

LC-ESI-TOF-MS ANALYSIS OF THE POLAR METABOLOME OF *SINORHIZOBIUM MELILOTI*

LC-ESI-TOF-MS ANALYSIS OF THE POLAR METABOLOME OF *SINORHIZOBIUM MELILOTI*

By

ELNA DAWN DEGLINT, B.Sc.

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AUTHOR: Elna Dawn Deglint, B.Sc. (University of the Fraser Valley)

SUPERVISOR: Professor B. E. McCarry

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## ABSTRACT

The goal of this thesis is to determine if *Sinorhizobium meliloti* can be useful as a sentinel soil microorganism for assessing the impacts of contaminant stressors on the metabolome of a microorganism. Not only is a good deal known about this organism, but it is an important organism in agriculture. Moreover, the currently available gene array and a large library of gene fusion can be used as facile pathways to explore genetic and genomic impacts in addition to metabolomic impacts of contaminants, should such studies be deemed worthwhile. In this study, the polar metabolome of the soil microorganism, *Sinorhizobium meliloti*, has been analyzed by LC-ESI-MS using a HILIC column coupled to a medium mass resolution time-of-flight mass spectrometer. This approach has resulted in the retention ( $k' > 0.7$ ) of over 300 polar metabolites as detected in both positive ion and negative ion modes. These data do not include ions corresponding to adduct ions, isotopic features or ions resulting from in-source decay processes. The retained peaks showed excellent linear responses and did not suffer from ion suppression, a common problem in flow-injection ESI analysis. This methodology has been applied to the analysis of *S. meliloti* exposed to fluorene, a common PAH contaminant, and to a coal tar fraction containing low molecular mass PAHs. Multiple cultures of *S. meliloti* were grown on M9 glucose minimal medium in the absence and presence of fluorene (0.14 mg/L and 1.4 mg/L) and a PAH mixture (total PAH concentrations of 0.14 mg/L and 1.4 mg/L). Analyses of biological replicates were performed in pentuplicate. The retention times of the resulting chromatograms were

aligned, peak areas determined and the resulting data processed using PCA and OPLS-DA methods. The retention time reproducibilities of peaks were within  $\pm 10$  seconds and the biological variabilities of over 700 components averaged  $23\% \pm 15\%$  (n=25). The impacts of fluorene exposures and PAH mixture exposures on the *S. meliloti* metabolomes (polar) caused significant changes in the metabolome. The lower concentration exposures had less of an impact than the higher dosages. Low dosages of both fluorene and the PAH mixture produced a similar metabolic response in *S. meliloti*, while at higher dosages the responses were more specific to each toxin. The use of SUS plots coupled with S-plots of the OPLS-DA analysis were particularly advantageous for the identification of metabolites of interest. Changes were seen in the levels of adenine, adenosine, glutamate, and aspartate, among others. In the future, the profiles of the non-polar metabolites of each of sample will be analyzed using a previously developed 'shotgun lipidomics' method.

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## ABBREVIATIONS

B&D	Bligh and Dyer
BaP	Benzo[a]pyrene
CE	Capillary electrophoresis
DI	Direction infusion
DMSO	Dimethylsulfoxide
ED	Entner–Dourdoroff pathway
EI	Electron ionization
EIC	Extracted ion chromatogram
ESI	Electrospray ionization
FT-ICR	Fourier-transform ion cyclotron resonance
GC	Gas chromatography
HILIC	Hydrophilic interaction chromatography
HMDB	Human Metabolome Database
k'	Capacity factor
LB <sub>mc</sub>	Luria broth containing 2.5 mM of MgSO <sub>4</sub> and CaCl <sub>2</sub>
LC	Liquid chromatography
m/z	Mass to charge ratio
MS	Mass spectrometry
MS/MS	Tandem mass spectrometry
NIST	National Institute of Standards and Technology
NMR	Nuclear magnetic resonance
OD <sub>600</sub>	Optical density measured at 600 nm
OPLS-DA	Orthogonal projections to latent structures - discriminant analysis
PAH	Polycyclic aromatic hydrocarbon
PCA	Principal component analysis
R <sub>2</sub> X	a measure of the variation in X which is correlated to Y
R <sub>2</sub> X(o <sub>x</sub> )	to the amount of variation in X that is uncorrelated to Y
R <sub>2</sub> Y	the total variation in Y explained by the statistical model



RPLC	Reversed phase liquid chromatography
SM	Streptomycin
SUS plot	Shared and unique structures plot
TIC	Total ion current chromatogram
TOF	Time of flight
$t_R$	Retention time

## Chapter One: Literature Review

### *Metabolomics*

In many organisms, the function of the majority of genes remains unknown. Even if the complete genome of a particular organism has been sequenced, the majority of genes have been assigned specific biochemical functions based only on sequence homologies with genes in other organisms or their function remains unknown<sup>1</sup>.

Although gene and protein expression are closely related, one modification in the genome can produce major changes in metabolites of seemingly unrelated biological pathways<sup>2</sup>. The metabolome (i.e., the complete suite of metabolites produced by an organism<sup>3</sup>) is also far more dependent on external factors than gene and protein expression. Much of the activity in the cell of an organism can be captured by studying metabolites that regulate cellular functioning and metabolic network operations. Genomics and proteomics may foreshadow cellular events, but the metabolome is the record of what has occurred at the cellular level<sup>4</sup>. In order to obtain a complete picture of cellular responses, a study of the expression of genes and proteins is needed, coupled with the analysis of all metabolites<sup>1</sup>.

### *Approaches to Studying Metabolomics*

In order to study the metabolome of an organism, a variety of approaches have been developed. Genome response levels can be an indication of the cellular response.

However, genomic studies can be extremely costly and for this reason, it is difficult to be thorough<sup>1</sup>. On the other hand, methods to study protein expression have been well developed and are relatively inexpensive, although quite labour intensive. Because small changes in protein expression can lead to significant changes in the metabolome, the proteomics analysis must be highly sensitive<sup>3</sup>. Although the metabolomic techniques for the direct detection and quantification of metabolites have been fairly developed, the identification of unknown metabolites remains a significant challenge due to the complexity and diversity of chemical structures<sup>1</sup>.

In order to answer questions pertaining to the metabolome, different approaches have been developed<sup>3</sup>. *Metabolite target analysis* is used to study a primary effect by only focusing on quantifying the substrate and/or product of interest. *Metabolite profiling* is used to study specific compounds, typically in specific biochemical pathways, where it is not intended to monitor effects on the entire metabolome. *Metabolomic fingerprinting* involves classification of samples according to their biological relevance, without identifying individual metabolites. *Metabolomics* is a comprehensive and quantitative analysis of all metabolites in a biological system. In this thesis, work will focus on using the metabolomics approach for untargeted metabolite analysis.

In an untargeted metabolomics approach, there is a strong need for thorough and robust chemical analyses of all metabolite classes, i.e., lipids, sugars, amino acids,

etc<sup>3</sup>. The method must be sensitive enough to analyze metabolites which are found at very low cellular concentrations, as well as compounds in high abundance. Because of the large number of metabolites present in a given biological sample, high resolution mass spectrometry methods have been shown to be valuable in distinguishing among species of the same nominal mass<sup>5</sup>. Untargeted metabolomics produces large and complex data sets, and efficient tools are needed to 'mine' these large data sets to produce biologically meaningful results<sup>6</sup>. There will always be the need for the identification of unknown compounds.

### *Methods of Analysis*

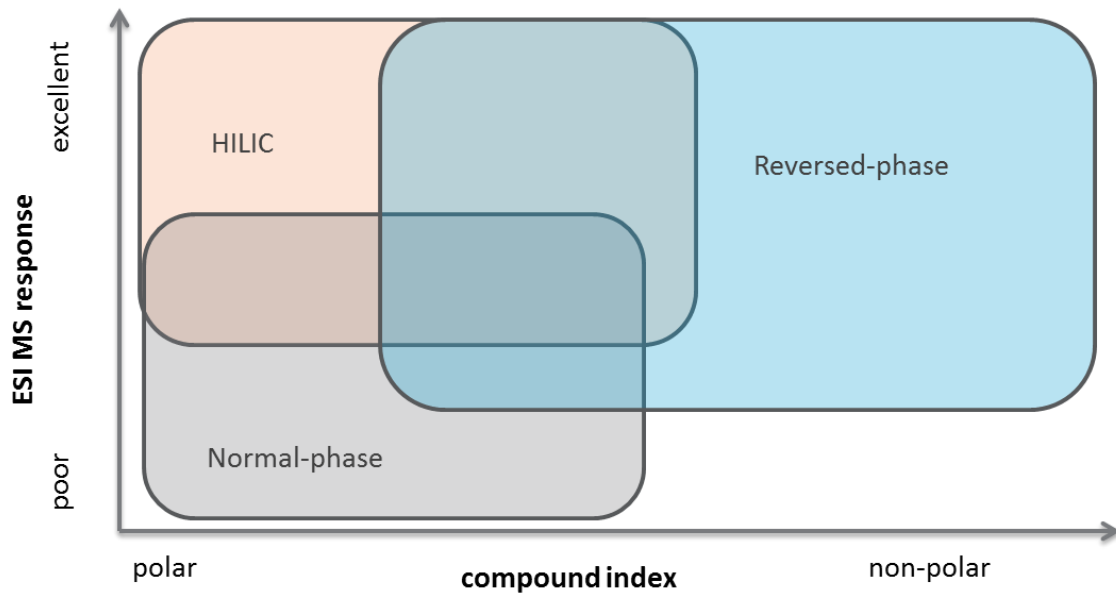
Although no technology can be relied upon to generate a complete picture of an organism's metabolome<sup>7</sup>, several methods of data acquisition have been developed, which can be grouped as spectroscopic methods and chromatographically mass spectrometric methods. The advantages of nuclear magnetic resonance (NMR) spectroscopy include minimal sample preparation, the ability to measure abundant metabolites accurately<sup>8</sup>, and its non-destructive nature<sup>5</sup>. However, this method lacks the sensitivity required for the quantification of a large number of metabolites<sup>8</sup>; peak clustering can make identification of metabolites difficult with certain matrices<sup>5</sup>. Mass spectrometry (MS) based techniques allow for high sensitivity and selectivity of detection. MS instruments with medium to high mass resolution can aid in the identification of unknown metabolites as well provide increased selectivity of detection.

Because MS-based methods generally require some degree of sample preparation, it is possible for metabolites to be 'lost' in the sample preparation process; certain classes of compounds maybe discriminated against.

When MS is coupled to a separation technique such as liquid chromatography (LC), capillary electrophoresis (CE) or gas chromatography (GC), the selectivity and sensitivity of the methods increases. Additional information about the physio-chemical properties of the metabolites can be obtained for use in identification<sup>5</sup>. In LC-MS, samples are usually introduced into the mass spectrometer via an electrospray ionization (ESI) source, while electron impact ionization (EI) is commonly used in GC-MS analyses. Reversed phase LC (RPLC) is most commonly used to analyze biological samples. Polar fractions contain primarily cytosolic materials, while non-polar fractions consist mainly of membrane components. However, because very polar compounds are poorly retained using RPLC, hydrophilic interaction chromatography (HILIC) has become a chromatographic option that has emerged as an alternative to reverse phase methods (see Figure 1.1). See Figure 1.2 for a summary of metabolomics analysis techniques.

In HILIC methods, polar analytes are partitioned into a layer of water which forms on the surface of the stationary phase<sup>5</sup>; by decreasing the amount of organic component in the stationary phase, more polar components tend to partition into the increasingly polar mobile phase. The non-polar fraction of the cellular extract (e.g.,

lipids and sterols) is typically analyzed on a reversed phase column or by direction infusion (DI) MS.



**Figure 1.1:** Polar fractions of cellular extracts can be analyzed by HILIC chromatography while the non-polar fraction can be effectively analyzed on a reversed-phase column.

Compound Class	NMR	ESI-MS (infusion or LC)	EI-GC-MS (with derivatization)	CE-MS
amino acids	✓	✓	✓	✓
sugars/ sugar alcohols	✓	-	✓	-
sugar phosphates	-	✓	✓	✓
nucleotides/nucleosides	-	✓	✓	✓
lipids	-	✓	-	-
sterols	-	-	✓	✓
<b>relative sensitivity</b>	+	++++		
<b># metabolites detected</b>	20-40	200-500		
<b>dynamic range</b>	~20	~10 <sup>3</sup>		

**Figure 1.2:** No single technique has the ability to analyze all compound classes present in an organism's metabolome, however MS-based techniques are more sensitive, comprehensive and robust than NMR methods<sup>5,9</sup>.

### *Quenching and Extraction of Metabolites*

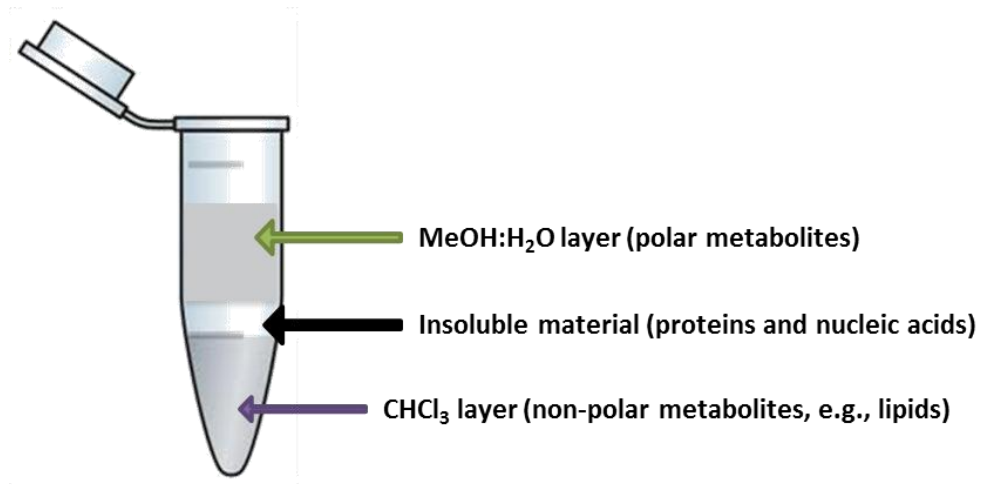
Sample preparation is crucial in gaining an accurate and complete picture of the metabolome at a given time, and is often the most overlooked part of metabolomic analyses. Proper sample preparation requires immediate quenching of cellular metabolic activity through the inactivation of enzymes<sup>10</sup>, and the complete extraction of the metabolites from the cell preparation. Extraction can be achieved through changes in temperature, extreme pH, organic solvents, mechanical stress or a combination of these approaches<sup>11</sup>. Sampling time is of crucial importance, as the metabolite turnover time can vary from milliseconds to hours<sup>12</sup>, and the inactivation process should not physically or chemically modify any metabolites present<sup>13</sup>.

Because metabolites vary in structure and properties, it is unlikely that any one method will, without bias, stop all metabolic processes and extract all classes of metabolites<sup>13</sup>. It is of crucial importance that the method of quenching and extraction is reproducible<sup>12</sup>; otherwise, changes in the metabolome may be due to other factors. While both the extraction and quenching of metabolites is dependent on the organism due to differences in cell membrane composition, the stability of metabolites should be similar to the stabilities observed in microbes<sup>11</sup>.

The Bligh and Dyer extraction, developed in 1959<sup>14</sup>, is a simple protocol that simultaneously extracts metabolites from cells and partitions them between two liquid



phases (methanol/water and chloroform, i.e., polar and non-polar phases), while the insoluble proteins are found as a band between the two solvent layers (see Figure 1.3). An advantage of the Bligh and Dyer procedure is that the extraction of both polar and non-polar metabolites occurs quickly and affords two reproducible fractions, a polar phase and a non-polar phase.



**Figure 1.3:** The Bligh and Dyer extraction method is a simple technique for the separation of polar and non-polar cellular metabolites by their partition coefficients.

### *Data Processing*

Analytical technologies used in metabolomics generate large amounts of raw data. The identification and quantification of metabolites can only be achieved by proper sample and data handling, which includes the use of internal and recovery standards, data processing and data analysis<sup>6</sup>.

Data processing is the process of transforming raw data files into useful chemical information. In the case of LC-MS data,  $m/z$  values and retention times for each ion present in the sample are meaningful<sup>6</sup>. Data processing should also be able to identify and differentiate the major ion(s) needed for quantification, but also adduct ions and/or fragment ions formed from each compound, as well as the isotopic peaks associated with these ions. Due to instrumental variations, which in turn cause variations in retention times across samples, alignment of chromatograms is necessary in order to make correct assignments and measurements of ions and ion clusters in samples<sup>15</sup>. Normalization of signal intensities is necessary to remove variations due to instrumental fluctuations; normalization is achieved using a set of internal standards<sup>6</sup>.

One package of open source software that is available for processing metabolic data sets is XCMS<sup>16</sup>. This package is capable of retention time alignment, peak detection and peak matching across multiple chromatograms. XCMS is used in conjunction with CAMERA, a program which is capable of identifying adduct ions and isotopic peaks in

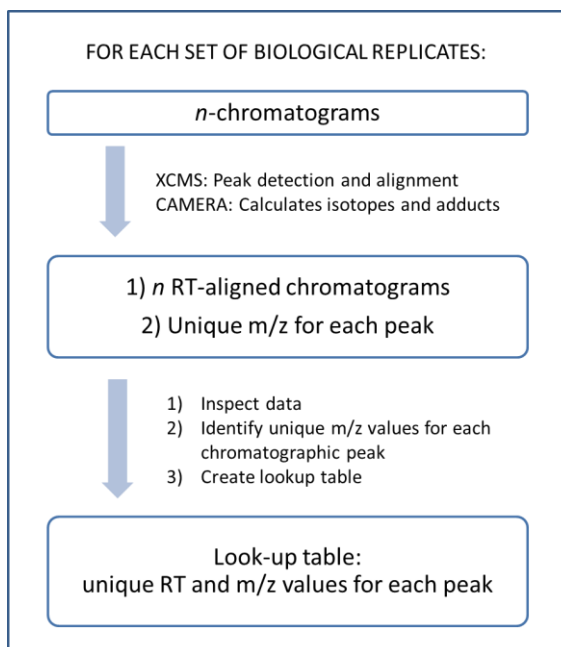
mass spectra<sup>17</sup>. Another commonly used open source software package for metabolomics analysis is mzMine<sup>18</sup>.

In order for data to be analyzed by the XCMS/CAMERA combination, the raw data file from the instrument is first converted to mzXML format, a format initially developed for the analysis of MS and MS/MS proteomics data by the Siuzdak group<sup>19</sup>. Once the files have been converted to the proper format, the chromatographic data can be deconvoluted and aligned using XCMS<sup>16</sup> and then annotated by CAMERA<sup>17</sup> to identify isotopic peaks, adduct ions and fragment ions from the peak list generated by XCMS. It is important to analyze data collected in positive ion and negative ion modes separately, as there will be no ions in common between these two file sets. As well, the solvent gradient and the LC column must be the same in all chromatograms used to collect this data.

XCMS contains four steps for pre-processing and analyzing LC-MS data. First, ion chromatograms are extracted for all ions present in the chromatographic run. From these extracted ion chromatograms, peaks are annotated and integrated to provide peak areas. Next, peaks are matched across a set of chromatographic runs and the grouping of peaks is based on mass-to-charge ratio. The greater the mass accuracy of the mass spectrometer, the greater the differentiation possible between masses of the same nominal value. From these groups, the retention time deviations are determined and chromatographic peaks are aligned to give a single mean retention time for a given

chromatographic peak. There may be peaks that are missing from some of the samples, and these can be filled in by reanalyzing the raw data files and integrating them across regions of missing peaks.

CAMERA contains four different steps for determining relationships among peaks. First, the peaks are grouped based on their retention times; secondly, the shapes of the peaks within a group are compared. Third, within these groups, isotopic peak profiles are calculated, and fourth, adduct ions and fragment ions are identified by computing hypothetical masses of adduct ions. Analyses using CAMERA is best achieved using high accuracy mass data.



**Figure 1.4:** Workflow for metabolomic data processing and data analysis.

There are some commercial software programs capable of performing similar types of data analysis for metabolic profiling. However, these programs are expensive (~\$20,000) and are specific to data sets generated on instrumentation of that vendor. Other freeware is available, such as metAlign; however, the algorithms used are not open source, and therefore cannot be scrutinized or improved upon by other research groups<sup>9</sup>.

The next step is data analysis, which is the interpretation of processed data, and includes some sort of multivariate analysis. In order to determine trends in data for large or small data sets in which the relationships between variables are unknown, an unsupervised method such as Principal Component Analysis (PCA) is used. PCA is a qualitative study of variance which leads to an understanding of what variables (loadings) and what samples (scores) are responsible for the variation observed in the data set. However, PCA does not take into account variations in the dependent variables, which can be caused by biological or instrumental variabilities<sup>6</sup>.

Supervised multivariate analysis methods, such as Orthogonal Partial Least Squares Discriminant Analysis (OPLS-DA), takes into account the variations and noise in the dependent variables and can more accurately assess which variations in the data are due to differences between sample classes<sup>20</sup>. Although OPLS-DA has the capability to separate significant variation from noise in the data, it is important to minimize experimental variation as much as possible through proper experimental design.

Variations in samples due to biological variability, sampling, sample preparation and analytical measurements should be monitored closely and minimized as much as possible<sup>15</sup>.

When metabolites have been identified as being significantly different between treated and control samples using multivariate analysis, it is necessary to identify or characterize these metabolites as best as possible. Structural characterization can be achieved by studying mass spectral fragmentation patterns using tandem mass spectrometry, while elemental composition can be obtained by determining the exact mass using high resolution mass spectrometry<sup>15</sup>. Using high resolution mass spectrometry, it is possible to narrow the number of potential elemental compositions of each ion; the higher the mass resolution, the fewer the number of elemental compositions which satisfy the mass value. In order to identify compounds, there are a number of metabolite databases available which have been organized according to different parameters, such as accurate mass values (see table 1.1)<sup>9</sup>. However, mass spectral databases do not contain retention times. Inconsistent nomenclature is also a problem.

In a paper published by the Metabolomics Standards Initiative, reporting standards were proposed for the identification of unknown metabolites<sup>21</sup>. For LC-MS analysis, a retention time and mass spectrum of a standard must be produced under identical experimental conditions on the same instrument as the initial analysis.

**Table 1.1:** MS-based databases and number of metabolites present in the databases

Database	Source	MS data available	Approximate number of records
Human metabolome database (HMDB)	Genome Alberta and Genome Canada	ESI	7900
Metlin	Scripps Research Institute	ESI	45,000
NIST mass spectral library	National Institute of Standards and Technology (NIST)	EI	163,000
Fiehn metabolite database	Agilent and LECO	EI	4000

### *Environmental Metabolomics*

Environmental metabolomics is an emerging discipline which applies the technologies of metabolomics analysis to characterize interactions of organisms with their environment<sup>22</sup>. This approach can be used to study the energetics, oxidative processes, or reproduction of an organism, or to characterize an organism's metabolic response to stressors, such as exposure to pollutant stress<sup>2</sup>. Traditional endpoints to determine toxicity are "mortality, tumour incidence, reproductive dysfunction, or behavioural effects<sup>2</sup>". However, because changes in the metabolome due to toxicity provides a very early picture of the effects of stressors, it is necessary to establish a link

between molecular responses (transcriptomics, metabolomics) and classical endpoints of survival (growth and reproduction at the population level)<sup>23</sup>.

Environmental metabolomic studies often aim to distinguish the metabolic fingerprints of the stressed organisms from that of the control, which in turn can potentially identify differences in biochemistry of the organism<sup>2</sup>, as the metabolic levels reflect the current state of the organism and can be related to the organism's phenotype<sup>22</sup>. However, it is possible that some metabolomic changes may be masked by inconsistent matrix effects, variations in extraction methods, and inadequate analytical resolution and sensitivity<sup>1</sup>. As well, it is possible that there are natural metabolomic variations within a population of organisms, which may lead to false conclusions.

There are many advantages to studying the metabolome of organisms under environmental stress. Metabolomics studies can lead to an understanding of physiological processes and whole organism responses as a result of exposure to different stressors<sup>24</sup>. This analysis can provide, for example, a metabolic picture of the mode of action of a particular toxin<sup>2,25</sup>. Due to the conservation of pathways and metabolism in many microorganisms, this strategy can also provide an understanding of toxicity in homologous systems<sup>26</sup>. Following identification of one or more biomarkers of exposure, targeted metabolomic methods can be applied as a quicker and less expensive analysis of metabolomic responses<sup>27</sup>.



Because changes in the metabolome are often observed much earlier than traditional phenotypic endpoints, such as reproductive changes<sup>25</sup>, metabolomics is a promising tool for ecotoxicology studies<sup>8</sup>. As well, different metabolic profiles often result from different dosages<sup>25</sup>. Because metabolomics studies are cheaper than genomics and transcriptomics studies<sup>28</sup>, more samples can be screened, resulting in better data quality.

#### *Current Environmental Metabolomics Studies*

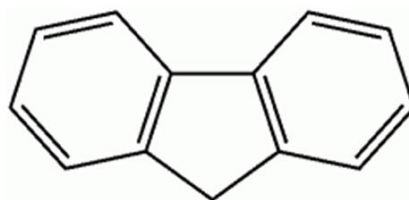
For a comprehensive list of current metabolomics studies, see Appendix 1. Most environmental metabolomics studies have been done on marine and soil organisms, with NMR being the most common method of data acquisition<sup>25,29,30</sup>. Most studies have taken an untargeted metabolomics approach to study the effects of various toxins<sup>8,31,25</sup>, either as single compounds or in binary forms. The number of metabolites observed in such studies ranges from 17 using a GC-MS method<sup>32</sup> to 4768, using FT-ICR-MS<sup>31</sup>. In most studies a larger number of metabolites were observed than could be assigned a specific chemical identity<sup>31,33</sup>. Some studies looked at both changes in the genome and the metabolome. In some cases, the transcriptomes of control and exposed organisms could not be distinguished, while the metabolomic profiles were very distinct<sup>23</sup>. In other cases, changes were observed both at the transcription level and in the metabolic profile<sup>32</sup>.

### *Polycyclic Aromatic Hydrocarbons*

Polycyclic aromatic hydrocarbons (PAH) are compounds that contain two or more fused benzene rings<sup>34</sup>, which are often formed as by-products of combustion processes. Natural sources such as volcanic eruptions and forest fires, as well anthropogenic sources, such as burning of fossil fuels, coal tar and wood contribute to the worldwide burden of PAH<sup>34</sup>. These compounds are harmful to both humans and organisms in the environment, since many PAH are mutagens, carcinogens, and/or teratogens<sup>35</sup>.

As the molecular mass of PAH increases, their solubilities in water diminish<sup>34</sup>; therefore PAH have a tendency to accumulate in soil by adsorption to humic materials<sup>35</sup>. Once present in the environment, PAH are degraded by light and by microorganisms. The physical measurements of PAH levels in soil do not provide an accurate picture of the effect of PAH and their degradation products on soil organisms. Often bioassays are used to assess toxicity, in which soil organisms, such as bacteria or earthworms, are exposed<sup>35</sup>.

For this study, the PAH fluorene was chosen as the stressor (see Figure 1.5). With a molecular mass of 166 g/mol, fluorene has a very low solubility in water (1.4 mg/L) and this value would theoretically be the maximum concentration that the organism would be exposed to in the environment.



**Molar mass:** 166.223 g/mol

**Solubility limit in water:** 1.4 mg/L

**Toxicity:** weak carcinogen

**Figure 1.5:** Fluorene, a tricyclic polycyclic aromatic hydrocarbon.

### *Mixtures*

The toxicity of mixtures is dependent both on the nature of the compounds themselves, as well as on the ratio and concentration of the compounds within the mixture. The ability of compounds within the mixture to interact with the test organism can result in additional effects<sup>36</sup>. For compounds with similar biological modes of action, it is assumed that the toxicity of the mixture can be predicted by concentration addition<sup>37</sup>, while individual compounds with dissimilar modes of action are assumed to have independent toxicity effects<sup>38</sup>.

When dealing with mixtures, three primary strategies have been developed to evaluate the toxicity of a mixture<sup>39</sup>. The integrative approach studies the mixture as a whole, while the dissective approach separates the mixture into its constituent effects

in an attempt to identify the toxic component(s) or fraction(s). The synthetic approach studies the interactions of compounds in simple mixtures with a given organism.

The most common way of assessing the toxicity of mixtures containing PAH is the synthetic approach<sup>40</sup>, where exposures to different levels of benzo[a]pyrene (BaP) have been traditionally used to predict the toxicity of the entire mixture. The toxicity of a given mixture of PAH is then expressed in BaP equivalent units. However, in a study done over a period of 18 years<sup>41</sup>, researchers concluded that despite the decrease in BaP in the environmental samples, the toxicity of a range of environmental samples remained relatively constant. In a similar study<sup>42</sup>, coal emission samples were collected and fractionated based on carbon number. Again, it was found the fraction containing BaP was not the most toxic.

Another study<sup>40</sup> evaluated different methods for predicting the toxicity of PAH. After fractionation of PAH extracted from coal tar, they found that there was no consistency as to which fraction was the most mutagenic. This may be due to interactions of PAH which lead to secondary effects in different test organisms. In another case, the three and four-membered rings were found to be the most mutagenic<sup>42</sup>.

*Environmental Studies of Mixtures*

Very few studies have been reported which study the effects of mixtures of contaminants on organisms. A synthetic approach was taken to study the combined effects of phenanthrene and cadmium on the organism *H. azteca*, a fresh water amphipod<sup>38</sup>. Compounds with different modes of action are assumed to be independent in their effects, as shown in earlier studies of *L. variegates* exposed to anthracene, fluoranthene, and pyrene<sup>43</sup>. However, this study found that sub-lethal concentrations of phenanthrene in the presence of cadmium caused an increase in mortality. Therefore, it is likely that joint toxicity between dissimilarly acting compounds can occur.

A study conducted in 2001<sup>44</sup> showed the effect of three PAH (phenanthrene, fluoranthene, and benzo[k]fluoranthene) on three freshwater organisms: *D. magna*, *H. azteca*, and *C. riparius*. Using a synthetic approach, a synergistic effect was seen, although the toxicity of these compounds was expected to be additive. They concluded that the principle of additivity, which is used to predict the toxicity of PAH, is inadequate in assessing environmental risk.

A very recent study<sup>23</sup> looked at changes in both the transcription and the metabolome of *D. magna* in response to exposures of pyrene and fluoranthene. Again, the results showed that the PAH mixture responses were more than additive. The transcriptomes of pyrene and fluoranthene could not be distinguished from each other,

while there were statistical significant differences in the metabolome profiles. It was concluded that the response of the mixture can be similar or different from the response of the single compound, based on the concentrations of the compounds in the mixture.

To truly assess the toxicity of a mixture, its effects must be studied as a whole<sup>41</sup>. This approach also gives a better picture of how organisms respond to complex mixtures in their environments, as they are rarely exposed to one toxin at time<sup>36</sup>.

#### *Sinorhizobium meliloti*, a Soil Microorganism

*Sinorhizobium meliloti* is a soil microorganism of the family Rhizobiaceae which forms a close metabolic association with leguminous plants such as alfalfa (*Medicago sativa*)<sup>45</sup>. Since the amount of available nitrogen in soils limits plant growth, the reduction of dinitrogen ( $N_2$ ) to ammonia ( $NH_3$ ) by *S. meliloti* allows the symbiotic plant to obtain nitrogen compounds necessary for metabolism<sup>46</sup>. In the agricultural industry, legumes which associate with *S. meliloti* do not require the addition of costly nitrogen-containing fertilizers to the soil<sup>47</sup>.

#### *Metabolism in S. meliloti*

*S. meliloti* is able to grow on several carbon sources, such as succinate, mannitol, glucose, sucrose, and maltose<sup>48</sup>. In presence of glucose, the organism uses the Entner –

Dourdoroff (ED) pathway, but not in the presence of succinate. As well, *S. meliloti* possesses the TCA cycle pathway (see Figure 1.6)<sup>48</sup>.

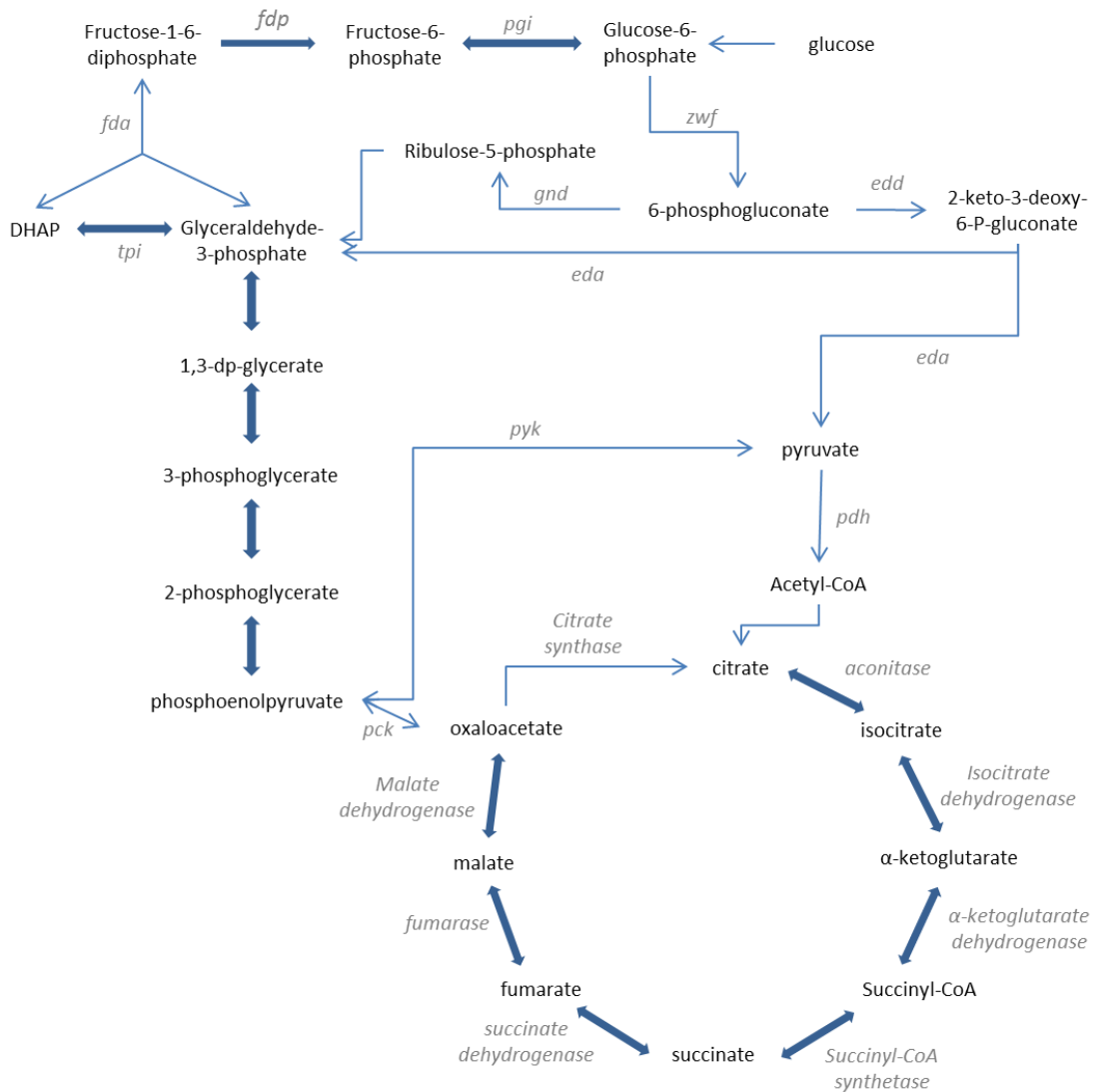
To date, several metabolomics studies have been conducted with *S. meliloti*. Initial research in 2003<sup>49</sup> used <sup>13</sup>C-NMR to study the metabolic carbon cycles by tracking <sup>13</sup>C-labeled glucose. They were able to determine the nature and diversity of the cycles by identifying polymers produced by intracellular metabolism, showing a much more complex biosynthetic route than had been previously understood.

In 2004, a study was published<sup>50</sup> (using strains *S. meliloti* 1021 and 2011, as well as *S. meliloti* *leuB::Tn5*, a leucine auxotrophic mutant), which focused on the methods of harvesting and extracting cellular metabolites, and the effect of the method on the metabolome. After a suitable method was developed, the metabolomic profiles of *S. meliloti* grown on different carbon sources using derivatization GC-MS were compared. Of the 200 peaks in the chromatogram, 65 were positively identified using standards. The samples grown on different carbon sources were distinguishable, and the identified metabolites were related to known metabolic pathways. The leucine auxotrophic mutant could not produce the enzyme 3-isopropylmalate dehydrogenase, and this mutation caused the accumulation of certain metabolites.

A study published in 2008<sup>51</sup> compared the comprehensive metabolomes of the strain sp. C4 grown on phenanthrene as a carbon source with samples grown on natural

carbon sources. The analysis by derivatization GC-MS observed 207 metabolites, 118 of which were identified using standards or mass spectral library hits. A large difference was seen between the metabolomes of cultures grown on phenanthrene compared to other carbon sources. The differences included metabolites involved in the TCA cycle, pyruvate metabolism, cofactor biosynthesis and fatty acid compositions.





**Figure 1.6:** TCA cycle and relate pathways<sup>52</sup>.

Abbreviations: DHAP (dihydroxyacetone phosphate), *dme* (diphosphopyridine-dependent malic enzyme), *eda* (2-keto-deoxy-6-phosphogluconate aldolase), *edd* (6-phosphogluconate dehydratase), *eno* (enolase), *fda* (fructose-1-6-P2 adolase), *fdp* (fructose-1-6-P2-phosphotase), *gap* (glyceraldehyde-3-phosphate dehydrogenase), *gnd* (6-phosphogluconate dehydrogenase), *pck* (phosphoenolpyruvate carboxykinase), *pdh* (pyruvate dehydrogenase), *pgi* (phosphoglucose isomerase), *pgk* (3-phosphoglycerate kinase), *pgm* (phosphoglycerate mutase), *pyk* (pyruvate kinase), *tme* (triphosphopyridine-dependent malic enzyme), *tpi* (triose phosphate isomerase), *zwf* (glucose-6-phosphate-1-dehydrogenase)

### *Project Goals*

The overarching goal of this thesis is to demonstrate whether *Sinorhizobium meliloti* can be useful as a sentinel soil microorganism for assessing the impacts of contaminant stressors on the metabolome of a microorganism. Not only is a good deal known about this organism, but it is an important organism in agriculture. Moreover, there is a gene array available and a large library of gene fusion so that there are facile pathways to explore genetic and genomic impacts in addition to metabolomic impacts of contaminants, should such studies be deemed worthwhile.

The specific goals of this thesis can be summarized as follows.

- 1) Previous work done in our research group has shown that HILIC methods are effective chromatographic approaches in the separation of polar metabolites in blood serum. This study will evaluate and optimize the HILIC chromatographic separation methods as applied for the analysis of the *S. meliloti* polar metabolome.
- 2) Since untargeted metabolomics studies produce large data sets, this project aims to evaluate and explore open source software packages such as XCMS and CAMERA as to their suitability to process *S. meliloti* metabolomic data sets.
- 3) To date, no study has examined the effect of PAH mixtures on the metabolome of *S. meliloti*. This study will evaluate the effects of both a single compound,

fluorene, and a complex mixture of low molecular mass PAH, on the non-polar and polar metabolome of *S. meliloti*.

- 4) No previous studies have simultaneously examined changes in both polar and non-polar metabolites. A method previously developed for the analysis of lipids in *S. meliloti*<sup>53</sup> will be applied to the analysis of lipids extracted from cultures exposed to fluorene and the PAH fraction prepared from coal tar.
- 5) This study will evaluate the effectiveness of unsupervised and supervised multivariate analysis methods (PCA and OPLS-DA), respectively, on metabolomic data to reveal relationships between the metabolisms of *S. meliloti* cultures exposed to PAH compounds at different exposure levels.
- 6) Metabolites identified as significant using multivariate analysis will be identified using high resolution mass spectrometry and tandem mass spectrometry techniques.
- 7) Following the identification of significant metabolites, this study will relate these metabolites to known biological pathways in *S. meliloti*, in order to understand the biological significance of these exposures to different PAH mixtures.

## Chapter Two: Materials and Methods

### *Solvents and Chemicals*

All solvents used (HPLC grade H<sub>2</sub>O, methanol and chloroform) for extractions and LCMS analysis were purchased from Caledon Laboratory Chemicals (Georgetown, ON). Standards L-methionine-d<sub>3</sub> (98%), L-tryptophan-d<sub>5</sub> (98%), L-phenylalanine-d<sub>8</sub> (98%), and the dipeptides glycine-phenylalanine (gly-phe), and phenylalanine-phenylalanine (phe-phe) were purchased from Cambridge Isotope Laboratories (Andover, MA). The coal tar sample was kindly provided by a local steel company and was fractionated by Fan Fei. The concentrations of PAH and PAH derivatives present in the coal tar fraction were determined by Fan via GC-MS analysis. The concentrations of PAH in a low molecular mass PAH fraction prepared from coal tar is shown in Table 2.1.

### *Bacterial Strains*

Frozen stocks of strains of *Sinorhizobium meliloti* RmP100 (wild type) were prepared by adding 600 µL of dense overnight culture to 600 µL of Luria broth (LB) containing 14% dimethylsulfoxide (DMSO). Cultures were stored at -80°C in glass vials<sup>52</sup>.

**Table 2.1:** Concentrations of individual PAH and PAH derivatives from coal tar fraction in growth media.

	1.4 mg/L concentration	0.14 mg/L concentration
<b>[PAH] mg/L</b>		
phenanthrene	6.05E-01	6.05E-02
biphenyl	2.60E-01	2.60E-02
fluorene	2.26E-01	2.26E-02
acenaphthylene	1.31E-01	1.31E-02
pyrene	5.47E-02	5.47E-03
acenaphthene	4.18E-02	4.18E-03
naphthalene	3.74E-02	3.74E-03
anthracene	3.07E-02	3.07E-03
fluoranthene	1.34E-02	1.34E-03
<b>PAH total</b>	<b>1.40E+00</b>	<b>1.40E-01</b>
<b>[PAH derivatives] mg/L</b>		
Me-PAH	8.84E-02	8.84E-03
PASH	3.57E-02	3.57E-03
NPAH	5.22E-03	5.22E-04

*Media Preparation, Growth Conditions and Growth Curves*

The Luria rich broth (LB, containing 10 g/L Difco Bacto Tryptone, 5 g/L Difco Yeast Extract and 5 g/L NaCl) was used as rich media source for *S. meliloti*. The pH of the broth was adjusted to 7.0 using 1N NaOH and the media autoclaved. After sterilization, a stock solution of 100 mL of LB broth was supplemented with 250  $\mu$ L of 1 M  $MgSO_4$  and 500  $\mu$ L of 0.5 M  $CaCl_2$  added to give final concentrations of 2.5 mM of both  $MgSO_4$  and  $CaCl_2$  ( $LB_{mc}$ )<sup>52</sup>.

The minimal growth medium for *S. meliloti* was prepared by adding 500  $\mu\text{L}$  of  $\text{MgSO}_4$  (1 M), 250  $\mu\text{L}$  of  $\text{CaCl}_2$  (0.5 M), 50  $\mu\text{L}$  of D-biotin (10 mg/mL), 5  $\mu\text{L}$  of  $\text{CoCl}_2$  (1 mg/mL), 5.00 mL of glucose (1.5 M), and 100.00 mL of 5x Difco M9-salts to a 500 mL volumetric flask and making up to volume using autoclaved distilled water. A solution of 1.5 M glucose was sterilized prior to addition using a 0.45  $\mu\text{m}$  Supor membrane filter (Acrodisc). A solution of 5x Difco M9-salts (33.9 g/L  $\text{NaHPO}_4$ , 15 g/L  $\text{NaH}_2\text{PO}_4$ , 2.5 g/L  $\text{NaCl}$  and 5 g/L  $\text{NH}_4\text{Cl}$ ) was prepared and autoclaved separately. The final minimal growth medium contained  $\text{MgSO}_4$  (1 mM),  $\text{CaCl}_2$  (0.25 mM), D-biotin (1  $\mu\text{g}/\text{mL}$ ),  $\text{CoCl}_2$  (0.01  $\mu\text{g}/\text{mL}$ ), glucose (15 mM) and 5x Difco M9-salts (20% v/v)<sup>52</sup>.

### *Antibiotics*

Streptomycin (SM) was purchased from Sigma and a stock solution of 200 mg/mL was prepared in  $\text{H}_2\text{O}$ . The agar plates were prepared with a final concentration of 200  $\mu\text{g}/\text{mL}$  SM. Approximately 25 mL of agar is required for one plate, therefore 25  $\mu\text{L}$  of the stock solution was added to each plate. LB was prepared to a concentration of 100  $\mu\text{g}/\text{mL}$  SM by adding 50  $\mu\text{L}$  of the 200 mg/mL stock to 100 mL of  $\text{LB}_{\text{MC}}$ <sup>52</sup>.

### *Growth conditions for Growth Curves and Metabolite Analysis*

Rich  $\text{LB}_{\text{mc}}$  (2 mL, containing SM) was inoculated with three to five colonies from an agar plate less than 10 days old and grown overnight. The cultures were centrifuged and washed once with 1000  $\mu\text{L}$  of 0.85%  $\text{NaCl}$  to prepare a stock culture. The optical

density ( $OD_{600}$ ) of the resuspended culture was measured by diluting the solution 100 fold and determining the  $OD_{600}$  using a Eppendorf Biophotometer (the  $OD_{600}$  of the stock culture was typically between 5 and 10)<sup>52</sup>.

The minimal media containing 0.14 or 1.40 mg/L of fluorene or two concentrations of PAH coal tar fraction (see Table 2.1 for concentrations) was prepared by adding 50  $\mu$ L of methanolic solutions of 14.0 or 140.0 mg/L solutions to 5.00 mL of minimal media to achieve a final concentration of 1% MeOH (v/v). Before inoculation, the minimal media containing the fluorene or PAH fraction was allowed to equilibrate to 30°C (the ideal growth temperature of *S. meliloti*). From the bacterial stock solution, an aliquot (approximately 20  $\mu$ L) was taken and added to the media containing either fluorene or the coal tar fraction in order to achieve an initial  $OD_{600}$  0.05. The 5 mL cultures (grown in pentuplicate) were incubated at 30°C with shaking (200 rpm) and grown to a final  $OD_{600}$  of approximately 0.75. For growth curve experiments,  $OD_{600}$  readings were taken every four hours using a Bausch and Lomb Spectronic 20 spectrophotometer.

#### *Extraction of Intracellular Metabolites*

Once the growth of the 5 mL cultures reached an  $OD_{600}$  of over 0.5, the cultures were individually centrifuged at 4400 rpm at 4°C in a Beckman Coulter Allegra X-22R Centrifuge and the supernatant discarded. The pellet was resuspended in 250  $\mu$ L 1:1

MeOH:H<sub>2</sub>O (v/v) followed by an addition of 250  $\mu$ L CHCl<sub>3</sub>. The recovery standards of L-methionine-d<sub>3</sub> (10  $\mu$ L, 4.28 mM), and L-tryptophan-d<sub>5</sub> (10  $\mu$ L, 2.10 mM) were added using a syringe. The samples were vortexed for 3 minutes and centrifuged at 4°C for 1 min at 13000 rpm in an Eppendorf Refrigerated Microcentrifuge Model 5415 R. The CHCl<sub>3</sub> layer was washed twice with 250  $\mu$ L 1:1 MeOH:H<sub>2</sub>O. The combined polar extracts were extracted with 250  $\mu$ L of CHCl<sub>3</sub>. The internal standards, of L-phenylalanine-d<sub>8</sub> (10  $\mu$ L, 0.67 mM), gly-phe (10  $\mu$ L of 1.16 mM), and phe-phe (10  $\mu$ L, 0.58 mM) were added to the combined MeOH:H<sub>2</sub>O layers (750  $\mu$ L) using a syringe.

#### *LC-MS Sample Analysis*

Metabolite analyses were conducted using an Agilent Technologies Model 1200 RR Series II liquid chromatogram coupled to a Bruker MicrOTOF II Mass Detector outfitted with an electrospray ionization (ESI) source, and run in both positive ion and negative ion modes. The parameters for the ESI were as follows: endplate offset, -500 V, capillary 3800 V, nebulizer, 2.0 bar, drying gas, 6.0 L/min, drying temperature, 180 °C, capillary exit voltage, 80.0 V, skimmer 1 voltage, 50.0 V, hexapole 1 voltage, 23.0 V, hexapole RF, 80.0 Vpp, and skimmer 2 voltage, 23.0 V. Full scan mass spectra were collected over the mass-to-charge (m/z) range 50 to 1000 Da, at a scan rate of 1.0 Hz (computed using a rolling average value of 2).



A ZIC HILIC Sulfonylbetaine column (50 x 2.1 mm, 3.5  $\mu\text{m}$  particles, pore size 100 Å, SeQuant, Umeå, Sweden), was used for all HILIC LC analyses. Mobile phases, delivered at 400  $\mu\text{L}/\text{min}$ , were (A) acetonitrile and (B) 5 mM ammonium acetate, pH 3. The column temperature was maintained at 25°C using a thermostated column oven. A gradient elution program was used which started at 95% solvent A and 5% solvent B, decreased to 90% solvent A, 10% B at 3 min, then to 25% A and 75% B at 13 min. This latter solvent composition was maintained for 3 min, before the system was returned to 95% A and 5% B over 1 min. The system was allowed to re-equilibrate for 5 min prior to the next injection. An injection volume of 2  $\mu\text{L}$  was used. The auto sampler and sample storage tray were held at 4°C.

#### *Instrumental Quality Assurance/Quality Control*

Prior to the analysis of any set of samples, a pooled sample was run in triplicate in both positive ion and negative ion modes. The retention times of the peaks were examined carefully for consistency in order to ensure that the instrument had stabilized and were performing well before the samples were analyzed. Once the instrument was judged to be in good working order, samples were run in random order, with the inclusion of several blank samples. A pooled sample was run after every sixth sample.

The MS was calibrated using a Bruker ESI-L low concentration tuning mix acquired from Agilent Technologies. This tuning mix was used to calibrate both positive

ion and negative ion modes. In order to ensure that no compounds remained on the column before a series of analyses, a blank run was performed and checked carefully.

Standards, L-methionine-d<sub>3</sub> (56 µM), L-tryptophan-d<sub>5</sub> (28 µM), L-phenylalanine-d<sub>8</sub> (9 µM), gly-phe (15 µM), and phe-phe (8 µM), were run to ensure that the column was performing well chromatographically and the MS system was producing adequate response.

#### *Metabolite Data Analysis*

Raw data files generated by the LC-ESI-MS Bruker MicroTOF instrument were converted to mzXML file format using the Bruker Compassxport program available from the Bruker website. The converted files were then analyzed using the XCMS/CAMERA packages (run in the R Project for Statistical Computing)<sup>54</sup>. See Appendix 2 for the XCMS/CAMERA script used to process these data. The XCMS and CAMERA software packages were downloaded from Bioconductor website (<http://www.bioconductor.org/>). The XCMS package deconvolutes and aligns the data and produces retention times (RT) and accurate mass-to-charge values (m/z) for all ions present in the chromatographic run, and reports peak areas of all masses detected. The CAMERA package calculates isotopic peaks present as well as identifying any adduct ions or fragment ions that have been formed via ESI. The R script produces a comma-separated values (CSV) file which can be imported to Microsoft Excel for further

manipulation and analysis. The CSV data files were then saved as a Microsoft XML formatted spreadsheets (XLSX).

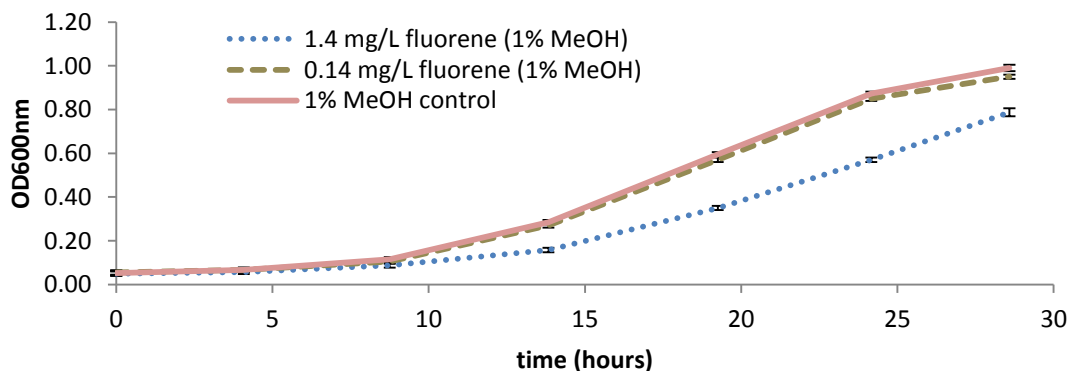
In Excel, apparent  $k'$  values of peaks ( $k' = \frac{(t_x - t_o)}{t_o}$ ) was calculated for all ions in the spreadsheet list. The resulting list was filtered by removing ions with apparent  $k' < 0.7$  and  $k' > 30$ . Ions with identical retention times were likely ions that were part of the mass spectrum of a given component. Careful inspection of the data set was required in order to identify the single ion that would be used for quantification of that peak. In other words, from each set of ions produced from one molecule (due to isotopic, adduct and fragment ions), one ion was chosen for quantification of that species. All other ions were discarded from the ion list. For metabolites at that retention time that appear in both ionization modes, the ion with the higher abundance was quantified. For each set of biological replicates, a lookup table was created which listed the retention time and the  $m/z$  value for a given peak. If there was ambiguity in the relationship of two ions, both were ions were left in the list. This sequence of steps was performed for each set of samples, i.e., control samples and treated samples in both positive ion and negative ion MS modes. The data from each set of samples in positive ion and negative ion modes were combined for statistical analysis. For species which appeared in both modes, the more responsive ion was chosen.

The peak areas of each ion in the lookup table were normalized based on OD<sub>600</sub> values of each culture prior to work up and extraction. Next the peak areas were normalized using the peak area of the internal standards. These data were analyzed using multivariate analysis (PCA and OPLS-DA) using the program SIMCA-P (Umetrics, Umeå, Sweden). Pareto scaling was used. Shared and unshared structure (SUS) plots were also generated using SIMCA-P. Metabolites which showed statistically significant changes were highlighted for identification and were tentatively identified according to accurate mass values of components listed in the Human Metabolome Database (HMDB) ([www.hmdb.ca](http://www.hmdb.ca)) or identified with authentic chemical standards.

### Chapter 3: Results and Discussion

#### Bacterial growth

Studies have shown that a change in the metabolism of an organism in response to stress is not always evident in the phenotype. If the response of an organism to stress results in a change of growth, there are also likely to be changes in the metabolome. In order to assess the effects of the PAH fluorene on *S. meliloti*, the growth of the bacterium in the presence of two concentrations of fluorene was investigated. Figure 3.1 shows the growth curves of *S. meliloti* in the presence of fluorene (in 1% MeOH) at concentrations near the solubility limit (1.4 mg/L) and at a dosage 10-fold lower (0.14 mg/L) in M9 minimal media containing glucose. Bacterial growth was affected by the 1.4 mg/L exposure, but not at 0.14 mg/L fluorene. From these data, it was expected that exposure of *S. meliloti* to fluorene 1.4 mg/L would produce a measureable change in the metabolome compared to the control.



**Figure 3.1:** Growth of *S. meliloti* in the presence of fluorene (1.4 and 0.14 mg/L) at 1% MeOH. Error bars indicate standard deviations (n=3).

*Extraction of intracellular metabolites*

In a previous study in the Finan lab, a bead beating extraction was used<sup>52</sup>. The cell pellet (collected from 5 mL of culture with an OD<sub>600</sub> of approximately 0.7), was treated with 800 µL of 1:1:1 ACN:H<sub>2</sub>O:MeOH<sup>55</sup> and the cells lysed by vortexing for 10 min with two ball bearings (3 mm in diameter). This extraction procedure was used initially in this work. LC-MS analysis showed that there were many non-polar metabolites (i.e., lipids) were present in the extracts and these lipids caused a number of interferences with the analysis of other metabolites.

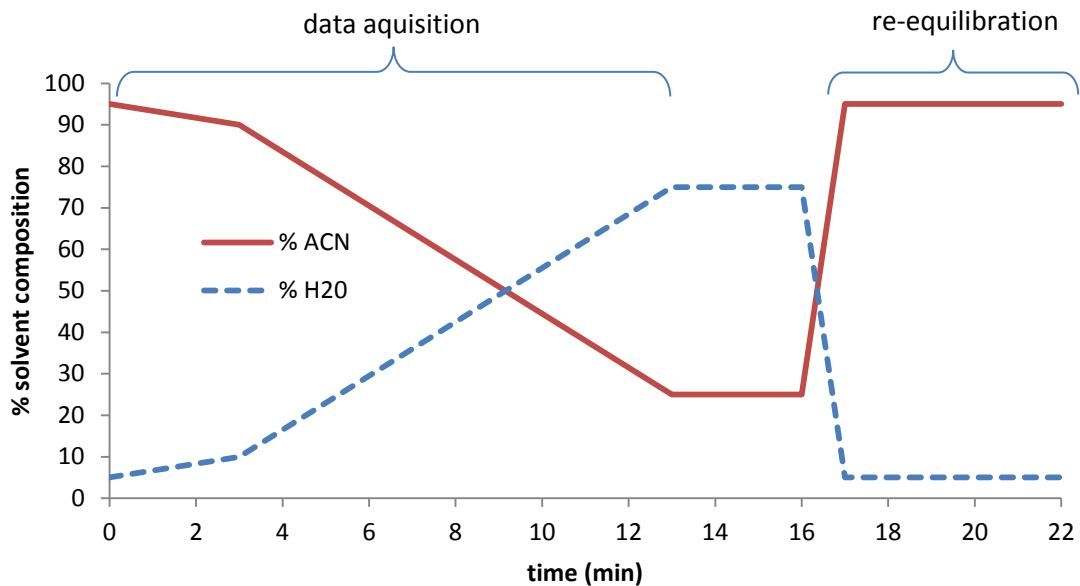
It was decided to try a Bligh and Dyer (B&D) extraction method as had been used in previous shotgun lipidomics analysis<sup>53</sup>. When the B&D extraction was performed on the bacterial cultures, the polar fractions did not contain the lipids. The B&D extraction method separates the polar and non-polar metabolites into two fractions; it was decided to analyse the polar fraction of *S. meliloti* by HILIC-LC-ESI-MS and analyse the non-polar fractions containing lipids using a previously developed 'shotgun' lipidomics approach<sup>53</sup>.

*HILIC-LC-ESI-MS analysis*

Based on research performed by another member of our group (K. Chalcraft), it has been shown that coupling two different LC columns in tandem was useful for analyzing complex samples, such as bacterial extracts containing polar metabolites and blood serum. In this set-up, a HILIC LC column, capable of separating polar compounds, was used as the first column and a reverse phase column as the second column. Optimally, non-polar compounds that would not be retained on the first column, would be retained and separated on the second reversed phase column. This column configuration achieves excellent separation of a wide range of metabolites.

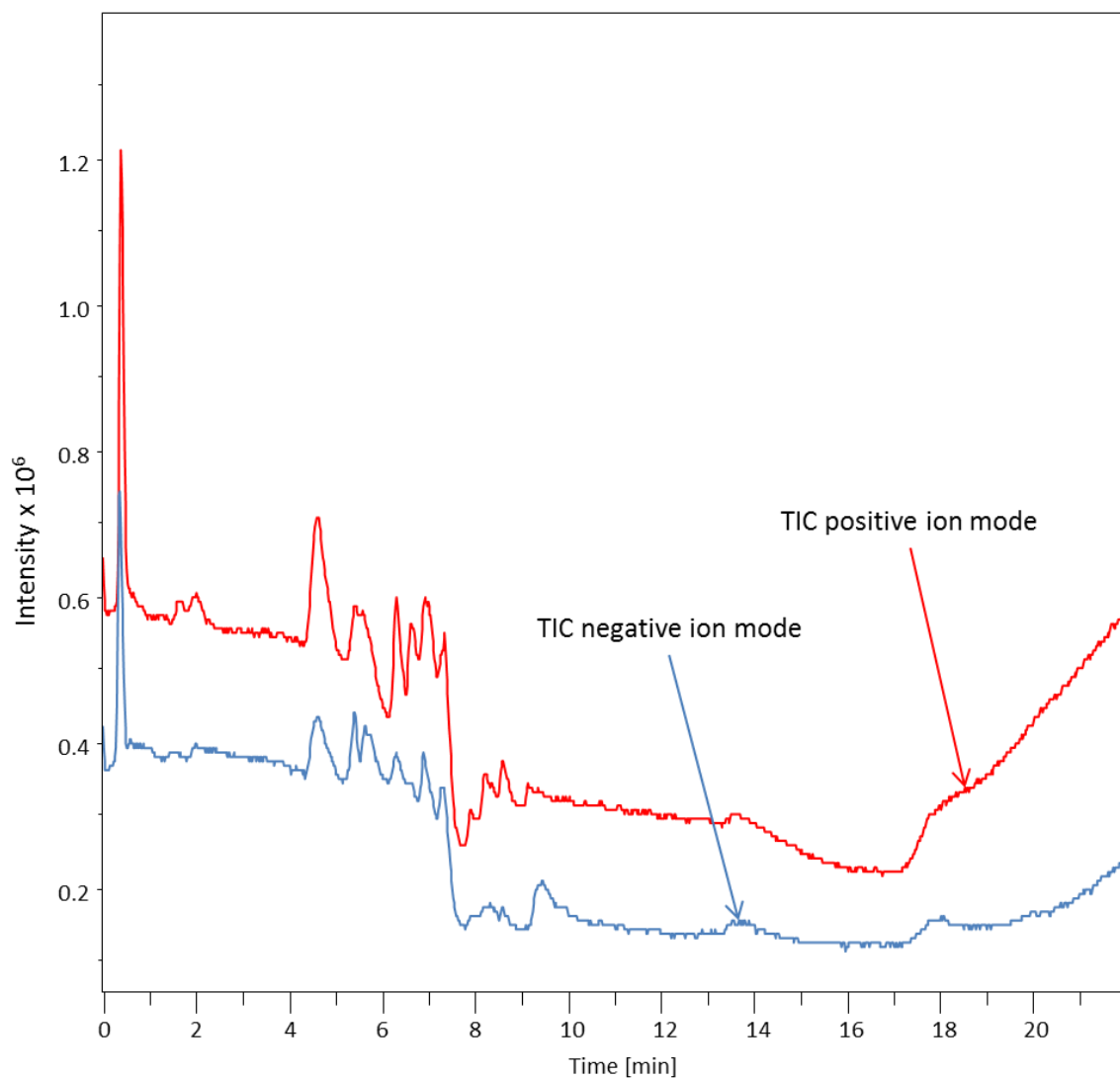
With the implementation of the Bligh and Dyer extraction, the tandem column setup was no longer necessary. It was decided to separate the polar metabolites using only the zic-HILIC column and the LC gradient was re-optimized. It was found that going from 95% ACN down to 25% ACN was necessary to remove all of the components from the column prior to a subsequent analysis (see Figure 3.2). A shallower gradient was used over the first three minutes to optimize the separation of early eluting compounds. The run time of the method including column equilibration was 22 minutes with data acquired for only 14 minutes. Chromatographic reproducibilities over many sequential runs was extremely good so it was concluded that the five minute column re-equilibration time (about 10 column volumes) was adequate.

Example total ion current chromatograms (plots of the total ion current signal over time) of *S. meliloti* RmP110 control samples analysed in negative ion and positive ion modes can be found in Figure 3.3. The peak at 0.4 minutes represents  $t_0$ . Extracted ion chromatograms in the negative ion mode (Figure 3.4) and the positive ion mode (Figure 3.5) show good peak shapes at both high and low peak intensities across a wide range of retention times.

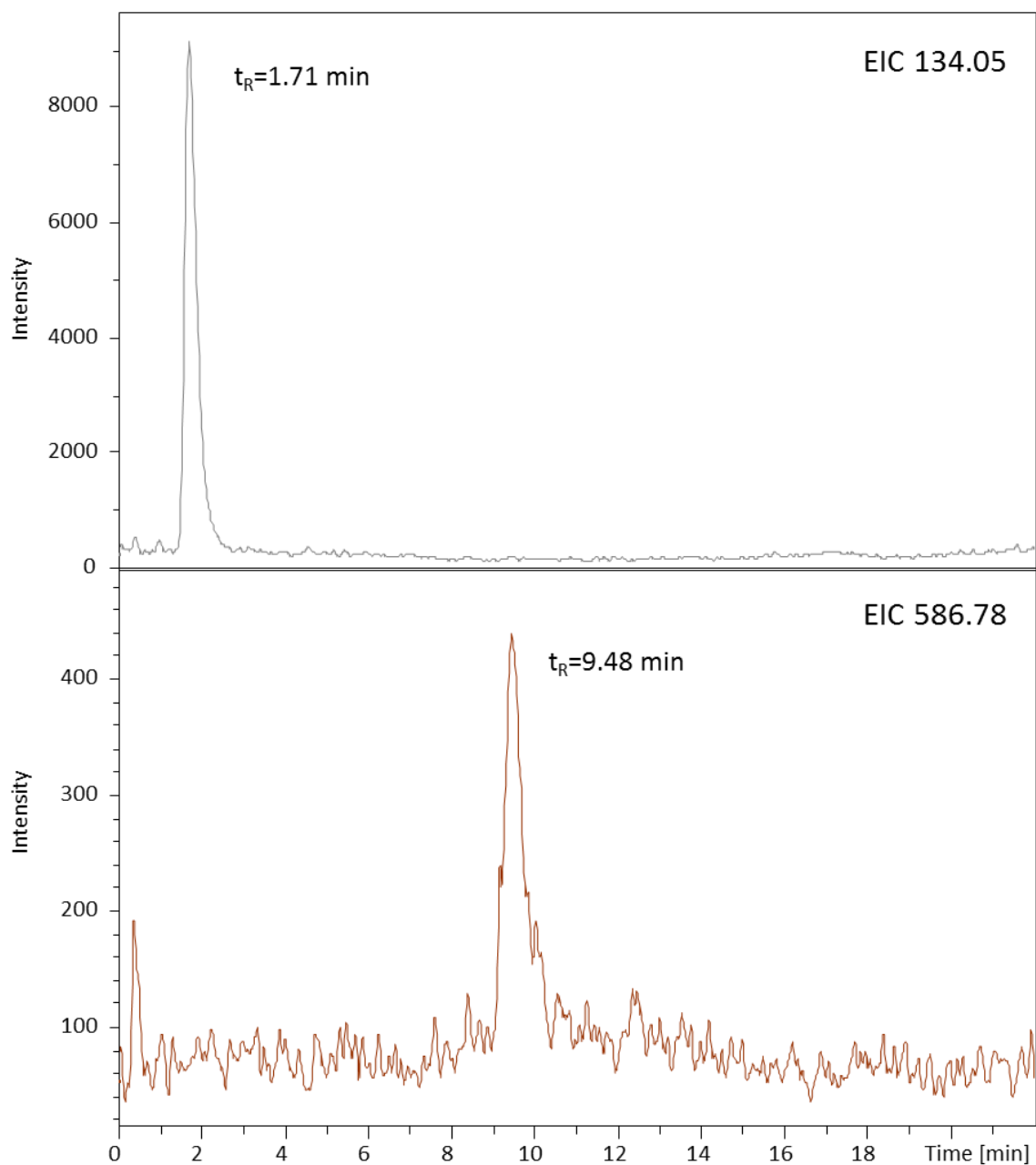


**Figure 3.2:** HILIC LC gradient used for analysis of polar metabolome of *S. meliloti*. The total run time is 22 minutes.

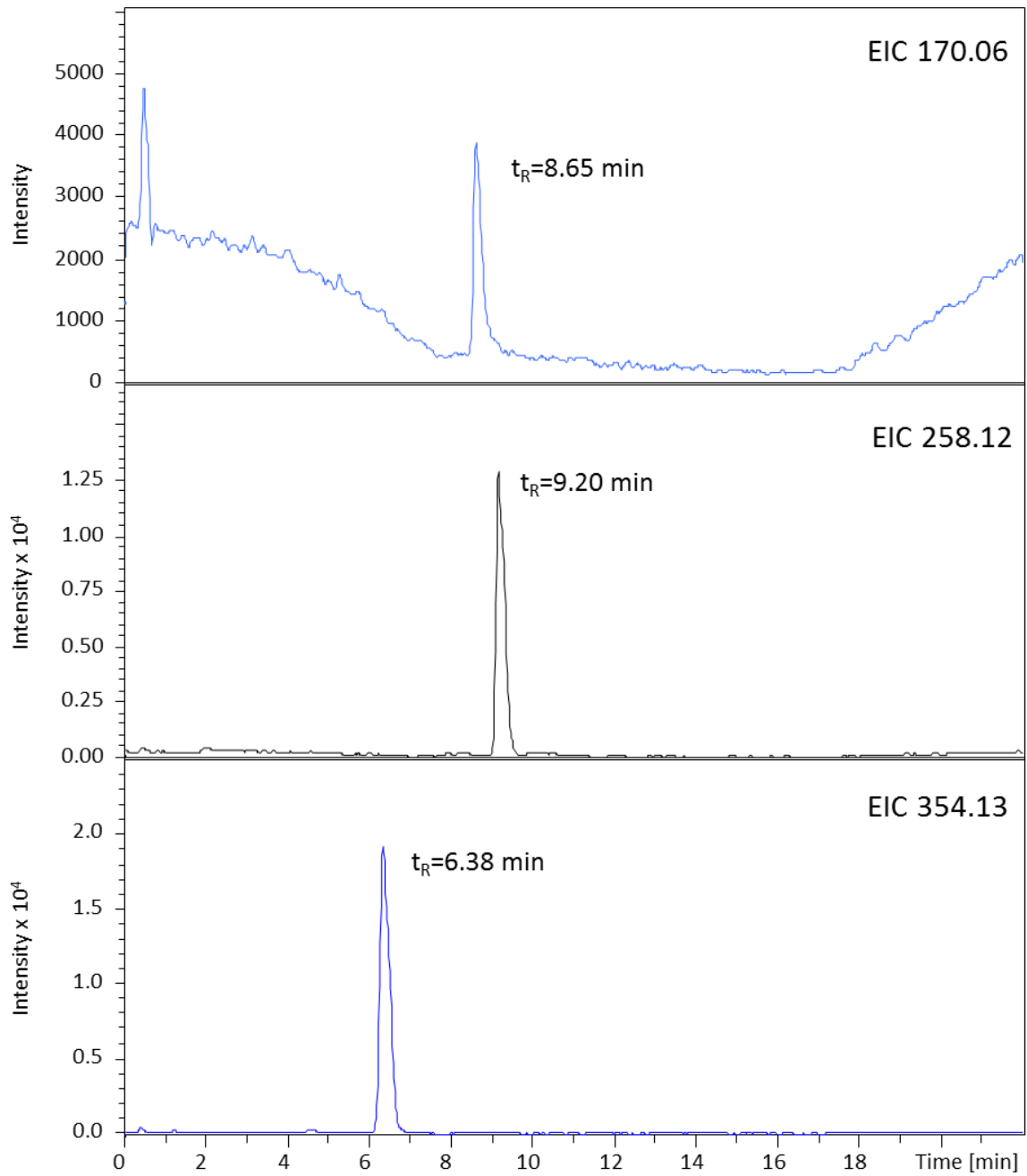




**Figure 3.3:** Total ion current chromatogram (TIC) from HILIC-LC-ESI-MS analysis of *S. meliloti* wild type run in negative ion and positive ion modes.



**Figure 3.4:** Extracted ion chromatograms (EIC) from a HILIC-LC-ESI-MS analysis of *S. meliloti* wild type run in the negative ion mode.



**Figure 3.5:** Extracted ion chromatograms (EIC) from a HILIC-LC-ESI-MS analysis of *S. meliloti* wild type run in the positive ion mode.

*Processing Raw Data Using XCMS/CAMERA*

LC-MS metabolomic analyses generate large data sets. For example, in a typical chromatogram of a polar extract of *S. meliloti* analysed using HILIC-ESI-LS-MS, over 1500 masses are observed, associated with over 300 chemical species. These mass spectra contain molecular ions  $[M+H]^+$  or  $[M-H]^-$  ions, together with various adduct ions (e.g.,  $[N+Na]^+$ ,  $[M+NH_4]^+$ ,  $[M-Cl]^-$ , etc.) and their associated isotopic masses.

Because these ions are formed in the ESI source, all ions related to a single chemical species will have identical chromatographic retention times. By using medium to high resolution mass analyzers, the accurate mass values, together with reproducible retention time data allows the unambiguous identification of the relationships between these ions and ultimately the identification of the molecular formulae.

The problem facing the researcher doing metabolomics analysis is how to tackle these large and complex mass spectral data sets so as to identify individual chemical constituents in the chromatogram and ultimately identify the chemical substances in the sample.

The first problem has been solved through the development of sophisticated software packages, which can align many chromatograms and associate the mass spectral features with those aligned chromatographic peaks.

The software packages XCMS and CAMERA are capable of mass spectral peak detection and chromatogram alignment, as well as assisting in identifying any adducts ions and isotopic ions which are present. Table 3.1 shows an example of the raw data output for selected ions in the  $m/z$  242-249 mass range in the negative ion mode following the analysis of five biological replicates of *S. melliloti*. The output in Table 3.1 provides the mean  $m/z$  value of each mass spectral peak (A) and mean retention time of the chromatographic feature (C, in seconds) as well as the range of  $m/z$  values (B) and the range of retention times (D, in seconds) of ions across all samples. The range of retention times and mass values results from variations in the instrumentation.

In Table 3.1, the column labeled 'npeaks' (E) is the number of peaks detected in all samples with peak area counts over 4000. In this example, only one sample class, 'control' is shown. The column 'control' (F) indicates the total number of peaks detected in all samples in the class 'control' with peak area counts over 4000. Because only one class of samples was analysed, 'npeaks' is equal to 'control'.

It is possible to compare two or more samples classes at a time, for example, control and treated samples. However, it was found that when more than one sample class was examined using XCMS/CAMERA, only peaks which were found in all sample classes were reported in the ion list. If an ion was not observed in the treated samples, for example, but was observed in the control samples, it was not included in the list. Previous metabolomics studies have shown that exposures of organisms to stress result

in the production of new, previously undetected metabolites and the disappearance of other peaks from the chromatogram. In order to accurately assess how the metabolome of *S. meliloti* changed in response to the presence of fluorene or the PAH fraction, it was decided to analyse one sample class at a time.

