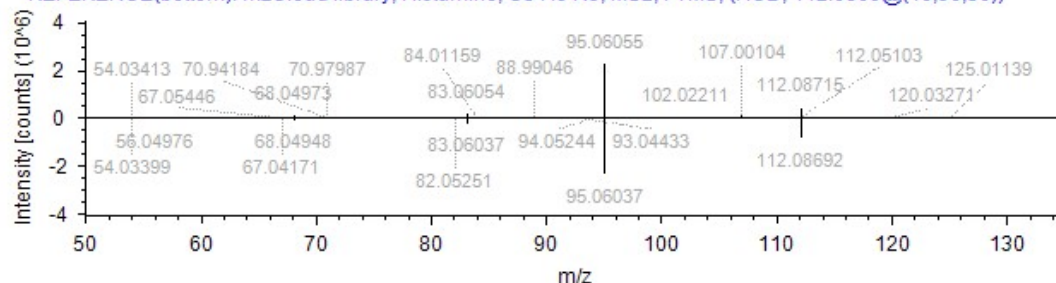


## MS2 information of DMs related to carbohydrate, lipid and AA metabolism

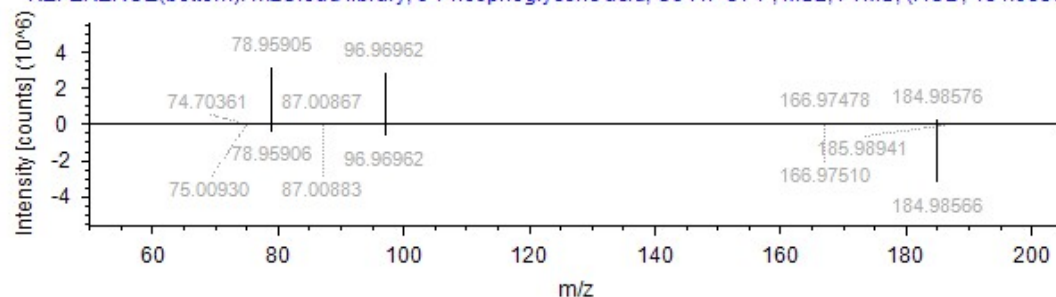
### Histamine

RAWFILE(top): 22P09130011\_BEHC18\_POS (F67) #207, RT=0.571 min, MS2, FTMS (+), (HCD, DDA, 112.0870@  
REFERENCE(bottom): mzCloud library, Histamine, C<sub>5</sub>H<sub>9</sub>N<sub>3</sub>, MS2, FTMS, (HCD, 112.0869@(10;30;50))



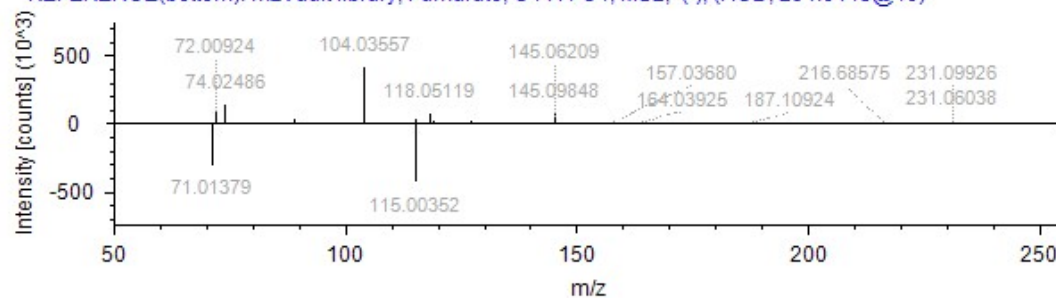
### 3-Phosphoglyceric acid

RAWFILE(top): 22P09130008\_BEHC18\_NEG (F19) #102, RT=0.589 min, MS2, FTMS (-), (HCD, DDA, 184.985  
REFERENCE(bottom): mzCloud library, 3-Phosphoglyceric acid, C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P, MS2, FTMS, (HCD, 184.9857@2



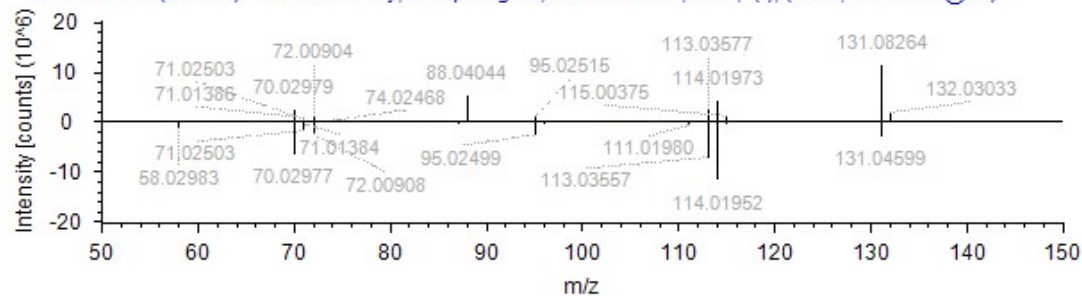
### Fumarate

RAWFILE(top): QC\_BEHC18\_NEG\_MSMS2 (F42) #125, RT=0.656 min, MS2, FTMS (-), (HCD, DDA, 231.0604  
REFERENCE(bottom): mzVault library, Fumarate, C<sub>4</sub>H<sub>4</sub>O<sub>4</sub>, MS2, (-), (HCD, 231.0145@40)



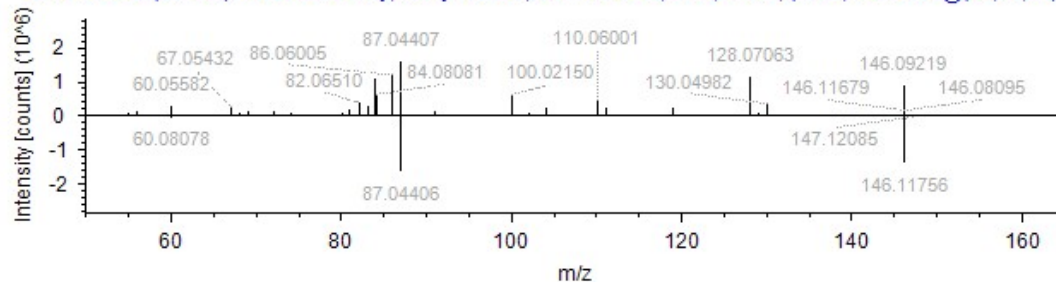
### L-Asparagine

RAWFILE(top): 22P08640015\_BEHC18\_NEG (F10) #127, RT=0.646 min, MS2, FTMS (-), (HCD, DDA, 131.046  
REFERENCE(bottom): mzVault library, L-Asparagine, C<sub>4</sub>H<sub>8</sub>N<sub>2</sub>O<sub>3</sub>, MS2, (-), (HCD, 131.0461@40)



