Electronic Supplementary Information

Beyond the Solvent Role: Discovery of DMSO as a Versatile Radical Reagent for Organic Transformations

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1. General information

All the reactions were carried out in dried pressure/sealed tubes. All the starting materials used for the reactions are purchased commercially (Sigma-Aldrich, Avra, BLD, SRL). The solvent DMSO (dried 99.5%) is purchased from Sisco-Research Laboratories (SRL) used for the reaction with atmost purity. Solvents like hexanes and ethyl acetate were distilled and used for column chromatography. Magnetic stirrers and silicone oil baths were used for the reactions. Thin layer chromatography (TLC) was used to monitor the reactions. Silica gels like (60-120) mesh and (100-200) mesh were used for the column chromatography which is used for the purification of organic compounds. ^{1}H spectra were recorded on a Bruker 400 MHz and 500 MHz spectrometer. ^{13}C were recorded on 100 MHZ and 125 MHZ spectrometers respectively. $CDCl_3$ and DMSO-d_6 solvents were used for NMR spectrum. Chemical shifts were reported in parts per million (ppm) and multiplicities are as written as: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), td (triplet of doublet) and ddd (doublet of doublet of doublet). Coupling constants (*J*) are reported in Hertz. Melting points were recorded on a CAPILLARY melting point apparatus. HRMS was performed in Bruker compass data analysis 4.2. LC-MS was performed in Schimadzu Labsolutions. GC-MS was performed in Schimadzu instrument.

2. General procedure

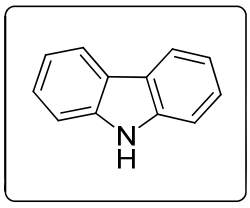
1,2,3,4-Tetrahydrocarbazoles were prepared using literature procedures [1-3].

General procedure for the aromatization of tetrahydrocarbazoles 2a-2u

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of 1,2,3,4-tetrahydro-1*H*-carbazoles (**2a**-**2s**) or tetrahydro-*β*-carboline (**2u**) or 2-anthracenyl-2,3-quino-4-one (**2t**) was dissolved in 2 mL of dry DMSO and the reaction mixture was pre-heated oil bath at 100 ºC for appropriate time. The reaction completion was monitored by TLC and the reaction mixture was quenched with water (50 mL), then cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

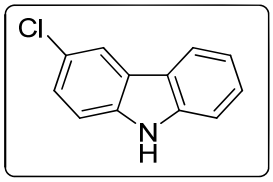
2.1 Characterisation of data for compounds 2a-2u

9*H*-Carbazole [4] (2a)



White solid; 39 mg, 80% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$): *δ* 8.08 (d, *J* = 8.0 Hz, 2H), 8.03 (br s, 1H), 7.43-7.39 (m, 4H), 7.24-7.22 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): *δ* 139.7, 125.7, 123.6, 120.2, 119.4, 110.4.

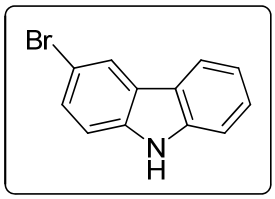
3-Chloro-9*H*-carbazole [4] (2b)



Pale-yellow solid; 36 mg, 73% yield; m.p. >200°C; ^{1}H NMR (400 MHz, $CDCl_3$): *δ* 8.08 (br s, 1H), 8.03 (d, *J*= 6.8 Hz, 2H), 7.45-7.43 (m, 2H), 7.38-

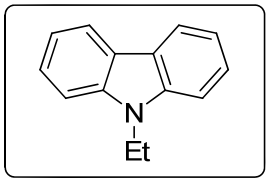
7.34 (m, 2H), 7.26 (s, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 140.8, 138.6, 126.8, 125.7, 124.2, 123.3, 122.0, 121.1, 120.2, 119.3, 112.8, 111.7

3-Bromo-9*H*-carbazole [4] **(2c)**



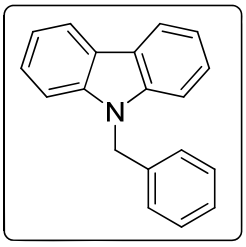
Pale-yellow solid; 25 mg, 51%yield; m.p. >200°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17 (s, 1H), 8.04-8.01 (m, 2H), 7.50-7.42 (m, 3H), 7.30-7.22 (m, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 139.8, 138.1, 128.5, 126.6, 125.2, 123.1, 122.4, 120.5, 119.9, 112.2, 112.0, 110.8.

9-Ethyl-9*H*-carbazole [5] **(2d)**



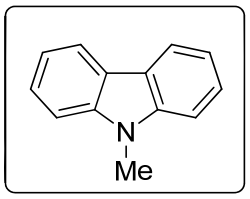
Off-white solid; 35 mg, 71 %yield; m.p. 111-114°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.11-8.09 (m, 2H), 7.46 (ddd, J = 15.0 Hz, 8.0 Hz, 1.2 Hz, 2H), 7.40 (d, J = 8.0 Hz, 2H), 7.22 (ddd, J = 14.5 Hz, 7.5 Hz, 1.2 Hz, 2H,), 4.37 (q, J = 22 Hz, 2H,), 1.43 (t, J = 14.5 Hz, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 140.1, 125.5, 122.9, 120.1, 118.6, 108.3, 37.6, 13.7.

9-Benzyl-9*H*-carbazole [5] **(2e)**



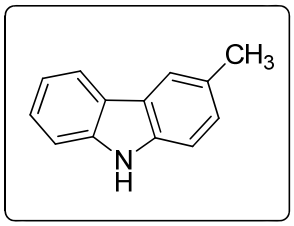
Pale-orange solid; 39 mg, 79%yield; m.p. 119-121°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, J = 7.6 Hz, 2H), 7.40 (ddd, J = 15.2 Hz, 8.0 Hz, 1.2 Hz, 2H), 7.3 (d, J = 8.0 Hz, 2H,), 7.24-7.18 (m, 5H), 7.12-7.10 (m, 2H), 5.46 (s, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 140.9, 137.3, 128.7, 127.4, 126.5, 125.8, 123.3, 120.3, 119.2, 108.9, 46.7

9-Methyl-9*H*-carbazole [5] **(2f)**



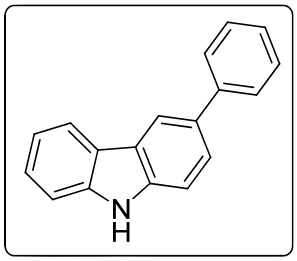
White solid; 32 mg 65%; m.p. 90-92°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.01 (d, J = 7.7 Hz, 2H,), 7.40-7.37 (m, 2H), 7.30 (d, J = 8.2 Hz, 2H), 7.16-7.13 (m, 2H), 3.74 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 139.9, 124.6, 121.7, 119.2, 117.7, 107.3, 27.9

3-Methyl-9*H*-carbazole [4] **(2h)**



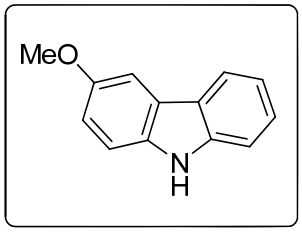
Off-white solid; 35 mg, 72%yield;m.p. >200°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, J= 7.6 Hz, 1H), 7.95 (br s, 1H), 7.87 (s, 1H), 7.38 (d, J= 4.4 Hz, 2H), 7.30 (d, J= 8.4 Hz, 1H), 7.24-7.18 (m, 2H), 2.52 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 140.0, 137.9, 128.7, 127.1, 125.6, 123.7, 123.4, 120.2, 120.1, 119.2, 110.4, 110.2, 21.2.

3-Phenyl-9*H*-carbazole [4] **(2i)**



Pale-yellow solid; 30 mg, 61%yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.29 (s, 1H), 8.13-8.08 (m, 2H), 7.71-7.66 (m, 3H), 7.48-7.43 (m, 5H), 7.35-7.32 (m, 2H), 7.25 (s, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 142.1, 140.0, 139.0, 133.1, 128.8, 127.3, 126.5, 126.1, 125.5, 123.9, 123.5, 120.4, 119.6, 118.9, 110.9, 110.8.

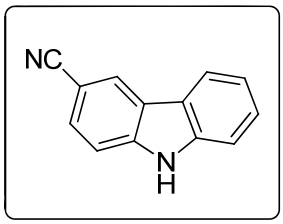
3-Methoxy-9*H*-carbazole [4] **(2j)**



Off-white solid; 20 mg, 41%yield; m.p. 150-153°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.06 (d, J = 8 Hz, 1H), 7.95 (s, 1H), 7.59 (d, J = 2.4 Hz, 1H,), 7.43-7.41 (m, 2H), 7.35 (d, J = 8.8 Hz, 1H), 7.26-7.22 (m, 1H), 7.10 (dd,

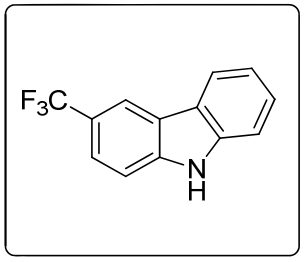
J = 8.8 Hz, 2.4 Hz, 1H,), 3.96 (s, 3H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.3, 140.6, 134.7, 125.7, 124.0, 123.6, 120.2, 119.1, 115.1, 111.1, 110.6, 103.8, 56.2.

9*H*-Carbazole-3-carbonitirile [5] (2k)



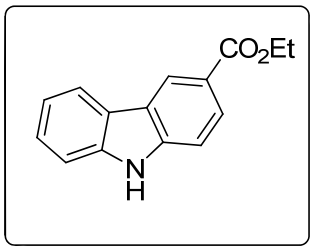
Brown solid; 25 mg, 51%yield; m.p. 182-185°C; ^{1}H NMR (400 MHz, $CDCl_3$ and DMSO-d_6): δ 10.75 (br s, 1H), 8.24 (d, J = 5.2 Hz, 1H,), 7.95 (d, J = 7.6 Hz, 1H,), 7.50 (dd, J = 8.4 Hz, 1.2 Hz, 1H), 7.41-7.33 (m, 3H), 7.17-7.13 (m, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$ and DMSO-d_6): δ 141.9, 140.5, 128.4, 126.8, 124.9, 123.2, 122.0, 120.5, 120.3, 120.0, 111.5, 111.3, 101.3.

3-(trifluoromethyl)-9*H*-carbazole [6] (2l)



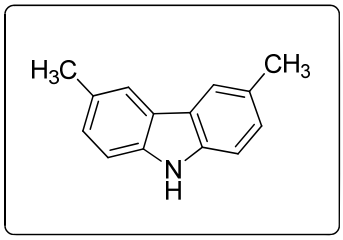
Pale-orange solid; 35 mg, 71%yield; m.p. 164-168°C; 1H NMR (400 MHz, $CDCl_3$): δ 8.37 (s, 1H), 8.27 (br s, 1H), 8.14 (d, J = 6.0 Hz, 1H,), 7.69 (d, J = 6.8 Hz, 1H), 7.52-7.49 (m, 3H), 7.34-7.31 (m, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 140.9, 139.9, 126.8, 123.0, 122.9, 122.7, 122.6, 120.6, 120.3, 118.0, 117.9, 110.9, 110.6.

Ethyl-9*H*-carbazole-3-carboxylate [4] (2m)



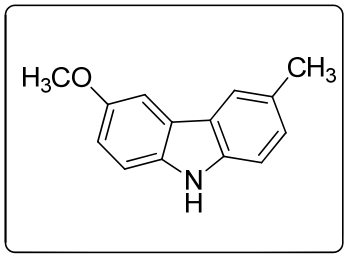
White solid; 40 mg, 82% yield; m.p. 156-159°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.82 (s, 1H), 8.30 (br s, 1H), 8.15-8.13 (m, 2H), 7.47-7.43 (m, 3H), 7.31-7.26 (m, 1H), 4.44 (q, J = 21.5 Hz, 2H), 1.46 (t, J = 14.0 Hz, 3H,). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 167.4, 142.2, 139.9, 127.5, 126.5, 123.4, 123.1, 122.8, 121.8, 120.7, 120.3, 110.9, 110.1, 60.7, 14.5.

3,3'-Dimethyl-9*H*-carbazole [5] (2n)



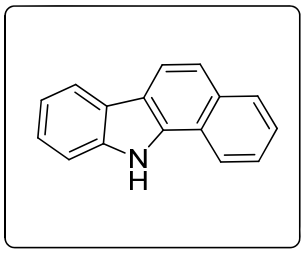
Off-white solid; 20 mg, 41% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.88 (s, 2H, 7.82 (br s, 1H), 7.31-7.24 (m, 4H), 2.56 (s, 6H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 138.1, 128.5, 127.0, 123.4, 120.2, 110.2, 21.4

3-Methoxy-6-methyl-9*H*-carbazole (Glycozoline) [5] (2o)



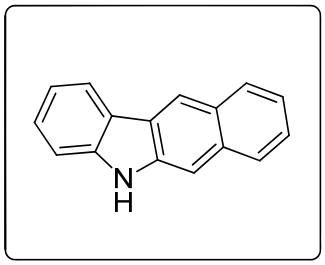
White solid; 31 mg, 62%yield; m.p. 178-180°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.86 (s, 1H), 7.83 (br s, 1H), 7.56 (d, J = 1.5 Hz, 1H), 7.32-7.29 (m, 2H), 7.25 (d, J = 8 Hz, 1H), 7.07 (dd, J = 8.5, 2 Hz, 1H), 3.95 (s, 3H), 2.56 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 153.8, 138.6, 134.8, 128.3, 127.2, 123.7, 123.5, 120.1, 114.9, 111.3, 110.4, 103.2, 56.1, 21.4.

11*H*-benzo[*a*]carbazole [6] (2p)



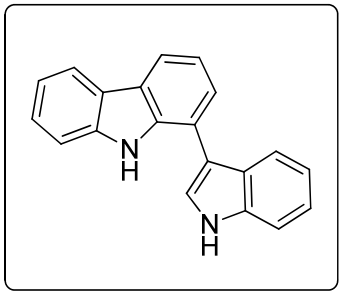
Light yellow solid; 36 mg, 73% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.85 (br s, 1H), 8.18-8.16 (m, 3H), 8.05 (d, J = 8.0 Hz, 1H), 7.70 (d, J = 8.5 Hz, 1H), 7.62 (d, J = 7.0 Hz, 3H), 7.57 (t, J = 7.4 Hz, 1H), 7.34 (t, J = 7.4 Hz, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 138.5, 134.9, 132.4, 129.1, 125.6, 125.2, 124.9, 124.2, 121.1, 120.5, 120.2, 120.0, 119.9, 119.3, 118.4, 111.1.

5*H*-benzo[*b*]carbazole [7](2q)



Off-white solid; 30 mg, 61%yield; m.p. >200°C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.82 (d, J = 8.4 Hz, 1H), 8.61 (d, J = 8.0 Hz, 1H), 8.38 (br s, 1H), 8.05 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.8 Hz, 1H), 7.77-7.73 (m, 1H), 7.62-7.41 (m, 5H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ 138.6, 137.2, 130.1, 129.4, 129.1, 127.4, 126.8, 124.3, 124.2, 123.2, 122.9, 122.0, 120.3, 115.7, 112.4, 111.0.

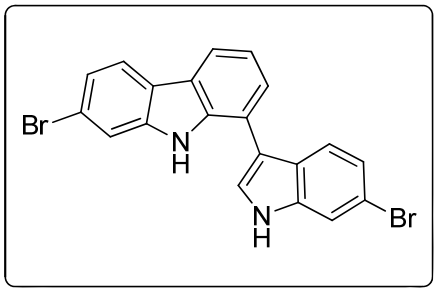
1-(1*H*-Indol-3-yl)-9*H*-carbazole [2] (2r)*



Pale-yellow solid; 27 mg, 45%yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.20 (s, 1H), 8.13 (d, J = 7.8 Hz, 1H), 8.08 (d, J = 7.7 Hz, 1H), 7.68 (d, J = 7.9 Hz, 1H), 7.56 (d, J = 8.2 Hz, 1H), 7.51 (d, J = 8.2 Hz, 1H), 7.46 (d, J = 1.9 Hz, 1H), 7.39 (t, J = 7.5 Hz, 1H), 7.38 – 7.29 (m, 3H), 7.26 – 7.22 (m, 1H), 7.19 (t, J = 7.2 Hz, 1H).^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 139.3, 138.2, 136.5, 126.3, 126.2, 125.8, 123.7, 123.4, 122.7, 122.6, 120.4 (2C), 120.1, 119.7, 119.4, 118.7, 118.3, 114.9, 111.6, 110.7.

* Solvent traces are difficult to remove completely, hence solvent peaks are observed in aliphatic region in the NMR spectra.

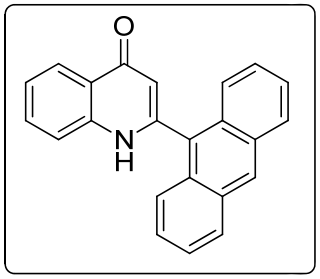
7-Bromo-1-(6-bromo-1*H*-indol-3-yl)-9*H*-carbazole [2] (2s)*



Colorless solid; 34 mg, 68% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.46 (br s, 1H), 8.13 (br s, 1H), 8.05 (br d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.68 (d, J = 1.5 Hz, 1H), 7.55 (dd, J = 7.5, 1.1 Hz, 1H), 7.53 (d, J = 1.5 Hz, 1H), 7.51 (d, J = 8.5 Hz, 1H), 7.46 (d, J = 2.5 Hz, 1H), 7.38-7.33 (m, 2H), 7.30 (dd, J = 8.5, 1.5 Hz, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 140.1, 138.2, 137.2, 126.6, 125.1, 123.9, 123.0, 122.9, 122.8, 122.7, 121.6, 121.1, 120.3, 119.3, 118.9, 117.9, 116.5, 114.8, 114.6, 113.8.

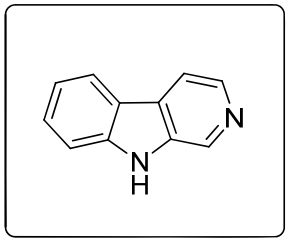
*Solvent traces are difficult to remove completely, hence solvent peaks are observed in aliphatic region in the NMR spectra.

2-(Anthracen-2-yl)quinolin-4(1*H*)-one [3] (2t)



Pale-orange solid; 32 mg, 64% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO) δ 12.22 (s, 1H), 8.85 (s, 1H), 8.27 (d, J = 7.9 Hz, 1H), 8.22 (d, J = 8.2 Hz, 2H), 7.80 (d, J = 8.5 Hz, 2H), 7.72 (t, J = 7.3 Hz, 1H), 7.61 – 7.55 (m, 5H), 7.44 (t, J = 7.5 Hz, 1H), 6.20 (s, 1H). ^{13}C {^{1}H} NMR (125 MHz, DMSO-d_6): δ 177.1, 148.3, 141.1, 132.4, 131.1, 129.6, 129.2, 129.1, 129.0, 127.7, 126.2, 125.7, 125.5, 124.0, 118.9, 112.6

9*H*-Pyrido[3,4-*b*]indole [6] (Norharmane) (2u)



White solid; 25 mg, 51% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6) δ 10.68 (br s, 1H), 8.83 (s, 1H), 8.83 (s, 1H), 8.31 (d, J = 4.0 Hz, 1H), 8.01 (d, J = 7.5 Hz, 1H), 7.85 (d, J = 4.5 Hz, 1H), 7.45-7.39

(m, 2H), 7.14 (t, J = 14.0 Hz, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$ and DMSO-d_6) δ 140.9, 138.3, 136.3, 133.9, 128.4, 128.1, 121.5, 121.1, 119.4, 114.5, 111.8

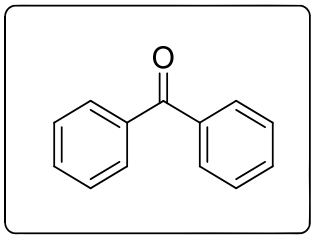
3. General procedure for the oxidation of alcohols 4a-j

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of aromatic alcohol was dissolved in 2 mL of dry DMSO and the reaction mixture was pre-heated oil bath at 120 ºC for appropriate time. The reaction completion was monitored by TLC and the reaction mixture was quenched with water (50 mL), then cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was used without purification.

Note: compound **4f** and **4j** was purified by column chromatography.

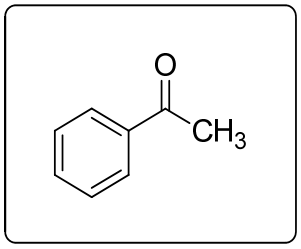
3.1. Characterisation of data for compounds 4a-4j

Benzophenone [8] **(4a)**



Colourless semi-solid; 45 mg 92% yield; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.82 (d, J = 5.0 Hz, 4H), 7.62 (t, J = 10.0 Hz, 2H), 7.51 (t, J = 10.0 Hz, 4H); ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 196.6, 137.1, 132.9, 130.1, 128.0.

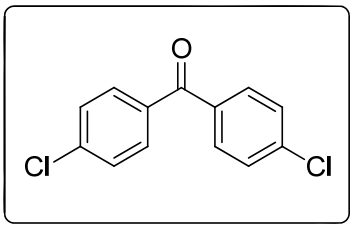
Acetophenone [8] **(4b)**



Colourless liquid; 41 mg, 83% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, J = 7.5 Hz, 1H), 7.57 (t, J = 14.5 Hz, 1H), 7.47 (t, J = 15.5 Hz, 1H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$) δ 198.1, 137.1, 133.1, 128.6,

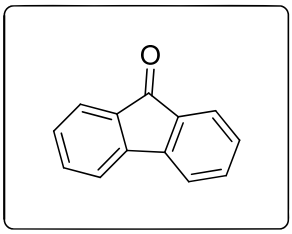
128.3, 26.6.

Bis(4-chlorophenyl)methanone [8] **(4c)**



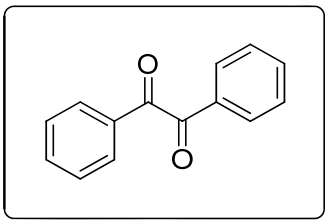
White solid; 48 mg 98% yield; m.p. 142-144 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.75 (d, J = 10.0 Hz, 4H), 6.98 (d, J = 10.0 Hz, 4H); ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 194. 8, 139.2, 135.6, 131.2, 128.7.

9*H*-Fluoren-9-one [8] **(4d)**



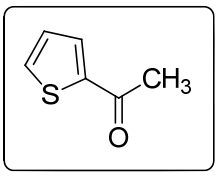
Flouroscent yellow solid; 48 mg, 97% yield; m.p. 81-84 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.68 (d, J = 7.3 Hz, 2H), 7.54 -7.48 (m, 4H), 7.32-7.28 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 193.9, 144.4, 134.7, 134.2, 129.1, 124.3, 1203.

Benzil [9] **(4e)**



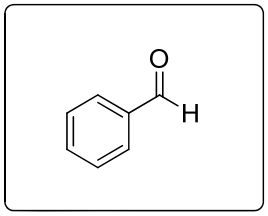
Pale-yellow solid; 48 mg, 97% yield; m.p. 93-95 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.0 (d, J = 10.0 Hz, 4H), 7.69 (t, J = 15.0 Hz, 2H), 7.54 (t, J = 15.0 Hz, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 194.6, 134.9, 133.0, 129.9, 129.0

1-(thiophen-2-yl)ethanone [9] **(4f)**



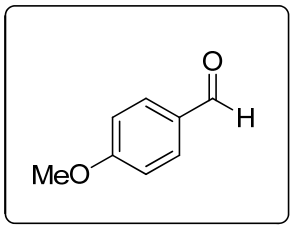
Brown liquid; 20 mg, 41% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (d, J = 3.5 Hz, 1H), 7.64 (d, J = 4.5 Hz, 1H), 7.13 (t, J = 8.5 Hz, 1H), 2.57 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 190.7, 144.6, 133.7, 132.4, 128.1, 26.9.

Benzaldehyde [10] **(4g)**



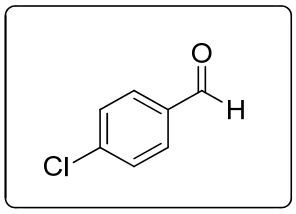
Colorless liquid; 47 mg, 96% Yield; ^{1}H NMR (500 MHz, $CDCl_3$); δ 10.01 (s, 1H), 7.88 (d, J = 7.5 Hz, 2H), 7.64 (t, J = 15.5 Hz, 1H), 7.54 (t, J = 15.0 Hz, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 192.3, 141.4, 134.4, 129.7, 129.0

4-Methoxybenzaldehyde [10] **(4h)**



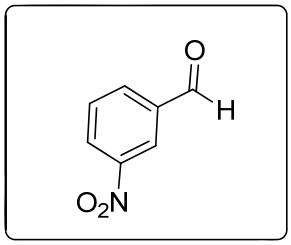
Colorless liquid; 45 mg, 92% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.91 (s, 1H), 7.87 (d, J = 9.0 Hz, 2H), 7.03 (d, J = 8.5 Hz, 2H), 3.92 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 190.8, 164.6, 132.3, 131.9, 114.3, 55.6.

4-Chlorobenzaldehyde [10] **(4i)**



White solid; 43 mg, 88% yield; m.p. 52-25°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.96 (s, 1H), 7.81 (d, J = 7.0 Hz, 2H), 7.50 (d, J = 8.0 Hz, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 190.9, 141.0, 134.7, 130.9, 129.5.

3-Nitrobenzaldehyde [11] **(4j)**



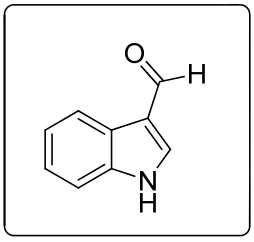
Yellowish crystalline solid; 24 mg, 49% yield; m.p. 53-56°C; ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.13 (s, 1H), 8.73 (s, 1H), 8.51-8.49 (m, 1H), 8.24 (d, J = 7.5 Hz, 1H), 7.78 (t, J = 16.0 Hz, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 189.6, 148.9, 137.5, 134.6, 130.4, 128.6, 124.5.

4. General procedure for the decarboxylation of keto acids (6a-f)

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of keto-acid and 0.3 mmol of *N*-methyl aniline was dissolved in 2 mL of dry DMSO and the reaction mixture was placed in the pre-heated oil bath at 100 ºC for appropriate time. The reaction completion was monitored by TLC, quenched with water (50 mL) and cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

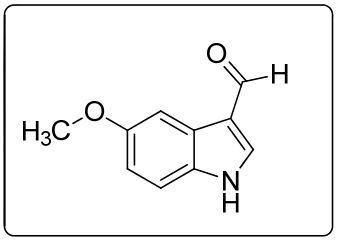
4.1 Characterization of data for the compounds (6a-f)

Indole-3-carbaldehyde [14] **(6a)**



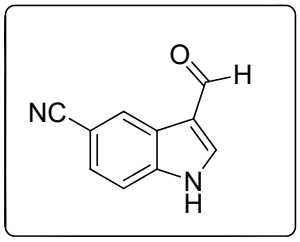
Yellow solid; 30 mg, 79% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.10 (br s, 1H), 9.94 (s, 1H), 8.29 (s, 1H), 8.10 (d, J = 7.5 Hz, 1H), 7.52 (d, J = 8.0 Hz, 1H), 7.28-7.21 (m, 2H). ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) δ 185.4, 138.9, 137.5, 124.6, 123.9, 122.6, 121.3, 118.6, 112.9

5-Methoxy indole-3-carbaldehyde [15] **(6b)**



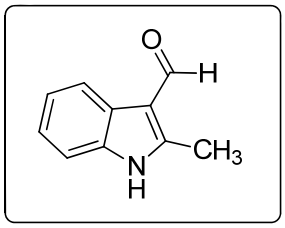
Pale-yellow solid; 26 mg, 65% yield; m.p. 179-181°C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.04 (br s, 1H), 9.90 (s, 1H), 8.22 (s, 1H), 7.59 (d, J = 2.5 Hz, 1H), 7.41 (d, J = 8.8 Hz, 1H), 6.89 (dd, J = 8.8, 2.5 Hz, 1H), 3.79 (s, 3H) ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$ and DMSO-d_6) δ 189.8, 160.9, 141.6, 136.9, 130.0, 123.5, 118.8, 117.6, 107.7, 60.4

5-Cyano indole-3-carbaldehyde [16] **(6c)**



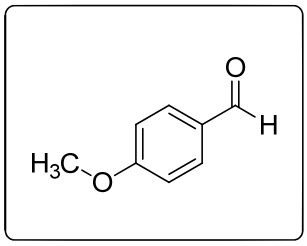
Brown solid; 22 mg, 56% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.57 (br s, 1H), 10.0 (s, 1H), 8.48 (d, J = 21.5 Hz, 2H), 7.71-7.63 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, DMSO-d_6) δ 185.8, 140.7, 139.3, 126.9, 126.2, 124.4, 120.4, 118.5, 114.4, 104.8

2-Methyl indole-3-carbaldehyde [17] **(6d)**



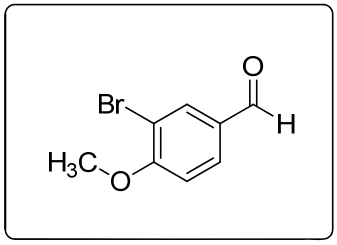
Brown solid; 28 mg, 72% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO-d_6) δ 12.01 (br s, 1H), 10.06 (s, 1H), 8.06-8.04 (m, 1H), 7.40-7.38 (m, 1H), 7.19-7.14 (m, 2H), 2.69 (s, 3H) ^{13}C{^{1}H} NMR (125 MHz, DMSO-d_6) δ 184.7, 148.9, 135.8, 126.0, 123.0, 122.3, 120.4, 114.1, 111.8, 11.9

4-Methoxy benzaldehyde [10] **(6e)**



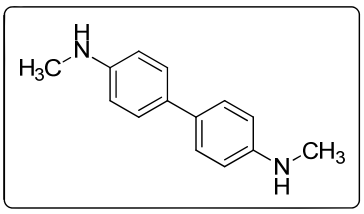
Clourless liquid; 23 mg, 62% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.89 (s, 1H), 7.85 (d, J = 8.8 Hz, 2H), 7.02 (d, J = 8.7 Hz, 2H), 3.89 (s, 3H) ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 190.7, 164.6, 131.9, 130.0, 114.3, 55.5

3-Bromo-4-methoxy benzaldehydes [13] **(6f)**



Pale-brown semi-solid; 25 mg, 61% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 9.86 (s, 1H), 8.10 (d, J = 2.0 Hz, 1H), 7.84 (dd, J = 8.5, 2.0 Hz, 1H), 7.03 (d, J = 8.5 HZ, 1H), 4.01 (s, 3H) ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$) δ 189.6, 160.6, 134.6, 131.2, 130.7, 112.6, 111.5, 56.6

***N,N'*-Dimethyl-[1,1'-biphenyl]-4,4'-diamine** [18] **(6')**



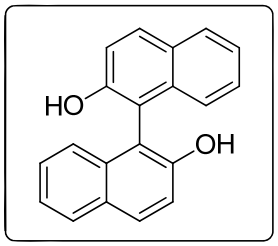
Reddish liquid; 24% yield; ^{1}H NMR (500 MHz, $CDCl_3$) δ 6.92 (d, J = 8.2 Hz, 4H), 6.47 (d, J = 8.4 Hz, 4H), 3.70 (br s, 2H), 2.73 (s, 6H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$) δ 147.5, 130.9, 129.5, 112.6, 31.0.

5. General procedures for the preparation of BINOLs (8a-c)

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of 2-naphthol was dissolved in 2 mL of dry DMSO and the reaction mixture was placed in the pre-heated oil bath at 120 ^{o}C for appropriate time. The reaction progress was monitored by TLC, after the reaction completion, the reaction mixture was quenched with water (50 mL) and cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

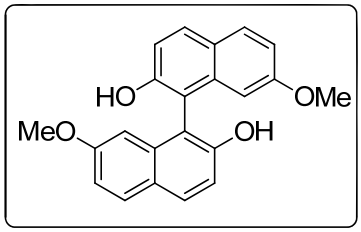
5.1 Characterization of data for the compounds (8a-c)

[2,2'-Binaphthalene]-1,3-diol (BINOL) [12] (8a)



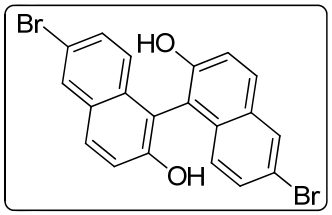
Off-white solid; 30 mg, 60% yield; m.p. >200°C; ^{1}H NMR (400 MHz, $CDCl_3$ and DMSO-d_6) δ 10.3 (d, J = 15.5 Hz, 1H), 8.19 (d, J = 10.5 Hz, 1H), 7.62 (d, J = 10.0 Hz, 2H), 7.56 (d, J = 10.5 Hz, 2H), 7.25 (d, J = 11.0 Hz, 2H), 7.18-7.15 (m, 2H), 7.10 (t, J = 18.5 Hz, 2H), 4.71 (br s, 2H). ^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$ and DMSO-d_6) δ 152.3, 134.3, 129.0, 128.4, 127.7, 125.7, 124.3, 122.4, 120.0, 118.7.

