

TENDER SPECIFICATION FOR THE SUPPLY, DELIVERY, INSTALLATION, COMMISSIONING AND TRAINING OF ONE UNIT OF ULTRA PERFORMANCE LIQUID CHROMATOGRAPH COUPLED TO A HIGH RESOLUTION MASS SPECTROMETER (UPLC-HRMS) SYSTEM**SCOPE OF TENDER:**

1. The system must be an ultra-performance liquid chromatograph (UPLC) coupled to a high resolution mass spectrometer (HRMS).
 - 1.1. UPLC must include the following stackable self-contained modules:
 - High pressure binary gradient solvent delivery system
 - Solvent rack with degasser
 - Autosampler/injector
 - Thermostatted column compartment
 - 1.2. High resolution mass spectrometer must be able to obtain MS information and MSMS fragments spectra with high mass accuracy, and the following operation modes shall be available:
 - Full scan MS, i.e. works like single quadrupole MS but with high mass accuracy with isotope pattern information
 - All ions fragmentation (AIF), i.e. acquire all MSMS fragment spectra
 - Data/Information dependent acquisition (IDA), i.e. acquire all MS data and trigger MSMS (fragment) spectra if present at above the set threshold; inclusion list can be set to prioritize the data search.
 - High resolution multiple reaction monitoring for quantitation, i.e. acquire targeted MS and MSMS ions for quantitation
2. The system should include a spectra library of at least 1,000 toxicology-relevant compounds.
3. The system should include tools to help elucidate the molecular structure or formula of an unknown from the observed MS and MSMS spectrum.
4. The tenderer must provide all the necessary arrangements for the commissioning of the system.
5. Tenderer should have a strong record in providing personalized and responsive after-sales support in Singapore. Tenderer is required to provide the reference list of installation in Singapore for similar units in the past 3 years. Please provide the details in Annex E Performance Summary.
6. The tenderer must provide training necessary to operate and use the system. Please refer Part D for the requirements.

PART A – ULTRA PERFORMANCE LIQUID CHROMATOGRAPHY**A.1 Binary gradient solvent delivery system**

1. The system must be equipped with two solvent selection valves to enable the choice of 4 different solvents.
2. There must be a switching valve to divert the mobile phase flow to waste, without going through the analytical column, for regular flushing of the system.
3. It must have a flow range of at least 0.1 – 2 ml/min.
4. Flow rate accuracy shall be within $\pm 1\%$.
5. Flow rate precision shall be $<0.1\%$ RSD or <0.02 min SD, whichever is greater

PART 3: REQUIREMENT SPECIFICATIONS**HSA000ETT17300002****Equipment 5: Ultra Performance Liquid Chromatograph - High Resolution Mass Spectrometer (UPLC-HRMS) System****Quantity: 1****Location: Analytical Toxicology Laboratory – Clinical & Forensic Toxicology (ATL-CFT)**

6. The operational pressure range should be up to at least 1,000 bar.
7. Solvent composition must be settable from 0-100%.
8. Solvent composition precision must be < 0.3% RSD or 0.05 min SD, whichever is greater and accuracy $\leq$ 0.5%.
9. Solvent resistant materials must be used in all areas which may have contact with the mobile phases.
10. There must be a real-time monitoring system and electronic log for the purpose of diagnostics/troubleshooting. For safety and maintenance, it must have leak detectors and voltage low enough for safe handling during routine maintenance areas.

A.2 Solvent rack with degasser

1. The solvent rack must have capacity of at least four (4) 1-L bottles.
2. It must have four (4) internal degassers with flow rate per channel of at least 2 ml/min.

A.3 Autosampler/injector

1. The sample injection shall have design such that there is zero loss injections.
2. Injection volume shall be settable from at least 0.1 – 10 μ l.
3. Injection volume accuracy should be within $\pm$ 1%, and precision should be < 0.5% RSD at 5 μ l.
4. The injector should have function for user to set the speed for drawing sample as well as the needle depth when injecting sample.
5. There shall be a feature for external and internal needle wash to prevent contamination.
6. Carryover must be no more than 0.005%.
7. The autosampler must be able to accommodate at least 100 positions for 2.0-ml vials.
8. It must be able to process samples automatically in any (random) sequence.
9. The autosampler shall be thermostatted; the temperature should be settable from at least 4°C to ambient temperature.
10. Solvent resistant materials must be used in all areas which may have contact with the mobile phases.
11. It must have leak detectors, autosampler (rack/tray) detector and electronic log.
12. It must have a safety feature when replacing the injection needle.