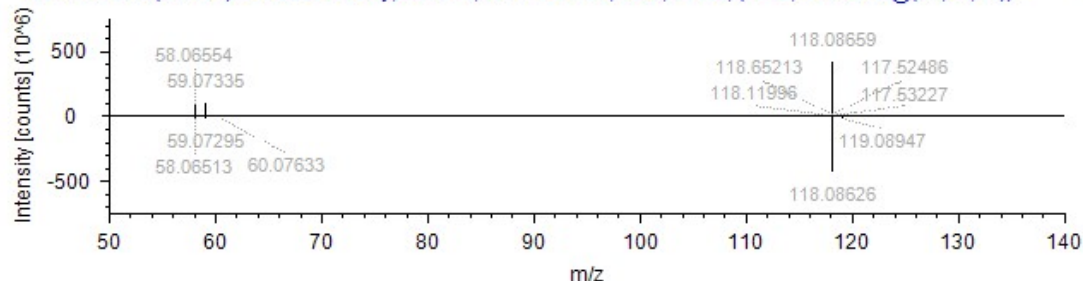
## Acetylcholine

RAWFILE(top): QC\_BEHC18\_POS\_MSMS1 (F86) #330, RT=0.722 min, MS2, FTMS (+), (HCD, DDA, 146.0809@2)  
REFERENCE(bottom): mzCloud library, Acetylcholine, C7 H15 N O2, MS2, FTMS, (HCD, 146.1176@(20;40;60))



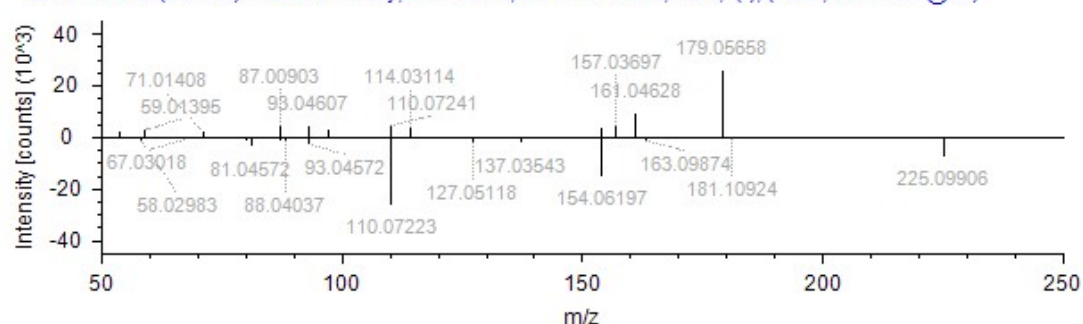
## Betaine

RAWFILE(top): 22P09130013\_BEHC18\_POS (F69) #246, RT=0.657 min, MS2, FTMS (+), (HCD, DDA, 118.0864@3)  
REFERENCE(bottom): mzCloud library, Betaine, C5 H11 N O2, MS2, FTMS, (HCD, 118.0863@(30;50;70))



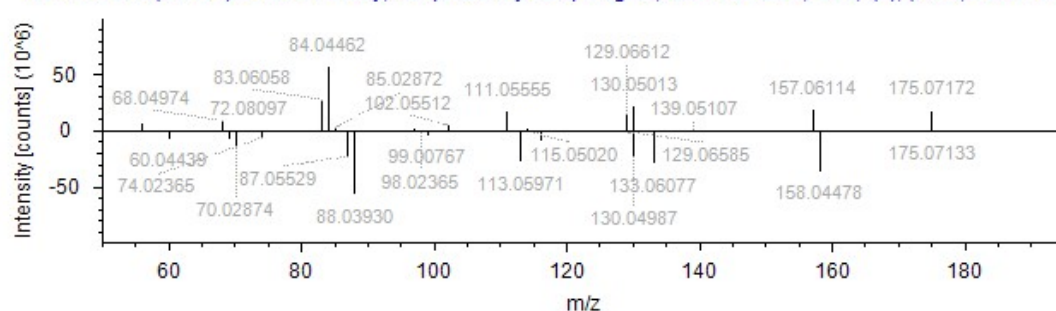
## Carnosine

RAWFILE(top): QC\_BEHC18\_NEG\_MSMS2 (F42) #163, RT=0.732 min, MS2, FTMS (-), (HCD, DDA, 225.0623@4)  
REFERENCE(bottom): mzVault library, Carnosine, C9 H14 N4 O3, MS2, (-), (HCD, 225.0991@40)



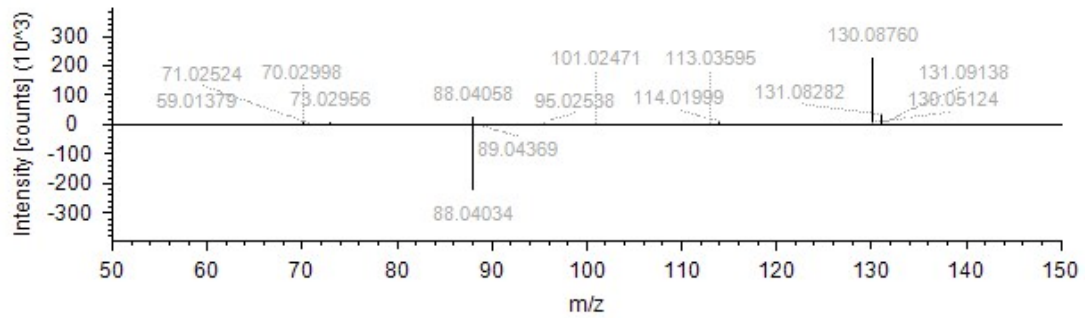
## N-alpha-acetyl-l-asparagine

RAWFILE(top): 22P08640010\_BEHC18\_POS (F52) #258, RT=0.687 min, MS2, FTMS (+), (HCD, DDA, 175.0714@5)  
REFERENCE(bottom): mzVault library, N-alpha-acetyl-l-asparagine, C6 H10 N2 O4, MS2, (+), (HCD, 175.0718@30)



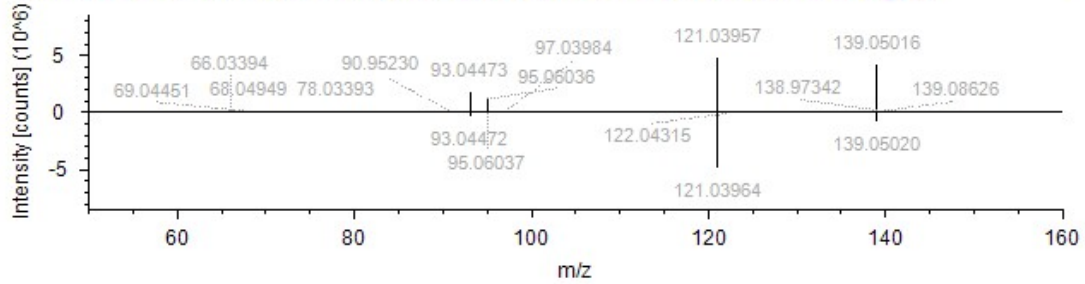
## Creatine

RAWFILE(top): QC\_BEHC18\_NEG\_MSMS1 (F41) #278, RT=0.903 min, MS2, FTMS (-), (HCD, DDA, 130.0876  
REFERENCE(bottom): mzVault library, Creatine, C4 H9 N3 O2, MS2, (-), (HCD, 130.0620@40)



