	C	W	22.4862	0.01497	0.00760
ASP	100	B	D	30.8157	0.37552	0.02245	ASP	100	C	W	23.4131	0.00975	0.00265
ASP	100	B	D	35.6190	0.02536	0.01192	ASP	100	C	W	23.5269	0.01160	0.00446
ASP	100	B	W	8.3877	0.08801	0.02272	ASP	100	C	W	23.6593	0.02232	0.00670
ASP	100	B	W	9.2107	0.04650	0.00512	ASP	100	C	W	24.8159	0.01350	0.00268
ASP	100	B	W	9.9333	0.11899	0.00862	ASP	100	C	W	26.3683	0.01708	0.00333
ASP	100	B	W	10.7945	0.18395	0.01416	ASP	100	C	W	26.7219	0.03096	0.00749
ASP	100	B	W	11.7006	0.02911	0.00157	ASP	100	C	W	27.8727	0.01020	0.00523
ASP	100	B	W	15.5690	0.02028	0.00377	ASP	100	C	W	28.7295	0.01342	0.00509
ASP	100	B	W	16.9944	0.01488	0.00260	ASP	100	C	W	28.7301	0.01482	0.00666
ASP	100	B	W	18.6208	0.02687	0.00405	ASP	100	C	W	29.0149	0.01686	0.00373
ASP	100	B	W	18.9953	0.01962	0.00195	ASP	100	C	W	30.2338	0.01872	0.00880
ASP	100	B	W	19.9388	0.14330	0.04878	ASP	100	C	W	30.4131	0.01162	0.00387
ASP	100	B	W	21.9475	0.01261	0.00331	ASP	100	C	W	30.6500	12.73785	0.00000
ASP	100	B	W	22.2487	0.01299	0.00214	ASP	100	C	W	31.4361	0.01110	0.00410
ASP	100	B	W	23.4121	0.01843	0.00207	ASP	100	C	W	34.4575	0.01072	0.00347

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	100	C	W	34.7784	0.01599	0.00406	ASP	100	D	D	37.7677	0.02605	0.01451
ASP	100	C	W	35.6129	0.01051	0.00352	ASP	100	D	D	37.9509	0.02365	0.00945
ASP	100	C	W	36.4474	0.01986	0.00251	ASP	100	D	W	9.2119	0.01259	0.00592
ASP	100	C	W	36.7882	0.02837	0.01516	ASP	100	D	W	11.7032	0.01037	0.00459
ASP	100	C	W	37.7625	0.02014	0.01129	ASP	100	D	W	14.2508	0.00778	0.00333
ASP	100	C	W	37.9425	0.01054	0.00584	ASP	100	D	W	15.5697	0.01365	0.00212
ASP	100	C	W	38.3204	0.01472	0.00315	ASP	100	D	W	16.9930	0.01147	0.00181
ASP	100	C	W	38.5377	0.00932	0.00586	ASP	100	D	W	18.6216	0.01494	0.00277
ASP	100	D	H	8.3828	0.09172	0.02593	ASP	100	D	W	18.9937	0.01065	0.00175
ASP	100	D	H	9.2079	0.03559	0.01515	ASP	100	D	W	22.2493	0.01646	0.00188
ASP	100	D	H	9.9320	0.07385	0.03404	ASP	100	D	W	23.4138	0.01186	0.00212
ASP	100	D	H	10.7828	0.14944	0.06587	ASP	100	D	W	23.5268	0.01618	0.00217
ASP	100	D	H	11.6992	0.02044	0.00246	ASP	100	D	W	23.6588	0.03693	0.01823
ASP	100	D	H	13.0119	0.14309	0.01939	ASP	100	D	W	24.2535	0.01434	0.00203
ASP	100	D	H	16.0549	0.14681	0.07483	ASP	100	D	W	24.8175	0.01758	0.00238
ASP	100	D	H	16.8105	0.08183	0.01652	ASP	100	D	W	26.3697	0.01309	0.00230
ASP	100	D	H	17.2482	0.10035	0.05383	ASP	100	D	W	26.7234	0.01275	0.00357
ASP	100	D	H	18.6217	0.03013	0.00313	ASP	100	D	W	27.6126	0.01338	0.00335
ASP	100	D	H	18.9949	0.02324	0.00231	ASP	100	D	W	27.8738	0.00809	0.00466
ASP	100	D	H	19.2044	0.19379	0.01424	ASP	100	D	W	28.7324	0.01544	0.00321
ASP	100	D	H	19.9425	0.12029	0.03060	ASP	100	D	W	29.0139	0.01169	0.00316
ASP	100	D	H	21.9469	0.02640	0.00600	ASP	100	D	W	30.4129	0.01000	0.00384
ASP	100	D	H	22.2492	0.01521	0.00339	ASP	100	D	W	33.8940	0.01187	0.00772
ASP	100	D	H	24.8143	0.01320	0.00445	ASP	100	D	W	34.3801	0.00580	0.00271
ASP	100	D	H	25.1416	0.04214	0.00727	ASP	100	D	W	34.4605	0.00970	0.00226
ASP	100	D	H	26.4830	0.18035	0.01454	ASP	100	D	W	34.7803	0.01683	0.00656
ASP	100	D	H	27.6154	0.02705	0.00633	ASP	1000	A	H	8.3813	0.19070	0.01494
ASP	100	D	H	29.0153	0.03013	0.01228	ASP	1000	A	H	9.9372	0.25487	0.01008
ASP	100	D	H	30.4125	0.01701	0.00848	ASP	1000	A	H	10.7881	0.22354	0.00789
ASP	100	D	H	31.1199	0.01964	0.00432	ASP	1000	A	H	11.6967	0.02575	0.00726
ASP	100	D	H	34.4608	0.01733	0.00462	ASP	1000	A	H	15.3418	0.78776	0.05150
ASP	100	D	H	34.7809	0.03854	0.01886	ASP	1000	A	H	15.5626	2.10431	0.09242
ASP	100	D	D	8.3840	0.09932	0.01248	ASP	1000	A	H	16.0595	0.19921	0.03465
ASP	100	D	D	9.2093	0.02219	0.00614	ASP	1000	A	H	16.8040	0.08173	0.02786
ASP	100	D	D	9.9369	0.11561	0.00953	ASP	1000	A	H	18.9909	0.02167	0.00474
ASP	100	D	D	10.7882	0.17278	0.00792	ASP	1000	A	H	19.2074	0.20966	0.01864
ASP	100	D	D	11.7050	0.01854	0.00225	ASP	1000	A	H	19.5584	0.14680	0.00971
ASP	100	D	D	13.0111	0.12851	0.00814	ASP	1000	A	H	19.9503	0.30004	0.01561
ASP	100	D	D	14.2513	0.01180	0.00357	ASP	1000	A	H	23.1449	0.28202	0.08819
ASP	100	D	D	15.5721	0.01035	0.00644	ASP	1000	A	H	26.4991	0.24438	0.02181
ASP	100	D	D	16.8120	0.08154	0.01940	ASP	1000	A	H	31.5331	0.15223	0.06453
ASP	100	D	D	16.9931	0.01648	0.00217	ASP	1000	A	H	32.4343	0.20881	0.03327
ASP	100	D	D	17.2470	0.09876	0.00649	ASP	1000	A	D	9.2081	0.05291	0.03191
ASP	100	D	D	18.6219	0.02068	0.00203	ASP	1000	A	D	9.9359	0.14552	0.00997
ASP	100	D	D	18.9950	0.01559	0.00220	ASP	1000	A	D	10.7876	0.18030	0.00732
ASP	100	D	D	19.2026	0.20406	0.01590	ASP	1000	A	D	11.6925	0.03346	0.00893
ASP	100	D	D	19.5631	0.15622	0.00768	ASP	1000	A	D	16.8140	0.05275	0.02897
ASP	100	D	D	19.9461	0.20581	0.01818	ASP	1000	A	D	16.9941	0.02427	0.01000
ASP	100	D	D	21.6654	0.17101	0.01384	ASP	1000	A	D	19.2049	0.13795	0.02414
ASP	100	D	D	21.9531	0.01864	0.00429	ASP	1000	A	D	19.9475	0.19804	0.04339
ASP	100	D	D	22.2484	0.01424	0.00233	ASP	1000	A	D	20.8395	0.45470	0.16988
ASP	100	D	D	22.4886	0.02129	0.01114	ASP	1000	A	D	24.8168	0.02770	0.00794
ASP	100	D	D	23.4177	0.01846	0.00360	ASP	1000	A	D	25.2829	0.49501	0.16324
ASP	100	D	D	23.5286	0.01308	0.00493	ASP	1000	A	D	26.8241	0.27551	0.06337
ASP	100	D	D	23.6373	0.22151	0.03459	ASP	1000	A	D	30.8131	0.13460	0.01851
ASP	100	D	D	23.6600	0.01905	0.00773	ASP	1000	A	D	31.3144	0.17942	0.00061
ASP	100	D	D	24.2584	0.01912	0.00700	ASP	1000	A	D	34.3763	0.03538	0.01712
ASP	100	D	D	24.8203	0.01413	0.00226	ASP	1000	A	W	8.3828	0.08369	0.02335
ASP	100	D	D	25.1419	0.01702	0.00561	ASP	1000	A	W	9.9391	0.09798	0.01195
ASP	100	D	D	25.2635	0.40199	0.05694	ASP	1000	A	W	10.7901	0.17064	0.00735
