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J. Serb. Chem. Soc. 85 (6) S224–S278 (2020) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

μ-Opioid/D_2 dopamine receptor pharmacophore containing ligands: Synthesis and pharmacological evaluation

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ISOLATED YIELDS AND SPECTROSCOPIC DATA OF THE SYNTHESIZED COMPOUNDS

*3-Bromo-1-(4-phenylpiperazin-1-yl)propan-1-one (**3a**).* Yield: 0.99 g (96%); pale yellow oil; IR (ATR, cm^{-1}): 3486, 2914, 2823, 1646, 1598, 1498, 1441, 1231, 1025, 761, 695; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.33 – 7.24 (2H, *m*), 6.99 – 6.89 (3H, *m*), 3.82 – 3.76 (2H, *m*), 3.71 – 3.64 (2H, *m*), 3.65 – – 3.59 (2H, *m*), 3.22 – 3.16 (4H, *m*), 2.96 (2H, *t*, J = 7.1 Hz); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 168.6, 150.9, 129.3, 120.7, 116.8, 49.8, 49.5, 45.5, 41.8, 36.4, 27.3.

*3-Bromo-1-(4-(2-methoxyphenyl)piperazin-1-yl) propan-1-one (**3b**).* Yield: 1.09 g (95.8%); pale yellow oil; IR (ATR, cm^{-1}): 3485, 2915, 2824, 1644, 1591, 1468, 1442, 1233, 1027, 762, 696; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.08 – – 7.00 (1H, *m*), 6.96 – 6.85 (3H, *m*), 3.88 (3H, *s*), 3.82 (2H, *t*, J = 5.0 Hz), 3.68 (2H, *t*, J = 7.1 Hz, partially overlapped), 3.64 (2H, *t*, J = 5.0 Hz, partially overlapped), 3.05 (4H, *dt*, J_1 = 17.5, J_2 = 5.0 Hz), 2.96 (2H, *t*, J = 7.1 Hz); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 170.0, 153.8, 142.1, 125.2, 122.6, 120.0, 112.9, 57.0, 52.5, 52.1, 47.3, 43.5, 37.9, 28.9.

*3-Bromo-1-(4-(2,3-dichlorophenyl)piperazin-1-yl) propan-1-one (**3c**).* Yield: 1.20 g (94,2%); pale yellow oil; IR (ATR, cm^{-1}): 3487, 2917, 2825, 1647, 1578, 1446, 1236, 958, 784; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.21 – 7.14 (2H, *m*), 6.90 (1H, *d*, J = 1.8 Hz), 3.80 (2H, *t*, J = 5.0 Hz), 3.66 (2H, *t*, J = 7.1 Hz), 3.63 (2H, *t*, J = 5.0 Hz), 3.04 – 2.97 (4H, *m*), 2.95 (2H, *t*, J = 7.1 Hz,); ^{13}C-NMR (126

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MHz, $CDCl_3$, δ / ppm): 168.8, 150.7, 150.7, 134.4, 128.3, 127.8, 127.6, 119.0, 51.3, 45.9, 36.5, 27.5.

4-Bromo-1-(4-(2-methoxyphenyl)piperazin-1-yl)butan-1-one ***(3d)***. Yield: 1.14 g (96,0 %); pale yellow oil; IR (ATR, cm^{-1}): 3394, 2920, 2495, 1637, 1592, 1500, 1454, 1243, 1028, 746; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.03 – 6.92 (1H, *m*), 6.89 – 6.76 (3H, *m*), 3.80 (3H, *s*), 3.76 – 3.66 (2H, *m*), 3.65 – 3.55 (4H, *m*), 2.96 (4H, *dt*, J_1 = 18.4, J_2 = 5.1 Hz), 2.48 (*2H*, *t*, J = 7.1 Hz), 2.13 – 2.03 (2H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 170.2, 152.3, 140.7, 123.6, 121.1, 118.5, 111.4, 55.5, 51.0, 50.6, 45.8, 44.9, 41.9, 29.8, 28.0.

5-Bromo-1-(4-phenylpiperazin-1-yl)pentan-1-one ***(3e)***. Yield: 1.11 g (97.9 %); pale yellow oil; IR (ATR, cm^{-1}): 3454, 2956, 1639, 1578, 1446, 1234, 1035, 775; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): δ = 7.33 – 7.27 (2H, *m*), 6.98 – 6.89 (3H, *m*), 3.82 – 3.77 (2H, *m*), 3.69 – 3.62 (2H, *m*), 3.59 (2H, *t*, J = 6.2 Hz), 3.23 – – 3.13 (4H, *m*), 2.45 – 2.39 (2H, *m*), 1.91 – 1.80 (4H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): δ = 172.4, 152.5, 130.8, 122.1, 118.2, 51.3, 51.0, 47.1, 46.3, 43.1, 33.9, 33.7, 24.1.

5-Bromo-1-(4-(2-methoxyphenyl)piperazin-1-yl) pentan-1-one ***(3f)***. Yield: 1.19 g (96.3 %); pale yellow oil: IR (ATR, cm^{-1}): 3453, 2954, 1630, 1577, 1448, 1236, 1036, 782; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.06 – 7.00 (1H, *m*), 6.94 – 6.84 (3H, *m*), 3.86 (3H, *s*), 3.80 (2H, *s*), 3.65 (2H, *s*), 3.55 (2H, *t*, J = 6.3 Hz), 3.04 (4H, *d*, J = 17.3 Hz), 2.42 – 2.35 (2H, *m*), 1.87 – 1.76 (4H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 172.5, 153.8, 125.5, 122.7, 120.3, 113.0, 57.0, 52.6, 52.2, 47.3, 46.3, 43.2, 33.8, 33.7, 24.1.

5-Bromo-1-(4-(2,3-dichlorophenyl)piperazin-1-yl) pentan-1-one ***(3g)***. Yield: 1.31 g (94.9 %); pale yellow oil; IR (ATR, cm^{-1}): 3451, 2957, 1619, 1579, 1449, 1235, 1035, 783; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.23 – 7.13 (2H, *m*), 6.93 (1H, *dd*, J_1 = 7.8, J_2 = 1.8 Hz), 3.80 (2H, br. *s*), 3.66 (2H, *t*, J = 5.0 Hz), 3.45 (2H, *t*, J = 6.6 Hz), 3.02 (4H, *dt*, J_1 = 16.1, J_2 = 5.0 Hz), 2.34 (2H, *t*, J = 7.3 Hz), 1.86 – 1.75 (4H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 171.3, 150.6, 134.2, 127.6, 125.3, 118.8, 51.2, 45.9, 33.5, 33.0, 32.1, 23.8.

6-Bromo-1-(4-phenylpiperazin-1-yl)hexan-1-one ***(3h)***. Yield: 1.16 g (98.0 %); pale yellow oil; IR (ATR, cm^{-1}): 3444, 2938, 2911, 2825, 1646, 1593, 1497, 1442, 1232, 1024, 763, 696; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.35 – 7.24 (2H, *m*), 6.96 – 6.87 (3H, *m*), 3.78 (2H, *t*, J = 5.3 Hz), 3.62 (2H, *t*, J = 5.2 Hz), 3.51 – 3.34 (2H, *m*), 3.22 – 3.08 (4H, *m*), 2.39 (2H, *t*, J = 7.5 Hz), 1.98 – 1.79 (2H, *m*), 1.76 – 1.62 (2H, *m*), 1.57 – 1.41 (2H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 171.3, 151.0, 129.3, 120.6, 116.7, 49.9, 49.5, 45.6, 41.6, 33.8, 33.0, 32.6, 28.0, 24.4.

6-Bromo-1-(4-(2-methoxyphenyl)piperazin-1-yl) hexan-1-one ***(3i)***. Yield: 1.26 g (97.7 %); pale yellow oil; IR (ATR, cm^{-1}): 3454, 2939, 2918, 2824, 1647, 1597, 1494, 1441, 1233, 1025, 762, 696: ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm):

7.07 – 7.00 (*m*, 1H), 6.96 – 6.86 (*m*, 3H), 3.88 (*s*, 3H), 3.80 (*t*, J = 5.1 Hz, 2H), 3.65 (*t*, J = 4.9 Hz, 2H), 3.42 (*t*, J = 6.7 Hz, 2H), 3.10 – 2.97 (*m*, 4H), 2.39 (*t*, J = 7.5 Hz, 2H), 1.75 – 1.64 (*m*, 2H), 1.57 – 1.47 (*m*, 2H), 1.44 (*t*, J = 7.3 Hz, 2H); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 172.8, 153.8, 142.1, 125.1, 122.6, 120.0, 112.9, 57.0, 52.6, 52.1, 47.4, 43.3, 35.3, 34.5, 34.1, 29.5, 25.9.

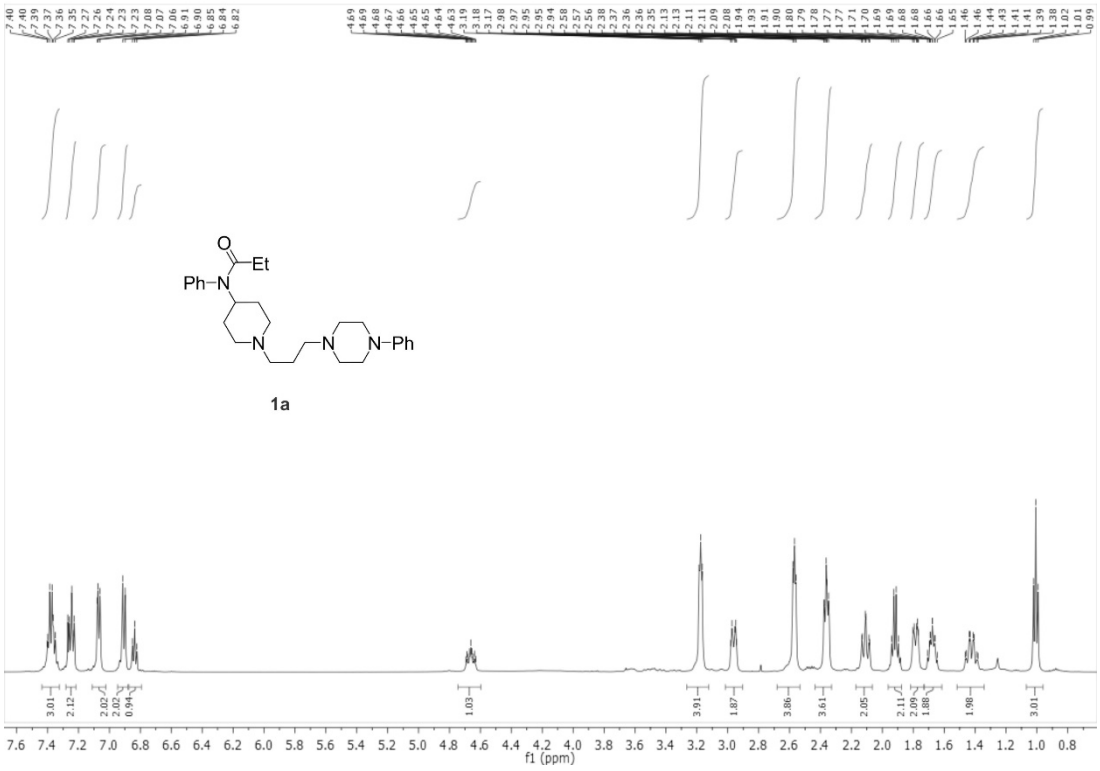
6-Bromo-1-(4-(2,3-dichlorophenyl) piperazin-1-yl)hexan-1-one ***(3j)***. Yield: 1.36 g (95.2 %); pale yellow oil; IR (ATR, cm^{-1}): 3467, 2938, 2862, 1645, 1450, 1236, 1032, 783, 736; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.22 – 7.11 (2H, *m*), 6.93 (1H, *dd*, J_1 = 7.8, J_2 = 1.9 Hz), 3.80 (2H, br. *s*), 3.65 (2H, *t*, J = 5.0 Hz), 3.43 – 3.37 (2H, *m*), 3.01 (4H, *dt*, J_1 = 13.7, J_2 = 5.1 Hz), 2.39 (2H, *t*, J = 7.5 Hz), 1.96 – 1.89 (2H, *m*), 1.79 – 1.68 (2H, *m*), 1.56 – 1.51 (2H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 171.4, 150.6, 134.2, 127.8, 127.6, 125.2, 118.8, 51.8, 51.2, 45.9, 41.8, 35.0, 33.8, 33.0, 28.0, 24.4.

7-Bromo-1-(4-phenylpiperazin-1-yl)heptan-1-one ***(3k)***. Yield: 1.19 g (97.1 %); pale yellow oil; IR (ATR, cm^{-1}): 3485, 2933, 2857, 1645, 1597, 1498, 1437, 1231, 1027, 760, 695; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.35 – 7.21 (2H, *m*), 7.02 – 6.85 (3H, *m*), 3.85 – 3.72 (2H, *m*), 3.62 (2H, *t*, J = 5.3 Hz), 3.48 – – 3.32 (2H, *m*), 3.16 (4H, *dt*, J_1 = 13.5, J_2 = 5.3 Hz), 2.37 (2H, *t*, J = 7.6 Hz), 1.93 – 1.79 (2H, *m*), 1.75 – 1.58 (2H, *m*), 1.55 – 1.43 (2H, *m*), 1.46 – 1.31 (2H, *m*); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 171.6, 151.0, 129.3, 120.6, 116.7, 49.9, 49.5, 45.6, 41.6, 34.0, 33.1, 32.6, 28.6, 28.0, 25.1.

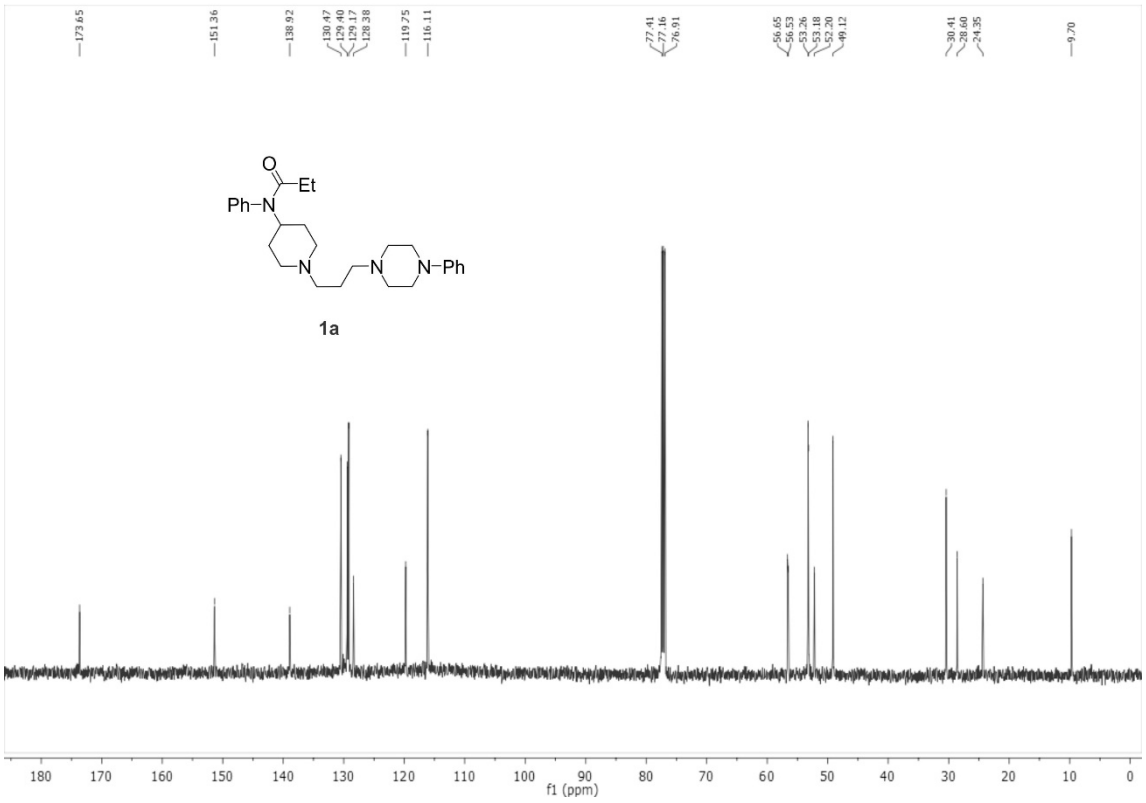
7-Bromo-1-(4-(2-methoxyphenyl)piperazin-1-yl)heptan-1-one ***(3l)***. Yield: 1.30 g (97.3 %); pale yellow oil; IR (ATR, cm^{-1}): 3441, 2935, 2858, 1643, 1501, 1460, 1242, 1029, 735; ^{1}H–NMR (500 MHz, $CDCl_3$, δ / ppm): 7.08 – 6.99 (1H, *m*), 6.94 – 6.85 (3H, *m*), 3.87 (3H, *s*), 3.79 (2H, *t,* J = 5.1 Hz), 3.64 (2H, *t*, J = 5.1 Hz), 3.44 – 3.37 (2H, *m*), 3.02 (4H, *dt*, J_1 = 16.2, J_2 = 5.1 Hz), 2.37 (2H, *t*, J = 7.6 Hz), 1.91 – 1.82 (2H, *m*), 1.71 – 1.62 (2H, *m*), 1.52 – 1.41 (2H, *m*, partially overlapped), 1.43 – 1.32 (2H, *m*, partially overlapped); ^{13}C–NMR (126 MHz, $CDCl_3$, δ / ppm): 171.6, 152.3, 140.

NMR spectra of the final compounds

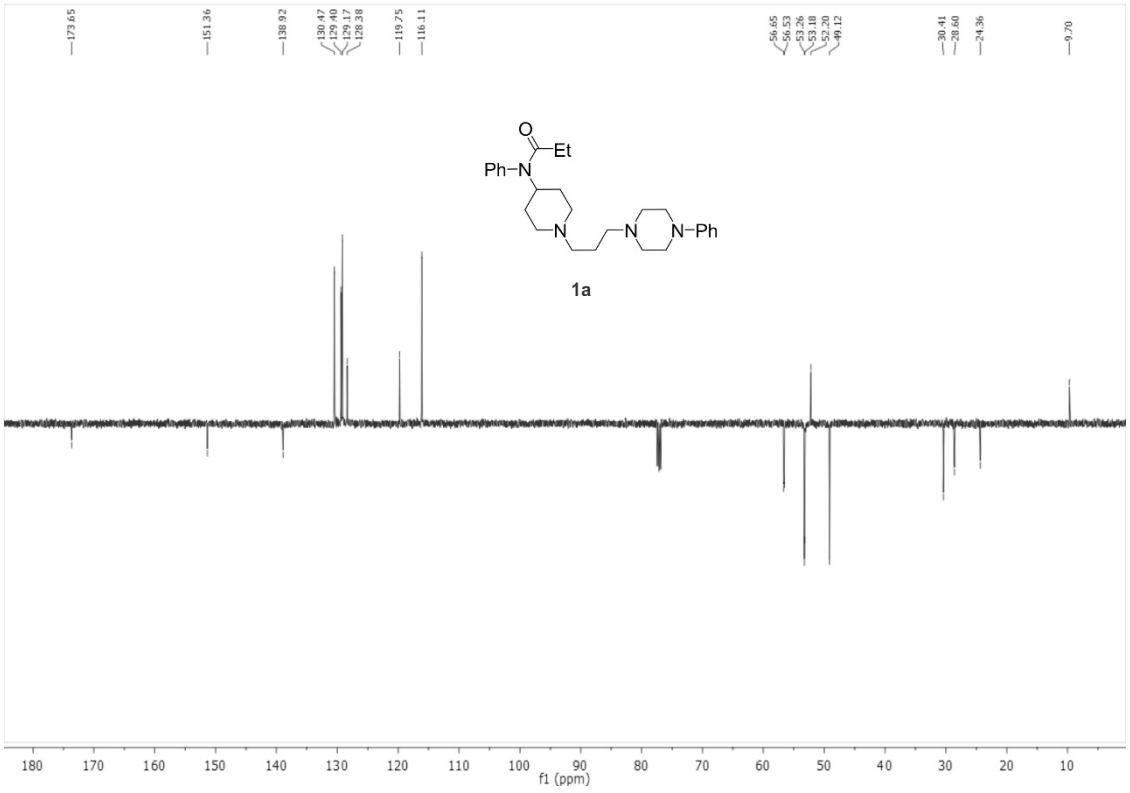
^{1}H NMR (500 MHz, $CDCl_3$)

