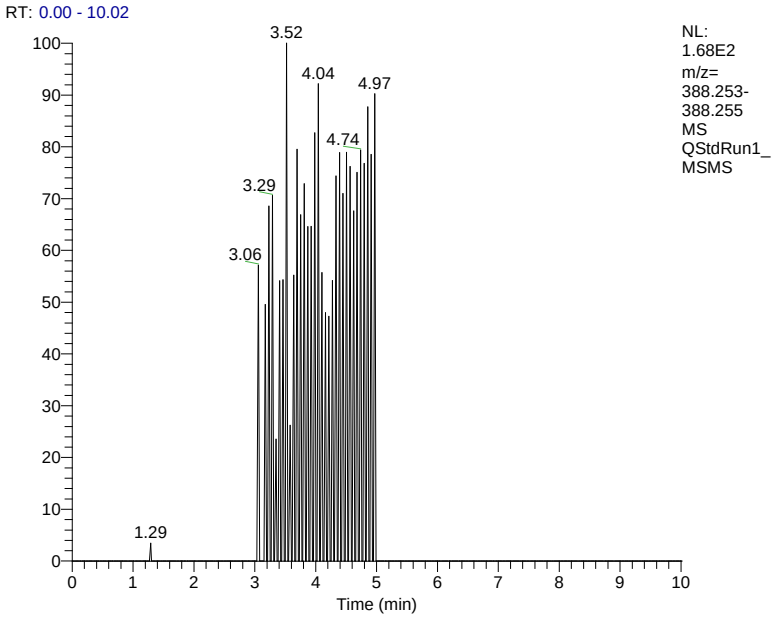
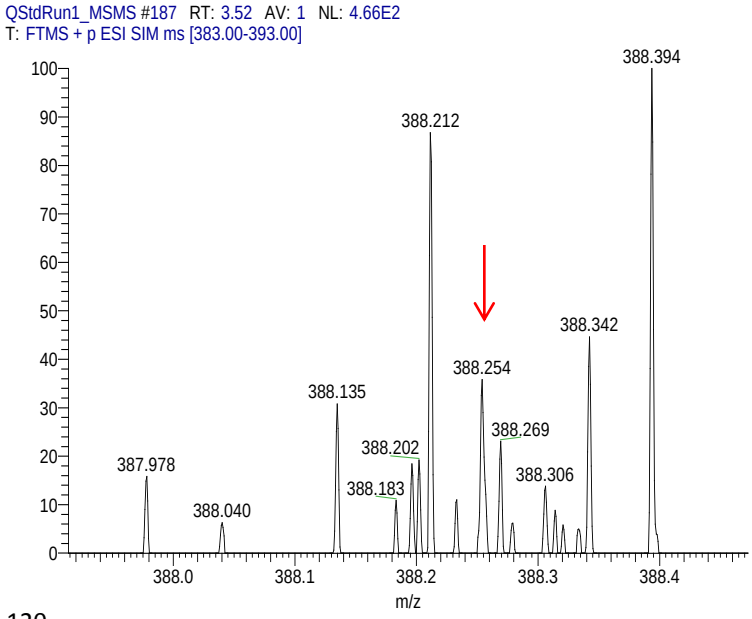
Additional File 11. MS/MS validation results for the 8 putative metabolites identified using DeconMSn. The first row shows the elution profile of the feature, middle row shows the full MS scan, and the last row shows the deconvoluted MS/MS spectrum obtained from DeconMSn.

