Electronic Supplementary Material (ESI) for MedChemComm.

Supporting Information

On-DNA Pd and Cu Promoted C-N Cross-Coupling Reactions

Instrumentation for "on-DNA" synthesis:

Analysis was performed by HPLC/ESI-MS. After reaction, an aliquot of the reaction mixture solution was diluted (typically a 1 μL aliquot diluted with 40 μL of water) for LC\MS. Reverse-phase chromatography column (Optimize Opti-Lynx Trap 20ul, C18AQ – 40u) was applied. The sample was eluted [Inject at 4%B, step 90%B at 0.1 min., 1 mL/min flow rate; Solvent A: 0.75% v/v hexafluoroisopropanol (HFIP)/0.038% v/v triethylamine /5 μM EDTA in deionized water; Solvent B: 0.75% v/v HFIP/0.038% triethylamine /5 μM EDTA in 90/10 methanol/ deionized water] with detection at UV 260 nm. Effluent was analyzed on an ESI-MS(LXQ) scanning at 525-1950 amu.

Materials for "on-DNA" synthesis:

DNA headpiece HP-NH_2(5′-/5Phos/GAGTCA/iSp9/iUniAmM/iSp9/TGACTCCC-3′, Figure 1) was obtained from Biosearch Technologies, Novato, CA.

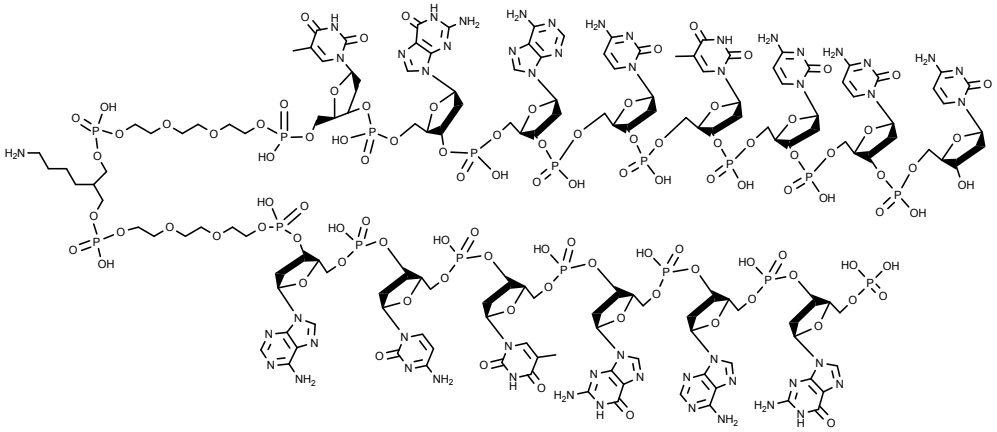


Figure 1. Headpiece: 5 -/5Phos/GAGTCA/iSp9/iUniAmM/iSp9/TGACTCCC-3, MW = 4937.20

The DNA-conjugated aryl iodides used in the studies were HP-SADO-ArI for Pd promoted C-N cross coupling and HP-ArI for Cu promoted C-N coupling. The protocol to prepare the HP-SADO-NH_2 was reported previously (Nat. Chem. Biol., 2009, 5, 647–654), and we used exact

the same protocol to prepare the HP-SADO-NH_2. The following is the detailed chemical structure of HP-SADO-NH_2 (Figure 2).

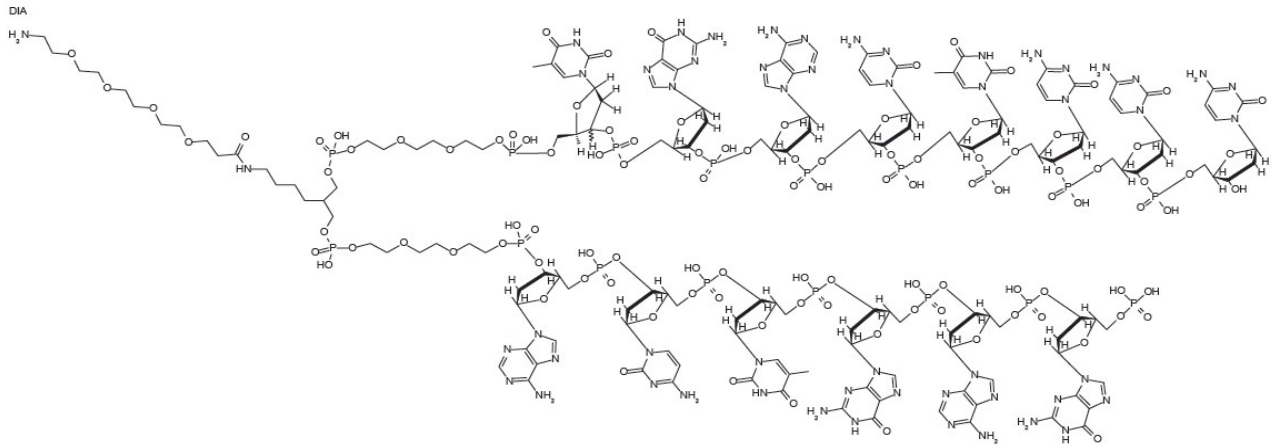
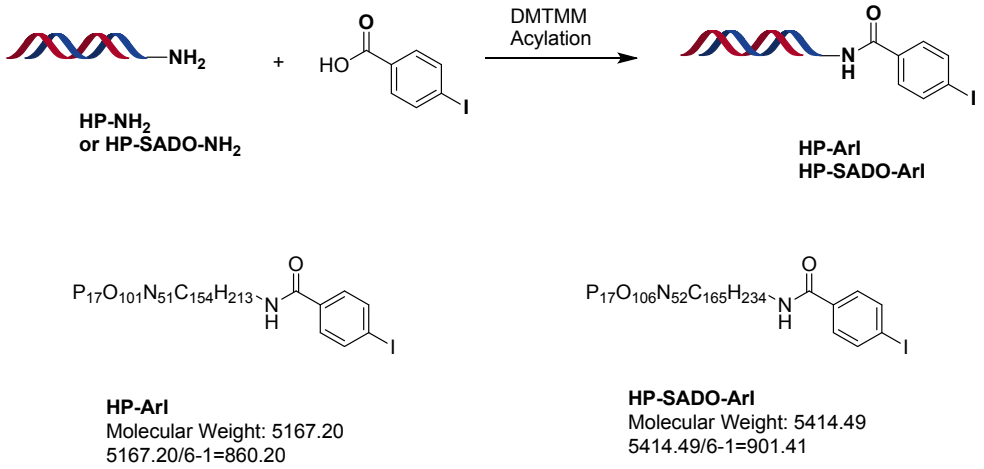


Figure 2. HP-SADO-NH_2, MW=5184.

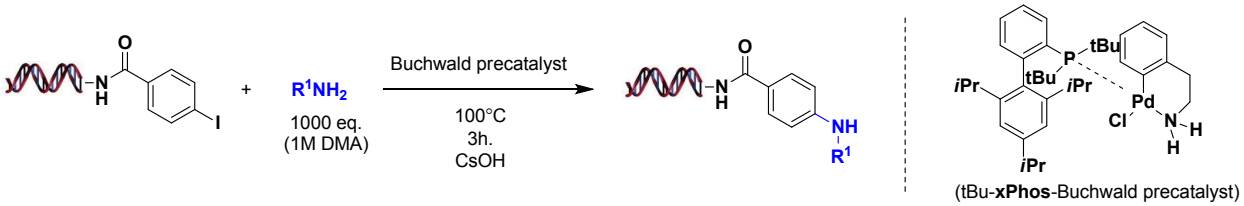


Scheme 1, HP-ArI and HP-SADO-ArI preparation

The above scheme described the preparation of HP-ArI an HP-SADO-ArI with simple amide coupling chemistry promoted by DMTMM. To the HP-NH_2 (1 mM) in pH 9.4 sodium borate buffer (250 mM), was added 40 equivalents of 4-iodo benzoic acid (200 mM in DMA), followed by 40 equivalents of DMTMM (200 mM in water). After being kept at rt for overnight, the reaction mixture was crashed by adding 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C). The mixture was stored at a -80°C freezer for more than 30 minutes. The sample was then centrifuged for around 30 minutes at 4°C in a microcentrifuge at

10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. The recovered pellet after lyophilization was dissolved in water (1 mM) and used directly for the next step C-N cross coupling reaction without further purification.

Pd promoted C-N coupling between DNA-conjugated ArI and primary aromatic amines



Materials

Oligo: 1 mM in water

Amine: 1 M in DMA (For example, when aromatic amine hydrochloride was employed as the amine source, equal amount of base was added, see note 1).

CsOH: 5 M in water

Buchwald precatalyst: 6.67 mM in DMA (degas by sonicating for ca. 5 minutes on the "degas" setting).

Scavenger: Sodium diethyldithiocarbamic acid 100 mM in H_2O

Procedure

1) To the oligo (10 nmol) starting material solution (10 ul, 1 mM in water) (note 2), was added 1000 equiv. of aromatic amine (10 ul, 1 M in DMA), followed by 1000 equiv. of CsOH (2 ul, 5 M in water) and 2 equiv. of degassed precatalyst (3 ul, 6.67 mM in DMA). The mixture was vortexed and centrifuged.

2) Heat the reaction mixture at 100° C for 3h (note 3).

3) After the reaction, add 30 equiv. of scavenger sodium diethyldithiocarbamic acid (30eq is compared with Pd precatalyst added, 6 ul 100 mM in water), and heat the reaction mixture at 80° C for at least 30 minutes (note 4).

4) Check the LC/MS of reaction mixture (note 5)

5) Add 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C). The mixture was stored at a -80°C freezer for more than 30 minutes.

6) Centrifuge the sample for around 30 minutes at 4°C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.

Note

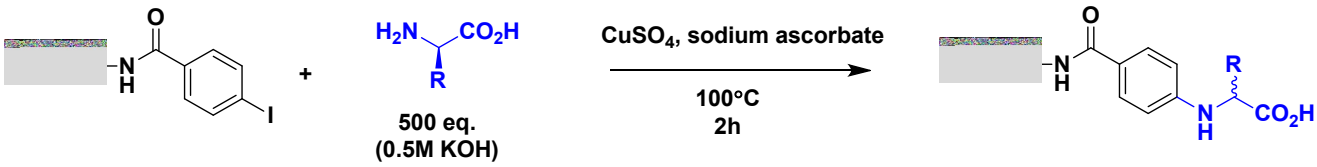
1) When amine salt was used, extra equal amount of base was added. For example, aromatic amine hydrochloride was employed as the amine source, instead of 1000 equiv. of CsOH, totally 2000 equiv. of CsOH was added.

2) For the library production, additional 5ul of water was added in order to reduce oligo decomposition.

3) Longer reaction time is detrimental for the oligo. For the library production, 2h heating time is sufficient.

4) Adding Pd scavenger followed by heating is necessary before the LC/MS, otherwise, the MS signal was messy.
5) In the MS spectrum, besides the major peaks such as the unreacted starting material and desired product, there were also small noise peaks observed. The exact reason why these noise peaks formed was not clear, likely due to the oligo decomposition during the reaction.

Cu(I) promoted C-N coupling between DNA-conjugated ArI and amino acids



Materials
Oligo: 1 mM in water
Amino aicd: 500 mM in KOH solution (directly dissolve the amino acid with 1:1 500 mM KOH solution, note 1)
$CuSO_4 \cdot 5H_2O$: 125 mM in H_2O
Sodium Ascorbate: 100 mM in H_2O
DMA
Scavenger: Sodium diethyldithiocarbamic acid 100 mM in H_2O

Procedure
1) To the oligo (10 ul 10 nmol, 1 mM in water) starting material solution, was added the same volume of DMA 10 ul (note 2), followed by 500 equiv. of amino acid (10 ul 500 mM in KOH solution). Then, 20 equiv. of $CuSO_4 \cdot 5H_2O$ (1.6 ul 125 mM in water) and 24 equiv. of sodium ascorbate (2.4 ul 100 mM in water) were added. The reaction mixture was vortexed and centrifuged.
2) Heat the reaction mixture at 100° C for 2h.
3) After the reaction, add the scavenger sodium diethyldithiocarbamic acid (2eq of the Cu amount, 4 ul 100 mM in water). Once scavenger was added, brown precipitate was observed (note 3). Vortex and centrifuge the sample, and collect the above supernatant.
4) For the recovered supernatant, add 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C). The mixture was stored at a -80°C freezer for more than 30 minutes.
5) Centrifuge the sample for around 30 minutes at 4°C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.
6) Check the LC\MS for the recovered dry pellet (note 4).