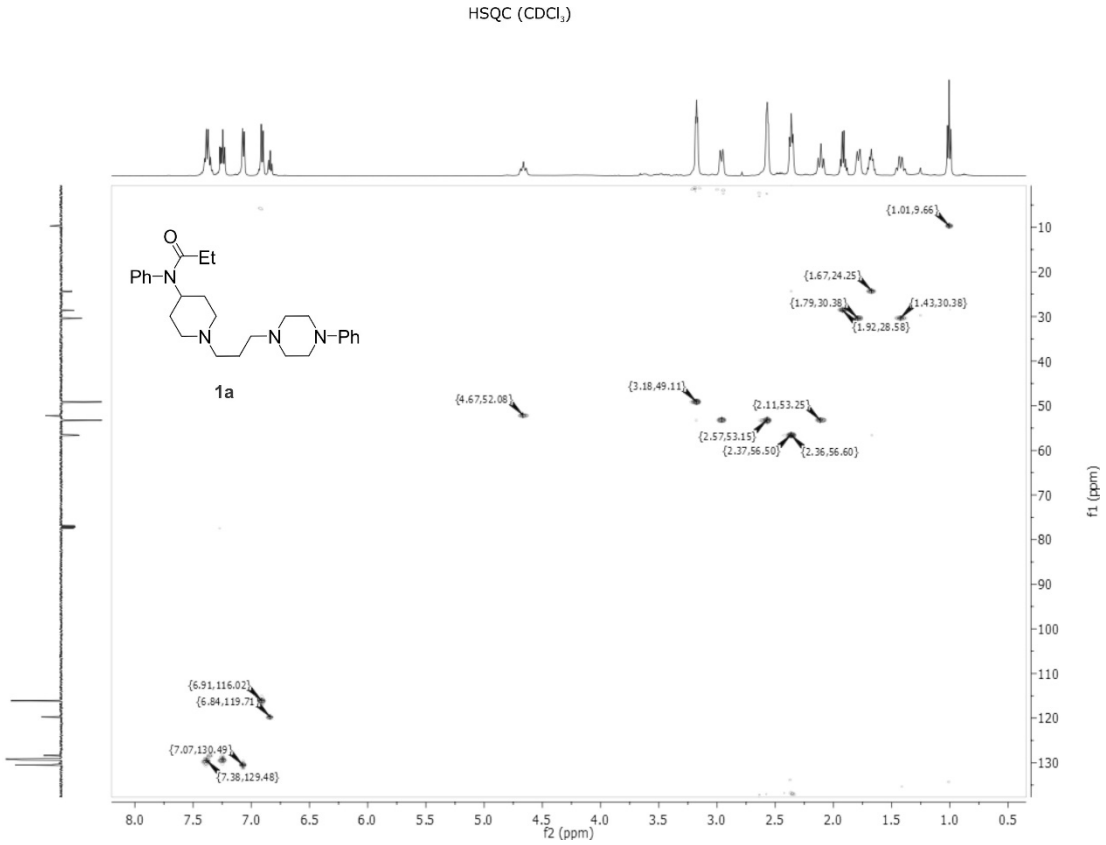


^{13}C NMR (126 MHz, $CDCl_3$)

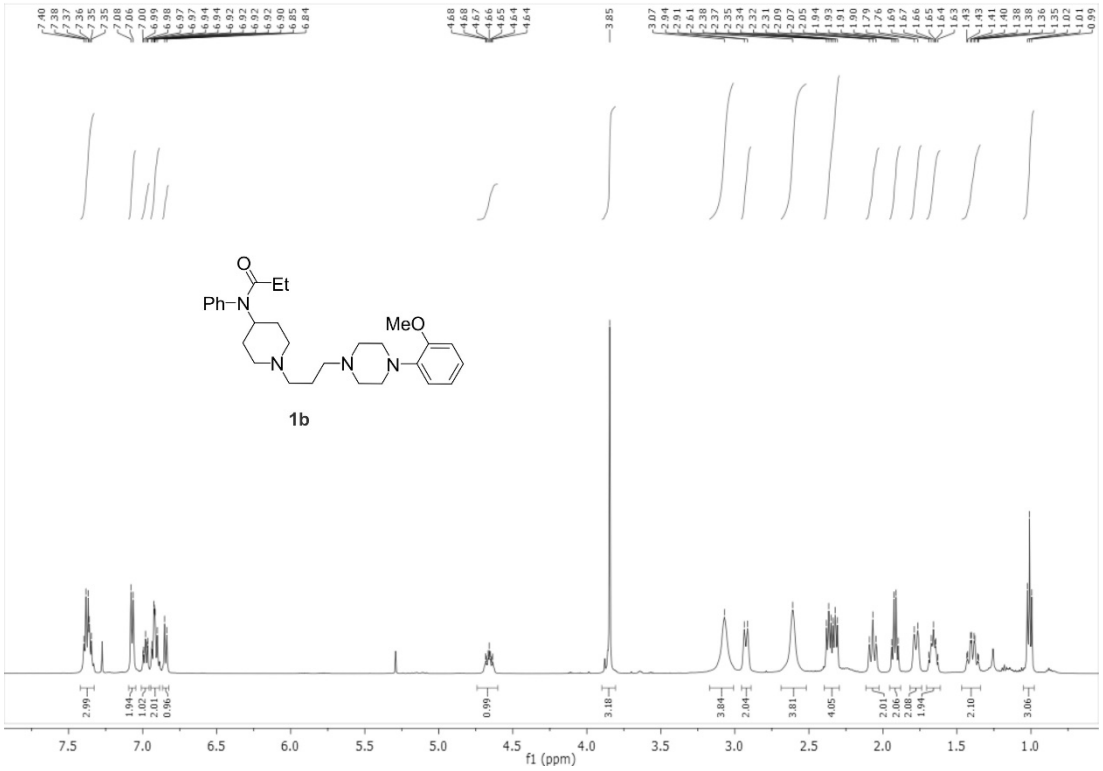


APT (126 MHz, $CDCl_3$)

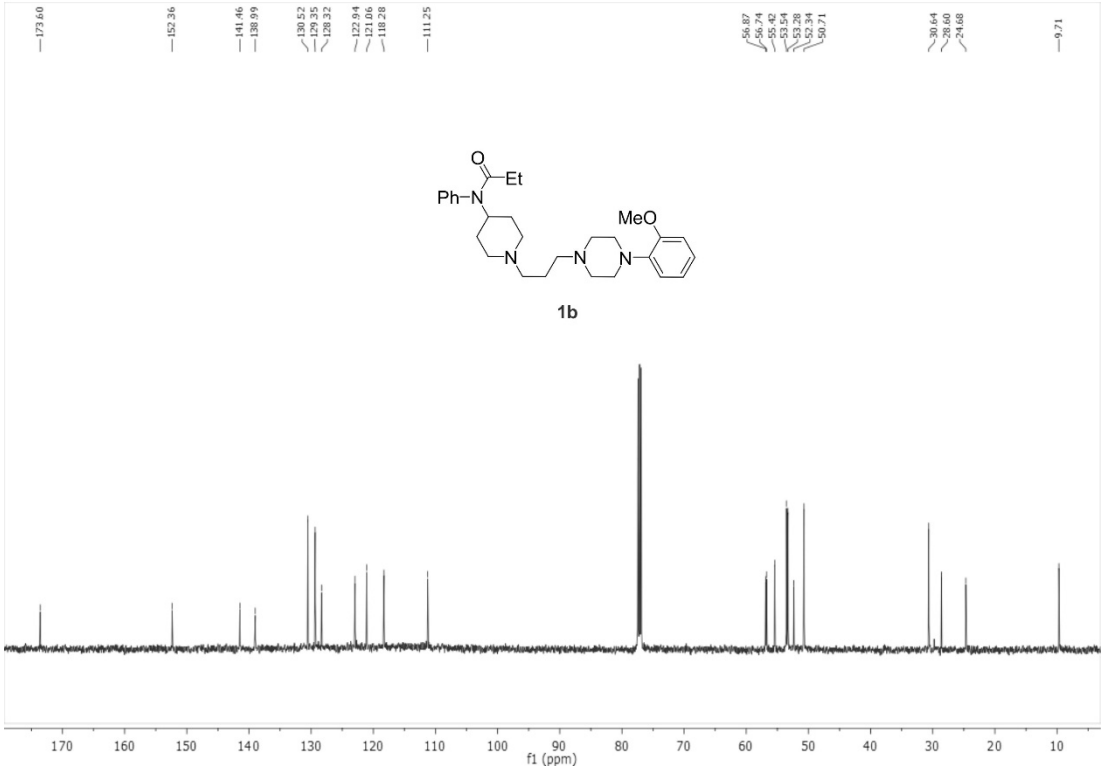



HSQC (CDCl3)
1a
{1.01,9.66}
{1.67,24.25}
{1.79,30.38}
{1.43,30.38}
{1.92,28.58}
{4.67,52.08}
{3.18,49.11}
{2.11,53.25}
{2.57,53.15}
{2.37,56.50}
{2.36,56.60}
{6.91,116.02}
{6.84,119.71}
{7.07,130.49}
{7.38,129.48}
f2 (ppm)
f1 (ppm)

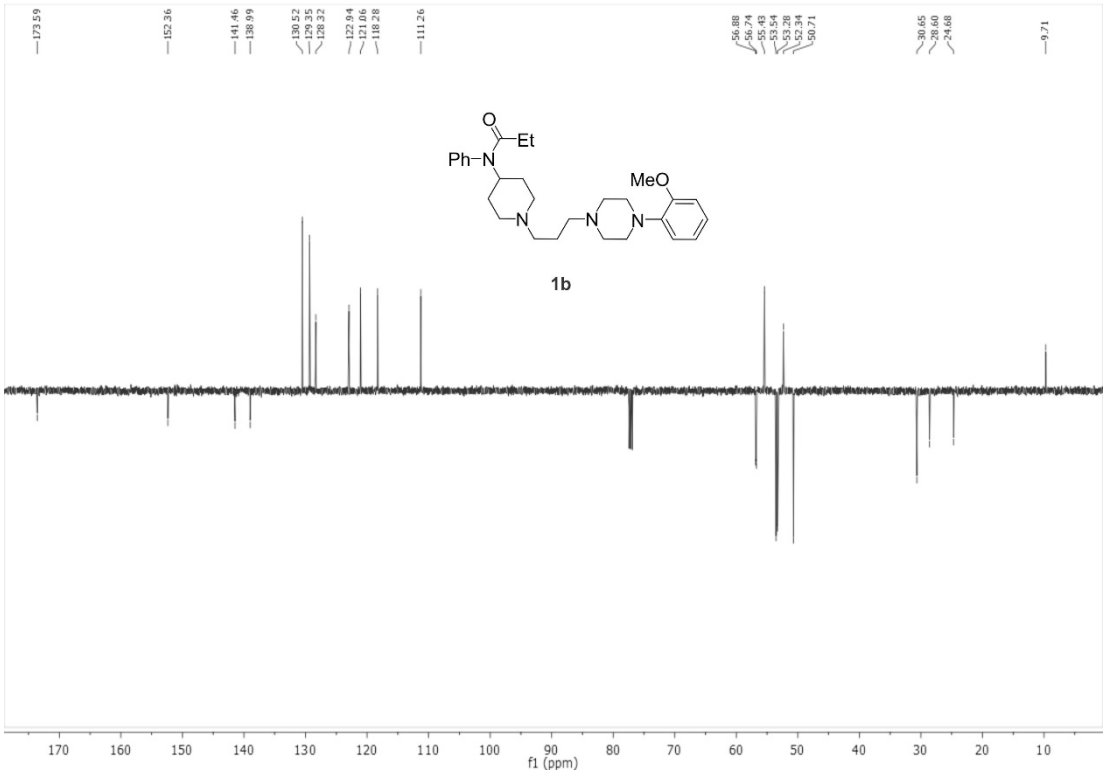
^{1}H NMR (500 MHz, $CDCl_3$)

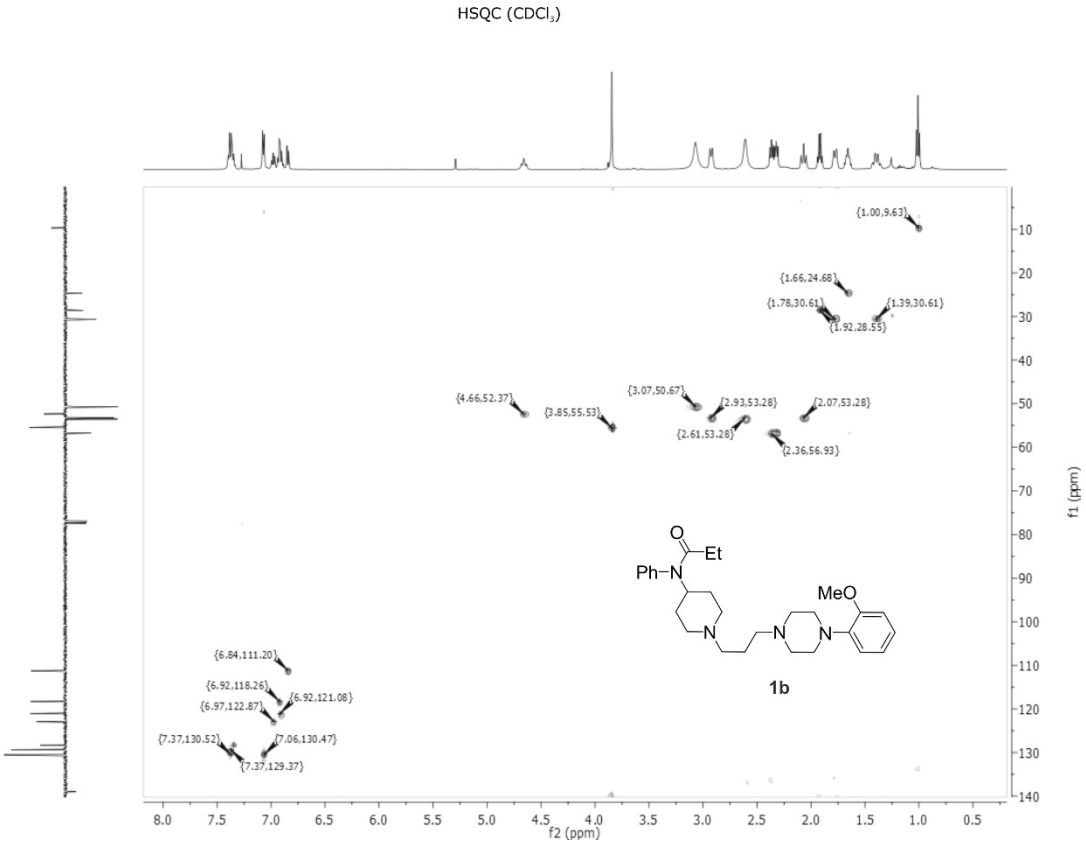


^{13}C NMR (126 MHz, $CDCl_3$)

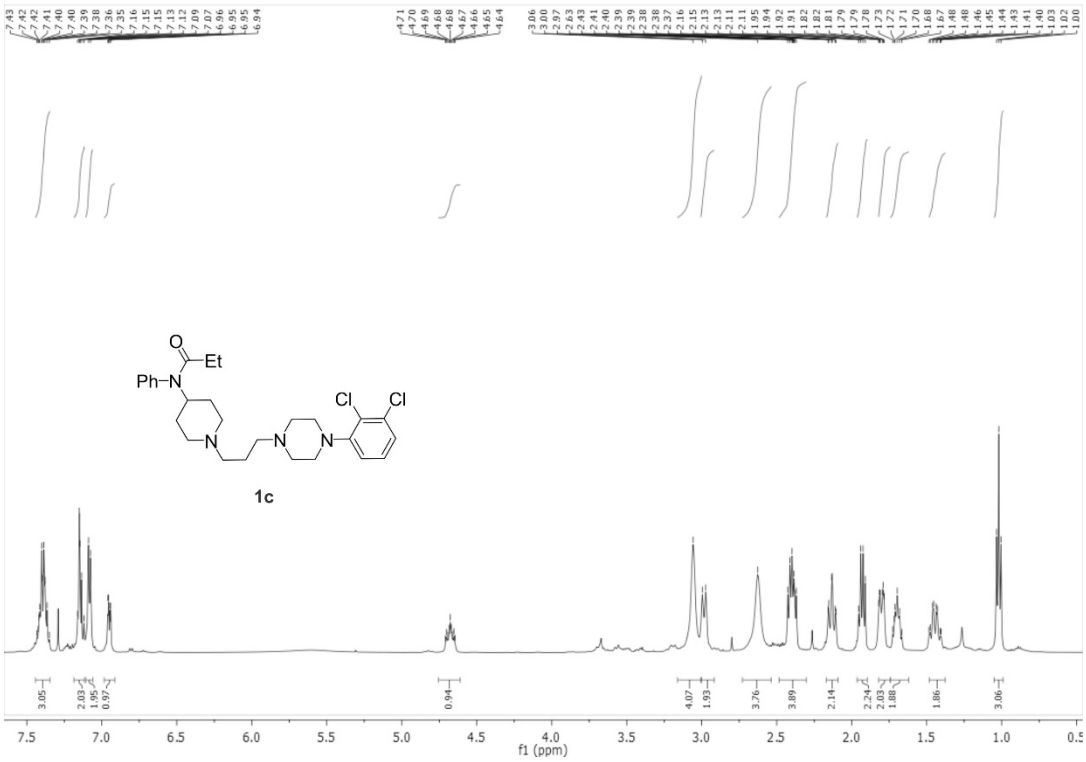


APT (126 MHz, $CDCl_3$)

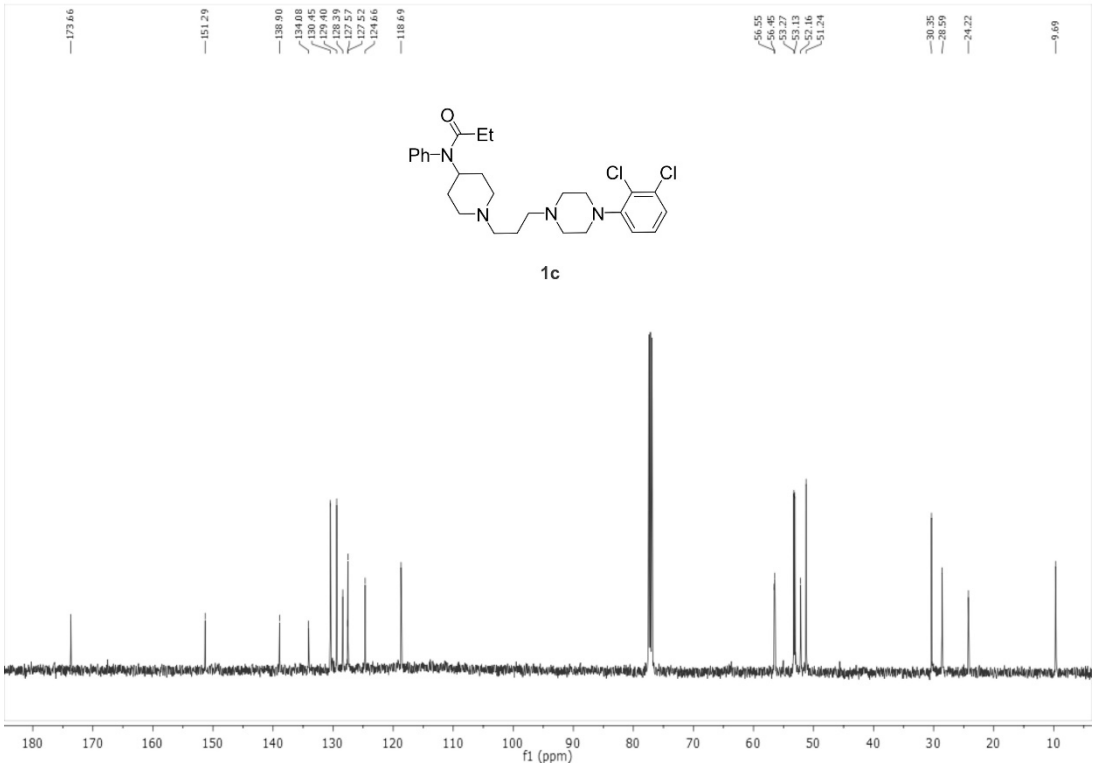



HSQC (CDCl3)
{1.00,9.63}
{1.66,24.68}
{1.78,30.61}
{1.39,30.61}
{1.92,28.55}
{4.66,52.37}
{3.85,55.53}
{3.07,50.67}
{2.93,53.28}
{2.07,53.28}
{2.61,53.28}
{2.36,56.93}
{6.84,111.20}
{6.92,118.26}
{6.92,121.08}
{6.97,122.87}
{7.37,130.52}
{7.06,130.47}
{7.37,129.37}
O
Et
Ph–N
MeO
N
N
N
1b
f1 (ppm)
f2 (ppm)

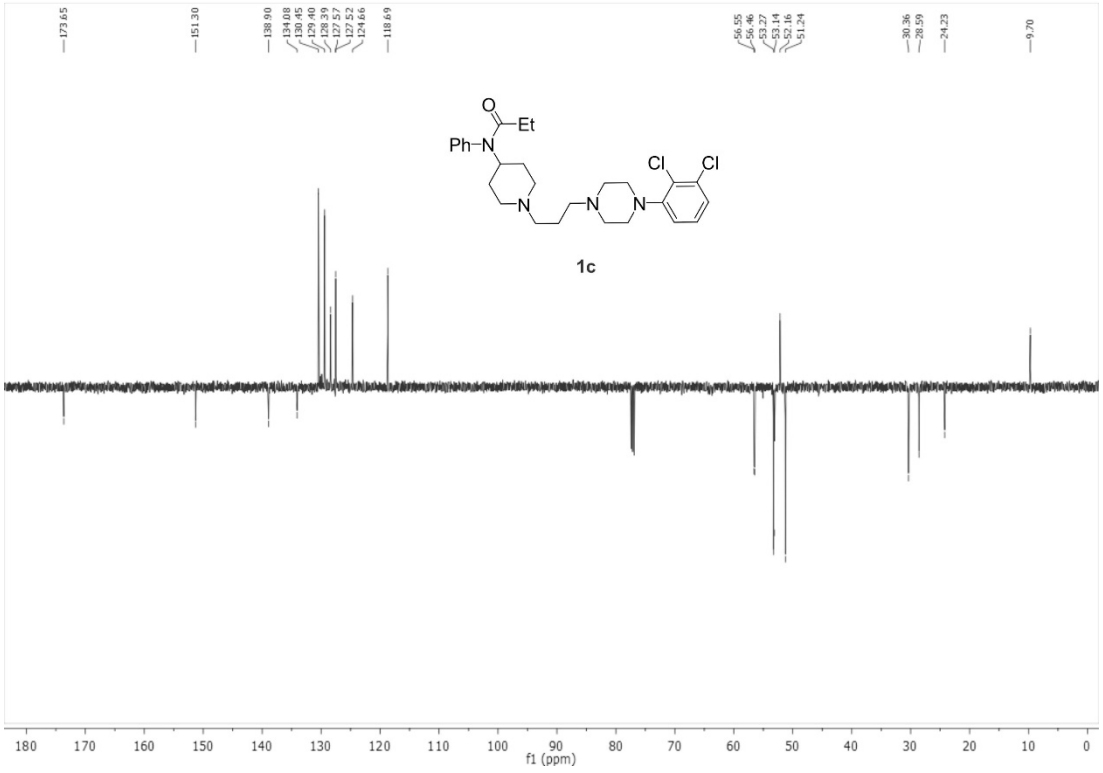
^{1}H NMR (500 MHz, $CDCl_3$)

