Supporting Information for:

One-pot multicomponent strategy for stereospecific construction of tricyclic pyrrolo[1,2-*a*]quinolines

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Contents

1. General Methods

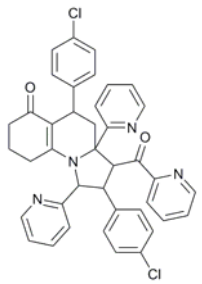
All reactions were carried out under a nitrogen atmosphere condition and solvents were dried according to established procedures. Thin layer chromatography was performed on silica gel GF254 plates. Silica gel (300-400 mesh) was used for column chromatography. Proton nuclear magnetic resonance (^{1}H NMR) spectra were recorded on a Brucker DPX 400 MHz spectrometer in $CDCl_3$ and carbon nuclear magnetic resonance (^{13}C NMR) spectra were recorded on Brucker 100 MHz spectrometer in $CDCl_3$ using tetramethylsilane (TMS) as internal standard. Data are presented as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet) and coupling constant in Hertz (Hz). Infrared (IR) spectra were recorded on a FT-IR-Tensor 27 spectrometer in KBr pellets and reported in cm^{-1}. HRMS (ESI) was measured with a miroTOF-QII HRMS/MS instrument (BRUKER). Melting points were measured on an X-4 melting point apparatus and were uncorrected. X-ray crystallographic analysis was performed with a Siemens SMART CCD and a Sismens P4 diffractometer.

2. General procedure for synthesis of Pyrrolo[1,2-a]quinoline Derivatives

A mixture of 3-aryl-1-azaaryl-prop-2-en-1-one (3) (2 mmol) prepared according to the literature methods[1], cyclohexane-1,3-dione (1) (1.0 mmol) or 5,5-dimethylcyclohexane-1,3-dione (1) (1.0 mmol) and 2-(aminomethyl)pyridine (2)(1.2 mmol) or pyrazin-2-ylmethanamine (2) (1.2 mmol) was dissolved in 6 mL of anhydrous methanol in a 25-mL 3-mouth flask, stirred with nitrogen incoming, heated to 45 ^{o}C progressively. The mixtures were stirred for a certain time (monitored by TLC). Then the solvent was removed in vacuo, and the residue was separated by column chromatography on silica gel (eluent, petroleum ether/ethyl acetate 4:1 v/v) to afford the producrts 4.

3. Characterization data of products

2,5-Bis-(4-chloro-phenyl)-3-(pyridine-2-carbonyl)-1,3*a*-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one (4a)



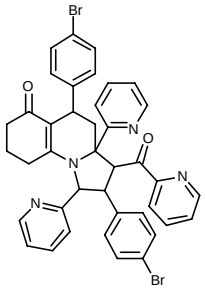
Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3369, 3050, 2926, 2884, 2358, 1697, 1613, 1588, 1543, 1489, 1466, 1433, 1413, 1350, 1321, 1289, 1250, 1198, 1107, 1089, 1051, 1012, 995, 879, 823, 790, 749, 660, 619, 555 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, J = 4.4 Hz, 1H, Py–H), 8.61 (d, J = 8.0 Hz, 1H, Py–H), 8.54 (d, J = 4.4 Hz, 1H, Py–H), 8.31 (d, J = 4.0 Hz, 1H, Py–H), 7.81–7.73 (m, 3H, Py–H + Ar–H), 7.56 (t, J = 7.2 Hz, 1H, Py–H), 7.38 (t, J = 6.0 Hz, 1H, Py–H), 7.26–7.24 (m, 1H, Py–H), 7.15–7.09 (m, 5H, Py–H + Ar–H), 7.02–6.96 (m, 4H, Py–H + Ar–H), 6.86 (d, J = 7.6 Hz, 1H, Ar–H), 5.50 (d, J = 13.2 Hz, 1H, C–H), 5.10 (d, J = 10.8 Hz, 1H, C–H), 3.91 (t, J = 11.6 Hz, 1H, C–H), 3.16 (dd, J = 13.2, 6.0 Hz, 1H, C–H), 2.86 (dd, J = 12.4, 5.6 Hz, 1H, CH_2), 2.39 (d, J = 11.6 Hz, 1H, CH_2), 2.16–1.92 (m, 3H, CH_2), 1.77–1.73 (m, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.49, 193.42, 160.42, 159.56, 159.08, 154.82, 150.11, 148.54, 148.14, 145.54, 136.81, 136.73, 136.48, 135.64, 133.13, 130.51, 129.63, 128.74, 128.07, 126.96, 124.02, 122.99, 122.54, 122.37, 122.30, 112.49, 73.17, 72.88, 58.88, 52.67, 46.57, 36.72, 36.08, 30.18, 20.81; HRMS (ESI) m/z: calcd. For $C_{40}H_{32}Cl_2N_4O_2Na$: 693.1800, $[M+Na]^+$ found: 693.1804.

2,5-Bis-(4-bromo-phenyl)-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one (4b)

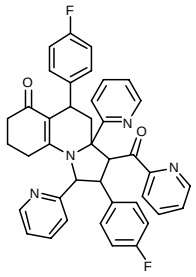
Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3448, 3050, 2873, 2361, 1698, 1661, 1575, 1488, 1451, 1437, 1355, 1291, 1252, 1221, 1153, 1072, 1053, 1010, 996, 971, 884, 874, 827, 789, 752, 723, 681, 619, 594, 549 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, J = 3.6 Hz, 1H, Py–H), 8.59 (d, J = 8.0 Hz, 1H, Py–H), 8.55 (d, J = 4.0 Hz, 1H, Py–H), 8.31 (d, J = 3.2 Hz, 1H,



Py–H), 7.81–7.72 (m, 3H, Py–H + Ar–H), 7.57 (t, *J* = 8.0 Hz, 1H, Py–H), 7.39 (t, *J* = 5.2 Hz, 1H, Py–H), 7.29–7.24 (m, 5H, Py–H + Ar–H), 7.14–7.11 (m, 1H, Py–H), 6.96–6.87 (m, 5H, Py–H + Ar–H), 5.50 (d, *J* = 12.8 Hz, 1H, C–H), 5.09 (d, *J* = 10.8 Hz, 1H, C–H), 3.90 (t, *J* = 11.6 Hz, 1H, C–H), 3.15 (dd, *J* = 12.8, 5.6 Hz, 1H, C–H), 2.84 (dd, *J* = 12.4, 5.6 Hz, 1H, CH_2), 2.39 (d, *J* = 11.2 Hz, 1H, CH_2), 2.15–2.04 (m, 2H, CH_2), 1.99–1.92 (m, 1H, CH_2), 1.77–1.73 (m, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.40, 193.35, 160.45, 159.45, 159.06, 154.84, 150.09, 148.54, 148.13, 146.03, 136.76, 136.70, 136.43, 136.17, 131.67, 130.97, 129.97, 128.52, 126.91, 123.98, 122.97, 122.53, 122.36, 122.28, 121.31, 118.65, 112.52, 73.15, 72.88, 58.86, 52.75, 46.54, 36.79, 36.07, 30.18, 20.80; HRMS (ESI) m/z: calcd. For $C_{40}H_{32}Br_2N_4O_2Na$: 783.0770, $[M+Na]^+$ found: 783.0765.

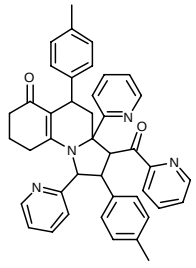
2,5-Bis-(4-fluoro-phenyl)-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one (4c)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3053, 3002, 2927, 2885, 2360, 1697, 1608, 1590, 1511, 1467, 1455, 1433, 1412, 1373, 1350, 1322, 1289, 1228, 1215, 1198, 1178, 1160, 1091, 1012, 995, 868, 837, 750, 664, 620, 561, 525 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.66 (d, *J* = 4.4 Hz, 1H, Py–H), 8.52 (d, *J* = 8.0 Hz, 1H, Py–H), 8.48 (d, *J* = 4.4 Hz, 1H, Py–H), 8.25 (d, *J* = 4.4 Hz, 1H, Py–H), 7.75–7.66 (m, 3H, Py–H + Ar–H), 7.52–7.48 (m, 1H, Py–H), 7.32 (t, *J* = 5.6 Hz, 1H, Py–H), 7.26–7.17 (m, 1H, Py–H), 7.06 (dd, *J* = 7.2, 4.8 Hz, 1H, Py–H), 6.97–6.91 (m, 4H, Py–H + Ar–H), 6.81–6.73 (m, 5H, Py–H + Ar–H), 5.43 (d, *J* = 13.2 Hz, 1H, C–H), 5.01 (d, *J* = 10.8 Hz, 1H, C–H), 3.85 (t, *J* = 11.8 Hz, 1H, C–H), 3.09 (dd, *J* = 13.2, 6.0 Hz, 1H, C-H), 2.80 (dd, *J* = 12.0, 5.6 Hz, 1H, CH_2), 2.34–2.29 (m, 1H, CH_2), 2.11–1.97 (m, 2H, CH_2), 1.94–1.85 (m, 1H, CH_2), 1.70–1.60 (m, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.57, 193.46, 160.64, 160.60, 159.38, 159.19, 154.93, 150.04, 148.49, 148.11, 142.39, 136.76, 136.62, 136.42, 132.78, 132.75, 129.79, 129.72, 127.95, 127.88, 126.88, 123.97, 122.90, 122.51, 122.37, 122.24, 115.54, 115.33, 114.71, 114.50, 112.84, 73.39, 72.88, 59.01, 52.58, 46.86, 36.52, 36.09, 30.20, 20.80; HRMS (ESI) m/z: calcd. For $C_{40}H_{32}F_2N_4O_2Na$: 661.2362, $[M+Na]^+$ found: 661.2362.

3-(Pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,5-di-p-tolyl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4d)

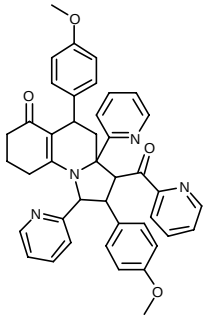


Petroleum ether : EtOAc (4:1); R_f =0.2; white solid, m.p. 273–275 ^{o}C.

IR(KBr): 3678, 3651, 3468, 3048, 2947, 2361, 1686, 1588, 1552, 1513, 1468, 1433, 1398, 1353, 1318, 1285, 1192, 1101, 1046, 995, 860, 812, 788, 751, 689, 679, 584, 535 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.75 (d, *J* = 3.6 Hz, 1H, Py–H), 8.69 (d, *J* = 2.8 Hz, 1H, Py–H), 8.45 (s, 1H, Py–H), 7.76 (s, 2H, Py–H + Ar–H), 7.70 (s, 1H, Py–H), 7.54–7.47 (m, 2H, Py–H + Ar–H), 7.26–7.19 (m, 2H, Py–H + Ar–H), 6.98–6.92 (m, 5H, Py–H + Ar–H), 6.61 (t, *J* = 5.6 Hz, 1H, Ar–H), 6.43 (d, *J* = 7.6 Hz, 2H, Ar–H), 6.33 (d, *J* = 7.2 Hz, 2H, Ar–H), 5.44 (d, *J* = 12.8 Hz, 1H, C–H), 5.13 (d, *J* = 10.8 Hz, 1H, C–H), 4.19 (d, *J* = 5.2 Hz, 1H, C–H), 3.67 (t, *J* = 11.2 Hz, 1H, C–H), 3.37 (d, *J* = 14.0 Hz, 1H, CH_2), 2.57–2.47 (m, 2H, CH_2), 2.36–2.30 (m, 2H, CH_2), 2.19–2.12 (m, 4H, CH_2 + CH_3), 1.99 (s, 3H, CH_3), 1.87 (s, 2H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.35, 194.60, 161.06, 160.00, 158.94, 155.34, 149.51, 148.26, 146.48, 139.66, 136.69, 136.63, 136.32, 134.71, 134.38, 132.68, 129.15, 128.22, 127.53, 127.37, 126.61, 124.69, 122.58, 122.50, 122.37, 121.56, 110.09, 74.05, 73.11, 60.93, 51.77, 40.62, 36.61, 34.48, 29.43, 22.20, 21.02, 20.69; HRMS (ESI) m/z: calcd. For $C_{42}H_{38}N_4O_2Na$: 653.2893, $[M+Na]^+$ found: 653.2911.

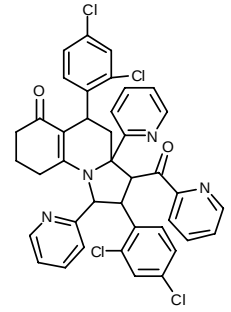
2,5-Bis-(4-methoxy-phenyl)-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4e)

Petroleum ether : EtOAc (4:1); R_f =0.2; white solid, m.p. 292–295 ^{o}C.



IR(KBr): 3443, 3050, 3000, 2930, 2878, 2833, 1696, 1612, 1588, 1512, 1466, 1434, 1411, 1349, 1322, 1297, 1248, 1196, 1181, 1149, 1124, 1110, 1094, 1037, 1009, 995, 953, 881, 866, 834, 795, 778, 749, 714, 689, 661, 620, 565, 529 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.72 (s, 1H, Py–H), 8.60 (d, J = 7.2 Hz, 1H, Py–H), 8.54 (s, 1H, Py–H), 8.32 (s, 1H, Py–H), 7.80–7.71 (m, 3H, Py–H + Ar–H), 7.54 (t, J = 6.8 Hz, 1H, Py–H), 7.35 (s, 1H, Py–H), 7.26–7.22(m, 1H, Py–H), 7.11 (s, 1H, Ar–H), 6.97 (dd, J = 20.0, 7.2 Hz, 4H, Py–H + Ar–H), 6.88 (d, J = 7.6 Hz, 1H, Ar–H), 6.73 (d, J = 7.2 Hz, 2H, Py–H + Ar–H), 6.65 (d, J = 7.6 Hz, 2H, Py–H + Ar–H), 5.51 (d, J = 12.8 Hz, 1H, C–H), 5.09 (d, J = 10.4 Hz, 1H, C–H), 3.88 (t, J = 11.2 Hz, 1H, C–H), 3.74 (s, 3H, OCH_3), 3.66 (s, 3H, OCH_3), 3.17 (dd, J = 13.6, 6.0 Hz, 1H, CH), 2.87–2.84 (m, 1H, CH_2), 2.39 (d, J = 12.0 Hz, 1H, CH_2), 2.20–2.06 (m, 2H, CH_2), 1.97–1.91 (m, 1H, CH_2), 1.77–1.71 (m, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.88, 193.45, 161.08, 159.53, 159.23, 158.66, 157.13, 155.05, 149.89, 148.51, 148.04, 139.04, 136.63, 136.48, 136.33, 129.25, 129.00, 127.58, 126.71, 124.02, 122.70, 122.56, 122.34, 122.09, 113.89, 113.35, 113.18, 73.43, 72.93, 59.03, 55.14, 55.09, 52.67, 46.97, 36.39, 36.19, 30.27, 20.84; HRMS (ESI) m/z: calcd. For $C_{42}H_{38}N_4O_4Na$: 685.2791, $[M+Na]^+$ found: 685.2761.

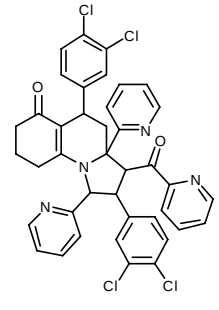
2,5-Bis-(2,4-dichloro-phenyl)-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4f)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^oC.

IR(KBr): 3050, 3008, 2926, 2882, 2361, 1703, 1608, 1588, 1544, 1470, 1433, 1413, 1374, 1347, 1322, 1293, 1242, 1197, 1178, 1148, 1120, 1105, 1044, 995, 954, 866, 825, 781, 770, 747, 689, 656, 619, 569 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.69 (s, 1H, Py–H), 8.55 (s, 1H, Py–H), 8.40 (d, J = 7.2 Hz, 1H, Py–H), 8.31 (s, 1H, Py–H), 7.81–7.70 (m, 3H, Py–H + Ar–H), 7.63–7.59 (m, 1H, Py–H), 7.40 (s, 2H, Py–H), 7.26 (m, 1H, Py–H), 7.22 (s, 1H, Py–H), 7.14–7.08 (m, 5H, Py–H + Ar–H), 7.04 (d, J = 8.0 Hz, 1H, Ar–H), 5.63 (d, J = 13.2 Hz, 1H, C–H), 5.13 (d, J = 12.0 Hz, 1H, C–H), 4.52–4.47 (m, 1H, C–H), 3.29 (d, J = 12.4 Hz, 1H, C–H), 3.21 (d, J = 10.4 Hz, 1H, CH_2), 2.41 (d, J = 16.0 Hz, 1H, CH_2), 2.11 (d, J = 16.4 Hz, 1H, CH_2), 2.02–1.96 (m, 2H, CH_2), 1.85–1.76 (m, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 193.06, 159.96, 158.44, 154.89, 150.01, 148.36, 148.01, 142.72, 136.92, 136.78, 136.28, 134.10, 133.44, 130.80, 129.71, 128.77, 127.52, 127.12, 126.89, 126.79, 123.45, 122.97, 122.40, 122.37, 121.87, 111.84, 72.93, 44.11, 35.96, 32.62, 30.18, 20.81; HRMS (ESI) m/z: calcd. For $C_{40}H_{30}Cl_4N_4O_2Na$: 763.0991, $[M+Na]^+$ found: 763.0976.

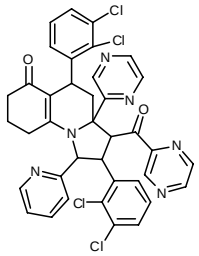
2,5-Bis-(3,4-dichloro-phenyl)-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4g)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^oC.

IR(KBr): 3708, 3686, 3667, 3646, 3626, 2353, 1697, 1611, 1588, 1542, 1469, 1434, 1415, 1371, 1354, 1321, 1292, 1197, 1175, 1130, 1029, 994, 877, 827, 793, 751, 708, 659 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.76 (s, 1H, Py–H), 8.58 (d, J = 5.2 Hz, 2H, Py–H), 8.32 (s, 1H, Py–H), 7.81–7.73 (m, 3H, Py–H + Ar–H), 7.61 (t, J = 7.6 Hz, 1H, Py–H), 7.42 (s, 1H, Py–H), 7.29–7.19 (m, 3H, Py–H + Ar–H), 7.15 (s, 3H, Py–H + Ar–H), 6.92–6.87 (m, 3H, Py–H + Ar–H), 5.47 (d, J = 12.8 Hz, 1H, C–H), 5.10 (d, J = 10.4 Hz, 1H, C–H), 3.91 (t, J = 11.6 Hz, 1H, C–H), 3.16 (dd, J = 13.2, 4.4 Hz, 1H, C–H), 2.84–2.80 (m, 1H, CH_2), 2.40 (d, J = 11.2 Hz, 1H, CH_2), 2.15–2.08 (m, 2H, CH_2), 1.99–1.93 (m, 1H, CH_2), 1.75 (d, J = 7.6 Hz, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.21, 193.43, 159.98, 159.64, 158.68, 154.64, 150.26, 148.64, 148.22, 147.43, 137.42, 136.92, 136.90, 136.56, 132.62, 131.73, 131.53, 130.53, 130.17, 129.91, 128.75, 128.45, 127.70, 127.15, 126.42, 123.96, 123.21, 122.55, 122.44, 122.40, 112.12, 72.92, 72.79, 58.76, 52.37, 46.20, 36.62, 35.96, 30.12, 20.75; HRMS (ESI) m/z: calcd. For $C_{40}H_{30}Cl_4N_4O_2Na$: 763.0991, $[M+Na]^+$ found: 763.1007.

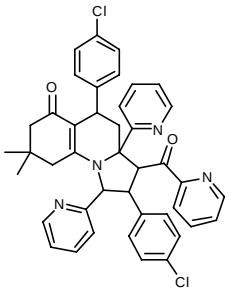
2,5-Bis-(2,3-dichloro-phenyl)-3-(pyrazine-2-carbonyl)-3a-pyrazin-2-yl-1-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4h)



Petroleum ether : EtOAc (4:1); R*f* = 0.2; white solid, m.p.>300 ^{o}C.

IR(KBr): 3752, 3713, 3691, 3677, 3650, 2967, 1724, 1664, 1642, 1607, 1500, 1422, 1344, 1274, 1215, 1188, 1150, 1077, 976, 817, 760, 669, 621, 522 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.95 (s, 1H, Py–H), 9.00 (s, 1H, Py–H), 8.82 (s, 1H, Py–H), 8.71 (s, 1H, Py–H), 8.53 (d, *J* = 15.2 Hz, 2H, Py–H + Ar–H), 8.33 (s, 1H, Py–H), 7.60–7.55 (m, 1H, Ar–H), 7.19–7.26 (3H, Py–H + Ar–H), 6.94–6.89 (m, 4H, Py–H + Ar–H), 6.78 (d, *J* = 6.8 Hz, 1H, Ar–H), 5.33 (d, *J* = 13.2 Hz, 1H, C–H), 5.11 (d, *J* = 11.2 Hz, 1H, C–H), 3.93 (t, *J* = 13.6 Hz, 1H, C–H), 3.04–2.99 (m, 1H, C–H), 2.80–2.76 (m, 1H, CH_2), 2.38 (d, *J* = 11.6 Hz, 1H, CH_2), 2.15–2.09 (m, 2H, CH_2), 1.99–1.95 (m, 1H, CH_2), 1.76 (s, 3H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$): δ 192.63, 157.55, 153.87, 150.58, 148.76, 147.81, 146.03, 145.98, 144.52, 143.84, 143.16, 142.74, 137.04, 137.02, 132.67, 131.67, 129.84, 127.51, 127.43, 126.74, 124.63, 123.34, 123.28, 121.72, 113.22, 110.55, 74.34, 71.79, 49.21, 44.17, 43.22, 34.00, 31.05, 30.57, 26.96; HRMS (ESI) m/z: calcd. For: $C_{38}H_{28}Cl_4N_6NaO_2$: 765.0896, $[M+Na]^+$ found: 765.0932.

