

Supplementary Information

Stability and transformation products of Rubber Derived Compounds in various storage conditions

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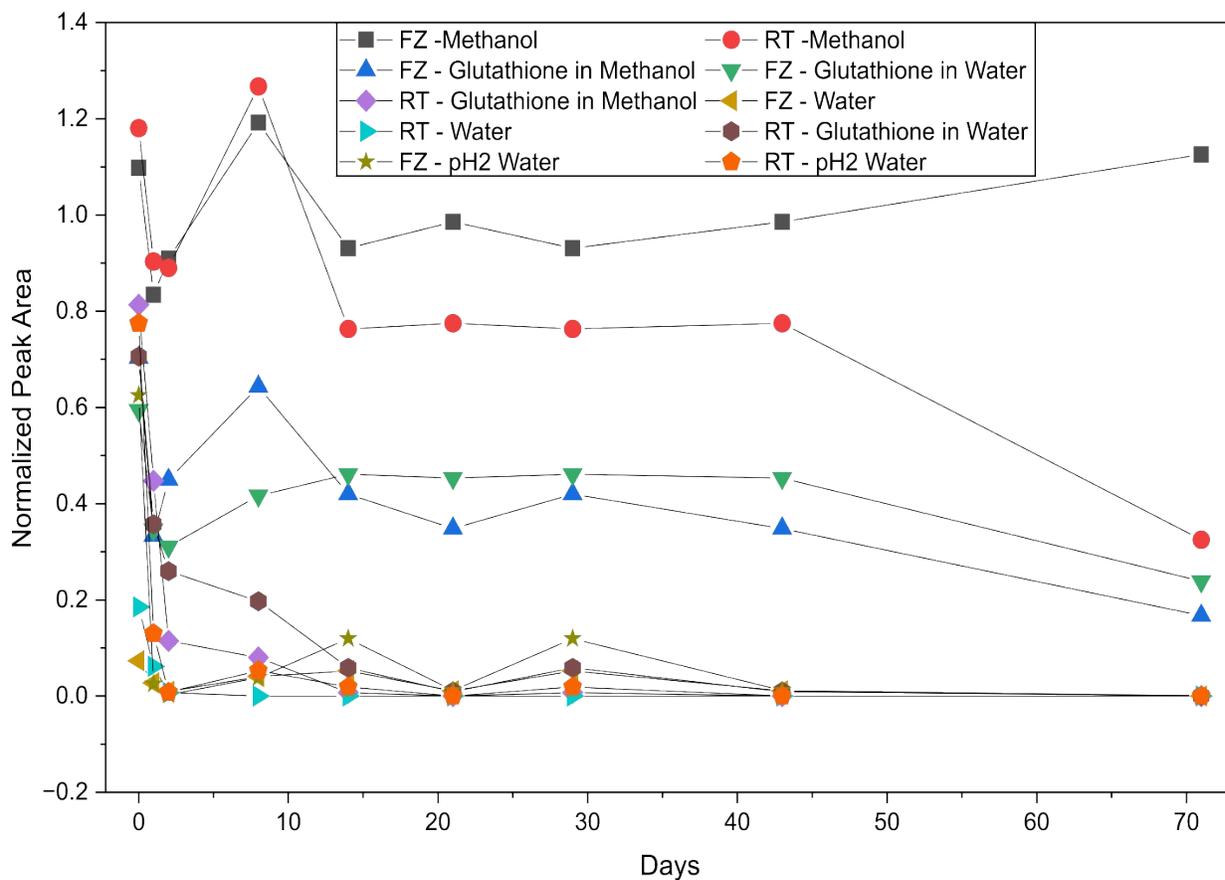


Figure S1. 6PPD normalized peak area data for FZ and RT conditions

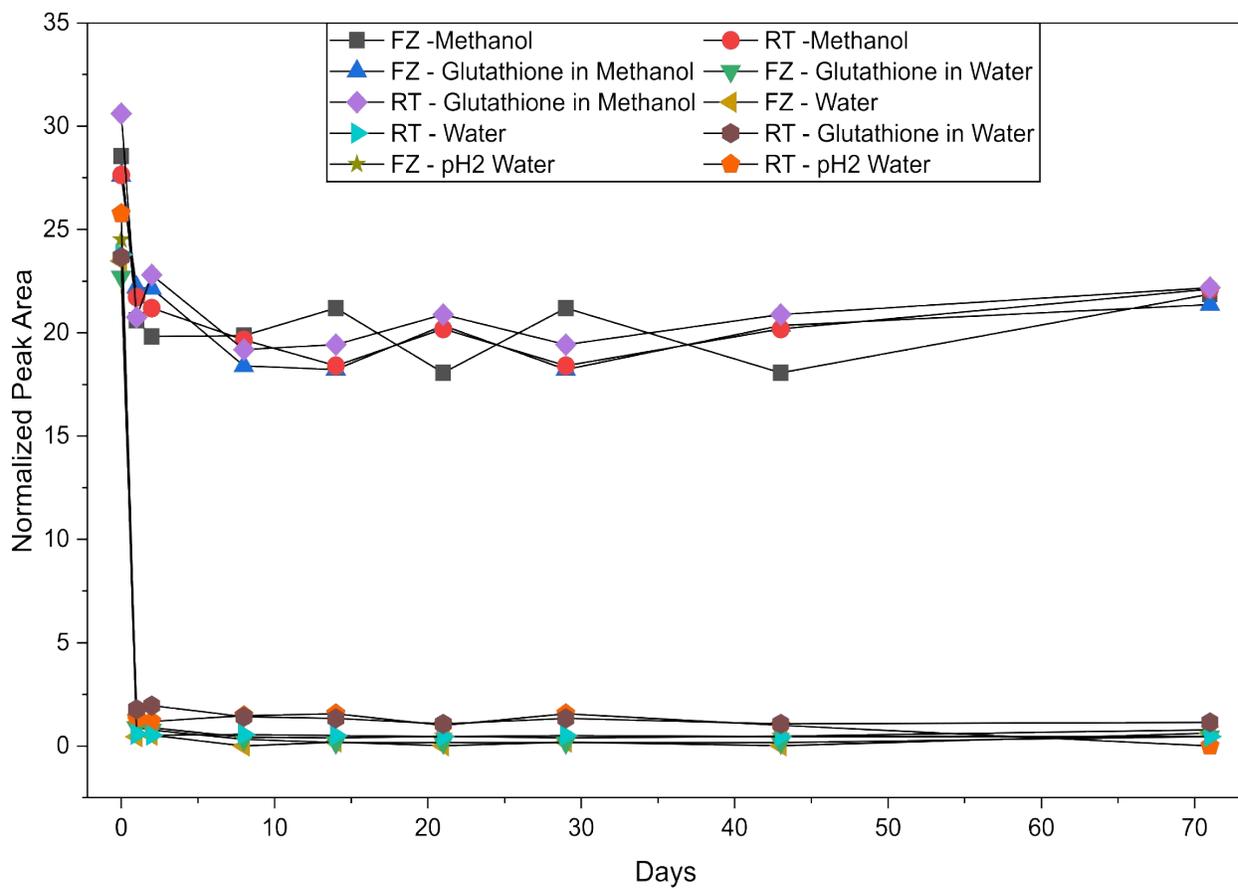


Figure S2. DTPD normalized peak area data for FZ and RT conditions

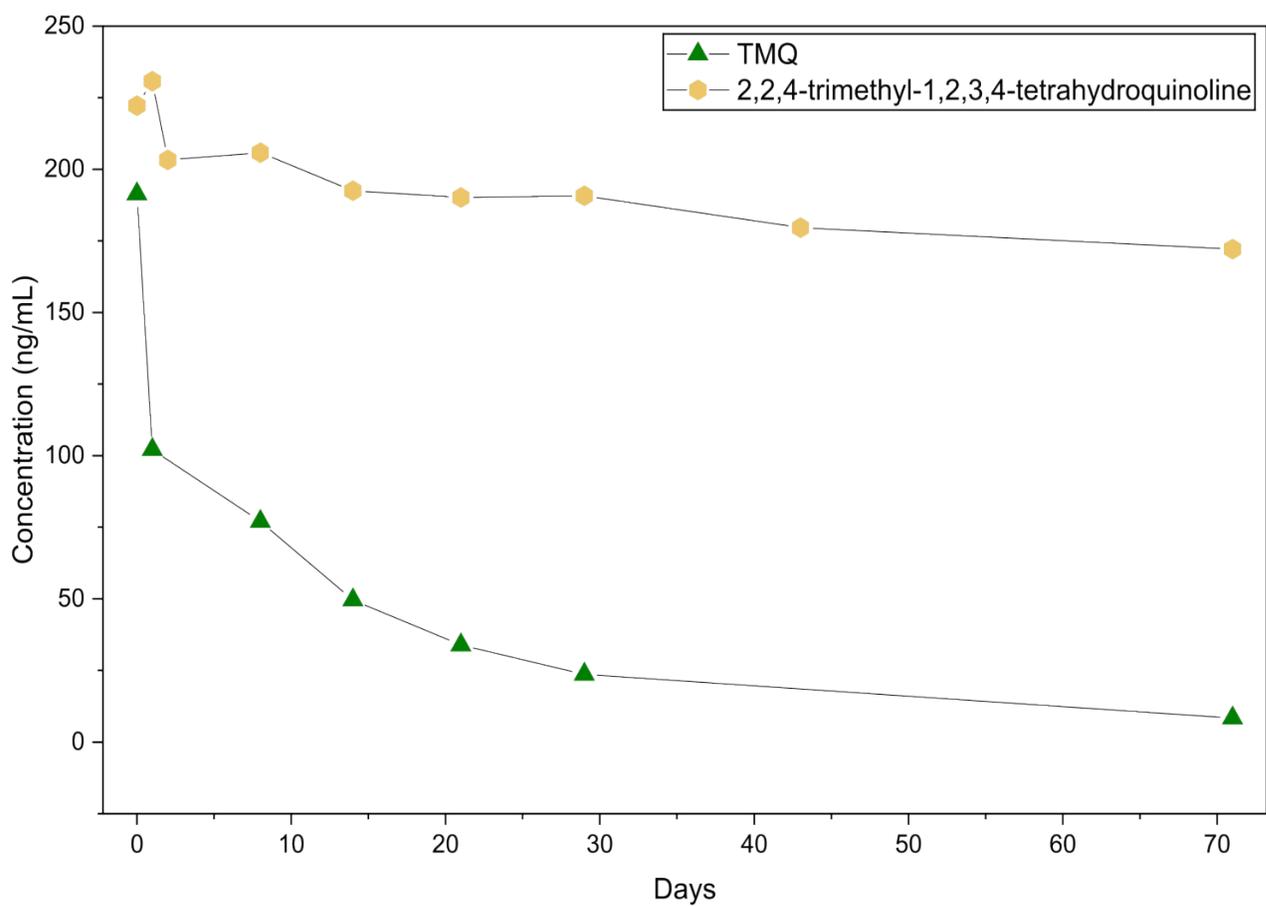


Figure S3. Trend data comparing TMQ and 2,2,4-trimethyl-1,2,3,4-tetrahydroquinoline in pH = 2 conditions

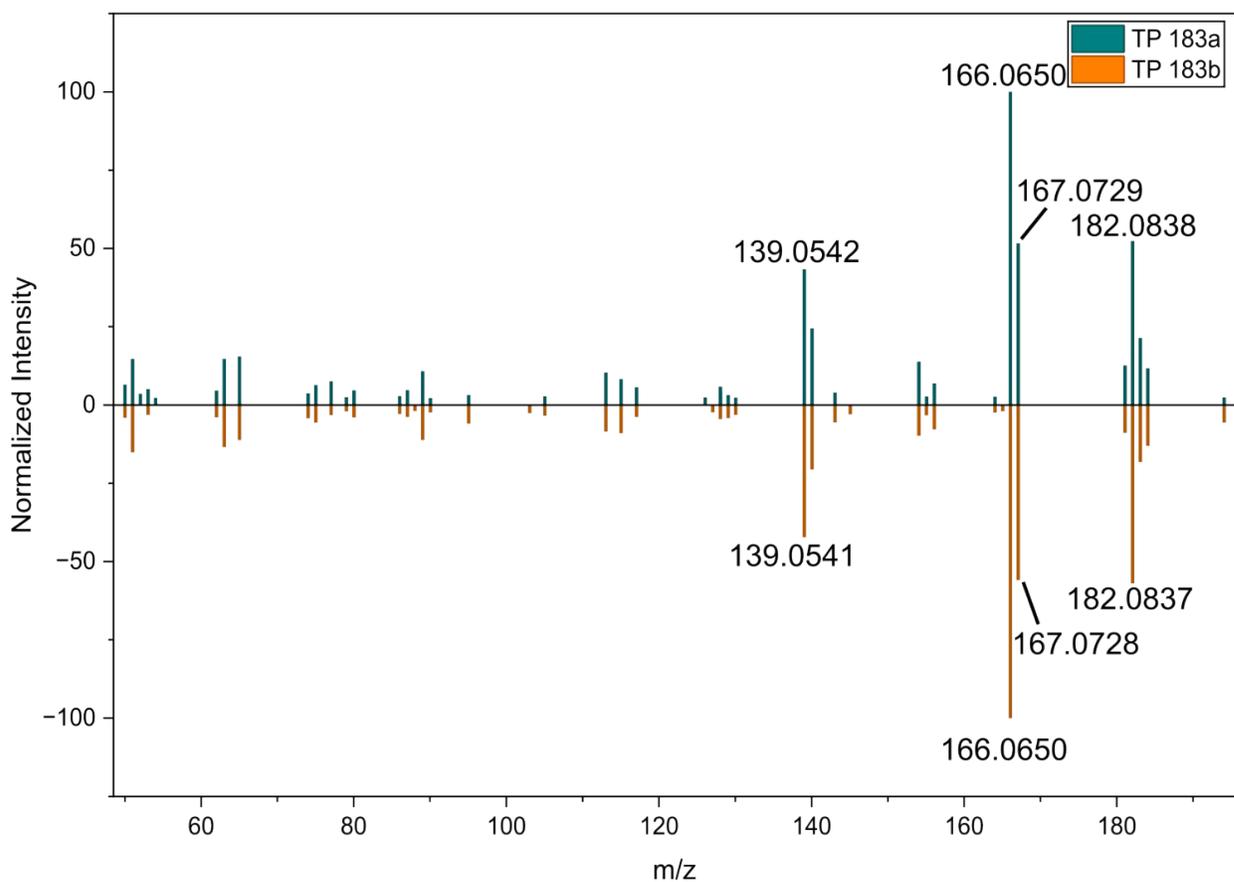


Figure S4. Comparison of TP 183a and TP 183b showing m/z fragments similar to 4-ADPA

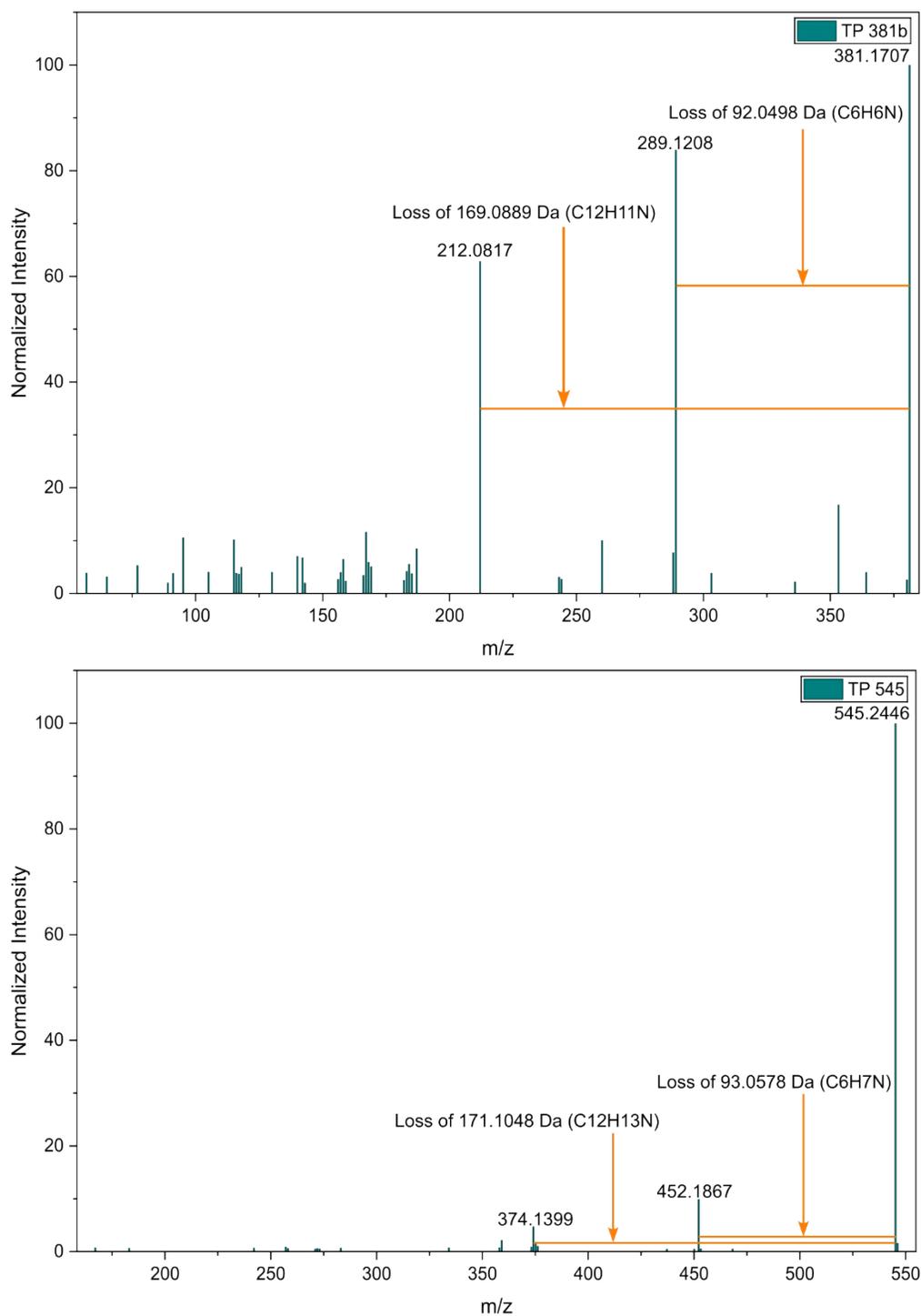


Figure S5. Comparison of TP 281b and TP 545 showing neutral losses that are shared with 4-ADPA

