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TOF-SIMS for Rapid Nuclear Forensics Evaluation of Uranium Oxide Particles

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THESIS

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ABSTRACT

Because of nuclear proliferation concerns, nuclear material must be safeguarded, and peaceful intentions verified. The field of nuclear forensics addresses these concerns. While established nuclear forensic techniques exist, quicker, more accurate and less expensive methods are of interest for nonproliferation applications. Currently a host of different analytical techniques, requiring a week or longer, are employed to obtain isotopic ratios, chemical abundances and morphology for forensic particulate samples. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) is a candidate technology for rapid evaluation of these properties for small amounts of nuclear materials. After a thorough investigation, this study found TOF-SIMS to be particularly useful to the nuclear forensic field as a triage technique, capable of quickly identifying and roughly assessing uranium containing materials for these properties. Uranium isotopic abundances can be determined to an accuracy of 1 percent. Uranium oxide particles are clearly distinguished from one another. TOF-SIMS imaging easily and quickly reveals the basic shape and composition of particles. Additionally the relative abundances of various secondary ions produced with TOF-SIMS may uncover new information on fundamental uranium oxide structures and properties.

Acknowledgments

Sir Issac Newton once said, "If I have seen further it is only by standing on the shoulders of giants." I am no Newton, and perhaps this statement is perhaps a bit of a reach for me. However, I am comfortable in saying that I could not hope to accomplish anything without the "giants" that surround me. Thank you, Dr. Burggraf for all the guidance and patience you showed me. Without your expertise and support I would have been lost. Thank you to Dr. Gardella and Brett Yatzor at SUNY Buffalo for the use of your TOF-SIMS and your expert knowledge. Thank you to Dr. Felker and Dr. Li for all your help in the lab. Thank you to Dr. Simons and Dr. Szakal for your clarification on a number of points I was confused on. Thank you to Linda Kasten for introducing me to TOF-SIMS. Last, but not least, thank you to my family, for your unwavering support and encouragement.

Capt Hannah E. Hocking

TABLE OF CONTENTS

Page

Page

LIST OF FIGURES

Figure Page

LIST OF TABLES

TOF-SIMS FOR RAPID NUCLEAR FORENSICS EVALUATION OF URANIUM OXIDE PARTICLES

I. Introduction

As more and more countries express interest in nuclear technology the need to monitor and assess nuclear activities is ever growing. Nuclear material must be safeguarded and peaceful intentions must be verified. Nuclear forensics, the technical means by which nuclear materials are characterized and interpreted [1], is an ongoing area of interest for the Department of Defense. While established nuclear forensic techniques exist [1], more accurate, less expensive and quicker methods are of continued interest. Rapid, actionable information is a priority.

Special nuclear material [2], plutonium and certain isotopic enrichments of uranium, is material which could be fashioned into a nuclear weapon and is of special regulatory interest. While plutonium is not commonly found in nature, uranium is much more widespread. Uranium ore is found in many locations across the globe. Uranium has many uses ranging from pottery glaze to nuclear weapon cores and uranium oxides are perhaps the most common nuclear reactor fuel. All this makes uranium a much more difficult material to monitor.

Currently, obtaining isotopic and chemical abundances of forensic samples requires a host of different analytical instruments and can take a week or more [1]. New

technology can provide breakthroughs in the endeavor to identify and characterize uranium containing particulates using isotopic, chemical, and morphological data.

Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) shows the potential to shorten the nuclear forensic timeline for uranium containing compounds. TOF-SIMS has the capability to gather isotopic and chemical information as well as gain a sense of the sample morphology. It can gather this information quickly and concurrently.

This study explores the potential of TOF-SIMS to be used as a nuclear forensic technique for the purpose of rapidly locating and describing uranium and uranium oxide particulate. Specifically the goal of this research was to determine if TOF-SIMS could be used to quickly achieve isotopic, chemical and morphological data on a uranium containing particle.

In this study, a novel sample mounting technique in which uranium oxide particulate samples were pressed into a clean gold surface was developed in hopes of reducing sample contamination. This technique calls for a minimum of sample preparation, which complements a quick forensic study. The gold mounted uranium oxide particulate samples were subjected to TOF-SIMS analysis using an IONTOF TOF-SIMS V with a Bi_3^{++} primary ion beam and a C_{60} sputtering beam which gathered mass spectrum data to 3000 amu.

The study found TOF-SIMS to be particularly useful to the nuclear forensic field as a sort of triage technique, capable of quickly identifying and roughly assessing particles of interest. The Isotope Calculator, created in this effort, can determine the isotopic abundance of uranium accurate to within 1%. Oxide identification is achievable

through a variety of mass spectrum analysis. Morphology information obtained with TOF-SIMS static imaging provides excellent insight into the sample particle and its environs. The gold sample mounting technique has both advantages and drawbacks, but is advantageous in situations where rapid analysis is desired. Additionally, TOF-SIMS may hold some merit as a tool in uncovering more information on fundamental uranium structure and properties.

II. Background

Uranium research perhaps reached its heyday in the 1950s. Prior to the Manhattan Project, relatively little interest was taken in uranium. Much of what is known about the basic science of uranium was discovered during the Manhattan Project and, later, for the development of nuclear reactors. Subsequent research efforts have been mainly focused on nuclear forensic applications. The relative sophistication of our nuclear forensic capabilities, however, will always depend on our understanding of the fundamental science underlying these techniques. For that reason it is imperative that both our sample material, uranium, and our proposed analysis technique, TOF-SIMS, be firmly understood.

Uranium

Uranium, being radioactive, exists in several isotopic forms. The majority (99.2742%) of naturally occurring uranium is U-238. A smaller percent (0.7204%) is found as U-235. The long half-life of uranium makes its natural isotopic abundance a practical constant [3].

Table 1. Natural Isotopic Abundance of Uranium.

	U-234	U-235	U-238
Abundance	0.0054%	0.7204%	99.2742%
Half-life	2.455E+5 y	7.04E+8 y	4.468E9 y

Nuclear reactors and enrichment facilities have the ability to alter the isotopic abundance of uranium. Enrichment facilities increase the U-235 content of uranium for use as

nuclear fuel or weapon material. Reactors will generally deplete the U-235 content of uranium fuel, though not necessarily below natural levels. Analysis of a forensic sample for isotopic abundance can tell of the sample's isotopic enrichment history.

Additionally the chemical nature of the uranium containing sample is important to this study. Fission fragments and impurities will contribute to a uranium containing sample. Uranium has oxidation states ranging from +3 to +6 and will form many compounds as well. Some of the most common chemicals which uranium reacts with are carbon, water, and oxygen. Chemical content can be related back to the processing history of a forensic sample.

Both uranium and uranium oxides will combine with carbon to form uranium carbides UC and UC_2. A third, less common, carbide is also possible; U_2C_3. Methane has also been shown to produce UC carbide on uranium. Carbon has a reducing effect on uranium and uranium oxides [4].

Water has been shown to react with uranium metal; oxidizing it. Uranium oxides show some affinity for water as well, existing as hydrates. $UO_2 * 2H_2O$, $U_3O_8 * H_2O$, $U_3O_8 * 2H_2O$, $UO_3 * H_2O$, $UO_3 * 2H_2O$, $2UO_3 * H_2O$, and $2UO_3 * 3H_2O$ are all noted in literature. As uranium oxidation state increases, hydrate formation becomes more probable. Adding energy to a uranium oxide hydrate can have the effect of further oxidation rather than dehydration [4].

Figure 1. Crystalline structure of UO_2, U_3O_8, and UO_3. [20]

Uranium metal is not chemically stable in an oxygen environment. Uranium oxidizes readily in the open atmosphere. The most common stoichiometric uranium oxides are UO_2, U_3O_8, and UO_3. Different crystalline structures exist for each of these oxides.

In an oxidizing environment uranium oxide will favor the UO_3 species. In a reducing environment UO_2 will be favored. In air, the intermediate form, U_3O_8, is favored. However, in reality uranium oxidation will produce a gradient of oxide composition with the stoichiometric oxides appearing merely as thin layers. Schueneman found that at low temperature, a gradient of amorphous defected oxide coating will form on UO_2 particles. Simple oxygen diffusion dynamics were found accountable for the oxide formation. The detailed characterization of uranium oxidation can be used to relate a particle's oxidation profile back to storage conditions and particle life [5].

Uranium's oxidation state, or valence, varies from +4, for pure UO_2, to +6, for pure UO_3. Determining the oxidation state of uranium helps to describe the chemical composition of the uranium oxide particle. In Plog et al. [6] the term fragment valence is

defined as the formal valence number of the metal atom in the fragment ion. For metal oxide, $Me_mO_n^q$, the average fragment valence is,

$$K = (q + 2n) / m. \quad (1)$$

In a mass spectrum, multiple types of fragments can be seen. Plog et al. shows, for a selection of metal oxides, that a plot of the abundance of each of these fragments against their average fragment valence yields two Gaussian curves; one for the positive ion spectrum and one for the negative ion spectrum. Averaging the mean of each curve gives G^0, which they define as the lattice valence. The authors put forth that this lattice valence could be used to determine oxide concentration for stoichiometry determination, but that the relation between lattice valence and metal valency must be known in considerable detail for a quantitative determination [6]. Schuler began using this principle to describe the average oxidation state of uranium [7]. In this work the change in lattice valence will be used as a relative measure of the average oxidation state of a uranium sample.

TOF-SIMS Capabilities

Sodhi states that "time-of-flight secondary ion mass spectrometry (TOF-SIMS) has emerged as one of the most important and versatile surface analytical techniques available for advanced materials research" [8]. Certain techniques even allow a three dimensional map of sample composition to be produced. TOF-SIMS requires a minimum of sample preparation, and is minimally destructive. All of this taken together makes TOF-SIMS a leading candidate for nuclear forensic analysis.

In general, all mass spectrometry includes the following steps. First the sample must be vaporized. Then these fragments are ionized and the ions are separated according to their mass-to-charge ratio (m/z). Either positive or negative ions may be selected to be examined with the positive ion analysis being more common. The abundance or intensity of each m/z is then determined to produce the mass spectrum of the sample. Analysis of the molecular fragments that comprise the mass spectrum is required to determine the contributing isotopic and chemical species. Various methods are used to atomize, ionize, and separate samples [9].

The most common methods of achieving atomization and ionization include the use of plasmas, sparks, lasers, and ion beams. Separation occurs by use of a quadrupole, magnetic sector, double focusing, ion trap, or time-of-flight mass analyzer. Currently magnetic sector SIMS instruments are used in state-of-the-art nuclear forensic analysis [10]. Magnetic sector SIMS makes use of an ion beam to fragment and ionize the sample. Ions are then separated by virtue of electromagnetics. Magnetic sector SIMS' advantage comes in the ultra high resolution that is achievable and the ability to completely fragment and consume the sample producing very high ion counts. Disadvantages include the extremely low m/z range and complete consumption of a forensic sample.

Time-of-flight SIMS (TOF-SIMS) mass analyzers also use an ion beam to fragment and ionize the sample. However, TOF-SIMS ion beams are much lower in fluence than the ones found in magnetic sector SIMS. A time-of-flight tube is used to separate the ions according to m/z. The time-flight-tube enables a virtually unlimited m/z range, the lower fluence primary ion beam allows spectra to be gathered from a single

monolayer of the sample, and preservation of a forensic sample as evidence. Tradeoffs are made in resolution and sensitivity [9].

Many different ion beams are available for TOF-SIMS instruments, each with its own advantages and disadvantages. Oxygen, cesium, and bismuth are commonly used ion beams. Ion beam selection must be tailored to the sample and study.

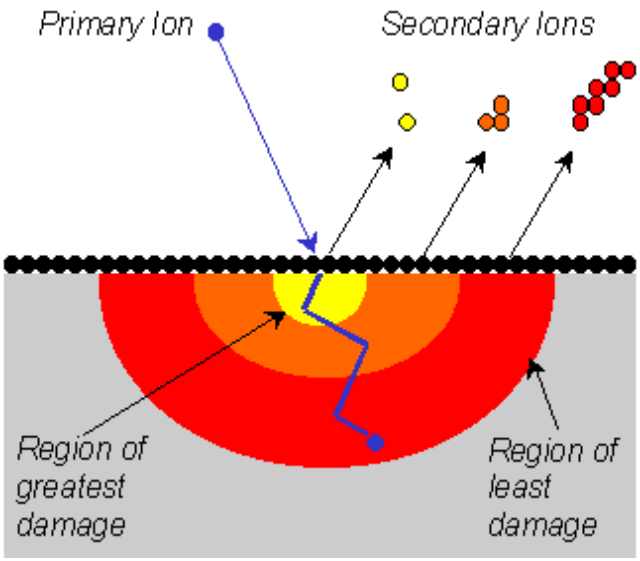


Figure 2. Schematic Diagram of the SIMS Process. [11]

The accelerated ion beam is momentarily pulsed at the sample surface. This beam of ions blasts away secondary ions from the sample. The secondary ions are then accelerated via electric field into a drift tube. All ions have nearly the same kinetic energy upon entering the drift tube. Heavier ions will therefore have a lower velocity than light ions. At the end of the drift tube is an ion detector. The high velocity light weight ions will reach the ion detector more quickly than the heavy ions. The time of arrival of each ion group is a result of their m/z ratio. A mass spectrum is constructed

from the information received at the ion detector. Once all the ions have cleared the drift tube the process can begin again. Each spectrum takes mere fractions of a second and most TOF-SIMS data is actually an aggragation of many of these brief spectra. The aggregate mass spectrum can be used to identify the compositions of the secondary ions given off by the sample surface, reflecting the composition of the sample itself [9].

TOF-SIMS is a versatile analysis method, and several techniques have been developed to fully exploit the capabilities of the instrument. Two of the most important are static imaging and dynamic depth profiling

Rastering the primary ion beam across the surface of the sample to be analyzed can effectively yield a two dimensional image of the sample composition. A spectrum is taken at each pixel in the image. Peaks of interest are selected and an image is constructed with the information gained from each point along the ion beam path highlighting the location of high and low intensity of the selected peak within a sample. This technique can be used to map out regions of chemical species with in a sample and provides some morphology data along with chemical and isotopic abundance.

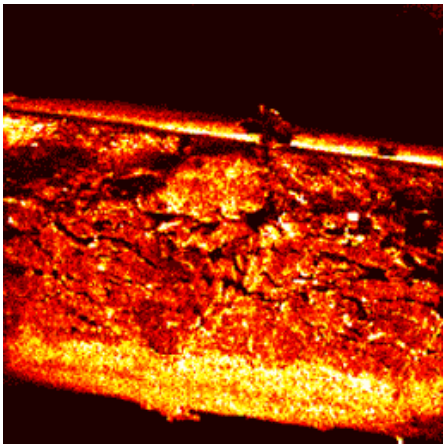


Figure 3. Two Dimensional Total Ion TOF-SIMS Image of a Coated Paper Cross-section. [11]

Further, dynamic depth profiling enables a three dimensional map of the sample composition to be produced. Dynamic TOF-SIMS depth profiling is achieved in a different method to magnetic sector SIMS. In magnetic sector SIMS the abundance of an ion is tracked real-time as the whole sample is eroded from the primary ion beam. In dynamic TOF-SIMS, two ion beams are used. The first ion beam is used exactly as described above. The second ion beam is alternated with the first. Its function is to sputter away large quantities of material from the sample surface. No spectrum is recorded during sputtering. This technique allows a series of spectra to be recorded at discrete depths within the sample [11]. Dynamic TOF-SIMS has found use in such varied applications as archeology and biotechnology [12] [13]. Along with the imaging technique described above, a three dimensional map of the sample composition can be assembled.

Certain issues arise with use of the sputtering gun, however. Unequal erosion rates for different elements, uneven erosion of the sample surface, and implantation can all occur.

Not all substances react to sputtering to the same degree. A multitude of factors go into determining an element's sputter yield. When a sample is made up of a combination of elements which do not all desorb the surface at the same rate nonstoichiometric sputtering occurs. Oxides are known to exhibit nonstoichiometric sputtering. The oxygen will preferentially desorb the surface of the sample resulting in a reduction process in the remaining sample [14].

When preferential sputtering occurs, surface roughness can also result. For example if a patch of low yield molecules cover the surface of a high yield substance an

island can form. The low yield molecules, resisting sputtering, and anything underneath them, will remain as an island while the surrounding high yield substance gets eroded away. These kinds of effects can play havoc with the assumption that sputtering will cleanly remove a layer of the sample at a time [14].

When a sputtering primary ion hits the sample surface the most likely interaction will not be for it to bounce away. Typically the sputtering ion will implant itself some distance into the surface of the sample. While this distance is usually greater than the monolayer that is analyzed after sputtering, with continued sputtering the implantation depth will be reached. The sputtering implantation pattern is dependent on many factors including sputtering species, sample species, sputtering ion energy, and sputtering angle [14].

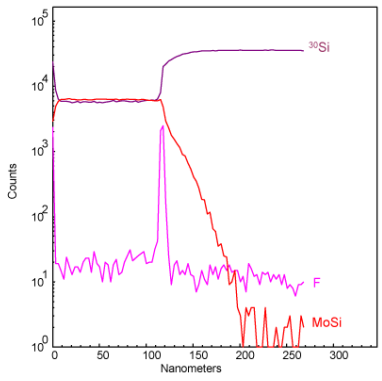


Figure 4. A TOF-SIMS sputter depth profile of a thin $MoSi_2$ film on silicon reveals the presence of a fluorine contaminant at the film / substrate interface. [11]

Previous Work

Because the half-life of uranium is so large, the isotopic distribution, and therefore the mass spectra, can be fairly well known. Previous studies have been conducted with uranium detailing its mass spectra.

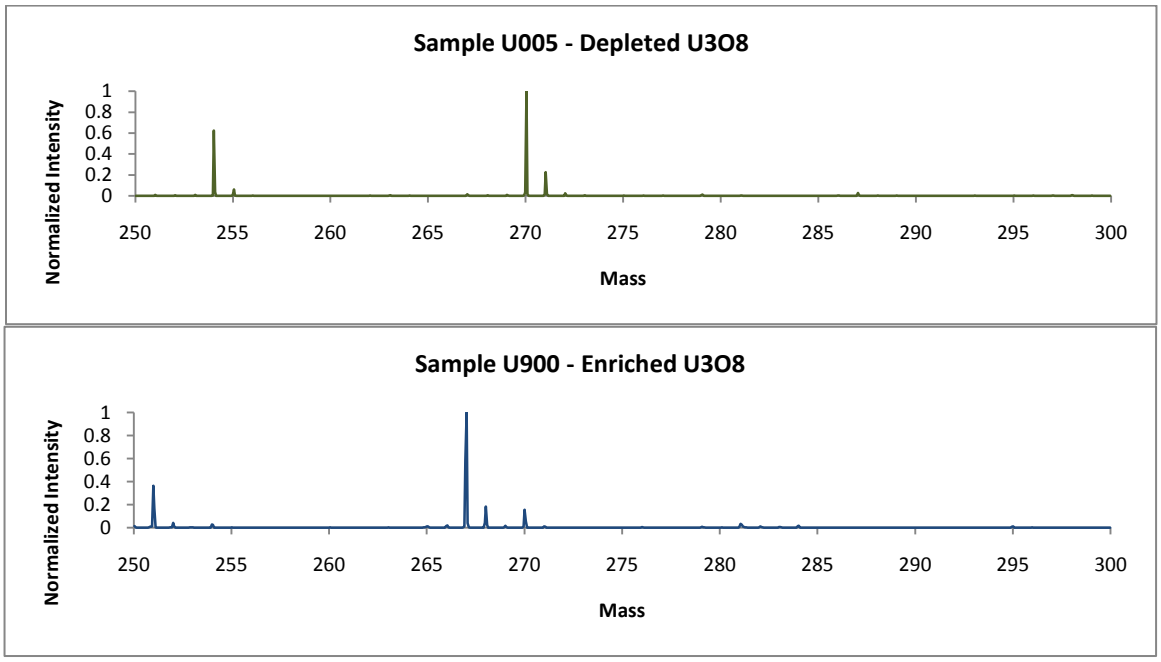


Figure 5. Partial TOF-SIMS mass spectra obtained from Schuler's study. [7]

In 2009 MSgt Schuler completed an extensive TOF-SIMS study of uranium oxides. UO_2, UO_3 and U_3O_8 samples were studied in isotopic abundances ranging from 0.5 to 90.0% U-235 [7]. Unfortunately, lack of a sputtering source to scour sample surfaces led to severe hydrocarbon surface contamination which influenced the data. Additionally without a sputtering source this study was limited to static SIMS methods yielding only surface information. Schuler was able to demonstrate the value of TOF-SIMS analysis as a potential nuclear forensic technique. He managed to overcome the

interfering effects of surface contamination and gather critical information from his data. Schuler also applied a very useful technique to determine the average oxidation state of TOF-SIMS samples [7].

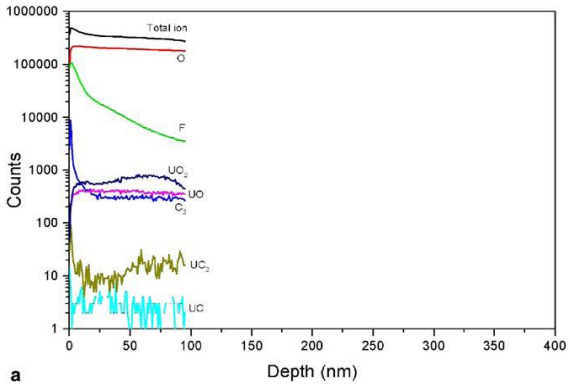


Figure 6. Chemical Composition of an Oxidized U-238 Particle from a Dynamic TOF-SIMS Study [15].

Lawrence Livermore National Laboratories (LLNL) has conducted a number of TOF-SIMS studies of uranium in recent years. In 2005 LLNL conducted a dynamic TOF-SIMS study of U-238 which had been implanted with C^+ ions. The control sample used in this 2005 study was a U-238 metal particle, exposed to the air for one year. The control provides a good estimation of what to expect from a dynamic TOF-SIMS study of uranium. However, dynamic TOF-SIMS analysis was performed on the control material only to a depth of 100 nm. The analysis suggests that the oxide layer was much thicker than 100 nm, and the oxide gradient is not properly seen. This study made no assessment of the suitability of this kind of technique for forensic analysis [15]. No treatment of higher mass ions, nor was the oxide layer characterized.

In 1998 LLNL published a study of the effect the TOF-SIMS primary ion beam has on uranium dioxide secondary ion emission [16]. A similar study was carried out in 2004 by Center Interdisciplinaire de Recherche Ions Lasers [17]. These studies show that there is a power law relationship for higher mass secondary ion yields. Different experimental parameters like primary ion beam species and degree of ionization can affect the power law exponent. Higher mass ions are believed to carry more accurate sample composition information whereas the abundance low mass ions are believed to be a product of volatilization conditions. Tailoring a TOF-SIMS operation to produce greater yields of high mass ions would be advantageous for determining the chemical composition of a sample.

In 2008 a group of scientists from the Japan Atomic Energy Agency published a magnetic sector SIMS study investigating the precision achieved for the isotopic ratio for uranium. It was determined that particle sizes of greater than 2 μm are sufficient to reduce the relative standard deviation of the U-235/U-238 ratio to 5.0% [18]. For a TOF-SIMS study, which produces lower secondary ion counts than magnetic sector SIMS, a particle size much greater than 2 μm must be analyzed for accurate results. From a forensic perspective this may limit the accuracy available for some sample analysis.

In 1999 a European static SIMS study of uranium and plutonium was carried out [19]. This study established that SIMS was a valuable tool for the forensic community. This study focused on trace chemicals contained within the nuclear material to determine the sample history. Oxide characteristics were not examined. While trace chemicals can go far to determine the bulk properties of samples, surface contamination may give

misleading results. Dynamic SIMS is required to verify trace chemical content and oxide layers give the history of a particular particle.

While studies of uranium and uranium oxide samples exist, TOF-SIMS analysis of uranium and uranium oxides has yet to be fully explored. Much more information can be gleaned from a forensic sample with proper use of this instrument. Not only could an isotopic abundance determination be achieved through TOF-SIMS, but analysis of the higher mass ions and a dynamic depth profile could yield chemical composition information enabling the oxide form of the sample to be identified.

III. Methodology

Gold Sample Mounting Technique

A previous TOF-SIMS study produced data that was contaminated by the presence of hydrocarbons. It was assumed that the high levels of protonation in U_xO_y ions were a result of this hydrocarbon contamination. In mounting uranium and uranium oxide particles for this study many precautions were taken to reduce the level of hydrocarbons present. This prohibited the use of plastics and adhesives in preparing the samples. Instead the sample particles were pressed into a clean gold surface. The sample preparation procedure can be found in Appendix A.

A thin layer of gold was placed on a copper substrate and heated to 915 degrees Celsius. An azeotrope occurs in the gold-copper phase diagram at 911 degrees. This allows a gold-copper alloy to form between the two layers without melting either layer. The heat treatment firmly attaches the gold to the copper without the use of hydrocarbon containing adhesives.

Subsequently a fine $1mm^2$ grid of lines was impressed into the soft gold surface using a machined carbide stamp. The gridlines serve as landmarks on the sample mount and facilitated the location of uranium containing particle using scanning TOF-SIMS. After the gridlines were placed on the gold and copper sample mount, uranium particles were placed on the gold surface and pressed into the surface using a hydraulic press.

For this study a total of eight different uranium containing particles were used. Uranium metal, UO_2, U_3O_8, and UO_3 particles were investigated in both natural and depleted $^{235}U/^{238}U$ isotopic ratios. Additionally data from two different enriched samples

were included in the study. See Table 2 for specific information on the samples used in this study.

Table 2: Sample Specifications

Sample	Material	Reference Name	Source	Type of Standard	Fraction U-234	Fraction U-235	Fraction U-236	Fraction U-238
nU	U metal	CRM 112-A	NBL	Metal Assay and Isotopic	.000052458	.0072017	---	.9927458
nUO_2	UO_2	---	NBL	Commercial material	.0000542	.007239	---	.99271
nU_3O_8	U_3O_8	CRM 129	NIST	Isotopic	.000052962	.0072087	.000000097	.9927382
nUO_3	UO_3	CRM 18	NIST	Uranium Assay	.000055	.0072	0	.992745
dU	U metal	CRM 115	NBL	Uranium Assay	.0000076	.0020291	.0000322	.9979311
dUO_2	UO_2	---	IBI Labs	Commercial material	---	.002-.0035	---	---
dU_3O_8	U_3O_8	---	IBI Labs	Commercial material	---	.002-.0035	---	---
dUO_3	UO_3	---	IBI Labs	Commercial material	---	.002-.0035	---	---
U500*	U_3O_8	CRM U500	NBL	Isotopic	.005181	.49696	.000755	.49711
U900*	U_3O_8	CRM U900	NBL	Isotopic	.007777	.90196	.003327	.08693

*Sample materials were not actually used in the course of this experiment, but spectra from these samples were utilized.

TOF-SIMS Parameters

The mounted samples were analyzed in an IONTOF TOF-SIMS V. A cycle time of 185 us was chosen allowing ion clusters of up to 3000 amu to be detected. The samples were analyzed using a Bi_3^{++} primary ion beam. The primary ion beam accelerated ions to 25 keV and 50 keV[1] at a target current of approximately 0.3 pA. A resolution of 256x256 was used for each image data collection. The sputtering beam used was a $C60^+$ gun. The $C60^+$ gun accelerated ions to 10 keV and a target current of approximately 1.4 nA. The sputtering area was 300x300 μm, greater than any of the analysis areas in this study.

[1] The TOF-SIMS required re-optimization of beam parameters part way through this study resulting in two different primary ion beam energies.

Data Collection Process and Parameters

For each sample a uranium-containing particle was located by scanning the gold surface using the primary ion beam monitoring U^+, UO^+, UO_2^+, and UO_3^+ ions. Once a particle was located, a 150 scan (30 minute) positive spectrum was recorded followed by a 150 scan (30 minute) negative spectrum. One scan samples data from each of the 256x256 pixels in the analysis area. The buckyball sputtering beam was then used to irradiate the particle for 5 scans in an effort off any surface contamination. Five scans of the sputtering gun translates very roughly to etching 0.5 nm of surface thickness. After this first sputtering period another positive/negative pair of spectra was recorded. The sputtering beam was then again directed onto the sample for 20 scans to erode some thickness into the particle. Twenty sputtering scan equates roughly to 2 nm of material. A third pair of positive/negative spectra was recorded. Again the sputtering beam was directed onto the sample for 20 scans and a fourth pair of spectra was recorded.[2]

[2] For the dUO2 sample a positive/negative pair of spectra was recorded followed by 2 sputtering scans, a second pair of spectra, 2 sputtering scans, a third pair of spectra, 2 sputtering scans, a fourth pair of spectra, 20 sputtering scans, and a final fifth pair of spectra. See Table 3.

Table 3: Collection Conditions for all Spectra Acquired in the Study.

Sample: nU		
Spectrum Name	**Positive**	**Negative**
nU001	X	
nU002		X
5 Sputtering Scans		
nU003	X	
nU004		X
20 Sputtering Scans		
nU005	X	
nU006		X
20 Sputtering Scans		
nU007	X	
nU008		X

Sample: dU		
Spectrum Name	**Positive**	**Negative**
dU001	X	
dU002		X
5 Sputtering Scans		
dU003	X	
dU004		X
20 Sputtering Scans		
dU005	X	
dU006		X
20 Sputtering Scans		
dU007	X	
dU008		X

Sample: nUO2		
Spectrum Name	**Positive**	**Negative**
nUO2001	X	
nUO2002		X
5 Sputtering Scans		
nUO2003	X	
nUO2004		X
20 Sputtering Scans		
nUO2005	X	
nUO2006		X
20 Sputtering Scans		
nUO2007*	X	
nUO2008*		X

*continued the next day

Sample: dUO2		
Spectrum Name	**Positive**	**Negative**
dUO2012	X	
dUO2013		X
2 Sputtering Scans		
dUO2014	X	
dUO2015		X
2 Sputtering Scans		
dUO2016	X	
dUO2017		X
2 Sputtering Scans		
dUO2018	X	
dUO2019		X
20 Sputtering Scans		
dUO2020	X	
dUO2021		X

Sample: nU3O8		
Spectrum Name	**Positive**	**Negative**
nU3O8001	X	
nU3O8002		X
5 Sputtering Scans		
nU3O8003	X	
nU3O8004		X
20 Sputtering Scans		
nU3O8005	X	
nU3O8006		X
20 Sputtering Scans		
nU3O8007	X	
nU3O8008		X

Sample: dU3O8		
Spectrum Name	**Positive**	**Negative**
dU3O8001	X	
dU3O8002		X
5 Sputtering Scans		
dU3O8003	X	
dU3O8004		X
20 Sputtering Scans		
dU3O8005	X	
dU3O8006		X
20 Sputtering Scans		
dU3O8007	X	
dU3O8008		X

Sample: nUO3		
Spectrum Name	**Positive**	**Negative**
nUO3001	X	
nUO3002		X
5 Sputtering Scans		
nUO3003	X	
nUO3004		X
20 Sputtering Scans		
nUO3005*	X	
nUO3006*		X
20 Sputtering Scans		
nUO3007*	X	
nUO3008*		X

*continued the next day

Sample: dUO3		
Spectrum Name	**Positive**	**Negative**
dUO3001	X	
dUO3002		X
5 Sputtering Scans		
dUO3003	X	
dUO3004		X
20 Sputtering Scans		
dUO3005	X	
dUO3006		X
20 Sputtering Scans		
dUO3007	X	

IV. Data Analysis/ Results

Isotope Determination

An isotopic calculator was developed in this study to evaluate TOF-SIMS capability to make a rapid isotopic determination. This information is both valuable to nuclear forensic community and essential for subsequent mass spectrum analysis of unknown samples.

The isotopic calculator was tested against the sample standards, nU3O8, U500, and U900, as described in Table 2. All three of these samples are U_3O_8 particles and they cover a range of enrichments from 0.72% to 90% U-235. Data from this experiment, spectrum nU3O8001, and data from a previous experiment, spectra U50001P and U90001P, were used for this analysis. The isotopic calculator inputs mass spectrum data for a given U_xO_y ion and reports the estimated uranium isotopics.

Each U_xO_y ion will result in a series of mass spectrum peaks due to the existence of multiple isotopes of both uranium and oxygen. This series of peaks holds the isotopic information for the sample particle. Most peaks have intensity contributions from multiple isomers having varying uranium and oxygen isotopes. Additionally, uranium oxide ions show a tendency to protonate, or take up a hydrogen atom, creating additional peaks. A linear equation summing each of these component intensity contributions can be constructed for each peak. A system of linear equations is formed by the equations for each individual peak which can be solved for the uranium isotopics and protonation percentage.

The system of equations for U^+ ion (with contributions from UH^+ and UH_2^+) are:

$$
\begin{aligned}
Peak_{234} &= fU234\cdot[1-(P1\cdot fH1)-(P1\cdot fH2)-(P2\cdot fH1)] \\
Peak_{235} &= fU235\cdot[1-(P1\cdot fH1)-(P1\cdot fH2)-(P2\cdot fH1)]+fU234\cdot[P1\cdot fH1] \\
Peak_{236} &= fU236\cdot[1-(P1\cdot fH1)-(P1\cdot fH2)-(P2\cdot fH1)]+fU235\cdot[P1\cdot fH1]+fU234\cdot[(P1\cdot fH2)+(P2\cdot fH1)] \\
Peak_{237} &= fU237\cdot[1-(P1\cdot fH1)-(P1\cdot fH2)-(P2\cdot fH1)]+fU236\cdot[P1\cdot fH1]+fU235\cdot[(P1\cdot fH2)+(P2\cdot fH1)] \\
Peak_{238} &= fU238\cdot[1-(P1\cdot fH1)-(P1\cdot fH2)-(P2\cdot fH1)]+fU237\cdot[P1\cdot fH1]+fU236\cdot[(P1\cdot fH2)+(P2\cdot fH1)] \\
Peak_{239} &= fU238\cdot[P1\cdot fH1]+fU237\cdot[(P1\cdot fH2)+(P2\cdot fH1)] \\
Peak_{240} &= fU238\cdot[(P1\cdot fH2)+(P2\cdot fH1)]
\end{aligned}
\tag{2}
$$

where $Peak_{XXX}$ is the total number of counts in peak XXX, fU234 is the atom fraction of U-234 in the sample, fU235 is the atom fraction of U-235 in the sample, fU236 is the atom fraction of U-236 in the sample, fU237 is the atom fraction of U-237 in the sample, fU238 is the atom fraction of U-238 in the sample, P1 is the percentage of uranium atoms that have protonated, P2 is the percentage of uranium atoms that have taken up two hydrogen atoms, or diprotonated, fH1 is the atom fraction of H-1, and fH2 is the atom fraction of deuterium.

The system of equations used for UO^+ and UO_2^+ ions can be found in Appendix B. As additional atoms are added to the ion the number of equations and the number of terms in each equation grows rapidly leaving this exercise best left to a computer for large ions.

Contamination can hinder efforts to make an accurate isotopic determination. Several commonly found metals can produce contributions to peaks in the UO_y peak range reducing the accuracy of an isotopic determination. Various isotopes of PbAl ions, PbSi ions, PbO_2 ions, and Sn_2 ions are likely to have produced peak interference in these spectra [10].

The isotope calculator presented in Appendix C was written in Matlab. It inputs mass spectrum data along with an initial assumption for the uranium isotopics and percentage of protonation and diprotonation. The spectrum to be analyzed is input into

the Select File textbox. Initial Assumptions for isotopics and protonation are entered in to the Initial Assumptions box. Natural isotopic abundance and 10 to 20 percent protonation are good starting assumptions. If the results show a marked difference from the initial assumptions, the assumptions can be refined to obtain the most accurate answer. The target U_xO_y ion which the isotopic determination will be obtained from is specified by the user in the Specify Ion box. "+" should be selected for positive spectra, "-" should be selected for negative spectra.

Once all data is entered, clicking the "Calculate" button begins the isotopic determination. The program uses the specified ion to selected relevant peaks. These peaks are located, have their background subtracted, and their peak counts calculated. The full system of equations for the input ion is constructed and the relative peak counts are fed into an iterative solver which settles on an isotopic determination for uranium, and the protonation percentage.

When the determination is complete the Results box and graph will update. The Results box reports the fractionation of the uranium; the fraction of protonation and diprotonation; R^2, a goodness of fit parameter, where 0 would be the ideal value; and the total counts for all peaks attributed to the ion. The estimated error reported by the calculator are one sigma values based on counting statistics.

The isotope calculator was tested against U_3O_8 particles of three different isotopic abundances. The isotopic determination for the most abundant ion for each uranium series is reported in Table 4.

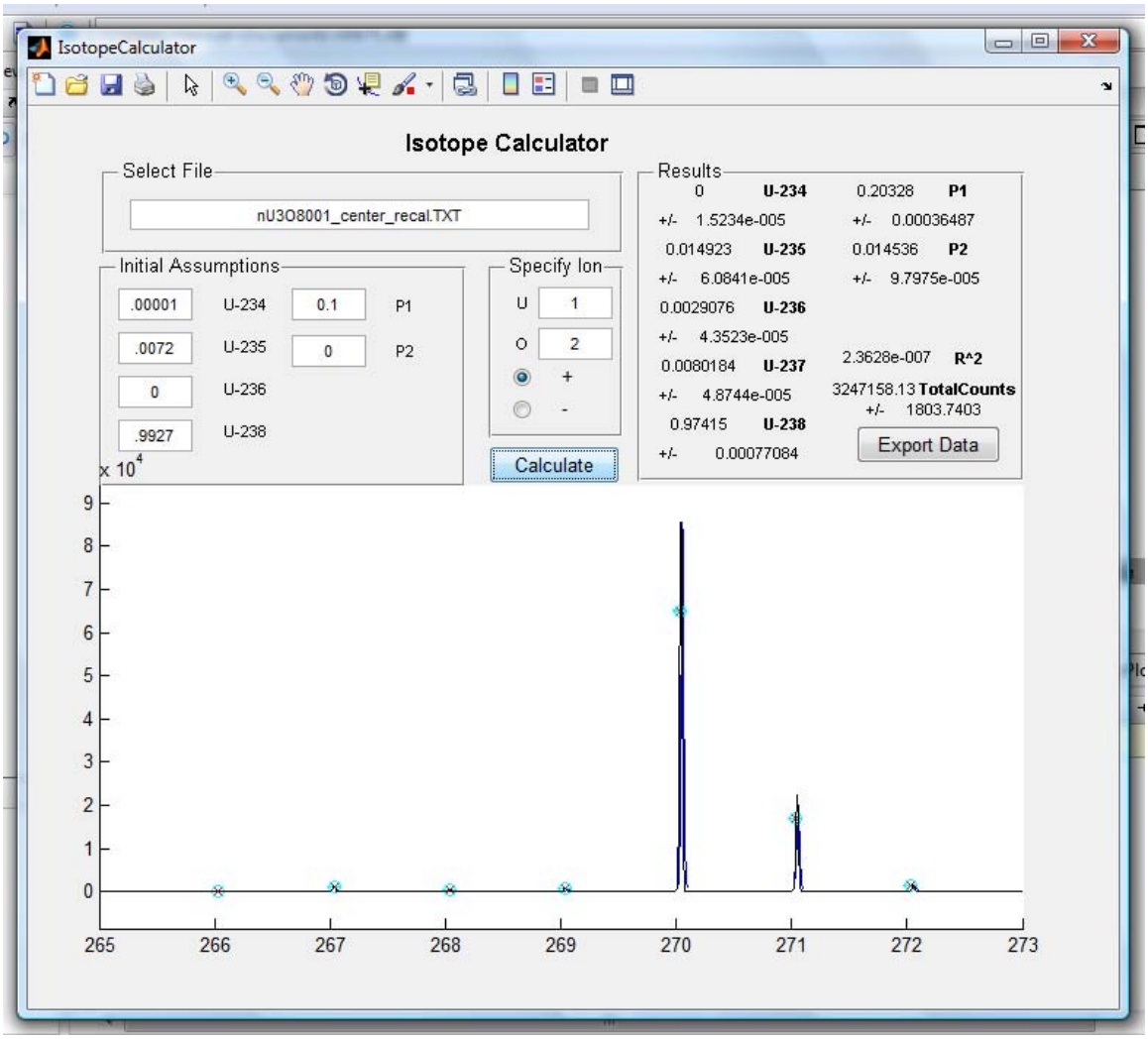


Figure 7: Screenshot of the Isotope Calculator interface. The graph displays a wealth of information in one easy to read format. The blue lines show the actual background subtracted data from the input spectrum. The cyan circles (with error bars) show the relative fraction of counts for each peak. The red "x" s show the relative fraction of counts calculated for each peak from the determined isotopics. The black line shows the recreated spectrum from the determined isotopics.

Table 4: Results of the Isotope Calculator for three samples of varying enrichments. The estimated errors are one sigma values based on counting statistics.

	fU234	fU235	fU236	fU237	fU238
Natural U3O8					
Standard	0.000052962	0.0072087	0.000000097	0.0000000	0.9927382
UO2+	0.00005 +/- 0.00002	0.01841 +/- 0.00006	0.00560 +/- 0.00004	0.01118 +/- 0.00005	0.96477 +/- 0.00077
U2O4+	0.00023 +/- 0.00000	0.00692 +/- 0.00022	0.00393 +/- 0.00019	0.00000 +/- 0.00010	0.98891 +/- 0.00244
U3O7+	0.00000 +/- 0.00013	0.00557 +/- 0.00045	0.00000 +/- 0.00030	0.00000 +/- -0.00020	0.99443 +/- 0.00417
U4O9+	0.00001 +/- 0.00000	0.00277 +/- 0.00117	0.00000 +/- -0.00136	0.00000 +/- 0.00000	0.99722 +/- 0.00921
U5O11+	0.00000 +/- 0.00000	0.00000 +/- 0.00000	0.00000 +/- 0.00000	0.00424 +/- 0.00412	0.99576 +/- 0.02264
50% Enriched U3O8					
Standard	0.00518	0.49696	0.00076	0.00000	0.49711
UO2+	0.01139 +/- 0.00005	0.50043 +/- 0.00041	0.00405 +/- 0.00017	0.00000 +/- -0.00007	0.48413 +/- 0.00040
U2O4+	0.00907 +/- 0.00064	0.49602 +/- 0.00259	0.00000 +/- -0.00148	0.00000 +/- 0.00104	0.49491 +/- 0.00430
U3O6+	0.00005 +/- ---	0.51097 +/- ---	0.00326 +/- ---	0.00000 +/- 0.00583	0.48572 +/- 5.19730
90% Enriched U3O8					
Standard	0.00778	0.90196	0.00333	0.00000	0.08693
UO2+	0.02333 +/- 0.00007	0.88434 +/- 0.00064	0.01166 +/- 0.00027	0.00000 +/- 0.00010	0.09233 +/- 0.00015
U2O4+	0.00005 +/- 0.00045	0.90651 +/- 0.00297	0.02622 +/- 0.00112	0.00010 +/- 0.00055	0.09324 +/- 0.00102
U3O6+	0.00001 +/- 0.00114	0.91444 +/- 0.00702	0.00000 +/- 0.00230	0.00000 +/- 0.00145	0.08531 +/- 11.26200
U4O8+	0.00564 +/- 0.38280	0.92707 +/- ---	0.00000 +/- ---	0.00000 +/- 0.00000	0.06729 +/- 0.45781

Table 5: Absolute error for Isotope Calculations.

	fU234	fU235	fU236	fU237	fU238
Natural U3O8					
UO2+	0.0000	0.0112	0.0056	0.0112	0.0280
U2O4+	0.0002	0.0003	0.0039	0.0000	0.0038
U3O7+	0.0001	0.0016	0.0000	0.0000	0.0017
U4O9+	0.0000	0.0044	0.0000	0.0000	0.0045
U5O11+	0.0001	0.0072	0.0000	0.0042	0.0030
50% Enriched U3O8					
UO2+	0.0062	0.0035	0.0033	0.0000	0.0130
U2O4+	0.0039	0.0009	0.0008	0.0000	0.0022
U3O6+	0.0051	0.0140	0.0025	0.0000	0.0114
90% Enriched U3O8					
UO2+	0.0156	0.0176	0.0083	0.0000	0.0054
U2O4+	0.0077	0.0046	0.0229	0.0001	0.0063
U3O6+	0.0078	0.0125	0.0033	0.0000	0.0016
U4O8+	0.0021	0.0251	0.0033	0.0000	0.0196

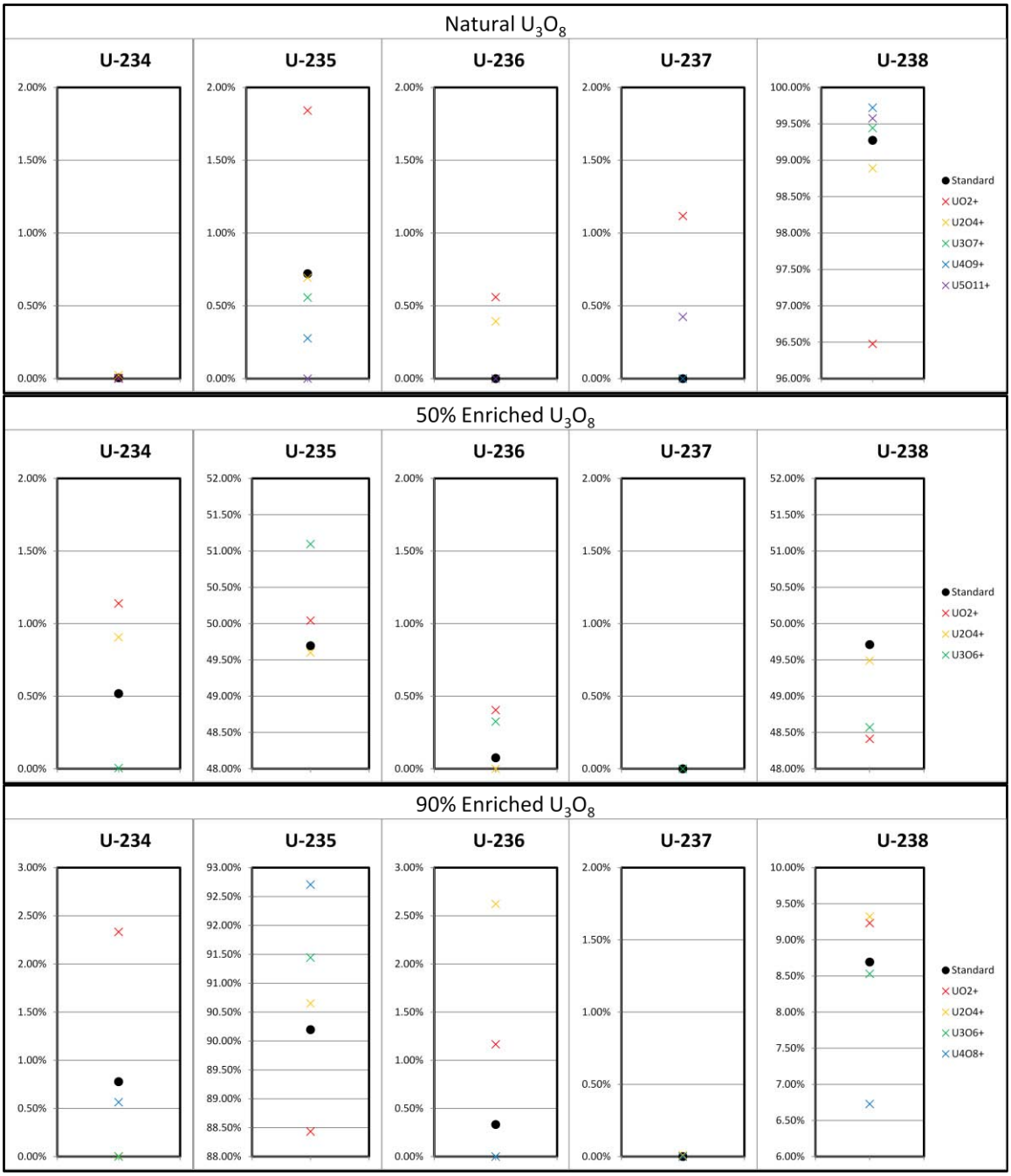


Figure 8: Graphical Representation of Table 4.

Protonation Determination

Any in-depth analysis of mass spectrum data requires that the degree of protonation for a given U_xO_y ion must be quantified. Most analysis requires that the total number of counts for the ion be known. The mass resolution necessary to distinguish the UxOy counts from the UxOyH counts is currently unattainable [10]. This leaves quantification of protonation to a mathematical exercise. Degree of protonation was calculated in two ways.

A Protonation Calculator, found in Appendix D, was developed. This calculator works in much the same way as the isotopic calculator. It inputs mass spectrum data along with the known uranium isotopics and an initial guess at the percentage of protonation and diprotonation. The spectrum to be analyzed is input into the Select File textbox. The known isotopics and initial assumptions for protonation are entered in to the Isotopics and Initial Assumptions box. Ten to 20 percent protonation is a good starting assumption. If the results show a marked difference from the initial assumptions, the assumptions can be refined to obtain the most accurate answer. The target U_xO_y ion, for which the protonation determination is calculated, is specified by the user in the Specify Ion box. "+" should be selected for positive spectra, "-" should be selected for negative spectra.

Once all data is entered clicking the "Calculate" button begins the protonation determination. The program uses the specified ion to selected relevant peaks. These peaks are located, have their background subtracted, and their peak counts calculated. The appropriate system of equations is constructed and the relative peak counts are fed into an iterative solver which settles on the protonation percentage for the ion.

When the determination is complete the Results box and graph will update. The Results box reiterates the fractionation of the uranium; and reports the fraction of protonation and diprotonation; R^2, a goodness of fit parameter, where zero would be the ideal value; and the total counts for all peaks attributed to the ion. The estimated error reported by the calculator are one sigma values based on counting statistics. Table 6 shows the protonation values for each prominate ion in the nU001 spectrum. Protonation values for all other spectra can be found in Appendix E.

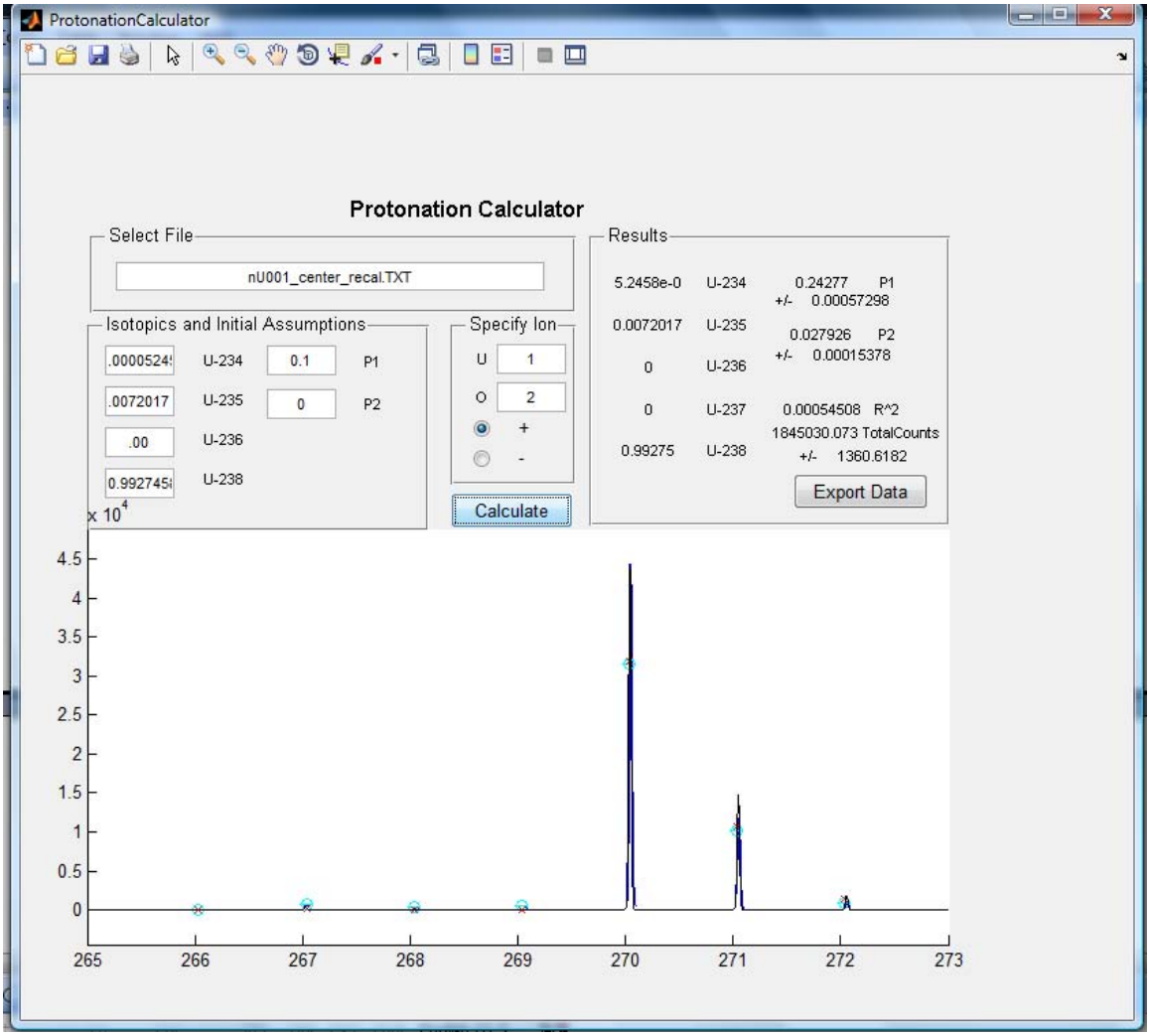


Figure 9: Screenshot of the Protonation Calculator interface. The graph displays a wealth of information in one easy to read format. The blue lines show the actual background subtracted data from the input spectrum. The cyan circles (with errorbars) show the relative fraction of counts for each peak. The red "x" s show the relative fraction of counts calculated for each peak from the determined isotopics. The black line shows the recreated spectrum from the determined isotopics.

Table 6: Tabulated protonation values and total counts for each prominate peak in the nU001 spectrum.

Spectrum:	nU001					
Isotopics:	**234:**	0.0000525	**235:**	0.0072017	**236:**	0.0000000
	237:	0.0000000	**238:**	0.9927458		

Ion		**P1**	**P2**	**TotalCounts**	**Residual**
U	**O**				
1	0	0.458810 +/- 0.011475	0.107030 +/- 0.003763	47563 +/- 241	0.022024
1	1	0.230960 +/- 0.001129	0.034217 +/- 0.000296	428354 +/- 661	0.002181
1	**2**	**0.242770 +/- 0.000573**	**0.027926 +/- 0.000154**	**1845030 +/- 1361**	**0.000545**
1	3	0.649830 +/- 0.658030	0.266440 +/- 0.233640	153616 +/- 402	0.026017
2	2	0.000000 +/- 0.000000	0.000000 +/- -0.017376	1721 +/- 85	0.000366
2	3	0.032250 +/- 0.001883	0.018359 +/- -0.000877	28256 +/- 197	0.000302
2	**4**	**0.138040 +/- 0.000968**	**0.002675 +/- 0.000251**	**243239 +/- 505**	**0.000110**
2	5	0.508100 +/- 0.006065	0.018695 +/- 0.001155	134100 +/- 381	0.000209
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.002636	7248 +/- 112	0.001102
3	6	0.051230 +/- 0.001221	0.000000 +/- -0.000536	62829 +/- 267	0.000251
3	**7**	**0.124470 +/- 0.001757**	**0.000000 +/- -0.000569**	**79185 +/- 299**	**0.000509**
3	8	0.607090 +/- 0.072334	0.000000 +/- -0.019976	3073 +/- 96	0.000761
4	7	0.000000 +/- 0.000000	0.000000 +/- -0.014290	1309 +/- 70	0.002004
4	8	0.000000 +/- 0.002462	0.000000 +/- -0.001701	15087 +/- 144	0.001046
4	**9**	**0.060749 +/- 0.002802**	**0.000000 +/- -0.001280**	**23113 +/- 174**	**0.001070**
4	10	0.219720 +/- 0.034577	0.000000 +/- -0.022164	1609 +/- 80	0.001190
5	9	0.000000 +/- 0.000000	0.000000 +/- -0.031659	248 +/- 51	0.003002
5	10	0.000000 +/- 0.000000	0.000000 +/- -0.004611	4802 +/- 94	0.003417
5	**11**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.004353**	**6093 +/- 108**	**0.003684**
5	12	0.000000 +/- 0.000000	0.000000 +/- -0.021605	1325 +/- 70	0.003960
6	12	0.000000 +/- 0.000000	0.000000 +/- -0.034727	859 +/- 57	0.004862
6	**13**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.028177**	**1095 +/- 69**	**0.005176**
6	14	0.000000 +/- 0.000000	0.000000 +/- -0.101590	373 +/- 55	0.005498
7	**15**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.036006**	**181 +/- 48**	**0.006898**

Additionally ratios of protonated and di-protonated peaks were ratio-ed to the high intensity U-238 peak for each ion. Table 7 shows these ratios for spectrum nU001. Values for all other spectra are located in Appendix F.

