

Minimum Technical Specification of High Resolution Mass Spectrometer System

High Resolution Mass Spectrometer for *proteomics and small biomolecules studies*. The instrument should essentially have High-Resolution Mass Spectrometer (HRMS) coupled to UHPLC/UPLC and NanoUPLC for MS and MS/MS experiments. All three instruments i.e., HRMS, NanoUPLC and UHPLC/UPLC should have compatibility with each other and software. The instrument should have all the features, software's including access to library and accessories required to carry out proteomics studies and capable of analyzing low molecular weight compounds, endogenous small molecule metabolite profiles and pharmaceuticals and bio transformed metabolites.

Analyzer: The geometry of the mass spectrometer should consist of quadrupole, collision cell followed by Time of Flight (TOF) or Orbital trap technology to perform high resolution MS and MS/MS experiments. It should be capable of connecting UHPLC and Nano LC for qualitative and quantitative analysis. It must be capable of performing MS and MS/MS experiments automatically in a single analysis.

Sources:

- System should have ESI and APCI ionization source.
- Ionization source must be capable of working in online manner with the UPLC/ nanoLC quoted and can also work with integrated syringe pump.
- Separate Nano ESI source should be provided.
- Flow rate: up to 2 ml/min or better without splitting.

Syringe Pump: A suitable syringe pump to introduce samples directly into the mass spectrometer should be provided.

Resolution in MS and MS/MS mode: 30000 or better for Q-TOF technology and 100000 or better for Orbitrap technology.

Mass Range:

Quadrupole mass range: 1200 m/z or better (For Singly Charged Ions)

TOF mass range for Q-TOF technology: 40000 m/z or more

Mass range for Orbitrap technology: 6000 m/z or more

Mass Accuracy: 1ppm or lower

Polarity Switching: The mass spectrometer must be capable of fast polarity switching acquiring one spectrum in positive and one in negative ionization mode.

Sensitivity: At least 1pg/ μ l with a minimum 200:1 S/N ratio

Dynamic range: 4 orders or better for Q-TOF and 3 orders or better for Orbitrap technology.

Scan Functions:

- Spectra speed in MS/MS mode: should be minimum 12 Hz or better for Orbitrap technology and 60 Hz or better for Q-TOF technology.
- The system should have variable window Q1 selection
- Must acquire and display Full Scan mass spectra @ MS/MS spectra
- Must acquire and display Selected Ion Monitoring (SIM/MRM) scan data for monitoring selected ions for target compound analysis

- Neutral-loss triggered data dependent MS/MS methodology, selecting predominantly precursor ions for MS/MS fragmentation, which show a predefined neutral loss under fragmenting conditions.

Vacuum system: Highly efficient vacuum systems consist of turbo molecular pumps followed by rotary mechanical pumps must be provided

Calibration: System should have complete Auto-calibration capability to set all relevant voltages automatically during external calibration.

UPLC/ UHPLC:

- Quaternary pumps with vacuum degasser and 100µl injection loop
- Operating Flow Rate Range: 0.05 to 2.000 mL/min
- Maximum Operating Pressure: 15,000 psi or better
- Auto sampler/Sample Manager Sample Capacity: 96 vials/samples or more with temperature control feature or programmable.
- Total system (including pump & Auto-sampler) should be capable of operating at 15,000 psi or better
- Column compartment temperature range: Up to 80⁰C or better.
- Photodiode array (PDA) detector capable of scanning from 190-600 nm range or better with flow cell volume of 2.5 microlitre or better.
- **Columns: quantity:** C18, 2.1x 100 mm, 1.8µm (05), C8, 2.1x 100 mm, 1.8µm (02), C18, 2.1 x 50 mm, 1.8 µM (02)

NanoLC:

- Binary pump with vacuum degasser and desalting functions.
- Flow rate range: 100-1000nl/min without splitting
- Working pressure of 10,000 psi or more
- Temperature-controlled column compartment (ambient +10⁰C to 60⁰C)
- Programmable injection with auto sampler with working pressure up to 10,000 psi.
- The auto-sampler should have the capacity to hold microtitre plates or multiple sample vial racks.
- NanoLC should have nanoSpray or equivalent parts.
- Auto sampler injection volume: up to 10 µl with 10 µl loop
- Auto-sampler temperature control 5 to 20⁰C or better.
- 5 columns for nanoLC

Note: Both LC systems should have single point software control with mass spectrometer

Software, Database and Computers

- Should be capable of performing all modes of operations of the LC-MS/MS instrument. Both LC and MS must be controlled with single software. Control software should be incorporated with elemental composition calculator as standard. Complete and most advanced version of software's should be quoted, which is capable of detecting, recording and analyzing the data.
- Should be able to perform real time multiple mass defect filter
- System should be supplied with software's to perform various workflow such as differential analysis, PCA analysis, comparing data between sequences.

- Software to predict the structure fragmentation data and create the tree for the fragments, structure editor etc.
- Software for metabolomics data analysis and interpretation along with metabolomics database should be provided
- Software for protein & peptide identification, peptide Sequencing, PTM with database for proteomics analysis utilizing High Mass Accuracy data recorded with HRMS mass analyser and also should be able to utilize fragmentation patterns generated from the High energy collision cell.
- More recent version of database for protein/peptide sequences, small biomolecules library/database (pesticides, environmental contaminants) should be provided with perpetual access.
- Small molecules metabolite identification (met id) software for different biotransformation pathways understanding should be provided
- Separate data stations for running the machine and data acquisition with most advanced configuration should be quoted
- Analysis softwares should be loaded on separate data system platform (Windows or MAC based) compatible with machine with following minimum features: For Windows: Intel Xeon E3 processor or better, minimum 32 GB RAM, 2TB or better storage, 27 inch display based with latest Windows software; For MAC: Quad-Core Intel Xeon E5 processor with 16 GB RAM, 2TB or better hard disk, 27 inch display supported with latest operating software. Color printer with duplexing, networking and Wi-Fi connectivity capabilities.
- This offline system should have all installed software required for small molecules and protein molecules for offline data processing

Training: Onsite training at installation place and offsite training at manufacturer or factory site for minimum two persons.

Pre-requisite and Accessories:

- **Nitrogen generator:** Nitrogen Generator along with in-built compressor should be supplied with system to take care of nitrogen gas requirements. Collision gas cylinder and pressure regulator, if needed should be supplied
- Gas cylinders, regulators, moisture/ hydrocarbon trap if required
- Online 15 KVA standard/branded UPS with 1hr backup (batteries of Exide or better brand)
- Vibration free table/ or base required for machine installation.

Warranty: Minimum 3 Years of comprehensive warranty on complete system for all components including third party items like UPS, batteries, computers etc.

Installations: All machines quoted should have at least 3 installations in India. All the additional items required for installation and proper functioning should be provided with machine.