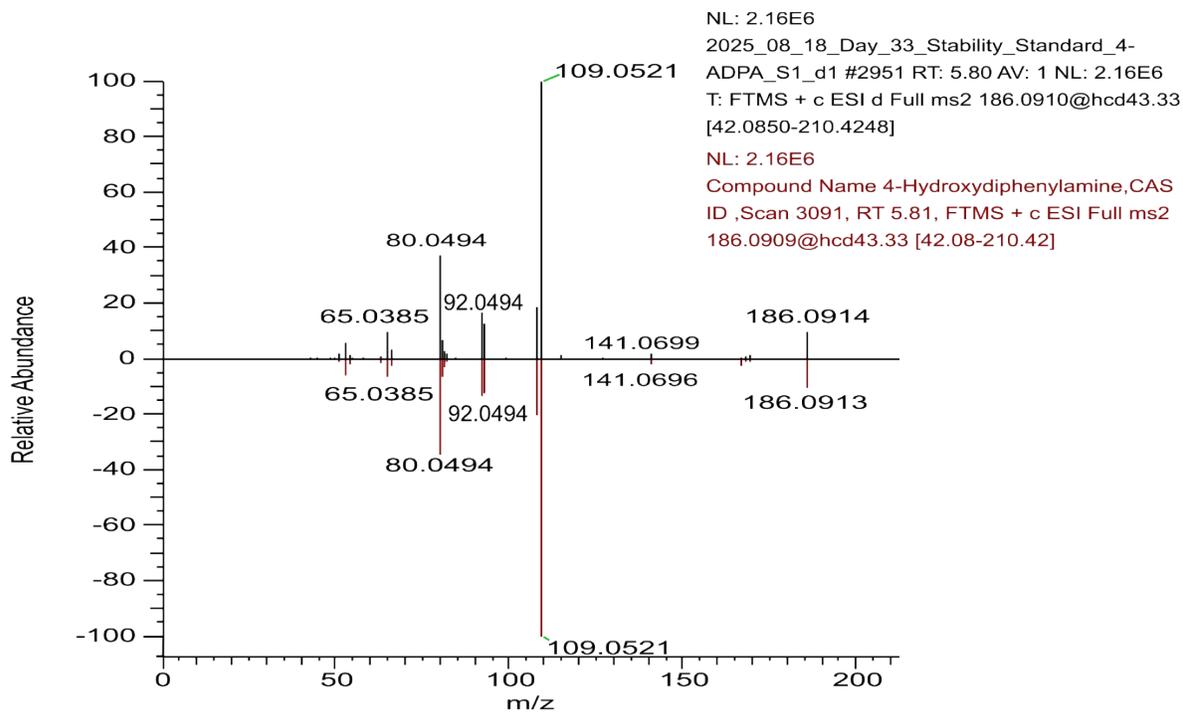
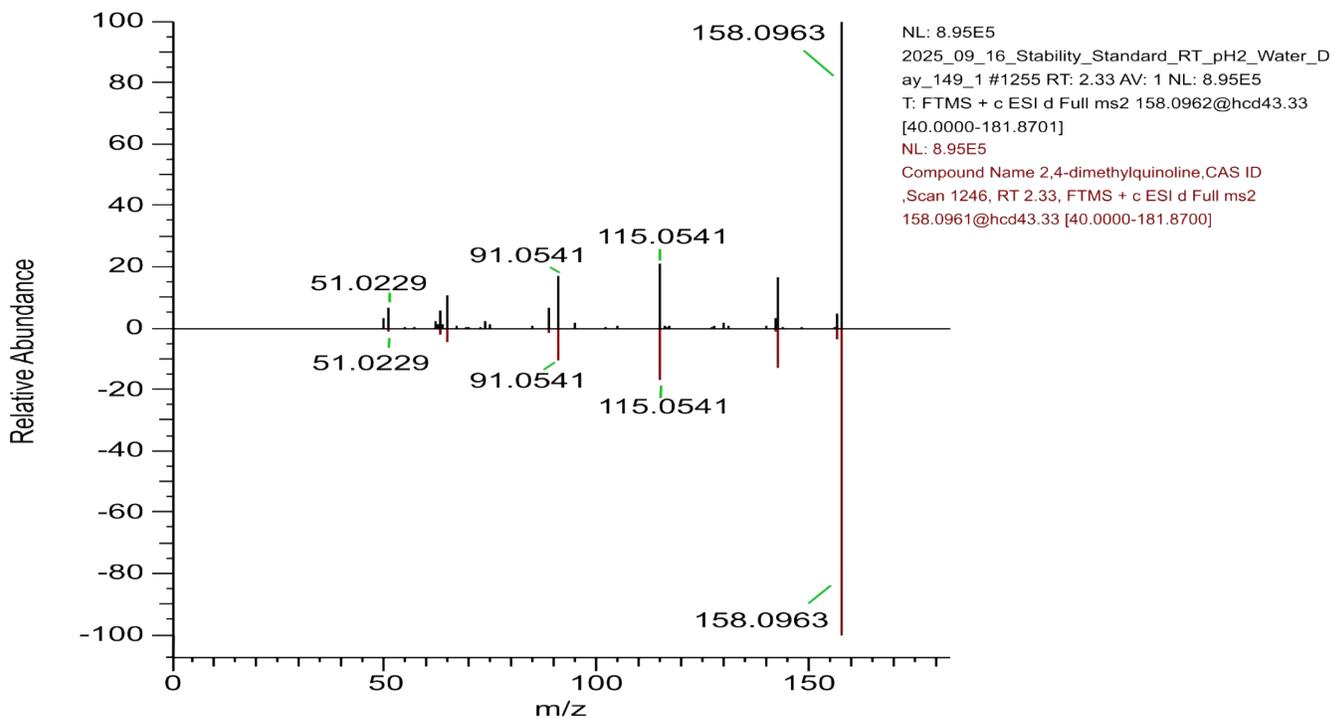
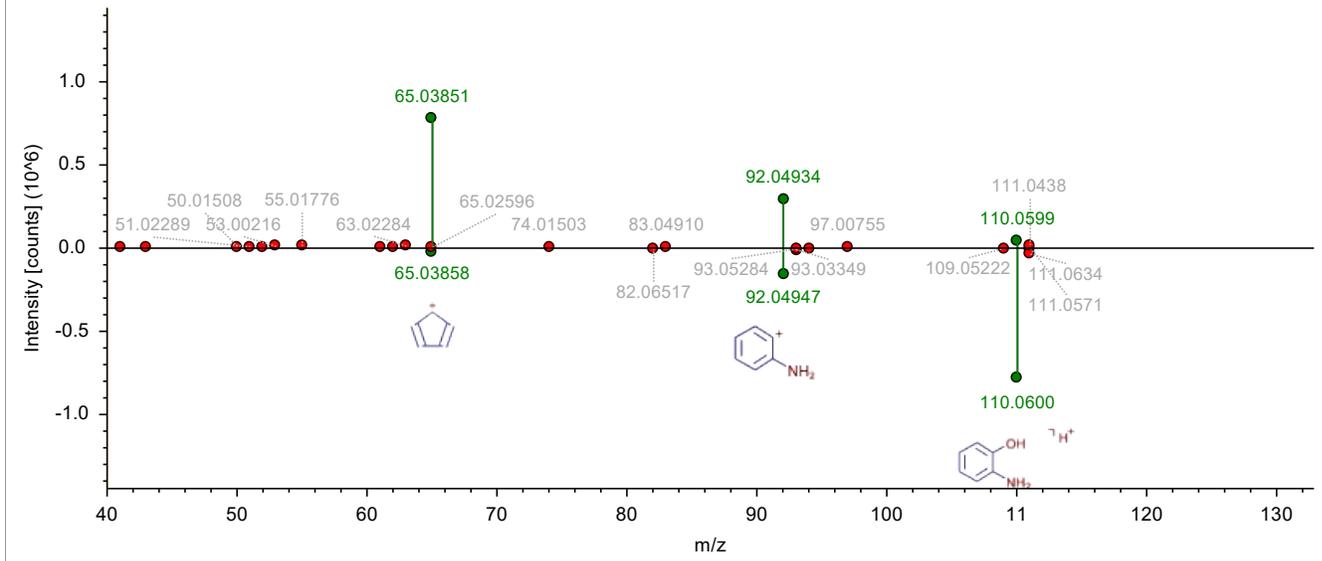


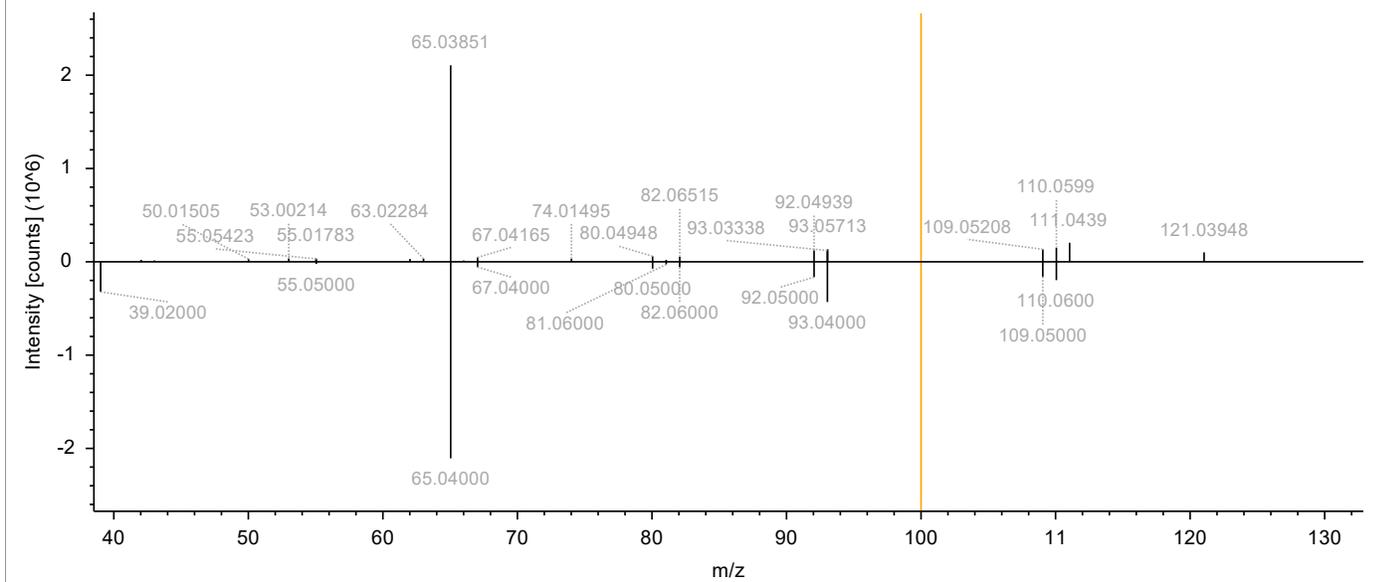
Figure S6. Comparison of experimental spectrum of 2,4-DMQ and 4-HDPA with in-house standard (Level 1 Identification)

RAWFILE(top): 2025_09_16_Stability_Standard_RT_Glutathione_Water_Day_149_1 (F54) #556, RT=1.012 min, MS2, FTMS (+), (HCD, DDA, 110.0598(+1))



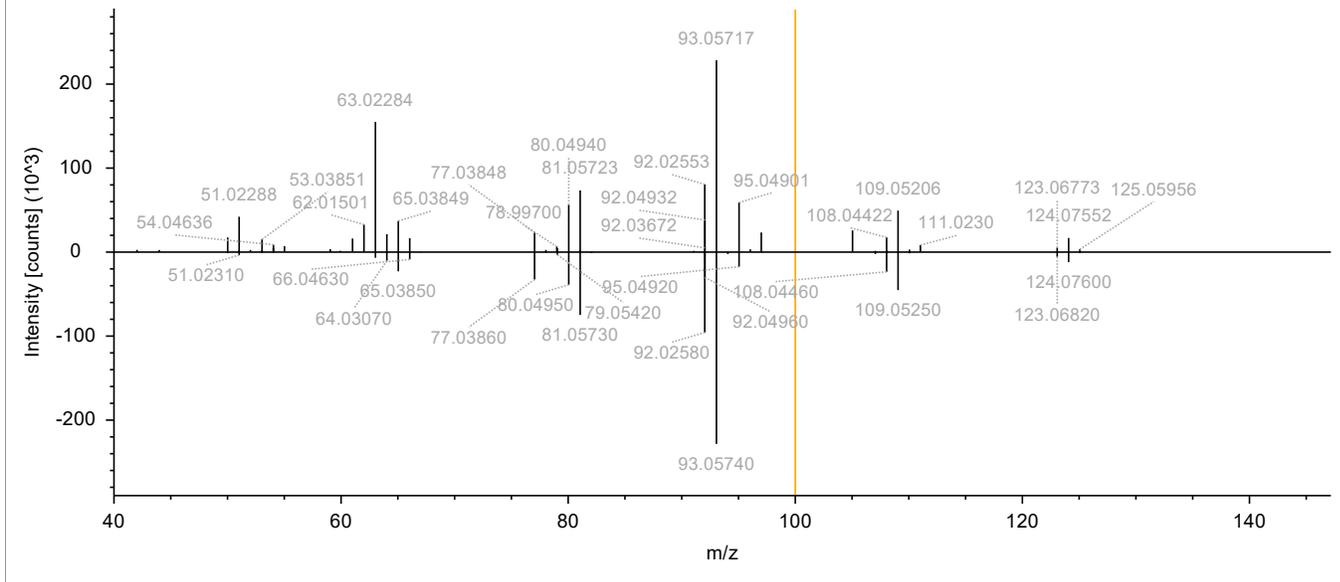
2-Aminophenol (78.7 match)

RAWFILE(top): 2025_08_08_Day_23_Stability_Standard_4sDPA_S2_d1 (F156) #342, RT=0.670 min, MS2, FTMS (+), (HCD, DDA, 110.0599@20;40;70+1)



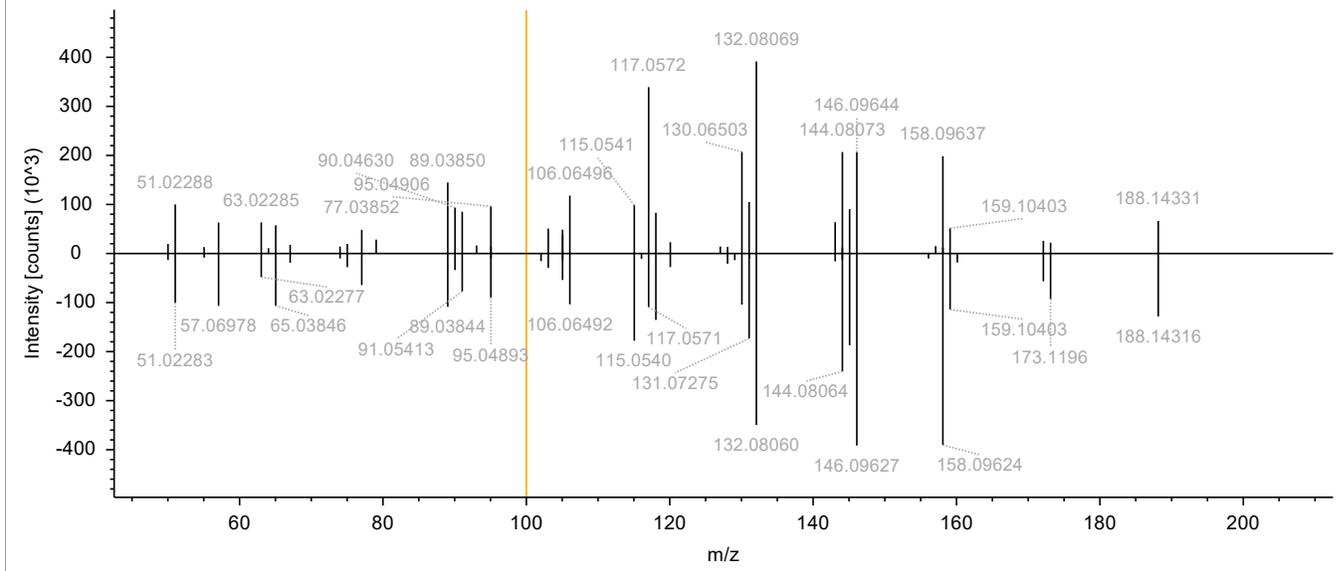
4-Aminophenol (88.9 match)

RAWFILE(top): 2025_09_16_Stability_Standard_RT_Glutathione_Methanol_Day_149_1 (F23) #862, RT=1.551 min, MS2, FTMS (+), (HCD, DDA, 124.07 +1)



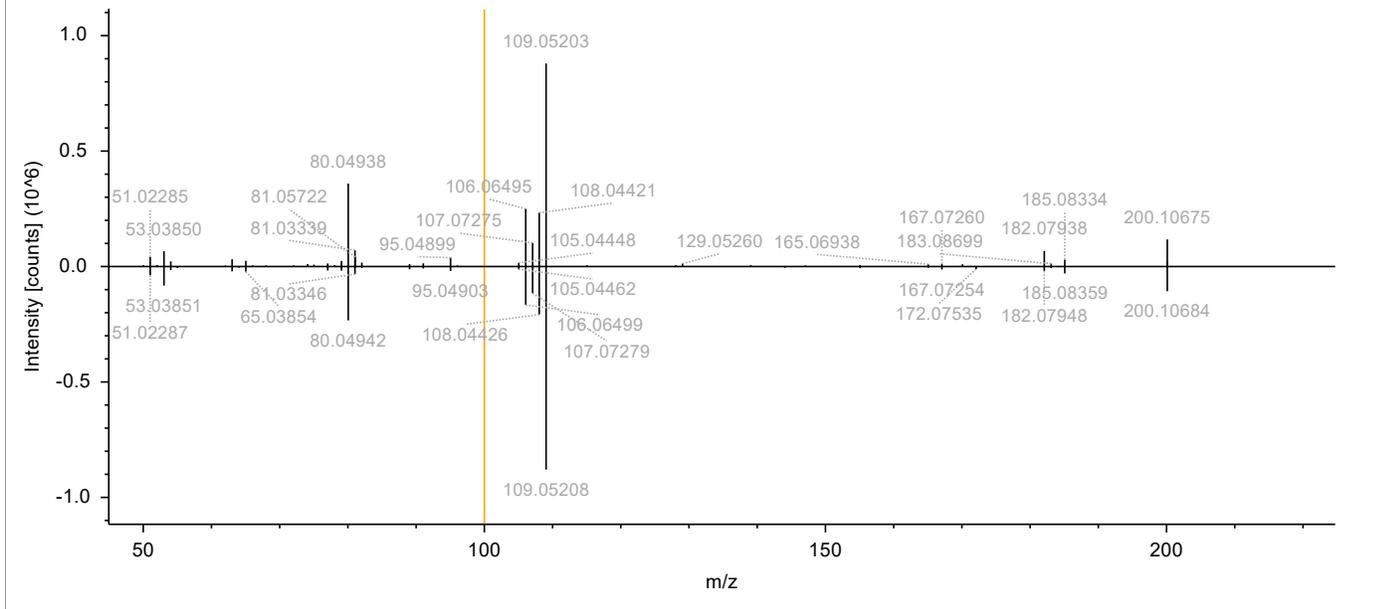
4-Methoxyaniline (83.6 match)

RAWFILE(top): 2025_07_23_Day_0_Stability_Standard_TMQ_S1_d1 (F101) #4100, RT=8.192 min, MS2, FTMS (+), (HCD, DDA, 188.1432@(20:40:70), +1)



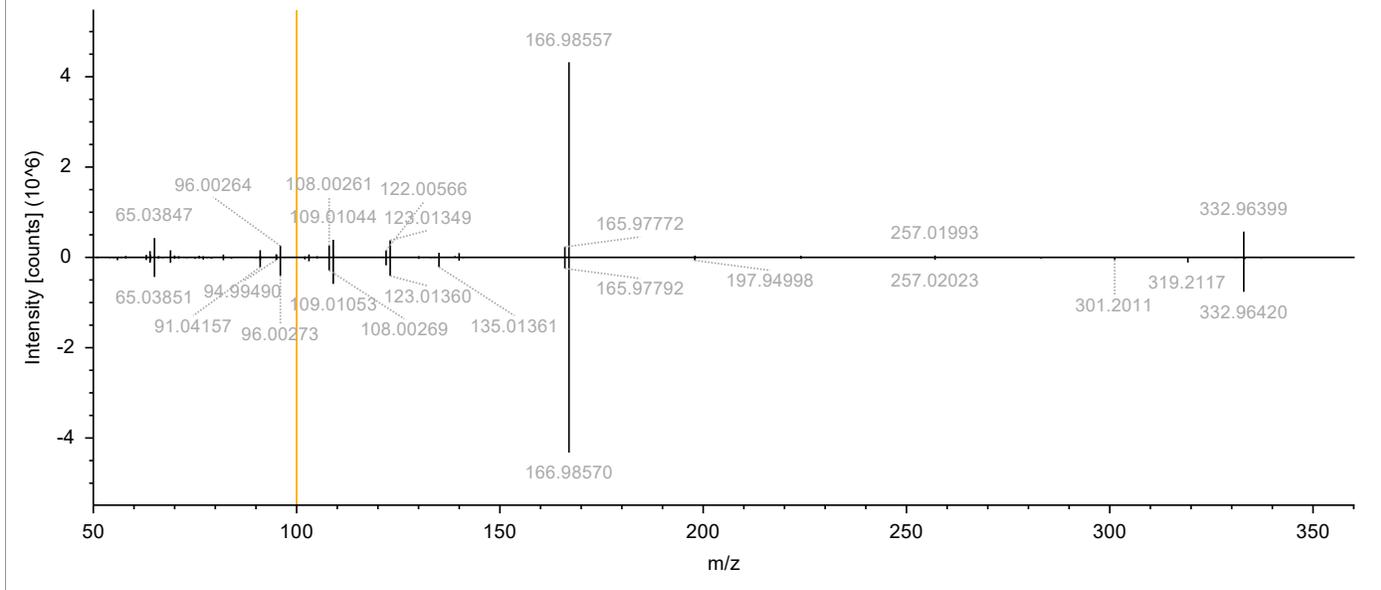
1,2-dihydro-2,2,4,7-tetramethylquinoline (91.2 match)

RAWFILE(top): 2025_09_16_Stability_Standard_RT_Water_Day_149_3 (F65) #3608, RT=6.804 min, MS2, FTMS (+), (HCD, DDA, 200.1066@(20;40;70)+1)



