

## Supplementary Information

### In-depth chemical profiling of tire and artificial turf crumb rubber: aging, transformation products, and transport pathways

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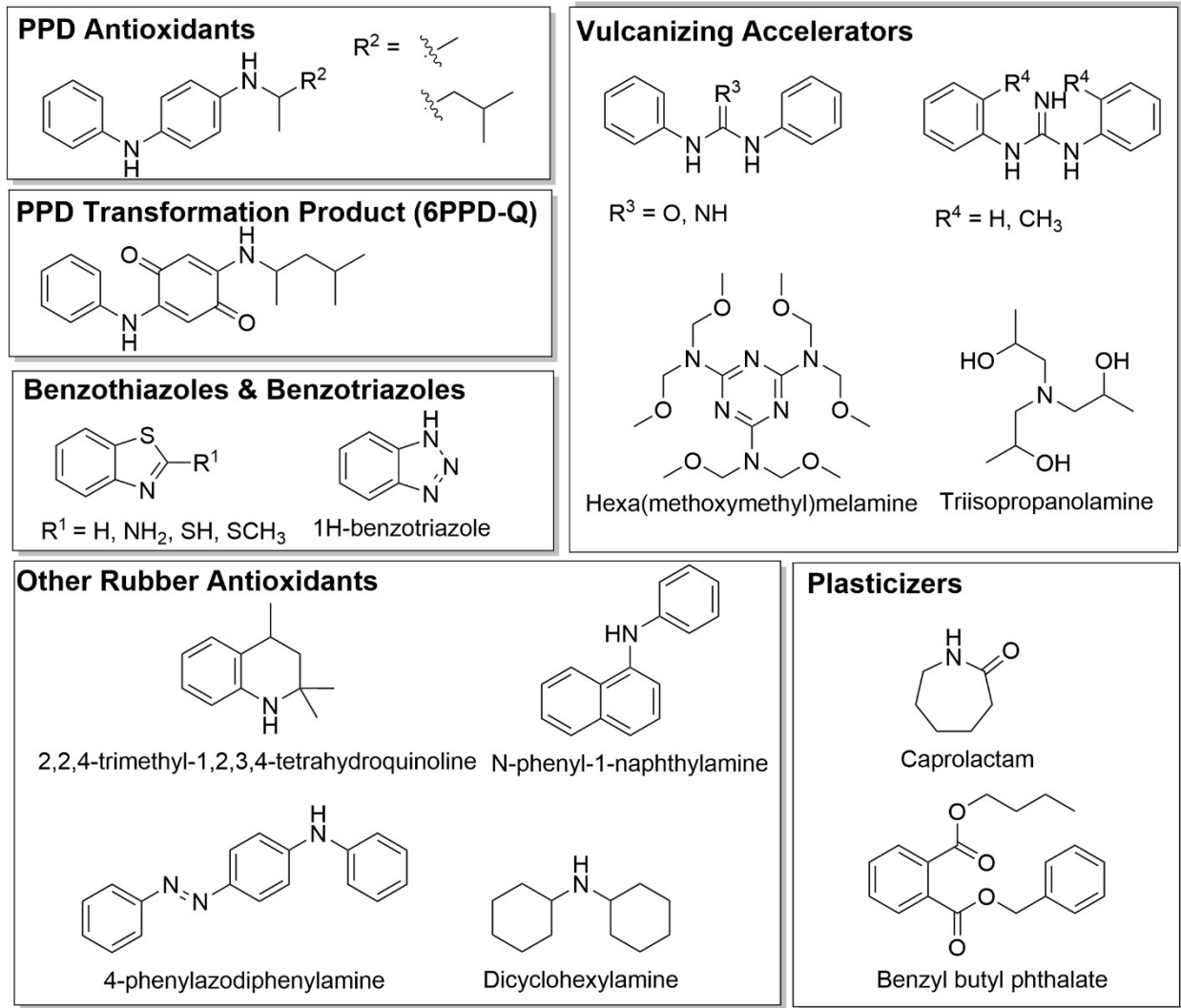
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<sup>b</sup> Barnett Institute for Chemical and Biological Analysis, College of Science, Northeastern University, Boston, MA, USA

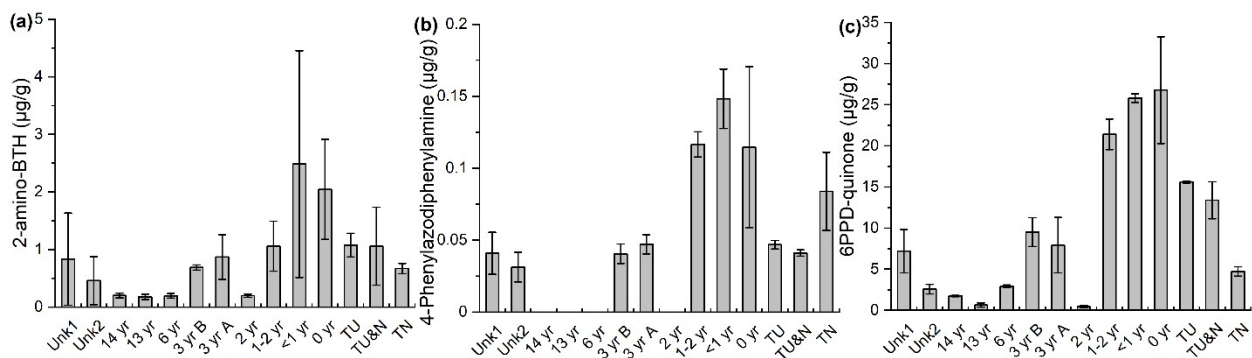
<sup>c</sup> Department of Civil and Environmental Engineering, University of Washington, Seattle, Washington, USA

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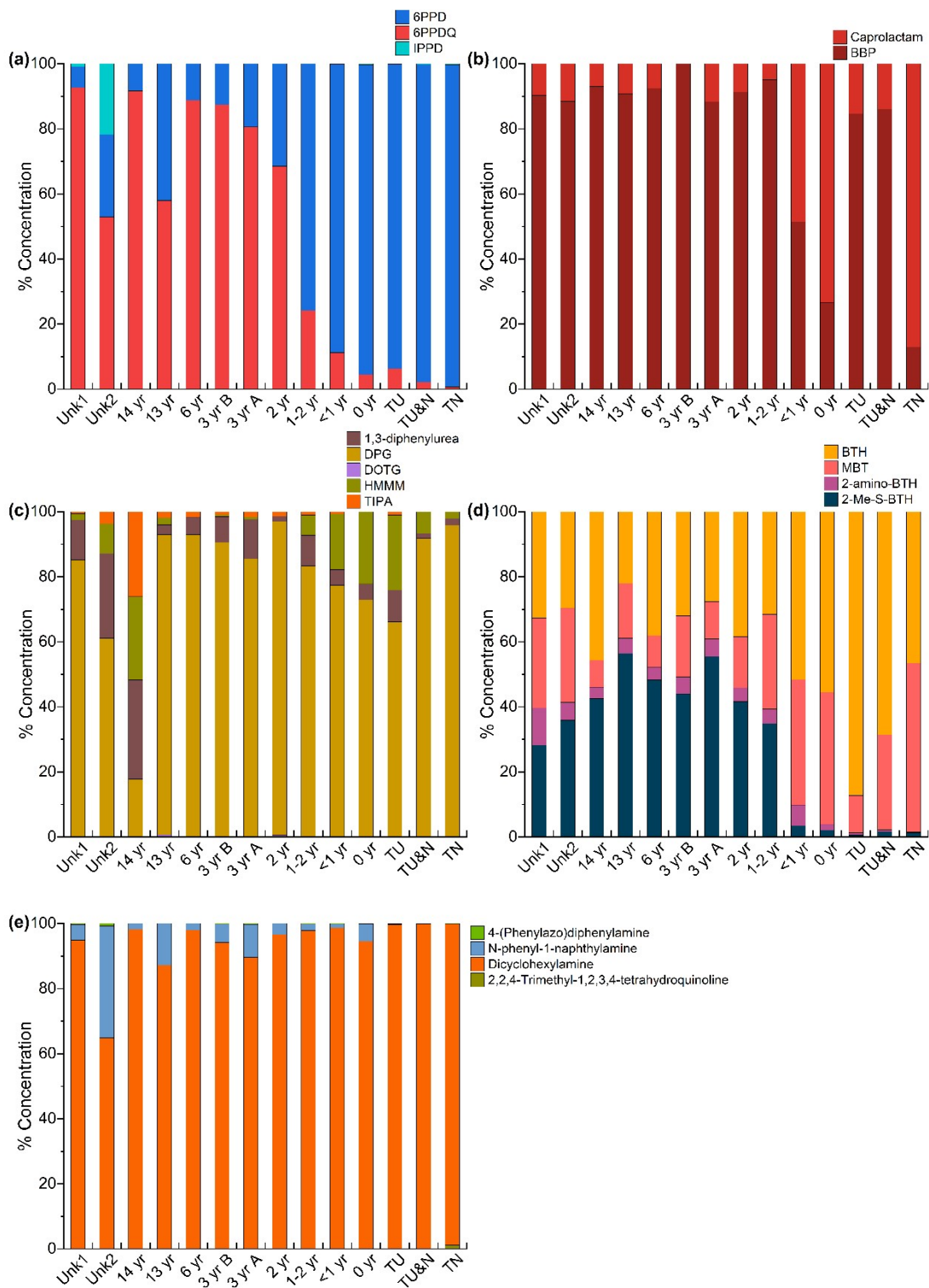
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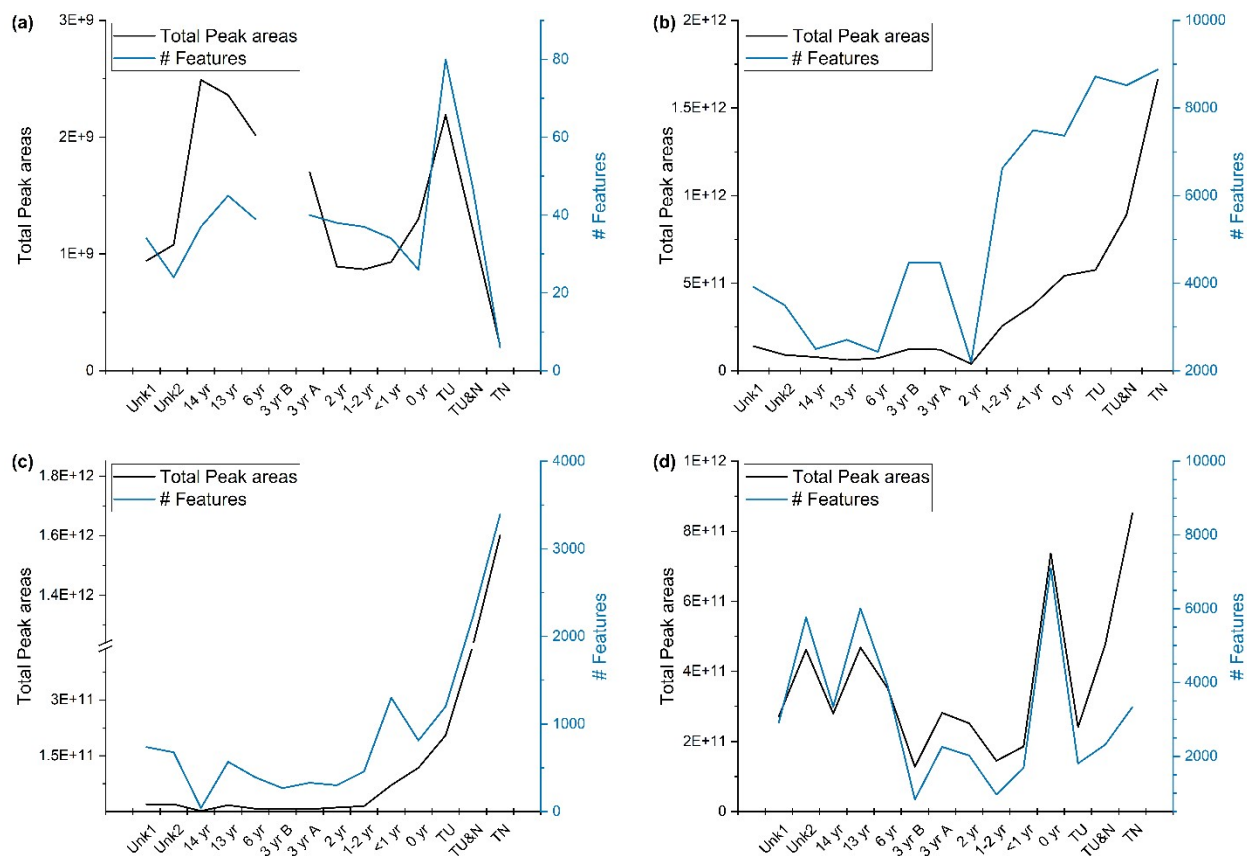
**Figure S1.** Chemical structure of compound classes selected for quantitation



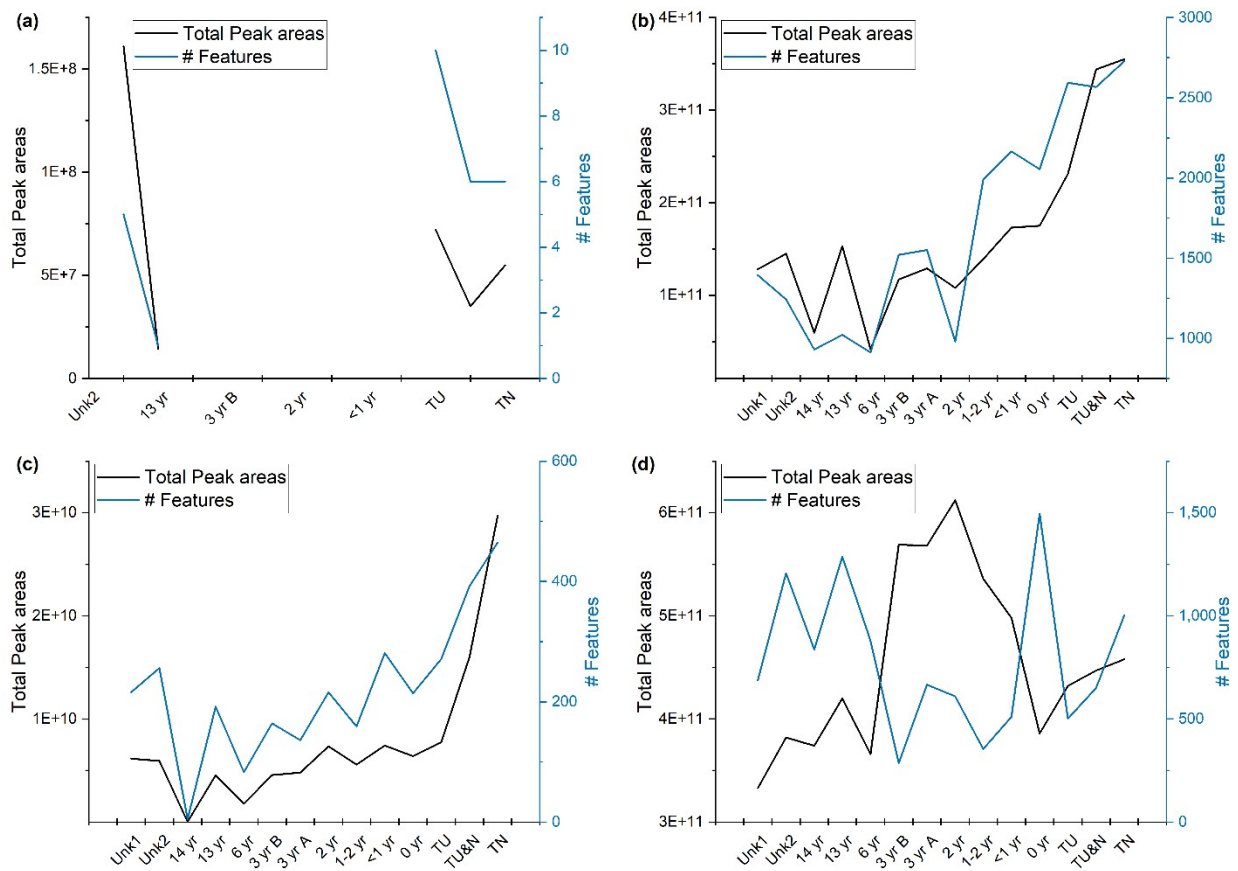
**Figure S2.** Quantitation in crumb rubber extractables of (a) 2-amino-BTH, (b) 4-phenylazodiphenylamine, and (c) 6PPD-quinone.



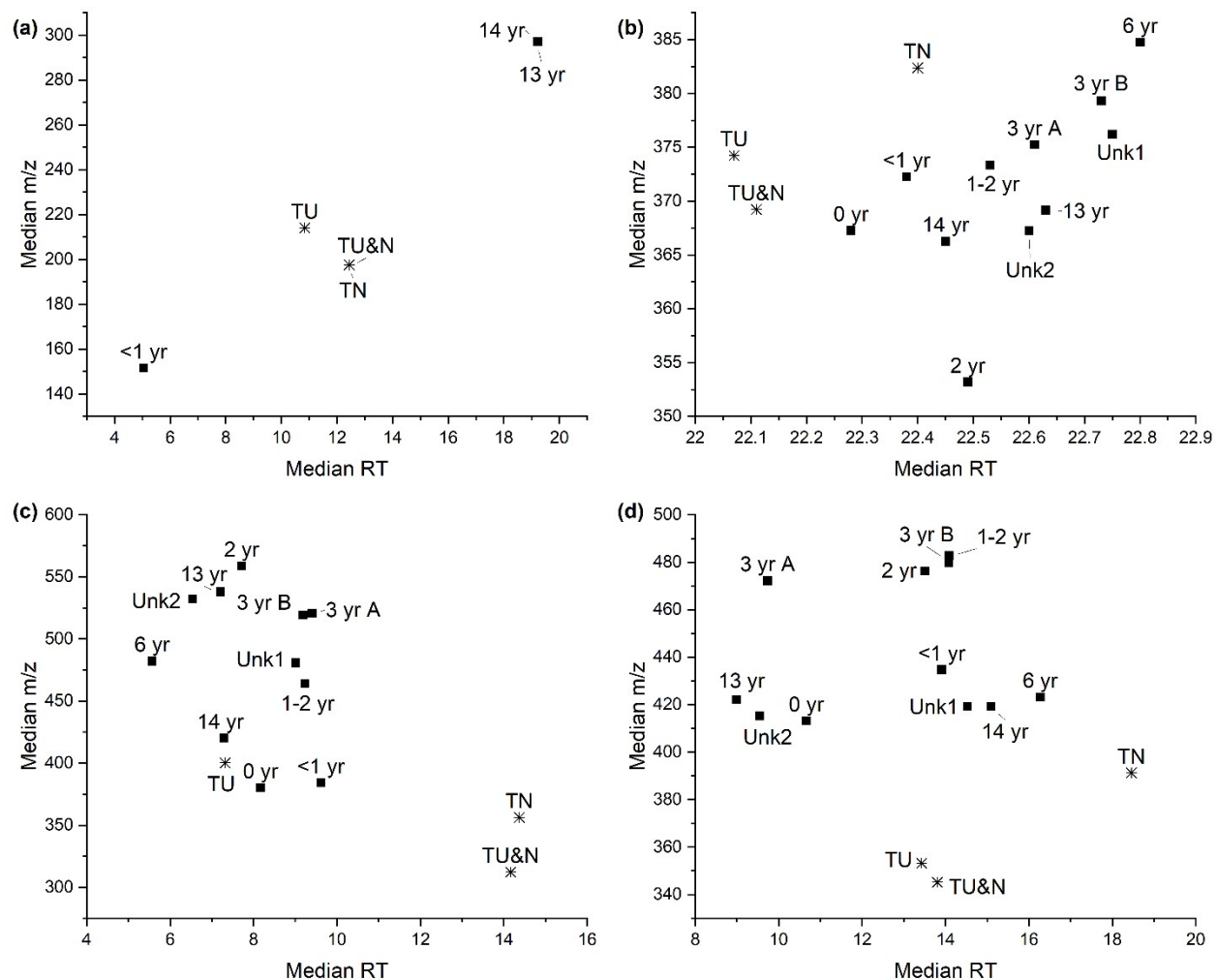
**Figure S3.** Relative concentrations of crumb rubber samples from extractables in (a) PPDs and PPD TPs, (b) plasticizers, (c) vulcanizing accelerators, (d) benzothiazoles and benzotriazoles and (e) other rubber antioxidants.



**Figure S4.** Relationship between total peak area and number of features with crumb rubber age in positive ion mode for (a) leachables, (b) extractables, (c) gastric and (d) gastrointestinal sample preparation methods.



**Figure S5.** Relationship between total peak area and number of features with crumb rubber age in negative ion mode for (a) leachables, (b) extractables, (c) gastric and (d) gastrointestinal sample preparation methods.



**Figure S6.** Relationship between median retention time (RT) and median  $m/z$  with crumb rubber age in negative ion mode for (a) leachables, (b) extractables, (c) gastric and (d) gastrointestinal sample preparation methods.

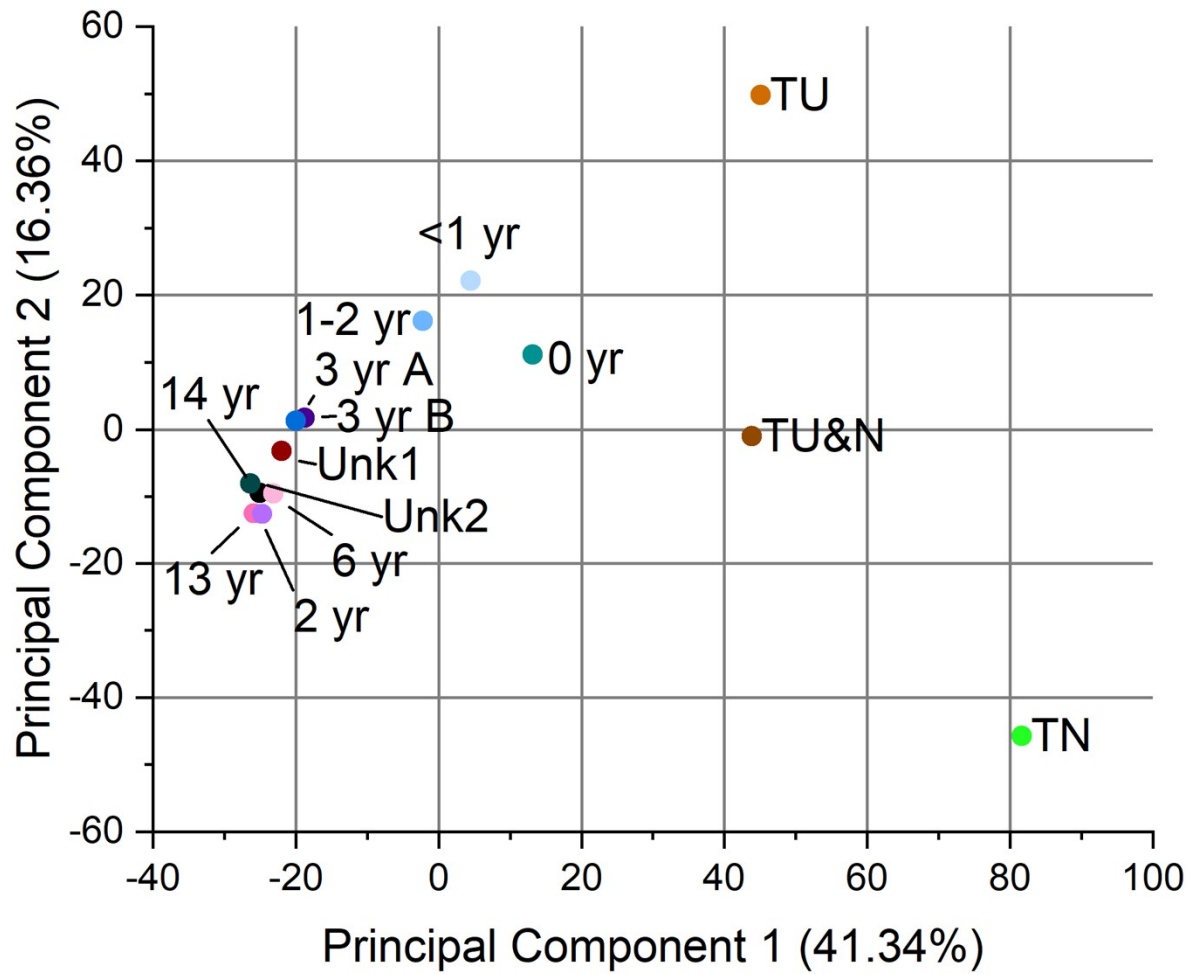
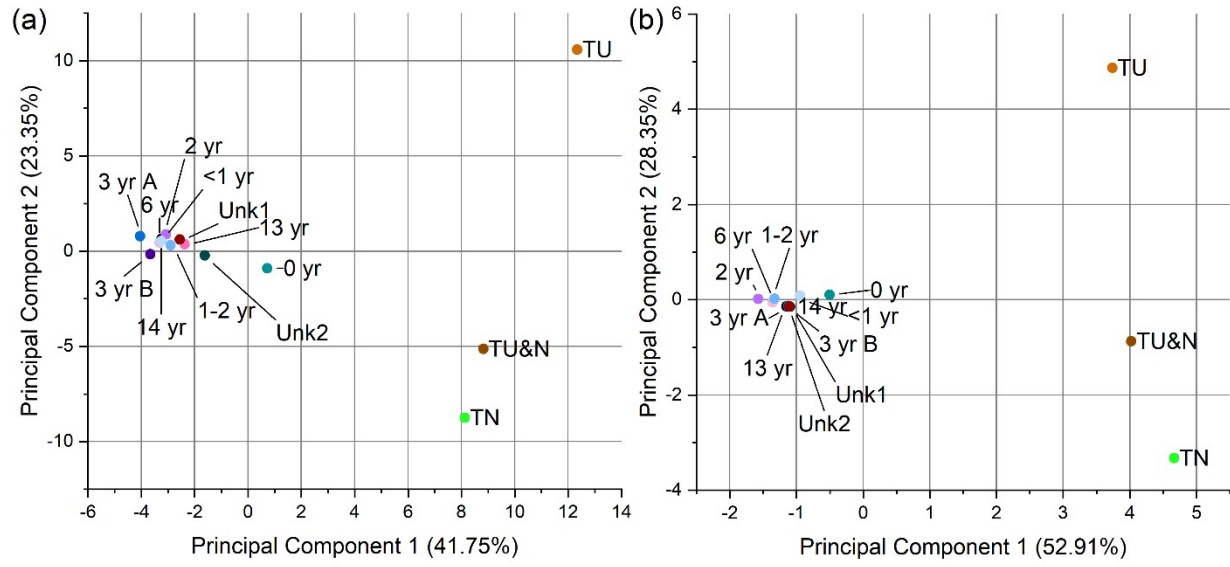


Figure S7. PCA of extractables in negative ion mode.

