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Market Research Survey of Commercial Off-The-Shelf (COTS) Portable MS Systems for IAEA Safeguards Applications

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February 2013



Pacific Northwest
NATIONAL LABORATORY

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Pacific Northwest National Laboratory
Richland, Washington 99352

Executive Summary

This report summarizes the results of a Market Research Survey of mass spectrometers that are deemed pertinent to International Atomic Energy Agency (IAEA) needs and strategic objectives. A compilation of all the MS instruments (43 in total) we found to meet these needs and strategic objectives are presented in this report, along with pertinent information regarding each instrument. The instruments in the compilation are categorized into two groups based on application, one for elemental/isotopic applications (22 instruments) and one for molecular applications (21 instruments). The main focus of this report is on MS instruments that represent currently available (or soon to be) commercial off-the shelf (COTS) technology and weigh less than 400 pounds. With these additional requirements, the main instrument list is culled down to 22 instruments which meet the requirements of being COTS and less than 400 pounds. This subset of instruments is then evaluated against a detailed set of criteria to determine whether each instrument significantly meets (green), meets (yellow), or significantly fails to meet (red) the needs of the IAEA safeguard community for in-field man-portable or field-deployable mass spectrometers. A detailed discussion of each of these instruments is also provided, summarizing the applications, strengths, and weaknesses of each MS configuration for IAEA safeguard purposes.

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1.0 Introduction

The goal of this report is to provide an independent Market Research Survey of COTS (commercial off-the-shelf) portable mass spectrometers (MS) that are deemed pertinent to International Atomic Energy Agency (IAEA) needs and strategic objectives. For this report, these IAEA needs were defined as man-portable and/or field-deployable MS instruments that are COTS (or near COTS) available, less than 400 pounds, and capable of providing isotopic, elemental, and organic analyses for IAEA in-field safeguard purposes.

The main reason for undertaking this survey was to compile and evaluate available MS technologies with current or future application to IAEA needs within the safeguards arena. Due to the broad spectrum of instrument types and configurations, this report draws upon the experience and expertise of the authors to provide an evaluation of the instruments, and provide a discussion of their applications, their strengths, and their weaknesses. In this report, there are 11 different ion sources (Table 1) and 5 different mass analyzers (Table 2) considered. The difficulty in evaluating these instruments arises from the many different ways that these components may be joined together for mass spectrometric needs. Figure 1 highlights these complexities and delineates the process and steps through which analyses may be obtained and components may be combined for an analysis.

2.0 Market Survey

2.1 Initial Market Survey and Requirements Assessment

This Market Research Survey was conducted in three phases. First, a list of available mass spectrometers (found in this study) with the potential to meet IAEA analysis requirements for isotopic, elemental, and organic analysis was compiled. This list of 43 instruments is broken into two broad categories: 1) 22 instruments for elemental/isotopic analyses (Table 3), and 2) 21 instruments for molecular analyses (Table 4). Within each of these categories, the mass spectrometers are further grouped by type of mass analyzer each instrument uses (quadrupole, magnetic sector, ion trap, time-of-flight, and ion cyclotron resonance). These tables capture many aspects of these instruments, such as mass analyzer, geometry, ion source, manufacture, inlet/sampling system, and application. These tables also show the evaluation of each mass spectrometer for COTS availability and weight. In order for the instruments to be considered for the next phase of the survey, both requirements have to be met (shown in green). Of the initial 43 instruments on the list, only 19 met both requirements. In addition, one instrument (the KORE MS-200) that did not meet the COTS readiness criteria (for UF₆) is included in this report due to current IAEA interest. Thus, 20 instruments are included in the next phase for evaluation and discussion.

2.2 Individual Mass Spectrometer Criteria Evaluation

The second phase of the market research survey was to evaluate each of the instruments that made it past the first phase against a broad set of performance based criteria (Table 5). These

criteria were developed in discussions between PNNL, LANL, SRNL, IAEA inspectors, and program headquarters. The criteria are designed to evaluate the applicability and potential development of each instrument for IAEA needs. These evaluations are provided in Table 6 for both the elemental/isotopic and the molecular instruments. Each cell of this table lists the best estimates for performance metrics, where available, of each instrument type. These estimates are based on a thorough study of the documentation for each instrument, along with discussions with the vendors and personal experience. The green (significantly meets), yellow (meets), and red (significantly fails) color coding of Table 5 were applied to each instruments in Table 6.

2.3 Individual Mass Spectrometer Discussion and Summary

The third phase of the market research survey was to provide a discussion and summary of each mass spectrometer. These discussions include a brief instrument description, its application, and its advantages and disadvantages.

3.0 Elemental and Isotope Ratio MS Instruments

3.1 General

This section provides general comments on known, atomic, mass spectrometers used for multi-elemental and/or isotope ratio (IR) analyses that could potentially be applied to the safeguards missions, i.e. elemental process-signatures and/or actinide isotope ratios. When the prerequisites of “COTS-ready” and a weight limit of 400 lbs were applied to this list, only 6 instrument groups qualified (5 from typical quadrupole ICP-MS manufactures, one a portable “molecular” TOF instrument being modified for UF₆ isotope ratio analysis, and one a bench-top SIMS instrument with either quadrupole or TOF mass analyzers). Specific comments on these instruments follow this discussion. Considering that the safeguards area is such a small niche market (10 off?), the commercial instrument companies will not likely address any special needs. Therefore, this section concludes with comments on instrument limitations (in regards to safeguards applications) that may be improved by directed research and development efforts.

The MS instrumentation technologies presented here are representative of what is available but are not exhaustive of what may have been experimentally tried. Several alternative mass spectrometric technologies have been applied to atomic ion (elemental and isotope ratio) and molecular ion (usually organic) analysis that have not been successful or are not yet successful. Some of these are briefly discussed here. Accelerator mass spectrometry (AMS) is a very sensitive isotope ratio technique with great accuracy, precision, and abundance sensitivity but, due to their cost, size, and complexity, this approach will not be discussed at all.

Quadrupole Ion Trap MS techniques have been applied to elemental and isotope ratio analysis a number of times with interesting results. However, a common result is that these ion traps, being accumulating/storage devices that hold the ions for a few milliseconds in the trapping volume at elevated pressure, offer multiple opportunities for ion-molecule reactions, especially for refractory elements such as the actinides. Thus, the atomic signals are often diluted into a

manifold of oxide/hydroxide products from the adventitious water present in the systems. Also, since these traps have a finite volume available, they have a limited maximum ion capacity before space charge effects are experienced. This limited ion capacity results in limits to the detection of low abundance ions in the presence of highly abundant ions. Thus, ion traps are not great devices for the detection and isotope ratio accuracy and precision of low abundance species/isotopes in the presence of more abundant species. The larger traps may be able to hold 10k to 100k ions. This limits the abundance sensitivity to E4-E5 at best. For the much smaller ion traps being developed for in-field use (some of which are presented in the ‘molecular’ section), the ion capacities are much smaller, perhaps <1000 ions. This means that there will be significant low abundant ion perturbation at the E3 level. This may be acceptable for detection of organic signatures and possibly for enriched uranium applications, but attention would also have to be paid to reaction possibilities and consequences.

Other Ion Trapping techniques, such as FT-ICR and DC IT (Thermo Scientific “Orbitrap”), utilize much better vacuums so do not suffer the reaction problem for reactive atomic ions but do suffer from space charge effects at near ion capacity. These techniques are not otherwise discussed here due to the much less than COTS status, the large instrument sizes, and experimental complexity.