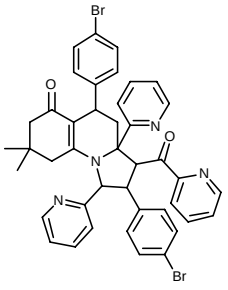
2,5-Bis-(4-chloro-phenyl)-8,8-dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4i)



Petroleum ether : EtOAc (4:1); R*f* = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3054, 2957, 2864, 2320, 1688, 1550, 1609, 1589, 1491, 1468, 1430, 1408, 1390, 1350, 1330, 1273, 1123, 1154, 1125, 1090, 1014, 995, 870, 830, 786, 747, 690, 658, 651, 579, 525 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, *J* = 4.4 Hz, 1H, Py–H), 8.54 (d, *J* = 4.4 Hz, 1H, Py–H), 8.50 (d, *J* = 8.0 Hz, 1H, Py–H), 8.32 (d, *J* = 4.4 Hz, 1H, Py–H), 7.82 (d, *J* = 8.0 Hz, 1H, Py–H), 7.79–7.72 (m, 2H, Py–H + Ar–H), 7.59 (t, *J* = 7.6 Hz, 1H, Py–H), 7.40 (t, *J* = 5.6 Hz, 1H, Py–H), 7.26 (m, 1H, Py–H), 7.15–7.10 (m, 5H, Py–H + Ar–H), 7.01 (d, *J* = 7.6 Hz, 4H, Py–H + Ar–H), 6.94 (d, *J* = 7.6 Hz, 1H, Ar–H), 5.51 (d, *J* = 13.2 Hz, 1H, C–H), 5.08 (d, *J* = 10.8 Hz, 1H, C–H), 3.93 (t, *J* = 12.0 Hz, 1H, C–H), 3.10 (dd, *J* = 13.2, 5.6 Hz, 1H, C–H), 2.81–2.77 (m, 1H, CH_2), 2.23–2.13 (m, 2H, CH_2), 1.92 (q, *J* = 16.4 Hz, 2H, CH_2), 1.72 (d, *J* = 16.8 Hz, 1H, CH_2), 1.08 (s, 3H, CH_3), 0.75 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.38, 192.84, 160.70, 159.12, 157.66, 154.90, 149.98, 148.47, 148.09, 145.45, 136.80, 136.68, 136.35, 135.65 133.14, 130.49, 129.60, 128.72, 128.38, 127.99, 126.92, 123.90, 122.94, 122.61, 122.39, 122.27, 111.10, 73.31, 73.11, 58.92, 52.70, 49.33, 46.36, 43.51, 36.97, 30.86, 30.68, 26.71; HRMS(ESI) m/z: calcd. for $C_{42}H_{36}Cl_2N_4O_2Na$: 721.211, $[M+Na]^+$ found: 721.2156.

2,5-Bis-(4-bromo-phenyl)-8,8-dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4j)

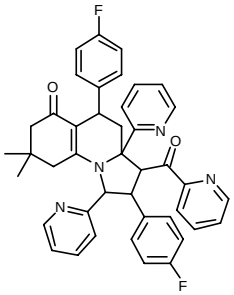


Petroleum ether : EtOAc (4:1); R$_f$ = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3053, 2960, 2860, 2320, 1694, 1618, 1590, 1550, 1487, 1428, 1407, 1360, 1332, 1273, 1246, 1153, 1124, 1088, 1010, 993, 825, 785, 748, 650, 620, 572, 535 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, *J* = 4.0 Hz, 1H, Py–H), 8.55 (d, *J* = 4.8 Hz, 1H, Py–H), 8.50 (d, *J* = 8.0 Hz, 1H, Py–H), 8.32 (d, *J* = 4.0 Hz, 1H, Py–H), 7.83–7.72 (m, 3H, Py–H + Ar–H), 7.61–7.57 (m, 1H, Py–H), 7.41–7.38 (m, 1H, Py–H), 7.30–7.26 (m, 4H, Py–H + Ar–H), 7.25 (s, 1H, Ar–H), 7.15–7.12(m, 1H, Ar–H), 6.96–6.93 (m, 5H, Py–H + Ar–H), 5.51 (d, *J* = 13.2 Hz, 1H, C–H), 5.08 (d, *J* = 10.8 Hz, 1H, C–H), 3.92 (t, *J* = 12.0 Hz, 1H, C–H), 3.10 (dd, *J* = 12.8, 5.6 Hz, 1H, C–H), 2.77 (dd, *J* = 12.0, 5.6 Hz, 1H, CH_2), 2.22–2.13 (m, 2H, CH_2), 2.01–1.86 (m, 2H, CH_2), 1.74–1.69 (m, 1H, CH_2), 1.07 (s, 3H, CH_3), 0.75 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.37, 192.82, 160.68, 159.09, 157.63, 154.88, 149.99, 148.50, 148.10, 145.98, 136.80, 136.69, 136.35, 136.17, 131.67, 130.91, 129.96, 128.82, 126.93, 123.89, 122.95, 122.60, 122.40, 122.28, 121.32, 118.64, 111.06, 73.25, 73.09, 58.85, 52.76, 49.31, 46.27, 43.50, 37.04, 30.86, 30.69, 26.70; HRMS (ESI) m/z: calcd. for

$C_{42}H_{36}Br_2N_4O_2Na$: 811.1082, $[M+Na]^+$ found: 811.1095.

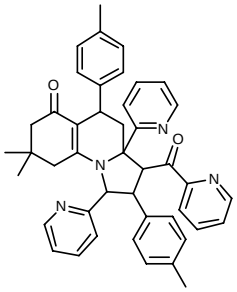
2,5-Bis-(4-fluoro-phenyl)-8,8-dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4k)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^oC.

IR (KBr): 3053, 2957, 2876, 2354, 1695, 1613, 1589, 1549, 1509, 1469, 1432, 1412, 1384, 1353, 1328, 1274, 1222, 1153, 1125, 1091, 1013, 995, 871, 833, 785, 750, 689, 656, 619, 575, 530 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.72 (d, J = 2.0 Hz, 1H, Py–H), 8.54 (d, J = 3.2 Hz, 1H, Py–H), 8.50 (d, J = 8.0 Hz, 1H, Py–H), 8.32 (d, J = 2.4 Hz, 1H, Py–H), 7.83–7.72 (m, 3H, Py–H + Ar–H), 7.58 (t, J = 7.2 Hz, 1H, Py–H), 7.38 (t, J = 4.8 Hz, 1H, Py–H), 7.26 (m, 1H, Py–H), 7.15–7.12 (m, 1H, Py–H), 7.02 (s, 4H, Py–H + Ar–H), 6.94 (d, J = 7.2 Hz, 1H, Py–H), 6.88–6.80 (m, 4H, Py–H + Ar–H), 5.52 (d, J = 12.8 Hz, 1H, C–H), 5.08 (d, J = 10.4 Hz, 1H, C–H), 3.94 (t, J = 11.6 Hz, 1H, C–H), 3.11 (dd, J = 12.8, 6.0 Hz, 1H, C–H), 2.83–2.78 (m, 1H, CH_2), 2.25–2.14 (m, 2H, CH_2), 1.99–1.86 (m, 2H, CH_2), 1.72 (d, J = 16.8 Hz, 1H, CH_2), 1.08 (s, 3H, CH_3), 0.75 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.51, 192.89, 160.87, 159.55, 159.25, 157.57, 154.98, 149.93, 148.43, 148.06, 142.36, 136.79, 136.61, 136.33, 132.81, 132.78, 129.79, 129.71, 128.27, 128.20, 126.88, 123.89, 122.88, 122.59, 122.41, 122.24, 115.54, 115.33, 114.65, 114.45, 111.34, 73.51, 73.11, 59.04, 52.60, 49.37, 46.62, 43.55, 36.79, 30.84, 30.71, 26.68; HRMS (ESI) m/z: calcd. for $C_{42}H_{36}F_2N_4O_2Na$: 689.2704, $[M+Na]^+$ found: 689.2777.

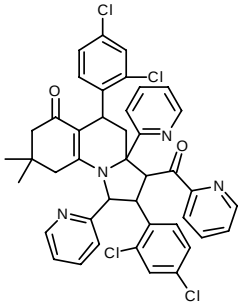
8,8-Dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,5-di-p-tolyl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one (4l)



Petroleum ether : EtOAc (4:1); R_f = 0.3; white solid, m.p. > 300 ^oC.

IR(KBr): 3054, 3018, 2963, 2923, 2884, 1693, 1620, 1591, 1553, 1512, 1469, 1426, 1407, 1362, 1334, 1321, 1275, 1243, 1218, 1178, 1153, 1124, 1088, 1055, 1040, 992, 820, 803, 785, 746, 686, 657, 596, 574, 534 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.70 (d, J = 4.4 Hz, 1H, Py–H), 8.54 (d, J = 4.0 Hz, 1H, Py–H), 8.50 (d, J = 7.6 Hz, 1H, Py–H), 8.32 (d, J = 4.4 Hz, 1H, Py–H), 7.80 (d, J = 7.6 Hz, 1H, Py–H), 7.72 (t, J = 7.6 Hz, 2H, Py–H + Ar–H), 7.56 (t, J = 7.6 Hz, 1H, Py–H), 7.34 (t, J = 6.0 Hz, 1H, Py–H), 7.23 (t, J = 6.0 Hz, 1H, Py–H), 7.11 (t, J = 6.0 Hz, 1H, Py–H), 6.97–6.91 (m, 9H, Py–H + Ar–H), 5.55 (d, J = 13.2 Hz, 1H, C–H), 5.10 (d, J = 10.8 Hz, 1H, C–H), 3.92 (t, J = 11.6 Hz, 1H, C–H), 3.14 (dd, J = 13.2 , 8.0 Hz, 1H, C–H), 2.79 (dd, J = 12.0, 5.6 Hz, 1H, CH_2), 2.28–2.21 (m, 4H, CH_2), 2.19–2.13 (m, 4H, CH_2 + CH_3), 1.90 (q, J = 16.4 Hz, 2H, CH_3), 1.70 (d, J = 17.2 Hz, 1H, CH_3), 1.08 (s, 3H, CH_3), 0.73 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.83, 192.85, 161.38, 159.62, 157.40, 155.15, 149.75, 148.49, 148.00, 143.79, 136.79, 136.59, 136.47, 136.20, 134.19, 134.03, 129.16, 128.55, 128.10, 126.99, 126.64, 123.89, 122.65, 122.38, 122.05, 111.76, 73.56, 73.24, 58.96, 53.09, 49.40, 46.54, 43.61, 37.14, 30.81, 30.78, 26.68, 21.15, 21.02; HRMS (ESI) m/z: calcd. For $C_{44}H_{42}N_4O_2Na$: 681.3206, $[M+Na]^+$ found: 681.3152.

2,5-Bis-(2,4-dichloro-phenyl)-8,8-dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4m)

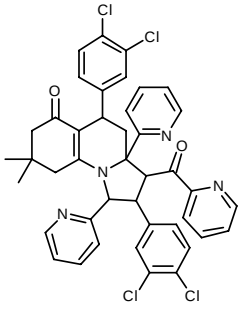


Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^oC.

IR(KBr): 3431, 3330, 2995, 2950, 2890, 1713, 1627, 1615, 1597, 1535, 1484, 1420, 1367, 1350, 1294, 1283, 1210, 1185, 1122, 1084, 1025, 945, 921, 871, 820, 804, 750, 689, 660, 577, 565, 537 cm^{-1}; ^1H NMR (400 MHz, $CDCl_3$): δ 8.67 (d, J = 4.4 Hz, 1H, Py–H), 8.54 (d, J = 4.0 Hz, 1H, Py–H), 8.33–8.31 (m, 2H, Py–H), 7.85 (d, J = 8.0 Hz, 1H, Py–H), 7.78 (t, J = 7.6 Hz, 1H, Py–H), 7.72 (t, J = 7.6 Hz, 1H, Py–H), 7.62 (t, J = 7.2 Hz, 1H, Py–H), 7.41 (t, J = 6.0 Hz, 1H, Py–H), 7.27–7.26 (m, 3H, Py–H + Ar–H), 7.21–7.05 (m, 6H,

Py–H + Ar–H), 5.62 (d, *J* = 12.4 Hz, 1H, C–H), 5.11 (s, 1H, C–H), 4.51 (t, *J* = 10.4 Hz, 1H, C–H), 3.30–3.26 (m, 1H, C–H), 3.10 (dd, *J* = 12.8, 5.6 Hz, 1H, CH_2), 2.21–1.88 (m, 4H, CH_2), 1.80 (d, *J* =17.2 Hz, 1H, CH_2), 1.07 (s, 3H, CH_3), 0.77 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.00, 192.55, 158.54, 158.19, 154.98, 149.90, 148.35, 148.02, 142.73, 136.95, 136.88, 136.23, 134.17, 133.47, 130.78, 129.73, 128.79, 127.58, 127.57, 126.94, 126.71, 123.43, 122.98, 122.50, 122.42, 121.95, 113.21, 110.39, 73.23, 49.28, 44.30, 43.39, 32.60, 31.05, 30.63, 26.79; HRMS (ESI) m/z: calcd. For $C_{42}H_{34}Cl_4N_4O_2Na$: 791.1304, $[M+Na]^+$ found: 791.1275.

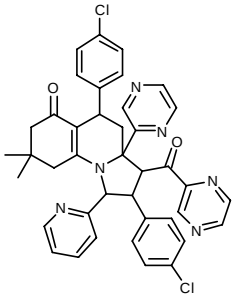
2,5-Bis-(3,4-dichloro-phenyl)-8,8-dimethyl-3-(pyridine-2-carbonyl)-1,3a-di-pyridin-2-yl-2,3,3a,4,5,7,8,9-octa hydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4n)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3154, 3028, 2955, 2910, 2875, 1693, 1612, 1589, 1550, 1469, 1430, 1409, 1354, 1326, 1271, 1300, 1223, 1149, 1129, 1092, 1030, 995, 840, 822, 788, 749, 680, 652, 647, 620 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.74 (d, *J* = 4.0 Hz, 1H, Py–H), 8.57 (d, *J* = 4.4 Hz, 1H, Py–H), 8.51 (d, *J* = 7.6 Hz, 1H, Py–H), 8.32 (d, *J* = 4.0 Hz, 1H, Py–H), 7.85–7.73 (m, 3H, Py–H + Ar–H), 7.62 (t, *J* = 7.6 Hz, 1H, Py–H), 7.42 (t, *J* = 5.6 Hz, 1H, Py–H), 7.30–7.29 (m, 1H, Py–H), 7.25–7.13 (m, 5H, Py–H + Ar–H), 6.97–6.89 (m, 3H, Py–H + Ar–H), 5.49 (d, *J* = 12.8 Hz, 1H, C–H), 5.08 (d, *J* = 10.8 Hz, 1H, C–H), 3.93 (t, *J* = 11.6 Hz, 1H, C–H), 3.11 (dd, *J* = 12.8, 5.6 Hz, 1H, C–H), 2.78–2.74 (m, 1H, CH_2), 2.22–2.14 (m, 2H, CH_2), 1.93 (q, *J* = 16.4 Hz, 2H, CH_2), 1.72 (d, *J* = 17.2 Hz, 1H, CH_2), 1.08 (s, 3H, CH_3), 0.76 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.14, 192.84, 160.22, 158.77, 157.86, 154.74, 150.16, 148.56, 148.18, 147.50, 137.50, 136.92, 136.87, 136.45, 132.62, 131.67, 131.52, 130.52, 130.18, 129.85, 128.91, 128.68, 127.74, 127.12, 126.67, 123.90, 123.19, 122.67, 122.43, 110.64, 73.04, 73.00, 58.81, 52.42, 49.29, 45.99, 43.43, 36.91, 30.93, 30.68, 26.69; HRMS (ESI) m/z: calcd. For $C_{42}H_{34}Cl_4N_4O_2Na$: 791.1304, $[M+Na]^+$ found: 791.1319.

2,5-Bis-(4-chloro-phenyl)-8,8-dimethyl-3-(pyrazine-2-carbonyl)-3a-pyrazin-2-yl-1-pyridin-2-yl-2,3,3a,4,5,7,8 ,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4o)



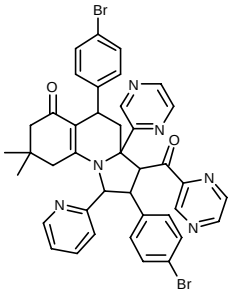
Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3569, 3449, 3127, 2950, 2361, 1686, 1619, 1609, 1588, 1552, 1513, 1491, 1468, 1433, 1408, 1399, 1330, 1352, 1319, 1285, 1273, 1192, 1092, 1046, 1019, 996, 860, 830, 813, 788, 751, 651, 579 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.91 (s, 1H, Py–H), 9.01 (s, 1H, Py–H), 8.82 (s, 1H, Py–H) , 8.71 (s, 1H, Py–H), 8.53 (d, *J* = 9.6 Hz, 2H, Py–H), 8.34 (s, 1H, Py–H), 7.60–7.56 (m, 1H, Py–H), 7.15 (t, *J* = 7.6 Hz, 5H, Py–H+ Ar–H), 6.99 (d, *J* = 7.6 Hz, 4H, Py–H + Ar–H), 6.82 (d, *J* = 7.2 Hz, 1H, Ar–H), 5.37 (d, *J* = 12.8 Hz, 1H, C–H), 5.09 (d, *J* = 10.4 Hz, 1H, C–H), 3.97 (t, *J* = 11.6 Hz, 1H, C–H), 3.01–2.97 (m, 1H, C–H), 2.75–2.73 (m, 1H, CH_2), 2.22–2.11 (m, 2H, CH_2), 1.94 (q, *J* = 16.8 Hz, 2H, CH_2), 1.75 (d, *J* = 17.6 Hz, 1H, CH_2), 1.07 (s, 3H, CH_3), 0.75 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.80, 193.10, 159.87, 157.19, 154.36, 150.57, 148.69, 147.80, 146.24, 144.83, 144.45, 143.72, 143.22, 142.84, 136.81, 134.79, 133.60, 130.85, 129.49, 128.98, 128.22, 128.18, 123.26, 122.54, 110.99, 72.92, 71.53, 59.25, 52.55, 49.20, 46.27, 43.32, 36.86, 30.86, 30.68, 26.74, 22.43; HRMS (ESI) m/z: calcd. For $C_{40}H_{34}Cl_2N_6O_2Na$: 723.2018, $[M+Na]^+$ found: 723.2019.

2,5-Bis-(4-bromo-phenyl)-8,8-dimethyl-3-(pyrazine-2-carbonyl)-3a-pyrazin-2-yl-1-pyridin-2-yl-2,3,3a,4,5,7, 8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4p)

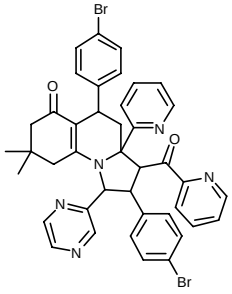
Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3429, 3109, 2882, 2358, 1697, 1619, 1589, 1548, 1542, 1485, 1477, 1420, 1410, 1349, 1320, 1290, 1208, 1187, 1180, 1107, 1104, 1081, 1052, 1032, 1017, 1007, 959, 927, 893, 860, 825, 821, 779, 778, 749, 667, 688, 554 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.91 (s, 1H, Py–H), 9.01 (s, 1H, Py–H), 8.82 (s, 1H, Py–H), 8.71 (s, 1H, Py–H), 8.53 (d, *J* = 12.0 Hz, 2H, Py–H), 8.34 (s, 1H, Py–H), 7.59 (t, *J* = 7.2 Hz, 1H, Py–H), 7.31–7.26 (m,



5H, Py–H + Ar–H), 6.93 (m, 4H, Py–H + Ar–H), 6.82 (d, *J* = 8.0 Hz, 1H, Ar–H), 5.36 (d, *J* = 12.8 Hz, 1H, C–H), 5.09 (d, *J* = 10.8 Hz, 1H, C–H), 3.96 (t, *J* = 12.0 Hz, 1H, C–H), 2.99 (dd, *J* = 13.2, 5.6 Hz, 1H, C–H), 2.73 (t, *J* = 6.8 Hz, 1H, CH_2), 2.22–2.11 (m, 2H, CH_2), 1.94 (q, *J* = 16.8 Hz, 2H, CH_2), 1.75 (d, *J* = 17.2 Hz, 1H, CH_2), 1.07 (s, 3H , CH_3), 0.76 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 196.78, 194.33, 193.08, 159.84, 158.85, 157.20, 154.33, 150.58, 148.68, 147.80, 146.24, 145.38, 144.44, 143.73, 143.24, 142.84, 136.83, 135.32, 131.92, 131.13, 129.84, 128.62, 123.26, 122.55, 121.75, 118.96, 110.94, 108.63, 72.85, 71.52, 59.19, 52.62, 49.19, 46.19, 43.31, 36.93, 30.86, 30.67, 26.75; HRMS (ESI) m/z: calcd. For $C_{40}H_{34}Br_2N_6O_2Na$: 813.0987, $[M+Na]^+$ found: 813.0973.

