附件一
【化驗設備技術規格】

1. 必需是一枱上高效液相色譜-高分辨率質譜儀聯用儀

1.1. 其必需包括 High Performance Liquid Chromatograph、High-Resolution Mass Spectrometry System、System Control and Data Processing Unit、Uninterupted power supply、Nitrogen generators 及兩台電腦。

1.2. 包括所提供的工作枱在內，其總高度不可超過 220 厘米。

2. High Performance Liquid Chromatography

2.1. **Solvent delivery unit**

2.1.1. A binary solvent delivery design, with an internal 4-solvent selection valve included, capable of delivering isocratic and binary gradients with smooth motion control.

2.1.2. With gradient operation, the unit shall be able to deliver at least 2 solvents and programmable from 0 to 100% in 1% increment, or finer, for each of the solvents with the total composition summing up to 100%.

2.1.3. Solvent composition precision should be < 0.3%RSD.

2.1.4. Solvent composition accuracy should be ±0.35% absolute or better.

2.1.5. The unit should have a software controllable automatic or manual priming function for module fluidic path.

2.1.6. The operation flow rate shall range from 0.001 ml/min to 5mL/min or wider in 0.001 mL/min increments or finer.

2.1.7. The flow precision shall be smaller than 0.1% RSD or <0.01 min SD or better, based on retention time.

2.1.8. Flow accuracy should be ±1% or 10 μL/min or greater.

2.1.9. The dead/delay/dwell volume after the LC column should be equal or <100 μL.

2.1.10. The operating pressure should be up to 1000 bar.

2.1.11. Leak detection system shall be available with leak safe handing design to assure isolation of electrical components from liquid flow path. Automatic shutdown of the pumping system should be initiated when leak is detected.

2.1.12. Information for diagnostic purpose shall be available for continuous tracking of instrument usage in terms of solvent utilization status associated with user defined limits.

2.1.13. System software should control operation of the entire unit.

2.1.14. An integrated solvent degassing with at least 2 channels.

2.1.15. The module should be able to run with LC column with sub-2 μm particle size column, at flow rates 0.5 mL/min without any hardware modifications.

2.2. **Solvent degassing unit**

2.2.1. Include a degassing device capable of eliminating gas generated during solvent blending for both isocratic and gradient elution.
2.2.2. The unit should include at least 2 solvent channels.
2.2.3. Each degassing channel shall be able to accommodate a flow rate from 0.001 mL/min to 5 mL/min or wider.

2.3. **Automated sample injection unit**
2.3.1. The unit shall be compatible with the liquid chromatograph and system control unit for fully automatic operation.
2.3.2. The unit should include automated injection syringe with an appropriate needle and a sample loop. (Support 2 ml, 105 and 96-well microtiter plate: 192)
2.3.3. Injection cycle time shall not be greater than 30 sec using default setting.
2.3.4. Injection range should be 0.1 to 50 µl or wider. In 0.1 μL increment without loop replacement or other hardware modification.
2.3.5. Injection precision should be <0.25% RSD or SD <10 nl.
2.3.6. Injection volume accuracy should be ±1% (50 μL, n = 10) max.
2.3.7. Carryover: <0.003% without washing, and <0.005% at 30 ppm or better.
2.3.8. Internal and external needle wash shall be available.
2.3.9. Injection port back-flush shall be available to reduce carry over.
2.3.10. The unit shall be able to operate from 4℃ to 40℃ or wider.
2.3.11. The temperature accuracy shall not be greater than ±2℃.
2.3.12. The temperature stability shall not be greater than ±1℃.

2.4. **Thermostatted column compartment**
2.4.1. The temperature rage shall be 5℃ to 80℃, or wider. The compartment can be pre-heated up to 150℃.
2.4.2. Temperature stability: ±0.1℃.
2.4.3. Temperature accuracy: ±0.5℃.
2.4.4. The unit shall be able to house at least four columns with 300 mm in length with pre-column. Corresponding column switching valve and drive for four columns switching shall be provided.
2.4.5. The unit shall be able to house at least eight columns with 100 mm in length with pre-column.
2.4.6. The system shall have leak detection and leak output signal for shutdown of pumping system.

3. High-Resolution Mass Spectrometry System
3.1. High performance accurate mass Q-TOF for toxicologist analysis. It shall include a mainframe with ion optics and electronics, vacuum system and the mass analyzer.
3.2. It shall be coupled to the HPLC system via an atmospheric pressure ionization interface for independent operation. The operation of the analyzer shall be controlled by the Workstation (section 4). The mass spectrometer shall be benchtop model or equivalent.

