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SUPPLEMENTARY MATERIAL TO

Synthetic route towards potential bivalent ligands possessing opioid and D_2/D_3 pharmacophores

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ISOLATED YIELDS AND SPECTROSCOPIC DATA OF SYNTHESIZED COMPOUNDS

*8-(*N*-Phenylpropionamido)-5-azaspiro [4.5] decan-5-ium chloride (**8a**).* Yield: 0.27 g (64.5 %); yellow oil; IR (ATR, cm^{-1}): 2977.3 (C–H aliphatic), 1645.1 (C=O), 1272.8 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.53–7.40 (3H, *m*, Ar-H), 7.14 (2H, *d*, J = 7.1 Hz, Ar-H), 4.82–4.59 (1H, *m*, CH-H), 4.02–3.74 (6H, *m*, CH_2-H), 3.66–3.51 (2H, *m*, CH_2-H), 2.23 (4H, *brs*), 2.12 (2H, *d*, J = 13.5 Hz, CH_2-2), 2.05–1.86 (4H, *m*, CH_2-H), 0.98 (3H, *t*, J = 7.4 Hz, CH_3-3); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 174.1, 139.1, 130.3, 129.7, 129.2, 67.1, 59.3, 57.7, 51.0, 41.2, 28.7, 26.0, 21.8, 21.2, 9.6; HRMS-HESI--Orbitrap: Calcd. for $C_{18}H_{27}N_2O^+$ $[M]^+$: 287.21179. Found: 287.21169.

*3-(*N*-Phenylpropionamido)-6-azaspiro [5.5] undecan-6-ium chloride (**8b**).* Yield: 0.29 g (66.2 %); yellow oil; IR (ATR, cm^{-1}): 2943.0 (C–H aliphatic), 1647.4 (C=O), 1269.7 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.53–7.37 (3H, *m*, Ar-H), 7.15 (2H, *dd*, J = 7.3 & 1.9 Hz, Ar-H), 4.61–4.49 (1H, *m*, CH-H), 4.03 (2H, *d*, J = 12.6 Hz, CH_2-H), 3.90–3.82 (2H, *m*, CH_2-H), 3.78 (2H, *t*, J = 12.2 Hz, CH_2-H), 3.59 (2H, *brs*, CH_2-H), 2.29–2.10 (2H, *m*, CH_2-H), 2.07 (2H, *d*, J = 13.1 Hz, CH_2-H), 1.98–1.87 (4H, *m*, CH_2-H), 1.79 (4H, *brs*, CH_2-H), 0.98 (3H, *t*, J = 7.4 Hz, CH_3-H); ^{13}C-NMR (126 MHz, $CDCl_3$,

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δ / ppm): 174.2, 139.8, 130.3, 129.3, 129.1, 64.2, 58.2, 53.7, 52.4, 28.8, 23.4, 21.3, 20.2, 19.7, 9.5; HRMS-HESI-Orbitrap: Calcd. for $C_{19}H_{29}N_2O^+$ $[M]^+$: 301.22744. Found: 301.22694.

N-*Phenylpiperidin-4-amine (**6**)*. Obtained from **9** *via* a three-step procedure already known from the literature.[4,5] Overall yield: 8.00 g (84.5 %); pale yellow oil; ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.21–7.09 (2H, *m*, Ar-H), 6.67 (1H, *t*, J = 7.3 Hz, Ar-H), 6.60 (2H, *d*, J = 7.7 Hz, Ar-H), 3.52 (1H, *brs*, NH-H), 3.36 (1H, *brs*, CH-H), 3.11 (2H, *dt*, J = 12.8 & 3.5 Hz, CH_2-H), 2.71 (2H, *td*, J = 12.5 & 2.5 Hz, CH_2-H), 2.07 (2H, *d*, J = 12.5 Hz, CH_2-H), 1.78 (1H, *brs*, NH-H), 1.40–1.21 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 146.9, 129.2, 117.1, 113.2, 50.3, 45.5, 33.9.

*4-Chloro-1-(4-phenylpiperazin-1-yl)butan-1-one (**7a**)*. Yield: 0.90 g (97.3 %); pale yellow oil; IR (ATR, cm^{-1}): 2916.3 (C–H aliphatic), 1644.4 (C=O), 869.9 (C–Cl); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.28–7.17 (2H, *m*, Ar-H), 6.97–6.77 (3H, *m*, Ar-H), 3.76–3.67 (2H, *m*, CH_2-H), 3.64–3.54 (4H, *m*, CH_2-H), 3.11 (4H, *dt*, J = 16.4 & 5.2 Hz, CH_2-H), 2.49 (2H, *t*, J = 7.1 Hz, CH_2-H), 2.13––2.05 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 170.3, 151.0, 129.4, 120.7, 116.7, 49.8, 49.5, 45.5, 45.0, 41.7, 29.8, 28.0.

*4-Chloro-1-(4-(3-methoxyphenyl)piperazin-1-yl)butan-1-one (**7b**)*. Yield: 0.99 g (95.9 %); pale yellow oil; IR (ATR, cm^{-1}): 2919.8 (C–H aliphatic), 1590.8 (C=O), 746.9 (C–Cl); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.05–6.97 (1H, *m*, Ar-H), 6.94–6.82 (3H, *m*, Ar-H), 3.86 (3H, *s*, OCH_3-H), 3.81–3.75 (2H, *m*, CH_2-H), 3.69–3.60 (4H, *m*, CH_2-H), 3.02 (4H, *dt*, J = 18.4 & 5.1 Hz, CH_2-H), 2.53 (2H, *t*, J = 7.1 Hz, CH_2-H), 2.14 (2H, *q*, J = 6.5 Hz, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 170.3, 152.4, 140.7, 123.7, 121.2, 118.5, 111.5, 55.5, 51.1, 50.7, 45.8, 45.0, 42.0, 29.9, 28.0.

*4-Chloro-1-(4-(2,3-dichlorophenyl)piperazin-1-yl)butan-1-one (**7c**)*. Yield: 1.14 g (97.9 %); pale yellow oil; IR (ATR, cm^{-1}): 2921.7 (C–H aliphatic), 1644.6 (C=O), 784.2 (C–Cl), 715.0 (C–Cl); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.24––7.13 (2H, *m*, Ar-H), 6.93 (1H, *dd*, J = 7.7 & 1.9 Hz, Ar-H), 3.84–3.77 (2H, *m*, CH_2-H), 3.69–3.65 (4H, *m*, CH_2-H), 3.07–2.98 (4H, *m*, CH_2-H), 2.56 (2H, *t*, J = 7.1 Hz, CH_2-H), 2.20–2.12 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 170.4, 150.7, 134.2, 127.7, 125.3, 118.9, 51.7, 45.9, 45.8, 44.9, 41.9, 29.8, 28.0.

*4-(4-(Phenylamino)piperidin-1-yl)-1-(4-phenylpiperazin-1-yl)butan-1-one (**13a**)*. Yield: 0.34 g (49.2 %); pale yellow oil. IR (ATR, cm^{-1}): 3340.7 (N–H amine), 3048.8 (C–H aromatic), 2939.2 (C–H aliphatic), 1637.7 (C=O), 1232.1 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.34–7.20 (2H, *m*, Ar-H), 7.22–7.07 (2H, *m*, Ar-H), 6.97–6.79 (3H, *m*, Ar-H), 6.76–6.63 (1H, *m*, Ar-H), 6.64–6.56 (2H, *m*, Ar-H), 3.86–3.73 (2H, *m*, CH_2-H), 3.70–3.60 (2H, *m*, CH_2-H), 3.51 (1H, *brs*, NH-H), 3.37–3.24 (1H, *m*, CH-H), 3.21–3.11 (4H, *m*, CH_2-H),

2.89 (2H, *d*, *J* = 11.4 Hz, CH_2-H), 2.51–2.34 (4H, *m*, CH_2-H), 2.25–2.10 (2H, *m*, CH_2-H), 2.06 (2H, *d*, *J* = 12.0 Hz, CH_2-H), 1.95–1.81 (2H, *m*, CH_2-H), 1.60––1.37 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, *δ* / ppm): 171.5, 151.1, 147.2, 129.4, 129.4, 120.7, 117.3, 116.7, 113.4, 58.0, 52.5, 50.0, 49.9, 49.5, 45.6, 41.6, 32.6, 31.1, 22.8.

*1-(4-(3-Methoxyphenyl)piperazin-1-yl)-4-(4-(phenylamino)piperidin-1-yl) butan-1-one (**13b**).* Yield: 0.33 g (45.1 %); pale yellow oil; IR (ATR, cm^{-1}): 3340.4 (N–H amine), 3050.8 (C–H aromatic), 2936.6 (C–H aliphatic), 1636.4 (C=O), 1241.5 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, *δ* / ppm): 7.21–7.11 (2H, *m*, Ar-H), 7.11–6.99 (1H, *m*, Ar-H), 6.96–6.87 (3H, *m*, Ar-H), 6.73–6.63 (1H, *m*, Ar-H), 6.62–6.56 (2H, *m*, Ar-H), 3.87 (3H, *s*, OCH_3-H), 3.83–3.77 (2H, *m*, CH_2-H), 3.73–3.61 (2H, *m*, CH_2-H), 3.52 (1H, *brs*, NH-H), 3.34–3.24 (1H, *m*, CH-H), 3.01–2.96 (4H, *m*, CH_2-H), 2.88 (2H, *d*, *J* = 11.0 Hz, 2H), 2.47–2.36 (4H, *m*, CH_2-H), 2.14 (2H, *t*, *J* = 11.0 Hz, CH_2-H), 2.05 (2H, *d*, *J* = 11.8 Hz, CH_2-H), 1.94–1.78 (2H, *m*, CH_2-H), 1.58–1.35 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, *δ* / ppm): 171.4, 152.3, 147.1, 140.7, 129.3, 123.6, 121.1, 118.4, 117.2, 113.3, 111.4, 57.9, 55.5, 52.4, 51.1, 50.6, 49.9, 45.9, 41.8, 32.5, 31.0, 22.7.