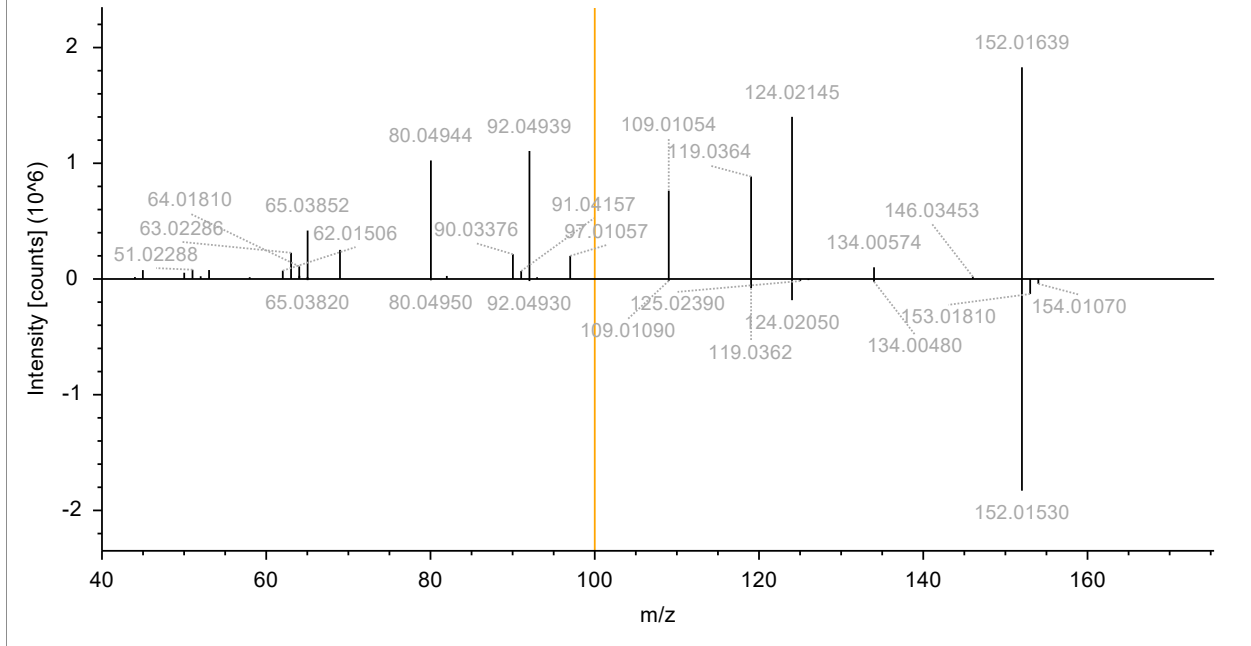


**Figure S8.** PCA of leachables in (a) positive and (b) negative ion mode.



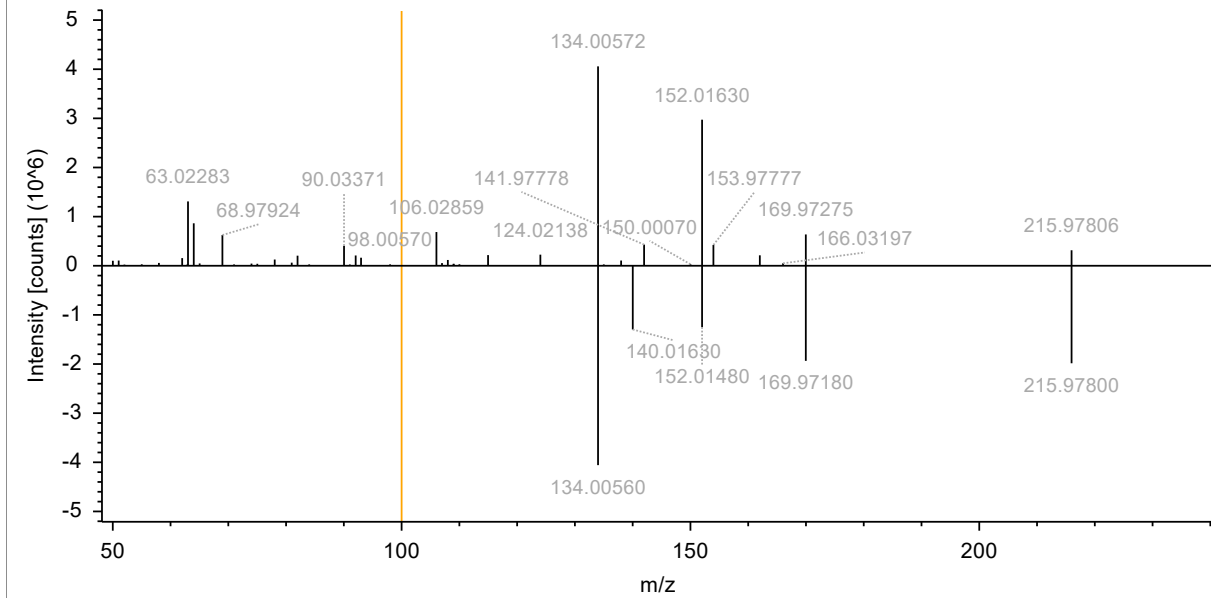
### 2-Hydroxybenzothiazole (Match 93.8)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_3\_20231031035408 (F45) #7247, RT=9.781 min, MS2, FTMS (+), (HCD, DDA, 15+1)



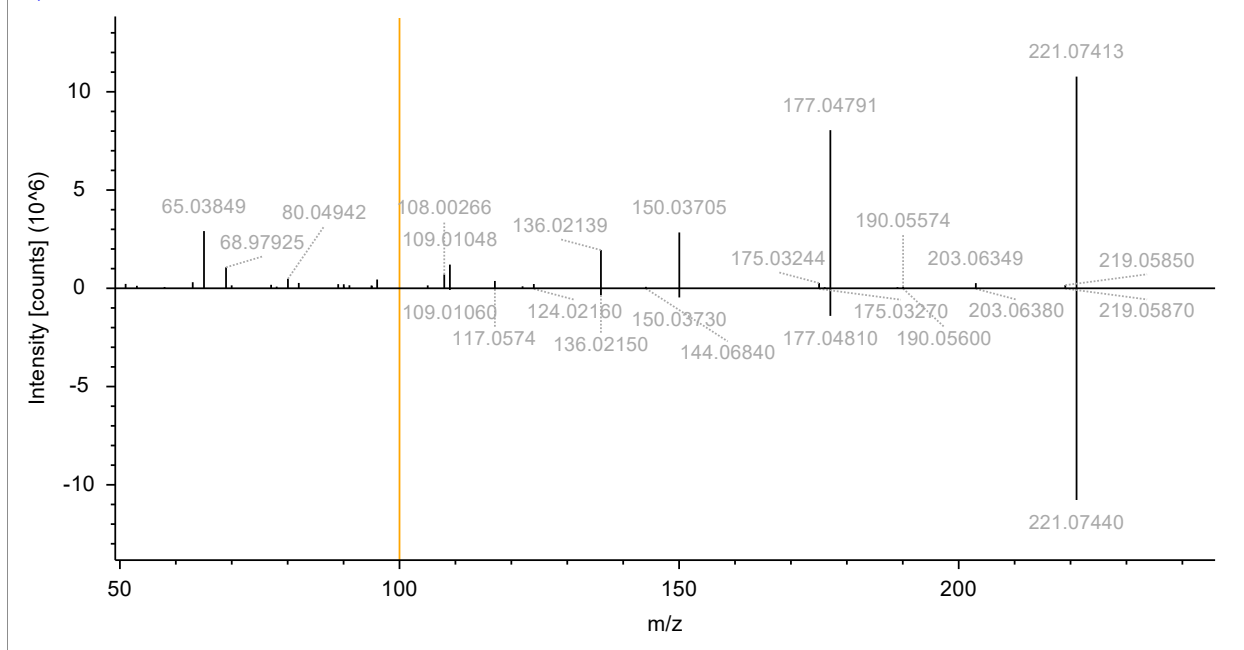
### 2-Benzothiazolesulfonic acid (Match 85.7)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_3\_20231031035408 (F45) #4236, RT=5.736 min, MS2, FTMS (+), (HCD, DDA, 21+1)



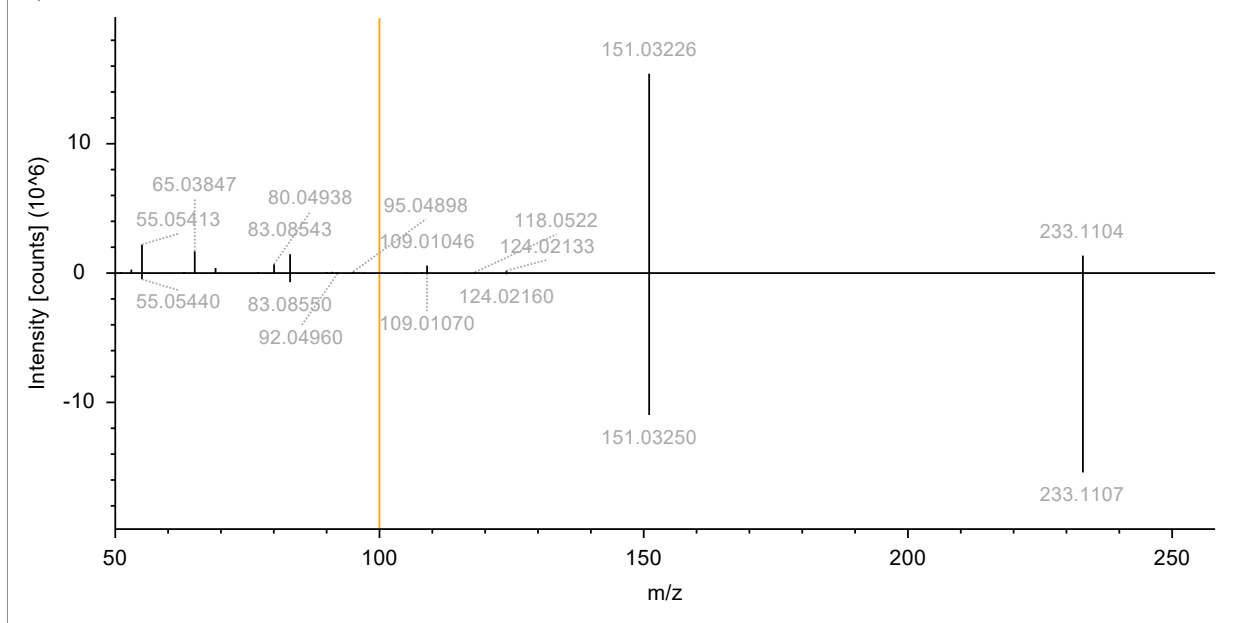
### 2-(4-morpholinyl)benzothiazole (Match 81.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_3\_20231030230527 (F33) #9171, RT=12.365 min, MS2, FTMS (+), (HCD, DDA, +1)



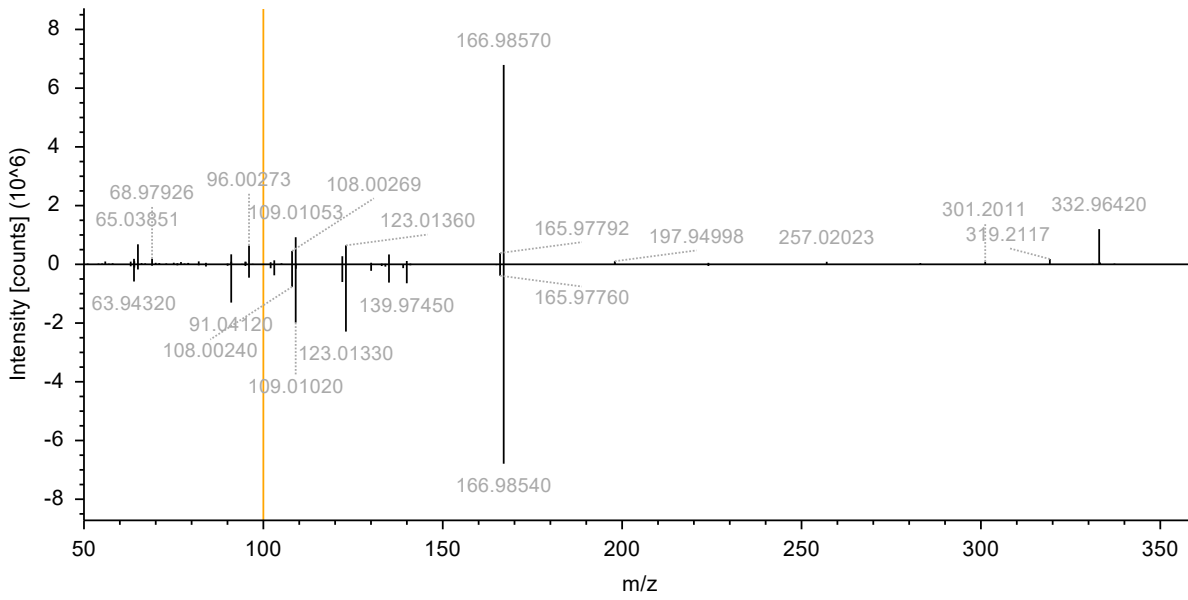
### N-cyclohexyl-2-benzothiazol-amine (Match 88.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_3\_20231031035408 (F45) #9962, RT=13.407 min, MS2, FTMS (+), (HCD, DDA, 2 +1)



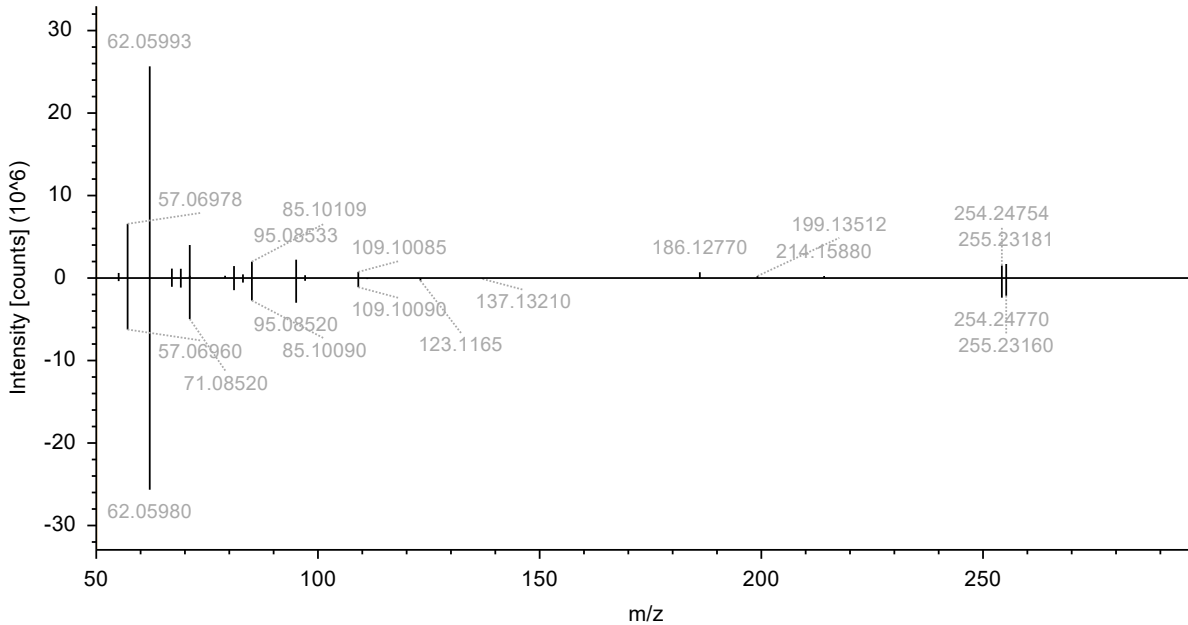
### 2,2-dithiobis(benzothiazole) (Match 88.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #15239, RT=20.417 min, MS2, FTMS (+), (HCD, DDA, +1)



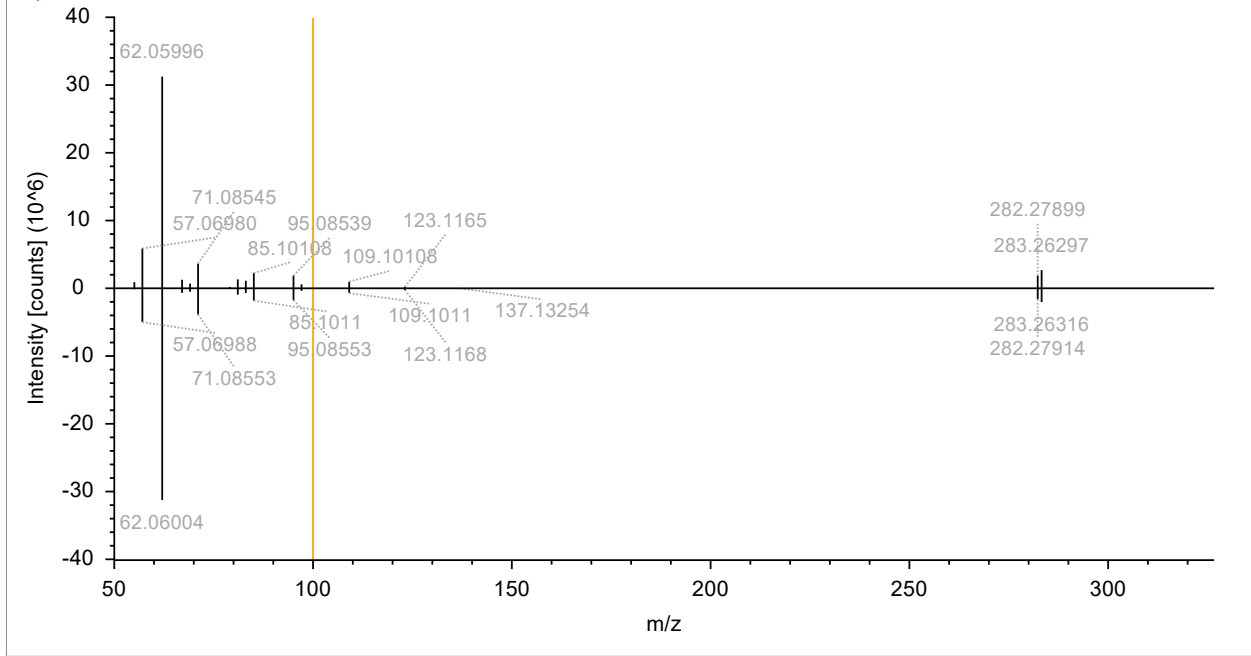
### Myristoyl ethanolamide (95.7)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #15774, RT=21.137 min, MS2, FTMS (+), (HCD, DDA, +1)



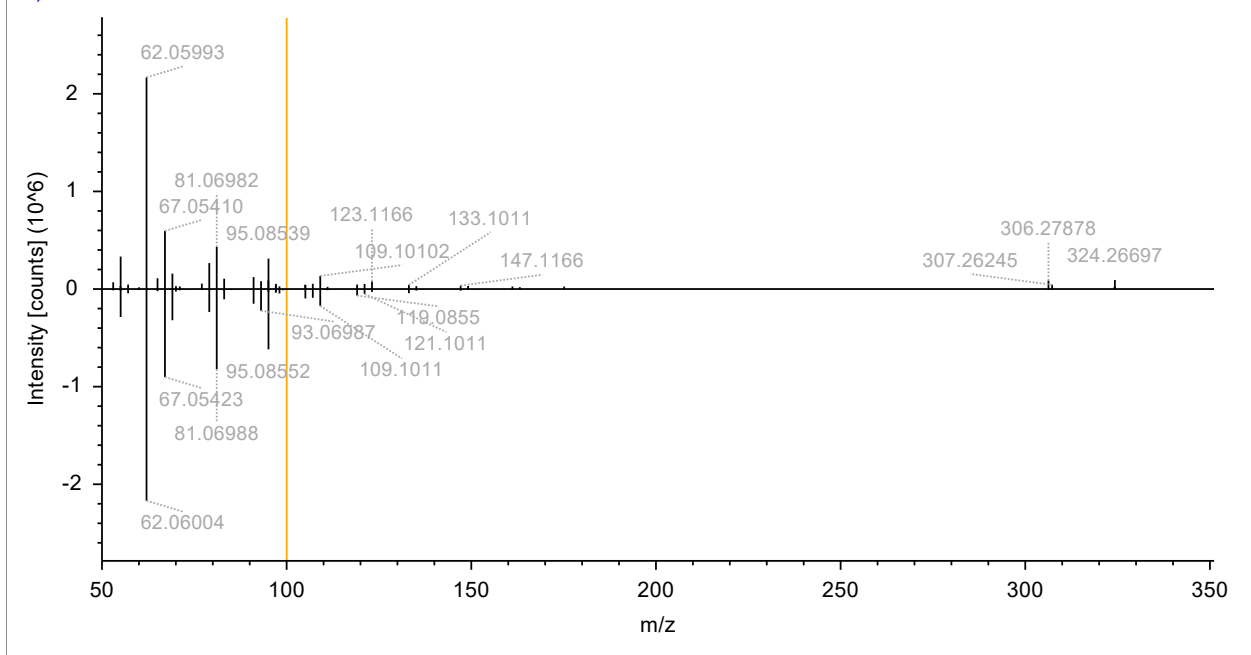
### Palmitoyl ethanolamide (Match 99.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #16966, RT=22.718 min, MS2, FTMS (+), (HCD, DDA, +1)



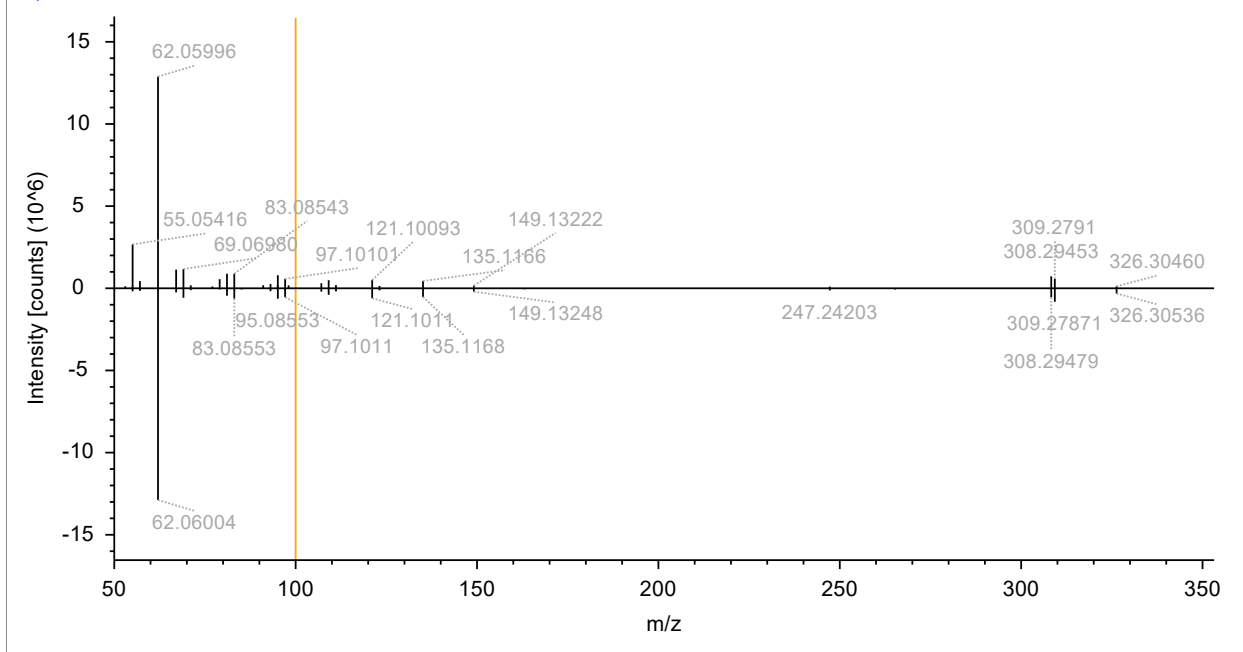
### Linoleyl ethanolamide (Match 87.7)

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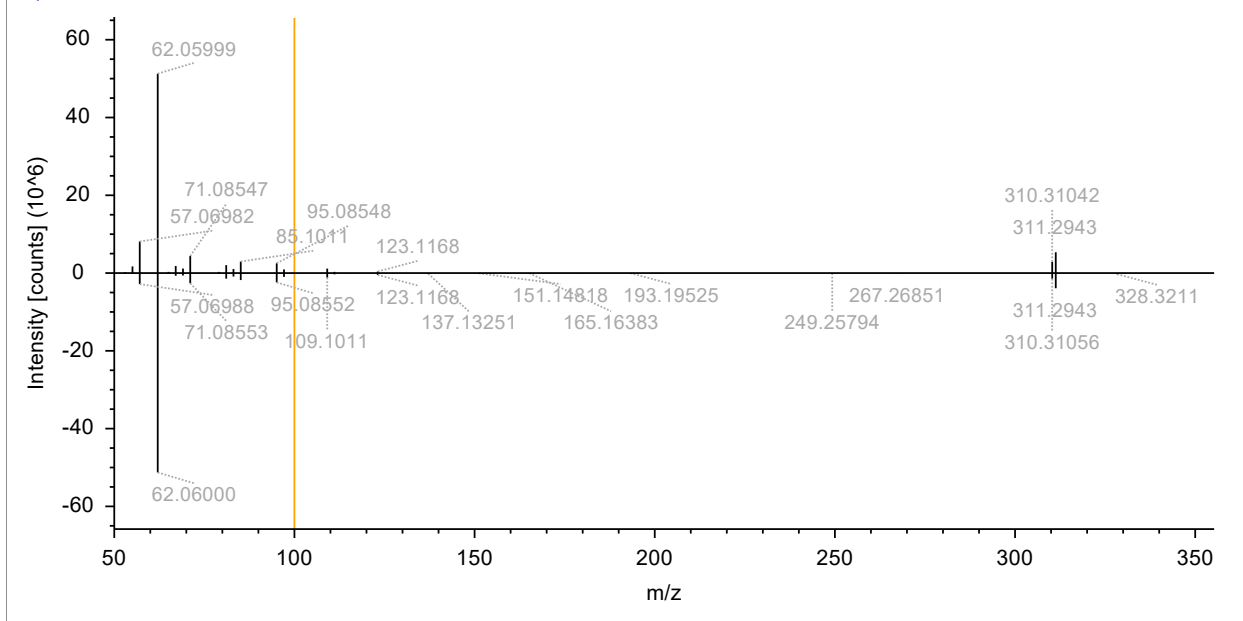
### Oleoyl ethanolamide (Match 91.1)

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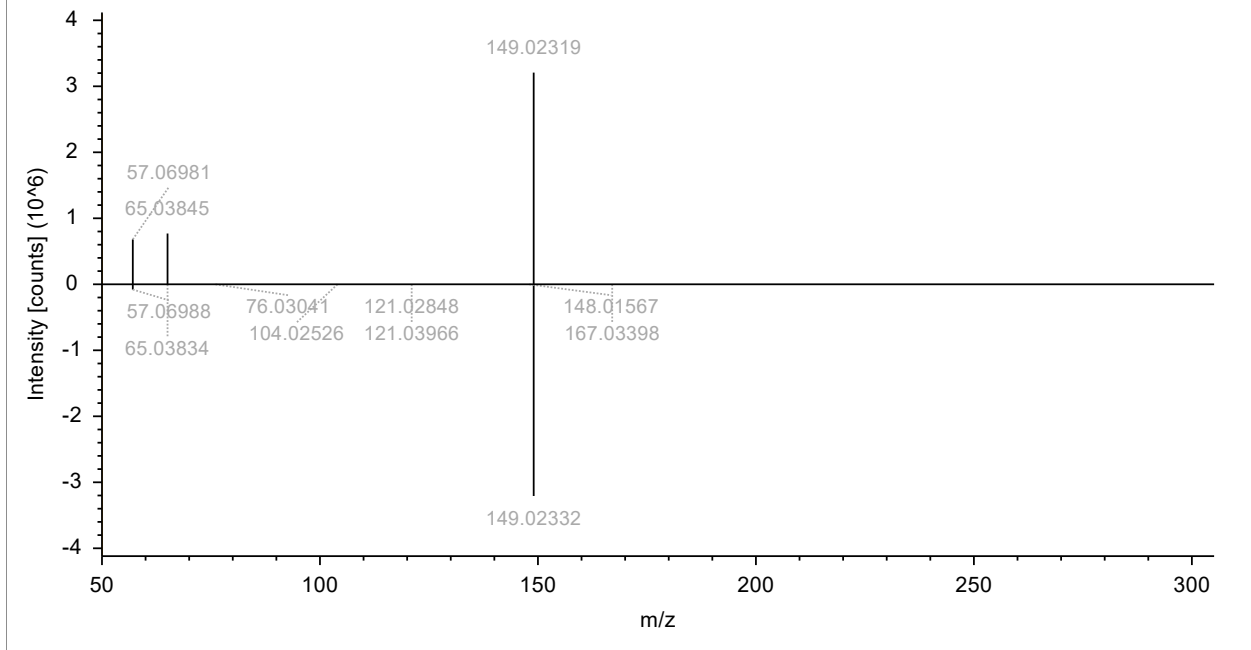
### Stearoyl ethanolamide (Match 93.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #17926, RT=23.983 min, MS2, FTMS (+), (HCD, DDA, +1)



