Battelle
The Business of Innovation

REQUEST FOR PROPOSAL NO. 108013

Offer Due: October 9, 2009

Delivery Required Date: October 31, 2010

CONTRACT REPRESENTATIVE	SHIP TO:
Tanya Smith MSIN: K9-15 Battelle Boulevard P.O. Box 999 RICHLAND, WA 99352-0999 Tel: 509/375-6823 Fax: 509/375-3818 E-mail: tanya.smith@pnl.gov	PO #TBD Battelle for US DOE 3335 Q Avenue Richland, WA 99354 United States

THE REQUIREMENTS IDENTIFIED HEREIN WILL BE FUNDED BY THE AMERICAN RECOVERY AND REINVESTMENT ACT OF 2009. (RECOVERY ACT)

This is a request for proposal for purchase of equipment as outlined in the attached techincal specifications. Proposals should be initially submitted on the most favorable price and technical terms which can be offered because of the possibility that award will be made without discussion of proposal received.

Submit all offers on the form below showing unit and total prices for meeting the stated required delivery date. If unable to meet stated date, offer best delivery date.

LINE ITEMS

Line	Qty	U/M	Description	Unit Price	Total Price
1	1	EA	Multi-collector inductively coupled plasma mass spectrometer per the attached specification. Shall include two spare torches, one spare load coil, and gaskets; one each of type of turbomolecular pumps and controllers, fuses, scroll pump rebuild kit, two spare PC detectors.	-	-
			OPTIONAL ACCESSORIES:		
			spare pulse counting detectors	-	-
			FC detector amplifiers	-	-
			High voltage power suppliers as identified in the Section V of the specification	-	-
				-	-
			High efficiency, commercial-off-the-shelf, de-solvating nebulizer	-	-
			autosampler fully integrated with the MC-ICPMS instrument's control and data acquisition software	-	-
			laser ablation system integrated into the MC-ICPMS instrument's control and data acquisition software.	-	-

2	1	EA	High-resolution inductively coupled plasma mass spectrometer (ICP-MS) per the attached specification	-	-
3	1	EA	ultra-high-resolution mass spectrometer per the attached specification	-	-
4	1	EA	Multi-Collector, High, ICP-MS, and ultra high resolution mass spectrometry package	-	-

BATTELLE CONTRACTS REPRESENTATIVE

The Battelle Contracts Representative, Tanya Smith, is the sole point of contact for any communications or questions regarding this acquisition.

PRICING INFORMATION

[ ] A. Prices proposed herein are substantiated with enclosed copy of published price lists and/or catalog price sheets including conditions of any available discounts and are not more than those offered our most favored purchasers for similar quantities under like conditions.

[ ] B. Published price list and/or catalog price sheets are not available. The prices proposed herein are not more than those offered our most favored purchasers including the United States Government for similar quantities under like conditions. If checked, include copies of recent invoices, sales slips, etc., for similar quantities of like material or services to at least two (2) other firms for verification.

Signed_____

Date_____

SUBMISSION OF PROPOSALS

Proposals should be prepared simply and economically, and provide a straightforward, concise delineation of the information required to be furnished. Emphasis should be on completeness and clarity. Elaborate brochures or other presentations are neither required nor desired.

Each proposal submitted should include:

1. A statement of acceptance of the conditions referenced in the General Provisions below.
2. Completed Representations and Certifications Form - Commercial Items found at http://www.pnl.gov/contracts/documents/solicitations.asp
   - The NAICS code for section 2(a)(1) is 423490
   - The size standard for section 2(a)(2) is 100 employees

Proposals are preferred to be electronically submitted to tanya.smith@pnl.gov. Transmittals containing proposals should include "Proposal to RFP No. 108013" in the subject line. Proposals must be received by Battelle no later than October 9, 2009.

Proposals may also be submitted via facsimile at the number above or by hard copy the address above. Correspondence must include "Proposal to RFP No. 108013." Proposals submitted by overnight mail must be mailed to

Battelle, Pacific Northwest Division
6th Street Warehouse
790 6th Street
ATTN: Tanya Smith, K9-15
Richland, WA 99354

GENERAL PROVISIONS

Each proposal submitted shall include a statement of acceptance of the conditions referenced below. The conditions may be viewed as at http://www.pnl.gov/contracts/documents/generalprovisions.asp:

- Fixed Price General Provisions for Commercial Items - Supplies/Services, Form A-409-CI- R1
- General Provisions Supplement - American Recovery and Reinvestment Act of 2009 titled Form A-409-ARRA Suppl - R1

RECOVERY ACT REQUIREMENTS

The following Recovery Act forms will be applicable to the successful offeror and may be viewed at http://www.pnl.gov/contracts/documents/

- Reporting Requirements (Form A-409-ARRA-Reporting)
- Monthly Contract Cost-to-Date Estimate (Form A-409-ARRA-Accrual)

EXPLANATION TO PROSPECTIVE OFFERORS

Any prospective offeror desiring an explanation or interpretation of the RFP must request it in writing soon enough to allow a reply to reach all prospective offerors before the submission of their offers. Oral explanations or instruction given before the award of the contract will not be binding. Any information given to a prospective offeror concerning the RFP will be furnished promptly to all other prospective offerors as an amendment of the solicitation, if that information is necessary in submitting offers or if the lack of it would be prejudicial to any other prospective offeror.

PROPOSAL DUE DATE AND VALIDITY PERIOD

Proposals shall be delivered to Battelle on or before the proposal due date and shall be valid for a minimum of 60 days.

AMENDMENTS TO RFP

If this RFP is amended, all provisions which are not modified remain unchanged.

Offerors shall acknowledge receipt of any amendment of this RFP (a) by signing and returning the form provided for such purpose; (b) by stating in its proposal that the amendment (date and number) was received and considered in formulating the proposal; or (c) by letter or E-mail. Battelle must receive the acknowledgement by the time specified for receipt of proposals.

SUBMISSION, MODIFICATION, REVISION, AND WITHDRAWAL OF PROPOSALS *(CL 605, OCT 2007)*

1. Offerors are responsible for submitting proposals, and any modifications or revisions, so as to reach the Battelle office designated in the solicitation by the time specified in the solicitation. If no time is specified in the solicitation, the time for receipt is 4:00 p.m., local time, for the designated Battelle office on the date that proposal or revision is due.

2. Any proposal, modification, or revision received at the Battelle office designated in the solicitation after the exact time specified for receipt of offers is "late" and will not be considered unless it is received before award is made, the Battelle Contracts Representative determines that accepting the late offer would not unduly delay the acquisition; and--

   A. If it was transmitted through an electronic commerce method authorized by the solicitation, it was received at the initial point of entry to the Battelle, Pacific Northwest Division, infrastructure not later than 5:00 p.m. one working day prior to the date specified for receipt of proposals; or

   B. There is acceptable evidence to establish that it was received at the Battelle site designated for receipt of offers and was under Battelle's control prior to the time set for receipt of offers; or

   C. It is the only proposal received.

3. However, a late modification of an otherwise successful proposal that makes its terms more favorable to the Battelle, will be considered at any time it is received and may be accepted.

A. Acceptable evidence to establish the time of receipt at the Battelle site includes the time/date stamp of that installation on the proposal wrapper, other documentary evidence of receipt maintained by the installation, or oral testimony or statements of Battelle personnel.

B. If an emergency or unanticipated event interrupts normal Battelle processes so that proposals cannot be received at the office designated for receipt of proposals by the exact time specified in the solicitation, and urgent Battelle requirements preclude amendment of the solicitation, the time specified for receipt of proposals will be deemed to be extended to the same time of day specified in the solicitation on the first work day on which normal Battelle processes resume.

C. Proposals may be withdrawn by written notice received at any time before award. Oral proposals in response to oral solicitations may be withdrawn orally. If the solicitation authorizes facsimile proposals, proposals may be withdrawn via facsimile received at any time before award. Proposals may be withdrawn in person by an offeror or an authorized representative, if the identity of the person requesting withdrawal is established and the person signs a receipt for the proposal before award.

D. Unless otherwise specified in the solicitation, the offeror may propose to provide any item or combination of items.

E. Offerors shall submit proposals in response to this solicitation in English and in U.S. dollars unless otherwise permitted by the solicitation.

F. Offerors may submit modifications to their proposals at any time before the solicitation closing date and time, and may submit modifications in response to an amendment, or to correct a mistake at any time before award.

G. Offerors may submit revised proposals only if requested or allowed by the Battelle Contracts Representative.

H. Proposals may be withdrawn at any time before award. Withdrawals are effective upon receipt of notice by the Battelle Contracts Representative

4. Offer expiration date. Proposals in response to this solicitation will be valid for the number of days specified on the solicitation cover sheet (unless a different period is proposed by the offeror).