Table 7: Counts in the intense U-238 peak and ratios of the U-238 protonated and diprotonated peaks to the U-238 peak for each prominate ion in the nU001 spectrum. The dominate ion for each uranium series is highlighted. A qualitative determination of the most probable dominate ion is made for the higher uranium series.

Spectrum: nU001				
Ion		**Counts (U-238 Peak)**	**(U-238+1) Peak / 238 Peak**	**(U-238+2) Peak / U-238 Peak**
U	**O**			
1	0	17856 +/- 137	1.06671 +/- 0.01147	0.13538 +/- 0.00377
1	1	303360 +/- 552	0.29566 +/- 0.00113	0.02163 +/- 0.00029
1	**2**	**1311957 +/- 1146**	**0.32466 +/- 0.00057**	**0.02973 +/- 0.00015**
1	3	2710 +/- 67	33.03191 +/- 0.82801	11.45472 +/- 0.29217
2	2	1721 +/- 49	0.0 +/- ---	0.0 +/- ---
2	3	26250 +/- 167	0.03496 +/- 0.00188	0.0 +/- ---
2	**4**	**203259 +/- 452**	**0.15876 +/- 0.00097**	**0.00756 +/- 0.00025**
2	5	61879 +/- 251	1.07504 +/- 0.00606	0.05204 +/- 0.00116
3	5	7248 +/- 89	0.0 +/- ---	0.0 +/- ---
3	6	57868 +/- 243	0.06192 +/- 0.00122	0.0 +/- ---
3	**7**	**67703 +/- 263**	**0.15704 +/- 0.00176**	**0.00067 +/- 0.00057**
3	8	1173 +/- 46	1.52952 +/- 0.07596	0.0 +/- ---
4	7	1309 +/- 46	0.0 +/- ---	0.0 +/- ---
4	8	14801 +/- 124	0.01934 +/- 0.00246	0.0 +/- ---
4	**9**	**21172 +/- 149**	**0.09168 +/- 0.00280**	**0.0 +/- ---**
4	10	1230 +/- 47	0.30825 +/- 0.03460	0.0 +/- ---
5	9	234 +/- 30	0.0 +/- ---	0.0 +/- ---
5	10	4802 +/- 76	0.0 +/- ---	0.0 +/- ---
5	**11**	**6093 +/- 84**	**0.0 +/- ---**	**0.0 +/- ---**
5	12	1272 +/- 47	0.0 +/- ---	0.0 +/- ---
6	12	859 +/- 42	0.0 +/- ---	0.0 +/- ---
6	**13**	**1095 +/- 50**	**0.0 +/- ---**	**0.0 +/- ---**
6	14	373 +/- 37	0.0 +/- ---	0.0 +/- ---
7	**15**	**172 +/- 33**	**0.0 +/- ---**	**0.0 +/- ---**
8	**17**	**--- +/- ---**	**--- +/- ---**	**--- +/- ---**
9	**19**	**--- +/- ---**	**--- +/- ---**	**--- +/- ---**
10	**21**	**--- +/- ---**	**--- +/- ---**	**--- +/- ---**

The degree of protonation that a given U_xO_y ion may experience was found to have some dependance on how favored that ion may be to form. Ions containing one more oxygen than the dominate ion were found to have a much higher degree of

protonation. The relative level of protonation an ion experiences may hold some information on the stability of ion coming off the surface. Ions containing a greater number of uranium atoms were also found to have a lower level of protonation.

Dominate Ion

The dominate ions were identified for each positive surface spectrum. It was found that the dominate three and four uranium ions for UO_2 contained less oxygen than the other oxides. While the abundance of low mass ions is generally considered to be more telling of instrument conditions than sample surfaces, high mass ions, like the ones here, may hold information on sample make-up.

Table 8: Dominate Ions for each positive surface spectrum.

Sample	Dominate Ion			
nUO2	UO_2^+	$U_2O_4^+$	**$U_3O_6^+$**	---
dUO2	UO_2^+	$U_2O_4^+$	**$U_3O_6^+$**	**$U_4O_8^+$**
nU3O8	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$
dU3O8	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$
nUO3	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$
dUO3	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$
nU	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$
dU	UO_2^+	$U_2O_4^+$	$U_3O_7^+$	$U_4O_9^+$

Protonation Depth Profile

It is commonly believed that the level of protonation observed in a spectrum is related to hydration. H_2O^+ ion abundance was determined for each spectrum in an effort

to relate the overall level of protonation back to relative hydration level. The fraction of H_2O^+ ions to total secondary ions was plotted as a function of sputtering depth. Likewise the fraction of protonated $U_xO_y^+$ ions to total $U_xO_y^+$ ions was plotted as a function of sputtering depth. It was found that the two trends do not correlate. A surface level dehydration is found for nearly all particles. This can be attributed to the ultra high vacuum conditions of the TOF-SIMS. This followed by a layer of increased hydration which may describe the traditional surface layer of the particle. This increased hydration layer is followed by a layer of decreased hydration, possibly describing the bulk hydration of the particle. Protonation on the other hand was found to be a surface phenomenon. In nearly all cases the highest levels of protonation were found on the surface of the particle. Both UO_2 and U_3O_8 particles then show a steep reduction in protonation while UO_3 particles have a nearly level region of protonation followed by a more moderate reduction in protonation. These trends may relate to the acid/base behavior of the oxides.

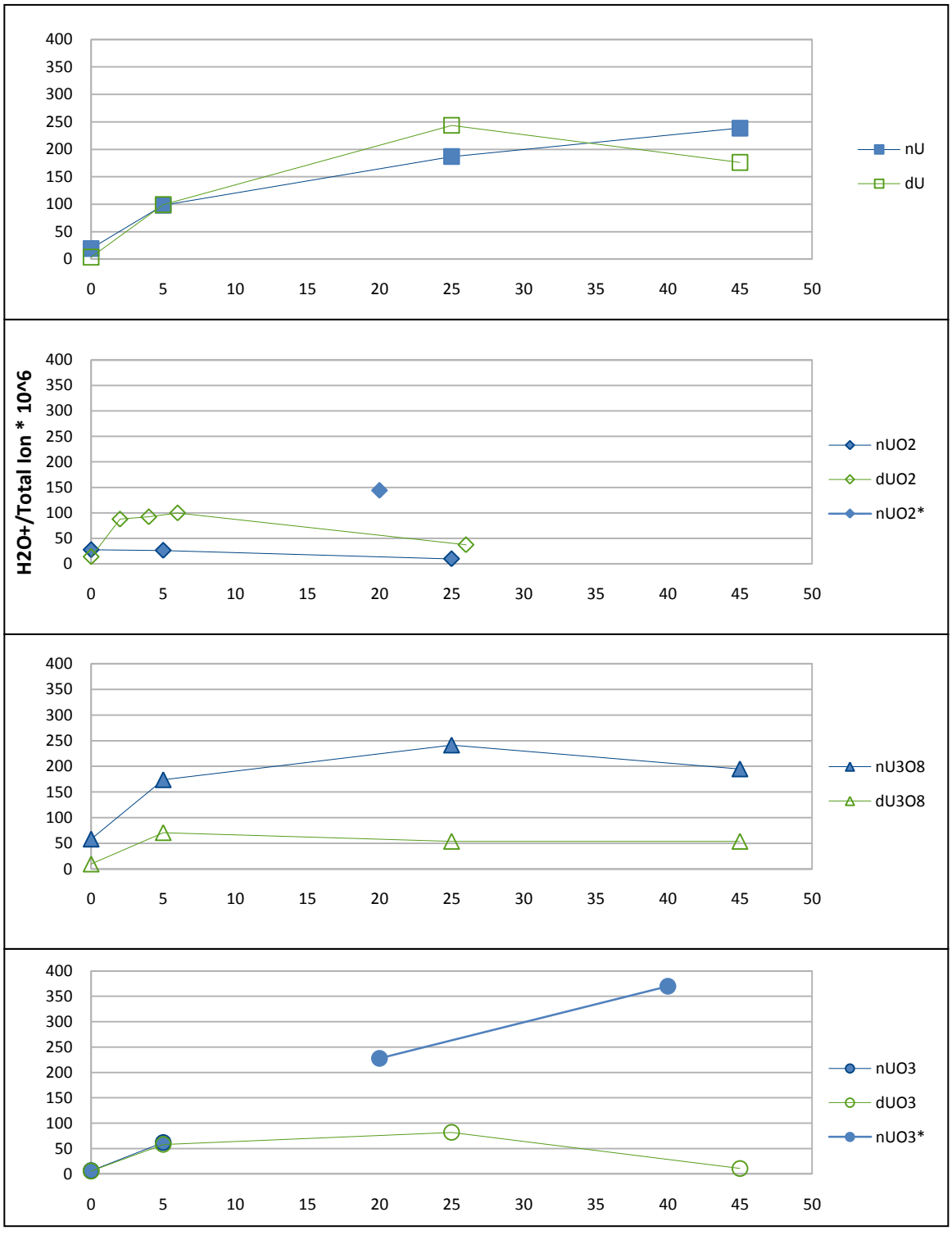


Figure 10: Micro-Fraction of H_2O^+ as compared to total ion count. In nearly all particles a surface level dehydration is seen. *A break in analysis where the samples were exposed to air occurred during the nUO2 and nUO3 data collection.

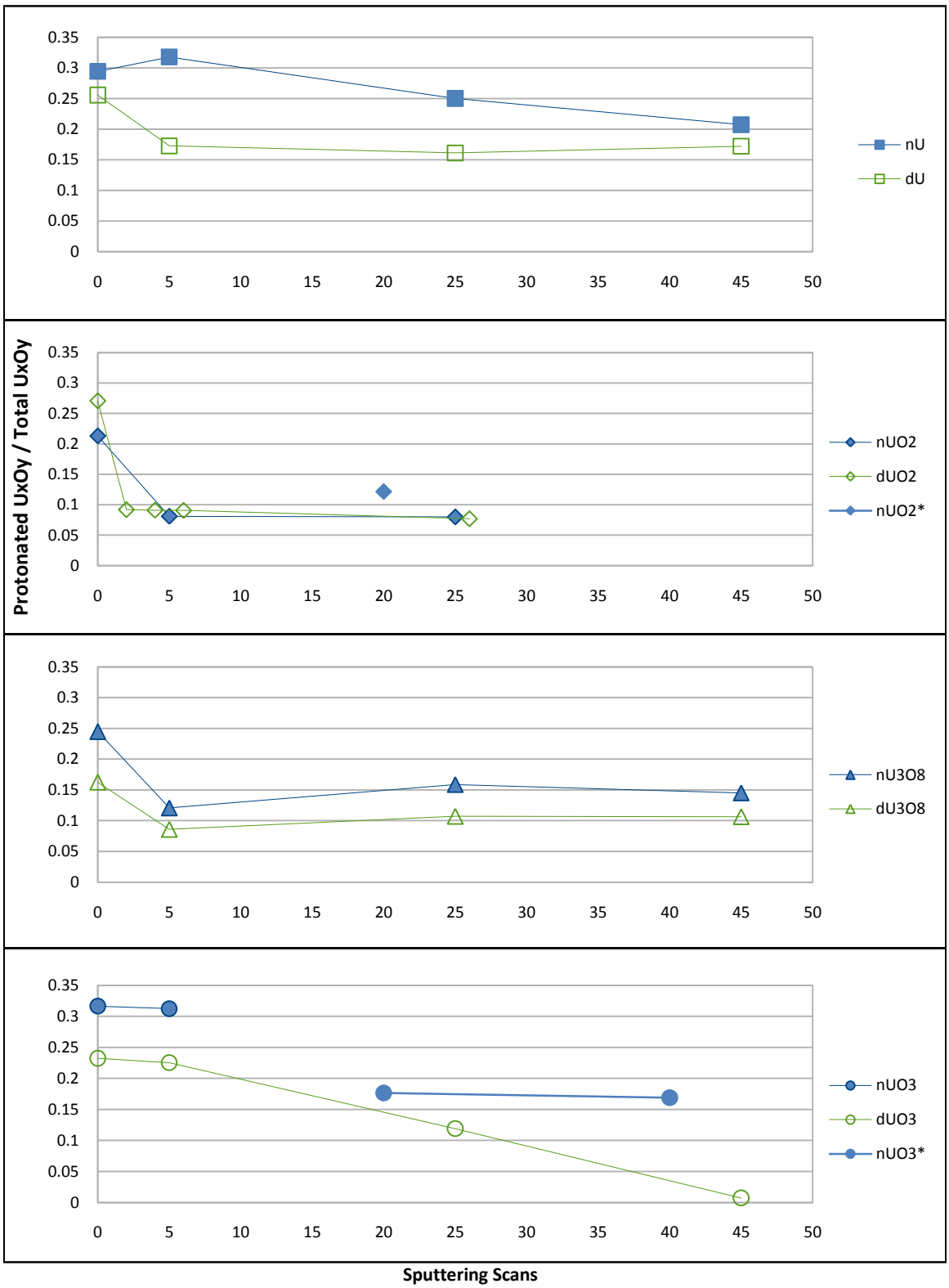


Figure 11: Fraction of protonated $UxOy^{+}$ ions as a function of depth for each particle. *A break in analysis where the samples were exposed to air occurred during the nUO2 and nUO3 data collection.

Lattice Valence

A fragment valence, K, was calculated for each U_xO_y ion and plotted against its intensity to obtain G^o, the lattice valence, as in Plog et al. [6]. The fragment valence can also be described as the average oxidation state of uranium in each ion. The lattice valence is assumed to hold some relation to the average oxidation state of the sample material, but that relationship has not been fully described. The data shows a decrease in lattice valence as particle depth increases. The valence graphs for spectra nU001 and nU002 is shown in Figure 12. Companion positive and negative log files generated by the Protonation Calculator are input into the Enter Data box. The Results box reports the Gaussian mean for the negative and positive ions in each uranium series for which there is three are more data points, G^+ and G^-. G^0, the lattice valence, is obtained by averaging the two. The left graph displays the positive spectrum data where the x-axis is the fragment valence for each ion and the y-axis is unprotonated counts for each ion. The right graph similarly displays the negative spectrum data. Gaussian curves are fit to each uranium series. Lattice valences are tabulated in Table 9.

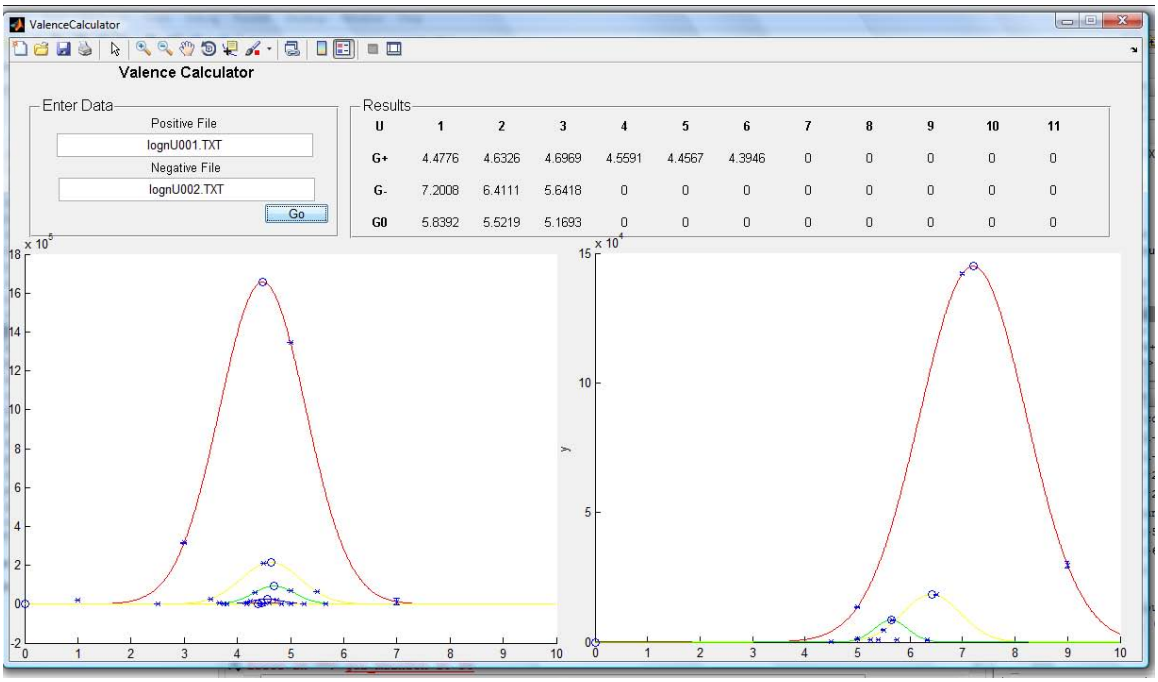


Figure 12: Screenshot of the Valence Calculator used to generate valence graphs as in Plog et al. [6]. The left graph displays the positive spectrum data where the x-axis is the fragment valence for each ion and the y-axis is unprotonated counts for each ion. The right graph similarly displays the negative spectrum data. Gaussian curves are fit to each uranium series. U1 – red, U2 – yellow, U3 – green, U4 – blue, U5 – red, U6 – yellow, U7 – green, U8 – blue, etc.

Table 9: Tabulated lattice valence for all spectra. Depth is measured in the cumulative number of C60 sputtering scans from the particle surface. A break in analysis where the samples were exposed to air occurred during the nUO2 and nUO3 data collection. It is probable that reoxidation occurred during these periods.

Particle	Depth-Sputtering Scans	U Series		
		1	2	3
nU	0	4.6936	5.1960	4.8441
	5	4.1322	4.3024	---
	25	4.0582	---	---
	45	4.0454	---	---
nUO2	0	4.6879	---	---
	5	4.3510	---	---
	25	3.7488	---	---
	45	4.5566	---	---
nU3O8	0	5.2418	5.0904	---
	5	5.0343	4.8980	---
	25	4.5267	4.5285	---
	45	4.3549	---	---
nUO3	0	4.9049	4.9653	4.9709
	5	4.4381	---	---
	25	4.8660	---	---
	45	4.6823	---	---
dU	0	4.9649	4.8592	4.8733
	5	4.6399	---	---
	25	4.5257	---	---
	45	4.4021	---	---
dUO2	0	5.2810	---	---
	2	4.8678	---	---
	4	4.7584	---	---
	6	4.7434	---	---
	26	4.6006	---	---
dU3O8	0	5.1875	5.0754	---
	5	5.0393	---	---
	25	4.4408	---	---
	45	4.3371	---	---
dUO3	0	5.2684	5.0578	4.9684
	5	4.6128	---	---
	25	4.3664	---	---
	45	---	---	---

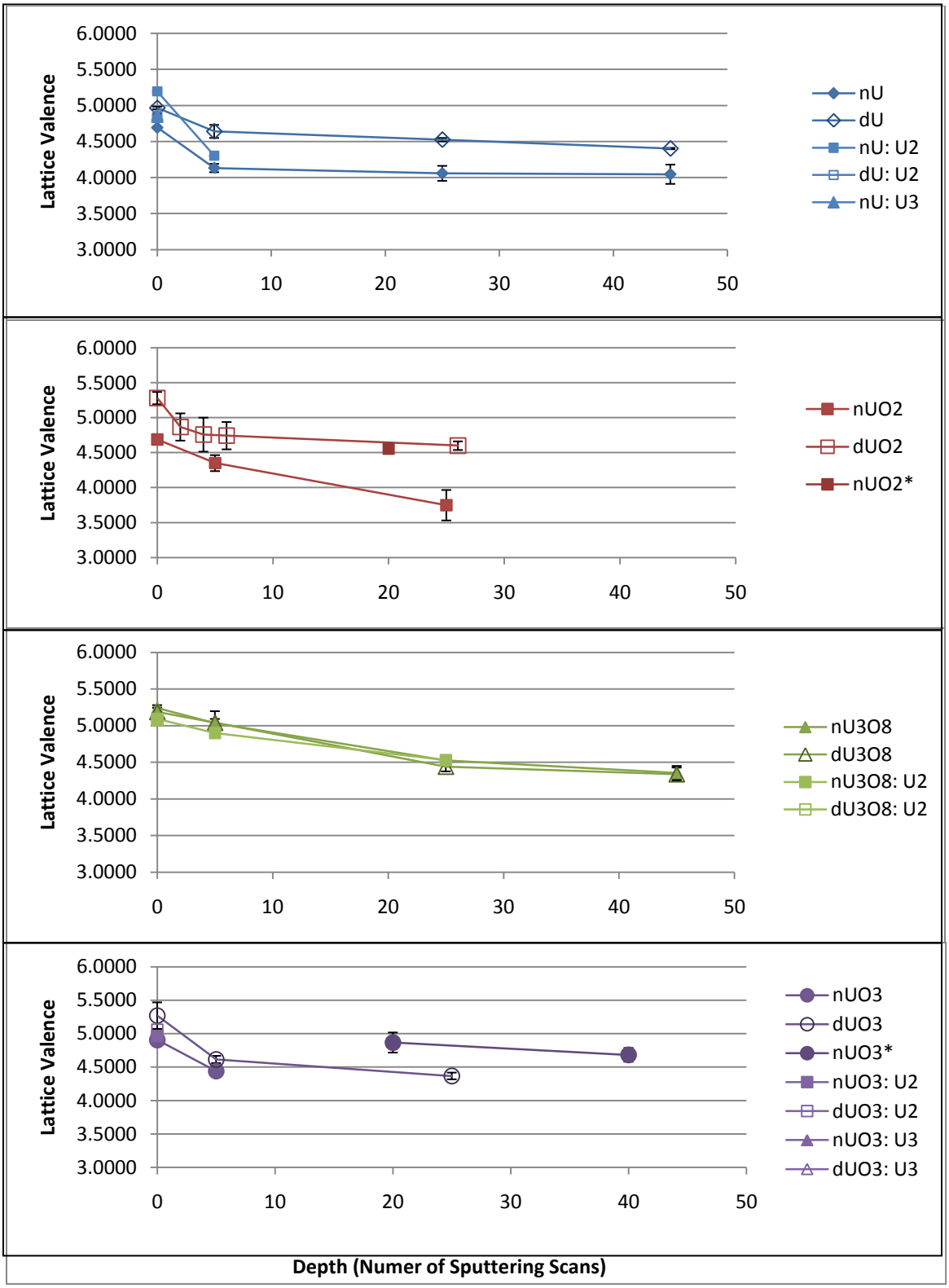


Figure 13: Lattice valence as a function of depth for each particle. *A break in analysis where the samples were exposed to air occurred during the nUO2 and nUO3 data collection. It is probable that reoxidation occurred during these periods as seen in the UO_2 and UO_3 graphs.

While all particles in Figure 11 show a reduction in lattice valence with sputtering depth, it is expected for UO_3 particles which should have a U_3O_8 surface layer due to exposure to the atmosphere, that a rise in average oxidation state would be present. Several factors may be at work here. Preferential oxygen sputtering may be causing a reduction in the sample. Carbon, a reducer, from the sputtering beam may be implanting itself into the particle surface and lowering the oxidation state of the uranium. The relative stability of the oxide and of secondary ions may be a factor. Here U_3O_8 shows the most moderate and most reproducible trend. This may be a result of the greater stability of U_3O_8 as compared to the other oxides.

Uranium Carbide Depth Profile

Carbon implantation was investigated as a possible cause of the lattice valence reduction trend. The fraction of UC^+ ions to U^+ ions was plotted as a function of sputtering depth. The surface spectra showed severe peak interference and reliable information was not attainable for this layer. The trends seen in carbide formation were modest at best and did not correlate to those seen in the lattice valence trends. Carbide formation is not likely the dominate factor in the reduction trend.

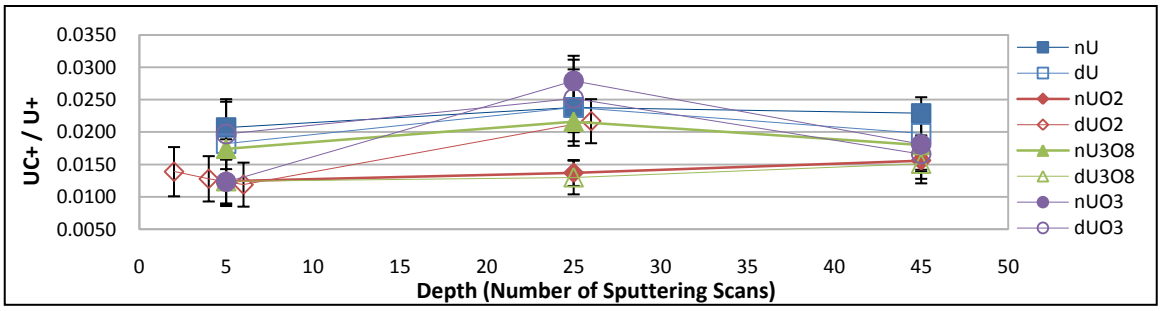


Figure 14: Fraction of uranium carbide as a function of sputtering depth for each particle.

Morphology

A distinct advantage of TOF-SIMS over other types of analytical instruments is the ability to obtain a sense of the elemental or chemical map of the sample. Images can be produced easily and quickly which show the basic shape of particles and sample features. The elemental or chemical makeup of major sample features or contamination is easily determined.

Figure 15 shows images from a pair of spectra for a natural uranium metal particle. The set of images on the left were produced from spectrum nU001, a positive spectrum. The set of images on the right were produced from spectrum nU002, a negative spectrum. These images clearly show two larger uranium containing particles; one approximately 50 um in diameter, and one approximately 100 um in diameter. Also apparent are regions of aluminum concentration, both on the particles and on the gold mounting surface. Hydrocarbons are found in all areas of these surface level spectra, but are present in much higher quantities on the uranium containing particles. Silicon ions are found throughout the area as well. A possible silica particle can be seen in the mid-right side of the negative images. Images for all spectra can be found in Appendix G.

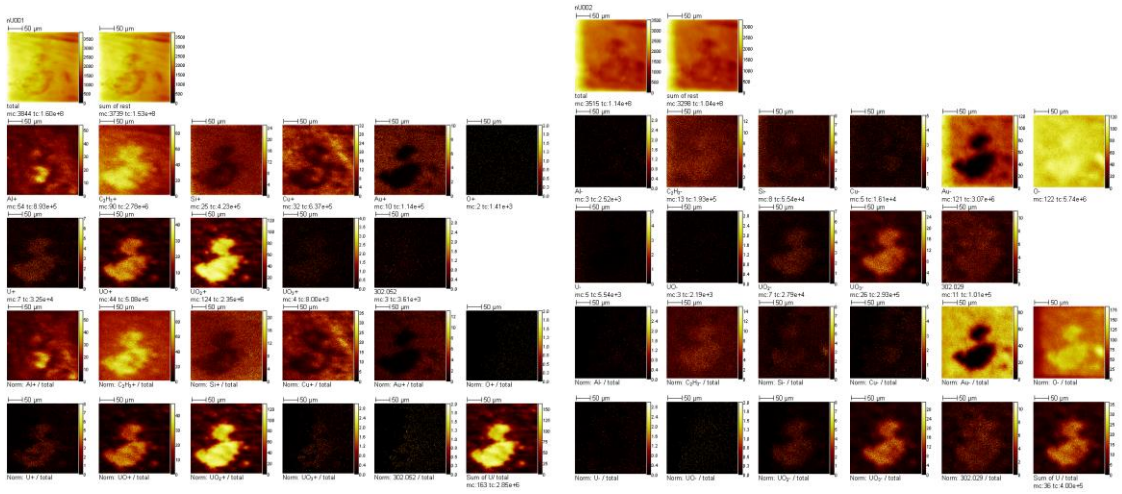


Figure 15: TOF-SIMS images of spectra nU001 and nU002.

Advantages and Disadvantages of Gold Mounting Technique

The gold sample mounting technique developed in this study was found to have several advantages and disadvantages over the previously used carbon tape mount. The gold mounting technique was developed in an effort to reduce the hydrocarbon contamination of samples. Hydrocarbon contamination was greatly reduced, with the gold surface cleaned of hydrocarbons after just a few scans of the buckyball sputtering beam. The actual sample material held on to hydrocarbon species much longer. Although hydrogen became much less abundant protonation of the U_xO_y ions continued.

Additionally other forms of contamination were introduced with the gold mounting technique. Major Au_x ion peaks and many minor gold containing ion peaks were observed. Minor aluminum containing ion peaks, perhaps from the aluminum wrapping material used with the samples in lieu of plastics, also littered the spectra. While it was easy to exclude major contaminate peaks, the multitudinous weak

contamination peaks cause more of a problem for data analysis, especially isotopic determination.

One advantage to the gold mounting technique was that the lack of volatile materials enabled the samples to be brought under vacuum in a very timely manner. Many times the samples were at sufficient vacuum before the TOF-SIMS machine had finished start-up procedures. A final unexpected advantage to the gold mounting technique was that the prominent Au_x ion peaks enabled high mass spectra calibrations.

V. Conclusions/Recommendations

Isotopic Calculation Performance

The isotopic calculator developed in this study was found to obtain an isotopic determination accurate to within 1%. For this study it was found that the U_2 series of ions were a more accurate predictor of isotopic composition. This is no doubt due to peak interference in the U_1 portion of the spectra. The U_2 ion series provided the highest number of ion counts while minimizing peak interference.

The accuracy of this isotopic determination, while by no means state of the art, can still provide a great deal of usefulness to the nuclear forensic community. TOF-SIMS is able to quickly and easily make the distinction between natural (or near natural) uranium, fuel grade enrichments, and weapons grade enrichments. Along with the inherent ease at which TOF-SIMS is able to scan and pick out particles of interest, this alone makes TOF-SIMS a powerful triage tool for the nuclear forensic community.

It is likely that the isotopic determination capability can be improved by studying and peak stripping common interference sources. There is also room for improvement in the error estimation piece of the calculator. Better isotopic determination and better understanding of the error are both valuable enhancements to a tool finding use in nuclear forensics.

Protonation Findings

A protonation calculator was developed which was found to estimate protonation of uranium oxide ions to a sufficient degree to allow relative abundances of each ion

species to found. It was also found that the probabilities of protonation for all uranium oxide ions are not equal. Adding additional oxygen atoms to the dominate ion will drastically increase the probability of protonation. With the help of quantum mechanical calculations this phenomenon may shed light on the structure of these ions as they are formed from the sample surface. Further it was discovered that different uranium oxides exhibit different overall protonation trends enabling a protonation depth profile to discern UO_3 from other oxides. Quantification of protonation levels also enabled the calculation of lattice valence for uranium oxide samples.

Lattice Valence Findings

Lattice valence was calculated for each uranium-containing particle (UO_2, U_3O_8, UO_3 and U metal) as a function of depth. A reduction in the average oxidation state of uranium was found for every particle. This reduction may be attributed to several factors. The buckyball sputtering beam may have reduced the samples due to carbon implantation or preferential sputtering of the oxygen. Secondary ions leaving the surface of the particle may have had more to do with the molecular structural stability of the particle and the ionization affinity of each secondary ion than with the stoichiometry of the uranium oxide. Uranium carbide signatures were found to be modest and carbon implantation is not likely the dominate factor in this reduction trend. It is probable that instead a combination of these factors produced the trend. More study is required to de-convolve the various factors at play. It is likely that with more study a greater understanding of the processes involved will be achieved. Nevertheless, U_3O_8 particles

were clearly distinguished from the rest. U_3O_8 particles showed a reproducible and much more modest reduction trend as a function of depth as compared to all other particles.

Oxide Determination

A combination of dominate ion identification, protonation depth profile trend, and lattice valence depth profile trend can be used to identify oxide composition. UO_2 can be distinguished by identification of the dominate $U_xO_y^+$ ions in a surface spectrum. UO_3 can be identified by its characteristic protonation depth profile as seen in

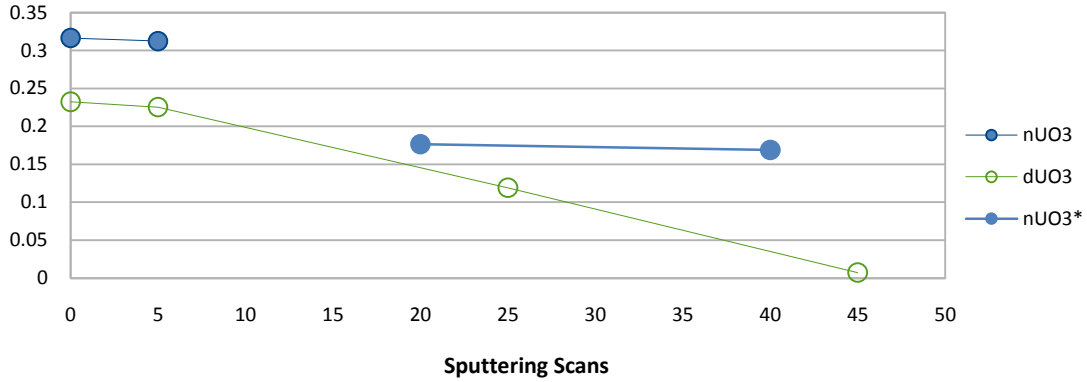


Figure 11. U_3O_8 can be detected by its characteristic lattice valence depth profile as seen in Figure 13. When applied to the surface oxide of metal uranium samples, dU and nU, it is found that the dU sample exhibits U_3O_8 behavior while the nU sample shows UO_3 behavior.

Morphology

While TOF-SIMS may only be able to provide rough outlines of the particles under study, other highly useful information is attained. Static imaging provides an elemental or chemical map of the analysis surface which is easily and quickly produced.

This allows the user to get a sense not only of the particle of interest, but also of major sources of contamination which may be present. Other methods of analysis do not provide the kind of imaging that is readily available with TOF-SIMS.

Success of the Gold Sample Mounting Procedure

The gold sample mounting procedure developed in this study did not reduce the protonation of uranium oxide ions as expected. However certain advantages did present themselves. Hydrocarbon contamination on the mounting surface was drastically reduced. The sample mounting procedure was very friendly to the TOF-SIMS ultra high vacuum system, reducing the pump down time to a matter of minutes, and the regular Au_x ions seen provided a means for spectrum calibration at the high mass end. Disadvantages include the presence of metal contamination especially in the U_1O_x ion range.

The gold sample mounting procedure would be well applied to samples where hydrocarbon contamination must be avoided, but metal contamination may be tolerated. Because of the lack of complex sample preparation and the quick pump down time, this sample mounting method may also be of use when quick answers are critical. The gold sample mounting procedure is not suggested for uranium containing samples where the most accurate TOF-SIMS isotopic determination is wanted.

Nuclear Forensic Utility of TOF-SIMS

TOF-SIMS would prove itself a powerful addition in the arsenal of a nuclear forensics expert. TOF-SIMS analysis would be found most useful as a quick and easy

method to triage forensic samples. With very little training a TOF-SIMS operator would be able to locate particles of interest, and obtain a rough isotopic determination. Images provide a sense of the particle and its environment. Major sources of contamination can be seen. A rudimentary depth profile enables the specific oxide to be determined. Additionally trace chemical analysis could be carried out with the spectrum obtained. Essentially TOF-SIMS quickly provides the user information on what to look for when using other more precise methods of analysis. This enables nuclear forensic analysis to be less of a "needle in a haystack" process. It is likely that with continued study TOF-SIMS will be able to provide more and quicker answers to the nuclear forensics expert as uranium containing samples are better characterized.

Appendix A. Sample Preparation Procedure

Materials:
¼ inch copper squares (approximately 1/32" thick)
¼ inch steel squares (approximately 1/32" thick)
¼ inch diameter gold foil circles (50 microns thick)
Aluminum foil for wrapping samples and lining sample container
Flat pressing surfaces (aluminum ingots were used)
Gold stamp[1]
Blue M oven with argon gas purge[2]
Methanol – HPLC grade (Fisher Scientific, Lot 070517)
Acetonitrile- 99.93+% HPLC grade
Sonicator- Branson 1210[3]
Hotplate
Tweezers
Spatula
Beaker
Sample container
Argon
Carver press[4]
Glove box[5]
PPE
Sample particulate

PPE: For non-glove box operations safety glasses and gloves must be worn.
For glove box operations and any handling of radioactive particulate a lab coat, gloves, TLD, and a 3M 6100/07024 HEPA respirator with 2091 filters is required.

1. Scribe corresponding identifying marks on the "dirtier" side of copper and steel piece pairs using a diamond tipped scribe (letters work well). These sides will be on the outside of the copper/gold/steel sandwich.
2. Cut or tear ¾ inch square pieces of aluminum foil and wrap then carefully remove each wrapper from a copper/steel sandwich set[6]. (This is to pre-crease the foil to allow for easier wrapping of a clean sample.)
3. Place copper squares, steel squares, aluminum wrappers, and pressing surfaces in small 100 mL beaker and fill with acetonitrile until items are covered (approximately 20 mL). Place the beaker in a sonicator set to degas and subject to sonication for 15 minutes.
4. Rinse sonicated items, sample container, aluminum container liner, gold stamp piece, and tweezers with a few mL of methanol using a squeeze bottle. Heat these items on a clean hotplate at 100 degrees Celsius for 10 minutes.
5. Place gold foil circles on copper squares and press between the clean pressing surfaces at 2500 lbs of pressure using the carver press.

6. Set BlueM oven to 915 degrees Celsius and insure that argon gas is flowing through the oven.
7. Once oven temperature has leveled out place one gold/copper piece on glass spatula and carefully insert into oven. Gold should be placed on the unmarked side of the copper.
8. After gold/copper piece has been in the oven at or above 911 degrees for 60 seconds remove and allow to cool.
9. Repeat steps seven and eight for each piece. The gold should become firmly attached to the copper piece without significant discoloration or distortion.
10. Using gold press tap coordinate lines into gold surface[7].
11. Pair gold/copper pieces with corresponding steel pieces and wrap in aluminum foil. Again, marked sides should be on the outside of the sandwich. Make corresponding marks on the aluminum foil to distinguish samples.
12. In glove box unwrap sample and use a cleaned spatula to place the smallest possible amount of uranium particulate onto unmarked side of steel sandwich piece.
13. Gently tap off all visible particulate from steel piece.
14. Place steel piece on gold/copper piece and rewrap with foil.
15. Press sample sandwich at 2500 lb pressure using the carver press.
16. Unwrap sample and inspect to ensure sample preparation was successful.
17. Rewrap sample, use additional aluminum foil if necessary.

Figure A- 1: Gold Stamp. The gold stamp consists of two machined aluminum blocks and a serrated carbide plunger. The sample is placed gold side up between the two aluminum blocks and the serrated tip is used to impress lines onto the gold surface. Subsequently turning the upper block 90 degrees and impressing a second set of lines will create a grid.

Figure A- 2: Blue M Oven.

Figure A- 3: Carver Press.

Figure A- 4: Sonicator.

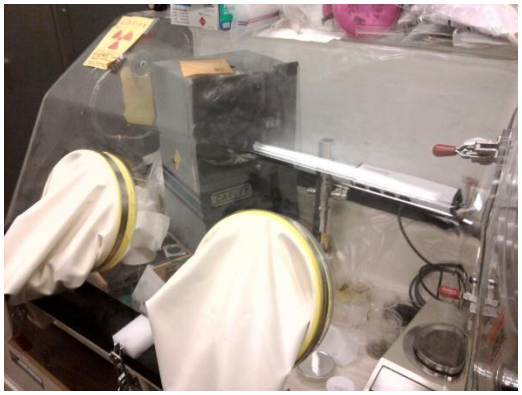


Figure A- 5: Glove Box.

Figure A- 6: Copper/Steel sandwich set on pre-creased aluminum foil wrapper.

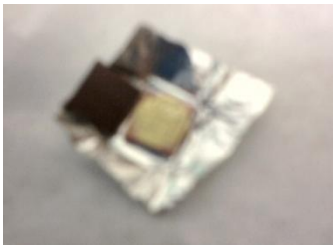


Figure A- 7: Copper/Gold/Steel sandwich showing prepared gold surface.

Appendix B. System of Equations for UO^+ and UO_2^+ Ions

System of linear equations for UO ions:

$$Peak_{250} = fU234 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)]$$
$$Peak_{251} = fU235 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO16 \cdot [P1 \cdot fH1]$$
$$+ fU234 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)]$$
$$Peak_{252} = fU236 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO16 \cdot [P1 \cdot fH1] + fU234 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU235 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO17 \cdot [P1 \cdot fH1]$$
$$+ fU234 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)]$$
$$Peak_{253} = fU237 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO16 \cdot [P1 \cdot fH1] + fU235 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU236 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO17 \cdot [P1 \cdot fH1] + fU234 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU235 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO18 \cdot [P1 \cdot fH1]$$
$$Peak_{254} = fU238 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO16 \cdot [P1 \cdot fH1] + fU236 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU237 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO17 \cdot [P1 \cdot fH1] + fU235 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU236 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO18 \cdot [P1 \cdot fH1] + fU234 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$Peak_{255} = fU238 \cdot fO16 \cdot [P1 \cdot fH1] + fU237 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU238 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO17 \cdot [P1 \cdot fH1] + fU236 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU237 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO18 \cdot [P1 \cdot fH1] + fU235 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$Peak_{255} = fU238 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU238 \cdot fO17 \cdot [P1 \cdot fH1] + fU237 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$
$$+ fU238 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO18 \cdot [P1 \cdot fH1] + fU236 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]$$

$Peak_{XXX}$ is the total number of counts in peak XXX, fU234 is the atom fraction of U-234 in the sample, fU235 is the atom fraction of U-235 in the sample, fU236 is the atom fraction of U-236 in the sample, fU237 is the atom fraction of U-237 in the sample, fU238 is the atom fraction of U-238 in the sample, P1 is the percentage of uranium atoms that have protonated, P2 is the percentage of uranium atoms that have taken up two hydrogen atoms, or diprotonated, fH1 is the atom fraction of H-1, and fH2 is the atom fraction of deuterium.

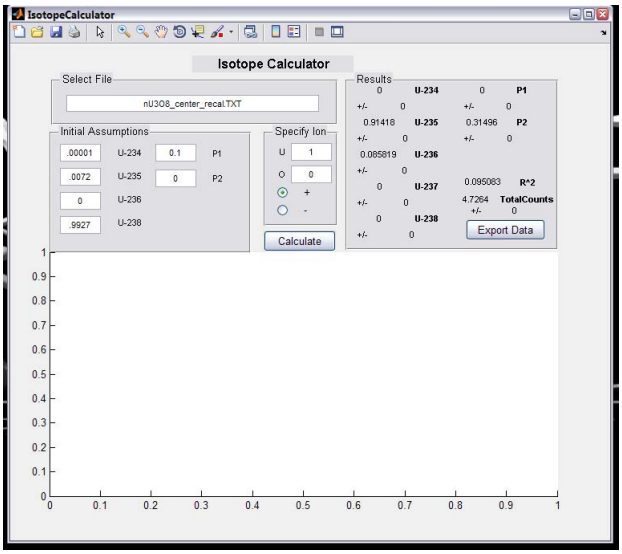
System of linear equations for UO_2 ions:

$$
\begin{aligned}
Peak_{266} &= fU234 \cdot fO16 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
Peak_{267} &= fU235 \cdot fO16 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO16 \cdot fO16 \cdot [P1 \cdot fH1] \\
&+ fU234 \cdot fO17 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
&+ fU234 \cdot fO16 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
Peak_{268} &= fU236 \cdot fO16 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO16 \cdot fO16 \cdot [P1 \cdot fH1] + fU234 \cdot fO16 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU235 \cdot fO17 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO17 \cdot fO16 \cdot [P1 \cdot fH1] \\
&+ fU234 \cdot fO18 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
&+ fU235 \cdot fO16 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO16 \cdot fO17 \cdot [P1 \cdot fH1] \\
&+ fU234 \cdot fO17 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
&+ fU234 \cdot fO16 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] \\
Peak_{269} &= fU237 \cdot fO16 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO16 \cdot fO16 \cdot [P1 \cdot fH1] + fU235 \cdot fO16 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO17 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO17 \cdot fO16 \cdot [P1 \cdot fH1] + fU234 \cdot fO17 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU235 \cdot fO18 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO18 \cdot fO16 \cdot [P1 \cdot fH1] \\
&+ fU237 \cdot fO16 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO16 \cdot fO17 \cdot [P1 \cdot fH1] + fU235 \cdot fO16 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO17 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO17 \cdot fO17 \cdot [P1 \cdot fH1] + fU234 \cdot fO17 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU235 \cdot fO18 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO18 \cdot fO17 \cdot [P1 \cdot fH1] \\
&+ fU237 \cdot fO16 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO16 \cdot fO18 \cdot [P1 \cdot fH1] + fU235 \cdot fO16 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO17 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO17 \cdot fO18 \cdot [P1 \cdot fH1] + fU234 \cdot fO17 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU235 \cdot fO18 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU234 \cdot fO18 \cdot fO18 \cdot [P1 \cdot fH1] \\
Peak_{270} &= fU238 \cdot fO16 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO16 \cdot fO16 \cdot [P1 \cdot fH1] + fU236 \cdot fO16 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO17 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO17 \cdot fO16 \cdot [P1 \cdot fH1] + fU235 \cdot fO17 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO18 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO18 \cdot fO16 \cdot [P1 \cdot fH1] + fU234 \cdot fO18 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO16 \cdot fO17 \cdot [P1 \cdot fH1] + fU236 \cdot fO16 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO17 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO17 \cdot fO17 \cdot [P1 \cdot fH1] + fU235 \cdot fO17 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO18 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO18 \cdot fO17 \cdot [P1 \cdot fH1] + fU234 \cdot fO18 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO16 \cdot fO18 \cdot [P1 \cdot fH1] + fU236 \cdot fO16 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO17 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO17 \cdot fO18 \cdot [P1 \cdot fH1] + fU235 \cdot fO17 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU236 \cdot fO18 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU235 \cdot fO18 \cdot fO18 \cdot [P1 \cdot fH1] + fU234 \cdot fO18 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
Peak_{271} &= fU238 \cdot fO16 \cdot fO16 \cdot [P1 \cdot fH1] + fU237 \cdot fO16 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO17 \cdot fO16 \cdot [P1 \cdot fH1] + fU236 \cdot fO17 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO18 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO18 \cdot fO16 \cdot [P1 \cdot fH1] + fU235 \cdot fO18 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO17 \cdot [P1 \cdot fH1] + fU237 \cdot fO16 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO17 \cdot fO17 \cdot [P1 \cdot fH1] + fU236 \cdot fO17 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO18 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO18 \cdot fO17 \cdot [P1 \cdot fH1] + fU235 \cdot fO18 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO18 \cdot [P1 \cdot fH1] + fU237 \cdot fO16 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO17 \cdot fO18 \cdot [P1 \cdot fH1] + fU236 \cdot fO17 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU237 \cdot fO18 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU236 \cdot fO18 \cdot fO18 \cdot [P1 \cdot fH1] + fU235 \cdot fO18 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
Peak_{272} &= fU238 \cdot fO16 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO16 \cdot [P1 \cdot fH1] + fU237 \cdot fO17 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO18 \cdot fO16 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO18 \cdot fO16 \cdot [P1 \cdot fH1] + fU236 \cdot fO18 \cdot fO16 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO17 \cdot [P1 \cdot fH1] + fU237 \cdot fO17 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO18 \cdot fO17 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO18 \cdot fO17 \cdot [P1 \cdot fH1] + fU236 \cdot fO18 \cdot fO17 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO16 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO17 \cdot fO18 \cdot [P1 \cdot fH1] + fU237 \cdot fO17 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)] \\
&+ fU238 \cdot fO18 \cdot fO18 \cdot [1-(P1 \cdot fH1)-(P1 \cdot fH2)-(P2 \cdot fH1)] + fU237 \cdot fO18 \cdot fO18 \cdot [P1 \cdot fH1] + fU236 \cdot fO18 \cdot fO18 \cdot [(P1 \cdot fH2)+(P2 \cdot fH1)]
\end{aligned}
$$

$Peak_{XXX}$ is the total number of counts in peak XXX, fU234 is the atom fraction of U-234 in the sample, fU235 is the atom fraction of U-235 in the sample, fU236 is the atom

fraction of U-236 in the sample, fU237 is the atom fraction of U-237 in the sample, fU238 is the atom fraction of U-238 in the sample, P1 is the percentage of uranium atoms that have protonated, P2 is the percentage of uranium atoms that have taken up two hydrogen atoms, or diprotonated, fH1 is the atom fraction of H-1, and fH2 is the atom fraction of deuterium.

