# **SPECIFICATION OF TRIPLE QUADRUPOLE LC-MS/MS SYSTEM**

Sr.	Specification
No.	
1.	Triple /Tandem Quadrupole Mass Spectrometer System:
	Latest Triple/Tandem Quadrupole LC-MS/MS Bench-Top System for high sensitivity
	trace level qualitative and quantitative analysis with complete software control.
a.	Liquid chromatography and the MS/MS should have been manufactured by the
	same company, should have a high degree of compatibility and should be operational
	with the single software, and there should be a written assurance from the competent
	authority of the manufacturing /supplying company to that effect and provide one-stop
	after- sales servicing, besides certifying that they will honor the bid conditions with Five
	Years Warranty followed by five years CMC.
2.	Ionization Source
a.	The instrument should have single/ dual orthogonal sources design to remove neutrals
	and matrix and should be able to perform ESI and APCI as well as +ve and -ve modes
	of ionization/applications using both sources simultaneously or alone.
b.	MS-System should be capable of performing analysis of all types of compounds of
	interest with a single-source platform in a single injection. Dedicated APCI probe
	should be provided.
3.	ESI and APCI source Flow rate range:
a.	The source must be capable of handling flow rate of 1ul to 2 ml/min without the need for
	use of flow splitter.
b.	Provision should be available to divert the flow to waste/MS through software
	before/during/after the analysis in order to reduce source fouling/contamination.
4.	Desolvation Temperature:
	The quoted ion source should have a desolvation temperature setting of 550°C or
	more for both ESI and APCI mode.
5.	Mass Range (AMU)
a.	m/z of 5 to 2000 amu for both quadrupoles or better.
b.	Scan Speed: should have a scan speed of 15,000 amu /sec or above

### **6. Polarity Switching time:** 20 m sec or less

#### 7. Interface:

Cone based source interface is required.

The interface should be such that it should be able to handle large batches of complex sample matrices over a long period without performance degradation. The cleaning of the sample Inlet within the source should be simple & should be done without venting the system and a facility to Vacuum Interlock should be available. Off axis / similar ion guide should be provided for further removal of matrix components resulting in lower source contamination.

### 8. Vacuum System:

- a. A robust high efficiency vacuum system with minimum maintenance and utility with low noise level.
- b. Vacuum system vent/pump cycles must be digitally monitored and controlled, to provide total software control and to ensure fail-safe operation in the event of power failure

### 9. Quadrupoles:

Quadrupoles having high standards of mechanical tolerances for high sensitivity and resolution in both the quadrupoles. The design including any other MS pre/post filters must be specified.

#### 10. Mass Resolution

Better than or equal to 0.8 amu over the entire Mass Range

#### 11. MRM/SRM Sensitivity

- a. The instrument should be capable of detection up to nano/pico mole levels.
- b. 1 pg of Reserpine in ESI +ve mode must have at least S/N 2,75,000:1 or more sensitivity (to be demonstrated on raw and unsmoothed data).
- c. 1 pg of chloramphenicol ESI Neg (-ve) mode must have at least S/N 65,000:1 or more sensitivity (to be demonstrated on raw and unsmoothed data).

#### 12. MRM channels

Must be able to measure 500 MRM/sec in one acquisition to enable Transition Studies within a single run.

#### 13. Collision Cell:

Specially designed collision cell to allow use of very low dwell times (1 millisecond or better) without sacrificing sensitivity and eliminate cross talk to enable Multiple MRM Transition studies within a single run.

### **14. Dynamic Range:** 5 orders of dynamic range or better

### 15. Integrated Auto-Tuning/Calibration device:

The calibration of the mass spectrometer should be fully automated without the use of a syringe pump. A built-in infusion device must be available to perform automatic calibration, auto tuning of molecules as well as for direct mass analysis. Automated optimization of ion optics and mass axis calibration in positive and negative ion modes should be provided.

Vendors should mandatorily quote Neonatal setup standards for method optimization in the mass range of 20 to 2000 Da and provide part numbers for those setup standards.