1) m/z 388.254

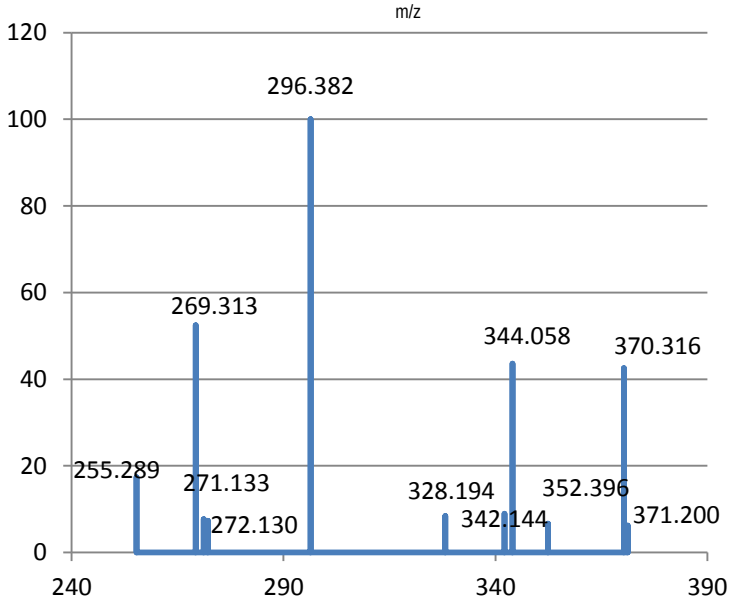
Elution profile



MS, FTMS

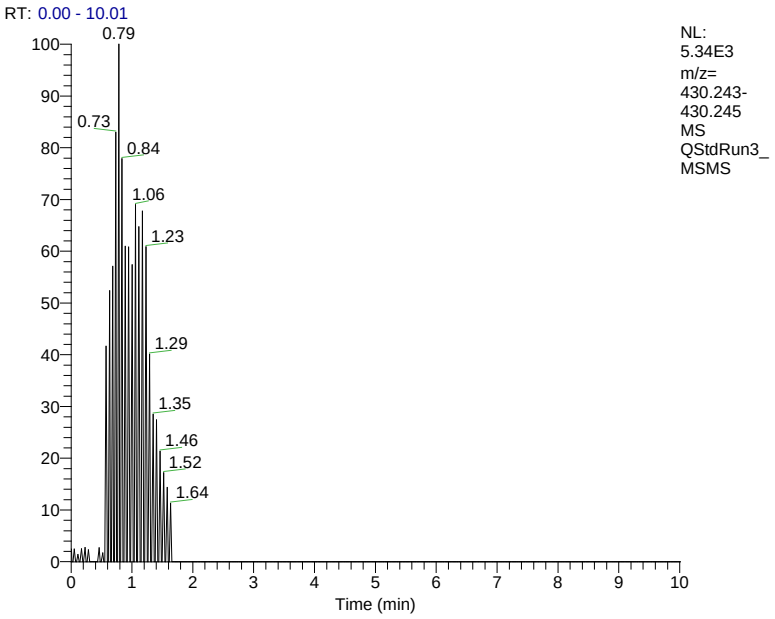


Deconvoluted MS/MS CID in Ion trap

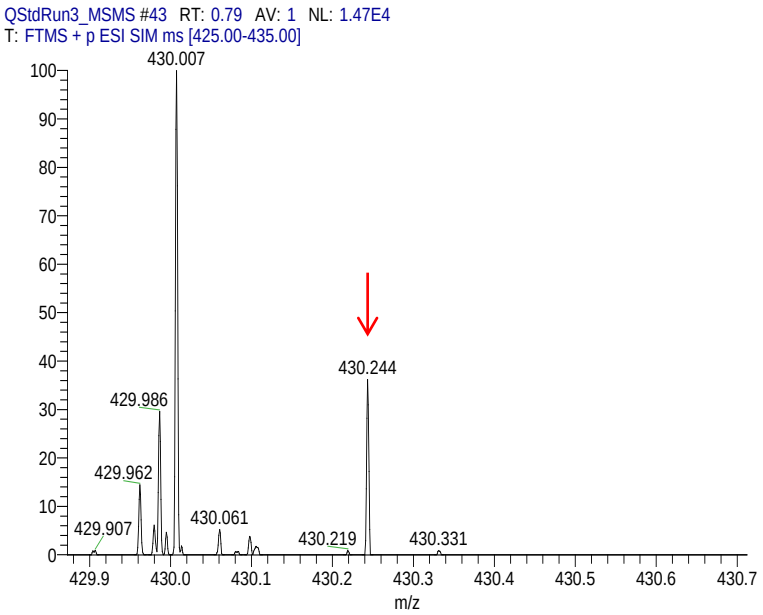


2) m/z 430.244

