Supporting Information for:

Probing 2-Aminobenzimidazole Small Molecule Library-RNA Motif Interactions Via Two-Dimensional Combinatorial Screening

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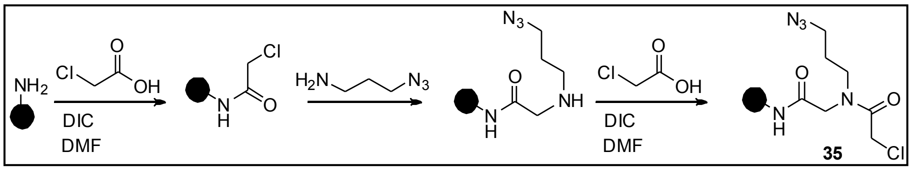
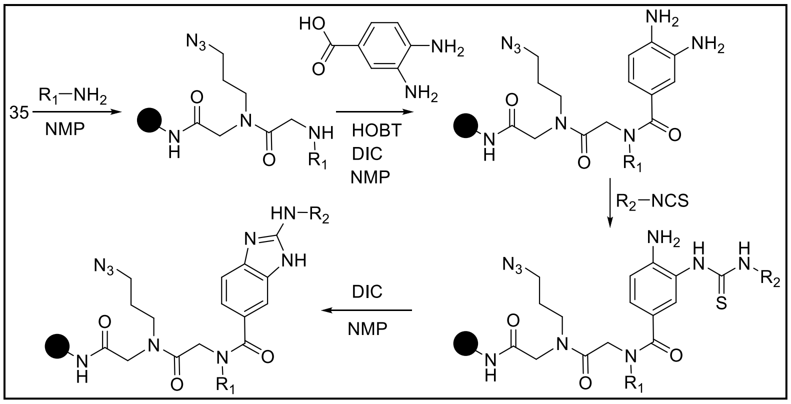
Section I: Synthesis of Libraries used in microarray screening

I(a) Synthesis of 2-aminobenzimidazole library: The library with the 2-(arylamino)benzimidazole scaffold was synthesized via the solid-phase approach. Initially an azidopropylamine modified resin **35** (Scheme S-1) was synthesized in a common reaction flask, and then it was split into individual vials for further modifications.



Scheme S-1: Synthesis of azido-propylamine-modified resin

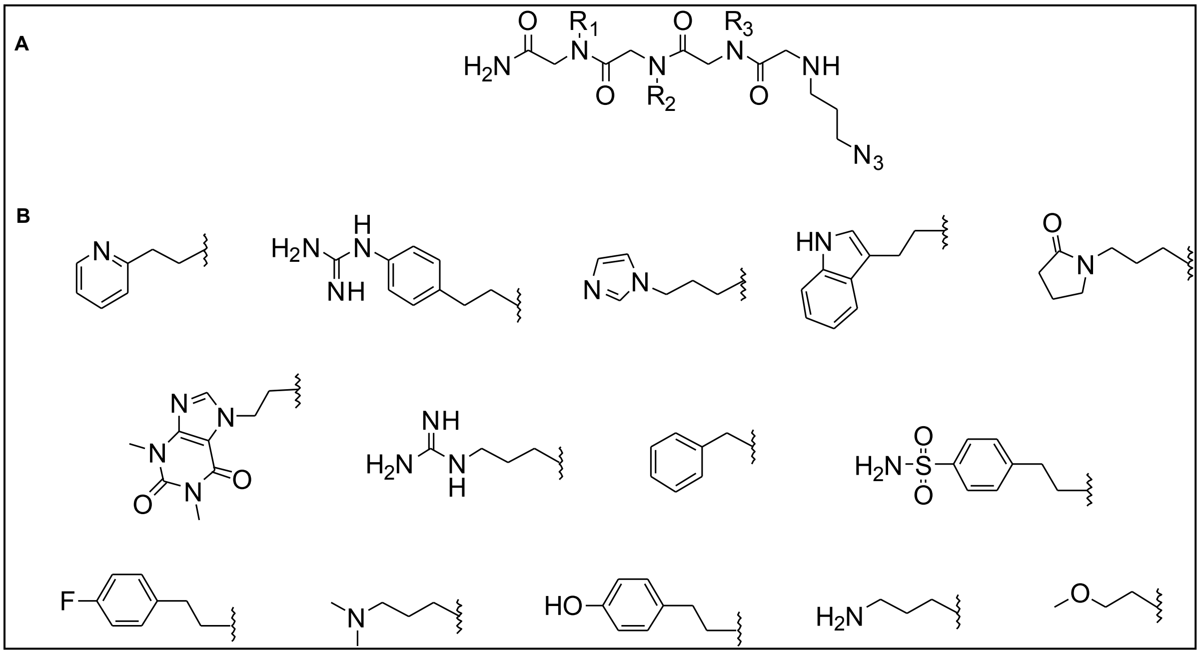
The resin-bound benzimidazole library was synthesized according to previously described approach (Scheme S-2).(*1, 2*) The utilized building blocks are presented in Figure 1.



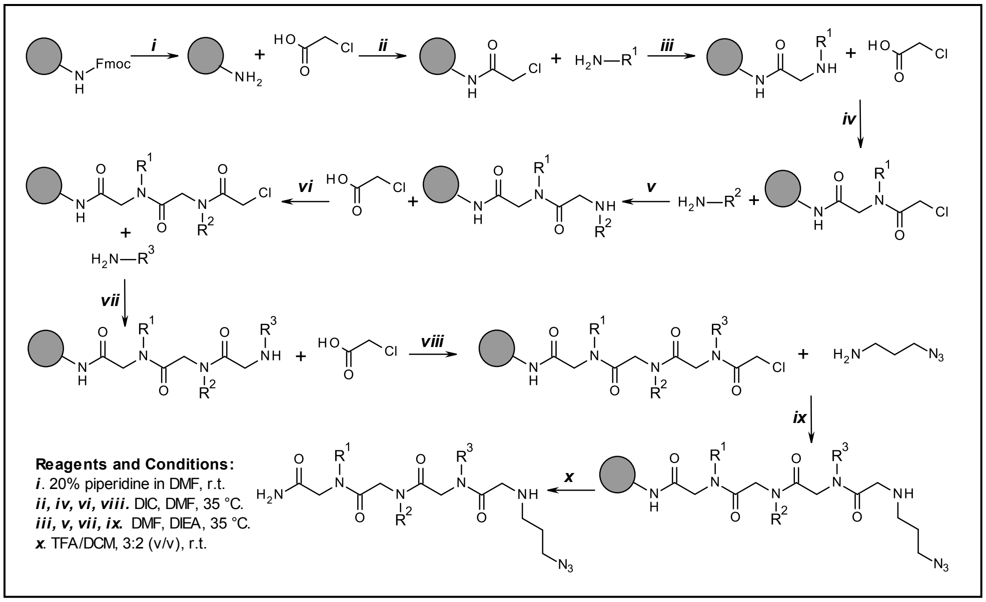
Scheme S-2: Synthesis of 2-aminobenzimidazole library

Vials were charged with the azide-modified resin **35** (15 mg, 10 µmol) and installed into the heating block. In the vials solutions of corresponding amines R^1NH_2 (0.35 mL, 1M in NMP) were loaded, and the displacement was carried out at 50 °C for 20 h, while shaken at 75 rpms. The liquids were evacuated; the beads were washed with DMF at 28°C, while shaking for 20 min at 150 rpm (2×1 mL), followed by wash with ethyl acetate (1.5 mL). Then, a solution of 3,4-diaminobezoic acid (0.8 g, 5.3 mmol), N-hydroxybenztriazole (0.85 g, 6.3 mmol), and DIC (1.9 mL, 12 mmol) in NMP (23 mL) was distributed into each vial (0.35 mL). The reaction was carried out at 37 °C for 36 h, while shaking at 75 rpm. The liquids were evacuated, and the beads were washed with DMF at 28 °C, while shaking for 20 min at 150 rpm (2×1 mL), followed by the wash with ethyl acetate (1.5 mL). Then into each vial NMP (0.35 mL), corresponding isothiocyanate R^2NCS (8 eq) and N,N-diisopropylethylamine (20 µl) were loaded. The reaction was carried out at 37°C for 20 h (shaking speed 75 rpm). The liquids were evacuated, the beads were washed with DMF at 28°C shaking for 20 min at 150 rpm (2×1 mL)), followed by the wash with ethyl acetate (1.5 mL). Then, into each vial 0.5 M DIC in NMP (0.5 mL) was loaded and the reactions were carried out at 37 °C for 20 h, while shaking at 75 rpm. The liquids were evacuated, the beads were washed with DMF at 28°C shaking for 20 min at 150 rpm (2×1 mL)), followed by the wash with ethyl acetate (1.5 mL). Reaction wells were further washed with 20% piperidine in DMF (1 mL, 1 h), and again with DMF, and ethyl acetate. The product was cleaved from the resin with a TFA/DCM/water mixture (60:40:2) at 28°C for 5 h, while shaking at 75 rpm. Liquids were separated and beads were washed with methanol (1 mL). Combined filtrates were evaporated under stream of air. The residues were dissolved in methanol (1 mL), and aliquots were taken for MS-ESI analyses, and the solutions were evaporated again. The samples were then dissolved in 1.2 mL of a methanol-water-glycerol (1:1:1, v/v/v) mixture, providing approximately 5.5 mM concentration. Out of 91 reactions, 79 compounds were successfully synthesized.

I(b) General Protocol for Peptoid Synthesis: The synthesis of peptoid library was accomplished using solid-phase methodology (Scheme S-4) as described by Zukermann *et al*,(*3*) and various primary amines were utilized as the sub-monomers at the displacement steps. These primary amines are denoted as NH_2-R_1, NH_2-R_2, and NH_2-R_3; and the entire selection of substituting groups R_1, R_2, and R_3 is presented in Scheme S-2. All library members were synthesized with an azide functional group. This allows for site-specific conjugation onto alkyne functionalized agarose slides by a copper(I) catalyzed 1,3 dipolar cycloaddition reaction.(*4-8*) This selection of amines is based on their structural similarities to known RNA binders, as described in the manuscript. 3-Azidopropylamine was synthesized as reported in literature.(*9*) The newly synthesized peptoid library well as a previously reported peptoid library (*10*) were studied.



Scheme S-3. (**A**) General structure of peptoid library members and submonomers used to construct them. (**B**) General structure of peptoid library members and the submonomers used.



Reagents and Conditions:
i. 20% piperidine in DMF, r.t.
ii, iv, vi, viii. DIC, DMF, 35 °C.
iii, v, vii, ix. DMF, DIEA, 35 °C.
x. TFA/DCM, 3:2 (v/v), r.t.

Scheme S-4: Solid phase synthetic protocol for peptoids.

Step *i:* Deprotection. Fmoc-Rink Amide MBHA Resin (62.5 mg, 25 µmol) with a substitution level of 0.40 meq/g was deprotected using 2×3 mL of 20% piperidine in DMF for 2×20 min with shaking at 550 rpm. The reaction wells were drained by flushing with nitrogen, and the resin was washed with 5×3 mL DMF for 5×2 min while shaking at 550 rpm.

Steps *ii, iv, vi,* and *viii*: Coupling with Chloroacetic acid. Coupling reactions were completed by adding 0.5 M chloroacetic acid in NMP (2 mL, 1 mmol, 40 equiv.) and 1 M DIC in NMP (1 mL, 1 mmol, 40 equiv.) into reaction wells containing resin-bound amines. Reaction mixtures were shaken at 550 rpm for 30 min at 35 ^{o}C. The reagents were then drained, and the coupling step was repeated. The resin was washed with 4×3 mL DMF for 4×2 min, while shaking at 550 rpm.

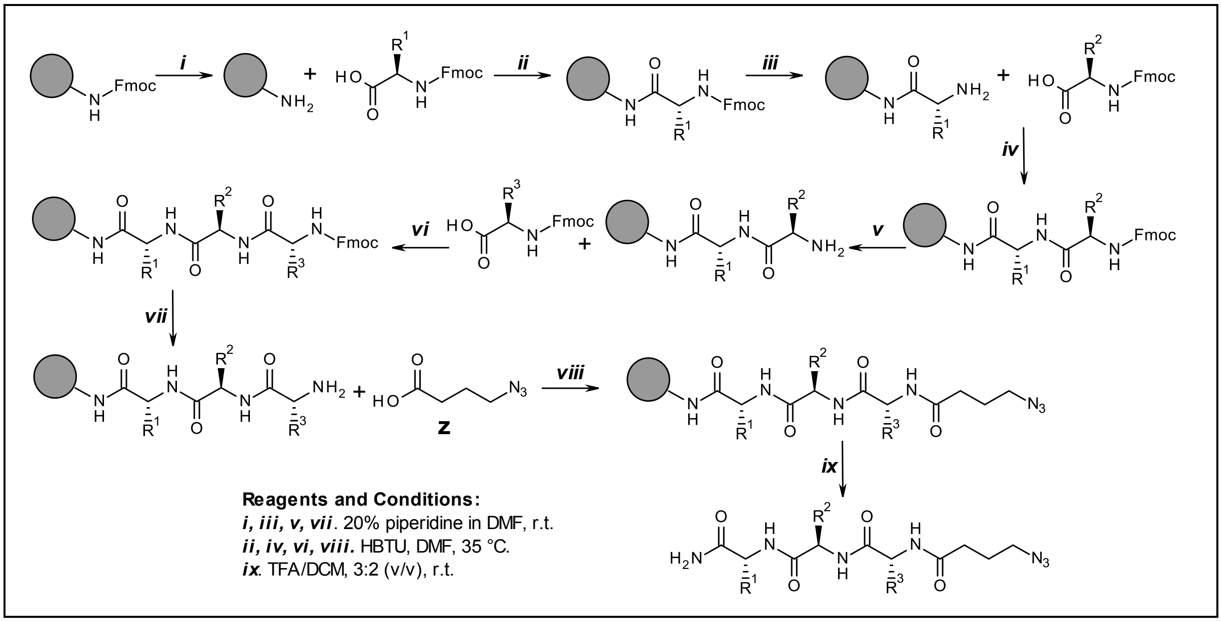
Steps *iii, v, vii,* and *ix*: Displacement with Primary Amines*.* Solutions of primary amines (0.5 M, 2 mL, 1 mmol, 40 equiv.) in NMP and 0.5 M solution of DIPEA in NMP (1 mL, 0.5 mmol, 20 equiv.) were added into the reaction wells. The reaction mixtures were shaken at 550 rpm for 30 min at 35 ^{o}C. After draining of the reagents, the displacement was repeated. The reaction wells were drained, and the resin was washed with 4×3 mL DMF for 4×2 min, while shaking at 550 rpm.

Final Wash: After completion of the last displacement step, the reaction wells were drained, and the resin was washed with 5×3 mL DMF for 5x2 min while shaking at 550 rpm. The resin was washed again with 4×3 mL methanol for 4×2 min.

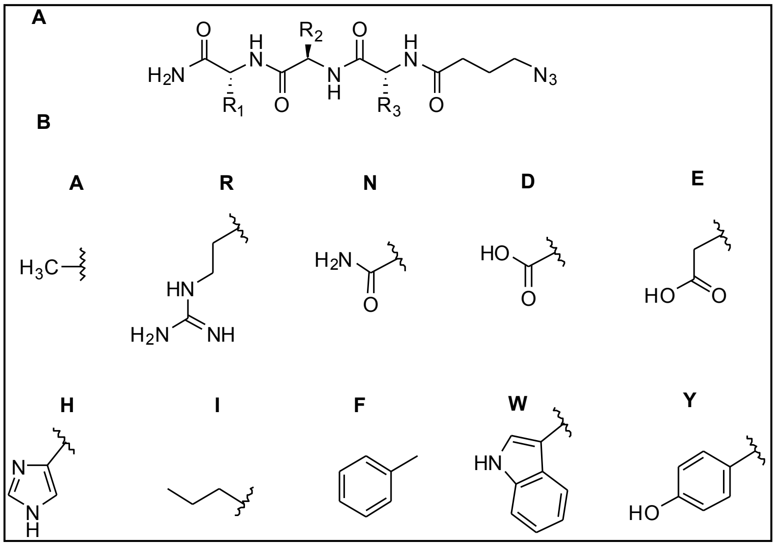
Step *x*: Cleavage from the Resin. The resin with bound peptoids was shaken in 2 mL of THF/DCM/H_2O (59:49:2, v/v/v) for 1 h. The supernatant containing cleaved peptoids was drained and collected. The resin was additionally washed with DCM (3 × 1mL). The volumes of combined cleavage solutions and DCM washes were reduced under stream of nitrogen. The oily residues were resuspended in water, and lyophilized to afford crude peptoids. The crude peptoids were dissolved in the minimal volume of methanol/water mixture (50:50, v/v). The solutions were centrifuged to remove insoluble solids, and supernatant solutions were subject to HPLC purifications using a 5% to 95% gradient of solvemt B (0.1% TFA in methanol) in solvent A (0.1% TFA in water) over 35min. LC fractions were analyzed using ESI-MS, and samples containing target products were combined and lyophilized. If additional purification of peptoids was necessary, the products were, resuspended in minimal volume of methanol-water (50:50, v/v) mixture, and samples were HPLC-purified using a 50% to 90% gradient of solvent B (0.1% TFA in methanol) in solvent A (0.1% TFA in water) over 40 min.

In total, 35 peptoids were successfully synthesized. Every compound from this peptoid library passed a mass spectral quality control (QC) analysis where the major peak $[M+H]^+$ corresponded to a 100% relative intensity compared to other by-product peaks, of which none demonstrated an intensity greater than 25% of the maximal intensity. Purity of the peptoids was estimated by HPLC using integration of the absorbance intensities at 254 nm. Average purity was greater than 60%.

I (c) General Protocol for Peptide Synthesis



Scheme S-5: Solid phase synthetic protocol for peptide library



Scheme S-6. (**A**) General structure of peptide library members and submonomers used to construct them. (**B**) General structure of peptide library members and the submonomers used.

The general scheme for solid-phase peptide synthesis utilized in this work is presented in Scheme S-5. The designed peptides contain three amino acid residues comprised by variations of 10 amino acids as in Scheme S-6, and the *N*-terminus of tripeptides is capped with 4-azidobutyrate. The starting material, 4-azidobutyric acid **Z** (Scheme S-5), was synthesized from commercially available ethyl 4-bromobutyrate in two steps according to previously published procedures.(*11, 12*) The sequences of 74 synthesized tripeptides were chosen from the list of sequences obtained using a Random Number Generator. All library members were synthesized with an azide functional group. This allows for site-specific conjugation onto alkyne functionalized agarose slides by a copper(I) catalyzed 1,3 dipolar cycloaddition reaction.(*4-8*)

Step *i:* Deprotection. Fmoc-Rink Amide MBHA Resin (62.5 mg, 25 μmol) with a substitution level of 0.40 meq/g was deprotected using 2×3 mL of 20% piperidine in DMF for 2×20 min with shaking at 550 rpm (Figure 13). The reaction wells were drained by flushing with nitrogen, and the resin was washed with 5×3 mL DMF for 5×2 min while shaking at 550 rpm.

Steps *ii, iv, vi,* and *viii*: Coupling with Fmoc-protected amino acids and 4-azidobutyric acid. Coupling reactions were completed by adding 0.5 M solutions of Fmoc-protected amino acids, or 4-azidobutyric acid in NMP (2 mL, 1 mmol, 40 equiv.) and 0.5 M HBTU in NMP (2 mL, 1 mmol, 40 equiv.) into reaction wells containing growing peptides on the resin. Reaction mixtures were shaken at 550 rpm for 30 min at 35 ^{o}C. The reagents were then drained, and the coupling step was repeated. The resin was washed with 4×3 mL DMF for 4×2 min, while shaking at 550 rpm.

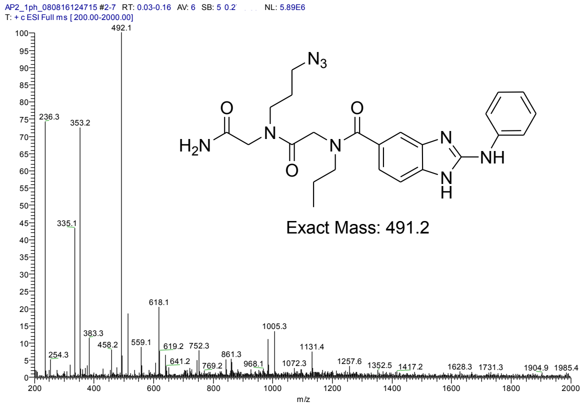
Steps *iii, v,* and *vii:* Deprotection of *N*-terminus of peptides. Piperidine (20% in DMF) was added to the reaction wells containing growing peptides on the resin. Reaction mixtures were shaken at 550 rpm for 20 min, the wells were drained, and deprotection procedure was repeated. The reaction wells were finally drained by flushing with nitrogen, and the resin was washed with 5×3 mL DMF for 5×2 min while shaking at 550 rpm.

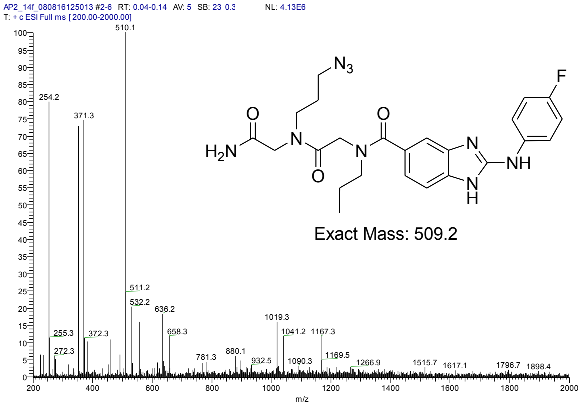
Final Wash: After completion of the last coupling step with 4-azidobutyric acid **z**, the reaction wells were drained, and the resin was washed with 5×3 mL DMF for 5×2 min while shaking at 550 rpm. The resin was washed again with 4×3 mL methanol for 4×2 min.

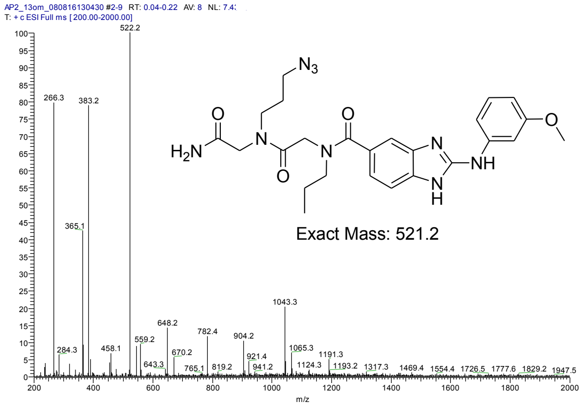
Step *ix*: Cleavage from the Resin. The resin with bound peptides was shaken in 2 mL of TFA/DCM/H_2O (59:49:2, v/v/v) for 1 h. The supernatant containing cleaved peptides was drained and collected. The resin was additionally washed with DCM (3×1 mL). The volumes of combined cleavage solutions and DCM washes were reduced under stream of nitrogen. The oily residues were resuspended in water, and lyophilized to afford crude peptides. The crude peptides were dissolved in the minimal volume of methanol/water mixtures. The solutions were centrifuged to remove insoluble solids, and supernatant solutions were subject to HPLC purifications using a 0% to 100% gradient of solvent B (0.1% TFA in methanol) in solvent A (0.1% TFA in water) over 50min. LC fractions were analyzed using ESI-MS, and samples containing target products were combined and lyophilized.

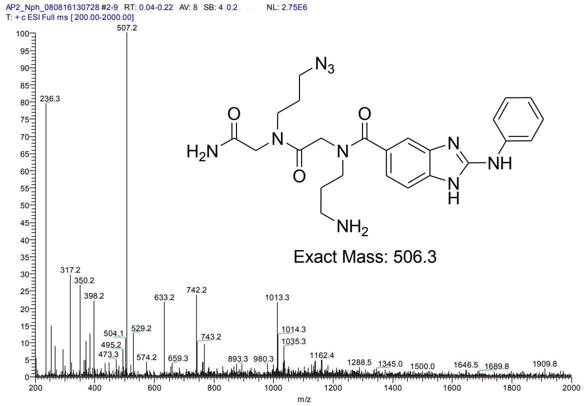
Section II: Spectroscopic Data for Compounds

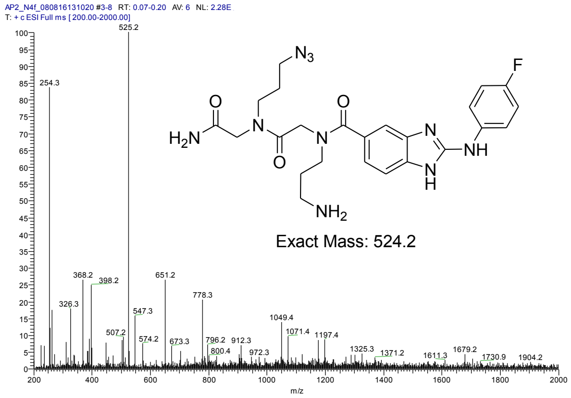
II (a) Mass Spectral Data for 2-Aminobenzimidazole Library Members