Appendix C. Isotope Calculator




```
function varargout = IsotopeCalculator(varargin)
% ISOTOPECALCULATOR M-file for IsotopeCalculator.fig
%      ISOTOPECALCULATOR, by itself, creates a new ISOTOPECALCULATOR or
raises the existing
%      singleton*.
%
%      H = ISOTOPECALCULATOR returns the handle to a new
ISOTOPECALCULATOR or the handle to
%      the existing singleton*.
%
%      ISOTOPECALCULATOR('CALLBACK',hObject,eventData,handles,...)
calls the local
%      function named CALLBACK in ISOTOPECALCULATOR.M with the given
input arguments.
%
%      ISOTOPECALCULATOR('Property','Value',...) creates a new
ISOTOPECALCULATOR or raises the
%      existing singleton*.  Starting from the left, property value
pairs are
%      applied to the GUI before IsotopeCalculator_OpeningFcn gets
called.  An
%      unrecognized property name or invalid value makes property
application
%      stop.  All inputs are passed to IsotopeCalculator_OpeningFcn via
varargin.
%
%      *See GUI Options on GUIDE's Tools menu.  Choose "GUI allows only
one
%      instance to run (singleton)".
%
```

```
% See also: GUIDE, GUIDATA, GUIHANDLES

% Edit the above text to modify the response to help IsotopeCalculator

% Last Modified by GUIDE v2.5 02-Dec-2010 12:06:33

% Begin initialization code - DO NOT EDIT
gui_Singleton = 1;
gui_State = struct('gui_Name',       mfilename, ...
                   'gui_Singleton',  gui_Singleton, ...
                   'gui_OpeningFcn', @IsotopeCalculator_OpeningFcn, ...
                   'gui_OutputFcn',  @IsotopeCalculator_OutputFcn, ...
                   'gui_LayoutFcn',  [] , ...
                   'gui_Callback',   []);
if nargin && ischar(varargin{1})
    gui_State.gui_Callback = str2func(varargin{1});
end

if nargout
    [varargout{1:nargout}] = gui_mainfcn(gui_State, varargin{:});
else
    gui_mainfcn(gui_State, varargin{:});
end
% End initialization code - DO NOT EDIT


% --- Executes just before IsotopeCalculator is made visible.
function IsotopeCalculator_OpeningFcn(hObject, eventdata, handles,
varargin)
% This function has no output args, see OutputFcn.
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
% varargin   command line arguments to IsotopeCalculator (see VARARGIN)

% Choose default command line output for IsotopeCalculator
handles.output = hObject;

% Update handles structure
set(hObject,'toolbar','figure');
guidata(hObject, handles);

% UIWAIT makes IsotopeCalculator wait for user response (see UIRESUME)
% uiwait(handles.figure1);


% --- Outputs from this function are returned to the command line.
function varargout = IsotopeCalculator_OutputFcn(hObject, eventdata,
handles)
% varargout  cell array for returning output args (see VARARGOUT);
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
```

```
% Get default command line output from handles structure
varargout{1} = handles.output;


% --- Executes on button press in calculate_pushbutton.
function calculate_pushbutton_Callback(hObject, eventdata, handles)
% hObject    handle to calculate_pushbutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

%Change calculate button
%set(handles.calculate_pushbutton, 'String', '...');
%guidata(hObject, handles);

%Get inputs
cla(handles.axes1,'reset')
guidata(hObject, handles);
axes(handles.axes1)

filename = get(handles.filename_editText,'String');
rawdata = dlmread(filename, '', 2, 0);
channel = rawdata(:,1);
mass = rawdata(:,2);
intensity = rawdata(:,3);

icU234 = str2double(get(handles.ic234_editText, 'String'));
icU235 = str2double(get(handles.ic235_editText, 'String'));
icU236 = str2double(get(handles.ic236_editText, 'String'));
icU237 = 0;
icU238 = str2double(get(handles.ic238_editText, 'String'));
icP1 = str2double(get(handles.icP1_editText, 'String'));
icP2 = str2double(get(handles.icP2_editText, 'String'));
nU = str2double(get(handles.nU_editText, 'String'));
nO = str2double(get(handles.nO_editText, 'String'));
p = get(handles.pos_radiobutton,'Value');
n = get(handles.neg_radiobutton,'Value');

if p==1 && n==0, pn = 1;
elseif p==0 && n==1, pn = 0;
else error('Correct charge')
end

%GetIsotopics
[fU234 fU235 fU236 fU237 fU238 P1 P2 R2 TotalCounts,...
    sigmaTotalCounts,sigma238, sigma237, sigma236, sigma235, sigma234,
sigmaP1, sigmaP2]...
    = GetIsotopics1(mass, intensity, icU234, icU235, icU236, icU237,
icU238, icP1, icP2, nU, nO, pn);
% [fU234 fU235 fU236 fU237 fU238 P1 P2 R2 TotalArea, sigmaTotalArea,
confidence, points] = GetIsotopics1(mass, intensity, icU234, ...
%     icU235, icU236, icU237, icU238, icP1, icP2, nU, nO, pn);
%Convert numbers to strings
```

```
sfU234 = num2str(fU234);
sfU235 = num2str(fU235);
sfU236 = num2str(fU236);
sfU237 = num2str(fU237);
sfU238 = num2str(fU238);
sP1 = num2str(P1);
sP2 = num2str(P2);
sR2 = num2str(R2);
sTotalCounts = num2str(TotalCounts);
seTotalCounts = num2str(sigmaTotalCounts);
seU234 = num2str(sigma234);
seU235 = num2str(sigma235);
seU236 = num2str(sigma236);
seU237 = num2str(sigma237);
seU238 = num2str(sigma238);
seP1 = num2str(sigmaP1);
seP2 = num2str(sigmaP2);

%Populate output
set(handles.fU234_text, 'String', sfU234);
set(handles.fU235_text, 'String', sfU235);
set(handles.fU236_text, 'String', sfU236);
set(handles.fU237_text, 'String', sfU237);
set(handles.fU238_text, 'String', sfU238);
set(handles.P1_text, 'String', sP1);
set(handles.P2_text, 'String', sP2);
set(handles.eU234_text, 'String', seU234);
set(handles.eU235_text, 'String', seU235);
set(handles.eU236_text, 'String', seU236);
set(handles.eU237_text, 'String', seU237);
set(handles.eU238_text, 'String', seU238);
set(handles.eP1_text, 'String', seP1);
set(handles.eP2_text, 'String', seP2);
set(handles.R2_text, 'String', sR2);
set(handles.TotalCounts_text, 'String', sTotalCounts);
set(handles.eTotalCounts_text, 'String', seTotalCounts);
%set(handles.calculate_pushbutton, 'String', 'Calculate');
guidata(hObject, handles);

function nU_editText_Callback(hObject, eventdata, handles)
% hObject    handle to nU_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of nU_editText as text
%        str2double(get(hObject,'String')) returns contents of
nU_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function nU_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to nU_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
```

```
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function nO_editText_Callback(hObject, eventdata, handles)
% hObject    handle to nO_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of nO_editText as text
%        str2double(get(hObject,'String')) returns contents of
nO_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function nO_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to nO_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function filename_editText_Callback(hObject, eventdata, handles)
% hObject    handle to filename_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of filename_editText as
text
%        str2double(get(hObject,'String')) returns contents of
filename_editText as a double
%get(hObject,'String')
guidata(hObject, handles);

% --- Executes during object creation, after setting all properties.
function filename_editText_CreateFcn(hObject, eventdata, handles)
```

```
% hObject    handle to filename_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic234_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic234_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic234_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic234_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic234_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic234_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic235_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic235_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic235_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic235_editText as a double
guidata(hObject, handles);
```

```
% --- Executes during object creation, after setting all properties.
function ic235_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic235_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic236_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic236_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic236_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic236_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic236_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic236_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic238_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic238_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic238_editText as
text
```

```
%        str2double(get(hObject,'String')) returns contents of
ic238_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic238_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic238_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function icP1_editText_Callback(hObject, eventdata, handles)
% hObject    handle to icP1_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of icP1_editText as
text
%        str2double(get(hObject,'String')) returns contents of
icP1_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function icP1_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to icP1_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function icP2_editText_Callback(hObject, eventdata, handles)
% hObject    handle to icP2_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
```

```
% Hints: get(hObject,'String') returns contents of icP2_editText as
text
%        str2double(get(hObject,'String')) returns contents of
icP2_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function icP2_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to icP2_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end


% --- Executes on button press in ExportData_pushbutton.
function ExportData_pushbutton_Callback(hObject, eventdata, handles)
% hObject    handle to ExportData_pushbutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

filename = get(handles.filename_editText,'String');
icU234 = get(handles.ic234_editText, 'String');
icU235 = get(handles.ic235_editText, 'String');
icU236 = get(handles.ic236_editText, 'String');
icU237 = '0';
icU238 = get(handles.ic238_editText, 'String');
icP1 = get(handles.icP1_editText, 'String');
icP2 = get(handles.icP2_editText, 'String');
nU = get(handles.nU_editText, 'String');
nO = get(handles.nO_editText, 'String');
p = num2str(get(handles.pos_radiobutton,'Value'));
n = num2str(get(handles.neg_radiobutton,'Value'));
IC = '1';
PC = '0';
fU234 = get(handles.fU234_text, 'String');
fU235 = get(handles.fU235_text, 'String');
fU236 = get(handles.fU236_text, 'String');
fU237 = get(handles.fU237_text, 'String');
fU238 = get(handles.fU238_text, 'String');
P1 = get(handles.P1_text, 'String');
P2 = get(handles.P2_text, 'String');
eU234 = get(handles.eU234_text, 'String');
eU235 = get(handles.eU235_text, 'String');
eU236 = get(handles.eU236_text, 'String');
eU237 = get(handles.eU237_text, 'String');
```

```
eU238 = get(handles.eU238_text, 'String');
eP1 = get(handles.eP1_text, 'String');
eP2 = get(handles.eP2_text, 'String');
R2 = get(handles.R2_text, 'String');
TotalCounts = get(handles.TotalCounts_text, 'String');
sigmaTotalCounts = get(handles.eTotalCounts_text, 'String');

% M = [filename, nU, nO, p, n, IC, PC,icU234,...
%     icU235,icU236,icU237,icU238,...
%     icP1, icP2, fU234, fU235, fU236, fU237, fU238, ...
%     P1, P2, R2, TotalCounts, eU234, eU235, eU236, eU237, eU238, ...
%     eP1, eP2, sigmaTotalCounts];
fileID = fopen('logdata.txt', 'a');
fprintf(fileID, '%s %s %s %s %s %s %s %s %s %s %s %s %s %s %s %s %s
%s %s %s %s %s %s %s %s %s %s %s %s \n',...
    filename, nU, nO, p, n, IC, PC,icU234,...
    icU235,icU236,icU237,icU238,...
    icP1, icP2, fU234, fU235, fU236, fU237, fU238, ...
    P1, P2, R2, TotalCounts, eU234, eU235, eU236, eU237, eU238, ...
    eP1, eP2, sigmaTotalCounts);
guidata(hObject, handles);



% --- Executes on button press in pos_radiobutton.
function pos_radiobutton_Callback(hObject, eventdata, handles)
% hObject    handle to pos_radiobutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hint: get(hObject,'Value') returns toggle state of pos_radiobutton


% --- Executes on button press in neg_radiobutton.
function neg_radiobutton_Callback(hObject, eventdata, handles)
% hObject    handle to neg_radiobutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hint: get(hObject,'Value') returns toggle state of neg_radiobutton
```

```
function [fU234 fU235 fU236 fU237 fU238 P1 P2 R2 TotalCounts,...
    sigmaTotalCounts,sigma238, sigma237, sigma236, sigma235, sigma234,
sigmaP1, sigmaP2]...
    = GetIsotopics1(mass, intensity, icU234, icU235, icU236, icU237,
icU238, icP1, icP2, nU, nO, pn)

%Get peaks of interest
peaks = GetPeaks(nU,nO);
peaksize = size(peaks);

hold on

%Get local variance-------------------------------------------------------
----
%Identify largest peak
loc1 = find (mass > (peaks(1)-0.4), 1, 'first');
loc2 = find (mass > (peaks(peaksize(1))+0.4), 1, 'first');
yvalues = intensity(loc1:loc2, 1);
xvalues = mass(loc1:loc2, 1);
[Pmax ploc] = max(yvalues);
bigpeak = xvalues(ploc);

%Get peak segment
loc1 = find (mass > (bigpeak-0.4), 1, 'first');
loc2 = find (mass > (bigpeak+0.4), 1, 'first');
yvalues = intensity(loc1:loc2, 1);
xvalues = mass(loc1:loc2, 1);

%Find local background
[min(1) location(1)] = GetMinimum(mass, intensity, bigpeak-0.5, .5);
[min(2) location(2)] = GetMinimum(mass, intensity, bigpeak+0.5, .5);
bg(1) = mean (intensity((location(1)-20):(location(1)+20)));
bg(2) = mean (intensity((location(2)-20):(location(2)+20)));
background = mean ([bg(1) bg(2)]);

%Subtract background
yvalues = yvalues-background;

%Fit regular gauss
gauss = fit(xvalues,yvalues,'gauss1');
%Get gaussian statistics
stats = coeffvalues(gauss);
c = stats(3);
sigma = c/sqrt(2);
%-------------------------------------------------------------------------
----

for i = 1:peaksize(1); %Find the counts for each peak

    %Find peak max
    peak = peaks(i);
    loc1 = find (mass > (peak-2*sigma), 1, 'first');
    loc2 = find (mass > (peak+2*sigma), 1, 'first');
```

```
    yvalues = intensity(loc1:loc2, 1);
    xvalues = mass(loc1:loc2, 1);
    [pmax ploc] = max(yvalues);
    %Recenter around max
    peak = xvalues(ploc);
    %Find local background and noise
    ploc = loc1+ploc;
    [min(1) location(1)] = GetMinimum(mass, intensity, peak-0.5, .5);
    [min(2) location(2)] = GetMinimum(mass, intensity, peak+0.5, .5);
    bg(1) = mean (intensity((location(1)-20):(location(1)+20)));
    bg(2) = mean (intensity((location(2)-20):(location(2)+20)));
    background = mean ([bg(1) bg(2)]);
    noise = ((bg(1)-min(1))*2 +(bg(2)-min(2))*2)/2;
    sigmaB(i) = sqrt(background*(loc2-loc1));
    %Find +/- 4 sigma peak segment
    loc1 = find (mass > (peak-4*sigma), 1, 'first');
    loc2 = find (mass > (peak+4*sigma), 1, 'first');
    yvalues = intensity(loc1:loc2, 1);
    xvalues = mass(loc1:loc2, 1);
    sigmaM(i) = sqrt(sum(yvalues));
    %Subtract background and plot peak segment
    yvalues = yvalues-background;
    sigmaX(i) = sqrt(sigmaM(i)^2 +sigmaB(i)^2);
    plot(xvalues,yvalues)
    %Total counts
    counts(i) = sum(yvalues);
    if counts(i) < 0; counts(i) = 0; end

end

%Get relative peak counts
TotalCounts = sum(counts);
sigmaTotalCounts = sqrt(sigmaX*sigmaX');
data = (counts/TotalCounts);
for i = 1:peaksize(1);
    if counts(i) == 0;
        sigmaData(i) =
sqrt((sigmaX(i)^2/1)+(sigmaTotalCounts^2/TotalCounts^2))*data(i);
    else
        sigmaData(i) =
sqrt((sigmaX(i)^2/counts(i)^2)+(sigmaTotalCounts^2/TotalCounts^2))*data
(i);
    end
end

%Weed out zero peaks
index1 = data==0;
doi = data;
poi = peaks;
poi(index1) = 0;
doi = nonzeros(doi);
poi = nonzeros(poi);

%Solve for isotopics, protonation
```

```
[fU234 fU235 fU236 fU237 fU238 P1 P2 R2] = Solver(doi, poi, ...
    icU234, icU235, icU236, icU237, icU238, icP1, icP2, nU, nO);

%Get calculated peak area from isotopics, protonation
[calc] = CalcArea([fU234 fU235 fU236 fU237 fU238 P1 P2], peaks, nU,
nO);

%Plot
multiplier = Pmax;
ylim([-Pmax/10 Pmax*1.1]);
legend('hide');
plot (peaks(:,1), data*multiplier, 'oc')
errorbar (peaks(:,1),data*multiplier, sigmaData*multiplier, 'oc')
plot (peaks(:,1), calc*multiplier, 'xr')
PlotSpectrum(fU234, fU235, fU236, fU237, fU238, P1, P2, nU, nO,...
   c, multiplier)

%Get isotopics, protonation error
[sigma238, sigma237, sigma236, sigma235, sigma234, sigmaP1, sigmaP2]...
    = GetError(i, counts, sigmaX, P1, P2);
```

```
function peaks = GetPeaks(nU,nO)

if nU == 0, error('invalid ion');
%U1 series
elseif nU == 1
        if nO == 0, peaks = (234:240)';
        elseif nO == 1, peaks = (250:256)';
        elseif nO == 2, peaks = (266:272)';
        elseif nO == 3, peaks = (282:288)';
        elseif nO == 4, peaks = (298:304)';
        else error('invalid ion')
        end
%U2 series
elseif nU == 2
        if nO == 2, peaks = (500:510)';
        elseif nO == 3, peaks = (516:526)';
        elseif nO == 4, peaks = (532:542)';
        elseif nO == 5, peaks = (548:558)';
        elseif nO == 6, peaks = (564:574)';
        elseif nO == 7, peaks = (580:590)';
        else error('invalid ion')
        end
%U3series
elseif nU == 3
        if nO == 4, peaks = (766:780)';
        elseif nO == 5, peaks = [782, 783, 784, 785, 786, 787, 789,
790,...
                791,792,793,794,795,796]';
        elseif nO == 6, peaks = (798:812)';
        elseif nO == 7, peaks = (814:828)';
        elseif nO == 8, peaks = (830:844)';
        elseif nO == 9, peaks = (846:860)';
        else error('invalid ion')
        end
%U4 series
elseif nU == 4
        if nO == 5, peaks = (1019:1034)';
        elseif nO == 6, peaks = (1035:1050)';
        elseif nO == 7, peaks = (1051:1066)';
        elseif nO == 8, peaks = (1067:1082)';
        elseif nO == 9, peaks = (1083:1098)';
        elseif nO == 10, peaks = (1099:1114)';
        elseif nO == 11, peaks = (1115:1130)';
        else error('invalid ion')
        end
%U5 series
elseif nU == 5
        if nO == 5, peaks = (1257:1272)';
        elseif nO == 6, peaks = (1273:1288)';
        elseif nO == 7, peaks = (1289:1304)';
        elseif nO == 8, peaks = (1305:1320)';
        elseif nO == 9, peaks = (1321:1336)';
        elseif nO == 10, peaks = (1337:1352)';
        elseif nO == 11, peaks = (1353:1368)';
```

```
        elseif nO == 12, peaks = [1369 1370 1371 1372 1373 1374 1375
1376 ...
                1377 1378 1380 1381 1382 1383 1384]';
        elseif nO == 13, peaks = (1385:1400)';
        elseif nO == 14, peaks = (1401:1416)';
        elseif nO == 15, peaks = (1417:1432)';
        else error('invalid ion')
        end
%U6 series
elseif nU == 6
        if nO == 6, peaks = (1511:1526)';
        elseif nO == 7, peaks = (1527:1542)';
        elseif nO == 8, peaks = (1543:1558)';
        elseif nO == 9, peaks = (1559:1574)';
        elseif nO == 10, peaks = [1575 1577 1578 1579 1580 1581 1582
...
                1583 1584 1585 1586 1587 1588 1589 1590]';
        elseif nO == 11, peaks = (1591:1606)';
        elseif nO == 12, peaks = (1607:1622)';
        elseif nO == 13, peaks = (1623:1638)';
        elseif nO == 14, peaks = (1639:1654)';
        elseif nO == 15, peaks = (1655:1670)';
        elseif nO == 16, peaks = (1671:1686)';
        elseif nO == 17, peaks = (1687:1702)';
        elseif nO == 18, peaks = (1703:1718)';
        else error('invalid ion')
        end
%U7 series
elseif nU == 7
        if nO == 7, peaks = [1765 1766 1767 1768 1769 1770 1771 1772
...
                1774 1775 1776 1777 1778 1779 1780]';
        elseif nO == 8, peaks = (1781:1796)';
        elseif nO == 9, peaks = (1797:1812)';
        elseif nO == 10, peaks = (1813:1828)';
        elseif nO == 11, peaks = (1829:1844)';
        elseif nO == 12, peaks = (1845:1860)';
        elseif nO == 13, peaks = (1861:1876)';
        elseif nO == 14, peaks = (1877:1892)';
        elseif nO == 15, peaks = (1893:1908)';
        elseif nO == 16, peaks = (1909:1924)';
        elseif nO == 17, peaks = (1925:1940)';
        elseif nO == 18, peaks = (1941:1956)';
        elseif nO == 19, peaks = [1957 1958 1959 1960 1961 1962 1963
1964 ...
                1965 1966 1967 1968 1969 1971 1972]';
        elseif nO == 20, peaks = (1973:1988)';
        elseif nO == 21, peaks = (1989:2004)';
        else error('invalid ion')
        end
%U8 series
elseif nU == 8
        if nO == 8, peaks = (2019:2034)';
        elseif nO == 9, peaks = (2035:2050)';
        elseif nO == 10, peaks = (2051:2066)';
```

```
        elseif nO == 11, peaks = (2067:2082)';
        elseif nO == 12, peaks = (2083:2098)';
        elseif nO == 13, peaks = (2099:2114)';
        elseif nO == 14, peaks = (2115:2130)';
        elseif nO == 15, peaks = (2131:2146)';
        elseif nO == 16, peaks = (2147:2162)';
        elseif nO == 17, peaks = [2163 2164 2165 2166 2168 2169 2170
2171 ...
                2172 2173 2174 2175 2176 2177 2178]';
        elseif nO == 18, peaks = (2179:2194)';
        elseif nO == 19, peaks = (2195:2210)';
        elseif nO == 20, peaks = (2211:2226)';
        elseif nO == 21, peaks = (2227:2242)';
        elseif nO == 22, peaks = (2243:2258)';
        elseif nO == 23, peaks = (2259:2274)';
        elseif nO == 24, peaks = (2275:2290)';
        else error('invalid ion')
        end
%U9 series
elseif nU == 9
        if nO == 9, peaks = (2273:2288)';
        elseif nO == 10, peaks = (2289:2304)';
        elseif nO == 11, peaks = (2305:2320)';
        elseif nO == 12, peaks = (2321:2336)';
        elseif nO == 13, peaks = (2337:2352)';
        elseif nO == 14, peaks = [2353 2354 2355 2356 2357 2358 2359
2360 ...
                2361 2362 2363 2365 2366 2367 2368]';
        elseif nO == 15, peaks = (2369:2384)';
        elseif nO == 16, peaks = (2385:2400)';
        elseif nO == 17, peaks = (2401:2416)';
        elseif nO == 18, peaks = (2417:2432)';
        elseif nO == 19, peaks = (2433:2448)';
        elseif nO == 20, peaks = (2449:2464)';
        elseif nO == 21, peaks = (2465:2480)';
        elseif nO == 22, peaks = (2481:2496)';
        elseif nO == 23, peaks = (2497:2512)';
        elseif nO == 24, peaks = (2513:2528)';
        elseif nO == 25, peaks = (2529:2544)';
        elseif nO == 26, peaks = (2545:2560)';
        elseif nO == 27, peaks = (2562:2576)';
        else error('invalid ion')
        end
%U10 series
elseif nU == 10
        if nO == 10, peaks = (2527:2542)';
        elseif nO == 11, peaks = (2543:2558)';
        elseif nO == 12, peaks = (2559:2574)';
        elseif nO == 13, peaks = (2575:2590)';
        elseif nO == 14, peaks = (2591:2606)';
        elseif nO == 15, peaks = (2607:2622)';
        elseif nO == 16, peaks = (2623:2638)';
        elseif nO == 17, peaks = (2639:2654)';
        elseif nO == 18, peaks = (2655:2670)';
        elseif nO == 19, peaks = (2671:2686)';
```

```
        elseif nO == 20, peaks = (2687:2702)';
        elseif nO == 21, peaks = (2703:2718)';
        elseif nO == 22, peaks = (2719:2734)';
        elseif nO == 23, peaks = (2735:2750)';
        elseif nO == 24, peaks = [2751 2752 2753 2754 2755 2756 2757
2759 ...
                2760 2761 2762 2763 2764 2765 2766]';
        elseif nO == 25, peaks = (2767:2782)';
        elseif nO == 26, peaks = (2783:2798)';
        elseif nO == 27, peaks = (2799:2814)';
        elseif nO == 28, peaks = (2815:2830)';
        elseif nO == 29, peaks = (2831:2846)';
        elseif nO == 30, peaks = (2847:2862)';
        else error('invalid ion')
        end
else
    error('invalid ion')
end
peaks = peaks - .0051*nO +.0460*nU;
```

```
function [I,loc] = GetMinimum(mass, intensity, massnumber, halfrange)

loc1 = find (mass > (massnumber-halfrange), 1, 'first');
loc2 = find (mass > (massnumber+halfrange), 1, 'first');
slice = intensity (loc1:loc2);
I = min(slice);
loc = find (slice == I, 1, 'first') + loc1;
```

```
function [fU234 fU235 fU236 fU237 fU238 P1 P2 r] = Solver(data, peaks,
...
    icU234, icU235, icU236, icU237, icU238, icP1, icP2, nU, nO)

initial = [icU234, icU235, icU236, icU237, icU238, icP1, icP2];

%pass parameters
data = data;
peaks = peaks;

options = optimset('Display', 'final', 'TolFun', .00000000000000000001,
...
    'TolX', .00000000000000000001,...
    'MaxFunEvals', 5000, 'MaxIter', 5000);

[s, r] = fminsearch (@(variables)Residuals(variables, data, peaks, nU,
nO)...
     , initial, options);

    fU234 = s(1);
    fU235 = s(2);
    fU236 = s(3);
    fU237 = s(4);
    fU238 = s(5);
    P1 = s(6);
    P2 = s(7);

%Correct for bad values- this is due to the solver scheme.
if fU234 < 0, fU234 = 0; end
if fU235 < 0, fU235 = 0; end
if fU236 < 0, fU236 = 0; end
if fU237 < 0, fU237 = 0; end
if fU238 < 0, fU238 = 0; end
if fU234 > 1, fU234 = 1; end
if fU235 > 1, fU235 = 1; end
if fU236 > 1, fU236 = 1; end
if fU237 > 1, fU237 = 1; end
if fU238 > 1, fU238 = 1; end
if P1 < 0, P1 = 0; end
if P1 > 1, P1 = 1; end
if P2 < 0, P2 = 0; end
if P2 > 1, P2 = 1; end
if (P1+P2)>1, P2 = 1-P1; end
U = fU234+fU235+fU236+fU237+fU238;
fU234 = fU234/U;
fU235 = fU235/U;
fU236 = fU236/U;
fU237 = fU237/U;
fU238 = fU238/U;
```

```
function res = Residuals(variables, data, peaks, nU, nO)

calc = CalcArea(variables, peaks, nU, nO);
datapoints = size(data);
res = 0;
for i = 1:datapoints(1)
    res = res +(abs(data(i)-calc(i)))^2;
end
```

```
function [calc] = CalcArea(variables, peaks, nU, nO)

%variables = [fU234 fU235 fU236 fU237 fU238 P1 P2];
fU234 = variables(1);
fU235 = variables(2);
fU236 = variables(3);
fU237 = variables(4);
fU238 = variables(5);
P1 = variables(6);
P2 = variables(7);

%Insure realistic values
if fU234 < 0, fU234 = 0; end
if fU235 < 0, fU235 = 0; end
if fU236 < 0, fU236 = 0; end
if fU237 < 0, fU237 = 0; end
if fU238 < 0, fU238 = 0; end
if fU234 > 1, fU234 = 1; end
if fU235 > 1, fU235 = 1; end
if fU236 > 1, fU236 = 1; end
if fU237 > 1, fU237 = 1; end
if fU238 > 1, fU238 = 1; end
if P1 < 0, P1 = 0; end
if P1 > 1, P1 = 1; end
if P2 < 0, P2 = 0; end
if P2 > 1, P2 = 1; end
if (P1+P2)>1, P2 = 1-P1; end

fU = [fU234, fU235, fU236, fU237, fU238];

%Check for fU = 1 and normalize if necessary
if sum(fU)~=1,
    fU234 = fU(1)/sum(fU);
    fU235 = fU(2)/sum(fU);
    fU236 = fU(3)/sum(fU);
    fU237 = fU(4)/sum(fU);
    fU238 = fU(5)/sum(fU);
    fU = [fU234, fU235, fU236, fU237, fU238];
end

[masses, fractions]=GetMF(nU,nO,fU, P1, P2);
calc = GetSumComponents(peaks, masses, fractions);
```

```
function [m, f] = GetMF(nU,nO,fU,P1,P2)

mU234 = 234.040951;
mU235 = 235.0439299;
mU236 = 236.045568;
mU237 = 237.0487302;
mU238 = 238.0507882;

fO16 = .99762;
fO17 = .00038;
fO18 = .00200;
mO16 = 15.99491462;
mO17 = 16.9991317;
mO18 = 17.999161;

%H
fH1 = 0.99985;
fH2 = 0.00015;
mH1 = 1.007825032;
mH2 = 2.01410178;
mH = [0 , mH1, mH2];
fP0 =  1-(P1*fH1)-(P1*fH2)-(P2*fH1);
fP1 =  P1*fH1;
fP2 =  P2*fH1+P1*fH2;
fP = [ fP0, fP1, fP2];

%O
mO = [mO16, mO17, mO18];
fO = [fO16, fO17, fO18];
%U
mU = [mU234, mU235, mU236, mU237, mU238];

m = 0;
f = 1;

for i = 1:nU;
    m = [mU(1)+m, mU(2)+m, mU(3)+m, mU(4)+m, mU(5)+m];
    f = [fU(1)*f, fU(2)*f, fU(3)*f, fU(4)*f, fU(5)*f];
    [f, m]=ReduceVector(f, m);
end

if nO>0;
    for j = 1:nO;
        m = [mO(1)+m, mO(2)+m, mO(3)+m];
        f = [fO(1)*f, fO(2)*f, fO(3)*f];
        [f, m]=ReduceVector(f, m);
    end
end

%Add protonation
m = [m+mH(1), m+mH(2), m+mH(3)];
f = [f*fP(1), f*fP(2), f*fP(3)];
[f, m]=ReduceVector(f, m);
```

```
function [output1, output2]=ReduceVector(input1, input2)
s = size(input1);
for i = 1: s(2);
    if input1(i)< 1e-5;
        input1(i) = 0;
        input2(i) = 0;
    end
end
output1 = (nonzeros(input1))';
output2 = (nonzeros(input2))';
```

```
function [calc] = GetSumComponents(peaks, masses, fractions)

peaknumber = size(peaks);
calc = zeros(1, peaknumber(1));

for i = 1: peaknumber(1);
    index = find(masses>(peaks(i,1)-0.5) & masses<(peaks(i,1)+0.5));
    components = size(index);
    for j = 1: components(2);
        calc(i) = calc(i)+fractions(index(j));
    end
end
```

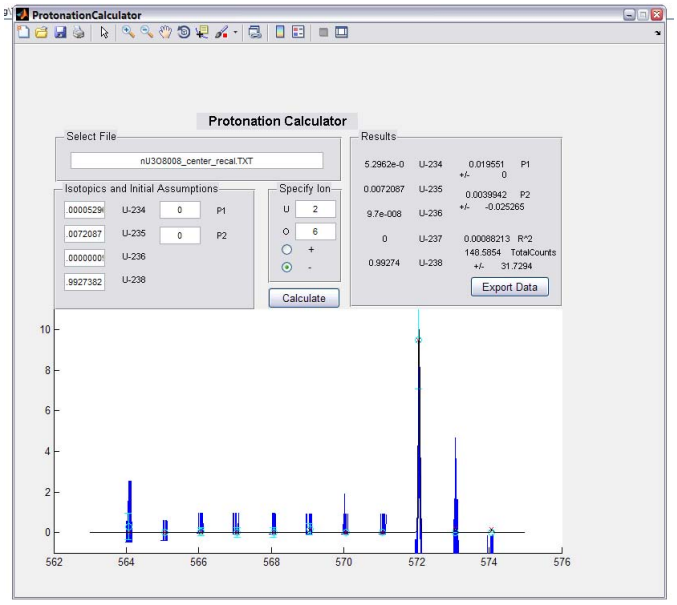
```
function PlotSpectrum(fU234, fU235, fU236, fU237, fU238, P1, P2, nU,
nO,...
    c, multiplier)

%Define Statistics
var = (c/sqrt(2))^2;

%Get Spectrum

xmin = 234*nU + 16*nO - 1;
xmax = 238*nU + 16*nO + 3;
X= xmin : .001 : xmax;

spectrum = GetCluster(fU234,fU235,fU236,fU237,fU238,...
        P1, P2, nU, nO, var);
curve = pdf(spectrum,X');
curve = curve/max(curve)*multiplier;

%Plot
plot(X', curve, 'k')
```

```
function[sigma238, sigma237, sigma236, sigma235, sigma234, sigmaP1,
sigmaP2]...
    = GetError(i, counts, sigmaX, P1, P2)

fO18 = .00200;
fH2 = 0.00015;
enrich = 0;

if i == 7 && counts(2)>counts(i-2); enrich = 1; j = 1; end
if i == 11 && counts(3)>counts(i-2); enrich = 1; j = 2; end
if i == 15 && counts(4)>counts(i-2); enrich = 1; j = 3; end
if i == 19 && counts(5)>counts(i-2); enrich = 1; j = 4; end
if i == 23 && counts(6)>counts(i-2); enrich = 1; j = 5; end
if i == 27 && counts(7)>counts(i-2); enrich = 1; j = 6; end
if i == 31 && counts(8)>counts(i-2); enrich = 1; j = 7; end
if i == 35 && counts(9)>counts(i-2); enrich = 1; j = 8; end
if i == 39 && counts(10)>counts(i-2); enrich = 1; j = 9; end
if i == 43 && counts(11)>counts(i-2); enrich = 1; j = 10; end

if enrich == 1;
    CountSum =
counts(1)+counts(2)+counts(3)+counts(4)+counts(5)+counts(6)+counts(7);

    est238 = ((counts(j+4) - (counts(j+2)*P2) - (counts(j+3)*P1)) / (1-
P1-P2)) ...
        /CountSum;
    est237 = ((counts(j+3) - (counts(j+1)*P2) - (counts(j+2)*P1)) / (1-
P1-P2))...
        / CountSum;
    est236 = ((counts(j+2) - (counts(j)*P2) - (counts(j+1)*P1)) / (1-
P1-P2))...
        / CountSum;
    est235 = ((counts(j+1) - (counts(j)*P1)) / (1-P1-P2)) / CountSum;
    est234 = counts(j) / CountSum;

    if counts(j) == 0; counts(1) = 1; end
    if counts(j+1) == 0; counts(2) = 1; end
    if counts(j+2) == 0; counts(3) = 1; end
    if counts(j+3) == 0; counts(4) = 1; end
    if counts(j+4) == 0; counts(5) = 1; end
    if counts(j+5) == 0; counts(6) = 1; end
    if counts(j+6) == 0; counts(7) = 1; end
    if P1 == 0; P1 = 1/CountSum; end
    if P2 == 0; P2 = 1/CountSum; end

    sigmaCountSum = sqrt(sigmaX(j)^2+sigmaX(j+1)^2+sigmaX(j+2)^2+...
        sigmaX(j+3)^2+sigmaX(j+4)^2+sigmaX(j+5)^2+sigmaX(j+6)^2);
    sigma234 = sqrt((sigmaX(j)^2/counts(j)^2) +
(sigmaCountSum^2/CountSum^2))*est234;
    sigmaP1 =
sqrt((sigmaX(j+2)/counts(j+2))^2+(sigmaX(j+1)/counts(j+1))^2)*...
        (counts(j+2)/counts(j+1));
    sigmaP2 =
sqrt((sigmaX(j+3)/counts(j+3))^2+(sigmaX(j+1)/counts(j+1))^2)*...
```

```
        (counts(j+3)/counts(j+1));
    sigma235 = sqrt(((sigmaX(j+1)^2 +
((sigmaX(j)/counts(j))^2+(sigmaP1/P1)^2)...
        *(counts(j)*P1)^2)/(counts(j+1)-counts(j)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est235;
   sigma236 =
sqrt(((sigmaX(j+2)^2+((sigmaX(j)/counts(j))^2+(sigmaP2/P2)^2)*(counts(j
)*P2)^2+...

((sigmaX(j+1)/counts(j+1))^2+(sigmaP1/P1)^2)*(counts(j+1)*P1)^2)/...
       (counts(j+2)-counts(j)*P2-counts(j+1)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est236;
   sigma237 =
sqrt(((sigmaX(j+3)^2+((sigmaX(j+1)/counts(j+1))^2+(sigmaP2/P2)^2)*(coun
ts(j+1)*P2)^2+...

((sigmaX(j+2)/counts(j+2))^2+(sigmaP1/P1)^2)*(counts(j+2)*P1)^2)/...
       (counts(j+3)-counts(j+1)*P2-counts(j+2)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est237;
   sigma238 =
sqrt(((sigmaX(j+4)^2+((sigmaX(j+2)/counts(j+2))^2+(sigmaP2/P2)^2)*(coun
ts(j+2)*P2)^2+...

((sigmaX(j+3)/counts(j+3))^2+(sigmaP1/P1)^2)*(counts(j+3)*P1)^2)/...
       (counts(j+4)-counts(j+2)*P2-counts(j+3)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est238;

elseif enrich == 0;
    CountSum = counts(i)+counts(i-1)+counts(i-2)+counts(i-3)+counts(i-
4)+counts(i-5)+counts(i-6);

    est238 = (counts(i-2)+counts(i-1)+counts(i))/CountSum;
    est237 = (counts(i-3) - (counts(i-5)*P2) - (counts(i-4)*P1)) /
CountSum;
    est236 = (counts(i-4) - (counts(i-6)*P2) - (counts(i-5)*P1)) /
CountSum;
    est235 = (counts(i-5) - (counts(i-6)*P1)) / CountSum;
    est234 = counts(i-6) / CountSum;
    estP1 = counts(i-1) / counts(i-2);
    estP2 = (counts(i) - counts(i-2)*fO18 - counts(i-1)*fH2) /
counts(i-2);

    if counts(i) == 0; counts(i) = 1; end
    if counts(i-1) == 0; counts(i-1) = 1; end
    if counts(i-2) == 0; counts(i-2) = 1; end
    if counts(i-3) == 0; counts(i-3) = 1; end
    if counts(i-4) == 0; counts(i-4) = 1; end
    if counts(i-5) == 0; counts(i-5) = 1; end
    if counts(i-6) == 0; counts(i-6) = 1; end
    if P1 == 0; P1 = 1/CountSum; end
    if P2 == 0; P2 = 1/CountSum; end
```

```
    sigmaCountSum = sqrt(sigmaX(i)^2+sigmaX(i-1)^2+sigmaX(i-2)^2+...
        sigmaX(i-3)^2+sigmaX(i-4)^2+sigmaX(i-5)^2+sigmaX(i-6)^2);

    sigma238 = sqrt(((sigmaX(i-2)^2+(sigmaX(i))^2+(sigmaX(i-1))^2)/...
        (counts(i-2)+counts(i-1)+counts(i))^2) +
(sigmaCountSum^2/CountSum^2))*est238;

    sigmaP1 = sqrt((sigmaX(i-1)^2/counts(i-1)^2) + (sigmaX(i-
2)^2/counts(i-2)^2))*estP1;

    sigmaP2 = sqrt(((sigmaX(i)^2+(sigmaX(i-2)*fO18)^2+(sigmaX(i-
1)*fH2)^2)...
        /(counts(i)-counts(i-2)*fO18-counts(i-1)*fH2)^2)+(sigmaX(i-
2)^2/counts(i-2)^2))*estP2;

    sigma234 = sqrt((sigmaX(i-6)^2/counts(i-6)^2) +
(sigmaCountSum^2/CountSum^2))*est234;

    sigma235 = sqrt((((sigmaX(i-5))^2+...
        (sqrt((sigmaX(i-6)^2/counts(i-
6)^2)+(sigmaP1^2/P1^2))*(counts(i-6)*P1))^2)...
        /(counts(i-5)-counts(i-
6)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est235;

    sigma236 = sqrt((((sigmaX(i-4))^2+...
        (sqrt((sigmaX(i-6)^2/counts(i-
6)^2)+(sigmaP2^2/P2^2))*(counts(i-6)*P2))^2 ...
        +(sqrt((sigmaX(i-5)^2/counts(i-
5)^2)+(sigmaP1^2/P1^2))*(counts(i-5)*P1))^2 ...
        )/(counts(i-4)-counts(i-6)*P2-counts(i-
5)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est236;

    sigma237 = sqrt((((sigmaX(i-3))^2+...
        (sqrt((sigmaX(i-5)^2/counts(i-
5)^2)+(sigmaP2^2/P2^2))*(counts(i-5)*P2))^2+...
        (sqrt((sigmaX(i-4)^2/counts(i-
4)^2)+(sigmaP1^2/P1^2))*(counts(i-4)*P1))^2 ...
        )/(counts(i-3)-counts(i-5)*P2-counts(i-
4)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est237;
end
```

Appendix D. Protonation Calculator




```
function varargout = ProtonationCalculator(varargin)
% PROTONATIONCALCULATOR M-file for ProtonationCalculator.fig
%      PROTONATIONCALCULATOR, by itself, creates a new
PROTONATIONCALCULATOR or raises the existing
%      singleton*.
%
%      H = PROTONATIONCALCULATOR returns the handle to a new
PROTONATIONCALCULATOR or the handle to
%      the existing singleton*.
%
%      PROTONATIONCALCULATOR('CALLBACK',hObject,eventData,handles,...)
calls the local
%      function named CALLBACK in PROTONATIONCALCULATOR.M with the
given input arguments.
%
%      PROTONATIONCALCULATOR('Property','Value',...) creates a new
PROTONATIONCALCULATOR or raises the
%      existing singleton*.  Starting from the left, property value
pairs are
%      applied to the GUI before ProtonationCalculator_OpeningFcn gets
called.  An
%      unrecognized property name or invalid value makes property
application
%      stop.  All inputs are passed to ProtonationCalculator_OpeningFcn
via varargin.
%
%      *See GUI Options on GUIDE's Tools menu.  Choose "GUI allows only
one
```

```
%      instance to run (singleton)".
%
% See also: GUIDE, GUIDATA, GUIHANDLES

% Edit the above text to modify the response to help
ProtonationCalculator

% Last Modified by GUIDE v2.5 02-Dec-2010 17:51:32

% Begin initialization code - DO NOT EDIT
gui_Singleton = 1;
gui_State = struct('gui_Name',       mfilename, ...
                   'gui_Singleton',  gui_Singleton, ...
                   'gui_OpeningFcn', @ProtonationCalculator_OpeningFcn,
...
                   'gui_OutputFcn',  @ProtonationCalculator_OutputFcn,
...
                   'gui_LayoutFcn',  [] , ...
                   'gui_Callback',   []);
if nargin && ischar(varargin{1})
    gui_State.gui_Callback = str2func(varargin{1});
end

if nargout
    [varargout{1:nargout}] = gui_mainfcn(gui_State, varargin{:});
else
    gui_mainfcn(gui_State, varargin{:});
end
% End initialization code - DO NOT EDIT


% --- Executes just before ProtonationCalculator is made visible.
function ProtonationCalculator_OpeningFcn(hObject, eventdata, handles,
varargin)
% This function has no output args, see OutputFcn.
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)
% varargin   command line arguments to ProtonationCalculator (see
VARARGIN)

% Choose default command line output for ProtonationCalculator
handles.output = hObject;

% Update handles structure
set(hObject,'toolbar','figure');
guidata(hObject, handles);

% UIWAIT makes ProtonationCalculator wait for user response (see
UIRESUME)
% uiwait(handles.figure1);
```

```
% --- Outputs from this function are returned to the command line.
function varargout = ProtonationCalculator_OutputFcn(hObject,
eventdata, handles)
% varargout  cell array for returning output args (see VARARGOUT);
% hObject    handle to figure
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Get default command line output from handles structure
varargout{1} = handles.output;


% --- Executes on button press in calculate_pushbutton.
function calculate_pushbutton_Callback(hObject, eventdata, handles)
% hObject    handle to calculate_pushbutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

%Change calculate button
%set(handles.calculate_pushbutton, 'String', '...');
%guidata(hObject, handles);

%Get inputs
cla(handles.axes1,'reset')
guidata(hObject, handles);
axes(handles.axes1)

filename = get(handles.filename_editText,'String');
rawdata = dlmread(filename, '', 2, 0);
channel = rawdata(:,1);
mass = rawdata(:,2);
intensity = rawdata(:,3);

fU234 = str2double(get(handles.ic234_editText, 'String'));
fU235 = str2double(get(handles.ic235_editText, 'String'));
fU236 = str2double(get(handles.ic236_editText, 'String'));
fU237 = 0;
fU238 = str2double(get(handles.ic238_editText, 'String'));
icP1 = str2double(get(handles.icP1_editText, 'String'));
icP2 = str2double(get(handles.icP2_editText, 'String'));
nU = str2double(get(handles.nU_editText, 'String'));
nO = str2double(get(handles.nO_editText, 'String'));
p = get(handles.pos_radiobutton,'Value');
n = get(handles.neg_radiobutton,'Value');

if p==1 && n==0, pn = 1;
elseif p==0 && n==1, pn = 0;
else error('Correct charge')
end

%GetProtonation
[P1 P2 R2 TotalCounts, sigmaTotalCounts, eP1, eP2]  =
GetProtonation1(mass, intensity, fU234, ...
```

```
    fU235, fU236, fU237, fU238, icP1, icP2, nU, nO, pn);
%Convert numbers to strings
sfU234 = num2str(fU234);
sfU235 = num2str(fU235);
sfU236 = num2str(fU236);
sfU237 = num2str(fU237);
sfU238 = num2str(fU238);
sP1 = num2str(P1);
sP2 = num2str(P2);
seP1 = num2str(eP1);
seP2 = num2str(eP2);
sR2 = num2str(R2);
sTotalCounts = num2str(TotalCounts);
seTotalCounts = num2str(sigmaTotalCounts);

%Populate output
set(handles.fU234_text, 'String', sfU234);
set(handles.fU235_text, 'String', sfU235);
set(handles.fU236_text, 'String', sfU236);
set(handles.fU237_text, 'String', sfU237);
set(handles.fU238_text, 'String', sfU238);
set(handles.P1_text, 'String', sP1);
set(handles.P2_text, 'String', sP2);
set(handles.eP1_text, 'String', seP1);
set(handles.eP2_text, 'String', seP2);
set(handles.R2_text, 'String', sR2);
set(handles.TotalCounts_text, 'String', sTotalCounts);
set(handles.eTotalCounts_text, 'String', seTotalCounts);
%set(handles.calculate_pushbutton, 'String', 'Calculate');
guidata(hObject, handles);

function nU_editText_Callback(hObject, eventdata, handles)
% hObject    handle to nU_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of nU_editText as text
%        str2double(get(hObject,'String')) returns contents of
nU_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function nU_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to nU_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
```

```
end



function nO_editText_Callback(hObject, eventdata, handles)
% hObject    handle to nO_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of nO_editText as text
%        str2double(get(hObject,'String')) returns contents of
nO_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function nO_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to nO_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function filename_editText_Callback(hObject, eventdata, handles)
% hObject    handle to filename_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of filename_editText as
text
%        str2double(get(hObject,'String')) returns contents of
filename_editText as a double
%get(hObject,'String')
guidata(hObject, handles);

% --- Executes during object creation, after setting all properties.
function filename_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to filename_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
```

```
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic234_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic234_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic234_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic234_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic234_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic234_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic235_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic235_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic235_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic235_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic235_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic235_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called
```

```
% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic236_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic236_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic236_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic236_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic236_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to ic236_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function ic238_editText_Callback(hObject, eventdata, handles)
% hObject    handle to ic238_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of ic238_editText as
text
%        str2double(get(hObject,'String')) returns contents of
ic238_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function ic238_editText_CreateFcn(hObject, eventdata, handles)
```

```
% hObject    handle to ic238_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function icP1_editText_Callback(hObject, eventdata, handles)
% hObject    handle to icP1_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of icP1_editText as
text
%        str2double(get(hObject,'String')) returns contents of
icP1_editText as a double
guidata(hObject, handles);


% --- Executes during object creation, after setting all properties.
function icP1_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to icP1_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end



function icP2_editText_Callback(hObject, eventdata, handles)
% hObject    handle to icP2_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hints: get(hObject,'String') returns contents of icP2_editText as
text
%        str2double(get(hObject,'String')) returns contents of
icP2_editText as a double
guidata(hObject, handles);
```

```
% --- Executes during object creation, after setting all properties.
function icP2_editText_CreateFcn(hObject, eventdata, handles)
% hObject    handle to icP2_editText (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    empty - handles not created until after all CreateFcns
called

% Hint: edit controls usually have a white background on Windows.
%       See ISPC and COMPUTER.
if ispc && isequal(get(hObject,'BackgroundColor'),
get(0,'defaultUicontrolBackgroundColor'))
    set(hObject,'BackgroundColor','white');
end


% --- Executes on button press in ExportData_pushbutton.
function ExportData_pushbutton_Callback(hObject, eventdata, handles)
% hObject    handle to ExportData_pushbutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

filename = get(handles.filename_editText,'String');
icU234 = get(handles.ic234_editText, 'String');
icU235 = get(handles.ic235_editText, 'String');
icU236 = get(handles.ic236_editText, 'String');
icU237 = '0';
icU238 = get(handles.ic238_editText, 'String');
icP1 = get(handles.icP1_editText, 'String');
icP2 = get(handles.icP2_editText, 'String');
nU = get(handles.nU_editText, 'String');
nO = get(handles.nO_editText, 'String');
p = num2str(get(handles.pos_radiobutton,'Value'));
n = num2str(get(handles.neg_radiobutton,'Value'));
IC = '0';
PC = '1';
fU234 = get(handles.fU234_text, 'String');
fU235 = get(handles.fU235_text, 'String');
fU236 = get(handles.fU236_text, 'String');
fU237 = get(handles.fU237_text, 'String');
fU238 = get(handles.fU238_text, 'String');
P1 = get(handles.P1_text, 'String');
P2 = get(handles.P2_text, 'String');
eU234 = '0';
eU235 = '0';
eU236 = '0';
eU237 = '0';
eU238 = '0';
eP1 = get(handles.eP1_text, 'String');
eP2 = get(handles.eP2_text, 'String');
R2 = get(handles.R2_text, 'String');
TotalCounts = get(handles.TotalCounts_text, 'String');
sigmaTotalCounts = get(handles.eTotalCounts_text, 'String');
```

```
% M = [filename, nU, nO, p, n, IC, PC,icU234,...
%     icU235,icU236,icU237,icU238,...
%     icP1, icP2, fU234, fU235, fU236, fU237, fU238, ...
%     P1, P2, R2, TotalCounts, eU234, eU235, eU236, eU237, eU238, ...
%     eP1, eP2, sigmaTotalCounts];
fileID = fopen('logdata.txt', 'a');
fprintf(fileID, '%s %s %s %s %s %s %s %s %s %s %s %s %s %s %s %s %s
%s %s %s %s %s %s %s %s %s %s %s %s \n',...
    filename, nU, nO, p, n, IC, PC,icU234,...
    icU235,icU236,icU237,icU238,...
    icP1, icP2, fU234, fU235, fU236, fU237, fU238, ...
    P1, P2, R2, TotalCounts, eU234, eU235, eU236, eU237, eU238, ...
    eP1, eP2, sigmaTotalCounts);
guidata(hObject, handles);



% --- Executes on button press in pos_radiobutton.
function pos_radiobutton_Callback(hObject, eventdata, handles)
% hObject    handle to pos_radiobutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hint: get(hObject,'Value') returns toggle state of pos_radiobutton


% --- Executes on button press in neg_radiobutton.
function neg_radiobutton_Callback(hObject, eventdata, handles)
% hObject    handle to neg_radiobutton (see GCBO)
% eventdata  reserved - to be defined in a future version of MATLAB
% handles    structure with handles and user data (see GUIDATA)

% Hint: get(hObject,'Value') returns toggle state of neg_radiobutton
```

```
function [P1 P2 R2 TotalCounts, sigmaTotalCounts, sigmaP1, sigmaP2] =
GetProtonation1...
    (mass, intensity, fU234, fU235, fU236, fU237, fU238, icP1, icP2, nU,
nO, pn)


%Get peaks of interest
peaks = GetPeaks(nU,nO);
peaksize = size(peaks);

hold on

%Get local variance-------------------------------------------------------
----
%Identify largest peak
loc1 = find (mass > (peaks(1)-0.4), 1, 'first');
loc2 = find (mass > (peaks(peaksize(1))+0.4), 1, 'first');
yvalues = intensity(loc1:loc2, 1);
xvalues = mass(loc1:loc2, 1);
[Pmax ploc] = max(yvalues);
bigpeak = xvalues(ploc);

%Get peak segment
loc1 = find (mass > (bigpeak-0.4), 1, 'first');
loc2 = find (mass > (bigpeak+0.4), 1, 'first');
yvalues = intensity(loc1:loc2, 1);
xvalues = mass(loc1:loc2, 1);

%Find local background
[min(1) location(1)] = GetMinimum(mass, intensity, bigpeak-0.5, .5);
[min(2) location(2)] = GetMinimum(mass, intensity, bigpeak+0.5, .5);
bg(1) = mean (intensity((location(1)-20):(location(1)+20)));
bg(2) = mean (intensity((location(2)-20):(location(2)+20)));
background = mean ([bg(1) bg(2)]);

%Subtract background
yvalues = yvalues-background;

%Fit regular gauss
gauss = fit(xvalues,yvalues,'gauss1');
%Get gaussian statistics
stats = coeffvalues(gauss);
c = stats(3);
sigma = c/sqrt(2);
%-------------------------------------------------------------------------
----

for i = 1:peaksize(1);  %Find the counts for each peak

    %Find peak max
    peak = peaks(i);
    loc1 = find (mass > (peak-2*sigma), 1, 'first');
    loc2 = find (mass > (peak+2*sigma), 1, 'first');
```

```
    yvalues = intensity(loc1:loc2, 1);
    xvalues = mass(loc1:loc2, 1);
    [pmax ploc] = max(yvalues);
    %Recenter around max
    peak = xvalues(ploc);
    %Find local background and noise
    ploc = loc1+ploc;
    [min(1) location(1)] = GetMinimum(mass, intensity, peak-0.5, .5);
    [min(2) location(2)] = GetMinimum(mass, intensity, peak+0.5, .5);
    bg(1) = mean (intensity((location(1)-20):(location(1)+20)));
    bg(2) = mean (intensity((location(2)-20):(location(2)+20)));
    background = mean ([bg(1) bg(2)]);
    noise = ((bg(1)-min(1))*2 +(bg(2)-min(2))*2)/2;
    sigmaB(i) = sqrt(background*(loc2-loc1));
    %Find +/- 4 sigma peak segment
    loc1 = find (mass > (peak-4*sigma), 1, 'first');
    loc2 = find (mass > (peak+4*sigma), 1, 'first');
    yvalues = intensity(loc1:loc2, 1);
    xvalues = mass(loc1:loc2, 1);
    sigmaM(i) = sqrt(sum(yvalues));
    %Subtract background and plot peak segment
    yvalues = yvalues-background;
    sigmaX(i) = sqrt(sigmaM(i)^2 +sigmaB(i)^2);
    plot(xvalues,yvalues)
    %Total counts
    counts(i) = sum(yvalues);
    if counts(i) < 0; counts(i) = 0; end

end

%Get relative peak counts
TotalCounts = sum(counts);
sigmaTotalCounts = sqrt(sigmaX*sigmaX');
data = (counts/TotalCounts);
for i = 1:peaksize(1);
    if counts(i) == 0;
        sigmaData(i) =
sqrt((sigmaX(i)^2/1)+(sigmaTotalCounts^2/TotalCounts^2))*data(i);
    else
        sigmaData(i) =
sqrt((sigmaX(i)^2/counts(i)^2)+(sigmaTotalCounts^2/TotalCounts^2))*data
(i);
    end
end

%Weed out zero peaks
index1 = data==0;
doi = data;
poi = peaks;
poi(index1) = 0;
doi = nonzeros(doi);
poi = nonzeros(poi);

%Solve for protonation
```

```
[P1 P2 R2] = PSolver(doi, poi, [fU234 fU235 fU236 fU237 fU238], ...
    icP1, icP2, nU, nO);

%Get calculated peak area from isotopics, protonation
[calc] = CalcArea([fU234 fU235 fU236 fU237 fU238 P1 P2], peaks, nU,
nO);

%Plot
multiplier = Pmax;
ylim([-Pmax/10 Pmax*1.1]);
legend('hide');
plot (peaks(:,1), data*multiplier, 'oc')
errorbar (peaks(:,1),data*multiplier, sigmaData*multiplier, 'oc')
plot (peaks(:,1), calc*multiplier, 'xr')
PlotSpectrum(fU234, fU235, fU236, fU237, fU238, P1, P2, nU, nO,...
    c, multiplier)

%Get protonation error
[sigma238, sigma237, sigma236, sigma235, sigma234, sigmaP1, sigmaP2]...
    = GetError(i, counts, sigmaX, P1, P2);
```

```
function peaks = GetPeaks(nU,nO)

if nU == 0, error('invalid ion');
%U1 series
elseif nU == 1
        if nO == 0, peaks = (234:240)';
        elseif nO == 1, peaks = (250:256)';
        elseif nO == 2, peaks = (266:272)';
        elseif nO == 3, peaks = (282:288)';
        elseif nO == 4, peaks = (298:304)';
        else error('invalid ion')
        end
%U2 series
elseif nU == 2
        if nO == 2, peaks = (500:510)';
        elseif nO == 3, peaks = (516:526)';
        elseif nO == 4, peaks = (532:542)';
        elseif nO == 5, peaks = (548:558)';
        elseif nO == 6, peaks = (564:574)';
        elseif nO == 7, peaks = (580:590)';
        else error('invalid ion')
        end
%U3series
elseif nU == 3
        if nO == 4, peaks = (766:780)';
        elseif nO == 5, peaks = [782, 783, 784, 785, 786, 787, 789,
790,...
                791,792,793,794,795,796]';
        elseif nO == 6, peaks = (798:812)';
        elseif nO == 7, peaks = (814:828)';
        elseif nO == 8, peaks = (830:844)';
        elseif nO == 9, peaks = (846:860)';
        else error('invalid ion')
        end
%U4 series
elseif nU == 4
        if nO == 5, peaks = (1019:1034)';
        elseif nO == 6, peaks = (1035:1050)';
        elseif nO == 7, peaks = (1051:1066)';
        elseif nO == 8, peaks = (1067:1082)';
        elseif nO == 9, peaks = (1083:1098)';
        elseif nO == 10, peaks = (1099:1114)';
        elseif nO == 11, peaks = (1115:1130)';
        else error('invalid ion')
        end
%U5 series
elseif nU == 5
        if nO == 5, peaks = (1257:1272)';
        elseif nO == 6, peaks = (1273:1288)';
        elseif nO == 7, peaks = (1289:1304)';
        elseif nO == 8, peaks = (1305:1320)';
        elseif nO == 9, peaks = (1321:1336)';
        elseif nO == 10, peaks = (1337:1352)';
        elseif nO == 11, peaks = (1353:1368)';
```

```
        elseif nO == 12, peaks = [1369 1370 1371 1372 1373 1374 1375
1376 ...
                1377 1378 1380 1381 1382 1383 1384]';
        elseif nO == 13, peaks = (1385:1400)';
        elseif nO == 14, peaks = (1401:1416)';
        elseif nO == 15, peaks = (1417:1432)';
        else error('invalid ion')
        end
%U6 series
elseif nU == 6
        if nO == 6, peaks = (1511:1526)';
        elseif nO == 7, peaks = (1527:1542)';
        elseif nO == 8, peaks = (1543:1558)';
        elseif nO == 9, peaks = (1559:1574)';
        elseif nO == 10, peaks = [1575 1577 1578 1579 1580 1581 1582
...
                1583 1584 1585 1586 1587 1588 1589 1590]';
        elseif nO == 11, peaks = (1591:1606)';
        elseif nO == 12, peaks = (1607:1622)';
        elseif nO == 13, peaks = (1623:1638)';
        elseif nO == 14, peaks = (1639:1654)';
        elseif nO == 15, peaks = (1655:1670)';
        elseif nO == 16, peaks = (1671:1686)';
        elseif nO == 17, peaks = (1687:1702)';
        elseif nO == 18, peaks = (1703:1718)';
        else error('invalid ion')
        end
%U7 series
elseif nU == 7
        if nO == 7, peaks = [1765 1766 1767 1768 1769 1770 1771 1772
...
                1774 1775 1776 1777 1778 1779 1780]';
        elseif nO == 8, peaks = (1781:1796)';
        elseif nO == 9, peaks = (1797:1812)';
        elseif nO == 10, peaks = (1813:1828)';
        elseif nO == 11, peaks = (1829:1844)';
        elseif nO == 12, peaks = (1845:1860)';
        elseif nO == 13, peaks = (1861:1876)';
        elseif nO == 14, peaks = (1877:1892)';
        elseif nO == 15, peaks = (1893:1908)';
        elseif nO == 16, peaks = (1909:1924)';
        elseif nO == 17, peaks = (1925:1940)';
        elseif nO == 18, peaks = (1941:1956)';
        elseif nO == 19, peaks = [1957 1958 1959 1960 1961 1962 1963
1964 ...
                1965 1966 1967 1968 1969 1971 1972]';
        elseif nO == 20, peaks = (1973:1988)';
        elseif nO == 21, peaks = (1989:2004)';
        else error('invalid ion')
        end
%U8 series
elseif nU == 8
        if nO == 8, peaks = (2019:2034)';
        elseif nO == 9, peaks = (2035:2050)';
        elseif nO == 10, peaks = (2051:2066)';
```

```
        elseif nO == 11, peaks = (2067:2082)';
        elseif nO == 12, peaks = (2083:2098)';
        elseif nO == 13, peaks = (2099:2114)';
        elseif nO == 14, peaks = (2115:2130)';
        elseif nO == 15, peaks = (2131:2146)';
        elseif nO == 16, peaks = (2147:2162)';
        elseif nO == 17, peaks = [2163 2164 2165 2166 2168 2169 2170
2171 ...
                2172 2173 2174 2175 2176 2177 2178]';
        elseif nO == 18, peaks = (2179:2194)';
        elseif nO == 19, peaks = (2195:2210)';
        elseif nO == 20, peaks = (2211:2226)';
        elseif nO == 21, peaks = (2227:2242)';
        elseif nO == 22, peaks = (2243:2258)';
        elseif nO == 23, peaks = (2259:2274)';
        elseif nO == 24, peaks = (2275:2290)';
        else error('invalid ion')
        end
%U9 series
elseif nU == 9
        if nO == 9, peaks = (2273:2288)';
        elseif nO == 10, peaks = (2289:2304)';
        elseif nO == 11, peaks = (2305:2320)';
        elseif nO == 12, peaks = (2321:2336)';
        elseif nO == 13, peaks = (2337:2352)';
        elseif nO == 14, peaks = [2353 2354 2355 2356 2357 2358 2359
2360 ...
                2361 2362 2363 2365 2366 2367 2368]';
        elseif nO == 15, peaks = (2369:2384)';
        elseif nO == 16, peaks = (2385:2400)';
        elseif nO == 17, peaks = (2401:2416)';
        elseif nO == 18, peaks = (2417:2432)';
        elseif nO == 19, peaks = (2433:2448)';
        elseif nO == 20, peaks = (2449:2464)';
        elseif nO == 21, peaks = (2465:2480)';
        elseif nO == 22, peaks = (2481:2496)';
        elseif nO == 23, peaks = (2497:2512)';
        elseif nO == 24, peaks = (2513:2528)';
        elseif nO == 25, peaks = (2529:2544)';
        elseif nO == 26, peaks = (2545:2560)';
        elseif nO == 27, peaks = (2562:2576)';
        else error('invalid ion')
        end
%U10 series
elseif nU == 10
        if nO == 10, peaks = (2527:2542)';
        elseif nO == 11, peaks = (2543:2558)';
        elseif nO == 12, peaks = (2559:2574)';
        elseif nO == 13, peaks = (2575:2590)';
        elseif nO == 14, peaks = (2591:2606)';
        elseif nO == 15, peaks = (2607:2622)';
        elseif nO == 16, peaks = (2623:2638)';
        elseif nO == 17, peaks = (2639:2654)';
        elseif nO == 18, peaks = (2655:2670)';
        elseif nO == 19, peaks = (2671:2686)';
```

```
        elseif nO == 20, peaks = (2687:2702)';
        elseif nO == 21, peaks = (2703:2718)';
        elseif nO == 22, peaks = (2719:2734)';
        elseif nO == 23, peaks = (2735:2750)';
        elseif nO == 24, peaks = [2751 2752 2753 2754 2755 2756 2757
2759 ...
                2760 2761 2762 2763 2764 2765 2766]';
        elseif nO == 25, peaks = (2767:2782)';
        elseif nO == 26, peaks = (2783:2798)';
        elseif nO == 27, peaks = (2799:2814)';
        elseif nO == 28, peaks = (2815:2830)';
        elseif nO == 29, peaks = (2831:2846)';
        elseif nO == 30, peaks = (2847:2862)';
        else error('invalid ion')
        end
else
    error('invalid ion')
end
peaks = peaks - .0051*nO +.0460*nU;
```

```
function [I,loc] = GetMinimum(mass, intensity, massnumber, halfrange)

loc1 = find (mass > (massnumber-halfrange), 1, 'first');
loc2 = find (mass > (massnumber+halfrange), 1, 'first');
slice = intensity (loc1:loc2);
I = min(slice);
loc = find (slice == I, 1, 'first') + loc1;
```

```
function [P1 P2 r] = PSolver(data, peaks, fU, icP1, icP2, nU, nO)

%initial values
initial = [icP1, icP2];

%pass parameters
data = data;
peaks = peaks;

options = optimset('Display', 'final', 'TolFun', .00000000000000000001,
...
    'TolX', .00000000000000000001,...
    'MaxFunEvals', 5000, 'MaxIter', 5000);

[solution, r] = fminsearch (@(variables) ...
        PResiduals(variables, data, peaks, fU, nU, nO), initial,
options);

    P1 = solution(1);
    P2 = solution(2);

%Correct for bad values- this is due to the solver scheme.
if P1 < 0, P1 = 0; end
if P1 > 1, P1 = 1; end
if P2 < 0, P2 = 0; end
if P2 > 1, P2 = 1; end
if (P1+P2)>1, P2 = 1-P1; end
```

```
function res = PResiduals(variables, data, peaks, fU, nU, nO)

calc = PCalcArea(variables, peaks, fU, nU, nO);
datapoints = size(data);
res = 0;
for i = 1:datapoints(1)
    res = res +(abs(data(i)-calc(i)))^2;
end
```

```
function calc = PCalcArea(variables, peaks, fU, nU, nO)

%variables = [P1 P2];
fU234 = fU(1);
fU235 = fU(2);
fU236 = fU(3);
fU237 = fU(4);
fU238 = fU(5);
P1 = variables(1);
P2 = variables(2);

%Insure realistic values
if fU234 < 0, fU234 = 0; end
if fU235 < 0, fU235 = 0; end
if fU236 < 0, fU236 = 0; end
if fU237 < 0, fU237 = 0; end
if fU238 < 0, fU238 = 0; end
if fU234 > 1, fU234 = 1; end
if fU235 > 1, fU235 = 1; end
if fU236 > 1, fU236 = 1; end
if fU237 > 1, fU237 = 1; end
if fU238 > 1, fU238 = 1; end
if P1 < 0, P1 = 0; end
if P1 > 1, P1 = 1; end
if P2 < 0, P2 = 0; end
if P2 > 1, P2 = 1; end
if (P1+P2)>1, P2 = 1-P1; end

fU = [fU234, fU235, fU236, fU237, fU238];

%Check for fU = 1 and normalize if necessary
if sum(fU)~=1,
    fU234 = fU(1)/sum(fU);
    fU235 = fU(2)/sum(fU);
    fU236 = fU(3)/sum(fU);
    fU237 = fU(4)/sum(fU);
    fU238 = fU(5)/sum(fU);
    fU = [fU234, fU235, fU236, fU237, fU238];
end

[masses fractions]=GetMF(nU,nO,fU, P1, P2);
calc = GetSumComponents(peaks, masses, fractions);
```

```
function [m, f] = GetMF(nU,nO,fU,P1,P2)

mU234 = 234.040951;
mU235 = 235.0439299;
mU236 = 236.045568;
mU237 = 237.0487302;
mU238 = 238.0507882;

fO16 = .99762;
fO17 = .00038;
fO18 = .00200;
mO16 = 15.99491462;
mO17 = 16.9991317;
mO18 = 17.999161;

%H
fH1 = 0.99985;
fH2 = 0.00015;
mH1 = 1.007825032;
mH2 = 2.01410178;
mH = [0 , mH1, mH2];
fP0 =  1-(P1*fH1)-(P1*fH2)-(P2*fH1);
fP1 =  P1*fH1;
fP2 =  P2*fH1+P1*fH2;
fP = [ fP0, fP1, fP2];

%O
mO = [mO16, mO17, mO18];
fO = [fO16, fO17, fO18];
%U
mU = [mU234, mU235, mU236, mU237, mU238];

m = 0;
f = 1;

for i = 1:nU;
    m = [mU(1)+m, mU(2)+m, mU(3)+m, mU(4)+m, mU(5)+m];
    f = [fU(1)*f, fU(2)*f, fU(3)*f, fU(4)*f, fU(5)*f];
    [f, m]=ReduceVector(f, m);
end

if nO>0;
    for j = 1:nO;
        m = [mO(1)+m, mO(2)+m, mO(3)+m];
        f = [fO(1)*f, fO(2)*f, fO(3)*f];
        [f, m]=ReduceVector(f, m);
    end
end

%Add protonation
m = [m+mH(1), m+mH(2), m+mH(3)];
f = [f*fP(1), f*fP(2), f*fP(3)];
[f, m]=ReduceVector(f, m);
```

```
function [output1, output2]=ReduceVector(input1, input2)
s = size(input1);
for i = 1: s(2);
    if input1(i)< 1e-5;
        input1(i) = 0;
        input2(i) = 0;
    end
end
output1 = (nonzeros(input1))';
output2 = (nonzeros(input2))';
```

```
function [calc] = GetSumComponents(peaks, masses, fractions)

peaknumber = size(peaks);
calc = zeros(1, peaknumber(1));

for i = 1: peaknumber(1);
    index = find(masses>(peaks(i,1)-0.5) & masses<(peaks(i,1)+0.5));
    components = size(index);
    for j = 1: components(2);
        calc(i) = calc(i)+fractions(index(j));
    end
end
```

```
function [calc] = CalcArea(variables, peaks, nU, nO)

%variables = [fU234 fU235 fU236 fU237 fU238 P1 P2];
fU234 = variables(1);
fU235 = variables(2);
fU236 = variables(3);
fU237 = variables(4);
fU238 = variables(5);
P1 = variables(6);
P2 = variables(7);

%Insure realistic values
if fU234 < 0, fU234 = 0; end
if fU235 < 0, fU235 = 0; end
if fU236 < 0, fU236 = 0; end
if fU237 < 0, fU237 = 0; end
if fU238 < 0, fU238 = 0; end
if fU234 > 1, fU234 = 1; end
if fU235 > 1, fU235 = 1; end
if fU236 > 1, fU236 = 1; end
if fU237 > 1, fU237 = 1; end
if fU238 > 1, fU238 = 1; end
if P1 < 0, P1 = 0; end
if P1 > 1, P1 = 1; end
if P2 < 0, P2 = 0; end
if P2 > 1, P2 = 1; end
if (P1+P2)>1, P2 = 1-P1; end

fU = [fU234, fU235, fU236, fU237, fU238];

%Check for fU = 1 and normalize if necessary
if sum(fU)~=1,
    fU234 = fU(1)/sum(fU);
    fU235 = fU(2)/sum(fU);
    fU236 = fU(3)/sum(fU);
    fU237 = fU(4)/sum(fU);
    fU238 = fU(5)/sum(fU);
    fU = [fU234, fU235, fU236, fU237, fU238];
end

[masses, fractions]=GetMF(nU,nO,fU, P1, P2);
calc = GetSumComponents(peaks, masses, fractions);
```

```
function PlotSpectrum(fU234, fU235, fU236, fU237, fU238, P1, P2, nU,
nO,...
    c, multiplier)

%Define Statistics
var = (c/sqrt(2))^2;

%Get Spectrum

xmin = 234*nU + 16*nO - 1;
xmax = 238*nU + 16*nO + 3;
X= xmin : .001 : xmax;

spectrum = GetCluster(fU234,fU235,fU236,fU237,fU238,...
        P1, P2, nU, nO, var);
curve = pdf(spectrum,X');
curve = curve/max(curve)*multiplier;

%Plot
plot(X', curve, 'k')
```

```
function[sigma238, sigma237, sigma236, sigma235, sigma234, sigmaP1,
sigmaP2]...
    = GetError(i, counts, sigmaX, P1, P2)

fO18 = .00200;
fH2 = 0.00015;
enrich = 0;

if i == 7 && counts(2)>counts(i-2); enrich = 1; j = 1; end
if i == 11 && counts(3)>counts(i-2); enrich = 1; j = 2; end
if i == 15 && counts(4)>counts(i-2); enrich = 1; j = 3; end
if i == 19 && counts(5)>counts(i-2); enrich = 1; j = 4; end
if i == 23 && counts(6)>counts(i-2); enrich = 1; j = 5; end
if i == 27 && counts(7)>counts(i-2); enrich = 1; j = 6; end
if i == 31 && counts(8)>counts(i-2); enrich = 1; j = 7; end
if i == 35 && counts(9)>counts(i-2); enrich = 1; j = 8; end
if i == 39 && counts(10)>counts(i-2); enrich = 1; j = 9; end
if i == 43 && counts(11)>counts(i-2); enrich = 1; j = 10; end

if enrich == 1;
    CountSum =
counts(1)+counts(2)+counts(3)+counts(4)+counts(5)+counts(6)+counts(7);

    est238 = ((counts(j+4) - (counts(j+2)*P2) - (counts(j+3)*P1)) / (1-
P1-P2)) ...
        /CountSum;
    est237 = ((counts(j+3) - (counts(j+1)*P2) - (counts(j+2)*P1)) / (1-
P1-P2))...
        / CountSum;
    est236 = ((counts(j+2) - (counts(j)*P2) - (counts(j+1)*P1)) / (1-
P1-P2))...
        / CountSum;
    est235 = ((counts(j+1) - (counts(j)*P1)) / (1-P1-P2)) / CountSum;
    est234 = counts(j) / CountSum;

    if counts(j) == 0; counts(1) = 1; end
    if counts(j+1) == 0; counts(2) = 1; end
    if counts(j+2) == 0; counts(3) = 1; end
    if counts(j+3) == 0; counts(4) = 1; end
    if counts(j+4) == 0; counts(5) = 1; end
    if counts(j+5) == 0; counts(6) = 1; end
    if counts(j+6) == 0; counts(7) = 1; end
    if P1 == 0; P1 = 1/CountSum; end
    if P2 == 0; P2 = 1/CountSum; end

    sigmaCountSum = sqrt(sigmaX(j)^2+sigmaX(j+1)^2+sigmaX(j+2)^2+...
        sigmaX(j+3)^2+sigmaX(j+4)^2+sigmaX(j+5)^2+sigmaX(j+6)^2);
    sigma234 = sqrt((sigmaX(j)^2/counts(j)^2) +
(sigmaCountSum^2/CountSum^2))*est234;
    sigmaP1 =
sqrt((sigmaX(j+2)/counts(j+2))^2+(sigmaX(j+1)/counts(j+1))^2)*...
        (counts(j+2)/counts(j+1));
    sigmaP2 =
sqrt((sigmaX(j+3)/counts(j+3))^2+(sigmaX(j+1)/counts(j+1))^2)*...
```

```
        (counts(j+3)/counts(j+1));
    sigma235 = sqrt(((sigmaX(j+1)^2 +
((sigmaX(j)/counts(j))^2+(sigmaP1/P1)^2)...
        *(counts(j)*P1)^2)/(counts(j+1)-counts(j)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est235;
   sigma236 =
sqrt(((sigmaX(j+2)^2+((sigmaX(j)/counts(j))^2+(sigmaP2/P2)^2)*(counts(j
)*P2)^2+...

((sigmaX(j+1)/counts(j+1))^2+(sigmaP1/P1)^2)*(counts(j+1)*P1)^2)/...
       (counts(j+2)-counts(j)*P2-counts(j+1)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est236;
   sigma237 =
sqrt(((sigmaX(j+3)^2+((sigmaX(j+1)/counts(j+1))^2+(sigmaP2/P2)^2)*(coun
ts(j+1)*P2)^2+...

((sigmaX(j+2)/counts(j+2))^2+(sigmaP1/P1)^2)*(counts(j+2)*P1)^2)/...
       (counts(j+3)-counts(j+1)*P2-counts(j+2)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est237;
   sigma238 =
sqrt(((sigmaX(j+4)^2+((sigmaX(j+2)/counts(j+2))^2+(sigmaP2/P2)^2)*(coun
ts(j+2)*P2)^2+...

((sigmaX(j+3)/counts(j+3))^2+(sigmaP1/P1)^2)*(counts(j+3)*P1)^2)/...
       (counts(j+4)-counts(j+2)*P2-counts(j+3)*P1)^2)+...
        ((sigmaP1^2+sigmaP2^2)/(1-P1-
P2)^2)+(sigmaCountSum/CountSum)^2)*est238;

elseif enrich == 0;
    CountSum = counts(i)+counts(i-1)+counts(i-2)+counts(i-3)+counts(i-
4)+counts(i-5)+counts(i-6);

    est238 = (counts(i-2)+counts(i-1)+counts(i))/CountSum;
    est237 = (counts(i-3) - (counts(i-5)*P2) - (counts(i-4)*P1)) /
CountSum;
    est236 = (counts(i-4) - (counts(i-6)*P2) - (counts(i-5)*P1)) /
CountSum;
    est235 = (counts(i-5) - (counts(i-6)*P1)) / CountSum;
    est234 = counts(i-6) / CountSum;
    estP1 = counts(i-1) / counts(i-2);
    estP2 = (counts(i) - counts(i-2)*fO18 - counts(i-1)*fH2) /
counts(i-2);

    if counts(i) == 0; counts(i) = 1; end
    if counts(i-1) == 0; counts(i-1) = 1; end
    if counts(i-2) == 0; counts(i-2) = 1; end
    if counts(i-3) == 0; counts(i-3) = 1; end
    if counts(i-4) == 0; counts(i-4) = 1; end
    if counts(i-5) == 0; counts(i-5) = 1; end
    if counts(i-6) == 0; counts(i-6) = 1; end
    if P1 == 0; P1 = 1/CountSum; end
    if P2 == 0; P2 = 1/CountSum; end
```

```
    sigmaCountSum = sqrt(sigmaX(i)^2+sigmaX(i-1)^2+sigmaX(i-2)^2+...
        sigmaX(i-3)^2+sigmaX(i-4)^2+sigmaX(i-5)^2+sigmaX(i-6)^2);

    sigma238 = sqrt(((sigmaX(i-2)^2+(sigmaX(i))^2+(sigmaX(i-1))^2)/...
        (counts(i-2)+counts(i-1)+counts(i))^2) +
(sigmaCountSum^2/CountSum^2))*est238;

    sigmaP1 = sqrt((sigmaX(i-1)^2/counts(i-1)^2) + (sigmaX(i-
2)^2/counts(i-2)^2))*estP1;

    sigmaP2 = sqrt(((sigmaX(i)^2+(sigmaX(i-2)*fO18)^2+(sigmaX(i-
1)*fH2)^2)...
        /(counts(i)-counts(i-2)*fO18-counts(i-1)*fH2)^2)+(sigmaX(i-
2)^2/counts(i-2)^2))*estP2;

    sigma234 = sqrt((sigmaX(i-6)^2/counts(i-6)^2) +
(sigmaCountSum^2/CountSum^2))*est234;

    sigma235 = sqrt((((sigmaX(i-5))^2+...
        (sqrt((sigmaX(i-6)^2/counts(i-
6)^2)+(sigmaP1^2/P1^2))*(counts(i-6)*P1))^2)...
        /(counts(i-5)-counts(i-
6)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est235;

    sigma236 = sqrt((((sigmaX(i-4))^2+...
        (sqrt((sigmaX(i-6)^2/counts(i-
6)^2)+(sigmaP2^2/P2^2))*(counts(i-6)*P2))^2 ...
        +(sqrt((sigmaX(i-5)^2/counts(i-
5)^2)+(sigmaP1^2/P1^2))*(counts(i-5)*P1))^2 ...
        )/(counts(i-4)-counts(i-6)*P2-counts(i-
5)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est236;

    sigma237 = sqrt((((sigmaX(i-3))^2+...
        (sqrt((sigmaX(i-5)^2/counts(i-
5)^2)+(sigmaP2^2/P2^2))*(counts(i-5)*P2))^2+...
        (sqrt((sigmaX(i-4)^2/counts(i-
4)^2)+(sigmaP1^2/P1^2))*(counts(i-4)*P1))^2 ...
        )/(counts(i-3)-counts(i-5)*P2-counts(i-
4)*P1)^2)+(sigmaCountSum^2/CountSum^2))*est237;
end
```