*1-(4-(2,3-Dichlorophenyl)piperazin-1-yl)-4-(4-(phenylamino)piperidin-1-yl) butan-1-one (**13c**).* Yield: 0.45 g (55 %); pale yellow oil; IR (ATR, cm^{-1}): 3341.4 (N–H amine), 3049.9 (C–H aromatic), 2940.6 (C–H aliphatic), 1638.1 (C=O), 1237.8 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, *δ* / ppm): 7.21–7.11 (3H, *m*, Ar-H), 7.01–6.88 (2H, *m*, Ar-H), 6.71–6.64 (1H, *m*, Ar-H), 6.62–6.56 (2H, *m*, Ar-H), 3.84–3.77 (2H, *m*, CH_2-H), 3.71–3.62 (2H, *m*, CH_2-H), 3.52 (1H, *brs*, NH-H), 3.36–3.28 (1H, *m*, CH-H), 3.05–2.97 (4H, *m*, CH_2-H), 2.94–2.85 (2H, *m*, CH_2-H), 2.46–2.36 (4H, *m*, CH_2-H), 2.22–2.11 (2H, *m*, CH_2-H), 2.10––2.02 (2H, *m*, CH_2-H), 1.93–1.80 (2H, *m*, CH_2-H), 1.60–1.41 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, *δ* / ppm): 171.5, 150.7, 147.2, 134.3, 129.4, 127.8, 127.7, 125.3, 118.8, 117.3, 113.3, 57.9, 52.5, 51.8, 51.2, 50.1, 45.9, 41.9, 32.6, 31.0, 22.7.

N-*Phenyl-1-(4-(4-phenylpiperazin-1-yl)butyl)piperidin-4-amine (**5a**).* Yield: 0.33 g (84.8 %); pale yellow oil; IR (ATR, cm^{-1}): 3397.6 (N–H amine), 3053.4 (C–H aromatic), 2938.4 (C–H aliphatic), 1601.4 (C=O), 1235.7 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, *δ* / ppm): 7.32–7.24 (2H, *m*, Ar-H), 7.21–7.14 (2H, *m*, Ar-H), 6.98–6.91 (2H, *m*, Ar-H), 6.91–6.83 (1H, *m*, Ar-H), 6.73–6.65 (1H, *m*, Ar-H), 6.65–6.57 (2H, *m*, Ar-H), 3.46 (1H, *brs*, NH-H), 3.39––3.28 (1H, *m*, CH-H), 3.27–3.18 (4H, *m*, CH_2-H), 2.92 (2H, *d*, *J* = 11.0 Hz, CH_2-H), 2.65–2.57 (4H, *m*, CH_2-H), 2.46–2.35 (4H, *m*, CH_2-H), 2.15 (2H, *t*, *J* = 11.1 Hz, CH_2-H), 2.08 (2H, *d*, *J* = 12.1 Hz, CH_2-H), 1.62–1.44 (6H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, *δ* / ppm): 151.3, 147.0, 129.3, 129.1, 119.6, 117.2, 116.0, 113.2, 58.5, 58.4, 53.2, 52.4, 49.1, 32.4, 25.0, 24.9.

1-(4-(4-(3-Methoxyphenyl)piperazin-1-yl)butyl)-N-*phenylpiperidin-4-amine (**5b**).* Yield: 0.42 g (84.2 %); pale yellow oil; IR (ATR, cm^{-1}): 3307.5 (N–H amine), 3052.1 (C–H aromatic), 2939.0 (C–H aliphatic), 1601.1 (C=O), 1241.2 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.19–7.12 (2H, *m*, Ar-H), 7.03–6.94 (1H, *m*, Ar-H), 6.97–6.89 (2H, *m*, Ar-H), 6.88–6.82 (1H, *m*, Ar-H), 6.72–6.64 (1H, *m*, Ar-H), 6.63–6.55 (2H, *m*, Ar-H), 3.85 (3H, *s*, OCH_3-H), 3.53 (1H, *brs*, NH-H), 3.40–3.24 (1H, *m*, CH-H), 3.10 (4H, *brs*, CH_2-H), 2.91 (2H, *d*, J = 11.2 Hz, CH_2-H), 2.66 (4H, *brs*, CH_2-H), 2.47–2.35 (4H, *m*, CH_2-H), 2.15 (2H, *t*, J = 11.0 Hz, CH_2-H), 2.07 (2H, *d*, J = 11.8 Hz, CH_2-H), 1.56 (4H, *brs*, CH_2-H), 1.55–1.44 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 153.8, 148.6, 142.9, 130.9, 124.5, 122.6, 119.8, 118.8, 114.8, 112.8, 60.1, 56.9, 55.0, 54.0, 52.2, 51.4, 33.9, 26.6.

1-(4-(4-(2,3-Dichlorophenyl)piperazin-1-yl)butyl)-N-*phenylpiperidin-4--amine (**5c**).* Yield: 0.46 g (83.1 %); pale yellow oil; IR (ATR, cm^{-1}): 3399.9 (N–H amine), 3051.9 (C–H aromatic), 2936.4 (C–H aliphatic), 1602.2 (C=O), 1242.3 (C–N amine), 781.3 (C–Cl); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.19––7.05 (4H, *m*, Ar-H), 6.70–6.63 (1H, *m*, Ar-H), 6.62–6.56 (3H, *m*, Ar-H), 3.50 (1H, *brs*, NH-H), 3.34–3.21 (1H, *m*, CH-H), 3.12–2.93 (4H, *m*, CH_2-H), 2.86 (4H, *d*, J = 10.7 Hz, CH_2-H), 2.39–2.29 (4H, *m*, CH_2-H), 2.15–1.99 (6H, *m*, CH_2-H), 1.55–1.47 (4H, *m*, CH_2-H), 1.50–1.41 (2H, *m*, CH_2-H); ^{13}C-NMR (126 MHz, $CDCl_3$. δ / ppm): ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 151.8, 147.2, 134.1, 129.4, 127.5, 124.7, 124.6, 118.8, 117.3, 113.3, 58.7, 52.6, 51.4, 50.1, 46.4, 32.7, 25.4.

N-*Phenyl*-N-*(1-(4-(4-phenylpiperazin-1-yl)butyl)piperidin-4-yl)propion-amide (**1a**).* Yield: 0.22 g (83 %); pale yellow oil; IR (ATR, cm^{-1}): 3058.6 (C–H aromatic); 2939.1 (C–H aliphatic); 1655.8 (C=O); 1238.4(C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.49–7.32 (3H, *m*, Ar-H), 7.29–7.20 (2H, *m*, Ar-H), 7.11–7.00 (2H, *m*, Ar-H), 6.94–6.88 (2H, *m*, Ar-H), 6.89–6.81 (1H, *m*, Ar-H), 4.73–4.58 (1H, *m*, CH-H), 3.22–3.15 (4H, *m*, CH_2-H), 2.94 (2H, *d*, J = 11.4 Hz, CH_2-H), 2.62–2.53 (4H, *m*, CH_2-H), 2.34 (4H, *dt*, J = 20.1, 6.2 Hz, CH_2-H), 2.08 (2H, *t*, J = 11.5 Hz, CH_2-H), 1.92 (2H, *q*, J = 7.3 Hz, CH_2-H), 1.78 (2H, *d*, J = 11.6 Hz, CH_2-H), 1.53–1.44 (4H, *m*, CH_2-H, partially overlapped), 1.44–1.35 (2H, *m*, CH_2-H, partially overlapped), 1.01 (3H, *t*, J = 7.4 Hz, CH_3-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 173.6, 151.4, 138.9, 130.5, 129.4, 129.2, 129.2, 128.4, 119.7, 116.1, 58.5, 58.4, 53.3, 53.2, 52.2, 49.1, 30.5, 28.6, 25.1, 24.9, 9.7. HRMS-HESI-Orbitrap: Calcd. for $C_{28}H_{40}N_4O$ $[M+H]^+$: 449.32749. Found: 449.32844.