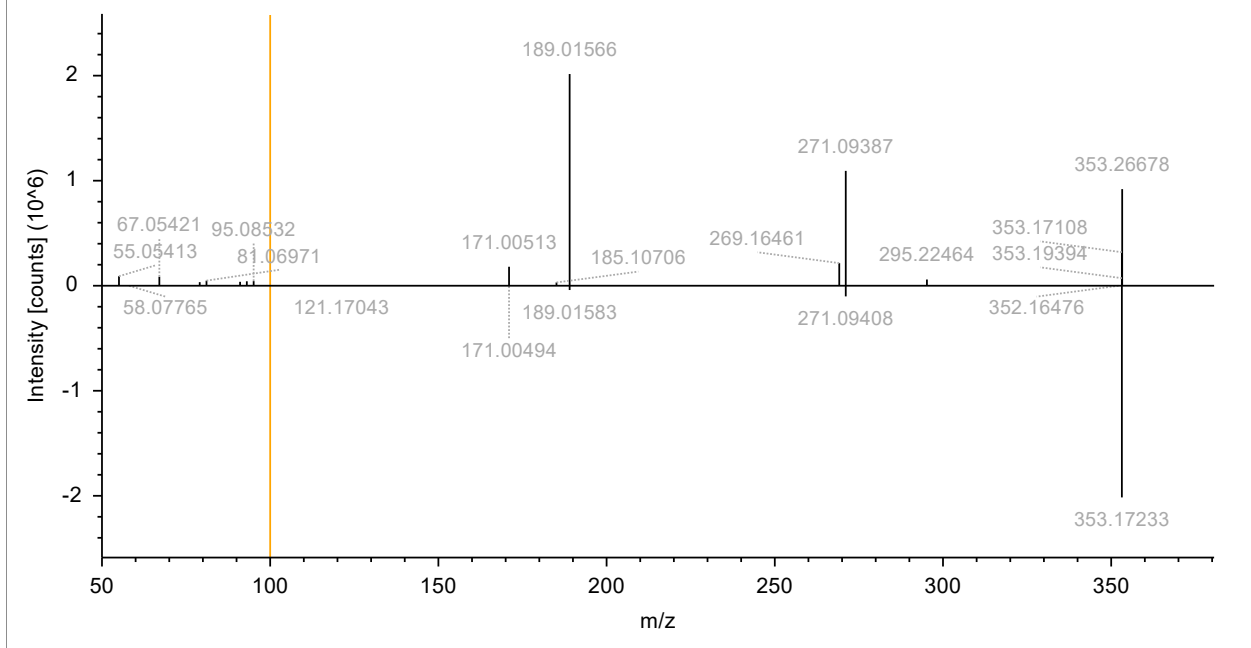
### Dibutyl phthalate (Match 93.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_3\_20231031021754 (F42) #14204, RT=19.076 min, MS2, FTMS (+), (HCD, DDA, +1)



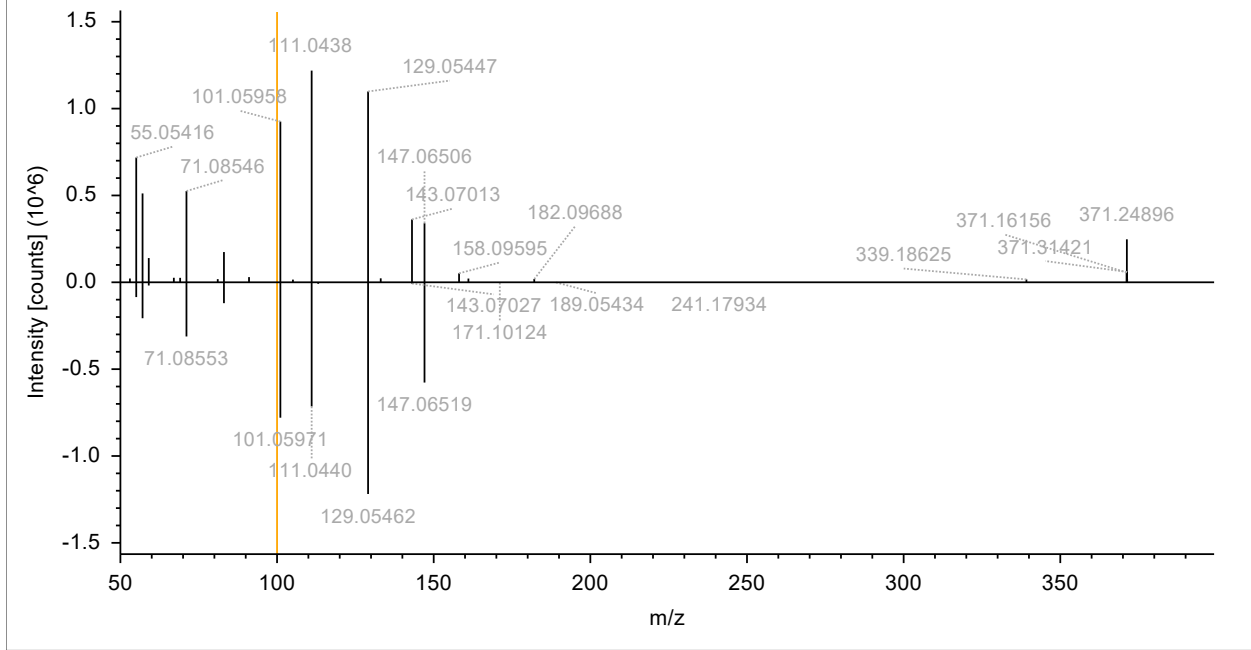
### Dicyclohexyl phthalate (Match 86.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C8\_2\_20231030174441 (F23) #15936, RT=21.404 min, MS2, FTMS (+), (HCD, DDA, +1)



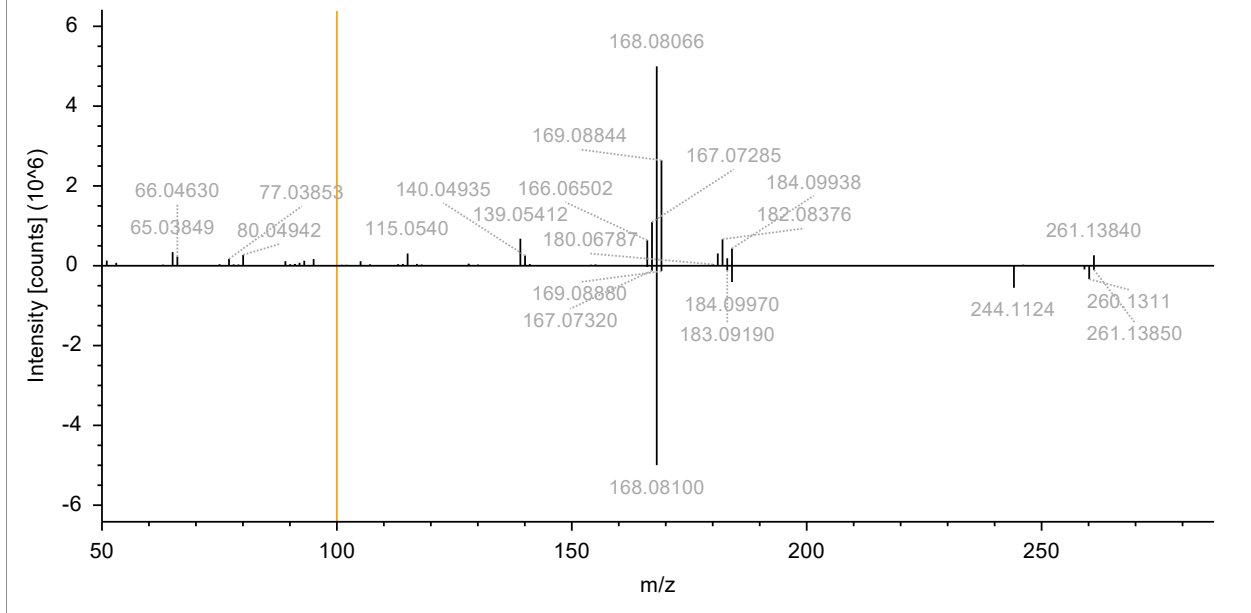
### Bis(2-ethylhexyl)adipate (Match 95.4)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_3\_20231031035408 (F45) #18510, RT=24.754 min, MS2, FTMS (+), (HCD, DDA, +1)



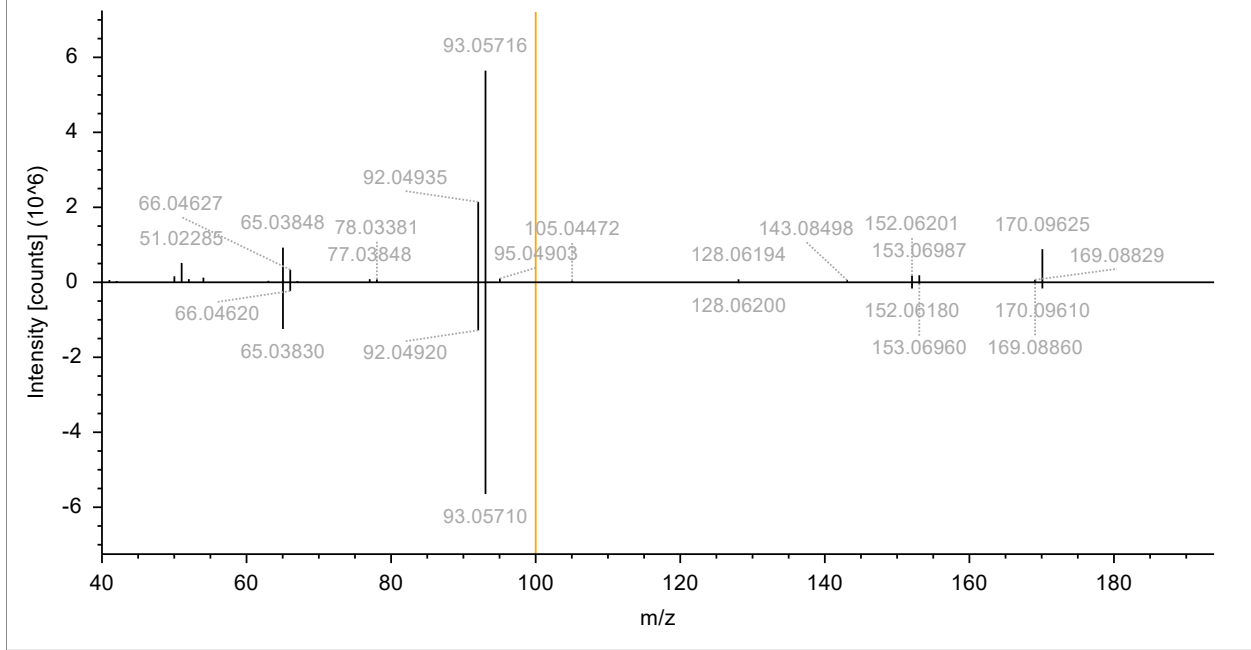
### Diphenyl-p-phenylenediamine (Match 79.1)

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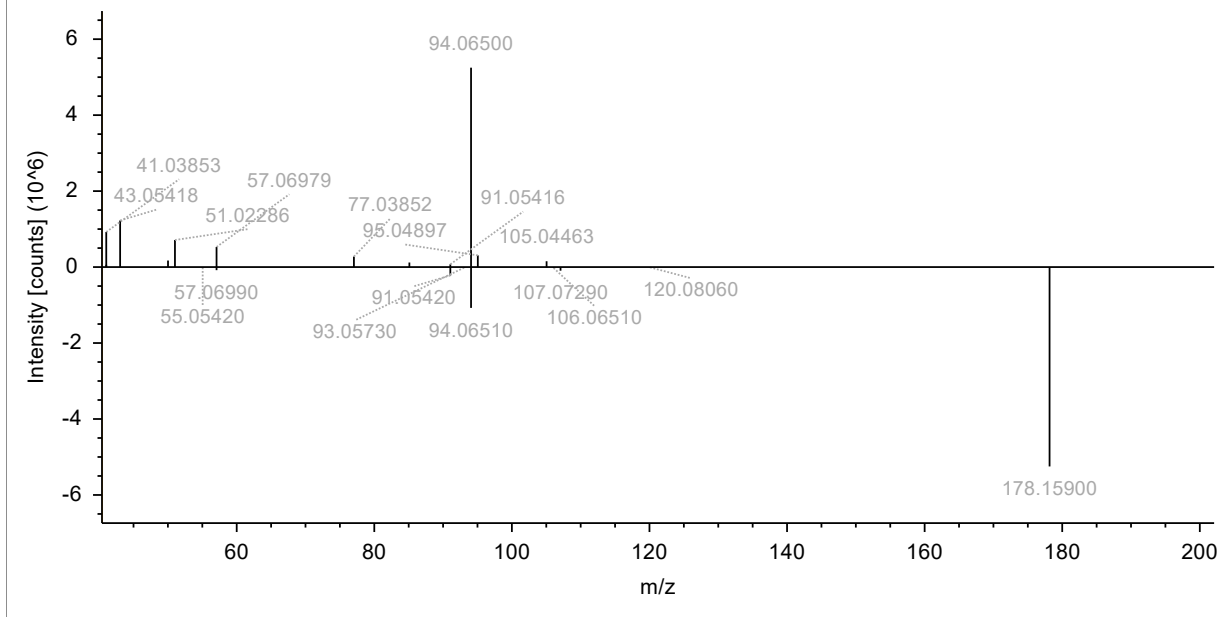
### Diphenylamine (Match 94.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #11619, RT=15.624 min, MS2, FTMS (+), (HCD, DDA, +1)



### 4-hexylaniline (Match 92.0)

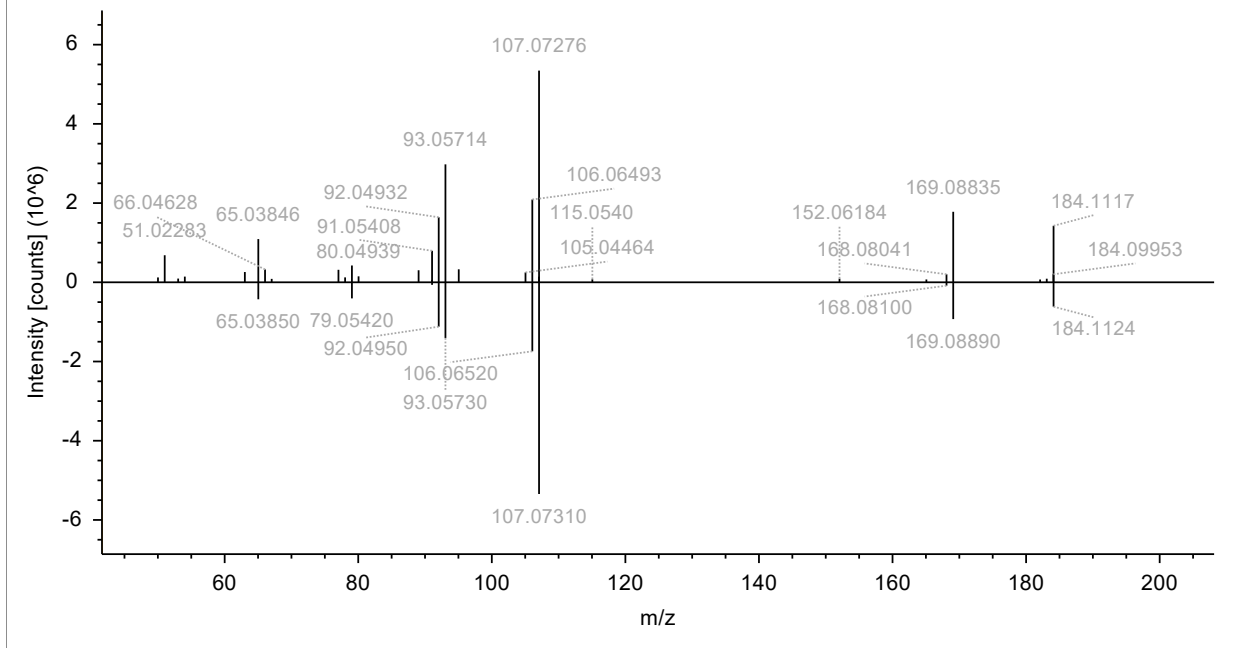
RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #7899, RT=10.653 min, MS2, FTMS (+), (HCD, DDA, 1 +1)





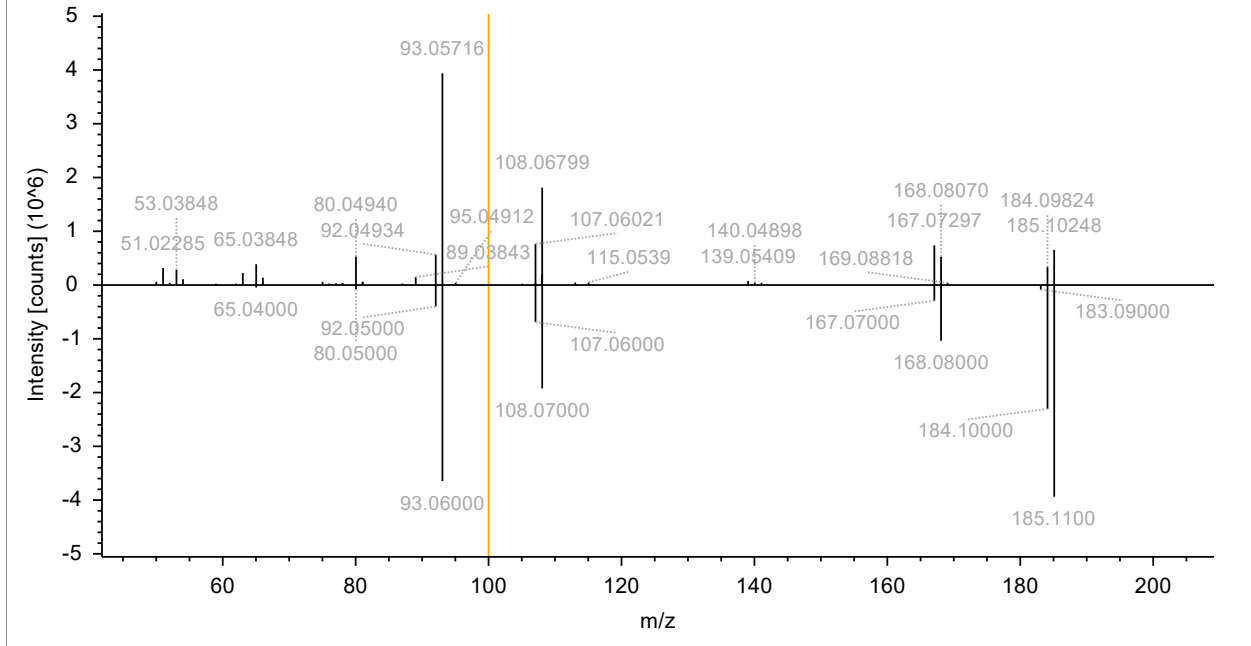
### Phenyl-p-tolyl-amine (Match 94.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #12747, RT=17.123 min, MS2, FTMS (+), (HCD, DDA, +1)



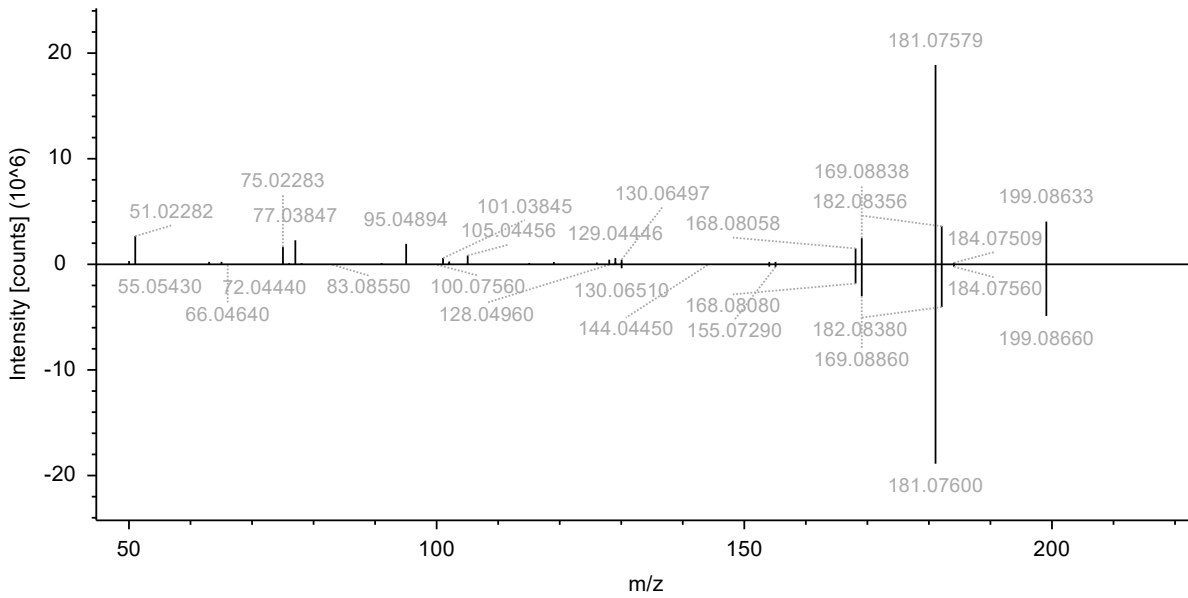
### 4-aminodiphenylamine (Match 91.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #13419, RT=18.014 min, MS2, FTMS (+), (HCD, DDA, +1)



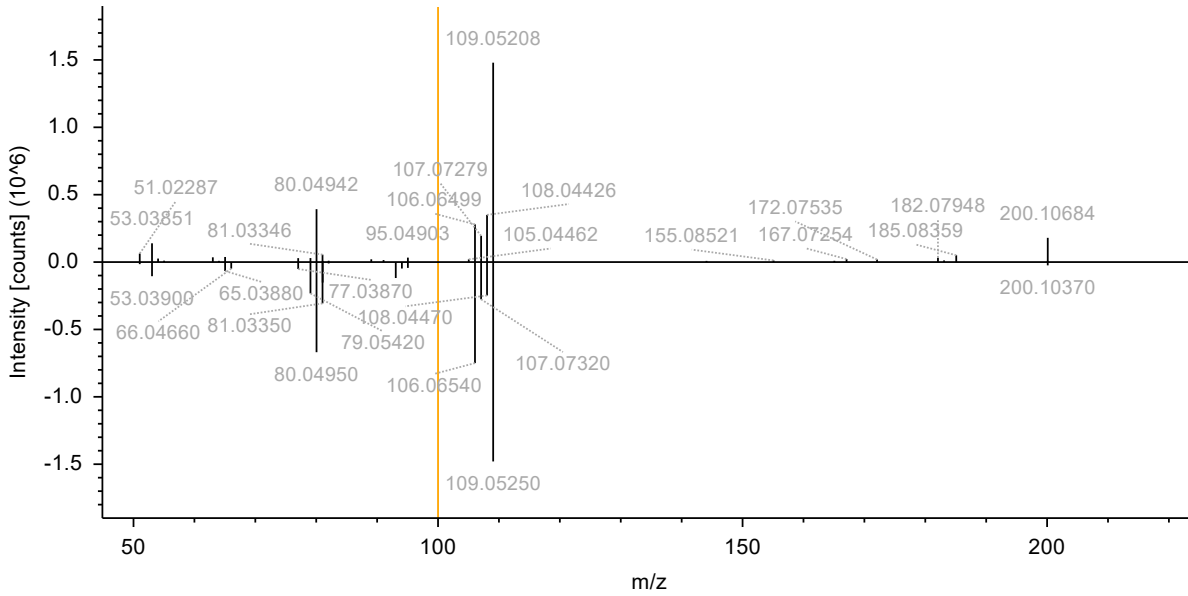
### 4-nitrosodiphenylamine (Match 90.4)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_1\_20231031011345 (F40) #9829, RT=13.251 min, MS2, FTMS (+), (HCD, DDA, 1+1)



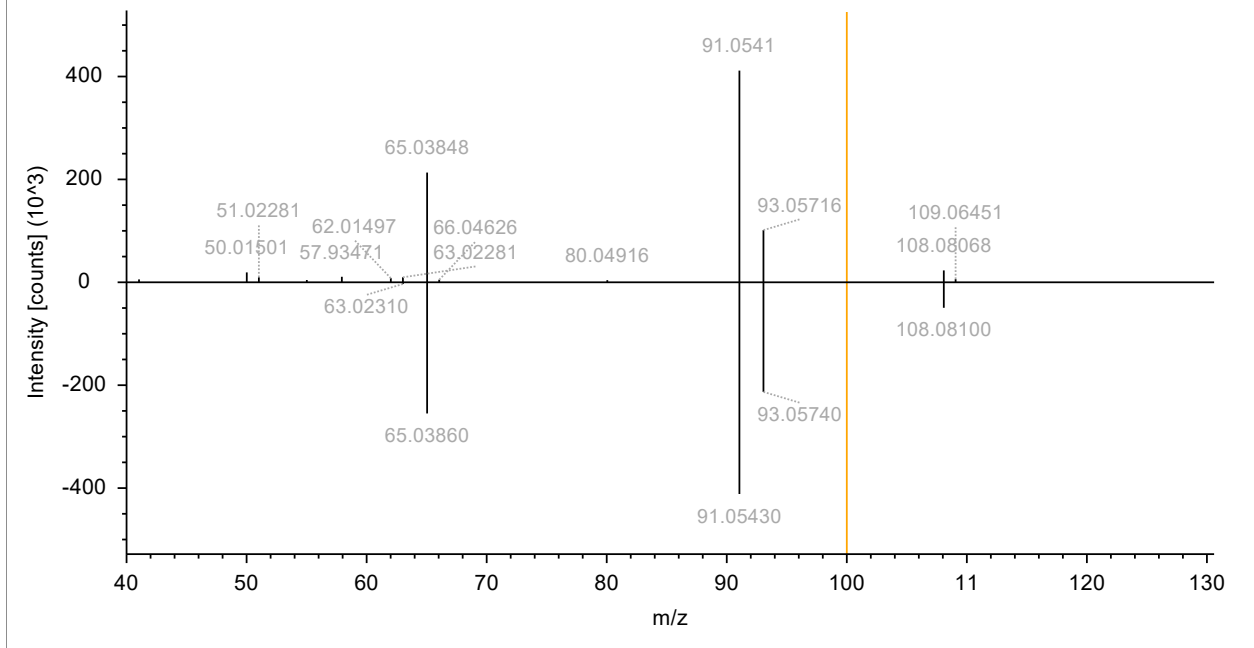
### 4-(4-methylanilino)phenol (Match 89.4)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #9930, RT=13.399 min, MS2, FTMS (+), (HCD, DDA, 1+1)