Appendix E. Protonation Values

The following tables report protonation values for U_xO_y ions in each spectrum as determined by the Protonation Calculator described in Appendix D. P1 denotes the fraction of ions with a single protonation. P2 denotes the fraction of ions which have di-protonated. The Total Counts column reports the total counts attributed to an ion including the protonated and di-protonated counts. The residual is the R^2 value reported by the Protonation Calculator. A smaller residual indicates a better fit from the Protonation Calculator. Reported errors are one sigma values based on counting statistics.

Spectrum:	nU001 Metal				
Isotopics:	**234:** 0.0000525	**235:** 0.0072017	**236:** 0.0000000		
	237: 0.0000000	**238:** 0.9927460			
Ion					
U **O**	**P1**	**P2**		**TotalCounts**	**Residual**
1 1	0.231696 +/- 0.001128	0.036655 +/- 0.000296		431902 +/- 661	0.002491
1 2	**0.242892 +/- 0.000573**	**0.028319 +/- 0.000154**		**1847520 +/- 1361**	**0.000572**
1 3	0.687916 +/- 0.006477	0.312084 +/- 0.006400		156862 +/- 402	0.039182
2 2	0.092638 +/- 0.014742	0.063403 +/- -0.014164		2408 +/- 85	0.002636
2 3	0.072982 +/- 0.001862	0.018666 +/- -0.000841		31018 +/- 197	0.003109
2 4	**0.145178 +/- 0.000968**	**0.000000 +/- 0.000251**		**247238 +/- 505**	**0.000331**
2 5	0.517463 +/- 0.006030	0.000000 +/- 0.001156		137955 +/- 381	0.001462
3 5	0.000000 +/- 0.000000	0.009244 +/- -0.002543		7822 +/- 112	0.000608
3 6	0.067229 +/- 0.001218	0.000000 +/- 0.000527		65121 +/- 267	0.000384
3 7	**0.137918 +/- 0.001752**	**0.000000 +/- 0.000564**		**82070 +/- 299**	**0.000063**
3 8	0.595741 +/- 0.054905	0.000000 +/- -0.013793		3895 +/- 96	0.000452
4 7	0.014113 +/- 0.000000	0.000000 +/- -0.010093		1748 +/- 70	0.001199
4 8	0.025473 +/- 0.002442	0.000000 +/- -0.001669		15944 +/- 144	0.000586
4 9	**0.085590 +/- 0.002789**	**0.000000 +/- -0.001254**		**24323 +/- 174**	**0.000982**
4 10	0.345043 +/- 0.029194	0.000000 +/- -0.014445		2576 +/- 80	0.000561
5 9	0.000000 +/- 0.000000	0.101641 +/- -1.192870		598 +/- 51	0.006223
5 10	0.000000 +/- 0.000000	0.000000 +/- -0.004243		5268 +/- 94	0.001825
5 11	**0.000000 +/- 0.000000**	**0.000000 +/- -0.004059**		**6624 +/- 108**	**0.001847**
5 12	0.016939 +/- 0.018219	0.000000 +/- -0.015452		1771 +/- 70	0.000651

6	12	0.000000 +/- 0.000000	0.000000 +/- -0.017138	1265 +/- 57	0.001817
6	**13**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.014723**	**1679 +/- 69**	**0.002535**
6	14	0.000000 +/- 0.000000	0.042407 +/- -0.050127	852 +/- 55	0.002555
7	**15**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.254068**	**594 +/- 48**	**0.000642**

Spectrum:	nU002				
Isotopics:	**234:** 0.0000525	**235:** 0.0072017	**236:** 0.000000		
	237: 0.0000000	**238:** 0.9927460			
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.152251 +/- 0.004713	0.171446 +/- 0.005055	20878 +/- 155	0.000226
1	**3**	**0.158658 +/- 0.001329**	**0.060699 +/- 0.000801**	**183134 +/- 432**	**0.000061**
1	4	0.661585 +/- 0.020900	0.117791 +/- 0.005325	139440 +/- 379	0.000557
2	5	0.396360 +/- 0.015981	0.000000 +/- -0.003994	8265 +/- 105	0.000160
2	**6**	**0.392629 +/- 0.007782**	**0.000000 +/- 0.001722**	**31499 +/- 193**	**0.000459**
2	4	0.260003 +/- 0.000000	0.086488 +/- 0.060748	337 +/- 42	0.011746
3	7	0.000000 +/- 0.000000	0.180018 +/- -0.018959	1602 +/- 63	0.012561
3	**8**	**0.100848 +/- 0.005071**	**0.000000 +/- -0.002595**	**9766 +/- 117**	**0.000873**
3	9	0.397665 +/- 0.041669	0.000000 +/- -0.023230	1953 +/- 77	0.000463
4	10	0.000000 +/- 0.000000	0.043154 +/- -0.023044	1250 +/- 60	0.001061
4	**11**	**0.000000 +/- 0.022755**	**0.043410 +/- -0.016572**	**1555 +/- 68**	**0.005956**
5	**13**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.019711**	**1318 +/- 60**	**0.001522**

Spectrum:	nU003				
Isotopics:	**234:** 0.0000525	**235:** 0.0072017	**236:** 0.000000		
	237: 0.0000000	**238:** 0.9927460			
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.360405 +/- 0.005486	0.069465 +/- 0.002140	62018 +/- 255	0.000020
1	**1**	**0.221754 +/- 0.001146**	**0.041317 +/- 0.000386**	**395170 +/- 632**	**0.001245**
1	2	0.297978 +/- 0.001804	0.093410 +/- 0.000826	369903 +/- 613	0.003544
2	2	0.101951 +/- 0.004038	0.065756 +/- -0.001422	16639 +/- 145	0.005060
2	**3**	**0.098004 +/- 0.001969**	**0.021819 +/- 0.000672**	**36610 +/- 205**	**0.005954**
2	4	0.133924 +/- 0.004035	0.152225 +/- -0.001784	24594 +/- 174	0.021836
3	4	0.255216 +/- 0.000000	0.048042 +/- -0.003435	4970 +/- 86	0.080379
3	**5**	**0.206848 +/- 0.000000**	**0.038777 +/- -0.003027**	**6723 +/- 99**	**0.040808**
3	6	0.032653 +/- 0.000000	0.005749 +/- -0.004825	3479 +/- 82	0.002644
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.036170	286 +/- 42	0.000859
4	**6**	**0.297022 +/- 0.000000**	**0.056310 +/- -0.029209**	**1104 +/- 54**	**0.144971**
4	7	0.000000 +/- 0.000000	0.000000 +/- -0.052836	608 +/- 48	0.000873

4	8	0.001504 +/- 0.000000	0.000281 +/- -0.058758	439 +/- 35	0.002376

Spectrum:	nU004				
Isotopics:	**234:** 0.0000525 **235:** 0.0072017 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927460				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.375068 +/- 0.020958	0.115327 +/- 0.011248	6604 +/- 95	0.000266
1	2	0.191338 +/- 0.003690	0.117503 +/- 0.002906	39772 +/- 206	0.000007
1	**3**	**0.129046 +/- 0.001668**	**0.058247 +/- 0.001140**	**86816 +/- 300**	**0.000012**
1	4	0.669583 +/- 0.116092	0.215784 +/- 0.042960	29521 +/- 181	0.000076
2	4	0.000000 +/- 0.000000	0.081520 +/- -0.119932	425 +/- 37	0.005193
2	**5**	**0.270459 +/- 0.040680**	**0.019376 +/- -0.034250**	**1204 +/- 54**	**0.000939**
2	7	0.000000 +/- 0.000000	0.141295 +/- -0.102961	480 +/- 56	0.021415

Spectrum:	nU005				
Isotopics:	**234:** 0.0000525 **235:** 0.0072017 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927460				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.209617 +/- 0.002909	0.024398 +/- 0.001086	57216 +/- 245	0.000007
1	**1**	**0.183310 +/- 0.001207**	**0.023812 +/- 0.000349**	**242224 +/- 498**	**0.000647**
1	2	0.253948 +/- 0.002002	0.071751 +/- 0.000917	192583 +/- 443	0.001282
2	2	0.015357 +/- 0.003423	0.118894 +/- -0.001480	13540 +/- 134	0.012519
2	**3**	**0.033371 +/- 0.001872**	**0.128510 +/- -0.000863**	**25880 +/- 172**	**0.015280**
2	4	0.087861 +/- 0.005261	0.206387 +/- -0.002654	13281 +/- 137	0.049256
3	4	0.268700 +/- 0.000000	0.049698 +/- -0.004367	3777 +/- 80	0.097731
3	**5**	**0.257336 +/- 0.000000**	**0.048032 +/- -0.003298**	**4574 +/- 85**	**0.062366**
3	6	0.018534 +/- 0.000000	0.004028 +/- -0.009064	1786 +/- 65	0.001729
4	**6**	**0.198336 +/- 0.000000**	**0.036242 +/- -0.045209**	**541 +/- 51**	**0.048963**

Spectrum:	nU006				
Isotopics:	**234:** 0.0000525 **235:** 0.0072017 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927460				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.336812 +/- 0.023075	0.073321 +/- 0.012293	3613 +/- 74	0.000820
1	2	0.187557 +/- 0.005289	0.098596 +/- 0.003712	19220 +/- 147	0.000003
1	**3**	**0.110715 +/- 0.001931**	**0.037926 +/- 0.001222**	**50760 +/- 230**	**0.000006**

1	4	0.705021 +/- 0.211075	0.197944 +/- 0.069005	16366 +/- 137	0.000024
2	5	0.000000 +/- 0.000000	0.000000 +/- -0.034689	267 +/- 37	0.000484
2	**6**	**0.319169 +/- 0.107327**	**0.279271 +/- -0.043251**	**647 +/- 42**	**0.087703**

Spectrum:	nU007				
Isotopics:	**234:** 0.0000525 **235:** 0.0072017 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927460				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.148659 +/- 0.002316	0.007488 +/- 0.000791	49792 +/- 228	0.000010
1	**1**	**0.158793 +/- 0.001241**	**0.014359 +/- 0.000287**	**178633 +/- 428**	**0.000410**
1	2	0.218642 +/- 0.002016	0.054115 +/- 0.000932	135632 +/- 375	0.000337
2	2	0.000000 +/- 0.002749	0.129596 +/- -0.001280	12369 +/- 124	0.010122
2	**3**	**0.017376 +/- 0.001900**	**0.128741 +/- -0.000985**	**19786 +/- 154**	**0.021098**
2	4	0.063984 +/- 0.005887	0.259498 +/- -0.002997	9975 +/- 116	0.062110
3	4	0.000000 +/- 0.000000	0.412801 +/- -0.005284	3372 +/- 73	0.109152
3	**5**	**0.265511 +/- 0.000000**	**0.048732 +/- -0.004151**	**3394 +/- 76**	**0.067801**
3	6	0.000000 +/- 0.000000	0.000000 +/- -0.009291	1264 +/- 58	0.000516

Spectrum:	nU008				
Isotopics:	**234:** 0.0000525 **235:** 0.0072017 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927460				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.318816 +/- 0.024371	0.023000 +/- 0.013872	2429 +/- 63	0.000430
1	2	0.187809 +/- 0.006040	0.068474 +/- 0.003989	13582 +/- 124	0.000023
1	**3**	**0.101480 +/- 0.002042**	**0.028517 +/- 0.001264**	**41233 +/- 209**	**0.000059**
1	4	0.702722 +/- 0.250370	0.200789 +/- 0.082132	12995 +/- 125	0.000023
2	**5**	**0.000000 +/- 0.064446**	**0.000000 +/- -0.034415**	**277 +/- 31**	**0.000352**

Spectrum:	nUO2001				
Isotopics:	**234:** 0.0000542 **235:** 0.0072390 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927100				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.215778 +/- 0.003868	0.014452 +/- 0.001106	33324 +/- 191	0.000224
1	**2**	**0.200088 +/- 0.001865**	**0.017989 +/- 0.000498**	**119555 +/- 350**	**0.000415**
1	3	0.944545 +/- ########	0.055455 +/- 10.291300	1792 +/- 76	0.000077
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.006224	1963 +/- 57	0.000210
2	**4**	**0.016756 +/- 0.003789**	**0.000000 +/- -0.002014**	**9193 +/- 108**	**0.000307**

2	5	0.365506 +/- 0.064886	0.005252 +/- -0.131166	973 +/- 51	0.000310
3	5	0.048465 +/- 0.000000	0.009042 +/- -0.010529	232 +/- 26	0.003087
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.009307**	**1585 +/- 51**	**0.000935**
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.045756	729 +/- 43	0.000975

Spectrum:	nUO2002					
Isotopics:	**234:**	0.0000542	**235:**	0.0072390	**236:**	0.000000
	237:	0.0000000	**238:**	0.9927100		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.037643 +/- 0.000000	0.033951 +/- 0.023879	937 +/- 49	0.000987
1	**3**	**0.098636 +/- 0.004281**	**0.020404 +/- 0.002598**	**10553 +/- 111**	**0.000124**
1	4	0.712731 +/- 0.073469	0.000000 +/- 0.014201	6825 +/- 96	0.000144

Spectrum:	nUO2003					
Isotopics:	**234:**	0.0000542	**235:**	0.0072390	**236:**	0.000000
	237:	0.0000000	**238:**	0.9927100		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.002699 +/- 0.000000	0.008064 +/- 0.002706	3741 +/- 68	0.000018
1	1	0.071098 +/- 0.003204	0.000000 +/- -0.001029	13873 +/- 125	0.000043
1	**2**	**0.120537 +/- 0.004091**	**0.000000 +/- 0.001951**	**14634 +/- 129**	**0.000040**
1	3	0.080134 +/- 0.000000	0.049901 +/- 0.045554	230 +/- 29	0.007804
2	2	0.018476 +/- 0.000000	0.004067 +/- -0.019793	761 +/- 42	0.001392
2	**3**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.007129**	**1214 +/- 47**	**0.000355**
2	4	0.004487 +/- 0.000000	0.000000 +/- -0.062485	587 +/- 42	0.000773

Spectrum:	nUO2004					
Isotopics:	**234:**	0.0000542	**235:**	0.0072390	**236:**	0.00000
	237:	0.0000000	**238:**	0.9927100		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.000000 +/- 0.000000	0.373140 +/- -0.123275	980 +/- 44	0.140776
1	**3**	**0.037279 +/- 0.004786**	**0.000000 +/- -0.003455**	**5305 +/- 80**	**0.000047**
1	4	0.858226 +/- 0.558964	0.000000 +/- -0.223125	1631 +/- 56	0.000096

Spectrum:	nUO2005					
Isotopics:	**234:**	0.0000542	**235:**	0.0072390	**236:**	0.000000
	237:	0.0000000	**238:**	0.9927100		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	0	0.002888 +/- 0.003714	0.003356 +/- 0.002134	6862 +/- 90	0.000070
1	**1**	**0.081152 +/- 0.003927**	**0.000000 +/- -0.001140**	**11937 +/- 119**	**0.000029**
1	2	0.146522 +/- 0.006313	0.000000 +/- -0.003350	8831 +/- 104	0.000403
1	3	0.000000 +/- 0.000000	0.039787 +/- 0.031572	396 +/- 35	0.000066
2	2	0.071177 +/- 0.000000	0.013106 +/- -0.145790	586 +/- 39	0.010371
2	**3**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.032538**	**715 +/- 45**	**0.000022**
2	4	0.007600 +/- 0.000000	0.001404 +/- -0.032449	366 +/- 37	0.000543

Spectrum:	nUO2006				
Isotopics:	**234:** 0.0000542	**235:** 0.0072390	**236:** 0.00000		
	237: 0.0000000	**238:** 0.9927100			
Ion U	**Ion O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	**3**	**0.000935 +/- 0.007486**	**0.006793 +/- -0.006217**	**2515 +/- 57**	**0.000068**
1	4	0.915963 +/- 3.843670	0.084037 +/- -0.079770	535 +/- 39	0.006446
1	2	0.000000 +/- 0.000000	0.586259 +/- -0.050819	820 +/- 40	0.339522

Spectrum:	nUO2007				
Isotopics:	**234:** 0.0000542	**235:** 0.0072390	**236:** 0.000000		
	237: 0.0000000	**238:** 0.9927100			
Ion U	**Ion O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.042505 +/- 0.007279	0.010047 +/- -0.004077	4245 +/- 74	0.000056
1	1	0.095378 +/- 0.002242	0.000000 +/- -0.000650	32373 +/- 187	0.000043
1	**2**	**0.142730 +/- 0.002361**	**0.017466 +/- 0.000954**	**48201 +/- 227**	**0.000021**
1	3	0.320031 +/- 0.101381	0.074117 +/- -0.059024	359 +/- 35	0.004677
2	2	0.032990 +/- 0.000000	0.005727 +/- -0.019697	806 +/- 38	0.001715
2	**3**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.003143**	**2922 +/- 62**	**0.000427**
2	4	0.000000 +/- 0.000000	0.000000 +/- -0.006522	2541 +/- 64	0.000401
3	**5**	**0.000000 +/- 0.000000**	**0.011427 +/- -0.028809**	**405 +/- 32**	**0.001332**
3	6	0.015587 +/- 0.000000	0.002939 +/- -0.017167	343 +/- 32	0.001314

Spectrum:	nUO2008				
Isotopics:	**234:** 0.0000542	**235:** 0.0072390	**236:** 0.000000		
	237: 0.0000000	**238:** 0.9927100			
Ion U	**Ion O**	**P1**	**P2**	**TotalCounts**	**Residual**

1	1	0.206392 +/- 0.000000	0.000000 +/- -0.021947	149 +/- 37	0.038110
1	2	0.163890 +/- 0.025258	0.217927 +/- 0.029930	1789 +/- 57	0.193169
1	**3**	**0.054505 +/- 0.003243**	**0.000000 +/- -0.001819**	**12018 +/- 120**	**0.000040**
1	4	0.734645 +/- 0.181428	0.092072 +/- 0.045687	4693 +/- 81	0.000065

Spectrum:	nU3O8001					
Isotopics:	**234:**	0.0000530	**235:**	0.0072087	**236:**	0.0000001
	237:	0.0000000	**238:**	0.9927400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.176680 +/- 0.000775	0.022115 +/- 0.000212	544710 +/- 741	0.000559
1	**2**	**0.205370 +/- 0.000365**	**0.020120 +/- 0.000098**	**3249680 +/- 1804**	**0.000199**
1	3	0.771120 +/- 0.130640	0.158530 +/- 0.027989	246558 +/- 501	0.001727
2	2	0.115030 +/- 0.015680	0.066844 +/- -0.017769	2283 +/- 81	0.003701
2	3	0.039074 +/- 0.001747	0.026166 +/- -0.000931	28854 +/- 186	0.000329
2	**4**	**0.074139 +/- 0.000549**	**0.002585 +/- 0.000191**	**330229 +/- 582**	**0.000071**
2	5	0.362140 +/- 0.002610	0.008925 +/- 0.000491	220452 +/- 478	0.000014
3	5	0.025116 +/- 0.000000	0.005178 +/- -0.004258	4285 +/- 85	0.001141
3	6	0.018249 +/- 0.000780	0.000000 +/- 0.000557	61064 +/- 258	0.000287
3	**7**	**0.050199 +/- 0.000831**	**0.000000 +/- 0.000424**	**116036 +/- 351**	**0.000093**
3	8	0.383210 +/- 0.011646	0.000000 +/- -0.002799	14037 +/- 137	0.000598
4	7	0.076697 +/- 0.000000	0.014502 +/- -0.702960	589 +/- 49	0.008745
4	8	0.000000 +/- 0.000000	0.000000 +/- -0.002227	10925 +/- 122	0.001448
4	**9**	**0.003808 +/- 0.001501**	**0.000000 +/- 0.001087**	**25879 +/- 175**	**0.000618**
4	10	0.114550 +/- 0.009341	0.000000 +/- -0.005047	5112 +/- 94	0.000551
4	11	0.259290 +/- 0.064524	0.111020 +/- -0.246480	908 +/- 64	0.007978
5	10	0.000000 +/- 0.000000	0.008263 +/- -0.005756	2959 +/- 76	0.003207
5	**11**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.004276**	**5373 +/- 96**	**0.001540**
5	12	0.000000 +/- 0.000000	0.042006 +/- -0.007288	3267 +/- 79	0.004509
6	12	0.000000 +/- 0.000000	0.231250 +/- -0.015993	177 +/- 39	0.033372
6	13	0.000000 +/- 0.000000	0.068880 +/- -0.086488	437 +/- 51	0.004349
6	**14**	**0.000000 +/- 0.000000**	**0.018805 +/- -0.029174**	**893 +/- 52**	**0.001056**
6	15	0.000000 +/- 0.000000	0.490790 +/- -0.014320	101 +/- 31	0.044240
7	**15**	**0.000000 +/- 0.000000**	**0.233680 +/- -0.013478**	**84 +/- 29**	**0.048848**
7	16	0 +/- 0	0.18204 +/- -0.009225	81.1951 +/- 23.0074	0.021041
7	17	0 +/- 0	0.3066 +/- -0.013979	45.6098 +/- 23.3042	0.041129

Spectrum:	nU3O8002					
Isotopics:	**234:**	0.0000530	**235:**	0.0072087	**236:**	0.0000001

		237: 0.0000000 **238:** 0.9927400			
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.056023 +/- 0.010022	0.226990 +/- 0.013531	4278 +/- 79	0.000499
1	3	0.100840 +/- 0.001251	0.018498 +/- 0.000597	98954 +/- 318	0.000012
1	**4**	**0.484910 +/- 0.004949**	**0.018654 +/- 0.000763**	**164753 +/- 410**	**0.000197**
2	5	0.295200 +/- 0.062204	0.015077 +/- -0.126830	637 +/- 40	0.000288
2	**6**	**0.156790 +/- 0.005297**	**0.000000 +/- -0.001858**	**12924 +/- 123**	**0.000308**
2	7	0.879600 +/- 1.043200	0.000000 +/- -0.075669	1196 +/- 56	0.000319
3	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.007306**	**2046 +/- 56**	**0.000395**
3	9	0.006556 +/- 0.000000	0.000000 +/- -0.043366	840 +/- 47	0.000510
4	10	0.000000 +/- 0.000000	0.307020 +/- -0.004492	23 +/- 13	0.032531
4	**11**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.188600**	**472 +/- 35**	**0.000394**
5	**14**	**0.000000 +/- 0.000000**	**0.185240 +/- -0.006588**	**21 +/- 13**	**0.018929**

Spectrum:		nU3O8003			
Isotopics:		**234:** 0.0000530 **235:** 0.0072087 **236:** 0.0000001			
		237: 0.0000000 **238:** 0.9927400			
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.093186 +/- 0.002772	0.026396 +/- 0.001836	20273 +/- 153	0.001151
1	1	0.059720 +/- 0.000313	0.000979 +/- 0.000065	747417 +/- 866	0.000003
1	**2**	**0.129920 +/- 0.000258**	**0.013123 +/- 0.000084**	**3.09878e6 +/- 1761**	**0.000019**
1	3	0.749590 +/- 0.054799	0.052901 +/- 0.007201	37518 +/- 201	0.001032
2	2	0.050443 +/- 0.000000	0.012179 +/- 0.002690	7152 +/- 94	0.001877
2	3	0.000000 +/- 0.000000	0.000000 +/- 0.000355	74768 +/- 279	0.000074
2	**4**	**0.012981 +/- 0.000276**	**0.000000 +/- 0.000195**	**255036 +/- 509**	**0.000007**
2	5	0.132670 +/- 0.003619	0.000000 +/- -0.001256	19494 +/- 149	0.000136
3	4	0.000000 +/- 0.000000	0.000000 +/- 0.004324	2021 +/- 58	0.000277
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.001166	13045 +/- 127	0.001049
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- 0.000560**	**54879 +/- 242**	**0.000243**
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.001462	16357 +/- 139	0.000469
4	6	0.000000 +/- 0.000000	0.000000 +/- -0.084748	456 +/- 41	0.000420
4	7	0.000000 +/- 0.000000	0.000000 +/- -0.004576	2630 +/- 66	0.000298
4	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- 0.001630**	**11005 +/- 115**	**0.001977**
4	9	0.000000 +/- 0.000000	0.000000 +/- -0.003316	4214 +/- 77	0.002358
5	9	0.038749 +/- 0.000000	0.000000 +/- 0.007882	906 +/- 45	0.005604
5	10	0.037925 +/- 0.000000	0.000000 +/- 0.003907	3192 +/- 75	0.007020
5	11	0.000000 +/- 0.000000	0.000000 +/- 0.008504	963 +/- 47	0.000899

Spectrum:	nU3O8004					
Isotopics:	**234:**	0.0000530	**235:**	0.0072087	**236:**	0.0000001
	237:	0.0000000	**238:**	0.9927400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.000000 +/- 0.000000	0.007121 +/- -0.012958	1858 +/- 55	0.000229
1	3	0.025712 +/- 0.000657	0.000555 +/- 0.000399	85160 +/- 295	0.000012
1	**4**	**0.519690 +/- 0.007699**	**0.023105 +/- 0.001441**	**92064 +/- 308**	**0.000014**
2	**6**	**0.075297 +/- 0.009036**	**0.000000 +/- -0.004534**	**2770 +/- 58**	**0.000219**
2	7	0.366830 +/- 0.000000	0.000000 +/- -0.008046	24 +/- 18	0.070764
2	5	0.231070 +/- 0.000000	0.000000 +/- -0.006494	27 +/- 16	0.022804

Spectrum:	nU3O8005					
Isotopics:	**234:**	0.0000530	**235:**	0.0072087	**236:**	0.0000001
	237:	0.0000000	**238:**	0.9927400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.088841 +/- 0.003123	0.000000 +/- -0.001076	17719 +/- 140	0.000050
1	1	0.119690 +/- 0.001289	0.000000 +/- -0.000268	109257 +/- 335	0.000023
1	**2**	**0.178070 +/- 0.001591**	**0.035439 +/- 0.000716**	**144182 +/- 384**	**0.000001**
1	3	0.275570 +/- 0.045853	0.162830 +/- 0.035411	1346 +/- 55	0.000034
2	2	0.060953 +/- 0.000000	0.000733 +/- -0.002710	6254 +/- 93	0.005519
2	**3**	**0.053131 +/- 0.000000**	**0.009562 +/- -0.001388**	**13989 +/- 130**	**0.006862**
2	4	0.009784 +/- 0.003683	0.084938 +/- -0.002229	10125 +/- 117	0.010949
2	5	0.269860 +/- 0.000000	0.000000 +/- -0.019646	146 +/- 37	0.038553
3	4	0.270740 +/- 0.000000	0.000000 +/- -0.003644	1820 +/- 59	0.085633
3	**5**	**0.112020 +/- 0.000000**	**0.021489 +/- -0.004771**	**2407 +/- 66**	**0.024985**
3	6	0.000000 +/- 0.000000	0.000000 +/- -0.005231	1817 +/- 55	0.001261
4	**8**	**0.053121 +/- 0.000000**	**0.006709 +/- 0.022960**	**187 +/- 26**	**0.001810**

Spectrum:	nU3O8006					
Isotopics:	**234:**	0.0000530	**235:**	0.0072087	**236:**	0.0000001
	237:	0.0000000	**238:**	0.9927400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.000000 +/- 0.000000	0.000000 +/- -2.262400	505 +/- 49	0.000093
1	2	0.120230 +/- 0.009840	0.004230 +/- -0.007157	3669 +/- 72	0.000232
1	**3**	**0.069528 +/- 0.001787**	**0.003979 +/- 0.000911**	**33602 +/- 189**	**0.000003**

1	4	0.702160 +/- 0.097788	0.127480 +/- 0.025459	15422 +/- 136	0.000065
2	**6**	**0.055776 +/- 0.000000**	**0.011110 +/- -0.025319**	**308 +/- 30**	**0.004540**
2	5	0.000000 +/- 0.000000	0.240570 +/- -0.009581	35 +/- 18	0.027110
2	7	0.000000 +/- 0.000000	0.303220 +/- -0.003780	11 +/- 7	0.022263

Spectrum:	nU3O8007			
Isotopics:	**234:** 0.0000530 **235:** 0.0072087 **236:** 0.0000001			
	237: 0.0000000 **238:** 0.9927400			
Ion				
U **O**	**P1**	**P2**	**TotalCounts**	**Residual**
1 0	0.067543 +/- 0.003083	0.000000 +/- -0.001113	15350 +/- 131	0.000065
1 1	0.112470 +/- 0.001636	0.000000 +/- -0.000405	66662 +/- 265	0.000009
1 2	**0.173970 +/- 0.002300**	**0.034148 +/- 0.001085**	**67984 +/- 266**	**0.000011**
1 3	0.072441 +/- 0.036566	0.037855 +/- 0.032284	700 +/- 45	0.000020
2 2	0.064782 +/- 0.000000	0.011752 +/- -0.003287	4384 +/- 79	0.007270
2 3	**0.050698 +/- 0.000000**	**0.009310 +/- -0.001889**	**8029 +/- 104**	**0.006433**
2 4	0.000000 +/- 0.006298	0.147140 +/- -0.003776	4810 +/- 84	0.025514
3 4	**0.274740 +/- 0.000000**	**0.000000 +/- 0.004755**	**1099 +/- 51**	**0.085259**
3 5	0.171970 +/- 0.000000	0.030978 +/- -0.020999	1072 +/- 55	0.050106
3 6	0.013799 +/- 0.000000	0.003138 +/- -0.019548	769 +/- 42	0.002111

Spectrum:	nU3O8008			
Isotopics:	**234:** 0.0000530 **235:** 0.0072087 **236:** 0.0000001			
	237: 0.0000000 **238:** 0.9927400			
Ion				
U **O**	**P1**	**P2**	**TotalCounts**	**Residual**
1 1	0.095117 +/- 0.027746	0.053063 +/- -0.037209	973 +/- 53	0.001390
1 2	0.107500 +/- 0.008442	0.059897 +/- -0.005172	5041 +/- 83	0.004773
1 3	**0.064235 +/- 0.001758**	**0.001711 +/- 0.000922**	**36252 +/- 199**	**0.000007**
1 4	0.713970 +/- 0.116170	0.138550 +/- 0.030752	15811 +/- 135	0.000067
2 6	**0.019551 +/- 0.000000**	**0.003994 +/- -0.025265**	**149 +/- 32**	**0.000882**

Spectrum:	nUO3001 UO3			
Isotopics:	**234:** 0.0000550 **235:** 0.0072000 **236:** 0.000000			
	237: 0.0000000 **238:** 0.9927450			
Ion				
U **O**	**P1**	**P2**	**TotalCounts**	**Residual**
1 1	0.294778 +/- 0.005102	0.051344 +/- 0.001517	39018 +/- 209	0.008070
1 2	**0.237430 +/- 0.001900**	**0.038237 +/- 0.000562**	**163450 +/- 411**	**0.002619**

1	3	0.551146 +/- 0.008883	0.292364 +/- 0.007685	25695 +/- 174	0.136948
2	3	0.013142 +/- 0.000000	0.000000 +/- -0.007886	1846 +/- 66	0.000272
2	**4**	**0.148944 +/- 0.003675**	**0.001700 +/- -0.001260**	**22990 +/- 167**	**0.000152**
2	5	0.470782 +/- 0.014111	0.000000 +/- -0.003486	17902 +/- 151	0.000338
3	5	0.051781 +/- 0.000000	0.000000 +/- -0.074312	460 +/- 41	0.003307
3	6	0.000000 +/- 0.000000	0.000000 +/- -0.003546	5981 +/- 100	0.000412
3	**7**	**0.086117 +/- 0.004177**	**0.000000 +/- -0.001997**	**11921 +/- 122**	**0.000775**
3	8	0.304839 +/- 0.046856	0.000000 +/- -0.045839	1124 +/- 55	0.000546
4	8	0.000000 +/- 0.000000	0.000000 +/- -0.014151	1196 +/- 55	0.001887
4	**9**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.006346**	**2991 +/- 75**	**0.001872**
4	10	0.000000 +/- 0.000000	0.025483 +/- -0.061271	385 +/- 41	0.001941
5	**11**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.049138**	**682 +/- 44**	**0.002109**

Spectrum:	nUO3002							
Isotopics:	**234:**	0.0000550	**235:**	0.0072000	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9927450				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	**3**	**0.126195 +/- 0.006360**	**0.019707 +/- 0.004375**	**7764 +/- 101**	**0.000038**
1	4	0.731761 +/- 0.204599	0.131247 +/- 0.051733	7288 +/- 97	0.000023
1	2	0.000000 +/- 0.000000	0.223956 +/- -0.209504	543 +/- 40	0.027379
2	5	0.000000 +/- 0.000000	0.000000 +/- -0.019303	132 +/- 31	0.000153
2	**6**	**0.278157 +/- 0.024488**	**0.000000 +/- -0.012896**	**2311 +/- 64**	**0.000156**
2	7	1.000000 +/- Inf	0.000000 +/- #NAME?	294 +/- 40	0.000216
3	7	0.757479 +/- 0.000000	0.000000 +/- -0.008389	49 +/- 18	0.098654
3	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.166543**	**562 +/- 41**	**0.000591**
3	9	0.080385 +/- 0.000000	0.014937 +/- -0.015832	143 +/- 31	0.005180
4	**11**	**0.040248 +/- 0.000000**	**0.008251 +/- -0.014168**	**125 +/- 27**	**0.006333**
5	**13**	**0.000000 +/- 0.000000**	**0.136581 +/- -0.009815**	**42 +/- 22**	**0.007894**
5	14	0.000000 +/- 0.000000	0.000000 +/- -0.003322	9 +/- 11	0.001781

Spectrum:	nUO3003							
Isotopics:	**234:**	0.0000550	**235:**	0.0072000	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9927450				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.403501 +/- 0.021137	0.032222 +/- 0.009378	6830 +/- 101	0.000025
1	1	0.216132 +/- 0.002694	0.033790 +/- 0.000976	68876 +/- 269	0.000291
1	**2**	**0.305171 +/- 0.003482**	**0.070531 +/- 0.001422**	**98198 +/- 319**	**0.000884**

1	3	0.316011 +/- 0.046896	0.448757 +/- 0.058091	1197 +/- 62	0.052699
2	2	0.024339 +/- 0.000000	0.004456 +/- -0.016032	922 +/- 46	0.002238
2	3	0.009375 +/- 0.006468	0.000000 +/- -0.002895	4592 +/- 84	0.000207
2	**4**	**0.102056 +/- 0.007820**	**0.000000 +/- -0.004227**	**5644 +/- 92**	**0.000205**
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.029045	624 +/- 38	0.000518
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.022511**	**869 +/- 44**	**0.000486**

Spectrum:	nUO3004				
Isotopics:	**234:** 0.0000550 **235:** 0.0072000 **236:** 0.00000				
	237: 0.0000000 **238:** 0.9927450				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.221011 +/- 0.025948	0.145812 +/- 0.018838	2038 +/- 58	0.102122
1	**3**	**0.100575 +/- 0.005043**	**0.024501 +/- 0.003619**	**7955 +/- 95**	**0.000033**
1	4	0.746836 +/- 0.280644	0.097782 +/- 0.066136	3301 +/- 71	0.000066
2	**6**	**0.111945 +/- 0.000000**	**0.000000 +/- -0.014734**	**80 +/- 19**	**0.009697**

Spectrum:	nUO3005				
Isotopics:	**234:** 0.0000550 **235:** 0.0072000 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927450				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.211796 +/- 0.009611	0.018691 +/- 0.004245	7575 +/- 102	0.001341
1	1	0.109990 +/- 0.000966	0.004045 +/- 0.000259	174168 +/- 423	0.000089
1	**2**	**0.186068 +/- 0.000867**	**0.023009 +/- 0.000296**	**496510 +/- 708**	**0.000031**
1	3	0.815942 +/- 3.130980	0.119206 +/- 0.419167	3983 +/- 89	0.003859
2	2	0.000000 +/- 0.000000	0.033446 +/- -0.027817	894 +/- 46	0.000598
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.001478	10731 +/- 116	0.000371
2	**4**	**0.016351 +/- 0.001493**	**0.000000 +/- -0.000896**	**31249 +/- 187**	**0.000231**
2	5	0.227611 +/- 0.031716	0.000000 +/- -0.022585	1323 +/- 56	0.000280
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.006479	1525 +/- 52	0.000429
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.002220**	**6162 +/- 88**	**0.000878**
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.009766	1317 +/- 51	0.001078
4	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.011923**	**1155 +/- 45**	**0.000881**

Spectrum:	nUO3006				
Isotopics:	**234:** 0.0000550 **235:** 0.0072000 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9927450				
Ion	**P1**		**P2**	**TotalCounts**	**Residual**

U	O								
1	2	0.072118	+/-	0.018239	0.183361	+/-	-0.024945	1550 +/- 50	0.035378
1	**3**	**0.023238**	**+/-**	**0.001390**	**0.000000**	**+/-**	**0.000988**	**26442 +/- 170**	**0.000008**
1	4	0.645216	+/-	0.026211	0.019086	+/-	0.004508	25781 +/- 170	0.000044
2	**6**	**0.000000**	**+/-**	**0.000000**	**0.000000**	**+/-**	**-0.029852**	**711 +/- 40**	**0.000903**

Spectrum:	nUO3007							
Isotopics:	**234:**	0.0000550	**235:**	0.0072000	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9927450				

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	0	0.062007	+/-	0.008745	0.019155	+/-	0.005300	3369 +/- 67	0.000417
1	1	0.110685	+/-	0.001512	0.000000	+/-	-0.000348	77669 +/- 284	0.000018
1	**2**	**0.185486**	**+/-**	**0.001520**	**0.031722**	**+/-**	**0.000672**	**168390 +/- 416**	**0.000005**
1	3	1.000000	+/-	Inf	0.000000	+/-	#NAME?	321 +/- 42	0.000210
2	2	0.000000	+/-	0.000000	0.061600	+/-	-0.007918	1205 +/- 46	0.002888
2	3	0.000000	+/-	0.000000	0.000000	+/-	-0.001653	7583 +/- 96	0.000457
2	**4**	**0.000000**	**+/-**	**0.000000**	**0.000000**	**+/-**	**-0.001867**	**9452 +/- 111**	**0.000410**
2	5	0.000000	+/-	0.000000	0.376438	+/-	-0.012860	37 +/- 24	0.066875
3	4	0.017293	+/-	0.000000	0.003494	+/-	-0.017842	336 +/- 34	0.001078
3	5	0.000000	+/-	0.000000	0.000000	+/-	-0.008341	1237 +/- 46	0.000859
3	**6**	**0.005805**	**+/-**	**0.000000**	**0.001138**	**+/-**	**-0.004462**	**2028 +/- 54**	**0.001469**
3	7	0.038066	+/-	0.000000	0.007046	+/-	-0.008730	123 +/- 23	0.002857

Spectrum:	nUO3008							
Isotopics:	**234:**	0.0000550	**235:**	0.0072000	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9927450				

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	2	0.016181	+/-	0.016306	0.364451	+/-	-0.017262	2482 +/- 62	0.129512
1	**3**	**0.056330**	**+/-**	**0.001574**	**0.000676**	**+/-**	**0.000838**	**36235 +/- 197**	**0.000005**
1	4	0.703318	+/-	0.072250	0.105993	+/-	0.017605	19087 +/- 149	0.000063
2	**6**	**0.000000**	**+/-**	**0.000000**	**0.000000**	**+/-**	**-0.041854**	**305 +/- 32**	**0.000809**
2	7	0.000000	+/-	0.000000	0.226790	+/-	-0.008236	49 +/- 16	0.030135

Spectrum:	dU001							
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322		
	237:	0.0000000	**238:**	0.9979310				

