



Technical Specifications :

Qualitative and Quantitative Analysis of Small Molecules using UHPLC with Mass Spectrometer

The technology provided should be able to meet the qualitative and quantitative analysis requirements of small molecules for environmental applications including pesticides, pharmaceuticals, metabolites and PAHs, in complex and real environmental matrices, viz. wastewater, river water, groundwater, sludge, soil etc. Setup should consist of following components as listed below. Entire set-up should be provided by the same vendor for seamless applications:

1. UHPLC (2 no.)

Analytical LC system should be provided with an integrated configuration for solvent and sample management with the following configuration:

- Binary gradient pump having maximum pressure 15000 psi or above.
- The system should be capable of being operated as HPLC and UHPLC both, compatible with columns of wide dimensions, up to sub 2 μm particle size.
- Capability of isocratic and gradient flow system.
- Vacuum Degasser with sufficient number of channels.
- Solvent delivery pump should be supplied with solvent tray, solvent bottles, filters, appropriate tubings and tool kit.
- Flow rate must be 0.01 – 1 mL/min (in 0.001 ml increment) or better suitable for LC-MS/MS operation.
- Flow precision must be $\leq 0.07\%$ RSD.
- Flow accuracy must be $\pm 1.0\%$ or better.
- Composition accuracy of 0.4% or better.
- Settable composition range should be 0-100%.
- Auto sampler must be supplied along with loop for Analytical purpose, and must be capable of holding 90 or more samples.
- Compatible vials (1000 nos.) with caps should be provided along with the auto sampler.
- Column oven temperature range: room temp. to 80°C or better, which is capable of holding multiple columns.
- Suitable PDA/UV-Vis detector (200-700nm or more) with accuracy 1nm or better (one for each UHPLC).

- Additionally, one suitable fluorescence detector (200-700nm or more) and one suitable RI detector should be included in the quote.
- Software to operate all the detectors should be provided with both the mass spectrometers.
- Single point software control for both LC and MS system.
- Compatible HPLC columns and guard columns (<2 µm) of C18 (4 no.), C8 (2 no.), and for environmentally relevant application including for pharmaceuticals (1 no.), pesticides (1 no.), PAHs (1 no.) and alcohols (1 no.) should be supplied.

2. High Resolution Mass Spectrometer (HRMS) (1 no.)

The HRMS system should have a Quadrupole in tandem with Time-of-Flight (TOF) (Q-TOF), or Orbitrap (Q-Orbitrap), or other equivalent HRMS technology for qualitative and quantitative analysis of small molecules for environmental applications with following specifications:

2a. Ionisation Source

- The system should include Electro Spray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) sources separately.
- ESI and APCI source with positive and negative modes of ionisation.
- The cleaning of source must be done without venting the system.
- Software controlled gas flow and heating facility.

2b. Mass Analyser and Detector

- Suitable analyser geometry which should have quadrupole as MS1 followed by TOF or Orbitrap or other equivalent HRMS technology as MS2 with a collision cell in between should be present.
- Mass range should be 50 - 2000 m/z or better.
- Mass resolution should be $\geq 60,000$ FWHM for HRMS.
- Mass accuracy should be <1.0 ppm in MS mode, and <2.0 ppm in MS/MS mode.
- Instrument should have picomole or higher sensitivity for standard sample in MS and MS/MS mode with proper documentation from company.
- Linear dynamic range should be of 4 orders or higher.
- Data acquisition rate must be ≥ 30 spectra/sec in MS and MS/MS mode for TOF, and ≥ 12 spectra/sec for Orbitrap or equivalent HRMS technology with proper documentation from company.
- Accuracy of 1 ppm or better should be maintained for a temperature range of 16-30 °C.
- Instrument should be supplied with a syringe pump with all necessary accessories for direct infusion of samples/standards, calibrant and reference compound.