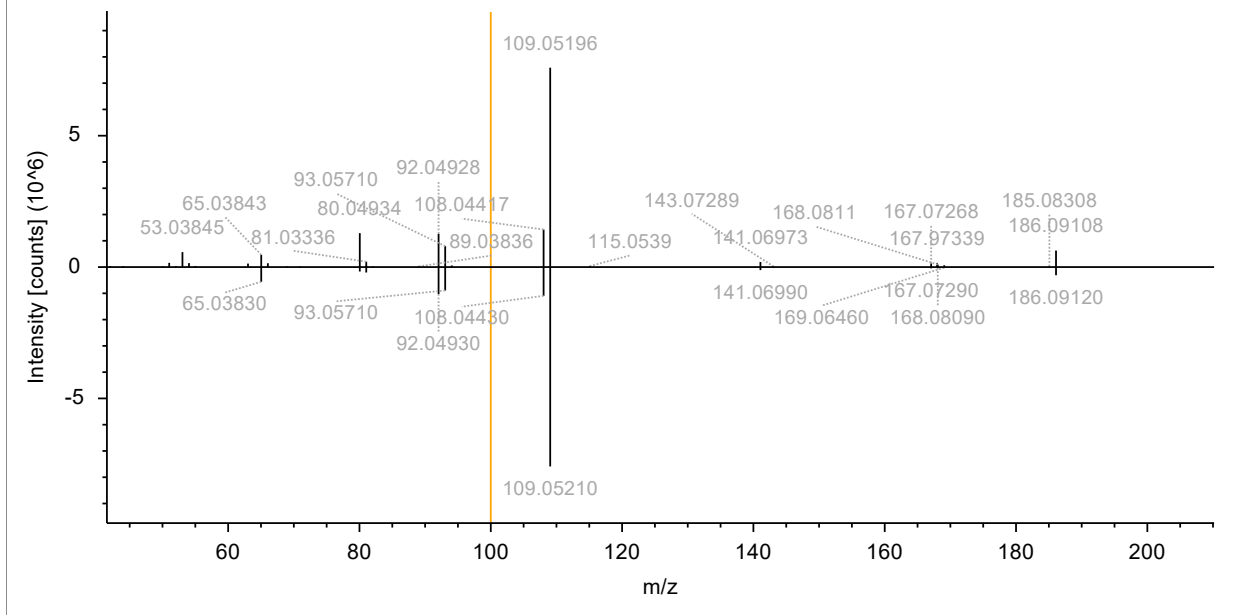
### 3-methylaniline (Match 97.7)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_2\_20231031032203 (F44) #1493, RT=2.049 min, MS2, FTMS (+), (HCD, DDA, 10+1)



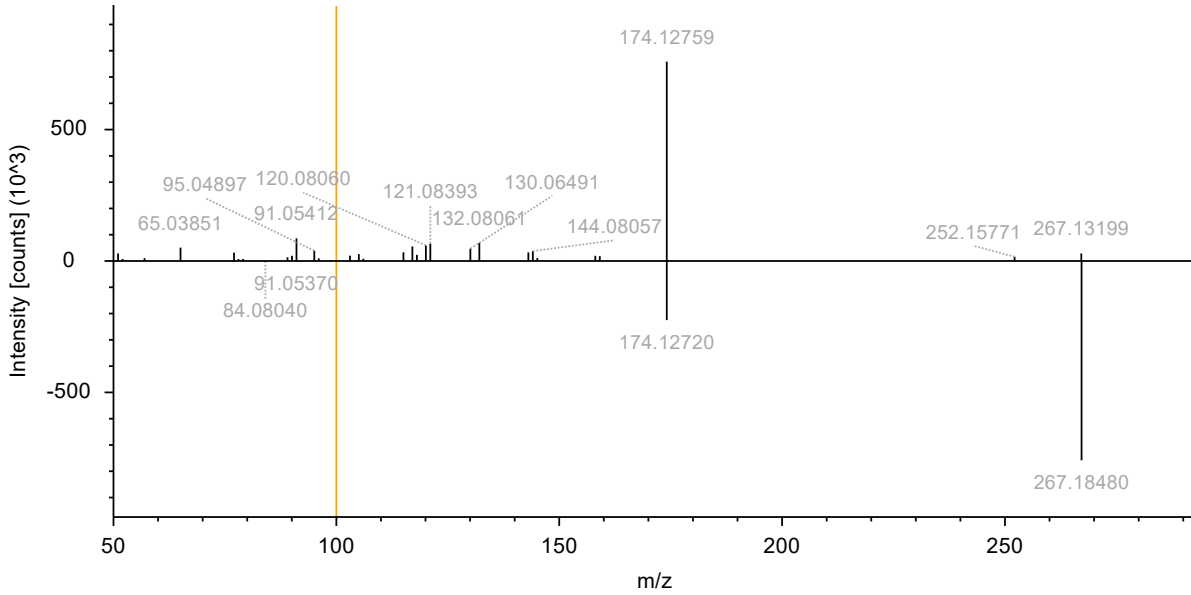
### 4-anilinophenol (Match 93.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #8596, RT=11.620 min, MS2, FTMS (+), (HCD, DDA, 10+1)



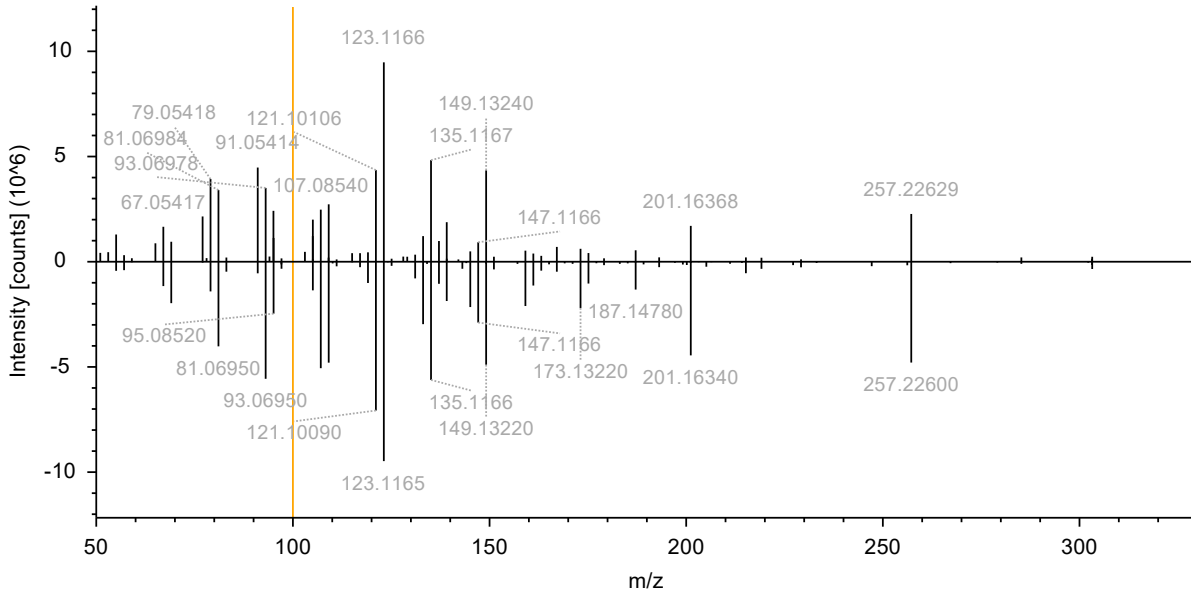
1-Benzyl-N-phenyl-4-piperidinamine (Match 87.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #6767, RT=9.147 min, MS2, FTMS (+), (HCD, DDA, 2f +1)



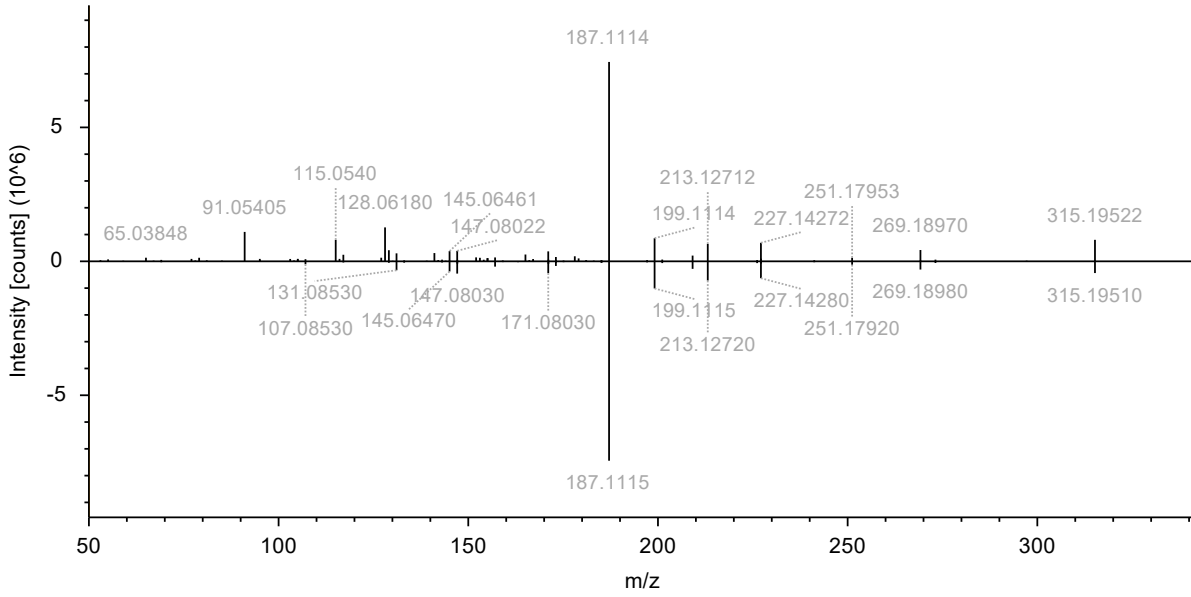
(-)-abietic acid (Match 87.6)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C8\_3\_20231030181646 (F24) #17278, RT=23.163 min, MS2, FTMS (+), (HCD, DDA, +1)



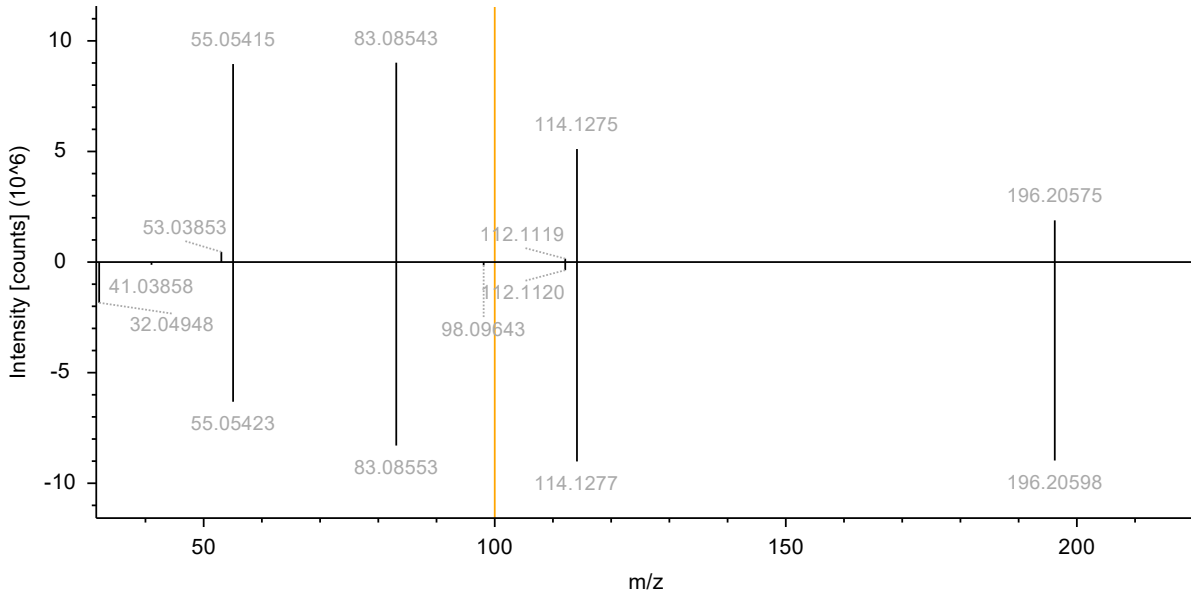
7-oxoabieta-8,11,13-trien-18-oic acid (Match 85.2)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C9\_3\_20231030195259 (F27) #14456, RT=19.467 min, MS2, FTMS (+), (HCD, DDA, +1)



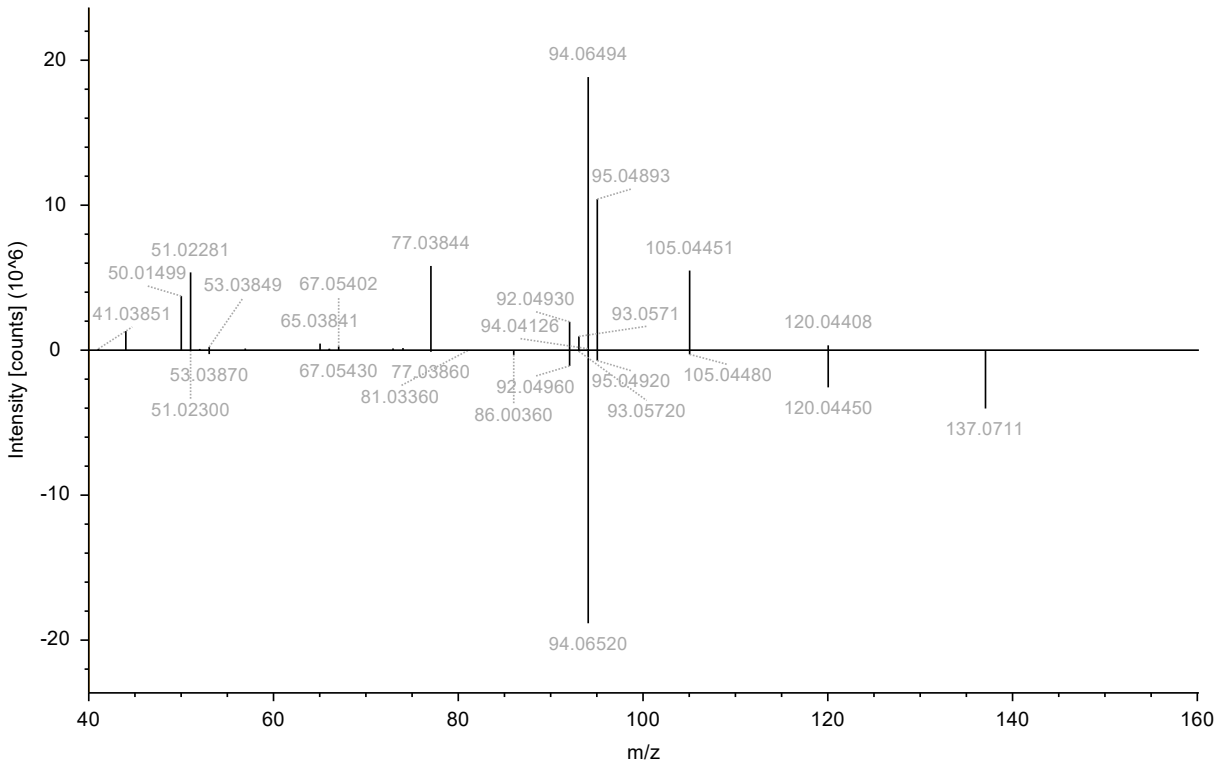
N-cyclohexyl-N-methylcyclohexanamine (Match 89.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #5745, RT=7.777 min, MS2, FTMS (+), (HCD, DDA, +1)



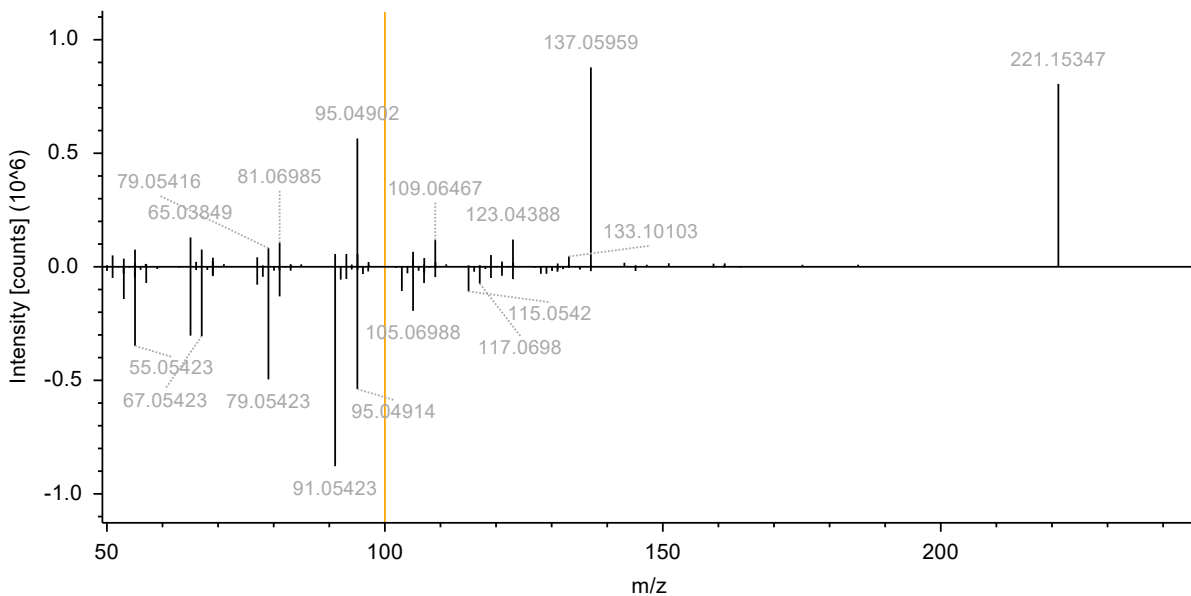
### 1-phenylurea (Match 80.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #3484, RT=4.730 min, MS2, FTMS (+), (HCD, DDA, 137.0706@+1)



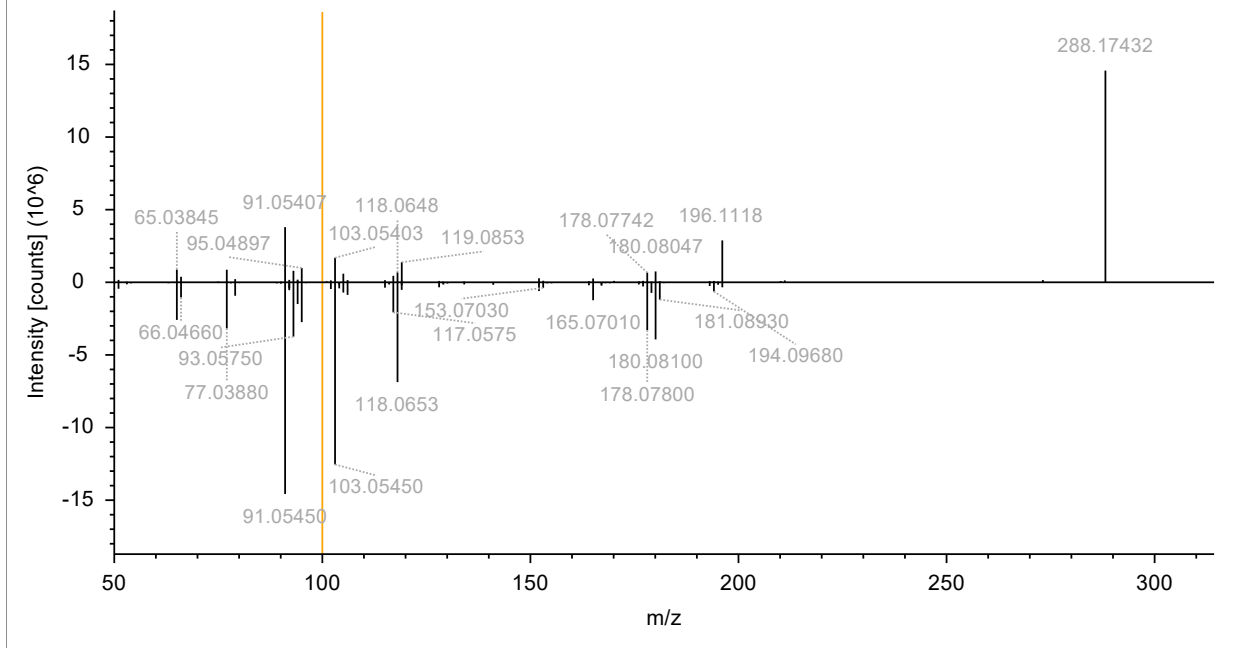
### 2,6-di-tert-butyl-1,4-benzoquinone (Match 77.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_3\_20231031035408 (F45) #14815, RT=19.863 min, MS2, FTMS (+), (HCD, DDA, +1)



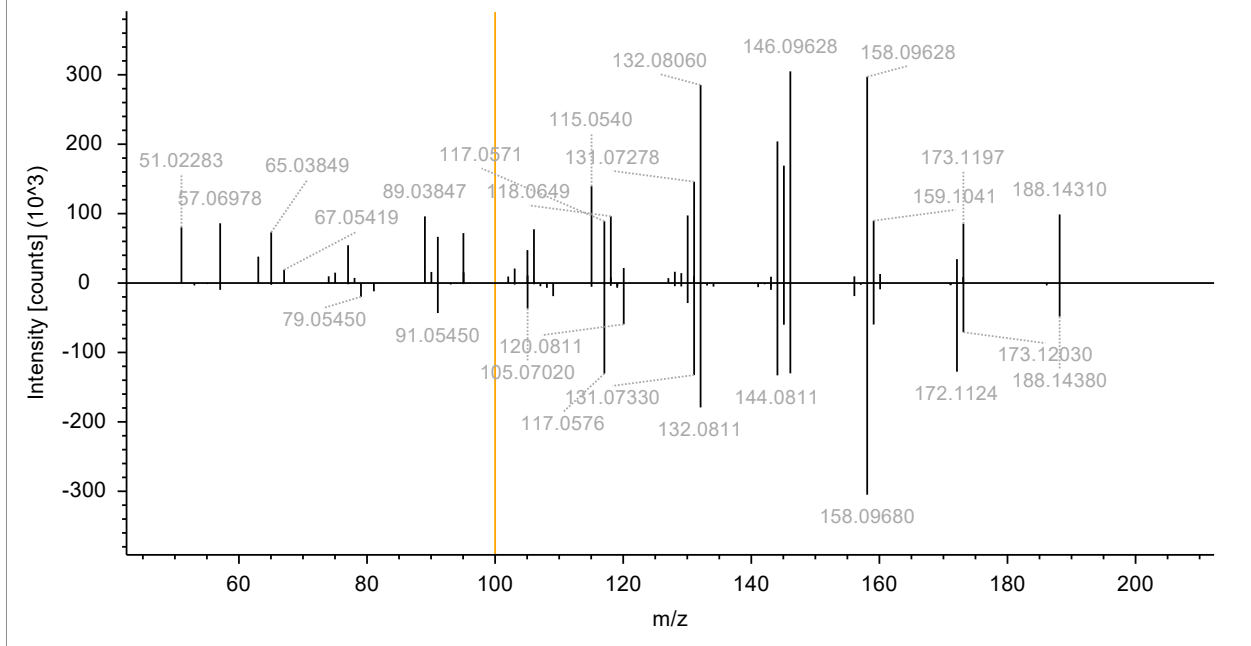
N-Phenyl-4-(2-phenyl-2-propanyl)aniline (Match 87.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C10\_1\_20231030202504 (F28) #15933, RT=21.403 min, MS2, FTMS (+), (HCD, DD/ +1)



1,2-dihydro-2,2,4,7-tetramethylquinoline (Match 84.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #9822, RT=13.223 min, MS2, FTMS (+), (HCD, DDA, 1 +1)

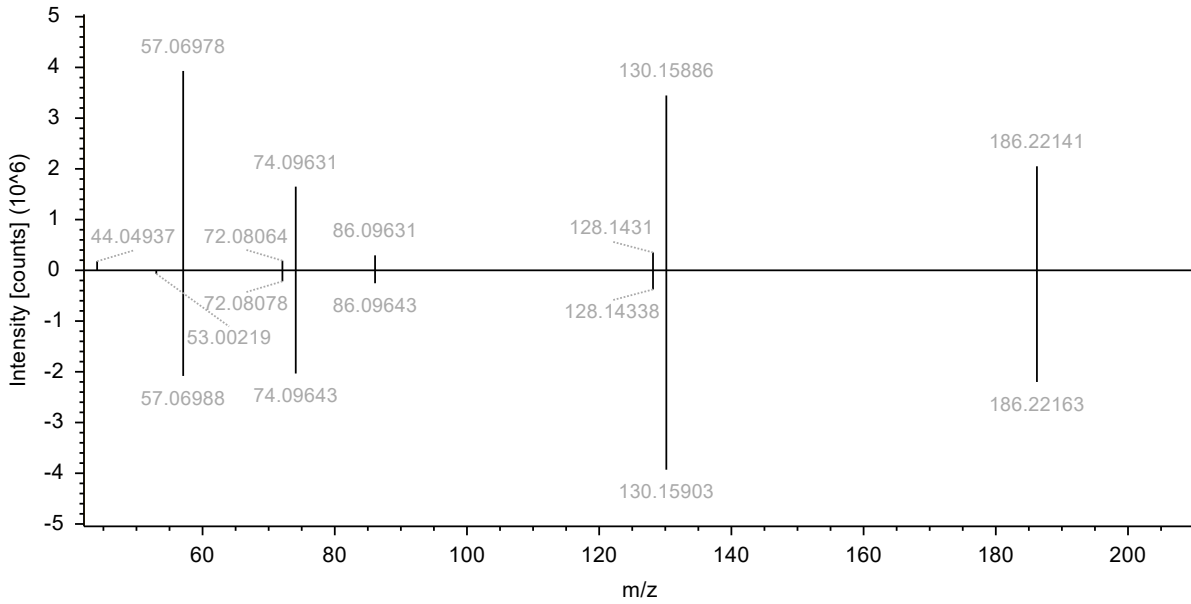






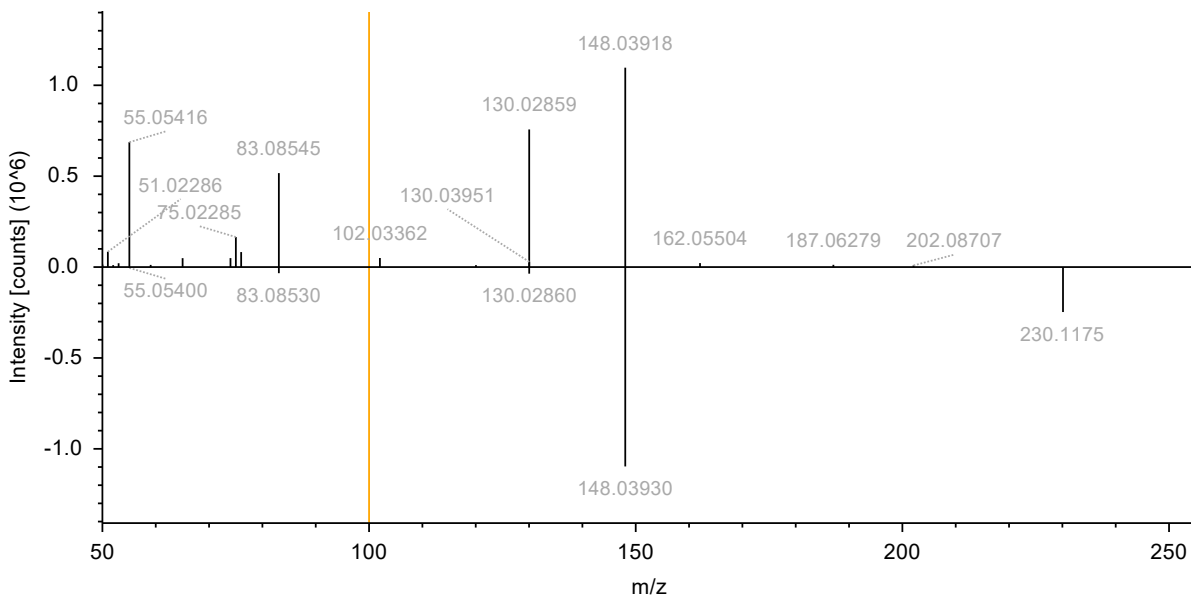
### Tributylamine (Match 97.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #6276, RT=8.479 min, MS2, FTMS (+), (HCD, DDA, 18+1)



