

Mass Spec Analysis for Small Molecule (Code D):

1. General Procedure.

The mass spectra are acquired on QTrap or Sciex API3+ (AB/MDS Sciex, Toronto, Canada). The sample is injected into the sample loop and delivered to the mass spectrometer by 65% acetonitrile/0.1% formic acid in water at 20 $\mu\text{l}/\text{min}$.

2. Mass accuracy and resolution.

The mass accuracy is less than ± 0.5 Da. The resolution is around 2000.

Resolution = $M / \Delta M$.

3. How to Read the Spectrum?

The mass spectrometer measures the mass-to-charge ratio (m/z). The molecule is protonated during the analysis and has one attached proton. Therefore, the molecular weight of the molecule should be the value of m/z in the spectrum minus 1.

Molecules can sometimes form adducts of ammonium ($M + \text{NH}_4$)⁺, sodium ($M + \text{Na}$)⁺, and potassium ($M + \text{K}$)⁺ during the MS analysis. The molecular weights of adducts is the mass of the molecule plus the masses of ammonium (18 Da), sodium (23 Da), or potassium (39 Da).