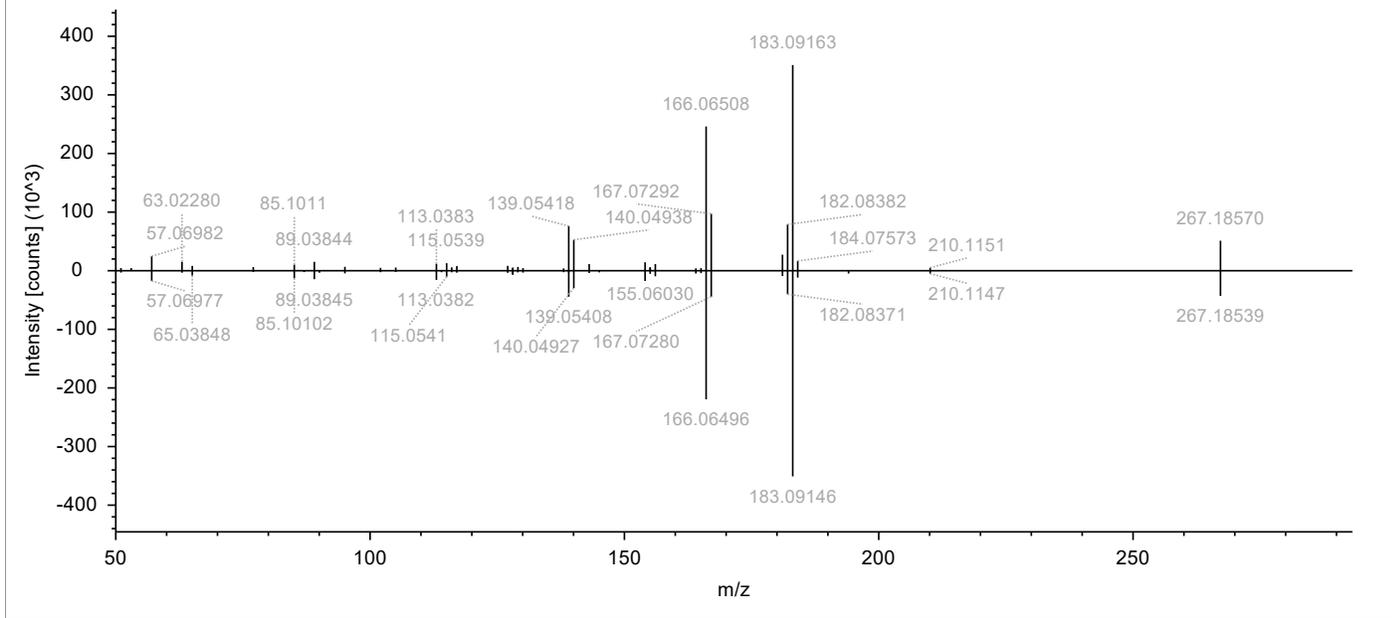
4-(4-methylanilino)phenol (95 match)

RAWFILE(top): 2025_08_08_Day_23_Stability_Standard_MBT_S3_d1 (F163) #5544, RT=10.700 min, MS2, FTMS (+), (HCD, DDA, 332.9639@(20;40;70)+1)



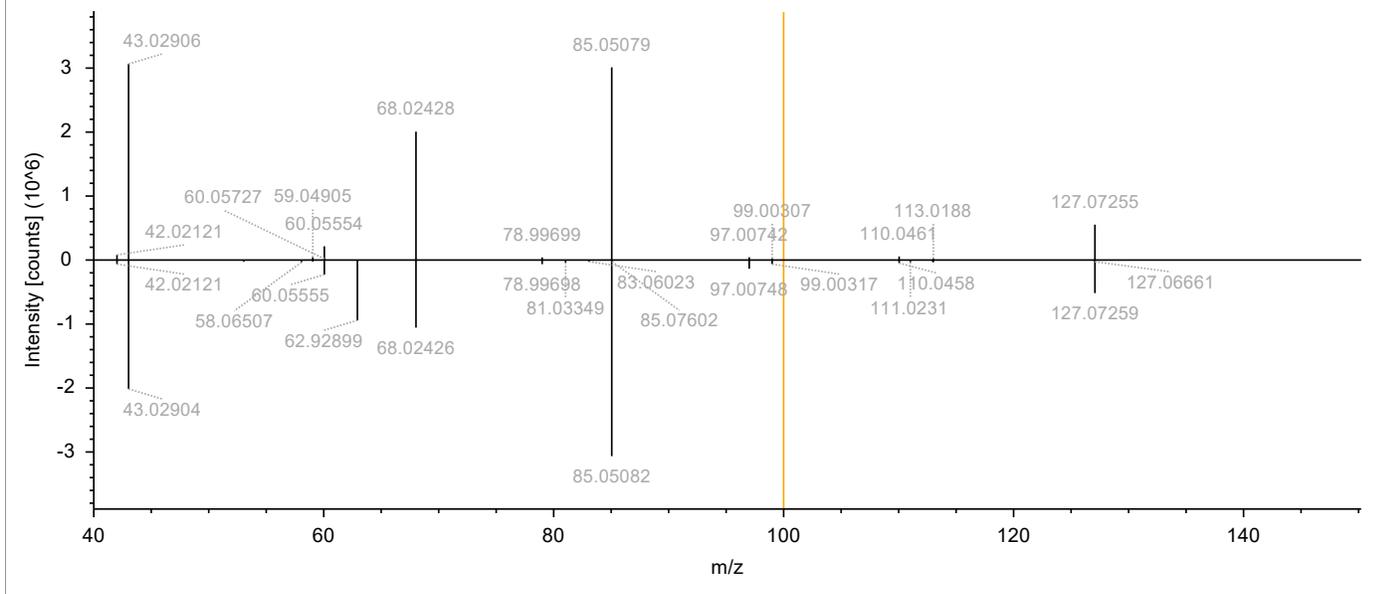
2,2-Dithiobis(benzothiazole) (93.4 match)

RAWFILE(top): 2025_07_23_Day_0_100_Cal_Check_STD_1 (F74) #2996, RT=5.936 min, MS2, FTMS (+), (HCD, DDA, 267.1855@(20;40;70), +1)



6QDI (91.9 match)

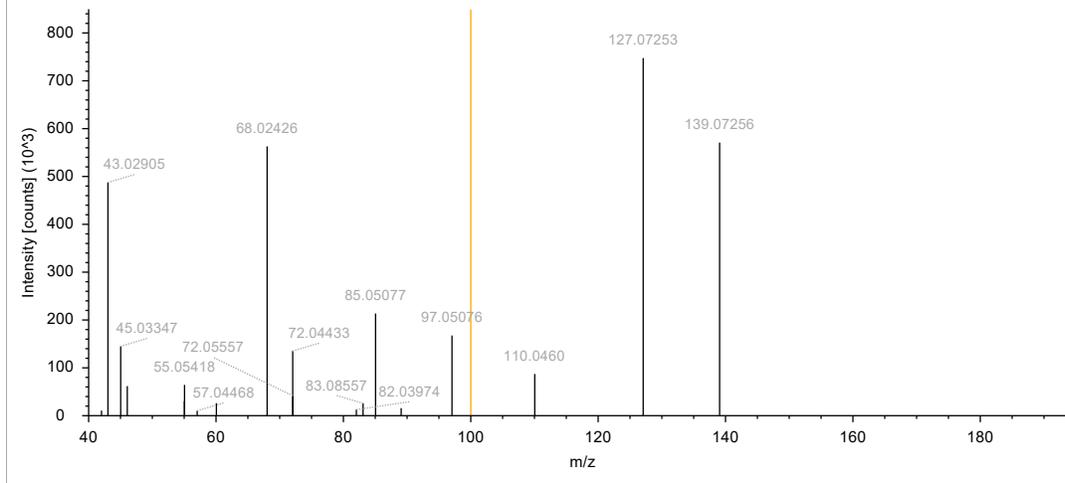
RAWFILE(top): 2025_09_16_Stability_Standard_RT_pH2_Water_Day_149_3 (F62) #338, RT=0.635 min, MS2, FTMS (+), (HCD, DDA, 127.0725@(20;40;70), +1)



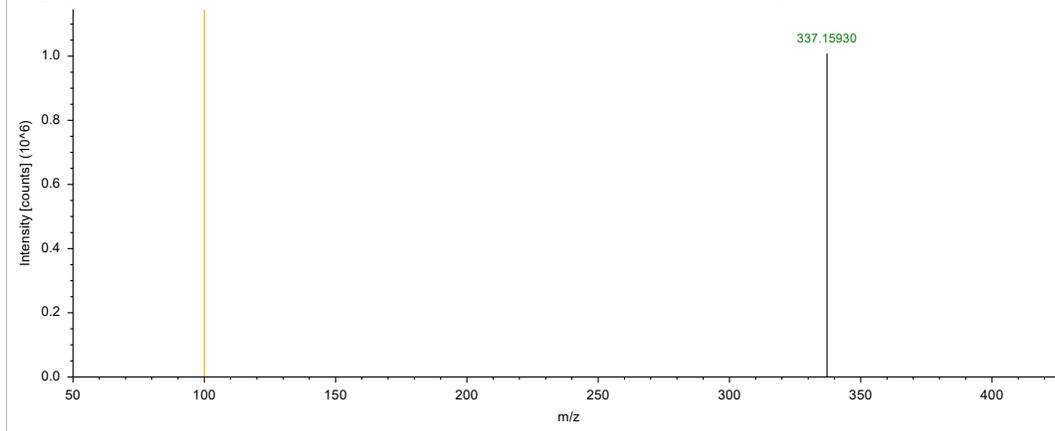
Melamine (88.6 match)

Figure S7. Comparison of experimental spectrum with mzVault, and mzCloud libraries in CD 3.3

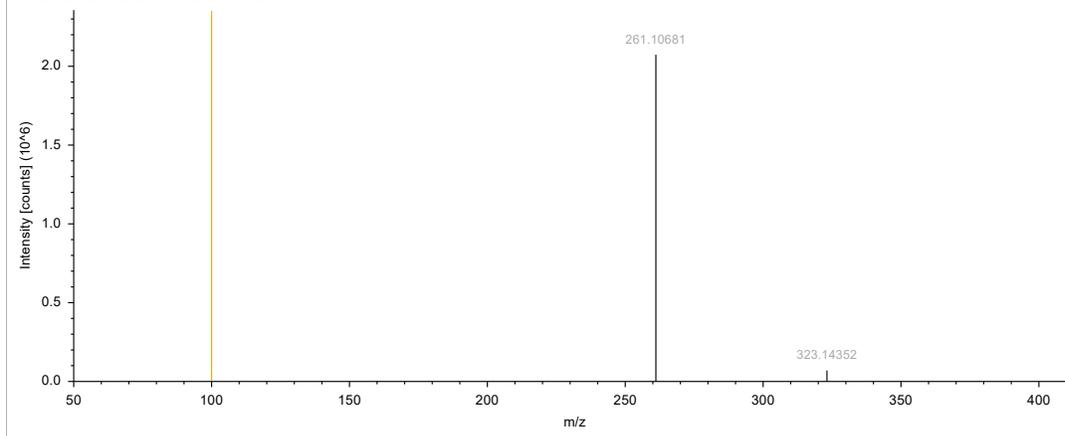
2025_08_18_Day_33_Stability_Standard_HMMM_S2_d1 (F128) #493, RT=0.936 min, MS2, FTMS (+), (HCD, DDA, 171.0987@(20;40;70),



2025_07_23_Day_0_Stability_Standard_HMMM_S2_d1 (F91) #2695, RT=5.295 min, MS2, FTMS (+), (HCD, DDA, 399.1957@(20;40;70),

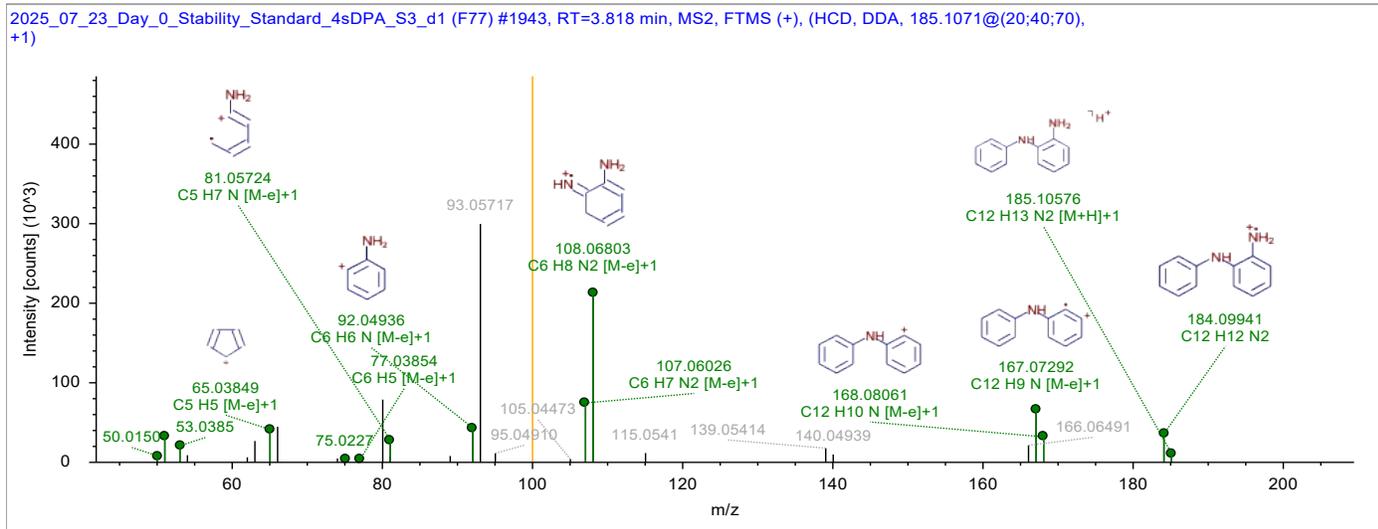


2025_07_23_Day_0_Stability_Standard_HMMM_S2_d1 (F91) #2238, RT=4.397 min, MS2, FTMS (+), (HCD, DDA, 385.1801@(20;40;70),

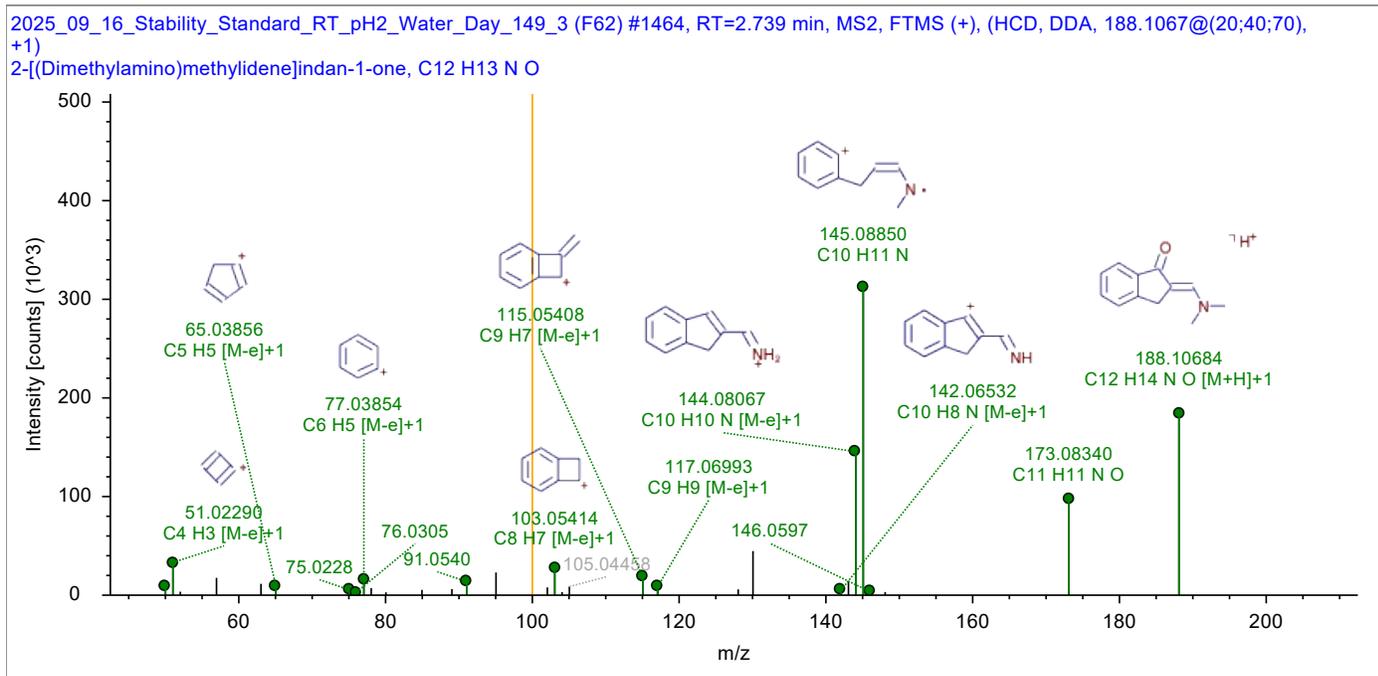


Methoxymethylmelamine (MonoMMM), TP 363, and TP 377 Matched with: Hexamethoxymethylmelamine - A precursor of persistent and mobile contaminants in municipal wastewater and the water cycle¹

Figure S8. Mass spectra of MonoMMM, TP363, and TP 377 with literature match citation (Level 2 Identification)

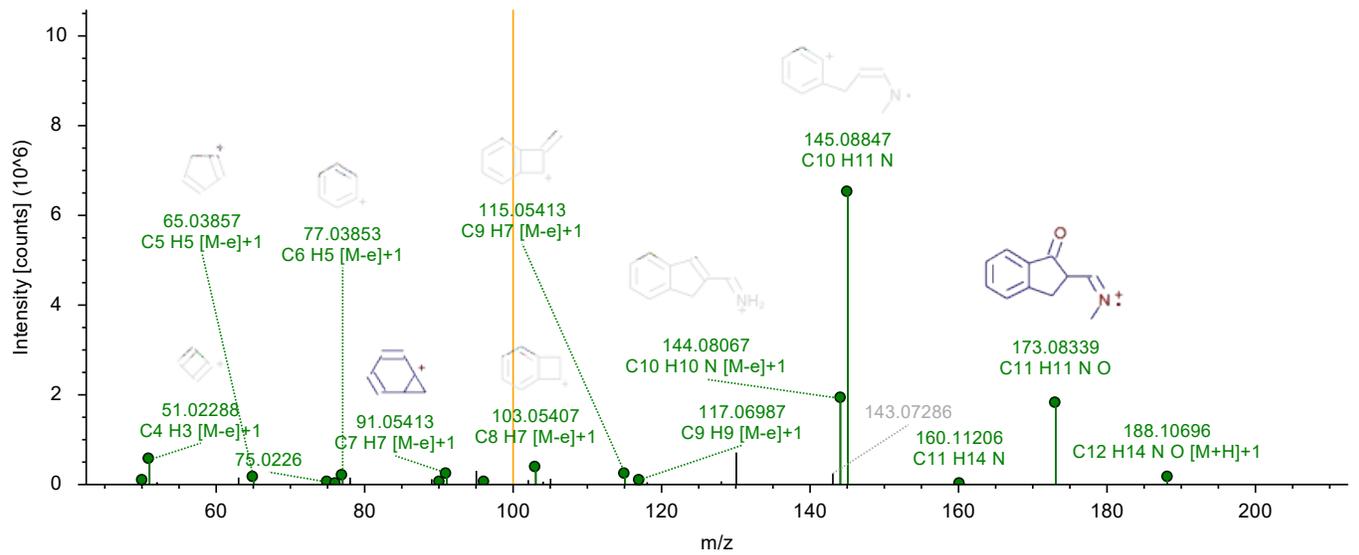


TP 185



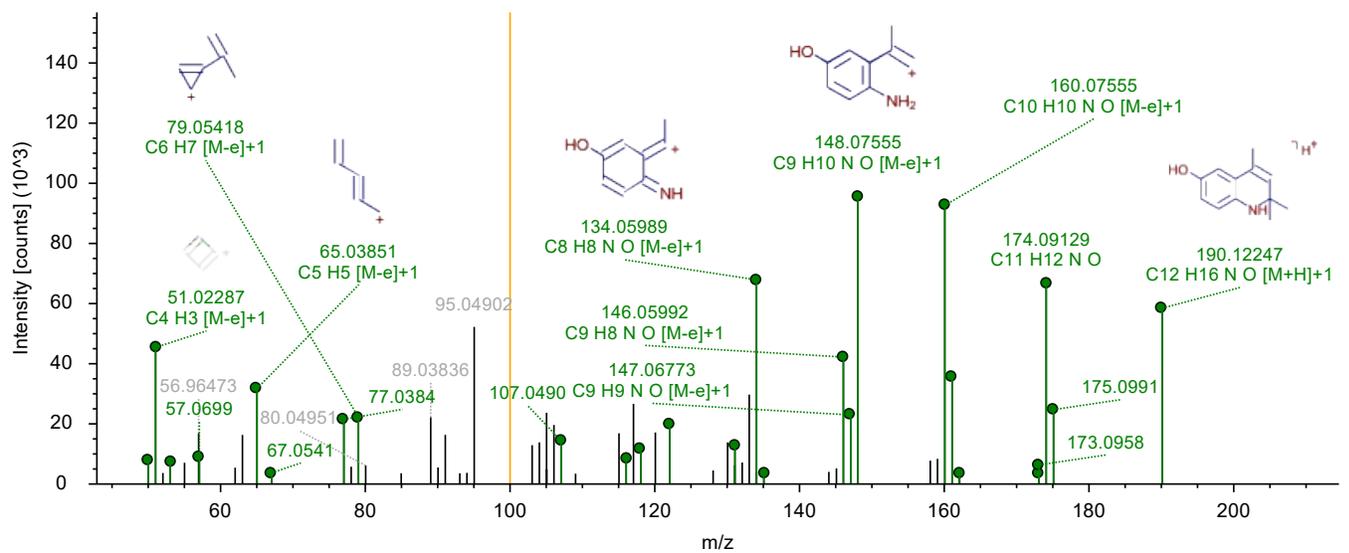
TP 188a

2025_08_18_Day_33_Stability_Standard_TMQ_S1_d1 (F31) #2985, RT=5.821 min, MS2, FTMS (+), (HCD, DDA, 188.1069@(20;40;70), +1)
2-[(Dimethylamino)methylidene]indan-1-one, C12 H13 N O



