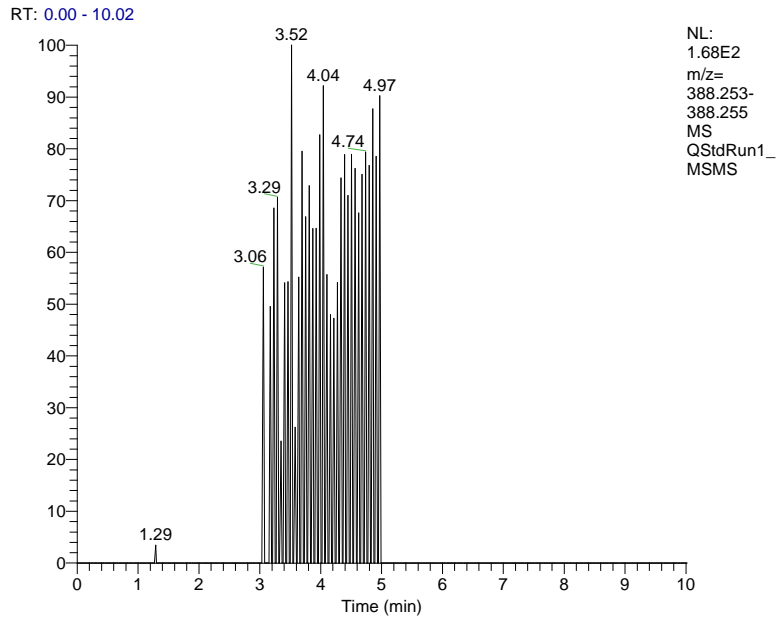


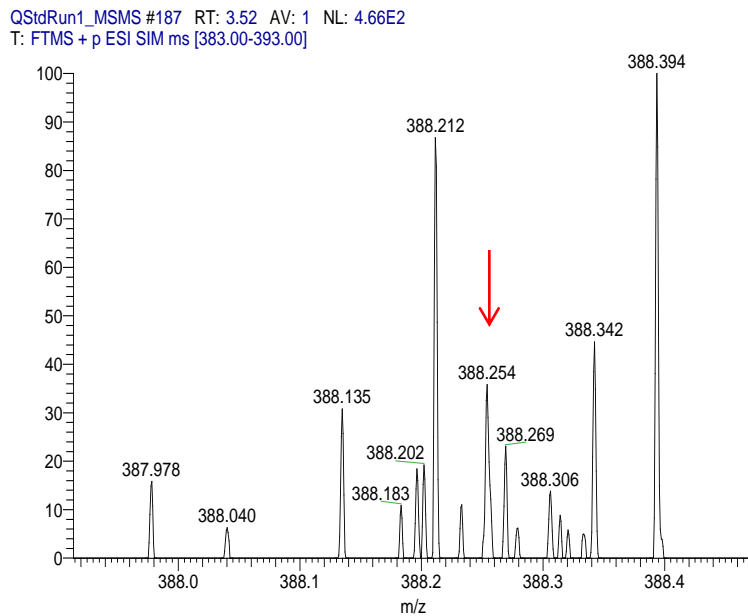
Additional File 11. MS/MS validation results for the 8 putative metabolites identified using DeconMSn. The first row shows the elution profile of the feature, middle row shows the full MS scan, and the last row shows the deconvoluted MS/MS spectrum obtained from DeconMSn.

