



INDIAN INSTITUTE OF TECHNOLOGY BOMBAY
MATERIALS MANAGEMENT DIVISION

PR No.: 1000039852

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Technical Specifications for Specifications for Gas ChromatographyHigh Resolution Mass Spectrometer – QTOF/Orbitrap (Qty-1)

Sr. No.	Content	Specification	Compliance (Yes/No)	Additional Information (if any)
1	General Specifications	<p>The mass spectrometer should be a high-resolution benchtop system.</p> <p>The mass spectrometer should have a hybrid configuration and should be capable of delivering high resolution and accurate masses for various modes of operation.</p> <p>The mass spectrometer must be capable of real-time data acquisition and data processing, and should ensure a high spectrum repetition rate.</p> <p>The mass spectrometer should utilize accelerated collision cell for generating the fragment spectra.</p> <p>The mass spectrometer should be a GC-MS/MS system utilizing a Quadrupole Mass Filter consisting of a segmented mass filter, providing variable and step-less precursor isolation width selection from 0.4 Da to full mass range.</p> <p>The mass spectrometer must be able to perform parallel filling and detection to increase the duty cycle.</p> <p>The mass spectrometer must be able to finish Auto Tune and mass calibration.</p> <p>The mass spectrometer should not require external gases except nitrogen and helium for electron ionization operation.</p> <p>The mass spectrometer must be a bench top system, as opposed to a floor /standing model.</p>		



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2	Performance Specifications:	Sensitivity EI Full MS: 1 μL of 100 $\text{fg}/\mu\text{L}$ octafluoronaphthalene (OFN) will produce a minimum signal-to-noise of 10000:1 or better .The area precision of eight sequential injections of 1 μL , 10 $\text{fg}/\mu\text{L}$ OFN will result in an instrument detection limit (IDL) of 6 fg or less (OFN) derived at the 99% confidence level or better.		
3	Mass Resolution	Maximum resolution should be 50000 (FWHM) or above at m/z 200 or at m/z 271.9867 for 1 pg of OFN.		
4	Scan Speed	Highest scan speed should be 40 scans per second (40 Hz) or better in Full MS Scan mode or SIM mode		
5	Mass Accuracy	The mass spectrometer must provide mass accuracies of less than 3 ppm RMS error with external calibration over 24 h and without any kind of mass recalibration. The mass spectrometer must provide mass accuracies of less than <2 ppm RMS error with internal calibration		
6	Dynamic Range	The mass spectrometer must have a dynamic range of greater than 5000:1 within one spectrum (single transient acquisition). The mass spectrometer must provide $>10^5$ analytical dynamic range or better.		
7	<i>m/z Range</i>	The mass spectrometer must have mass range of 30 - 3000 Da or better.		
8	Scan Functions	The mass spectrometer must be capable of Full MS, Selected Ion Monitoring (SIM) and MS/MS experiments		
9.	Ion Source	The mass spectrometer must have sources capable of electron ionization, and chemical ionization		



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10.	Ion Optics and Mass Analyzer	<p>The mass spectrometer must have a RF only quadrupole device with axial field for most robust operation and highest transmission.</p> <p>The mass spectrometer must have a segmented hyperbolic Quad mass filter, enabling it to select a variable and step-less precursor isolation width from 0.4 to 50 u.</p> <p>The mass spectrometer must have an electrostatic orbital trap or a TOF as its mass-analyzing device.</p>		
11	Vacuum System	<p>The mass spectrometer must have no more than one turbo molecular pump.</p> <p>The mass spectrometer must have a differentially pumped vacuum system with pressures ranging from 5 to 5×10^{-10} mbar in the mass analyzer.</p> <p>The mass spectrometer must have a high-vacuum aluminum manifold.</p>		
12	Detection System	<p>Mass spectra must be detected by an image current detection system or photo multiplier device.</p>		
13	High Resolution Accurate Mass Analyzer	<p>Must have an electrostatic orbital trap or a High-resolution Q-TOF. Must have very low electronic capacitance for high signal to noise ratio of ions.</p>		
14	Software	<p>Appropriate software along with libraries for qualitative and quantitative analysis of small molecules and statistical analysis capabilities. Latest licensed copy of NIST 2023.</p> <p>Four more licensed copy of software has to be provided, over and above the one associated with the main Instrument.</p>		
15	GC Specifications	<p>The GC must feature an external color touch screen to provide easy accessibility to the GC and immediate interactions with it. The touch screen of the GC should provide all data required, including all temperature and pressure/flow parameters, type of carrier gas, carrier gas column pressure, flow rates, split flow, detector gas flow rates and all detector parameters.</p>		