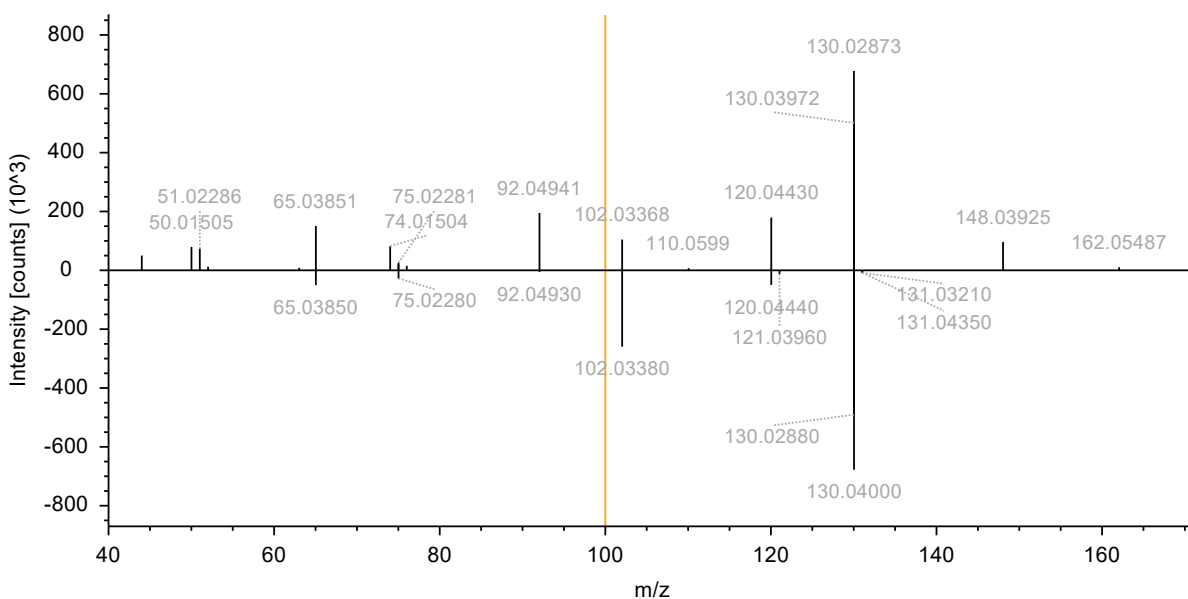
### N-cyclohexylphthalimide (Match 94.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #7306, RT=9.861 min, MS2, FTMS (+), (HCD, DDA, 23+1)



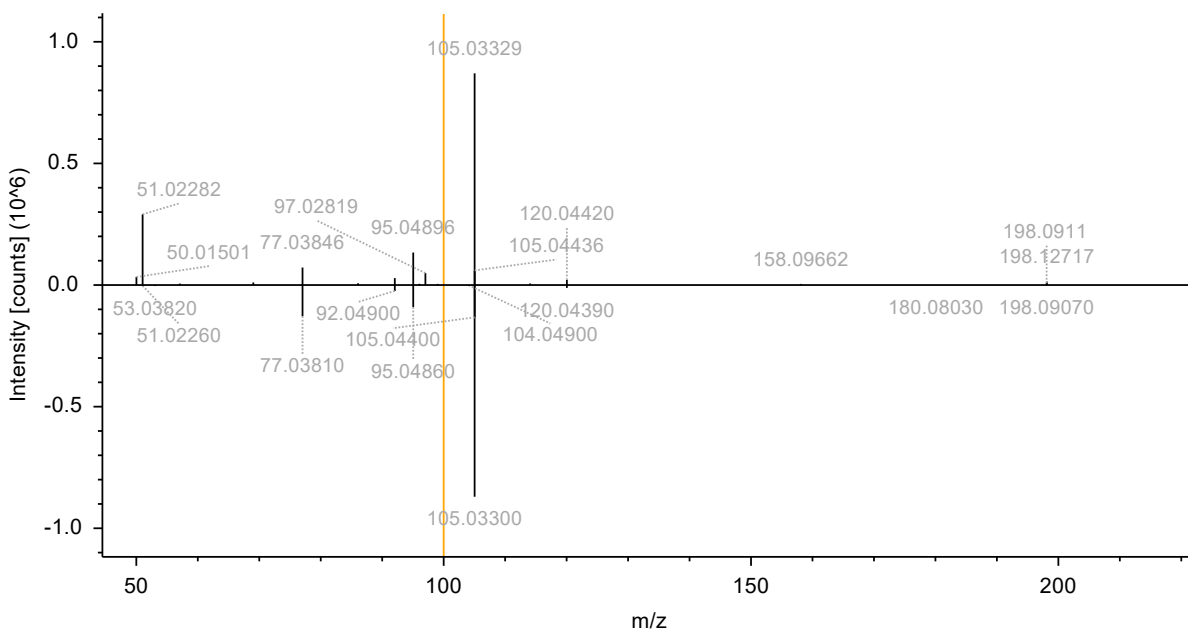
### Phthalimide (Match 88.4)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #3632, RT=4.915 min, MS2, FTMS (+), (HCD, DDA, 14+1)



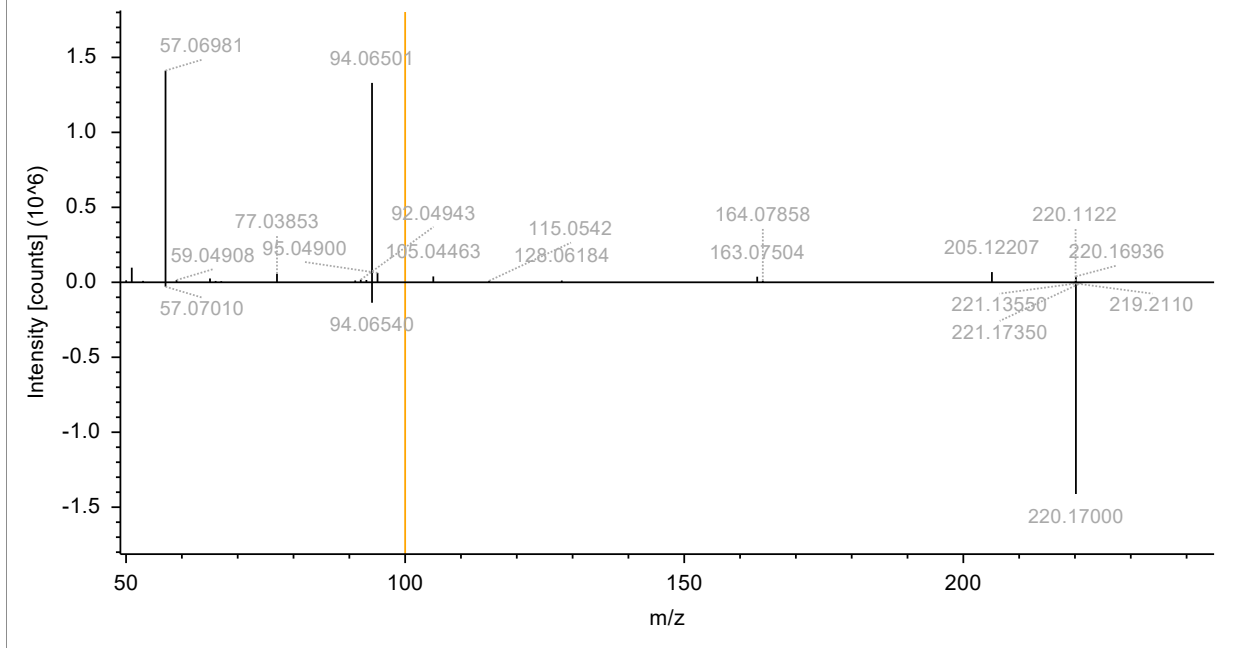
### Benzanilide (Match 85.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_1\_20231031024959 (F43) #8838, RT=11.912 min, MS2, FTMS (+), (HCD, DDA, 14+1)



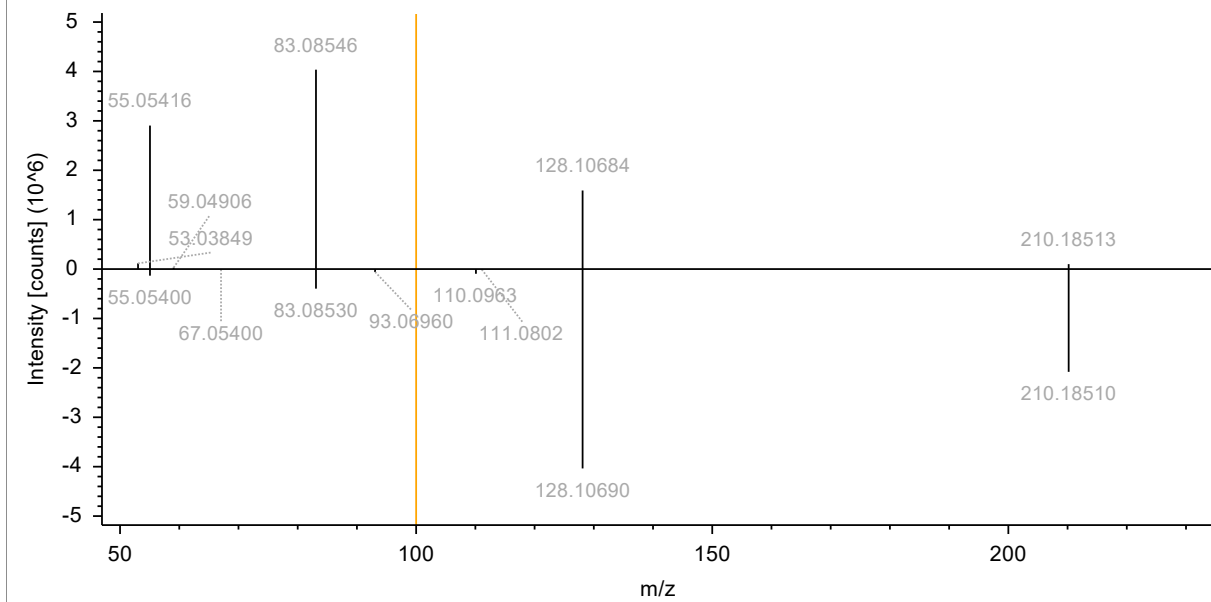
### 2-ethyl-N-phenylhexanamide (Match 89.6)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #11722, RT=15.748 min, MS2, FTMS (+), (HCD, DDA, +1)



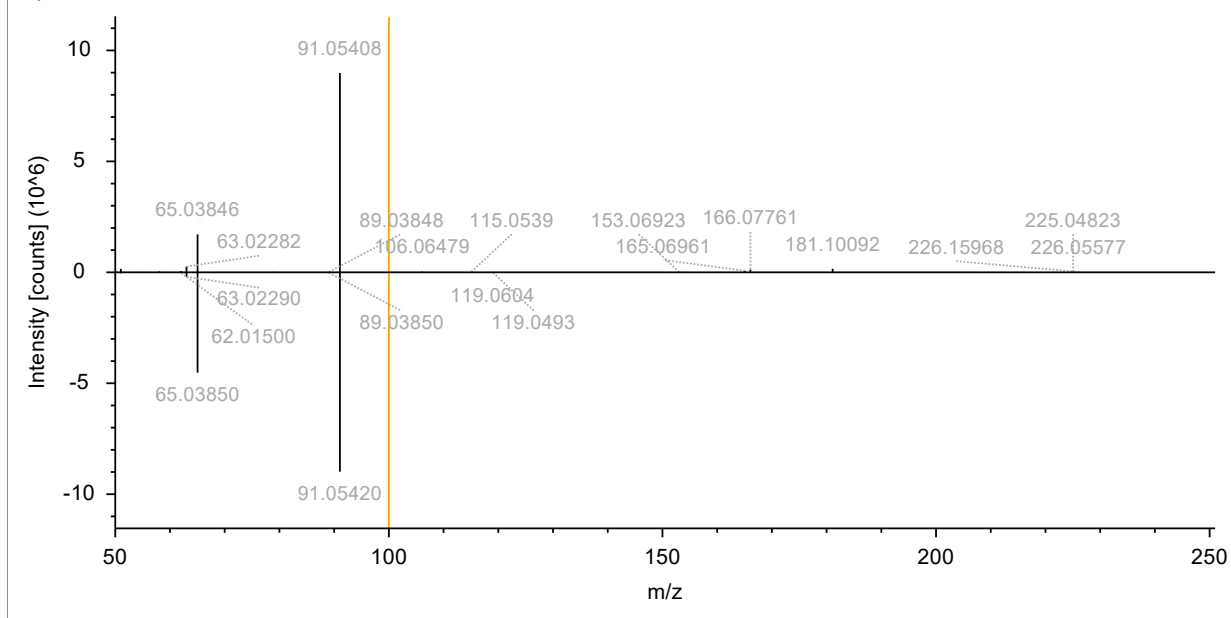
### N-Cyclohexylcyclohexanecarboxamide (Match 89.4)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_3\_20231030230527 (F33) #12931, RT=17.424 min, MS2, FTMS (+), (HCD, DDA, +1)



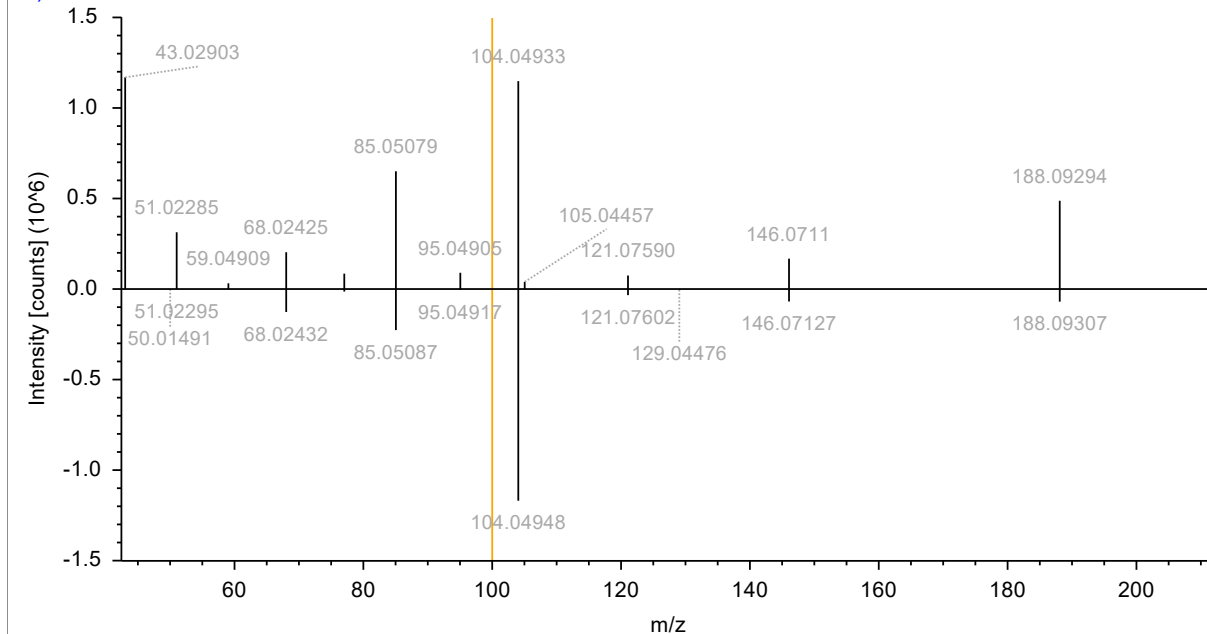
### N-benzyl-2-methylbenzamide (Match 99.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T2\_2\_20231031032203 (F44) #11045, RT=14.856 min, MS2, FTMS (+), (HCD, DDA, +1)



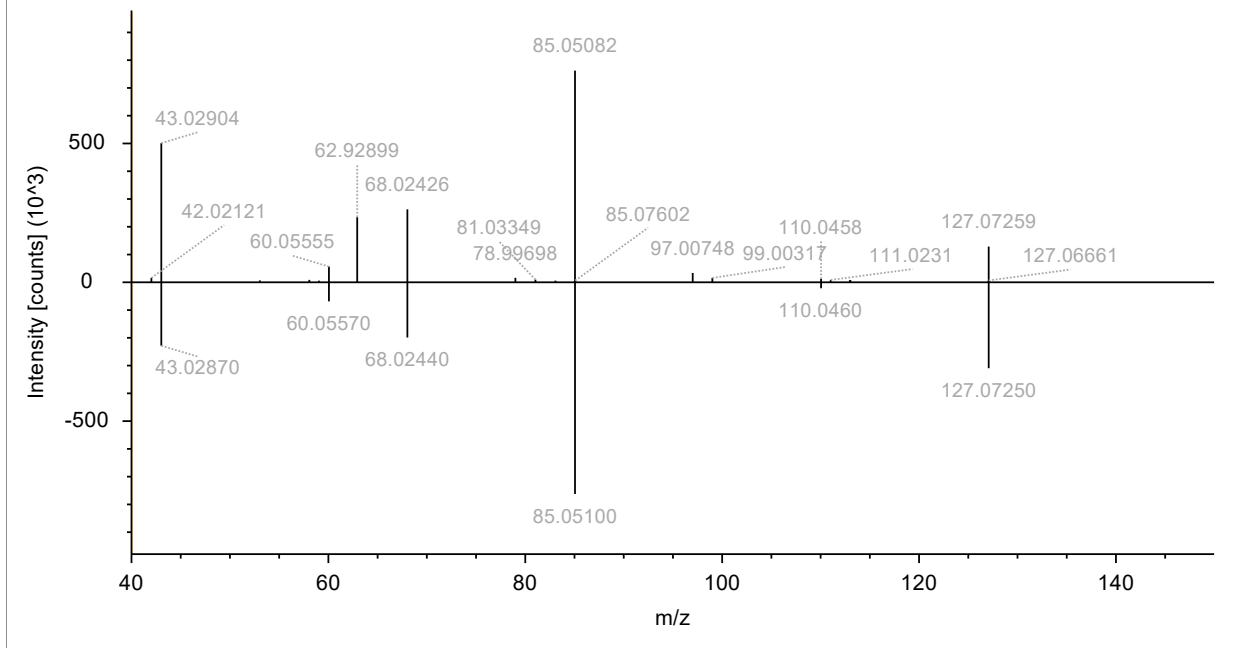
### Benzoguanamine (Match 73.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C5\_1\_20231030052657 (F13) #3903, RT=5.295 min, MS2, FTMS (+), (HCD, DDA, 18 +1)



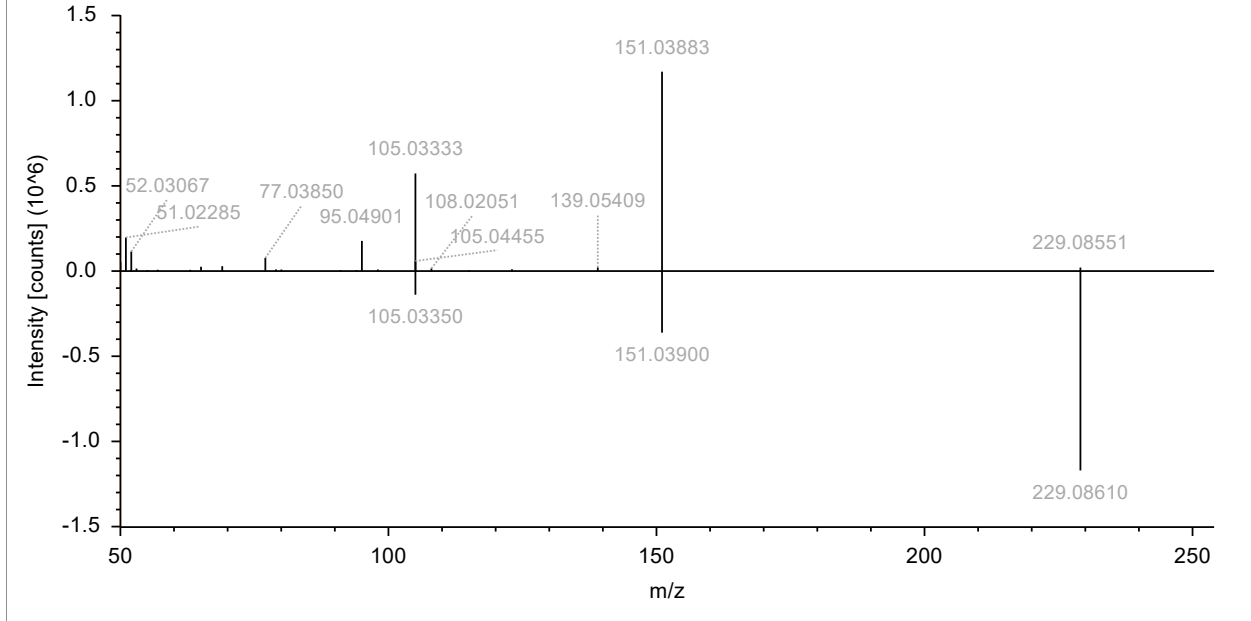
### Melamine (Match 90.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C8\_3\_20231030181646 (F24) #369, RT=0.541 min, MS2, FTMS (+), (HCD, DDA, 127+1)



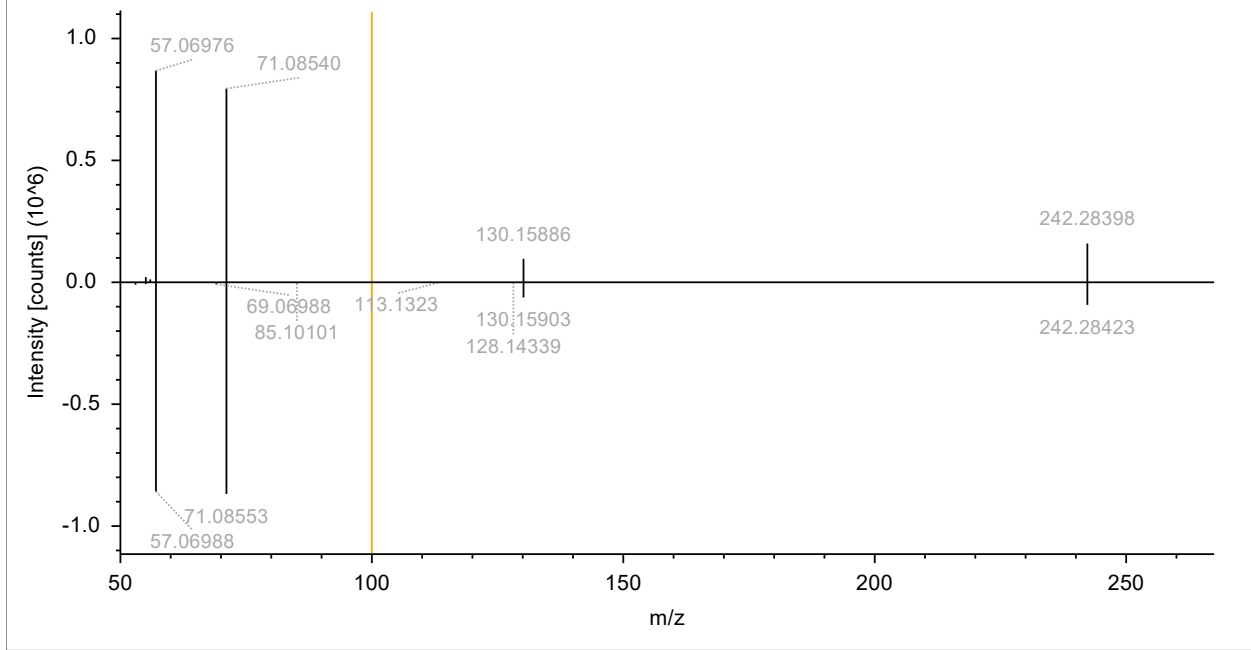
### Benzophenone-3 (Match 91.8)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C2\_1\_20231030003815 (F4) #12389, RT=16.673 min, MS2, FTMS (+), (HCD, DDA, 229+1)



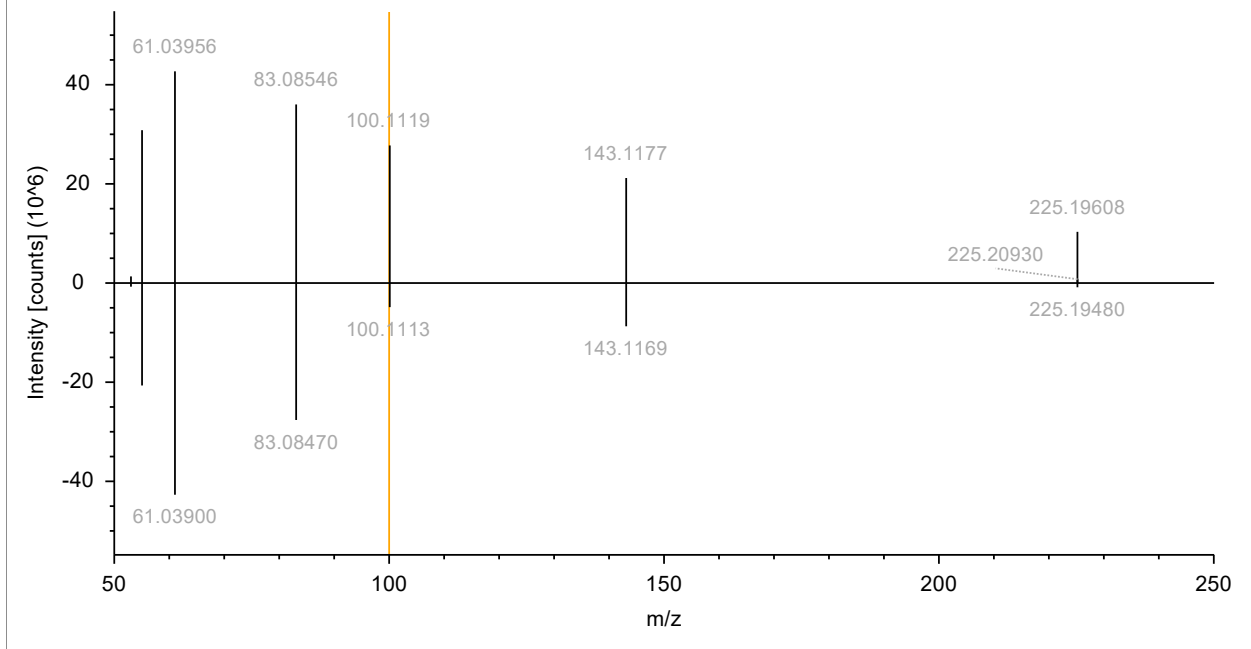
Bis(2-ethylhexyl) amine (Match 93.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #11212, RT=15.130 min, MS2, FTMS (+), (HCD, DD/ +1)