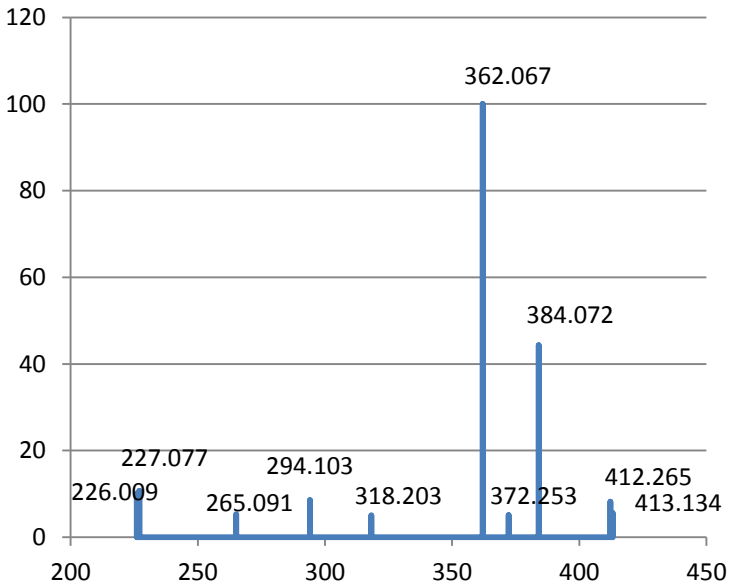
Elution profile



MS, FTMS

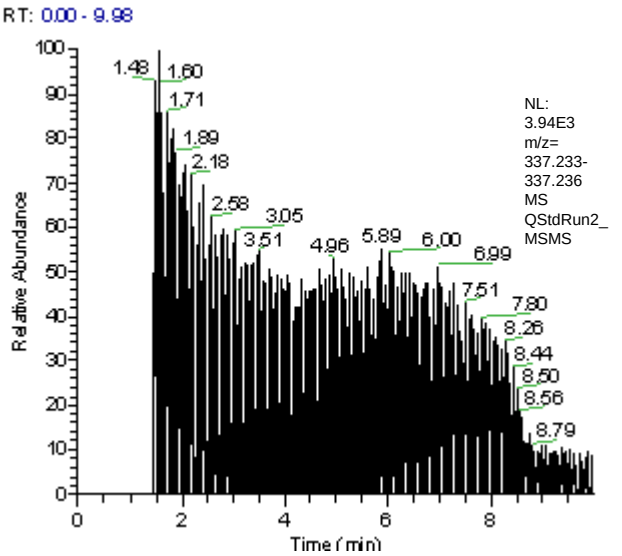


Deconvoluted MS/MS
CID in Ion trap

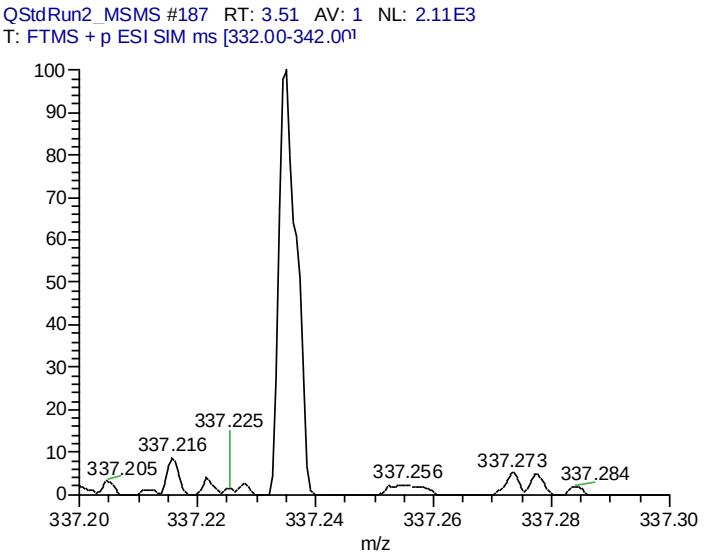


3) m/z 337.235