3.2 Elemental/Isotopic MS Instruments

There are several atomic mass spectrometers for elemental and/or isotope ratio analysis (see Table 3). The variety comes from ion source types, mass separator types, and detector types and/or arrangements. Most are commercially available for a variety of elemental analyses, including but not limited to environmental (air/water quality); drinking water; foodstuffs; geological; quality assurance (metals, semiconductors, pharmaceuticals, etc.); etc. Most elemental/IR instruments (but not all) utilize inductively coupled plasma ion sources (ICP) due to the robust nature and high ionization efficiency of this source. The instruments designed for elemental analysis and isotope ratio analysis are typically scanning types that cover the entire atomic mass range and have a single detector. The listed SIMS instruments are capable of producing molecular ions and atomic ions from sample surfaces and can produce isotope ratio analysis of elements as atomic or molecular ions. While the portable TOF instrument is available as an EI-source molecular instrument, it is also being modified and evaluated for uranium isotope ratio applications for UF₆. The instruments specifically designed for high quality isotope ratio analysis are double focusing, multi-collector (detector) instruments such that all the isotopes for a single element are focused on to individual detectors and determined simultaneously for the best accuracy and precision. These simultaneous, isotope ratio instruments are all large and expensive and all do not meet the weight prerequisite

3.3 Comments for Instruments Making the COTS/Weight Cut-off

Seven instrument groups from five manufacturers made the COTS/weight cut (see Table 3). The reader is reminded that the weights quoted for these instruments are the instrument weights alone and do not include one or more of the following depending on the instrument: rotary-vane rough vacuum pumps, a recirculating chiller, a compressed argon gas source (facility, dewar, or

compressed gas bottles), compressed collision/reaction gas(s), a control-and-acquisition computer, and sample handling/preparation equipment.

All of the qualified quadrupole ICP-MS instruments are scanning type instruments utilizing ICP ion sources, linear quadrupole mass separators, and single secondary-electron-multiplier detectors. Since they use ICP sources the samples must be presented as a liquid (typically dissolved in an aqueous nitric acid solution) or as very small solid particles from a laser ablation sample introduction accessory (separate component) for solid samples. The sample types for the SIMS instruments are small, electrically conductive, solid materials whose surface constituents may be analyzed and/or near-surface composition may be bored into. The portable TOF instrument is designed for sampling gaseous atmospheres and, in its modified form, for gaseous UF_6 analysis.

All of the quadrupole ICP-MS instruments offer some type of collision/reaction cell technology that can be effective in removing or significantly reducing interferences to the analyte signal caused by isobaric polyatomic ions. There are three ways this is achieved: collisionally, reactively, or by energy dissipation. Ion collisions with a non-reactive gas (e.g. He) can dissociate interfering polyatomic ions. Ion-molecule reactions can resolve interferences by: 1) charge exchange between interferent ions and the reactive gas (e.g., plasma gas ion (Ar^+/H_2 , NH_3), matrix ion (Xe^+/O_2)), and 2) by creating a polyatomic ion of the analyte or interferent, thus moving it to a higher m/z ratio resolved by the quadrupole (e.g. S^+ or $\text{Se}^+ + \text{O}_2 \rightarrow \text{SO}^+$ or SeO^+). And lastly, ion energy dissipation through collision with a non-reactive gas (e.g., He) can produce selectively greater kinetic energy loss for polyatomic ions than for atomic ions allowing separation by kinetic energy discrimination (KED). Depending on the sample matrix or other factors, one of these techniques may be required to get the best detection and/or isotope ratio analysis. These techniques of course add complexity and may require more than just a moderately trained operator.

Again, these instruments provide adequate or more than adequate performance for safeguards applications for minimum detectable quantity (concentration), sensitivity, dynamic range, and abundance sensitivity. For the purpose of this report, we feel that the minimum detectable quantity (MDQ) assessment is best captured using subcategories of concentration (ng/mL) and sensitivity (kcps/ppb, kilo-counts-per-second/part-per-billion).

We divided the ‘measurement uncertainty’ category into two columns, ‘element concentration’ and ‘isotope ratio’ in order to compare the elemental vs. isotope ratio performance. For these criteria, the scanning quadrupole instruments are rated ‘yellow’ or medium since they will not be as stable, accurate, and precise as the multi-collector, sector instruments. Although the sector instruments would provide ‘green’ or high precision and accuracy, they all fail the weight requirement by many hundredweight and are considerably more expensive.

All the quadrupole instruments are highly evolved (3rd, 4th, 5th generation depending on how one defines a generation) and are thus rated ‘green’ for a well-established maturity level. Any customization that may be necessary for safeguards’ needs will involve significant instrument development efforts or less expensive efforts in sample preparation techniques to more closely match sample types with the preferred instrument input form.

Instrument automation is fairly advanced for all, however none should be left to an ‘unskilled’ operator (see criteria definitions, table 5). Thus, this criteria is rated ‘yellow’. A trained and skilled operator who also acts as an inspector would be much preferred to an inspector who was trained to operate one of these instruments.

Data-processing automation for the quadrupole instruments is in a similar state, however a particular processing sequence and reporting format could be set up by a skilled/trained person and then operated by one less skilled – as long as nothing went wrong. Thus we code this criteria ‘green’.

Although these instruments are much smaller, more robust and stable, and more transportable (not portable) than their predecessors, skilled, knowledgeable staff are still required to take-down, move, and re-install these instruments. A better scenario would be to set up one of these instruments in a fixed- or mobile-lab and leave it there. Thus we rate this category ‘yellow’ for all.

As these types of instruments have evolved, their maintenance requirements have decreased, driven especially by the needs of contract labs and the semiconductor industry. Some issues can be resolved by technicians (green), some by skilled operators (yellow), and some only by specialized staff (red). For the most part a ‘yellow’ rating should cover this criteria.

Improvements in reliability have also dramatically improved with the evolution, however operation in other than a very robust laboratory/staffing setting will not yield 24/7 availability. A ‘yellow’ – dependable with some maintenance and repair is the appropriate rating.

All of these instruments, except the portable TOF, operate on 120-240 VAC, 20-30A electrical supplies, which are common in nearly any laboratory setting – ‘yellow’. None of these are even close to battery powered, although they can be fitted with ‘uninterruptable power supplies’ that could power the instruments long enough for an orderly shut down. This provision would of course add weight and cost. The portable TOF instrument is powered by a 12V battery.

3.4 Specific Comments for Elemental/Isotopic MS Instruments

3.4.1 Agilent 7700s

The Agilent 7700 ICP-MS series is comprised of three very similar instruments. All use a 2-cone sample inlet system, chicane lens to separate UV photons and neutral atoms from the ion beam, an octopole collision/reaction cell, and a linear quadrupole. All utilize helium as the collision gas and remove the interfering polyatomic ions by kinetic energy discrimination (KED). The 7700e uses only He KED for simple, high-throughput of unknown samples. The 7700s, designed specifically for the special needs of the semiconductor industry, also has provision for a reactive gas in the collision cell and for operation in the “cool plasma” mode. (Cool plasma is a lower power operational mode of the ICP resulting in fewer argon-based polyatomic interferences.) The 7700x is designed for more

problematic sample types. In addition to the added features of the 7700s it also has a unique interface arrangement for high-matrix samples.

3.4.2 Agilent 8800

The Agilent 8800 is a relatively new model similar to the 7700 series except that it has a mass resolving quadrupole between the interface lens and the collision/reaction cell (CRC) that is followed by a resolving quadrupole as in the 7700. This additional quad and the capability to add a few different collision/reaction gasses to the CRC provide considerable flexibility (also added complexity) to analysis of samples with unusual interferences. The greater complexity and cost of this instrument precludes its use for safeguards except, perhaps, in an R&D setting for matrix characterization or special/unusual sample analysis.