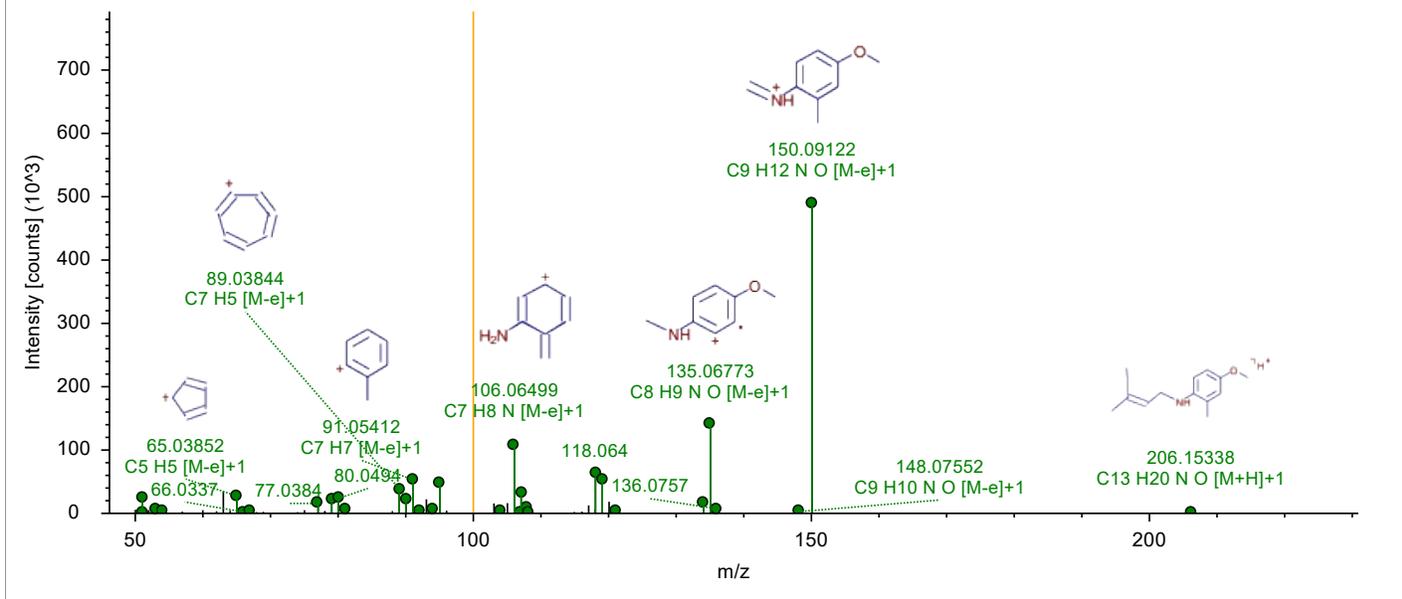
TP 188c

2025_09_16_Stability_Standard_RT_Water_Day_149_3 (F37) #1509, RT=2.831 min, MS2, FTMS (+), (HCD, DDA, 190.1224@(20;40;70), +1)
2,2,4-Trimethyl-1,2-dihydro-6-quinolinol, C12 H15 N O

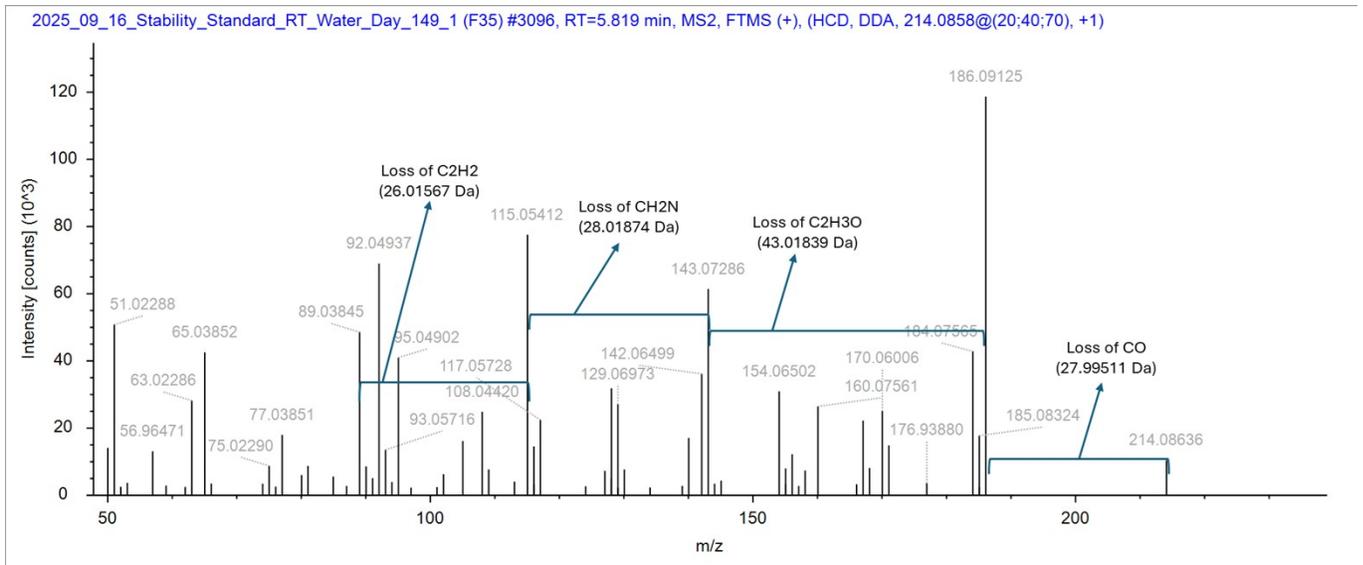


TP 190

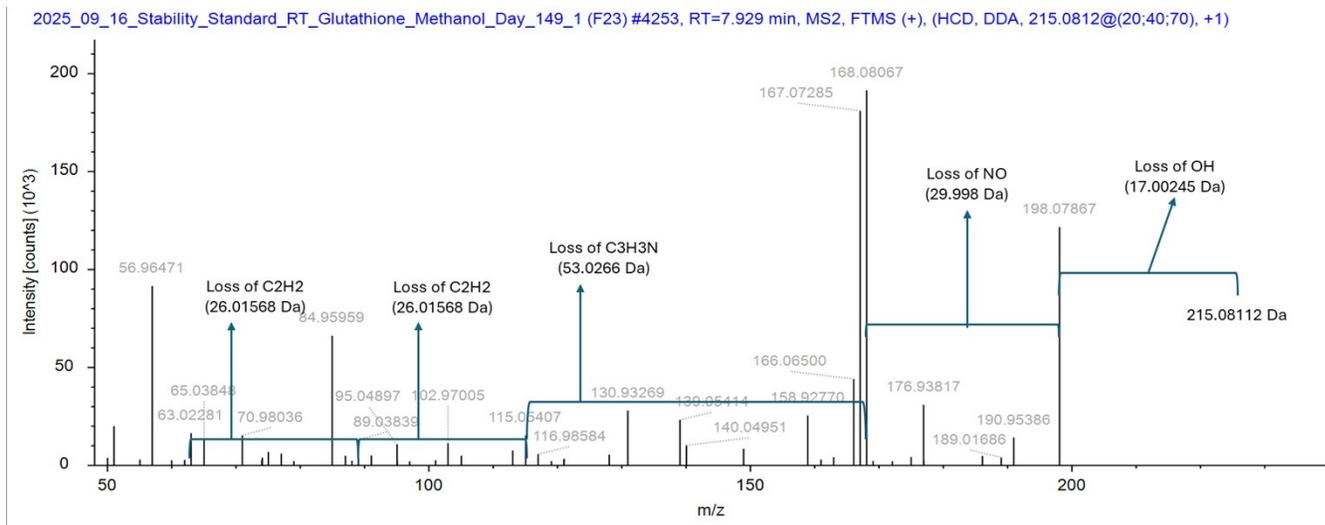
2025_09_16_Stability_Standard_RT_pH2_Water_Day_149_2 (F33) #1899, RT=3.545 min, MS2, FTMS (+), (HCD, DDA, 206.1536@(20;40;70), +1)
 C13 H19 N O



