

INDIAN INSTITUTE OF TECHNOLOGY BOMBAY MATERIALS MANAGEMENT DIVISION

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Technical specification for High Resolution Mass Spectrometer

The system should have Quadrupole and Time of flight (Q-Tof)/Quadrupole with Time of Flight Equivalent technology for qualitative and quantitative analysis.

No.	Item	Specifications
1.	Ionisation source	 Dedicated Electro-spray ionisation (ESI) source with positive and negative modes of ionisation. ESI source permits switching between the two ionisation modes during a single run. The cleaning of source must be done without venting the system. Software controlled gas flow and heating facility. ESI flow rate range without splitter: up to 2ml/min Dedicated APCI source should be included
2.	Mass Range	 TOF: m/z up to 10,000 Da or better Quadrupole: m/z up to 2,000 Da or more
3.	Mass resolution	• 30,000 FWHM or better for TOF. In case of equivalent technology other than TOF, the resolution of the mass analyser must be more than 1,20,000 FWHM or better
4.	Analyzer type	 Suitable analyser geometry which should have quadrupole as MS1 followed by TOF as MS2 with a collision cell in between should be present and capable of providing resolution 30,000 FWHM. Detector should be equipped with the latest technology
5.	Mass Accuracy	• <1.0 ppm in MS mode and <2.0 ppm in MS/MS mode
6.	Mass Sensitivity	• Instrument should have sensitivity for standard sample (at picogram level) with S/N 500:1 (RMS) in MS or better and S/N 1500:1 (RMS) or betterin MS/MS mode with proper documentation from company.
7.	Spectral acquisition rate	 Data acquisition rate must be 30 spectra/sec; 30 Hz or better in MS and MS/MS mode and for equivalent technology mass analyser of minimum 12 spectra or better with proper documentation from company. Higher spectral acquisition rate will be desirable.
8.	Temperature Stability	 Need to maintain 1 ppm accuracy even at temp of 18-28 °C for 24 hours
9.	Calibrant Delivery	Provision for infusion of calibrant and reference compound.
10.	Reference /lock mass	 System should be capable of internal reference mass correction / lock mass for MS and MSMS operation. Chemical reference kit for mass calibration should be supplied.
11.	Vacuum System	 Highly efficient vacuum systems consist of turbo molecular pumps followed by rotary mechanical pump must be provide. All accessories required for the proper functioning of the vacuum system should

		be supplied.
12.	Optimization	• Flexible automated optimization for protein, peptide, oligonucleotides and small molecule analysis.
13.	Software/hardware system	 Branded PC(Dell/HP/IBM or substantially equivalent) 16GB RAM, 3 TB Hard Drive, with 24 inch monitor, laser printer, work station facility, data handling and reporting with Licensed software for full control of the LC and MS systems. 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, a) Automated mass calibration, resolution, sensitivity check should be performed by software. b) Elemental composition calculator for the HRMS data. c) Simulation of isotopic pattern for a given molecular formula. d) De-convolution tool for the determination of Mol. Wt. of high molecular weight compounds. e) Appropriate software tools for addressing screening, compound identification and structural elucidation workflows. f) Appropriate software for small molecules and nucleotide analysis that can perform both qualitative and quantitative analyses along with statistical tests, should be provided g) Soft copy (PDF/ ASCII etc.) of all the operations and maintenance /trouble shooting manuals of the instrument and software must be supplied. h) Free software upgradation for at least five years.
14.	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 vender.
15.	Accessories	 Any other gas cylinders for the working of the system shall be provided with all accessories such as regulator, gas purification panel unit, cylinder cage / bracket etc. should be supplied and fitted with FOC by vender.
16.	UPS	 A suitable online UPS of 10Kva capacity or more with at least 60 min back up for the complete system (including LC) should be provided. Battery and battery rack should be provided along with UPS.
17.	LC system	 Analytical LC system should be provided for solvent and sample management with the following configuration,,
17(a)	Pump	 High Pressure Binary pump having maximum pressure 15000 PSI or better. The system should be capable of being operated as HPLC and UHPLC both, compatible with columns of wide dimensions, up to sub 2 micron 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.
17(b)	Flow rate	 Must be 0.001 – 2 mL/min (in 0.001 ml increment) suitable for LC-MS/MS operation.
17(c)	Flow Precision	• Must be less than 0.07% RSD.
17(d)	Flow Accuracy	Must be better than 1%
17(e)	Composition Accuracy	• <u>+</u> 0.5% or better

17(f)	Composition range	Settable range should be 0-100%
17(g)	Auto sampler	 It must be supplied along with loop for Analytical purpose. Must be capable of holding 90 or more samples. 1.5 mL vials (1000 nos) with caps should be provided with the auto sampler It should have Peltier sample cooler from 4-40°C
17(h)	Column oven	• Temperature range: room temp. to 80°C or better, which is capable of holding multiple columns.
17(i)	Detector	• Suitable PDA detector (190-800nm or more) with accuracy 1nm or better. It should have dual light source with temperature controlled flow cell
17(j)	Control	Single point software control for both LC and MS system
17(k)	Hardware	Both LC and MS should be from same manufacturer.
17(1)	Columns	 HPLC columns and guard columns of C18 and C8 (<2um) 4 nos each, also suitable columns to analyse peptide/proteins/oligonucleotide should be provided.
18.	Training/Maintenan ce	 Free training for operations and maintenance of the spectrometer at the time of installation and subsequent periodic training (two times/year) during the warranty period. Service engineer should visit 2 times a year for annual maintenance of the system during the warranty period.
19.	Specification sheet	A detailed specification sheet highlighting all above specifications along with detailed experimental conditions must be attached.
20.	User Reference List	 At least 10 Global Academic customer list with complete contact details should be provided.
21.	Warranty	 5 years complete comprehensive maintenance warranty on the entire system (UPLC, MS, Nitrogen generator, UPS etc.) with spares, electronic boards and hardware consumables. 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.