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778.3
547.3
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574.2
673.3
796.2
912.3
800.4
972.3
1049.4
1071.4
1197.4
1325.3
1371.2
1611.3
1679.2
1730.9
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N
H
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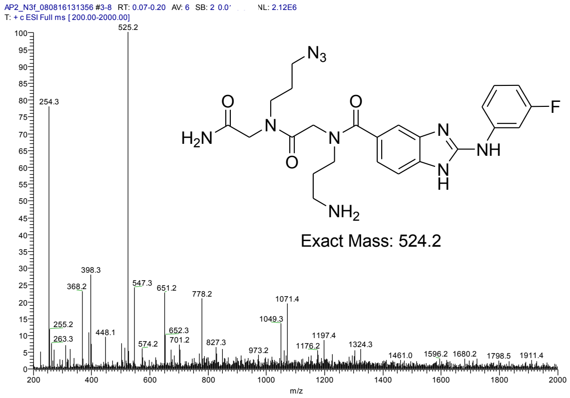
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398.3
368.2
547.3
651.2
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263.3
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652.3
701.2
574.2
827.3
1071.4
1049.3
1197.4
1176.2
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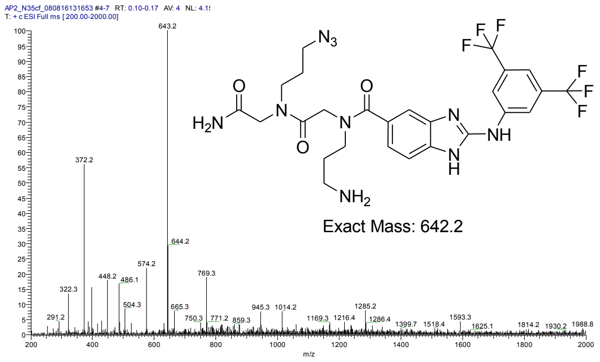
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771.2
859.3
945.3
1014.2
1169.3
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1285.2
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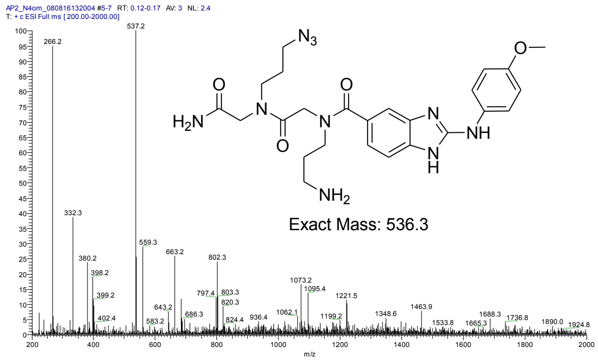
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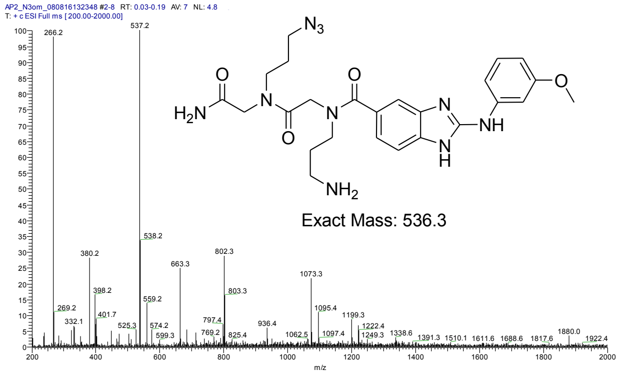
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269.2
559.2
401.7
332.1
525.3
574.2
599.3
797.4
769.2
825.4
936.4
1073.3
1095.4
1199.3
1222.4
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1097.4
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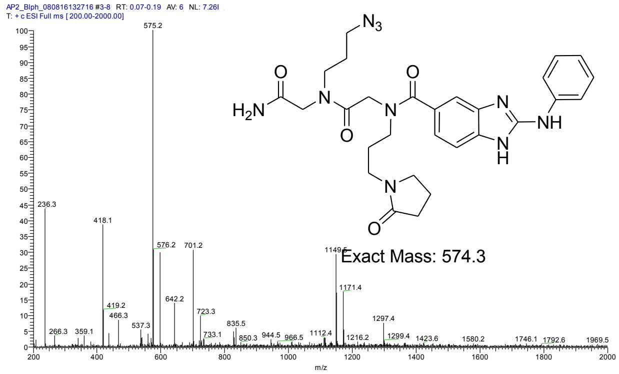
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642.2
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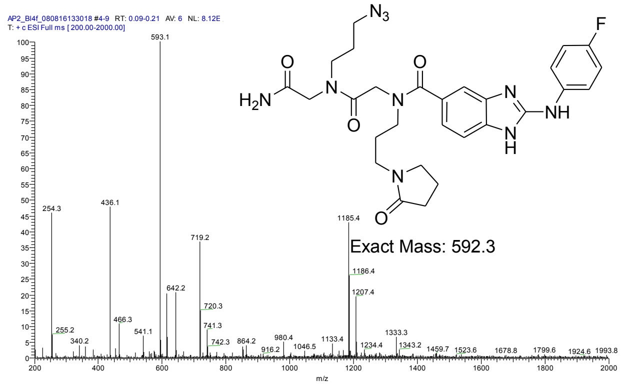
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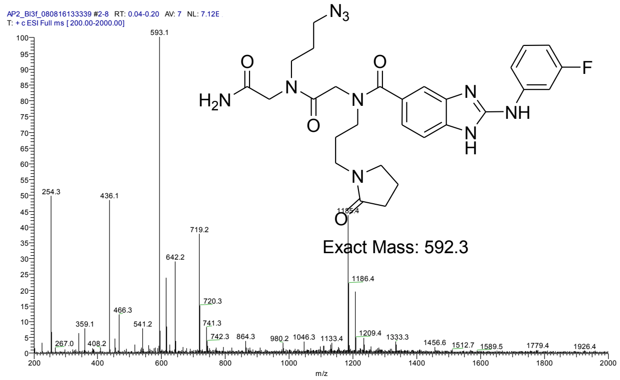
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742.3
267.0
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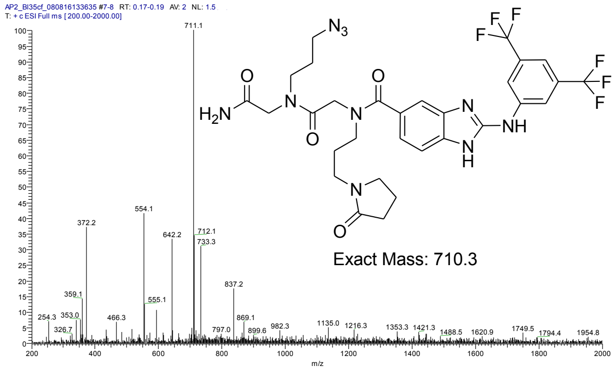
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326.7
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869.1
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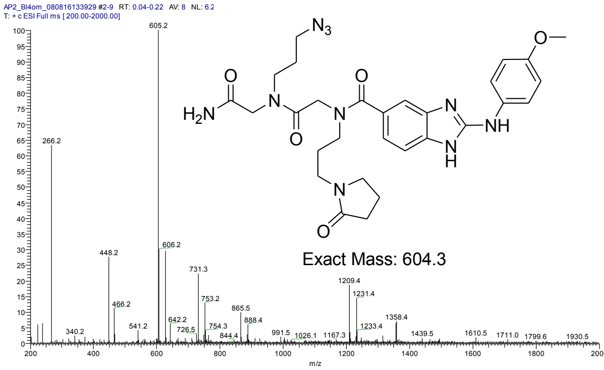
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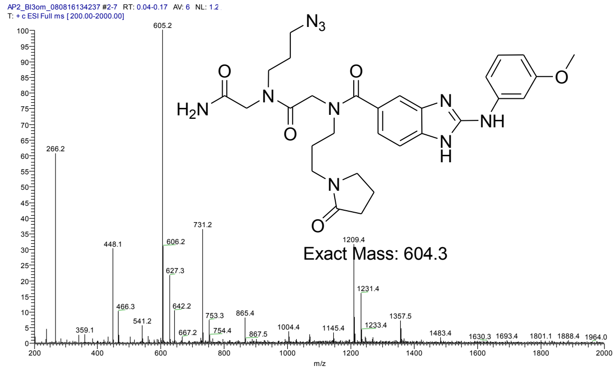
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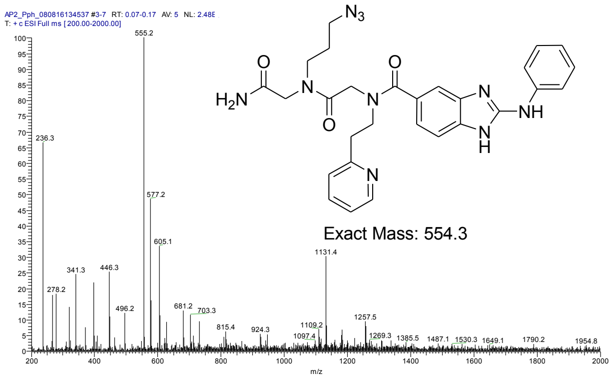
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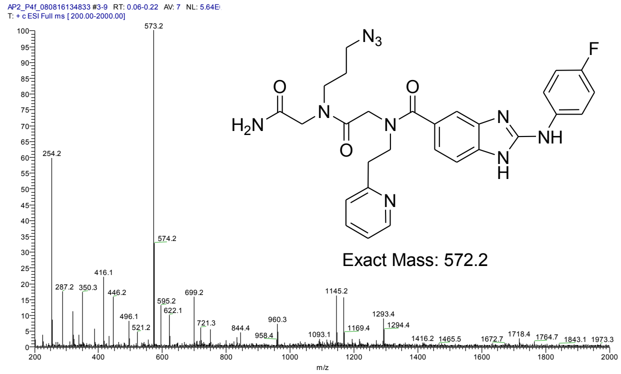
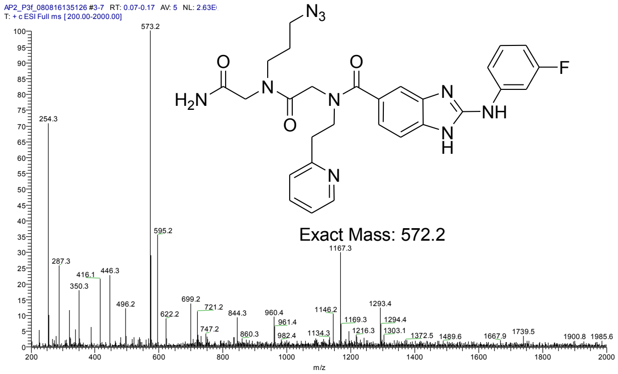
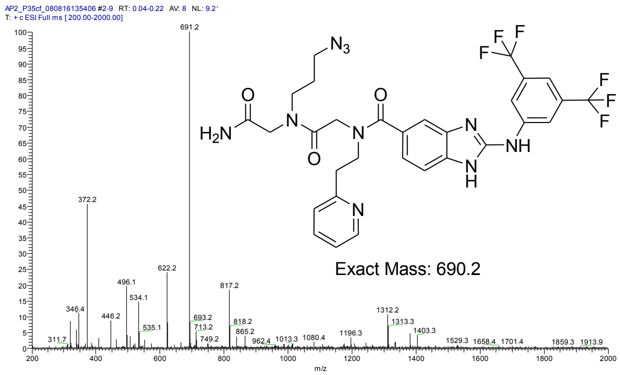
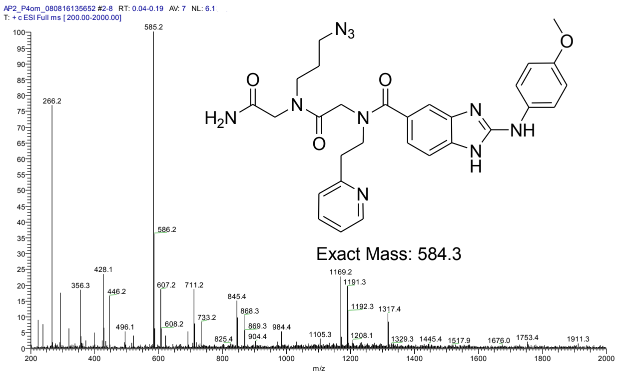
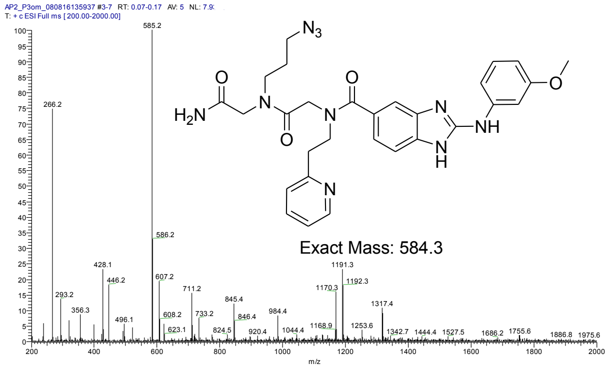
703.3
815.4
924.3
1109.2
1097.4
1257.5
1269.3
1385.5
1487.1
1530.3
1649.1
1790.2
1954.8
m/z
N3
H2N
NH
Exact Mass: 554.3

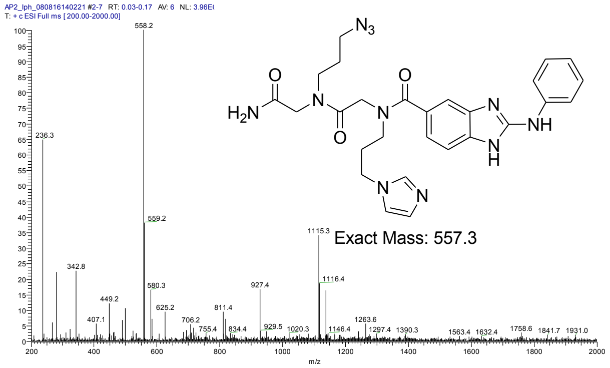

AP2_P4f_080816134833 #3-9 RT: 0.06-0.22 AV: 7 NL: 5.64E
T: + c ESI Full ms [200.00-2000.00]
573.2
254.2
574.2
416.1
287.2
350.3
446.2
496.1
521.2
595.2
622.1
699.2
721.3
844.4
958.4
960.3
1093.1
1145.2
1169.4
1293.4
1294.4
1416.2
1465.5
1672.7
1718.4
1764.7
1843.1
1973.3
m/z
N3
H2N
NH
F
Exact Mass: 572.2

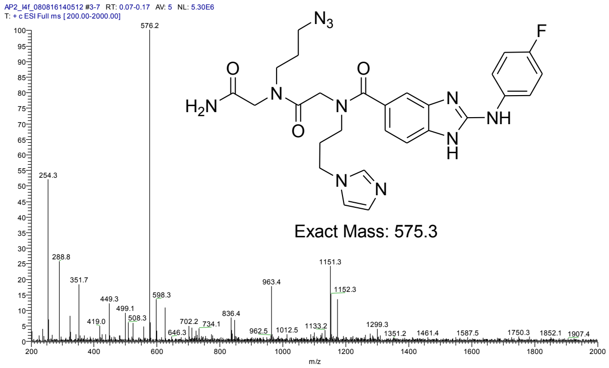

AP2_P3f_080816135126 #3-7 RT: 0.07-0.17 AV: 5 NL: 2.63E
T: + c ESI Full ms [200.00-2000.00]
573.2
254.3
595.2
1167.3
287.3
416.1
446.3
350.3
496.2
622.2
699.2
721.2
747.2
844.3
860.3
960.4
961.4
982.4
1134.3
1146.2
1169.3
1216.3
1293.4
1294.4
1303.1
1372.5
1489.6
1667.9
1739.5
1900.8
1985.6
m/z
N3
H2N
NH
F
Exact Mass: 572.2

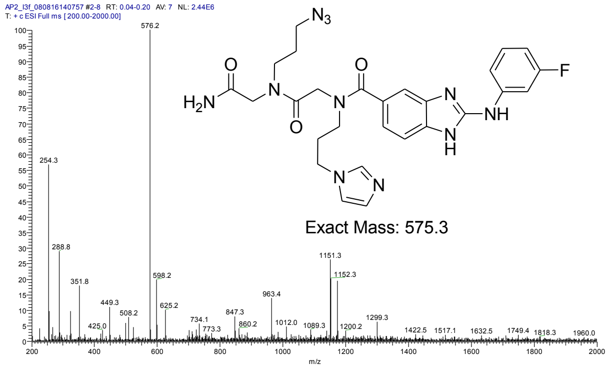

AP2_P35cf_080816135406 #2-9 RT: 0.04-0.22 AV: 8 NL: 9.2
T: + c ESI Full ms [200.00-2000.00]
691.2
372.2
622.2
496.1
534.1
346.4
446.2
535.1
311.7
817.2
693.2
713.2
749.2
818.2
865.2
962.4
1013.3
1080.4
1196.3
1312.2
1313.3
1403.3
1529.3
1658.4
1701.4
1859.3
1913.9
m/z
N3
H2N
NH
F
Exact Mass: 690.2

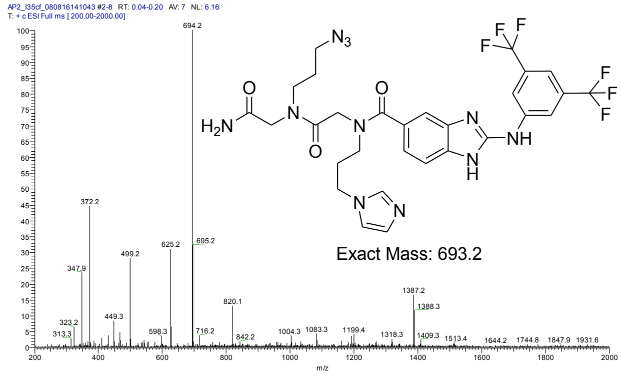

AP2_P4om_080816135652 #2-8 RT: 0.04-0.19 AV: 7 NL: 6.1
T: + c ESI Full ms [200.00-2000.00]
585.2
266.2
586.2
428.1
356.3
446.2
496.1
607.2
608.2
711.2
733.2
845.4
868.3
825.4
869.3
904.4
984.4
1105.3
1169.2
1191.3
1192.3
1208.1
1317.4
1329.3
1445.4
1517.9
1676.0
1753.4
1911.3
m/z
N3
H2N
NH
Exact Mass: 584.3

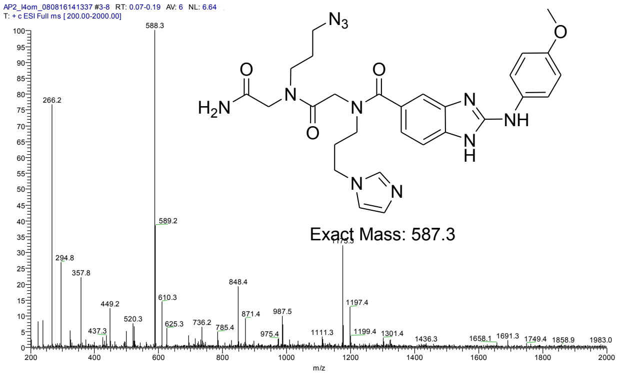

AP2_P3om_080816135937 #3-7 RT: 0.07-0.17 AV: 5 NL: 7.9
T: + c ESI Full ms [200.00-2000.00]
585.2
266.2
586.2
428.1
446.2
607.2
293.2
356.3
496.1
608.2
623.1
711.2
733.2
824.5
845.4
846.4
920.4
984.4
1044.4
1168.9
1170.3
1191.3
1192.3
1253.6
1317.4
1342.7
1444.4
1527.5
1686.2
1755.6
1886.8
1975.6
m/z
N3
O
H2N
N
O
N
N
NH
O
N
H
N
Exact Mass: 584.3

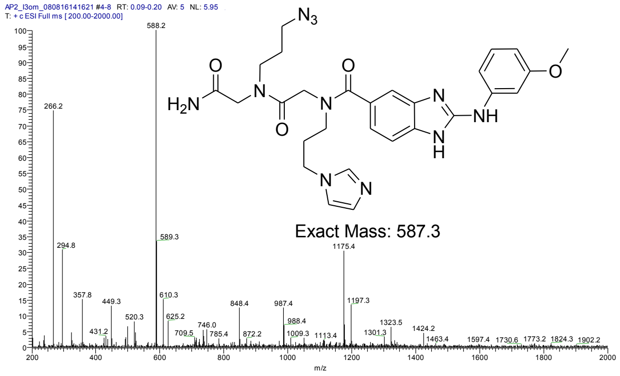

AP2_Iph_080816140221 #2-7 RT: 0.03-0.17 AV: 6 NL: 3.96E
T: + c ESI Full ms [200.00-2000.00]
558.2
236.3
559.2
342.8
580.3
449.2
407.1
625.2
706.2
755.4
811.4
834.4
927.4
929.5
1020.3
1115.3
1116.4
1146.4
1263.6
1297.4
1390.3
1563.4
1632.4
1758.6
1841.7
1931.0
m/z
N3
O
H2N
N
O
N
N
NH
N
H
N
N
Exact Mass: 557.3

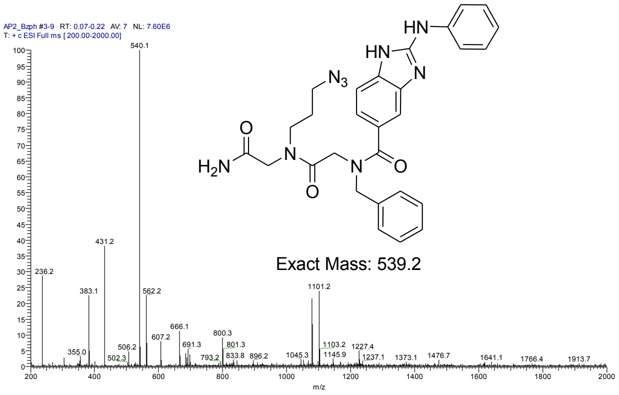

AP2_I4f_080816140512 #3-7 RT: 0.07-0.17 AV: 5 NL: 5.30E6
T: + c ESI Full ms [200.00-2000.00]
576.2
254.3
288.8
351.7
449.3
499.1
508.3
419.0
598.3
646.3
702.2
734.1
836.4
962.5
963.4
1012.5
1133.2
1151.3
1152.3
1299.3
1351.2
1461.4
1587.5
1750.3
1852.1
1907.4
m/z
N3
F
O
O
H2N
N
N
N
NH
O
N
H
N
N
Exact Mass: 575.3

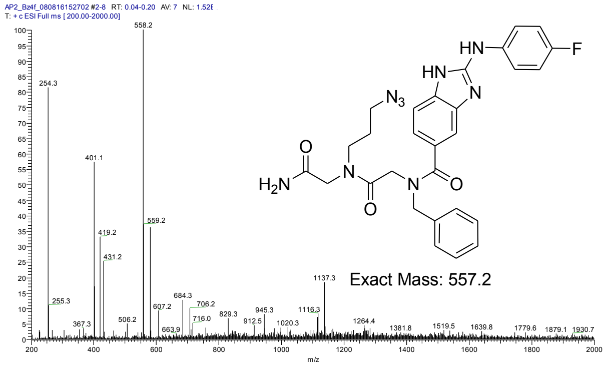

AP2_I3f_080816140757 #2-8 RT: 0.04-0.20 AV: 7 NL: 2.44E6
T: + c ESI Full ms [200.00-2000.00]
576.2
254.3
288.8
351.8
598.2
449.3
425.0
508.2
625.2
734.1
773.3
847.3
860.2
963.4
1012.0
1089.3
1151.3
1152.3
1200.2
1299.3
1422.5
1517.1
1632.5
1749.4
1818.3
1960.0
m/z
N3
O
O
F
H2N
N
N
N
NH
O
N
H
N
N
Exact Mass: 575.3


AP2_I35cf_080816141043 #2-8 RT: 0.04-0.20 AV: 7 NL: 6.16
T: + c ESI Full ms [200.00-2000.00]
694.2
372.2
347.9
499.2
625.2
695.2
323.2
313.3
449.3
598.3
716.2
820.1
842.2
1004.3
1083.3
1199.4
1318.3
1387.2
1388.3
1409.3
1513.4
1644.2
1744.8
1847.9
1931.6
m/z
N3
F
F
F
F
F
F
O
O
H2N
N
N
N
NH
O
N
H
N
N
Exact Mass: 693.2

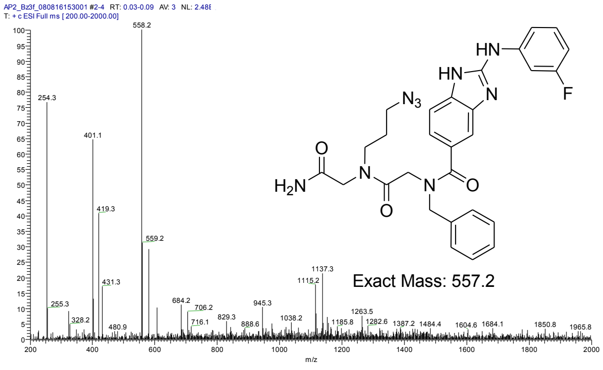

AP2_I4om_080816141337 #3-8 RT: 0.07-0.19 AV: 6 NL: 6.64
T: + c ESI Full ms [200.00-2000.00]
588.3
266.2
589.2
294.8
357.8
610.3
449.2
520.3
437.3
625.3
736.2
785.4
848.4
871.4
975.4
987.5
1111.3
1175.3
1197.4
1199.4
1301.4
1436.3
1658.1
1691.3
1749.4
1858.9
1983.0
m/z
N3
O
O
O
H2N
N
N
N
NH
O
N
H
N
N
Exact Mass: 587.3


AP2_I3om_080816141621 #4-8 RT: 0.09-0.20 AV: 5 NL: 5.95
T: + c ESI Full ms [200.00-2000.00]
588.2
266.2
589.3
294.8
357.8
449.3
610.3
520.3
625.2
431.2
709.5
746.0
785.4
848.4
872.2
987.4
988.4
1009.3
1113.4
1175.4
1197.3
1301.3
1323.5
1424.2
1463.4
1597.4
1730.6
1773.2
1824.3
1902.2
m/z
N3
O
O
O
H2N
N
N
N
NH
O
N
H
N
N
Exact Mass: 587.3

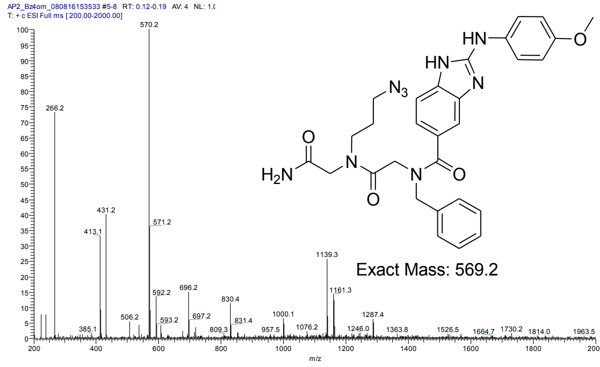

AP2_Bzph #3-9 RT: 0.07-0.22 AV: 7 NL: 7.60E6
T: + c ESI Full ms [200.00-2000.00]
540.1
431.2
236.2
383.1
562.2
355.0
502.3
506.2
607.2
666.1
691.3
793.2
800.3
801.3
833.8
896.2
1045.3
1101.2
1103.2
1145.9
1227.4
1237.1
1373.1
1476.7
1641.1
1766.4
1913.7
m/z
HN
HN
N
N3
O
H2N
N
N
O
O
Exact Mass: 539.2



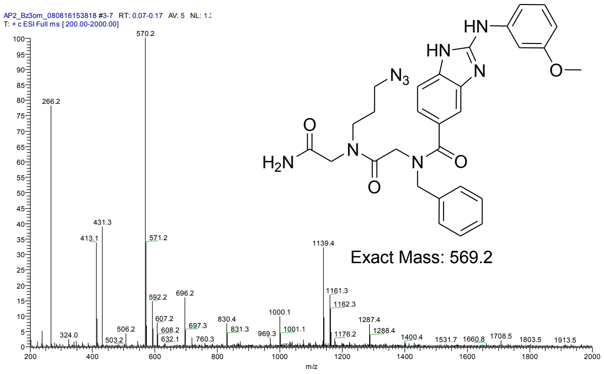
Exact Mass: 557.2



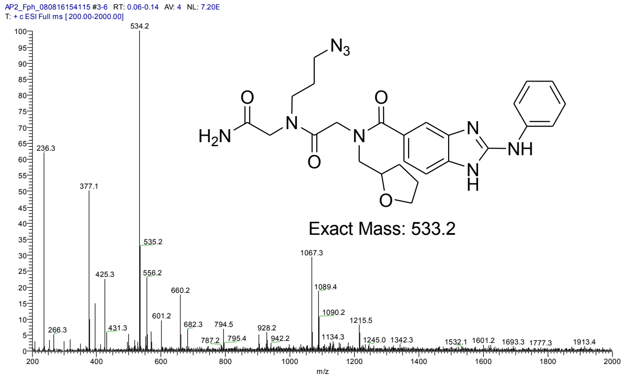
Exact Mass: 557.2



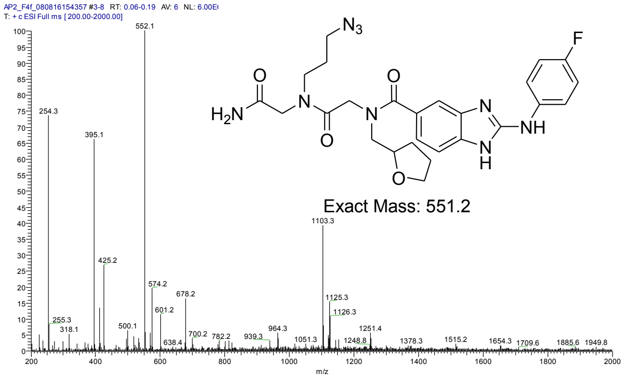
Exact Mass: 569.2



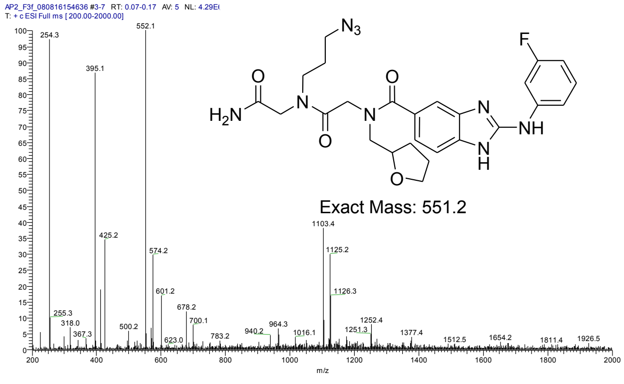
Exact Mass: 569.2



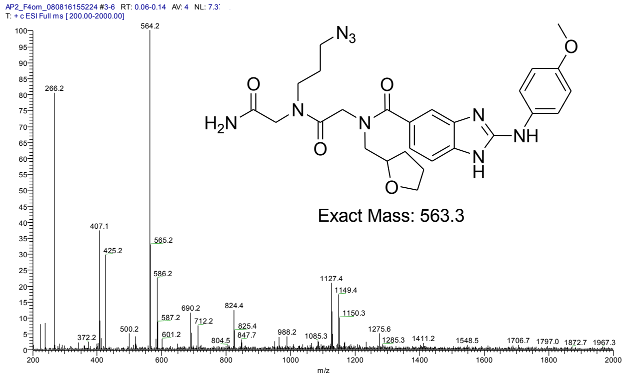
Exact Mass: 533.2



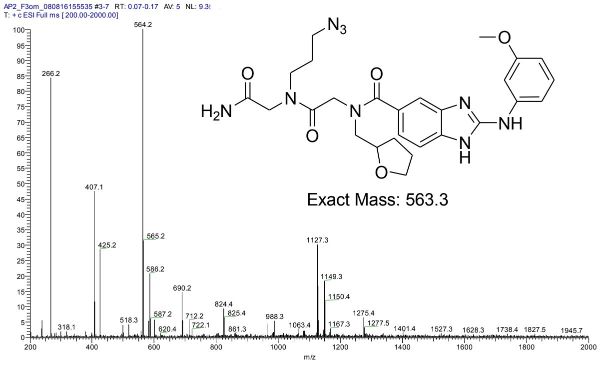
Exact Mass: 551.2

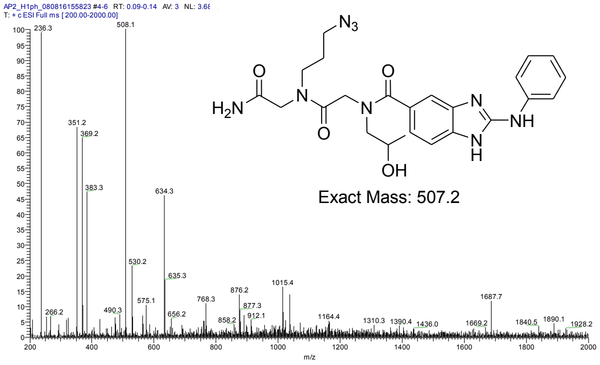


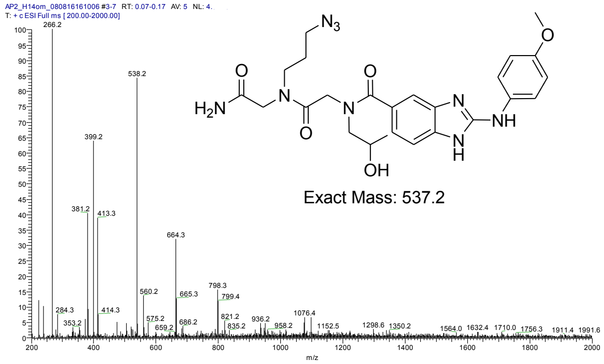
Exact Mass: 551.2

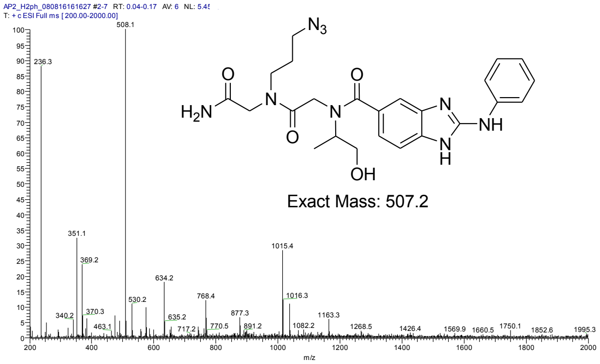


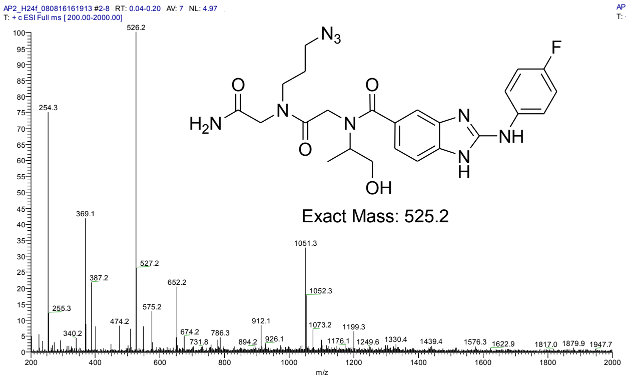
Exact Mass: 563.3

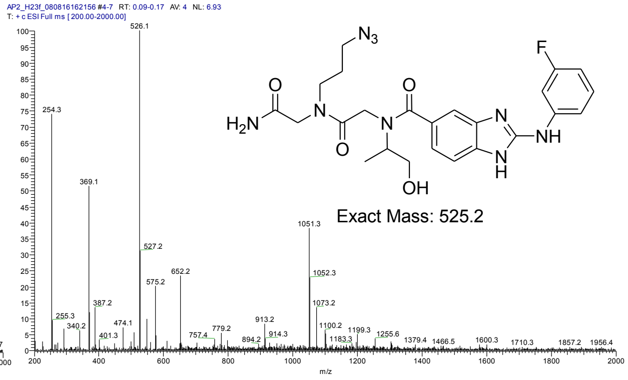

AP2_F3om_080816155535 #3-7 RT: 0.07-0.17 AV: 5 NL: 9.3
T: + c ESI Full ms [200.00-2000.00]
564.2
266.2
407.1
425.2
565.2
586.2
1127.3
1149.3
1150.4
690.2
824.4
1275.4
N3
H2N
O
N
NH
H
O
Exact Mass: 563.3
m/z