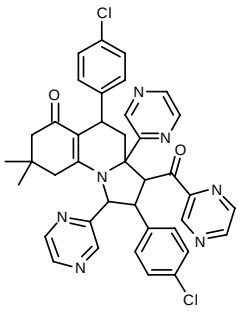
2,5-Bis-(4-bromo-phenyl)-8,8-dimethyl-1-pyrazin-2-yl-3-(pyridine-2-carbonyl)-3a-pyridin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one (4q)



Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

IR(KBr): 3568, 3293, 3051, 2953, 2869, 1693, 1618, 1587, 1553, 1487, 1467, 1396, 1348, 1320, 1270, 1225, 1175, 1124, 1102, 1072, 1010, 995, 823, 787, 752, 698, 661, 642, 618, 564, 510 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (s, 1H, Py–H), 8.57 (d, *J* = 2.4 Hz, 1H, Py–H), 8.54 (d, *J* = 4.0 Hz, 1H, Py–H), 8.33 (s, 1H, Py–H), 8.29 (s, 1H, Py–H), 8.25 (d, *J* = 7.6 Hz, 1H, Py–H), 7.81 (d, *J* = 7.6 Hz, 1H, Py–H), 7.78–7.76 (m, 1H, Py–H), 7.75–7.71 (m, 1H, Py–H), 7.39 (t, *J* = 5.6 Hz, 1H, Py–H), 7.30 (d, *J* = 2.0 Hz, 2H, Py–H + Ar–H), 7.28 (d, *J* = 2.0 Hz, 2H, Ar–H), 7.14 (t, *J* = 5.6 Hz, 1H, Ar–H), 6.96–6.93 (m, 4H, Ar–H), 5.53 (d, *J* = 12.8 Hz, 1H, C–H), 5.18 (d, *J* = 10.8 Hz, 1H, C–H), 3.90 (t, *J* = 12.0 Hz, 1H, C–H), 3.14–3.09 (m, 1H, C–H), 2.80–2.77 (m, 1H, CH_2), 2.22 (t, *J* = 12.8 Hz, 1H, CH_2), 2.09 (d, *J* = 17.2 Hz, 1H, CH_2), 1.99–1.88 (m, 2H, CH_2), 1.72–1.69 (m, 1H, CH_2), 1.09 (s, 3H, CH_3), 0.77 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 197.00, 192.89, 158.73, 156.65, 156.59, 154.65, 148.52, 148.24, 145.63, 144.59, 144.21, 144.01, 136.85, 136.43, 135.20, 131.98, 130.97, 129.82, 128.76, 127.03, 123.30, 122.41, 122.38, 121.76, 118.75, 111.57, 73.24, 70.53, 59.01, 52.97, 49.21, 46.12, 43.99, 36.96, 30.94, 30.79, 26.62; HRMS (ESI) m/z: calcd. For $C_{41}H_{35}Br_2N_5O_2Na$: 812.1035, $[M+Na]^+$ found: 812.1032.

2,5-Bis-(4-chloro-phenyl)-8,8-dimethyl-3-(pyrazine-2-carbonyl)-1-pyrazin-2-yl-3a-pyrimidin-2-yl-2,3,3a,4,5,7,8,9-octahydro-1*H*-pyrrolo[1,2-*a*]quinolin-6-one(4r)

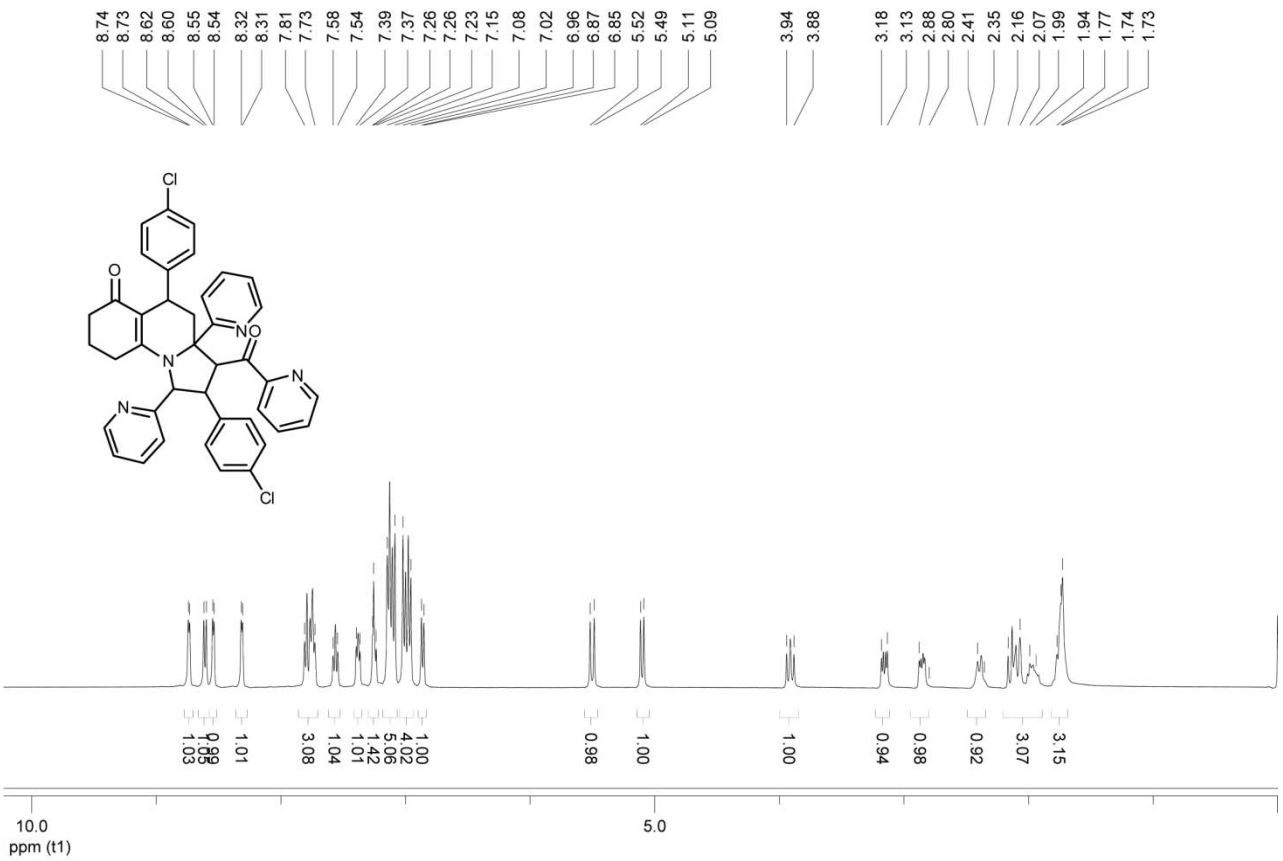


Petroleum ether : EtOAc (4:1); R_f = 0.2; white solid, m.p. > 300 ^{o}C.

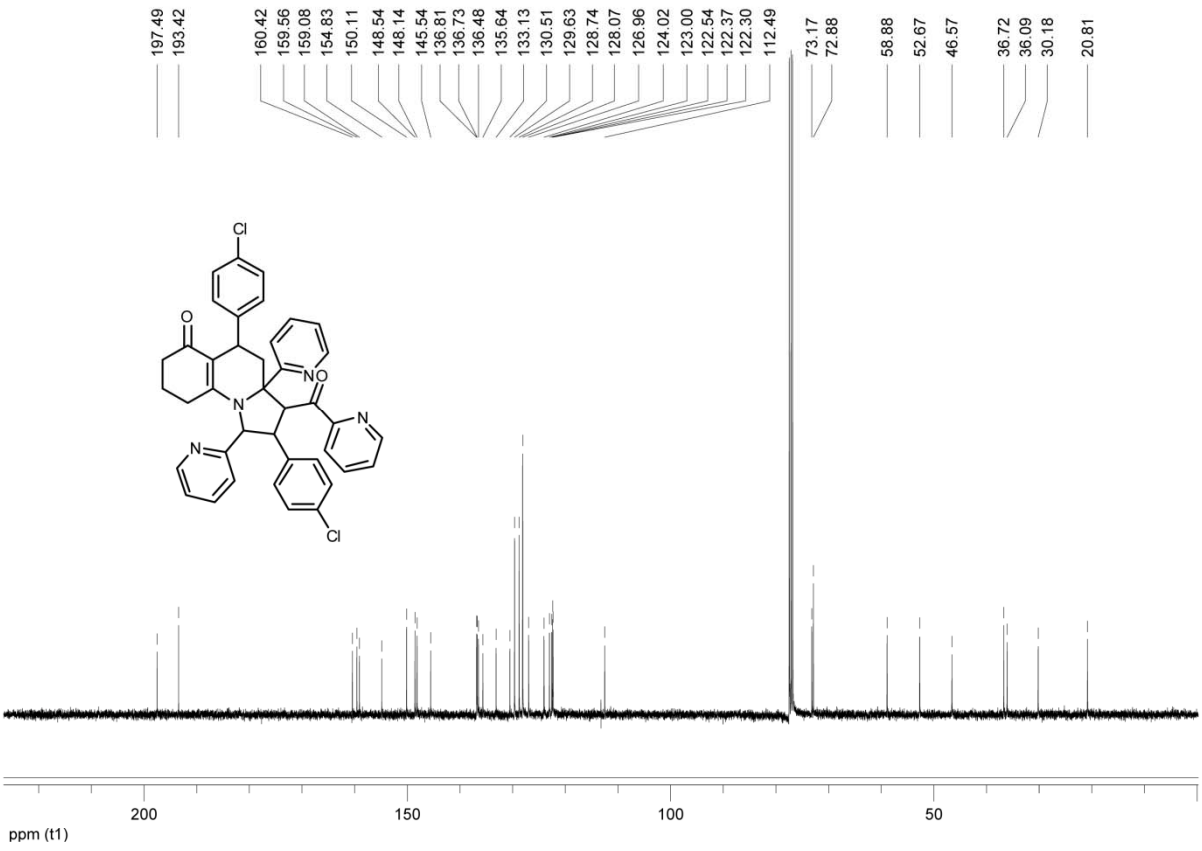
IR(KBr): 3422, 3044, 2957, 2869, 1694, 1637, 1561, 1490, 1468, 1406, 1392, 1314, 1227, 1178, 1091, 1053, 1017, 974, 940, 911, 841, 763, 724, 698, 665, 616, 581, 566, 527 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.79 (s, 1H, Py–H), 8.98 (s, 1H, Py–H), 8.82 (s, 2H, Py–H), 8.74 (s, 1H, Py–H), 8.60 (d, *J* = 2.0 Hz, 1H, Py–H), 8.08 (d, *J* = 2.0 Hz, 1H, Py–H), 8.01 (s, 1H, Py–H), 7.65 (s, 1H, Py–H), 7.18 (d, *J* = 8.0 Hz, 2H, Ar–H), 6.98 (d, *J* = 8.0 Hz, 2H, Ar–H), 6.69 (d, *J* = 8.0 Hz, 2H, Ar–H), 6.36 (d, *J* = 8.0 Hz, 2H, Ar–H), 5.33 (d, *J* = 12.8 Hz, 1H, C–H), 5.19 (d, *J* = 10.4 Hz, 1H, C–H), 4.22 (s, 1H, C–H), 3.72 (t, *J* = 11.2 Hz, 1H, C–H), 3.24 (d, *J* = 12.8 Hz, 1H, CH_2), 2.57–2.55 (m, 1H, CH_2), 2.31–2.22 (m, 2H, CH_2), 2.14 (d, *J* = 16.0 Hz, 1H, CH_2), 1.98 (d, *J* = 16.0 Hz, 1H, CH_2), 1.02 (s, 3H, CH_3), 0.92 (s, 3H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$): δ 195.92, 194.14, 180.35, 157.03, 155.72, 153.73, 148.66, 147.92, 145.81, 144.92, 144.63, 144.53, 143.62, 143.15, 142.83, 141.90, 140.88, 134.10, 133.91, 129.99, 129.55, 129.35, 128.69, 128.65, 127.48, 113.21, 108.89, 71.78, 70.78, 60.96, 51.67, 49.84, 43.27, 41.09, 34.14, 32.23, 29.82, 27.72; HRMS (ESI) m/z: calcd. For $C_{39}H_{33}Cl_2N_7O_2Na$: 724.1970, $[M+Na]^+$ found: 724.1972.