3.4.3 Thermo Scientific iCAP Q

The Thermo Scientific iCAP Q also consists of a series of 3 related instruments. All are based on a dual cone interface, a 90° deflection of ions (removes photons and neutrals), and the mass-resolving quad. The iCAP Qa operates as a standard ICP-MS with no CRC technology. The iCAP Qc includes a collision cell that operates in the KED mode of interference reduction and is optimized for high sensitivity. The iCAP Qs has special modification for the semiconductor industry and has a CRC that can operate in KED mode or in the collision/reaction modes.

3.4.4 Perkin-Elmer Sciex NexION 300

The Perkin-Elmer Sciex NexION 300 series consists of 4 similar instruments. All are based on a triple cone interface, a quadrupole ion deflector (removes photons and neutrals), and a mass-resolving quadrupole. The 300Q is a standard ICP-MS without any collision/reaction technology, although a CRC can be retrofitted. The 300X has a CRC that can operate in 3 modes (standard, KED, reaction) under computer control. The standard ICP-MS mode operates without any collision/reaction gas, the KED mode uses helium collision gas, and the reaction mode uses a variety of reactive gases depending on the desired interferences to be removed. In the 300D the CRC can also operate as a resolving quadrupole thus eliminating certain interfering reaction products before they are sent to the main quadrupole (more flexibility, more complexity). The 300S has the capabilities of the 300D and has been expressly optimized for maximum sensitivity for semiconductor applications

3.4.5 SAI Millbrook Mini-SIMS Alpha and ToF

The Mini-SIMS by SAI is the one instrument type reviewed in this study that can be used for both types of analyses (atomic and molecular). SIMS is known for its

ability for elemental studies along with molecular information from the upper most layers of a surface. Even though molecular signals are greatly enhanced in large SIMS instruments when a cluster source is employed for primary ions, monatomic projectiles (used in these smaller Alpha and TOF SIMS instruments) can produce molecular information, especially when employed in the static mode. The Mini-SIMS comes in two configurations. The alpha model employs a quadrupole mass analyzer and the ToF model used a time-of-flight mass analyzer. Both instruments provide surface data from the sample surface. The ToF analyzer does permit the recording of unexpected elements or molecules, due to the ability of the ToF mass analyzer to detect all ions per event. The Mini-SIMS has the advantage of being relatively small and simple to operate when compared to a typical commercial SIMS instrument. However, it is not as sensitive or capable of providing as much detail when compared to a larger instrument. These small instrument will require a technician of a higher skill level to operate, but may provide the best chance for capturing reasonable isotope ratio information without an ICP.

3.4.6 KORE MS-200

The KORE MS-200 was originally designed for portable, in-field analysis of volatile organic compounds (VOCs). Its primary use being volatile and semi-volatile organic analysis of atmospheric gases. It produces analyte pre-concentration (actually matrix exclusion) by the use of two semi-permeable membranes through which the volatile organic components pass. The low permeation rate of the membrane permits the use of a low-power ion pump to maintain vacuum. Ionization is by an annular ring-type electron impact source, which was chosen to allow the use of KORE's patented "converging annular TOF" design. The ring-of-ions formed in the source are accelerated into a field-free region towards an ion reflector in such a way that the ring-of-ions is focused to a point just before the single detector. This clever design is intriguing and probably quite useable for in-field organic analysis. However, how well its inlet, membrane, and ion sources components can be passivated for and resistant to the corrosive, fluorinating atmosphere of UF_6 is unknown. Its detection limit for UF_6 will be limited by the permeation rate of whatever membranes are selected. Low permeation rates will also lead to long transition times from one sample to another. We include this instrument in the COTS/weight qualified list only because it is currently under development and evaluation by KORE and IAEA for UF_6 application. We do not consider the instrument UF_6 COTS at this time.

3.5 Capability Improvement Opportunities

For safeguard applications, uranium detectability is a significant parameter followed by isotope ratio determination. In these areas, the 4 different qualified instrument designs show little significant difference. The Agilent 8800 may be down-graded a bit for its greater complexity (thus flexibility). The desires of the safeguards community for a man-portable detection system will not provide a large enough potential market for one of the existing commercial

manufacturers to develop the capability. The main limitation for a man-portable instrument is an ion source with enough power/energy to atomize and ionize analytes at atmospheric pressure: a) dissolved in an aqueous solution or b) as solids from a surface or imbedded on a swipe. The latter may be a viable approach toward the desired capability. Using existing bench-top ICP-MS instruments, a miniature laser ablation system may be developed that could produce small aerosol particles from a variety of surfaces and materials and deliver these to an atomizing/ionizing source. It may be conceivable that a LA design may in fact be able to do both if coupled closely enough to the ion inlet of the MS. More than likely though, a separate, small atomization/ionization ion source will also need to be developed. Given success in these efforts, attention could be turned to an appropriate MS design followed by the appropriate software development and system ruggedization for a man-portable, in-field elemental/IR-MS for trained but unskilled operator.

4.0 Molecular MS Instruments

4.1 General

This section provides general comments on known mass spectrometers capable of molecular and organic analyses of samples of interest to the safeguards missions, i.e. compound identification and/or compound presence indications. When the prerequisites of “COTS-ready” and a weight limit of 400 lbs were applied to this list, only 13 instrument groups qualified. Specific comments on these instruments follow this discussion. Unlike the elemental and isotopic instruments, there may be significant interest in these organic molecular MS instruments by commercial and governmental entities. Broader application space exists outside of the IAEA needs for commitment of development funds and potentially directed collaboration. These types of instruments are typically smaller, lighter, and more user friendly, making them more ubiquitous in the market place.

4.2 Molecular MS Instruments

There are several different mass spectrometers for molecular and organic analysis needs (see Table 4). Like the atomic MS instruments, but to a larger degree, variability in the source, mass analyzer, detector and cost drives a vast array of instrument types and designs. Most are commercially available for a variety of analytical needs including but not limited to environmental (air/water quality); drinking water; foodstuffs; geological (minor); quality assurance (metals, semiconductors, pharmaceuticals, etc.); etc.

4.3 Comments for Instruments Making the COTS/Weight Cut-off

A major driver in the wide spectrum of these types of instruments is the variable ion sources available for this instrument. Electron impact and electrospray are the dominant ion sources on the market for these instruments, but other sources also include chemical ionization, DART, DESI, and laser ablation (see Table 1 for description of ion sources). The instruments are

typically designed for fast, reliable analyses with a single detector optimized for the signal of interest. These instruments are small and low-cost, making them attractive to the needs of the IAEA and safeguards community.

4.4 Specific Comments for Molecular MS Instrument

4.4.1 MicroSaic 3500 MiD

MicroSaic claims the 3500 MiD is the smallest fully integrated mass spectrometer. It is designed to be integrated with a LC (liquid chromatography) system. With its small footprint it can actually be the base for many smaller LC systems on the market. The manufacturers of this system also claim this instrument is 100% maintainable by the operator. The system is completely modular. The spray system, quadrupole and vacuum interface are chip based. As the user's needs change, the operator can change chipsets to update the 3500 MiD. This instrument is truly limited by its small three orders of magnitude dynamic range. The modular technology is unlike any presented on any other instrument in this study. Questions regarding the instrument's long-term reliability with this unproven new technology would be warranted.

4.4.2 Inficon HAPSITE ER

The folks at Inficon claim their HAPSITE ER instrument is the world's only person portable GC/MS. It requires minimal training. The operator can undergo 10 minutes of training and is capable of producing laboratory quality results in the field. They claim that the operator need only push one button and the instrument will begin identifying volatile organic compounds, toxic industrial chemicals, toxic industrial materials, chemical warfare agents and semi-volatile organic compounds. Inficon claims species can be detected at the ppm-ppt levels. This is a battery operated system and can operate for 2-3 hours on a single charge. Vacuum is maintained using a non-evaporative getter pump. Results are recorded on the instrument's panel and can be correlated to an exact location with on-board GPS.