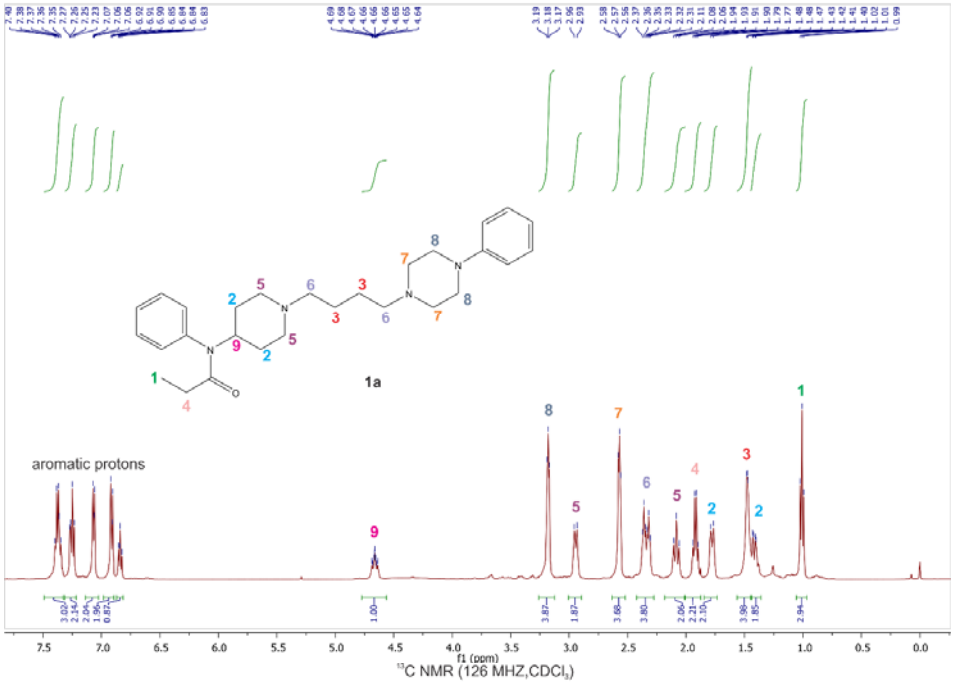
N-*(1-(4-(4-(3-Methoxyphenyl)piperazin-1-yl)butyl)piperidin-4-yl)*-N-*phe-nylpropionamide (**1b**).* Yield: 0.25 g (85.6 %); pale yellow oil; IR (ATR, cm^{-1}): 3058.2 (C–H aromatic); 2939.1 (C–H alkane); 1655.5 (C=O); 1241.4 (C–N amine); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.44–7.34 (3H, *m*, Ar-H), 7.11–

–7.04 (2H, *m*, Ar-H), 7.03–6.97 (1H, *m*, Ar-H), 6.96–6.90 (2H, *m*, Ar-H), 6.89––6.83 (1H, *m*, Ar-H), 4.78–4.54 (1H, *m*, CH-H), 3.86 (3H, *s*, OCH_3-H), 3.09 (4H, *s*, CH_2-H), 2.95 (2H, *d*, *J* = 11.4 Hz, CH_2-H), 2.64 (4H, *s*, CH_2-H), 2.44–2.36 (2H, *m*, CH_2-H), 2.37–2.28 (2H, *m*, CH_2-H), 2.08 (2H, *t*, *J* = 11.3 Hz, CH_2-H), 1.93 (2H, *q*, *J* = 7.3 Hz, CH_2-H), 1.79 (2H, *d*, *J* = 11.5 Hz, CH_2-H), 1.58–1.44 (4H, *m*, CH_2-H, partially overlapped), 1.46–1.34 (2H, *m*, CH_2-H, partially overlapped), 1.02 (3H, *t*, *J* = 7.4 Hz, CH_3-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 173.6, 152.3, 141.4, 138.9, 130.5, 129.4, 128.3, 123.0, 121.1, 118.3, 111.3, 58.6, 58.5, 55.4, 53.5, 53.2, 52.3, 50.6, 30.5, 28.6, 25.2, 24.9, 9.7; HRMS-HESI--Orbitrap: Calcd. for $C_{29}H_{42}N_4O_2$ $[M+H]^+$: 479.33805. Found: 479.33886.

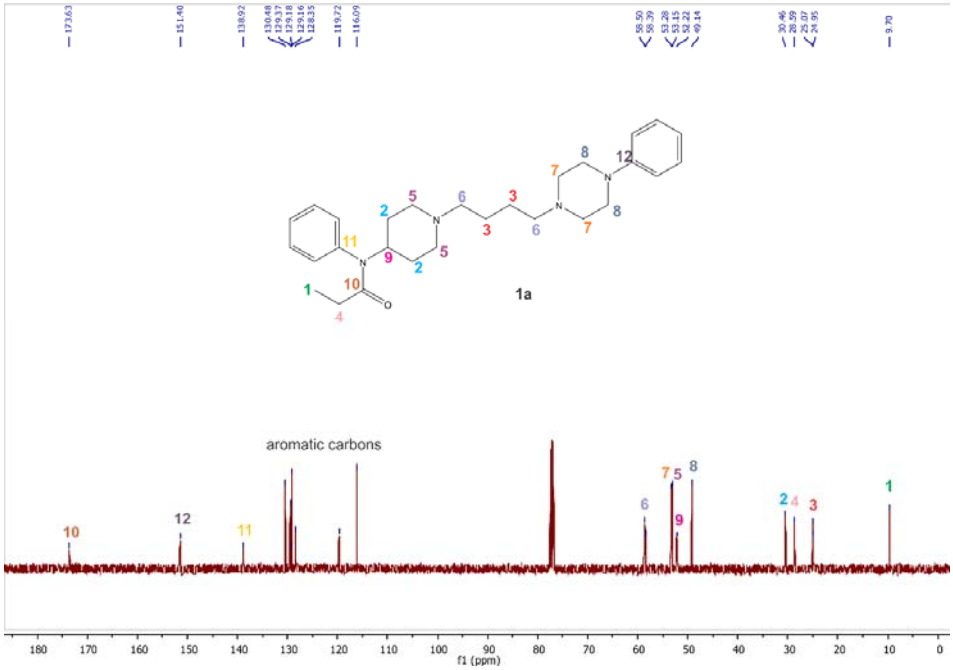
N-*(1-(4-(4-(2,3-Dichlorophenyl)piperazin-1-yl)butyl)piperidin-4-yl)*-N-*phenylpropionamide (**1c**)*. Yield: 0.26 g (84.2 %); pale yellow oil; IR (ATR, cm^{-1}): 3057.9 (C–H aromatic); 2940.2 (C–H aliphatic); 1653.8 (C=O); 1242.7 (C–N amine), 735.7 (C–Cl); ^{1}H-NMR (500 MHz, $CDCl_3$, δ / ppm): 7.45–7.33 (3H, *m*, Ar-H), 7.16–7.10 (2H, *m*, Ar-H), 7.10–7.02 (2H, *m*, Ar-H), 6.99–6.89 (1H, *m*, Ar-H), 4.71–4.60 (1H, *m*, CH-H), 3.05 (4H *s*, CH_2-H), 2.96 (2H, *d*, *J* = 11.5 Hz, CH_2-H), 2.62 (4H *s*, CH_2-H), 2.47–2.37 (2H, *m*, CH_2-H), 2.37–2.30 (2H, *m*, CH_2-H), 2.10 (2H, *t*, *J* = 11.6 Hz, CH_2-H), 1.97–1.88 (2H, *m*, CH_2-H), 1.78 (2H, *d*, *J* = 12.6 Hz, CH_2-H), 1.53–1.46 (4H, *m*, CH_2-H, partially overlapped), 1.46–1.35 (2H, *m*, CH_2-H, partially overlapped), 1.01 (3H, *t*, *J* = 7.4 Hz, CH_3-H); ^{13}C-NMR (126 MHz, $CDCl_3$, δ / ppm): 173.6, 151.3, 138.9, 134.1, 130.4, 129.4, 128.4, 127.5, 124.6, 118.7, 58.4, 58.3, 53.3, 53.1, 52.2, 51.2, 30.4, 28.6, 24.9, 24.8, 9.7; HRMS-Heated ESI-Orbitrap: Calcd. for $C_{28}H_{38}Cl_2N_4O$ $[M+H]^+$: 517.24954. Found: 517.25082.