3.3. **Ionization source**

3.3.1. All source parameters are under computer control except sprayer position.

3.3.2. The system should be equipped with separate ionization sources and capable to operate in electrospray ionization (ESI) source and an atmospheric pressure chemical ionization (APCI) source with both positive and negative ion mode.

3.3.3. Venting the instrument shall not be required when switching between ESI and APCI modes.

3.3.4. The ESI and the APCI source shall be interchangeable in the same housing.

3.3.5. The source should have orthogonal spraying for improved robustness. And should have self-cleaning ceramic heaters with embedded temperature sensor.

3.3.6. The source should have flow rate compatibility in ESI mode from 5 µl/min to 3,000µl/min, and APCI mode from 50µl/min to 3,000µl/min without flow splitting.

3.3.7. The solvent compatibility is from 100 % aqueous to 100 % organic at flow rate up to 1 mL/min for ESI and APCI mode.

3.3.8. The desolvation temperature is user selectable from ambient to 750℃.

3.3.9. The nebulized spray of the ion source shall be positioned off-axis to reduce contamination of the mass spectrometer.

3.3.10. The ESI and APCI probes should be with two inlet channels for separate delivery of calibrant and sample solutions to the ionization chamber.

3.4. **High-Resolution Mass Spectrometer (HRMS)**

3.4.1. The mass spectrometer shall include a quadrupole mass filter, a collision cell for MS/MS fragmentation and a second mass analyzer for accurate mass measurement.

3.4.2. The full scan mass range shall be 50-40,000 m/z or wider

3.4.3. The quadrupole mass range for precursor selection shall be 50-2200 m/z or wider.

3.4.4. The system shall include a calibrant delivery system (CDS) to deliver calibration standards via a separate ionization probe that functions independently from the main probe/electrode.

3.4.5. The system shall be capable of optimizing quadrupole parameters automatically.

3.4.6. The system shall be capable of calibration mass accuracy and resolution automatically.

3.4.7. The mass spectrometer shall be able to, but not limited to, perform the functions as stipulated below.

(a) Full ion scan MS
(b) Q1 Scan
(c) MS/MS
(d) Product ion scan

3.4.8. Able to perform Data Dependent Acquisition (DDA), Information Dependent Acquisition (IDA) or equivalent.
   (a) Able to perform neutral loss triggered DDA/IDA
   (b) Able to perform DDA/IDA in precursor isolation window
   (c) The collision energy applied to DDA/IDA scan shall be user controllable.
   (d) Spectral library matching shall be feasible with the MS/MS spectrum acquired in DDA/IDA scan.

3.4.9. Able to perform Data Independent Acquistion (DIA), Information Independent Acquisition (IIA) or equivalent.
   (a) The system shall acquire a high resolution, accurate mass MS/MS full spectrum in a specified Q1 window in DIA/IIA scan.
   (b) Shall be able to acquire by fragmenting all ions that enter the mass spectrometer with high-resolution, accurate mass detection.
   (c) Spectral library matching shall be feasible with the MS/MS spectrum acquired in DIA/IIA scan.
   (d) The system shall acquired up to 200 Q1 windows per cycle during DIA/IIA scan.
   (e) The collision energy applied to DDA/IDA and DIA/IIA scan shall be user controllable.
   (f) The tandem mass spectra could be acquired by sequentially isolating and fragmenting ranges of m/z.

3.4.10. Able to quantitate using MS/MS data.

3.4.11. Sensitivity of exact mass measurement: signal to noise (S/N) for 1pg reserpine in ESI mode on column with positive ionization shall be 750:1 (RWS) or better.

3.4.12. MS/MS sensitivity: 1pg reserpine in ESI mode on column with positive ionization should produce S/N>1,500:1 RMS.

3.4.13. Scan speed:
   (a) MS: at least 25Hz
   (b) MS/MS: at least 100Hz

3.4.14. Mass resolution should be equal to or greater than 42,000 (FWHM).

3.4.15. Internal mass accuracy should be equal or less than 1 ppm.

3.4.16. Internal mass accuracy should be equal or less than 0.5 ppm.

3.4.17. Mass accuracy over time shall be less than 2ppm RMS over 12 hours or better.

3.4.18. Dynamic range should be equal to or greater than 4 orders of magnitude.

3.4.19. Computer controlled polarity switching shall be available.

3.4.20. The system shall include dynamic background subtraction technology to minimize collection of background ions during MS/MS analysis.

