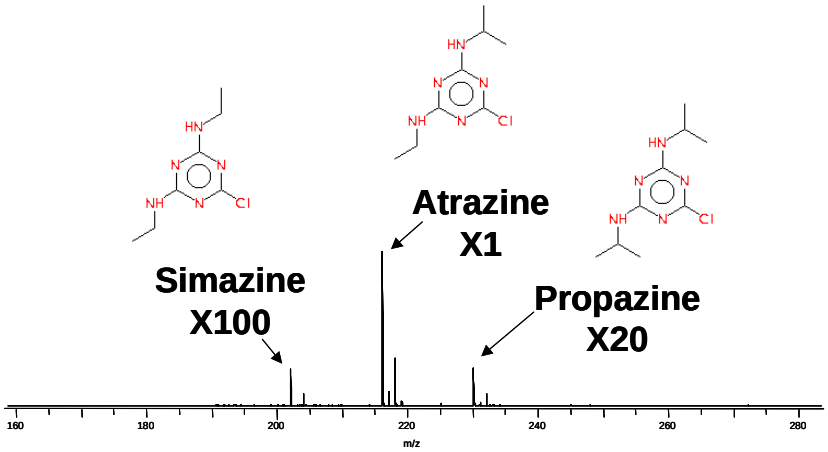
Rapid Detection and Exact Mass Measurements of Trace Components in an Herbicide

Analytical chemists are often asked to identify trace components in manufactured compounds such as drugs, consumer products, and agricultural chemicals. A common approach to the identification of minor components is to use gas or liquid chromatography coupled with high-resolution mass spectrometry. Although this approach is effective, it may be time-consuming and difficult to set up.

The AccuTOF with Direct Analysis in Real Time (DART™) provides a rapid solution. The high dynamic range of both source and detector permit the determination of minor components in the presence of a major component. The AccuTOF always provides high-resolution data with exact mass measurements and accurate isotope ratios that can provide elemental composition assignments for unknown compounds.

In this example, a few dust particles from a sample of atrazine herbicide containing 1% propazine and 0.2% simazine were deposited on a glass rod and placed in front of the DART. The mass spectrum shown below was measured in seconds. All three components were detected with good signal-to-noise and excellent mass accuracy and isotopic abundances.



Exact Mass Measurements

Compound	[M+H]$^+$	Measured	Calculated	Diff. (mmu)
Atrazine	$C_8H_{15}N_5Cl$	216.10159	216.10160	-0.01
Propazine	$C_9H_{17}N_5Cl$	230.11760	230.11725	+0.35
Simazine	$C_7H_{13}N_5Cl$	202.08440	202.08595	+1.60

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