5. Restriction on disclosure and use of data. Offerors that include in their proposals data that they do not want disclosed to the public for any purpose, or used by Battelle except for evaluation purposes, shall--

A. Mark the title page with the following legend:

This proposal includes data that shall not be disclosed outside Battelle and shall not be duplicated, used, or disclosed--in whole or in part--for any purpose other than to evaluate this proposal. If, however, a contract is awarded to this offeror as a result of--or in connection with--the submission of this data, Battelle shall have the right to duplicate, use, or disclose the data to the extent provided in the resulting contract. This restriction does not limit Battelle's right to use information contained in this data if it is obtained from another source without restriction. The data subject to this restriction are contained in sheets [*insert numbers or other identification of sheets*]; and

B. Mark each sheet of data it wishes to restrict with the following legend:

Use or disclosure of data contained on this sheet is subject to the restriction on the title page of this proposal.

TREATMENT OF PROPOSAL DATA

A. Although not specifically requested by the RFP, the proposal may include technical data and other data, including trade secrets and/or privileged or confidential commercial or financial information, which the Offeror does not want disclosed to the public or used by PNNL or the Government for any purpose other than proposal evaluation. To protect such data, the Offeror will specifically identify each page including each line or paragraph thereof containing the data to be protected and mark the cover sheet of the proposal with the following notice:

NOTICE

> The data contained in pages _____ of this proposal have been submitted in confidence and contain trade secrets and/or privileged or confidential commercial or financial information, and such data shall be used or disclosed only for evaluation purposes. PNNL and the Government shall have the right to use or disclose the data herein to the extent provided in the contract. This restriction does not limit PNNL's and the Government's right to use or disclose data obtained without restriction from any source, including the Offeror.

Reference to this notice on the cover sheet should be placed on each page to which the notice applies. PNNL assumes no liability for disclosure or use of unmarked data and may use or disclose such data for any purpose.

B. Should a contract be awarded based on a proposal, it is policy, in consideration of the award, to obtain unlimited rights for the Government in technical data contained in the proposal unless the prospective contractor marks those portions of the technical information that he asserts as "proprietary data," or specifies those portions of such technical data that are not directly related to or will not be utilized in the work to be funded under this subcontract. "Proprietary data" are defined as technical data which embody trade secrets developed at private expense, such as design procedures or techniques, chemical composition of materials, or manufacturing methods, processes, or treatments, including minor modifications thereof, provided that such data: (1) are not generally known or available from other sources without obligation concerning their confidentiality; (2) have not been made available by the owner to others without obligation concerning their confidentiality; and (3) are not already available to the Government without obligation concerning their confidentiality. An Offeror who receives a contract award shall mark the data identified as proprietary by specifying the appropriate proposal page number to be inserted in the Rights to Proposal Data clause below. Subject to the concurrence of PNNL, information unrelated to the subject may be deleted from the proposal by the Offeror. The responsibility, however, of identifying technical data as proprietary or deleting it as unrelated rests with the Offeror.

C. The following clause shall be included in any contract based on a proposal. This clause is intended to apply only to technical data and not to other data, such as privileged or confidential commercial or financial information

RIGHTS TO PROPOSAL DATA

> Except for technical data contained on pages _____of the contractor's proposal dated _____, which are asserted by the Contractor as being proprietary data, it is agreed that as a condition of the award of this contract, notwithstanding the provisions of any notice appearing on the proposal, the Government shall have the right to use, duplicate, and disclose and have others do so for any purpose whatsoever, the technical data contained in the proposal upon which this contract is based.

ANTI-KICKBACK PROCEDURES *(CL 398 - JUL 1995)*

A. **Definitions**

"Kickback," as used in this clause, means any money, fee, commission, credit, gift, gratuity, thing of value, or compensation of any kind which is provided, directly or indirectly, to Battelle, Battelle employees, subcontractor, or subcontractor employees for the purpose of improperly obtaining or rewarding favorable treatment in connection with a prime contract or in connection with a subcontract relating to a prime contract.

"Person," as used in this clause, means a corporation, partnership, business association of any kind, trust, joint-stock company, or individual.

"Prime contract," as used in this clause, means a contract or contractual action entered into by Battelle for the purpose of obtaining supplies, materials, equipment, or services of any kind.

"Prime Contractor," as used in this clause, means a person who has entered into a prime contract with Battelle.

"Prime Contractor employee," as used in this clause, means any officer, partner, employee, or agent of a prime Contractor.

"Subcontract," as used in this clause, means a contract or contractual action entered into by Battelle or a subcontractor for the purpose of obtaining supplies, materials, equipment, or services of any kind under a prime contract.

"Subcontractor," as used in this clause, (1) means any person, other than Battelle, who offers to furnish or furnishes any supplies, materials, equipment, or services of any kind under a prime contract or a subcontract entered into in connection with such prime contract, and (2) includes any person who offers to furnish or furnishes general supplies to Battelle or a higher tier subcontractor.

"Subcontractor employee," as used in this clause, means any officer, partner, employee, or agent of a subcontractor.

B. **The Anti-Kickback Act of 1986** (41 U.S.C. 51-58) (the Act), prohibits any person from -

1. Providing or attempting to provide or offering to provide any kickback;
2. Soliciting, accepting, or attempting to accept any kickback; or
3. Including, directly or indirectly, the amount of any kickback in the contract price charged by a prime contractor to the United States or in the contract price charged by a subcontractor to a prime contractor or higher tier subcontractor.

C. 1. When the Contractor has reasonable grounds to believe that a violation described in paragraph B of this clause may have occurred, the Contractor shall promptly report to the Battelle Contracts Representative in writing the possible violation. Such reports shall be made to the inspector general of Battelle, and Battelle shall forward such reports to DOE, or the Department of Justice.

2. The Contractor shall cooperate fully with any Federal agency investigating a possible violation described in paragraph B of this clause.

3. The Battelle Contracts Representative may (i) offset the amount of kickback against any monies owed by Battelle under the prime contract and/or (ii) direct that the prime Contractor withhold from sums owed a subcontractor under the prime contract, the amount of the kickback. The Battelle Contracts Representative may order that monies withheld under subdivision C.3.(ii) of this clause be paid over to DOE unless Battelle has already offset those monies under subdivision C.3.(i) of this clause. In either case, the Prime Contractor shall notify the Battelle Contracts Representative when the monies are withheld.

4. The Contractor agrees to incorporate the substance of this clause, including this subparagraph C.4, in all subcontracts under this contract which exceed $100,000.

BID AND PROPOSAL COSTS

Battelle is not obligated to pay any cost incurred in the preparation and submission of a proposal, nor to enter into a contract or any other arrangement with any Offeror.

TYPE OF CONTRACT

Battelle contemplates awarding a fixed price contract for this request.

TECHNICAL SPECIFICATIONS

The enclosed Technical Specification outlines the requirements for this solicitation. Offerors may propose on any or all of the items listed above.

INSURANCE /PRELIMINARY HAZARDS ASSESSMENT (PHA)

As required in the referenced general provisions the Contractor must provide a valid insurance certificate and completed PHA prior to any work performed on-site.

PROMPT PAYMENT DISCOUNTS

In addition to normal payment terms, please advise amount and details of other cash discounts or savings available to Battelle for more expeditious or favorable methods of payment or for other reasons.

AUTHORIZED NEGOTIATORS

If a negotiation meeting is held, the Offeror shall designate as its negotiator a person who is authorized to make legally binding commitments without further review or approval. If, for any reason, it is impractical for the Offeror to be represented at a negotiation meeting by other than a person fully authorized to act in its behalf, Battelle shall be notified sufficiently in advance to allow a decision to be made whether the negotiations should proceed as scheduled or be postponed. The Offeror's notice, if originally given orally, shall be confirmed in writing.

CONTRACT AWARD

a) Battelle may evaluate proposals received in response to this solicitation without discussion. Contract award, if any, will be made to the responsive, responsible offeror whose evaluated proposal will be most advantageous to Battelle, considering only price and any price-related factors specified elsewhere in the solicitation, or

(b) Battelle may reject any or all proposals, and waive informalities or minor irregularities in proposals received, or

(c) Battelle may accept any item or combination of items, unless doing so is precluded by a restrictive limitation in the solicitation or the proposal, or

(d) Battelle may reject a proposal as non-responsive if the prices proposed are materially unbalanced between line items or sub-line items. A proposal is materially unbalanced when it is based on prices significantly less than prices for some items and prices which are significantly overstated in relation to prices for other items, and if there is a reasonable doubt that the proposal will result in the lowest overall price to Battelle even though it may be the low evaluated proposal, or if it is so unbalanced as to be tantamount to allowing an advance payment.

(e) Funding is obligated for this action. However, contract award is subject to Availability of Funds at the time of award.