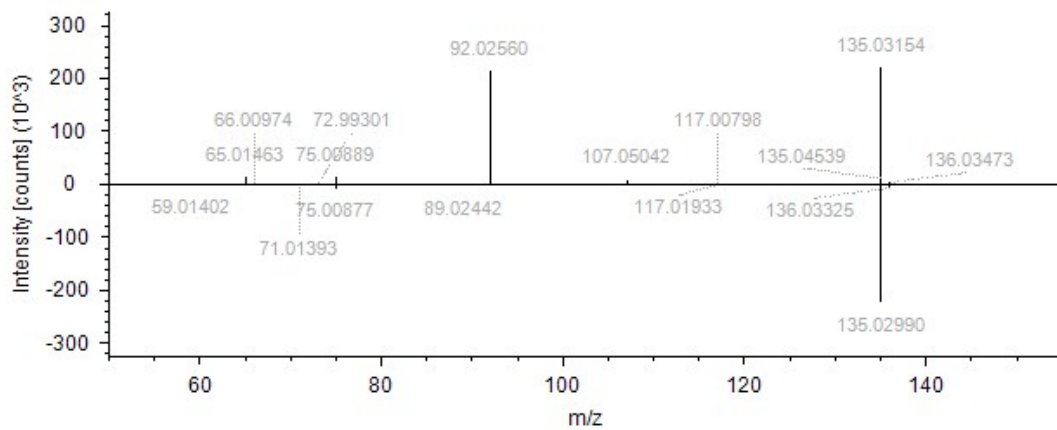
## Urocanate

RAWFILE(top): QC\_BEHC18\_POS\_MSMS5 (F90) #361, RT=0.713 min, MS2, FTMS (+), (HCD, DDA, 139.0500@2)  
REFERENCE(bottom): mzVault library, Urocanate, C6 H6 N2 O2, MS2, (+), (HCD, 139.0505@30)



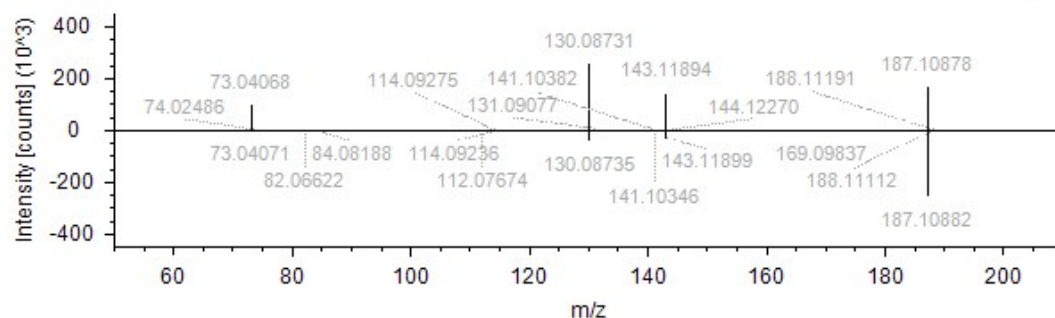
## L-Threonic acid

RAWFILE(top): QC\_BEHC18\_NEG\_MSMS1 (F41) #203, RT=0.743 min, MS2, FTMS (-), (HCD, DDA, 135.0315@2)  
REFERENCE(bottom): mzCloud library, L-Threonic acid, C4 H8 O5, MS2, FTMS, (HCD, 135.0299@(10;30;50))



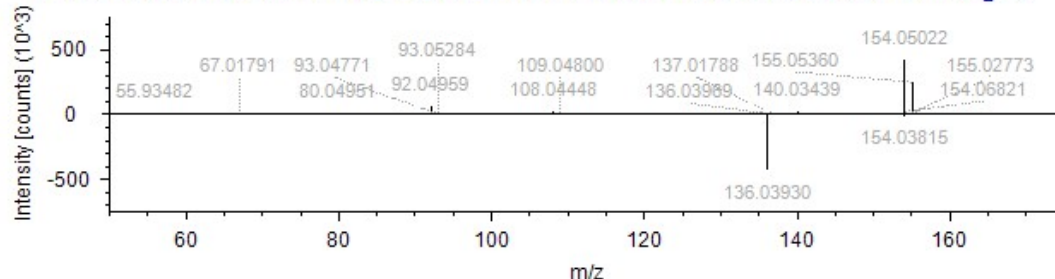
### Glycyl-L-leucine

RAWFILE(top): 22P08640015\_BEHC18\_NEG (F10) #513, RT=1.614 min, MS2, FTMS (-), (HCD, DDA, 187.108  
REFERENCE(bottom): mzCloud library, Glycyl-L-leucine, C8 H16 N2 O3, MS2, FTMS, (HCD, 187.1088@(30;50



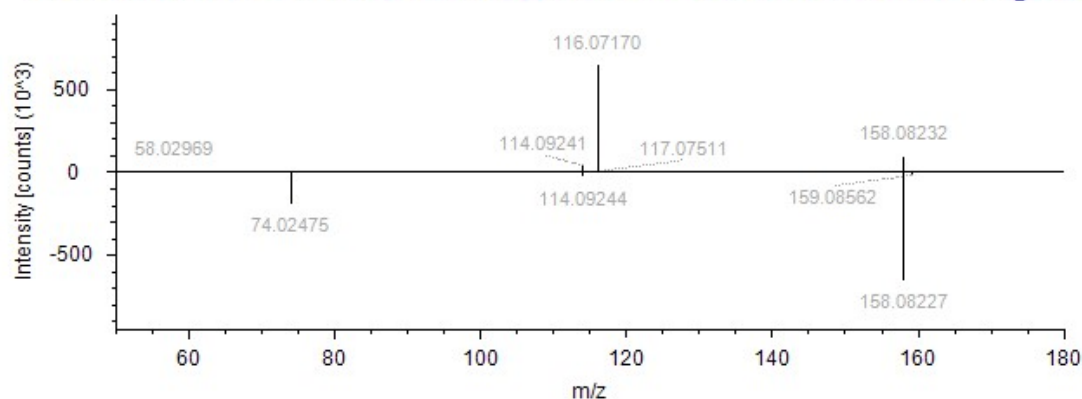
### 3-hydroxyanthranilate

RAWFILE(top): 22P09130006\_BEHC18\_POS (F62) #740, RT=1.821 min, MS2, FTMS (+), (HCD, DDA, 154.0500@(  
REFERENCE(bottom): mzVault library, 3-hydroxyanthranilate, C7 H7 N O3, MS2, (+), (HCD, 154.0503@30)