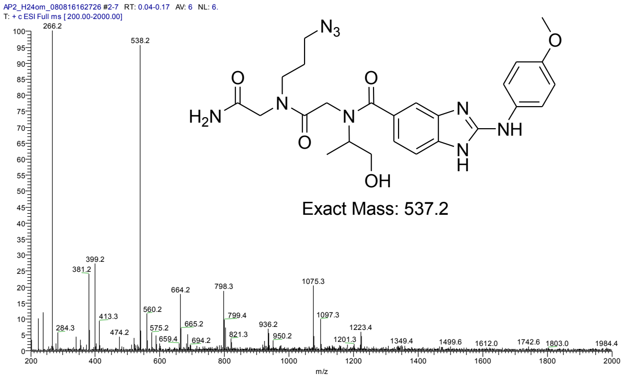

AP2_H1ph_080816155823 #4-6 RT: 0.09-0.14 AV: 3 NL: 3.6
T: + c ESI Full ms [200.00-2000.00]
236.3
508.1
351.2
369.2
383.3
634.3
530.2
635.3
1015.4
1687.7
N3
H2N
OH
NH
Exact Mass: 507.2
m/z

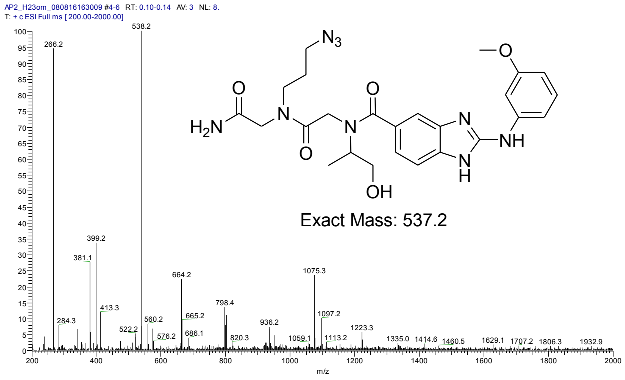

AP2_H14om_080816161006 #3-7 RT: 0.07-0.17 AV: 5 NL: 4.
T: + c ESI Full ms [200.00-2000.00]
266.2
538.2
399.2
381.2
413.3
664.3
798.3
1076.4
N3
H2N
OH
NH
Exact Mass: 537.2
m/z

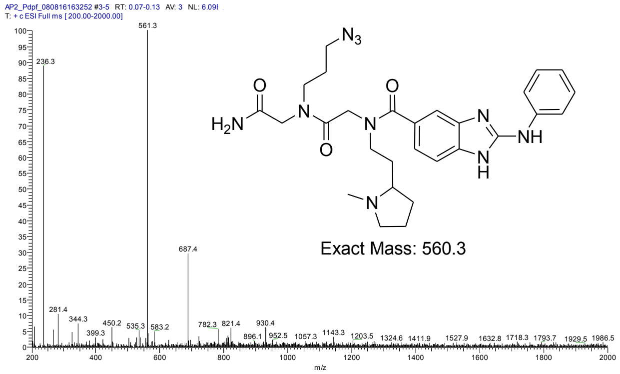

AP2_H2ph_080816161627 #2-7 RT: 0.04-0.17 AV: 6 NL: 5.4
T: + c ESI Full ms [200.00-2000.00]
508.1
236.3
351.1
369.2
634.2
768.4
1015.4
1016.3
N3
H2N
OH
NH
Exact Mass: 507.2
m/z

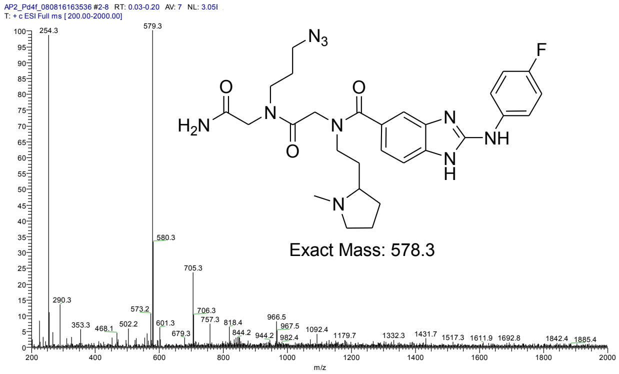

AP2_H24f_080816161913 #2-8 RT: 0.04-0.20 AV: 7 NL: 4.97
T: + c ESI Full ms [200.00-2000.00]
526.2
254.3
369.1
527.2
387.2
652.2
1051.3
1052.3
F
N3
H2N
OH
NH
Exact Mass: 525.2
m/z

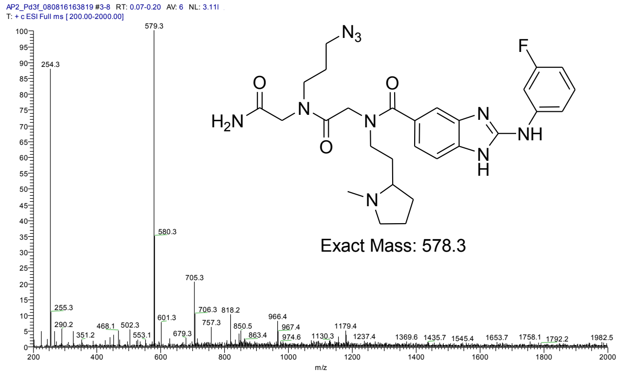

AP2_H23f_080816162156 #4-7 RT: 0.09-0.17 AV: 4 NL: 6.93
T: + c ESI Full ms [200.00-2000.00]
526.1
254.3
369.1
527.2
575.2
652.2
1051.3
1052.3
F
N3
H2N
OH
NH
Exact Mass: 525.2
m/z

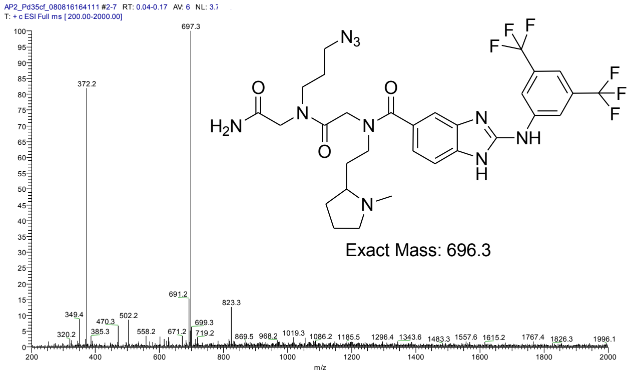

AP2_H24om_080816162726 #2-7 RT: 0.04-0.17 AV: 6 NL: 6.
T: + c ESI Full ms [200.00-2000.00]
266.2
538.2
399.2
381.2
664.2
798.3
1075.3
N3
H2N
OH
NH
Exact Mass: 537.2
m/z

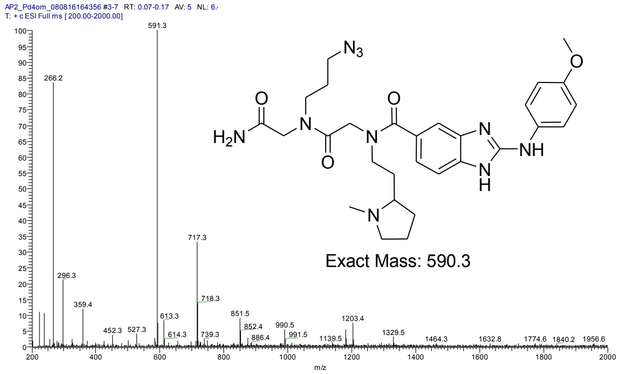

AP2_H23om_080816163009 #4-6 RT: 0.10-0.14 AV: 3 NL: 8.
T: + c ESI Full ms [200.00-2000.00]
538.2
266.2
399.2
381.1
664.2
798.4
1075.3
N3
H2N
OH
NH
Exact Mass: 537.2
m/z

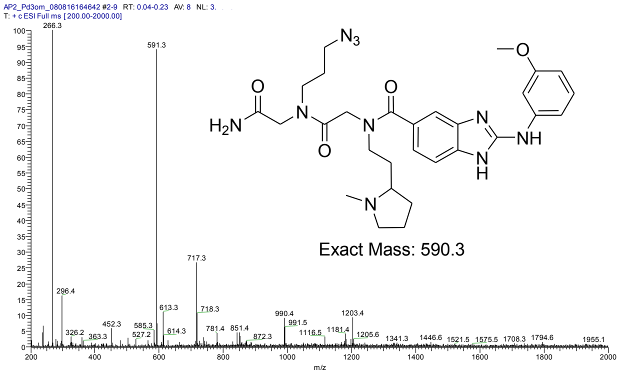

AP2_Pdpf_080816163252 #3-5 RT: 0.07-0.13 AV: 3 NL: 6.09E
T: + c ESI Full ms [200.00-2000.00]
561.3
236.3
687.4
281.4
344.3
399.3
450.2
535.3
583.2
782.3
821.4
930.4
896.1
952.5
1057.3
1143.3
1203.5
1324.6
1411.9
1527.9
1632.8
1718.3
1793.7
1929.5
1986.5
m/z
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 560.3

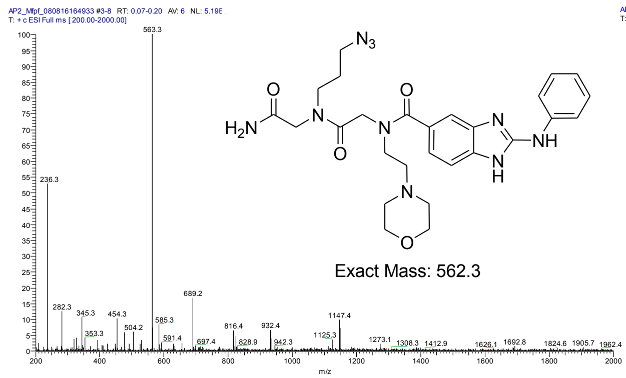

AP2_Pd4f_080816163536 #2-8 RT: 0.03-0.20 AV: 7 NL: 3.05E
T: + c ESI Full ms [200.00-2000.00]
579.3
254.3
580.3
705.3
290.3
353.3
468.1
502.2
573.2
601.3
679.3
706.3
757.3
818.4
844.2
944.2
966.5
967.5
982.4
1092.4
1179.7
1332.3
1431.7
1517.3
1611.9
1692.8
1842.4
1885.4
m/z
F
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 578.3

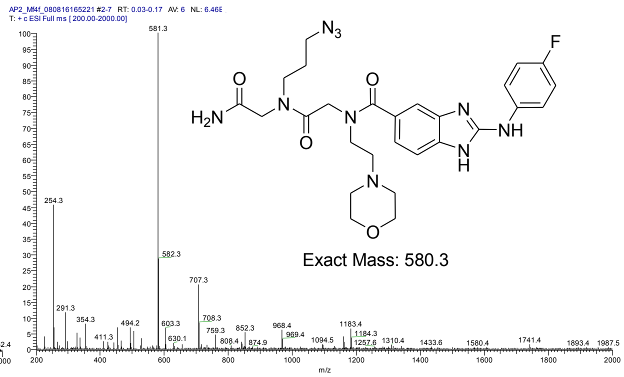

AP2_Pd3f_080816163819 #3-8 RT: 0.07-0.20 AV: 6 NL: 3.11E
T: + c ESI Full ms [200.00-2000.00]
579.3
254.3
580.3
705.3
255.3
290.2
351.2
468.1
502.3
553.1
601.3
679.3
706.3
757.3
818.2
850.5
863.4
966.4
967.4
974.6
1130.3
1179.4
1237.4
1369.6
1435.7
1545.4
1653.7
1758.1
1792.2
1982.5
m/z
F
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 578.3

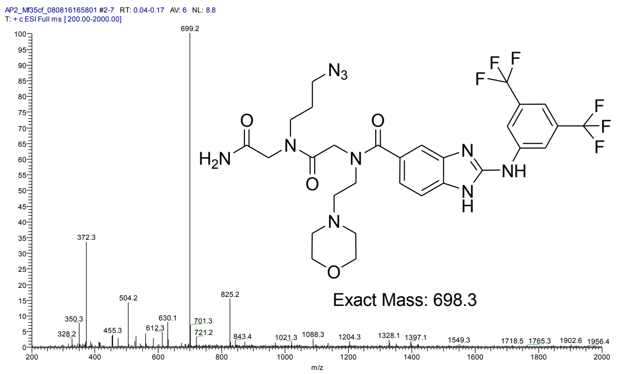

AP2_Pd35cf_080816164111 #2-7 RT: 0.04-0.17 AV: 6 NL: 3.1
T: + c ESI Full ms [200.00-2000.00]
697.3
372.2
349.4
320.2
385.3
470.3
502.2
558.2
671.2
691.2
699.3
719.2
823.3
869.5
968.2
1019.3
1086.2
1185.5
1296.4
1343.6
1483.3
1557.6
1615.2
1767.4
1826.3
1996.1
m/z
F
F
F
F
F
F
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 696.3

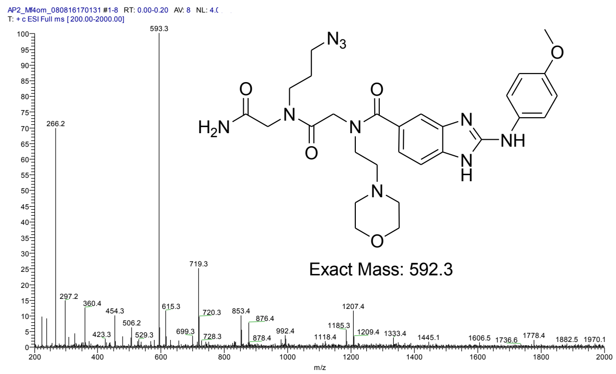

AP2_Pd4om_080816164356 #3-7 RT: 0.07-0.17 AV: 5 NL: 6.
T: + c ESI Full ms [200.00-2000.00]
591.3
266.2
717.3
296.3
359.4
452.3
527.3
613.3
614.3
718.3
739.3
851.5
852.4
886.4
990.5
991.5
1139.5
1203.4
1329.5
1464.3
1632.8
1774.6
1840.2
1956.6
m/z
O
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 590.3

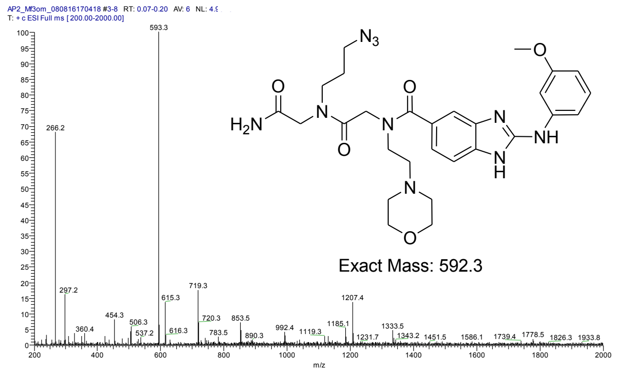

AP2_Pd3om_080816164642 #2-9 RT: 0.04-0.23 AV: 8 NL: 3.
T: + c ESI Full ms [200.00-2000.00]
266.3
591.3
717.3
296.4
326.2
363.3
452.3
527.2
585.3
613.3
614.3
718.3
781.4
851.4
872.3
990.4
991.5
1116.5
1181.4
1203.4
1205.6
1341.3
1446.6
1521.5
1575.5
1708.3
1794.6
1955.1
m/z
O
N3
H2N
O
N
O
N
O
N
NH
N
H
N
Exact Mass: 590.3

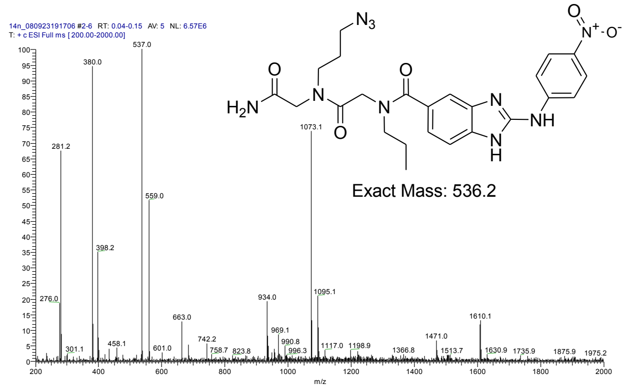

AP2_Mfpf_080816164933 #3-8 RT: 0.07-0.20 AV: 6 NL: 5.19E
T: + c ESI Full ms [200.00-2000.00]
563.3
236.3
689.2
282.3
345.3
353.3
454.3
504.2
585.3
591.4
697.4
816.4
828.9
932.4
942.3
1125.3
1147.4
1273.1
1308.3
1412.9
1626.1
1692.8
1824.6
1905.7
1962.4
m/z
N3
H2N
O
N
O
N
O
N
NH
N
H
N
O
Exact Mass: 562.3

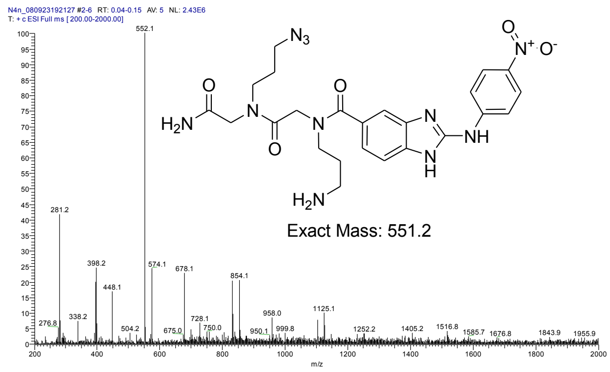

AP2_Mf4f_080816165221 #2-7 RT: 0.03-0.17 AV: 6 NL: 6.46E
T: + c ESI Full ms [200.00-2000.00]
581.3
254.3
582.3
707.3
291.3
354.3
411.3
494.2
603.3
630.1
708.3
759.3
808.4
852.3
874.9
968.4
969.4
1094.5
1183.4
1184.3
1257.6
1310.4
1433.6
1580.4
1741.4
1893.4
1987.5
m/z
F
N3
H2N
O
N
O
N
O
N
NH
N
H
N
O
Exact Mass: 580.3

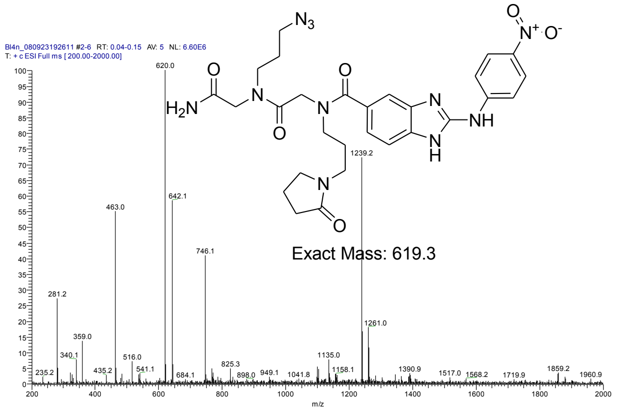

AP2_Mf35cf_080816165801 #2-7 RT: 0.04-0.17 AV: 6 NL: 8.8
T: + c ESI Full ms [200.00-2000.00]
699.2
372.3
504.2
825.2
350.3
328.2
455.3
612.3
630.1
701.3
721.2
843.4
1021.3
1088.3
1204.3
1328.1
1397.1
1549.3
1718.5
1765.3
1902.6
1956.4
m/z
N3
F
H2N
O
N
NH
Exact Mass: 698.3

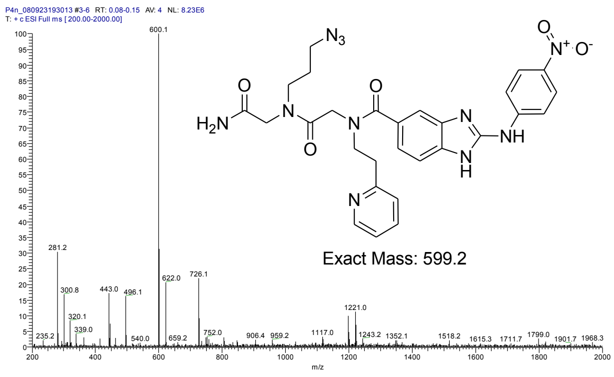

AP2_Mf4om_080816170131 #1-8 RT: 0.00-0.20 AV: 8 NL: 4.0
T: + c ESI Full ms [200.00-2000.00]
593.3
266.2
719.3
297.2
360.4
454.3
423.3
506.2
529.3
615.3
699.3
720.3
728.3
853.4
876.4
878.4
992.4
1118.4
1185.3
1207.4
1209.4
1333.4
1445.1
1606.5
1736.6
1778.4
1882.5
1970.1
m/z
N3
H2N
O
N
NH
Exact Mass: 592.3

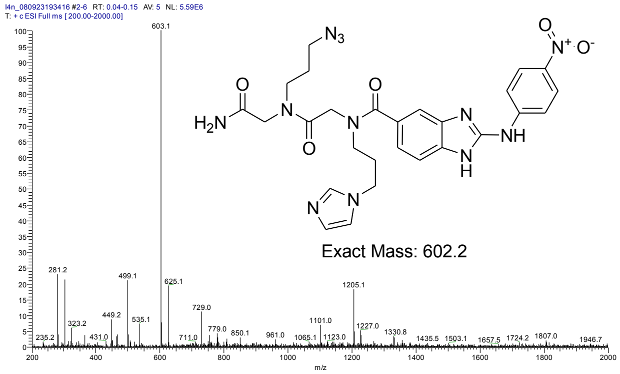

AP2_Mf3om_080816170418 #3-8 RT: 0.07-0.20 AV: 6 NL: 4.9
T: + c ESI Full ms [200.00-2000.00]
593.3
266.2
297.2
360.4
454.3
506.3
537.2
615.3
616.3
719.3
720.3
783.5
853.5
890.3
992.4
1119.3
1185.1
1207.4
1231.7
1333.5
1343.2
1451.5
1586.1
1739.4
1778.5
1826.3
1933.8
m/z
N3
H2N
O
N
NH
Exact Mass: 592.3

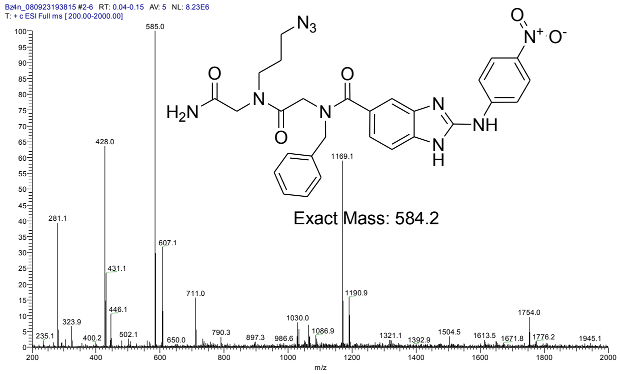

14n_080923191706 #2-6 RT: 0.04-0.15 AV: 5 NL: 6.57E6
T: + c ESI Full ms [200.00-2000.00]
537.0
380.0
281.2
1073.1
559.0
398.2
276.0
301.1
458.1
601.0
663.0
742.2
758.7
823.8
934.0
969.1
990.8
996.3
1095.1
1117.0
1198.9
1366.8
1471.0
1513.7
1610.1
1630.9
1735.9
1875.9
1975.2
m/z
N3
N+
O-
H2N
O
N
NH
Exact Mass: 536.2

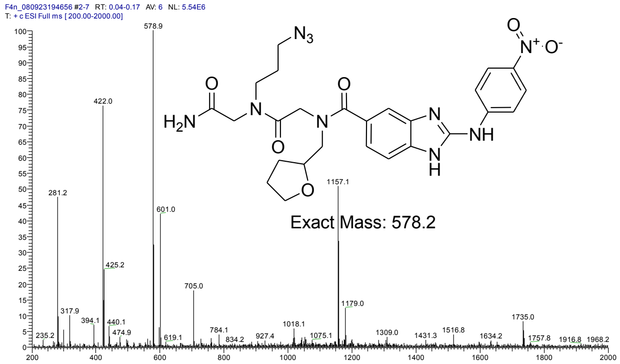

N4n_080923192127 #2-6 RT: 0.04-0.15 AV: 5 NL: 2.43E6
T: + c ESI Full ms [200.00-2000.00]
552.1
281.2
398.2
448.1
574.1
678.1
854.1
276.8
338.2
504.2
675.0
728.1
750.0
958.0
950.1
999.8
1125.1
1252.2
1405.2
1516.8
1585.7
1676.8
1843.9
1955.9
m/z
N3
N+
O-
H2N
O
N
NH
Exact Mass: 551.2

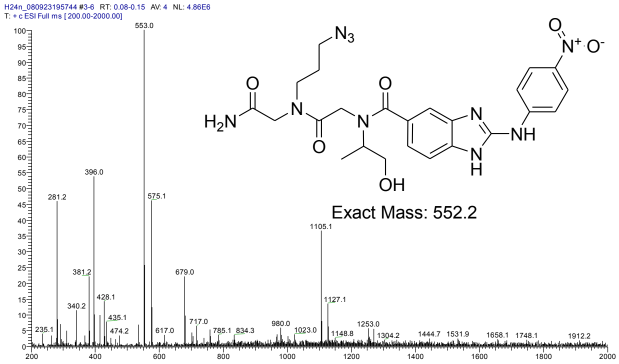

Bl4n_080923192611 #2-6 RT: 0.04-0.15 AV: 5 NL: 6.60E6
T: + c ESI Full ms [200.00-2000.00]
620.0
1239.2
463.0
642.1
746.1
281.2
359.0
340.1
235.2
435.2
516.0
541.1
684.1
825.3
898.0
949.1
1041.8
1135.0
1158.1
1261.0
1390.9
1517.0
1568.2
1719.9
1859.2
1960.9
m/z
N3
N+
O-
H2N
O
N
NH
Exact Mass: 619.3

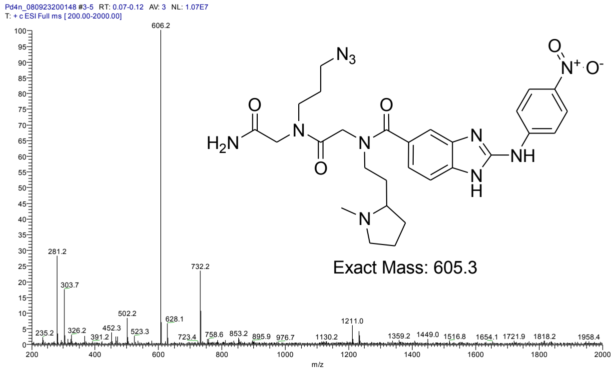

P4n_080923193013 #3-6 RT: 0.08-0.15 AV: 4 NL: 8.23E6
T: + c ESI Full ms [200.00-2000.00]
600.1
281.2
300.8
320.1
339.0
235.2
443.0
496.1
540.0
622.0
659.2
726.1
752.0
906.4
959.2
1117.0
1221.0
1243.2
1352.1
1518.2
1615.3
1711.7
1799.0
1901.7
1968.3
m/z
N3
N+
O-
H2N
O
N
NH
Exact Mass: 599.2

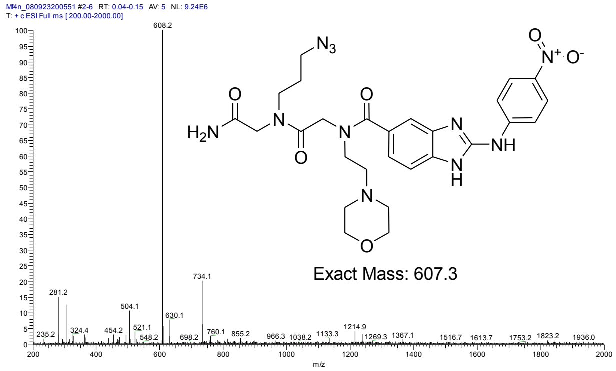

I4n_080923193416 #2-6 RT: 0.04-0.15 AV: 5 NL: 5.59E6
T: + c ESI Full ms [200.00-2000.00]
603.1
281.2
499.1
625.1
1205.1
Exact Mass: 602.2
m/z

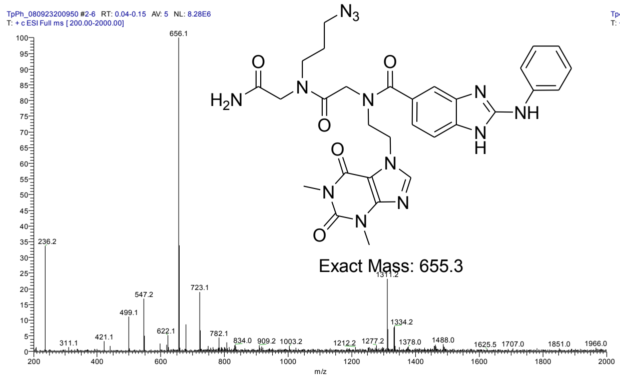

Bz4n_080923193815 #2-6 RT: 0.04-0.15 AV: 5 NL: 8.23E6
T: + c ESI Full ms [200.00-2000.00]
585.0
428.0
281.1
607.1
1169.1
Exact Mass: 584.2
m/z

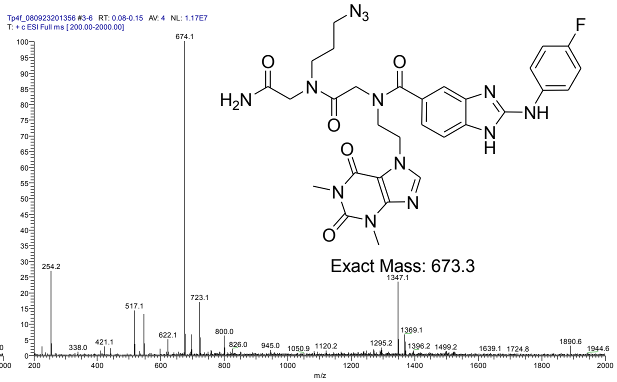

F4n_080923194656 #2-7 RT: 0.04-0.17 AV: 6 NL: 5.54E6
T: + c ESI Full ms [200.00-2000.00]
578.9
422.0
281.2
601.0
1157.1
Exact Mass: 578.2
m/z

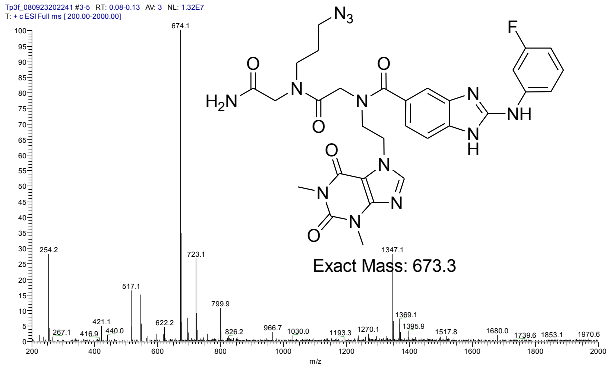

H24n_080923195744 #3-6 RT: 0.08-0.15 AV: 4 NL: 4.86E6
T: + c ESI Full ms [200.00-2000.00]
553.0
396.0
281.2
575.1
1105.1
Exact Mass: 552.2
m/z