Ion	P1	P2	TotalCounts	Residual

U	O				
1	0	0.427994 +/- 0.041102	0.102138 +/- 0.013542	3469 +/- 78	0.069717
1	1	0.212393 +/- 0.003370	0.055189 +/- 0.001017	40316 +/- 209	0.013919
1	**2**	**0.187421 +/- 0.001289**	**0.038018 +/- 0.000387**	**216493 +/- 470**	**0.004116**
2	3	0.154728 +/- 0.000000	0.000000 +/- -0.005718	3192 +/- 84	0.011064
2	**4**	**0.088631 +/- 0.002462**	**0.013799 +/- -0.000992**	**30546 +/- 193**	**0.000319**
2	5	0.498966 +/- 0.017970	0.000000 +/- -0.004339	13197 +/- 129	0.000113
3	5	0.012470 +/- 0.000000	0.002644 +/- -0.045238	682 +/- 45	0.000549
3	6	0.008400 +/- 0.002955	0.016003 +/- -0.002130	9277 +/- 109	0.000884
3	**7**	**0.071792 +/- 0.003976**	**0.000000 +/- -0.002048**	**12035 +/- 122**	**0.000146**
3	8	0.050707 +/- 0.000000	0.010058 +/- -0.032781	135 +/- 43	0.004805
4	8	0.000000 +/- 0.000000	0.000000 +/- -0.006979	2175 +/- 65	0.000059
4	**9**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.005105**	**3924 +/- 77**	**0.000649**
4	10	0.000000 +/- 0.000000	0.050290 +/- -0.046192	245 +/- 40	0.003197
5	10	0.000000 +/- 0.000000	0.000000 +/- -0.423648	489 +/- 43	0.000484
5	**11**	**0.010754 +/- 0.000000**	**0.002018 +/- -0.017187**	**1204 +/- 49**	**0.000544**
1	3	0.486715 +/- 0.006751	0.283109 +/- 0.004912	26267 +/- 173	0.338177

Spectrum:	dU002					
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322
	237:	0.0000000	**238:**	0.9979310		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.180589 +/- 0.012119	0.183099 +/- 0.011869	5226 +/- 88	0.010305
1	**3**	**0.145789 +/- 0.002122**	**0.064802 +/- 0.001381**	**63375 +/- 257**	**0.000298**
1	4	0.686958 +/- 0.052604	0.141045 +/- 0.013601	55818 +/- 243	0.001581
2	5	0.323496 +/- 0.020715	0.000000 +/- -0.007577	3547 +/- 75	0.000097
2	**6**	**0.389720 +/- 0.010066**	**0.000000 +/- 0.002189**	**18453 +/- 149**	**0.000029**
2	7	0.870540 +/- 41.360300	0.129460 +/- 36.702700	1422 +/- 78	0.006595
3	7	0.420060 +/- 0.000000	0.004970 +/- -0.164631	1015 +/- 54	0.037910
3	**8**	**0.074505 +/- 0.006081**	**0.000000 +/- -0.003444**	**6694 +/- 99**	**0.000109**
3	9	0.412165 +/- 0.044534	0.000000 +/- -0.028056	1684 +/- 63	0.000239
4	10	0.000000 +/- 0.000000	0.000000 +/- -0.253659	567 +/- 53	0.000115
4	**11**	**0.132975 +/- 0.021169**	**0.000000 +/- -0.014331**	**1721 +/- 63**	**0.000243**
5	**13**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.017533**	**1294 +/- 55**	**0.000605**

Spectrum:	dU003					
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322
	237:	0.0000000	**238:**	0.9979310		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	0	0.189729 +/- 0.015625	0.008996 +/- -0.008658	2539 +/- 59	0.000054
1	1	0.122650 +/- 0.001918	0.007144 +/- 0.000560	52161 +/- 235	0.000206
1	**2**	**0.180778 +/- 0.001765**	**0.031401 +/- 0.000696**	**116580 +/- 346**	**0.000133**
1	3	0.737836 +/- Inf	0.000000 +/- #NAME?	503 +/- 47	0.072225
2	2	0.000000 +/- 0.000000	0.000000 +/- -0.242749	531 +/- 33	0.000034
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.002568	4432 +/- 76	0.000081
2	**4**	**0.014517 +/- 0.003452**	**0.000000 +/- -0.002049**	**8290 +/- 101**	**0.000073**
2	5	0.006116 +/- 0.000000	0.001322 +/- -0.027560	187 +/- 35	0.000442
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.016970	746 +/- 40	0.000114
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.005481**	**1977 +/- 50**	**0.000327**
4	6	0.150741 +/- 0.000000	0.000000 +/- 0.056471	52 +/- 14	0.023383
4	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.007779**	**236 +/- 28**	**0.000272**

Spectrum:	dU004					
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322
	237:	0.0000000	**238:**	0.9979310		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	2	0.070500 +/- 0.009614	0.002434 +/- -0.009147	2817 +/- 63	0.000045
1	**3**	**0.034898 +/- 0.001587**	**0.001715 +/- 0.001074**	**26779 +/- 171**	**0.000007**
1	4	0.665625 +/- 0.057188	0.086584 +/- 0.013781	13273 +/- 124	0.000022
2	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.102168**	**617 +/- 42**	**0.000334**

Spectrum:	dU005					
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322
	237:	0.0000000	**238:**	0.9979310		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	0	0.050812 +/- 0.013286	0.004124 +/- -0.008363	1838 +/- 51	0.000010
1	1	0.116846 +/- 0.002513	0.000000 +/- -0.000641	30190 +/- 180	0.000008
1	**2**	**0.189621 +/- 0.003064**	**0.035869 +/- 0.001427**	**44099 +/- 215**	**0.000009**
2	2	0.000000 +/- 0.000000	0.000000 +/- -0.006244	1293 +/- 45	0.000065
2	**3**	**0.007135 +/- 0.000000**	**0.001640 +/- -0.002623**	**3716 +/- 67**	**0.000305**
2	4	0.022228 +/- 0.000000	0.004057 +/- -0.005063	2898 +/- 63	0.001561
3	4	0.000000 +/- 0.000000	0.148144 +/- -0.023630	451 +/- 34	0.017513
3	**5**	**0.093582 +/- 0.000000**	**0.000000 +/- -0.033658**	**718 +/- 37**	**0.007583**
3	6	0.000000 +/- 0.000000	0.000000 +/- -1.872480	499 +/- 32	0.000347

Spectrum:	dU006								
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322			
	237:	0.0000000	**238:**	0.9979310					

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	1	0.000000	+/-	0.046744	0.074706	+/-	-0.079470	397 +/- 39	0.005915
1	2	0.108510	+/-	0.009830	0.000000	+/-	-0.006763	3649 +/- 72	0.000014
1	**3**	**0.054042**	**+/-**	**0.001733**	**0.000000**	**+/-**	**0.000945**	**31713 +/- 185**	**0.000007**
1	4	0.689997	+/-	0.131187	0.153257	+/-	0.040654	9682 +/- 108	0.000027
2	**6**	**0.012481**	**+/-**	**0.000000**	**0.002011**	**+/-**	**-0.029599**	**161 +/- 31**	**0.001056**

Spectrum:	dU007								
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322			
	237:	0.0000000	**238:**	0.9979310					

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	0	0.043835	+/-	0.016642	0.001981	+/-	-0.010881	1379 +/- 46	0.000006
1	1	0.117589	+/-	0.003721	0.000000	+/-	-0.001395	18237 +/- 144	0.000002
1	**2**	**0.209712**	**+/-**	**0.004897**	**0.039728**	**+/-**	**0.002360**	**21876 +/- 154**	**0.000003**
2	2	0.003497	+/-	0.000000	0.000836	+/-	-0.043932	422 +/- 29	0.000093
2	**3**	**0.000000**	**+/-**	**0.000000**	**0.000000**	**+/-**	**-0.005618**	**1649 +/- 48**	**0.000066**
2	4	0.012169	+/-	0.000000	0.002335	+/-	-0.018005	1069 +/- 44	0.000717

Spectrum:	dU008								
Isotopics:	**234:**	0.0000076	**235:**	0.0020291	**236:**	0.0000322			
	237:	0.0000000	**238:**	0.9979310					

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	2	0.156717	+/-	0.013539	0.047204	+/-	0.007590	2918 +/- 65	0.018437
1	**3**	**0.076287**	**+/-**	**0.002670**	**0.009821**	**+/-**	**0.001486**	**18853 +/- 143**	**0.000004**
1	4	0.696990	+/-	0.241496	0.183211	+/-	0.078879	6610 +/- 90	0.000019

Spectrum:	dUO2012								
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000			
	237:	0.0000000	**238:**	0.9972400					

Ion									
U	**O**	**P1**			**P2**			**TotalCounts**	**Residual**
1	0	0.368346	+/-	0.023649	0.231512	+/-	-0.009743	9389 +/- 114	0.026950

1	1	0.321307 +/- 0.003967	0.037537 +/- 0.000883	75276 +/- 283	0.003820
1	**2**	**0.199305 +/- 0.001618**	**0.030612 +/- 0.000501**	**154950 +/- 400**	**0.002400**
2	3	0.003948 +/- 0.000000	0.000906 +/- -0.004741	2591 +/- 68	0.000078
2	**4**	**0.077129 +/- 0.004457**	**0.000000 +/- -0.002106**	**10323 +/- 118**	**0.000078**
2	5	0.458016 +/- 0.039302	0.000000 +/- -0.017530	2774 +/- 72	0.000079
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.056372	427 +/- 34	0.000256
3	**6**	**0.002874 +/- 0.000000**	**0.000679 +/- -0.006535**	**2061 +/- 59**	**0.000181**
3	7	0.003484 +/- 0.000000	0.000820 +/- -0.006900	1665 +/- 53	0.000204
4	**8**	**0.018445 +/- 0.000000**	**0.023947 +/- 0.015748**	**310 +/- 32**	**0.000194**

Spectrum:	dUO2013							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.00000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	**3**	**0.000000 +/- 0.004510**	**0.025727 +/- -0.003386**	**6159 +/- 92**	**0.000393**
1	4	0.563565 +/- 0.036431	0.000000 +/- -0.010339	6072 +/- 92	0.000058
1	2	0.292149 +/- 0.067796	0.248835 +/- 0.060872	1208 +/- 50	0.093822
2	**6**	**0.000000 +/- 0.000000**	**0.031219 +/- -0.032615**	**255 +/- 32**	**0.000735**

Spectrum:	dUO2014							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.012974 +/- 0.007653	0.021338 +/- -0.003873	3857 +/- 74	0.000291
1	1	0.061944 +/- 0.000973	0.000000 +/- -0.000227	92781 +/- 309	0.000006
1	**2**	**0.099257 +/- 0.000695**	**0.006449 +/- 0.000245**	**297355 +/- 549**	**0.000001**
1	3	0.860534 +/- 0.807814	0.005054 +/- -0.111222	1426 +/- 54	0.000217
2	2	0.049491 +/- 0.000000	0.001793 +/- 0.008373	638 +/- 35	0.001667
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.001725	5678 +/- 82	0.000132
2	**4**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.001309**	**13745 +/- 126**	**0.000201**
3	5	0.000000 +/- 0.000000	0.000000 +/- 0.004135	900 +/- 38	0.000067
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.004163**	**2693 +/- 60**	**0.000374**
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.038604	643 +/- 35	0.000394
3	8	1.000000 +/- 0.000000	0.000000 +/- -0.018954	4 +/- 6	0.376499

Spectrum:	dUO2015					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000

		237:	0.0000000	**238:**	0.9972400	
Ion						
U	**O**	**P1**		**P2**	**TotalCounts**	**Residual**
1	2	0.048253 +/- 0.000000		0.004146 +/- 0.020973	542 +/- 34	0.002665
1	**3**	**0.025251 +/- 0.001837**		**0.000000 +/- -0.001128**	**16528 +/- 133**	**0.000023**
1	4	0.624137 +/- 0.035998		0.037591 +/- 0.007508	12903 +/- 120	0.000014
2	**6**	**0.014848 +/- 0.000000**		**0.000000 +/- -0.042308**	**312 +/- 29**	**0.000358**

Spectrum:	dUO2016					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		
Ion						
U	**O**	**P1**		**P2**	**TotalCounts**	**Residual**
1	0	0.024418 +/- 0.000000		0.012259 +/- 0.003835	3220 +/- 66	0.000328
1	1	0.057172 +/- 0.001117		0.000000 +/- -0.000317	69922 +/- 269	0.000011
1	**2**	**0.102733 +/- 0.000899**		**0.007406 +/- 0.000338**	**189669 +/- 439**	**0.000004**
1	3	0.894597 +/- 3.680440		0.105403 +/- -0.047879	531 +/- 41	0.008721
2	2	0.006249 +/- 0.000000		0.008295 +/- 0.006161	1054 +/- 41	0.000088
2	3	0.000000 +/- 0.000000		0.000000 +/- -0.001750	5380 +/- 80	0.000118
2	**4**	**0.000000 +/- 0.000000**		**0.000000 +/- -0.001644**	**8827 +/- 101**	**0.000166**
2	5	0.051752 +/- 0.000000		0.000000 +/- -0.038853	312 +/- 29	0.001654
3	5	0.000000 +/- 0.000000		0.000000 +/- 0.005197	717 +/- 39	0.000046
3	**6**	**0.024726 +/- 0.000000**		**0.004448 +/- -0.005553**	**1692 +/- 52**	**0.002348**
3	7	0.000000 +/- 0.000000		0.000000 +/- -0.014045	230 +/- 26	0.000232

Spectrum:	dUO2017					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		
Ion						
U	**O**	**P1**		**P2**	**TotalCounts**	**Residual**
1	2	0.199160 +/- 0.000000		0.009387 +/- 0.014305	835 +/- 37	0.040824
1	**3**	**0.028327 +/- 0.002092**		**0.000000 +/- -0.001232**	**16416 +/- 134**	**0.000027**
1	4	0.689043 +/- 0.065933		0.045949 +/- 0.014086	9834 +/- 111	0.000018
2	**6**	**0.000000 +/- 0.000000**		**0.000000 +/- -0.016120**	**200 +/- 25**	**0.000123**

Spectrum:	dUO2018					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		
Ion		**P1**		**P2**	**TotalCounts**	**Residual**

U	O				
1	0	0.009794 +/- 0.000000	0.014657 +/- 0.004354	3041 +/- 68	0.000096
1	1	0.058259 +/- 0.001120	0.000000 +/- -0.000304	67846 +/- 264	0.000017
1	**2**	**0.103017 +/- 0.000947**	**0.008107 +/- 0.000369**	**170422 +/- 416**	**0.000003**
1	3	0.910933 +/- 3.037230	0.089067 +/- -0.045385	517 +/- 39	0.009635
2	2	0.032957 +/- 0.000000	0.007486 +/- 0.007072	1230 +/- 46	0.000851
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.001699	5825 +/- 85	0.000119
2	**4**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.001806**	**8474 +/- 98**	**0.000219**
2	5	0.066589 +/- 0.000000	0.011858 +/- -0.012778	181 +/- 26	0.002896
3	5	0.003701 +/- 0.000000	0.000000 +/- 0.005598	933 +/- 41	0.000145
3	**6**	**0.021825 +/- 0.000000**	**0.004085 +/- -0.005728**	**1969 +/- 49**	**0.001940**
3	8	0.130090 +/- Inf	0.000000 +/- #NAME?	3 +/- 4	0.295846

Spectrum:	dUO2019							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.000000 +/- 0.000000	0.038368 +/- -0.001646	36 +/- 8	0.001855
1	2	0.345091 +/- 0.000000	0.007107 +/- 0.013882	953 +/- 40	0.120819
1	**3**	**0.025551 +/- 0.002196**	**0.000000 +/- -0.001180**	**16315 +/- 134**	**0.000025**
1	4	0.693071 +/- 0.072841	0.064695 +/- 0.016007	9475 +/- 104	0.000017

Spectrum:	dUO2020							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.010113 +/- 0.000000	0.006185 +/- 0.003630	4483 +/- 80	0.000042
1	1	0.051595 +/- 0.001525	0.000000 +/- -0.000478	34959 +/- 192	0.000008
1	**2**	**0.096401 +/- 0.001712**	**0.006942 +/- 0.000678**	**51154 +/- 230**	**0.000003**
1	3	0.000000 +/- 0.000000	0.077805 +/- 0.079960	185 +/- 37	0.000010
2	2	0.013662 +/- 0.000000	0.003187 +/- -0.004717	1661 +/- 54	0.000440
2	**3**	**0.000000 +/- 0.000000**	**0.075844 +/- -0.002940**	**3039 +/- 63**	**0.006732**
2	4	0.041512 +/- 0.000000	0.000000 +/- -0.002301	2074 +/- 57	0.001952
3	**4**	**0.062842 +/- 0.000000**	**0.001946 +/- 0.010787**	**304 +/- 33**	**0.001798**
3	5	0.017035 +/- 0.000000	0.000000 +/- -0.012047	258 +/- 34	0.000554
3	6	0.058835 +/- 0.000000	0.010834 +/- -0.012554	283 +/- 28	0.007565
3	8	0.610049 +/- Inf	0.147946 +/- Inf	7 +/- 7	0.032795

Spectrum:	dUO2021					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.00000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.000000 +/- 0.000000	0.176302 +/- -0.042147	868 +/- 38	0.032932
1	**3**	**0.027968 +/- 0.003349**	**0.000000 +/- -0.001904**	**8295 +/- 98**	**0.000025**
1	4	0.759664 +/- 0.145089	0.000000 +/- -0.068196	3402 +/- 75	0.000075

Spectrum:	dU3O8001					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.415310 +/- 0.031007	0.048161 +/- 0.010771	3558 +/- 74	0.001377
1	1	0.148310 +/- 0.001875	0.013415 +/- 0.000496	70298 +/- 269	0.000285
1	**2**	**0.131600 +/- 0.000717**	**0.010245 +/- 0.000195**	**401156 +/- 637**	**0.000105**
1	3	0.812490 +/- 1.907300	0.147570 +/- 0.353960	12360 +/- 127	0.000562
2	3	0.008781 +/- 0.000000	0.001978 +/- -0.007758	1865 +/- 58	0.000169
2	**4**	**0.053050 +/- 0.002205**	**0.000000 +/- -0.001079**	**21080 +/- 155**	**0.000025**
2	5	0.339700 +/- 0.011742	0.000000 +/- -0.003290	9611 +/- 107	0.000044
3	6	0.000000 +/- 0.000000	0.000000 +/- -0.004599	3243 +/- 69	0.000111
3	**7**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.003605**	**5386 +/- 87**	**0.000390**
3	8	0.052792 +/- 0.000000	0.000000 +/- -0.012151	92 +/- 29	0.001978
3	5	0.021876 +/- 0.000000	0.008035 +/- 0.023042	185 +/- 19	0.000297
4	8	0.019013 +/- 0.000000	0.003836 +/- -0.035184	354 +/- 39	0.000572
4	**9**	**0.000000 +/- 0.000000**	**0.000000 +/- 0.006723**	**1021 +/- 47**	**0.000391**
4	10	0.264430 +/- 0.000000	0.048509 +/- -0.008047	50 +/- 22	0.045058

Spectrum:	dU3O8002					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.026456 +/- 0.013295	0.183940 +/- 0.017073	2347 +/- 63	0.001399
1	3	0.093613 +/- 0.001408	0.013423 +/- 0.000713	71513 +/- 272	0.000008
1	**4**	**0.481380 +/- 0.005847**	**0.023957 +/- 0.000957**	**117769 +/- 347**	**0.000582**
2	5	0.159030 +/- 0.070357	0.053141 +/- -0.055107	419 +/- 37	0.001372

2	**6**	**0.164090 +/- 0.005604**	**0.000000 +/- -0.001830**	**11446 +/- 115**	**0.000079**
2	7	0.806840 +/- 0.369610	0.000000 +/- -0.079199	1214 +/- 50	0.000167
3	**8**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.008110**	**1932 +/- 55**	**0.000315**
3	9	0.043766 +/- 0.033358	0.000000 +/- -0.056814	753 +/- 43	0.000121
4	10	0.000000 +/- 0.000000	0.453030 +/- -0.005327	32 +/- 15	0.037341
4	**11**	**0.002071 +/- 0.000000**	**0.000610 +/- -0.080852**	**397 +/- 36**	**0.000194**
5	**13**	**0.000000 +/- 0.000000**	**0.053973 +/- -0.012993**	**212 +/- 25**	**0.003126**
5	14	0.147840 +/- 0.000000	0.147820 +/- -0.006417	20 +/- 14	0.026739

Spectrum:	dU3O8003							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.005399 +/- 0.000000	0.001073 +/- -0.007103	1820 +/- 51	0.000022
1	1	0.057247 +/- 0.001109	0.000198 +/- -0.000273	60204 +/- 248	0.000006
1	**2**	**0.090646 +/- 0.000716**	**0.005532 +/- 0.000243**	**243175 +/- 496**	**0.000017**
1	3	0.853970 +/- 0.651850	0.000000 +/- -0.088556	1226 +/- 46	0.000029
2	3	0.000000 +/- 0.000000	0.000000 +/- -0.002260	2754 +/- 57	0.000159
2	**4**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.001392**	**11494 +/- 114**	**0.000204**
2	5	0.000000 +/- 0.000000	0.000000 +/- -0.072387	572 +/- 36	0.000220
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.006351	380 +/- 28	0.000402
3	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.004052**	**2414 +/- 55**	**0.000242**
3	7	0.000000 +/- 0.000000	0.000000 +/- -0.085761	551 +/- 38	0.000229
4	**8**	**0.019547 +/- 0.000000**	**0.000000 +/- 0.009817**	**309 +/- 29**	**0.000958**
5	**10**	**0.193270 +/- 0.000000**	**0.053180 +/- 0.103540**	**47 +/- 19**	**0.024038**

Spectrum:	dU3O8004							
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000		
	237:	0.0000000	**238:**	0.9972400				

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.004915 +/- 0.000000	0.001151 +/- -0.041740	892 +/- 44	0.000108
1	3	0.018013 +/- 0.000844	0.000000 +/- 0.000541	49596 +/- 227	0.000000
1	**4**	**0.494010 +/- 0.008695**	**0.017226 +/- 0.001502**	**56611 +/- 242**	**0.000016**
2	**6**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.008672**	**1731 +/- 54**	**0.000359**
2	7	0.392120 +/- 0.736440	0.115580 +/- -0.006152	22 +/- 9	0.005606
3	**8**	**0.017504 +/- 0.000000**	**0.011256 +/- 0.018597**	**191 +/- 24**	**0.000185**
3	9	0.103690 +/- 0.000000	0.000000 +/- -0.007480	35 +/- 14	0.006299

Spectrum:	dU3O8005									
Isotopics:	234:	0.0000100	235:	0.0027500	236:	0.000000				
	237:	0.0000000	238:	0.9972400						

Ion												
U	O	P1			P2			TotalCounts			Residual
1	0	0.000000	+/-	0.000000	0.000000	+/-	-0.002379	4331	+/-	75	0.000008
1	1	0.096566	+/-	0.002496	0.000000	+/-	-0.000687	25966	+/-	166	0.000002
1	**2**	**0.127180**	**+/-**	**0.002889**	**0.016744**	**+/-**	**0.001440**	**27521**	**+/-**	**171**	**0.000008**
1	3	0.079761	+/-	0.000000	0.088003	+/-	0.074081	109	+/-	19	0.003936
2	2	0.000000	+/-	0.000000	0.035383	+/-	-0.036753	658	+/-	35	0.001230
2	**3**	**0.000000**	**+/-**	**0.000000**	**0.000000**	**+/-**	**-0.004491**	**1544**	**+/-**	**49**	**0.000110**
2	4	0.032428	+/-	0.000000	0.005924	+/-	-0.021506	986	+/-	45	0.001820

Spectrum:	dU3O8006									
Isotopics:	234:	0.0000100	235:	0.0027500	236:	0.000000				
	237:	0.0000000	238:	0.9972400						

Ion												
U	O	P1			P2			TotalCounts			Residual
1	2	0.131970	+/-	0.010196	0.000000	+/-	-0.006786	3680	+/-	71	0.000024
1	**3**	**0.066867**	**+/-**	**0.001867**	**0.007308**	**+/-**	**0.000980**	**31648**	**+/-**	**183**	**0.000001**
1	4	0.702120	+/-	0.104040	0.130740	+/-	0.029815	12964	+/-	124	0.000026
2	**6**	**0.052927**	**+/-**	**0.000000**	**0.010185**	**+/-**	**-0.018327**	**146**	**+/-**	**28**	**0.004798**

Spectrum:	dU3O8007									
Isotopics:	234:	0.0000100	235:	0.0027500	236:	0.000000				
	237:	0.0000000	238:	0.9972400						

Ion												
U	O	P1			P2			TotalCounts			Residual
1	0	0.041572	+/-	0.004688	0.000000	+/-	-0.002448	5696	+/-	80	0.000004
1	**1**	**0.097574**	**+/-**	**0.002529**	**0.000000**	**+/-**	**-0.000651**	**25038**	**+/-**	**163**	**0.000012**
1	2	0.123580	+/-	0.003058	0.018004	+/-	0.001525	23521	+/-	158	0.000005
1	3	0.022942	+/-	0.000000	0.059248	+/-	0.035226	211	+/-	22	0.000419
2	2	0.019453	+/-	0.000000	0.003986	+/-	-0.018490	734	+/-	36	0.001118
2	**3**	**0.009637**	**+/-**	**0.000000**	**0.002030**	**+/-**	**-0.006321**	**1417**	**+/-**	**49**	**0.000466**
2	4	0.059453	+/-	0.000000	0.010428	+/-	-0.041978	750	+/-	42	0.005057

Spectrum:	dU3O8008									
Isotopics:	234:	0.0000100	235:	0.0027500	236:	0.000000				
	237:	0.0000000	238:	0.9972400						

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	1	0.008448 +/- 0.048285	0.103190 +/- -0.071999	432 +/- 38	0.003909
1	2	0.096800 +/- 0.011190	0.000742 +/- -0.007579	2997 +/- 66	0.000057
1	**3**	**0.074166 +/- 0.002246**	**0.007558 +/- 0.001141**	**24412 +/- 161**	**0.000002**
1	4	0.712780 +/- 0.161000	0.146660 +/- 0.044593	9554 +/- 105	0.000021
2	**6**	**0.000000 +/- 0.000000**	**0.075055 +/- -0.020139**	**125 +/- 25**	**0.006636**

Spectrum:	dUO3001					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	0	0.384300 +/- 0.148250	0.306690 +/- -0.100850	970 +/- 54	0.051516
1	1	0.262060 +/- 0.007867	0.038375 +/- 0.002388	13043 +/- 127	0.006119
1	**2**	**0.208500 +/- 0.002406**	**0.031078 +/- 0.000683**	**76922 +/- 284**	**0.002567**
2	3	0.093454 +/- 0.000000	0.000000 +/- -0.035648	759 +/- 42	0.003333
2	**4**	**0.096084 +/- 0.004847**	**0.000000 +/- -0.002252**	**10448 +/- 118**	**0.000075**
2	5	0.431010 +/- 0.020450	0.000000 +/- -0.006186	7277 +/- 103	0.000110
2	6	1.000000 +/- Inf	0.000000 +/- #NAME?	321 +/- 39	0.000214
3	5	0.127290 +/- 0.000000	0.000000 +/- -0.008468	190 +/- 22	0.011781
3	6	0.000000 +/- 0.000000	0.000000 +/- -0.007166	2492 +/- 67	0.000172
3	**7**	**0.037042 +/- 0.006468**	**0.000000 +/- -0.003619**	**5025 +/- 85**	**0.000203**
3	8	0.051462 +/- 0.000000	0.010320 +/- -0.045839	232 +/- 40	0.002679
4	7	0.384810 +/- 0.000000	0.000000 +/- -0.001248	22 +/- 13	0.060345
4	8	0.000000 +/- 0.000000	0.000000 +/- -0.812690	511 +/- 37	0.000392
4	**9**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.021050**	**916 +/- 51**	**0.000653**
4	10	0.000000 +/- 0.000000	0.025364 +/- -0.014534	117 +/- 27	0.000797
5	10	0.093674 +/- 0.000000	0.017852 +/- -0.008590	82 +/- 22	0.006317
5	**11**	**0.003407 +/- 0.000000**	**0.000621 +/- -0.022763**	**295 +/- 29**	**0.000382**
1	4	0.599080 +/- 4.446700	0.252930 +/- 1.188200	0 +/- 114	0.130940

Spectrum:	dUO3002					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion U	Ion O	P1	P2	TotalCounts	Residual
1	3	0.169940 +/- 0.003508	0.069919 +/- 0.002221	30656 +/- 182	0.000228
1	**4**	**0.693880 +/- 0.051626**	**0.118050 +/- 0.012446**	**40023 +/- 208**	**0.000354**

1	2	0.037855 +/- 0.028249	0.222130 +/- 0.031007	1210 +/- 57	0.003683
2	5	0.287690 +/- 0.024965	0.000000 +/- -0.011247	2241 +/- 62	0.000063
2	**6**	**0.343920 +/- 0.009595**	**0.000000 +/- -0.002600**	**14810 +/- 136**	**0.000093**
2	7	0.796390 +/- 0.548580	0.100530 +/- -0.388620	3523 +/- 82	0.013419
3	7	0.207860 +/- 0.000000	0.000000 +/- -0.110120	551 +/- 41	0.010905
3	**8**	**0.055482 +/- 0.007467**	**0.000000 +/- -0.004411**	**4560 +/- 85**	**0.000153**
3	9	0.295950 +/- 0.024348	0.000000 +/- -0.012616	2576 +/- 71	0.000221
4	**11**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.017119**	**1474 +/- 63**	**0.000960**
5	**13**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.027228**	**970 +/- 48**	**0.000300**
5	14	0.143260 +/- 0.000000	0.000000 +/- -0.022411	88 +/- 36	0.007881
4	10	0.000000 +/- 0.000000	0.000000 +/- -0.114880	442 +/- 43	0.000374

Spectrum:	dUO3003				
Isotopics:	**234:** 0.0000100 **235:** 0.0027500 **236:** 0.000000				
	237: 0.0000000 **238:** 0.9972400				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	0	0.261760 +/- 0.019537	0.020093 +/- -0.013468	2525 +/- 59	0.000199
1	1	0.159580 +/- 0.003257	0.009499 +/- 0.001263	28737 +/- 178	0.000009
1	**2**	**0.228860 +/- 0.003434**	**0.049802 +/- 0.001499**	**51079 +/- 232**	**0.000244**
1	3	0.353720 +/- 0.137980	0.139560 +/- 0.080651	340 +/- 32	0.004562
2	2	0.004960 +/- 0.000000	0.001317 +/- -3.616300	510 +/- 35	0.000142
2	3	0.000477 +/- 0.000000	0.000252 +/- -0.005127	2253 +/- 61	0.000107
2	**4**	**0.043861 +/- 0.008621**	**0.000000 +/- -0.006020**	**3001 +/- 66**	**0.000062**
3	5	0.000000 +/- 0.000000	0.000000 +/- -0.034389	395 +/- 29	0.000308
3	**6**	**0.004734 +/- 0.000000**	**0.001148 +/- -0.074926**	**430 +/- 34**	**0.000343**
3	7	0.150320 +/- 0.000000	0.027987 +/- -0.006914	29 +/- 18	0.027642

Spectrum:	dUO3004				
Isotopics:	**234:** 0.0000100 **235:** 0.0027500 **236:** 0.00000				
	237: 0.0000000 **238:** 0.9972400				
Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	1	0.403970 +/- 0.000000	0.000000 +/- -0.016180	71 +/- 19	0.071713
1	2	0.062879 +/- 0.026648	0.010008 +/- -0.066328	801 +/- 40	0.000235
1	**3**	**0.023858 +/- 0.003432**	**0.005011 +/- 0.002410**	**8115 +/- 98**	**0.000002**
1	4	0.650250 +/- 0.097720	0.047678 +/- 0.031654	2874 +/- 66	0.000014
2	**5**	**0.283120 +/- 0.000000**	**0.000000 +/- -0.004881**	**15 +/- 12**	**0.048793**

Spectrum:	dUO3005					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
2	**3**	**0.048205 +/- 0.000000**	**0.010140 +/- 0.006845**	**659 +/- 39**	**0.001768**
2	4	0.007273 +/- 0.000000	0.000000 +/- -0.053394	368 +/- 32	0.000217
2	2	0.011660 +/- 0.000000	0.000000 +/- -0.019404	248 +/- 31	0.000467
3	6	0.234790 +/- 0.000000	0.000000 +/- -0.001826	18 +/- 15	0.014520
1	0	0.000395 +/- 0.000000	0.019093 +/- 0.005180	1399 +/- 48	0.000000
1	1	0.100300 +/- 0.004523	0.000000 +/- -0.001967	9755 +/- 106	0.000012
1	**2**	**0.160650 +/- 0.006054**	**0.000000 +/- 0.003233**	**9987 +/- 109**	**0.000035**
1	3	0.158630 +/- 0.000000	0.070732 +/- 0.091013	119 +/- 21	0.010539

Spectrum:	dUO3006					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	2	0.165080 +/- 0.020220	0.043617 +/- -0.024032	1477 +/- 48	0.002482
1	**3**	**0.071749 +/- 0.003898**	**0.001322 +/- 0.002550**	**9302 +/- 104**	**0.000057**
1	4	0.753470 +/- 0.342670	0.098747 +/- 0.087309	2903 +/- 71	0.000120

Spectrum:	dUO3007					
Isotopics:	**234:**	0.0000100	**235:**	0.0027500	**236:**	0.000000
	237:	0.0000000	**238:**	0.9972400		

Ion					
U	**O**	**P1**	**P2**	**TotalCounts**	**Residual**
1	**0**	**0.000000 +/- 0.000000**	**0.002749 +/- 0.000743**	**13616 +/- 126**	**0.000006**
1	1	0.008741 +/- 0.000000	0.001762 +/- -0.000942	9273 +/- 106	0.000243
1	2	0.015351 +/- 0.000000	0.003396 +/- -0.005088	2311 +/- 54	0.000682
1	3	0.000000 +/- 0.000000	0.026339 +/- 0.016473	503 +/- 32	0.000008
2	**2**	**0.000000 +/- 0.000000**	**0.000000 +/- -0.015597**	**346 +/- 34**	**0.000062**

Appendix F. Protonation Ratios

The following tables report the number of counts in the intense U-238 containing peak for each U_xO_y ion, the ratio of the counts in the peak one mass number greater than the U-238 peak to the U-238 peak and the ratio of the counts in the peak two mass numbers higher than the U-238 peak to the U-238 peak. Reported errors are one sigma values based on counting statistics.

Spectrum: nU001				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	303885 +/- 552	0.29655 +/- 0.00113	0.02312 +/- 0.00029
1	2	1312296 +/- 1146	0.32481 +/- 0.00057	0.02994 +/- 0.00015
1	3	3437 +/- 67	26.25461 +/- 0.52157	9.19024 +/- 0.18743
2	2	1994 +/- 49	0.11059 +/- 0.01474	0.00000 +/- NaN
2	3	26844 +/- 167	0.05632 +/- 0.00186	0.00027 +/- 0.000839
2	4	203797 +/- 452	0.16093 +/- 0.00097	0.00963 +/- 0.000251
2	5	62302 +/- 251	1.07714 +/- 0.00603	0.06275 +/- 0.00116
3	5	7492 +/- 89	0.00000 +/- NaN	0.00000 +/- NaN
3	6	58321 +/- 243	0.06953 +/- 0.001218	0.00637 +/- 0.000528
3	7	68369 +/- 263	0.16604 +/- 0.00175	0.00906 +/- 0.000565
3	8	1551 +/- 46	1.46022 +/- 0.05583	0.00000 +/- NaN
4	7	1646 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
4	8	15076 +/- 124	0.04644 +/- 0.002444	0.00000 +/- NaN
4	9	21599 +/- 149	0.11555 +/- 0.00279	0.00000 +/- NaN
4	10	1618 +/- 47	0.53578 +/- 0.02921	0.00000 +/- NaN
5	9	507 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
5	10	5175 +/- 76	0.00000 +/- NaN	0.00000 +/- NaN
5	11	6499 +/- 84	0.00000 +/- NaN	0.00000 +/- NaN
5	12	1642 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
6	12	1228 +/- 42	0.00000 +/- NaN	0.00000 +/- NaN
6	13	1638 +/- 50	0.00000 +/- NaN	0.00000 +/- NaN
6	14	757 +/- 37	0.00000 +/- NaN	0.00000 +/- NaN
7	15	542 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU002				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	13940 +/- 120	0.22367 +/- 0.00474	0.25376 +/- 0.00507
1	3	140432 +/- 376	0.20155 +/- 0.00133	0.08084 +/- 0.00080
1	4	29185 +/- 172	3.07303 +/- 0.02088	0.52844 +/- 0.00533
2	5	4926 +/- 73	0.66315 +/- 0.01599	0.00000 +/- NaN
2	6	18460 +/- 139	0.64624 +/- 0.007783	0.01827 +/- 0.001723
2	4	217 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN
3	7	1277 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
3	8	8589 +/- 95	0.13128 +/- 0.00507	0.00000 +/- NaN
3	9	1139 +/- 41	0.66720 +/- 0.041669	0.00000 +/- NaN
4	10	1135 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
4	11	1407 +/- 45	0.08788 +/- 0.02276	0.00000 +/- NaN
5	13	1255 +/- 43	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU003				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	35227 +/- 189	0.63330 +/- 0.00549	0.12498 +/- 0.00214
1	1	282859 +/- 533	0.28739 +/- 0.00115	0.03956 +/- 0.00039
1	2	214864 +/- 465	0.47200 +/- 0.00180	0.12752 +/- 0.00083
2	2	13584 +/- 120	0.12323 +/- 0.00404	0.00000 +/- NaN
2	3	30630 +/- 177	0.08615 +/- 0.001969	0.00213 +/- 0.000673
2	4	17139 +/- 134	0.18910 +/- 0.00404	0.00000 +/- NaN
3	4	3356 +/- 60	0.00000 +/- NaN	0.00000 +/- NaN
3	5	4903 +/- 73	0.00000 +/- NaN	0.00000 +/- NaN
3	6	3227 +/- 61	0.00000 +/- NaN	0.00000 +/- NaN
3	7	283 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN
4	6	683 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
4	7	595 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
4	8	417 +/- 26	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU004				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	3301 +/- 61	0.73385 +/- 0.02096	0.22126 +/- 0.01126
1	2	27149 +/- 166	0.27726 +/- 0.00369	0.17387 +/- 0.00291
1	3	69483 +/- 265	0.15911 +/- 0.00167	0.07703 +/- 0.00114

1	4	3312 +/- 61	5.88147 +/- 0.11698	1.90581 +/- 0.04323
2	4	382 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
2	5	833 +/- 35	0.38267 +/- 0.04062	0.00000 +/- NaN
2	7	398 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum:		**nU005**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	43566 +/- 210	0.27455 +/- 0.00291	0.03276 +/- 0.00108
1	1	187612 +/- 434	0.22084 +/- 0.00121	0.01868 +/- 0.00035
1	2	125955 +/- 356	0.36549 +/- 0.00200	0.09375 +/- 0.00092
2	2	11500 +/- 111	0.01849 +/- 0.00342	0.00000 +/- NaN
2	3	21226 +/- 148	0.04095 +/- 0.001872	0.00000 +/- NaN
2	4	9151 +/- 99	0.12599 +/- 0.00526	0.00000 +/- NaN
3	4	2495 +/- 53	0.00000 +/- NaN	0.00000 +/- NaN
3	5	3072 +/- 59	0.00000 +/- NaN	0.00000 +/- NaN
3	6	1682 +/- 45	0.00000 +/- NaN	0.00000 +/- NaN
4	6	397 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum:		**nU006**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	1	2069 +/- 48	0.56272 +/- 0.02306	0.10902 +/- 0.01228
1	2	13567 +/- 119	0.26410 +/- 0.00529	0.14309 +/- 0.00372
1	3	42643 +/- 207	0.13209 +/- 0.00193	0.05174 +/- 0.00123
1	4	1603 +/- 45	7.11554 +/- 0.21253	2.02724 +/- 0.06928
2	5	264 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
2	6	252 +/- 21	0.79673 +/- 0.10733	0.00000 +/- NaN

Spectrum:		**nU007**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	41771 +/- 205	0.17726 +/- 0.00232	0.01013 +/- 0.00079
1	1	144735 +/- 382	0.18372 +/- 0.00124	0.00895 +/- 0.00029
1	2	96726 +/- 312	0.29599 +/- 0.00202	0.07152 +/- 0.00093
2	2	10560 +/- 104	0.02150 +/- 0.00275	0.00000 +/- NaN
2	3	16536 +/- 131	0.02146 +/- 0.0019	0.00000 +/- NaN
2	4	6588 +/- 83	0.09608 +/- 0.00589	0.00000 +/- NaN
3	4	1919 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
3	5	2251 +/- 51	0.00000 +/- NaN	0.00000 +/- NaN

3	6	1237 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU008				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	1566 +/- 42	0.47919 +/- 0.02439	0.02680 +/- 0.01392
1	2	10018 +/- 101	0.25606 +/- 0.00604	0.09970 +/- 0.00399
1	3	35470 +/- 189	0.12049 +/- 0.00204	0.04191 +/- 0.00127
1	4	1260 +/- 42	7.16384 +/- 0.25398	2.07389 +/- 0.08294
2	5	273 +/- 21	0.00939 +/- 0.064446	0.00000 +/- NaN

Spectrum: nUO2001				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	25214 +/- 161	0.27527 +/- 0.00387	0.01050 +/- 0.00105
1	2	91452 +/- 303	0.24918 +/- 0.00187	0.01745 +/- 0.00050
1	3	51 +/- 18	33.08100 +/- 11.53036	4.42961 +/- 1.63826
2	3	1946 +/- 48	0.00000 +/- NaN	0.00000 +/- NaN
2	4	8912 +/- 97	0.02819 +/- 0.003789	0.00000 +/- NaN
2	5	580 +/- 32	0.52469 +/- 0.06599	0.00000 +/- NaN
3	5	211 +/- 21	0.00000 +/- NaN	0.00000 +/- NaN
3	6	1576 +/- 44	0.00000 +/- NaN	0.00000 +/- NaN
3	7	724 +/- 35	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO2002				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	862 +/- 34	0.00000 +/- NaN	0.04800 +/- 0.02364
1	3	9135 +/- 97	0.11022 +/- 0.00428	0.02627 +/- 0.00260
1	4	1917 +/- 48	2.49443 +/- 0.07353	0.05801 +/- 0.01409

Spectrum: nUO2003				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3674 +/- 62	0.00000 +/- NaN	0.00000 +/- NaN
1	1	12827 +/- 115	0.08156 +/- 0.00320	0.00000 +/- NaN
1	2	12780 +/- 114	0.14216 +/- 0.00409	0.00277 +/- 0.00195
1	3	202 +/- 21	0.00000 +/- NaN	0.00000 +/- NaN
2	2	729 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN

2	3	1211 +/- 39	0.00000 +/- NaN	0.00000 +/- NaN
2	4	570 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO2004				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	623 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
1	3	5039 +/- 72	0.04085 +/- 0.00480	0.00000 +/- NaN
1	4	241 +/- 22	5.76362 +/- 0.54611	0.01324 +/- 0.10141

Spectrum: nUO2005				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	6765 +/- 84	0.00228 +/- 0.00371	0.00000 +/- NaN
1	1	10897 +/- 107	0.09157 +/- 0.00393	0.00000 +/- NaN
1	2	7409 +/- 89	0.16740 +/- 0.00631	0.00093 +/- 0.00335
1	3	373 +/- 25	0.00000 +/- NaN	0.08612 +/- 0.03339
2	2	527 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
2	3	702 +/- 35	0.00000 +/- NaN	0.00000 +/- NaN
2	4	354 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO2006				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	3	2459 +/- 51	0.00210 +/- 0.00751	0.00000 +/- NaN
1	4	51 +/- 14	9.94998 +/- 2.77068	0.00000 +/- NaN
1	2	336 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO2007				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3992 +/- 65	0.04486 +/- 0.00728	0.00000 +/- NaN
1	1	29153 +/- 171	0.11041 +/- 0.00224	0.00000 +/- NaN
1	2	40079 +/- 202	0.17244 +/- 0.00236	0.02702 +/- 0.00096
1	3	212 +/- 19	0.27685 +/- 0.10073	0.00000 +/- NaN
2	2	760 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
2	3	2919 +/- 56	0.00000 +/- NaN	0.00000 +/- NaN
2	4	2525 +/- 53	0.00000 +/- NaN	0.00000 +/- NaN
3	5	387 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN

3	6	325 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO2008				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	120 +/- 17	0.00000 +/- NaN	0.00000 +/- NaN
1	2	871 +/- 34	0.07291 +/- 0.02470	0.05228 +/- 0.02434
1	3	11221 +/- 108	0.06053 +/- 0.00325	0.00000 +/- NaN
1	4	824 +/- 33	4.14598 +/- 0.18030	0.56550 +/- 0.04558

Spectrum: nU3O8001				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	426796 +/- 654	0.21096 +/- 0.00078	0.01650 +/- 0.00021
1	2	2468544 +/- 1571	0.26045 +/- 0.00037	0.02306 +/- 0.00010
1	3	13178 +/- 118	13.97150 +/- 0.12945	2.64593 +/- 0.02776
2	2	1834 +/- 47	0.14224 +/- 0.01568	0.00600 +/- 0.01245
2	3	26391 +/- 165	0.04286 +/- 0.001746	0.00000 +/- NaN
2	4	296819 +/- 546	0.07916 +/- 0.00055	0.00821 +/- 0.000191
2	5	135140 +/- 369	0.57800 +/- 0.00261	0.02620 +/- 0.00049
3	5	4048 +/- 68	0.00000 +/- NaN	0.00000 +/- NaN
3	6	57627 +/- 242	0.01708 +/- 0.00078	0.00555 +/- 0.000557
3	7	106516 +/- 328	0.05949 +/- 0.00083	0.00681 +/- 0.000425
3	8	8552 +/- 95	0.63494 +/- 0.01165	0.00000 +/- NaN
4	7	512 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
4	8	10822 +/- 106	0.00000 +/- NaN	0.00000 +/- NaN
4	9	24827 +/- 160	0.01940 +/- 0.00150	0.00542 +/- 0.001087
4	10	4372 +/- 69	0.14899 +/- 0.00934	0.00000 +/- NaN
4	11	512 +/- 32	0.33413 +/- 0.06801	0.00000 +/- NaN
5	10	2769 +/- 61	0.00000 +/- NaN	0.00000 +/- NaN
5	11	5187 +/- 77	0.00000 +/- NaN	0.00000 +/- NaN
5	12	2935 +/- 60	0.00000 +/- NaN	0.00000 +/- NaN
6	12	136 +/- 28	0.00000 +/- NaN	0.00000 +/- NaN
6	13	378 +/- 36	0.00000 +/- NaN	0.00000 +/- NaN
6	14	813 +/- 38	0.00000 +/- NaN	0.00000 +/- NaN
6	15	43 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
7	15	66 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
7	16	61.41463 +/- 16.681	0 +/- NaN	0.146148 +/- 0.084538
7	17	28.14634 +/- 16.06	0 +/- NaN	0 +/- NaN

Spectrum: nU3O8002				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	3003 +/- 59	0.07041 +/- 0.01000	0.31414 +/- 0.01355
1	3	85834 +/- 294	0.11496 +/- 0.00125	0.02646 +/- 0.00060
1	4	79826 +/- 284	0.97785 +/- 0.00495	0.03981 +/- 0.00076
2	5	428 +/- 27	0.42975 +/- 0.06220	0.00000 +/- NaN
2	6	10747 +/- 106	0.20032 +/- 0.005299	0.00000 +/- NaN
2	7	169 +/- 23	6.22693 +/- 0.86656	0.00000 +/- NaN
3	8	2000 +/- 48	0.00000 +/- NaN	0.00000 +/- NaN
3	9	799 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN
4	10	16 +/- 9	0.00000 +/- NaN	0.00000 +/- NaN
4	11	448 +/- 28	0.00000 +/- NaN	0.00000 +/- NaN
5	14	8 +/- 10	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU3O8003				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	17485 +/- 134	0.09544 +/- 0.00275	0.00000 +/- NaN
1	1	694767 +/- 834	0.06324 +/- 0.00031	0.00233 +/- 0.00007
1	2	2619573 +/- 1619	0.15102 +/- 0.00026	0.01793 +/- 0.00008
1	3	6877 +/- 85	3.97096 +/- 0.05484	0.22698 +/- 0.00714
2	2	6575 +/- 83	0.00000 +/- NaN	0.00000 +/- NaN
2	3	73693 +/- 272	0.00000 +/- NaN	0.00201 +/- 0.000355
2	4	246044 +/- 496	0.01591 +/- 0.00028	0.00648 +/- 0.00020
2	5	16585 +/- 130	0.16086 +/- 0.00362	0.00000 +/- NaN
3	4	1985 +/- 48	0.00000 +/- NaN	0.00575 +/- 0.004286
3	5	13034 +/- 118	0.00000 +/- NaN	0.00000 +/- NaN
3	6	53073 +/- 232	0.00000 +/- NaN	0.00588 +/- 0.00056
3	7	16060 +/- 130	0.00000 +/- NaN	0.00000 +/- NaN
4	6	451 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
4	7	2540 +/- 57	0.00000 +/- NaN	0.00000 +/- NaN
4	8	10957 +/- 107	0.00000 +/- NaN	0.00272 +/- 0.00163
4	9	4176 +/- 69	0.00000 +/- NaN	0.00000 +/- NaN
5	9	824 +/- 37	0.00000 +/- NaN	0.00370 +/- 0.007869
5	10	2892 +/- 63	0.00000 +/- NaN	0.00287 +/- 0.003911
5	11	916 +/- 36	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU3O8004				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1823 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
1	3	81824 +/- 286	0.02859 +/- 0.00066	0.00766 +/- 0.00040
1	4	41454 +/- 204	1.13823 +/- 0.00771	0.06318 +/- 0.00145
2	6	2511 +/- 52	0.09173 +/- 0.00904	0.00000 +/- NaN
2	7	15 +/- 9	0.00000 +/- NaN	0.00000 +/- NaN
2	5	20 +/- 11	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU3O8005				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	16078 +/- 128	0.10027 +/- 0.00312	0.00000 +/- NaN
1	1	95010 +/- 309	0.13410 +/- 0.00129	0.00085 +/- 0.00027
1	2	112056 +/- 336	0.22725 +/- 0.00159	0.04940 +/- 0.00072
1	3	725 +/- 35	0.50239 +/- 0.04783	0.27863 +/- 0.03601
2	2	5756 +/- 78	0.00000 +/- NaN	0.00000 +/- NaN
2	3	12831 +/- 115	0.00000 +/- NaN	0.00000 +/- NaN
2	4	8948 +/- 97	0.01232 +/- 0.00368	0.00000 +/- NaN
2	5	104 +/- 18	0.00000 +/- NaN	0.00000 +/- NaN
3	4	1286 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
3	5	2017 +/- 49	0.00000 +/- NaN	0.00000 +/- NaN
3	6	1817 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
4	8	167 +/- 21	0.00000 +/- NaN	0.01139 +/- 0.021218

Spectrum: nU3O8006				
Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	505 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
1	2	3174 +/- 59	0.13817 +/- 0.00984	0.00000 +/- NaN
1	3	30709 +/- 176	0.07687 +/- 0.00179	0.01114 +/- 0.00091
1	4	2669 +/- 58	4.01729 +/- 0.09648	0.77120 +/- 0.02531
2	6	279 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
2	5	30 +/- 12	0.00000 +/- NaN	0.00000 +/- NaN
2	7	9 +/- 7	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU3O8007			
Ion	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak

U	O			
1	0	14260 +/- 121	0.07567 +/- 0.00308	0.00000 +/- NaN
1	1	58556 +/- 243	0.12650 +/- 0.00164	0.00000 +/- NaN
1	2	53294 +/- 232	0.22191 +/- 0.00230	0.04915 +/- 0.00109
1	3	612 +/- 31	0.07718 +/- 0.03674	0.01025 +/- 0.03159
2	2	3971 +/- 65	0.00000 +/- NaN	0.00000 +/- NaN
2	3	7385 +/- 89	0.00000 +/- NaN	0.00000 +/- NaN
2	4	4004 +/- 66	0.00911 +/- 0.00629	0.00000 +/- NaN
3	4	772 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
3	5	826 +/- 38	0.00000 +/- NaN	0.00000 +/- NaN
3	6	729 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nU3O8008

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	821 +/- 34	0.11223 +/- 0.02775	0.00000 +/- NaN
1	2	4198 +/- 67	0.14555 +/- 0.00883	0.00000 +/- NaN
1	3	33411 +/- 185	0.07089 +/- 0.00176	0.00899 +/- 0.00092
1	4	2367 +/- 53	4.72195 +/- 0.11604	0.95887 +/- 0.03080
2	6	144 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3001

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	23868 +/- 156	0.41926 +/- 0.00510	0.02420 +/- 0.00148
1	2	113612 +/- 338	0.30871 +/- 0.00190	0.02914 +/- 0.00056
1	3	411 +/- 30	25.35579 +/- 1.86996	9.48261 +/- 0.71265
2	3	1783 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
2	4	19063 +/- 141	0.17664 +/- 0.003674	0.00000 +/- NaN
2	5	9439 +/- 102	0.89364 +/- 0.01411	0.00000 +/- NaN
3	5	420 +/- 28	0.00000 +/- NaN	0.00000 +/- NaN
3	6	5830 +/- 82	0.00000 +/- NaN	0.00000 +/- NaN
3	7	10663 +/- 106	0.11171 +/- 0.004177	0.00000 +/- NaN
3	8	768 +/- 33	0.45480 +/- 0.04685	0.00000 +/- NaN
4	8	1192 +/- 43	0.00000 +/- NaN	0.00000 +/- NaN
4	9	2975 +/- 61	0.00000 +/- NaN	0.00000 +/- NaN
4	10	356 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
5	11	672 +/- 34	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3002				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	3	6554 +/- 84	0.14729 +/- 0.00636	0.02747 +/- 0.00438
1	4	1007 +/- 37	5.24131 +/- 0.20550	0.93732 +/- 0.05123
1	2	419 +/- 26	0.00000 +/- NaN	0.00000 +/- NaN
2	5	130 +/- 21	0.00000 +/- NaN	0.00000 +/- NaN
2	6	1656 +/- 45	0.39643 +/- 0.024451	0.00000 +/- NaN
2	7	17 +/- 9	17.98709 +/- 9.28766	0.00000 +/- NaN
3	7	22 +/- 11	0.00000 +/- NaN	0.00000 +/- NaN
3	8	560 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
3	9	128 +/- 21	0.00000 +/- NaN	0.00000 +/- NaN
4	11	115 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
5	13	34 +/- 17	0.00000 +/- NaN	0.00000 +/- NaN
5	14	0 +/- 47	NaN +/- NaN	NaN +/- NaN

Spectrum: nUO3003				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3831 +/- 68	0.71532 +/- 0.02114	0.05665 +/- 0.00938
1	1	50711 +/- 226	0.28202 +/- 0.00269	0.03858 +/- 0.00098
1	2	59666 +/- 246	0.48160 +/- 0.00348	0.10392 +/- 0.00143
1	3	28 +/- 19	15.35330 +/- 10.45334	21.53568 +/- 14.64442
2	2	879 +/- 35	0.00000 +/- NaN	0.00000 +/- NaN
2	3	4498 +/- 72	0.01954 +/- 0.00647	0.00000 +/- NaN
2	4	4968 +/- 73	0.11886 +/- 0.00782	0.00000 +/- NaN
3	5	611 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
3	6	851 +/- 36	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3004				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1093 +/- 38	0.24072 +/- 0.02595	0.10245 +/- 0.01885
1	3	6870 +/- 84	0.11741 +/- 0.00505	0.03541 +/- 0.00362
1	4	539 +/- 28	4.48130 +/- 0.25481	0.72547 +/- 0.06475
2	6	54 +/- 16	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3005			
Ion	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak

U	O			
1	0	5679 +/- 79	0.26147 +/- 0.00962	0.00000 +/- NaN
1	1	152154 +/- 391	0.12064 +/- 0.00097	0.00224 +/- 0.00026
1	2	387061 +/- 623	0.23411 +/- 0.00087	0.03092 +/- 0.00030
1	3	241 +/- 25	13.18585 +/- 1.41094	1.59992 +/- 0.20249
2	2	844 +/- 36	0.00000 +/- NaN	0.00000 +/- NaN
2	3	10706 +/- 107	0.00000 +/- NaN	0.00000 +/- NaN
2	4	30278 +/- 175	0.02683 +/- 0.00149	0.00000 +/- NaN
2	5	1011 +/- 38	0.30744 +/- 0.03171	0.00000 +/- NaN
3	5	1504 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
3	6	6124 +/- 82	0.00000 +/- NaN	0.00000 +/- NaN
3	7	1311 +/- 43	0.00000 +/- NaN	0.00000 +/- NaN
4	8	1132 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3006

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1142 +/- 36	0.09928 +/- 0.01824	0.00000 +/- NaN
1	3	25445 +/- 161	0.02446 +/- 0.00139	0.00498 +/- 0.00099
1	4	8601 +/- 95	1.91369 +/- 0.02621	0.07795 +/- 0.00451
2	6	708 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3007

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3047 +/- 57	0.05946 +/- 0.00875	0.00000 +/- NaN
1	1	68606 +/- 263	0.12733 +/- 0.00151	0.00000 +/- NaN
1	2	130433 +/- 362	0.23882 +/- 0.00152	0.04618 +/- 0.00067
1	3	22 +/- 14	17.73311 +/- 11.48832	0.00000 +/- NaN
2	2	1109 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
2	3	7582 +/- 90	0.00000 +/- NaN	0.00000 +/- NaN
2	4	9415 +/- 100	0.00000 +/- NaN	0.00000 +/- NaN
2	5	10 +/- 16	0.00000 +/- NaN	0.00000 +/- NaN
3	4	318 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN
3	5	1232 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
3	6	1942 +/- 49	0.00000 +/- NaN	0.00000 +/- NaN
3	7	113 +/- 18	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: nUO3008

