Electronic Supplementary Information:

Friedländer synthesis of polysubstituted quinolines and naphthyridines promoted by propylphosphonic anhydride (T3P®) under mild conditions

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1. General information

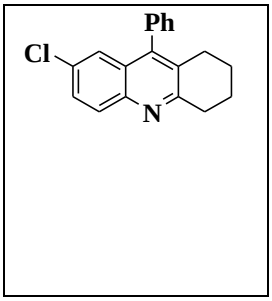
^{1}H NMR and ^{13}C NMR were recorded at room temperature on a Bruker™ DPX 300 at 300 and 75 MHz, respectively. Chemical shifts are in parts per million (ppm). The assignments were made using one dimensional (1D) ^{1}H and ^{13}C spectra or two-dimensional (2D) HSQC and COSY spectra. Melting points were determined on a Büchi B-540 apparatus and are uncorrected. Mass spectra were recorded with a LCMS-MS analysis was performed on a Waters Alliance Micromass ZQ 2000, using a C18 X-Bridge 5 μm particle size column, dimensions 50 mm * 4.6 mm. A gradient starting from 100% H_2O/0.1% formic acid and reaching 5% H_2O/95% CH_3CN/0.1% formic acid within 3 min at a flow rate of 2 mL/min was used. Purity (%) was determined by reversed phase HPLC, using UV detection (215 nm), and all compound showed purity greater than 95%. All commercial reagents and solvents were used without further purification. HRMS analysis was performed on a LCT Premier XE Micromass, using a C18 X-Bridge 3.5 μm particle size column, dimensions 50 mm * 4.6 mm. A gradient starting from 98% H_2O 5 mM Ammonium Formate pH=9.2 and reaching 100% CH_3CN 5 mM Ammonium Formate pH=9.2 within 3 min at a flow rate of 1 mL/min was used. Reactions were performed using a Discover™ microwave from CEM™.

2. General Procedure for Friedländer reaction promoted by Propylphosphonic Anhydride (T3P®).

To a mixture of 2-Aminoaryl Ketone (0.5 mmol) and Ketone (0.5 mmol) was added T3P® (50% in EtOAc) (0.5 mmol) in drops. The mixture was heated to 60°C without added solvent for 0.5-1h in air. After completion the reaction observed by LC-MS, water (3 ml) was added to the reaction mixture and was shaken to dissolve the T3P®. The crude product was easily purified and isolated by recrystallization from hot methanol (2 ml) for more purification to give the pure polysubstituted quinolines. In all cases, the resulting products were isolated in total purity, as determined by LC-MS and afforded analytically pure products in excellent to good yields in 85-96% as a off-white or light yellow solid.

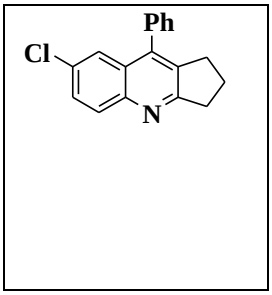
3. Characterization of compounds.

2-chloro-5,6,7,8-tetrahydro-9-phenylacridine (1):



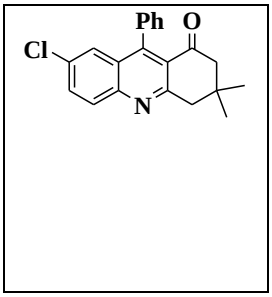
Yield (137 mg, 94%); white solid; mp= 165-167 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.94 (d, J = 9.0 Hz, 1H), 7.55-7.45 (m, 4H), 7.28 (d, J = 2.1 Hz, 1H), 7.19 (dd, J = 7.8, 1.5 Hz, 2H), 3.17 (t, J = 6.6 Hz, 2H), 2.58 (t, J = 6.6 Hz, 2H), 1.99-1.91 (m, 2H), 1.80-173 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.47 (Cq), 145.72 (Cq), 144.68 (Cq), 136.37 (Cq), 131.14 (Cq), 130.08, 129.44 (Cq), 129.24, 129.01, 128.83, 128.06, 127.38 (Cq), 124.53, 34.21, 28.13, 22.90, 22.81; rt(LCMS) = 3.83 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{19}H_{17}NCl$ 294.1050; found 294.1057.

7-chloro-2,3-dihydro-9-phenyl-1*H*-cyclopenta[*b*]quinoline (2):



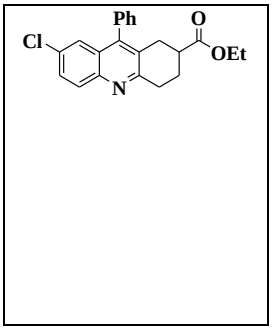
Yield (126 mg, 90%); white solid; mp= 96-98 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.96 (d, J = 8.7 Hz, 1H), 7.56 (d, J = 2.1 Hz, 1H); 7.51-7.40 (m, 4H), 7.29 (dd, J = 7.8, 1.5 Hz, 2H), 3.18 (t, J = 7.5 Hz, 2H), 2.85 (t, J = 7.5 Hz, 2H), 2.16-2.06 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.80 (Cq), 146.33 (Cq), 141.84 (Cq), 135.98 (Cq), 134.65 (Cq), 131.30 (Cq), 130.37, 129.15, 128.96, 128.70, 128.28, 126.98 (Cq), 124.46, 35.11, 30.36, 23.41; rt(LCMS) = 3.64 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{18}H_{15}NCl$ 280.0893; found 280.0893.

7-chloro-3,4-dihydro-3,3-dimethyl-9-phenylacridin-1(2*H*)-one (3):



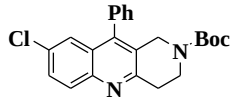
Yield (151 mg, 90%); white solid; mp= 211-213 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.98 (d, J = 9.0 Hz, 1H), 7.64 (dd, J = 9.0, 2.1 Hz, 1H), 7.53-7.47 (m, 3H), 7.43 (d, J = 2.4 Hz, 1H), 7.18-7.14 (m, 2H), 3.24 (s, 2H), 2.55 (s, 2H), 1.14 (s, 6H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 197.59 (Cq), 161.45 (Cq), 150.04 (Cq), 147.39 (Cq), 136.82 (Cq), 132.46, 132.39 (Cq), 130.25, 128.37, 128.24, 128.04 (Cq), 127.91, 126.76, 123.30, 54.17, 48.31, 32.25, 28.37; rt(LCMS) = 3.58 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{21}H_{19}NOCl$ 336.1155; found 336.1149.

ethyl 7-chloro-1,2,3,4-tetrahydro-9-phenylacridine-2-carboxylate (4):



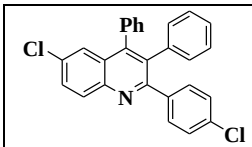
Yield (170 mg, 93%); white solid; mp= 114-116 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, J = 9.0 Hz, 1H), 7.55-7.47 (m, 4H), 7.27 (d, J = 2.4 Hz, 1H), 7.24-7.17 (m, 2H), 4.18-4.03 (m, 2H), 3.34-3.12 (m, 2H), 2.93-2.71 (m, 3H), 2.36-2.26 (m, 1H), 2.17-2.03 (m, 1H), 1.21 (t, J = 7.2 Hz,3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 174.76 (Cq), 157.92 (Cq), 146.19 (Cq), 144.83 (Cq), 135.87 (Cq), 131.43 (Cq), 130.11, 129.58, 129.11, 129.06. 128.86, 128.82, 128.28, 127.39, 127.30 (Cq), 124.63, 60.67, 39.63, 32.78, 30.04, 25.65, 14.19; rt(LCMS) = 3.66 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{22}H_{21}NO_2Cl$ 366.1261; found 366.1261.

tert-butyl 8-chloro-3,4-dihydro-10-phenylbenzo[*b*][1,6]naphthyridine-2(1*H*)-carboxylate (5):



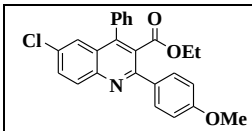
Yield (187 mg, 95%); white solid; mp= 183-185 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.92 (d, J = 9.0 Hz, 1H), 7.53-7.46 (m, 4H), 7.31 (d, J = 1.5 Hz, 1H), 7.21 (dd, J = 7.8, 1.5 Hz, 2H), 4.40 (s, 2H), 3.79 (t, J = 6.0 Hz, 2H), 3.21 (t, J = 6.0 Hz, 2H), 1.40 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.37 (Cq), 154.51 (Cq), 145.06 (Cq), 134.64 (Cq), 131.80 (Cq), 130.23, 129.94, 129.10, 128.75, 128.64, 127.25 (Cq), 125.95 (Cq), 124.56, 80.08 (Cq), 44.28, 41.45, 33.50, 28.34; rt(LCMS) = 3.80 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{23}H_{24}N_2O_2Cl$ 395.1526; found 395.1538.

6-chloro-2-(4-chlorophenyl)-3,4-diphenylquinoline (6):



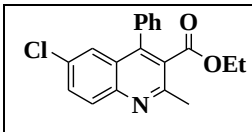
Yield (199 mg, 94%); white solid; mp= 213-215 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.19 (d, J = 9.0 Hz, 1H), 7.69 (dd, J = 9.0, 2.4 Hz, 1H), 7.58 (d, J = 2.4 Hz, 1H), 7.37-7.28 (m, 5H), 7.24-7.19 (m, 2H), 7.15-7.12 (m, 2H), 7.09-7.05 (m, 3H), 6.92-6.89 (m, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.88 (Cq), 147.23 (Cq), 145.77 (Cq), 139.27 (Cq), 137.72 (Cq), 136.10 (Cq), 134.06 (Cq), 133.61 (Cq), 132.71 (Cq), 131.35, 131.32, 131.18, 130.49, 130.16, 128.08, 127.98, 127.69, 127.52 (Cq), 126.80, 125.41; rt(LCMS) = 4.22 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{27}H_{18}NCl_2$ 426.0816; found 426.0823.

ethyl 6-chloro-2-(4-methoxyphenyl)-4-phenylquinoline-3-carboxylate (7):



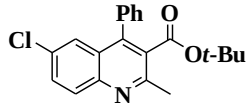
Yield (198 mg, 95%); white solid; mp= 133-135 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15 (d, J = 9.0 Hz, 1H), 7.75 (d, J = 8.7 Hz, 2H), 7.67 (dd, J = 8.7, 2.4 Hz, 1H), 7.56 (d, J = 2.4 Hz, 1H), 7.54-7.50 (m, 3H), 7.42-7.39 (m, 2H), 7.01 (d, J = 8.7 Hz, 2H), 3.93 (q, J = 7.2 Hz, 2H), 3.85 (s, 3H), 0.87 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.13 (Cq), 160.52 (Cq), 155.69 (Cq), 146.28 (Cq), 134.95 (Cq), 132.74 (Cq), 132.32 (Cq), 131.36, 130.04, 129.35, 128.83, 128.46, 127.85 (Cq), 126.15 (Cq), 125.25, 114.01, 61.43, 55.37, 13.55; rt(LCMS) = 3.95 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{25}H_{21}NO_3Cl$ 418.1210; found 418.1227.

ethyl 6-chloro-2-methyl-4-phenylquinoline-3-carboxylate (8):



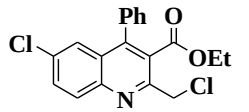
Yield (151 mg, 93%); white solid; mp= 101-103 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.96 (d, J = 9.0 Hz, 1H), 7.59 (dd, J = 9.0, 2.4 Hz, 1H), 7.50 (d, J = 2.4 Hz, 1H), 7.47-7.45 (m, 3H), 7.33 (d, J = 4.2 Hz, 1H), 7.30 (d, J = 1.8 Hz, 1H), 4.04 (q, J = 7.2 Hz, 2H), 2.74 (s, 3H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 168.03 (Cq), 154.96 (Cq), 146.04 (Cq), 145.33 (Cq), 135.02 (Cq), 132.31 (Cq), 131.06, 130.53, 129.28, 128.75, 128.43, 128.14 (Cq), 125.90 (Cq), 125.16, 61.43, 23.75, 13.63; rt(LCMS) = 3.65 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{19}H_{17}NO_2Cl$ 326.0984; found 326.0964.

tert-butyl 6-chloro-2-methyl-4phenylquinoline-3-carboxylate (9):



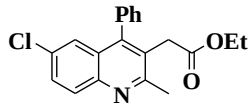
Yield (162 mg, 92%); white solid; mp= 142-144 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.94 (d, J = 9.0 Hz, 1H), 7.56 (dd, J = 9.0, 2.4 Hz, 1H), 7.45-7.42 (m, 4H), 7.35-7.30 (m, 2H), 2.75 (s, 3H), 1.20 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.05 (Cq), 154.87 (Cq), 145.79 (Cq), 144.51 (Cq), 135.02 (Cq), 132.13 (Cq), 130.77, 130.44, 129.51, 129.26 (Cq), 128.63, 128.35, 126.14 (Cq), 125.08, 82.54 (Cq), 27.55, 23.60; rt(LCMS) = 3.93 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{21}H_{21}NO_2Cl$ 354.1261; found 354.1269.

ethyl 6-chloro-2-(chloromethyl)-4-phenylquinoline-3-carboxylate (10):



Yield (162 mg, 90%); white solid; mp= 107-109 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.03 (d, J = 9.0 Hz, 1H), 7.64 (dd, J = 9.0, 2.1 Hz, 1H), 7.57 (d, J = 2.1 Hz, 1H), 7.51-7.47 (m, 3H), 7.35-7.31 (m, 2H), 5.00 (s, 2H), 4.04 (q, J = 7.2 Hz, 2H), 0.89 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.26 (Cq), 153.41 (Cq), 147.30 (Cq), 145.68 (Cq), 135.00 (Cq), 133.85 (Cq), 131.67, 131.22, 129.19, 128.91, 128.52, 127.00 (Cq), 125.37, 61.72, 45.76, 13.49; rt(LCMS) = 3.82 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{19}H_{16}NO_2Cl_2$ 360.0558; found 360.0568.

ethyl 2-(6-chloro-2-methyl-4-phenylquinolin-3-yl)acetate (11):



Yield (154 mg, 91%); white solid; mp= 135-137 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.97 (d, J = 9.0 Hz, 1H), 7.57-7.49 (m, 4H), 7.28-7.23 (m, 3H), 4.11 (q, J = 7.2 Hz, 2H), 3.59 (s, 2H), 2.72 (s, 3H), 1.19 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 170.68 (Cq), 158.91 (Cq), 147.31 (Cq), 145.15 (Cq), 136.06 (Cq), 131.57 (Cq), 130.27, 129.84, 129.16, 128.79, 128.49, 127.52 (Cq), 125.70 (Cq), 125.24, 61.10, 36.55, 24.12, 14.17; rt(LCMS) = 3.51 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{20}H_{19}NO_2Cl$ 340.1104; found 340.1103.

ethyl 2-((ethoxycarbonyl)methyl)-6-chloro-4-phenylquinoline-3-carboxylate (12):

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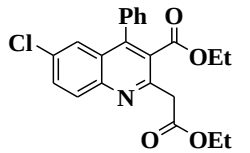
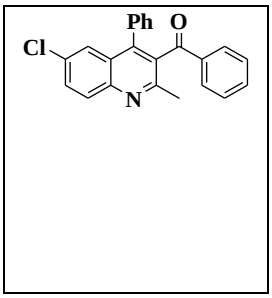


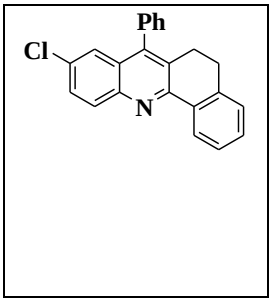
Yield (181 mg, 91%); yellow solid; mp= 57-59 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.99 (d, J = 9.0 Hz, 1H), 7.60 (dd, J = 9.0, 2.4 Hz, 1H), 7.52 (d, J = 2.4 Hz, 1H), 7.46-7.42 (m, 3H), 7.31-7.28 (m, 2H), 4.18 (s, 2H), 4.13 (q, J = 7.2 Hz, 2H), 3.94 (q, J = 7.2 Hz, 2H), 1.23 (t, J = 7.2 Hz, 3H), 1.21 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 169.92 (Cq), 167.66 (Cq), 151.97 (Cq), 146.84 (Cq), 146.05 (Cq), 135.48 (Cq), 133.02 (Cq), 131.32, 131.01, 129.19, 128.65, 128.39, 127.31 (Cq), 126.58(Cq), 125.32, 61.39, 48.93, 43.25, 14.10, 13.36 rt(LCMS) = 3.70 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{22}H_{21}NO_4Cl$ 398.1159; found 398.1160.

(6-chloro-2-methyl-4-phenylquinolin-3-yl)(phenyl)methanone (13):



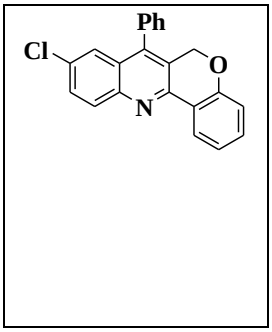
Yield (168 mg, 94%); white solid; mp= 216-218 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.05 (d, J = 9.0 Hz, 1H), 7.63 (dd, J = 9.0, 2.4 Hz, 1H), 7.58-7.54 (m, 3H), 7.44-7.38 (m, 1H), 7.28-7.14 (m, 7H), 2.60 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 197.34 (Cq), 155.09 (Cq), 146.24 (Cq), 144.74 (Cq), 136.89 (Cq), 134.16 (Cq), 133.73, 133.24 (Cq), 132.46 (Cq), 130.98, 130.64, 129.93, 129.24, 128.55, 128.27, 126.12 (Cq), 125.00, 24.04; rt(LCMS) = 3.64 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{23}H_{17}NOCl$ 358.0999; found 358.1014.

9-chloro-5,6-dihydro-7-phenylbenzo[*c*]acridine (14):



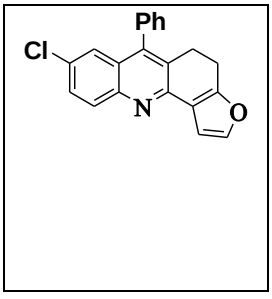
Yield (163 mg, 96%); white solid; mp= 146-148 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.63 (dd, J = 7.5, 1.2 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 7.61-7.54 (m, 4H), 7.49-7.37 (m, 3H), 7.33-7.24 (m, 3H), 2.91-2.83 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.41 (Cq), 145.61 (Cq), 144.62 (Cq), 139.30 (Cq), 136.24 (Cq), 134.80 (Cq), 131.75 (Cq), 131.26, 129.92, 129.46, 129.41, 129.09 (Cq), 128.83, 128.27, 128.02 (Cq), 127.80, 127.36, 126.39, 124.88, 28.14, 26.56; rt(LCMS) = 4.42 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{23}H_{17}NCl$ 342.1050; found 342.1059.

9-chloro-7-phenyl-6*H*-chromeno[4,3-b]quinoline (15):



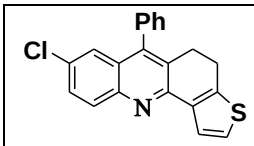
Yield (163 mg, 95%); white solid; mp= 181-183 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.50 (dd, J = 7.8, 1.8 Hz, 1H), 8.08 (d, J = 9.0 Hz, 1H), 7.60-7.54 (m, 4H), 7.45 (d, J = 2.1 Hz, 1H), 7.40-7.34 (m, 1H), 7.31-7.27 (m, 2H), 7.20-7.15 (m, 1H), 6.97 (dd, J = 8.4, 0.9 Hz, 1H), 5.07 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.26 (Cq), 148.93 (Cq), 146.41 (Cq), 142.83 (Cq), 134.21 (Cq), 132.09, 132.01 (Cq), 131.22, 130.18, 129.20, 129.01, 128.87, 127.74 (Cq), 125.79, 124.93, 123.62 (Cq), 123.16 (Cq), 122.54, 117.24, 66.61; rt(LCMS) = 4.42 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{22}H_{15}NOCl$ 344.0842; found 344.0840.

8-chloro-4,5-dihydro-6phenylfuro[2,3-*c*]acridine (16):



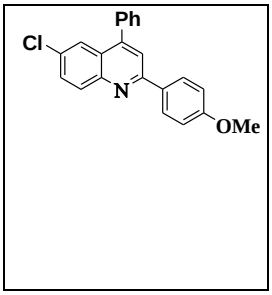
Yield (155 mg, 94%); white solid; mp= 144-146 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.99 (d, J = 9.0 Hz, 1H), 7.59-7.50 (m, 4H), 7.44 (d, J = 1.8 Hz, 1H), 7.29-7.26 (m, 3H), 7.11 (d, J = 2.1 Hz, 1H), 2.98-2.85 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.01 (Cq), 151.57 (Cq), 145.33 (Cq), 144.41 (Cq), 142.84, 136.38 (Cq), 131.01 (Cq), 130.30, 129.26, 129.20, 128.87,128.24, 127.62 (Cq), 126.38 (Cq), 124.99, 120.78 (Cq), 107.34, 26.51, 21.72; rt(LCMS) = 3.87 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{21}H_{15}NOCl$ 332.0842; found 332.0838.

8-chloro-4,5-dihydro-6-phenylthieno[2,3-*c*]acridine (17):



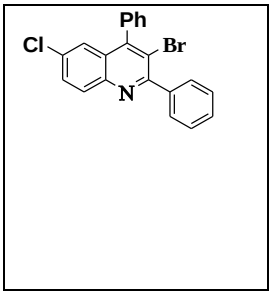
Yield (161 mg, 93%); white solid; mp= 182-184 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.02 (d, J = 9.0 Hz, 1H), 7.92 (d, J = 5.4 Hz, 1H), 7.59-7.51 (m, 4H), 7.34 (d, J = 2.4 Hz, 1H), 7.31-7.27 (m, 2H), 7.21 (d, J = 5.4 Hz, 1H), 2.93 (s, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.43 (Cq), 145.42 (Cq), 144.55 (Cq), 143.47 (Cq), 137.47 (Cq), 136.38 (Cq), 131.30 (Cq), 130.79, 129.37, 128.87, 128.27, 127.75 (Cq), 126.87 (Cq), 125.29, 124.95, 123.29, 27.34, 23.25; rt(LCMS) = 4.22 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{21}H_{15}NSCl$ 348.0614; found 348.0621.

6-chloro-2-(4-methoxyphenyl)-4-phenylquinoline (18):



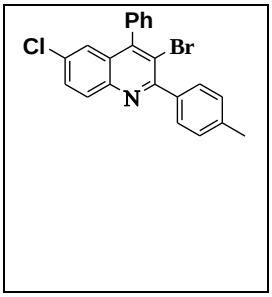
Yield (159 mg, 93%); white solid; mp= 116-118 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18-8.13 (m, 3H), 7.85 (d, J = 2.4 Hz, 1H), 7.80 (s, 1H), 7.65 (dd, J = 9.0, 2.4 Hz, 1H), 7.58-7.53 (m, 5H), 7.05 (dd, J = 6.9, 2.1 Hz, 2H), 3.89 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.04 (Cq), 156.60 (Cq), 148.25 (Cq), 147.25 (Cq), 137.88 (Cq), 131.75 (Cq), 131.53, 130.33, 129.46, 128.89, 128.81, 128.66, 126.23 (Cq), 124.47, 119.54, 114.29, 55.41; rt(LCMS) = 3.89 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{22}H_{17}NOCl$ 346.0999; found 346.0997.

3-bromo-6-chloro-2,4-diphenylquinoline (19):



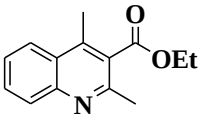
Yield (189 mg, 96%); yellow solid; mp= 151-153 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.14 (d, J = 9.0 Hz, 1H), 7.77 (dd, J = 7.8, 2.1 Hz, 2H), 7.67 (dd, J = 9.0, 2.4 Hz, 1H), 7.64-7.50 (m, 6H), 7.43 (d, J = 2.4 Hz, 1H), 7.37 (dd, J =7.8, 2.1 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.26 (Cq), 148.95 (Cq), 144.91 (Cq), 140.68 (Cq), 137.48 (Cq), 133.34 (Cq), 131.31, 130.80, 129.44, 129.22, 128.92, 128.83, 128.58 (Cq), 128.09, 125.15, 119.76 (Cq); rt(LCMS) = 3.85 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{21}H_{14}NClBr$ 393.9998; found 394.0013.

3-bromo-6-chloro-4-phenyl-2-*p*-tolylquinoline (20):



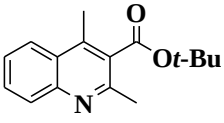
Yield (194 mg, 95%); light yellow solid; mp= 160-162 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.12 (d, J = 9.0 Hz, 1H), 7.68-7.56 (m, 6H), 7.40-7.27 (m, 5H), 2.46 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.27 (Cq), 148.84 (Cq), 144.92 (Cq), 138.88 (Cq), 137.83 (Cq), 137.56 (Cq), 133.15 (Cq), 131.26, 130.69, 129.35, 129.20, 128.79, 128.75, 128.49 (Cq), 125.10, 119.84 (Cq), 21.44; rt(LCMS) = 3.97 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{22}H_{16}NClBr$ 408.0155; found 408.0162.

ethyl 2,4-dimethylquinoline-3-carboxylate (21):



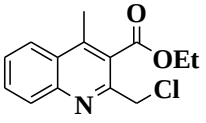
Yield (108 mg, 95%); white solid; mp= 205-207 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.68 (d, J = 8.4 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 7.83 (t, J = 7.8 Hz, 1H), 7.71 (t, J = 7.8 Hz, 1H), 4.44 (q, J = 7.2 Hz, 2H), 2.95 (s, 3H), 2.76 (s, 3H), 1.35 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.51 (Cq), 153.46 (Cq), 150.94 (Cq), 139.01 (Cq), 133.84, 129.23, 128.61 (Cq), 126.25 (Cq), 124.87, 123.28, 62.88, 19.70, 17.06, 14.13; rt(LCMS) = 2.30 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{14}H_{16}NO_2$ 230.1181; found 230.1188.

***tert*-butyl 2,4-dimethylquinoline-3-carboxylate (22):**



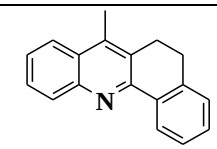
Yield (114 mg, 89%); white solid; mp= 223-225 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.88 (d, J = 8.4 Hz, 1H), 8.18 (d, J = 8.4 Hz, 1H), 7.91 (t, J = 7.8 Hz, 1H), 7.80 (t, J = 7.8 Hz, 1H), 3.07 (s, 3H), 2.84 (s, 3H), 1.60 (s, 9H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 164.01 (Cq), 153.07 (Cq), 151.80 (Cq), 137.39 (Cq), 134.35, 130.00 (Cq), 129.71, 126.50 (Cq), 124.93, 122.24, 85.44 (Cq), 28.08, 18.73, 17.00; rt(LCMS) = 3.11 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{16}H_{20}NO_2$ 258.1494; found 258.1490.

ethyl 2-(chloromethyl)-4-methylquinoline-3-carboxylate (23):



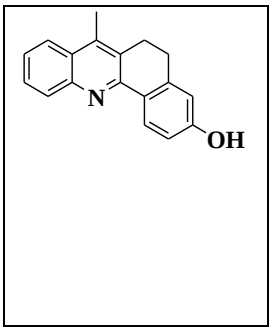
Yield (126 mg, 95%); deliquescent yellow solid; mp= 105-107 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.00 (d, J = 8.4 Hz, 1H), 7.92 (d, J = 8.4 Hz, 1H), 7.67 (t, J = 8.4 Hz, 1H), 7.51 (t, J = 7.8 Hz, 1H), 4.92 (s, 2H), 4.47 (q, J = 7.2 Hz, 2H), 2.64 (s, 3H), 1.41 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 167.83 (Cq), 152.70 (Cq), 146.36 (Cq), 144.17 (Cq), 130.63, 129.71, 127.68, 126.78 (Cq), 126.49 (Cq), 124.13, 62.05, 46.10, 15.86, 14.10; rt(LCMS) = 2.88 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{14}H_{15}NO_2Cl$ 264.0791; found 264.0802.

5,6-dihydro-7-methylbenzo[*c*]acridine (24):



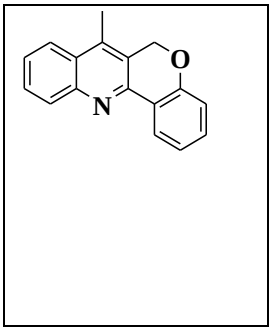
Yield (115 mg, 94%); grey solid; mp= 92-94 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.68 (d, J = 7.5 Hz, 1H), 8.22 (d, J = 8.4 Hz, 1H), 7.95 (d, J = 8.4 Hz, 1H), 7.68 (dd, J = 9.6, 6.9 Hz, 1H), 7.53-7.38 (m, 3H), 7.28 (d, J = 7.5 Hz, 1H), 3.11-2.95 (m, 4H), 2.59 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.62 (Cq), 146.88 (Cq), 139.77 (Cq), 139.11 (Cq), 135.28 (Cq), 130.25, 129.49, 128.40 (Cq), 128.26, 127.76 (Cq), 127.61, 127.25, 126.48, 125.83, 123.68, 28.17, 25.35, 13.91; rt(LCMS) = 3.33 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{18}H_{16}N$ 246.1283; found 246.1295.

5,6-dihydro-7-methylbenzo[*c*]acridin-3-ol (25):



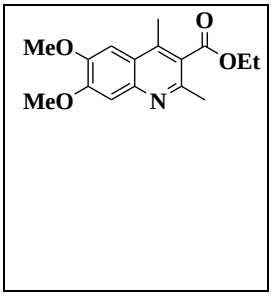
Yield (113 mg, 86%); grey solid; mp= 185-187 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.95 (d, J = 7.5 Hz, 1H), 7.68 (dd, J = 6.9, 1.5 Hz, 1H), 7.64 (dd, J = 6.9, 1.5 Hz, 1H), 7.53 (dd, J = 6.9, 1.5 Hz, 1H), 7.50 (dd, J = 6.9, 1.5 Hz, 1H), 6.81 (dd, J = 8.4, 1.5 Hz, 1H), 6.72 (d, J = 2.1 Hz, 1H), 3.01-3.05 (m, 2H), 2.90-2.85 (m, 2H), 2.63 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 159.54 (Cq), 152.52 (Cq), 146.31 (Cq), 141.54 (Cq), 140.35 (Cq), 129.39, 128.87, 128.24, 128.11 (Cq), 127.29 (Cq), 126.12 (Cq), 125.87, 124.53, 114.77, 114.45, 28.01, 25.19, 14.16; rt(LCMS) = 2.35 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{18}H_{16}NO$ 262.1232; found 262.1229.

7-methyl-6*H*-chromeno[4,3-b]quinoline (26):



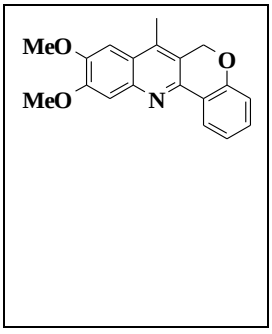
Yield (113 mg, 92%); yellow solid; mp= 111-113 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.48 (dd, J = 7.8, 1.8 Hz, 1H), 8.11 (dd, J = 8.7, 0.9 Hz, 1H), 7.91 (dd, J = 8.7, 0.9 Hz, 1H), 7.69-7.64 (m, 1H), 7.51-7.45 (m, 1H), 7.40-7.34 (m, 1H), 7.16 (dt, J = 8.7, 1.2 Hz, 1H), 7.01 (dd, J = 8.1, 1.2 Hz, 1H), 5.37 (s, 2H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.03 (Cq), 148.12 (Cq), 147.54 (Cq), 138.04, 131.61, 130.12, 129.04, 127.53 (Cq), 125.98, 125.74, 123.60, 123.38 (Cq), 123.20 (Cq), 122.40, 117.00, 66.21, 13.03; rt(LCMS) = 3.48 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{17}H_{14}NO$ 248.1075; found 248.1081.

ethyl 6,7-dimethoxy-2,4-dimethylquinoline-3-carboxylate (27):



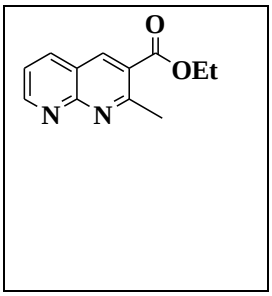
Yield (138 mg, 96%); yellow solid; mp= 128-130 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.19 (s, 1H), 4.43 (q, J = 7.2 Hz, 2H), 4.03 (s, 3H), 4.00 (s, 3H), 2.82 (s, 3H), 2.69 (s, 3H), 1.38 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 166.51 (Cq), 155.24 (Cq), 150.97 (Cq), 149.92 (Cq), 146.70 (Cq), 138.10 (Cq), 126.34 (Cq), 121.95 (Cq), 102.64, 102.35, 62.39, 56.83, 56.39, 19.93, 16.97, 14.15; rt(LCMS) = 2.28 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{16}H_{20}NO_4$ 290.1392; found 290.1404.