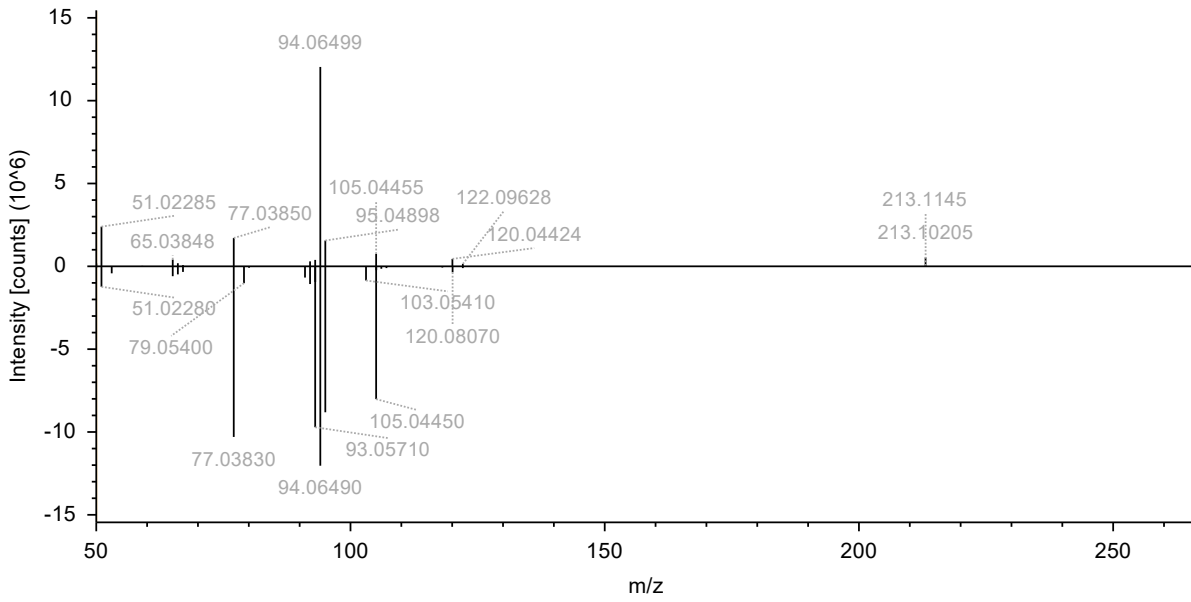
1,3-dicyclohexylurea (Match 99.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_3\_20231031021754 (F42) #11103, RT=14.953 min, MS2, FTMS (+), (HCD, DDA, +1)



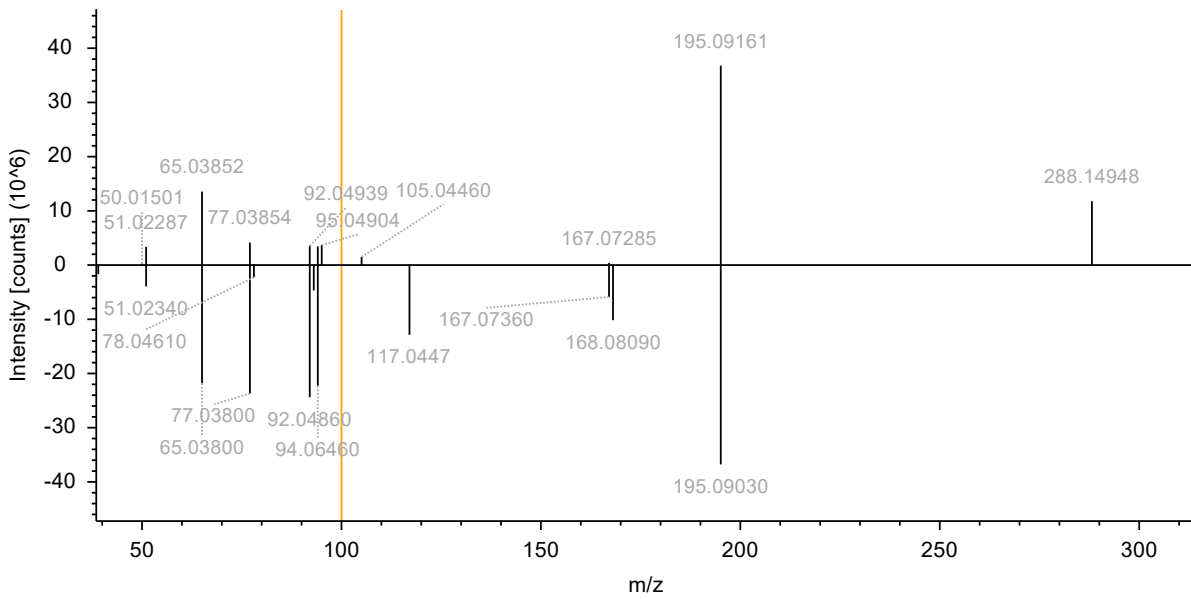
### 1-(2-ethylphenyl)-3-phenylurea (Match 88.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #6349, RT=8.585 min, MS2, FTMS (+), (HCD, DDA, 24 +1)



### Triphenylguanidine (Match 81.1)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #7695, RT=10.382 min, MS2, FTMS (+), (HCD, DDA, 2 +1)



1,1-diethyl-3-phenylurea (Match 85.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #8943, RT=12.083 min, MS2, FTMS (+), (HCD, DDA, 1+1)

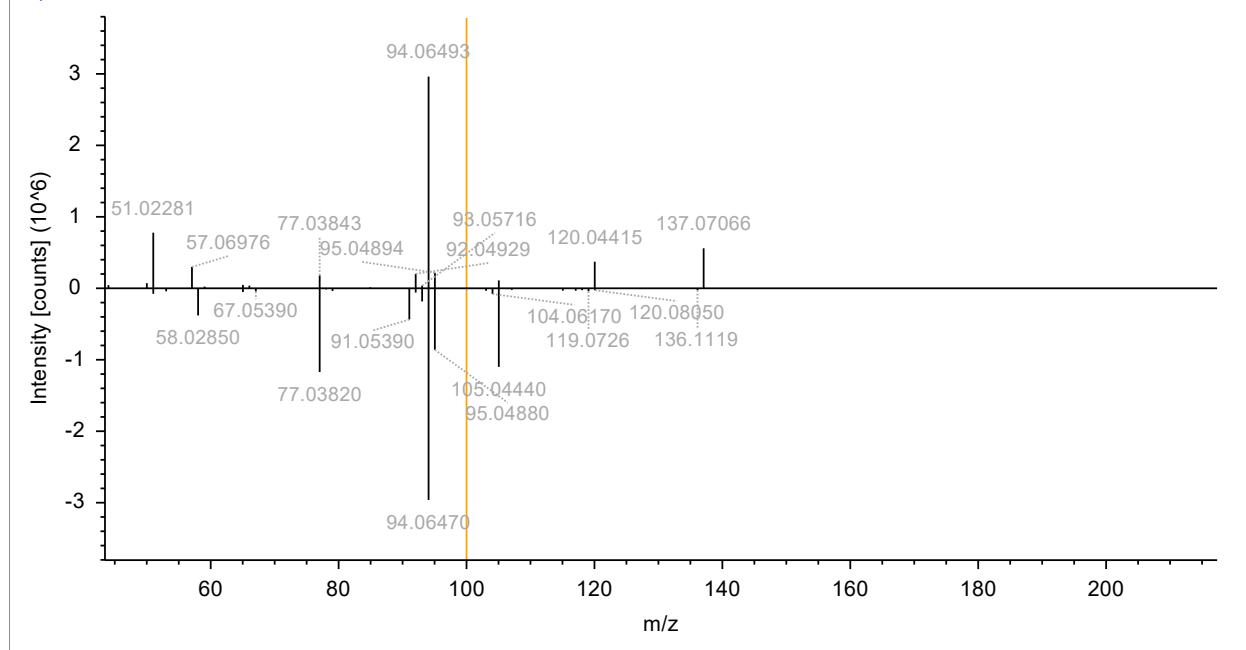
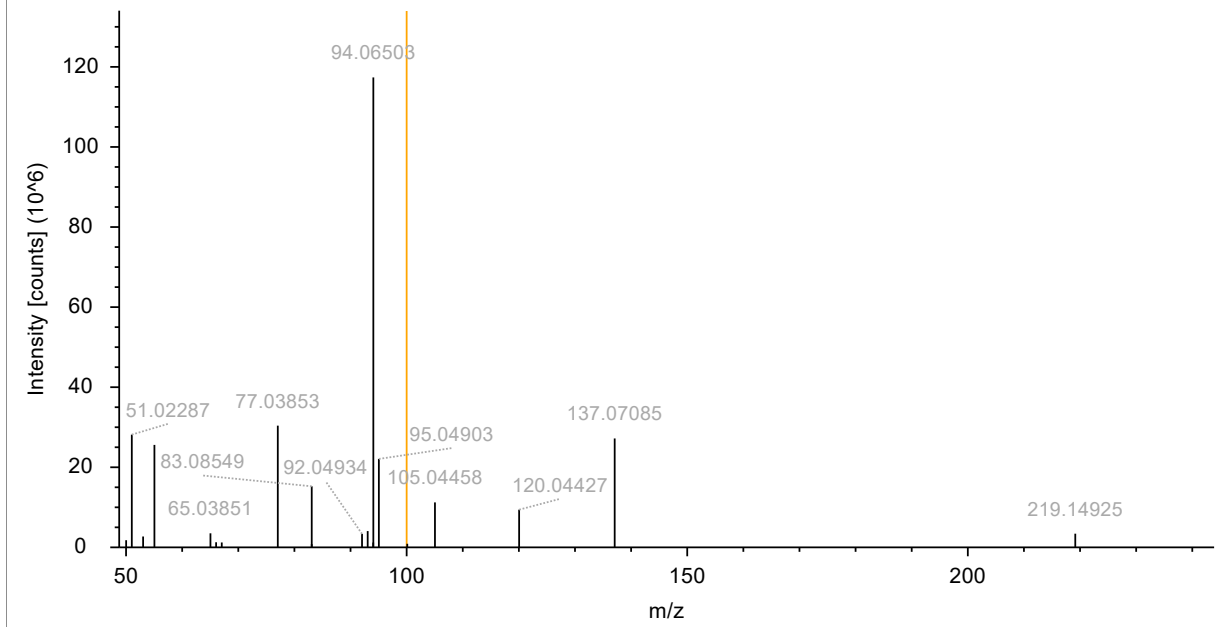


Figure S9. Comparison between experimental and mzVault library MS/MS spectra in CD 3.3.



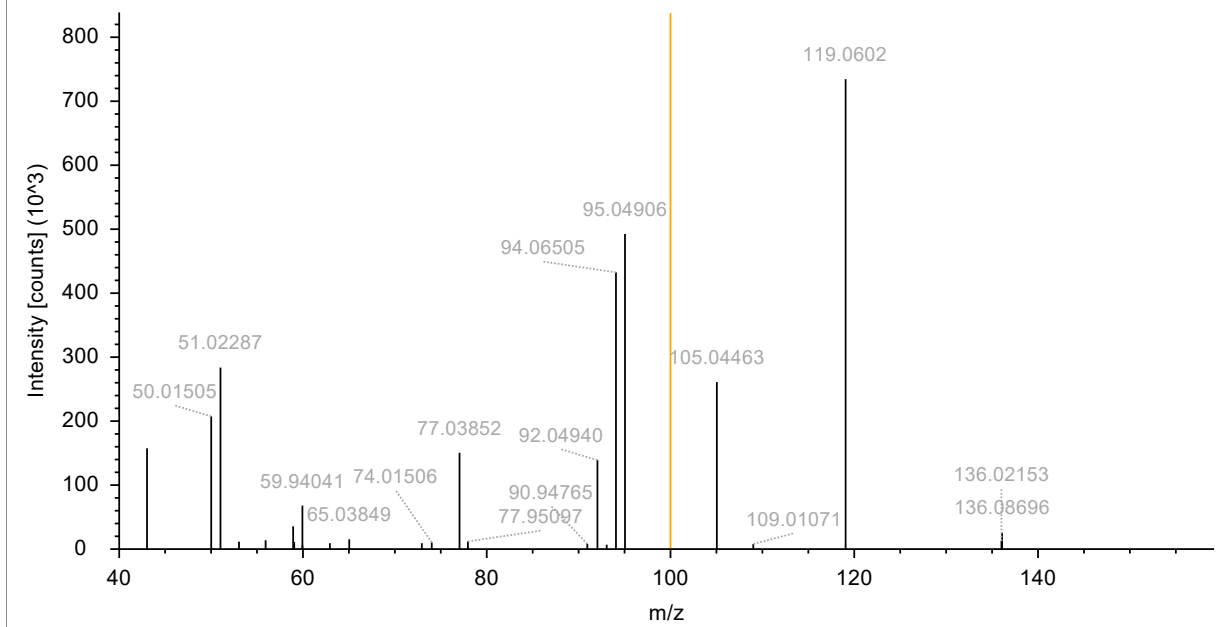
### 1-cyclohexyl-3-phenylurea

2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #10310, RT=13.879 min, MS2, FTMS (+), (HCD, DDA, 219.1489@(20;



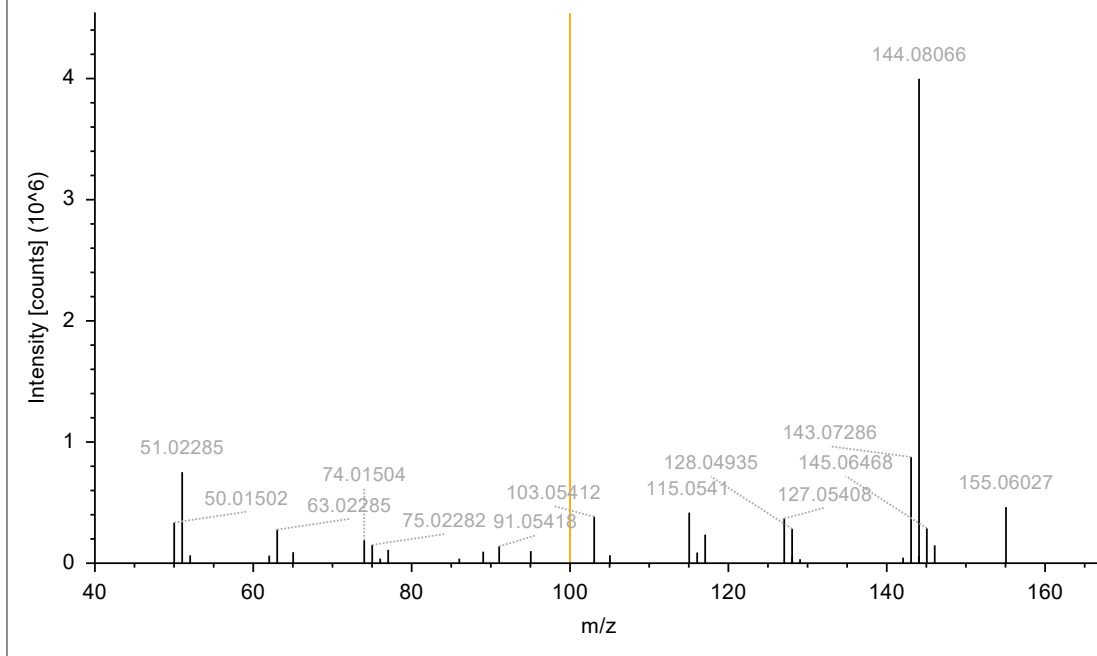
### 1-phenylguanidine

2023\_10\_26\_Quant\_Ext\_T1\_1\_20231031011345 (F40) #1134, RT=1.569 min, MS2, FTMS (+), (HCD, DDA, 136.0868@(20;60



### Naphthalen-2-amine

2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #13148, RT=17.655 min, MS2, FTMS (+), (HCD, DDA, 144.0)



### N,N-dicyclohexyl-2-benzothiazolesulfenamide

2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #18419, RT=24.659 min, MS2, FTMS (+), (HCD, DDA, 347

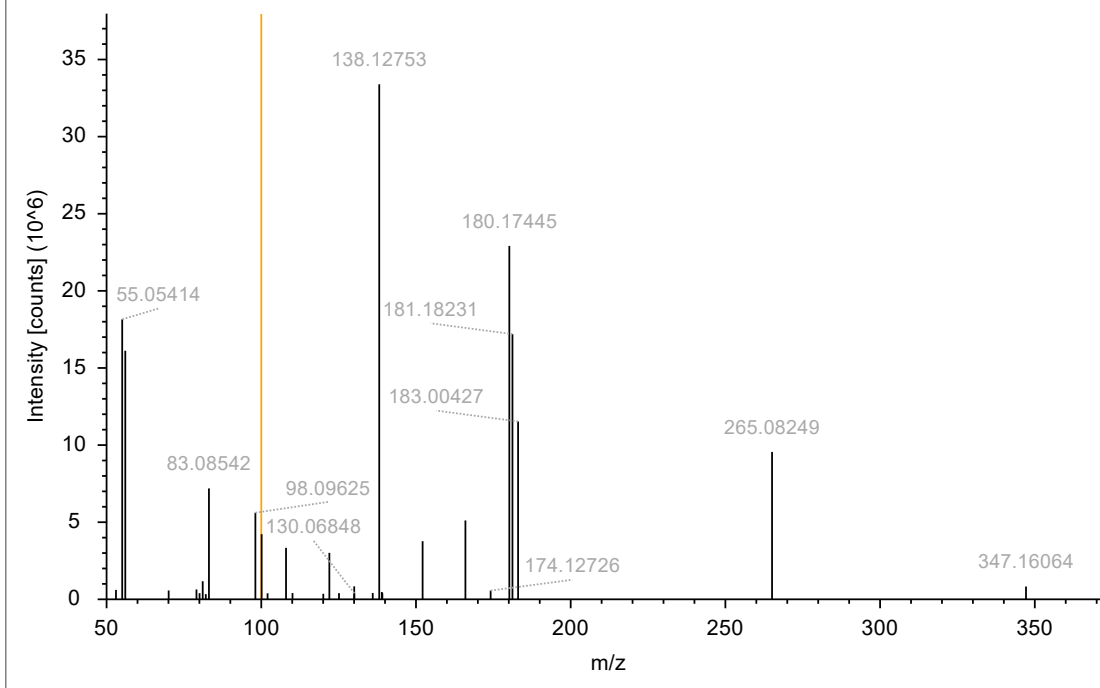
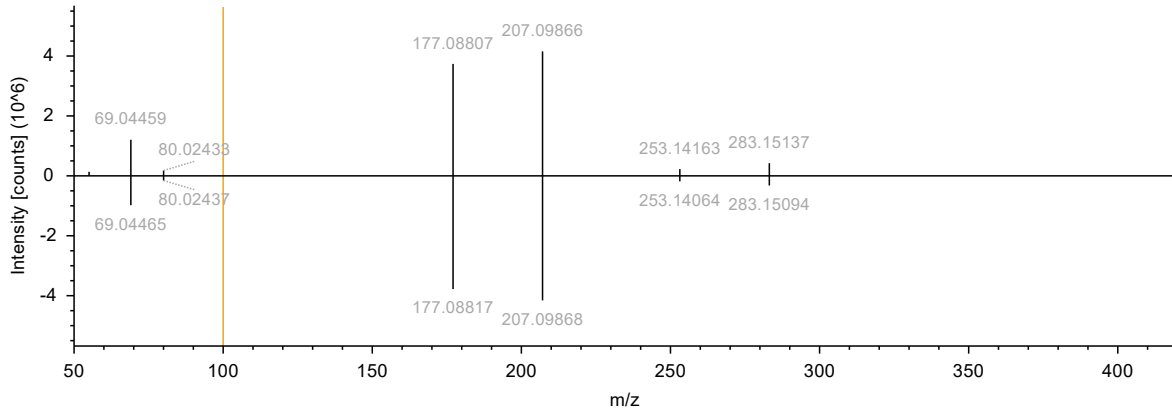


Figure S10. MS/MS Compounds identified from other sources (Level 2a).

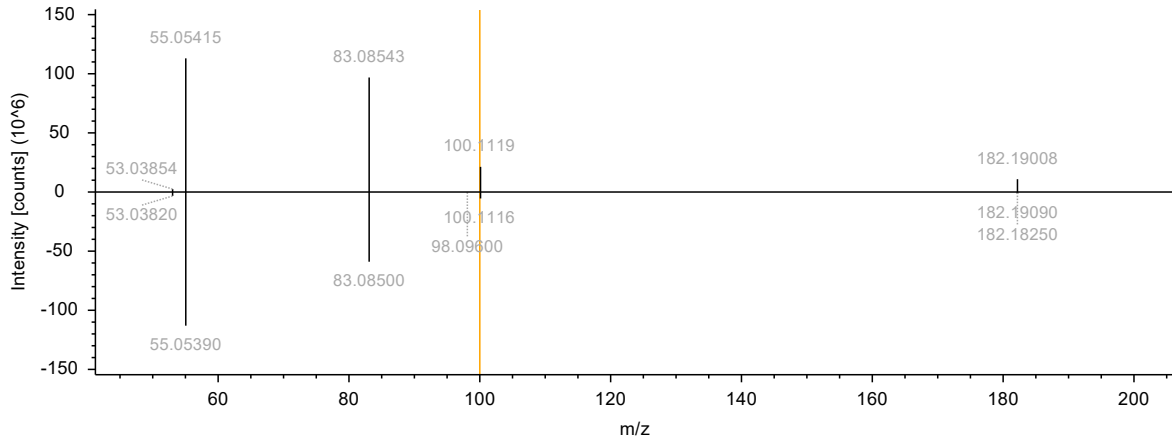
### Hexa(methoxymethyl)melamine (Match 99.8)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_1\_20231031011345 (F40) #9540, RT=12.864 min, MS2, FTMS (+), (HCD, DDA, 391.2292@(20;60), +1)



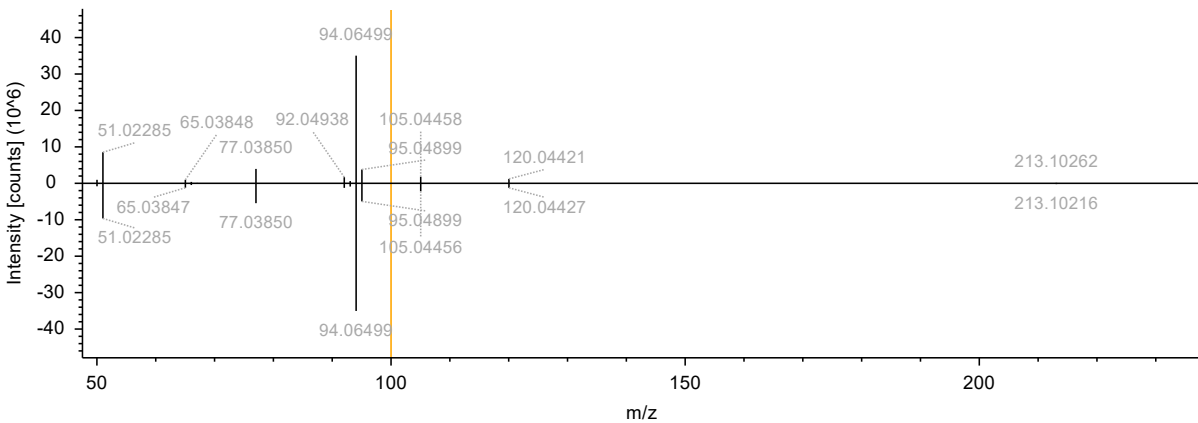
### Dicyclohexylamine (Match 99.6)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #5993, RT=8.110 min, MS2, FTMS (+), (HCD, DDA, 182.1900@(20;60), +1)



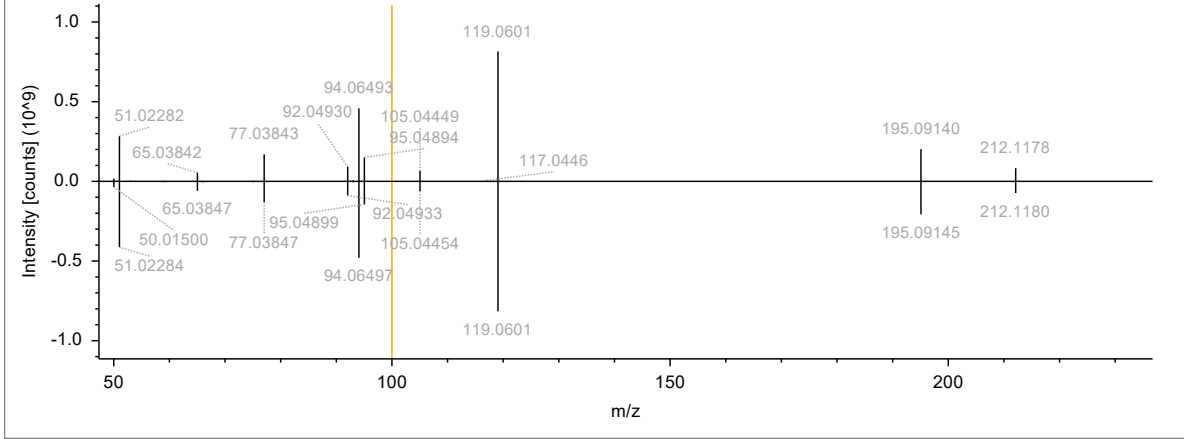
### 1,3-diphenylurea (Match 99.5)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_1\_20231031011345 (F40) #9484, RT=12.790 min, MS2, FTMS (+), (HCD, DDA, 213.1019@(20;60), +1)



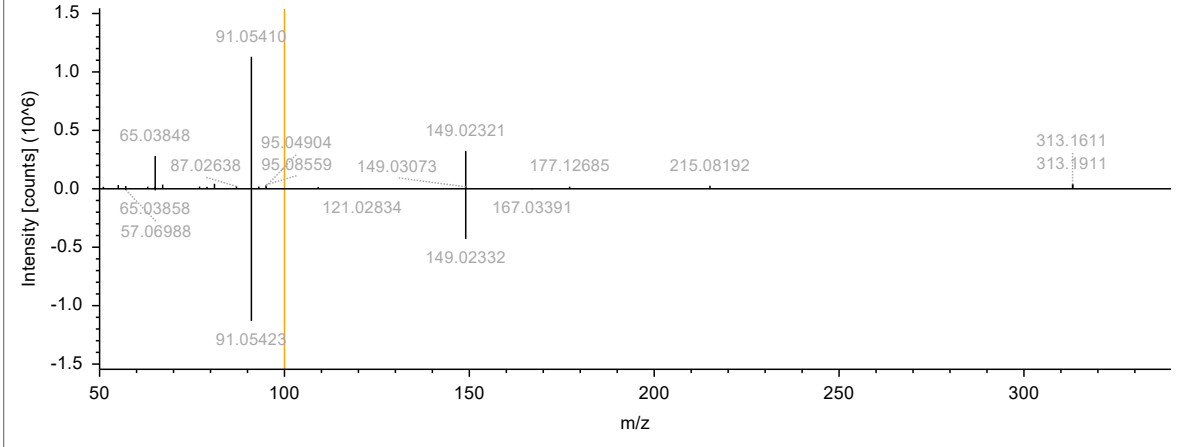
### 1,3-diphenylguanidine (Match 99.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #4737, RT=6.425 min, MS2, FTMS (+), (HCD, DDA, 212.1178@(20;60), +1)



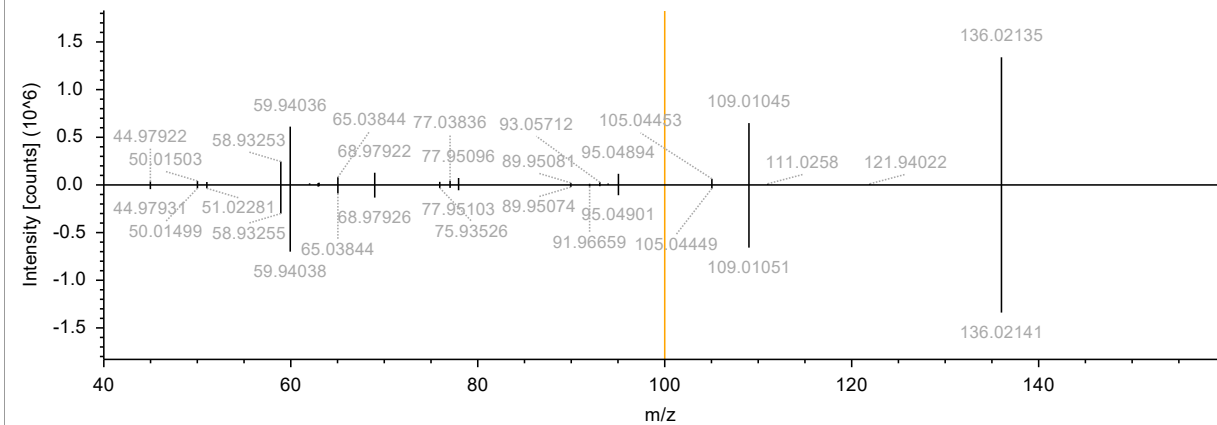
### Benzyl butyl phthalate (Match 99.2)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T1\_3\_20231031021754 (F42) #14293, RT=19.194 min, MS2, FTMS (+), (HCD, DDA, 313.1433@(20;60), +1)