<table>
<tr><td colspan="2" rowspan="3">We offer to sell the above items (or alternate items as specified) at the prices indicated, on the terms and conditions stated and the referenced general provisions which will be a part of any resulting order.</td><td colspan="2">F.O.B. DESTINATION</td></tr>
<tr><td colspan="2">Delivery Date at F.O.B. Point October 31, 2010</td></tr>
<tr><td colspan="2">Terms of Payment Payment terms shall be 80% at receipt of system and 20% after installation and acceptance of system to be completed within the timeframe identified in the technical specification. Payment shall be Net 30 upon receipt of invoice. If prompt payment discounts are available, please state</td></tr>
<tr><td>Offer Date</td><td>Firm Name</td><td>Weight</td><td>Recommended Carrier</td></tr>
<tr><td>Dimensions</td><td>Number of Boxes</td><td colspan="2">Origin Zip Code</td></tr>
<tr><td>Name/Title</td><td colspan="3">Signature</td></tr>
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Technical Specifications Overview

September 11, 2009

The Environmental Molecular Sciences Laboratory (EMSL), a part of Pacific Northwest National Laboratory (PNNL), desires to obtain enhanced capability for the determination of elemental and isotopic abundances and ratios in a variety of sample matrices and types. The EMSL currently possesses conventional inductively coupled plasma mass spectrometry (ICPMS) capability (quadrupole ICPMS) for metal and metalloid determination, but plans to augment that capability with high-precision multi-collector ICPMS (MC-ICPMS), high-resolution ICPMS (HR-ICPMS), and ultra-high-resolution ICPMS (UHR-ICPMS). Accordingly, bids are sought for each of these capabilities, with specifications as detailed below. PNNL reserves the right to make awards for these items either separately or as a package, and prospective offerers are encouraged to bid for any and all items.

Item 1 MC-ICPMS

A multi-collector, magnetic-sector ICPMS instrument is desired with multiple, moveable faraday and discrete dynode detectors enabling a wide range of precise isotopic ratios to be determined. The desired collector configuration is 10 faraday collectors, 3 full-size dynode detectors, and 2 compact dynode detectors. The MC-ICPMS must be configured to provide very high sensitivity (detection efficiencies of at least 0.3% for ^{238}U). Detailed specifications and needs are detailed in Appendix 1.

Item 2, HR-ICPMS

A high-resolution, magnetic sector ICPMS instrument is desired for interference free ICPMS determinations. Low-, medium-, and high-resolution modes of operation, allowing for 300, 4000, and 10,000 mass resolution measurements are required. Measurement linearity of $>10^{12}$, using both analog and pulse counting detection, and detection sensitivity of $< 1 \times 10^{9}$ counts per second/ppm concentration is also required. Detailed specifications and needs are given in Appendix 2.

Item 3, UHR-ICPMS

EMSL desires to develop ultra-high resolution ICPMS capability, following on PNNL's ground-breaking research involving the interfacing of orbital trapping mass spectrometry with ICP ionization sources. EMSL desires to interface ICP ionization sources to second-generation orbital trapping instrumentation, and thus requires an Orbitrap (or equivalent) mass spectrometer capable of delivering mass resolution of 100,000 R at mass ranges of 100-300 daltons. Detailed specifications and needs are given in Appendix 3.

Delivery Requirements

All equipment shall be installed in the Environmental and Molecular Sciences Laboratory, a national scientific user facility, at PNNL's Richland, WA location The instruments shall be delivered, installed, and PNNL staff trained not later than six months after receipt of a purchase order.

Technical Specification for a Multi-Collector Inductively Coupled Plasma Mass Spectrometer

Section I. General Requirements.

The mass spectrometer is intended for high precision isotopic analysis of small amounts of actinides, primarily uranium and plutonium, and other elements and isotopes. The proposed instrument's performance must be demonstrated using analytical protocols in which the sample analyte amount is limited. Thus, we request the offeror to provide data that meets performance specifications for various absolute amounts of analyte in the solution presented to the instrument. For uranium, these levels of interest are 1 picogram (pg), 10 pg, and 1000 pg . For plutonium, these levels are 1 femtogram (fg), 10 fg, and 1000 fg. If the offeror facility is unable to handle plutonium, then this requirement can be met by combining uranium performance data with background data at key plutonium isotope masses. Typically, these analytes would be presented to the instrument as 1 mL aqueous solutions of 1-5% nitric acid containing the above amounts of uranium or plutonium. Such small volumes minimize chemical blanks and are compatible with high efficiency, desolvating nebulizing systems. In addition, several isotopic compositions are of interest including uranium that is depleted in its abundance of ^{235}U relative to isotopically natural uranium, uranium that is isotopically natural, and uranium that is isotopically enriched.

There shall be a sufficient number of ion detectors to simultaneously measure as many as five isotopes of uranium (233, 234, 235, 236, and 238). These detectors, possibly augmented with additional detectors, shall also be usable for detection of as many as six isotopes of plutonium (238, 239, 240, 241, 242, and 244). At least three pulse counting (PC) detectors are required. These PC detectors will typically be accompanied by Faraday Cup (FC) detectors to enable monitoring of all isotopes of interest for a first element of interest and possibly for other elements whose isotopic masses overlap those of the first element of interest. Additional FC detectors beyond those needed for U and Pu shall be required to measure the isotopic composition of other elements in the Periodic Table (Li to Cm) without changing the number or sequence of detector types in the detector array. The instrument shall be capable of rapid changeover of either the magnetic field, cup positions, and optics potentials such that isotopes of multiple elements can be measured using a single, small aliquot of sample. That is, the magnetic field and optics switching and settling times as well as cup repositioning time (if applicable) must be short compared to data acquisition times so as to maximize utilization of the sample. The instrument must have very low detector dark currents and detector cross talk. Other background must also be very low, such as background from scattered ions, unstructured (continuous) by mass ions and spectral peaks at the masses of the isotopes analyzed. This is further defined in the section III.8

For uranium isotope dilution mass spectrometric (IDMS) analysis, ^{233}U is used as the spike. The isotopes in the sample which are of interest to be measured include ^{234}U, ^{235}U, ^{236}U, and ^{238}U. $^{235}U/^{238}U$ ratios range from 0.002 up to ~20 which will require the capability to accurately measure ^{234}U and ^{236}U in the presence of high levels of ^{235}U and ^{238}U.

The plutonium isotopes to be measured are ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, and ^{244}Pu. Plutonium-244 is used as the spike for IDMS measurements. Spiking levels may range from 1 to 100 fg. Quantities of ^{241}Pu and ^{242}Pu in the samples are normally much lower than the ^{239}Pu and ^{240}Pu levels. Care should be taken in the fabrication and testing of this instrument to minimize contamination or other issues that would lead to spectral background at these actinide masses of interest. The above Pu isotopes shall all be measured using PC detectors to provide maximum sensitivity. It is required that all Pu isotopes of interest must be measurable using PC detectors with at most two central axis mass settings (magnet field settings). PNNL requests a bid for a separately priced option for a detector array that enables simultaneous measurement of ^{239}Pu,

^{240}Pu, ^{241}Pu, and ^{242}Pu on PC detectors without compromising the ability to measure uranium isotopes as specified herein and without compromising the ability to measure other elements from Li to Cm.

Various other elements and isotopes are also desired to be analyzed. The instrument shall provide suitable flexibility to provide a wide range and number of environmental isotope determinations. The instrument, instrument control and data acquisition, analysis and output protocol must be optimized for high sensitivity, high precision isotopic measurements. Some of the following general requirements will be specified more fully in subsequent sections of this document.

Vacuum construction shall use state-of-the-art ultrahigh vacuum materials and techniques including non-magnetic, weldable, bakeable stainless steel wherever appropriate. The use of metal-gasketed, ultra-high vacuum compatible flanges is required in the instrument's vacuum chambers, except for the foreline vacuum sections, although metal gasketed flanges are preferred here as well. Equipment for baking the instrument must be included with the instrument.

The instrument is intended for analysis of small amounts of actinides and other environmental isotopes. It shall be possible to simultaneously monitor all Pu (238-244, excluding 243) or all U isotopes (233-238, excluding 237) on PC detectors using a maximum of two magnet settings.

Section II. Performance metrics

Performance metrics shall be demonstrated using solutions of standard reference materials where appropriate. Such test materials shall be provided by the offeror. Where signal intensities are stated in terms of ion currents, it shall be understood that this does not restrict measurement of such peaks to either a PC detector or to a FC detector.

II.1. Mass range

The instrument shall be capable of routinely detecting positive ions with mass-to-charge ratios between 1 and 280 Da/charge to enable the measurement of actinide molecular ions.

II.2. Mass resolving power and mass spectral peak shape.

The mass spectrum is defined as the plot of detected ion current as a linear function of mass-to-charge ratio. The mass peak is the shape of the spectral response as the magnetic field is scanned across a single isotope. The mass resolving power for each detector must be at least M/DM = 400 at 238 amu. DM shall be measured at mass M using the mass peak width at 10% of peak height. The mass peak top is defined as the portion of the peak between the points at which the ion signal is 99% of maximum on the high and low mass sides of the peak, respectively. The (mass) width of the peak top shall be no less than 50% of the (mass) width of the peak measured at 50% of peak maximum for both PC and FC detectors. Peaks must be flat with signal intensity variation less than 0.01% on all FC collectors over at least the central 50% of the peak top (determined as the relative standard deviation of 10 one second integrations of the signal across the peak top). Peak flatness must be 0.1% or better for all PC detectors.

II.3. Abundance Sensitivity.

