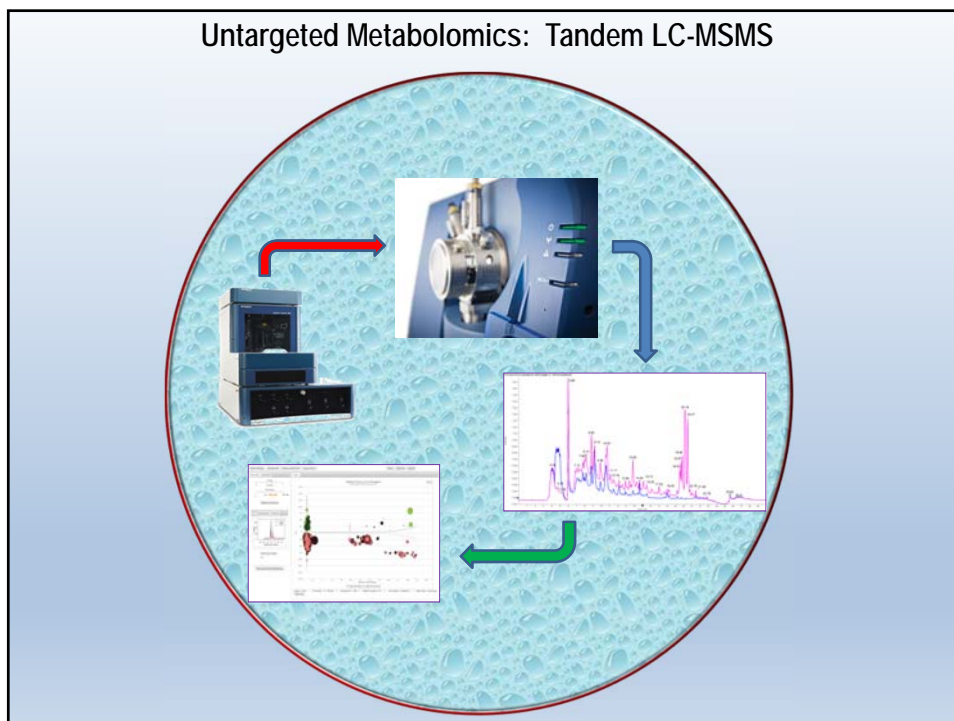
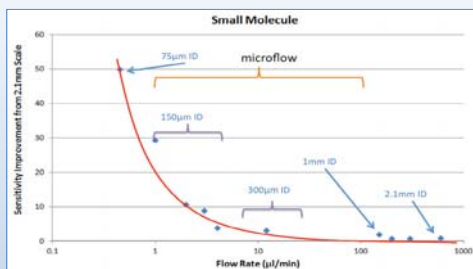


Untargeted Metabolomics: Tandem LC-MSMS



Column and Flow Rate Selection



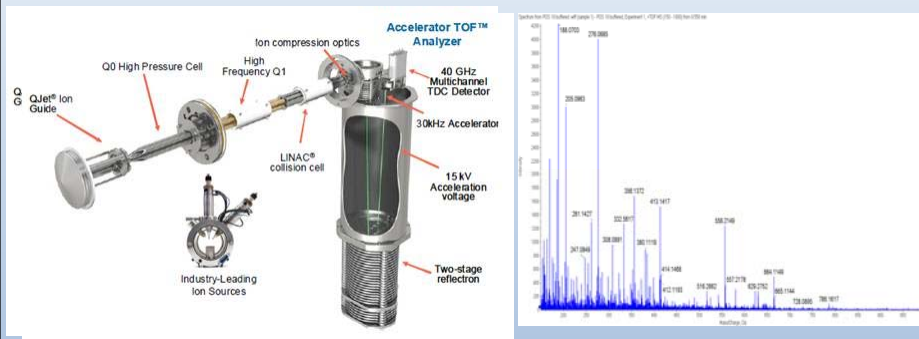
Reverse Phase and Normal Phase Selections:

- Reverse Phase (C4, C8, C18, etc...)
- Normal Phase (Silica, Amide, Amido, etc...)