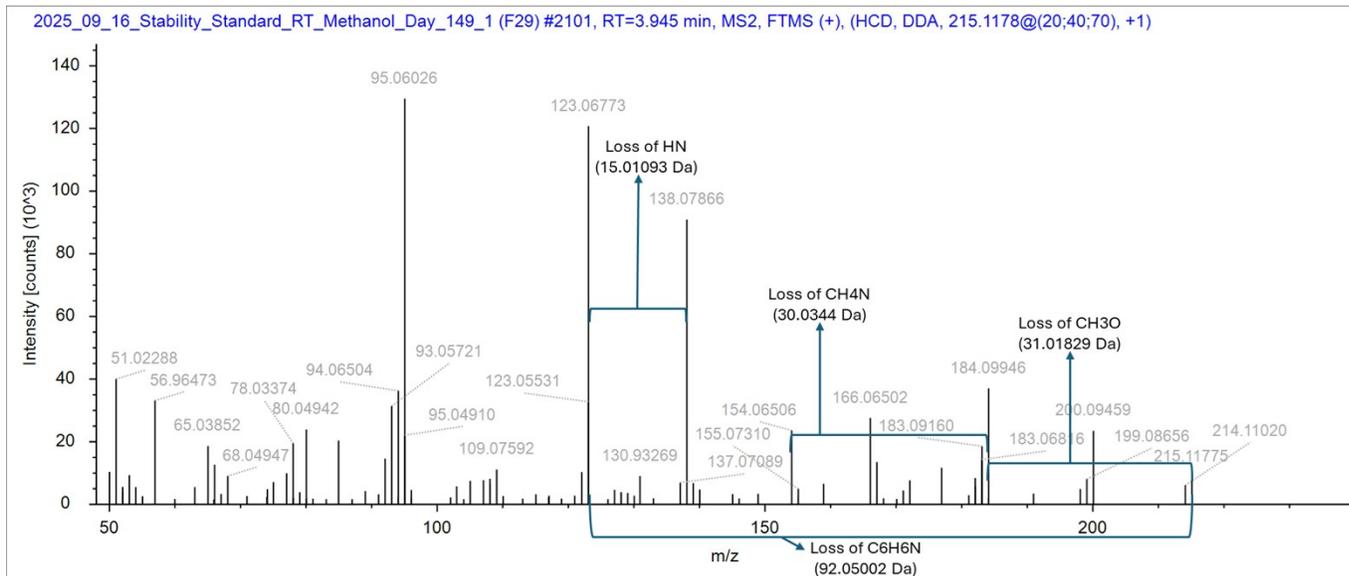
Feature 206



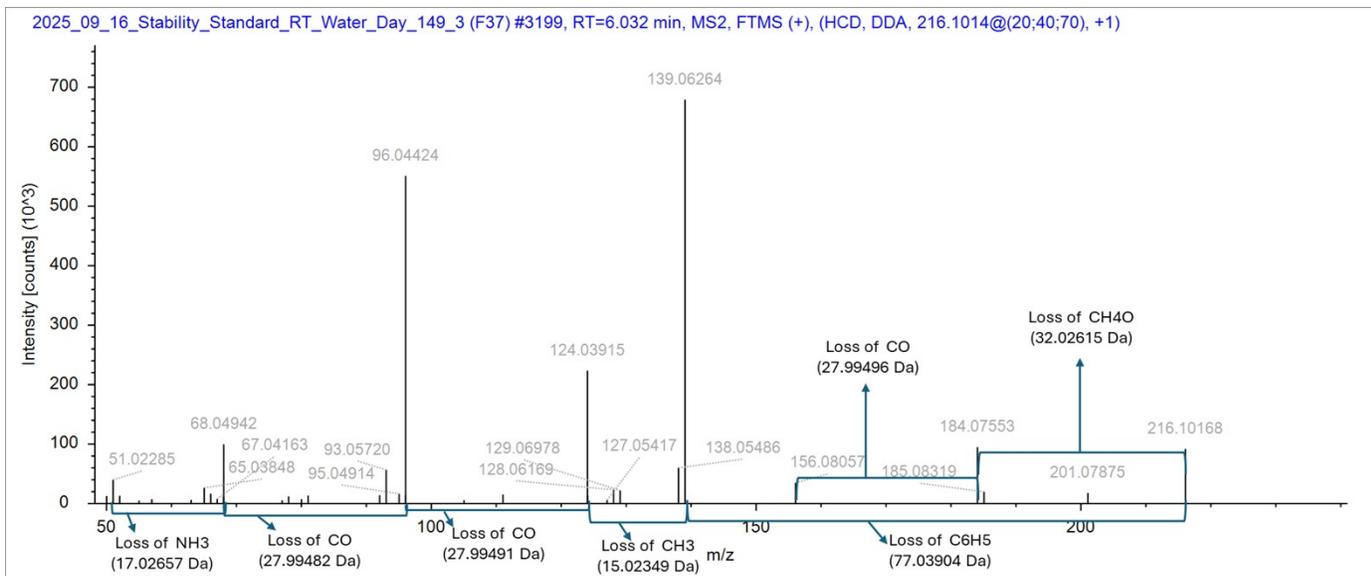
TP 214



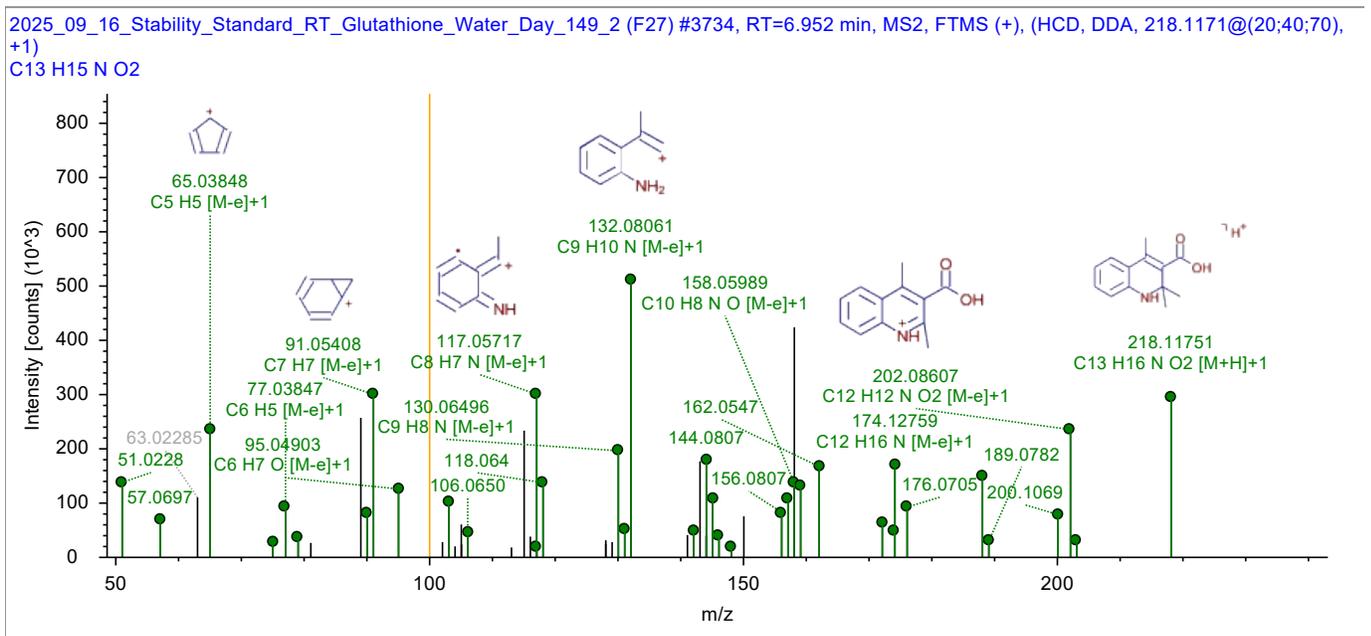
Impurity 215



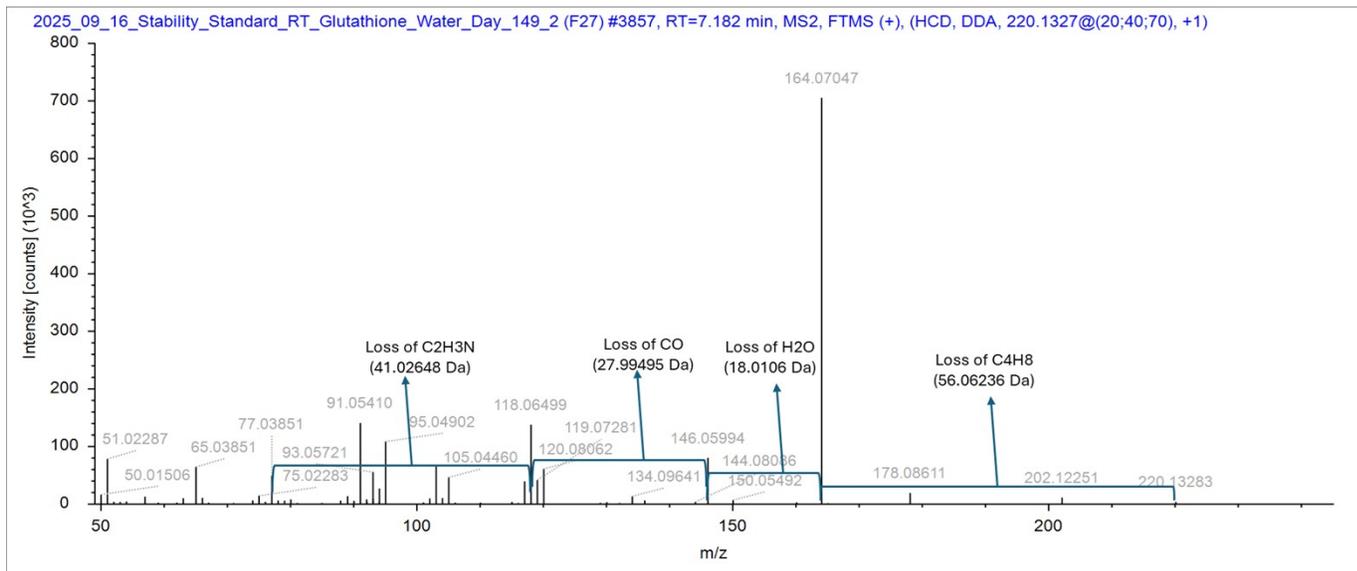
Feature 215a



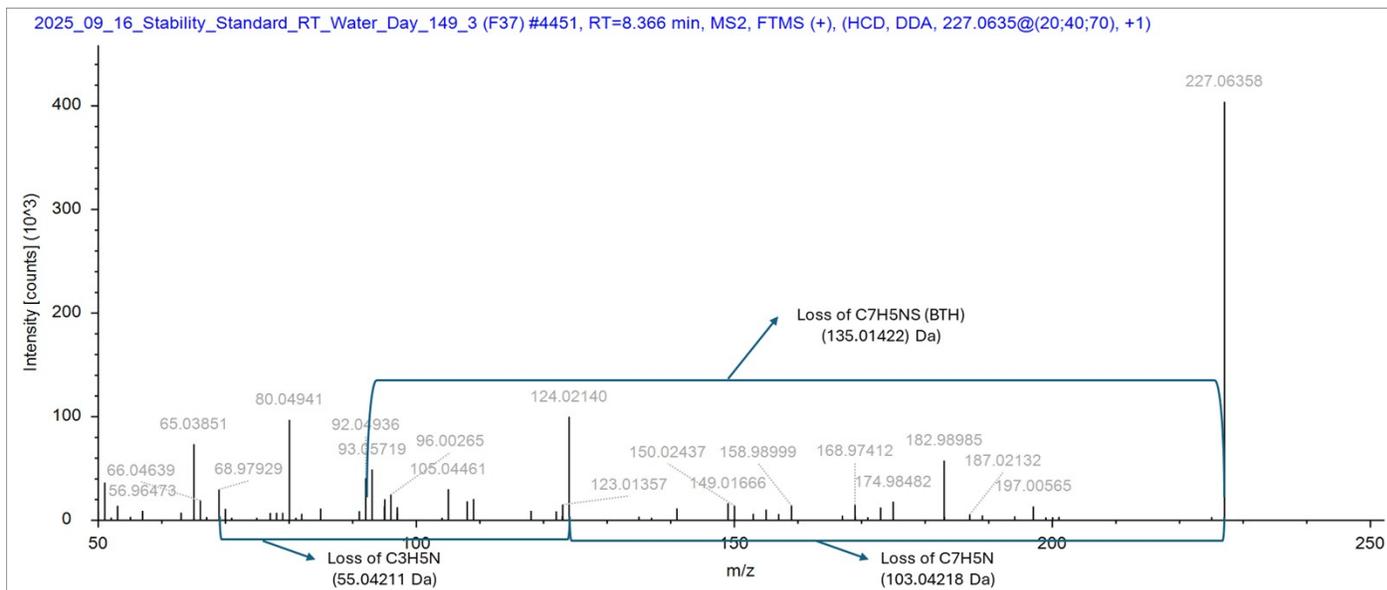
TP 216a



Feature 218a

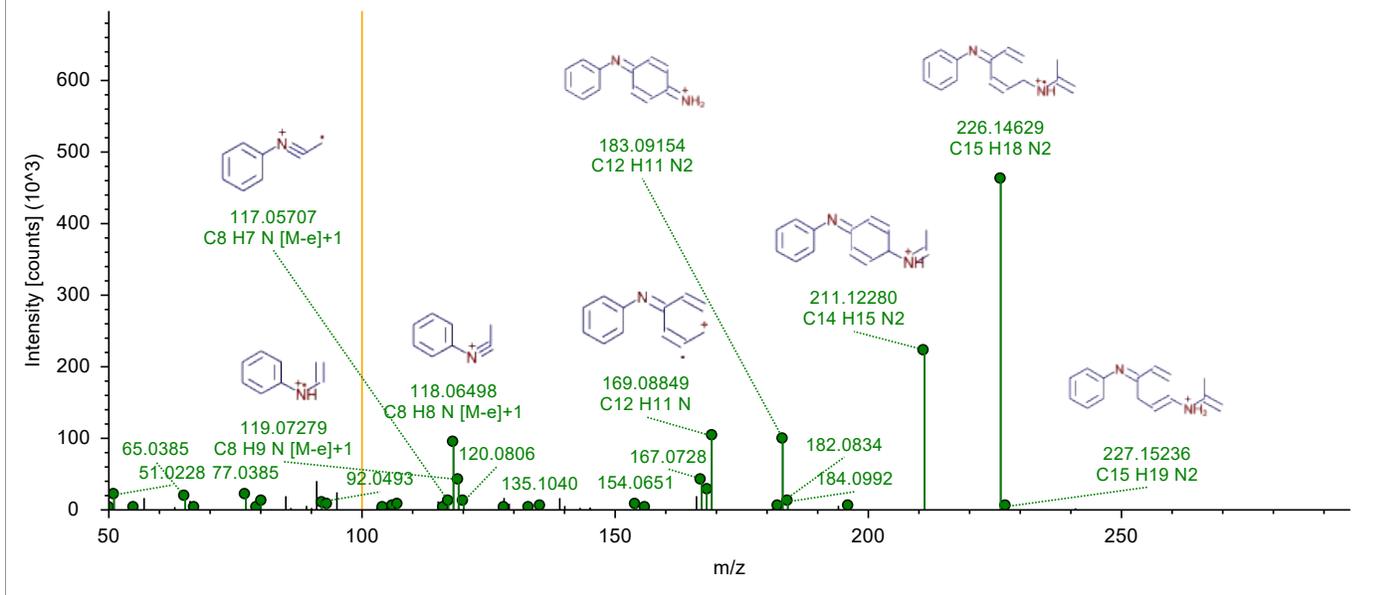


Feature 220b



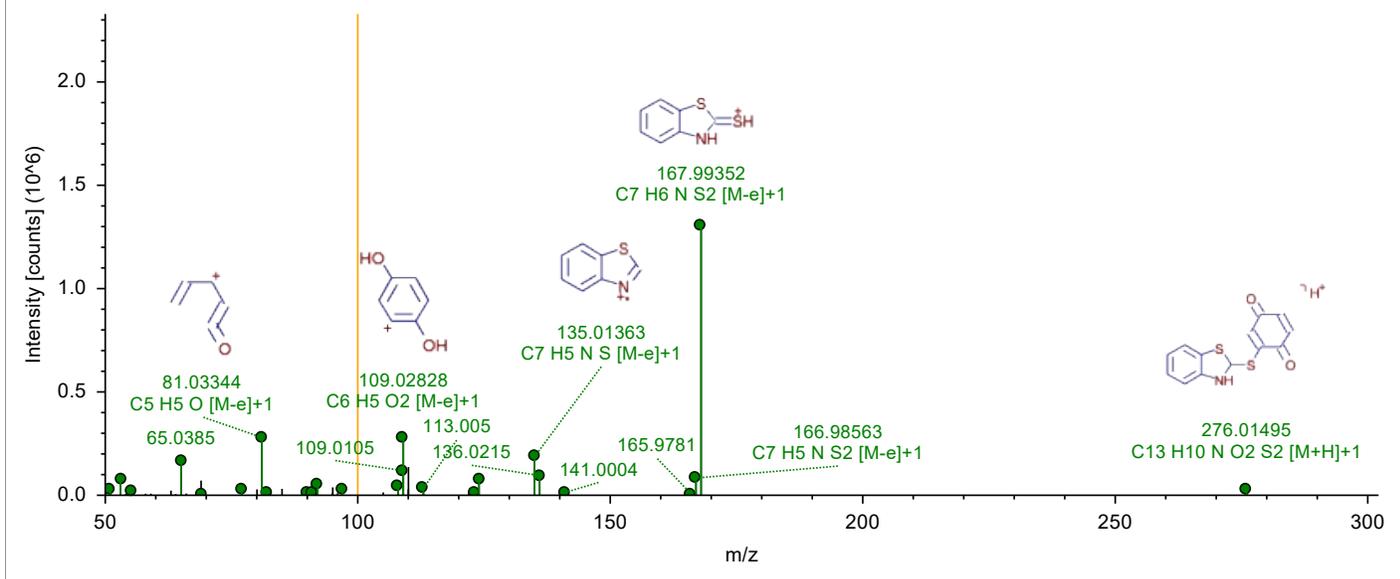
Impurity 227

2025_09_16_Stability_Standard_RT_Methanol_Day_149_3 (F31) #2563, RT=4.822 min, MS2, FTMS (+), (HCD, DDA, 269.2009@(20;40;70), +1)
C18 H24 N2

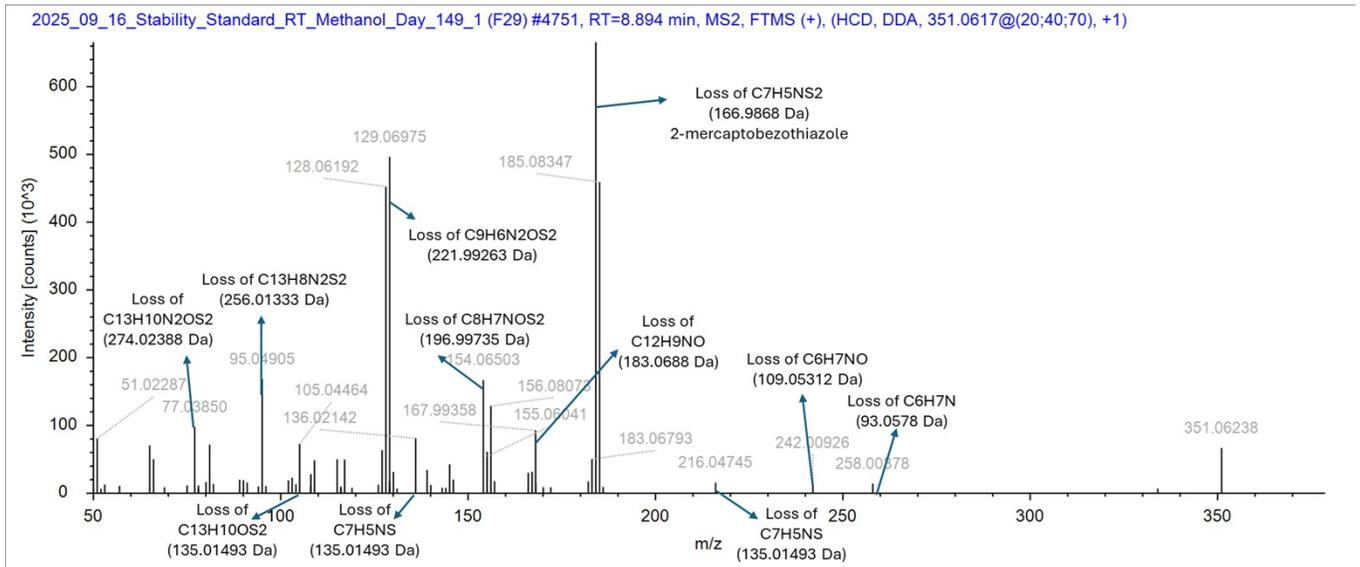


Feature 269b

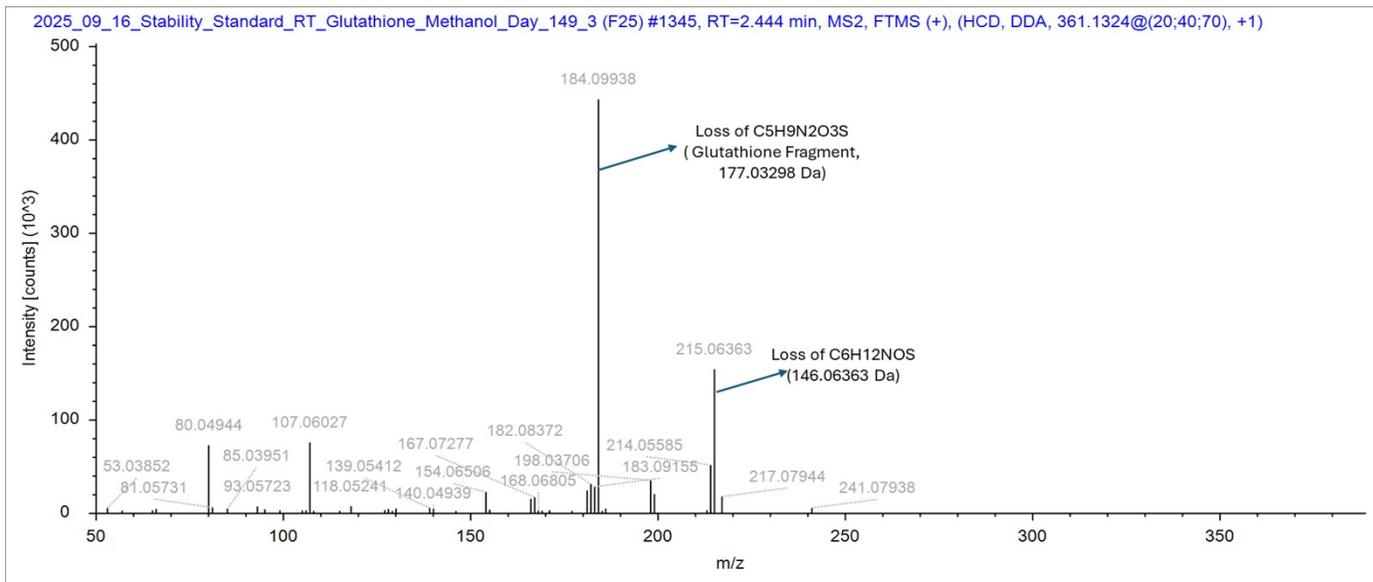
2025_09_16_Stability_Standard_RT_pH2_Water_Day_149_1 (F32) #3137, RT=5.873 min, MS2, FTMS (+), (HCD, DDA, 276.0143@(20;40;70), +1)
C13 H9 N O2 S2