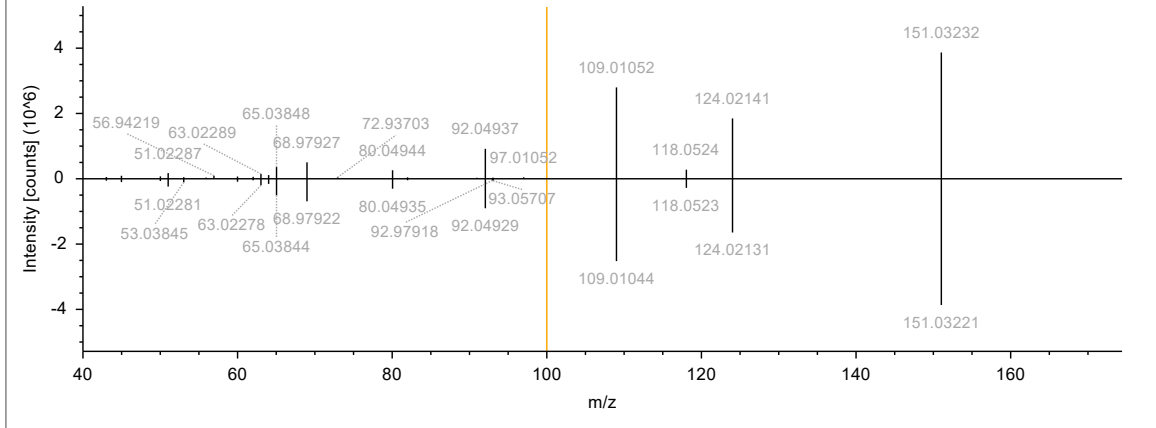
### Benzothiazole (Match 98.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #7330, RT=9.901 min, MS2, FTMS (+), (HCD, DDA, 136.0215@(20;60), +1)



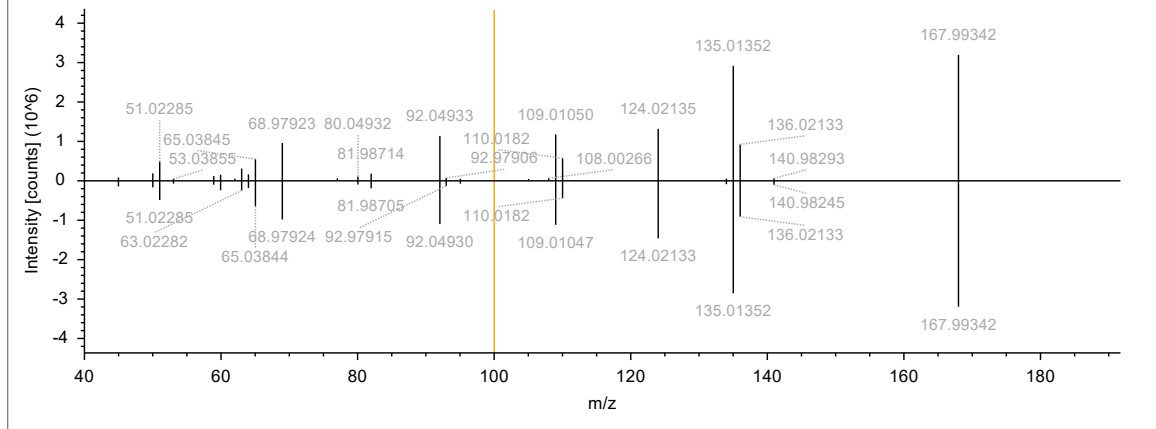
### 2-aminobenzothiazole (Match 98.0)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C8\_3\_20231030181646 (F24) #3111, RT=4.227 min, MS2, FTMS (+), (HCD, DDA, 151.0323@(20;60, +1)



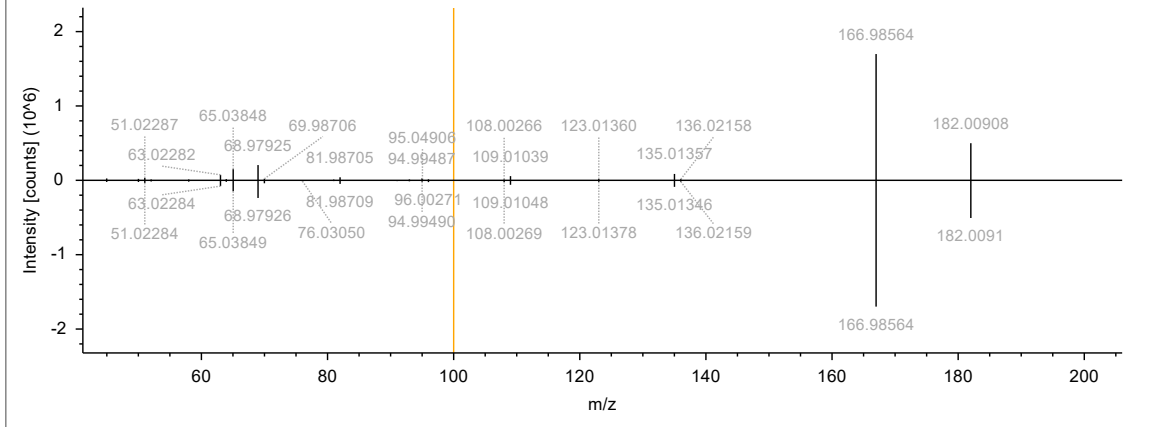
### 2-Mercaptobenzothiazole (Match 97.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #7782, RT=10.504 min, MS2, FTMS (+), (HCD, DDA, 167.9933@(20;60, +1)



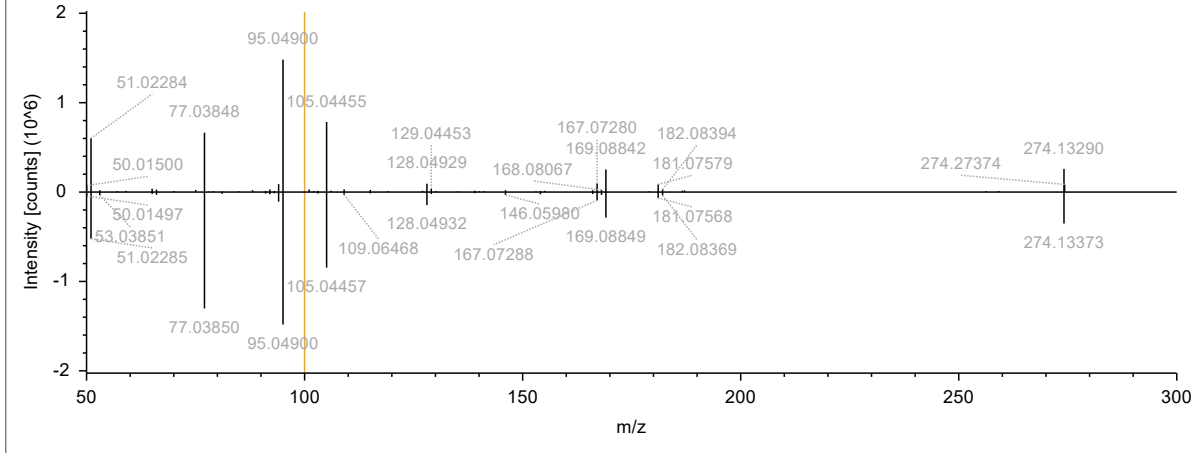
### 2-(methylthio)benzothiazole (Match 96.7)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C7\_1\_20231030153623 (F19) #10873, RT=14.678 min, MS2, FTMS (+), (HCD, DDA, 182.0090@(20;60, +1)



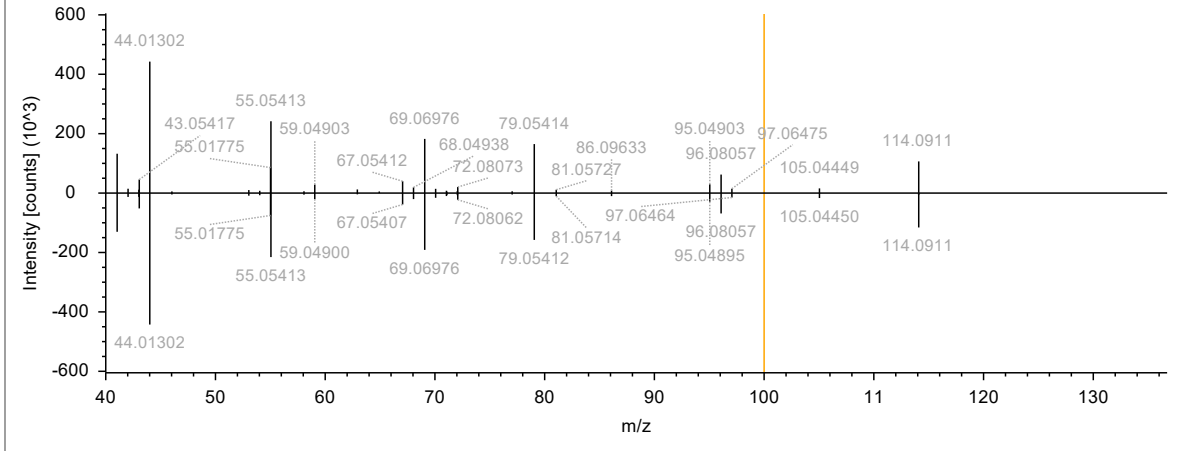
### 4-phenylazodiphenylamine (Match 96.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_2\_20231030223322 (F32) #15124, RT=20.309 min, MS2, FTMS (+), (HCD, DDA, 274.1337@(20;6+1)



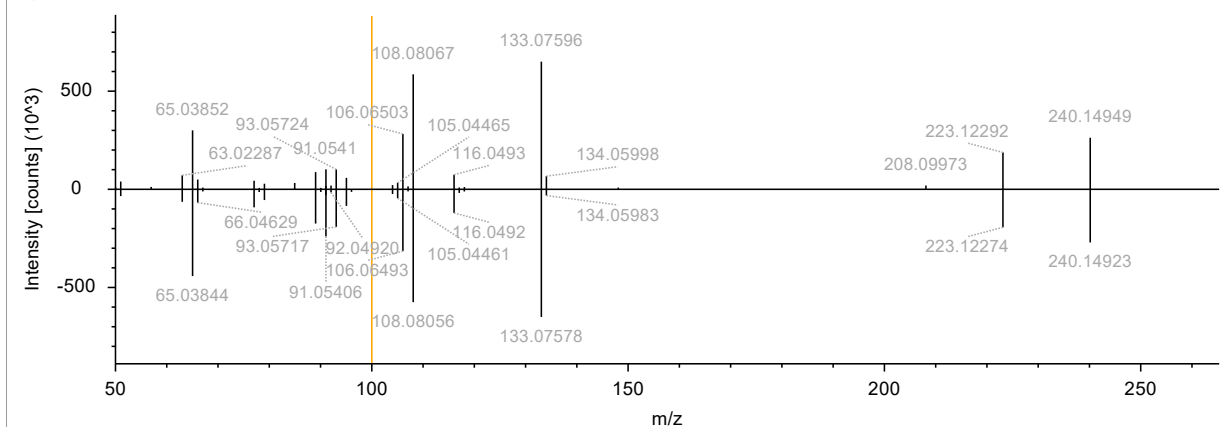
### Caprolactam (Match 96.2)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_2\_20231030223322 (F32) #3309, RT=4.500 min, MS2, FTMS (+), (HCD, DDA, 114.0912@(20;60+1)



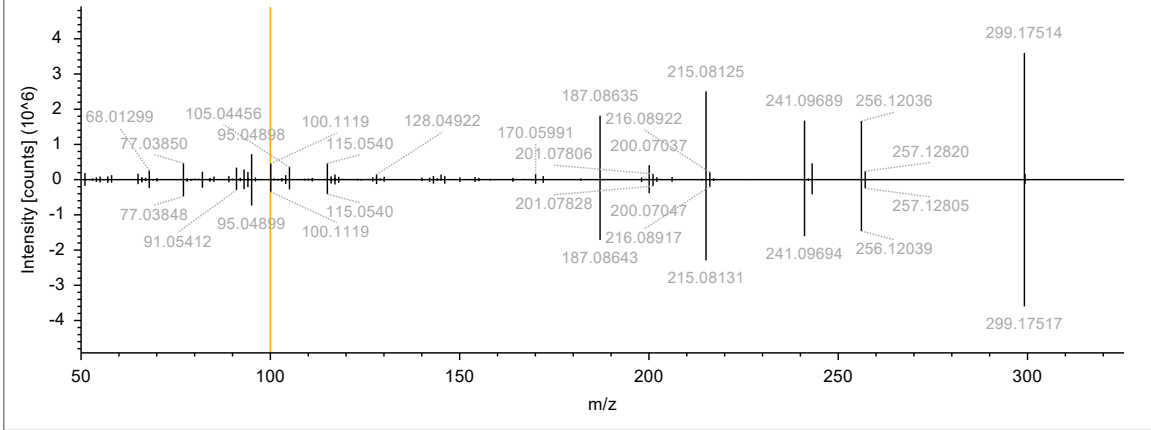
### 1,3-di-o-tolylguanidine (Match 95.6)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_3\_20231030230527 (F33) #6005, RT=8.125 min, MS2, FTMS (+), (HCD, DDA, 240.1493@(20;60+1)



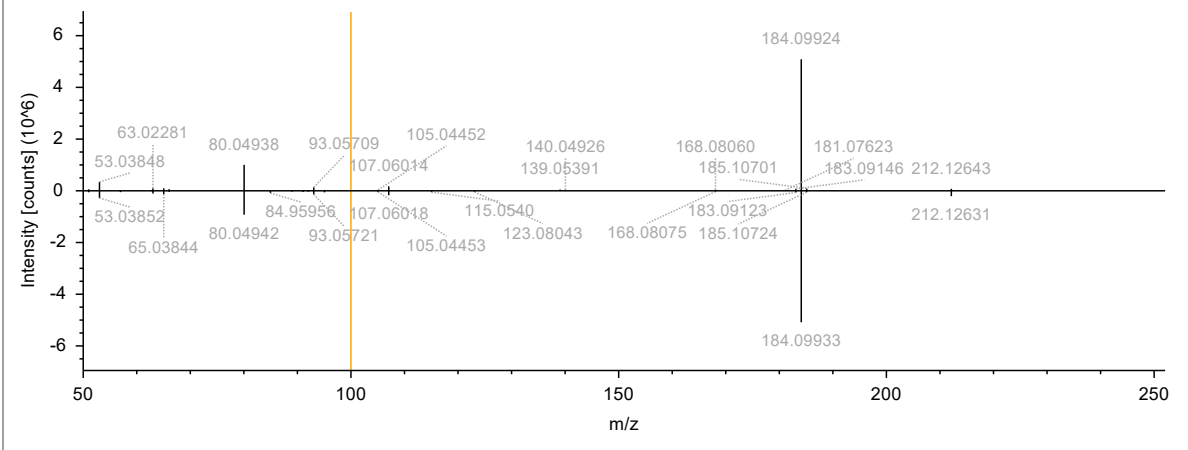
### 6PPD-quinone (Match 95.3)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C11\_2\_20231030223322 (F32) #13362, RT=17.983 min, MS2, FTMS (+), (HCD, DDA, 299.1750@(20;6 +1)



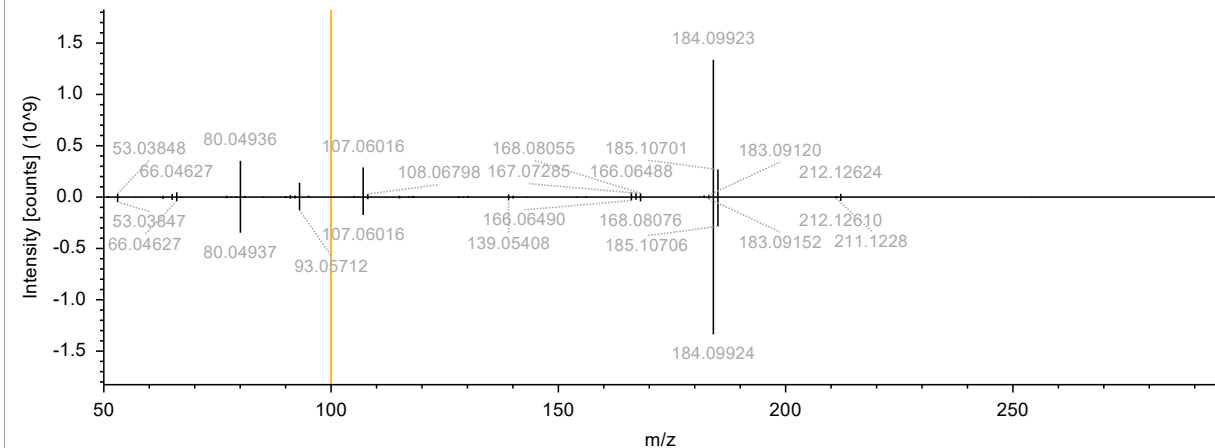
### N-isopropyl-N'-phenyl-1,4-phenylenediamine (IPPD) (Match 93.2)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_C8\_2\_20231030174441 (F23) #7231, RT=9.737 min, MS2, FTMS (+), (HCD, DDA, 227.1542@(20;60, +1)



### N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) (Match 91.7)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #9602, RT=12.927 min, MS2, FTMS (+), (HCD, DDA, 269.2006@(20;60, +1)



### 2,2,4-trimethyl-1,2,3,4-tetrahydroquinoline (TMQ) (Match 84.9)

RAWFILE(top): 2023\_10\_26\_Quant\_Ext\_T3\_3\_20231031053030 (F48) #6563, RT=8.874 min, MS2, FTMS (+), (HCD, DDA, 176.1431@(20;60), +1)

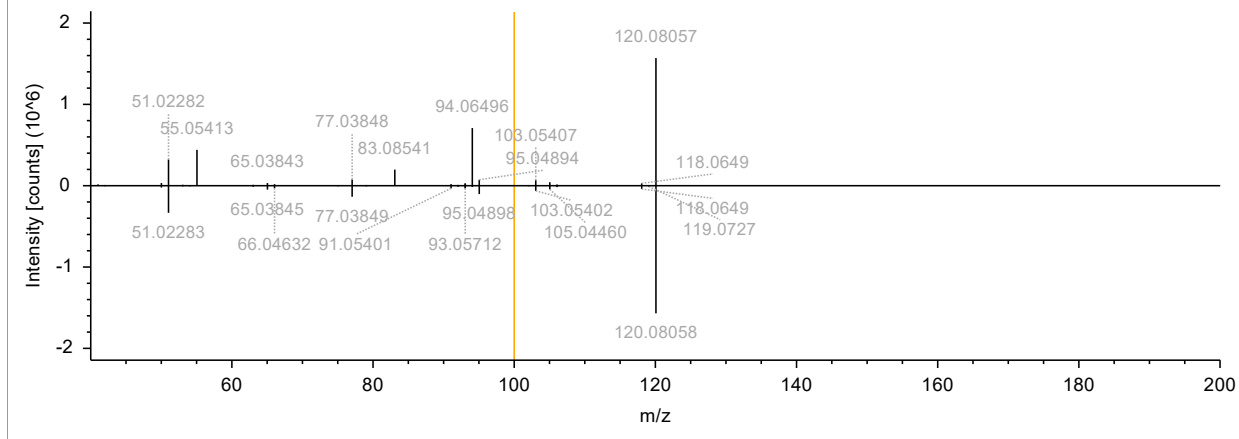
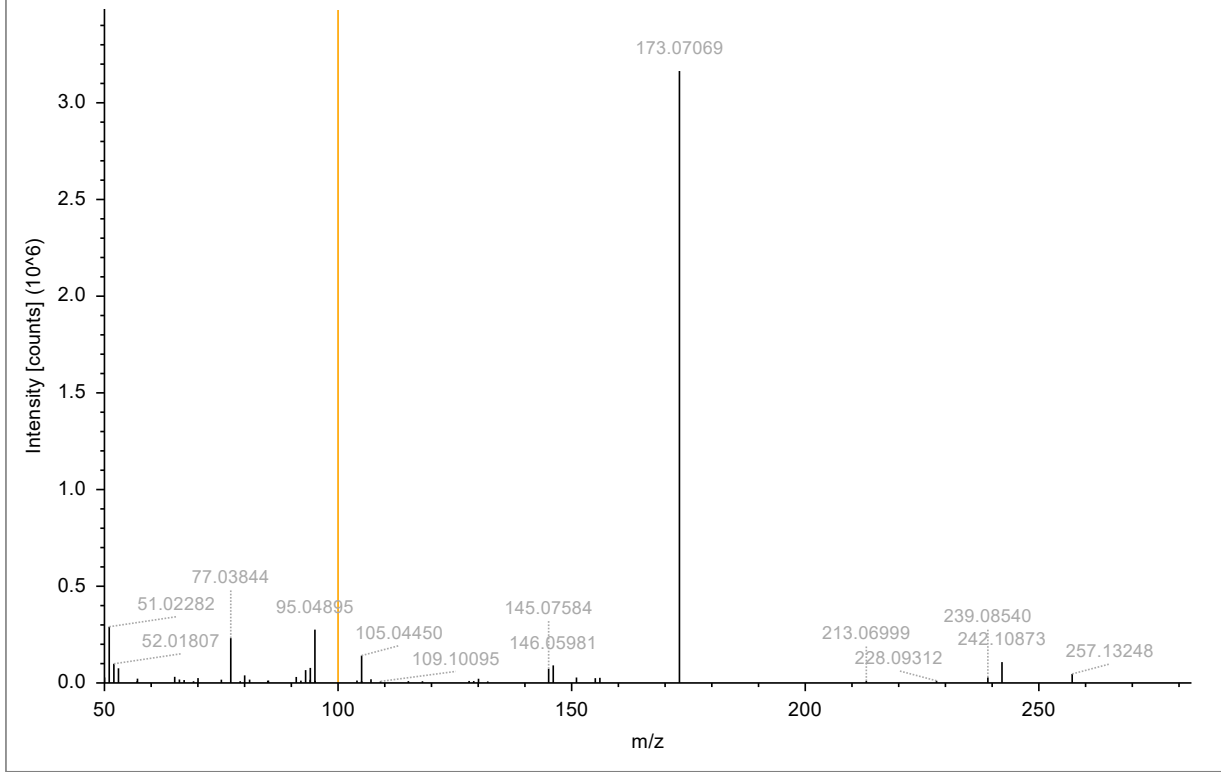


Figure S11. Comparison between experimental and in-house standard (Level 1).



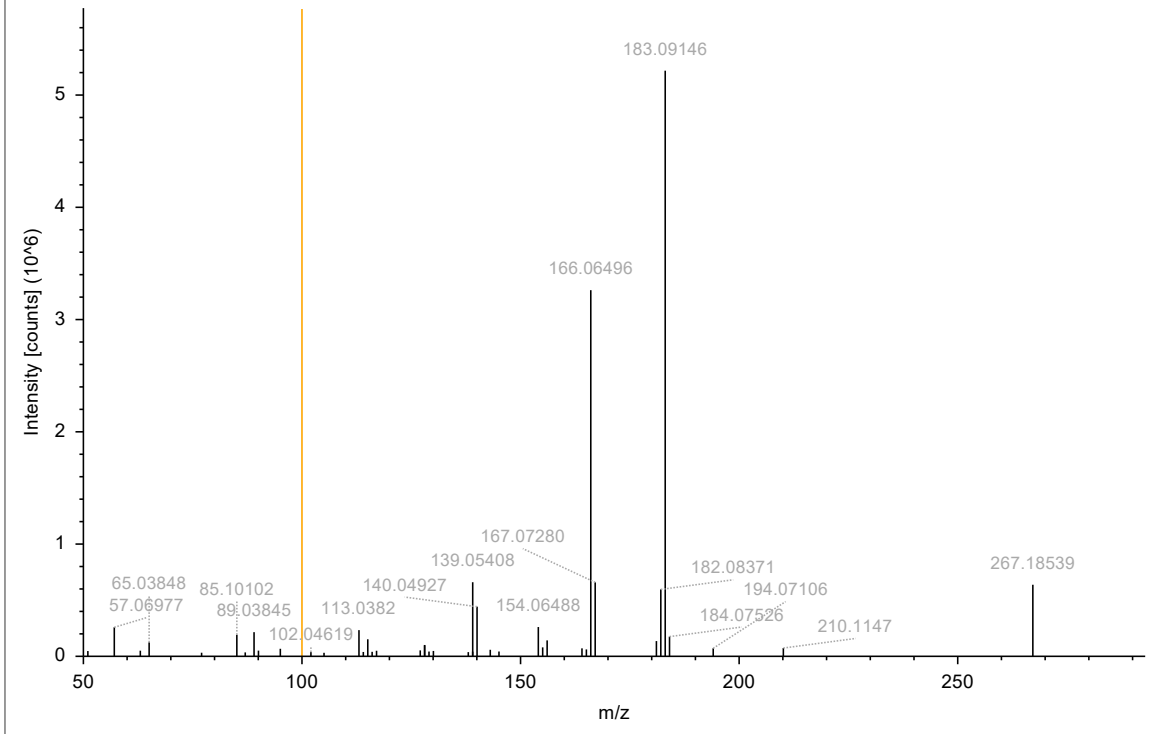
### TP 256

2023\_10\_26\_Quant\_Ext\_C11\_2\_20231030223322 (F32) #14642, RT=19.675 min, MS2, FTMS (+), (HCD, DDA, 257.1646@(20;60),



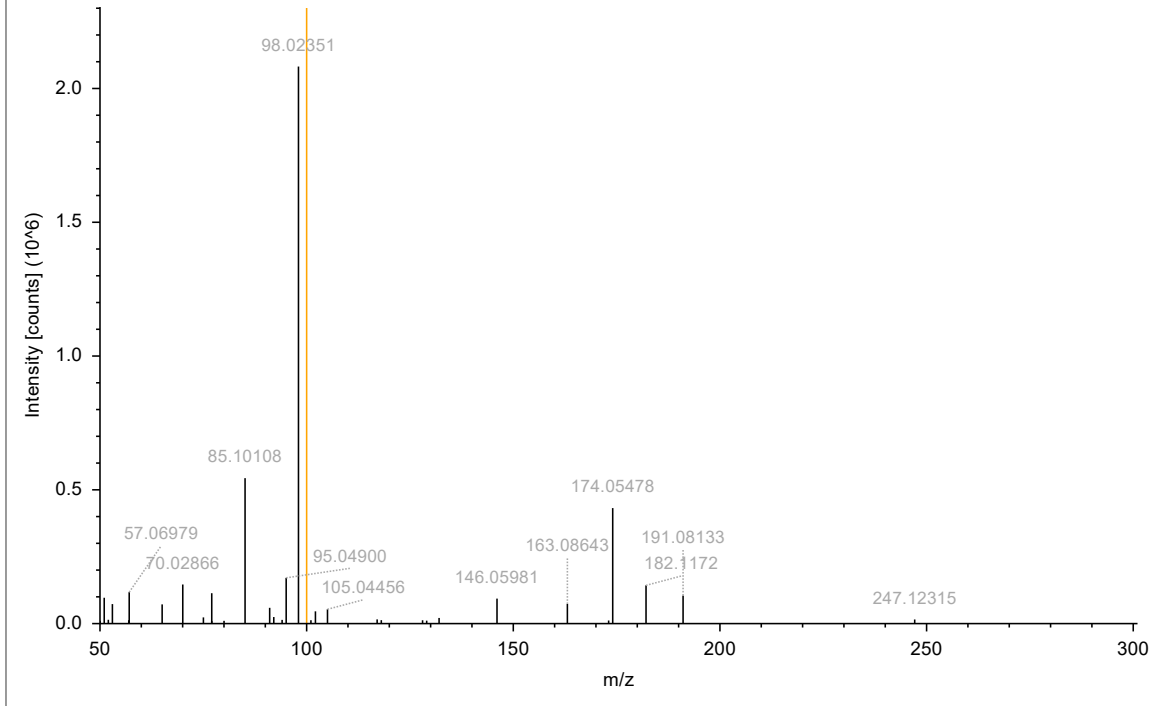
### 6QDI

2023\_10\_26\_Quant\_Ext\_T3\_2\_20231031045821 (F47) #13394, RT=17.981 min, MS2, FTMS (+), (HCD, DDA, 267.1853@(20;60),