7,7'-Dimethoxy-[1,1'-binaphthalene]-2,2'-diol [19] (8b)



White solid; 31 mg, 62% yield; m.p. >200°C ; ^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6) δ 7.53-7.43 (m, 6H), 6.98 (d, J = 8.5 Hz, 2H), 6.80 (t, J = 9.0 Hz, 2H), 4.68 (br s, 2H), 3.62 (s, 6H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$ and DMSO-d_6) δ 158.0, 152.7, 135.1, 130.0, 127.7, 124.5, 117.4, 115.6, 114.8, 102.9, 55.2

6,6'-Dibromo-[1,1'-binaphthalene]-2,2'-diol [20] (8c)



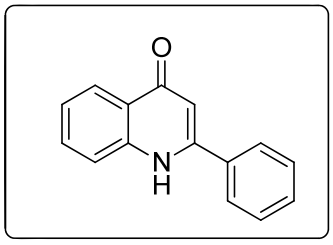
Pale-orange solid; 33 mg, 63% yield; m.p 115-118°C; ^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6) δ 8.10 (d, J = 7.5 Hz, 2H), 7.79 (s, 2H), 7.47 (d, J = 7.0 Hz, 2H), 7.34–7.33 (m, 2H), 7.23-7.21 (m, 2H), 4.73 (br s, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$ and DMSO-d_6) δ 152.4, 132.3, 130.2, 130.0, 128.9, 126.9, 125.6, 119.3, 119.0, 115.9

6. General procedure for the cyclization of amino chalcones (10a-f)

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of aminochalcone was dissolved in 2 mL of dry DMSO and the reaction mixture was placed in the pre-heated oil bath at 120 ºC for appropriate time. The reaction progress was monitored by TLC, after the reaction completion, the reaction mixture was quenched with water (50 mL) and cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

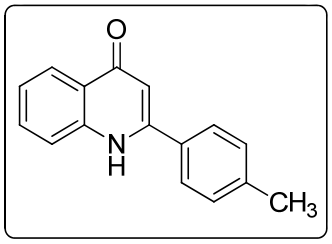
6.1 Characterisation of data for compounds 10a-f

2-phenylquinolin-4(1*H*)-one [21] **(10a)**



White powder; 30 mg, 61% yield; m.p. >200°C; ^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6): δ 11.48 (br s, 1H), 8.23 (d, J = 6.8 Hz, 1H), 7.74-7.60 (m, 3H), 7.54-7.51 (m, 1H), 7.44-7.40 (m, 3H), 7.26-7.23 (m, 1H), 6.39 (s, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$ and DMSO-d_6): δ 178.6, 150.5, 140.6, 134.7, 131.6, 130.2, 128.7, 127.4, 125.2, 125.1, 123.2, 118.5, 108.1

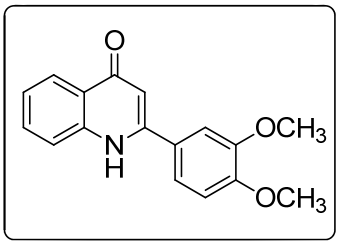
2-(*p*-Tolyl)quinolin-4(1*H*)-one [21] **(10b)**



Yellow solid; 17 mg, 34% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.74 (br s, 1H), 8.18 (d, J = 7.9 Hz, 1H), 7.83 (dd, J = 19.2, 7.9 Hz, 3H), 7.74 (t, J = 7.4 Hz, 1H), 7.47 (d, J = 7.8 Hz, 2H), 7.41 (t, J = 7.3 Hz, 1H), 6.41 (s, 1H), 2.47 (s, 3H). ^{13}C {^{1}H} NMR

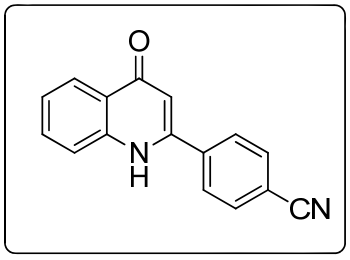
(125 MHz, DMSO-d_6): δ 177.4, 150.4, 140.9, 140.8, 132.2, 131.7, 130.0, 127.7, 125.3, 125.2, 123.6, 119.1, 107.4, 21.3

2-(3,4-Dimethoxyphenyl)quinolin-4(1*H*)-one [21] **(10c)**



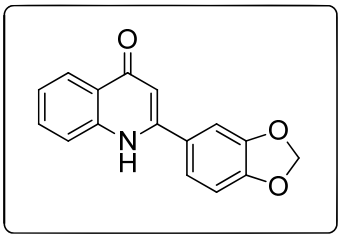
White solid; 35 mg, 71 % yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO-d_6): δ 11.57 (br s, 1H), 8.10 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 8.3 Hz, 1H), 7.67 (t, J = 8.2 Hz,1H), 7.43-7.39 (m, 2H), 7.33 (t, J = 7.4 Hz, 1H), 7.15 (d, J = 8.4 Hz, 1H), 6.39 (s, 1H), 3.90 (s, 3H), 3.85 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, DMSO-d_6): δ 177.4, 151.2, 150.3, 149.3, 140.9, 132.1, 126.9, 125.3, 125.2, 123.5, 120.6, 119.0, 112.2, 111.2, 107.2, 56.2, 56.1.

4-(4-Oxo-1,4-dihydroquinolin-2-yl)benzonitrile [21] **(10d)**



Off-white solid; 24 mg, 49% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.86 (br s, 1H), 8.12-8.06 (m, 5H), 7.75-7.68 (m, 2H), 7.36 (s, 1H), 6.42 (s, 1H); ^{13}C{^{1}H} NMR (125 MHz, DMSO- d_6): δ 177.4, 148.6, 141.0, 139.0, 133.3, 133.0, 132.6, 128.9, 125.4, 125.2, 124.0, 119.3, 118.8, 113.3, 108.7.

2-(benzo[*d*][1,3]dioxol-5-yl)quinolin-4(1*H*)-one [21] **(10f)**



Yellow solid; 29 mg, 60% yield; m.p. >200°C; ^{1}H NMR (500 MHz, DMSO- d_6): δ 11.55 (br s, 1H), 8.09-8.07 (m, 1H), 7.75 (d, J = 8.3 Hz, 1H), 7.67-7.64 (m, 1H), 7.43 (d, J = 1.8 Hz, 1H), 7.38 (dd, J = 8.1, 1.9 Hz, 1H), 7.34-7.31 (m, 1H), 7.13 (d, J = 8.1 Hz, 1H), 6.30 (s, 1H), 6.15 (s, 2H). ^{13}C {^{1}H}

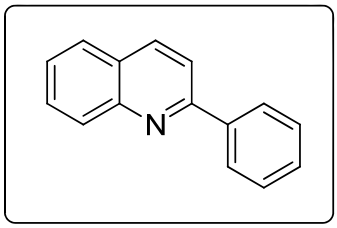
NMR (125 MHz, DMSO- d_6): δ 177.3, 150.0, 149.6, 148.3, 140.9, 132.2, 128.4, 125.3, 125.1, 123.6, 122.3, 119.1, 109.1, 108.1, 107.3, 102.3

7. General procedure for C-C bond formation of Povarov reaction 12a-f

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of Benzylidene aniline and butyl vinyl ether (1.25 equiv) were dissolved in 2 mL of dry DMSO and the reaction mixture was pre-heated oil bath at 100 ºC for appropriate time. The reaction completion was monitored by TLC and the reaction mixture was quenched with water (50 mL), then cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

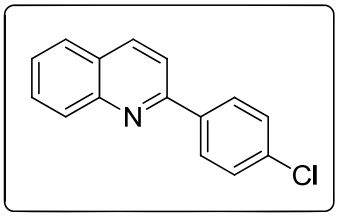
7.1 Characterization of data for the compounds (12a-f)

2-Phenylquinoline[22] **(12a)**



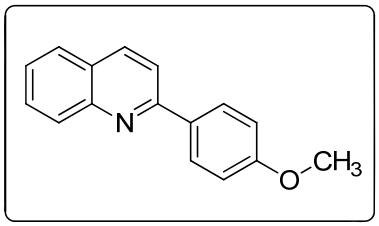
White solid; (35 mg), 62% yield; m.p. 79-81°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25-8.23 (m, 1H), 8.21-8.19 (m, 3H), 7.91 (d, J = 8.5 Hz, 1H), 7.86 (d, J = 8.5 Hz, 1H), 7.78-7.74 (m, 1H), 7.58-7.54(m, 3H), 7.52-7.48 (m, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.4, 148.3, 139.7, 136.8, 129.8, 129.7, 129.3, 128.8, 127.6, 127.5, 127.2, 126.3, 119.0.

2-(4-Chlorophenyl)quinolone [22] **(12b)**



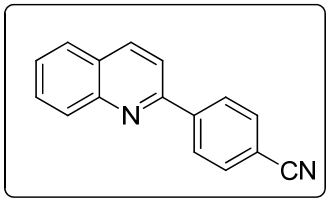
White solid; (28 mg), 51% yield; m.p. 104-106°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23 (d, J = 8.6 Hz, 1H), 8.19 (d, J = 8.5 Hz, 1H), 8.15-8.12 (m, 2H), 7.85 (d, J = 8.5 Hz, 2H), 7.78-7.74 (m, 1H), 7.58-7.54 (m, 1H), 7.53-7.51 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.0, 148.2, 138.0, 136.9, 135.5, 129.8, 129.7, 129.0, 128.8, 127.5, 127.2, 126.5, 118.6.

2-(4-Methoxyphenyl)quinolone [22] **(12c)**



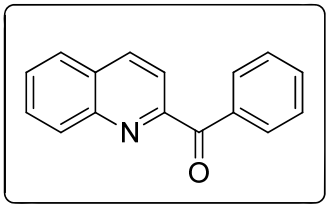
Off-white solid; (39 mg), 70% yield; m.p. 121-124°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.21 (d, J = 8.6 Hz, 1H), 8.17-8.15 (m, 3H), 7.87 (d, J = 8.6 Hz, 1H), 7.83 (dd, J = 8.1, 0.9 Hz, 1H), 7.75-7.72 (m, 1H), 7.54-7.51 (m, 1H), 7.09-7.06 (m, 2H), 3.92 (s, 3H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 160.8, 156.9, 148.3, 136.7, 132.2, 129.6, 128.9, 127.4, 126.9, 125.9, 118.6, 114.2, 55.4.

2-(4-cyanophenyl)quinolone [23] **(12d)**



Colourless solid; 30 mg, 54% yield; m.p. 89-91°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.23-8.20 (m, 3H), 8.10 (d, J = 8.5 Hz, 1H), 7.80 (dd, J = 12.5, 8.4 Hz, 2H), 7.75-7.73 (m, 2H), 7.71-7.68 (m, 1H), 7.53-7.49 (m, 1H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 154.9, 148.3, 143.7, 137.3, 132.6, 130.2, 129.9, 128.1, 127.6, 127.5, 127.1, 118.8, 118.6, 112.7.

Phenyl(quinolin-2-yl)methanone[24] **(12f)**



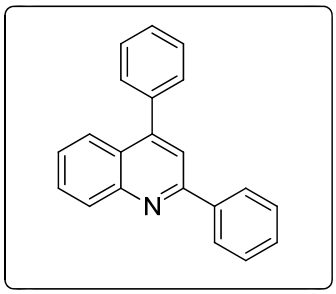
Yellow solid; (23 mg), 42% yield; m.p. 102-104°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.28 (d, J = 8.5 Hz, 1H), 8.17-8.15 (m, 2H), 8.13 (d, J = 8.4 Hz, 1H), 8.04 (d, J = 8.5 Hz, 1H), 7.84 (d, J = 8.1 Hz, 1H), 7.73-7.69 (m, 1H), 7.60-7.53 (m, 2H), 7.46-7.43 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 193.8, 154.7, 146.7, 137.1, 136.2, 133.1, 131.5, 130.6, 130.1, 128.9, 128.4, 128.1, 127.6, 120.8.

8. General procedure for C-C bond formation of Friedlander's synthesis 14a-d

In a 25 mL of pressure tube, 50 mg (0.3 mmol) of 2-aminobenzophenone and acetophenone (1 equiv.) was dissolved in 2 mL of dry DMSO and the reaction mixture was placed in the pre-heated oil bath at 120 ºC for appropriate time. The reaction progress was monitored by TLC, after the reaction completion, the reaction mixture was quenched with water (50 mL) and cooled it to room temperature. Then it was extracted with ethyl acetate (3 × 10 mL) and the separated organic layer was dried over anhydrous Na_2SO_4. The organic layer was evaporated under reduced pressure and the crude product was purified by column chromatography using silica gel (60-120 mesh), eluted with ethyl acetate and hexane mixture.

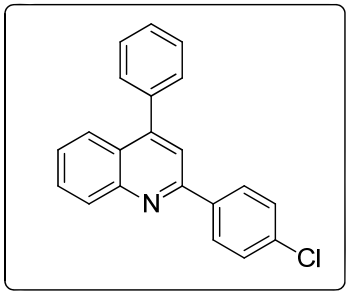
8.1 Characterization of data for the compounds (14a-d)

2,4-Diphenylquinoline [25] (14a)



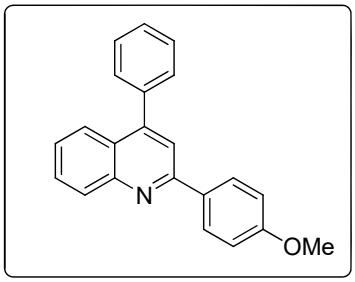
White solid; 48 mg, 66% yield; m.p. 105-108°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.17 (d, J = 8.4 Hz, 1H), 8.12-8.10 (m, 2H), 7.82 (d, J = 8.3 Hz, 1H), 7.74 (s, 1H), 7.67-7.63 (m, 1H), 7.49-7.46 (m, 4H), 7.45-7.43 (m, 3H), 7.41-7.36 (m, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.9, 149.2, 148.8, 139.6, 138.4, 130.1, 129.6 (2C), 129.4, 128.8, 128.6, 128.4, 127.6, 126.4, 125.8, 125.7, 119.4.

2-(4-Chlorophenyl)-4-phenylquinoline [26] (14b)



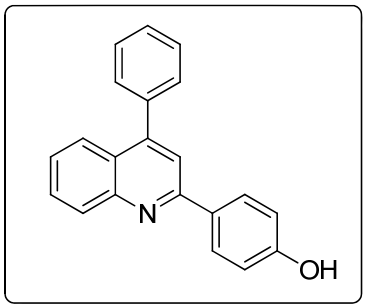
White solid; 51 mg, 64% yield; m.p. 113-115°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (d, J = 8.5 Hz, 1H), 8.19-8.17 (, 2H), 7.93 (dd, J = 8.5, 1.0 Hz, 1H), 7.81 (s, 1H), 7.79-7.75 (m, 1H), 7.59-7.57 (m, 4H), 7.56-7.50 (m, 4H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 155.5, 149.4, 148.8, 138.3, 138.0, 135.6, 130.1, 129.7, 129.5, 129.0, 128.8, 128.6, 128.5, 126.5, 125.8, 125.7, 118.9.

2-(4-Methoxyphenyl)-4-phenylquinoline [26] (14c)



Yellow solid; 57 mg, 73% yield; m.p. 118-121°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.25 (d, J = 8.5 Hz, 1H), 8.20 (d, J = 8.7 Hz, 2H), 7.91 (d, J = 8.3 Hz, 1H), 7.81 (s, 1H), 7.75 (t, J = 7.6 Hz, 1H), 7.59-7.54 (m, 5H), 7.49-7.46 (m, 1H), 7.08 (d, J = 8.6 Hz, 2H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 160.9, 156.4, 149.1, 148.8, 138.5, 132.2, 129.9, 129.6, 129.5, 128.9, 128.6, 128.4, 126.0, 125.6, 125.5, 118.9, 114.2, 55.4.

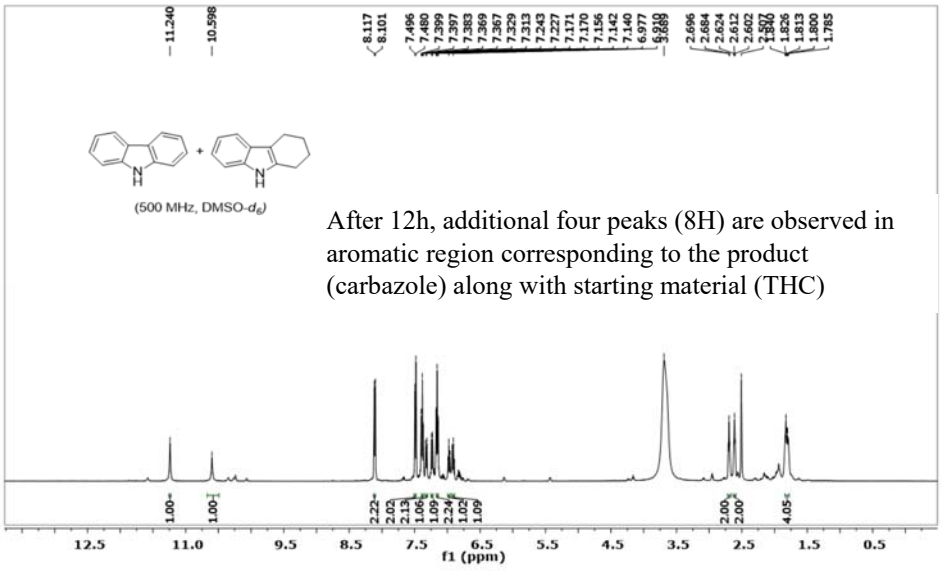
4-(4-Phenylquinolin-2-yl)phenol[26] **(14d)**

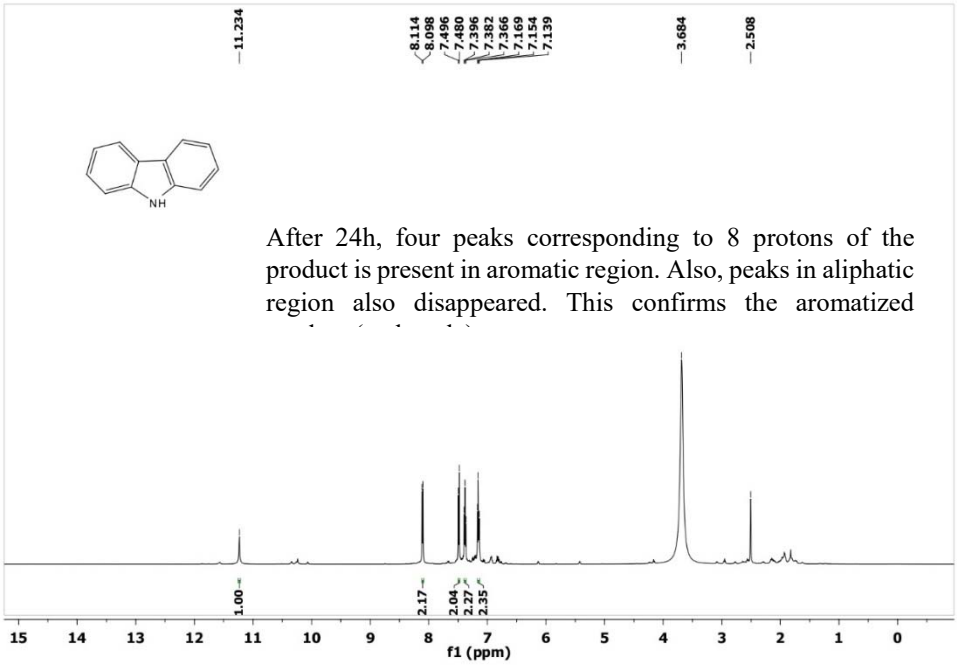


Orange solid; 35 mg, 47%; m.p. 114-117°C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.35 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 6.6 Hz, 2H), 7.92 (d, J = 8.4 +Hz, 1H), 7.78-7.74 (m, 2H), 7.58-7.53 (m, 5H), 7.49 (t, J = 7.6Hz, 1H), 6.92 (d, J = 7.4 Hz, 2H). ^{13}C {^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.9, 157.2, 149.6, 148.4, 138.3, 131.3, 129.8, 129.5, 129.3, 129.1, 128.6, 128.5, 126.1, 125.7, 125.5, 119.6, 116.0.

8. Mechanistic study:

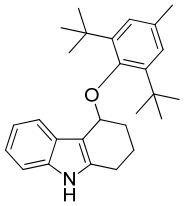
The reaction of 1,2,3,4-tetrahydrocarbazole (10 mg) and 0.5 mL of DMSO-d_6 in NMR tube was heated at 100ºC in a closed condition. After 12 hours and 24 hours, the reaction was analysed directly (without any workup) by NMR. It has clearly shown that the carbazole product (**2a**) was completely formed at 24 hours while in 12 hours, there was a peak for both THC (**1a)** and carbazole (**2a)** in NMR.


11.240
10.598
8.117
8.101
7.496
7.480
7.399
7.397
7.383
7.369
7.367
7.329
7.313
7.243
7.227
7.171
7.170
7.156
7.142
7.140
6.977
3.689
2.696
2.684
2.624
2.612
2.602
1.826
1.813
1.800
1.785
(500 MHz, DMSO-d_6)
After 12h, additional four peaks (8H) are observed in aromatic region corresponding to the product (carbazole) along with starting material (THC)
1.00
1.00
2.22
2.02
2.13
1.06
1.09
2.24
1.02
1.09
2.00
2.00
4.05
12.5
11.0
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


11.234
8.114
8.098
7.496
7.480
7.396
7.382
7.366
7.169
7.154
7.139
3.684
2.508
NH
After 24h, four peaks corresponding to 8 protons of the product is present in aromatic region. Also, peaks in aliphatic region also disappeared. This confirms the aromatized
1.00
2.17
2.04
2.27
2.35
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

8.1 Radical trapping experiments

HRMS of compound 1ab

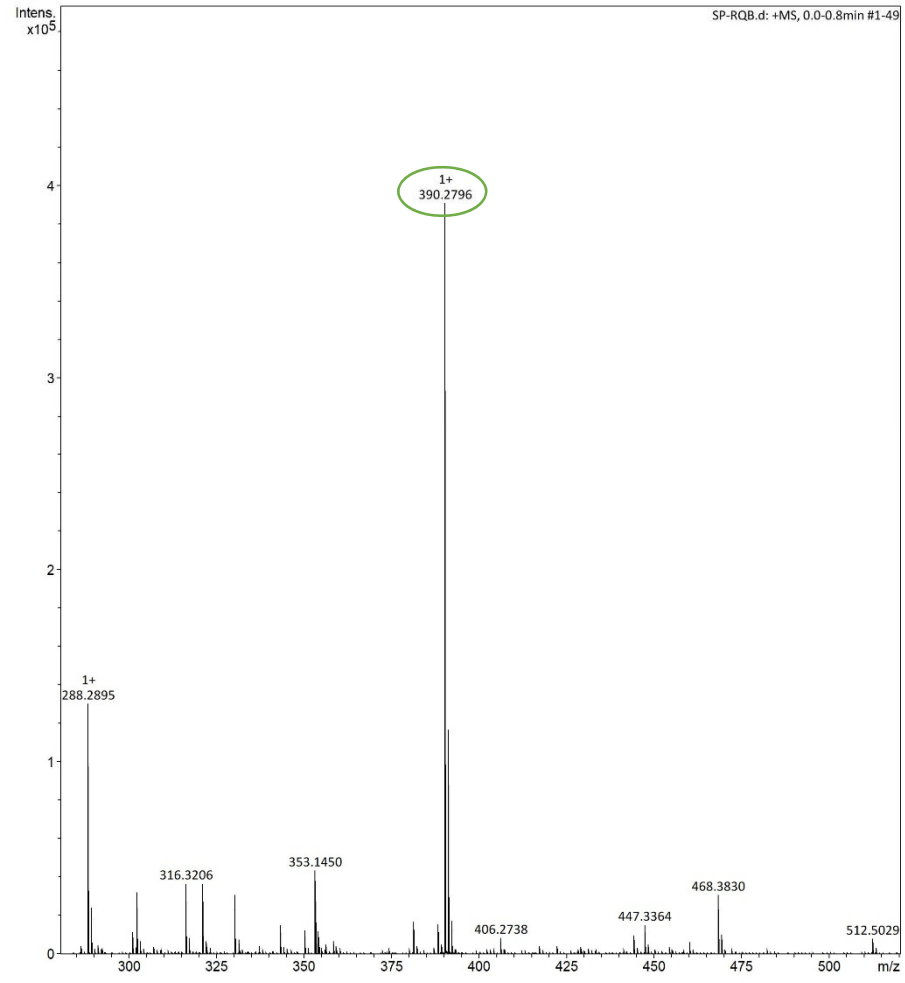


1ab

Generic Display Report

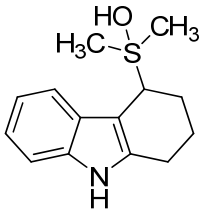
Analysis Info

Analysis Name	\\10.2.4.74\rn\HRMS DATA\RN LAB\PREETHIKA\SP-RQB.d	Acquisition Date	28-Oct-25 3:26:55 PM
Method	tune_low_Pos.m	Operator	UOH
Sample Name	SP-RQB	Instrument	maXis
Comment			



Bruker Compass DataAnalysis 4.2 printed: 28-Oct-25 4:00:24 PM by: RN LAB Page 1 of 1

LC-MS data for the intermediate IV in Fig. 2



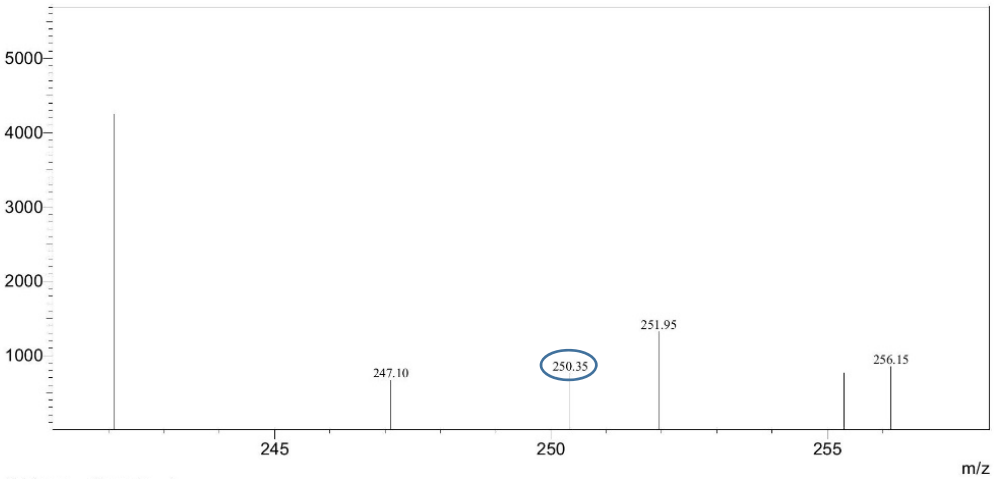
==== Shimadzu Labsolutions Data Report ====

Sample Information

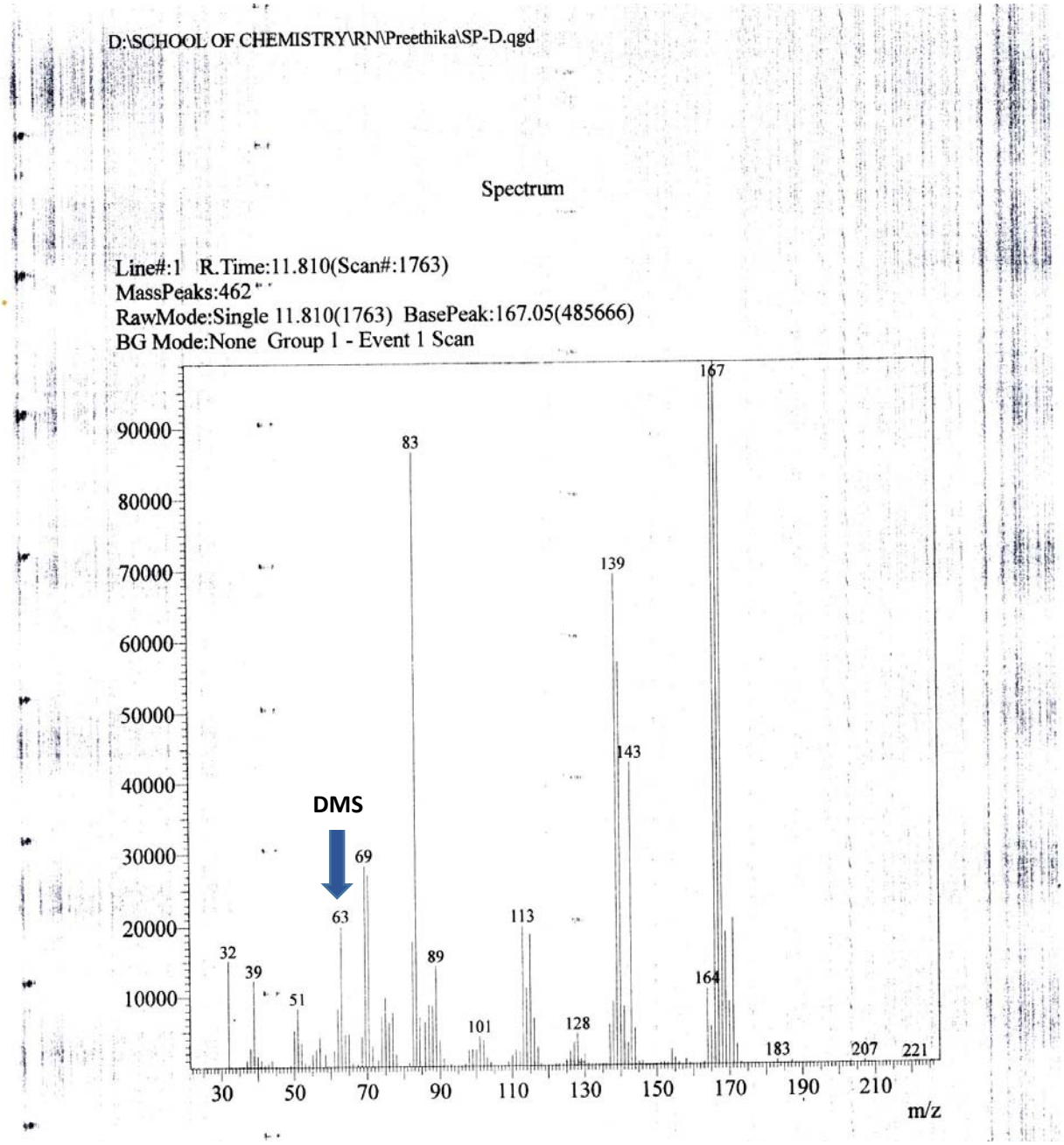
Sample Name	: SP-I
Injection Volume	: 2
Method File	: 170919-MASTER METHOD1-Q1.lcm
Data File	: 14102025-SP-I-ESI-002.lcd

<Spectrum>

R.Time:----(Scan#:----)
MassPeaks:102 BasePeak:220.10(13072)
Spectrum Mode:Averaged 0.171-1.573(63-573)
BG Mode:Averaged 1.392-1.980(507-721) Polarity:Positive Segment 1 - Event 1



GC-MS data for the confirmation of dimethyl sulfide



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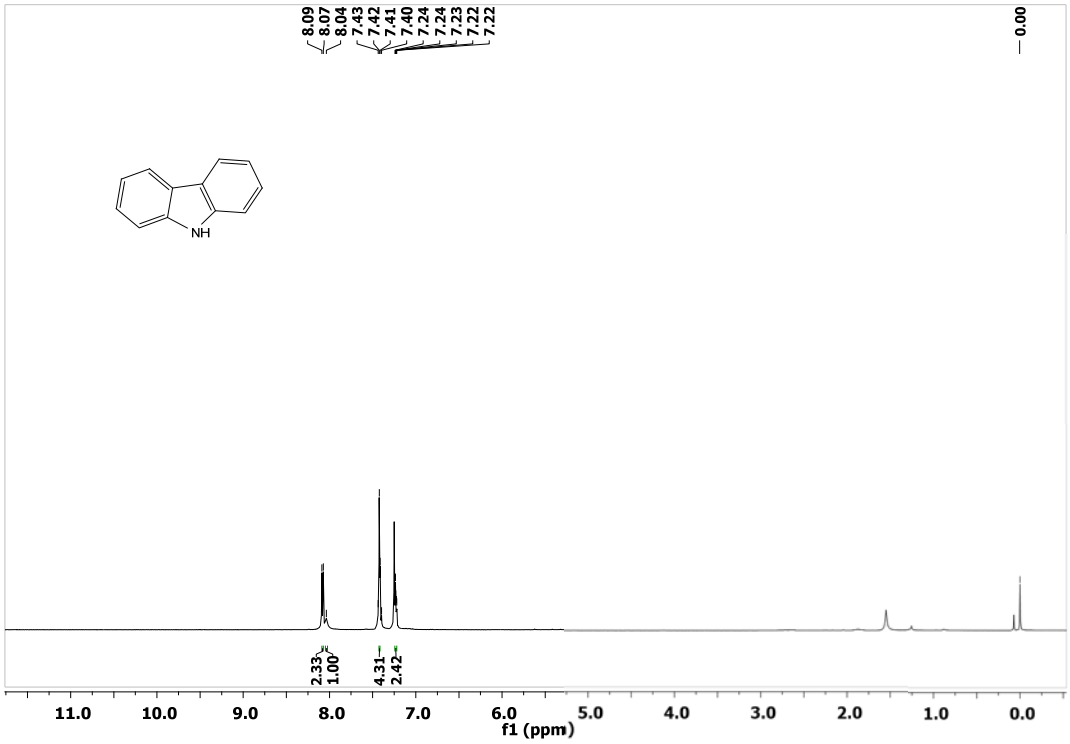
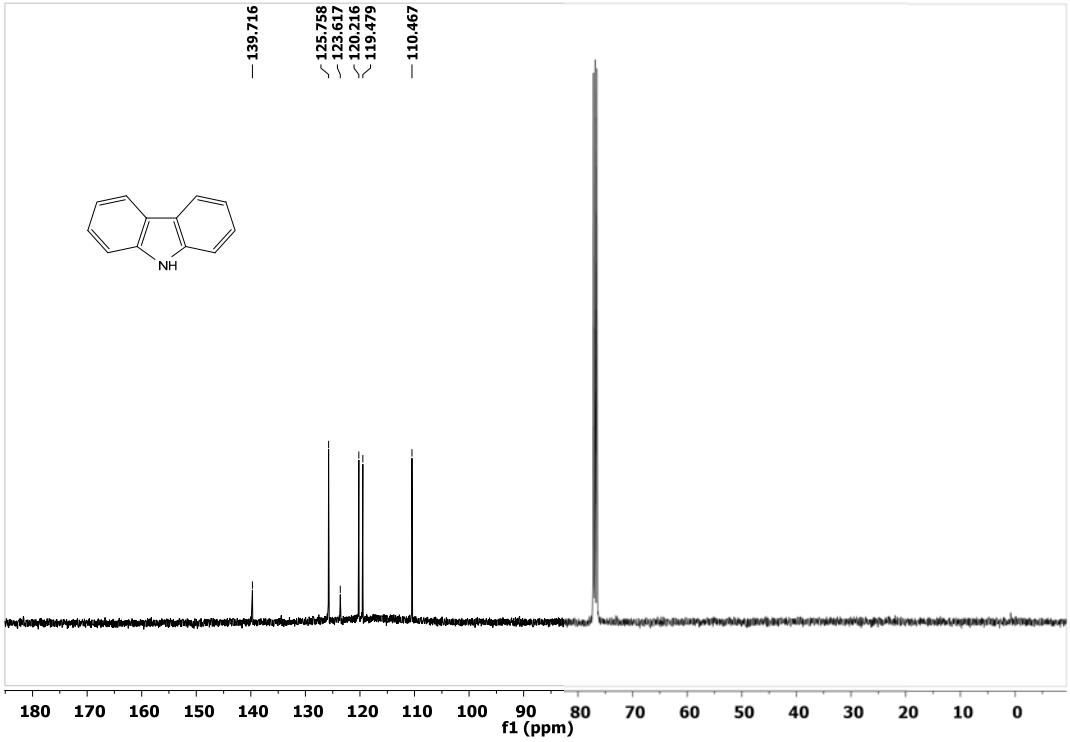
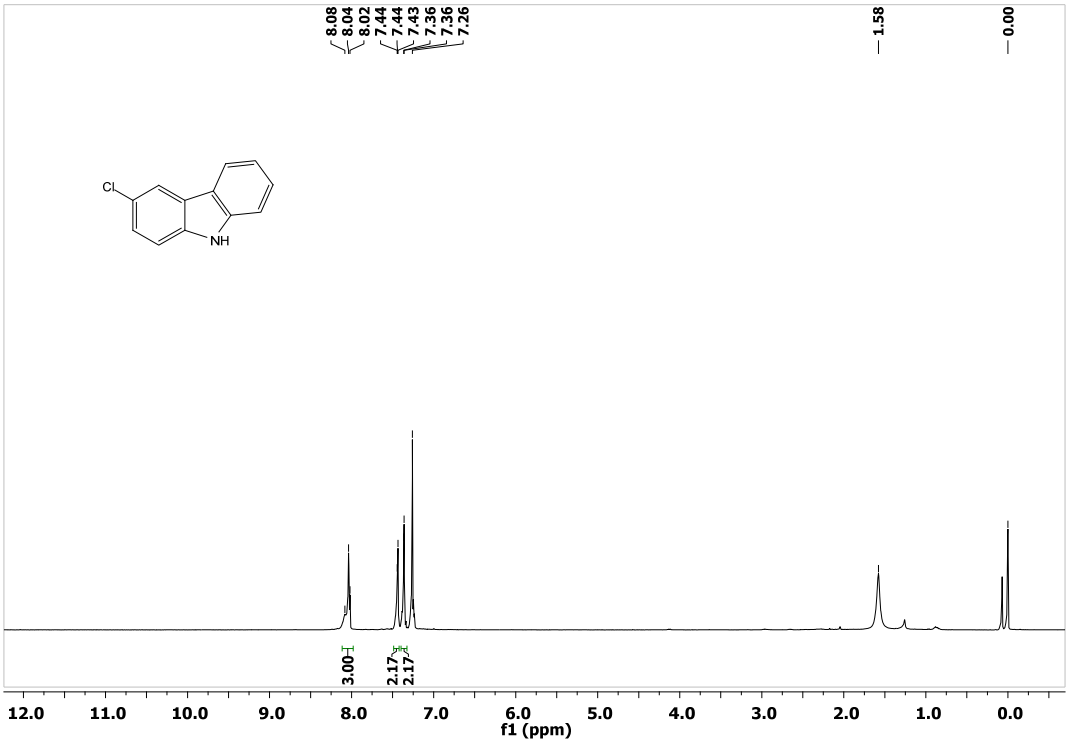
^{1}H NMR (500 MHz, $CDCl_3$) (**2a**)