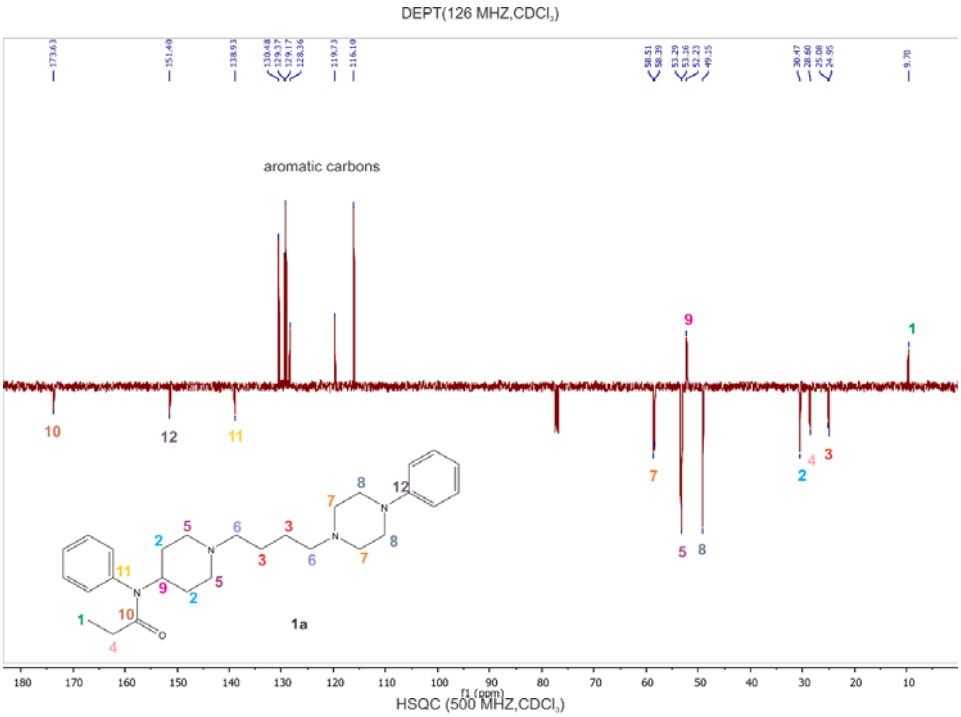
SPECTRA OF THE FINAL COMPOUNDS

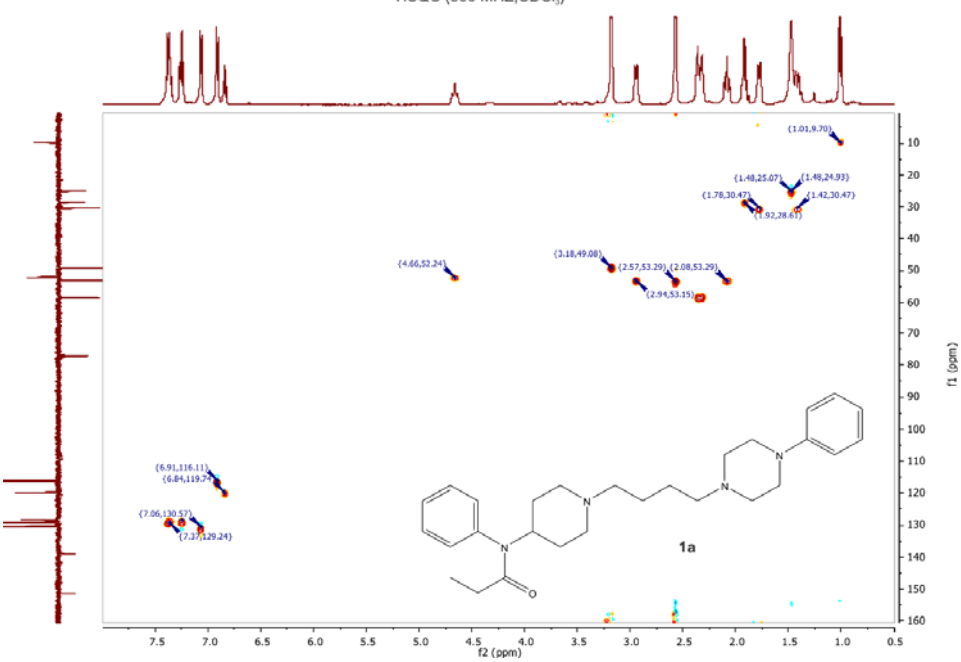
^{1}H NMR (500 MHZ,CDCl$_3$)

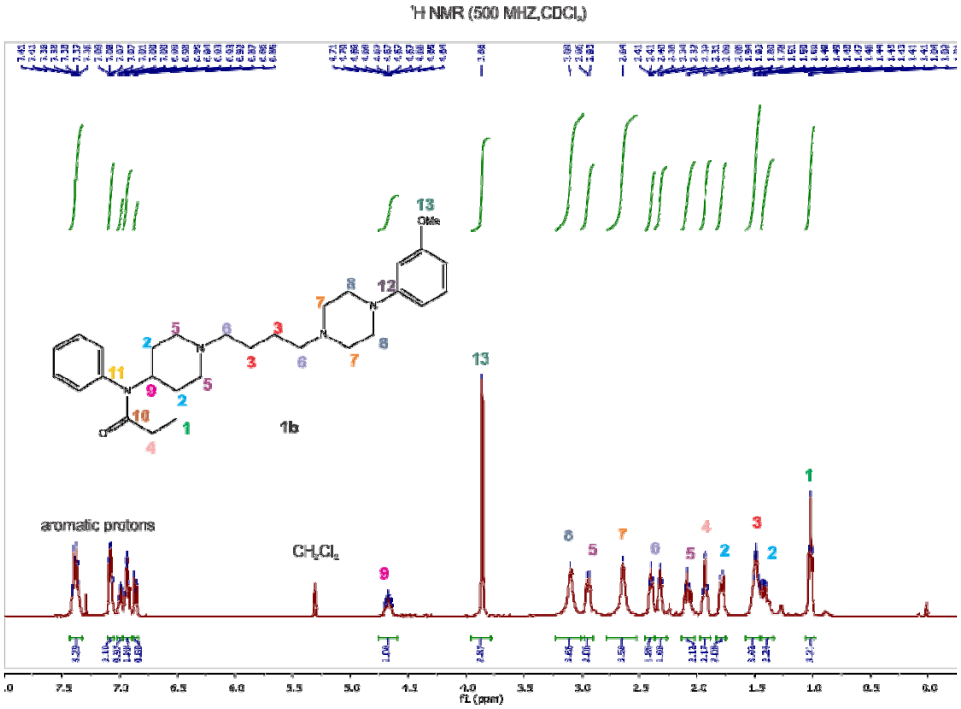


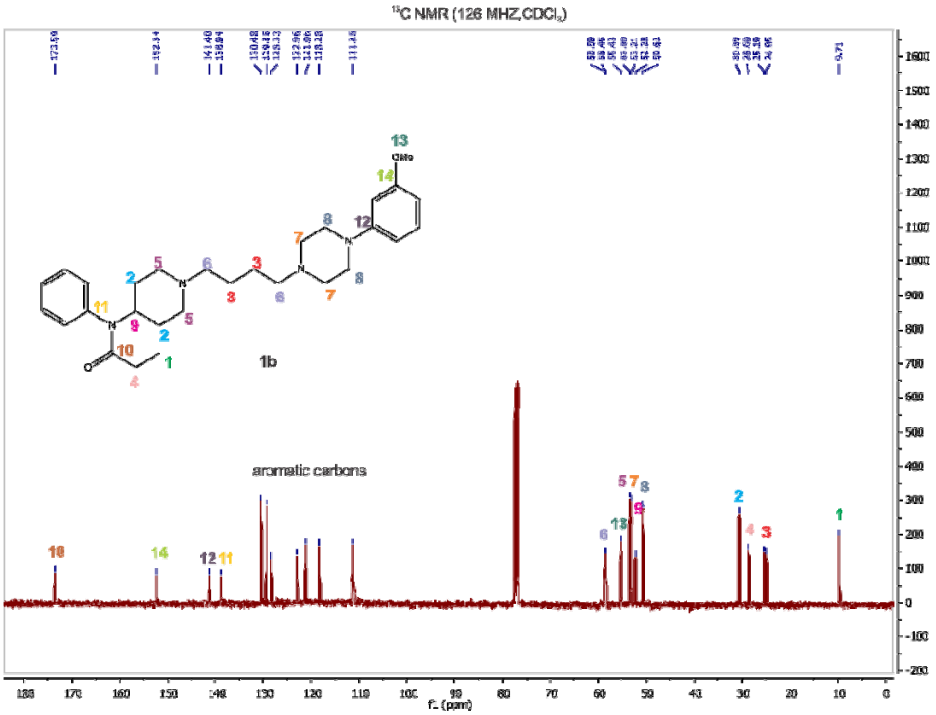
^{13}C NMR (126 MHZ,CDCl$_3$)

