# Korea Basic Science Institute COMMODITY DESCRIPTION

Commodity Ti	ommodity Tiple Quadrupole LC/MS System					
L HSK No. I	027.30-1000 479.89-9099	Page 1 of 7	Date			
Description					Q'ty	
detection 2. By using compoirm conducter 3. Should procedure collision 4. Fast scan UHPLC 5. Ultranger features 6. Compatent nano-ES for robe volumes 7. Compatent composition method reporting 8. Archieve 9. Provide 10. Provide 11. Provide 11. Provide 12. Capillat utilized	on and quantitation fing MRM quantitation of MRM quantitation of screening, confined.  provide software lare to optimize Mare to optimize Mare energies, automatican speeds allow to the chromatography.  ast MRM acquisition ensure compatibility with a wider of the compatibility with a wider of the confined and th	ty enabling the lowest for most demanding applion and product ion rmation and quantitation and quantitation and fally.  The speeds and ion polar with UHPLC analyses, are range of ionization PPI, Multi-mode source tive quantitation with the system contractically enhances proacquisition to data the for challenging separation uncompromised data quacity per bench space, thou transfer between the system could be the system coul	plications. scan profiling, ion should be ompound setup ragmentor and high throughput larity switching sources - ESI, es, and MALDI small smaple rol and data ductivity from processing and ations. uality.  LCs, regardless interfaced and mental requests.	set	1	
<ol> <li>Triple Quadrupole LC/MS</li> <li>Ion source</li> </ol>			set	1		

1) Electro Spray Ion Source		1
2) Atmospheric Pressure Chemical Ionization Source		1
3. Ultra High Performance Liquid Chromatography System		1
4. System control and acquisition system		1
5. Accessories	set	1

## C. Specification

### 1. Triple Quadrupole LC/MS

#### 1) Interface

- a) Off-axies geometry & heated counter-current desolvation gas should design for rugged performance.
- b) Should provide capable of analyzing large batches of complex urine, plasma and plant extracts over long periods of time without maintenance degradation or equivalent.
- c) The ESI, APCI, APPI, Nanospray, Multimode and Maldi interface could be mounted on the system as simple detachable hinge, which provides for fast, easy switching of interface.

### 2) Analyzer

- a) The quadrupole mass filter should separates ions according to their mass-to-charge ratio (m/z), allowing only one m/z to travel the length of the quadrupole at a time. The RF beam shaper, post filter, or equivalent devices should be necessary because of the quadrupole's close proximity to the collision cell.
- b) The quadrupole consists of four parallel rods through which selected ions should be filtered before reaching a collision cell where they are fragmented.
- c) High pressure collision cell with applying of acceleration voltages should optimize MS/MS fragmentation while eliminating cross talk, even at very low dwell times.
- d) Quadrupole 2 should use four parallel rods again to optimize ion transmission and spectral resolution.
- e) An automatic instrument tunning protocol should be applicable to adjust the operational parameters of the mass analyzer for optimum performance, while a calinrant solution of known composition should be infused into the ion source, resulting in an new tune file that contains new tune parameters.

### 3) Vacuum system

- a) Number of pump system (i.e., roughing & turbo molecular pumps should be required to maintain deep pressure vacuum.
- b) Maintaining the required rough and high vacuum should be essential for optimum performance.
- c) Vacuum readings should be monitored regularly in the

Acuqisition SW's actuals display.

- 4) Acquisition Capabilities: following acquisition mode should be provided.
  - a) Selected ion monitoring (SIM) for quantitation/low level detection.
  - b) Collision induced dissociation tandem MS (CID/MS/MS) for structural elucidation.
  - c) Alterative positive and negative ion scanning
  - d) Product ion scans
  - e) Precursor ion scans
  - f) Neutral loss scans
  - g) Single and multiple ion selected reaction monitoring (SRM/MRM) in the MS/MS mode for ultra high sensitivity quantitation. MRM transitions could be also triggered by their specific RT parameters.
  - h) In order to perform library searching and compound screening and confirmation, combination of fast and sensitive MRM quantitation and evaluation of a product ion spectrum should be feasible.
- 5) System Performance
  - a) Mass range: m/z 5 to 2,000 or more in Q1 and Q3
  - b) Scanning speed: 12,000 u/sec or faster
  - c) Dynamic range :  $1.0 \times 10^6$  or wider
  - d) Mass accuracy: 0.1 amu or less from 5-1,000 m/z
  - e) Mass stability : less than 0.1 Da in 24 hours at constant temperature
  - f) Mass resolution: 0.6 Da or less (FWHM)
  - g) Polarity switching: Switch from positive ion mode to negative ion mode in 40 ms or faster
  - h) Minimum dwell time: 1 ms or faster
  - i) Maximum MRM transition rates : 250 or more per time segment
  - j) RT informed MRM transitions : 3,000 or more ion transitions per methods
  - k) Collision cell ion clearance: 1 ms or faster
  - 1) MRM sensitivity ESI Positive
  - 1 pg of reserpine injected on column, quantifying on the transition m/z 609 to 195 with Signal-to-noise ratio more than 80,000:1. (RMS x1)
  - m) MRM sensitivity ESI Negative
  - 1 pg of reserpine injected on column, quantifying on the transition m/z 321 to 152 with Signal-to-noise ratio more than 80,000:1. (RMS x1)
- 2. Ion Source