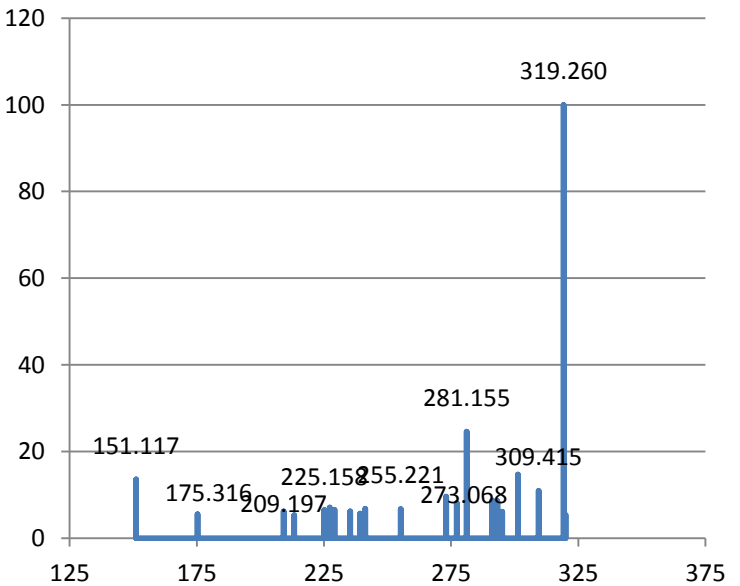
Elution profile



MS, FTMS

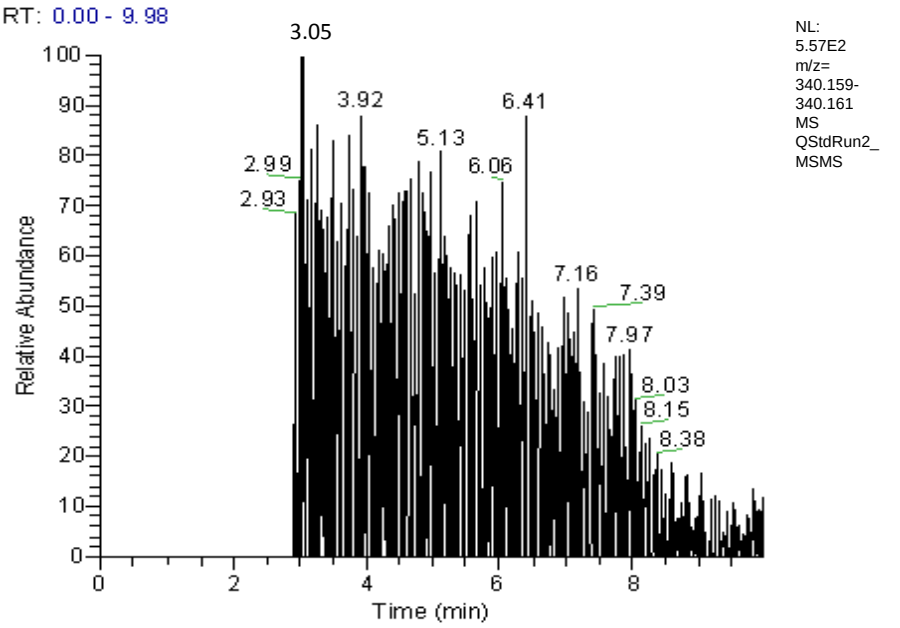


Deconvoluted MS/MS
CID in Ion trap

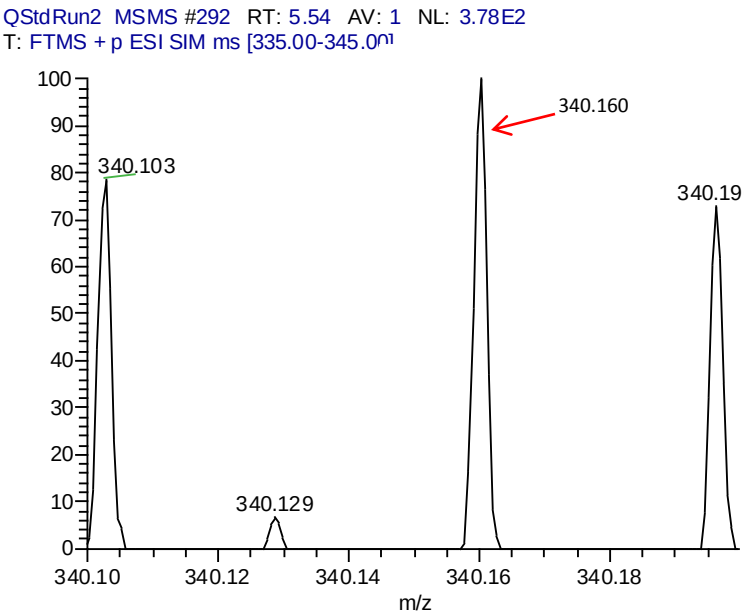


4) m/z 340.160