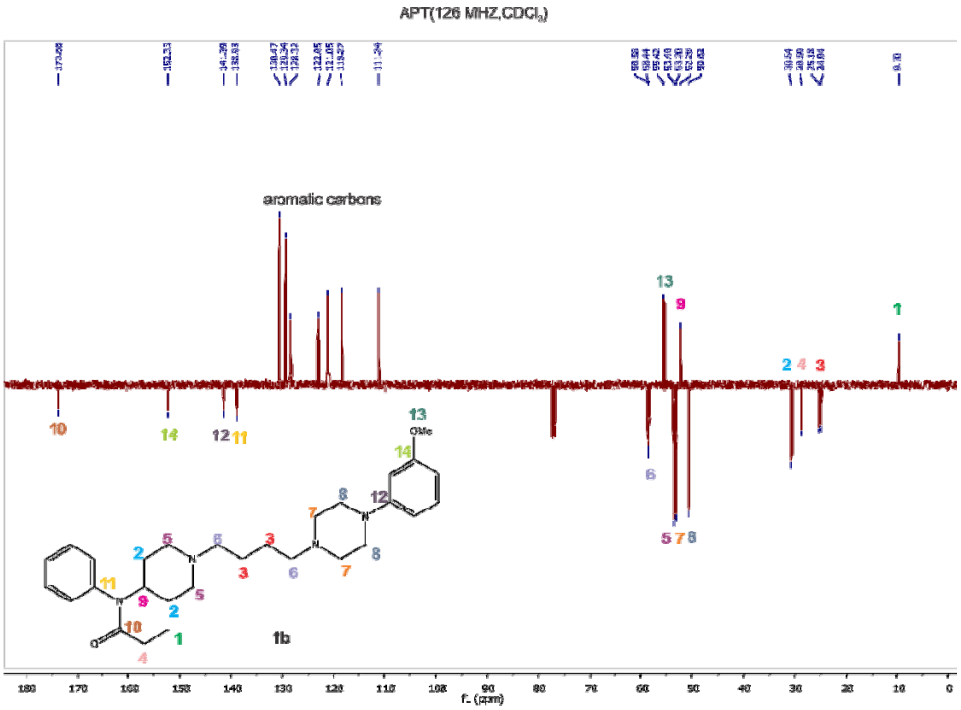


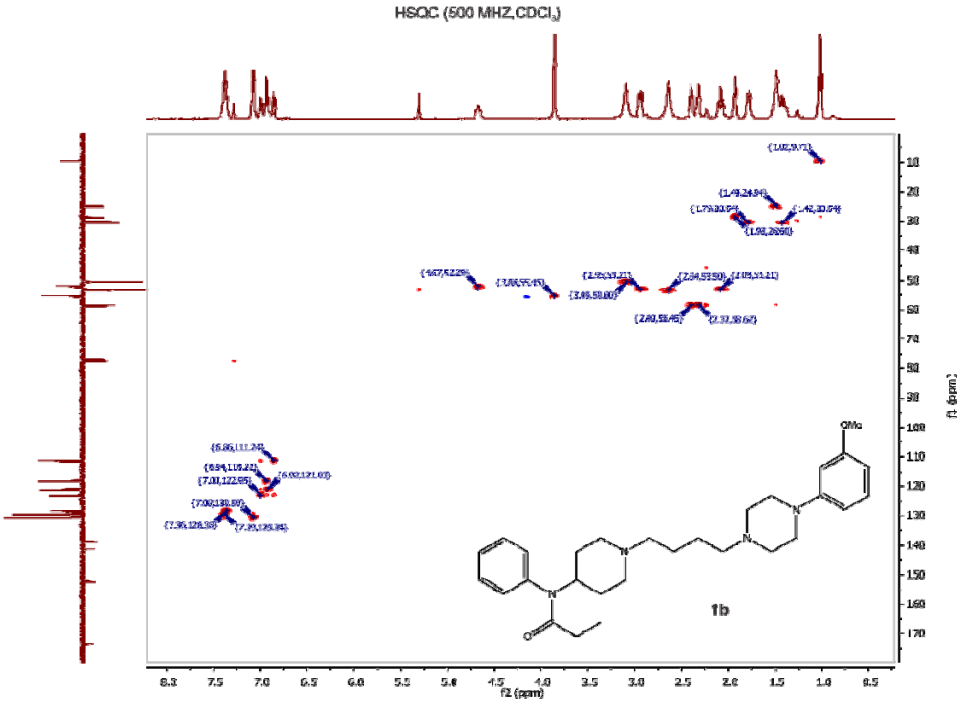

DEPT(126 MHZ,CDCl3)
aromatic carbons
1a
f1 (ppm)


HSQC (500 MHZ,CDCl3)
1a
f2 (ppm)
f1 (ppm)

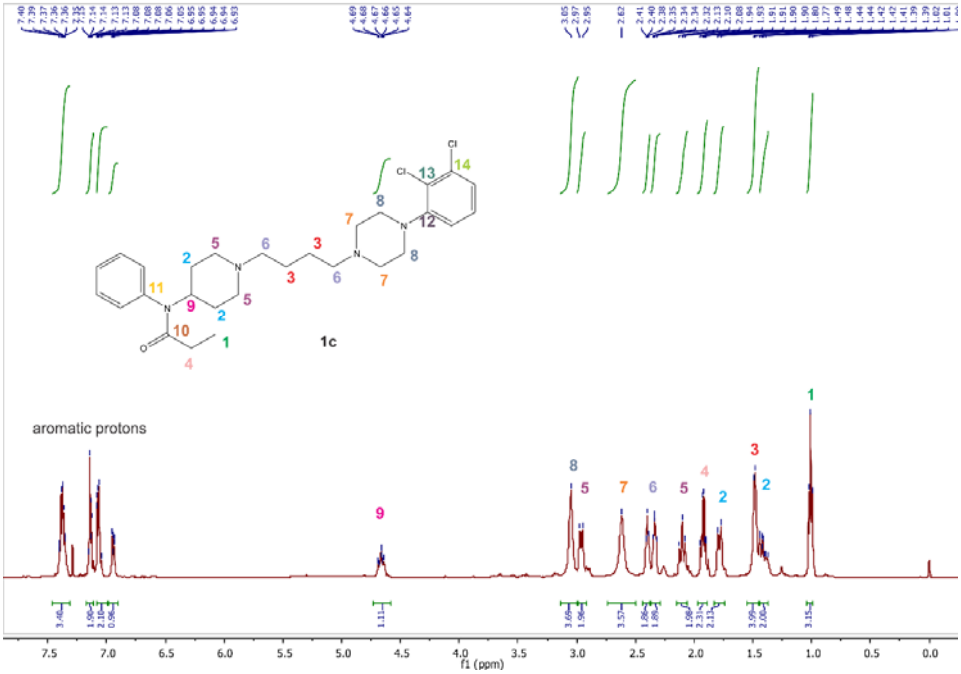

^{1}H NMR (500 MHZ,CDCl$_3$)
aromatic protons
CH$_2$Cl$_2$
1b
f1 (ppm)


^{13}C NMR (126 MHZ,CDCl$_3$)
aromatic carbons
1b
f1 (ppm)

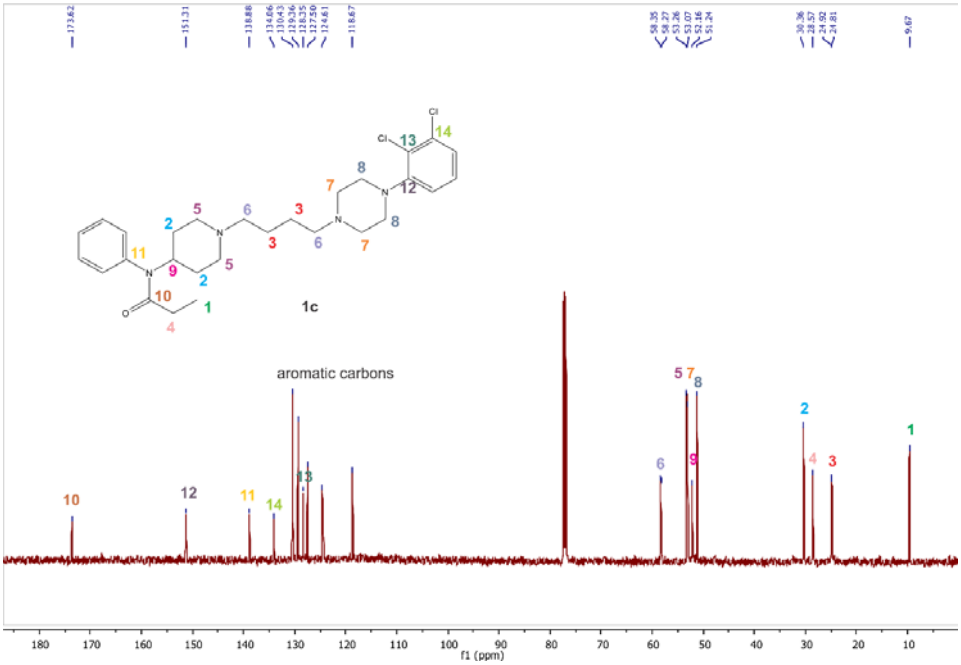

APT(126 MHZ,CDCl3)
aromatic carbons
1b
f1 (ppm)

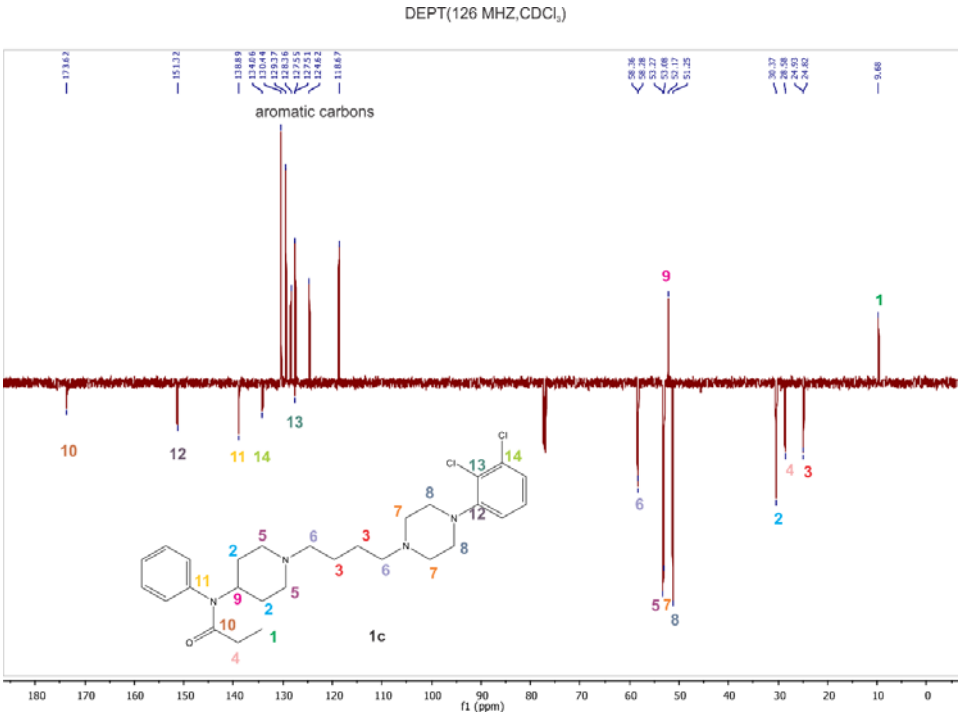

HSQC (500 MHZ,CDCl3)
1b
f2 (ppm)
f1 (ppm)