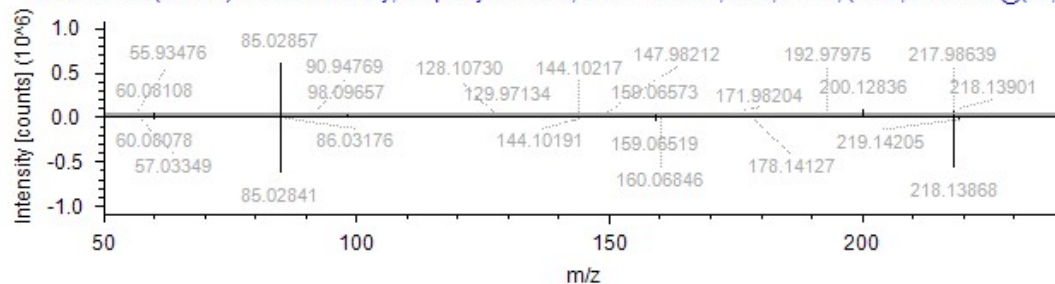
### N-Isovalerylglycine

RAWFILE(top): 22P08640003\_BEHC18\_NEG (F2) #591, RT=1.847 min, MS2, FTMS (-), (HCD, DDA, 158.0823@(  
REFERENCE(bottom): mzCloud library, N-Isovalerylglycine, C7 H13 N O3, MS2, FTMS, (HCD, 158.0823@(30;50;7



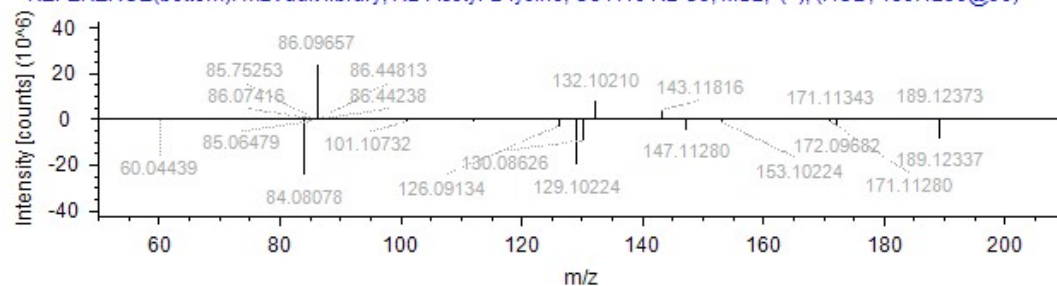
### Propionylcarnitine

RAWFILE(top): 22P09130009\_BEHC18\_POS (F65) #771, RT=1.900 min, MS2, FTMS (+), (HCD, DDA, 218.1388@(  
REFERENCE(bottom): mzCloud library, Propionylcarnitine, C10 H19 N O4, MS2, FTMS, (HCD, 218.1387@(20;40;6)



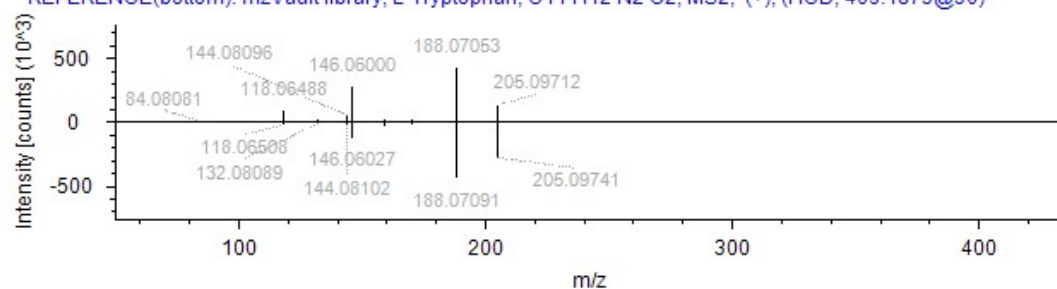
## N2-Acetyl-L-lysine

RAWFILE(top): 22P08640015\_BEHC18\_POS (F55) #1286, RT=3.114 min, MS2, FTMS (+), (HCD, DDA, 189.1235@  
REFERENCE(bottom): mzVault library, N2-Acetyl-L-lysine, C8 H16 N2 O3, MS2, (+), (HCD, 189.1239@30)



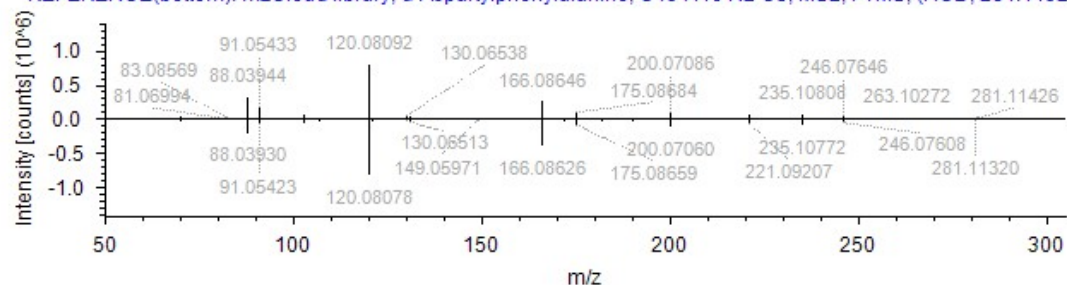
## L-Tryptophan

RAWFILE(top): QC\_BEHC18\_POS\_MSMS5 (F90) #1745, RT=3.310 min, MS2, FTMS (+), (HCD, DDA, 409.1863@(  
REFERENCE(bottom): mzVault library, L-Tryptophan, C11 H12 N2 O2, MS2, (+), (HCD, 409.1873@30)



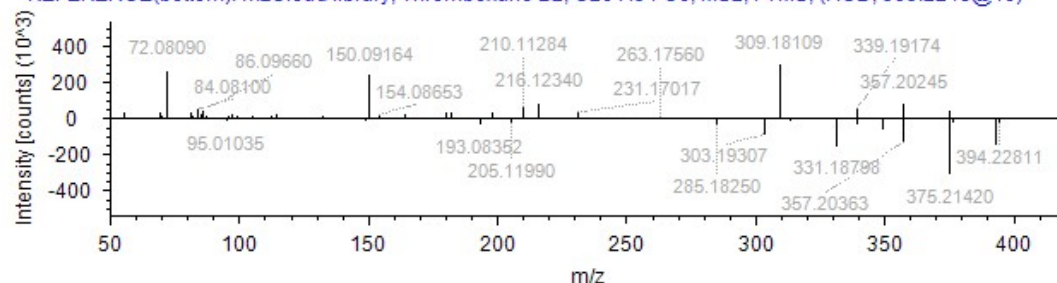
## $\alpha$ -Aspartylphenylalanine

RAWFILE(top): 22P08640015\_BEHC18\_POS (F55) #1460, RT=3.531 min, MS2, FTMS (+), (HCD, DDA, 281.1132@  
REFERENCE(bottom): mzCloud library,  $\alpha$ -Aspartylphenylalanine, C13 H16 N2 O5, MS2, FTMS, (HCD, 281.1132@30)