A.4 Thermostatted column compartment

1. The operational temperature should range from at least 25-60°C.
2. It must provide precise and homogenous column thermostat within the operational temperature range.
3. The temperature shall have accuracy within $\pm$ 0.5°C, stability/precision within $\pm$ 0.1°C.
4. It should have the capacity of holding at least 2 x 10 cm analytical columns with guard columns.
5. It must come with automatic column switching valve to at least 2 different analytical columns according to user setting, without the need to remove and re-attach the columns.
6. There must be solvent leak sensor and real time temperature monitoring.

PART B – HIGH RESOLUTION MASS SPECTROMETER**B.1 Acquisition Method**

1. The mass spectrometer must be able to perform these acquisition method:
 - a) Full scan MS, i.e. works like a single quadrupole MS but with high mass accuracy
 - b) All ions fragmentation (AIF), i.e. acquire all MS and MSMS (fragment) spectra
 - c) Data/information dependent acquisition (IDA), i.e. acquire all MS data and trigger MSMS (fragment) spectra if above the set threshold; inclusion list can be set to prioritize.

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- d) High resolution multiple reaction monitoring for quantitation, i.e. acquire targeted MS and MSMS ions for quantitation

B.2 Ion Source

1. The system must be equipped with Electrospray Ionization (ESI) source as the standard, operable at both positive and negative polarity, with the possibility to change to other ion sources.
2. The ion source must come with grounded and fixed nebulizer needle for safety and easy/optimized alignment.
3. The ion source must have orthogonal spraying for improved robustness.
4. Capable of handling LC mobile phase flow rate of up to 1 ml/min, with gradient from 100% aqueous to 100% organic, with complete vaporization of solvent and good ionization.
5. The introduction of tuning mixture or internal mass calibration solution must not interfere with sample introduction.
6. The ionization voltage must be settable from at least -4kV (for negative polarity) to +5kV (for positive polarity).
7. Changing or maintaining the ion source must be possible without breaking the vacuum and simple for the user to perform.
8. Opening/removing the ion source chamber should shut down the gas and power supply automatically, otherwise other safety measure must be demonstrated for safe routine maintenance.

B.3 High Resolution Mass Analyzer

1. The mass analyser must be either a quadrupole-time of flight mass spectrometer (QTOF-MS) with stable vacuum system and temperature control or an Orbitrap mass spectrometer.
2. The mass analyser must be able to produce accurate and reproducible mass determination, isotopic pattern and accurate mass fragment (MSMS) ions.
3. The mass analyser running on IDA mode must be able to produce MSMS spectra of at least the top 5 most intense ions. An inclusion list for IDA mode must be possible to prioritize the analysis of the drugs in the list.
4. The scan speed for MS and MSMS must be settable at no less than 10 Hz.
5. The m/z range for both MS and MSMS must be at least 50 – 1,500.
6. The mass accuracy for the range 100 – 600 m/z must be within 3 ppm with external mass calibration for MS acquisition.
7. At m/z range 100 – 600, the MS mass resolution must be at least 15,000.
8. The system should be able to provide sensitivity for reserpine on column with S/N > 100:1 at 1 pg in MS mode and MS/MS mode.
9. The collision energy must be settable from at least 10 – 50 eV for low to high fragmentation.
10. Tuning and mass calibration must be possible in both positive and negative polarity, and done automatically.
11. Mass calibration must be possible in between sample run, either before every run or user-defined intervals so as not to interfere with sample analysis.
12. The system should have a standby mode when it is not acquiring data to save on resources.

PART C – DATA MANAGEMENT SYSTEM**C.1 Computer and Accessories**

1. At least Intel Core i5 3.2 GHz processor or equivalent.
2. At least 8 GB RAM.
3. At least 1 TB hard disk.
4. Pre-installed Windows 7 (64-bit) professional or higher with MS Word and MS Excel.
5. Computer must have at least 3 years warranty and must be accompanied with its system recovery CDs or DVDs.

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6. At least a 20" LCD colour monitor, a 101-key keyboard, an optical mouse and a DVD-ROM.
7. At least 2 Ethernet for the installation of LAN.
8. One black and white laser printer with the capability to print duplex and capacity of 500 sheets of paper or better.