Notes

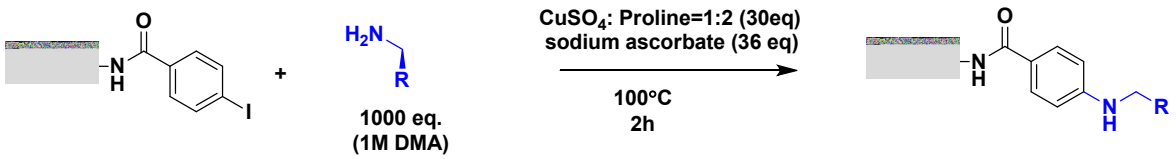
1) For specific amino acids, extra attention was needed. For example, for the Serine and Threonine, it's better to directly dissolve them in water; for the Tyrosine, it's better to add extra equivalent of base to dissolve the acid; for the Asparic acid and Glutamic acid, extra amount of base is also necessary.

2) DMA is beneficial for the side chain R group which has the aliphatic group like the phenylalanine and proline. For Lys, Arg, Gly which easily dissolved in water, DMA is not necessary.

3) Scavenger is necessary to remove the Cu after the reaction.

4) In the MS spectrum, besides the major peaks such as the unreacted starting material and desired product, there were also many small noise peaks observed. The exact reason why these noise peaks formed was not clear, likely due to the oligo decomposition during the reaction.

Cu(I) promoted C-N coupling between DNA-conjugated ArI and aliphatic amine



Materials

Oligo: 1 mM in water

Amine: 1 M in DMA (when amine salt such as benzylamine hydrochloride was carried out for reactions, equal amount of base was added, see note 1).

$CuSO_4 \cdot 5H_2O$: 125 mM in H_2O

Sodium Ascorbate: 100 mM in H_2O

Proline: 1 M in KOH solution (proline:KOH=1:1)

Scavenger: Sodium diethyldithiocarbamic acid 100 mM in H_2O

Procedure

1) Mix the $CuSO_4$: proline = 1 : 2 by volume together to prepare the 100 mM Cu/proline complex (deep blue color). For example, 100 ul of $CuSO_4 \cdot 5H_2O$ (125 mM in H_2O) was mixed with 25 ul of proline (1 M in KOH solution, proline : KOH = 1 : 1) to generate the 125 ul of 100 mM Cu\proline complex (note 2).

2) To the oligo starting material solution (10 ul, 10 nmol, 1 mM in water), was added 1000 equiv. of amine (10 ul 1 M in DMA), followed by 30 equiv. of 100 mM Cu\proline complex 3.0 ul and 36 equiv. of sodium ascorbate solution 3.6 ul. The reaction mixture was vortexed and centrifuged.

3) Heat the reaction mixture at 100° C for 2h.

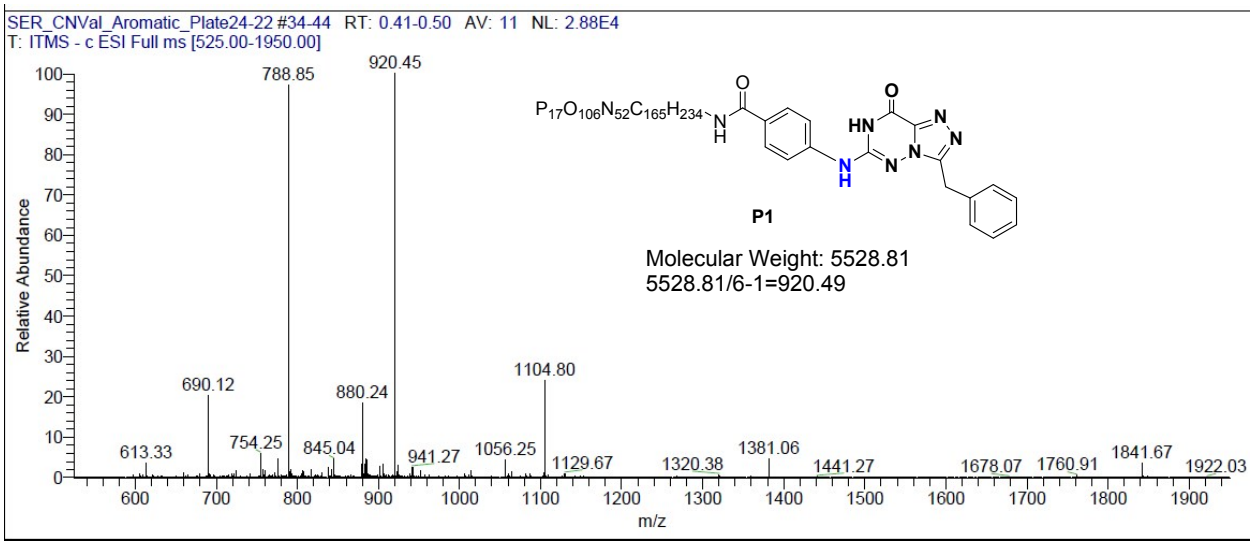
4) After the reaction, add the scavenger sodium diethyldithiocarbamic acid (2eq of the Cu amount, 6 ul 100 mM in water). Once scavenger was added, brown precipitate was observed (note 3). Vortex and centrifuge the sample, and collect the above supernatant.

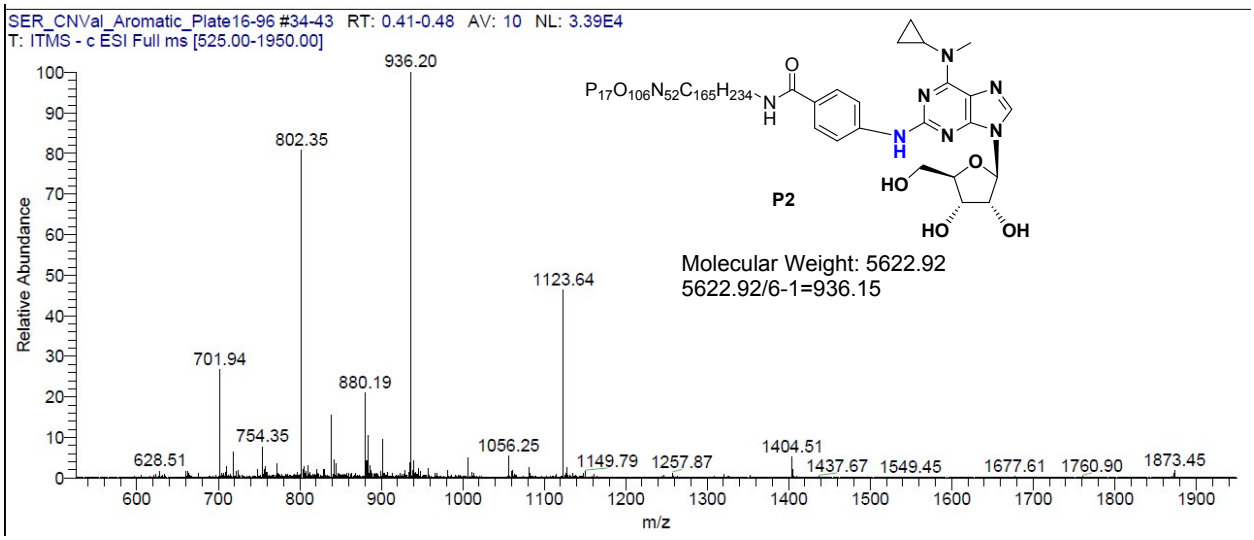
5) For the recovered supernatant, add 5 M NaCl solution (10% by volume) and cold ethanol (2.5 times by volume, ethanol stored at -20°C). The mixture was stored at a -80°C freezer for more than 30 minutes.
6) Centrifuge the sample for around 30 minutes at 4°C in a microcentrifuge at 10000 rpm. The above supernatant was removed and the pellet (precipitate) was cooled in liquid nitrogen and then placed on a lyophilizer. After lyophilization, the dry pellet was recovered.
7) Check the LC\MS for the recovered dry pellet (note 3, 4).

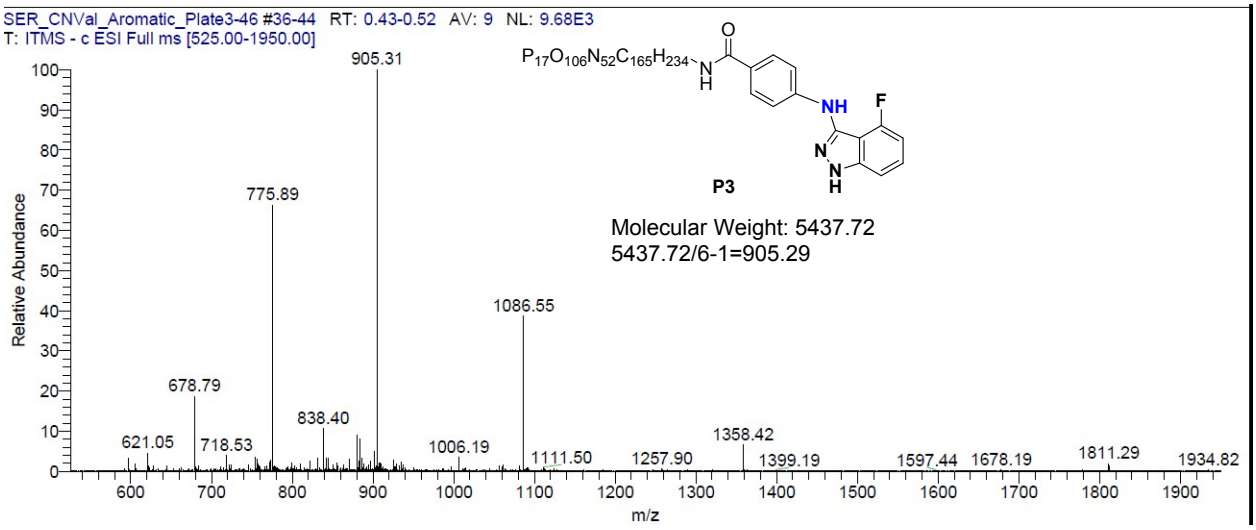
Notes

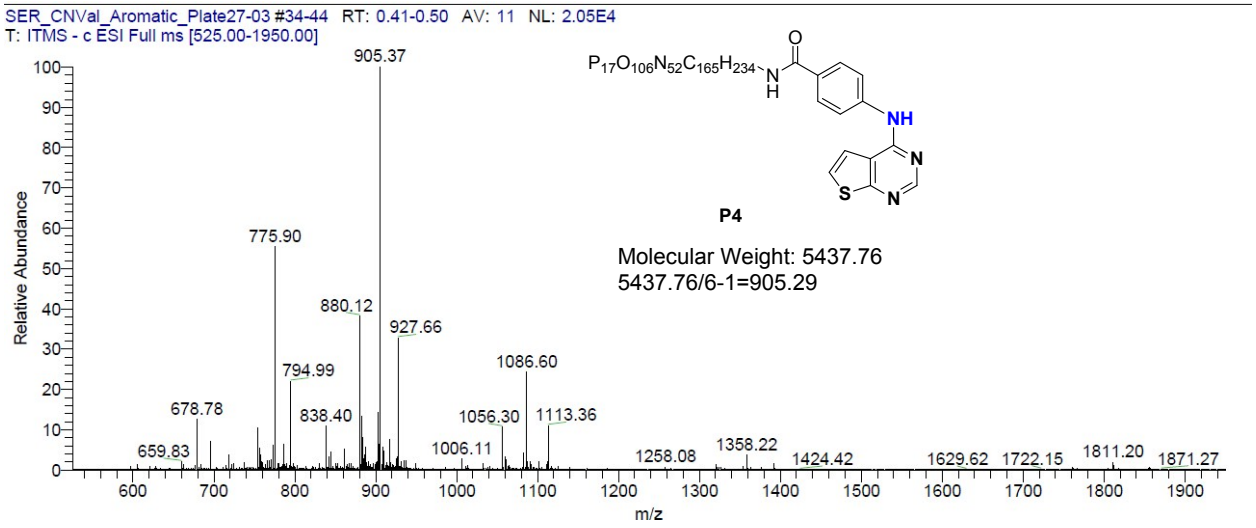
1) When amine salt was used, extra equal amount of base was added. For example, if benzylamine hydrochloride was employed, another 1000 equiv. of NaOH 2 ul (5 M in water) was added.
2) Proline is necessary for the reaction as the ligand. But because excessive amount of proline was used, the proline could also react with DNA-conjugated aryl iodide to form the side product.
3) In the MS spectrum, besides the major peaks such as the unreacted starting material and desired product, there were also many small noise peaks observed. The exact reason why these noise peaks formed was not clear, likely due to the oligo decomposition during the reaction. It's very obvious for aliphatic amines.
4) HPLC purification of recovered dry pellet was also carried out for 100 nmol of oligo starting materials; around 50 nmol oligo could be recovered after HPLC purification.