Copies of NMR spectra of Products

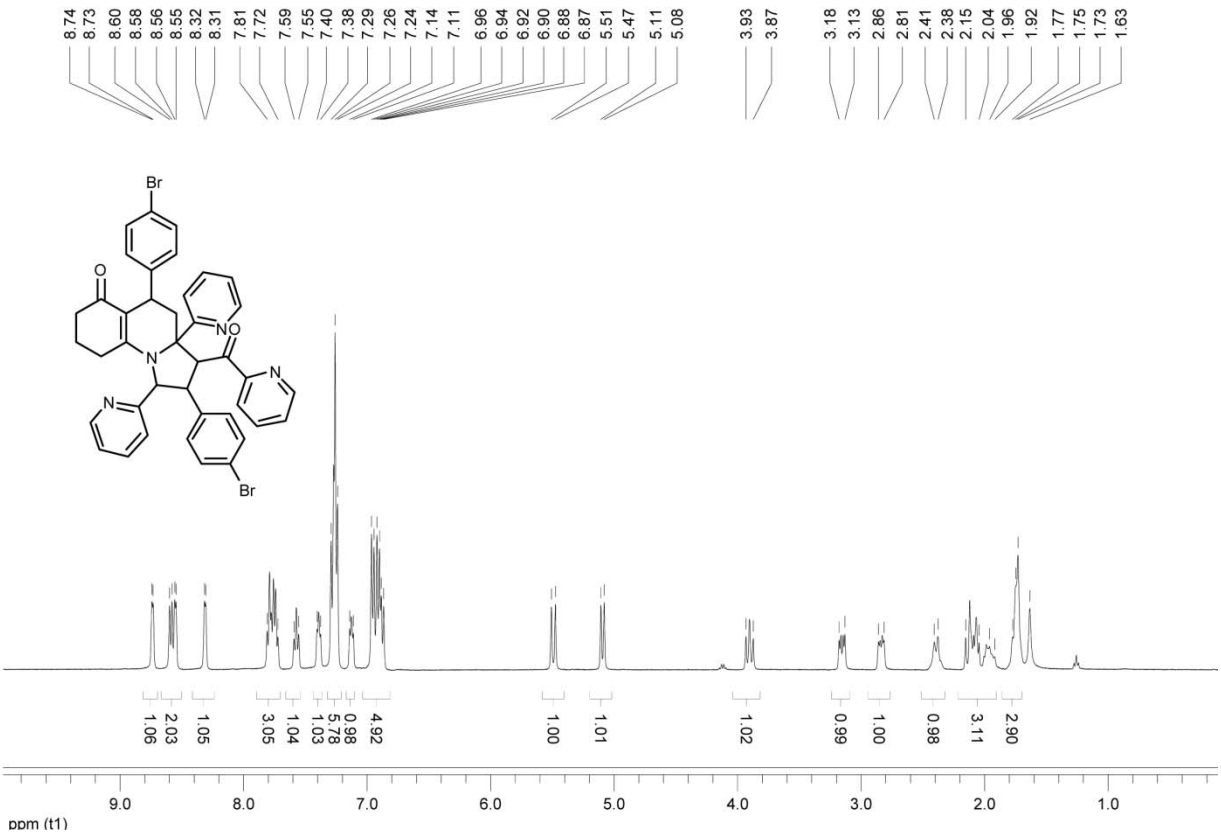
Product 4a, ^{1}H NMR 400 MHz, $CDCl_3$



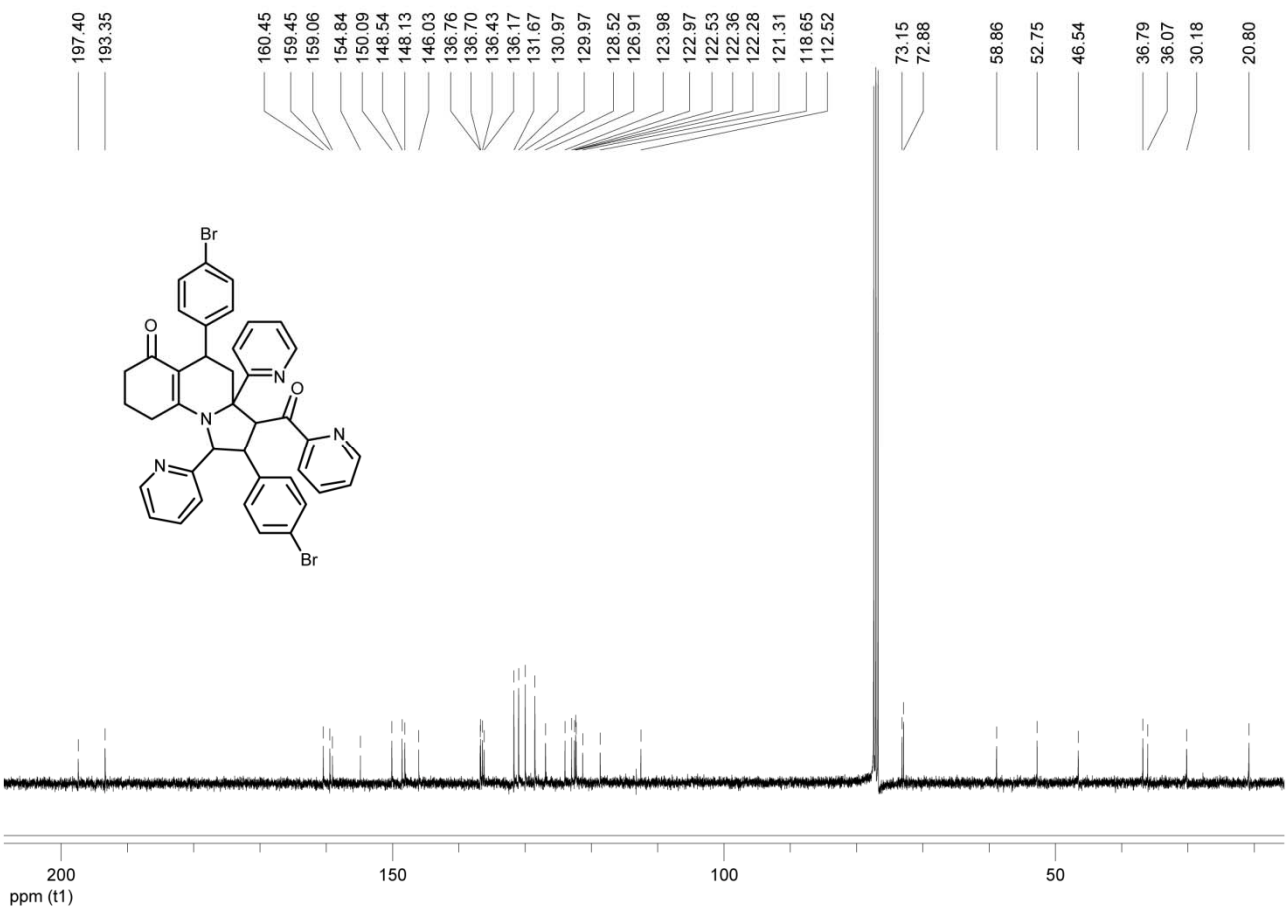
^{13}C NMR 100 MHz, $CDCl_3$



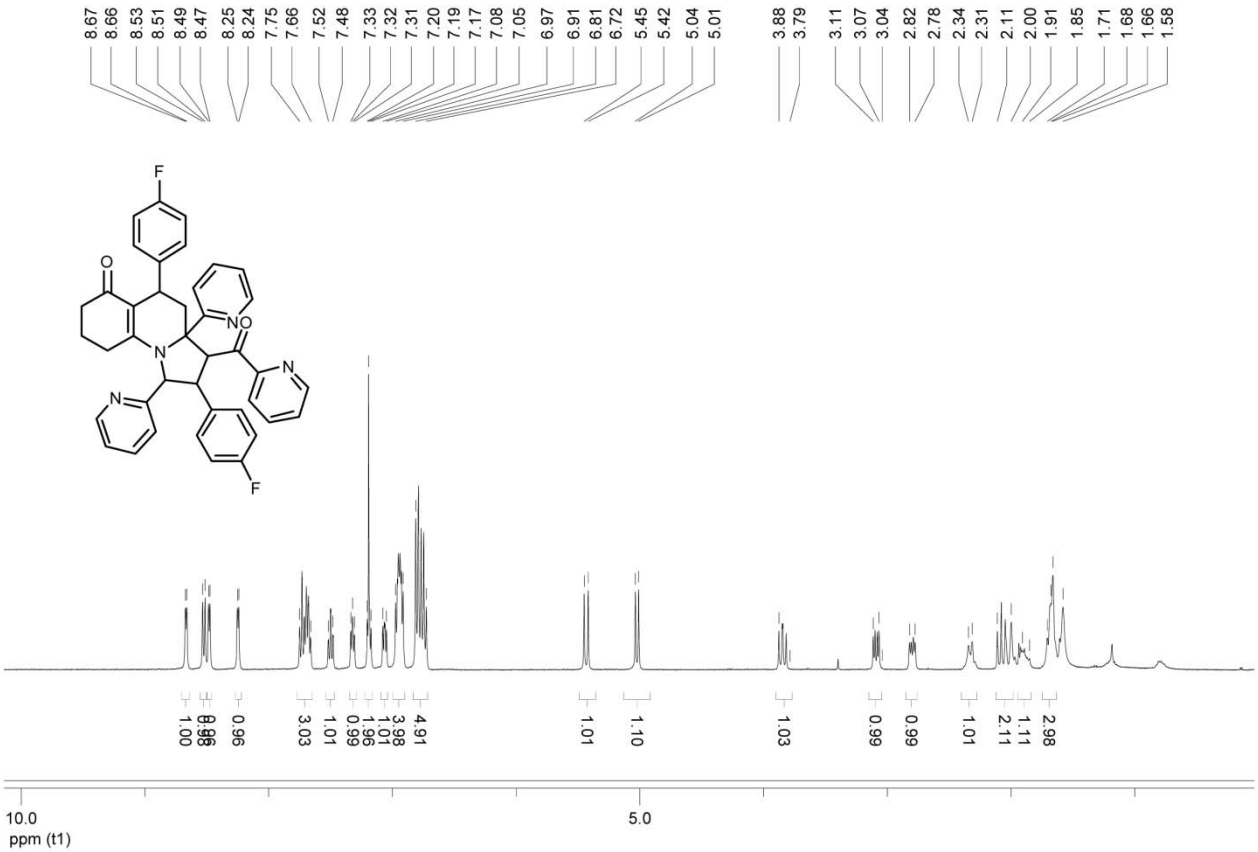
Product 4b, ^{1}H NMR 400 MHz, $CDCl_3$



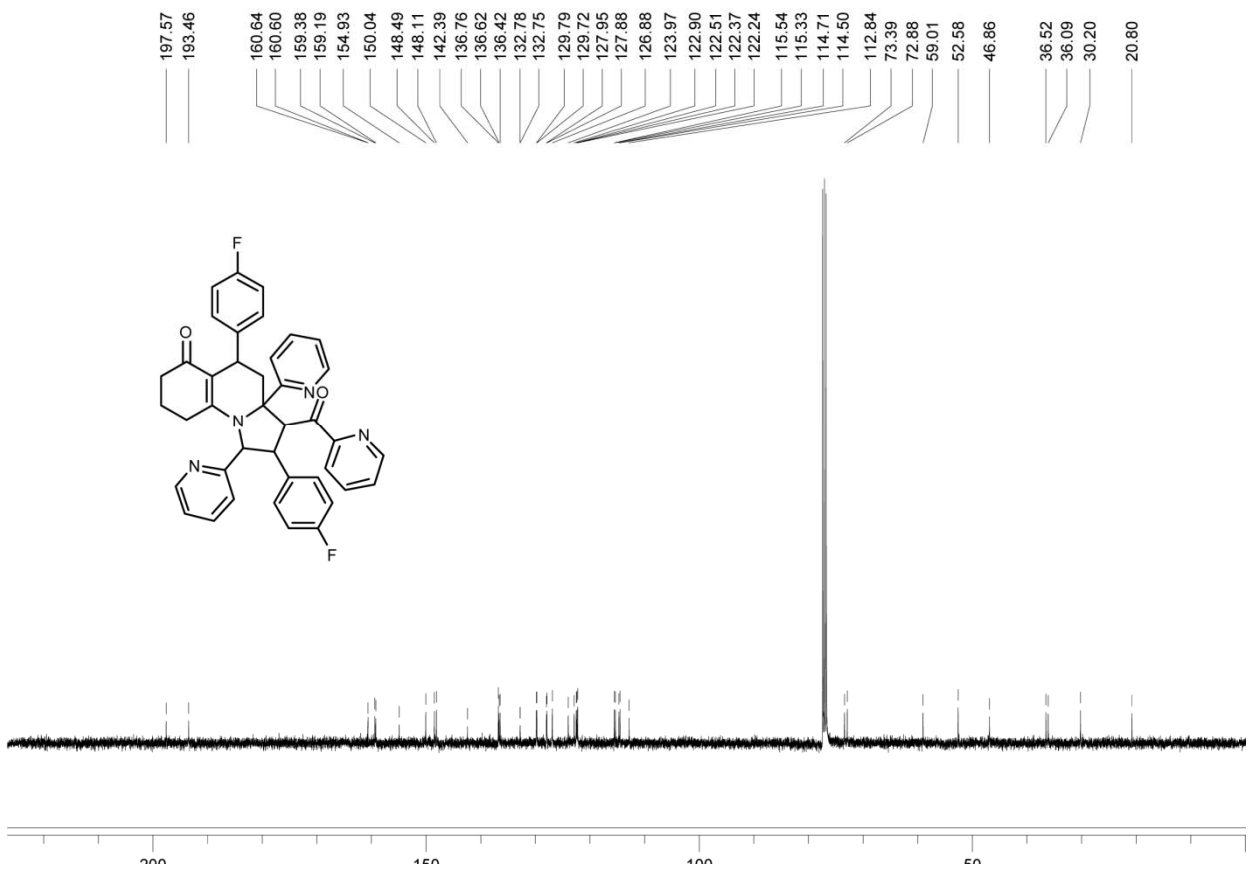
^{13}C NMR 100 MHz, $CDCl_3$



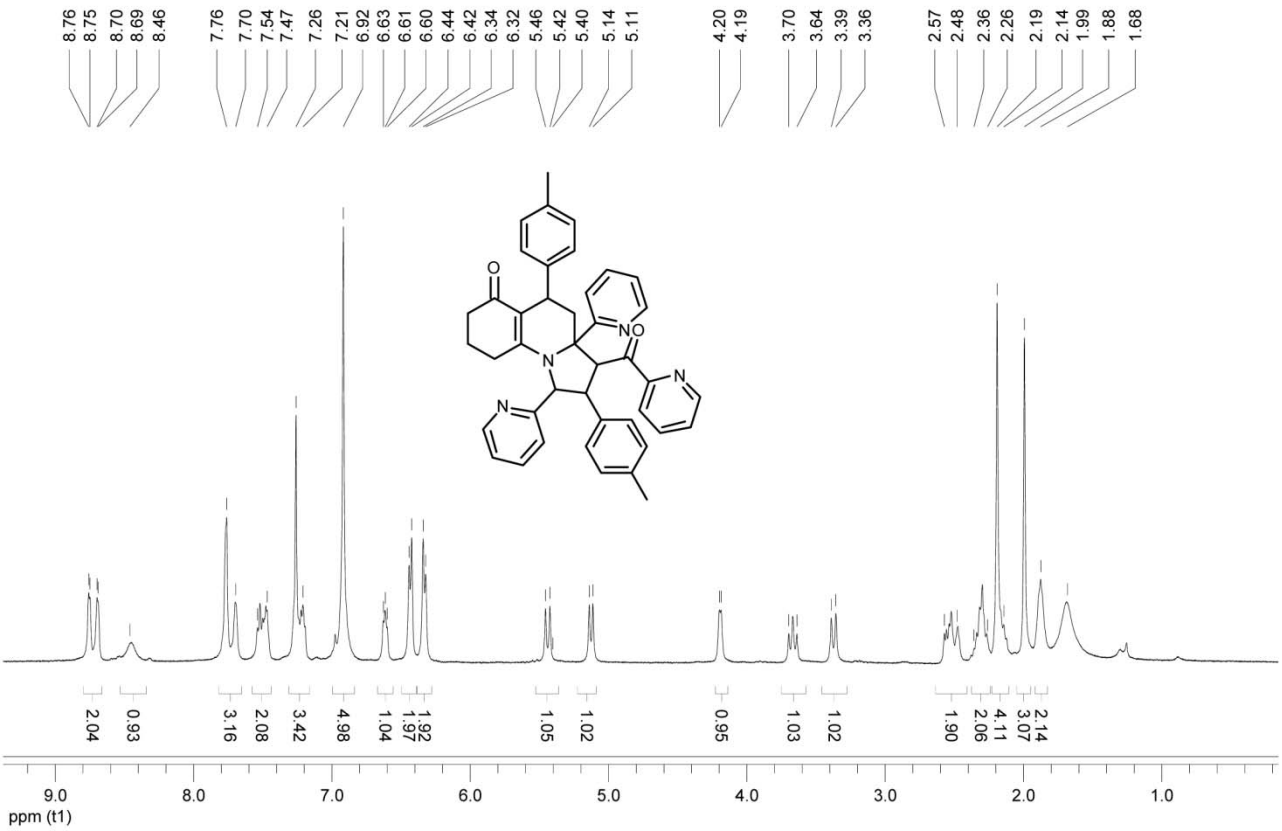
Product 4c, ^{1}H NMR 400 MHz, $CDCl_3$



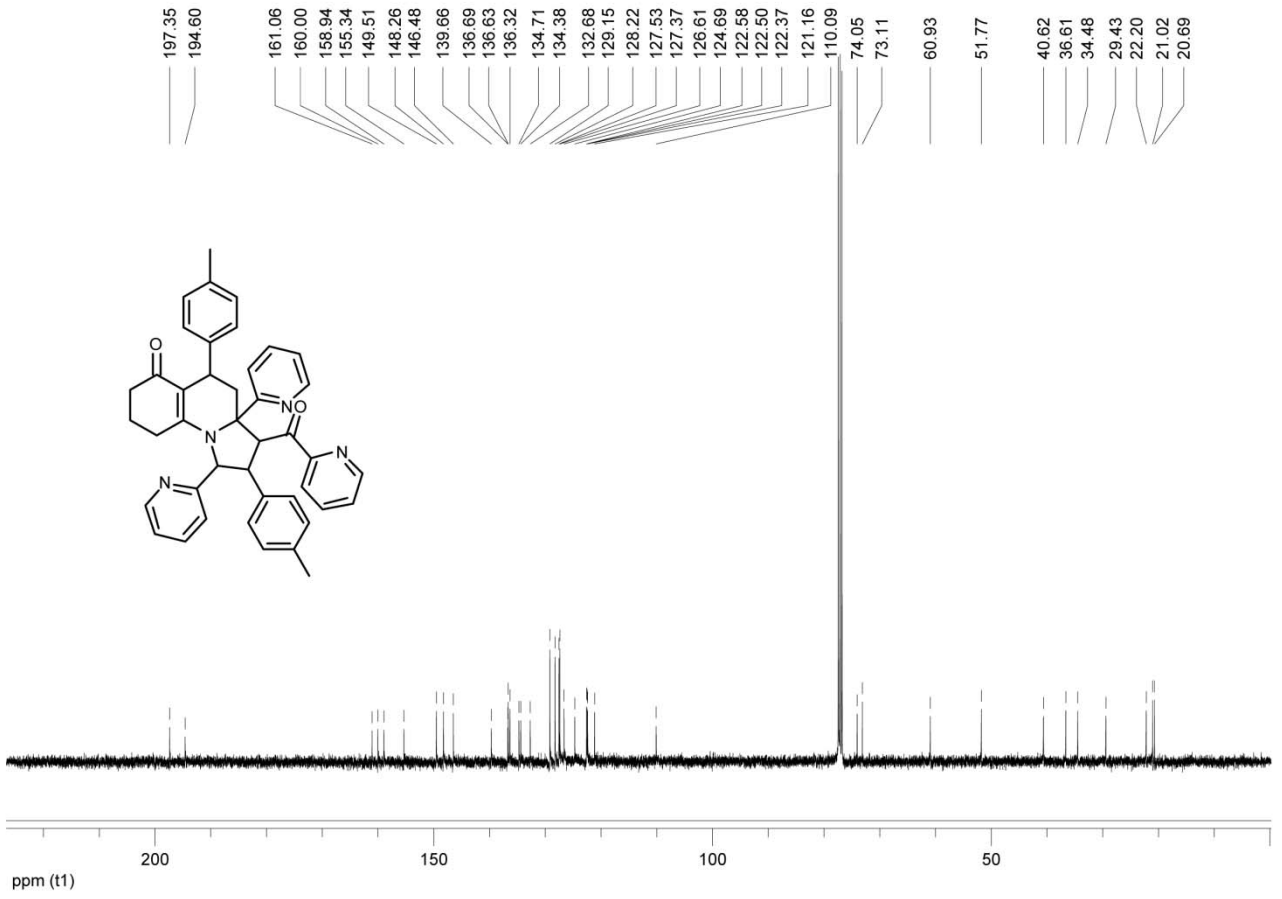
^{13}C NMR 100 MHz, $CDCl_3$



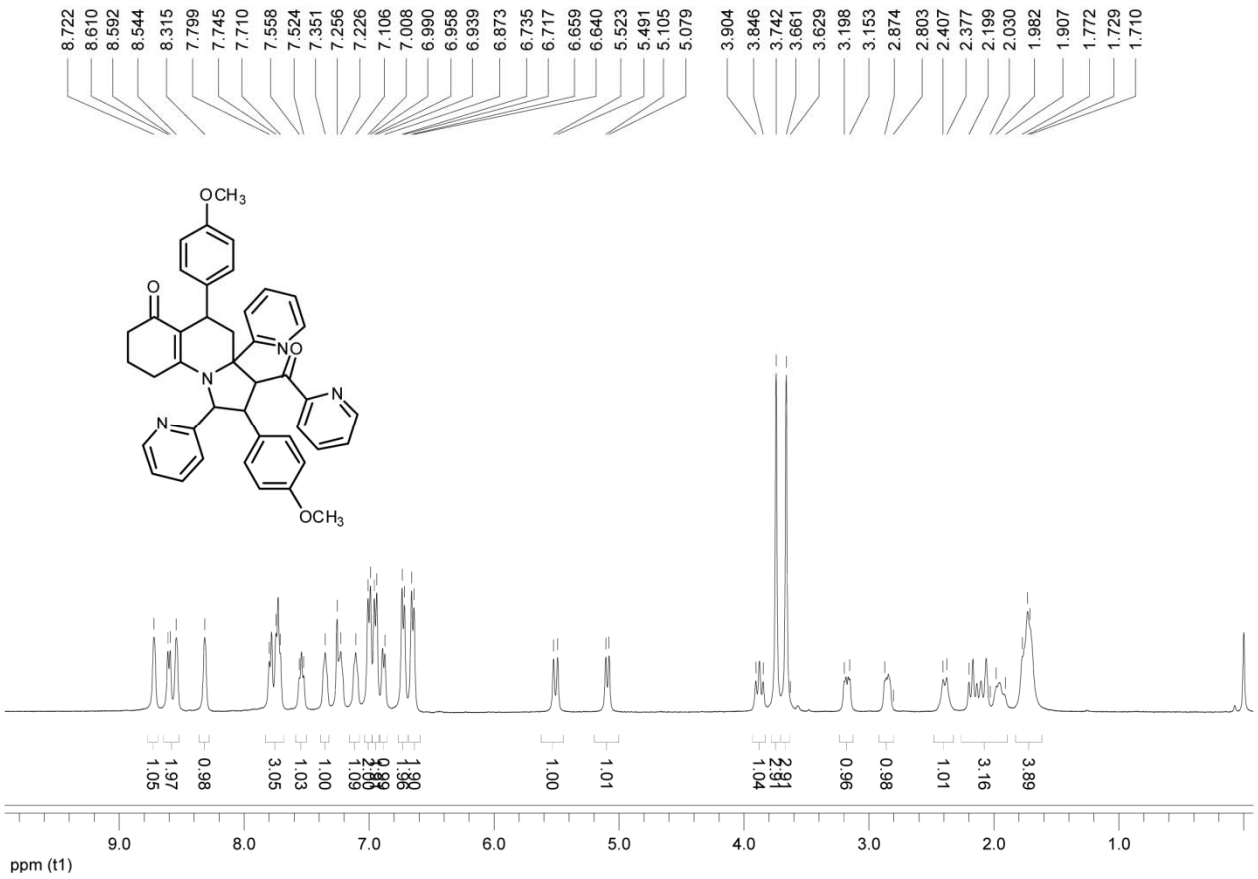
Product 4d, ^{1}H NMR 400 MHz, $CDCl_3$