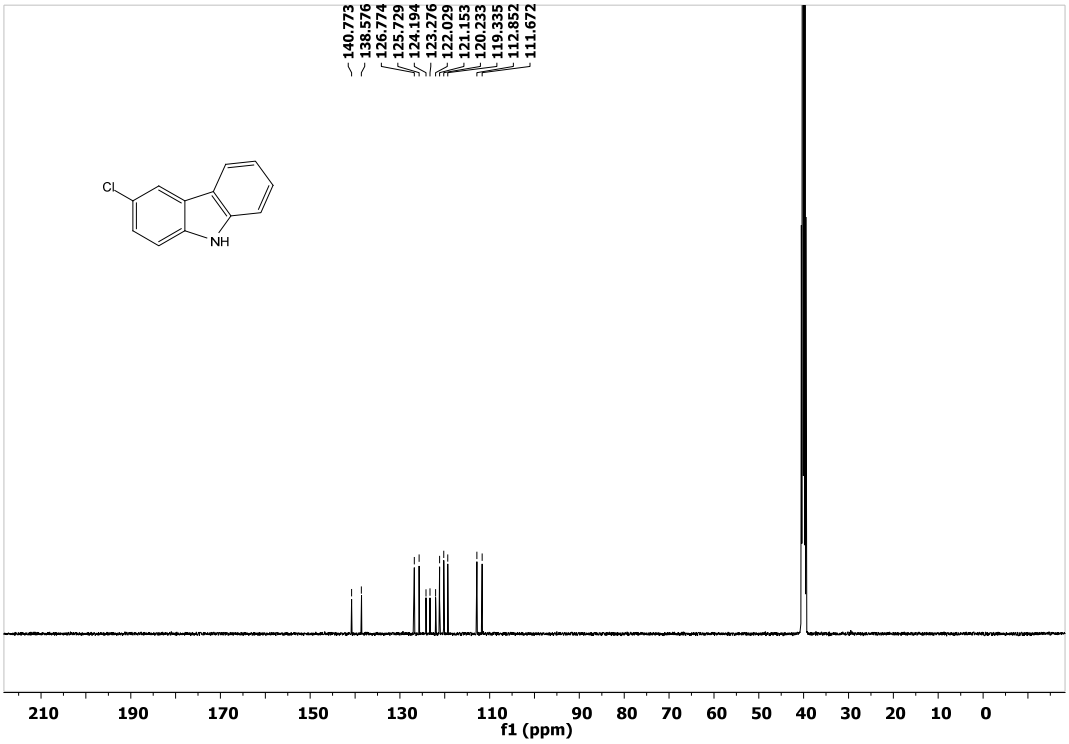
^{13}C NMR (125 MHz, $CDCl_3$) (**2a**)



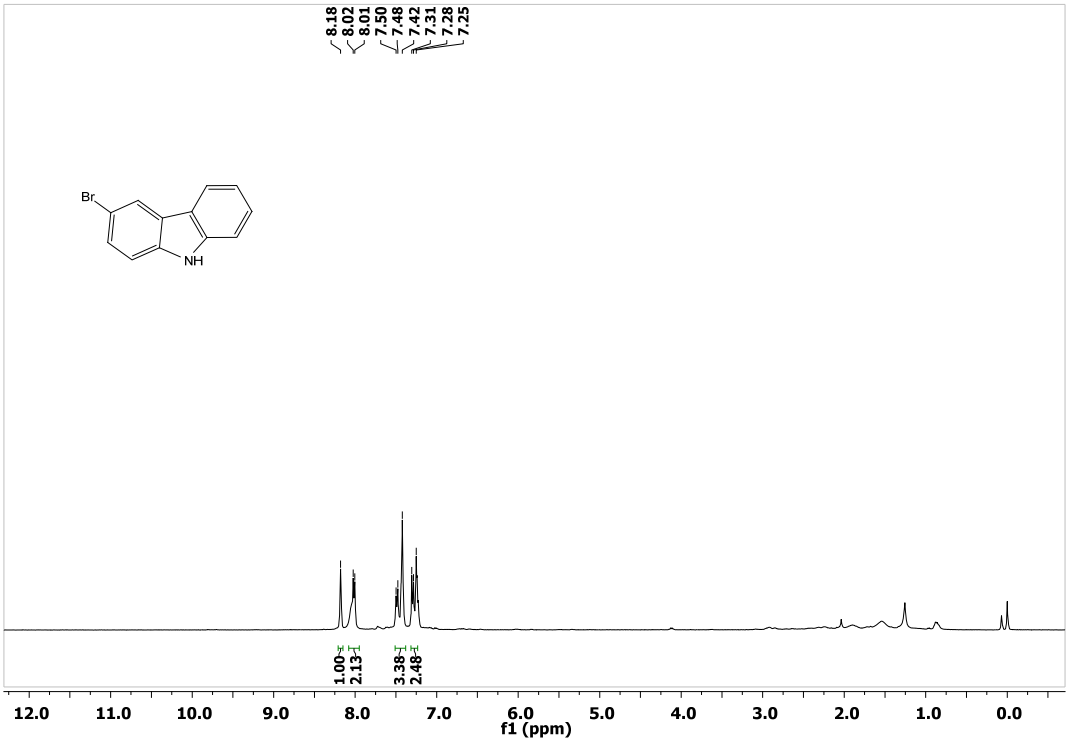
^{1}H NMR (400 MHz, $CDCl_3$) (**2b**)



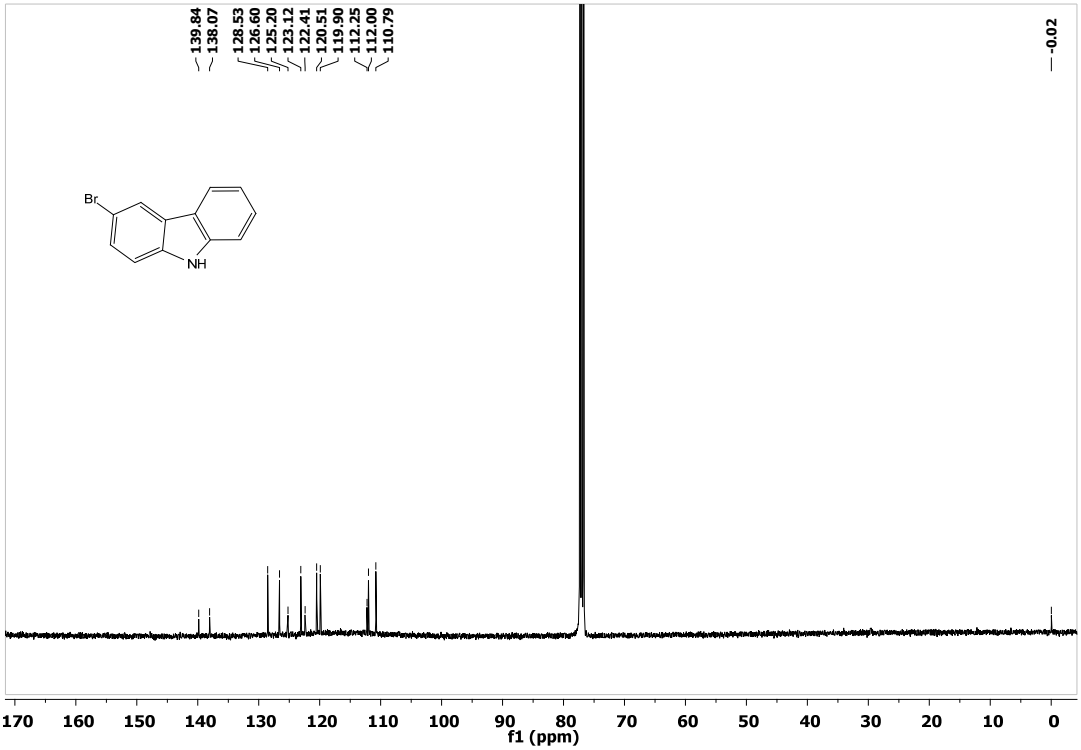
^{1}H NMR (400 MHz, $CDCl_3$) (**2b**)



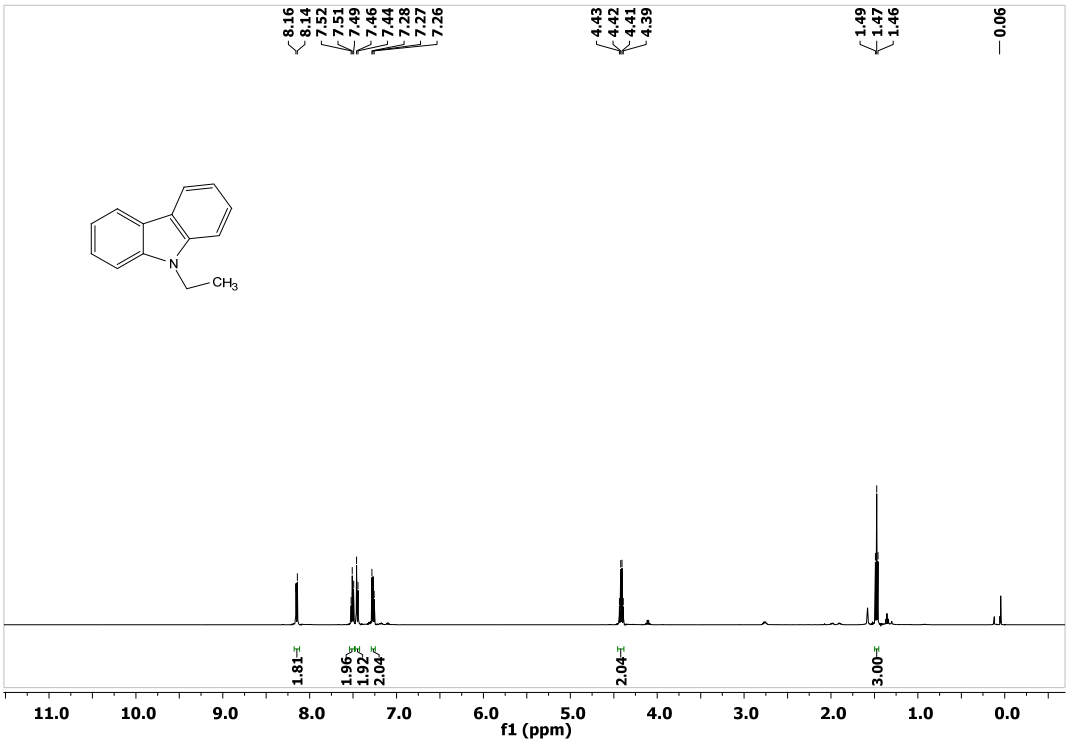
^{1}H NMR (400 MHz, $CDCl_3$) (**2c**)



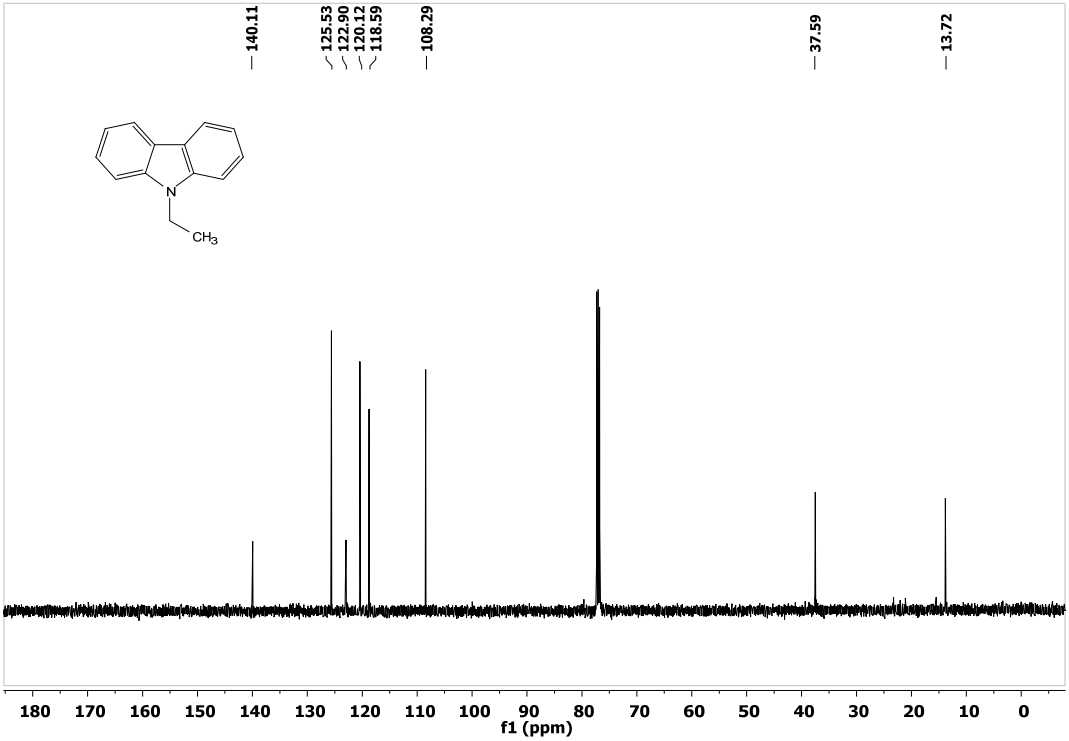
^{13}C NMR (100 MHz, $CDCl_3$) (**2c**)



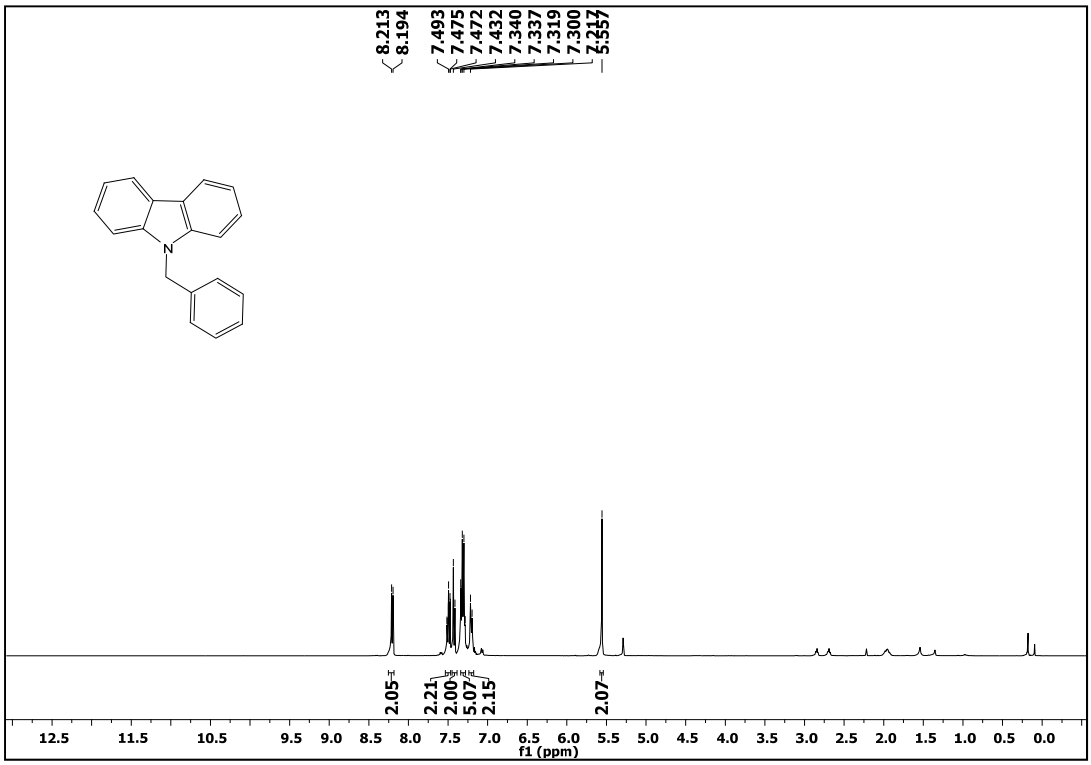
^{1}H NMR (500 MHz, $CDCl_3$) (**2d**)



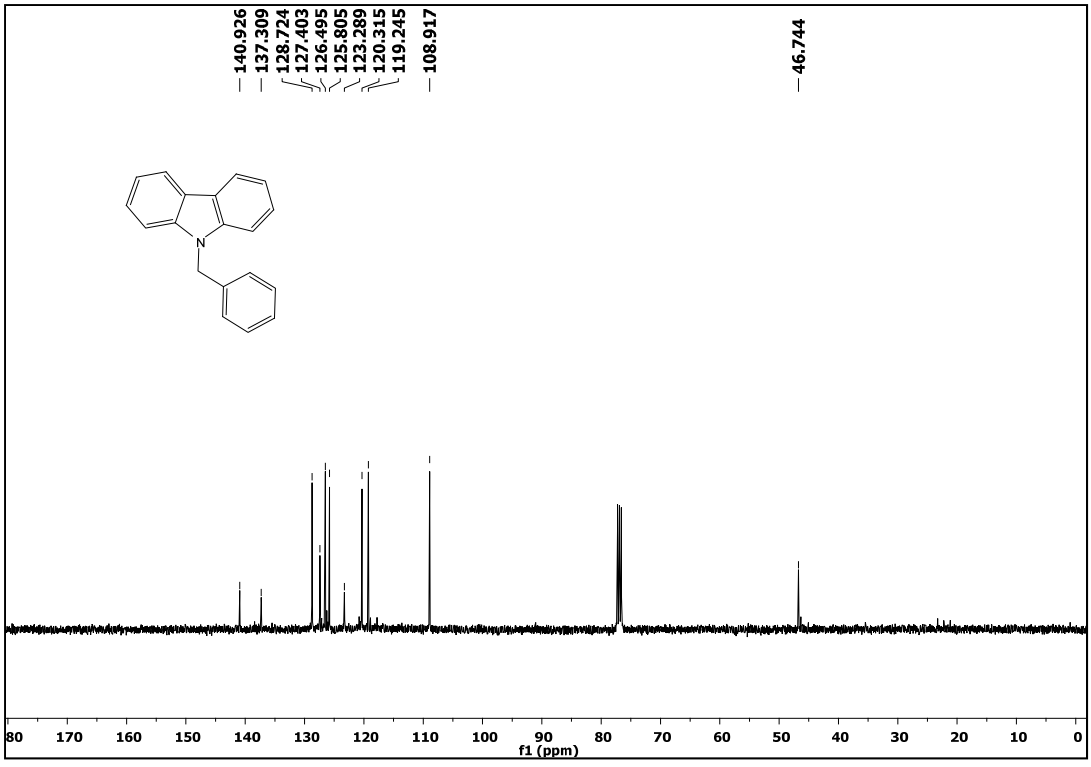
^{13}C NMR (125 MHz, $CDCl_3$) (**2d**)



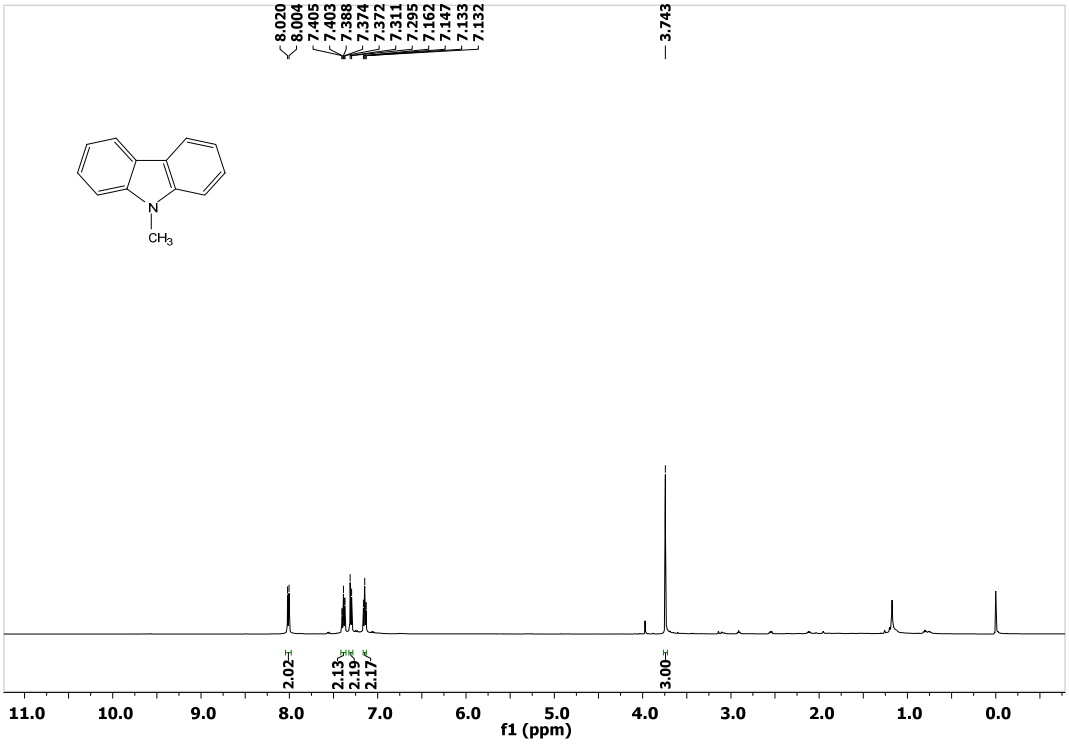
^{1}H NMR (400 MHz, $CDCl_3$) (**2e**)



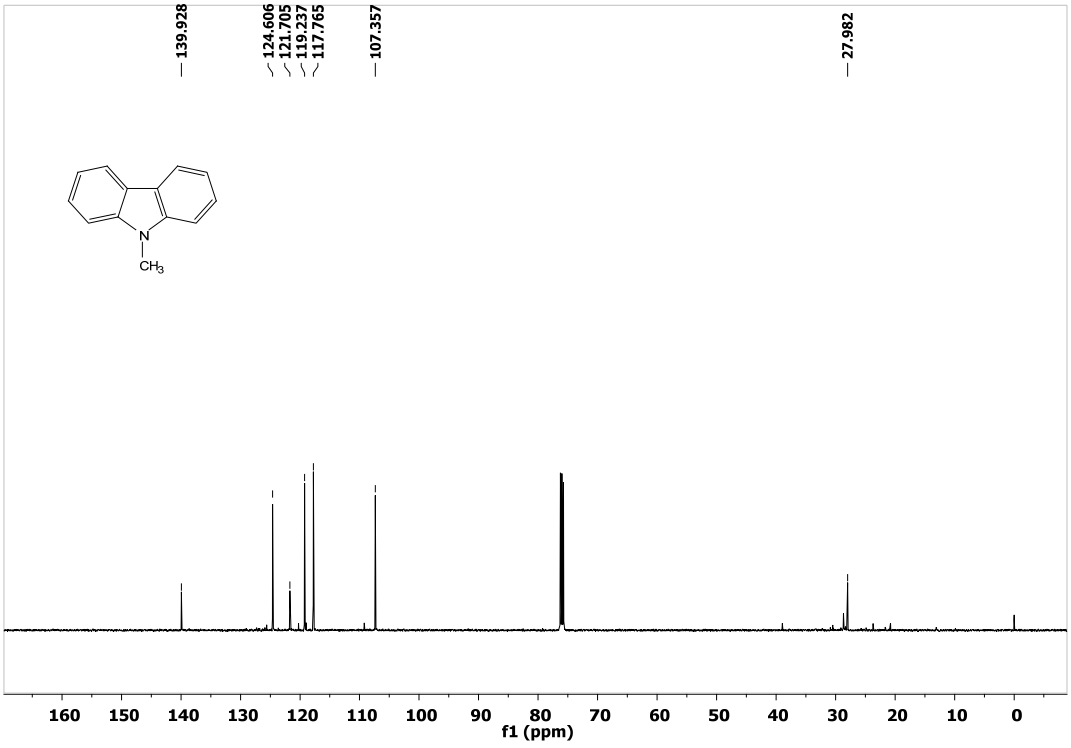
^{13}C NMR (125 MHz, $CDCl_3$) (**2e**)



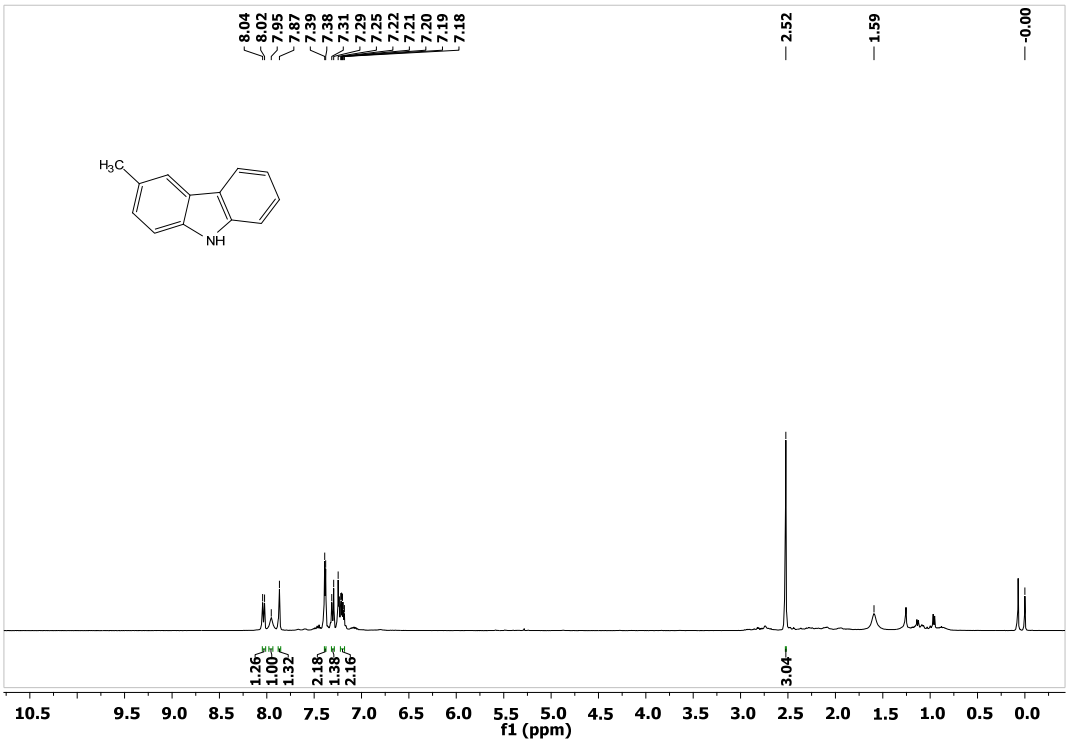
^{1}H NMR (500 MHz, $CDCl_3$) (**2f**)



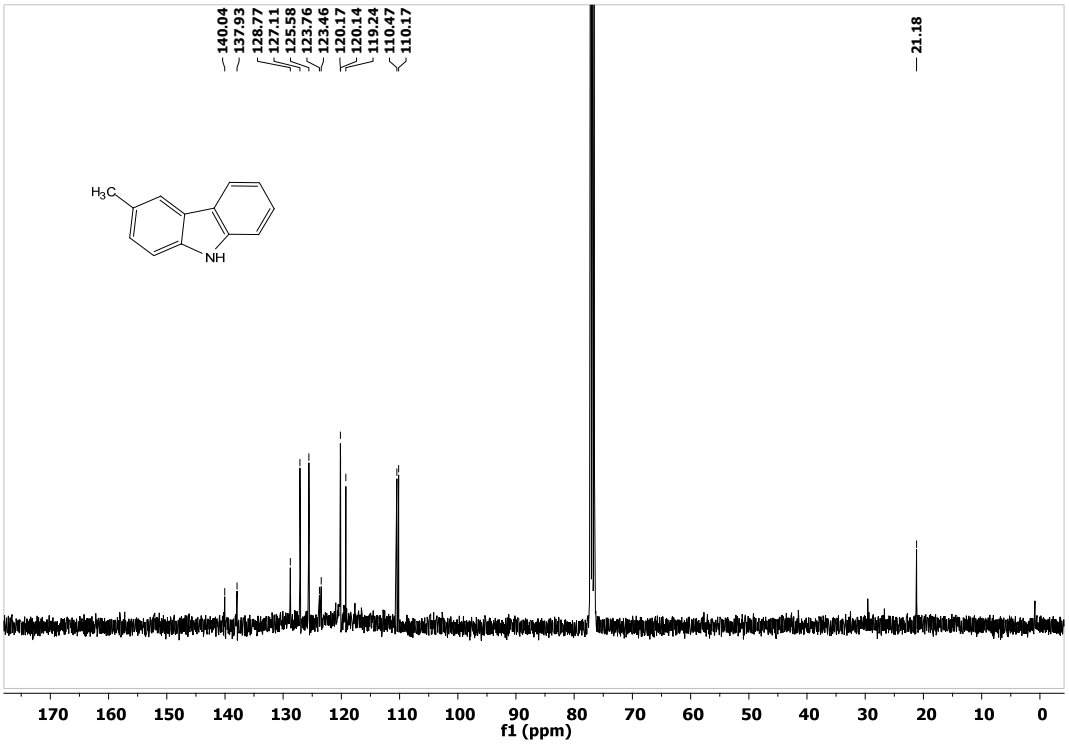
^{13}C NMR (125 MHz, $CDCl_3$) (**2f**)



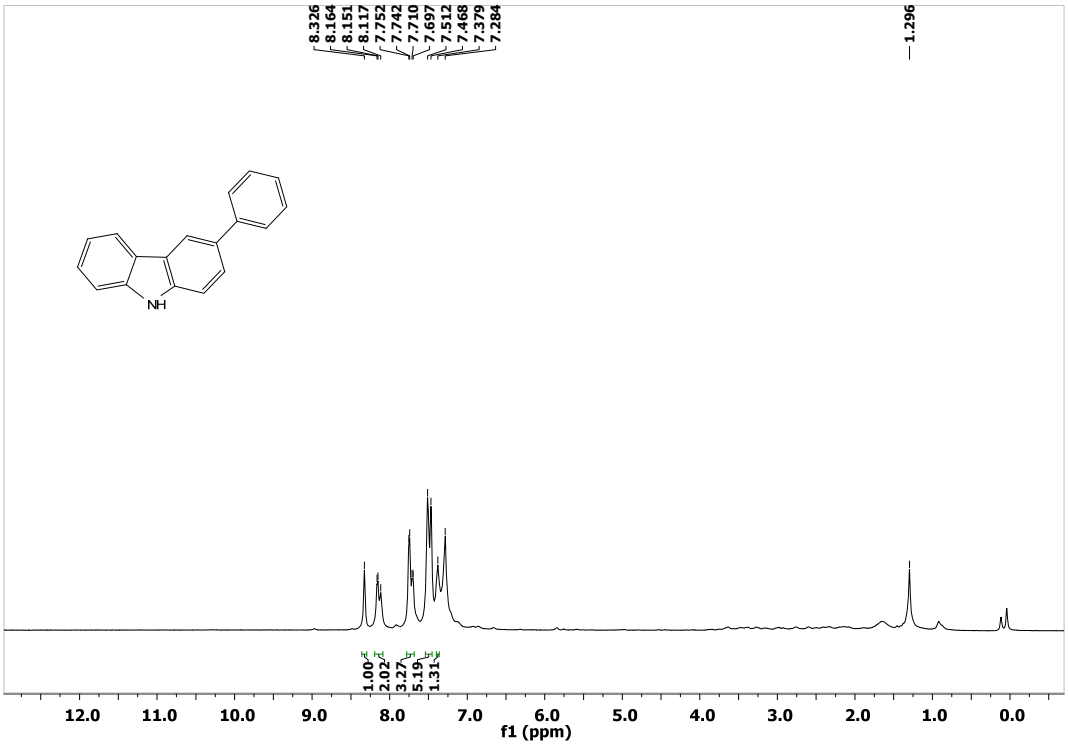
^{1}H NMR (400 MHz, $CDCl_3$) (**2h**)



