Market Consultation

Ion mobility-mass spectrometer

Datum versie: 30 August 2023

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1. Background information regarding the application

The Vrije Universiteit Amsterdam (VU) is a large innovative university which actively contributes to developments in education and research. For more information about the VU, see https://www.vu.nl/en

The Division of BioAnalytical Chemistry (BAC) of the Chemistry and Pharmaceutical Sciences department, has the intention to acquire a state-of-the-art ion mobility mass spectrometer for the characterization, identification, and accurate quantitation of a large variety of molecules such as metabolites, oligonucleotides, peptides and (glyco)proteins either direct or from complex samples/mixtures.

The purpose of this market consultation is to find potential suppliers of such an instrument, which fulfill our specific demands (listed below) and price point, in order to give direction on which procurement procedure the Vrije Universiteit Amsterdam should follow for this purchase.

Therefore, we ask the potential suppliers to respond based on the information provided in this document regarding technical product specifications, functional specifications of the listed main applications, delivery, service provision and other conditions. If, after requesting the information, you decide not to respond further, we kindly request you to notify us. To be clear: this is NOT a quote request.

2. Required specifications for the ion mobility mass spectrometer

2.1 General description

We request a highly sensitive, high-resolution ion mobility mass spectrometer with high mass accuracy, fast MS2 acquisition speed for the identification and accurate quantitation of thousands of (glyco)peptides, and an ion-mobility option for structure elucidation. This instrument will be used for several main research lines within BAC and therefore it needs to fulfil a wide range of criteria covering all our key demands. The research within BAC focus on small molecule/metabolite characterization, aggregation of proteins and peptides, bottom-up proteomics (specifically for venom identification), glycoproteomics, and native protein characterization. Each research direction requires specific demands that needs to be filled by the instrument, which are described below. The minimal system requirements are listed in section 2.2.

(1) Peptide and protein aggregation and small molecule characterization:

The research on peptide and protein aggregation relies heavily on adjustable, soft (low voltage) parameters throughout the instrument. For both aggregation studies and small molecule characterization require high-resolution ion mobility separation and structure elucidation (by CCS) as an integrated dimension to the mass spectrometer.

(2) Bottom-up Proteomics and Glycoproteomics:

The instrument needs to enable the unambiguous identification of peptides in complex matrices such as snake venoms or human body fluids, using conventional fragmentation approaches, such as collision-induced dissociation (CID). It should be able to allow a high throughput of samples with high

identification rates while using short liquid chromatography gradients below 30 minutes per sample. To archive this, the MS2 acquisition rate should be above 100 Hz. In addition, the instrument must be able to specifically identify a large number of unique glycopeptides among a vast majority of peptides.

(3) Native (large) protein characterization:

The ion mobility mass spectrometer must have an m/z range of up to 20,000 to measure large proteins (above 150 kDa) in their native form.

2.2 The mass spectrometer should include the following features:

1. Mass spectrometers

1.1 Analyzer

The instrument must contain a high-resolution time of flight-based analyzer with a repetition rate of up to 10 Hz. Flight tube and electronics must be temperature controlled by a water chiller for unparalleled stability.

1.2 Quadrupole

The instrument must contain a high-pressure quadrupole collision cell. The quad must have an isolation window of up to 3.000 m/z. The analytical quadrupole is synchronized with ion elution from the ion mobility tunnel device for highly efficient parallel precursor isolation in all PASEF acquisition modes (PASEF, dia-PASEF, prm-PASEF).

1.3 Multipole

The MS instrument has an Ion Beam Conditioning multipole for highly efficient ion transfer and quadrupole injection.

1.4 Mass range

The instrument must have a 20,000 m/z in rf-only mode.

1.5 Mass resolution

The instrument must have a mass resolution that is equal to or greater than 60,000 (full sensitivity resolution at 1222 m/z.

1.6 Scan speed TOF MS

The instrument must have a maximum scan speed of up to 50 Hz MS.