ASP	100	D	D	26.3741	0.01788	0.00526	ASP	1000	A	W	11.6904	0.02249	0.01441
ASP	100	D	D	26.4843	0.15926	0.01538	ASP	1000	A	W	11.6936	0.03837	0.02024
ASP	100	D	D	26.7247	0.01717	0.00739	ASP	1000	A	W	13.0107	0.06845	0.02003
ASP	100	D	D	26.8234	0.17530	0.05769	ASP	1000	A	W	15.3408	0.70407	0.03964
ASP	100	D	D	27.2788	0.18033	0.01814	ASP	1000	A	W	15.5447	2.30300	0.09572
ASP	100	D	D	27.6143	0.02160	0.00259	ASP	1000	A	W	16.0513	0.19109	0.00782
ASP	100	D	D	28.7356	0.02267	0.00476	ASP	1000	A	W	16.8083	0.04025	0.02385
ASP	100	D	D	29.0156	0.01903	0.00478	ASP	1000	A	W	17.2462	0.06546	0.00766
ASP	100	D	D	30.4136	0.00882	0.00484	ASP	1000	A	W	18.5933	0.04301	0.01212
ASP	100	D	D	30.5973	0.04093	0.01098	ASP	1000	A	W	19.1989	0.13223	0.02245
ASP	100	D	D	31.1202	0.00740	0.00452	ASP	1000	A	W	19.9392	0.14943	0.02415
ASP	100	D	D	31.4430	0.01785	0.00619	ASP	1000	A	W	23.6350	0.28881	0.04376
ASP	100	D	D	31.9481	0.02410	0.01262	ASP	1000	A	W	26.4801	0.15238	0.04510
ASP	100	D	D	34.3802	0.00885	0.00427	ASP	1000	A	W	26.8211	0.12788	0.05382
ASP	100	D	D	34.4637	0.01731	0.00253	ASP	1000	A	W	32.4278	0.17903	0.03678
ASP	100	D	D	34.7838	0.03332	0.00841	ASP	1000	B	H	8.3799	0.13373	0.02144
ASP	100	D	D	35.6200	0.01510	0.00574	ASP	1000	B	H	8.3809	0.15427	0.02506
ASP	100	D	D	36.7960	0.02527	0.01020	ASP	1000	B	H	9.9352	0.20434	0.01165
ASP	100	D	D	37.3929	0.01520	0.00924	ASP	1000	B	H	9.9368	0.24120	0.01175

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	1000	B	H	10.7861	0.21242	0.00829	ASP	1000	C	W	9.9378	0.10262	0.00907
ASP	1000	B	H	13.0124	0.07034	0.02085	ASP	1000	C	W	10.7891	0.18366	0.00607
ASP	1000	B	H	15.6021	1.88859	0.24865	ASP	1000	C	W	13.0158	0.17153	0.01511
ASP	1000	B	H	16.8035	0.05196	0.03401	ASP	1000	C	W	15.3404	0.60183	0.29742
ASP	1000	B	H	17.2516	0.13713	0.00864	ASP	1000	C	W	15.6852	1.72844	1.12599
ASP	1000	B	H	19.2066	0.15442	0.01851	ASP	1000	C	W	16.4515	1.20396	0.08600
ASP	1000	B	H	19.2080	0.15171	0.03232	ASP	1000	C	W	19.2046	0.21439	0.01567
ASP	1000	B	H	19.5585	0.15441	0.00928	ASP	1000	C	W	19.9479	0.23448	0.01290
ASP	1000	B	H	19.5622	0.17177	0.01242	ASP	1000	C	W	26.4849	0.19634	0.01620
ASP	1000	B	H	19.9464	0.17283	0.05316	ASP	1000	C	W	27.2767	0.12913	0.02180
ASP	1000	B	H	20.3859	0.18913	0.11626	ASP	1000	C	W	27.8238	0.13575	0.02101
ASP	1000	B	H	22.2942	0.01323	0.00287	ASP	1000	C	W	31.5252	0.20676	0.07366
ASP	1000	B	H	23.1393	0.36540	0.08034	ASP	1000	C	W	32.4341	0.21882	0.04394
ASP	1000	B	H	25.2771	0.34385	0.15588	ASP	1000	D	D	8.3828	0.09499	0.01665
ASP	1000	B	H	26.8258	0.21294	0.04675	ASP	1000	D	D	9.9349	0.13059	0.00861
ASP	1000	B	H	30.1161	0.16418	0.07441	ASP	1000	D	D	10.7865	0.17386	0.00629
ASP	1000	B	H	39.4190	0.01912	0.00967	ASP	1000	D	D	13.0144	0.06546	0.01563
ASP	1000	B	D	8.3830	0.07446	0.02552	ASP	1000	D	D	15.3432	0.70925	0.04476
ASP	1000	B	D	9.9359	0.14754	0.00922	ASP	1000	D	D	15.5927	2.20541	0.13941
ASP	1000	B	D	10.7874	0.18207	0.00656	ASP	1000	D	D	16.4475	1.18366	0.07490
ASP	1000	B	D	13.0153	0.08179	0.01418	ASP	1000	D	D	16.8143	0.04638	0.02900
ASP	1000	B	D	16.8142	0.06751	0.01726	ASP	1000	D	D	17.2485	0.08234	0.00918
ASP	1000	B	D	17.2496	0.10873	0.00614	ASP	1000	D	D	19.2045	0.17747	0.01568
ASP	1000	B	D	19.2057	0.18231	0.01338	ASP	1000	D	D	20.3862	0.30033	0.03382
ASP	1000	B	D	19.5642	0.07742	0.01138	ASP	1000	D	D	34.1611	0.75588	0.14786
ASP	1000	B	D	19.9470	0.23771	0.01200	ASP	1000	D	D	37.4087	0.05036	0.00645
ASP	1000	B	D	20.3856	0.23046	0.10573	ASP	1000	D	W	8.3878	0.11902	0.01395
ASP	1000	B	D	25.2166	0.34847	0.11704	ASP	1000	D	W	9.9370	0.08599	0.00944
ASP	1000	B	D	26.4874	0.22225	0.06101	ASP	1000	D	W	10.7886	0.16836	0.00592
ASP	1000	B	D	27.2778	0.12141	0.01882	ASP	1000	D	W	11.9306	2.87518	0.30779
ASP	1000	B	D	34.1412	0.52125	0.11745	ASP	1000	D	W	13.0161	0.07970	0.01752
ASP	1000	B	D	38.3613	0.17051	0.04520	ASP	1000	D	W	15.3510	0.79386	0.13092
ASP	1000	B	D	38.9786	0.35724	0.18531	ASP	1000	D	W	15.6156	0.81852	0.44999
ASP	1000	B	D	39.7564	0.34330	0.03127	ASP	1000	D	W	17.2491	0.06857	0.00909
ASP	1000	B	W	8.3821	0.08828	0.01825	ASP	1000	D	W	18.9853	0.04285	0.01570
ASP	1000	B	W	9.9373	0.11758	0.00841	ASP	1000	D	W	19.2049	0.18224	0.01556
ASP	1000	B	W	10.7889	0.18944	0.00606	ASP	1000	D	W	19.5641	0.15074	0.00774
ASP	1000	B	W	11.8533	3.31422	0.30350	ASP	1000	D	W	19.9442	0.14725	0.03572
ASP	1000	B	W	13.0088	0.17072	0.01535	ASP	1000	D	W	20.8561	0.35482	0.10898
ASP	1000	B	W	15.3556	0.72513	0.08645	ASP	1000	D	W	23.5142	0.03001	0.01239
ASP	1000	B	W	16.8083	0.07469	0.01872	ASP	1000	D	W	26.4830	0.15964	0.05894
ASP	1000	B	W	17.2446	0.09044	0.00691	ASP	1000	D	W	26.8250	0.20712	0.01630
ASP	1000	B	W	19.2002	0.18518	0.01197	ASP	1000	D	W	27.6012	0.01899	0.01204
ASP	1000	B	W	19.5584	0.15518	0.00645	ASP	1000	D	W	32.4277	0.31157	0.02778
ASP	1000	B	W	19.9454	0.21809	0.01412	ASP	1000	D	W	34.0066	0.00744	0.00065
ASP	1000	B	W	21.2060	0.78799	0.11548	ASP	1000	D	W	34.2525	0.75701	0.22777
ASP	1000	B	W	21.6630	0.09358	0.00057	ASP	1000	D	W	34.6726	0.33540	0.06737
ASP	1000	B	W	23.1257	0.34383	0.02951	ASP	1000	D	W	37.3983	0.15052	0.08916
ASP	1000	B	W	23.6315	0.31290	0.03121	ASP	1000	E	D	8.3831	0.10246	0.01416
ASP	1000	B	W	24.1813	0.18383	0.03615	ASP	1000	E	D	9.9353	0.12972	0.00754
ASP	1000	B	W	26.4826	0.17304	0.01335	ASP	1000	E	D	10.7870	0.16276	0.00575
ASP	1000	B	W	26.8201	0.11685	0.06316	ASP	1000	E	D	11.9187	3.83913	0.22657
ASP	1000	B	W	27.2709	0.11940	0.02018	ASP	1000	E	D	13.0148	0.03429	0.02184
ASP	1000	B	W	30.7988	0.17698	0.10463	ASP	1000	E	D	15.3413	0.68335	0.03439