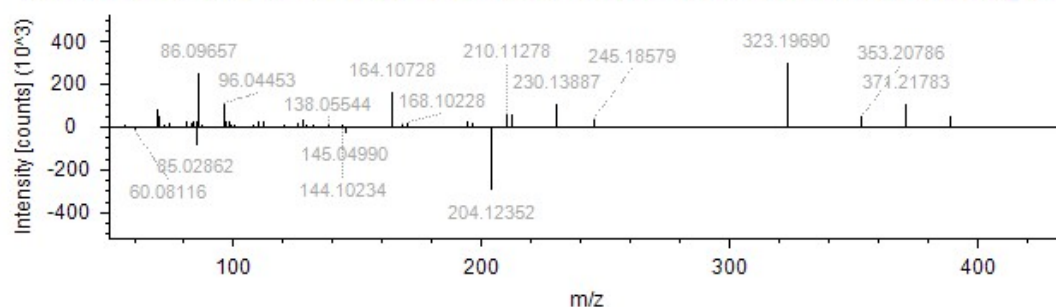
## Thromboxane B2

RAWFILE(top): 22P08640016\_BEHC18\_POS (F56) #1563, RT=3.803 min, MS2, FTMS (+), (HCD, DDA, 393.2231@  
REFERENCE(bottom): mzCloud library, Thromboxane B2, C20 H34 O6, MS2, FTMS, (HCD, 393.2248@40)



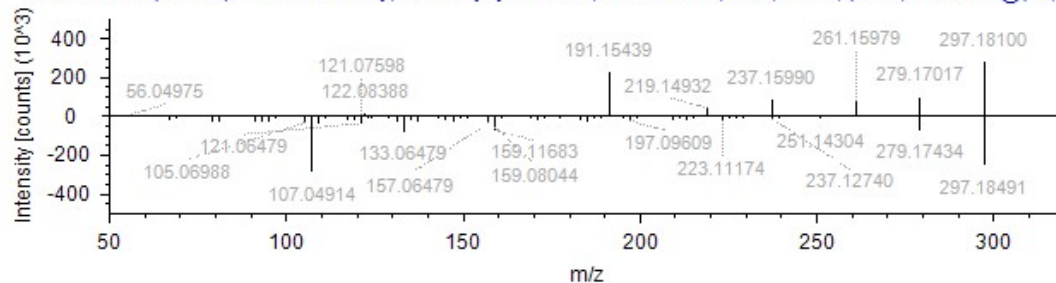
## O-ACETYLCARNITINE

RAWFILE(top): 22P08640016\_BEHC18\_POS (F56) #1782, RT=4.367 min, MS2, FTMS (+), (HCD, DDA, 407.2388@  
REFERENCE(bottom): mzVault library, O-ACETYLCARNITINE, C9 H17 N O4, MS2, (+), (HCD, 407.2393@30)



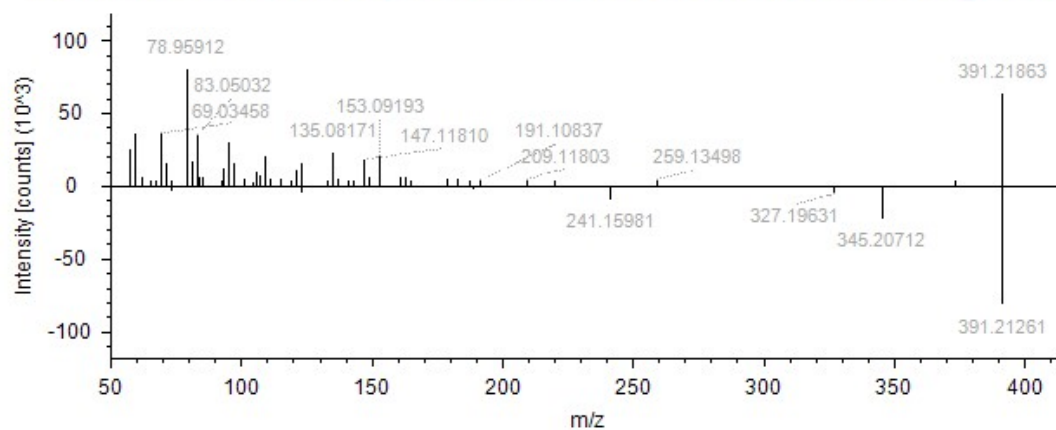
## 17 $\alpha$ -Ethinylestradiol

RAWFILE(top): 22P08640010\_BEHC18\_POS (F52) #1862, RT=4.554 min, MS2, FTMS (+), (HCD, DDA, 297.1802@  
REFERENCE(bottom): mzCloud library, 17 $\alpha$ -Ethinylestradiol, C20 H24 O2, MS2, FTMS, (HCD, 297.1849@(15;30;6)



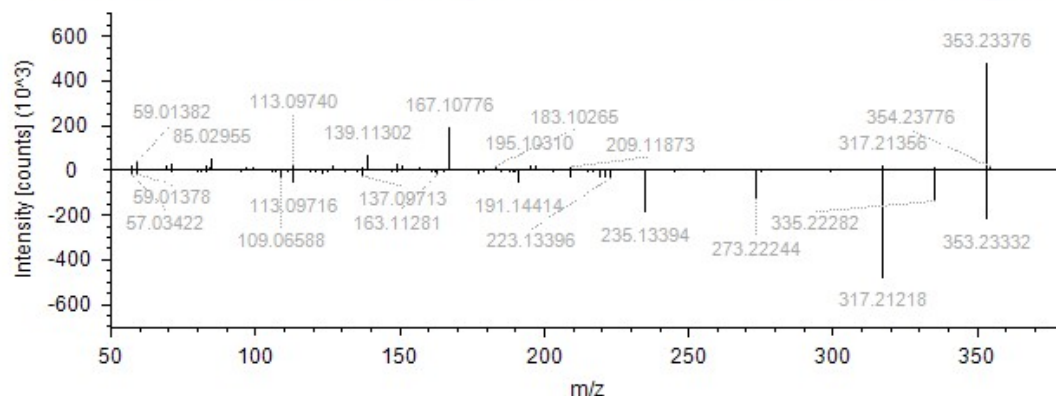
## Corticosterone

RAWFILE(top): 22P08640012\_BEHC18\_NEG (F8) #1978, RT=6.396 min, MS2, FTMS (-), (HCD, DDA, 391.2129@  
REFERENCE(bottom): mzCloud library, Corticosterone, C21 H30 O4, MS2, FTMS, (HCD, 391.2119@(20;40;60)