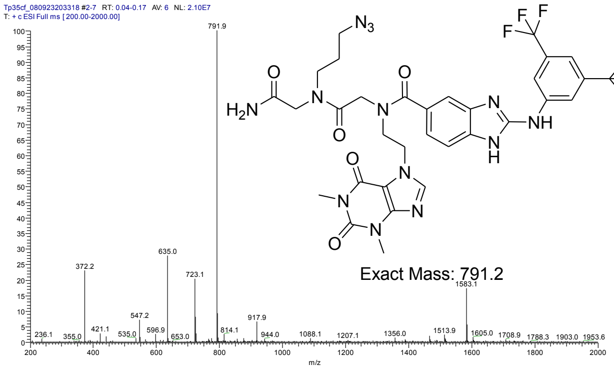

Pd4n_080923200148 #3-5 RT: 0.07-0.12 AV: 3 NL: 1.07E7
T: + c ESI Full ms [200.00-2000.00]
606.2
281.2
732.2
Exact Mass: 605.3
m/z

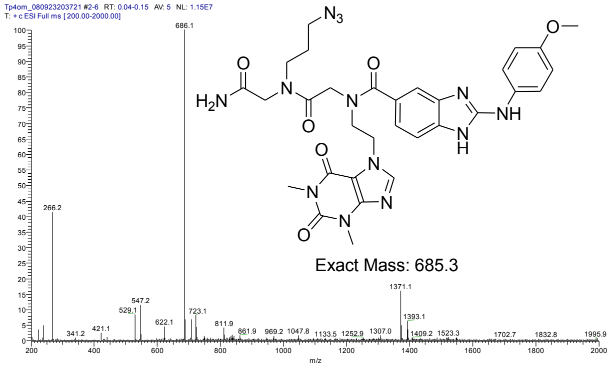

Mf4n_080923200551 #2-6 RT: 0.04-0.15 AV: 5 NL: 9.24E6
T: + c ESI Full ms [200.00-2000.00]
608.2
734.1
Exact Mass: 607.3
m/z

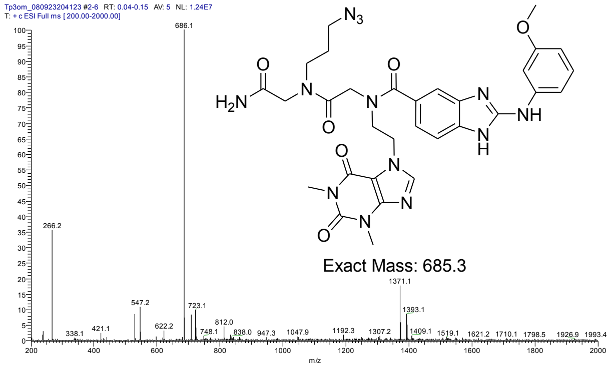

TpPh_080923200950 #2-6 RT: 0.04-0.15 AV: 5 NL: 8.28E6
T: + c ESI Full ms [200.00-2000.00]
656.1
236.2
1311.2
Exact Mass: 655.3
m/z

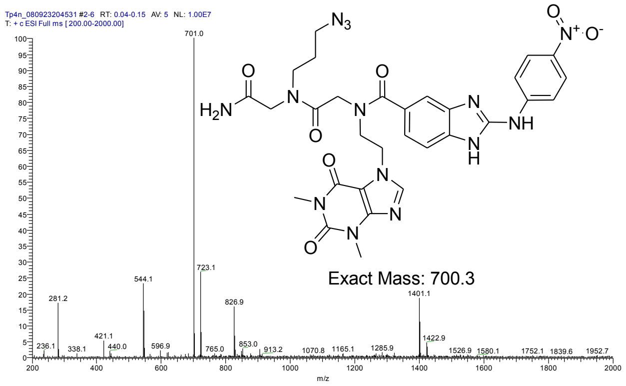

Tp4f_080923201356 #3-6 RT: 0.08-0.15 AV: 4 NL: 1.17E7
T: + c ESI Full ms [200.00-2000.00]
674.1
254.2
1347.1
Exact Mass: 673.3
m/z

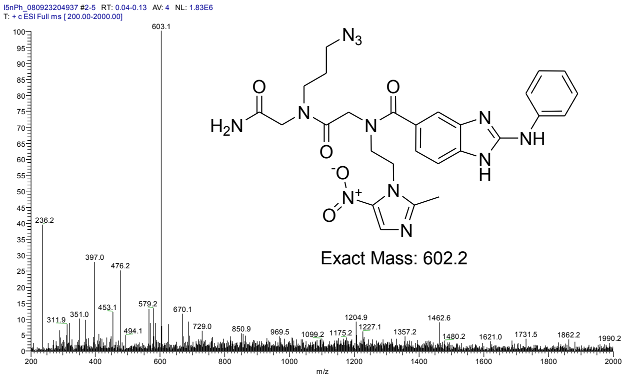

Tp3f_080923202241 #3-5 RT: 0.08-0.13 AV: 3 NL: 1.32E7
T: + c ESI Full ms [200.00-2000.00]
674.1
254.2
723.1
1347.1
517.1
799.9
1369.1
267.1
416.9
421.1
440.0
622.2
826.2
966.7
1030.0
1193.3
1270.1
1395.9
1517.8
1680.0
1739.6
1853.1
1970.6
m/z
N3
F
O
H2N
N
NH
N
H
Exact Mass: 673.3

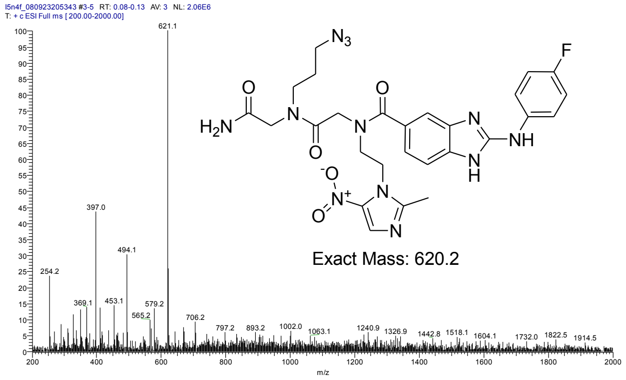

Tp35cf_080923203318 #2-7 RT: 0.04-0.17 AV: 6 NL: 2.10E7
T: + c ESI Full ms [200.00-2000.00]
791.9
372.2
635.0
723.1
1583.1
917.9
547.2
236.1
355.0
421.1
535.0
596.9
653.0
814.1
944.0
1088.1
1207.1
1356.0
1513.9
1605.0
1708.9
1788.3
1903.0
1953.6
m/z
N3
F
F
F
F
F
F
Exact Mass: 791.2

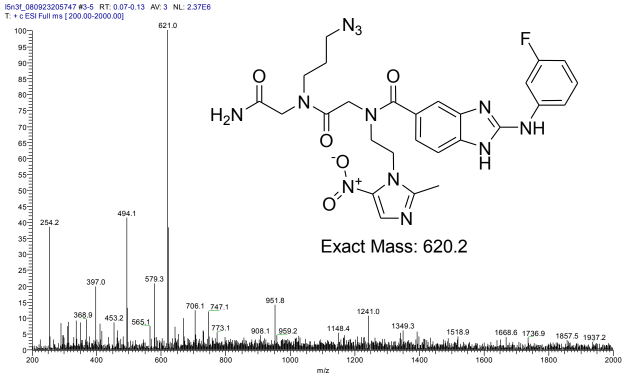

Tp4om_080923203721 #2-6 RT: 0.04-0.15 AV: 5 NL: 1.15E7
T: + c ESI Full ms [200.00-2000.00]
686.1
266.2
1371.1
547.2
529.1
723.1
1393.1
341.2
421.1
622.1
811.9
861.9
969.2
1047.8
1133.5
1252.9
1307.0
1409.2
1523.3
1702.7
1832.8
1995.9
m/z
N3
Exact Mass: 685.3

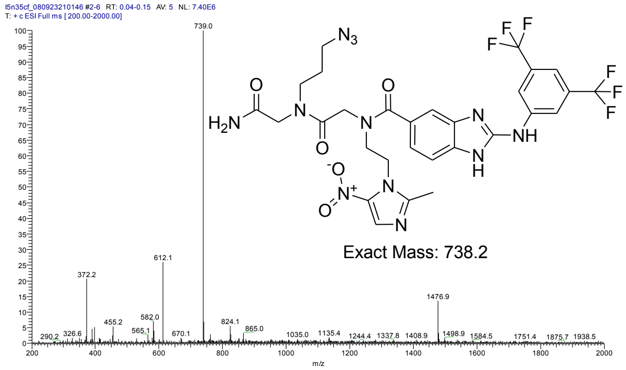

Tp3om_080923204123 #2-6 RT: 0.04-0.15 AV: 5 NL: 1.24E7
T: + c ESI Full ms [200.00-2000.00]
686.1
266.2
1371.1
547.2
723.1
1393.1
812.0
338.1
421.1
622.2
748.1
838.0
947.3
1047.9
1192.3
1307.2
1409.1
1519.1
1621.2
1710.1
1798.5
1926.9
1993.4
m/z
N3
Exact Mass: 685.3

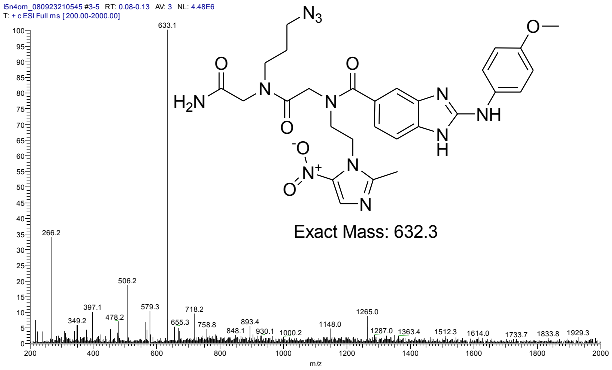

Tp4n_080923204531 #2-6 RT: 0.04-0.15 AV: 5 NL: 1.00E7
T: + c ESI Full ms [200.00-2000.00]
701.0
544.1
723.1
281.2
1401.1
826.9
1422.9
421.1
236.1
338.1
440.0
596.9
765.0
853.0
913.2
1070.8
1165.1
1285.9
1526.9
1580.1
1752.1
1839.6
1952.7
m/z
N3
N+
O-
Exact Mass: 700.3

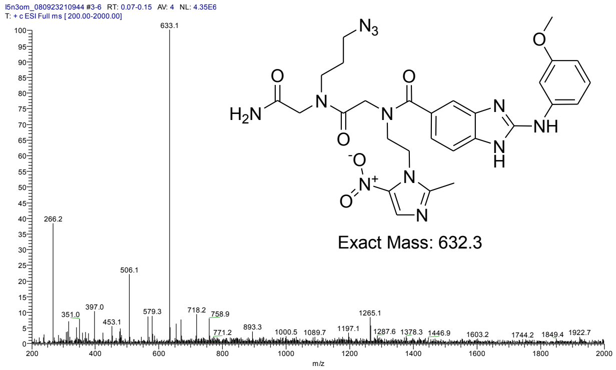

I5nPh_080923204937 #2-5 RT: 0.04-0.13 AV: 4 NL: 1.83E6
T: + c ESI Full ms [200.00-2000.00]
603.1
236.2
397.0
476.2
579.2
453.1
670.1
311.9
351.0
494.1
729.0
850.9
969.5
1099.2
1175.2
1204.9
1227.1
1357.2
1462.6
1480.2
1621.0
1731.5
1862.2
1990.2
m/z
N3
N+
O-
O
Exact Mass: 602.2

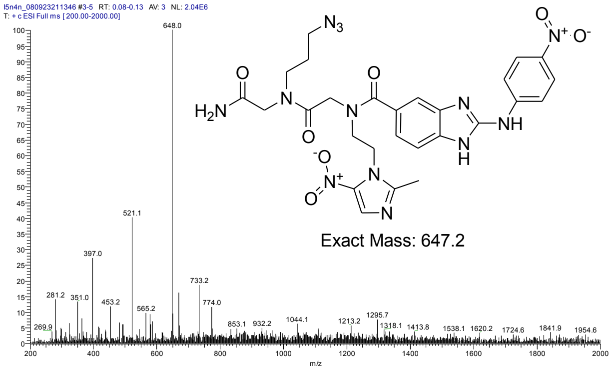

I5n4f_080923205343 #3-5 RT: 0.08-0.13 AV: 3 NL: 2.06E6
T: + c ESI Full ms [200.00-2000.00]
621.1
397.0
494.1
254.2
369.1
453.1
579.2
565.2
706.2
797.2
893.2
1002.0
1063.1
1240.9
1326.9
1442.8
1518.1
1604.1
1732.0
1822.5
1914.5
m/z
N3
F
Exact Mass: 620.2


I5n3f_080923205747 #3-5 RT: 0.07-0.13 AV: 3 NL: 2.37E6
T: + c ESI Full ms [200.00-2000.00]
621.0
254.2
494.1
397.0
579.3
388.9
453.2
565.1
706.1
747.1
773.1
951.8
908.1
959.2
1148.4
1241.0
1349.3
1518.9
1668.6
1736.9
1857.5
1937.2
m/z
N3
F
Exact Mass: 620.2

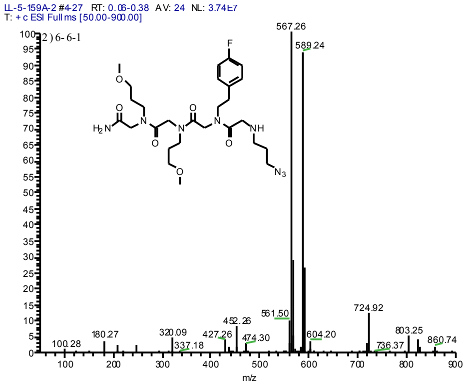

l5n35cf_080923210146 #2-6 RT: 0.04-0.15 AV: 5 NL: 7.40E6
T: + c ESI Full ms [200.00-2000.00]
739.0
612.1
372.2
455.2
582.0
565.1
290.2
326.6
670.1
824.1
865.0
1476.9
1035.0
1135.4
1244.4
1337.8
1408.9
1498.9
1584.5
1751.4
1875.7
1938.5
m/z
N3
H2N
O
N
NH
H
F
-O
N+
Exact Mass: 738.2

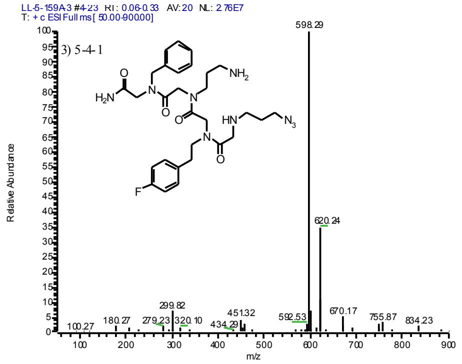

l5n4om_080923210545 #3-5 RT: 0.08-0.13 AV: 3 NL: 4.48E6
T: + c ESI Full ms [200.00-2000.00]
633.1
266.2
506.2
397.1
349.2
478.2
579.3
655.3
718.2
758.8
848.1
893.4
930.1
1000.2
1148.0
1265.0
1287.0
1363.4
1512.3
1614.0
1733.7
1833.8
1929.3
m/z
N3
H2N
O
N
NH
H
-O
N+
Exact Mass: 632.3

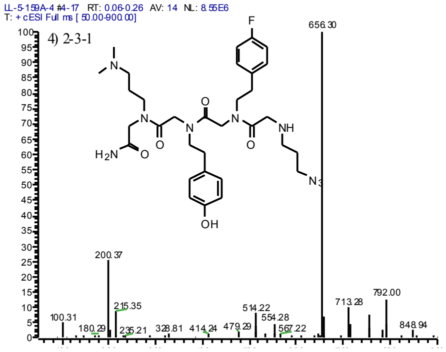

l5n3om_080923210944 #3-6 RT: 0.07-0.15 AV: 4 NL: 4.35E6
T: + c ESI Full ms [200.00-2000.00]
633.1
266.2
506.1
351.0
397.0
453.1
579.3
718.2
758.9
771.2
893.3
1000.5
1089.7
1197.1
1265.1
1287.6
1378.3
1446.9
1603.2
1744.2
1849.4
1922.7
m/z
N3
H2N
O
N
NH
H
-O
N+
Exact Mass: 632.3

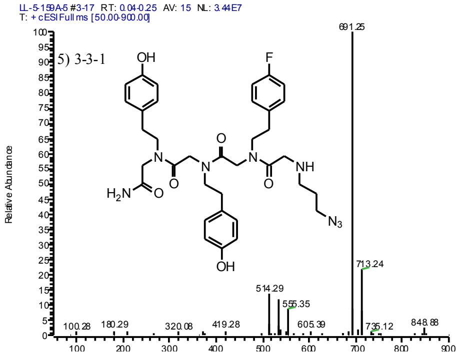

l5n4n_080923211346 #3-5 RT: 0.08-0.13 AV: 3 NL: 2.04E6
T: + c ESI Full ms [200.00-2000.00]
648.0
521.1
397.0
281.2
351.0
453.2
565.2
269.9
733.2
774.0
853.1
932.2
1044.1
1213.2
1295.7
1318.1
1413.8
1538.1
1620.2
1724.6
1841.9
1954.6
m/z
N3
H2N
O
N
NH
H
N+
O-
-O
Exact Mass: 647.2

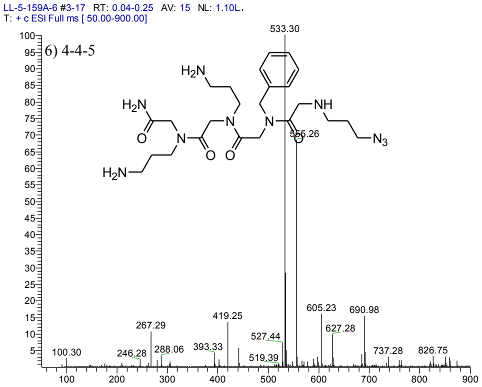
II (b) Mass Spectral Data for Peptoid Library Members

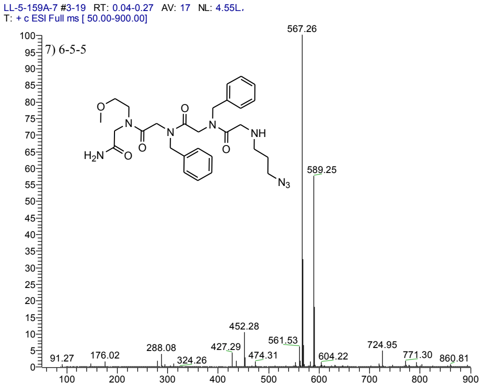


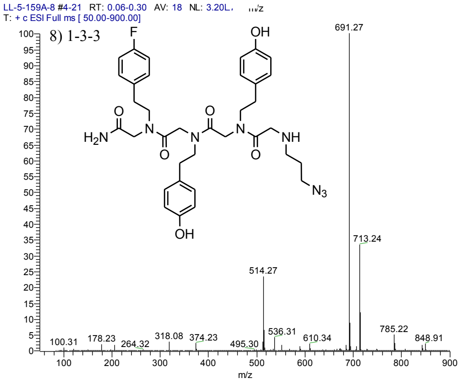


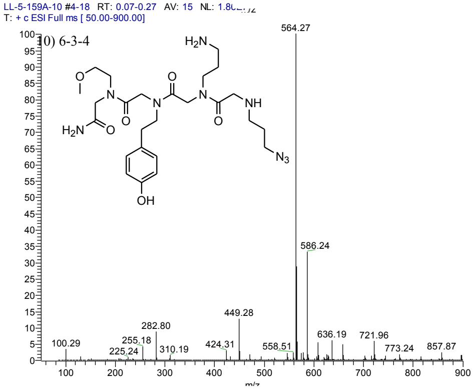


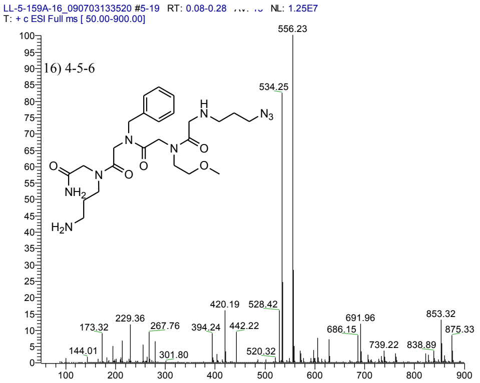




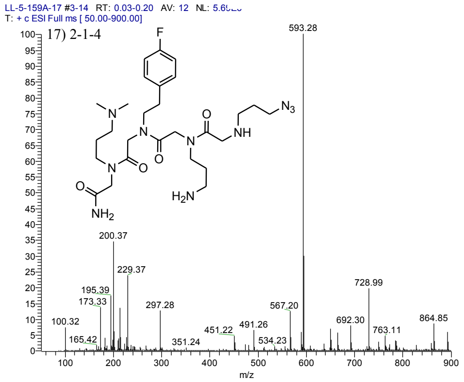




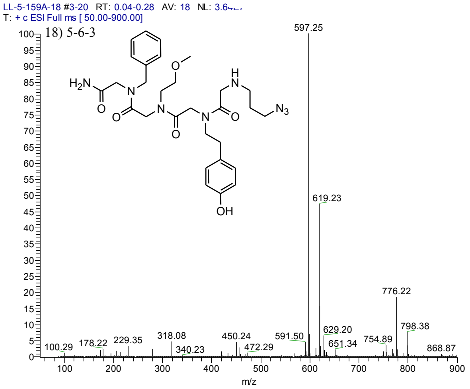




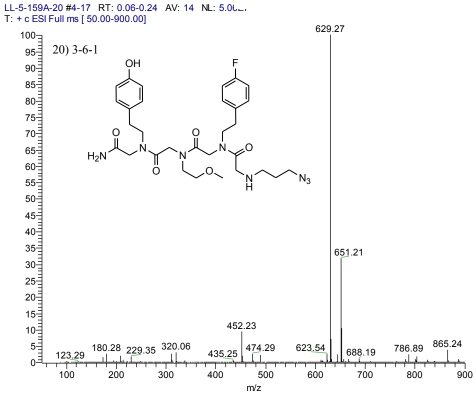
LL-5-159A-16_090703133520 #5-19 RT: 0.08-0.28 NL: 1.25E7
T: + c ESI Full ms [50.00-900.00]
16) 4-5-6
556.23
534.25
173.32
229.36
267.76
144.01
301.80
394.24
420.19
442.22
528.42
520.32
691.96
686.15
739.22
838.89
853.32
875.33



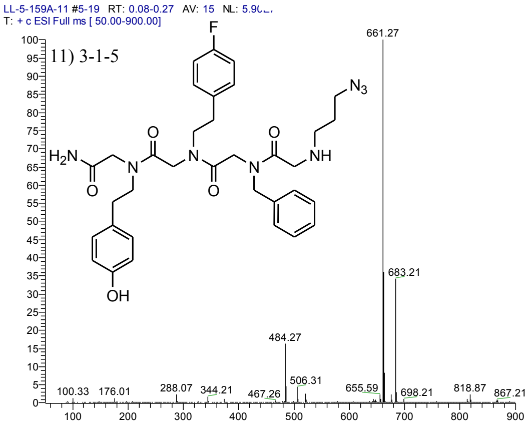
LL-5-159A-17 #3-14 RT: 0.03-0.20 AV: 12
T: + c ESI Full ms [50.00-900.00]
17) 2-1-4
593.28
200.37
229.37
195.39
173.33
100.32
165.42
297.28
351.24
451.22
491.26
534.23
567.20
692.30
728.99
763.11
864.85
m/z



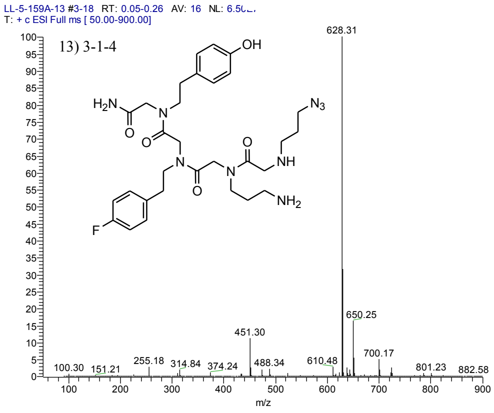
LL-5-159A-18 #3-20 RT: 0.04-0.28 AV: 18
T: + c ESI Full ms [50.00-900.00]
18) 5-6-3
597.25
619.23
100.29
178.22
229.35
318.08
340.23
450.24
472.29
591.50
629.20
651.34
754.89
776.22
798.38
868.87
m/z



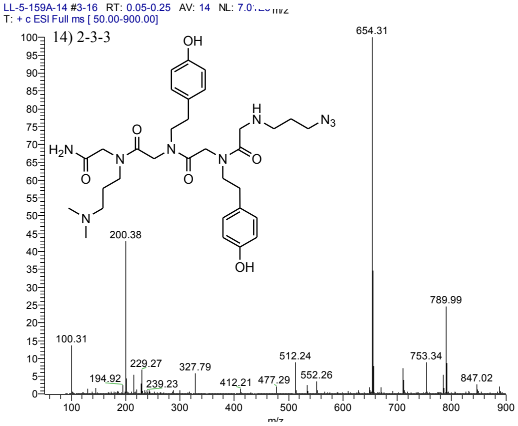
LL-5-159A-20 #4-17 RT: 0.06-0.24 AV: 14
T: + c ESI Full ms [50.00-900.00]
20) 3-6-1
629.27
651.21
123.29
180.28
229.35
320.06
435.25
452.23
474.29
623.54
688.19
786.89
865.24
m/z



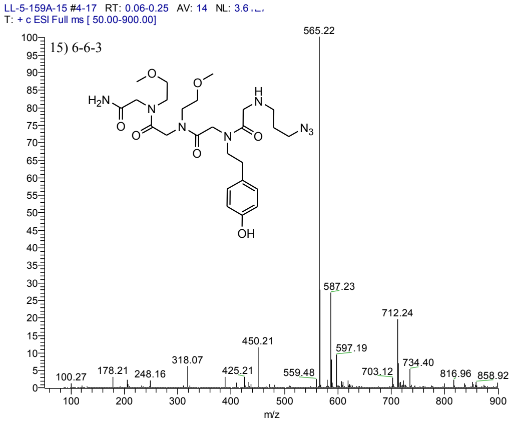
LL-5-159A-11 #5-19 RT: 0.08-0.27 AV: 15
T: + c ESI Full ms [50.00-900.00]
11) 3-1-5
661.27
683.21
484.27
100.33
176.01
288.07
344.21
467.26
506.31
655.59
698.21
818.87
867.21



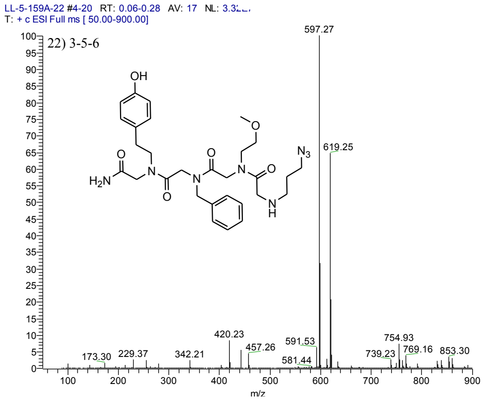
LL-5-159A-13 #3-18 RT: 0.05-0.26 AV: 16
T: + c ESI Full ms [50.00-900.00]
13) 3-1-4
628.31
650.25
700.17
451.30
100.30
151.21
255.18
314.84
374.24
488.34
610.48
801.23
882.58
m/z

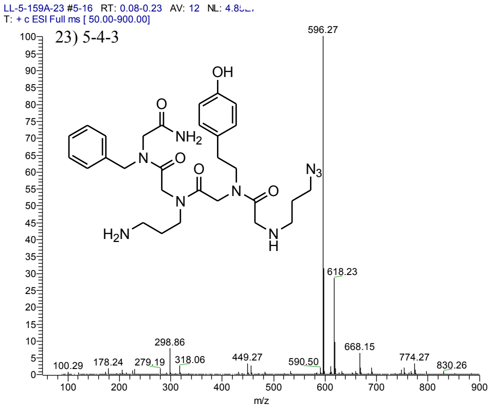


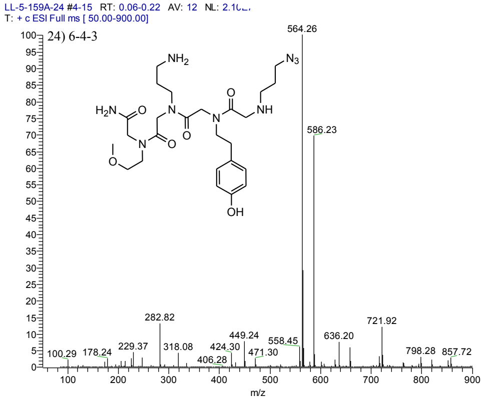
LL-5-159A-14 #3-16 RT: 0.05-0.25 AV: 14
T: + c ESI Full ms [50.00-900.00]
14) 2-3-3
654.31
200.38
789.99
753.34
100.31
194.92
229.27
239.23
327.79
412.21
477.29
512.24
552.26
847.02

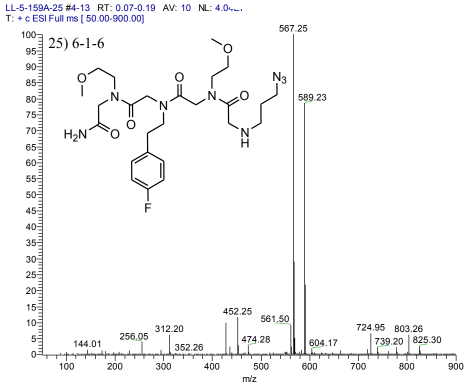


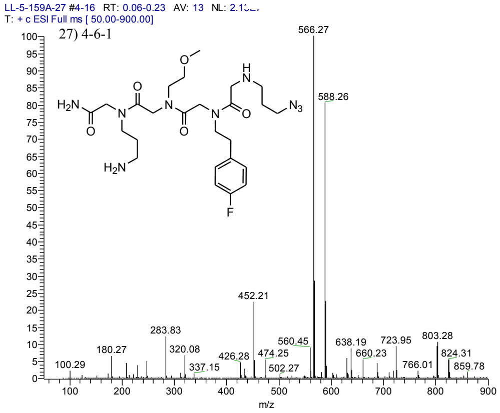
LL-5-159A-15 #4-17 RT: 0.06-0.25 AV: 14
T: + c ESI Full ms [50.00-900.00]
15) 6-6-3
565.22
587.23
597.19
712.24
734.40
100.27
178.21
248.16
318.07
425.21
450.21
559.48
703.12
816.96
858.92
m/z