9,10-dimethoxy-7-methyl-6*H*-chromeno[4,3-b]quinoline (28):



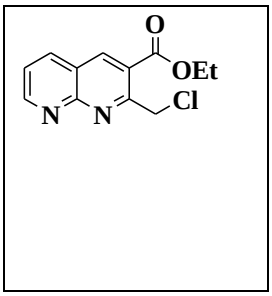
Yield (140 mg, 92%); yellow solid; mp= 273-275 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.25 (d, J = 7.8 Hz, 1H), 9.06 (s, 1H), 7.49 (t, J = 7.8 Hz, 1H), 7.29 (t, J = 7.8 Hz, 1H), 7.14 (s, 1H), 7.00 (d, J = 7.8 Hz, 1H), 5.40 (s, 2H), 4.14 (s, 3H), 4.04 (s, 3H), 2.72 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.16 (Cq), 155.55 (Cq), 151.27 (Cq), 146.96 (Cq), 140.98 (Cq), 135.71 (Cq), 135.35, 128.33, 123.73, 123.37 (Cq), 121.88 (Cq), 117.69, 115.02 (Cq), 101.90, 101.83, 65.01, 57.40, 56.36, 15.44; rt(LCMS) = 2.91 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{19}H_{18}NO_3$ 308.1287; found 308.1277.

ethyl 2-methyl-1,8-naphthyridine-3-carboxylate (29):



Yield (93 mg, 87%); light red solid; mp= 152-154 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.14 (dd, J = 4.2, 1.8 Hz, 1H), 8.76 (s, 1H), 8.25 (dd, J = 8.1, 1.8 Hz, 1H), 7.49 (dd, J = 8.1, 4.2 Hz, 1H), 4.47 (q, J = 7.2 Hz, 2H), 3.08 (s, 3H), 1.47 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.57 (Cq), 162.23 (Cq), 155.92 (Cq), 155.24, 140.65, 137.51, 124.81 (Cq), 122.08, 119.95 (Cq), 61.49, 25.84, 14.14; rt(LCMS) = 2.00 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{12}H_{13}N_2O_2$ 217.0977; found 217.0986.

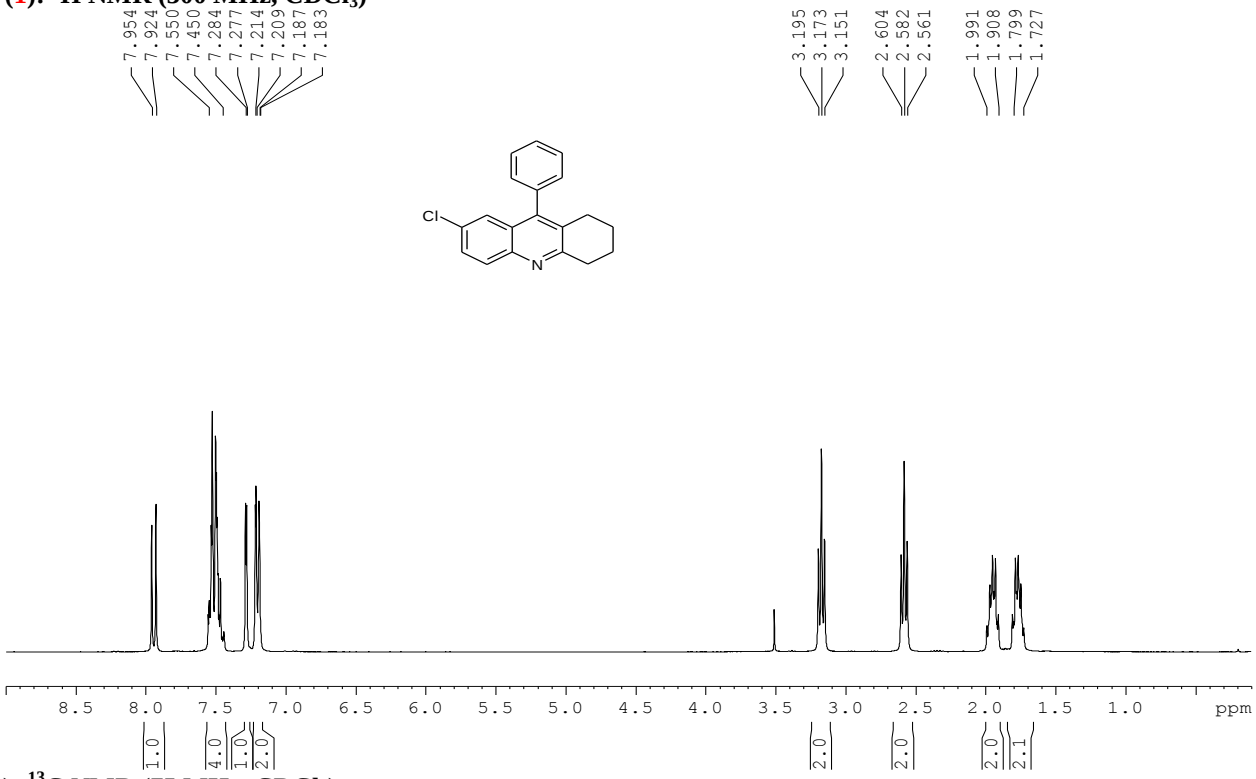
ethyl 2-(chloromethyl)-1,8-naphthyridine-3-carboxylate (30):



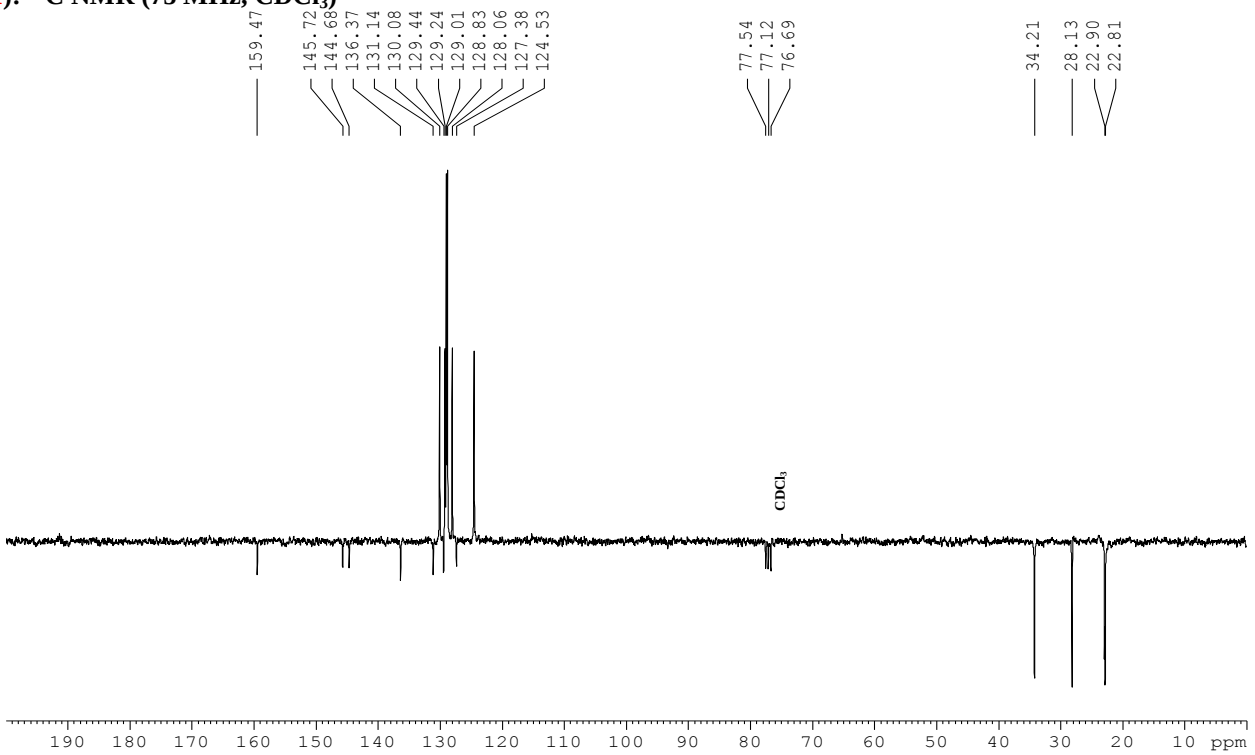
Yield (107 mg, 85%); light red solid; mp= 203-205 °C; Purity: 100%; ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.22 (dd, J = 4.2, 1.8 Hz, 1H), 8.85 (s, 1H), 8.31 (dd, J = 8.1, 1.8 Hz, 1H), 7.59 (dd, J = 8.1, 4.2 Hz, 1H), 5.32 (s, 2H), 4.51 (q, J = 7.2 Hz, 2H), 1.49 (t, J = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.00 (Cq), 159.33 (Cq), 156.00, 155.76 (Cq), 142.01, 137.61, 124.62 (Cq), 123.39, 121.39 (Cq), 62.22, 46.39, 14.17; rt(LCMS) = 2.26 min (5 min, PH = 3.8); HRMS-ESI (m/z): $[M+H]^+$ calcd. for $C_{12}H_{12}N_2O_2Cl$ 251.0587; found 251.0598.

4. XNMR Spectra

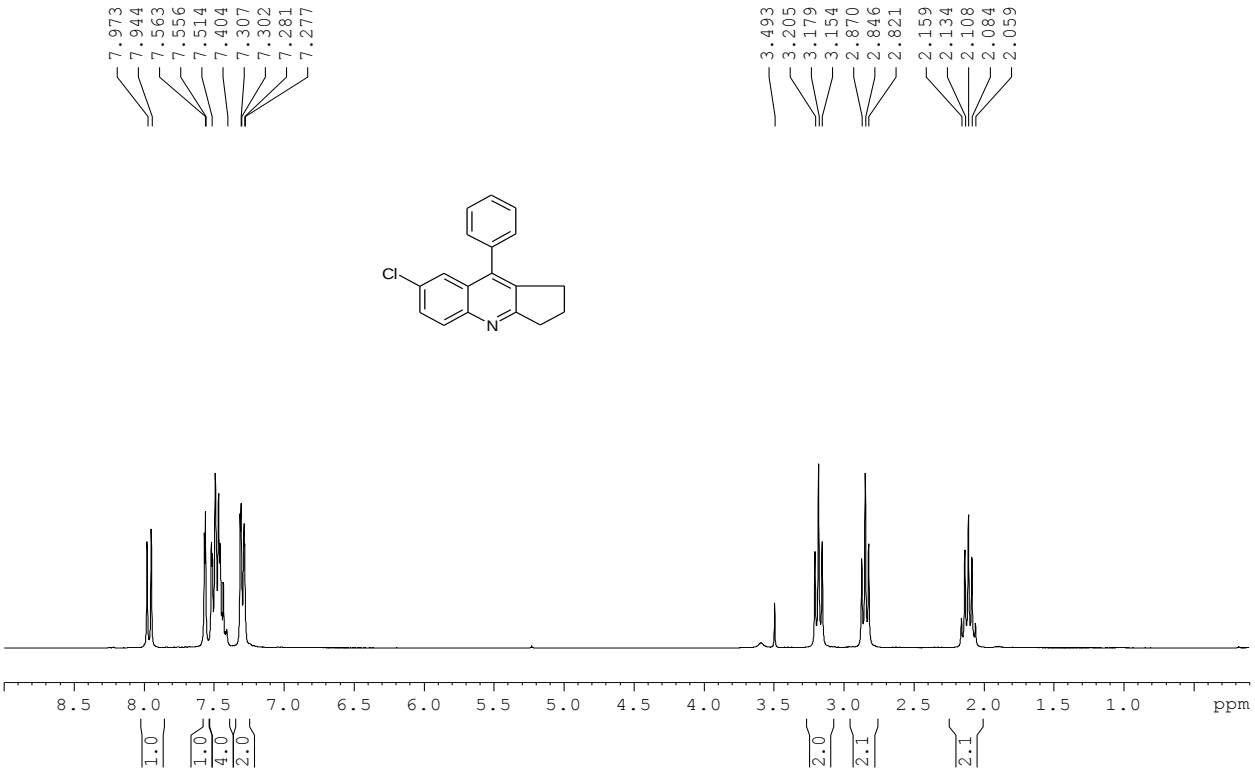
(1): ^{1}H NMR (300 MHz, $CDCl_3$)



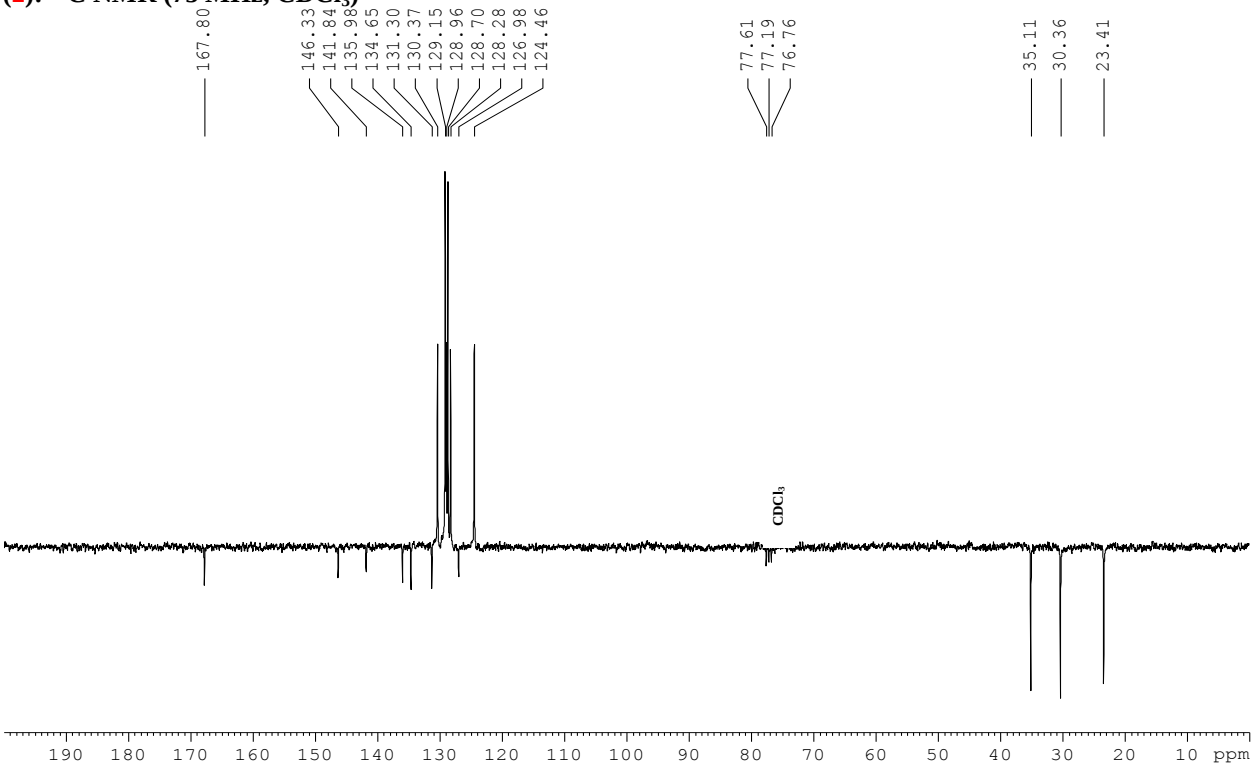
(1): ^{13}C NMR (75 MHz, $CDCl_3$)



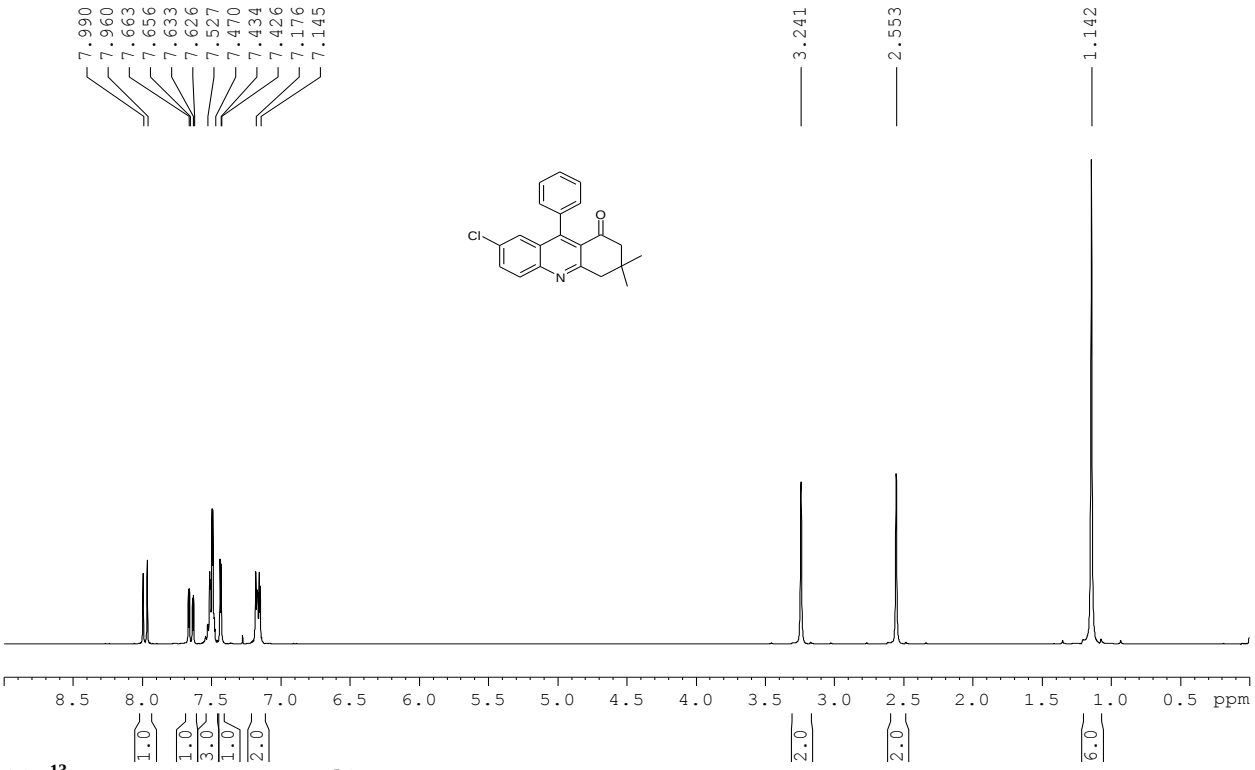
(2): ^{1}H NMR (300 MHz, $CDCl_3$)



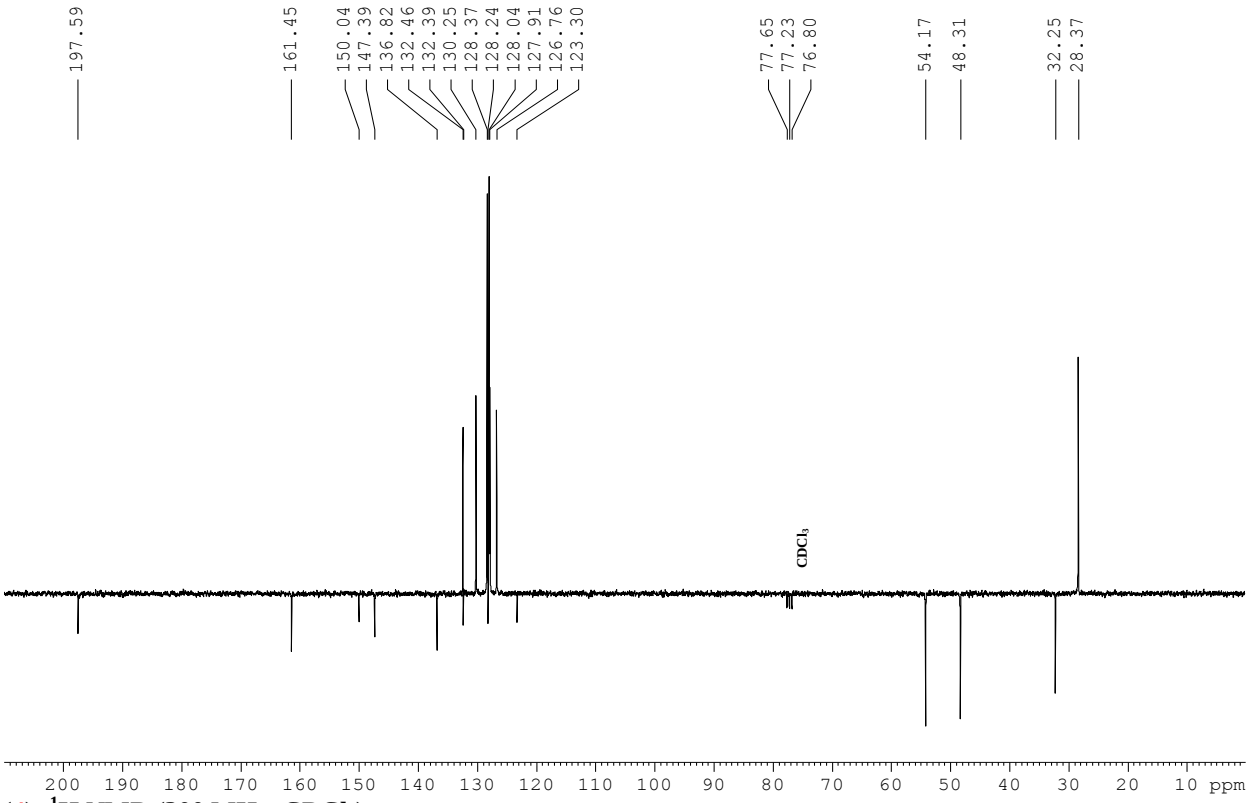
(2): ^{13}C NMR (75 MHz, $CDCl_3$)



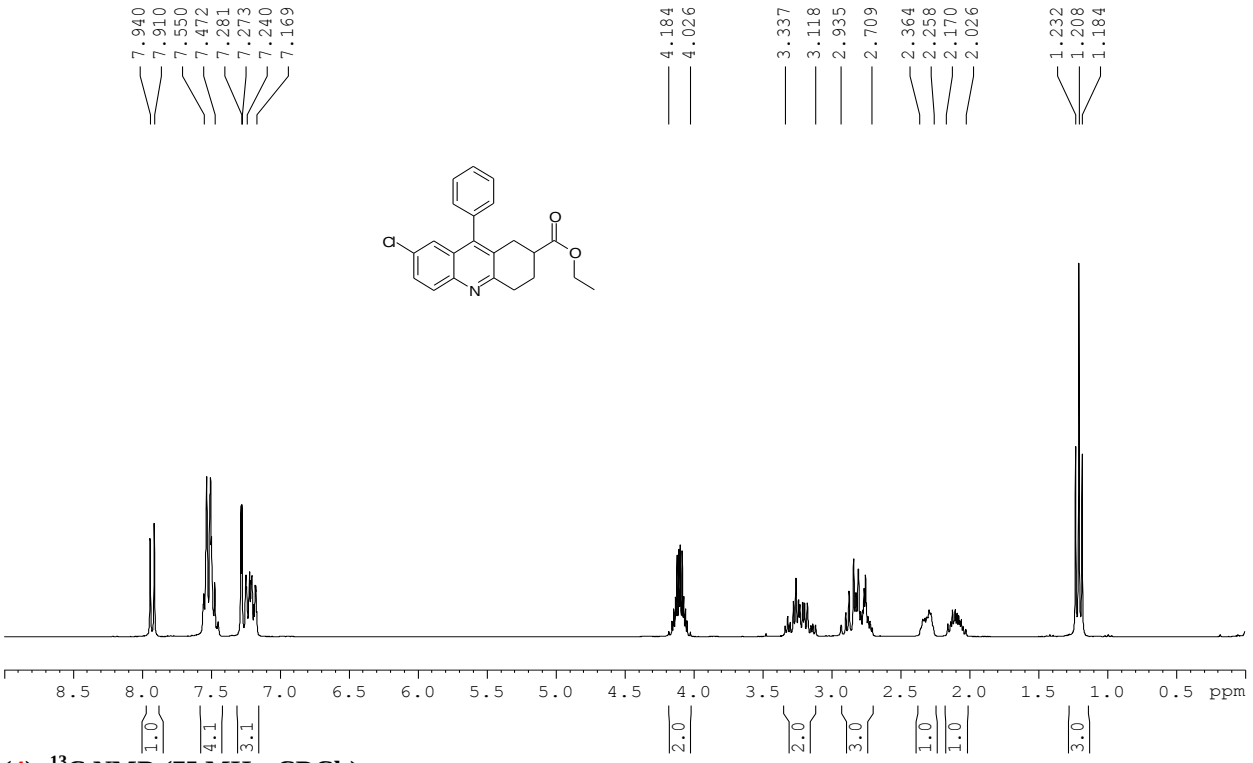
(3): ^{1}H NMR (300 MHz, $CDCl_3$)



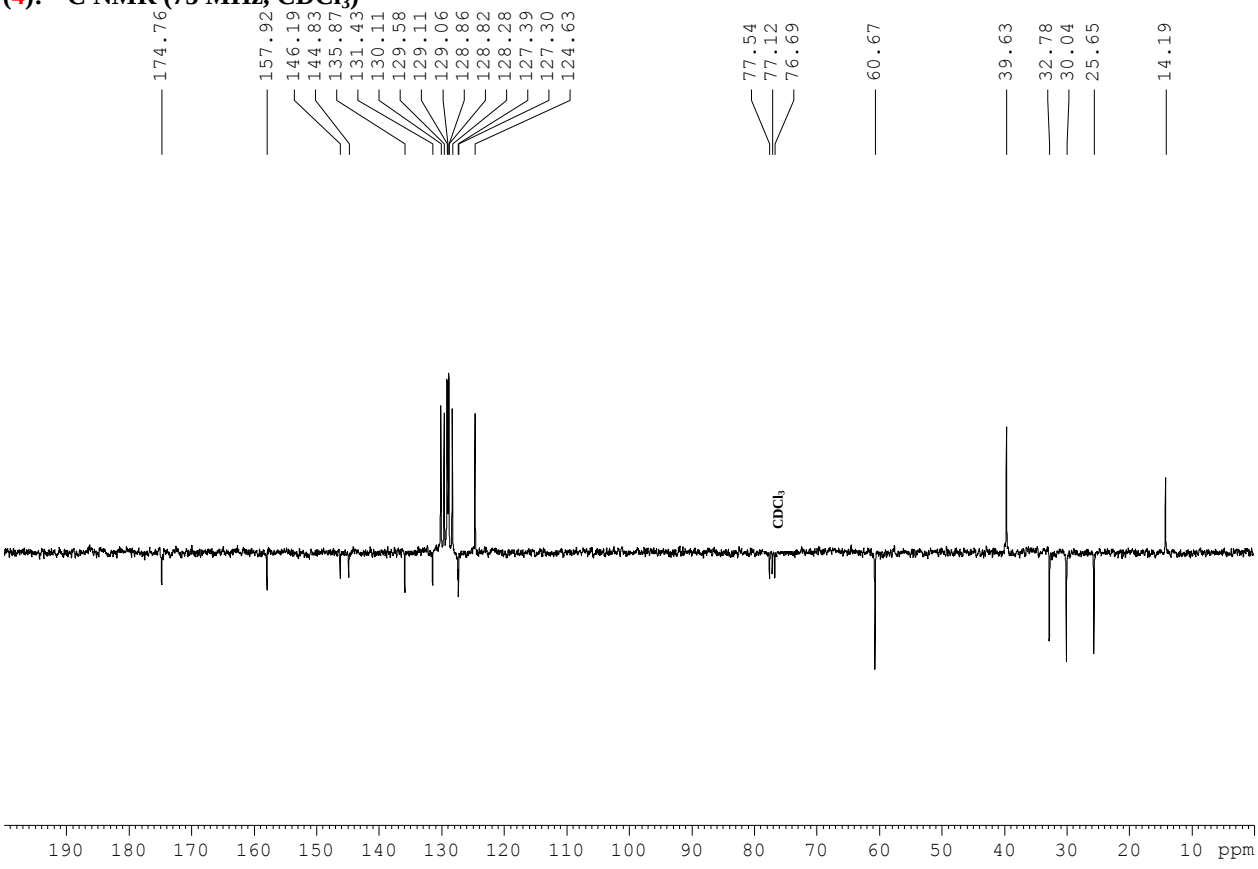
(3): ^{13}C NMR (75 MHz, $CDCl_3$)



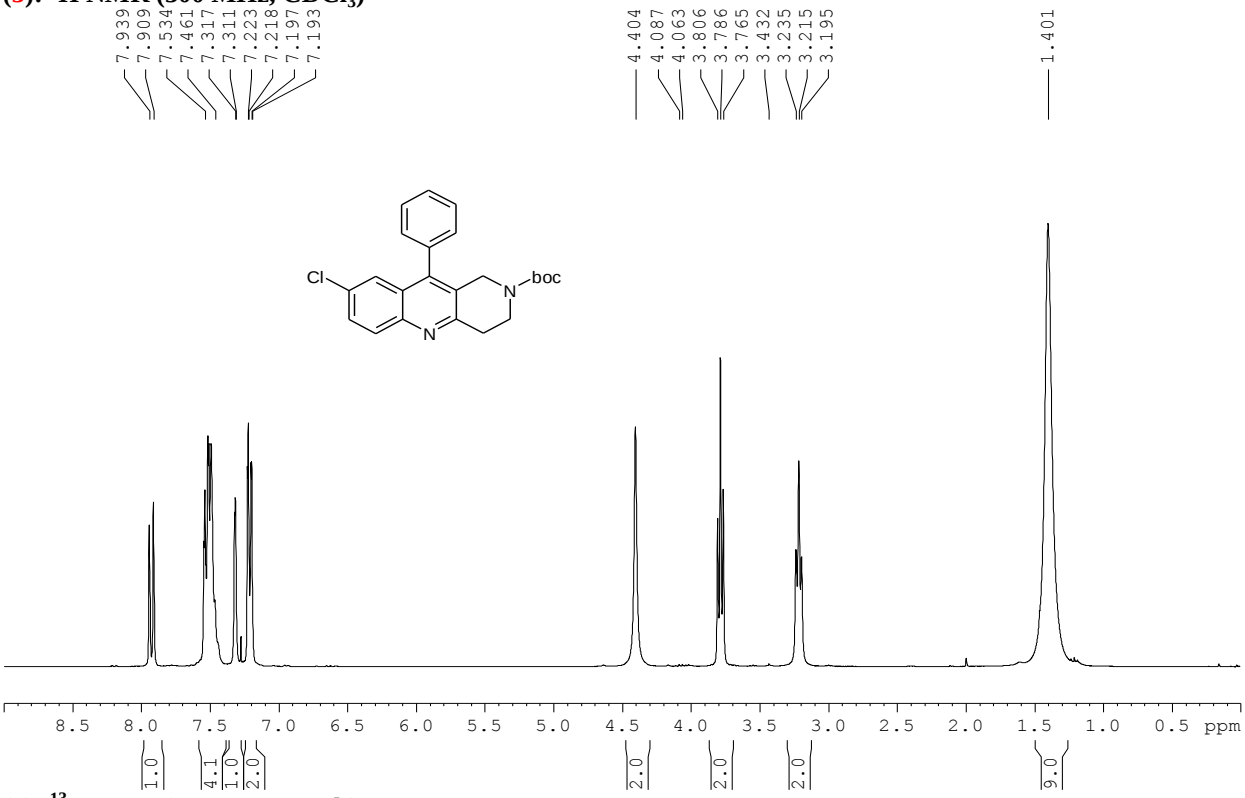
(4): ^{1}H NMR (300 MHz, $CDCl_3$)



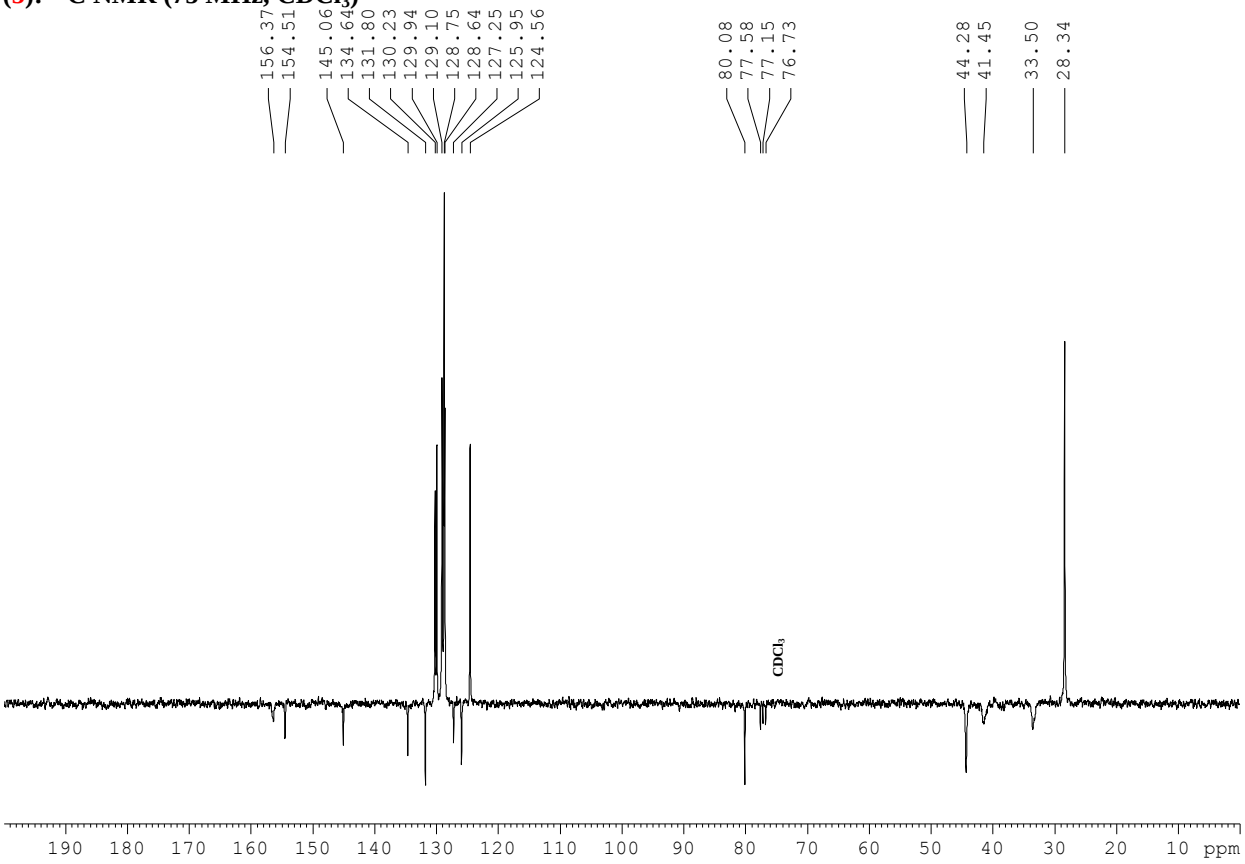
(4): ^{13}C NMR (75 MHz, $CDCl_3$)