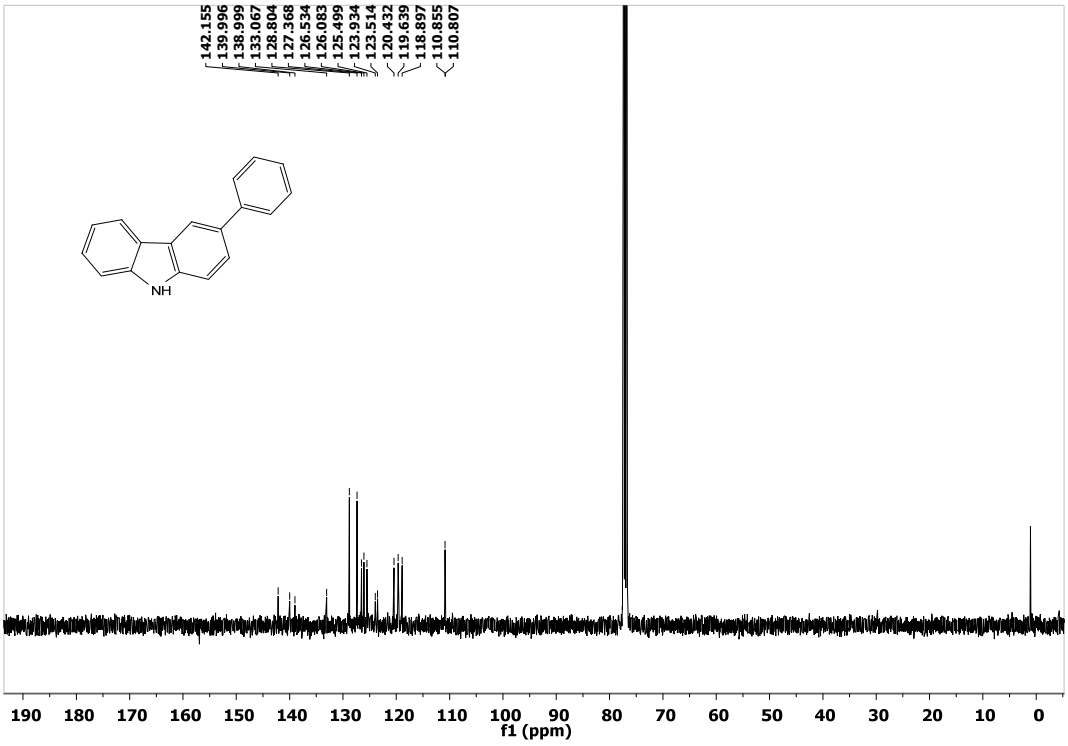
^{13}C NMR (100 MHz, $CDCl_3$) (**2h**)



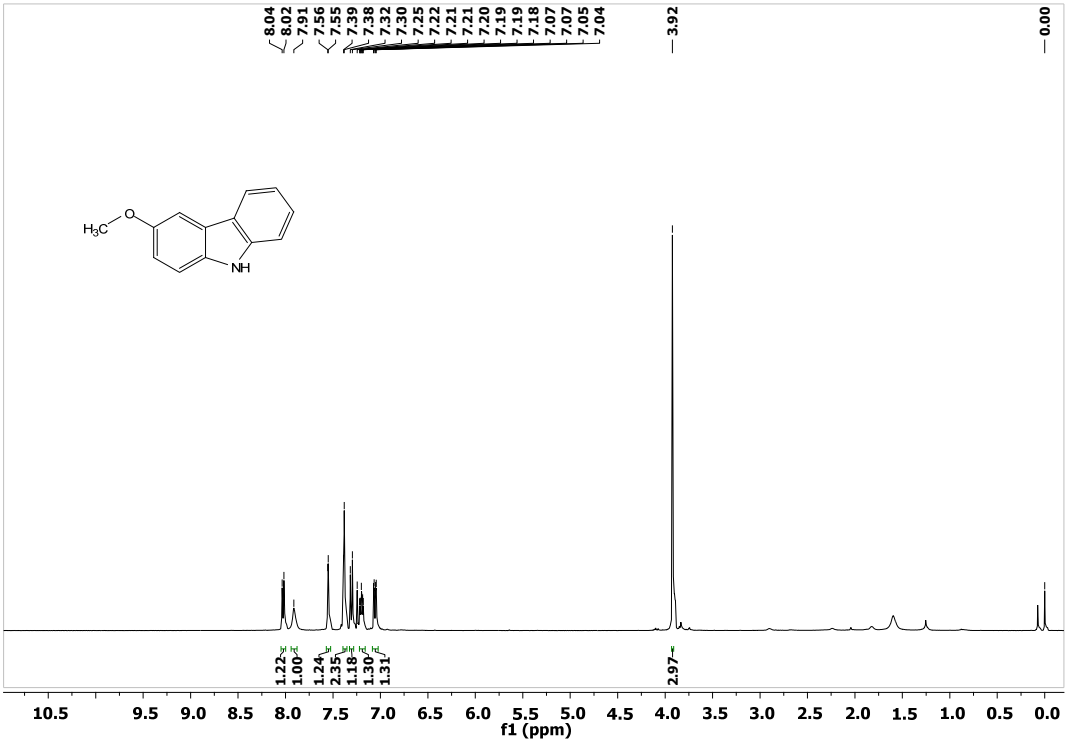
^{1}H NMR (500 MHz, $CDCl_3$) (**2i**)



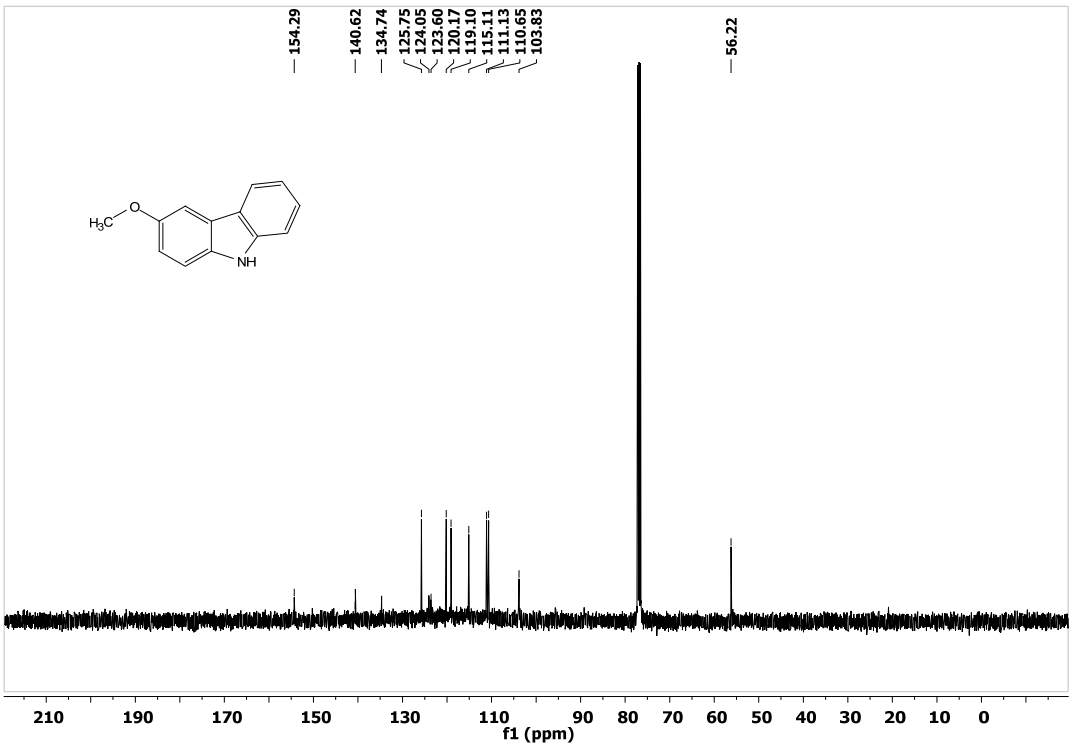
^{13}C NMR (125 MHz, $CDCl_3$) (**2i**)



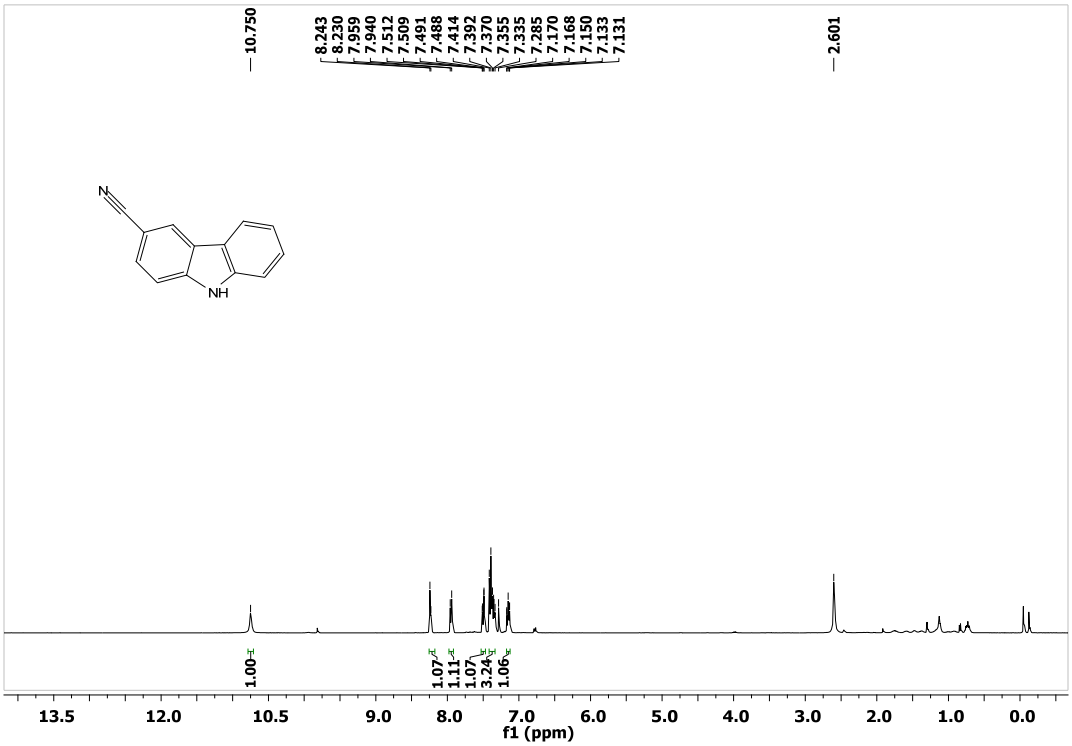
^{1}H NMR (400 MHz, $CDCl_3$) (**2j**)



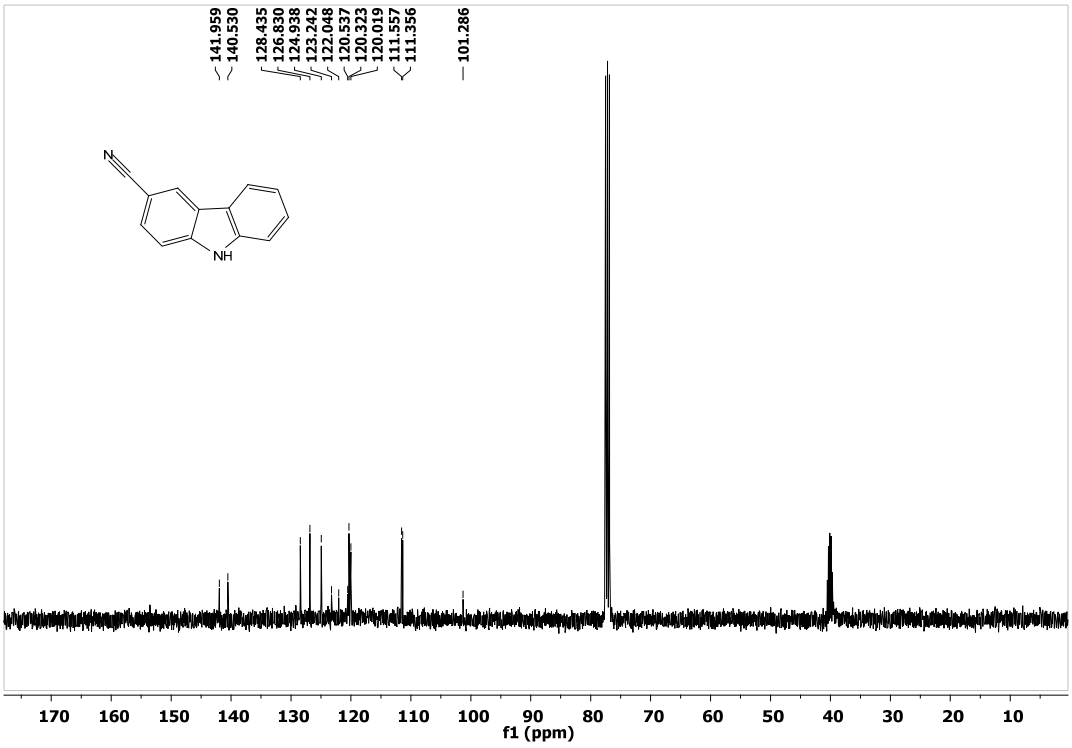
^{13}C NMR (100 MHz, $CDCl_3$) (**2j**)



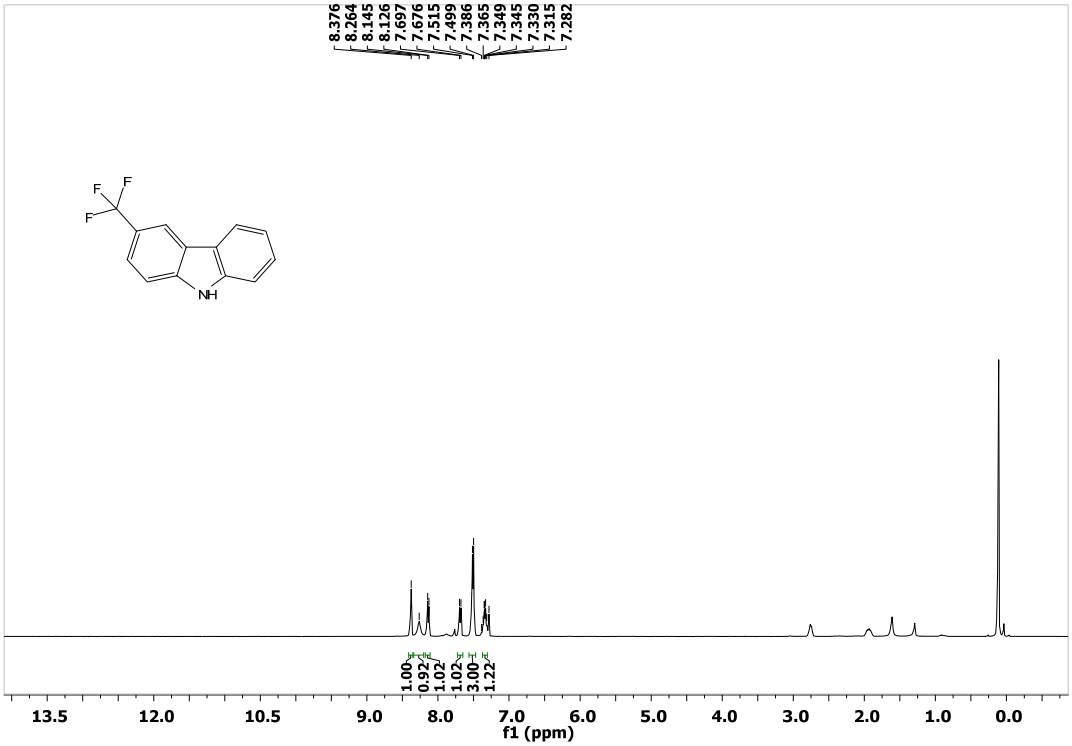
^{1}H NMR (400 MHz, $CDCl_3$ and DMSO-d_6) (**2k**)



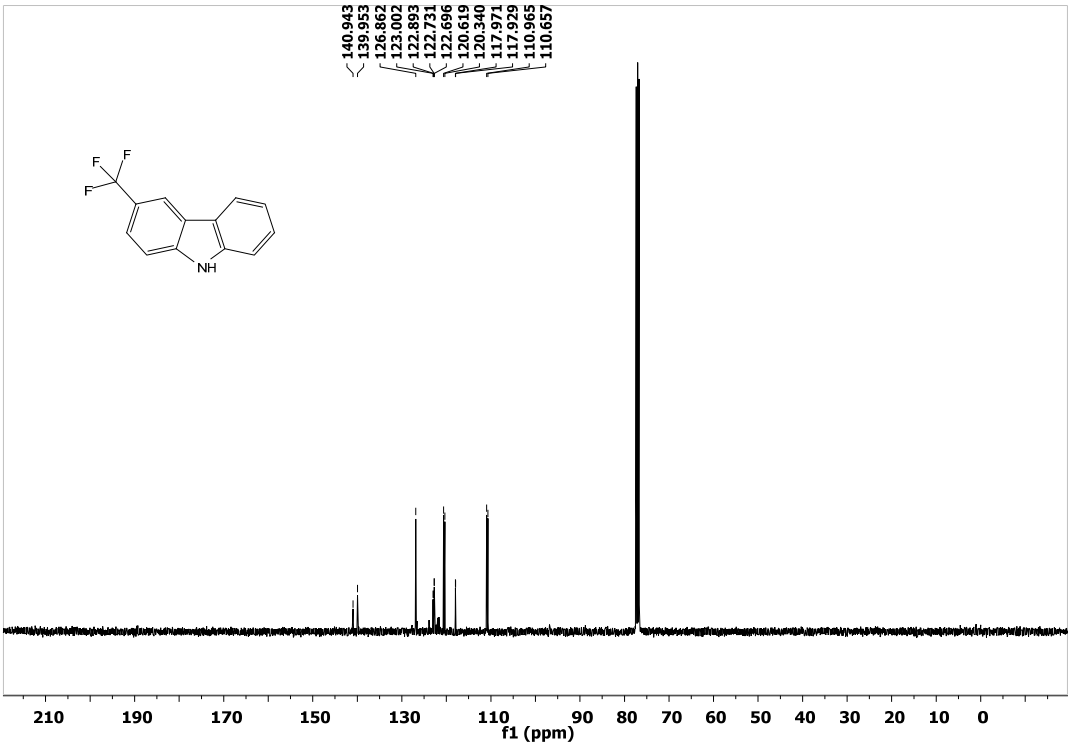
^{13}C NMR (100 MHz, $CDCl_3$ and DMSO-d_6) (**2k**)



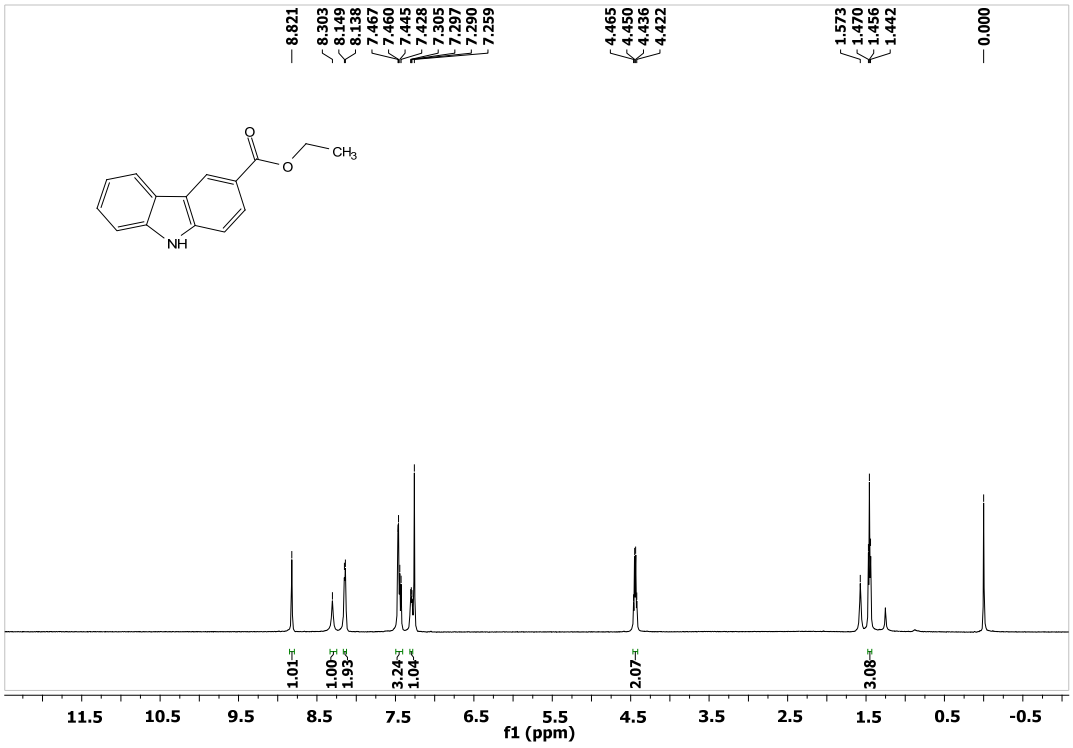
^{1}H NMR (400 MHz, $CDCl_3$) (**2l**)



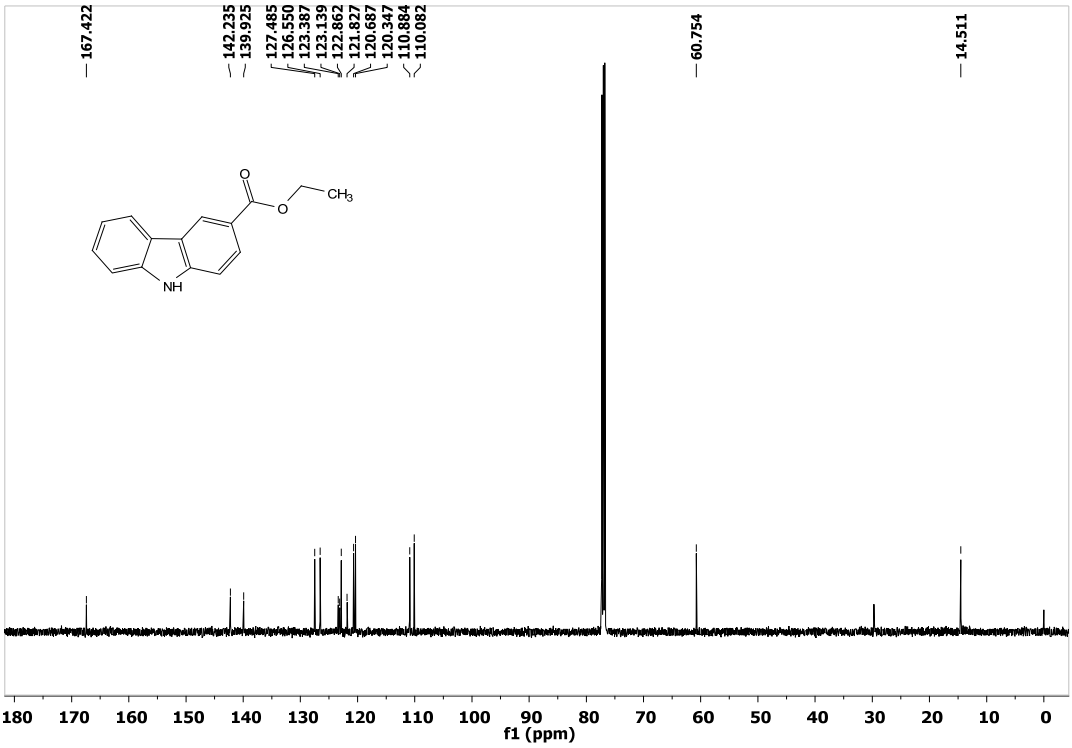
^{13}C NMR (100 MHz, $CDCl_3$) (**2l**)



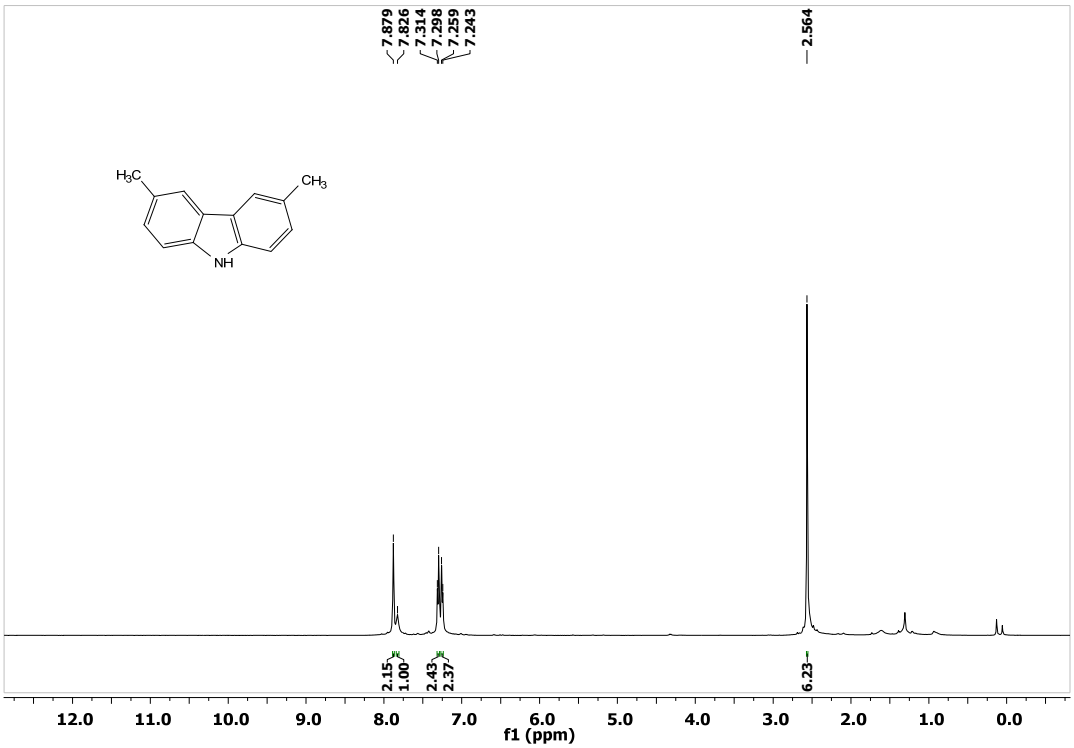
^{1}H NMR (500 MHz, $CDCl_3$) (**2m**)



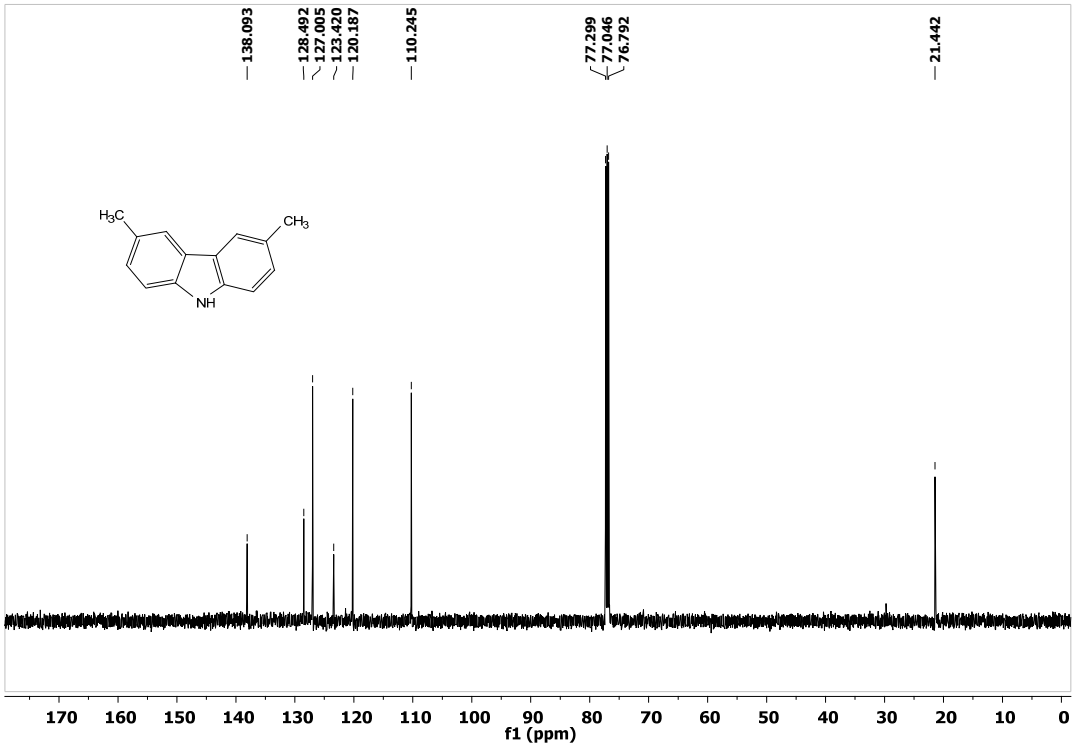
^{13}C NMR (125 MHz, $CDCl_3$) (**2m**)



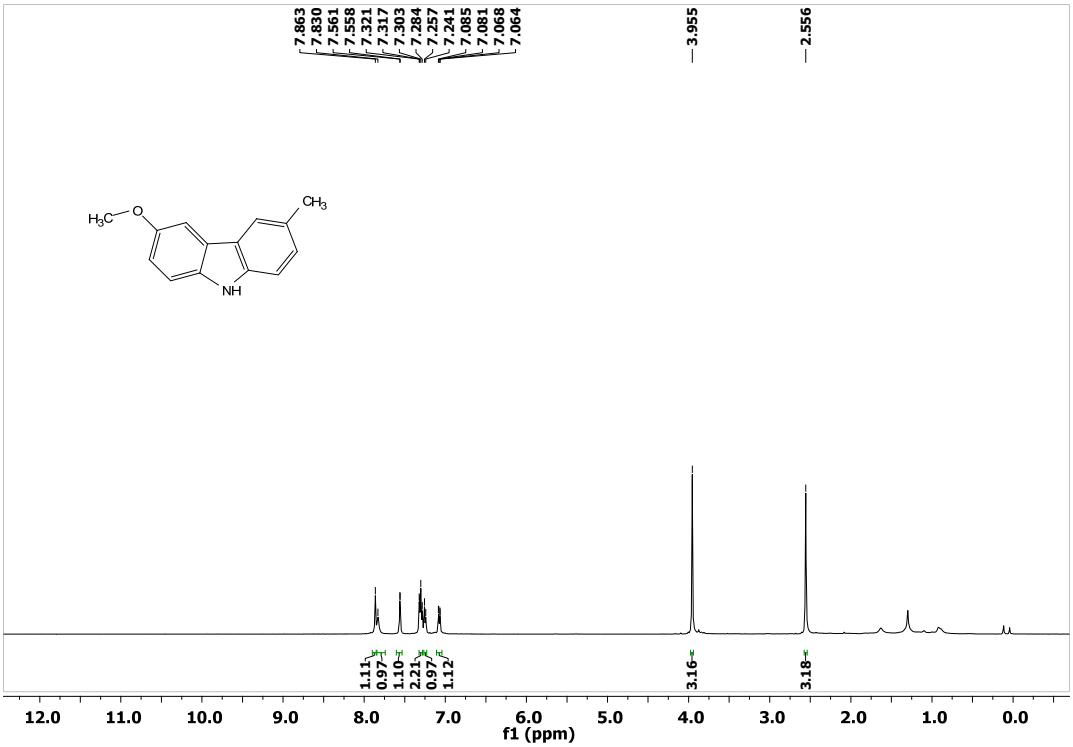
^{1}H NMR (500 MHz, $CDCl_3$) (**2n**)



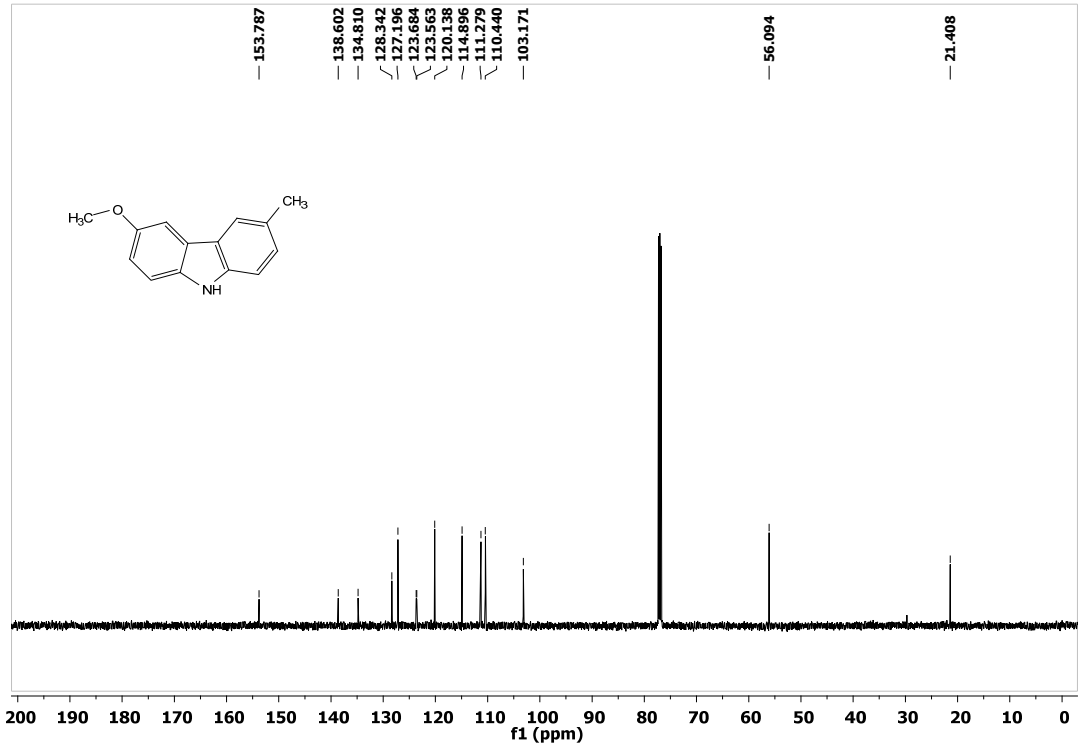
^{13}C NMR (125 MHz, $CDCl_3$) (**2n**)