4.4.3 SAI Millbrook Mini-SIMS Alpha and ToF

The Mini-SIMS by SAI is the one instrument type reviewed in this study that can be used for both types of analyses (atomic and molecular). SIMS is known for its ability for elemental studies along with molecular information from the upper most layers of a surface. Even though molecular signals are greatly enhanced in large SIMS instruments when a cluster source is employed for primary ions, monatomic projectiles (used in these smaller Alpha and TOF SIMS instruments) can produce molecular information, especially when employed in the static mode. The Mini-SIMS comes in two configurations. The alpha model employs a quadrupole mass analyzer and the ToF model used a time-of-flight mass analyzer. Both instruments provide surface data from the sample surface. The ToF analyzer does permit the

recording of unexpected elements or molecules, due to the ability of the ToF mass analyzer to detect all ions per event. The Mini-SIMS has the advantage of being relatively small and simple to operate when compared to a typical commercial SIMS instrument. However, it is not as sensitive or capable of providing as much detail when compared to a larger instrument. These small instrument will require a technician of a higher skill level to operate, but may provide the best chance for capturing reasonable isotope ratio information without an ICP.

4.4.4 Agilent 6400 Series

The Agilent 6400 Series consists of 4 instruments based on a well-evolved linear triple-quadrupole system for MS/MS interrogation of analyte ions. The interface utilizes ESI, API, and APCI to ionize LC and IC eluant streams. The standard interface optics in the base instrument yield good performance with a simple design. For fg level sensitivity, which is achievable in the top-of-the-line model, dual RF ion funnels are required to collect, desolvate, and transmit the ions to the quadrupole optics. Although this system probably has greater capability than may be needed for safeguards, it provides a vision of what is possible.

4.4.5 Thermo Scientific LCQ Fleet

The Thermo LCQ is considered by many as the standard for API-MS. It offers good overall sensitivity along with good abundance sensitivity. Like most ion traps, it offers the scientist chemical structure information. The utility of such information in a field lab scenario is unknown. The ion source is Thermo's Ion Max API source which offers the analyst the choice of ESI and APCI. This instrument performs best when coupled to a LC front-end. The Thermo LCQ instrument is at the top end of the weight range criterion for this survey; with the roughing pump included it will be close to the cut-off limit of 400 pounds. While one of the top performers in ion trap mass spectrometers, there are better choices regarding portability than the LCQ.

4.4.6 Torion Tridion 9-GC-TMS

The Tridion is another ion trap mass spectrometer housed in a self-contained package designed for portability. In this MS instrument the ions move in a toroidal path according to their m/z ratio. The vacuum system is a turbo pump backed by a diaphragm roughing pump. This instrument's ionization source is located in the ion trap and regulates the number of ions created based on the analyte's concentration as directed by its AutoIon software. The instrument also has AutoTune and AutoCal functions for ease of operation. The Tridion's battery life is about 2.5 hours on a full charge. The onboard (and disposable) He cartridge holds enough gas for 100-150 acquisitions. The instruments onboard electronics has a large library of known compounds and can be updated with new ones.

4.4.7 FLIR Griffin 400 & 460

Both of these instruments are GC/MS and are nearly identical. Their only difference is the 400 is strictly a GC/MS whilst the Griffin 460 has the added ability for direct atmosphere sampling. Both systems are designed for transport between locales. The internal shock mounting system maintains system integrity through the most rugged transportation. These instruments can be operated with either AC or DC power. The vacuum system of these instruments is completely self-contained. Vacuum is maintained using a miniature turbo pump backed with a miniature quad diaphragm pump. This arrangement ensures that there are no issues with oil spillage during transport. There is little remarkable or novel about this system, it is mature technology taken on the road.

4.4.8 Flir Griffin 824

The Griffin 824 is similar to the 400 & 460 in the fact that they both use ion traps as a means of mass separation. Instead of using a GC front end or sampling directly from atmosphere, the 824 samples swipes for explosives or narcotics only. A swipe is placed into the instrument and heated, whereupon the explosives/narcotics volatilize, ionized and detected in the ion trap. This instrument is very limited in its application, but performs its role very well due to its high sensitivity in the ng range. The Griffin 824 only operates on 120VAC, making it somewhat limited in portability and fieldability.

4.4.9 MassTech Explorer 50 & 100

The MassTech Explorer 50 and 100 are ion trap mass spectrometers. These instruments allow for structural elucidation by allowing the user to employ MSn. Both instruments are equipped with an atmospheric pressure interface, which allows the user to employ a series of different ionization techniques such as AP-MALDI, ESI and APCI. Both instruments have sensitivities similar to larger, more expensive ion traps such as Thermo Scientific's LCQ. Where these instruments stand out from their competition is their size. The Explorer 100 only weighs 150 pounds and is MassTech's first entry into mass spectrometers. The Explorer 50 is their second generation API-Ion Trap and weighs only 75 pounds.

4.4.10 OI Analytical IonCam

The IonCam is the only magnetic sector mass spectrometer that meets the COTS and weight criteria for inclusion in this report. The IonCam is also the only mass spectrometer in the group that can be qualified as a multi-collector instrument. At its core, it is a field-portable GC-MS with alternate direct air injection and an EI source. Such a combination is ideal for volatile organic compound (VOC) analytical needs. The mass analyzer is an EB sector of Mattauch-Herzog configuration that has its focal plane at the 5 cm exit face of the permanent magnet. This focal plane is where the array detector is placed for simultaneous detection of

the ions exiting the magnet. The detector is a charged coupled device (CCD) consisting of an array of 2126 discrete detector elements (24 μm pitch, 5 cm length) that cover the full focal plane of the magnet. The 7 to 250 m/z range is covered in approximately 20% windows by adjusting the acceleration potential.

4.4.11 MSI-Tokyo InfiToF

The InfiToF is a unique instrument as it is only one of two instruments described here that use a time of flight mass analyzer. With instruments this small, there is typically a trade-off between sensitivity and resolution. The engineers at MSI-Tokyo have developed an instrument that maximizes resolution in a small package. They use a series of four electrostatic lenses to direct the ions in a “figure-8” orbit. The number of orbits can vary from 3-20, with maximum mass resolution was recorded at 30,000. This instrument was designed to connect to a GC, with an EI (electron impact) ion source. For greater usefulness, it would be desirable for the instrument to have a dynamic range for signal handling greater than 1023. Currently, we are unaware if this is a COTS instrument due to our inability to reach this Japan based company.

4.4.12 Alternative Ionization Sources (DESI and DART)

Most instruments with application to molecular analysis require an LC or GC front end to make the most of the mass analyzer. Other than the Griffin 824 and Mini-SIMS, there are no other solid phase sampling instruments included in this molecular instrument section. Thermally labile compounds are not identified or analyzed in any of the aforementioned techniques. Research over the last decade has resulted in two similar but different techniques for examining organic molecules on a surface at atmospheric pressure. These techniques are known as DESI and DART (described in Table 1). DESI has a documented sensitivity of 50 ng of sample, whereas DART is in the ppm level for detection. These ion sources are not complete instruments, but need to be coupled with a mass spectrometer to form a complete system. Discussions with Thermo Scientific staff indicate that a single or triple quadrupole system would be ideal for either DESI or DART sources. For this reason, we have included instrument data for Thermo’s MSQ+ and TSQ Max in Tables 4 and 6.

4.5 Capability Improvement Opportunities

The material within this last section of this report contains a wide variety of instrument designs and layouts. Some of these instruments incorporate technology which is mature and well established, whereas some of the technology is new and unproven. There are a couple instruments from smaller vendors that push the envelope in regards to bringing new technology alongside mature technologies, resulting in exciting new configurations. The problem is that they all typically detect the same type of molecules, which are organics, have higher vapor pressures, and usually are susceptible to chromatographic methods, and are amendable to

electron impact ionization. For any of these instruments to be useful in the realm of Safeguards there needs to be an investment in how to study compounds and/or elements with the aforementioned mass spectrometers.