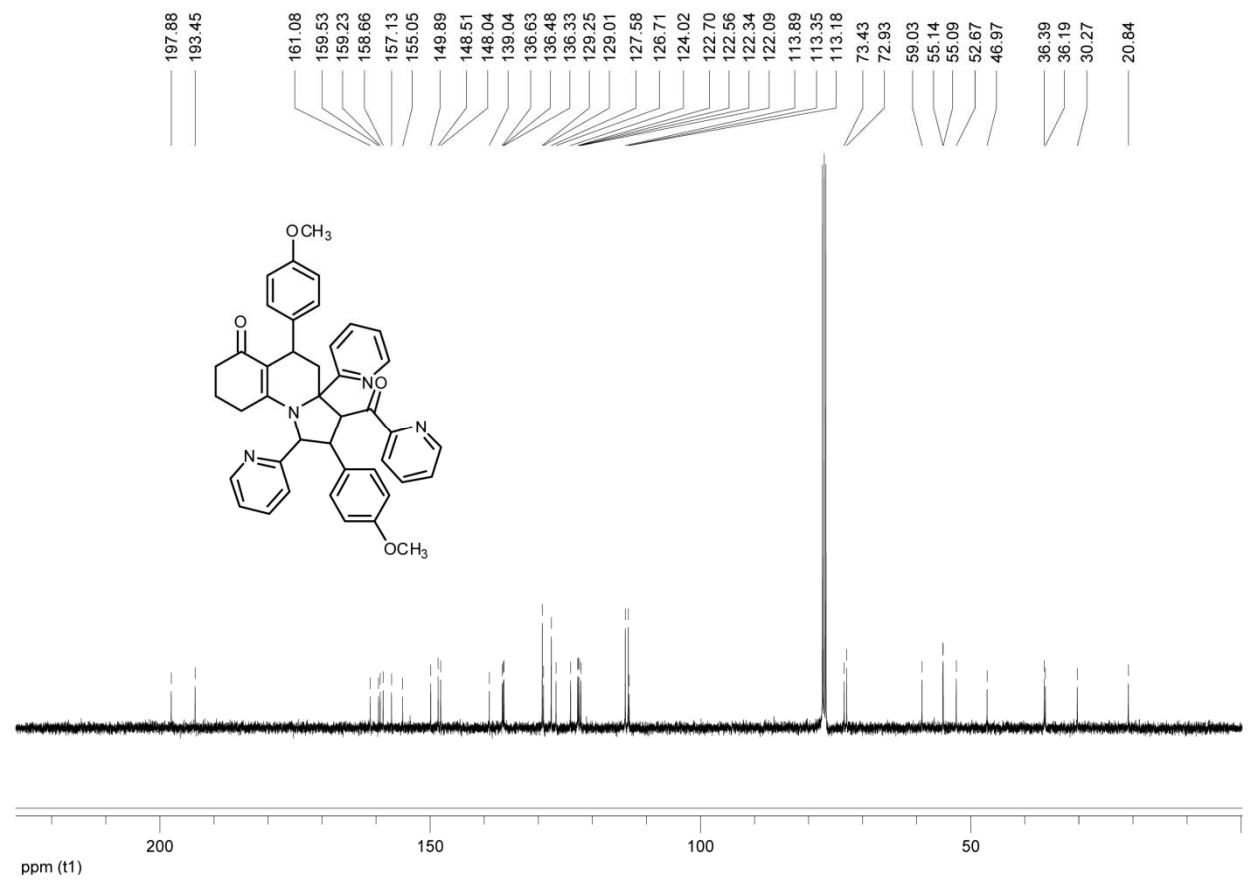
^{13}C NMR 100 MHz, $CDCl_3$



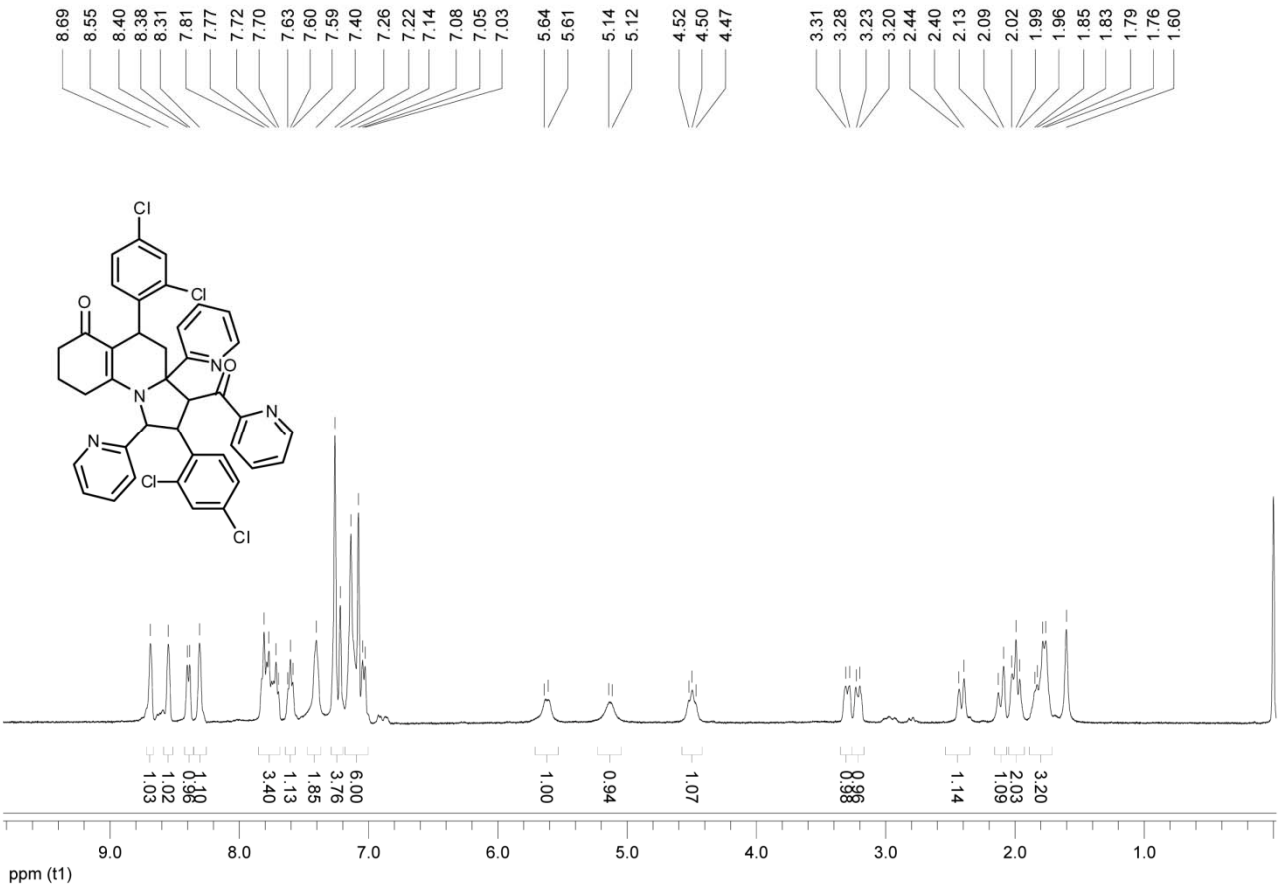
Product 4e, ^{1}H NMR 400 MHz, $CDCl_3$



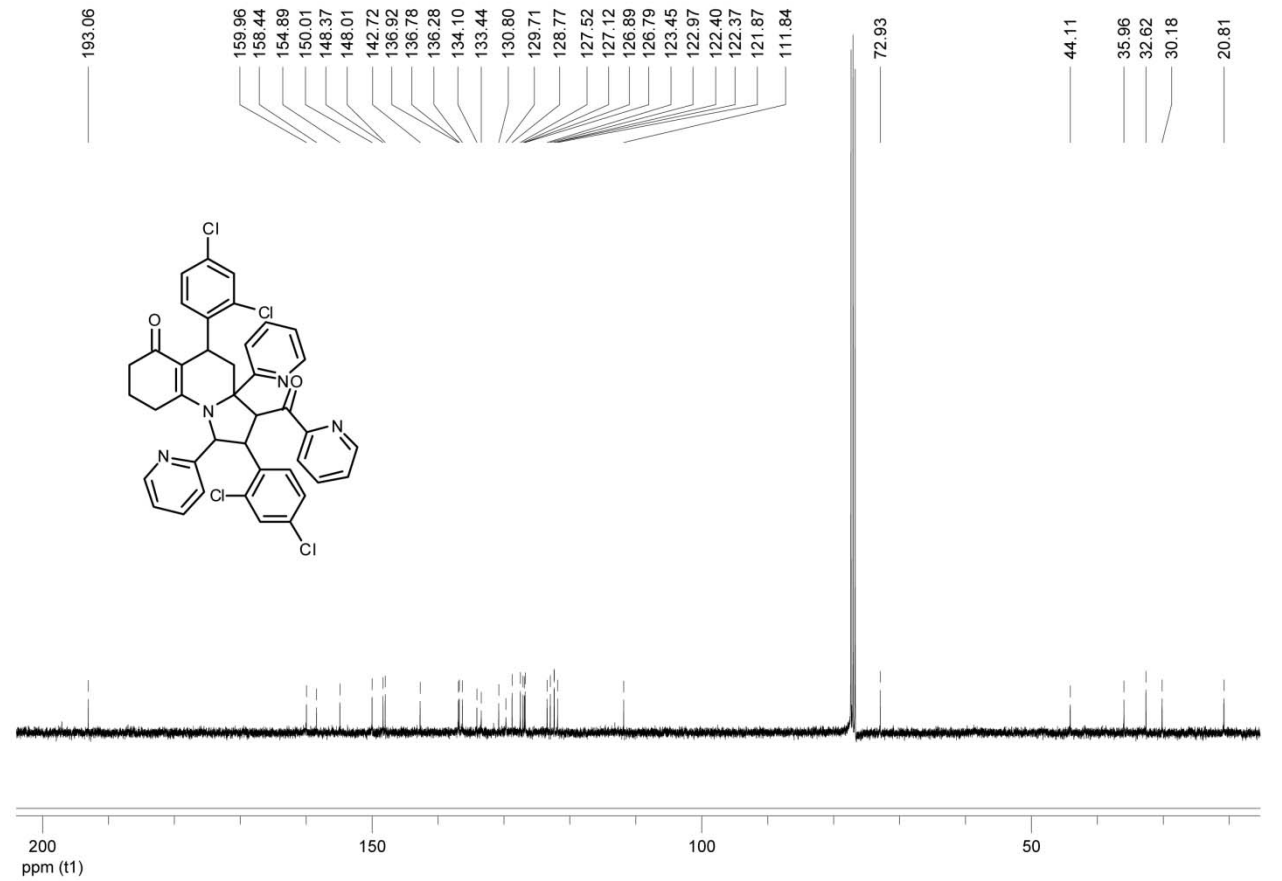
^{13}C NMR 100 MHz, $CDCl_3$



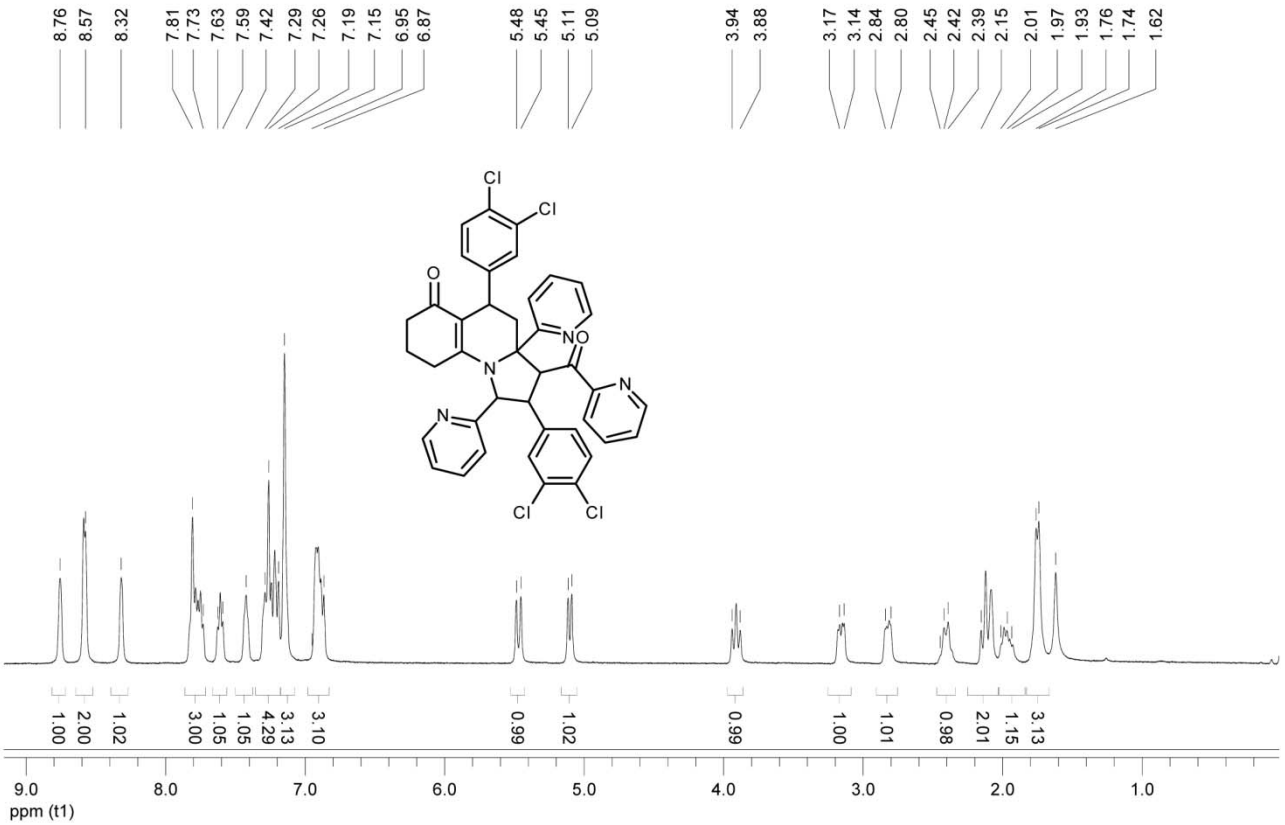
Product 4f, ^{1}H NMR 400 MHz, $CDCl_3$



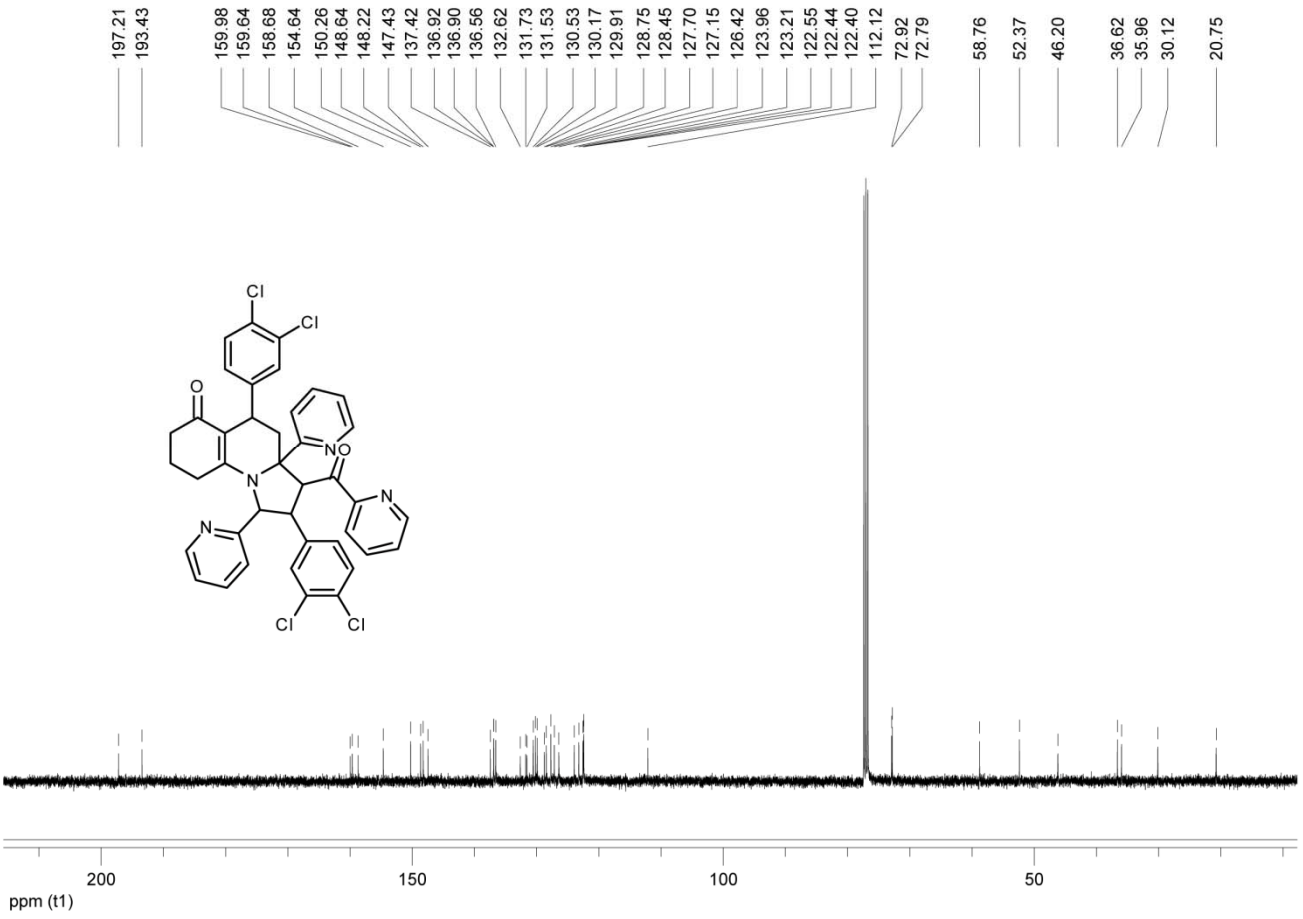
^{13}C NMR 100 MHz, $CDCl_3$



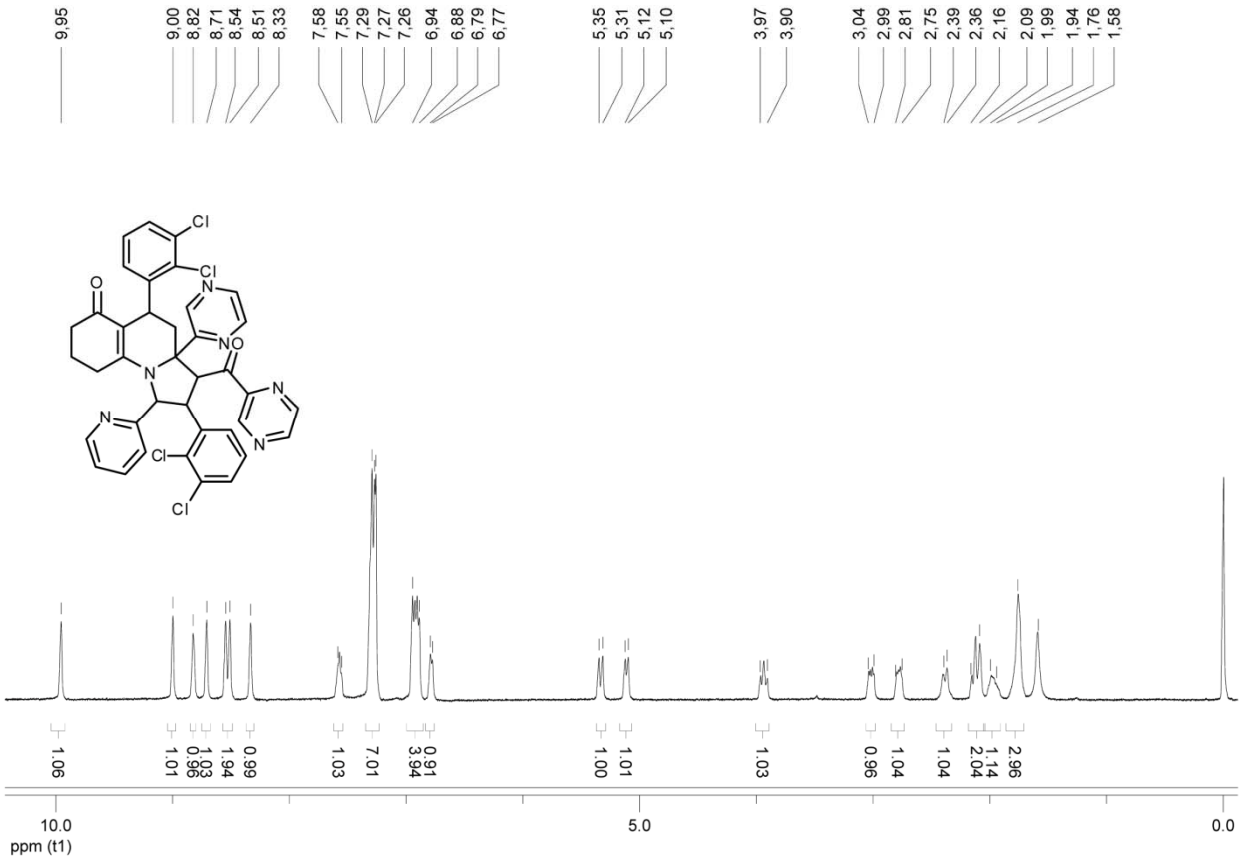
Product 4g, ^{1}H NMR 400 MHz, $CDCl_3$



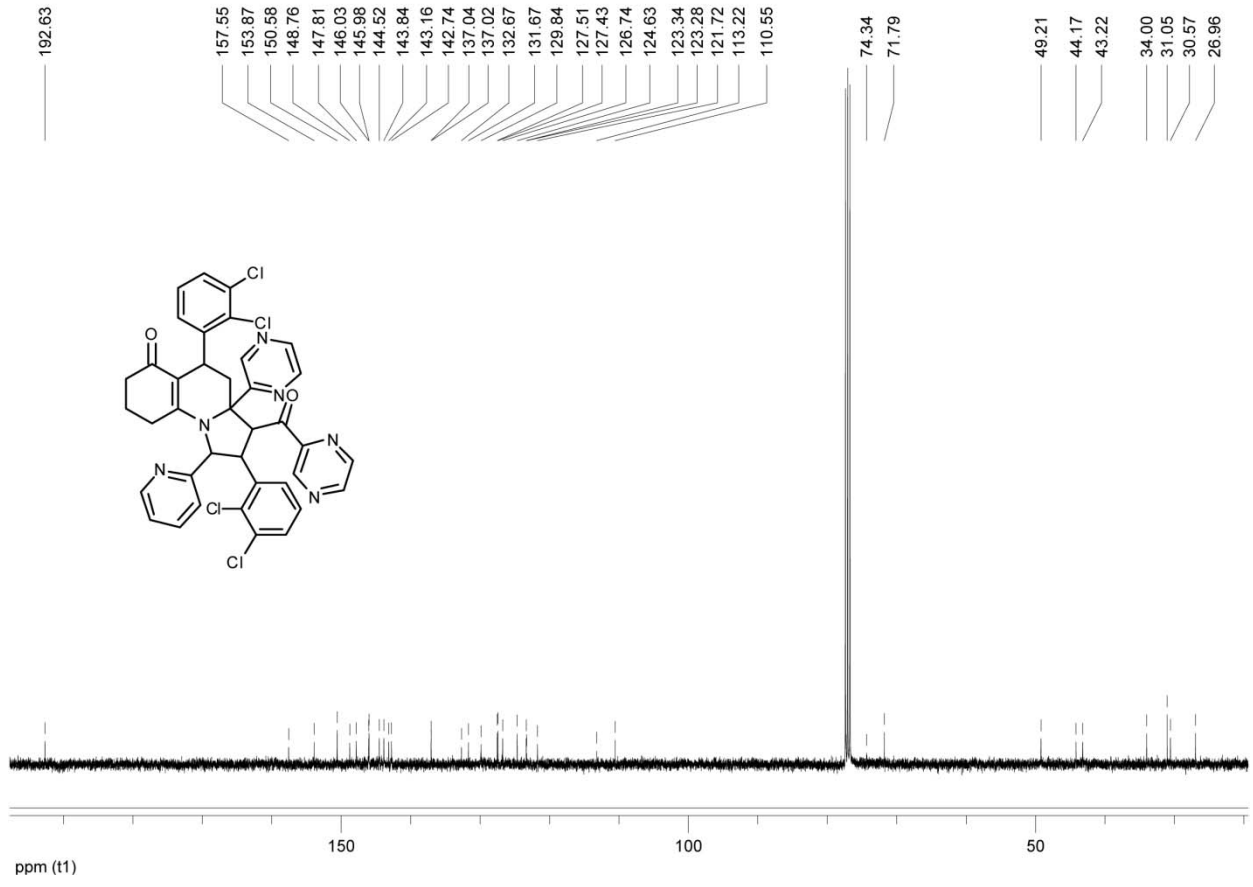
^{13}C NMR 100 MHz, $CDCl_3$



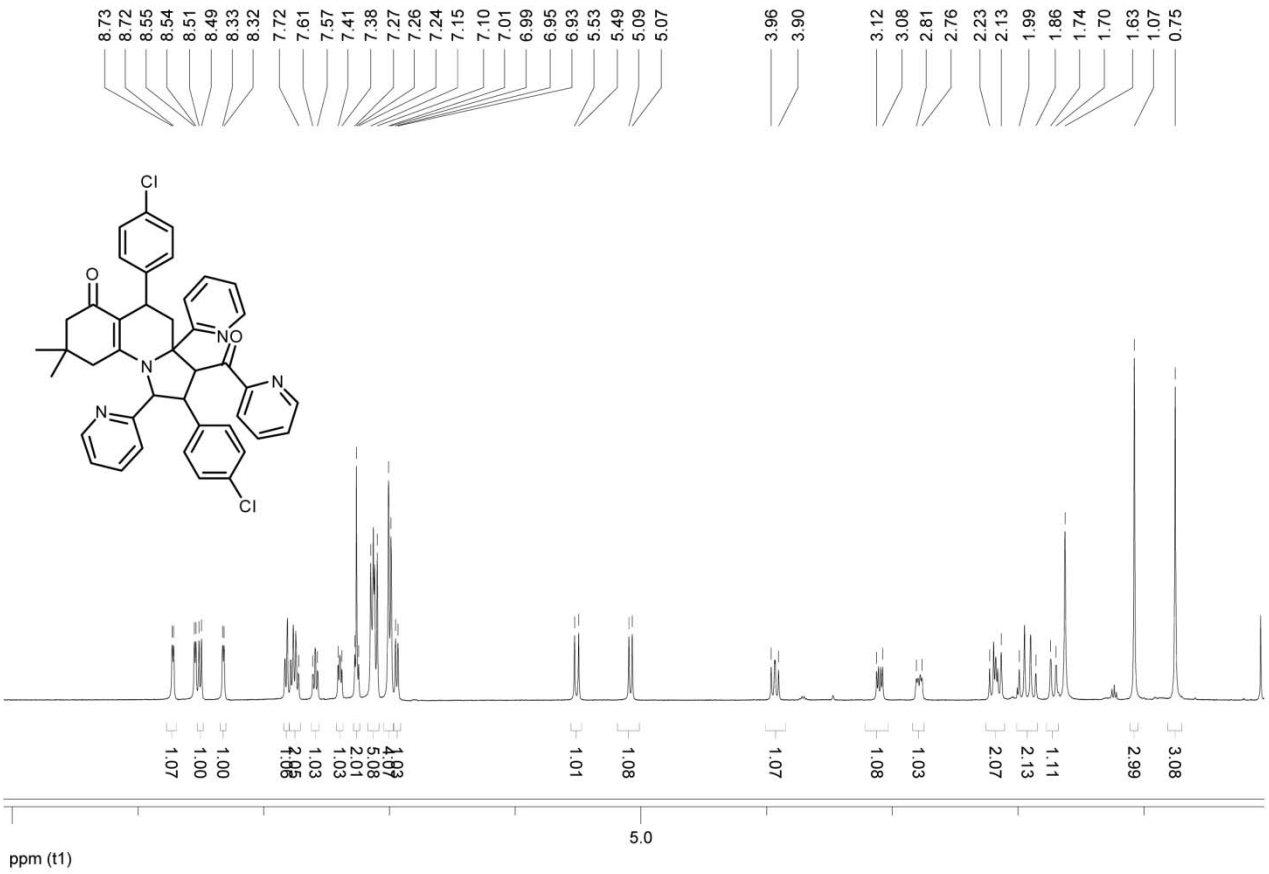