1) m/z 388.254

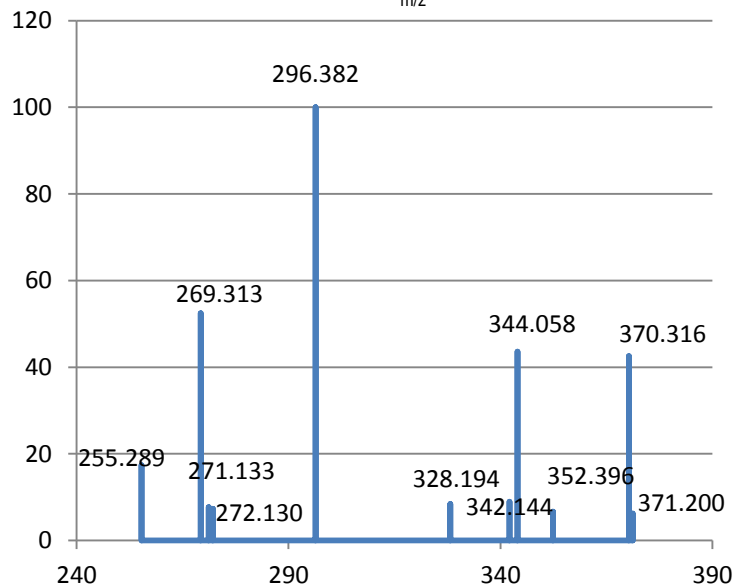
Elution profile



MS, FTMS

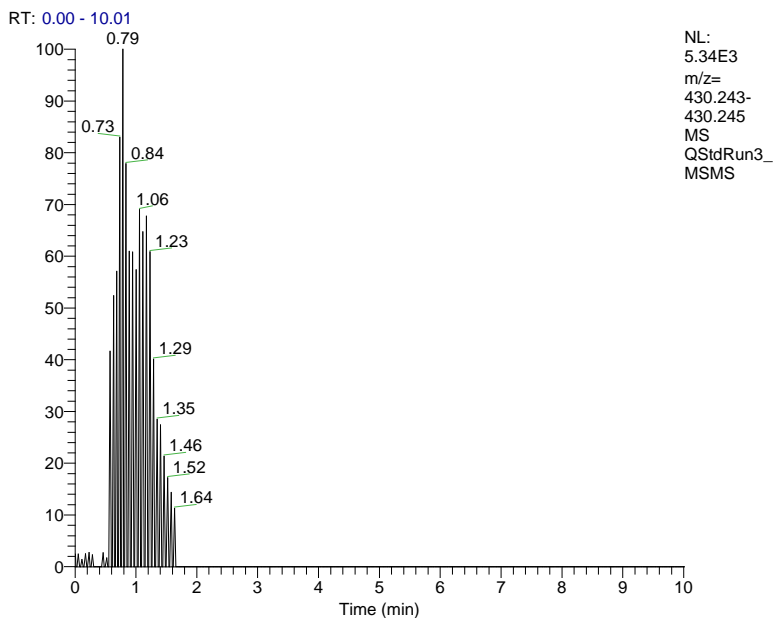


Deconvoluted MS/MS
CID in Ion trap

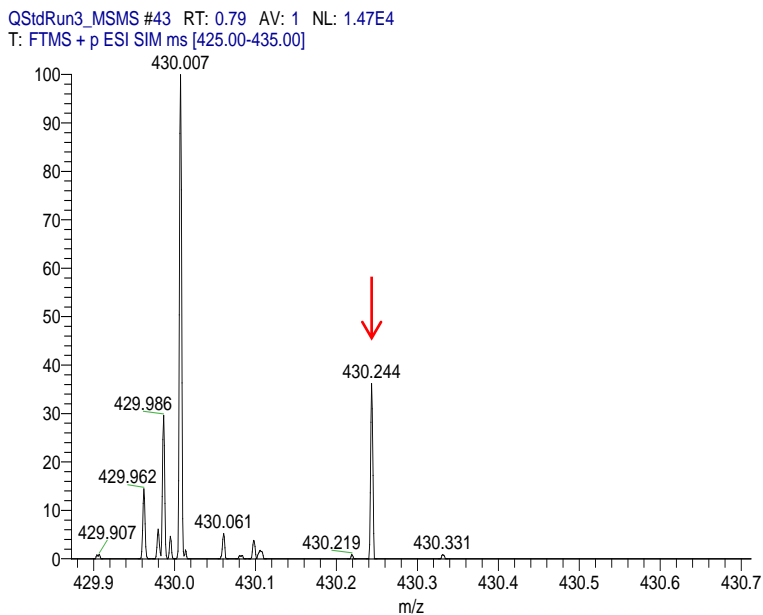


2) m/z 430.244

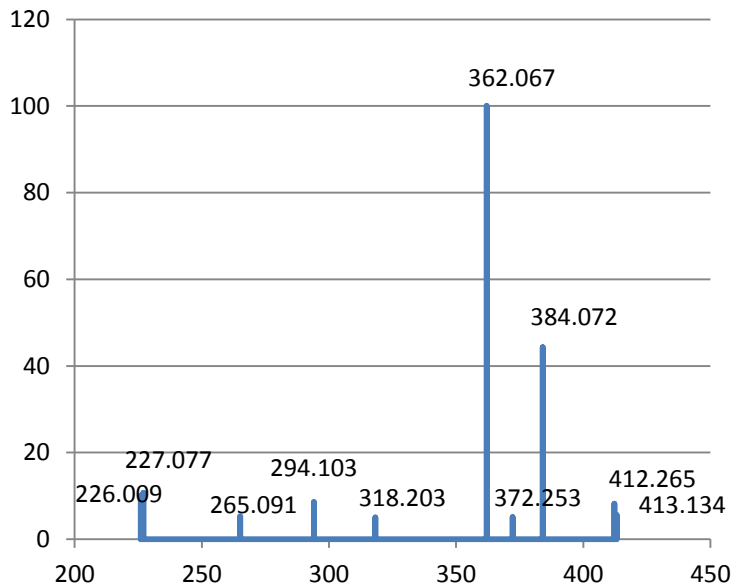
Elution profile