- 1) Electrospray Ionization source
  - a) The source need to be designed to enhance ionization productivity such as improving the desolvation and spatial focusing of ions. Various technologies such as thermal gradient focusing with super-heated gas (i.e., N2, Ar, or equivalent) might be co-utilized.
  - b) Flow rate compatibility: more than 1,000 ul/min
  - c) Sprayer configuration: Off-axies.
- 2) Atmosperic Pressure chemical Ionization (APCI) source
  - a) The APCI source is a popular complement to electrospray. Because APCI does not generate multiply charged ions, and operates at higher temperatures, it is commonly used to analyze smaller, thermally stable polar and non-polar compounds.
  - b) The source need to be designed to enhance ionization productivity such as improving the desolvation and spatial focusing of ions. Various technologies such as thermal gradient focusing with super-heated gas (i.e., N2, Ar, or else) might be co-utilized.
  - c) Sprayer configuration: Off-axies
  - d) Flow rate compatibility: more than 1,000 ul/min
  - e) Gradient compatibility: Full gradient capability
- 3) Ultra high performance liquid chromatography system
  - a) Binary gradient pump
  - Type : Two dual pistons in series pumps with proprietary servo-controlled variable stroke design and smooth motion control
  - Flow range: Setpoints from 0.001 5 ml/min, in 0.001 ml/min increments or less
  - Flow precision: 0.07 % RSD or 0.005 min SD, whatever is greater (0.2-5.0 ml/min)
  - Flow accuracy : ± 1% or 10 ul/min, whatever is greater
  - Maximum operating pressure : up to 130 MPa (1,300 bar) or higher
  - Pressure pulsation : Less than 1% amplitide, or less than 0.5 MPa (5 bar) whatever is greater
  - Compressibility compensation : Automatic, pre-defined, based on mobile phase selection
  - pH-range : 1.0-12.5 or wider
  - Gradient formation : High pressure binary mixing
  - Delay volume: less than 75ul
  - Composition range: Settable range 0.0 100.0 %
  - Composition precision: Less than 0.15 % RSD, or 0.01 min SD whatever is greater from 0.2 5 ml/min
  - Composition accuracy : ± 0.35 % absolute from 5-95 %, from

- 0.2-5.0 ml/min
- Solvent selection valve : Included
- Number of channels: 2
- Internal volume per channel : 1.5 ml or less
- Materilas in contact with solvent : Telflon AF, FEP, PPS
- Control: By the LC/MS/MS comtrol and acquisition software
- Communications : Through controller-area network (CAN), RS232C, and/or APG remote : communte signals such as ready, start, stop and shutdown
- Safety and maintenance: Error detection (e.g., leak detection, safe leak handling, leak output signal for shutdown of the pumping system) and display should be made through the LC/MS/MS control and acquisition software
- b) Automatic sample organizer
- Injection range : 0.1 20 ul or more in 0.1 ul increments
- Precision: Less than 0.15 % RSD from 5 20 ul volumn
- Accuracy : ± 1% (10 ul, n-10)
- Pressure range: up to 130 MPa (1,300 bar) or higher
- Sample viscosity range : 0.2-5 cp or wider
- Sample capacity: 2 ml vial 400 ea or more : 96 well plate - 8 ea or more
- Carry over, flow through design : Typically < 0.001 % with a optional washing device
- Temperature accuracy :  $-1^{\circ}$ C to  $+4^{\circ}$ C at a set point of  $4^{\circ}$ C
- Control and data evaluation : By the LC/MS/MS control and acquisiton software
- Communications : Throuth controller-area network (CAN), RS232C, and/or APG remote: commute sugnals such as ready, start, stop and shutdown
- Safety and maintenance: Error detection (e.g., leak detection, safe leak handling, leak output signal for shutdown of the pumping system) and display should be made through the LC/MS/MS control and acquisition software
- c) Thermostatted Column Compartment
- Temperature range :  $4^{\circ}$ C to  $100^{\circ}$ C or wider
- Temperature stability :  $\pm$  0.05  $^{\circ}$ C or less
- Temperature accuracy :  $\pm$  0.5  $^{\circ}$ C or less with calibration
- Column capacity: 30cm; 4ea or more / 15cm: 8ea or more
- Control : By the LC/MS/MS control and acqusition software
- Communications : Through controller-area network (CAN), RC232C, and/or APG remote: communte signals such as ready, start, stop and shutdown
- Safety and maintenance : Error detection (e.g., leak detection,