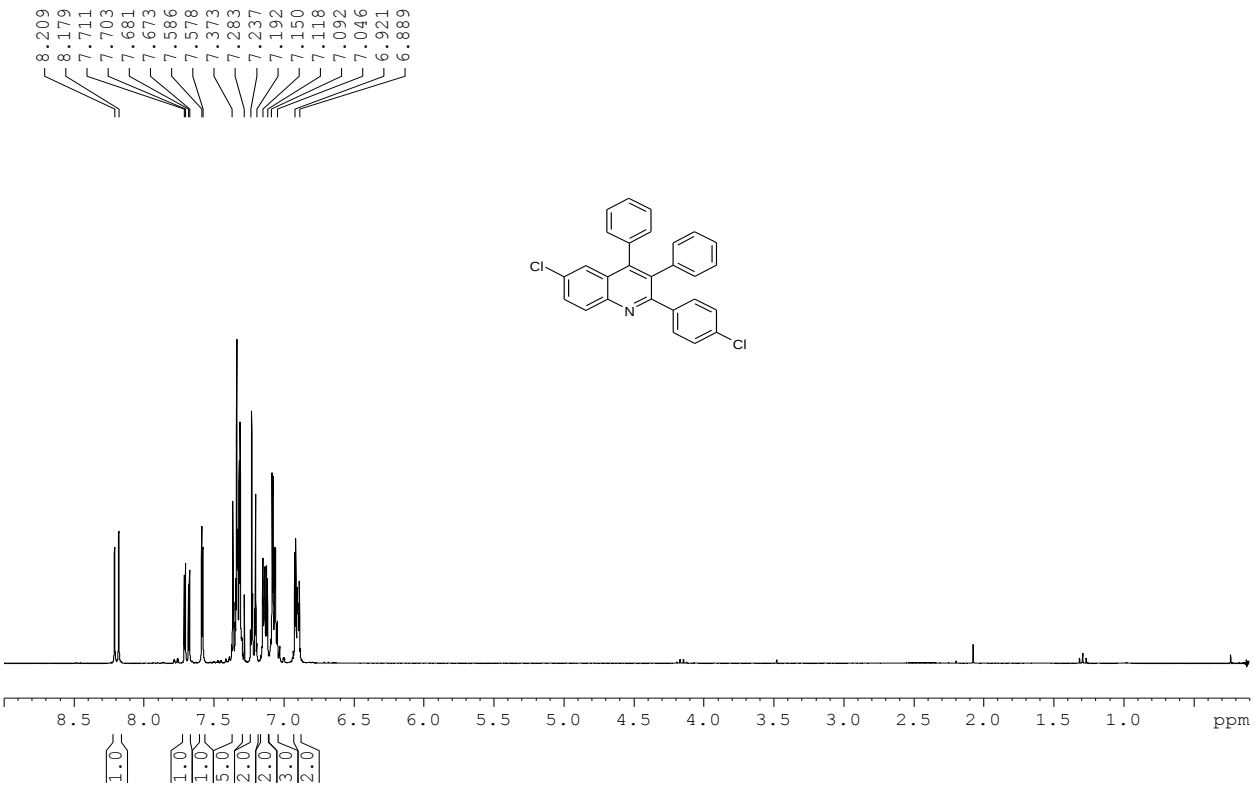
(5): ^{1}H NMR (300 MHz, $CDCl_3$)



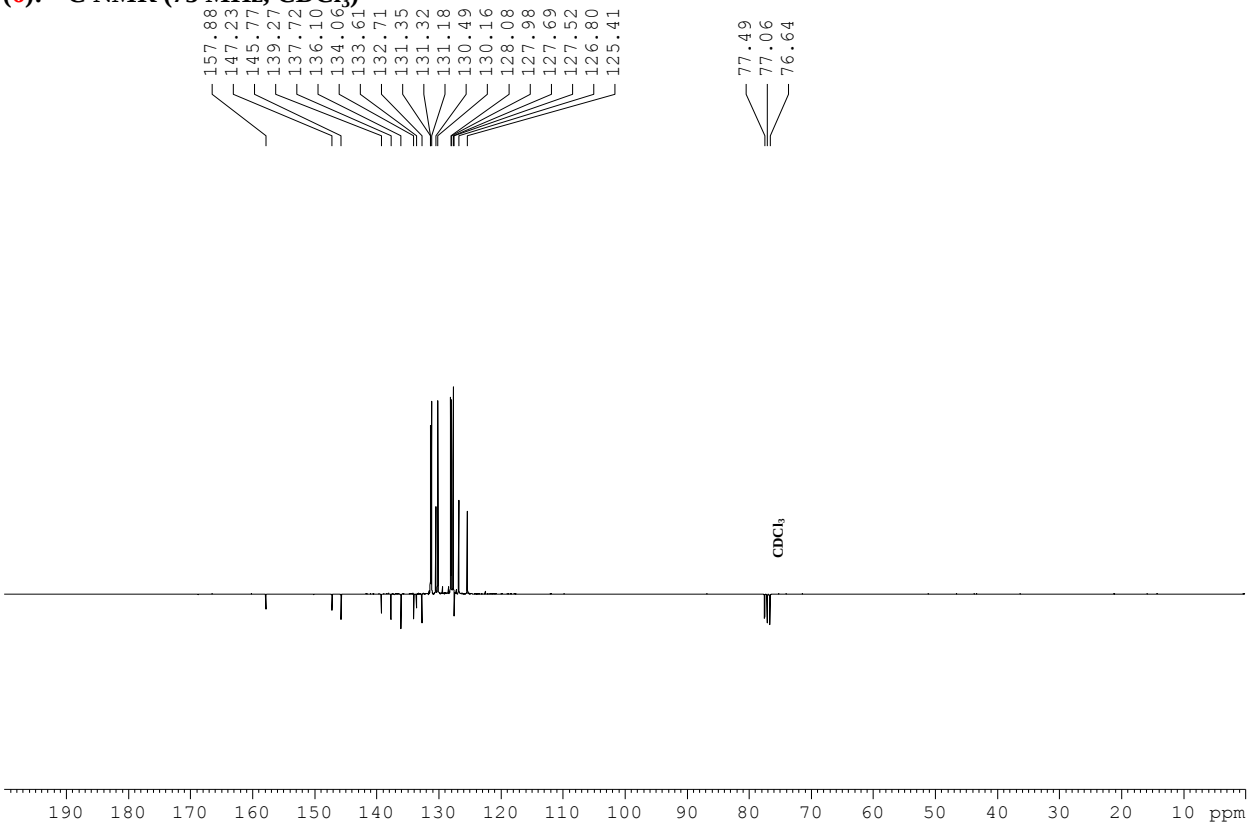
(5): ^{13}C NMR (75 MHz, $CDCl_3$)



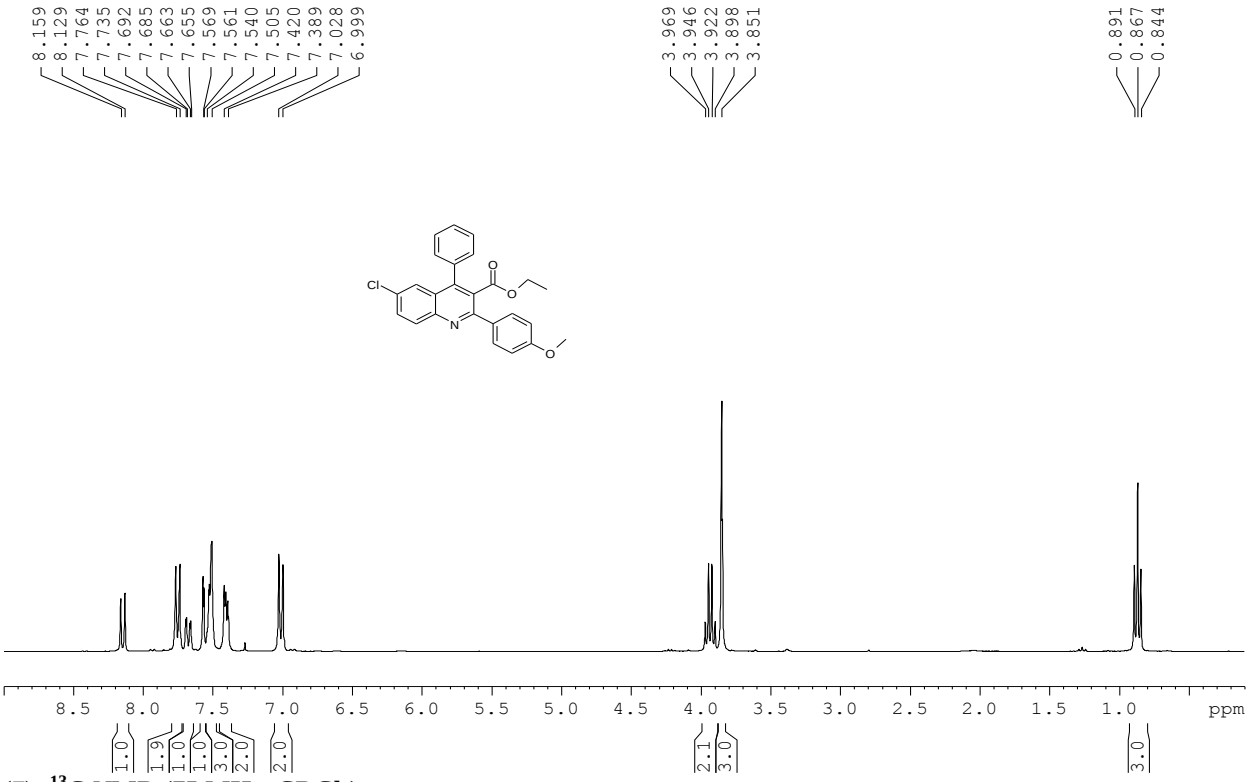
(6): ^{1}H NMR (300 MHz, $CDCl_3$)



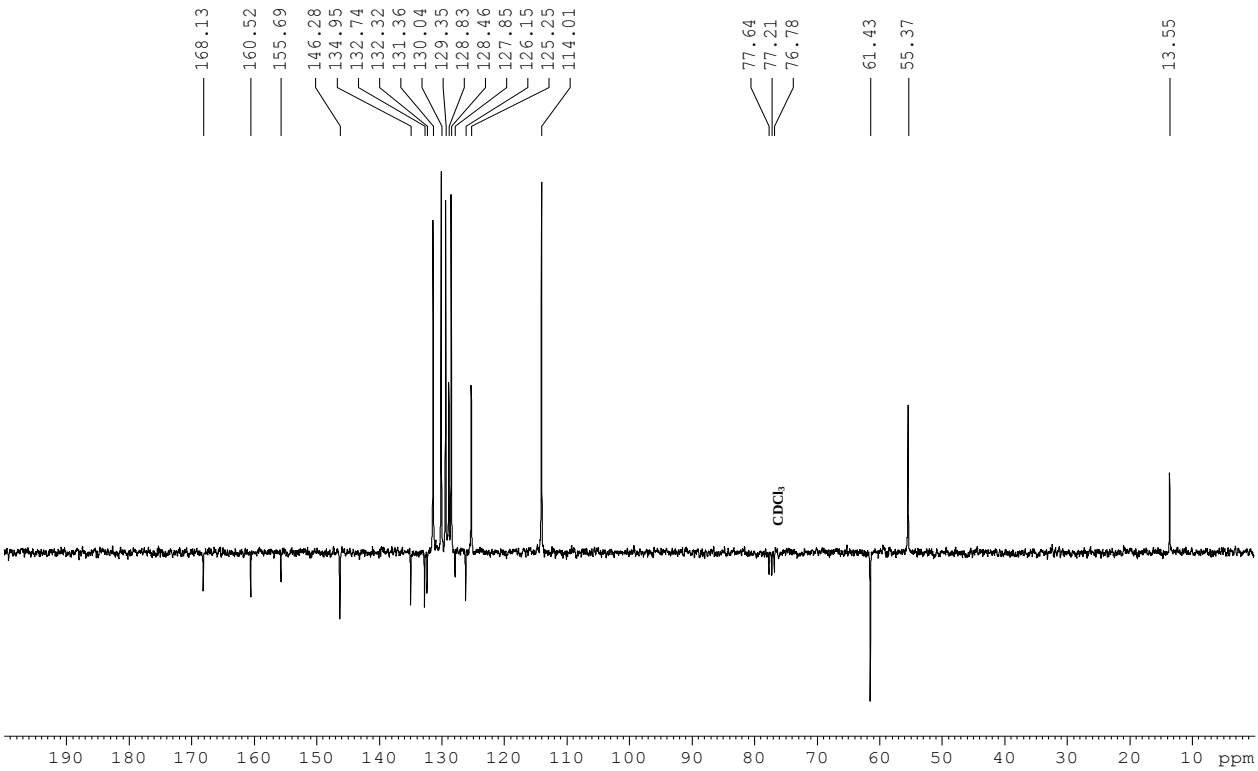
(6): ^{13}C NMR (75 MHz, $CDCl_3$)



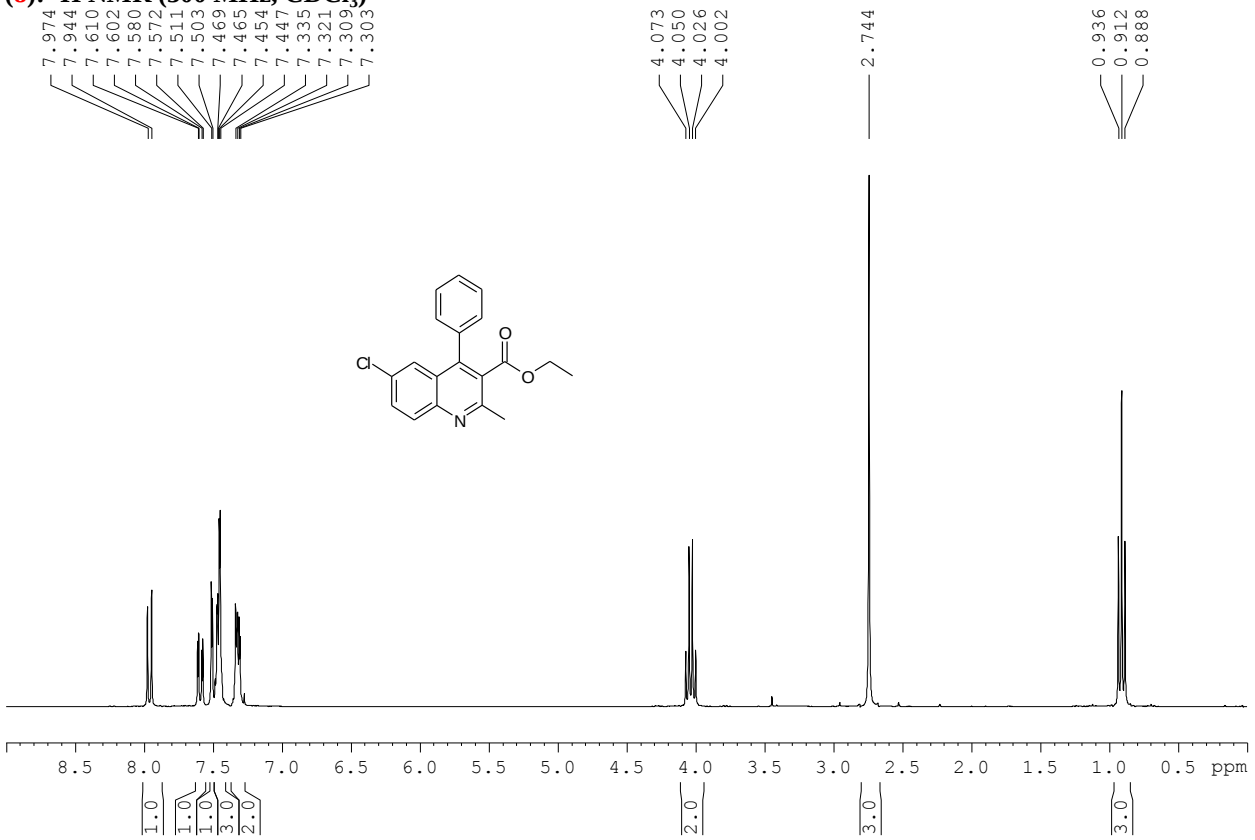
(7): ^{1}H NMR (300 MHz, $CDCl_3$)



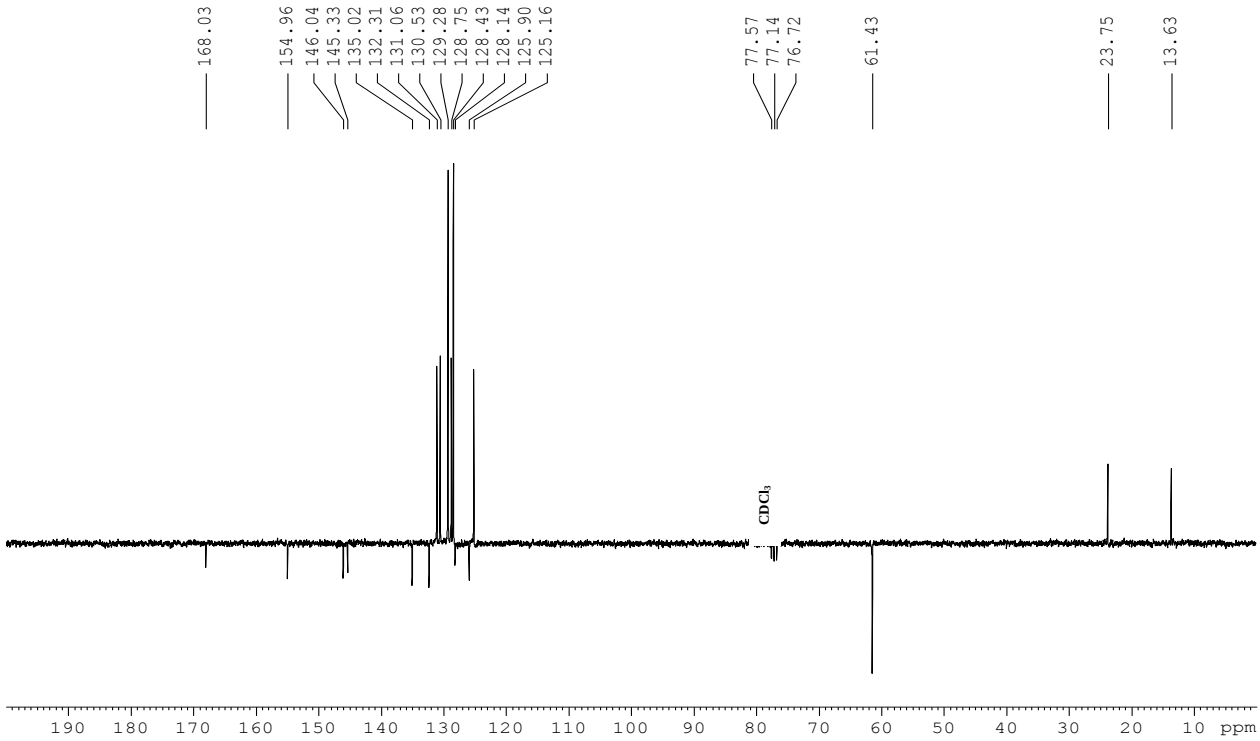
(7): ^{13}C NMR (75 MHz, $CDCl_3$)



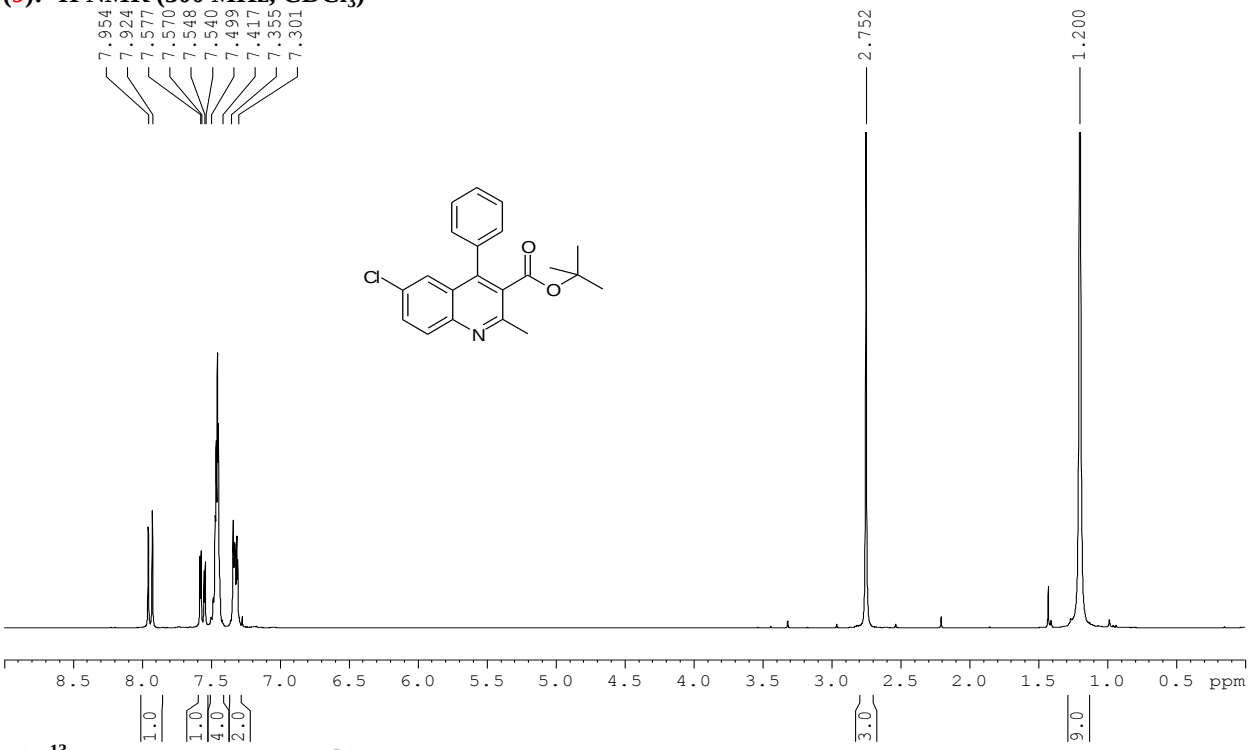
(8): ^{1}H NMR (300 MHz, $CDCl_3$)



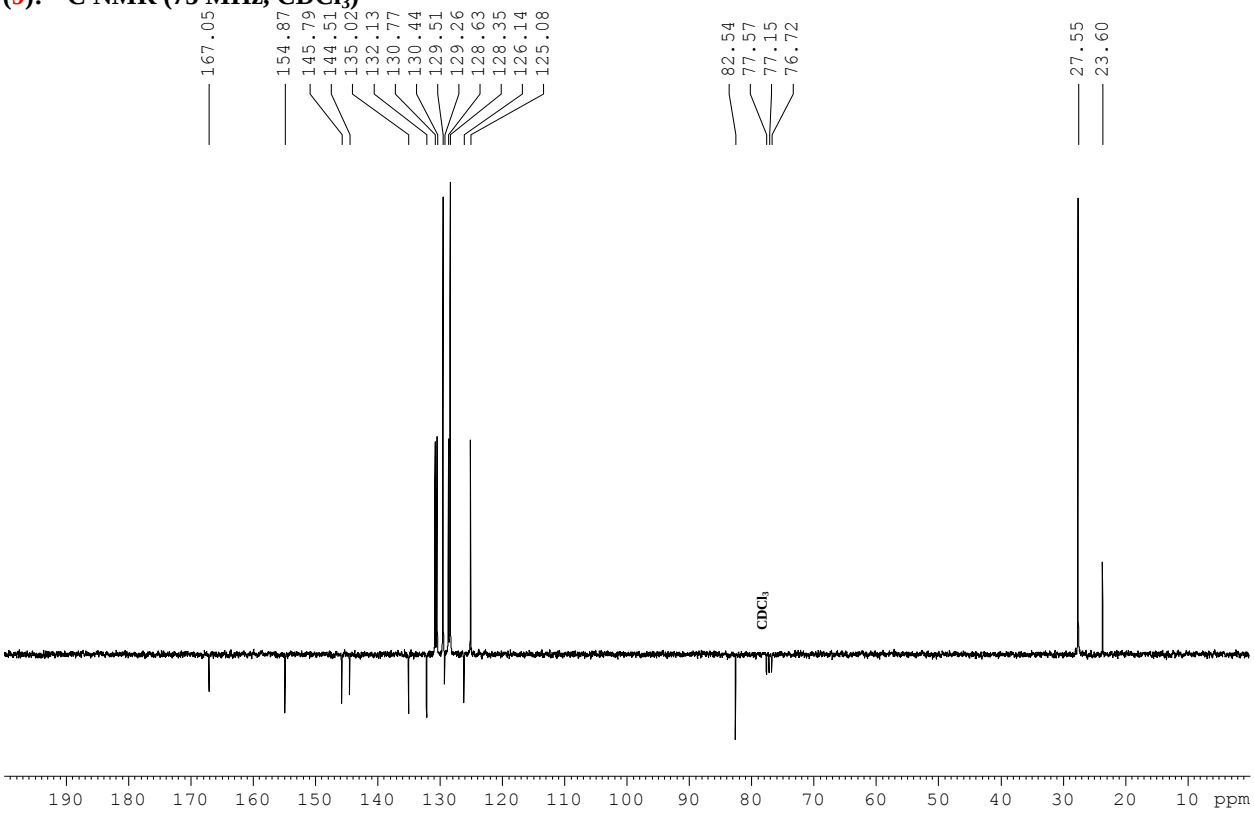
(8): ^{13}C NMR (75 MHz, $CDCl_3$)



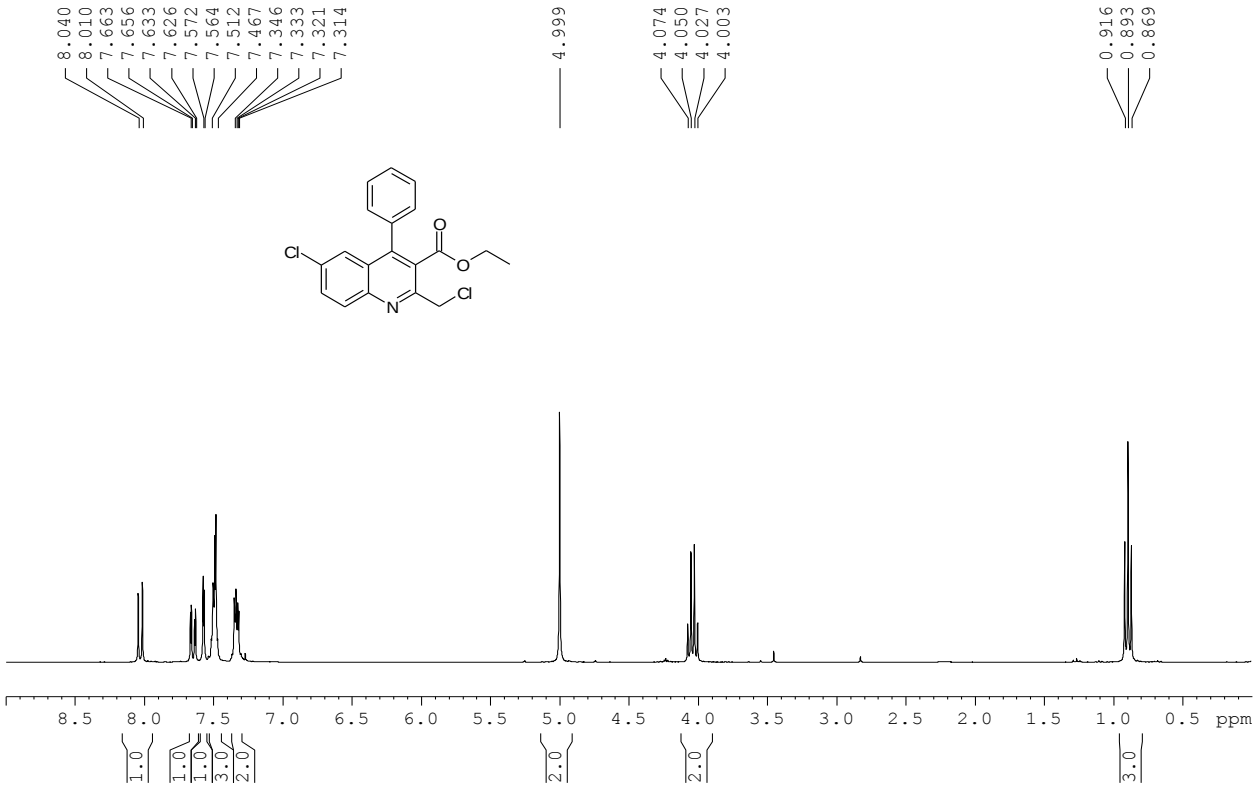
(9): ^{1}H NMR (300 MHz, $CDCl_3$)



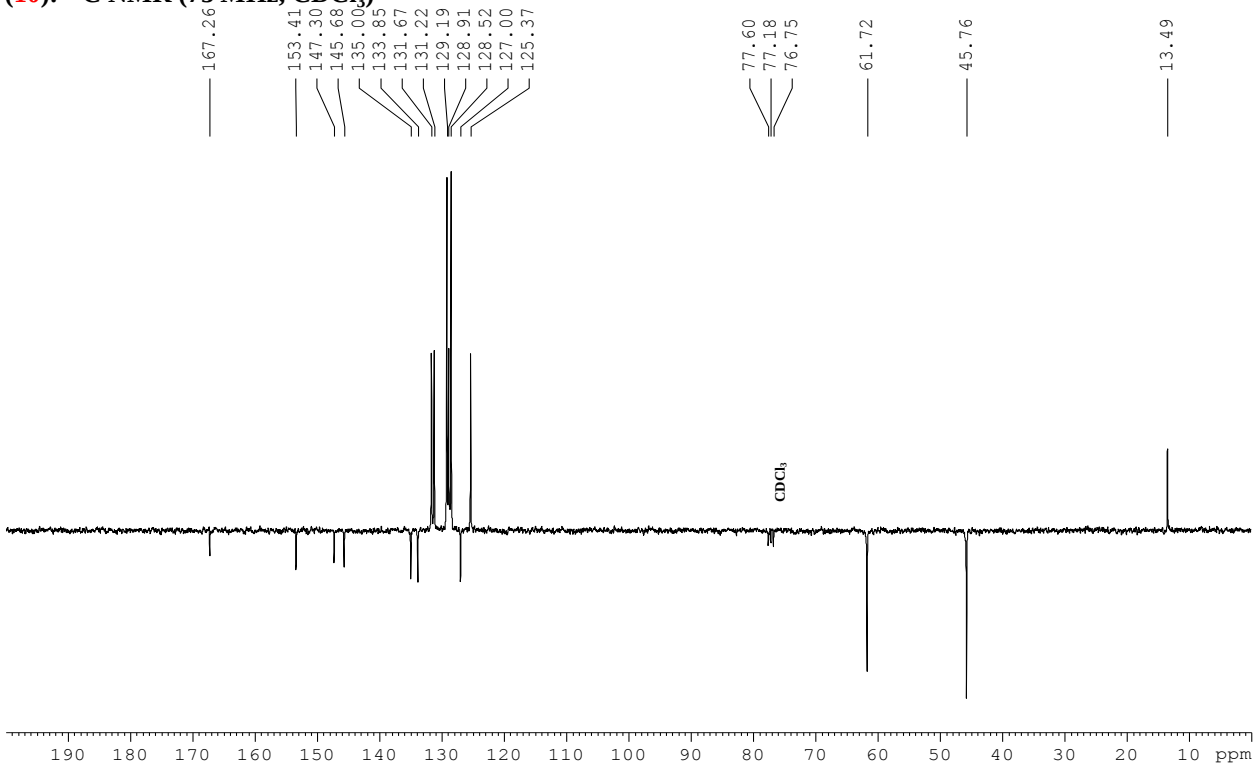
(9): ^{13}C NMR (75 MHz, $CDCl_3$)



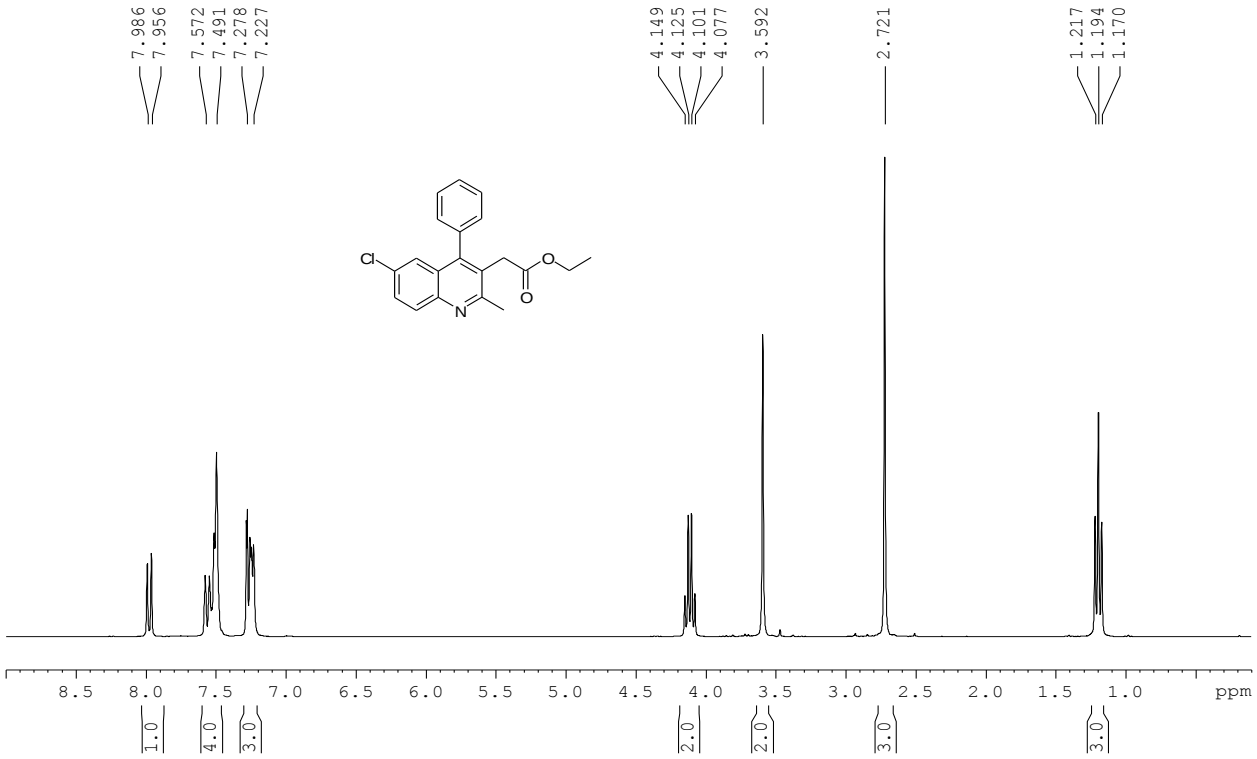
(10): ^{1}H NMR (300 MHz, $CDCl_3$)



