# **GUIDELINE FOR LC-MS USERS**

Liquid chromatography-mass spectrometry (LC-MS, or alternatively HPLC-MS) is an analytical chemistry technique that combines the physical separation capabilities of liquid chromatography (or HPLC) with the mass analysis capabilities of mass spectrometry (MS). LC-MS is a powerful technique that has very high sensitivity and selectivity and so is useful in many applications.

SAIF CSIR-CDRI, Lucknow is providing only small molecule qualitative analysis service to our SAIF Users.

#### **Experiments**

1. LC-ESI-MS analysis: Liquid chromatography-mass spectrometry (LC-MS) as a widely used technique for identification and quantification of molecules/compounds/analytes separated by liquid chromatography.

It provides separation of compounds and detection by MS (provide molecular weight of compounds).

2. LC-ESI-MS/MS analysis: Liquid chromatography-tandem mass spectrometry (LC-MS/MS) is technique in which fragmentation of molecules/compounds/analytes use to identify/ confirm the chemical structure.

Note-The charges will be for acquiring and providing you the data, not for data analysis.

## INFORMATION REQUIREMENTS FOR ANALYSIS

S.N0.	Analysis	Information require for analysis	
1.	Liquid chromatography- mass spectrometry (LC-MS)	Nature of sample: plant extracts/chemical reaction products/pure isolated compound from column Or Fraction of plant extract: like hexane, chloroform, ethyl acetate etc. Solubility: Acetonitrile, Methanol or water Expected : Molecular weight of analytes	
2.	Liquid chromatography- mass spectrometry (LC-MS/MS)	SAIF/ Lot Number (previous LC-MS Analysis) 2. Peak list: which required (MS/MS fragmentation)	
		Retention time:	3.51 min (m/z 395) 5.43 min (m/z 275) 6.86 min (m/z 520)

Note- without require information analysis can't be performed

## LC-MS/MS Instrument



Developed for integrated UPLC MS/MS qualitative and quantitative applications, the Waters ACQUITY<sup>®</sup> TQD features the highest levels of tandem quadrupole MS selectivity, robustness, speed, and accuracy.

Specification:

- 1. ZSpray<sup>™</sup> dual-orthogonal API source
- 2. Mass scan range: *m/z* 50-2000 Th
- 3. Acquisition speed: 10 scan/second
- 4. Polarity switching(ES+/ ES-): 20 ms
- 5. ESCi mode switching: 20 ms
- 6. MRM Sensitivity : 1 pico gram (Reserpine S/N 2000:1)

Example: Sample preparation

Keywords: Extraction; Liquid-liquid extraction;



LC-MS and LC-MS/MS for phytochemical analysis.

- 1. Weight out 10 mg of solvent free plant extract's fraction in eppendorf tube.
- 2. Label with sample code and properly packed in a thermocol box.
- 3. Send for analysis along with all necessary details.

## **Contact:**

### Dr. Sanjeev Kanojiya

Principal Scientist & Assoc Prof. AcSIR Email: sanjeev\_kanojiya@cdri.res.in Telephone Numbers: +91-522-2772450 EPABX-4510 Fax No: +91-522-2771941