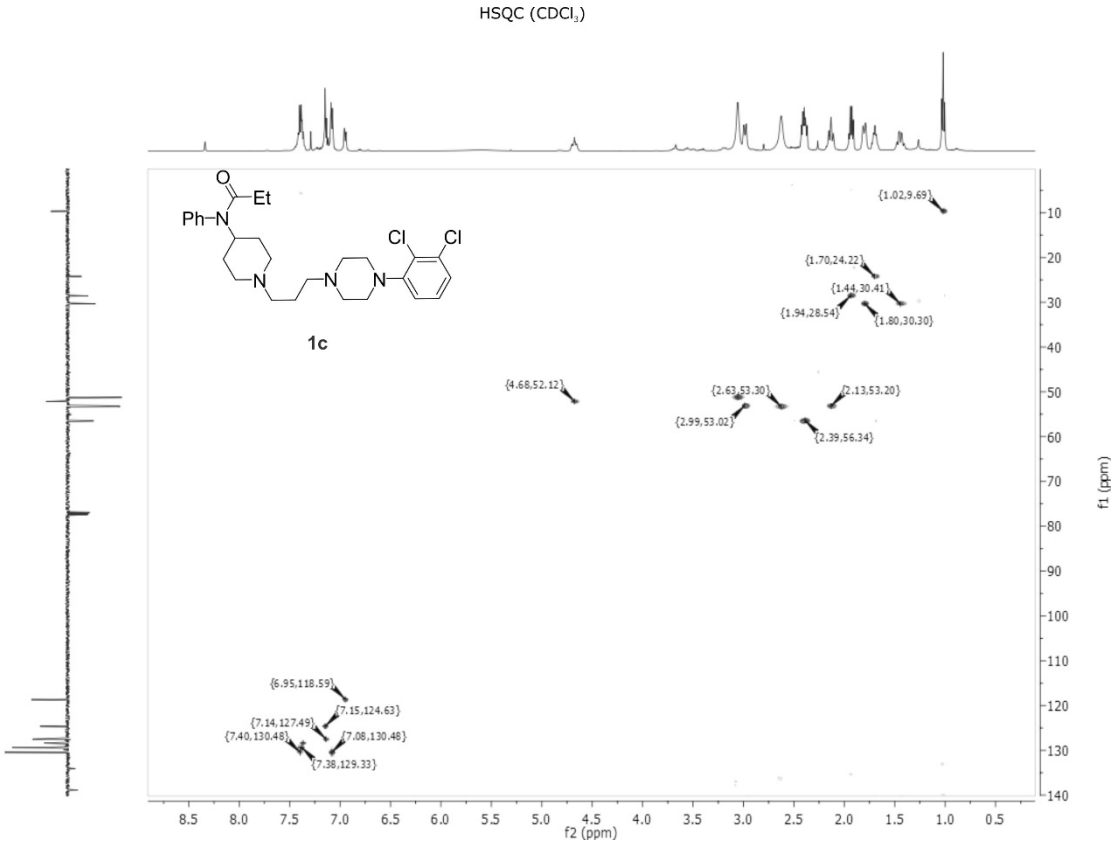


^{13}C NMR (126 MHz, $CDCl_3$)

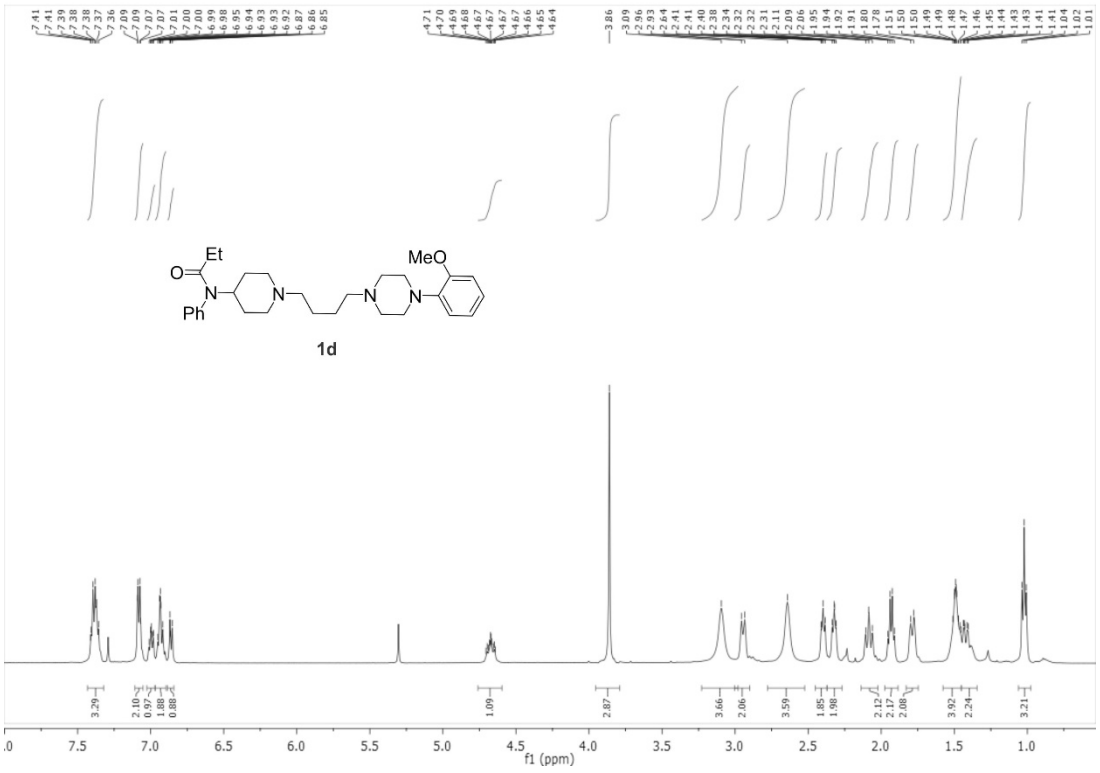


APT (126 MHz, $CDCl_3$)

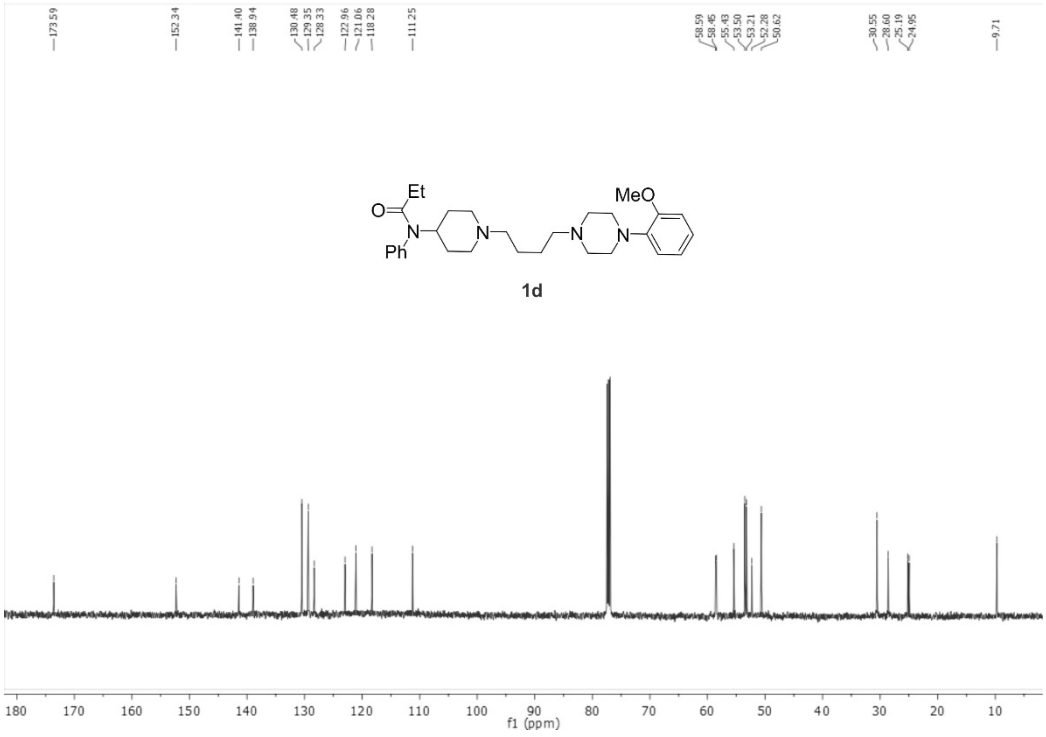



HSQC (CDCl3)
O
Et
Ph–N
Cl
Cl
N
N
N
1c
{1.02,9.69}
{1.70,24.22}
{1.44,30.41}
{1.94,28.54}
{1.80,30.30}
{4.68,52.12}
{2.63,53.30}
{2.13,53.20}
{2.99,53.02}
{2.39,56.34}
{6.95,118.59}
{7.15,124.63}
{7.14,127.49}
{7.40,130.48}
{7.08,130.48}
{7.38,129.33}
f2 (ppm)
f1 (ppm)

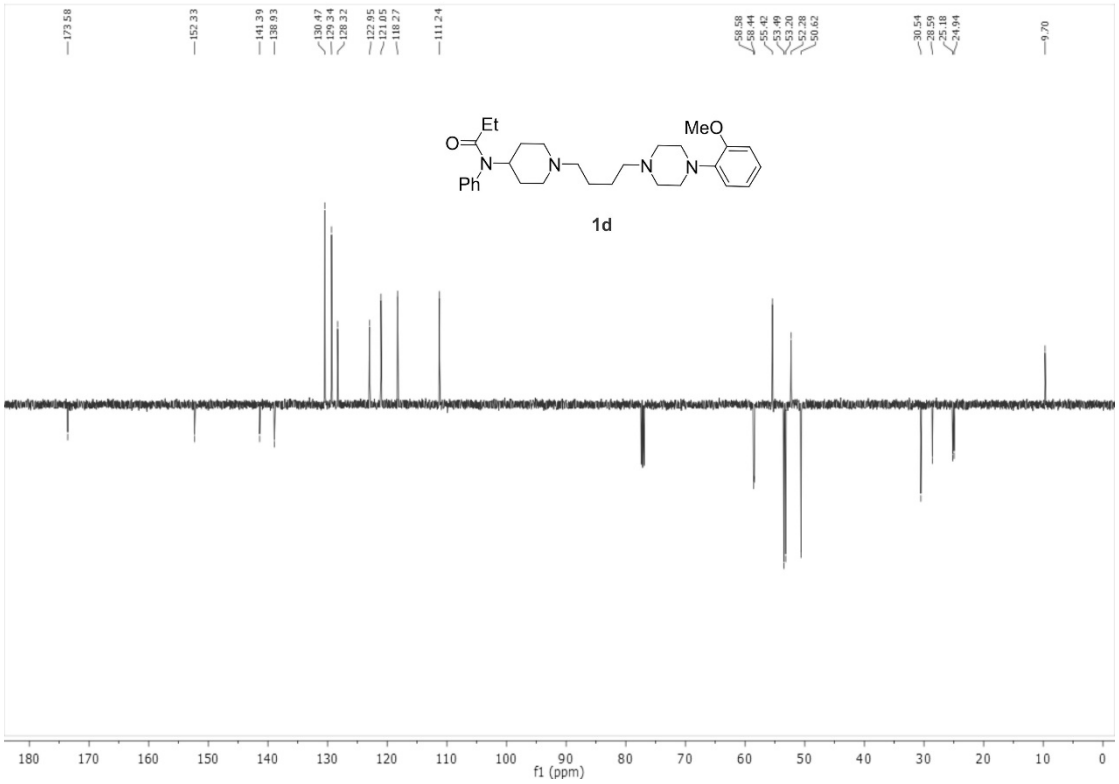
^{1}H NMR (500 MHz, $CDCl_3$)

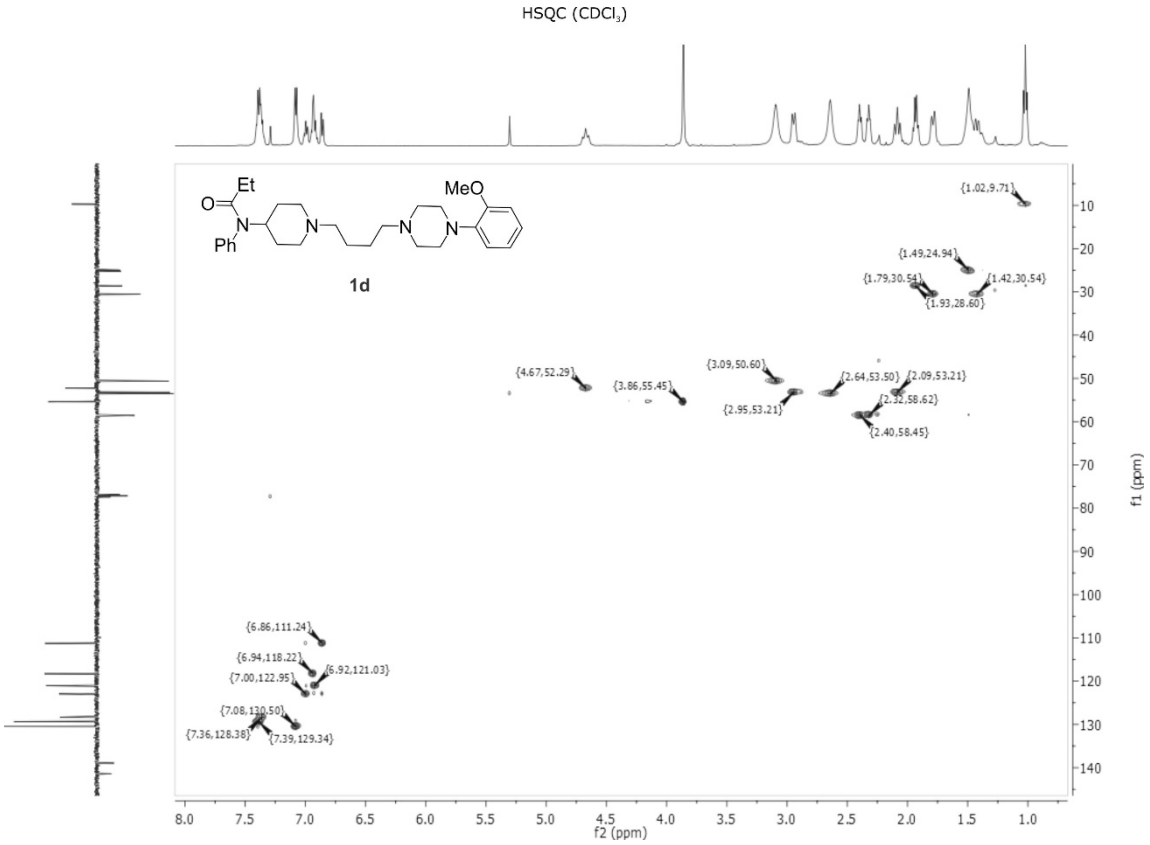


^{13}C NMR (126 MHz, $CDCl_3$)

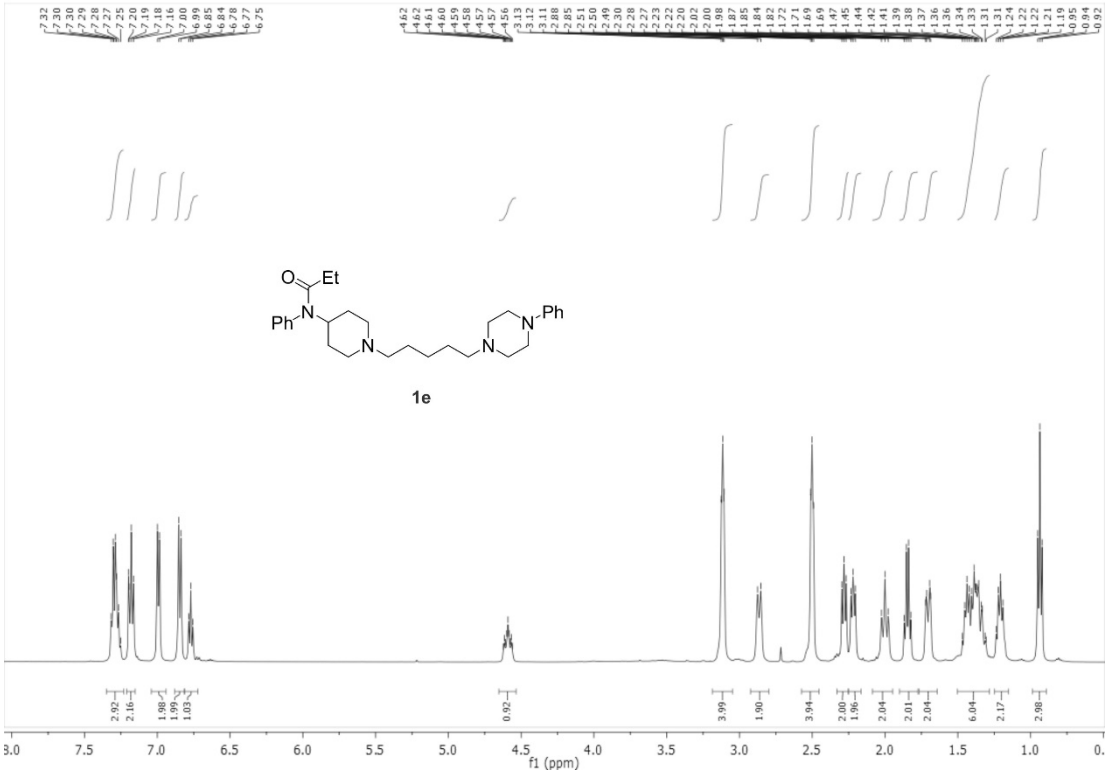


APT (126 MHz, $CDCl_3$)