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16	GC Oven	<p>The column oven should have an operating range of ambient plus 5°C to 450°C. Heat-up time from 50°C to 450°C within 4 minutes (230 VAC version). Cool-down time from 450°C to 50°C in less than 4 minutes.</p> <p>The heating rate should be 120 °C/min. The oven temperature stability should be within 0.01 °C/°C of actual temperature.</p>		
17	SSL Injector- Qty-2	<p>The SSL injector should be user-installable within a few minutes, and without any special tool.</p> <p>Maximum Temperature: 400 °C.</p> <p>Split Ratio: up to 12500:1.</p> <p>Pressure Range: 0-150 PSI.</p> <p>Total Flow Setting:</p> <ul style="list-style-type: none"> – Control of split flow in 1 mL/min from 0 to 1250 mL/min. – Purge flow from 0 to 50 mL/min. 		
18	Specifications of liquid autosampler, Headspace, SPME Arrow	<p>It should have more than 160 vials capacity for 2 ml sample vials & more than 45 vial capacity for headspace and SPME arrow. It should have liquid, Headspace, and high sensitivity SPME Arrow capabilities. Syringe changing should be fully automatic for headspace mode/liquid mode and SPME Arrow.</p> <p>Detectors other than mass: FID should be provided.</p> <p>Flame Ionization Detector (FID)</p> <p>:Flameout detection and automatic re-ignition, Maximum temperature: 450°C settable in 0.1°C steps, Sensitivity: 0.03 Coulombs/gC.</p>		
19	Consumables for GC/HRMS should be quoted for trouble free operation	<ul style="list-style-type: none"> - Vials (2ml capacity) /septas/screw caps for liquid autosampler- 400 nos. - Vials for Headspace (20 ml capacity) /septas/caps for headspace vials-300 nos. - Septas for injector ports- 200 nos. - Liquid syringes – 10ul – qty-7 - Gas tight Syringe 100ul to 1ml. - qty-5 		



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		<ul style="list-style-type: none"> - Ferrules-50 - Liners & seals for injector ports- 10 each for SSL & PTV - Column nuts- 10 each for SSL & PTV - Vacuum Pump oil- 5 litre - MS filaments- 5 filaments - Crimper & decrimper for HS vials- two each - Split Line & Carrier line filter- 2 each - GC capillary column – 5% Phenyl Methyl Polysiloxane or equivalent, 30 mts, 0.25 mm id, 0.25 um film- qty-3. 1 wax column and appropriate column for FAME analysis - Deactivated glass wool-qty-10 g. - Ceramic column cutter- qty -2 - Replacement triple trap for Carrier gas - Aluminium Oxide for cleaning - Calibration compound FC 43 - SPME arrows of different types of Fiber compositions 3 sets of 5 fibers 		
20	Local purchase	<ol style="list-style-type: none"> 1. UPS with 1 hour back up 2. Two computers one for instrument operation and the other for data processing; the one for data processing should have higher RAM (64 bit or better) 3. Gas purification panel, gas cylinders with regulators and filters should be provided with tubing fittings for all the gases. Gas cylinders for Methane (10 L wc) and Helium , Hydrogen, Nitrogen and zero Air (47 L wc) should be included. Hydrocarbon trap should be included. 4. Laser jet Color Printer. 		
21	Training and Warranty	<p>Training for Technician: 5 persons training in IIT Bombay lab by Application scientists for 15 days</p> <p>Five years Warranty</p> <p>Instrument Delivered must be manufactured within past 1 year from</p>		



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		date of delivery		
		The system should be quoted on DDP basis.		