The abundance sensitivity is the ratio of the signal contribution from an intense peak at a mass M measured at one mass unit higher or lower, (i.e., at an adjacent isotope's mass, M±1) to the signal of the parent peak at M. Abundance sensitivity is typically measured on the low mass side of a peak to account for scattered, reduced energy ions and to eliminate confusion that may arise from the presence of hydrides or other interfering ion peaks when measuring the high mass peak tail. Alternatively, abundance sensitivity can be measured at fractional mass positions and the value at

the mass of isotopes of interest interpolated. For at least one of the high sensitivity, PC detectors, abundance sensitivity shall be better than 0.5 ppm while meeting the sensitivity, peak shape and flatness requirements defined herein. Abundance sensitivity shall be measured as the ratio of mass ^{237}U ion current to the ^{238}U ion current under sampling conditions in which the signal at mass 238 is dominated by uranium and the signal at mass 237 is dominated by scattered uranium ions. The intensity of this scattered ^{238}U ion beam measured at mass 237 shall be at least 10 times the background at mass 237 so that the measured abundance sensitivity is dominated by scatter and not by other effects. Such low abundance sensitivity shall be provided on one or more PC detectors situated such that when the ^{234}U or ^{236}U beams are measured on the low abundance sensitivity PC detector, the ^{235}U beam can be measured on a second PC detector and the ^{238}U beam on either a PC or FC detector.

II.4. Sensitivity

The instrument must demonstrate high efficiency where efficiency is defined as the number of valid counts registered by the data system per atom in the sample introduced into the instrument. Such efficiencies are typically ~0.1% for the actinides in state-of-the-art ICP/MS instruments. These efficiencies are typically lower for light elements. The required performance for the PNNL MC-ICPMS is 0.3% (3 counts for every 1000 atoms in the solution being analyzed) for ^{238}U under conditions that simultaneously meet the peak shape, isotope ratio precision, mass resolving power, stability, and abundance sensitivity requirements set forth herein. When tuned for this high actinide efficiency, the instrument need not meet stringent sensitivity requirements for lighter elements. However, the response for Li, Sr, and U shall be at least 0.002%, 0.05%, and 0.1%, respectively, using a single instrument tuning optimized for this broad elemental mass range.

II.5. Stability.

Stability of high voltage power supplies shall be better than +/- 20 ppm over a 30 minute period. Ripple and noise shall not exceed 50 mV peak-to-peak. Critical ion optical components shall have voltage stability of 1 ppm, e.g., 5 mV lens bias stability relative to a source bias of 5000V.

Detected ion beam currents shall be stable over both short and long time periods under conditions optimized for other key performance metrics, especially sensitivity and abundance sensitivity. Short term stability shall be better than 0.5% (relative internal precision, 1-sigma) of 10 replicate 5 second integrations of a uranium isotope signal. Such stability shall be demonstrated over a period of at least 10 minutes. Long term stability shall be better than 2% measured using no more than one minute integrations of the same signal used for the short term stability measurement and shall be demonstrated for a period of at least 4 hours. All of the above stability measurements shall be demonstrated using both FC and PC detectors.

II.6. Uranium and Plutonium Background.

The instrument must be fabricated, assembled, maintained, operated, and delivered in an extremely clean condition with respect to uranium and plutonium contamination. The intensities of background peaks on all PC detectors in the mass spectral regions of interest (233 amu to 244 amu) shall be lower than 1 count/second (cps), except for the peak at mass-to-charge ratio 238, which shall have intensity less than 5 cps. Such backgrounds shall be demonstrated while introducing 1% nitric acid into sample introduction system associated with the ion source under normal sample uptake conditions. Non-spectral background, e.g., signals measured at “half-mass” position, in this region shall be less than 0.1 cps.

Actinide hydride levels must be kept very low. Uranium shall be used to characterize the hydride level. Uranium hydride ($^{238}UH^{+}$) abundance relative to $^{238}U^{+}$ shall be demonstrated to be lower than 20 ppm using the standard sample nebulizer and better than 5 ppm using a high efficiency, desolvating nebulizer such as a DSN, APEX, or PFA.

II.7. Non-actinide Background

While introducing a blank solution of nitric acid into the instrument, the background in the mass region 233-244 shall demonstrate that no actinides are detectable, except for uranium and then only at the ^{238}U isotope. The ^{238}U signal in such a background measurement shall be as low as possible, but in no case greater than 5 cps. This background shall be demonstrated to be stable; in particular, the standard deviation of this background signal shall be no worse than twice the Poisson counting statistics limit. For example, the background might be measured using 10 one minute integrations. At 5 cps, each such integration would yield an average of 300 counts. If these replicate integrated values are Poisson distributed, the standard deviation of the 10 replicate integrations will be $(300)^{-1/2}$, or 5.8%. Thus, the instrument must demonstrate a standard deviation no worse than twice this value or ~12%

II.8. Magnetic Field

The magnetic field must be stable and computer controlled. The magnetic field must be stable to +/- 50 ppm over a 30 minute period. A sensor to accurately measure the magnetic field, such as a Hall Effect probe, shall be included and the output of this sensor shall be recorded routinely with the data acquired for various scans. The output of this sensor shall also be available for measurement external to the instrument. The magnetic field control system must use a single, high resolution digital-to-analog converter to control the instrument mass setting across each mass range of interest. The smallest mass step of the computer controlled magnetic field shall be no larger than 0.001 amu in the mass region of uranium. Settling time shall be fast, such that rapid switching between the elements of interest (U, Pu) can be performed without sacrificing data acquisition time. This magnet switching and settling time between elements is taken as the time for a user selected mass position to be reached within ±0.005 amu. Any voltages that are changed in connection with this mass change shall also be stable within this magnet settling time as well as Faraday amplifier settling time. This time shall be less than 5 seconds and the magnet position shall be stable to ±0.01 amu for a period of at least 30 minutes. It is required that the instrument be capable of measuring at least 3 isotopes of each of these elements at a single mass setting, and to measure additional isotopes of other elements using additional magnet settings and do so with the aforementioned rapid magnet switching.

II.9. Detectors

PNNL requires that multiple detectors of each type, PC and FC, be provided such that simultaneous detection of the isotopes of interest is possible. The stability, noise characteristics, and dynamic range of these detectors must be sufficient to ensure that the precision of isotope ratio measurements for small samples is not detector limited, but are instead limited primarily by the counting statistics of the minor isotopes detected. Of course for higher count rates (exceeding 100K cps for conventional, large format electron multipliers), detector stability and/or linearity can begin to limit precision and accuracy. It is necessary that a sufficient number of PC detectors be provided so that all five uranium isotopes of interest (233, 234, 235, 236, and 238) can be measured using at most two magnet settings. Similarly, this same detector array shall be capable of measuring the six plutonium isotopes (238, 239, 240, 241, 242, and 244) of interest using at most two magnet settings. At a minimum, it shall be possible to simultaneously measure 234, 235, and 238 isotopes at a single magnet setting using PC detectors; this configuration is required for the lowest of the analyte levels of interest for this instrument. It is required that the detector

array contain additional FC and/or PC detectors to enable a wide range of elements from Li to Pu to be analyzed. Each detector must have separate amplifiers or pulse counting circuits as appropriate and data acquisition channels for simultaneous data acquisition of all detectors.

The PC detectors are to be spaced so as to allow for the simultaneous measurement of various actinide isotopes as described above. One possible configuration of detectors is shown in the Table below. The Table shows a subset of the full detector array in the vicinity of the detectors that would be used for actinide analysis; the full array will require additional detectors to cover the full elemental range of interest. The ability to analyze spiked samples using either a PC or FC detector for the spike is required; it is also desirable to analyze unspiked samples. For plutonium analyses, all isotopes of interest shall be measured on PC detectors. For uranium analyses, various configurations may be used depending on the amount and isotopic composition of the uranium to be measured. The offeror is requested and encouraged to suggest alternative detector configurations that may better meet the measurement requirements set forth herein. Inherent flexibility in detector placement, movement, and interchanging is desired so as to allow maximum flexibility in isotopic determinations across the elemental mass range previously defined.

Collector Configurations in the Vicinity of Actinide Ion Beams

Sample	**PC**	**PC**	**PC**	**XX**	**PC**	**FC**	**PC**	**XX**	**FC**
Pu-1	239	240	241			244			
Pu-2	240	241	242		244				
U low – un-spiked	234	235	236		238				
U low – spiked			238			235	234	233	
U high					234	235	236		238

Provision must be made for the inter-calibration of FC detector amplifiers on a routine basis using the same reference voltage. PC detector gains must be measurable to an accuracy of 1 part in one thousand. PC detector response must not deviate from a linear function by more than 1% for detected analyte signals covering the full response range of the detector, i.e., up to maximum count rates corresponding to the maximum routinely usable count rate specified by the detector manufacturer. A documented method, including all necessary hardware and software, for routinely calibrating the FC and PC detectors, must be provided. Calibration shall include calibration of detector linearity, absolute response, and cross calibrations to include FC to FC and PC to FC. FC detector amplifier circuits must be linear to better than 0.001% of full scale plus 0.02% of signal. Ion current measurement circuitry must have short time constants and low voltage coefficients at all gains to enable precise data acquisition within several (<5) seconds of applying an ion current to a detector. Cross talk between detectors must be sufficiently low such that there is no significant effect on key performance requirements set forth herein.