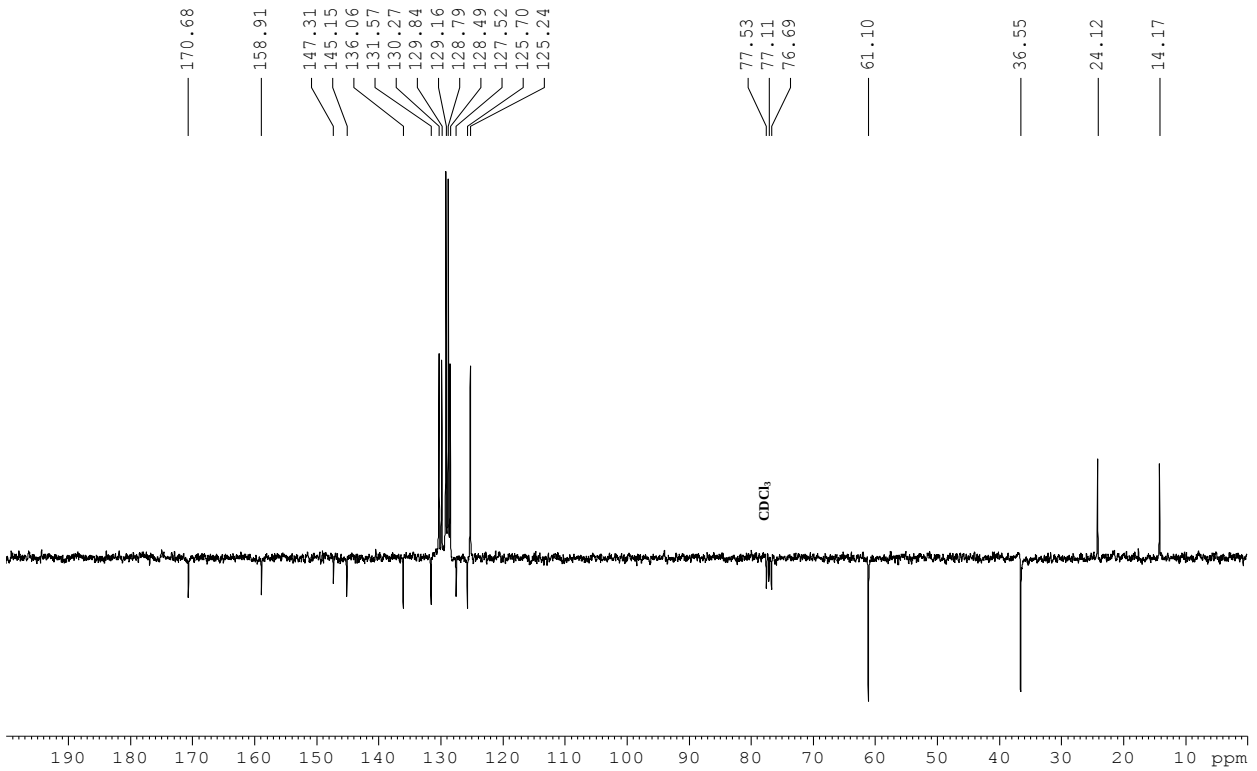
(10): ^{13}C NMR (75 MHz, $CDCl_3$)



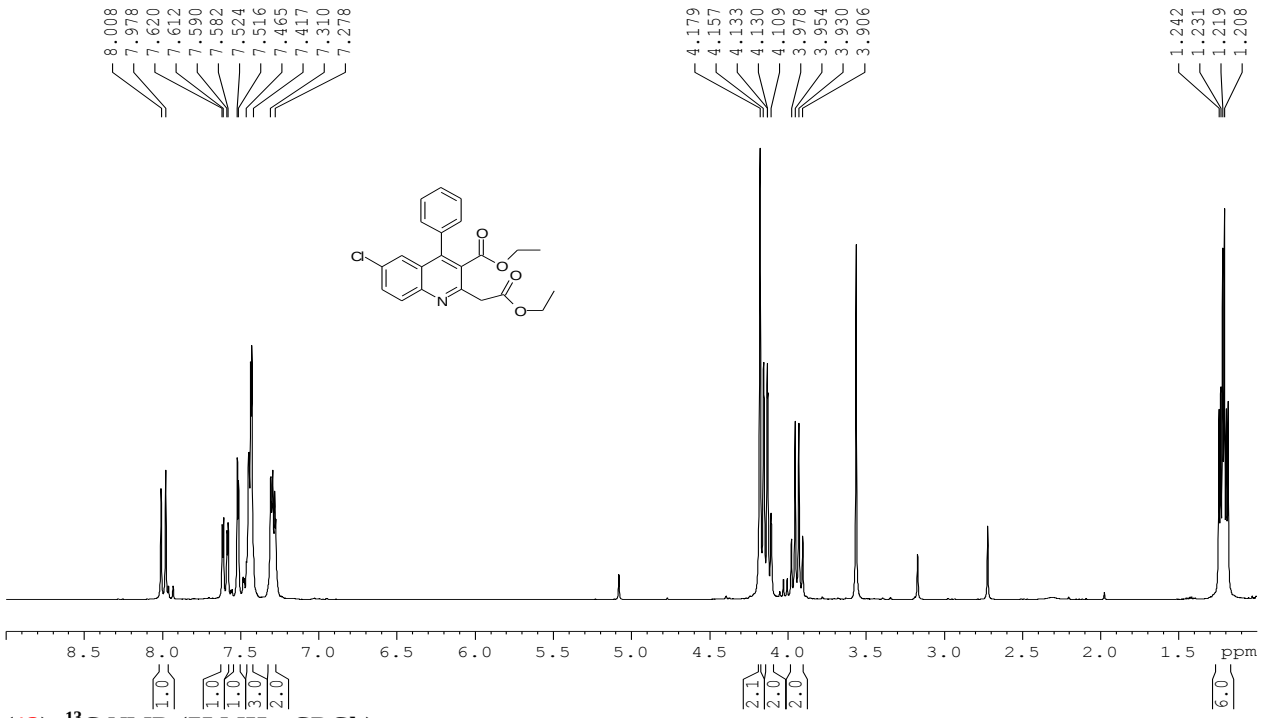
(11): ^{1}H NMR (300 MHz, $CDCl_3$)



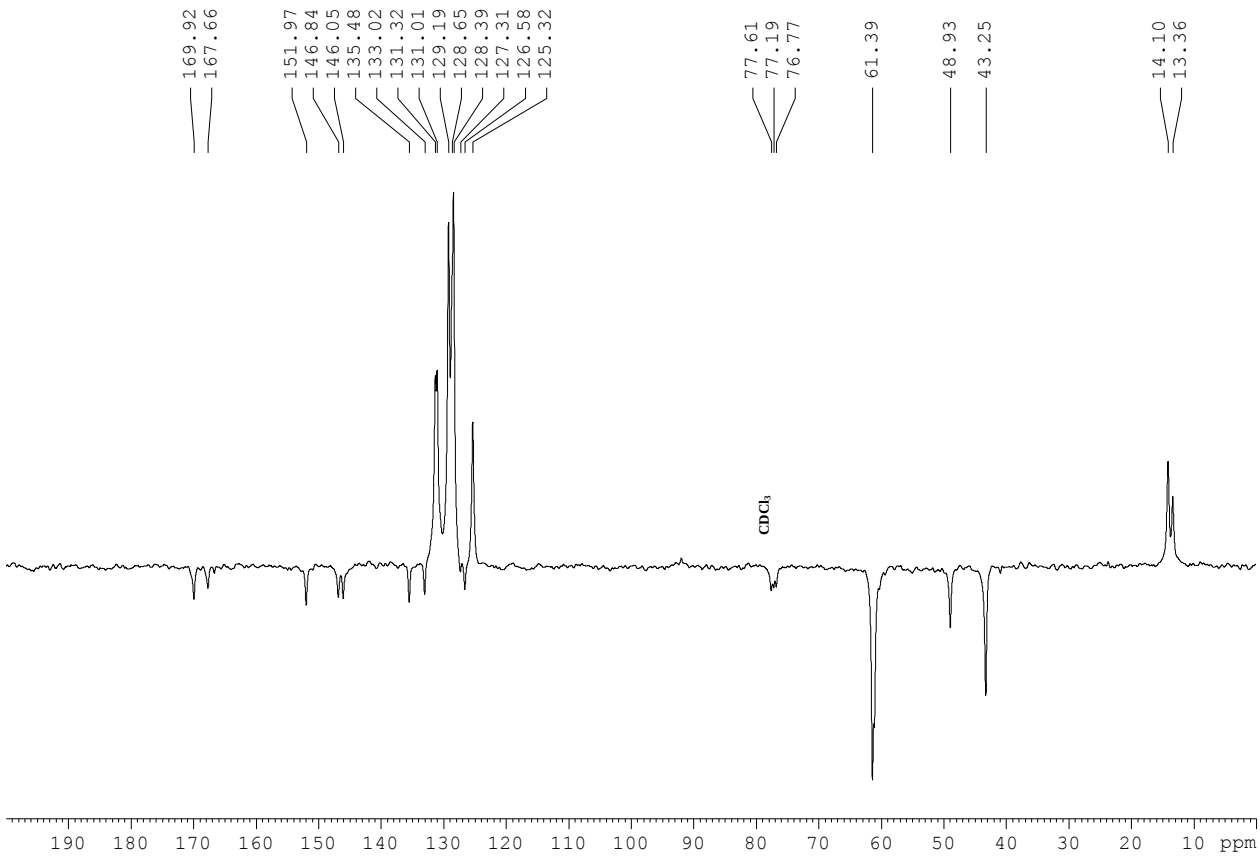
(11): ^{13}C NMR (75 MHz, $CDCl_3$)



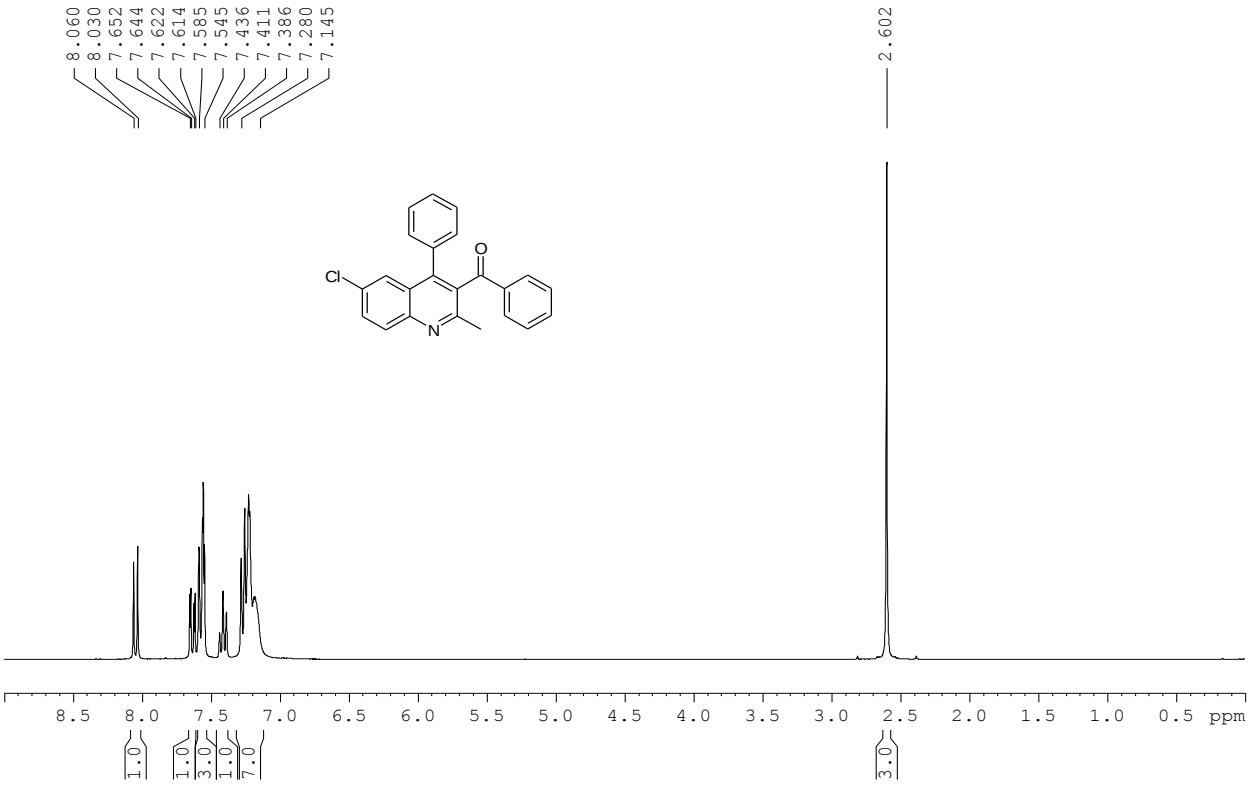
(12): ^{1}H NMR (300 MHz, $CDCl_3$)



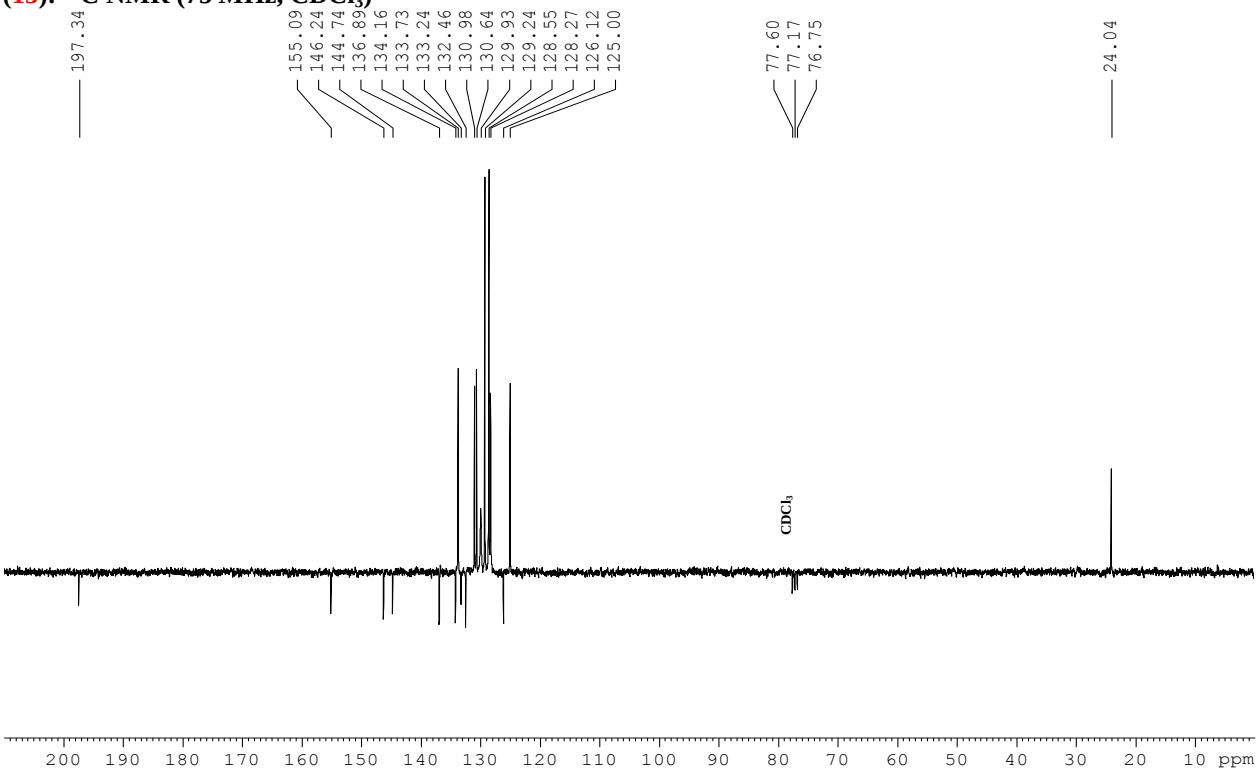
(12): ^{13}C NMR (75 MHz, $CDCl_3$)



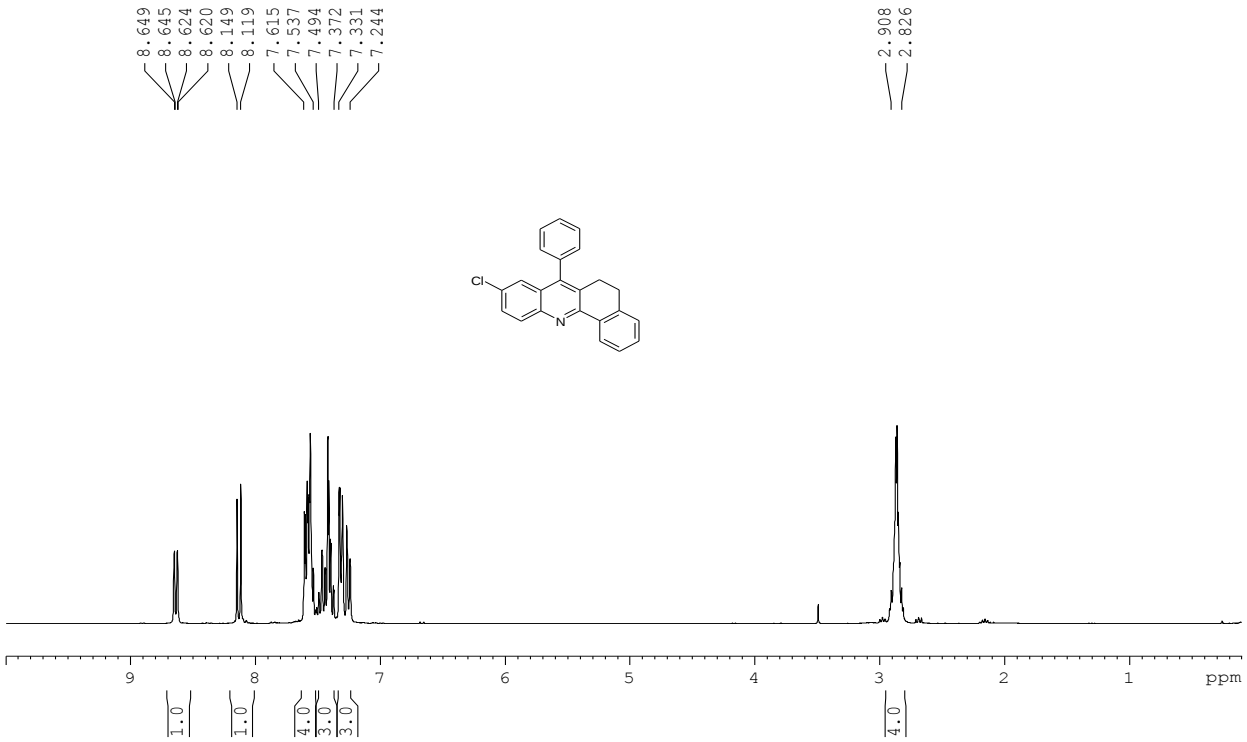
(13): ^{1}H NMR (300 MHz, $CDCl_3$)



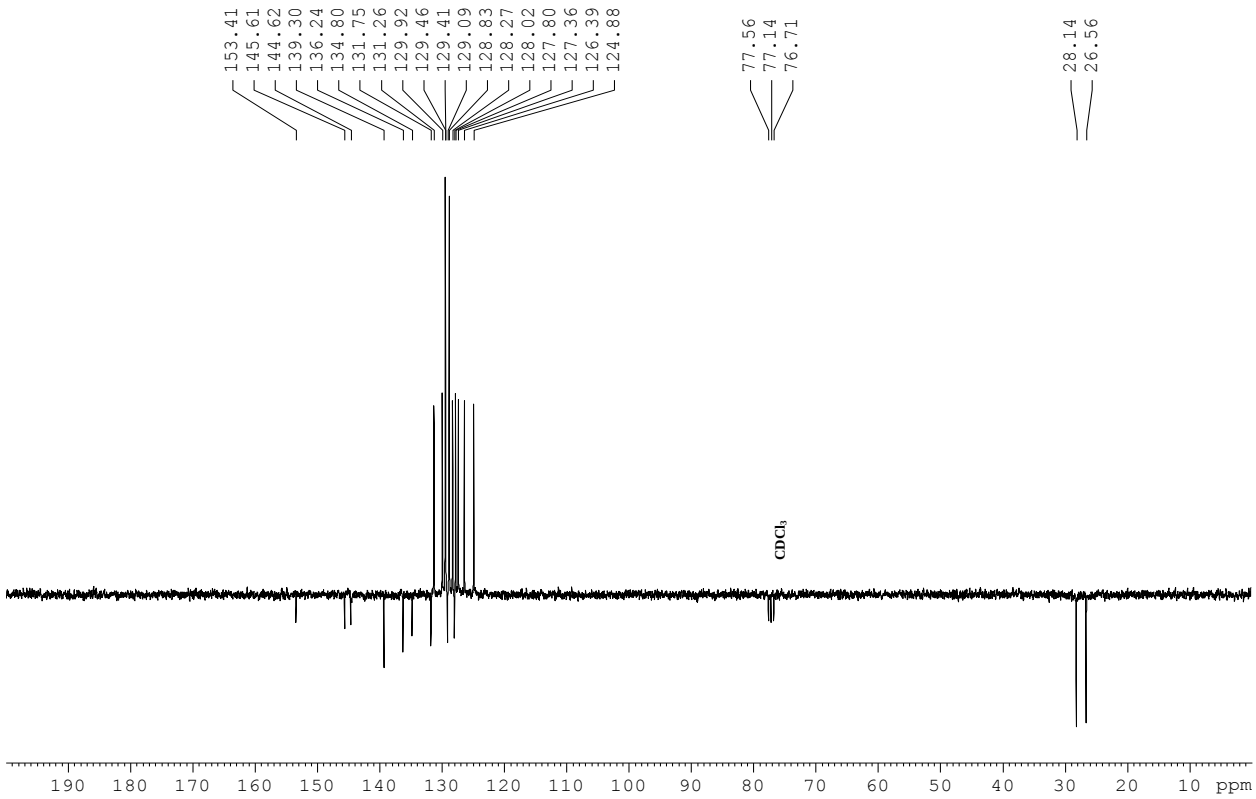
(13): ^{13}C NMR (75 MHz, $CDCl_3$)



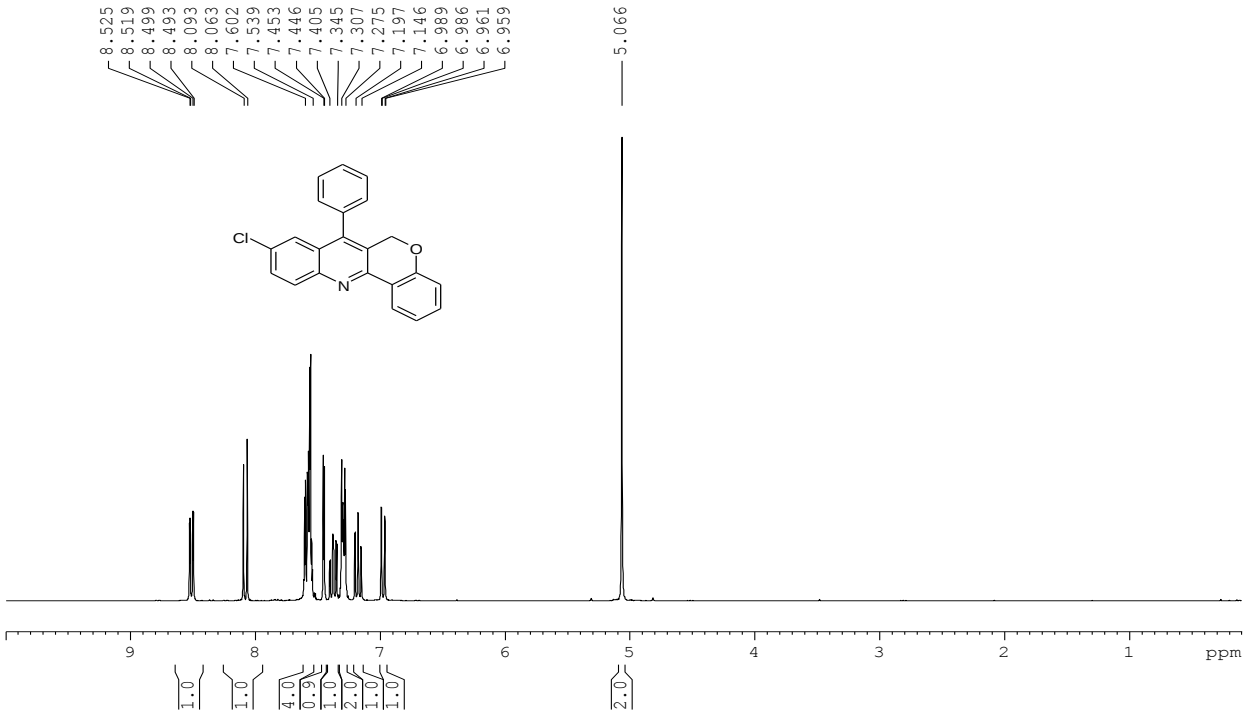
(14): ^{1}H NMR (300 MHz, $CDCl_3$)



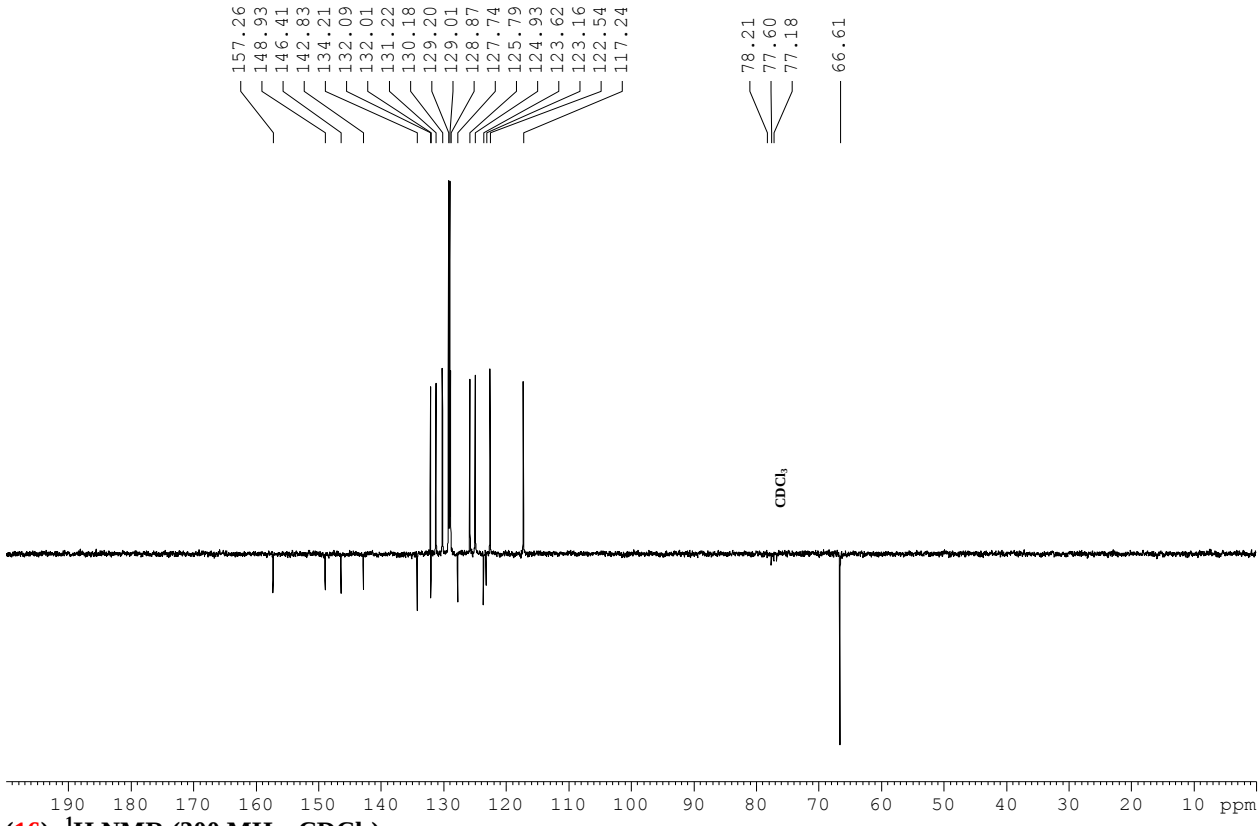
(14): ^{13}C NMR (75 MHz, $CDCl_3$)



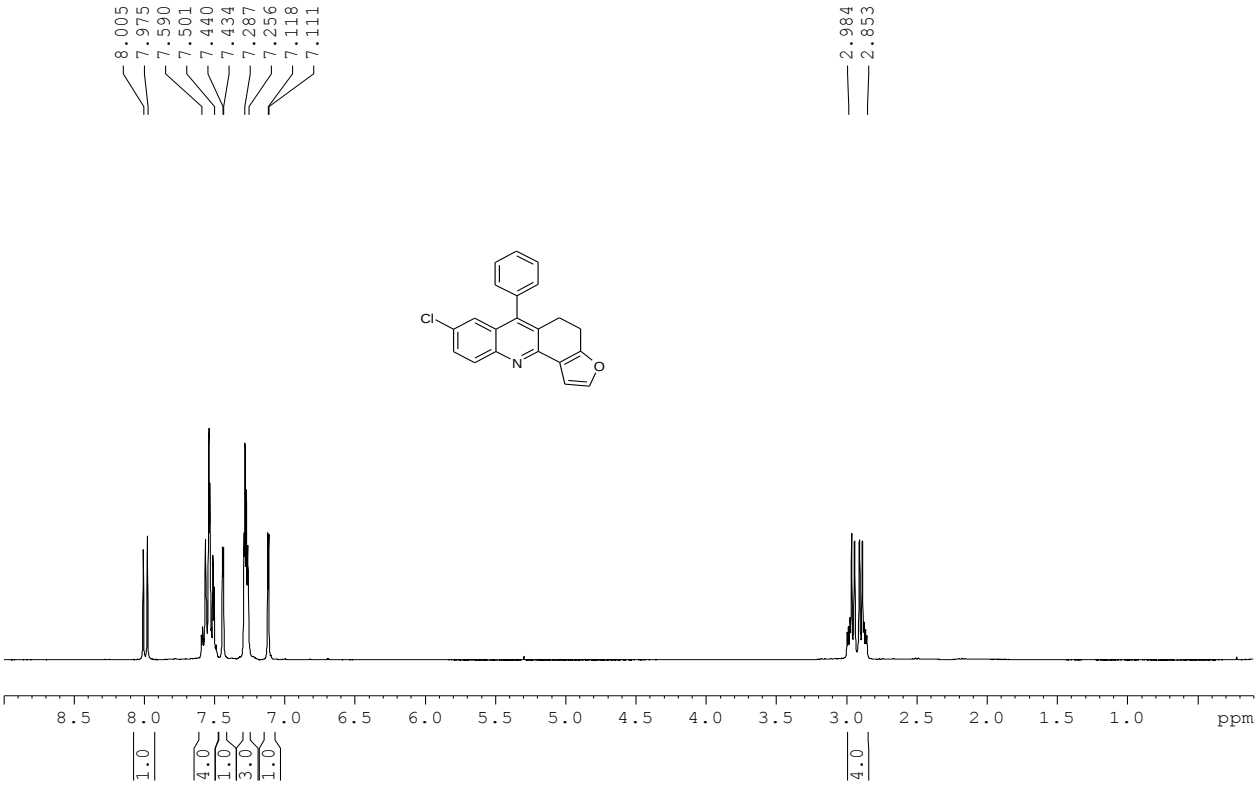
(15): ^{1}H NMR (300 MHz, $CDCl_3$)