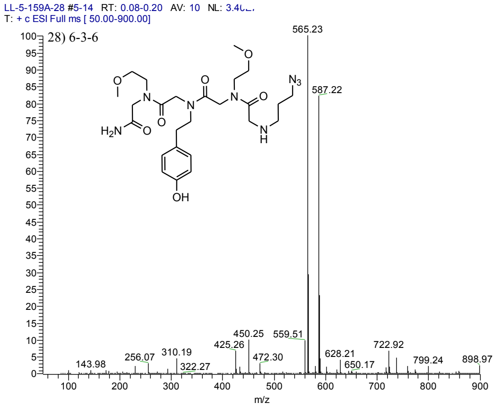

22) 3-5-6

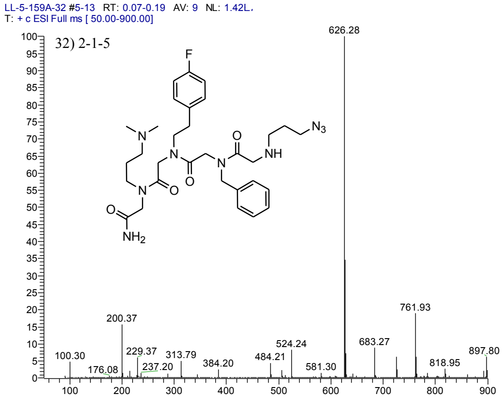

23) 5-4-3

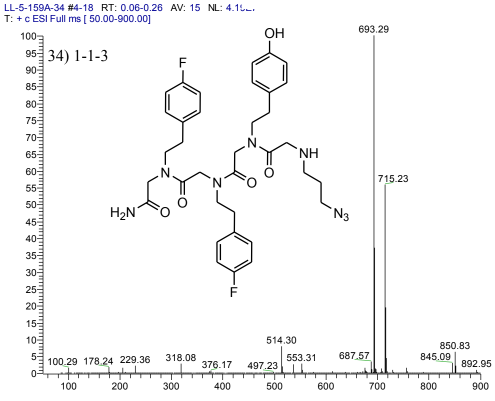

24) 6-4-3

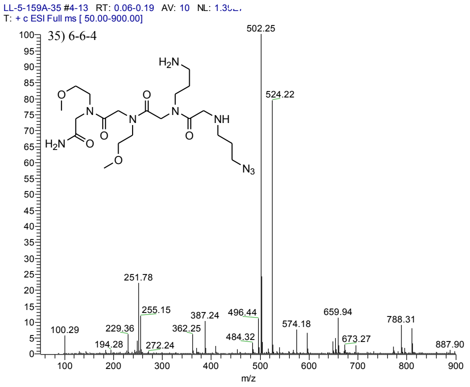

25) 6-1-6

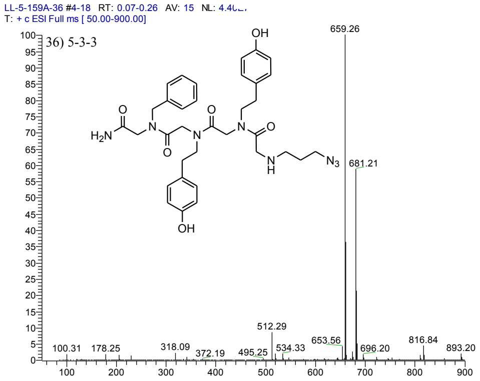

27) 4-6-1

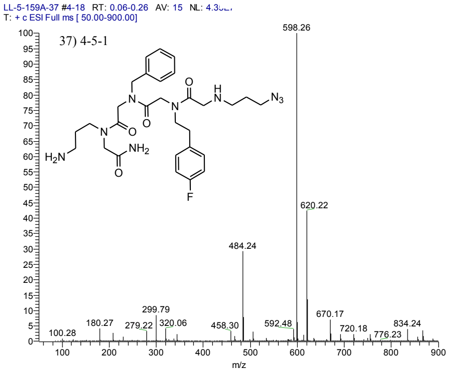

28) 6-3-6

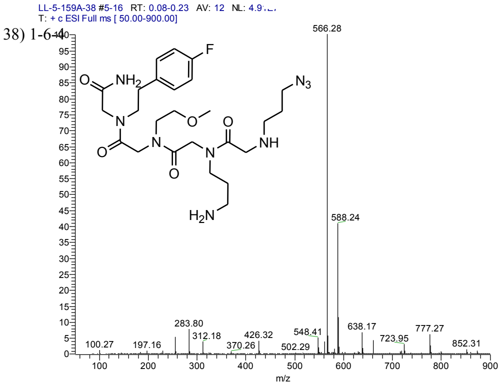

32) 2-1-5

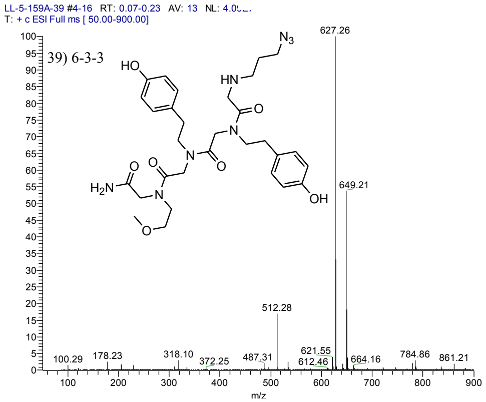

34) 1-1-3

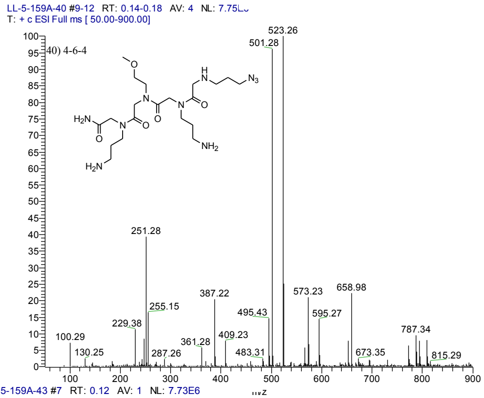

LL-5-159A-35 #4-13 RT: 0.06-0.19 AV: 10 NL: 1.39
T: + c ESI Full ms [50.00-900.00]
35) 6-6-4
H2N
NH
N3
O
N
H2N
502.25
524.22
251.78
255.15
387.24
496.44
659.94
229.36
362.25
574.18
788.31
100.29
194.28
272.24
484.32
673.27
887.90
m/z

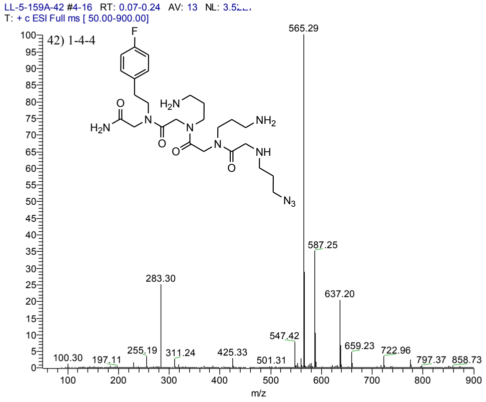

LL-5-159A-36 #4-18 RT: 0.07-0.26 AV: 15 NL: 4.40
T: + c ESI Full ms [50.00-900.00]
36) 5-3-3
OH
H2N
N
H
N3
OH
659.26
681.21
512.29
100.31
178.25
318.09
372.19
495.25
534.33
653.56
696.20
816.84
893.20

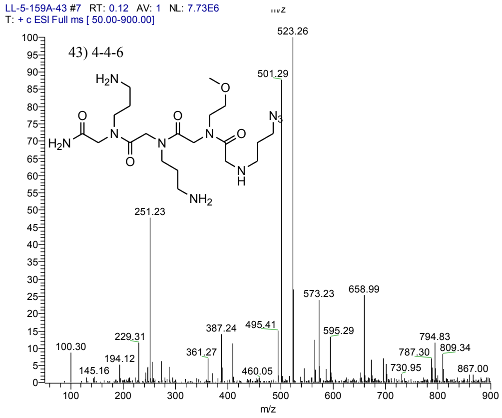

LL-5-159A-37 #4-18 RT: 0.06-0.26 AV: 15 NL: 4.38
T: + c ESI Full ms [50.00-900.00]
37) 4-5-1
H
N
N3
H2N
NH2
F
598.26
620.22
484.24
299.79
180.27
279.22
320.06
458.30
592.48
670.17
720.18
834.24
776.23
100.28
m/z

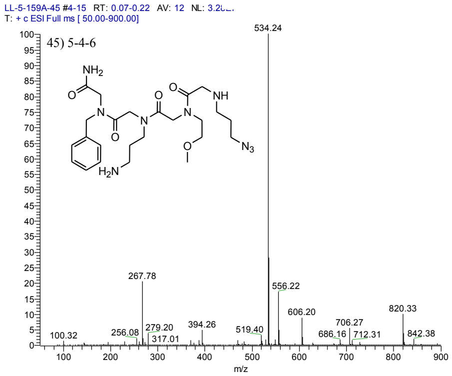

LL-5-159A-38 #5-16 RT: 0.08-0.23 AV: 12 NL: 4.91
T: + c ESI Full ms [50.00-900.00]
38) 1-6-4
F
O NH2
N3
NH
H2N
566.28
588.24
283.80
312.18
426.32
548.41
638.17
777.27
723.95
100.27
197.16
370.26
502.29
852.31
m/z

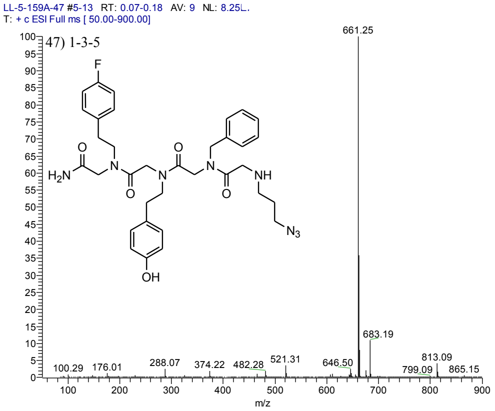

LL-5-159A-39 #4-16 RT: 0.07-0.23 AV: 13 NL: 4.09
T: + c ESI Full ms [50.00-900.00]
39) 6-3-3
HO
HN
N3
H2N
OH
627.26
649.21
512.28
100.29
178.23
318.10
372.25
487.31
621.55
612.46
664.16
784.86
861.21
m/z

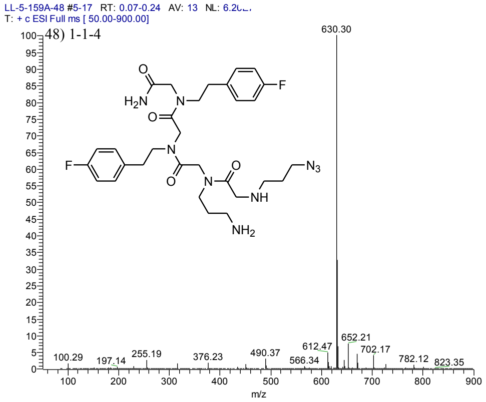

LL-5-159A-40 #9-12 RT: 0.14-0.18 AV: 4 NL: 7.75
T: + c ESI Full ms [50.00-900.00]
40) 4-6-4
H2N
NH2
N3
523.26
501.28
251.28
387.22
573.23
658.98
255.15
229.38
495.43
595.27
361.28
409.23
787.34
100.29
130.25
287.26
483.31
673.35
815.29


LL-5-159A-42 #4-16 RT: 0.07-0.24 AV: 13 NL: 3.52
T: + c ESI Full ms [50.00-900.00]
42) 1-4-4
F
H2N
NH2
NH
N3
565.29
587.25
637.20
283.30
547.42
659.23
100.30
197.11
255.19
311.24
425.33
501.31
722.96
797.37
858.73
m/z

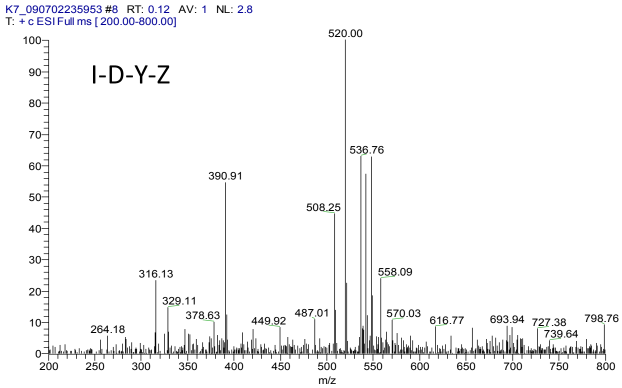

LL-5-159A-43 #7 RT: 0.12 AV: 1 NL: 7.73E6
T: + c ESI Full ms [50.00-900.00]
43) 4-4-6
H2N
H2N
N3
N
H
NH2
523.26
501.29
251.23
573.23
658.99
229.31
387.24
495.41
595.29
794.83
100.30
361.27
787.30
809.34
194.12
145.16
460.05
730.95
867.00
m/z

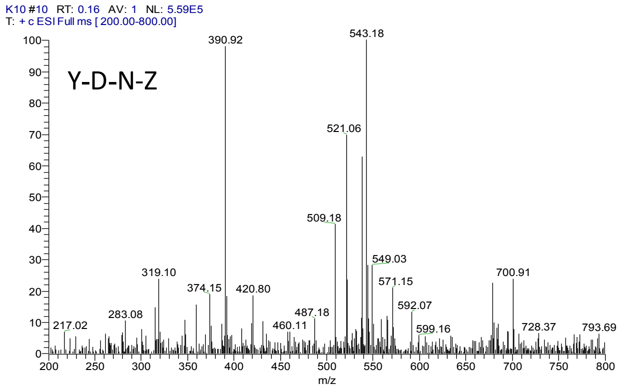

LL-5-159A-45 #4-15 RT: 0.07-0.22 AV: 12 NL: 3.2
T: + c ESI Full ms [50.00-900.00]
45) 5-4-6
NH2
O
N
O
N
O
O
N
NH
H2N
O
N3
534.24
267.78
556.22
606.20
820.33
100.32
256.08
279.20
317.01
394.26
519.40
686.16
706.27
712.31
842.38
m/z

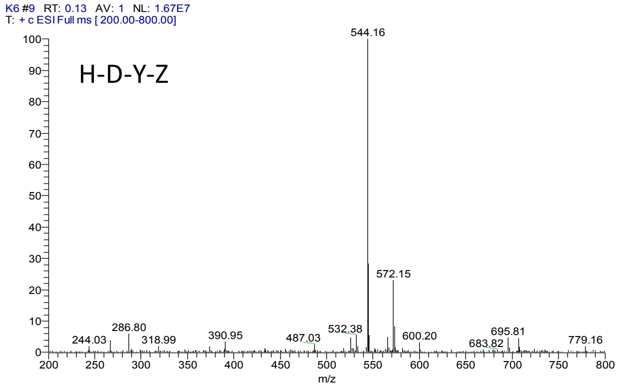

LL-5-159A-47 #5-13 RT: 0.07-0.18 AV: 9 NL: 8.25
T: + c ESI Full ms [50.00-900.00]
47) 1-3-5
F
H2N
O
N
O
N
O
N
O
NH
OH
N3
661.25
683.19
100.29
176.01
288.07
374.22
482.28
521.31
646.50
799.09
813.09
865.15
m/z

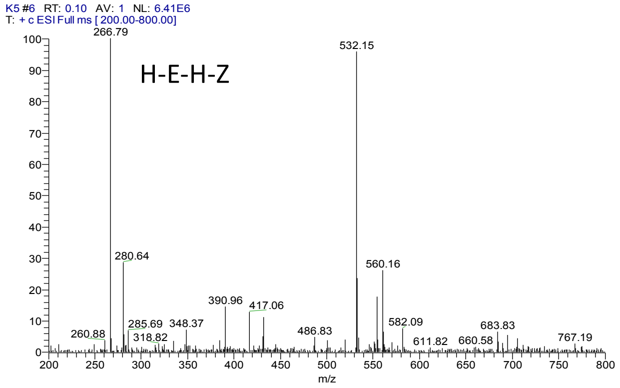

LL-5-159A-48 #5-17 RT: 0.07-0.24 AV: 13 NL: 6.2
T: + c ESI Full ms [50.00-900.00]
48) 1-1-4
O
H2N
N
F
O
N
F
O
N
O
NH
N3
NH2
630.30
100.29
197.14
255.19
376.23
490.37
566.34
612.47
652.21
702.17
782.12
823.35
m/z

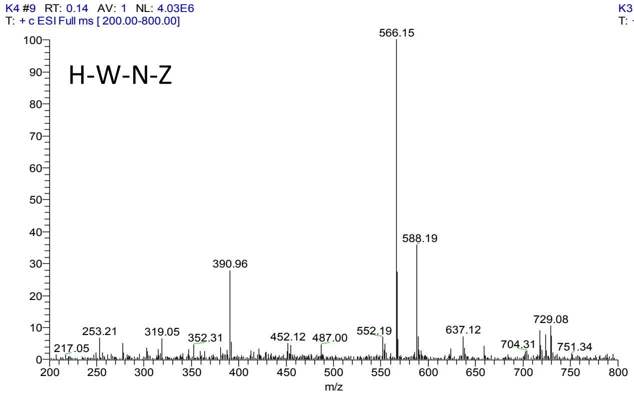
II (c) Mass Spectral Data for Peptides Library Members

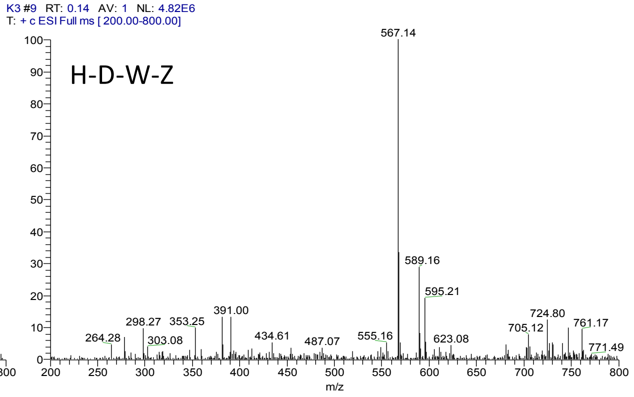


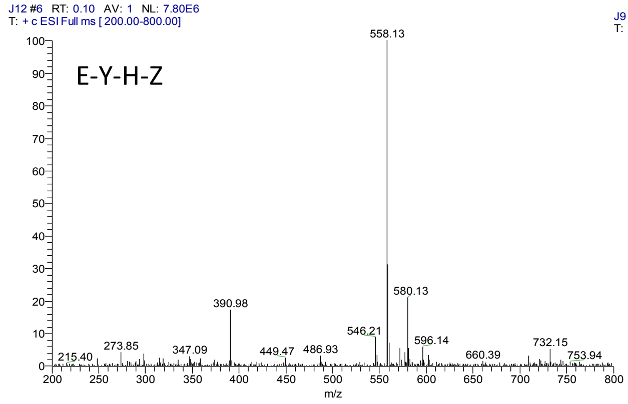


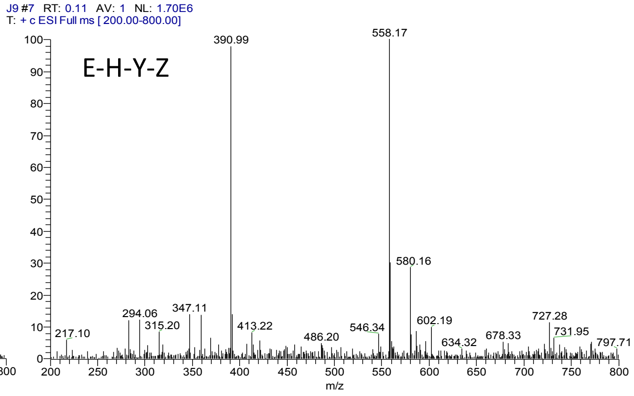


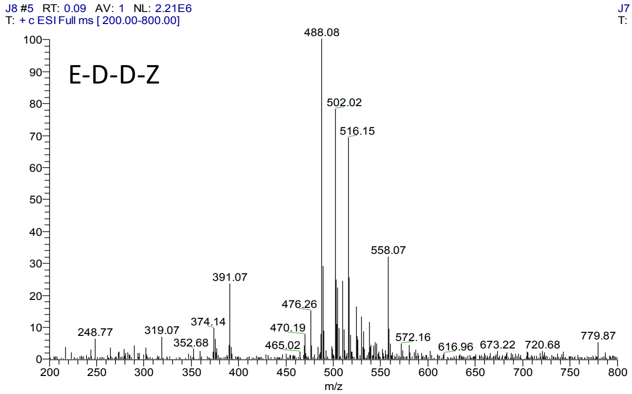


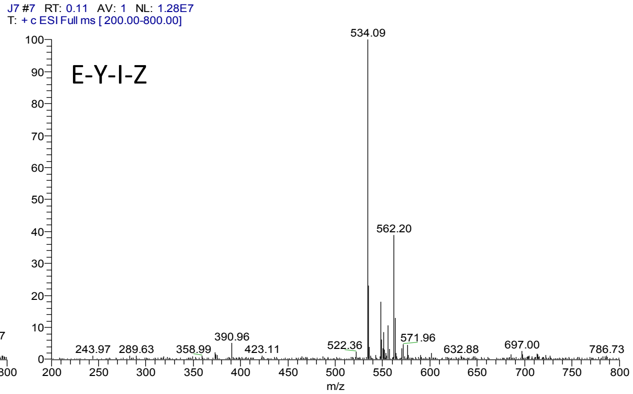


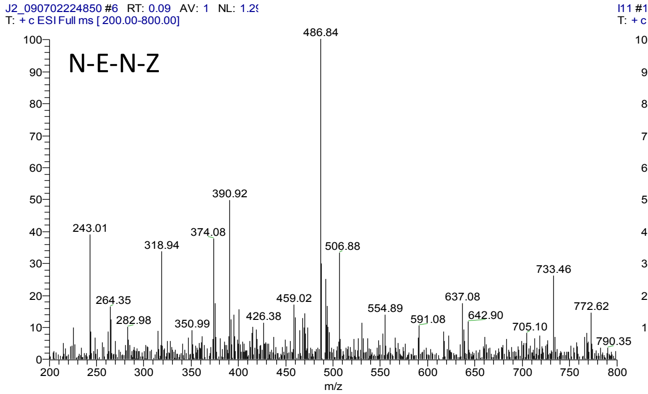


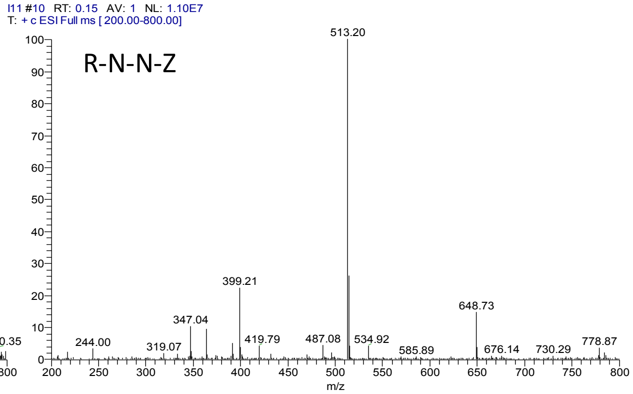


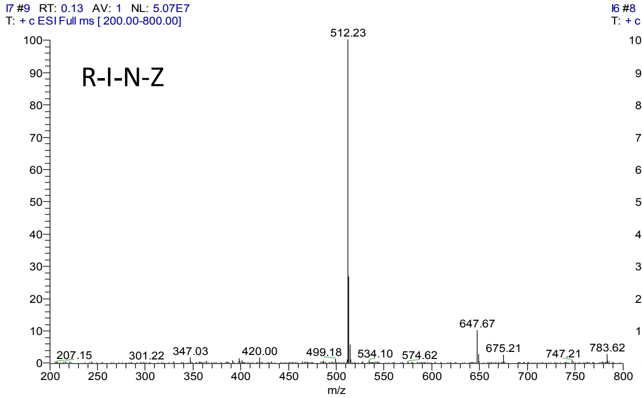


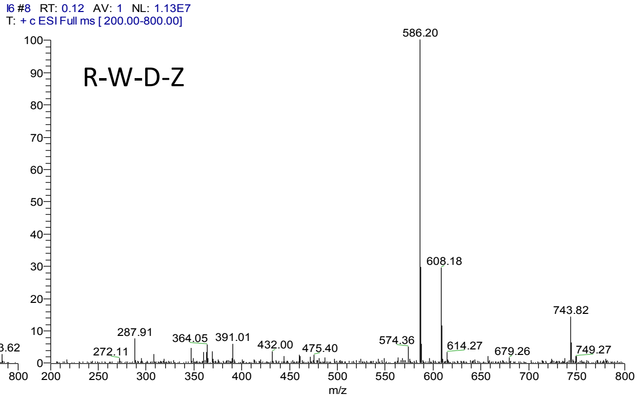

J8 #5 RT: 0.09 AV: 1 NL: 2.21E6
T: + c ESI Full ms [200.00-800.00]
E-D-D-Z
488.08
502.02
516.15
558.07
391.07
476.26
374.14
470.19
319.07
248.77
352.68
465.02
572.16
616.96
673.22
720.68
779.87
m/z

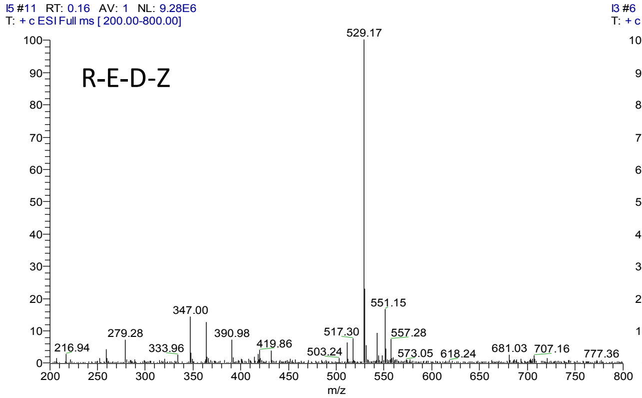

J7 #7 RT: 0.11 AV: 1 NL: 1.28E7
T: + c ESI Full ms [200.00-800.00]
E-Y-I-Z
534.09
562.20
390.96
243.97
289.63
358.99
423.11
522.36
571.96
632.88
697.00
786.73
m/z

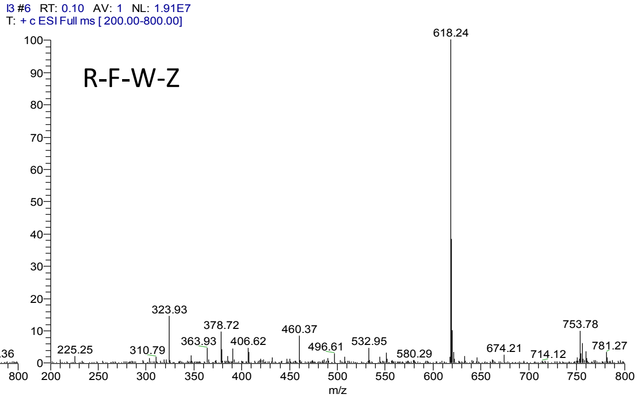

J2_090702224850 #6 RT: 0.09 AV: 1 NL: 1.2
T: + c ESI Full ms [200.00-800.00]
N-E-N-Z
486.84
390.92
243.01
374.08
318.94
506.88
733.46
264.35
459.02
637.08
772.62
282.98
426.38
554.89
591.08
642.90
350.99
705.10
790.35
m/z

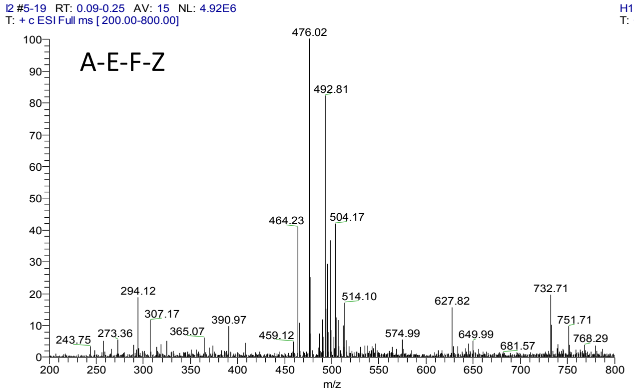

I11 #10 RT: 0.15 AV: 1 NL: 1.10E7
T: + c ESI Full ms [200.00-800.00]
R-N-N-Z
513.20
399.21
648.73
347.04
244.00
319.07
419.79
487.08
534.92
585.89
676.14
730.29
778.87
m/z


I7 #9 RT: 0.13 AV: 1 NL: 5.07E7
T: + c ESI Full ms [200.00-800.00]
R-I-N-Z
512.23
647.67
675.21
207.15
301.22
347.03
420.00
499.18
534.10
574.62
747.21
783.62
m/z


I6 #8 RT: 0.12 AV: 1 NL: 1.13E7
T: + c ESI Full ms [200.00-800.00]
R-W-D-Z
586.20
608.18
743.82
287.91
364.05
391.01
432.00
475.40
574.36
614.27
679.26
749.27
272.11
m/z


I5 #11 RT: 0.16 AV: 1 NL: 9.28E6
T: + c ESI Full ms [200.00-800.00]
R-E-D-Z
529.17
551.15
347.00
279.28
390.98
517.30
557.28
216.94
333.96
419.86
503.24
573.05
618.24
681.03
707.16
777.36
m/z


I3 #6 RT: 0.10 AV: 1 NL: 1.91E7
T: + c ESI Full ms [200.00-800.00]
R-F-W-Z
618.24
323.93
378.72
460.37
753.78
363.93
406.62
532.95
781.27
225.25
310.79
496.61
580.29
674.21
714.12
m/z