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1525 +/- 42	0.03101 +/- 0.01631	0.00000 +/- NaN
1	3	33698 +/- 185	0.06138 +/- 0.00157	0.00735 +/- 0.00084
1	4	3671 +/- 65	3.62157 +/- 0.07208	0.57962 +/- 0.01759
2	6	305 +/- 23	0.00000 +/- NaN	0.00000 +/- NaN
2	7	53 +/- 9	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU001

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	1305 +/- 41	0.88972 +/- 0.04110	0.02965 +/- 0.01368
1	1	27449 +/- 167	0.23994 +/- 0.00337	0.01165 +/- 0.00101
1	2	160956 +/- 402	0.21633 +/- 0.00129	0.02035 +/- 0.00039
2	3	2668 +/- 55	0.00000 +/- NaN	0.00000 +/- NaN
2	4	27045 +/- 167	0.10017 +/- 0.002462	0.00000 +/- NaN
2	5	6615 +/- 84	0.99559 +/- 0.01795	0.00000 +/- NaN
3	5	659 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
3	6	8867 +/- 96	0.01071 +/- 0.00296	0.00000 +/- NaN
3	7	11019 +/- 107	0.08841 +/- 0.003973	0.00000 +/- NaN
3	8	124 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN
4	8	2125 +/- 53	0.00000 +/- NaN	0.00000 +/- NaN
4	9	3909 +/- 65	0.00000 +/- NaN	0.00000 +/- NaN
4	10	224 +/- 23	0.00000 +/- NaN	0.00000 +/- NaN
5	10	483 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN
5	11	1146 +/- 39	0.00000 +/- NaN	0.00000 +/- NaN
1	3	246 +/- 27	28.10860 +/- 3.13433	6.67519 +/- 0.762416

Spectrum: dU002

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	3115 +/- 59	0.23340 +/- 0.01151	0.25930 +/- 0.01172
1	3	49161 +/- 223	0.17895 +/- 0.00212	0.08068 +/- 0.00138
1	4	8683 +/- 96	4.27514 +/- 0.05247	0.81131 +/- 0.01358
2	5	2367 +/- 53	0.48129 +/- 0.02072	0.00000 +/- NaN
2	6	11048 +/- 108	0.64056 +/- 0.010066	0.01793 +/- 0.002191
2	7	59 +/- 19	20.77372 +/- 6.83501	0.00000 +/- NaN
3	7	570 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
3	8	6079 +/- 81	0.08932 +/- 0.00608	0.00000 +/- NaN

3	9	971 +/- 36	0.67902 +/- 0.045037	0.00000 +/- NaN
4	10	548 +/- 35	0.00000 +/- NaN	0.00000 +/- NaN
4	11	1458 +/- 44	0.16669 +/- 0.02117	0.00000 +/- NaN
5	13	1272 +/- 42	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU003				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	2030 +/- 48	0.23676 +/- 0.01562	0.00000 +/- NaN
1	1	44891 +/- 213	0.13557 +/- 0.00192	0.00372 +/- 0.00056
1	2	90856 +/- 304	0.22624 +/- 0.00176	0.03935 +/- 0.00070
1	3	0 +/- 1180	NaN +/- NaN	NaN +/- NaN
2	2	527 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN
2	3	4420 +/- 70	0.00000 +/- NaN	0.00000 +/- NaN
2	4	8109 +/- 92	0.02234 +/- 0.00345	0.00000 +/- NaN
2	5	124 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
3	5	740 +/- 34	0.00000 +/- NaN	0.00000 +/- NaN
3	6	1972 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
4	6	0 +/- 13	NaN +/- NaN	NaN +/- NaN
4	8	205 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU004				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	2	2594 +/- 53	0.07680 +/- 0.00961	0.00000 +/- NaN
1	3	25543 +/- 161	0.03662 +/- 0.00159	0.00709 +/- 0.00108
1	4	3286 +/- 61	2.66839 +/- 0.05734	0.36591 +/- 0.01383
2	6	618 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU005				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	1734 +/- 44	0.05376 +/- 0.01324	0.00000 +/- NaN
1	1	26597 +/- 164	0.13439 +/- 0.00251	0.00000 +/- NaN
1	2	33923 +/- 185	0.24556 +/- 0.00306	0.05054 +/- 0.00143
2	2	1292 +/- 39	0.00000 +/- NaN	0.00000 +/- NaN
2	3	3642 +/- 62	0.00000 +/- NaN	0.00000 +/- NaN
2	4	2783 +/- 54	0.00000 +/- NaN	0.00000 +/- NaN
3	4	378 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN
3	5	639 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN

3	6	498 +/- 28	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU006				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	363 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
1	2	3239 +/- 60	0.12446 +/- 0.00983	0.00000 +/- NaN
1	3	29762 +/- 174	0.05949 +/- 0.00173	0.00441 +/- 0.00094
1	4	1528 +/- 42	4.33418 +/- 0.13138	0.98406 +/- 0.04062
2	6	161 +/- 19	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU007				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	1313 +/- 40	0.04593 +/- 0.01664	0.00000 +/- NaN
1	1	16041 +/- 128	0.13467 +/- 0.00372	0.00000 +/- NaN
1	2	16330 +/- 129	0.28112 +/- 0.00490	0.05849 +/- 0.00236
2	2	417 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN
2	3	1642 +/- 43	0.00000 +/- NaN	0.00000 +/- NaN
2	4	1039 +/- 36	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU008				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	2196 +/- 51	0.15654 +/- 0.01354	0.01524 +/- 0.00759
1	3	17075 +/- 132	0.08480 +/- 0.00267	0.01708 +/- 0.00149
1	4	794 +/- 31	5.74377 +/- 0.24364	1.53221 +/- 0.07937

Spectrum: dUO2012				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3746 +/- 66	0.92124 +/- 0.02364	0.00000 +/- NaN
1	1	46106 +/- 216	0.31322 +/- 0.00303	0.02181 +/- 0.00088
1	2	115313 +/- 341	0.23945 +/- 0.00162	0.01803 +/- 0.00050
2	3	2545 +/- 53	0.00000 +/- NaN	0.00000 +/- NaN
2	4	9448 +/- 100	0.09127 +/- 0.004453	0.00000 +/- NaN
2	5	1463 +/- 45	0.82221 +/- 0.03995	0.00000 +/- NaN
3	5	418 +/- 26	0.00000 +/- NaN	0.00000 +/- NaN
3	6	2008 +/- 50	0.00000 +/- NaN	0.00000 +/- NaN
3	7	1617 +/- 44	0.00000 +/- NaN	0.00000 +/- NaN

4	8	288 +/- 26	0.00000 +/- NaN	0.00169 +/- 0.016885

Spectrum: dUO2013				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	3	5942 +/- 81	0.00168 +/- 0.00450	0.00000 +/- NaN
1	4	2647 +/- 55	1.28725 +/- 0.03648	0.00000 +/- NaN
1	2	444 +/- 26	0.13690 +/- 0.04970	0.00379 +/- 0.03965
2	6	238 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dUO2014				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3715 +/- 64	0.01343 +/- 0.00765	0.00000 +/- NaN
1	1	86738 +/- 296	0.06803 +/- 0.00097	0.00000 +/- NaN
1	2	264057 +/- 514	0.11217 +/- 0.00070	0.01180 +/- 0.00025
1	3	186 +/- 23	6.47632 +/- 0.83706	0.00000 +/- NaN
2	2	599 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
2	3	5672 +/- 78	0.00000 +/- NaN	0.00000 +/- NaN
2	4	13735 +/- 120	0.00000 +/- NaN	0.00000 +/- NaN
3	5	887 +/- 35	0.00000 +/- NaN	0.00140 +/- 0.00449
3	6	2684 +/- 56	0.00000 +/- NaN	0.00000 +/- NaN
3	7	640 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
3	8	0 +/- 41	NaN +/- NaN	NaN +/- NaN

Spectrum: dUO2015				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	510 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN
1	3	15987 +/- 127	0.02917 +/- 0.00183	0.00000 +/- NaN
1	4	4339 +/- 68	1.84103 +/- 0.03599	0.12779 +/- 0.00752
2	6	301 +/- 23	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dUO2016				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	3093 +/- 59	0.00000 +/- NaN	0.00000 +/- NaN
1	1	65753 +/- 257	0.06340 +/- 0.00112	0.00000 +/- NaN
1	2	167654 +/- 410	0.11694 +/- 0.00090	0.01327 +/- 0.00034

1	3	62 +/- 17	7.97667 +/- 2.30521	0.00000 +/- NaN
2	2	1028 +/- 37	0.00000 +/- NaN	0.01933 +/- 0.005793
2	3	5366 +/- 77	0.00000 +/- NaN	0.00000 +/- NaN
2	4	8808 +/- 96	0.00000 +/- NaN	0.00000 +/- NaN
2	5	291 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN
3	5	705 +/- 35	0.00000 +/- NaN	0.00412 +/- 0.005224
3	6	1606 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
3	7	226 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dUO2017

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	659 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
1	3	15848 +/- 127	0.03357 +/- 0.00209	0.00000 +/- NaN
1	4	2601 +/- 57	2.58660 +/- 0.06573	0.19535 +/- 0.01407
2	6	197 +/- 19	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dUO2018

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	2955 +/- 61	0.00000 +/- NaN	0.00000 +/- NaN
1	1	63723 +/- 253	0.06455 +/- 0.00112	0.00000 +/- NaN
1	2	150465 +/- 388	0.11733 +/- 0.00095	0.01401 +/- 0.00037
1	3	67 +/- 16	7.33588 +/- 1.80594	0.00000 +/- NaN
2	2	1168 +/- 40	0.00000 +/- NaN	0.00000 +/- NaN
2	3	5814 +/- 81	0.00000 +/- NaN	0.00000 +/- NaN
2	4	8473 +/- 93	0.00000 +/- NaN	0.00000 +/- NaN
2	5	164 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
3	5	912 +/- 37	0.00000 +/- NaN	0.00008 +/- 0.005842
3	6	1875 +/- 45	0.00000 +/- NaN	0.00000 +/- NaN
3	8	0 +/- 59	NaN +/- NaN	NaN +/- NaN

Spectrum: dUO2019

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	1	95 +/- 17	0.00000 +/- NaN	0.00000 +/- NaN
1	2	617 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
1	3	15798 +/- 128	0.03082 +/- 0.00220	0.00000 +/- NaN
1	4	2286 +/- 51	2.84768 +/- 0.07287	0.28912 +/- 0.01605

Spectrum: dUO2020				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	4398 +/- 73	0.00000 +/- NaN	0.00000 +/- NaN
1	1	33052 +/- 183	0.05672 +/- 0.00152	0.00000 +/- NaN
1	2	45577 +/- 215	0.10932 +/- 0.00171	0.01303 +/- 0.00068
1	3	165 +/- 21	0.00000 +/- NaN	0.00000 +/- NaN
2	2	1616 +/- 45	0.00000 +/- NaN	0.00000 +/- NaN
2	3	2774 +/- 55	0.00000 +/- NaN	0.00000 +/- NaN
2	4	1958 +/- 48	0.00000 +/- NaN	0.00000 +/- NaN
3	4	278 +/- 23	0.00000 +/- NaN	0.01028 +/- 0.01088
3	5	249 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
3	6	257 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
3	8	0 +/- 299	NaN +/- NaN	NaN +/- NaN

Spectrum: dUO2021				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	710 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
1	3	7991 +/- 91	0.03073 +/- 0.00335	0.00000 +/- NaN
1	4	814 +/- 34	3.08797 +/- 0.14782	0.00000 +/- NaN

Spectrum: dU3O8001				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	1858 +/- 48	0.76038 +/- 0.03083	0.07498 +/- 0.01100
1	1	58150 +/- 242	0.17039 +/- 0.00187	0.01074 +/- 0.00051
1	2	340067 +/- 584	0.15007 +/- 0.00072	0.01141 +/- 0.00020
1	3	397 +/- 33	24.83851 +/- 2.06846	4.26065 +/- 0.37240
2	3	1821 +/- 47	0.00000 +/- NaN	0.00000 +/- NaN
2	4	19735 +/- 142	0.06099 +/- 0.00220	0.00000 +/- NaN
2	5	6275 +/- 81	0.51931 +/- 0.01174	0.00000 +/- NaN
3	6	3196 +/- 61	0.00000 +/- NaN	0.00000 +/- NaN
3	7	5358 +/- 77	0.00000 +/- NaN	0.00000 +/- NaN
3	8	62 +/- 19	0.00000 +/- NaN	0.00000 +/- NaN
3	5	184 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
4	8	335 +/- 31	0.00000 +/- NaN	0.00000 +/- NaN
4	9	993 +/- 39	0.00000 +/- NaN	0.00000 +/- NaN

4	10	30 +/- 15	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8002				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1784 +/- 47	0.00000 +/- NaN	0.20427 +/- 0.01777
1	3	63168 +/- 252	0.10509 +/- 0.00141	0.02023 +/- 0.00071
1	4	56708 +/- 239	0.97450 +/- 0.00585	0.04443 +/- 0.00096
2	5	340 +/- 24	0.25434 +/- 0.06567	0.00000 +/- NaN
2	6	9451 +/- 99	0.20464 +/- 0.005604	0.00000 +/- NaN
2	7	246 +/- 20	3.98611 +/- 0.35510	0.00000 +/- NaN
3	8	1913 +/- 48	0.00000 +/- NaN	0.00000 +/- NaN
3	9	701 +/- 30	0.05241 +/- 0.03336	0.00000 +/- NaN
4	10	6 +/- 11	0.00000 +/- NaN	0.00000 +/- NaN
4	11	385 +/- 28	0.00000 +/- NaN	0.00000 +/- NaN
5	13	192 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
5	14	16 +/- 8	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8003				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	1803 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
1	1	56453 +/- 238	0.06111 +/- 0.00111	0.00016 +/- 0.00026
1	2	217858 +/- 467	0.09989 +/- 0.00072	0.00895 +/- 0.00024
1	3	205 +/- 19	5.26355 +/- 0.52428	0.00000 +/- NaN
2	3	2754 +/- 55	0.00000 +/- NaN	0.00000 +/- NaN
2	4	11486 +/- 109	0.00000 +/- NaN	0.00000 +/- NaN
2	5	570 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
3	5	379 +/- 25	0.00000 +/- NaN	0.00103 +/- 0.00635
3	6	2396 +/- 52	0.00000 +/- NaN	0.00000 +/- NaN
3	7	545 +/- 33	0.00000 +/- NaN	0.00000 +/- NaN
4	8	294 +/- 27	0.00000 +/- NaN	0.00465 +/- 0.00982
5	10	37 +/- 15	0.00000 +/- NaN	0.09115 +/- 0.094859

Spectrum: dU3O8004				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	953 +/- 34	0.00000 +/- NaN	0.00000 +/- NaN
1	3	48232 +/- 221	0.01969 +/- 0.00084	0.00548 +/- 0.00054

1	4	27322 +/- 167	1.01211 +/- 0.00869	0.04462 +/- 0.00150
2	6	1729 +/- 46	0.00000 +/- NaN	0.00000 +/- NaN
2	7	5 +/- 8	0.00000 +/- NaN	0.00000 +/- NaN
3	8	181 +/- 21	0.00000 +/- NaN	0.00338 +/- 0.02122
3	9	30 +/- 9	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8005				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	4326 +/- 69	0.00000 +/- NaN	0.00000 +/- NaN
1	1	23342 +/- 154	0.10742 +/- 0.00249	0.00000 +/- NaN
1	2	23409 +/- 154	0.15025 +/- 0.00289	0.02479 +/- 0.00144
1	3	127 +/- 16	0.00000 +/- NaN	0.00000 +/- NaN
2	2	629 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
2	3	1540 +/- 42	0.00000 +/- NaN	0.00000 +/- NaN
2	4	934 +/- 35	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8006				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	2	3183 +/- 58	0.15614 +/- 0.01020	0.00000 +/- NaN
1	3	29010 +/- 172	0.07332 +/- 0.00187	0.01396 +/- 0.00098
1	4	2178 +/- 49	4.15070 +/- 0.10372	0.81862 +/- 0.02998
2	6	134 +/- 18	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8007				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	5449 +/- 75	0.04420 +/- 0.00469	0.00000 +/- NaN
1	1	22507 +/- 151	0.10971 +/- 0.00253	0.00000 +/- NaN
1	2	20058 +/- 142	0.14549 +/- 0.00306	0.02600 +/- 0.00153
1	3	186 +/- 16	0.00000 +/- NaN	0.00000 +/- NaN
2	2	709 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
2	3	1383 +/- 41	0.00000 +/- NaN	0.00000 +/- NaN
2	4	687 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dU3O8008				
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**

1	1	382 +/- 26	0.00990 +/- 0.04851	0.00000 +/- NaN
1	2	2684 +/- 55	0.10801 +/- 0.01119	0.00000 +/- NaN
1	3	22189 +/- 150	0.08165 +/- 0.00224	0.01408 +/- 0.00114
1	4	1367 +/- 40	4.93917 +/- 0.15696	1.06107 +/- 0.04398
2	6	115 +/- 16	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum: dUO3001

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	298 +/- 25	1.23113 +/- 0.14210	0.00000 +/- NaN
1	1	8715 +/- 96	0.47867 +/- 0.00952	0.01440 +/- 0.00238
1	2	56528 +/- 239	0.25530 +/- 0.00241	0.01927 +/- 0.00068
2	3	679 +/- 30	0.00000 +/- NaN	0.00000 +/- NaN
2	4	9332 +/- 99	0.11060 +/- 0.004847	0.00000 +/- NaN
2	5	4122 +/- 71	0.76244 +/- 0.02045	0.00000 +/- NaN
2	6	0 +/- 816	NaN +/- NaN	NaN +/- NaN
3	5	140 +/- 17	0.00000 +/- NaN	0.00000 +/- NaN
3	6	2467 +/- 54	0.00000 +/- NaN	0.00000 +/- NaN
3	7	4770 +/- 72	0.05129 +/- 0.00647	0.00000 +/- NaN
3	8	212 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
4	7	13 +/- 8	0.00000 +/- NaN	0.00000 +/- NaN
4	8	505 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
4	9	910 +/- 41	0.00000 +/- NaN	0.00000 +/- NaN
4	10	110 +/- 18	0.00000 +/- NaN	0.00000 +/- NaN
5	10	70 +/- 17	0.00000 +/- NaN	0.00000 +/- NaN
5	11	282 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN
1	4	0 +/- 8	NaN +/- NaN	NaN +/- NaN

Spectrum: dUO3002

Ion U	Ion O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	3	22925 +/- 153	0.21961 +/- 0.00351	0.09242 +/- 0.00223
1	4	7233 +/- 89	3.76767 +/- 0.05153	0.62643 +/- 0.01244
1	2	1029 +/- 42	0.28421 +/- 0.03605	0.29039 +/- 0.03149
2	5	1572 +/- 43	0.40716 +/- 0.02497	0.00000 +/- NaN
2	6	9616 +/- 101	0.53085 +/- 0.009593	0.00000 +/- NaN
2	7	358 +/- 24	7.65510 +/- 0.53806	0.00000 +/- NaN
3	7	424 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN
3	8	4229 +/- 69	0.07021 +/- 0.00747	0.00000 +/- NaN

3	9	1787 +/- 45	0.43227 +/- 0.024349	0.00000 +/- NaN
4	11	1465 +/- 45	0.00000 +/- NaN	0.00000 +/- NaN
5	13	933 +/- 37	0.00000 +/- NaN	0.00000 +/- NaN
5	14	74 +/- 20	0.00000 +/- NaN	0.00000 +/- NaN
4	10	432 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum:		**dUO3003**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	0	1809 +/- 44	0.36448 +/- 0.01954	0.00000 +/- NaN
1	1	23729 +/- 155	0.19150 +/- 0.00326	0.01239 +/- 0.00126
1	2	36313 +/- 193	0.31314 +/- 0.00343	0.06672 +/- 0.00150
1	3	134 +/- 18	0.71390 +/- 0.17310	0.00000 +/- NaN
2	2	502 +/- 27	0.00000 +/- NaN	0.00000 +/- NaN
2	3	2223 +/- 53	0.00000 +/- NaN	0.00000 +/- NaN
2	4	2839 +/- 55	0.05150 +/- 0.00862	0.00000 +/- NaN
3	5	387 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
3	6	418 +/- 29	0.00000 +/- NaN	0.00000 +/- NaN
3	7	32 +/- 14	0.00000 +/- NaN	0.00000 +/- NaN

Spectrum:		**dUO3004**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
1	1	42 +/- 12	0.00000 +/- NaN	0.00000 +/- NaN
1	2	735 +/- 31	0.04137 +/- 0.02808	0.00000 +/- NaN
1	3	7799 +/- 90	0.02525 +/- 0.00344	0.01071 +/- 0.00242
1	4	859 +/- 32	2.13662 +/- 0.09829	0.15416 +/- 0.03201
2	5	2 +/- 7	0.00000 +/- NaN	0.00000 +/- NaN

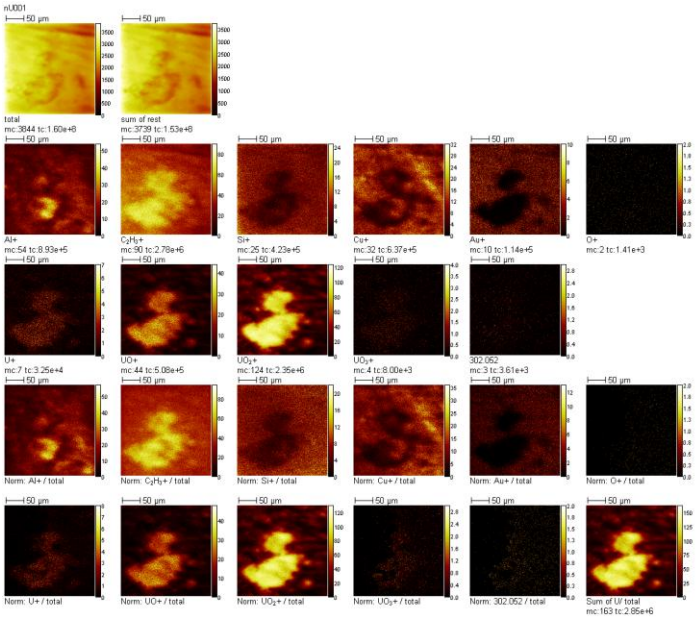
Spectrum:		**dUO3005**		
Ion				
U	**O**	**Counts(U-238Peak)**	**(U-238+1)Peak/U-238Peak**	**(U-238+2)Peak/U-238Peak**
2	3	612 +/- 32	0.00000 +/- NaN	0.00000 +/- NaN
2	4	360 +/- 24	0.00000 +/- NaN	0.00000 +/- NaN
2	2	242 +/- 25	0.00000 +/- NaN	0.00000 +/- NaN
3	6	13 +/- 12	0.00000 +/- NaN	0.00000 +/- NaN
1	0	1368 +/- 42	0.00000 +/- NaN	0.00000 +/- NaN
1	1	8755 +/- 95	0.11434 +/- 0.00453	0.00000 +/- NaN
1	2	8312 +/- 93	0.19045 +/- 0.00605	0.00316 +/- 0.00325

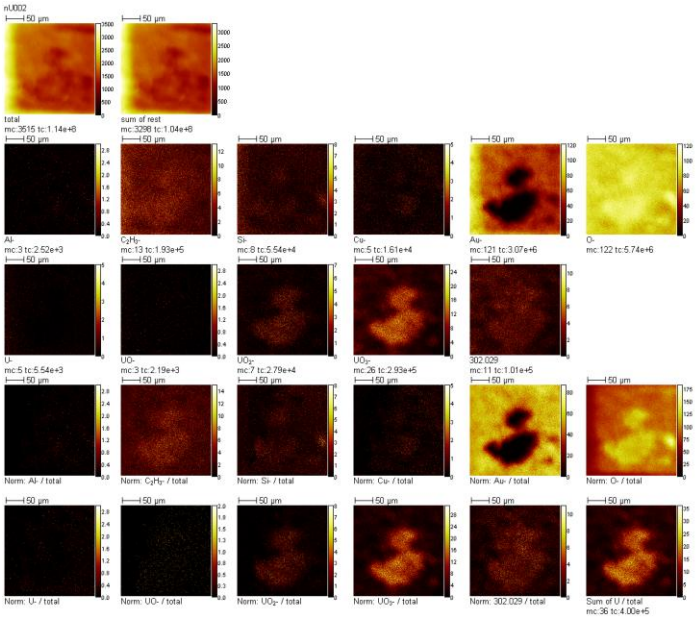
1	3	95 +/- 14	0.00000 +/- NaN	0.00000 +/- NaN

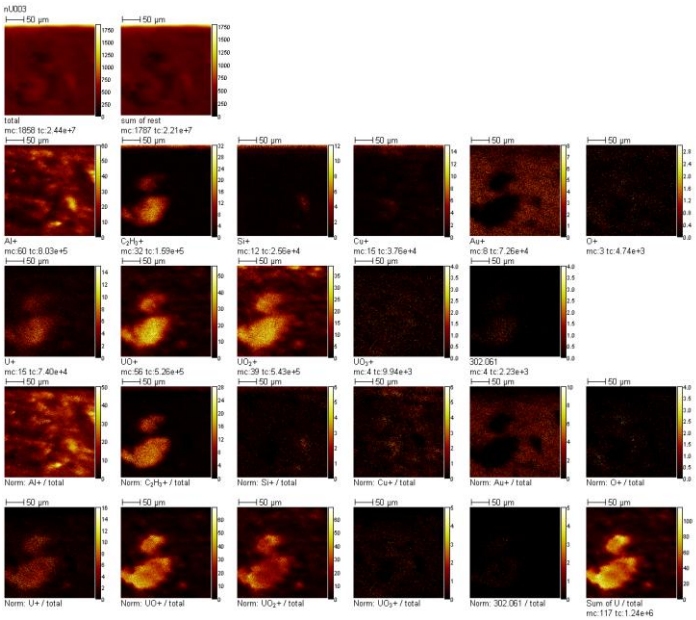
Spectrum: dUO3006				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	2	1236 +/- 37	0.20288 +/- 0.02017	0.00000 +/- NaN
1	3	8510 +/- 93	0.07558 +/- 0.00389	0.00436 +/- 0.00255
1	4	418 +/- 26	5.13731 +/- 0.34615	0.66550 +/- 0.08764

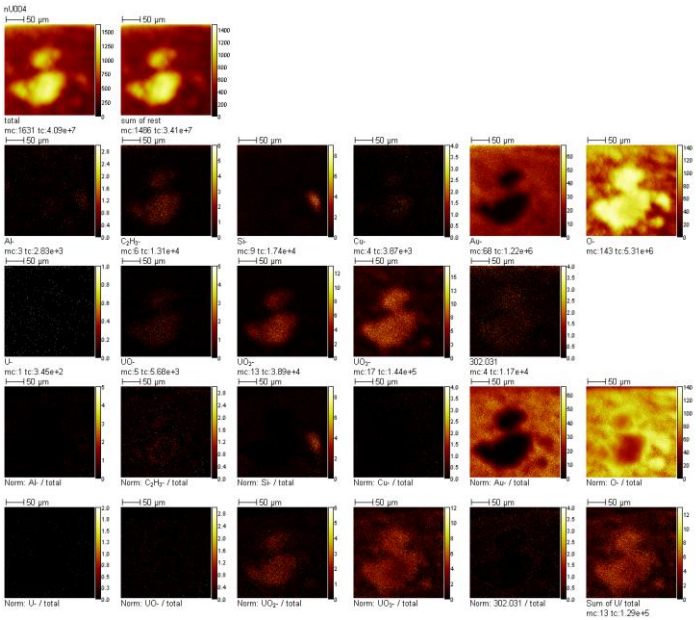
Spectrum: dUO3007				
Ion				
U	O	Counts(U-238Peak)	(U-238+1)Peak/U-238Peak	(U-238+2)Peak/U-238Peak
1	0	13553 +/- 122	0.00000 +/- NaN	0.00000 +/- NaN
1	1	9128 +/- 100	0.00000 +/- NaN	0.00000 +/- NaN
1	2	2280 +/- 50	0.00000 +/- NaN	0.00000 +/- NaN
1	3	482 +/- 28	0.00000 +/- NaN	0.04253 +/- 0.01650
2	2	343 +/- 22	0.00000 +/- NaN	0.00000 +/- NaN

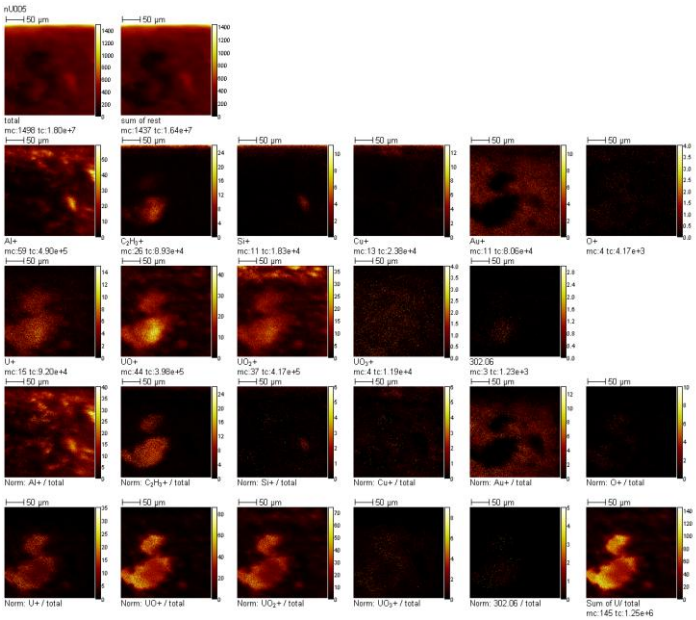
Appendix G. TOF-SIMS Images

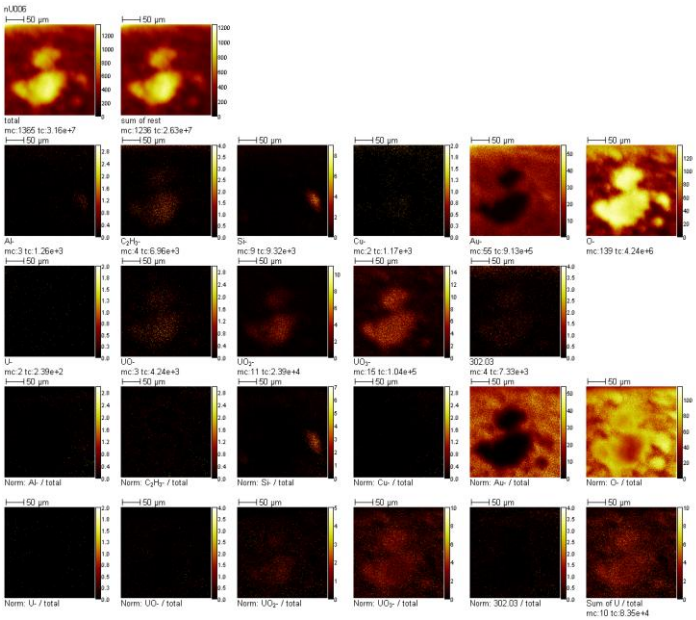


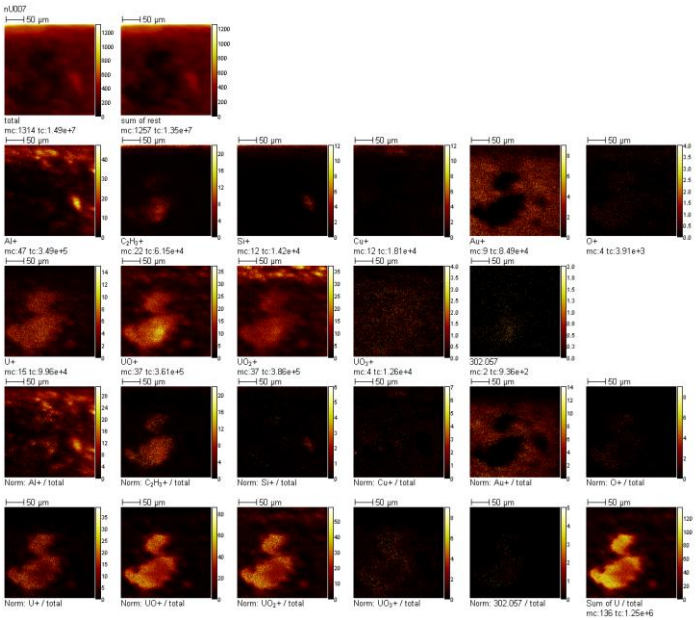


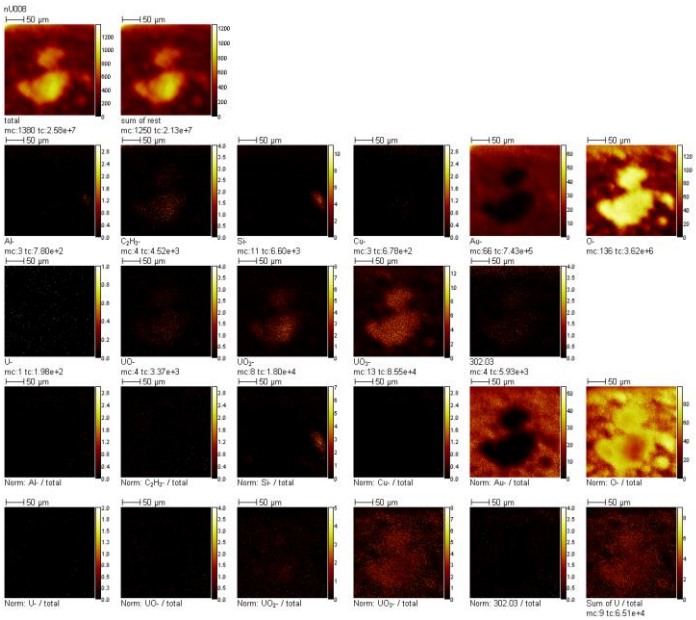

nU003
total
mc:1858 tc:2.44e+7
sum of rest
mc:1787 tc:2.21e+7
Al+
mc:60 tc:8.03e+5
C2H2+
mc:32 tc:1.59e+5
Si+
mc:12 tc:2.66e+4
Cu+
mc:15 tc:3.76e+4
Au+
mc:8 tc:7.26e+4
O+
mc:3 tc:4.74e+3
U+
mc:15 tc:7.40e+4
UO+
mc:56 tc:5.26e+5
UO2+
mc:39 tc:5.43e+5
UO3+
mc:4 tc:9.94e+3
302.061
mc:4 tc:2.23e+3
Norm: Al+ / total
Norm: C2H2+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.061 / total
Sum of U / total
mc:117 tc:1.24e+6

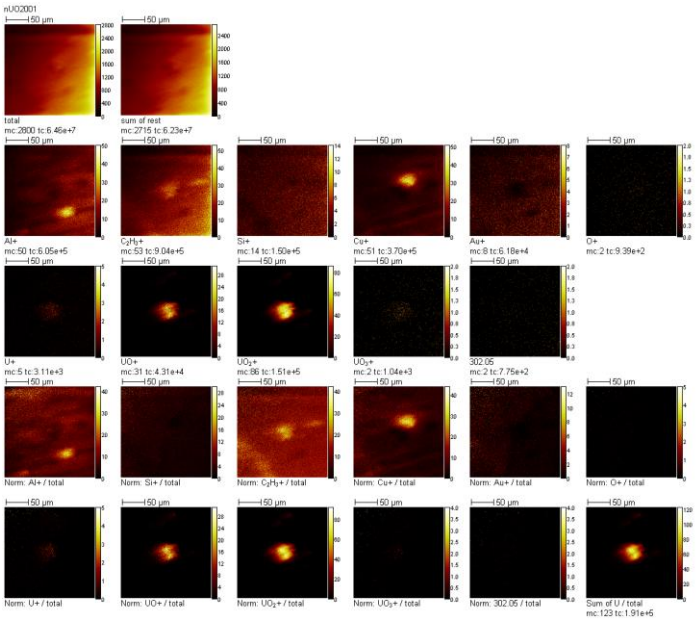

nU004
total
mc:1631 tc:4.09e+7
sum of rest
mc:1496 tc:3.41e+7
Al-
mc:3 tc:2.83e+3
C2H2-
mc:6 tc:1.31e+4
Si-
mc:9 tc:1.74e+4
Cu-
mc:4 tc:3.87e+3
Au-
mc:68 tc:1.22e+6
O-
mc:143 tc:5.31e+6
U-
mc:1 tc:3.45e+2
UO-
mc:5 tc:5.68e+3
UO2-
mc:13 tc:3.89e+4
UO3-
mc:17 tc:1.44e+5
302.031
mc:4 tc:1.17e+4
Norm: Al- / total
Norm: C2H2- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.031 / total
Sum of Uf total
mc:13 tc:1.29e+5

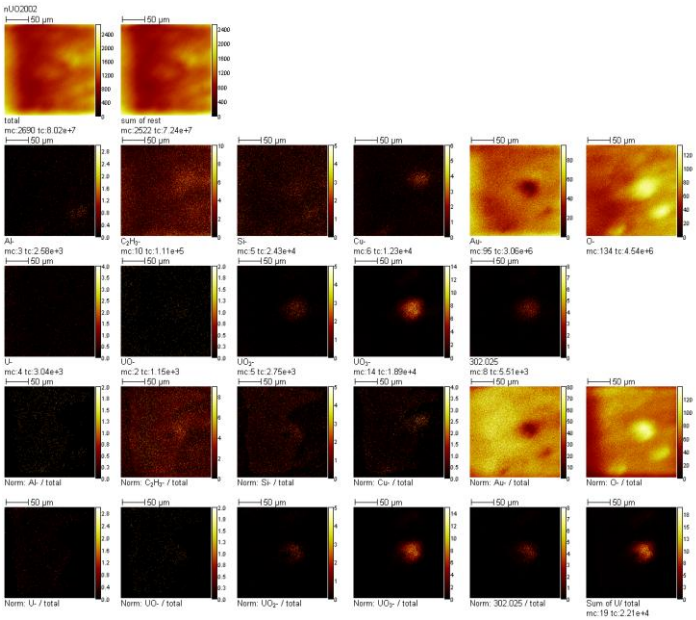

nU005
150 µm
total
mc:1498 tc:1.80e+7
sum of rest
mc:1437 tc:1.64e+7
Al+
mc:59 tc:4.90e+5
C2H2+
mc:26 tc:8.93e+4
Si+
mc:11 tc:1.83e+4
Cu+
mc:13 tc:2.38e+4
Au+
mc:11 tc:8.08e+4
O+
mc:4 tc:4.17e+3
U+
mc:15 tc:9.20e+4
UO+
mc:44 tc:3.98e+5
UO2+
mc:37 tc:4.17e+5
UO3+
mc:4 tc:1.19e+4
302.06
mc:3 tc:1.23e+3
Norm: Al+ / total
Norm: C2H2+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.06 / total
Sum of U/ total
mc:145 tc:1.25e+6

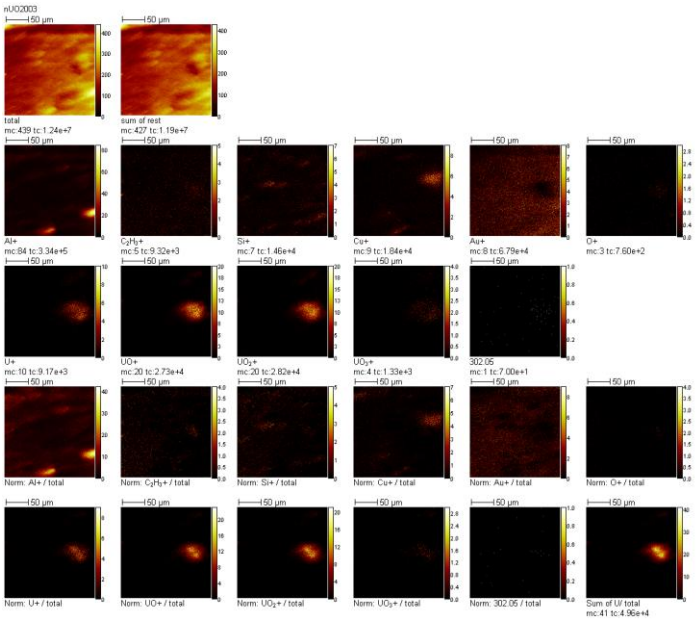

nU006
150 µm
total
mc:1365 tc:3.16e+7
sum of rest
mc:1236 tc:2.63e+7
Al-
mc:3 tc:1.26e+3
C2H2-
mc:4 tc:6.96e+3
Si-
mc:9 tc:9.32e+3
Cu-
mc:2 tc:1.17e+3
Au-
mc:55 tc:9.13e+5
O-
mc:139 tc:4.24e+6
U-
mc:2 tc:2.39e+2
UO-
mc:3 tc:4.24e+3
UO2-
mc:11 tc:2.39e+4
UO3-
mc:15 tc:1.04e+5
302.03
mc:4 tc:7.33e+3
Norm: Al- / total
Norm: C2H2- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.03 / total
Sum of U / total
mc:10 tc:8.35e+4

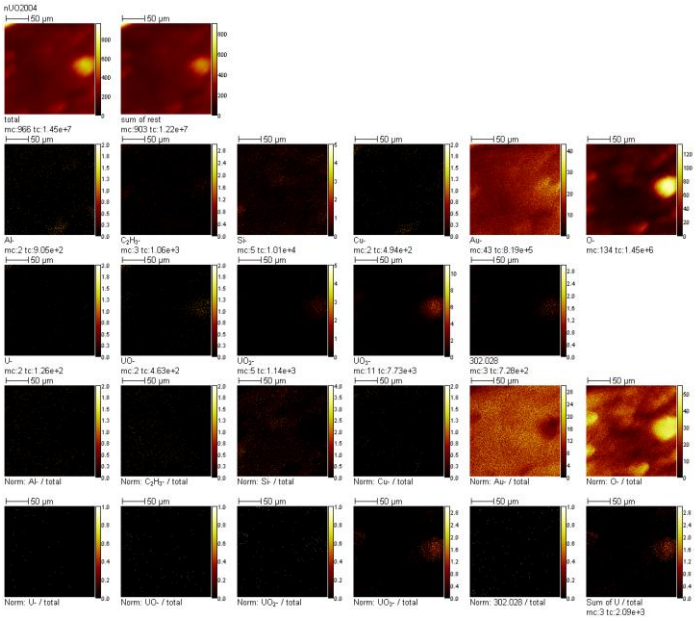

nU007
150 µm
total
mc:1314 tc:1.49e+7
sum of rest
mc:1257 tc:1.35e+7
Al+
mc:47 tc:3.49e+5
C2H2+
mc:22 tc:6.15e+4
Si+
mc:12 tc:1.42e+4
Cu+
mc:12 tc:1.81e+4
Au+
mc:9 tc:8.49e+4
O+
mc:4 tc:3.91e+3
U+
mc:15 tc:9.96e+4
UO+
mc:37 tc:3.61e+5
UO2+
mc:37 tc:3.86e+5
UO3+
mc:4 tc:1.26e+4
302.057
mc:2 tc:9.36e+2
Norm: Al+ / total
Norm: C2H2+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.057 / total
Sum of U / total
mc:136 tc:1.25e+6

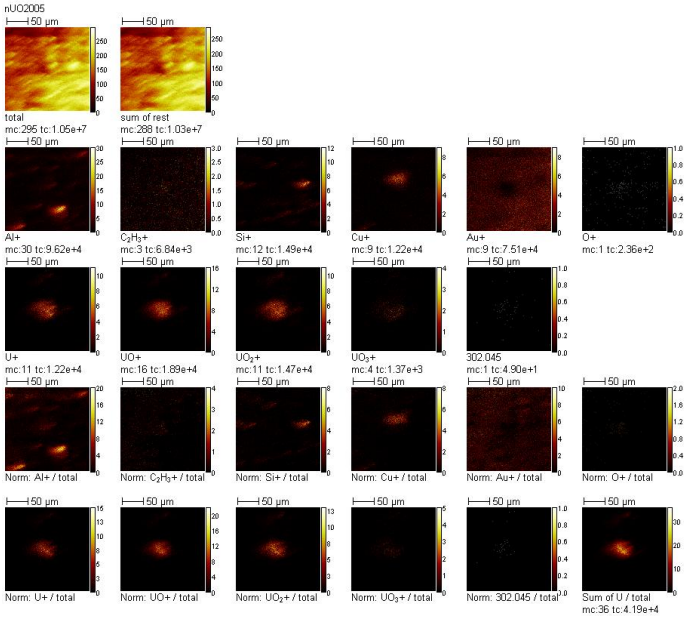

nU008
150 µm
total
mc:1380 tc:2.58e+7
sum of rest
mc:1250 tc:2.13e+7
Al-
mc:3 tc:7.80e+2
C2H2-
mc:4 tc:4.52e+3
Si-
mc:11 tc:6.60e+3
Cu-
mc:3 tc:6.78e+2
Au-
mc:66 tc:7.43e+5
O-
mc:136 tc:3.62e+6
U-
mc:1 tc:1.98e+2
UO-
mc:4 tc:3.37e+3
UO2-
mc:8 tc:1.80e+4
UO3-
mc:13 tc:8.55e+4
302.03
mc:4 tc:5.93e+3
Norm: Al- / total
Norm: C2H2- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.03 / total
Sum of U / total
mc:9 tc:6.51e+4

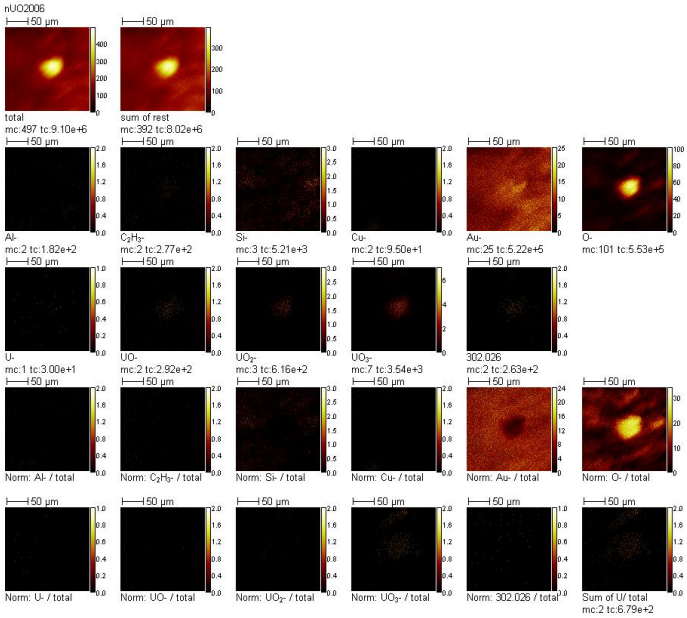

nUO2001
total
mc:2800 tc:6.46e+7
sum of rest
mc:2715 tc:6.23e+7
Al+
mc:50 tc:6.05e+5
C2H2+
mc:53 tc:9.04e+5
Si+
mc:14 tc:1.60e+5
Cu+
mc:51 tc:3.70e+5
Au+
mc:8 tc:6.18e+4
O+
mc:2 tc:9.39e+2
U+
mc:5 tc:3.11e+3
UO+
mc:31 tc:4.31e+4
UO2+
mc:86 tc:1.51e+5
UO2+
mc:2 tc:1.04e+3
302.05
mc:2 tc:7.75e+2
Norm: Al+ / total
Norm: Si+ / total
Norm: C2H2+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO2+ / total
Norm: 302.05 / total
Sum of U / total
mc:123 tc:1.91e+6

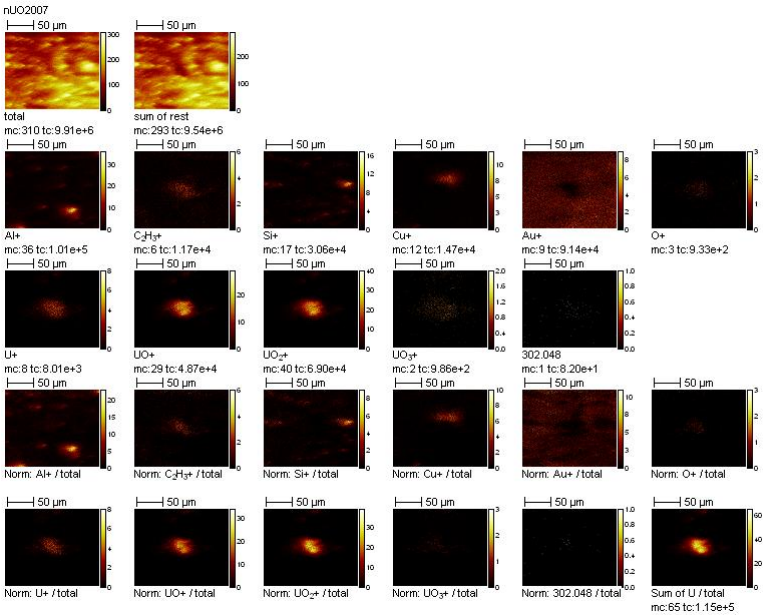

nUO2002
total
mc:2690 tc:8.02e+7
sum of rest
mc:2522 tc:7.24e+7
Al-
mc:3 tc:2.58e+3
C2H2-
mc:10 tc:1.11e+5
Si-
mc:5 tc:2.43e+4
Cu-
mc:6 tc:1.23e+4
Au-
mc:95 tc:3.06e+6
O-
mc:134 tc:4.54e+6
U-
mc:4 tc:3.04e+3
UO-
mc:2 tc:1.15e+3
UO2-
mc:5 tc:2.75e+3
UO2-
mc:14 tc:1.89e+4
302.025
mc:8 tc:5.51e+3
Norm: Al- / total
Norm: C2H2- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO2- / total
Norm: 302.025 / total
Sum of U- total
mc:19 tc:2.21e+4

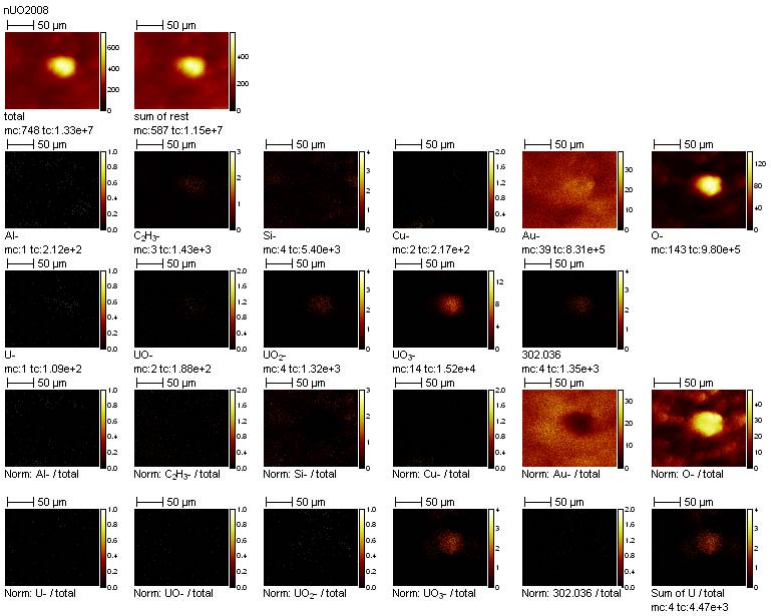

nU02003
total
mc:439 tc:1.24e+7
sum of rest
mc:427 tc:1.19e+7
Al+
mc:84 tc:3.34e+5
C2H2+
mc:5 tc:9.32e+3
Si+
mc:7 tc:1.46e+4
Cu+
mc:9 tc:1.84e+4
Au+
mc:8 tc:6.79e+4
O+
mc:3 tc:7.60e+2
U+
mc:10 tc:9.17e+3
UO+
mc:20 tc:2.73e+4
UO2+
mc:20 tc:2.82e+4
UO3+
mc:4 tc:1.33e+3
302.05
mc:1 tc:7.00e+1
Norm: Al+ / total
Norm: C2H2+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.05 / total
Sum of U/ total
mc:41 tc:4.96e+4

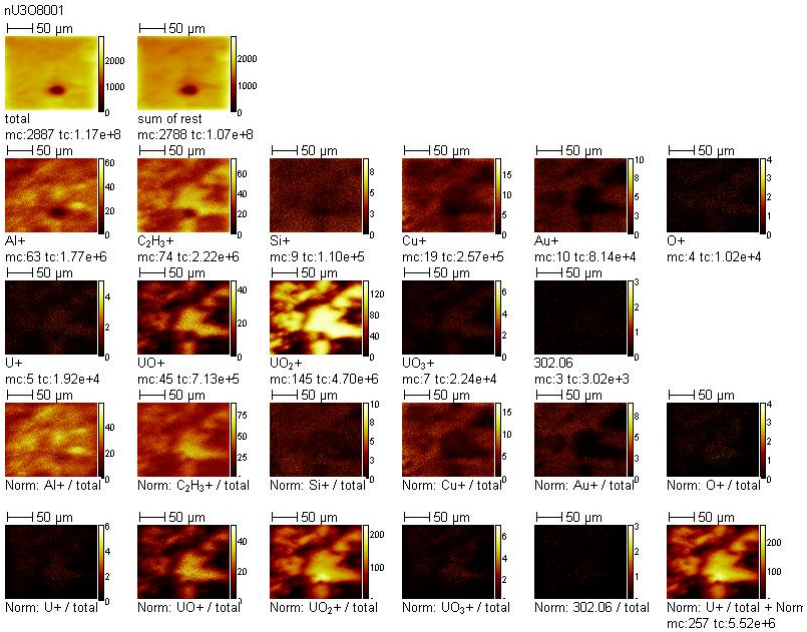

nU02004
total
mc:966 tc:1.45e+7
sum of rest
mc:903 tc:1.22e+7
Al-
mc:2 tc:9.05e+2
C2H2-
mc:3 tc:1.06e+3
Si-
mc:5 tc:1.01e+4
Cu-
mc:2 tc:4.94e+2
Au-
mc:43 tc:8.19e+5
O-
mc:134 tc:1.45e+6
U-
mc:2 tc:1.26e+2
UO-
mc:2 tc:4.63e+2
UO2-
mc:5 tc:1.14e+3
UO3-
mc:11 tc:7.73e+3
302.028
mc:3 tc:7.28e+2
Norm: Al- / total
Norm: C2H2- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.028 / total
Sum of U / total
mc:3 tc:2.09e+3

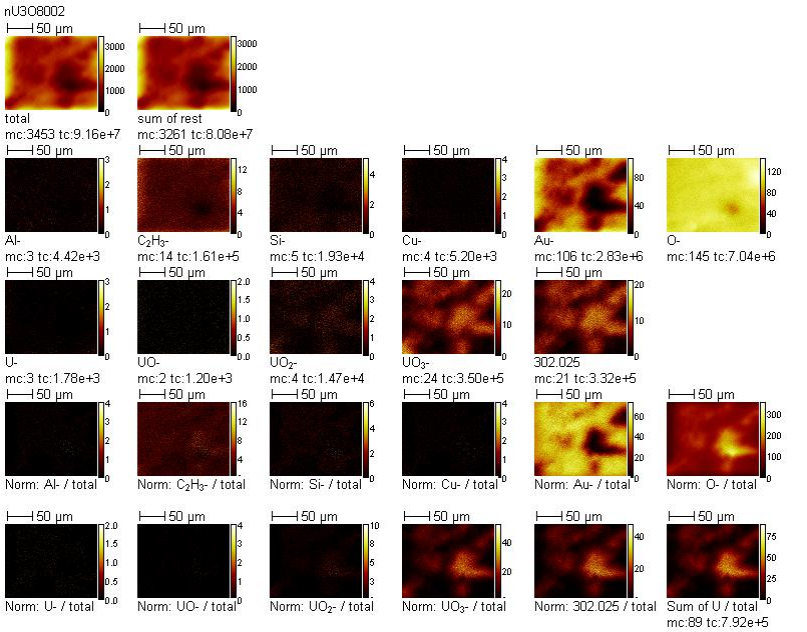

nUO2005
50 µm
total
mc:295 tc:1.05e+7
sum of rest
mc:288 tc:1.03e+7
Al+
mc:30 tc:9.62e+4
C3H3+
mc:3 tc:6.84e+3
Si+
mc:12 tc:1.49e+4
Cu+
mc:9 tc:1.22e+4
Au+
mc:9 tc:7.51e+4
O+
mc:1 tc:2.36e+2
U+
mc:11 tc:1.22e+4
UO+
mc:16 tc:1.89e+4
UO2+
mc:11 tc:1.47e+4
UO3+
mc:4 tc:1.37e+3
302.045
mc:1 tc:4.90e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.045 / total
Sum of U / total
mc:36 tc:4.19e+4