**Table 3.1:** Example of XCMS/CAMERA raw data output (*S. meliloti* control, 5 biological replicates, negative ion mode) together with explanations.

Peak areas														
mean m/z	mzmin	mzmax	mean rt	rtmin	rtmax	npeaks	control	sample 1	sample 2	sample 3	sample 4	sample 5	isotopes	adduct
242.18	242.18	242.19	28.03	27.98	28.22	6	6	30777	14555	15429	30910	20783	[92][M] <sup>+</sup>	
243.07	243.07	243.07	148.69	147.85	149.32	6	6	60416	94272	87335	147282	91683	[89][M] <sup>+</sup>	[M-H] <sup>-</sup> -244.077
243.09	243.09	243.09	61.37	61.13	62.15	5	5	12994	13897	21039	32273	22126		
243.18	243.18	243.19	28.03	26.98	28.22	6	6	4957	3304	2880	5652	4432	[92][M+1] <sup>+</sup>	
243.90	243.89	243.91	74.48	74.34	74.53	6	6	15668	21439	9254	12730	12558		
244.07	244.07	244.07	148.95	148.58	149.32	6	6	7749	12322	11232	17633	11898	[89][M+1] <sup>+</sup>	
244.10	244.10	244.10	400.75	399.78	401.08	6	6	17760	32065	23081	28352	39105	[63][M] <sup>+</sup>	[M+Cl] <sup>-</sup> -209.128
245.05	245.05	245.06	487.53	484.09	487.88	4	4	1300	9175	3226	7736	7717		
245.10	245.10	245.10	400.48	399.78	400.97	6	6	3548	5338	3761	4849	5862	[63][M+1] <sup>+</sup>	
245.91	245.90	245.91	74.49	73.48	75.32	6	6	7528	9956	3894	5384	6155		
246.09	246.09	246.09	399.74	399.07	399.99	6	6	7832	13461	8789	11282	13858	[63][M+2] <sup>+</sup>	
246.99	246.99	246.99	333.47	332.87	333.97	6	6	13971	15003	18076	25579	19635		
247.92	247.92	247.93	74.49	73.42	75.32	4	4	4059	4596	5639	2138	2999		

The XCMS package computes the peak areas of each ion in each sample (G). As well, the CAMERA package computes the isotopic ion values based on accurate mass data. The column labeled 'isotopes' lists information in the format [x] [M+y]<sup>+</sup> (Table 3.1, H), where [x] is solely a numbering system for relating isotopic peaks which belong to the same species (Table 3.1, H). The notation [M]<sup>+</sup> refers to the molecular ion, while [M+1]<sup>+</sup> refers to the A+1 isotopic peak (Table 3.1, I). The '+' notation has no relation to the ionization mode in which the sample was run.

The CAMERA package also computes values for potential adduct ions and fragment ions based on retention time windows and accurate mass data. In Table 3.1, the column labeled 'adduct' suggests relationships between ions. The first item in the column (J) suggests the type of adduct, while the number indicates the mass of the neutral species from which the adduct was formed (K).

The task for the researcher is to sift through all of the 1000-1500 ions using their associated retention times to identify which ion one wishes to use as the 'identification ion' for a given chemical species. While this task can be rather tedious, it is essential to providing a top quality data set for statistical analysis. It is critical that this part of the data analysis be done properly and accurately.

*Adducts and Isotopes Explained Using L-tryptophan-d<sub>5</sub> as an Example*

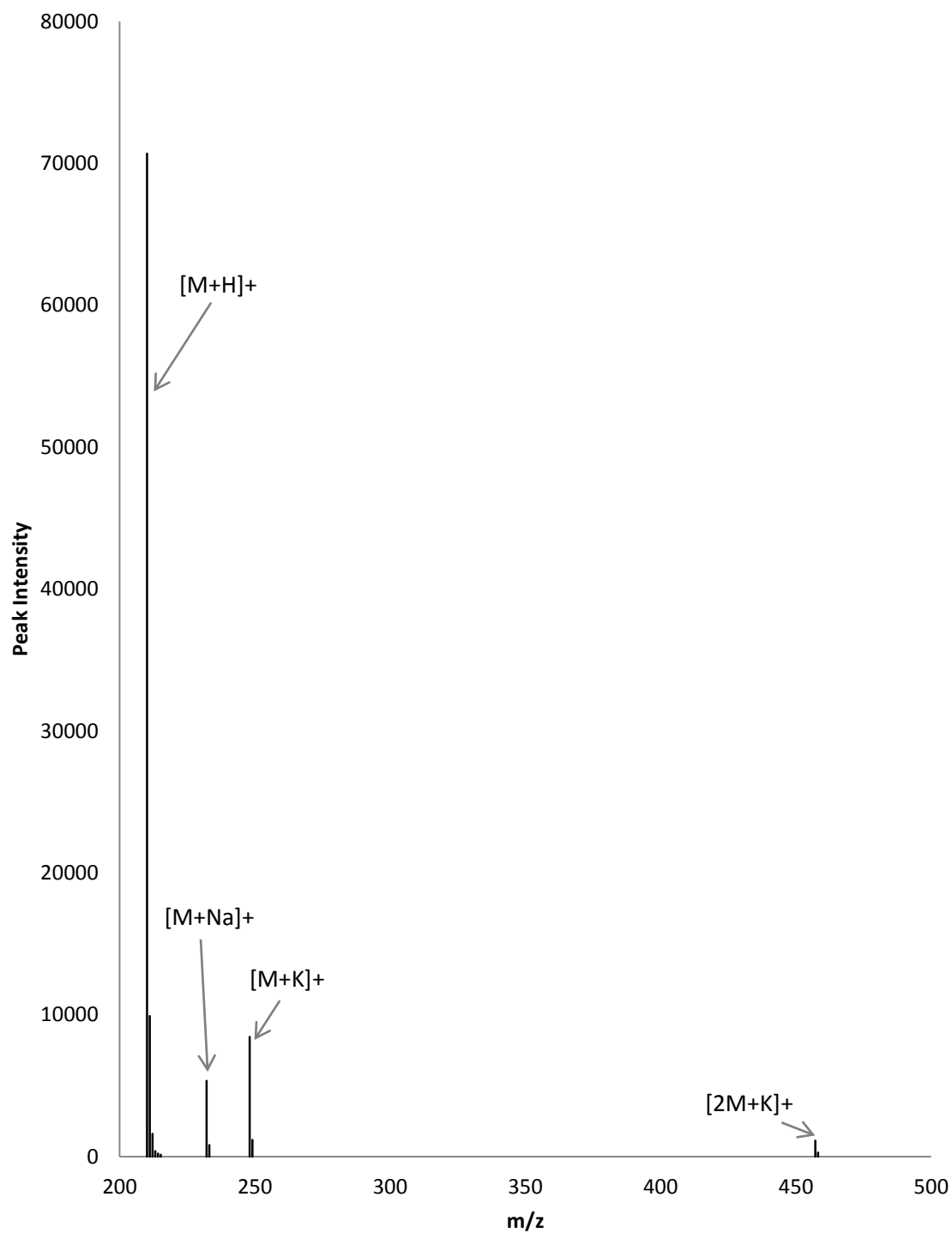
The standard L-tryptophan-d<sub>5</sub> ionized well in both positive and negative modes. As expected for an amino acid, there was large protonated molecular ion [M+H]<sup>+</sup> found in the positive ion mode at m/z 210.14 and a deprotonated molecular ion [M-H]<sup>-</sup> in the negative ion mode at m/z 208.12 (see Table 3.2). Both the [M+H]<sup>+</sup> ion and [M-H]<sup>-</sup> ion have a mean retention time of 6.71 minutes ± 0.03 min in the five positive ion and five negative ion chromatograms. The XCMS/CAMERA software package identified eleven ions in the positive ion mass spectra and eight ions in the negative ion mass spectra, all of which shared the same retention time. All these ions were attributed to arising from L-tryptophan-d<sub>5</sub> (Table 3.2). Two reconstructed mass showing the adduct ions and isotopic peaks ions of L-tryptophan-d<sub>5</sub> are shown in Figure 3.6 (positive ion mode) and in Figure 3.7 (negative ion mode).

The inset of Figure 3.7 shows detail of the adduct ions of [M-Cl]<sup>-</sup>. Chlorine has two isotopes, <sup>35</sup>Cl and <sup>37</sup>Cl, in the approximate ratio of 3 to 1. In addition to retention times and accurate masses of the ions, relative isotope intensities can be used to identify relationships between ions.

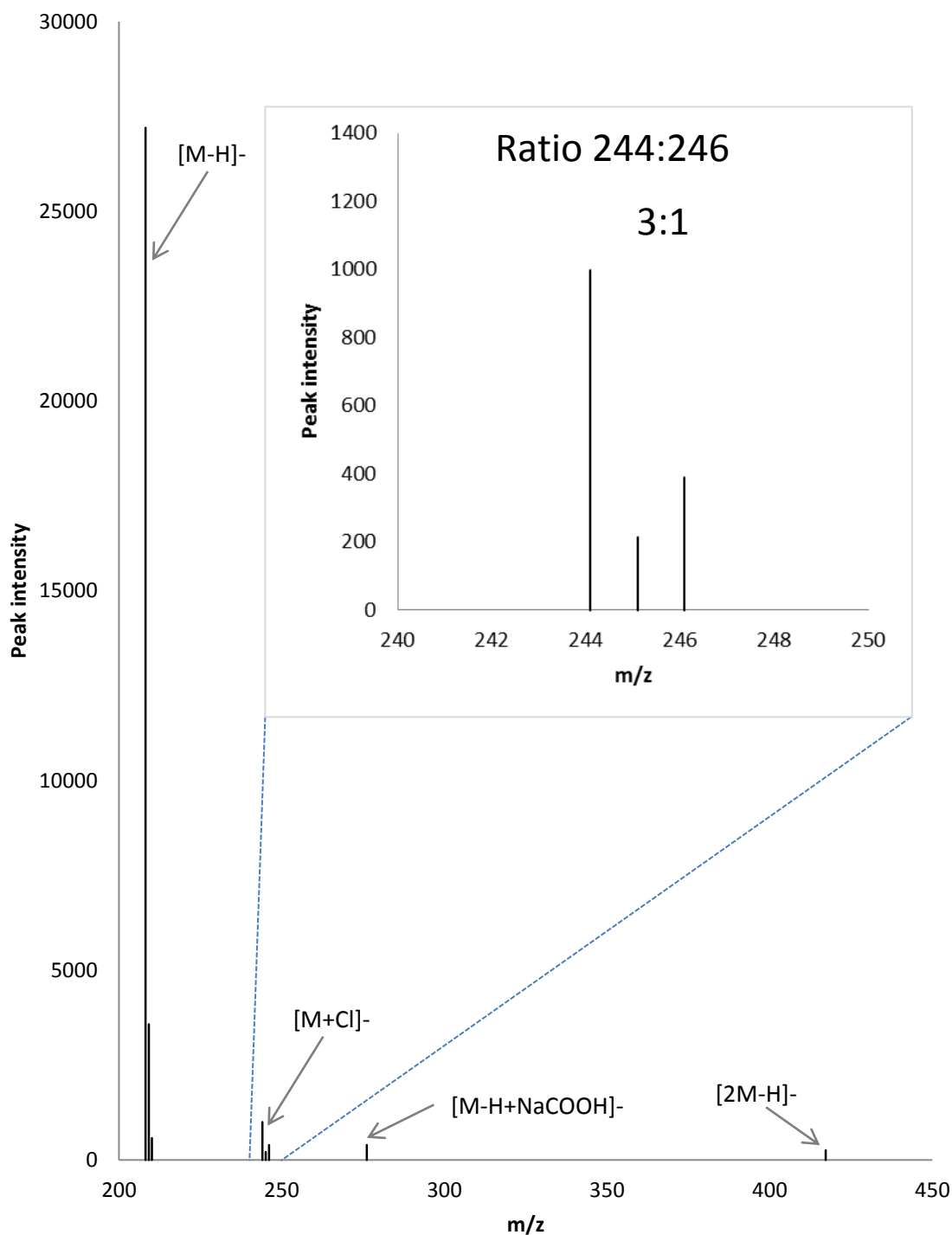


**Table 3.2:** Isotopic peaks present and adducts formed from L-tryptophan-d<sub>5</sub> in both positive and negative ion modes.

m/z	LC Retention Time (min)	Nature of ion	Isotope	MS Peak intensity
Positive ion mode				
210.14	6.71	[M+H] <sup>+</sup>	M	70675
211.15	6.71		M+1	9924
212.14	6.68		M+2	1605
213.14	6.70		M+3	402
214.14	6.70		M+4	229
232.13	6.73	[M+Na] <sup>+</sup>	M	5344
233.13	6.71		M+1	815
248.10	6.71	[M+K] <sup>+</sup>	M	8449
249.10	6.71		M+1	1188
457.24	6.68	[2M+K] <sup>+</sup>	M	1132
458.24	6.68		M+1	293
Negative ion mode				
208.12	6.70	[M-H] <sup>-</sup>	M	27198
209.13	6.70		M+1	3577
210.13	6.70		M+2	577
244.10	6.68	[M+Cl] <sup>-</sup>	M	998
245.10	6.67		M+1	214
246.09	6.66		M+2	390
276.11	6.71	[M-H+NaCOOH] <sup>-</sup>		391
417.24	6.68	[2M-H] <sup>-</sup>		257



**Figure 3.6:** Reconstructed mass spectrum (positive ion mode) of L-tryptophan-d<sub>5</sub> showing adduct ions and isotopic peaks.



**Figure 3.7:** Reconstructed mass spectrum (negative ion mode) of L-tryptophan-d<sub>5</sub> showing adduct ions and isotopic peaks.

Table 3.3 lists the number of ions detected by XCMS/CAMERA in positive and negative ions modes. The number of ions detected in both ion modes ranges from 1948 to 2285. This number includes adduct ions and isotopic ions of many compounds, however, only one ion is required to quantify a given metabolite. Approximately 35% of the ions present in the original list were found to be unique for a given chemical species. The number of ions present in the final lookup table ranged from 633 to 711.

**Table 3.3:** Total number of ions detected by XCMS/CAMERA in positive and negative ion modes, and number of metabolites found in the final lookup table (positive and negative ion modes) in each sample class.

	# of ions detected by XCMS/CAMERA			# of ions in lookup table		
	positive ion mode	negative ion mode	sum of both ion modes	positive ion mode	negative ion mode	sum of both ion modes
control	1216	824	2040	423	251	674
0.14 mg/L fluorene	1298	859	2157	448	255	703
1.4 mg/L fluorene	1374	911	2285	446	259	705
0.14 mg/L PAH	1355	919	2274	454	257	711
1.4 mg/L PAH	1167	781	1948	399	234	633

Despite the numerous adducts ions and isotopic ions present, only one ion is required to quantify a given metabolite. Therefore, it is important that the relative abundances of the related ions remain constant from one sample to the next. Table 3.4 lists the ratios for the major ions present in Figures 3.1 and 3.2. Note that while the percent variability is quite low, the relative abundances contribute to the total variability in the concentrations of the metabolite.

**Table 3.4:** Reproducibilities in five biological replicates of *S. meliloti* WT control (positive ion and negative ion modes).

Adduct ratio	m/z ratio	Average	% variability
Positive ion mode			
[M+H] <sup>+</sup> : [M+Na] <sup>+</sup>	210.14 : 232.13	14.2	6.8%
[M+H] <sup>+</sup> : [M+K] <sup>+</sup>	210.14 : 248.10	9.4	6.7%
Negative ion mode			
[M-H] <sup>-</sup> : [M+Cl] <sup>-</sup>	208.12 : 244.10	25.3	20.5%

*Comparison of Bruker DataAnalysis and XCMS/CAMERA Packages*

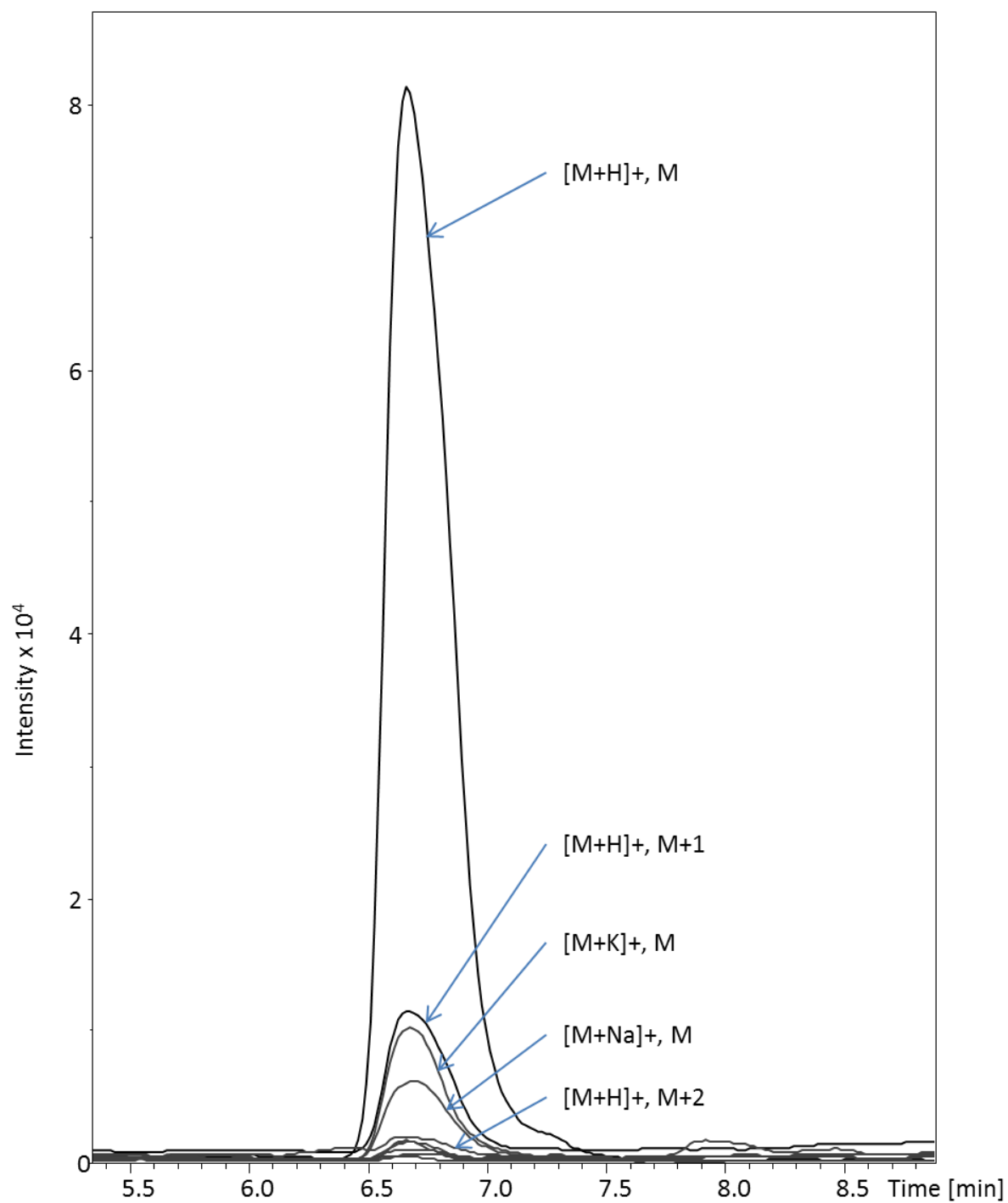
In order to analyse experimental data produced from ESI-LC-MS, runs performed on the Agilent LC coupled to the Bruker MicrOTOF II Mass Detector, a program called Bruker DataAnalysis is provided by the manufacturer. DataAnalysis uses only the original data files produced by the LC-MS instrument. This program is capable of extracting ion chromatograms from chromatographic files and providing data, such as integrated peak areas, peak widths, retention times, etc., in an Excel file format. Analysis of the same data files by the XCMS/CAMERA package requires the raw data file to be converted to another file format. It was decided to compare the quality of integrated peak areas from DataAnalysis and from the XCMS/CAMERA packages to determine whether one package gave better data than the other.

Table 3.5 lists the peak areas of adduct ions and isotopic ions of L-tryptophan-d<sub>5</sub> formed in both positive ion and negative ion modes, calculated using DataAnalysis and XCMS/CAMERA. In the positive ion mode, the comparison shows low percent variabilities, with the exception of the M+2 isotopic peak of the [M+H]<sup>+</sup> adduct . However, in the negative ion mode, the DataAnalysis package provided significantly different peak areas than the XCMS/CAMERA package. The reason for this difference was found to be in the nature of the extracted ion chromatograms (EIC) produced by DataAnalysis software. In positive ion mode (Figure 3.8), the EICs from the DataAnalysis package have the same retention times, peak widths and shapes. However, in the EICs

in the negative ion mode (Figure 3.9) showed one ugly ‘double peak’ for the M+1 isotopic peak of the [M-H]<sup>-</sup> ion.

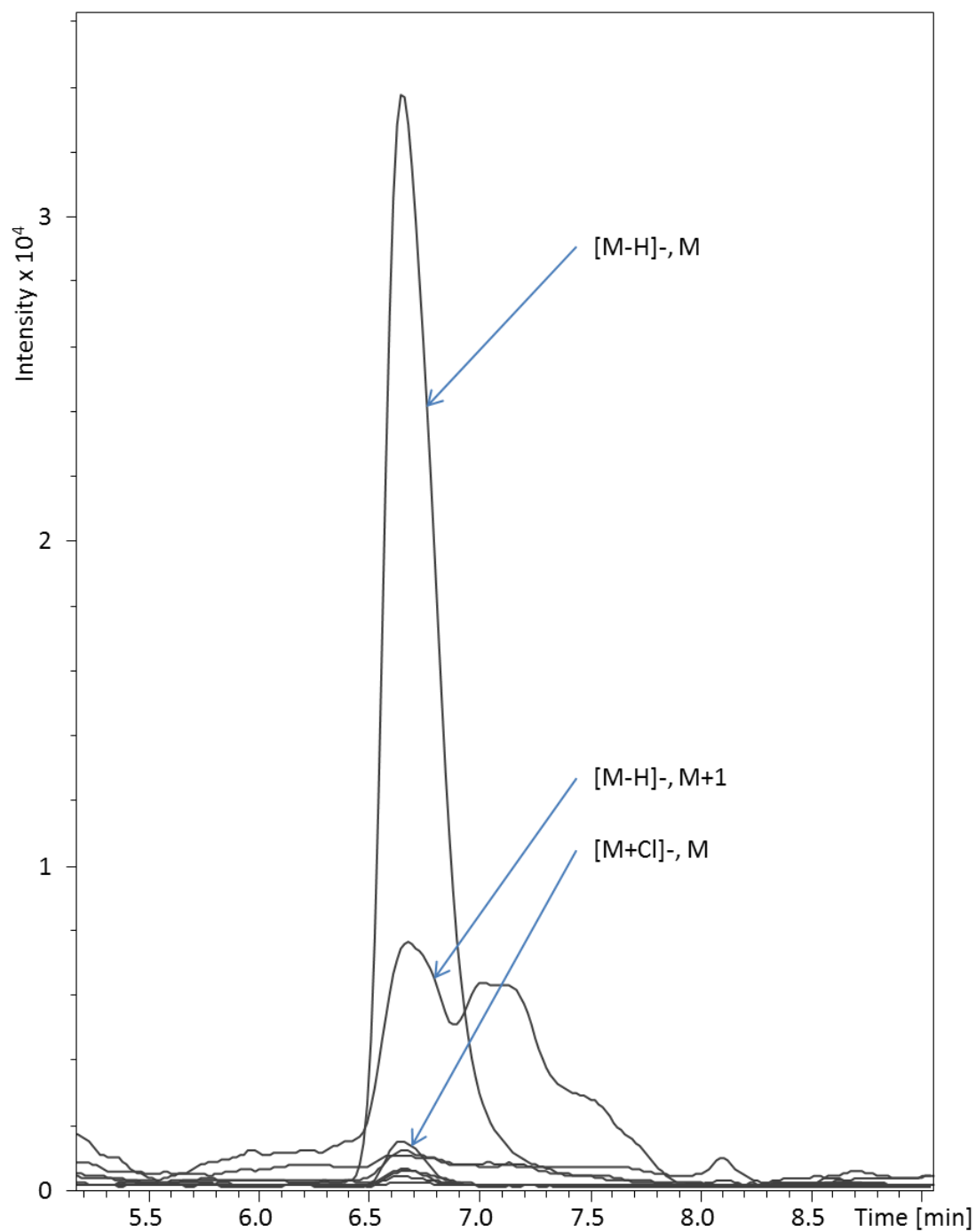
**Table 3.5:** Comparison on integration in Bruker DataAnalysis and XCMS/CAMERA of adducts and isotopes peaks of L-tryptophan-d<sub>5</sub> formed in positive ion and negative ion modes

m/z	XCMS area	DataAnalysis area	adduct	isotope	percent variability
positive ion mode					
210.14	1447069	1542156	[M+H] <sup>+</sup>	M	4.5%
211.15	203925	201813		M+1	0.7%
212.14	46370	28636		M+2	33.4%
232.13	112061	121453	[M+Na] <sup>+</sup>	M	5.7%
233.13	17744	14267		M+1	15.4%
248.10	168695	178888	[M+K] <sup>+</sup>	M	4.1%
249.10	23684	20766		M+1	9.3%
457.24	20592	21158	[2M+K] <sup>+</sup>	M	1.9%
458.24	5690	5454		M+1	3.0%
negative ion mode					
208.12	522281	562580	[M-H] <sup>-</sup>	M	5.3%
209.13	69629	150326		M+1	51.9%
210.13	11585	22806		M+2	46.1%
244.10	17760	16897	[M+Cl] <sup>-</sup>	M	3.5%
246.09	7832	6320		M+2	15.1%
276.11	8055	7696	[M-H+NaCOOH] <sup>-</sup>		3.2%
417.24	4689	5682	[2M-H] <sup>-</sup>		13.5%



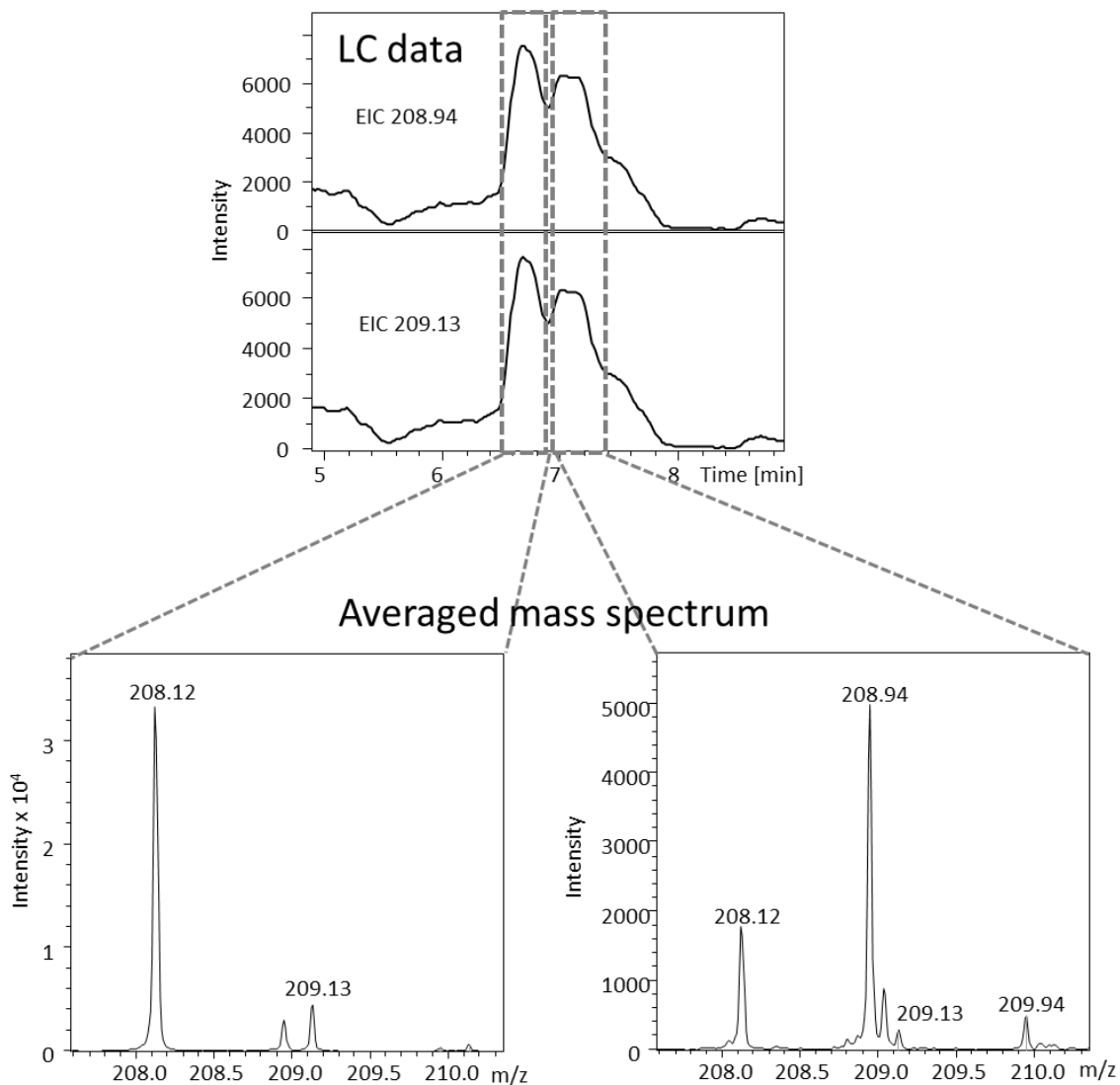
**Figure 3.8:** LC chromatograms extracted using Bruker DataAnalysis program of adducts and isotopic peaks of L-tryptophan-d<sub>5</sub> in positive ion mode.





**Figure 3.9:** LC chromatograms extracted using Bruker DataAnalysis program of adducts and isotopic peaks of L-tryptophan-d<sub>5</sub> in negative ion mode.

The unusual peak shape of the EIC for the M+1 isotope of [M-H]<sup>-</sup> ion in Figure 3.9 appears to be due to the fact that the Bruker software does not use narrow enough mass windows to extract ion chromatograms for species that have similar mass spectral values. In other words, the 'additional' peaks seem to be due to interferences from other species in the sample. Figure 3.10 shows two EICs corresponding to m/z 208.94 and 209.13. The EICs have identical chromatographic profiles. However, the high resolution mass spectra show these ions are well resolved. Clearly the Bruker software cannot distinguish between mass spectral peaks differing by 0.19 mass units, or 1000 ppm. For this reason, data work up and peak integrations were performed using XCMS/CAMERA, and not the Bruker's DataAnalysis software.

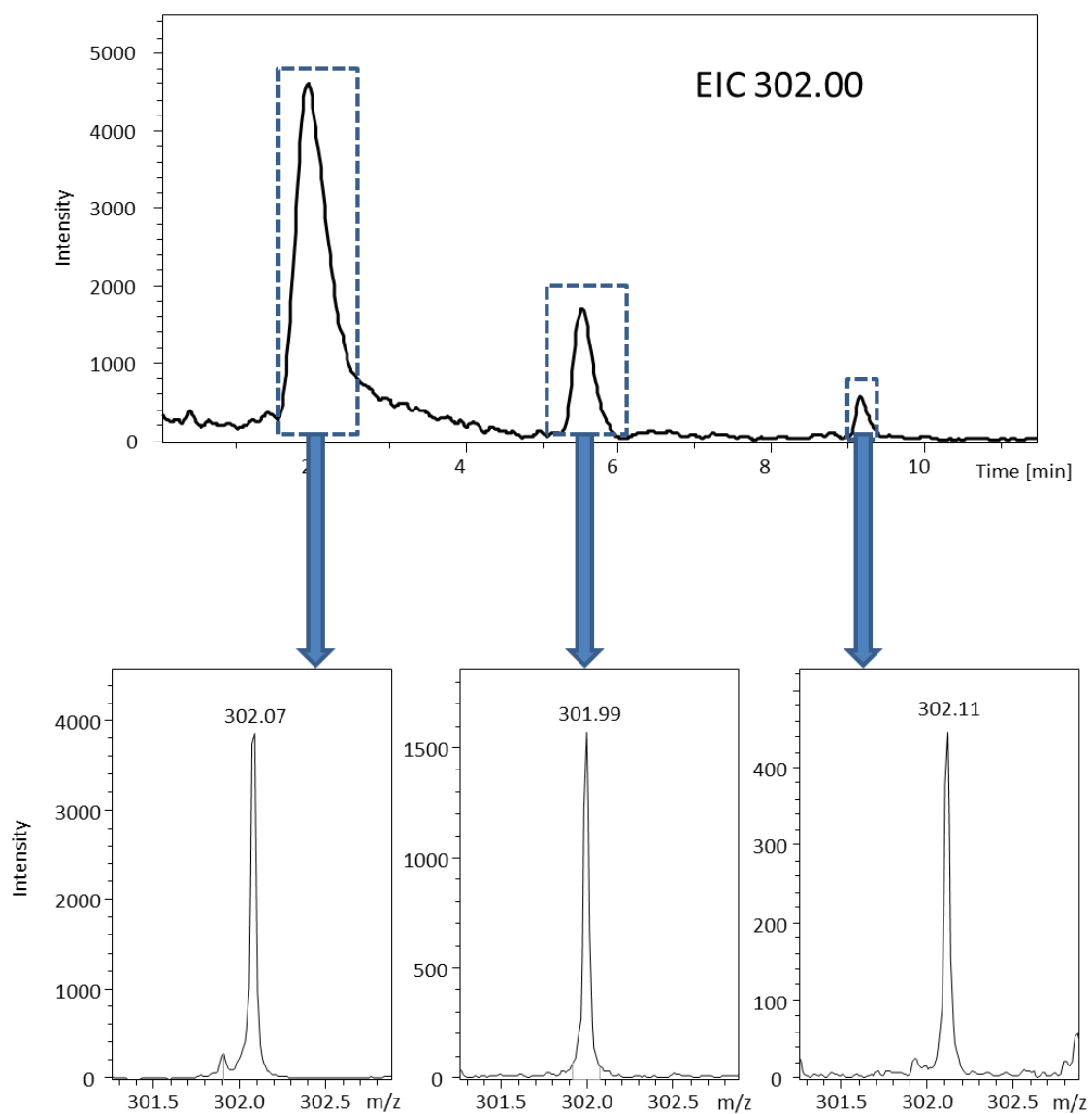


**Figure 3.10:** Extracted ion chromatograms prepared using the Bruker DataAnalysis software package. It was not possible to set a narrow enough mass window to provide separate mass chromatograms for peaks with masses differing by 0.19 Da.

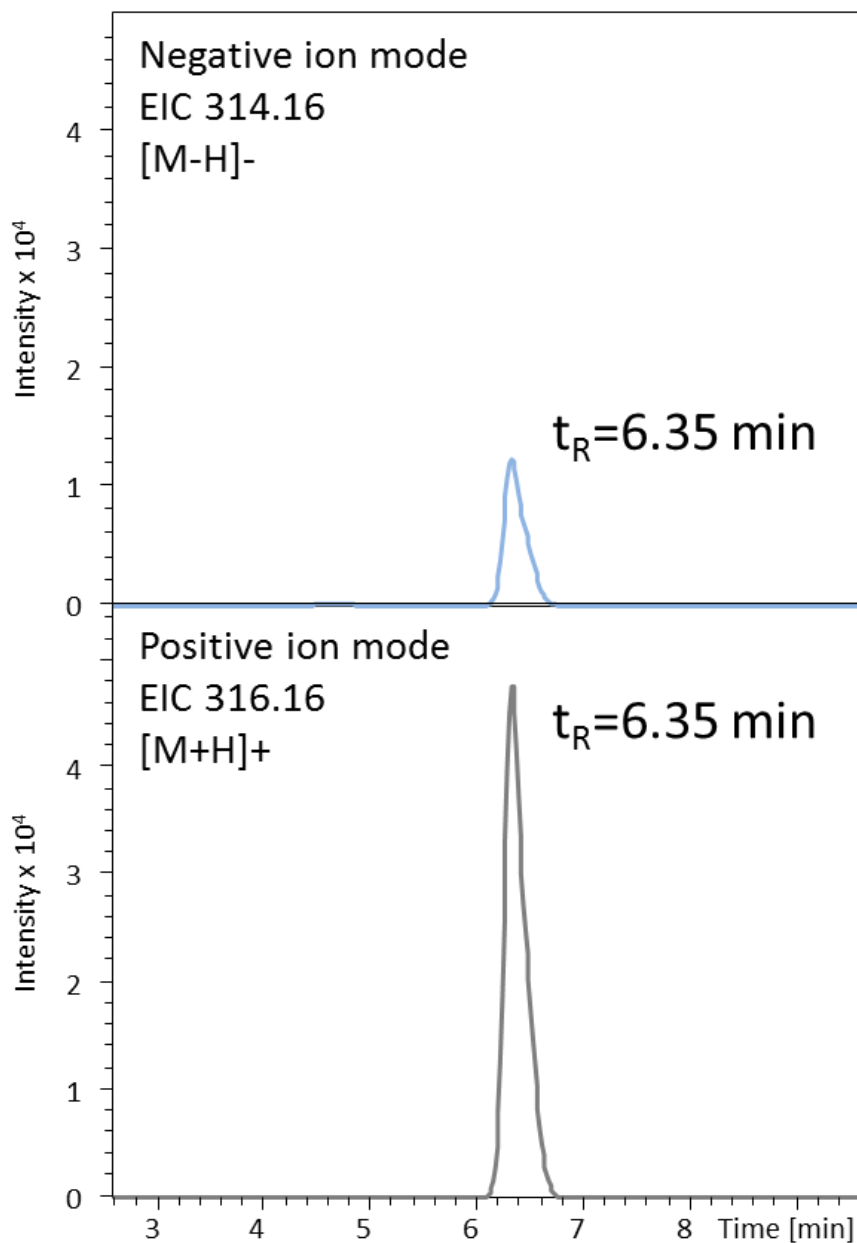
### *Creation of Lookup Tables*

Once a unique  $m/z$  value has been determined for a given species, this mass value together with a narrow mass range were placed in a lookup table along with the peak's retention time. Thus, each ion in the lookup table was identified by an accurate mass value, and a retention time. The mass range was determined by examining mass ranges of peaks in the XCMS/CAMERA data output. The retention time range was also determined from the same XCMS/CAMERA data output (Table 3.1). The final lookup tables often contained 600-700 listings. Due to the mass accuracy of the mass spectral data and the retention time reproducibility of the method, each entry in the lookup table was associated with a single chemical substance. Three different chemical species were identified which had nearly identical mass values but very different retention times; their EICs with  $m/z$  302.00 are shown in Figure 3.11. These three species are listed as three different entries in the lookup table and are identified separately in the data analysis.

When the finalized ion lists from both negative ion and positive ion modes are combined into a single lookup table, it is necessary to identify which ionization mode would be used to quantify a given compound; in this way, the same species would not be quantified twice (see Figure 3.12). The more responsive ion was usually chosen for quantification.



**Figure 3.11:** EIC of  $m/z$  302.00 produces three peaks at different retention times but with nearly identical mass values. These three peaks are due to three different chemical species with very similar  $m/z$  values.



**Figure 3.12:** EICs of molecular ions in both negative ion  $[M-H]^-$  and positive ion  $[M+H]^+$  modes. The molecular ions were related using accurate mass values and identical retention times.

*Extraction Efficiencies*

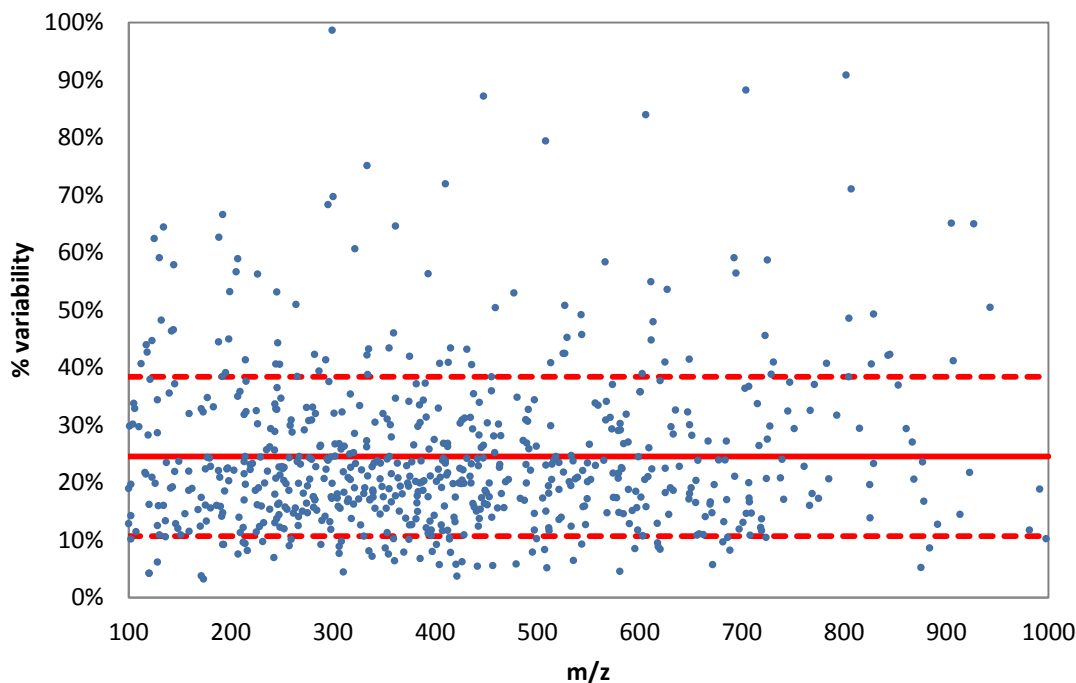
In order to determine the efficiency of extraction of metabolites, two recovery standards were used, L-methionine-d<sub>3</sub> and L-tryptophan-d<sub>5</sub>. Table 3.6 lists the percent recoveries for the two standards in five experiments. Recoveries between 84 and 119% are considered acceptable, but these values do not necessarily represent the recoveries of all metabolite classes in the sample.

**Table 3.6:** Percent recoveries for internal standards in five samples.

Sample class	positive ion mode		Negative ion mode	
	% Recovery	St dev (n=5)	% Recovery	St dev (n=5)
L-methionine-d <sub>3</sub>				
control	115%	10%	96%	3%
0.14 mg/L fluorene	116%	5%	92%	5%
1.4 mg/L fluorene	120%	7%	94%	3%
0.14 mg/L PAH	114%	8%	95%	5%
1.4 mg/L PAH	119%	7%	95%	2%
L-tryptophan-d <sub>5</sub>				
control	89%	5%	103%	5%
0.14 mg/L fluorene	89%	7%	102%	8%
1.4 mg/L fluorene	85%	2%	101%	1%
0.14 mg/L PAH	84%	5%	102%	9%
1.4 mg/L PAH	89%	8%	103%	5%

*Variabilities in metabolome analyses of S. meliloti*

A major contribution in the variability in metabolite levels is the biological variability, which is defined as the physiological differences among organisms or cultures<sup>56</sup>. Figure 3.13 shows the biological variabilities of 674 ions (both in positive ion and negative ion modes) present in the control sample class. The mean value for all samples in five experiments ranged between 19.2% and 26.9% , with standard deviations between 12.4% to 19.4% (Table 3.7).



**Figure 3.13:** Percent biological variability for 674 ions present in control samples from both positive ion and negative ion modes. The solid line indicates the mean and dashed lines indicate one standard deviation ( $\pm 14.3\%$ ) away from the mean (24.6%).

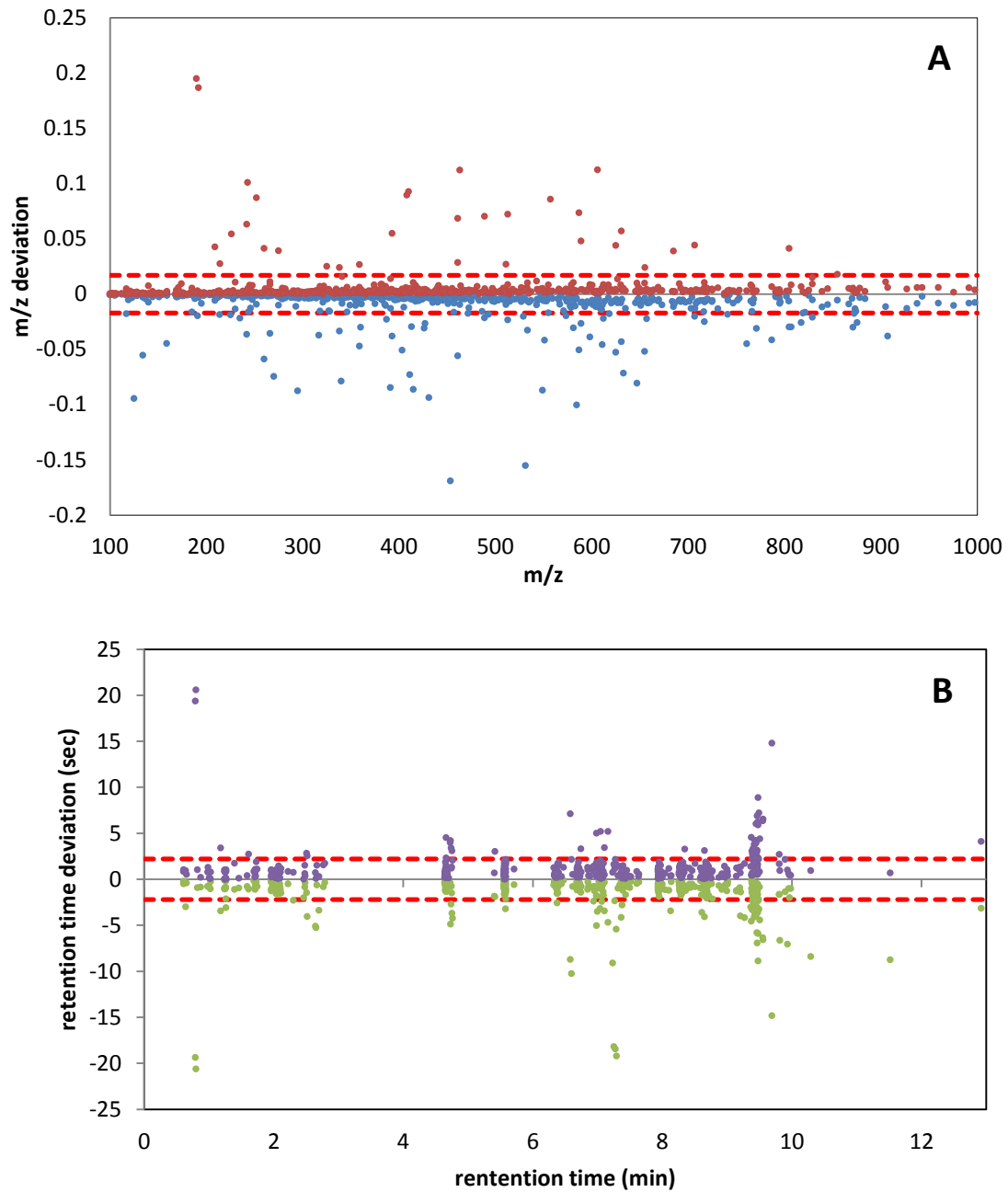


**Table 3.7:** Mean biological variabilities for five sample classes.

Sample class	Mean biological variability	st dev (n=5)
control	24.6%	14.3%
0.14 mg/L fluorene	19.2%	12.4%
1.4 mg/l fluorene	21.9%	13.3%
0.14 mg/L PAH	26.9%	19.4%
1.4 mg/L PAH	24.5%	15.4%

Variations in instrument performance also contribute to the variability in metabolite levels. Figure 3.14A shows the instrumental variations in the mass accuracies (m/z deviation) over a mass range from 100 to 1000 for 674 ions detected in the control sample class. The standard deviation of mass values was found to be  $\pm 0.02$  m/z units. The range of retention times, also computed by XCMS/CAMERA, had a standard deviation of  $\pm 2$  seconds for the 674 ions detected in the control samples (Figure 3.14B). These deviations were typical for all sample classes.

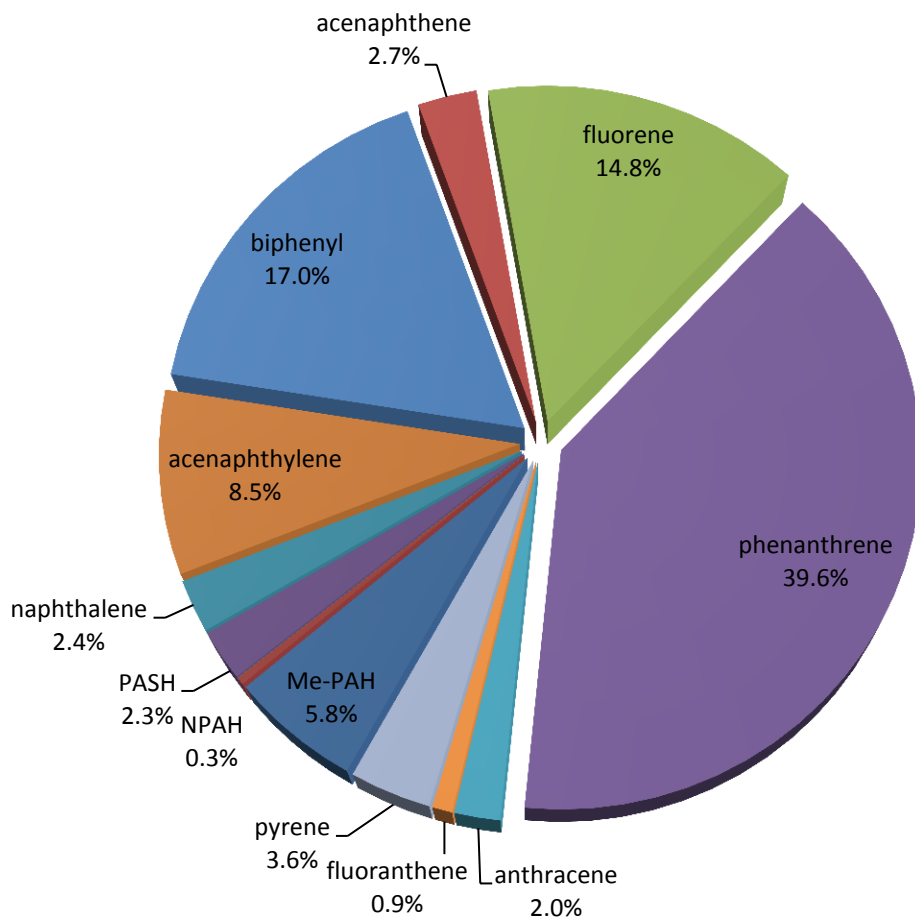
Figure 3.14B reveals an interesting characteristic of separations using the zic-HILIC column. It appears as though ions are separated into zones or bands. There are 11 zones of elution in which roughly 90% of the ions elute, while over some parts of the gradient, no ions were retained (e.g., range of 3-4 minutes). Plotting the retention time against the retention time deviations as reported by XCMS/CAMERA can be used to visualize the chromatographic results and develop new chromatographic methods for separation of complex mixtures.



**Figure 3.14:** Deviations in mass-to-charge ratios (A) and retention time values (B) for 674 peaks detected in the control sample (both in positive ion and negative ion modes). Dashed lines indicate one standard deviation.

*PAH exposure of S. meliloti*

The HILIC-LC-ESI-MS method and data mining procedure was applied to the analysis of *S. meliloti* exposed to fluorene (0.14 mg/L and 1.4 mg/L), and to a coal tar PAH fraction containing 15% fluorene and various lower molecular mass PAHs (total PAH concentrations of 0.14 mg/L and 1.4 mg/L, see Figure 3.15 for PAH composition of coal tar fraction). The fraction was prepared from coal tar and analyzed by GC-MS by Fan Fei.



**Figure 3.15:** Profile of PAH compounds in low molecular mass PAH fraction prepared from coal tar that was used in metabolomics experiment.

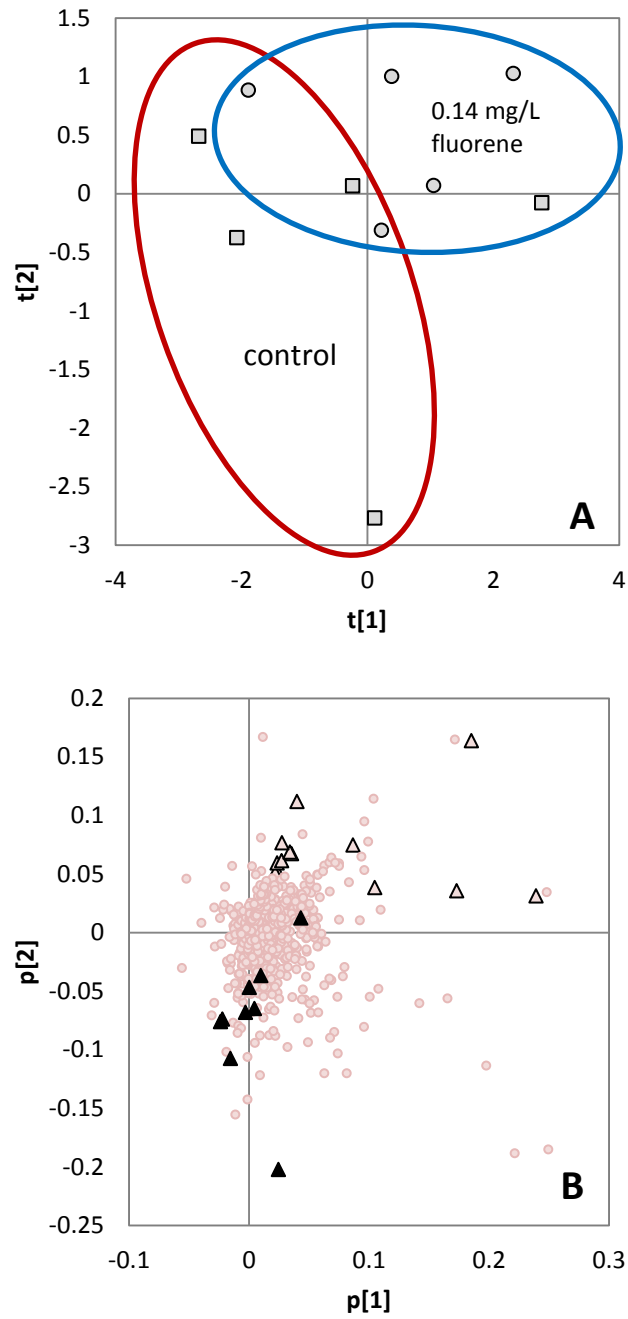
### *Multivariate Analysis – Principal Component Analysis*

Principal component analysis (PCA) was used to analyze data from control and PAH-exposed samples of *S. meliloti*. Although instrumental and biological variations may contribute to overall variations in metabolite levels, PCA is useful in revealing hidden trends in these data. PCA is used as an initial check of the metabolomic data, primarily to ensure that there is indeed statistically meaningful separation of data in the sample groups. If PCA does not produce a separation of the sample classes, then moving on to a supervised statistical method, such as OPLS-DA, will not produce meaningful results. For multivariate data analysis, the sample data sets contained the following number of ions: control, 674; 0.14 mg/L fluorene, 703; 1.4 mg/L fluorene, 705; 0.14 mg/L PAH, 711 and 1.4 mg/L PAH, 633). All normalized peak areas with m/z values and retention times can be found in Appendix 4.

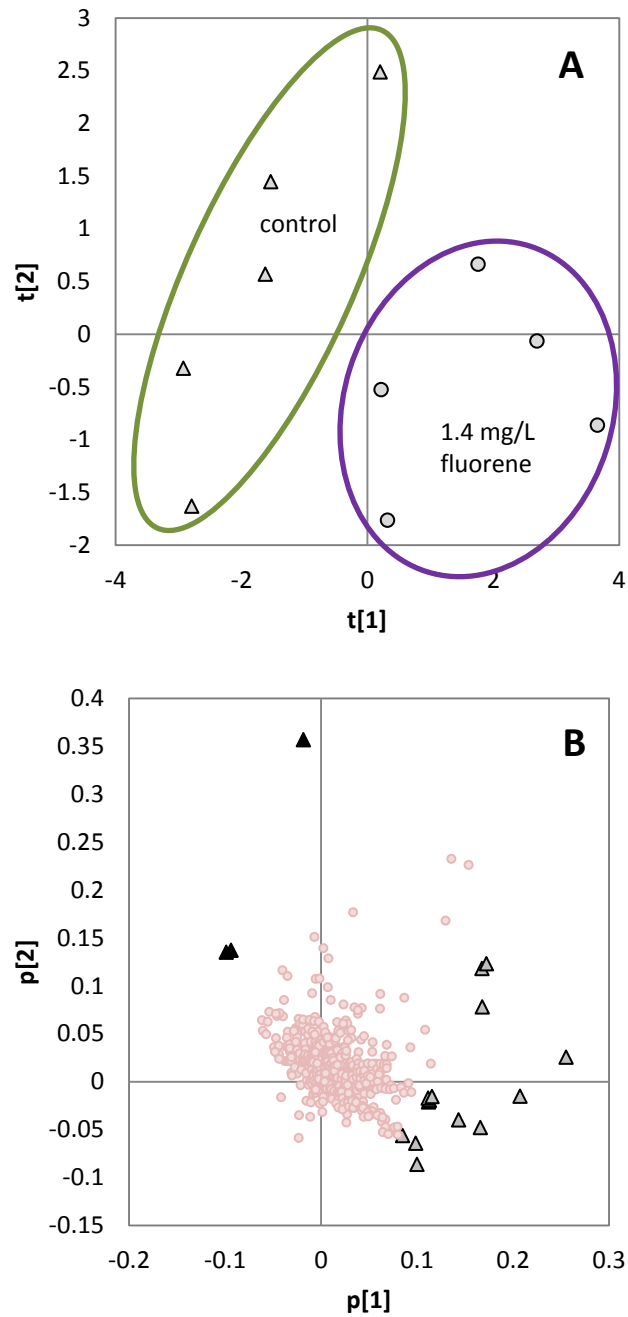
PCA is a qualitative study of variance which leads to understanding of what samples (scores) and what variables (loadings) and are responsible for the variations observed in the data. The PCA plots of *S. meliloti* exposed to fluorene at a concentration of 0.14 mg/L are shown in Figure 3.16 (A, scores plot, B, loadings plot). The loadings plot shows how metabolites in the samples contribute to the separation between the control and treated samples. The triangles in Figure 3.16 B indicate those metabolites which were identified as significant in the subsequent OPLS-DA analysis (see Figure 3.19). Figure 3.17 shows the scores plot (A) and loadings plot (B) of the control samples versus

samples exposed to fluorene at 1.4 mg/L. In both instances, the PCA loadings plots do not provide information to predict the significant metabolites. The 'significant' metabolites, subsequently identified by OPLS-DA analysis, are found on the 'periphery' of the PCA loadings plot but so are a number of other 'insignificant' compounds in the same region of the plot.

In the case of the lower dosage 0.14 mg/L fluorene, the first principal component accounted for 47.8% of the variation within the data set while the second component accounted for an additional 17.8% of the variance for a total of 65.6%. In the case of the higher fluorene exposure (1.4 mg/L), the first component accounted for 54.9% of the variance and the second component, 19.4%. The total numbers of principal components in the PCA analyses were 3 (0.14 mg/L) and 2 (1.4 mg/L).



**Figure 3.16:** PCA scores plot (A) and loadings plot (B) of control vs 0.14mg/L fluorene. The triangles indicate those ions which were identified as significant in the subsequent OPLS-DA analysis.



**Figure 3.17:** PCA scores plot (A) and loadings plot (B) of control vs 1.4mg/L fluorene. The triangles indicate those ions which were identified as significant in the subsequent OPLS-DA analysis.

*Multivariate analysis – Orthogonal Partial Least Squares Discriminant Analysis*

To get a clearer understanding of which metabolites are undergoing the most significant changes due to PAH exposures, a supervised statistical analysis method, OPLS-DA, was used. In this approach, the noise in the dependent variables is taken into account and the method can more accurately assess which variations in the data are actually due to differences between sample classes.

OPLS-DA was performed on the data of sets of *S. meliloti* control bacterial extracts and extracts from bacteria exposed to fluorene at 0.14 mg/L and 1.4 mg/L. The scores plots (Figure 3.18) show excellent separations of the control biological samples from those exposed to fluorene. These separations are much greater than was seen in the PCA scores plots.

The  $R^2Y$  value is the total variation in Y explained by the statistical model. The  $R^2Y$  values for the control samples and samples exposed to fluorene were  $R^2Y=.999$  for both the 0.14 and 1.4 mg/L fluorene exposures, indicating an excellent separation of the samples. This result is not surprising given that OPLS-DA is a supervised method and the method 'knows' there are two different sample classes.

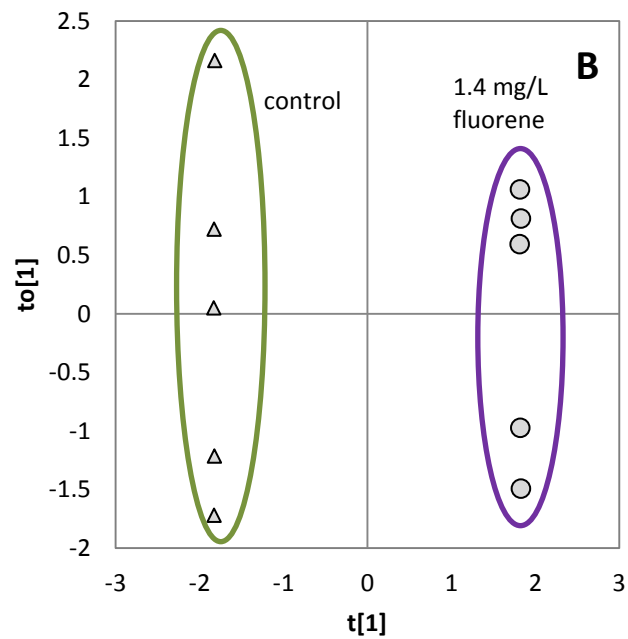
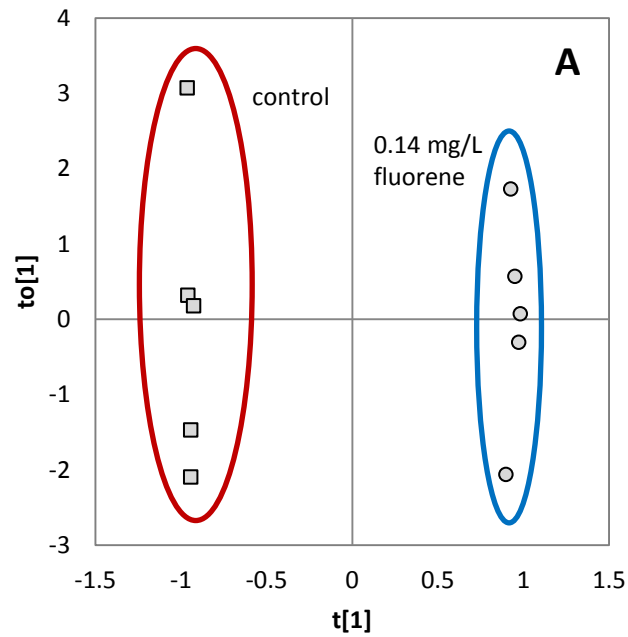
The  $R^2X$  value is a measure of the variation in X which is correlated to Y. In this case,  $R^2X$  for the separation of control samples and samples exposed to 0.14 mg/L fluorene was 14.5%, while the  $R^2X$  for the separation control samples and those exposed



to 1.4 mg/L fluorene was much greater at 40.4%. These values reflect the amount of variation in the level of metabolites that can be related to the differences between the sample classes. The smaller  $R^2X$  value indicates that the variability in the levels of metabolites in control and treated samples is higher in samples exposed to 1.4 mg/L fluorene. The  $R^2X(o_x)$ , (where  $o_x$  corresponds to the  $x^{\text{th}}$  orthogonal component value) corresponds to the amount of variation in X that is uncorrelated to Y. In other words, it is the measure of in-class variation seen in the scores plots.  $R^2X(o_1)$  for the separation of control samples and samples exposed to 0.14 mg/L fluorene is 45.6%, while the  $R^2X(o_1)$  for the separation control samples and those exposed to 1.4 mg/L fluorene is 28.5%. This in-class variation is due mainly to biological variability among samples in the same class. Table 3.8 summarizes the statistical values for all multivariate analyses performed on all sample classes.

**Table 3.8:** Statistical summary of multivariate analyses performed on cultures of *S. meliloti* exposed to fluorene and PAH mixture at concentrations of 0.14 and 1.4 mg/L

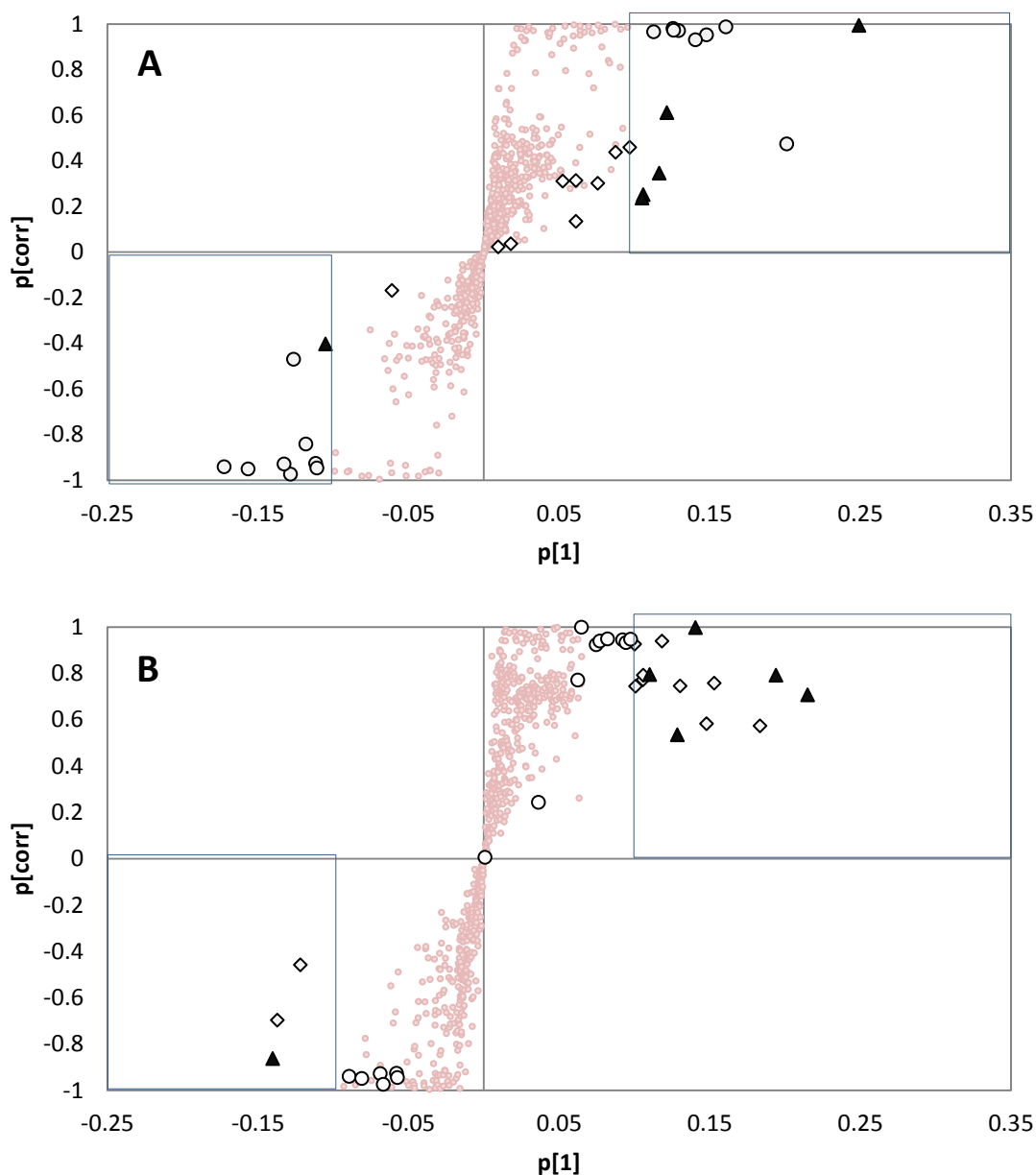
	PCA		OPLS-DA			
	model	$R^2X(1+2)$	model	$R^2X$	$R^2Y$	$R^2X(o_1)$
0.14 mg/L fluorene	3	65.6%	1+4	14.5%	99.9%	45.6%
1.4 mg/L fluorene	2	74.3%	1+5	40.4%	99.9%	28.5%
0.14 mg/L PAH	4	66.8%	1+2	24.3%	99.2%	25.5%
1.4 mg/L PAH	4	71.4%	1+1	41.9%	95.7%	26.0%



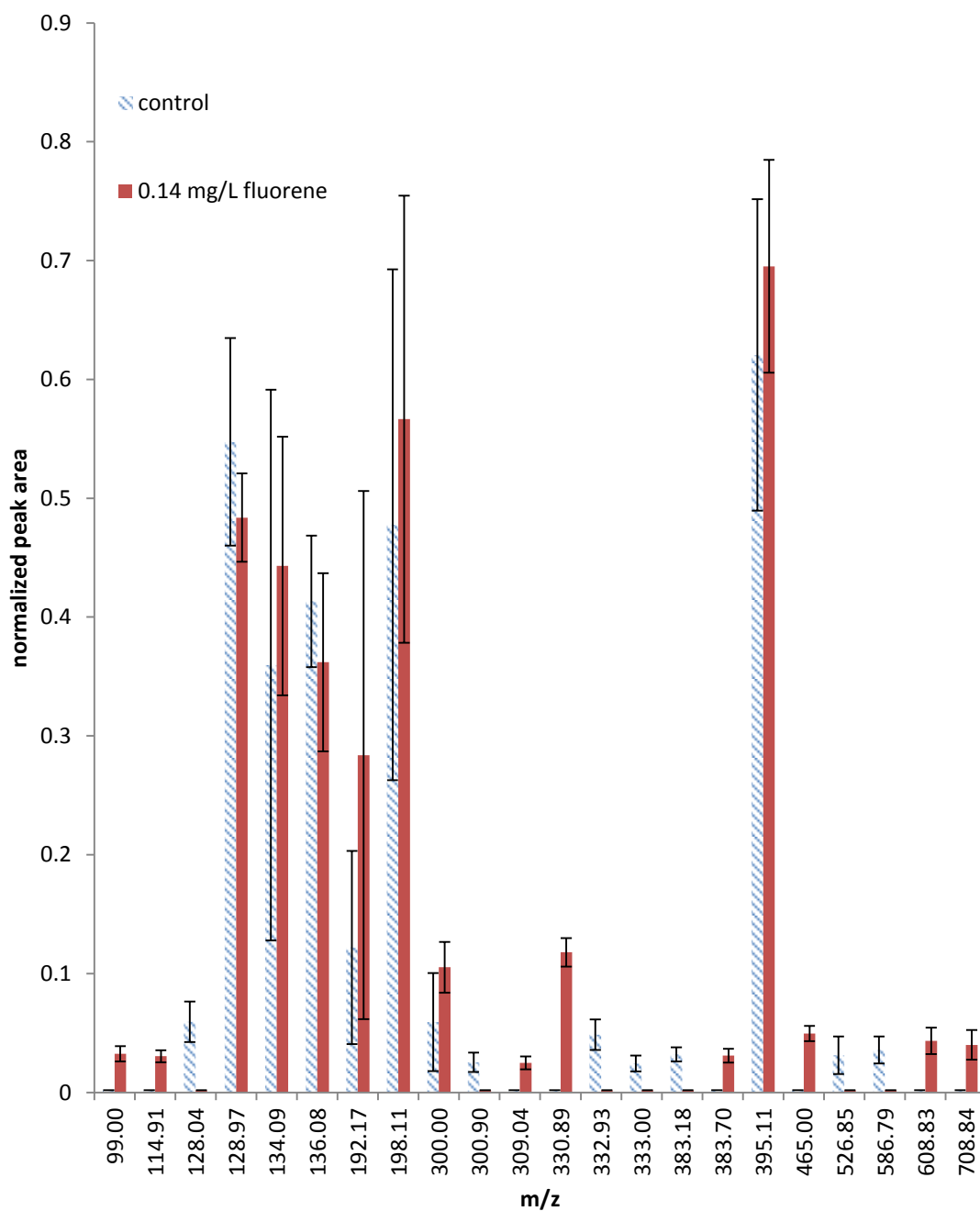
**Figure 3.18:** OPLS-DA scores plots of control bacteria versus bacteria exposed to (A) 0.14 mg/L fluorene and (B) 1.4 mg/L fluorene.

In OPLS-DA analyses, the S-plot is a useful tool for visualizing and interpreting the outcome of the multivariate analysis. The S-plot plots the covariance and correlation between the metabolites and the sample classes and is very useful in identifying statistically significant variables, i.e., significant metabolites. The metabolites of greatest interest are found at the top right and the bottom left of the S-plots with  $|p| > 0.1$ . It must be remembered that a compound with a large change between treated and control samples will not necessarily be important in the S-plot if its biological variability is large. Additionally, the differences between levels of control and treated compounds that are not detected in one sample set be treated differently in the software.

Figure 3.19 shows the S-plots of control versus 0.14 mg/L fluorene (A) and 1.4 mg/L fluorene (B). The boxes indicate areas where  $|p| > 0.1$ , which contain ions which were found to be significant by the OPLS-DA analysis. Figure 3.20 shows the ions that were determined to be statistically significant between the control and the samples exposed to 0.14 mg/L fluorene (Table 3.9 lists values with respective retention times). Figure 3.21 shows the ions that were determined to be statistically significant between the control and the samples exposed to 1.4 mg/L fluorene (Table 3.10 lists values with respective retention times). In total, six ions of significance were in common between the two exposures; these had masses of 134.09, 136.08, 198.11, 300.00, 330.89 and 395.11.