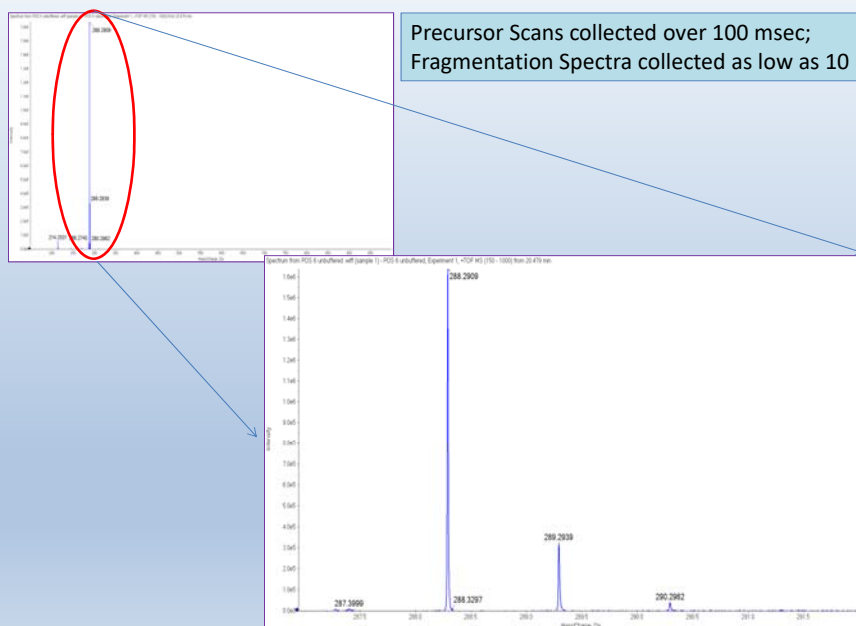
Instrument Configuration

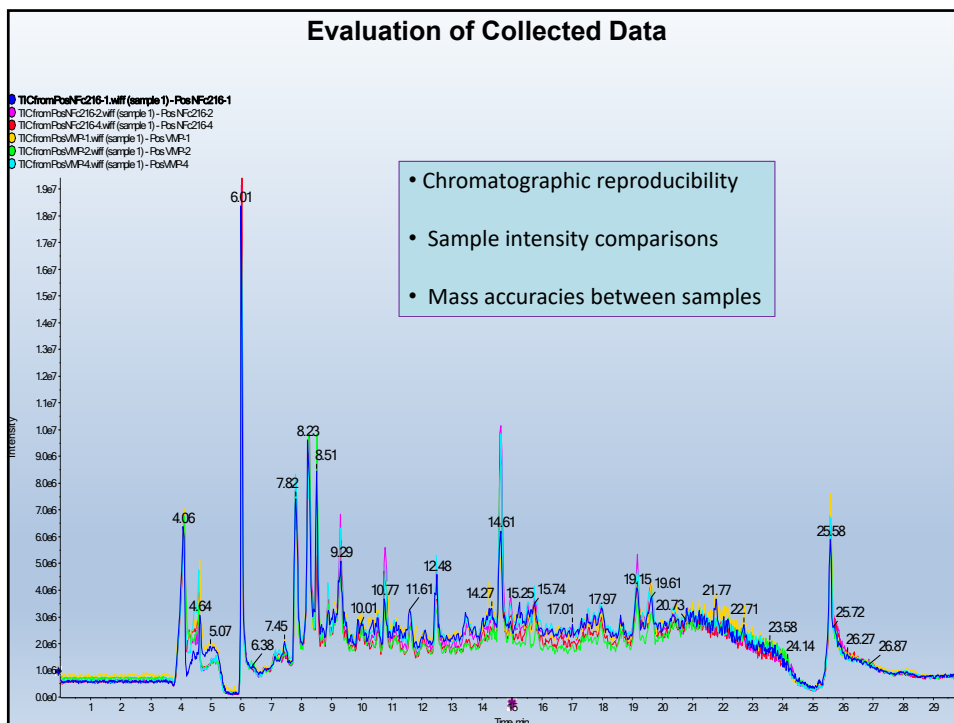