I2 #5-19 RT: 0.09-0.25 AV: 15 NL: 4.92E6
T: + c ESI Full ms [200.00-800.00]
A-E-F-Z
476.02
492.81
464.23
504.17
294.12
514.10
627.82
732.71
307.17
751.71
390.97
365.07
243.75
273.36
459.12
574.99
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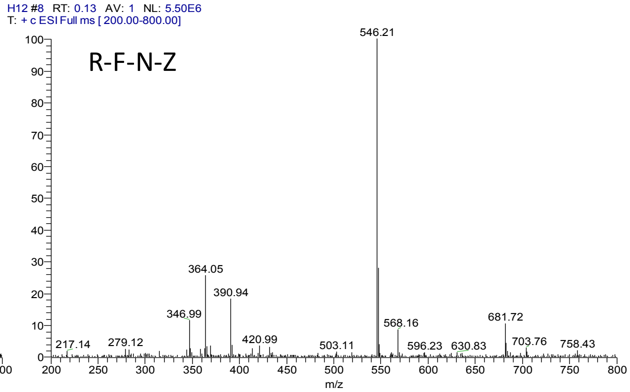
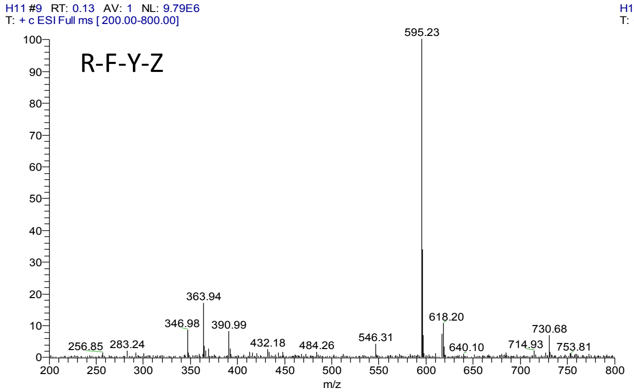
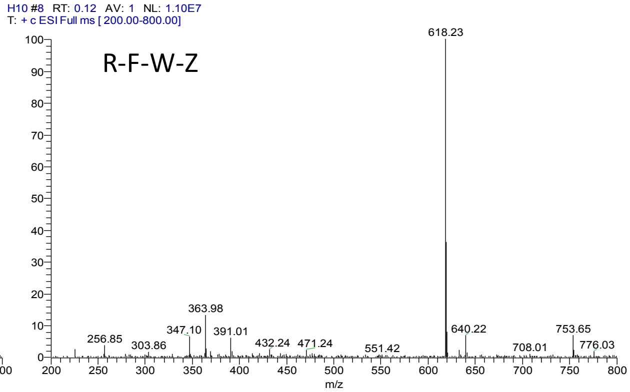
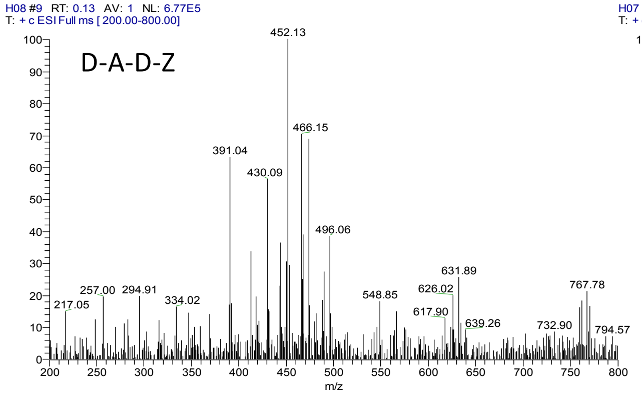
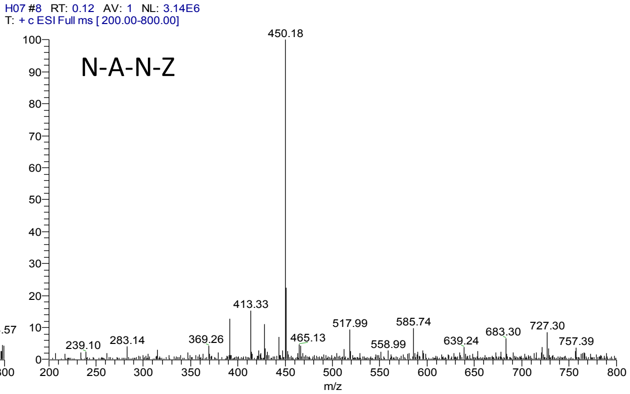
768.29
681.57
m/z

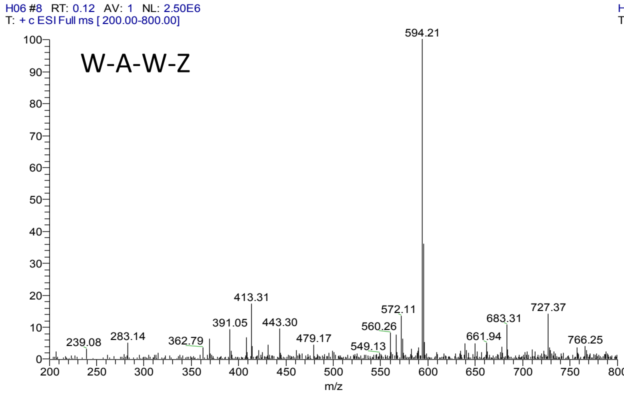

H12 #8 RT: 0.13 AV: 1 NL: 5.50E6
T: + c ESI Full ms [200.00-800.00]
R-F-N-Z
546.21
364.05
390.94
346.99
568.16
681.72
217.14
279.12
420.99
503.11
596.23
630.83
703.76
758.43
m/z

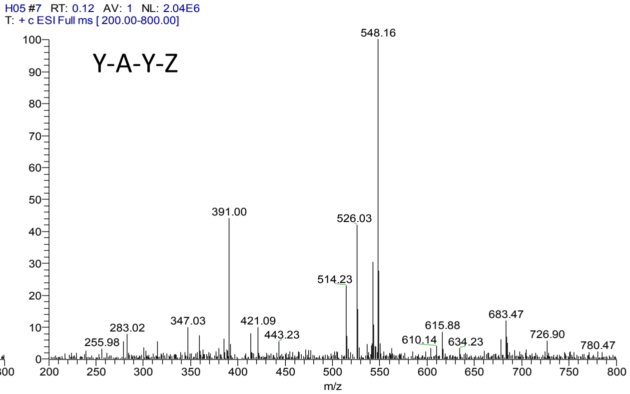

H11 #9 RT: 0.13 AV: 1 NL: 9.79E6
T: + c ESI Full ms [200.00-800.00]
R-F-Y-Z
595.23
363.94
346.98
390.99
618.20
730.68
256.85
283.24
432.18
484.26
546.31
640.10
714.93
753.81
m/z

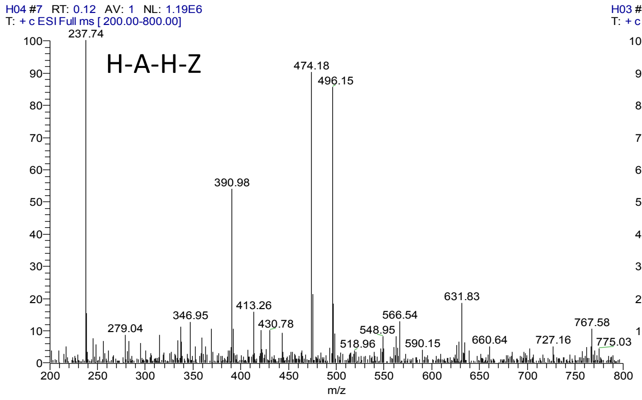

H10 #8 RT: 0.12 AV: 1 NL: 1.10E7
T: + c ESI Full ms [200.00-800.00]
R-F-W-Z
618.23
363.98
347.10
391.01
640.22
753.65
256.85
303.86
432.24
471.24
551.42
708.01
776.03
m/z

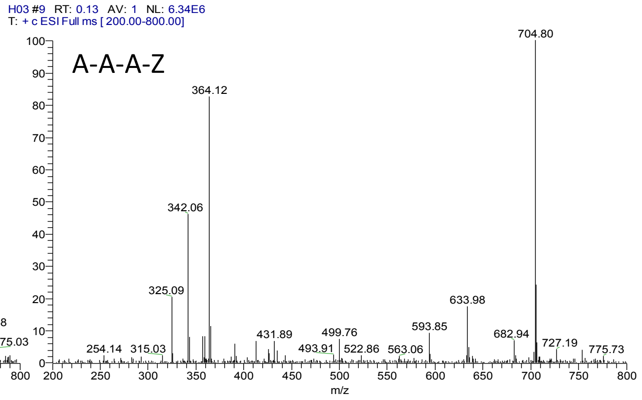

H08 #9 RT: 0.13 AV: 1 NL: 6.77E5
T: + c ESI Full ms [200.00-800.00]
D-A-D-Z
452.13
466.15
391.04
430.09
496.06
631.89
767.78
257.00
294.91
548.85
626.02
217.05
334.02
617.90
639.26
732.90
794.57
m/z

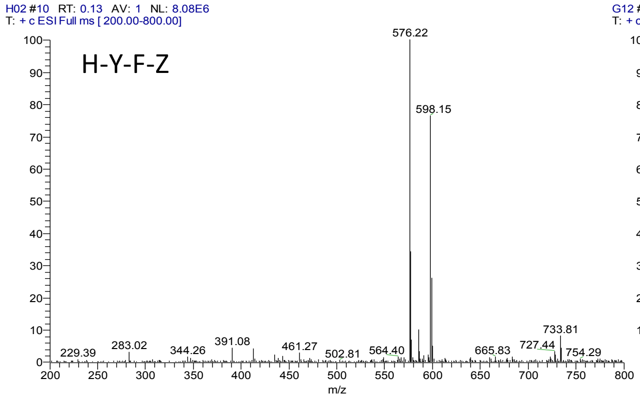

H07 #8 RT: 0.12 AV: 1 NL: 3.14E6
T: + c ESI Full ms [200.00-800.00]
N-A-N-Z
450.18
413.33
517.99
585.74
727.30
369.26
465.13
683.30
239.10
283.14
558.99
639.24
757.39
m/z

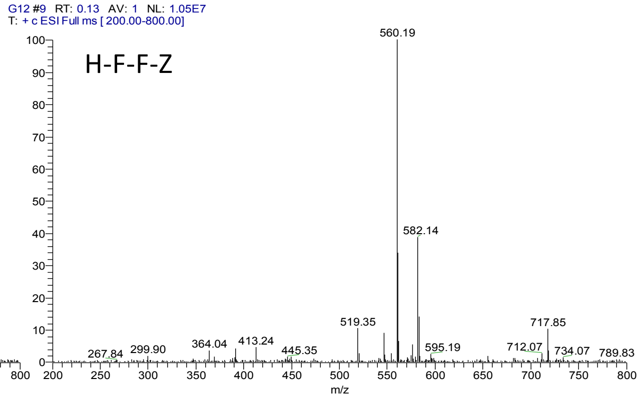

H06 #8 RT: 0.12 AV: 1 NL: 2.50E6
T: + c ESI Full ms [200.00-800.00]
W-A-W-Z
594.21
413.31
572.11
727.37
391.05
443.30
560.26
683.31
239.08
283.14
362.79
479.17
549.13
661.94
766.25
m/z

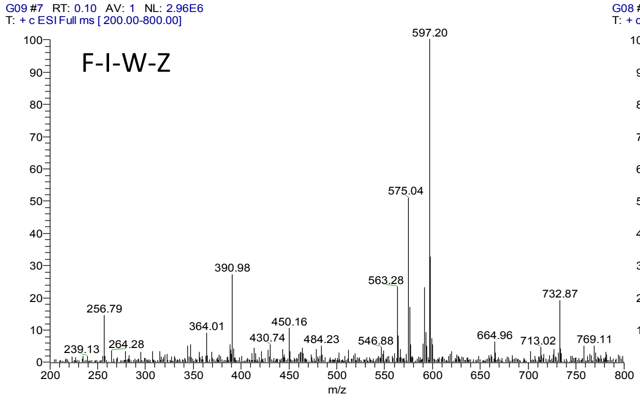

H05 #7 RT: 0.12 AV: 1 NL: 2.04E6
T: + c ESI Full ms [200.00-800.00]
Y-A-Y-Z
548.16
391.00
526.03
514.23
683.47
283.02
347.03
421.09
615.88
255.98
443.23
610.14
634.23
726.90
780.47
m/z

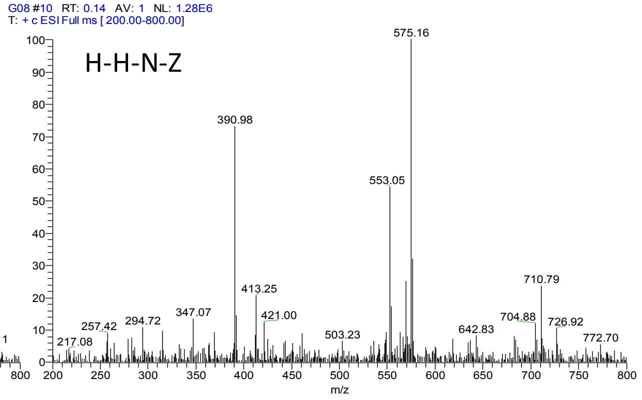

H04 #7 RT: 0.12 AV: 1 NL: 1.19E6
T: + c ESI Full ms [200.00-800.00]
H-A-H-Z
237.74
474.18
496.15
390.98
413.26
430.78
346.95
279.04
631.83
566.54
548.95
518.96
590.15
660.64
727.16
767.58
775.03
m/z

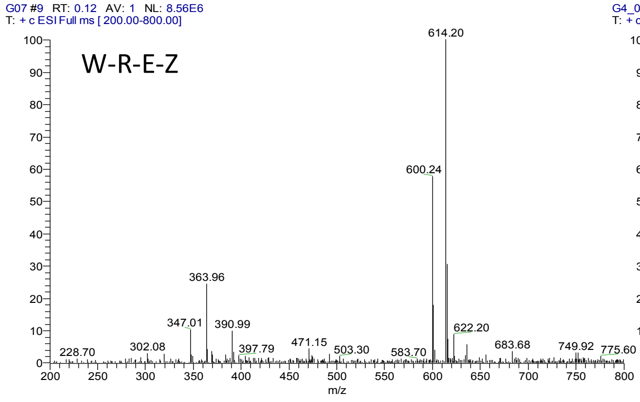

H03 #9 RT: 0.13 AV: 1 NL: 6.34E6
T: + c ESI Full ms [200.00-800.00]
A-A-A-Z
704.80
364.12
342.06
325.09
633.98
593.85
431.89
499.76
254.14
315.03
493.91
522.86
563.06
682.94
727.19
775.73
m/z

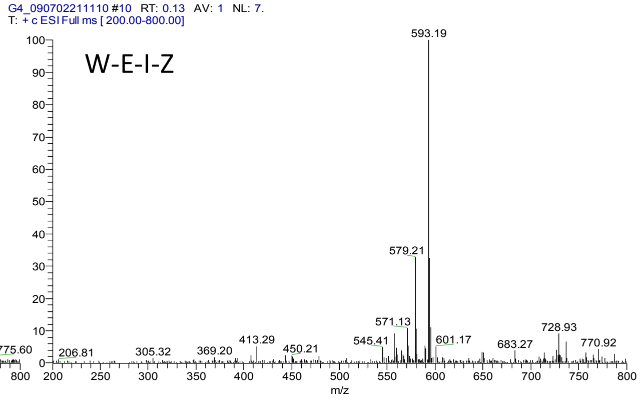

H02 #10 RT: 0.13 AV: 1 NL: 8.08E6
T: + c ESI Full ms [200.00-800.00]
H-Y-F-Z
576.22
598.15
733.81
229.39
283.02
344.26
391.08
461.27
502.81
564.40
665.83
727.44
754.29
m/z

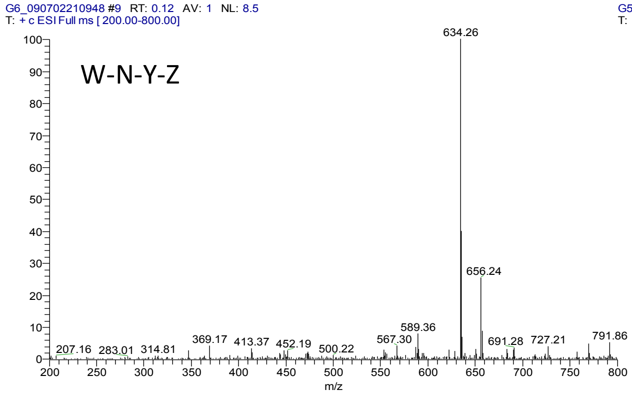

G12 #9 RT: 0.13 AV: 1 NL: 1.05E7
T: + c ESI Full ms [200.00-800.00]
H-F-F-Z
560.19
582.14
519.35
717.85
267.84
299.90
364.04
413.24
445.35
595.19
712.07
734.07
789.83
m/z

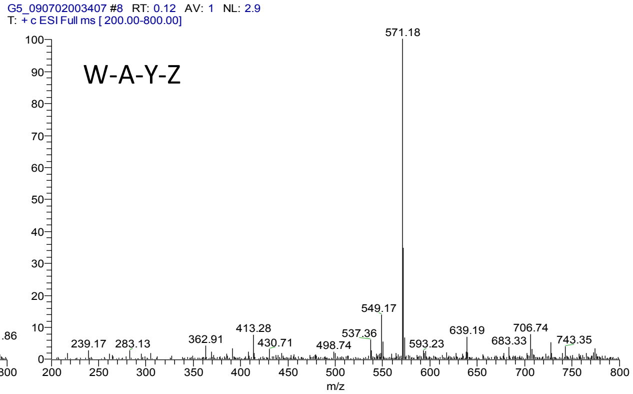

G09 #7 RT: 0.10 AV: 1 NL: 2.96E6
T: + c ESI Full ms [200.00-800.00]
F-I-W-Z
597.20
575.04
563.28
390.98
732.87
256.79
364.01
450.16
430.74
484.23
239.13
264.28
546.88
664.96
713.02
769.11
m/z

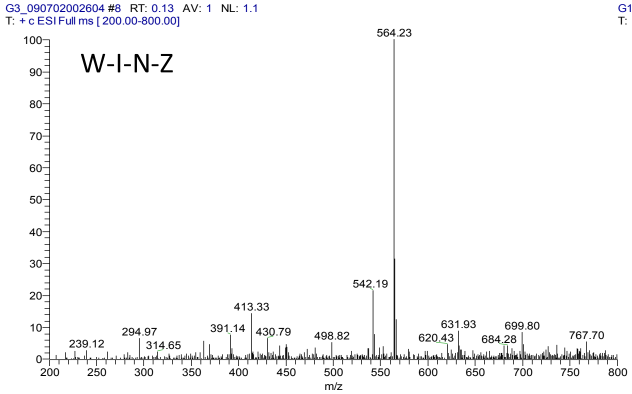

G08 #10 RT: 0.14 AV: 1 NL: 1.28E6
T: + c ESI Full ms [200.00-800.00]
H-H-N-Z
575.16
390.98
553.05
710.79
413.25
421.00
347.07
294.72
257.42
217.08
503.23
642.83
704.88
726.92
772.70
m/z

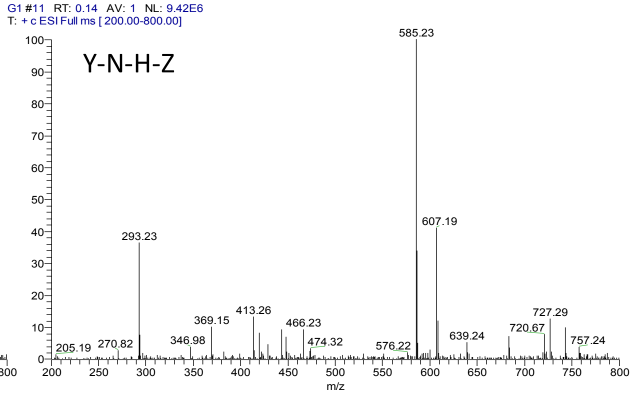

G07 #9 RT: 0.12 AV: 1 NL: 8.56E6
T: + c ESI Full ms [200.00-800.00]
W-R-E-Z
614.20
600.24
363.96
347.01
390.99
622.20
228.70
302.08
397.79
471.15
503.30
583.70
683.68
749.92
775.60
m/z

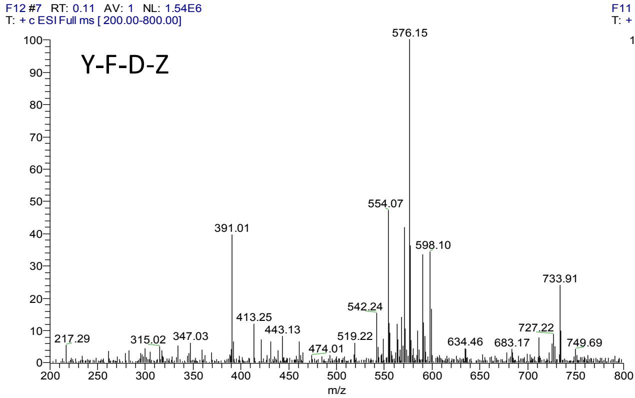

G4_090702211110 #10 RT: 0.13 AV: 1 NL: 7.
T: + c ESI Full ms [200.00-800.00]
W-E-I-Z
593.19
579.21
571.13
545.41
601.17
728.93
206.81
305.32
369.20
413.29
450.21
683.27
770.92
m/z


G6_090702210948 #9 RT: 0.12 AV: 1 NL: 8.5
T: + c ESI Full ms [200.00-800.00]
W-N-Y-Z
634.26
656.24
589.36
567.30
691.28
727.21
791.86
207.16
283.01
314.81
369.17
413.37
452.19
500.22
m/z


G5_090702003407 #8 RT: 0.12 AV: 1 NL: 2.9
T: + c ESI Full ms [200.00-800.00]
W-A-Y-Z
571.18
549.17
537.36
413.28
639.19
706.74
239.17
283.13
362.91
430.71
498.74
593.23
683.33
743.35
m/z


G3_090702002604 #8 RT: 0.13 AV: 1 NL: 1.1
T: + c ESI Full ms [200.00-800.00]
W-I-N-Z
564.23
542.19
413.33
391.14
294.97
239.12
314.65
430.79
498.82
631.93
620.43
699.80
684.28
767.70
m/z


G1 #11 RT: 0.14 AV: 1 NL: 9.42E6
T: + c ESI Full ms [200.00-800.00]
Y-N-H-Z
585.23
607.19
293.23
413.26
369.15
466.23
346.98
474.32
205.19
270.82
576.22
639.24
727.29
720.67
757.24
m/z


F12 #7 RT: 0.11 AV: 1 NL: 1.54E6
T: + c ESI Full ms [200.00-800.00]
Y-F-D-Z
576.15
554.07
391.01
598.10
733.91
413.25
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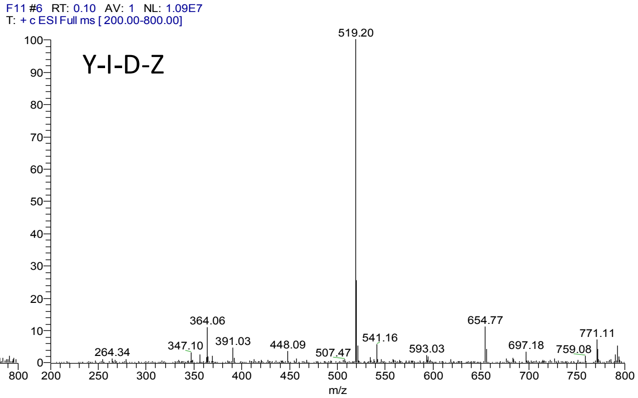
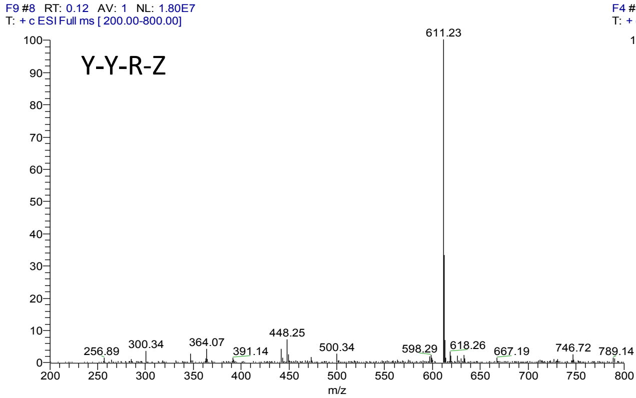
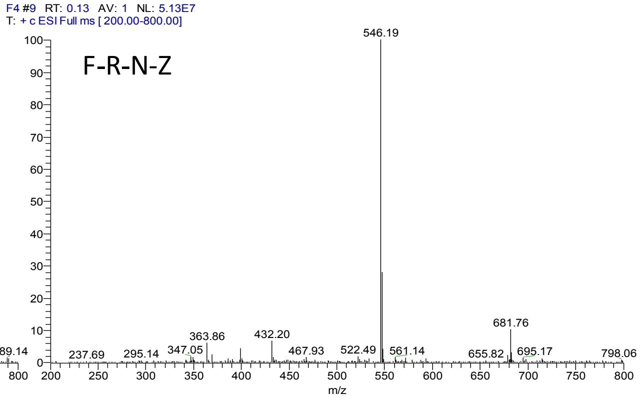
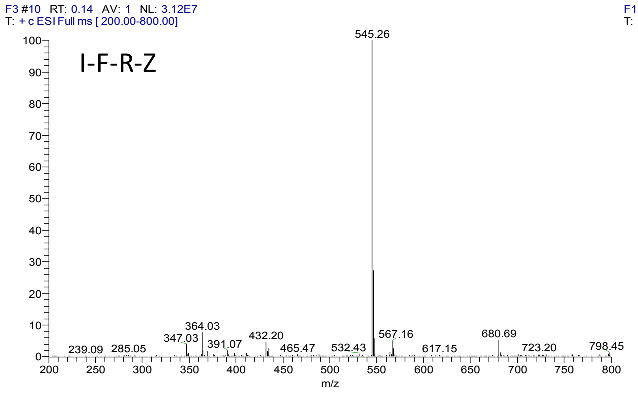
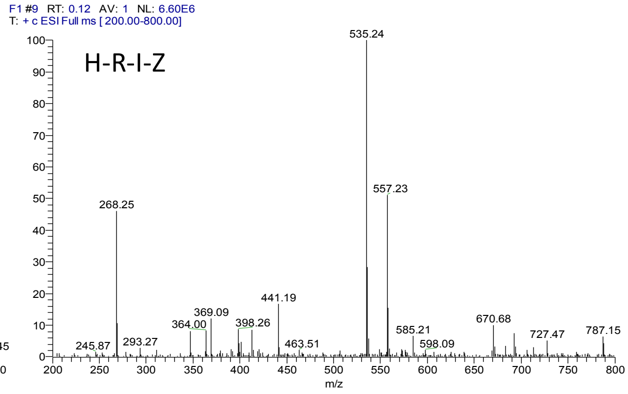
727.22
217.29
315.02
347.03
474.01
519.22
634.46
683.17
749.69
m/z

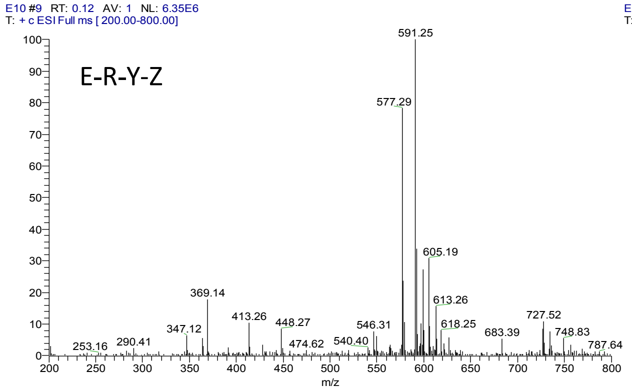

F11 #6 RT: 0.10 AV: 1 NL: 1.09E7
T: + c ESI Full ms [200.00-800.00]
Y-I-D-Z
519.20
364.06
347.10
391.03
448.09
507.47
541.16
593.03
654.77
697.18
759.08
771.11
264.34
m/z

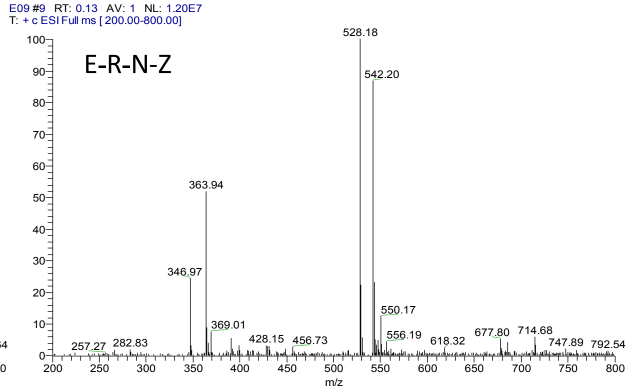

F9 #8 RT: 0.12 AV: 1 NL: 1.80E7
T: + c ESI Full ms [200.00-800.00]
Y-Y-R-Z
611.23
448.25
364.07
300.34
256.89
391.14
500.34
598.29
618.26
667.19
746.72
789.14
m/z

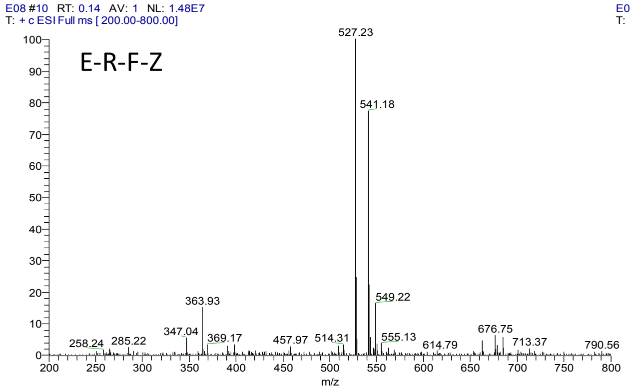

F4 #9 RT: 0.13 AV: 1 NL: 5.13E7
T: + c ESI Full ms [200.00-800.00]
F-R-N-Z
546.19
681.76
432.20
363.86
347.05
295.14
237.69
467.93
522.49
561.14
655.82
695.17
798.06
m/z

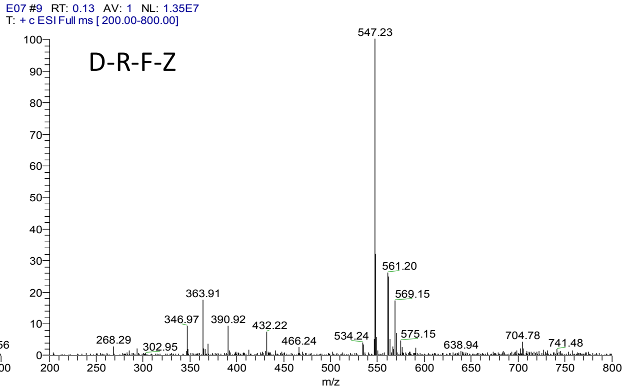

F3 #10 RT: 0.14 AV: 1 NL: 3.12E7
T: + c ESI Full ms [200.00-800.00]
I-F-R-Z
545.26
239.09
285.05
347.03
364.03
391.07
432.20
465.47
532.43
567.16
617.15
680.69
723.20
798.45
m/z

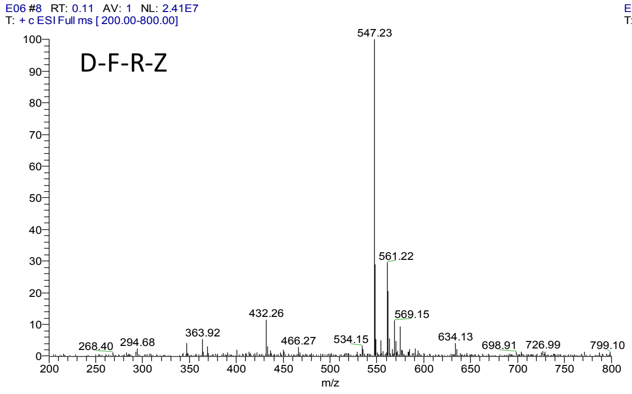

F1 #9 RT: 0.12 AV: 1 NL: 6.60E6
T: + c ESI Full ms [200.00-800.00]
H-R-I-Z
535.24
557.23
268.25
245.87
293.27
364.00
369.09
398.26
441.19
463.51
585.21
598.09
670.68
727.47
787.15
m/z