5.0 Conclusion

The findings of this market research survey indicate that there are no instruments that meet the general requirements of being COTS and < 400 pounds that also meet all of the man-portable and/or field-deployable criteria for the IAEA needs. None of the instruments in the evaluation matrix (Table 6) are green all the way across the board. The four quadrupole elemental and isotope MS instruments are the best fit in terms of criteria evaluation, with nearly half of the criteria matrix in green and the other half in yellow. These instruments represent an area of potential future interest due to the relatively minor limitations of these instruments. With some strategic planning and focused research, there is a high probability that these instruments could be green across the evaluation criteria matrix.

In the molecular and organic MS instrument part of this survey, the instruments ranked overall lower, with more yellows and reds, and quite a few unknowns. While these instruments enjoy broad application in many arenas and are relatively low cost, application to actinide analysis is not seen at this time in COTS instruments. Analysts working on molecular and organic species of interest to the IAEA certainly have many instruments to choose from, but there are also trade-offs, such as sensitivity and precision, that have to be evaluated.

The specific challenges and analytical requirements the IAEA safeguards effort pose for mass spectrometry are significant. It is clear that further research and development in mass spectrometry are needed to overcome these obstacles. This research has highlighted the need for a multi-pronged approach to MS analysis; one that addresses the interplay between sampling needs and preparation, ion source abilities, mass analyzer, and detector. Changes made to one of these steps (see Fig. 1), changes the influence the other steps have on the whole process. Such a balanced approach holds the best chance for us to make significant in-roads to these challenging analytical needs of a man-portable device capable of high precision and sensitivity.

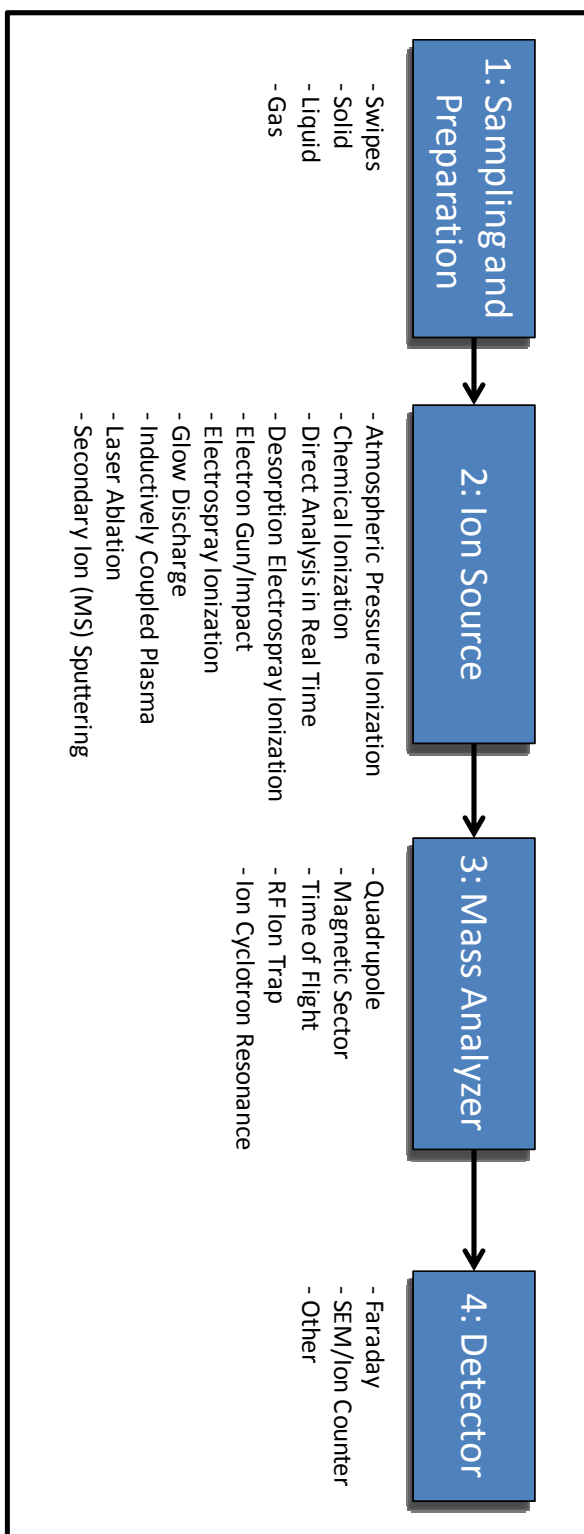


Figure 1: MS Analysis Flow Chart. This flow-chart illustrates the steps involved in mass spectrometer based analyses. The lists below each step identify the different types of each component evaluated in this report.

Table 1. List of different types of ion sources and their descriptions.	
API	<u>Atmospheric Pressure Ionization</u> : This is a generic term for an ion source that operates at atmospheric pressure. Examples of this include ESI, atmospheric matrix assisted laser desorption ionization (AMALDI), and atmospheric pressure chemical ionization (APCI).
CI	<u>Chemical Ionization</u> : This ion source uses EI or corona discharge to ionize a reagent gas (methane, oxygen, water, etc.), which, in turn ionize the analyte species by proton or electron transfer, adduct formation, etc.
DART	<u>Direct Analysis in Real Time</u> : This ion source uses molecular excited species to react with the analyte via contact. This collision creates a radical cation of the analyte which is swept into the mass spectrometer. The novel concept of this technique is that no sample preparation is needed. The analyte can be adsorbed to a solid and still be ionized.
DESI	<u>Desorption Electrospray Ionization</u> : This ion source occurs at atmospheric pressure and utilizes an electrospray source that directs its charged droplet towards a surface. The electrosprayed solvent reacts with analyte on the surface and facilitates its desorption and ionization. The analyte ions are swept into the mass spectrometer where they are detected.
EG	<u>Electron Gun</u> : This device is commonly used in SIMS instruments that may be analyzing insulating material in the negative mode. Positive ion bombardment and negative ion emission can result in analyte charging creating degradation in mass spectrum quality. An electron gun can mitigate positive sample charging allowing for extended analysis time for insulating species.
EI	<u>Electron Impact</u> : Electrons formed from thermionic emission interact with gas phase atoms or molecules generally forming positive ions with a single charge. This technique is often called a hard ionization technique where the analyte often undergoes significant fragmentation.
ESI	<u>Electrospray Ionization</u> : This ion source is one of the softest on the market. It works when a highly charged capillary sprays a fine mist of highly charged droplets. As the solvent evaporates the droplets become smaller to the point where the repulsive forces of the droplets charge are stronger than the bonds that hold the droplet together. When this point is reached the droplet undergoes a coulombic explosion which produces smaller multi-charged droplets. This process continues until all that's left is desolvated analyte ions with multiple charges each.
GD	<u>Glow Discharge</u> : This ion source uses two charged plates at relatively low pressure with the analyte of interest deposited on the plates. As the potential between the plates grows there is a transfer of ions and electrons between the two plates which in turn sputters the sample from the cathode. Once these atoms are in the gas phase interaction with electrons and other ions can ionize the analyte of interest. The ions are quickly accelerated into a mass spectrometer where they are detected.
ICP	<u>Inductively Coupled Plasma</u> : Is a robust ionization source used for predominately atomic species. The plasma is a high temperature source that receives its energy from electrical current induced by a time varied magnetic field. This source typically results in most elements being ionized to a +1 charge with 100% efficiency.
LA	<u>Laser Ablation</u> : This technique employs laser energy to ablate a small area/volume from the sample surface. The resultant debris is swept into an ICP with an argon (typical) gas stream. This technique provides high spatial resolution of solid samples for elemental analysis.
SIMS	<u>Secondary Ion Mass Spectrometry</u> : These instruments use an ion gun to sputter analyte from a surface. These sputtered secondary ions are repelled into a mass spectrometer where they are separated by their m/z ratio and detected. This technique is surface specific.