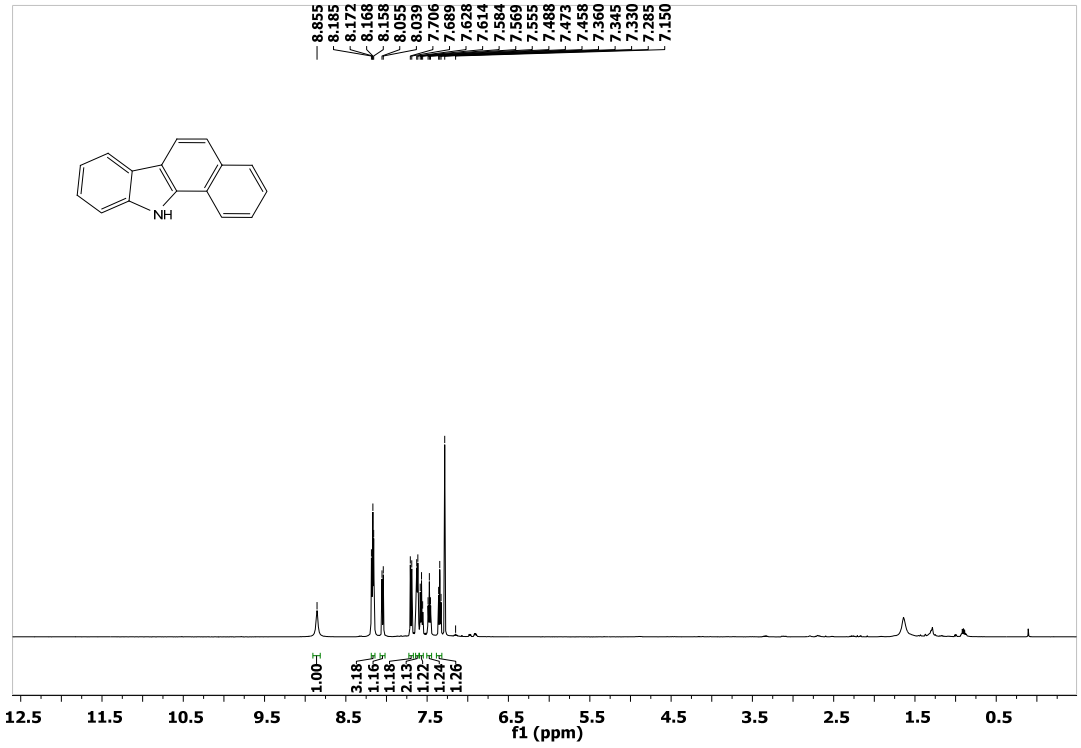
^{1}H NMR (500 MHz, $CDCl_3$) (**2o**)



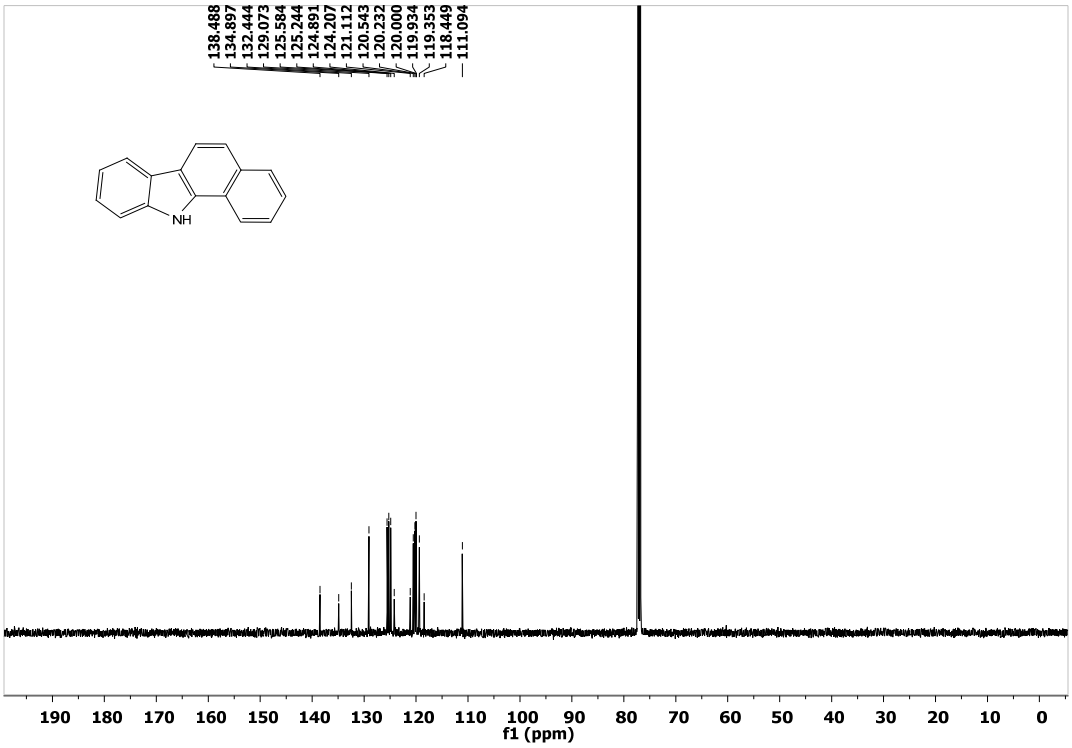
^{13}C NMR (125 MHz, $CDCl_3$) (**2o**)



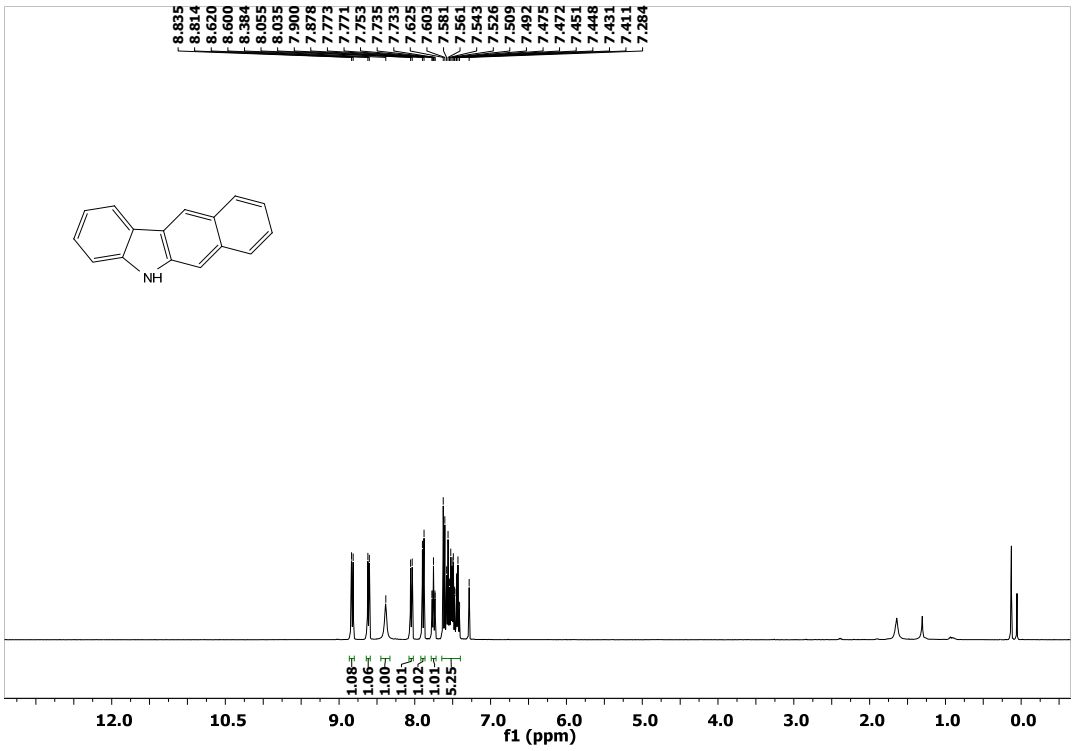
^{1}H NMR (500 MHz, $CDCl_3$) (**2p**)



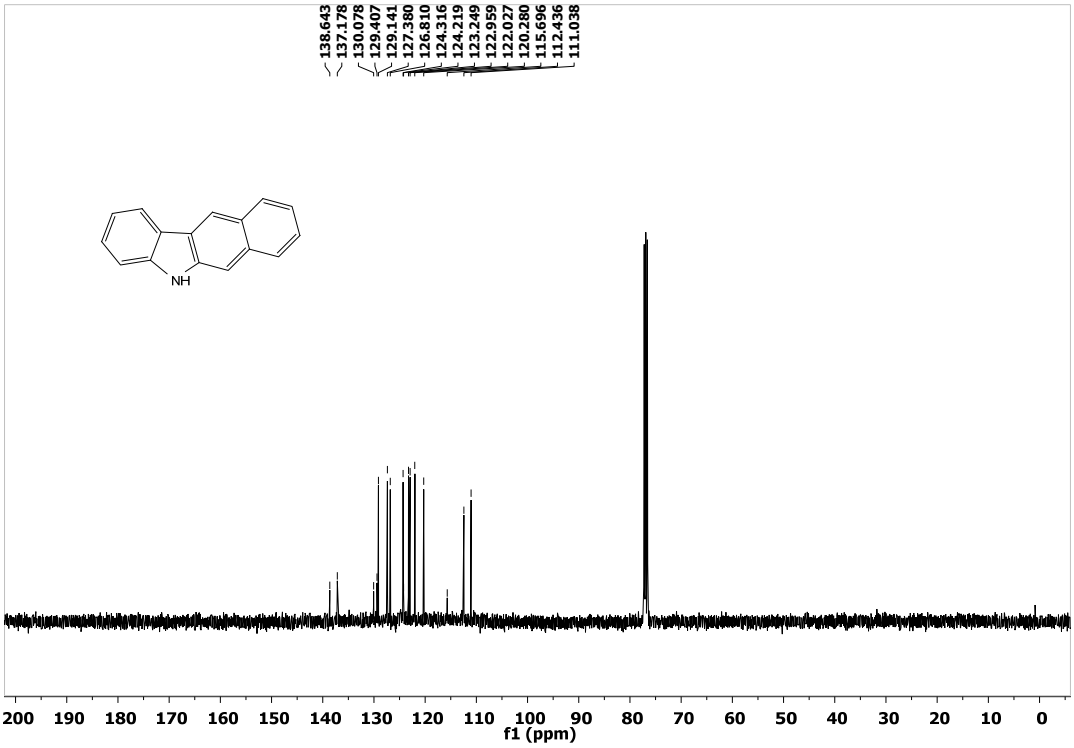
^{13}C NMR (125 MHz, $CDCl_3$) (**2p**)



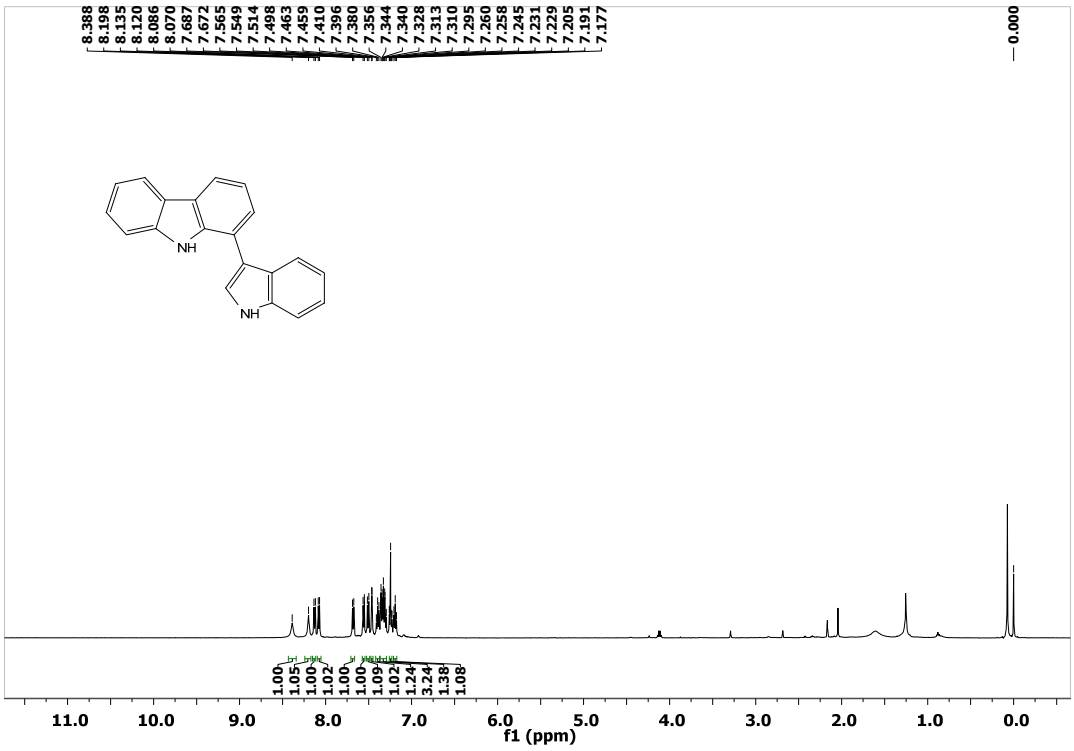
^{1}H NMR (400 MHz, $CDCl_3$) (**2q**)



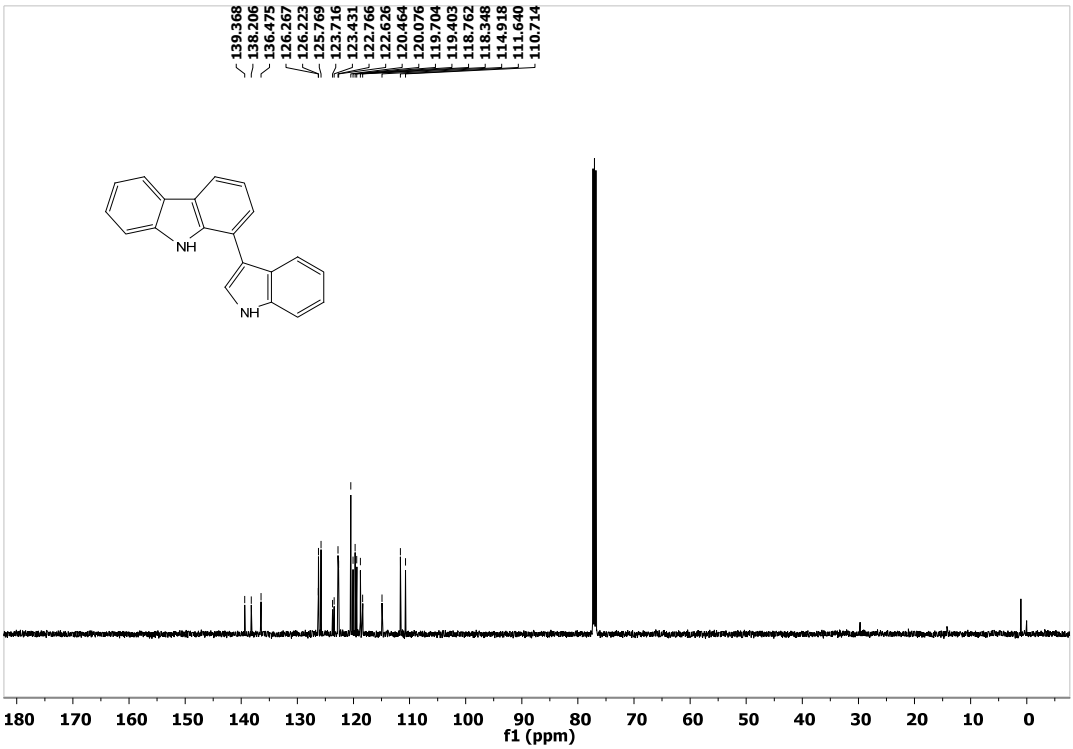
^{13}C NMR (100 MHz, $CDCl_3$) (**2q**)



^{1}H NMR (500 MHz, $CDCl_3$) (**2r**)



^{13}C NMR (125 MHz, $CDCl_3$) (**2r**)



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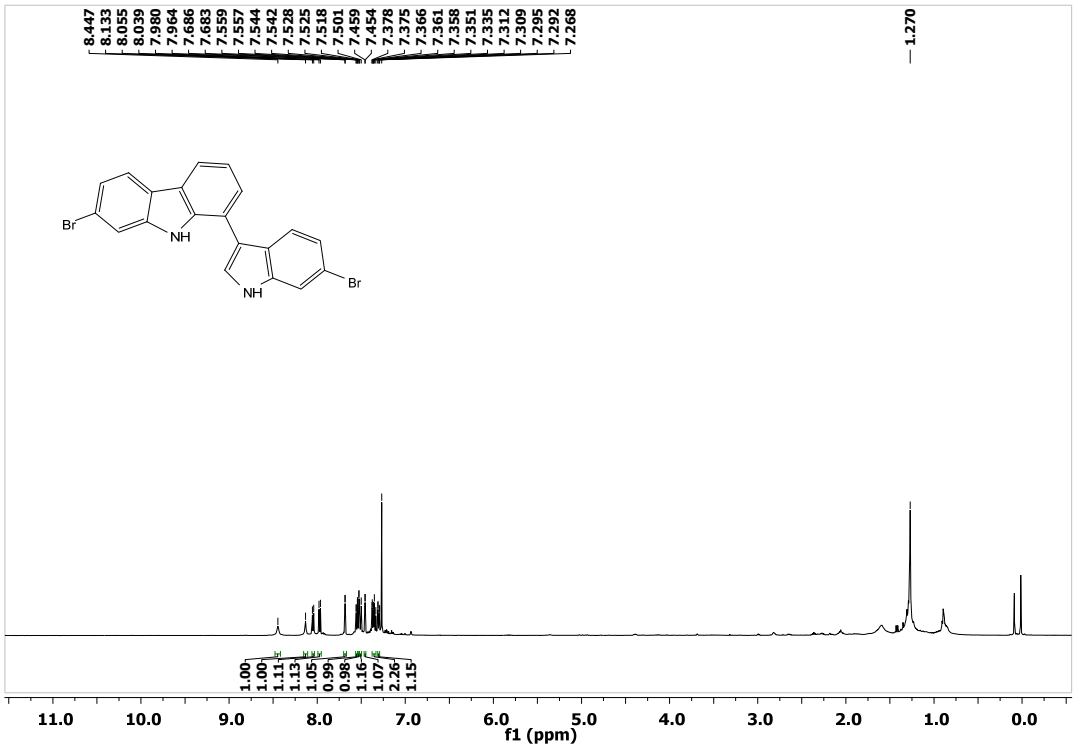
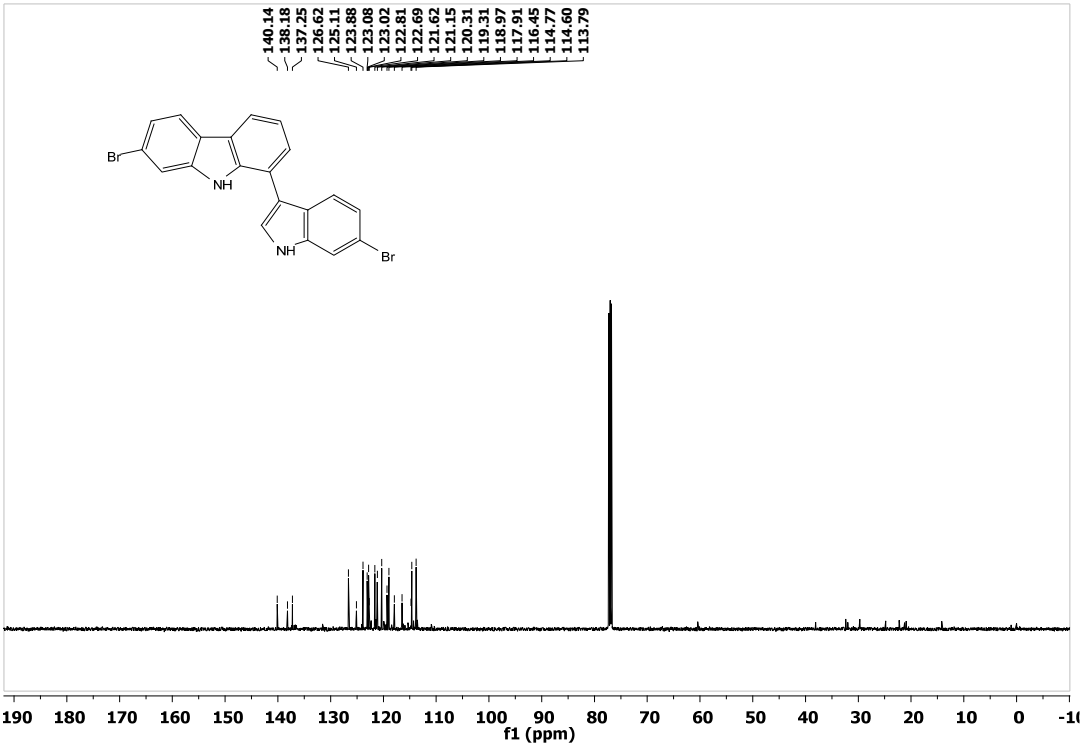


^{13}C NMR (125 MHz, $CDCl_3$) (**2s**)



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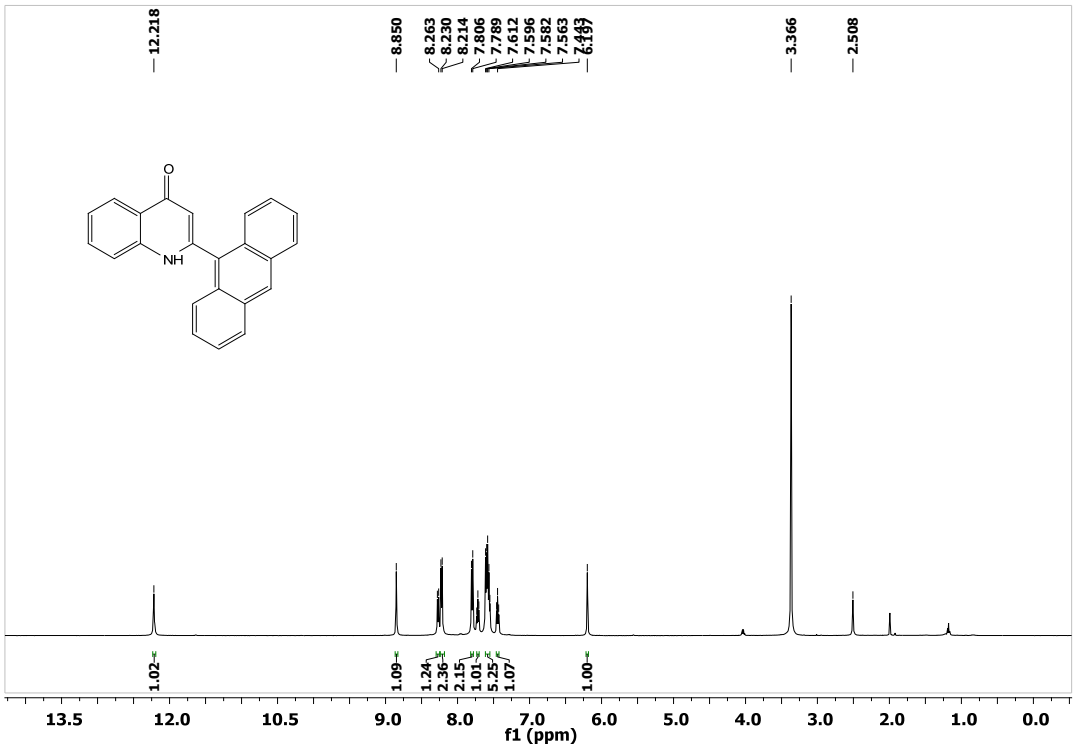

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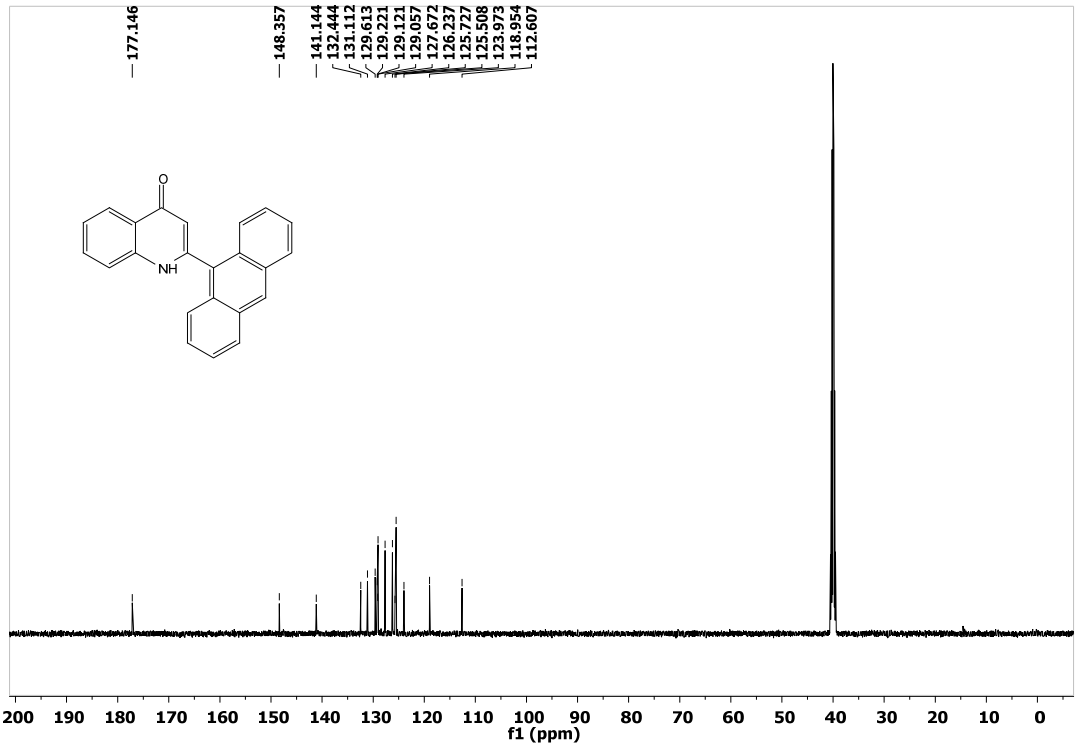

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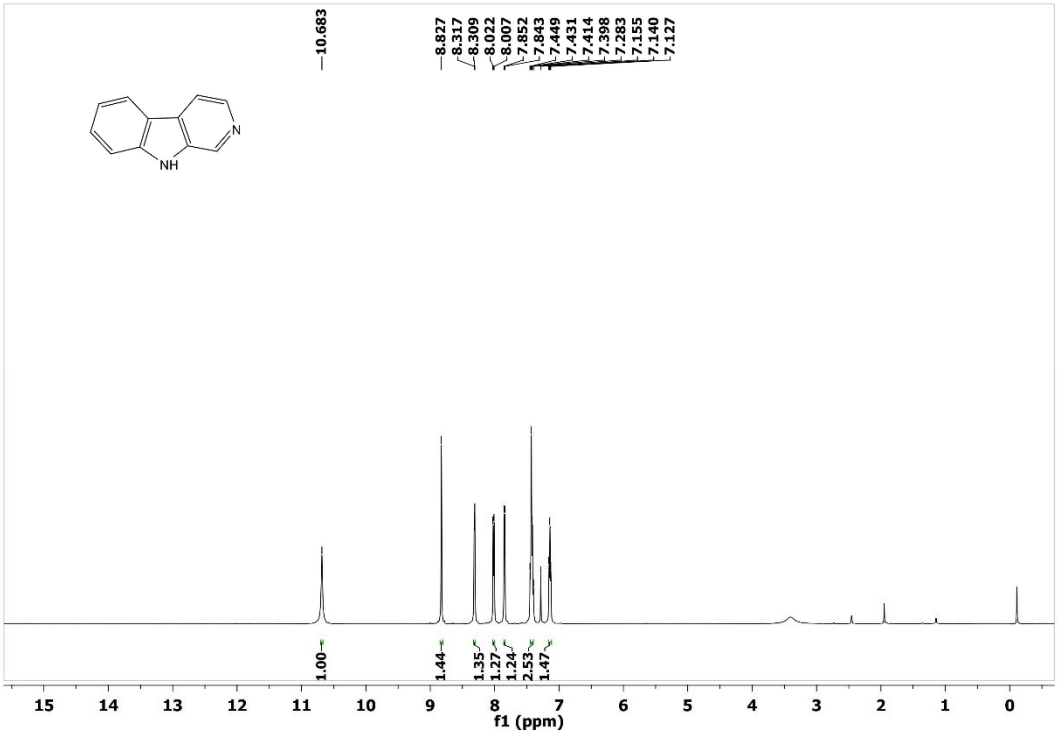

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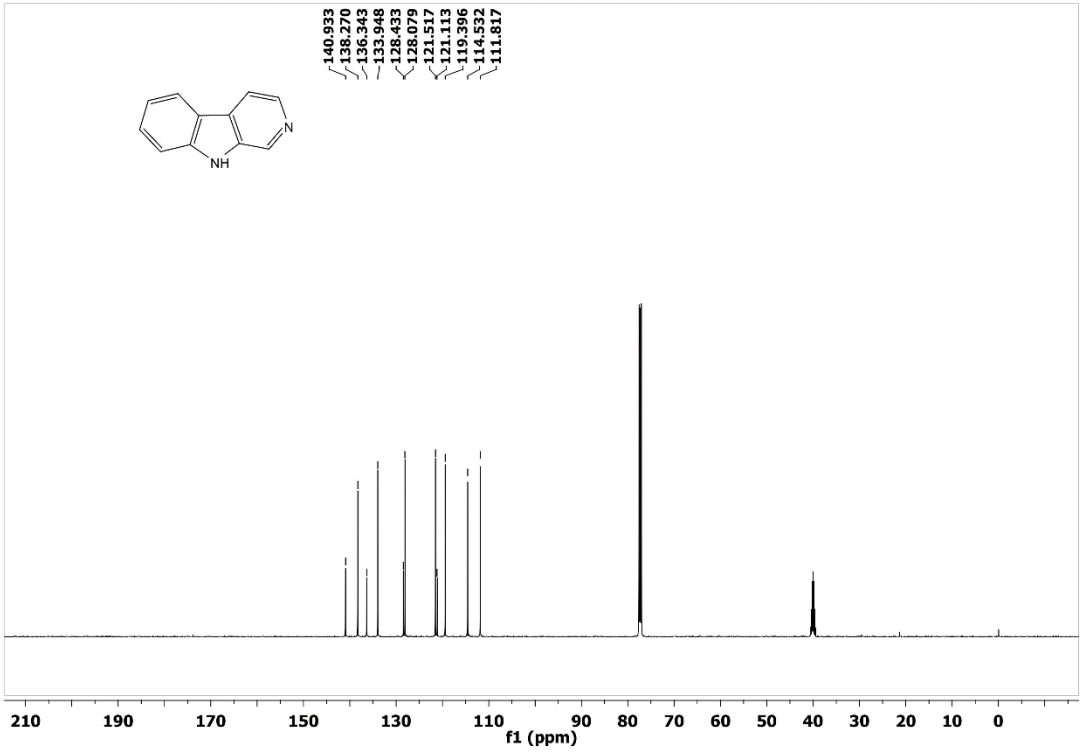
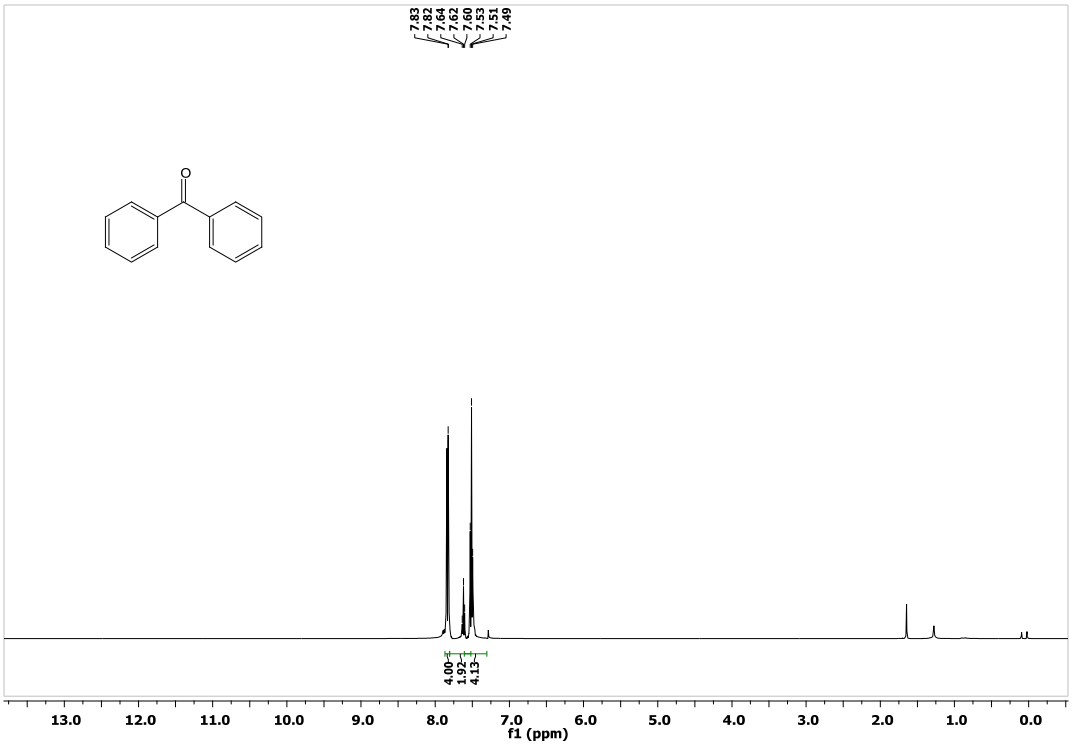
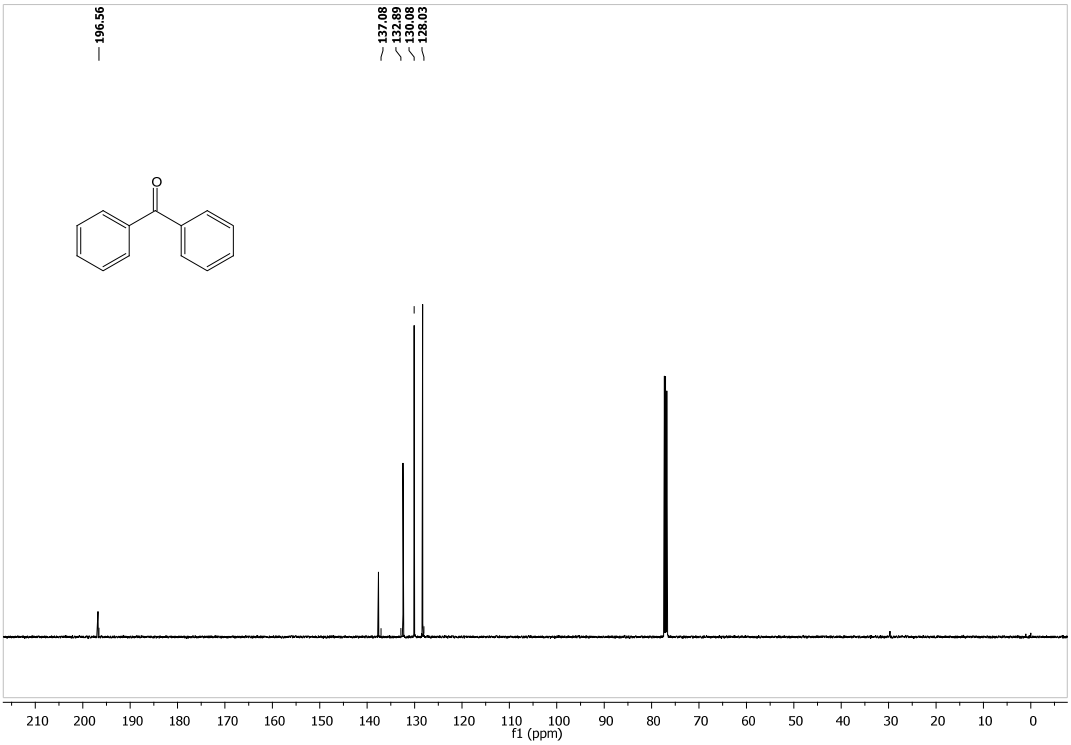