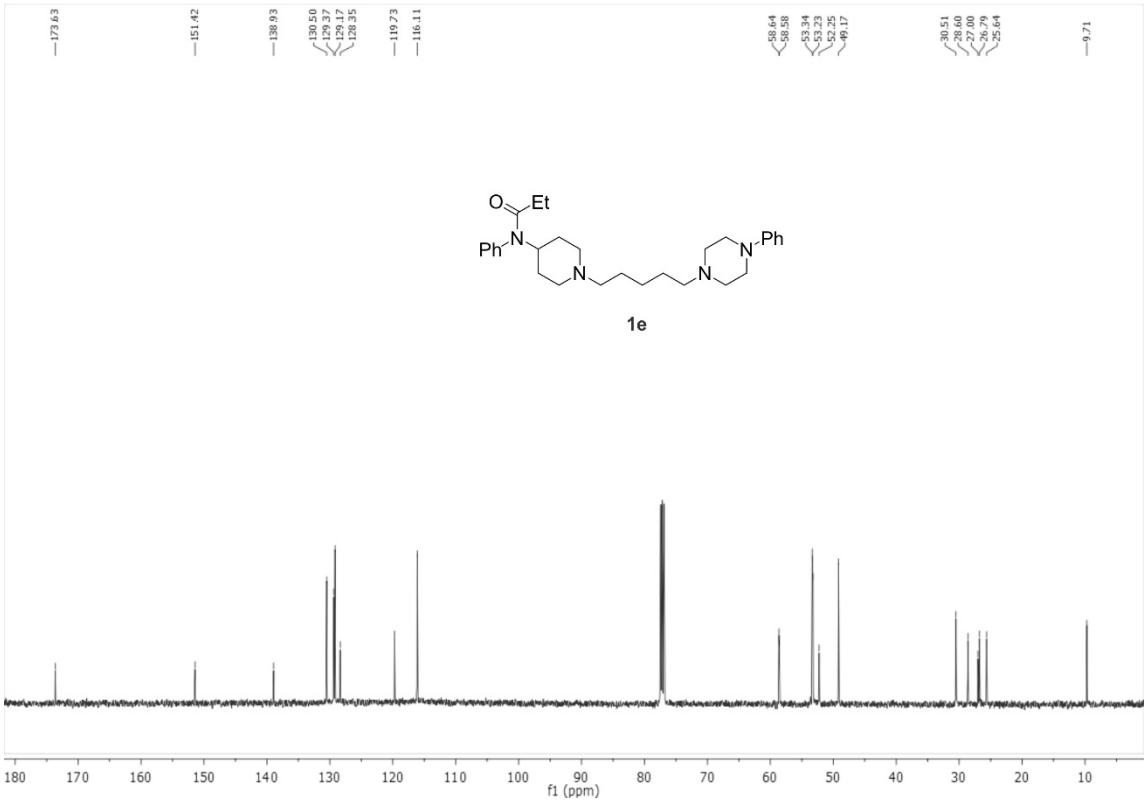


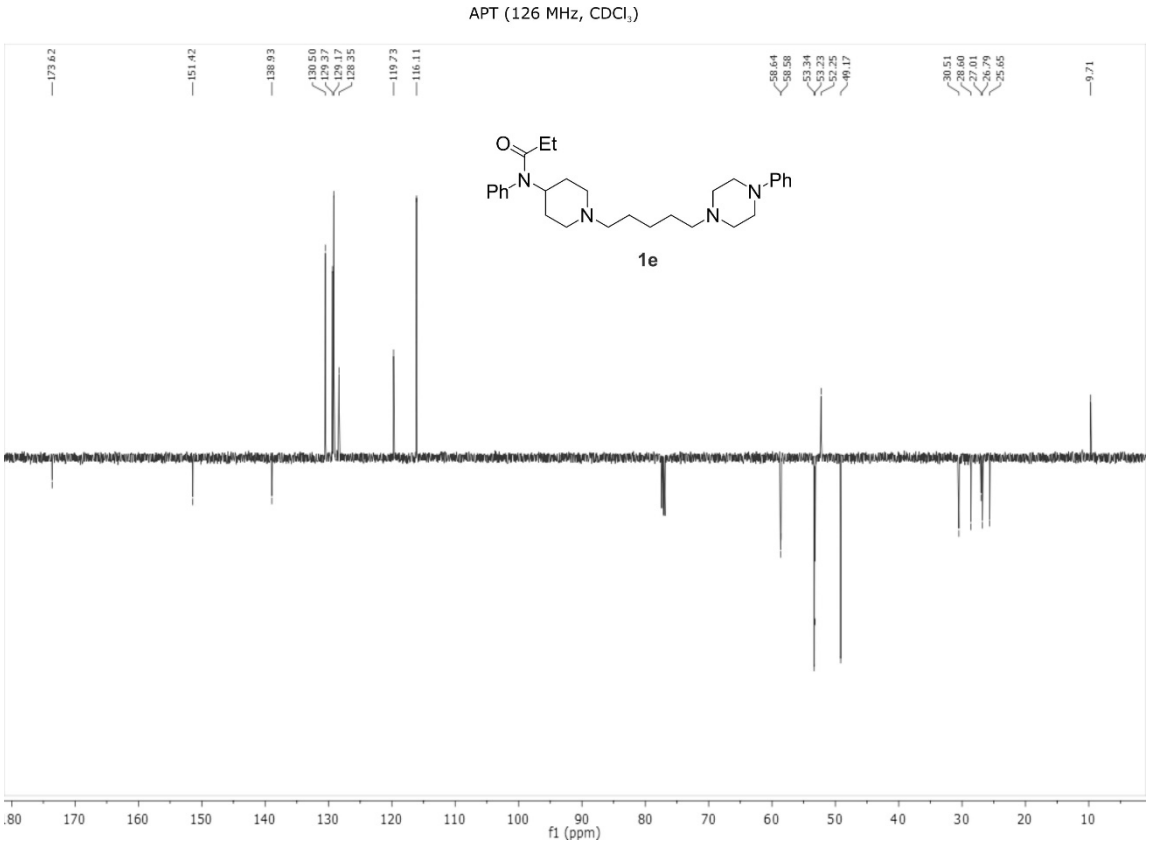

HSQC (CDCl3)
Et
O
N
Ph
N
N
N
MeO
1d
{1.02,9.71}
{1.49,24.94}
{1.79,30.54}
{1.42,30.54}
{1.93,28.60}
{4.67,52.29}
{3.86,55.45}
{3.09,50.60}
{2.95,53.21}
{2.64,53.50}
{2.09,53.21}
{2.32,58.62}
{2.40,58.45}
{6.86,111.24}
{6.94,118.22}
{6.92,121.03}
{7.00,122.95}
{7.08,130.50}
{7.36,128.38}
{7.39,129.34}
f1 (ppm)
f2 (ppm)

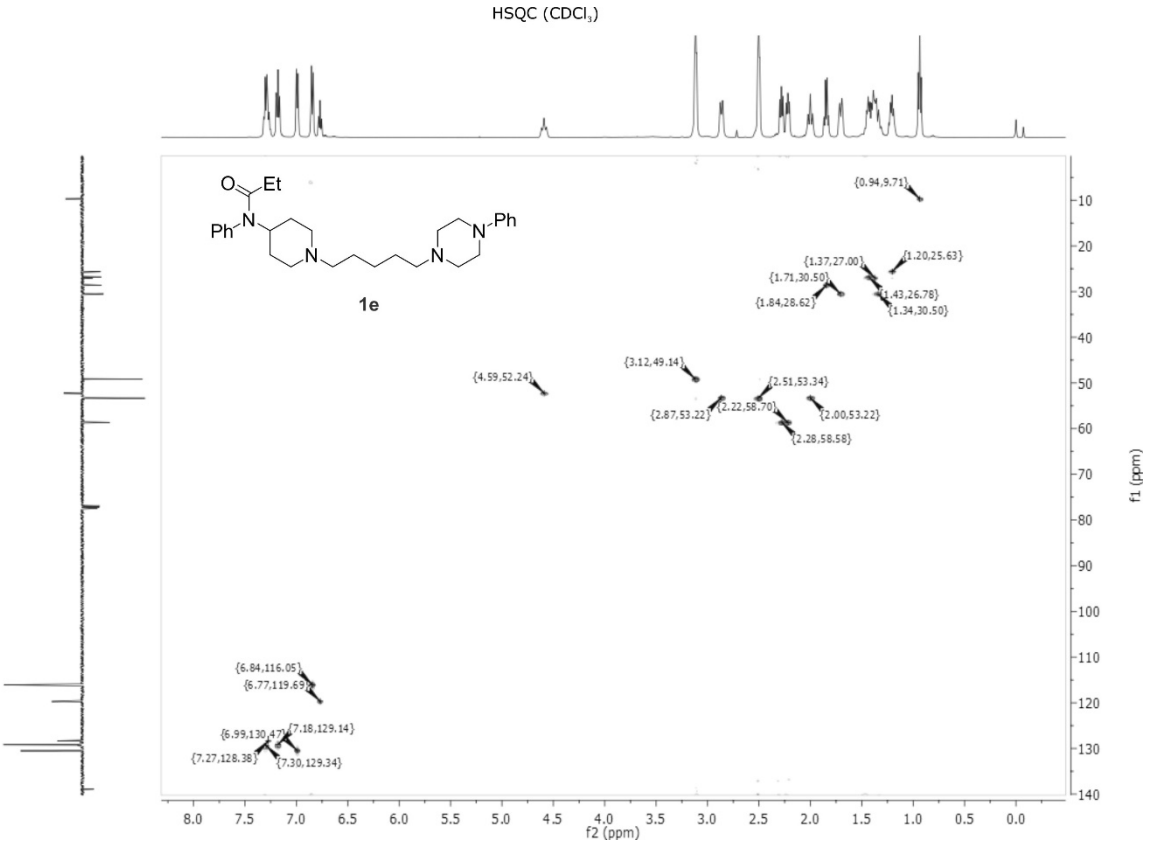
^{3}H NMR (500 MHz, $CDCl_3$)



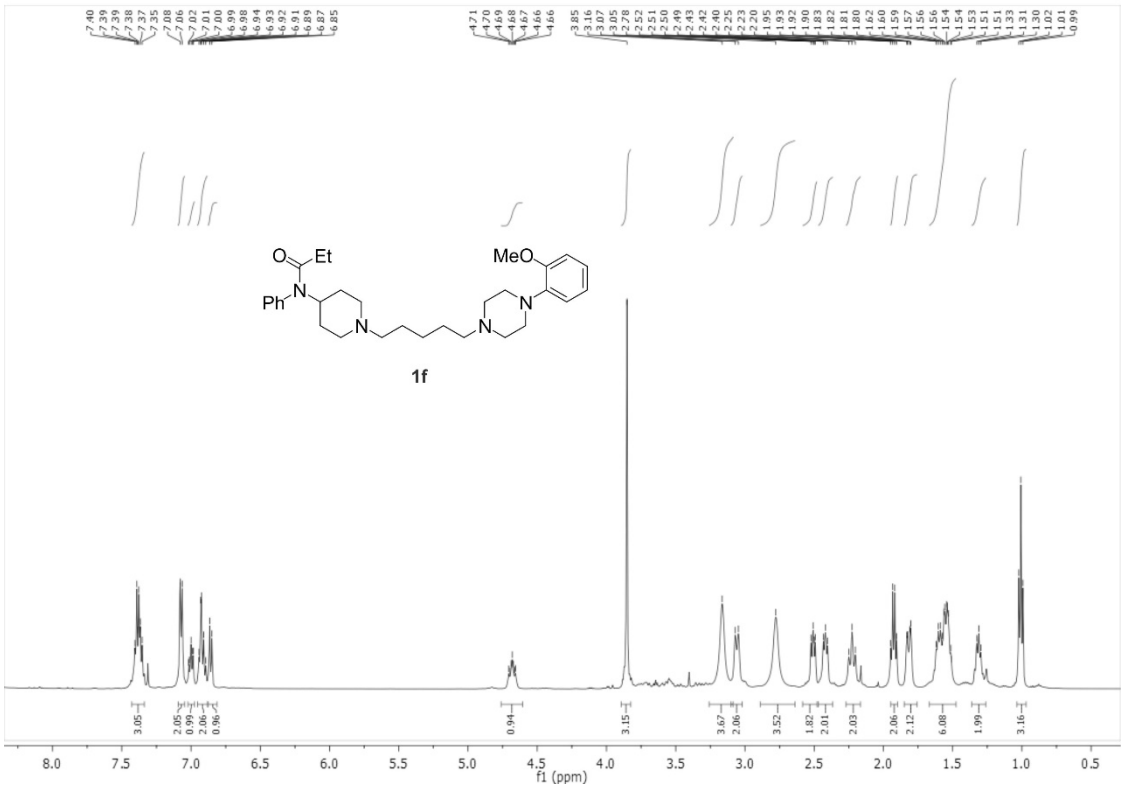
^{13}C NMR (126 MHz, $CDCl_3$)



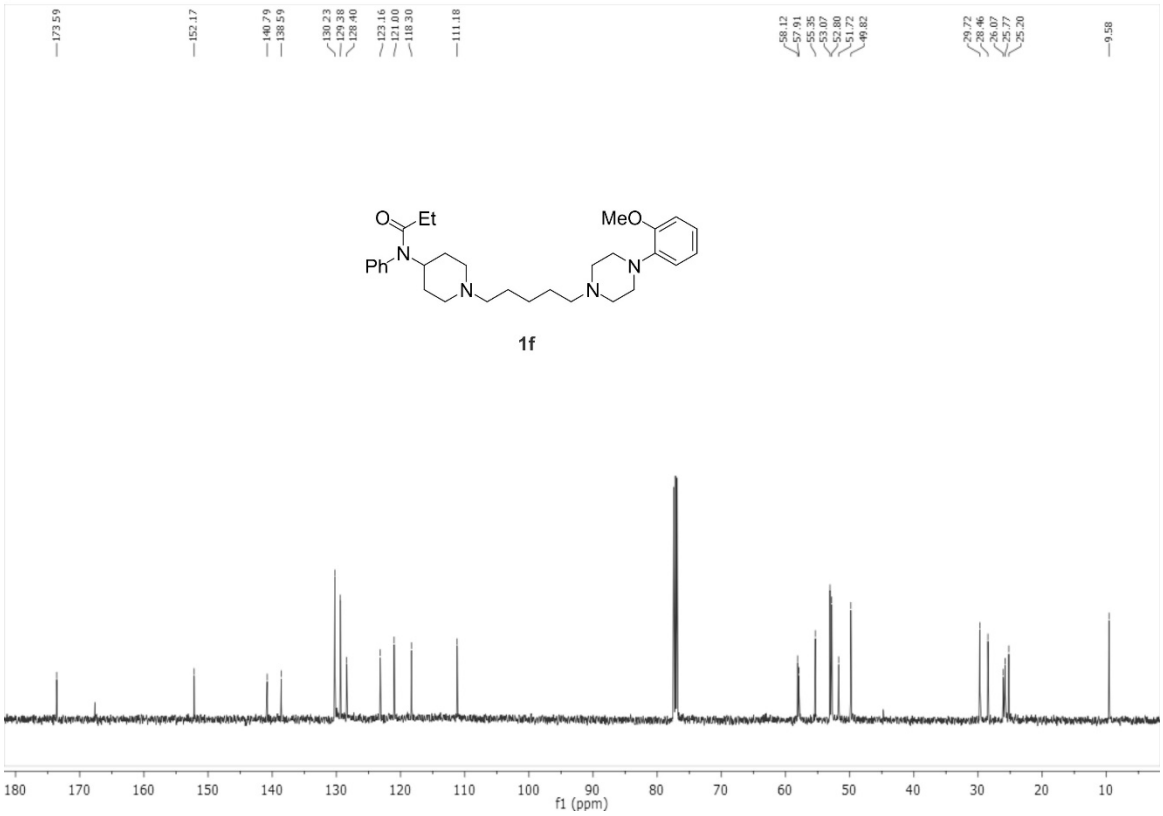

APT (126 MHz, CDCl3)
173.62
151.42
138.93
130.50
129.37
129.17
128.35
119.73
116.11
58.64
58.58
53.34
53.23
52.25
49.17
30.51
28.60
27.01
26.79
25.65
9.71
O
Et
N
Ph
N
N
N
Ph
1e
f1 (ppm)


HSQC (CDCl3)
O
Et
Ph
N
N
N
Ph
1e
{0.94,9.71}
{1.37,27.00}
{1.20,25.63}
{1.71,30.50}
{1.43,26.78}
{1.84,28.62}
{1.34,30.50}
{4.59,52.24}
{3.12,49.14}
{2.51,53.34}
{2.87,53.22}
{2.22,58.70}
{2.00,53.22}
{2.28,58.58}
{6.84,116.05}
{6.77,119.69}
{6.99,130.47}
{7.18,129.14}
{7.27,128.38}
{7.30,129.34}
f2 (ppm)
f1 (ppm)

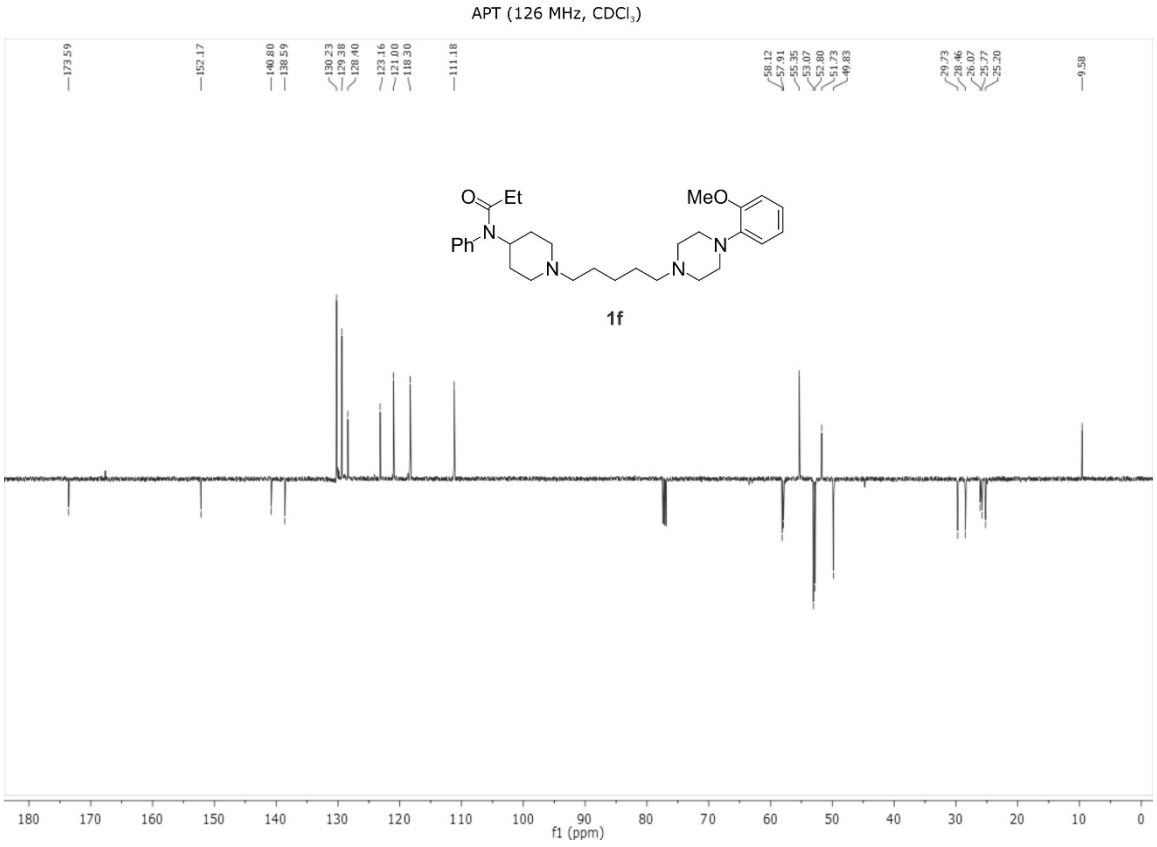
^{1}H NMR (500 MHz, $CDCl_3$)

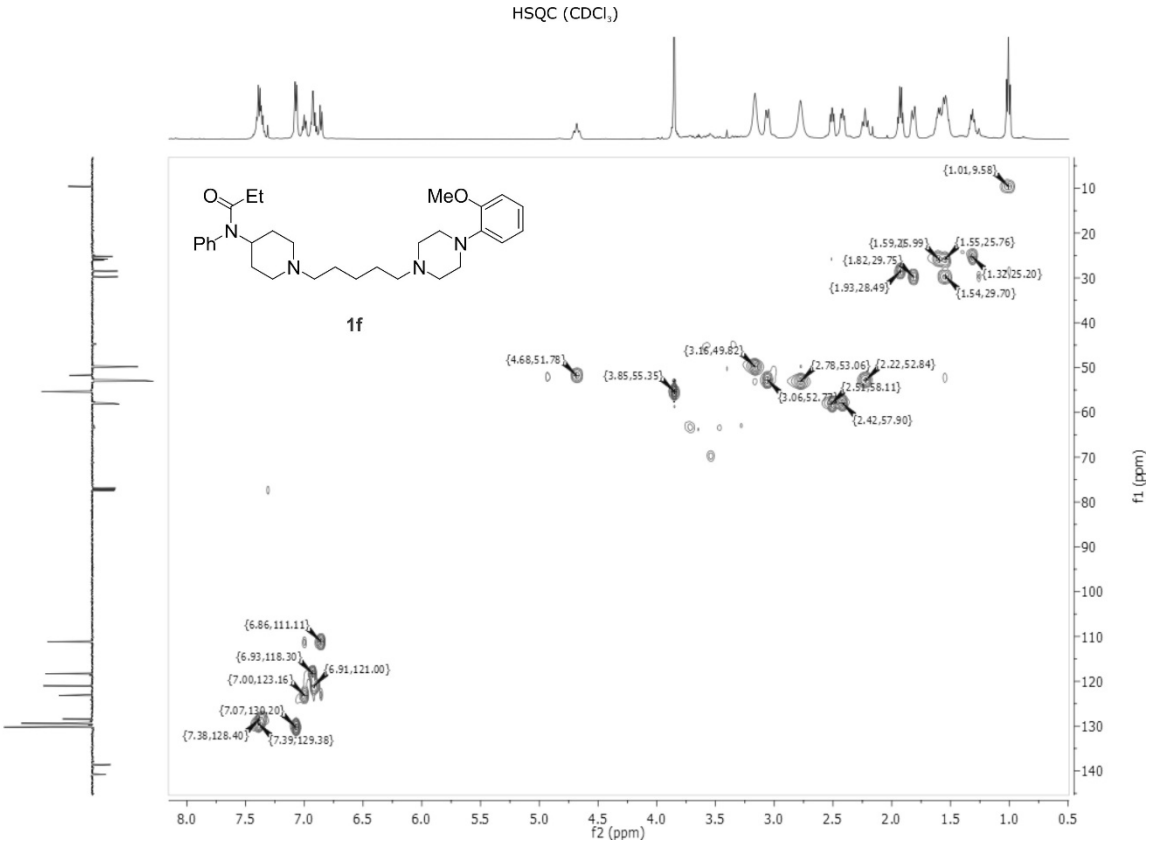


^{13}C NMR (126 MHz, $CDCl_3$)