Product 4h, ^{1}H NMR 400 MHz, $CDCl_3$



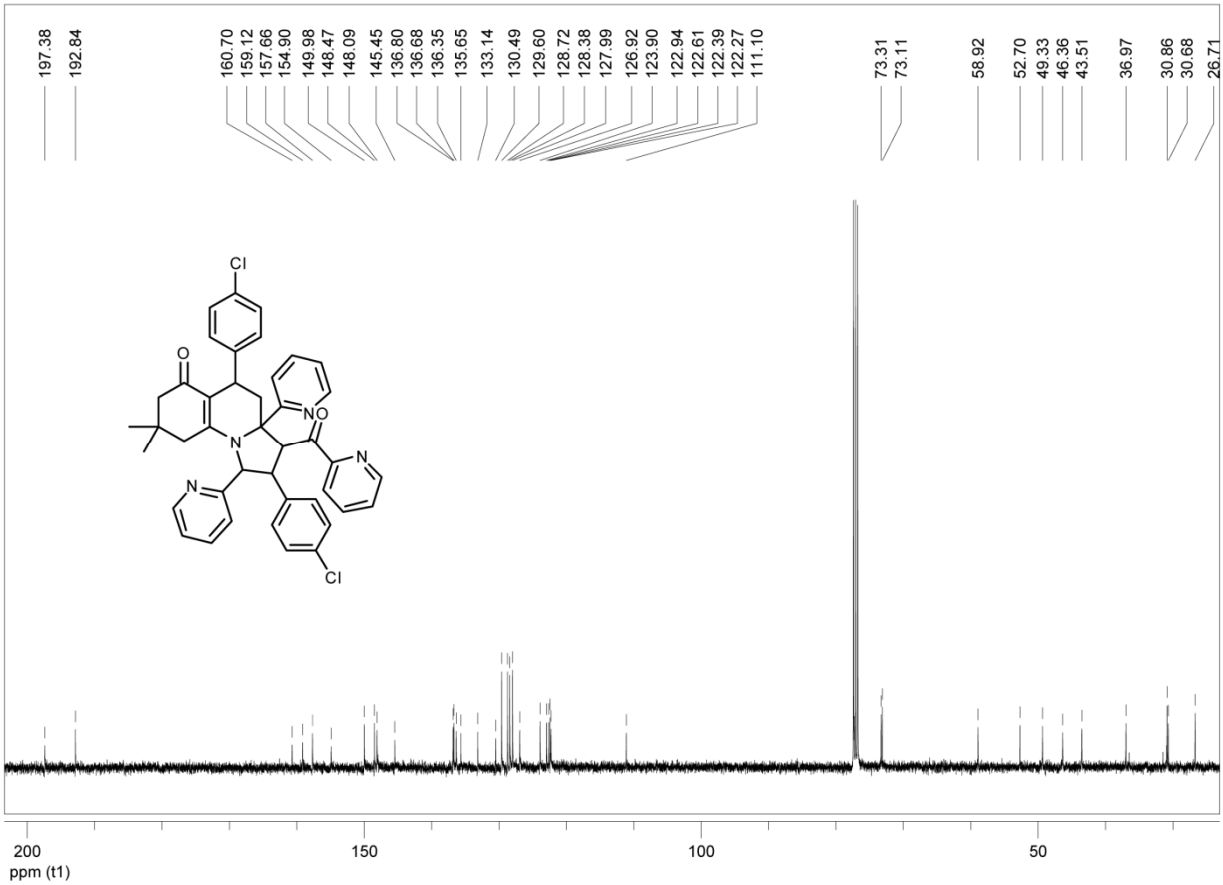
^{13}C NMR 100 MHz, $CDCl_3$



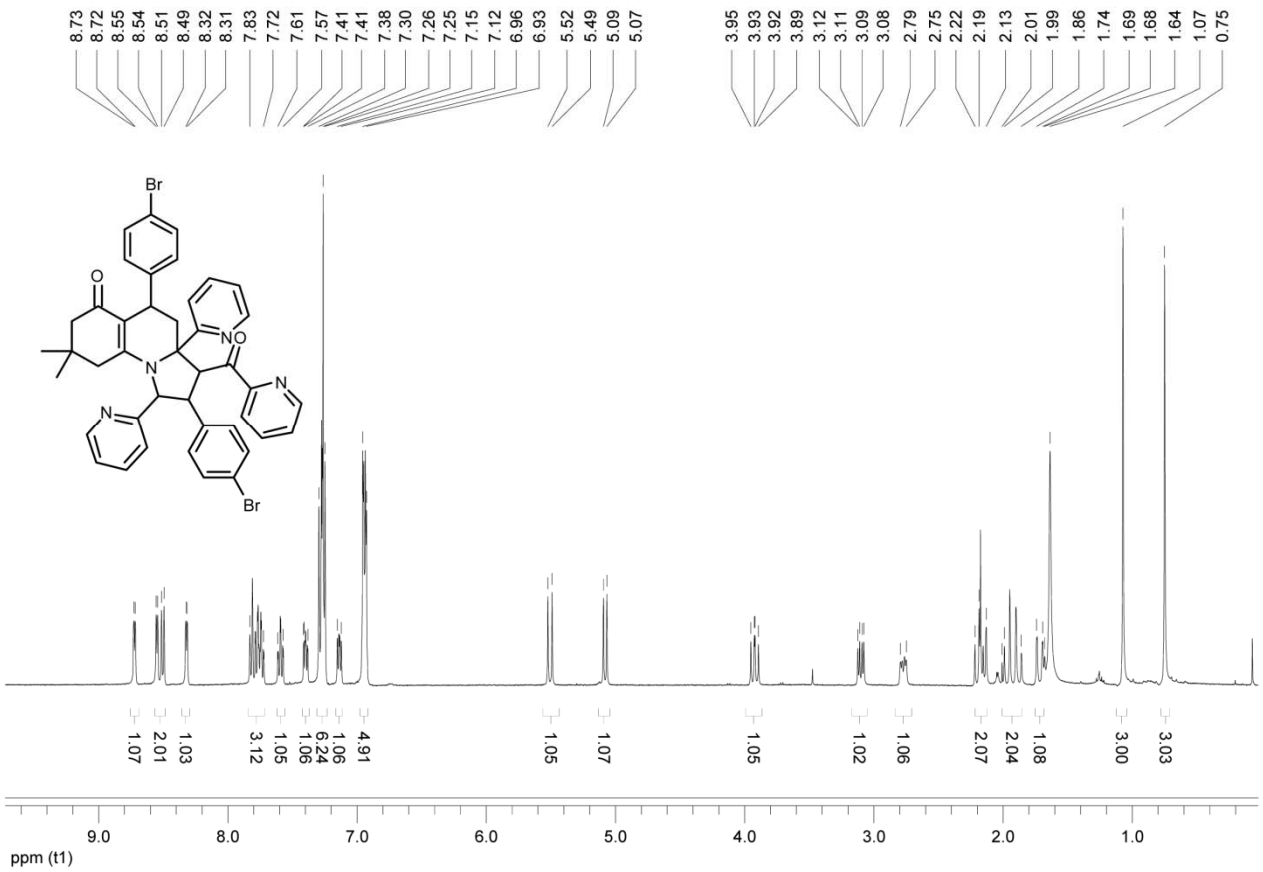
Product 4i, ^{1}H NMR 400 MHz, $CDCl_3$



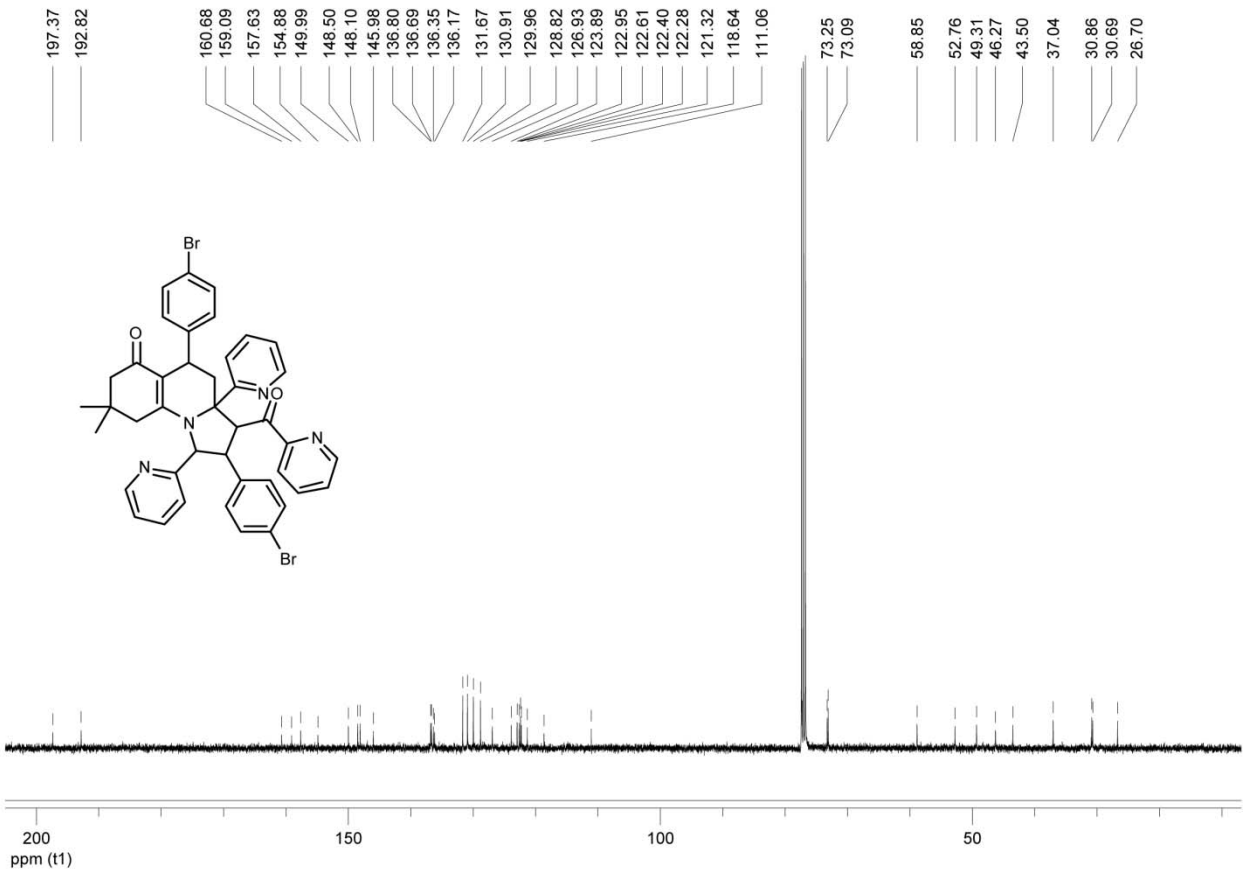
^{13}C NMR 100 MHz, $CDCl_3$



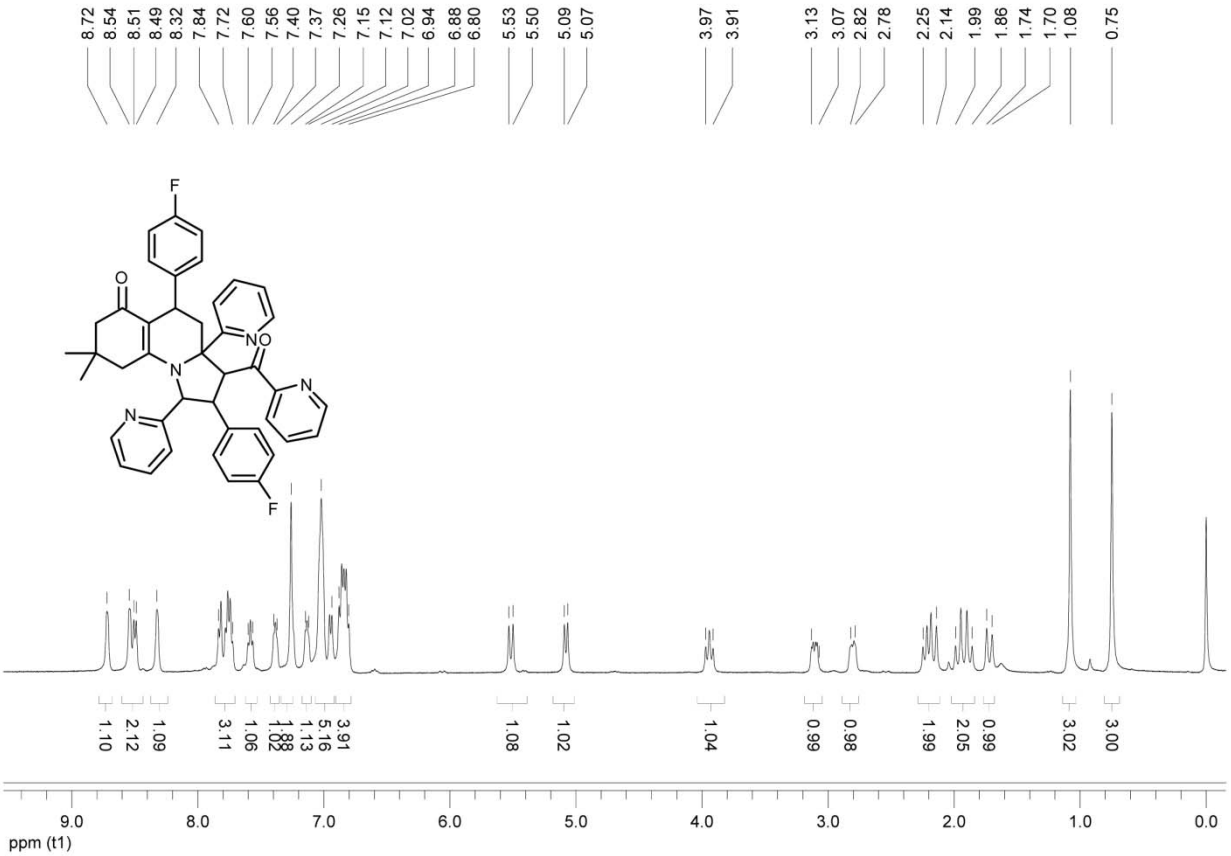
Product 4j, ^{1}H NMR 400 MHz, $CDCl_3$



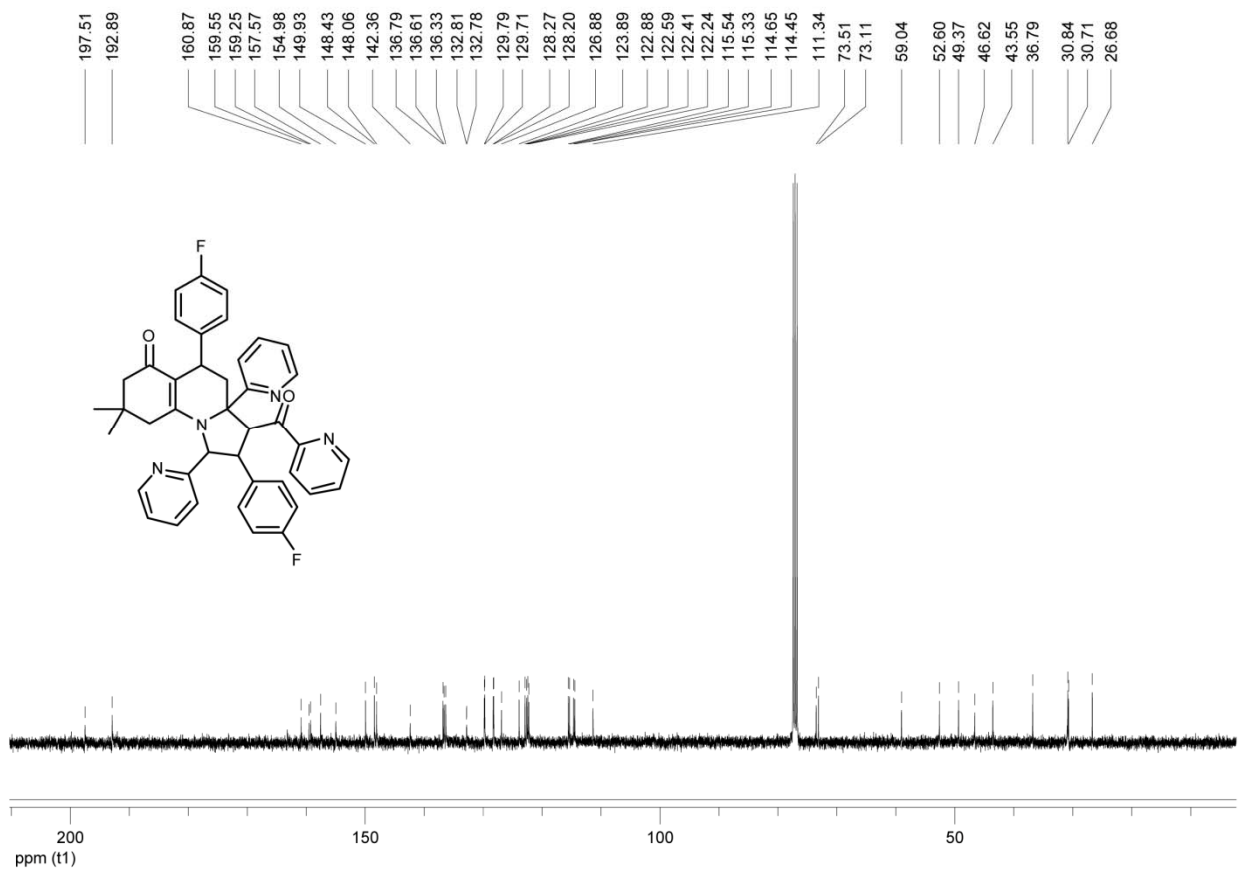
^{13}C NMR 100 MHz, $CDCl_3$



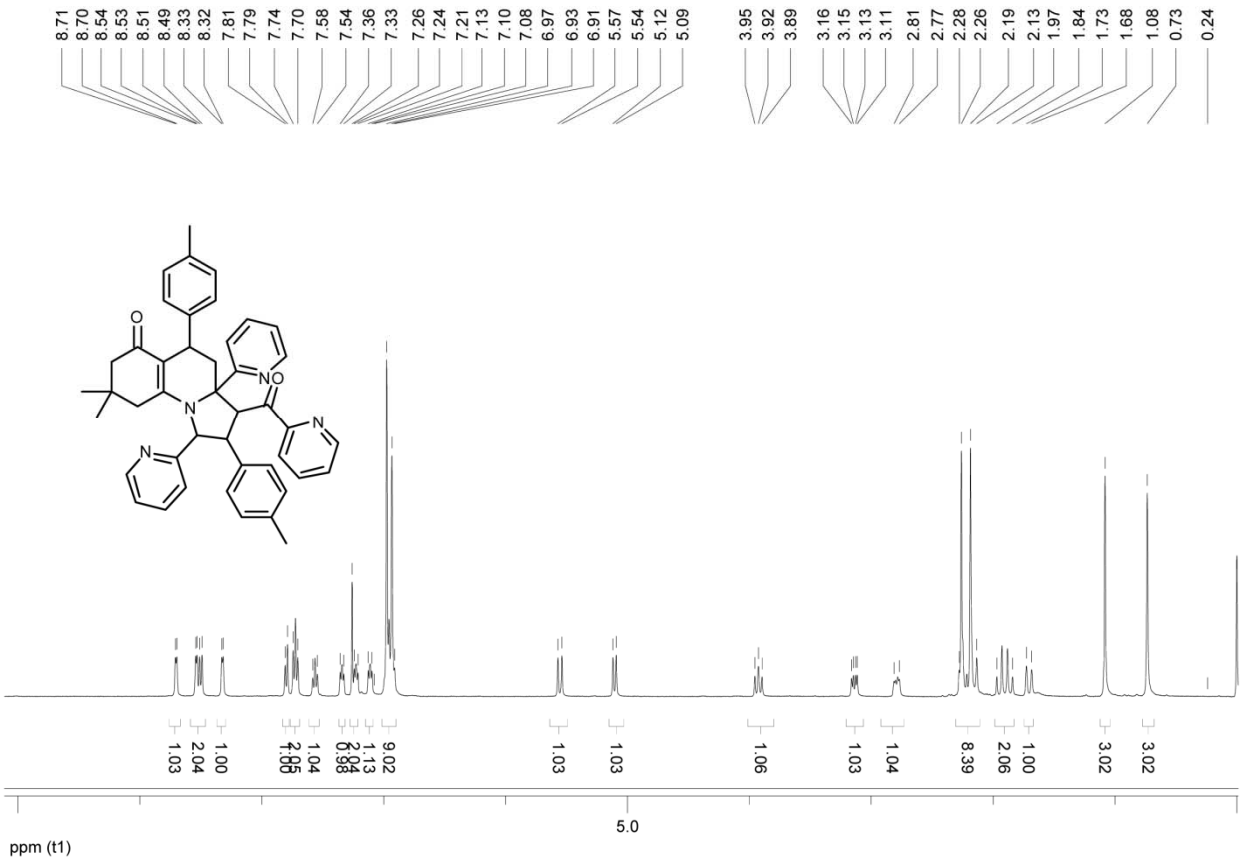
Product 4k, ^{1}H NMR 400 MHz, $CDCl_3$



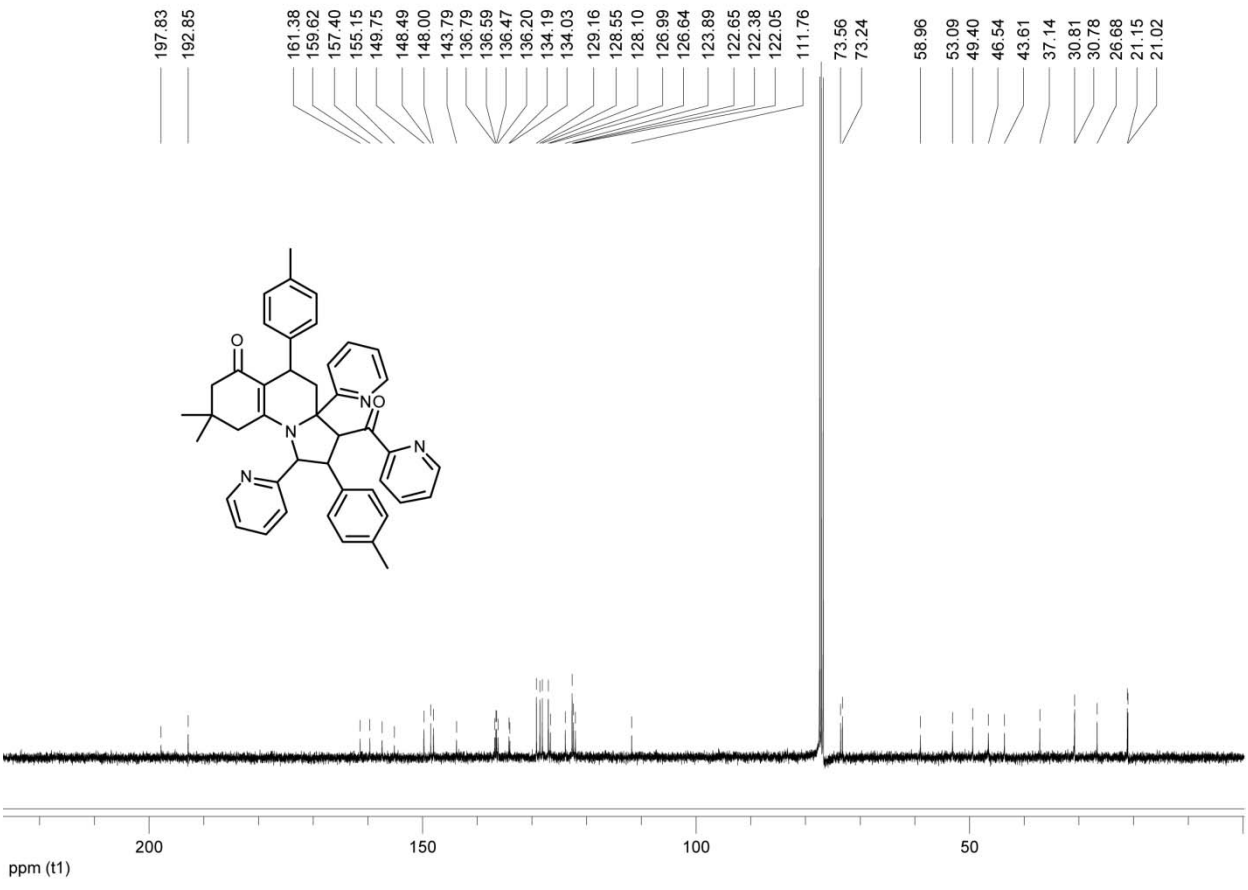
^{13}C NMR 100 MHz, $CDCl_3$