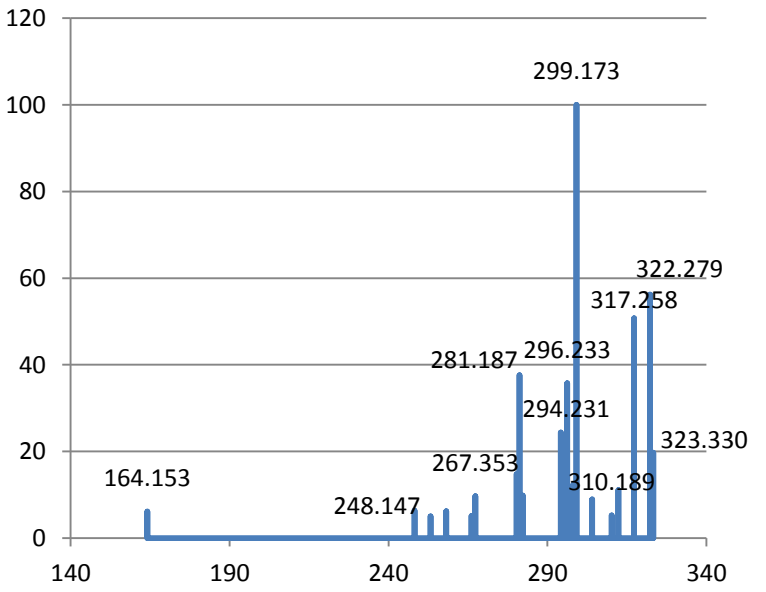
Elution profile



MS, FTMS

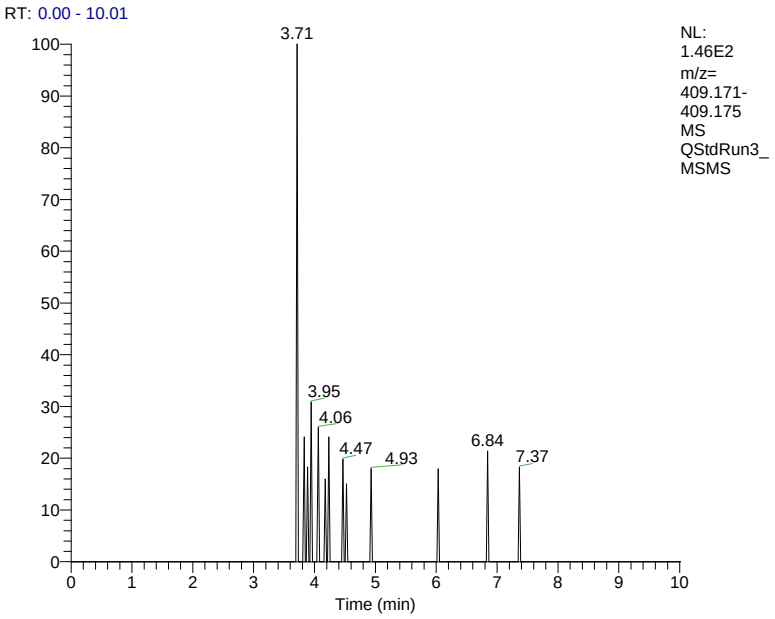


Deconvoluted MS/MS CID in Ion trap

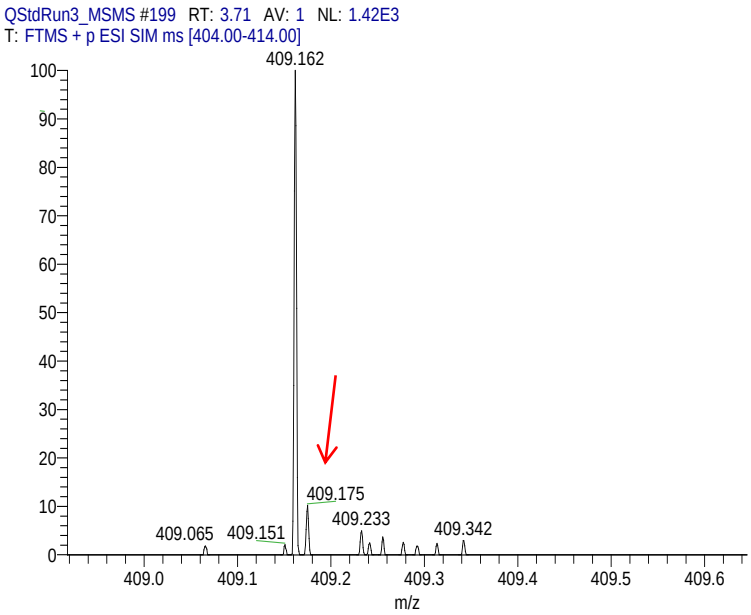


5) m/z 409.173

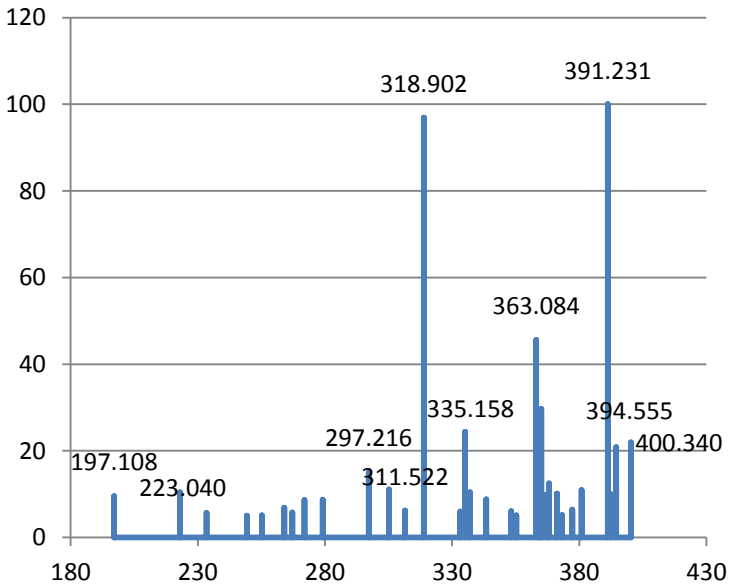