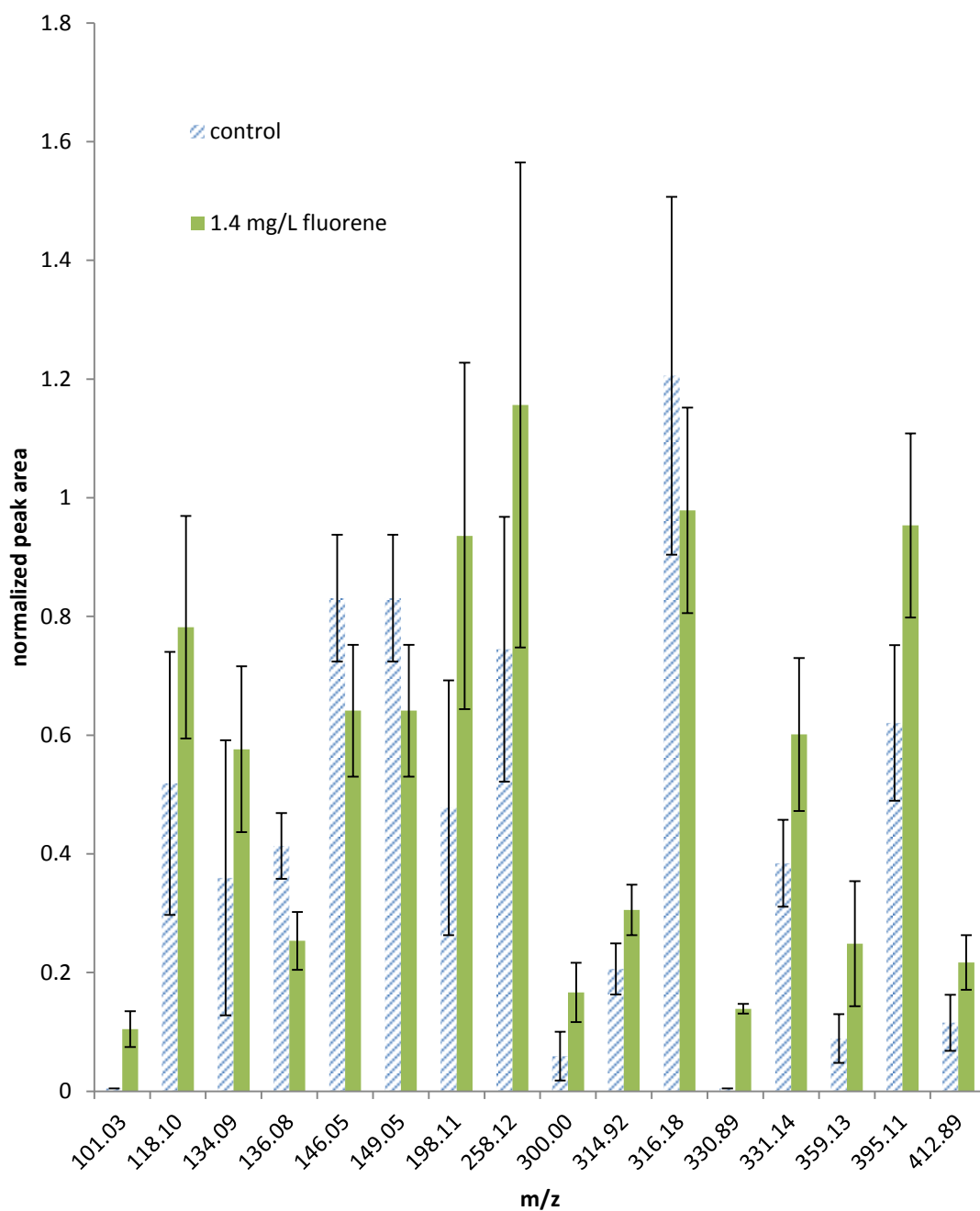
**Figure 3.19:** S-plots of control versus 0.14 mg/L fluorene (A) and 1.4 mg/L fluorene (B). Black triangles indicate ions with  $|p| > 0.1$  in both samples, circles indicate ions with  $|p| > 0.1$  in samples exposed to 0.14 mg/L fluorene, and diamonds indicate ions with  $|p| > 0.1$  in samples exposed to 1.4 mg/L fluorene. (A) contains 703 data features and (B) contains 705 data features.



**Figure 3.20:** Relative normalized peak areas of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 0.14 mg/L fluorene experiments. Error bars indicate standard deviations ( $n=5$ ).

**Table 3.9:** List of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 0.14 mg/L fluorene exposure experiments. These ions indicated in bold face are common with ions in Table 3.10.

m/z	R <sub>t</sub> (min)	ion mode
0.14 mg/L fluorene		
99.00	9.37	pos
114.91	7.77	pos
128.04	7.86	neg
128.97	7.94	neg
<b>134.09</b>	<b>7.37</b>	<b>pos</b>
<b>136.08</b>	<b>1.71</b>	<b>pos</b>
192.17	5.40	pos
<b>198.11</b>	<b>6.93</b>	<b>pos</b>
<b>300.00</b>	<b>5.79</b>	<b>neg</b>
300.90	9.50	neg
309.04	7.33	neg
<b>330.89</b>	<b>9.43</b>	<b>neg</b>
332.93	8.27	neg
333.00	9.02	pos
383.18	5.60	neg
383.70	5.58	neg
<b>395.11</b>	<b>7.02</b>	<b>neg</b>
465.00	5.59	neg
526.85	9.37	neg
586.79	9.48	neg
608.83	9.38	neg
708.84	9.36	pos



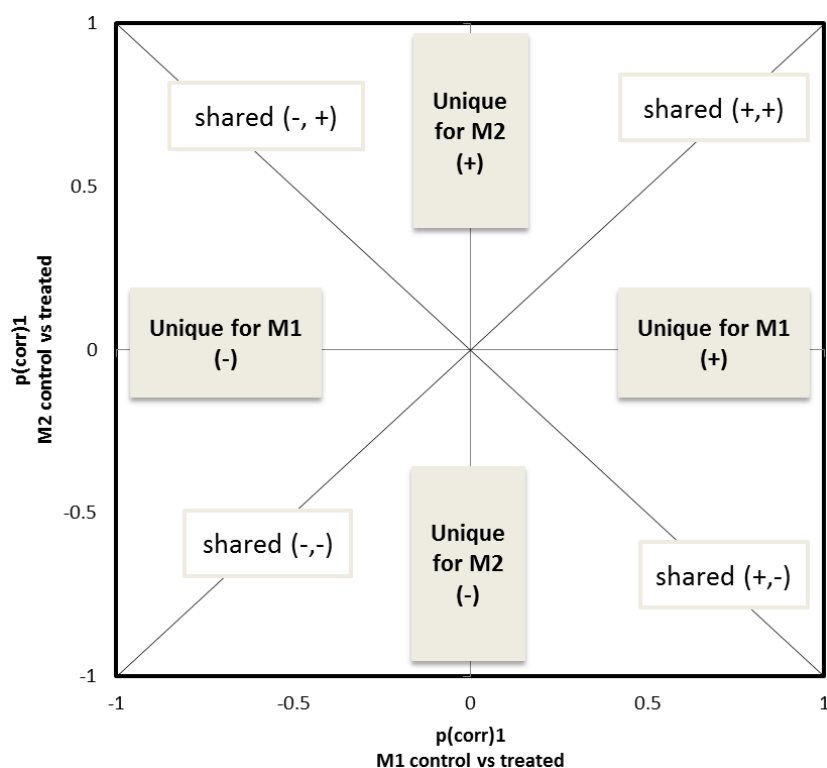
**Figure 3.21:** Relative normalized peak areas of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 1.4 mg/L fluorene experiments. Error bars indicate standard deviations ( $n=5$ ).

**Table 3.10:** List of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 1.4 mg/L fluorene experiments. Those ions indicated in bold face are common with those ions in Table 3.9.

m/z	R <sub>t</sub> (min)	ion mode
1.4 mg/L fluorene		
101.03	6.99	neg
118.10	7.52	pos
<b>134.09</b>	<b>7.37</b>	<b>pos</b>
<b>136.08</b>	<b>1.71</b>	<b>pos</b>
146.05	8.65	neg
149.05	6.98	neg
<b>198.11</b>	<b>6.93</b>	<b>pos</b>
258.12	9.20	pos
<b>300.00</b>	<b>5.79</b>	<b>neg</b>
314.92	9.42	neg
316.18	6.35	pos
<b>330.89</b>	<b>9.43</b>	<b>neg</b>
331.14	7.06	neg
359.13	7.31	neg
<b>395.11</b>	<b>7.02</b>	<b>neg</b>
412.89	9.40	neg

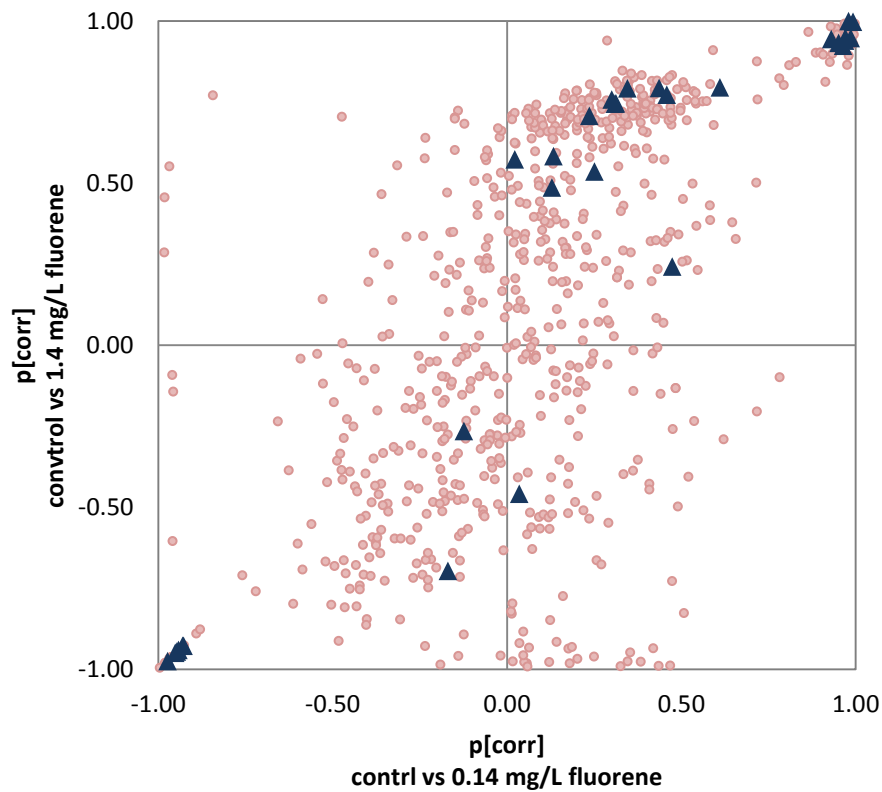


S-plots are useful for identifying significant features which account for the variation between two sample classes. More than two classes can be compared using OPLS2-DA. However, the S-plot would not clearly communicate which features of interest were contributing to the separation between multiple sample classes. Three sample classes, however, can be compared using shared and unshared structures (SUS) plots, which are plots of the  $p(\text{corr})$  values from the analysis of two models (Figure 3.22)<sup>20</sup>.



**Figure 3.22:** A shared and unique structures plot (SUS plot) is used to compare the outcome of multiple classification models compared to a common control. It can be used to identify compounds of interest which are causing variations between samples classes.

Figure 3.23 shows the SUS plot comparing three sample classes: control and samples exposed to fluorene at 0.14 mg/L and at 1.4 mg/L fluorene. Data points in the top right corner indicate those ions whose levels are elevated resulting from both exposures to fluorene, while data points in the bottom left corner indicate ions which have decreased in both exposed sample classes.

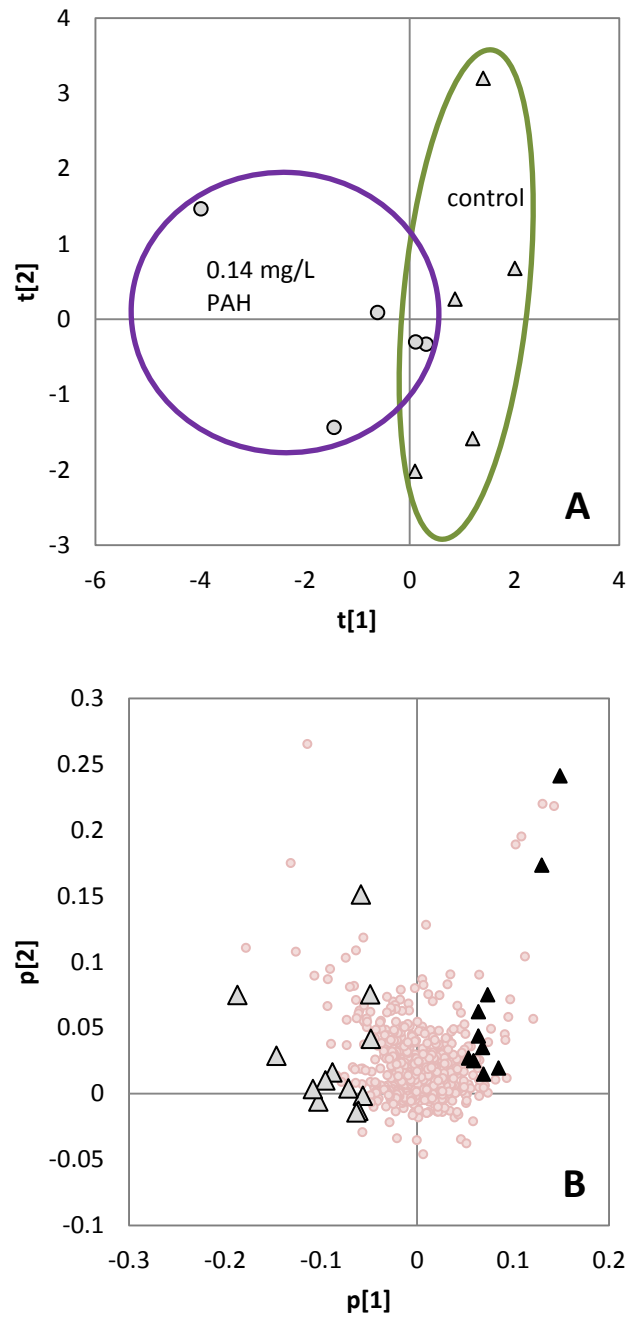


**Figure 3.23:** SUS plot of comparing samles classes exposed to fluorene at 0.14 mg/L and 1.4 mg/L. Triangles indicate ions which were identified as significant (i.e.,  $|p| > 0.1$ ) from their respective S-plots.

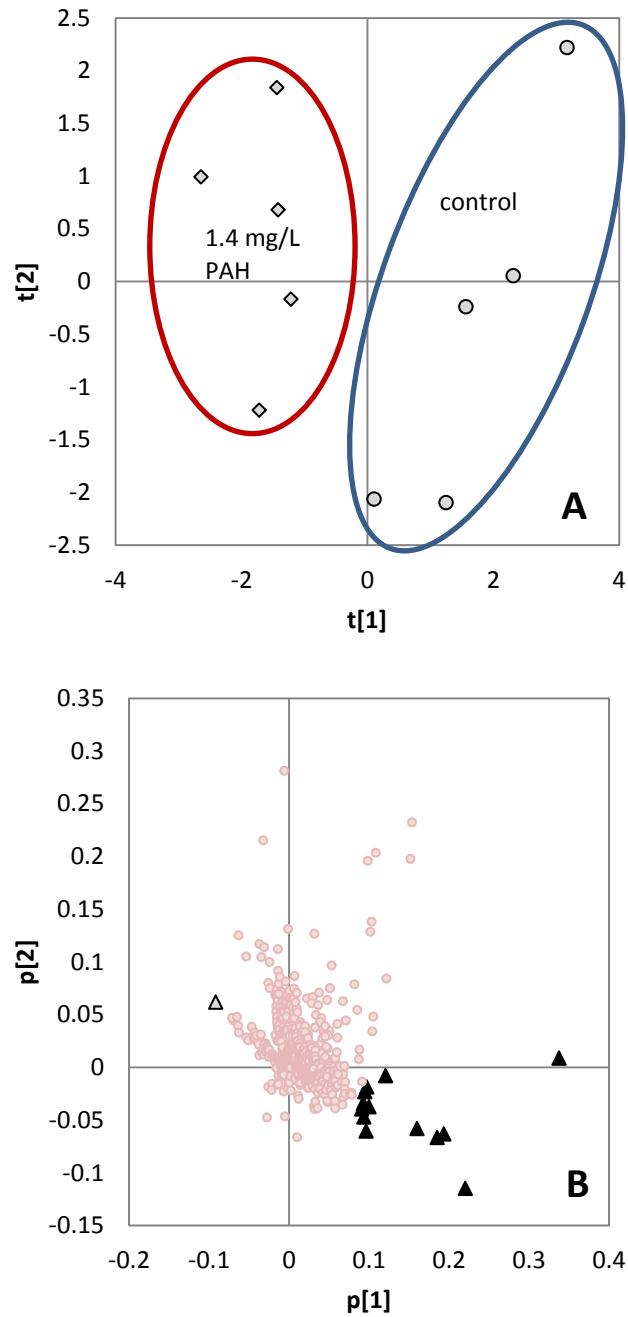
Both the S-plots and the SUS plot provide information on which ions are significant between sample classes. In the S-plot, an ion is found to be significant if  $|p| > 0.1$ , while the SUS plot determines relationships between sample classes based solely on  $p(\text{corr})$  values of ions. Some ions which were identified as significant because of their  $p$  value, had low  $p(\text{corr})$  values. The low  $p(\text{corr})$  values led these species to be judged as insignificant in the SUS plot. In the same way, certain compounds with high  $p(\text{corr})$  values in the S-plot were not always considered significant, because their  $p$  values fell just below the  $|p| > 0.1$  cutoff. For these reasons, it is difficult to interpret both the S-plots and SUS plots simultaneously. Perhaps the  $|p| > 0.1$  cutoff for identifying significant components is too simple an approach and should be correlated with information from the SUS plots.

#### *Exposures of S. meliloti to a mixture of PAH*

Cultures of *S. meliloti* were also exposed to a mixture of low molecular mass PAH. Figure 3.24 shows the scores plot (A) and the loading plot (B) of *S. meliloti* exposed to the PAH mixture derived from coal tar at concentrations of 0.14 mg/L PAH mixture, while Figure 3.25 shows the scores plot (A) and loadings plot (B) of the control sample class versus samples exposed to 1.4 mg/L PAH mixture. The first two principal components,  $t[1]$  and  $t[2]$ , accounted for 66.8% of the total variation observed in the data set in the case of the 0.14 mg/L PAH experiment, while the first two principal components accounted for 71.4% of the variability in the 1.4 mg/L PAH experiment.

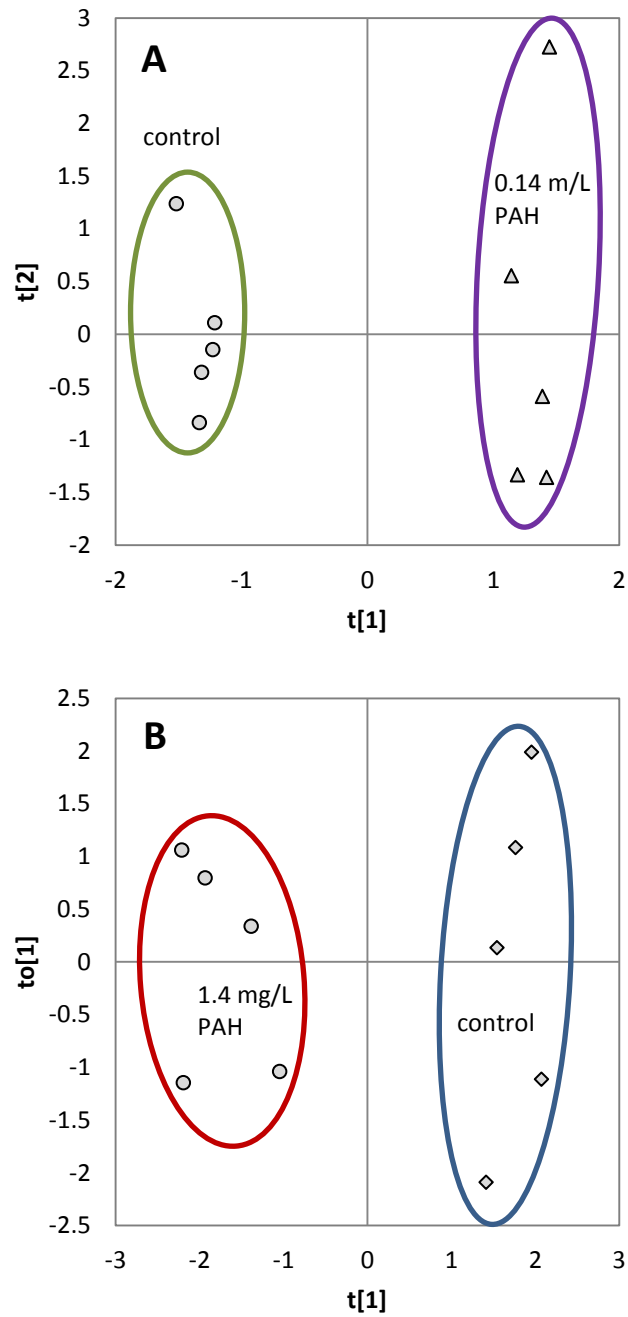


**Figure 3.24:** PCA scores plot (A) and loadings plot (B) of control vs 0.14mg/L PAH. The triangles indicate those ions which were identified as significant in the subsequent OPLS-DA analysis.



**Figure 3.25:** PCA scores plot (A) and loadings plot (B) of control vs 1.4 mg/L PAH. The triangles indicate those ions which were identified as significant in the subsequent OPLS-DA analysis.

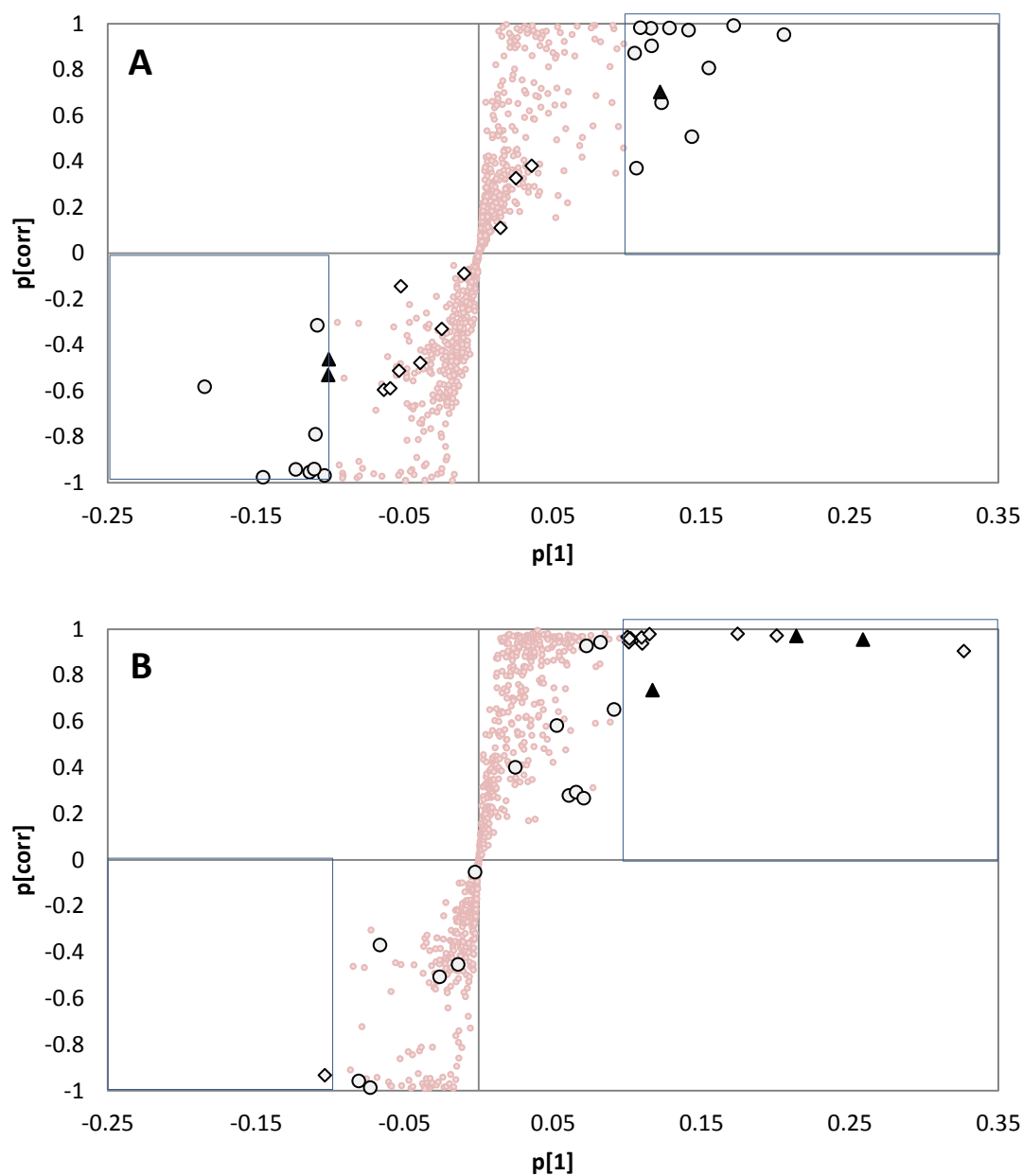
OPLS-DA was performed on the data from the PAH mixture exposures. The scores plots (Figure 3.26) show excellent separation of the control and exposed samples. The  $R^2X$  value values reflect the amount of variation in the level of metabolites that can be related to the differences between the sample classes. In this case,  $R^2X$  for the separation of control samples and samples exposed to 0.14 mg/L PAH was 24.3%, and the  $R^2X$  for the separation control samples and those exposed to 1.4 mg/L PAH was 41.9%. The  $R^2X(o_x)$  is the measure of in class variation seen in the scores plots.  $R^2X(o_1)$  for samples exposed to 0.14 mg/L PAH was 25.5%, and the  $R^2X(o_1)$  and for 1.4 mg/L PAH was 26.0%.



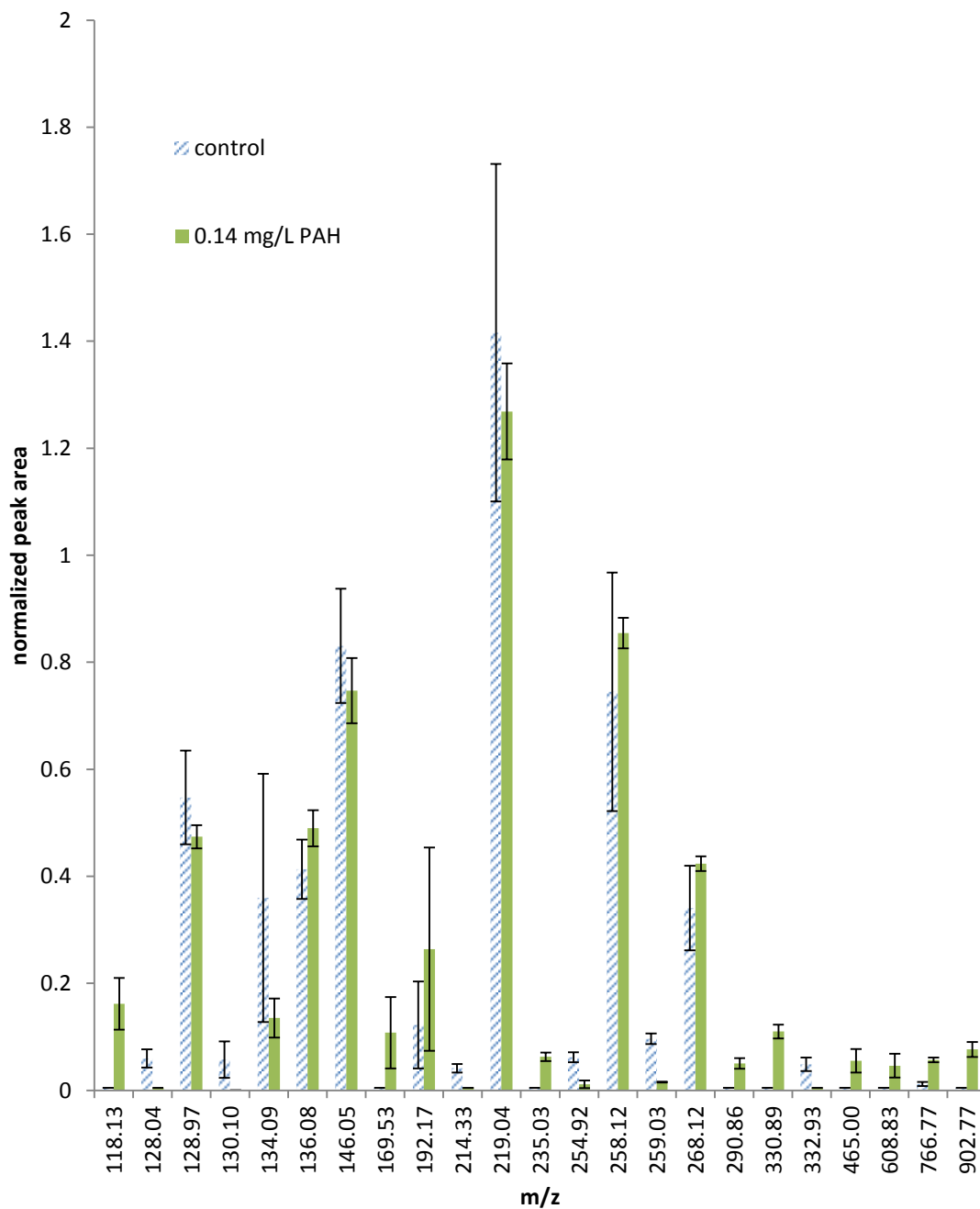
**Figure 3.26:** OPLS-DA scores plots of control bacteria versus bacteria exposed to (A) 0.14 mg/L PAH and (B) 1.4 mg/L PAH.

Figure 3.27 shows the S-plots for control versus 0.14 mg/L (A) and 1.4 mg/L (B) PAH mixture. Figure 3.28 lists the ions of components that were determined to be statistically significant between the control and the sample classes exposed to 0.14 mg/L PAH (Table 3.11 lists values with respective retention times), while Figure 3.29 lists the significant components for samples exposed to 1.4 mg/L PAH (Table 3.12 lists values with respective retention times). The three ions which were in common to both exposures had masses of 128.97, 136.08, and 146.05. Figure 3.30 shows the SUS plot comparing three sample classes, control, samples exposed to PAH at 0.14 mg/L and at 1.4 mg/L.





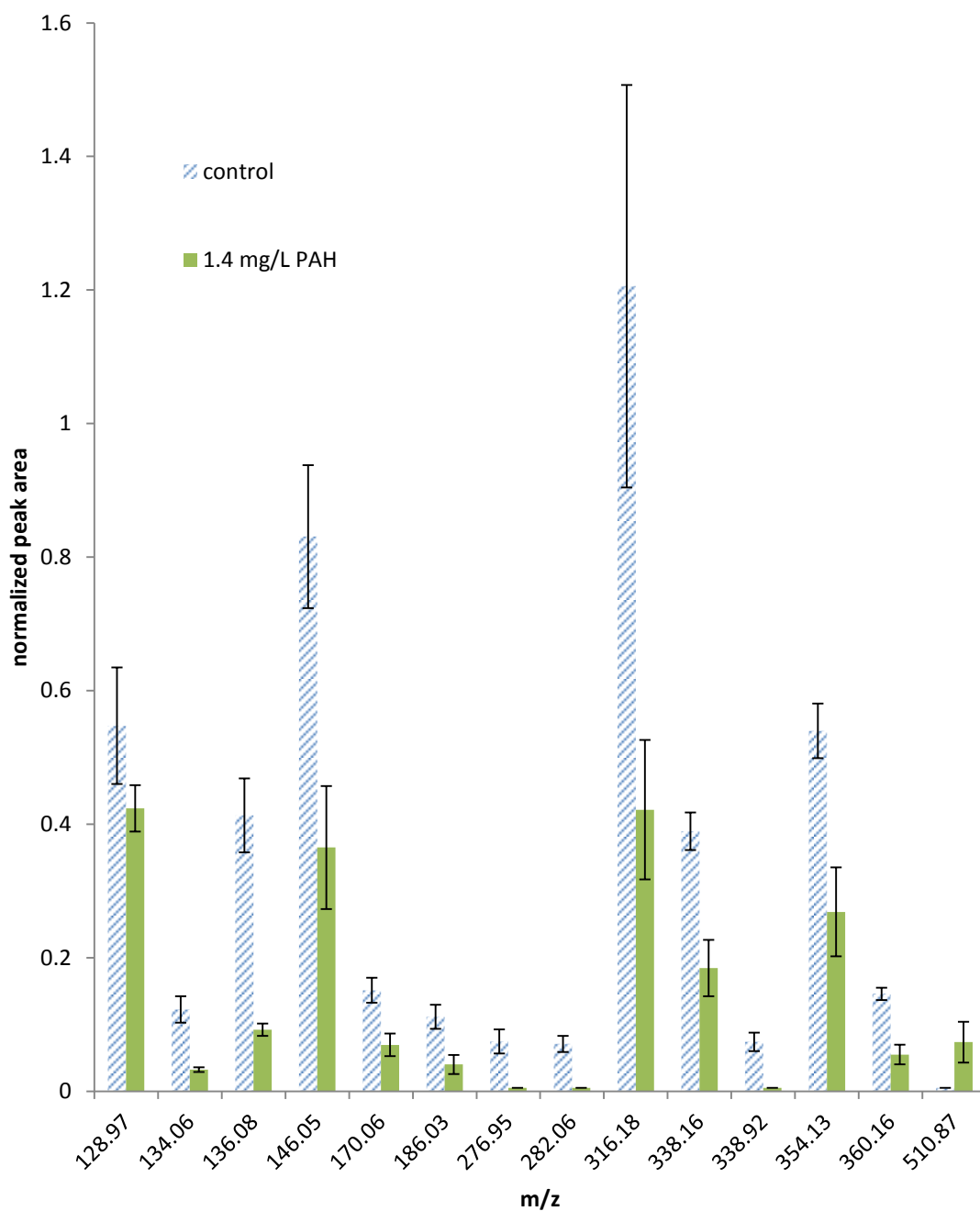
**Figure 3.27:** S-plots of control versus 0.14 mg/L PAH (A) and 1.4 mg/L PAH (B). Black triangles indicate ions with  $|p| > 0.1$  in both samples, circles indicate ions with  $|p| > 0.1$  in samples exposed to 0.14 mg/L fluorene, and diamonds indicate ions with  $|p| > 0.1$  in samples exposed to 1.4 mg/L fluorene. (A) is a plot of 711 features, and (B) contains 633 features.



**Figure 3.28:** Relative normalized peak areas of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 0.14 mg/L PAH experiments. Error bars indicate standard deviations (n=5).

**Table 3.11:** List of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 0.14 mg/L PAH experiments. These ions indicated in bold face are common with ions in Table 3.12.

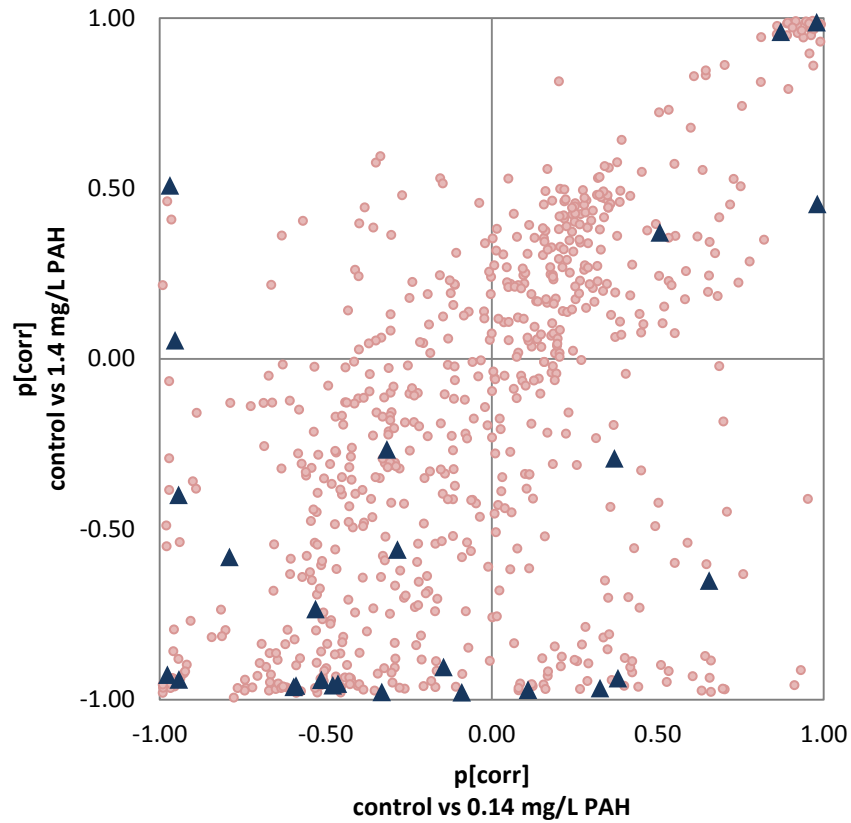
m/z	R <sub>t</sub> (min)	ion mode
0.14 mg/L PAH		
118.13	6.04	pos
128.04	7.86	neg
<b>128.97</b>	<b>7.94</b>	<b>neg</b>
130.10	6.56	neg
134.09	7.37	pos
<b>136.08</b>	<b>1.71</b>	<b>pos</b>
<b>146.05</b>	<b>8.65</b>	<b>neg</b>
169.53	9.96	neg
192.17	5.40	pos
214.33	6.99	neg
219.04	7.06	pos
235.03	7.08	neg
254.92	9.42	neg
258.12	9.20	pos
259.03	9.21	neg
268.12	1.96	pos
290.86	7.93	pos
330.89	9.43	neg
332.93	8.27	neg
465.00	5.59	neg
608.83	9.38	neg
766.77	9.43	neg
902.77	9.30	neg



**Figure 3.29:** Relative normalized peak areas of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 1.4 mg/L PAH experiments. Error bars indicate standard deviations ( $n=5$ ).

**Table 3.12:** List of ions determined to be statistically significant from OPLS-DA S plot ( $|p| > 0.1$ ) from comparison of control and 1.4 mg/L PAH experiments. These ions indicated in bold face are common with ions in Table 3.11.

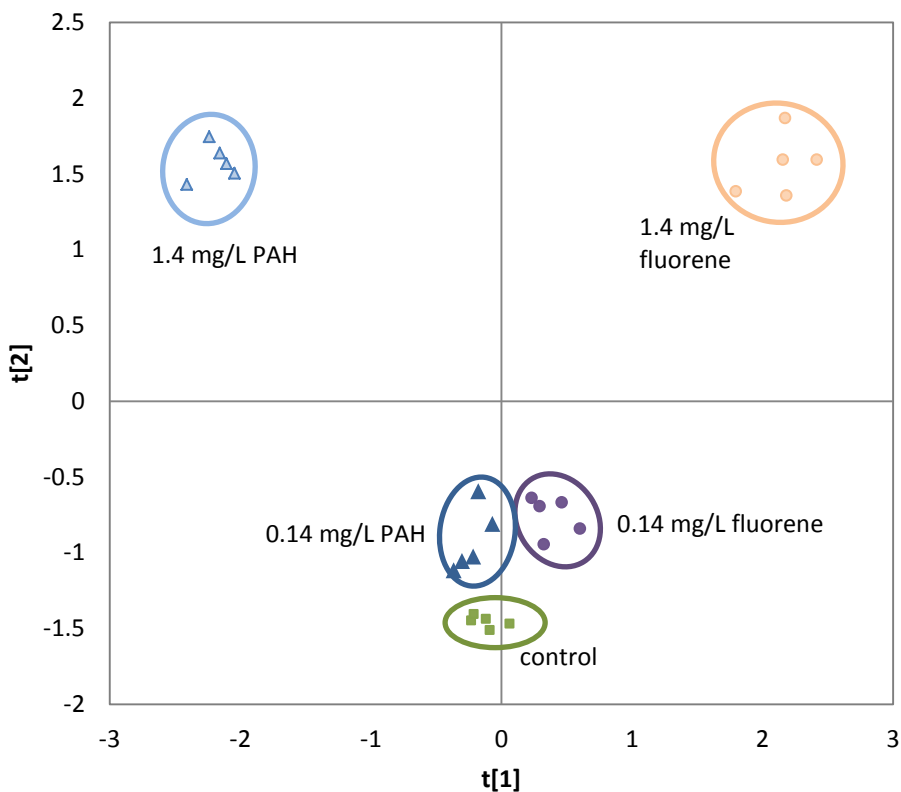
m/z	R <sub>t</sub> (min)	ion mode
1.4 mg/L PAH		
<b>128.97</b>	<b>7.94</b>	<b>neg</b>
134.06	1.71	neg
<b>136.08</b>	<b>1.71</b>	<b>pos</b>
<b>146.05</b>	<b>8.65</b>	<b>neg</b>
170.06	8.65	pos
186.03	8.65	pos
276.95	7.07	neg
282.06	6.69	neg
316.18	6.35	pos
338.16	6.38	pos
338.92	9.58	pos
354.13	6.38	pos
360.16	6.36	neg
510.87	9.34	neg



**Figure 3.30:** SUS plot of comparing samples exposed to PAH at 0.14 mg/L and 1.4 mg/L. Triangles indicate ions which were identified as significant (i.e.,  $|p| > 0.1$ ) from their respective S-plots.

*Comparing S. meliloti Grown in the Presence of Fluorene or PAH Mixture*

Multiple cultures of *S. meliloti* were grown in the absence and presence of fluorene (0.14 mg/L and 1.4 mg/L) and a PAH mixture (total PAH concentrations of 0.14 mg/L and 1.4 mg/L). The impacts of fluorene exposures and PAH mixture exposures on the *S. meliloti* caused significant changes in the metabolome. An OPLS2-DA analysis reveals important trends among the sample classes.



**Figure 3.31:** OPLS2-DA analysis of 5 classes of samples with 5 replicates in each class: control, 0.14 and 1.4 mg/L fluorene, 0.14 and 1.4 mg/L PAH. Data analysis includes 711 features.

The samples of *S. meliloti* exposed to fluorene or the PAH mixture at 0.14 mg/L were metabolically different from each other and from the control. The samples exposed at 1.4 mg/L fluorene or PAH mixture were very different from each other and from the other three sample sets. The S-plots of these two exposures (Figure 3.19) clearly showed the effect of dosage on the metabolome. Metabolites identified as significant ( $|p| > 0.1$ ) for the 1.4 mg/L fluorene exposure were plotted on the S-plot for 0.14 mg/L as circles. As the fluorene dosage increase, the metabolites identified as circles become more significant (i.e., had larger absolute p values in the 1.4 mg/L S-plot). This implies that a higher fluorene dosage induces similar, but more pronounced changes on the metabolism of *S. meliloti*. This is also evident in the SUS plot (Figure 3.23), as the general trend of data is along the diagonal from bottom left to top right; overall, many ions were either elevated in both exposed sample relative to control, or were decreased in exposed samples relative to control.

Because of the inconsistencies between the S-plots and SUS plots, it is difficult to determine which ions (i.e., compounds) are most significant. Certain ions appeared as significant ( $|p| < 0.1$ ) in both exposures, e.g., the m/z 134.09 ion (detected in positive ion mode), and the m/z 300.00 ion (detected in negative ion mode). These ions were elevated in both exposures compared to control, and were attributed to aspartic acid and N-acetyl-glucosamine-1-phosphate, respectively. The ions at m/z 146.05 (detected in negative ion mode) and m/z 118.10 (detected in positive ion mode) were significantly



decreased in the 1.4 mg/L fluorene exposure. These metabolites are assigned as glutamic acid and valine, respectively.

The effects of exposure to PAH mixtures at high and low dosages appear to have very different effects on the metabolome compared to fluorene. The S-plots comparing the control to samples exposed to 0.14 and 1.4 mg/L PAH produced few common ions. Some ions were significant ( $|p| > 0.1$ ) in both exposures, such as  $m/z$  136.08 (detected in positive ion mode). This ion corresponds to adenine and was elevated in the lower dosage of PAH, but decreased in the higher dosage of 1.4 mg/L PAH exposure. The ion at  $m/z$  146.05 (i.e., glutamate and detected in negative ion mode) decreased in both exposed samples, while the ion at  $m/z$  268.12 (detected in positive ion mode) was elevated in the lower dosage of PAH, and was identified as adenosine. Aspartic acid levels were elevated in both fluorene exposures; however, in samples exposed to 0.14 mg/L PAH, the levels of aspartic acid were decreased compared to control.

In the case of fluorene, it appeared as though the higher dosage had a similar, but more pronounced change on the metabolism of *S. meliloti*. However, in the case of PAH, it appears as though the effects of the PAH fraction at different concentrations has different effects on the metabolome of *S. meliloti*.

Not only is it difficult to understand which levels of ions are significantly contributing to the variation between classes, it is also challenging to confirm the

identity of an ion. Some ions identified as significant in this analysis had different  $m/z$  values but shared retention times. Although these ions may be related, the relationship cannot be determined. This problem can be resolved using high resolution and tandem mass spectrometry, as adduct ions should produce the same fragmentation patterns.

## Chapter 4: Conclusions and Future Work

The work in this thesis has developed an untargeted analytical approach to the metabolome of *S. meliloti* using HILIC-LC-ESI-MS. In order to analyse the large data sets produced, a methodology using open source software packages (XCMS and CAMERA) has been developed, which identifies specific ions for quantification of metabolites. Multivariate analysis was used to identify those metabolites which contributed to variation between wild type *S. meliloti* grown in the absence and presence of fluorene and a PAH mixture.

The first goal of this thesis was to investigate the effectiveness of HILIC chromatography to separate polar metabolites present in *S. meliloti*. The LC analysis run time was optimized to 22 minutes, which included 14 minutes of data acquisition and 5 minutes of re-equilibration. The chromatography produced bands of elution, as revealed by retention time deviations computed by XCMS/CAMERA. These retention time deviations will be used in the future for the optimization of chromatographic conditions of complex mixtures.

The second goal of this project was to explore and implement open source software in order to handle the large amount of data produced by HILIC-LC-ESI-MS. The XCMS/CAMERA package was successfully used to align chromatograms and calculate related adduct ions and isotopic ions. Approximately 2000 ions were detected by

XCMS/CAMERA in each sample class. It was found that the XCMS/CAMERA package was more effective than Bruker's DataAnalysis in integrating peak areas due to the inability of the DataAnalysis software to distinguish between mass spectrometrically resolved peaks with similar mass values. The relationships between ions as computed by XCMS/CAMERA were used to develop a lookup table which identified a unique mass and retention time for a unique species present in the bacterial extract. Approximately 35%, or 700 ions of the 2000 detected, were listed in the final lookup table.

Third, this study aimed to examine the effects of PAH in single and complex mixtures on the metabolome of *S. meliloti* using the multivariate statistical approaches. PCA was used as an initial check to ensure separation of sample classes. OPLS-DA analysis was performed on the approximately 700 ions listed in the lookup table. Both the S-plots and the SUS plots provided information on ions found to be significant between sample classes, although it was difficult to examine the plots simultaneously. It appears as though the  $|p| > 0.1$  cutoff for identifying significant components in the S-plots is too simplistic an approach and should be correlated with information from the SUS plots.

The S-plots identified several ions as significant. In the fluorene exposures, 22 ions were found to be significant in the 0.14 mg/L exposure and 16 in the 1.4 mg/L exposure, 6 of which were found in both samples. In the PAH mixture exposures, 23 ions were found to be significant in the 0.14 mg/L exposure, and 14 in the higher dosage of

1.4 mg/L, with 3 ions in common. Several ions were identified, including glutamate, aspartate, adenine, adenosine and N-acetyl-glucosamine-1-phosphate. From the multivariate analyses, it appeared as though the lower concentration exposures had less of an impact than the higher dosages. Low dosages of both fluorene and the PAH mixture produced a similar metabolic response in *S. meliloti*, while at higher dosages; the responses seemed to be more specific to each exposure.

Many of the ions identified as significant were not positively identified. The next task is to determine the molecular identities of these ions. One way to achieve this is to perform high resolution mass spectrometry on an instrument such as an Orbitrap. High resolution mass spectrometry can be used to determine elemental compositions while tandem mass spectrometry can be used to elucidate the structure of unknown metabolites by studying fragmentation patterns.

Once the chemical identity of these metabolites has been confirmed, they will be understood in terms of the biological relevance by relating them to known metabolic pathways in *S. meliloti*.

This project aimed to analyse both the polar and non-polar fraction of *S. meliloti* exposed to fluorene and PAH mixtures. This study only examined the polar fraction. This analysis, however, will not require too much additional work, as the extraction methods and analytical methods have already been developed.

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## APPENDICES

**Appendix 1: Literature review of environmental metabolomics**

Organism	Compound/ Mixture	Type of study	What do we need to know?	Number of compounds identified	Conclusion
<i>Daphnia magna</i> <sup>23, 31</sup>	fluoranthene, pyrene and mixtures (0.062, 0.125, 0.250 Toxic units)	transcriptomics, metabolomic profiling (NMR, GC-MS)	<i>D. magna</i> is commonly used for toxicological tests. Acute exposure of compounds was used to measure changes in gene expression and metabolism.	mRNA: 34 (fluoranthene), 27 (pyrene)(14 common to both), 127 mRNA fragments (mixtures)  Metabolites: 25 (NMR), 86 (GC-MS)	mRNA results showed the PAH mixture responses were more than additive. While the transcriptomes of pyrene and fluoranthene showed no differences, the metabolome profiles could be statistically separated. It was found that the response of the mixture can be similar or different from the response of the individual compounds depending on the concentrations of compounds in a mixture.
	copper (0, 5, 10, 25, 50 ug/L)	untargeted metabolomics (FT-ICR MS)	Because no previous metabolomics studies had been done using <i>D. magna</i> , this study focused on developing an effective MS metabolomics method for toxicity testing.	Metabolites: 4768 (assigned an empirical formula), 1017 (putatively identified)	The observed changes in the metabolome in response to Cu exposure were consistent with previous work. A novel marker for Cu toxicity was identified.
<i>Caenorhabditis elegans</i> <sup>57</sup> (Wild type used, as well as gk125 strain, with metallothionein deletions)	cadmium (12 uM)	metabolomic fingerprinting (NMR, UPLC-MS), knock out organism	<i>C. elegans</i> is a model organism and the complete genome has been sequenced. This study focused to compare metabolic fingerprints of both Ca exposed and mutant organisms.	-	The genotype did not modify the metabolomic profile, even though it is known that metallothionein is known to protect against cadmium. It was shown that the biological response is not controlled by changes in gene expression.

<i>Lumbricus rubellus</i> <sup>25, 8</sup> (earthworm)	cadmium, atrazine, fluoranthrene, and combinations (different ranges of toxins at sub-lethal effect range)	untargeted metabolomics (NMR)	The goal of this study was to distinguish the effects of different compounds, and assign modes of action.	-	Samples were discriminated using chemometrics, and individual biomarkers. The high doses showed higher variation and the results showed a relationship between metabolomic response and reproduction rate.
	pyrene (0, 10, 40, 160, 640 mg/kg soil)	untargeted metabolomics (NMR, GC-MS)	This study aimed to assess the metabolic changes due to exposure of earthworms to environmentally relevant concentrations of pyrene.	Metabolites: 32 (NMR), 51 (GC-MS)	Pyrene was found to cause a dose dependent effect, although the effects of pyrene seemed non-specific. Relating patterns of toxicity is difficult because the metabolism of pyrene varies among organisms.
<i>onchorhynchus tshawytscha</i> <sup>29</sup> (smolts of 2 or 3 year old were used)	water-accommodated (WAF) (0.39-6.25 g/L), chemical-enhanced (CE WAF) (0.063-1.0 g/L) fraction of Prudhoe Bay crude oil	metabolomics (NMR)	This study aimed to compare the effect of water-accommodated fraction of crude oil (naturally source), with the chemically enhanced water fraction.	Metabolites: 18 (smolt muscle), 21 (smolt liver)	Two potential sub lethal biomarkers were discovered. Both CEWAF and WAF exposure produced similar, but distinct metabolomic patterns.
<i>Pseudomonas pseudoalcaligenes</i> <sup>26</sup> (KF707, and KF707 strain T5 with hyper-resistance to tellurite)	tellurite (25 ug/mL)	genomics, targeted metabolomics (NMR)	The metabolomic analysis of an isolated KF707 mutant with hyper resistance to tellurite was done, as well as microarray analysis in order to determine the mechanism of resistance.	mRNA: 26 Metabolites: 27	The mutant T5, in the absence of tellurite, produced a similar metabolomic profile to the exposed wild type. However, when T5 was exposed, a different profile was observed.

<i>Eisenia fetida</i> <sup>58</sup> (earthworms)	dichlorodiph enyltrichloro ethane (DDT), endosulfan (0.5, 1.0, 2.0 ug/cm <sup>2</sup> )	metabolomics (NMR, GC-MS)	The goal of this study was to use NMR metabolomics to identify an appropriate biomarker, as well as use GC/MS metabolomics to quantify metabolite concentrations.	-	This study found that by using the metabolomic profile of earthworms, biomarkers can be used to determine the contaminant concentration in soil from contaminated sites.
<i>Mytilus edulis</i> <sup>30</sup> (marine mussels, sourced from Scottish waters)	atrazine (3 mg/L, 5 ug/L), lindane (1 mg/L, 5 ug/L)	metabolomics (NMR)	Metabolomics was used to identify the impact of each toxicant and distinguish its effects from those of the natural environmental stresses.	Metabolites: 21	Mussels exposed to atrazine could be separated by their metabolomic profile from those starved and subjected to hypoxia, as well as high and low doses of atrazine. The response of the mussels to lindane was consistent with previous work.
<i>Sinorhizobium</i> <i>sp. C4</i> <sup>59</sup> (Isolated from PAH contaminated soils in Hawaii)	phenanthren e (300 mg/L)	untargeted metabolomics (GC-MS)	The goal of study was to understand the pathway of phenanthrene degradation using untargeted metabolomics.	Metabolites: 118	Large metabolomic differences were observed between cultures grown on phenanthrene and natural carbon sources.
<i>Saccharomyces</i> <i>cerevisiae</i> S244C <sup>32</sup>	cadmium (0.03 mM CdCl <sub>2</sub> )	genomics, metabolomics (CE-MS)	Using <i>S. cerevisiae</i> , this study aimed to integrate genomics and metabolomics studies.	mRNA: 310 genes up regulated, 322 genes down regulated Metabolites: 17	The observed changes in genome suggest that Cd causes oxidative stress, and induction of the pathway of sulphur amino acid. Different metabolites were identified as responding to cadmium toxicity.
<i>Pimephales</i> <i>promelas</i> <sup>28</sup> (fathead minnow)	17(alpha)- ethynylestra diol (EE2) (synthetic estrogen) (0, 10, 100 ng/L)	metabolomic profiling (NMR)	In the environment, fish are exposed to varibel levels of toxin mixtures. The mode of action is also dependent on gender and duration of exposure.	-	Metabolomic data showed that male fish can compensate and recover from low EE2 exposure. This can be useful for regulators to be able to differentiate exposure concentrations that produce short term affects, and those that produce long term damage.

<i>apodemus sylvaticus</i> (wood mice) <i>myodes glareolus</i> (bank voles) <sup>22</sup>	cadmium (33.5 mg/L)	metabolomics (NMR)	The goal was to study the biochemical consequences of Cd. No studies have looked at long term environmentally realistic exposure.	-	The metabolic responses to toxin were similar in both voles and mice. As well, the metabolic changes were likely due to a response to liver tissue damage, and not directly due to exposure to Cd.
<i>onchorhynchus mykiss</i> <sup>60</sup> (rainbow trout)	ethinylestradiol (EE2, a contraceptive estrogen) (0.87 and 10 ng/L)	untargeted metabolomics (NMR)	Because he affects of estrogen in fish is well documented, this system can be used as a model for metabolomics studies.	-	Many of the identified metabolites were related to previous knowledge of effect of estrogen on fish, however, the low dosage of 1 ng/L did not show any significant difference from the control.
<i>onchorhynchus tshawytscha</i> <sup>27</sup> (exposed eggs, and alevins))	dinoseb(50-750 ppb), diazinon (10-100 ppm), esfenvalerate (1-100 ppb)	metabolomics (NMR, HPLC-UV)	This study aimed to use metabolomics to determine the effects of pesticides in storm-water run-offs on the health of eggs and alevins.	-	The metabolic effects of diazinon corresponded to the know mechanism of action.
<i>scendesmus vaculoatus</i> <sup>33</sup> (green algae)	prometryn (herbicide which inhibits photosystem II) (0.1 umol/L)	Metabolomics (GC-MS)	The goal of this study was to link physiological markers and changes in the metabolome, in order to detect effects of chemicals at sub-acute toxic levels.	mRNA: 51 differences, 29 identified	It was found that changes in the metabolome were seen at much lower dose levels than perturbations in growth.
<i>Diporeia</i> <sup>24</sup> (species collected from Lake Michigan and Lake Superior)	atrazine (.03-3000 ppb)	metabolomic profiling (GCxGC/TOF-MS)	The metabolomes of species taken from Lake Superior and Michigan were compared. The affects of atrazine on the organism was also investigated.	Total metabolites identified: 76 (lake comparison), 302 (atrazine) Changed: 72 (lake comparison), 35 (atrazine)	GCxGC/TOF-MS was useful tool for the detection and identification of a large number of metabolites. However, the differences in the metabolomic profiles of species taken from the different lakes may be attributed to differences in populations, gender or age.

*Pseudomonas putida*,  
*Pseudomonas aeruginosa*,  
*Micrococcus luteus*,  
*Blastomonas nataroria*<sup>61</sup>

atenolol, propranolol (chiral pharmaceuticals) (10-130 ug/mL)	fingerprint metabolomics (FT-IR)	Although their mode of action of active pharmaceutical ingredients (API) is well understood in humans, similar targets in microorganisms may control different processes.	Fingerprint metabolomics was done, so only changes in classes as a whole were observed.	The authors presented FT-IR coupled with chemometrics as a useful method to investigate the phenotypes and metabolic differences for a microorganism's response to APIs.
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**Appendix 2: XCMS/CAMERA script executed in RProject for Statistical Computing:**

```
myDir = "C:/Users/..."
### ++++++
### change working directory to your files, see +++ section
setwd(myDir)
### get working directory
(WD <- getwd())
### load the xcms package
library(xcms)
### finds peaks
xset <- xcmsSet()
### print used files and memory usage
xset
### Group peaks together across samples
xset <- group(xset, sleep=.0001)
### Calculate retention time deviations for every time
xset2 <- retcor(xset, family="s", plotype="m")
### Group peaks together across samples, set bandwidth, change important m/z parameters here
### Syntax: group(object, bw = 30, minfrac = 0.5, minsamp= 1, mzwid = 0.25, max = 5, sleep = 0)
xset2 <- group(xset2, bw =30, minfrac = 0.5, minsamp= 1, mzwid = 0.25, max = 5, sleep = 0)
### identify peak groups and integrate samples
xset3 <- fillPeaks(xset2)
### print statistics
xset3
### load the CAMERA package
library(CAMERA)
### create an xsAnnotate object
xsa <- xsAnnotate(xset3)
### group after RT value of the xcms grouped peak
xsaF <- groupFWHM(xsa, perfwhm=0.6)
### annotate isotopes
### note: this can be done before grouping
xsaFI <- findIsotopes(xsaF, mzabs=0.01, maxcharge=3, maxiso=3, ppm=5)
### verify grouping
xsaC <- groupCorr(xsaFI, cor_eic_th=0.75, polarity="negative")
### annotate adducts
xsaFA <- findAdducts(xsaFI, polarity="negative", ppm=5, multiplier=3)
### get final peaktable and store on drive
write.csv(getPeaklist(xsaFA), file="result_Camera.csv")
```



**Appendix 3: Metabolites detected in *E. coli* and their cellular concentrations**<sup>55</sup>

Metabolite	compound class	mol/L	molar mass
Glutamic acid	amino acid	9.6E-02	147.05
Glutathione	tripeptide	1.7E-02	307.08
Fructose-1,6-bisphosphate	sugar	1.5E-02	340.00
ATP	nucleotide	9.6E-03	507.00
UDP-N-acetylglucosamine		9.2E-03	607.08
Hexose-Pa		8.8E-03	260.03
UTP	nucleotide	8.3E-03	483.97
GTP	nucleotide	4.9E-03	522.99
TTP	nucleoside	4.6E-03	497.98
Aspartic acid	amino acid	4.2E-03	133.04
Valine	amino acid	4.0E-03	117.08
Glutamine	amino acid	3.8E-03	146.07
6-Phosphogluconate	Entner–Doudoroff pathway	3.8E-03	276.02
CTP	nucleotide	2.7E-03	482.98
Alanine	amino acid	2.6E-03	89.05
NAD +	coenzyme	2.6E-03	663.11
UDP-glucose	nucleotide sugar	2.5E-03	566.06
Glutathione disulfide	disulfide	2.4E-03	612.15
Uridine	nucleoside	2.1E-03	244.07
Citric acid	TCA intermediate	2.0E-03	192.03
UDP	nucleotide	1.8E-03	404.00
malic acid (malate)	TCA intermediate	1.7E-03	134.02
3-Phosphoglyceric acid	glycolysis pathway	1.5E-03	185.99
Glyceric acid	sugar	1.4E-03	106.03
Citrulline	amino acid	1.4E-03	175.10
Coenzyme A	TCA intermediate	1.4E-03	767.12
Pentose-Pc		1.3E-03	230.02
Glucosamine-6-phosphate		1.2E-03	259.05
Acetylphosphate		1.1E-03	139.99
Gluconolactone		1.0E-03	178.05
GDP	nucleotide	6.8E-04	443.02
Acetyl-CoA	TCA intermediate	6.1E-04	809.13
Carbamoyl aspartic acid	modified amino acid	5.9E-04	176.04
Succinic acid	TCA intermediate	5.7E-04	118.03
Arginine	amino acid	5.7E-04	174.11
UDP-glucuronate		5.7E-04	580.03
ADP	nucleotide	5.6E-04	427.03
Asparagine	amino acid	5.1E-04	132.05
alpha-Ketoglutaric acid	TCA intermediate	4.4E-04	146.02
Lysine	amino acid	4.1E-04	146.11
Proline	amino acid	3.9E-04	115.06
dTDP	deoxynucleotide	3.8E-04	402.02

Homocysteine	modified amino acid	3.7E-04	135.04
Dihydroxyacetone phosphate		3.7E-04	170.00
CMP	nucleotide	3.6E-04	323.05
Isoleucine + leucine	amino acid	3.0E-04	131.09
Deoxyribose-5-Phosphate		3.0E-04	214.02
AMP	nucleotide	2.8E-04	347.06
Inosine monophosphate		2.7E-04	348.05
PRPP		2.6E-04	389.95
Succinyl-CoA	TCA intermediate	2.3E-04	867.13
Inosine triphosphate		2.1E-04	507.98
Guanine	nucleobase	1.9E-04	151.05
Threonine	amino acid	1.8E-04	119.06
Phosphoenolpyruvic acid		1.8E-04	167.98
S-Adenosyl-L-methionine	modified amino acid	1.8E-04	398.14
FAD		1.7E-04	755.15
Methionine	amino acid	1.5E-04	149.05
2,3-Dihydroxybenzoic acid		1.4E-04	154.03
Fumaric acid	TCA intermediate	1.2E-04	116.01
NADPH	coenzyme	1.2E-04	745.09
Phenylpyruvic acid		9.0E-05	164.05
NADH	coenzyme	8.3E-05	665.12
N-Acetyl-glucosamine-1P		8.2E-05	301.06
Serine	amino acid	6.8E-05	105.04
Histidine	amino acid	6.8E-05	155.07
Flavin mononucleotide		5.4E-05	442.09
4-Hydroxybenzoate		5.2E-05	138.03
Glycerol-3-phosphate		4.9E-05	172.01
N-Acetyl-ornithine		4.3E-05	174.10
Gluconic acid		4.2E-05	196.06
Cyclic AMP		3.5E-05	329.05
dCTP	deoxynucleotide	3.5E-05	466.99
Malonyl-CoA		3.5E-05	853.12
Tyrosine	amino acid	2.9E-05	181.07
GMP	nucleotide	2.4E-05	363.06
Inosine diphosphate		2.4E-05	428.01
Acetoacetyl-CoA		2.2E-05	851.14
Riboflavin		1.9E-05	374.12
Phenylalanine	amino acid	1.8E-05	165.08
cis-Aconitic acid		1.6E-05	174.02
dATP	deoxynucleotide	1.6E-05	491.00
Cytosine	nucleobase	1.4E-05	111.04
Shikimic acid		1.4E-05	174.05
Histidinol		1.3E-05	141.09
Dihydroorotic acid		1.2E-05	158.03
Quinolinic acid		1.2E-05	167.02
Tryptophan	amino acid	1.2E-05	204.09

Ornithine	amino acid	1.0E-05	132.09
dAMP	deoxynucleotide	8.8E-06	331.07
Adenosine phosphosulfate		6.6E-06	427.02
Myo-inositol		5.7E-06	180.06
Propionyl-CoA		5.3E-06	823.14
ADP-glucose		4.3E-06	589.08
Anthranilic acid	amino acid	3.5E-06	137.05
Deoxyadenosine		2.8E-06	251.10
Cytidine	nucleoside	2.6E-06	243.09
NADP +	coenzyme	2.1E-06	744.08
Guanosine	nucleoside	1.6E-06	283.09
Adenine	nucleobase	1.5E-06	135.05
Deoxyguanosine		5.2E-07	267.10
Adenosine	nucleoside	1.3E-07	267.10

**Appendix 4: Normalized peak areas of all ions used in multivariate analyses**Look up table for *S. meliloti* control samples

avg(mz)	avg(rt)	ionization mode	sample 1	sample 2	sample 3	sample 4	sample 5
78.97	9.38	neg	1.58E-02	1.13E-02	1.57E-02	1.94E-02	1.62E-02
87.98	5.58	neg	2.98E-03	2.19E-03	2.47E-03	3.64E-03	2.84E-03
90.99	8.29	pos	3.76E-02	2.57E-02	2.63E-02	4.08E-02	2.91E-02
100.05	7.07	neg	2.51E-02	2.13E-02	1.73E-02	2.19E-02	2.16E-02
100.12	4.66	pos	2.73E-02	2.23E-02	1.78E-02	2.21E-02	2.90E-02
101.08	2.05	pos	9.28E-03	4.37E-03	5.52E-03	7.37E-03	8.84E-03
102.06	8.65	neg	6.89E-02	7.49E-02	6.92E-02	9.58E-02	8.06E-02
102.07	7.12	pos	7.38E-02	6.84E-02	5.47E-02	9.48E-02	7.72E-02
102.07	8.65	pos	4.91E-02	5.20E-02	4.37E-02	5.80E-02	5.01E-02
104.12	7.04	pos	5.16E-02	4.79E-02	3.12E-02	7.34E-02	4.70E-02
105.00	8.26	pos	2.01E-02	1.60E-02	1.68E-02	3.45E-02	2.46E-02
106.10	7.63	pos	2.52E-02	1.68E-02	1.07E-02	2.73E-02	2.20E-02
107.08	7.08	pos	4.61E-01	4.05E-01	3.55E-01	4.77E-01	4.39E-01
110.02	12.93	pos	1.69E-02	1.21E-02	8.49E-03	1.95E-02	1.63E-02
112.07	4.74	pos	1.27E-02	2.34E-02	1.27E-02	8.11E-03	1.27E-02
116.08	7.60	pos	4.60E-02	3.98E-02	3.06E-02	5.65E-02	4.33E-02
117.02	1.45	neg	2.15E-02	2.54E-02	2.14E-02	3.47E-02	2.41E-02
117.11	7.49	pos	2.10E-02	1.83E-02	1.28E-02	3.91E-02	2.10E-02
118.10	7.52	pos	4.84E-01	3.97E-01	2.88E-01	8.74E-01	5.50E-01
119.08	2.04	pos	2.81E-02	1.47E-02	1.67E-02	2.42E-02	2.80E-02
120.09	4.65	pos	6.48E-02	6.96E-02	6.40E-02	6.28E-02	6.78E-02
120.09	4.65	pos	6.48E-02	6.96E-02	6.40E-02	6.28E-02	6.78E-02
120.09	7.40	pos	4.26E-02	4.01E-02	3.00E-02	4.80E-02	4.08E-02
121.06	0.86	pos	2.02E-02	2.09E-02	2.90E-02	4.32E-02	1.94E-02
122.90	1.24	neg	4.42E-03	3.36E-03	8.76E-04	3.15E-03	2.70E-03
122.94	7.96	pos	1.72E-01	1.38E-01	1.18E-01	2.02E-01	1.48E-01
124.99	1.25	neg	8.96E-03	7.36E-03	1.22E-02	4.20E-03	1.23E-03
125.95	5.57	neg	4.35E-03	3.14E-03	3.40E-03	4.90E-03	3.34E-03
128.03	12.92	pos	2.12E-02	1.29E-02	9.41E-03	2.07E-02	1.27E-02
128.04	7.86	neg	5.34E-02	4.22E-02	6.14E-02	8.75E-02	5.32E-02
128.04	8.65	neg	4.81E-02	5.35E-02	4.97E-02	6.54E-02	5.40E-02
128.14	6.39	pos	2.71E-01	2.67E-01	2.38E-01	2.82E-01	2.61E-01
128.97	7.94	neg	6.96E-01	5.00E-01	4.87E-01	5.57E-01	4.97E-01
130.06	1.37	neg	2.80E-03	3.34E-03	2.62E-03	3.36E-03	2.94E-03
130.09	6.56	neg	3.12E-02	4.04E-02	3.63E-02	1.13E-01	6.67E-02
132.07	7.42	neg	2.65E-02	3.94E-02	2.47E-02	7.58E-02	5.02E-02
134.05	1.71	neg	1.19E-01	1.17E-01	1.49E-01	1.31E-01	9.54E-02
134.09	7.37	pos	1.75E-01	3.05E-01	1.63E-01	7.26E-01	4.30E-01
136.06	7.08	pos	4.43E-01	3.92E-01	3.38E-01	4.39E-01	4.13E-01
136.08	1.71	pos	3.87E-01	4.58E-01	3.82E-01	4.85E-01	3.55E-01
137.09	2.04	pos	1.23E-01	7.49E-02	7.51E-02	1.08E-01	1.19E-01
139.88	1.26	neg	6.93E-03	4.39E-03	2.30E-03	5.48E-03	4.68E-03
140.99	5.58	neg	2.09E-02	1.50E-02	1.52E-02	2.27E-02	1.71E-02
141.88	1.26	neg	1.12E-01	7.36E-02	1.98E-02	8.75E-02	7.19E-02
142.98	5.57	neg	1.97E-02	1.40E-02	1.49E-02	2.20E-02	1.65E-02

143.87	1.26	neg	7.15E-02	4.63E-02	1.23E-02	5.84E-02	4.76E-02
144.18	2.31	pos	1.92E-03	4.62E-03	1.46E-03	5.16E-03	7.07E-03
145.06	6.96	pos	1.19E-01	7.44E-02	7.89E-02	1.80E-01	1.18E-01
145.07	8.51	neg	3.86E-02	3.48E-02	3.33E-02	2.04E-02	3.67E-02
146.05	8.65	neg	6.54E-01	8.49E-01	8.41E-01	9.45E-01	8.63E-01
149.05	6.98	neg	1.09E-01	8.24E-02	1.08E-01	1.58E-01	1.18E-01
151.03	2.22	neg	1.92E-02	1.95E-02	2.46E-02	2.23E-02	2.00E-02
155.09	7.07	pos	2.04E-01	1.72E-01	1.58E-01	2.30E-01	1.97E-01
158.98	8.31	pos	1.14E-01	7.76E-02	7.09E-02	1.14E-01	8.60E-02
158.99	12.92	neg	6.48E-02	4.75E-02	4.28E-02	6.56E-02	5.29E-02
159.08	2.05	pos	1.28E-02	5.71E-03	7.70E-03	1.04E-02	1.30E-02
159.08	8.65	neg	2.21E-02	2.23E-02	2.04E-02	1.67E-02	1.92E-02
162.05	3.07	neg	1.70E-02	1.53E-02	1.66E-02	2.29E-02	1.47E-02
168.04	8.67	neg	9.01E-02	7.13E-02	6.18E-02	7.90E-02	6.58E-02
170.06	8.65	pos	1.29E-01	1.54E-01	1.38E-01	1.77E-01	1.59E-01
171.05	2.05	neg	5.25E-02	1.96E-02	5.10E-02	3.69E-02	4.57E-02
171.10	6.34	pos	3.78E-02	3.35E-02	2.49E-02	4.08E-02	3.52E-02
171.12	6.40	neg	1.24E-01	1.13E-01	1.23E-01	1.19E-01	1.22E-01
173.05	2.05	neg	1.69E-02	6.48E-03	1.66E-02	1.21E-02	1.55E-02
173.14	6.39	pos	1.17E-01	1.14E-01	1.16E-01	1.24E-01	1.17E-01
175.08	7.08	pos	8.62E-02	8.17E-02	5.84E-02	6.57E-02	6.82E-02
175.13	10.29	pos	1.15E-01	1.02E-01	9.36E-02	1.59E-01	1.07E-01
176.05	1.39	neg	5.70E-03	5.40E-03	6.78E-03	5.99E-03	4.71E-03
176.94	9.39	neg	6.62E-02	4.79E-02	7.35E-02	1.21E-01	8.19E-02
177.05	2.79	neg	1.61E-02	1.15E-02	1.73E-02	9.26E-03	1.33E-02
180.15	0.66	pos	4.41E-02	5.04E-02	5.60E-02	6.44E-02	6.38E-02
183.04	1.25	neg	7.17E-03	5.92E-03	8.21E-03	3.82E-03	3.99E-03
186.03	8.65	pos	8.63E-02	1.18E-01	1.04E-01	1.35E-01	1.14E-01
187.87	1.26	neg	5.06E-02	3.71E-02	9.19E-03	3.82E-02	3.55E-02
188.03	8.65	pos	8.14E-03	1.15E-02	8.37E-03	1.37E-02	1.03E-02
188.19	11.52	pos	4.32E-02	3.55E-02	4.62E-02	1.41E-01	8.42E-02
189.10	9.81	neg	1.92E-02	2.17E-02	1.77E-02	1.95E-02	2.90E-02
189.87	1.26	neg	3.27E-02	2.39E-02	2.42E-02	2.45E-02	2.26E-02
191.10	6.70	pos	1.78E-01	1.74E-01	1.24E-01	1.55E-01	1.48E-01
191.87	1.26	neg	6.98E-03	5.43E-03	1.91E-03	5.46E-03	4.52E-03
192.04	8.67	pos	1.77E-01	1.46E-01	1.28E-01	1.84E-01	1.50E-01
192.11	6.71	pos	6.78E-01	6.05E-01	5.31E-01	6.62E-01	6.33E-01
192.17	5.40	pos	2.27E-01	6.55E-02	6.34E-02	6.09E-02	1.93E-01
193.12	6.70	pos	4.01E-01	3.49E-01	3.12E-01	3.78E-01	3.63E-01
193.99	5.57	neg	2.50E-02	1.77E-02	1.81E-02	2.66E-02	2.10E-02
195.98	5.57	neg	3.01E-02	2.07E-02	2.12E-02	3.42E-02	2.46E-02
196.96	7.98	neg	1.55E-01	1.07E-01	9.09E-02	1.13E-01	9.73E-02
197.98	5.58	neg	1.48E-02	1.07E-02	1.11E-02	1.71E-02	1.26E-02
198.11	6.93	pos	5.02E-01	2.80E-01	2.97E-01	8.13E-01	4.96E-01
199.05	7.63	neg	7.52E-02	3.19E-02	3.45E-02	2.96E-02	8.79E-02
203.07	7.10	pos	1.48E+00	9.64E-01	9.09E-01	1.44E+00	1.16E+00
205.08	7.39	pos	1.07E-01	5.30E-02	4.16E-02	6.95E-02	1.63E-01
206.80	5.92	neg	2.16E-01	7.78E-02	8.69E-02	7.21E-02	7.38E-02
206.90	7.94	pos	2.61E-02	2.65E-02	1.95E-02	4.76E-02	3.17E-02
207.12	6.70	neg	3.12E-01	2.72E-01	2.68E-01	2.57E-01	2.76E-01
208.01	8.69	pos	6.70E-02	5.59E-02	4.81E-02	6.49E-02	5.26E-02
208.90	7.93	pos	6.00E-03	6.18E-03	4.80E-03	1.15E-02	8.18E-03

