

Equipment 6: Liquid Chromatography – High Resolution Quadrupole Time-of-Flight Tandem Mass Spectrometry (LC-QTOF-MS) System
Quantity: 1
Location: Analytical Toxicology Laboratory- Drug Abuse Testing (ATL-DAT)

1 Functional Requirements

The equipment is intended to be used to perform comprehensive drug analysis in biological samples.

2 General Requirements

The system must be a high resolution quadrupole time-of-flight tandem mass spectrometer (QTOF MS) coupled with an ultra-high performance liquid chromatograph (UHPLC), and comprises the configurations and requirements as follows:

Part A Liquid chromatograph mainframe

1. Binary gradient pump
2. Autosampler / injector
3. Thermostatted column compartment

Part B Quadrupole time-of-flight mass spectrometer

1. Ion source
2. Mass Analyser

Part C Data management software system

1. Computer hardware and accessories
2. Software
3. MS spectral database or library

Part D Miscellaneous

1. Other requirements
2. Accessories
3. Optional Accessories

Part E Warranty & Post warranty comprehensive maintenance services

The system must be able to operate on these conditions:

- Ambient operating temperature: minimum 15- 35 °C
- Line voltage requirements: 230V $\pm$ 10%
- Conforms to minimally one the following safety standards: CSA, IEC, EN
- Conforms to ISO9001 quality management standard.

3 Technical Requirements

Part A – Ultra High Performance Liquid Chromatography

A.1 Binary Gradient Pump

- The pump system must be equipped with two solvent selection valves to enable the choice of up to four solvents, in combination of two.
- The delay volume must be less than 150 μ L.
- The flow rate must be settable within the range of 10 μ L/min to 2 mL/min in minimum of 1 μ L/min increments.
- The flow accuracy must be within $\pm$ 1%.
- The flow precision must be less than 0.1% RSD.
- The gradient composition accuracy must be within $\pm$ 0.5%.
- The gradient composition precision must be less than 0.2% RSD.
- The flow and gradient settings must be user settable using programmable software.
- The pressure tolerance must be at least 1000 bar.
- The system pressure must be able to be digitally monitored.

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- The pump system must be equipped with integrated vacuum degasser.
- The pump system must be equipped with automatic purge and seal wash.

A.2 Autosampler / Injector

- The sample injection volume must be variable between 0.1 µL to 20 µL in minimum of 0.1 µL increments.
- The injection accuracy must be within $\pm 1\%$.
- The injection precision must be less than 0.2% RSD.
- The pressure tolerance must be at least 1000 bar.
- The sample capacity must have at least 120 positions for 2 mL vials. For volumes less than 300 µL, plastic or glass inserts can be used.
- The autosampler must have a cooling capability with temperature range covering 4 °C to 40 °C.
- The injection and autosampler settings must be user settable using programmable software.

A.3 Thermostatted Column Compartment

- The temperature control range must cover the range of 20 °C to 90 °C.
- The temperature set point accuracy must be within ± 0.5 °C without the need to calibrate.
- The temperature set point precision must be no larger than 0.1 °C.
- The temperature stability must be within ± 0.3 °C.
- The compartment must be able to be installed with at least four columns, each column of length up to 15 cm, with pre-filter or guard columns.
- The compartment must be fitted with switching valves for the selection of the installed columns.
- The switch and selection of the installed columns must be user settable using programmable software.
- The pressure tolerance must be at least 1000 bar.

Part B – High Resolution Quadrupole Time-of-Flight Mass Spectrometer**B.1 Ion Source**

- The system must be equipped with an electrospray ionisation (ESI) source as standard.
- The ion source should be compatible with both electrospray ionisation (ESI) and atmospheric pressure chemical ionisation (APCI) probes.
- The switching of ionisation probes must be simple and tool free.
- The ion source must have feature for improved robustness, such as but not limited to orthogonal spraying.
- The ion source must have self-cleaning  with temperature sensor.
- The ion source must have a flow rate compatibility in ESI mode which covers the range from 5 µL/min to 1000 µL/min.
- The solvent compatibility for the ion source must be from 100% aqueous to 100% organic, with full gradient capability.
- All ion source parameters except sprayer positioning must be computer-controllable.
- The source must be able to be removed from the host system without tools and without breaking the vacuum.