3.5. **Vacuum system**

3.5.1. The mass spectrometer shall include a differentially pumped vacuum system or equivalent.

3.5.2. The pumping vacuum system should preferably have fail-safe protection in case of power failures.

3.5.3. Vaccum read-backs and system vent/pump cycles shall be digitally monitored to provide software control.

3.5.4. Oil and mist traps for the roughing pumps, if required, shall be provided.

3.5.5. The exhaust waste generated from the vacuum venting system shall be connected with the existing venting system at no extra cost.

4. System control, Data Management and Data Processing Unit

4.1. The workstation shall include, but not limited to the following units:

(a) The system control unit (online workstation, section 4.2) for controlling the operation and handling of data.

(b) A set of standalone offline data processing unit (offline workstation, section 4.3)

4.2. **System control and data handling unit (online workstation)**

4.2.1. All the interfaces and software necessary for the control and data processing of the HPLC-HRMS system shall be provided.

4.2.2. The online workstation shall be networked to the offline data processing unit. The installation of the local area network shall be provided without any additional cost.

4.2.3. The minimum hardware configuration of the online workstation is listed as follow:

(a) Intel® core i5, quad core processor of speed 2.9 GHz
(b) 32GB DDR3 RAM memory
(c) Two sets of 2TB hard disk for storage of data
(d) Three ethernet 10/100 Mbps LAN adapter cards with 3 ethernet ports
(e) Four USB 3.0 ports
(f) One sound card
(g) Graphic card(s) with 64 MB memory or above, supporting dual monitor display
(h) One 22-inch LED monitor or better
(i) DVD-rewritable drive with 8X speed or above
(j) One set of keyboard and mouse
(k) One laser printer for automatic both sides printing with printing speed of up to 40 A4-pages per minute and up to 1200 x 1200 dpi resolution

4.2.4. The online workstation shall include:

(a) A licensed system control and data handling software (section 4.2.5)
(b) A licensed operating system such as Microsoft® Windows® 7 or its latest version, or equivalent. Vendor is responsible for any update required throughout the life of the analyzer.
(c) Data processing software such as Microsoft® Office 2013 professional or higher version or equivalent with perpetual license for data processing and handling through database, spreadsheet, word processing and reporting.

(d) Fully licensed anti-virus software such as Norton Anti-virus or equivalent software which is fully compatible with the workstation.

4.2.5. The system control and data handling software of the online workstation shall have the following features:

(a) The software shall be able to operate and control the HPLC and HRMS system, enable instrument set-up, data acquisition, processing and reporting.

(b) The software shall have true multi-tasking capacity to display, review and manipulate previously acquired data files while acquisition of new data is in progress.

(c) The software shall be capable of displaying the complete timed event methods and real time display of instrument parameters and signals of the HPLC and HRMS systems.

(d) Licensed software for generating system mirror image files for the workstation shall be provided for system recovery in case of computer break down. The system mirror image files shall contain the operating system, all licensed software, equipment settings and control parameters and acquired data.

(e) All software shall come with official licenses. The licensed software shall be fully compatible with the operating system.

(f) The workstation software should be based on Microsoft® Windows® platform, compatible with Windows® 7 or higher version. Multitasking suite of analytical applications and instrument management software should be included for data processing and handling.

(g) Complete data processing program including manual and automatic integration of chromatographic peaks/ noise threshold / baseline control parameters shall be provided.

(h) The software shall be able to calculate the elemental composition. A goodness of fit from actual to theoretical isotopes or similar indicators shall be included. The software shall be able to filter out incorrect elemental composition calculations through the use of intelligent algorithms or other equivalent methodologies.

(i) The software shall enable calibration using MS/MS data with linear or quadratic fits. Calibration information for each compound shall be accessible on screen, and shall include target and qualifier ions, retention time windows and regression outputs.

(j) The software shall be capable of providing database searching function for matching of HR-MS and HR-MS/MS spectra.

(k) Data analysis software for drug screening and quantitation shall be included.

(l) The software shall be able to generate qualitative as well as quantitative reports. The report format shall be customized according to user’s requirement at no extra cost.

(m) Comprehensive self-diagnostic and extensive on-line help programs for fast troubleshooting of the whole system shall be provided.
(n) Free upgrade of system software within 2 years after installation shall be provided.

4.3. **A set of standalone offline data processing unit**

4.3.1. All the interfaces and software necessary for the control and data processing of the HPLC-HRMS system (section 2 to 3) shall be provided.

4.3.2. The data processing unit shall be networked to the online workstation. The installation of the local area network shall be provided without any additional cost.

