AIMS Instrumentation & Sample Report Documentation

AB Sciex QStar XL

AIMS Mass Spectrometry Laboratory
Department of Chemistry, University of Toronto
80 St. George Street, Toronto ON, M5S 3H6
QStar XL Q-TOF MS

Manufacturer: AB Sciex, Concord, ON

Features

Mass Analyzer: Quadrupole time-of-flight (Q-TOF)
Ion Source: Ionspray source (ESI)
Source Interface: HSID interface (IONICS, Bolton, ON)
Ion Polarity: Positive and negative
Mass range: 20-40 000 Da
Resolution: Up to 8 000 mass resolution
Mass Accuracy: +/- ~2.5 mDa
HPLC: Agilent 1100 Series HPLC

QStar XL Sample Results Format

Low Resolution ESI Spectrum

The low resolution QStar XL ESI-MS report consists of a profile mass spectrum showing m/z versus intensity. Spectral peaks are labeled with m/z values rounded to one decimal place. The standard data acquisition range is m/z 90-1000 Da but printed mass spectra are normally expanded to display an appropriate region of interest.

Accurate Mass Report

The QStar XL accurate mass report is generated using the Elemental Composition Calculator as implemented in the Analyst QS software package. The report provides the high resolution mass spectrometry (HRMS) value and a list of possible molecular formulae with calculated exact m/z values. All of the values contained in the report correspond to the ionic species of interest and the given ionic formula includes the charging agent – e.g. [M+H+]+. Therefore, both the measured and calculated values are corrected for the mass of the electron (0.00054 Da) and should be reported as m/z.

Suggested reporting format for compound characterization:
“HRMS (ESI-QTOF+): m/z [M+H+]+ calc’d for C_{21}H_{35}N_{10}O_{5}+ 507.2786 Da, measured 507.2793 Da.”
Sample Name: mb-2-22

Acq. Date: Thursday, July 11, 2013
Acq. Time: 10:15

Polarity/Scan Type: Positive
Elemental composition calculator

Target m/z: +507.2793 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 100
Min DBE: -0.5000 Max DBE: +50.0000
Electron state: Even
Num of charges: 1
Add water: N/A
Add proton: N/A
File Name: 130711_0874.wiff

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<th>PPM Error</th>
<th>DBE</th>
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* ESI - QStar XL
QStar XL Biomolecule Compound Report

The protein compound report summarizes results from ESI-MS analyses of intact proteins or peptides for the purpose of molecular weight determination. The raw mass spectral data is processed using the Protein or Peptide Reconstruct algorithms as implemented in the BioAnalyst v1.1.5 software package. The report is composed of three sections:

(1) Mass Spectrum
Panel (1) shows the averaged and background-subtracted mass spectrum in a plot of $m/z$ versus intensity. Spectral peaks are labeled with $m/z$ values rounded to one decimal place. The standard $m/z$ acquisition range for biomolecular analysis is 200-2000 Da; however, the printed mass spectrum is often expanded to highlight the appropriate region of interest.

(2) Mass List
Panel (2) contains the compound mass list generated by the Protein or Peptide Reconstruct algorithms and includes the following columns:

- Mass (Avg) the centroid average neutral mass in Da
- Mass (mono) the monoisotopic neutral mass in Da (peptides only)
- Apex Mass the apex neutral mass in Da
- Area the peak area
- Start Scan start of peak
- Stop Scan end of peak
- Score reconstruction fit score
- Evidence $\mathcal{C}$ indicates compound molecular weight determined via identification of consecutive charge states
  $I$ indicates compound molecular weight determined via identification of charge state from a resolved isotopic envelope

(3) Reconstructed Mass Spectrum
Panel (3) shows the reconstructed mass spectrum generated by the Protein or Peptide Reconstruction algorithms in a plot of neutral mass (Da) versus intensity. Spectral peaks are labeled with mass values rounded to one decimal place.

Mass Accuracy
The mass accuracy associated with protein molecular weight determinations varies according to several factors including molecular weight, charge states observed, signal intensity and signal complexity (e.g. adducts, multiple proteins, etc.). The ‘rule of thumb’ for a relative measure of protein mass accuracy is +/- 0.01% of the protein molecular weight; however, in practice the observed mass accuracy is typically less than 1 Da for proteins up to ~30 kDa.
QStar XL Protein Compound Report

Sample Name: L197E 10x

* ESI - QStar XL

Acq. Date: Thursday, March 07, 2013

Acq. Time: 10:16

Max. 24.8 counts.

Max. 739.0 cps.

Acq. File: 130307_CHM379_Intact.wiff

Polarity/Scan Type: Positive