B.2 Mass Analyzer

- The mass analyzer must consist of a quadrupole mass filter, a quadrupole collision cell and a high performance time-of-flight (TOF) analyzer.
- The mass analyzer must be able to perform full scan MS and MS/MS, product ion scan and multiple reaction monitoring (MRM).
- The mass analyzer must be able to perform data independent MS/MS acquisition for variable precursor's mass range windows.
- The mass analyzer must be able to perform data dependent MS/MS acquisition, with or without an inclusion list of precursor ions.

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- Sensitivity in positive MS mode: the signal-to-noise must be equal to or higher than 750:1 for reserpine 1 pg on column, or equivalent.
- Sensitivity in positive MS/MS mode: the signal-to-noise must be equal to or higher than 1750:1, for reserpine 1 pg on column, or equivalent.
- The scan speed must be at least 25 Hz for MS scan, and at least 500 Hz for MS/MS scan.
- The MS mass resolution must be 40000 [full width half height (FWHM)] or better at m/z around 1000.
- The mass accuracy must be less than or equal to 800 ppb root mean square (RMS) error by internal calibration, and 2 ppm RMS error by external calibration for MS mode.
- The inter-scan linear dynamic range must be equal to or greater than 4 orders of magnitude without signal reduction.
- The mass range must cover 20 to 40000 m/z for high resolution MS.
- The precursor ion selection range must cover 20 to 2200 m/z.
- The system must allow for polarity switching, and polarity switching must be computer-controllable.

Part C – Data Management System**C.1 Computer and Accessories**

- Minimum configuration: Intel Core i7 3.2GHz or equivalent, 16GB RAM, 4 TB hard drive, DVD RW (CD RW capable), USB optical scroll mouse, keyboard, high resolution 22 inch widescreen flat panel colour monitor.
- Microsoft® Windows® 7 Professional 64 bit (upgradable to Windows 10 in the future) must be installed.
- System Documentation Kit must be provided.
- Microsoft office software must be installed.
- The PC(s) must be under 3-year full warranty and accompanied with their system recovery CDs or DVDs.
- Laser jet printer with duplex printing capability must be provided.
- All computer interfaces, cables and software drivers must be provided.
- Ethernet slots to support inter-computer and network data transfer function must be installed.

C.2 Software

- A single software platform for control of all modules and functions of the LC and MS, including data acquisition and processing.
- The software must include full digital instrument control, tuning, qualitative analysis, report creation and diagnostics.
- The software should have a compound database generation tool for the creation of accurate mass libraries.
- The software should be able to screen for compounds using a mass spectral library.
- The software should also be able to perform targeted and non-targeted screening using “data dependent” acquisition.
- The software should be able to perform both mass spectral library matching and precursor/fragment ion matching in the absence of a mass spectral library.
- The software should have a flexible and easy-to-use report template for the creation of any report format.
- The software should have a fragmentation interpretation tool module.
- The software should have built-in capability for automated searching of accurate MS, isotope pattern and assigned elemental formula with online databases.
- Software revisions or upgrades in the future, if any, should be provided at no additional cost.

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C.3 Mass Spectral Database / Library

- The spectral library must contain reproducible accurate mass MS/MS spectra that can be used for the identification of unknown compounds.
- The spectral library should contain at least 150 toxicology-relevant compounds, which should comprise of drugs of abuse (including the new psychoactive substances such as synthetic cathinones, synthetic cannabinoids, etc), pharmaceutical drugs and their metabolites.
- All the toxicology-relevant compounds should have compound theoretical mass information and MS/MS spectra.
- The identification of a compound should be based on the compound's retention time as well as high resolution accurate mass MS/MS profile, and a matching score must be included.
- The weightage of the match criteria for identification of compounds should be user-settable.
- The spectral library should be updated at no additional cost during warranty period whenever there is a new revision.
- Users should be able to create and add-on high resolution mass spectral library (MS/MS) for any new compound.
- The identification of compounds should be able to be based on multiple libraries, including in-built and user created libraries.

Part D – Miscellaneous

The proposed system shall include and fulfil the following requirements.

D.1 Other requirements

- **Electrical Requirements**
 - i) The unit shall operate directly on the Agency's existing electrical switched socket of rating 230V ac $\pm 10\%$, 50 Hz ± 2 Hz, single phase/triple phase ac supply.
 - ii) The unit shall be protected from transient power disruption during use. The disruption shall not affect the unit's performance.
- **Delivery, installation, commissioning**
 - i) The equipment shall be delivered, installed and fully commissioned before 31 Mar 2018.
 - ii) The Tenderer must oversee overall systems integration, site preparation, installation and necessary configuration of the system.
- **Risk Assessment**
 - i) The Contractor must perform on-site risk assessment. Risk Assessment Report in 5x5 matrix shall be submitted and approved prior to the delivery of the unit.