1.6 Scan speed TOF MS/MS and DIA acquisition

The instrument must have a maximum scan speed of up to 120 Hz (120 MS/MS spectra per second) for mass- and mobility-selected ions and a fast quadrupole switching time to enable efficient fragmentation of ions from multiple mobility windows This must include a superior DIA analysis with mass and ion mobility window stepping for highest data quality with background ion interference removal (e.g. isobaric+1 background ions) allowing for library or library free DIA with unrivalled proteome depth and ID confidence. It must incorporate true CCS values in addition to retention times and m/z values for unambiguous assignment of the MS/MS from the DIA-PASEF run to the library. The instrument must allow a collision energy ramping on mass-to-charge ratio and charge state or ion mobility.

1.7 MS/MS duty cycle

The instrument must contain a ≥90% duty cycle for TOFMS/MS acquisition.

1.8 dynamic range (LDR)

The instrument must have a dynamic range of ≥5 orders of magnitude. High-resolution Extracted Ion Chromatogram technology with better than +/- 0.5 - 1.0 mDa stability on centroid data values over a typical LC peak. This must include a 10-bit ADC for high quantitative dynamic range, sampling rate: 5 G Sample/sec ADC with 50 Gbit/sec.

1.9 Mass accuracy

The instrument must have a mass accuracy better than 800 ppb RMS error and better than 2 ppm RMS error with an external calibrant.

1.10 Positive and negative mode TOF MS

The instrument must have the ability to change between positive and negative mode measurements within a single run.

1.11 Scan type and sensitivity

The instrument must offer full-scan TOF MS with an S/N >100:1 for Reserpine 1 pg. The scan mode in MS/MS must be better than 1000 counts based on the consumption of 2.5 fmol of Glu-fibrinopeptide B. This shall correspond to a signal-to-noise ratio better than 50:1. The MS/MS sensitivity specification is while using quadrupole isolation of the pre-cursor ion demonstrating that there is minimal transmission loss through the isolating quad. The instrument must allow parallel MS/MS events from each ion mobility scan leading to 1000+ precursor transitions in under 30-minute gradients.

1.12 Fragmentation modes

The instrument must have a CID cell with scalable (ramp) collision energies based on one ion mobility or m/z value. The CID mode must have an operating range from 0 eV to 150 eV.

2. Ion mobility

The system contains an ion mobility analyser delivering high mobility resolution of R= 200 in a single pass at a 350 msec mobility scan time and reproducible CCS (Collisional Cross Section) determination with a standard deviation of = 0.5% RSD between experiments.

The ion mobility must contain a high capacity dual-Stacked Ring Ion Guide (SRIG) enabling Parallel Accumulation and Serial Fragmentation (PASEF) and accurate, reproducible ion mobility separation and Collisional Cross Section (CCS) determination. CCS and mass calibration are achieved with the same calibrant reagent and can be applied to all compounds regardless of chemical class. The system must include a parallel ion mobility analyser allowing accumulation and analyses in parallel. The ion mobility should allow for close to 100% duty cycle, with ion accumulation and sequencing speed>120 Hz and 60,000 (FWHM) resolution at 1222 m/z. The sensitivity of the MS with ion mobility should be <15% RSD based on 50 fg/ul of Reserpine.

3. Ion source

The instrument must contain an ion source, or equivalent providing the same performance.

The ion source needs to have three requirements.

- The ion source must have an ESI-based source compatible with a flow rate of 1 µL/min to 1 mL/min.
- The ion source must have a probe for nanoflow workflows, for minimal sample consumption and high sensitivity and it must be capable of the use of dopant-enriched nitrogen gas with different organic solvents. The nano flow ion source needs to be optimized for ~50 nL flow rates with no need to make any sprayer adjustments. A true "plug and play" nano source for easy operation is necessary.
- The system must be compatible with in-house-made sources.
- The source parameters must be able to be controlled for soft ionization.
- The source must be temperature regulated.
- ESI source must allow positive and negative ion detection with the needle of the ESI source grounded for safer operation.
- The nano source must be compatible with LC separation and include a column oven directly connected to the source to guarantee a temperature-controlled separation with ideal peak widths.

4. Software and operating system

1.The system must include a Windows-based data acquisition and editing software package that incorporates a graphical user interface utilizing multi-pane windows for easy data acquisition and analysis. MS instrument must provide a real-time data acquisition and data processing interface, enabling a high spectrum ID rate.