ASP	1000	C	H	8.3808	0.17943	0.01928	ASP	1000	E	D	16.8150	0.06471	0.01839
ASP	1000	C	H	9.9368	0.20617	0.01174	ASP	1000	E	D	19.5648	0.24602	0.07933
ASP	1000	C	H	10.7882	0.21314	0.00848	ASP	1000	E	D	26.8252	0.15787	0.00124
ASP	1000	C	H	13.0150	0.10106	0.01667	ASP	1000	E	D	27.8281	0.10179	0.02266
ASP	1000	C	H	16.4516	0.04555	0.00682	ASP	1000	E	D	30.1102	0.12156	0.04780
ASP	1000	C	H	16.8100	0.09833	0.02936	ASP	1000	E	D	30.8095	0.21239	0.07901
ASP	1000	C	H	19.1663	0.36383	0.13659	ASP	1000	E	D	31.3153	0.02068	0.00050
ASP	1000	C	H	22.2945	0.01586	0.00268	ASP	1000	E	W	8.3878	0.07225	0.01989
ASP	1000	C	H	26.8333	0.27285	0.09601	ASP	1000	E	W	9.9367	0.06805	0.01122
ASP	1000	C	H	38.3619	0.17507	0.05729	ASP	1000	E	W	10.7883	0.15464	0.00635
ASP	1000	C	D	9.9354	0.13161	0.00774	ASP	1000	E	W	13.0152	0.13414	0.01415
ASP	1000	C	D	10.7870	0.17246	0.00562	ASP	1000	E	W	15.3381	0.62019	0.11189
ASP	1000	C	D	11.6930	0.03560	0.00926	ASP	1000	E	W	15.5713	1.78874	0.33769
ASP	1000	C	D	14.2521	0.04184	0.01333	ASP	1000	E	W	16.4486	1.28553	0.09392
ASP	1000	C	D	15.3464	0.69363	0.20827	ASP	1000	E	W	17.2490	0.06876	0.00878
ASP	1000	C	D	15.5788	2.31458	0.15159	ASP	1000	E	W	19.2048	0.17201	0.01637
ASP	1000	C	D	16.4500	1.16037	0.06348	ASP	1000	E	W	19.5637	0.15822	0.00789
ASP	1000	C	D	16.9932	0.03234	0.00801	ASP	1000	E	W	19.9419	0.20030	0.02920
ASP	1000	C	D	19.2046	0.17890	0.01411	ASP	1000	E	W	20.3815	0.20971	0.03092
ASP	1000	C	D	19.9476	0.23738	0.01070	ASP	1000	E	W	24.1875	0.22379	0.05745
ASP	1000	C	D	20.3808	0.18611	0.10220	ASP	1000	E	W	26.4824	0.13388	0.05693
ASP	1000	C	D	24.8167	0.03332	0.01175	ASP	1000	E	W	26.8244	0.17165	0.06807
ASP	1000	C	D	30.1116	0.11747	0.04357	ASP	1000	E	W	27.2774	0.11041	0.02983
ASP	1000	C	D	34.3740	0.05112	0.01883	ASP	1000	E	W	35.9340	0.49791	0.04709
ASP	1000	C	W	8.3881	0.06888	0.02084	ASP	1000	E	W	37.3925	0.22934	0.05383

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
ASP	1000	F	D	8.3829	0.10700	0.01401
ASP	1000	F	D	9.9352	0.11343	0.00836
ASP	1000	F	D	10.7867	0.14754	0.00609
ASP	1000	F	D	13.0137	0.11351	0.01300
ASP	1000	F	D	15.3465	0.65280	0.03529
ASP	1000	F	D	15.5586	2.39266	0.09008
ASP	1000	F	D	16.0591	0.03213	0.00679
ASP	1000	F	D	16.4513	1.19778	0.05707
ASP	1000	F	D	19.2048	0.15781	0.01400
ASP	1000	F	D	19.5636	0.13604	0.00705
ASP	1000	F	D	19.9450	0.22642	0.01246
ASP	1000	F	D	20.3817	0.25386	0.03719
ASP	1000	F	D	26.4851	0.16525	0.06417
ASP	1000	F	D	27.2766	0.11447	0.02045
ASP	1000	F	D	30.8101	0.22301	0.07747
ASP	1000	F	D	34.1626	0.59693	0.15657
ASP	1000	F	W	8.3877	0.08930	0.01845
ASP	1000	F	W	9.9367	0.09976	0.00890
ASP	1000	F	W	10.7882	0.18082	0.00618
ASP	1000	F	W	11.9244	2.57914	0.32860
ASP	1000	F	W	13.0153	0.15654	0.01503
ASP	1000	F	W	15.3429	0.65539	0.04276
ASP	1000	F	W	15.5598	2.27219	0.10751
ASP	1000	F	W	16.0573	0.08414	0.01274
ASP	1000	F	W	16.4474	1.20677	0.07502
ASP	1000	F	W	16.8166	0.05725	0.02681
ASP	1000	F	W	19.2033	0.21030	0.01615
ASP	1000	F	W	19.9448	0.21235	0.03556
ASP	1000	F	W	20.3813	0.24491	0.03891
ASP	1000	F	W	21.1947	0.70040	0.16003
ASP	1000	F	W	26.4820	0.15779	0.06171
ASP	1000	F	W	31.4754	0.68082	0.12766
ASP	1000	F	W	34.9070	0.19037	0.04857

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	10	A	H	8.3870	0.12210	0.01165	GLU	10	E	H	19.5677	0.13418	0.00669
GLU	10	A	H	9.9343	0.12725	0.00637	GLU	10	E	H	19.9443	0.17772	0.02720
GLU	10	A	H	10.7856	0.21632	0.00809	GLU	10	E	H	31.1244	0.01272	0.00480
GLU	10	A	H	11.7037	0.00960	0.00455	GLU	10	E	H	31.5224	0.23727	0.08424
GLU	10	A	H	12.4965	0.02966	0.01012	GLU	10	E	H	34.3850	0.01155	0.00447
GLU	10	A	H	13.0151	0.11746	0.01287	GLU	100	A	H	8.3867	0.10940	0.01634
GLU	10	A	H	14.2542	0.01773	0.00406	GLU	100	A	H	9.9345	0.15562	0.00642
GLU	10	A	H	16.8175	0.06636	0.01857	GLU	100	A	H	10.7859	0.20181	0.00528
GLU	10	A	H	16.9972	0.01611	0.00256	GLU	100	A	H	16.8156	0.09873	0.01904
GLU	10	A	H	17.2508	0.07981	0.00750	GLU	100	A	H	17.2511	0.11087	0.00744
GLU	10	A	H	19.0000	0.00746	0.00337	GLU	100	A	H	18.9989	0.01939	0.00223
GLU	10	A	H	19.2058	0.17257	0.01830	GLU	100	A	H	19.9471	0.22125	0.01776
GLU	10	A	H	19.5684	0.13061	0.00856	GLU	100	A	H	22.2527	0.00949	0.00536
GLU	10	A	H	19.9456	0.11783	0.03689	GLU	100	A	H	24.8175	0.01434	0.00684
GLU	10	A	H	24.8189	0.00601	0.00383	GLU	100	A	H	27.6199	0.01593	0.00815
GLU	10	A	H	25.1483	0.01319	0.00423	GLU	100	A	H	29.0183	0.01471	0.00522
GLU	10	A	H	29.0216	0.01049	0.00382	GLU	100	A	H	31.1242	0.01623	0.00734
GLU	10	A	H	33.9069	0.00843	0.00522	GLU	100	A	H	34.8551	0.74245	0.08237
GLU	10	A	H	34.3861	0.01284	0.00317	GLU	100	A	D	9.9314	0.09919	0.01383
GLU	10	A	H	34.7931	0.01514	0.00710	GLU	100	A	D	10.7830	0.12872	0.01423
GLU	10	B	H	8.3865	0.09431	0.01043	GLU	100	A	D	11.7021	0.01731	0.00282
GLU	10	B	H	9.2105	0.02318	0.01425	GLU	100	A	D	13.0130	0.15570	0.01724
GLU	10	B	H	9.9328	0.17248	0.00699	GLU	100	A	D	18.6245	0.01007	0.00413
GLU	10	B	H	10.7844	0.18432	0.00655	GLU	100	A	D	18.9976	0.01086	0.00290
GLU	10	B	H	13.0142	0.08700	0.01545	GLU	100	A	D	21.6569	0.20814	0.03501
GLU	10	B	H	16.8177	0.07122	0.01192	GLU	100	A	D	24.8181	0.00977	0.00353
GLU	10	B	H	17.2493	0.12380	0.00443	GLU	100	A	D	29.0184	0.01103	0.00411
GLU	10	B	H	18.9994	0.00804	0.00426	GLU	100	A	D	34.7877	0.02792	0.00324
GLU	10	B	H	19.2053	0.17307	0.01344	GLU	100	A	W	11.7049	0.01143	0.00593
GLU	10	B	H	19.5683	0.13180	0.00618	GLU	100	A	W	12.4947	0.01613	0.00656
GLU	10	B	H	19.9438	0.20040	0.02359	GLU	100	A	W	14.2560	0.01446	0.00286
GLU	10	B	H	21.9502	0.01150	0.00734	GLU	100	A	W	15.5719	0.01118	0.00268
GLU	10	B	H	26.8302	0.23370	0.04216	GLU	100	A	W	16.9979	0.01356	0.00511