Specific detector systems:

III.9.a. Faraday Cup detection systems

FC detectors shall be shielded and the effects of secondary electron or ion emission suppressed. Stray ion beams shall not be able to impinge on FCs or on the components associated with the FC detector or signal leads (shielded case, suppressor plates, entrance aperture plates, in-vacuum amplifier leads, etc). The noise on each FC detector shall be less than 0.1 fA measured using a 1 second integration of the FC current. Such noise measurement shall be made with the plasma on and all instrument high voltages and magnet current applied.

III.9.b. Ion counting detection system

The PC ion detector systems (PC detector and associated amplifier, discriminator and pulse counting circuits) shall have absolute efficiencies (quantum efficiency) of at least 85%, i.e., at least 85% of ions impinging on the detectors shall produce a count under amplifier-discriminator settings which yield a dark count rate no greater than 1 count per minute. Apart from this efficiency requirement, the PC ion detector systems shall have dark count rates lower than 1 count per minute. The aggregated dead time for the PC detectors, associated amplifiers, and counting electronics as an overall PC detection system shall be $\leq$20 nanoseconds. The signal range of the PC detector shall be from the dark count rate to a count rate sufficient to achieve the isotope ratio precision requirements given herein. Specifically, the dynamic range of the PC detectors shall be sufficiently large to not limit the isotope ratio performance of the instrument for the analyte amounts of interest stated herein. This is especially important for intermediate ranges of analyte amount where the major isotope is clearly best measured using an FC detector, the minor isotope(s) are best measured with a PC detector, but isotopes of intermediate abundance can be measured with either an FC or PC detector. The maximum count rate of the PC detectors shall be given as the maximum rate that the PC detectors can sustain as part of routine analyses without unduly shortening the life of the detector. The maximum count rate of the PC detectors shall be included in the instrument performance specifications section of the offeror's response to this RFP.

Section III. Software and Host Computer

The host computer, its operating system, and the instrument control, data acquisition, data reduction, and data output shall be Microsoft Windows compatible. The host computer shall be US standard compatible and have the following minimum hardware components: 100 GB of free hard disk space on the delivered system, at least 3 GHz CPU operating speed, 2 GB RAM, Microsoft operating system (XP preferred), two LCD monitors (each at least 20 inches wide), at least three USB ports on the front of the CPU case with additional USB ports on the back of case, and a DVD burner.

The instrument must be delivered with computer-controlled ion source, ion optics, magnet and detector electronics. The instrument control software must be integrated with software that controls data acquisition and post-acquisition data reduction. The source code for instrumental control, data acquisition, storage, reduction, and display shall be provided. It is required that source code and complete algorithm descriptions associated with data acquisition, post-acquisition processing, and processing be provided. The latter is intended to enable the user to perform all data manipulations to obtain fully corrected and calibrated isotope ratio results independent of the offeror's software. The program must provide an accurate timebase for all operations and data will be acquired and stored as high precision (time, mass, integrated signal from all detectors) records with appropriate indexing and supporting parameters (e.g., dwell time, amplifier gain range, number of scans). The data acquisition software must include provision to acquire, store, recall, and export mass spectra over defined mass ranges, displaying detected ion current data acquired in real time on linear or logarithmic scales versus mass. The mass range for

such “mass scans” shall be over any user selected scan start and end values including up to the full mass range of the instrument. The software will also provide capability to acquire ion currents as a function of time at a single magnetic field setting and display such acquired data in real time during the acquisition. Such real time display of detector signals shall be possible for any number of detectors simultaneously including for all detectors (PC or FC). In either the mass scan mode or temporal scan mode, the software shall provide for both numeric and graphical display of the data being acquired for any number of detectors up to and including for all detectors.

The software shall provide for both graphical and numeric display of data, analysis of data (eg, isotope ratio calculation, baseline drift correction, fitting of data to simple functional forms), and exportation of data to commercial spreadsheet software. Data and displays from all scan types and calculation results, numeric or graphical, shall be fully displayable and fully exportable. Common mass bias correction functions (linear, power law, exponential) shall be incorporated into the data reduction/correction software. The PC detector deadtime used in calculations shall be able to be changed by the user. Isobaric and molecular ion interference corrections shall be built in to the software enabling interference corrections to be made without exporting the data. Calculated values such as isotope ratios, interference corrected signals (count rates or ion currents), ratios of interference corrected signals, shall be able to be displayed in real time. Such display of calculated values shall include current as well as recent history of such values, for example, a display showing a user selectable time window of such data from the present back to 10 minutes earlier, 1 hour earlier, etc.

Section IV. Additional requirements and specifications

IV.1. Power.

PNNL requires that the instrument be supplied ready for use with United States standard electrical power. If transformers are required for operation with U.S. standard electrical power, such transformers shall be included with the instrument.

IV.2. Pumping System.

The high vacuum pumps shall be turbomolecular pumps and shall be provided from a commercial vacuum pump manufacturer along with required controllers. The foreline pump for the turbomolecular pumps shall be a scroll pump. All tubes, chambers, valves, and other vacuum components of the foreline pumping system shall be thoroughly degreased prior to assembly and use so as to eliminate hydrocarbon contaminants. All such components be of stainless steel construction and/or UHV compatible (all metal gasket seals) or alternative that provides high vacuum conditions with low levels of atmospheric contaminants. With these provisions, the components of the foreline and forepump system will be interchangeable with other mass spectrometers at PNNL.

IV.3. Datalogging.

Provision shall be made for recording data acquisition setups, instrument status, and tuning parameters for each analysis (i.e., for each mass spectral or temporal scan recorded by the instrument). Provision shall also be made for logging the following instrument parameters during each analysis: the magnetic field strength measured with at least 16 bits of resolution and the critical high voltages that affect ion beam stability and mass position.

IV.4. Instrument Design, Fabrication, and Testing.

Only oil-free vacuum pumps (high vacuum and foreline) will be used in all stages of fabrication, assembly, testing, and use. All spectrometer components shall be fabricated from non-magnetic materials.

At no time during assembly and testing shall the instrument be exposed to large amounts of substantially non-natural isotopic composition elements of interest. By "large amounts", we mean the largest aliquot sizes listed herein for the various performance tests.

Section V. Spare parts, options and consumables

The delivered system shall include the following spare parts and consumables:

1. ICP parts to include at least two spare torches, one spare load coil, and gaskets

2. one each of the various types of turbomolecular pumps (and controllers) used in the instrument.

3. Fuses

4. Scroll pump rebuild kit

5. Two spare PC detectors

In addition, PNNL requests that the bid include pricing and delivery for an option to purchase additional spare pulse counting detectors, FC detector amplifiers, and the following high voltage Power supplies

1. Ion accelerating potential
2. Ion optics (focusing and steering)
3. Pulse counting detector power supply

PNNL also requests pricing and delivery for the following optional accessory items.

1. High efficiency, commercial-off-the-shelf, de-solvating nebulizer.
2. An autosampler whose operation and control is fully integrated with the MC-ICPMS instrument's control and data acquisition software. This autosampler should accommodate a range of sample vial volumes from at least as low as 1 mL to at least as large as 10 mL.
3. A laser ablation system integrated into the MC-ICPMS instrument's control and data acquisition software.

Section VI. Documentation and Training

VI.1. Documentation

Documentation and manuals shall be provided describing all aspects of operations, data reduction methods, data calculations, maintenance, and troubleshooting of every sub-system of which the instrument is comprised. Typically these sub-systems are the vacuum system, low and high voltage power supplies, magnet power supplies, data acquisition electronics, and software. These systems also include various controlling electronics associated with each sub-system. Software refers to all instrument control, host computer to instrument computer/controller interface, and data acquisition, reduction, and display functions. Firmware components and code shall be documented where these are not described in other hardware or software documentation. Two

copies each of both electronic and paper (hardcopy) versions of all manuals and drawings shall be provided.

VI.2. User Training

Training shall be provided for up to three PNNL staff, such training to include at a minimum all aspects of instrument start-up, shutdown, procedures for recovery from a facility power or other utility failure, hardware and software setup, data acquisition, data display, export and processing, instrument tuning, operation, and maintenance. Training shall include a demonstration of the uninterruptible power supply capability. Training shall be provided covering all instrument setup, tuning, and operations required to demonstrate the required performance metrics set forth herein as well as to perform analysis of samples. Training shall include incidental aspects of instrument operation such as display and analysis of data both in real time and using stored data, exporting of data files into commercial software programs, and the creation and use of programmed sequences of analyses.

VI.3 Offeror Training.

Offeror training will be required for the laboratory work associated with installation and testing on-site. The instrument shall be installed in the Environmental and Molecular Sciences Laboratory, a national scientific user facility, at PNNL's Richland, WA location. Safety and other operational training specific to that building will be required prior to the start of laboratory work at PNNL. Such training will be provided by PNNL.