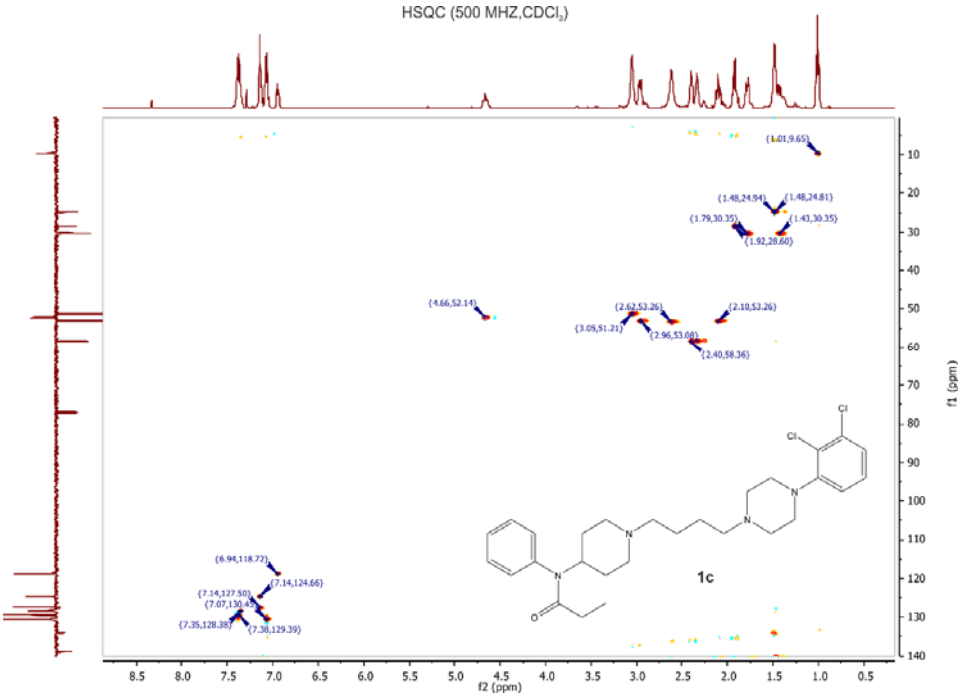
^{1}H NMR (500 MHZ,CDCl$_3$)



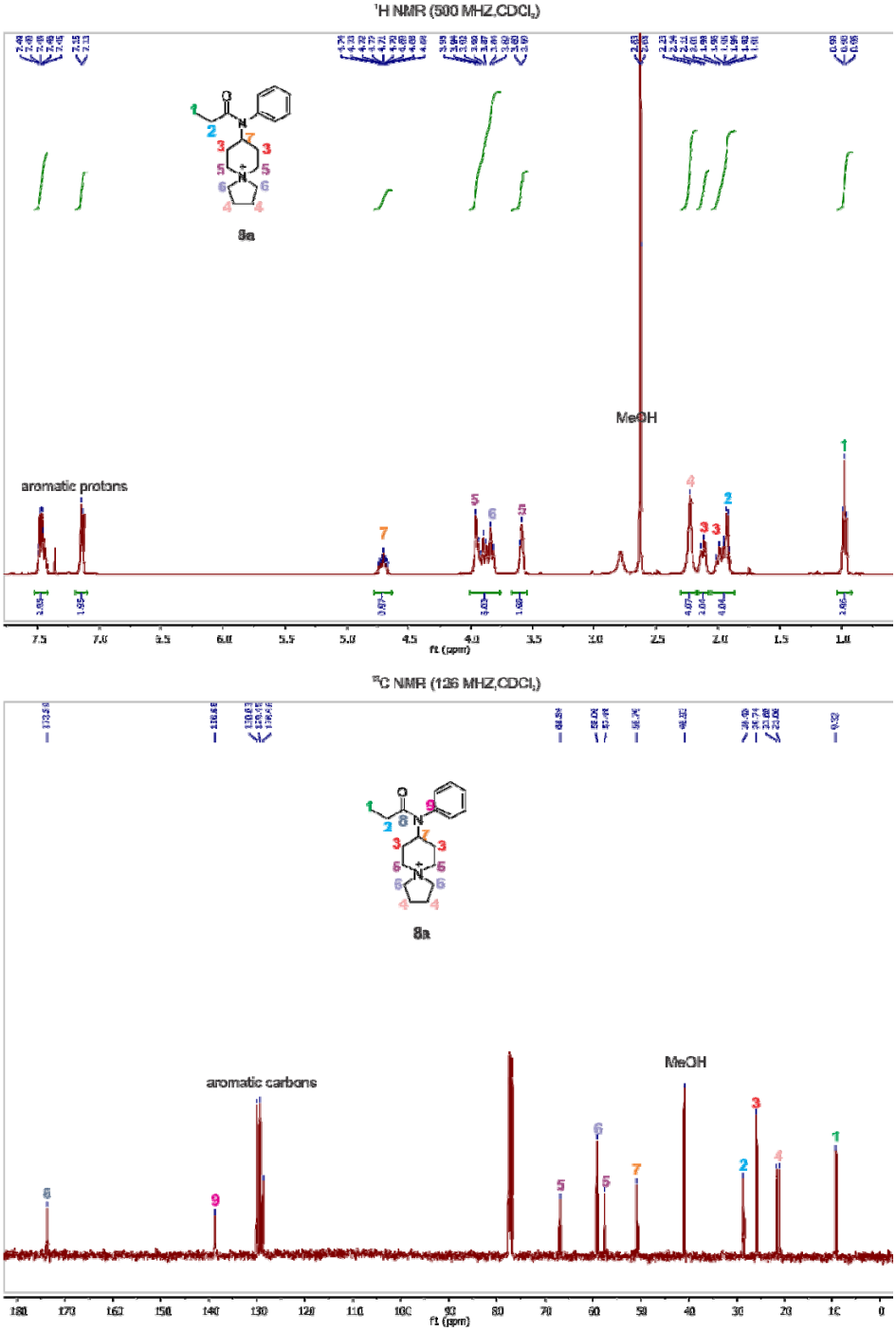
^{13}C NMR (126 MHZ,CDCl$_3$)