4.3.3. The minimum hardware configuration of the online workstation is listed as follow:

(a) Intel® Xeon Processor (20MB Cache, 3.2 GHz) or above
(b) 32GB DDR3 RAM memory
(c) Two sets of 2TB hard disk for storage of data
(d) Three ethernet 10/100 Mbps LAN adapter cards with 3 ethernet ports
(e) Four USB 3.0 ports
(f) One sound card
(g) Graphic card(s) with 64 MB memory or above, supporting dual monitor display
(h) One 23-inch LED monitor or better
(i) DVD-rewritable drive with 8X speed or above
(j) One set of keyboard and mouse
(k) One laser printer for automatic both sides printing with printing speed of up to 40 A4-pages per minute and up to 1200 x 1200 dpi resolution

4.3.4. The offline data processing unit shall include:

(a) A licensed system control and data handling software (section 4.2.5)
(b) A licensed operating system such as Microsoft® Windows® 7 or its latest version, or equivalent. Vendor is responsible for any update required throughout the life of the analyzer.
(c) Data processing software such as Microsoft® Office 2013 professional or higher version or equivalent with perpetual license for data processing and handling through database, spreadsheet, word processing and reporting.
(d) Fully licensed anti-virus software such as Norton Anti-virus or equivalent software which is fully compatible with the workstation.

5. Method package for clinica/forensic toxicology screening

5.1. A validated data acquisition method of the high resolution mass spectrometer (HRMS) for forensic/clinical toxicology screening of urine and blood matrix shall be provided.

5.2. The method shall be compatible with the hardware and software described in section 2, 3 and 4.

5.3. The details of mass spectrometric detection method shall include but not be limited to the followings:

5.3.1. Details of chromatographic separation which include the composition and gradient of the mobile phase solutions, flow rate, injection volume, total run time, column type and temperature setting.

5.3.2. Details of mass spectrometric parameter settings.

5.3.3. A forensic/clinical drug and metabolite database that contains high resolution MS/MS spectrum of least 600 drug and metabolites in positive and negative ionization mode.

The information provided in the library shall include but not be limited to the retention time (in connection with the proposed chromatographic method), the accurate mass of molecular ions and fragmented ions. Fragment mass spectra of parent drugs shall be generated experimentally using authentic drug standards. Fragment mass spectra of metabolites are generated using authentic standards or biological samples with known clinical history in the presence of corresponding parent drugs.

5.3.4. A designated result interpretation method and corresponding customized report format.

5.3.5. Additional database/library shall be provided (if available)

(a) High resolution MS/MS library of pesticides
(b) High resolution MS/MS library of natural products
(c) High resolution MS/MS library of mycotoxins
(d) High resolution MS/MS library of antibiotics

6. Nitrogen generation system

6.1. An integrated nitrogen generation system, or a standalone nitrogen generator equipped with an air compressor, or other equivalent gas generator shall be provided to supply nitrogen gas for the operation of the HPLC-MS system.

6.2. The nitrogen gas generators shall be fully compatible with the system. All accessories for installation such as tee(s). Teflon® connection tubing(s) required shall be provided.

6.3. Nitrogen flow and purity shall be compatible with the MS operation.

6.4. Noise level generated shall be lower than 60 dB within 10 meters during operation.

6.5. The nitrogen gas generators shall be connected with the existing nitrogen gas back-up system at no extra cost.

6.6. All necessary regulators and gas transfer lines for the connection between the instruments and gas supplies shall be provided.

6.7. Any license required for the operation nitrogen generator or related shall be provided.

7. Uninterrupted power supply (UPS)

7.1. A constant and uninterrupted power supply (UPS) shall be assured to the LC-MS/MS (including HPLC, HRMS and workstations) for a minimum of 8 minutes of electricity backup time.
7.2. The UPS shall comply with IEC 62040, or equivalent standards, for electromagnetic compatibility requirements.

8. **配件、安裝及測試**
8.1. 必需為 HPLC (section 2)、HRMS (section 3)及 workstation system (section 4) 提供一個定制的工作枱，以便準確安裝儀器；
8.2. 必需包括一個以非易燃材料製成的通風隔音罩，以容納真空泵；
8.3. 工作台必需包括一減振設備,以避免 primary vacuum pump 對 MS 所造成的振動；
8.4. 應提供儀器的所有必要的校準和 performance check kits；
8.5. 應提供用於儀器的日常及定期維護的專用工具；
8.6. 投標人應當確定電力需求，其環境溫度濕度，以優化儀器安裝的運作程序及其他特殊要求；
8.7. 儀器設備的電源操作應 220V, 50Hz；以及適合用於 IEC 60309 (30A) 之插頭；
8.8. 在測試期間遇到問題時，應提供所有必要的協助，諮詢，時間和資源，以確保整個系統在整個系統的整個使用壽命期間完成安裝和平穩運行。