All MS examples





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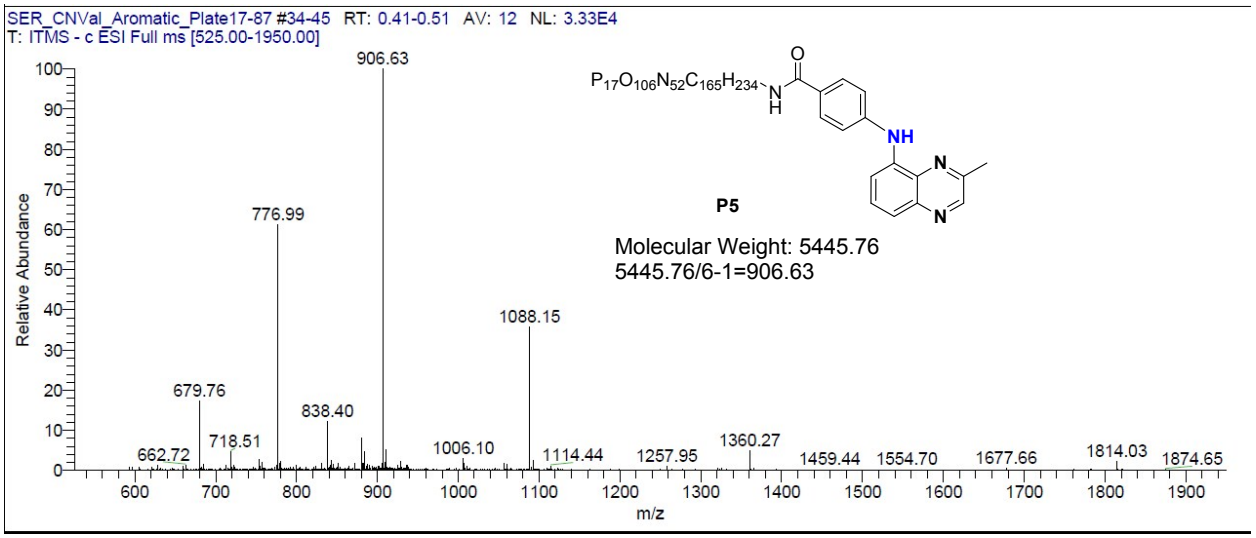
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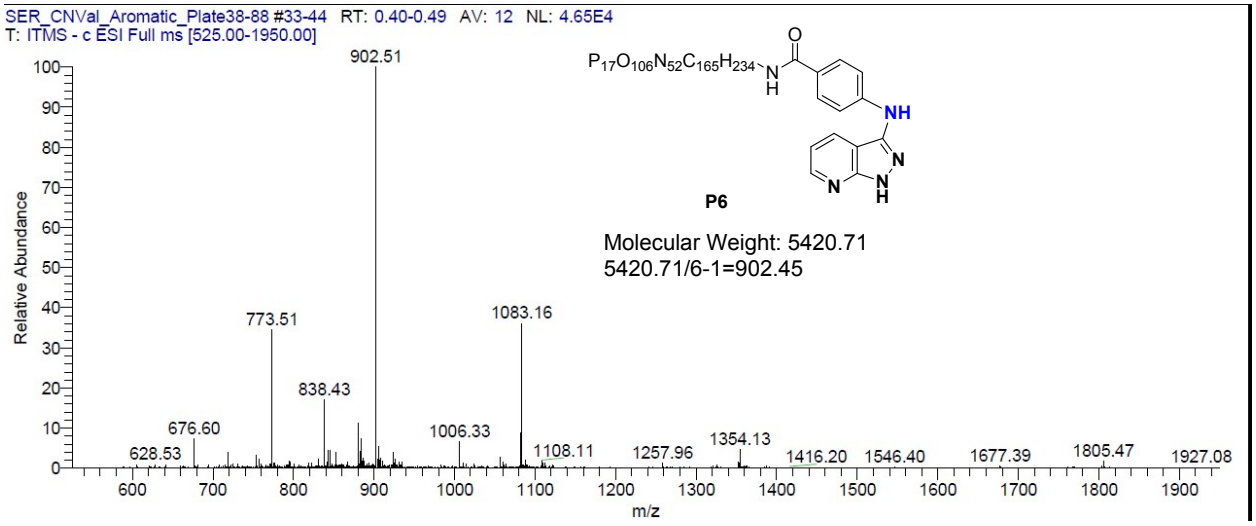
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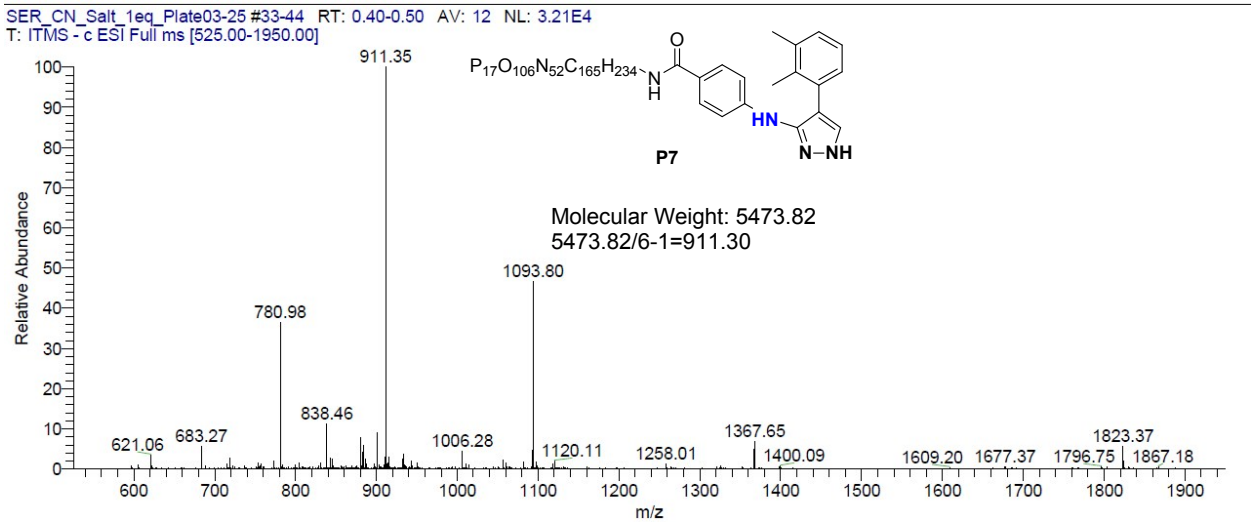
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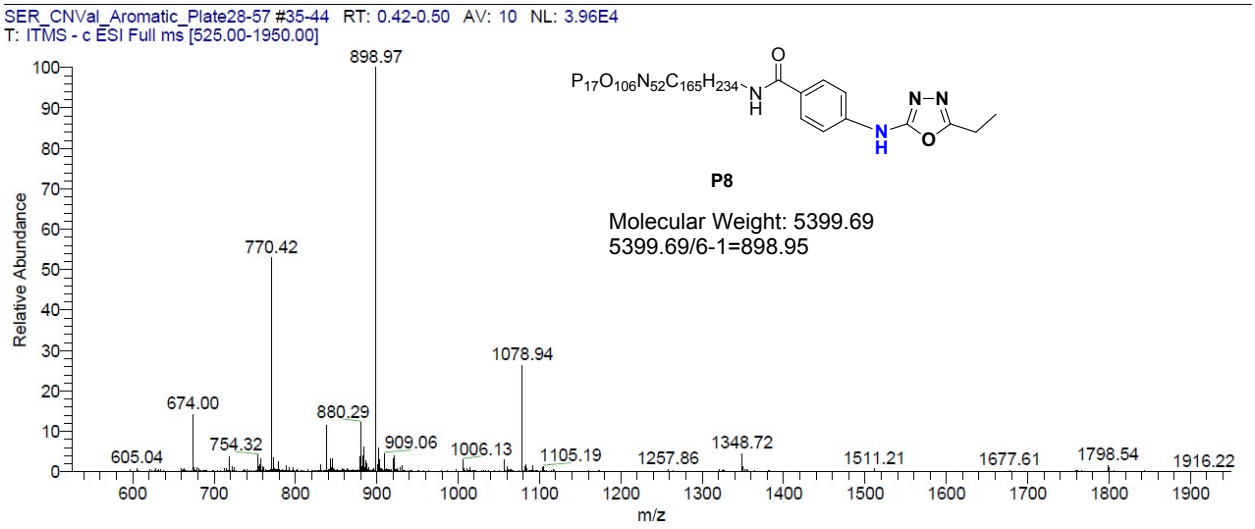
Relative Abundance
m/z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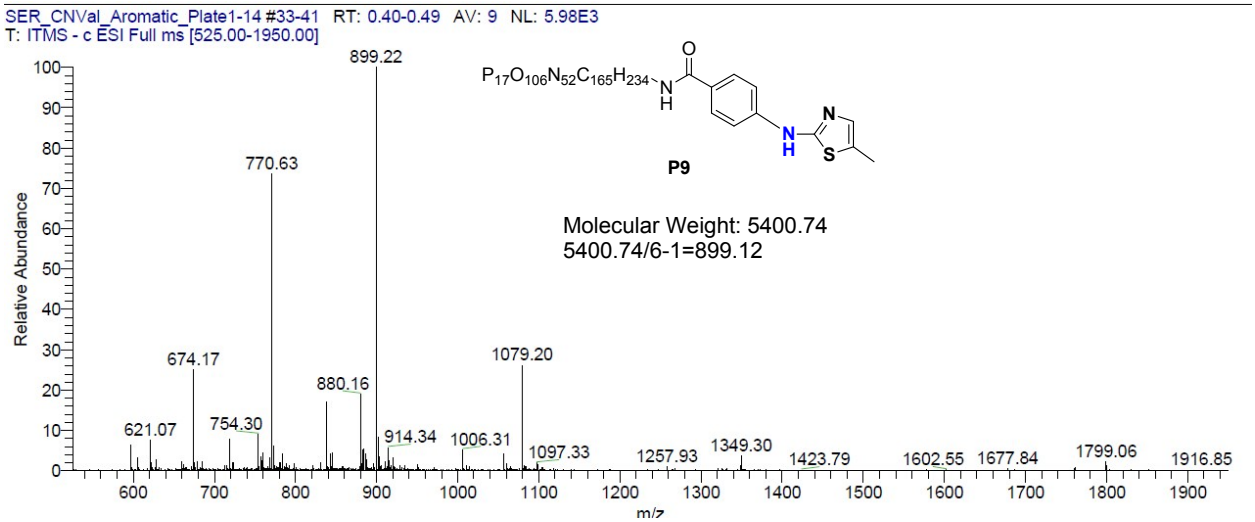
Relative Abundance
m/z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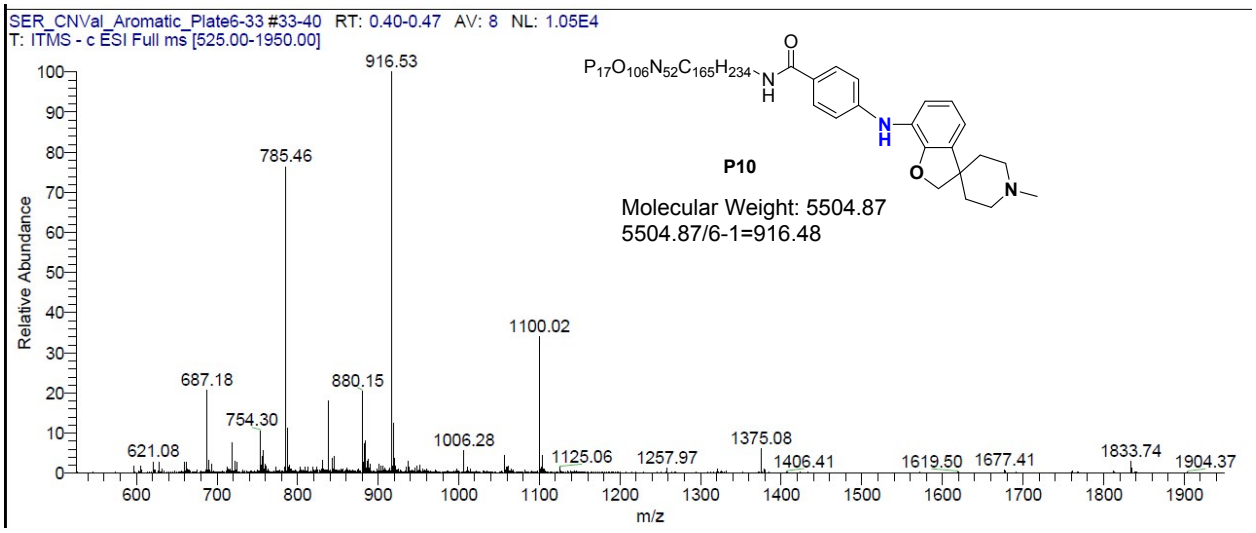
Relative Abundance
m/z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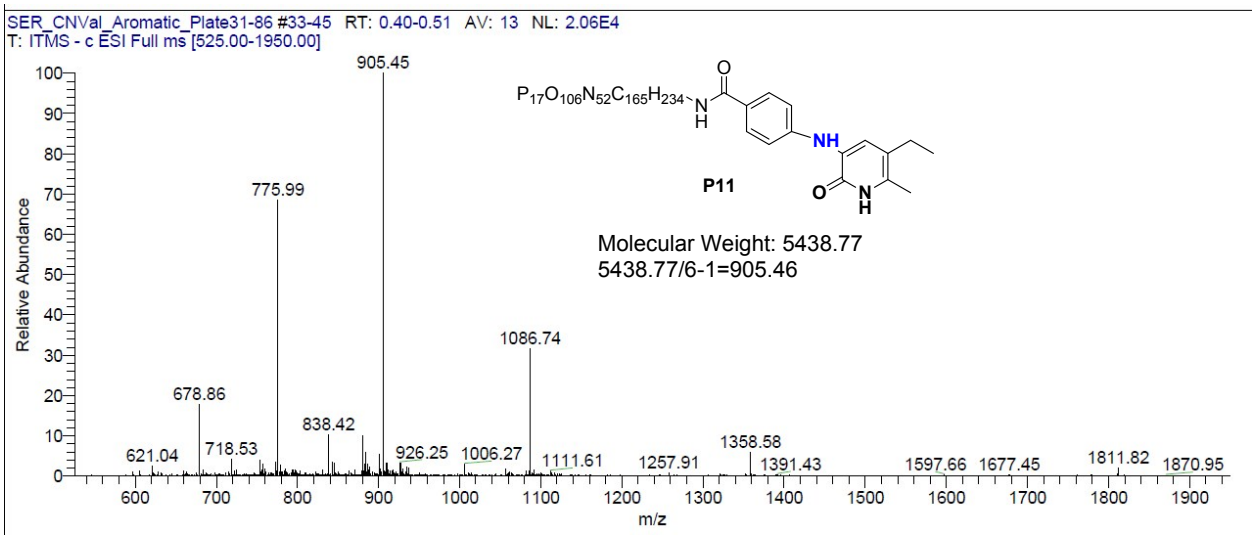