MS, FTMS

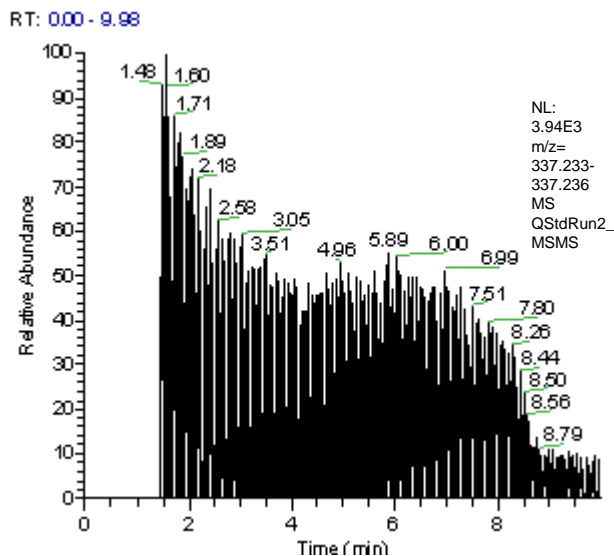


Deconvoluted MS/MS CID in Ion trap

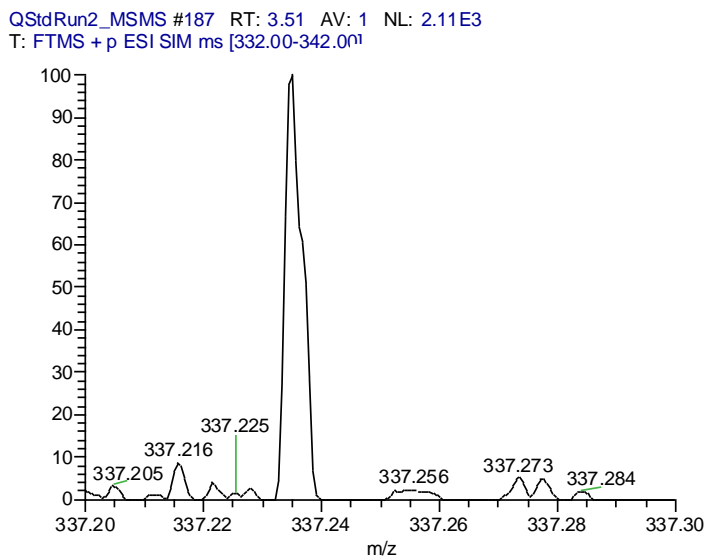


3) m/z 337.235

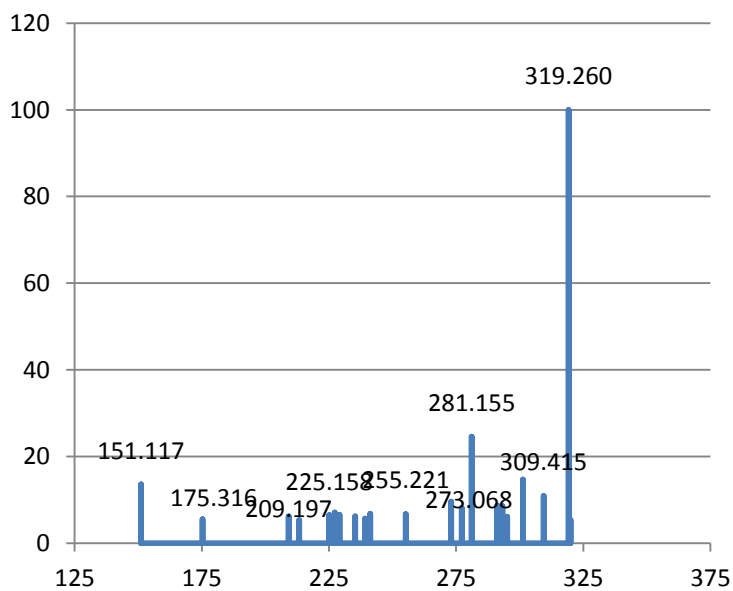
Elution profile



MS, FTMS



Deconvoluted MS/MS
CID in Ion trap

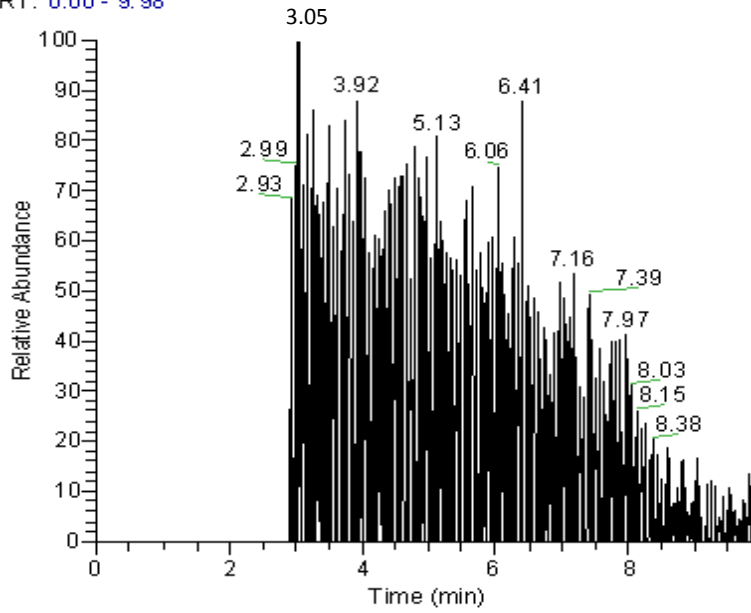