#### 17 Scan Modes

- a. The following scan modes should be available
  - MS scanning
  - Selected ion monitoring/recording (SIM/SIR)
  - Product ion scanning
  - Precursor ion scanning
  - Neutral loss/gain scanning
  - Multiple reaction monitoring
  - Advanced scan modes
- b. The system should have background MS scan or suitable advanced mode along with MRM for robust method development specially to get better understanding on matrix interferences with minimum MS to MS/MS switching time.
- c. MSMS Data along with MRM to confirm the compound of interest to avoid false positive

#### 18 Detector:

PMT/EMT detector having the highest sensitivity system should be quoted. The detector quoted should be with 10-year performance guarantee (Letter/confirmation to be provided by OEM and not by bidder).

#### 19 Data Management System

- a. The software must be provided for seamless control of standalone MS and LC-MS/MS. The software should also have feature of giving warning messages in case of errors/malfunctioning during operations and should stop automatically to prevent further damage to the system.
- b. The software should have features required to control LC-MS/MS for clinical applications
- C. The quantification software must provide the QC and patient sample variations monitoring to address the deviation flags.

### **20** Generator with in-built Compressor & Negative Exhaust

- a. A suitable noise free gas generator, compressor, filters, or any other accessory required for the functioning of system, should be supplied to take care of gas requirements for ionization source.
- b. Also, a gas cylinder for fragmentation purposes including regulators, tubing's, filters, etc. should be supplied
- c. Required Capacity Nitrogen generator for the proper functioning of the system along with external compressor and PM kit should be supplied.
- **21 UPS:** A compatible online UPS of 10 KVA capacity or more with at least 30 minutes or more back up for the complete system should be provided.

### 22 Computer System

The Factory fitted personal computer with latest processor/ configuration should be supplied along with the instrument. The latest OS (windows 10 or better software which is compatible with the chromatography / MS / MS software) should be supplied along with original license key of windows and Microsoft office. Processor should be Intel Processor i7 or better. 10TB Hard Disc/Drive and 512GB SSD should be standard. RAM – 32GB or better. 1GB dedicated graphics card or better.

Software should provide long term storage capacity of Results.

MS System should preferably be compatible with Ion mobility / third dimensional separation for analyzing complex matrices.

The system should also be compatible with Nano and Micro flow for the future applications

There should preferably be an option for future upgrades connecting GC to existing software

and hardware. Documentary evidence of the same must be submitted along with the technical

bid.

Neonatal screening applications software should be provided which can calculate the measured analytical values, reporting and interpretation.

The provided operating software should have the capability to create formula customization for intensity-based calculations, and results should export to Excel.

## 25 Chromatographic system to the Mass spectrometer with following specifications:

- a. Quaternary/Binary operating pump(s) with low pressure mixing with an operating pressure of a minimum of 15000 psi or better.
- It should deliver constant and pulse free solvent ranging from 0.010 to 2.000 mL/min, in 0.001
   mL increments or better

C.	The instrument should have in-built Vacuum degasser facility with minimum four lines and
9	should be efficient to remove dissolved air online.
d.	System Delay Volume should be less than 400ul, independent of system backpressure & with
9	standard mixer.
e.	The chromatography system should be capable of being operated both as a HPLC $\&$ Fast HPLC
ŀ	by interchanging the column chemistries.
f.	Auto sampler should be available with a capacity of approx. 90 vials or more of 2 ml or better
	capacity
g.	The auto sampler should have cooling facility up to 4 degrees or better and heating up to 40
C	degrees or better.
h. I	Programmable injection volume from 0.5 ul to 20 ul or better must be available.
i.	The carryover of the auto sampler must be less than 0.002% or better.
j. (	Column Temperature Control should be from ambient to 80 deg. C or less.
K. ]	Instrument should be capable to perform gradient curve for method development.
L.	The tracking of column injection incidents should be supported by the specified system.
26	Onsite training should be provided whenever required free of cost.
<b>27</b> l	LC-MS/MS reference spectral library for an expansive and chemically diverse compound
	collection.
28	Sonicator to be provided.
29	Accessories to be provided as below:
ļ	i. PEEK ferrules: Minimum 5 Qty.
ļ	ii. Vacuum pump oil: Atleast 1L.
30	Should be BIS/ISO certified.
31	System should have LIS facility.