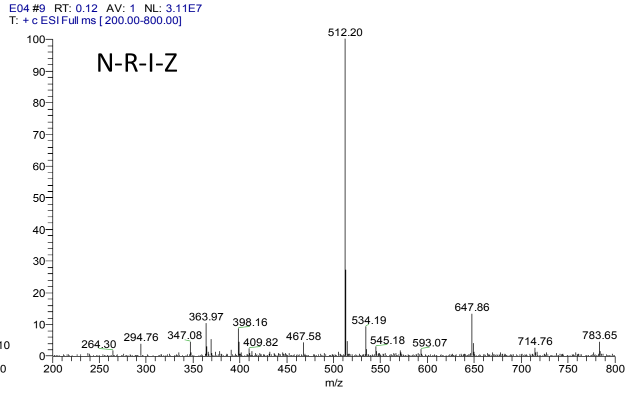

E10 #9 RT: 0.12 AV: 1 NL: 6.35E6
T: + c ESI Full ms [200.00-800.00]
E-R-Y-Z
591.25
577.29
605.19
369.14
413.26
448.27
347.12
613.26
618.25
727.52
748.83
253.16
290.41
474.62
540.40
546.31
683.39
787.64
m/z

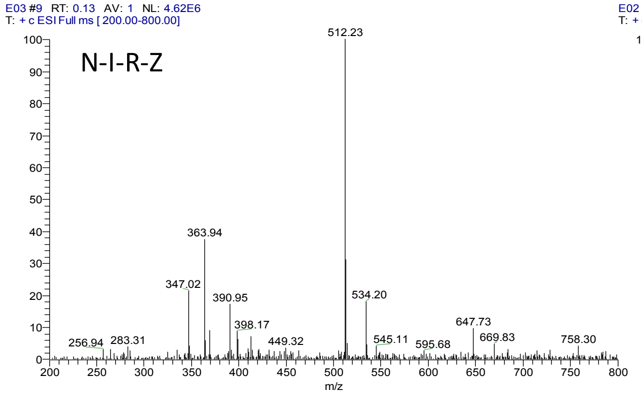

E09 #9 RT: 0.13 AV: 1 NL: 1.20E7
T: + c ESI Full ms [200.00-800.00]
E-R-N-Z
528.18
542.20
363.94
346.97
369.01
550.17
556.19
257.27
282.83
428.15
456.73
618.32
677.80
714.68
747.89
792.54
m/z

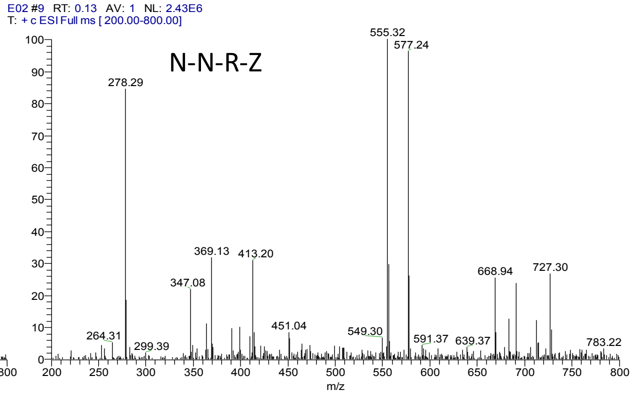

E08 #10 RT: 0.14 AV: 1 NL: 1.48E7
T: + c ESI Full ms [200.00-800.00]
E-R-F-Z
527.23
541.18
549.22
363.93
347.04
369.17
555.13
258.24
285.22
457.97
514.31
614.79
676.75
713.37
790.56
m/z

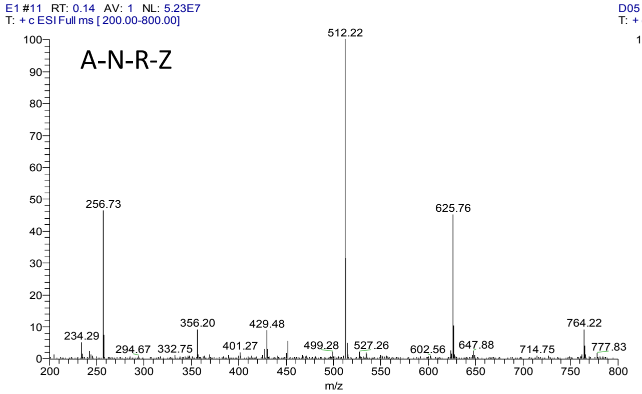

E07 #9 RT: 0.13 AV: 1 NL: 1.35E7
T: + c ESI Full ms [200.00-800.00]
D-R-F-Z
547.23
561.20
569.15
363.91
346.97
390.92
432.22
575.15
268.29
302.95
466.24
534.24
638.94
704.78
741.48
m/z

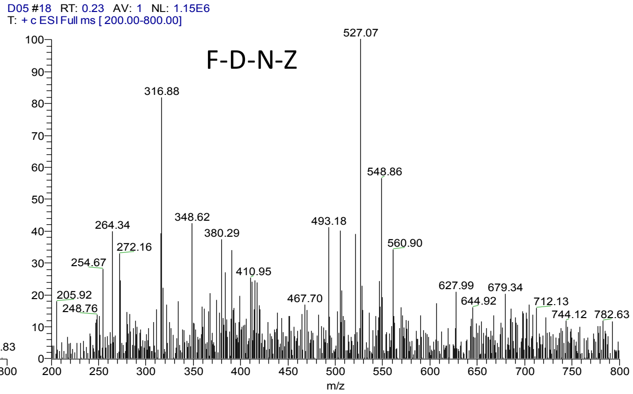

E06 #8 RT: 0.11 AV: 1 NL: 2.41E7
T: + c ESI Full ms [200.00-800.00]
D-F-R-Z
547.23
561.22
569.15
432.26
363.92
268.40
294.68
466.27
534.15
634.13
698.91
726.99
799.10
m/z

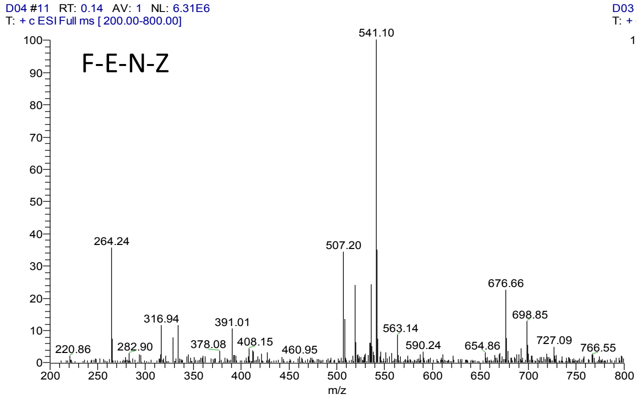

E04 #9 RT: 0.12 AV: 1 NL: 3.11E7
T: + c ESI Full ms [200.00-800.00]
N-R-I-Z
512.20
647.86
363.97
398.16
534.19
264.30
294.76
347.08
409.82
467.58
545.18
593.07
714.76
783.65
m/z

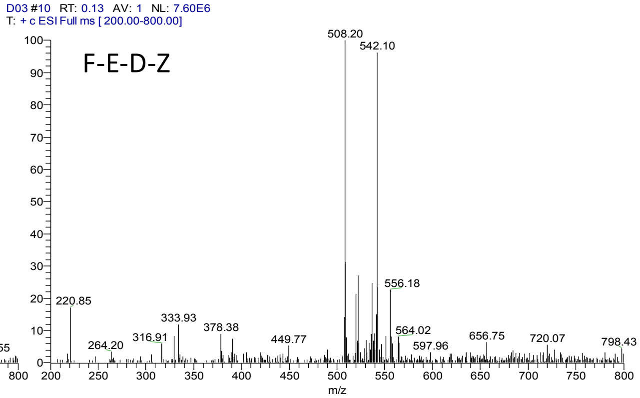

E03 #9 RT: 0.13 AV: 1 NL: 4.62E6
T: + c ESI Full ms [200.00-800.00]
N-I-R-Z
512.23
363.94
347.02
390.95
398.17
534.20
256.94
283.31
449.32
545.11
595.68
647.73
669.83
758.30
m/z

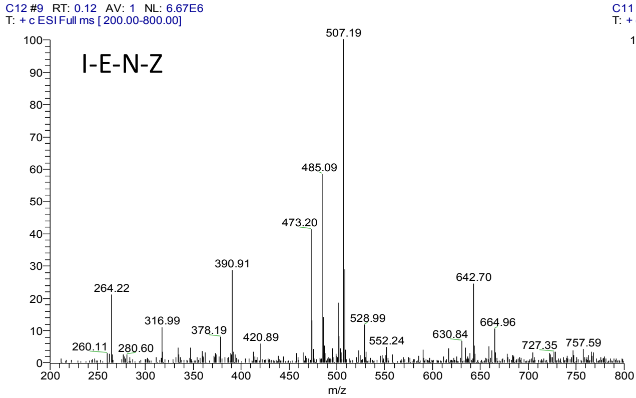

E02 #9 RT: 0.13 AV: 1 NL: 2.43E6
T: + c ESI Full ms [200.00-800.00]
N-N-R-Z
555.32
577.24
278.29
369.13
413.20
347.08
264.31
299.39
451.04
549.30
591.37
639.37
668.94
727.30
783.22
m/z

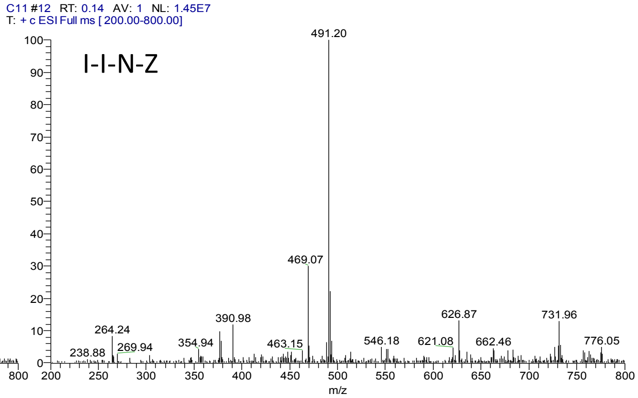

E1 #11 RT: 0.14 AV: 1 NL: 5.23E7
T: + c ESI Full ms [200.00-800.00]
A-N-R-Z
512.22
256.73
625.76
234.29
294.67
332.75
356.20
401.27
429.48
499.28
527.26
602.56
647.88
714.75
764.22
777.83
m/z

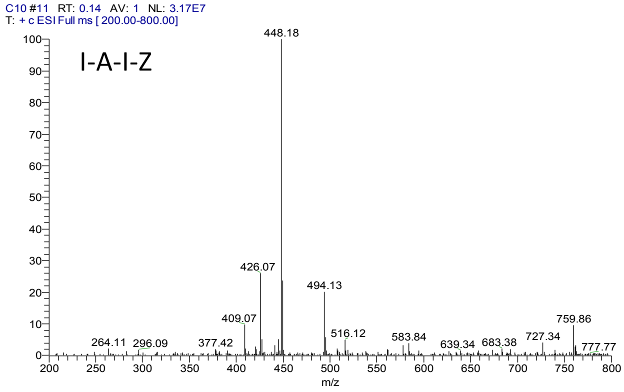

D05 #18 RT: 0.23 AV: 1 NL: 1.15E6
T: + c ESI Full ms [200.00-800.00]
F-D-N-Z
527.07
316.88
548.86
264.34
348.62
380.29
493.18
560.90
254.67
272.16
410.95
205.92
248.76
467.70
627.99
644.92
679.34
712.13
744.12
782.63
m/z

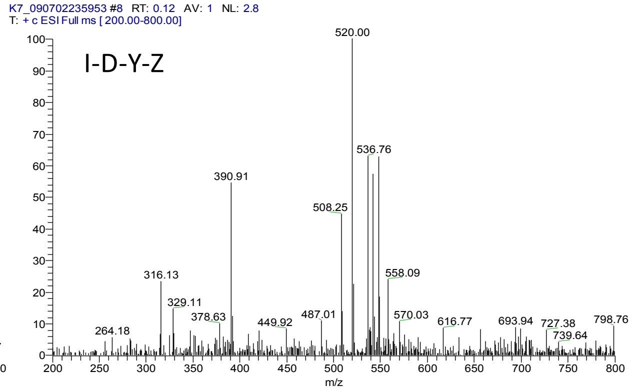

D04 #11 RT: 0.14 AV: 1 NL: 6.31E6
T: + c ESI Full ms [200.00-800.00]
F-E-N-Z
541.10
264.24
507.20
676.66
316.94
391.01
698.85
563.14
220.86
282.90
378.08
408.15
460.95
590.24
654.86
727.09
766.55
m/z

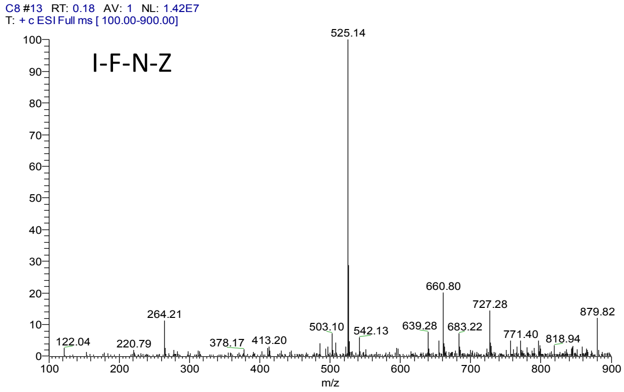

D03 #10 RT: 0.13 AV: 1 NL: 7.60E6
T: + c ESI Full ms [200.00-800.00]
F-E-D-Z
508.20
542.10
556.18
220.85
333.93
316.91
264.20
378.38
449.77
564.02
597.96
656.75
720.07
798.43
m/z

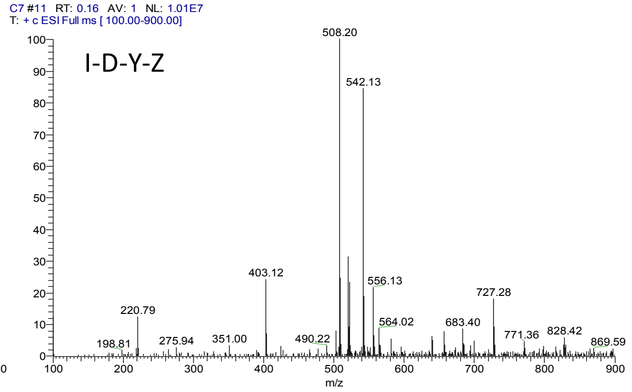

C12 #9 RT: 0.12 AV: 1 NL: 6.67E6
T: + c ESI Full ms [200.00-800.00]
I-E-N-Z
507.19
485.09
473.20
390.91
264.22
642.70
316.99
378.19
528.99
664.96
260.11
280.60
420.89
552.24
630.84
727.35
757.59
m/z

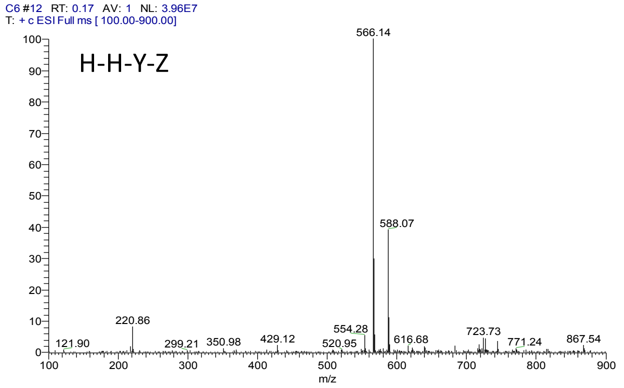

C11 #12 RT: 0.14 AV: 1 NL: 1.45E7
T: + c ESI Full ms [200.00-800.00]
I-I-N-Z
491.20
469.07
390.98
264.24
238.88
269.94
354.94
463.15
546.18
621.08
626.87
662.46
731.96
776.05
m/z

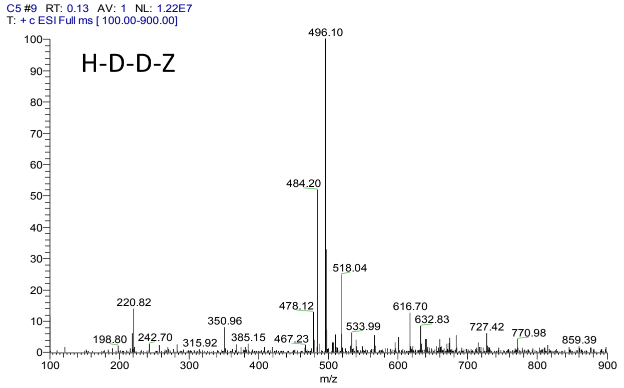

C10 #11 RT: 0.14 AV: 1 NL: 3.17E7
T: + c ESI Full ms [200.00-800.00]
I-A-I-Z
448.18
426.07
494.13
409.07
516.12
264.11
296.09
377.42
583.84
639.34
683.38
727.34
759.86
777.77
m/z

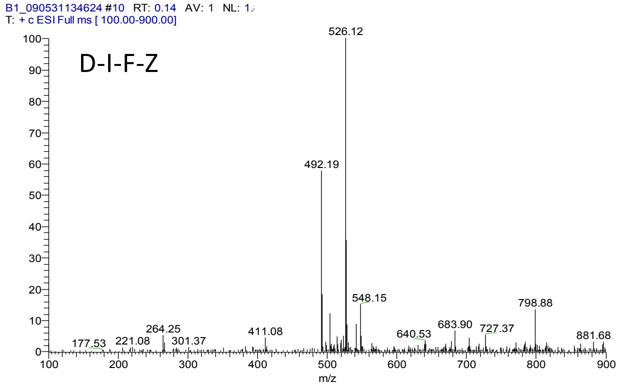

K7_090702235953 #8 RT: 0.12 AV: 1 NL: 2.8
T: + c ESI Full ms [200.00-800.00]
I-D-Y-Z
520.00
536.76
390.91
508.25
316.13
558.09
329.11
378.63
570.03
264.18
449.92
487.01
616.77
693.94
727.38
739.64
798.76
m/z

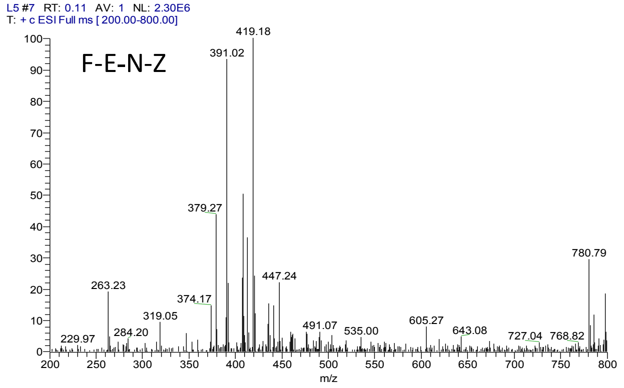

C8 #13 RT: 0.18 AV: 1 NL: 1.42E7
T: + c ESI Full ms [100.00-900.00]
I-F-N-Z
525.14
660.80
727.28
264.21
879.82
503.10
542.13
639.28
683.22
771.40
122.04
220.79
378.17
413.20
818.94
m/z

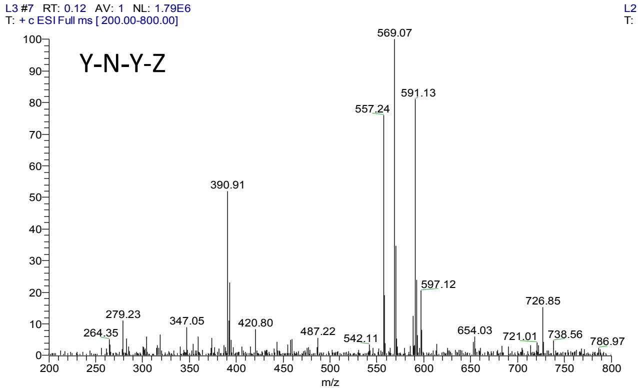

C7 #11 RT: 0.16 AV: 1 NL: 1.01E7
T: + c ESI Full ms [100.00-900.00]
I-D-Y-Z
508.20
542.13
403.12
556.13
727.28
220.79
564.02
683.40
198.81
275.94
351.00
490.22
771.36
828.42
869.59
m/z

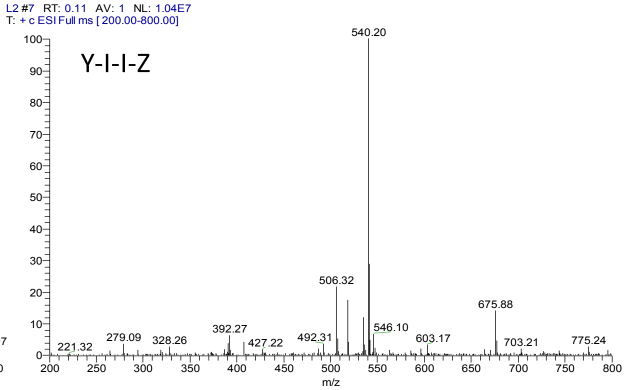

C6 #12 RT: 0.17 AV: 1 NL: 3.96E7
T: + c ESI Full ms [100.00-900.00]
H-H-Y-Z
566.14
588.07
220.86
554.28
723.73
121.90
299.21
350.98
429.12
520.95
616.68
771.24
867.54
m/z

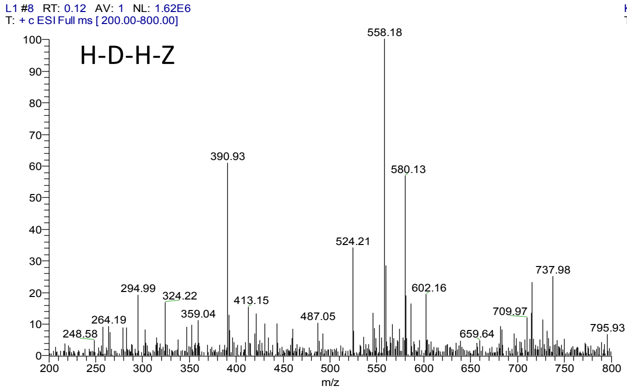

C5 #9 RT: 0.13 AV: 1 NL: 1.22E7
T: + c ESI Full ms [100.00-900.00]
H-D-D-Z
496.10
484.20
518.04
220.82
478.12
616.70
350.96
632.83
198.80
242.70
315.92
385.15
467.23
533.99
727.42
770.98
859.39
m/z

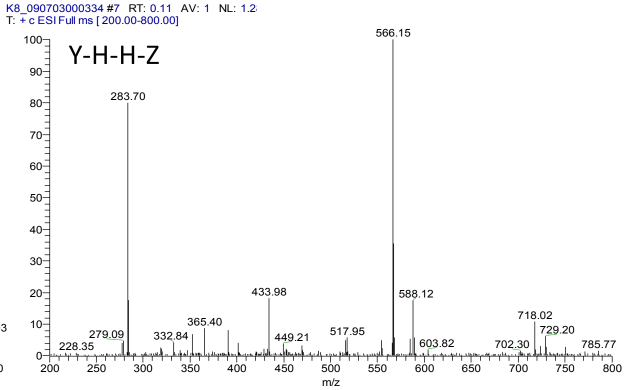

B1_090531134624 #10 RT: 0.14 AV: 1 NL: 1.
T: + c ESI Full ms [100.00-900.00]
D-I-F-Z
526.12
492.19
548.15
798.88
264.25
411.08
683.90
727.37
177.53
221.08
301.37
640.53
881.68
m/z

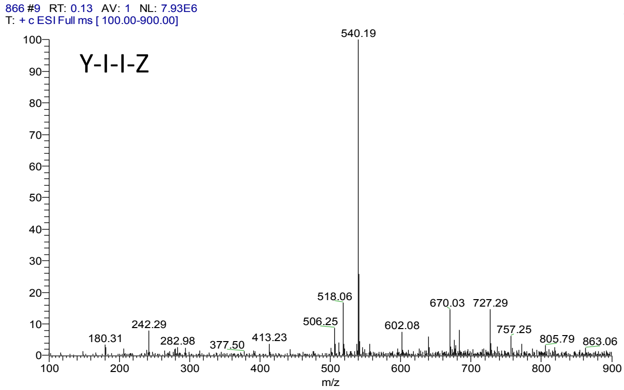

L5 #7 RT: 0.11 AV: 1 NL: 2.30E6
T: + c ESI Full ms [200.00-800.00]
F-E-N-Z
419.18
391.02
379.27
780.79
447.24
263.23
374.17
319.05
605.27
229.97
284.20
491.07
535.00
643.08
727.04
768.82
m/z

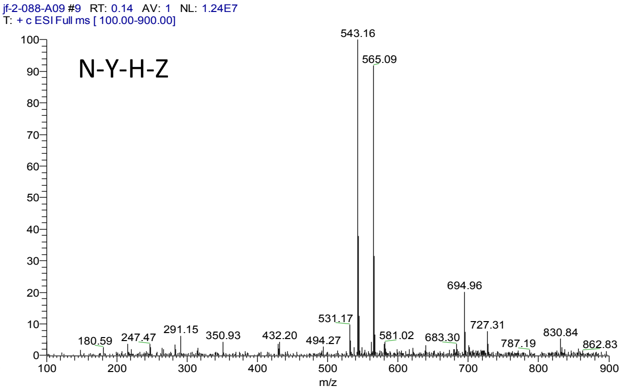

L3 #7 RT: 0.12 AV: 1 NL: 1.79E6
T: + c ESI Full ms [200.00-800.00]
Y-N-Y-Z
569.07
591.13
557.24
390.91
597.12
279.23
264.35
347.05
420.80
487.22
542.11
654.03
726.85
721.01
738.56
786.97
m/z

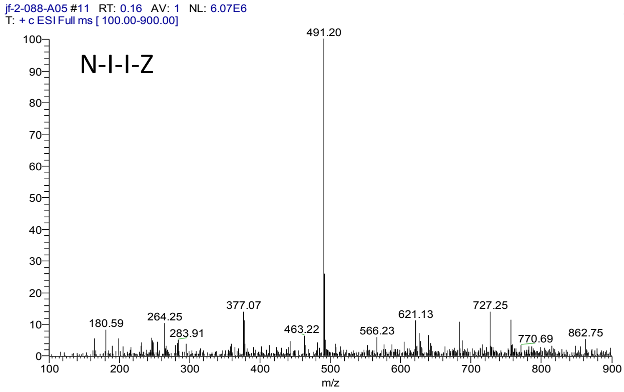

L2 #7 RT: 0.11 AV: 1 NL: 1.04E7
T: + c ESI Full ms [200.00-800.00]
Y-I-I-Z
540.20
506.32
675.88
221.32
279.09
328.26
392.27
427.22
492.31
546.10
603.17
703.21
775.24
m/z

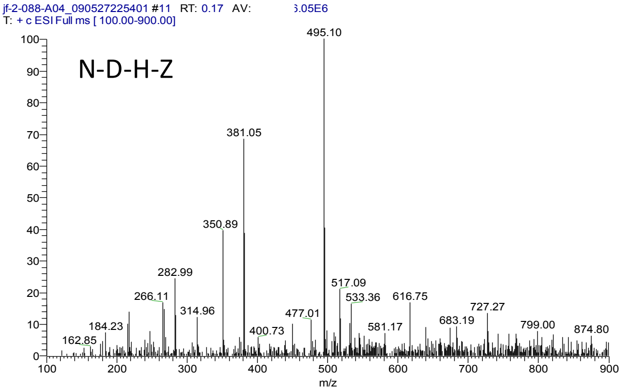

L1 #8 RT: 0.12 AV: 1 NL: 1.62E6
T: + c ESI Full ms [200.00-800.00]
H-D-H-Z
558.18
390.93
580.13
524.21
737.98
294.99
324.22
264.19
359.04
413.15
248.58
487.05
602.16
709.97
659.64
795.93
m/z

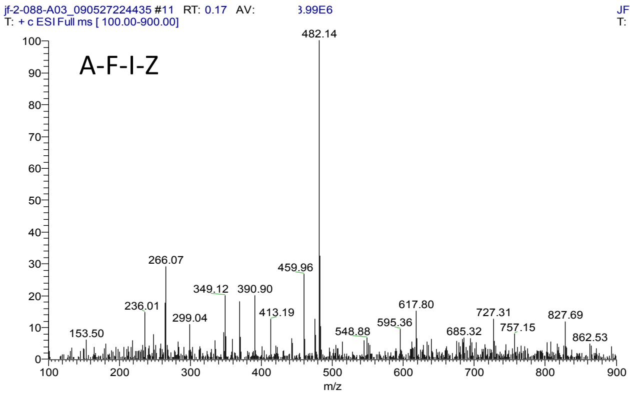

K8_090703000334 #7 RT: 0.11 AV: 1 NL: 1.2
T: + c ESI Full ms [200.00-800.00]
Y-H-H-Z
566.15
283.70
433.98
588.12
365.40
332.84
279.09
228.35
449.21
517.95
603.82
718.02
729.20
702.30
785.77
m/z