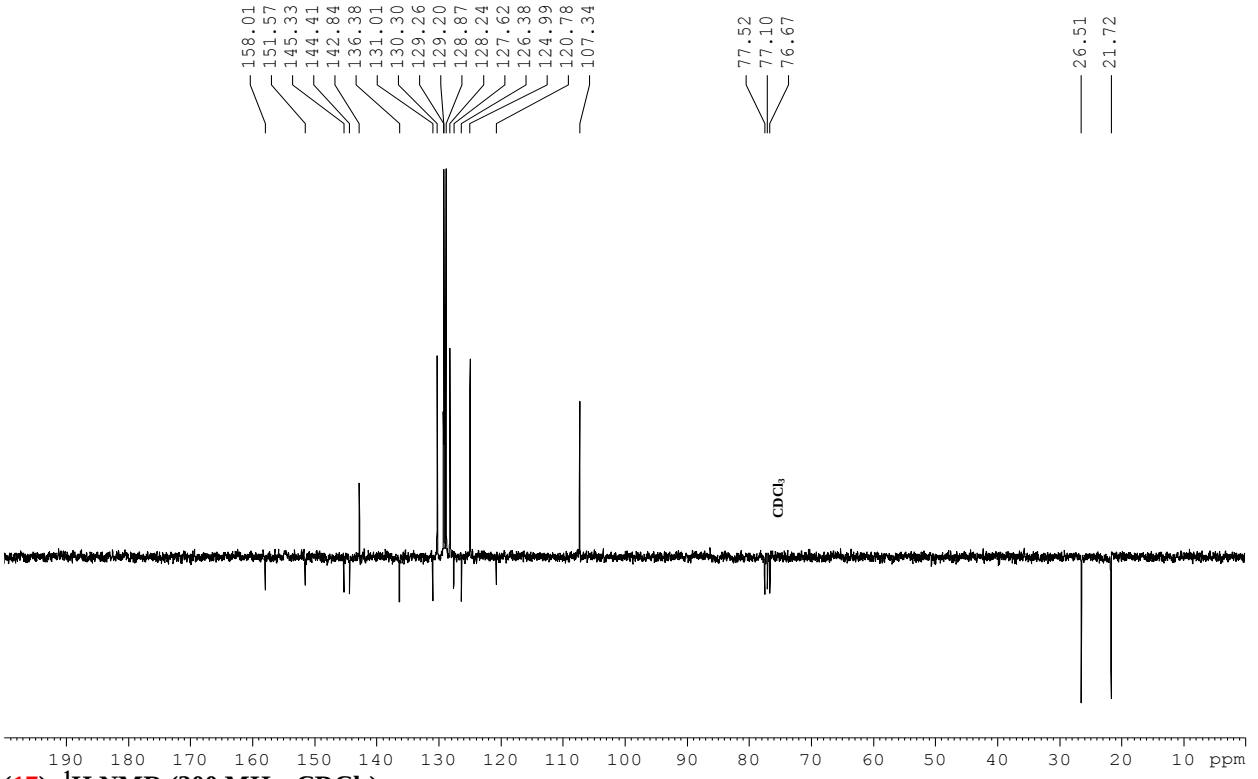
(15): ^{13}C NMR (75 MHz, $CDCl_3$)



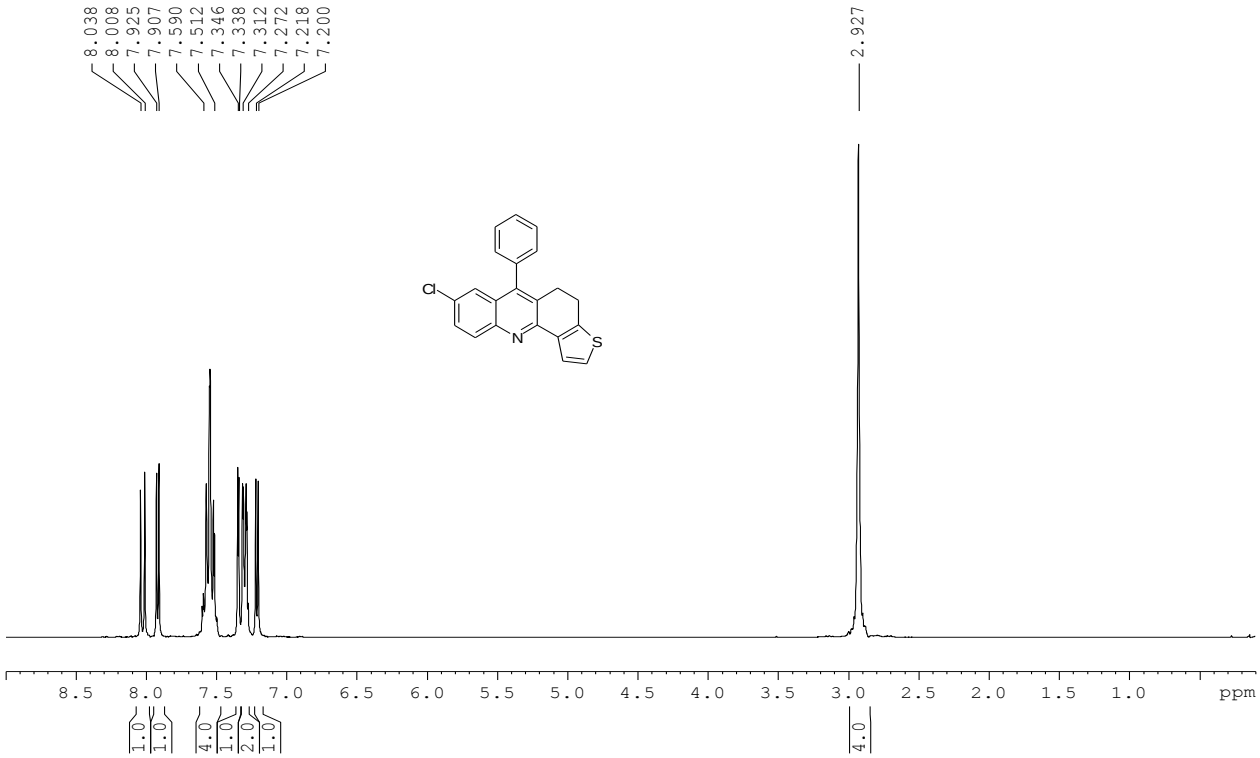
(16): ^{1}H NMR (300 MHz, $CDCl_3$)



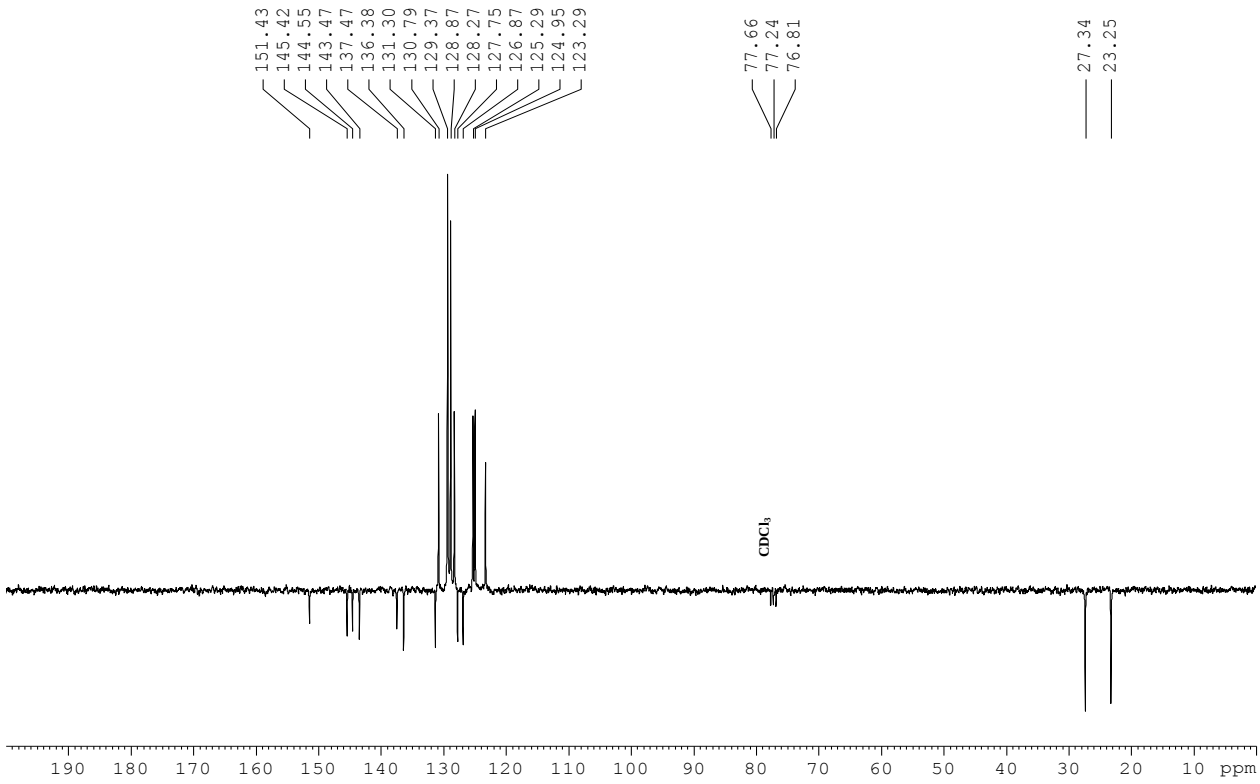
(16): ^{13}C NMR (75 MHz, $CDCl_3$)



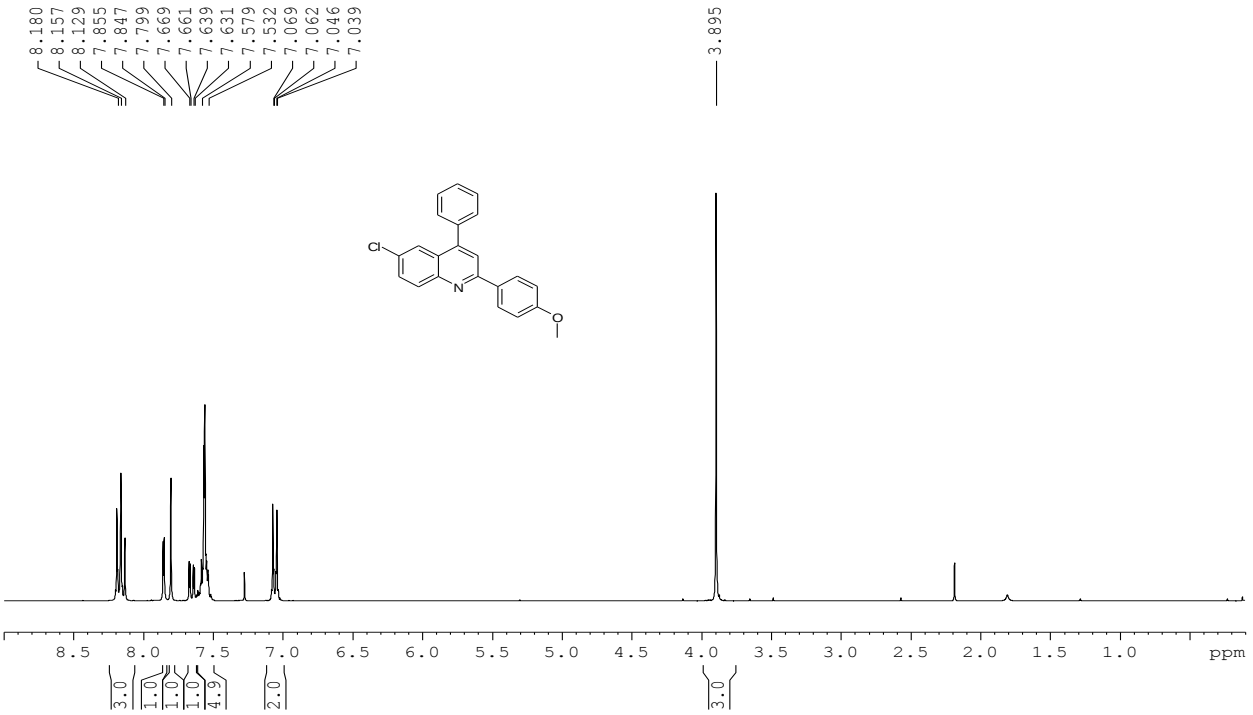
(17): ^{1}H NMR (300 MHz, $CDCl_3$)



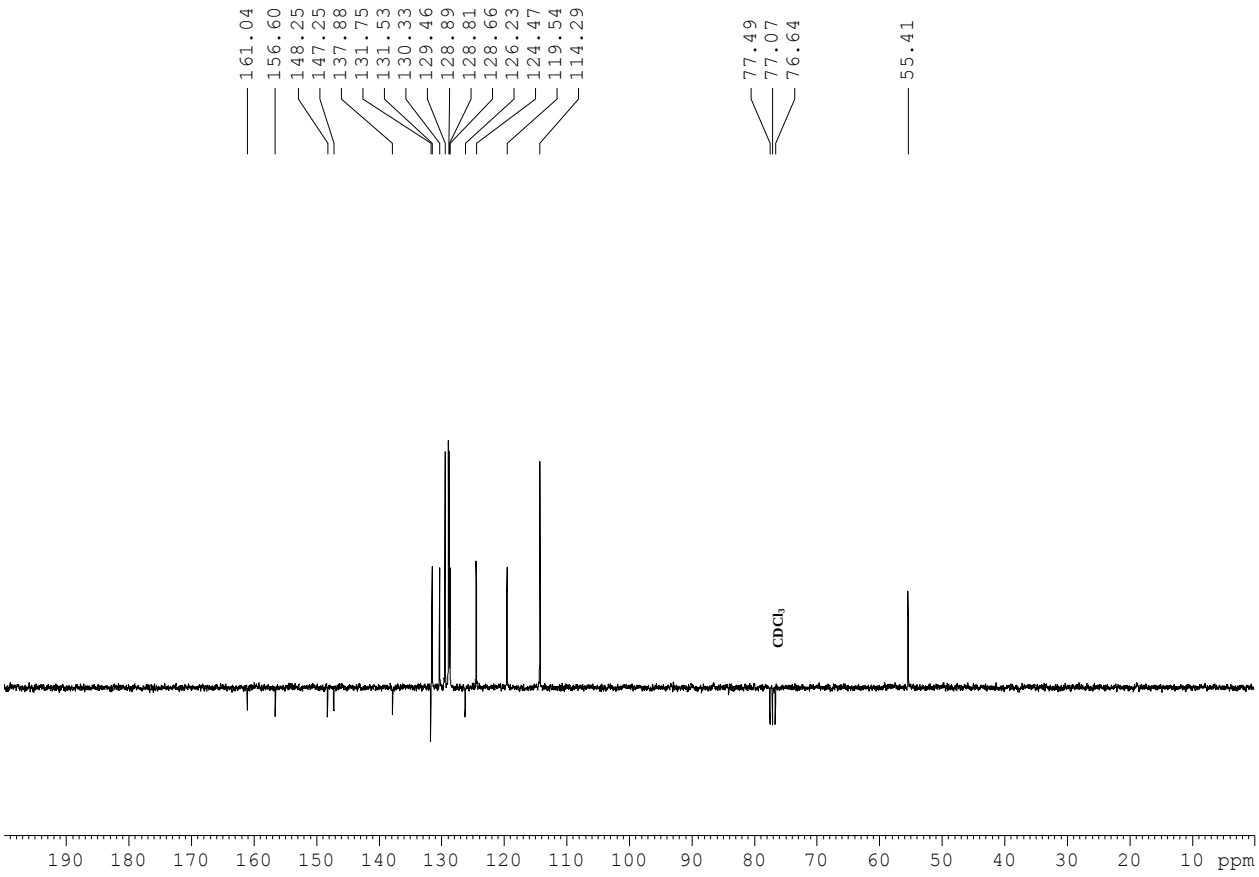
(17): ^{13}C NMR (75 MHz, $CDCl_3$)



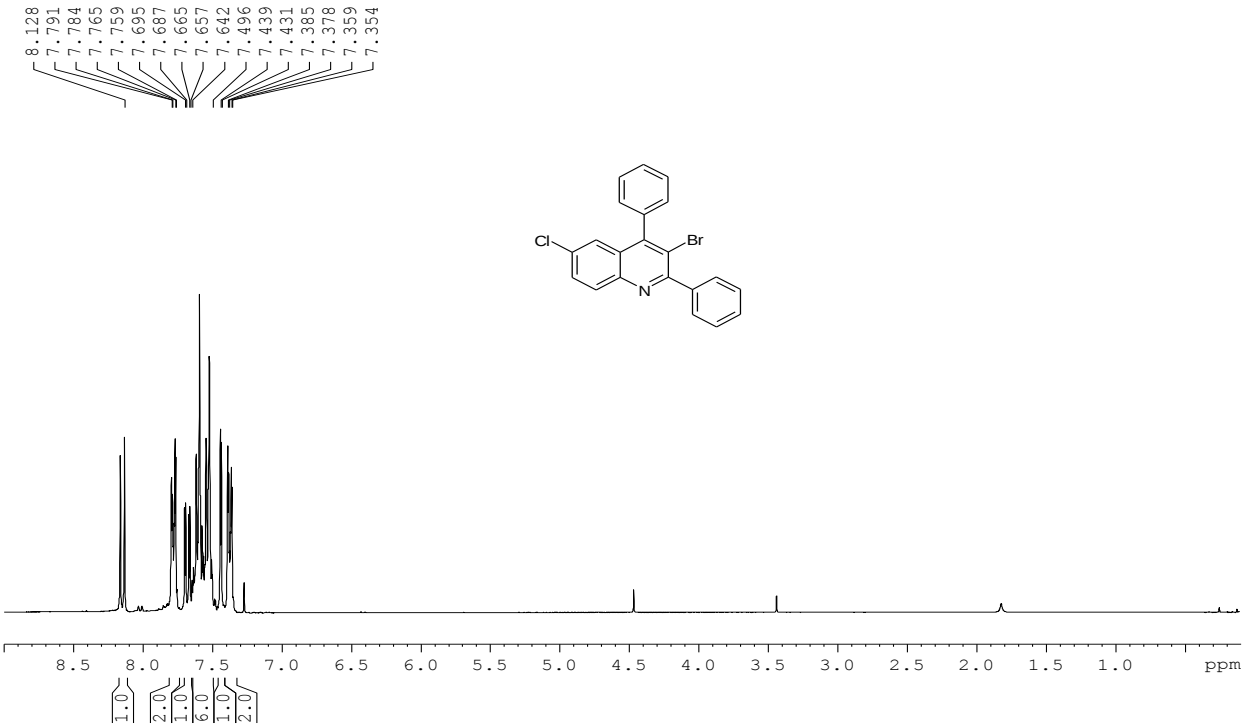
(18): ^{1}H NMR (300 MHz, $CDCl_3$)



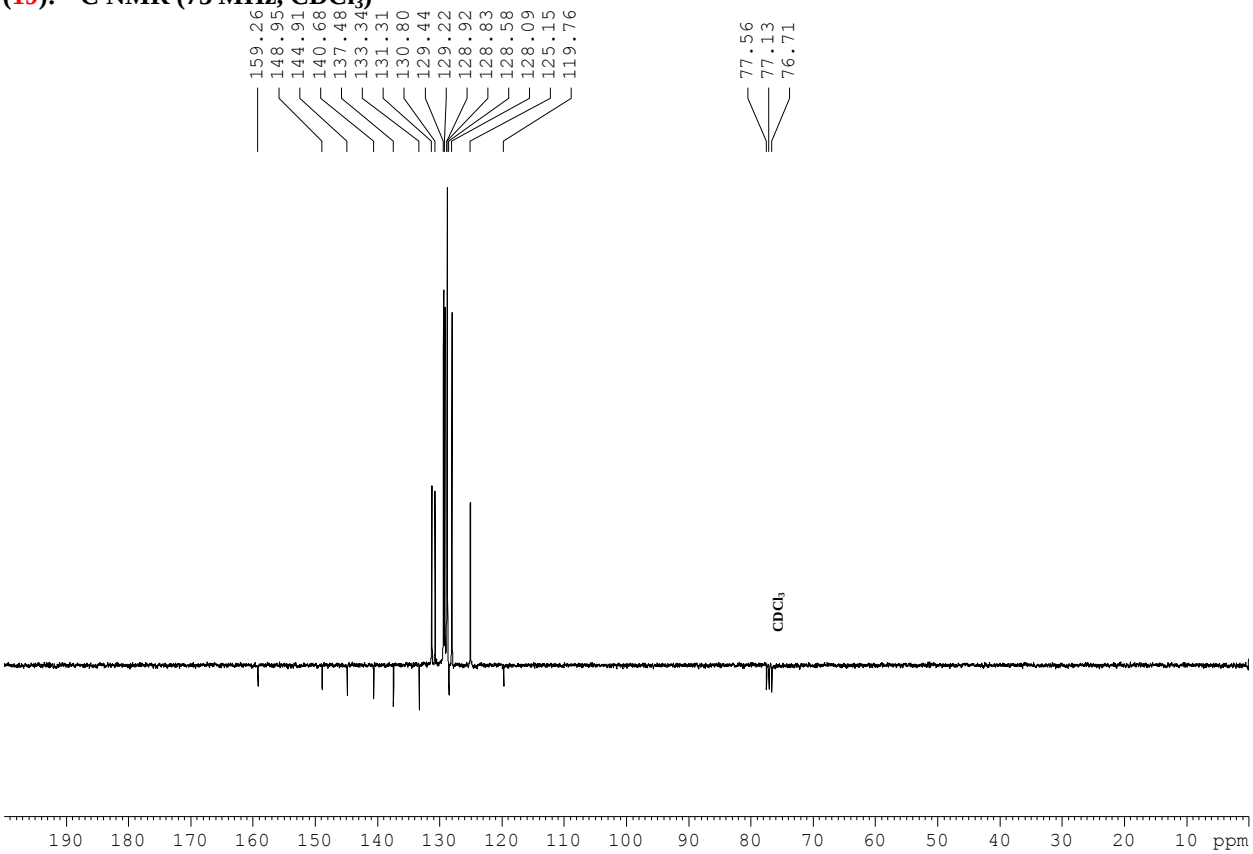
(18): ^{13}C NMR (75 MHz, $CDCl_3$)



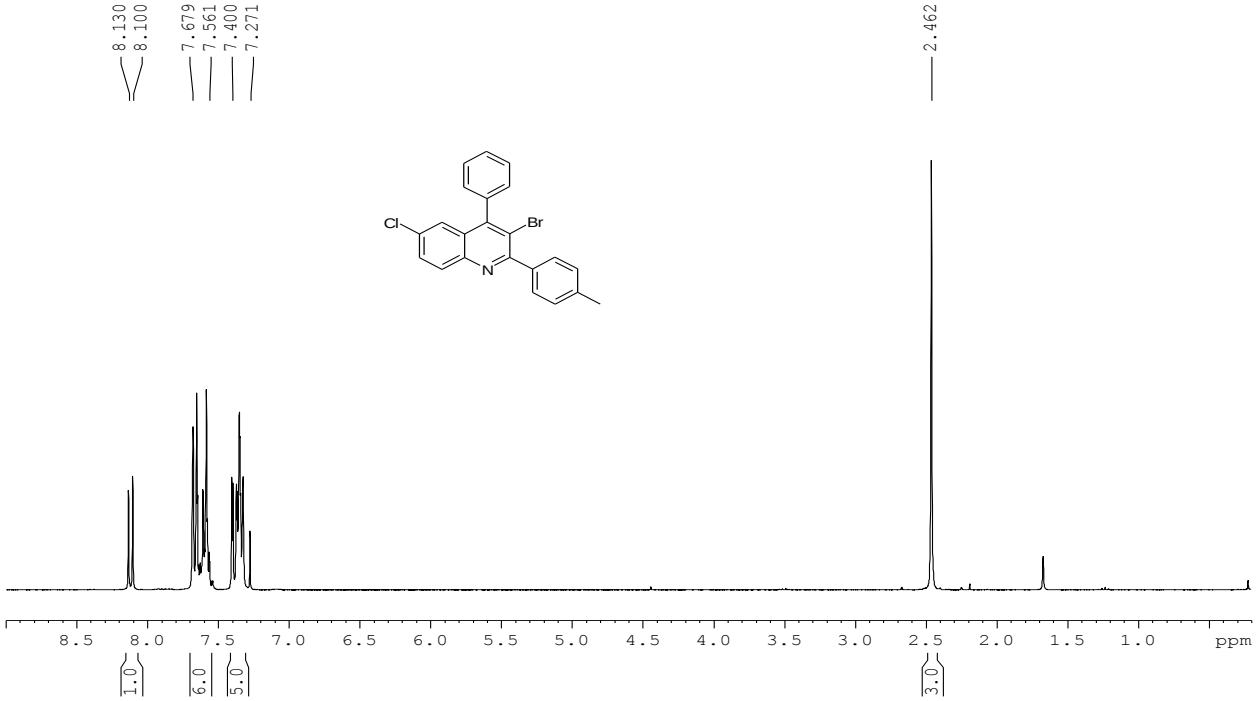
(19): ^{1}H NMR (300 MHz, $CDCl_3$)



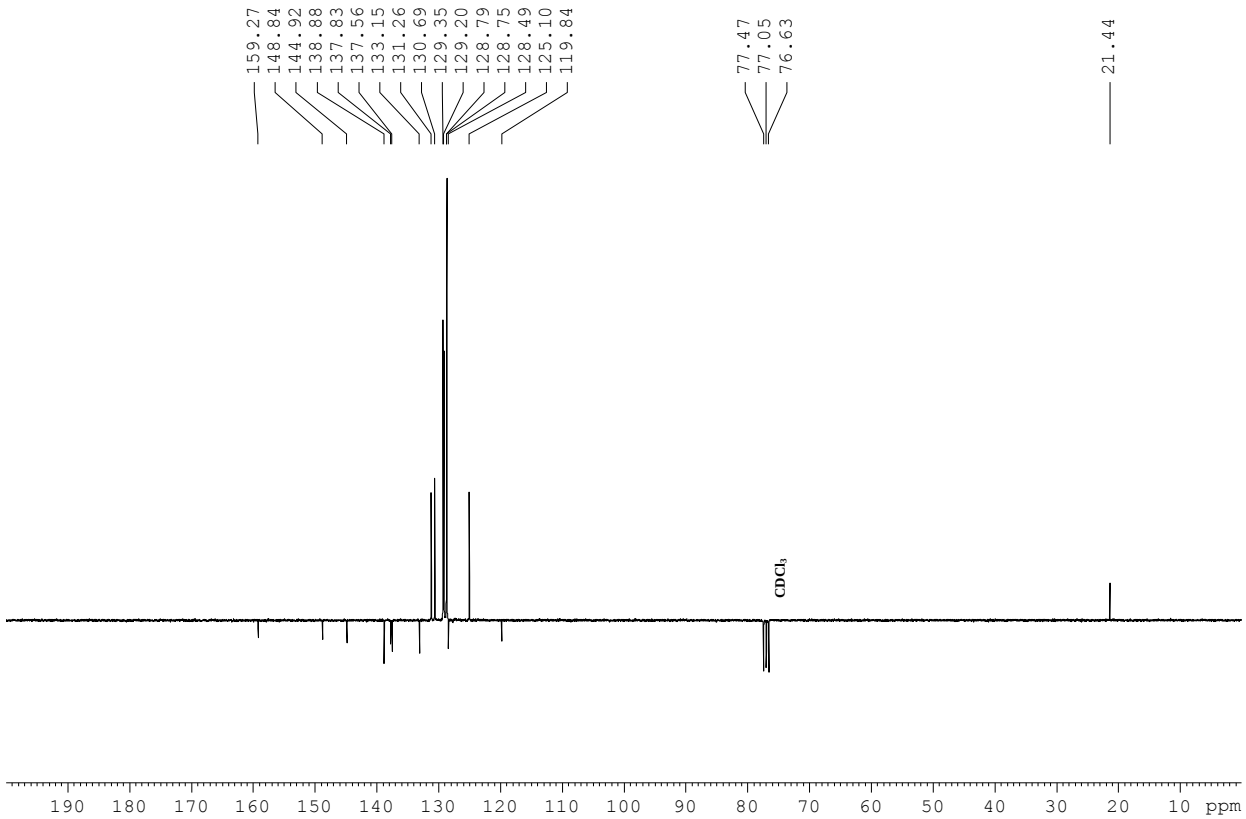
(19): ^{13}C NMR (75 MHz, $CDCl_3$)



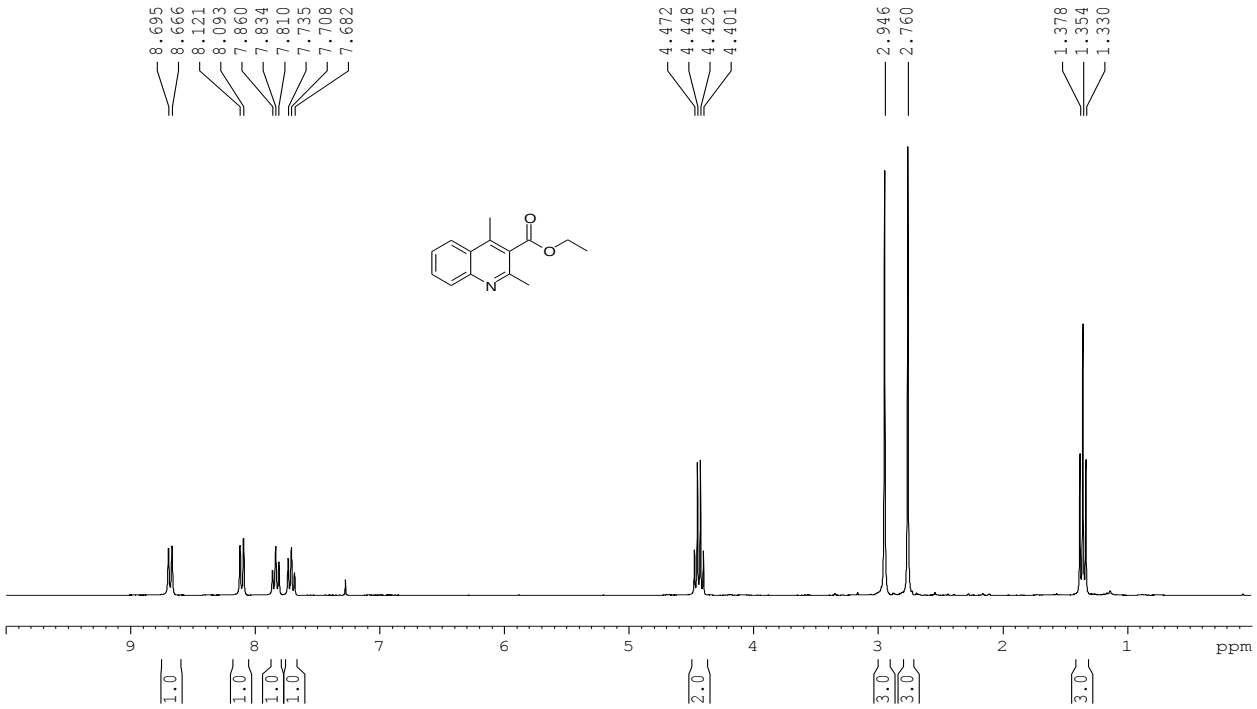
(20): ^{1}H NMR (300 MHz, $CDCl_3$)



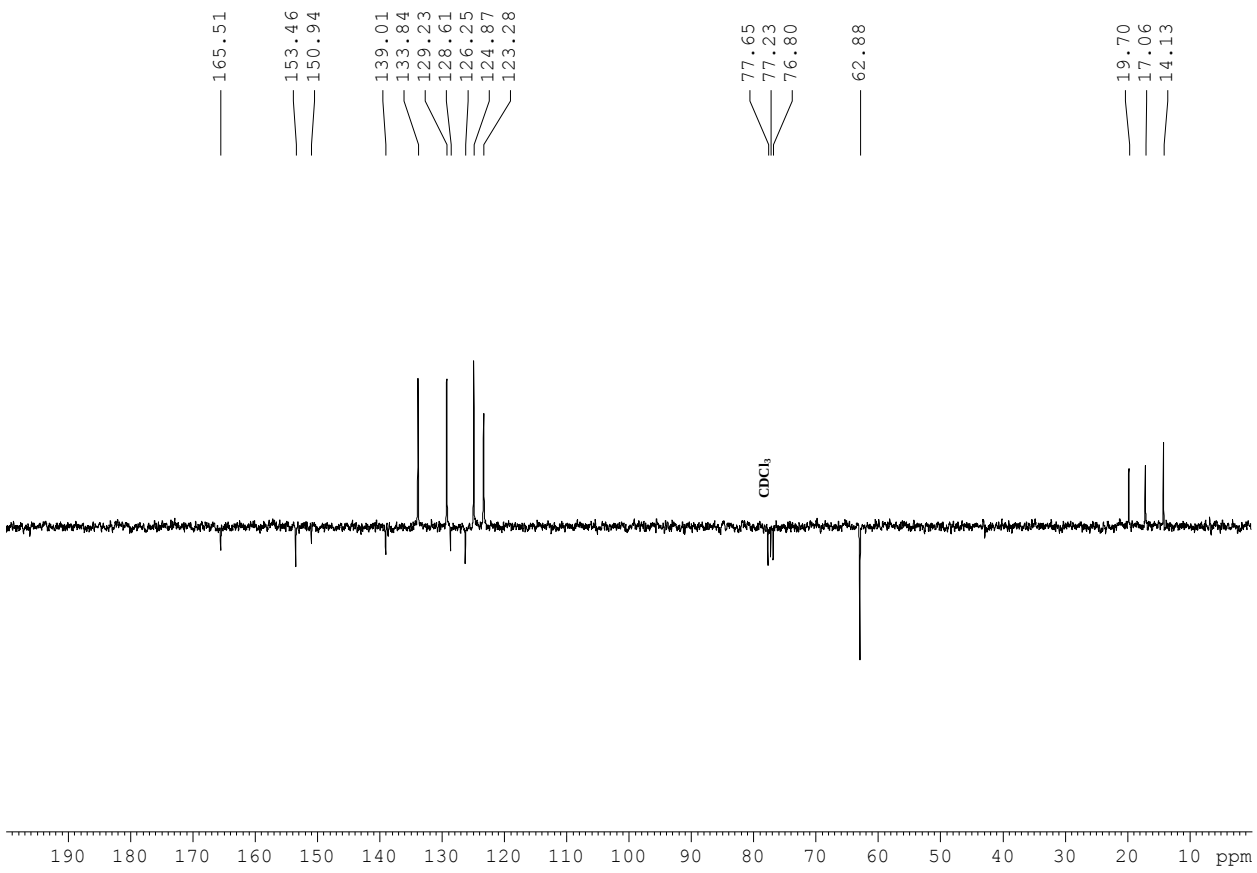
(20): ^{13}C NMR (75 MHz, $CDCl_3$)