Table 2. List of mass analyzers and their descriptions.	
ICR	<u>Ion Cyclotron Resonance</u> : Ion Cyclotron Resonance (FT ICR or FTMS) and DC ion traps (Orbitrap). These ion traps have trapping cells designed such that ions entering them orbit around or along some central point or axis at frequencies related to the ion's m/z. The ions are detected by sensing their image currents in the frequency domain and converting the frequency information to a mass-to-charge spectrum by a Fast Fourier Transform.
IT	<u>Ion Trap</u> : This type of mass analyzer uses oscillating radiofrequency (RF) fields to store ions according to their m/z value and then to sequentially cause them to escape confinement as the RF potential is increased according to an established trajectory which allows the ions to be counted on a detector. The RF fields are typically configured in a series of cylindrically symmetrical electrodes, a ring electrode arraignment, and two end-cap electrodes. Ion traps have the potential for high resolution.
MS	<u>Magnetic Sector</u> : These instruments use a magnetic field to deflect the ions in a specific trajectory based on their mass-to-charge ratio. Lighter isotopes will be deflected more in a given field, resulting in a separation of isotopes or a mass spectrum from low to high across the detector configuration. Ion sources for this type of instrument can vary greatly from solid to liquid to gas, each with their own benefits and caveats.
QP	<u>Quadrupole</u> : This type of mass analyzer uses combined oscillating radiofrequency (RF) and DC potentials applied to four parallel hyperbolic rods to steer the ions along a path tuned for a specific mass onto a detector. These analyzers have the ability to scan the mass range very rapidly, and generate good elemental and ratio analyses.
ToF	<u>Time-of-Flight</u> : This is a technique utilized to separate ions based on their mass to charge ratios. All ions are accelerated to the same kinetic energy. Lighter masses will have a higher velocity than their heavier counterparts, thus reaching the detector earlier.

Table 3. Instruments for Elemental/Isotope Ratio Analyses (Group A)													
Mass Analyzer	Instr. Number	Geometry	Ion Source	Manufacturer	Model	Production Type	Inlet/Sampling System	Atm. Inlet	Application	COTS ?	<400 (lbs)	wt (lbs) / mounting	Ref
Quadrupole	A1	Quad - linear	ICP	Agilent	7700e/7700s/7700x	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	Y	254 / bench	1
	A2	Triple Quad - linear	ICP	Agilent	8800	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	Y	316 / bench	2
	A3	Quad - linear	ICP	Bruker Corp	Aurora M90	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	N	est >400 / floor	3
	A4	Quad - linear	ICP	Thermo Scientific	iCAP Q	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	Y	313 / bench	4
	A5	Quad - linear	ICP	PE Sciex	NexION 300 series	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	Y	400 / bench	5
	A6	Quad - linear	EI	LANL (1994)	R&D	Molecule	Gas	N	UF6 Isotope Ratio	N	Y	<400?	6
	A7	Quad - linear	EI	In Process Insts	IMU 200	Molecular UF6	Gas	Y	Solid UX/ UF6 Isotope Ratio	Y	N	~1600	7
	A8	Quad - linear	SIMS	Millbrook/SAI	Mini-SIMS alpha	Molecular/Atomic	Vacuum	N	Solid Surface/Elem/IR	Y	Y	220 / bench	8
Magnetic Sector	A9	Double Focusing/Mattauch-Herzog/Array detector	ICP	Spectro Analytical Instruments Inc	Spectro MS	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	N	1490 / floor	9
	A10	Double Focusing/EB/Single detector	ICP	Thermo Scientific	Element 2, Element XR	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	N	many cwt/ floor	10
	A11	Double Focusing/EB/Single detector	GD	Thermo Scientific	Element GD	Atomic	Solids	N	Elemental/Isotope Ratio	Y	N	many cwt/ floor	11
	A12	Double Focusing/EB/Multi-detector	ICP	Thermo Scientific	Neptune / Neptune+	Atomic	Liquid/Solid (LA)	Y	Isotope Ratio	Y	N	many cwt/ floor	12
	A13	Single Focusing/B/Multi-collector	TI	Thermo Scientific	Triton / Triton+	Atomic	Solids (purified)	N	Isotope Ratio	Y	N	many cwt/ floor	13
	A14	Double Focusing/EB/Single detector	ICP	Nu Instruments	Attom	Atomic	Liquid/Solid (LA)	Y	Elemental/Isotope Ratio	Y	N	many cwt/ floor	14
	A15	Double Focusing/EB/Multi-detector	ICP	Nu Instruments	Plasma II	Atomic	Liquid/Solid (LA)	Y	Isotope Ratio	Y	N	many cwt/ floor	15
	A16	Double Focusing/EB/Multi-detector	ICP	Nu Instruments	Plasma 1700	Atomic	Liquid/Solid (LA)	Y	Isotope Ratio	Y	N	many cwt/ floor	16
	A17	Double Focusing/EB/Single detector	GD	nu Instruments	Astrum	Atomic	Solids	N	Elemental/Isotope Ratio	Y	N	many cwt/ floor	17
Ion Trap	A18	Micro Ion Trap	EI	ORNL	Prototype	ORNL/Develop.	Gas	N	UF6 Isotope Ratio	N	Y	~ 40	18
Time-of-Flight	A19	Linear	GD	KORE	GD-TOF	Atomic	Solids	N	Elemental/Isotope Ratio	Y	N	est >400 / cart	19
	A20	Orthogonal	ICP	GBC Scientific	OptiMass 9500	Atomic	Liquid/LA Solids	Y	Elemental/Isotope Ratio	Y	N	595	20
	A21*	Reflectron TOF	EI	KORE	MS-200	Molecular UF6	Gas	Y	UF6 Isotope Ratio	N	Y	55	21
	A22	Linear TOF	SIMS	Millbrook/SAI	Mini-SIMS ToF	Molecular/Atomic	Vacuum	N	Solid Surface/Elem/IR	Y	Y	220 / bench	22
* This instrument does not meet the COTS criteria (for UF6) but is included for evaluation in Table 6 due to IAEA interest.													
References	Hyperlinks												
1	www.chem.agilent.com/en-US/products-services/Instruments-Systems/Atomic-Spectroscopy/Pages/default.aspx												
2	www.chem.agilent.com/en-US/products-services/Instruments-Systems/Atomic-Spectroscopy/8800-Triple-Quadrupole-ICP-MS/Pages/default.aspx												
3	www.bruker.com/products/mass-spectrometry-and-separations/icp-ms/aurora-m90/overview.html												
4	www.thermoscientific.com/ecomm/servlet/promotions?storeId=11152&contentId=54604&ca=dramatic												
5	www.perkinelmer.com/Catalog/Family/ID/NexION												
6	www.sciencedirect.com/science/article/pii/S058485470100235X												
7	www.in-process.com/products-imu-200-93.html?pro=12&PHPSESSID=tnnhlrhs												
8	www.minisims.com/minisims-alpha.htm												
9	www.spectro.com/pages/e/p010402tab_overview.htm												
10	www.thermoscientific.com/ecomm/servlet/productsdetail_11152__11961723_-1												
11	www.thermoscientific.com/ecomm/servlet/productsdetail_11152_L10380_87279_11962735_-1												
12	www.thermoscientific.com/ecomm/servlet/productsdetail_11152_L10608_98065_11961870_-1												
13	www.thermoscientific.com/ecomm/servlet/productsdetail?productId=11962736&groupType=PRODUCT&searchType=0&storeId=11152&from=search												
14	www.nu-ins.com/index.php/plasma-source												
15	www.nu-ins.com/index.php/plasma-source/the-nu-plasma-ii												
16	www.nu-ins.com/index.php/plasma-source/the-nu-plasma-1700												
17	www.nu-ins.com/index.php/plasma-source/the-nu-astrum												
18	Reference to Whitten paper 2004 (published?)												
19	www.kore.co.uk/bucharest.htm												
20	gbcsci.com/products/icp_tof/optimass.asp												
21	www.kore.co.uk/ms-200.htm												
22	www.saiman.co.uk/minisims-tof-mass-spectrometer.html												