GLU	10	B	H	27.6210	0.01155	0.00576	GLU	100	A	W	18.4811	0.01570	0.00383
GLU	10	C	H	8.3874	0.09921	0.01152	GLU	100	A	W	18.6230	0.02381	0.00218
GLU	10	C	H	9.9332	0.12883	0.00475	GLU	100	A	W	18.9999	0.01345	0.00234
GLU	10	C	H	10.7848	0.16804	0.00439	GLU	100	A	W	21.9517	0.01150	0.00353
GLU	10	C	H	11.7032	0.01256	0.00312	GLU	100	A	W	22.2520	0.01488	0.00202
GLU	10	C	H	13.0144	0.08074	0.01052	GLU	100	A	W	23.4172	0.01006	0.00202
GLU	10	C	H	16.8183	0.06325	0.01492	GLU	100	A	W	23.5285	0.01173	0.00312
GLU	10	C	H	17.2494	0.09965	0.00553	GLU	100	A	W	23.6613	0.01392	0.00297
GLU	10	C	H	18.6268	0.01023	0.00381	GLU	100	A	W	24.2569	0.01492	0.00287
GLU	10	C	H	18.9996	0.00813	0.00511	GLU	100	A	W	24.8198	0.01152	0.00360
GLU	10	C	H	19.5690	0.14406	0.00673	GLU	100	A	W	25.1362	0.02059	0.00388
GLU	10	C	H	19.9440	0.14969	0.02560	GLU	100	A	W	26.3715	0.01329	0.00292
GLU	10	C	H	27.6207	0.01990	0.00317	GLU	100	A	W	26.7258	0.01359	0.00457
GLU	10	C	H	34.1210	0.52434	0.10777	GLU	100	A	W	27.6162	0.01069	0.00334
GLU	10	C	H	34.7911	0.02011	0.00719	GLU	100	A	W	27.8774	0.01427	0.00604
GLU	10	D	H	8.3861	0.08255	0.02032	GLU	100	A	W	29.0156	0.01080	0.00411
GLU	10	D	H	9.9334	0.11647	0.00745	GLU	100	A	W	30.2363	0.01287	0.00538
GLU	10	D	H	10.7846	0.16251	0.00594	GLU	100	A	W	30.4148	0.02613	0.00843
GLU	10	D	H	11.7022	0.00980	0.00248	GLU	100	A	W	31.1227	0.01330	0.00169
GLU	10	D	H	16.8171	0.08410	0.02206	GLU	100	A	W	31.4409	0.00915	0.00282
GLU	10	D	H	16.9969	0.01113	0.00280	GLU	100	A	W	33.9002	0.01335	0.00459
GLU	10	D	H	17.2502	0.07790	0.00936	GLU	100	A	W	34.3817	0.00825	0.00325
GLU	10	D	H	18.6261	0.01382	0.00192	GLU	100	A	W	34.4624	0.01289	0.00205
GLU	10	D	H	18.9994	0.01477	0.00218	GLU	100	A	W	34.7864	0.02811	0.00468
GLU	10	D	H	19.2062	0.19692	0.01861	GLU	100	A	W	35.6167	0.01024	0.00254
GLU	10	D	H	19.5680	0.11769	0.00969	GLU	100	A	W	36.6397	0.00976	0.00371
GLU	10	D	H	24.8184	0.01029	0.00372	GLU	100	A	W	36.9444	0.01200	0.00410
GLU	10	D	H	25.1460	0.01138	0.00310	GLU	100	A	W	37.3920	0.01461	0.00403
GLU	10	D	H	29.0215	0.01197	0.00535	GLU	100	A	W	37.4660	0.01278	0.00308
GLU	10	D	H	31.1247	0.01061	0.00314	GLU	100	A	W	38.3250	0.00607	0.00314
GLU	10	D	H	33.9042	0.01560	0.00579	GLU	100	A	W	38.5427	0.01473	0.00372
GLU	10	D	H	34.7909	0.01925	0.00389	GLU	100	B	H	8.3866	0.10304	0.01018
GLU	10	E	H	8.3859	0.12569	0.01041	GLU	100	B	H	9.9333	0.13996	0.00458
GLU	10	E	H	9.2110	0.02867	0.01101	GLU	100	B	H	10.7848	0.16828	0.00391
GLU	10	E	H	9.9333	0.17389	0.00500	GLU	100	B	H	13.0140	0.07230	0.01101
GLU	10	E	H	10.7847	0.19608	0.00434	GLU	100	B	H	16.8166	0.05769	0.01517
GLU	10	E	H	11.7028	0.00856	0.00531	GLU	100	B	H	17.2496	0.11816	0.00456
GLU	10	E	H	13.0141	0.12126	0.01340	GLU	100	B	H	19.2050	0.20771	0.01183
GLU	10	E	H	13.1475	1.28531	0.50037	GLU	100	B	H	19.9445	0.20768	0.01958
GLU	10	E	H	15.3418	0.70746	0.03523	GLU	100	B	H	20.3839	0.21486	0.07255
GLU	10	E	H	15.5921	1.97323	0.07656	GLU	100	B	H	20.8488	0.36115	0.22256
GLU	10	E	H	16.8166	0.06844	0.01684	GLU	100	B	D	9.2108	0.01736	0.00648
GLU	10	E	H	16.9966	0.02092	0.00361	GLU	100	B	D	11.7019	0.00856	0.00239
GLU	10	E	H	17.2500	0.13496	0.00500	GLU	100	B	D	23.4175	0.00826	0.00180
GLU	10	E	H	18.9996	0.01677	0.00332	GLU	100	B	D	23.6620	0.00752	0.00350
GLU	10	E	H	19.1936	0.50186	0.07505	GLU	100	B	D	25.1420	0.00957	0.00275

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	100	B	D	29.0170	0.00558	0.00357	GLU	100	C	W	19.0018	0.02729	0.00362
GLU	100	B	D	31.4431	0.00542	0.00332	GLU	100	C	W	21.9515	0.00670	0.00401
GLU	100	B	W	11.7043	0.01497	0.00413	GLU	100	C	W	22.2522	0.01127	0.00200
GLU	100	B	W	14.2553	0.01179	0.00317	GLU	100	C	W	22.4897	0.01311	0.00318
GLU	100	B	W	18.4819	0.01548	0.00407	GLU	100	C	W	23.4172	0.00826	0.00214
GLU	100	B	W	18.6243	0.01436	0.00328	GLU	100	C	W	23.6612	0.01195	0.00248
GLU	100	B	W	18.9996	0.01427	0.00160	GLU	100	C	W	24.2573	0.00659	0.00371
GLU	100	B	W	21.9523	0.00890	0.00499	GLU	100	C	W	24.8199	0.01335	0.00199
GLU	100	B	W	22.2521	0.01168	0.00306	GLU	100	C	W	25.1414	0.01541	0.00266
GLU	100	B	W	23.4172	0.02279	0.00712	GLU	100	C	W	26.3715	0.01027	0.00288
GLU	100	B	W	24.2571	0.01385	0.00280	GLU	100	C	W	27.6169	0.01220	0.00238
GLU	100	B	W	24.8193	0.01088	0.00279	GLU	100	C	W	28.7354	0.01487	0.00250
GLU	100	B	W	25.1430	0.02861	0.00903	GLU	100	C	W	29.0192	0.01778	0.00142
GLU	100	B	W	26.3717	0.01360	0.00300	GLU	100	C	W	30.4150	0.00830	0.00187
GLU	100	B	W	26.7275	0.01017	0.00525	GLU	100	C	W	31.1235	0.01170	0.00124
GLU	100	B	W	27.6173	0.01183	0.00256	GLU	100	C	W	31.4404	0.00537	0.00335
GLU	100	B	W	27.8773	0.01122	0.00469	GLU	100	C	W	34.4626	0.00747	0.00194
GLU	100	B	W	29.0170	0.01333	0.00307	GLU	100	C	W	34.7860	0.02330	0.00391
GLU	100	B	W	30.2359	0.01000	0.00508	GLU	100	C	W	35.6181	0.00750	0.00162
GLU	100	B	W	30.4149	0.00936	0.00190	GLU	100	C	W	36.6393	0.00908	0.00245
GLU	100	B	W	31.1233	0.01034	0.00177	GLU	100	C	W	36.7935	0.01344	0.00835
GLU	100	B	W	31.4412	0.01118	0.00278	GLU	100	C	W	37.3922	0.00845	0.00334
GLU	100	B	W	34.3828	0.00874	0.00223	GLU	100	C	W	38.3262	0.00658	0.00228
GLU	100	B	W	34.4636	0.00605	0.00296	GLU	100	C	W	38.5436	0.00835	0.00348
GLU	100	B	W	34.7862	0.02318	0.00447	GLU	100	D	H	8.3858	0.11301	0.01517
GLU	100	B	W	35.6166	0.00849	0.00267	GLU	100	D	H	9.2110	0.02784	0.00847
GLU	100	B	W	36.6412	0.00895	0.00322	GLU	100	D	H	9.9338	0.12850	0.00636
GLU	100	B	W	37.4679	0.00965	0.00595	GLU	100	D	H	10.7852	0.16755	0.00516
GLU	100	C	H	8.3865	0.10476	0.01461	GLU	100	D	H	11.7025	0.02083	0.00185
GLU	100	C	H	9.2114	0.04873	0.01674	GLU	100	D	H	12.4965	0.03843	0.01115