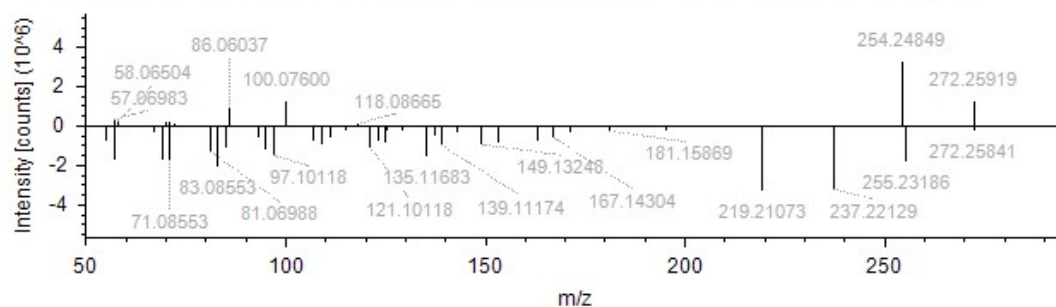
## Prostaglandin E1

RAWFILE(top): 22P08640012\_BEHC18\_NEG (F8) #2320, RT=7.312 min, MS2, FTMS (-), (HCD, DDA, 353.2336@  
REFERENCE(bottom): mzCloud library, Prostaglandin E1, C20 H34 O5, MS2, FTMS, (HCD, 353.2334@(10;30;50)



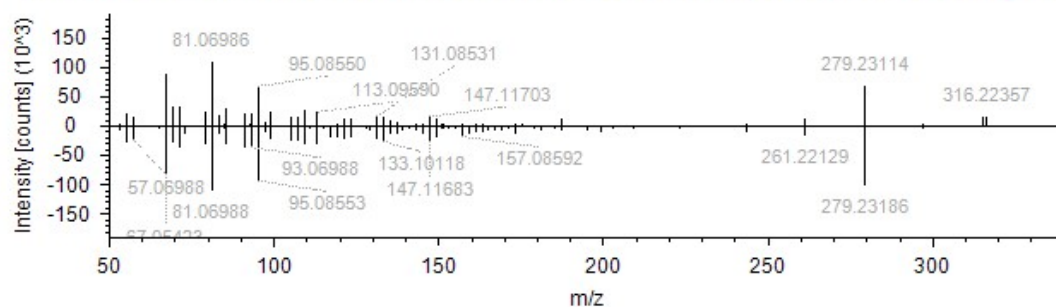
## Palmitoleic acid

RAWFILE(top): 22P08640001\_BEHC18\_POS (F46) #3083, RT=7.725 min, MS2, FTMS (+), (HCD, DDA, 272.2592@  
REFERENCE(bottom): mzVault library, Palmitoleic acid, C16 H30 O2, MS2, (+), (HCD, 272.2592@30)



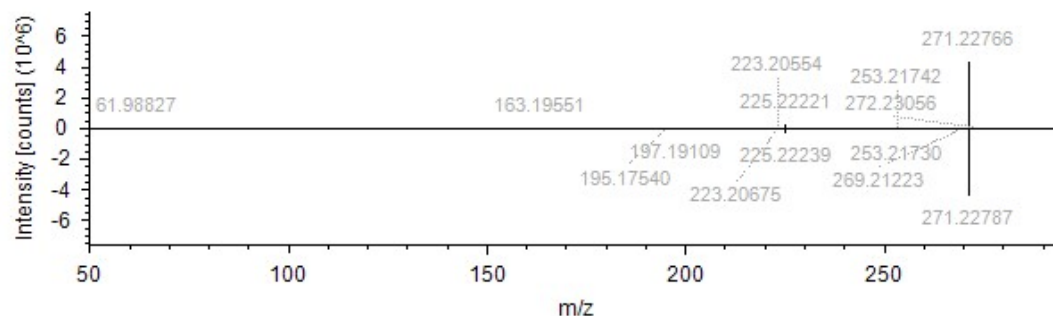
## (+/-)12(13)-DiHOME

RAWFILE(top): QC\_BEHC18\_POS\_MSMS5 (F90) #4254, RT=8.376 min, MS2, FTMS (+), (HCD, DDA, 315.2521@  
REFERENCE(bottom): mzCloud library, (+/-)12(13)-DiHOME, C18 H34 O4, MS2, FTMS, (HCD, 315.2530@(20;40;60)



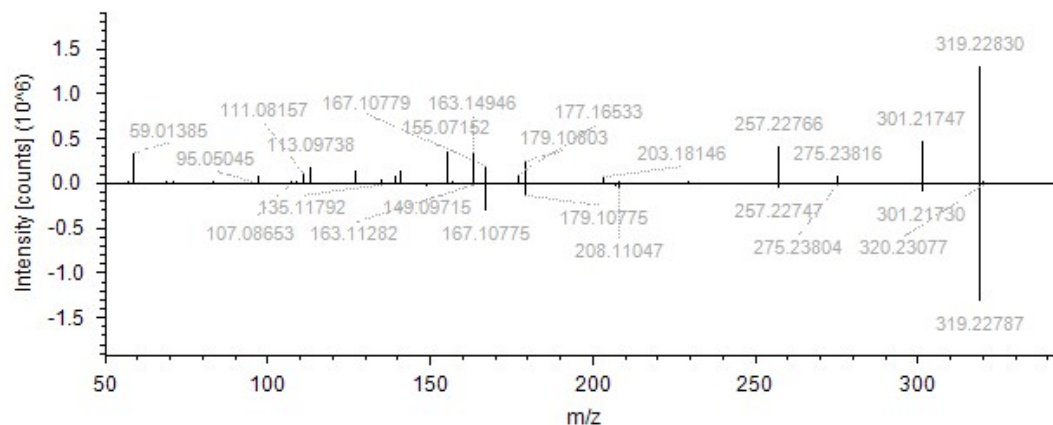
## 16-Hydroxyhexadecanoic acid

RAWFILE(top): 22P08640001\_BEHC18\_NEG (F1) #2332, RT=8.400 min, MS2, FTMS (-), (HCD, DDA, 271.227  
REFERENCE(bottom): mzCloud library, 16-Hydroxyhexadecanoic acid, C16 H32 O3, MS2, FTMS, (HCD, 271.2



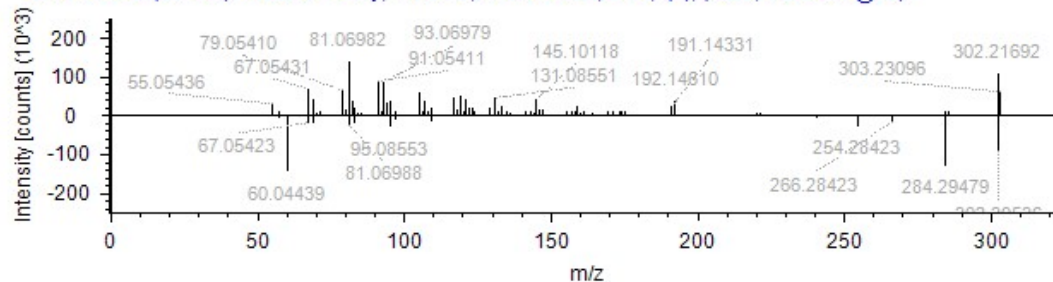
## 11,12-Epoxy-(5Z,8Z,11Z)-icosatrienoic acid