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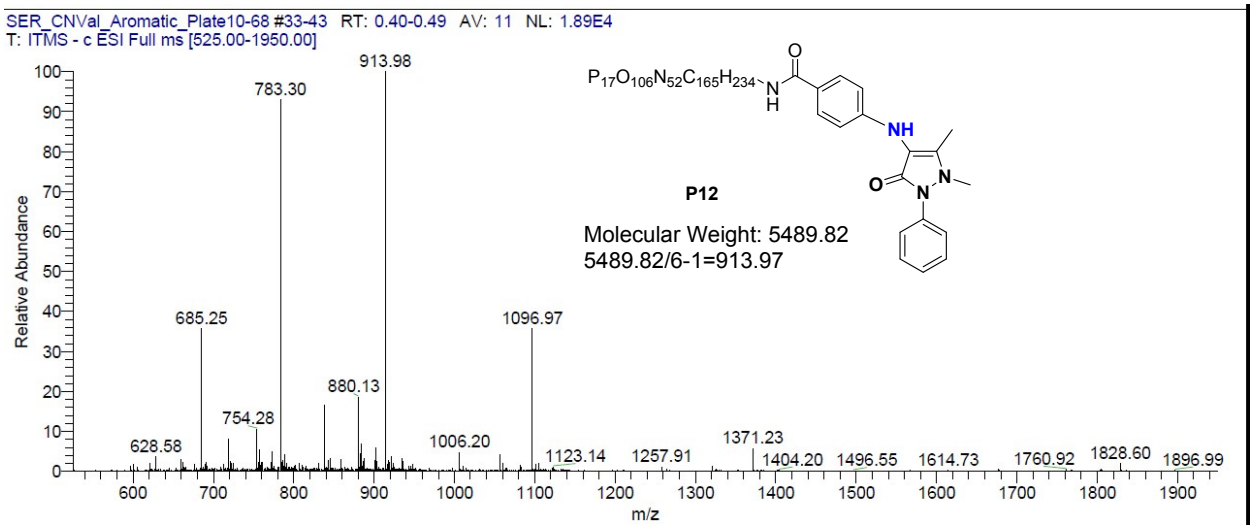
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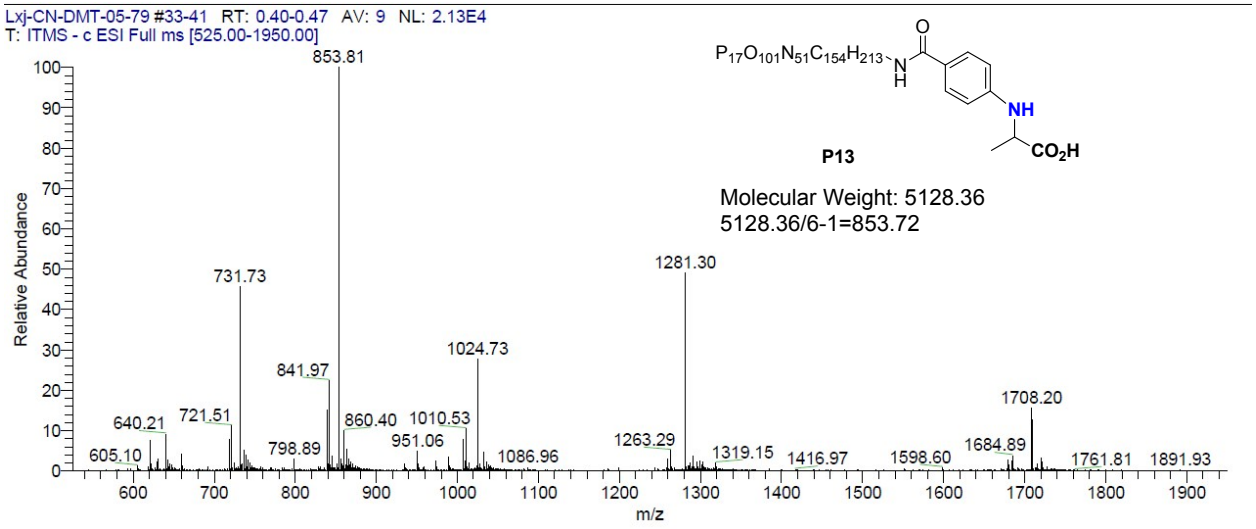
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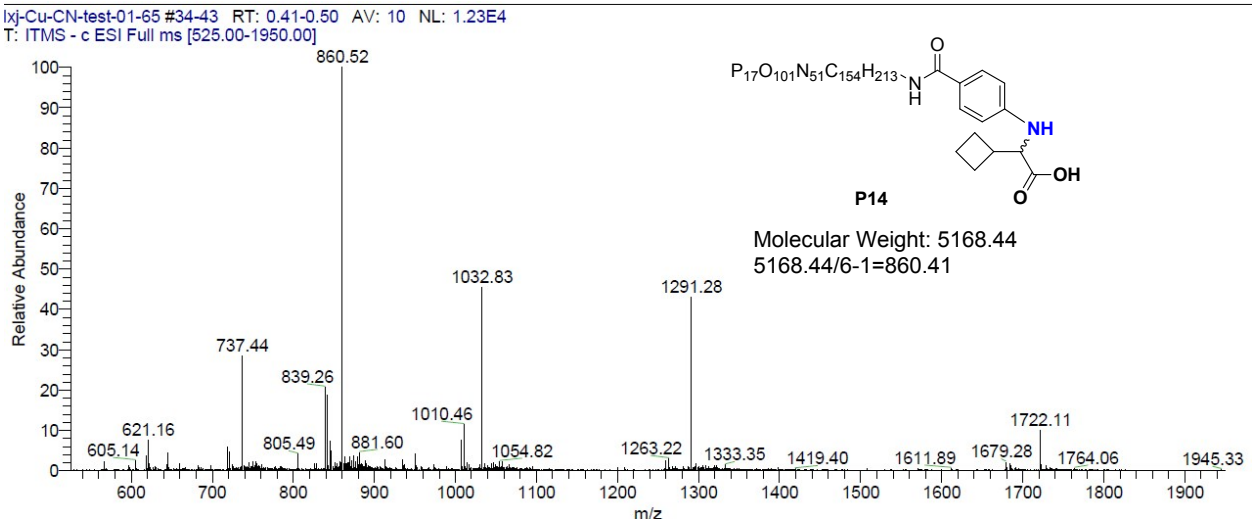
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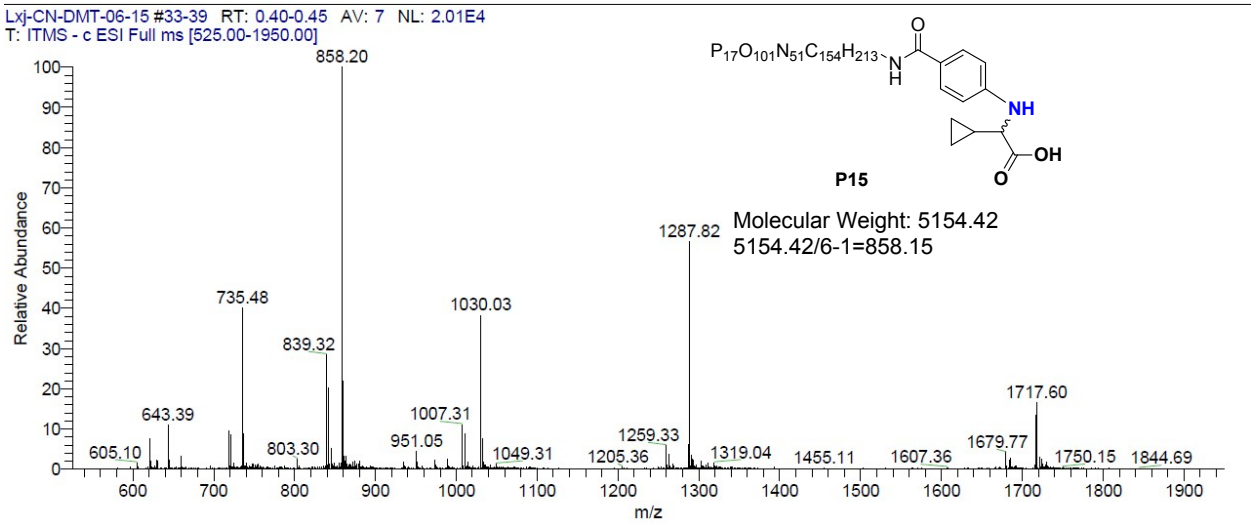
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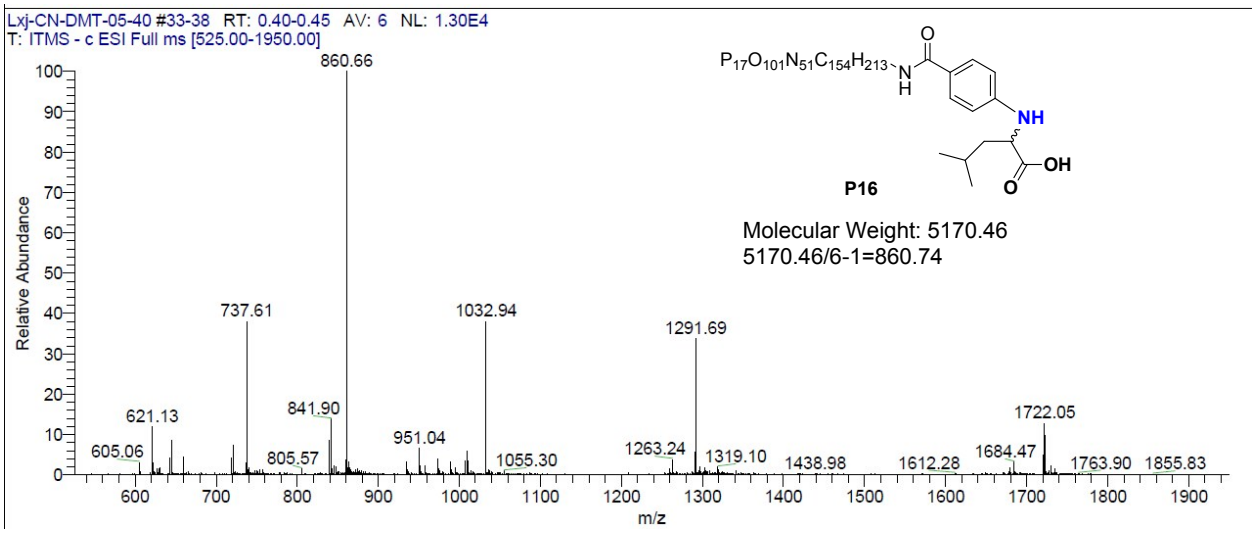
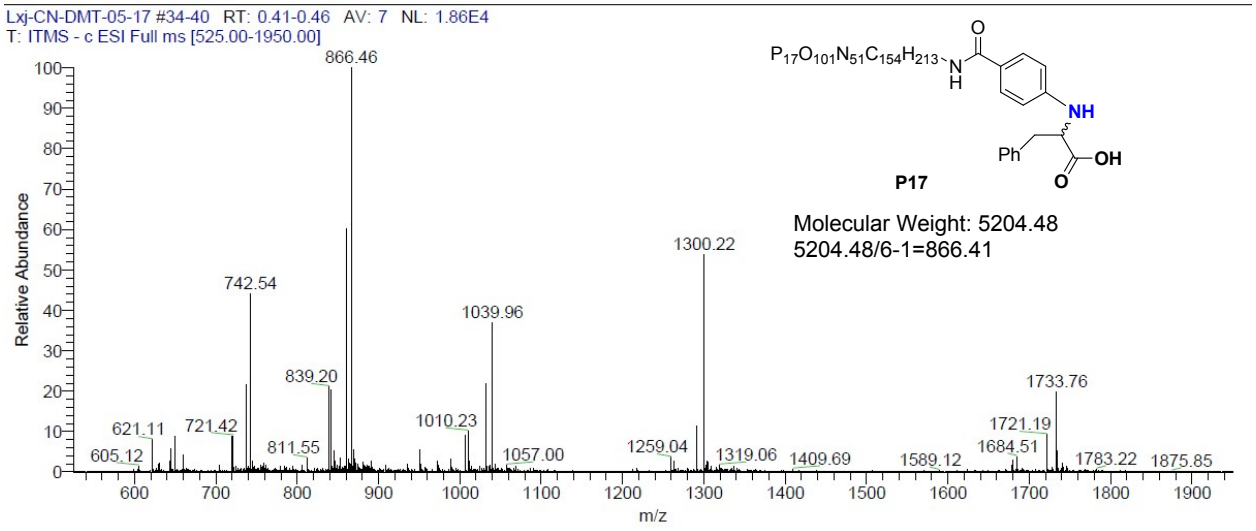
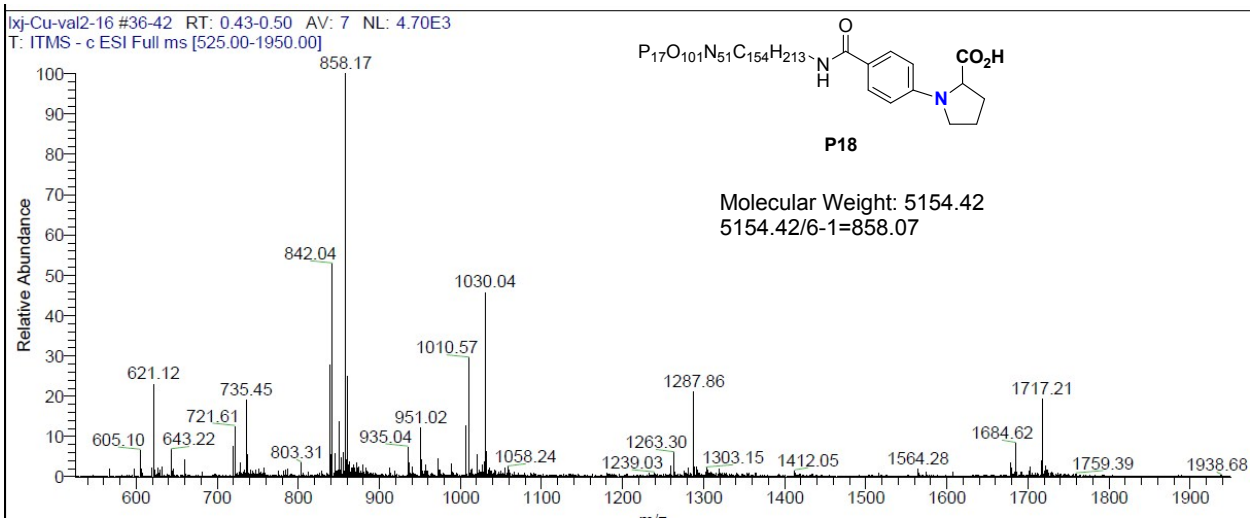
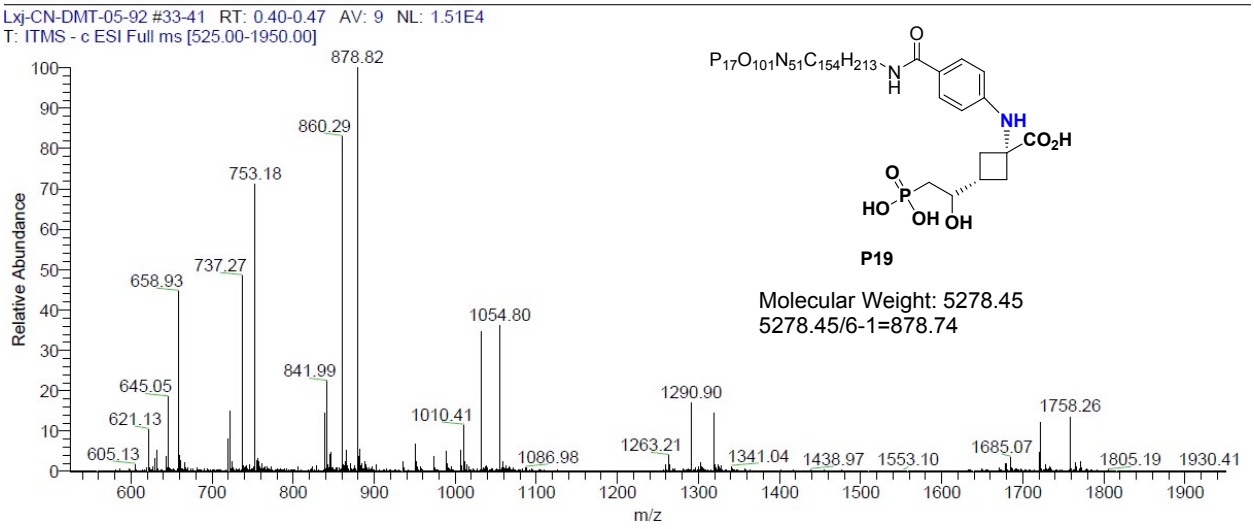
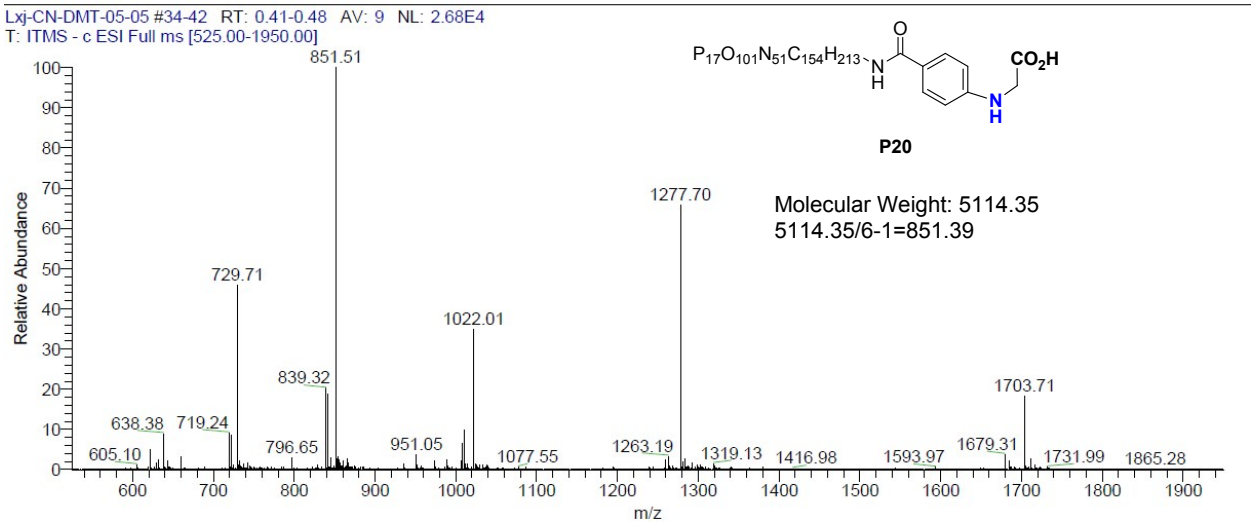
Molecular Weight: 5154.42
5154.42/6-1=858.15

