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Detailed Technical Specifications for GCMS-MS (QQQ) with HS:

A. System level Requirements

1. GCMS-MS (QQQ) with HS: We require a triple quadrupole mass spectrometer coupled to Gas chromatography (GC) system, autosampler, headspace sampler, software, desktop computer, UPS, gas cylinders, gas purification panels and all the necessary accessories, the latest NIST libraries.
2. The instrument needs to be a standard product of the vendor with List of at least 20 global installations of the quoted instrument and description of the users with details and additional user details for 3 installations within India need to be provided. We are not looking for a custom-built product based on the specifications provided herein and such quotations will be rejected.
3. The various components of the above system need to be quoted by the same vendor for seamless integration, installation, and post-sales services.
4. The vendor needs to certify that the quoted instrument is complete. No additional accessories should be required for full functionality of the GC-MS/MS. Incomplete quotes will be rejected.
5. All the specifications must be available on the manufacturer's specification sheet. Any supporting document or lab report regarding GC-MS/MS specifications will not be accepted.

B. Gas Chromatography system.

A GC system should have the capability of:

1. One Split/Splitless capillary column injection unit
2. One PTV capillary column injection unit
3. Maximum Injector temperature: 400 °C
4. Split ratio: 7000:1 or more
5. Carrier gas Flow Control should have Constant flow, constant pressure, Constant linear velocity modes
6. Pressure program ramps: minimum 3 steps
7. Operating temp range for oven from near ambient to 450°C
8. Maximum temp rate 115°C/min or higher
9. Cooling rate: 450°C to 50°C within 4 mins or lesser with optional cooling ramp
10. Temperature ramps Minimum 5 or more
11. Adjust pressure in increments of 0.001 psi, pressure setting range of 0-95 psi
12. Flow sensor for control and storage of split ratio

13. Inlet should be capable of taking total flow of upto 500 mL/min with N₂ and 1000 mL/min with H₂ or He.
14. Use capillary columns of 25, 50, 100, 250, 320 microns
15. GC should have a display unit.
16. The system should have post column backflush

C. Liquid Autosampler

1. Electronic motor actuated automatic injection system
2. Should have an auto injector tray of minimum 100 vials capacity
3. Vendors must supply GC syringes for liquid injection for 10uL (5 nos. each) preferably of the same brand.

D. Head Space Sampler

1. Head Space (HS) Sampler should be transfer line based with loop and trap adsorbent system for precise quantification
2. Trap should be electronic cooling temperature range upto -20°C
3. Headspace sampler should have a separate inlet, i.e., other than Split and PTV inlet mentioned above
4. Headspace sampler with minimum 40 vials capacity to be provided with compatibility with vials of 10 mL and 20 mL sizes of crimp top closure.
5. The HS system should have minimum 10 vials heated independently in overlapping mode with adjustable shaking options.
6. Carry over lesser than 0.001%.
7. All temperature should be programmable up to 250 °C or higher.
8. Vial pressurization should be fully controlled by software using suitable Flow/pressure control system
9. Headspace must be configured independent channel of liquid injection module to avoid cross-contamination.
10. The Software should be a single operation software for both GC and HS system.
11. Suitable accessories for the HS connection should be included in the quote

E. Triple Quadrupole Mass Spectrometer

A triple quadrupole mass spectrometer conforming to international safety standards, designed and manufactured under a quality system registered to ISO 9001 with appropriate computer to support the system from original manufacturer.

1. Mass range: Quadrupole 10 to 1000 amu or higher
2. Mass resolution: minimum 0.7 (width at half height).
3. Mass axis stability: ± 0.1 amu over 24 hours or more
4. Linear Dynamic range: minimum 6 order of magnitude.