GLU	100	C	H	9.9330	0.13589	0.00428	GLU	100	D	H	13.0146	0.07546	0.01295
GLU	100	C	H	10.7845	0.17562	0.00457	GLU	100	D	H	16.8153	0.10868	0.01640
GLU	100	C	H	11.7024	0.01930	0.00568	GLU	100	D	H	16.9963	0.01617	0.00303
GLU	100	C	H	12.4959	0.03719	0.01088	GLU	100	D	H	18.4822	0.01403	0.00728
GLU	100	C	H	13.0141	0.08129	0.01084	GLU	100	D	H	18.6259	0.02574	0.00178
GLU	100	C	H	14.2533	0.00998	0.00600	GLU	100	D	H	18.9986	0.02396	0.00226
GLU	100	C	H	16.8167	0.08388	0.01641	GLU	100	D	H	19.5670	0.16330	0.00762
GLU	100	C	H	16.9960	0.01573	0.00249	GLU	100	D	H	19.9453	0.15817	0.03470
GLU	100	C	H	17.2492	0.09311	0.00616	GLU	100	D	H	20.3868	0.21755	0.11466
GLU	100	C	H	18.6267	0.01962	0.00219	GLU	100	D	H	21.9497	0.01108	0.00646
GLU	100	C	H	18.9986	0.01741	0.00212	GLU	100	D	H	24.2581	0.02550	0.01052
GLU	100	C	H	19.9435	0.19277	0.01955	GLU	100	D	H	26.3746	0.01619	0.00853
GLU	100	C	H	21.9501	0.01565	0.00446	GLU	100	D	H	29.0213	0.01787	0.00767
GLU	100	C	H	22.2519	0.01101	0.00366	GLU	100	D	H	31.1237	0.01269	0.00438
GLU	100	C	H	24.8174	0.01480	0.00305	GLU	100	D	H	34.3852	0.00987	0.00433
GLU	100	C	H	25.1476	0.02004	0.00661	GLU	100	D	H	34.4655	0.00849	0.00417
GLU	100	C	H	26.7293	0.01967	0.00782	GLU	100	D	H	34.7896	0.01977	0.00807
GLU	100	C	H	27.6201	0.01344	0.00533	GLU	100	D	D	25.1408	0.01338	0.00366
GLU	100	C	H	29.0214	0.01376	0.00474	GLU	100	D	D	26.7255	0.00920	0.00566
GLU	100	C	D	8.3871	0.07852	0.02650	GLU	100	D	D	34.4646	0.00629	0.00332
GLU	100	C	D	9.2106	0.02674	0.00670	GLU	100	D	W	14.2543	0.01213	0.00271
GLU	100	C	D	9.9329	0.09628	0.00964	GLU	100	D	W	15.5705	0.01390	0.00240
GLU	100	C	D	10.7842	0.12501	0.00858	GLU	100	D	W	18.4803	0.06325	0.01932
GLU	100	C	D	11.7021	0.01612	0.00160	GLU	100	D	W	18.6229	0.01270	0.00253
GLU	100	C	D	15.5712	0.01296	0.00205	GLU	100	D	W	18.9991	0.01381	0.00219
GLU	100	C	D	16.9959	0.01541	0.00142	GLU	100	D	W	22.2521	0.01232	0.00267
GLU	100	C	D	17.2485	0.07844	0.01021	GLU	100	D	W	22.4890	0.01843	0.00470
GLU	100	C	D	18.4807	0.01766	0.00268	GLU	100	D	W	23.5297	0.01414	0.00296
GLU	100	C	D	18.6237	0.01729	0.00191	GLU	100	D	W	23.6616	0.01190	0.00306
GLU	100	C	D	18.9983	0.01712	0.00119	GLU	100	D	W	24.2573	0.00864	0.00361
GLU	100	C	D	19.2053	0.13040	0.03321	GLU	100	D	W	24.8187	0.05407	0.00734
GLU	100	C	D	19.5683	0.09648	0.01608	GLU	100	D	W	26.3715	0.00602	0.00349
GLU	100	C	D	21.9502	0.00870	0.00297	GLU	100	D	W	26.7251	0.01523	0.00268
GLU	100	C	D	22.2517	0.01362	0.00164	GLU	100	D	W	27.6159	0.01319	0.00488
GLU	100	C	D	23.4180	0.01257	0.00153	GLU	100	D	W	27.8772	0.00892	0.00380
GLU	100	C	D	24.8182	0.01285	0.00138	GLU	100	D	W	29.0178	0.01042	0.00303
GLU	100	C	D	25.1447	0.01652	0.00477	GLU	100	D	W	30.2362	0.01136	0.00368
GLU	100	C	D	26.3732	0.01059	0.00390	GLU	100	D	W	30.4143	0.01039	0.00212
GLU	100	C	D	26.7261	0.01183	0.00309	GLU	100	D	W	30.5918	0.01737	0.00867
GLU	100	C	D	27.6181	0.01524	0.00228	GLU	100	D	W	31.1226	0.01144	0.00165
GLU	100	C	D	29.0168	0.01884	0.00335	GLU	100	D	W	31.4423	0.00973	0.00229
GLU	100	C	D	30.2362	0.01039	0.00463	GLU	100	D	W	31.7869	0.22375	0.13475
GLU	100	C	D	31.1231	0.00732	0.00207	GLU	100	D	W	31.9449	0.01644	0.00529
GLU	100	C	D	34.7863	0.03288	0.00718	GLU	100	D	W	31.9462	0.02624	0.01432
GLU	100	C	W	11.7038	0.01256	0.00312	GLU	100	D	W	33.9006	0.01342	0.00483
GLU	100	C	W	15.5716	0.00922	0.00230	GLU	100	D	W	34.3830	0.01160	0.00174
GLU	100	C	W	16.9982	0.00763	0.00275	GLU	100	D	W	34.4630	0.00861	0.00197
GLU	100	C	W	18.4807	0.01403	0.00327	GLU	100	D	W	34.7872	0.02461	0.00345
GLU	100	C	W	18.6235	0.02637	0.00850	GLU	100	D	W	36.4502	0.01147	0.00440

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	100	D	W	36.6401	0.01022	0.00288	GLU	1000	B	H	16.4494	1.12620	0.09169
GLU	100	D	W	36.7933	0.02019	0.01023	GLU	1000	B	H	16.8162	0.09205	0.02261
GLU	100	D	W	36.9447	0.00804	0.00341	GLU	1000	B	H	16.8173	0.13247	0.02171
GLU	100	D	W	37.3931	0.00853	0.00395	GLU	1000	B	H	17.2492	0.12726	0.00578
GLU	100	D	W	37.4659	0.01037	0.00276	GLU	1000	B	H	18.6113	0.07470	0.02220
GLU	100	D	W	37.7620	0.01208	0.00682	GLU	1000	B	H	18.9913	0.04682	0.01742
GLU	100	D	W	38.3261	0.00859	0.00184	GLU	1000	B	H	19.2054	0.17310	0.01402
GLU	100	D	W	38.5434	0.01563	0.00248	GLU	1000	B	H	19.2067	0.23713	0.01663
GLU	1000	A	H	8.3844	0.12267	0.01716	GLU	1000	B	H	19.5635	0.14068	0.00617
GLU	1000	A	H	9.2094	0.05376	0.02670	GLU	1000	B	H	19.5682	0.17108	0.01032
GLU	1000	A	H	9.9351	0.15206	0.00855	GLU	1000	B	H	19.9424	0.12549	0.03272
GLU	1000	A	H	10.7861	0.18524	0.00664	GLU	1000	B	H	19.9503	0.25738	0.01483
GLU	1000	A	H	11.6966	0.04710	0.00413	GLU	1000	B	H	20.3846	0.18591	0.09110
GLU	1000	A	H	13.0136	0.12877	0.01253	GLU	1000	B	H	20.8602	0.54014	0.33854
GLU	1000	A	H	14.2548	0.03567	0.00890	GLU	1000	B	H	21.2172	0.67752	0.10980
GLU	1000	A	H	15.3443	0.72625	0.16076	GLU	1000	B	H	21.2290	0.81994	0.10929
GLU	1000	A	H	15.5776	2.34006	0.33804	GLU	1000	B	H	22.2944	0.01590	0.00238
GLU	1000	A	H	16.8102	0.06642	0.03045	GLU	1000	B	H	24.8196	0.02451	0.00788
GLU	1000	A	H	17.2509	0.11164	0.00904	GLU	1000	B	H	25.2830	0.51609	0.04265
GLU	1000	A	H	19.2065	0.16107	0.01666	GLU	1000	B	H	25.2839	0.50270	0.03303
GLU	1000	A	H	19.5630	0.15095	0.00708	GLU	1000	B	H	26.1922	0.19124	0.11659
GLU	1000	A	H	19.9453	0.16850	0.03255	GLU	1000	B	H	26.4873	0.19913	0.01828
GLU	1000	A	H	20.3851	0.36121	0.03076	GLU	1000	B	H	26.5002	0.23324	0.01936
GLU	1000	A	H	25.2833	0.44589	0.04410	GLU	1000	B	H	26.8263	0.29437	0.02242
GLU	1000	A	H	26.8272	0.24608	0.06167	GLU	1000	B	H	26.8312	0.31941	0.01713
GLU	1000	A	H	32.4361	0.12234	0.06067	GLU	1000	B	H	27.2757	0.09520	0.02042
