Guideline for LC-MS data analysis for facility users

Liquid chromatography–mass spectrometry (**LC-MS**, or alternatively **HPLC-MS**) is an analytical tool 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.

Experiment

1. LC-ESI-MS analysis: **Liquid chromatography-mass spectrometry (LC-MS)** as a widely used technique for determination of molecular weights of compounds/analytes separated by liquid chromatography in LC-MS system.

Data interpretation/analysis

It provides separation of compounds (Retention Time) and detection of compounds (as different adduct formation due to ESI source) by MS (provide molecular weight of compounds/analytes).

Basic information obtains by LC-MS data

1. How many number of compounds present in the sample?
2. What are their molecular weights?

Example-1

Table -1: Chromatographic retention time and detection of compound with adduct formation.

S.No.	RT	M.W.	ESI (+)		ESI (-)		
			$[M+H]^+$	$[M+NH_4]^+$	$[M-H]^-$	$[M+Cl]^-$	$[M+CH_3COO]^-$
1	4.24	**404**	405	422	403	439	463
2	4.30	**578**	579	596	577	-	-
3	4.33	**548**	549	566	547	583	607
4	4.50	**520**	-	538	519	555	-
5	4.81	**548**	549	566	547	583	607
6	5.06	**546**	547	564	545	581	-
7	5.54	**548**	549	566	547	583	607

1. Note- On the basis of previously known compounds and their molecular weight information in literature (published paper on similar sample like plant/microbes/animals) user can predict the possible compounds present in sample.
2. After getting possibility from LC-MS data molecular weight information, user need MS/MS and LC-HRMS data to identify the compound detected in MS.
3. User should do thoroughly literature search so that maximum number of compounds can be identify in sample. Without literature support, LC-MS data analysis is not possible.
4. User can use ESI/APCI ion calculator to confirm molecular weight of compounds detected in LC-MS Run. http://plantmetabolome.cdri.res.in/public/frm_AductIonCalc.aspx
5. MS/MS spectra library can be used for reference spectra. Like https://massbank.eu/MassBank , https://metlin.scripps.edu/landing_page.php?pgcontent=mainPage
6. Data analysis is part of end user, it will not provide by SAIF