Technical Specification for:

Ultra-High-Resolution (>200,000 FWHM at m/z 400), Ultra-High Range (m/z 80,000) Hybrid Quadrupole-Orbitrap Mass Spectrometer

An ultra-high-resolution, ultra-high-range mass spectrometry system with MS/MS capability including a high performance chromatography system, suited for qualitative & quantitative analysis of molecules and materials.

Sources:

- System should have dedicated ESI source capable of handling flow rates from 1ul/min to 2ml/min.
- APCI source should be capable of handling flow rate from 50ul/min to 2ml/min.

Mass Range:

- System should have the mass range up to m/z 80,000 or better for singly charged ions with high mass resolution.
- The mass isolation should be up to m/z 25,000 for MS, MS/MS and beyond. experiments.

Mass Resolution:

• System should have min. resolution of 80,000 FWHM at m/z 350 or higher.

Mass Accuracy:

• System should demonstrate the mass accuracy measurement of <1ppm with internal calibration and < 3ppm with external calibration.

Scan Functions:

- Must acquire and display full scan mass spectra.
- Must acquire and display selected ion monitoring (SIM) with high resolution MS data.
- Must acquire and display full scan MS/MS and higher order tandem mass spectra for selected ions.
- Data independent analysis with variable quadrupole isolation.

Dynamic Range:

• System should demonstrate a dynamic range of >5000:1.

Calibration:

• System should have complete Auto-calibration capability to set all relevant voltages automatically during external and internal calibration.

System Software:

- System software should acquire data from MS and HPLC/UHPLC and should have qualitative and quantitative features.
- Should capable of doing elemental composition, high resolution MS extraction, etc.
- Modifications in the software, manuals, MS database (see below) must be supplied and installed free of cost.

High Pressure Quaternary LC System

- The ultra fast liquid chromatography should have high pressure pump with minimum back pressure of 15000 psi.
- The pump should have flow rate from 0.001-5ml/min and flow accuracy of \pm 0.1%.
- The pump should have flow precession of <0.5% RSD.
- The ultrafast LC should be supplied with autosampler with minimum sample capacity of 100 x1.5-2 ml vials capacity also should accommodate 96/384 well plates.
- The autosampler should have injection volume range of $0.1 100 \mu l$.
- Injection volume accuracy of +/-1.0%.
- The auto sampler sample carry-over: $\leq 0.005\%$.
- The auto sampler should have temperature range from 4° C to 40° C.
- The column compartment: should accommodate 2 columns with temperature range from 20^oC below ambient to 90^oC.
- The ultrafast LC should be supplied with PDA detector with wavelength range 190-800nm. PDA data to be available separately.
- Standard columns such as Agilent Poroshell 120 Phenyl-Hexyl (4.6 mm \times 150 mm \times 2.7 μ m), Agilent Eclipse Plus C18 (4.6 \times 150 mm; 3.5 μ m), and Phenomenex Lunar C8 (4.6 \times 250 mm; 5 μ m), etc., to enable multiple analyses to be supplied.
- Software should be capable of combining/analyzing LC and MS data together.

Pre-requisites:

- Imported nitrogen generator with compressor to supply the required flow at required pressure of nitrogen at appropriate purity.
- Any other gases and consumables for routine operation for 5 years to be supplied, along with regulators, tubings, etc.

Warranty

• The HRMS, UHPLC and N2 generator should be quoted with 3 years warranty and 2 years AMC. Appropriate spares and consumables must be available at site (and not at vendors office) for quick maintenance.

Manuals

Operation and service manuals to be provided.

MS Database and other accessories

- MS database to be provided for pesticide, antibiotics, endocrine disrupting agents, drugs, common industrial and household chemicals and their metabolites to analyze water and wastewater samples leading to an understanding of geographical changes in consumption trends in a population, as part of a study commonly referred to as wastewater-based epidemiology, to be supplied.
- Accessories needed for sampling, preconcentration and analysis of such studies to be included.

Computers

• The system to be supplied with appropriate computers for data acquisition, display and control. Additional computer has to be supplied for data analysis without affecting the computers used for data acquisition.

Training

• Supplier should provide training on operation and routine maintenance during installation and once every year for 5 years for new students/postdocs. Training for MS and LC to be provided separately.

Installation

• The supplier should provide high quality, noise-free UPS for the whole system to handle power shutdowns of 2 hours duration with additional surge suppressors. Appropriate precision air conditioners as per the ambience requirements suiting the ambience of the laboratory to be supplied.

Remote Operation

• The systems are expected to have features enabling remote operation for most of the functions so that users from across the globe can access the instrument for their requirements.

Additional feature

 The supplier should be look after the existing mass spectrometer (Thermo LTQ MS, housed in the TUE building of IIT Madras) till December 2025.

Terms and Conditions:

Vendor Eligibility Criteria:

• Supplier should have supplied multiple instruments of similar kind to Research Institutions.