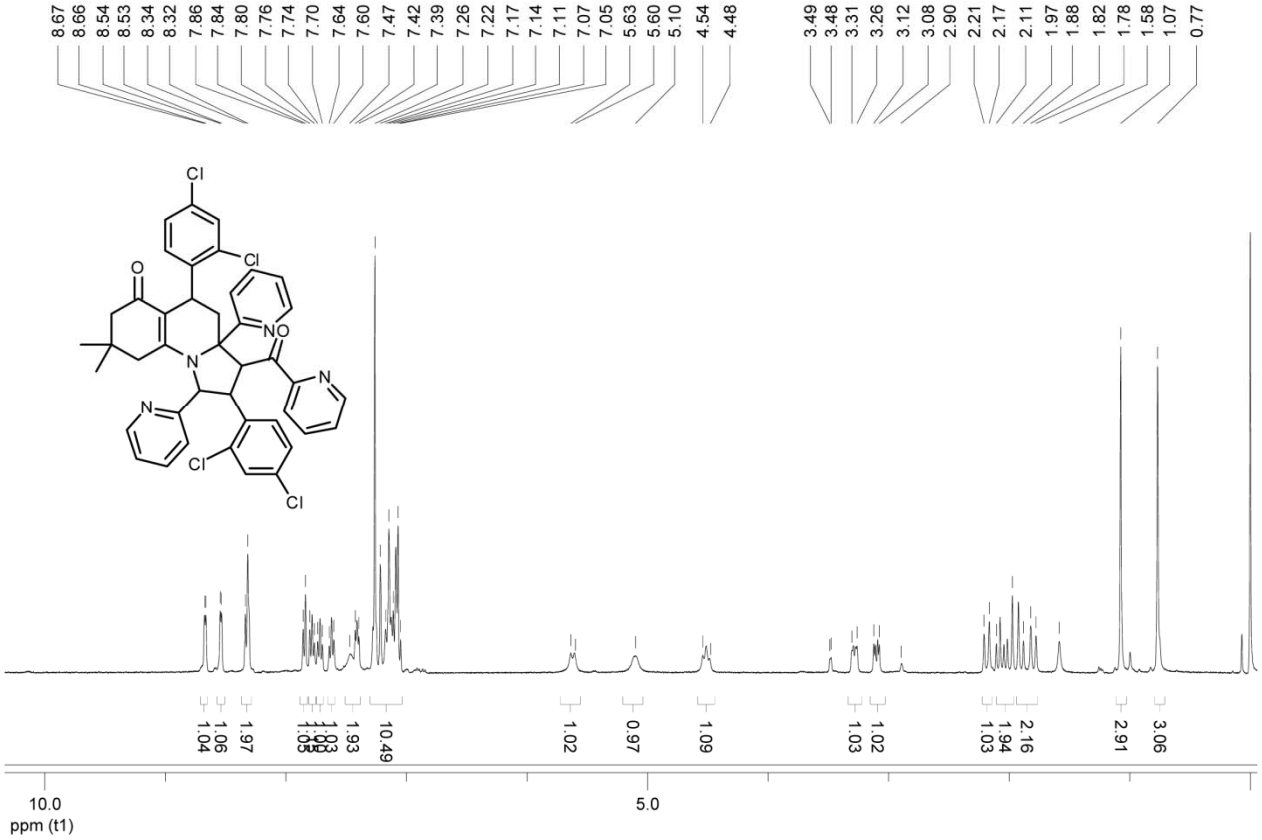
Product 4l, ^{1}H NMR 400 MHz, $CDCl_3$



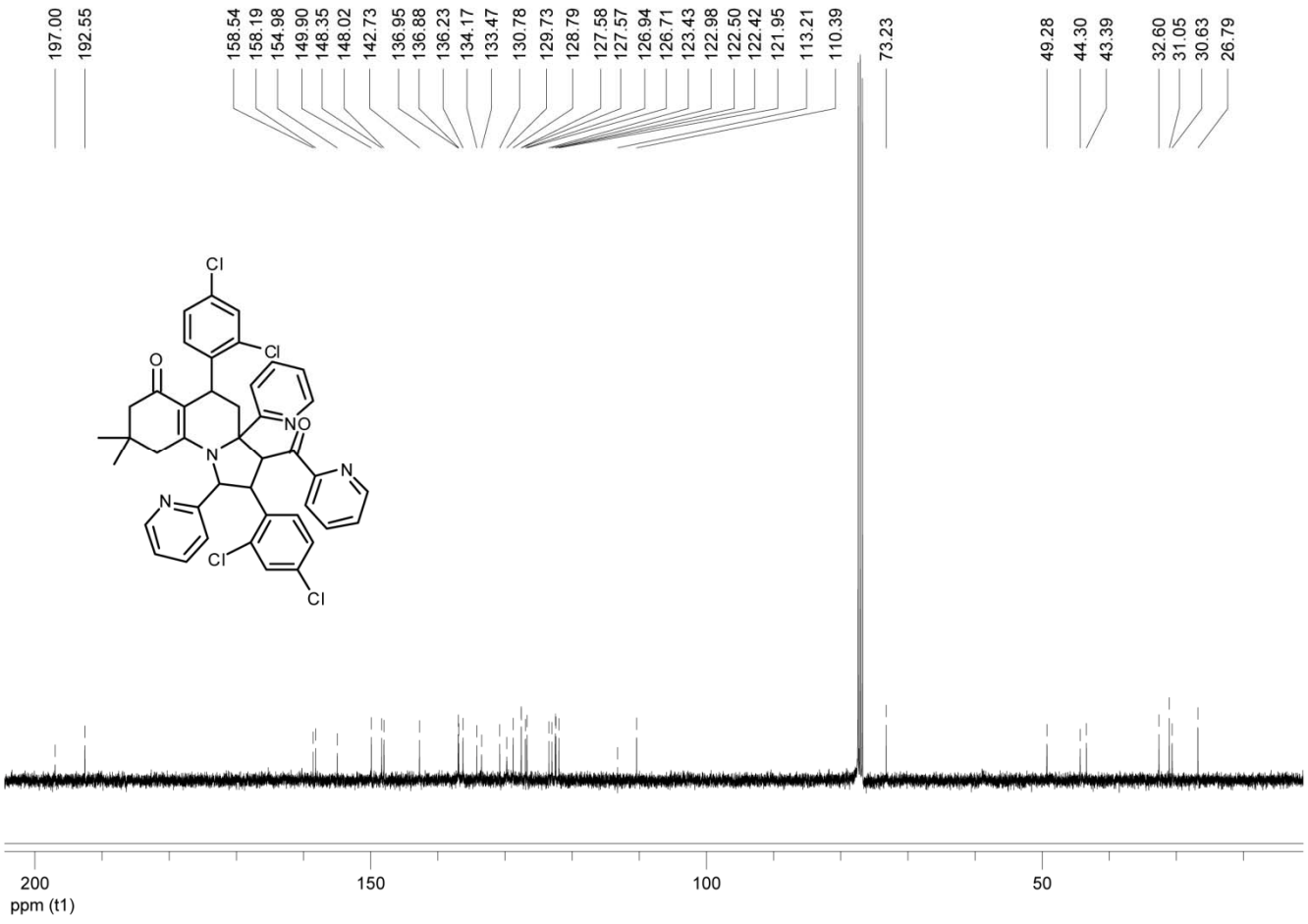
^{13}C NMR 100 MHz, $CDCl_3$



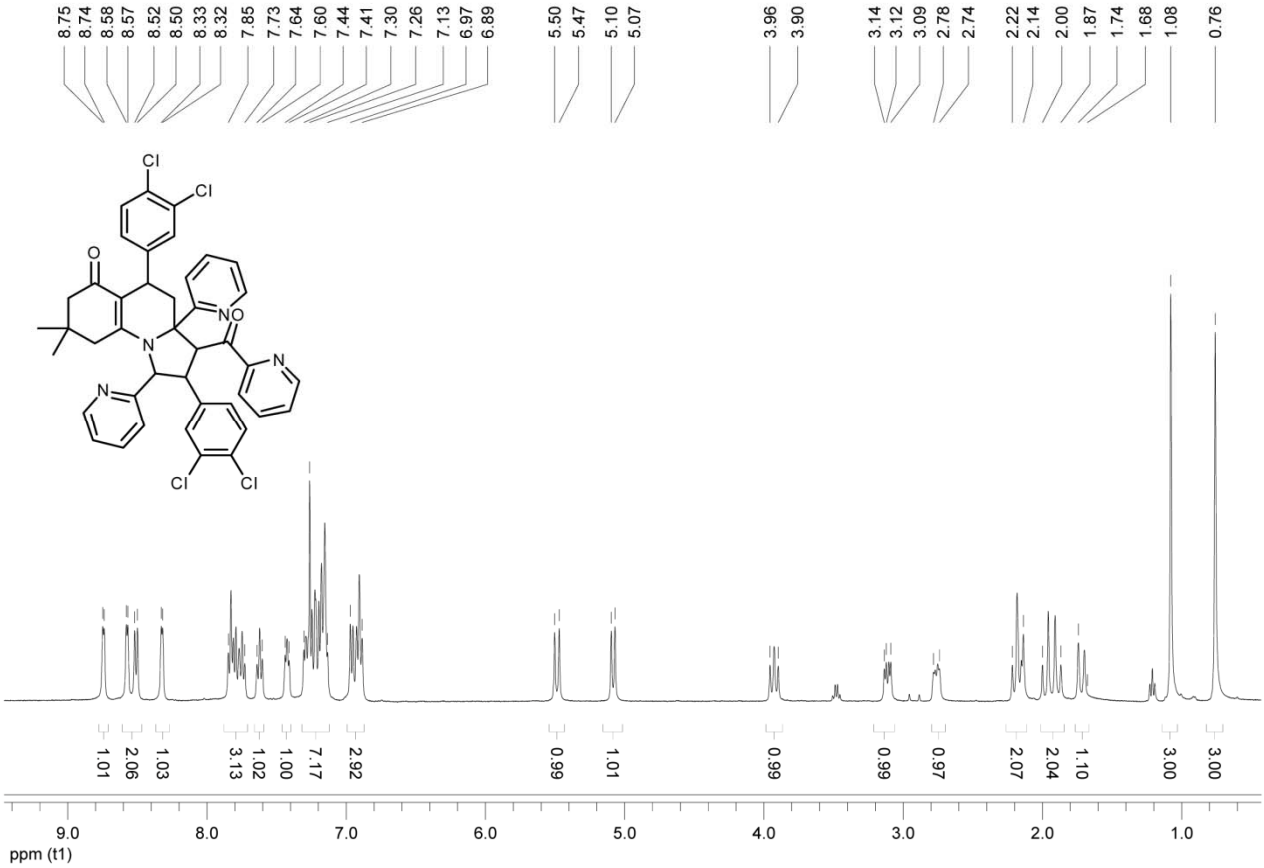
Product 4m, ^{1}H NMR 400 MHz, $CDCl_3$



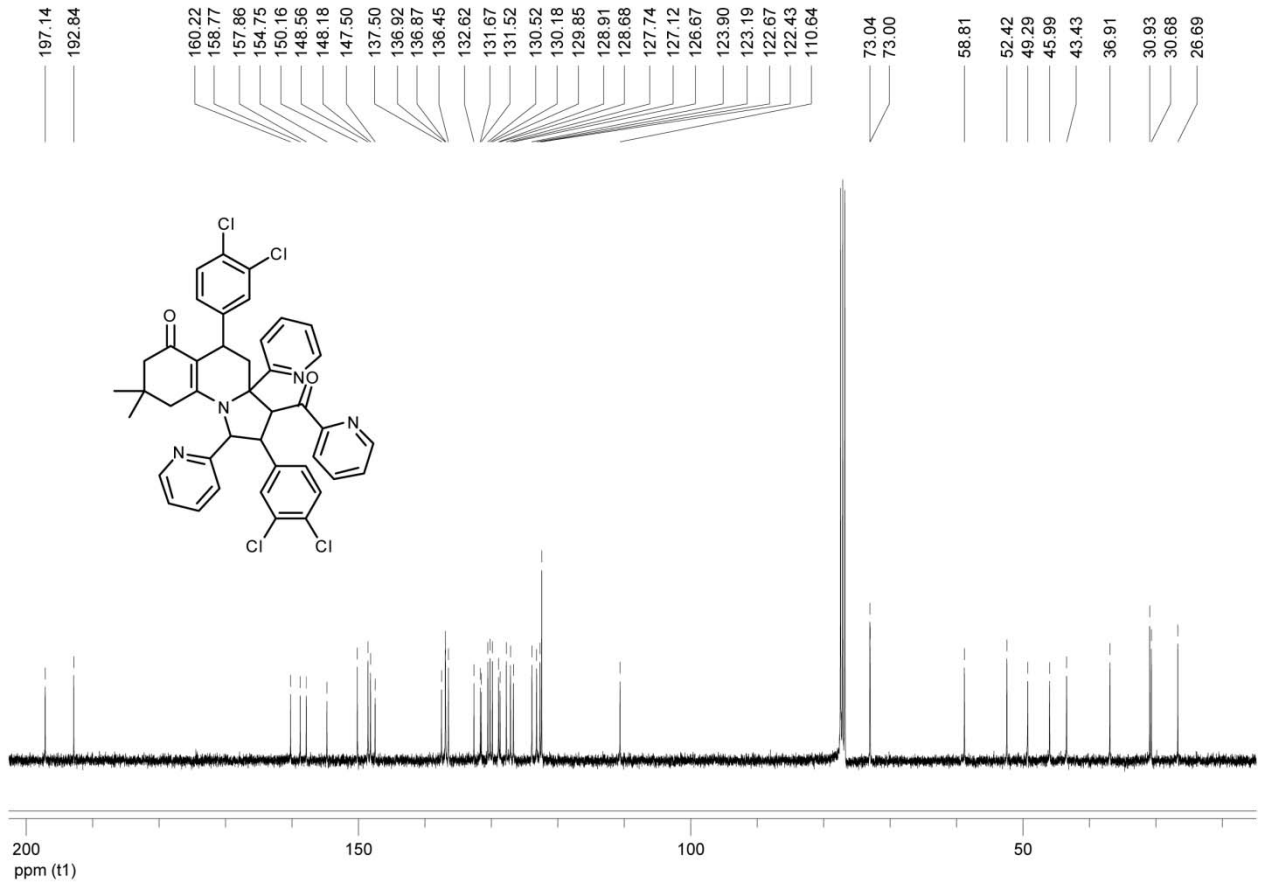
^{13}C NMR 100 MHz, $CDCl_3$



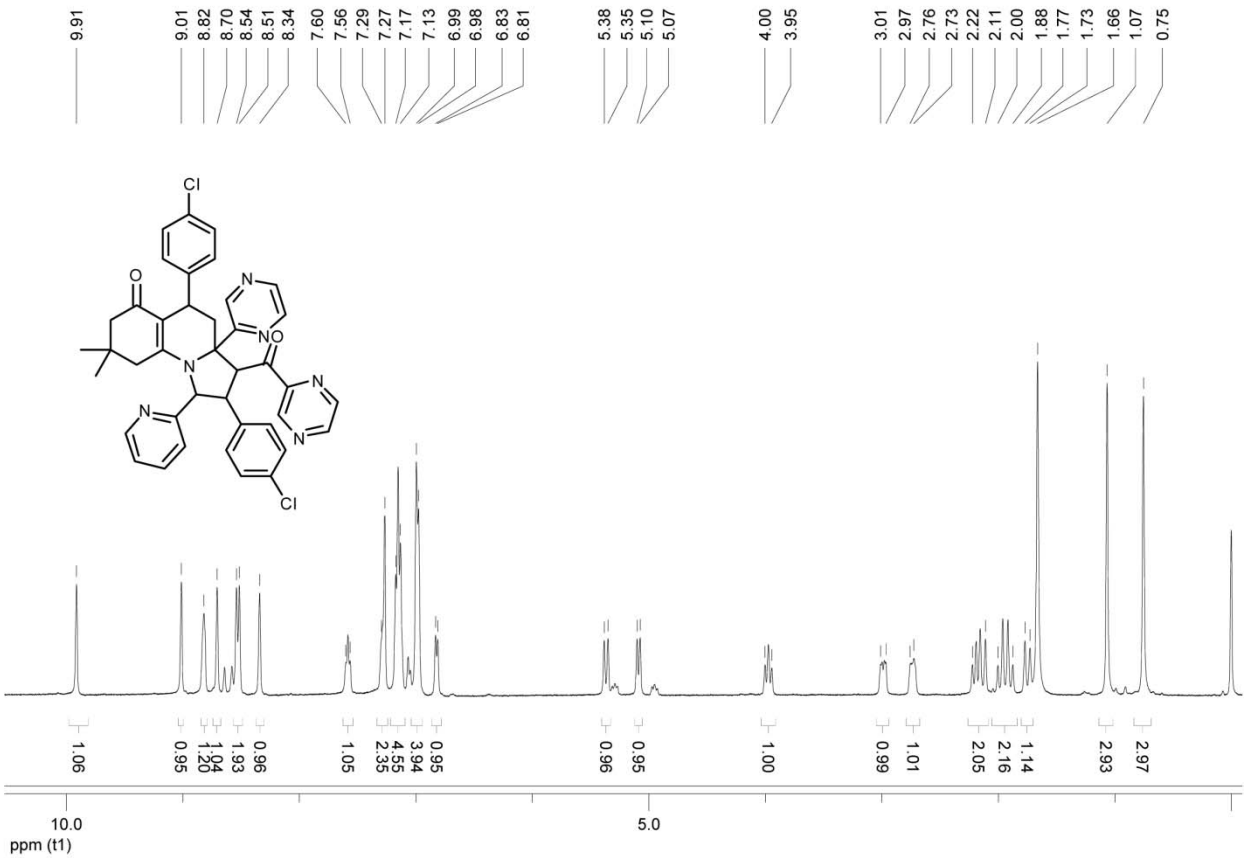
Product 4n, ^{1}H NMR 400 MHz, $CDCl_3$



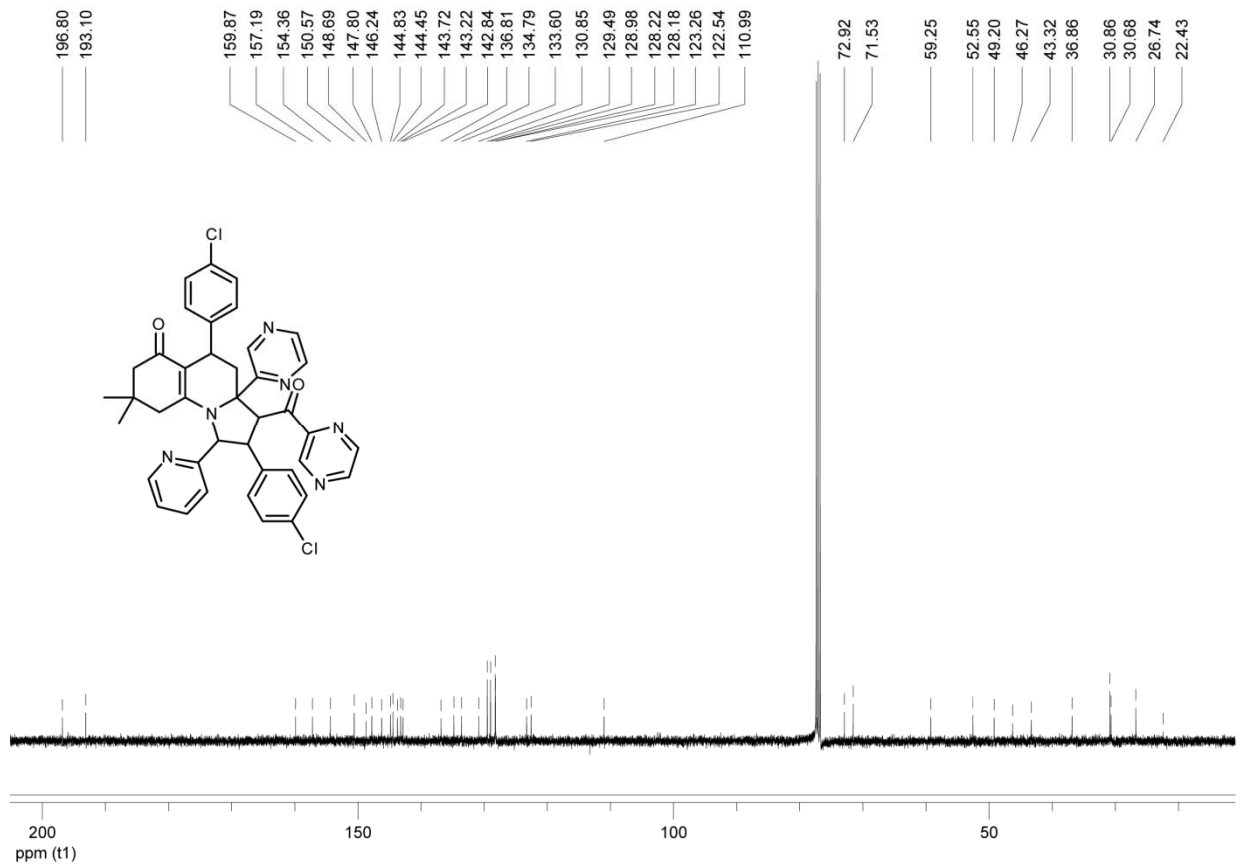
^{13}C NMR 100 MHz, $CDCl_3$



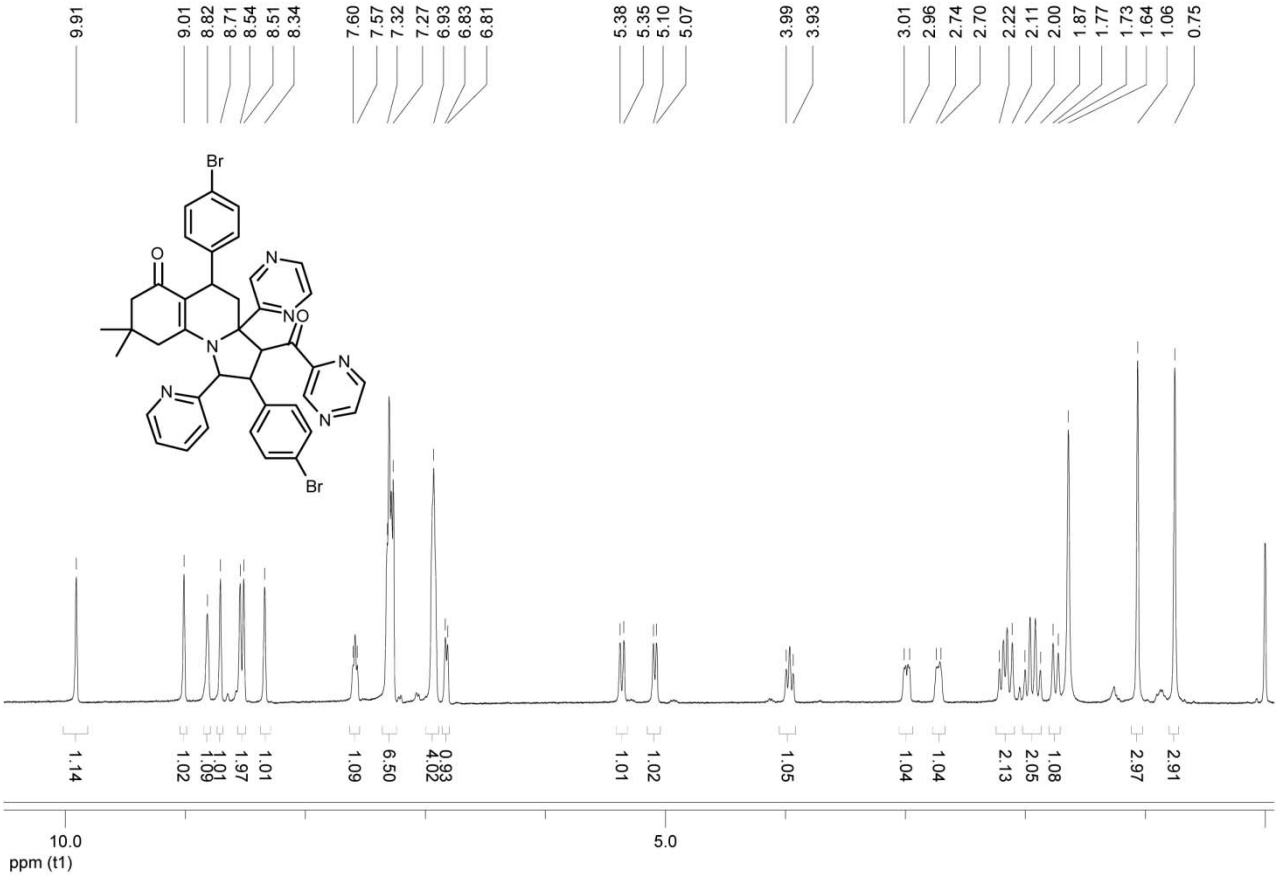
Product 4o, ^{1}H NMR 400 MHz, $CDCl_3$



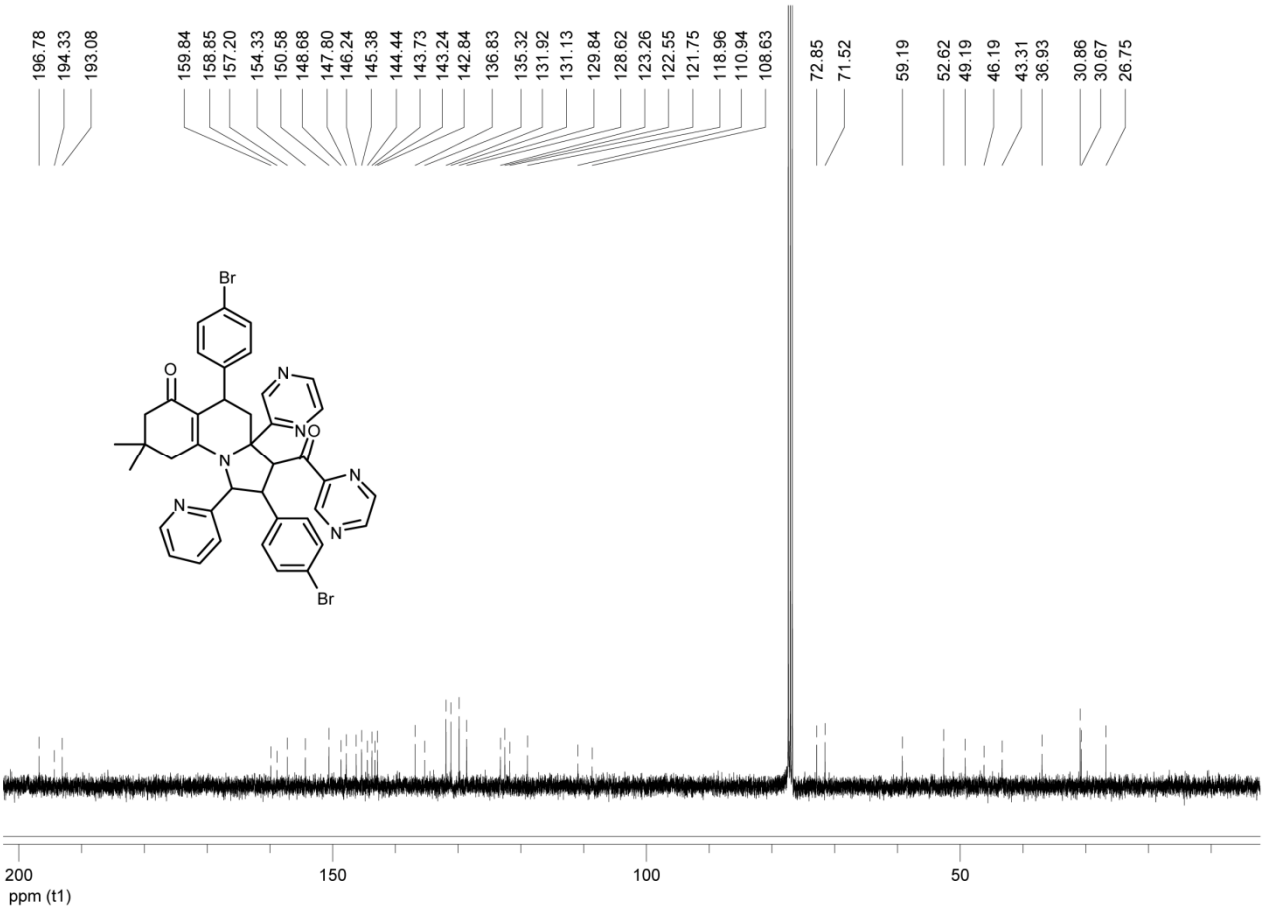