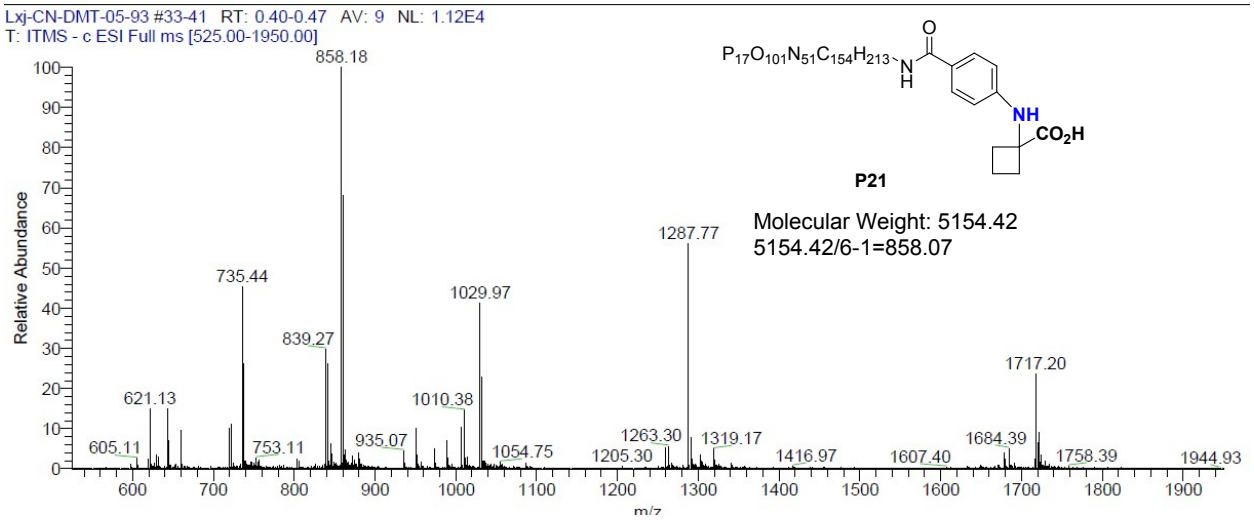

Lxj-CN-DMT-05-40 #33-38 RT: 0.40-0.45 AV: 6 NL: 1.30E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
860.66
737.61
1032.94
1291.69
621.13
841.90
951.04
605.06
805.57
1055.30
1263.24
1319.10
1438.98
1612.28
1684.47
1722.05
1763.90
1855.83
P16
Molecular Weight: 5170.46
5170.46/6-1=860.74

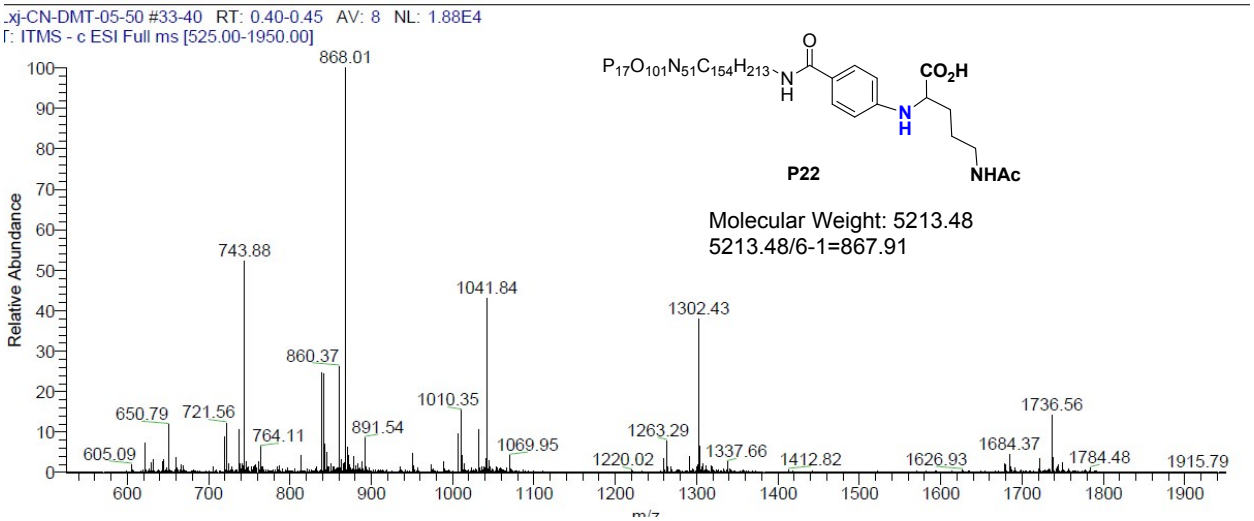

Lxj-CN-DMT-05-17 #34-40 RT: 0.41-0.46 AV: 7 NL: 1.86E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
866.46
742.54
1300.22
1039.96
839.20
621.11
721.42
1010.23
605.12
811.55
1057.00
1259.04
1319.06
1409.69
1589.12
1684.51
1733.76
1721.19
1783.22
1875.85
P17
Molecular Weight: 5204.48
5204.48/6-1=866.41