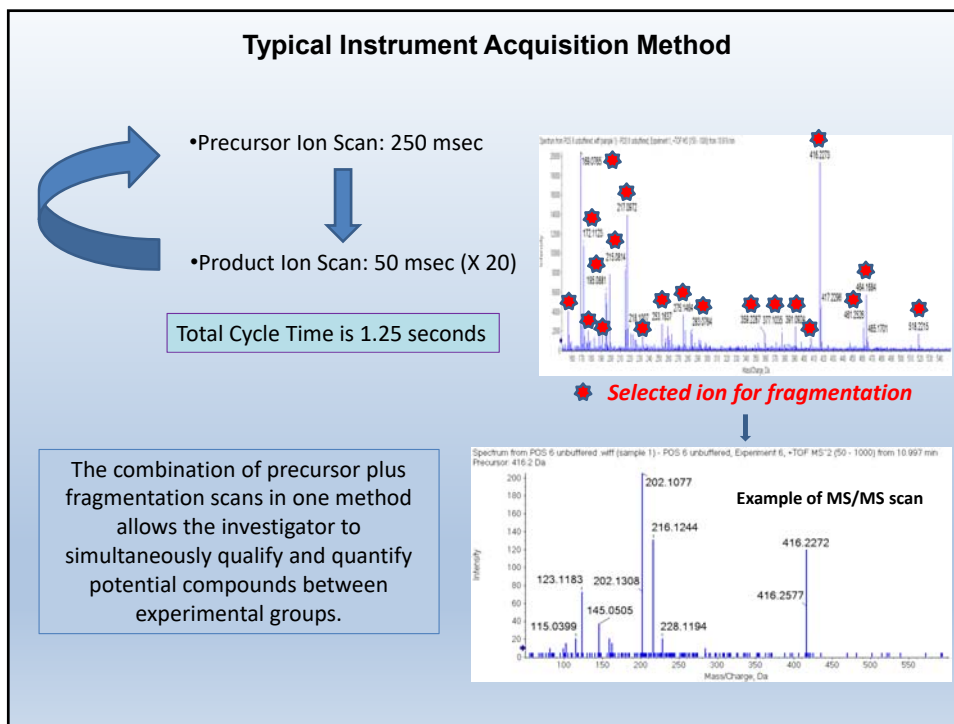
AB Sciex 5600 Triple ToF Mass Spectrometer (Q-ToF MS)