209.14	6.71	pos	2.14E-01	1.85E-01	1.70E-01	2.27E-01	2.04E-01
212.13	6.65	pos	8.26E-02	6.66E-02	6.08E-02	6.99E-02	6.41E-02
212.14	2.68	pos	1.07E-02	9.61E-03	9.05E-03	8.28E-03	9.19E-03
212.93	7.94	neg	1.17E-01	8.08E-02	8.31E-02	9.11E-02	7.98E-02
213.03	7.10	pos	3.00E-02	2.46E-02	1.91E-02	2.06E-02	1.82E-02
213.06	8.46	neg	1.92E-02	1.62E-02	1.17E-02	7.63E-03	1.43E-02
213.09	0.86	neg	4.85E-03	3.67E-03	5.24E-03	3.71E-03	2.88E-03
214.01	8.94	pos	8.53E-02	5.71E-02	4.64E-02	6.34E-02	5.27E-02
214.05	8.75	neg	4.06E-02	4.63E-02	3.55E-02	4.16E-02	4.21E-02
214.14	0.98	neg	1.65E-02	1.65E-02	3.31E-02	1.53E-02	1.40E-02
214.33	6.99	neg	4.18E-02	3.12E-02	3.96E-02	5.39E-02	4.00E-02
214.89	1.24	neg	5.96E-03	6.23E-03	1.92E-03	4.62E-03	4.15E-03
215.02	7.09	pos	8.27E-03	6.58E-03	1.21E-02	6.10E-03	6.16E-03
216.16	0.98	pos	9.99E-03	9.68E-03	8.50E-03	9.33E-03	8.24E-03
219.04	7.06	pos	1.74E+00	1.15E+00	1.07E+00	1.74E+00	1.38E+00
219.05	7.14	neg	1.67E-01	1.17E-01	1.10E-01	1.53E-01	1.92E-01
221.04	7.07	pos	1.64E-01	1.04E-01	9.27E-02	1.50E-01	1.38E-01
224.11	7.34	neg	1.25E-02	1.39E-02	1.21E-02	1.88E-02	1.43E-02
225.03	9.34	pos	1.31E-02	1.56E-02	1.18E-02	1.22E-02	1.39E-02
226.00	8.70	neg	3.95E-02	2.84E-02	2.64E-02	3.16E-02	3.02E-02
226.14	7.29	pos	4.77E-02	1.94E-02	1.04E-02	5.66E-02	3.65E-02
226.97	8.30	pos	3.48E-01	2.54E-01	2.48E-01	3.81E-01	2.96E-01
228.06	8.60	neg	2.79E-02	3.21E-02	2.27E-02	2.67E-02	2.66E-02
229.06	2.67	neg	6.52E-03	4.73E-03	7.93E-03	4.75E-03	4.97E-03
230.03	8.66	pos	6.51E-02	5.38E-02	4.13E-02	5.45E-02	5.14E-02
231.12	6.71	pos	2.08E-02	1.72E-02	1.65E-02	1.78E-02	1.67E-02
232.13	6.72	pos	2.00E-01	1.67E-01	1.41E-01	1.76E-01	1.57E-01
233.09	7.96	pos	7.94E-02	5.81E-02	4.84E-02	7.72E-02	6.38E-02
234.93	9.44	pos	3.88E-02	2.69E-02	3.18E-02	5.22E-02	3.60E-02
235.97	9.95	pos	2.42E-02	1.61E-02	1.51E-02	2.44E-02	1.93E-02
238.05	2.02	neg	5.89E-03	5.12E-03	8.48E-03	4.65E-03	5.13E-03
238.06	8.76	pos	1.41E-02	1.49E-02	9.70E-03	1.35E-02	1.32E-02
239.05	2.03	neg	1.29E-02	5.79E-03	1.32E-02	9.23E-03	1.19E-02
242.02	8.67	neg	2.26E-02	2.53E-02	2.63E-02	2.73E-02	2.55E-02
242.61	8.30	pos	1.43E-01	9.26E-02	7.53E-02	1.23E-01	9.45E-02
242.99	7.06	pos	1.74E-02	1.29E-02	1.73E-02	1.77E-02	1.82E-02
243.07	2.47	neg	4.28E-02	4.41E-02	4.04E-02	7.19E-02	3.88E-02
243.09	1.02	neg	9.20E-03	6.50E-03	9.73E-03	1.58E-02	9.37E-03
243.12	0.82	pos	2.76E-03	3.30E-03	2.32E-03	2.92E-03	2.09E-03
243.90	1.24	neg	1.11E-02	1.00E-02	4.28E-03	6.22E-03	5.32E-03
244.11	8.63	pos	1.62E-02	2.31E-02	1.39E-02	2.21E-02	2.12E-02
244.12	5.94	pos	8.91E-03	2.01E-02	1.96E-02	2.04E-02	1.22E-02
245.05	8.13	neg	9.35E-03	4.28E-02	1.48E-02	3.75E-02	3.38E-02
245.09	2.48	pos	1.49E-02	1.94E-02	1.29E-02	2.75E-02	1.49E-02
245.10	7.40	pos	1.31E-01	1.26E-01	9.36E-02	1.34E-01	1.14E-01
245.12	1.00	pos	1.53E-02	1.21E-02	1.46E-02	2.88E-02	1.94E-02
245.90	1.24	neg	5.33E-03	4.66E-03	1.80E-03	2.63E-03	2.61E-03
245.97	8.73	pos	1.68E-02	1.28E-02	1.17E-02	1.46E-02	1.17E-02
246.99	5.57	neg	9.89E-03	7.02E-03	8.36E-03	1.25E-02	8.31E-03
247.08	8.13	pos	1.35E-02	1.24E-02	8.80E-03	1.01E-02	1.17E-02
247.09	6.70	pos	2.69E-02	2.15E-02	1.88E-02	2.25E-02	1.97E-02
247.92	1.23	neg	2.87E-03	2.15E-03	2.61E-03	1.04E-03	1.27E-03

248.04	9.94	pos	8.23E-03	5.74E-03	6.83E-03	1.01E-02	8.52E-03
248.10	6.71	pos	3.00E-01	2.52E-01	2.17E-01	2.60E-01	2.37E-01
248.89	8.06	pos	1.61E-02	1.08E-02	7.33E-03	9.21E-03	7.73E-03
250.00	8.70	pos	1.36E-02	9.04E-03	7.41E-03	1.07E-02	9.84E-03
250.99	5.57	neg	1.19E-02	7.68E-03	8.78E-03	1.33E-02	9.52E-03
251.94	9.95	pos	7.41E-03	4.94E-03	5.87E-03	8.38E-03	6.31E-03
252.00	8.70	neg	4.15E-02	3.35E-02	3.23E-02	3.74E-02	3.13E-02
252.13	1.23	pos	7.91E-03	1.08E-02	6.59E-03	1.01E-02	6.81E-03
252.99	9.96	pos	1.48E-02	1.03E-02	1.08E-02	1.42E-02	1.29E-02
254.11	6.71	pos	1.70E-02	1.18E-02	1.20E-02	1.22E-02	1.04E-02
254.92	9.42	neg	6.85E-02	4.56E-02	6.44E-02	6.87E-02	6.18E-02
256.91	9.67	pos	1.10E-01	7.62E-02	6.94E-02	9.13E-02	7.86E-02
257.08	1.88	neg	4.65E-03	3.94E-03	3.78E-03	4.40E-03	3.90E-03
257.12	2.04	pos	3.13E-03	1.91E-03	1.89E-03	3.06E-03	2.94E-03
258.12	9.20	pos	5.38E-01	6.47E-01	5.99E-01	1.08E+00	8.62E-01
258.91	8.11	pos	4.78E-02	3.13E-02	2.22E-02	3.74E-02	2.57E-02
259.03	9.21	neg	9.45E-02	1.04E-01	8.05E-02	1.04E-01	9.88E-02
260.12	9.21	pos	1.06E-02	2.49E-02	1.90E-02	2.10E-02	1.67E-02
261.08	7.40	pos	1.55E-01	1.52E-01	1.09E-01	1.58E-01	1.32E-01
263.07	7.40	pos	1.73E-02	1.57E-02	1.12E-02	1.58E-02	1.42E-02
263.81	1.28	neg	1.86E-03	1.39E-03	2.35E-04	1.41E-03	1.05E-03
264.86	8.00	pos	3.40E-02	2.57E-02	1.88E-02	2.93E-02	2.12E-02
264.94	8.07	neg	1.58E-01	9.38E-02	7.01E-02	8.35E-02	6.97E-02
266.06	8.65	pos	1.05E-02	1.14E-02	8.75E-03	1.17E-02	1.22E-02
266.08	6.71	neg	7.47E-02	6.60E-02	5.16E-02	6.84E-02	7.46E-02
266.11	1.95	neg	1.32E-02	1.69E-02	1.30E-02	1.97E-02	1.32E-02
266.86	8.00	pos	1.95E-02	1.28E-02	1.08E-02	1.58E-02	1.20E-02
268.12	1.96	pos	3.29E-01	3.87E-01	2.46E-01	4.48E-01	2.93E-01
270.08	6.73	pos	3.27E-02	2.67E-02	2.37E-02	2.61E-02	2.25E-02
270.99	8.36	pos	1.30E-02	9.88E-03	1.09E-02	7.84E-03	9.79E-03
271.98	8.70	pos	3.17E-02	1.92E-02	1.63E-02	2.11E-02	1.74E-02
273.92	9.97	pos	1.69E-02	8.48E-03	7.95E-03	1.17E-02	9.70E-03
274.10	2.09	neg	6.23E-02	5.56E-02	6.36E-02	7.63E-02	4.93E-02
274.89	7.98	pos	6.22E-02	5.10E-02	4.06E-02	6.81E-02	5.24E-02
275.06	2.06	neg	9.88E-03	7.49E-03	9.37E-03	1.09E-02	8.14E-03
276.13	2.08	pos	3.62E-02	3.99E-02	2.51E-02	5.84E-02	3.70E-02
276.95	7.07	neg	1.06E-01	7.21E-02	6.56E-02	7.01E-02	5.91E-02
277.12	7.96	pos	7.38E-02	5.80E-02	4.66E-02	7.98E-02	6.09E-02
279.03	2.02	pos	2.69E-03	1.31E-03	1.76E-03	2.51E-03	2.98E-03
279.06	7.42	neg	8.35E-02	6.79E-02	4.83E-02	5.21E-02	5.29E-02
280.11	9.14	pos	5.68E-02	6.19E-02	3.03E-02	3.02E-02	4.24E-02
280.57	7.11	pos	9.99E-03	6.35E-03	7.67E-03	7.32E-03	8.85E-03
280.83	7.95	pos	1.52E-02	1.35E-02	1.16E-02	1.77E-02	1.39E-02
280.92	7.97	neg	1.43E-01	1.08E-01	9.72E-02	1.21E-01	9.51E-02
282.02	8.64	pos	2.06E-02	9.34E-03	9.59E-03	1.91E-02	9.26E-03
282.06	6.69	neg	8.35E-02	6.81E-02	5.19E-02	7.77E-02	7.36E-02
282.13	6.35	pos	1.87E-02	1.47E-02	1.21E-02	1.84E-02	1.63E-02
282.83	7.94	pos	6.96E-03	5.11E-03	3.34E-03	8.44E-03	6.10E-03
283.06	7.44	pos	2.92E-02	2.41E-02	1.63E-02	2.41E-02	1.85E-02
284.05	6.70	neg	3.37E-02	2.92E-02	2.17E-02	2.87E-02	2.98E-02
286.15	1.00	neg	1.61E-03	9.99E-04	1.80E-03	1.64E-03	5.66E-04
287.07	9.80	neg	7.37E-03	6.31E-03	6.42E-03	1.06E-02	1.06E-02

287.95	8.75	pos	2.75E-02	1.69E-02	1.48E-02	2.09E-02	1.65E-02
288.13	6.67	pos	7.39E-03	6.47E-03	7.61E-03	7.31E-03	6.12E-03
289.07	9.05	neg	2.00E-02	2.73E-02	2.04E-02	2.49E-02	2.26E-02
291.13	8.92	pos	1.23E-02	1.46E-02	1.02E-02	1.41E-02	1.79E-02
292.09	6.72	neg	5.48E-02	4.24E-02	3.88E-02	4.08E-02	4.64E-02
292.86	7.93	pos	1.17E-02	1.31E-02	9.97E-03	2.61E-02	1.70E-02
293.10	8.62	neg	1.18E-02	2.14E-02	2.28E-02	2.00E-02	2.06E-02
293.98	8.70	neg	2.31E-02	1.45E-02	1.35E-02	1.54E-02	1.47E-02
294.95	9.37	pos	1.15E-02	1.18E-02	3.08E-02	6.21E-02	3.71E-02
294.95	8.31	pos	5.02E-02	3.21E-02	3.05E-02	5.13E-02	4.03E-02
296.08	9.13	pos	4.31E-02	4.98E-02	2.22E-02	2.14E-02	3.14E-02
296.89	7.94	neg	1.35E-01	1.13E-01	1.09E-01	1.47E-01	1.15E-01
297.98	8.67	pos	1.60E-02	1.13E-02	8.47E-03	1.40E-02	1.07E-02
298.00	6.39	neg	6.90E-02	5.42E-02	5.60E-02	6.36E-02	5.24E-02
298.12	0.81	pos	1.57E-02	1.35E-02	9.91E-03	1.30E-02	1.12E-02
298.89	7.94	neg	3.23E-02	2.61E-02	2.51E-02	3.79E-02	2.92E-02
299.03	7.43	pos	1.80E-02	1.67E-02	1.16E-02	1.75E-02	1.23E-02
299.17	0.61	pos	4.72E-02	6.46E-02	1.91E-02	4.46E-02	2.10E-01
300.00	5.79	neg	4.79E-02	4.23E-02	3.93E-02	1.32E-01	3.40E-02
300.90	9.50	neg	3.73E-02	2.72E-02	2.65E-02	1.58E-02	2.03E-02
301.99	5.58	neg	2.12E-02	1.46E-02	1.65E-02	2.65E-02	1.74E-02
302.04	6.70	pos	8.96E-03	6.15E-03	4.18E-03	8.05E-03	7.60E-03
304.01	8.66	neg	4.89E-02	3.59E-02	3.05E-02	3.88E-02	3.54E-02
304.11	6.69	neg	3.83E-02	4.48E-02	5.34E-02	3.37E-02	4.46E-02
305.01	9.03	pos	1.22E-02	1.29E-02	8.50E-03	1.02E-02	1.06E-02
305.99	5.58	neg	6.89E-03	4.74E-03	5.83E-03	9.27E-03	5.68E-03
306.09	8.64	neg	6.91E-02	6.51E-02	6.05E-02	5.83E-02	6.92E-02
306.13	4.73	neg	8.00E-03	7.91E-03	7.84E-03	9.51E-03	8.97E-03
307.04	7.02	pos	1.28E-02	9.58E-03	1.02E-02	9.18E-03	8.85E-03
307.98	5.58	neg	1.97E-03	1.17E-03	1.26E-03	2.09E-03	1.55E-03
308.11	8.64	pos	5.96E-02	5.82E-02	4.82E-02	5.28E-02	6.17E-02
308.93	8.38	neg	2.64E-02	1.69E-02	1.39E-02	1.37E-02	1.38E-02
309.96	8.74	neg	1.57E-02	1.01E-02	1.03E-02	1.10E-02	9.73E-03
310.10	4.66	neg	4.28E-03	4.44E-03	3.98E-03	4.44E-03	4.33E-03
310.57	5.58	pos	1.42E-03	9.21E-04	1.39E-03	1.56E-03	1.44E-03
310.93	8.31	pos	1.89E-02	1.25E-02	9.60E-03	1.66E-02	1.27E-02
314.91	9.42	neg	2.04E-01	1.51E-01	1.95E-01	2.70E-01	2.11E-01
315.09	8.64	neg	5.18E-02	7.53E-02	7.40E-02	8.40E-02	8.01E-02
316.18	6.35	pos	1.15E+00	1.11E+00	8.14E-01	1.64E+00	1.32E+00
316.93	9.42	pos	4.04E-02	2.93E-02	3.86E-02	7.20E-02	4.84E-02
316.96	8.31	neg	3.30E-01	2.16E-01	2.09E-01	2.73E-01	2.23E-01
317.12	8.62	pos	2.21E-02	3.41E-02	3.00E-02	4.23E-02	3.53E-02
318.05	6.58	neg	2.29E-02	3.30E-02	2.76E-02	3.07E-02	2.67E-02
319.99	8.70	neg	3.00E-02	2.16E-02	2.14E-02	2.24E-02	2.09E-02
320.03	6.68	neg	1.74E-02	1.38E-02	7.98E-03	1.43E-02	1.44E-02
320.99	9.04	pos	1.16E-02	1.14E-02	6.96E-03	9.38E-03	9.78E-03
321.15	7.96	pos	3.59E-02	1.88E-02	2.25E-02	3.65E-02	2.57E-02
321.18	2.07	pos	7.60E-03	4.86E-03	1.51E-03	1.32E-02	8.95E-03
322.06	6.48	pos	5.67E-03	5.32E-03	4.66E-03	8.20E-03	5.42E-03
325.05	7.08	neg	8.59E-02	7.86E-02	8.92E-02	5.53E-02	7.83E-02
325.99	6.92	pos	1.34E-02	6.07E-03	6.52E-03	1.16E-02	1.04E-02
327.08	8.87	neg	1.48E-02	1.64E-02	1.23E-02	1.72E-02	1.46E-02



328.02	5.56	neg	4.13E-03	2.71E-03	2.90E-03	2.45E-03	2.72E-03
330.02	5.58	neg	6.86E-02	4.89E-02	4.94E-02	4.40E-02	5.05E-02
330.09	8.65	pos	3.68E-02	3.49E-02	2.79E-02	3.39E-02	3.66E-02
331.14	7.06	neg	3.30E-01	2.99E-01	3.89E-01	4.85E-01	4.17E-01
332.93	8.27	neg	6.94E-02	5.00E-02	3.67E-02	4.65E-02	4.03E-02
333.00	9.02	pos	2.17E-02	2.13E-02	1.91E-02	3.59E-02	2.40E-02
333.12	0.65	neg	1.83E-02	2.42E-02	2.64E-02	1.79E-02	7.56E-02
333.16	7.03	pos	5.05E-02	3.42E-02	3.27E-02	8.68E-02	5.46E-02
333.95	9.93	pos	9.05E-03	5.97E-03	7.10E-03	1.53E-02	8.94E-03
334.00	6.70	neg	1.13E-01	7.76E-02	7.90E-02	8.76E-02	6.56E-02
334.89	9.37	neg	1.07E-02	8.53E-03	1.51E-02	2.55E-02	1.62E-02
335.15	4.68	pos	6.46E-02	5.48E-02	5.31E-02	5.42E-02	5.75E-02
335.99	6.69	neg	7.06E-02	5.49E-02	5.44E-02	6.05E-02	4.42E-02
336.07	5.58	pos	3.28E-03	2.17E-03	3.14E-03	3.54E-03	3.17E-03
338.11	6.67	neg	2.62E-02	2.07E-02	1.41E-02	1.79E-02	2.29E-02
338.16	6.38	pos	3.89E-01	3.81E-01	3.52E-01	4.30E-01	3.94E-01
338.92	9.58	pos	9.03E-02	6.20E-02	5.99E-02	8.64E-02	7.17E-02
339.07	5.58	pos	4.82E-03	3.82E-03	5.25E-03	6.28E-03	5.14E-03
339.09	8.64	pos	3.63E-02	4.41E-02	3.90E-02	5.74E-02	4.53E-02
340.07	6.67	neg	2.01E-02	1.74E-02	1.03E-02	1.44E-02	1.69E-02
340.99	7.43	pos	8.26E-03	5.60E-03	4.25E-03	4.73E-03	4.38E-03
341.06	5.58	pos	1.82E-03	1.87E-03	2.14E-03	2.65E-03	2.18E-03
343.31	5.39	pos	3.48E-03	2.22E-03	2.41E-03	1.95E-03	2.30E-03
346.07	8.41	neg	2.44E-02	2.47E-02	2.19E-02	3.20E-02	2.59E-02
346.07	8.67	pos	1.03E-02	1.04E-02	9.19E-03	1.52E-02	1.22E-02
346.29	4.66	pos	1.89E-02	1.40E-02	1.09E-02	1.23E-02	1.77E-02
348.09	8.43	pos	1.89E-02	1.96E-02	1.48E-02	2.54E-02	1.92E-02
348.90	8.04	neg	7.51E-02	5.00E-02	3.53E-02	4.48E-02	3.95E-02
349.14	7.95	pos	1.15E-02	9.00E-03	7.52E-03	1.14E-02	9.28E-03
351.13	4.67	pos	9.70E-02	8.11E-02	8.38E-02	7.77E-02	8.38E-02
352.07	8.65	pos	1.93E-02	1.44E-02	1.28E-02	1.50E-02	1.56E-02
352.91	8.35	pos	2.76E-02	1.80E-02	1.56E-02	1.88E-02	1.73E-02
353.00	5.58	neg	4.31E-03	2.96E-03	3.44E-03	6.40E-03	4.13E-03
353.05	8.65	neg	1.91E-02	2.07E-02	1.88E-02	2.28E-02	2.43E-02
354.13	6.38	pos	5.46E-01	5.24E-01	4.91E-01	6.03E-01	5.35E-01
354.85	7.98	neg	3.40E-02	2.34E-02	1.83E-02	1.91E-02	9.15E-03
354.89	9.57	pos	6.29E-02	4.36E-02	4.10E-02	5.84E-02	4.71E-02
355.00	5.58	neg	1.04E-02	7.90E-03	9.37E-03	1.49E-02	1.06E-02
356.14	6.36	pos	1.80E-02	4.15E-02	3.94E-02	4.70E-02	4.16E-02
356.98	7.46	pos	6.58E-03	5.70E-03	3.95E-03	5.33E-03	4.11E-03
356.99	5.58	neg	1.05E-02	7.78E-03	9.64E-03	1.59E-02	1.05E-02
357.01	9.33	neg	3.58E-02	4.20E-02	3.96E-02	5.14E-02	5.25E-02
359.07	7.04	pos	1.68E-02	1.29E-02	1.61E-02	1.54E-02	1.66E-02
359.13	7.31	neg	7.46E-02	4.60E-02	8.18E-02	1.57E-01	8.55E-02
360.16	6.36	neg	1.30E-01	1.54E-01	1.49E-01	1.45E-01	1.50E-01
361.08	8.64	pos	5.32E-02	4.87E-02	4.05E-02	6.49E-02	4.75E-02
361.08	7.05	pos	9.88E-03	9.52E-03	3.61E-03	1.14E-02	1.09E-02
361.24	6.36	pos	1.64E-01	8.84E-02	1.46E-02	2.46E-01	1.65E-01
362.94	8.29	pos	7.75E-02	5.39E-02	5.29E-02	9.08E-02	6.89E-02
363.74	5.59	pos	2.20E-03	1.64E-03	2.51E-03	2.95E-03	2.23E-03
364.88	7.97	neg	8.98E-02	6.71E-02	6.62E-02	7.70E-02	6.31E-02
365.73	5.58	pos	4.53E-03	3.88E-03	5.24E-03	6.49E-03	4.88E-03

367.56	5.58	pos	2.14E-03	1.74E-03	2.64E-03	2.75E-03	2.63E-03
369.11	4.67	neg	3.68E-02	3.13E-02	2.99E-02	3.24E-02	3.25E-02
371.11	7.09	pos	4.00E-02	4.12E-02	2.92E-02	3.53E-02	3.33E-02
372.00	8.65	neg	2.42E-02	1.55E-02	1.42E-02	2.03E-02	1.60E-02
373.11	4.78	pos	9.41E-03	5.91E-03	7.15E-03	6.11E-03	6.66E-03
374.06	8.66	pos	1.44E-02	1.05E-02	8.50E-03	1.10E-02	1.06E-02
374.14	4.65	neg	2.04E-03	2.51E-03	2.45E-03	2.41E-03	2.71E-03
374.23	6.36	pos	1.22E-02	1.16E-02	7.52E-03	1.97E-02	1.52E-02
374.83	7.93	pos	3.59E-03	3.20E-03	2.59E-03	7.07E-03	4.41E-03
374.99	8.59	neg	4.73E-02	3.84E-02	3.39E-02	4.29E-02	3.88E-02
375.20	7.38	pos	5.49E-03	5.89E-03	3.97E-03	7.05E-03	4.87E-03
377.03	8.65	pos	2.92E-02	2.75E-02	2.39E-02	3.31E-02	2.55E-02
377.15	6.36	neg	5.89E-02	6.79E-02	4.24E-02	7.71E-02	8.09E-02
378.92	8.30	pos	3.40E-02	2.35E-02	1.86E-02	3.46E-02	2.34E-02
380.85	7.94	neg	7.21E-02	6.32E-02	5.87E-02	9.67E-02	7.27E-02
381.07	7.06	pos	6.75E-03	6.81E-03	9.14E-03	7.94E-03	8.67E-03
381.50	5.58	neg	2.06E-03	1.25E-03	1.82E-03	3.42E-03	2.15E-03
382.09	6.75	neg	2.77E-02	2.54E-02	3.09E-02	2.31E-02	3.51E-02
382.24	1.70	pos	1.02E-02	1.04E-02	8.03E-03	1.16E-02	7.62E-03
382.85	7.93	neg	2.57E-02	2.11E-02	2.25E-02	3.07E-02	2.40E-02
383.13	7.00	pos	7.78E-01	4.50E-01	4.24E-01	8.26E-01	6.08E-01
383.18	5.60	neg	4.02E-02	3.04E-02	3.19E-02	2.39E-02	3.36E-02
384.49	5.58	neg	1.66E-03	1.33E-03	1.62E-03	2.97E-03	1.89E-03
384.95	8.31	neg	1.43E-01	9.30E-02	9.55E-02	1.40E-01	1.16E-01
385.08	4.67	neg	3.16E-02	2.76E-02	2.66E-02	2.98E-02	2.81E-02
385.14	7.29	pos	4.12E-02	2.42E-02	1.91E-02	3.81E-02	3.78E-02
386.07	1.69	pos	1.39E-03	1.66E-03	1.06E-03	2.03E-03	1.42E-03
387.07	7.06	pos	9.84E-03	7.30E-03	7.13E-03	1.12E-02	1.04E-02
387.98	8.68	neg	1.92E-02	1.45E-02	1.20E-02	1.37E-02	1.35E-02
388.19	6.88	neg	5.05E-02	4.46E-02	5.84E-02	1.01E-01	7.57E-02
389.01	7.03	neg	9.93E-02	7.09E-02	6.47E-02	6.67E-02	6.41E-02
390.21	6.84	pos	3.21E-02	2.00E-02	1.83E-02	4.53E-02	3.00E-02
391.07	5.59	pos	4.53E-03	3.43E-03	4.43E-03	4.81E-03	4.37E-03
391.17	6.93	pos	7.85E-03	7.30E-03	8.94E-03	1.51E-02	1.06E-02
392.92	9.39	pos	2.01E-02	1.10E-02	1.82E-02	4.74E-02	2.60E-02
393.03	7.06	neg	5.57E-02	4.87E-02	4.89E-02	5.31E-02	4.11E-02
393.07	5.59	pos	4.56E-03	3.45E-03	4.97E-03	5.71E-03	5.01E-03
394.01	6.69	neg	4.73E-02	3.08E-02	3.59E-02	3.17E-02	2.35E-02
395.06	7.05	pos	9.70E-03	7.16E-03	8.67E-03	9.85E-03	1.01E-02
395.11	7.02	neg	6.52E-01	4.55E-01	5.51E-01	8.08E-01	6.36E-01
396.12	6.37	pos	1.27E-02	9.53E-03	1.18E-02	1.21E-02	1.08E-02
396.23	1.71	pos	3.16E-03	3.22E-03	2.91E-03	3.27E-03	2.42E-03
397.05	7.06	pos	9.70E-03	1.03E-02	1.13E-02	1.05E-02	1.19E-02
399.03	8.66	pos	3.30E-02	2.77E-02	2.28E-02	3.18E-02	2.71E-02
399.11	7.11	pos	2.09E-01	1.29E-01	1.17E-01	2.22E-01	1.72E-01
401.05	4.65	neg	5.75E-03	4.44E-03	4.52E-03	5.51E-03	3.37E-03
401.17	7.39	neg	1.27E-01	1.22E-01	1.48E-01	1.51E-01	1.36E-01
403.03	7.09	neg	1.90E-02	1.59E-02	2.01E-02	1.44E-02	1.12E-02
403.19	7.37	pos	1.48E-02	1.23E-02	1.36E-02	2.62E-02	1.95E-02
404.03	8.58	pos	8.13E-03	7.50E-03	7.40E-03	7.02E-03	7.91E-03
404.20	2.01	pos	3.19E-03	1.70E-03	1.58E-03	4.26E-03	3.18E-03
405.03	8.62	pos	1.98E-02	1.72E-02	1.28E-02	2.23E-02	1.56E-02

406.00	5.58	neg	3.22E-03	2.59E-03	2.99E-03	3.67E-03	3.09E-03
406.08	6.36	pos	1.94E-02	1.54E-02	1.65E-02	2.49E-02	1.99E-02
407.09	7.03	pos	1.02E-02	8.37E-03	1.08E-02	1.11E-02	9.09E-03
407.13	4.66	neg	3.32E-03	4.61E-03	5.30E-03	2.90E-03	4.06E-03
408.02	5.58	neg	7.41E-03	5.54E-03	5.97E-03	9.99E-03	7.02E-03
408.09	6.35	neg	2.98E-02	2.77E-02	1.59E-02	3.59E-02	3.25E-02
409.00	5.58	neg	5.04E-03	3.81E-03	3.88E-03	5.45E-03	4.41E-03
409.96	9.38	pos	2.00E-02	1.59E-02	2.71E-02	8.19E-02	4.10E-02
410.00	5.58	neg	8.65E-03	6.63E-03	7.38E-03	1.19E-02	8.28E-03
410.09	6.35	neg	2.16E-02	2.04E-02	1.13E-02	2.04E-02	2.22E-02
411.07	4.66	neg	9.34E-03	6.94E-03	6.72E-03	8.27E-03	5.26E-03
412.00	5.58	neg	5.05E-03	3.50E-03	4.82E-03	7.21E-03	4.86E-03
412.09	6.37	pos	1.55E-02	1.24E-02	1.61E-02	1.68E-02	1.43E-02
412.19	6.84	pos	2.77E-02	2.17E-02	1.65E-02	3.35E-02	2.19E-02
412.28	4.65	pos	2.39E-03	2.09E-03	1.44E-03	1.87E-03	2.60E-03
412.89	9.40	neg	8.19E-02	6.95E-02	1.10E-01	1.90E-01	1.26E-01
413.99	5.58	neg	1.96E-03	1.83E-03	1.99E-03	2.38E-03	1.96E-03
414.09	6.37	pos	6.73E-03	5.52E-03	6.33E-03	7.30E-03	6.11E-03
415.01	8.68	pos	1.08E-02	1.03E-02	9.35E-03	1.07E-02	9.07E-03
417.57	5.58	pos	4.99E-03	3.54E-03	5.02E-03	6.34E-03	5.16E-03
418.26	6.68	pos	2.96E-02	2.92E-02	2.24E-02	3.36E-02	2.97E-02
419.27	6.68	pos	1.59E-01	1.71E-01	1.41E-01	1.98E-01	1.86E-01
419.57	5.58	pos	5.91E-03	5.19E-03	7.17E-03	8.21E-03	6.75E-03
420.29	6.60	pos	8.24E-02	9.62E-02	9.41E-02	9.09E-02	9.26E-02
421.30	6.54	pos	2.14E-02	2.32E-02	2.33E-02	2.34E-02	2.32E-02
423.06	7.05	pos	9.15E-03	6.06E-03	8.32E-03	1.05E-02	1.01E-02
424.07	6.35	neg	2.77E-02	2.49E-02	1.66E-02	3.15E-02	2.98E-02
424.22	4.70	pos	2.13E-03	3.62E-03	2.00E-03	1.78E-03	2.39E-03
425.17	7.39	pos	3.83E-02	3.27E-02	2.42E-02	4.17E-02	3.21E-02
426.06	6.35	neg	1.74E-02	1.70E-02	9.69E-03	2.09E-02	2.46E-02
426.17	4.50	neg	1.98E-03	2.06E-03	2.10E-03	1.80E-03	1.88E-03
426.31	0.62	pos	1.40E-03	1.46E-03	1.64E-03	2.23E-03	2.00E-03
427.01	8.61	neg	1.27E-02	9.58E-03	9.34E-03	1.56E-02	1.39E-02
428.07	6.37	pos	6.27E-03	5.01E-03	6.35E-03	6.51E-03	5.49E-03
428.16	6.84	pos	1.15E-02	1.06E-02	8.93E-03	1.51E-02	1.11E-02
428.87	9.41	neg	5.19E-02	3.80E-02	5.89E-02	8.90E-02	6.14E-02
430.89	9.42	pos	2.07E-02	1.61E-02	2.20E-02	4.55E-02	2.84E-02
430.93	8.29	pos	7.31E-02	5.11E-02	5.44E-02	9.22E-02	6.98E-02
434.18	6.84	pos	5.40E-03	3.85E-03	3.61E-03	5.59E-03	3.89E-03
434.30	5.58	neg	1.45E-03	1.07E-03	1.22E-03	2.30E-03	1.57E-03
434.87	9.48	neg	7.34E-02	4.92E-02	5.99E-02	8.44E-02	6.77E-02
435.31	7.26	neg	2.47E-02	1.74E-02	3.31E-02	2.32E-02	2.32E-02
435.50	5.58	neg	1.53E-03	1.34E-03	1.93E-03	3.51E-03	2.37E-03
436.50	5.58	neg	2.01E-02	1.62E-02	1.93E-02	3.25E-02	2.84E-02
436.89	9.59	pos	5.66E-02	4.31E-02	4.24E-02	6.15E-02	5.12E-02
437.50	5.58	neg	1.72E-03	1.24E-03	1.72E-03	3.10E-03	2.15E-03
438.02	4.65	neg	3.23E-03	2.54E-03	2.49E-03	3.27E-03	2.35E-03
440.25	6.68	pos	6.72E-03	7.59E-03	5.94E-03	8.86E-03	7.13E-03
441.12	7.34	pos	2.39E-02	1.80E-02	1.71E-02	2.99E-02	1.99E-02
441.25	6.69	pos	4.27E-02	4.16E-02	3.72E-02	4.18E-02	3.93E-02
442.08	5.58	pos	2.51E-03	1.79E-03	2.08E-03	2.25E-03	2.28E-03
442.13	7.36	pos	4.26E-03	3.95E-03	2.98E-03	5.67E-03	4.15E-03

442.81	7.95	pos	8.74E-03	7.84E-03	7.24E-03	1.40E-02	9.48E-03
443.04	4.74	neg	9.30E-03	7.18E-03	6.58E-03	7.15E-03	7.45E-03
443.09	7.24	pos	1.06E-02	5.34E-03	5.92E-03	1.15E-02	7.41E-03
444.08	5.58	pos	8.42E-03	6.26E-03	8.02E-03	9.73E-03	8.52E-03
444.94	8.28	pos	1.45E-02	1.05E-02	1.10E-02	1.97E-02	1.48E-02
445.23	7.38	pos	3.69E-02	4.61E-02	3.50E-02	5.32E-02	4.71E-02
446.91	8.29	pos	3.36E-02	2.20E-02	2.01E-02	3.34E-02	2.39E-02
447.13	0.87	neg	3.45E-03	2.51E-03	1.71E-03	2.58E-03	2.09E-03
447.28	6.44	pos	3.06E-03	5.10E-03	3.06E-03	2.03E-02	1.04E-02
448.07	5.58	pos	5.32E-03	4.61E-03	5.54E-03	7.14E-03	5.73E-03
448.84	7.96	neg	4.72E-02	3.63E-02	2.97E-02	3.92E-02	3.20E-02
450.15	6.85	pos	3.80E-03	3.09E-03	3.15E-03	4.74E-03	3.50E-03
450.85	9.49	neg	8.43E-02	6.11E-02	6.87E-02	9.23E-02	7.60E-02
451.05	7.20	pos	1.27E-02	7.82E-03	1.18E-02	1.85E-02	1.57E-02
452.87	9.53	pos	5.10E-02	3.75E-02	3.67E-02	5.44E-02	4.51E-02
452.94	8.30	neg	8.59E-02	5.75E-02	6.59E-02	9.49E-02	7.35E-02
454.99	9.35	neg	9.22E-03	1.11E-02	1.49E-02	2.40E-02	1.90E-02
455.05	7.06	pos	9.40E-03	6.32E-03	4.72E-03	1.25E-02	8.69E-03
455.21	6.69	neg	2.33E-02	2.37E-02	1.78E-02	2.12E-02	2.61E-02
456.31	6.70	pos	6.31E-02	6.19E-02	6.49E-02	7.12E-02	6.66E-02
457.07	7.26	pos	1.40E-02	8.40E-03	8.73E-03	1.61E-02	1.18E-02
458.07	2.02	pos	1.68E-03	8.42E-04	1.19E-03	1.13E-03	1.17E-03
458.79	7.92	pos	4.55E-03	4.21E-03	3.24E-03	1.07E-02	6.75E-03
461.00	5.58	neg	4.00E-03	3.06E-03	3.56E-03	4.64E-03	3.60E-03
462.00	5.58	neg	2.51E-03	1.44E-03	1.82E-03	3.24E-03	2.46E-03
463.00	5.58	neg	5.33E-02	4.09E-02	4.44E-02	7.18E-02	5.43E-02
463.13	7.34	pos	1.08E-02	7.79E-03	7.07E-03	1.21E-02	8.37E-03
464.00	5.57	neg	2.16E-03	1.83E-03	2.30E-03	3.68E-03	2.64E-03
464.82	7.94	neg	3.59E-02	3.10E-02	3.18E-02	4.67E-02	3.29E-02
467.21	7.39	pos	2.15E-02	2.85E-02	1.91E-02	2.49E-02	2.18E-02
468.91	8.32	neg	3.92E-02	2.78E-02	2.44E-02	3.41E-02	2.64E-02
471.57	5.59	pos	1.72E-03	1.22E-03	1.90E-03	2.23E-03	1.86E-03
477.01	4.77	pos	5.77E-03	2.15E-03	1.95E-03	3.18E-03	2.11E-03
479.21	6.70	pos	7.25E-03	6.64E-03	6.35E-03	6.81E-03	6.29E-03
480.07	6.59	pos	6.55E-03	2.96E-03	4.55E-03	7.14E-03	4.00E-03
483.18	7.39	pos	1.26E-02	1.65E-02	1.04E-02	1.36E-02	1.23E-02
486.15	8.62	pos	6.75E-03	1.18E-02	1.01E-02	1.51E-02	1.18E-02
487.30	6.35	pos	3.23E-03	4.04E-03	3.18E-03	4.75E-03	3.90E-03
488.50	5.58	neg	1.51E-03	1.09E-03	1.45E-03	2.46E-03	1.76E-03
488.90	8.34	pos	2.22E-02	1.52E-02	1.27E-02	1.95E-02	1.46E-02
489.19	7.39	pos	3.74E-03	6.01E-03	4.16E-03	4.06E-03	4.37E-03
489.50	5.58	neg	1.69E-03	1.41E-03	1.69E-03	2.72E-03	1.77E-03
490.50	5.59	neg	1.90E-02	1.29E-02	1.45E-02	2.64E-02	2.47E-02
490.90	9.34	pos	2.41E-02	1.44E-02	1.92E-02	3.46E-02	2.23E-02
491.50	5.58	neg	1.16E-03	1.05E-03	1.14E-03	1.90E-03	1.34E-03
493.08	7.38	pos	3.56E-03	4.70E-03	4.64E-03	6.35E-03	5.94E-03
495.08	5.57	pos	4.36E-03	3.66E-03	4.01E-03	4.47E-03	4.01E-03
496.83	9.80	pos	3.80E-02	2.08E-02	1.76E-02	2.18E-02	2.02E-02
497.02	4.65	neg	3.95E-03	2.97E-03	3.21E-03	3.18E-03	2.69E-03
497.08	5.57	pos	1.20E-02	9.17E-03	1.17E-02	1.27E-02	1.15E-02
498.92	8.28	pos	4.92E-02	3.66E-02	3.56E-02	6.64E-02	4.93E-02
499.08	5.57	pos	1.61E-02	1.24E-02	1.49E-02	1.63E-02	1.50E-02

505.16	7.40	pos	9.40E-03	1.14E-02	7.40E-03	1.05E-02	8.24E-03
507.14	6.69	neg	4.68E-02	4.17E-02	4.42E-02	4.25E-02	3.72E-02
507.94	9.38	pos	1.06E-02	1.12E-02	1.93E-02	6.12E-02	2.94E-02
508.13	8.63	pos	1.13E-02	1.56E-02	1.39E-02	2.10E-02	1.70E-02
508.15	6.70	pos	4.02E-03	3.53E-03	3.83E-03	3.15E-03	4.70E-03
509.30	2.50	neg	1.74E-02	1.68E-02	1.58E-02	1.82E-02	1.71E-02
510.79	9.94	neg	2.41E-02	1.42E-02	1.83E-02	1.77E-02	1.76E-02
511.09	4.65	neg	1.46E-03	2.05E-03	2.29E-03	1.59E-03	2.00E-03
511.16	6.73	pos	1.44E-02	1.34E-02	1.58E-02	1.75E-02	1.78E-02
511.33	2.50	pos	7.52E-03	9.12E-03	6.84E-03	8.49E-03	8.81E-03
512.88	9.39	pos	2.20E-02	2.74E-02	2.25E-02	5.31E-02	3.18E-02
512.92	8.27	pos	1.30E-02	8.92E-03	9.10E-03	1.80E-02	1.27E-02
514.00	5.59	neg	2.05E-02	1.45E-02	1.59E-02	2.34E-02	1.62E-02
514.29	1.97	pos	6.05E-03	6.35E-03	4.36E-03	7.66E-03	4.64E-03
516.01	5.58	neg	2.55E-03	1.77E-03	2.23E-03	3.40E-03	2.45E-03
518.01	5.58	neg	2.27E-03	1.52E-03	1.80E-03	2.87E-03	2.03E-03
520.92	8.30	neg	6.20E-02	4.17E-02	4.86E-02	6.79E-02	5.69E-02
521.08	8.64	pos	8.70E-03	8.08E-03	6.14E-03	7.28E-03	8.52E-03
521.13	7.38	pos	6.17E-03	5.90E-03	6.28E-03	9.94E-03	7.78E-03
523.41	7.07	pos	1.09E-02	8.72E-03	8.35E-03	1.16E-02	1.03E-02
525.30	6.61	pos	1.61E-02	2.29E-02	1.53E-02	4.04E-02	2.44E-02
525.58	5.58	pos	1.24E-03	8.33E-04	1.42E-03	1.51E-03	1.11E-03
526.78	7.94	pos	5.43E-03	4.72E-03	3.40E-03	1.01E-02	6.07E-03
526.85	9.37	neg	2.34E-02	1.20E-02	3.02E-02	5.49E-02	3.57E-02
528.87	9.40	pos	1.42E-02	1.16E-02	1.58E-02	3.35E-02	2.10E-02
531.15	6.71	pos	6.26E-03	4.03E-03	4.50E-03	4.02E-03	4.36E-03
532.80	7.96	neg	2.31E-02	1.62E-02	1.54E-02	2.30E-02	1.77E-02
532.85	9.42	neg	3.78E-02	2.67E-02	3.71E-02	5.33E-02	4.45E-02
533.12	7.06	pos	6.20E-03	6.67E-03	8.40E-03	7.85E-03	7.85E-03
534.87	9.48	pos	4.59E-02	3.30E-02	3.70E-02	6.04E-02	4.61E-02
535.13	7.37	pos	5.88E-03	5.85E-03	5.45E-03	6.23E-03	6.45E-03
536.90	8.32	neg	4.18E-02	2.89E-02	2.50E-02	3.11E-02	2.85E-02
539.18	7.32	neg	6.87E-03	7.29E-03	7.24E-03	1.09E-02	7.33E-03
542.76	7.92	pos	4.13E-03	4.22E-03	3.50E-03	1.03E-02	5.93E-03
543.23	2.03	pos	1.62E-03	2.96E-03	1.64E-03	4.52E-03	2.36E-03
543.38	7.07	pos	5.55E-03	4.46E-03	4.82E-03	4.71E-03	5.39E-03
544.27	2.07	pos	1.95E-03	2.32E-03	1.86E-03	2.64E-03	1.46E-03
544.46	6.38	pos	3.99E-03	4.96E-03	6.13E-03	5.69E-03	4.99E-03
546.08	8.65	pos	6.60E-03	8.58E-03	7.66E-03	1.02E-02	8.35E-03
547.13	6.70	pos	8.74E-03	6.18E-03	7.74E-03	7.73E-03	7.02E-03
548.78	7.93	neg	1.72E-02	1.61E-02	1.67E-02	2.40E-02	1.90E-02
548.83	9.45	neg	4.54E-02	3.39E-02	4.11E-02	6.32E-02	4.93E-02
549.09	5.58	pos	1.27E-03	9.81E-04	1.40E-03	1.73E-03	1.50E-03
550.85	9.47	pos	3.57E-02	2.48E-02	2.90E-02	4.93E-02	3.54E-02
552.10	8.63	pos	1.98E-02	1.84E-02	1.75E-02	2.78E-02	1.87E-02
556.33	4.65	pos	9.83E-04	1.18E-03	1.74E-03	6.86E-04	1.09E-03
556.88	8.33	pos	2.28E-02	1.47E-02	1.33E-02	1.99E-02	1.55E-02
559.34	4.64	pos	3.66E-02	4.71E-02	7.10E-02	3.40E-02	3.81E-02
565.06	9.19	neg	2.46E-02	2.57E-02	2.62E-02	3.73E-02	4.02E-02
566.09	5.60	pos	1.49E-03	7.04E-04	2.30E-04	1.90E-03	1.56E-03
566.91	8.28	pos	4.50E-02	3.04E-02	3.58E-02	6.64E-02	4.53E-02
567.33	0.60	pos	1.70E-03	1.61E-03	7.70E-04	1.24E-03	2.11E-03

568.07	8.65	pos	1.49E-02	1.46E-02	1.21E-02	1.80E-02	1.35E-02
571.18	7.01	pos	2.38E-03	1.98E-03	3.43E-03	4.46E-03	3.59E-03
572.87	8.34	pos	1.64E-02	1.07E-02	7.59E-03	1.15E-02	9.52E-03
573.32	4.64	pos	5.96E-03	7.56E-03	1.18E-02	5.36E-03	5.61E-03
574.08	8.63	pos	1.65E-02	1.74E-02	1.37E-02	2.39E-02	1.66E-02
574.36	1.00	pos	8.85E-03	1.11E-02	6.85E-03	9.78E-03	8.58E-03
577.58	5.58	pos	2.22E-03	1.64E-03	2.19E-03	2.72E-03	2.27E-03
578.91	8.37	neg	2.03E-02	1.36E-02	1.25E-02	1.48E-02	1.33E-02
579.04	9.90	neg	1.54E-02	1.55E-02	1.52E-02	2.79E-02	2.04E-02
579.21	6.36	pos	8.13E-03	6.41E-03	6.92E-03	1.10E-02	8.60E-03
579.58	5.58	pos	3.22E-03	2.47E-03	3.08E-03	3.77E-03	3.12E-03
580.46	6.71	pos	5.76E-03	5.67E-03	6.09E-03	5.58E-03	5.38E-03
580.91	8.27	pos	1.45E-02	9.32E-03	1.05E-02	1.99E-02	1.38E-02
581.21	6.37	pos	6.38E-03	7.08E-03	3.70E-03	9.09E-03	7.33E-03
582.21	5.72	neg	3.62E-02	2.10E-02	2.29E-02	2.66E-02	3.14E-02
582.88	8.29	pos	2.61E-02	1.90E-02	1.60E-02	2.76E-02	2.02E-02
584.11	9.17	pos	1.98E-02	2.08E-02	1.46E-02	1.93E-02	2.20E-02
584.24	5.72	pos	2.19E-02	1.38E-02	1.11E-02	1.98E-02	2.03E-02
586.79	9.48	neg	3.74E-02	2.56E-02	2.80E-02	5.43E-02	3.29E-02
588.86	9.40	pos	2.04E-02	1.33E-02	1.14E-02	2.19E-02	1.59E-02
588.91	8.29	neg	4.30E-02	3.47E-02	3.66E-02	5.51E-02	4.52E-02
590.05	8.65	pos	1.36E-02	1.30E-02	1.08E-02	1.56E-02	1.32E-02
592.79	9.66	neg	4.04E-02	3.11E-02	3.03E-02	2.97E-02	2.82E-02
595.33	0.84	neg	4.23E-03	4.32E-03	3.74E-03	3.86E-03	3.52E-03
596.06	8.64	pos	1.35E-02	1.19E-02	1.01E-02	1.61E-02	1.12E-02
597.30	4.66	pos	3.33E-03	2.22E-03	2.56E-03	2.68E-03	2.47E-03
598.12	9.92	pos	1.80E-02	1.94E-02	1.49E-02	1.84E-02	2.07E-02
598.87	8.30	pos	1.38E-02	9.32E-03	7.45E-03	1.19E-02	9.01E-03
600.38	0.80	pos	6.32E-03	6.92E-03	4.82E-03	7.28E-03	1.19E-02
600.57	0.79	pos	6.32E-03	6.92E-03	4.82E-03	7.28E-03	1.19E-02
601.19	6.37	pos	6.22E-03	5.25E-03	8.05E-03	7.84E-03	6.37E-03
602.39	0.85	pos	5.91E-03	6.57E-03	2.34E-03	3.40E-03	6.33E-03
602.84	5.59	pos	9.63E-03	7.50E-03	9.32E-03	1.01E-02	9.17E-03
603.09	5.58	pos	9.63E-03	7.50E-03	9.32E-03	1.01E-02	9.17E-03
604.89	8.31	neg	3.33E-02	2.45E-02	1.98E-02	2.86E-02	2.26E-02
605.92	9.37	pos	7.71E-03	7.76E-03	1.39E-02	4.66E-02	2.02E-02
606.09	8.98	neg	7.91E-03	8.41E-03	8.42E-03	1.15E-02	9.50E-03
608.10	8.13	pos	6.96E-03	8.74E-03	6.88E-03	1.13E-02	9.22E-03
608.90	8.32	pos	1.17E-02	7.43E-03	7.25E-03	1.29E-02	9.15E-03
610.87	9.38	pos	3.04E-02	1.72E-02	2.75E-02	7.00E-02	3.77E-02
611.16	9.80	neg	7.08E-03	8.44E-03	7.32E-03	1.71E-02	7.77E-03
612.02	8.63	pos	1.23E-02	9.33E-03	8.03E-03	1.33E-02	8.81E-03
613.18	9.81	pos	9.52E-03	1.29E-02	9.61E-03	2.53E-02	1.15E-02
614.38	0.80	pos	3.43E-03	4.47E-03	2.71E-03	3.49E-03	2.14E-02
617.17	6.36	pos	6.27E-03	4.83E-03	6.47E-03	6.84E-03	5.75E-03
617.55	5.66	pos	2.56E-03	2.07E-03	2.66E-03	2.57E-03	2.45E-03
618.12	8.59	neg	1.32E-02	1.27E-02	1.46E-02	1.15E-02	1.37E-02
620.09	5.60	pos	2.31E-03	1.32E-03	1.02E-03	2.73E-03	2.33E-03
620.14	8.59	pos	1.69E-02	1.74E-02	1.49E-02	1.47E-02	1.48E-02
624.80	9.41	neg	1.62E-02	9.47E-03	1.77E-02	3.06E-02	1.96E-02
624.87	8.32	pos	2.05E-02	1.51E-02	1.45E-02	2.14E-02	1.64E-02
625.12	8.96	pos	6.66E-03	7.08E-03	6.14E-03	1.05E-02	7.54E-03

626.84	9.39	pos	1.21E-02	7.90E-03	1.20E-02	2.96E-02	1.69E-02
628.40	6.67	pos	2.90E-03	3.31E-03	3.82E-03	4.03E-03	4.15E-03
630.08	8.96	pos	6.80E-03	8.43E-03	7.41E-03	1.09E-02	9.33E-03
630.80	9.49	neg	3.38E-02	1.79E-02	2.29E-02	3.93E-02	2.87E-02
632.75	7.92	neg	1.58E-02	1.25E-02	1.34E-02	1.99E-02	1.65E-02
632.85	9.44	pos	3.38E-02	2.57E-02	2.89E-02	5.16E-02	3.82E-02
634.90	8.27	pos	3.86E-02	2.70E-02	2.98E-02	5.96E-02	4.30E-02
638.87	8.31	pos	1.15E-02	7.23E-03	7.07E-03	1.03E-02	7.85E-03
646.80	9.44	neg	2.44E-02	1.75E-02	2.52E-02	4.16E-02	3.03E-02
648.30	8.67	pos	1.76E-02	1.98E-02	1.30E-02	1.84E-02	2.10E-02
648.37	6.32	pos	5.50E-03	6.56E-03	4.33E-03	1.22E-02	8.24E-03
648.83	9.46	pos	2.60E-02	1.97E-02	2.29E-02	4.12E-02	2.72E-02
648.87	9.41	neg	1.96E-02	1.33E-02	1.38E-02	1.33E-02	1.69E-02
650.38	6.68	pos	2.33E-03	3.26E-03	3.84E-03	3.90E-03	3.70E-03
650.87	8.29	pos	2.42E-02	1.53E-02	1.36E-02	2.59E-02	1.77E-02
654.82	9.55	pos	2.47E-02	1.85E-02	1.62E-02	2.16E-02	1.84E-02
655.20	8.62	pos	7.15E-03	9.74E-03	8.36E-03	1.23E-02	1.01E-02
656.09	5.58	pos	6.09E-03	4.78E-03	5.37E-03	6.28E-03	5.37E-03
656.90	8.29	neg	2.15E-02	1.63E-02	1.97E-02	3.05E-02	2.29E-02
658.09	5.57	pos	1.05E-02	8.16E-03	9.02E-03	1.08E-02	9.62E-03
662.12	9.00	neg	1.20E-02	1.42E-02	1.32E-02	1.60E-02	1.32E-02
664.14	9.00	pos	4.31E-02	4.40E-02	3.83E-02	5.56E-02	4.44E-02
666.85	8.30	pos	1.55E-02	9.19E-03	7.77E-03	1.27E-02	1.06E-02
668.79	9.50	neg	2.31E-02	1.86E-02	2.42E-02	2.96E-02	2.43E-02
669.29	4.67	pos	3.91E-03	2.66E-03	3.39E-03	2.67E-03	3.17E-03
670.81	9.57	pos	2.74E-02	2.04E-02	2.12E-02	2.83E-02	2.36E-02
671.49	4.64	pos	2.32E-03	2.37E-03	2.54E-03	2.17E-03	2.33E-03
672.88	8.31	neg	1.92E-02	1.41E-02	1.29E-02	2.06E-02	1.64E-02
677.18	8.62	pos	5.61E-03	8.58E-03	7.88E-03	1.12E-02	8.33E-03
681.26	4.66	neg	1.43E-03	1.60E-03	1.82E-03	1.48E-03	1.67E-03
682.30	6.69	pos	5.15E-03	4.20E-03	5.66E-03	5.98E-03	4.98E-03
683.49	4.64	pos	1.84E-03	2.05E-03	3.03E-03	1.82E-03	1.91E-03
684.78	9.43	neg	1.79E-02	1.23E-02	1.72E-02	2.57E-02	1.63E-02
685.26	4.67	pos	8.09E-03	5.40E-03	6.30E-03	5.59E-03	6.06E-03
686.12	8.98	pos	2.06E-02	2.02E-02	1.83E-02	2.43E-02	2.13E-02
688.32	6.69	pos	3.41E-03	3.43E-03	2.95E-03	3.15E-03	2.86E-03
692.33	1.62	neg	5.66E-03	3.37E-03	2.43E-03	1.78E-03	1.31E-03
692.86	8.32	pos	2.30E-02	1.49E-02	1.43E-02	1.99E-02	1.61E-02
694.36	1.60	pos	1.38E-02	1.02E-02	6.24E-03	4.40E-03	3.51E-03
697.24	4.66	neg	2.70E-03	3.50E-03	3.36E-03	2.85E-03	3.50E-03
701.24	4.67	pos	3.48E-03	2.49E-03	3.01E-03	2.65E-03	2.97E-03
702.89	8.27	pos	3.22E-02	2.38E-02	2.61E-02	5.59E-02	3.82E-02
703.89	9.34	pos	6.27E-03	4.67E-03	9.67E-03	3.45E-02	1.34E-02
704.29	6.69	pos	3.40E-03	2.83E-03	4.24E-03	3.46E-03	3.32E-03
706.77	9.48	neg	1.93E-02	8.52E-03	1.60E-02	2.60E-02	1.62E-02
706.86	8.30	pos	1.19E-02	8.34E-03	8.05E-03	1.14E-02	8.16E-03
707.10	5.56	pos	5.53E-03	3.82E-03	3.97E-03	5.41E-03	4.38E-03
707.24	4.71	pos	1.82E-03	1.31E-03	1.18E-03	1.49E-03	1.52E-03
708.10	8.98	pos	1.28E-02	1.18E-02	9.51E-03	1.22E-02	1.15E-02
709.10	5.57	pos	1.95E-02	1.44E-02	1.65E-02	2.12E-02	1.82E-02
715.23	4.66	pos	1.13E-02	5.77E-03	5.84E-03	8.38E-03	5.60E-03
716.88	8.27	pos	1.35E-02	9.98E-03	9.96E-03	1.81E-02	1.21E-02

718.29	6.69	pos	4.09E-03	3.53E-03	4.29E-03	4.91E-03	3.97E-03
719.22	4.67	neg	1.82E-03	1.49E-03	1.39E-03	1.64E-03	1.80E-03
719.34	8.58	pos	2.96E-02	3.02E-02	2.22E-02	2.34E-02	2.80E-02
722.79	9.37	neg	9.16E-03	5.12E-03	4.46E-03	1.38E-02	8.59E-03
723.56	5.62	pos	2.03E-03	1.62E-03	1.99E-03	1.70E-03	1.69E-03
724.08	8.97	pos	9.57E-03	8.90E-03	5.66E-03	9.75E-03	7.48E-03
724.82	9.39	pos	7.43E-03	5.42E-03	9.25E-03	2.26E-02	1.31E-02
724.89	8.27	neg	1.27E-02	9.36E-03	1.12E-02	1.88E-02	1.56E-02
727.27	6.35	pos	3.91E-03	2.69E-03	3.40E-03	5.91E-03	4.42E-03
728.79	9.40	neg	1.05E-02	7.96E-03	1.34E-02	2.20E-02	1.45E-02
730.83	9.43	pos	2.19E-02	1.73E-02	2.24E-02	4.60E-02	3.07E-02
737.60	5.58	pos	2.25E-03	1.52E-03	2.42E-03	2.74E-03	2.03E-03
739.20	4.69	pos	1.99E-03	1.40E-03	1.12E-03	1.49E-03	1.17E-03
740.86	8.29	neg	1.21E-02	9.87E-03	8.72E-03	1.31E-02	9.71E-03
744.78	9.40	neg	1.06E-02	8.87E-03	1.26E-02	2.00E-02	1.33E-02
746.81	9.44	pos	1.73E-02	1.36E-02	1.70E-02	3.34E-02	2.18E-02
751.21	4.66	pos	3.98E-03	2.51E-03	2.13E-03	2.88E-03	2.00E-03
760.85	8.30	pos	1.41E-02	1.01E-02	1.11E-02	1.78E-02	1.27E-02
766.09	5.58	pos	1.97E-03	1.43E-03	2.04E-03	2.27E-03	1.95E-03
766.77	9.43	neg	1.23E-02	6.50E-03	1.10E-02	1.74E-02	1.26E-02
768.79	9.52	pos	2.23E-02	1.51E-02	1.72E-02	2.34E-02	1.85E-02
770.87	8.27	pos	1.98E-02	1.58E-02	1.68E-02	3.63E-02	2.29E-02
774.85	8.30	pos	9.94E-03	6.89E-03	7.56E-03	1.02E-02	7.97E-03
782.77	9.40	neg	8.81E-03	3.83E-03	7.82E-03	1.19E-02	5.62E-03
784.87	8.28	pos	1.08E-02	7.38E-03	7.93E-03	1.21E-02	9.58E-03
792.87	8.27	neg	8.49E-03	4.79E-03	6.76E-03	1.15E-02	7.33E-03
801.88	9.36	pos	3.67E-03	4.28E-03	7.02E-03	2.77E-02	1.20E-02
804.48	6.33	pos	4.70E-03	8.71E-03	7.81E-03	1.41E-02	1.15E-02
804.78	9.37	neg	8.10E-03	5.30E-03	3.36E-03	1.33E-02	9.15E-03
806.83	9.38	pos	8.74E-03	8.10E-03	1.49E-02	4.00E-02	2.00E-02
815.09	5.56	pos	1.85E-03	9.67E-04	1.16E-03	1.99E-03	1.48E-03
825.09	5.58	pos	2.34E-03	1.51E-03	1.75E-03	2.47E-03	2.09E-03
825.29	4.65	pos	1.46E-03	1.21E-03	1.59E-03	1.14E-03	1.47E-03
826.78	9.38	neg	6.89E-03	4.84E-03	3.20E-03	1.01E-02	7.63E-03
828.81	9.41	pos	1.31E-02	1.25E-02	1.47E-02	3.52E-02	2.09E-02
828.83	8.29	pos	1.14E-02	7.68E-03	7.37E-03	1.26E-02	1.04E-02
842.76	9.38	neg	6.17E-03	3.85E-03	3.50E-03	9.73E-03	6.39E-03
844.79	9.41	pos	9.33E-03	9.28E-03	1.29E-02	2.38E-02	1.55E-02
852.86	8.27	pos	8.21E-03	6.22E-03	7.15E-03	1.22E-02	4.65E-03
860.86	8.26	neg	3.79E-03	2.88E-03	3.37E-03	5.92E-03	3.84E-03
866.77	9.49	pos	1.40E-02	1.04E-02	1.20E-02	2.06E-02	1.49E-02
868.23	5.58	pos	1.08E-03	7.27E-04	9.61E-04	1.30E-03	1.16E-03
875.32	4.64	pos	1.44E-03	1.38E-03	1.26E-03	1.41E-03	1.41E-03
876.60	5.58	pos	3.39E-03	2.83E-03	4.45E-03	5.27E-03	4.44E-03
878.10	5.59	pos	1.69E-03	1.31E-03	1.75E-03	2.13E-03	1.74E-03
883.58	5.62	pos	1.50E-03	1.34E-03	1.63E-03	1.61E-03	1.40E-03
891.44	6.68	pos	3.02E-03	3.25E-03	3.84E-03	4.13E-03	3.83E-03
904.80	9.37	pos	7.47E-03	5.74E-03	8.93E-03	2.53E-02	1.28E-02
906.85	8.26	pos	8.20E-03	4.23E-03	5.50E-03	1.24E-02	7.81E-03
913.42	6.69	pos	2.29E-03	2.41E-03	3.27E-03	2.91E-03	2.79E-03
922.82	8.27	pos	7.08E-03	5.57E-03	4.27E-03	7.55E-03	5.66E-03
926.79	9.39	pos	5.60E-03	5.61E-03	9.88E-03	2.39E-02	1.32E-02



942.77	9.40	pos	7.04E-03	5.04E-03	8.21E-03	1.77E-02	1.05E-02
981.45	4.64	pos	1.22E-03	1.03E-03	1.35E-03	1.05E-03	1.27E-03
991.41	4.64	pos	2.78E-03	1.97E-03	2.05E-03	2.78E-03	1.94E-03
997.43	4.65	pos	1.62E-03	1.43E-03	1.82E-03	1.45E-03	1.69E-03
1002.78	9.36	pos	6.35E-03	4.43E-03	5.40E-03	1.33E-02	6.66E-03

Look up table for *S. meliloti* samples exposed to 0.14 mg/L fluorene

avg(mz)	avg(rt)	ionization mode	sample 1	sample 2	sample 3	sample 4	sample 5
78.97	9.38	neg	1.45E-02	1.82E-02	2.05E-02	1.96E-02	2.39E-02
87.98	5.58	neg	2.20E-03	3.23E-03	3.17E-03	2.88E-03	3.44E-03
90.99	8.29	pos	2.68E-02	3.21E-02	3.71E-02	3.85E-02	3.82E-02
99.00	9.37	pos	2.45E-02	3.21E-02	3.52E-02	2.94E-02	4.17E-02
100.05	7.07	neg	1.94E-02	2.08E-02	2.07E-02	2.21E-02	1.92E-02
100.12	4.66	pos	2.50E-02	2.68E-02	2.60E-02	3.84E-02	4.80E-02
101.08	2.05	pos	6.61E-03	6.49E-03	5.56E-03	1.01E-02	1.01E-02
102.06	8.65	neg	7.11E-02	8.90E-02	7.16E-02	6.20E-02	8.19E-02
102.07	7.12	pos	6.14E-02	7.89E-02	7.45E-02	8.28E-02	8.55E-02
102.07	8.65	pos	4.50E-02	5.97E-02	4.79E-02	4.37E-02	5.04E-02
104.12	7.04	pos	3.59E-02	5.37E-02	5.31E-02	5.40E-02	6.54E-02
105.00	8.26	pos	1.84E-02	2.62E-02	2.72E-02	2.20E-02	3.67E-02
106.10	7.63	pos	1.12E-02	1.44E-02	1.54E-02	1.96E-02	1.62E-02
107.08	7.08	pos	3.54E-01	4.17E-01	4.35E-01	4.61E-01	4.52E-01
110.02	12.93	pos	1.18E-02	1.44E-02	1.76E-02	1.71E-02	1.90E-02
112.07	4.74	pos	1.40E-02	1.05E-02	7.90E-03	7.93E-03	6.88E-03
114.91	7.77	pos	2.44E-02	2.60E-02	3.56E-02	3.46E-02	3.16E-02
116.08	7.60	pos	3.21E-02	5.04E-02	5.13E-02	3.99E-02	5.24E-02
117.02	1.45	neg	2.18E-02	3.29E-02	2.56E-02	2.15E-02	2.99E-02
117.11	7.49	pos	1.48E-02	2.98E-02	2.70E-02	2.05E-02	3.97E-02
118.10	7.52	pos	3.38E-01	5.62E-01	5.52E-01	9.15E-01	4.73E-01
119.08	2.04	pos	2.03E-02	1.90E-02	1.64E-02	3.38E-02	3.40E-02
120.09	4.65	pos	6.36E-02	6.61E-02	7.09E-02	6.86E-02	6.78E-02
120.09	4.65	pos	6.36E-02	6.61E-02	7.09E-02	6.86E-02	6.78E-02
120.09	7.40	pos	3.14E-02	4.01E-02	4.28E-02	4.64E-02	4.44E-02
121.06	0.86	pos	7.42E-03	1.01E-02	3.52E-02	8.82E-03	2.04E-02
122.90	1.24	neg	4.91E-04	2.71E-03	4.14E-03	2.43E-03	5.52E-03
122.94	7.96	pos	1.35E-01	1.61E-01	1.60E-01	1.49E-01	1.76E-01
124.99	1.25	neg	8.85E-03	5.66E-03	6.05E-03	5.75E-03	7.18E-03
125.95	5.57	neg	3.20E-03	4.55E-03	4.96E-03	3.72E-03	5.22E-03
128.03	12.92	pos	1.13E-02	1.73E-02	1.60E-02	1.62E-02	1.99E-02
128.04	8.65	neg	5.03E-02	6.24E-02	5.07E-02	4.25E-02	5.65E-02
128.14	6.39	pos	2.47E-01	2.64E-01	2.77E-01	2.93E-01	3.09E-01
128.97	7.94	neg	4.70E-01	5.14E-01	5.32E-01	4.49E-01	4.54E-01
130.06	1.37	neg	2.45E-03	3.04E-03	3.21E-03	3.05E-03	3.11E-03
130.09	6.56	neg	4.72E-02	9.62E-02	7.76E-02	4.92E-02	6.15E-02
132.07	7.42	neg	4.40E-02	6.34E-02	4.83E-02	4.49E-02	5.14E-02
134.05	1.71	neg	1.10E-01	1.40E-01	9.47E-02	6.47E-02	1.11E-01
134.09	7.37	pos	3.08E-01	5.63E-01	4.34E-01	3.70E-01	5.40E-01

136.06	7.08	pos	3.37E-01	3.99E-01	4.20E-01	4.28E-01	3.93E-01
136.08	1.71	pos	3.31E-01	4.19E-01	3.78E-01	2.49E-01	4.34E-01
137.09	2.04	pos	8.74E-02	8.92E-02	7.59E-02	1.36E-01	1.34E-01
139.88	1.26	neg	9.48E-04	4.54E-03	5.17E-03	4.96E-03	5.84E-03
140.99	5.58	neg	1.57E-02	1.86E-02	2.13E-02	1.65E-02	2.12E-02
141.88	1.26	neg	1.21E-02	6.92E-02	9.11E-02	7.02E-02	9.71E-02
142.98	5.57	neg	1.51E-02	1.80E-02	1.97E-02	1.50E-02	1.98E-02
143.87	1.26	neg	8.32E-03	4.39E-02	5.64E-02	4.47E-02	6.08E-02
144.18	2.31	pos	3.15E-03	9.89E-03	6.94E-03	6.10E-03	7.19E-03
145.06	6.96	pos	8.26E-02	1.20E-01	1.50E-01	1.35E-01	2.03E-01
145.07	8.51	neg	2.96E-02	2.94E-02	2.71E-02	3.00E-02	3.41E-02
146.05	8.65	neg	7.84E-01	1.04E+00	7.43E-01	5.94E-01	7.79E-01
149.05	6.98	neg	9.63E-02	1.25E-01	1.43E-01	1.19E-01	1.77E-01
151.03	2.22	neg	2.23E-02	2.33E-02	3.05E-02	1.39E-02	1.75E-02
155.09	7.07	pos	1.61E-01	1.87E-01	2.05E-01	2.03E-01	2.09E-01
158.98	8.31	pos	8.00E-02	8.75E-02	9.62E-02	9.53E-02	9.93E-02
158.99	12.92	neg	4.77E-02	5.37E-02	5.87E-02	5.21E-02	7.43E-02
159.08	2.05	pos	9.33E-03	8.54E-03	7.70E-03	1.14E-02	1.18E-02
159.08	8.65	neg	1.89E-02	1.64E-02	2.02E-02	1.62E-02	2.22E-02
162.05	3.07	neg	1.63E-02	1.87E-02	1.56E-02	1.34E-02	1.97E-02
168.04	8.67	neg	6.68E-02	7.63E-02	7.28E-02	6.32E-02	7.32E-02
170.06	8.65	pos	1.40E-01	1.80E-01	1.37E-01	1.14E-01	1.42E-01
171.05	2.05	neg	5.84E-02	3.87E-02	2.68E-02	5.45E-02	4.92E-02
171.10	6.34	pos	2.56E-02	3.65E-02	3.59E-02	3.57E-02	4.44E-02
171.12	6.40	neg	1.15E-01	1.17E-01	1.16E-01	1.24E-01	1.18E-01
173.05	2.05	neg	1.98E-02	1.30E-02	9.65E-03	1.84E-02	1.72E-02
173.14	6.39	pos	1.13E-01	1.15E-01	1.16E-01	1.28E-01	1.28E-01
175.08	7.08	pos	6.01E-02	6.29E-02	7.12E-02	7.24E-02	5.23E-02
175.13	10.29	pos	9.83E-02	1.46E-01	1.07E-01	9.25E-02	1.21E-01
176.05	1.39	neg	7.17E-03	6.29E-03	4.57E-03	3.54E-03	4.74E-03
176.94	9.39	neg	6.81E-02	1.03E-01	1.04E-01	8.61E-02	1.19E-01
177.05	2.79	neg	1.60E-02	1.41E-02	1.09E-02	8.35E-03	7.39E-03
180.15	0.66	pos	5.34E-02	5.80E-02	4.90E-02	5.64E-02	5.66E-02
183.04	1.25	neg	6.25E-03	4.87E-03	5.08E-03	5.03E-03	6.01E-03
186.03	8.65	pos	1.05E-01	1.34E-01	9.63E-02	7.74E-02	1.02E-01
187.87	1.26	neg	6.07E-03	3.36E-02	4.29E-02	3.55E-02	4.29E-02
188.03	8.65	pos	9.65E-03	1.07E-02	8.84E-03	6.88E-03	8.91E-03
188.19	11.52	pos	5.01E-02	9.67E-02	9.43E-02	6.22E-02	1.59E-01
189.10	9.81	neg	2.55E-02	2.41E-02	2.34E-02	2.35E-02	2.67E-02
189.87	1.26	neg	2.45E-02	2.18E-02	2.73E-02	2.19E-02	2.76E-02
191.10	6.70	pos	1.29E-01	1.43E-01	1.54E-01	1.62E-01	1.51E-01
191.87	1.26	neg	1.11E-03	4.90E-03	6.09E-03	5.03E-03	6.00E-03
192.04	8.67	pos	1.39E-01	1.46E-01	1.56E-01	1.49E-01	1.53E-01
192.11	6.71	pos	5.37E-01	6.22E-01	6.31E-01	6.25E-01	6.05E-01
192.17	5.40	pos	1.39E-01	1.39E-01	1.23E-01	3.90E-01	6.28E-01
193.12	6.70	pos	3.10E-01	3.65E-01	3.73E-01	3.68E-01	3.68E-01
193.99	5.57	neg	1.90E-02	2.29E-02	2.51E-02	1.87E-02	2.51E-02
195.98	5.57	neg	2.13E-02	2.79E-02	3.01E-02	2.49E-02	3.11E-02
196.96	7.98	neg	9.42E-02	8.95E-02	1.05E-01	9.87E-02	8.84E-02
197.98	5.58	neg	1.14E-02	1.38E-02	1.50E-02	1.24E-02	1.54E-02
198.11	6.93	pos	3.32E-01	4.97E-01	6.33E-01	5.30E-01	8.42E-01
199.05	7.63	neg	5.47E-02	6.23E-02	4.22E-02	1.17E-01	1.38E-01