Elution profile



MS, FTMS

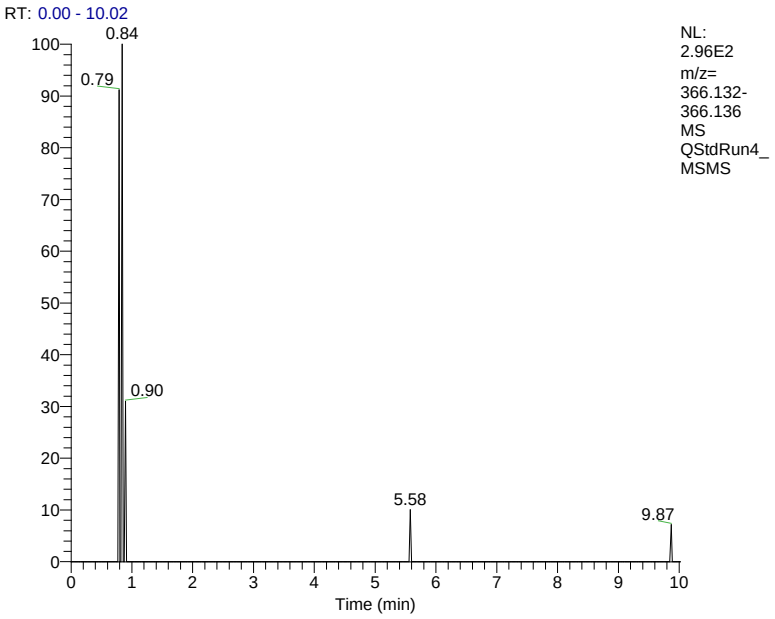


Deconvoluted MS/MS
CID in Ion trap

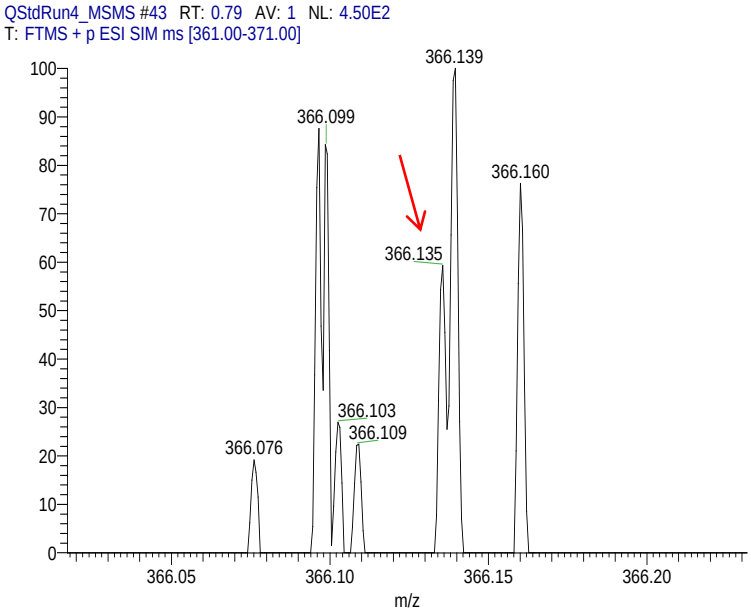


6) m/z 366.133

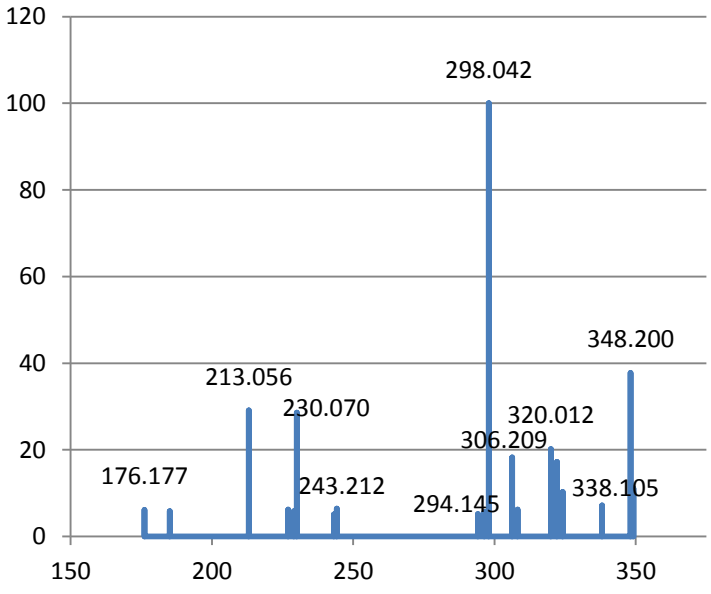