4) m/z 340.160

RT: 0.00 - 9.98

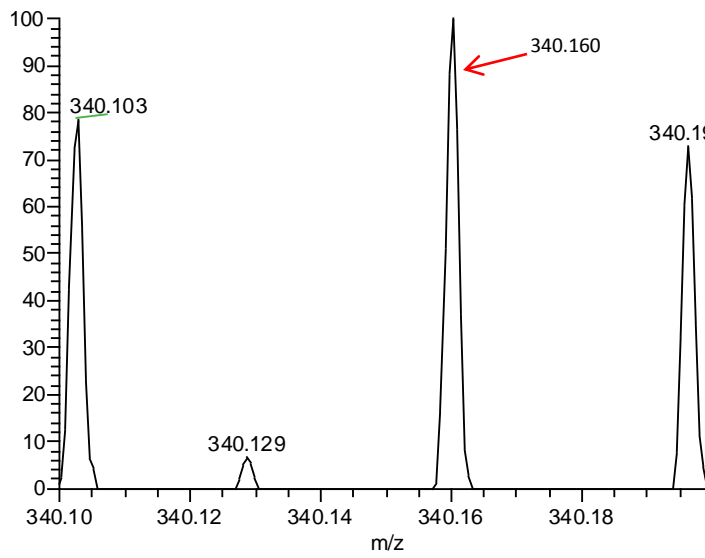
NL:
5.57E2
m/z=
340.159-
340.161
MS
QStdRun2_
MSMS

Elution profile

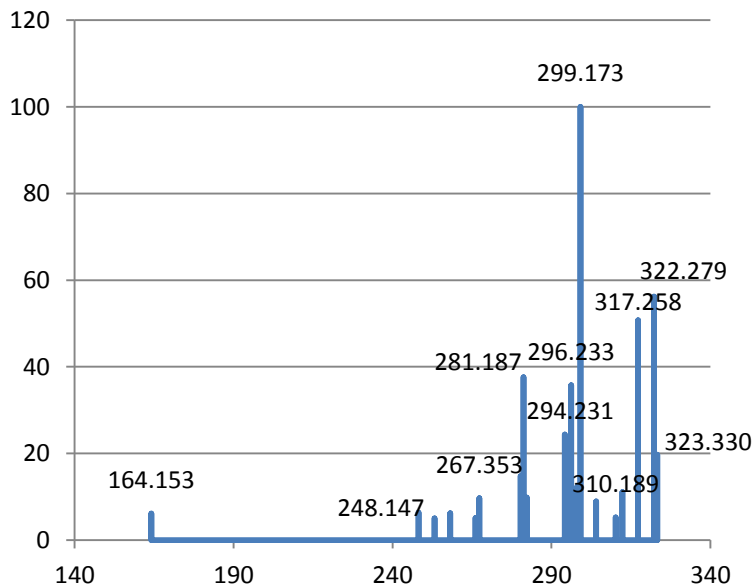


MS, FTMS

QStdRun2_MSMS #292 RT: 5.54 AV: 1 NL: 3.78E2
T: FTMS + p ESI SIM ms [335.00-345.00]