Table 4. Instruments for Molecular MS Analysis (Group B)

Mass Analyzer	Instr. Number	Geometry	IonSource	Manufacturer	Model	Production Type	Inlet/ Sampling System	Atm. Inlet	Application	COTS ?	<400 (lbs)	wt (lbs) / mounting	Ref
Quadrupole	B1	Linear Quad/TOF	Electrospray	Waters	Xevo G2-S QToF	Molecule	Liquid	Y	Chem. Signature	Y	N	586/bench	1
	B2	Linear/Chip Based	ESI	Microsaic	3500 MiD	Molecule	Liquid	Y	Chem. Signature	Y	Y	60	2
	B3	Linear	EI	Inficon	Hapsite	Molecule	GC	Y	Chem. Signature	Y	Y	42	3
	B4	Linear	SIMS	Millbrook/SAI	Mini-SIMS alpha	Molecular/Atomic	Vacuum	N	Solid Surface Analysis	Y	Y	220/bench	4
	B5	Linear LCMS	API/ESI/APCI	Thermo	MSQ +	Molecular	Varies	Y	Chem. Signature	Y	Y	132/bench	5
	B6	Linear Triple Quad LCMS	API/ESI/APCI	Thermo	TSQ MAZ	Molecular	LC	Y	Chem. Signature	Y	Y		6
	B7	Linear Triple Quad LCMS	API/ESI/APCI	Agilent	6400 series	Molecular	LC	Y	Chem. Signature	Y	Y	255/bench	7
Ion Trap	B8	Linear Quadrupole Ion Trap	ESI, APCI	Thermo Scientific	LTQ XL*, LCQ	Molecule	GC, LC /API, ESI, APCI	Y	Chem. Signature	Y	Y	264/bench	8
	B9	Toroidal	EI/CI	Torion	Tridion 9 GC-TMS	Molecule	SPME/GC	N	Chem. Signature	Y	Y	32/bench	9
	B10	Cylindrical	EI	Flir	Griffin 824, 460, 400	Molecule	Atmospheric	Y	Chem. Signature	Y	Y	50, 98, 82 b	10
	B11	3D Quadrupole	ESI, API	MassTech, Inc	Explorer 50; 100	Molecule	Atmospheric	Y	Chem. Signature	Y	Y	75, 150	11
	B12	Cylindrical (2 mm, 4-disk)	electron gun	AIRI Seoul, Korea	No Info.	Molecule	Atmospheric (pulsed)	Y	Chem. Signature	N	Y	3	12
Magnetic Sector	B13	Double Focusing Sector Field Mattauch-Herzog	EI	OI Analytical	IonCam	Molecule	GC/ Atmospheric	Vac.	Chem. Signature	Y	Y	42 / bench	13
	B14	Double Focusing Sector Field	EI/CI	JEOL	GCmate	Molecule	GC/ Atmospheric	Vac.	Chem. Signature	Discont.	Y	400/bench	14
	B15	Double Focusing Sector Field	EI/CI	JEOL	JMS-700 MStation	Molecule	GC/ Atmospheric	Vac.	Chem. Signature	Y	N	6000 / floor	15
Time-of-Flight	B16	Linear/Reflectron	DART, ESI	JEOL	AccuTOF	Molecule	Atmospheric	Y	Chem. Signature	Y	N	>400/floor	16
	B17	Spiral	Maldi	JEOL	SpiralTOF	Molecule	MALDI	N	UF6 Isotope Ratio Analysis/ Chem. Sig	Y	N	>400/bench	17
	B18	Multi-Turn/Figure 8	EI/ Photoionization	MSI Tokyo	InfITOF	Molecular	Vacuum	N	Chem. Signature	Y	Y	88 / bench	18
	B19	Linear	SIMS	Millbrook/SAI	Mini-SIMS ToF	Molecular/Atomic	vacuum	N	Solid Surface Analysis	Y	Y	220/bench	19
Ion Cyclotron Resonance	B20	Fourier Transform-ICR	EI	Siemens	Quanta	Molecular/Atomic	Gas Phase/ GC	N	Chem. Signature	N	N	500/floor	20
	B21	No Info.	No Info.	Frinnov	No Info.	No Info.	No Info.	No Info.	No Info.	N	No Info.	No Info.	21
References	Hyperlinks												
1	www.waters.com/waters/nav.htm?cid=134672594&locale=en_US												
2	www.microsaic.com/products												
3	www.inficonemergencyresponse.com/en/hapsite_er/index.html												
4	www.minisims.com/minisims-alpha.htm												
5	www.thermoscientific.com/												
6	www.thermoscientific.com/												
7	www.chem.agilent.com/en-US/products-services/Instruments-Systems												
8	www.thermoscientific.com/ecom/servlet/productsdetail_11152___11960637_-1												
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10	gs.flir.com/detection/chemical/mass-spec/mobile-labs/cit												
11	Anal. Chem., 2012, 84 (22), pp 10105–10112 Publication Date (Web): November 1, 2012 (Article)												
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16	www.jeol.com/PRODUCTS/AnalyticalInstruments/MassSpectrometers/AccuTOFDART/tabid/141/Default.aspx												
17	www.jeol.com/PRODUCTS/AnalyticalInstruments/MassSpectrometers/JMSS3000SpiralTOF/tabid/752/Default.aspx												
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19	www.saiman.co.uk/minisims-tof-mass-spectrometer.html												
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21	www.fist.fr/en/measuring-instruments/a-compact-ftms-mass-spectrometer.html												

Table 5: Evaluation Criteria Guidelines for Mass Spectrometer Matrix			
Color Code	Significantly Meets	Meets	Significantly Fails to Meet
Minimum Detectable Quantity	<ng	ng-ug	>ug
Dynamic Range	>10 ⁶	10 ⁶ -10 ³	<10 ³
Maturity Level	Well established, common in laboratories, readily available, little or no customization	Basic principle is well established, common in well-equipped or specialized labs, some-what available, customization common	First generation or prototype, special order, built to order, highly customized, only found in specialized or select labs
Instrument Automation	Push-button operation, all tuning is automated and computer controlled, unskilled but trained operator can operate, no detailed knowledge of MS principals needed to run, unattended operation	Mostly computer controlled operation and tuning, skilled or trained operator required to maximize performance, some operator input or decisions required to maximize performance, unattended operation with oversight	Some or no computer control of tuning and operation, highly dependent on operator input and decisions, detailed knowledge of instrument principals required to run, no unattended operation
Data Processing Automation	Automatic data processing, results are automatically produced in report format, no decision points, automated QA	Automatic data processing with input or decision required by operator, calculations or formatting to produce report	Manual data processing and reporting, data interpretation required
Measurement Uncertainty	High precision and/or accuracy	medium precision and/or accuracy	low Precision and/or accuracy
Abundance Sensitivity	High, Adequate for depleted 235U/238U isotopic ratio	Medium, Adequate for LEU isotopic ratio measurements	Low, May or maybe not adequate for HEU isotopic ratio measurements
Mechanical Robustness	Transportable, easily broken down and set-up, mechanically stable, works in wide range of environmental conditions including non-lab and field use	Can be broken down, transported, and set-up without special support, requires special packaging for transport, requires normal lab environment for operation	Can not be broken down and transported without great difficulties, skilled personnel required to disassemble and assemble, Highly specialized, controlled lab environment required
Maintenance	Well established maintenance, trained technician can perform maintenance, all tools and parts reliability available, second source vendors available for parts and supplied, requires periodic vendor support	Maintenance performed by highly skilled/trained operator, specialized skill and knowledge needed, parts available from vendor, vendor support common	Specialized or vendor-supplied maintenance required, parts and supplies specialized and sometimes difficult to source, may require custom or one-time parts fabrication
Reliability	Always available, available 24/7 with minimal down-time	Dependable, expect some down-time for maintenance and repair	Finicky, expect more down-time than up-time
Electrical Requirements	Independent of AC line source, battery operated or built-in power transformer or conditioning incorporated for use with unstable line sources	Normal laboratory AC power required	Special or high-powered electrical requirements
Cost	<\$130K	\$130K-\$500K	>\$500K