Elution profile



MS, FTMS

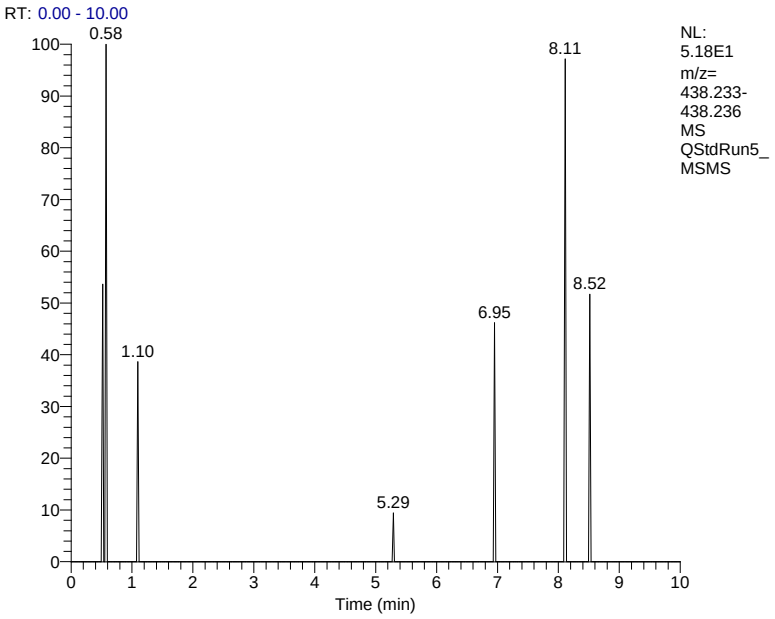


Deconvoluted MS/MS
CID in Ion trap

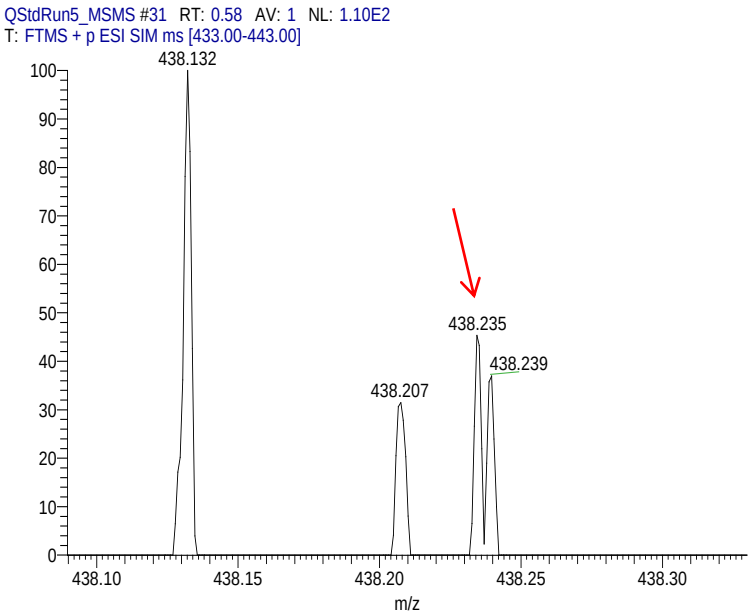


7) m/z 438.234

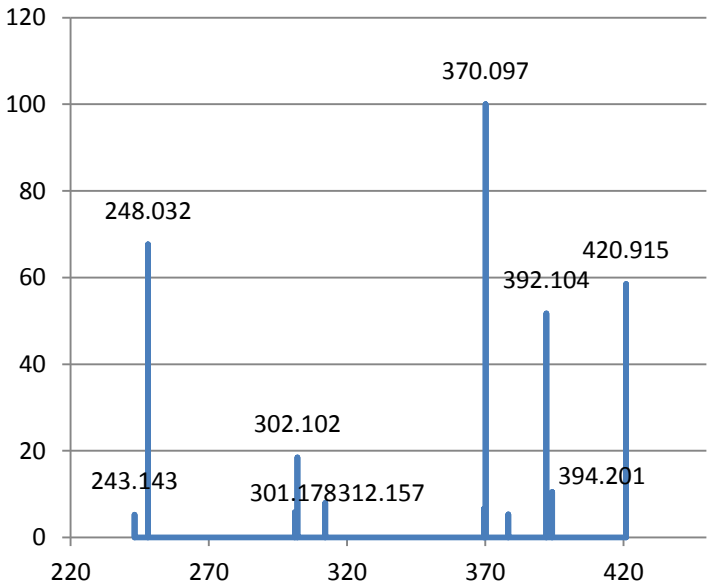
Elution profile