C.2 Software

1. The software must include full digital instrument control, mass calibration and tuning, acquisition, qualitative and quantitative analysis, report creation and diagnostics as well as molecular structure or molecular formula elucidation.
2. The instrument control software should have at least user and administrator access rights.
3. It should be able to save the acquisition parameters and data analysis method (if any) together with every data file.
4. Should be able to import/export sample sequence or calibration information minimally to Excel
5. High resolution XIC must be possible within 20 ppm of the stated m/z.
6. The qualitative identification of a compound should be based on at least the mass accuracy, isotopic pattern, retention time, diagnostic fragment ions/spectral library match (if applicable).
7. User should be able to flexibly choose which parameter to use and set weightage (if applicable) for each parameter. The software should be able to give a combined match quality for all the parameters used for identification.
8. In AIF mode where there is no isolation of ion, the software must be able to show that the diagnostic fragment ions are correlated to the parent ion, e.g. by overlaying the fragment ion peaks with the parent ion. Tenderer must show ways to ensure confidence in the identification on top of using diagnostic fragment ions.
9. For data analysis in IDA mode, library spectrum match must be possible.
10. Quantification must be possible by using historical calibration data or calibration from different sequences.
11. Quantification software must allow for multiple internal standards to be processed in a single data analysis method.
12. For quantitation, at least 2 qualifier ions must be possible if the quantification is based on a single ion (either parent or daughter ion).
13. The software must be able to search for online public chemical databases for an unknown compound, based on the observed MS and MSMS spectrum.
14. A tool to generate molecular formula or structure and provide in-silico fragmentation to help elucidate the unknown compound shall be available.
15. Audit trail must be available.
16. Output for importation to LIMS system must be possible for result uploading.
17. Online help should be available for users in each of the software.

C.3 Database/Spectra Library

1. The spectra library must contain reproducible MSMS spectra at preferably different collision energies for the identification of unknown compounds.
2. There should be editable fields to include information like molecular formula, auto-calculated monoisotopic mass, structure, diagnostic fragment ions, and retention time.
3. It must contain at least 1,000 toxicology-relevant compounds.
4. User must be able to edit the library provided, e.g. remove and add compounds, add retention time information, etc.
5. User should be able to create own library for different acquisition method
6. Addition of new compound spectra to the library should be easy with minimum steps.

C.4 Report Template

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1. Tenderer must provide the initial report templates for qualitative and quantitative analysis as required by the user.
2. Report template software must be available for user to customize or modify the templates.
3. For qualitative analysis, the template must include information such as XIC chromatogram, observed m/z and its error in ppm, isotopic pattern, retention time and its deviation from library, MSMS spectrum match, abundance and molecular formula.
4. For quantitative analysis, the template must include additional information such as area of analyte, area of internal standard, calculated concentration, calibration curve, calibration type and equation, and method name in one report.
5. In general, the report template must include basic sample information such as sample name, operator, acquisition date and time, sample vial position, injection volume, data file name/path, acquisition and data analysis method as well as any user comment.
6. The report template should be customised to only print positive result meeting the pre-set criteria.

PART D – MISCELLANEOUS**D.1 Training, Warranty and Support**

1. In-house training for at least 4 persons must be provided that shall minimally include routine hardware maintenance and troubleshooting, software to operate the system and basic and advance data analysis.
2. One classroom-type lecture on the principles of the instrument with familiarization of the different workflows must be provided.
3. The system shall come with at least one-year warranty upon successful commissioning. The warranty must include the following:
 - a. At least 1 preventive maintenance (PM) inclusive of PM kit;
 - b. Provision of unlimited breakdown calls, on-site services and troubleshooting;
 - c. Supply of all replacement parts; and
 - d. Provide system update or upgrade of software version if any.
4. Tenderer shall guarantee that the spare parts, consumables and services for the system will be available for a period of 7 years from the date of discontinuation of the system.
5. Option to purchase comprehensive maintenance contract for 3 years after the warranty period must be quoted. The price quoted must include:
 - a. one preventive maintenance per year,
 - b. unlimited breakdown calls and on-site services,
 - c. all consumables and parts for servicing
 - d. software and library updates
6. Tenderer must be able to provide at least 2 hardware engineer locally for the provision of technical support.
7. Tenderer shall submit the contacts, names and years of experience for at least 2 system hardware engineers and 2 application chemists who will be dedicated for customer support in Annex E.

D3. Site preparation

1. The complete system includes computer and printer, LC and MS shall be placed on existing bench with the available space of 280 cm (width) x 84 cm (depth) x 200 cm (height). Additional or customized bench with the additional of not more than 15cm for the depth shall be provided if it is required.
2. Tenderer shall ensure the proposed system can be installed and connected to existing facility such as power and gas lines.