GLU	1000	A	D	8.3860	0.10819	0.01786	GLU	1000	B	H	27.8241	0.15230	0.01958
GLU	1000	A	D	9.9361	0.13713	0.00748	GLU	1000	B	H	29.0601	0.01410	0.00696
GLU	1000	A	D	10.7878	0.18765	0.00540	GLU	1000	B	H	29.0601	0.01050	0.00645
GLU	1000	A	D	11.6976	0.02464	0.01129	GLU	1000	B	H	29.0601	0.01207	0.00055
GLU	1000	A	D	13.0169	0.11696	0.01159	GLU	1000	B	H	29.4395	1.00261	0.11024
GLU	1000	A	D	15.3410	0.62604	0.04491	GLU	1000	B	H	29.4420	0.96319	0.13059
GLU	1000	A	D	15.5524	2.11098	0.08481	GLU	1000	B	H	30.1077	0.14823	0.05967
GLU	1000	A	D	16.4542	1.03496	0.04916	GLU	1000	B	H	30.7995	0.29698	0.10139
GLU	1000	A	D	16.8209	0.03857	0.00077	GLU	1000	B	H	30.7995	0.29217	0.08912
GLU	1000	A	D	16.9998	0.02761	0.00900	GLU	1000	B	H	30.7995	0.29698	0.10139
GLU	1000	A	D	17.2508	0.09056	0.00932	GLU	1000	B	H	31.1311	0.02551	0.01364
GLU	1000	A	D	18.9952	0.04095	0.01885	GLU	1000	B	H	34.6814	0.05919	0.02821
GLU	1000	A	D	19.2080	0.19016	0.01498	GLU	1000	B	H	34.8946	0.23788	0.13628
GLU	1000	A	D	19.5699	0.16048	0.00701	GLU	1000	B	H	34.8948	0.19837	0.12541
GLU	1000	A	D	19.9468	0.11079	0.04023	GLU	1000	B	H	34.9077	0.22905	0.03576
GLU	1000	A	D	21.2227	0.78924	0.09885	GLU	1000	B	H	34.9144	0.21716	0.07138
GLU	1000	A	D	23.6419	0.02383	0.00041	GLU	1000	B	D	8.3852	0.10056	0.01394
GLU	1000	A	D	25.2868	0.50320	0.04046	GLU	1000	B	D	9.9348	0.12257	0.00630
GLU	1000	A	D	26.8318	0.26545	0.07557	GLU	1000	B	D	10.7868	0.16584	0.00439
GLU	1000	A	D	29.4293	1.35173	0.11256	GLU	1000	B	D	13.0165	0.10220	0.00973
GLU	1000	A	D	29.4317	1.28555	0.11089	GLU	1000	B	D	15.3524	0.72576	0.08472
GLU	1000	A	D	34.4629	0.02732	0.01798	GLU	1000	B	D	15.6387	1.56330	0.35371
GLU	1000	A	D	39.0071	0.47458	0.05865	GLU	1000	B	D	16.8214	0.06560	0.01784
GLU	1000	A	D	39.0084	0.45660	0.06202	GLU	1000	B	D	17.2500	0.09413	0.00598
GLU	1000	A	W	8.3854	0.10799	0.01827	GLU	1000	B	D	19.2075	0.16814	0.01544
GLU	1000	A	W	9.9334	0.13894	0.00779	GLU	1000	B	D	19.5704	0.15606	0.00676
GLU	1000	A	W	10.7849	0.20363	0.00585	GLU	1000	B	D	19.9476	0.07296	0.04033
GLU	1000	A	W	11.6958	0.02575	0.01374	GLU	1000	B	D	25.2853	0.46201	0.03654
GLU	1000	A	W	13.0140	0.13036	0.01036	GLU	1000	B	D	26.4906	0.17186	0.01555
GLU	1000	A	W	18.9912	0.02841	0.00807	GLU	1000	B	D	27.2892	0.15610	0.01748
GLU	1000	A	W	19.9450	0.21002	0.03447	GLU	1000	B	W	8.3860	0.10346	0.01831
GLU	1000	A	W	23.6425	0.29981	0.10943	GLU	1000	B	W	8.3860	0.09579	0.01564
GLU	1000	A	W	26.8239	0.15546	0.09269	GLU	1000	B	W	9.2100	0.04376	0.02458
GLU	1000	A	W	27.2802	0.12642	0.02995	GLU	1000	B	W	9.9333	0.11052	0.00631
GLU	1000	A	W	27.8259	0.19214	0.02437	GLU	1000	B	W	9.9349	0.14963	0.00952
GLU	1000	A	W	32.4358	0.26024	0.04613	GLU	1000	B	W	10.7848	0.16563	0.00459
GLU	1000	B	H	8.3842	0.13118	0.01033	GLU	1000	B	W	10.7868	0.20454	0.00575
GLU	1000	B	H	8.3847	0.16344	0.01820	GLU	1000	B	W	13.0128	0.15492	0.01189
GLU	1000	B	H	9.9340	0.15288	0.00633	GLU	1000	B	W	13.0167	0.12810	0.01022
GLU	1000	B	H	9.9364	0.21527	0.00739	GLU	1000	B	W	15.3410	0.64957	0.06619
GLU	1000	B	H	10.7874	0.18078	0.00589	GLU	1000	B	W	15.3434	0.66094	0.08479
GLU	1000	B	H	10.7877	0.22596	0.00704	GLU	1000	B	W	15.5764	1.92445	0.11576
GLU	1000	B	H	11.7001	0.03956	0.00744	GLU	1000	B	W	15.6116	1.81433	0.20915
GLU	1000	B	H	13.0129	0.11372	0.01098	GLU	1000	B	W	16.8180	0.07509	0.00955
GLU	1000	B	H	13.0164	0.11761	0.01223	GLU	1000	B	W	16.8217	0.08136	0.02269
GLU	1000	B	H	14.2573	0.06332	0.02938	GLU	1000	B	W	17.0008	0.03156	0.02030
GLU	1000	B	H	15.3386	0.65275	0.04160	GLU	1000	B	W	17.2486	0.07195	0.00748
GLU	1000	B	H	15.3583	0.76364	0.08694	GLU	1000	B	W	19.2033	0.20296	0.01584
GLU	1000	B	H	15.5417	2.16816	0.07074	GLU	1000	B	W	19.2072	0.17340	0.01756
GLU	1000	B	H	15.5549	1.97092	0.11937	GLU	1000	B	W	19.5646	0.15210	0.00687
GLU	1000	B	H	16.0604	0.19835	0.01882	GLU	1000	B	W	19.5705	0.16591	0.00756
GLU	1000	B	H	16.0611	0.02112	0.00765	GLU	1000	B	W	19.9440	0.17980	0.02820
GLU	1000	B	H	16.4491	1.13386	0.06119	GLU	1000	B	W	19.9475	0.09106	0.04088

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	1000	B	W	20.8502	0.47384	0.08934	GLU	1000	C	W	19.2041	0.15640	0.01709
GLU	1000	B	W	20.8505	0.49393	0.09835	GLU	1000	C	W	19.5645	0.16683	0.00695
GLU	1000	B	W	21.2149	0.77385	0.11679	GLU	1000	C	W	19.9426	0.14219	0.03148
GLU	1000	B	W	21.2248	0.75342	0.09278	GLU	1000	C	W	23.6330	0.32547	0.03789
GLU	1000	B	W	22.2952	0.01281	0.00259	GLU	1000	C	W	26.8233	0.17632	0.06232
GLU	1000	B	W	23.6349	0.30131	0.06687	GLU	1000	D	H	8.3840	0.13177	0.01655
GLU	1000	B	W	25.2843	0.49798	0.03478	GLU	1000	D	H	9.9351	0.14298	0.00925
GLU	1000	B	W	26.1881	0.17866	0.08432	GLU	1000	D	H	10.7861	0.18376	0.00684
GLU	1000	B	W	26.4877	0.17750	0.05200	GLU	1000	D	H	11.6954	0.02025	0.00694
GLU	1000	B	W	26.8266	0.14260	0.04557	GLU	1000	D	H	13.0137	0.09144	0.01435
GLU	1000	B	W	27.2799	0.11208	0.00066	GLU	1000	D	H	15.3416	0.74146	0.04956
GLU	1000	B	W	27.2881	0.16503	0.01707	GLU	1000	D	H	16.8102	0.07189	0.02556
GLU	1000	B	W	27.8237	0.14180	0.01858	GLU	1000	D	H	18.6076	0.04718	0.01991
GLU	1000	B	W	29.4377	1.11047	0.09595	GLU	1000	D	H	19.9458	0.24776	0.01295
GLU	1000	B	W	29.4452	1.05613	0.10935	GLU	1000	D	H	23.6428	0.30272	0.04520
GLU	1000	B	W	31.9756	0.01967	0.00937	GLU	1000	D	H	26.8285	0.22115	0.08931
GLU	1000	B	W	32.4365	0.21636	0.04108	GLU	1000	D	H	27.2756	0.10524	0.02236
GLU	1000	B	W	36.3755	0.03039	0.00836	GLU	1000	D	H	32.4366	0.38749	0.00974
GLU	1000	B	W	38.3640	0.28277	0.04482	GLU	1000	D	D	8.3857	0.10408	0.01923
GLU	1000	B	W	38.3643	0.21747	0.04051	GLU	1000	D	D	9.9366	0.14753	0.00816