- System should be capable of internal reference mass correction / lock mass for MS and MS/MS operation. Chemical reference kit for mass calibration should be supplied.
- Flexible automated optimization small molecule analysis should be present.
- LC-MS/MS start-up kit should be supplied as standard.
- Mass calibration and tuning kits should be supplied.
- All consumables required for initial demonstration and training of users should be provided.

2c. Vacuum System

- High efficiency vacuum system with low noise and maintenance must be provided. All accessories required for the proper functioning of the vacuum system should be supplied.

2d. Nitrogen Generator and Air Compressor

- A noise free Nitrogen gas generator with in-built compressor which is capable to deliver the 99.99% pure gas required to run the system.
- Cooling moisture trap, all pipe/tubing connections and fittings will be done by vendor.
- N₂ and other gas cylinders, i.e. Argon, for the working of the system shall be provided with all accessories such as regulator, gas purification panel unit, cylinder cage / bracket etc. and fitted with FOC by vendor.

2e. Software/Hardware System

- A high-end workstation facility with branded PC (Dell/HP/IBM etc.) 16GB RAM, 3 TB Hard Drive, with 24-inch monitor, laser printer, data handling and reporting with Licensed software for full control of the LC and HRMS systems.
- Another high-end workstation facility for offline data analysis of UHPLC-HRMS setup with branded PC (Dell/HP/IBM etc.) 16GB RAM, 3 TB Hard Drive, with 24-inch monitor, laser printer, data handling and reporting with Licensed software.
- Suitable software for instrument operation, scan and data processing of all scan function should be provided in CD`s with legal licenses.
- The software should have the following features,
 - i. Automated mass calibration, resolution, sensitivity check should be performed by software.
 - ii. Elemental composition calculator for the HRMS data.
 - iii. Simulation of isotopic pattern for a given molecular formula.
 - iv. Appropriate software tools for addressing screening, compound identification and structural elucidation workflows.
- Specific libraries for water screening and environmental samples should be provided.

- Soft copy (PDF/ ASCII etc.) of all the operations and maintenance /trouble shooting manuals of the instrument and software must be supplied.
 - The workstation should be able to monitor the performance of all the individual components of the LC-MS with alerts for any errors.
 - Software to operate all the detectors should be provided.
 - Free software upgradation on both workstations for at least five years.
- Equipment should be supplied with suitable power backup system with at least 60 minutes back up for the complete system (including LC) should be provided. Battery and battery rack should be provided along with system.

3. Triple Quadrupole Mass Spectrometer (1 no.)

The Triple Quadrupole Mass Spectrometer (LC-MS/MS) for targeted quantification of small molecules for environmental applications must include appropriate separation devices, high sensitivity triple quadrupole mass spectrometer, appropriate software and accessories as per following specifications:

3a. Ionization Source

- The system should include Electro Spray Ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI) sources separately.
- ESI and APCI source with positive and negative modes of ionisation.
- The cleaning of source must be done without venting the system.
- Software controlled gas flow and heating facility.

3b. Mass Analyser and Detector

- Quadrupoles should have high quality mechanical tolerance and minimum coefficient of thermal expansion for high standard of mass stability in varying lab temperature conditions.
- Mass Range: 50-2000 m/z or better.
- Resolution: ≤ 0.7 FWHM.
- Linear dynamic range: ≥ 5 orders of magnitude.
- Mass stability: 0.1Da 12 hours or better.
- Sensitivity: MRM ESI Positive mode: Injection of 1pg of reserpine onto a column should yield signal to noise ratio $\geq 1,50,000:1$.
- Sensitivity: MRM ESI Negative mode: Injection of 1pg of chloramphenicol onto a column should yield signal to noise ratio $\geq 1,00,000:1$.
- Scan speed: 15,000 amu/sec or above.
- Operating modes: Full scan, SIM, SIR, Precursor ion scan, product ion scan, Neutral loss scan, MRM, simultaneous full scan and MRM.
- MS and MS/MS can be performed in a single run.
- Instrument should be supplied with a syringe pump with all necessary accessories for direct infusion of samples/standards, calibrant and reference compound.
- LC-MS/MS start-up kit should be supplied as standard.