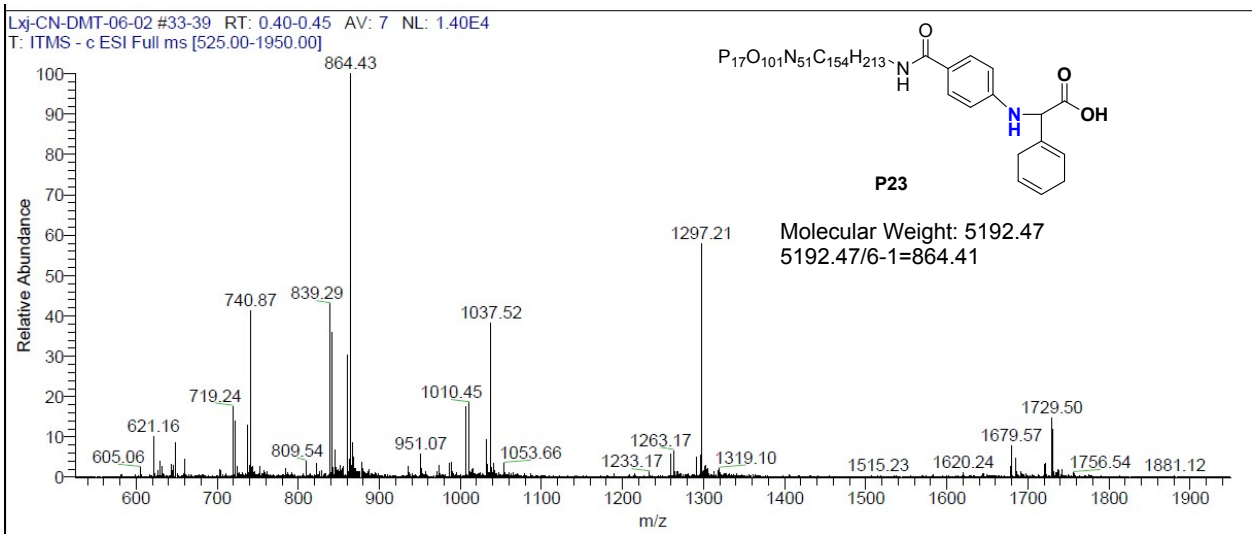

lxj-Cu-val2-16 #36-42 RT: 0.43-0.50 AV: 7 NL: 4.70E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
858.17
842.04
1030.04
1010.57
621.12
735.45
1287.86
721.61
951.02
605.10
643.22
935.04
803.31
1058.24
1263.30
1239.03
1303.15
1412.05
1564.28
1717.21
1684.62
1759.39
1938.68
P18
Molecular Weight: 5154.42
5154.42/6-1=858.07

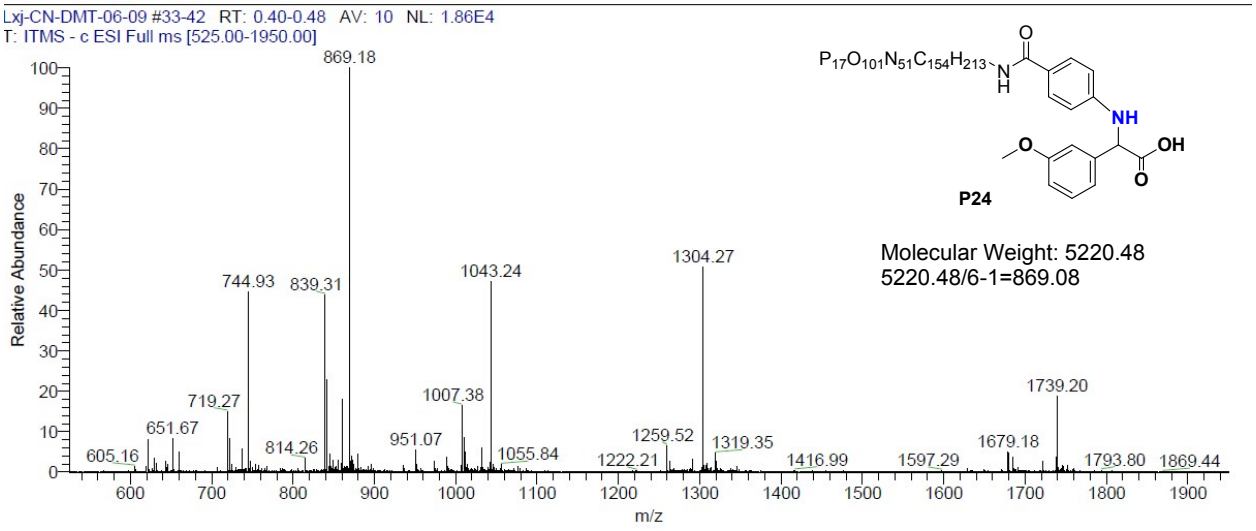

Lxj-CN-DMT-05-92 #33-41 RT: 0.40-0.47 AV: 9 NL: 1.51E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
878.82
860.29
753.18
737.27
658.93
1054.80
841.99
645.05
621.13
605.13
1010.41
1086.98
1290.90
1263.21
1341.04
1438.97
1553.10
1685.07
1758.26
1805.19
1930.41
$P_{17}O_{101}N_{51}C_{154}H_{213}$
P19
Molecular Weight: 5278.45
5278.45/6-1=878.74

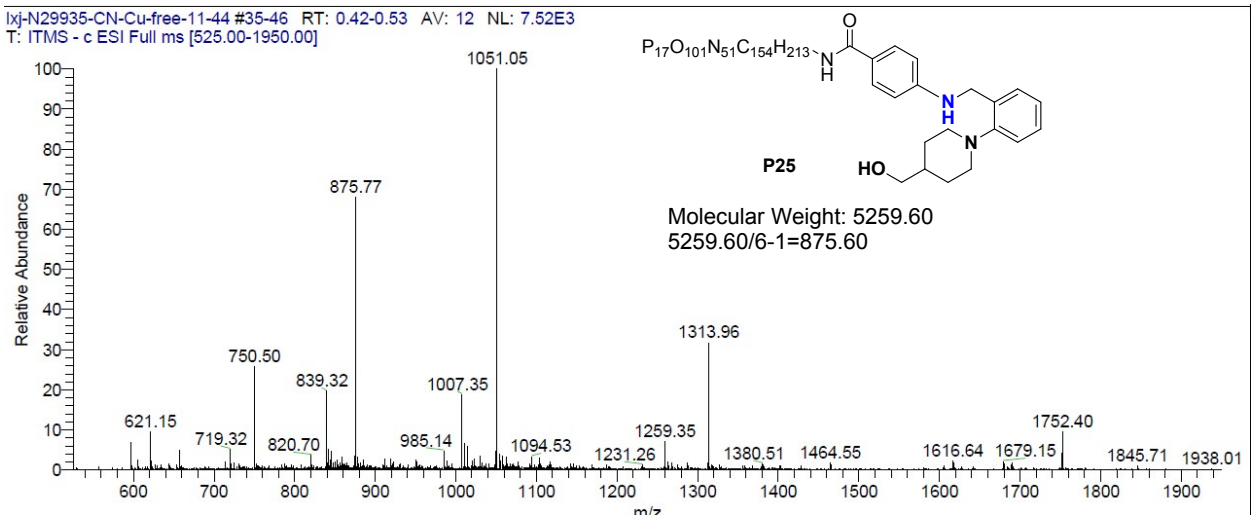

Lxj-CN-DMT-05-05 #34-42 RT: 0.41-0.48 AV: 9 NL: 2.68E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
851.51
1277.70
729.71
1022.01
839.32
638.38
719.24
605.10
796.65
951.05
1077.55
1263.19
1319.13
1416.98
1593.97
1679.31
1703.71
1731.99
1865.28
$P_{17}O_{101}N_{51}C_{154}H_{213}$
P20
Molecular Weight: 5114.35
5114.35/6-1=851.39

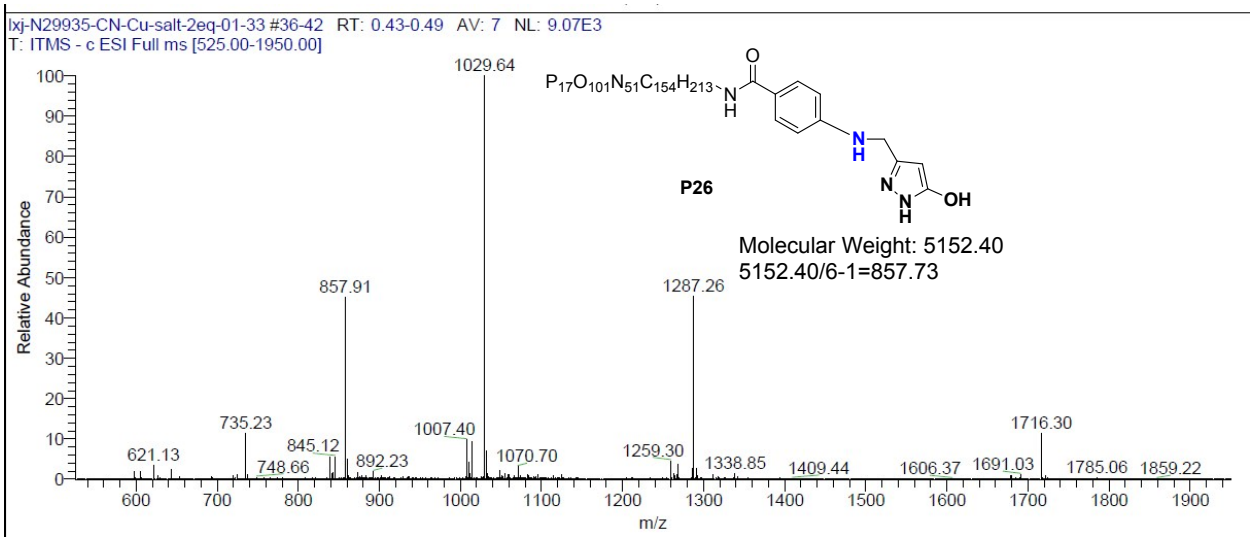

Lxj-CN-DMT-05-93 #33-41 RT: 0.40-0.47 AV: 9 NL: 1.12E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
858.18
1287.77
735.44
1029.97
839.27
621.13
1010.38
605.11
753.11
935.07
1054.75
1205.30
1263.30
1319.17
1416.97
1607.40
1684.39
1717.20
1758.39
1944.93
$P_{17}O_{101}N_{51}C_{154}H_{213}$
P21
Molecular Weight: 5154.42
5154.42/6-1=858.07

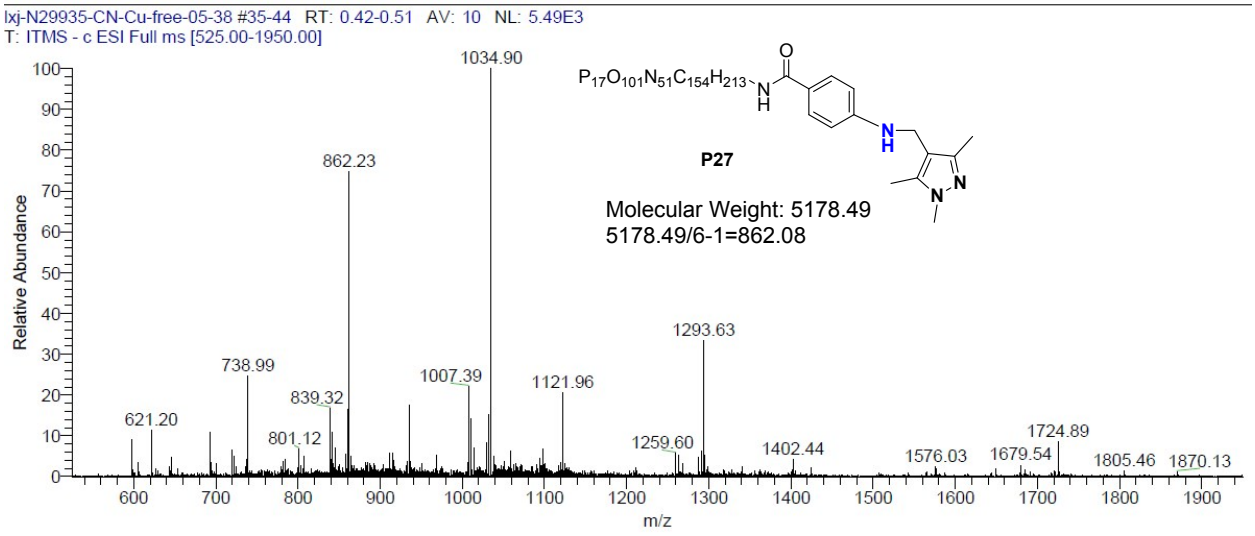

xj-CN-DMT-05-50 #33-40 RT: 0.40-0.45 AV: 8 NL: 1.88E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
868.01
743.88
1041.84
1302.43
860.37
1010.35
650.79
721.56
891.54
764.11
1069.95
1263.29
1736.56
605.09
1220.02
1337.66
1412.82
1626.93
1684.37
1784.48
1915.79
m/z
P22
NHAc
Molecular Weight: 5213.48
5213.48/6-1=867.91