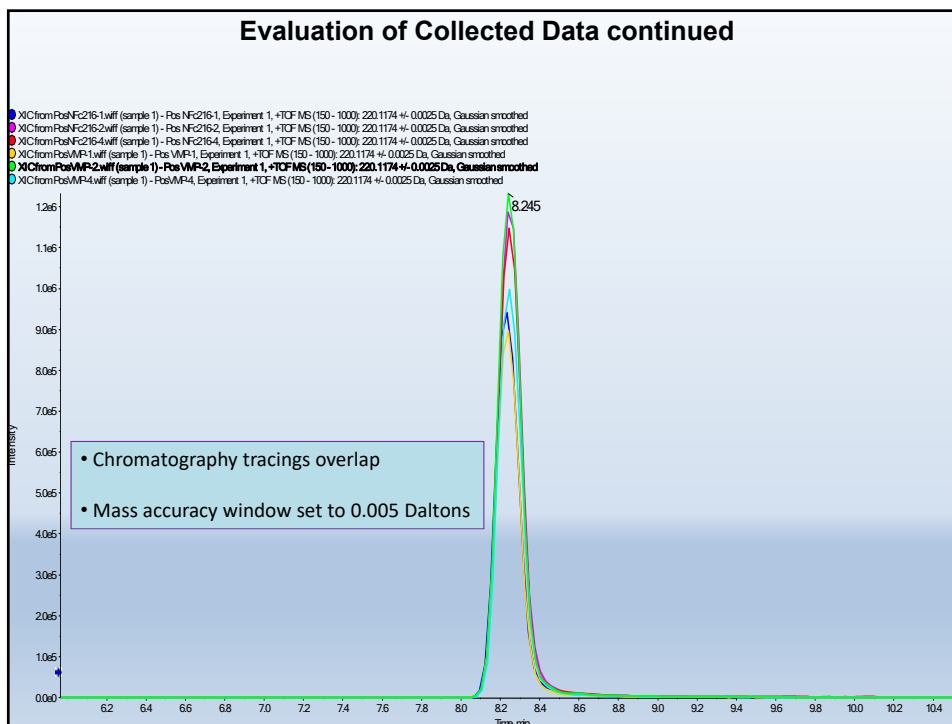


The Time of Flight (ToF) chamber allows for rapid detection and high mass accuracy as compared to traditional triple quadrupole instrumentation. All fragments are detected simultaneously instead of a precursor (parent ion) > fragment (daughter ion) pair.

High Resolution and Acquisition Speed





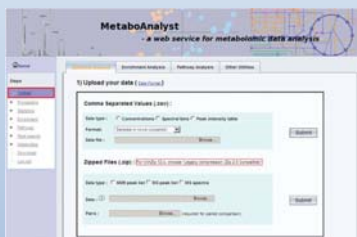


Exporting Data to Statistical Programs

Programs like MS Convert can transform instrument raw files (.wiff, .dta, etc) in usable formats such as mzXML. Keep in mind when transforming the raw data, the size of the files can increase significantly.

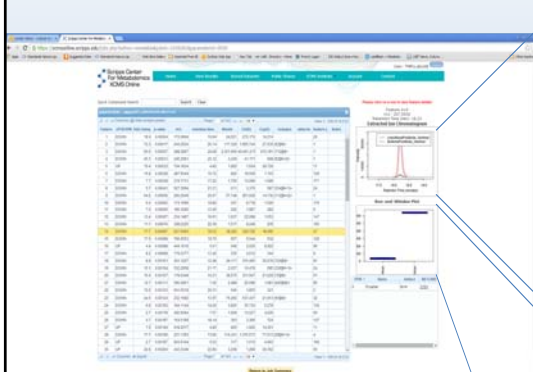
File Name	Size	Type	Date Modified
PosNF216-1.mzXML	1,244 MB	mzXML	5/12/2014 10:26:57
PosNF216-1.wiff	4,132 KB	ABSciex.WI...	5/11/2014 4:50:51 P
PosNF216-2.mzXML	1,145 MB	mzXML	5/12/2014 10:26:48
PosNF216-2.wiff	4,083 KB	ABSciex.WI...	5/11/2014 6:09:23 P
PosNF216-4.mzXML	1,168 MB	mzXML	5/12/2014 10:29:22
PosNF216-4.wiff	4,128 KB	ABSciex.WI...	5/11/2014 7:25:59 P
VMP-1.mzXML	1,225 MB	mzXML	5/12/2014 10:29:43
VMP-1.wiff	4,182 KB	ABSciex.WI...	5/11/2014 12:58:08
VMP-2.mzXML	1,095 MB	mzXML	5/12/2014 10:31:15
VMP-2.wiff	3,874 KB	ABSciex.WI...	5/11/2014 2:15:43 P
VMP-4.mzXML	1,114 MB	mzXML	5/12/2014 10:31:38
VMP-4.wiff	3,952 KB	ABSciex.WI...	5/11/2014 3:30:18 P

Data Analyses Software



There are a host of software platforms ranging from free online resources to company specific programs.

Data Analyses Software continued



XCMS Online aligns chromatography and outputs user friendly schematics from uploaded data including PCA graphs, t-test, etc.