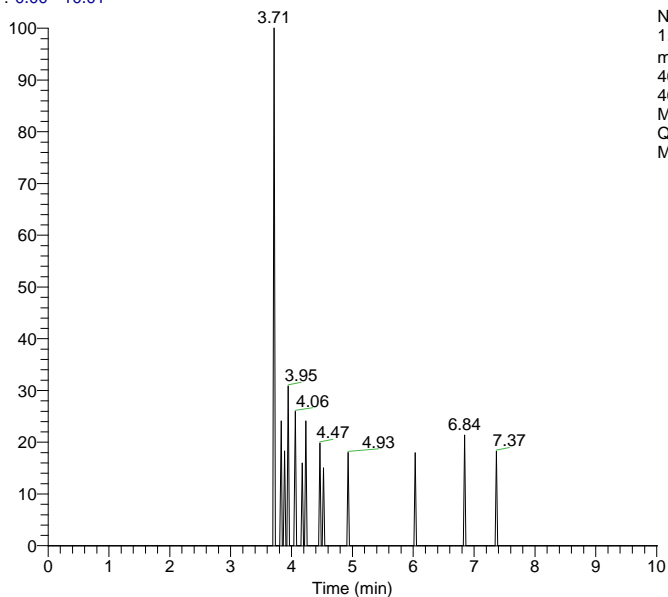


Deconvoluted MS/MS
CID in Ion trap



5) m/z 409.173

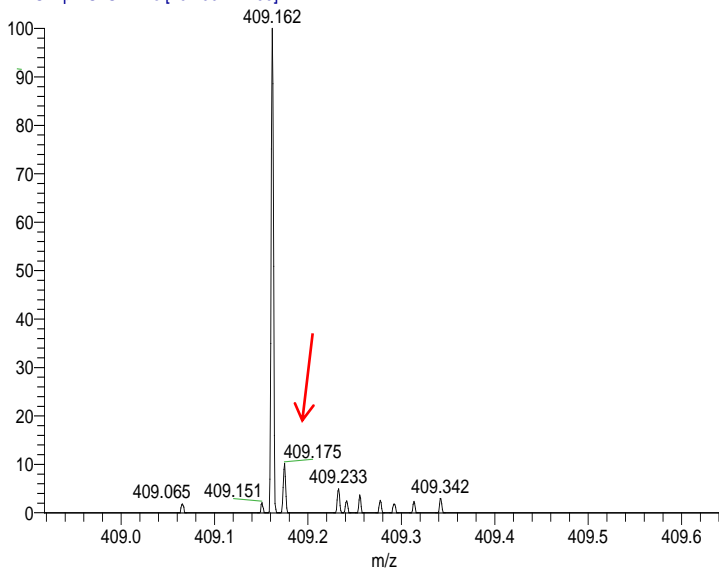
RT: 0.00 - 10.01



NL:
1.46E2
m/z=
409.171-
409.175
MS
QStdRun3_
MSMS

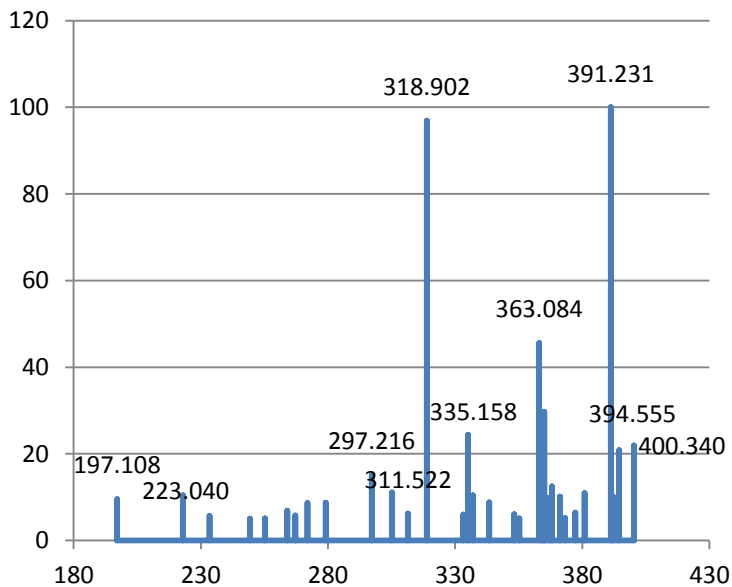
Elution profile

QStdRun3_MSMS #199 RT: 3.71 AV: 1 NL: 1.42E3
T: FTMS + p ESI SIM ms [404.00-414.00]