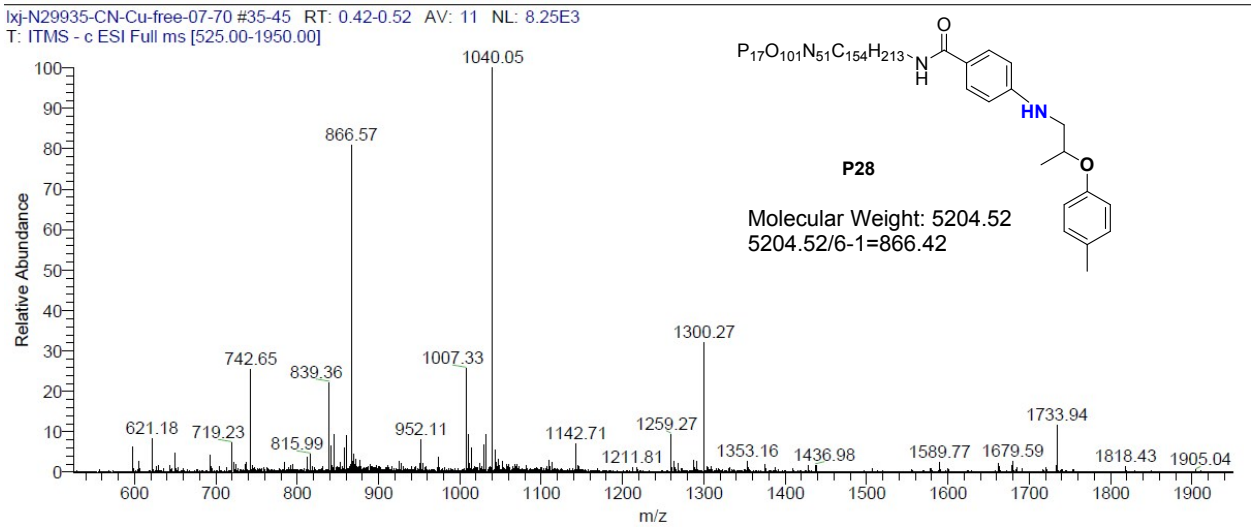

Lxj-CN-DMT-06-02 #33-39 RT: 0.40-0.45 AV: 7 NL: 1.40E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
864.43
1297.21
740.87
839.29
1037.52
719.24
1010.45
621.16
809.54
951.07
1053.66
1263.17
1729.50
605.06
1233.17
1319.10
1515.23
1620.24
1679.57
1756.54
1881.12
m/z
P23
Molecular Weight: 5192.47
5192.47/6-1=864.41

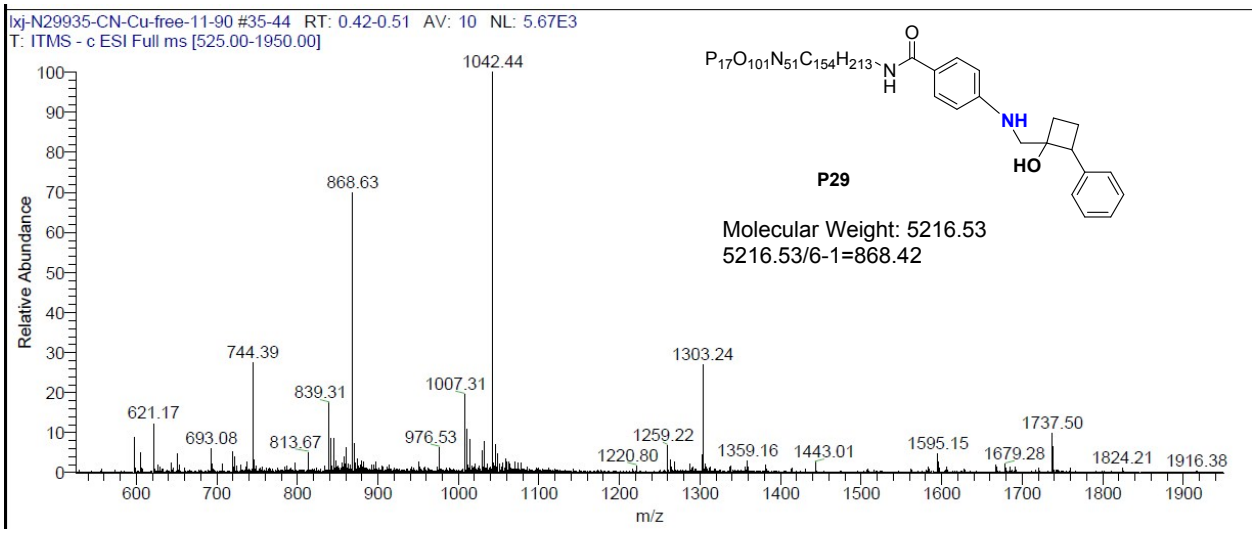

Lxj-CN-DMT-06-09 #33-42 RT: 0.40-0.48 AV: 10 NL: 1.86E4
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
869.18
1304.27
744.93
839.31
1043.24
719.27
1007.38
651.67
814.26
951.07
1055.84
1259.52
1319.35
1739.20
605.16
1222.21
1416.99
1597.29
1679.18
1793.80
1869.44
m/z
P24
Molecular Weight: 5220.48
5220.48/6-1=869.08

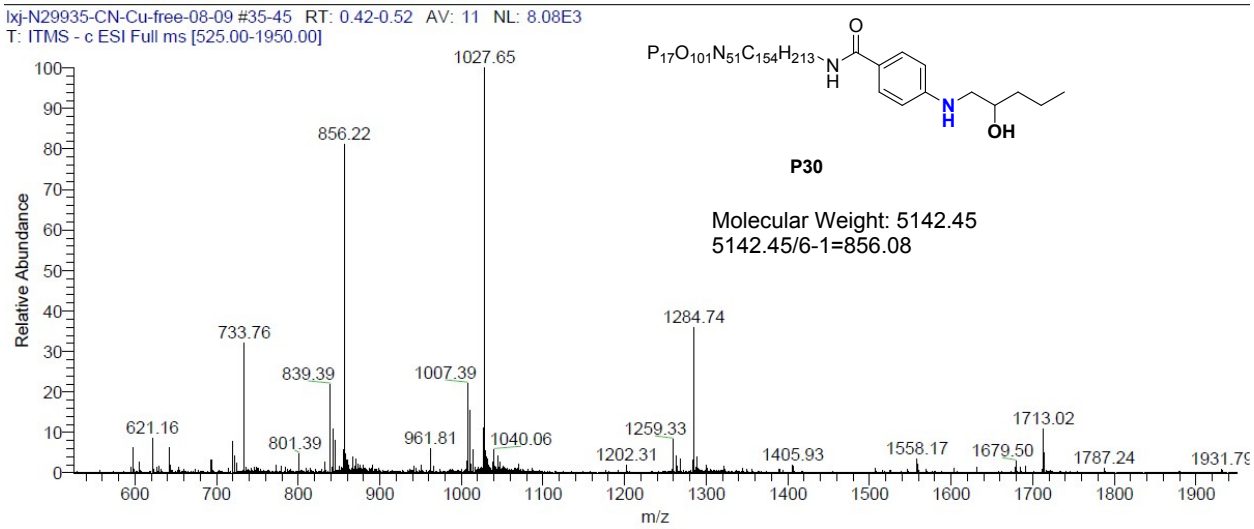

lxj-N29935-CN-Cu-free-11-44 #35-46 RT: 0.42-0.53 AV: 12 NL: 7.52E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1051.05
875.77
1313.96
750.50
839.32
1007.35
621.15
719.32
820.70
985.14
1094.53
1231.26
1259.35
1380.51
1464.55
1616.64
1679.15
1752.40
1845.71
1938.01
P17O101N51C154H213
P25
HO
Molecular Weight: 5259.60
5259.60/6-1=875.60

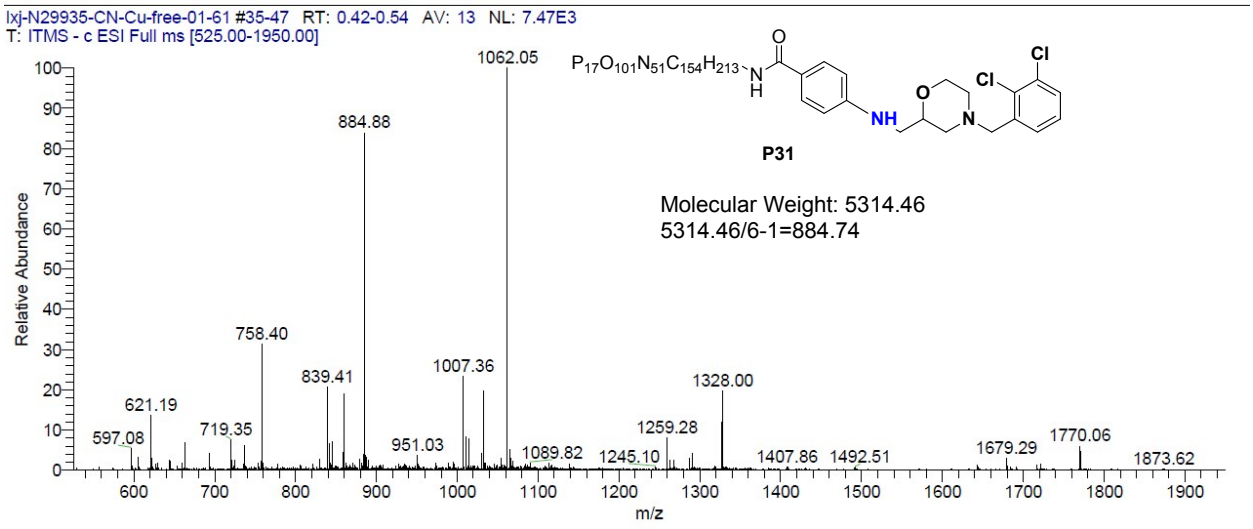

lxj-N29935-CN-Cu-salt-2eq-01-33 #36-42 RT: 0.43-0.49 AV: 7 NL: 9.07E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1029.64
857.91
1287.26
735.23
845.12
1007.40
621.13
748.66
892.23
1070.70
1259.30
1338.85
1409.44
1606.37
1691.03
1716.30
1785.06
1859.22
P17O101N51C154H213
P26
OH
Molecular Weight: 5152.40
5152.40/6-1=857.73

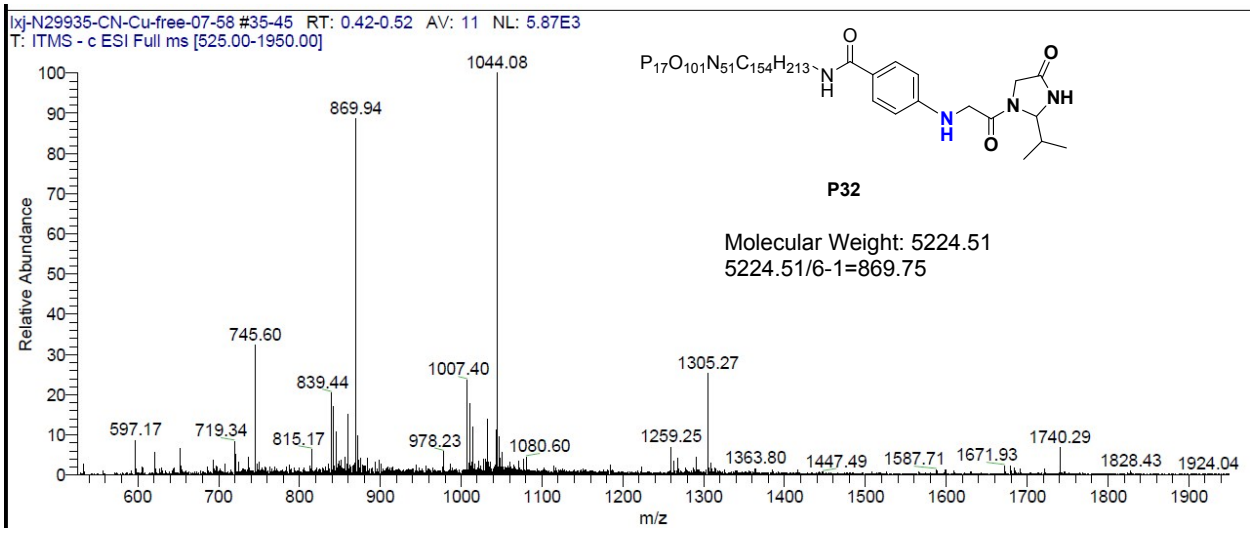

lxj-N29935-CN-Cu-free-05-38 #35-44 RT: 0.42-0.51 AV: 10 NL: 5.49E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1034.90
862.23
1293.63
738.99
1007.39
1121.96
839.32
621.20
801.12
1259.60
1402.44
1576.03
1679.54
1724.89
1805.46
1870.13
P17O101N51C154H213
P27
Molecular Weight: 5178.49
5178.49/6-1=862.08