203.07	7.10	pos	9.61E-01	1.12E+00	1.33E+00	1.25E+00	1.40E+00
205.08	7.39	pos	9.66E-02	1.43E-01	5.25E-02	2.08E-01	1.15E-01
206.80	5.92	neg	6.47E-02	1.22E-01	6.46E-02	7.13E-02	4.50E-02
206.90	7.94	pos	2.09E-02	3.20E-02	3.78E-02	3.00E-02	4.79E-02
207.12	6.70	neg	2.65E-01	2.71E-01	2.64E-01	2.81E-01	2.49E-01
208.01	8.69	pos	5.27E-02	5.58E-02	5.52E-02	5.19E-02	5.05E-02
208.90	7.93	pos	5.01E-03	7.85E-03	8.54E-03	6.38E-03	1.06E-02
209.14	6.71	pos	1.73E-01	2.04E-01	2.08E-01	2.17E-01	2.13E-01
212.13	6.65	pos	6.60E-02	7.33E-02	7.41E-02	8.38E-02	7.76E-02
212.14	2.68	pos	9.25E-03	8.64E-03	1.03E-02	7.61E-03	1.07E-02
212.93	7.94	neg	8.01E-02	8.77E-02	9.35E-02	7.06E-02	8.02E-02
213.03	7.10	pos	2.06E-02	1.95E-02	2.14E-02	2.25E-02	1.43E-02
213.06	8.46	neg	1.44E-02	1.14E-02	9.77E-03	1.41E-02	1.21E-02
213.09	0.86	neg	4.37E-03	3.43E-03	3.37E-03	3.42E-03	5.16E-03
214.01	8.94	pos	5.08E-02	7.38E-02	5.72E-02	7.46E-02	1.12E-01
214.05	8.75	neg	3.77E-02	4.17E-02	3.64E-02	3.66E-02	3.53E-02
214.14	0.98	neg	2.64E-02	1.76E-02	1.50E-02	1.74E-02	1.70E-02
214.33	6.99	neg	3.88E-02	5.00E-02	5.68E-02	4.45E-02	5.62E-02
214.89	1.24	neg	9.53E-04	4.77E-03	7.25E-03	4.17E-03	7.73E-03
219.04	7.06	pos	1.14E+00	1.35E+00	1.61E+00	1.44E+00	1.67E+00
219.05	7.14	neg	1.55E-01	2.02E-01	1.44E-01	2.17E-01	1.73E-01
221.04	7.07	pos	1.05E-01	1.35E-01	1.44E-01	1.66E-01	1.61E-01
224.11	7.34	neg	1.22E-02	1.94E-02	1.53E-02	1.71E-02	2.24E-02
225.03	9.34	pos	1.13E-02	1.31E-02	1.17E-02	1.19E-02	1.38E-02
226.00	8.70	neg	2.95E-02	3.03E-02	2.90E-02	3.09E-02	3.07E-02
226.14	7.29	pos	9.17E-03	2.63E-02	5.02E-02	4.91E-02	5.38E-02
226.97	8.30	pos	2.76E-01	3.12E-01	3.52E-01	3.06E-01	3.43E-01
228.06	8.60	neg	2.46E-02	2.59E-02	2.15E-02	2.29E-02	2.37E-02
229.06	2.67	neg	8.63E-03	5.10E-03	5.36E-03	4.09E-03	5.25E-03
230.03	8.66	pos	4.30E-02	4.60E-02	4.88E-02	5.26E-02	5.14E-02
231.02	9.94	pos	7.53E-03	7.36E-03	8.82E-03	8.10E-03	1.19E-02
231.12	6.71	pos	1.77E-02	1.68E-02	1.96E-02	1.75E-02	1.77E-02
232.13	6.72	pos	1.54E-01	1.78E-01	1.84E-01	1.87E-01	1.70E-01
233.09	7.96	pos	5.17E-02	6.59E-02	6.56E-02	7.20E-02	7.01E-02
234.93	9.44	pos	3.44E-02	4.27E-02	5.04E-02	4.78E-02	4.96E-02
235.14	7.05	pos	1.38E-02	1.34E-02	8.83E-03	1.26E-02	1.37E-02
235.97	9.95	pos	1.82E-02	1.91E-02	2.20E-02	1.96E-02	2.29E-02
238.05	2.02	neg	6.77E-03	6.09E-03	4.45E-03	5.35E-03	5.94E-03
238.06	8.76	pos	1.12E-02	1.27E-02	9.59E-03	1.23E-02	1.01E-02
239.05	2.03	neg	1.39E-02	1.00E-02	7.91E-03	1.38E-02	1.28E-02
242.02	8.67	neg	2.34E-02	2.81E-02	2.25E-02	3.06E-02	2.26E-02
242.61	8.30	pos	8.77E-02	9.06E-02	1.09E-01	1.27E-01	1.10E-01
242.99	7.06	pos	1.79E-02	1.89E-02	1.43E-02	2.01E-02	1.94E-02
243.07	2.47	neg	3.97E-02	6.37E-02	4.72E-02	3.73E-02	5.30E-02
243.09	1.02	neg	8.19E-03	1.11E-02	1.25E-02	1.10E-02	1.66E-02
243.12	0.82	pos	2.12E-03	2.64E-03	2.92E-03	1.94E-03	3.52E-03
243.90	1.24	neg	2.56E-03	7.12E-03	9.49E-03	7.16E-03	1.14E-02
244.11	8.63	pos	1.93E-02	2.39E-02	1.80E-02	1.52E-02	1.82E-02
244.12	5.94	pos	1.77E-02	2.68E-02	1.15E-02	5.46E-03	2.78E-02
245.05	8.13	neg	3.87E-02	2.44E-02	2.88E-02	3.09E-03	2.63E-03
245.09	2.48	pos	1.51E-02	2.23E-02	1.90E-02	1.41E-02	2.07E-02
245.10	7.40	pos	9.44E-02	1.06E-01	1.32E-01	1.23E-01	1.26E-01

245.12	1.00	pos	1.44E-02	2.01E-02	2.47E-02	1.90E-02	3.05E-02
245.90	1.24	neg	1.08E-03	3.67E-03	4.31E-03	3.13E-03	4.81E-03
245.97	8.73	pos	1.20E-02	1.24E-02	1.26E-02	1.42E-02	1.21E-02
246.99	5.57	neg	7.07E-03	1.02E-02	1.13E-02	8.35E-03	1.18E-02
247.09	6.70	pos	2.03E-02	2.37E-02	2.25E-02	2.30E-02	1.98E-02
248.04	9.94	pos	7.85E-03	8.50E-03	1.02E-02	8.20E-03	1.09E-02
248.10	6.71	pos	2.35E-01	2.72E-01	2.66E-01	2.67E-01	2.37E-01
248.89	8.06	pos	9.12E-03	7.26E-03	9.48E-03	1.15E-02	7.29E-03
250.00	8.70	pos	1.00E-02	7.35E-03	8.53E-03	1.10E-02	9.01E-03
250.99	5.57	neg	7.69E-03	1.12E-02	1.14E-02	8.05E-03	1.24E-02
251.94	9.95	pos	5.78E-03	5.91E-03	6.72E-03	6.08E-03	8.37E-03
252.00	8.70	neg	2.98E-02	3.27E-02	3.14E-02	3.29E-02	3.03E-02
252.13	1.23	pos	7.39E-03	8.69E-03	8.33E-03	5.60E-03	9.54E-03
254.11	6.71	pos	1.31E-02	1.39E-02	1.12E-02	1.22E-02	1.08E-02
254.92	9.42	neg	6.30E-02	6.70E-02	6.84E-02	6.73E-02	5.57E-02
256.91	9.67	pos	7.51E-02	8.16E-02	8.37E-02	9.61E-02	7.10E-02
257.08	1.88	neg	3.42E-03	4.18E-03	3.65E-03	3.97E-03	4.31E-03
258.12	9.20	pos	6.50E-01	8.08E-01	7.11E-01	6.33E-01	9.61E-01
258.91	8.11	pos	2.52E-02	2.54E-02	3.32E-02	3.95E-02	3.07E-02
259.03	9.21	neg	8.44E-02	9.59E-02	7.62E-02	8.37E-02	8.42E-02
260.12	9.21	pos	2.17E-02	1.55E-02	2.16E-02	2.26E-02	1.61E-02
261.08	7.40	pos	1.13E-01	1.22E-01	1.53E-01	1.59E-01	1.55E-01
262.11	5.36	neg	2.47E-03	1.41E-03	9.84E-04	4.73E-03	4.62E-03
263.07	7.40	pos	1.12E-02	1.34E-02	1.59E-02	1.55E-02	1.44E-02
263.81	1.28	neg	1.14E-04	9.05E-04	1.59E-03	8.98E-04	1.35E-03
264.86	8.00	pos	2.24E-02	2.31E-02	2.45E-02	2.71E-02	2.39E-02
264.94	8.07	neg	7.58E-02	7.02E-02	8.66E-02	8.67E-02	6.40E-02
266.06	8.65	pos	9.86E-03	1.24E-02	8.17E-03	8.71E-03	8.50E-03
266.08	6.71	neg	7.06E-02	6.33E-02	6.80E-02	6.23E-02	5.33E-02
266.11	1.95	neg	1.19E-02	1.84E-02	1.38E-02	1.28E-02	1.86E-02
266.86	8.00	pos	1.15E-02	1.26E-02	1.37E-02	1.46E-02	1.29E-02
268.12	1.96	pos	2.92E-01	3.70E-01	3.26E-01	2.79E-01	4.05E-01
270.08	6.73	pos	2.56E-02	2.70E-02	2.60E-02	2.78E-02	2.17E-02
270.99	8.36	pos	1.15E-02	9.29E-03	7.40E-03	1.38E-02	6.21E-03
271.98	8.70	pos	1.66E-02	1.70E-02	2.18E-02	2.57E-02	2.00E-02
273.92	9.97	pos	9.55E-03	8.70E-03	1.17E-02	1.76E-02	1.09E-02
274.10	2.09	neg	7.37E-02	6.98E-02	6.13E-02	4.38E-02	8.45E-02
274.89	7.98	pos	4.68E-02	5.80E-02	6.09E-02	5.16E-02	6.00E-02
275.06	2.06	neg	1.13E-02	9.79E-03	8.69E-03	9.75E-03	1.15E-02
276.13	2.08	pos	3.07E-02	4.29E-02	4.64E-02	3.04E-02	6.07E-02
276.95	7.07	neg	5.60E-02	5.95E-02	7.09E-02	6.70E-02	5.23E-02
277.12	7.96	pos	5.46E-02	6.44E-02	6.41E-02	7.37E-02	7.70E-02
279.03	2.02	pos	2.20E-03	2.01E-03	1.91E-03	3.17E-03	3.07E-03
279.06	7.42	neg	5.69E-02	5.03E-02	5.55E-02	6.73E-02	4.89E-02
280.11	9.14	pos	4.04E-02	3.19E-02	2.89E-02	4.79E-02	2.03E-02
280.57	7.11	pos	9.39E-03	8.29E-03	6.94E-03	9.85E-03	9.22E-03
280.83	7.95	pos	1.34E-02	1.59E-02	1.59E-02	1.40E-02	1.65E-02
280.92	7.97	neg	1.00E-01	1.03E-01	1.13E-01	9.03E-02	9.85E-02
282.02	8.64	pos	1.04E-02	9.10E-03	1.91E-02	1.80E-02	1.78E-02
282.06	6.69	neg	7.52E-02	7.02E-02	7.17E-02	6.01E-02	6.36E-02
282.13	6.35	pos	1.36E-02	1.82E-02	1.61E-02	1.63E-02	1.75E-02
282.83	7.94	pos	4.40E-03	5.45E-03	6.98E-03	6.22E-03	7.28E-03

283.06	7.44	pos	1.67E-02	1.69E-02	2.36E-02	2.59E-02	2.23E-02
284.05	6.70	neg	2.64E-02	2.38E-02	2.88E-02	2.45E-02	2.03E-02
284.12	6.47	pos	7.27E-04	9.63E-03	1.68E-03	4.67E-04	1.02E-02
286.15	1.00	neg	1.90E-03	1.78E-03	1.73E-03	2.11E-03	2.36E-03
287.07	9.80	neg	8.69E-03	1.04E-02	1.03E-02	9.72E-03	1.34E-02
287.95	8.75	pos	1.71E-02	1.62E-02	1.81E-02	2.29E-02	1.81E-02
288.13	6.67	pos	7.04E-03	6.80E-03	5.02E-03	6.51E-03	5.34E-03
289.07	9.05	neg	2.41E-02	2.56E-02	2.78E-02	2.22E-02	2.82E-02
291.13	8.92	pos	1.71E-02	1.22E-02	1.59E-02	1.54E-02	2.23E-02
292.09	6.72	neg	4.29E-02	4.30E-02	4.51E-02	4.45E-02	3.86E-02
292.86	7.93	pos	1.10E-02	1.85E-02	2.00E-02	1.35E-02	2.37E-02
293.98	8.70	neg	1.35E-02	1.39E-02	1.57E-02	1.67E-02	1.37E-02
294.95	9.37	pos	5.43E-02	4.26E-02	4.89E-02	3.56E-02	6.40E-02
294.95	8.31	pos	3.46E-02	4.13E-02	4.61E-02	3.77E-02	4.38E-02
296.08	9.13	pos	3.23E-02	2.25E-02	2.22E-02	3.62E-02	1.64E-02
296.89	7.94	neg	1.12E-01	1.31E-01	1.27E-01	8.86E-02	1.23E-01
297.98	8.67	pos	1.04E-02	9.62E-03	1.24E-02	1.66E-02	1.26E-02
298.00	6.39	neg	4.25E-02	5.67E-02	5.19E-02	4.58E-02	4.90E-02
298.12	0.81	pos	1.05E-02	1.04E-02	1.46E-02	1.18E-02	1.75E-02
298.89	7.94	neg	2.73E-02	2.99E-02	2.89E-02	2.40E-02	2.72E-02
299.03	7.43	pos	1.20E-02	1.16E-02	1.72E-02	1.75E-02	1.60E-02
299.17	0.61	pos	4.70E-02	9.92E-02	6.09E-02	1.18E-01	4.03E-02
300.00	5.79	neg	8.58E-02	1.03E-01	1.15E-01	8.56E-02	1.36E-01
301.99	5.58	neg	1.47E-02	2.14E-02	2.43E-02	1.72E-02	2.61E-02
302.04	6.70	pos	4.12E-03	6.20E-03	7.31E-03	7.16E-03	7.53E-03
304.01	8.66	neg	3.22E-02	3.37E-02	3.95E-02	3.76E-02	3.88E-02
304.11	6.69	neg	4.29E-02	4.60E-02	3.63E-02	3.20E-02	2.72E-02
305.01	9.03	pos	9.77E-03	1.05E-02	8.34E-03	1.09E-02	8.74E-03
305.99	5.58	neg	4.84E-03	7.30E-03	7.88E-03	6.21E-03	8.73E-03
306.09	8.64	neg	7.49E-02	8.57E-02	5.76E-02	5.35E-02	6.17E-02
306.13	4.73	neg	1.29E-02	8.34E-03	7.40E-03	8.16E-03	9.03E-03
307.04	7.02	pos	9.64E-03	8.42E-03	1.02E-02	9.56E-03	8.21E-03
307.98	5.58	neg	1.04E-03	1.75E-03	1.78E-03	1.23E-03	2.13E-03
308.11	8.64	pos	6.22E-02	7.20E-02	5.23E-02	4.93E-02	4.52E-02
308.15	4.67	pos	4.97E-03	6.01E-03	5.33E-03	5.08E-03	6.33E-03
308.93	8.38	neg	1.46E-02	1.38E-02	1.41E-02	1.55E-02	1.18E-02
309.04	7.33	neg	1.79E-02	2.38E-02	3.02E-02	2.20E-02	3.05E-02
309.08	8.62	pos	1.07E-02	1.36E-02	7.23E-03	1.01E-02	8.87E-03
309.96	8.74	neg	1.02E-02	1.14E-02	1.18E-02	1.14E-02	1.07E-02
310.10	4.66	neg	4.22E-03	3.94E-03	4.19E-03	4.45E-03	3.99E-03
310.23	6.66	pos	9.25E-03	9.57E-03	1.07E-02	2.08E-02	2.65E-02
310.57	5.58	pos	1.35E-03	1.40E-03	1.53E-03	1.16E-03	1.66E-03
310.93	8.31	pos	1.11E-02	1.33E-02	1.42E-02	1.50E-02	1.40E-02
314.91	9.42	neg	1.97E-01	2.47E-01	2.69E-01	2.14E-01	2.68E-01
315.09	8.64	neg	6.67E-02	9.28E-02	6.45E-02	4.71E-02	6.67E-02
315.13	2.48	pos	3.19E-03	4.07E-03	3.83E-03	2.49E-03	5.19E-03
316.18	6.35	pos	9.24E-01	1.36E+00	1.22E+00	1.12E+00	1.48E+00
316.93	9.42	pos	4.13E-02	5.08E-02	6.00E-02	5.35E-02	6.79E-02
316.96	8.31	neg	2.24E-01	2.42E-01	2.69E-01	2.50E-01	2.61E-01
317.12	8.62	pos	2.96E-02	4.27E-02	2.59E-02	2.28E-02	2.99E-02
317.55	6.01	neg	2.23E-03	4.25E-03	3.91E-03	3.18E-03	4.02E-03
318.05	6.58	neg	2.90E-02	3.00E-02	3.23E-02	2.84E-02	2.83E-02

319.99	8.70	neg	2.18E-02	2.27E-02	2.31E-02	2.15E-02	2.12E-02
320.03	6.68	neg	1.49E-02	1.21E-02	1.44E-02	1.31E-02	1.26E-02
320.99	9.04	pos	8.31E-03	8.82E-03	7.96E-03	9.84E-03	7.07E-03
321.15	7.96	pos	2.52E-02	2.43E-02	2.45E-02	3.13E-02	3.14E-02
321.18	2.07	pos	1.42E-03	6.84E-03	1.02E-02	7.25E-03	1.10E-02
322.06	6.48	pos	6.17E-03	8.28E-03	6.02E-03	5.36E-03	7.90E-03
323.41	6.96	pos	1.21E-02	1.04E-02	1.03E-02	1.08E-02	1.56E-02
325.05	7.08	neg	8.38E-02	6.97E-02	5.66E-02	5.43E-02	4.99E-02
325.06	8.60	pos	6.58E-03	1.07E-02	7.08E-03	7.37E-03	7.84E-03
325.99	6.92	pos	8.80E-03	9.85E-03	9.79E-03	1.19E-02	1.40E-02
327.08	8.87	neg	1.39E-02	1.88E-02	1.26E-02	1.18E-02	1.42E-02
327.49	5.58	neg	1.57E-03	2.30E-03	2.33E-03	1.74E-03	2.56E-03
328.49	5.58	neg	3.01E-03	3.69E-03	4.31E-03	2.92E-03	4.94E-03
330.02	5.58	neg	5.52E-02	5.28E-02	5.84E-02	5.13E-02	4.50E-02
330.09	8.65	pos	3.83E-02	4.29E-02	3.04E-02	3.00E-02	2.92E-02
330.89	9.43	neg	1.03E-01	1.20E-01	1.36E-01	1.12E-01	1.19E-01
331.14	7.06	neg	3.65E-01	4.35E-01	4.62E-01	3.65E-01	4.73E-01
333.12	0.65	neg	4.19E-02	4.01E-02	2.17E-02	4.79E-02	1.45E-02
333.16	7.03	pos	3.38E-02	5.56E-02	6.78E-02	5.65E-02	8.17E-02
333.95	9.93	pos	7.89E-03	9.27E-03	1.15E-02	1.02E-02	1.40E-02
334.00	6.70	neg	6.37E-02	7.98E-02	8.23E-02	6.67E-02	6.59E-02
334.89	9.37	neg	1.47E-02	2.21E-02	2.13E-02	1.73E-02	2.78E-02
335.15	4.68	pos	5.51E-02	5.69E-02	5.85E-02	5.65E-02	5.56E-02
335.99	6.69	neg	4.17E-02	5.17E-02	5.62E-02	4.64E-02	3.99E-02
336.07	5.58	pos	3.02E-03	3.35E-03	3.57E-03	2.71E-03	3.44E-03
338.11	6.67	neg	2.30E-02	1.85E-02	2.10E-02	1.88E-02	1.44E-02
338.16	6.38	pos	3.91E-01	4.59E-01	3.72E-01	3.52E-01	4.26E-01
338.92	9.58	pos	7.01E-02	6.77E-02	7.59E-02	8.67E-02	7.41E-02
339.07	5.58	pos	5.34E-03	6.20E-03	6.32E-03	4.94E-03	6.21E-03
339.09	8.64	pos	4.15E-02	5.05E-02	4.29E-02	3.41E-02	4.43E-02
341.06	5.58	pos	2.16E-03	2.52E-03	2.70E-03	1.98E-03	2.28E-03
346.07	8.41	neg	2.41E-02	2.96E-02	2.33E-02	2.29E-02	2.57E-02
346.07	8.67	pos	1.19E-02	1.42E-02	1.17E-02	1.37E-02	9.70E-03
346.29	4.66	pos	1.66E-02	1.80E-02	1.47E-02	1.96E-02	2.57E-02
348.03	2.04	neg	1.50E-03	1.71E-03	1.45E-03	1.19E-03	1.99E-03
348.09	8.43	pos	1.74E-02	2.19E-02	1.82E-02	1.69E-02	1.75E-02
348.90	8.04	neg	3.82E-02	3.53E-02	4.47E-02	4.61E-02	3.95E-02
349.14	7.95	pos	8.68E-03	1.08E-02	1.08E-02	1.13E-02	1.17E-02
350.97	9.94	pos	4.79E-03	6.56E-03	8.31E-03	6.02E-03	9.50E-03
351.13	4.67	pos	8.58E-02	9.11E-02	8.53E-02	8.30E-02	8.06E-02
352.07	8.65	pos	1.85E-02	1.62E-02	1.49E-02	1.45E-02	1.42E-02
352.91	8.35	pos	1.72E-02	1.54E-02	1.94E-02	1.88E-02	1.42E-02
353.00	5.58	neg	3.25E-03	4.81E-03	5.20E-03	3.25E-03	5.63E-03
353.05	8.65	neg	1.90E-02	2.39E-02	1.78E-02	1.49E-02	1.91E-02
354.13	6.38	pos	5.54E-01	6.64E-01	5.22E-01	5.10E-01	5.93E-01
354.89	9.57	pos	4.36E-02	4.60E-02	5.11E-02	6.27E-02	4.57E-02
355.00	5.58	neg	8.27E-03	1.20E-02	1.36E-02	9.51E-03	1.51E-02
356.14	6.36	pos	4.39E-02	5.44E-02	3.73E-02	3.65E-02	4.87E-02
356.98	7.46	pos	4.55E-03	3.65E-03	5.14E-03	5.68E-03	4.43E-03
356.99	5.58	neg	8.34E-03	1.20E-02	1.26E-02	9.06E-03	1.51E-02
357.01	9.33	neg	4.51E-02	4.88E-02	4.09E-02	4.16E-02	4.46E-02
359.07	7.04	pos	1.67E-02	1.77E-02	1.50E-02	1.70E-02	1.67E-02

359.13	7.31	neg	7.44E-02	1.11E-01	1.06E-01	9.68E-02	1.71E-01
360.16	6.36	neg	1.47E-01	1.67E-01	1.31E-01	1.22E-01	1.45E-01
361.08	8.64	pos	4.46E-02	5.03E-02	5.14E-02	4.90E-02	5.63E-02
361.08	7.05	pos	3.80E-03	9.97E-03	1.11E-02	1.09E-02	1.06E-02
361.24	6.36	pos	1.58E-02	1.26E-01	1.97E-01	1.90E-01	2.02E-01
362.94	8.29	pos	6.24E-02	7.42E-02	8.02E-02	6.62E-02	8.05E-02
363.32	17.69	pos	2.67E-03	3.05E-03	1.58E-02	2.58E-02	2.21E-02
363.74	5.59	pos	2.51E-03	2.95E-03	3.03E-03	1.88E-03	2.71E-03
364.88	7.97	neg	6.02E-02	6.91E-02	7.63E-02	6.06E-02	6.37E-02
365.73	5.58	pos	5.58E-03	6.30E-03	5.68E-03	4.17E-03	6.40E-03
367.56	5.58	pos	2.51E-03	3.08E-03	2.80E-03	1.91E-03	2.89E-03
369.11	4.67	neg	3.32E-02	2.99E-02	3.21E-02	3.30E-02	3.26E-02
370.07	8.45	pos	7.90E-03	9.24E-03	7.29E-03	7.25E-03	7.22E-03
371.11	7.09	pos	2.97E-02	3.30E-02	3.66E-02	4.06E-02	2.78E-02
372.00	8.65	neg	1.50E-02	1.66E-02	2.06E-02	1.90E-02	2.00E-02
373.11	4.78	pos	7.41E-03	7.95E-03	6.57E-03	7.74E-03	7.09E-03
374.06	8.66	pos	1.19E-02	1.09E-02	1.10E-02	1.27E-02	1.05E-02
374.14	4.65	neg	3.10E-03	2.56E-03	2.98E-03	3.16E-03	3.19E-03
374.23	6.36	pos	8.66E-03	1.41E-02	1.41E-02	1.33E-02	1.72E-02
374.83	7.93	pos	2.90E-03	4.47E-03	5.28E-03	3.63E-03	5.68E-03
374.99	8.59	neg	3.69E-02	3.84E-02	3.79E-02	3.63E-02	3.40E-02
375.20	7.38	pos	4.27E-03	5.21E-03	6.97E-03	7.24E-03	6.93E-03
377.03	8.65	pos	2.60E-02	2.68E-02	2.69E-02	3.15E-02	3.61E-02
377.12	7.09	pos	9.89E-03	1.14E-02	1.21E-02	1.16E-02	9.70E-03
377.15	6.36	neg	8.16E-02	6.53E-02	6.83E-02	6.62E-02	6.88E-02
378.18	7.30	pos	9.64E-03	1.46E-02	1.92E-02	1.47E-02	3.77E-02
378.92	8.30	pos	2.15E-02	2.43E-02	2.96E-02	3.01E-02	2.85E-02
380.85	7.94	neg	6.76E-02	8.11E-02	8.14E-02	5.06E-02	7.68E-02
381.07	7.06	pos	1.02E-02	8.41E-03	6.31E-03	8.12E-03	7.21E-03
381.50	5.58	neg	1.81E-03	2.29E-03	3.04E-03	1.77E-03	2.78E-03
382.09	6.75	neg	3.63E-02	3.09E-02	2.30E-02	2.59E-02	2.30E-02
382.24	1.70	pos	7.64E-03	9.15E-03	9.26E-03	5.42E-03	9.48E-03
382.85	7.93	neg	2.00E-02	2.68E-02	2.66E-02	6.73E-03	2.49E-02
383.13	7.00	pos	4.75E-01	5.85E-01	7.12E-01	6.68E-01	7.92E-01
383.69	5.58	neg	2.79E-02	2.68E-02	3.70E-02	2.57E-02	3.76E-02
384.49	5.58	neg	1.75E-03	2.14E-03	2.48E-03	1.64E-03	2.73E-03
384.95	8.31	neg	1.05E-01	1.18E-01	1.33E-01	1.13E-01	1.32E-01
385.08	4.67	neg	2.86E-02	2.72E-02	2.87E-02	3.21E-02	2.87E-02
385.14	7.29	pos	2.69E-02	3.59E-02	3.14E-02	4.62E-02	4.25E-02
386.07	1.69	pos	8.84E-04	1.54E-03	1.89E-03	8.74E-04	1.51E-03
387.07	7.06	pos	7.68E-03	8.51E-03	1.01E-02	1.05E-02	1.18E-02
387.98	8.68	neg	1.22E-02	1.29E-02	1.48E-02	1.53E-02	1.57E-02
388.19	6.88	neg	6.13E-02	8.14E-02	8.67E-02	1.15E-01	1.33E-01
389.01	7.03	neg	7.04E-02	6.63E-02	7.01E-02	6.09E-02	5.96E-02
390.21	6.84	pos	2.01E-02	2.99E-02	3.66E-02	4.78E-02	5.81E-02
391.07	5.59	pos	4.66E-03	5.19E-03	4.94E-03	4.00E-03	4.81E-03
391.17	6.93	pos	8.68E-03	1.14E-02	1.22E-02	1.21E-02	1.60E-02
392.91	9.34	neg	7.68E-03	1.52E-02	1.80E-02	9.64E-03	2.91E-02
392.92	9.39	pos	2.41E-02	3.12E-02	3.63E-02	2.80E-02	5.31E-02
393.03	7.06	neg	3.51E-02	5.00E-02	5.05E-02	4.30E-02	3.84E-02
393.07	5.59	pos	5.01E-03	5.62E-03	5.83E-03	4.05E-03	5.36E-03
394.01	6.69	neg	2.37E-02	3.07E-02	3.27E-02	2.56E-02	2.27E-02

395.06	7.05	pos	9.75E-03	1.04E-02	7.97E-03	8.31E-03	8.22E-03
395.11	7.02	neg	5.89E-01	6.62E-01	7.72E-01	6.48E-01	8.04E-01
396.12	6.37	pos	1.29E-02	1.62E-02	1.05E-02	1.07E-02	1.11E-02
396.23	1.71	pos	2.65E-03	2.72E-03	2.45E-03	1.73E-03	2.78E-03
397.05	7.06	pos	1.18E-02	1.15E-02	1.02E-02	1.28E-02	9.83E-03
399.03	8.66	pos	2.60E-02	2.59E-02	2.86E-02	2.59E-02	2.65E-02
399.11	7.11	pos	1.33E-01	1.67E-01	2.06E-01	1.84E-01	2.10E-01
401.05	4.65	neg	1.49E-03	5.11E-03	4.54E-03	4.01E-03	4.23E-03
401.17	7.39	neg	1.32E-01	1.44E-01	1.51E-01	1.06E-01	1.33E-01
403.19	7.37	pos	1.29E-02	1.85E-02	2.18E-02	1.39E-02	2.22E-02
404.03	8.58	pos	6.19E-03	7.26E-03	5.87E-03	5.54E-03	7.21E-03
404.20	2.01	pos	2.47E-03	3.08E-03	2.47E-03	3.33E-03	3.89E-03
405.03	8.62	pos	1.50E-02	1.37E-02	1.92E-02	1.77E-02	1.76E-02
406.00	5.58	neg	2.59E-03	3.08E-03	3.68E-03	2.77E-03	3.51E-03
406.08	6.36	pos	1.96E-02	2.51E-02	1.74E-02	1.72E-02	2.06E-02
407.09	7.03	pos	1.05E-02	1.06E-02	1.12E-02	1.05E-02	1.05E-02
407.13	4.66	neg	3.85E-03	3.99E-03	3.34E-03	3.57E-03	3.30E-03
408.02	5.58	neg	5.81E-03	8.09E-03	8.10E-03	6.09E-03	9.31E-03
408.09	6.35	neg	3.68E-02	2.74E-02	2.74E-02	2.59E-02	3.25E-02
409.00	5.58	neg	3.74E-03	4.15E-03	4.92E-03	4.04E-03	4.91E-03
409.96	9.38	pos	2.99E-02	4.73E-02	5.87E-02	4.11E-02	8.48E-02
410.00	5.58	neg	6.43E-03	1.01E-02	1.04E-02	7.25E-03	1.09E-02
410.09	6.35	neg	2.43E-02	1.81E-02	1.92E-02	1.55E-02	1.92E-02
411.04	5.12	neg	3.15E-03	8.08E-03	3.88E-03	3.13E-03	3.82E-03
411.19	1.96	pos	6.49E-04	1.08E-03	1.06E-03	7.29E-04	1.75E-03
412.00	5.58	neg	3.95E-03	5.52E-03	6.12E-03	4.31E-03	6.78E-03
412.09	6.37	pos	1.76E-02	2.34E-02	1.32E-02	1.60E-02	1.74E-02
412.19	6.84	pos	2.03E-02	2.54E-02	3.20E-02	3.55E-02	3.30E-02
412.28	4.65	pos	1.83E-03	2.31E-03	2.39E-03	2.83E-03	3.47E-03
412.89	9.40	neg	1.09E-01	1.53E-01	1.79E-01	1.31E-01	1.98E-01
413.99	5.58	neg	1.76E-03	2.30E-03	2.66E-03	1.63E-03	2.34E-03
414.09	6.37	pos	7.71E-03	1.05E-02	7.21E-03	6.52E-03	6.53E-03
415.01	8.68	pos	9.34E-03	9.38E-03	9.02E-03	1.02E-02	9.66E-03
415.07	7.30	pos	5.78E-03	7.37E-03	5.68E-03	6.14E-03	1.27E-02
417.57	5.58	pos	5.07E-03	5.92E-03	6.07E-03	4.64E-03	6.01E-03
418.26	6.68	pos	2.41E-02	3.24E-02	3.19E-02	3.26E-02	2.92E-02
419.08	2.02	neg	1.09E-03	1.16E-03	7.80E-04	1.50E-03	1.65E-03
419.27	6.68	pos	1.41E-01	1.95E-01	1.87E-01	1.80E-01	1.67E-01
419.57	5.58	pos	7.19E-03	8.57E-03	7.85E-03	5.69E-03	7.67E-03
420.17	0.63	pos	1.20E-03	2.01E-03	1.35E-03	2.16E-03	9.73E-04
420.29	6.60	pos	9.63E-02	9.86E-02	8.74E-02	8.03E-02	8.60E-02
421.30	6.54	pos	2.35E-02	2.37E-02	2.09E-02	2.04E-02	2.18E-02
423.06	7.05	pos	9.29E-03	1.04E-02	8.76E-03	9.97E-03	1.31E-02
424.07	6.35	neg	3.23E-02	2.45E-02	2.66E-02	2.64E-02	2.89E-02
424.22	4.70	pos	2.17E-03	2.00E-03	1.63E-03	1.82E-03	1.89E-03
425.17	7.39	pos	2.51E-02	3.12E-02	4.08E-02	3.32E-02	4.18E-02
426.06	6.35	neg	2.42E-02	1.76E-02	2.12E-02	2.09E-02	2.50E-02
426.17	4.50	neg	2.22E-03	1.88E-03	1.95E-03	1.87E-03	2.06E-03
427.01	8.61	neg	8.36E-03	1.40E-02	1.61E-02	1.49E-02	1.47E-02
428.07	6.37	pos	7.45E-03	9.42E-03	5.36E-03	5.38E-03	6.04E-03
428.16	6.84	pos	8.98E-03	2.26E-02	1.40E-02	1.75E-02	1.53E-02
428.87	9.41	neg	5.70E-02	7.78E-02	9.37E-02	6.09E-02	9.31E-02



430.89	9.42	pos	2.62E-02	3.33E-02	3.71E-02	3.27E-02	4.20E-02
430.93	8.29	pos	6.19E-02	7.09E-02	7.92E-02	6.90E-02	8.43E-02
434.18	6.84	pos	4.04E-03	6.49E-03	5.09E-03	6.62E-03	5.11E-03
434.30	5.58	neg	1.26E-03	1.80E-03	1.96E-03	1.35E-03	2.22E-03
434.87	9.48	neg	6.37E-02	7.19E-02	8.56E-02	7.69E-02	8.21E-02
435.31	7.26	neg	2.63E-02	2.67E-02	2.19E-02	1.28E-02	2.22E-02
435.50	5.58	neg	1.89E-03	2.37E-03	3.01E-03	1.78E-03	3.42E-03
436.50	5.58	neg	2.66E-02	2.33E-02	3.24E-02	2.17E-02	3.14E-02
436.89	9.59	pos	4.64E-02	5.39E-02	5.97E-02	6.00E-02	5.38E-02
437.50	5.58	neg	1.89E-03	2.22E-03	2.59E-03	1.59E-03	2.99E-03
438.02	4.65	neg	9.06E-04	3.15E-03	2.50E-03	2.05E-03	2.31E-03
438.50	5.59	neg	1.62E-02	1.38E-02	1.83E-02	1.29E-02	1.87E-02
440.25	6.68	pos	7.15E-03	8.38E-03	7.91E-03	7.83E-03	6.36E-03
441.12	7.34	pos	1.66E-02	2.20E-02	2.75E-02	2.62E-02	2.74E-02
441.25	6.69	pos	4.07E-02	4.88E-02	4.67E-02	4.21E-02	3.61E-02
442.08	5.58	pos	2.12E-03	2.48E-03	2.42E-03	2.20E-03	2.61E-03
442.13	7.36	pos	3.19E-03	4.32E-03	5.35E-03	5.37E-03	4.90E-03
442.81	7.95	pos	7.84E-03	9.95E-03	9.32E-03	9.16E-03	1.13E-02
443.04	4.74	neg	8.54E-03	6.77E-03	7.70E-03	8.29E-03	7.57E-03
443.09	7.24	pos	6.50E-03	7.86E-03	1.19E-02	9.30E-03	9.28E-03
444.08	5.58	pos	8.74E-03	9.65E-03	9.72E-03	7.25E-03	9.78E-03
444.94	8.28	pos	1.32E-02	1.73E-02	1.73E-02	1.60E-02	2.06E-02
445.23	7.38	pos	3.68E-02	4.32E-02	4.92E-02	4.44E-02	4.93E-02
446.91	8.29	pos	2.33E-02	2.44E-02	3.23E-02	3.09E-02	3.05E-02
447.13	0.87	neg	2.23E-03	2.64E-03	3.10E-03	3.35E-03	2.88E-03
447.28	6.44	pos	6.53E-03	1.66E-02	7.75E-03	4.90E-03	1.06E-02
448.07	5.58	pos	5.87E-03	6.32E-03	6.11E-03	5.51E-03	7.31E-03
448.24	0.57	pos	8.57E-04	1.51E-03	1.40E-03	2.24E-03	1.52E-03
448.84	7.96	neg	3.25E-02	3.46E-02	3.83E-02	2.83E-02	2.91E-02
450.15	6.85	pos	3.78E-03	4.08E-03	4.56E-03	5.06E-03	4.57E-03
450.85	9.49	neg	6.85E-02	8.82E-02	9.27E-02	8.17E-02	9.08E-02
451.05	7.20	pos	1.36E-02	1.70E-02	1.48E-02	1.62E-02	2.52E-02
452.87	9.53	pos	4.48E-02	4.64E-02	5.16E-02	5.27E-02	4.68E-02
452.94	8.30	neg	6.72E-02	7.97E-02	9.01E-02	7.54E-02	9.09E-02
454.99	9.35	neg	1.42E-02	2.02E-02	1.84E-02	1.65E-02	2.37E-02
455.05	7.06	pos	5.14E-03	7.38E-03	1.17E-02	1.08E-02	1.33E-02
455.21	6.69	neg	2.84E-02	2.36E-02	2.04E-02	2.27E-02	2.10E-02
456.31	6.70	pos	6.89E-02	6.49E-02	5.79E-02	6.27E-02	6.85E-02
457.07	7.26	pos	9.99E-03	1.16E-02	1.64E-02	1.25E-02	1.48E-02
458.07	2.02	pos	1.49E-03	1.09E-03	1.10E-03	1.37E-03	1.29E-03
458.79	7.92	pos	3.62E-03	6.52E-03	7.81E-03	5.15E-03	9.28E-03
461.00	5.58	neg	3.08E-03	3.97E-03	4.65E-03	3.08E-03	4.47E-03
462.00	5.58	neg	2.32E-03	2.32E-03	2.94E-03	1.83E-03	3.02E-03
463.00	5.58	neg	5.37E-02	5.79E-02	6.70E-02	4.54E-02	7.16E-02
463.13	7.34	pos	7.52E-03	8.63E-03	1.20E-02	9.02E-03	1.06E-02
464.00	5.57	neg	2.19E-03	2.79E-03	3.15E-03	2.32E-03	3.58E-03
464.82	7.94	neg	3.12E-02	3.97E-02	4.04E-02	2.75E-02	3.67E-02
465.00	5.59	neg	4.51E-02	4.87E-02	5.57E-02	4.20E-02	5.63E-02
466.20	0.88	pos	1.56E-03	1.46E-03	1.79E-03	1.74E-03	1.98E-03
467.21	7.39	pos	1.82E-02	2.06E-02	2.39E-02	2.46E-02	2.31E-02
468.91	8.32	neg	2.48E-02	2.92E-02	3.25E-02	3.27E-02	2.94E-02
471.57	5.59	pos	1.69E-03	2.17E-03	1.92E-03	1.54E-03	2.07E-03

477.01	4.77	pos	2.21E-03	2.54E-03	2.87E-03	2.78E-03	2.90E-03
478.29	0.63	pos	9.14E-04	1.75E-03	1.13E-03	2.13E-03	1.34E-03
479.21	6.70	pos	7.34E-03	7.97E-03	7.52E-03	6.84E-03	6.66E-03
480.07	6.59	pos	5.32E-03	6.66E-03	5.68E-03	4.85E-03	4.50E-03
483.18	7.39	pos	1.16E-02	1.18E-02	1.45E-02	1.54E-02	1.32E-02
486.15	8.62	pos	1.08E-02	1.57E-02	8.97E-03	8.15E-03	1.00E-02
487.30	6.35	pos	3.91E-03	4.67E-03	3.19E-03	3.23E-03	4.41E-03
488.50	5.58	neg	1.38E-03	1.71E-03	2.07E-03	1.28E-03	2.08E-03
488.90	8.34	pos	1.41E-02	1.51E-02	1.72E-02	1.89E-02	1.64E-02
489.19	7.39	pos	4.53E-03	3.62E-03	5.40E-03	6.15E-03	4.62E-03
489.50	5.58	neg	1.42E-03	2.21E-03	2.73E-03	1.73E-03	2.69E-03
490.50	5.59	neg	2.01E-02	2.00E-02	2.33E-02	1.64E-02	2.33E-02
490.90	9.34	pos	6.17E-03	2.45E-02	2.83E-02	2.61E-02	3.97E-02
491.50	5.58	neg	1.16E-03	1.57E-03	1.79E-03	1.44E-03	2.20E-03
493.08	7.38	pos	4.84E-03	5.48E-03	5.12E-03	5.70E-03	5.61E-03
495.08	5.57	pos	4.11E-03	4.57E-03	4.53E-03	4.06E-03	4.45E-03
496.83	9.80	pos	1.93E-02	2.01E-02	2.29E-02	2.60E-02	1.91E-02
497.02	4.65	neg	1.55E-03	3.51E-03	3.13E-03	2.42E-03	2.65E-03
497.08	5.57	pos	1.14E-02	1.29E-02	1.24E-02	1.09E-02	1.31E-02
498.92	8.28	pos	4.03E-02	5.14E-02	5.54E-02	4.75E-02	6.26E-02
499.08	5.57	pos	1.47E-02	1.66E-02	1.63E-02	1.37E-02	1.60E-02
505.16	7.40	pos	7.65E-03	7.43E-03	1.00E-02	1.01E-02	9.19E-03
507.14	6.69	neg	3.17E-02	4.59E-02	4.26E-02	3.42E-02	3.52E-02
507.94	9.38	pos	1.95E-02	3.81E-02	4.47E-02	2.92E-02	6.87E-02
508.13	8.63	pos	1.59E-02	1.93E-02	1.50E-02	1.13E-02	1.65E-02
508.15	6.70	pos	4.21E-03	5.00E-03	3.29E-03	3.98E-03	4.06E-03
509.30	2.50	neg	1.61E-02	1.91E-02	1.67E-02	1.63E-02	1.77E-02
510.79	9.94	neg	1.61E-02	1.65E-02	1.90E-02	2.33E-02	1.76E-02
511.09	4.65	neg	2.20E-03	2.20E-03	2.20E-03	1.86E-03	2.00E-03
511.16	6.73	pos	1.67E-02	1.96E-02	1.61E-02	1.76E-02	1.68E-02
511.33	2.50	pos	8.54E-03	9.06E-03	9.18E-03	8.48E-03	9.29E-03
512.80	9.98	pos	1.33E-02	1.44E-02	1.42E-02	1.51E-02	1.48E-02
512.84	9.31	neg	7.61E-03	1.29E-02	1.43E-02	9.40E-03	2.04E-02
512.88	9.39	pos	2.35E-02	3.52E-02	4.22E-02	2.98E-02	5.08E-02
512.92	8.27	pos	1.01E-02	1.32E-02	1.36E-02	1.32E-02	1.56E-02
514.00	5.59	neg	1.86E-02	1.98E-02	2.20E-02	1.53E-02	1.87E-02
514.29	1.97	pos	5.23E-03	6.04E-03	5.59E-03	4.60E-03	6.24E-03
516.01	5.58	neg	2.03E-03	2.84E-03	3.38E-03	2.19E-03	2.79E-03
518.01	5.58	neg	1.69E-03	2.15E-03	2.40E-03	1.85E-03	2.46E-03
520.92	8.30	neg	4.74E-02	6.16E-02	6.59E-02	5.35E-02	6.73E-02
521.08	8.64	pos	8.85E-03	1.04E-02	7.70E-03	6.87E-03	7.92E-03
521.13	7.38	pos	5.36E-03	4.41E-03	9.18E-03	6.42E-03	8.43E-03
523.41	7.07	pos	9.47E-03	9.96E-03	1.04E-02	1.39E-02	1.30E-02
525.30	6.61	pos	1.68E-02	2.76E-02	2.97E-02	1.75E-02	2.62E-02
525.58	5.58	pos	1.37E-03	1.72E-03	1.51E-03	1.22E-03	1.55E-03
526.78	7.94	pos	4.05E-03	6.20E-03	7.63E-03	6.15E-03	8.16E-03
528.87	9.40	pos	1.78E-02	2.38E-02	2.80E-02	2.33E-02	3.34E-02
531.15	6.71	pos	4.84E-03	5.39E-03	4.32E-03	4.95E-03	4.84E-03
532.80	7.96	neg	1.72E-02	2.21E-02	2.18E-02	1.42E-02	1.82E-02
532.85	9.42	neg	4.03E-02	4.56E-02	5.31E-02	4.81E-02	5.72E-02
533.12	7.06	pos	9.62E-03	8.48E-03	7.85E-03	8.60E-03	6.95E-03
534.87	9.48	pos	4.28E-02	4.75E-02	5.42E-02	5.20E-02	5.10E-02

535.13	7.37	pos	5.79E-03	6.86E-03	4.51E-03	6.41E-03	6.19E-03
536.90	8.32	neg	2.53E-02	3.10E-02	3.24E-02	2.93E-02	2.88E-02
539.18	7.32	neg	7.07E-03	1.05E-02	9.86E-03	8.44E-03	1.35E-02
541.19	1.98	neg	9.10E-04	9.56E-04	8.08E-04	3.33E-04	1.10E-03
542.76	7.92	pos	3.60E-03	6.56E-03	7.76E-03	5.44E-03	1.06E-02
543.23	2.03	pos	2.32E-03	3.52E-03	2.85E-03	1.63E-03	4.87E-03
543.38	7.07	pos	5.17E-03	5.03E-03	4.28E-03	4.60E-03	3.83E-03
544.27	2.07	pos	2.14E-03	2.25E-03	2.16E-03	1.33E-03	2.66E-03
546.08	8.65	pos	7.24E-03	8.72E-03	8.33E-03	6.80E-03	8.00E-03
547.13	6.70	pos	7.92E-03	8.51E-03	7.29E-03	7.68E-03	6.96E-03
548.78	7.93	neg	1.72E-02	2.06E-02	2.18E-02	1.36E-02	2.06E-02
548.83	9.45	neg	4.38E-02	5.51E-02	5.90E-02	5.12E-02	6.28E-02
549.09	5.58	pos	1.53E-03	1.66E-03	1.52E-03	1.43E-03	1.77E-03
550.85	9.47	pos	3.29E-02	3.83E-02	4.60E-02	4.31E-02	4.30E-02
552.10	8.63	pos	1.96E-02	1.99E-02	2.10E-02	1.71E-02	2.27E-02
556.33	4.65	pos	1.85E-03	1.41E-03	1.01E-03	7.73E-04	7.96E-04
556.88	8.33	pos	1.69E-02	1.53E-02	1.89E-02	1.94E-02	1.84E-02
559.34	4.64	pos	7.24E-02	5.61E-02	3.40E-02	3.14E-02	3.37E-02
565.06	9.19	neg	2.90E-02	3.73E-02	2.86E-02	3.68E-02	3.10E-02
566.09	5.60	pos	1.35E-04	1.09E-03	2.15E-03	1.82E-03	1.51E-03
566.91	8.28	pos	3.77E-02	4.89E-02	5.43E-02	4.33E-02	5.75E-02
567.33	0.60	pos	1.39E-03	1.80E-03	1.68E-03	2.27E-03	1.19E-03
568.07	8.65	pos	1.39E-02	1.34E-02	1.43E-02	1.29E-02	1.46E-02
571.18	7.01	pos	3.99E-03	4.64E-03	4.20E-03	3.59E-03	3.98E-03
572.87	8.34	pos	8.99E-03	7.79E-03	1.12E-02	1.10E-02	9.06E-03
573.32	4.64	pos	1.27E-02	8.70E-03	4.99E-03	4.95E-03	5.98E-03
574.08	8.63	pos	1.65E-02	1.60E-02	1.94E-02	1.81E-02	2.02E-02
574.36	1.00	pos	8.21E-03	8.69E-03	9.21E-03	3.55E-03	5.69E-03
577.58	5.58	pos	2.12E-03	2.76E-03	2.73E-03	1.93E-03	2.81E-03
578.91	8.37	neg	1.31E-02	1.38E-02	1.45E-02	1.57E-02	1.41E-02
579.04	9.90	neg	1.67E-02	2.30E-02	1.87E-02	1.79E-02	2.29E-02
579.21	6.36	pos	8.34E-03	1.15E-02	7.63E-03	6.99E-03	8.48E-03
579.58	5.58	pos	3.30E-03	3.91E-03	3.46E-03	2.59E-03	3.97E-03
580.46	6.71	pos	5.93E-03	5.61E-03	4.71E-03	6.85E-03	6.58E-03
580.91	8.27	pos	1.17E-02	1.49E-02	1.67E-02	1.46E-02	1.82E-02
581.21	6.37	pos	4.32E-03	6.42E-03	7.22E-03	6.32E-03	7.27E-03
582.21	5.72	neg	1.72E-02	2.03E-02	2.07E-02	1.58E-02	2.65E-02
582.88	8.29	pos	1.79E-02	2.03E-02	2.55E-02	2.34E-02	2.60E-02
583.96	8.55	pos	9.33E-03	6.72E-03	9.22E-03	1.00E-02	5.12E-03
584.11	9.17	pos	1.77E-02	1.86E-02	1.49E-02	2.14E-02	1.40E-02
584.24	5.72	pos	9.91E-03	1.27E-02	1.47E-02	1.16E-02	2.00E-02
588.86	9.40	pos	1.38E-02	2.06E-02	1.78E-02	1.85E-02	2.39E-02
588.91	8.29	neg	3.68E-02	4.58E-02	5.26E-02	3.90E-02	4.97E-02
589.20	2.07	pos	7.73E-04	9.68E-04	7.41E-04	2.66E-04	1.19E-03
590.05	8.65	pos	1.22E-02	1.31E-02	1.41E-02	1.29E-02	1.38E-02
592.79	9.66	neg	3.18E-02	3.30E-02	3.70E-02	3.53E-02	2.82E-02
594.80	9.79	pos	1.62E-02	1.58E-02	1.71E-02	2.18E-02	1.65E-02
595.33	0.84	neg	5.88E-03	3.68E-03	3.71E-03	3.95E-03	3.60E-03
595.98	0.66	pos	7.59E-04	1.12E-03	9.14E-04	1.13E-03	8.45E-04
596.06	8.64	pos	1.13E-02	1.07E-02	1.42E-02	1.44E-02	1.57E-02
597.30	4.66	pos	2.66E-03	2.69E-03	2.44E-03	2.71E-03	2.37E-03
598.12	9.92	pos	1.55E-02	2.13E-02	1.64E-02	1.62E-02	1.87E-02

598.87	8.30	pos	9.20E-03	8.66E-03	1.05E-02	1.30E-02	1.06E-02
600.38	0.80	pos	1.18E-02	1.10E-02	6.66E-03	1.21E-02	8.10E-03
600.57	0.79	pos	1.18E-02	1.10E-02	6.66E-03	1.21E-02	8.10E-03
601.19	6.37	pos	9.59E-03	1.24E-02	6.42E-03	5.84E-03	7.24E-03
602.39	0.85	pos	5.23E-03	2.81E-03	3.32E-03	2.81E-03	4.16E-03
602.84	5.59	pos	9.57E-03	1.03E-02	1.04E-02	8.06E-03	1.08E-02
603.09	5.58	pos	9.57E-03	1.03E-02	1.04E-02	8.06E-03	1.08E-02
604.89	8.31	neg	2.37E-02	2.48E-02	2.72E-02	2.56E-02	2.57E-02
605.92	9.37	pos	1.41E-02	2.69E-02	3.23E-02	1.95E-02	4.82E-02
606.09	8.98	neg	9.05E-03	1.16E-02	8.74E-03	9.03E-03	9.81E-03
608.10	8.13	pos	7.48E-03	1.13E-02	6.86E-03	7.65E-03	8.63E-03
608.83	9.38	neg	2.92E-02	3.97E-02	4.52E-02	4.28E-02	5.99E-02
608.90	8.32	pos	8.10E-03	8.54E-03	1.16E-02	9.66E-03	9.90E-03
610.87	9.38	pos	3.05E-02	4.32E-02	5.63E-02	4.03E-02	6.75E-02
611.16	9.80	neg	4.81E-03	9.93E-03	8.98E-03	5.29E-03	1.26E-02
612.02	8.63	pos	8.69E-03	9.31E-03	1.20E-02	1.13E-02	1.15E-02
613.18	9.81	pos	8.68E-03	1.27E-02	1.23E-02	8.73E-03	1.58E-02
614.38	0.80	pos	5.15E-03	4.12E-03	5.27E-03	5.42E-03	5.62E-03
617.17	6.36	pos	6.59E-03	9.25E-03	4.85E-03	4.48E-03	6.21E-03
617.55	5.66	pos	2.66E-03	2.46E-03	2.46E-03	2.36E-03	1.89E-03
618.12	8.59	neg	1.16E-02	1.35E-02	1.03E-02	1.08E-02	1.16E-02
620.09	5.60	pos	3.48E-04	2.08E-03	2.55E-03	2.07E-03	1.93E-03
620.14	8.59	pos	1.27E-02	1.47E-02	1.25E-02	1.26E-02	1.40E-02
624.80	9.41	neg	1.64E-02	2.51E-02	3.03E-02	1.70E-02	3.43E-02
624.87	8.32	pos	1.67E-02	1.62E-02	1.99E-02	2.08E-02	2.02E-02
625.12	8.96	pos	6.06E-03	7.75E-03	4.92E-03	7.42E-03	6.80E-03
626.84	9.39	pos	1.26E-02	1.91E-02	2.26E-02	1.69E-02	2.94E-02
630.08	8.96	pos	6.75E-03	1.07E-02	7.55E-03	9.37E-03	8.00E-03
630.80	9.49	neg	2.63E-02	3.35E-02	3.78E-02	3.16E-02	3.84E-02
632.75	7.92	neg	1.25E-02	1.64E-02	1.82E-02	1.06E-02	1.64E-02
632.85	9.44	pos	3.35E-02	3.89E-02	4.57E-02	4.19E-02	4.68E-02
634.90	8.27	pos	3.27E-02	4.37E-02	5.10E-02	3.91E-02	5.18E-02
638.87	8.31	pos	8.20E-03	8.09E-03	8.87E-03	8.44E-03	8.50E-03
646.80	9.44	neg	2.66E-02	3.55E-02	4.11E-02	3.10E-02	4.25E-02
648.30	8.67	pos	1.94E-02	1.74E-02	1.85E-02	1.48E-02	2.31E-02
648.37	6.32	pos	5.83E-03	9.97E-03	6.14E-03	6.09E-03	1.04E-02
648.83	9.46	pos	2.41E-02	3.20E-02	3.86E-02	3.37E-02	3.59E-02
648.87	9.41	neg	1.65E-02	1.56E-02	1.76E-02	1.92E-02	1.55E-02
650.38	6.68	pos	4.06E-03	5.40E-03	4.25E-03	4.17E-03	3.00E-03
650.87	8.29	pos	1.88E-02	1.85E-02	2.46E-02	2.30E-02	2.52E-02
654.82	9.55	pos	1.82E-02	1.67E-02	1.95E-02	2.21E-02	1.74E-02
655.20	8.62	pos	8.50E-03	1.08E-02	8.36E-03	5.14E-03	9.12E-03
656.09	5.58	pos	5.42E-03	5.72E-03	6.02E-03	5.62E-03	6.32E-03
656.90	8.29	neg	2.06E-02	2.45E-02	3.01E-02	2.34E-02	3.09E-02
658.09	5.57	pos	9.32E-03	1.04E-02	1.07E-02	8.89E-03	1.09E-02
662.12	9.00	neg	1.22E-02	1.56E-02	1.27E-02	1.31E-02	1.33E-02
664.14	9.00	pos	4.13E-02	4.88E-02	4.08E-02	3.95E-02	4.27E-02
666.85	8.30	pos	8.01E-03	9.20E-03	1.16E-02	1.29E-02	1.04E-02
668.79	9.50	neg	2.47E-02	2.80E-02	3.17E-02	2.78E-02	2.93E-02
669.29	4.67	pos	3.35E-03	3.75E-03	2.81E-03	3.37E-03	2.98E-03
670.81	9.57	pos	2.36E-02	2.54E-02	2.73E-02	2.86E-02	2.10E-02
671.49	4.64	pos	2.68E-03	2.52E-03	2.10E-03	2.05E-03	2.15E-03

672.88	8.31	neg	1.37E-02	1.61E-02	1.84E-02	1.72E-02	1.79E-02
676.88	8.29	pos	7.91E-03	9.26E-03	1.06E-02	8.27E-03	1.03E-02
677.18	8.62	pos	8.41E-03	1.07E-02	8.26E-03	6.63E-03	8.32E-03
681.26	4.66	neg	1.70E-03	1.34E-03	1.62E-03	1.55E-03	1.58E-03
682.30	6.69	pos	5.97E-03	7.09E-03	5.75E-03	6.06E-03	5.60E-03
683.49	4.64	pos	3.01E-03	2.53E-03	1.78E-03	1.95E-03	2.22E-03
684.78	9.43	neg	1.47E-02	1.93E-02	2.12E-02	1.89E-02	2.95E-02
685.26	4.67	pos	6.62E-03	7.39E-03	6.13E-03	6.58E-03	6.25E-03
686.12	8.98	pos	1.75E-02	2.18E-02	1.76E-02	2.02E-02	1.90E-02
688.32	6.69	pos	3.54E-03	4.47E-03	3.64E-03	4.15E-03	3.10E-03
692.33	1.62	neg	1.99E-03	1.64E-03	1.76E-03	1.65E-03	1.15E-03
692.86	8.32	pos	1.47E-02	1.66E-02	1.83E-02	1.90E-02	1.92E-02
694.36	1.60	pos	5.73E-03	3.87E-03	5.24E-03	4.31E-03	3.38E-03
697.24	4.66	neg	3.65E-03	2.81E-03	3.24E-03	3.15E-03	3.01E-03
701.24	4.67	pos	3.16E-03	3.50E-03	2.86E-03	3.37E-03	3.02E-03
702.89	8.27	pos	2.94E-02	3.80E-02	4.53E-02	3.51E-02	5.09E-02
703.89	9.34	pos	1.06E-02	1.96E-02	2.34E-02	1.47E-02	3.81E-02
704.29	6.69	pos	4.09E-03	4.59E-03	3.45E-03	3.87E-03	3.17E-03
704.87	8.28	pos	5.81E-03	6.86E-03	6.95E-03	6.87E-03	7.30E-03
706.77	9.48	neg	1.51E-02	1.96E-02	2.44E-02	1.84E-02	3.00E-02
706.86	8.30	pos	7.74E-03	9.27E-03	1.01E-02	1.02E-02	9.35E-03
707.10	5.56	pos	4.47E-03	4.84E-03	5.01E-03	4.32E-03	4.97E-03
707.24	4.71	pos	1.13E-03	1.29E-03	1.68E-03	1.58E-03	1.42E-03
708.10	8.98	pos	9.85E-03	1.11E-02	1.09E-02	1.06E-02	1.10E-02
708.84	9.36	pos	2.45E-02	3.83E-02	4.67E-02	3.35E-02	5.72E-02
709.10	5.57	pos	1.77E-02	2.01E-02	1.99E-02	1.66E-02	1.97E-02
715.23	4.66	pos	5.61E-03	7.25E-03	7.32E-03	6.71E-03	7.04E-03
716.88	8.27	pos	1.08E-02	1.35E-02	1.52E-02	1.40E-02	1.62E-02
718.29	6.69	pos	4.72E-03	5.37E-03	3.96E-03	4.61E-03	4.67E-03
719.22	4.67	neg	1.86E-03	1.57E-03	1.53E-03	1.86E-03	1.79E-03
719.34	8.58	pos	2.59E-02	2.10E-02	2.65E-02	2.03E-02	3.27E-02
722.79	9.37	neg	5.03E-03	1.19E-02	1.52E-02	5.07E-03	1.57E-02
723.56	5.62	pos	2.11E-03	2.18E-03	2.02E-03	1.88E-03	1.02E-03
724.08	8.97	pos	7.08E-03	7.68E-03	8.24E-03	7.12E-03	6.70E-03
724.82	9.39	pos	1.01E-02	1.66E-02	1.87E-02	1.34E-02	2.41E-02
724.89	8.27	neg	1.21E-02	1.58E-02	1.76E-02	1.39E-02	1.99E-02
727.27	6.35	pos	4.49E-03	7.54E-03	4.59E-03	3.62E-03	5.71E-03
728.79	9.40	neg	1.36E-02	1.63E-02	2.12E-02	1.82E-02	2.26E-02
730.83	9.43	pos	2.31E-02	3.24E-02	3.86E-02	3.63E-02	3.70E-02
737.60	5.58	pos	2.16E-03	2.67E-03	2.50E-03	2.22E-03	2.85E-03
739.20	4.69	pos	1.08E-03	1.39E-03	1.57E-03	1.26E-03	1.23E-03
740.86	8.29	neg	8.87E-03	1.12E-02	1.34E-02	1.14E-02	1.24E-02
744.78	9.40	neg	1.04E-02	1.71E-02	2.05E-02	1.41E-02	2.30E-02
746.81	9.44	pos	2.21E-02	2.37E-02	2.99E-02	2.56E-02	3.13E-02
751.21	4.66	pos	2.03E-03	2.49E-03	2.61E-03	2.35E-03	2.46E-03
760.85	8.30	pos	1.17E-02	1.36E-02	1.70E-02	1.66E-02	1.64E-02
766.09	5.58	pos	1.63E-03	2.39E-03	2.56E-03	1.93E-03	2.48E-03
766.77	9.43	neg	1.15E-02	1.32E-02	1.76E-02	1.50E-02	1.64E-02
768.79	9.52	pos	1.90E-02	2.00E-02	2.47E-02	2.47E-02	1.90E-02
770.87	8.27	pos	2.03E-02	2.54E-02	3.16E-02	2.31E-02	3.36E-02
774.85	8.30	pos	7.87E-03	9.59E-03	9.03E-03	9.58E-03	9.67E-03
782.77	9.40	neg	6.97E-03	9.39E-03	1.04E-02	1.02E-02	1.34E-02

784.87	8.28	pos	8.74E-03	1.09E-02	1.11E-02	1.04E-02	1.27E-02
792.87	8.27	neg	7.03E-03	9.69E-03	1.10E-02	6.33E-03	1.06E-02
801.88	9.36	pos	7.69E-03	1.63E-02	1.89E-02	1.15E-02	3.08E-02
804.48	6.33	pos	9.10E-03	1.76E-02	8.17E-03	6.48E-03	1.36E-02
804.78	9.37	neg	3.88E-03	1.00E-02	1.28E-02	4.13E-03	1.53E-02
806.83	9.38	pos	1.54E-02	2.57E-02	3.05E-02	2.34E-02	4.00E-02
815.09	5.56	pos	1.57E-03	1.74E-03	1.67E-03	9.76E-04	1.60E-03
825.09	5.58	pos	2.02E-03	2.01E-03	2.31E-03	1.62E-03	1.86E-03
825.29	4.65	pos	1.60E-03	1.59E-03	1.30E-03	1.14E-03	1.23E-03
826.78	9.38	neg	3.91E-03	9.02E-03	1.06E-02	4.49E-03	1.24E-02
828.81	9.41	pos	1.71E-02	2.39E-02	2.87E-02	2.44E-02	3.22E-02
828.83	8.29	pos	9.01E-03	9.20E-03	1.11E-02	1.08E-02	1.09E-02
842.76	9.38	neg	3.35E-03	7.70E-03	9.07E-03	7.15E-03	1.12E-02
844.79	9.41	pos	1.46E-02	1.85E-02	2.27E-02	1.91E-02	2.63E-02
852.86	8.27	pos	7.71E-03	1.03E-02	9.57E-03	9.81E-03	1.23E-02
860.86	8.26	neg	3.27E-03	4.59E-03	5.07E-03	3.40E-03	6.34E-03
866.77	9.49	pos	1.39E-02	1.71E-02	1.91E-02	1.77E-02	1.70E-02
868.23	5.58	pos	1.20E-03	1.37E-03	1.24E-03	1.13E-03	1.38E-03
875.32	4.64	pos	1.36E-03	1.54E-03	1.67E-03	1.76E-03	1.78E-03
876.60	5.58	pos	4.84E-03	5.57E-03	4.87E-03	3.94E-03	5.51E-03
877.30	5.59	pos	3.78E-03	4.44E-03	4.02E-03	3.15E-03	4.75E-03
878.10	5.59	pos	1.71E-03	2.15E-03	2.17E-03	1.56E-03	1.97E-03
883.58	5.62	pos	1.68E-03	1.72E-03	1.73E-03	1.42E-03	1.86E-03
891.44	6.68	pos	3.97E-03	5.37E-03	3.90E-03	4.04E-03	3.79E-03
899.86	9.34	pos	5.22E-03	9.89E-03	1.24E-02	7.34E-03	2.40E-02
902.77	9.30	neg	4.07E-03	4.94E-03	3.69E-03	5.49E-03	8.38E-03
904.80	9.37	pos	1.05E-02	1.64E-02	1.87E-02	1.50E-02	2.68E-02
906.85	8.26	pos	6.73E-03	8.32E-03	1.11E-02	7.76E-03	1.23E-02
913.42	6.69	pos	3.67E-03	4.53E-03	3.08E-03	3.40E-03	3.36E-03
922.82	8.27	pos	5.23E-03	5.58E-03	6.97E-03	7.22E-03	7.29E-03
926.79	9.39	pos	1.12E-02	1.61E-02	1.98E-02	1.75E-02	2.33E-02
942.77	9.40	pos	9.93E-03	1.36E-02	1.43E-02	1.34E-02	1.85E-02
953.62	5.58	pos	9.40E-04	9.88E-04	9.19E-04	6.97E-04	1.08E-03
974.83	8.25	pos	3.58E-03	5.78E-03	6.47E-03	4.59E-03	8.09E-03
979.11	5.58	pos	1.02E-03	1.09E-03	1.23E-03	1.15E-03	1.52E-03
981.45	4.64	pos	1.41E-03	1.56E-03	1.15E-03	1.47E-03	1.22E-03
991.41	4.64	pos	2.17E-03	2.43E-03	2.38E-03	2.33E-03	2.63E-03
997.43	4.65	pos	1.81E-03	1.98E-03	1.67E-03	1.94E-03	1.91E-03
997.84	9.33	pos	3.27E-03	6.41E-03	7.34E-03	4.10E-03	1.39E-02
1002.78	9.36	pos	5.79E-03	8.65E-03	1.13E-02	8.74E-03	1.60E-02

Look up table for *S. meliloti* samples exposed to 1.4 mg/L fluorene

avg(mz)	avg(rt)	ionization mode	sample 1	sample 2	sample 3	sample 4	sample 5
78.97	9.38	neg	3.14E-02	3.59E-02	2.28E-02	1.79E-02	2.48E-02
87.98	5.58	neg	4.94E-03	5.55E-03	3.56E-03	3.21E-03	4.24E-03
90.99	8.29	pos	4.73E-02	5.06E-02	3.45E-02	3.55E-02	4.34E-02
99.00	9.37	pos	5.39E-02	5.93E-02	3.01E-02	3.27E-02	4.61E-02
100.05	7.07	neg	1.98E-02	2.30E-02	2.21E-02	2.04E-02	2.13E-02
100.12	4.66	pos	2.74E-02	3.88E-02	1.84E-02	2.16E-02	2.59E-02
101.03	6.99	neg	1.16E-01	1.47E-01	8.44E-02	6.86E-02	1.07E-01
102.06	8.65	neg	7.53E-02	5.00E-02	5.94E-02	5.90E-02	8.43E-02
102.07	7.12	pos	8.19E-02	8.11E-02	6.45E-02	7.79E-02	8.46E-02
102.07	8.65	pos	4.31E-02	3.66E-02	3.13E-02	4.44E-02	5.39E-02
104.11	9.19	pos	2.37E-02	1.60E-02	1.39E-02	2.29E-02	2.33E-02
104.12	7.04	pos	8.43E-02	4.69E-02	3.85E-02	7.41E-02	7.59E-02
105.00	8.26	pos	5.47E-02	6.29E-02	2.99E-02	2.64E-02	4.22E-02
106.10	7.63	pos	4.41E-02	3.96E-02	4.71E-02	1.66E-02	4.13E-02
107.08	7.08	pos	3.98E-01	4.11E-01	3.64E-01	4.12E-01	4.16E-01
110.02	12.93	pos	2.43E-02	2.80E-02	1.39E-02	1.60E-02	2.22E-02
112.07	4.74	pos	1.20E-02	5.05E-03	8.08E-03	1.72E-02	9.60E-03
114.91	7.77	pos	2.80E-02	2.91E-02	2.89E-02	3.03E-02	3.10E-02
116.08	7.60	pos	3.72E-02	3.07E-02	2.78E-02	3.89E-02	4.30E-02
117.02	1.45	neg	2.75E-02	2.33E-02	2.09E-02	1.78E-02	2.78E-02
117.11	7.49	pos	3.29E-02	2.07E-02	1.44E-02	1.66E-02	2.86E-02
118.10	7.52	pos	5.82E-01	1.03E+00	6.25E-01	8.90E-01	7.78E-01
119.08	2.04	pos	2.00E-02	1.98E-02	1.15E-02	1.84E-02	2.00E-02
120.09	4.65	pos	6.69E-02	6.98E-02	6.04E-02	6.97E-02	6.88E-02
120.09	4.65	pos	6.69E-02	6.98E-02	6.04E-02	6.97E-02	6.88E-02
120.09	7.40	pos	4.13E-02	4.02E-02	3.58E-02	4.06E-02	4.34E-02
121.06	0.86	pos	6.56E-03	8.18E-03	5.91E-03	7.11E-03	1.34E-02
122.90	1.24	neg	3.54E-03	4.71E-03	3.75E-03	3.86E-03	3.03E-03
122.94	7.96	pos	1.95E-01	2.03E-01	1.39E-01	1.53E-01	1.89E-01
124.99	1.25	neg	5.57E-03	7.09E-03	1.54E-03	4.88E-03	6.18E-03
125.95	5.57	neg	7.04E-03	7.87E-03	4.71E-03	3.91E-03	5.55E-03
128.03	12.92	pos	2.34E-02	2.53E-02	1.44E-02	1.58E-02	2.03E-02
128.04	8.65	neg	5.10E-02	3.63E-02	4.19E-02	4.31E-02	5.40E-02
128.14	6.39	pos	2.79E-01	2.61E-01	2.59E-01	2.74E-01	2.82E-01
128.97	7.94	neg	5.48E-01	6.15E-01	5.41E-01	4.83E-01	5.55E-01
130.06	1.37	neg	3.42E-03	3.22E-03	2.72E-03	2.17E-03	3.27E-03
130.09	6.56	neg	7.10E-02	7.09E-02	4.44E-02	5.12E-02	8.99E-02
132.07	7.42	neg	7.40E-02	7.28E-02	5.05E-02	5.72E-02	8.35E-02
134.05	1.71	neg	8.52E-02	5.29E-02	5.65E-02	7.77E-02	8.67E-02
134.09	7.37	pos	6.84E-01	6.46E-01	3.88E-01	4.68E-01	6.95E-01
136.06	7.08	pos	3.91E-01	3.93E-01	3.47E-01	4.00E-01	4.09E-01
136.08	1.71	pos	3.03E-01	1.94E-01	2.09E-01	2.80E-01	2.82E-01
137.09	2.04	pos	8.75E-02	8.18E-02	5.29E-02	7.94E-02	8.93E-02
139.88	1.26	neg	5.02E-03	5.78E-03	5.80E-03	5.55E-03	4.56E-03
140.99	5.58	neg	3.05E-02	3.42E-02	2.33E-02	2.01E-02	2.56E-02
141.88	1.26	neg	8.10E-02	9.39E-02	8.83E-02	8.41E-02	7.66E-02
142.98	5.57	neg	2.99E-02	3.30E-02	2.14E-02	2.04E-02	2.36E-02
143.87	1.26	neg	5.01E-02	5.71E-02	5.34E-02	5.16E-02	4.80E-02