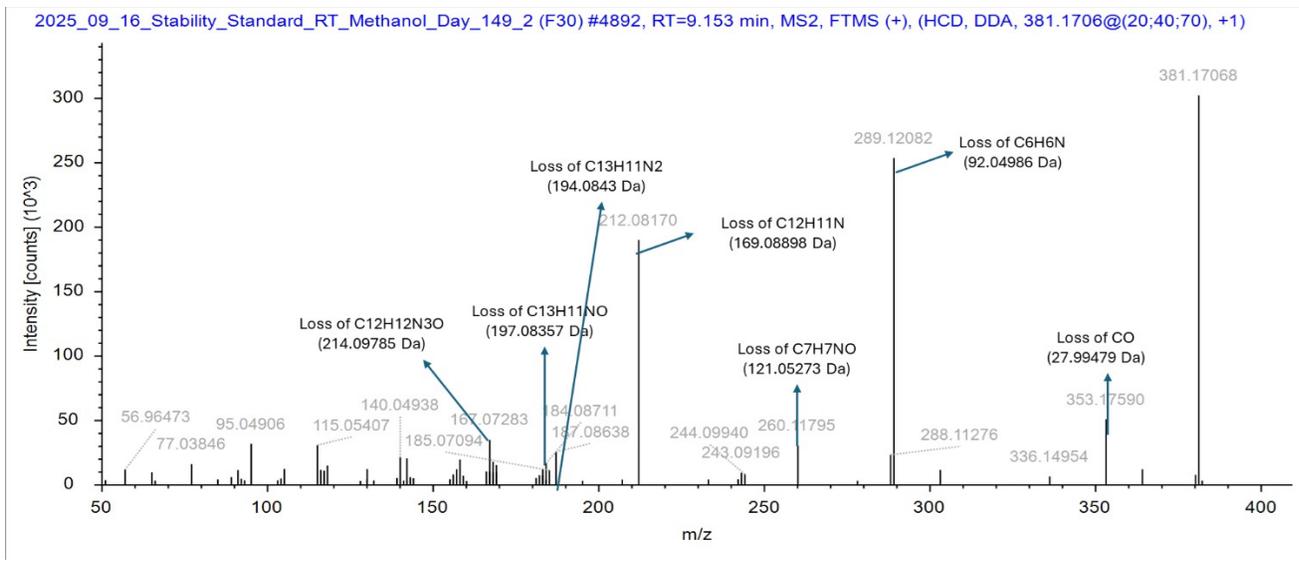
Feature 276



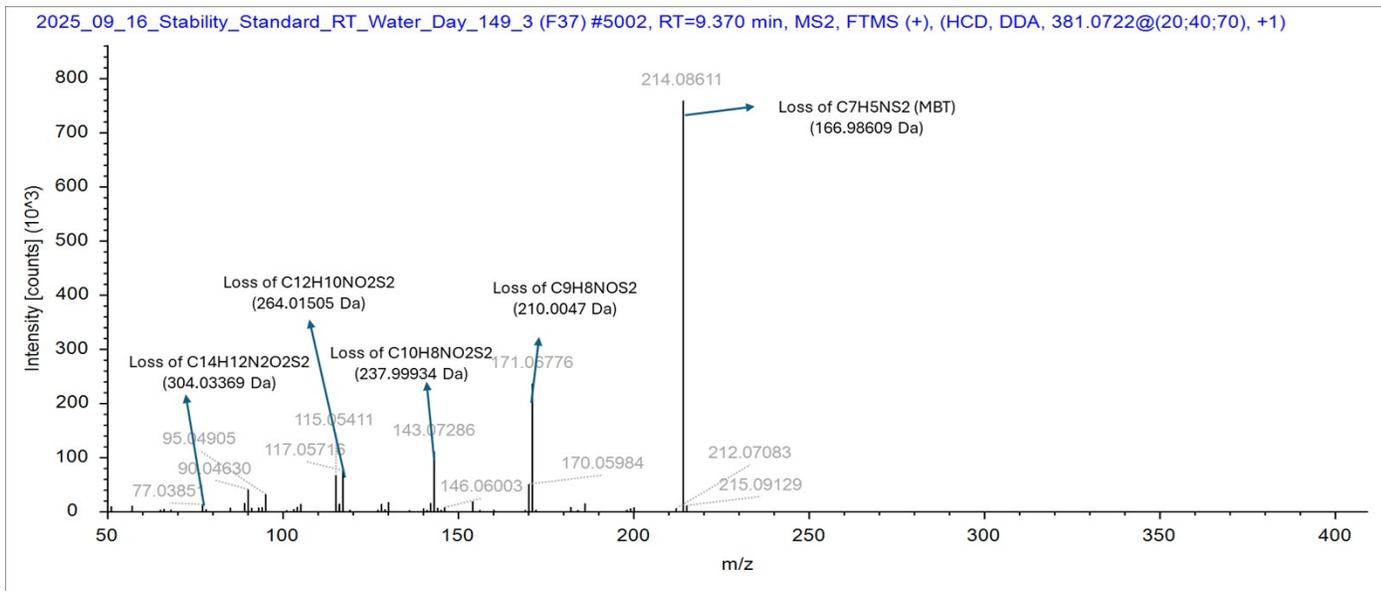
Feature 351



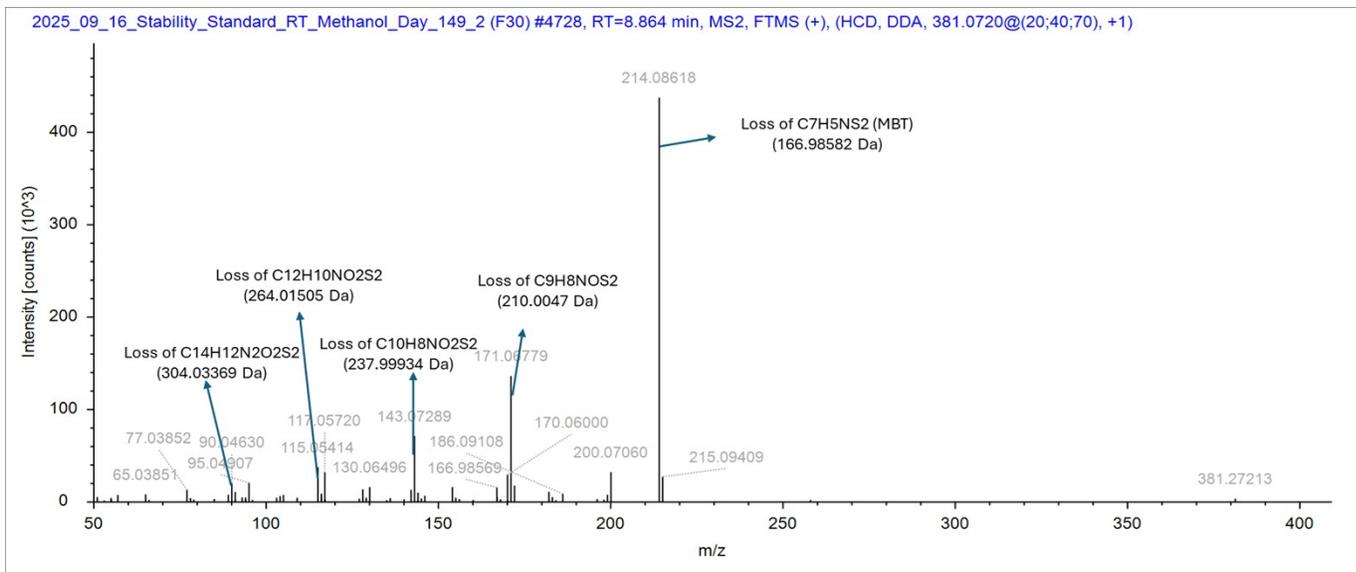
Feature 261a



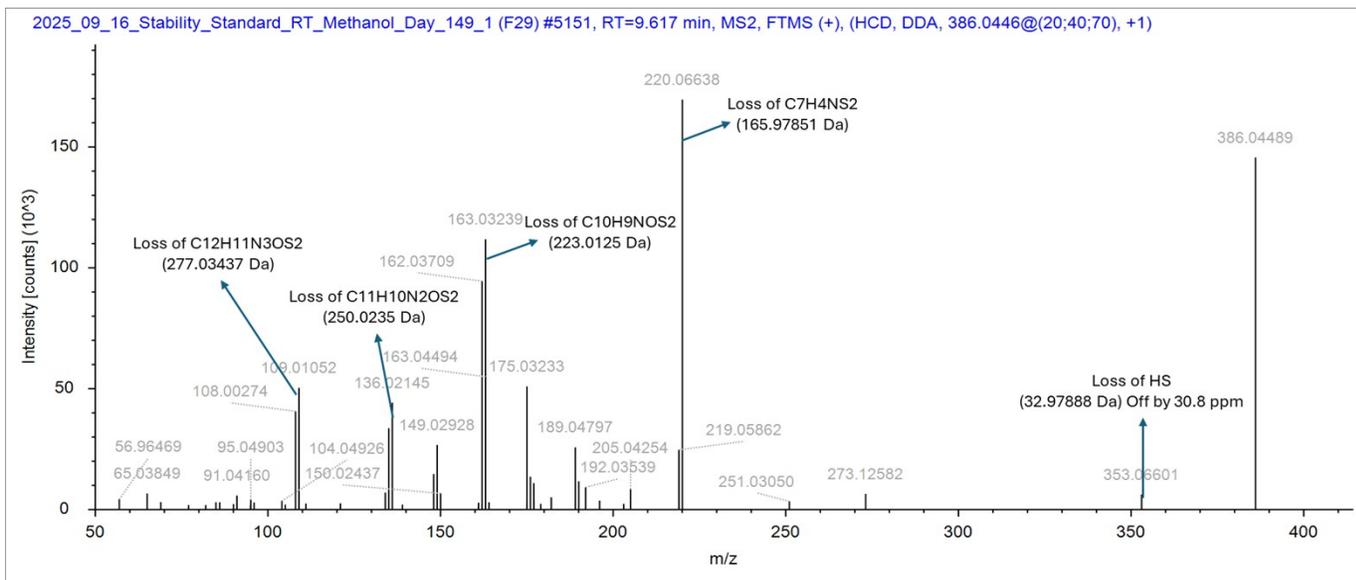
TP 381



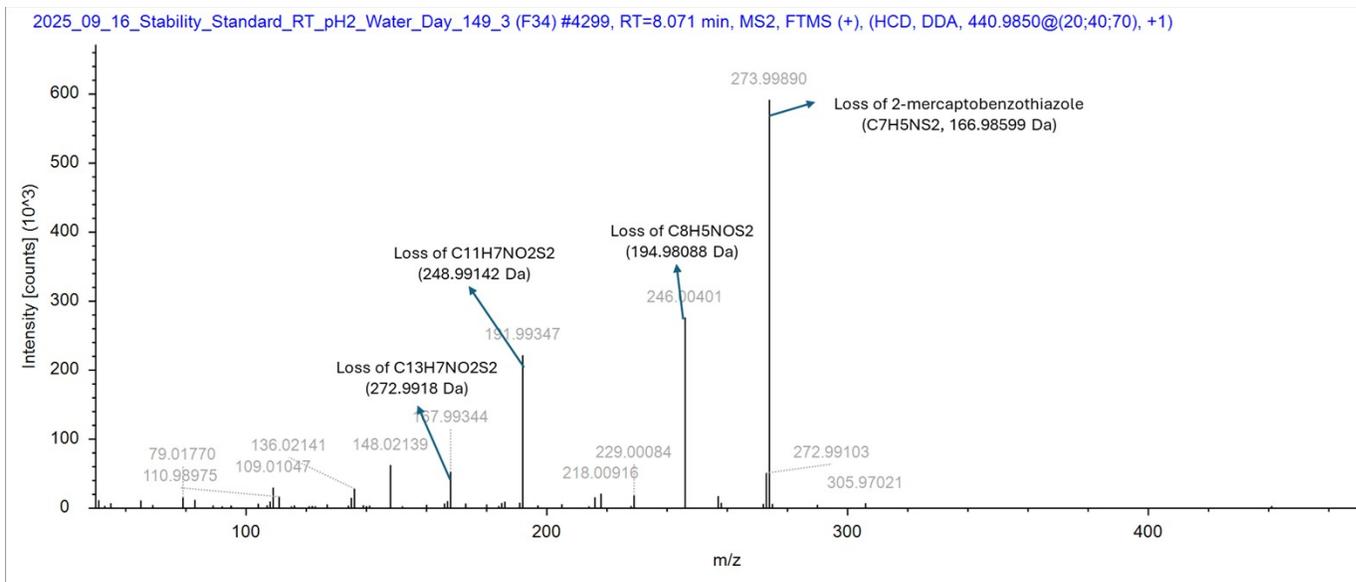
Feature 381a



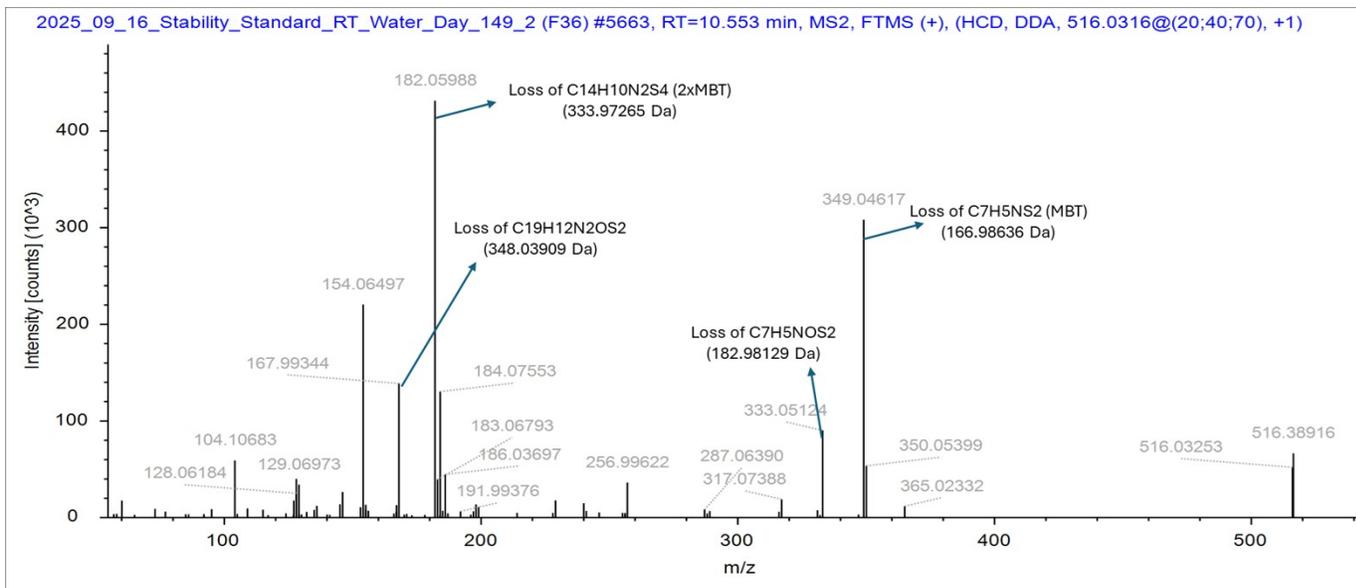
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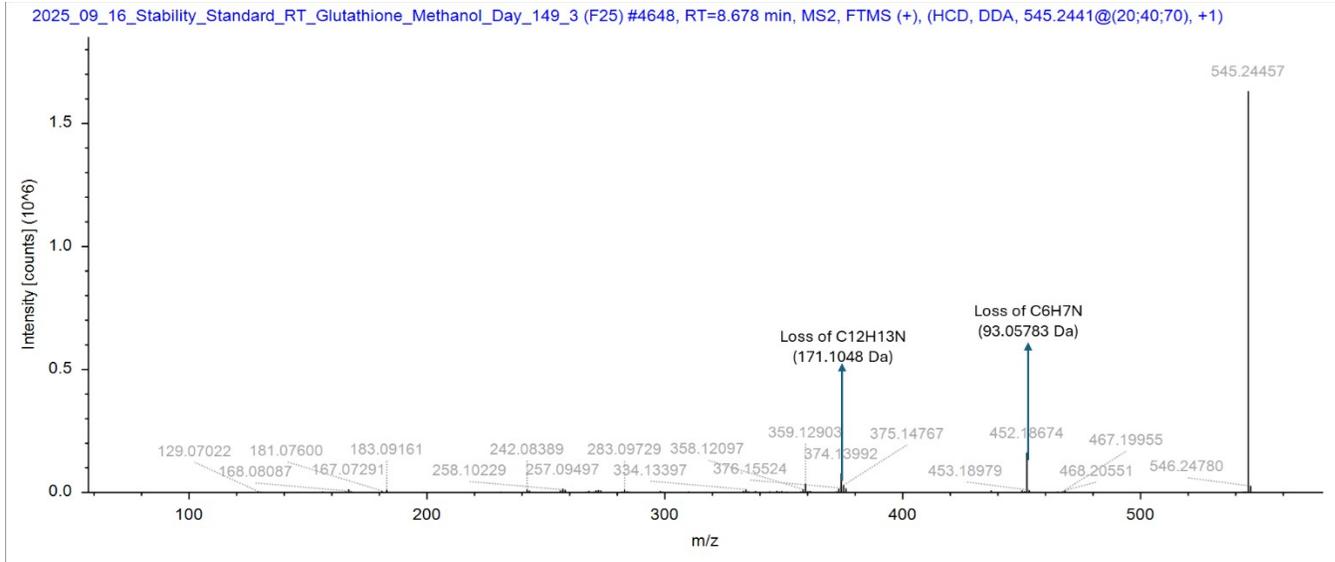
Feature 386



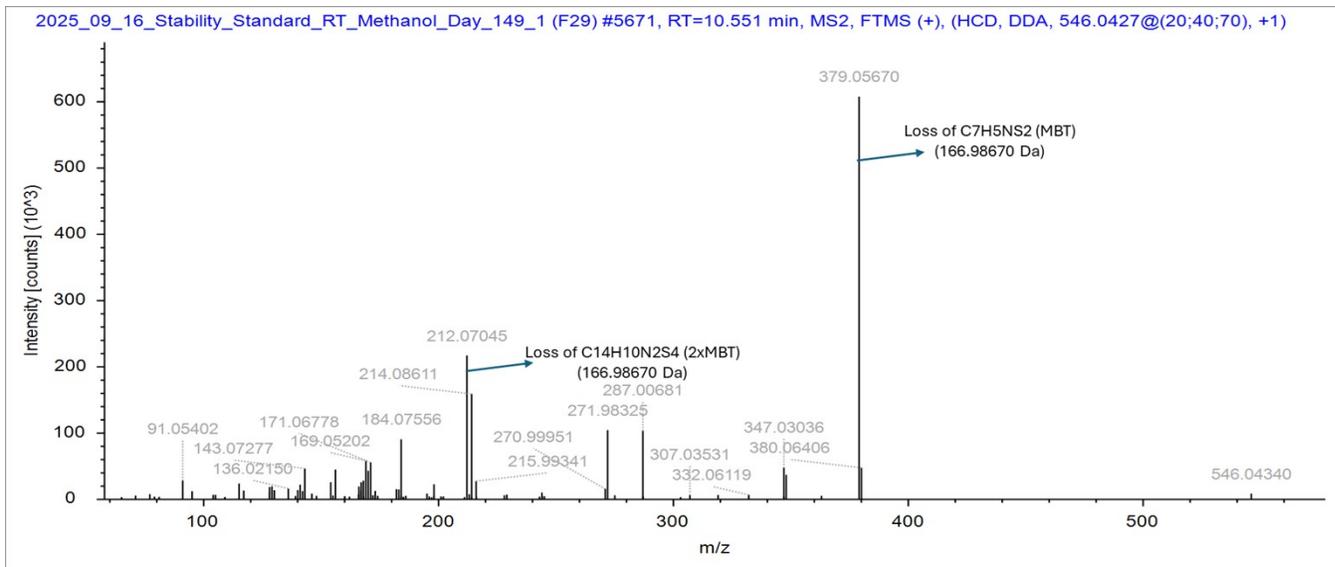
Feature 440



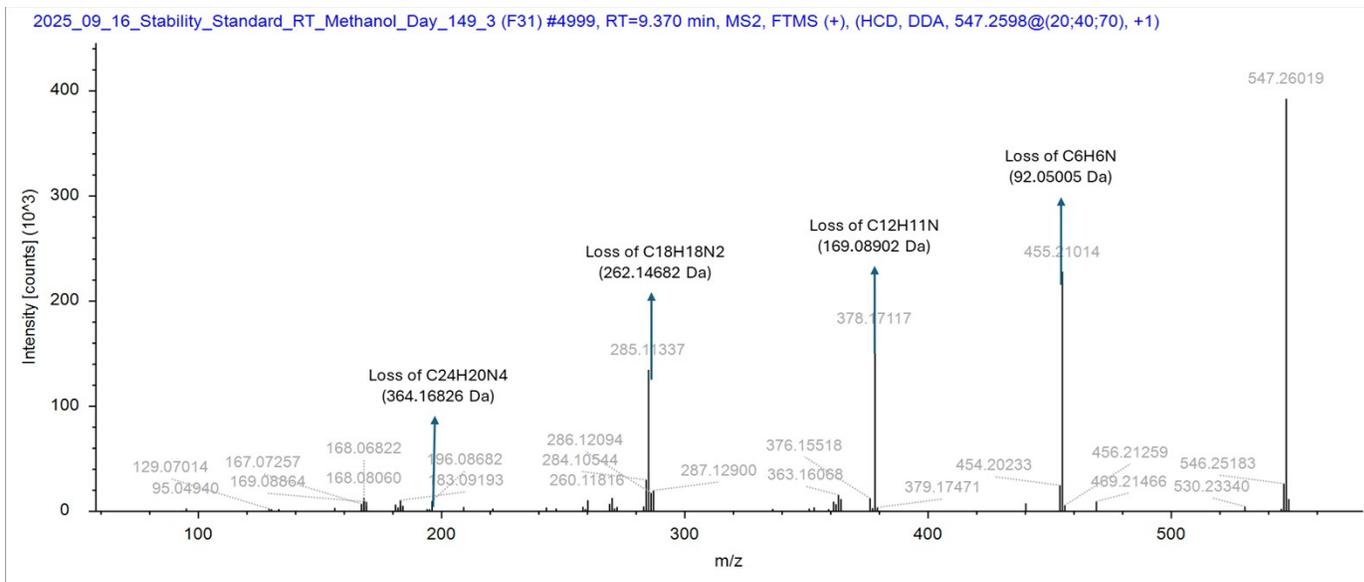
Feature 516



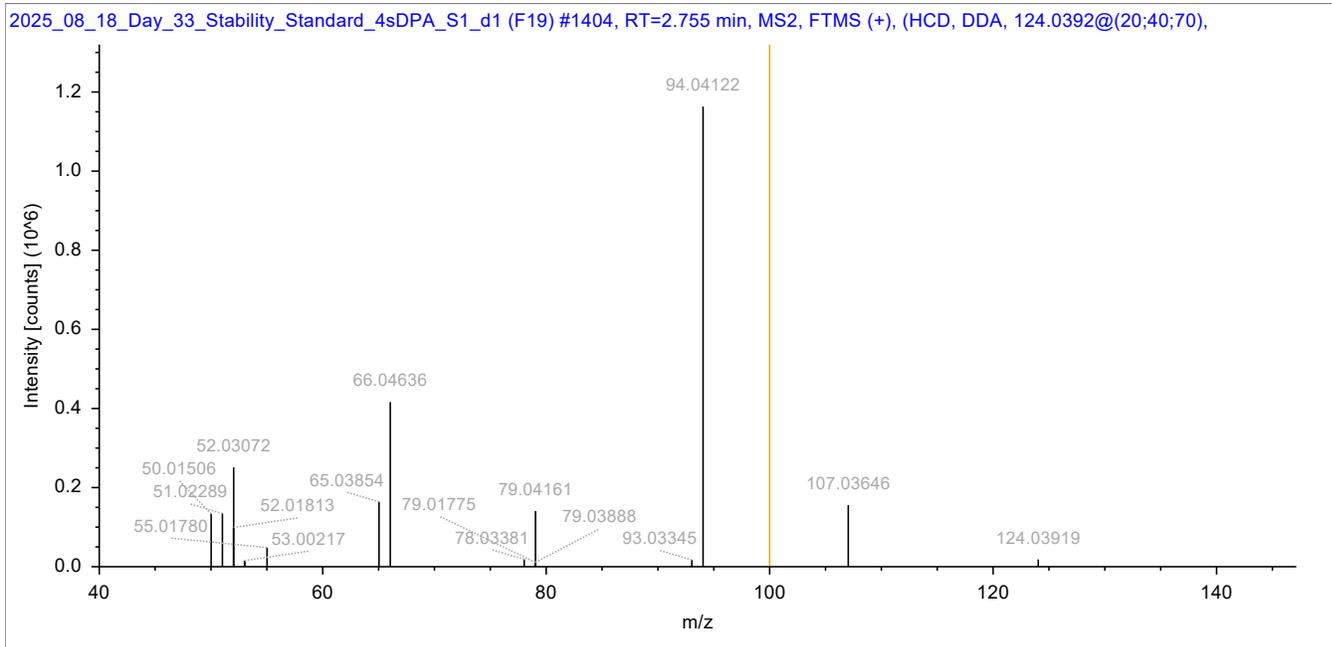
Feature 545

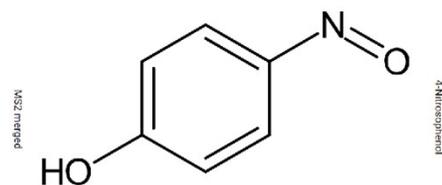
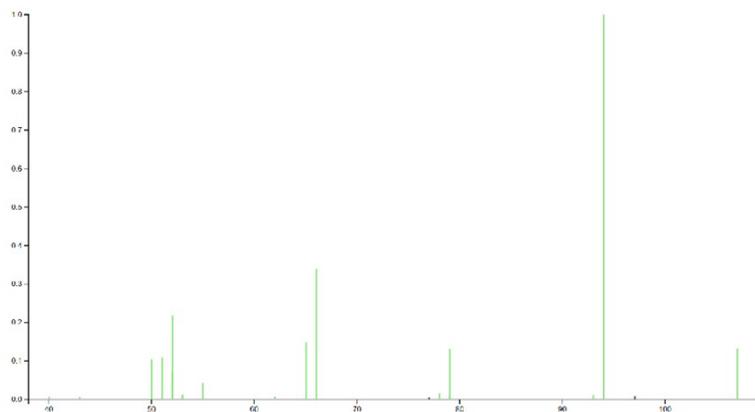