Section VII. Performance Test Plan

The offeror shall demonstrate instrument performance on the instrument after installation at PNNL that meets all of the offerors published specifications for the instrument. In addition to the offeror performance tests, the following specific measurements and resulting data, unless they are equivalent to a published offeror specification, shall be provided at various phases of the award process. Where offeror published performance specifications and performance tests described herein differ in their stringency, the more stringent test or specification shall be demonstrated. For each measurement required, the raw data shall be provided as well as the final calculated parameters, e.g., stability, sensitivity, etc. These measurements will require work to be performed at both the offeror's site and at PNNL in Richland, WA. An equivalent measurement protocol can be offered by the offeror as part of the offeror's bid, but it's suitability for determining the performance metric of interest shall be determined by PNNL. Prior to shipping, the offeror shall provide in writing to PNNL a description of how their instrument will be operated to achieve each of the performance tests required.

VII.1. Sensitivity.

The required sensitivity (section III.3) shall be demonstrated by performing replicate analyses of an isotopically certified uranium standard solution. For this test, the solution can be of natural or near-natural isotopic composition. Sensitivity shall not be increased at the expense of resolution or isotope ratio precision; PNNL requires an optimization of these and other performance metrics which maximizes precision and accuracy of isotopic composition measurements when the amount of analyte element is highly limited, e.g., when the total amount of available actinide element is 1 picogram or less.

VII.2. Mass Resolving Power and Peak Shapes.

The required mass resolving power and peak shape shall be demonstrated by mass spectral scans of ^{6}Li, ^{23}Na, ^{88}Sr, ^{144}Nd, and ^{238}U. These scans shall be acquired using at least six decades of

detector dynamic range, that is, the maximum signal for each peak shall be at least 1,000,000-fold larger than the adjacent half-mass background signal. In this way, the shape of the peak tails can be quantified.

VII.3. Abundance Sensitivity

The required abundance sensitivity shall be demonstrated by mass spectral scans of the 235-240 mass range while introducing isotopically natural uranium. Such scans shall be acquired at a mass increment no greater than 0.02 amu, i.e., there shall be at least 50 channels of data per amu in the mass spectral scan. The concentration of the uranium solution shall be selected such that the intensity of the $^{238}U^{+}$ peak during such scans shall be sufficient to obtain scattered $^{238}U^{+}$ signals at mass 237 that are at least 10 times the background.

VII.4. Stability

The required voltage stabilities shall be measured by appropriately configured recording oscilloscope and/or multimeter. The ion beam current variations shall be documented using a mass peak no more intense than required to meet the stability specification.

VII.5. Non-Actinide Background

The required low background for non-actinide masses shall be demonstrated by acquiring mass spectral scans over appropriate regions under conditions for which the instrument meets all other performance specifications, especially mass resolution, peak shape, sensitivity, stability, isotope ratio precision, and abundance sensitivity. The test shall be done both with and without uranium introduced into the ion source. For the purposes of this test, the flow rate of uranium into the instrument shall be sufficient to yield ^{238}U ion current of 10 pA.

VII.6. Actinide Background

The required background for key actinide masses shall be demonstrated by data acquisition at the appropriate masses. At the conclusion of on-site testing at PNNL, the background at mass 238 shall be no more than 5 counts/sec when introducing 1% nitric acid into the instrument. The background for all other masses of interest in actinide analysis (mass 233 to 244 inclusive) shall be less than 0.1 counts/sec. Sufficient dwell time on each mass shall be used in this measurement to provide an uncertainty (1-sigma) on the background measurement that is no greater than 10% of the background signal.

VII.7. Magnetic Field

The required magnetic field stability, settling time, and reproducibility shall be demonstrated by monitoring ion currents on the sides of appropriate mass peaks during mass peak switching between elements, e.g., monitoring the side of the ^{238}U peak after having switched from monitoring of a nearby mass such as ^{233}U.

VII.8. Detector Performance Demonstration

The required performance for detectors shall be demonstrated for each detector by performing the following series of measurements. Data shall be acquired which is sufficient to determine the FC dark current and ion counting detector dark count rates to an accuracy of 10% or less. The offeror shall provide a written description of tests that will be utilized to demonstrate and quantify:

VII.8.1. Low cross talk. It is suggested that low cross talk be demonstrated by recording mass spectral scans on all detectors simultaneously while scanning an intense beam such as that from ^{209}Bi or another mono-isotopic element across the entire detector array. In this way any cross talk from the large signal associated with ^{209}Bi striking a given detector can be simultaneously registered on all other detectors. While the offeror need not use this method, a comparable data set shall be required which satisfactorily demonstrates low cross talk. Low cross-talk is defined herein to mean that the signal on a given detector under test shall be no greater than 50% above its dark count/current while scanning a beam over any other detector that is 10^7-fold more intense than the dark count/current of the detector under test. For example, if a PC detector is being assessed (dark count rate is 0.1 cps), then a 10^6 cps beam is scanned across all other detectors. If a FC detector is being assessed (noise level 0.1 fA), then a 1 nA beam is scanned across all other FC detectors (clearly one would not expose a PC detector to such an intense beam).

VII.8.2. Linearity of the response of the detectors and their associated amplifiers and other electronics shall be demonstrated including measures of the maximum counting rate for ion counting detectors before they depart from linearity in response.

VII.8.3. Inter-calibration of the gains of FC and PC detectors. It is suggested that this measurement can be made using an isotopically natural certified reference material such as U129a (formerly U950). In this measurement, an FC detector is used to measure $^{238}U^+$ and a PC detector to measure $^{234}U^+$. The measured ratio is corrected for mass bias (determined internally or externally) and then compared with the certified isotope ratio. This measurement is then repeated with other combinations of the FC and PC detectors in a sequence that provides inter-calibration of any detector (FC or PC) with any other detector. With PNNL concurrence, the offeror may use an alternative method to demonstrate inter-calibration.

VII.9. Actinide Isotope ratio Determinations

The isotopic ratios of selected uranium reference materials shall be demonstrated to be accurately measured for total uranium amounts ranging from 1 picogram to 10 nanograms. These amounts refer to the amount of uranium consumed during a single analysis, not necessarily to the amount present in the solution presented to the instrument for such analysis. Accuracy shall in all instances be demonstrated to be within the statistical precision of the measuring devices and the appropriate corrections (e.g. dead time and PC quantum efficiencies), but in no case shall the total uncertainty (random and systematic sources of uncertainty appropriately propagated) in the measured $^{235}U/^{238}U$ isotopic ratios be worse than 0.1% of the measured ratio and in no case shall the measured $^{234}U/^{238}U$ total uncertainty be worse than 1%.

Isotope ratio precision shall also be demonstrated with elements spanning the full elemental range of the instrument. In addition to U and Pu, these other elements shall include at least Li, Sr, Nd, and Pb.

Section VIII. Consumables Spare Parts, and Options

While certain spare parts and consumables are to be included with the instrument, the offeror is requested to provide separate bids for additional consumables, optional equipment, spare parts, extended warranty, and annual maintenance and service plans.

Section IX. Requirements by Award Stage

It is our intent to procure a commercially available instrument that meets the specifications in response to this request. The following information must therefore be provided as part of any response to this RFP:

a. example data corresponding to tests VIII.1, VIII.2, VIII.3, VIII.6, and VIII.9 in the Test Plan. These data can be from any instrument comparable to the one to be fabricated in response to this request. These data are to be representative of the performance of the instrument proposed to be built.

b. a list of customers who have purchased the same or comparable instruments in the last three years.

IX.1 Pre-shipping Stage

a. Provide test data for tests VIII.1 through VIII.9 in the Test Plan. Data corresponding to each of the tests VIII.1 through VIII.9 inclusive shall be provided in an electronic format that is readable in commercial spreadsheet software as well as in hardcopy format (graphs and plots of data, narrative of the testing performed). The instrument shall not be shipped until PNNL provides a written statement that the above data have been received and are acceptable.

b. A listing of all items to be shipped shall be provided, including documentation, manuals, drawings, accessories, spares, and consumables. Items not available for shipping with the main instrument, but that are intended to be shipped at a later time, shall be specifically called out and identified along with a guaranteed date of shipment.

IX.2 , Installation, and On-Site Training Dates

. The offeror shall install, test, and train in accordance with the requirements set forth herein not later than 8 months after receipt of the purchase order.

IX.3 Final Acceptance

Prior to final acceptance of the instrument by PNNL, the following shall be demonstrated or delivered:

a. A fully functional instrument, including all components, spares, accessories, consumables, and related hardware shall be delivered, installed, and tested in accordance with the Test Plan described herein.

b. All performance metrics shall be successfully demonstrated on the delivered instrument as described in the Test Plan.

c. All documentation shall be delivered in both electronic and hardcopy formats.

d. All training shall be completed.

Section X. Software Upgrades and System Warranty

The offeror shall provide to PNNL at no charge all software modifications and software upgrades that occur during the warranty period.