3. A vacuum pump stand with adjustable legs and non-vibration isolators should also be provided to avoid vibration to the bench.

D4. Performance of Services

1. The Contractor shall perform the Services in the manner as specified in the Contract in order to maintain the Equipment in Good Working Order.
2. The Services to be performed by the Contractor shall consist of Preventive Maintenance and Corrective Maintenance as described below for during warranty and post-warranty maintenance services.

2.1 Preventive Maintenance

- a) The Preventive Maintenance shall consist of:

Routine maintenance of the Equipment, including but not limited to the testing of functions and inspecting of the condition of the Equipment in order to keep the Equipment safe for use and in Good Working Order; and

Adjustment and/or repair of any defect in or malfunction of the Equipment discovered by the Contractor's representatives during the course of routine maintenance checks.

- b) The Preventive Maintenance performed shall be in compliance with the maintenance procedures and safety tests specified by the manufacturer.
- c) The Preventive Maintenance shall be carried out during Operating Hours i.e. Monday to Friday from 8:30 am to 6pm excluding Saturday, Sunday and Public Holiday.

2.2 Corrective Maintenance

- a) Upon receipt of oral or written notice from the Authority, the Contractor shall use its best endeavours to ensure that the Contractor's suitably qualified and duly authorised representatives attends to the Authority on-site, within the response time of not more than 24 hours upon receipt of oral/written notification if the request is made on a Working Day. If the request is made on a non-Working Day, the Contractor shall be on-site within the response time within the first twenty-four (24) hours of the beginning of the next Working Day (if extended coverage is not provided).
- b) The Contractor shall complete any repair, or replacement or adjustment of components within three (3) if the replacement part is available locally and seven (7) working days if the replacement part is not available locally from and including the date on which the Contractor was given notice pursuant to Clause D4-2.2(a) unless the Authority had agrees in writing to have the time period extended.

3 REPLACEMENT AND PURCHASE OF COMPONENTS

- 3.1 The Contractor shall inform the Authority of any part or component of the Equipment that needs to be replaced. Prior approval must be issued by the Authority before the replacement may be effected unless the replacement required is deemed urgent by the Authority in which case a verbal approval (which shall subsequently be confirmed in writing) obtained from an authorised officer of the Authority shall suffice.
- 3.2 The Contractor shall use all reasonable endeavours to supply only original or genuine replacement components, which are required to maintain the Equipment in Good Working Order. All replacement components which are provided free-of-charge and chargeable to the Authority are specified in the Price Summary.

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4 GUARANTEE

- 4.1 The Contractor hereby warrants that all the Equipment and every part or unit thereof serviced by the Contractor shall conform to the requirements of this Contract and be free from any defect or deficiency in their performance or workmanship for a period of three (3) months from the date of acceptance of the Services by the Authority (hereinafter referred to as "the Equipment Guarantee Period"). The Contractor hereby also warrants that all materials and every part or unit thereof, used for the Services shall be free from any defect in manufacture or any defect arising out of design, workmanship or materials used or any failure or malfunction due to quality of material, workmanship, design, assembly, installation or integration for a period of three (3) months from the date of acceptance of the materials by the Authority (hereinafter referred to as "the Materials Guarantee Period"). The Equipment Guarantee Period and the Materials Guarantee Period shall collectively be known as the "Guarantee Period".
- 4.2 Where during the Guarantee Period, any part or unit of the Equipment serviced by the Contractor or materials used for the Services or supplied therefor are found to be defective of any of the reasons specific in Clause D4-4.1 above, the Contractor shall at the written request of the Authority replace the same at the expense (including freight charges, transportation costs or other incidental charges) of the Contractor or if the Authority so agrees make good or repair the same at the expense (including freight charges, transportation costs and other incidental charges) within the turn-around-time as defined in Clause D4-2.2(b). The Equipment or materials or part or unit thereof so replaced or repaired shall be subject to the Guarantee under this Clause for the Authority or three (3) months whichever is later and such balance of the Guarantee Period shall begin to run only from the date of receipt of the part or unit so replaced or repaired by the Authority.
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I hereby confirm that I can meet all the Requirement Specifications as stated in Part 3: Requirement Specifications – Equipment 5.

Tenderer's (as *Principal/Agent)
Company or Business Registration No:

Tenderer's official
Stamp:

Authorized Signature
Name:

Designation:

(*Delete whichever is not applicable)

Please indicate any remarks here should there be any.

Reference To	Remarks