RAWFILE(top): 22P08640012\_BEHC18\_NEG (F8) #2862, RT=8.698 min, MS2, FTMS (-), (HCD, DDA, 319.2280@  
REFERENCE(bottom): mzCloud library, 11,12-Epoxy-(5Z,8Z,11Z)-icosatrienoic acid, C20 H32 O3, MS2, FTMS, (H



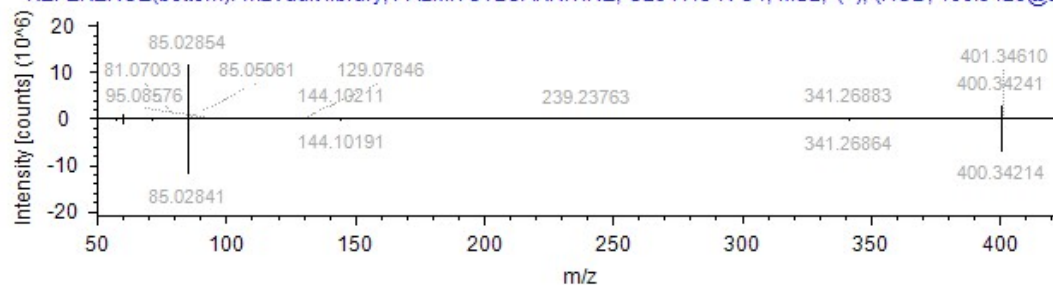
## Stearate

RAWFILE(top): QC\_BEHC18\_POS\_MSMS5 (F90) #4499, RT=8.856 min, MS2, FTMS (+), (HCD, DDA, 302.2184@  
REFERENCE(bottom): mzVault library, Stearate, C18 H36 O2, MS2, (+), (HCD, 302.3061@30)



## PALMITOYL CARNITINE

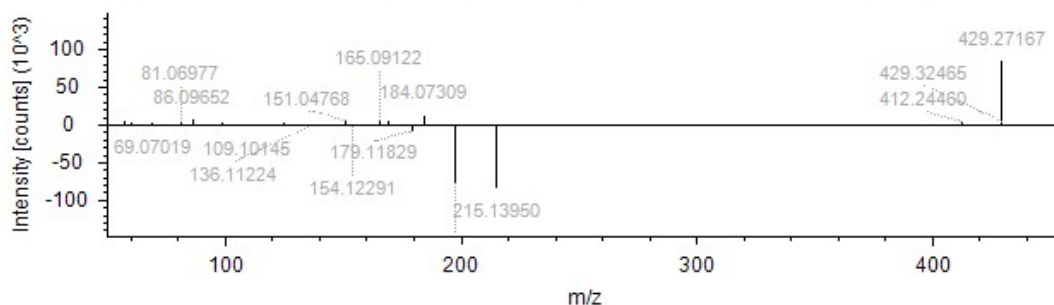
RAWFILE(top): 22P09130009\_BEHC18\_POS (F65) #3467, RT=8.838 min, MS2, FTMS (+), (HCD, DDA, 400.3417@  
REFERENCE(bottom): mzVault library, PALMITOYL CARNITINE, C23 H45 N O4, MS2, (+), (HCD, 400.3429@30)





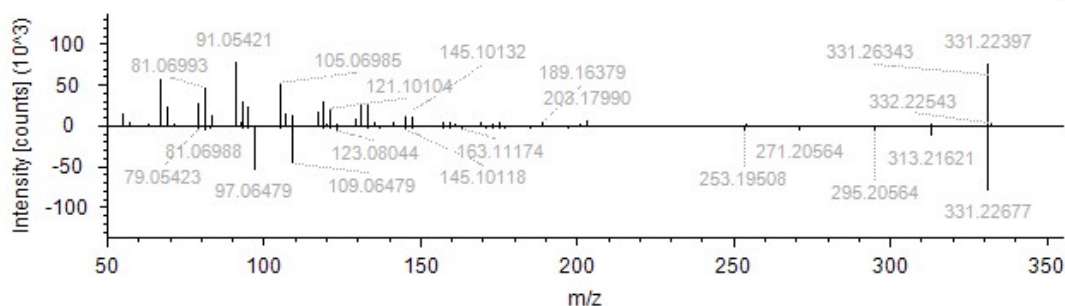
## Dethiobiotin

RAWFILE(top): QC\_BEHC18\_POS\_MSMS3 (F88) #1754, RT=8.998 min, MS2, FTMS (+), (HCD, DDA, 429.2739@  
REFERENCE(bottom): mzVault library, Dethiobiotin, C10 H18 N2 O3, MS2, (+), (HCD, 429.2714@30)



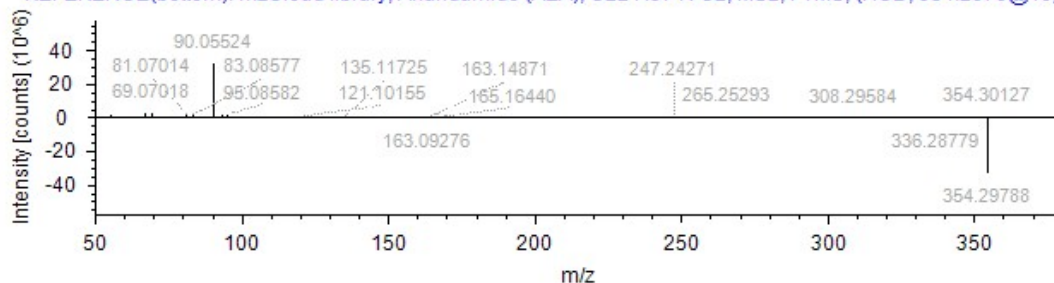
## 17 $\alpha$ -Hydroxyprogesterone

RAWFILE(top): QC\_BEHC18\_POS\_MSMS2 (F87) #3701, RT=9.157 min, MS2, FTMS (+), (HCD, DDA, 331.2630@  
REFERENCE(bottom): mzCloud library, 17 $\alpha$ -Hydroxyprogesterone, C21 H30 O3, MS2, FTMS, (HCD, 331.2268@20)



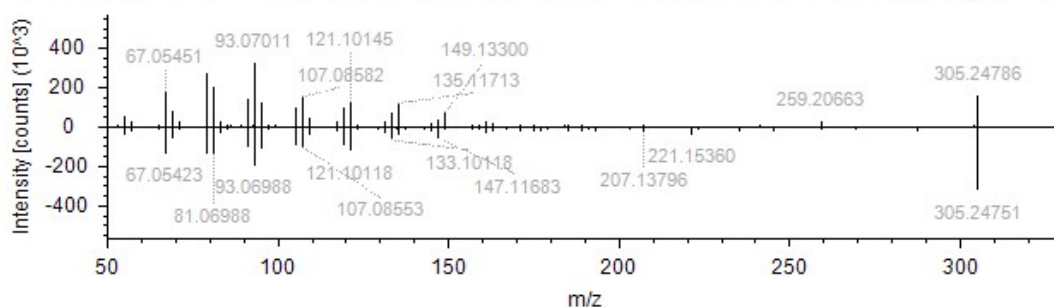
## Anandamide (AEA)