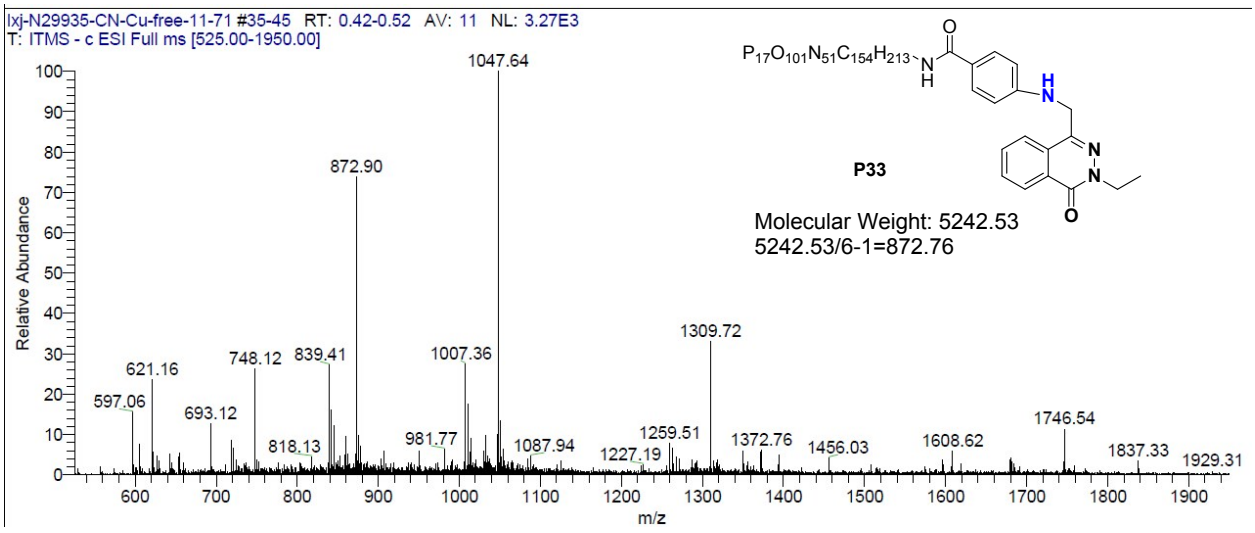

lxj-N29935-CN-Cu-free-07-70 #35-45 RT: 0.42-0.52 AV: 11 NL: 8.25E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1040.05
866.57
742.65
839.36
1007.33
1300.27
621.18
719.23
815.99
952.11
1142.71
1259.27
1211.81
1353.16
1436.98
1589.77
1679.59
1733.94
1818.43
1905.04
$P_{17}O_{101}N_{51}C_{154}H_{213}$
HN
O
P28
Molecular Weight: 5204.52
5204.52/6-1=866.42

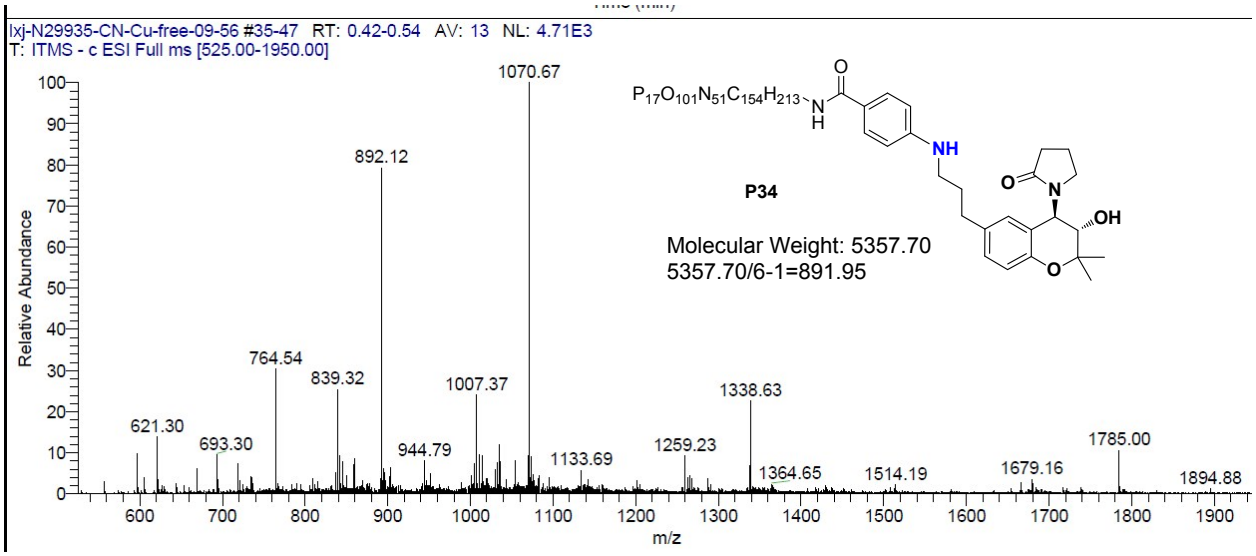

lxj-N29935-CN-Cu-free-11-90 #35-44 RT: 0.42-0.51 AV: 10 NL: 5.67E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1042.44
868.63
744.39
839.31
1007.31
1303.24
621.17
693.08
813.67
976.53
1220.80
1259.22
1359.16
1443.01
1595.15
1679.28
1737.50
1824.21
1916.38
$P_{17}O_{101}N_{51}C_{154}H_{213}$
NH
HO
P29
Molecular Weight: 5216.53
5216.53/6-1=868.42

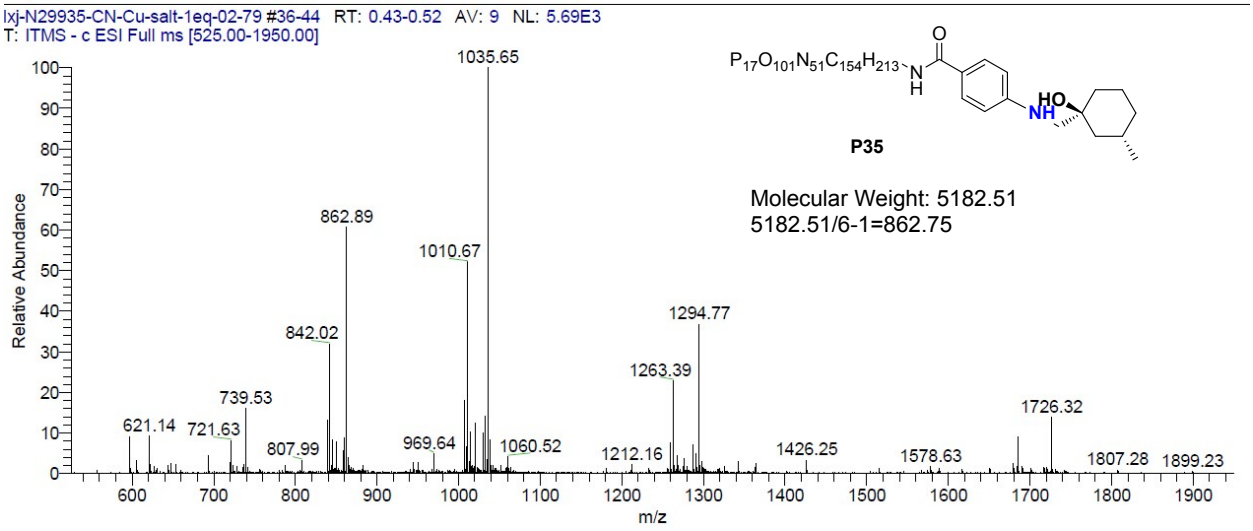

lxj-N29935-CN-Cu-free-08-09 #35-45 RT: 0.42-0.52 AV: 11 NL: 8.08E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1027.65
856.22
733.76
839.39
1007.39
1284.74
621.16
801.39
961.81
1040.06
1202.31
1259.33
1405.93
1558.17
1679.50
1713.02
1787.24
1931.79
$P_{17}O_{101}N_{51}C_{154}H_{213}$
N
H
OH
P30
Molecular Weight: 5142.45
5142.45/6-1=856.08

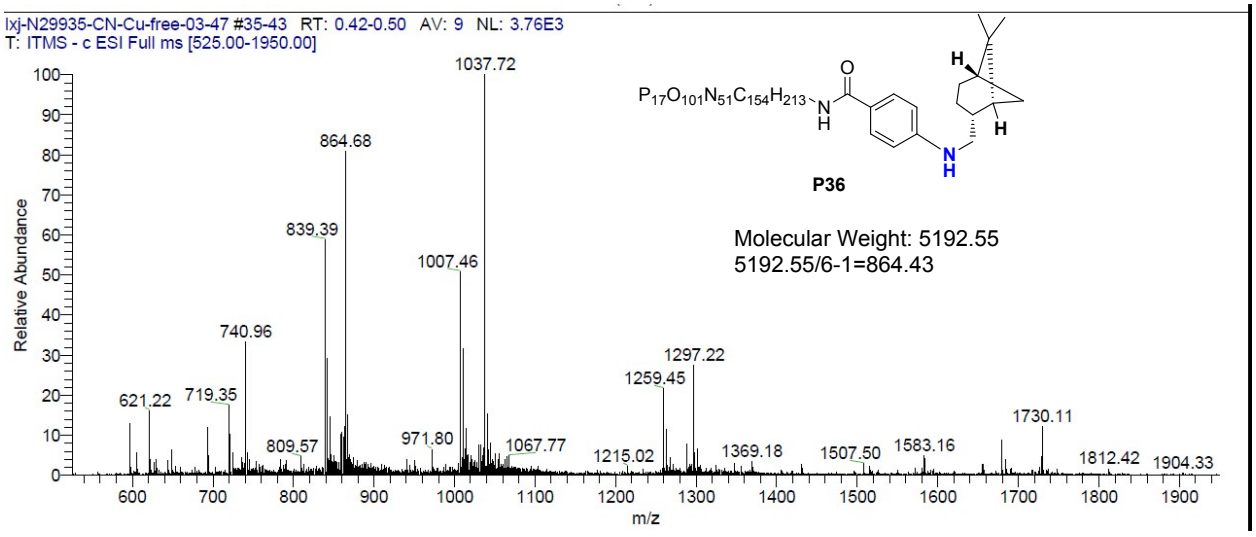

lxj-N29935-CN-Cu-free-01-61 #35-47 RT: 0.42-0.54 AV: 13 NL: 7.47E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1062.05
884.88
758.40
839.41
1007.36
1328.00
621.19
719.35
597.08
951.03
1089.82
1245.10
1259.28
1407.86
1492.51
1679.29
1770.06
1873.62
P17O101N51C154H213
P31
Molecular Weight: 5314.46
5314.46/6-1=884.74


lxj-N29935-CN-Cu-free-07-58 #35-45 RT: 0.42-0.52 AV: 11 NL: 5.87E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1044.08
869.94
745.60
839.44
1007.40
1305.27
597.17
719.34
815.17
978.23
1080.60
1259.25
1363.80
1447.49
1587.71
1671.93
1740.29
1828.43
1924.04
P17O101N51C154H213
P32
Molecular Weight: 5224.51
5224.51/6-1=869.75


lxj-N29935-CN-Cu-free-11-71 #35-45 RT: 0.42-0.52 AV: 11 NL: 3.27E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1047.64
872.90
1309.72
621.16
748.12
839.41
1007.36
597.06
693.12
818.13
981.77
1087.94
1227.19
1259.51
1372.76
1456.03
1608.62
1746.54
1837.33
1929.31
P17O101N51C154H213
P33
Molecular Weight: 5242.53
5242.53/6-1=872.76


lxj-N29935-CN-Cu-free-09-56 #35-47 RT: 0.42-0.54 AV: 13 NL: 4.71E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1070.67
892.12
764.54
839.32
1007.37
621.30
693.30
944.79
1133.69
1259.23
1338.63
1364.65
1514.19
1679.16
1785.00
1894.88
P34
Molecular Weight: 5357.70
5357.70/6-1=891.95


lxj-N29935-CN-Cu-salt-1eq-02-79 #36-44 RT: 0.43-0.52 AV: 9 NL: 5.69E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1035.65
862.89
1010.67
842.02
1294.77
1263.39
739.53
621.14
721.63
807.99
969.64
1060.52
1212.16
1426.25
1578.63
1726.32
1807.28
1899.23
P35
Molecular Weight: 5182.51
5182.51/6-1=862.75


lxj-N29935-CN-Cu-free-03-47 #35-43 RT: 0.42-0.50 AV: 9 NL: 3.76E3
T: ITMS - c ESI Full ms [525.00-1950.00]
Relative Abundance
m/z
1037.72
864.68
839.39
1007.46
740.96
621.22
719.35
809.57
971.80
1067.77
1215.02
1259.45
1297.22
1369.18
1507.50
1583.16
1730.11
1812.42
1904.33
P36
Molecular Weight: 5192.55
5192.55/6-1=864.43