The offeror shall warrant the complete instrument and associated components or systems to be free of defects in materials and workmanship including software for a period of two years from

the date of final acceptance. Power supplies and electronics shall be warranted for a period of three years from the date of final acceptance. During the warranty period, the offeror will repair or replace any defective structures, components, or sub-systems in the instrument and will bear all costs, including travel, labor, and per diem, associated with such repair or replacement. Replacement parts shall be reasonably available, but in no case shall more than 30 days be required to provide such parts with the 30 days measured from the date of the determination by PNNL and the offeror that such parts are needed.

Technical Specification for a High-Resolution Inductively Coupled Plasma Mass Spectrometer

Section I. Introductions and General Requirements.

The diversity of sample types encountered from the wide range users of the EMSL facility demands a HR-ICP/MS that pushes the edge of the elemental analysis envelope. The HR-ICP/MS acquired for the EMSL user facility must handle sample concentrations ranging from ultra-trace, parts per quadrillion levels, to levels in excess of several parts per million. These samples may arrive in solid, liquid or gaseous form requiring novel sample introduction techniques that place even further demands on the flexibility of HR-ICP/MS instrument. The complexities of samples of biological origin, for example, place demands on the ultimate resolution in order to resolve interferences, but also require that a lower resolution, quick scan method be available to rapidly map the composition and possible interfering species so an appropriate sample introduction and analysis method can be developed and applied. The ability to detect transient signals is absolutely critical for novel introduction methods such as laser ablation of minute biological samples. Instrumental backgrounds must be sufficiently low to not interfere with required detection limits. Large numbers of samples must often be analyzed over long periods of time, demanding extremely stable instrument performance. Control and tuning of the instrument must be routine to allow use by a number of EMSL users, and the instrument's parameters must be easily accessible through software to allow accurate documentation and reporting. Data must be exportable in a number of data formats to allow easy dissemination of results in reports and publications. Finally, the instrument should match as closely as possible the available space, power, cooling and water requirements of the designated space in the ESML facility to minimize facility modification costs.

These specifications are summarized below:

Section II. Specifications

II.1 Dyanamic Range

The HR-ICP/MS must have a dynamic range of at least 10^{12}, 2 fg/g – 2000 ug/g , extendable by up to a factor of 50 by running the lowest concentration elements in low resolution mode and the higher concentration elements in a high resolution mode. This dynamic range shall be rapidly accessible, without instrumental hardware changes, to allow accommodation and analysis of samples containing elements of interest over a dynamic range of at least 10^{12}. Ideally the full dynamic range would be accessible by an automated software implementation.

II.2 Detection Circuits

Particle counting, analog detection and Faraday current modes should be available not only as a means of extending dynamic range, but for possible cross checking of calibrations and trouble shooting procedures. The switching of each mode shall overlap by at least two orders of magnitude and there should be provision for automatic cross-calibration between the three measurement modes

II.3 Specifications Relating to Detection and Dynamic Range

1. Signal integration times as low as 1 ms
2. No decay time after exposure to high intensity signals
3. Automatic switching between detection modes with a delay less than 1 ms
4. Cross-over ranges between modes of greater than 2 orders of magnitude
5. Automatic cross-calibration between detector modes
6. Dynamic Range
   - Faraday: 5×10^{7} cps – 1×10^{12} cps - 1 ms sample time
   - Analog Detector: 5×10^{4} – 1×10^{9} - 1 ms sample time
   - Pulse Counting Dectection: 0.2 cps - 5×10^{6} cps – 100 □s

- Dynamic Range for Electron Multiplier: > 9 orders of magnitude
- Dynamic range of detector system including Faraday collector: > 12 orders of magnitude

7. Dark noise less than 0.2 cps, and independent of "interference removal mode
8. SEM plateau on the order of 300V

II.4 Measurement Stability

1. Better than 1% RSD in 10 minutes
2. Better than 2% RSD in 1 hour

II.5 Scan Speed and Stability

- The high demands placed on the ESML HR-ICP/MS for the analysis of repetitive, transient signals as well as long term slowly varying sample concentrations dictate stringent specifications in these areas.

II.6 Magnet Characteristics, Scan Speed, Stability and Reproducibility

1. Mass range must meet or exceed 2-260 at full accelerating voltage
2. Full accelerating voltage must be 8-kV
3. Scan speed of range from m/z 7 to m/z 240 in less than 150 ms
4. Stability/reproducibility during scanning better than 25 ppm in 8 hours
5. BE sector geometry, with ability to add retardation lens for best abundance sensitivity (< 25 ppm)
6. Scan modes:

A. *SCAN MODES*: The instrument shall offer a wide variety of scan modes, which will allow the Laboratory to optimize experimental design, including

A. B-scan (*magnetic field scan*)

a. normal operation:

i.<350 ms, all isotopes between 23-240-23 amu with scan time 1 ms per amu

ii.600 ms, all isotopes between 6-238-6 amu

b. Rapid magnet scan option

i.7Li-238U-7Li in 125 ms

B. B-jump (*magnet field peak jump,* to change between regions in the periodic table):

1. 1 ms/amu: jump from 100 to 140 takes 40 ms
2. In order to jump between regions in the periodic table, the magnet must support extremely rapid peak jumps, with mass range switching time (at low resolution) between *30 and 50 ms* depending on mass jump, including settling time. *Settling time* is on the order of *10 ms*, but depends on range that has been jumped, and is expected to be on the order of 1 ms/amu.
3. NOTE: FAST MASS CONTROL: To obtain peak-to-peak transfer speeds <1ms, the capacitive loading of the power supply is kept to a minimum by not floating the RF generator, the torch, and the cone system at accelerating voltage potential

C. HV-scan *(high voltage scan, =E scan*): <10 ms for +30% above magnet rest mass

1. Park magnet at 100 and scan to mass 130 in 10 ms
2. It is possible to scan all Ba isotopes at 10 passes/second with >90% on-peak duty cycle

D. HV-jump (*high voltage peak jump, =E jump*): Peak to peak transfer speed <1 ms, for rapid and precise measurement of isotope ratios

E. Optimization of acquisition windows: Multielement analysis shall routinely be done with acquisition windows no greater than 10% (Low Resolution), 30% (Medium Resolution) and 50% (High Resolution).

II.7 Resolution

1. Resolution (R) shall be variable
2. Low Resolution (R=300) for analysis of isolated isotopes and quick analysis of unknowns. Flat top peak shape is highly desireable for high-precision isotope ratio measurements
3. Medium Resolution (R=4000) for most elements in simple sample matrices
4. High Resolution (R=10000) for analysis of elements in complex samples anticipated to be encountered frequently in ESML use facility

II.8 Software Control

1. Auto tuning of all major ICP parameters
2. Automated auto-sample and start and stop sequences
3. Easy display and access to isotopes of interest for creation of acquisition routines
4. Easy or automated isobaric corrections
5. Easy creation and modification of data acquisition sequences
6. Software must allow collection of data in multiple resolution settings during a single analysis

II.9 Analytical Figures of Merit (to be demonstrated at installation)

1. Detection limits <0.1 ng/l In at 3s of the background, R=300 (100 ppq)
2. Sensitivity:
    a. R=300: count rates $\geq 1x10^9$ counts per second per ppm Indium with standard PFA low flow (100 uL) nebulizer (ESI sample introduction system), without need for ultrasonic or desolvating nebulizers *(to be demonstrated at installation*)
    b. R=4000: count rates $\geq 5x10^7$counts per second per ppm Fe *(to be demonstrated at installation)*
    c. R>10000: count rates $>5x10^6$ per second per ppm (to be demonstrated at installation)
3. Isotope ratio precision:
    a. $^{235}U/^{238}U < 0.1\%$ RSD, for U nat, U005 and U010
    b. $^{234}U/^{238}U < 0.3\%$ RSD, for U010
    c. (n=10 measurements, > 10 ppb U)
4. Hydride formation: $^{238}UH/^{238}U$: < 0.0002 (20 ppm) for natural uranium
5. BaO/Ba ratio: 0.2%
6. $M2^+/M^+$ Ba <0.03
7. Cold Plasma Mode: operation down to 600 W
8. Dark noise: The average count rate across 10 neighboring channels of the electron multiplier is < 0.2 cps.
9. Pulse discriminator dead time <20 ns

II.10 Transient Signal Analysis

1. It shall be possible to collect rapid scans across the detector during a transient signal: Rapid magnet scan option, 7Li-238U-7Li in 125 ms
    - HV-scan *(high voltage scan*): <10 ms for +30% above magnet rest mass

2. The detector system shall have a dynamic range approaching or greater than 9 orders of magnitude in order to deal with the variation in abundance expected from real samples.

II.11 Vacuum System

1. Analyzer pressure is $<1x10^{-7}$ mbar.
2. This pressure shall be achieved with (at least) a five stage differential pumping system using turbomolecular pumps
3. Turbomolecular pumps shall be state of the art, with ceramic bearings.
4. The vacuum system shall be safety protected with a hard-wired vacuum integrity system with start-up and shutdown sequencing. The vacuum shall be monitored in the lens stack and the forevacuum
5. It shall be possible to monitor the pressure in the ESA. (In the ELEMENT2, this is performed by moving a gauge head from the lens stack to an existing plug-in in the ESA region).