144.18	2.31	pos	1.10E-02	1.38E-02	8.36E-03	6.54E-03	9.36E-03
145.06	6.96	pos	2.42E-01	2.90E-01	1.42E-01	1.39E-01	1.99E-01
145.07	8.51	neg	2.14E-02	1.92E-02	2.21E-02	2.20E-02	2.79E-02
146.05	8.65	neg	7.03E-01	4.83E-01	5.82E-01	6.71E-01	7.68E-01
149.05	6.98	neg	2.58E-01	2.88E-01	1.68E-01	1.39E-01	2.00E-01
151.03	2.22	neg	1.10E-02	8.13E-03	1.45E-02	1.21E-02	1.55E-02
155.09	7.07	pos	2.03E-01	2.19E-01	1.79E-01	1.96E-01	2.04E-01
158.98	8.31	pos	1.20E-01	1.36E-01	9.16E-02	9.39E-02	1.10E-01
158.99	12.92	neg	8.47E-02	1.04E-01	6.17E-02	5.87E-02	7.41E-02
159.08	2.05	pos	8.97E-03	8.84E-03	5.00E-03	8.38E-03	8.09E-03
159.08	8.65	neg	1.46E-02	9.40E-03	1.26E-02	1.27E-02	1.64E-02
162.05	3.07	neg	2.48E-02	1.77E-02	1.52E-02	1.39E-02	1.86E-02
168.04	8.67	neg	7.42E-02	6.89E-02	6.84E-02	6.54E-02	7.96E-02
170.06	8.65	pos	1.28E-01	8.10E-02	9.45E-02	1.23E-01	1.48E-01
171.05	2.05	neg	3.47E-02	3.03E-02	1.94E-02	3.07E-02	3.39E-02
171.10	6.34	pos	3.03E-02	2.48E-02	2.14E-02	2.77E-02	3.62E-02
171.12	6.40	neg	1.15E-01	1.22E-01	1.18E-01	1.19E-01	1.19E-01
172.99	8.26	pos	2.59E-02	3.26E-02	1.47E-02	1.35E-02	2.03E-02
173.05	2.05	neg	1.19E-02	1.01E-02	5.96E-03	1.02E-02	1.25E-02
173.14	6.39	pos	1.14E-01	1.17E-01	1.22E-01	1.18E-01	1.19E-01
175.08	7.08	pos	4.14E-02	4.10E-02	6.60E-02	5.82E-02	5.31E-02
175.13	10.29	pos	1.15E-01	9.45E-02	8.45E-02	1.05E-01	1.23E-01
176.05	1.39	neg	4.74E-03	2.96E-03	2.53E-03	2.81E-03	5.22E-03
176.94	9.39	neg	1.54E-01	1.77E-01	1.21E-01	1.01E-01	1.25E-01
177.05	2.79	neg	1.69E-02	1.45E-02	1.52E-02	1.53E-02	9.34E-03
179.06	5.58	pos	6.78E-02	7.22E-02	5.76E-02	5.41E-02	5.72E-02
180.15	0.66	pos	7.60E-02	8.28E-02	9.62E-02	4.95E-02	4.18E-02
183.04	1.25	neg	5.27E-03	6.12E-03	3.54E-03	4.81E-03	4.19E-03
186.03	8.65	pos	8.07E-02	4.64E-02	6.23E-02	8.58E-02	1.03E-01
187.87	1.26	neg	3.76E-02	4.39E-02	3.85E-02	4.13E-02	3.34E-02
188.03	8.65	pos	7.80E-03	5.42E-03	5.07E-03	9.42E-03	9.64E-03
188.19	11.52	pos	1.91E-01	1.56E-01	8.66E-02	7.94E-02	1.49E-01
189.10	9.81	neg	1.53E-02	1.22E-02	1.31E-02	1.36E-02	1.85E-02
189.87	1.26	neg	2.38E-02	2.74E-02	2.47E-02	2.55E-02	2.29E-02
191.10	6.70	pos	1.40E-01	1.38E-01	1.33E-01	1.42E-01	1.40E-01
191.87	1.26	neg	5.79E-03	6.28E-03	5.20E-03	5.46E-03	5.43E-03
192.04	8.67	pos	1.44E-01	1.32E-01	1.18E-01	1.42E-01	1.64E-01
192.11	6.71	pos	5.88E-01	5.87E-01	5.25E-01	6.20E-01	6.10E-01
192.17	5.40	pos	2.28E-01	2.67E-01	5.76E-02	9.02E-02	1.58E-01
193.12	6.70	pos	3.44E-01	3.45E-01	3.12E-01	3.65E-01	3.60E-01
193.99	5.57	neg	3.59E-02	4.09E-02	2.61E-02	2.32E-02	2.99E-02
195.98	5.57	neg	4.33E-02	5.04E-02	3.25E-02	2.73E-02	3.66E-02
196.10	2.25	pos	4.74E-02	3.93E-02	2.06E-02	1.25E-02	2.13E-02
196.96	7.98	neg	9.61E-02	1.10E-01	1.05E-01	1.00E-01	1.03E-01
197.98	5.58	neg	2.13E-02	2.44E-02	1.62E-02	1.42E-02	1.81E-02
198.11	6.93	pos	1.15E+00	1.30E+00	7.51E-01	5.74E-01	9.10E-01
199.05	7.63	neg	5.81E-02	4.23E-02	3.10E-02	4.11E-02	5.79E-02
203.07	7.10	pos	1.38E+00	1.44E+00	1.04E+00	1.23E+00	1.40E+00
205.08	7.39	pos	4.17E-02	5.76E-02	5.26E-02	7.47E-02	7.23E-02
206.80	5.92	neg	7.23E-02	2.05E-02	5.86E-02	6.91E-02	7.25E-02
206.90	7.94	pos	4.78E-02	4.81E-02	2.84E-02	3.24E-02	4.23E-02
207.12	6.70	neg	2.72E-01	2.81E-01	2.83E-01	2.68E-01	2.86E-01



208.01	8.69	pos	4.65E-02	3.96E-02	4.30E-02	5.00E-02	5.47E-02
208.90	7.93	pos	1.12E-02	1.14E-02	6.20E-03	7.09E-03	1.06E-02
209.14	6.71	pos	1.98E-01	2.07E-01	1.90E-01	1.98E-01	2.09E-01
212.13	6.65	pos	7.35E-02	7.55E-02	1.08E-01	8.21E-02	7.77E-02
212.14	2.68	pos	1.13E-02	9.15E-03	9.42E-03	8.66E-03	1.24E-02
212.93	7.94	neg	9.92E-02	1.16E-01	8.82E-02	8.76E-02	9.17E-02
213.03	7.10	pos	1.04E-02	9.91E-03	2.19E-02	1.81E-02	1.49E-02
213.09	0.86	neg	3.60E-03	3.30E-03	5.14E-03	3.07E-03	3.58E-03
214.01	8.94	pos	1.53E-01	1.76E-01	4.85E-02	5.39E-02	6.20E-02
214.05	8.75	neg	4.48E-02	2.95E-02	3.36E-02	5.91E-02	5.05E-02
214.14	0.98	neg	1.65E-02	1.47E-02	1.37E-02	1.50E-02	1.63E-02
214.33	6.99	neg	7.10E-02	8.32E-02	5.79E-02	4.94E-02	6.93E-02
214.89	1.24	neg	5.59E-03	6.81E-03	5.18E-03	6.06E-03	4.05E-03
219.04	7.06	pos	1.68E+00	1.67E+00	1.42E+00	1.45E+00	1.63E+00
219.05	7.14	neg	1.53E-01	1.86E-01	1.53E-01	1.54E-01	1.84E-01
221.04	7.07	pos	1.45E-01	1.48E-01	1.26E-01	1.31E-01	1.49E-01
224.11	7.34	neg	2.43E-02	3.05E-02	2.65E-02	1.46E-02	1.22E-02
225.03	9.34	pos	1.09E-02	8.01E-03	8.48E-03	1.10E-02	1.42E-02
226.00	8.70	neg	2.93E-02	3.24E-02	2.75E-02	3.02E-02	3.08E-02
226.14	7.29	pos	5.96E-02	5.35E-02	4.09E-02	4.18E-02	4.78E-02
226.97	8.30	pos	4.01E-01	4.71E-01	3.12E-01	3.46E-01	3.87E-01
228.06	8.60	neg	2.93E-02	1.74E-02	2.10E-02	3.47E-02	3.15E-02
229.06	2.67	neg	6.71E-03	4.82E-03	4.75E-03	4.11E-03	5.40E-03
230.03	8.66	pos	5.03E-02	4.17E-02	4.07E-02	5.31E-02	5.50E-02
231.02	9.94	pos	1.68E-02	1.72E-02	8.39E-03	8.46E-03	1.28E-02
231.12	6.71	pos	1.44E-02	1.64E-02	1.92E-02	1.78E-02	1.65E-02
232.13	6.72	pos	1.59E-01	1.66E-01	2.17E-01	1.68E-01	1.68E-01
233.09	7.96	pos	7.42E-02	7.37E-02	5.76E-02	6.30E-02	7.47E-02
234.93	9.44	pos	5.28E-02	5.88E-02	4.36E-02	4.39E-02	5.56E-02
235.03	7.08	neg	5.35E-02	6.36E-02	5.82E-02	6.01E-02	6.39E-02
235.14	7.05	pos	9.09E-03	4.35E-03	1.76E-02	1.07E-02	9.67E-03
235.97	9.95	pos	2.62E-02	3.18E-02	2.25E-02	2.14E-02	2.53E-02
238.05	2.02	neg	5.86E-03	4.35E-03	3.28E-03	3.54E-03	6.44E-03
238.06	8.76	pos	1.31E-02	7.84E-03	7.22E-03	1.76E-02	1.59E-02
239.05	2.03	neg	9.26E-03	8.26E-03	6.24E-03	7.71E-03	9.70E-03
242.02	8.67	neg	1.99E-02	1.36E-02	1.82E-02	1.82E-02	2.25E-02
242.61	8.30	pos	9.95E-02	1.04E-01	8.55E-02	1.02E-01	1.11E-01
242.99	7.06	pos	1.78E-02	9.08E-03	1.14E-03	1.82E-02	1.63E-02
243.07	2.47	neg	7.03E-02	4.81E-02	3.90E-02	5.99E-02	6.35E-02
243.09	1.02	neg	2.29E-02	2.60E-02	1.35E-02	1.16E-02	1.87E-02
243.12	0.82	pos	4.63E-03	2.85E-03	2.61E-03	3.71E-03	3.69E-03
243.90	1.24	neg	8.36E-03	1.02E-02	5.73E-03	7.97E-03	7.20E-03
244.11	8.63	pos	2.32E-02	5.92E-03	1.04E-02	2.50E-02	2.68E-02
244.12	5.94	pos	3.51E-02	4.81E-04	1.96E-02	2.83E-02	2.94E-02
245.05	8.13	neg	3.47E-02	3.05E-02	2.74E-02	3.93E-02	4.20E-02
245.09	2.48	pos	2.71E-02	2.04E-02	1.57E-02	2.34E-02	2.64E-02
245.10	7.40	pos	9.41E-02	9.94E-02	1.14E-01	1.07E-01	1.18E-01
245.12	1.00	pos	4.69E-02	5.35E-02	2.80E-02	2.35E-02	3.44E-02
245.90	1.24	neg	3.61E-03	4.65E-03	3.00E-03	3.95E-03	3.06E-03
245.97	8.73	pos	1.09E-02	1.07E-02	1.08E-02	1.06E-02	1.30E-02
246.99	5.57	neg	1.71E-02	1.99E-02	1.13E-02	1.02E-02	1.38E-02
247.09	6.70	pos	2.00E-02	1.99E-02	2.87E-02	2.02E-02	2.03E-02

248.04	9.94	pos	1.50E-02	1.87E-02	1.05E-02	9.52E-03	1.25E-02
248.10	6.71	pos	2.30E-01	2.41E-01	3.46E-01	2.53E-01	2.37E-01
248.89	8.06	pos	6.89E-03	8.91E-03	7.09E-03	8.39E-03	8.47E-03
250.00	8.70	pos	8.80E-03	8.57E-03	9.72E-03	9.02E-03	9.66E-03
250.99	5.57	neg	1.82E-02	2.14E-02	1.27E-02	1.08E-02	1.39E-02
251.94	9.95	pos	9.09E-03	8.24E-03	7.86E-03	7.29E-03	1.02E-02
252.00	8.70	neg	3.21E-02	3.06E-02	3.30E-02	3.04E-02	3.17E-02
252.13	1.23	pos	1.12E-02	7.33E-03	6.48E-03	1.04E-02	1.03E-02
252.99	9.96	pos	1.56E-02	1.79E-02	1.25E-02	1.24E-02	1.44E-02
254.11	6.71	pos	1.08E-02	1.04E-02	1.96E-02	1.10E-02	1.05E-02
256.91	9.67	pos	6.93E-02	8.38E-02	7.12E-02	8.16E-02	6.63E-02
257.08	1.88	neg	3.53E-03	4.23E-03	2.91E-03	3.32E-03	3.77E-03
257.12	2.04	pos	2.62E-03	3.05E-03	1.54E-03	2.11E-03	2.81E-03
258.12	9.20	pos	1.52E+00	8.24E-01	6.56E-01	1.21E+00	1.57E+00
258.91	8.11	pos	2.64E-02	2.86E-02	2.22E-02	2.77E-02	3.45E-02
259.03	9.21	neg	7.94E-02	8.12E-02	8.15E-02	8.37E-02	9.70E-02
260.12	9.21	pos	2.81E-02	1.59E-02	1.16E-02	2.26E-02	2.83E-02
261.08	7.40	pos	1.05E-01	1.01E-01	1.55E-01	1.27E-01	1.40E-01
262.14	2.44	pos	4.50E-03	5.79E-05	1.31E-03	2.33E-03	2.43E-03
263.07	7.40	pos	1.09E-02	1.16E-02	1.52E-02	1.33E-02	1.38E-02
263.81	1.28	neg	1.23E-03	1.29E-03	1.14E-03	1.09E-03	1.00E-03
264.86	8.00	pos	2.00E-02	2.31E-02	2.08E-02	2.41E-02	2.58E-02
264.94	8.07	neg	6.10E-02	7.38E-02	7.30E-02	7.70E-02	7.88E-02
266.06	8.65	pos	9.59E-03	5.23E-03	7.00E-03	1.09E-02	1.22E-02
266.08	6.71	neg	6.96E-02	6.97E-02	7.45E-02	7.23E-02	7.12E-02
266.11	1.95	neg	2.37E-02	1.52E-02	1.20E-02	2.15E-02	2.32E-02
266.86	8.00	pos	1.13E-02	1.23E-02	1.11E-02	1.31E-02	1.47E-02
268.12	1.96	pos	5.24E-01	3.93E-01	2.92E-01	4.62E-01	4.94E-01
270.08	6.73	pos	2.18E-02	2.36E-02	4.05E-02	2.22E-02	2.32E-02
270.99	8.36	pos	7.47E-03	7.50E-03	8.69E-03	9.09E-03	6.86E-03
271.98	8.70	pos	1.91E-02	2.19E-02	1.84E-02	2.04E-02	2.15E-02
273.92	9.97	pos	1.01E-02	1.20E-02	1.10E-02	1.06E-02	1.23E-02
274.10	2.09	neg	7.90E-02	4.20E-02	3.14E-02	4.32E-02	6.96E-02
274.89	7.98	pos	6.73E-02	6.87E-02	4.90E-02	5.23E-02	6.25E-02
275.06	2.06	neg	1.05E-02	6.69E-03	4.71E-03	6.35E-03	9.33E-03
276.13	2.08	pos	5.38E-02	3.38E-02	2.37E-02	3.24E-02	5.11E-02
276.95	7.07	neg	5.94E-02	6.27E-02	6.23E-02	6.82E-02	7.06E-02
277.12	7.96	pos	6.78E-02	7.35E-02	5.09E-02	5.82E-02	8.14E-02
279.06	7.42	neg	4.19E-02	1.00E-01	5.18E-02	5.11E-02	4.68E-02
280.11	9.14	pos	1.18E-02	5.68E-03	1.98E-02	4.66E-02	3.01E-02
280.57	7.11	pos	1.78E-02	2.29E-02	2.24E-02	1.60E-02	1.84E-02
280.83	7.95	pos	1.66E-02	1.83E-02	1.33E-02	1.52E-02	1.69E-02
280.92	7.97	neg	1.07E-01	1.18E-01	1.12E-01	1.02E-01	1.11E-01
282.02	8.64	pos	1.99E-02	2.56E-02	1.51E-02	1.69E-02	2.03E-02
282.06	6.69	neg	8.01E-02	7.95E-02	7.94E-02	7.66E-02	8.00E-02
282.13	6.35	pos	1.48E-02	1.27E-02	1.24E-02	1.26E-02	1.49E-02
282.83	7.94	pos	7.00E-03	7.32E-03	5.16E-03	5.94E-03	6.85E-03
283.06	7.44	pos	1.48E-02	1.55E-02	2.24E-02	1.83E-02	2.10E-02
284.05	6.70	neg	2.91E-02	3.09E-02	2.76E-02	2.70E-02	2.22E-02
284.12	6.47	pos	1.58E-02	9.27E-03	7.21E-03	1.49E-02	1.87E-02
286.15	1.00	neg	1.83E-03	3.37E-03	2.53E-03	1.06E-03	5.37E-04
287.07	9.80	neg	7.33E-03	6.29E-03	6.94E-03	6.35E-03	1.02E-02

287.95	8.75	pos	1.68E-02	1.95E-02	1.66E-02	1.84E-02	1.72E-02
288.13	6.67	pos	3.49E-03	5.45E-03	8.58E-03	5.78E-03	5.90E-03
289.07	9.05	neg	2.55E-02	2.11E-02	2.26E-02	2.14E-02	2.63E-02
290.86	7.93	pos	9.12E-02	8.64E-02	5.09E-02	5.42E-02	7.45E-02
291.13	8.92	pos	1.49E-02	1.54E-02	9.41E-03	1.01E-02	1.86E-02
292.09	6.72	neg	4.32E-02	5.01E-02	4.78E-02	4.24E-02	5.00E-02
292.86	7.93	pos	2.80E-02	2.72E-02	1.48E-02	1.74E-02	2.43E-02
293.98	8.70	neg	1.54E-02	1.75E-02	1.57E-02	1.43E-02	1.46E-02
294.95	9.37	pos	8.60E-02	1.02E-01	4.52E-02	4.59E-02	7.25E-02
296.08	9.13	pos	6.78E-03	3.84E-03	1.52E-02	3.47E-02	2.02E-02
296.89	7.94	neg	1.58E-01	1.89E-01	1.36E-01	1.23E-01	1.44E-01
297.98	8.67	pos	1.32E-02	1.47E-02	1.02E-02	1.16E-02	1.38E-02
298.00	6.39	neg	5.60E-02	5.92E-02	5.56E-02	5.37E-02	5.94E-02
298.12	0.81	pos	1.00E-02	1.02E-02	8.17E-03	9.53E-03	1.27E-02
298.89	7.94	neg	3.70E-02	4.36E-02	3.09E-02	2.90E-02	3.60E-02
299.03	7.43	pos	9.45E-03	1.04E-02	1.41E-02	1.33E-02	1.47E-02
299.17	0.61	pos	2.53E-02	2.76E-02	7.45E-02	7.43E-02	6.42E-02
300.00	5.79	neg	1.89E-01	2.38E-01	1.35E-01	1.09E-01	1.60E-01
301.99	5.58	neg	4.14E-02	4.63E-02	2.65E-02	2.18E-02	2.97E-02
302.04	6.70	pos	6.68E-03	6.59E-03	2.15E-03	7.30E-03	7.07E-03
304.01	8.66	neg	4.29E-02	4.80E-02	3.86E-02	3.79E-02	4.07E-02
304.11	6.69	neg	3.86E-02	3.86E-02	3.97E-02	4.32E-02	3.14E-02
305.01	9.03	pos	7.47E-03	8.53E-03	7.12E-03	9.69E-03	9.51E-03
305.99	5.58	neg	1.37E-02	1.54E-02	9.01E-03	7.36E-03	9.90E-03
306.09	8.64	neg	4.65E-02	4.53E-02	4.78E-02	4.55E-02	5.92E-02
306.13	4.73	neg	1.02E-02	7.43E-03	8.97E-03	7.66E-03	1.04E-02
307.04	7.02	pos	7.93E-03	7.30E-03	1.17E-02	8.58E-03	7.90E-03
307.98	5.58	neg	3.05E-03	3.38E-03	2.02E-03	1.77E-03	2.36E-03
308.11	8.64	pos	3.18E-02	3.18E-02	3.43E-02	4.02E-02	5.15E-02
308.93	8.38	neg	1.19E-02	1.24E-02	1.37E-02	1.39E-02	1.35E-02
309.04	7.33	neg	4.72E-02	6.40E-02	3.26E-02	2.89E-02	3.91E-02
309.96	8.74	neg	1.11E-02	1.23E-02	1.20E-02	1.07E-02	1.11E-02
310.10	4.66	neg	4.19E-03	4.17E-03	4.05E-03	3.95E-03	4.16E-03
310.57	5.58	pos	2.26E-03	2.49E-03	1.89E-03	1.50E-03	1.67E-03
310.93	8.31	pos	1.25E-02	1.44E-02	1.15E-02	1.37E-02	1.48E-02
314.91	9.42	neg	3.26E-01	3.67E-01	2.90E-01	2.55E-01	2.89E-01
315.09	8.64	neg	5.84E-02	3.78E-02	4.90E-02	5.71E-02	6.53E-02
315.13	2.48	pos	5.22E-03	3.79E-03	3.29E-03	4.19E-03	4.60E-03
316.18	6.35	pos	1.09E+00	8.48E-01	8.06E-01	9.30E-01	1.22E+00
316.93	9.42	pos	6.95E-02	7.76E-02	5.83E-02	5.74E-02	7.61E-02
316.96	8.31	neg	3.07E-01	3.49E-01	2.91E-01	2.59E-01	2.86E-01
317.12	8.62	pos	2.80E-02	1.54E-02	2.48E-02	2.66E-02	3.24E-02
318.05	6.58	neg	3.02E-02	3.81E-02	2.03E-02	3.22E-02	4.02E-02
319.99	8.70	neg	2.37E-02	2.17E-02	2.13E-02	2.23E-02	2.27E-02
320.03	6.68	neg	1.27E-02	1.41E-02	1.27E-02	1.39E-02	1.22E-02
320.99	9.04	pos	5.33E-03	5.78E-03	7.10E-03	8.47E-03	7.97E-03
321.15	7.96	pos	3.37E-02	3.53E-02	2.52E-02	2.71E-02	3.44E-02
321.18	2.07	pos	1.13E-02	4.61E-03	2.81E-03	7.33E-03	9.99E-03
322.06	6.48	pos	1.00E-02	8.34E-03	7.93E-03	8.15E-03	9.66E-03
323.41	6.96	pos	9.16E-03	8.67E-03	1.11E-02	1.09E-02	1.01E-02
325.05	7.08	neg	5.97E-02	5.92E-02	6.58E-02	6.48E-02	6.07E-02
325.06	8.60	pos	6.07E-03	4.73E-03	4.32E-03	5.25E-03	6.80E-03

325.99	6.92	pos	1.40E-02	8.77E-03	1.19E-03	9.66E-03	1.34E-02
327.08	8.87	neg	1.27E-02	1.02E-02	1.26E-02	1.31E-02	1.74E-02
327.49	5.58	neg	4.14E-03	4.88E-03	2.85E-03	2.41E-03	3.22E-03
328.49	5.58	neg	7.13E-03	7.78E-03	5.14E-03	4.27E-03	5.14E-03
329.00	9.91	pos	1.37E-02	1.60E-02	7.52E-03	6.81E-03	1.18E-02
329.49	5.60	neg	8.58E-02	1.12E-01	6.02E-02	4.94E-02	7.23E-02
330.09	8.65	pos	2.00E-02	1.83E-02	2.11E-02	2.45E-02	3.20E-02
330.89	9.43	neg	1.38E-01	1.49E-01	1.45E-01	1.30E-01	1.33E-01
331.14	7.06	neg	6.63E-01	7.91E-01	5.07E-01	4.73E-01	5.71E-01
333.12	0.65	neg	6.97E-03	8.55E-03	2.51E-02	2.52E-02	2.30E-02
333.16	7.03	pos	9.67E-02	1.00E-01	6.82E-02	6.23E-02	8.51E-02
333.95	9.93	pos	1.74E-02	1.85E-02	1.16E-02	1.09E-02	1.61E-02
334.00	6.70	neg	7.73E-02	8.52E-02	7.76E-02	7.90E-02	7.71E-02
334.89	9.37	neg	3.17E-02	3.55E-02	2.60E-02	2.04E-02	2.90E-02
335.15	4.68	pos	5.91E-02	5.87E-02	5.87E-02	6.06E-02	5.48E-02
335.99	6.69	neg	5.13E-02	5.64E-02	6.02E-02	5.34E-02	6.13E-02
336.07	5.58	pos	4.61E-03	4.92E-03	3.94E-03	3.53E-03	3.95E-03
338.11	6.67	neg	1.67E-02	2.00E-02	2.02E-02	2.31E-02	1.87E-02
338.16	6.38	pos	3.46E-01	3.11E-01	3.34E-01	3.12E-01	3.64E-01
338.92	9.58	pos	5.92E-02	5.86E-02	6.66E-02	7.73E-02	7.87E-02
339.07	5.58	pos	8.26E-03	8.77E-03	6.99E-03	6.69E-03	6.84E-03
339.09	8.64	pos	3.76E-02	2.40E-02	2.89E-02	3.54E-02	4.41E-02
340.07	6.67	neg	1.50E-02	1.54E-02	1.58E-02	1.57E-02	1.50E-02
341.06	5.58	pos	3.27E-03	3.88E-03	3.09E-03	2.78E-03	3.00E-03
343.31	5.39	pos	1.31E-03	1.56E-03	1.96E-03	2.51E-03	1.26E-03
346.07	8.41	neg	2.41E-02	1.96E-02	2.19E-02	2.47E-02	2.97E-02
346.29	4.66	pos	1.73E-02	2.49E-02	1.47E-02	1.28E-02	1.42E-02
348.03	2.04	neg	2.06E-03	1.24E-03	9.96E-04	1.51E-03	1.88E-03
348.09	8.43	pos	1.84E-02	1.24E-02	1.33E-02	1.65E-02	1.98E-02
348.90	8.04	neg	4.09E-02	4.82E-02	4.57E-02	4.48E-02	4.43E-02
349.14	7.95	pos	1.15E-02	1.22E-02	8.09E-03	9.24E-03	1.14E-02
350.97	9.94	pos	1.17E-02	1.24E-02	7.61E-03	7.23E-03	1.01E-02
351.13	4.67	pos	9.43E-02	8.50E-02	9.64E-02	9.46E-02	7.50E-02
352.91	8.35	pos	1.57E-02	1.70E-02	1.68E-02	1.89E-02	1.81E-02
353.00	5.58	neg	8.81E-03	9.94E-03	5.73E-03	4.99E-03	6.52E-03
353.05	8.65	neg	1.77E-02	1.14E-02	1.66E-02	1.65E-02	1.92E-02
354.00	5.57	neg	3.71E-03	4.43E-03	2.60E-03	2.36E-03	3.18E-03
354.13	6.38	pos	5.04E-01	4.34E-01	5.35E-01	4.60E-01	5.22E-01
354.89	9.57	pos	4.13E-02	4.16E-02	4.51E-02	5.43E-02	4.92E-02
355.00	5.58	neg	2.38E-02	2.70E-02	1.51E-02	1.35E-02	1.67E-02
356.00	1.94	neg	3.45E-03	2.34E-03	2.56E-03	3.19E-03	3.25E-03
356.14	6.36	pos	3.37E-02	3.35E-02	4.24E-02	2.87E-02	3.79E-02
356.98	7.46	pos	2.82E-03	2.72E-03	5.11E-03	3.55E-03	4.75E-03
356.99	5.58	neg	2.39E-02	2.67E-02	1.48E-02	1.27E-02	1.68E-02
357.01	9.33	neg	3.96E-02	3.67E-02	4.23E-02	4.10E-02	4.64E-02
359.07	7.04	pos	1.44E-02	1.23E-02	1.54E-03	1.63E-02	1.42E-02
359.13	7.31	neg	3.13E-01	3.97E-01	1.83E-01	1.34E-01	2.17E-01
360.16	6.36	neg	1.14E-01	1.05E-01	9.45E-02	1.04E-01	1.25E-01
360.99	5.60	neg	3.34E-02	3.96E-02	2.38E-02	2.02E-02	2.71E-02
361.08	8.64	pos	4.90E-02	3.72E-02	3.99E-02	4.73E-02	5.70E-02
361.08	7.05	pos	1.07E-02	1.04E-02	1.40E-03	1.06E-02	1.08E-02
361.24	6.36	pos	1.62E-01	9.67E-02	6.61E-02	1.43E-01	1.81E-01

362.94	8.29	pos	1.04E-01	1.20E-01	7.94E-02	7.82E-02	9.06E-02
363.32	17.69	pos	9.42E-03	1.16E-02	3.07E-03	4.95E-03	2.01E-02
363.74	5.59	pos	4.02E-03	4.22E-03	3.23E-03	2.98E-03	3.20E-03
364.88	7.97	neg	7.57E-02	9.07E-02	7.60E-02	7.00E-02	7.60E-02
365.73	5.58	pos	8.03E-03	8.95E-03	7.06E-03	6.23E-03	6.93E-03
367.56	5.58	pos	3.73E-03	4.00E-03	3.32E-03	2.91E-03	3.26E-03
369.11	4.67	neg	3.27E-02	3.36E-02	3.13E-02	3.15E-02	3.10E-02
371.11	7.09	pos	1.92E-02	1.90E-02	3.33E-02	3.21E-02	2.81E-02
372.00	8.65	neg	2.18E-02	2.63E-02	2.23E-02	1.74E-02	2.11E-02
373.11	4.78	pos	7.71E-03	6.24E-03	8.19E-03	7.82E-03	5.98E-03
374.06	8.66	pos	7.97E-03	1.00E-02	8.35E-03	8.66E-03	1.22E-02
374.14	4.65	neg	4.93E-04	3.08E-03	2.25E-03	2.67E-03	2.96E-03
374.23	6.36	pos	1.40E-02	9.25E-03	8.37E-03	1.13E-02	1.47E-02
374.83	7.93	pos	7.66E-03	7.56E-03	4.41E-03	4.53E-03	6.35E-03
374.99	8.59	neg	3.24E-02	2.91E-02	3.56E-02	3.52E-02	3.61E-02
375.20	7.38	pos	4.37E-03	4.43E-03	7.00E-03	5.54E-03	6.63E-03
377.03	8.65	pos	4.80E-02	2.49E-02	3.99E-02	2.45E-02	3.04E-02
377.12	7.09	pos	8.36E-03	8.91E-03	1.72E-02	1.05E-02	1.08E-02
377.15	6.36	neg	6.10E-02	5.63E-02	5.71E-02	5.96E-02	7.69E-02
378.18	7.30	pos	5.27E-02	6.53E-02	3.17E-02	1.60E-02	3.91E-02
378.92	8.30	pos	2.85E-02	2.96E-02	2.40E-02	2.54E-02	3.08E-02
380.85	7.94	neg	1.09E-01	1.14E-01	8.27E-02	7.31E-02	8.94E-02
381.07	7.06	pos	5.57E-03	2.77E-03	1.50E-03	8.10E-03	6.50E-03
381.50	5.58	neg	4.87E-03	5.22E-03	3.28E-03	2.72E-03	3.36E-03
382.09	6.75	neg	3.52E-02	2.88E-02	2.97E-02	2.77E-02	2.58E-02
382.24	1.70	pos	7.74E-03	4.84E-03	7.37E-03	6.05E-03	7.30E-03
382.85	7.93	neg	3.32E-02	3.71E-02	2.56E-02	2.44E-02	3.09E-02
383.13	7.00	pos	7.91E-01	7.86E-01	6.34E-01	6.58E-01	7.93E-01
383.69	5.58	neg	5.80E-02	6.78E-02	4.37E-02	3.36E-02	4.64E-02
384.49	5.58	neg	4.36E-03	4.25E-03	2.53E-03	2.21E-03	3.14E-03
384.95	8.31	neg	1.62E-01	1.83E-01	1.43E-01	1.23E-01	1.47E-01
385.08	4.67	neg	2.61E-02	2.97E-02	2.84E-02	2.83E-02	2.89E-02
385.14	7.29	pos	3.39E-02	3.43E-02	3.04E-02	3.29E-02	3.72E-02
386.07	1.69	pos	1.00E-03	6.38E-04	6.85E-04	1.00E-03	1.28E-03
387.07	7.06	pos	1.17E-02	7.31E-03	1.80E-03	1.15E-02	1.07E-02
387.98	8.68	neg	1.50E-02	1.62E-02	1.39E-02	1.57E-02	1.41E-02
388.19	6.88	neg	1.50E-01	1.85E-01	1.03E-01	9.03E-02	1.53E-01
389.01	7.03	neg	5.58E-02	6.07E-02	6.77E-02	6.59E-02	6.45E-02
390.21	6.84	pos	5.17E-02	5.41E-02	4.34E-02	3.25E-02	5.93E-02
391.07	5.59	pos	6.87E-03	7.41E-03	6.04E-03	5.37E-03	5.31E-03
391.17	6.93	pos	1.52E-02	1.65E-02	1.81E-02	1.03E-02	1.49E-02
392.91	9.34	neg	4.34E-02	5.43E-02	2.33E-02	1.78E-02	3.04E-02
392.92	9.39	pos	7.49E-02	8.46E-02	3.69E-02	3.59E-02	5.78E-02
393.03	7.06	neg	4.58E-02	4.46E-02	4.71E-02	4.38E-02	4.91E-02
393.07	5.59	pos	7.68E-03	8.31E-03	6.36E-03	5.80E-03	5.77E-03
394.01	6.69	neg	2.68E-02	3.22E-02	3.09E-02	2.94E-02	2.97E-02
395.06	7.05	pos	8.30E-03	4.25E-03	1.68E-03	8.72E-03	9.75E-03
395.11	7.02	neg	1.02E+00	1.17E+00	8.75E-01	7.55E-01	9.45E-01
396.12	6.37	pos	1.02E-02	8.88E-03	1.90E-02	9.49E-03	1.13E-02
396.23	1.71	pos	2.42E-03	1.55E-03	2.36E-03	1.69E-03	2.37E-03
397.05	7.06	pos	8.43E-03	5.13E-03	3.61E-03	1.07E-02	8.95E-03
399.03	8.66	pos	2.32E-02	2.06E-02	2.28E-02	2.63E-02	2.93E-02

399.11	7.11	pos	2.12E-01	2.05E-01	1.69E-01	1.84E-01	2.14E-01
401.05	4.65	neg	4.78E-03	4.78E-03	4.68E-03	4.77E-03	4.73E-03
401.17	7.39	neg	1.86E-01	1.97E-01	1.60E-01	1.46E-01	1.58E-01
403.19	7.37	pos	3.30E-02	3.35E-02	2.61E-02	2.09E-02	2.24E-02
404.03	8.58	pos	6.26E-03	3.70E-03	5.00E-03	5.54E-03	7.21E-03
404.20	2.01	pos	4.17E-03	2.79E-03	2.38E-03	3.33E-03	4.19E-03
405.03	8.62	pos	1.88E-02	1.87E-02	1.53E-02	1.76E-02	1.98E-02
406.00	5.58	neg	5.65E-03	5.28E-03	3.84E-03	3.64E-03	3.79E-03
406.08	6.36	pos	1.73E-02	1.14E-02	3.83E-03	1.62E-02	1.91E-02
407.09	7.03	pos	9.19E-03	9.75E-03	1.48E-02	9.29E-03	1.05E-02
407.13	4.66	neg	3.38E-03	3.52E-03	3.65E-03	4.33E-03	2.91E-03
408.02	5.58	neg	1.46E-02	1.63E-02	9.21E-03	8.64E-03	1.05E-02
408.09	6.35	neg	2.75E-02	2.65E-02	2.54E-02	2.50E-02	3.33E-02
409.00	5.58	neg	6.86E-03	6.63E-03	5.32E-03	4.91E-03	5.74E-03
409.96	9.38	pos	1.21E-01	1.51E-01	6.19E-02	5.63E-02	9.60E-02
410.00	5.58	neg	1.87E-02	2.07E-02	1.20E-02	1.03E-02	1.30E-02
410.09	6.35	neg	1.92E-02	1.85E-02	1.82E-02	1.60E-02	2.08E-02
411.04	5.12	neg	7.57E-03	6.95E-03	7.14E-03	4.10E-03	6.85E-03
411.19	1.96	pos	1.26E-03	5.91E-04	4.66E-04	9.27E-04	1.02E-03
412.00	5.58	neg	1.11E-02	1.17E-02	6.70E-03	5.92E-03	7.35E-03
412.19	6.84	pos	3.03E-02	3.38E-02	4.11E-02	2.47E-02	3.41E-02
412.19	2.00	pos	1.79E-03	1.07E-03	5.99E-04	1.33E-03	2.16E-03
412.28	4.65	pos	2.51E-03	2.98E-03	2.03E-03	2.33E-03	1.88E-03
412.89	9.40	neg	2.41E-01	2.83E-01	1.89E-01	1.66E-01	2.06E-01
413.05	7.28	neg	5.76E-02	7.01E-02	3.10E-02	2.07E-02	3.98E-02
413.99	5.58	neg	4.07E-03	4.11E-03	2.35E-03	2.62E-03	2.84E-03
414.09	6.37	pos	6.31E-03	6.04E-03	1.19E-02	6.01E-03	6.19E-03
415.01	8.68	pos	6.91E-03	6.71E-03	7.69E-03	8.49E-03	9.18E-03
417.57	5.58	pos	8.25E-03	8.90E-03	7.69E-03	6.18E-03	6.54E-03
418.26	6.68	pos	2.88E-02	2.91E-02	3.68E-02	3.00E-02	3.02E-02
419.27	6.68	pos	1.71E-01	1.71E-01	2.09E-01	1.86E-01	1.77E-01
419.57	5.58	pos	1.13E-02	1.23E-02	9.91E-03	8.14E-03	8.95E-03
420.17	0.63	pos	5.29E-04	7.64E-04	1.61E-03	1.67E-03	1.59E-03
420.29	6.60	pos	8.51E-02	8.83E-02	1.13E-01	8.36E-02	8.29E-02
421.30	6.54	pos	2.16E-02	2.13E-02	2.71E-02	2.19E-02	2.14E-02
423.06	7.05	pos	1.27E-02	7.44E-03	1.63E-03	1.13E-02	1.08E-02
424.07	6.35	neg	2.53E-02	2.78E-02	2.35E-02	2.22E-02	2.90E-02
424.22	4.70	pos	2.93E-03	1.07E-03	2.01E-03	3.54E-03	1.95E-03
425.17	7.39	pos	3.57E-02	3.30E-02	4.28E-02	3.49E-02	3.94E-02
426.06	6.35	neg	1.84E-02	1.99E-02	1.62E-02	1.60E-02	2.25E-02
426.17	4.50	neg	2.21E-03	2.08E-03	2.01E-03	2.02E-03	1.84E-03
426.31	0.62	pos	2.95E-03	3.79E-03	3.42E-03	1.55E-03	1.60E-03
427.01	8.61	neg	1.58E-02	1.61E-02	1.48E-02	1.38E-02	1.56E-02
428.16	6.84	pos	1.19E-02	1.41E-02	1.72E-02	1.12E-02	1.49E-02
428.87	9.41	neg	1.24E-01	1.39E-01	1.00E-01	8.41E-02	1.05E-01
430.06	6.34	pos	3.20E-03	6.83E-03	5.71E-03	3.16E-03	3.16E-03
430.89	9.42	pos	4.44E-02	5.16E-02	3.63E-02	3.56E-02	4.65E-02
430.93	8.29	pos	1.06E-01	1.23E-01	7.85E-02	7.94E-02	9.87E-02
434.18	6.84	pos	4.57E-03	4.85E-03	8.90E-03	3.98E-03	5.02E-03
434.30	5.58	neg	3.17E-03	3.33E-03	2.42E-03	2.14E-03	2.51E-03
434.87	9.48	neg	9.24E-02	9.87E-02	8.83E-02	7.99E-02	8.50E-02
435.31	7.26	neg	3.81E-02	4.29E-02	3.34E-02	2.76E-02	2.66E-02

435.50	5.58	neg	4.86E-03	5.03E-03	3.21E-03	2.70E-03	3.57E-03
436.50	5.58	neg	5.41E-02	5.98E-02	3.89E-02	3.31E-02	3.97E-02
436.89	9.59	pos	4.85E-02	4.39E-02	4.67E-02	5.51E-02	5.69E-02
437.50	5.58	neg	4.28E-03	4.97E-03	3.22E-03	2.23E-03	3.39E-03
438.02	4.65	neg	2.67E-03	2.64E-03	2.58E-03	2.70E-03	2.56E-03
438.50	5.59	neg	2.86E-02	3.66E-02	2.01E-02	1.88E-02	2.56E-02
440.25	6.68	pos	6.48E-03	7.38E-03	1.21E-02	7.68E-03	7.48E-03
441.12	7.34	pos	2.52E-02	2.65E-02	2.85E-03	2.10E-02	2.89E-02
441.25	6.69	pos	3.84E-02	4.20E-02	7.41E-02	4.18E-02	3.65E-02
442.08	5.58	pos	3.08E-03	3.36E-03	2.89E-03	2.57E-03	2.35E-03
442.81	7.95	pos	1.38E-02	1.44E-02	9.56E-03	9.05E-03	1.31E-02
443.04	4.74	neg	7.19E-03	7.61E-03	7.10E-03	7.42E-03	7.79E-03
443.09	7.24	pos	9.71E-03	1.26E-02	1.25E-02	8.22E-03	1.03E-02
444.08	5.58	pos	1.22E-02	1.31E-02	1.20E-02	9.83E-03	1.06E-02
444.94	8.28	pos	2.55E-02	2.78E-02	1.79E-02	1.71E-02	2.21E-02
445.23	7.38	pos	3.81E-02	3.61E-02	5.10E-02	4.48E-02	4.63E-02
446.91	8.29	pos	2.92E-02	3.29E-02	2.44E-02	2.69E-02	3.36E-02
447.28	6.44	pos	9.46E-03	7.99E-03	5.55E-03	5.60E-03	1.14E-02
448.07	5.58	pos	8.22E-03	8.78E-03	8.39E-03	6.28E-03	7.45E-03
448.24	0.57	pos	1.40E-03	1.26E-03	1.42E-03	1.73E-03	1.80E-03
448.84	7.96	neg	3.94E-02	4.65E-02	3.48E-02	3.60E-02	3.82E-02
450.15	6.85	pos	3.95E-03	4.00E-03	7.03E-03	3.33E-03	4.75E-03
450.85	9.49	neg	9.83E-02	9.80E-02	9.39E-02	8.96E-02	9.09E-02
451.05	7.20	pos	2.96E-02	1.55E-02	3.70E-03	1.88E-02	2.18E-02
452.87	9.53	pos	4.21E-02	4.07E-02	4.32E-02	4.89E-02	5.15E-02
452.94	8.30	neg	1.12E-01	1.23E-01	9.35E-02	8.66E-02	9.66E-02
454.99	9.35	neg	2.12E-02	2.01E-02	2.03E-02	1.84E-02	2.56E-02
455.05	7.06	pos	1.34E-02	1.43E-02	1.43E-03	1.06E-02	1.39E-02
455.21	6.69	neg	2.41E-02	2.36E-02	2.44E-02	2.60E-02	2.33E-02
456.31	6.70	pos	6.02E-02	6.63E-02	7.54E-02	5.53E-02	6.76E-02
457.07	7.26	pos	1.86E-02	2.06E-02	2.07E-02	1.28E-02	1.73E-02
458.07	2.02	pos	1.06E-03	1.15E-03	1.26E-03	1.14E-03	1.16E-03
458.79	7.92	pos	1.24E-02	1.15E-02	5.49E-03	6.18E-03	9.88E-03
461.00	5.58	neg	7.28E-03	8.30E-03	5.20E-03	4.61E-03	5.02E-03
462.00	5.58	neg	4.87E-03	5.42E-03	3.63E-03	3.07E-03	3.72E-03
463.00	5.58	neg	1.08E-01	1.23E-01	7.52E-02	6.53E-02	8.63E-02
463.13	7.34	pos	9.99E-03	1.13E-02	1.31E-02	9.86E-03	1.11E-02
464.00	5.57	neg	4.99E-03	5.61E-03	3.77E-03	2.90E-03	4.05E-03
464.82	7.94	neg	5.64E-02	5.56E-02	3.98E-02	3.53E-02	4.54E-02
465.00	5.59	neg	8.28E-02	9.65E-02	5.90E-02	4.95E-02	6.49E-02
467.21	7.39	pos	1.35E-02	1.29E-02	2.49E-02	2.00E-02	2.22E-02
468.91	8.32	neg	2.87E-02	3.21E-02	2.86E-02	2.94E-02	2.94E-02
471.57	5.59	pos	2.82E-03	3.02E-03	3.01E-03	1.86E-03	2.33E-03
477.01	4.77	pos	3.26E-03	2.28E-03	2.41E-04	3.16E-03	2.87E-03
479.21	6.70	pos	6.55E-03	7.68E-03	1.36E-02	7.23E-03	6.30E-03
480.12	6.79	pos	7.36E-03	5.80E-03	3.60E-03	5.90E-03	7.57E-03
483.18	7.39	pos	7.43E-03	7.03E-03	1.42E-02	1.27E-02	1.30E-02
486.15	8.62	pos	8.60E-03	5.75E-03	7.28E-03	8.10E-03	1.15E-02
488.50	5.58	neg	3.09E-03	3.65E-03	2.35E-03	2.11E-03	2.38E-03
488.80	9.88	neg	3.40E-02	3.40E-02	2.98E-02	2.59E-02	3.38E-02
488.90	8.34	pos	1.47E-02	1.80E-02	1.63E-02	1.70E-02	1.80E-02
489.19	7.39	pos	1.66E-03	2.29E-03	5.35E-03	3.43E-03	2.91E-03

489.50	5.58	neg	3.87E-03	4.21E-03	2.77E-03	2.36E-03	2.75E-03
490.50	5.59	neg	3.76E-02	4.54E-02	2.79E-02	2.42E-02	2.76E-02
490.89	9.30	neg	2.24E-02	2.88E-02	8.76E-03	5.12E-03	1.27E-02
490.90	9.34	pos	5.91E-02	6.66E-02	2.65E-02	2.71E-02	4.46E-02
491.50	5.58	neg	2.82E-03	3.25E-03	2.17E-03	1.94E-03	2.15E-03
493.08	7.38	pos	6.72E-03	2.28E-03	7.67E-04	5.89E-03	5.88E-03
495.08	5.57	pos	5.44E-03	5.69E-03	4.79E-03	4.71E-03	4.59E-03
496.83	9.80	pos	1.87E-02	2.01E-02	1.92E-02	2.31E-02	2.33E-02
497.02	4.65	neg	3.21E-03	3.51E-03	3.16E-03	3.07E-03	2.79E-03
497.08	5.57	pos	1.51E-02	1.57E-02	1.38E-02	1.27E-02	1.42E-02
498.92	8.28	pos	7.98E-02	9.06E-02	5.80E-02	5.39E-02	7.20E-02
499.08	5.57	pos	2.02E-02	2.08E-02	1.77E-02	1.68E-02	1.77E-02
505.16	7.40	pos	4.64E-03	5.35E-03	1.06E-02	7.10E-03	8.83E-03
507.14	6.69	neg	3.75E-02	4.13E-02	4.19E-02	3.64E-02	4.30E-02
507.94	9.38	pos	1.01E-01	1.19E-01	4.99E-02	4.29E-02	7.77E-02
508.13	8.63	pos	1.41E-02	7.63E-03	9.97E-03	1.31E-02	1.62E-02
508.15	6.70	pos	4.97E-03	3.57E-03	1.69E-03	4.40E-03	4.18E-03
509.30	2.50	neg	1.14E-02	1.02E-02	1.08E-02	8.09E-03	1.29E-02
510.79	9.94	neg	2.17E-02	2.79E-02	1.94E-02	1.65E-02	1.84E-02
511.09	4.65	neg	1.74E-03	2.10E-03	2.08E-03	2.08E-03	1.88E-03
511.16	6.73	pos	1.78E-02	1.16E-02	2.48E-03	1.84E-02	1.68E-02
511.33	2.50	pos	5.68E-03	5.44E-03	5.67E-03	4.28E-03	7.04E-03
512.80	9.98	pos	1.72E-02	1.70E-02	1.55E-02	1.31E-02	1.51E-02
512.84	9.31	neg	3.12E-02	3.94E-02	2.03E-02	1.44E-02	2.37E-02
512.88	9.39	pos	5.85E-02	6.99E-02	3.98E-02	4.10E-02	5.39E-02
512.92	8.27	pos	2.14E-02	2.38E-02	1.42E-02	1.56E-02	1.70E-02
514.00	5.59	neg	2.66E-02	3.16E-02	2.14E-02	2.03E-02	2.34E-02
514.29	1.97	pos	8.20E-03	7.47E-03	6.83E-03	7.38E-03	8.31E-03
516.01	5.58	neg	4.87E-03	4.75E-03	3.59E-03	3.03E-03	3.58E-03
517.01	5.61	neg	2.55E-02	2.61E-02	1.80E-02	1.86E-02	1.96E-02
518.01	5.58	neg	3.69E-03	3.39E-03	2.71E-03	2.41E-03	2.79E-03
520.92	8.30	neg	9.06E-02	1.03E-01	7.50E-02	6.84E-02	7.15E-02
521.08	8.64	pos	5.37E-03	5.74E-03	5.65E-03	5.02E-03	7.93E-03
521.17	7.19	pos	8.02E-03	8.28E-03	1.14E-02	8.18E-03	4.45E-03
523.41	7.07	pos	1.04E-02	1.12E-02	9.85E-03	9.71E-03	1.26E-02
525.30	6.61	pos	2.46E-02	2.29E-02	1.53E-02	2.00E-02	2.06E-02
525.58	5.58	pos	2.13E-03	2.31E-03	1.65E-03	1.60E-03	1.58E-03
526.78	7.94	pos	9.22E-03	1.03E-02	6.22E-03	6.36E-03	8.47E-03
526.85	9.37	neg	7.88E-02	8.74E-02	5.55E-02	4.52E-02	6.73E-02
528.87	9.40	pos	3.96E-02	4.24E-02	2.67E-02	2.76E-02	3.75E-02
531.15	6.71	pos	3.75E-03	2.59E-03	6.13E-03	4.30E-03	4.01E-03
532.80	7.96	neg	2.18E-02	2.82E-02	2.24E-02	2.07E-02	2.34E-02
532.85	9.42	neg	5.94E-02	6.65E-02	5.71E-02	5.04E-02	6.10E-02
534.87	9.48	pos	4.87E-02	4.86E-02	4.91E-02	5.13E-02	5.63E-02
535.13	7.37	pos	4.56E-03	2.95E-03	1.71E-03	6.01E-03	5.33E-03
536.90	8.32	neg	2.89E-02	3.24E-02	2.90E-02	3.07E-02	3.02E-02
539.18	7.32	neg	2.76E-02	3.54E-02	1.39E-02	1.02E-02	1.67E-02
541.19	1.98	neg	1.39E-03	6.71E-04	4.81E-04	1.02E-03	1.19E-03
542.76	7.92	pos	1.35E-02	1.18E-02	6.18E-03	6.01E-03	1.00E-02
543.23	2.03	pos	4.96E-03	2.31E-03	1.83E-03	2.91E-03	4.43E-03
543.38	7.07	pos	4.75E-03	4.38E-03	4.71E-03	4.69E-03	4.47E-03
544.27	2.07	pos	2.61E-03	1.92E-03	1.70E-03	1.62E-03	2.50E-03



546.08	8.65	pos	6.79E-03	4.04E-03	5.61E-03	6.36E-03	8.08E-03
547.13	6.70	pos	6.60E-03	4.43E-03	1.07E-03	7.36E-03	7.13E-03
548.78	7.93	neg	2.96E-02	3.19E-02	2.18E-02	1.89E-02	2.28E-02
548.83	9.45	neg	6.69E-02	7.46E-02	5.99E-02	6.08E-02	6.62E-02
549.09	5.58	pos	2.33E-03	2.55E-03	2.02E-03	1.76E-03	2.05E-03
550.85	9.47	pos	3.96E-02	4.00E-02	4.13E-02	4.25E-02	4.58E-02
552.10	8.63	pos	1.96E-02	1.51E-02	1.54E-02	1.84E-02	2.25E-02
556.88	8.33	pos	1.81E-02	1.98E-02	1.68E-02	1.85E-02	2.02E-02
559.34	4.64	pos	3.76E-02	4.10E-02	5.38E-02	3.63E-02	3.22E-02
563.19	7.29	pos	5.48E-03	7.31E-03	3.37E-03	3.76E-03	5.89E-03
565.06	9.19	neg	2.52E-02	3.21E-02	3.51E-02	3.42E-02	3.89E-02
566.09	5.60	pos	2.39E-03	1.61E-03	1.65E-03	2.24E-03	2.04E-03
566.91	8.28	pos	8.01E-02	9.21E-02	5.63E-02	5.48E-02	7.05E-02
567.33	0.60	pos	1.22E-03	1.19E-03	1.63E-03	1.52E-03	1.44E-03
568.07	8.65	pos	1.31E-02	1.03E-02	1.24E-02	1.24E-02	1.53E-02
571.18	7.01	pos	5.53E-03	5.25E-03	6.44E-03	3.56E-03	5.45E-03
572.87	8.34	pos	8.73E-03	1.01E-02	9.61E-03	1.03E-02	1.00E-02
573.32	4.64	pos	5.85E-03	6.07E-03	8.11E-03	5.61E-03	5.59E-03
574.08	8.63	pos	1.84E-02	1.65E-02	1.60E-02	1.61E-02	2.22E-02
574.36	1.00	pos	4.04E-03	2.97E-03	3.08E-03	3.64E-03	5.38E-03
577.58	5.58	pos	3.63E-03	4.12E-03	3.30E-03	2.90E-03	2.88E-03
578.91	8.37	neg	1.51E-02	1.80E-02	1.60E-02	1.64E-02	1.42E-02
579.04	9.90	neg	2.47E-02	2.34E-02	1.82E-02	1.86E-02	2.64E-02
579.21	6.36	pos	7.54E-03	5.12E-03	1.06E-03	6.45E-03	7.09E-03
579.58	5.58	pos	5.47E-03	5.84E-03	4.59E-03	3.89E-03	4.13E-03
580.46	6.71	pos	5.33E-03	5.79E-03	5.47E-03	4.58E-03	6.93E-03
580.91	8.27	pos	2.37E-02	2.76E-02	1.68E-02	1.72E-02	2.04E-02
581.21	6.37	pos	6.48E-03	5.14E-03	1.27E-03	5.72E-03	6.21E-03
582.21	5.72	neg	3.27E-02	2.13E-02	2.35E-02	1.38E-02	2.25E-02
582.88	8.29	pos	2.53E-02	2.80E-02	2.08E-02	2.28E-02	2.69E-02
584.11	9.17	pos	1.10E-02	1.28E-02	1.40E-02	1.58E-02	1.76E-02
584.24	5.72	pos	2.18E-02	1.07E-02	1.12E-02	8.79E-03	1.25E-02
588.86	9.40	pos	3.62E-02	4.52E-02	1.74E-02	1.96E-02	2.70E-02
588.91	8.29	neg	7.00E-02	8.68E-02	5.85E-02	5.03E-02	5.79E-02
590.05	8.65	pos	1.20E-02	9.05E-03	1.01E-02	1.13E-02	1.41E-02
592.79	9.66	neg	3.08E-02	3.12E-02	3.02E-02	2.59E-02	2.89E-02
594.80	9.79	pos	1.68E-02	1.63E-02	1.60E-02	1.71E-02	1.72E-02
595.32	0.81	pos	9.42E-04	1.09E-03	6.79E-04	4.01E-04	1.30E-03
595.33	0.84	neg	2.76E-03	2.37E-03	4.80E-03	5.16E-03	6.99E-03
595.98	0.66	pos	9.42E-04	1.09E-03	6.79E-04	4.01E-04	1.30E-03
596.06	8.64	pos	1.63E-02	1.42E-02	1.13E-02	1.28E-02	1.65E-02
597.30	4.66	pos	2.92E-03	2.58E-03	3.45E-03	2.91E-03	2.25E-03
598.12	9.92	pos	1.16E-02	9.99E-03	1.22E-02	1.46E-02	1.99E-02
598.87	8.30	pos	1.02E-02	1.22E-02	8.08E-03	8.70E-03	1.25E-02
600.38	0.80	pos	6.83E-03	4.52E-03	9.34E-03	6.12E-03	7.73E-03
600.57	0.79	pos	6.83E-03	4.52E-03	9.34E-03	6.12E-03	7.73E-03
602.39	0.85	pos	3.18E-03	2.32E-03	4.27E-03	2.86E-03	3.69E-03
602.84	5.59	pos	1.34E-02	1.41E-02	1.16E-02	1.04E-02	1.11E-02
603.09	5.58	pos	1.34E-02	1.41E-02	1.16E-02	1.04E-02	1.11E-02
604.89	8.31	neg	2.76E-02	3.16E-02	2.57E-02	2.58E-02	2.79E-02
605.92	9.37	pos	8.49E-02	9.87E-02	3.66E-02	3.16E-02	5.69E-02
606.09	8.98	neg	9.63E-03	8.66E-03	8.31E-03	7.91E-03	1.01E-02

608.10	8.13	pos	3.46E-03	7.29E-03	5.75E-03	6.90E-03	8.95E-03
608.83	9.38	neg	7.76E-02	9.67E-02	5.66E-02	4.30E-02	6.21E-02
608.90	8.32	pos	1.28E-02	1.32E-02	1.03E-02	1.03E-02	1.17E-02
610.74	7.93	pos	6.04E-03	6.29E-03	3.89E-03	4.59E-03	6.04E-03
610.78	10.01	pos	1.01E-02	1.21E-02	9.39E-03	9.18E-03	9.85E-03
610.87	9.38	pos	8.29E-02	9.17E-02	5.28E-02	4.78E-02	7.38E-02
611.16	9.80	neg	1.41E-02	9.11E-03	6.28E-03	7.09E-03	1.21E-02
612.02	8.63	pos	9.65E-03	1.01E-02	9.76E-03	9.23E-03	1.26E-02
613.18	9.81	pos	1.65E-02	8.64E-03	7.53E-03	1.02E-02	1.44E-02
614.38	0.80	pos	2.99E-03	2.50E-03	5.48E-03	4.16E-03	4.49E-03
617.17	6.36	pos	5.48E-03	4.16E-03	1.93E-04	4.99E-03	5.25E-03
617.55	5.66	pos	3.07E-03	2.66E-03	3.08E-03	2.70E-03	1.81E-03
618.12	8.59	neg	1.13E-02	8.34E-03	9.86E-03	8.32E-03	1.32E-02
619.08	5.65	pos	2.21E-03	1.54E-03	1.74E-03	2.38E-03	2.21E-03
620.09	5.60	pos	3.33E-03	2.11E-03	2.16E-03	2.84E-03	2.57E-03
620.14	8.59	pos	1.23E-02	8.68E-03	1.08E-02	1.14E-02	1.61E-02
624.80	9.41	neg	4.78E-02	5.63E-02	3.31E-02	2.60E-02	3.72E-02
624.87	8.32	pos	2.00E-02	2.10E-02	1.73E-02	1.80E-02	1.86E-02
625.12	8.96	pos	6.83E-03	6.70E-03	5.82E-03	5.16E-03	6.74E-03
626.84	9.39	pos	3.66E-02	3.73E-02	2.30E-02	2.29E-02	3.21E-02
628.40	6.67	pos	3.00E-03	3.69E-03	6.51E-03	4.37E-03	3.42E-03
630.08	8.96	pos	8.15E-03	6.77E-03	6.63E-03	7.88E-03	8.98E-03
630.80	9.49	neg	4.35E-02	4.79E-02	3.92E-02	3.44E-02	4.13E-02
632.75	7.92	neg	2.32E-02	2.75E-02	1.52E-02	1.82E-02	2.03E-02
632.85	9.44	pos	4.76E-02	4.98E-02	4.09E-02	4.29E-02	4.91E-02
634.90	8.27	pos	7.49E-02	8.81E-02	5.13E-02	4.88E-02	6.28E-02
638.87	8.31	pos	1.00E-02	1.01E-02	8.95E-03	9.31E-03	1.05E-02
646.80	9.44	neg	4.59E-02	5.28E-02	3.96E-02	3.68E-02	4.47E-02
648.37	6.32	pos	5.07E-03	3.44E-03	4.44E-03	4.13E-03	6.99E-03
648.83	9.46	pos	3.64E-02	3.88E-02	3.42E-02	3.54E-02	3.92E-02
648.90	8.27	pos	2.34E-02	2.32E-02	1.42E-02	1.61E-02	1.84E-02
650.38	6.68	pos	3.38E-03	4.02E-03	8.02E-03	4.02E-03	3.94E-03
650.87	8.29	pos	2.46E-02	2.74E-02	1.92E-02	2.09E-02	2.67E-02
654.82	9.55	pos	1.81E-02	2.17E-02	1.76E-02	2.18E-02	1.89E-02
655.20	8.62	pos	7.90E-03	3.19E-03	6.28E-03	6.90E-03	9.30E-03
656.09	5.58	pos	7.13E-03	7.78E-03	6.37E-03	6.31E-03	6.83E-03
656.90	8.29	neg	4.53E-02	5.12E-02	3.59E-02	2.87E-02	3.20E-02
658.09	5.57	pos	1.27E-02	1.36E-02	1.14E-02	1.05E-02	1.17E-02
662.12	9.00	neg	1.15E-02	1.00E-02	9.94E-03	1.11E-02	1.31E-02
664.14	9.00	pos	3.46E-02	2.66E-02	2.87E-02	3.62E-02	4.46E-02
666.85	8.30	pos	1.02E-02	1.24E-02	8.27E-03	1.03E-02	1.21E-02
668.79	9.50	neg	2.60E-02	2.96E-02	3.28E-02	2.86E-02	2.96E-02
669.29	4.67	pos	3.72E-03	2.64E-03	4.46E-03	4.19E-03	2.56E-03
670.81	9.57	pos	2.01E-02	2.35E-02	2.30E-02	2.62E-02	2.43E-02
671.49	4.64	pos	2.32E-03	2.17E-03	2.62E-03	2.08E-03	2.02E-03
672.35	6.69	pos	2.51E-03	2.71E-03	5.93E-03	2.92E-03	2.41E-03
672.88	8.31	neg	1.82E-02	2.29E-02	2.00E-02	1.79E-02	1.89E-02
676.88	8.29	pos	1.39E-02	1.49E-02	9.42E-03	1.01E-02	1.32E-02
681.26	4.66	neg	1.64E-03	1.48E-03	1.45E-03	1.58E-03	1.52E-03
682.30	6.69	pos	5.84E-03	3.82E-03	1.41E-03	5.32E-03	5.77E-03
683.49	4.64	pos	1.78E-03	1.79E-03	2.09E-03	1.75E-03	1.87E-03
684.78	9.43	neg	7.78E-03	9.48E-03	2.70E-02	1.90E-02	3.18E-02

685.26	4.67	pos	7.71E-03	6.01E-03	8.22E-03	8.12E-03	5.25E-03
686.12	8.98	pos	1.60E-02	1.15E-02	1.38E-02	1.41E-02	2.04E-02
688.32	6.69	pos	3.55E-03	3.26E-03	6.87E-03	3.32E-03	3.01E-03
690.77	9.63	neg	1.49E-02	1.71E-02	1.45E-02	1.51E-02	1.50E-02
692.86	8.32	pos	1.99E-02	2.32E-02	1.76E-02	1.87E-02	2.07E-02
694.36	1.60	pos	2.70E-03	2.19E-03	2.42E-03	3.19E-03	2.21E-03
697.24	4.66	neg	3.01E-03	3.10E-03	2.79E-03	3.16E-03	3.04E-03
701.24	4.67	pos	3.71E-03	2.85E-03	3.69E-03	3.68E-03	2.74E-03
702.89	8.27	pos	7.05E-02	8.24E-02	4.73E-02	4.49E-02	5.67E-02
703.89	9.34	pos	6.36E-02	7.80E-02	2.72E-02	2.18E-02	4.45E-02
704.29	6.69	pos	3.22E-03	2.82E-03	2.20E-03	3.52E-03	3.65E-03
704.87	8.28	pos	9.42E-03	1.18E-02	7.26E-03	6.58E-03	8.40E-03
706.77	9.48	neg	6.85E-03	9.77E-03	2.71E-02	7.03E-03	3.39E-02
706.86	8.30	pos	1.07E-02	1.19E-02	9.14E-03	1.03E-02	1.33E-02
707.10	5.56	pos	5.95E-03	6.20E-03	6.51E-03	5.45E-03	5.46E-03
707.24	4.71	pos	1.55E-03	1.29E-03	1.67E-03	1.58E-03	1.47E-03
708.10	8.98	pos	8.83E-03	6.11E-03	6.86E-03	9.21E-03	1.07E-02
708.84	9.36	pos	7.41E-02	8.56E-02	4.79E-02	4.42E-02	6.40E-02
709.10	5.57	pos	2.46E-02	2.62E-02	2.43E-02	2.03E-02	2.24E-02
715.23	4.66	pos	9.27E-03	6.13E-03	4.58E-05	8.78E-03	7.58E-03
716.88	8.27	pos	2.25E-02	2.73E-02	1.37E-02	1.48E-02	2.01E-02
718.29	6.69	pos	3.96E-03	2.51E-03	1.11E-03	4.10E-03	4.02E-03
718.86	8.28	pos	2.41E-02	2.75E-02	1.75E-02	2.12E-02	2.69E-02
719.22	4.67	neg	1.73E-03	1.79E-03	1.73E-03	1.57E-03	1.67E-03
722.79	9.37	neg	2.45E-02	2.81E-02	1.38E-02	1.13E-02	1.73E-02
724.08	8.97	pos	5.90E-03	4.01E-03	5.24E-03	5.98E-03	8.80E-03
724.82	9.39	pos	2.89E-02	3.20E-02	1.85E-02	1.67E-02	2.57E-02
724.89	8.27	neg	2.78E-02	3.54E-02	2.10E-02	1.76E-02	2.18E-02
728.79	9.40	neg	2.73E-02	3.15E-02	2.05E-02	1.84E-02	2.19E-02
730.83	9.43	pos	4.08E-02	4.44E-02	3.43E-02	3.54E-02	4.38E-02
737.60	5.58	pos	3.85E-03	4.11E-03	3.21E-03	2.86E-03	2.88E-03
739.20	4.69	pos	1.63E-03	1.44E-03	5.70E-04	1.63E-03	1.33E-03
740.86	8.29	neg	1.55E-02	1.65E-02	1.34E-02	1.22E-02	1.41E-02
744.78	9.40	neg	2.83E-02	3.18E-02	2.16E-02	1.79E-02	2.25E-02
746.81	9.44	pos	3.26E-02	3.64E-02	2.87E-02	2.82E-02	3.76E-02
751.21	4.66	pos	3.01E-03	2.35E-03	3.84E-04	3.10E-03	2.93E-03
760.85	8.30	pos	1.77E-02	1.70E-02	1.42E-02	1.48E-02	1.83E-02
766.09	5.58	pos	3.26E-03	3.39E-03	2.82E-03	2.44E-03	2.61E-03
766.77	9.43	neg	2.05E-02	1.97E-02	1.51E-02	1.63E-02	1.81E-02
768.79	9.52	pos	1.73E-02	1.98E-02	2.00E-02	2.25E-02	2.17E-02
770.87	8.27	pos	5.21E-02	6.11E-02	3.26E-02	2.89E-02	4.06E-02
774.85	8.30	pos	1.05E-02	1.17E-02	8.88E-03	9.98E-03	1.12E-02
782.77	9.40	neg	1.74E-02	2.11E-02	1.06E-02	1.06E-02	1.38E-02
784.87	8.28	pos	1.85E-02	1.97E-02	1.13E-02	1.13E-02	1.49E-02
785.21	1.96	pos	1.34E-03	8.89E-04	6.75E-04	1.06E-03	1.37E-03
792.87	8.27	neg	1.74E-02	2.29E-02	1.35E-02	1.10E-02	1.22E-02
801.88	9.36	pos	5.68E-02	6.60E-02	2.25E-02	1.80E-02	3.79E-02
804.48	6.33	pos	7.11E-03	4.47E-03	6.85E-03	6.44E-03	7.70E-03
804.78	9.37	neg	2.28E-02	2.71E-02	1.30E-02	9.29E-03	1.56E-02
806.83	9.38	pos	5.52E-02	6.16E-02	3.23E-02	2.79E-02	4.64E-02
815.09	5.56	pos	2.10E-03	2.19E-03	2.34E-03	1.96E-03	1.54E-03
822.81	9.35	pos	2.37E-02	2.61E-02	1.43E-02	1.37E-02	2.09E-02

825.09	5.58	pos	2.67E-03	3.09E-03	2.65E-03	2.20E-03	2.57E-03
825.29	4.65	pos	1.48E-03	1.24E-03	1.80E-03	1.66E-03	1.12E-03
826.78	9.38	neg	1.36E-02	1.59E-02	1.05E-02	9.37E-03	1.21E-02
828.81	9.41	pos	3.26E-02	3.50E-02	2.60E-02	2.70E-02	3.35E-02
828.83	8.29	pos	1.21E-02	1.30E-02	1.04E-02	1.05E-02	1.29E-02
842.76	9.38	neg	1.20E-02	1.39E-02	9.61E-03	8.20E-03	1.09E-02
844.79	9.41	pos	2.47E-02	2.73E-02	2.03E-02	2.10E-02	2.63E-02
852.86	8.27	pos	1.57E-02	1.86E-02	9.72E-03	1.00E-02	1.37E-02
860.86	8.26	neg	1.02E-02	1.26E-02	6.73E-03	5.80E-03	7.86E-03
866.77	9.49	pos	1.36E-02	1.50E-02	1.62E-02	1.85E-02	1.80E-02
868.23	5.58	pos	1.78E-03	1.91E-03	1.86E-03	1.28E-03	1.42E-03
875.32	4.64	pos	1.66E-03	1.53E-03	1.60E-03	1.71E-03	1.57E-03
876.60	5.58	pos	7.99E-03	8.52E-03	7.33E-03	5.23E-03	5.98E-03
877.30	5.59	pos	1.52E-03	1.52E-03	1.75E-03	1.28E-03	1.39E-03
878.10	5.59	pos	2.77E-03	3.00E-03	2.39E-03	2.23E-03	2.40E-03
883.58	5.62	pos	1.82E-03	1.96E-03	2.52E-03	1.76E-03	1.85E-03
891.44	6.68	pos	3.87E-03	2.48E-03	1.09E-03	3.49E-03	3.66E-03
899.86	9.34	pos	4.05E-02	4.61E-02	1.53E-02	1.12E-02	2.66E-02
902.77	9.30	neg	1.10E-02	1.44E-02	4.23E-03	3.18E-03	8.36E-03
904.80	9.37	pos	3.69E-02	4.32E-02	2.02E-02	1.95E-02	3.16E-02
906.85	8.26	pos	1.92E-02	2.26E-02	1.03E-02	1.07E-02	1.40E-02
913.42	6.69	pos	2.91E-03	2.20E-03	1.26E-03	3.07E-03	3.07E-03
922.82	8.27	pos	9.77E-03	1.08E-02	6.03E-03	6.44E-03	8.37E-03
926.79	9.39	pos	2.59E-02	2.73E-02	1.82E-02	1.85E-02	2.45E-02
942.77	9.40	pos	1.96E-02	2.19E-02	1.31E-02	1.46E-02	2.05E-02
953.62	5.58	pos	1.62E-03	1.54E-03	1.21E-03	1.13E-03	1.17E-03
974.83	8.25	pos	1.06E-02	1.37E-02	5.99E-03	5.50E-03	8.32E-03
979.11	5.58	pos	1.45E-03	1.83E-03	1.61E-03	1.31E-03	1.31E-03
981.45	4.64	pos	1.39E-03	9.92E-04	1.83E-03	1.59E-03	1.06E-03
991.41	4.64	pos	3.04E-03	2.00E-03	9.20E-05	2.92E-03	2.17E-03
997.43	4.65	pos	2.20E-03	1.41E-03	2.61E-03	2.20E-03	1.52E-03
997.84	9.33	pos	2.52E-02	3.07E-02	8.65E-03	6.98E-03	1.60E-02
1002.78	9.36	pos	2.05E-02	2.46E-02	1.14E-02	1.05E-02	1.80E-02