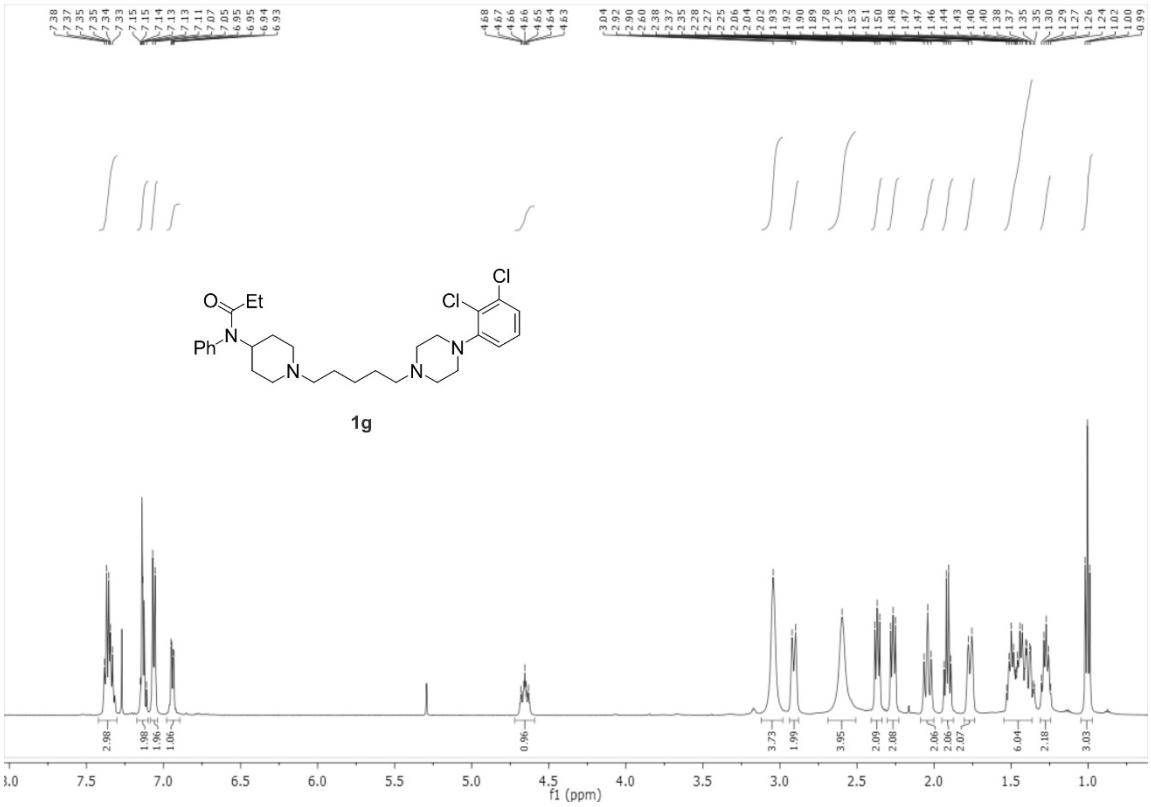


1f

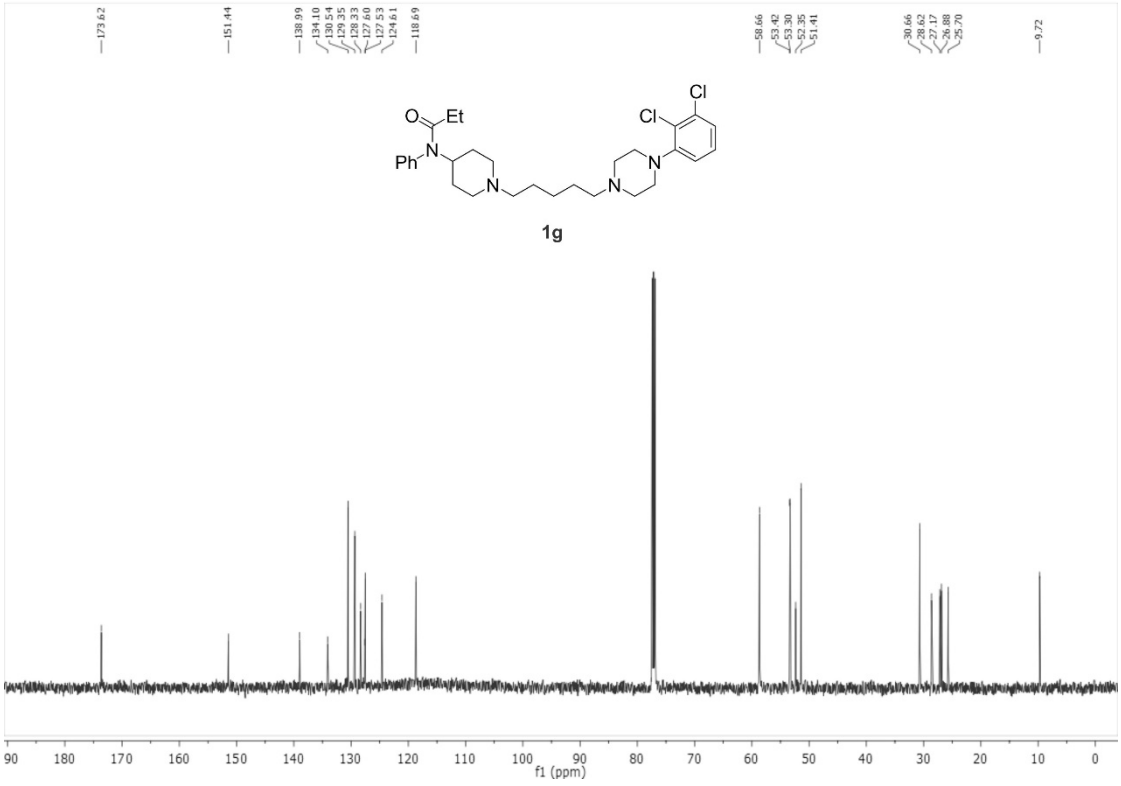

APT (126 MHz, CDCl3)
173.59
152.17
140.80
138.59
130.23
129.38
128.40
123.16
121.00
118.30
111.18
58.12
57.91
55.35
53.07
52.80
51.73
49.83
29.73
28.46
26.07
25.77
25.20
9.58
O
Et
N
Ph
MeO
N
N
N
1f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


HSQC (CDCl3)
O
Et
Ph
N
MeO
N
N
1f
{1.01,9.58}
{1.59,25.99}
{1.55,25.76}
{1.82,29.75}
{1.32,25.20}
{1.93,28.49}
{1.54,29.70}
{4.68,51.78}
{3.85,55.35}
{3.16,49.82}
{2.78,53.06}
{2.22,52.84}
{3.06,52.77}
{2.51,58.11}
{2.42,57.90}
{6.86,111.11}
{6.93,118.30}
{6.91,121.00}
{7.00,123.16}
{7.07,120.20}
{7.38,128.40}
{7.39,129.38}
f2 (ppm)
f1 (ppm)

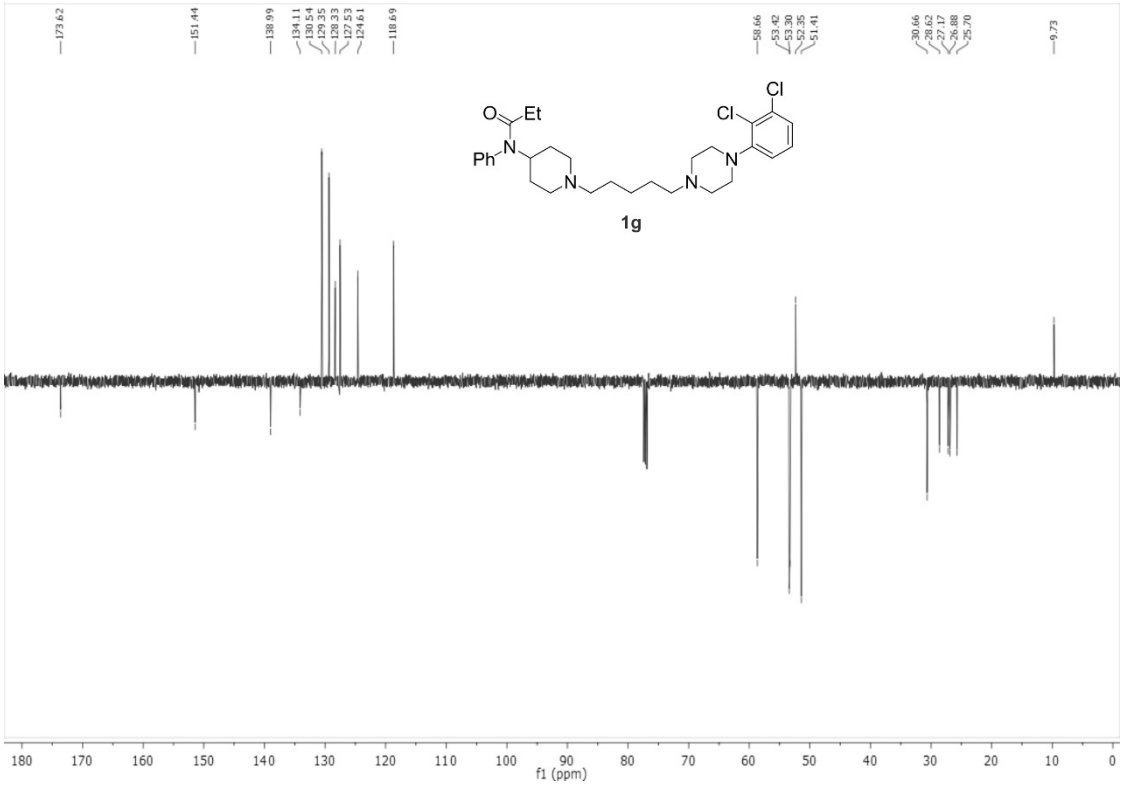
^{1}H NMR (500 MHz, $CDCl_3$)

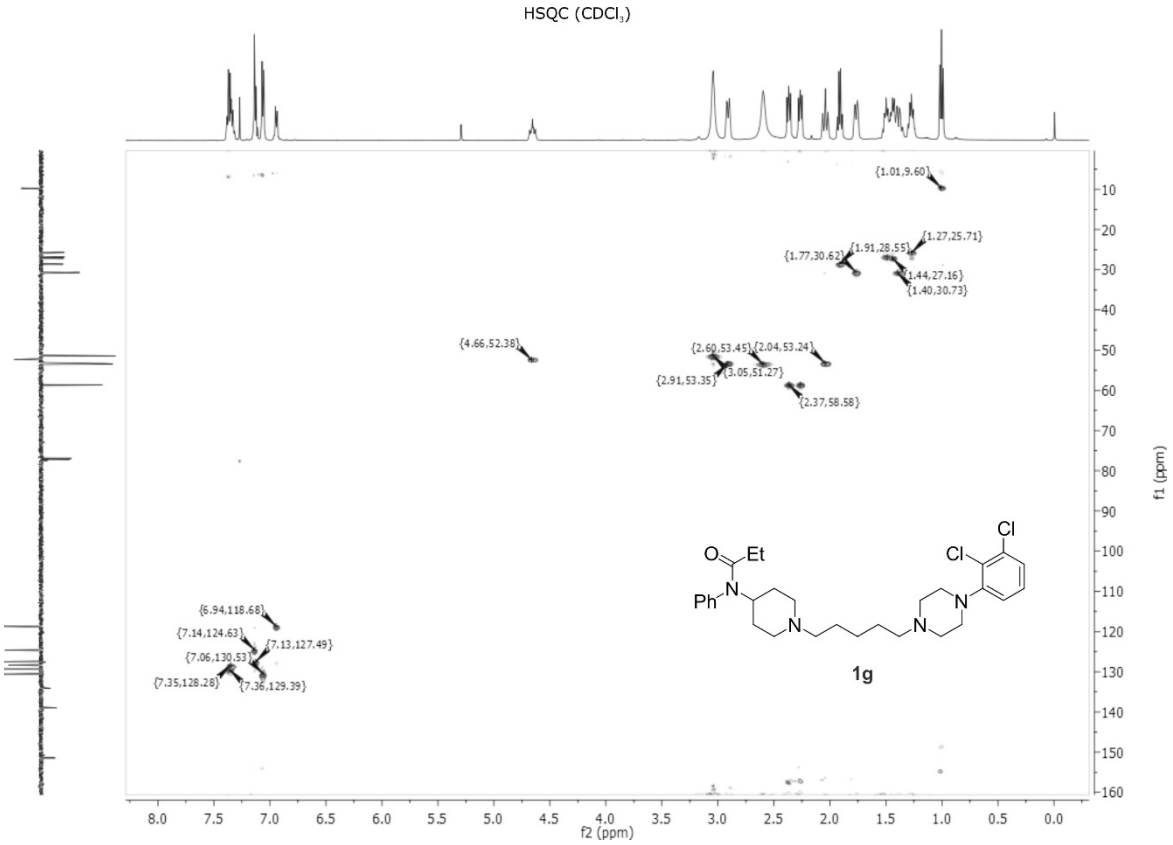


^{13}C NMR (126 MHz, $CDCl_3$)

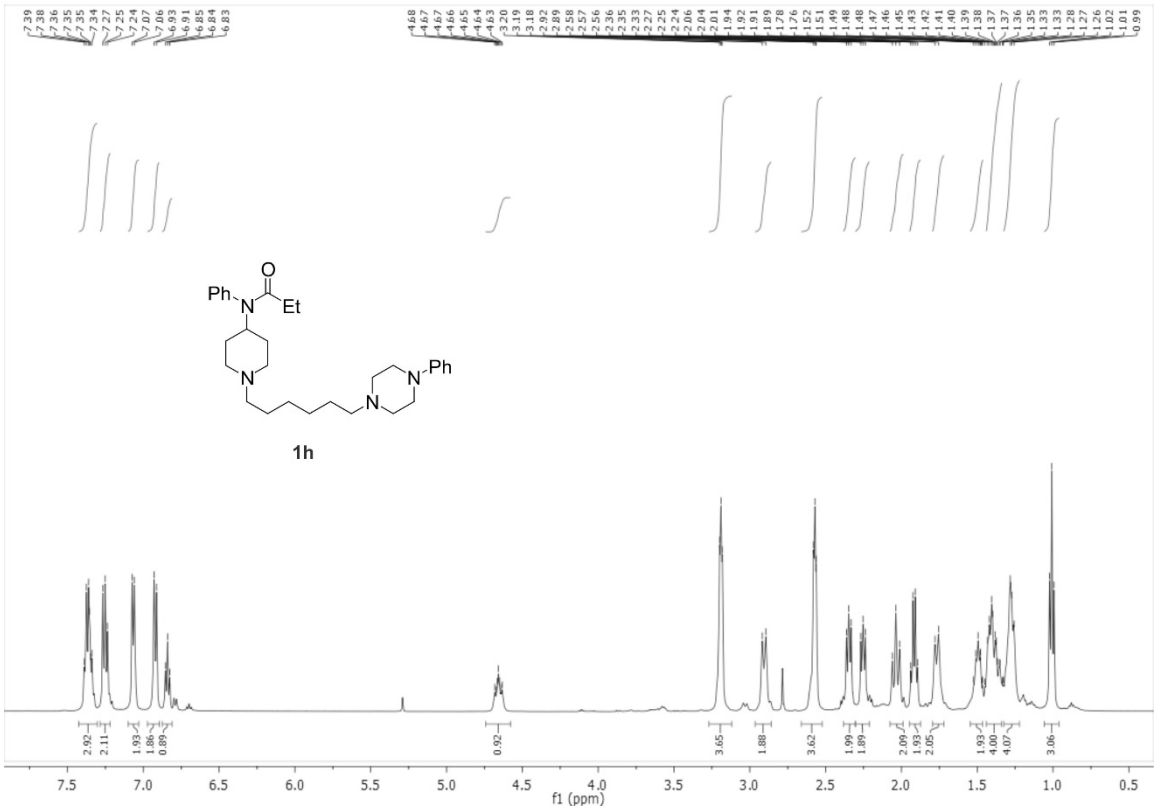


APT (126 MHz, $CDCl_3$)

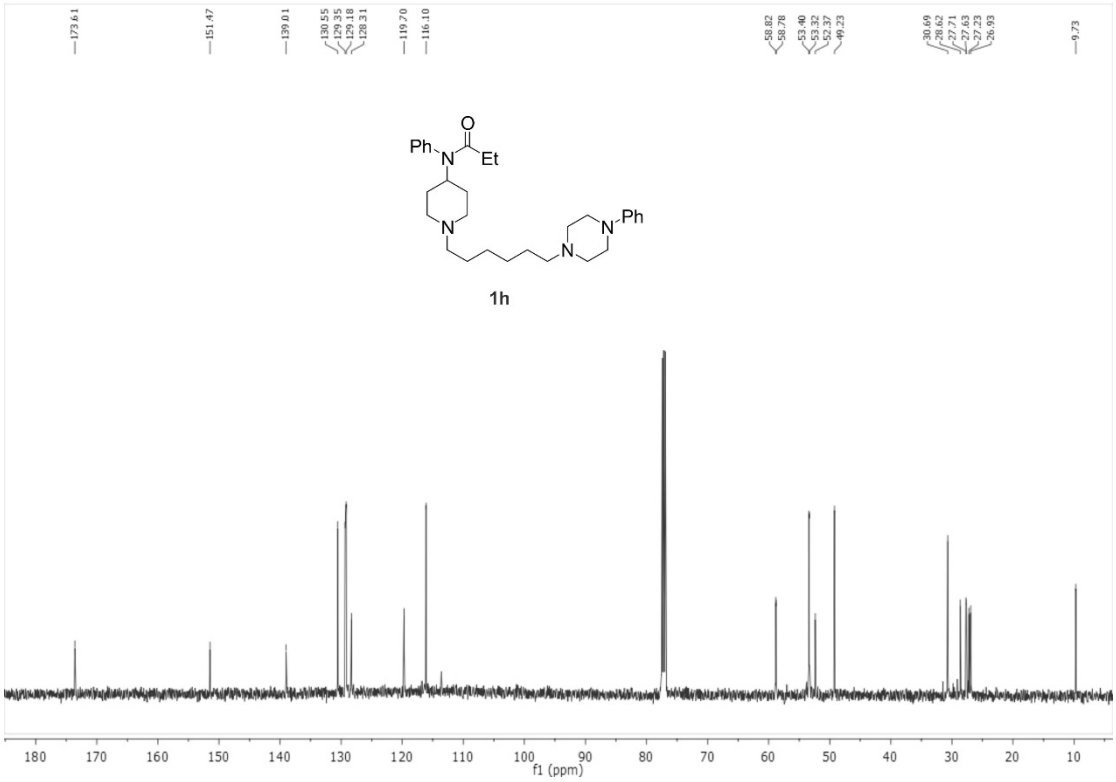



HSQC (CDCl3)
{1.01,9.60}
{1.27,25.71}
{1.91,28.55}
{1.77,30.62}
{1.44,27.16}
{1.40,30.73}
{4.66,52.38}
{2.60,53.45}
{2.04,53.24}
{3.05,51.27}
{2.91,53.35}
{2.37,58.58}
{6.94,118.68}
{7.14,124.63}
{7.13,127.49}
{7.06,130.53}
{7.35,128.28}
{7.36,129.39}
O
Et
N
Ph
Cl
Cl
N
N
1g
f2 (ppm)
f1 (ppm)

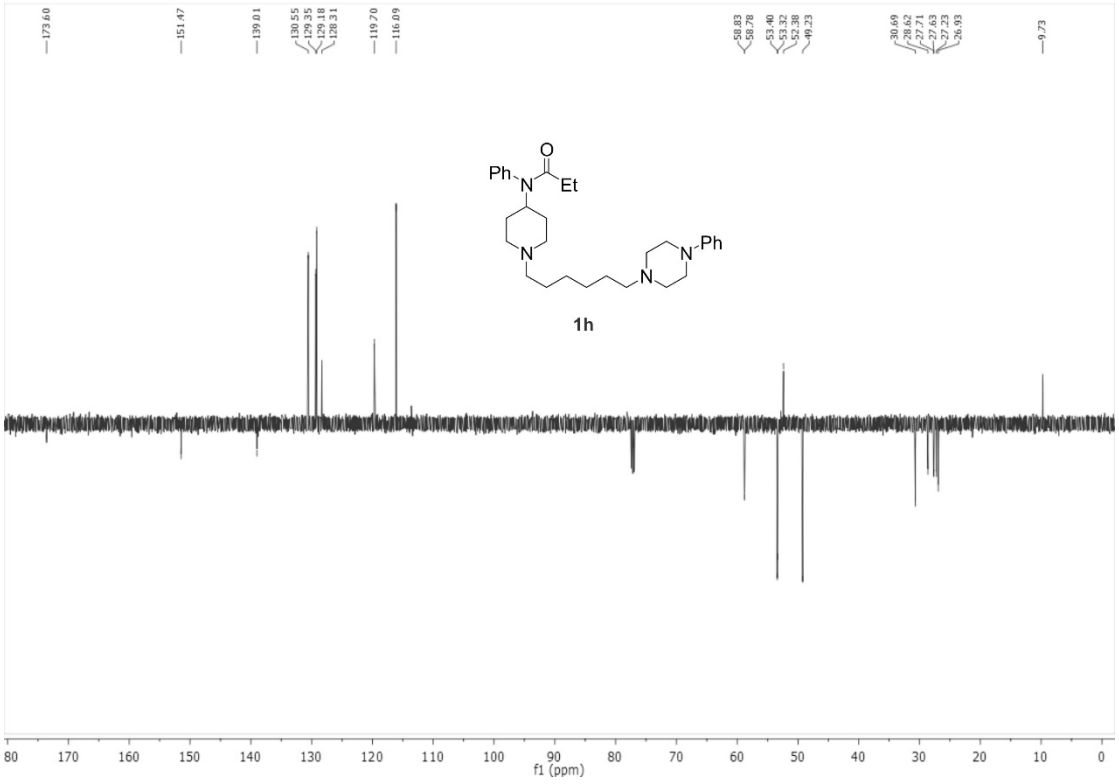
^{1}H NMR (500 MHz, $CDCl_3$)