RAWFILE(top): 22P08640016\_BEHC18\_POS (F56) #3884, RT=9.658 min, MS2, FTMS (+), (HCD, DDA, 354.3006@  
REFERENCE(bottom): mzCloud library, Anandamide (AEA), C22 H37 N O2, MS2, FTMS, (HCD, 354.2979@10)



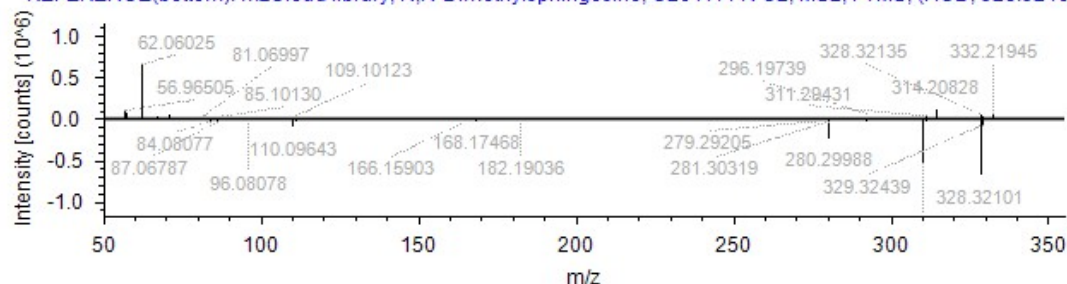
## Arachidonic acid

RAWFILE(top): 22P08640014\_BEHC18\_POS (F54) #3695, RT=9.181 min, MS2, FTMS (+), (HCD, DDA, 305.2473@  
REFERENCE(bottom): mzCloud library, Arachidonic acid, C20 H32 O2, MS2, FTMS, (HCD, 305.2475@(20;40;60))



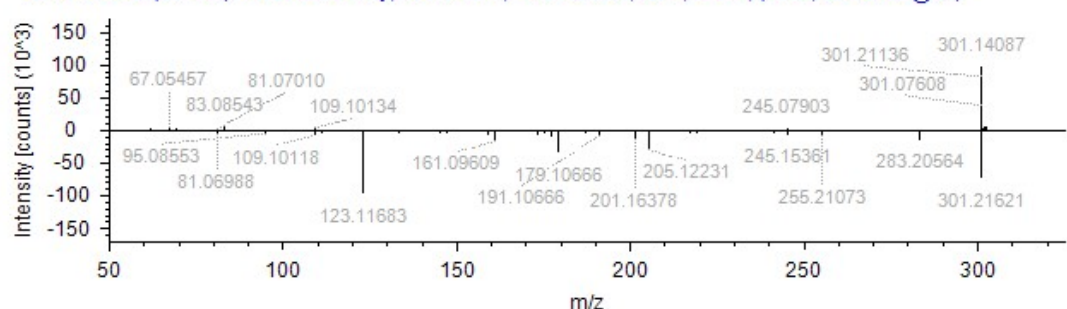
### N,N-Dimethylsphingosine

RAWFILE(top): 22P09130012\_BEHC18\_POS (F68) #3908, RT=9.910 min, MS2, FTMS (+), (HCD, DDA, 328.3206@  
REFERENCE(bottom): mzCloud library, N,N-Dimethylsphingosine, C20 H41 N O2, MS2, FTMS, (HCD, 328.3210@



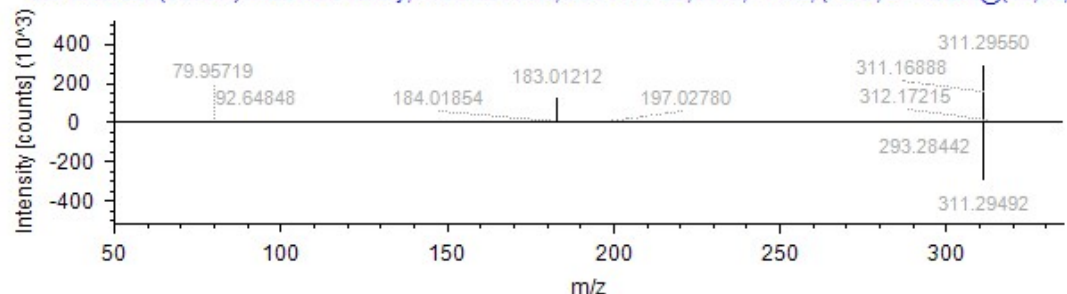
### Isotretinoin

RAWFILE(top): QC\_BEHC18\_POS\_MSMS2 (F87) #4099, RT=9.921 min, MS2, FTMS (+), (HCD, DDA, 301.2112@  
REFERENCE(bottom): mzCloud library, Isotretinoin, C20 H28 O2, MS2, FTMS, (HCD, 301.2159@10)



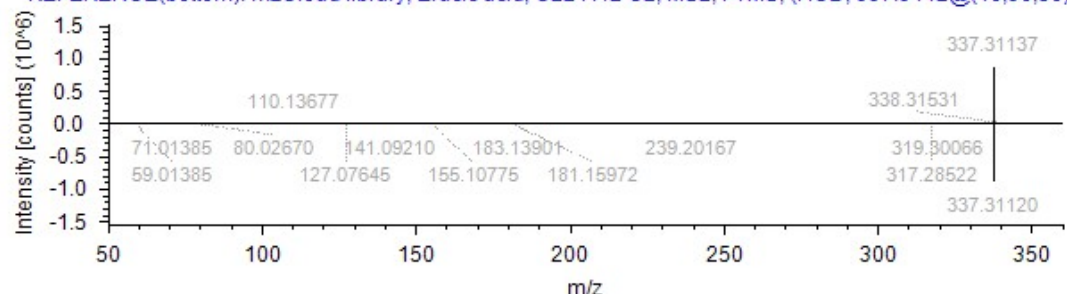
### Arachidic acid

RAWFILE(top): QC\_BEHC18\_NEG\_07 (F32) #2868, RT=10.308 min, MS2, FTMS (-), (HCD, DDA, 311.2956@  
REFERENCE(bottom): mzCloud library, Arachidic acid, C20 H40 O2, MS2, FTMS, (HCD, 311.2956@(10;30;50)



### Erucic acid

RAWFILE(top): 22P08640001\_BEHC18\_NEG (F1) #3063, RT=10.357 min, MS2, FTMS (-), (HCD, DDA, 337.31  
REFERENCE(bottom): mzCloud library, Erucic acid, C22 H42 O2, MS2, FTMS, (HCD, 337.3112@(10;30;50)



## Nervonic acid

RAWFILE(top): 22P09130004\_BEHC18\_NEG (F15) #2744, RT=10.719 min, MS2, FTMS (-), (HCD, DDA, 365.3  
REFERENCE(bottom): mzCloud library, Nervonic acid, C24 H46 O2, MS2, FTMS, (HCD, 365.3425@(20;40;60);