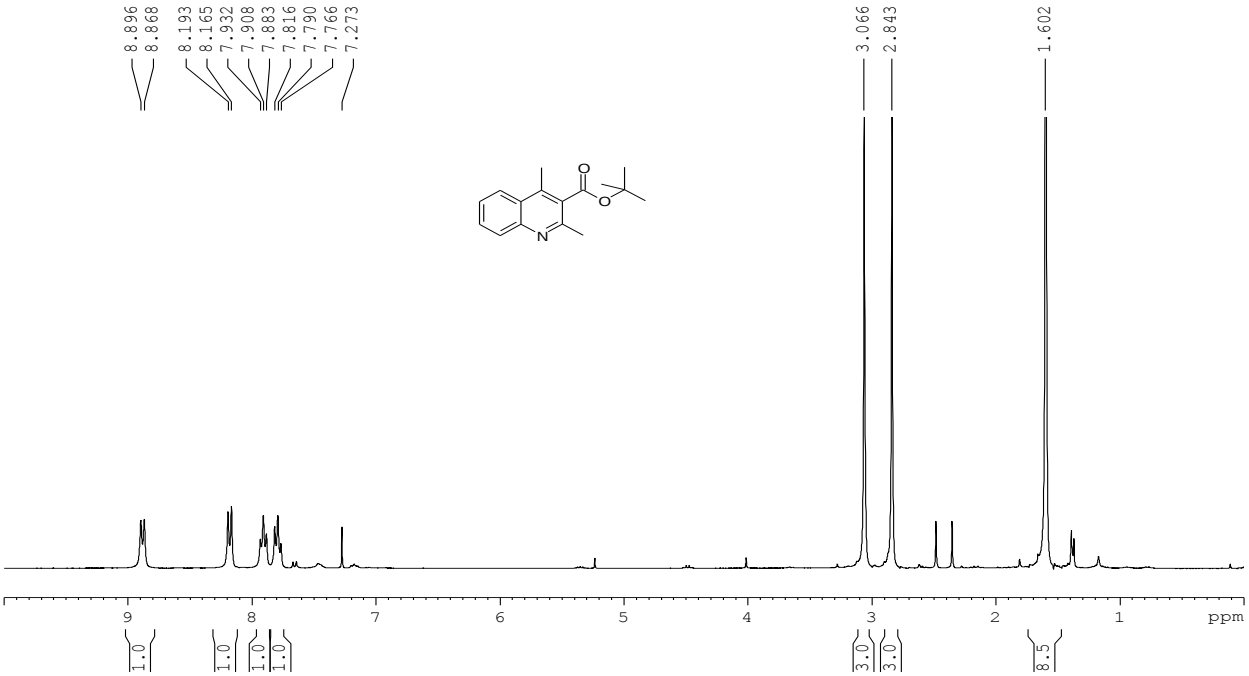
(21): ^{1}H NMR (300 MHz, $CDCl_3$)



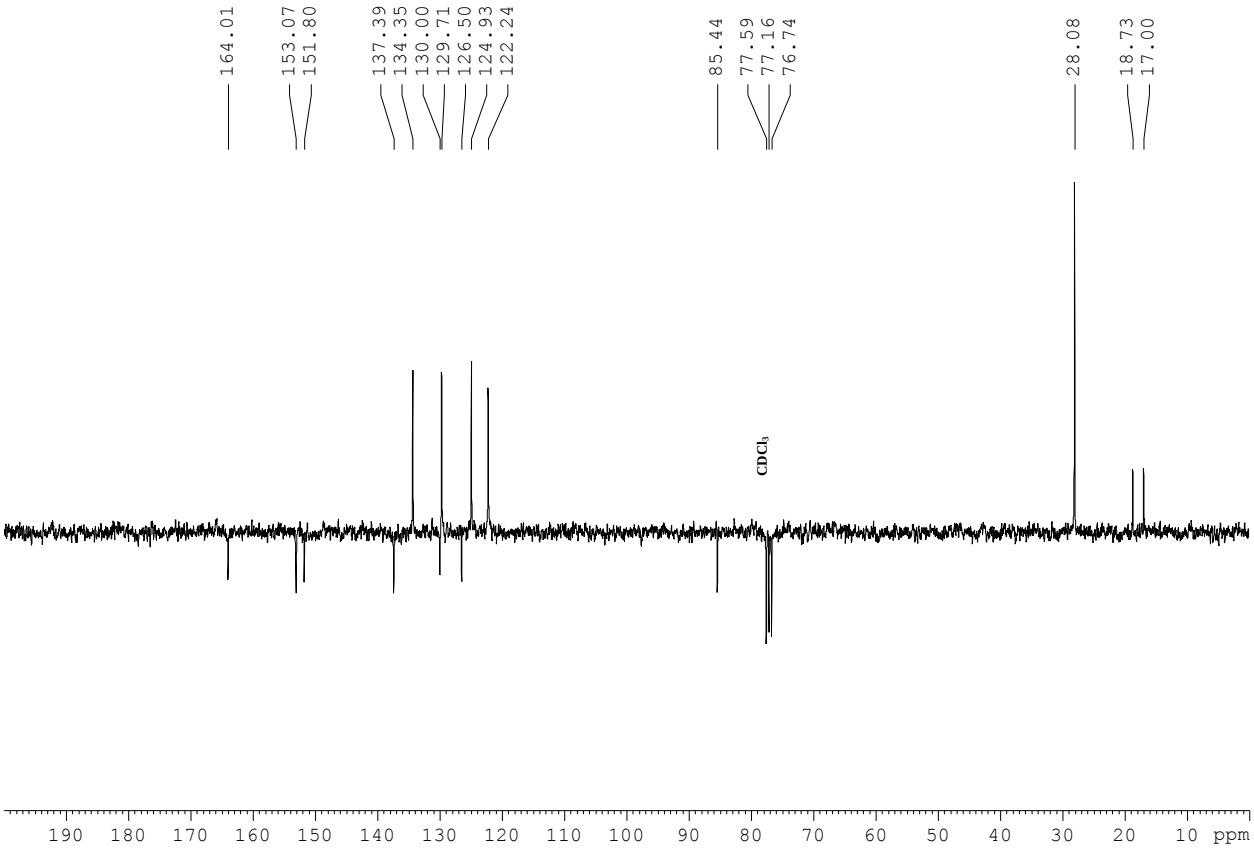
(21): ^{13}C NMR (75 MHz, $CDCl_3$)



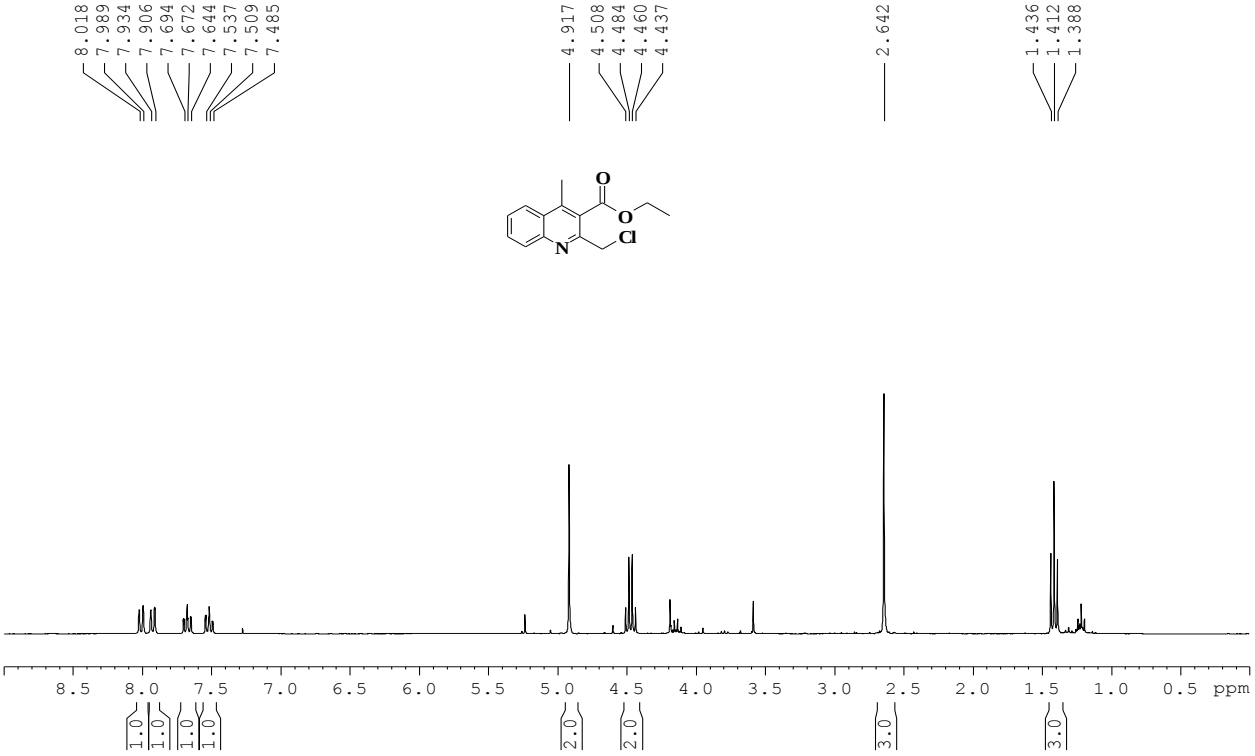
(22): ^{1}H NMR (300 MHz, $CDCl_3$)



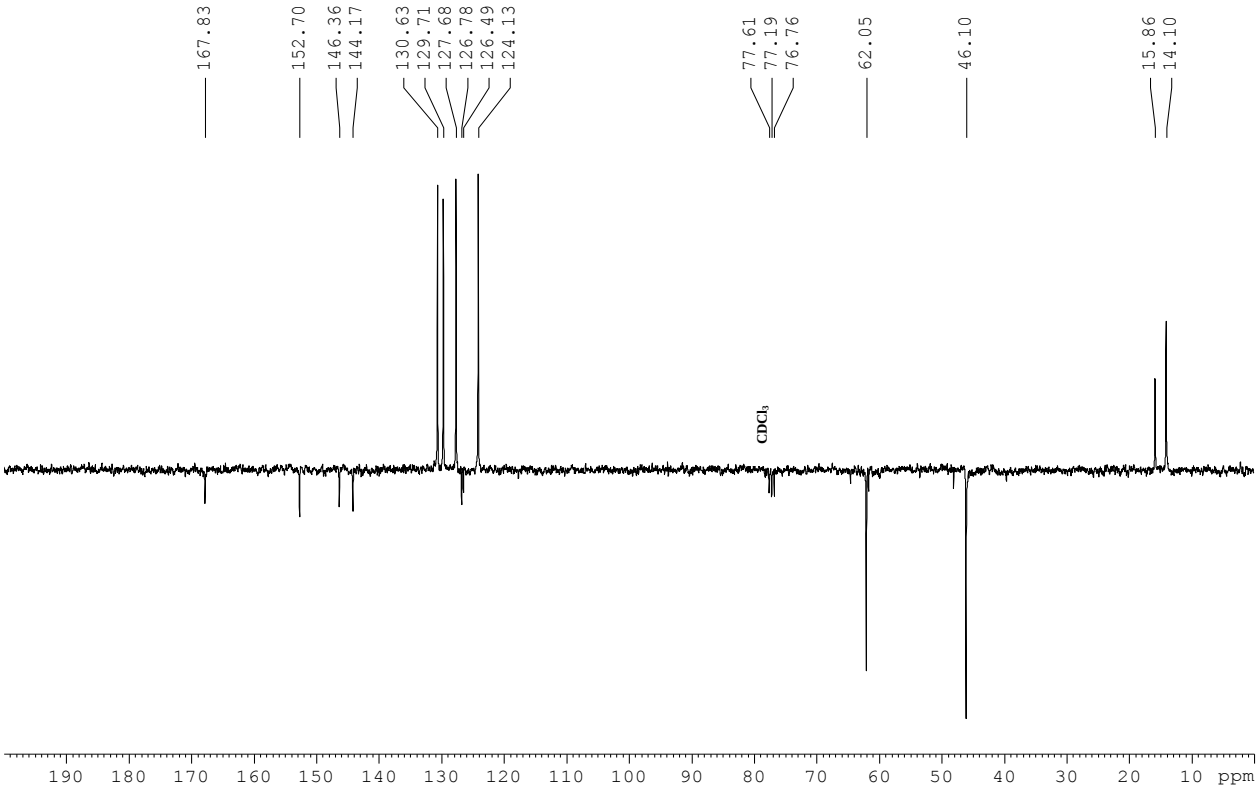
(22): ^{13}C NMR (75 MHz, $CDCl_3$)



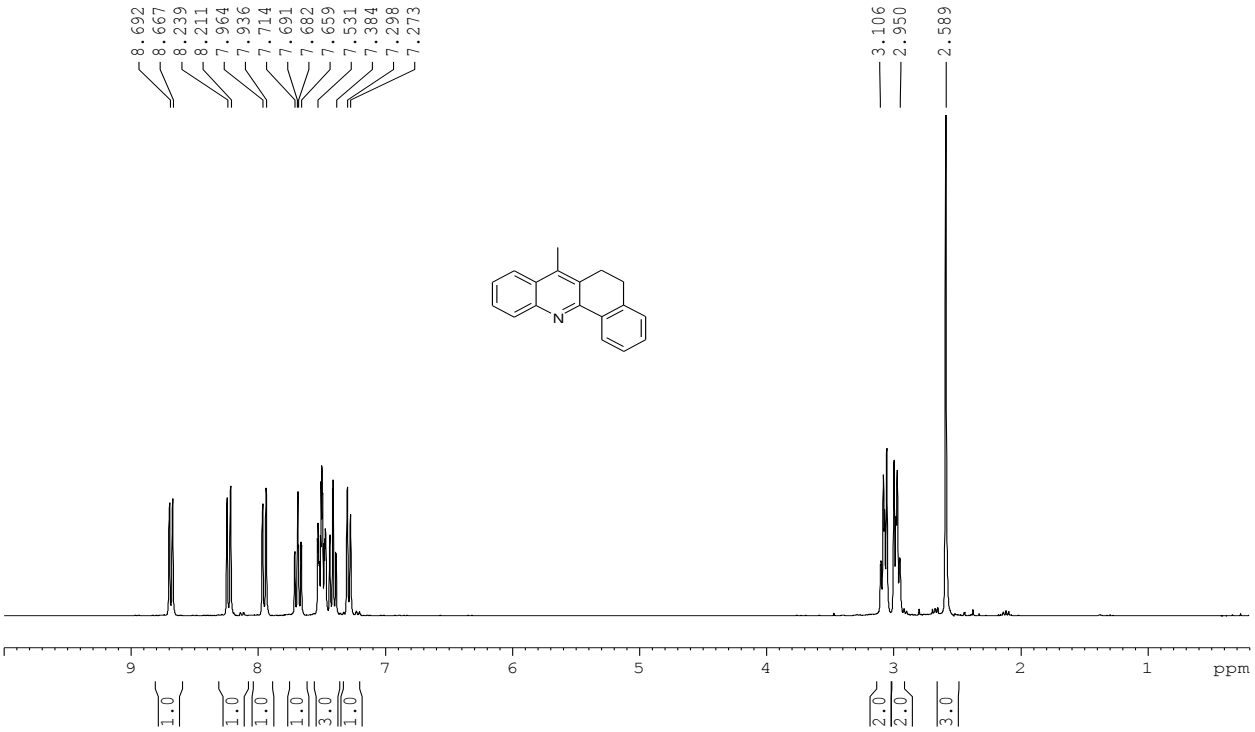
(23): ^{1}H NMR (300 MHz, $CDCl_3$)



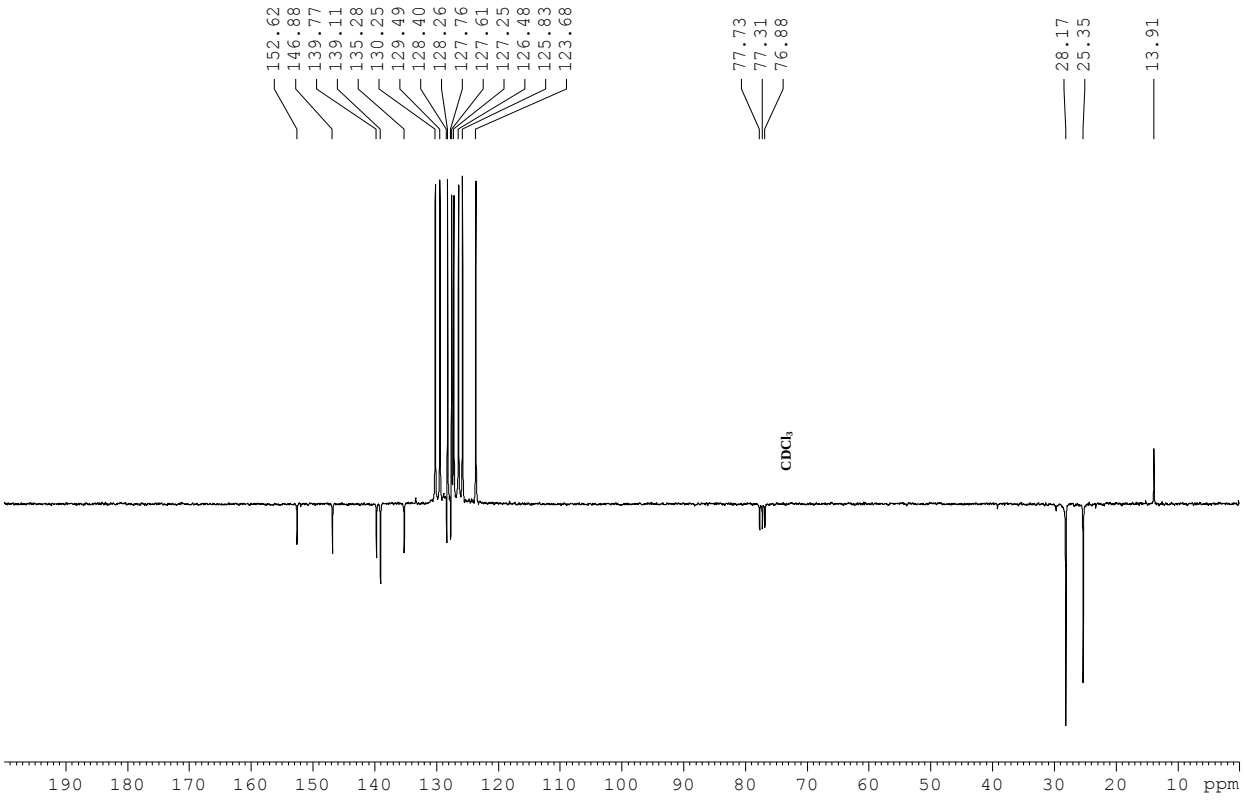
(23): ^{13}C NMR (75 MHz, $CDCl_3$)



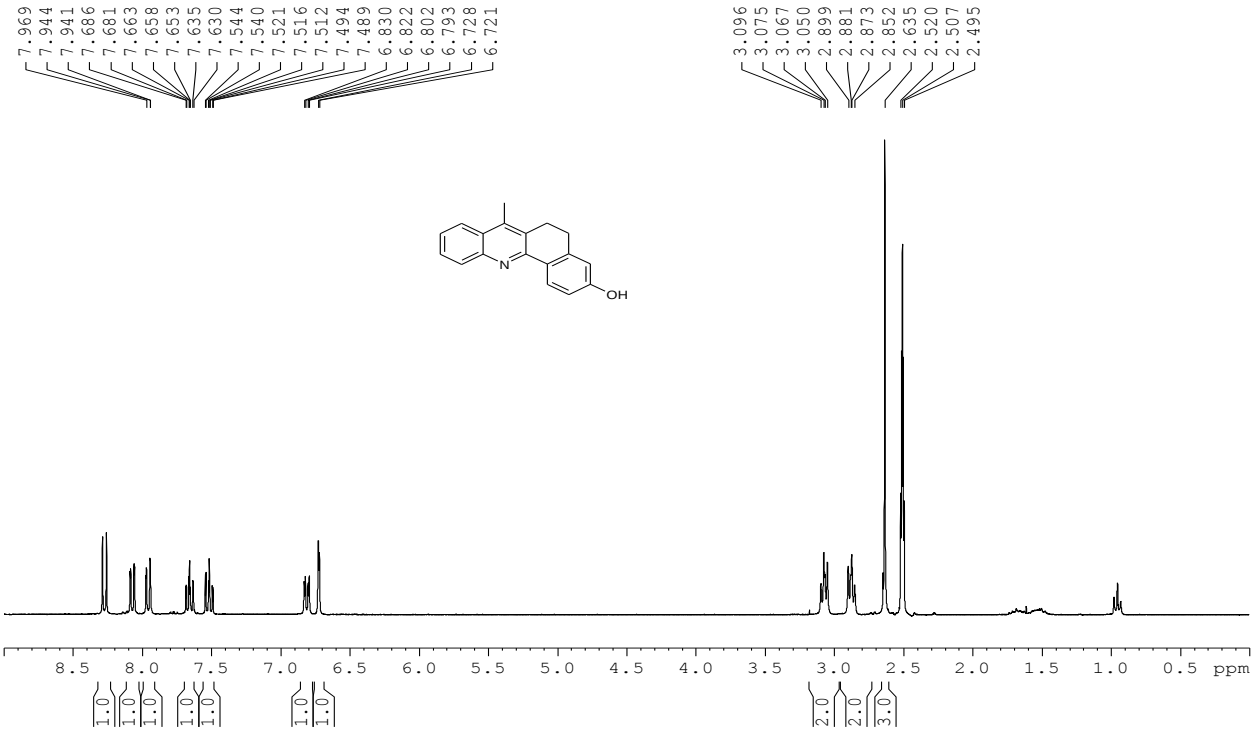
(24): ^{1}H NMR (300 MHz, $CDCl_3$)



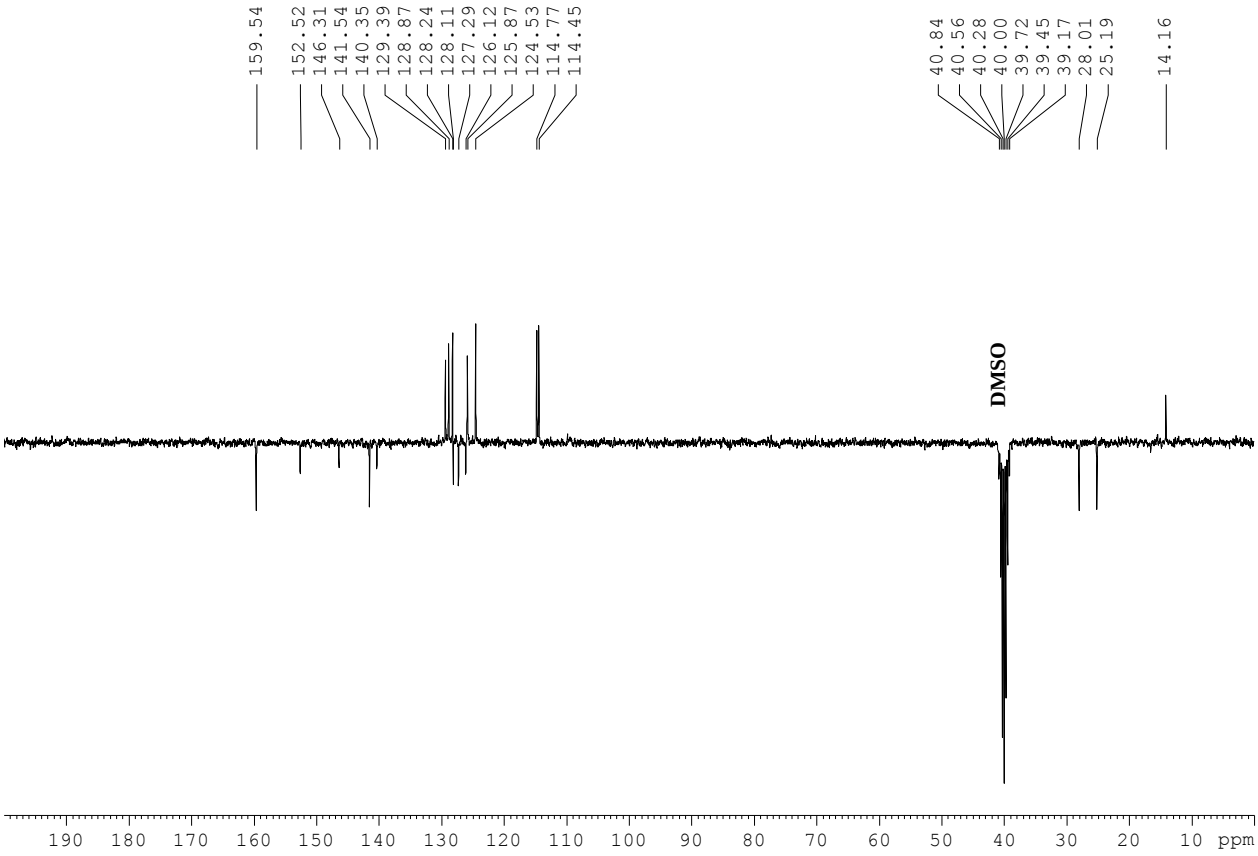
(24): ^{13}C NMR (75 MHz, $CDCl_3$)



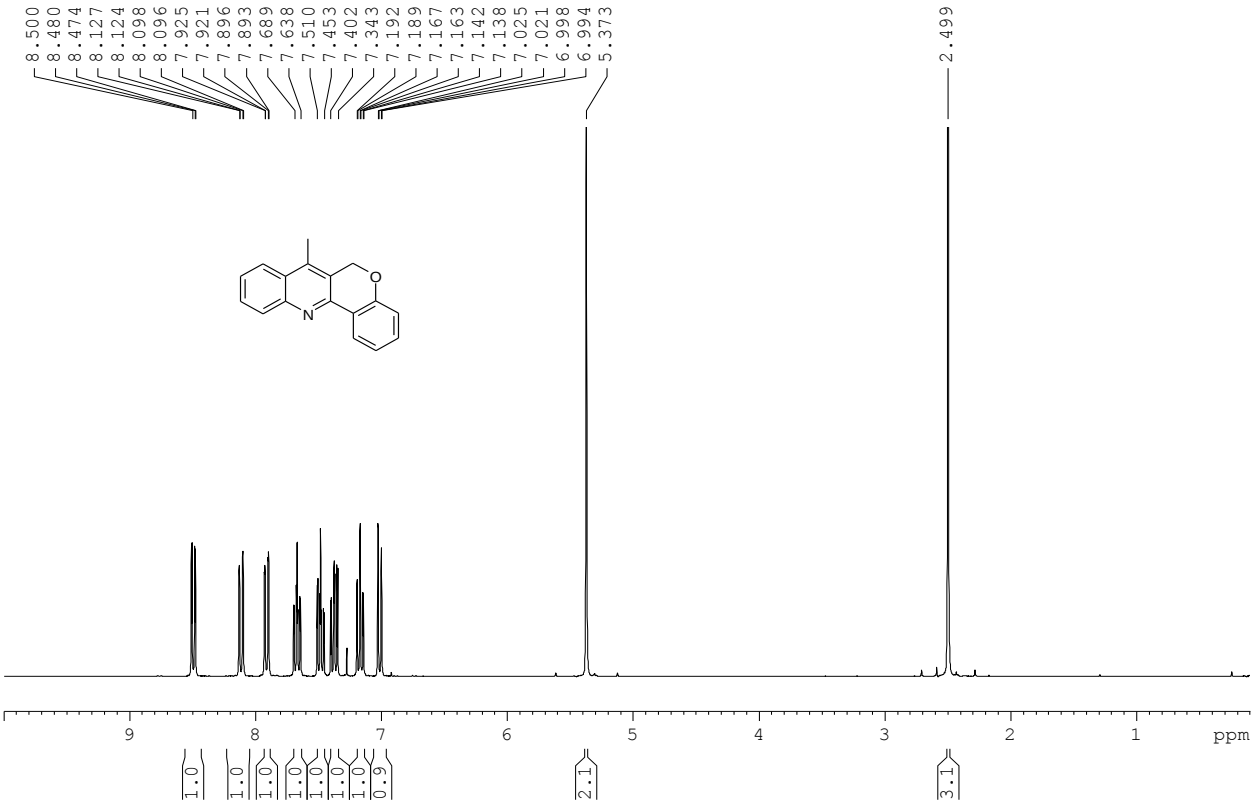
(25): ^{1}H NMR (300 MHz, DMSO)



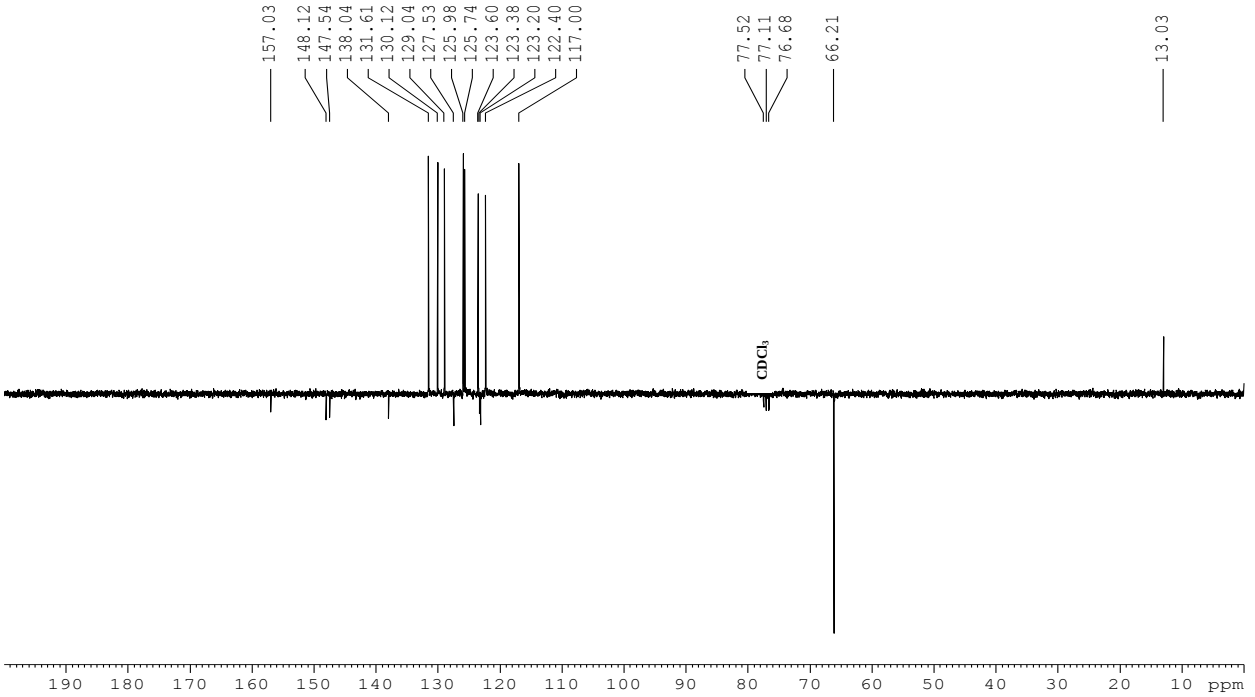
(25): ^{13}C NMR (75 MHz, DMSO)



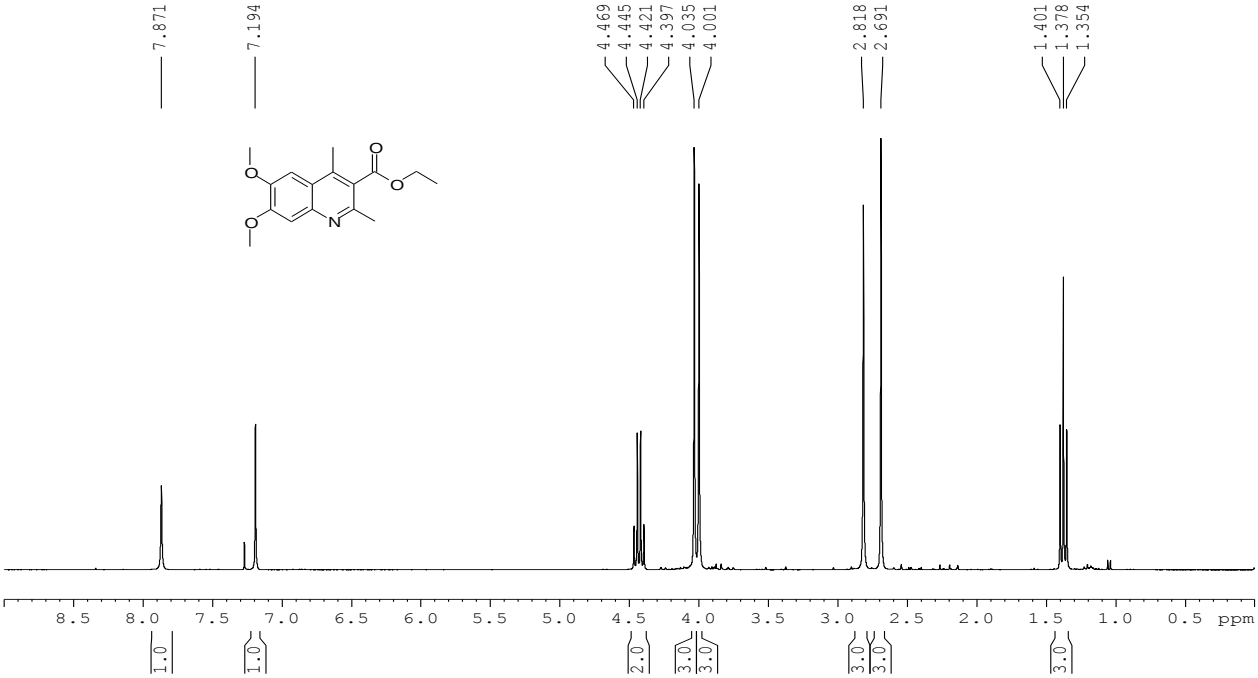
(26): ^{1}H NMR (300 MHz, $CDCl_3$)