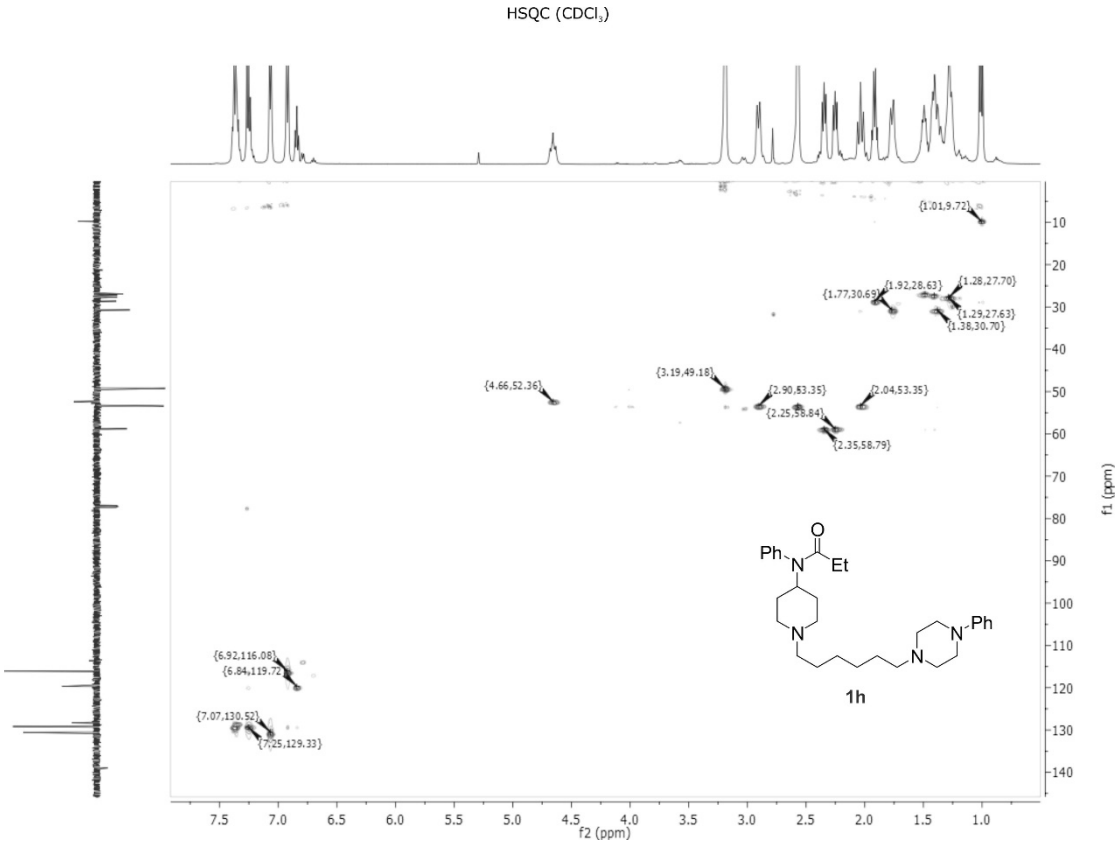


^{13}C NMR (126 MHz, $CDCl_3$)

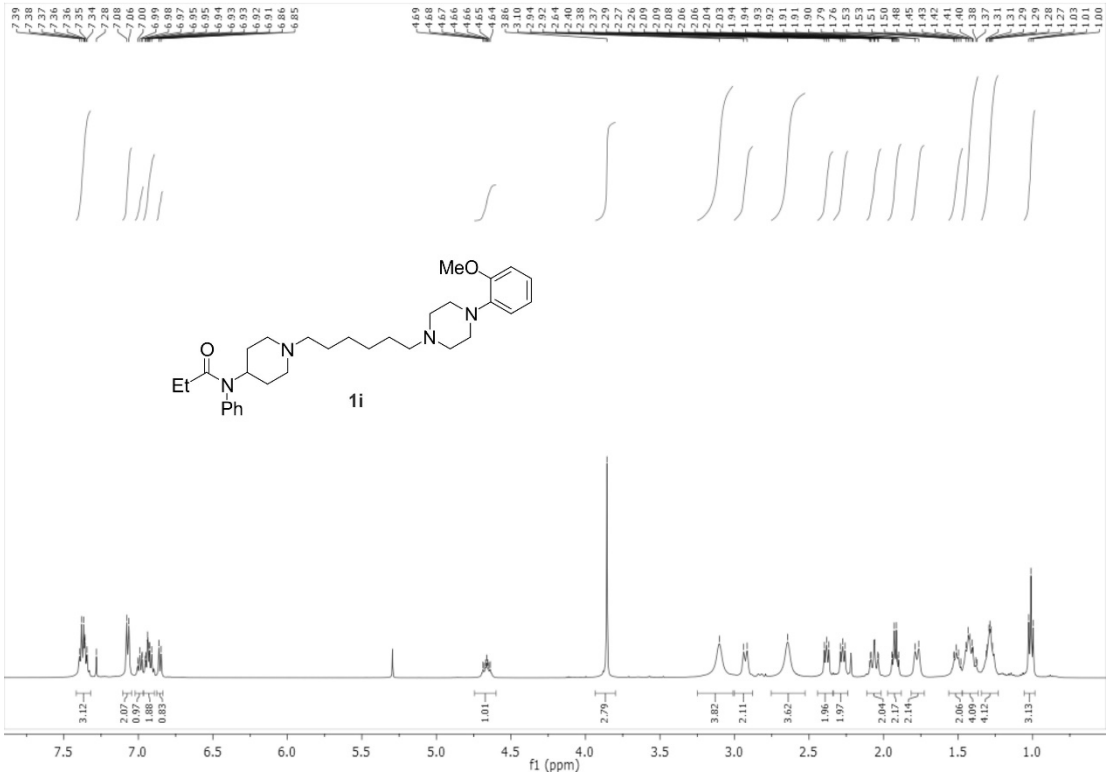


APT (126 MHz, $CDCl_3$)

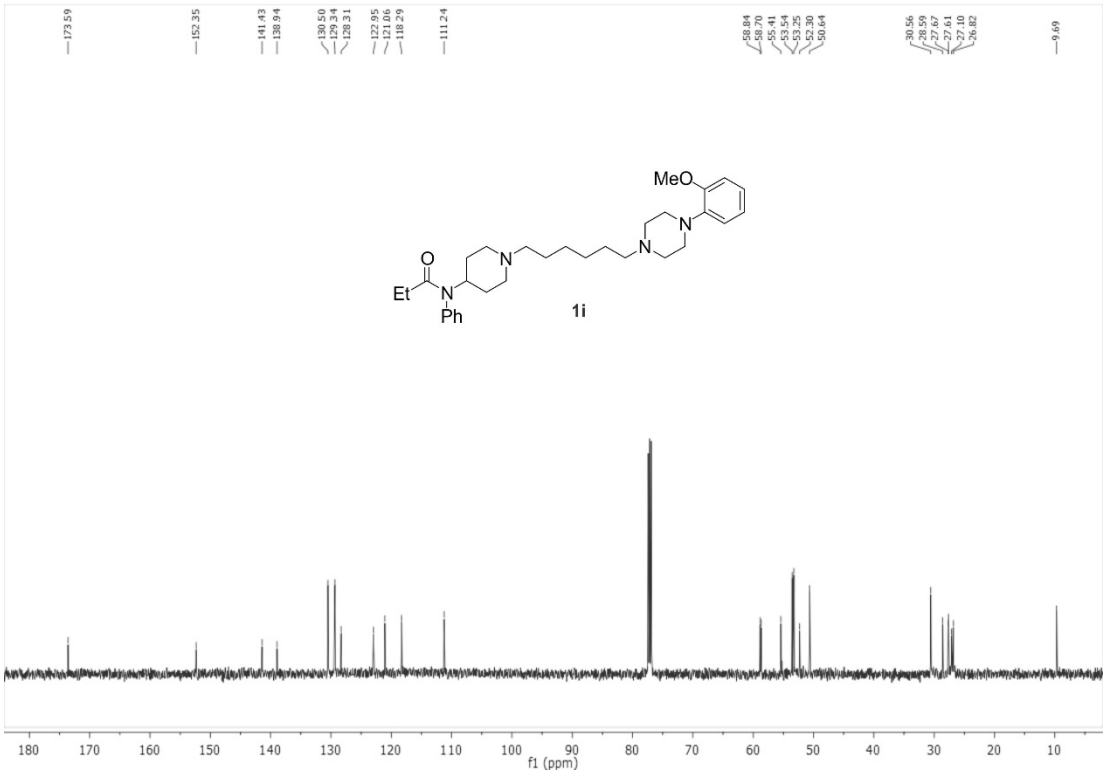



HSQC (CDCl3)
{1.01,9.72}
{1.77,30.69}
{1.92,28.63}
{1.28,27.70}
{1.29,27.63}
{1.38,30.70}
{4.66,52.36}
{3.19,49.18}
{2.90,53.35}
{2.04,53.35}
{2.25,58.84}
{2.35,58.79}
{6.92,116.08}
{6.84,119.72}
{7.07,130.52}
{7.25,129.33}
Ph
N
O
Et
N
N
N
Ph
1h
f2 (ppm)
f1 (ppm)

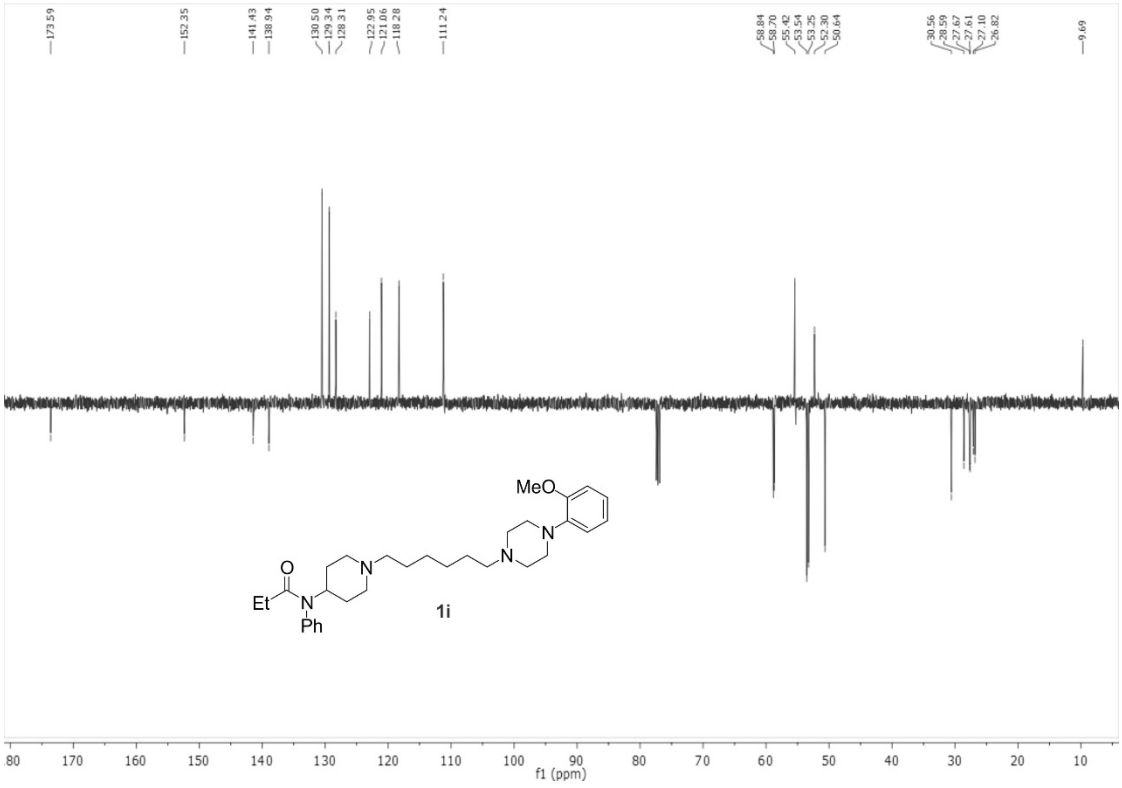
^{1}H NMR (500 MHz, $CDCl_3$)

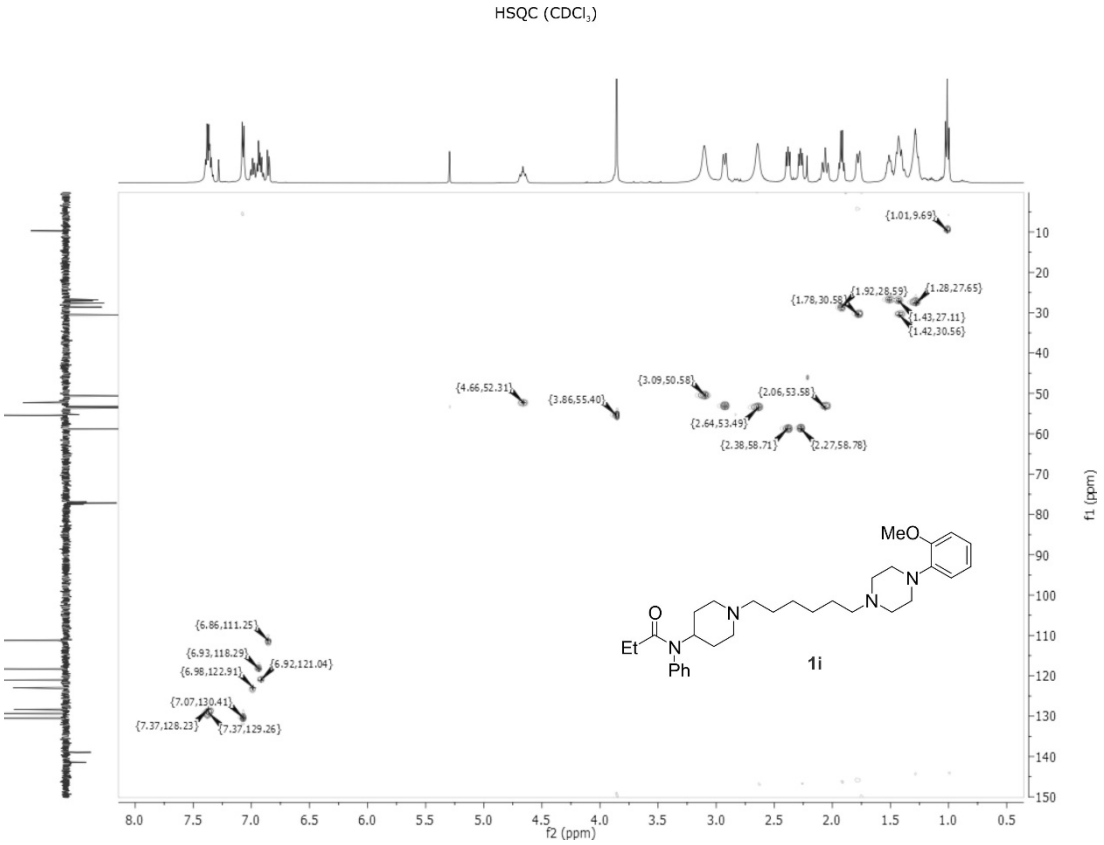


^{13}C NMR (126 MHz, $CDCl_3$)

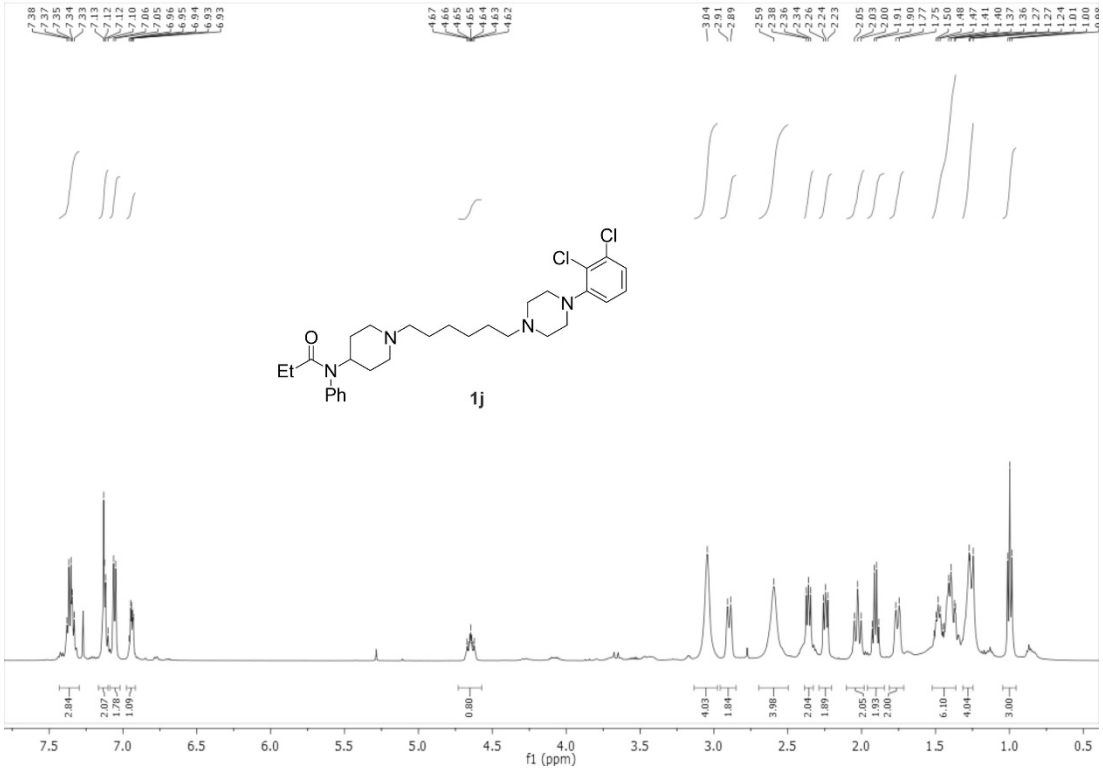


APT (126 MHz, $CDCl_3$)

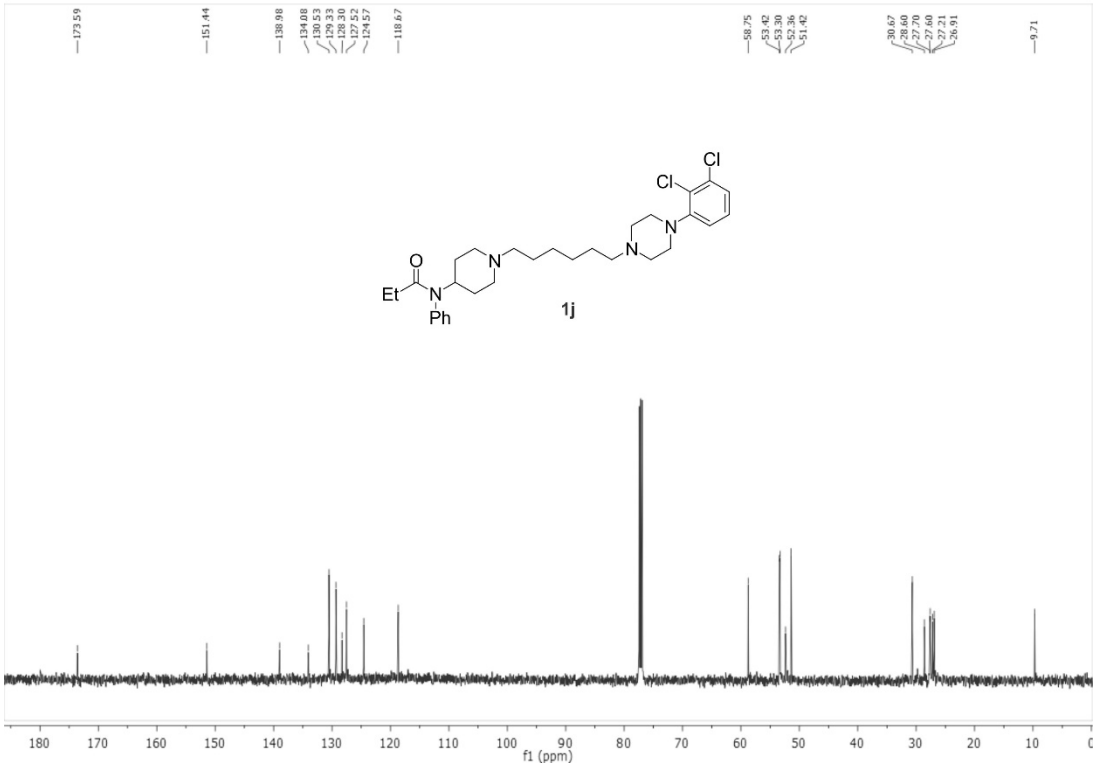



HSQC (CDCl3)
{1.01,9.69}
{1.78,30.58}
{1.92,28.59}
{1.28,27.65}
{1.43,27.11}
{1.42,30.56}
{4.66,52.31}
{3.86,55.40}
{3.09,50.58}
{2.06,53.58}
{2.64,53.49}
{2.38,58.71}
{2.27,58.78}
{6.86,111.25}
{6.93,118.29}
{6.92,121.04}
{6.98,122.91}
{7.07,130.41}
{7.37,128.23}
{7.37,129.26}
MeO
N
N
N
O
Et
N
Ph
1i
f2 (ppm)
f1 (ppm)