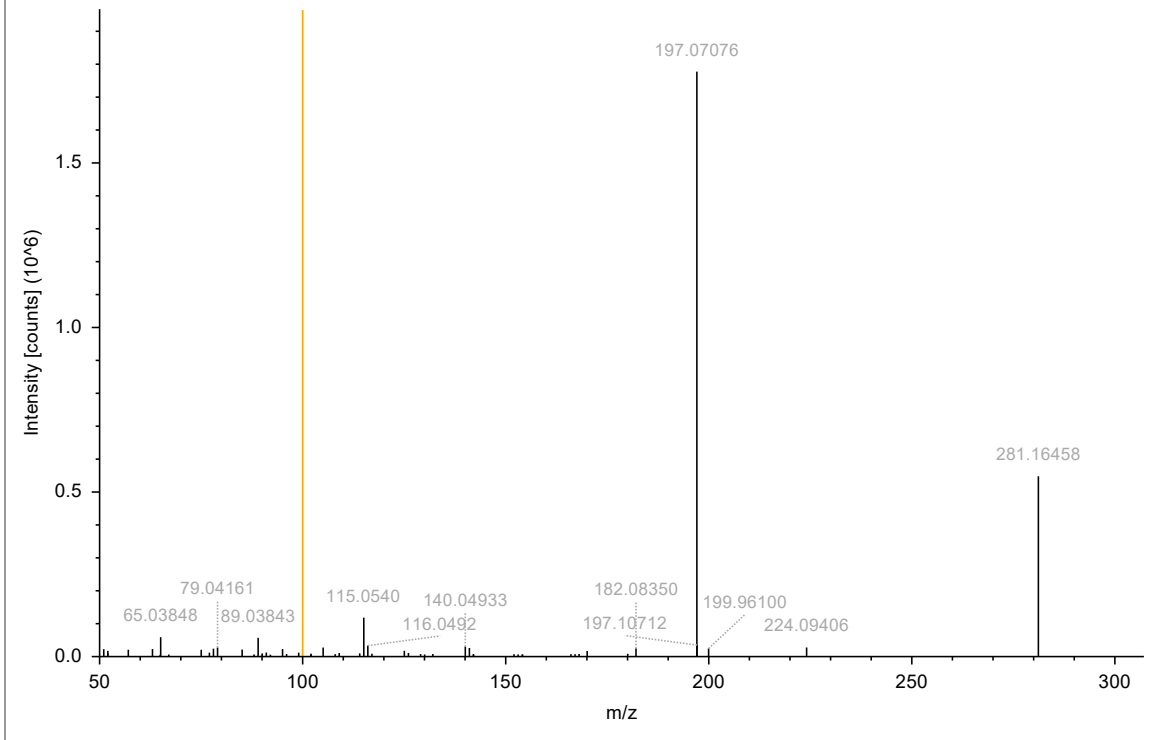
### TP 274

2023\_10\_26\_Quant\_Ext\_C8\_2\_20231030174441 (F23) #12783, RT=17.245 min, MS2, FTMS (+), (HCD, DDA, 275.1750@(20;60),



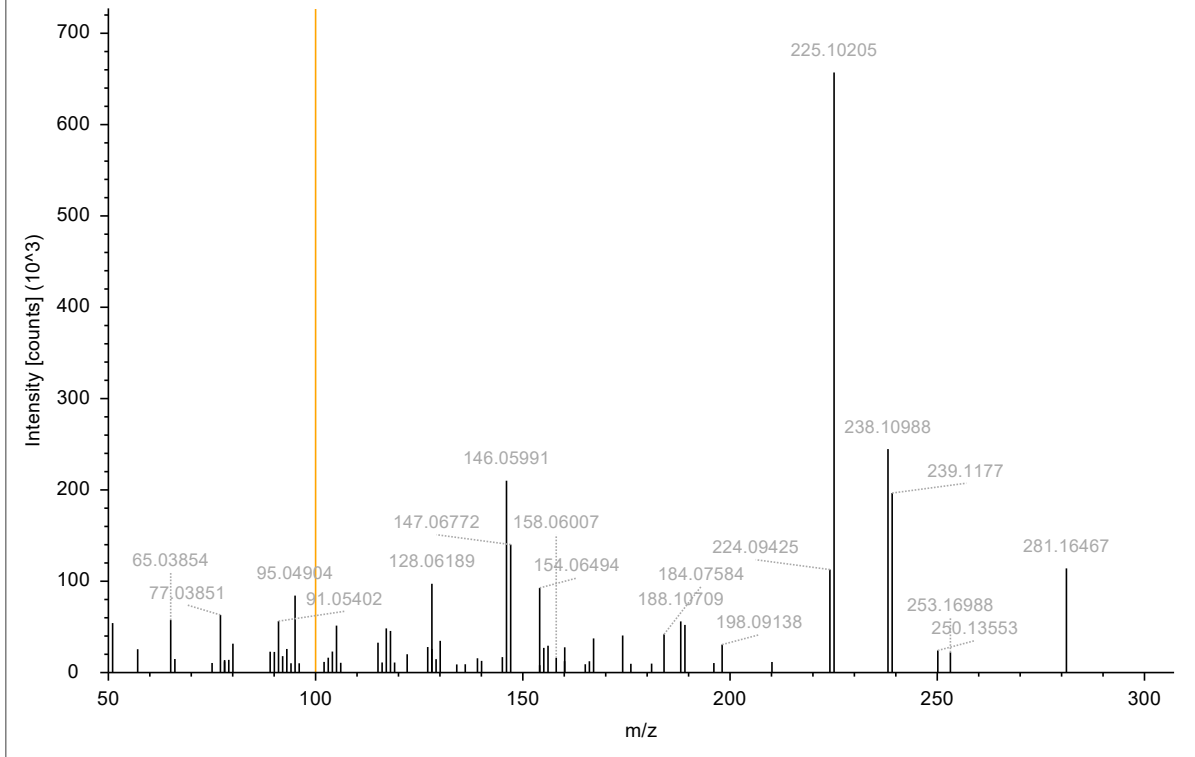
### TP280a

2023\_10\_26\_Quant\_Ext\_C11\_1\_20231030220118 (F31) #8460, RT=11.398 min, MS2, FTMS (+), (HCD, DDA, 281.1644@(20;60),



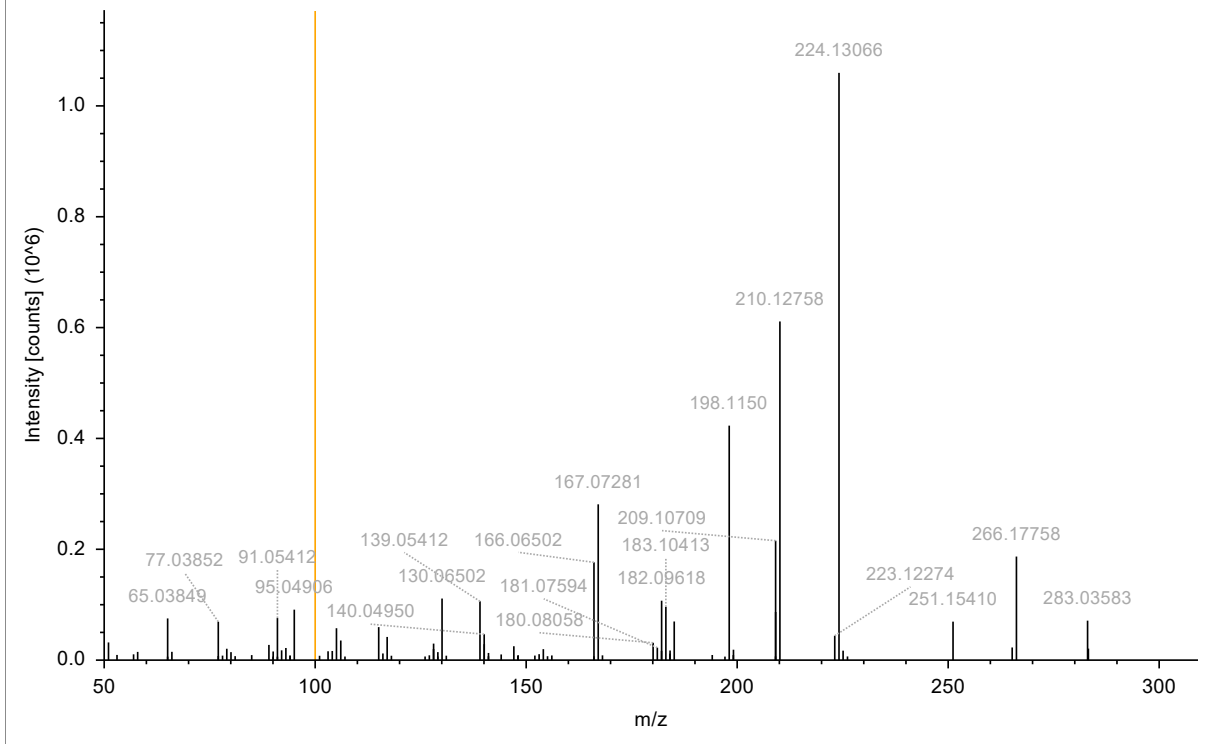
### TP280b

2023\_10\_26\_Quant\_Ext\_C11\_3\_20231030230527 (F33) #13139, RT=17.699 min, MS2, FTMS (+), (HCD, DDA, 281.1643@(20;60),



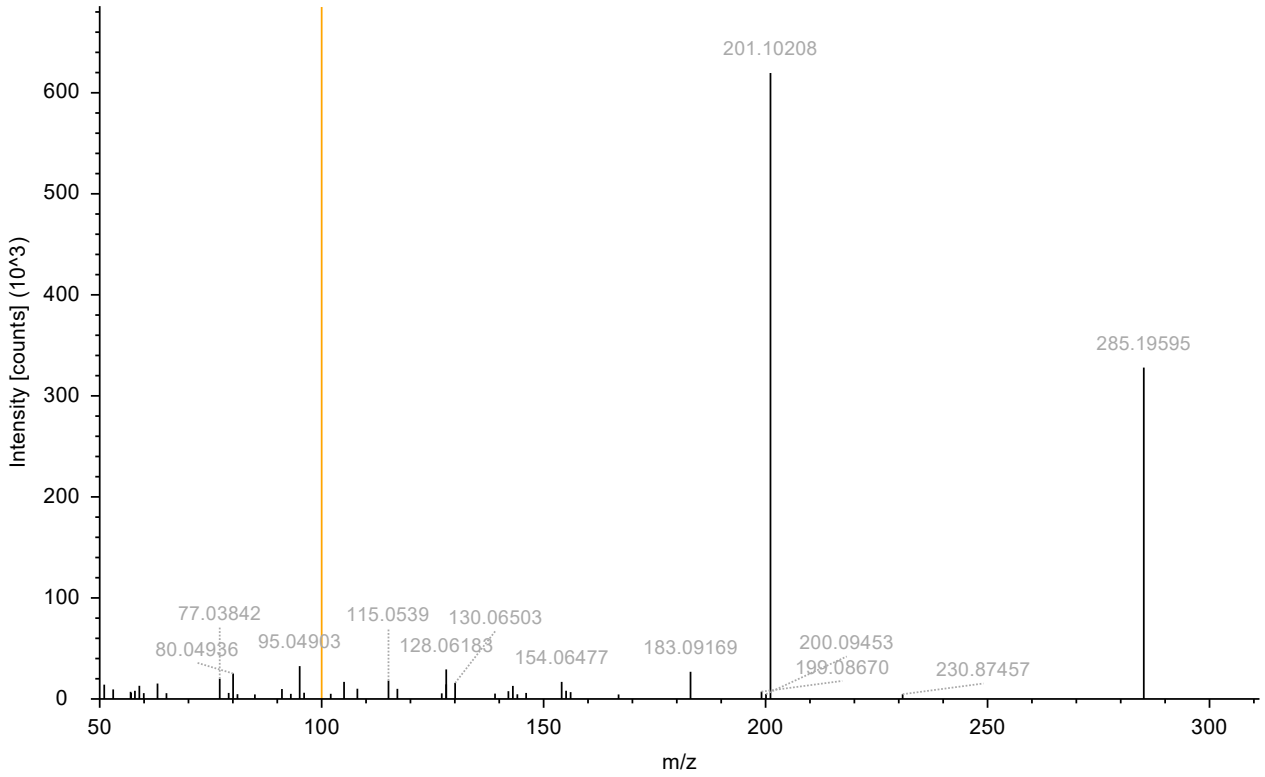
### TP282b

2023\_10\_26\_Quant\_Ext\_T3\_1\_20231031042613 (F46) #11269, RT=15.156 min, MS2, FTMS (+), (HCD, DDA, 283.1802@(20;60),



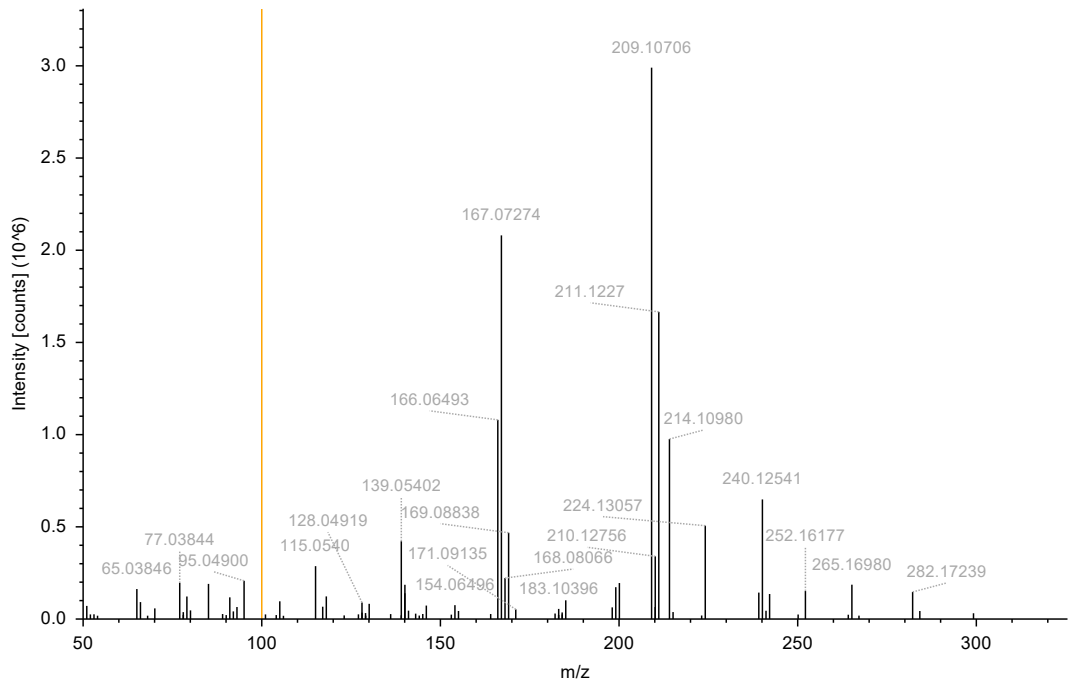
### TP284a

2023\_10\_26\_Quant\_Ext\_C11\_3\_20231030230527 (F33) #12047, RT=16.247 min, MS2, FTMS (+), (HCD, DDA, 285.1958@(20;60),



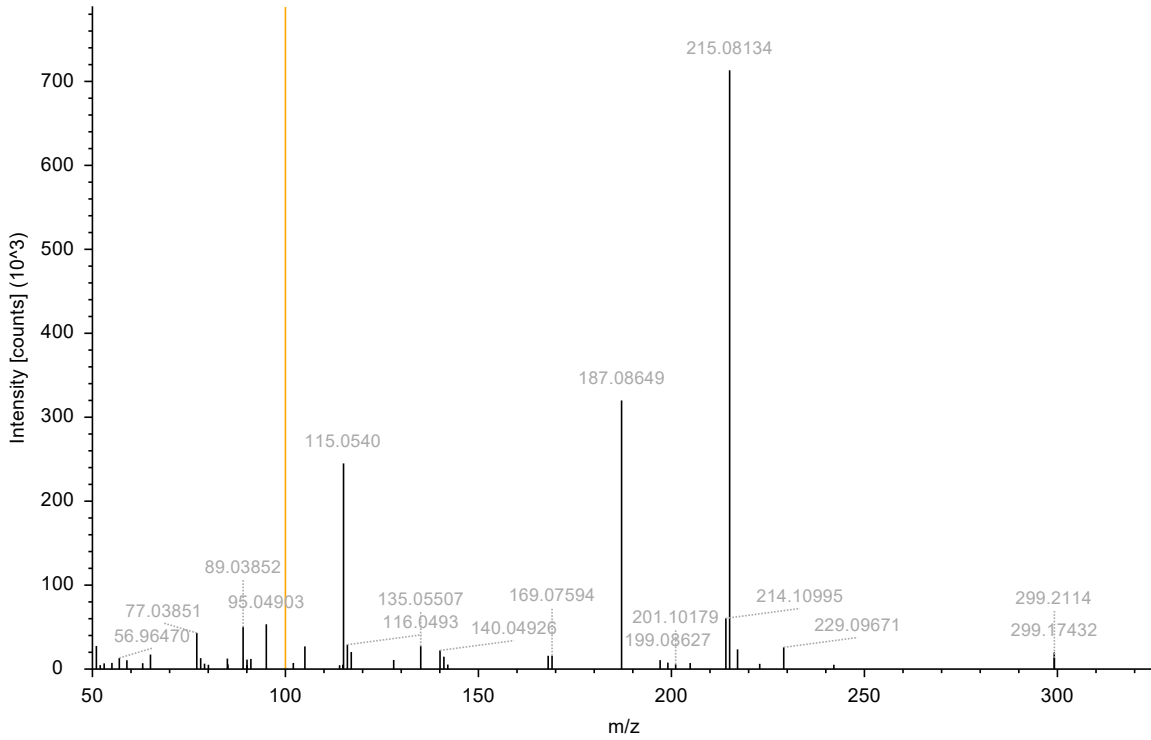
### TP298b

2023\_10\_26\_Quant\_Ext\_T1\_1\_20231031011345 (F40) #10003, RT=13.483 min, MS2, FTMS (+), (HCD, DDA, 299.1750@(20;60),



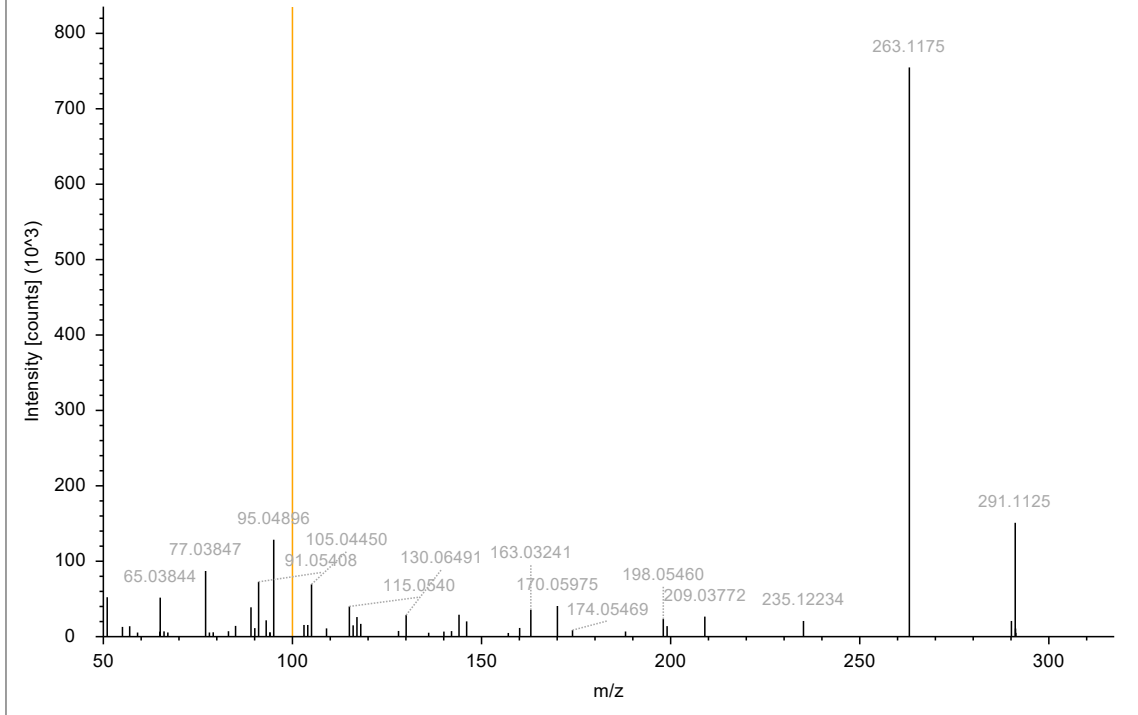
### TP298c

2023\_10\_26\_Quant\_Ext\_T2\_2\_20231031032203 (F44) #8774, RT=11.836 min, MS2, FTMS (+), (HCD, DDA, 299.1747@(20;60),



### DPPD-quinone

2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #12112, RT=16.287 min, MS2, FTMS (+), (HCD, DDA, 291.1124@(20;60),



# DTPD-quinone

2023\_10\_26\_Quant\_Ext\_T1\_2\_20231031014550 (F41) #13162, RT=17.680 min, MS2, FTMS (+), (HCD, DDA, 319.1436@(20;60),

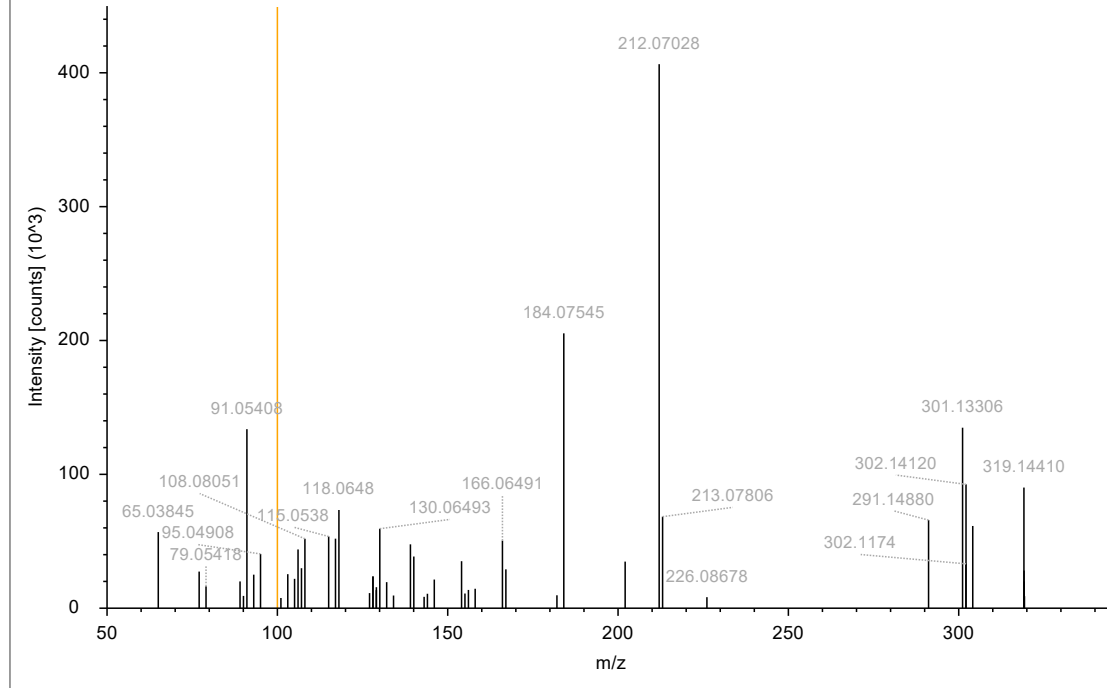
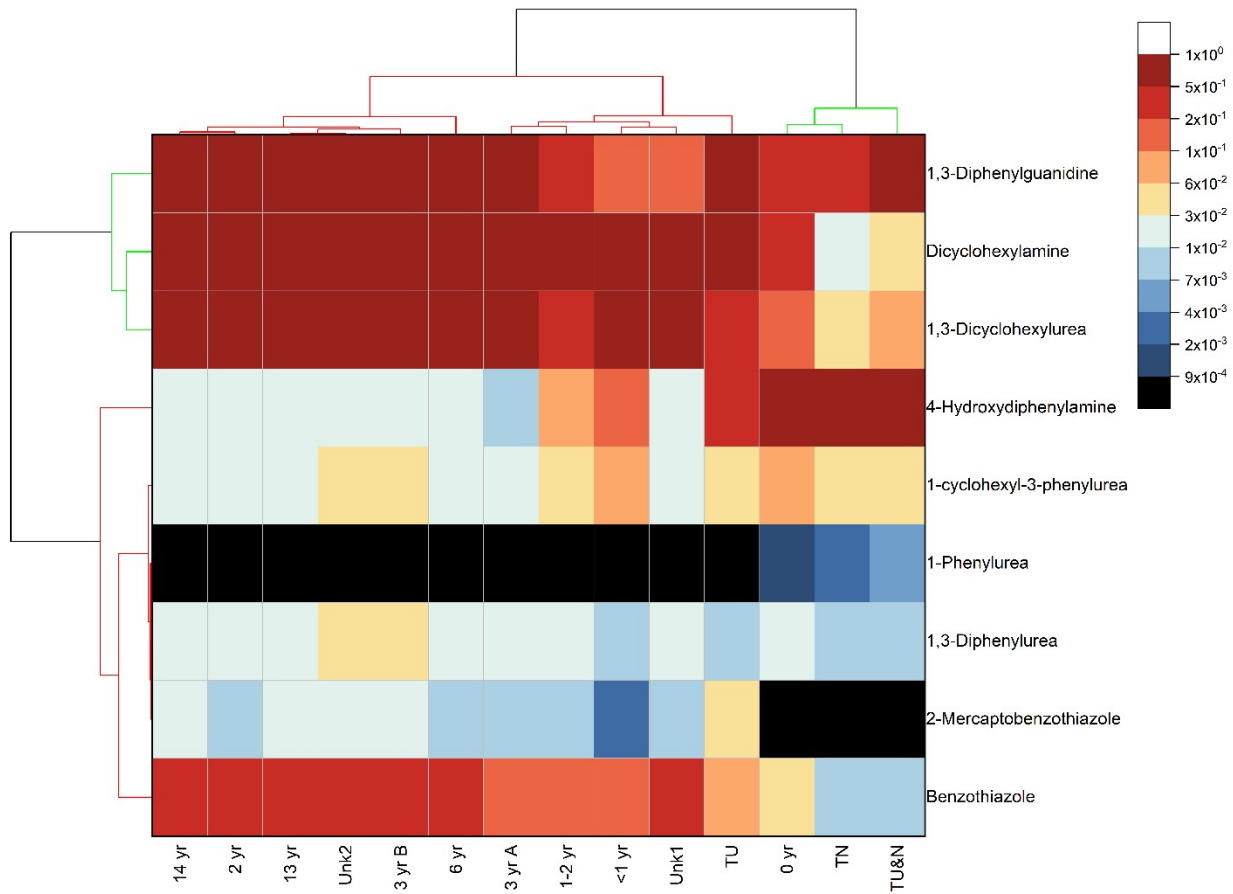


Figure S12. MS/MS of PPD transformation products in extractables.



**Figure S13.** Hierarchical clustering of tire and turf crumb rubber leachables in positive ion mode.