- Mass calibration and tuning kits should be supplied.
- All consumables required for initial demonstration and training of users should be provided.

3c. Vacuum System

- High efficiency vacuum system with low noise and maintenance.
- Instrument should perform multiple MRMs without cross talk in a single run.
- Gas flow levels must be controlled by the software.
- Accessories required for proper function of the vacuum system should be included.

3d. Nitrogen Generator and Air Compressor

- A noise free Nitrogen gas generator with in- built compressor which is capable to deliver the 99.99% pure gas required to run the system.
- Cooling moisture trap, all pipe/tubing connections and fittings will be done by vendor.
- N₂ and other gas cylinders, i.e. Argon, for the working of the system shall be provided with all accessories such as regulator, gas purification panel unit, cylinder cage / bracket etc. and fitted with FOC by vender.

3e. Software/Hardware System

- A high-end workstation facility with branded PC (Dell/HP/IBM etc.) 16GB RAM, 3 TB Hard Drive, with 24-inch monitor, laser printer, data handling and reporting with Licensed software for full control of the LC and triple quadrupole mass spectrometer systems.
- Another high-end workstation facility for offline data analysis of UHPLC-QQQMS setup with branded PC (Dell/HP/IBM etc.) 16GB RAM, 3 TB Hard Drive, with 24-inch monitor, laser printer, data handling and reporting with Licensed software.
- Suitable software for instrument operation, scan and data processing of all scan function should be provided in CD`s with legal licenses.
- Soft copy (PDF/ ASCII etc.) of all the operations and maintenance /trouble shooting manuals of the instrument and software must be supplied.
- The software should be able to acquire and process the data simultaneously and should be able to control the UHPLC, detector and auto sampler.
- The workstation should be able to acquire, store and reproduce the data.
- The system should be able to control gas flow and the software should be having options for automated calibration and quantitative optimization.
- The workstation should be able to monitor the performance of all the individual components of the LC-MS with alerts for any errors.
- Software to operate all the detectors should be provided.
- Single point software control for both LC and MS system.

- Automated mass calibration, sample tuning, SIR, MRM method development.
- Software for small molecules data acquisition.
- Software for targeted quantitative analysis of small molecules.
- Free software upgradation on both workstations for at least five years.
- Equipment should be supplied with suitable power backup system with at least 30 minutes back up for the complete system (including LC) should be provided. Battery and battery rack should be provided along with system.

Terms and conditions

- **Supplier's selection of incoterm FOB/FCA will be treated as DDP for this tender. Hence suppliers should quote the final amount of equipment as per DDP incoterm.**
- The duty exemption certificate, if needed, will be provided by the IIT Mumbai, as per applicability.
- System performance should be demonstrated with necessary standards, and calibration kits which will be provided by the vendor.
- All the system components supplied, should have warranty for three years from date of installations and 2 years AMC including all labour cost. Payment of spare parts if necessary will be made as and when required basis.
- Warranty should include preventive maintenance kit, calibration kit for LC-MS/MS system, and compressor of nitrogen generator without any further cost to the institute.
- No conditional warranty will be accepted.
- Basic training for a period of one week after installation & commissioning of the equipment to technical personnel to be provided at our site.
- On-site training of staff and students (at least twice in a year for 7 days each) during the first 3 years.
- Good technical support should be provided after the installation of the instrument and the service engineer should be able to attend unlimited breakdown calls and should visit the installation site within 24 hours without fail.
- Service support should be available for 6 days a week.
- Training on troubleshooting the issues associated with instrumentation or application should be provided free of cost whenever required by the user.
- Manufacturer should provide the service support details in Mumbai and India. Details of the service engineers and application specialists should be provided along with their experience in the mass spectrometry field and their association with manufacturer's company.
- Details of the users (name, phone number and email ID) in India for the quoted instrument in the bid should be provided.
- Instrument performance, quality of service and application support certificates from at least three existing users should be provided.