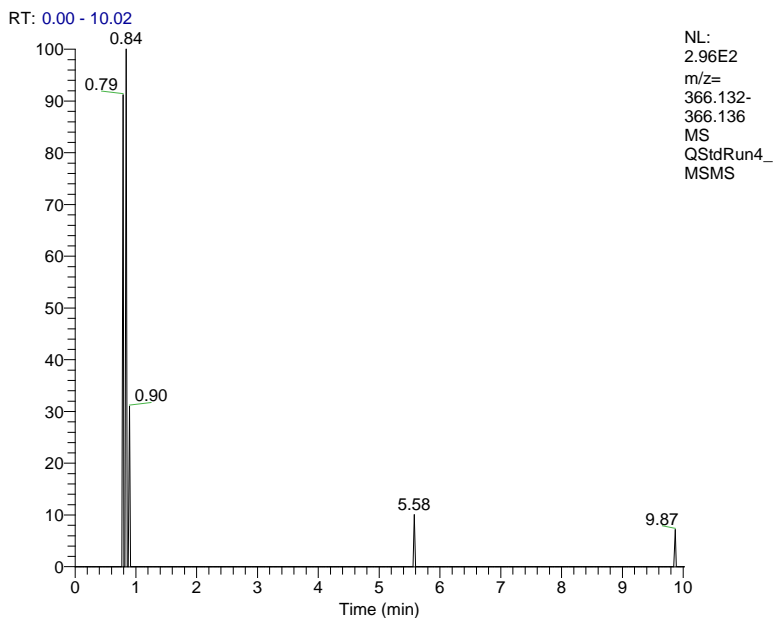


MS, FTMS

Deconvoluted MS/MS
CID in Ion trap

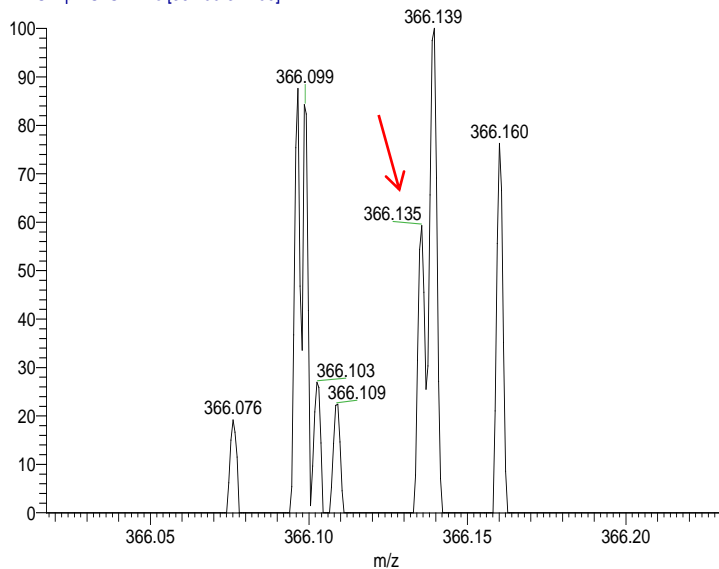


6) m/z 366.133

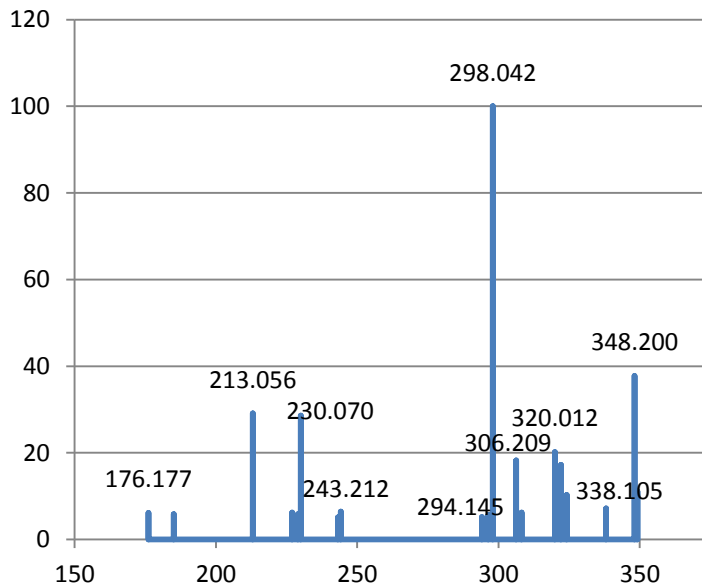


QStdRun4_MSMS #43 RT: 0.79 AV: 1 NL: 4.50E2
T: FTMS + p ESI SIM ms [361.00-371.00]