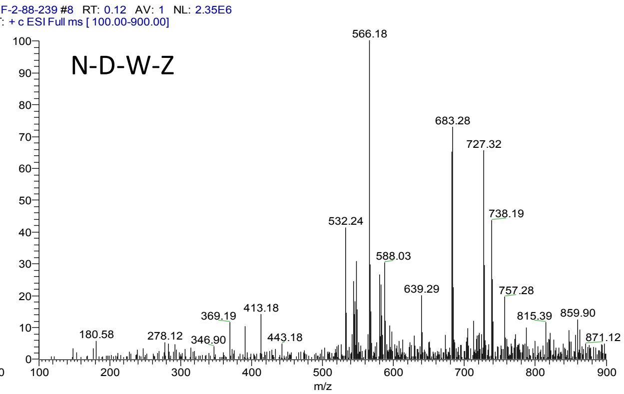

866 #9 RT: 0.13 AV: 1 NL: 7.93E6
T: + c ESI Full ms [100.00-900.00]
Y-I-I-Z
540.19
518.06
506.25
670.03
727.29
757.25
602.08
180.31
242.29
282.98
377.50
413.23
805.79
863.06
m/z


jf-2-088-A09 #9 RT: 0.14 AV: 1 NL: 1.24E7
T: + c ESI Full ms [100.00-900.00]
N-Y-H-Z
543.16
565.09
694.96
727.31
531.17
180.59
247.47
291.15
350.93
432.20
494.27
581.02
683.30
787.19
830.84
862.83
m/z


jf-2-088-A05 #11 RT: 0.16 AV: 1 NL: 6.07E6
T: + c ESI Full ms [100.00-900.00]
N-I-I-Z
491.20
377.07
180.59
264.25
283.91
463.22
566.23
621.13
727.25
770.69
862.75
m/z


jf-2-088-A04_090527225401 #11 RT: 0.17 AV:
5.05E6
T: + c ESI Full ms [100.00-900.00]
N-D-H-Z
495.10
381.05
350.89
282.99
266.11
314.96
184.23
162.85
400.73
477.01
517.09
533.36
581.17
616.75
727.27
683.19
799.00
874.80
m/z


jf-2-088-A03_090527224435 #11 RT: 0.17 AV: 3.99E6
T: + c ESI Full ms [100.00-900.00]
A-F-I-Z
482.14
266.07
459.96
236.01
349.12
390.90
299.04
413.19
617.80
595.36
548.88
727.31
827.69
685.32
757.15
862.53
153.50
0
10
20
30
40
50
60
70
80
90
100
100
200
300
400
500
600
700
800
900
m/z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T: + c ESI Full ms [100.00-900.00]
N-D-W-Z
566.18
683.28
727.32
532.24
738.19
588.03
639.29
757.28
369.19
413.18
815.39
859.90
180.58
278.12
346.90
443.18
871.12
0
10
20
30
40
50
60
70
80
90
100
100
200
300
400
500
600
700
800
900
m/z

II (d) NMR, IR, and HR-MS characterization of

ABI (**15-AB-21**)

HRMS: Calculated mass: 588.2684 (M+H); observed mass: 558.2677

^{1}H (CD_3OD, 400MHz) δ 9.01 (2H, d, J=6.91), 7.7-7.38 (9H, m), 4.92 (4H, s), 4.52 (2H, t, J=13.07), 3.32 (6H, m), 1.30 (4H, m)

^{13}C-NMR (CD_3OD, 100MHz) δ 173.09, 171.00, 162.72, 162.36, 151.08, 136.86, 136.79, 136.66, 133.06, 132.29, 128.75, 128.70, 124.01, 123.40, 121.14, 121.10, 113.04, 112.77, 111.82, 111.56, 52.98, 52.89, 46.86, 46.37, 45.89, 29.30, 27.92

IR (thin film): 981, 1026, 1121, 1232, 1370, 2072, 2236, 2487, 2909, 2977, 3334 cm^{-1}

ABII (**11-AB-25**)

HRMS: Calculated mass: 697.2792 (M+H); observed mass: 697.2784

^{1}H (CD_3OD, 400MHz) δ 8.14 (2H, d, J= 6.02), 7.91 (1H, s), 7.56-7.38 (3H, m), 4.94 (4H, s), 3.73 (1H, m), 3.32 (6H, m), 3.09 (2H, m), 2.99 (3H, d, J=5.95), 1.93-1.63 (4H, m), 1.3 (4H,m)

^{13}C-NMR (CD_3OD, 100MHz) δ 172.42, 171.58, 171.08,162.47,162.12, 150.71, 140.21, 134.55, 134.20, 128.54, 125.84, 123.74, 113.67, 112.50, 112.25, 68.87, 57.27, 53.44, 46.52, 46.41, 30.77, 30.59, 29.98, 27.88, 23.75

IR (thin film): 981, 1028, 1122, 1231, 1448, 2072, 2222, 2489, 2832, 2909, 2936, 2956, 3322 cm^{-1}

ABIII (**15-AB-25**)

HRMS: Calculated mass: 694.2431 (M+H); observed mass: 694.2430

^{1}H (CD_3OD, 400MHz) δ 9.01 (2H, d, J=6.91), 7.66-7.10 (7H, m), 4.92 (4H, s), 4.52 (2H, t, J=13.07), 3.32 (6H, m), 1.30 (4H, m)

IR (thin film): 982, 1025, 1122, 1231, 1445, 2072, 2489, 2830, 2944, 3320 cm^{-1}

ABIV (**19-AB-25**)

HRMS: Calculated mass: 643.2322 (M+H); observed mass: 643.2315

^{1}H (CD_3OD, 400MHz) δ 8.14 (2H, d, J=6.84), 7.94 (1H, s), 8.13-7.41 (3H, m), 4.93 (4H, s), 3.33 (6H, m), 2.06 (2H, m), 1.33 (4H, m)

IR (thin film): 979, 1027, 1122, 1232, 1366, 2072, 2234, 2482, 2900, 2972, 3316 cm^{-1}

ABV (**15-AB-26**)

HRMS: Calculated mass: 588.2789 (M+H); observed mass: 588.2782

^{1}H (CD_3OD, 400MHz) δ 9.01 (2H, d, J=6.91), 7.66-7.10 (7H, m), 4.92 (4H, s), 4.52 (2H, t, J=13.99), 3.88 (3H, s) 3.32 (6H, m), 1.30 (4H, m)

IR (thin film): 981, 1025, 1122, 1155, 1232, 1446, 2072, 2253, 2832, 2913, 2941, 3335 cm^{-1}

Section III

III (a) Screening of Small molecule libraries via microarray

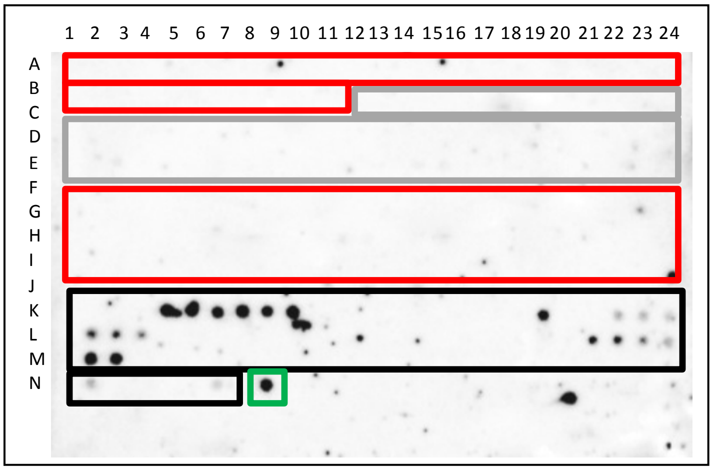
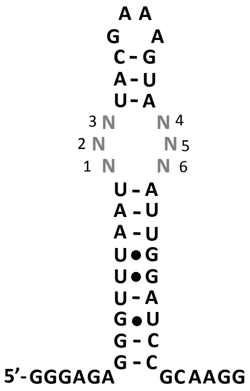


Figure S-1: Microarray screening of a small molecule library containing peptoids, peptides, and 2-aminobenzimidazoles for binding **1**. Image of the microarray with all 284 ligands after hybridization with ^{32}P-labeled **1**. The peptoid library members are outlined in red (0 hits), peptide library members are outlined in grey (0 hits), 2-aminobenzimidazole members are outlined in black (19 hits), and the positive control is outlined in green.

Section IV. RNA-PSP analysis: Sum Z-scores for **ABI – ABV**



1

Table S-1: Sequences of all selected loops for **ABI** and their corresponding sum Z-scores. The position where each nucleotide occurs is indicated in secondary structure of **1** above.

S. No	Loop	1	2	3	4	5	6	Σ Z-Score
1	AB I IL 1	G	C	U	C	C	G	51.37
2	AB I IL 2	G	C	U	C	U	G	51.41
3	AB I IL 3	A	C	C	G	U	C	55.73
4	AB I IL 4	A	U	G	G	U	C	51.24
5	AB I IL 5	G	G	U	C	C	C	49.30
6	AB I IL 6	G	C	U	C	A	C	48.77
7	AB I IL 7	A	G	G	G	U	C	48.56
8	AB I IL 8	A	C	G	G	C	C	47.27
9	AB I IL 9	U	A	U	C	A	U	44.90
10	AB I IL 10	U	A	U	C	A	U	44.90
11	AB I IL 11	G	A	U	C	C	A	43.52
12	AB I IL 12	A	C	A	G	A	C	41.13
13	AB I IL 13	U	C	C	G	G	C	40.19
14	AB I IL 14	G	C	U	C	U	U	39.45
15	AB I IL 15	G	G	A	G	C	C	36.91
16	AB I IL 16	C	G	A	C	C	C	36.60
17	AB I IL 17	A	A	A	G	C	C	35.95
18	AB I IL 18	A	C	A	U	U	C	32.39

19	AB I IL 19	G	G	A	C	A	C	31.98
20	AB I IL 20	G	A	C	U	G	G	31.04
21	AB I IL 21	G	A	G	C	C	A	29.34
22	AB I IL 22	U	C	G	G	G	G	27.37
23	AB I IL 23	C	G	A	C	U	C	25.53
24	AB I IL 24	A	G	U	G	A	C	25.29
25	AB I IL 25	G	A	U	U	G	G	24.92
26	AB I IL 26	G	U	C	U	G	G	24.86
27	AB I IL 27	U	C	U	G	G	G	24.28
28	AB I IL 28	G	A	G	A	C	C	23.16
29	AB I IL 29	G	A	A	G	C	A	23.16
30	AB I IL 30	U	C	C	C	G	C	22.98
31	AB I IL 31	G	U	U	U	G	C	22.32
32	AB I IL 32	G	C	C	A	U	C	20.96
33	AB I IL 33	A	U	G	C	A	C	20.91
34	AB I IL 34	A	U	U	U	C	C	20.42
35	AB I IL 35	A	U	A	C	A	G	19.80
36	AB I IL 36	U	A	U	A	A	C	19.35
37	AB I IL 37	G	U	C	A	G	C	19.17
38	AB I IL 38	G	G	U	G	C	U	18.87
39	AB I IL 39	G	G	G	A	U	C	18.76
40	AB I IL 40	A	C	U	U	G	C	18.64
41	AB I IL 41	A	U	A	G	U	G	17.61
42	AB I IL 42	A	U	C	A	C	C	17.33
43	AB I IL 43	A	U	A	U	A	G	16.71
44	AB I IL 44	G	C	U	G	G	A	16.68
45	AB I IL 45	A	C	C	A	U	U	14.16
46	AB I IL 46	C	A	A	A	C	C	13.71
47	AB I IL 47	C	U	U	C	A	C	13.30
48	AB I IL 48	A	C	A	A	U	A	11.07
49	AB I IL 49	G	A	C	U	A	A	10.83
50	AB I IL 50	U	G	U	A	A	U	10.53
51	AB I IL 51	C	C	A	C	C	G	8.87
52	AB I IL 52	C	C	G	G	A	A	8.38
53	AB I IL 53	G	U	U	G	A	A	8.21
54	AB I IL 54	G	U	A	A	C	G	6.85
55	AB I IL 55	U	U	G	A	A	C	6.14
56	AB I IL 56	U	U	G	G	G	U	5.78
57	AB I IL 57	C	C	C	C	A	G	5.78
58	AB I IL 58	A	G	C	U	U	U	5.29
59	AB I IL 59	A	G	G	C	U	A	5.29

60	AB I IL 60	C	C	U	G	U	A	5.29
61	AB I IL 61	G	A	C	G	A	U	5.06
62	AB I IL 62	A	G	C	G	C	G	4.88
63	AB I IL 63	C	C	G	U	G	A	3.09
64	AB I IL 64	U	G	A	A	G	A	3.09
65	AB I IL 65	C	A	C	C	U	A	3.09
66	AB I IL 66	C	A	C	U	U	U	3.09
67	AB I IL 67	U	A	G	A	G	A	3.09
68	AB I IL 68	U	A	A	C	C	G	2.68
69	AB I IL 69	U	G	G	G	C	A	2.68
70	AB I IL 70	G	G	G	U	A	U	1.97
71	AB I IL 71	C	A	C	G	G	G	0.00

Table S-2: Sequences of all selected loops for **ABII** and their corresponding sum Z-scores. The position where each nucleotide occurs is indicated in secondary structure of **1** above.

S. No	Loop	1	2	3	4	5	6	Σ Z-Score
1	AB II IL 1	C	A	A	G	G	C	108.7257
2	AB II IL 2	A	C	A	C	G	C	90.45831
3	AB II IL 2	A	C	A	C	G	C	90.45831
4	AB II IL 3	A	C	A	G	G	C	127.0134
5	AB II IL 4	U	A	U	C	C	C	99.50588
6	AB II IL 5	A	C	U	U	G	C	83.68124
7	AB II IL 6	U	A	U	C	C	C	99.50588
8	AB II IL 7	A	C	U	U	G	C	83.68124
9	AB II IL 8	A	C	A	C	C	C	75.81603
10	AB II IL 9	C	C	A	U	G	C	70.51098
11	AB II IL 10	A	C	G	G	C	C	70.49602
12	AB II IL 11	A	C	A	G	U	C	68.58954
13	AB II IL 12	A	A	U	C	C	C	66.36061
14	AB II IL 13	A	C	G	U	C	C	64.37825
15	AB II IL 14	C	U	G	G	G	C	64.08398
16	AB II IL 15	C	A	G	G	G	A	63.68153
17	AB II IL 16	A	C	A	G	G	U	58.85229
18	AB II IL 17	C	U	G	G	G	A	53.8375
19	AB II IL 18	U	G	U	C	C	G	53.66045
20	AB II IL 19	C	C	G	G	G	A	52.30268
21	AB II IL 20	U	C	G	C	C	C	52.09154
22	AB II IL 21	C	C	U	U	C	C	46.2309
23	AB II IL 22	A	U	C	C	C	G	46.15653
24	AB II IL 23	C	A	C	G	A	C	43.56854
25	AB II IL 24	C	C	C	C	G	C	42.99221
26	AB II IL 25	C	U	C	C	C	C	42.31909
27	AB II IL 26	U	G	U	G	C	G	39.80401
28	AB II IL 27	U	A	C	G	A	C	38.73227
29	AB II IL 28	A	U	U	G	C	G	38.62622
30	AB II IL 29	C	A	G	U	G	C	36.80919
31	AB II IL 30	G	G	U	C	C	G	36.72488
32	AB II IL 31	C	C	U	C	A	C	34.11721
33	AB II IL 32	A	U	C	G	U	G	33.19806
34	AB II IL 33	A	A	C	G	U	C	32.81723
35	AB II IL 34	U	U	C	C	C	A	30.59095
36	AB II IL 35	A	U	U	A	C	G	30.54924
37	AB II IL 36	U	U	C	G	C	G	29.93345

38	AB II IL 37	C	U	C	U	U	G	29.17484
39	AB II IL 38	G	C	C	G	C	C	28.59302
40	AB II IL 39	U	A	A	G	G	G	28.44814
41	AB II IL 40	C	G	A	C	C	C	27.62759
42	AB II IL 41	A	C	G	U	G	U	26.32669
43	AB II IL 42	C	U	C	U	U	A	25.84852
44	AB II IL 43	G	U	G	C	C	G	25.24977
45	AB II IL 44	U	A	C	U	A	C	23.38641
46	AB II IL 45	C	U	C	G	U	U	23.19288
47	AB II IL 46	A	C	U	G	U	A	22.83427
48	AB II IL 47	C	C	U	C	C	U	21.60898
49	AB II IL 48	C	A	G	G	C	G	19.73308
50	AB II IL 49	A	C	U	A	C	A	19.00961
51	AB II IL 50	C	U	U	A	G	C	18.79137
52	AB II IL 51	G	A	G	U	C	C	18.54762
53	AB II IL 52	U	C	A	C	C	A	18.3637
54	AB II IL 53	A	U	C	G	G	U	16.15647
55	AB II IL 54	G	U	C	C	G	G	13.96435
56	AB II IL 55	G	A	C	U	C	G	13.27155
57	AB II IL 56	U	C	U	G	G	U	12.68937
58	AB II IL 57	U	G	C	A	A	G	11.17
59	AB II IL 58	U	G	C	A	G	G	11.17
60	AB II IL 59	U	A	A	G	U	U	10.9789
61	AB II IL 60	U	A	A	C	U	A	10.73233
62	AB II IL 61	C	G	C	U	U	A	10.71936
63	AB II IL 62	G	A	A	A	C	G	10.36964
64	AB II IL 63	G	G	A	C	G	G	10.18376
65	AB II IL 64	C	G	C	C	U	G	8.692479
66	AB II IL 65	A	G	A	C	G	A	8.581568
67	AB II IL 66	A	A	A	A	G	G	8.143905
68	AB II IL 67	U	A	C	C	G	A	7.830417
69	AB II IL 68	U	G	A	G	C	U	7.808588
70	AB II IL 69	U	C	G	G	A	G	7.528411
71	AB II IL 70	G	C	A	G	A	G	7.528411
72	AB II IL 71	A	C	C	U	A	A	7.03778
73	AB II IL 72	A	U	C	A	A	A	5.271867
74	AB II IL 73	U	G	C	G	U	A	5.175071
75	AB II IL 74	A	U	A	U	A	G	3.326313
76	AB II IL 75	G	G	G	G	A	G	2.710819
77	AB II IL 76	U	U	U	C	G	U	2.464251
78	AB II IL 77	G	A	A	U	A	A	0

Table S-3: Sequences of all selected loops for **ABIII** and their corresponding sum Z-scores. The position where each nucleotide occurs is indicated in secondary structure of **1** above.

S. No	Loop	1	2	3	4	5	6	Σ Z-Score
1	AB III IL 1	U	U	U	G	C	G	167.2105
2	AB III IL 1	U	U	U	G	C	G	167.2105
3	AB III IL 1	U	U	U	G	C	G	167.2105
4	AB III IL 3	C	C	C	C	G	C	132.6968
5	AB III IL 4	C	A	C	C	G	C	118.8408
6	AB III IL 5	C	C	C	C	G	G	110.1144
7	AB III IL 6	C	C	C	C	G	A	102.5067
8	AB III IL 7	G	C	C	C	U	G	102.1979
9	AB III IL 8	C	U	C	U	G	C	97.97974
10	AB III IL 9	C	C	U	G	C	C	95.47503
11	AB III IL 10	A	U	U	G	C	C	94.61297
12	AB III IL 11	C	A	C	G	G	C	82.70202
13	AB III IL 12	G	A	U	G	C	C	77.27151
14	AB III IL 13	C	C	A	G	C	C	65.41424
15	AB III IL 14	A	A	U	G	C	G	64.08981
16	AB III IL 15	A	A	A	G	C	C	61.5774
17	AB III IL 16	A	U	A	G	C	G	58.59703
18	AB III IL 17	G	C	G	G	C	C	56.31616
19	AB III IL 18	A	C	C	C	U	G	55.60781
20	AB III IL 19	G	A	C	C	U	G	53.58299
21	AB III IL 20	U	C	U	C	C	C	51.0001
22	AB III IL 21	C	U	C	U	G	G	50.68067
23	AB III IL 22	C	U	C	U	U	C	49.12005
24	AB III IL 23	A	A	U	G	A	C	48.27477
25	AB III IL 24	C	A	G	U	G	C	42.30723
26	AB III IL 25	C	C	C	C	A	U	40.33884
27	AB III IL 26	G	C	U	C	G	G	39.32911
28	AB III IL 27	A	A	C	C	G	A	38.21291
29	AB III IL 28	A	A	C	C	U	C	38.07573
30	AB III IL 29	G	G	C	C	G	G	36.39911
31	AB III IL 30	G	C	A	G	G	C	35.27423
32	AB III IL 31	G	G	U	G	G	C	34.65379
33	AB III IL 32	G	C	C	U	U	C	32.87606
34	AB III IL 33	U	A	U	C	G	C	31.3478
35	AB III IL 34	U	U	C	A	C	G	29.29945

36	AB III IL 35	A	G	A	C	C	C	28.7186
37	AB III IL 36	G	U	A	C	C	G	28.20733
38	AB III IL 37	C	C	U	C	C	U	28.15913
39	AB III IL 38	U	G	A	C	C	C	25.58265
40	AB III IL 39	A	C	C	A	G	A	24.84736
41	AB III IL 40	G	C	U	G	A	G	22.28189
42	AB III IL 41	G	U	U	A	C	A	22.02245
43	AB III IL 42	U	C	C	U	G	A	21.36464
44	AB III IL 43	G	C	G	C	U	U	20.68479
45	AB III IL 44	A	C	G	A	C	C	19.41213
46	AB III IL 45	U	G	U	U	G	C	17.2434
47	AB III IL 46	C	G	G	U	A	C	15.96144
48	AB III IL 47	G	G	C	U	A	C	11.95376
49	AB III IL 48	G	C	U	A	U	A	11.56154
50	AB III IL 49	G	U	A	A	U	G	10.03327
51	AB III IL 50	G	C	A	C	A	A	9.800836
52	AB III IL 51	G	U	G	U	C	A	8.948716
53	AB III IL 52	C	U	A	A	C	A	7.598639
54	AB III IL 53	U	G	G	U	A	G	3.482721
55	AB III IL 54	A	U	G	G	U	U	2.132644
56	AB III IL 55	U	U	G	A	U	A	0
57	AB III IL 56	C	G	G	G	U	G	0
58	AB III IL 57	C	U	A	G	A	U	0
59	AB III IL 58	C	A	U	U	A	A	0

Table S-4: Sequences of all selected loops for **ABIV** and their corresponding sum Z-scores. The position where each nucleotide occurs is indicated in secondary structure of **1** above.

S. No	Loop	1	2	3	4	5	6	Σ Z-Score
1	AB IV IL 1	C	A	C	C	C	C	242.2054
2	AB IV IL 1	C	A	C	C	C	C	242.2054
3	AB IV IL 2	G	C	C	C	C	C	202.111
4	AB IV IL 3	C	C	C	C	G	C	181.8436
5	AB IV IL 4	A	A	C	C	C	C	173.9718
6	AB IV IL 5	U	C	C	C	C	C	172.1775
7	AB IV IL 6	C	C	A	C	C	C	154.7534
8	AB IV IL 7	C	G	C	C	C	C	148.835
9	AB IV IL 8	A	C	A	C	C	C	143.1652
10	AB IV IL 9	G	C	C	C	C	A	133.8437
11	AB IV IL 10	C	A	C	C	C	A	128.9347
12	AB IV IL 11	A	C	A	C	C	U	126.7522
13	AB IV IL 12	A	C	A	C	C	U	126.7522
14	AB IV IL 13	G	A	C	C	G	C	121.3406
15	AB IV IL 14	G	C	C	A	G	C	111.7298
16	AB IV IL 15	G	A	A	C	C	U	109.5441
17	AB IV IL 16	G	A	A	C	C	U	109.5441
18	AB IV IL 17	C	C	C	A	U	C	105.1149
19	AB IV IL 18	U	C	C	C	C	A	103.9101
20	AB IV IL 19	C	C	C	C	G	U	102.0903
21	AB IV IL 20	C	C	C	C	U	G	95.94266
22	AB IV IL 21	G	C	C	C	G	G	92.61426
23	AB IV IL 22	G	C	C	A	U	G	83.67924
24	AB IV IL 23	C	C	U	C	G	C	78.26131
25	AB IV IL 24	C	C	U	A	C	C	76.16101
26	AB IV IL 25	A	C	C	A	U	G	75.54361
27	AB IV IL 26	G	A	C	G	G	C	73.75705
28	AB IV IL 27	C	C	C	G	C	U	72.02102
29	AB IV IL 28	C	C	C	A	A	G	71.77256
30	AB IV IL 29	A	A	C	A	G	C	67.86459
31	AB IV IL 30	A	C	C	U	U	C	67.73314
32	AB IV IL 31	C	C	A	A	C	G	65.81675
33	AB IV IL 32	A	C	C	U	A	C	63.8935
34	AB IV IL 33	U	A	C	G	C	C	61.9152
35	AB IV IL 34	A	A	A	U	C	C	60.53193
36	AB IV IL 35	C	C	G	A	C	U	55.41654
37	AB IV IL 36	C	C	G	A	U	G	53.45111

38	AB IV IL 37	A	G	C	A	C	C	52.90231
39	AB IV IL 38	A	U	U	C	C	C	51.07062
40	AB IV IL 39	G	G	A	C	C	A	50.72157
41	AB IV IL 40	C	U	C	A	G	C	50.42849
42	AB IV IL 41	G	C	C	U	G	U	48.49781
43	AB IV IL 42	G	A	A	C	A	C	42.11249
44	AB IV IL 43	G	C	U	A	C	A	38.22589
45	AB IV IL 44	G	C	U	U	C	U	37.76128
46	AB IV IL 45	G	C	A	G	C	G	36.0352
47	AB IV IL 46	A	A	A	U	C	A	32.46398
48	AB IV IL 47	U	C	G	U	G	C	30.43735
49	AB IV IL 48	C	A	A	C	A	U	27.59238
50	AB IV IL 49	A	G	G	U	G	C	27.2205
51	AB IV IL 50	A	C	C	G	A	A	23.98193
52	AB IV IL 51	G	U	C	G	C	A	23.86896
53	AB IV IL 52	U	A	C	A	G	A	21.48489
54	AB IV IL 53	G	G	G	U	G	C	20.01644
55	AB IV IL 54	C	A	G	C	U	A	16.62942
56	AB IV IL 55	A	C	G	U	G	U	16.58814
57	AB IV IL 56	C	A	U	G	C	U	15.5313
58	AB IV IL 57	A	U	G	U	A	C	13.0502
59	AB IV IL 58	C	G	C	U	U	A	8.4331
60	AB IV IL 59	U	U	G	G	C	U	6.660679
61	AB IV IL 60	G	G	G	C	A	U	5.532998
62	AB IV IL 61	G	A	U	G	G	G	3.274131
63	AB IV IL 62	U	A	G	G	G	A	3.274131
64	AB IV IL 63	A	G	A	A	U	G	2.896678
65	AB IV IL 64	A	U	A	G	U	G	0

Table S-5: Sequences of all selected loops for **ABV** and their corresponding sum Z-scores. The position where each nucleotide occurs is indicated in secondary structure of **1** above.

S. No	Loop	1	2	3	4	5	6	Σ Z-Score
1	AB II IL 1	C	C	A	G	C	C	140.814
2	AB II IL 2	C	C	A	G	G	C	121.3676
3	AB II IL 3	G	C	A	G	C	C	100.831
4	AB II IL 4	U	C	G	G	C	C	94.48154
5	AB II IL 5	G	C	A	G	C	G	89.77421
6	AB II IL 6	U	C	G	G	C	G	87.41722
7	AB II IL 7	C	G	G	G	G	C	79.1738
8	AB II IL 7	C	G	G	G	G	C	79.1738
9	AB II IL 8	A	C	A	C	C	C	78.78228
10	AB II IL 9	A	U	A	C	G	C	76.58505
11	AB II IL 10	A	C	G	G	C	G	73.45406
12	AB II IL 11	C	C	U	G	G	G	69.61515
13	AB II IL 12	U	C	U	G	C	C	66.77411
14	AB II IL 13	C	C	C	C	A	C	66.66362
15	AB II IL 14	U	C	G	G	G	G	65.91786
16	AB II IL 15	C	C	A	G	A	G	65.40177
17	AB II IL 16	U	C	C	C	A	C	64.52784
18	AB II IL 17	C	A	C	G	C	C	63.31238
19	AB II IL 18	C	G	A	C	G	A	61.59054
20	AB II IL 19	A	U	U	C	G	C	60.83244
21	AB II IL 20	A	C	U	G	C	G	59.41227
22	AB II IL 21	U	C	C	A	A	C	58.6343
23	AB II IL 22	A	U	A	C	U	C	58.10317
24	AB II IL 23	C	G	A	C	U	A	56.34204
25	AB II IL 24	C	U	A	C	C	C	55.42108
26	AB II IL 25	C	A	C	A	C	C	54.12517
27	AB II IL 26	U	A	C	A	A	C	54.00406
28	AB II IL 27	C	C	A	A	U	C	53.10803
29	AB II IL 28	C	A	A	U	G	C	52.69586
30	AB II IL 29	C	U	C	G	C	C	52.5659
31	AB II IL 30	G	C	A	G	U	G	50.92732
32	AB II IL 31	G	A	U	C	G	C	49.52502
33	AB II IL 32	A	G	U	C	G	C	47.52243
34	AB II IL 33	A	A	C	A	A	C	46.54892
35	AB II IL 34	G	U	G	A	G	C	46.53094
36	AB II IL 35	G	U	G	A	G	C	46.53094
37	AB II IL 36	G	A	U	A	G	C	43.16996

38	AB II IL 37	C	A	A	G	G	G	42.78958
39	AB II IL 38	A	C	U	C	A	C	41.91104
40	AB II IL 39	C	C	U	U	G	G	39.18691
41	AB II IL 40	C	G	C	A	G	A	38.99532
42	AB II IL 41	C	G	C	A	G	A	38.99532
43	AB II IL 42	U	C	G	G	G	A	38.94698
44	AB II IL 43	C	G	A	U	A	C	38.493
45	AB II IL 44	C	C	C	C	A	A	35.41436
46	AB II IL 45	G	U	G	G	C	C	35.22257
47	AB II IL 46	A	A	A	A	A	C	34.37191
48	AB II IL 47	C	G	A	U	A	A	33.17941
49	AB II IL 48	A	U	A	C	C	G	30.42607
50	AB II IL 49	C	C	U	A	U	G	29.50805
51	AB II IL 50	U	A	U	G	G	C	29.48397
52	AB II IL 51	C	C	U	C	U	A	28.69195
53	AB II IL 52	C	A	A	A	G	U	28.34383
54	AB II IL 53	A	G	A	C	C	A	27.93193
55	AB II IL 54	C	G	U	C	U	C	27.05586
56	AB II IL 55	U	G	C	C	C	C	25.60949
57	AB II IL 56	C	A	A	G	U	A	25.19527
58	AB II IL 57	G	C	U	C	G	G	23.49063
59	AB II IL 58	U	A	G	A	C	C	22.60402
60	AB II IL 59	A	C	A	G	G	U	22.57239
61	AB II IL 60	U	G	C	U	G	C	22.08027
62	AB II IL 61	G	U	U	C	U	C	21.62477
63	AB II IL 62	C	U	A	A	G	U	21.32293
64	AB II IL 63	G	C	A	A	C	U	19.98707
65	AB II IL 64	G	G	G	G	A	C	18.55294
66	AB II IL 65	C	U	C	C	U	A	17.90524
67	AB II IL 66	A	A	U	G	C	G	16.95783
68	AB II IL 67	U	C	C	U	A	A	12.91696
69	AB II IL 68	G	C	G	A	U	G	10.8329
70	AB II IL 69	G	G	A	C	U	U	8.034321
71	AB II IL 70	U	G	A	C	A	U	8.034321
72	AB II IL 71	A	A	C	C	C	G	5.855824
73	AB II IL 72	G	U	A	U	G	G	4.550322
74	AB II IL 73	G	U	U	A	U	A	2.927429
75	AB II IL 74	A	A	G	A	G	U	2.275161
76	AB II IL 75	G	A	G	U	G	G	2.275161
77	AB II IL 76	G	G	U	A	C	G	0

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