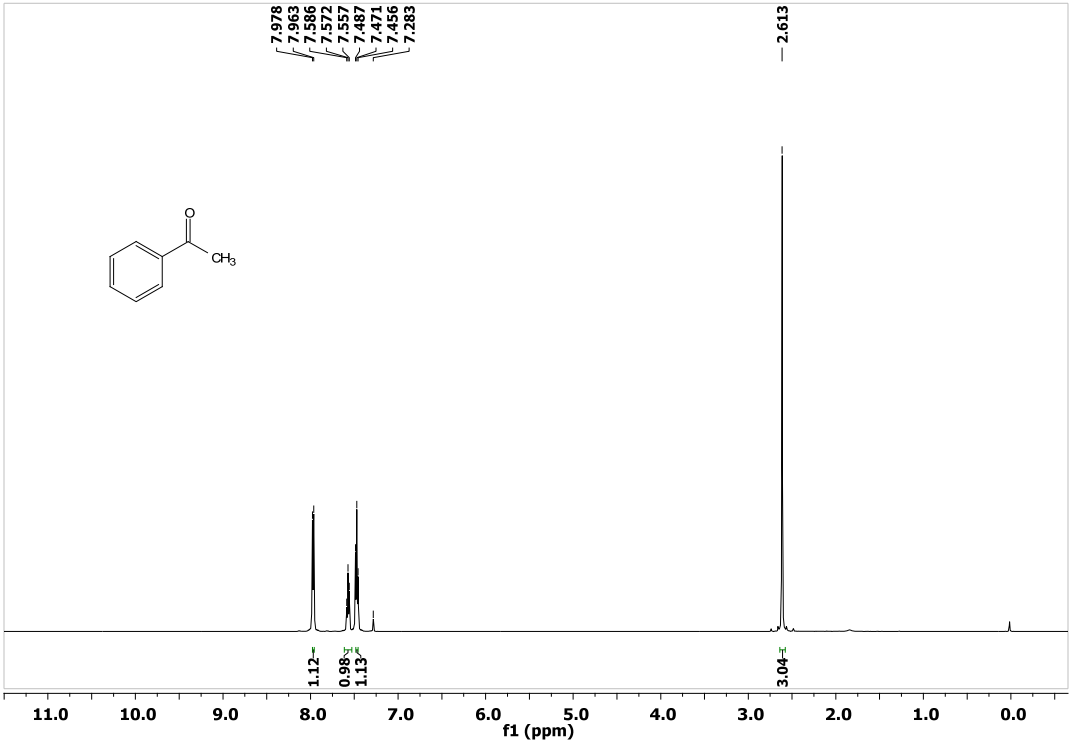
^{1}H NMR (500 MHz, $CDCl_3$) (**4a**)



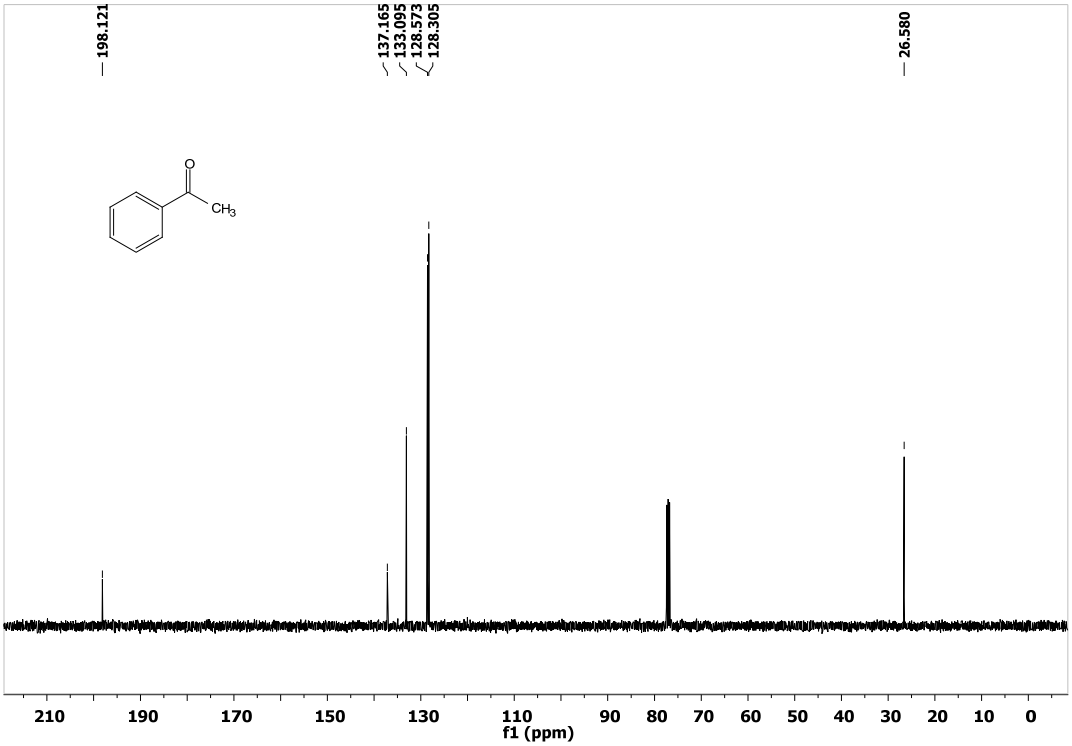
^{13}C NMR (125 MHz, $CDCl_3$) (**4a**)



^{1}H NMR (500 MHz, $CDCl_3$) (**4b**)



^{13}C NMR (100 MHz, $CDCl_3$) (**4b**)



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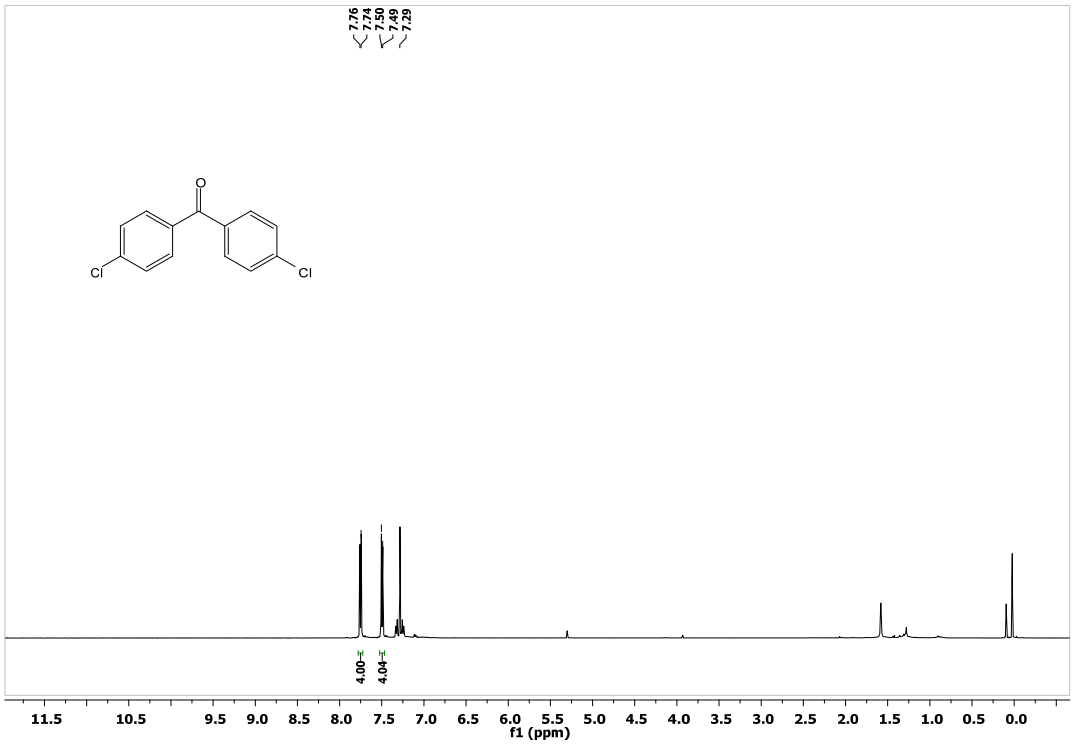
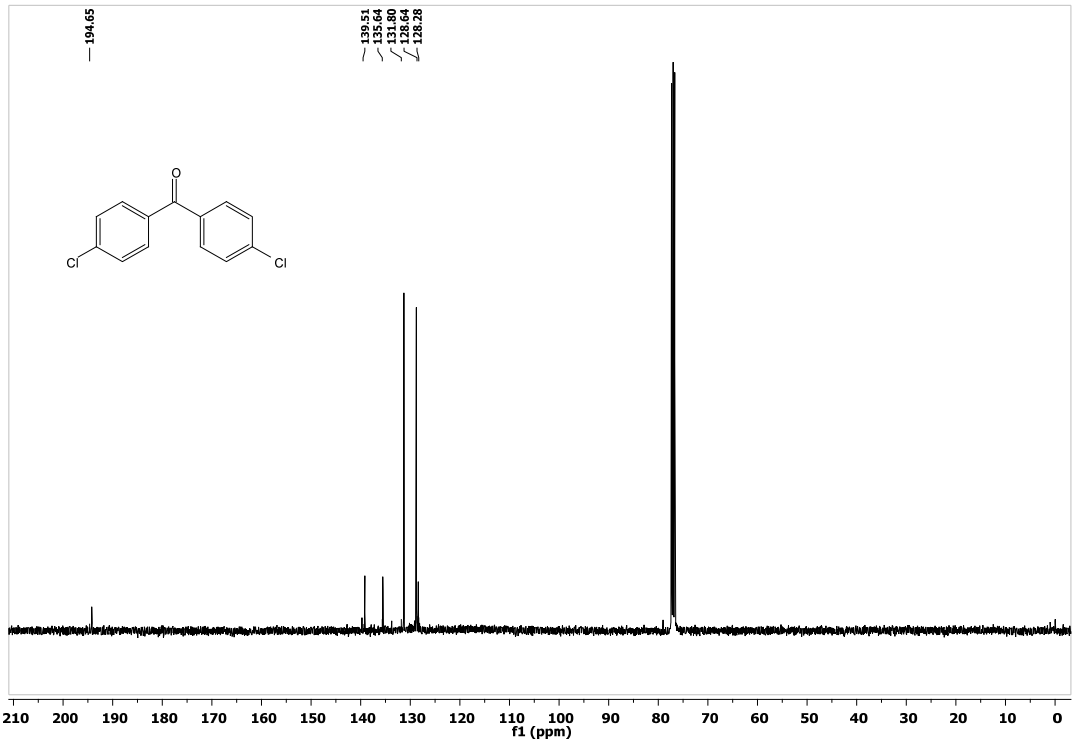


^{13}C NMR (125 MHz, $CDCl_3$) (**4c**)



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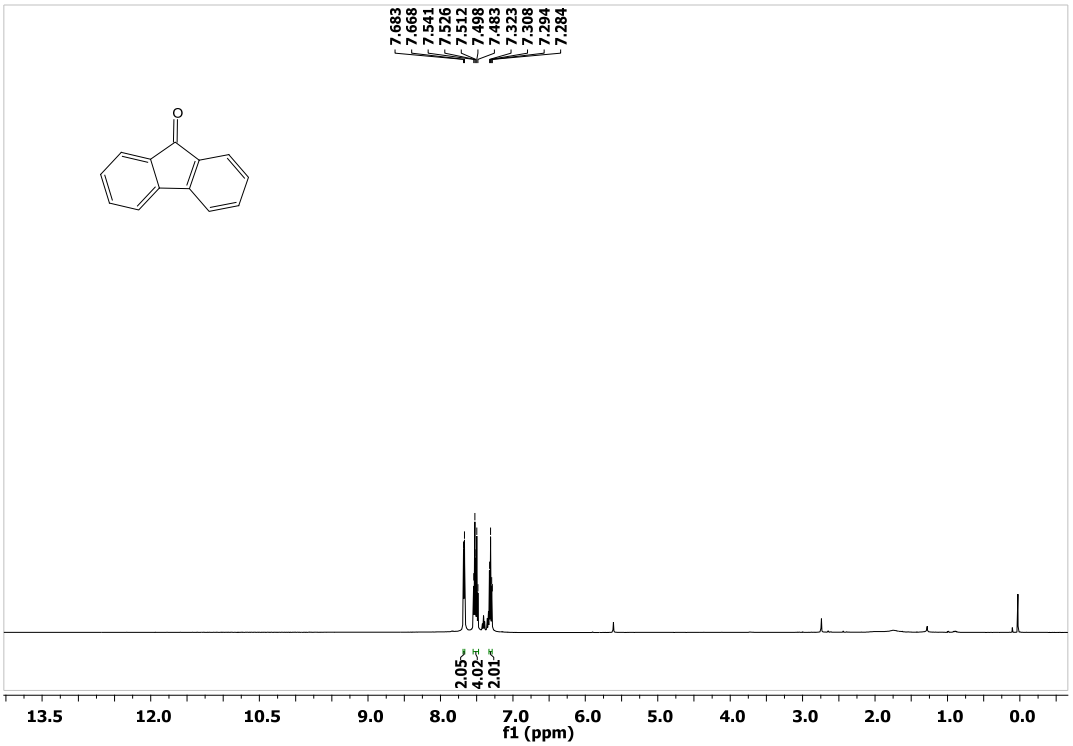

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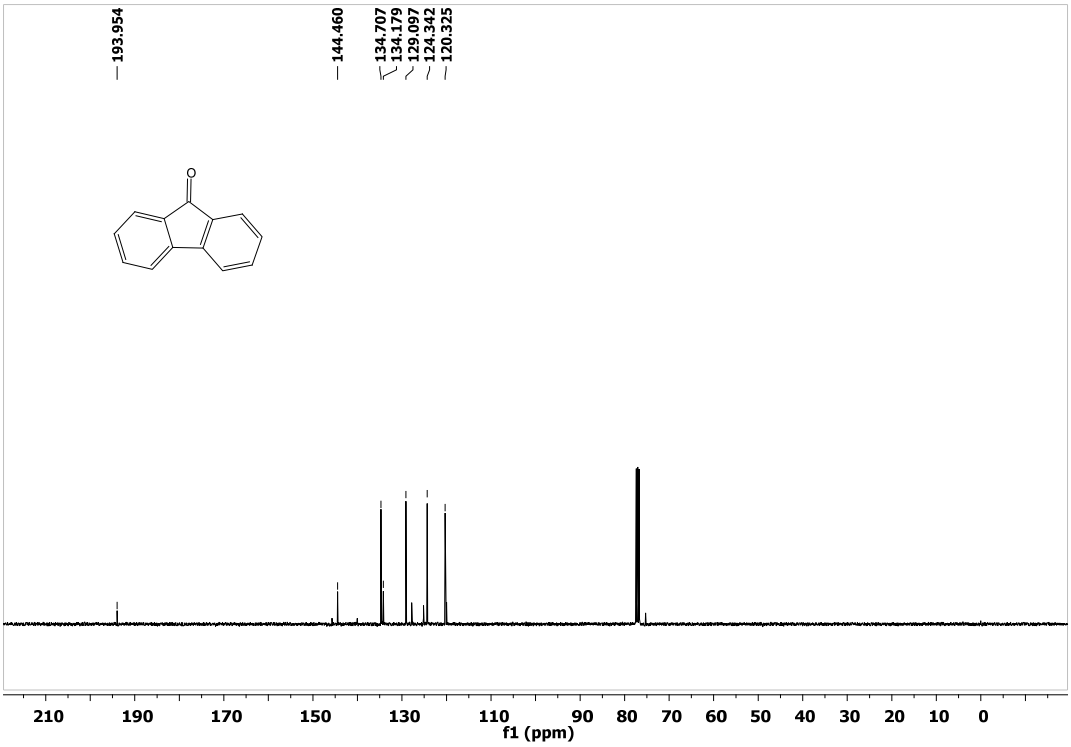
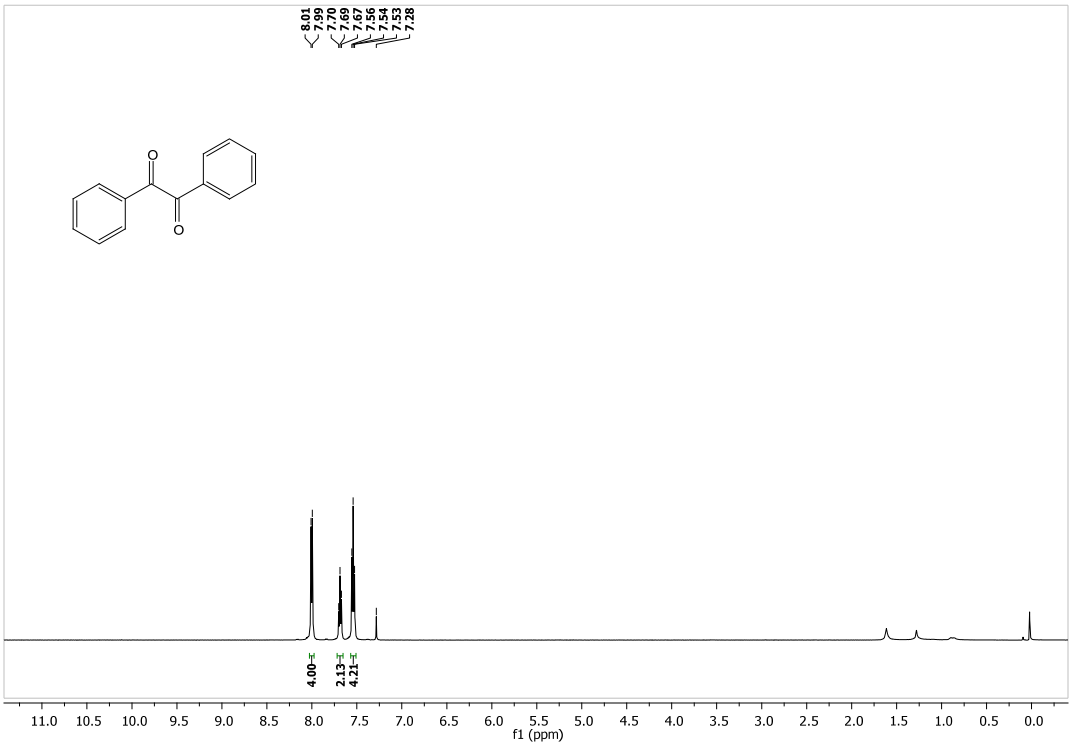
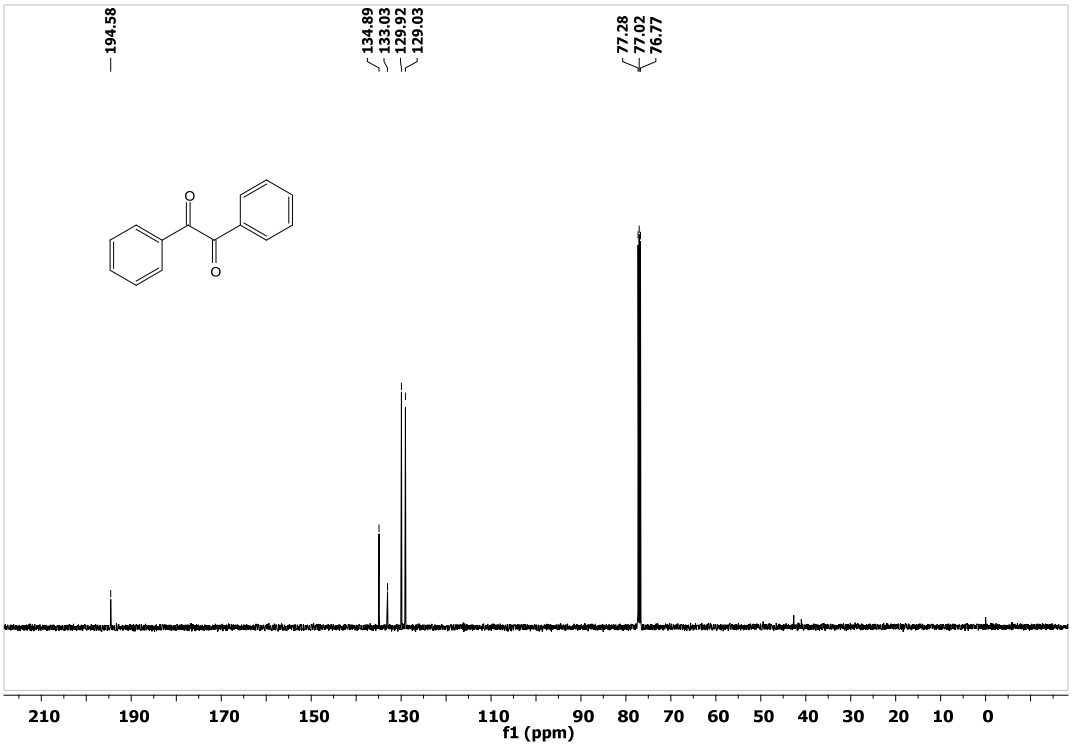


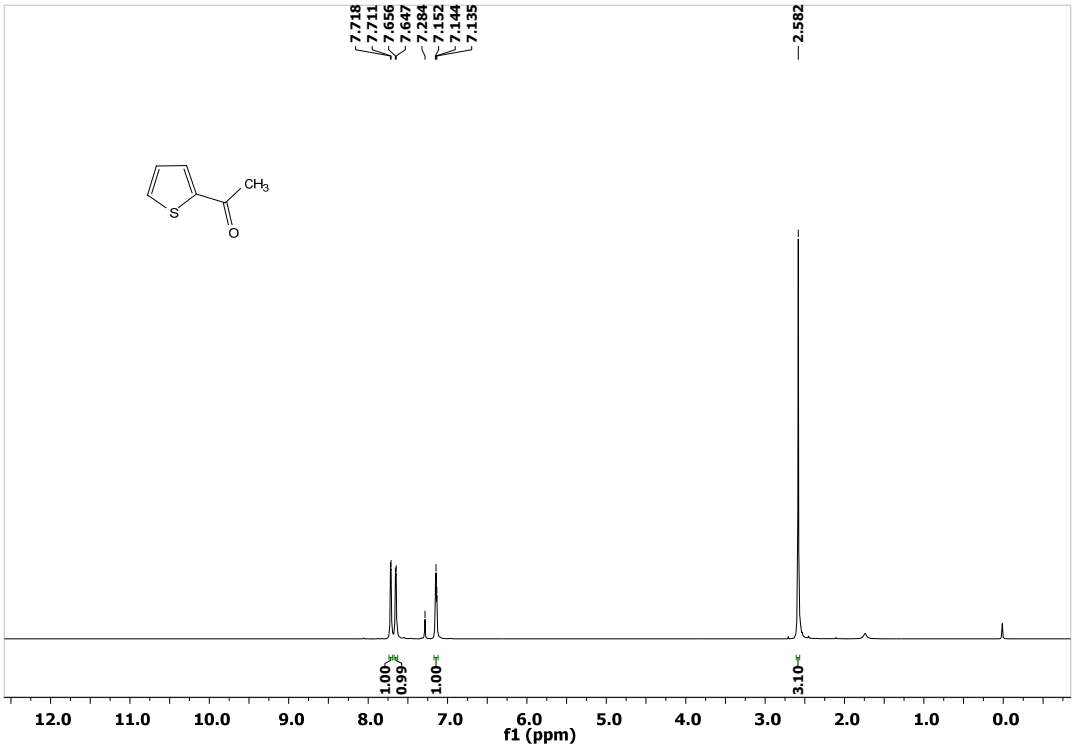
^{1}H NMR (500 MHz, $CDCl_3$) (**4e**)



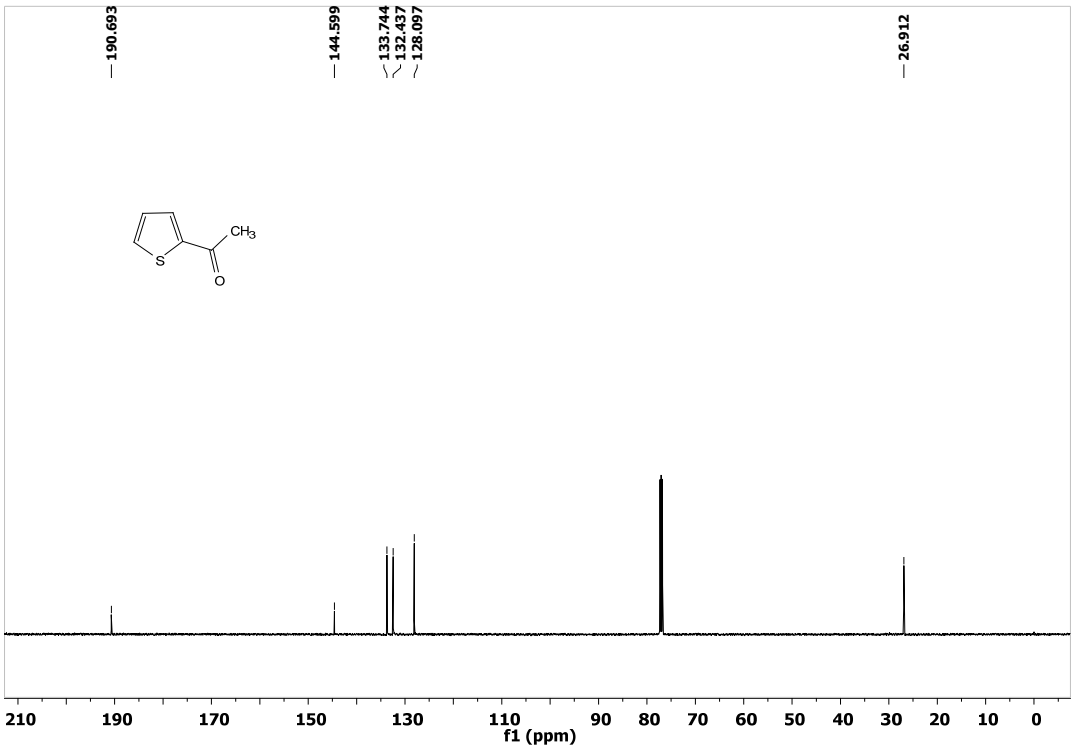
^{13}C NMR (125 MHz, $CDCl_3$) (**4e**)



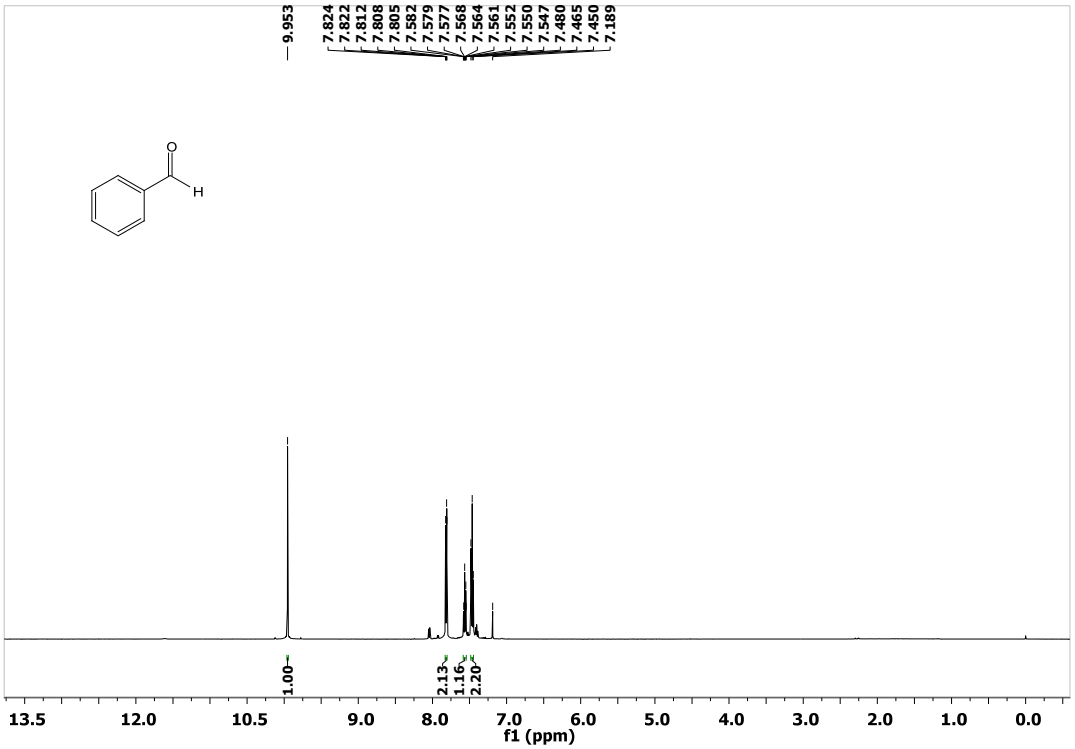
^{1}H NMR (500 MHz, $CDCl_3$) (**4f**)



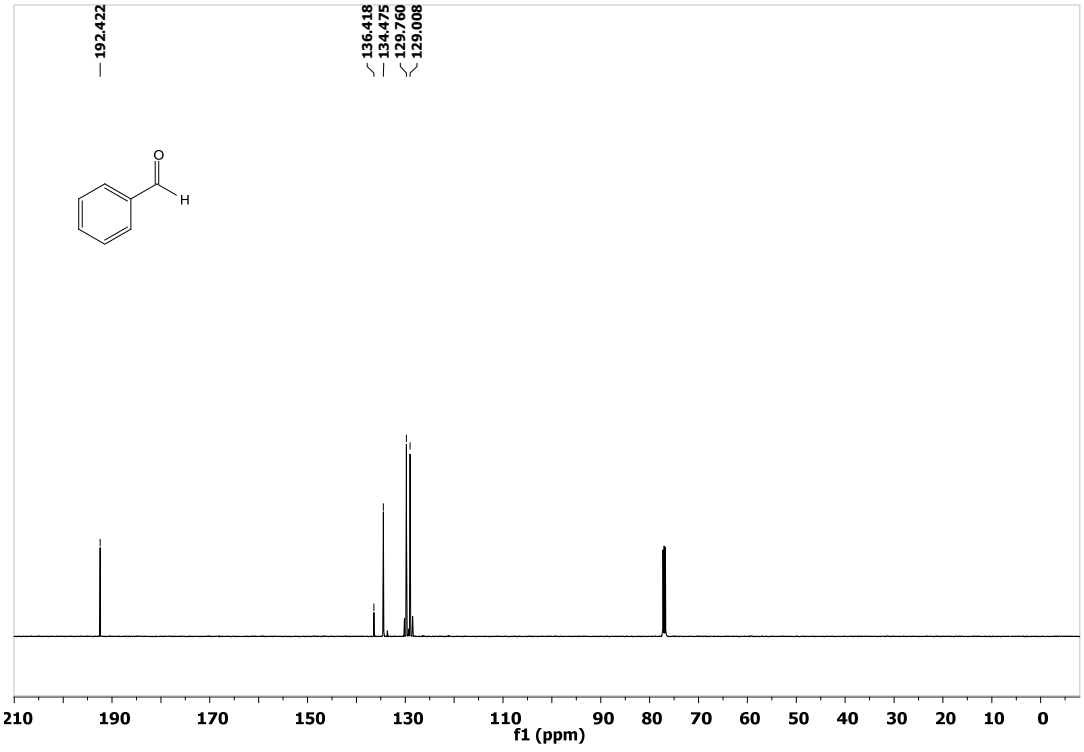
^{13}C NMR (125 MHz, $CDCl_3$) (**4f**)



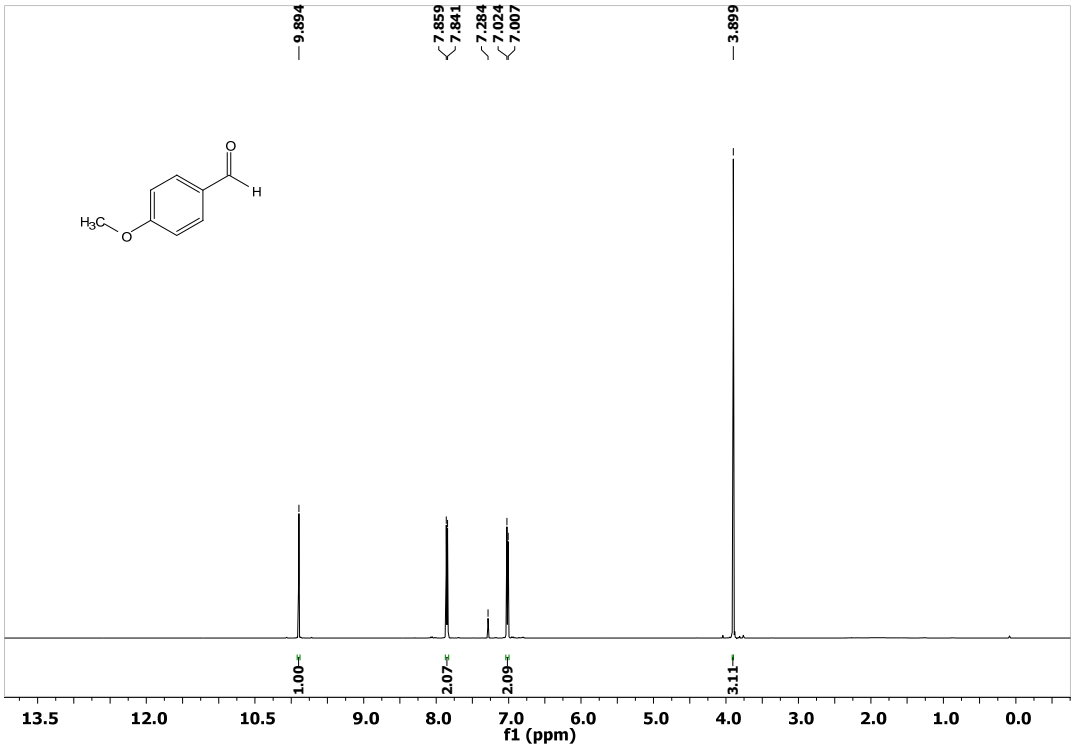
^{1}H NMR (500 MHz, $CDCl_3$) (**4g**)