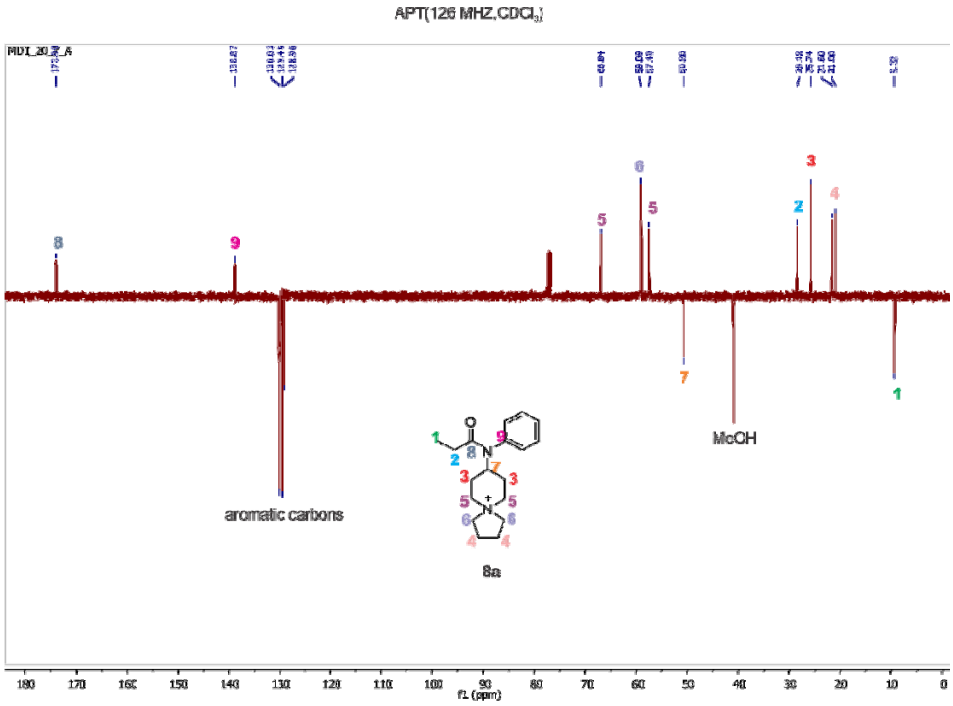


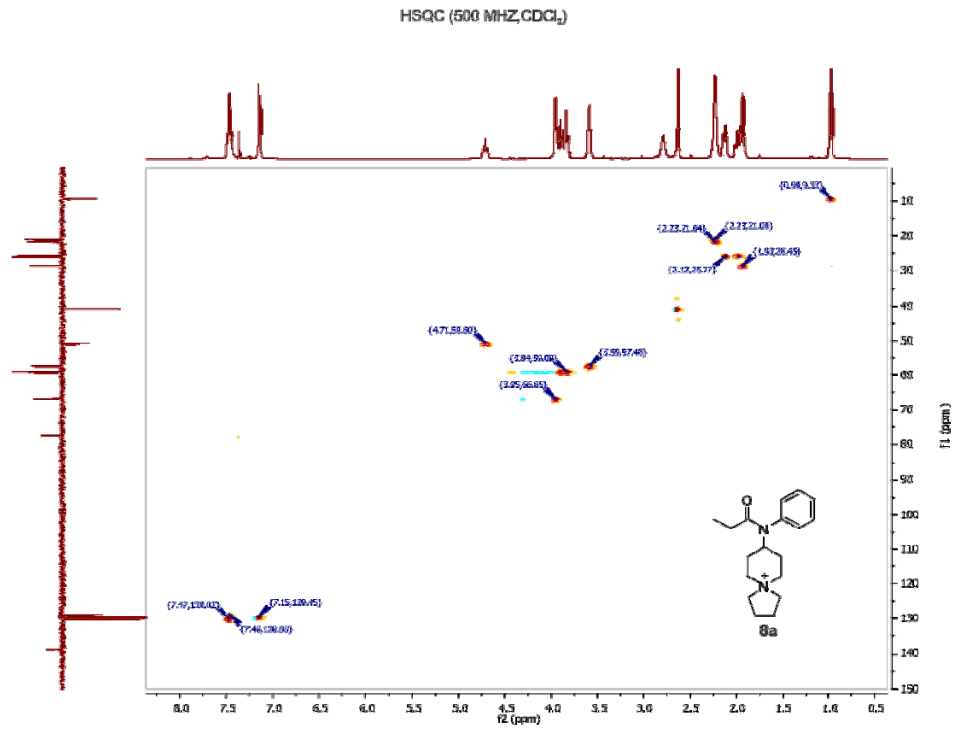

DEPT(126 MHZ,CDCl3)
aromatic carbons
1c
f1 (ppm)

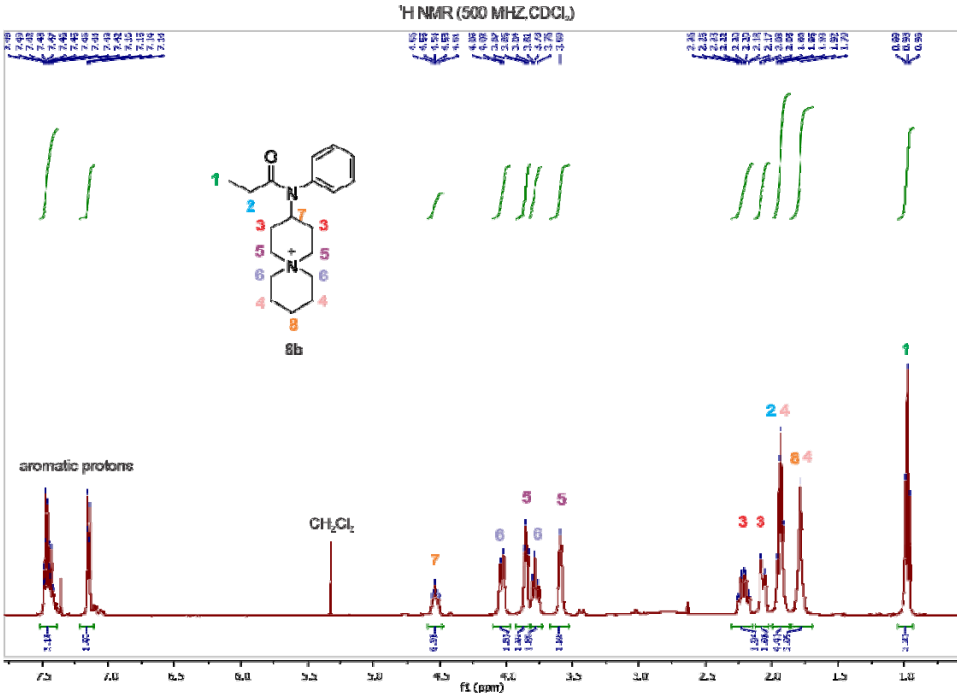

HSQC (500 MHZ,CDCl3)
1c
f2 (ppm)
f1 (ppm)