2.The software must Full PASEF and dia-PASEF GUI integration into the acquisition software to set up customized methods in mobility and m/z space.

3.. Biopharma Compass for the characterization of Biologics with automated workflows for intact, top-down or bottom-up analysis. Routine QC using MALDI or LC-MS, e.g., for synthetic peptides and oligonucleotides. Include OligoQuest™ for the MS2 analysis of RNA and DNA. Integrated control for QTOF and timsTOF systems enables automated data acquisition and processing.

4.The system must be compatible with a variety of commercially available LC systems present within BAC including parts such as pumps, autosamplers and detectors. The MS instrument must be able to integrate LC systems in a complete workflow in an easy manner using suitable plugins. LC-MS(/MS) measurements should be easily scheduled in samples tables that integrate MS and LC parameters. Data interpretation should be possible from a single data file that includes LC and MS results.

5.The system must be capable of easy, automated optimization of quadrupole and TOF calibration and resolution as well as optimized detector settings.

6. DataAnalysis software for processing MS and LC-MS analyses acquired should be included. This software needs to be accessible by multiple users at the same time with at least five floating licences.

5. Service

Warranty of 1 year for the instrument. Remote support is available.

6. Delivery

The Ion mobility mass spectrometer is deliverable within 6 weeks of purchase.

7. Budget

The budget available for this purchase is a maximum of 553,719.00 euros (excl. VAT or 670,000.00 incl. VAT). This absolute maximum budget includes all costs such as installation and implementation, delivery, warranties, training and documentation, possible additional costs for travel, accommodation, and testing.

3. Procedure and timeline of the market consultation

During the market consultation, all communication with regard to this subject is conducted via the purchasing management department of the Vrije Universiteit Amsterdam. Contact details, see below:

Name:	Purchasing Management Department
Faculty / Department	Finance Department
Address:	Van der Boechorststraat 1 1083 BT Amsterdam
E-Mail:	aanbestedingen.fpc@vu.nl
Citing	Market Consultation: Ion mobility mass spectrometer

Timetable Market Consultation:

Description	Deadline
Publication on www.tenderned.nl	01 September 2023
Publication Memorandum of Information	10 September 2023
Deadline for questions	07 September 2023, 11:00 a.m.
Last moment to submit answers	14 September 2023, 11:00 a.m.
Sending summary to participants and closing the market consultation process	01 October 2023

You are requested to respond to this market consultation no later than 11:00 am on 14-09-2023. Responses received after this period will no longer be considered.

The VU would like to give you the opportunity to ask any questions you may have about this market consultation. You can do this by e-mail until 07-09-2023, 11:00 a.m. at the latest. You should send your application and questions by e-mail to aanbestedingen.fpc@vu.nl for the attention of the Purchasing Management department. When submitting your response, please include "**Ion mobility mass spectrometry**" in the subject line.

Answers to the questions will be published on Tenderned by means of an information memorandum by 10-09-2023 at the latest.

The VU will keep the option open to invite parties, in response to the submitted responses, to provide additional explanations to your answers orally and/or by means of a presentation. The VU will contact these parties and schedule a meeting in consultation.

The results of the market consultation can be used as input for any tender to be followed. After the market consultation has ended, written feedback of the market consultation is provided to all respondents in the form of a summary of the answers, taking into account any commercial interests of the parties. This feedback does not affect the obligation of the market consultation. Prices and/or rates are excluded from publication.

Candidates who have participated in this market consultation and who have answered the questions will receive the summary by e-mail, no later than 01-10-2023.

This summary will also be published as an appendix to any tender to be followed.

4. Other terms and conditions

In addition to the terms and conditions stated elsewhere in this document, this market consultation is subject to the following terms and conditions:

• Parties cannot derive any (mutual) obligations or rights towards the VU from this market consultation;

• Participation in this market consultation does not guarantee a role as supplier;

• Any costs for participating in this market consultation will not be reimbursed by the VU;

• The official language during this market consultation is in principle English;

• the VU is in no way bound by the results of the market consultation or obliged to realize and/or tender for the subject to which the market consultation relates;

• Claims about the use of information, confidentiality or requests for compensation in connection therewith will not be honored;

• The VU reserves the right to suspend this market consultation temporarily or permanently.