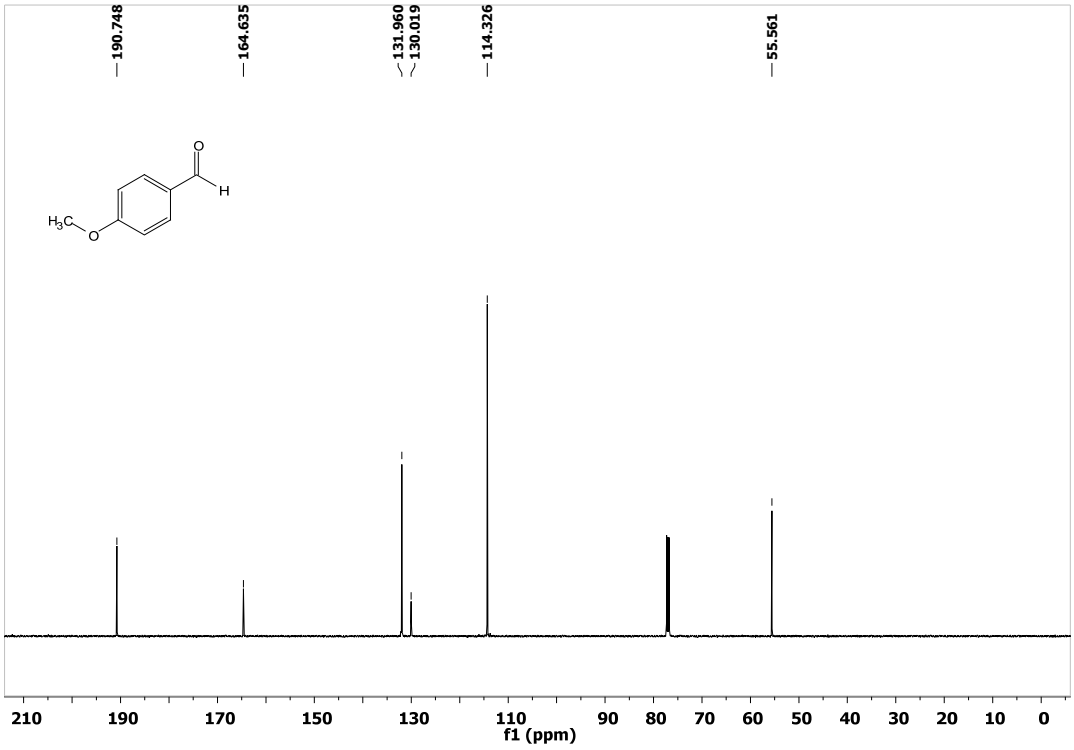
^{13}C NMR (125 MHz, $CDCl_3$) (**4g**)



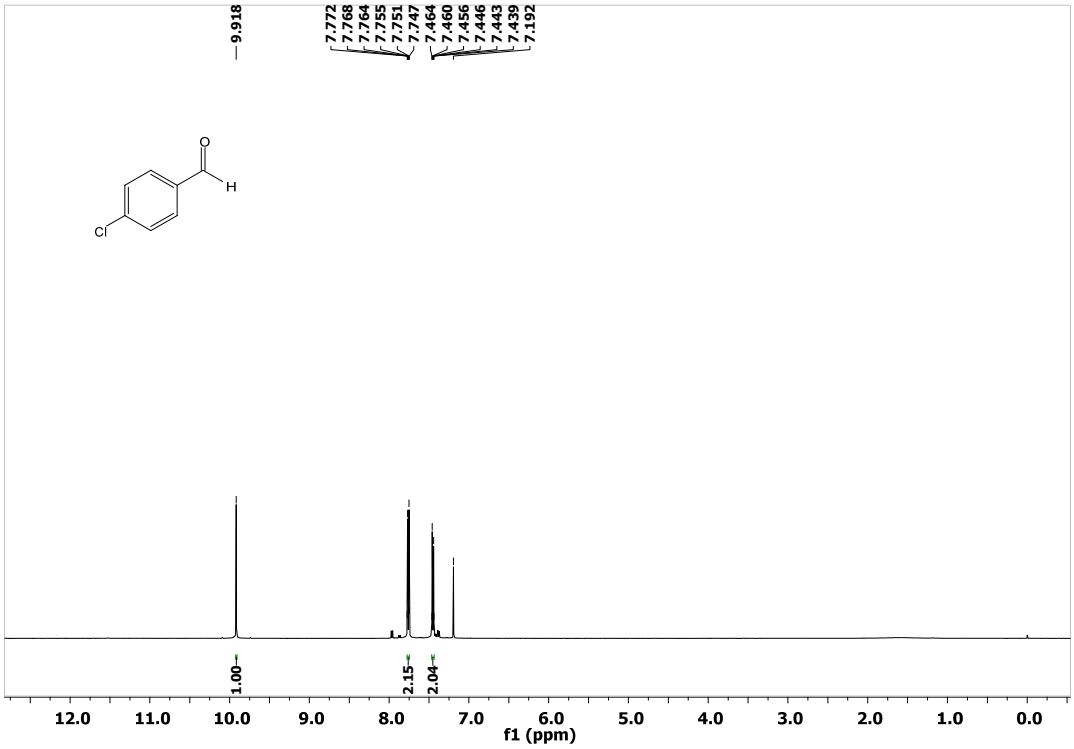
^{1}H NMR (500 MHz, $CDCl_3$) (**4h**)



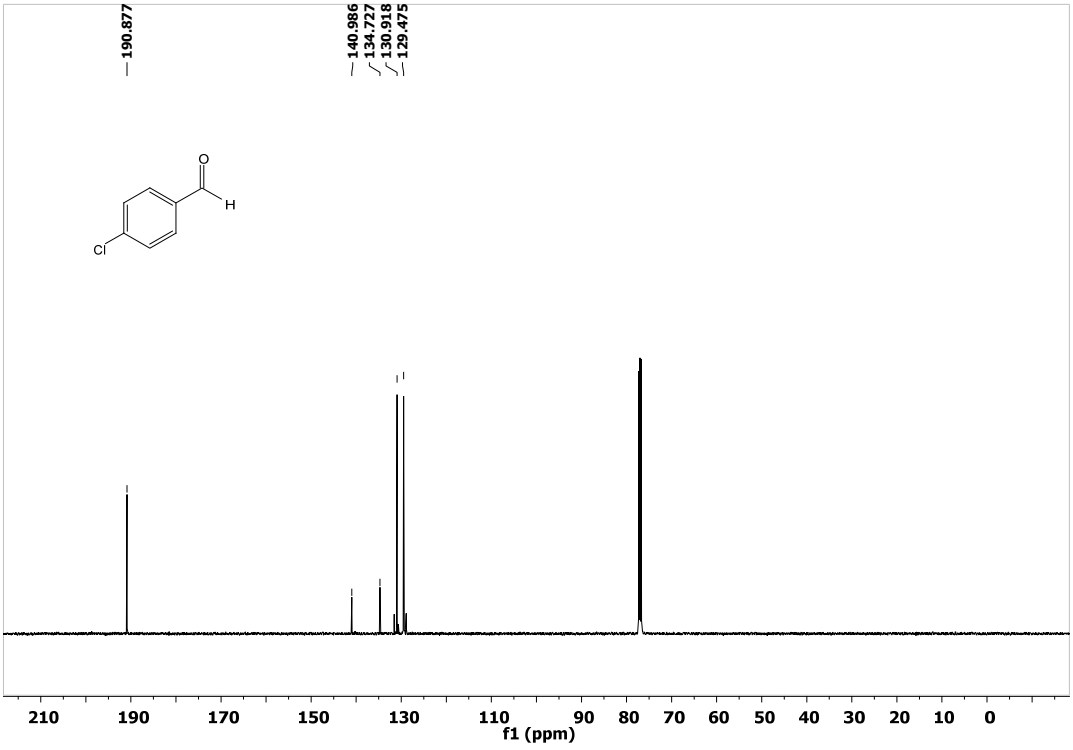
^{13}C NMR (125 MHz, $CDCl_3$) (**4h**)



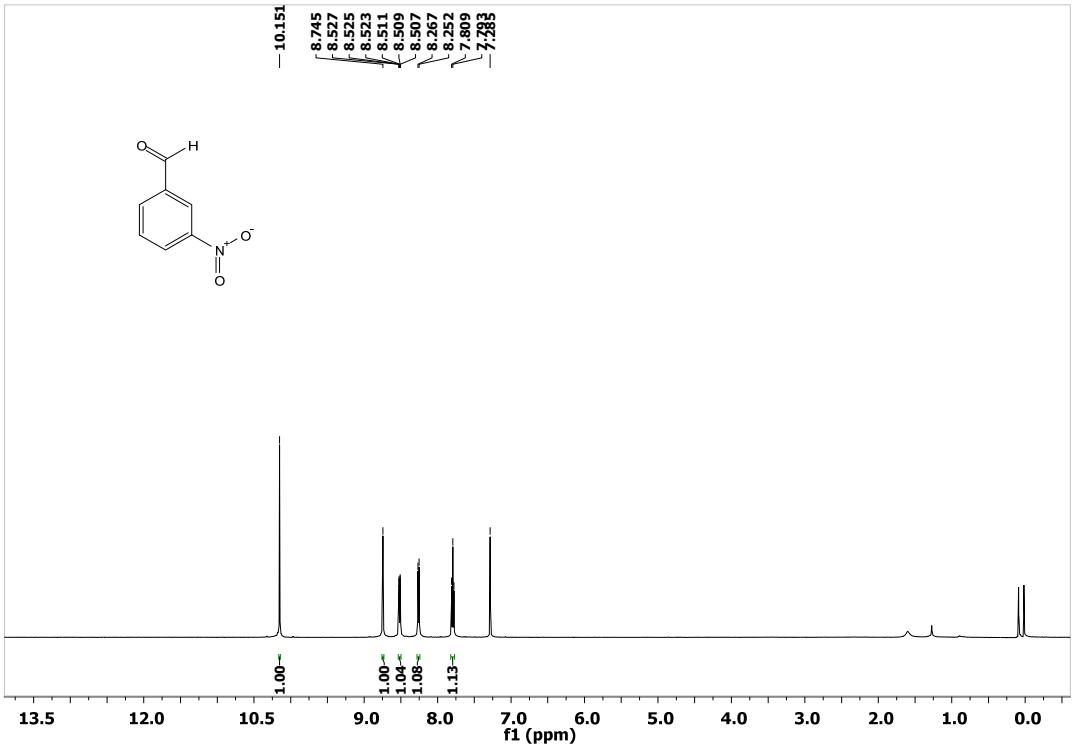
^{1}H NMR (500 MHz, $CDCl_3$) (**4i**)



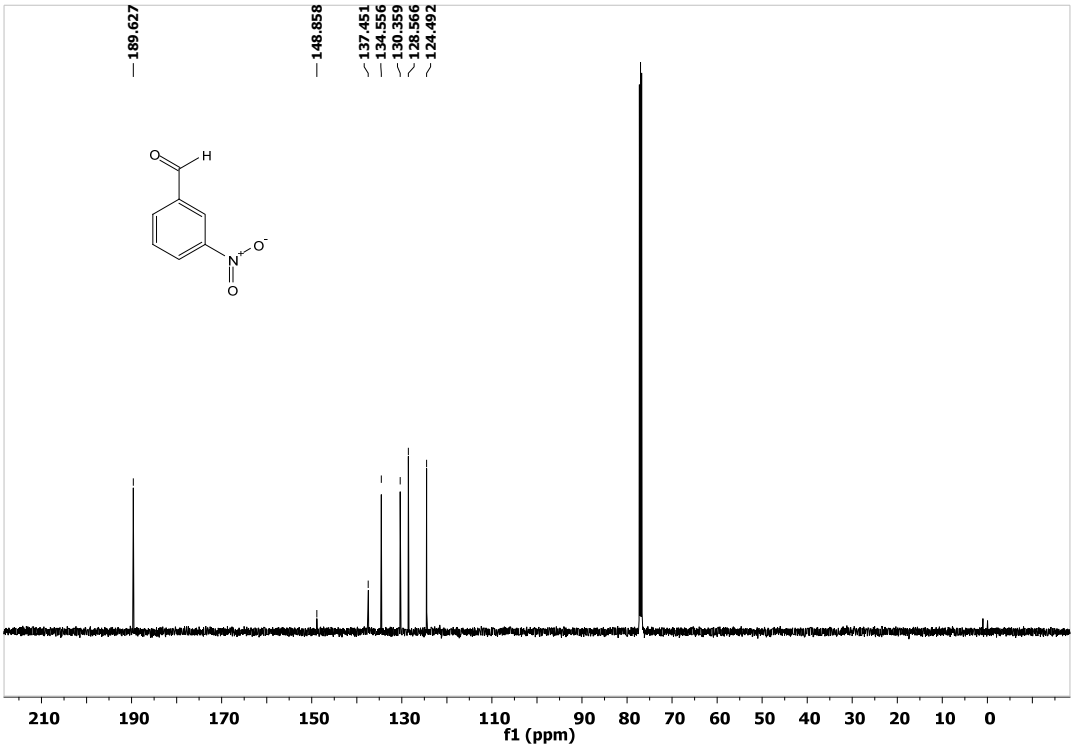
^{13}C NMR (125 MHz, $CDCl_3$) (**4i**)



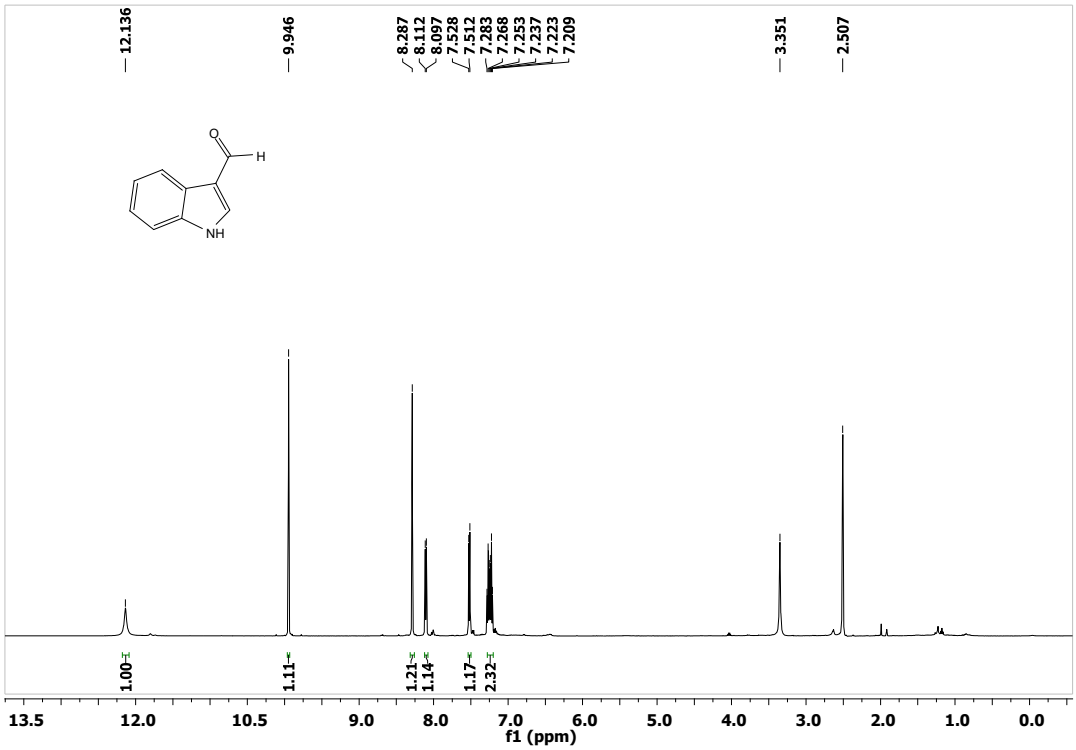
^{1}H NMR (500 MHz, $CDCl_3$) (**4j**)



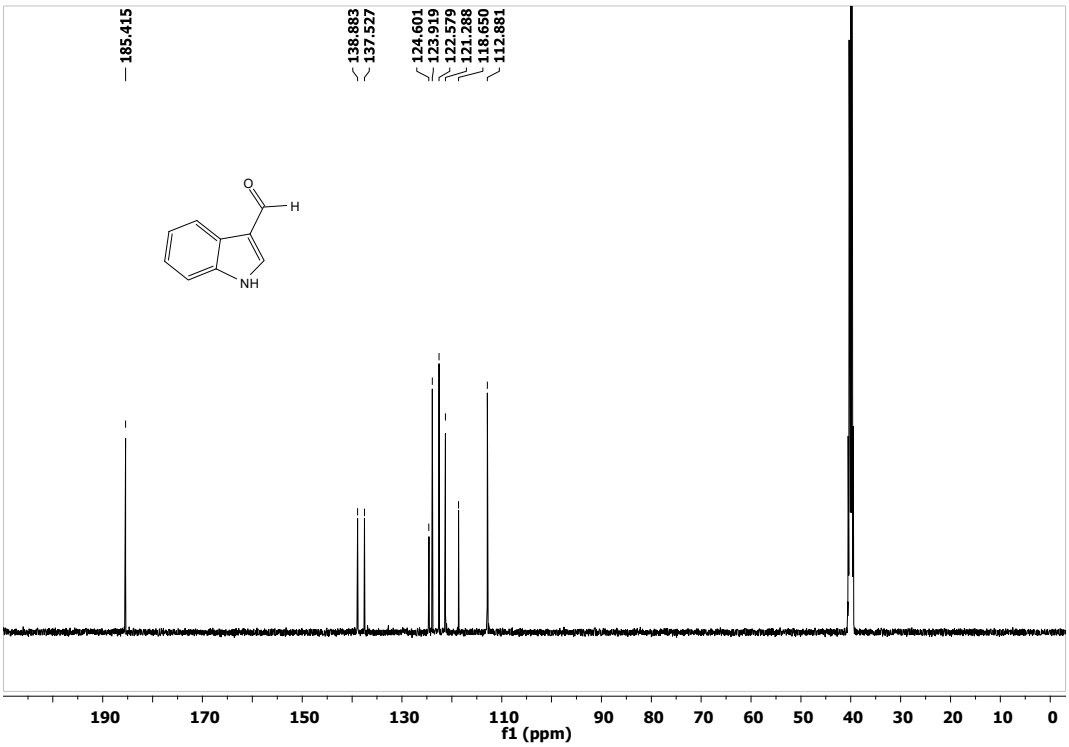
^{13}C NMR (125 MHz, $CDCl_3$) (**4j**)



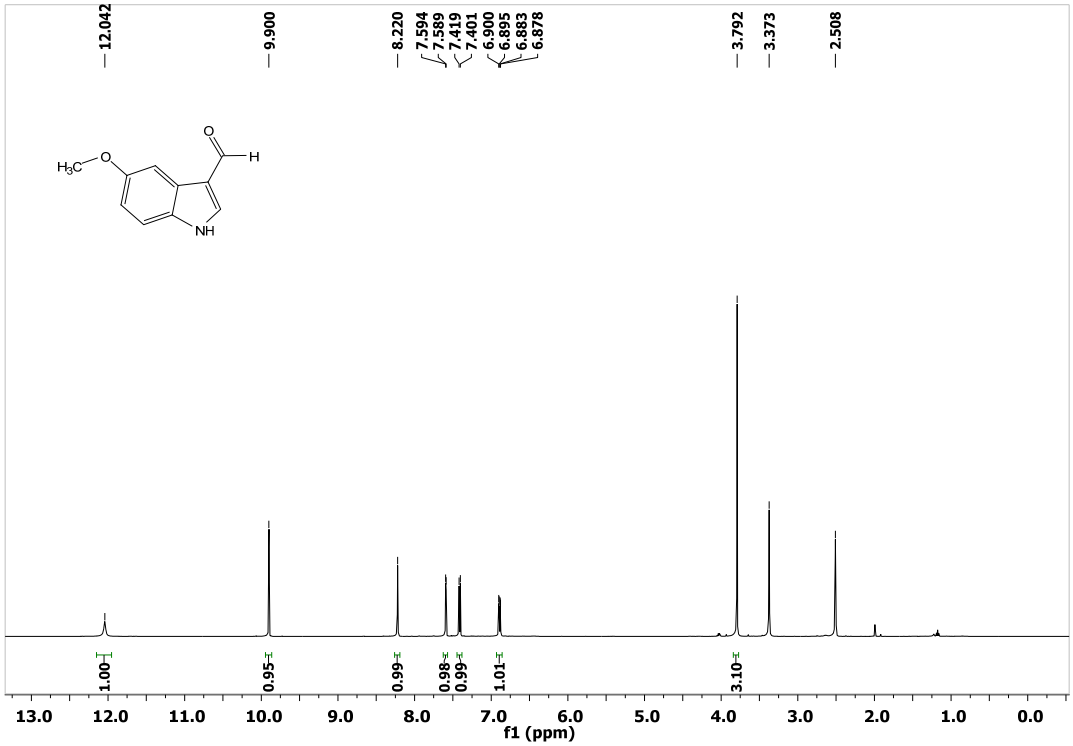
^{1}H NMR (500 MHz, $CDCl_3$) (**6a**)



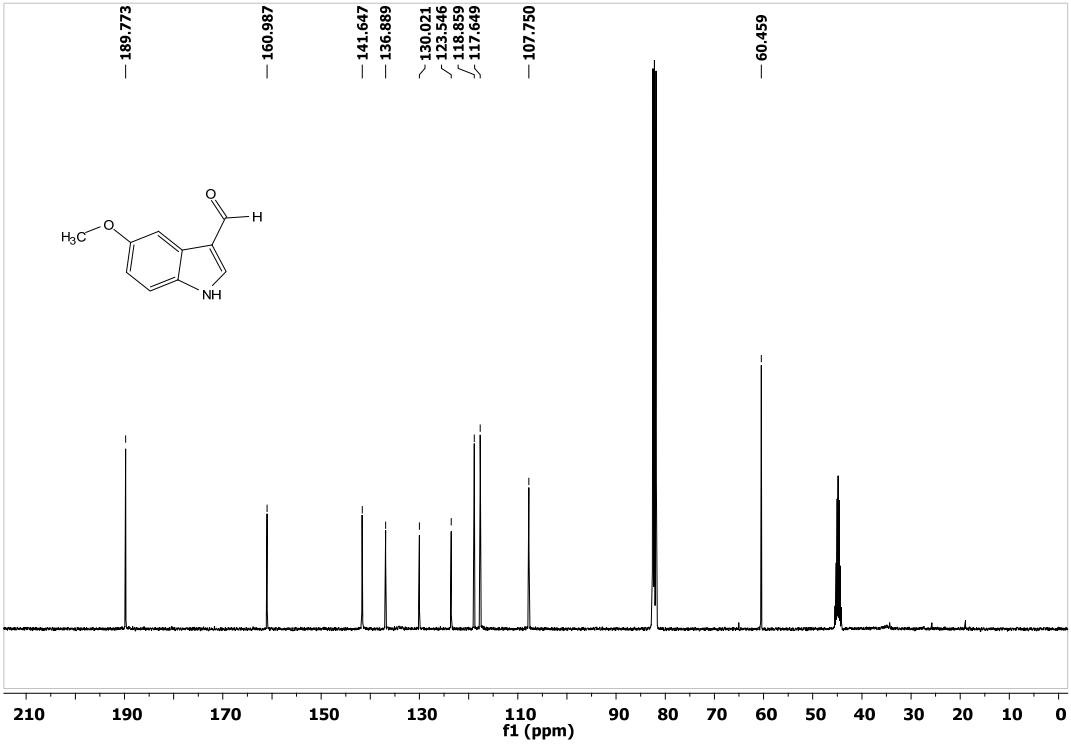
^{13}C NMR (125 MHz, $CDCl_3$) (**6a**)



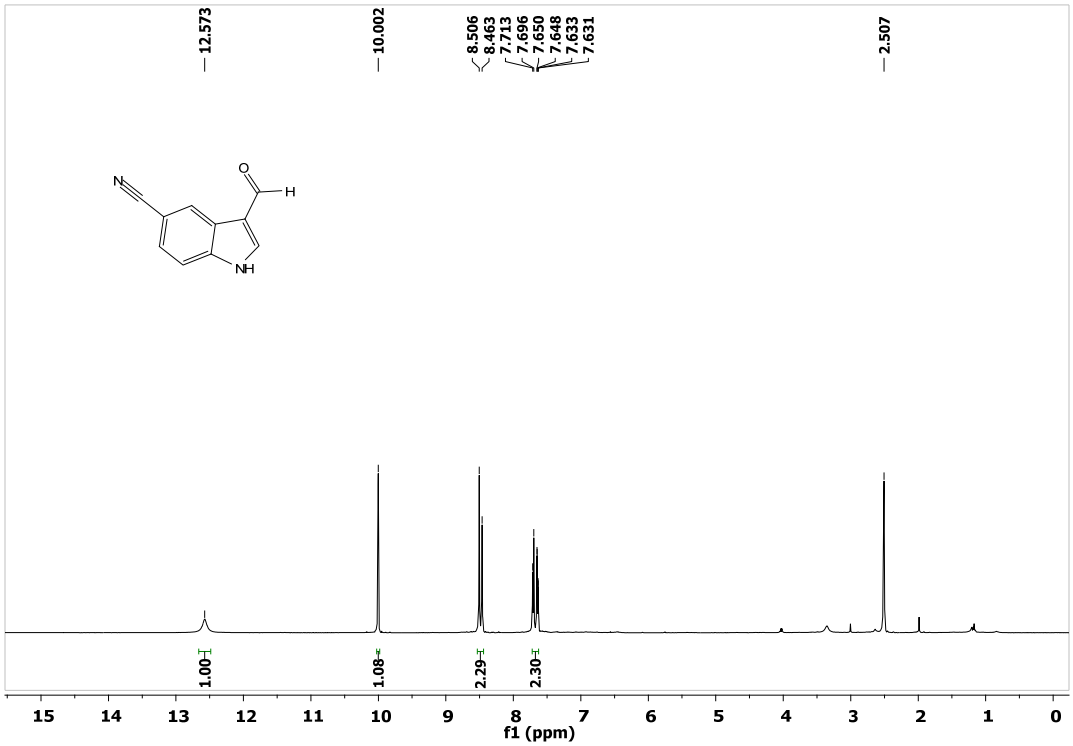
^{1}H NMR (500 MHz, $CDCl_3$) (**6b**)



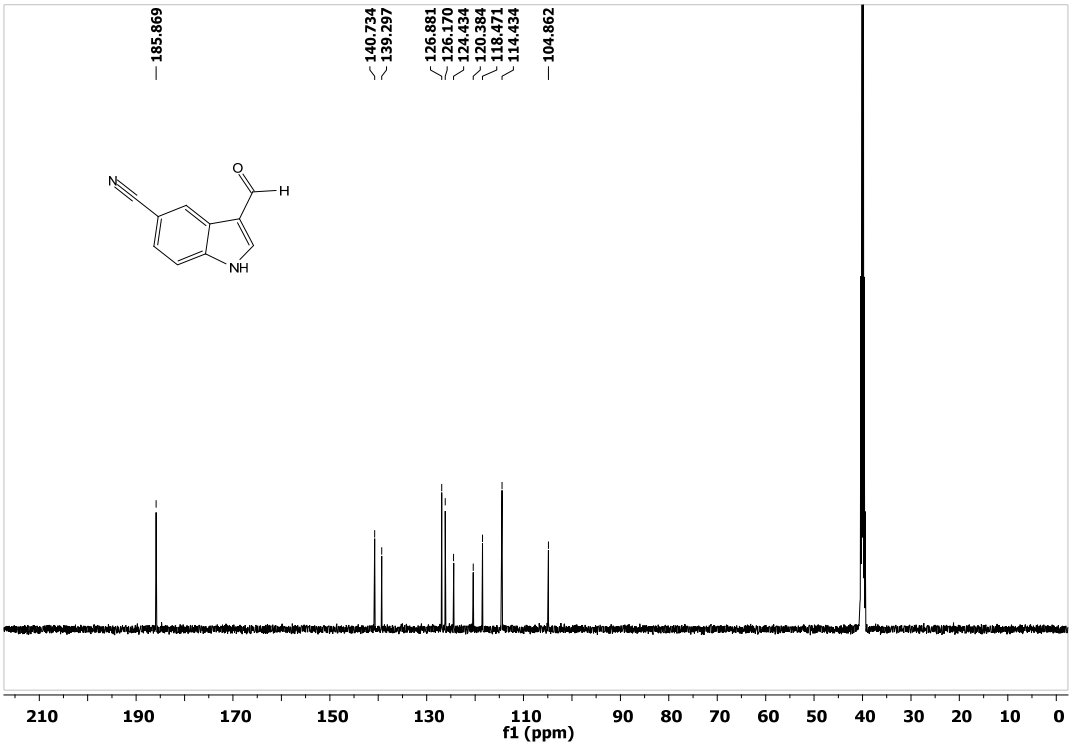
^{13}C NMR (125 MHz, $CDCl_3$) (**6b**)



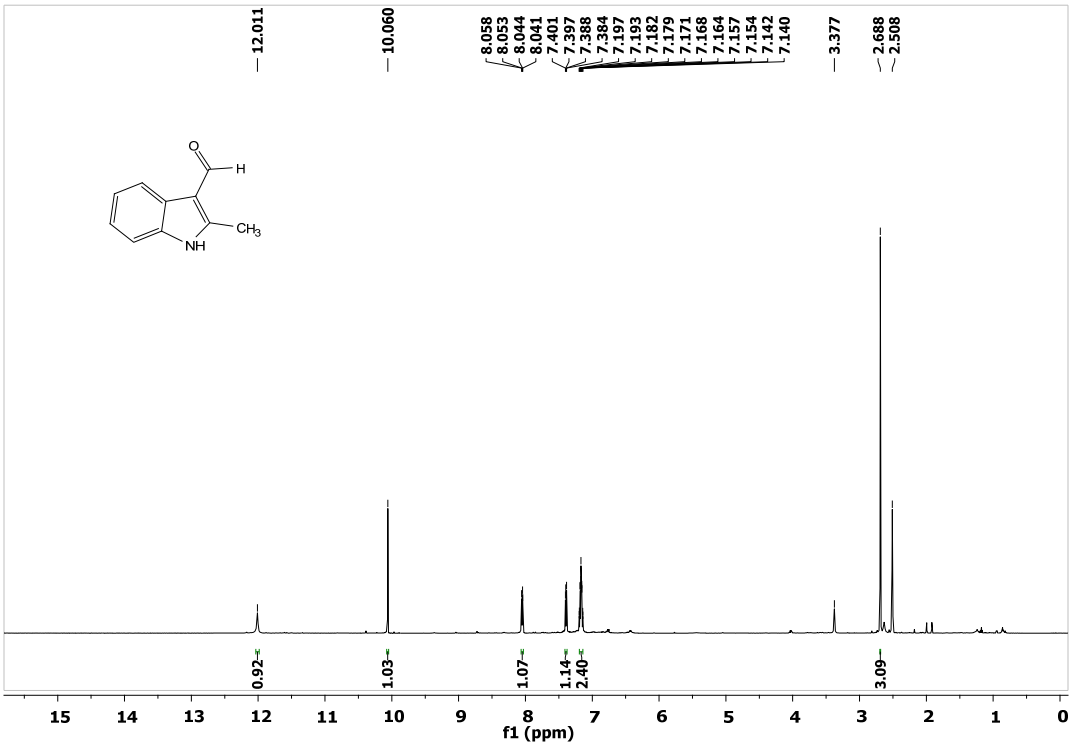
^{1}H NMR (500 MHz, $CDCl_3$) (**6c**)



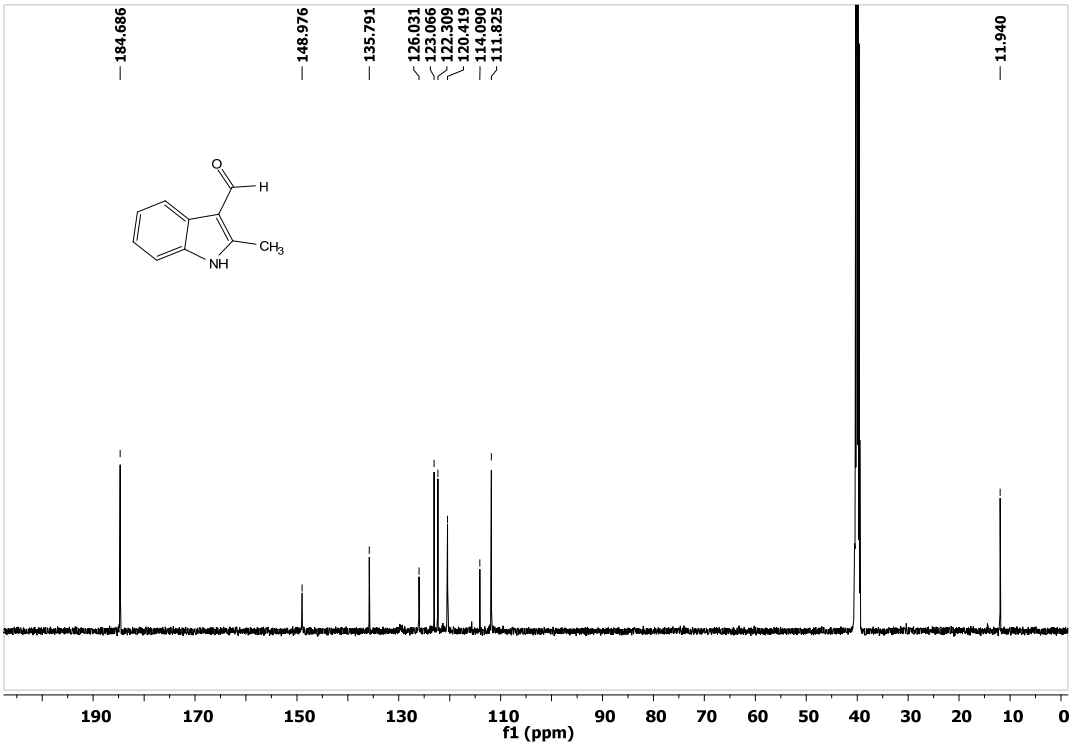
^{13}C NMR (125 MHz, $CDCl_3$) (**6c**)