GLU	1000	C	H	8.3837	0.14083	0.02010	GLU	1000	D	D	10.7883	0.20423	0.00622
GLU	1000	C	H	8.3844	0.09799	0.01472	GLU	1000	D	D	11.7002	0.04322	0.00724
GLU	1000	C	H	9.9341	0.10327	0.00750	GLU	1000	D	D	13.0178	0.13104	0.01091
GLU	1000	C	H	9.9360	0.19058	0.00869	GLU	1000	D	D	15.3566	0.79826	0.03629
GLU	1000	C	H	10.7855	0.15738	0.00519	GLU	1000	D	D	16.4638	0.96797	0.04129
GLU	1000	C	H	10.7875	0.23446	0.00646	GLU	1000	D	D	16.8206	0.05891	0.02314
GLU	1000	C	H	11.6956	0.04294	0.00680	GLU	1000	D	D	17.0020	0.02817	0.00526
GLU	1000	C	H	11.6978	0.03678	0.00647	GLU	1000	D	D	17.2519	0.11059	0.00649
GLU	1000	C	H	13.0131	0.11153	0.01262	GLU	1000	D	D	18.9970	0.03783	0.00499
GLU	1000	C	H	13.0162	0.13740	0.01135	GLU	1000	D	D	19.2083	0.16150	0.01681
GLU	1000	C	H	14.2507	0.04565	0.01387	GLU	1000	D	D	19.5702	0.16775	0.00731
GLU	1000	C	H	15.3457	0.44729	0.08989	GLU	1000	D	D	19.9491	0.16842	0.03134
GLU	1000	C	H	15.5796	1.84959	0.16282	GLU	1000	D	D	21.2296	0.69708	0.08657
GLU	1000	C	H	15.6245	1.87093	0.23398	GLU	1000	D	D	24.8277	0.04477	0.01007
GLU	1000	C	H	16.0621	0.17875	0.00952	GLU	1000	D	D	29.3999	0.82636	0.22402
GLU	1000	C	H	16.8110	0.06206	0.02161	GLU	1000	D	D	29.4056	0.89977	0.20577
GLU	1000	C	H	16.8171	0.11528	0.02394	GLU	1000	D	D	30.1178	0.03523	0.01684
GLU	1000	C	H	16.9996	0.03045	0.01411	GLU	1000	D	D	31.1317	0.03256	0.00944
GLU	1000	C	H	16.9997	0.02954	0.00578	GLU	1000	D	D	32.4356	0.27230	0.03533
GLU	1000	C	H	17.2500	0.09347	0.00676	GLU	1000	D	D	34.4648	0.03993	0.02589
GLU	1000	C	H	18.9943	0.04523	0.01649	GLU	1000	D	D	34.6469	0.14845	0.06178
GLU	1000	C	H	19.2062	0.14674	0.01560	GLU	1000	D	D	35.5722	0.22794	0.14736
GLU	1000	C	H	19.2087	0.19864	0.02302	GLU	1000	D	D	35.5965	0.04124	0.02097
GLU	1000	C	H	19.5633	0.14884	0.00682	GLU	1000	D	D	35.9433	0.43267	0.09253
GLU	1000	C	H	19.5679	0.16339	0.01049	GLU	1000	D	D	38.3600	0.13661	0.05498
GLU	1000	C	H	19.9437	0.13068	0.03252	GLU	1000	D	D	38.3600	0.13886	0.05472
GLU	1000	C	H	19.9513	0.14631	0.05580	GLU	1000	D	D	38.3600	0.13661	0.05498
GLU	1000	C	H	22.2945	0.00916	0.00396	GLU	1000	D	D	39.7507	0.36264	0.02909
GLU	1000	C	H	25.1062	0.02500	0.00839	GLU	1000	D	D	39.7508	0.36369	0.03069
GLU	1000	C	H	26.8282	0.23140	0.05450	GLU	1000	D	W	8.3856	0.10236	0.01619
GLU	1000	C	H	31.1299	0.03839	0.01650	GLU	1000	D	W	9.9330	0.09090	0.00852
GLU	1000	C	H	31.1300	0.03899	0.01460	GLU	1000	D	W	10.7846	0.17365	0.00514
GLU	1000	C	D	8.3857	0.13188	0.01642	GLU	1000	D	W	11.6966	0.03666	0.00381
GLU	1000	C	D	9.2111	0.05422	0.03449	GLU	1000	D	W	13.0135	0.11715	0.00974
GLU	1000	C	D	9.9366	0.14583	0.00965	GLU	1000	D	W	16.0561	0.19602	0.01094
GLU	1000	C	D	10.7882	0.20219	0.00708	GLU	1000	D	W	16.8142	0.07370	0.01950
GLU	1000	C	D	11.6990	0.03302	0.01822	GLU	1000	D	W	19.2038	0.18598	0.01629
GLU	1000	C	D	15.5720	1.99716	0.11637	GLU	1000	D	W	19.5643	0.16640	0.00639
GLU	1000	C	D	16.8208	0.06192	0.02621	GLU	1000	D	W	19.9418	0.16154	0.02480
GLU	1000	C	D	17.2517	0.04256	0.01705	GLU	1000	D	W	23.6412	0.27112	0.07471
GLU	1000	C	D	18.9956	0.02502	0.01524	GLU	1000	D	W	25.2767	0.34518	0.13831
GLU	1000	C	D	19.9518	0.24534	0.01668	GLU	1000	D	W	26.4875	0.10619	0.06387
GLU	1000	C	D	21.2297	0.71821	0.10395	GLU	1000	D	W	26.8254	0.17962	0.05510
GLU	1000	C	D	23.6486	0.30015	0.04110	GLU	1000	D	W	28.9973	0.01160	0.00347
GLU	1000	C	D	26.4922	0.14243	0.06118	GLU	1000	E	H	8.3843	0.15944	0.01687
GLU	1000	C	D	31.1320	0.03371	0.01946	GLU	1000	E	H	8.3862	0.16607	0.01325
GLU	1000	C	D	34.0236	0.12050	0.07685	GLU	1000	E	H	9.9341	0.13630	0.00877
GLU	1000	C	D	34.1705	0.63435	0.13207	GLU	1000	E	H	9.9352	0.18008	0.00769
GLU	1000	C	D	34.1826	0.61276	0.18843	GLU	1000	E	H	10.7867	0.19970	0.00633
GLU	1000	C	D	35.9454	0.51197	0.05044	GLU	1000	E	H	10.7872	0.17935	0.00608
GLU	1000	C	D	35.9464	0.50499	0.04544	GLU	1000	E	H	13.0154	0.09607	0.01302
GLU	1000	C	W	8.3861	0.08570	0.02402	GLU	1000	E	H	15.3379	0.72403	0.04082
GLU	1000	C	W	9.9336	0.12373	0.00921	GLU	1000	E	H	15.3393	0.63484	0.19660
GLU	1000	C	W	10.7850	0.18393	0.00693	GLU	1000	E	H	15.5687	1.99322	0.18688
GLU	1000	C	W	11.6971	0.01755	0.00649	GLU	1000	E	H	16.0583	0.23191	0.03685
GLU	1000	C	W	13.0138	0.13200	0.01194	GLU	1000	E	H	16.4518	1.11788	0.08135
GLU	1000	C	W	16.0530	0.20337	0.01225	GLU	1000	E	H	16.8152	0.10954	0.01816
GLU	1000	C	W	16.8141	0.07728	0.01763	GLU	1000	E	H	16.8176	0.07850	0.03001
GLU	1000	C	W	17.2491	0.07779	0.00783	GLU	1000	E	H	17.2493	0.15058	0.00725

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd	Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	1000	E	H	17.2497	0.11588	0.00736	GLU	1000	F	H	19.2047	0.16937	0.01559
GLU	1000	E	H	19.2050	0.16686	0.01555	GLU	1000	F	H	19.5633	0.14542	0.00750
GLU	1000	E	H	19.2063	0.19713	0.01783	GLU	1000	F	H	19.5647	0.15413	0.00625
GLU	1000	E	H	19.5628	0.14645	0.00780	GLU	1000	F	H	19.9459	0.24364	0.04542
GLU	1000	E	H	19.5674	0.15670	0.00912	GLU	1000	F	H	20.3802	0.27544	0.12898
GLU	1000	E	H	19.9434	0.11868	0.04108	GLU	1000	F	H	21.0928	1.33571	0.28550
GLU	1000	E	H	19.9450	0.08043	0.04828	GLU	1000	F	H	21.0982	1.27989	0.29720
GLU	1000	E	H	19.9464	0.17893	0.04207	GLU	1000	F	H	21.2214	0.72887	0.08861
GLU	1000	E	H	20.3806	0.29255	0.04879	GLU	1000	F	H	26.4842	0.08849	0.05240
GLU	1000	E	H	20.3866	0.18951	0.12269	GLU	1000	F	H	26.4885	0.17408	0.06446
GLU	1000	E	H	22.2929	0.01653	0.00232	GLU	1000	F	H	26.8242	0.14693	0.05682
GLU	1000	E	H	25.2782	0.47944	0.03378	GLU	1000	F	H	26.8253	0.25633	0.02024
GLU	1000	E	H	25.2805	0.50343	0.05640	GLU	1000	F	H	27.2805	0.14472	0.01911
GLU	1000	E	H	26.4877	0.23457	0.02138	GLU	1000	F	H	27.8247	0.17713	0.01760