^{13}C NMR 100 MHz, $CDCl_3$



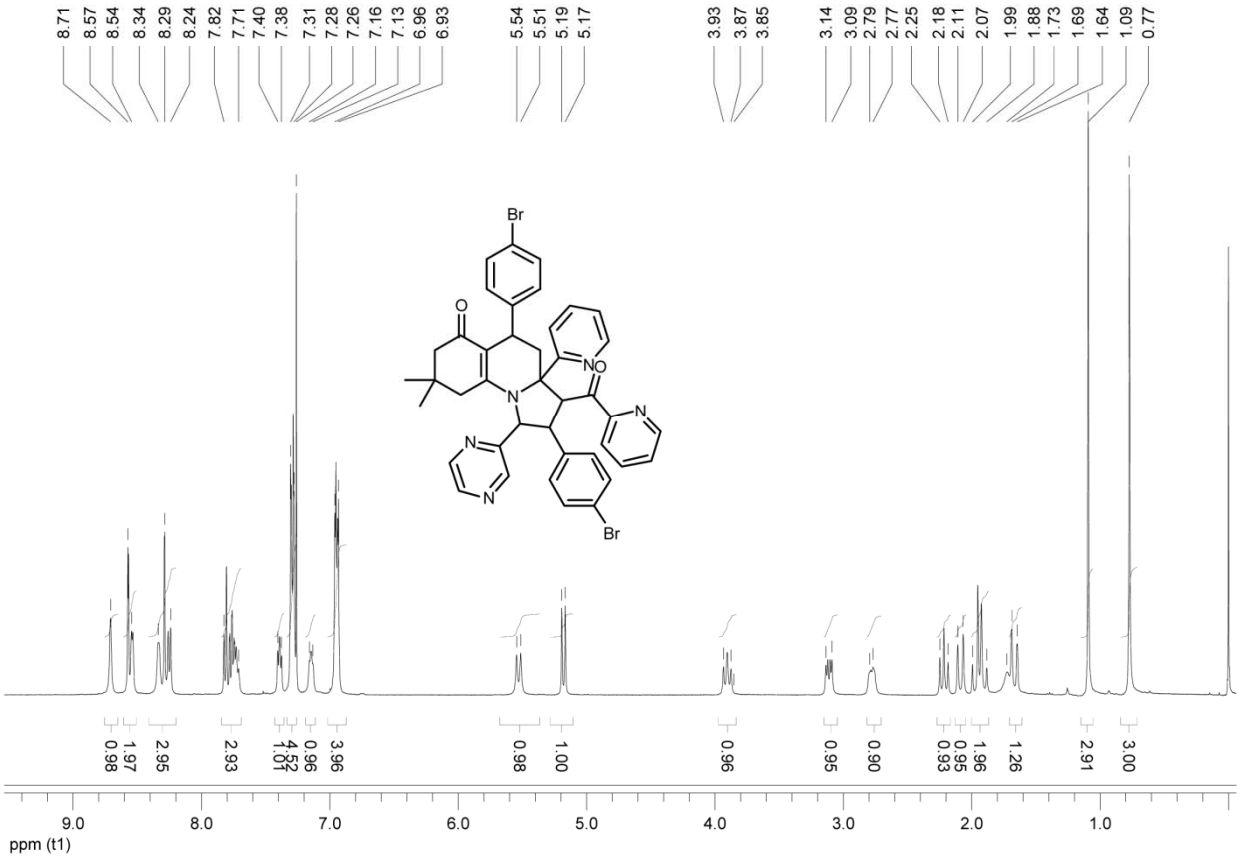
Product 4p, ^{1}H NMR 400 MHz, $CDCl_3$



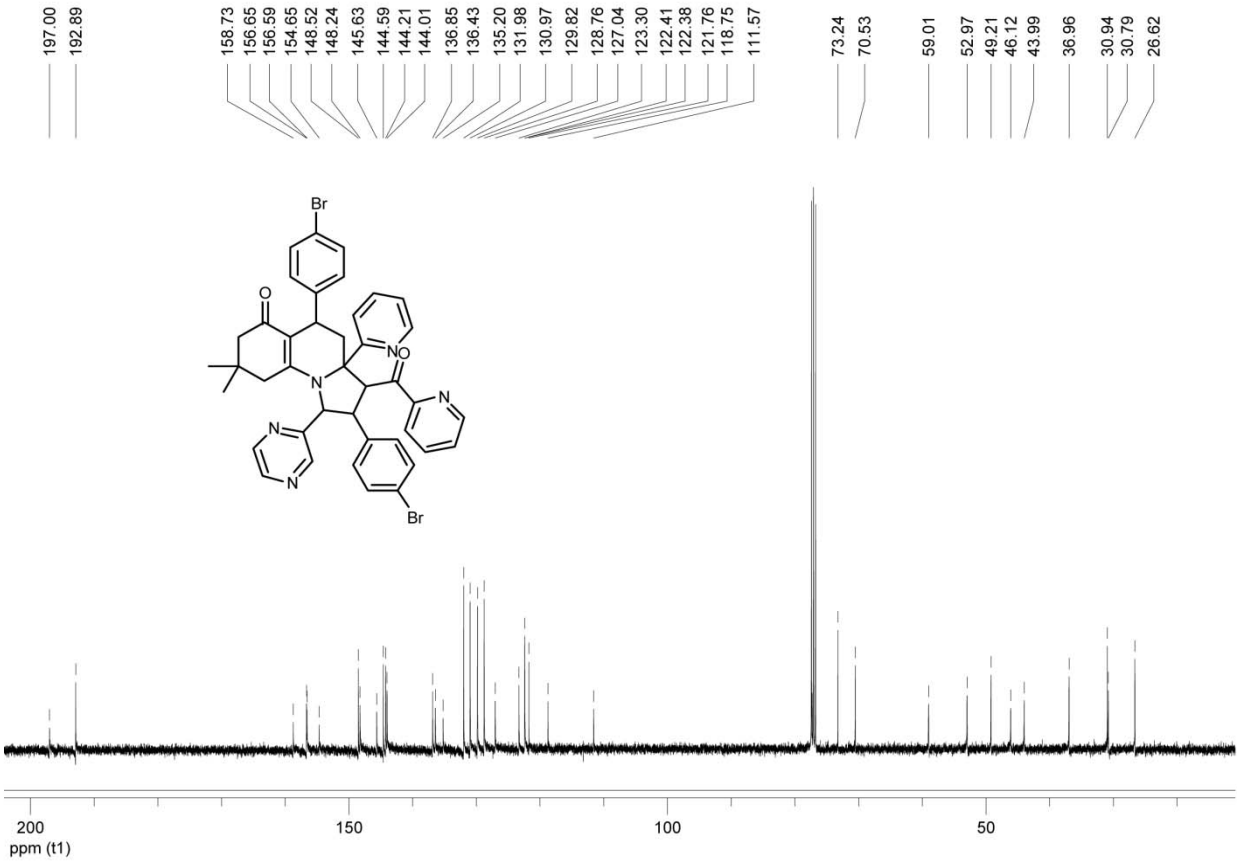
^{13}C NMR 100 MHz, $CDCl_3$



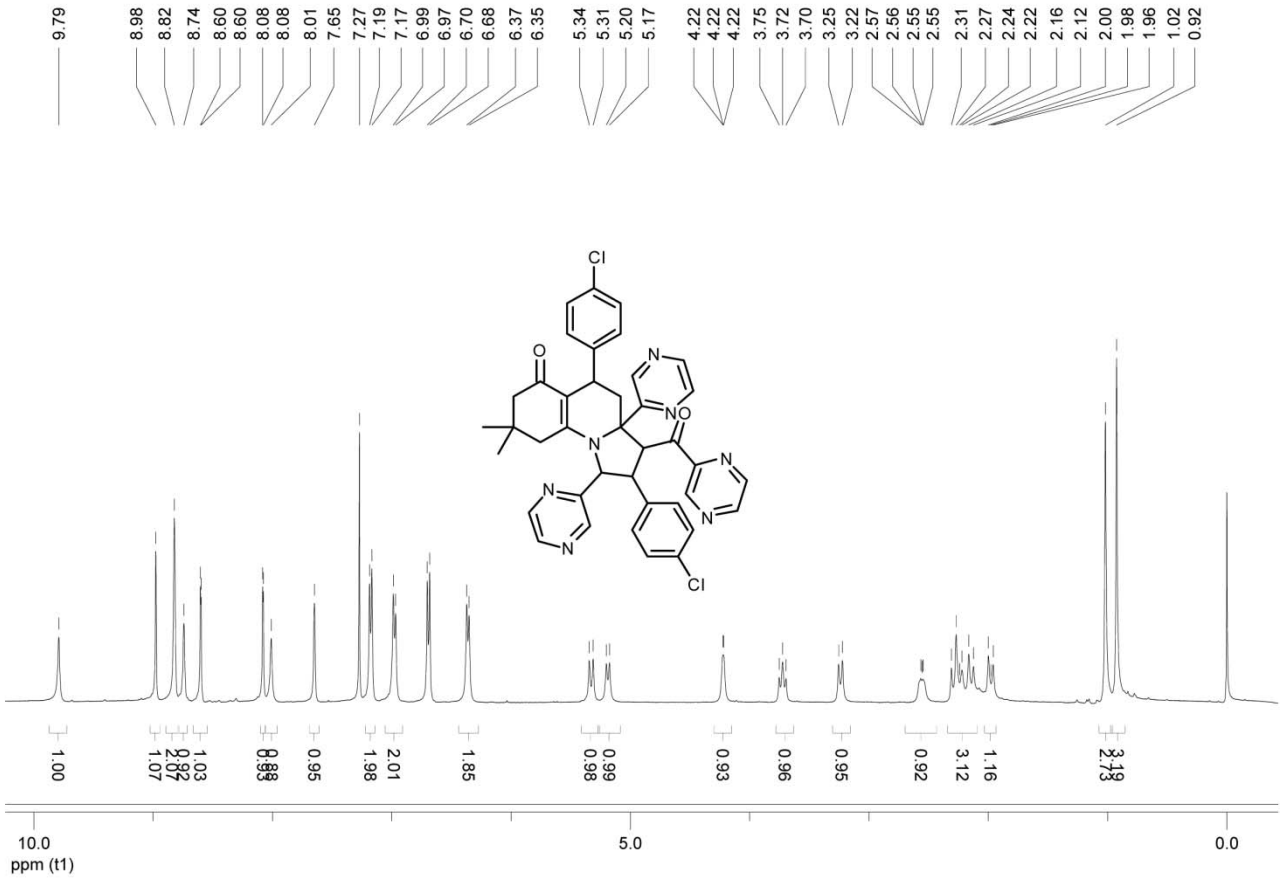
Product 4q, ^{1}H NMR 400 MHz, $CDCl_3$



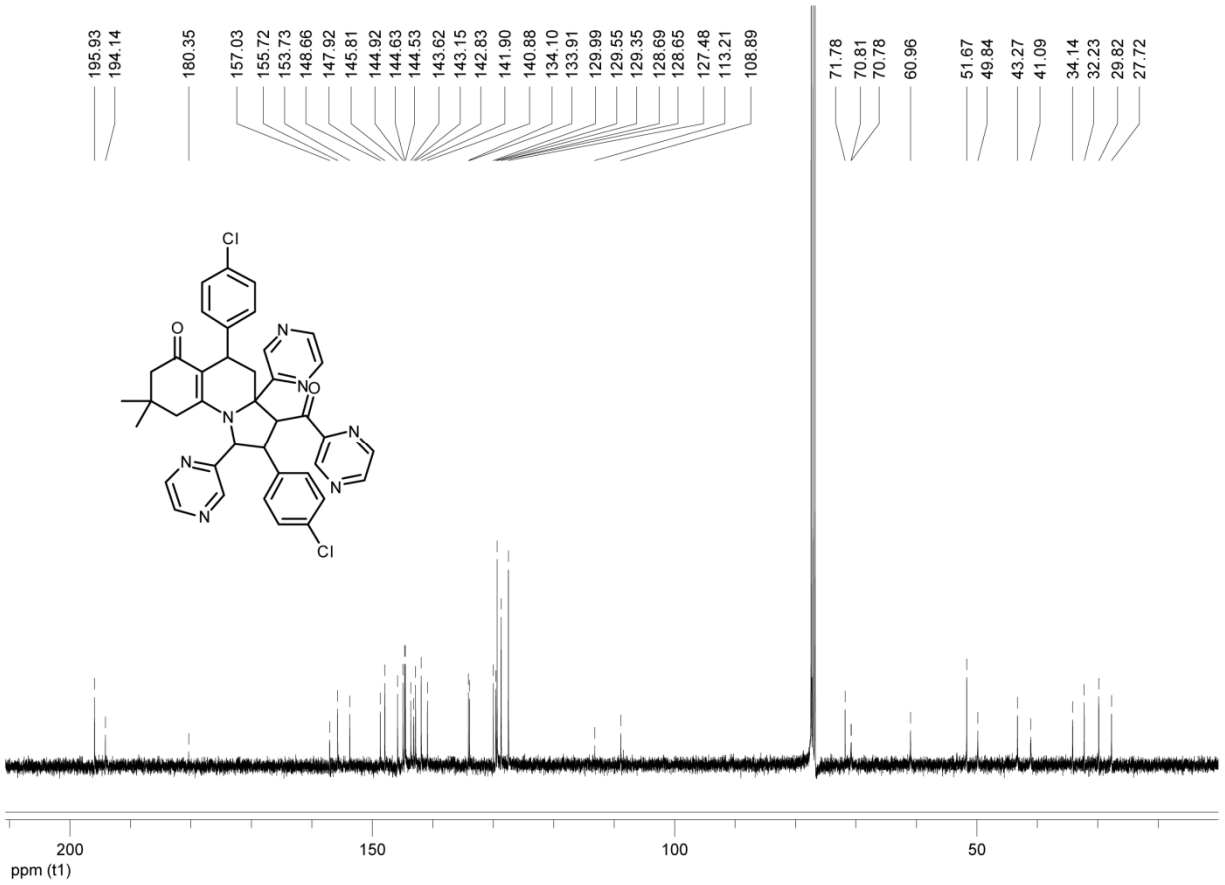
^{13}C NMR 100 MHz, $CDCl_3$



Product 4r, ^{1}H NMR 400 MHz, $CDCl_3$



^{13}C NMR 100 MHz, $CDCl_3$



5.Reference for the preparation of 3-aryl-1-azaaryl-prop-2-en-1-one (3)

1. G.-W. Wang, Y.-W. Dong, P. Wu, T.-T.Yuan, Y.-B. Shen. *J. Org. Chem.* **2008**, *73*, 7088–7095.