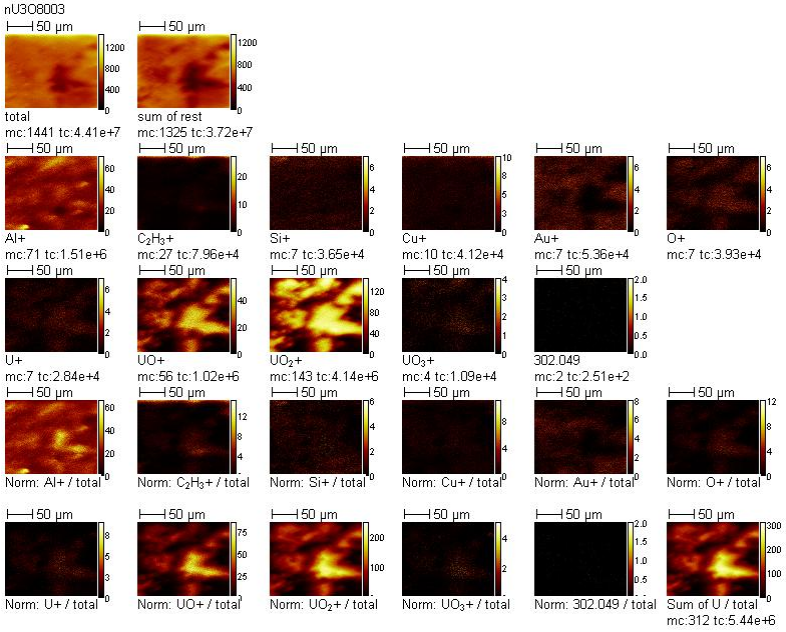

nUO2006
50 µm
total
mc:497 tc:9.10e+6
sum of rest
mc:392 tc:8.02e+6
Al-
mc:2 tc:1.82e+2
C3H3-
mc:2 tc:2.77e+2
Si-
mc:3 tc:5.21e+3
Cu-
mc:2 tc:9.50e+1
Au-
mc:25 tc:5.22e+5
O-
mc:101 tc:5.53e+5
U-
mc:1 tc:3.00e+1
UO-
mc:2 tc:2.92e+2
UO2-
mc:3 tc:6.16e+2
UO3-
mc:7 tc:3.54e+3
302.026
mc:2 tc:2.63e+2
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.026 / total
Sum of U/ total
mc:2 tc:6.79e+2

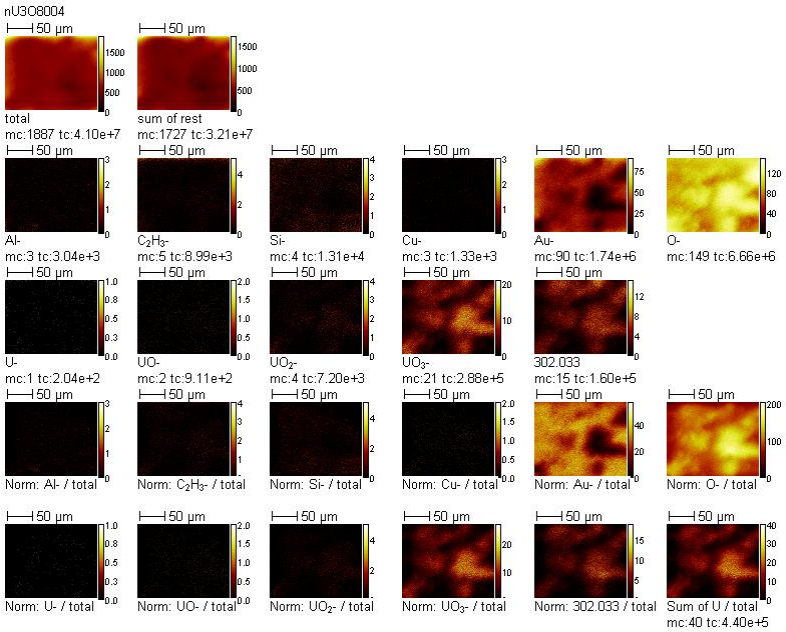

nUO2007
50 µm
total
mc:310 tc:9.91e+6
sum of rest
mc:293 tc:9.54e+6
Al+
mc:36 tc:1.01e+5
C2H3+
mc:6 tc:1.17e+4
Si+
mc:17 tc:3.06e+4
Cu+
mc:12 tc:1.47e+4
Au+
mc:9 tc:9.14e+4
O+
mc:3 tc:9.33e+2
U+
mc:8 tc:8.01e+3
UO+
mc:29 tc:4.87e+4
UO2+
mc:40 tc:6.90e+4
UO3+
mc:2 tc:9.86e+2
302.048
mc:1 tc:8.20e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.048 / total
Sum of U / total
mc:65 tc:1.15e+5

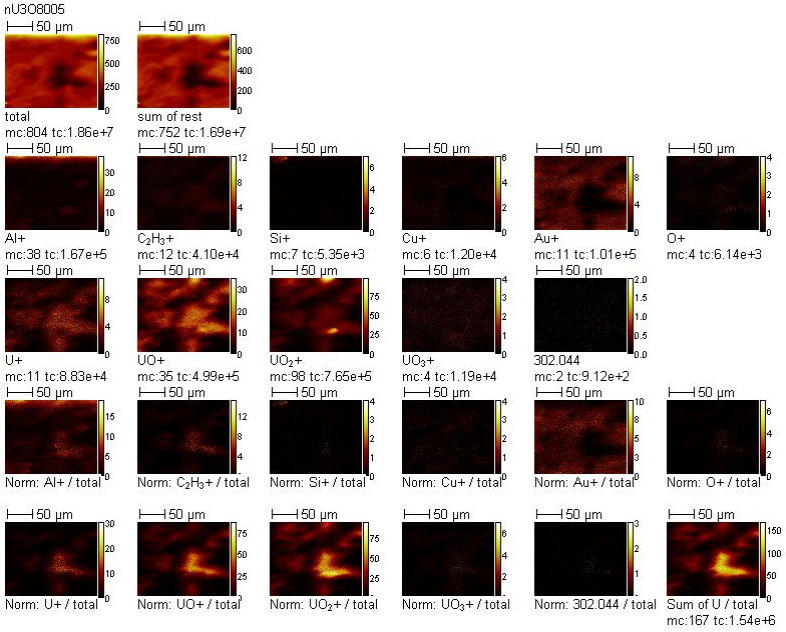

nUO2008
50 µm
total
mc:748 tc:1.33e+7
sum of rest
mc:587 tc:1.15e+7
Al-
mc:1 tc:2.12e+2
C2H3-
mc:3 tc:1.43e+3
Si-
mc:4 tc:5.40e+3
Cu-
mc:2 tc:2.17e+2
Au-
mc:39 tc:8.31e+5
O-
mc:143 tc:9.80e+5
U-
mc:1 tc:1.09e+2
UO-
mc:2 tc:1.88e+2
UO2-
mc:4 tc:1.32e+3
UO3-
mc:14 tc:1.52e+4
302.036
mc:4 tc:1.35e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.036 / total
Sum of U / total
mc:4 tc:4.47e+3

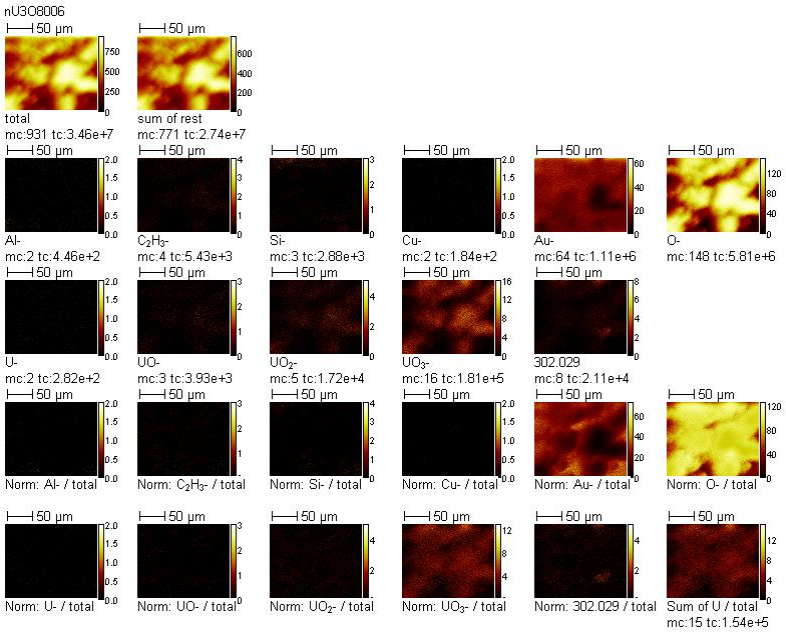

nU3O8001
50 µm
total
mc:2887 tc:1.17e+8
sum of rest
mc:2788 tc:1.07e+8
Al+
mc:63 tc:1.77e+6
C2H3+
mc:74 tc:2.22e+6
Si+
mc:9 tc:1.10e+5
Cu+
mc:19 tc:2.57e+5
Au+
mc:10 tc:8.14e+4
O+
mc:4 tc:1.02e+4
U+
mc:5 tc:1.92e+4
UO+
mc:45 tc:7.13e+5
UO2+
mc:145 tc:4.70e+6
UO3+
mc:7 tc:2.24e+4
302.06
mc:3 tc:3.02e+3
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.06 / total
Norm: U+ / total + Norm
mc:257 tc:5.52e+6

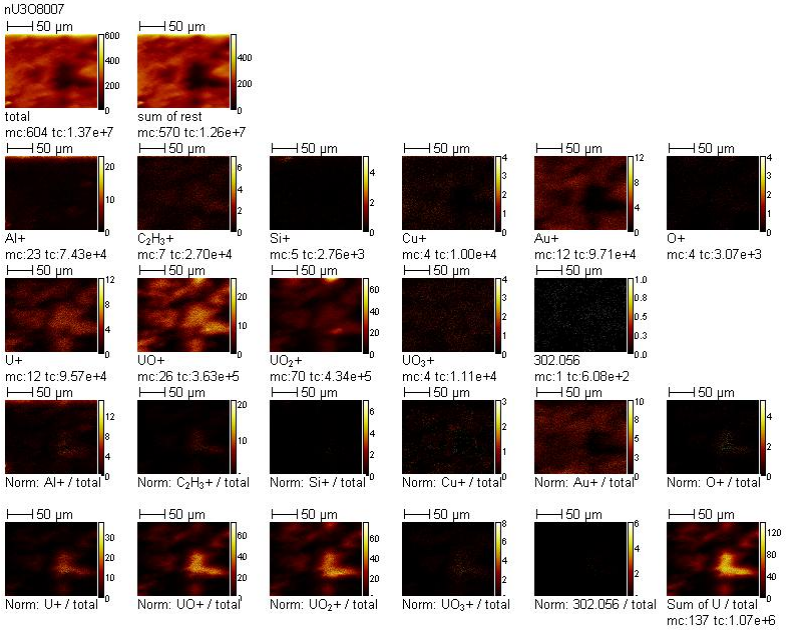

nU3O8002
50 µm
total
mc:3453 tc:9.16e+7
sum of rest
mc:3261 tc:8.08e+7
Al-
mc:3 tc:4.42e+3
C2H3-
mc:14 tc:1.61e+5
Si-
mc:5 tc:1.93e+4
Cu-
mc:4 tc:5.20e+3
Au-
mc:106 tc:2.83e+6
O-
mc:145 tc:7.04e+6
U-
mc:3 tc:1.78e+3
UO-
mc:2 tc:1.20e+3
UO2-
mc:4 tc:1.47e+4
UO3-
mc:24 tc:3.50e+5
302.025
mc:21 tc:3.32e+5
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.025 / total
Sum of U / total
mc:89 tc:7.92e+5

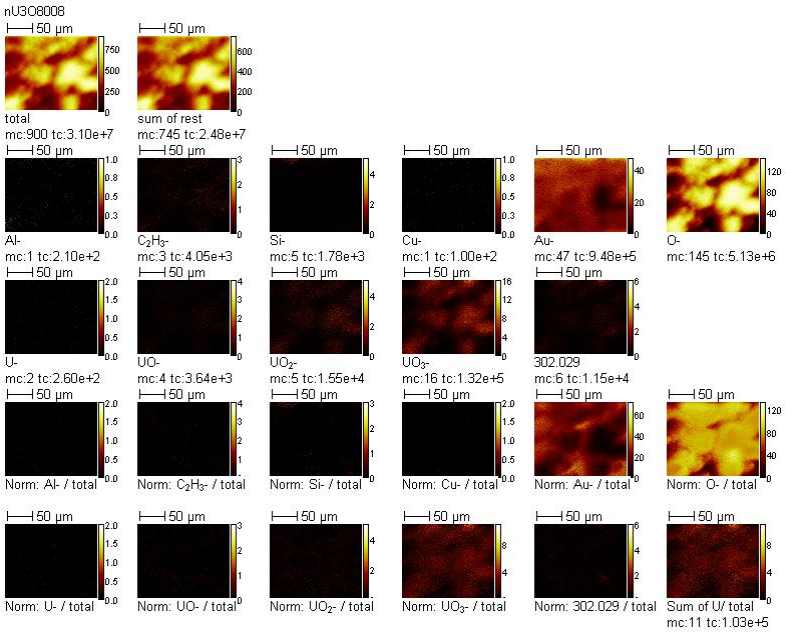

nU3O8003
50 µm
total
mc:1441 tc:4.41e+7
sum of rest
mc:1325 tc:3.72e+7
Al+
mc:71 tc:1.51e+6
C2H3+
mc:27 tc:7.96e+4
Si+
mc:7 tc:3.65e+4
Cu+
mc:10 tc:4.12e+4
Au+
mc:7 tc:5.36e+4
O+
mc:7 tc:3.93e+4
U+
mc:7 tc:2.84e+4
UO+
mc:56 tc:1.02e+6
UO2+
mc:143 tc:4.14e+6
UO3+
mc:4 tc:1.09e+4
302.049
mc:2 tc:2.51e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.049 / total
Sum of U / total
mc:312 tc:5.44e+6

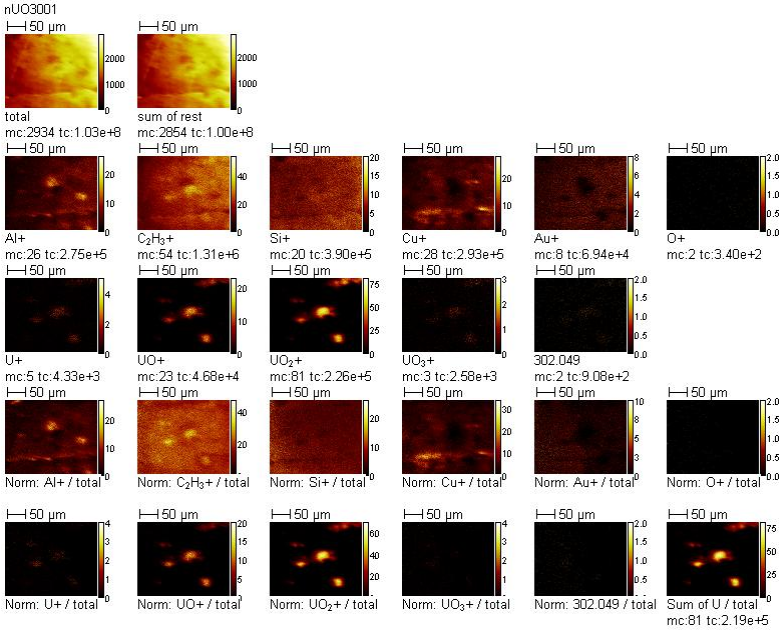

nU3O8004
50 µm
total
mc:1887 tc:4.10e+7
sum of rest
mc:1727 tc:3.21e+7
Al-
mc:3 tc:3.04e+3
C2H3-
mc:5 tc:8.99e+3
Si-
mc:4 tc:1.31e+4
Cu-
mc:3 tc:1.33e+3
Au-
mc:90 tc:1.74e+6
O-
mc:149 tc:6.66e+6
U-
mc:1 tc:2.04e+2
UO-
mc:2 tc:9.11e+2
UO2-
mc:4 tc:7.20e+3
UO3-
mc:21 tc:2.88e+5
302.033
mc:15 tc:1.60e+5
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.033 / total
Sum of U / total
mc:40 tc:4.40e+5

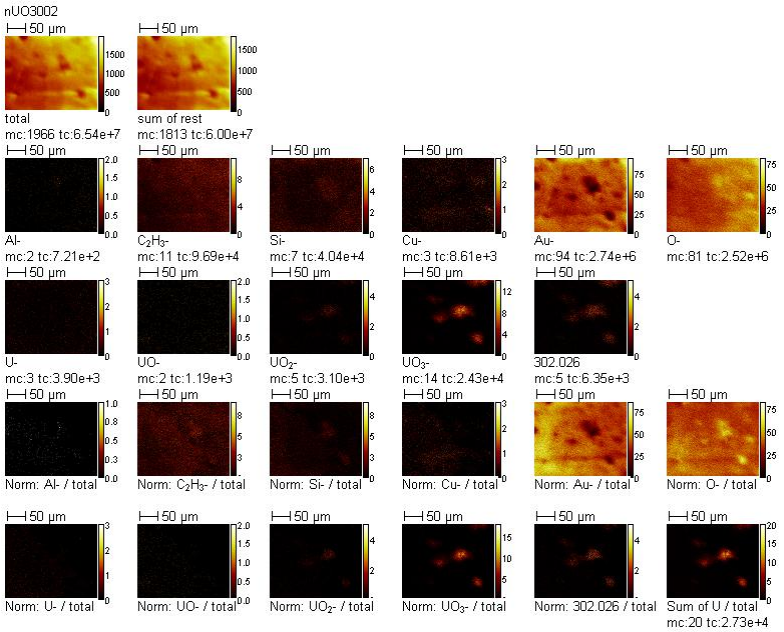

nU3O8005
50 µm
total
mc:804 tc:1.86e+7
sum of rest
mc:752 tc:1.69e+7
Al+
mc:38 tc:1.67e+5
C2H3+
mc:12 tc:4.10e+4
Si+
mc:7 tc:5.35e+3
Cu+
mc:6 tc:1.20e+4
Au+
mc:11 tc:1.01e+5
O+
mc:4 tc:6.14e+3
U+
mc:11 tc:8.83e+4
UO+
mc:35 tc:4.99e+5
UO2+
mc:98 tc:7.65e+5
UO3+
mc:4 tc:1.19e+4
302.044
mc:2 tc:9.12e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.044 / total
Sum of U / total
mc:167 tc:1.54e+6

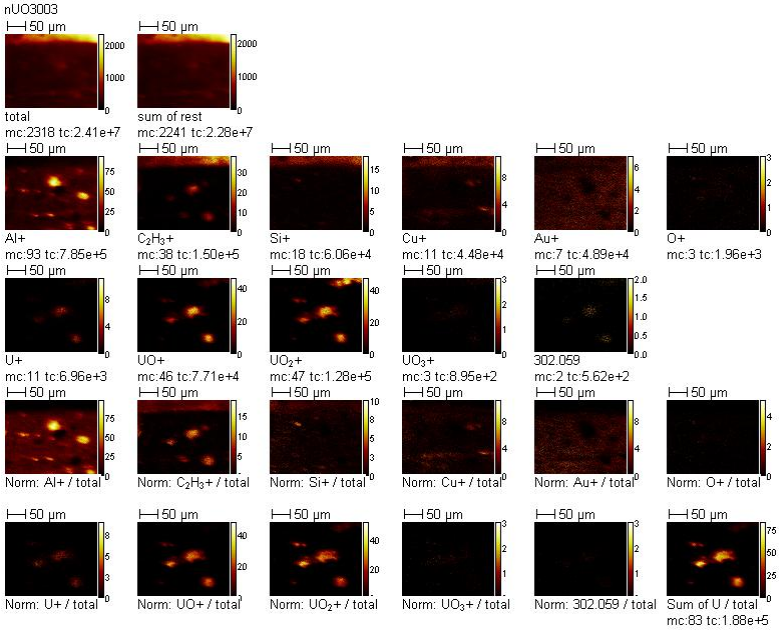

nU3O8006
50 µm
total
mc:931 tc:3.46e+7
sum of rest
mc:771 tc:2.74e+7
Al-
mc:2 tc:4.46e+2
C2H3-
mc:4 tc:5.43e+3
Si-
mc:3 tc:2.88e+3
Cu-
mc:2 tc:1.84e+2
Au-
mc:64 tc:1.11e+6
O-
mc:148 tc:5.81e+6
U-
mc:2 tc:2.82e+2
UO-
mc:3 tc:3.93e+3
UO2-
mc:5 tc:1.72e+4
UO3-
mc:16 tc:1.81e+5
302.029
mc:8 tc:2.11e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.029 / total
Sum of U / total
mc:15 tc:1.54e+5

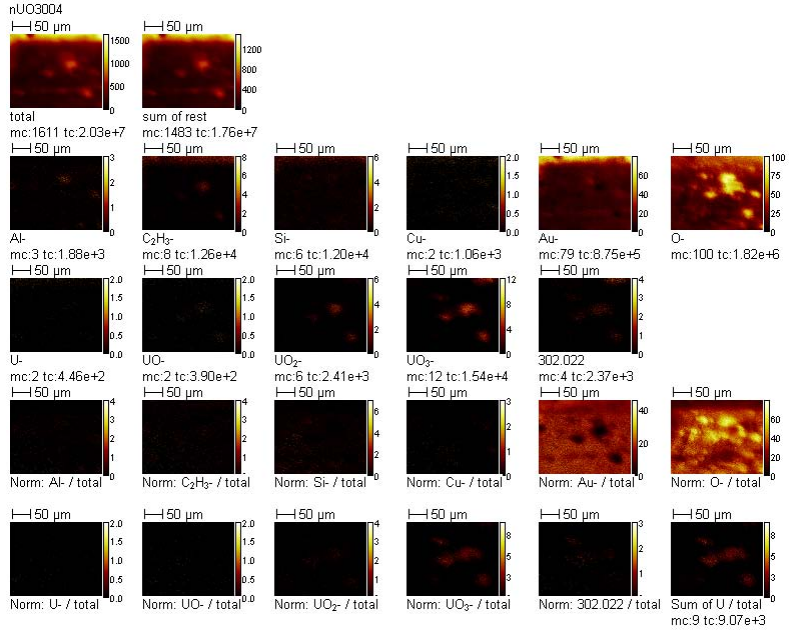

nU3O8007
50 µm
total
mc:604 tc:1.37e+7
sum of rest
mc:570 tc:1.26e+7
Al+
mc:23 tc:7.43e+4
C2H3+
mc:7 tc:2.70e+4
Si+
mc:5 tc:2.76e+3
Cu+
mc:4 tc:1.00e+4
Au+
mc:12 tc:9.71e+4
O+
mc:4 tc:3.07e+3
U+
mc:12 tc:9.57e+4
UO+
mc:26 tc:3.63e+5
UO2+
mc:70 tc:4.34e+5
UO3+
mc:4 tc:1.11e+4
302.056
mc:1 tc:6.08e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.056 / total
Sum of U / total
mc:137 tc:1.07e+6

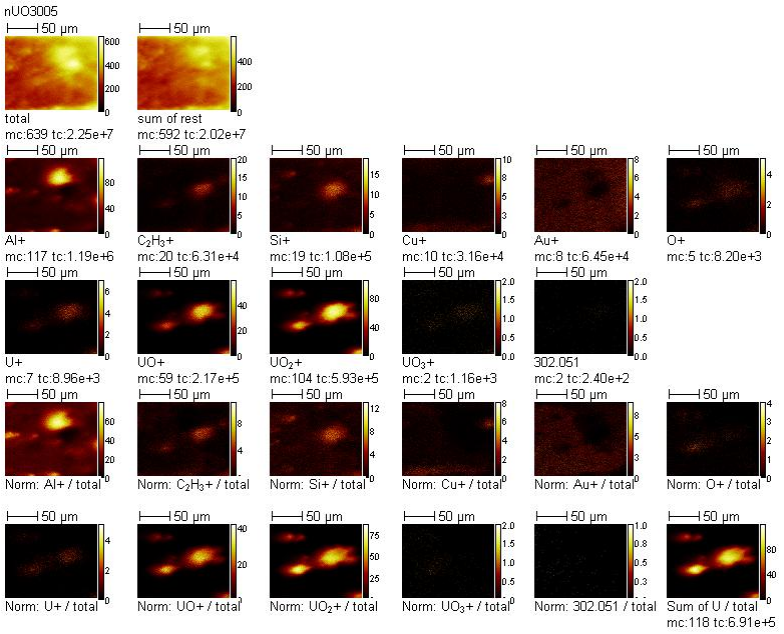

nU3O8008
50 µm
total
mc:900 tc:3.10e+7
sum of rest
mc:745 tc:2.48e+7
Al-
mc:1 tc:2.10e+2
C2H3-
mc:3 tc:4.05e+3
Si-
mc:5 tc:1.78e+3
Cu-
mc:1 tc:1.00e+2
Au-
mc:47 tc:9.48e+5
O-
mc:145 tc:5.13e+6
U-
mc:2 tc:2.60e+2
UO-
mc:4 tc:3.64e+3
UO2-
mc:5 tc:1.55e+4
UO3-
mc:16 tc:1.32e+5
302.029
mc:6 tc:1.15e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.029 / total
Sum of U/ total
mc:11 tc:1.03e+5

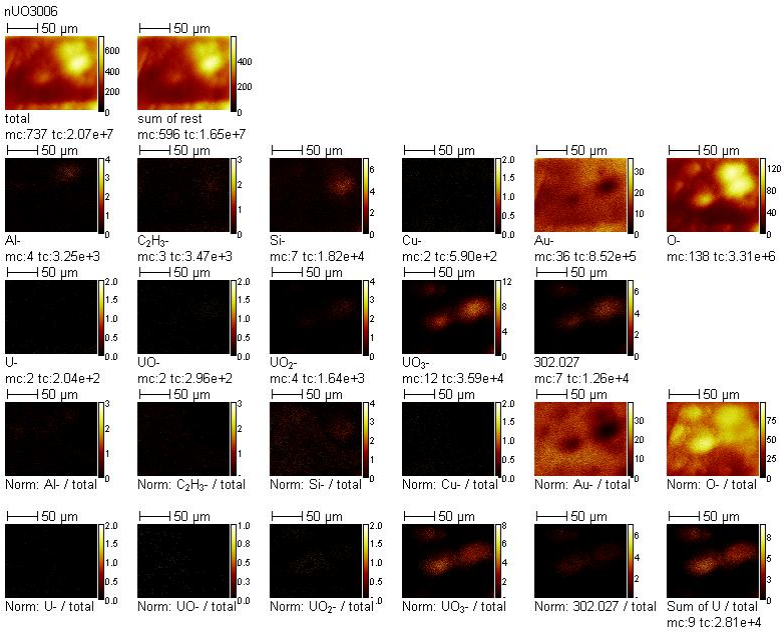

nUO3001
50 µm
total
mc:2934 tc:1.03e+8
sum of rest
mc:2854 tc:1.00e+8
Al+
mc:26 tc:2.75e+5
C2H3+
mc:54 tc:1.31e+6
Si+
mc:20 tc:3.90e+5
Cu+
mc:28 tc:2.93e+5
Au+
mc:8 tc:6.94e+4
O+
mc:2 tc:3.40e+2
U+
mc:5 tc:4.33e+3
UO+
mc:23 tc:4.68e+4
UO2+
mc:81 tc:2.26e+5
UO3+
mc:3 tc:2.58e+3
302.049
mc:2 tc:9.08e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.049 / total
Sum of U / total
mc:81 tc:2.19e+5

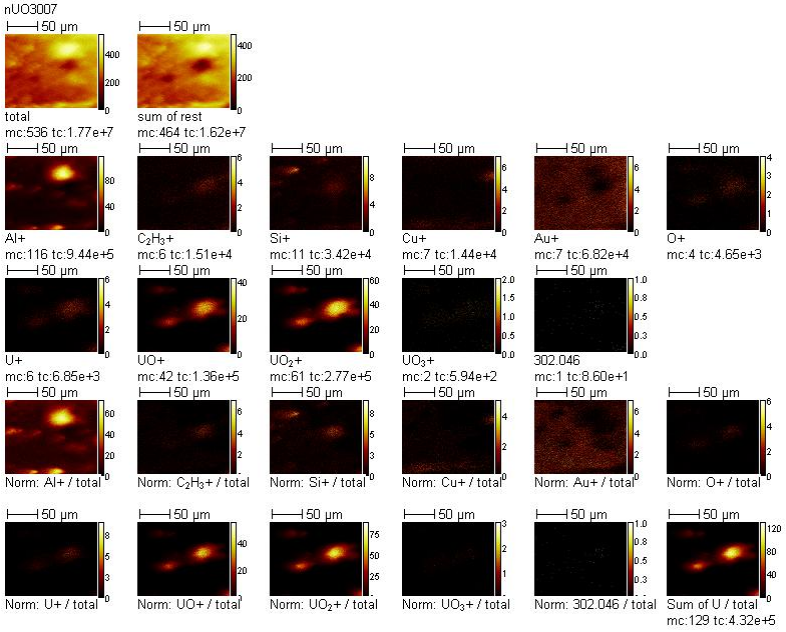

nUO3002
50 µm
total
mc:1966 tc:6.54e+7
sum of rest
mc:1813 tc:6.00e+7
Al-
mc:2 tc:7.21e+2
C2H3-
mc:11 tc:9.69e+4
Si-
mc:7 tc:4.04e+4
Cu-
mc:3 tc:8.61e+3
Au-
mc:94 tc:2.74e+6
O-
mc:81 tc:2.52e+6
U-
mc:3 tc:3.90e+3
UO-
mc:2 tc:1.19e+3
UO2-
mc:5 tc:3.10e+3
UO3-
mc:14 tc:2.43e+4
302.026
mc:5 tc:6.35e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.026 / total
Sum of U / total
mc:20 tc:2.73e+4

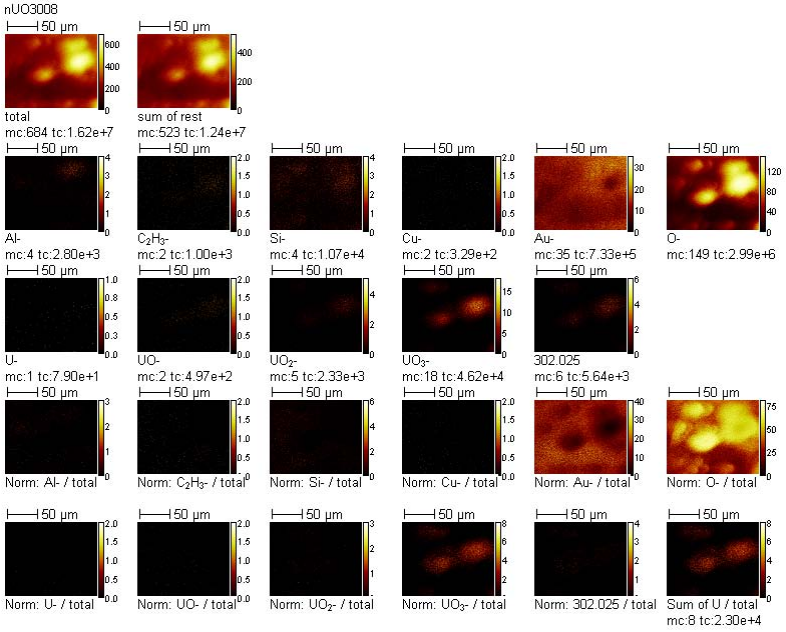

nUO3003
50 µm
total
mc:2318 tc:2.41e+7
sum of rest
mc:2241 tc:2.26e+7
Al+
mc:93 tc:7.85e+5
C2H3+
mc:38 tc:1.50e+5
Si+
mc:18 tc:6.06e+4
Cu+
mc:11 tc:4.48e+4
Au+
mc:7 tc:4.89e+4
O+
mc:3 tc:1.96e+3
U+
mc:11 tc:6.96e+3
UO+
mc:46 tc:7.71e+4
UO2+
mc:47 tc:1.28e+5
UO3+
mc:3 tc:8.95e+2
302.059
mc:2 tc:5.62e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.059 / total
Sum of U / total
mc:83 tc:1.88e+5

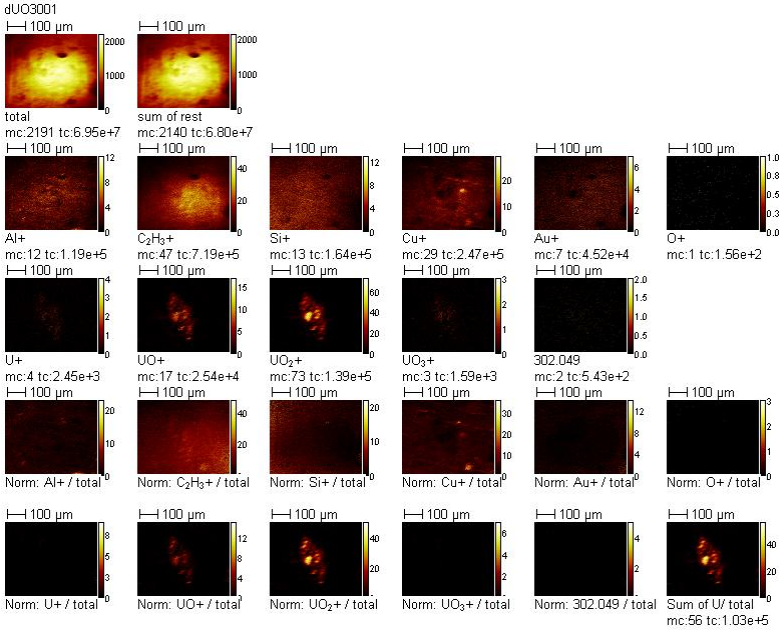

nUO3004
50 µm
total
mc:1611 tc:2.03e+7
sum of rest
mc:1483 tc:1.76e+7
Al-
mc:3 tc:1.88e+3
C2H3-
mc:8 tc:1.26e+4
Si-
mc:6 tc:1.20e+4
Cu-
mc:2 tc:1.06e+3
Au-
mc:79 tc:8.75e+5
O-
mc:100 tc:1.82e+6
U-
mc:2 tc:4.46e+2
UO-
mc:2 tc:3.90e+2
UO2-
mc:6 tc:2.41e+3
UO3-
mc:12 tc:1.54e+4
302.022
mc:4 tc:2.37e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.022 / total
Sum of U / total
mc:9 tc:9.07e+3

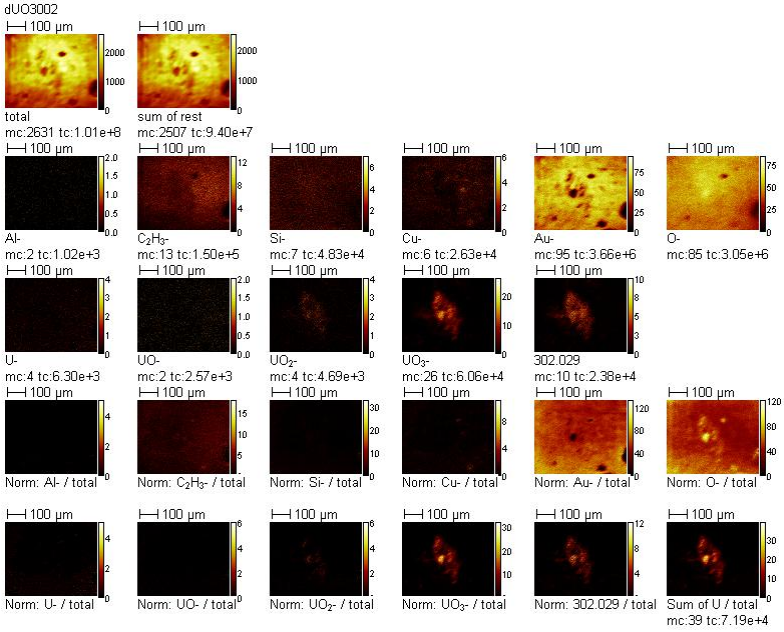

nUO3005
50 µm
total
mc:639 tc:2.25e+7
sum of rest
mc:592 tc:2.02e+7
Al+
mc:117 tc:1.19e+6
C2H3+
mc:20 tc:6.31e+4
Si+
mc:19 tc:1.08e+5
Cu+
mc:10 tc:3.16e+4
Au+
mc:8 tc:6.45e+4
O+
mc:5 tc:8.20e+3
U+
mc:7 tc:8.96e+3
UO+
mc:59 tc:2.17e+5
UO2+
mc:104 tc:5.93e+5
UO3+
mc:2 tc:1.16e+3
302.051
mc:2 tc:2.40e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.051 / total
Sum of U / total
mc:118 tc:6.91e+5

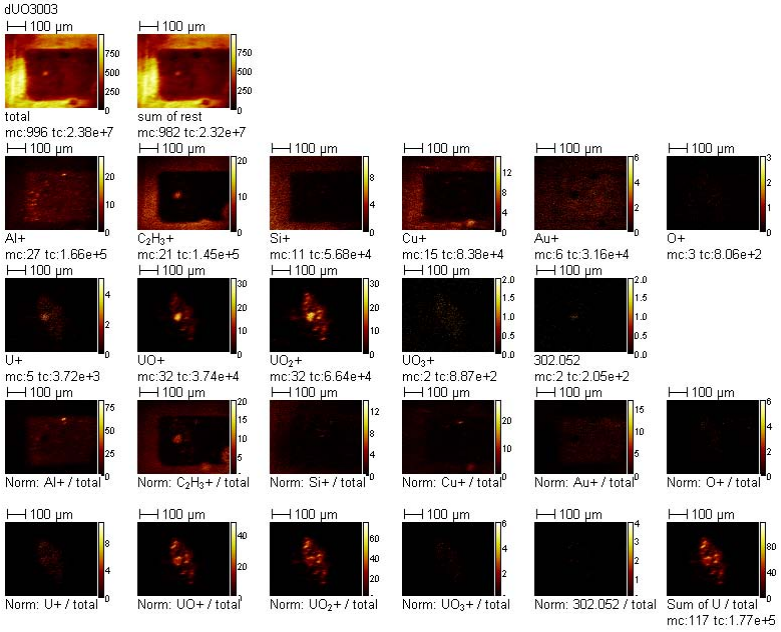

nUO3006
50 µm
total
mc:737 tc:2.07e+7
sum of rest
mc:596 tc:1.65e+7
Al-
mc:4 tc:3.25e+3
C2H3-
mc:3 tc:3.47e+3
Si-
mc:7 tc:1.82e+4
Cu-
mc:2 tc:5.90e+2
Au-
mc:36 tc:8.52e+5
O-
mc:138 tc:3.31e+6
U-
mc:2 tc:2.04e+2
UO-
mc:2 tc:2.96e+2
UO2-
mc:4 tc:1.64e+3
UO3-
mc:12 tc:3.59e+4
302.027
mc:7 tc:1.26e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.027 / total
Sum of U / total
mc:9 tc:2.81e+4

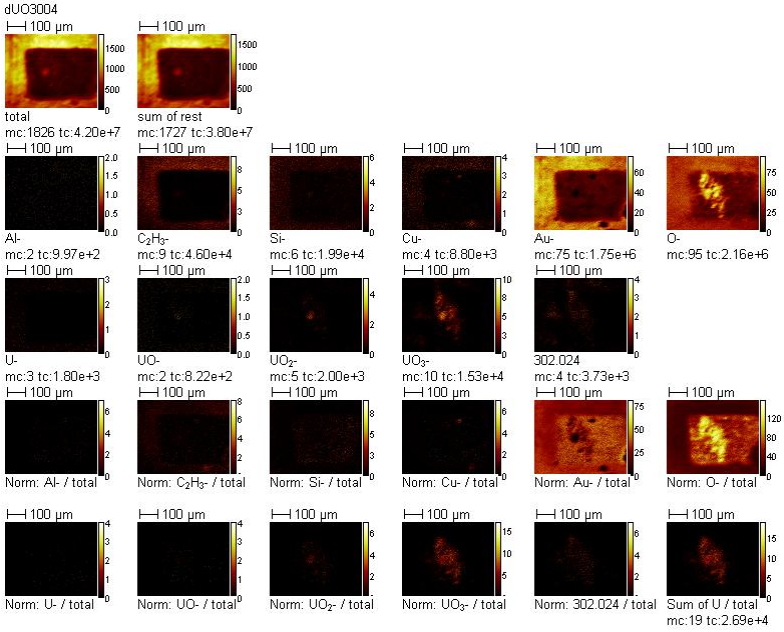

nUO3007
50 µm
total
mc:536 tc:1.77e+7
sum of rest
mc:464 tc:1.62e+7
Al+
mc:116 tc:9.44e+5
C2H3+
mc:6 tc:1.51e+4
Si+
mc:11 tc:3.42e+4
Cu+
mc:7 tc:1.44e+4
Au+
mc:7 tc:6.82e+4
O+
mc:4 tc:4.65e+3
U+
mc:6 tc:6.85e+3
UO+
mc:42 tc:1.36e+5
UO2+
mc:61 tc:2.77e+5
UO3+
mc:2 tc:5.94e+2
302.046
mc:1 tc:8.60e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.046 / total
Sum of U / total
mc:129 tc:4.32e+5

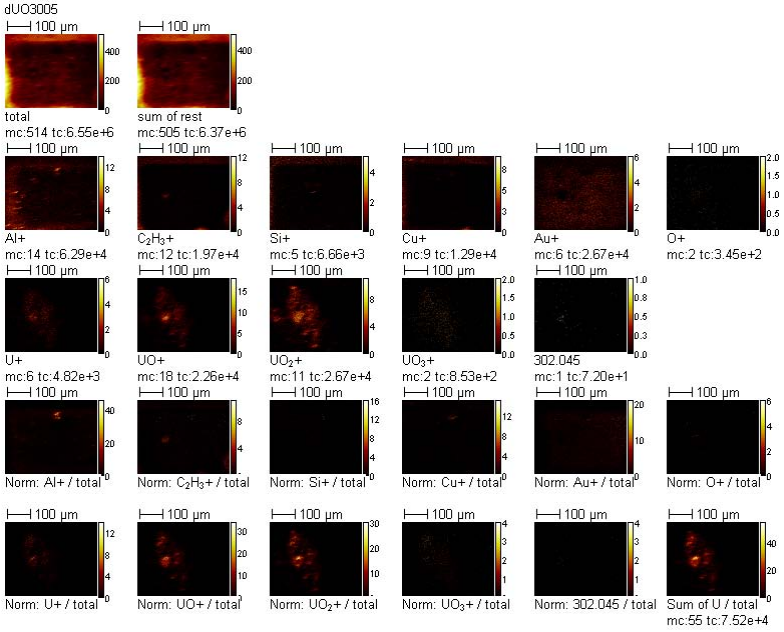

nUO3008
50 µm
total
mc:684 tc:1.62e+7
sum of rest
mc:523 tc:1.24e+7
Al-
mc:4 tc:2.80e+3
C2H3-
mc:2 tc:1.00e+3
Si-
mc:4 tc:1.07e+4
Cu-
mc:2 tc:3.29e+2
Au-
mc:35 tc:7.33e+5
O-
mc:149 tc:2.99e+6
U-
mc:1 tc:7.90e+1
UO-
mc:2 tc:4.97e+2
UO2-
mc:5 tc:2.33e+3
UO3-
mc:18 tc:4.62e+4
302.025
mc:6 tc:5.64e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.025 / total
Sum of U / total
mc:8 tc:2.30e+4

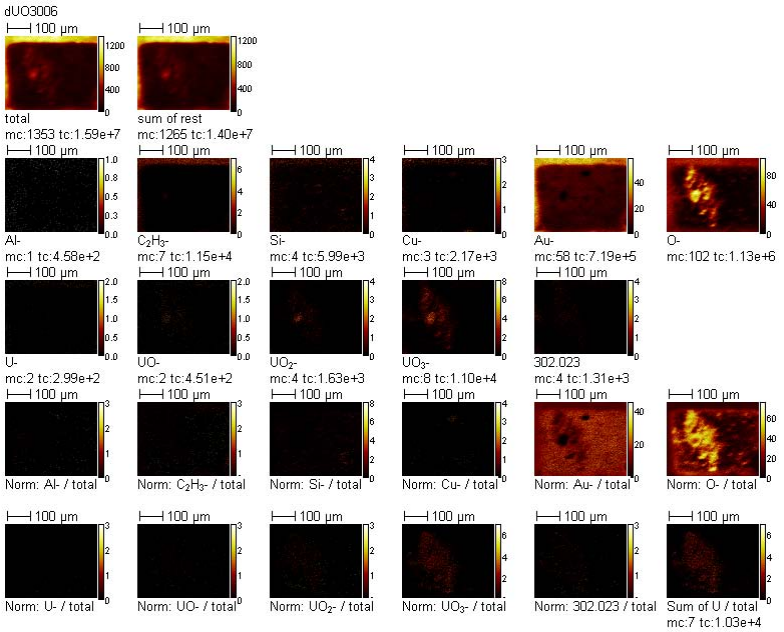

dUO3001
100 µm
total
mc:2191 tc:6.95e+7
sum of rest
mc:2140 tc:6.80e+7
Al+
mc:12 tc:1.19e+5
C2H3+
mc:47 tc:7.19e+5
Si+
mc:13 tc:1.64e+5
Cu+
mc:29 tc:2.47e+5
Au+
mc:7 tc:4.52e+4
O+
mc:1 tc:1.56e+2
U+
mc:4 tc:2.45e+3
UO+
mc:17 tc:2.54e+4
UO2+
mc:73 tc:1.39e+5
UO3+
mc:3 tc:1.59e+3
302.049
mc:2 tc:5.43e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.049 / total
Sum of U/ total
mc:56 tc:1.03e+5

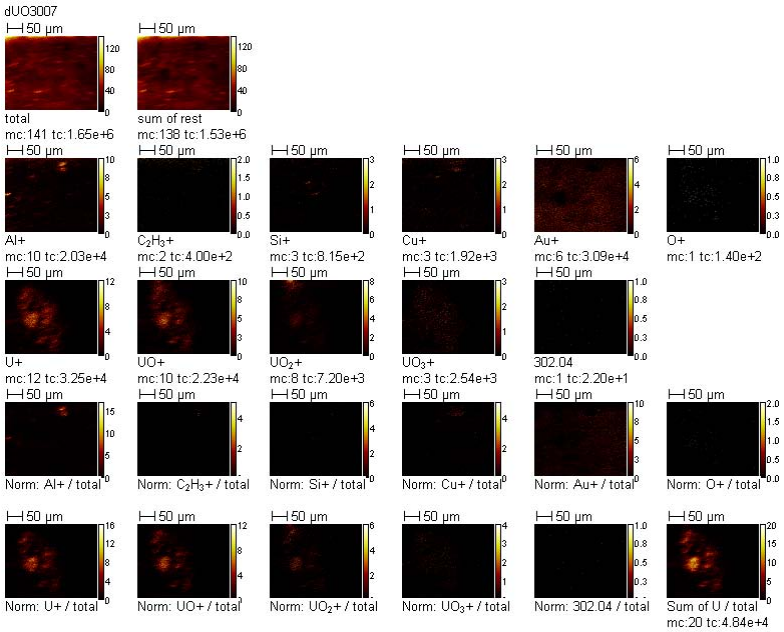

dUO3002
100 µm
total
mc:2631 tc:1.01e+8
sum of rest
mc:2507 tc:9.40e+7
Al-
mc:2 tc:1.02e+3
C2H3-
mc:13 tc:1.50e+5
Si-
mc:7 tc:4.83e+4
Cu-
mc:6 tc:2.63e+4
Au-
mc:95 tc:3.66e+6
O-
mc:85 tc:3.05e+6
U-
mc:4 tc:6.30e+3
UO-
mc:2 tc:2.57e+3
UO2-
mc:4 tc:4.69e+3
UO3-
mc:26 tc:6.06e+4
302.029
mc:10 tc:2.38e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.029 / total
Sum of U / total
mc:39 tc:7.19e+4

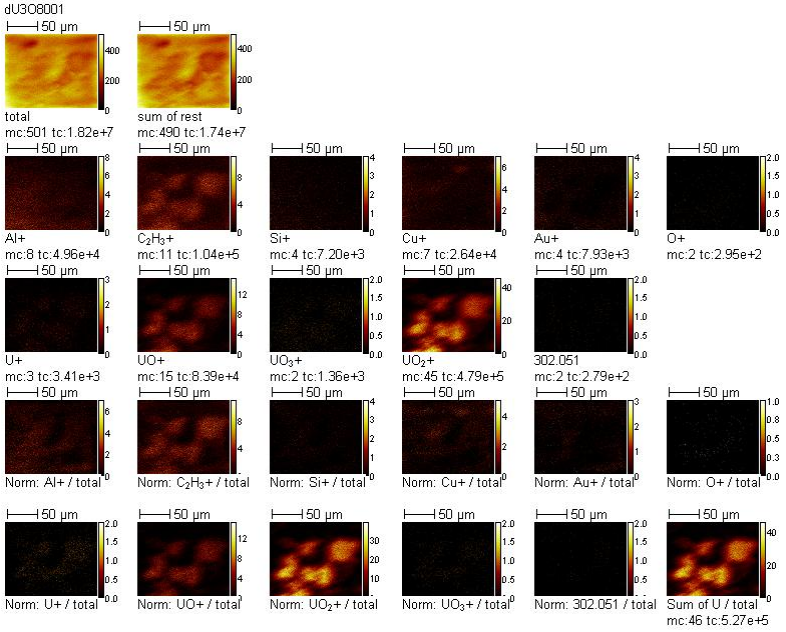

dUO3003
100 µm
total
mc:996 tc:2.38e+7
sum of rest
mc:982 tc:2.32e+7
Al+
mc:27 tc:1.66e+5
C2H3+
mc:21 tc:1.45e+5
Si+
mc:11 tc:5.68e+4
Cu+
mc:15 tc:8.38e+4
Au+
mc:6 tc:3.16e+4
O+
mc:3 tc:8.06e+2
U+
mc:5 tc:3.72e+3
UO+
mc:32 tc:3.74e+4
UO2+
mc:32 tc:6.64e+4
UO3+
mc:2 tc:8.87e+2
302.052
mc:2 tc:2.05e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.052 / total
Sum of U / total
mc:117 tc:1.77e+5

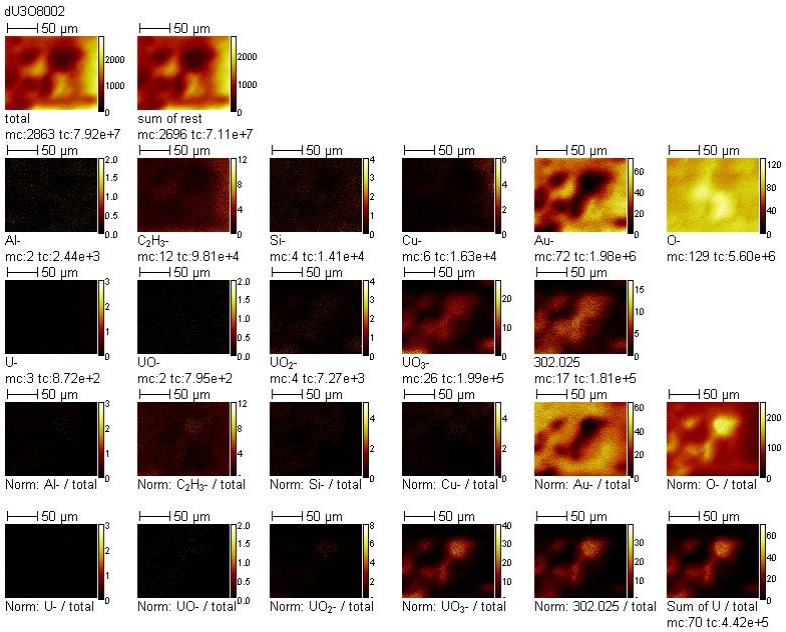

dUO3004
100 µm
total
mc:1826 tc:4.20e+7
sum of rest
mc:1727 tc:3.80e+7
Al-
mc:2 tc:9.97e+2
C2H3-
mc:9 tc:4.60e+4
Si-
mc:6 tc:1.99e+4
Cu-
mc:4 tc:8.80e+3
Au-
mc:75 tc:1.75e+6
O-
mc:95 tc:2.16e+6
U-
mc:3 tc:1.80e+3
UO-
mc:2 tc:8.22e+2
UO2-
mc:5 tc:2.00e+3
UO3-
mc:10 tc:1.53e+4
302.024
mc:4 tc:3.73e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.024 / total
Sum of U / total
mc:19 tc:2.69e+4

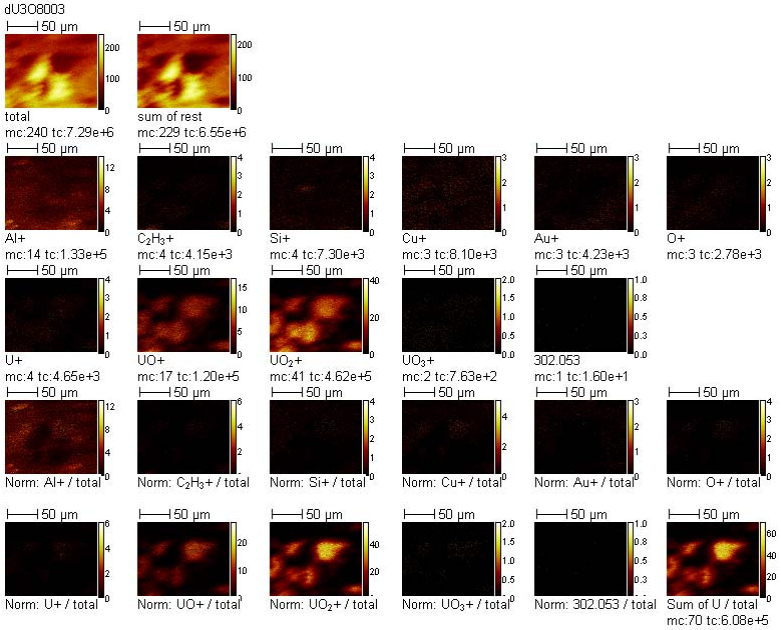

dUO3005
100 µm
total
mc:514 tc:6.55e+6
sum of rest
mc:505 tc:6.37e+6
Al+
mc:14 tc:6.29e+4
C2H3+
mc:12 tc:1.97e+4
Si+
mc:5 tc:6.66e+3
Cu+
mc:9 tc:1.29e+4
Au+
mc:6 tc:2.67e+4
O+
mc:2 tc:3.45e+2
U+
mc:6 tc:4.82e+3
UO+
mc:18 tc:2.26e+4
UO2+
mc:11 tc:2.67e+4
UO3+
mc:2 tc:8.53e+2
302.045
mc:1 tc:7.20e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.045 / total
Sum of U / total
mc:55 tc:7.52e+4

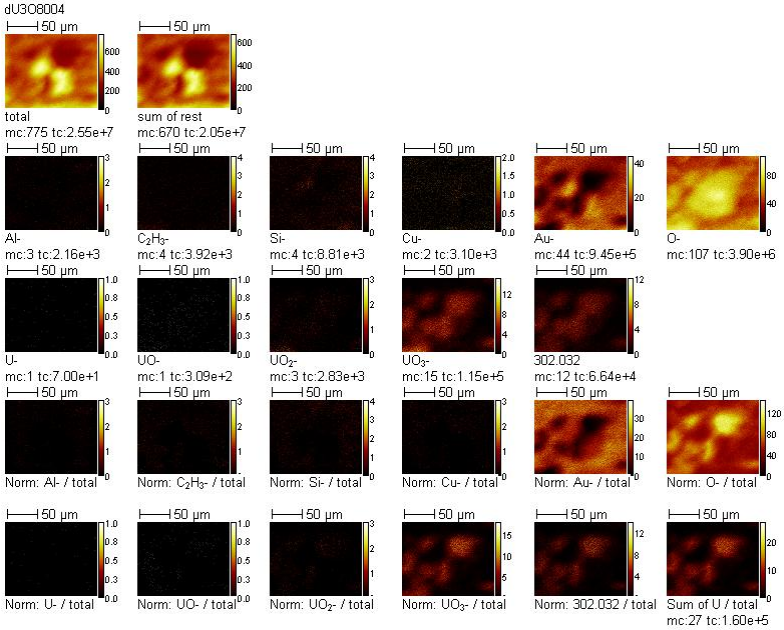

dUO3006
100 µm
total
mc:1353 tc:1.59e+7
sum of rest
mc:1265 tc:1.40e+7
Al-
mc:1 tc:4.58e+2
C2H3-
mc:7 tc:1.15e+4
Si-
mc:4 tc:5.99e+3
Cu-
mc:3 tc:2.17e+3
Au-
mc:58 tc:7.19e+5
O-
mc:102 tc:1.13e+6
U-
mc:2 tc:2.99e+2
UO-
mc:2 tc:4.51e+2
UO2-
mc:4 tc:1.63e+3
UO3-
mc:8 tc:1.10e+4
302.023
mc:4 tc:1.31e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.023 / total
Sum of U / total
mc:7 tc:1.03e+4