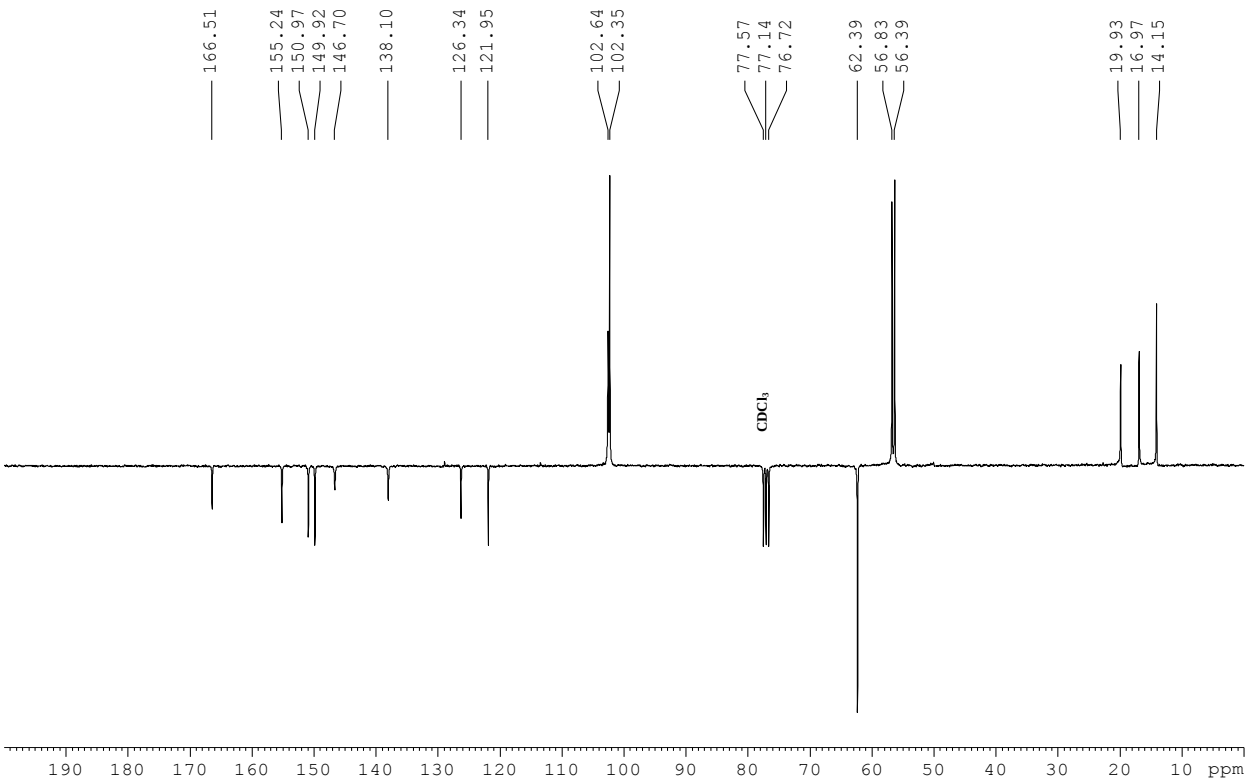
(26): ^{13}C NMR (75 MHz, $CDCl_3$)



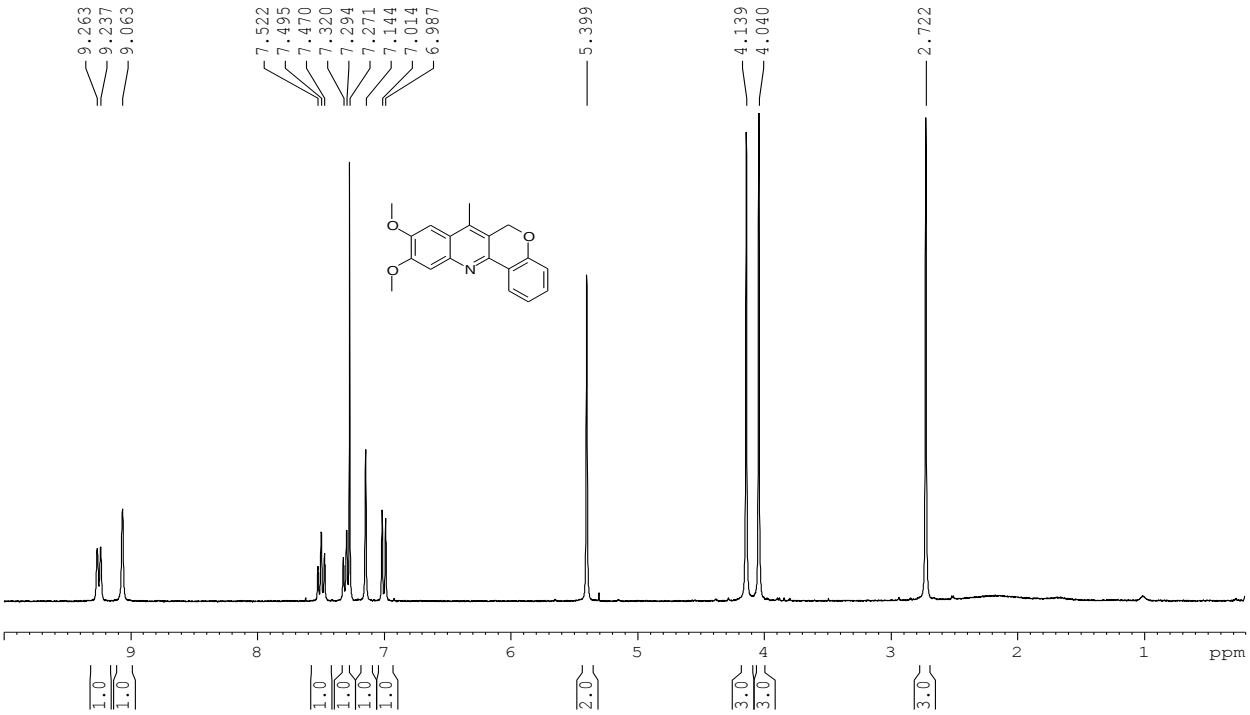
(27): ^{1}H NMR (300 MHz, $CDCl_3$)



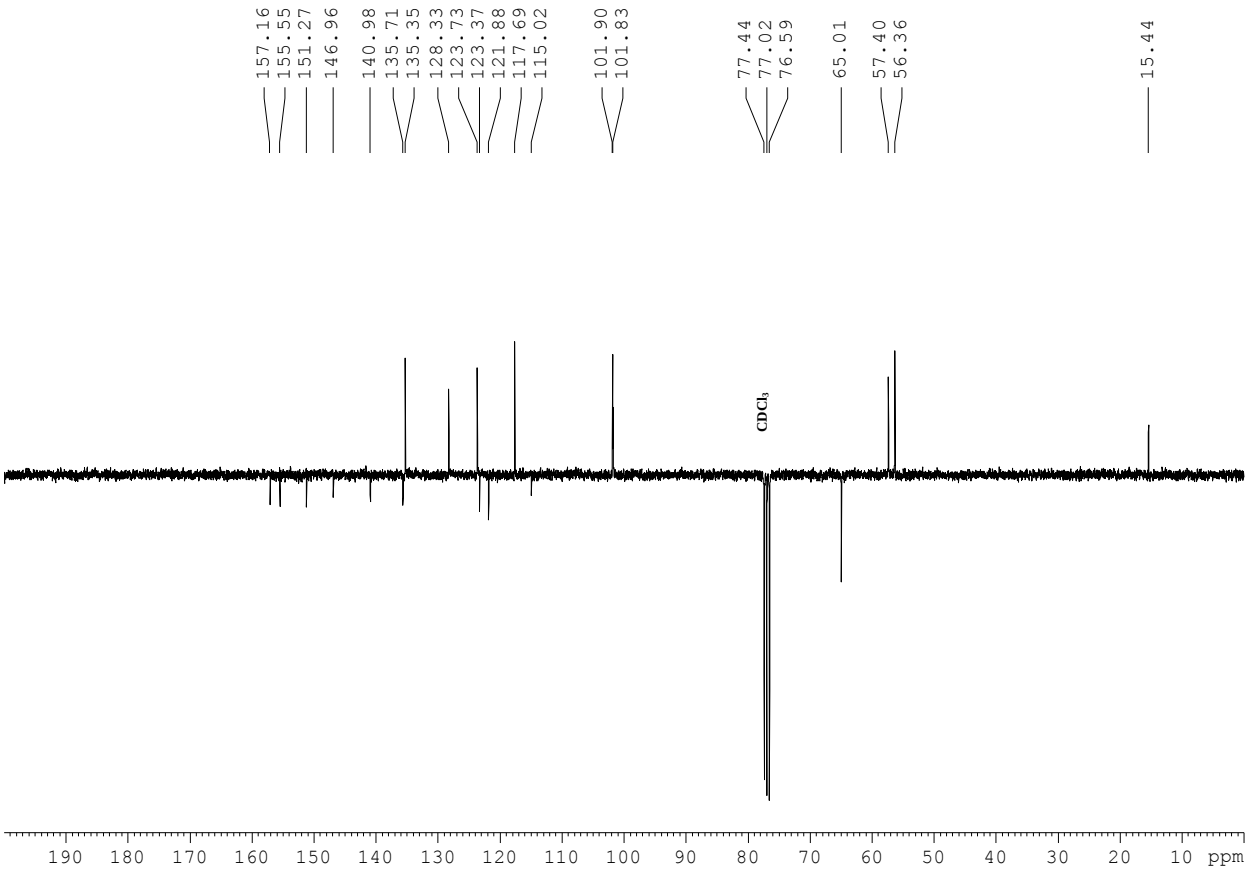
(27): ^{13}C NMR (75 MHz, $CDCl_3$)



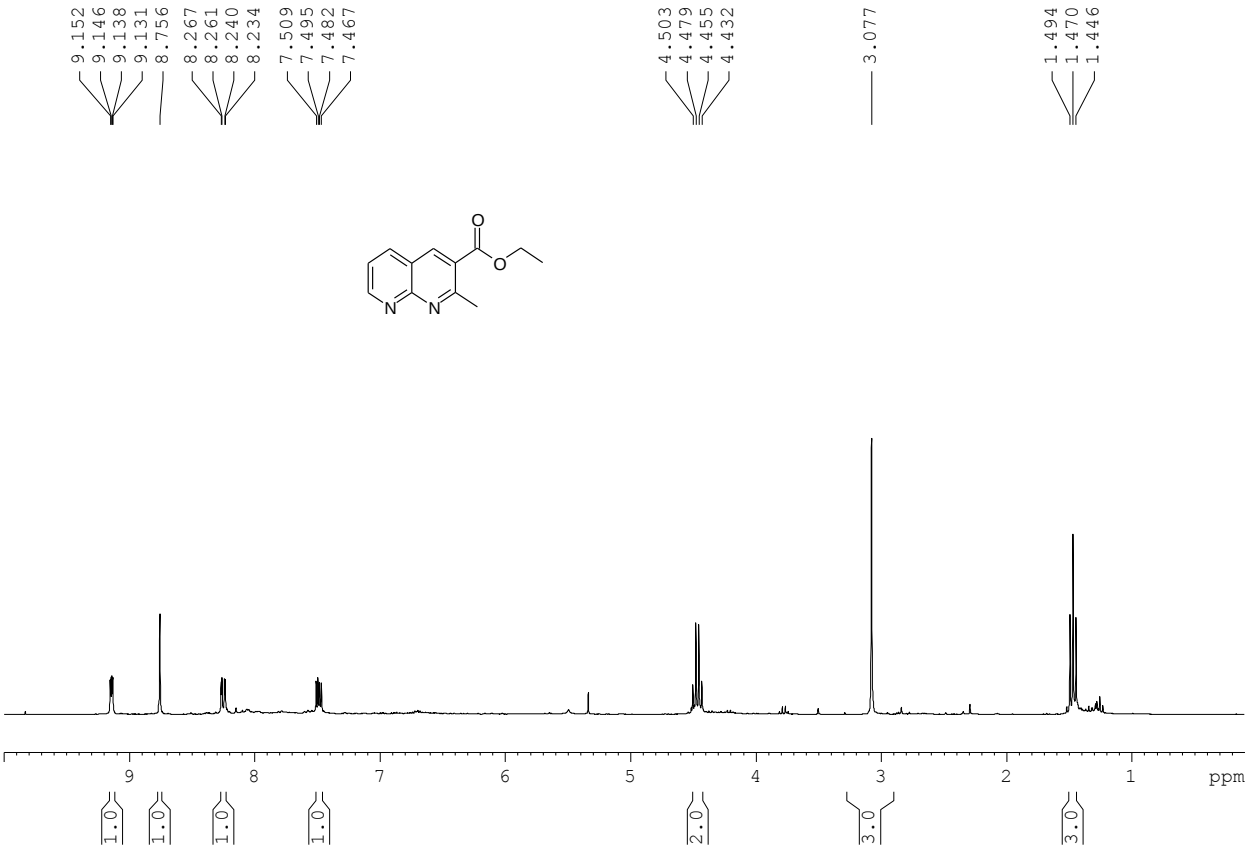
(28): ^{1}H NMR (300 MHz, $CDCl_3$)



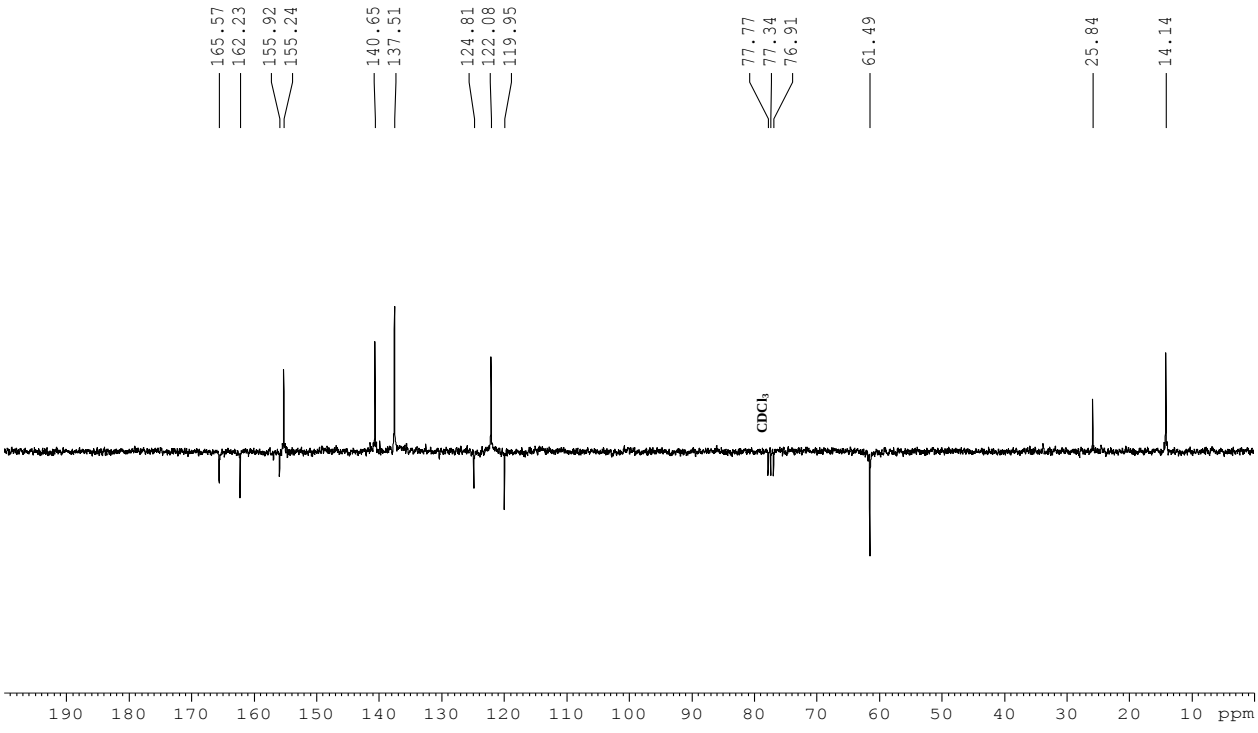
(28): ^{13}C NMR (75 MHz, $CDCl_3$)



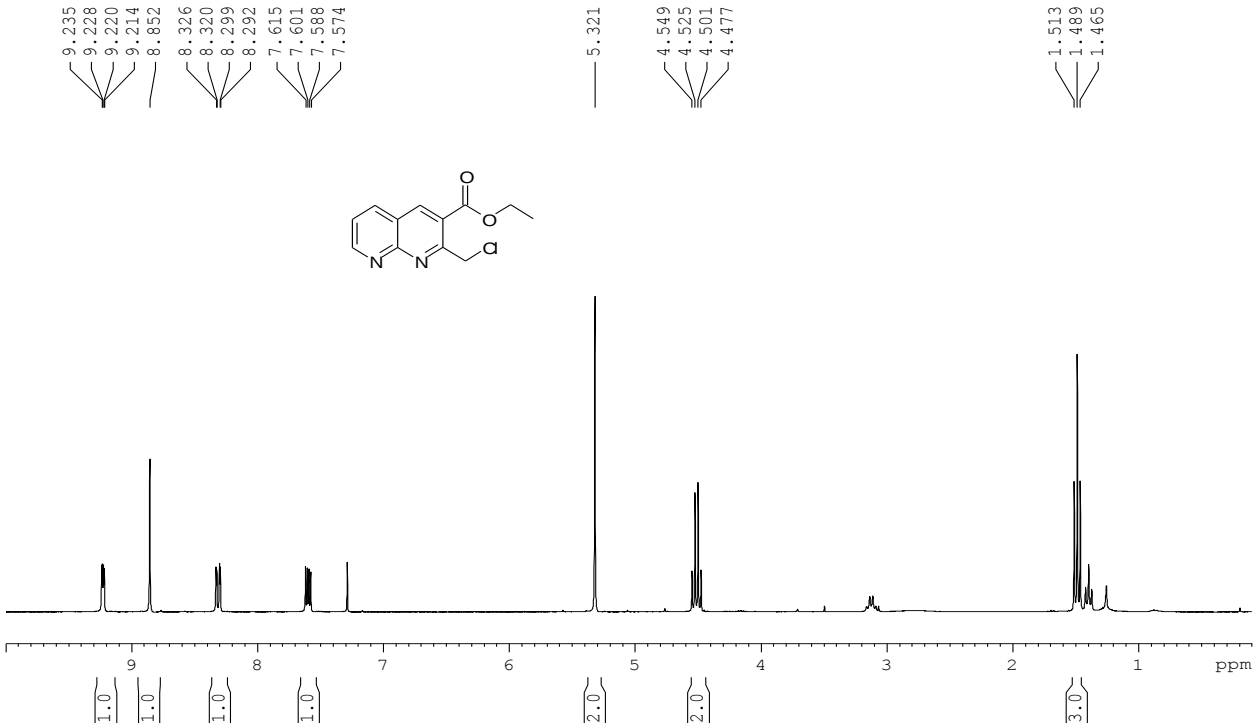
(29): ^{1}H NMR (300 MHz, $CDCl_3$)



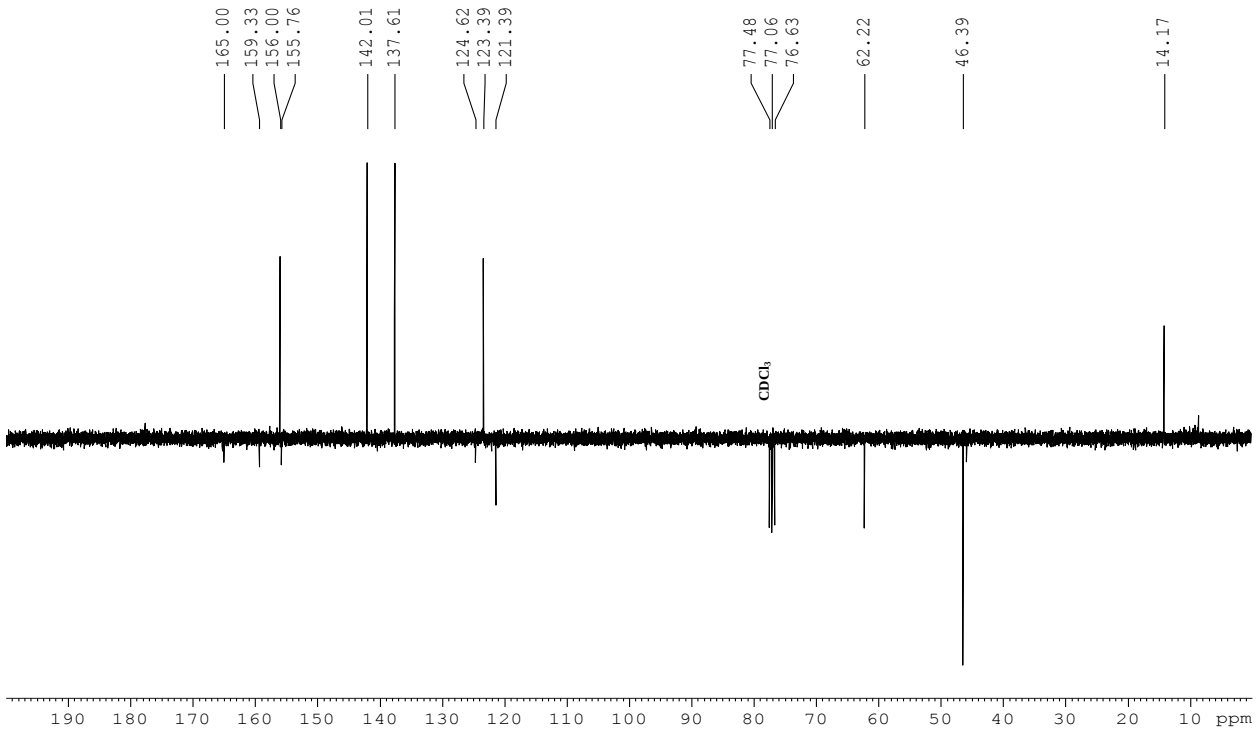
(29): ^{13}C NMR (75 MHz, $CDCl_3$)



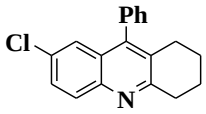
(30): ^{1}H NMR (300 MHz, $CDCl_3$)



(30): ^{13}C NMR (75 MHz, $CDCl_3$)



5. HRMS-ESI (m/z): $[M+H]^+$ for all compounds

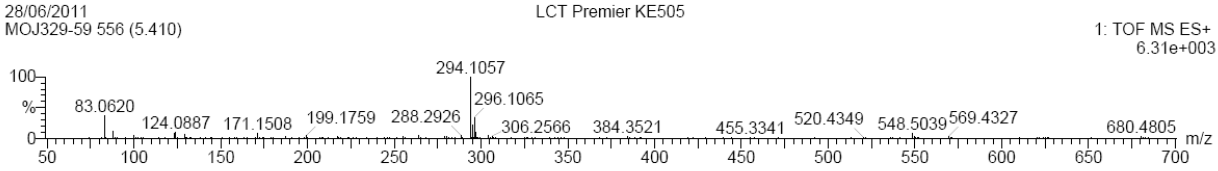


Elemental Composition Report **Page 1**

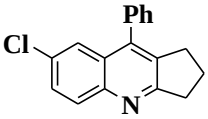
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
16504 formula(e) evaluated with 31 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

28/06/2011
MOJ329-59 556 (5.410)



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
294.1057	294.1050	0.7	2.4	11.5	1.4	C19 H17 N Cl
	294.1061	-0.4	-1.4	7.5	17.9	C16 H18 N O F Cl
	294.1043	1.4	4.8	2.5	98.0	C11 H21 N3 O2 S Cl
	294.1048	0.9	3.1	0.5	116.1	C11 H18 N F5 Cl

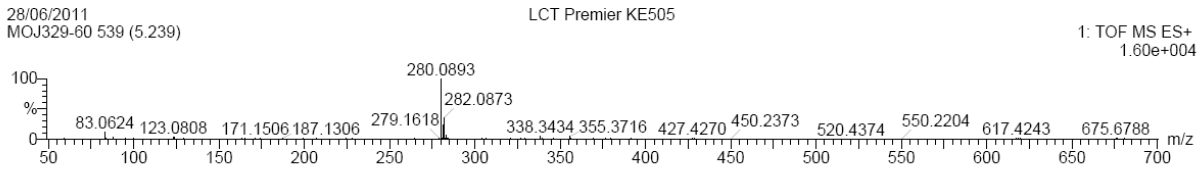


Elemental Composition Report **Page 1**

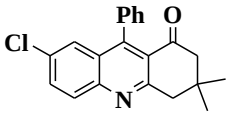
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
13292 formula(e) evaluated with 29 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

28/06/2011
MOJ329-60 539 (5.239)



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
280.0893	280.0893	0.0	0.0	11.5	16.5	C18 H15 N Cl
	280.0904	-1.1	-3.9	7.5	96.6	C15 H16 N O F Cl
	280.0887	0.6	2.1	2.5	320.5	C10 H19 N3 O2 S Cl

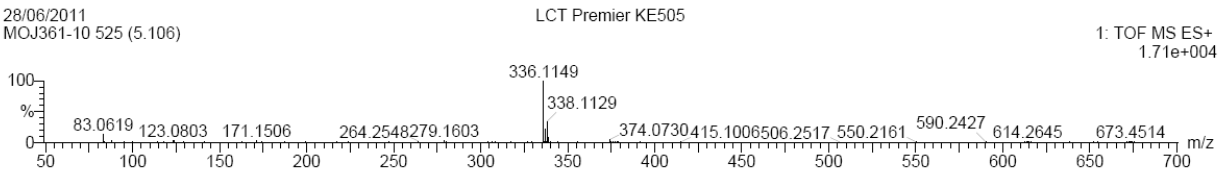


Elemental Composition Report **Page 1**

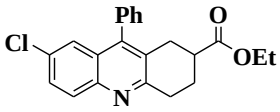
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
30038 formula(e) evaluated with 53 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

28/06/2011
MOJ361-10 525 (5.106)



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
336.1149	336.1155	-0.6	-1.8	12.5	13.2	C21 H19 N O Cl
	336.1142	0.7	2.1	5.5	48.0	C16 H19 N F4 Cl
	336.1140	0.9	2.7	9.5	50.2	C14 H16 N7 F Cl
	336.1149	0.0	0.0	3.5	167.6	C13 H23 N3 O3 S Cl
	336.1154	-0.5	-1.5	1.5	172.1	C13 H20 N O F5 Cl
	336.1151	-0.2	-0.6	5.5	175.7	C11 H17 N7 O F2 Cl
	336.1138	1.1	3.3	0.5	326.0	C10 H21 N3 O5 F2 Cl

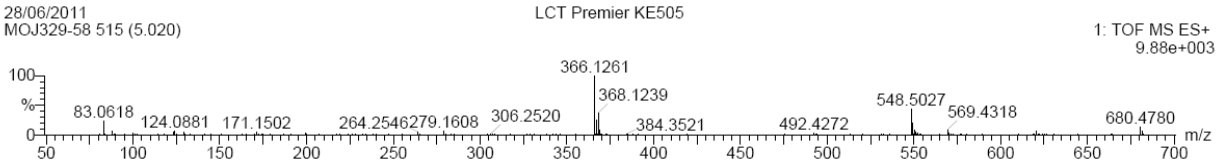


Elemental Composition Report **Page 1**

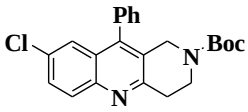
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
44211 formula(e) evaluated with 84 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

28/06/2011
MOJ329-58 515 (5.020)



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
366.1261	366.1261	0.0	0.0	12.5	5.2	C22 H21 N O2 Cl
	366.1272	-1.1	-3.0	8.5	11.4	C19 H22 N O3 F Cl
	366.1270	-0.9	-2.5	4.5	32.3	C17 H24 N F3 S Cl
	366.1268	-0.7	-1.9	8.5	33.7	C15 H21 N7 S Cl
	366.1248	1.3	3.6	5.5	42.0	C17 H21 N O F4 Cl
	366.1245	1.6	4.4	9.5	43.7	C15 H18 N7 O F Cl



Elemental Composition Report **Page 1**

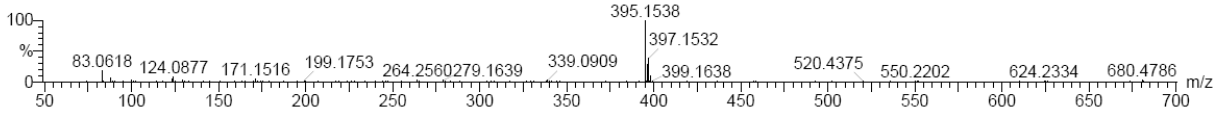
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
62448 formula(e) evaluated with 101 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

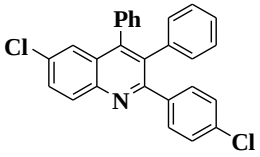
28/06/2011
MOJ329-57 530 (5.152)

LCT Premier KE505

1: TOF MS ES+
1.10e+004



Minimum:				-1.5							
Maximum:		2.0	5.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
395.1538	395.1526	1.2	3.0	12.5	8.2	C23	H24	N2	O2	Cl	
	395.1538	0.0	0.0	8.5	35.7	C20	H25	N2	O3	F	Cl
	395.1536	0.2	0.5	4.5	62.8	C18	H27	N2	F3	S	Cl
	395.1533	0.5	1.3	8.5	64.4	C16	H24	N8	S	Cl	
	395.1549	-1.1	-2.8	4.5	104.7	C17	H26	N2	O4	F2	Cl
	395.1520	1.8	4.6	3.5	130.2	C15	H28	N4	O4	S	Cl



Elemental Composition Report **Page 1**

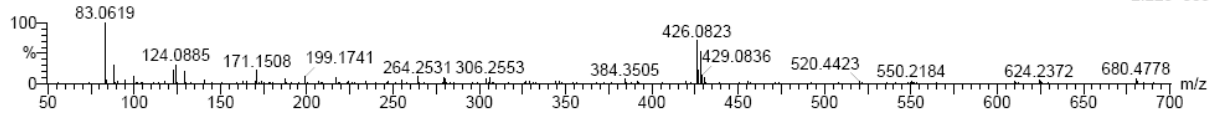
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
88223 formula(e) evaluated with 272 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

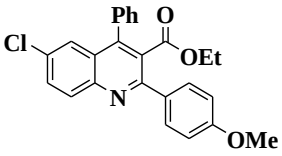
28/06/2011
MOJ329-52 635 (6.157)

LCT Premier KE505

1: TOF MS ES+
2.22e+003



Minimum:				-1.5							
Maximum:		2.0	5.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
426.0823	426.0816	0.7	1.6	18.5	1.4	C27	H18	N	Cl2		
	426.0828	-0.5	-1.2	14.5	3.4	C24	H19	N	O	F	Cl2
	426.0839	-1.6	-3.8	10.5	10.6	C21	H20	N	O2	F2	Cl2
	426.0810	1.3	3.1	9.5	12.7	C19	H22	N3	O2	S	Cl2
	426.0815	0.8	1.9	7.5	19.3	C19	H19	N	F5	Cl2	
	426.0812	1.1	2.6	11.5	19.5	C17	H16	N7	F2	Cl2	



Elemental Composition Report **Page 1**

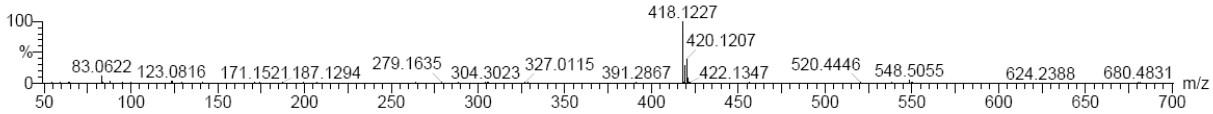
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
80701 formula(e) evaluated with 177 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

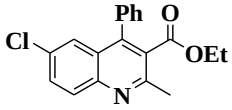
28/06/2011
MOJ329-63 578 (5.605)

LCT Premier KE505

1: TOF MS ES+
1.67e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
418.1227	418.1210	1.7	4.1	15.5	7.3	C25 H21 N O3 Cl
	418.1235	-0.8	-1.9	16.5	14.0	C23 H18 N5 F Cl
	418.1208	1.9	4.5	11.5	17.8	C23 H23 N F2 S Cl
	418.1244	-1.7	-4.1	10.5	32.5	C22 H25 N O3 S Cl
	418.1221	0.6	1.4	11.5	36.9	C22 H22 N O4 F Cl
	418.1246	-1.9	-4.5	12.5	60.6	C20 H19 N5 O F2 Cl
	418.1219	0.8	1.9	7.5	74.7	C20 H24 N O F3 S Cl



Elemental Composition Report **Page 1**

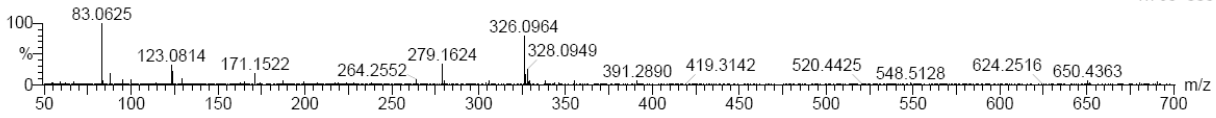
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
26293 formula(e) evaluated with 60 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