Feature 546



TP 547





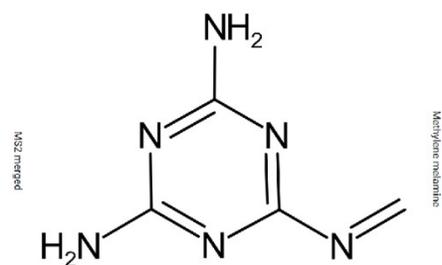
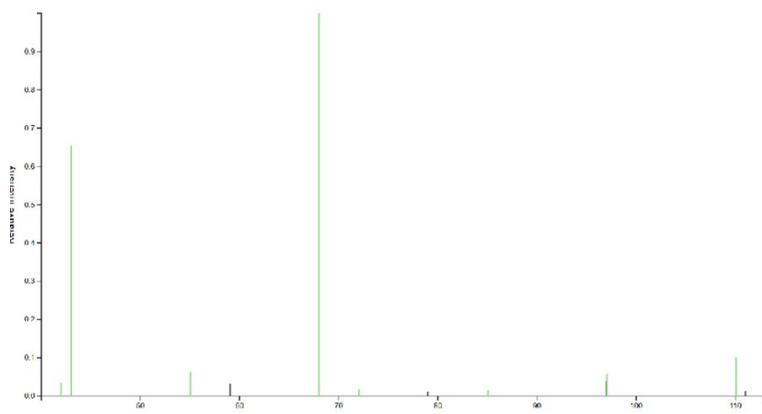
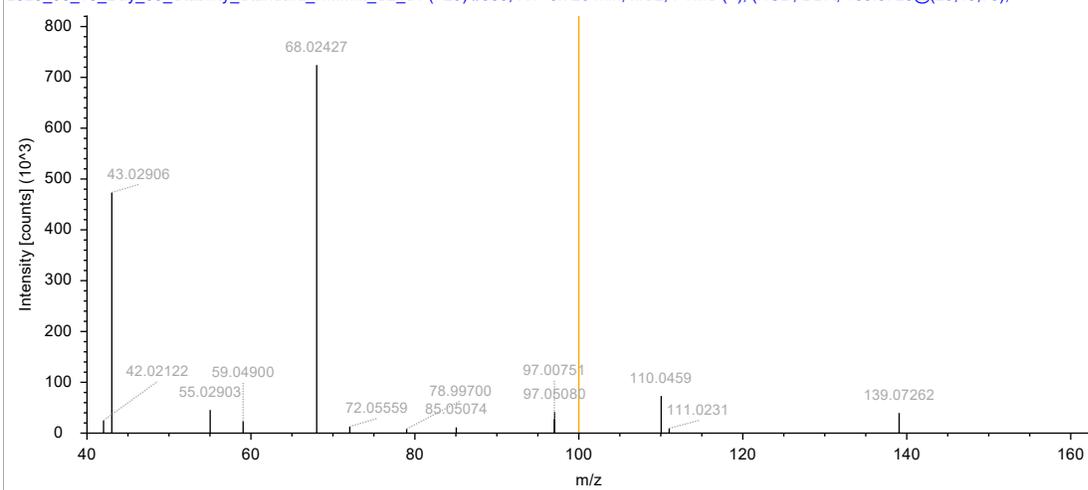
License: Academic Institutions (Academic License)

Quota: UNLIMITED

Jobs: 83

4-Nitrosophenol – Annotated with SIRIUS

2025_08_18_Day_33_Stability_Standard_HMMM_S2_d1 (F23) #358, RT=0.720 min, MS2, FTMS (+), (HCD, DDA, 139.0725@(20:40:70),



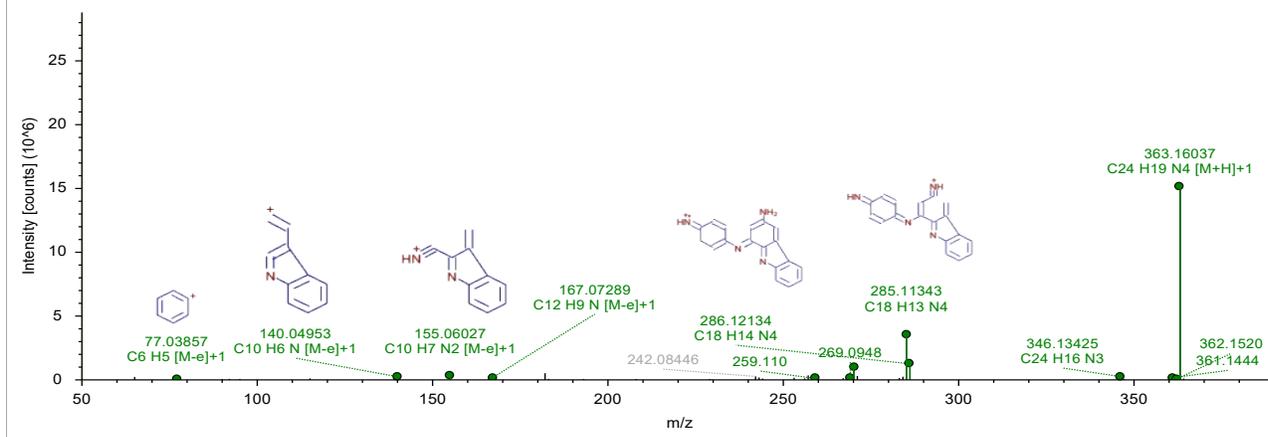
License: Academic Institutions (Academic License)

Quota: UNLIMITED

Jobs: 0

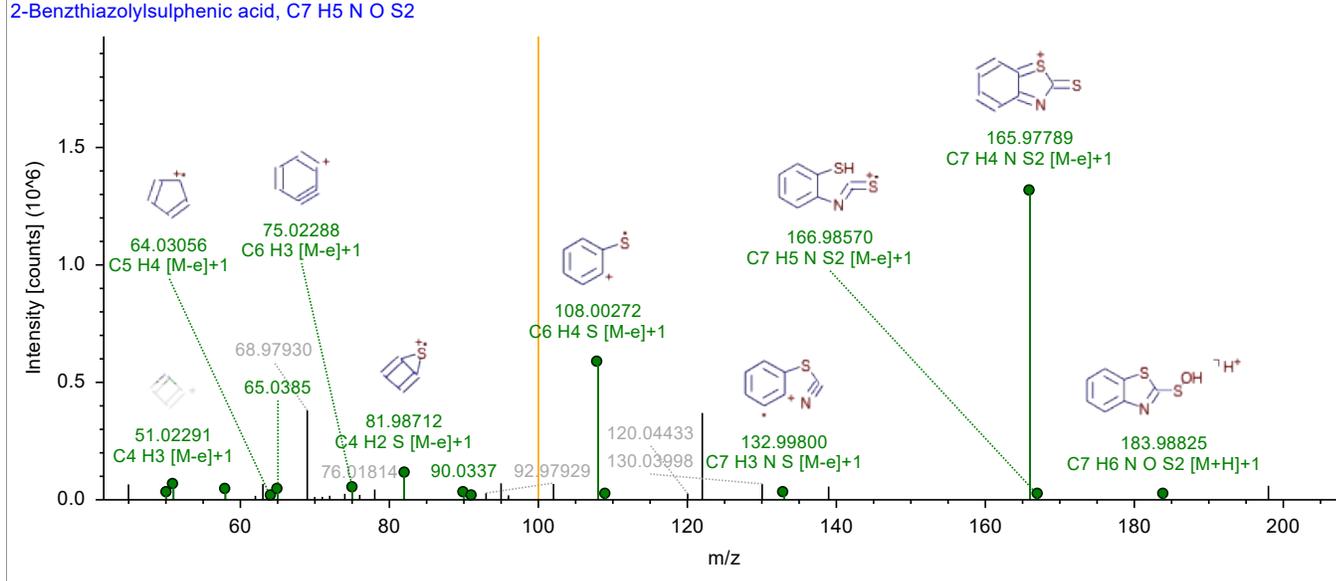
Methylene melamine – Annotated with SIRIUS

2025_08_08_Day_23_Stability_Standard_4-ADPA_S3_d1 (F7) #2911, RT=5.609 min, MS2, FTMS (+), (HCD, DDA, 363.1600@(20;40;70), +1)
 C24 H18 N4



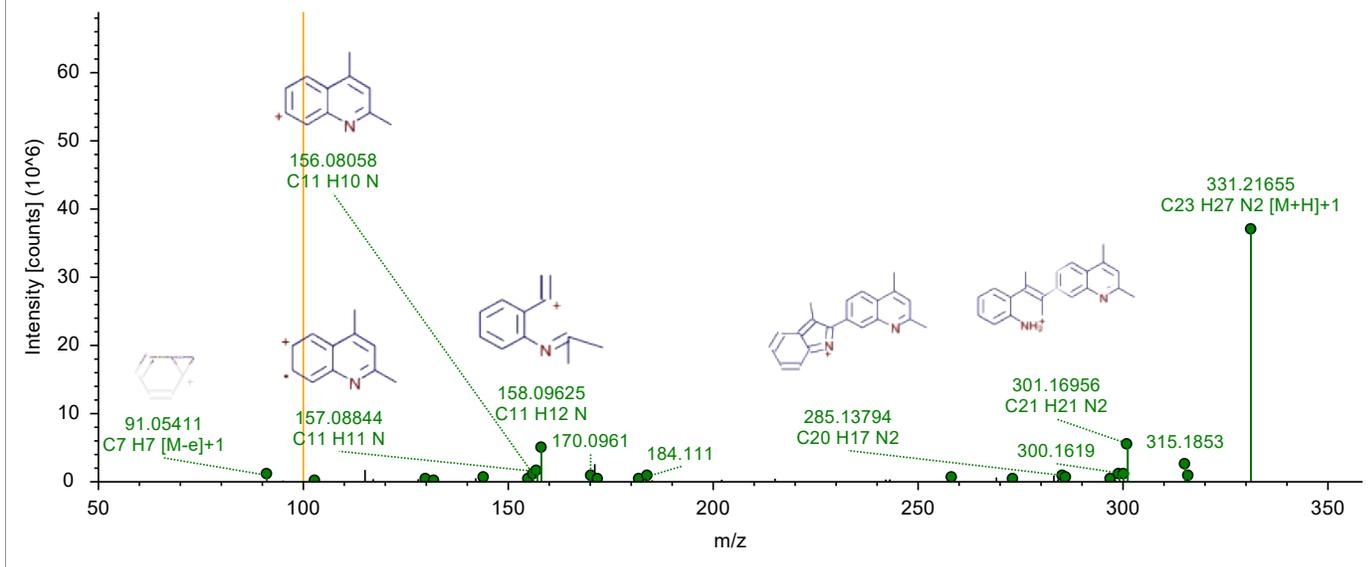
TP 363

2025_08_08_Day_23_Stability_Standard_MBT_S1_d1 (F28) #2988, RT=5.761 min, MS2, FTMS (+), (HCD, DDA, 183.9884@(20;40;70), +1)
 2-Benzthiazolylsulphenic acid, C₇H₅N O S₂



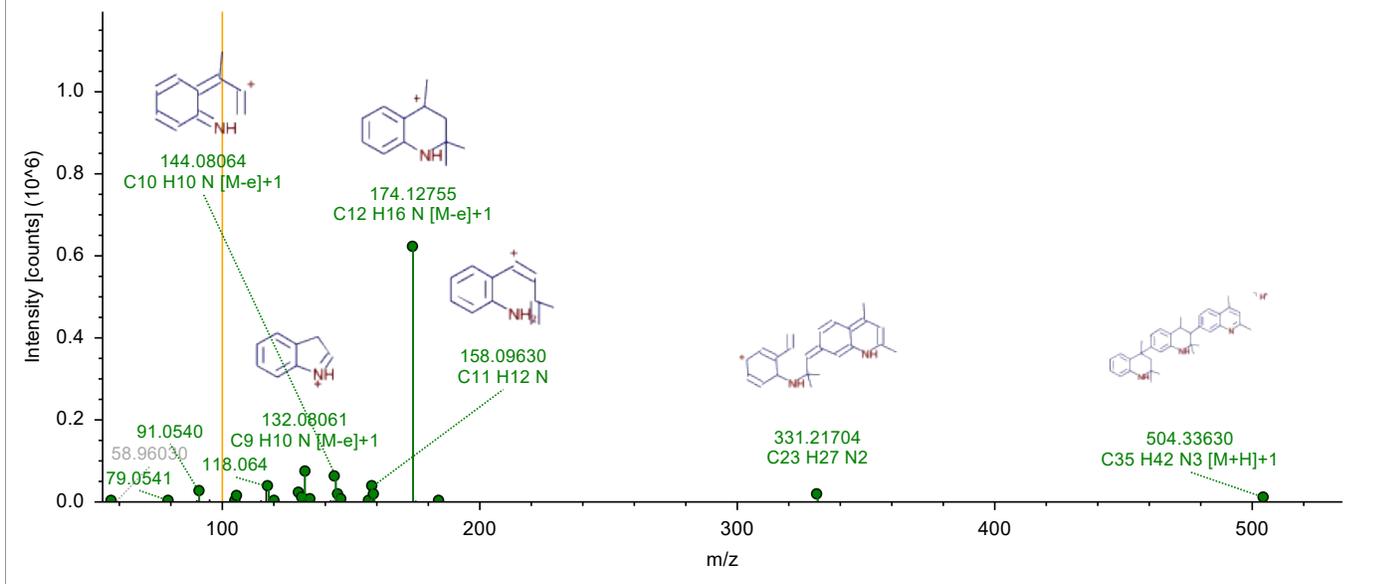
2-Benzthiazolylsulphenic acid

2025_08_18_Day_33_Stability_Standard_PolyTMQ_S2_d1 (F134) #2865, RT=5.616 min, MS2, FTMS (+), (HCD, DDA, 331.2164@(20;40;70), +1)
C23 H26 N2



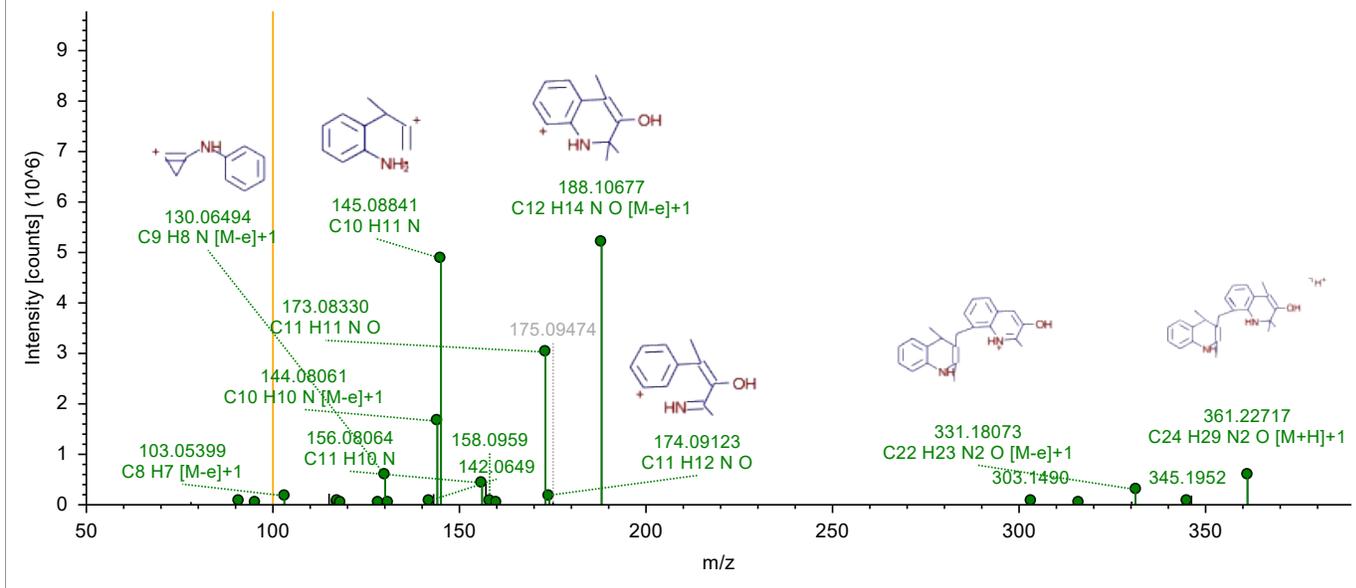
TP 331

2025_08_08_Day_23_Stability_Standard_PolyTMQ_S2_d1 (F20) #4549, RT=8.747 min, MS2, FTMS (+), (HCD, DDA, 504.3368@(20;40;70), +1)
C35 H41 N3



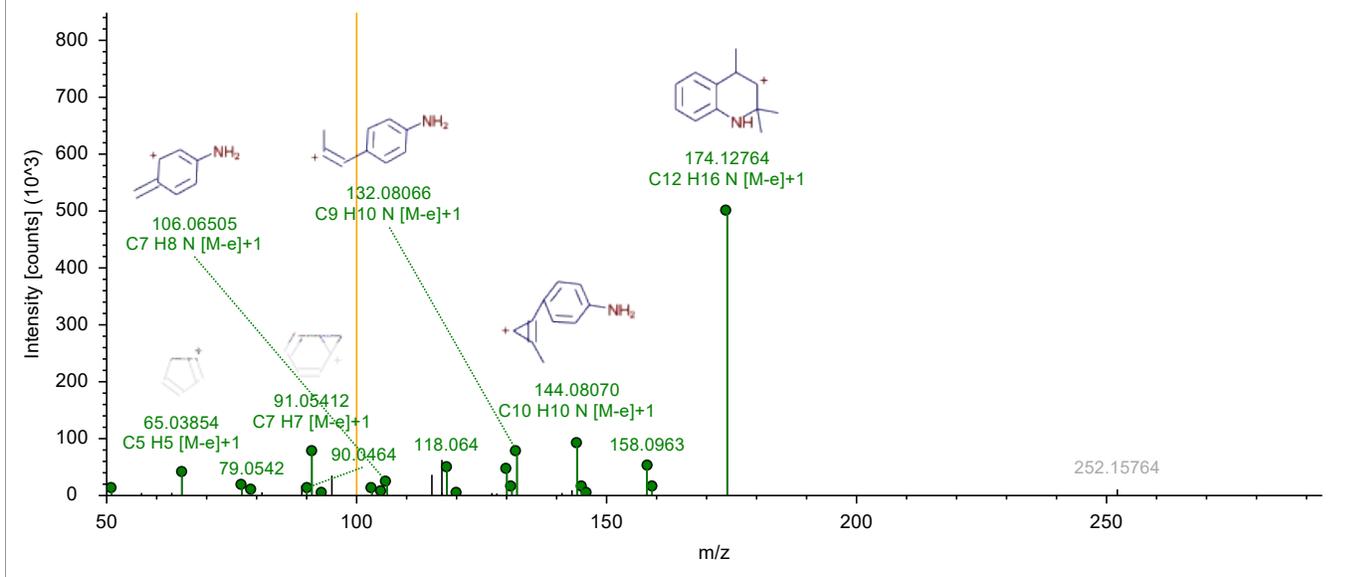
TP 504

2025_08_18_Day_33_Stability_Standard_TMQ_S2_d1 (F137) #4701, RT=9.162 min, MS2, FTMS (+), (HCD, DDA, 361.2269@(20;40;70), +1)
C24 H28 N2 O



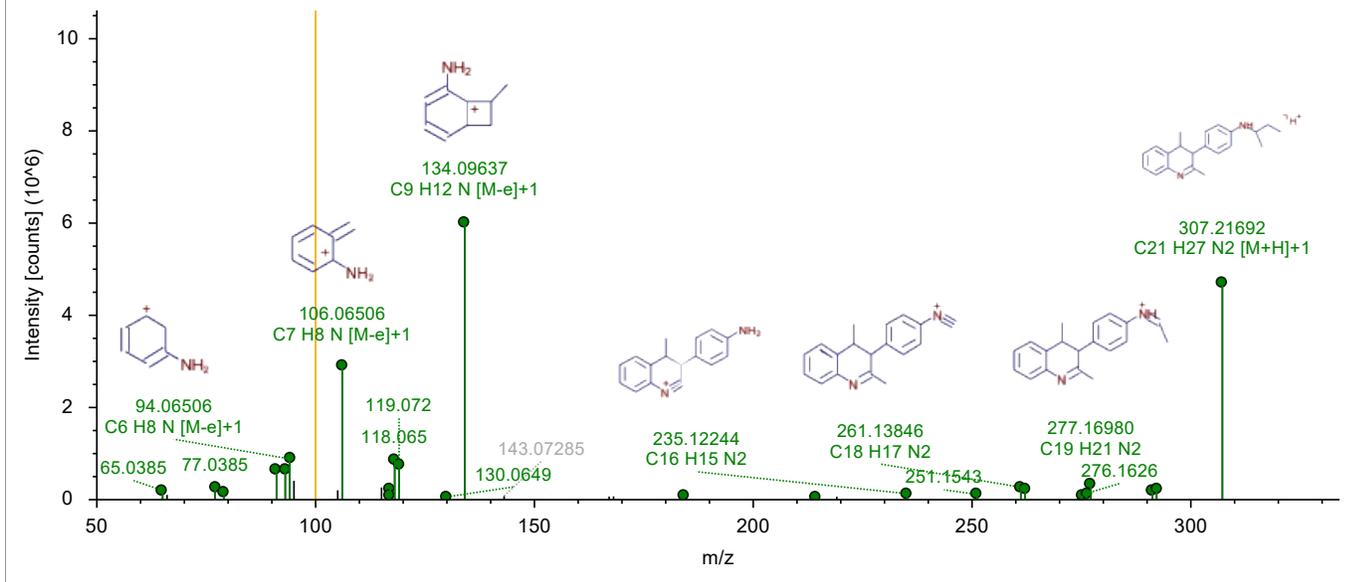
TP 361

2025_08_08_Day_23_Stability_Standard_PolyTMQ_S1_d1 (F26) #2164, RT=4.171 min, MS2, FTMS (+), (HCD, DDA, 267.1853@(20;40;70), +1)
C18 H22 N2