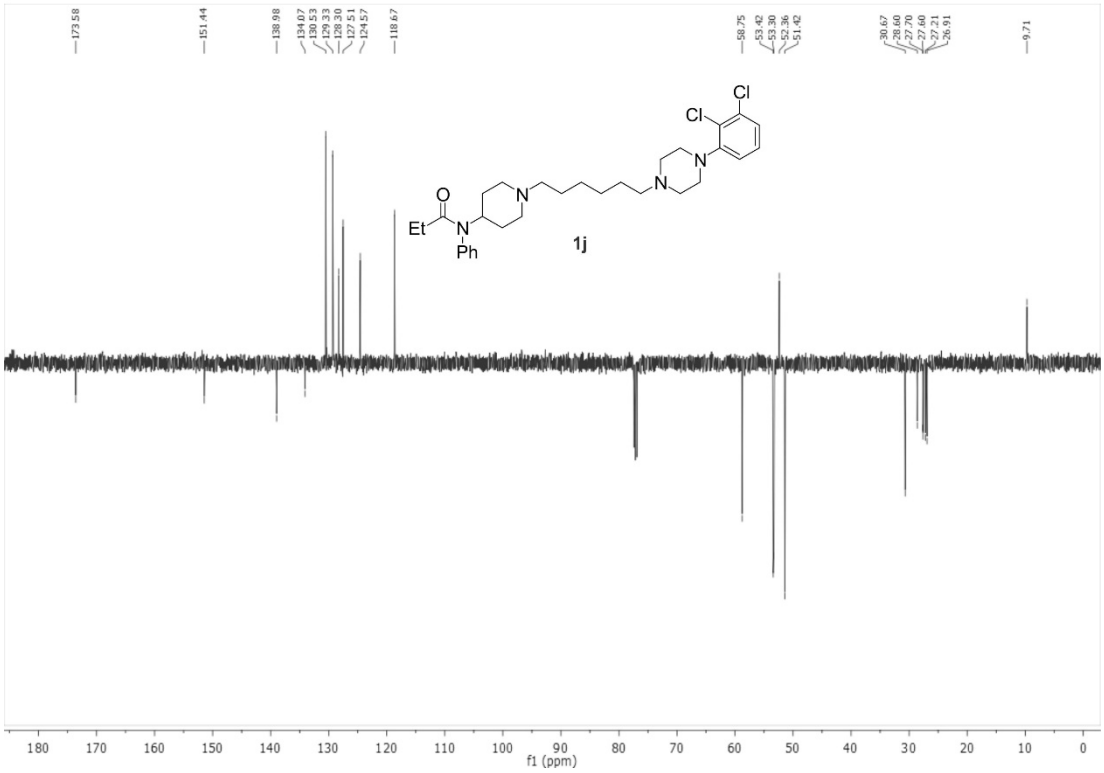
^{1}H NMR (500 MHz, $CDCl_3$)

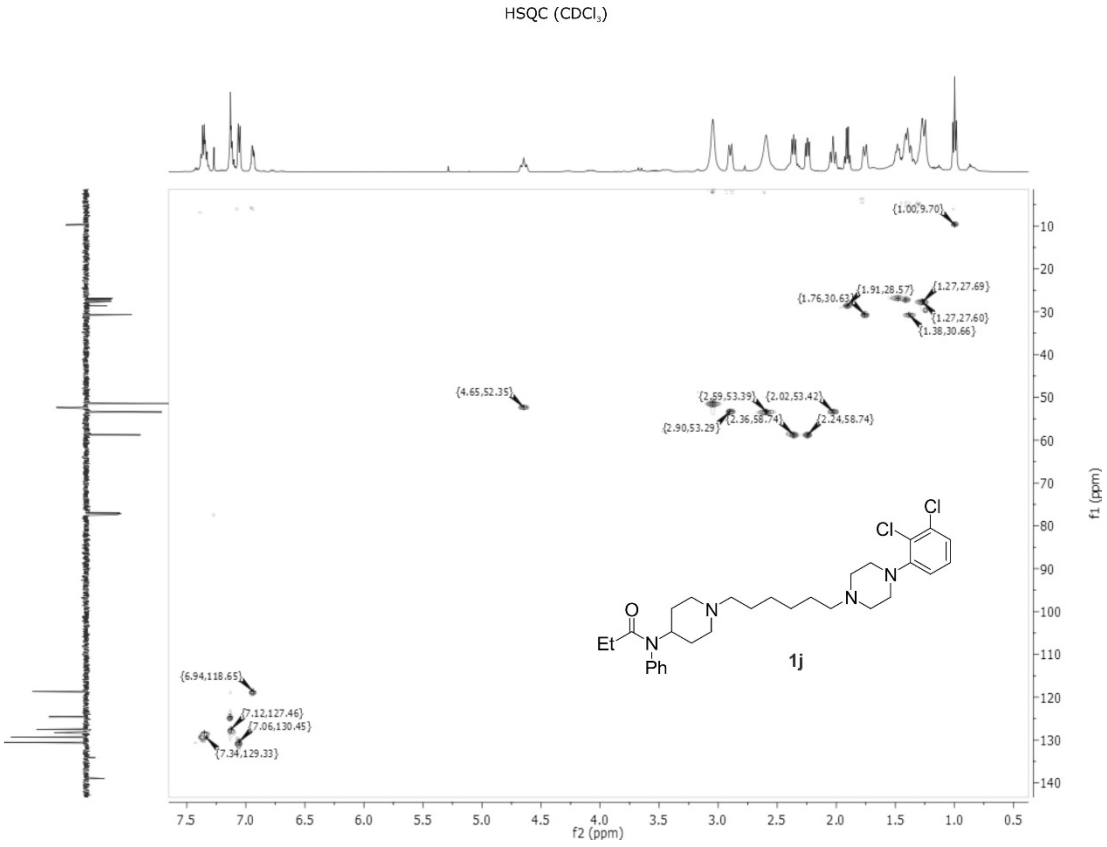


^{13}C NMR (126 MHz, $CDCl_3$)

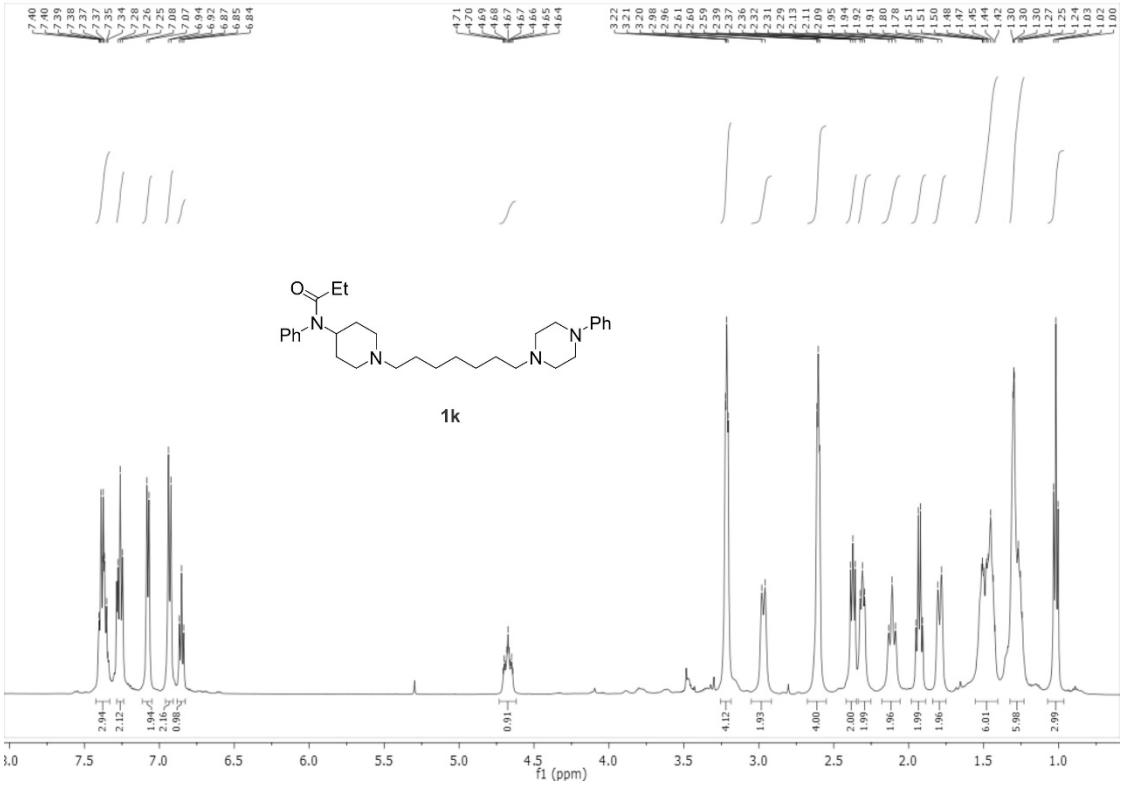


APT (126 MHz, $CDCl_3$)

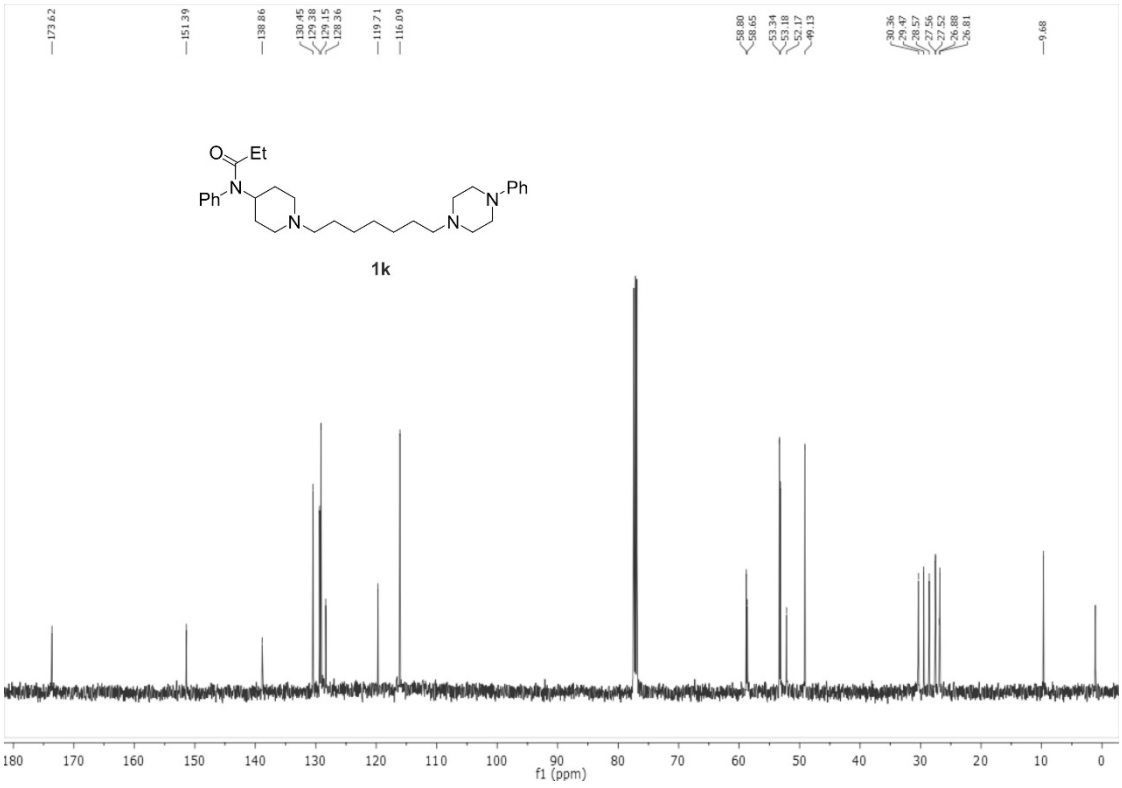



HSQC (CDCl3)
{1.00,9.70}
{1.91,28.57}
{1.27,27.69}
{1.76,30.63}
{1.27,27.60}
{1.38,30.66}
{4.65,52.35}
{2.59,53.39}
{2.02,53.42}
{2.90,53.29}
{2.36,58.74}
{2.24,58.74}
{6.94,118.65}
{7.12,127.46}
{7.06,130.45}
{7.34,129.33}
Cl
Cl
N
N
N
O
Et
N
Ph
1j
f2 (ppm)
f1 (ppm)

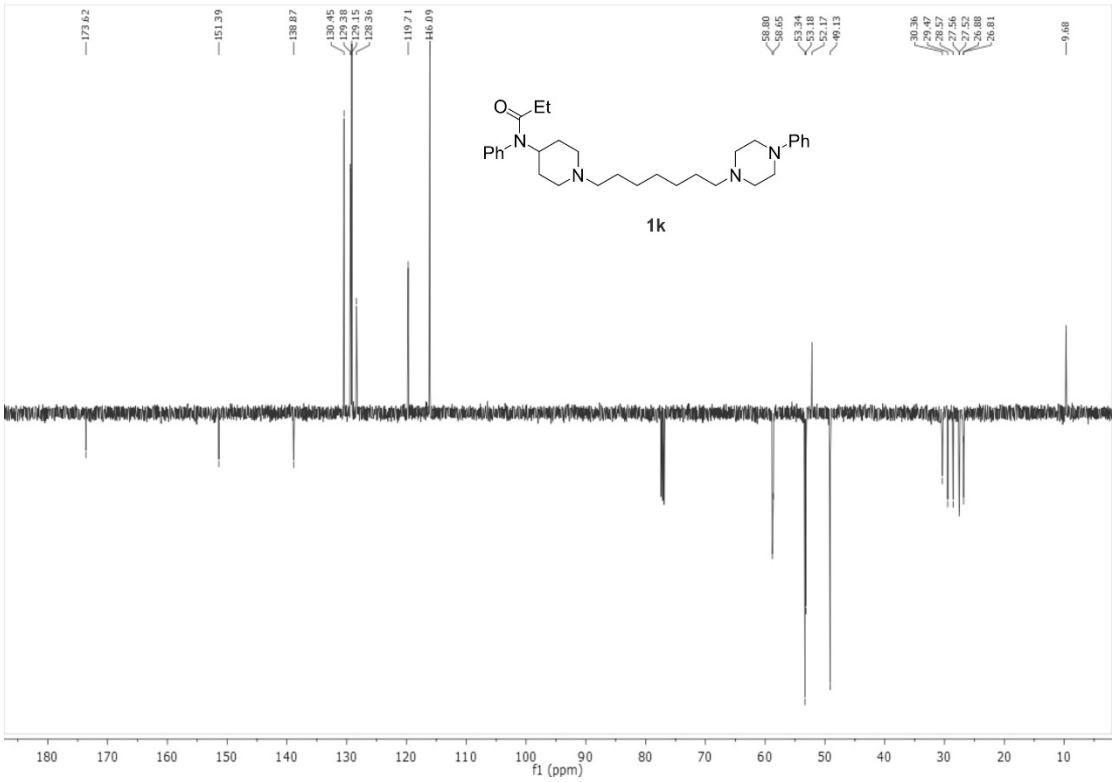
^{1}H NMR (500 MHz, $CDCl_3$)

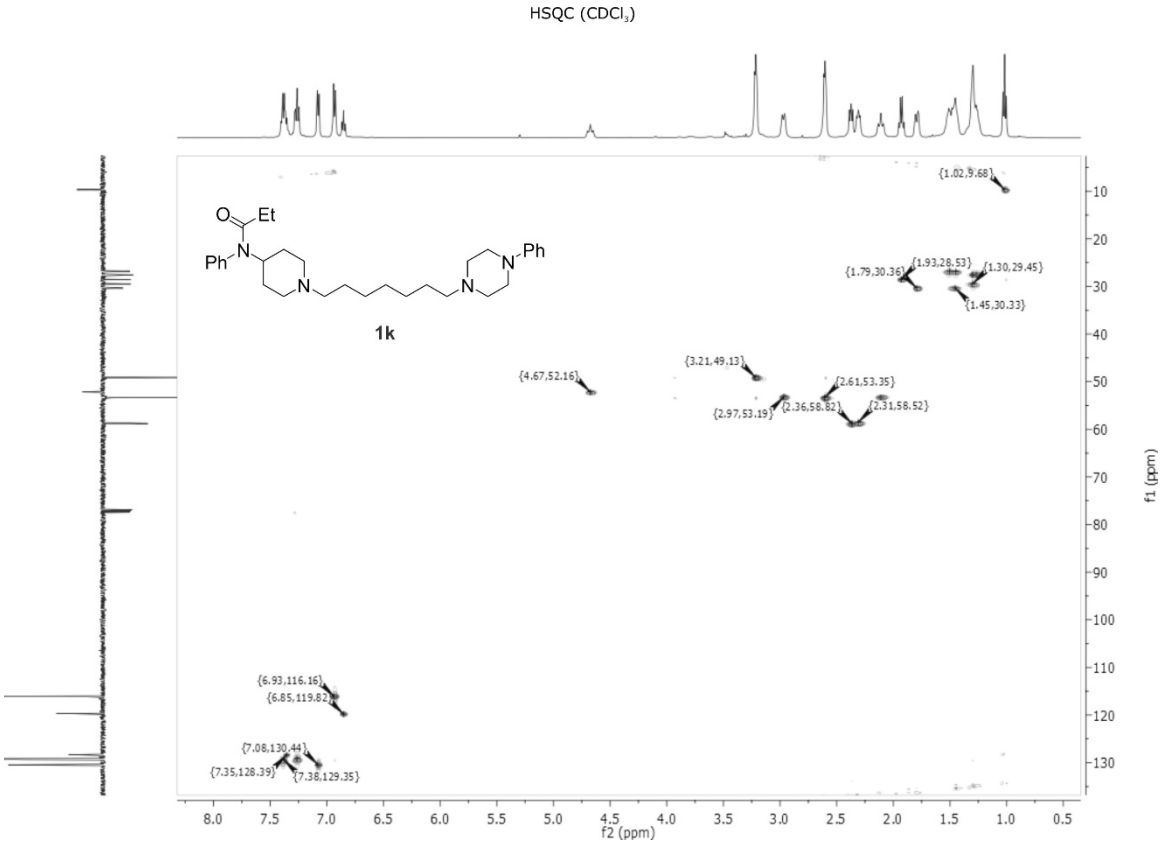


^{13}C NMR (126 MHz, $CDCl_3$)

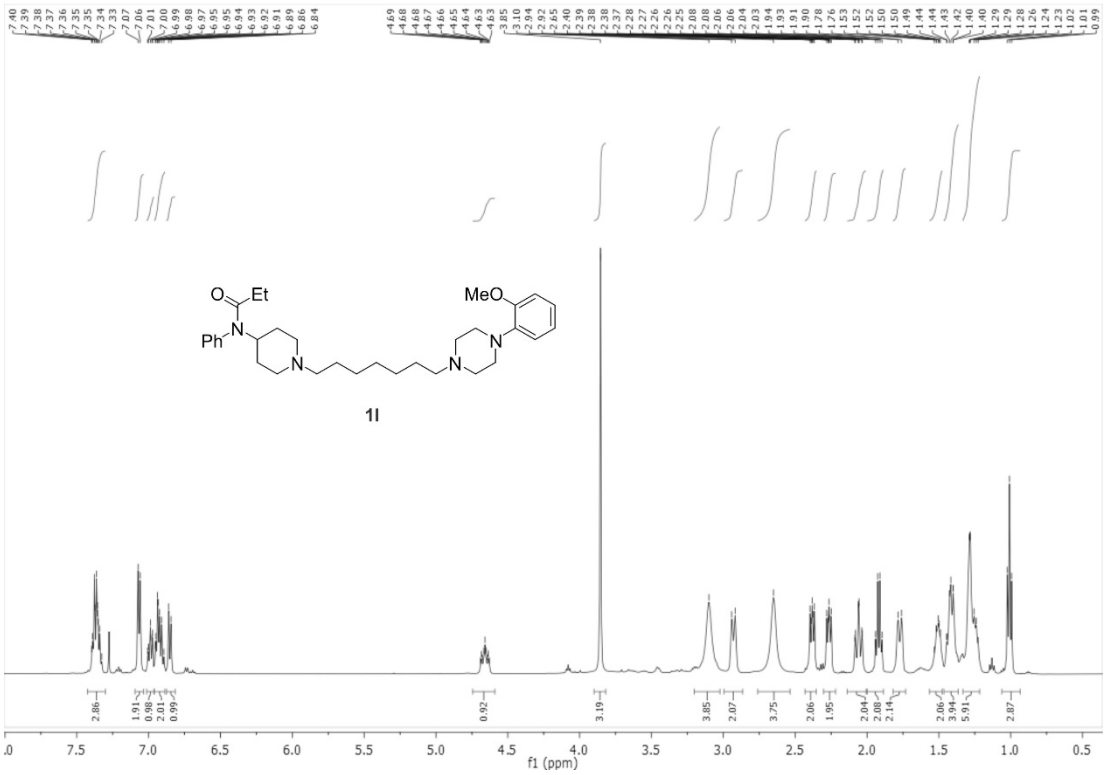


APT (126 MHz, $CDCl_3$)