Look up table for *S. meliloti* samples exposed to 0.14 mg/L PAH mixture

avg(mz)	avg(rt)	ionization mode	sample 1	sample 2	sample 3	sample 4	sample 5
78.97	9.38	neg	1.39E-02	1.40E-02	3.41E-02	1.68E-02	1.77E-02
87.98	5.58	neg	2.11E-03	2.56E-03	4.64E-03	2.74E-03	2.71E-03
90.99	8.29	pos	2.67E-02	2.67E-02	3.97E-02	2.84E-02	3.00E-02
100.05	7.07	neg	1.83E-02	2.12E-02	1.85E-02	1.94E-02	1.92E-02
100.12	4.66	pos	2.56E-02	2.58E-02	4.93E-02	4.45E-02	3.95E-02
101.08	2.05	pos	7.80E-03	8.71E-03	1.05E-02	8.15E-03	9.09E-03
102.06	8.65	neg	5.45E-02	7.16E-02	6.58E-02	7.55E-02	6.67E-02
102.07	7.12	pos	5.19E-02	6.68E-02	4.90E-02	6.70E-02	6.41E-02
102.07	8.65	pos	3.81E-02	5.13E-02	3.41E-02	5.02E-02	4.25E-02
104.11	9.19	pos	1.77E-02	1.67E-02	1.80E-02	1.53E-02	1.50E-02
104.12	7.04	pos	4.32E-02	6.76E-02	3.77E-02	4.97E-02	5.39E-02
105.00	8.26	pos	1.89E-02	1.77E-02	5.61E-02	1.96E-02	2.34E-02
106.10	7.63	pos	4.23E-02	3.14E-02	2.88E-02	2.73E-02	2.44E-02
107.08	7.08	pos	3.58E-01	4.36E-01	3.43E-01	4.40E-01	4.15E-01
110.02	12.93	pos	1.11E-02	1.25E-02	2.36E-02	1.13E-02	1.49E-02
112.07	4.74	pos	2.71E-02	1.92E-02	9.12E-03	1.51E-02	1.56E-02
116.08	7.60	pos	2.66E-02	4.66E-02	3.08E-02	4.67E-02	4.43E-02
117.02	1.45	neg	1.19E-02	1.65E-02	1.42E-02	1.61E-02	1.44E-02
117.11	7.49	pos	1.49E-02	2.66E-02	3.49E-02	2.47E-02	2.03E-02
118.10	7.52	pos	3.08E-01	5.52E-01	3.24E-01	4.85E-01	7.80E-01
118.13	6.04	pos	9.40E-02	1.48E-01	1.79E-01	2.27E-01	1.61E-01
119.08	2.04	pos	2.76E-02	2.92E-02	3.77E-02	2.71E-02	3.22E-02
120.09	4.65	pos	6.46E-02	6.94E-02	6.25E-02	6.77E-02	6.83E-02
120.09	4.65	pos	6.46E-02	6.94E-02	6.25E-02	6.77E-02	6.83E-02
120.09	7.40	pos	3.38E-02	4.86E-02	3.13E-02	4.42E-02	4.18E-02
122.90	1.24	neg	2.64E-04	1.90E-03	2.13E-04	1.76E-03	2.61E-03
122.94	7.96	pos	1.24E-01	1.41E-01	1.48E-01	1.41E-01	1.45E-01
124.99	1.25	neg	6.81E-03	4.86E-03	5.62E-03	9.05E-03	4.88E-03
125.95	5.57	neg	3.18E-03	3.66E-03	7.13E-03	3.59E-03	4.27E-03
128.03	12.92	pos	1.22E-02	1.35E-02	2.50E-02	1.26E-02	1.22E-02
128.04	8.65	neg	3.88E-02	5.33E-02	4.78E-02	5.39E-02	4.73E-02
128.14	6.39	pos	2.50E-01	2.79E-01	2.40E-01	2.81E-01	2.63E-01
128.97	7.94	neg	4.50E-01	4.69E-01	5.02E-01	4.59E-01	4.90E-01
130.06	1.37	neg	2.05E-03	3.24E-03	3.31E-03	2.83E-03	2.79E-03
132.07	7.42	neg	1.56E-02	1.64E-02	1.30E-02	1.43E-02	2.35E-02
134.05	1.71	neg	1.28E-01	1.42E-01	1.54E-01	1.35E-01	1.21E-01
134.09	7.37	pos	9.87E-02	1.63E-01	1.03E-01	1.30E-01	1.81E-01
136.06	7.08	pos	3.39E-01	4.20E-01	3.26E-01	4.16E-01	3.98E-01
136.08	1.71	pos	4.34E-01	5.09E-01	4.95E-01	5.22E-01	4.90E-01
137.09	2.04	pos	1.13E-01	1.28E-01	1.58E-01	1.21E-01	1.41E-01
139.88	1.26	neg	4.40E-04	3.71E-03	2.81E-04	3.82E-03	4.25E-03
140.99	5.58	neg	1.67E-02	1.60E-02	2.68E-02	1.71E-02	1.81E-02
141.88	1.26	neg	2.69E-03	5.74E-02	3.28E-03	6.31E-02	7.17E-02
142.98	5.57	neg	1.51E-02	1.57E-02	2.68E-02	1.68E-02	1.81E-02
143.87	1.26	neg	1.26E-03	3.52E-02	1.80E-03	3.92E-02	4.36E-02
144.18	2.31	pos	6.24E-03		6.16E-03		
145.06	6.96	pos	8.46E-02	1.01E-01	2.17E-01	1.14E-01	1.14E-01
146.05	8.65	neg	6.79E-01	8.13E-01	7.37E-01	8.06E-01	7.00E-01

149.05	6.98	neg	1.11E-01	9.19E-02	2.53E-01	1.01E-01	1.22E-01
151.03	2.22	neg	8.79E-03	1.02E-02	9.40E-03	1.27E-02	1.07E-02
155.09	7.07	pos	1.62E-01	1.89E-01	1.86E-01	2.01E-01	1.86E-01
157.12	6.39	pos	2.21E-02	2.46E-02	2.13E-02	2.31E-02	2.34E-02
158.98	8.31	pos	7.30E-02	8.38E-02	9.80E-02	8.62E-02	8.46E-02
158.99	12.92	neg	4.79E-02	4.65E-02	9.32E-02	4.65E-02	5.36E-02
159.08	2.05	pos	1.20E-02	1.33E-02	1.66E-02	9.68E-03	1.44E-02
159.08	8.65	neg	1.97E-02	2.68E-02	2.93E-02	2.79E-02	2.31E-02
162.05	3.07	neg	1.65E-02	1.82E-02	1.86E-02	1.91E-02	2.02E-02
168.04	8.67	neg	5.72E-02	6.52E-02	6.65E-02	6.88E-02	6.76E-02
169.53	9.96	neg	8.72E-02	6.47E-02	2.26E-01	7.64E-02	8.50E-02
170.06	8.65	pos	1.11E-01	1.51E-01	1.03E-01	1.35E-01	1.28E-01
171.05	2.05	neg	8.03E-02	4.63E-02	1.02E-01	4.58E-02	5.07E-02
171.10	6.34	pos	2.47E-02	3.81E-02	2.79E-02	3.76E-02	2.74E-02
171.12	6.40	neg	1.19E-01	1.22E-01	1.13E-01	1.21E-01	1.20E-01
172.99	8.26	pos	9.77E-03	9.74E-03	2.54E-02	1.09E-02	1.34E-02
173.05	2.05	neg	2.78E-02	1.61E-02	3.36E-02	1.56E-02	1.76E-02
173.14	6.39	pos	1.15E-01	1.18E-01	1.14E-01	1.25E-01	1.17E-01
174.13	0.63	pos	1.85E-02	8.77E-03	1.67E-02	7.57E-03	8.11E-03
175.08	7.08	pos	6.78E-02	8.16E-02	3.20E-02	8.00E-02	7.16E-02
175.13	10.29	pos	9.16E-02	1.23E-01	1.13E-01	1.26E-01	1.06E-01
176.05	1.39	neg	5.96E-03	4.92E-03	7.46E-03	4.79E-03	3.47E-03
176.94	9.39	neg	7.73E-02	6.89E-02	1.60E-01	7.50E-02	9.00E-02
177.05	2.79	neg	1.28E-02	1.26E-02	2.12E-02	8.34E-03	1.19E-02
180.15	0.66	pos	5.56E-02	5.29E-02	5.72E-02	5.85E-02	6.27E-02
183.04	1.25	neg	6.50E-03	4.03E-03	4.51E-03	3.70E-03	4.33E-03
186.03	8.65	pos	8.19E-02	1.10E-01	6.84E-02	1.01E-01	8.50E-02
187.87	1.26	neg	1.39E-03	2.96E-02	1.70E-03	3.15E-02	3.36E-02
188.03	8.65	pos	7.19E-03	1.00E-02	6.16E-03	9.86E-03	7.51E-03
188.19	11.52	pos	4.78E-02	4.59E-02	1.71E-01	5.03E-02	6.39E-02
189.10	9.81	neg	1.23E-02	1.70E-02	1.04E-02	1.43E-02	1.48E-02
190.06	1.22	neg	2.15E-02	2.08E-02	2.63E-02	2.04E-02	2.13E-02
191.10	6.70	pos	1.31E-01	1.61E-01	1.13E-01	1.62E-01	1.40E-01
191.87	1.26	neg	1.98E-03	4.65E-03	2.40E-03	4.73E-03	5.26E-03
192.04	8.67	pos	1.13E-01	1.49E-01	1.08E-01	1.56E-01	1.42E-01
192.11	6.71	pos	5.31E-01	6.49E-01	4.95E-01	6.32E-01	6.01E-01
192.17	5.40	pos	2.24E-01	1.31E-01	5.96E-01	1.53E-01	2.14E-01
193.12	6.70	pos	3.07E-01	3.71E-01	2.89E-01	3.66E-01	3.43E-01
193.99	5.57	neg	1.88E-02	1.89E-02	3.20E-02	1.87E-02	2.24E-02
195.98	5.57	neg	2.23E-02	2.24E-02	3.82E-02	2.42E-02	2.55E-02
196.10	2.25	pos	1.50E-02	1.91E-02	2.34E-02	2.38E-02	2.55E-02
196.96	7.98	neg	9.17E-02	9.55E-02	7.37E-02	9.48E-02	9.88E-02
197.98	5.58	neg	1.10E-02	1.17E-02	1.92E-02	1.17E-02	1.24E-02
198.11	6.93	pos	3.37E-01	4.08E-01	9.49E-01	4.56E-01	4.77E-01
199.05	7.63	neg	6.90E-02	4.89E-02	1.70E-01	7.26E-02	6.63E-02
203.07	7.10	pos	9.37E-01	1.13E+00	1.06E+00	1.14E+00	1.10E+00
205.08	7.39	pos	4.53E-02	1.25E-01	1.27E-01	2.05E-01	1.18E-01
206.80	5.92	neg	1.99E-02	5.51E-02	1.88E-02	7.86E-02	7.17E-02
206.90	7.94	pos	2.13E-02	3.10E-02	3.34E-02	3.13E-02	2.89E-02
207.12	6.70	neg	2.48E-01	2.66E-01	2.51E-01	2.66E-01	2.67E-01
208.01	8.69	pos	4.16E-02	5.17E-02	3.69E-02	5.08E-02	4.81E-02
208.90	7.93	pos	5.71E-03	6.70E-03	8.02E-03	7.54E-03	6.99E-03

209.14	6.71	pos	1.76E-01	2.03E-01	1.80E-01	2.11E-01	1.98E-01
212.13	6.65	pos	7.33E-02	7.15E-02	7.25E-02	7.34E-02	7.10E-02
212.14	2.68	pos	1.01E-02	1.08E-02	1.36E-02	1.32E-02	1.12E-02
212.93	7.94	neg	8.02E-02	8.34E-02	9.03E-02	6.79E-02	8.12E-02
213.03	7.10	pos	2.31E-02	2.30E-02	7.79E-03	2.40E-02	2.15E-02
213.06	8.46	neg	1.04E-02	1.38E-02	8.10E-03	9.91E-03	9.20E-03
213.09	0.86	neg	3.78E-03	3.45E-03	4.09E-03	3.42E-03	3.13E-03
214.01	8.94	pos	4.49E-02	5.31E-02	1.37E-01	6.17E-02	5.36E-02
214.05	8.75	neg	4.60E-02	4.42E-02	2.84E-02	4.15E-02	3.83E-02
214.14	0.98	neg	2.86E-02	1.70E-02	2.77E-02	1.71E-02	1.49E-02
214.89	1.24	neg	2.31E-04	3.32E-03	3.17E-04	2.78E-03	4.43E-03
219.04	7.06	pos	1.13E+00	1.35E+00	1.22E+00	1.32E+00	1.32E+00
219.05	7.14	neg	1.39E-01	1.63E-01	2.30E-01	1.98E-01	1.86E-01
221.04	7.07	pos	1.01E-01	1.27E-01	1.15E-01	1.47E-01	1.25E-01
224.11	7.34	neg	1.54E-02	1.40E-02	1.41E-02	1.77E-02	2.04E-02
225.03	9.34	pos	9.05E-03	1.32E-02	7.30E-03	1.30E-02	1.05E-02
226.00	8.70	neg	2.71E-02	2.76E-02	2.83E-02	3.25E-02	2.82E-02
226.14	7.29	pos	1.07E-02	3.88E-02	1.19E-02	4.45E-02	2.36E-02
226.97	8.30	pos	2.63E-01	2.67E-01	3.32E-01	2.68E-01	3.04E-01
228.06	8.60	neg	3.06E-02	3.10E-02	1.85E-02	2.80E-02	2.53E-02
229.06	2.67	neg	9.84E-03	5.32E-03	1.38E-02	6.73E-03	5.68E-03
230.03	8.66	pos	4.35E-02	5.01E-02	3.27E-02	5.27E-02	4.60E-02
231.02	9.94	pos	6.35E-03	5.52E-03	1.49E-02	7.25E-03	8.25E-03
231.12	6.71	pos	1.64E-02	1.66E-02	1.31E-02	1.76E-02	1.60E-02
232.13	6.72	pos	1.74E-01	1.75E-01	1.45E-01	1.80E-01	1.70E-01
233.09	7.96	pos	4.97E-02	5.83E-02	5.48E-02	6.04E-02	6.01E-02
234.93	9.44	pos	3.24E-02	3.62E-02	3.75E-02	3.74E-02	4.11E-02
235.03	7.08	neg	6.09E-02	7.04E-02	5.09E-02	7.02E-02	6.17E-02
235.14	7.05	pos	1.28E-02	8.48E-03	1.97E-02	1.58E-02	9.00E-03
235.97	9.95	pos	1.48E-02	1.81E-02	2.14E-02	1.67E-02	2.01E-02
238.05	2.02	neg	7.69E-03	5.27E-03	1.11E-02	5.41E-03	5.12E-03
238.06	8.76	pos	1.27E-02	1.32E-02	4.98E-03	1.12E-02	1.21E-02
239.05	2.03	neg	1.69E-02	1.20E-02	2.12E-02	1.22E-02	1.21E-02
242.02	8.67	neg	1.81E-02	2.52E-02	2.05E-02	2.37E-02	2.01E-02
242.61	8.30	pos	8.21E-02	9.66E-02	6.74E-02	1.13E-01	1.00E-01
242.99	7.06	pos	1.24E-02	1.69E-02	8.13E-03	1.38E-02	7.26E-03
243.07	2.47	neg	4.23E-02	5.54E-02	4.73E-02	4.57E-02	4.95E-02
243.09	1.02	neg	8.04E-03	8.41E-03	2.16E-02	1.00E-02	9.98E-03
243.12	0.82	pos	3.77E-03	3.59E-03	3.51E-03	2.94E-03	2.93E-03
243.90	1.24	neg	7.04E-04	4.96E-03	7.34E-04	4.43E-03	7.00E-03
244.11	8.63	pos	2.28E-02	2.52E-02	1.29E-02	2.36E-02	1.52E-02
244.12	5.94	pos	4.38E-02	4.58E-02	3.93E-02	3.81E-02	3.81E-02
245.05	8.13	neg	4.13E-02	3.99E-02	3.29E-02	1.69E-02	2.87E-02
245.09	2.48	pos	1.84E-02	2.04E-02	1.93E-02	1.72E-02	2.04E-02
245.10	7.40	pos	1.09E-01	1.30E-01	7.21E-02	1.40E-01	1.23E-01
245.12	1.00	pos	1.81E-02	1.69E-02	4.85E-02	1.71E-02	2.05E-02
245.90	1.24	neg	8.36E-04	2.47E-03	1.06E-03	2.45E-03	2.86E-03
245.97	8.73	pos	8.81E-03	1.26E-02	8.19E-03	1.20E-02	1.19E-02
246.99	5.57	neg	7.12E-03	8.13E-03	1.48E-02	7.93E-03	9.61E-03
247.09	6.70	pos	2.17E-02	2.19E-02	1.85E-02	2.31E-02	2.04E-02
248.04	9.94	pos	6.55E-03	6.83E-03	1.56E-02	6.85E-03	9.18E-03
248.10	6.71	pos	2.64E-01	2.67E-01	2.21E-01	2.60E-01	2.54E-01

248.89	8.06	pos	7.46E-03	1.00E-02	3.50E-03	1.11E-02	8.37E-03
250.00	8.70	pos	6.35E-03	8.43E-03	6.05E-03	9.85E-03	8.35E-03
250.99	5.57	neg	7.42E-03	8.60E-03	1.57E-02	8.43E-03	1.01E-02
251.94	9.95	pos	4.96E-03	4.86E-03	8.47E-03	6.21E-03	4.76E-03
252.00	8.70	neg	2.94E-02	3.36E-02	2.97E-02	3.39E-02	3.10E-02
252.13	1.23	pos	1.19E-02	1.11E-02	1.03E-02	9.93E-03	1.05E-02
252.99	9.96	pos	9.97E-03	9.20E-03	1.48E-02	1.04E-02	1.16E-02
254.11	6.71	pos	1.42E-02	1.18E-02	1.03E-02	1.27E-02	1.12E-02
254.92	9.42	neg	8.99E-03	6.41E-03	2.42E-02	9.49E-03	7.25E-03
256.91	9.67	pos	6.26E-02	7.96E-02	6.44E-02	8.20E-02	8.13E-02
257.08	1.88	neg	3.41E-03	3.78E-03	4.47E-03	4.03E-03	3.74E-03
257.12	2.04	pos	2.78E-03	4.46E-03	3.82E-03	3.21E-03	3.46E-03
258.12	9.20	pos	8.82E-01	8.83E-01	8.58E-01	8.21E-01	8.29E-01
258.91	8.11	pos	2.45E-02	2.83E-02	1.55E-02	3.24E-02	3.25E-02
259.03	9.21	neg	1.47E-02	1.55E-02	1.50E-02	1.54E-02	1.69E-02
260.12	9.21	pos	2.75E-02	2.59E-02	1.67E-02	1.61E-02	1.61E-02
261.08	7.40	pos	1.40E-01	1.71E-01	7.63E-02	1.94E-01	1.62E-01
262.14	2.44	pos	2.72E-04	1.68E-03	4.69E-05	1.03E-03	1.23E-03
263.07	7.40	pos	1.31E-02	1.70E-02	8.17E-03	1.63E-02	1.53E-02
263.81	1.28	neg	2.01E-04	1.07E-03	6.24E-05	9.31E-04	1.16E-03
264.86	8.00	pos	1.99E-02	2.56E-02	1.25E-02	2.47E-02	2.44E-02
264.94	8.07	neg	6.76E-02	8.71E-02	4.62E-02	8.68E-02	8.14E-02
266.06	8.65	pos	1.05E-02	1.13E-02	6.17E-03	1.15E-02	9.04E-03
266.08	6.71	neg	9.10E-02	6.73E-02	7.30E-02	6.56E-02	7.33E-02
266.11	1.95	neg	1.28E-02	2.01E-02	1.49E-02	1.93E-02	1.84E-02
266.86	8.00	pos	1.02E-02	1.32E-02	7.00E-03	1.39E-02	1.30E-02
268.12	1.96	pos	4.07E-01	4.33E-01	4.30E-01	4.11E-01	4.37E-01
270.08	6.73	pos	2.91E-02	2.50E-02	2.25E-02	2.65E-02	2.32E-02
270.99	8.36	pos	7.52E-03	7.56E-03	7.60E-03	7.24E-03	6.22E-03
271.98	8.70	pos	1.58E-02	1.88E-02	1.40E-02	2.05E-02	1.79E-02
273.92	9.97	pos	9.24E-03	1.14E-02	8.59E-03	9.26E-03	1.42E-02
274.10	2.09	neg	5.74E-02	4.85E-02	8.17E-02	4.82E-02	5.06E-02
274.89	7.98	pos	4.75E-02	5.12E-02	4.53E-02	5.21E-02	5.56E-02
275.06	2.06	neg	9.43E-03	8.09E-03	1.35E-02	8.07E-03	8.49E-03
276.13	2.08	pos	2.67E-02	3.66E-02	3.34E-02	3.37E-02	3.81E-02
276.95	7.07	neg	4.16E-02	6.58E-02	2.30E-02	6.58E-02	7.27E-02
277.12	7.96	pos	4.75E-02	5.88E-02	5.18E-02	6.09E-02	5.70E-02
279.03	2.02	pos	2.58E-03	2.93E-03	3.37E-03	2.62E-03	3.05E-03
279.06	7.42	neg	6.43E-02	5.61E-02	3.50E-02	5.24E-02	5.75E-02
280.11	9.14	pos	4.83E-02	5.91E-02	4.62E-03	5.87E-02	4.02E-02
280.57	7.11	pos	5.68E-03	7.79E-03	3.34E-03	6.96E-03	3.82E-03
280.83	7.95	pos	1.20E-02	1.26E-02	1.26E-02	1.26E-02	1.48E-02
280.92	7.97	neg	9.79E-02	1.00E-01	8.46E-02	9.15E-02	1.07E-01
282.02	8.64	pos	1.04E-02	1.38E-02	1.18E-02	1.49E-02	1.68E-02
282.06	6.69	neg	9.54E-02	7.31E-02	8.13E-02	6.76E-02	7.30E-02
282.13	6.35	pos	1.27E-02	1.63E-02	1.36E-02	1.67E-02	1.38E-02
282.83	7.94	pos	4.35E-03	5.78E-03	4.47E-03	7.21E-03	5.52E-03
283.06	7.44	pos	1.98E-02	2.50E-02	9.88E-03	2.63E-02	2.50E-02
284.05	6.70	neg	3.67E-02	2.71E-02	3.42E-02	2.70E-02	2.85E-02
284.12	6.47	pos	7.33E-03	1.02E-02	1.32E-02	4.89E-03	9.41E-03
286.15	1.00	neg	2.17E-03	1.53E-03	1.69E-03	2.82E-03	2.59E-03
287.07	9.80	neg	5.00E-03	5.08E-03	5.71E-03	6.00E-03	5.94E-03



287.95	8.75	pos	1.37E-02	1.81E-02	1.34E-02	1.69E-02	1.58E-02
288.13	6.67	pos	6.16E-03	5.31E-03	7.22E-03	6.71E-03	5.08E-03
289.07	9.05	neg	1.57E-02	2.20E-02	1.99E-02	1.96E-02	2.26E-02
290.86	7.93	pos	3.61E-02	5.15E-02	6.39E-02	4.98E-02	5.13E-02
291.13	8.92	pos	7.25E-03	1.05E-02	7.63E-03	1.04E-02	1.07E-02
292.09	6.72	neg	4.63E-02	4.23E-02	4.28E-02	4.05E-02	4.25E-02
292.86	7.93	pos	1.13E-02	1.71E-02	1.92E-02	1.60E-02	1.53E-02
293.98	8.70	neg	1.29E-02	1.46E-02	1.43E-02	1.59E-02	1.55E-02
294.95	9.37	pos	4.10E-02	3.32E-02	8.50E-02	3.10E-02	4.02E-02
294.95	8.31	pos	3.22E-02	3.60E-02	4.05E-02	3.19E-02	4.08E-02
296.08	9.13	pos	3.49E-02	4.67E-02	2.92E-03	4.45E-02	2.81E-02
296.89	7.94	neg	1.09E-01	1.13E-01	1.58E-01	9.77E-02	1.21E-01
297.98	8.67	pos	9.00E-03	1.10E-02	8.70E-03	1.13E-02	1.18E-02
298.00	6.39	neg	2.51E-02	5.77E-02	2.08E-02	5.40E-02	5.66E-02
298.12	0.81	pos	1.17E-02	1.52E-02	1.10E-02	1.87E-02	1.46E-02
298.89	7.94	neg	2.56E-02	2.59E-02	3.41E-02	2.51E-02	2.91E-02
299.03	7.43	pos	1.40E-02	1.71E-02	7.13E-03	1.77E-02	1.60E-02
299.17	0.61	pos	3.02E-02	1.29E-01	8.91E-02	2.21E-01	2.61E-01
300.00	5.79	neg	9.44E-02	8.05E-02	2.21E-01	8.10E-02	1.04E-01
300.90	9.50	neg	1.51E-02	1.57E-02	7.17E-03	1.77E-02	1.84E-02
301.99	5.58	neg	1.54E-02	1.71E-02	3.65E-02	1.67E-02	2.06E-02
302.04	6.70	pos	3.31E-03	7.39E-03	1.94E-03	7.50E-03	5.14E-03
304.01	8.66	neg	3.53E-02	3.42E-02	3.95E-02	3.25E-02	3.71E-02
304.11	6.69	neg	5.81E-02	3.71E-02	4.61E-02	3.14E-02	3.63E-02
305.01	9.03	pos	6.77E-03	9.03E-03	4.78E-03	1.06E-02	8.31E-03
305.99	5.58	neg	4.92E-03	5.78E-03	1.20E-02	5.41E-03	6.89E-03
306.09	8.64	neg	5.42E-02	5.75E-02	5.90E-02	5.66E-02	5.37E-02
306.13	4.73	neg	1.33E-02	6.22E-03	1.19E-02	9.00E-03	8.06E-03
307.04	7.02	pos	8.70E-03	9.04E-03	7.77E-03	9.23E-03	8.15E-03
307.98	5.58	neg	1.22E-03	1.31E-03	2.89E-03	1.44E-03	1.72E-03
308.11	8.64	pos	4.13E-02	5.35E-02	3.93E-02	4.78E-02	4.46E-02
308.93	8.38	neg	1.42E-02	1.45E-02	7.92E-03	1.49E-02	1.39E-02
309.04	7.33	neg	2.16E-02	2.03E-02	4.34E-02	2.10E-02	2.69E-02
309.96	8.74	neg	1.03E-02	1.00E-02	1.01E-02	1.19E-02	1.04E-02
310.10	4.66	neg	4.46E-03	4.09E-03	4.60E-03	4.69E-03	4.26E-03
310.23	6.66	pos	1.22E-02	4.00E-03	1.89E-02	7.71E-03	6.70E-03
310.57	5.58	pos	1.35E-03	1.09E-03	2.35E-03	1.03E-03	1.36E-03
310.93	8.31	pos	1.08E-02	1.34E-02	9.04E-03	1.29E-02	1.39E-02
314.91	9.42	neg	2.07E-01	1.85E-01	3.09E-01	1.91E-01	2.44E-01
315.09	8.64	neg	5.74E-02	7.24E-02	6.33E-02	6.56E-02	6.27E-02
315.13	2.48	pos	3.85E-03	3.82E-03	3.73E-03	3.21E-03	3.61E-03
316.18	6.35	pos	8.67E-01	1.40E+00	1.00E+00	1.31E+00	1.03E+00
316.93	9.42	pos	3.77E-02	3.91E-02	5.53E-02	4.76E-02	4.99E-02
316.96	8.31	neg	2.14E-01	2.24E-01	2.83E-01	2.26E-01	2.52E-01
317.12	8.62	pos	2.37E-02	3.44E-02	2.46E-02	3.05E-02	2.43E-02
318.05	6.58	neg	3.53E-02	3.20E-02	3.08E-02	2.78E-02	3.05E-02
319.99	8.70	neg	2.00E-02	2.20E-02	2.11E-02	2.24E-02	2.30E-02
320.03	6.68	neg	2.40E-02	1.50E-02	1.82E-02	1.28E-02	1.25E-02
320.99	9.04	pos	6.00E-03	8.26E-03	3.36E-03	9.38E-03	6.82E-03
321.15	7.96	pos	1.95E-02	2.34E-02	2.24E-02	2.72E-02	2.63E-02
321.18	2.07	pos	1.41E-03	8.20E-03	1.44E-03	5.68E-03	4.98E-03
322.06	6.48	pos	6.47E-03	7.32E-03	8.17E-03	6.49E-03	6.55E-03

323.41	6.96	pos	6.87E-03	8.89E-03	7.09E-03	7.58E-03	5.13E-03
325.05	7.08	neg	9.12E-02	6.39E-02	6.55E-02	5.59E-02	6.01E-02
325.99	6.92	pos	4.92E-03	8.72E-03	5.16E-03	9.14E-03	6.13E-03
327.08	8.87	neg	1.26E-02	1.35E-02	1.25E-02	1.59E-02	1.21E-02
327.49	5.58	neg	1.67E-03	1.62E-03	3.74E-03	1.64E-03	2.23E-03
328.49	5.58	neg	3.30E-03	2.61E-03	6.89E-03	3.09E-03	3.82E-03
329.00	9.91	pos	5.07E-03	5.21E-03	1.18E-02	5.79E-03	6.45E-03
330.02	5.58	neg	4.80E-02	4.69E-02	4.63E-02	4.70E-02	5.38E-02
330.09	8.65	pos	2.54E-02	3.26E-02	2.29E-02	3.27E-02	2.66E-02
330.89	9.43	neg	1.07E-01	9.51E-02	1.19E-01	1.02E-01	1.27E-01
331.14	7.06	neg	4.76E-01	3.33E-01	7.66E-01	3.31E-01	4.42E-01
333.12	0.65	neg	2.42E-02	5.50E-02	7.78E-02	1.07E-01	1.09E-01
333.16	7.03	pos	3.52E-02	5.26E-02	6.50E-02	5.16E-02	5.77E-02
333.95	9.93	pos	8.13E-03	5.71E-03	1.48E-02	1.09E-02	9.64E-03
334.00	6.70	neg	3.41E-02	7.43E-02	2.30E-02	7.13E-02	8.14E-02
334.89	9.37	neg	1.43E-02	1.01E-02	3.74E-02	1.58E-02	1.84E-02
335.15	4.68	pos	5.51E-02	5.99E-02	5.71E-02	4.81E-02	5.33E-02
335.99	6.69	neg	2.79E-02	5.30E-02	1.70E-02	4.98E-02	5.67E-02
336.07	5.58	pos	2.95E-03	2.96E-03	4.53E-03	2.52E-03	3.02E-03
338.11	6.67	neg	3.07E-02	2.00E-02	2.54E-02	1.61E-02	2.06E-02
338.16	6.38	pos	3.77E-01	4.12E-01	3.99E-01	3.71E-01	3.65E-01
338.92	9.58	pos	5.53E-02	6.60E-02	4.72E-02	6.95E-02	7.12E-02
339.07	5.58	pos	5.54E-03	4.54E-03	8.78E-03	4.19E-03	5.38E-03
339.09	8.64	pos	3.00E-02	4.22E-02	2.92E-02	4.23E-02	3.79E-02
339.16	0.58	pos	1.42E-03	7.61E-03	1.11E-03	5.21E-03	5.64E-03
340.07	6.67	neg	2.46E-02	1.80E-02	2.01E-02	1.59E-02	1.67E-02
341.06	5.58	pos	2.12E-03	1.89E-03	3.67E-03	1.99E-03	2.17E-03
346.07	8.41	neg	1.80E-02	2.22E-02	1.48E-02	2.20E-02	2.06E-02
346.07	8.67	pos	8.53E-03	9.90E-03	7.35E-03	8.73E-03	8.93E-03
346.29	4.66	pos	1.64E-02	1.57E-02	3.05E-02	2.33E-02	2.48E-02
348.03	2.04	neg	2.50E-03	1.77E-03	2.19E-03	1.46E-03	1.56E-03
348.09	8.43	pos	1.16E-02	1.73E-02	9.64E-03	1.65E-02	1.50E-02
348.90	8.04	neg	3.77E-02	4.44E-02	2.57E-02	4.64E-02	4.28E-02
349.14	7.95	pos	7.81E-03	9.00E-03	9.03E-03	1.12E-02	7.00E-03
350.97	9.94	pos	6.21E-03	5.21E-03	1.06E-02	6.09E-03	7.44E-03
351.13	4.67	pos	8.85E-02	9.01E-02	9.23E-02	7.73E-02	7.85E-02
352.07	8.65	pos	1.21E-02	1.56E-02	1.06E-02	1.54E-02	1.28E-02
352.91	8.35	pos	1.45E-02	1.68E-02	1.05E-02	1.73E-02	1.83E-02
353.00	5.58	neg	3.63E-03	3.66E-03	7.43E-03	3.26E-03	4.61E-03
353.05	8.65	neg	1.73E-02	2.04E-02	1.63E-02	1.92E-02	1.81E-02
354.00	5.57	neg	1.88E-03	1.71E-03	3.71E-03	1.70E-03	2.32E-03
354.10	6.42	neg	3.37E-02	3.56E-02	3.38E-02	2.69E-02	2.82E-02
354.13	6.38	pos	5.40E-01	5.78E-01	5.60E-01	5.61E-01	4.94E-01
354.85	7.98	neg	8.30E-04	2.09E-02	1.51E-03	9.78E-03	6.12E-03
354.89	9.57	pos	4.09E-02	4.92E-02	3.28E-02	4.81E-02	4.80E-02
355.00	5.58	neg	9.48E-03	9.69E-03	2.12E-02	9.65E-03	1.17E-02
356.00	1.94	neg	1.56E-03	2.63E-03	1.62E-03	3.29E-03	3.05E-03
356.14	6.36	pos	4.26E-02	4.69E-02	4.82E-02	4.40E-02	3.48E-02
356.98	7.46	pos	3.99E-03	5.18E-03	2.09E-03	6.36E-03	5.19E-03
356.99	5.58	neg	9.07E-03	8.79E-03	2.14E-02	1.01E-02	1.15E-02
357.01	9.33	neg	3.63E-02	3.74E-02	2.18E-02	4.43E-02	4.08E-02
359.07	7.04	pos	1.30E-02	1.63E-02	7.94E-03	1.36E-02	1.03E-02

359.13	7.31	neg	7.75E-02	6.12E-02	3.43E-01	6.21E-02	8.65E-02
360.16	6.36	neg	1.51E-01	1.40E-01	1.51E-01	1.30E-01	1.23E-01
360.27	4.66	pos	3.35E-03	2.94E-03	5.77E-03	4.56E-03	4.60E-03
361.08	8.64	pos	3.69E-02	4.73E-02	3.93E-02	5.07E-02	4.54E-02
361.08	7.05	pos	2.84E-03	1.16E-02	1.86E-03	1.10E-02	9.82E-03
361.24	6.36	pos	1.60E-02	2.13E-01	1.69E-02	1.59E-01	7.83E-02
362.94	8.29	pos	6.22E-02	6.10E-02	8.30E-02	5.82E-02	7.56E-02
363.32	17.69	pos	2.06E-03	1.11E-02	1.41E-03	1.80E-02	1.23E-02
363.74	5.59	pos	4.86E-03	3.77E-03	7.51E-03	3.56E-03	4.50E-03
364.88	7.97	neg	6.36E-02	6.50E-02	6.37E-02	6.42E-02	6.60E-02
365.73	5.58	pos	4.55E-03	3.39E-03	7.11E-03	3.44E-03	4.13E-03
367.56	5.58	pos	2.76E-03	2.21E-03	4.33E-03	1.99E-03	2.43E-03
369.11	4.67	neg	3.36E-02	3.05E-02	3.14E-02	3.22E-02	3.11E-02
371.11	7.09	pos	3.49E-02	3.93E-02	1.33E-02	4.06E-02	3.86E-02
372.00	8.65	neg	1.56E-02	1.70E-02	1.74E-02	1.78E-02	1.95E-02
373.11	4.78	pos	7.42E-03	7.48E-03	7.59E-03	5.69E-03	5.78E-03
374.06	8.66	pos	9.00E-03	9.68E-03	8.82E-03	9.08E-03	9.55E-03
374.14	4.65	neg	3.95E-03	2.59E-03	2.80E-03	2.93E-03	2.80E-03
374.23	6.36	pos	7.86E-03	1.63E-02	9.87E-03	1.40E-02	1.13E-02
374.83	7.93	pos	3.08E-03	4.15E-03	5.23E-03	4.02E-03	4.29E-03
374.99	8.59	neg	3.20E-02	3.60E-02	2.97E-02	4.22E-02	3.71E-02
375.20	7.38	pos	6.06E-03	7.11E-03	3.74E-03	8.28E-03	7.62E-03
377.03	8.65	pos	2.17E-02	2.55E-02	2.01E-02	2.66E-02	2.34E-02
377.12	7.09	pos	1.28E-02	1.17E-02	7.65E-03	1.31E-02	1.32E-02
377.15	6.36	neg	1.19E-01	7.52E-02	1.04E-01	6.62E-02	6.54E-02
378.18	7.30	pos	1.06E-02	9.82E-03	4.66E-02	1.13E-02	1.40E-02
378.92	8.30	pos	2.12E-02	2.48E-02	1.83E-02	2.57E-02	2.69E-02
380.85	7.94	neg	6.64E-02	6.77E-02	9.67E-02	6.18E-02	7.39E-02
381.07	7.06	pos	7.02E-03	8.69E-03	2.68E-03	7.16E-03	4.36E-03
381.50	5.58	neg	2.15E-03	1.91E-03	4.13E-03	1.92E-03	2.32E-03
382.09	6.75	neg	4.46E-02	2.55E-02	5.17E-02	2.40E-02	2.21E-02
382.24	1.70	pos	9.63E-03	1.13E-02	1.08E-02	1.22E-02	1.11E-02
382.85	7.93	neg	2.28E-02	2.29E-02	3.21E-02	2.06E-02	2.48E-02
383.13	7.00	pos	4.33E-01	5.80E-01	5.15E-01	5.73E-01	5.59E-01
383.69	5.58	neg	3.34E-02	2.03E-02	7.07E-02	2.07E-02	2.95E-02
384.49	5.58	neg	1.85E-03	1.92E-03	4.16E-03	1.71E-03	2.04E-03
384.95	8.31	neg	1.04E-01	1.04E-01	1.48E-01	1.07E-01	1.25E-01
385.08	4.67	neg	2.90E-02	2.67E-02	2.71E-02	2.99E-02	2.75E-02
385.14	7.29	pos	2.04E-02	3.10E-02	3.07E-02	3.92E-02	3.10E-02
386.07	1.69	pos	1.29E-03	2.18E-03	1.43E-03	2.19E-03	1.86E-03
387.07	7.06	pos	4.98E-03	1.05E-02	4.27E-03	8.89E-03	7.10E-03
387.98	8.68	neg	2.81E-02	3.29E-02	2.95E-02	3.23E-02	2.68E-02
388.19	6.88	neg	8.76E-02	6.02E-02	1.75E-01	8.61E-02	8.89E-02
389.01	7.03	neg	6.59E-02	6.14E-02	5.43E-02	6.21E-02	5.80E-02
390.21	6.84	pos	1.95E-02	2.80E-02	3.64E-02	3.98E-02	3.17E-02
391.07	5.59	pos	4.56E-03	4.10E-03	6.98E-03	3.62E-03	4.37E-03
391.17	6.93	pos	1.08E-02	8.95E-03	1.36E-02	1.17E-02	1.15E-02
392.91	9.34	neg	1.10E-02	5.95E-03	4.97E-02	8.20E-03	1.51E-02
392.92	9.39	pos	2.10E-02	2.17E-02	6.86E-02	2.72E-02	3.09E-02
393.03	7.06	neg	2.44E-02	4.60E-02	1.91E-02	4.79E-02	5.05E-02
393.07	5.59	pos	4.97E-03	4.44E-03	7.63E-03	3.75E-03	4.64E-03
394.01	6.69	neg	2.65E-02	3.11E-02	1.72E-02	2.67E-02	3.11E-02

395.06	7.05	pos	7.20E-03	1.10E-02	3.84E-03	8.84E-03	5.45E-03
395.11	7.02	neg	6.97E-01	5.25E-01	9.41E-01	5.34E-01	6.83E-01
396.12	6.37	pos	1.35E-02	1.19E-02	1.48E-02	1.08E-02	1.01E-02
396.23	1.71	pos	3.15E-03	3.32E-03	3.48E-03	3.68E-03	3.52E-03
397.05	7.06	pos	8.55E-03	1.18E-02	4.15E-03	1.09E-02	5.87E-03
399.03	8.66	pos	1.99E-02	2.72E-02	1.98E-02	2.56E-02	2.44E-02
399.11	7.11	pos	1.26E-01	1.68E-01	1.30E-01	1.70E-01	1.60E-01
401.05	4.65	neg	7.72E-04	5.22E-03	8.41E-04	4.36E-03	4.46E-03
401.17	7.39	neg	1.52E-01	1.22E-01	2.03E-01	1.09E-01	1.42E-01
403.19	7.37	pos	1.42E-02	1.74E-02	2.91E-02	1.51E-02	1.89E-02
404.03	8.58	pos	7.48E-03	8.46E-03	7.65E-03	9.05E-03	5.97E-03
404.20	2.01	pos	3.51E-03	4.12E-03	5.02E-03	3.99E-03	4.57E-03
405.03	8.62	pos	1.30E-02	1.62E-02	1.48E-02	1.75E-02	1.60E-02
406.00	5.58	neg	2.77E-03	2.60E-03	4.43E-03	2.65E-03	3.25E-03
406.05	1.91	neg	2.26E-03	1.83E-03	2.02E-03	2.00E-03	8.44E-04
406.08	6.36	pos	1.29E-02	2.26E-02	8.87E-03	1.69E-02	1.11E-02
407.09	7.03	pos	1.14E-02	1.00E-02	9.18E-03	9.81E-03	9.64E-03
407.13	4.66	neg	4.92E-03	3.88E-03	3.78E-03	3.15E-03	3.42E-03
408.02	5.58	neg	6.49E-03	6.06E-03	1.39E-02	6.39E-03	6.99E-03
408.09	6.35	neg	4.15E-02	2.86E-02	4.18E-02	2.70E-02	2.77E-02
409.00	5.58	neg	3.34E-03	3.79E-03	5.98E-03	3.97E-03	4.28E-03
409.96	9.38	pos	3.23E-02	2.98E-02	1.14E-01	3.00E-02	4.84E-02
410.00	5.58	neg	7.47E-03	7.43E-03	1.67E-02	7.17E-03	8.59E-03
410.09	6.35	neg	3.02E-02	1.86E-02	3.28E-02	1.95E-02	1.90E-02
411.01	5.56	neg	3.00E-03	2.97E-03	4.49E-03	3.19E-03	3.54E-03
411.19	1.96	pos	1.12E-03	1.19E-03	1.34E-03	1.35E-03	1.43E-03
412.00	5.58	neg	4.38E-03	4.20E-03	9.57E-03	4.60E-03	5.64E-03
412.09	6.37	pos	1.98E-02	1.74E-02	2.15E-02	1.50E-02	1.38E-02
412.19	6.84	pos	2.36E-02	2.61E-02	4.35E-02	3.28E-02	2.85E-02
412.19	2.00	pos	2.26E-03	2.23E-03	3.27E-03	2.18E-03	2.46E-03
412.28	4.65	pos	2.01E-03	2.43E-03	3.80E-03	3.20E-03	3.01E-03
412.89	9.40	neg	1.33E-01	1.02E-01	2.35E-01	1.13E-01	1.53E-01
413.99	5.58	neg	1.84E-03	1.99E-03	3.39E-03	1.85E-03	2.03E-03
414.09	6.37	pos	8.71E-03	7.83E-03	9.55E-03	6.39E-03	6.03E-03
415.01	8.68	pos	7.26E-03	9.22E-03	5.89E-03	1.03E-02	8.77E-03
415.07	7.30	pos	4.59E-03	6.30E-03	7.26E-03	5.41E-03	4.09E-03
417.57	5.58	pos	5.83E-03	4.24E-03	8.89E-03	4.21E-03	5.25E-03
418.26	6.68	pos	2.59E-02	3.39E-02	2.59E-02	3.18E-02	3.20E-02
419.08	2.02	neg	2.91E-03	3.45E-03	2.20E-03	2.97E-03	3.26E-03
419.27	6.68	pos	1.60E-01	2.05E-01	1.47E-01	1.90E-01	1.97E-01
419.57	5.58	pos	7.12E-03	5.71E-03	1.18E-02	5.37E-03	6.30E-03
420.17	0.63	pos	1.01E-03	2.16E-03	2.07E-03	3.28E-03	3.70E-03
420.29	6.60	pos	9.74E-02	9.53E-02	1.01E-01	9.18E-02	1.00E-01
421.30	6.54	pos	2.46E-02	2.33E-02	2.47E-02	2.26E-02	2.50E-02
423.06	7.05	pos	7.37E-03	7.91E-03	6.24E-03	7.23E-03	5.21E-03
424.07	6.35	neg	3.70E-02	2.87E-02	4.35E-02	2.50E-02	2.49E-02
424.22	4.70	pos	4.69E-03	4.06E-03	1.21E-03	2.96E-03	3.06E-03
425.17	7.39	pos	2.81E-02	3.67E-02	2.30E-02	3.81E-02	3.48E-02
426.06	6.35	neg	2.64E-02	1.73E-02	3.03E-02	1.98E-02	1.74E-02
426.17	4.50	neg	2.67E-03	1.93E-03	2.40E-03	2.04E-03	1.90E-03
426.31	0.62	pos	1.67E-03	1.74E-03	1.98E-03	1.98E-03	2.53E-03
427.01	8.61	neg	7.97E-03	1.51E-02	1.38E-02	1.52E-02	1.56E-02

428.07	6.37	pos	7.68E-03	6.29E-03	8.65E-03	6.43E-03	5.17E-03
428.16	6.84	pos	1.26E-02	1.30E-02	1.99E-02	1.65E-02	1.38E-02
428.87	9.41	neg	6.83E-02	5.17E-02	1.12E-01	6.11E-02	8.04E-02
430.06	6.34	pos	4.59E-03	4.02E-03	5.40E-03	3.48E-03	3.12E-03
430.89	9.42	pos	2.38E-02	2.53E-02	3.64E-02	2.64E-02	3.17E-02
430.93	8.29	pos	6.02E-02	5.89E-02	8.90E-02	5.60E-02	7.14E-02
434.18	6.84	pos	5.48E-03	4.51E-03	1.17E-02	5.98E-03	4.93E-03
434.30	5.58	neg	1.71E-03	1.42E-03	3.02E-03	1.49E-03	1.69E-03
434.87	9.48	neg	7.18E-02	6.30E-02	7.57E-02	6.92E-02	7.93E-02
435.50	5.58	neg	2.41E-03	1.82E-03	4.35E-03	1.83E-03	2.55E-03
436.50	5.58	neg	3.29E-02	1.98E-02	6.18E-02	1.93E-02	2.76E-02
436.89	9.59	pos	4.21E-02	4.66E-02	3.16E-02	5.39E-02	5.25E-02
437.50	5.58	neg	2.39E-03	1.74E-03	4.12E-03	1.84E-03	2.00E-03
438.02	4.65	neg	2.44E-03	2.87E-03	6.27E-04	2.39E-03	2.61E-03
438.50	5.59	neg	1.79E-02	1.15E-02	3.24E-02	1.09E-02	1.62E-02
440.25	6.68	pos	8.44E-03	8.22E-03	7.04E-03	8.00E-03	7.58E-03
441.12	7.34	pos	1.98E-02	2.07E-02	1.79E-02	2.36E-02	2.34E-02
441.25	6.69	pos	4.91E-02	4.58E-02	4.09E-02	4.48E-02	4.74E-02
442.08	5.58	pos	2.25E-03	2.19E-03	3.00E-03	1.90E-03	2.12E-03
442.13	7.36	pos	3.52E-03	4.32E-03	3.22E-03	4.18E-03	4.58E-03
442.81	7.95	pos	7.81E-03	9.17E-03	1.12E-02	9.95E-03	9.87E-03
443.04	4.74	neg	8.30E-03	6.19E-03	7.95E-03	8.70E-03	6.75E-03
443.09	7.24	pos	7.85E-03	7.32E-03	8.95E-03	8.22E-03	8.35E-03
444.08	5.58	pos	8.68E-03	7.67E-03	1.22E-02	6.82E-03	8.31E-03
444.94	8.28	pos	1.23E-02	1.33E-02	2.15E-02	1.38E-02	1.38E-02
445.23	7.38	pos	4.29E-02	5.31E-02	3.17E-02	5.25E-02	5.09E-02
446.91	8.29	pos	2.09E-02	2.44E-02	1.99E-02	2.63E-02	2.63E-02
448.07	5.58	pos	6.02E-03	5.03E-03	8.26E-03	5.18E-03	5.75E-03
448.24	0.57	pos	1.16E-03	1.73E-03	1.40E-03	2.26E-03	1.62E-03
448.84	7.96	neg	3.24E-02	3.47E-02	3.23E-02	3.07E-02	3.28E-02
450.15	6.85	pos	4.21E-03	3.25E-03	3.84E-03	4.49E-03	4.23E-03
450.85	9.49	neg	7.88E-02	6.96E-02	8.32E-02	7.50E-02	8.29E-02
451.05	7.20	pos	9.60E-03	1.23E-02	1.44E-02	1.06E-02	7.98E-03
452.10	6.95	pos	3.26E-03	3.38E-03	2.00E-03	3.06E-03	2.11E-03
452.87	9.53	pos	3.54E-02	4.29E-02	2.98E-02	4.37E-02	4.71E-02
452.94	8.30	neg	7.11E-02	6.76E-02	1.03E-01	6.64E-02	7.91E-02
454.99	9.35	neg	1.41E-02	1.24E-02	1.60E-02	1.80E-02	1.72E-02
455.05	7.06	pos	3.37E-03	8.19E-03	2.10E-03	9.59E-03	8.79E-03
455.21	6.69	neg	3.90E-02	2.65E-02	3.10E-02	2.31E-02	2.73E-02
456.31	6.70	pos	6.81E-02	6.20E-02	7.20E-02	6.65E-02	7.35E-02
457.07	7.26	pos	1.08E-02	1.00E-02	1.39E-02	1.18E-02	1.25E-02
458.07	2.02	pos	1.50E-03	1.30E-03	1.59E-03	1.37E-03	1.17E-03
458.79	7.92	pos	4.18E-03	5.32E-03	9.04E-03	5.00E-03	5.72E-03
459.17	6.66	pos	8.06E-03	9.38E-03	6.58E-03	4.77E-03	6.59E-03
461.00	5.58	neg	3.40E-03	3.07E-03	6.68E-03	2.98E-03	3.96E-03
462.00	5.58	neg	2.45E-03	1.83E-03	4.52E-03	2.27E-03	2.56E-03
463.00	5.58	neg	6.54E-02	4.74E-02	1.28E-01	4.45E-02	5.79E-02
463.13	7.34	pos	9.53E-03	8.93E-03	6.54E-03	9.71E-03	1.11E-02
464.00	5.57	neg	2.53E-03	1.94E-03	4.78E-03	2.03E-03	2.72E-03
464.82	7.94	neg	3.51E-02	3.13E-02	5.44E-02	3.00E-02	3.43E-02
465.00	5.59	neg	5.26E-02	4.15E-02	9.32E-02	4.06E-02	4.78E-02
467.21	7.39	pos	2.22E-02	2.89E-02	8.90E-03	3.04E-02	2.79E-02

468.91	8.32	neg	2.62E-02	2.79E-02	2.32E-02	3.02E-02	2.96E-02
471.57	5.59	pos	1.97E-03	1.65E-03	2.73E-03	1.30E-03	1.72E-03
477.01	4.77	pos	1.79E-03	3.19E-03	8.39E-04	2.53E-03	1.72E-03
478.29	0.63	pos	9.74E-04	1.79E-03	1.74E-03	3.46E-03	5.08E-03
479.21	6.70	pos	8.24E-03	7.69E-03	7.25E-03	7.15E-03	6.32E-03
480.12	6.79	pos	5.15E-03	5.34E-03	5.14E-03	6.41E-03	3.77E-03
483.18	7.39	pos	1.31E-02	1.82E-02	4.58E-03	1.82E-02	1.61E-02
486.15	8.62	pos	7.39E-03	1.13E-02	7.47E-03	1.05E-02	8.02E-03
487.30	6.35	pos	3.42E-03	4.34E-03	4.20E-03	4.21E-03	3.55E-03
488.50	5.58	neg	1.69E-03	1.44E-03	3.11E-03	1.39E-03	1.67E-03
488.80	9.88	neg	2.97E-02	2.96E-02	2.87E-02	3.51E-02	2.94E-02
488.90	8.34	pos	1.36E-02	1.49E-02	1.09E-02	1.42E-02	1.64E-02
489.19	7.39	pos	6.14E-03	5.84E-03	7.83E-05	6.87E-03	6.01E-03
489.50	5.58	neg	1.87E-03	1.46E-03	3.91E-03	1.70E-03	2.35E-03
490.50	5.59	neg	2.45E-02	1.45E-02	4.43E-02	1.53E-02	2.19E-02
490.82	9.88	pos	7.87E-03	7.92E-03	8.93E-03	2.19E-02	1.02E-02
490.90	9.34	pos	1.85E-02	2.01E-02	5.16E-02	6.87E-03	2.31E-02
491.50	5.58	neg	1.56E-03	1.17E-03	2.53E-03	1.27E-03	1.80E-03
493.08	7.38	pos	2.98E-03	5.85E-03	2.84E-03	2.53E-03	2.58E-03
495.08	5.57	pos	4.35E-03	3.86E-03	5.42E-03	3.50E-03	4.04E-03
496.83	9.80	pos	1.67E-02	2.55E-02	1.20E-02	2.13E-02	1.81E-02
497.02	4.65	neg	1.15E-03	3.30E-03	1.24E-03	3.22E-03	3.04E-03
497.08	5.57	pos	1.16E-02	1.06E-02	1.50E-02	1.03E-02	1.11E-02
498.92	8.28	pos	4.14E-02	4.19E-02	6.35E-02	4.15E-02	5.00E-02
499.08	5.57	pos	1.54E-02	1.37E-02	2.00E-02	1.25E-02	1.47E-02
505.16	7.40	pos	9.79E-03	9.35E-03	3.54E-03	1.22E-02	1.09E-02
507.14	6.69	neg	2.20E-02	4.66E-02	1.45E-02	3.92E-02	4.32E-02
507.94	9.38	pos	2.26E-02	2.01E-02	9.46E-02	2.24E-02	3.58E-02
508.13	8.63	pos	1.04E-02	1.59E-02	1.17E-02	1.65E-02	1.38E-02
509.30	2.50	neg	5.87E-03	1.19E-02	7.61E-03	1.60E-02	1.00E-02
510.79	9.94	neg	2.20E-02	2.20E-02	2.98E-02	2.40E-02	2.78E-02
511.09	4.65	neg	2.25E-03	2.12E-03	1.86E-03	1.96E-03	1.85E-03
511.16	6.73	pos	1.30E-02	1.85E-02	8.56E-03	1.62E-02	1.15E-02
511.33	2.50	pos	4.03E-03	5.78E-03	4.29E-03	7.43E-03	6.03E-03
512.80	9.98	pos	9.13E-03	9.36E-03	9.91E-03	1.12E-02	1.30E-02
512.84	9.31	neg	6.95E-03	5.61E-03	3.97E-02	6.95E-03	1.25E-02
512.88	9.39	pos	2.68E-02	2.36E-02	4.83E-02	2.64E-02	3.50E-02
512.92	8.27	pos	1.01E-02	1.07E-02	1.70E-02	1.02E-02	1.27E-02
514.00	5.59	neg	1.58E-02	1.47E-02	2.63E-02	1.46E-02	1.66E-02
514.29	1.97	pos	7.02E-03	7.04E-03	7.29E-03	7.06E-03	7.76E-03
516.01	5.58	neg	2.29E-03	2.30E-03	3.83E-03	2.25E-03	2.91E-03
518.01	5.58	neg	1.76E-03	1.87E-03	3.25E-03	1.71E-03	2.15E-03
520.92	8.30	neg	5.62E-02	4.97E-02	8.66E-02	4.90E-02	5.82E-02
521.08	8.64	pos	5.75E-03	7.02E-03	5.92E-03	6.66E-03	6.42E-03
521.13	7.38	pos	8.06E-03	6.10E-03	5.36E-03	6.45E-03	8.62E-03
523.41	7.07	pos	7.85E-03	9.09E-03	9.88E-03	1.22E-02	9.68E-03
525.30	6.61	pos	2.36E-02	3.43E-02	2.08E-02	2.77E-02	3.37E-02
525.58	5.58	pos	1.37E-03	1.17E-03	2.25E-03	8.74E-04	1.11E-03
526.78	7.94	pos	3.82E-03	6.79E-03	6.55E-03	5.56E-03	5.38E-03
526.85	9.37	neg	3.53E-02	2.64E-02	7.30E-02	3.24E-02	4.27E-02
528.87	9.40	pos	1.59E-02	1.62E-02	3.12E-02	2.02E-02	2.43E-02
531.15	6.71	pos	3.91E-03	4.74E-03	2.57E-03	3.91E-03	2.41E-03

532.80	7.96	neg	1.81E-02	1.95E-02	1.91E-02	1.69E-02	2.01E-02
532.85	9.42	neg	4.41E-02	3.75E-02	5.87E-02	3.84E-02	5.05E-02
533.12	7.06	pos	7.23E-03	7.79E-03	4.03E-03	7.50E-03	5.52E-03
534.87	9.48	pos	3.67E-02	4.17E-02	3.00E-02	4.39E-02	4.88E-02
535.13	7.37	pos	4.14E-03	6.28E-03	2.30E-03	5.57E-03	2.79E-03
536.90	8.32	neg	2.80E-02	2.84E-02	2.52E-02	2.73E-02	3.22E-02
539.18	7.32	neg	7.52E-03	7.75E-03	3.56E-02	6.05E-03	8.16E-03
541.19	1.98	neg	1.12E-03	9.18E-04	1.02E-03	9.56E-04	8.62E-04
542.42	17.59	pos	3.43E-03	1.00E-02	1.57E-03	2.50E-02	1.64E-02
542.76	7.92	pos	3.90E-03	5.75E-03	9.65E-03	6.05E-03	5.89E-03
543.23	2.03	pos	2.84E-03	3.58E-03	3.56E-03	2.86E-03	3.54E-03
544.27	2.07	pos	1.97E-03	1.74E-03	2.39E-03	1.61E-03	2.12E-03
544.46	6.38	pos	5.57E-03	4.55E-03	6.09E-03	4.93E-03	5.26E-03
546.08	8.65	pos	6.30E-03	7.86E-03	6.34E-03	8.13E-03	6.48E-03
547.13	6.70	pos	5.36E-03	7.75E-03	4.18E-03	6.34E-03	5.02E-03
548.78	7.93	neg	1.82E-02	1.73E-02	3.08E-02	1.46E-02	1.68E-02
548.83	9.45	neg	5.15E-02	4.14E-02	5.99E-02	4.61E-02	5.54E-02
549.09	5.58	pos	1.51E-03	1.16E-03	2.67E-03	1.18E-03	1.53E-03
550.85	9.47	pos	3.11E-02	3.34E-02	2.66E-02	3.52E-02	4.01E-02
552.10	8.63	pos	1.55E-02	2.01E-02	1.68E-02	2.08E-02	1.93E-02
556.33	4.65	pos	1.83E-03	1.15E-03	1.81E-03	9.10E-04	9.50E-04
556.88	8.33	pos	1.51E-02	1.60E-02	1.14E-02	1.62E-02	1.64E-02
559.34	4.64	pos	6.94E-02	3.60E-02	7.54E-02	3.37E-02	4.65E-02
565.06	9.19	neg	1.99E-02	2.29E-02	1.20E-02	2.57E-02	2.16E-02
566.09	5.60	pos	6.16E-04	1.62E-03	6.80E-04	1.26E-03	9.95E-04
566.91	8.28	pos	3.91E-02	3.86E-02	6.47E-02	3.86E-02	4.84E-02
567.33	0.60	pos	1.14E-03	2.30E-03	1.59E-03	2.44E-03	2.72E-03
568.07	8.65	pos	1.11E-02	1.44E-02	1.09E-02	1.40E-02	1.32E-02
571.18	7.01	pos	3.82E-03	2.89E-03	4.64E-03	2.78E-03	3.41E-03
572.87	8.34	pos	9.23E-03	1.02E-02	5.28E-03	1.12E-02	1.07E-02
573.32	4.64	pos	1.17E-02	5.42E-03	1.18E-02	5.41E-03	7.39E-03
574.08	8.63	pos	1.25E-02	1.80E-02	1.57E-02	1.75E-02	1.72E-02
574.36	1.00	pos	6.27E-03	9.18E-03	5.03E-03	9.11E-03	6.92E-03
577.58	5.58	pos	2.39E-03	2.00E-03	3.97E-03	2.07E-03	2.19E-03
578.91	8.37	neg	1.34E-02	1.28E-02	1.31E-02	1.44E-02	1.42E-02
579.04	9.90	neg	1.35E-02	1.47E-02	1.56E-02	1.41E-02	1.47E-02
579.21	6.36	pos	6.34E-03	9.93E-03	4.16E-03	7.09E-03	5.06E-03
579.58	5.58	pos	3.41E-03	2.65E-03	5.89E-03	2.54E-03	3.28E-03
580.46	6.71	pos	5.37E-03	5.49E-03	5.86E-03	6.99E-03	5.47E-03
580.91	8.27	pos	1.29E-02	1.09E-02	2.24E-02	1.15E-02	1.38E-02
581.21	6.37	pos	3.43E-03	7.92E-03	2.74E-03	6.94E-03	6.26E-03
582.21	5.72	neg	1.65E-02	1.59E-02	4.32E-02	2.34E-02	1.58E-02
582.88	8.29	pos	1.81E-02	2.03E-02	1.75E-02	2.06E-02	2.13E-02
583.96	8.55	pos	4.23E-03	6.15E-03	6.45E-03	7.99E-03	3.87E-03
584.11	9.17	pos	1.07E-02	1.56E-02	4.57E-03	1.63E-02	1.15E-02
584.24	5.72	pos	9.60E-03	1.12E-02	1.95E-02	1.48E-02	8.97E-03
588.86	9.40	pos	1.31E-02	1.26E-02	3.73E-02	1.38E-02	1.76E-02
588.91	8.29	neg	4.15E-02	3.98E-02	6.98E-02	3.73E-02	4.64E-02
589.20	2.07	pos	7.06E-04	6.15E-04	9.22E-04	5.28E-04	7.42E-04
590.05	8.65	pos	9.43E-03	1.20E-02	1.10E-02	1.28E-02	1.21E-02
595.33	0.84	neg	3.42E-03	3.92E-03	2.16E-03	4.02E-03	3.24E-03
595.98	0.66	pos	8.99E-04	1.58E-03	1.28E-03	2.55E-03	2.58E-03

596.06	8.64	pos	1.02E-02	1.30E-02	1.16E-02	1.44E-02	1.34E-02
597.30	4.66	pos	2.56E-03	2.86E-03	2.52E-03	2.08E-03	2.32E-03
598.12	9.92	pos	1.13E-02	1.52E-02	9.90E-03	1.54E-02	1.35E-02
598.87	8.30	pos	7.86E-03	9.46E-03	6.76E-03	1.04E-02	9.68E-03
600.38	0.80	pos	8.09E-03	1.12E-02	5.35E-03	5.32E-03	9.81E-03
601.19	6.37	pos	7.86E-03	8.06E-03	5.74E-03	5.70E-03	4.52E-03
602.39	0.85	pos	3.29E-03	5.83E-03	2.31E-03	5.95E-03	3.93E-03
603.09	5.58	pos	9.96E-03	8.39E-03	1.38E-02	7.75E-03	9.08E-03
604.89	8.31	neg	2.50E-02	2.32E-02	2.27E-02	2.49E-02	2.82E-02
605.92	9.37	pos	1.68E-02	1.40E-02	7.82E-02	1.47E-02	2.60E-02
606.09	8.98	neg	5.70E-03	7.14E-03	7.11E-03	7.04E-03	7.89E-03
608.10	8.13	pos	4.92E-02	3.59E-02	7.06E-02	3.72E-02	4.23E-02
608.83	9.38	neg	3.25E-02	3.36E-02	8.55E-02	3.88E-02	3.98E-02
608.90	8.32	pos	8.01E-03	7.97E-03	9.05E-03	7.78E-03	9.43E-03
610.74	7.93	pos	2.75E-03	4.21E-03	4.60E-03	4.92E-03	3.68E-03
610.87	9.38	pos	3.05E-02	2.78E-02	6.69E-02	3.51E-02	4.36E-02
611.16	9.80	neg	5.49E-03	8.01E-03	6.86E-03	9.33E-03	9.61E-03
612.02	8.63	pos	7.87E-03	9.13E-03	8.52E-03	1.04E-02	9.35E-03
613.18	9.81	pos	6.25E-03	1.15E-02	5.43E-03	1.28E-02	1.16E-02
614.38	0.80	pos	2.31E-03	8.97E-03	4.97E-03	2.48E-02	3.20E-02
617.17	6.36	pos	5.63E-03	6.42E-03	4.09E-03	5.04E-03	3.73E-03
617.55	5.66	pos	2.69E-03	2.19E-03	2.86E-03	1.98E-03	2.02E-03
618.12	8.59	neg	1.43E-02	1.73E-02	1.70E-02	1.69E-02	1.23E-02
619.08	5.65	pos	9.23E-04	2.10E-03	9.07E-04	1.55E-03	8.01E-04
620.14	8.59	pos	1.43E-02	1.94E-02	1.51E-02	1.84E-02	1.31E-02
624.80	9.41	neg	2.00E-02	1.50E-02	5.12E-02	1.76E-02	2.57E-02
624.87	8.32	pos	1.51E-02	1.64E-02	1.32E-02	1.81E-02	1.74E-02
625.12	8.96	pos	3.49E-03	6.36E-03	3.45E-03	6.39E-03	5.71E-03
626.84	9.39	pos	1.41E-02	1.37E-02	3.02E-02	1.41E-02	1.99E-02
628.40	6.67	pos	5.04E-03	4.48E-03	4.82E-03	3.91E-03	5.57E-03
630.08	8.96	pos	4.93E-03	6.96E-03	3.73E-03	7.16E-03	7.29E-03
630.80	9.49	neg	2.88E-02	2.41E-02	3.96E-02	2.61E-02	3.39E-02
632.75	7.92	neg	1.47E-02	1.47E-02	2.20E-02	1.30E-02	1.64E-02
632.85	9.44	pos	2.94E-02	3.30E-02	2.94E-02	3.71E-02	4.03E-02
634.90	8.27	pos	3.39E-02	3.42E-02	6.36E-02	3.10E-02	4.24E-02
638.87	8.31	pos	8.26E-03	7.83E-03	7.03E-03	8.57E-03	8.84E-03
646.80	9.44	neg	3.11E-02	2.38E-02	4.29E-02	2.72E-02	3.39E-02
648.30	8.67	pos	1.16E-02	1.54E-02	1.13E-02	1.61E-02	1.37E-02
648.37	6.32	pos	5.42E-03	9.80E-03	7.10E-03	8.19E-03	5.74E-03
648.83	9.46	pos	2.42E-02	2.69E-02	2.38E-02	2.91E-02	3.26E-02
648.87	9.41	neg	1.23E-02	1.32E-02	1.40E-02	1.46E-02	1.33E-02
650.38	6.68	pos	5.37E-03	4.43E-03	5.29E-03	4.39E-03	4.10E-03
650.87	8.29	pos	1.62E-02	1.99E-02	1.64E-02	1.82E-02	2.07E-02
654.82	9.55	pos	1.46E-02	1.92E-02	1.55E-02	1.88E-02	1.78E-02
655.20	8.62	pos	6.18E-03	9.67E-03	6.28E-03	9.37E-03	7.06E-03
656.09	5.58	pos	5.83E-03	5.27E-03	7.31E-03	4.95E-03	5.23E-03
656.90	8.29	neg	2.26E-02	2.17E-02	4.38E-02	2.01E-02	2.65E-02
658.09	5.57	pos	9.96E-03	9.04E-03	1.21E-02	8.43E-03	9.30E-03
662.12	9.00	neg	1.10E-02	1.38E-02	1.14E-02	1.42E-02	1.23E-02
664.14	9.00	pos	2.87E-02	3.99E-02	2.52E-02	4.16E-02	3.44E-02
666.85	8.30	pos	9.03E-03	9.49E-03	6.87E-03	1.04E-02	9.87E-03
668.79	9.50	neg	2.69E-02	2.27E-02	2.71E-02	2.65E-02	2.88E-02



669.29	4.67	pos	3.70E-03	3.44E-03	3.89E-03	2.61E-03	2.41E-03
670.81	9.57	pos	1.90E-02	2.41E-02	1.53E-02	2.61E-02	2.66E-02
671.49	4.64	pos	2.89E-03	2.21E-03	3.01E-03	2.04E-03	2.22E-03
672.35	6.69	pos	5.15E-03	5.02E-03	5.14E-03	4.57E-03	4.61E-03
672.88	8.31	neg	1.58E-02	1.50E-02	1.56E-02	1.67E-02	1.96E-02
676.88	8.29	pos	7.45E-03	6.95E-03	9.66E-03	5.79E-03	9.52E-03
681.26	4.66	neg	2.05E-03	1.35E-03	1.79E-03	1.45E-03	1.44E-03
682.30	6.69	pos	5.36E-03	5.81E-03	3.62E-03	5.16E-03	3.68E-03
683.49	4.64	pos	2.81E-03	1.67E-03	2.99E-03	1.95E-03	1.91E-03
684.78	9.43	neg	1.26E-02	1.14E-02	1.47E-02	1.28E-02	1.53E-02
685.26	4.67	pos	6.73E-03	7.63E-03	7.52E-03	5.35E-03	5.06E-03
686.12	8.98	pos	1.34E-02	1.86E-02	1.22E-02	2.13E-02	1.62E-02
688.32	6.69	pos	4.01E-03	3.64E-03	3.59E-03	3.88E-03	3.64E-03
692.86	8.32	pos	1.49E-02	1.57E-02	1.33E-02	1.69E-02	1.82E-02
697.24	4.66	neg	4.07E-03	2.91E-03	3.73E-03	2.96E-03	3.05E-03
701.24	4.67	pos	3.19E-03	3.59E-03	3.30E-03	2.59E-03	2.40E-03
702.89	8.27	pos	3.09E-02	3.00E-02	6.16E-02	3.16E-02	3.88E-02
703.89	9.34	pos	1.21E-02	8.74E-03	6.33E-02	1.10E-02	1.99E-02
704.29	6.69	pos	4.00E-03	3.77E-03	2.64E-03	3.87E-03	2.47E-03
704.87	8.28	pos	4.97E-03	5.41E-03	8.91E-03	5.39E-03	5.68E-03
706.77	9.48	neg	1.78E-02	1.44E-02	5.17E-02	1.65E-02	2.04E-02
706.86	8.30	pos	7.43E-03	8.26E-03	8.05E-03	8.48E-03	1.00E-02
707.10	5.56	pos	4.53E-03	4.15E-03	5.83E-03	3.99E-03	4.27E-03
707.24	4.71	pos	1.19E-03	1.48E-03	1.49E-03	1.41E-03	1.54E-03
708.10	8.98	pos	7.59E-03	1.06E-02	6.74E-03	1.16E-02	9.38E-03
708.84	9.36	pos	2.53E-02	2.53E-02	6.13E-02	2.60E-02	3.84E-02
709.10	5.57	pos	1.79E-02	1.72E-02	2.44E-02	1.55E-02	1.75E-02
715.23	4.66	pos	5.18E-03	8.92E-03	2.20E-03	6.06E-03	5.42E-03
716.88	8.27	pos	1.07E-02	9.39E-03	2.03E-02	1.09E-02	1.26E-02
718.29	6.69	pos	4.00E-03	5.00E-03	2.59E-03	3.86E-03	2.95E-03
719.22	4.67	neg	2.01E-03	1.69E-03	1.95E-03	1.95E-03	1.57E-03
719.34	8.58	pos	2.15E-02	2.84E-02	2.05E-02	2.82E-02	1.88E-02
722.79	9.37	neg	8.70E-03	4.91E-03	2.71E-02	3.20E-03	1.02E-02
723.56	5.62	pos	2.21E-03	1.40E-03	1.54E-03	1.45E-03	1.83E-03
724.08	8.97	pos	4.77E-03	7.24E-03	4.03E-03	7.90E-03	7.18E-03
724.82	9.39	pos	1.04E-02	9.98E-03	2.39E-02	1.10E-02	1.54E-02
724.89	8.27	neg	1.32E-02	1.26E-02	2.84E-02	1.20E-02	1.67E-02
727.27	6.35	pos	5.32E-03	5.79E-03	6.87E-03	3.71E-03	5.30E-03
728.79	9.40	neg	1.49E-02	1.32E-02	2.46E-02	1.57E-02	1.67E-02
730.83	9.43	pos	2.24E-02	2.50E-02	2.82E-02	2.91E-02	3.29E-02
737.60	5.58	pos	2.35E-03	2.12E-03	4.20E-03	1.77E-03	2.06E-03
739.20	4.69	pos	1.07E-03	1.65E-03	6.67E-04	1.14E-03	1.20E-03
740.86	8.29	neg	1.06E-02	1.05E-02	1.23E-02	9.80E-03	1.28E-02
744.78	9.40	neg	1.46E-02	1.15E-02	2.52E-02	1.25E-02	1.62E-02
746.81	9.44	pos	1.81E-02	1.89E-02	2.25E-02	2.23E-02	2.61E-02
751.21	4.66	pos	2.04E-03	2.96E-03	1.13E-03	2.51E-03	2.11E-03
760.85	8.30	pos	1.10E-02	1.26E-02	1.08E-02	1.42E-02	1.36E-02
766.09	5.58	pos	1.79E-03	1.99E-03	2.97E-03	1.59E-03	1.89E-03
766.77	9.43	neg	5.90E-02	5.36E-02	5.11E-02	5.87E-02	6.25E-02
768.79	9.52	pos	1.69E-02	1.92E-02	1.34E-02	2.10E-02	2.16E-02
770.87	8.27	pos	2.11E-02	1.92E-02	4.46E-02	1.85E-02	2.45E-02
774.85	8.30	pos	7.53E-03	8.06E-03	8.76E-03	8.57E-03	8.24E-03