safe leak handling, leak output signal for shutdown of the pumping system) and display should be made through the LC/MS/MS control and acquisition software

- Column switching valve : for Auto -filtration, Concentration
   : 8pos/18port or more, 8-column selector, 130 MPa (1,300 bar)
- 4) System control and acquisition system
  - a) Workstation
  - Hardware Configuration (similar or better than below)
  - CPU: Intel Xeon E5-1620 3.6GHz 10MB/1600 4C CPU
  - Memory: 8GB (4x2GB) DDR3-1333 ECC RAM
  - HDD: 2 x 500 GB SATA (Raid 1)
  - CD ROM: HP 16 x DVD+-RW SuperMulti SATA Drive
  - OS: MS Windows 7 Professional 64-bit English
  - Microsoft Excel 2013 English
  - NVIDIA Quadro 400 512MB Graphics
  - 2nd Braodcom Gigabit Ethernet Card
  - Display Resolution: 1680 \* 1050 (WSXGA)
  - Display Response time: 5ms
  - Warranty : at least 3 Years
  - b) Data processing and system control software
  - (1) The Software consists of four major components
    - (a) Acquisition
      - All LC and MS parameters should be immediately visible
      - Real-time plots should show the status of whole connected instruments/parts at work
      - Running multiple samples need to be easily handled through
      - Automatic instrument tune protocol should be available
      - Control whole LC and MS system simultaneously with no trouble
    - (b) Quantitative Analysis
      - The Quantitative analysis program should provides Batch-at-a-Glance views that let users see quantitation results immediately for the entire batch of data that the users choose to open
    - (c) Qualitative Analysis
      - The Qualitative analysis program should allows users to operate on many data files at once from a single screen. Typically, qyalitative analysis is used to determine the precursor and product ions associated with a particular compound. This MRM transition information can be used to create the acquisition method and, later, the quantitation method
    - (d) MRM transition methods setup software

- the software should be fully automated for multiple compounds one or a few says of unattended work
- The software should have features of selection and optimization of precursor and its product ions.
- Should support multiple MRM method setup with multiple target compounds.
- Should create a compounds database with setuped parameters for re-use.

#### D. Standard Acc's

1. UHPLC system Tool Kit		1
2. LC/MS/MS System Tool Kit	ea	1
3. Solvent Safty cap for LC solvent bottle (1L) 4 units/1pk	pk	1
4. LC capillary kit (0.12mm ID)	ea	1
5. Clear vial, screw cap, slit PTFE/Si septa, 500vials/pk	pk	1
6. Quick connect LC fitting set	ea	4
7. MS tunning solution	ea	3
8. Big Universal Trap, 1/4" fttgs, Nitrogen	ea	4
9. Big Universal Trap, 1/8" fttgs, Nitrogen	ea	1
10. Additional 22" LCD monitor	ea	1
11. UPS (12KW, 30Min back up)	ea	1
12. N2 Gas Generator (64L/min)	ea	1
13. Rotary pump cover	ea	2
14. UPLC Column (C18)	ea	1

## E. Optional Acc's or Equivalent parts

#### F. Remarks

- 1. The installation and performance test should be carries out by bidder/supplier's responsibility at end user's site.
- 2. Annual maintenance contract (including all consumables and parts) for two years should be provided supplier after the performance test
- 3. The bidder/supplier need to provide the highest-end LC-MS/MS Spectrometer system of their products at the supplement.