GLU	1000	E	H	26.4913	0.20913	0.02002	GLU	1000	F	H	30.1077	0.08762	0.04139
GLU	1000	E	H	26.7997	0.02667	0.00788	GLU	1000	F	H	31.5256	0.12625	0.06568
GLU	1000	E	H	27.2780	0.12143	0.02143	GLU	1000	F	H	32.4354	0.23325	0.03409
GLU	1000	E	H	27.2829	0.14901	0.02073	GLU	1000	F	H	34.6875	0.30319	0.05043
GLU	1000	E	H	29.4150	1.59543	0.14483	GLU	1000	F	D	8.3850	0.11322	0.01981
GLU	1000	E	H	30.1123	0.17952	0.05743	GLU	1000	F	D	8.5456	1.97704	0.56380
GLU	1000	E	H	30.1684	0.01868	0.00921	GLU	1000	F	D	9.9341	0.13367	0.00622
GLU	1000	E	H	30.4193	0.36300	0.11485	GLU	1000	F	D	10.7857	0.17531	0.00514
GLU	1000	E	H	30.4219	0.38180	0.11325	GLU	1000	F	D	13.0148	0.10209	0.01047
GLU	1000	E	H	30.8016	0.26009	0.10857	GLU	1000	F	D	13.0149	0.09388	0.01108
GLU	1000	E	H	30.8019	0.26356	0.10552	GLU	1000	F	D	15.3365	0.63840	0.04447
GLU	1000	E	H	31.9280	0.01683	0.00907	GLU	1000	F	D	15.5627	1.55047	0.29734
GLU	1000	E	H	34.0093	0.01983	0.00039	GLU	1000	F	D	16.8185	0.07215	0.01873
GLU	1000	E	H	34.3122	0.61492	0.40558	GLU	1000	F	D	17.2473	0.10363	0.00628
GLU	1000	E	H	34.3311	0.60878	0.35598	GLU	1000	F	D	19.2030	0.18225	0.01494
GLU	1000	E	H	34.6666	0.30198	0.13189	GLU	1000	F	D	19.9443	0.19339	0.02851
GLU	1000	E	H	34.6696	0.32021	0.13088	GLU	1000	F	D	25.2803	0.41976	0.09974
GLU	1000	E	W	5.7645	1.31031	0.46508	GLU	1000	F	D	29.4335	1.04815	0.09531
GLU	1000	E	W	8.3848	0.11113	0.01789	GLU	1000	F	D	29.4391	1.07261	0.08349
GLU	1000	E	W	9.9328	0.11670	0.00734	GLU	1000	F	D	30.1093	0.10303	0.05225
GLU	1000	E	W	9.9398	0.12229	0.00717	GLU	1000	F	D	30.8132	0.36165	0.01662
GLU	1000	E	W	10.7842	0.15310	0.00559	GLU	1000	F	D	30.8135	0.37089	0.01760
GLU	1000	E	W	10.7913	0.18191	0.00503	GLU	1000	F	D	31.1272	0.04461	0.02636
GLU	1000	E	W	13.0199	0.09164	0.01112	GLU	1000	F	W	8.3837	0.11526	0.02041
GLU	1000	E	W	15.3371	0.70129	0.03420	GLU	1000	F	W	8.3857	0.09727	0.01461
GLU	1000	E	W	16.0603	0.14689	0.06104	GLU	1000	F	W	9.9347	0.16158	0.00913
GLU	1000	E	W	16.8127	0.09338	0.01636	GLU	1000	F	W	9.9396	0.11706	0.00438
GLU	1000	E	W	17.2482	0.09024	0.00631	GLU	1000	F	W	10.7859	0.19316	0.00701
GLU	1000	E	W	19.2034	0.16802	0.01403	GLU	1000	F	W	10.7910	0.18449	0.00340
GLU	1000	E	W	19.5639	0.14763	0.00626	GLU	1000	F	W	11.6967	0.04750	0.00241
GLU	1000	E	W	19.9425	0.08857	0.03391	GLU	1000	F	W	13.0135	0.12050	0.00932
GLU	1000	E	W	20.8562	0.21621	0.00265	GLU	1000	F	W	13.0203	0.11370	0.00654
GLU	1000	E	W	21.2221	0.70533	0.08987	GLU	1000	F	W	15.6342	1.70602	0.13491
GLU	1000	E	W	22.2534	0.01726	0.01005	GLU	1000	F	W	16.4548	1.10575	0.03684
GLU	1000	E	W	25.2789	0.39266	0.12353	GLU	1000	F	W	16.8100	0.07752	0.02233
GLU	1000	E	W	25.2802	0.47360	0.12184	GLU	1000	F	W	16.8210	0.07601	0.01603
GLU	1000	E	W	26.4864	0.09251	0.06040	GLU	1000	F	W	16.8230	0.01906	0.00078
GLU	1000	E	W	26.8222	0.09066	0.01628	GLU	1000	F	W	16.9958	0.02143	0.00442
GLU	1000	E	W	27.2780	0.11909	0.01701	GLU	1000	F	W	17.0028	0.04156	0.01211
GLU	1000	E	W	29.3685	0.87764	0.24032	GLU	1000	F	W	17.2510	0.11884	0.00740
GLU	1000	E	W	29.3698	0.85467	0.24114	GLU	1000	F	W	17.2528	0.08085	0.00486
GLU	1000	E	W	30.1113	0.12339	0.06422	GLU	1000	F	W	18.9875	0.03868	0.00275
GLU	1000	E	W	30.4169	1.67602	0.54796	GLU	1000	F	W	19.2055	0.16330	0.01561
GLU	1000	E	W	30.4529	2.06604	0.72434	GLU	1000	F	W	19.2085	0.17524	0.00937
GLU	1000	E	W	30.8137	0.31340	0.02811	GLU	1000	F	W	19.5628	0.15209	0.00656
GLU	1000	E	W	30.8146	0.31982	0.02836	GLU	1000	F	W	19.5704	0.14979	0.00481
GLU	1000	E	W	32.4346	0.21292	0.03309	GLU	1000	F	W	19.9448	0.10646	0.04420
GLU	1000	E	W	34.9024	0.17721	0.03526	GLU	1000	F	W	19.9494	0.15745	0.01893
GLU	1000	E	W	34.9091	0.17314	0.03690	GLU	1000	F	W	20.3869	0.22898	0.09652
GLU	1000	E	W	38.3646	0.22041	0.04312	GLU	1000	F	W	20.8468	0.38589	0.09954
GLU	1000	F	H	8.3841	0.13072	0.01956	GLU	1000	F	W	21.1015	1.54218	0.76079
GLU	1000	F	H	8.3857	0.08817	0.01389	GLU	1000	F	W	21.1202	1.76613	0.47695
GLU	1000	F	H	8.3858	0.10942	0.02062	GLU	1000	F	W	21.2232	0.69662	0.21373
GLU	1000	F	H	9.9321	0.11857	0.00612	GLU	1000	F	W	23.6430	0.26896	0.00194
GLU	1000	F	H	9.9355	0.17673	0.00801	GLU	1000	F	W	25.2820	0.50490	0.02676
GLU	1000	F	H	10.7836	0.16445	0.00498	GLU	1000	F	W	26.1262	0.91445	0.07716
GLU	1000	F	H	10.7870	0.21051	0.00631	GLU	1000	F	W	26.1934	0.26461	0.09471
GLU	1000	F	H	11.6974	0.13182	0.06310	GLU	1000	F	W	26.4898	0.15782	0.04170
GLU	1000	F	H	13.0126	0.10669	0.00839	GLU	1000	F	W	26.8310	0.17906	0.03582
GLU	1000	F	H	13.0159	0.11939	0.01197	GLU	1000	F	W	27.2864	0.12641	0.01378
GLU	1000	F	H	15.3384	0.69432	0.03946	GLU	1000	F	W	29.4092	1.33159	0.11487
GLU	1000	F	H	16.8137	0.04652	0.02426	GLU	1000	F	W	30.4148	0.03142	0.01160
GLU	1000	F	H	16.8175	0.05698	0.03159	GLU	1000	F	W	31.1300	0.02471	0.00981
GLU	1000	F	H	17.2472	0.09421	0.00562	GLU	1000	F	W	31.3201	0.14266	0.06101
GLU	1000	F	H	19.2029	0.14249	0.01494	GLU	1000	F	W	38.9811	0.48405	0.03945

Amino Acid	Conc mg/L	Method	Time	2 Θ°	Micro-strain	2*esd
GLU	1000	F	W	38.9820	0.48493	0.04024
GLU	1000	F	W	40.2977	0.57887	0.05617
GLU	1000	F	W	40.3005	0.56927	0.05336
GLU	1000	F	W	41.0118	0.37083	0.05014
GLU	1000	F	W	41.0134	0.36976	0.04852
GLU	1000	F	W	41.0225	0.28997	0.04398
GLU	1000	F	W	41.4842	0.37126	0.04209
GLU	1000	F	W	41.4848	0.38776	0.04365
GLU	1000	F	W	42.3301	0.37401	0.05953
GLU	1000	F	W	42.9074	0.47918	0.07120
GLU	1000	F	W	42.9120	0.49619	0.28658
GLU	1000	F	W	43.6074	0.38376	0.04084
GLU	1000	F	W	43.6086	0.37678	0.00197
GLU	1000	F	W	45.0519	0.98461	0.09451
GLU	1000	F	W	46.0289	0.33968	0.04351
GLU	1000	F	W	46.5831	0.54947	0.04709
GLU	1000	F	W	50.0320	0.42093	0.10948