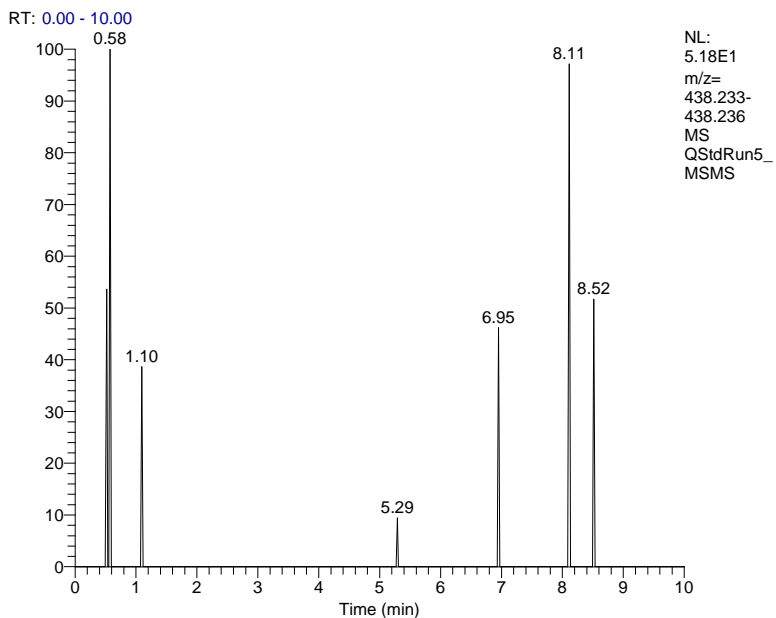
MS, FTMS



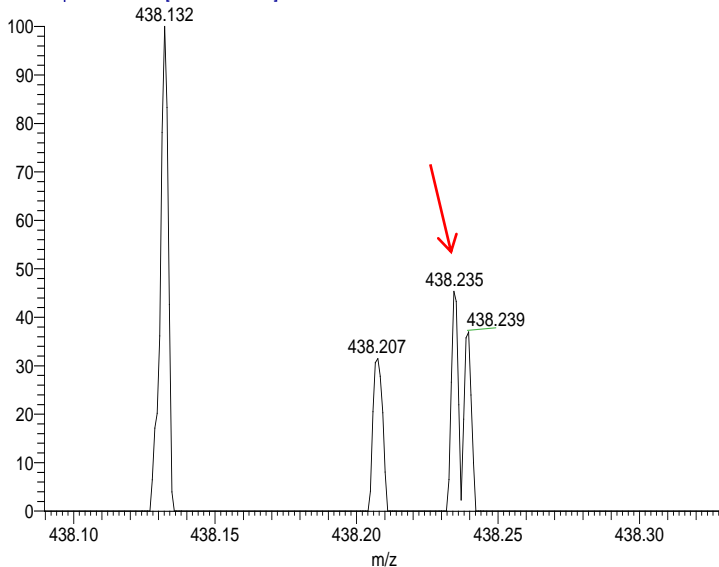
Deconvoluted MS/MS
CID in Ion trap



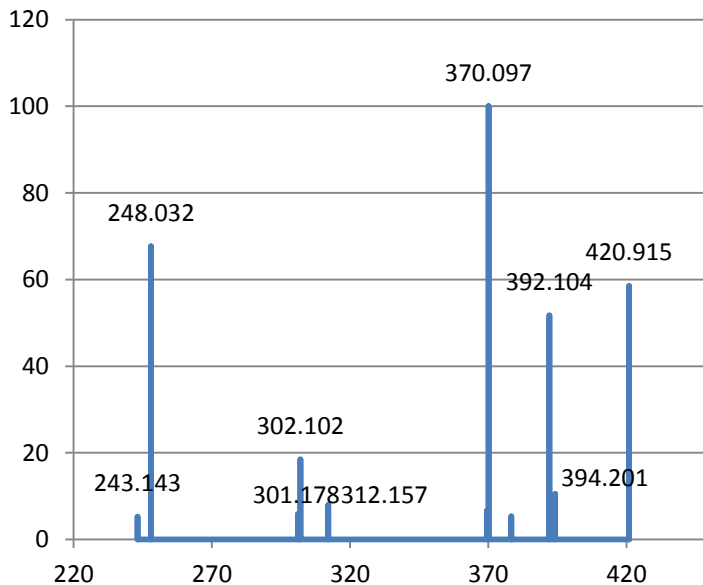
7) m/z 438.234



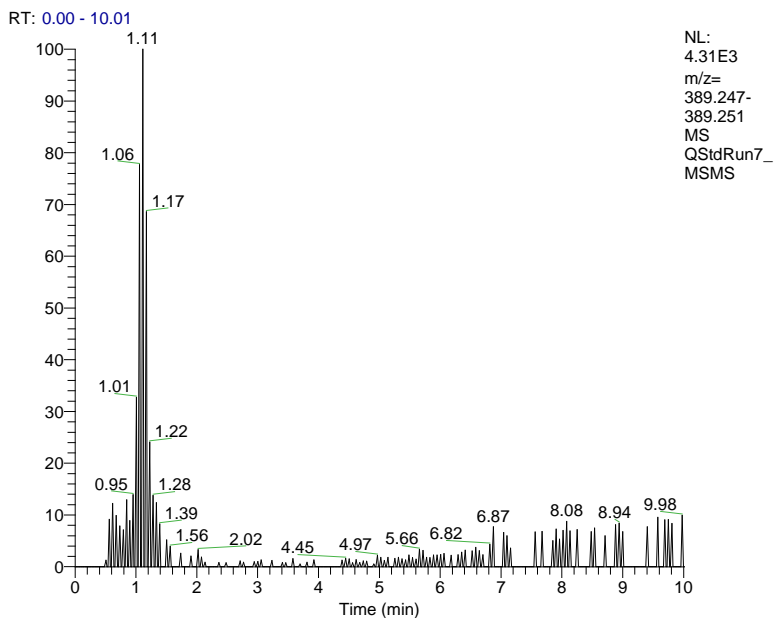
QStdRun5_MSMS #31 RT: 0.58 AV: 1 NL: 1.10E2