Table 6. Criteria Evaluation Matrix

Elemental / Isotope Ratio Instruments		Minimum Detectable										Meas. Unc. (%RSD)													
		Conc. (ng/mL)	Sensitivity (kps/ppb)	Dynamic Range	Maturity Level	Instrument Automation	Data Processing Automation	Analyte conc.	Isotope Ratio	Abundance Sensitivity	Mechanical Robustness	Maintenance	Reliability	Electrical Reqs (VAC / A)	Cost (\$k)	Weight (lbs)									
Mass Analyzer	Instrument Number	Geometry	Ion Source	Manufacturer	Model	Data										Meas. Uncertainty									
						Maturity Level										Isotope Abundance Sensitivity									
						Instrument Automation										Mechanical Robustness									
						Data Processing Automation										Maintenance Reliability									
						Analyte conc.										Electrical Reqs									
						Isotope Ratio										Cost (\$k)									
						Abundance Sensitivity										Weight (lbs)									
						Maturity Level										Reliability									
A1	Quad - linear	ICP	Agilent	7700e/7700s/7700k	0.01	~90	E9	~3rd gen	Rel. Good	Good	Good	<4	<0.1	E7	Rel. Good	Rel. Good	Dependable	200-240 / 30	197	253					
A2	Triple Quad - linear	ICP	Agilent	8800	0.05	~200	E10	~3rd gen	More Complex	Good	Good	<3	<0.2	E10	Rel. Good	Rel. Good	Dependable	200-240 / 24	290	314					
A4	Quad - linear	ICP	Thermo Scientific	ICAP Q	<0.1	~300	E9	~3rd gen	Rel. Good	Good	Good	<3	<0.1	E7	Rel. Good	Rel. Good	Dependable	200-240 / 30	115	312					
A5	Quad - linear	ICP	PE Sciox	NexION 300 series	<0.5	40	E9	~3rd gen	Rel. Good	Good	Good	<4	~0.08	E7	Rel. Good	Rel. Good	Dependable	200-240 / 22	160	400					
A8	Quad - linear	SIMS	Millbrook/SAI	Mini-SIMS alpha	Matrix dep.	No info.	E7	Medium	Limited	PC	No info.	No info.	No info.	No info.	Med	User	Good	120 / 10	350	220					
Time-of-Flight	A21+	Reflection TOF	EI	KORE	MS-200	1-1000	No info.	No info.	Underv.	Limited	Limited	30	No info.	No info.	No info.	Med	User	Good	12 V Battery	64	55				
	A22	Linear TOF	SIMS	Millbrook/SAI	Mini-SIMS ToF	Matrix dep.	No info.	No info.	Medium	Limited	PC	No info.	No info.	No info.	Med	User	Good	120 / 10	350	220					
Molecular Instruments																									
Mass Analyzer										Minimum Detectable															
Geometry										Meas. Uncertainty															
Ion Source										Isotope Abundance Sensitivity															
Manufacturer										Mechanical Robustness															
Model										Maintenance Reliability															
Mass										Electrical Reqs															
Maturity Level										Cost (\$k)															
Dynamic Range										Weight (lbs)															
Quadrupole	B2	Linear/chip Based	EI	Microsaic	3500 MID	10 pg	E3	New	Little	On Board	No info.	NA	NA	NA	Good	Modular	Good	100-220 / 300W	No info.	60					
	B3	Linear	EI	Inftcon	Hapstra	<pg	E7	New	Good	On Board	No info.	NA	NA	NA	Good	Simple Field	Good	Battery / 15	150	42					
	B4	Linear	SIMS	Millbrook/SAI	Mini-SIMS alpha	Matrix dep.	E7	Medium	Limited	PC	No info.	NA	NA	NA	Med	User	Good	120 / 10	350	220					
	B5	Linear LCMS	AP/ESI/APCI	Thermo Scientific	MSQ+	20 pg	E7	Good	Good	Good	Good	No info.	NA	NA	Good	Good	Good	230 / 15	160	132					
	B6	Linear Triple Quad LCMS	AP/ESI/APCI	Thermo Scientific	TSQ Max	fg	E7	Good	Good	PC	No info.	NA	E10	Med	Level dep.	Good	Good	230 / 20	160	250					
	B7	Linear Triple Quad LCMS	AP/ESI/APCI	Agilent	6400 series	10 fg	E7	Good	Good	Good	Good	No info.	NA	NA	Good	Good	Good	230 / 15	225-475	255					
	B8	Linear 3D	GC, LC /AP/ESI, APCI	Thermo Scientific	LTO XL*, LCQ	<ng	No info.	Good	Good	PC	No info.	NA	NA	NA	Med	Level dep.	Good	Good	230 / 20	120	250				
Ion Trap	B9	Toroidal	EI/CI	Toron	Trition 9 GC-TMS	ppb-pptm (VOC)	No info.	New	Good	Good	Good	No info.	NA	NA	Good	Field	Good	Battery	85	32					
	B10.1	Cylindrical	EI	FLUR	Griffin 400	ug	No info.	New	Good	On Board	No info.	NA	NA	NA	Good	Level dep.	Good	Battery	87	82					
	B10.2	Cylindrical	EI	FLUR	Griffin 460	ug	No info.	New	Good	On Board	No info.	NA	NA	NA	Good	Level dep.	Good	Battery	130	98					
	B10.3	Cylindrical	EI	FLUR	Griffin824	ng	No info.	New	Good	On Board	No info.	NA	NA	NA	Good	Level dep.	Good	120	75	50					
	B11.1	3D Quadrupole	ESI, AP-MA/LDI, APCI	MassTech	Explorer 50	ng	No info.	New	Little	PC	No info.	NA	NA	NA	Good	No info.	Good	AC/DC	120	75					
B11.2	3D Quadrupole	ESI, AP-MA/LDI, APCI	MassTech	Explorer 100	ng	No info.	New	No info.	No info.	No info.	No info.	NA	NA	Good	No info.	Good	AC/DC	165	150						
Magnetic Sector	B13	Double Focusing/ Mattauch-Herzog/ Array detector	EI	OI	IonCam	ng	2000	New	Limited	On Board	No info.	NA	NA	NA	Good	Level dep.	Good	Battery	50	42					
	Time-of-Flight	B18	Multi-Turn/ Figure 8	EI/Photoion.	MSI Tokyo	p mol	E3	New	Limited	PC	No info.	NA	NA	Wf = 30,000	Good	Level dep.	Good	No info.	No info.	88					
B19		Linear	SIMS	Millbrook/SAI	MiniSIMS TOF	Matrix dep.	E6	Medium	Limited	PC	No info.	NA	No info.	Med	User	Good	Good	120 / 10	350	220					

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