MS, FTMS

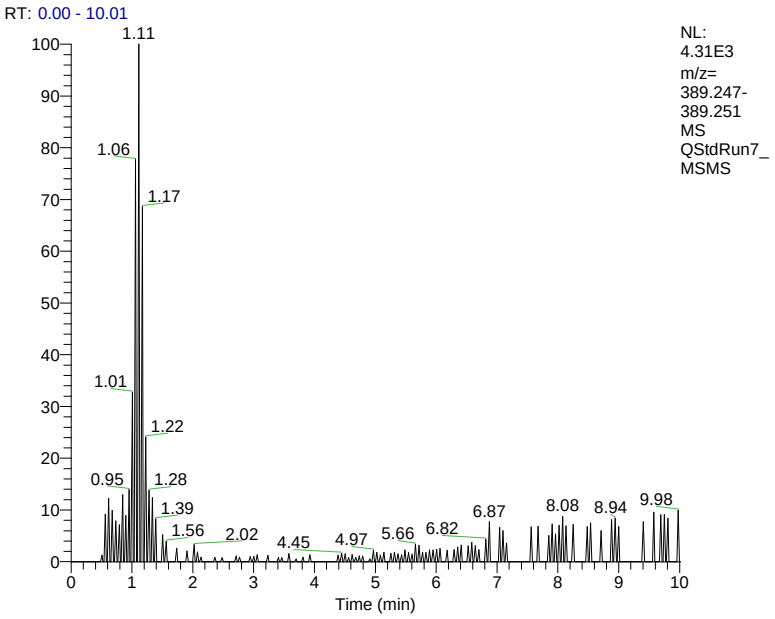


Deconvoluted MS/MS
CID in Ion trap

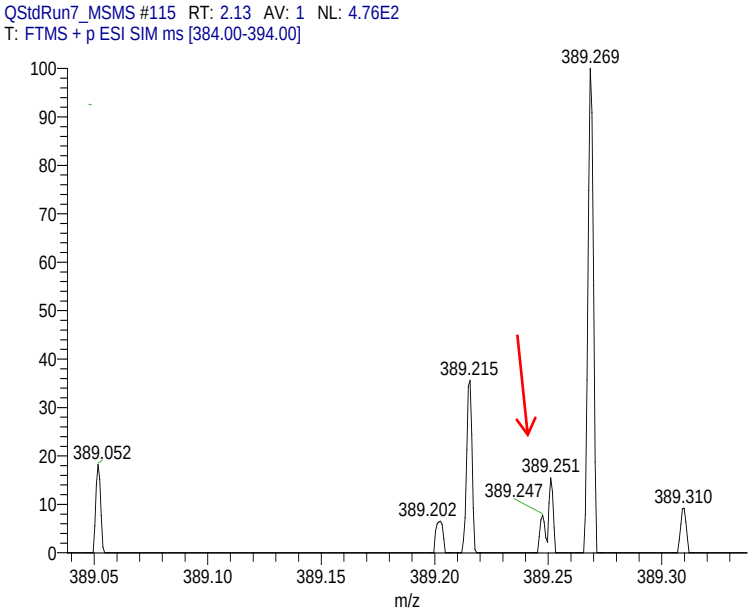


8) m/z 389.249

Elution profile



MS, FTMS



Deconvoluted MS/MS
CID in Ion trap