II.12 Electronics

All control and acquisition electronics shall utilize complete fiber optic opto-isolation between digital and analogue circuitry in order to avoid ground loops and to prevent any damage to the digital electronics due to high voltage arcing.

II.13 Computer Hardware & Data Acquisition

1. The MS shall utilize a distributed processing systems using a 32-bit front-end microprocessor for instrument control and a work station for data processing.
2. Connection between the work station and the mass spectrometer shall be via an industry-standard Local Area Network (LAN) connection (e.g. ETHERNET).
3. With addition of a second Ethernet card, it shall be possible to process the data via a laboratory network
4. All acquired data shall be in spreadsheet compatible format for easy export to external packages.
5. The operating system shall be Windows NT
6. The software shall be written in C++
7. The tuning screen shall allow display of up to six peaks at a time.
8. Autotune of all instrument parameters for automated tuning
9. Full remote control via Internet/Modem/LAN
10. Full LIMS connectivity
11. Method Wizard for automatic method development
12. Full QA/QC procedure
13. EPA 200.8 compliant
14. Real time monitoring of an unlimited number of transient signals
15. Laser triggering

II.14 Serviceability

1. Instrument control via modem shall be enabled, to allow remote real time operation for purposes of trouble shooting, using diagnostics, or running pre-specified routines. This capability is a routine function, and is supported by both computer software and instrument electronics. This shall be setup and demonstrated on the 2nd tool controller.
2. All printed circuit boards (PCB) shall provide generalized input/output connections, test points for measurement of signals, and LED go-nogo diagnostic indicators for all vital PCB parameters.
3. All instrument parameters as well as all go/no PCB diagnostic indicators shall be computer settable and/or computer readable to facilitate complete computer-driven diagnostics as well as storage of this information for QA/QC procedures.
4. All computer hardware shall be of non-proprietary, standard PC design to facilitate easy system expansion and to allow connection with laboratory information management systems (LIMS).

5. Diagnostics software shall run in the background, concurrent with normal instrument operation.
6. Cones shall be readily accessible, allowing easy examination and exchange. The cones shall be threaded and shall not have screws.
7. It shall be easy to exactly and quantitatively align the torch in X,Y and Z directions.

II.15 Physical Parameters

1. Power 3-phase 230/400V 50/60 Hz fused at 32 A per phase. Consumption 9 kVA. PNNL requires that the instrument be supplied ready for use with United States standard electrical power. If transformers are required for operation with U.S. standard electrical power, such transformers shall be included with the instrument.
2. Temperature 18-24 ºC , Humidity 50-60%
3. Cooling Water 10 – 20 ºC, 43 – 65 psi
4. Argon purity 99.996% minimum, uninterrupted at 116 – 145 psi
5. Exhaust total flow of 900 m^3/hr
6. Dimensions 92" x 176" x 148" or less

III. Documentation

Documentation and manuals shall be provided describing all aspects of operations, data reduction methods, data calculations, maintenance, and troubleshooting of every sub-system of which the instrument is comprised. Software refers to all instrument control, host computer to instrument computer/controller interface, and data acquisition, reduction, and display functions. Two copies each of both electronic and paper (hardcopy) versions of all manuals and drawings shall be provided.

IV. User Training

Training shall be provided for up to three PNNL staff, such training to include at a minimum all aspects of instrument start-up, shutdown, procedures for recovery from a facility power or other utility failure, hardware and software setup, data acquisition, data display, export and processing, instrument tuning, operation, and maintenance. Training shall be provided covering all instrument setup, tuning, and operations required to demonstrate the required performance metrics set forth herein as well as to perform analysis of samples. Training shall include incidental aspects of instrument operation such as display and analysis of data both in real time and using stored data, exporting of data files into commercial software programs, and the creation and use of programmed sequences of analyses.

V Final Acceptance

Prior to final acceptance of the instrument by PNNL, the following shall be demonstrated or delivered:

1. A fully functional instrument, including all components, spares, accessories, consumables, and related hardware shall be delivered, installed, and tested in accordance with the Test Plan described herein.
2. All performance metrics shall be successfully demonstrated on the delivered instrument as described in the Test Plan.
3. All documentation shall be delivered in both electronic and hardcopy formats.
4. All training shall be completed.

Section VI. System Warranty

The offeror shall warrant the complete instrument and associated components or systems to be free of defects in materials and workmanship for a period of two years from the date of final acceptance. Power supplies and electronics shall be warranted for a period of three years from the date of final acceptance.

During the warranty period, the offeror will repair or replace any defective structures, components, or sub-systems in the instrument and will bear all costs, including travel, labor, and per diem, associated with such repair or replacement. Replacement parts shall be reasonably available, but in no case shall more than 30 days be required to provide such parts with the 30 days measured from the date of the determination by PNNL and the offeror that such parts are needed.

Specifications for EMSL Ultra-High-Resolution ICPMS Capability

Section I. Introductions and General requirements.

In addition to MC-ICPMS and HR-ICPMS capabilities, EMSL also desires to develop and demonstrate ultra-high resolution ICPMS capability (ie R > 100,000). Proof of principle for such capability has been demonstrated by PNNL using orbital trapping MS techniques combined with plasma source ionization, with very high elemental and isotopic spectral resolution being achieved. To further demonstrate this capability and to make it routinely available for EMSL user access, EMSL desires to build a second-generation system of this type.

Accordingly, the offerer shall provide a mass spectrometer with general characteristics that include atmospheric pressure ionization and facile sample introduction capabilities (suitable for inductively coupled plasma source retrofitting and adaption), differential pumping to enable such interfacing, very high mass resolution and mass accuracy at high scan rates, a mass range of at least 50-300 mass/charge (m/z) ratio, and a high efficiency collision cell for dissociation of interfering molecular ions.

Offerer will demonstrate system performance using a standard electrospray ion source. PNNL will subsequently adapt and modify the system for prototypical ICPMS use and demonstration, and accepts that such adaption may alter the original, demonstrated operating specifications.

Specific performance requirements for the ultra-high-resolution MS capability are as follows:

Resolution

A mass resolution of at least 100,000 R (m/delta m) shall be demonstrated.

Mass Range:

A minimum operating mass range from mass/charge (m/z) 50 to 300 shall be demonstrated. An operating mass range of 5 to 300 m/z is preferred.

Mass Accuracy

Mass accuracy of < 5 parts per million (external mass calibration) shall be demonstrated.

Dynamic Range

An operating dynamic range of at least 4000 shall be demonstrated.

Mass Scan Modes

Two scan modes shall be provided: 1) normal, full scan mode, 1-10 Hz, and 2) fragmentation mode, using supplied high-efficiency collision cell

Sensitivity

Detection limits of 500 femtograms (fg) of model organic or biomolecular compounds shall be demonstrated at the above specified conditions.

II. Documentation

Documentation and manuals shall be provided describing all aspects of operations, data reduction methods, data calculations, maintenance, and troubleshooting of every sub-system of which the instrument is comprised. Software refers to all instrument control, host computer to instrument computer/controller interface, and data acquisition, reduction, and display functions. Two copies each of both electronic and paper (hardcopy) versions of all manuals and drawings shall be provided.

III. User Training

Training shall be provided for up to three PNNL staff, such training to include at a minimum all aspects of instrument start-up, shutdown, procedures for recovery from a facility power or other utility failure, hardware and software setup, data acquisition, data display, export and processing, instrument tuning, operation, and maintenance. Training shall be provided covering all instrument setup, tuning, and operations required to demonstrate the required performance metrics set forth herein as well as to perform analysis of samples. Training shall include incidental aspects of instrument operation such as display and analysis of data both in real time and using stored data, exporting of data files into commercial software programs, and the creation and use of programmed sequences of analyses.

IV Final Acceptance

Prior to final acceptance of the instrument by PNNL, the following shall be demonstrated or delivered:

1. A fully functional instrument, including all components, spares, accessories, consumables, and related hardware shall be delivered, installed, and tested in accordance with the Test Plan described herein. PNNL requires that the instrument be supplied ready for use with United States standard electrical power. If transformers are required for operation with U.S. standard electrical power, such transformers shall be included with the instrument

2. All performance metrics shall be successfully demonstrated on the delivered instrument as described in the Test Plan.

3. All documentation shall be delivered in both electronic and hardcopy formats.

4. All training shall be completed.

Section V. System Warranty

The offeror shall warrant the complete instrument and associated components or systems to be free of defects in materials and workmanship for a period of two years from the date of final acceptance. Power supplies and electronics shall be warranted for a period of three years from the date of final acceptance. During the warranty period, the offeror will repair or replace any defective structures, components, or sub-systems in the instrument and will bear all costs, including travel, labor, and per diem, associated with such repair or replacement. Replacement parts shall be reasonably available, but in no case shall more than 30 days be required to provide such parts with the 30 days measured from the date of the determination by PNNL and the offeror that such parts are needed.