782.77	9.40	neg	6.89E-03	4.89E-03	1.30E-02	6.60E-03	7.69E-03
784.87	8.28	pos	7.36E-03	7.98E-03	1.50E-02	8.04E-03	8.92E-03
792.87	8.27	neg	8.06E-03	7.50E-03	1.91E-02	5.79E-03	1.02E-02
801.88	9.36	pos	8.74E-03	8.02E-03	5.46E-02	8.39E-03	1.44E-02
804.48	6.33	pos	1.10E-02	1.47E-02	1.40E-02	1.04E-02	9.27E-03
804.78	9.37	neg	9.81E-03	8.42E-03	2.63E-02	8.51E-03	1.08E-02
806.83	9.38	pos	1.64E-02	1.54E-02	4.66E-02	1.75E-02	2.60E-02
815.09	5.56	pos	1.25E-03	1.41E-03	1.24E-03	1.23E-03	1.59E-03
822.81	9.35	pos	7.93E-03	6.92E-03	1.88E-02	7.30E-03	1.10E-02
825.09	5.58	pos	1.87E-03	1.87E-03	2.55E-03	1.74E-03	1.99E-03
825.29	4.65	pos	1.36E-03	1.43E-03	1.54E-03	1.06E-03	1.05E-03
826.78	9.38	neg	9.35E-03	3.36E-03	1.50E-02	5.93E-03	8.56E-03
828.81	9.41	pos	1.69E-02	1.68E-02	2.28E-02	1.99E-02	2.34E-02
828.83	8.29	pos	8.37E-03	8.72E-03	8.13E-03	9.16E-03	9.87E-03
842.76	9.38	neg	2.79E-03	3.07E-03	1.22E-02	2.48E-03	3.38E-03
844.79	9.41	pos	1.29E-02	1.36E-02	1.80E-02	1.55E-02	1.94E-02
852.86	8.27	pos	7.14E-03	6.67E-03	1.41E-02	7.74E-03	7.86E-03
860.86	8.26	neg	4.20E-03	3.37E-03	1.16E-02	3.00E-03	4.92E-03
866.77	9.49	pos	1.28E-02	1.42E-02	1.08E-02	1.35E-02	1.70E-02
875.32	4.64	pos	1.41E-03	1.54E-03	1.49E-03	1.61E-03	1.42E-03
876.60	5.58	pos	1.87E-03	1.53E-03	2.82E-03	1.33E-03	1.68E-03
877.30	5.59	pos	2.68E-03	2.06E-03	4.62E-03	2.00E-03	2.50E-03
878.10	5.59	pos	1.87E-03	1.53E-03	2.82E-03	1.33E-03	1.68E-03
883.58	5.62	pos	1.73E-03	1.44E-03	1.52E-03	1.30E-03	1.46E-03
891.44	6.68	pos	3.57E-03	3.91E-03	2.71E-03	3.58E-03	2.99E-03
899.86	9.34	pos	5.88E-03	4.95E-03	3.79E-02	5.95E-03	9.20E-03
902.77	9.30	neg	6.92E-02	8.12E-02	5.84E-02	9.57E-02	7.78E-02
904.80	9.37	pos	1.06E-02	1.01E-02	3.07E-02	1.14E-02	1.64E-02
906.85	8.26	pos	6.14E-03	6.57E-03	1.79E-02	6.20E-03	7.92E-03
913.42	6.69	pos	3.68E-03	3.48E-03	2.45E-03	2.75E-03	2.55E-03
922.82	8.27	pos	5.06E-03	6.08E-03	6.75E-03	5.57E-03	6.50E-03
926.79	9.39	pos	1.14E-02	1.08E-02	1.72E-02	1.32E-02	1.59E-02
942.77	9.40	pos	9.44E-03	9.48E-03	1.31E-02	1.13E-02	1.27E-02
953.62	5.58	pos	8.59E-04	6.74E-04	1.40E-03	7.89E-04	9.49E-04
974.83	8.25	pos	3.63E-03	4.21E-03	1.03E-02	4.12E-03	4.93E-03
991.41	4.64	pos	1.99E-03	3.02E-03	1.01E-03	2.22E-03	1.81E-03
997.43	4.65	pos	1.81E-03	2.29E-03	2.13E-03	1.38E-03	1.45E-03
997.84	9.33	pos	3.34E-03	3.22E-03	2.64E-02	3.34E-03	6.19E-03
1002.78	9.36	pos	6.69E-03	4.66E-03	1.74E-02	3.31E-03	1.07E-02

Look up table for *S. meliloti* samples exposed to 1.4 mg/L PAH mixture

avg(mz)	avg(rt)	ionization mode	sample 1	sample 2	sample 3	sample 4	sample 5
78.97	9.38	neg	1.65E-02	1.38E-02	1.50E-02	2.31E-02	2.20E-02
87.98	5.58	neg	2.78E-03	2.38E-03	2.28E-03	3.17E-03	3.45E-03
90.99	8.29	pos	3.70E-02	3.18E-02	2.70E-02	3.09E-02	4.19E-02
100.05	7.07	neg	2.20E-02	2.12E-02	2.07E-02	1.93E-02	2.16E-02
100.12	4.66	pos	4.18E-02	2.67E-02	2.31E-02	1.79E-02	4.30E-02
101.08	2.05	pos	9.88E-03	8.55E-03	8.16E-03	3.65E-03	1.04E-02
102.06	8.65	neg	3.57E-02	3.97E-02	4.95E-02	3.36E-02	3.82E-02
102.07	7.12	pos	7.17E-02	6.58E-02	6.04E-02	5.44E-02	7.37E-02
104.12	7.04	pos	4.21E-02	4.00E-02	3.29E-02	2.93E-02	4.74E-02
105.00	8.26	pos	2.42E-02	1.89E-02	1.86E-02	3.44E-02	3.61E-02
106.10	7.63	pos	3.70E-02	4.40E-02	1.56E-02	2.33E-02	3.71E-02
107.08	7.08	pos	4.33E-01	3.90E-01	3.26E-01	3.54E-01	4.17E-01
110.02	12.93	pos	1.46E-02	1.38E-02	1.22E-02	1.46E-02	1.87E-02
114.91	7.77	pos	3.04E-02	3.11E-02	2.00E-02	2.29E-02	2.68E-02
116.08	7.60	pos	2.09E-02	2.00E-02	2.01E-02	1.90E-02	2.34E-02
117.02	1.45	neg	1.39E-02	1.53E-02	1.95E-02	1.22E-02	2.25E-02
118.10	7.52	pos	5.63E-01	5.11E-01	3.40E-01	3.57E-01	5.51E-01
119.08	2.04	pos	3.32E-02	2.55E-02	2.81E-02	6.87E-03	3.51E-02
120.09	4.65	pos	6.63E-02	6.94E-02	6.29E-02	5.95E-02	7.08E-02
120.09	4.65	pos	6.63E-02	6.94E-02	6.29E-02	5.95E-02	7.08E-02
120.09	7.40	pos	4.33E-02	4.18E-02	2.98E-02	3.39E-02	4.13E-02
121.06	0.86	pos	4.34E-03	1.42E-02	1.61E-02	1.13E-02	9.88E-03
122.90	1.24	neg	2.92E-03	3.76E-03	3.55E-04	2.21E-04	2.79E-03
122.94	7.96	pos	1.29E-01	1.24E-01	1.19E-01	1.18E-01	1.51E-01
124.99	1.25	neg	5.57E-03	6.80E-03	1.16E-02	5.99E-03	5.48E-03
125.95	5.57	neg	3.29E-03	3.29E-03	2.33E-03	4.54E-03	4.71E-03
128.03	12.92	pos	1.38E-02	1.12E-02	1.01E-02	1.62E-02	1.52E-02
128.04	7.86	neg	4.43E-02	5.28E-02	6.42E-02	4.20E-02	5.07E-02
128.04	8.65	neg	2.46E-02	2.73E-02	3.34E-02	2.40E-02	2.80E-02
128.14	6.39	pos	3.20E-01	2.77E-01	2.42E-01	2.54E-01	2.97E-01
128.97	7.94	neg	3.78E-01	4.74E-01	4.22E-01	4.34E-01	4.11E-01
130.06	1.37	neg	1.60E-03	1.95E-03	1.68E-03	1.23E-03	2.35E-03
130.09	6.56	neg	1.61E-02	3.11E-02	5.03E-02	1.24E-02	3.31E-02
132.07	7.42	neg	2.92E-02	3.75E-02	6.36E-02	1.70E-02	4.42E-02
134.05	1.71	neg	2.83E-02	2.89E-02	3.55E-02	3.55E-02	3.43E-02
134.09	7.37	pos	2.47E-01	2.86E-01	3.76E-01	1.61E-01	3.77E-01
136.06	7.08	pos	3.86E-01	3.74E-01	3.08E-01	3.46E-01	3.69E-01
136.08	1.71	pos	8.40E-02	8.05E-02	9.58E-02	1.01E-01	9.88E-02
137.09	2.04	pos	1.20E-01	1.08E-01	1.13E-01	3.23E-02	1.33E-01
139.88	1.26	neg	5.15E-03	5.37E-03	3.13E-04	3.32E-04	5.33E-03
140.99	5.58	neg	1.59E-02	1.70E-02	1.53E-02	2.01E-02	1.96E-02
141.88	1.26	neg	7.71E-02	8.50E-02	3.95E-03	3.16E-03	7.26E-02
142.98	5.57	neg	1.54E-02	1.61E-02	1.35E-02	1.94E-02	1.95E-02
143.87	1.26	neg	5.06E-02	5.22E-02	2.21E-03	2.04E-03	4.47E-02
144.18	2.31	pos	8.12E-03	6.91E-03	2.45E-03	4.35E-03	9.43E-03
145.06	6.96	pos	1.38E-01	1.04E-01	7.46E-02	1.67E-01	1.73E-01
145.07	8.51	neg	1.41E-02	1.70E-02	2.00E-02	1.29E-02	1.59E-02
146.05	8.65	neg	2.85E-01	3.70E-01	5.21E-01	3.31E-01	3.19E-01

149.05	6.98	neg	1.27E-01	1.02E-01	1.02E-01	1.86E-01	1.63E-01
155.09	7.07	pos	1.87E-01	1.69E-01	1.46E-01	1.81E-01	1.87E-01
157.12	6.39	pos	2.54E-02	2.42E-02	2.22E-02	2.17E-02	2.70E-02
158.98	8.31	pos	9.49E-02	9.25E-02	7.81E-02	8.46E-02	9.74E-02
158.99	12.92	neg	5.14E-02	4.88E-02	4.46E-02	6.56E-02	6.12E-02
159.08	2.05	pos	1.20E-02	1.22E-02	1.24E-02	3.30E-03	1.36E-02
162.05	3.07	neg	8.89E-03	8.10E-03	1.05E-02	7.85E-03	1.26E-02
164.13	6.74	pos	7.13E-02	6.98E-02	3.28E-02	3.46E-02	6.91E-02
168.04	8.67	neg	4.43E-02	5.84E-02	5.35E-02	4.62E-02	4.93E-02
170.06	8.65	pos	6.26E-02	7.59E-02	9.40E-02	4.85E-02	6.63E-02
171.05	2.05	neg	4.76E-02	4.56E-02	7.96E-02	2.34E-02	5.45E-02
171.12	6.40	neg	1.22E-01	1.14E-01	1.17E-01	1.21E-01	1.21E-01
173.05	2.05	neg	1.70E-02	1.47E-02	2.74E-02	8.21E-03	1.79E-02
173.14	6.39	pos	1.26E-01	1.15E-01	1.17E-01	1.16E-01	1.17E-01
175.08	7.08	pos	6.48E-02	6.89E-02	5.28E-02	4.18E-02	5.17E-02
175.13	10.29	pos	6.33E-02	6.56E-02	6.65E-02	4.81E-02	7.26E-02
176.94	9.39	neg	7.96E-02	6.51E-02	7.70E-02	1.21E-01	1.07E-01
177.05	2.79	neg	9.02E-03	1.28E-02	1.99E-02	2.07E-02	1.08E-02
183.04	1.25	neg	4.73E-03	5.55E-03	7.85E-03	4.41E-03	4.63E-03
186.03	8.65	pos	3.40E-02	4.30E-02	6.31E-02	2.63E-02	3.43E-02
187.87	1.26	neg	3.60E-02	4.09E-02	1.84E-03	1.88E-03	3.24E-02
188.19	11.52	pos	3.92E-02	2.67E-02	4.46E-02	4.88E-02	7.27E-02
189.87	1.26	neg	2.36E-02	2.59E-02	7.67E-03	5.41E-03	2.05E-02
191.10	6.70	pos	1.51E-01	1.50E-01	1.18E-01	1.16E-01	1.31E-01
191.87	1.26	neg	5.53E-03	6.33E-03	7.52E-04	8.20E-04	4.63E-03
192.04	8.67	pos	1.11E-01	1.20E-01	1.15E-01	8.04E-02	1.20E-01
192.11	6.71	pos	5.94E-01	5.92E-01	4.97E-01	4.99E-01	5.74E-01
192.17	5.40	pos	3.56E-01	1.10E-01	1.25E-01	3.40E-02	3.27E-01
193.12	6.70	pos	3.64E-01	3.40E-01	2.88E-01	2.91E-01	3.49E-01
193.99	5.57	neg	2.01E-02	2.03E-02	1.72E-02	2.38E-02	2.32E-02
195.98	5.57	neg	2.37E-02	2.47E-02	1.98E-02	2.78E-02	2.84E-02
196.96	7.98	neg	8.67E-02	1.17E-01	8.52E-02	7.79E-02	9.02E-02
197.98	5.58	neg	1.19E-02	1.19E-02	1.01E-02	1.35E-02	1.40E-02
198.11	6.93	pos	5.26E-01	4.29E-01	3.09E-01	8.27E-01	7.03E-01
199.05	7.63	neg	1.16E-01	7.15E-02	6.55E-02	1.47E-02	1.09E-01
203.07	7.10	pos	1.17E+00	1.11E+00	8.22E-01	9.74E-01	1.17E+00
205.08	7.39	pos	1.63E-01	1.18E-01	9.32E-02	1.40E-02	1.36E-01
206.80	5.92	neg	9.03E-02	7.61E-02	2.33E-02	1.90E-02	6.34E-02
206.90	7.94	pos	2.13E-02	1.91E-02	1.59E-02	2.63E-02	2.65E-02
207.12	6.70	neg	2.70E-01	2.70E-01	2.54E-01	2.50E-01	2.77E-01
208.01	8.69	pos	4.06E-02	4.30E-02	4.20E-02	2.72E-02	4.14E-02
208.90	7.93	pos	5.50E-03	4.97E-03	4.55E-03	6.20E-03	6.79E-03
209.14	6.71	pos	1.98E-01	1.89E-01	1.65E-01	1.76E-01	2.04E-01
212.13	6.65	pos	8.69E-02	8.42E-02	7.84E-02	6.47E-02	8.59E-02
212.14	2.68	pos	6.33E-03	5.74E-03	6.00E-03	9.56E-03	7.26E-03
212.93	7.94	neg	5.78E-02	6.98E-02	6.83E-02	7.15E-02	6.77E-02
213.03	7.10	pos	1.83E-02	2.10E-02	1.71E-02	1.18E-02	1.29E-02
213.09	0.86	neg	4.76E-03	3.58E-03	4.20E-03	4.43E-03	3.36E-03
214.01	8.94	pos	5.76E-02	5.80E-02	4.44E-02	9.55E-02	5.94E-02
214.05	8.75	neg	2.52E-02	2.48E-02	3.10E-02	2.02E-02	2.38E-02
214.14	0.98	neg	1.63E-02	1.55E-02	3.01E-02	2.92E-02	1.84E-02
214.33	6.99	neg	4.55E-02	3.84E-02	4.15E-02	6.29E-02	5.51E-02

214.89	1.24	neg	4.92E-03	6.42E-03	3.67E-04	3.52E-04	4.17E-03
219.04	7.06	pos	1.40E+00	1.33E+00	9.85E-01	1.25E+00	1.39E+00
219.05	7.14	neg	1.86E-01	1.74E-01	1.75E-01	1.18E-01	2.07E-01
221.04	7.07	pos	1.45E-01	1.30E-01	9.17E-02	1.08E-01	1.36E-01
224.11	7.34	neg	9.31E-03	1.06E-02	1.11E-02	1.15E-02	1.19E-02
226.00	8.70	neg	2.37E-02	2.68E-02	2.66E-02	2.23E-02	2.25E-02
226.14	7.29	pos	4.26E-02	3.57E-02	7.99E-03	1.04E-02	4.00E-02
226.97	8.30	pos	3.22E-01	3.09E-01	2.75E-01	2.90E-01	3.63E-01
228.06	8.60	neg	1.87E-02	1.92E-02	2.14E-02	1.43E-02	1.69E-02
229.06	2.67	neg	3.34E-03	2.99E-03	5.23E-03	7.30E-03	3.76E-03
230.03	8.66	pos	4.22E-02	4.33E-02	3.67E-02	2.78E-02	4.20E-02
231.02	9.94	pos	9.97E-03	7.85E-03	5.54E-03	1.00E-02	1.19E-02
231.12	6.71	pos	1.72E-02	1.75E-02	1.33E-02	1.35E-02	1.61E-02
232.13	6.72	pos	1.71E-01	1.72E-01	1.38E-01	1.28E-01	1.53E-01
233.09	7.96	pos	5.94E-02	5.76E-02	4.72E-02	4.32E-02	6.33E-02
234.93	9.44	pos	4.03E-02	3.52E-02	3.37E-02	3.87E-02	5.11E-02
235.14	7.05	pos	1.28E-02	9.54E-03	1.16E-02	2.20E-02	1.91E-02
235.97	9.95	pos	2.12E-02	1.84E-02	1.73E-02	1.95E-02	2.28E-02
238.05	2.02	neg	4.60E-03	4.25E-03	6.70E-03	4.53E-03	5.22E-03
238.06	8.76	pos	7.38E-03	8.10E-03	8.58E-03	5.14E-03	6.85E-03
239.05	2.03	neg	1.42E-02	1.18E-02	1.87E-02	6.72E-03	1.63E-02
241.97	8.70	neg	1.22E-02	1.45E-02	1.55E-02	1.11E-02	1.12E-02
242.61	8.30	pos	1.14E-01	1.08E-01	8.42E-02	6.85E-02	1.12E-01
242.99	7.06	pos	1.74E-02	1.72E-02	1.79E-02	1.15E-02	1.73E-02
243.07	2.47	neg	3.09E-02	2.89E-02	3.64E-02	2.54E-02	3.77E-02
243.09	1.02	neg	1.07E-02	8.04E-03	7.27E-03	1.44E-02	1.78E-02
243.90	1.24	neg	7.83E-03	1.06E-02	1.50E-03	8.52E-04	6.72E-03
244.11	8.63	pos	1.34E-02	1.10E-02	1.50E-02	7.52E-03	1.16E-02
245.10	7.40	pos	1.26E-01	1.18E-01	8.31E-02	9.18E-02	1.11E-01
245.12	1.00	pos	1.89E-02	1.57E-02	1.50E-02	3.35E-02	2.90E-02
245.90	1.24	neg	3.48E-03	4.79E-03	6.93E-04	7.23E-04	3.32E-03
245.97	8.73	pos	9.84E-03	9.87E-03	9.63E-03	6.29E-03	9.86E-03
246.99	5.57	neg	8.41E-03	8.25E-03	6.23E-03	9.86E-03	1.06E-02
247.09	6.70	pos	2.17E-02	2.07E-02	1.79E-02	1.62E-02	1.86E-02
247.92	1.23	neg	1.32E-03	1.94E-03	2.30E-03	1.01E-03	1.50E-03
248.04	9.94	pos	9.17E-03	8.65E-03	6.58E-03	9.53E-03	1.03E-02
248.10	6.71	pos	2.41E-01	2.51E-01	2.12E-01	1.94E-01	2.04E-01
248.89	8.06	pos	1.13E-02	1.22E-02	8.76E-03	6.94E-03	9.38E-03
250.00	8.70	pos	1.00E-02	9.11E-03	8.00E-03	6.67E-03	8.91E-03
250.99	5.57	neg	8.53E-03	9.49E-03	7.24E-03	1.05E-02	1.20E-02
251.94	9.95	pos	6.83E-03	5.78E-03	5.28E-03	7.13E-03	9.43E-03
252.00	8.70	neg	2.34E-02	2.82E-02	2.56E-02	2.44E-02	2.28E-02
252.13	1.23	pos	4.30E-03	5.33E-03	5.39E-03	4.50E-03	4.20E-03
252.99	9.96	pos	1.19E-02	1.19E-02	1.07E-02	1.25E-02	1.44E-02
254.11	6.71	pos	1.03E-02	1.20E-02	1.09E-02	8.63E-03	8.47E-03
254.92	9.42	neg	6.86E-02	6.08E-02	6.40E-02	5.53E-02	6.26E-02
256.91	9.67	pos	8.82E-02	8.95E-02	6.99E-02	4.98E-02	7.49E-02
257.08	1.88	neg	2.13E-03	2.14E-03	2.18E-03	2.07E-03	2.45E-03
258.12	9.20	pos	6.90E-01	4.76E-01	7.03E-01	5.55E-01	7.92E-01
258.91	8.11	pos	3.24E-02	3.28E-02	2.36E-02	1.62E-02	2.89E-02
259.03	9.21	neg	5.87E-02	6.43E-02	7.82E-02	4.06E-02	6.16E-02
260.12	9.21	pos	1.35E-02	1.78E-02	1.48E-02	1.05E-02	1.59E-02

261.08	7.40	pos	1.48E-01	1.40E-01	9.81E-02	1.06E-01	1.31E-01
262.11	5.36	neg	4.19E-03	9.12E-04	2.54E-03	7.98E-04	2.37E-03
263.07	7.40	pos	1.49E-02	1.37E-02	9.57E-03	1.12E-02	1.21E-02
263.81	1.28	neg	1.11E-03	1.32E-03	1.69E-03	1.38E-04	1.06E-03
264.86	8.00	pos	2.67E-02	2.54E-02	1.92E-02	1.63E-02	2.38E-02
264.94	8.07	neg	7.72E-02	9.40E-02	6.59E-02	5.11E-02	6.42E-02
266.08	6.71	neg	5.98E-02	7.49E-02	8.53E-02	7.88E-02	5.52E-02
266.11	1.95	neg	1.07E-02	1.10E-02	9.73E-03	6.56E-03	1.41E-02
266.86	8.00	pos	1.35E-02	1.43E-02	1.15E-02	8.61E-03	1.23E-02
268.12	1.96	pos	2.40E-01	2.50E-01	2.88E-01	2.35E-01	3.02E-01
270.08	6.73	pos	2.32E-02	2.43E-02	2.23E-02	1.77E-02	2.01E-02
270.99	8.36	pos	1.53E-02	8.37E-03	1.13E-02	7.37E-03	6.46E-03
271.98	8.70	pos	2.37E-02	2.22E-02	1.61E-02	1.56E-02	2.25E-02
273.92	9.97	pos	1.38E-02	1.14E-02	1.22E-02	7.96E-03	1.39E-02
274.10	2.09	neg	1.05E-02	1.26E-02	3.44E-02	1.55E-02	1.54E-02
274.89	7.98	pos	4.18E-02	4.53E-02	4.24E-02	4.12E-02	4.99E-02
275.06	2.06	neg	8.81E-03	7.02E-03	1.10E-02	3.95E-03	9.56E-03
276.13	2.08	pos	7.93E-03	8.83E-03	1.40E-02	7.31E-03	1.11E-02
279.03	2.02	pos	3.03E-03	2.60E-03	2.64E-03	8.37E-04	3.59E-03
279.06	7.42	neg	6.41E-02	6.74E-02	5.50E-02	3.93E-02	4.64E-02
280.11	9.14	pos	4.59E-02	3.82E-02	3.75E-02	7.82E-03	2.50E-02
280.57	7.11	pos	8.76E-03	8.99E-03	8.03E-03	4.41E-03	8.51E-03
280.83	7.95	pos	1.12E-02	1.10E-02	1.17E-02	1.25E-02	1.28E-02
280.92	7.97	neg	8.24E-02	1.09E-01	8.95E-02	7.90E-02	8.53E-02
282.02	8.64	pos	1.74E-02	1.68E-02	1.16E-02	1.36E-02	1.94E-02
282.13	6.35	pos	8.70E-03	8.01E-03	9.37E-03	6.36E-03	8.10E-03
282.83	7.94	pos	5.33E-03	4.88E-03	3.57E-03	4.09E-03	6.00E-03
283.06	7.44	pos	2.18E-02	2.08E-02	1.45E-02	1.45E-02	1.84E-02
287.95	8.75	pos	1.92E-02	2.00E-02	1.48E-02	1.34E-02	1.91E-02
288.13	6.67	pos	6.71E-03	5.43E-03	6.93E-03	8.45E-03	6.54E-03
289.07	9.05	neg	1.27E-02	1.21E-02	2.04E-02	1.05E-02	1.60E-02
290.86	7.93	pos	3.27E-02	3.05E-02	2.66E-02	4.37E-02	4.40E-02
291.13	8.92	pos	5.62E-03	5.94E-03	1.11E-02	3.04E-03	8.42E-03
292.09	6.72	neg	3.76E-02	4.66E-02	4.56E-02	4.01E-02	3.99E-02
292.86	7.93	pos	1.05E-02	9.96E-03	8.25E-03	1.24E-02	1.36E-02
293.98	8.70	neg	1.47E-02	1.61E-02	1.30E-02	1.40E-02	1.45E-02
294.95	9.37	pos	3.73E-02	3.65E-02	3.40E-02	5.20E-02	5.87E-02
294.95	8.31	pos	3.86E-02	4.26E-02	3.54E-02	3.92E-02	3.93E-02
296.08	9.13	pos	3.20E-02	2.67E-02	2.57E-02	4.00E-03	1.78E-02
296.89	7.94	neg	6.71E-02	9.93E-02	9.37E-02	1.08E-01	9.49E-02
297.98	8.67	pos	1.43E-02	1.22E-02	9.52E-03	8.87E-03	1.44E-02
298.00	6.39	neg	4.96E-02	5.53E-02	2.32E-02	2.53E-02	4.98E-02
298.12	0.81	pos	8.77E-03	9.53E-03	5.24E-03	5.24E-03	7.98E-03
298.89	7.94	neg	1.93E-02	2.39E-02	2.53E-02	2.49E-02	2.21E-02
299.03	7.43	pos	1.61E-02	1.45E-02	1.09E-02	1.02E-02	1.42E-02
299.17	0.61	pos	9.27E-02	9.43E-02	1.11E-01	4.85E-03	1.48E-01
300.00	5.79	neg	8.10E-02	8.35E-02	8.35E-02	1.31E-01	1.20E-01
301.99	5.58	neg	1.61E-02	1.80E-02	1.33E-02	2.22E-02	2.37E-02
302.04	6.70	pos	6.64E-03	6.92E-03	3.86E-03	5.85E-03	6.40E-03
304.01	8.66	neg	3.12E-02	3.62E-02	3.20E-02	3.42E-02	3.25E-02
304.11	6.69	neg	3.15E-02	3.95E-02	5.03E-02	4.54E-02	3.08E-02
305.01	9.03	pos	7.73E-03	7.24E-03	9.22E-03	3.63E-03	6.84E-03

305.99	5.58	neg	5.65E-03	5.96E-03	4.34E-03	7.55E-03	8.06E-03
306.09	8.64	neg	2.81E-02	3.14E-02	4.44E-02	2.83E-02	2.79E-02
306.13	4.73	neg	4.84E-03	4.78E-03	9.94E-03	1.18E-02	5.79E-03
307.04	7.02	pos	8.35E-03	9.76E-03	7.95E-03	8.40E-03	6.77E-03
307.98	5.58	neg	1.50E-03	1.46E-03	1.13E-03	1.81E-03	2.05E-03
308.11	8.64	pos	2.53E-02	2.84E-02	3.76E-02	1.97E-02	2.59E-02
308.93	8.38	neg	1.45E-02	1.60E-02	1.23E-02	1.30E-02	1.37E-02
309.04	7.33	neg	2.16E-02	2.38E-02	1.92E-02	3.26E-02	2.45E-02
309.96	8.74	neg	9.13E-03	1.09E-02	1.10E-02	9.49E-03	1.18E-02
310.10	4.66	neg	4.07E-03	3.99E-03	4.36E-03	4.32E-03	4.10E-03
310.23	6.66	pos	2.12E-02	1.06E-02	7.72E-03	3.51E-03	1.84E-02
310.57	5.58	pos	1.17E-03	1.20E-03	1.30E-03	1.74E-03	1.47E-03
310.93	8.31	pos	1.38E-02	1.43E-02	1.01E-02	9.37E-03	1.33E-02
314.91	9.42	neg	1.97E-01	1.90E-01	2.02E-01	2.80E-01	2.58E-01
315.09	8.64	neg	2.02E-02	2.94E-02	4.28E-02	2.42E-02	2.47E-02
316.18	6.35	pos	4.29E-01	4.34E-01	5.10E-01	2.45E-01	4.90E-01
316.93	9.42	pos	5.48E-02	4.37E-02	3.91E-02	5.40E-02	6.60E-02
316.96	8.31	neg	2.29E-01	2.60E-01	2.22E-01	2.61E-01	2.53E-01
318.05	6.58	neg	2.68E-02	2.86E-02	3.40E-02	3.17E-02	2.75E-02
319.99	8.70	neg	1.87E-02	2.23E-02	1.85E-02	1.82E-02	1.58E-02
320.03	6.68	neg	9.89E-03	1.48E-02	2.12E-02	1.86E-02	1.22E-02
320.99	9.04	pos	7.15E-03	7.47E-03	7.73E-03	3.13E-03	6.36E-03
322.06	6.48	pos	5.88E-03	6.19E-03	6.19E-03	6.51E-03	6.26E-03
323.41	6.96	pos	1.08E-02	9.68E-03	9.68E-03	8.22E-03	7.69E-03
325.05	7.08	neg	5.56E-02	6.63E-02	8.90E-02	6.65E-02	5.22E-02
325.99	6.92	pos	1.14E-02	9.62E-03	6.90E-03	6.41E-03	1.09E-02
327.49	5.58	neg	1.67E-03	1.66E-03	1.52E-03	2.45E-03	2.25E-03
328.49	5.58	neg	3.39E-03	2.99E-03	2.90E-03	4.78E-03	4.35E-03
330.02	5.58	neg	4.99E-02	5.19E-02	4.71E-02	4.39E-02	5.38E-02
330.09	8.65	pos	1.61E-02	1.63E-02	2.29E-02	1.08E-02	1.42E-02
331.14	7.06	neg	3.80E-01	3.60E-01	4.10E-01	6.43E-01	4.77E-01
333.12	0.65	neg	4.02E-02	3.04E-02	1.17E-01	8.70E-03	6.82E-02
333.16	7.03	pos	5.80E-02	5.08E-02	3.31E-02	7.25E-02	6.90E-02
333.95	9.93	pos	1.23E-02	9.23E-03	8.21E-03	1.07E-02	1.45E-02
334.00	6.70	neg	6.77E-02	7.61E-02	2.80E-02	3.29E-02	6.20E-02
334.89	9.37	neg	1.85E-02	1.16E-02	1.68E-02	3.07E-02	2.62E-02
335.15	4.68	pos	5.37E-02	6.29E-02	5.25E-02	3.71E-02	5.31E-02
335.99	6.69	neg	4.41E-02	5.51E-02	2.12E-02	2.15E-02	4.35E-02
336.07	5.58	pos	2.50E-03	2.95E-03	2.94E-03	3.81E-03	2.96E-03
338.11	6.67	neg	1.72E-02	2.26E-02	3.31E-02	2.63E-02	1.64E-02
338.16	6.38	pos	1.61E-01	1.81E-01	2.53E-01	1.42E-01	1.86E-01
339.07	5.58	pos	4.30E-03	4.99E-03	5.58E-03	7.15E-03	6.49E-03
339.09	8.64	pos	1.68E-02	2.05E-02	2.74E-02	1.39E-02	1.88E-02
340.07	6.67	neg	1.28E-02	1.78E-02	2.41E-02	2.05E-02	1.21E-02
341.06	5.58	pos	1.86E-03	1.94E-03	2.01E-03	2.76E-03	2.37E-03
343.31	5.39	pos	5.95E-04	1.43E-03	1.83E-03	1.37E-03	1.28E-03
346.07	8.41	neg	1.29E-02	1.28E-02	1.77E-02	1.12E-02	1.45E-02
346.29	4.66	pos	1.95E-02	1.66E-02	1.46E-02	1.38E-02	2.11E-02
347.28	6.38	pos	9.56E-03	8.16E-03	6.10E-03	5.32E-03	9.54E-03
348.09	8.43	pos	1.01E-02	1.02E-02	1.30E-02	3.03E-03	1.09E-02
348.90	8.04	neg	3.87E-02	4.77E-02	3.73E-02	2.99E-02	3.85E-02
350.97	9.94	pos	8.09E-03	7.34E-03	5.54E-03	7.44E-03	9.07E-03

351.13	4.67	pos	8.55E-02	9.67E-02	8.57E-02	5.91E-02	8.36E-02
352.91	8.35	pos	1.99E-02	2.04E-02	1.59E-02	1.36E-02	1.76E-02
353.00	5.58	neg	3.17E-03	3.47E-03	2.73E-03	5.38E-03	4.83E-03
354.00	5.57	neg	2.03E-03	1.80E-03	1.75E-03	2.44E-03	2.04E-03
354.13	6.38	pos	2.45E-01	2.62E-01	3.75E-01	1.92E-01	2.69E-01
354.85	7.98	neg	1.40E-02	2.21E-02	8.02E-04	1.34E-03	1.38E-02
354.89	9.57	pos	6.05E-02	5.02E-02	4.45E-02	3.50E-02	5.29E-02
355.00	5.58	neg	9.57E-03	9.45E-03	8.03E-03	1.45E-02	1.37E-02
356.14	6.36	pos	4.58E-03	9.01E-03	2.85E-02	4.88E-03	9.76E-03
356.98	7.46	pos	5.08E-03	3.96E-03	3.56E-03	3.43E-03	2.85E-03
356.99	5.58	neg	9.20E-03	8.95E-03	7.82E-03	1.38E-02	1.32E-02
357.01	9.33	neg	3.04E-02	2.76E-02	4.08E-02	2.27E-02	3.17E-02
359.07	7.04	pos	1.61E-02	1.56E-02	1.79E-02	1.21E-02	1.66E-02
359.13	7.31	neg	8.65E-02	7.25E-02	7.42E-02	2.26E-01	1.68E-01
360.16	6.36	neg	4.52E-02	5.01E-02	8.03E-02	4.43E-02	5.48E-02
361.08	8.64	pos	2.91E-02	3.32E-02	3.47E-02	2.34E-02	3.01E-02
361.08	7.05	pos	1.04E-02	9.71E-03	3.60E-03	3.09E-03	1.09E-02
361.24	6.36	pos	7.55E-02	7.34E-02	1.02E-02	5.62E-03	7.46E-02
362.22	6.98	pos	8.51E-03	1.53E-02	5.02E-03	5.03E-03	8.65E-03
362.94	8.29	pos	6.89E-02	7.16E-02	6.19E-02	7.58E-02	8.32E-02
363.74	5.59	pos	2.08E-03	2.26E-03	2.15E-03	3.14E-03	2.70E-03
364.88	7.97	neg	5.14E-02	6.31E-02	5.82E-02	5.64E-02	5.37E-02
365.73	5.58	pos	3.96E-03	4.58E-03	5.10E-03	6.76E-03	5.76E-03
367.56	5.58	pos	2.11E-03	2.25E-03	2.57E-03	3.13E-03	2.52E-03
369.11	4.67	neg	3.23E-02	3.24E-02	3.17E-02	3.13E-02	3.21E-02
371.11	7.09	pos	3.29E-02	3.41E-02	2.63E-02	1.86E-02	2.57E-02
372.00	8.65	neg	1.68E-02	1.81E-02	1.55E-02	1.63E-02	1.98E-02
373.11	4.78	pos	7.22E-03	8.29E-03	7.24E-03	3.90E-03	6.80E-03
374.06	8.66	pos	7.75E-03	8.11E-03	8.71E-03	5.01E-03	7.38E-03
374.14	4.65	neg	3.35E-03	2.47E-03	2.45E-03	2.82E-03	3.21E-03
374.83	7.93	pos	3.09E-03	2.65E-03	2.20E-03	3.54E-03	3.84E-03
375.20	7.38	pos	7.10E-03	4.64E-03	3.76E-03	5.36E-03	6.55E-03
377.03	8.65	pos	2.48E-02	1.65E-02	1.90E-02	2.01E-02	2.79E-02
377.12	7.09	pos	1.04E-02	1.15E-02	9.60E-03	1.09E-02	9.15E-03
377.15	6.36	neg	2.94E-02	3.35E-02	6.61E-02	7.66E-02	3.26E-02
378.18	7.30	pos	1.43E-02	1.12E-02	8.07E-03	3.78E-02	2.86E-02
378.92	8.30	pos	2.81E-02	2.57E-02	2.02E-02	1.98E-02	2.86E-02
380.85	7.94	neg	4.04E-02	5.50E-02	5.48E-02	6.78E-02	5.69E-02
381.07	7.06	pos	8.79E-03	7.43E-03	9.71E-03	5.00E-03	6.48E-03
381.50	5.58	neg	1.91E-03	1.88E-03	1.80E-03	3.08E-03	2.48E-03
382.09	6.75	neg	2.30E-02	2.67E-02	4.57E-02	4.59E-02	2.26E-02
382.24	1.70	pos	2.01E-03	2.43E-03	2.45E-03	3.58E-03	2.38E-03
382.85	7.93	neg	1.55E-02	1.79E-02	1.85E-02	2.10E-02	1.85E-02
383.13	7.00	pos	6.09E-01	5.90E-01	4.05E-01	5.80E-01	6.23E-01
383.18	5.60	neg	2.93E-02	3.47E-02	3.27E-02	2.15E-02	2.50E-02
383.69	5.58	neg	2.58E-02	2.06E-02	3.35E-02	4.80E-02	3.73E-02
384.49	5.58	neg	1.89E-03	1.60E-03	1.73E-03	2.72E-03	2.23E-03
384.95	8.31	neg	1.02E-01	1.22E-01	9.85E-02	1.30E-01	1.19E-01
385.08	4.67	neg	3.07E-02	2.88E-02	2.80E-02	2.82E-02	2.87E-02
385.14	7.29	pos	3.87E-02	3.56E-02	2.40E-02	2.16E-02	3.85E-02
387.07	7.06	pos	1.07E-02	1.02E-02	6.95E-03	5.00E-03	1.04E-02
387.98	8.68	neg	1.29E-02	1.49E-02	1.32E-02	1.18E-02	1.31E-02



388.19	6.88	neg	1.29E-01	6.54E-02	7.54E-02	1.37E-01	1.72E-01
389.01	7.03	neg	6.24E-02	6.61E-02	6.56E-02	5.15E-02	5.72E-02
390.21	6.84	pos	4.78E-02	2.74E-02	1.94E-02	4.53E-02	5.39E-02
391.07	5.59	pos	3.99E-03	4.16E-03	4.44E-03	5.74E-03	4.72E-03
391.17	6.93	pos	1.26E-02	8.87E-03	8.86E-03	1.65E-02	1.48E-02
392.91	9.34	neg	1.10E-02	5.71E-03	1.01E-02	3.35E-02	2.35E-02
392.92	9.39	pos	3.21E-02	3.07E-02	2.17E-02	4.47E-02	5.35E-02
393.03	7.06	neg	4.12E-02	4.68E-02	2.33E-02	1.99E-02	4.57E-02
393.07	5.59	pos	3.76E-03	4.52E-03	4.62E-03	6.32E-03	5.12E-03
394.01	6.69	neg	2.35E-02	3.00E-02	1.34E-02	9.27E-03	2.26E-02
395.06	7.05	pos	9.18E-03	8.47E-03	9.49E-03	6.50E-03	8.03E-03
395.11	7.02	neg	6.56E-01	6.24E-01	6.19E-01	8.23E-01	8.15E-01
396.12	6.37	pos	6.61E-03	6.87E-03	9.95E-03	4.25E-03	6.04E-03
397.05	7.06	pos	1.11E-02	1.02E-02	1.09E-02	6.24E-03	9.51E-03
399.03	8.66	pos	1.84E-02	2.05E-02	2.02E-02	1.41E-02	1.87E-02
399.11	7.11	pos	1.79E-01	1.61E-01	1.14E-01	1.46E-01	1.72E-01
401.05	4.65	neg	4.36E-03	5.13E-03	6.11E-04	7.99E-04	4.07E-03
401.17	7.39	neg	1.22E-01	1.30E-01	1.33E-01	1.70E-01	1.32E-01
403.03	7.09	neg	9.87E-03	1.53E-02	2.07E-02	1.40E-02	1.36E-02
403.19	7.37	pos	1.39E-02	1.71E-02	1.28E-02	3.05E-02	1.80E-02
404.20	2.01	pos	2.75E-03	2.53E-03	2.83E-03	1.17E-03	3.35E-03
405.03	8.62	pos	1.36E-02	1.46E-02	1.26E-02	1.11E-02	1.59E-02
406.00	5.58	neg	2.75E-03	3.03E-03	2.27E-03	3.08E-03	3.11E-03
406.08	6.36	pos	7.97E-03	8.49E-03	9.57E-03	1.30E-02	7.27E-03
407.09	7.03	pos	1.07E-02	8.87E-03	9.44E-03	1.06E-02	9.61E-03
407.13	4.66	neg	3.33E-03	3.73E-03	3.71E-03	3.46E-03	3.56E-03
408.02	5.58	neg	5.97E-03	6.10E-03	5.34E-03	8.68E-03	8.02E-03
409.00	5.58	neg	3.69E-03	4.33E-03	2.82E-03	4.39E-03	4.28E-03
409.96	9.38	pos	4.42E-02	2.76E-02	3.33E-02	7.50E-02	7.98E-02
410.00	5.58	neg	6.52E-03	7.62E-03	6.18E-03	1.07E-02	9.90E-03
410.09	6.35	neg	1.00E-02	1.05E-02	2.05E-02	1.23E-02	7.76E-03
411.01	5.56	neg	2.93E-03	3.20E-03	2.70E-03	4.15E-03	3.32E-03
412.00	5.58	neg	4.13E-03	4.76E-03	3.52E-03	6.21E-03	5.95E-03
412.19	6.84	pos	3.48E-02	2.44E-02	1.66E-02	2.47E-02	3.24E-02
412.28	4.65	pos	3.27E-03	2.52E-03	1.94E-03	1.44E-03	2.92E-03
412.89	9.40	neg	1.24E-01	1.00E-01	1.22E-01	2.07E-01	1.89E-01
413.99	5.58	neg	1.69E-03	2.11E-03	1.45E-03	2.28E-03	2.35E-03
414.09	6.37	pos	3.36E-03	3.76E-03	5.15E-03	2.01E-03	3.90E-03
415.07	7.30	pos	8.17E-03	5.16E-03	5.48E-03	7.90E-03	1.03E-02
417.57	5.58	pos	4.24E-03	4.53E-03	4.97E-03	7.17E-03	5.43E-03
418.26	6.68	pos	2.88E-02	2.89E-02	2.48E-02	2.62E-02	2.99E-02
419.08	2.02	neg	1.61E-03	1.36E-03	1.81E-03	5.73E-04	2.12E-03
419.27	6.68	pos	1.74E-01	1.75E-01	1.47E-01	1.55E-01	1.70E-01
419.57	5.58	pos	5.54E-03	6.27E-03	7.26E-03	9.21E-03	7.17E-03
420.17	0.63	pos	1.58E-03	1.92E-03	2.42E-03	3.98E-04	2.37E-03
420.29	6.60	pos	7.59E-02	7.70E-02	9.35E-02	9.32E-02	7.57E-02
421.30	6.54	pos	1.93E-02	1.95E-02	2.36E-02	2.28E-02	1.98E-02
423.06	7.05	pos	1.03E-02	8.57E-03	9.27E-03	8.71E-03	1.14E-02
424.07	6.35	neg	7.28E-03	1.35E-02	2.61E-02	2.46E-02	2.03E-02
424.22	4.70	pos	1.41E-03	1.42E-03	1.66E-03	7.00E-04	8.96E-04
425.17	7.39	pos	3.40E-02	3.41E-02	2.27E-02	3.27E-02	3.20E-02
426.17	4.50	neg	2.08E-03	2.09E-03	2.55E-03	2.31E-03	1.94E-03

428.07	6.37	pos	3.59E-03	3.13E-03	4.57E-03	1.73E-03	2.75E-03
428.16	6.84	pos	1.67E-02	1.13E-02	9.04E-03	9.43E-03	1.49E-02
428.87	9.41	neg	6.70E-02	5.46E-02	6.04E-02	1.06E-01	8.82E-02
430.89	9.42	pos	3.32E-02	2.47E-02	2.32E-02	3.34E-02	4.42E-02
430.93	8.29	pos	7.18E-02	6.86E-02	6.24E-02	7.55E-02	8.68E-02
434.18	6.84	pos	5.56E-03	3.82E-03	3.27E-03	1.10E-02	5.03E-03
434.30	5.58	neg	8.55E-04	9.50E-04	7.80E-04	1.13E-03	1.00E-03
434.87	9.48	neg	6.98E-02	6.27E-02	6.92E-02	8.43E-02	7.82E-02
435.31	7.26	neg	8.62E-03	1.99E-02	2.51E-02	4.15E-02	1.65E-02
435.50	5.58	neg	2.13E-03	1.93E-03	1.84E-03	3.34E-03	2.76E-03
436.50	5.58	neg	2.00E-02	2.02E-02	2.88E-02	4.07E-02	2.94E-02
436.89	9.59	pos	6.00E-02	5.40E-02	4.48E-02	4.09E-02	5.91E-02
440.25	6.68	pos	7.82E-03	7.68E-03	6.97E-03	6.64E-03	6.37E-03
441.12	7.34	pos	2.41E-02	1.96E-02	1.70E-02	1.48E-02	2.36E-02
441.25	6.69	pos	4.05E-02	4.24E-02	4.03E-02	3.65E-02	3.52E-02
442.08	5.58	pos	2.14E-03	2.01E-03	2.05E-03	2.47E-03	2.52E-03
442.13	7.36	pos	3.94E-03	4.15E-03	2.99E-03	4.59E-03	4.31E-03
442.81	7.95	pos	7.12E-03	6.57E-03	7.15E-03	6.64E-03	8.26E-03
443.04	4.74	neg	7.74E-03	8.03E-03	7.99E-03	7.93E-03	7.74E-03
443.09	7.24	pos	9.17E-03	7.26E-03	5.89E-03	8.34E-03	8.15E-03
444.08	5.58	pos	7.43E-03	8.06E-03	7.78E-03	1.05E-02	8.84E-03
444.94	8.28	pos	1.55E-02	1.45E-02	1.31E-02	1.75E-02	1.89E-02
445.23	7.38	pos	5.01E-02	4.43E-02	3.48E-02	4.61E-02	4.48E-02
446.91	8.29	pos	2.92E-02	2.64E-02	2.07E-02	2.04E-02	3.04E-02
447.13	0.87	neg	2.26E-03	1.92E-03	1.30E-03	1.32E-03	2.20E-03
448.07	5.58	pos	5.27E-03	5.40E-03	5.88E-03	7.34E-03	6.33E-03
448.24	0.57	pos	2.11E-03	1.65E-03	8.28E-04	9.55E-04	2.52E-03
448.84	7.96	neg	2.48E-02	3.28E-02	2.79E-02	2.88E-02	2.76E-02
450.15	6.85	pos	4.67E-03	4.11E-03	2.85E-03	4.01E-03	3.60E-03
450.85	9.49	neg	7.69E-02	7.30E-02	7.11E-02	9.05E-02	8.66E-02
451.05	7.20	pos	1.57E-02	1.23E-02	1.29E-02	1.55E-02	1.99E-02
452.10	6.95	pos	5.92E-03	4.15E-03	4.24E-03	3.46E-03	4.02E-03
452.87	9.53	pos	5.26E-02	4.77E-02	4.02E-02	3.59E-02	5.17E-02
452.94	8.30	neg	6.85E-02	7.46E-02	6.70E-02	9.18E-02	8.18E-02
454.99	9.35	neg	1.21E-02	8.53E-03	1.55E-02	1.16E-02	1.69E-02
455.05	7.06	pos	1.07E-02	9.45E-03	4.62E-03	2.43E-03	1.17E-02
455.21	6.69	neg	1.99E-02	2.48E-02	3.26E-02	3.23E-02	2.23E-02
456.31	6.70	pos	5.88E-02	5.59E-02	6.60E-02	8.76E-02	6.26E-02
457.07	7.26	pos	1.20E-02	1.15E-02	9.28E-03	1.48E-02	1.25E-02
458.07	2.02	pos	1.24E-03	1.45E-03	1.72E-03	8.14E-04	1.58E-03
458.79	7.92	pos	3.99E-03	3.04E-03	2.72E-03	5.11E-03	5.79E-03
459.17	6.66	pos	4.84E-03	5.21E-03	6.07E-03	5.93E-03	5.11E-03
461.00	5.58	neg	2.88E-03	3.15E-03	2.98E-03	4.53E-03	4.08E-03
462.00	5.58	neg	2.09E-03	2.15E-03	1.89E-03	3.21E-03	2.87E-03
463.00	5.58	neg	4.23E-02	4.64E-02	5.31E-02	8.43E-02	5.96E-02
463.13	7.34	pos	9.16E-03	8.89E-03	6.32E-03	9.74E-03	8.97E-03
464.00	5.57	neg	2.15E-03	2.10E-03	2.15E-03	3.61E-03	3.04E-03
464.82	7.94	neg	2.32E-02	2.40E-02	2.95E-02	3.36E-02	2.88E-02
467.21	7.39	pos	2.45E-02	2.24E-02	1.69E-02	1.63E-02	2.14E-02
468.91	8.32	neg	2.84E-02	3.28E-02	2.23E-02	2.54E-02	2.88E-02
471.57	5.59	pos	1.62E-03	1.70E-03	2.01E-03	2.38E-03	1.85E-03
477.01	4.77	pos	2.06E-03	3.46E-03	1.77E-03	5.30E-03	2.00E-03

479.21	6.70	pos	7.01E-03	6.73E-03	6.64E-03	5.53E-03	5.88E-03
480.12	6.79	pos	7.77E-03	3.61E-03	5.32E-03	7.85E-03	8.65E-03
483.18	7.39	pos	1.51E-02	1.45E-02	1.01E-02	8.51E-03	1.09E-02
488.50	5.58	neg	1.26E-03	1.32E-03	1.33E-03	2.24E-03	1.82E-03
488.90	8.34	pos	1.86E-02	1.81E-02	1.51E-02	1.22E-02	1.67E-02
489.19	7.39	pos	5.56E-03	4.25E-03	3.43E-03	3.31E-03	4.26E-03
489.50	5.58	neg	1.57E-03	1.51E-03	1.60E-03	3.02E-03	2.03E-03
490.50	5.59	neg	1.75E-02	1.65E-02	2.01E-02	3.29E-02	2.18E-02
490.90	9.34	pos	2.62E-02	2.25E-02	1.94E-02	3.35E-02	3.54E-02
491.50	5.58	neg	1.20E-03	1.23E-03	1.43E-03	1.94E-03	1.51E-03
493.08	7.38	pos	5.99E-03	5.72E-03	4.44E-03	2.58E-03	5.39E-03
495.08	5.57	pos	3.87E-03	4.35E-03	3.81E-03	4.20E-03	4.56E-03
496.83	9.80	pos	2.59E-02	2.86E-02	1.99E-02	1.51E-02	2.39E-02
497.02	4.65	neg	2.87E-03	3.23E-03	1.00E-03	1.04E-03	2.58E-03
497.08	5.57	pos	1.08E-02	1.08E-02	1.10E-02	1.13E-02	1.28E-02
498.92	8.28	pos	4.64E-02	4.53E-02	4.16E-02	5.72E-02	6.06E-02
499.08	5.57	pos	1.46E-02	1.49E-02	1.47E-02	1.57E-02	1.62E-02
505.16	7.40	pos	1.04E-02	8.85E-03	6.58E-03	6.77E-03	8.26E-03
507.14	6.69	neg	3.72E-02	3.84E-02	1.89E-02	2.17E-02	3.78E-02
507.94	9.38	pos	3.03E-02	1.73E-02	2.24E-02	5.96E-02	5.94E-02
508.13	8.63	pos	4.42E-03	5.93E-03	8.93E-03	3.87E-03	6.38E-03
508.15	6.70	pos	4.29E-03	4.00E-03	3.96E-03	5.15E-03	3.83E-03
509.30	2.50	neg	5.92E-03	8.07E-03	8.33E-03	5.03E-03	5.62E-03
510.79	9.94	neg	1.83E-02	1.86E-02	1.80E-02	2.01E-02	2.06E-02
510.87	9.34	neg	5.94E-02	4.14E-02	5.54E-02	1.14E-01	9.76E-02
511.09	4.65	neg	2.03E-03	1.97E-03	2.01E-03	2.06E-03	2.15E-03
511.16	6.73	pos	1.86E-02	1.57E-02	1.63E-02	1.69E-02	1.64E-02
511.33	2.50	pos	2.84E-03	4.53E-03	4.88E-03	2.75E-03	3.10E-03
512.80	9.98	pos	1.54E-02	1.31E-02	1.13E-02	1.22E-02	1.62E-02
512.84	9.31	neg	9.55E-03	6.23E-03	8.70E-03	2.88E-02	1.98E-02
512.88	9.39	pos	3.29E-02	2.54E-02	2.58E-02	4.05E-02	4.73E-02
512.92	8.27	pos	1.23E-02	1.09E-02	9.65E-03	1.36E-02	1.53E-02
514.00	5.59	neg	1.58E-02	1.12E-02	1.91E-02	2.27E-02	1.84E-02
514.29	1.97	pos	4.02E-03	4.38E-03	5.43E-03	4.98E-03	4.59E-03
516.01	5.58	neg	2.13E-03	2.28E-03	1.92E-03	2.80E-03	2.32E-03
518.01	5.58	neg	1.86E-03	1.85E-03	1.46E-03	2.37E-03	2.15E-03
520.92	8.30	neg	5.12E-02	6.03E-02	5.00E-02	7.12E-02	6.19E-02
521.13	7.38	pos	5.58E-03	5.84E-03	7.02E-03	8.24E-03	8.46E-03
521.17	7.19	pos	5.58E-03	5.84E-03	7.02E-03	8.24E-03	8.46E-03
523.41	7.07	pos	1.35E-02	8.73E-03	8.71E-03	1.14E-02	1.45E-02
525.30	6.61	pos	7.82E-03	9.94E-03	1.03E-02	6.25E-03	9.39E-03
525.58	5.58	pos	1.18E-03	1.15E-03	1.28E-03	1.53E-03	1.45E-03
526.78	7.94	pos	4.20E-03	4.11E-03	2.98E-03	4.92E-03	5.27E-03
526.85	9.37	neg	3.62E-02	2.49E-02	3.28E-02	5.57E-02	5.63E-02
528.87	9.40	pos	2.34E-02	1.77E-02	1.69E-02	2.69E-02	3.29E-02
531.15	6.71	pos	4.73E-03	4.67E-03	4.31E-03	4.75E-03	3.67E-03
532.80	7.96	neg	1.41E-02	1.67E-02	1.34E-02	1.80E-02	1.45E-02
532.85	9.42	neg	4.83E-02	3.87E-02	4.19E-02	5.68E-02	5.66E-02
533.12	7.06	pos	7.74E-03	8.48E-03	8.84E-03	6.89E-03	6.91E-03
534.87	9.48	pos	5.09E-02	4.44E-02	3.99E-02	4.17E-02	5.60E-02
535.13	7.37	pos	6.56E-03	5.60E-03	5.66E-03	3.44E-03	6.20E-03
536.90	8.32	neg	2.83E-02	3.33E-02	2.41E-02	2.64E-02	2.86E-02

539.18	7.32	neg	9.11E-03	6.56E-03	6.46E-03	1.97E-02	1.20E-02
542.76	7.92	pos	3.74E-03	4.22E-03	2.66E-03	4.97E-03	5.62E-03
546.08	8.65	pos	2.49E-03	3.80E-03	5.24E-03	2.80E-03	3.76E-03
547.13	6.70	pos	7.67E-03	7.09E-03	7.36E-03	8.46E-03	6.17E-03
548.83	9.45	neg	5.17E-02	4.23E-02	4.62E-02	6.20E-02	6.28E-02
549.09	5.58	pos	1.40E-03	1.36E-03	1.56E-03	1.95E-03	1.61E-03
550.85	9.47	pos	4.35E-02	3.41E-02	3.30E-02	3.36E-02	4.28E-02
552.10	8.63	pos	9.34E-03	1.03E-02	1.37E-02	8.87E-03	1.20E-02
556.88	8.33	pos	2.01E-02	2.08E-02	1.54E-02	1.37E-02	1.87E-02
559.34	4.64	pos	2.89E-02	3.73E-02	7.62E-02	6.90E-02	3.28E-02
565.06	9.19	neg	3.47E-02	3.38E-02	5.23E-02	2.12E-02	4.03E-02
566.09	5.60	pos	1.89E-03	2.04E-03	8.49E-04	5.24E-04	1.71E-03
566.91	8.28	pos	4.39E-02	4.38E-02	3.96E-02	5.39E-02	5.64E-02
567.33	0.60	pos	1.82E-03	1.74E-03	2.03E-03	7.11E-04	1.99E-03
568.07	8.65	pos	6.49E-03	8.75E-03	9.48E-03	6.36E-03	8.76E-03
571.18	7.01	pos	3.64E-03	2.70E-03	3.61E-03	5.36E-03	4.47E-03
572.87	8.34	pos	1.11E-02	1.16E-02	8.12E-03	5.90E-03	1.17E-02
573.32	4.64	pos	5.03E-03	5.69E-03	1.30E-02	1.28E-02	5.72E-03
574.08	8.63	pos	1.08E-02	1.15E-02	1.30E-02	9.15E-03	1.25E-02
574.36	1.00	pos	2.09E-03	2.26E-03	5.00E-03	1.80E-03	2.48E-03
577.58	5.58	pos	1.81E-03	1.95E-03	2.21E-03	2.83E-03	2.48E-03
578.91	8.37	neg	1.27E-02	1.58E-02	1.38E-02	1.34E-02	1.34E-02
579.04	9.90	neg	1.21E-02	1.13E-02	1.70E-02	1.15E-02	1.59E-02
579.21	6.36	pos	3.50E-03	3.49E-03	5.03E-03	5.88E-03	3.68E-03
579.58	5.58	pos	2.59E-03	2.87E-03	3.33E-03	4.48E-03	3.78E-03
580.46	6.71	pos	6.93E-03	4.88E-03	5.95E-03	6.51E-03	7.17E-03
580.91	8.27	pos	1.30E-02	1.27E-02	1.23E-02	1.63E-02	1.76E-02
581.21	6.37	pos	3.12E-03	3.34E-03	2.45E-03	2.66E-03	3.51E-03
582.21	5.72	neg	1.40E-02	9.38E-03	1.60E-02	1.34E-02	1.25E-02
582.88	8.29	pos	2.09E-02	2.06E-02	1.80E-02	1.65E-02	2.57E-02
584.11	9.17	pos	2.15E-02	2.29E-02	2.80E-02	6.96E-03	1.80E-02
584.24	5.72	pos	9.98E-03	5.68E-03	7.55E-03	6.26E-03	7.60E-03
588.86	9.40	pos	1.11E-02	1.33E-02	1.48E-02	2.13E-02	2.26E-02
588.91	8.29	neg	3.80E-02	4.24E-02	3.88E-02	6.02E-02	4.91E-02
590.05	8.65	pos	7.44E-03	8.04E-03	9.05E-03	6.17E-03	9.23E-03
592.79	9.66	neg	2.48E-02	3.45E-02	2.38E-02	2.55E-02	2.86E-02
595.33	0.84	neg	2.96E-03	2.57E-03	4.13E-03	1.16E-03	2.81E-03
596.06	8.64	pos	8.93E-03	8.69E-03	9.64E-03	7.71E-03	1.06E-02
597.30	4.66	pos	2.43E-03	3.00E-03	2.51E-03	2.07E-03	2.33E-03
598.12	9.92	pos	6.51E-03	8.52E-03	1.05E-02	4.55E-03	7.76E-03
598.87	8.30	pos	1.14E-02	9.81E-03	8.52E-03	6.72E-03	1.09E-02
600.38	0.80	pos	5.58E-03	4.86E-03	1.04E-02	4.25E-03	4.85E-03
600.57	0.79	pos	5.58E-03	4.86E-03	1.04E-02	4.25E-03	4.85E-03
601.19	6.37	pos	3.98E-03	3.80E-03	5.68E-03	5.73E-03	2.89E-03
602.39	0.85	pos	2.31E-03	2.12E-03	3.63E-03	2.11E-03	1.92E-03
602.84	5.59	pos	8.42E-04	1.41E-03	1.26E-03	1.64E-03	1.56E-03
603.09	5.58	pos	7.81E-03	9.46E-03	8.62E-03	1.02E-02	9.76E-03
604.89	8.31	neg	2.35E-02	2.52E-02	2.20E-02	2.23E-02	2.50E-02
605.92	9.37	pos	2.05E-02	1.32E-02	1.49E-02	4.93E-02	4.38E-02
606.09	8.98	neg	4.80E-03	5.76E-03	6.77E-03	4.54E-03	5.62E-03
608.83	9.38	neg	3.48E-02	3.33E-02	3.14E-02	6.28E-02	5.78E-02
608.90	8.32	pos	8.69E-03	1.00E-02	8.27E-03	8.61E-03	1.01E-02

610.87	9.38	pos	4.33E-02	2.86E-02	3.42E-02	5.51E-02	6.57E-02
611.16	9.80	neg	4.27E-03	3.62E-03	4.93E-03	3.93E-03	5.55E-03
612.02	8.63	pos	6.76E-03	7.21E-03	6.57E-03	6.13E-03	8.50E-03
614.38	0.80	pos	5.53E-03	4.99E-03	8.03E-03	1.54E-03	1.14E-02
617.17	6.36	pos	2.67E-03	2.86E-03	4.40E-03	3.96E-03	2.94E-03
617.55	5.66	pos	2.02E-03	2.47E-03	2.53E-03	1.99E-03	2.09E-03
618.12	8.59	neg	5.61E-03	7.22E-03	6.17E-03	4.17E-03	7.20E-03
619.08	5.65	pos	1.66E-03	2.17E-03	1.09E-03	1.52E-03	2.07E-03
620.09	5.60	pos	2.04E-03	2.39E-03	9.80E-04	1.04E-03	2.19E-03
620.14	8.59	pos	7.68E-03	7.93E-03	9.06E-03	4.84E-03	8.46E-03
624.80	9.41	neg	1.71E-02	1.58E-02	1.92E-02	4.07E-02	3.19E-02
624.87	8.32	pos	2.09E-02	1.89E-02	1.69E-02	1.44E-02	2.07E-02
626.84	9.39	pos	1.66E-02	1.27E-02	1.42E-02	2.50E-02	2.68E-02
628.40	6.67	pos	4.27E-03	3.28E-03	4.33E-03	4.07E-03	4.80E-03
630.08	8.96	pos	4.91E-03	4.41E-03	6.55E-03	2.97E-03	4.97E-03
632.85	9.44	pos	4.53E-02	3.41E-02	3.20E-02	3.69E-02	5.03E-02
634.90	8.27	pos	4.00E-02	3.81E-02	3.53E-02	5.25E-02	5.17E-02
638.87	8.31	pos	8.65E-03	9.45E-03	6.71E-03	6.91E-03	1.03E-02
646.80	9.44	neg	3.12E-02	2.44E-02	2.78E-02	4.21E-02	4.02E-02
648.83	9.46	pos	3.45E-02	2.82E-02	2.54E-02	2.88E-02	4.06E-02
648.87	9.41	neg	1.42E-02	1.73E-02	1.58E-02	1.58E-02	1.19E-02
648.90	8.27	pos	1.38E-02	1.19E-02	1.12E-02	1.53E-02	1.81E-02
650.38	6.68	pos	4.09E-03	3.39E-03	4.31E-03	4.08E-03	3.86E-03
650.87	8.29	pos	2.20E-02	2.05E-02	1.65E-02	1.54E-02	2.45E-02
654.82	9.55	pos	2.14E-02	2.31E-02	1.86E-02	1.29E-02	1.75E-02
656.09	5.58	pos	5.07E-03	5.75E-03	5.51E-03	5.26E-03	5.98E-03
656.90	8.29	neg	2.23E-02	2.39E-02	2.12E-02	3.51E-02	3.00E-02
658.09	5.57	pos	8.62E-03	9.44E-03	9.02E-03	1.05E-02	1.00E-02
662.12	9.00	neg	6.72E-03	7.22E-03	9.10E-03	5.91E-03	7.92E-03
664.14	9.00	pos	2.05E-02	2.56E-02	2.83E-02	1.50E-02	2.24E-02
666.85	8.30	pos	1.12E-02	1.04E-02	7.99E-03	7.62E-03	1.15E-02
668.79	9.50	neg	2.84E-02	2.53E-02	2.54E-02	3.06E-02	3.02E-02
669.29	4.67	pos	3.06E-03	4.23E-03	3.81E-03	1.87E-03	3.08E-03
670.81	9.57	pos	2.96E-02	2.59E-02	2.11E-02	1.60E-02	2.55E-02
671.49	4.64	pos	1.88E-03	2.30E-03	2.61E-03	2.61E-03	2.24E-03
672.35	6.69	pos	2.57E-03	2.74E-03	3.47E-03	2.64E-03	2.35E-03
672.88	8.31	neg	1.76E-02	1.73E-02	1.43E-02	1.50E-02	1.81E-02
676.88	8.29	pos	8.41E-03	8.15E-03	7.73E-03	9.66E-03	1.06E-02
681.26	4.66	neg	1.33E-03	1.42E-03	1.74E-03	1.49E-03	1.36E-03
682.30	6.69	pos	6.51E-03	4.58E-03	5.51E-03	7.93E-03	6.17E-03
683.49	4.64	pos	2.13E-03	1.89E-03	3.03E-03	2.90E-03	2.12E-03
684.78	9.43	neg	1.78E-02	1.57E-02	1.45E-02	3.64E-02	2.51E-02
685.26	4.67	pos	6.70E-03	8.75E-03	6.49E-03	5.13E-03	6.22E-03
686.12	8.98	pos	9.70E-03	1.12E-02	1.27E-02	6.74E-03	1.10E-02
688.32	6.69	pos	4.06E-03	3.58E-03	3.27E-03	2.96E-03	3.30E-03
692.86	8.32	pos	1.83E-02	1.78E-02	1.45E-02	1.47E-02	1.94E-02
697.24	4.66	neg	3.10E-03	3.10E-03	3.86E-03	3.46E-03	3.30E-03
701.24	4.67	pos	3.23E-03	3.77E-03	3.04E-03	1.91E-03	2.98E-03
702.89	8.27	pos	3.55E-02	3.10E-02	3.09E-02	4.79E-02	5.09E-02
703.89	9.34	pos	1.71E-02	8.28E-03	1.14E-02	3.82E-02	3.57E-02
704.29	6.69	pos	3.96E-03	3.68E-03	3.86E-03	4.93E-03	3.38E-03
704.87	8.28	pos	6.52E-03	7.54E-03	6.40E-03	7.41E-03	8.19E-03

706.77	9.48	neg	1.97E-02	1.50E-02	1.53E-02	3.70E-02	2.85E-02
706.86	8.30	pos	1.03E-02	8.82E-03	8.10E-03	8.19E-03	1.07E-02
707.10	5.56	pos	4.21E-03	4.48E-03	4.23E-03	5.14E-03	4.81E-03
707.24	4.71	pos	1.64E-03	1.62E-03	1.22E-03	9.34E-04	1.40E-03
708.10	8.98	pos	6.46E-03	6.80E-03	7.33E-03	5.07E-03	5.77E-03
708.84	9.36	pos	3.42E-02	2.35E-02	2.67E-02	5.14E-02	5.74E-02
709.10	5.57	pos	1.61E-02	1.87E-02	1.71E-02	1.98E-02	1.88E-02
715.23	4.66	pos	6.57E-03	9.76E-03	4.55E-03	1.87E-02	5.57E-03
716.88	8.27	pos	1.34E-02	1.25E-02	1.04E-02	1.48E-02	1.81E-02
718.29	6.69	pos	4.66E-03	4.28E-03	4.06E-03	6.08E-03	4.14E-03
718.86	8.28	pos	2.06E-02	1.74E-02	1.41E-02	1.65E-02	2.40E-02
719.22	4.67	neg	1.93E-03	2.08E-03	1.94E-03	1.81E-03	2.02E-03
722.79	9.37	neg	4.94E-03	4.95E-03	6.94E-03	1.90E-02	1.50E-02
723.56	5.62	pos	1.87E-03	1.70E-03	1.96E-03	1.71E-03	1.20E-03
724.82	9.39	pos	1.49E-02	9.49E-03	1.09E-02	1.93E-02	2.36E-02
724.89	8.27	neg	1.28E-02	1.37E-02	1.28E-02	2.19E-02	1.71E-02
728.79	9.40	neg	1.75E-02	1.51E-02	1.53E-02	2.16E-02	2.22E-02
730.83	9.43	pos	3.60E-02	2.72E-02	2.46E-02	2.99E-02	4.35E-02
737.60	5.58	pos	2.03E-03	2.12E-03	2.50E-03	3.07E-03	2.61E-03
739.20	4.69	pos	1.11E-03	1.73E-03	9.91E-04	2.00E-03	1.18E-03
740.86	8.29	neg	1.10E-02	1.07E-02	9.67E-03	1.04E-02	1.21E-02
744.78	9.40	neg	1.56E-02	1.30E-02	1.30E-02	2.47E-02	2.16E-02
746.81	9.44	pos	2.73E-02	2.08E-02	1.87E-02	2.44E-02	3.26E-02
751.21	4.66	pos	2.24E-03	3.07E-03	1.92E-03	7.03E-03	1.99E-03
760.85	8.30	pos	1.63E-02	1.39E-02	1.13E-02	1.24E-02	1.69E-02
766.09	5.58	pos	1.79E-03	2.17E-03	1.93E-03	2.15E-03	2.45E-03
766.77	9.43	neg	1.36E-02	1.10E-02	1.34E-02	1.70E-02	1.70E-02
768.79	9.52	pos	2.62E-02	2.04E-02	1.78E-02	1.45E-02	2.18E-02
770.87	8.27	pos	2.30E-02	2.36E-02	2.03E-02	3.44E-02	3.63E-02
774.85	8.30	pos	1.00E-02	7.60E-03	7.14E-03	8.37E-03	1.07E-02
782.77	9.40	neg	9.76E-03	8.05E-03	7.50E-03	1.36E-02	1.16E-02
784.87	8.28	pos	1.04E-02	9.09E-03	8.87E-03	1.13E-02	1.34E-02
792.87	8.27	neg	7.10E-03	6.69E-03	6.30E-03	1.50E-02	1.01E-02
801.88	9.36	pos	1.26E-02	6.59E-03	8.18E-03	3.03E-02	2.81E-02
804.78	9.37	neg	1.04E-02	7.62E-03	8.59E-03	1.74E-02	1.46E-02
806.83	9.38	pos	2.38E-02	1.67E-02	1.67E-02	3.61E-02	4.15E-02
815.09	5.56	pos	1.04E-03	1.68E-03	1.41E-03	1.74E-03	1.29E-03
825.09	5.58	pos	1.92E-03	2.12E-03	1.93E-03	2.28E-03	2.14E-03
825.29	4.65	pos	1.26E-03	1.59E-03	1.60E-03	1.10E-03	1.38E-03
826.78	9.38	neg	4.97E-03	3.28E-03	7.63E-03	1.15E-02	1.16E-02
828.81	9.41	pos	2.62E-02	1.69E-02	1.71E-02	2.48E-02	3.40E-02
828.83	8.29	pos	1.06E-02	1.05E-02	8.71E-03	8.54E-03	1.23E-02
842.76	9.38	neg	7.58E-03	5.42E-03	6.59E-03	1.03E-02	1.04E-02
844.79	9.41	pos	2.05E-02	1.43E-02	1.27E-02	1.83E-02	2.61E-02
860.86	8.26	neg	3.87E-03	4.02E-03	3.40E-03	8.18E-03	6.53E-03
866.77	9.49	pos	2.01E-02	1.50E-02	1.20E-02	1.30E-02	1.80E-02
868.23	5.58	pos	1.04E-03	8.63E-04	1.14E-03	1.59E-03	1.33E-03
875.32	4.64	pos	1.81E-03	1.71E-03	1.30E-03	1.09E-03	1.75E-03
876.60	5.58	pos	1.67E-03	1.78E-03	1.87E-03	2.25E-03	2.05E-03
877.30	5.59	pos	2.18E-03	2.28E-03	2.57E-03	3.60E-03	2.90E-03
878.10	5.59	pos	1.67E-03	1.78E-03	1.87E-03	2.25E-03	2.05E-03
883.58	5.62	pos	1.32E-03	1.62E-03	1.76E-03	1.59E-03	1.46E-03

891.44	6.68	pos	4.18E-03	4.11E-03	4.40E-03	6.00E-03	3.69E-03
899.86	9.34	pos	7.75E-03	3.97E-03	5.19E-03	2.17E-02	1.98E-02
904.80	9.37	pos	1.66E-02	1.04E-02	1.09E-02	2.34E-02	2.75E-02
906.85	8.26	pos	8.12E-03	7.90E-03	6.30E-03	1.19E-02	1.37E-02
913.42	6.69	pos	3.71E-03	3.47E-03	3.15E-03	4.71E-03	3.52E-03
922.82	8.27	pos	6.12E-03	6.24E-03	5.21E-03	5.07E-03	8.72E-03
926.79	9.39	pos	1.76E-02	1.34E-02	1.18E-02	1.88E-02	2.34E-02
942.77	9.40	pos	1.35E-02	9.16E-03	8.55E-03	1.40E-02	1.87E-02
974.83	8.25	pos	5.51E-03	3.60E-03	3.95E-03	7.01E-03	6.99E-03
981.45	4.64	pos	1.43E-03	1.79E-03	1.51E-03	7.50E-04	1.26E-03
991.41	4.64	pos	2.22E-03	3.16E-03	1.70E-03	5.91E-03	2.06E-03
997.43	4.65	pos	2.03E-03	2.24E-03	1.89E-03	1.00E-03	1.81E-03
1002.78	9.36	pos	1.02E-02	5.76E-03	5.50E-03	1.25E-02	1.63E-02