5. Scan rate (electronic): 20000 amu/sec or higher
6. Ionization modes: EI (Electron ionization) and System should have dual filament with automatic filament switching.
7. Ionization potential from 10 eV to 200 eV or more for better dissociation of Ions
9. Collision energy must be variable; nitrogen/argon as a collision gas is required.
10. Should be able to do Scan, SIM, MRM/SRM, Parent ion scan, Product ion Scan, and Neutral loss scan
11. Should be able to do Simultaneous Full Scan -SIM or Full Scan/MRM or SRM whenever required.
12. SRM/MRM Speed: minimum of 800 MRM/sec
13. Minimum MRM dwell time of 0.5 milliseconds or lower.
14. A rotary-vane foreline pump supporting the turbo molecular pump should be quoted.
15. Installation checkout sensitivity must be better than –Instrument detection limit. EI MRM IDL: 0.5 fg OFN, statistically derived at 99% confidence level from the area precision of eight sequential splitless injections of 1 μ L, 10 fg/ μ L OFN standard. MS/MS transition of m/z 272 and 222. The required sensitivity of the system should be demonstrated at the site after installation of the facility.
17. EI MRM Sensitivity: 1 μ L of 100 fg/ μ L Octafluoronaphthalene (OFN) should produce the following minimum signal - to -noise for the transition from m/z 272 to m/z 222: 30,000:1 or better.
18. EI Scan Sensitivity: 1 μ L of 100 fg/ μ L Octafluoronaphthalene (OFN) should produce the following minimum signal - to -noise for m/z 272: 2000:1 or better.

F. Workstations Specifications

1. Data acquisition computer interfacing hardware and software for instrument control, data acquisition, and data processing must be supplied compatible with the GC-MS system and should be quoted by the same vendor.
2. 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

1. 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.
2. 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
3. **NIST Library:** Original licenced version NIST 2020 or latest version should be quoted

4. Metabolomics Database to be quoted to identify small metabolites measured by scan and MRM along with Retention time/retention indices. Suitable column and method generation compounds to be supplied specified in metabolomics database.
5. Inborn Errors of metabolism method set for screening 36 Organic acids disorders using 130+ metabolites in urine should be provided

H. Essential accessories required to run GC-MS/MS

1. 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, computer hardware and software installations, extra electrical wiring, switches, and so on, to bring the instrument to PQ level.
2. Any additional accessory for easy switch of liquid autosampler between PTV and split
3. Compatible UPS (minimum 10 KVA) with a good backup time of ≥ 1 hour and a data logger should be supplied by the vendor. Warranty (comprehensive) for UPS and Battery system for Two years.
4. Tool kit
5. i) Gas purification panel with moisture trap for GC-MS ii) Gas regulators for Helium iii) Cylinder filled with Helium gas
6. i) Gas regulators for CID gas ii) Cylinder filled with CID gas
7. Gas linings and other accessories for end-to-end connections.

I. Consumables:

1. GC columns:
 - DB-5 : 30m x 0.250mm x 1.0 μm (01 no.),
 - SP2560 : 100m x 0.25mm x 0.20 μm (0.1 no)
 - Rxi 624 Sil MS : 30m x 0.250mm x 1.4 μm (01 no.)
2. Additional EI Filaments (2 No.)
3. Liquid Auto sampler vials: 500 vials (2 ml capacity) with screw cap.
5. Headspace Auto sampler vials: 500 vials (20 ml capacity) with cap and septa.
6. Decrimper and crimper
7. Column Ferrules- injector end (Split-40 No. and PTV -20 No.), interface end (20 No. each) compatible with the above mentioned column.
8. Septa for injector (100 No.)
9. Appropriate nuts to fit capillary columns to the injector and MS interface (10 nos.)
10. Split liners (with glass/quartz wool at optimum position) (10 No. each)
11. PTV liners (with glass/quartz wool at optimum position) (10 No. each)
12. O-ring for injector liner (20 No.)
13. Split vent trap (2 No.)

14. Column cutter (2 No.)
15. Oil mist trap for pump (2 No.).
16. Suitable n-alkane mixture for Retention index determination

J. User training

Free of cost installation, onsite training for 10 days with respect to metabolomics application

Instrument operation and data analysis training at the customer site to be included (at least once per year for 3 years).

K. Additional Mandatory Requirements

1. The vendor must have a service center in India, and the vendor should provide the address of certified and authorized service center.
2. Instruments must be attended to within 48hr 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.
3. 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.
4. The vendor must highlight the specification in their technical brochure sheet and mention compliance with the specifications in the tender document.
5. The vendor must demonstrate the claimed GC, MS, and software capabilities on site at the time of installation.
6. The equipment should come with a certificate of analysis and conformity.
7. Original Equipment Manufacturer (OEM) Certificate is required.

L. Warranty and CMC.

2 Years warranty should be provided by vendor for entire instrument, including all accessories and offline systems.