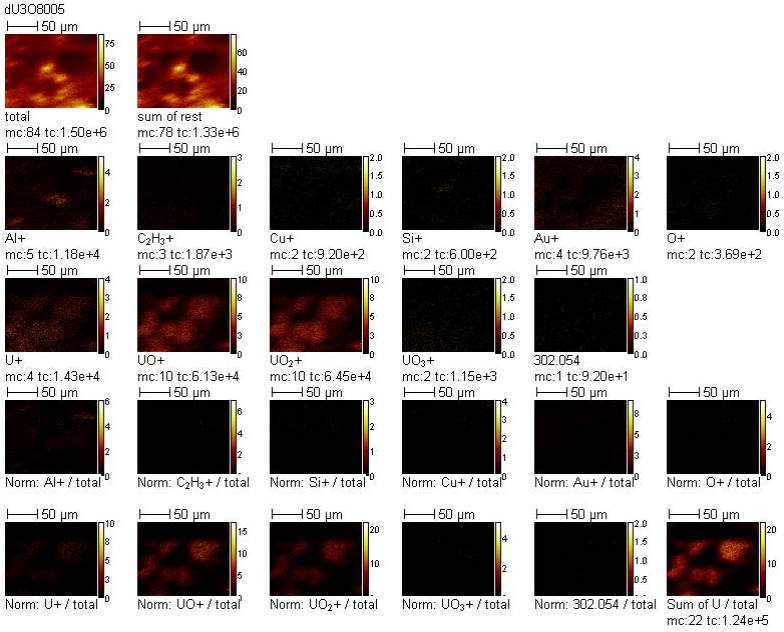

dUO3007
50 µm
total
mc:141 tc:1.65e+6
50 µm
sum of rest
mc:138 tc:1.53e+6
50 µm
Al+
mc:10 tc:2.03e+4
50 µm
C2H3+
mc:2 tc:4.00e+2
50 µm
Si+
mc:3 tc:8.15e+2
50 µm
Cu+
mc:3 tc:1.92e+3
50 µm
Au+
mc:6 tc:3.09e+4
50 µm
O+
mc:1 tc:1.40e+2
50 µm
U+
mc:12 tc:3.25e+4
50 µm
UO+
mc:10 tc:2.23e+4
50 µm
UO2+
mc:8 tc:7.20e+3
50 µm
UO3+
mc:3 tc:2.54e+3
50 µm
302.04
mc:1 tc:2.20e+1
50 µm
Norm: Al+ / total
50 µm
Norm: C2H3+ / total
50 µm
Norm: Si+ / total
50 µm
Norm: Cu+ / total
50 µm
Norm: Au+ / total
50 µm
Norm: O+ / total
50 µm
Norm: U+ / total
50 µm
Norm: UO+ / total
50 µm
Norm: UO2+ / total
50 µm
Norm: UO3+ / total
50 µm
Norm: 302.04 / total
50 µm
Sum of U / total
mc:20 tc:4.84e+4

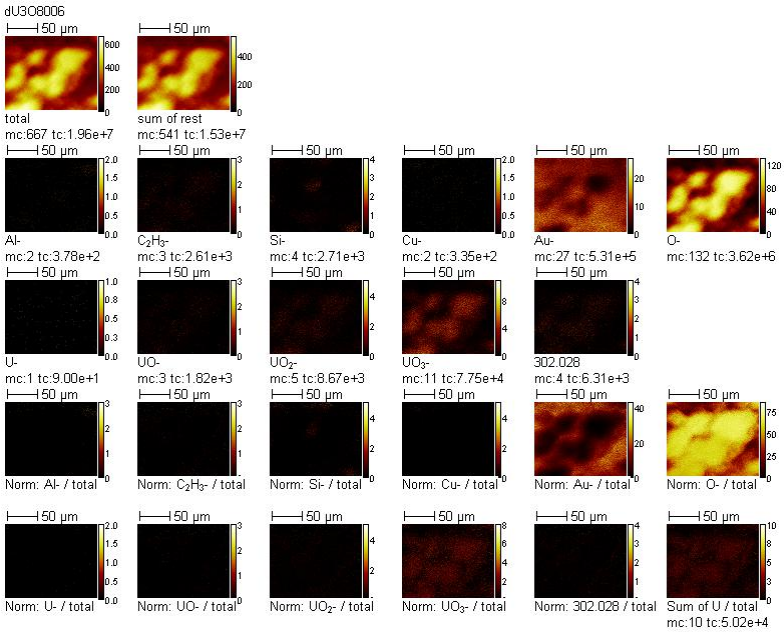

dU3O8001
50 µm
total
mc:501 tc:1.82e+7
sum of rest
mc:490 tc:1.74e+7
Al+
mc:8 tc:4.96e+4
C2H3+
mc:11 tc:1.04e+5
Si+
mc:4 tc:7.20e+3
Cu+
mc:7 tc:2.64e+4
Au+
mc:4 tc:7.93e+3
O+
mc:2 tc:2.95e+2
U+
mc:3 tc:3.41e+3
UO+
mc:15 tc:8.39e+4
UO3+
mc:2 tc:1.36e+3
UO2+
mc:45 tc:4.79e+5
302.051
mc:2 tc:2.79e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.051 / total
Sum of U / total
mc:46 tc:5.27e+5

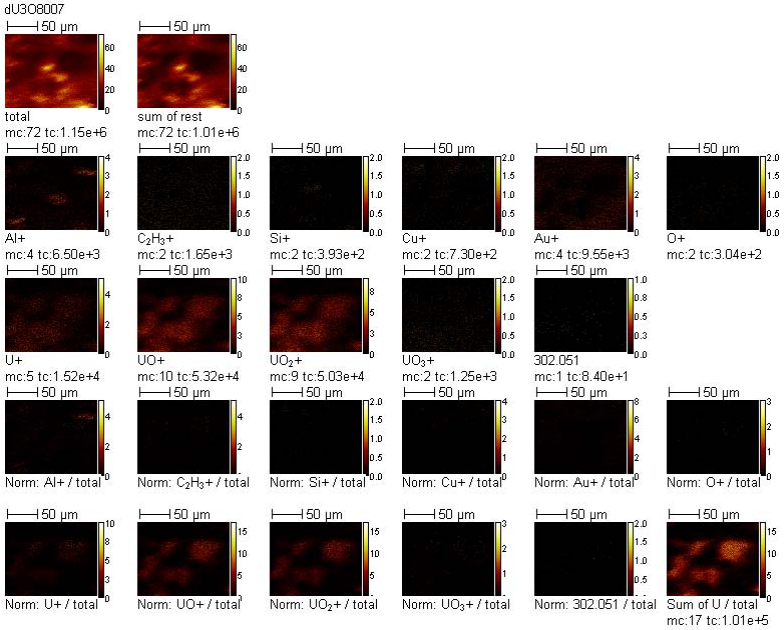

dU3O8002
50 µm
total
mc:2863 tc:7.92e+7
sum of rest
mc:2696 tc:7.11e+7
Al-
mc:2 tc:2.44e+3
C2H3-
mc:12 tc:9.81e+4
Si-
mc:4 tc:1.41e+4
Cu-
mc:6 tc:1.63e+4
Au-
mc:72 tc:1.98e+6
O-
mc:129 tc:5.60e+6
U-
mc:3 tc:8.72e+2
UO-
mc:2 tc:7.95e+2
UO2-
mc:4 tc:7.27e+3
UO3-
mc:26 tc:1.99e+5
302.025
mc:17 tc:1.81e+5
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.025 / total
Sum of U / total
mc:70 tc:4.42e+5

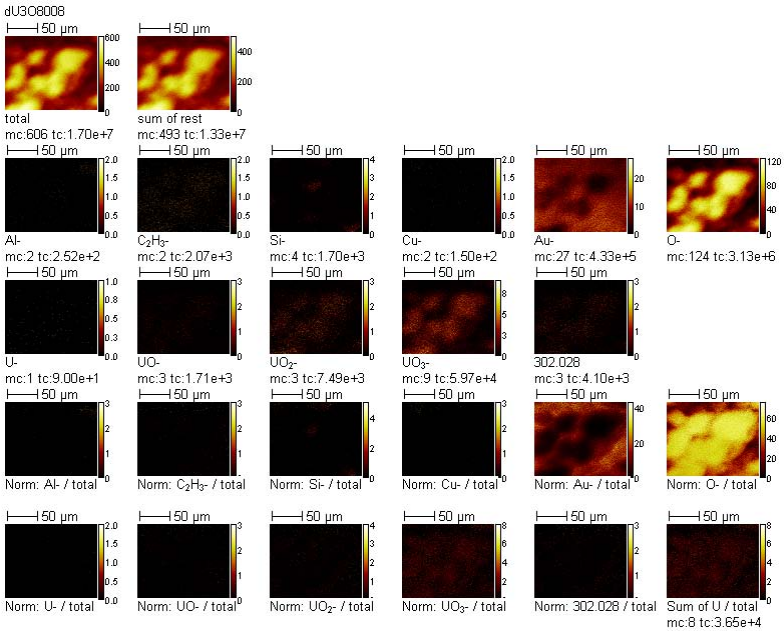

dU3O8003
50 µm
total
mc:240 tc:7.29e+6
sum of rest
mc:229 tc:6.55e+6
Al+
mc:14 tc:1.33e+5
C2H3+
mc:4 tc:4.15e+3
Si+
mc:4 tc:7.30e+3
Cu+
mc:3 tc:8.10e+3
Au+
mc:3 tc:4.23e+3
O+
mc:3 tc:2.78e+3
U+
mc:4 tc:4.65e+3
UO+
mc:17 tc:1.20e+5
UO2+
mc:41 tc:4.62e+5
UO3+
mc:2 tc:7.63e+2
302.053
mc:1 tc:1.60e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.053 / total
Sum of U / total
mc:70 tc:6.08e+5

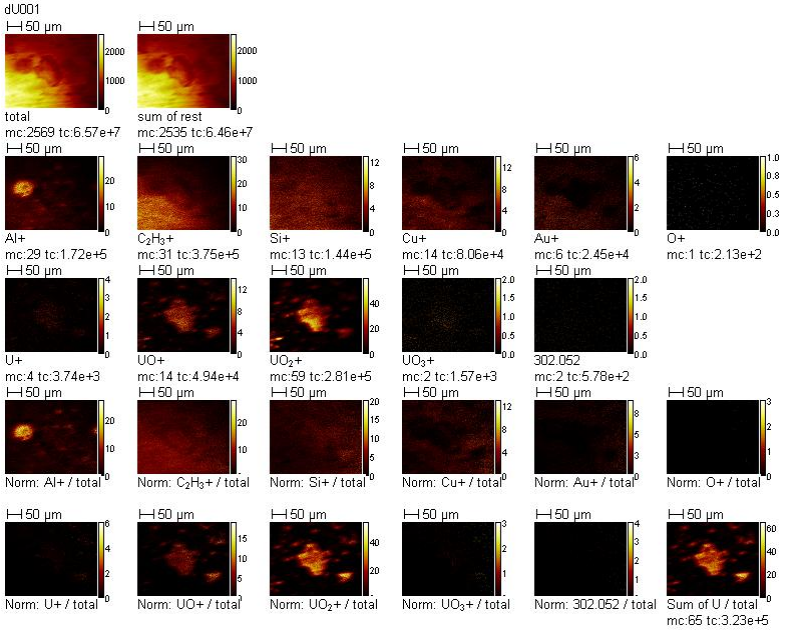

dU3O8004
50 µm
total
mc:775 tc:2.55e+7
sum of rest
mc:670 tc:2.05e+7
Al-
mc:3 tc:2.16e+3
C2H3-
mc:4 tc:3.92e+3
Si-
mc:4 tc:8.81e+3
Cu-
mc:2 tc:3.10e+3
Au-
mc:44 tc:9.45e+5
O-
mc:107 tc:3.90e+6
U-
mc:1 tc:7.00e+1
UO-
mc:1 tc:3.09e+2
UO2-
mc:3 tc:2.83e+3
UO3-
mc:15 tc:1.15e+5
302.032
mc:12 tc:6.64e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.032 / total
Sum of U / total
mc:27 tc:1.60e+5

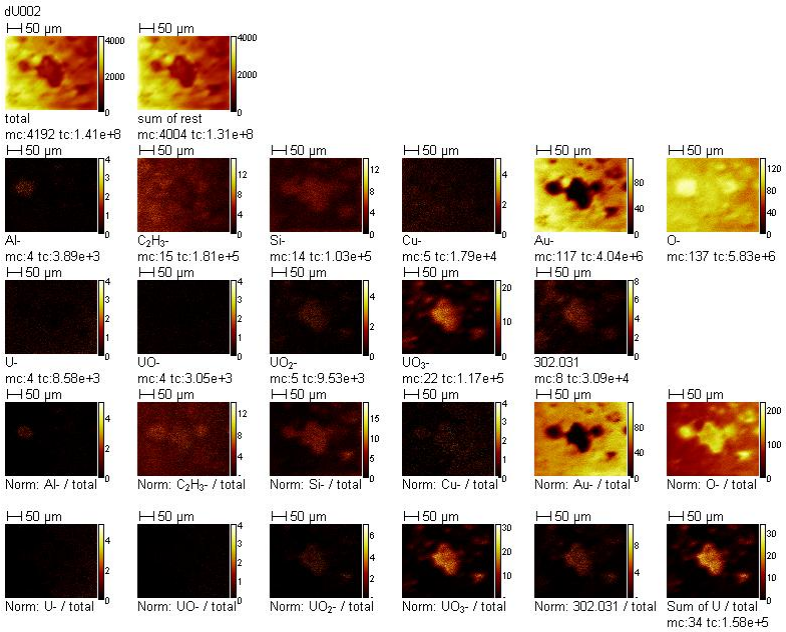

dU3O8005
50 µm
total
mc:84 tc:1.50e+6
sum of rest
mc:78 tc:1.33e+6
Al+
mc:5 tc:1.18e+4
C2H3+
mc:3 tc:1.87e+3
Cu+
mc:2 tc:9.20e+2
Si+
mc:2 tc:6.00e+2
Au+
mc:4 tc:9.76e+3
O+
mc:2 tc:3.69e+2
U+
mc:4 tc:1.43e+4
UO+
mc:10 tc:6.13e+4
UO2+
mc:10 tc:6.45e+4
UO3+
mc:2 tc:1.15e+3
302.054
mc:1 tc:9.20e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.054 / total
Sum of U / total
mc:22 tc:1.24e+5

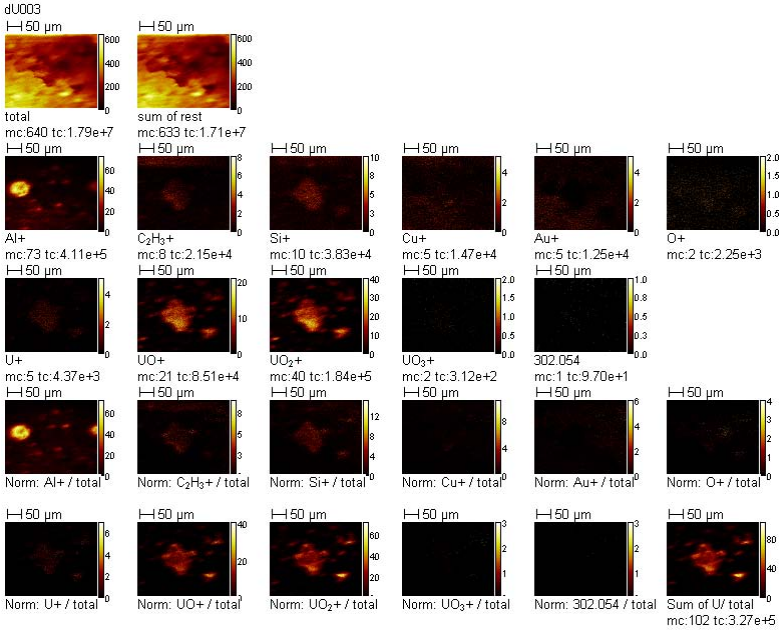

dU3O8006
50 µm
total
mc:667 tc:1.96e+7
sum of rest
mc:541 tc:1.53e+7
Al-
mc:2 tc:3.78e+2
C2H3-
mc:3 tc:2.61e+3
Si-
mc:4 tc:2.71e+3
Cu-
mc:2 tc:3.35e+2
Au-
mc:27 tc:5.31e+5
O-
mc:132 tc:3.62e+6
U-
mc:1 tc:9.00e+1
UO-
mc:3 tc:1.82e+3
UO2-
mc:5 tc:8.67e+3
UO3-
mc:11 tc:7.75e+4
302.028
mc:4 tc:6.31e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.028 / total
Sum of U / total
mc:10 tc:5.02e+4

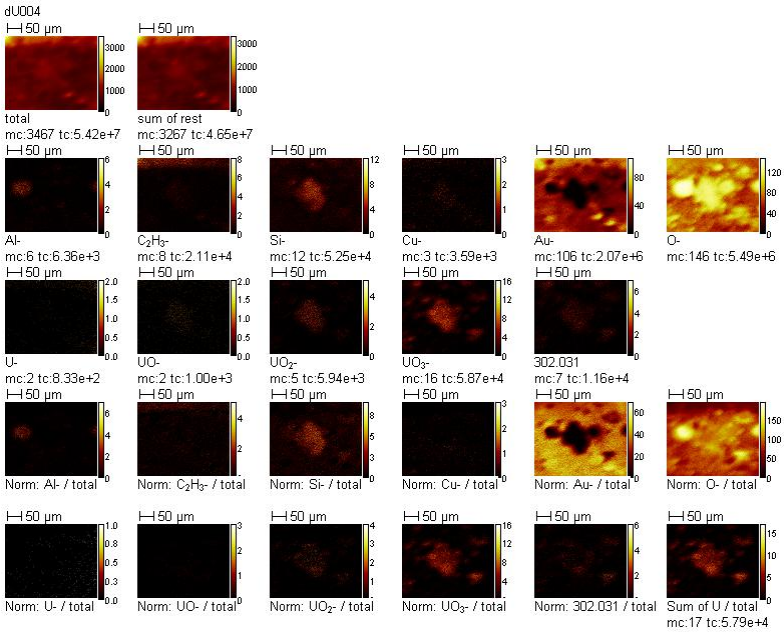

dU3O8007
50 µm
total
mc:72 tc:1.15e+6
sum of rest
mc:72 tc:1.01e+6
Al+
mc:4 tc:6.50e+3
C2H3+
mc:2 tc:1.65e+3
Si+
mc:2 tc:3.93e+2
Cu+
mc:2 tc:7.30e+2
Au+
mc:4 tc:9.55e+3
O+
mc:2 tc:3.04e+2
U+
mc:5 tc:1.52e+4
UO+
mc:10 tc:5.32e+4
UO2+
mc:9 tc:5.03e+4
UO3+
mc:2 tc:1.25e+3
302.051
mc:1 tc:8.40e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.051 / total
Sum of U / total
mc:17 tc:1.01e+5

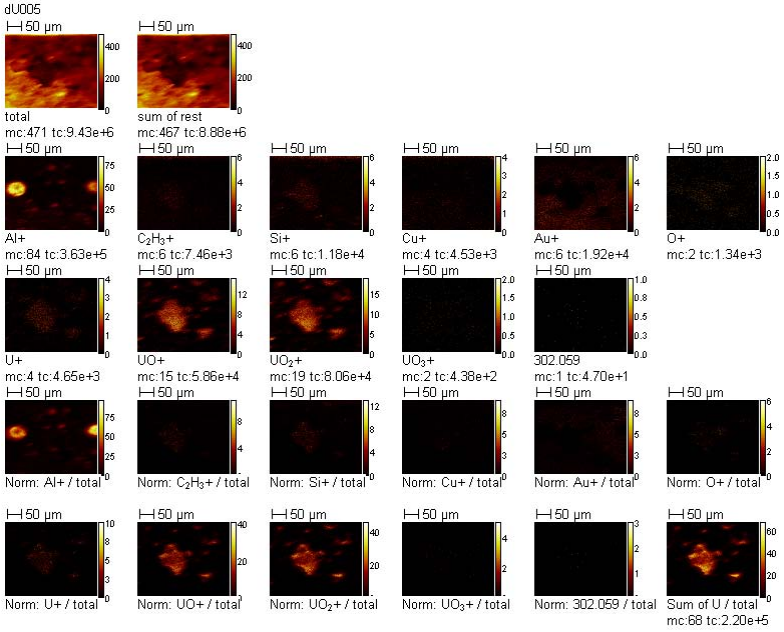

dU3O8008
50 µm
total
mc:606 tc:1.70e+7
sum of rest
mc:493 tc:1.33e+7
Al-
mc:2 tc:2.52e+2
C2H3-
mc:2 tc:2.07e+3
Si-
mc:4 tc:1.70e+3
Cu-
mc:2 tc:1.50e+2
Au-
mc:27 tc:4.33e+5
O-
mc:124 tc:3.13e+6
U-
mc:1 tc:9.00e+1
UO-
mc:3 tc:1.71e+3
UO2-
mc:3 tc:7.49e+3
UO3-
mc:9 tc:5.97e+4
302.028
mc:3 tc:4.10e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.028 / total
Sum of U / total
mc:8 tc:3.65e+4

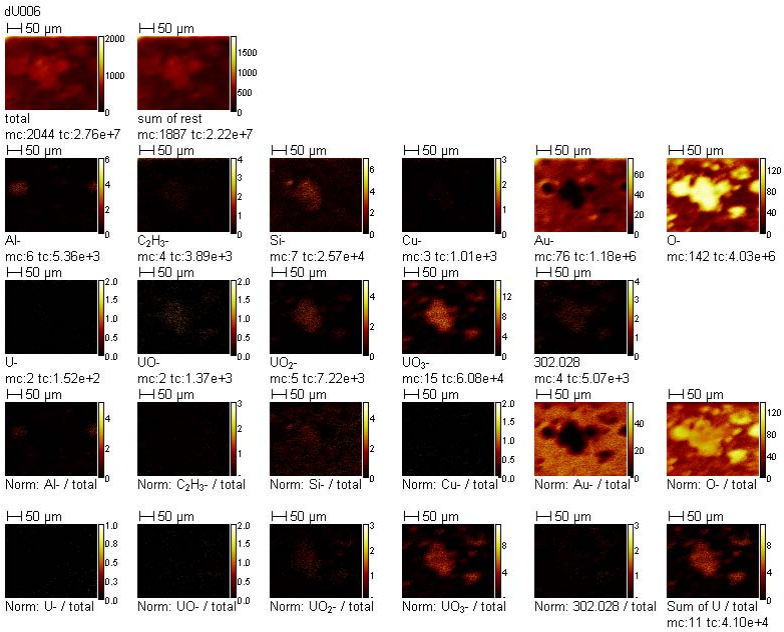

dU001
50 µm
total
mc:2569 tc:6.57e+7
sum of rest
mc:2535 tc:6.46e+7
Al+
mc:29 tc:1.72e+5
C2H3+
mc:31 tc:3.75e+5
Si+
mc:13 tc:1.44e+5
Cu+
mc:14 tc:8.06e+4
Au+
mc:6 tc:2.45e+4
O+
mc:1 tc:2.13e+2
U+
mc:4 tc:3.74e+3
UO+
mc:14 tc:4.94e+4
UO2+
mc:59 tc:2.81e+5
UO3+
mc:2 tc:1.57e+3
302.052
mc:2 tc:5.78e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.052 / total
Sum of U / total
mc:65 tc:3.23e+5

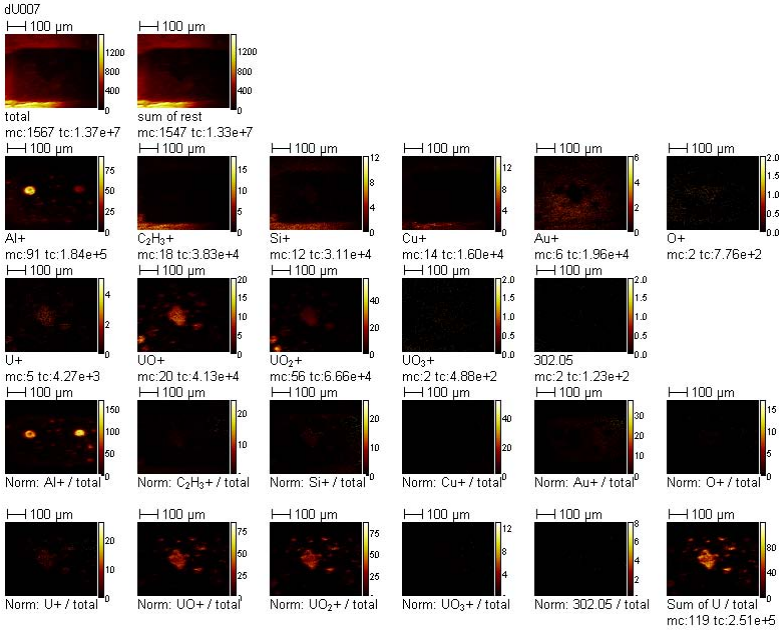

dU002
50 µm
total
mc:4192 tc:1.41e+8
sum of rest
mc:4004 tc:1.31e+8
Al-
mc:4 tc:3.89e+3
C2H3-
mc:15 tc:1.81e+5
Si-
mc:14 tc:1.03e+5
Cu-
mc:5 tc:1.79e+4
Au-
mc:117 tc:4.04e+6
O-
mc:137 tc:5.83e+6
U-
mc:4 tc:8.58e+3
UO-
mc:4 tc:3.05e+3
UO2-
mc:5 tc:9.53e+3
UO3-
mc:22 tc:1.17e+5
302.031
mc:8 tc:3.09e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.031 / total
Sum of U / total
mc:34 tc:1.58e+5

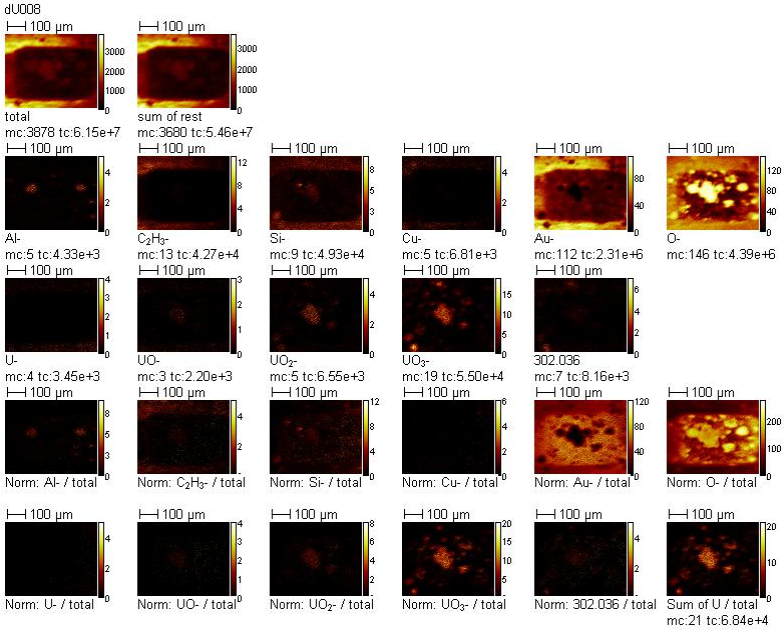

dU003
50 µm
total
mc:640 tc:1.79e+7
sum of rest
mc:633 tc:1.71e+7
Al+
mc:73 tc:4.11e+5
C2H3+
mc:8 tc:2.15e+4
Si+
mc:10 tc:3.83e+4
Cu+
mc:5 tc:1.47e+4
Au+
mc:5 tc:1.25e+4
O+
mc:2 tc:2.25e+3
U+
mc:5 tc:4.37e+3
UO+
mc:21 tc:8.51e+4
UO2+
mc:40 tc:1.84e+5
UO3+
mc:2 tc:3.12e+2
302.054
mc:1 tc:9.70e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.054 / total
Sum of U/ total
mc:102 tc:3.27e+5

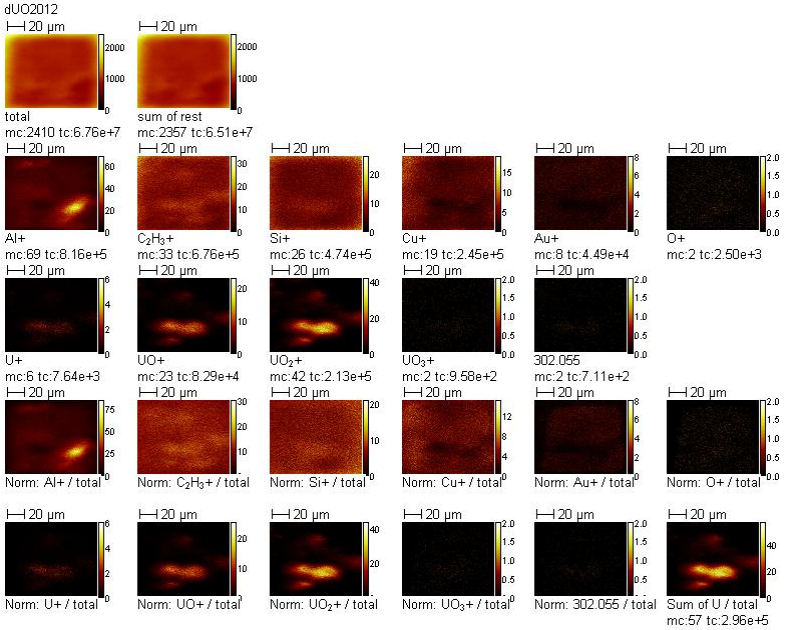

dU004
50 µm
total
mc:3467 tc:5.42e+7
sum of rest
mc:3267 tc:4.65e+7
Al-
mc:6 tc:6.36e+3
C2H3-
mc:8 tc:2.11e+4
Si-
mc:12 tc:5.25e+4
Cu-
mc:3 tc:3.59e+3
Au-
mc:106 tc:2.07e+6
O-
mc:146 tc:5.49e+6
U-
mc:2 tc:8.33e+2
UO-
mc:2 tc:1.00e+3
UO2-
mc:5 tc:5.94e+3
UO3-
mc:16 tc:5.87e+4
302.031
mc:7 tc:1.16e+4
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.031 / total
Sum of U / total
mc:17 tc:5.79e+4

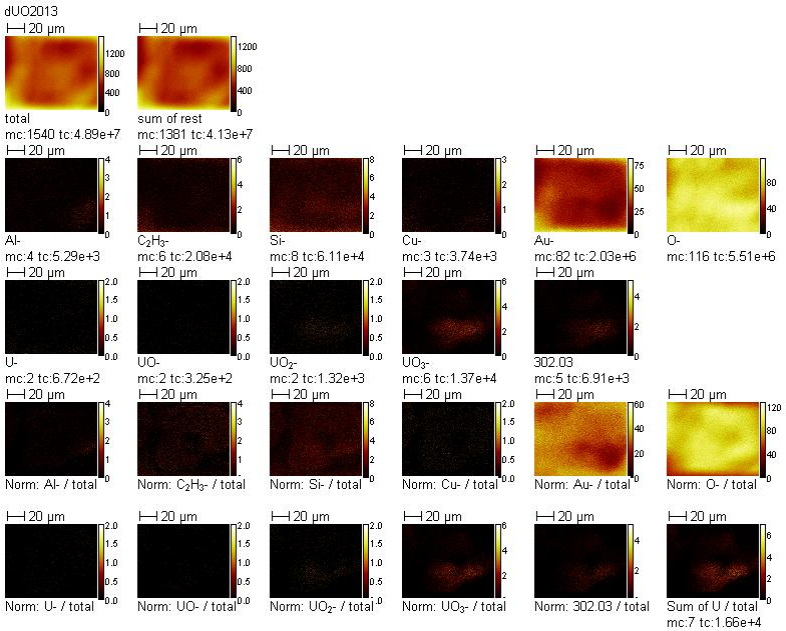

dU005
50 µm
total
mc:471 tc:9.43e+6
sum of rest
mc:467 tc:8.88e+6
Al+
mc:84 tc:3.63e+5
C2H3+
mc:6 tc:7.46e+3
Si+
mc:6 tc:1.18e+4
Cu+
mc:4 tc:4.53e+3
Au+
mc:6 tc:1.92e+4
O+
mc:2 tc:1.34e+3
U+
mc:4 tc:4.65e+3
UO+
mc:15 tc:5.86e+4
UO2+
mc:19 tc:8.06e+4
UO3+
mc:2 tc:4.38e+2
302.059
mc:1 tc:4.70e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.059 / total
Sum of U / total
mc:68 tc:2.20e+5

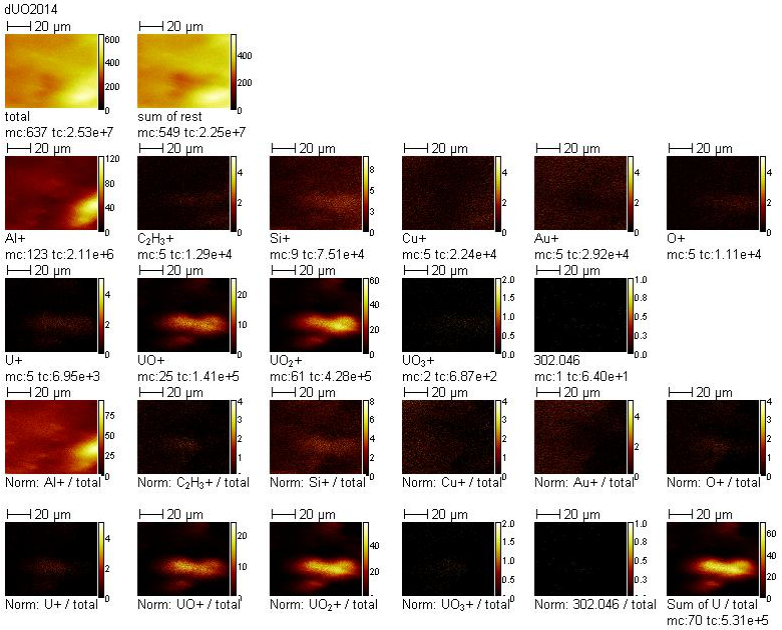

dU006
50 µm
total
mc:2044 tc:2.76e+7
sum of rest
mc:1887 tc:2.22e+7
Al-
mc:6 tc:5.36e+3
C2H3-
mc:4 tc:3.89e+3
Si-
mc:7 tc:2.57e+4
Cu-
mc:3 tc:1.01e+3
Au-
mc:76 tc:1.18e+6
O-
mc:142 tc:4.03e+6
U-
mc:2 tc:1.52e+2
UO-
mc:2 tc:1.37e+3
UO2-
mc:5 tc:7.22e+3
UO3-
mc:15 tc:6.08e+4
302.028
mc:4 tc:5.07e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.028 / total
Sum of U / total
mc:11 tc:4.10e+4

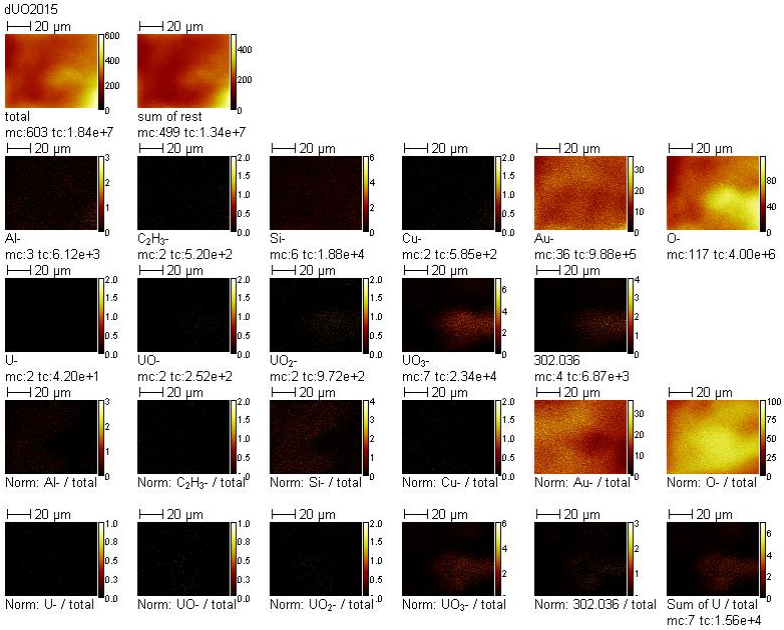

dU007
100 µm
total
mc:1567 tc:1.37e+7
sum of rest
mc:1547 tc:1.33e+7
Al+
mc:91 tc:1.84e+5
C2H3+
mc:18 tc:3.83e+4
Si+
mc:12 tc:3.11e+4
Cu+
mc:14 tc:1.60e+4
Au+
mc:6 tc:1.96e+4
O+
mc:2 tc:7.76e+2
U+
mc:5 tc:4.27e+3
UO+
mc:20 tc:4.13e+4
UO2+
mc:56 tc:6.66e+4
UO3+
mc:2 tc:4.88e+2
302.05
mc:2 tc:1.23e+2
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.05 / total
Sum of U / total
mc:119 tc:2.51e+5

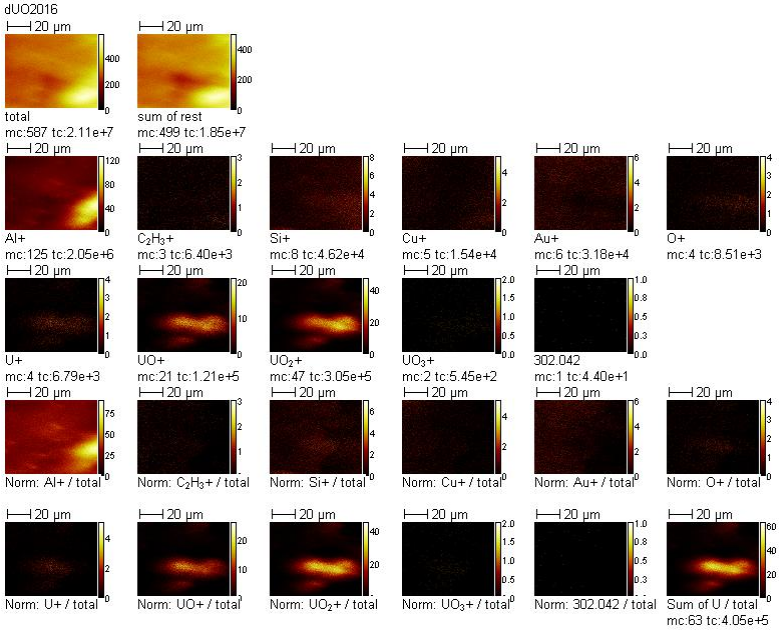

dU008
100 µm
total
mc:3878 tc:6.15e+7
sum of rest
mc:3680 tc:5.46e+7
Al-
mc:5 tc:4.33e+3
C2H3-
mc:13 tc:4.27e+4
Si-
mc:9 tc:4.93e+4
Cu-
mc:5 tc:6.81e+3
Au-
mc:112 tc:2.31e+6
O-
mc:146 tc:4.39e+6
U-
mc:4 tc:3.45e+3
UO-
mc:3 tc:2.20e+3
UO2-
mc:5 tc:6.55e+3
UO3-
mc:19 tc:5.50e+4
302.036
mc:7 tc:8.16e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.036 / total
Sum of U / total
mc:21 tc:6.84e+4

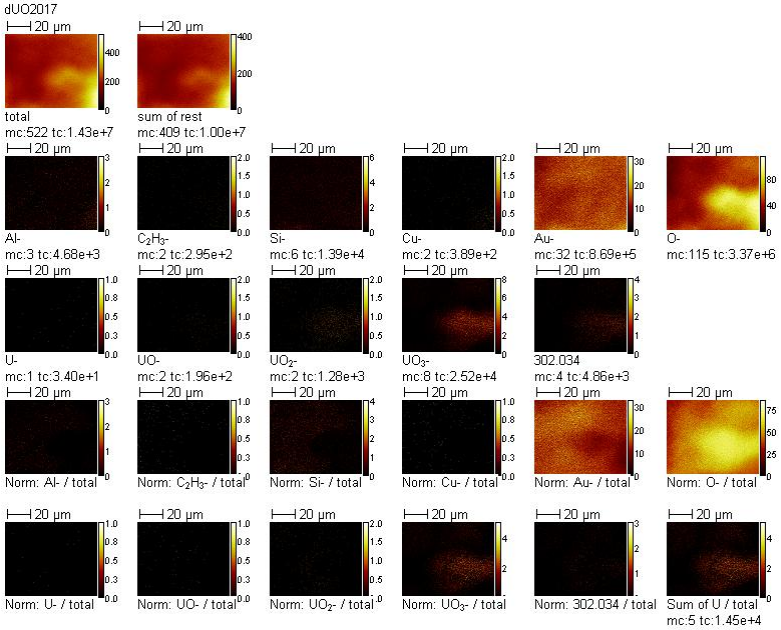

dUO2012
20 µm
total
mc:2410 tc:6.76e+7
20 µm
sum of rest
mc:2357 tc:6.51e+7
20 µm
Al+
mc:69 tc:8.16e+5
20 µm
C2H3+
mc:33 tc:6.76e+5
20 µm
Si+
mc:26 tc:4.74e+5
20 µm
Cu+
mc:19 tc:2.45e+5
20 µm
Au+
mc:8 tc:4.49e+4
20 µm
O+
mc:2 tc:2.50e+3
20 µm
U+
mc:6 tc:7.64e+3
20 µm
UO+
mc:23 tc:8.29e+4
20 µm
UO2+
mc:42 tc:2.13e+5
20 µm
UO3+
mc:2 tc:9.58e+2
20 µm
302.055
mc:2 tc:7.11e+2
20 µm
Norm: Al+ / total
20 µm
Norm: C2H3+ / total
20 µm
Norm: Si+ / total
20 µm
Norm: Cu+ / total
20 µm
Norm: Au+ / total
20 µm
Norm: O+ / total
20 µm
Norm: U+ / total
20 µm
Norm: UO+ / total
20 µm
Norm: UO2+ / total
20 µm
Norm: UO3+ / total
20 µm
Norm: 302.055 / total
20 µm
Sum of U / total
mc:57 tc:2.96e+5

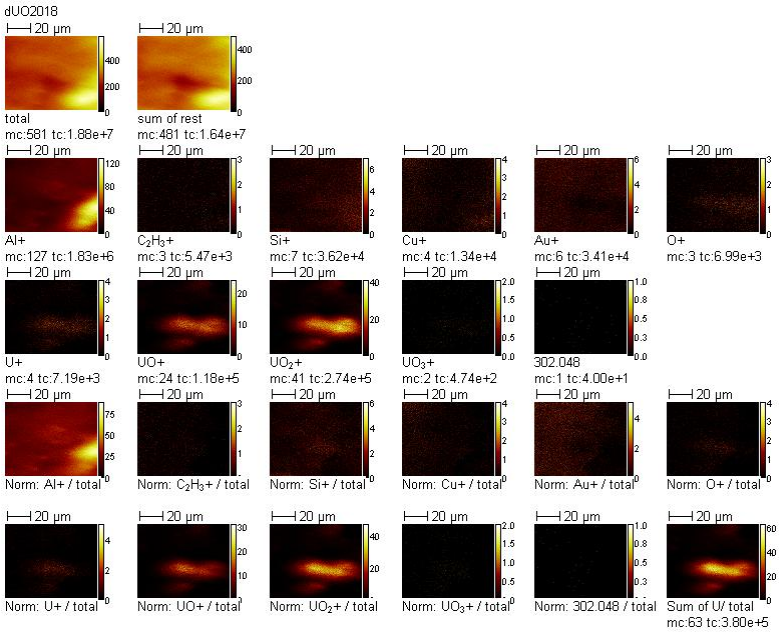

dUO2013
20 µm
total
mc:1540 tc:4.89e+7
20 µm
sum of rest
mc:1381 tc:4.13e+7
20 µm
Al-
mc:4 tc:5.29e+3
20 µm
C2H3-
mc:6 tc:2.08e+4
20 µm
Si-
mc:8 tc:6.11e+4
20 µm
Cu-
mc:3 tc:3.74e+3
20 µm
Au-
mc:82 tc:2.03e+6
20 µm
O-
mc:116 tc:5.51e+6
20 µm
U-
mc:2 tc:6.72e+2
20 µm
UO-
mc:2 tc:3.25e+2
20 µm
UO2-
mc:2 tc:1.32e+3
20 µm
UO3-
mc:6 tc:1.37e+4
20 µm
302.03
mc:5 tc:6.91e+3
20 µm
Norm: Al- / total
20 µm
Norm: C2H3- / total
20 µm
Norm: Si- / total
20 µm
Norm: Cu- / total
20 µm
Norm: Au- / total
20 µm
Norm: O- / total
20 µm
Norm: U- / total
20 µm
Norm: UO- / total
20 µm
Norm: UO2- / total
20 µm
Norm: UO3- / total
20 µm
Norm: 302.03 / total
20 µm
Sum of U / total
mc:7 tc:1.66e+4

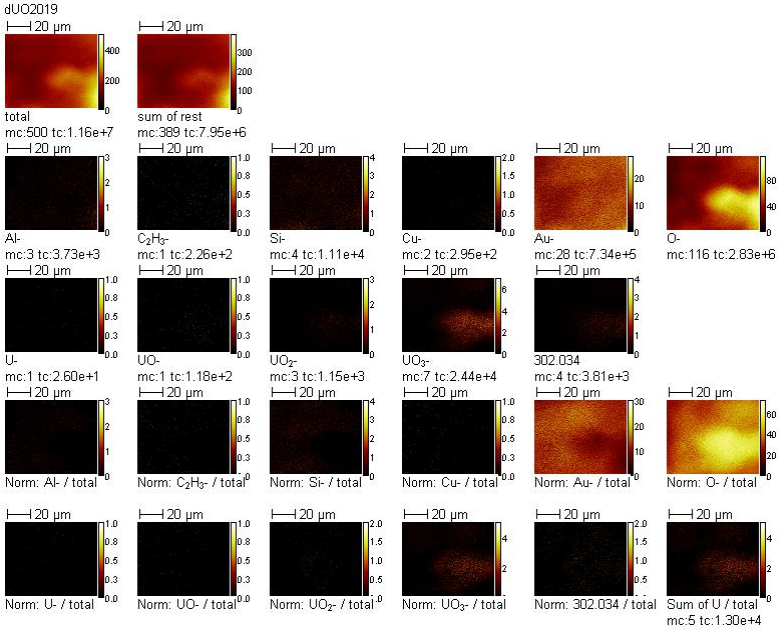

dUO2014
20 µm
total
mc:637 tc:2.53e+7
sum of rest
mc:549 tc:2.25e+7
Al+
mc:123 tc:2.11e+6
C2H3+
mc:5 tc:1.29e+4
Si+
mc:9 tc:7.51e+4
Cu+
mc:5 tc:2.24e+4
Au+
mc:5 tc:2.92e+4
O+
mc:5 tc:1.11e+4
U+
mc:5 tc:6.95e+3
UO+
mc:25 tc:1.41e+5
UO2+
mc:61 tc:4.28e+5
UO3+
mc:2 tc:6.87e+2
302.046
mc:1 tc:6.40e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.046 / total
Sum of U / total
mc:70 tc:5.31e+5

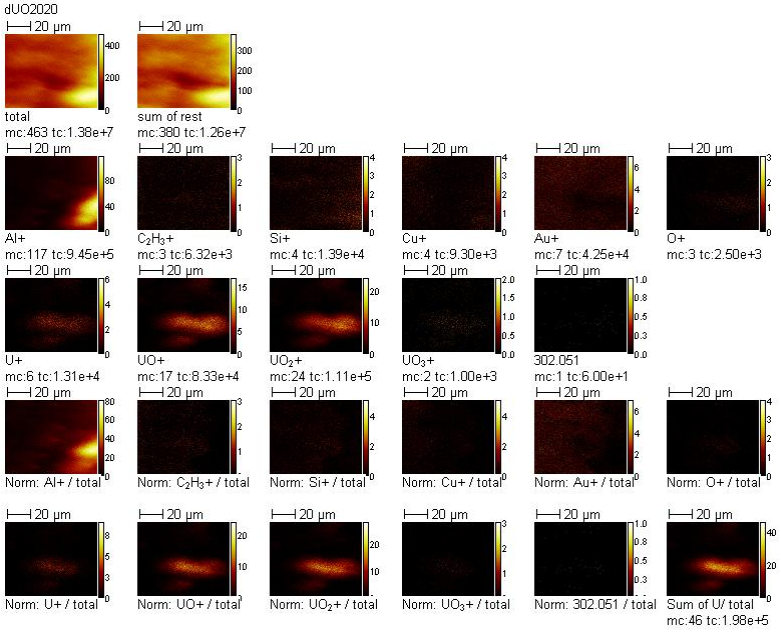

dUO2015
20 µm
total
mc:603 tc:1.84e+7
sum of rest
mc:499 tc:1.34e+7
Al-
mc:3 tc:6.12e+3
C2H3-
mc:2 tc:5.20e+2
Si-
mc:6 tc:1.88e+4
Cu-
mc:2 tc:5.85e+2
Au-
mc:36 tc:9.88e+5
O-
mc:117 tc:4.00e+6
U-
mc:2 tc:4.20e+1
UO-
mc:2 tc:2.52e+2
UO2-
mc:2 tc:9.72e+2
UO3-
mc:7 tc:2.34e+4
302.036
mc:4 tc:6.87e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.036 / total
Sum of U / total
mc:7 tc:1.56e+4

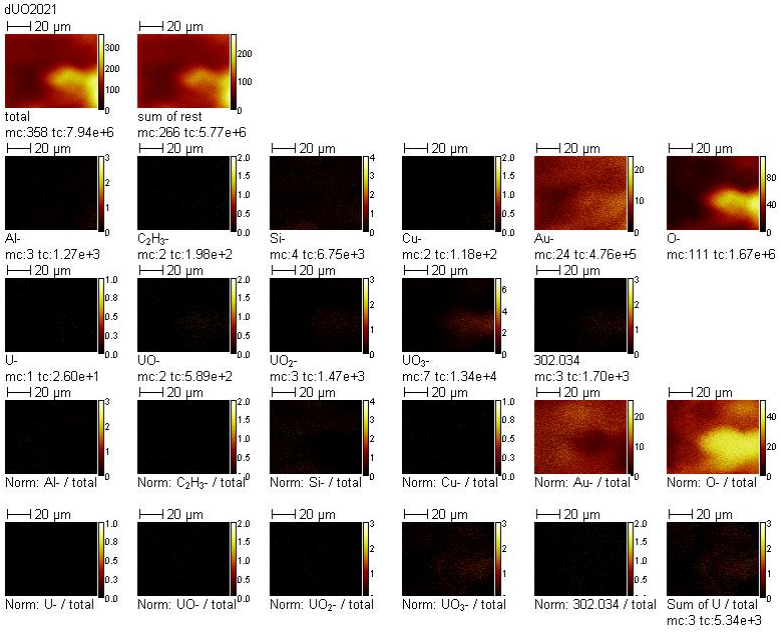

dUO2016
20 µm
total
mc:587 tc:2.11e+7
sum of rest
mc:499 tc:1.85e+7
Al+
mc:125 tc:2.05e+6
C2H3+
mc:3 tc:6.40e+3
Si+
mc:8 tc:4.62e+4
Cu+
mc:5 tc:1.54e+4
Au+
mc:6 tc:3.18e+4
O+
mc:4 tc:8.51e+3
U+
mc:4 tc:6.79e+3
UO+
mc:21 tc:1.21e+5
UO2+
mc:47 tc:3.05e+5
UO3+
mc:2 tc:5.45e+2
302.042
mc:1 tc:4.40e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.042 / total
Sum of U / total
mc:63 tc:4.05e+5


dUO2017
20 µm
total
mc:522 tc:1.43e+7
sum of rest
mc:409 tc:1.00e+7
Al-
mc:3 tc:4.68e+3
C2H3-
mc:2 tc:2.95e+2
Si-
mc:6 tc:1.39e+4
Cu-
mc:2 tc:3.89e+2
Au-
mc:32 tc:8.69e+5
O-
mc:115 tc:3.37e+6
U-
mc:1 tc:3.40e+1
UO-
mc:2 tc:1.96e+2
UO2-
mc:2 tc:1.28e+3
UO3-
mc:8 tc:2.52e+4
302.034
mc:4 tc:4.86e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.034 / total
Sum of U / total
mc:5 tc:1.45e+4


dUO2018
20 µm
total
mc:581 tc:1.88e+7
sum of rest
mc:481 tc:1.64e+7
Al+
mc:127 tc:1.83e+6
C2H3+
mc:3 tc:5.47e+3
Si+
mc:7 tc:3.62e+4
Cu+
mc:4 tc:1.34e+4
Au+
mc:6 tc:3.41e+4
O+
mc:3 tc:6.99e+3
U+
mc:4 tc:7.19e+3
UO+
mc:24 tc:1.18e+5
UO2+
mc:41 tc:2.74e+5
UO3+
mc:2 tc:4.74e+2
302.048
mc:1 tc:4.00e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.048 / total
Sum of U/ total
mc:63 tc:3.80e+5


dUO2019
20 µm
total
mc:500 tc:1.16e+7
sum of rest
mc:389 tc:7.95e+6
Al-
mc:3 tc:3.73e+3
C2H3-
mc:1 tc:2.26e+2
Si-
mc:4 tc:1.11e+4
Cu-
mc:2 tc:2.95e+2
Au-
mc:28 tc:7.34e+5
O-
mc:116 tc:2.83e+6
U-
mc:1 tc:2.60e+1
UO-
mc:1 tc:1.18e+2
UO2-
mc:3 tc:1.15e+3
UO3-
mc:7 tc:2.44e+4
302.034
mc:4 tc:3.81e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.034 / total
Sum of U / total
mc:5 tc:1.30e+4


dUO2020
20 µm
total
mc:463 tc:1.38e+7
sum of rest
mc:380 tc:1.26e+7
Al+
mc:117 tc:9.45e+5
C2H3+
mc:3 tc:6.32e+3
Si+
mc:4 tc:1.39e+4
Cu+
mc:4 tc:9.30e+3
Au+
mc:7 tc:4.25e+4
O+
mc:3 tc:2.50e+3
U+
mc:6 tc:1.31e+4
UO+
mc:17 tc:8.33e+4
UO2+
mc:24 tc:1.11e+5
UO3+
mc:2 tc:1.00e+3
302.051
mc:1 tc:6.00e+1
Norm: Al+ / total
Norm: C2H3+ / total
Norm: Si+ / total
Norm: Cu+ / total
Norm: Au+ / total
Norm: O+ / total
Norm: U+ / total
Norm: UO+ / total
Norm: UO2+ / total
Norm: UO3+ / total
Norm: 302.051 / total
Sum of U/ total
mc:46 tc:1.98e+5


dUO2021
20 µm
total
mc:358 tc:7.94e+6
sum of rest
mc:266 tc:5.77e+6
Al-
mc:3 tc:1.27e+3
C2H3-
mc:2 tc:1.98e+2
Si-
mc:4 tc:6.75e+3
Cu-
mc:2 tc:1.18e+2
Au-
mc:24 tc:4.76e+5
O-
mc:111 tc:1.67e+6
U-
mc:1 tc:2.60e+1
UO-
mc:2 tc:5.89e+2
UO2-
mc:3 tc:1.47e+3
UO3-
mc:7 tc:1.34e+4
302.034
mc:3 tc:1.70e+3
Norm: Al- / total
Norm: C2H3- / total
Norm: Si- / total
Norm: Cu- / total
Norm: Au- / total
Norm: O- / total
Norm: U- / total
Norm: UO- / total
Norm: UO2- / total
Norm: UO3- / total
Norm: 302.034 / total
Sum of U / total
mc:3 tc:5.34e+3

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14. ABSTRACT

Because of nuclear proliferation concerns, nuclear material must be safeguarded, and peaceful intentions verified. The field of nuclear forensics addresses these concerns. While established nuclear forensic techniques exist, quicker, more accurate and less expensive methods are of interest for nonproliferation applications. Currently a host of different analytical techniques, requiring a week or longer, are employed to obtain isotopic ratios, chemical abundances and morphology for forensic particulate samples. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) is a candidate technology for rapid evaluation of these properties for small amounts of nuclear materials. After a thorough investigation, this study found TOF-SIMS to be particularly useful to the nuclear forensic field as a triage technique, capable of quickly identifying and roughly assessing uranium containing materials for these properties. Uranium isotopic abundances can be determined to an accuracy of 1 percent. Uranium oxide particles are clearly distinguished from one another. TOF-SIMS imaging easily and quickly reveals the basic shape and composition of particles. Additionally the relative abundances of various secondary ions produced with TOF-SIMS may uncover new information on fundamental uranium oxide structures and properties.

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