



INDIAN INSTITUTE OF TECHNOLOGY BOMBAY
MATERIALS MANAGEMENT DIVISION
Powai, Mumbai - 400076

Technical specification of LC-MS/MS

PR No. 1000027488

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A. System level Requirements

1. We require a triple quadrupole mass spectrometer, gas generator, ultra-performance liquid chromatography (UHPLC) system, autosampler, column oven, software, desktop computer, UPS, and all the necessary accessories, libraries, and method packages for metabolomics applications.
2. The various components of the above system need to be quoted by the same vendor for seamless integration, installation, and post-sales services.
3. The vendor needs to certify that the quoted instrument is complete. No additional accessories should be required for full functionality of the LC-MS/MS. Incomplete quotes will be rejected.
4. All the specifications must be available on the manufacturer's specification sheet. Any supporting document or lab report regarding LC-MS/MS specifications will not be accepted.

B. Ultra-High-Performance Liquid Chromatography (UHPLC) System

1. Binary gradient pump with high-pressure mixing, equipped with in-line degasser
2. The operating flow rate range is 5 -3000 uL/min or more, in 1-uL or smaller increments.
3. The pressure rating of 18000 psi or higher.
4. The UHPLC system should have a single-point software-based control with MS.
5. Gradient profile: step and linear gradient at multiple levels
6. Capability to run columns from 1.6 – 5 μm particle size range.

C. Autosampler

1. Injection volume: 0.1 to 20 μL (or higher) in 0.1 μL increments.
2. Sample capacity of at least 90 vials of 1.5/2 ml.



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3. Sample cooling range from 4 – 40 °C
4. The pressure rating of 18000 psi or higher.

D. Column Oven

1. The oven should accommodate 1-2 columns of 25 cm with 5 cm of guard column.
2. Temperature range: 10 °C below room temperature to 80 °C or more.
3. The column oven should preferably work on forced air circulation to maintain a uniform temperature.

E. Triple Quadrupole Mass Spectrometer

- **MS ionization source:** The instrument ionization source should have an interchangeable APCI (Atmospheric Pressure Chemical Ionization) and ESI (Electro-Spray Ionization) probe. Each probe should be coded for automatic identification by the software/firmware of the host system. There should be a provision available to divert the flow to waste/MS through the software before/during/after the analysis to reduce source fouling/contamination.

Mass Analyzer and Detector

- Required Resolution: 0.5-0.7 Da or better. Vendors must provide resolution for complete mass range for the QQQ in the technical manufacturer's specification sheet
- Quadrupole mass range: at least 5 – 1200 m/z or higher
- Scan speed: 12,000 Da/sec or higher
- MRM dwell time: 1 ms or less
- Linear dynamic range: ≥ 6 orders of magnitude.
- Data acquisition should be possible in full scan, selected ion monitoring/recording (SIM/SIR), product ion scan, precursor ion scan, neutral loss/gain scan, and multiple reaction monitoring (MRM) modes.
- MRM acquisition rate: 500 MRMs/sec or more
- Sensitivity: For positive ionization mode, 1pg of reserpine should have a signal to noise of



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$\geq 15,00,000:1$. For negative ionization mode, 1pg of chloramphenicol should have a signal to noise of $\geq 15,00,000:1$. These specifications should be present in the manufacturer's official specification sheet and should be demonstrated to the end user after installation.

- Polarity switching: Positive and negative mode spectral acquisition should be possible in a single run with a polarity switching time of ≤ 15 ms or less
- Vacuum interlock system: An in-built system that allows source and optionally even capillary cleaning and maintenance while maintaining the system vacuum
- Detector: High energy, high sensitivity detector

F. Workstations Specifications

- Data acquisition computer interfacing hardware and software for instrument control, data acquisition, and data processing must be supplied compatible with the LC-MS system and should be quoted by the same vendor.
- A separate high configuration workstation should be quoted for offline data processing. Minimum computer specifications for each computer: 64 GB RAM, 10 TB hard disk. The most recent version of Windows compatible with acquisition and offline data processing software, mouse, English keyboard, and a 24 inches screen should be provided. All software and potential upgrades should be compatible with the operating system.

G. Software and data analysis tools

- Software for data acquisition, processing, and analysis suited for metabolomics applications, as well as other related and relevant applications, should be provided. The quoted software should be capable of both qualitative and quantitative analyses with statistical tests.
- The software should be capable of multitasking with single-point control over the system. Capable of performing automated calibration, extracting mass spectra and retention time of an analyte and searching/matching them against the library spectra, and quantitative estimation
- All the software must be fully compliant with 21 CFR Part 11.



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H. Accessories

- Prerequisite for MS: It will be the vendor's responsibility to install the equipment and the accessories to run the instrument. It may include but is not restricted to plumbing, wiring, cylinders, piping, gas generators, computer hardware and software installations, extra electrical wiring, switches, and so on, to bring the instrument to PQ level.
- A suitable nitrogen generator should be supplied by the vendor and quoted. The generator must have a trouble-free compressor with the appropriate capacity to deliver gas for the appropriate functioning of LCMS/MS.
- Compatible UPS (≥ 15 KVA) with a good backup time of at least ≥ 1 hour and a data logger should be supplied by the vendor.

I. User training

- Instrument operation and data analysis training at the customer site to be included (at least two times per year for 4 years).

J. Additional Mandatory Requirements

- The vendor must have a service center in India, and the vendor should provide the address of certified and authorized service center.
- List of at least 10 global installations of the quoted instrument and description of the users with details. Optionally, additional user details for 5 installations within India may be provided.
- Instruments must be attended to within 48 hr in case of any breakdown. The uptime for the system should be $> 95\%$ per year. The vendor should assure the availability of the spares for the next 5 years from the installation date.



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- Technical /application support should be provided by a competent person of the supplier as and when required. This should be extended without any conditions or additional costs throughout the instrument use at IIT Bombay.
- The vendor must highlight the specification in their technical brochure sheet and mention compliance with the specifications in the tender document.
- The vendor must demonstrate the claimed LC, MS, and software capabilities on site after installation.
- The equipment should come with a certificate of analysis and conformity.
- Original Equipment Manufacturer (OEM) Certificate is required.

K. Warranty

- One year of warranty and a Comprehensive Maintenance Contract (CMC) for 3 years is required for the entire system, including all accessories and offline systems.