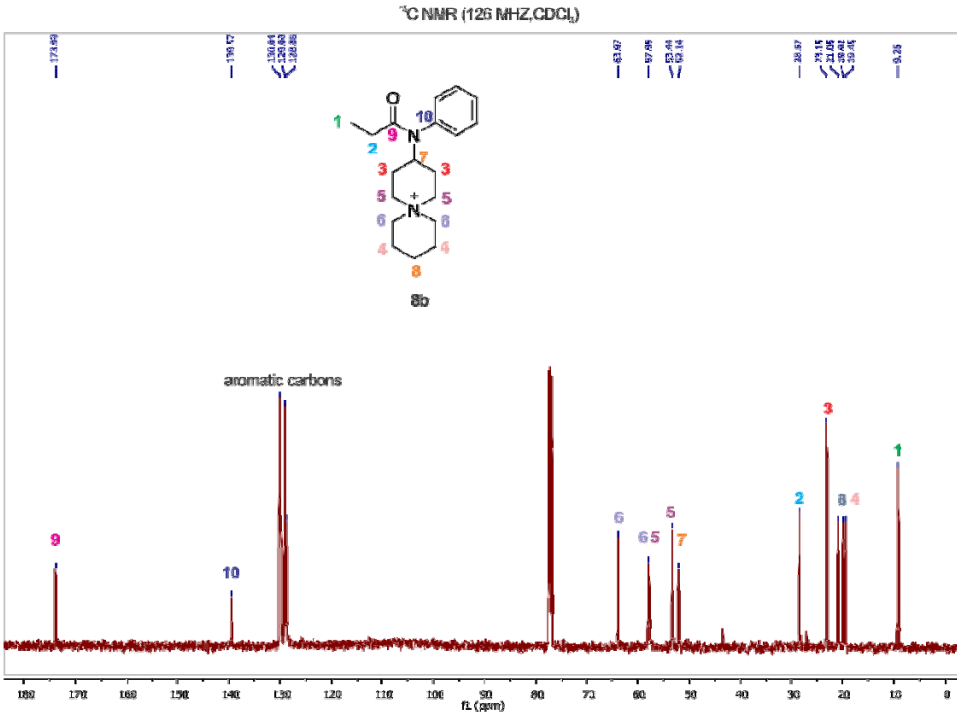
SPECTRA OF THE UNDESIRED PRODUCTS

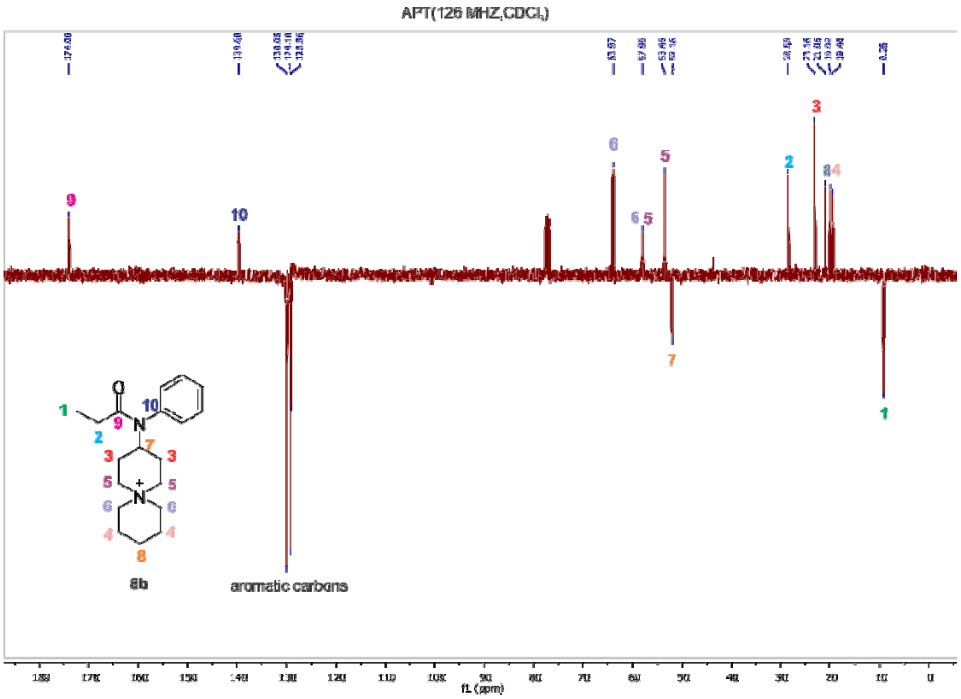


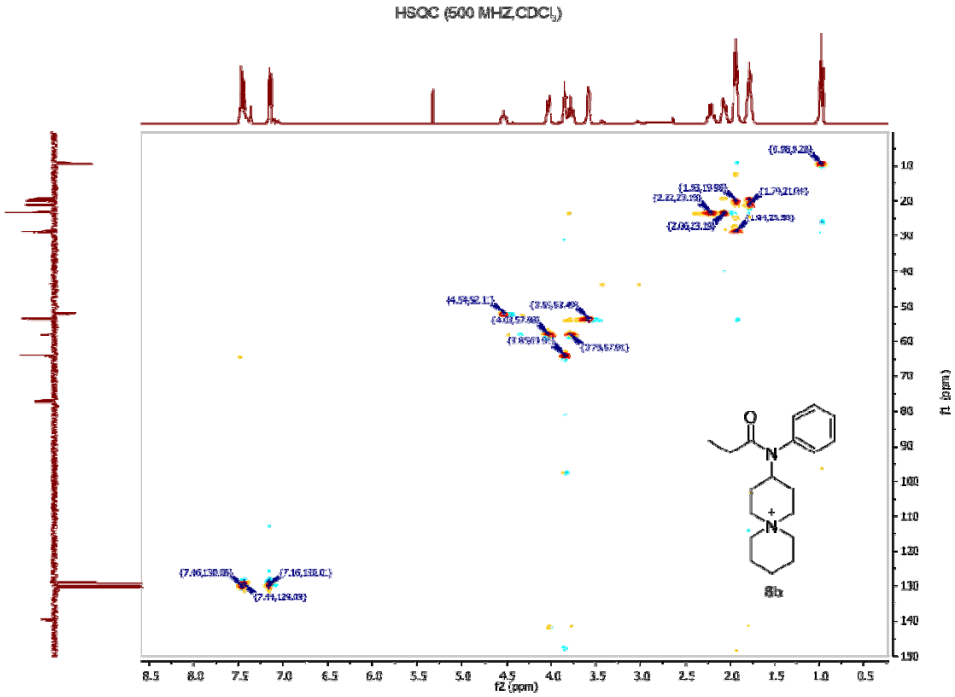

APT(126 MHZ,CDCl3)
aromatic carbons
MeOH
8a
f1 (ppm)

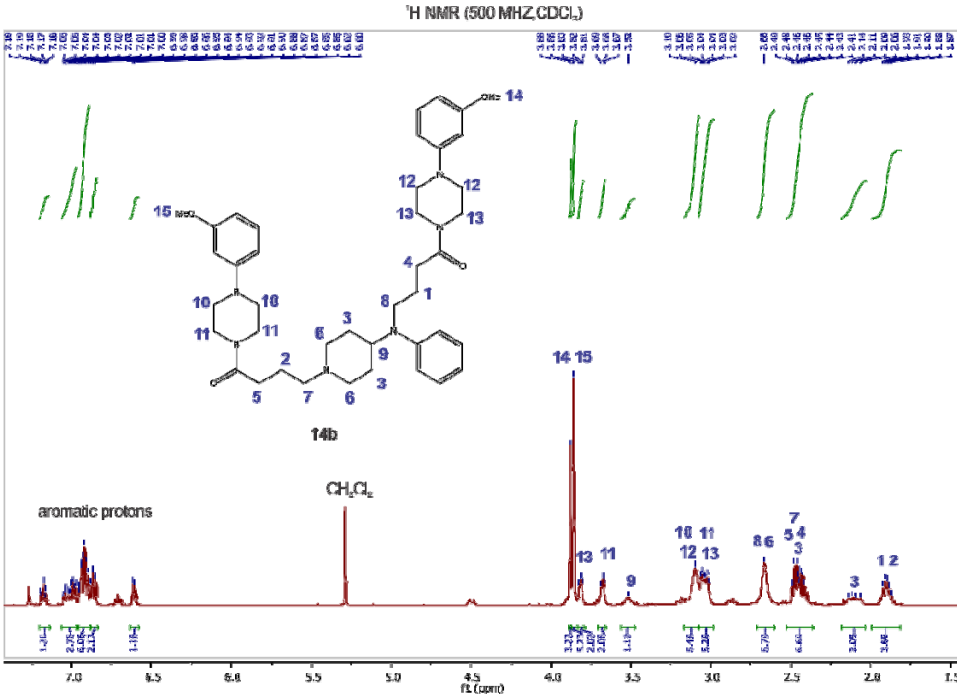

HSQC (500 MHZ,CDCl3)
8a
f2 (ppm)
f1 (ppm)

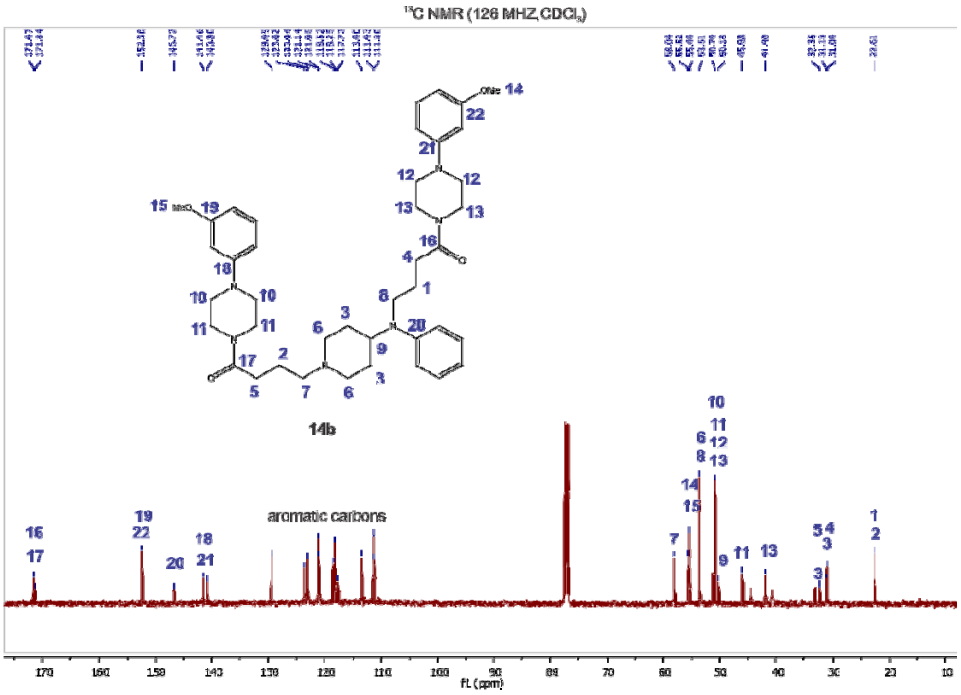

^{1}H NMR (500 MHZ,CDCl$_3$)
8b
aromatic protons
CH_2Cl_2
f1 (ppm)

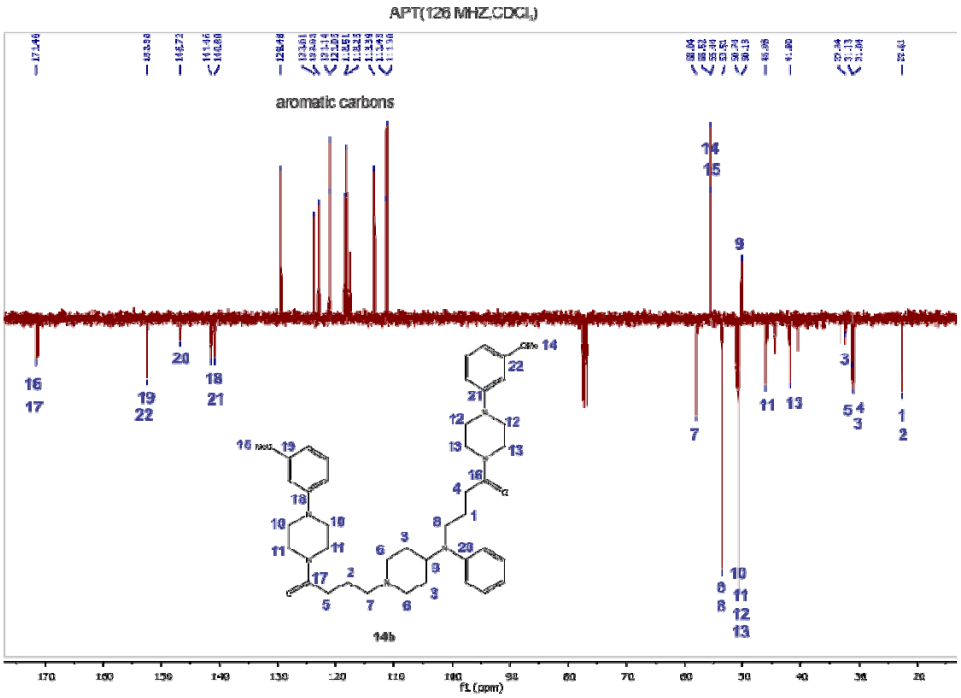

^{13}C NMR (126 MHZ,CDCl$_3$)
8b
aromatic carbons
f1 (ppm)


APT(126 MHZ,CDCl3)
9
10
6
5
2
3
4
7
1
aromatic carbons
8b
f1 (ppm)


HSQC (500 MHZ,CDCl3)
8b
f2 (ppm)
f1 (ppm)


^{1}H NMR (500 MHZ,CDCl$_3$)
14b
aromatic protons
CH_2Cl_2
f1 (ppm)


^{13}C NMR (126 MHZ,CDCl$_3$)
14b
aromatic carbons
f1 (ppm)



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