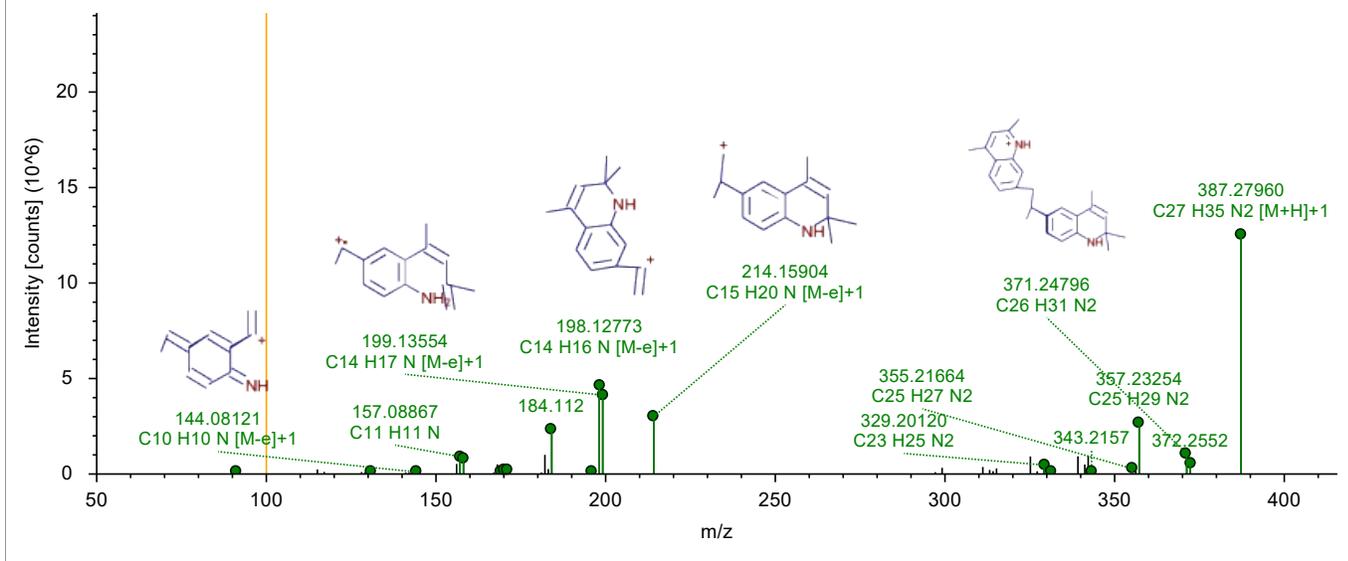
Impurity 267

2025_07_23_Day_0_Stability_Standard_PolyTMQ_S2_d1 (F92) #3454, RT=6.797 min, MS2, FTMS (+), (HCD, DDA, 307.2167@(20;40;70), +1)
C21 H26 N2



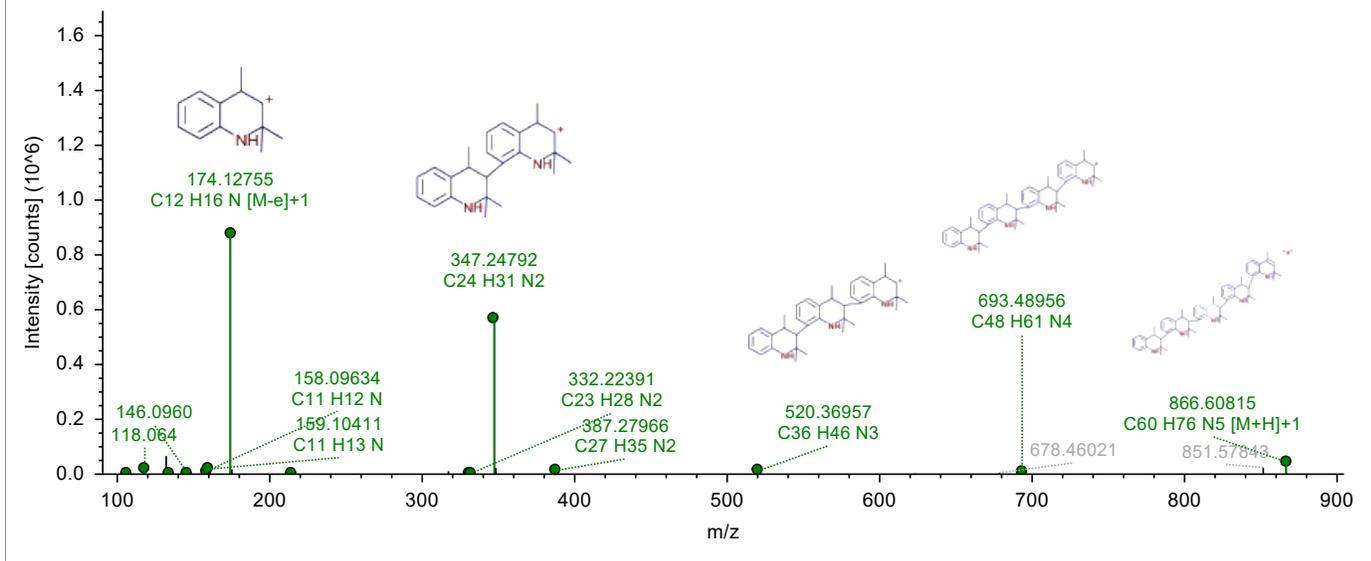
TP 307

2025_07_23_Day_0_Stability_Standard_PolyTMQ_S2_d1 (F92) #5239, RT=10.276 min, MS2, FTMS (+), (HCD, DDA, 387.2793@(20;40;70), +1)
C27 H34 N2



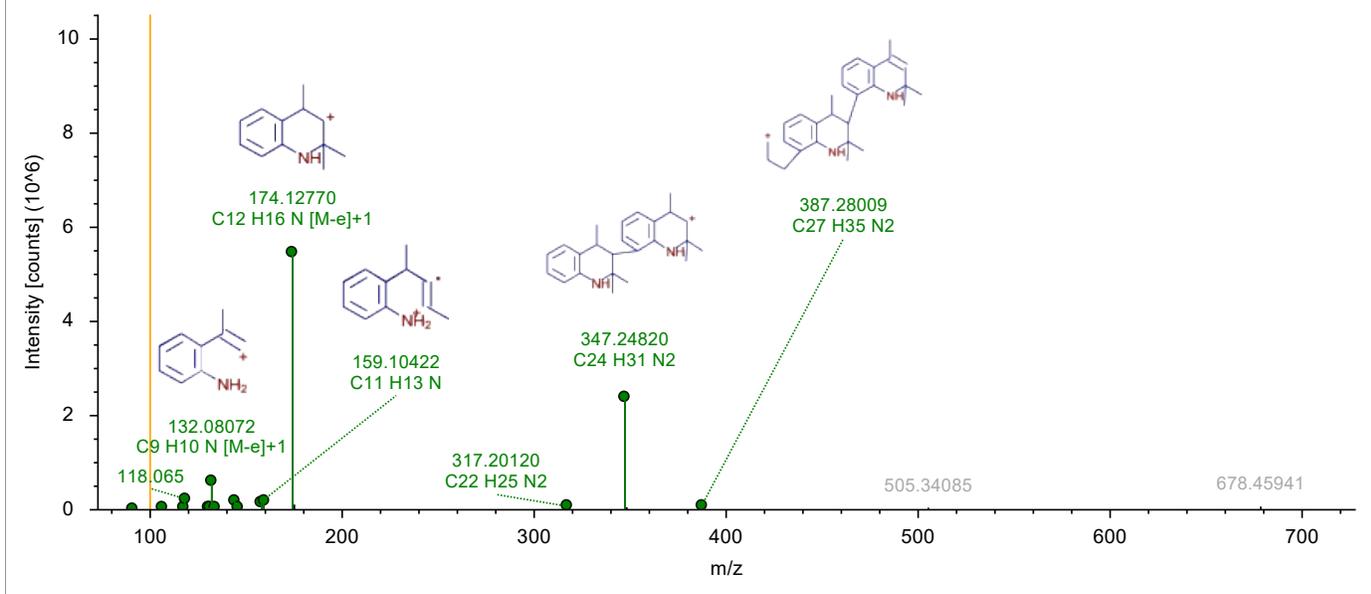
TP 387

2025_07_25_Day_2_Stability_Standard_PolyTMQ_S1_d1 (F59) #5473, RT=10.548 min, MS2, FTMS (+), (HCD, DDA, 866.6081@(20;40;70), +1)
C60 H75 N5



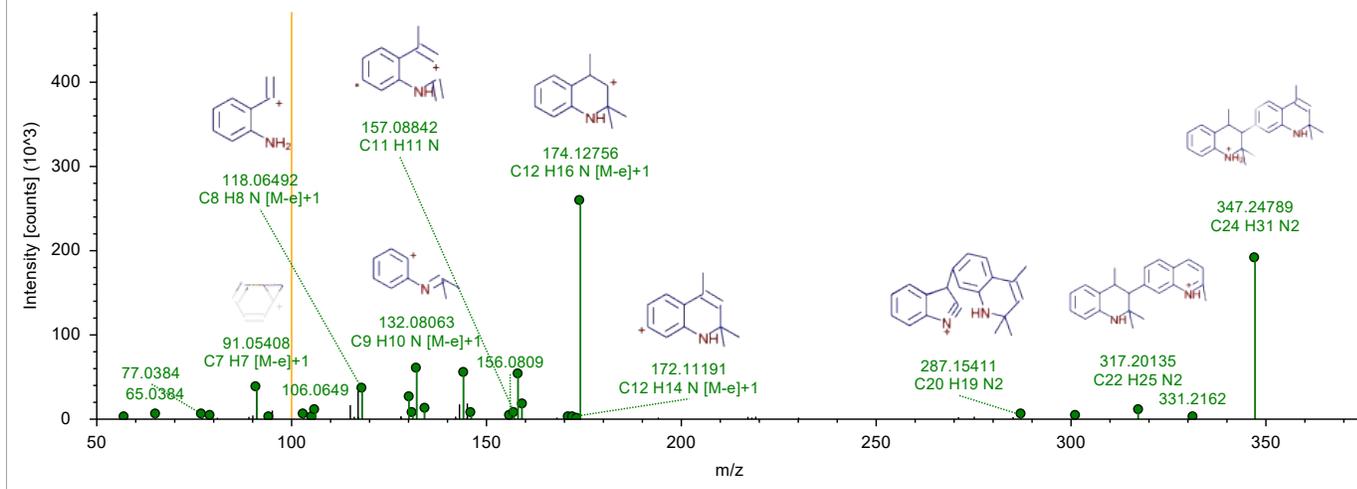
Feature 866

2025_07_23_Day_0_Stability_Standard_PolyTMQ_S2_d1 (F92) #5170, RT=10.142 min, MS2, FTMS (+), (HCD, DDA, 693.4883@(20;40;70), +1)
C48 H60 N4



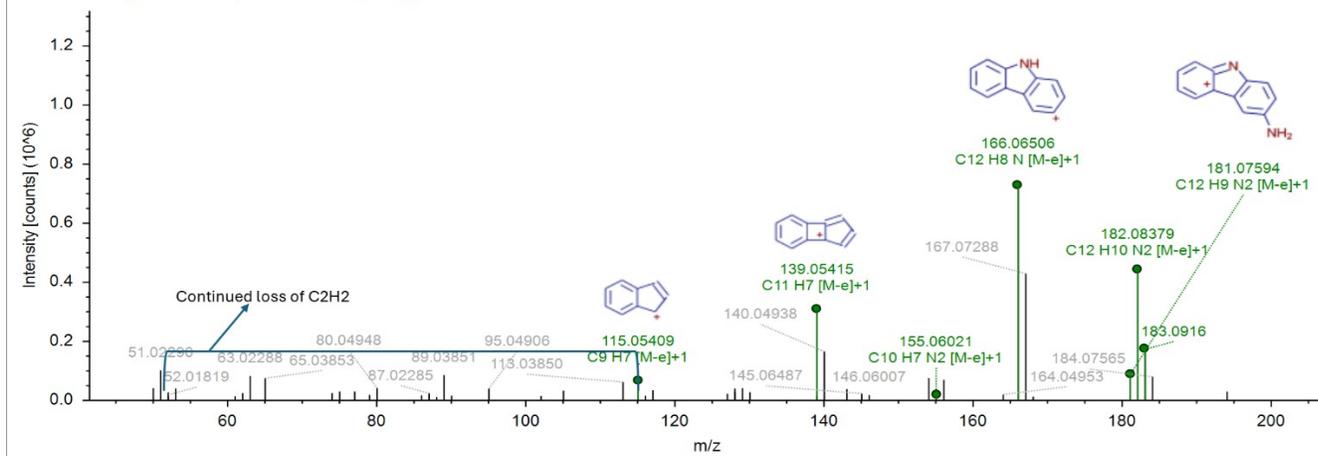
Feature 693

2025_07_23_Day_0_Stability_Standard_PolyTMQ_S1_d1 (F100) #4099, RT=8.051 min, MS2, FTMS (+), (HCD, DDA, 347.2480@(20;40;70), +1)
C24 H30 N2



Feature 347

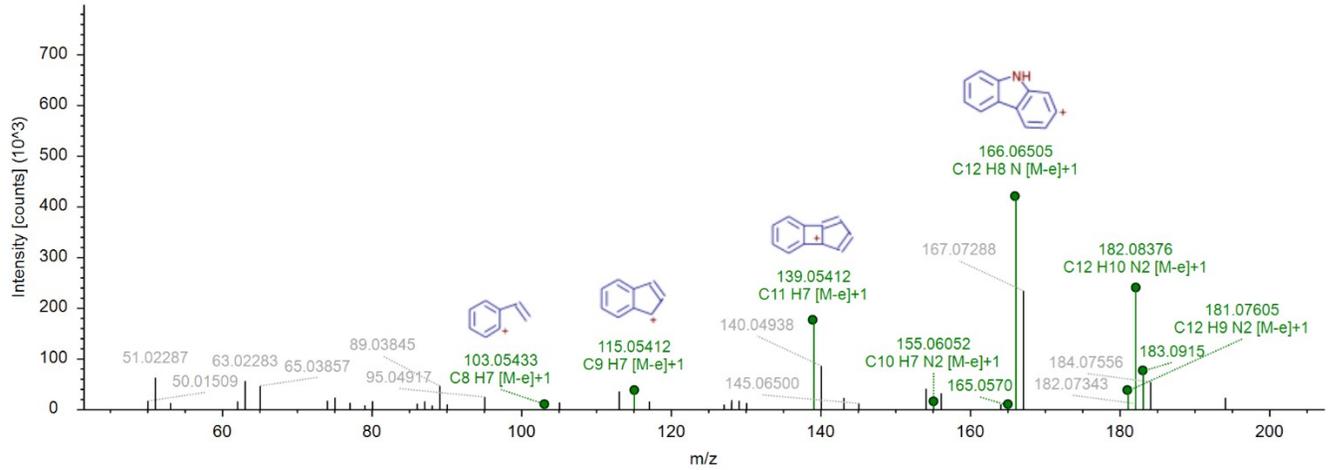
2025_07_23_Day_0_Stability_Standard_4sDPA_S1_d1 (F96) #1387, RT=2.725 min, MS2, FTMS (+), (HCD, DDA, 183.0915@(20;40;70), +1)
C12 H10 N2
FISH Coverage: 7 Matched, 42 Unmatched, 0 Skipped



TP 183a

2025_07_23_Day_0_Stability_Standard_4sDPA_S3_d1 (F77) #1820, RT=3.576 min, MS2, FTMS (+), (HCD, DDA, 183.0915@ (20;40;70), +1)

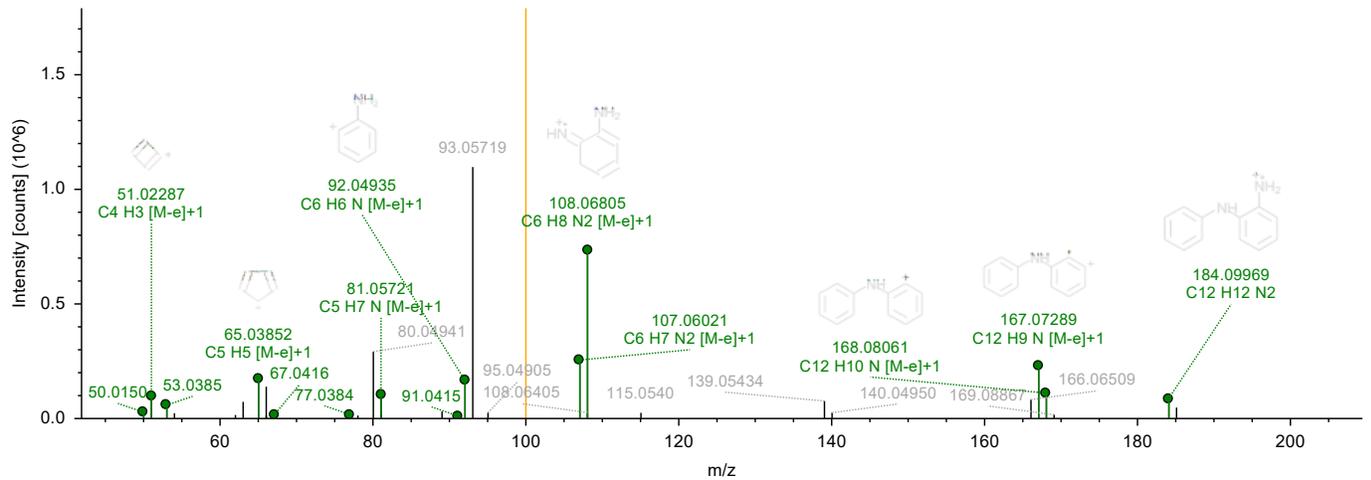
FISH Coverage: 9 Matched, 35 Unmatched, 0 Skipped



TP 183b

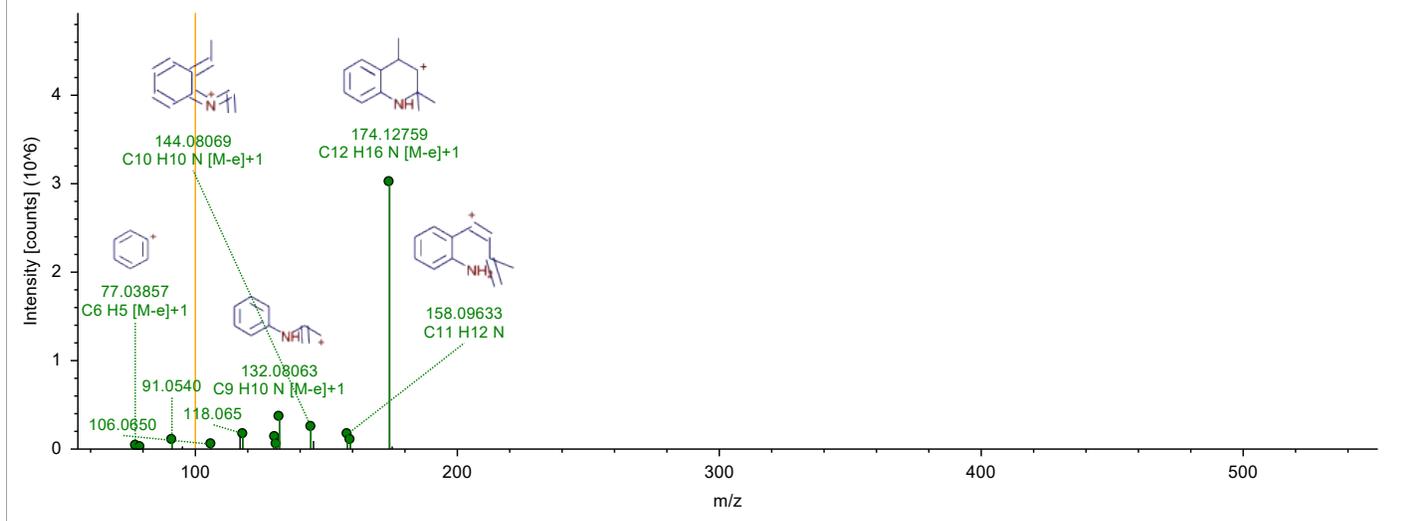
2025_07_23_Day_0_Stability_Standard_4sDPA_S3_d1 (F77) #1904, RT=3.741 min, MS2, FTMS (+), (HCD, DDA, 185.1072@ (20;40;70), +1)

2-Aminodiphenylamine, C12 H12 N2



TP 185

2025_08_18_Day_33_Stability_Standard_PolyTMQ_S2_d1 (F134) #4875, RT=9.512 min, MS2, FTMS (+), (HCD, DDA, 520.3680@(20;40;70), +1)
C36 H45 N3



Feature 520

Figure S9. Mass spectrum with annotations of features (Level 3 Identification)