D.2 Accessories

The price quoted shall also include the following:

- Syringe pump for direct infusion of sample;
- Roughing pump with enclosure box equipped with sound proof walls for minimization of pump noise;
- Uninterrupted Power Supply (UPS) which enables the system to operate for at least 15 minutes must be supplied; and
- Essential accessories required for operating the unit.

D.3 Optional Accessories

The Tenderer shall quote for the following optional accessories:

- i) Atmospheric Chemical Ionisation (APCI) source

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- ii) Additional 1 unit of PC that shall be used to perform data processing. The PC shall minimally meet the following requirement: Intel Core i7, high resolution 22 inch widescreen LCD Monitor, Windows 10 Professional 64 bit, 2.4 GHz Processor, 16 GB RAM, DVD drive, 1 TB hard drive (NTFS), NTFS format, 1 serial port (RS232), 3 ethernet port (for LC, MS and user network), keyboard & mouse
- iii) Additional software and/or license for data processing where applicable.

Please state if the software as described in Clause C.2 can be installed on more than 1 PC. :

All prices quoted for the optional accessories above shall be valid throughout the warranty period.

Part E Warranty, Post warranty Maintenance and Training**E.1 Warranty and Maintenance**

- The system shall come with at least one (1) year warranty for the whole system that comprises equipment hardware, software, UPS and etc. The warranty must include the following at no additional cost:
 - (i) Annual preventive maintenance (PM) with PM kit;
 - (ii) Annual preventive maintenance (PM) for UPS;
 - (iii) Unlimited breakdown calls and on-site services;
 - (iv) Supply of replacement of parts;
 - (v) Update and upgrade of software version and mass spectral library
- The Tenderer must ensure service parts and consumables are readily available and provide assurance that all parts can be obtained at least 10 years after delivery of the instrument.

E.2 Training and Technical Support

- The Tenderer must provide after-sales support from service engineers and application chemists in Singapore.
- Approximately 1 month upon successful of commissioning, on-site basic training for users (4 – 6 pax) should be provided. The training shall be conducted by trained personnel, and topics should include theory, equipment overview, method setup, data acquisition, data processing, report formatting and general maintenance. A proposed training schedule and agenda must be appended with the tender submission.
- Advanced training should be provided within one (1) year from the completion of on-site basic training including advanced functions of the system and software, troubleshooting and advanced maintenance of the system for 4 pax.
- The Tenderer must send its application specialist(s) to HSA Analytical Toxicology Laboratory to complete the following required method setup onsite post equipment full commissioning.
 - (i) Screening workflow using data independent or data dependent acquisition with mass spectral libraries
 - (ii) Confirmation workflow using high resolution MRM acquisition

E.3 3-Year Post warranty comprehensive maintenance

- Tenderer is required to quote comprehensive maintenance contract for three (3) years after the warranty period. The comprehensive maintenance contract shall provide coverage for overall system including hardware and software and UPS. The price quoted shall minimally include the following:
 - (i) provision of unlimited breakdown calls and on-site services
 - (ii) provision of replacement parts

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- (iii) to provide one (1) preventive maintenance per year
- (iv) to provide two (2) preventive maintenance per year for UPS
- (v) any software or library revisions

E.4 Performance of Services

E4.1 The Services to be performed by the Contractor shall consist of Preventive Maintenance and Corrective Maintenance as described below.

E4.1.1 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.

E4.1.2 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, 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 respond within 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 5 working days if parts are available locally or 10 working days if parts are not available locally from and including the date on which the Contractor was given notice pursuant to Clause 4.1.2(a), unless the Authority had agrees in writing to have the time period extended.
If the repair, or replacement or adjustment of components for longer than 30 working days, corresponding extension of the warranty and comprehensive maintenance contract must be offered for the affected period.

E.5 Replacement and Purchase of Components

- E5.1 The Contractor shall inform the Authority of any part or component of the Equipment that needs to be replaced.
- E5.2 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.

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E.6 GUARANTEE

- E6.1 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".
- E6.2 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 E6.1 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 a Guarantee Turn-Around-Time of 7 days . 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 6.

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 non-compliance here should there be any.

Reference To	Remarks