T: FTMS + p ESI SIM ms [433.00-443.00]



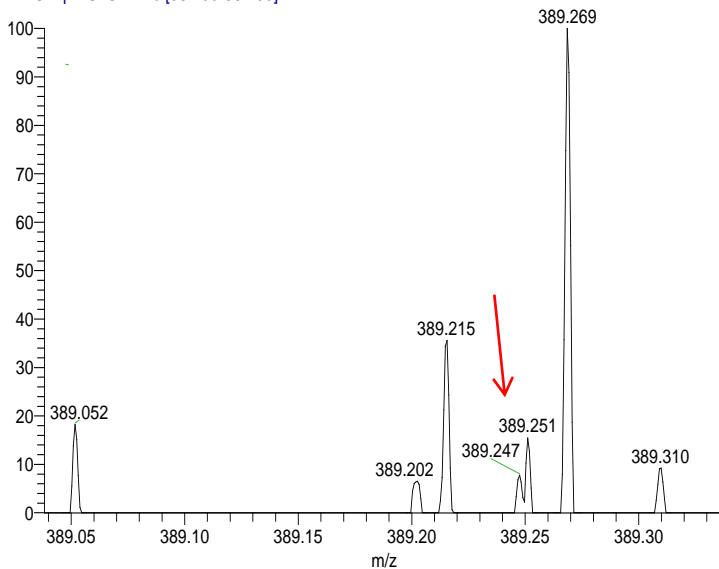
Deconvoluted MS/MS
CID in Ion trap



8) m/z 389.249



QStdRun7_MSMS #115 RT: 2.13 AV: 1 NL: 4.76E2
T: FTMS + p ESI SIM ms [384.00-394.00]



Deconvoluted MS/MS
CID in Ion trap