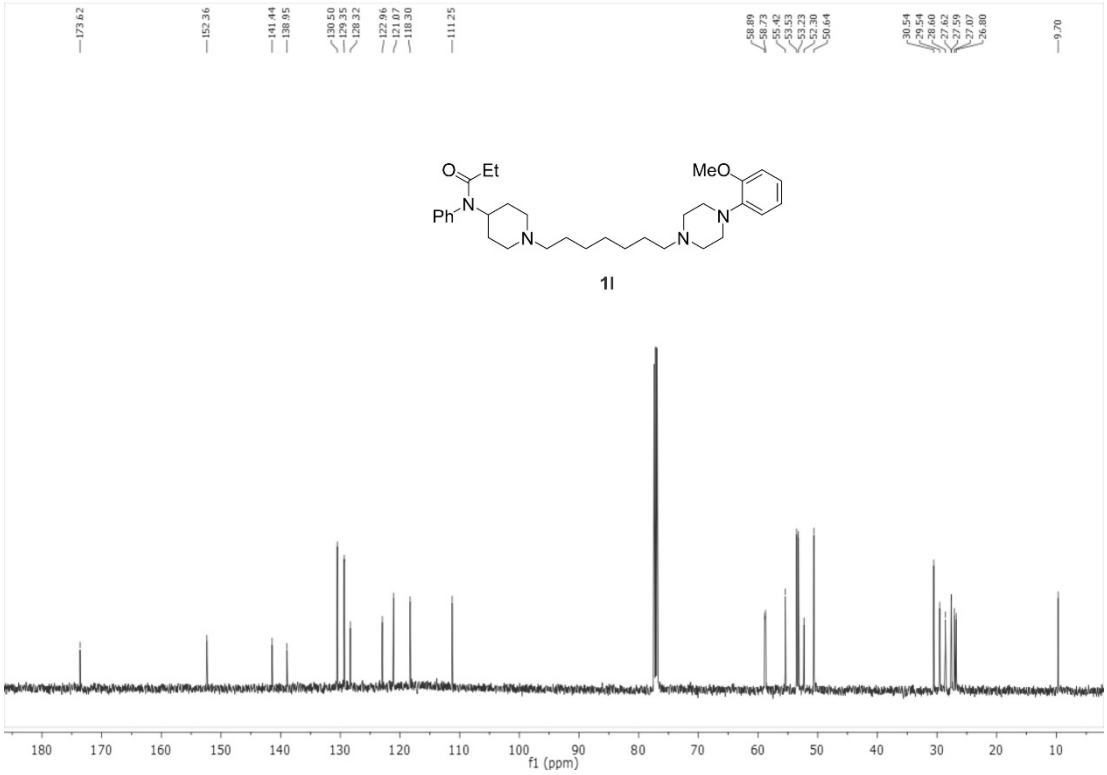



HSQC (CDCl3)
O
Et
N
Ph
N
N
Ph
1k
{1.02,9.68}
{1.79,30.36}
{1.93,28.53}
{1.30,29.45}
{1.45,30.33}
{4.67,52.16}
{3.21,49,13}
{2.61,53.35}
{2.97,53.19}
{2.36,58.82}
{2.31,58.52}
{6.93,116.16}
{6.85,119.82}
{7.08,130.44}
{7.35,128.39}
{7.38,129.35}
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f2 (ppm)
10 20 30 40 50 60 70 80 90 100 110 120 130
f1 (ppm)

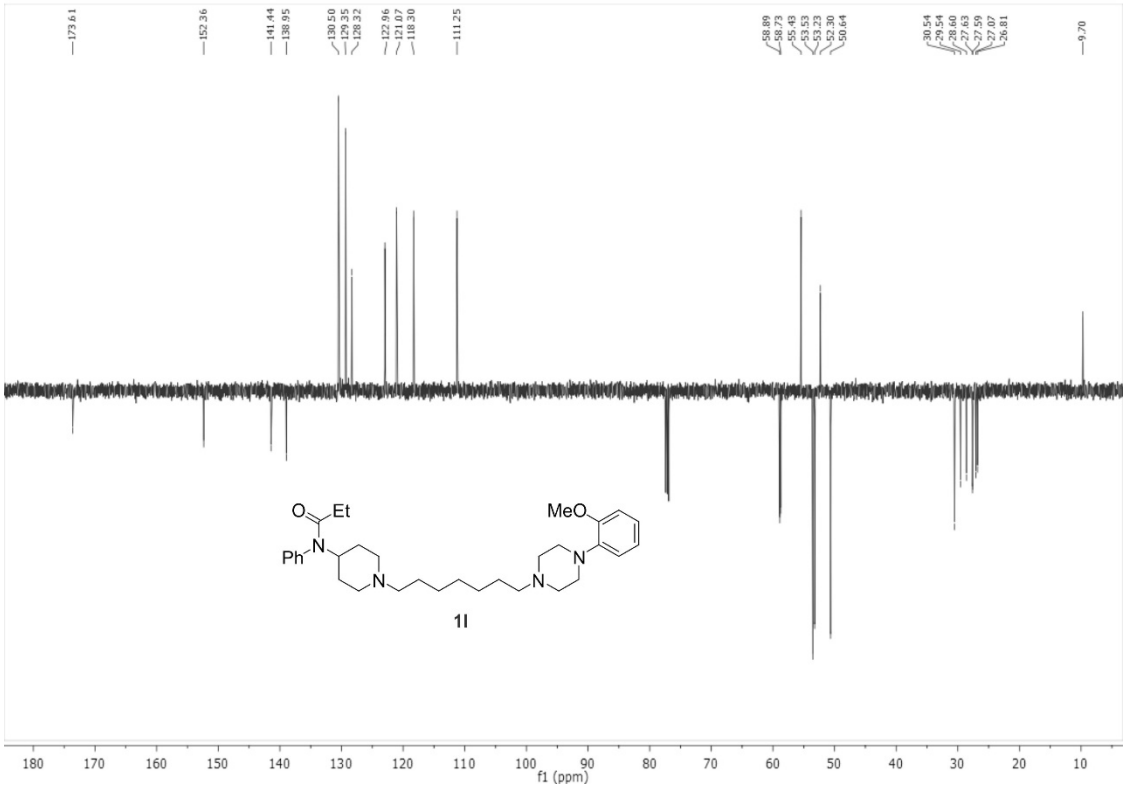
^{1}H NMR (500 MHz, $CDCl_3$)



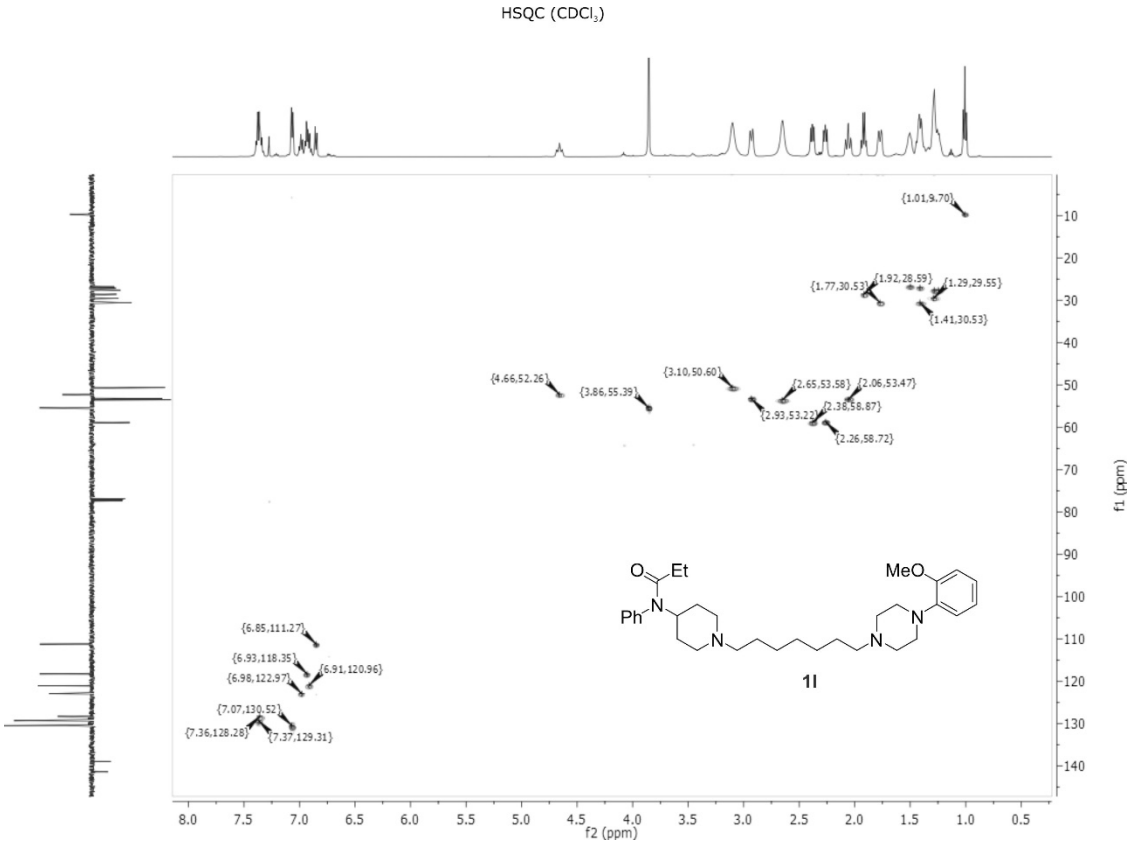
^{13}C NMR (126 MHz, $CDCl_3$)



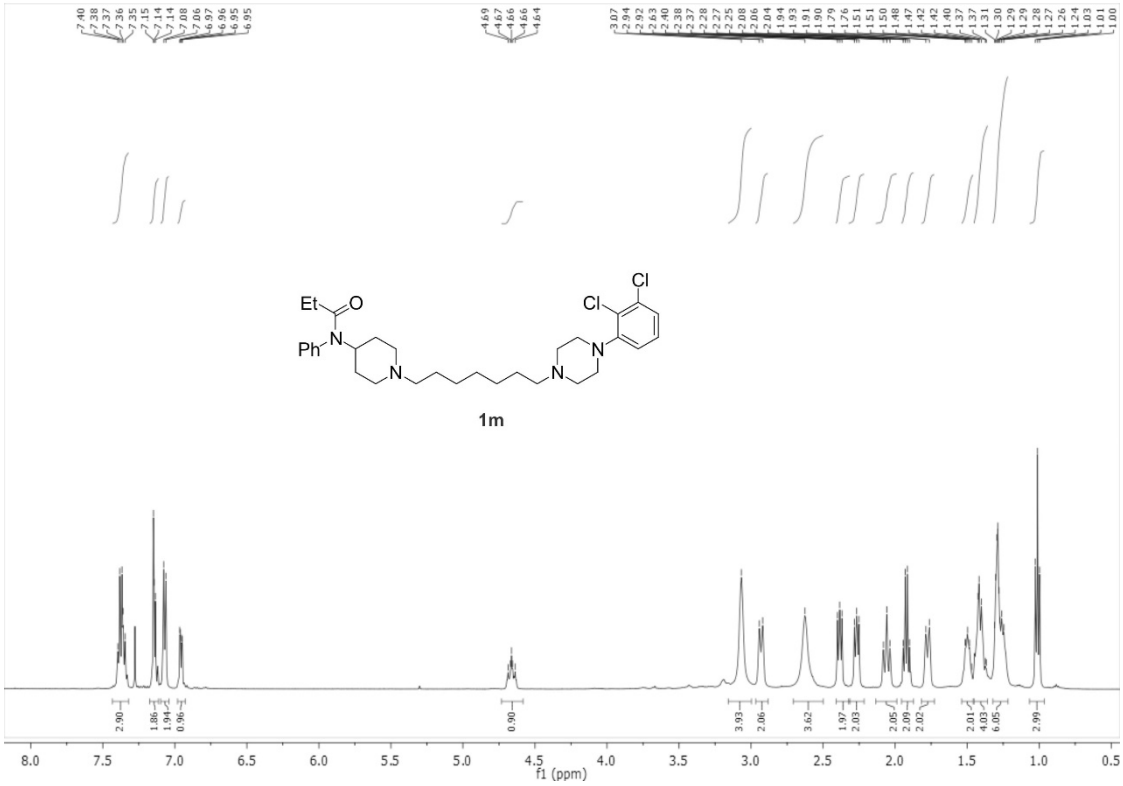
APT (126 MHz, $CDCl_3$)



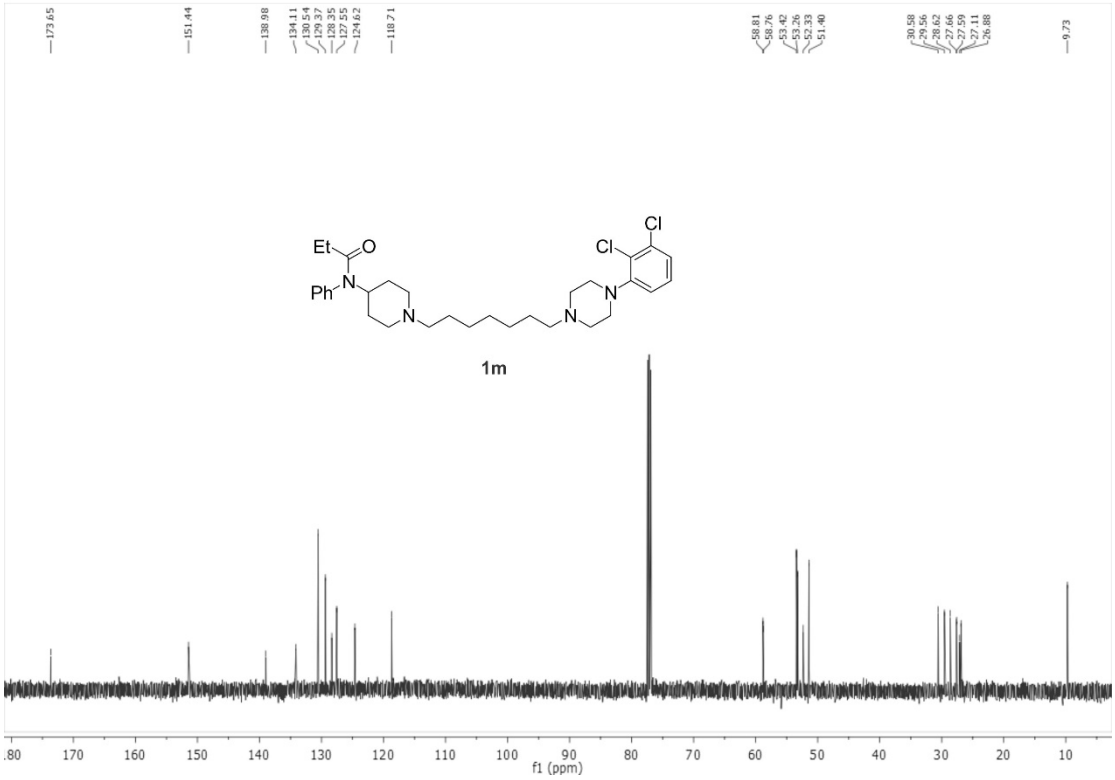
1l


HSQC (CDCl3)
{1.01,9.70}
{1.77,30.53}
{1.92,28.59}
{1.29,29.55}
{1.41,30.53}
{4.66,52.26}
{3.86,55.39}
{3.10,50.60}
{2.65,53.58}
{2.06,53.47}
{2.93,53.22}
{2.38,58.87}
{2.26,58.72}
{6.85,111.27}
{6.93,118.35}
{6.91,120.96}
{6.98,122.97}
{7.07,130.52}
{7.36,128.28}
{7.37,129.31}
O
Et
Ph
N
MeO
1I
f1 (ppm)
f2 (ppm)

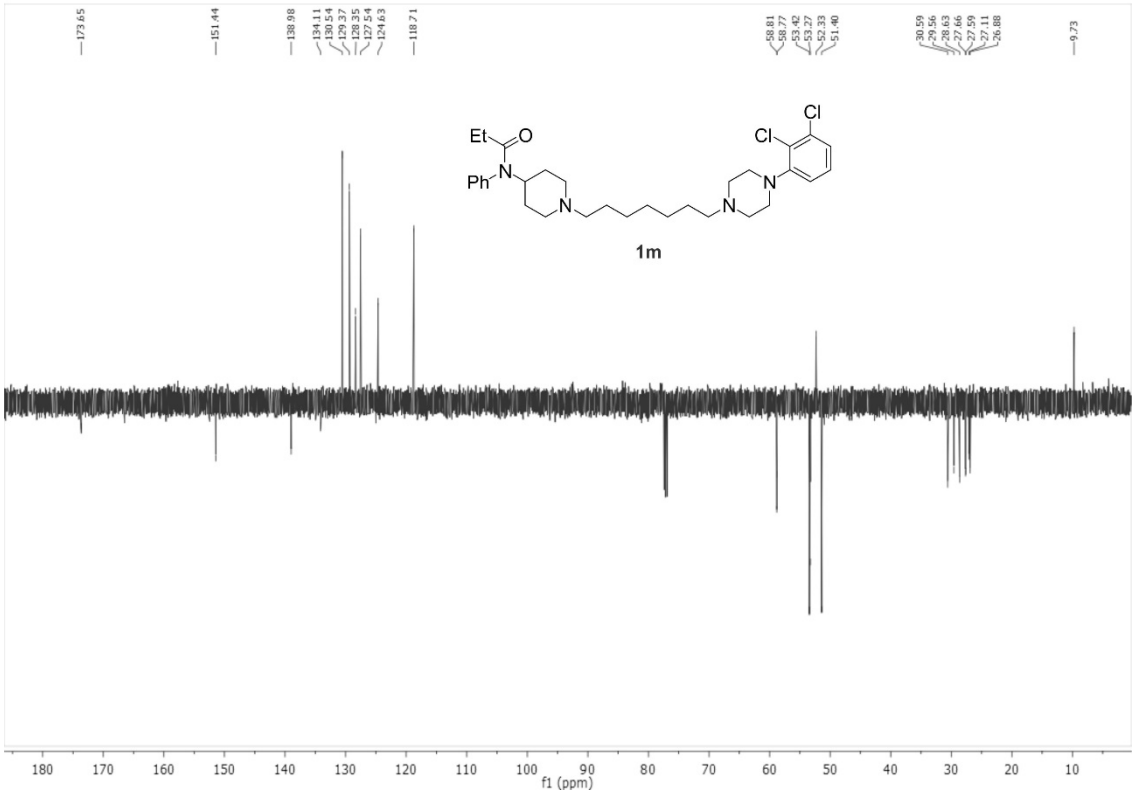
^{1}H NMR (500 MHz, $CDCl_3$)

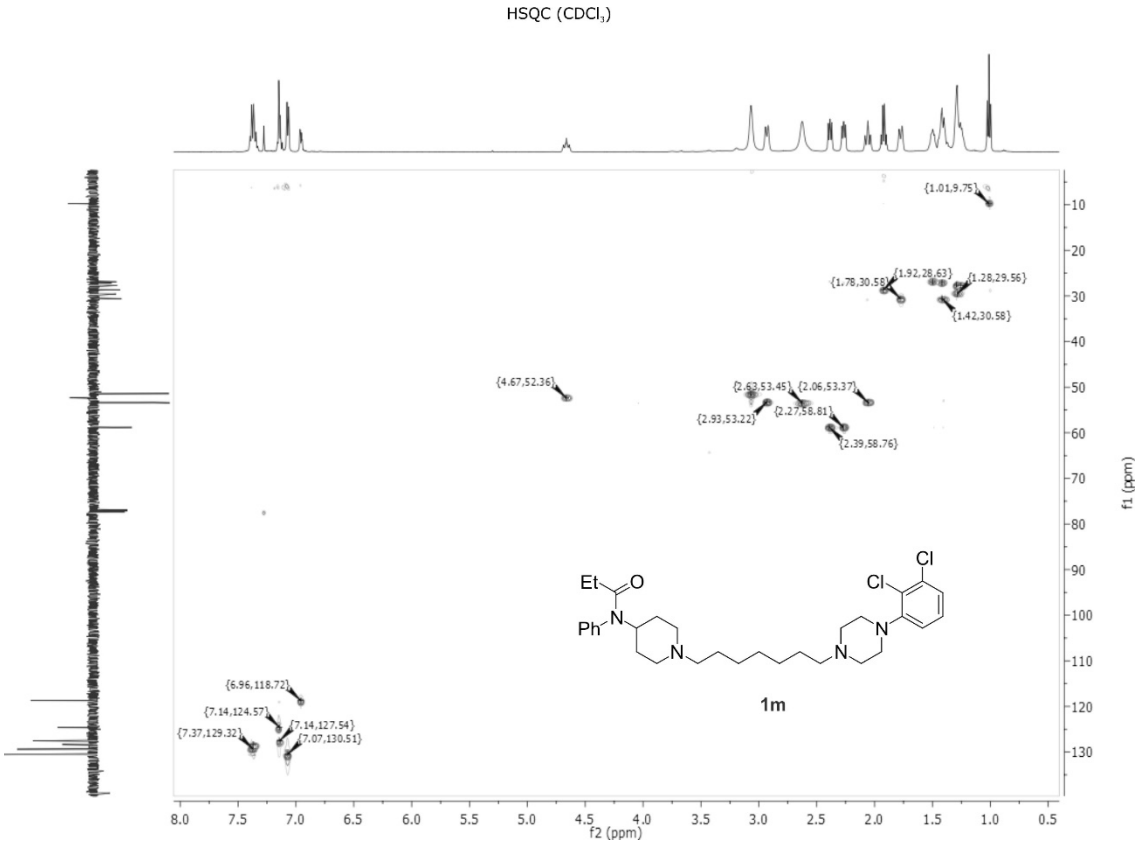


^{13}C NMR (126 MHz, $CDCl_3$)



APT (126 MHz, $CDCl_3$)




HSQC (CDCl3)
{1.01,9.75}
{1.78,30.58}
{1.92,28.63}
{1.28,29.56}
{1.42,30.58}
{4.67,52.36}
{2.63,53.45}
{2.06,53.37}
{2.93,53.22}
{2.27,58.81}
{2.39,58.76}
{6.96,118.72}
{7.14,124.57}
{7.14,127.54}
{7.37,129.32}
{7.07,130.51}
Et
O
N
Ph
Cl
Cl
N
N
1m
f2 (ppm)
f1 (ppm)