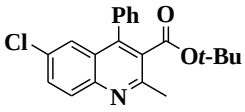
28/06/2011
MOJ329-61 529 (5.135)

LCT Premier KE505

1: TOF MS ES+
1.76e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
326.0964	326.0948	1.6	4.9	11.5	1.8	C19 H17 N O2 Cl
	326.0959	0.5	1.5	7.5	4.3	C16 H18 N O3 F Cl
	326.0971	-0.7	-2.1	3.5	13.4	C13 H19 N O4 F2 Cl
	326.0957	0.7	2.1	3.5	14.3	C14 H20 N F3 S Cl
	326.0955	0.9	2.8	7.5	14.6	C12 H17 N7 S Cl



Elemental Composition Report

Single Mass Analysis

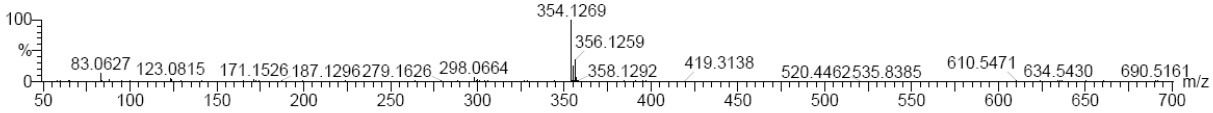
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
38006 formula(e) evaluated with 68 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

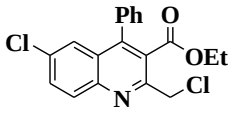
28/06/2011
MOJ329-68 580 (5.622)

LCT Premier KE505

1: TOF MS ES+
1.40e+004



Minimum:				-1.5							
Maximum:		2.0	5.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
354.1269	354.1261	0.8	2.3	11.5	6.3	C21	H21	N	O2	Cl	
	354.1272	-0.3	-0.8	7.5	51.2	C18	H22	N	O3	F	Cl
	354.1270	-0.1	-0.3	3.5	131.2	C16	H24	N	F3	S	Cl
	354.1268	0.1	0.3	7.5	133.4	C14	H21	N7	S	Cl	
	354.1284	-1.5	-4.2	3.5	153.3	C15	H23	N	O4	F2	Cl
	354.1254	1.5	4.2	2.5	235.9	C13	H25	N3	O4	S	Cl



Elemental Composition Report

Single Mass Analysis

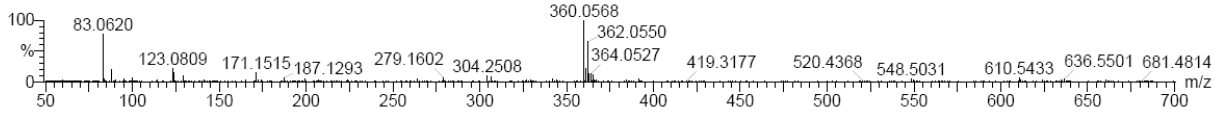
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
41287 formula(e) evaluated with 137 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

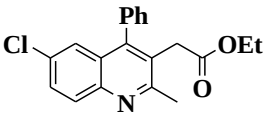
28/06/2011
MOJ329-69 557 (5.411)

LCT Premier KE505

1: TOF MS ES+
2.51e+003



Minimum:				-1.5							
Maximum:		2.0	5.0	50.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula					
360.0568	360.0558	1.0	2.8	11.5	0.8	C19	H16	N	O2	Cl2	
	360.0570	-0.2	-0.6	7.5	7.3	C16	H17	N	O3	F	Cl2
	360.0567	0.1	0.3	3.5	19.2	C14	H19	N	F3	S	Cl2
	360.0565	0.3	0.8	7.5	19.7	C12	H16	N7	S	Cl2	
	360.0581	-1.3	-3.6	3.5	25.5	C13	H18	N	O4	F2	Cl2
	360.0552	1.6	4.4	2.5	37.9	C11	H20	N3	O4	S	Cl2
	360.0579	-1.1	-3.1	-0.5	43.6	C11	H20	N	O	F4	S Cl2



Elemental Composition Report

Single Mass Analysis

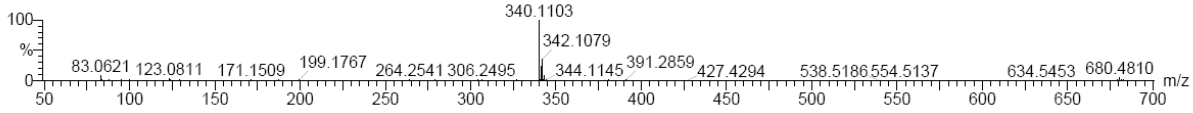
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
31718 formula(e) evaluated with 62 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

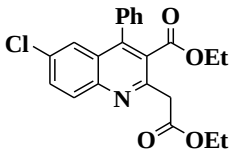
28/06/2011
MOJ329-64 516 (5.025)

LCT Premier KE505

1: TOF MS ES+
2.92e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
340.1103	340.1104	-0.1	-0.3	11.5	1.1	C20 H19 N O2 Cl
	340.1116	-1.3	-3.8	7.5	52.0	C17 H20 N O3 F Cl
	340.1091	1.2	3.5	4.5	164.9	C15 H19 N O F4 Cl
	340.1114	-1.1	-3.2	3.5	167.8	C15 H22 N F3 S Cl
	340.1089	1.4	4.1	8.5	170.1	C13 H16 N7 O F Cl
	340.1111	-0.8	-2.4	7.5	172.2	C13 H19 N7 S Cl



Elemental Composition Report

Single Mass Analysis

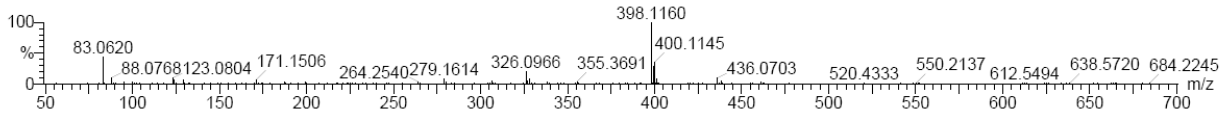
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
64668 formula(e) evaluated with 144 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

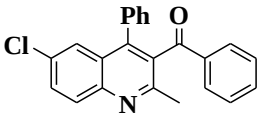
28/06/2011
MOJ361-06 532 (5.168)

LCT Premier KE505

1: TOF MS ES+
5.82e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
398.1160	398.1172	-1.2	-3.0	17.5	1.4	C23 H17 N5 Cl
	398.1159	0.1	0.3	12.5	11.1	C22 H21 N O4 Cl
	398.1146	1.4	3.5	12.5	19.0	C23 H22 N F S Cl
	398.1157	0.3	0.8	8.5	38.4	C20 H23 N O F2 S Cl
	398.1171	-1.1	-2.8	8.5	40.7	C19 H22 N O5 F Cl
	398.1179	-1.9	-4.8	7.5	69.0	C20 H26 N F S2 Cl



Elemental Composition Report

Single Mass Analysis

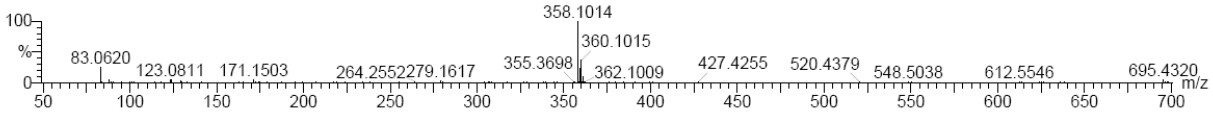
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
40117 formula(e) evaluated with 88 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-3 Cl: 0-5 Br: 0-8 F: 0-5

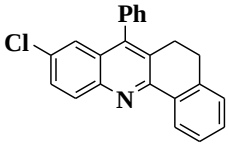
28/06/2011
MOJ361-11 533 (5.192)

LCT Premier KE505

1: TOF MS ES+
1.11e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
358.1014	358.1010	0.4	1.1	11.5	2.5	C20 H18 N O2 Cl F
	358.1022	-0.8	-2.2	7.5	21.6	C17 H19 N O3 Cl F2
	358.0999	1.5	4.2	15.5	27.6	C23 H17 N O Cl
	358.1019	-0.5	-1.4	3.5	57.6	C15 H21 N S Cl F4
	358.1017	-0.3	-0.8	7.5	59.3	C13 H18 N7 S Cl F
	358.0997	1.7	4.7	4.5	67.0	C15 H18 N O Cl F5



Elemental Composition Report

Single Mass Analysis

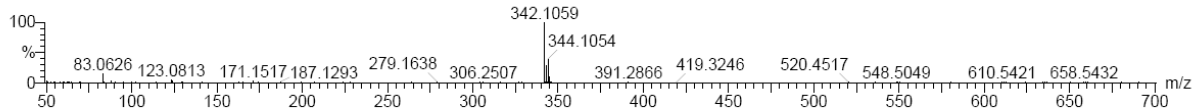
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
32615 formula(e) evaluated with 67 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

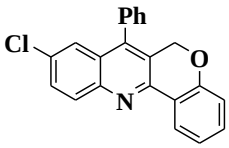
28/06/2011
MOJ329-65 691 (6.677)

LCT Premier KE505

1: TOF MS ES+
1.04e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
342.1059	342.1050	0.9	2.6	15.5	18.9	C23 H17 N Cl
	342.1061	-0.2	-0.6	11.5	57.9	C20 H18 N O F Cl
	342.1072	-1.3	-3.8	7.5	136.7	C17 H19 N O2 F2 Cl
	342.1043	1.6	4.7	6.5	157.0	C15 H21 N3 O2 S Cl
	342.1048	1.1	3.2	4.5	222.7	C15 H18 N F5 Cl
	342.1046	1.3	3.8	8.5	226.6	C13 H15 N7 F2 Cl
	342.1054	0.5	1.5	2.5	284.3	C12 H22 N3 O3 F S Cl



Elemental Composition Report **Page 1**

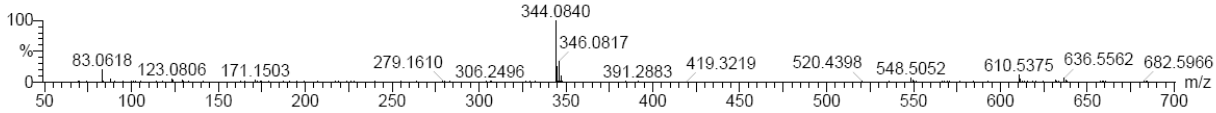
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
33554 formula(e) evaluated with 86 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

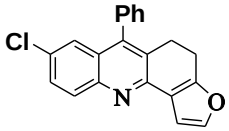
28/06/2011
MOJ329-70 648 (6.278)

LCT Premier KE505

1: TOF MS ES+
1.08e+004



Minimum:		2.0	5.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
344.0840	344.0842	-0.2	-0.6	15.5	1.9	C22 H15 N O Cl
	344.0854	-1.4	-4.1	11.5	21.8	C19 H16 N O2 F Cl
	344.0829	1.1	3.2	8.5	57.7	C17 H15 N F4 Cl
	344.0827	1.3	3.8	12.5	59.3	C15 H12 N7 F Cl
	344.0836	0.4	1.2	6.5	141.4	C14 H19 N3 O3 S Cl
	344.0841	-0.1	-0.3	4.5	150.9	C14 H16 N O F5 Cl
	344.0838	0.2	0.6	8.5	153.4	C12 H13 N7 O F2 Cl



Elemental Composition Report **Page 1**

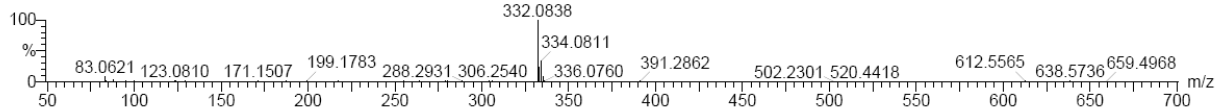
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
28579 formula(e) evaluated with 68 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

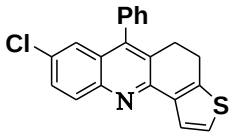
28/06/2011
MOJ361-09 570 (5.530)

LCT Premier KE505

1: TOF MS ES+
2.62e+004



Minimum:		2.0	5.0	-1.5		
Maximum:				50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
332.0838	332.0842	-0.4	-1.2	14.5	10.0	C21 H15 N O Cl
	332.0854	-1.6	-4.8	10.5	43.1	C18 H16 N O2 F Cl
	332.0829	0.9	2.7	7.5	121.3	C16 H15 N F4 Cl
	332.0827	1.1	3.3	11.5	124.6	C14 H12 N7 F Cl
	332.0836	0.2	0.6	5.5	335.5	C13 H19 N3 O3 S Cl
	332.0841	-0.3	-0.9	3.5	344.9	C13 H16 N O F5 Cl
	332.0838	0.0	0.0	7.5	350.3	C11 H13 N7 O F2 Cl



Elemental Composition Report

Single Mass Analysis

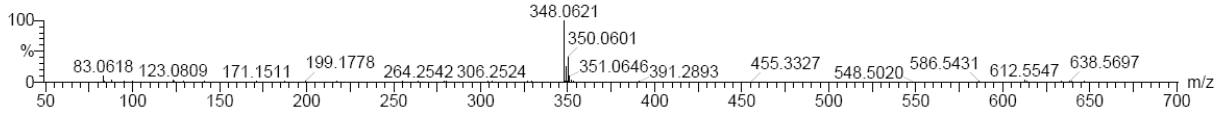
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
35404 formula(e) evaluated with 104 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

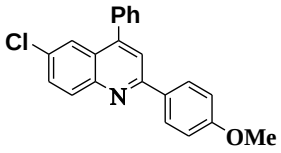
28/06/2011
MOJ361-07 644 (6.237)

LCT Premier KE505

1: TOF MS ES+
2.30e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
348.0621	348.0614	0.7	2.0	14.5	5.2	C21 H15 N S Cl
	348.0625	-0.4	-1.1	10.5	51.5	C18 H16 N O F S Cl
	348.0637	-1.6	-4.6	6.5	193.2	C15 H17 N O2 F2 S Cl
	348.0607	1.4	4.0	5.5	265.2	C13 H19 N3 O2 S2 Cl
	348.0614	0.7	2.0	7.5	300.8	C15 H14 N O3 F3 Cl
	348.0612	0.9	2.6	11.5	306.5	C13 H11 N7 O3 Cl
	348.0612	0.9	2.6	3.5	355.7	C13 H16 N F5 S Cl



Elemental Composition Report

Single Mass Analysis

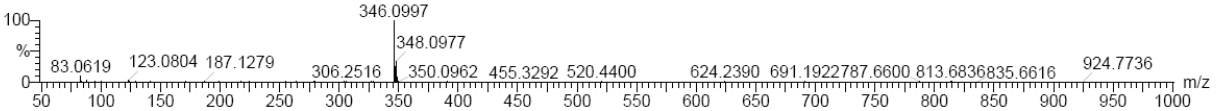
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
34420 formula(e) evaluated with 76 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

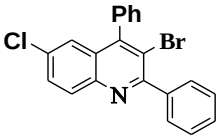
28/06/2011
MOJ361-22 620 (6.011)

LCT Premier KE505

1: TOF MS ES+
2.15e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.0997	346.0999	-0.2	-0.6	14.5	6.3	C22 H17 N O Cl
	346.1010	-1.3	-3.8	10.5	25.8	C19 H18 N O2 F Cl
	346.0986	1.1	3.2	7.5	85.5	C17 H17 N F4 Cl
	346.0983	1.4	4.0	11.5	89.2	C15 H14 N7 F Cl
	346.0992	0.5	1.4	5.5	244.0	C14 H21 N3 O3 S Cl
	346.0997	0.0	0.0	3.5	254.3	C14 H18 N O F5 Cl
	346.0995	0.2	0.6	7.5	258.2	C12 H15 N7 O F2 Cl



Elemental Composition Report

Single Mass Analysis

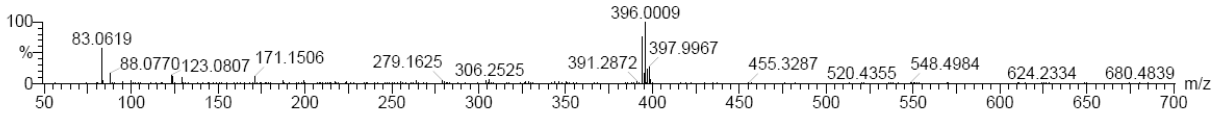
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
62346 formula(e) evaluated with 283 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

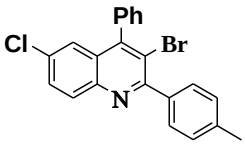
28/06/2011
MOJ361-28 599 (5.814)

LCT Premier KE505

1: TOF MS ES+
3.67e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
394.0013	393.9998	1.5	3.8	14.5	2.0	C21 H14 N Cl Br
	394.0010	0.3	0.8	10.5	2.1	C18 H15 N O F Cl Br
	394.0032	-1.9	-4.8	9.5	2.4	C18 H18 N S Cl Br
	394.0021	-0.8	-2.0	6.5	15.1	C15 H16 N O2 F2 Cl Br
	393.9997	1.6	4.1	3.5	32.8	C13 H15 N F5 Cl Br
	393.9994	1.9	4.8	7.5	33.6	C11 H12 N7 F2 Cl Br
	394.0025	-1.2	-3.0	6.5	34.3	C16 H19 N S2 Cl3



Elemental Composition Report

Single Mass Analysis

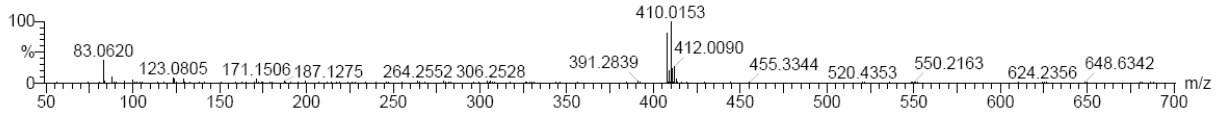
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
72911 formula(e) evaluated with 313 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

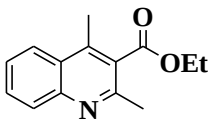
28/06/2011
MOJ361-33 636 (6.169)

LCT Premier KE505

1: TOF MS ES+
6.04e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
408.0162	408.0155	0.7	1.7	14.5	5.2	C22 H16 N Cl Br
	408.0166	-0.4	-1.0	10.5	16.1	C19 H17 N O F Cl Br
	408.0181	-1.9	-4.7	6.5	35.8	C17 H21 N S2 Cl3
	408.0170	-0.8	-2.0	14.5	45.1	C20 H15 N3 S Br
	408.0177	-1.5	-3.7	6.5	46.5	C16 H18 N O2 F2 Cl Br
	408.0181	-1.9	-4.7	10.5	47.9	C17 H16 N3 O F S Br
	408.0147	1.5	3.7	11.5	51.9	C20 H17 N S Cl3



Elemental Composition Report **Page 1**

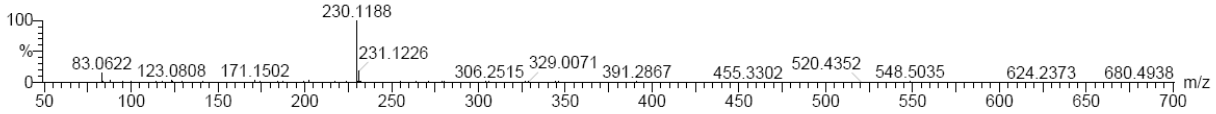
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
5565 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

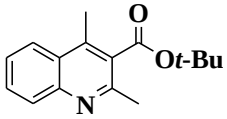
28/06/2011
MOJ329-76 445 (4.346)

LCT Premier KE505

1: TOF MS ES+
1.58e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
230.1188	230.1181	0.7	3.0	7.5	31.2	C14 H16 N O2
	230.1192	-0.4	-1.7	3.5	87.1	C11 H17 N O3 F
	230.1177	1.1	4.8	0.5	454.3	C4 H14 N7 O2 F2
	230.1190	-0.2	-0.9	-0.5	1204.3	C9 H19 N F3 S
	230.1188	0.0	0.0	3.5	1208.9	C7 H16 N7 S
	230.1199	-1.1	-4.8	-0.5	1393.7	C4 H17 N7 O F S
	230.1184	0.4	1.7	-0.5	7914.1	C6 H18 N5 O F Cl



Elemental Composition Report **Page 1**

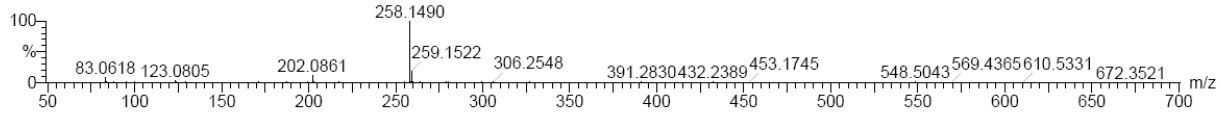
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9163 formula(e) evaluated with 9 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

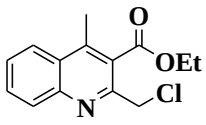
28/06/2011
MOJ329-78 479 (4.675)

LCT Premier KE505

1: TOF MS ES+
2.73e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
258.1490	258.1494	-0.4	-1.5	7.5	1.1	C16 H20 N O2
	258.1481	0.9	3.5	0.5	281.0	C11 H20 N O F4
	258.1479	1.1	4.3	4.5	287.6	C9 H17 N7 O F
	258.1490	0.0	0.0	0.5	654.7	C6 H18 N7 O2 F2
	258.1501	-1.1	-4.3	3.5	963.1	C9 H20 N7 S
	258.1499	-0.9	-3.5	0.5	1196.1	C H16 N13 O3
	258.1488	0.2	0.8	-1.5	1419.3	C8 H24 N3 O4 S
	258.1485	0.5	1.9	3.5	12075.6	C11 H21 N5 Cl



Elemental Composition Report **Page 1**

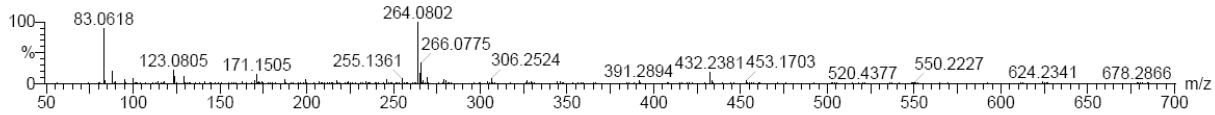
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
10239 formula(e) evaluated with 22 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

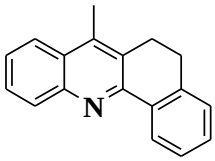
28/06/2011
MOJ329-80 468 (4.561)

LCT Premier KE505

1: TOF MS ES+
2.69e+003



Minimum:		2.0	5.0	-1.5		
Maximum:				50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
264.0802	264.0791	1.1	4.2	7.5	0.4	C14 H15 N O2 Cl
	264.0803	-0.1	-0.4	3.5	10.2	C11 H16 N O3 F Cl
	264.0801	0.1	0.4	-0.5	26.8	C9 H18 N F3 S Cl
	264.0798	0.4	1.5	3.5	27.6	C7 H15 N7 S Cl
	264.0814	-1.2	-4.5	-0.5	37.8	C8 H17 N O4 F2 Cl
	264.0810	-0.8	-3.0	-0.5	64.0	C4 H16 N7 O F S Cl
	264.0814	-1.2	-4.5	3.5	249.5	C5 H14 N9 S2



Elemental Composition Report **Page 1**

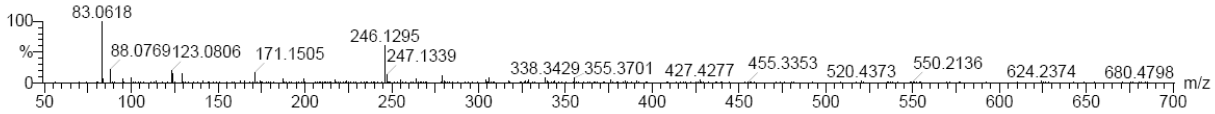
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7460 formula(e) evaluated with 11 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

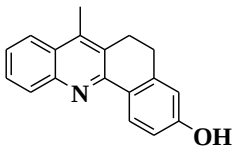
28/06/2011
MOJ361-26 533 (5.193)

LCT Premier KE505

1: TOF MS ES+
2.65e+003



Minimum:		2.0	5.0	-1.5		
Maximum:				50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
246.1295	246.1283	1.2	4.9	11.5	1.4	C18 H16 N
	246.1294	0.1	0.4	7.5	8.5	C15 H17 N O F
	246.1306	-1.1	-4.5	3.5	24.0	C12 H18 N O2 F2
	246.1301	-0.6	-2.4	-1.5	65.7	C6 H20 N3 O7
	246.1290	0.5	2.0	0.5	76.4	C5 H15 N7 O F3
	246.1288	0.7	2.8	4.5	77.4	C3 H12 N13 O



Elemental Composition Report **Page 1**

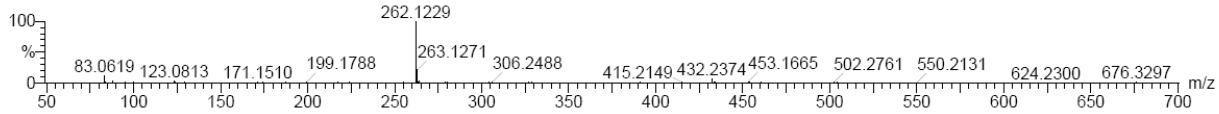
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9858 formula(e) evaluated with 15 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

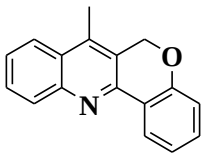
28/06/2011
MOJ361-01 462 (4.512)

LCT Premier KE505

1: TOF MS ES+
2.05e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
262.1229	262.1232	-0.3	-1.1	11.5	7.6	C18 H16 N O
	262.1219	1.0	3.8	4.5	240.3	C13 H16 N F4
	262.1216	1.3	5.0	8.5	245.9	C11 H13 N7 F
	262.1230	-0.1	-0.4	0.5	495.9	C10 H17 N O F5
	262.1228	0.1	0.4	4.5	502.4	C8 H14 N7 O F2
	262.1225	0.4	1.5	2.5	658.3	C10 H20 N3 O3 S



Elemental Composition Report **Page 1**

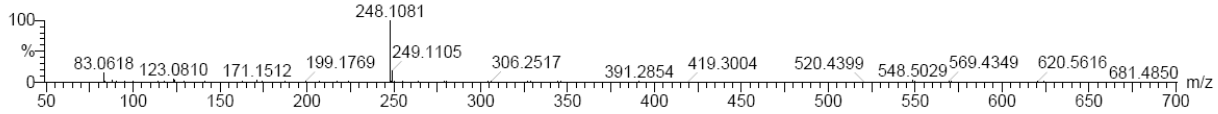
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
7745 formula(e) evaluated with 11 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

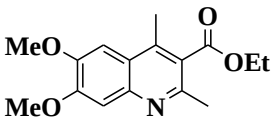
28/06/2011
MOJ329-79 511 (4.973)

LCT Premier KE505

1: TOF MS ES+
1.55e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
248.1081	248.1075	0.6	2.4	11.5	5.4	C17 H14 N O
	248.1087	-0.6	-2.4	7.5	21.4	C14 H15 N O2 F
	248.1074	0.7	2.8	0.5	294.5	C9 H15 N O F5
	248.1071	1.0	4.0	4.5	299.3	C7 H12 N7 O F2
	248.1083	-0.2	-0.8	0.5	570.0	C4 H13 N7 O2 F3
	248.1080	0.1	0.4	4.5	577.2	C2 H10 N13 O2



Elemental Composition Report **Page 1**

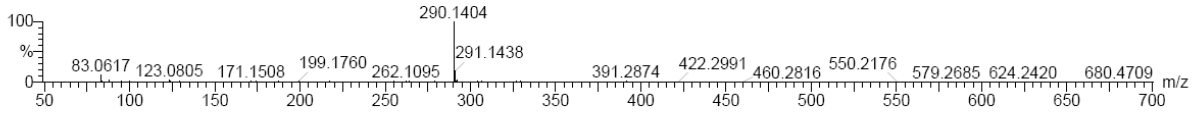
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
15449 formula(e) evaluated with 20 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

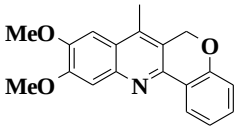
28/06/2011
MOJ361-24 425 (4.156)

LCT Premier KE505

1: TOF MS ES+
2.33e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
290.1404	290.1392	1.2	4.1	7.5	7.0	C16 H20 N O4
	290.1417	-1.3	-4.5	8.5	28.8	C14 H17 N5 O F
	290.1404	0.0	0.0	3.5	36.7	C13 H21 N O5 F
	290.1406	-0.2	-0.7	12.5	66.0	C17 H16 N5
	290.1415	-1.1	-3.8	-0.5	205.7	C10 H22 N O6 F2
	290.1404	0.0	0.0	1.5	333.1	C9 H17 N5 F5



Elemental Composition Report **Page 1**

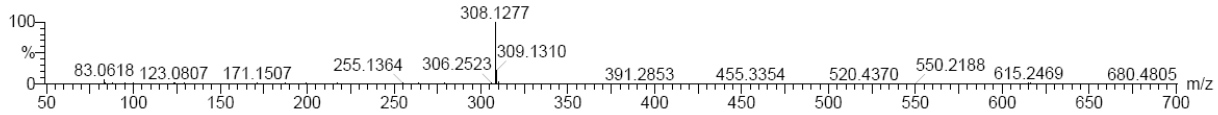
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
20280 formula(e) evaluated with 33 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

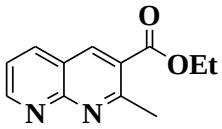
28/06/2011
MOJ361-21 481 (4.693)

LCT Premier KE505

1: TOF MS ES+
3.56e+004



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
308.1277	308.1287	-1.0	-3.2	11.5	9.1	C19 H18 N O3
	308.1262	1.5	4.9	8.5	44.5	C17 H17 N O F3
	308.1274	0.3	1.0	4.5	242.9	C14 H18 N O2 F4
	308.1271	0.6	1.9	8.5	248.2	C12 H15 N7 O2 F
	308.1285	-0.8	-2.6	0.5	625.5	C11 H19 N O3 F5
	308.1283	-0.6	-1.9	4.5	635.4	C9 H16 N7 O3 F2
	308.1285	-0.8	-2.6	7.5	922.9	C17 H20 N F2 S
	308.1269	0.8	2.6	-0.5	943.2	C8 H20 N3 O7 F2
	308.1292	-1.5	-4.9	4.5	1221.1	C4 H14 N13 O4



Elemental Composition Report **Page 1**

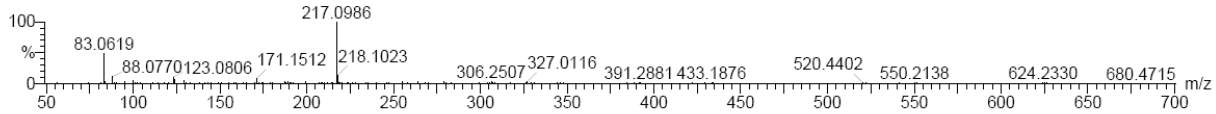
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4348 formula(e) evaluated with 8 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

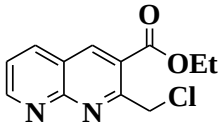
28/06/2011
MOJ361-18 385 (3.779)

LCT Premier KE505

1: TOF MS ES+
5.12e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
217.0986	217.0977	0.9	4.1	7.5	1.0	C12 H13 N2 O2
	217.0988	-0.2	-0.9	3.5	14.0	C9 H14 N2 O3 F
	217.0986	0.0	0.0	-0.5	222.9	C7 H16 N2 F3 S
	217.0984	0.2	0.9	3.5	224.5	C5 H13 N8 S
	217.0995	-0.9	-4.1	-0.5	294.5	C2 H14 N8 O F S
	217.0995	-0.9	-4.1	2.5	2327.2	C11 H18 O2 Cl
	217.0980	0.6	2.8	-0.5	2353.2	C4 H15 N6 O F Cl
	217.0987	-0.1	-0.5	-1.5	2694.8	C6 H19 N4 Cl2



Elemental Composition Report **Page 1**

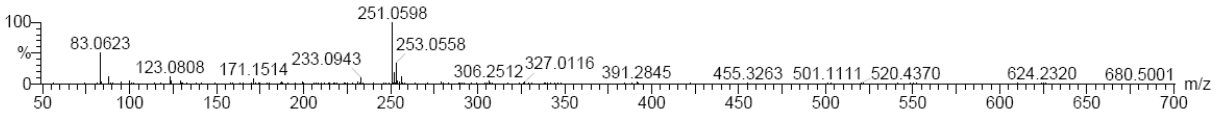
Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
8221 formula(e) evaluated with 26 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 F: 0-5 S: 0-3 Cl: 0-5 Br: 0-8

28/06/2011
MOJ361-25 405 (3.966)

LCT Premier KE505

1: TOF MS ES+
4.95e+003



Minimum:				-1.5		
Maximum:		2.0	5.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
251.0598	251.0587	1.1	4.4	7.5	16.7	C12 H12 N2 O2 Cl
	251.0599	-0.1	-0.4	3.5	61.8	C9 H13 N2 O3 F Cl
	251.0597	0.1	0.4	-0.5	103.9	C7 H15 N2 F3 S Cl
	251.0594	0.4	1.6	3.5	105.9	C5 H12 N8 S Cl
	251.0610	-1.2	-4.8	-0.5	139.2	C6 H14 N2 O4 F2 Cl
	251.0606	-0.8	-3.2	-0.5	197.8	C2 H13 N8 O F S Cl