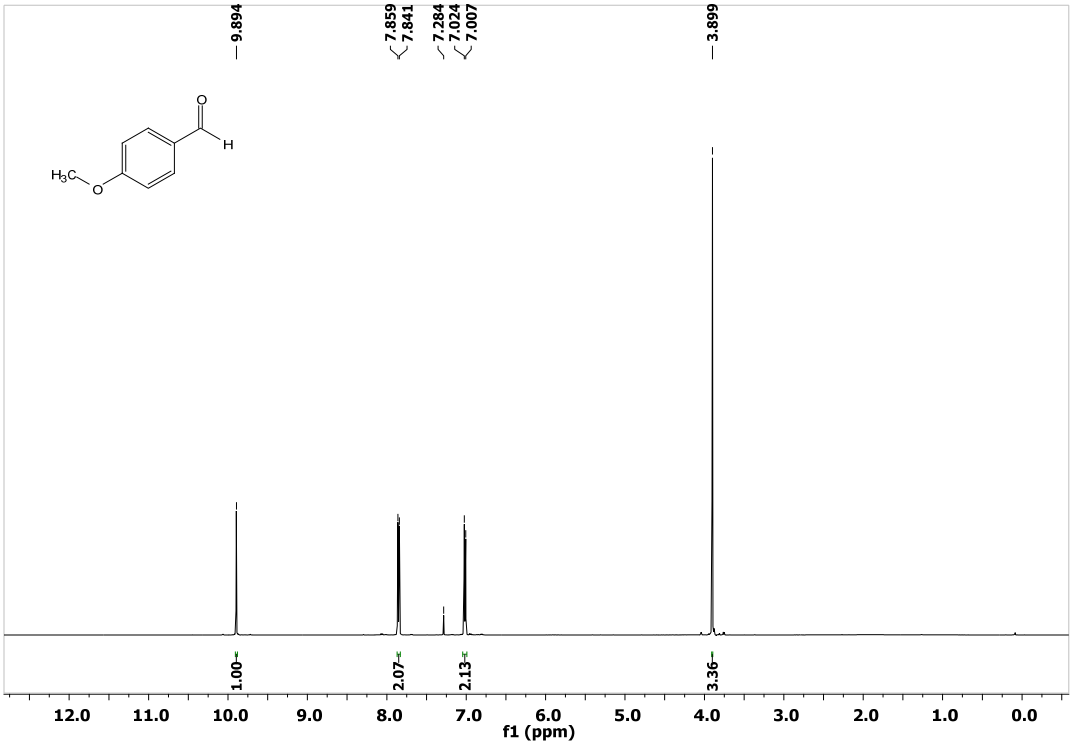
^{1}H NMR (500 MHz, $CDCl_3$) (**6d**)



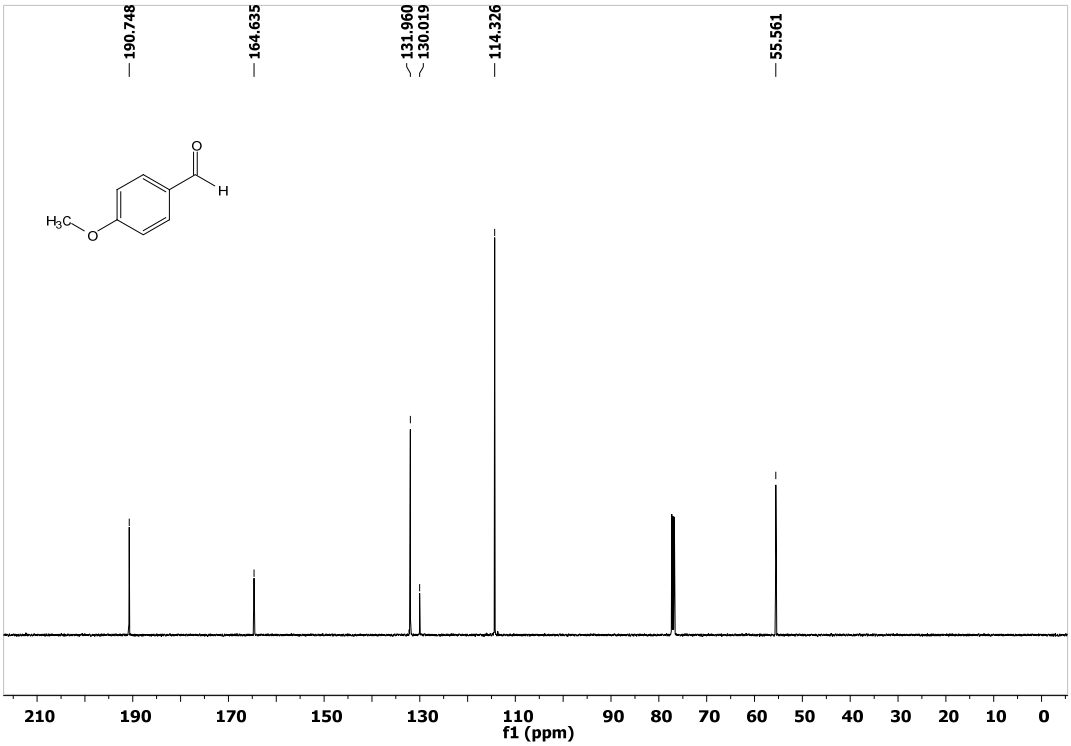
^{13}C NMR (125 MHz, $CDCl_3$) (**6d**)



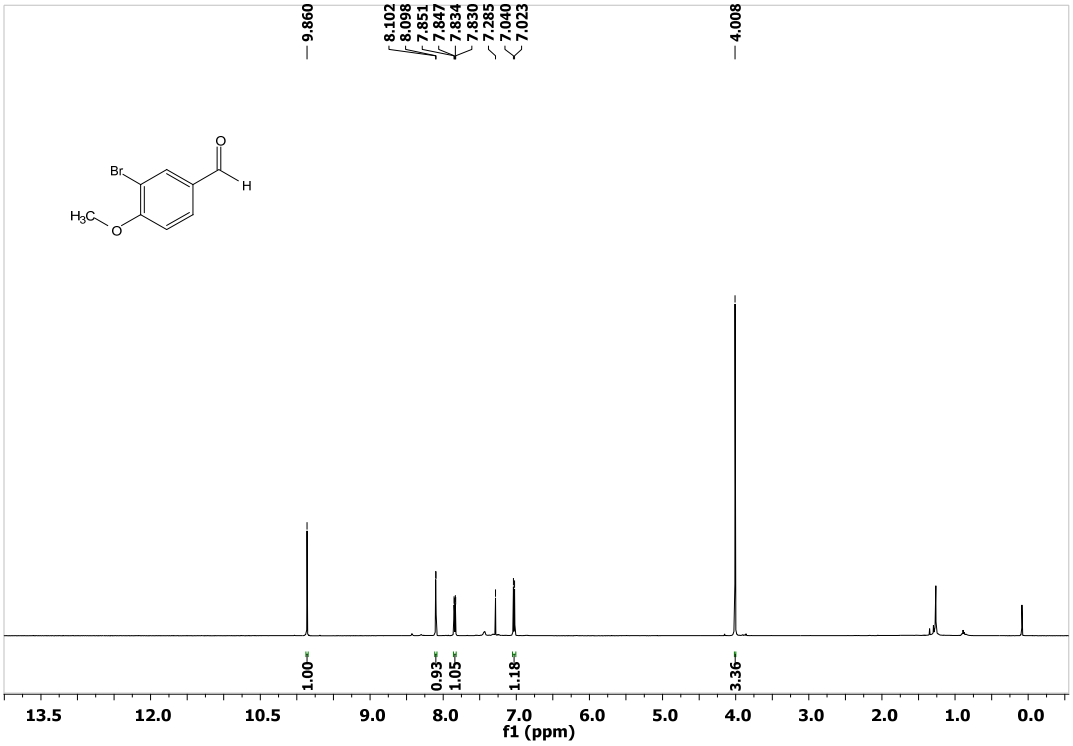
^{1}H NMR (500 MHz, $CDCl_3$) (**6e**)



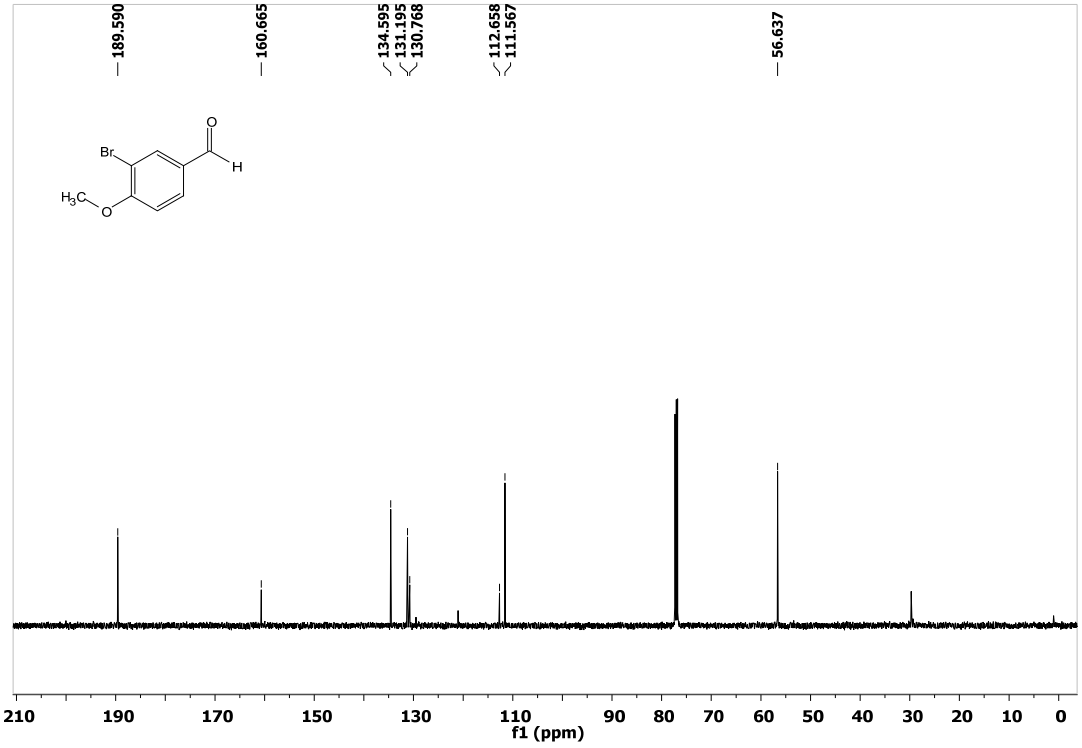
^{13}C NMR (125 MHz, $CDCl_3$) (**6e**)



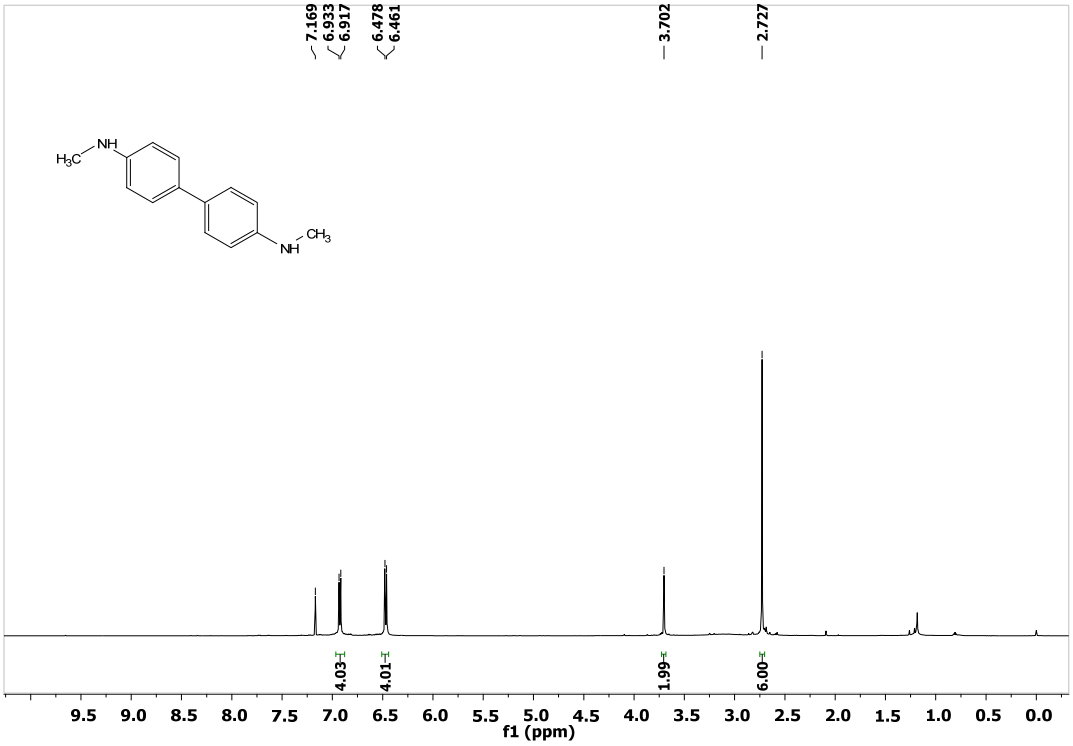
^{1}H NMR (500 MHz, $CDCl_3$) (**6f**)



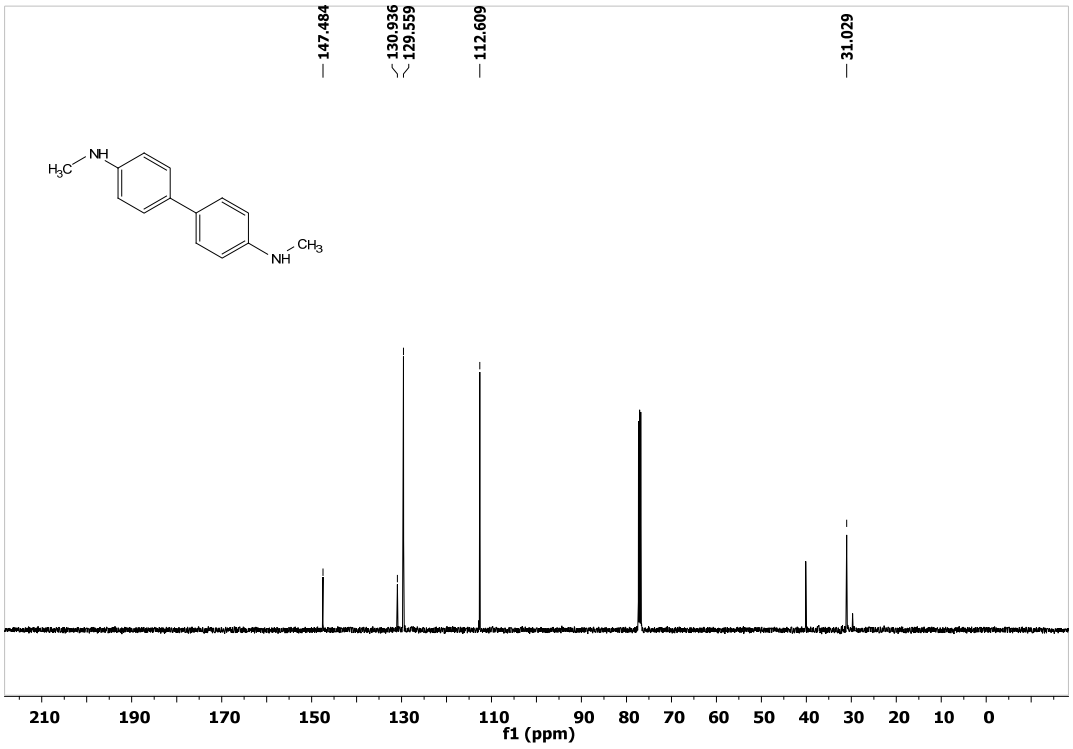
^{13}C NMR (125 MHz, $CDCl_3$) (**6f**)



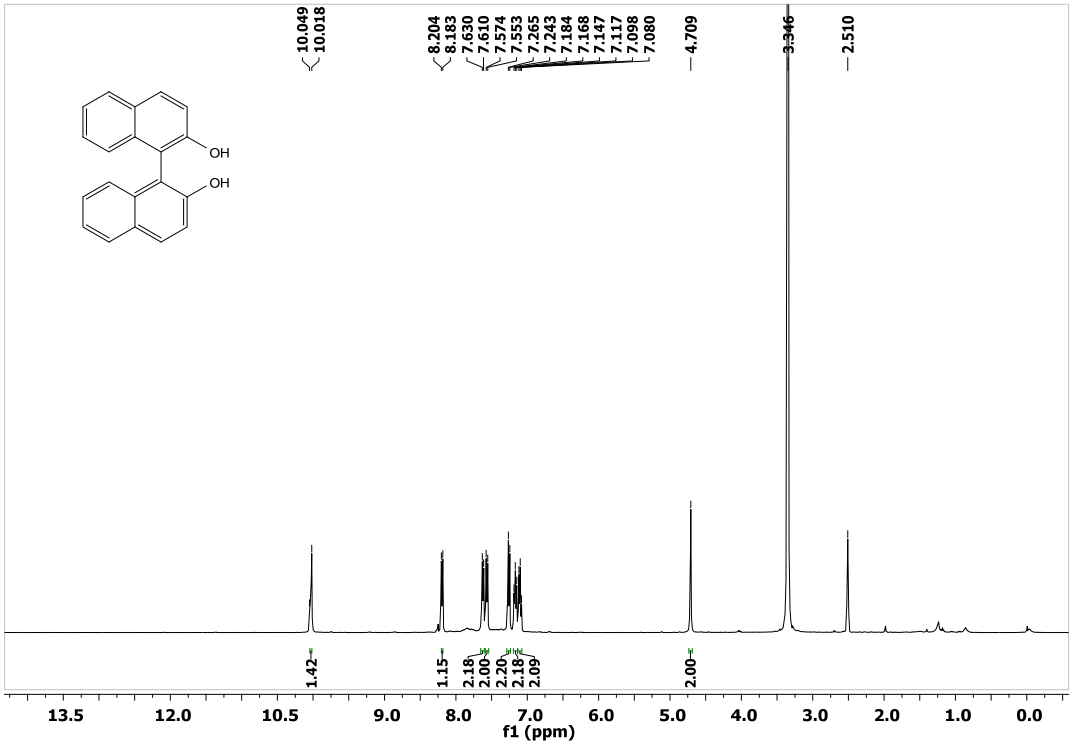
^{1}H NMR (500 MHz, $CDCl_3$) (**6'**)



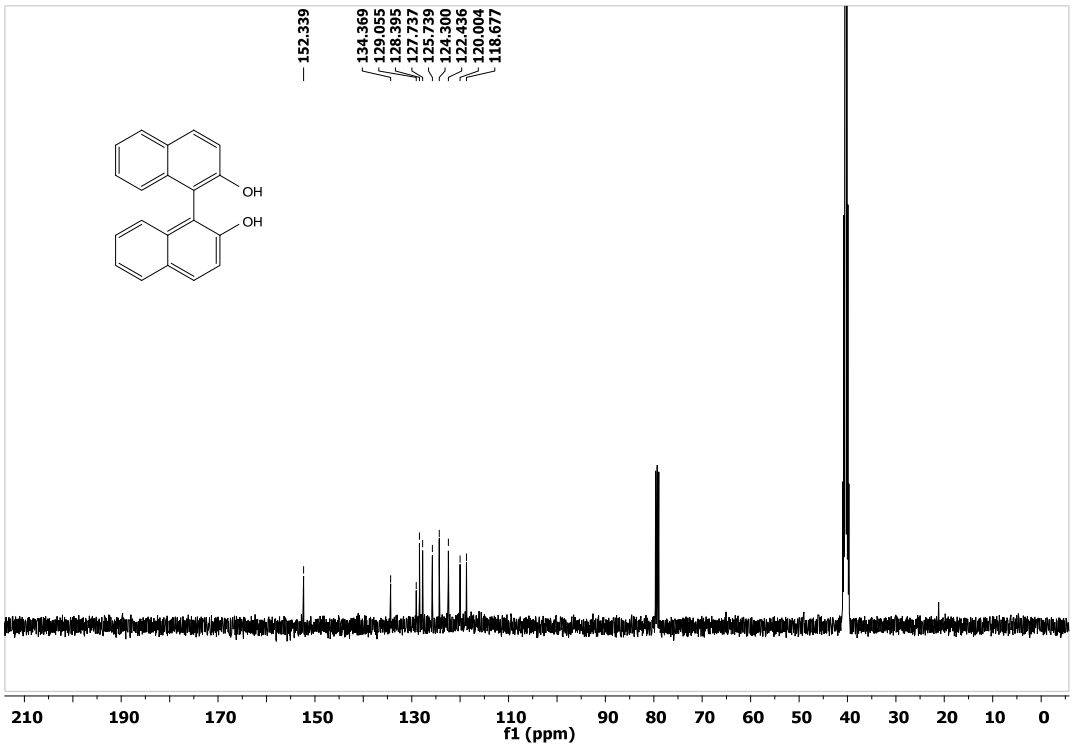
^{13}C NMR (125 MHz, $CDCl_3$) (**6'**)



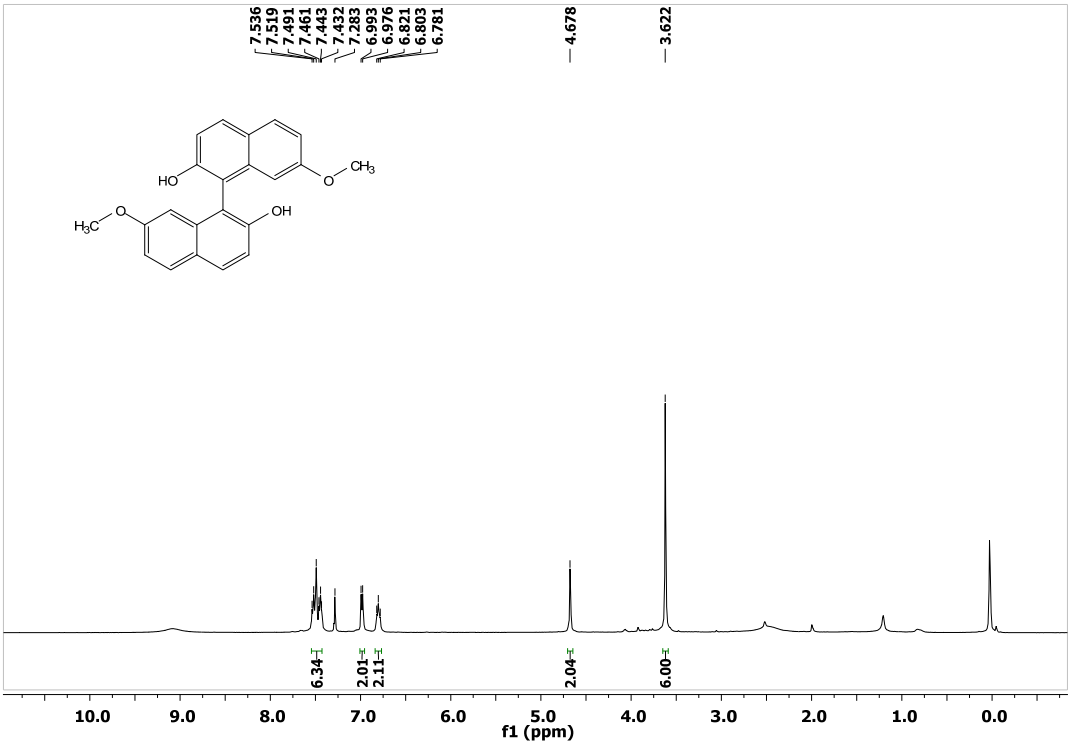
^{1}H NMR (400 MHz, $CDCl_3$ and DMSO-d_6) (**8a**)



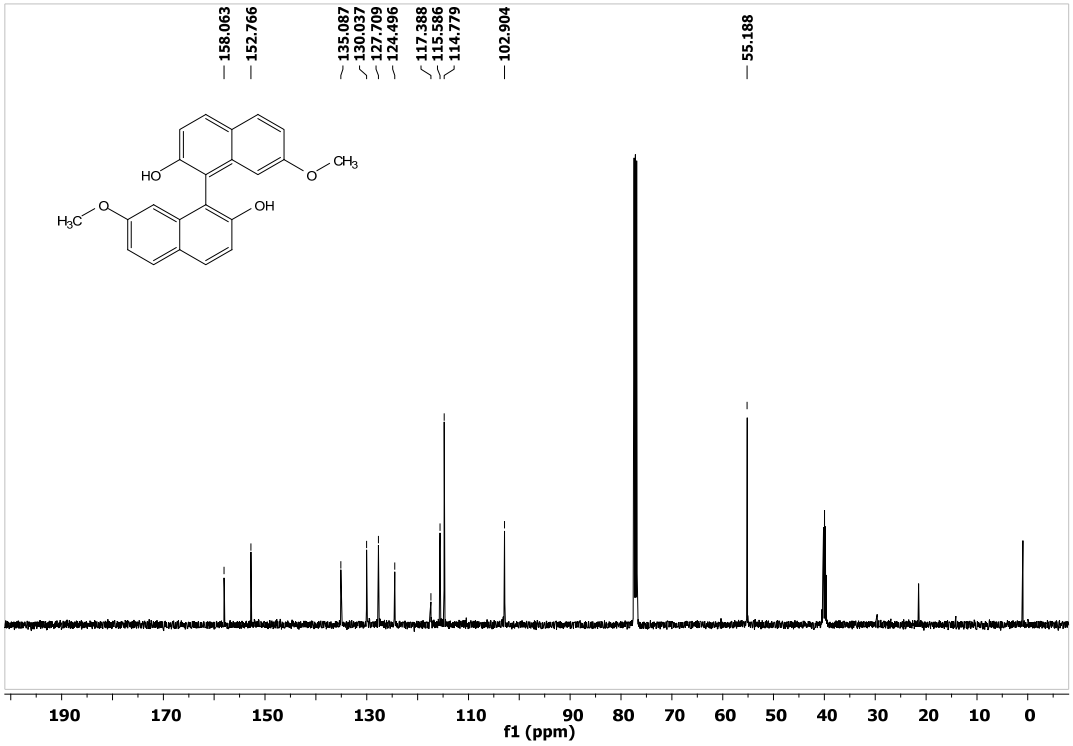
^{13}C NMR (100 MHz, $CDCl_3$ and DMSO-d_6) (**8a**)



^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6) (**8b**)

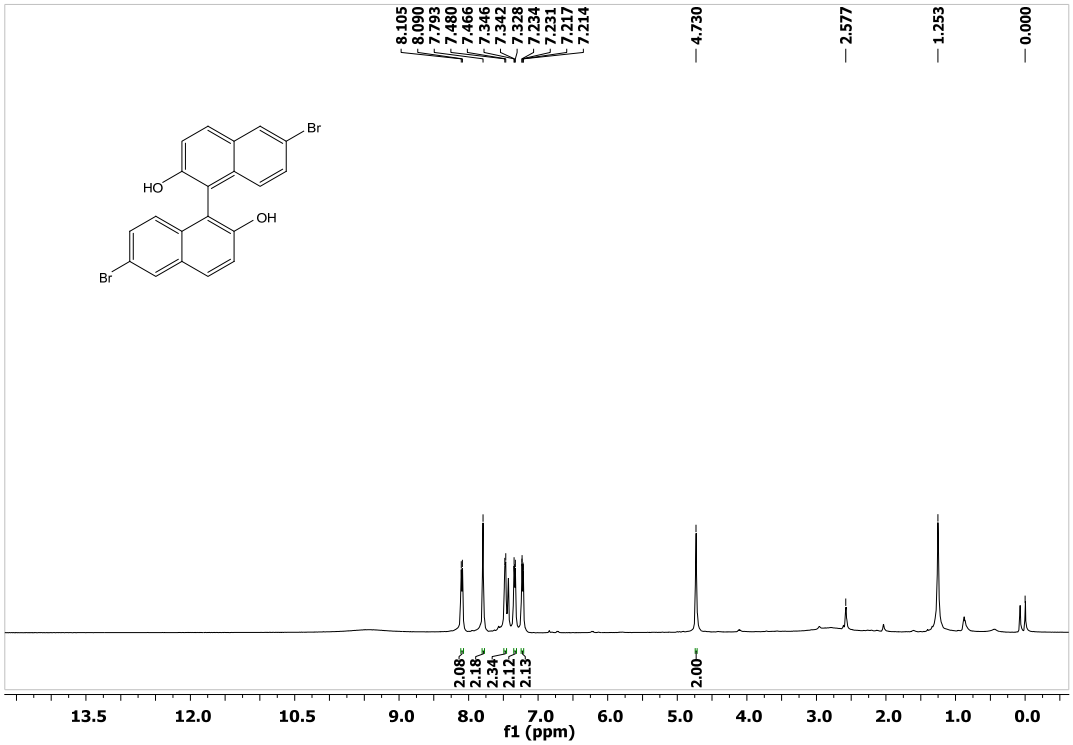


^{13}C NMR (125 MHz, $CDCl_3$ and DMSO-d_6) (**8b**)

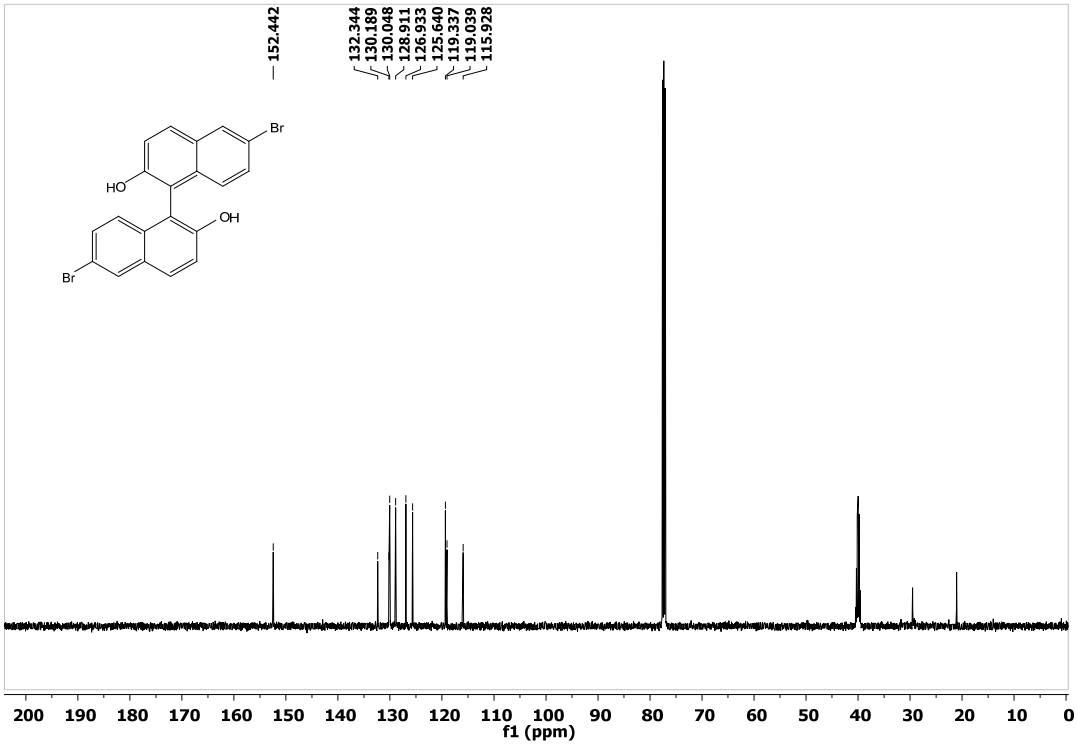


^{1}H NMR

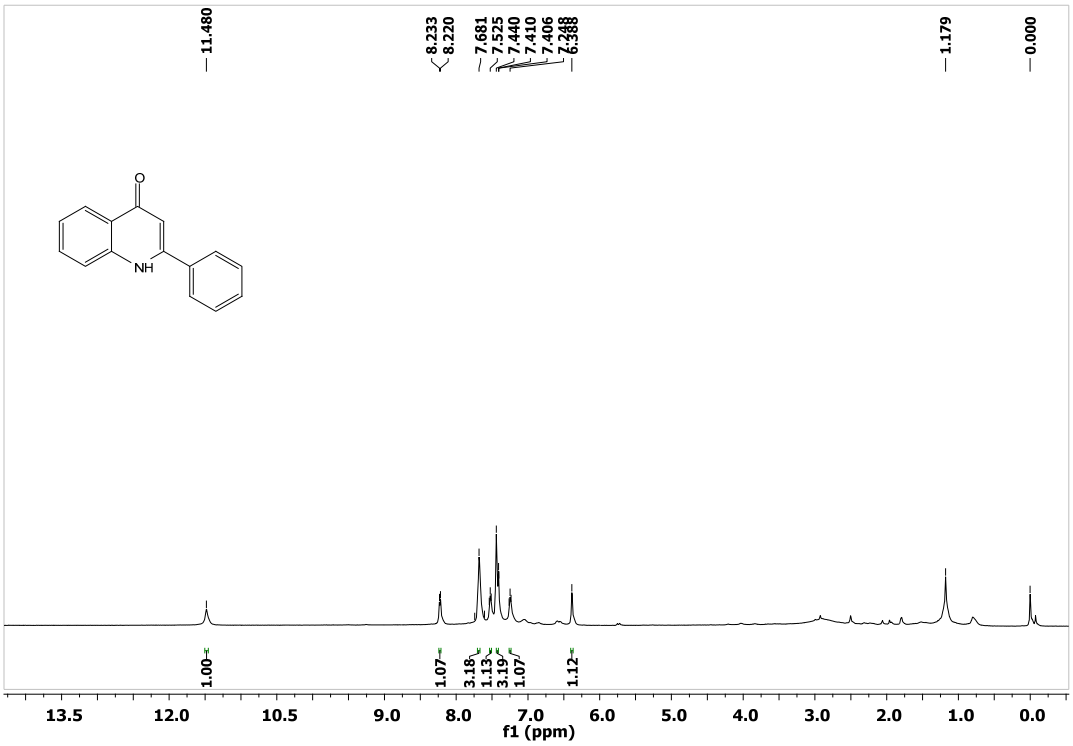
(500 MHz, $CDCl_3$ and DMSO-d_6) (**8c**)



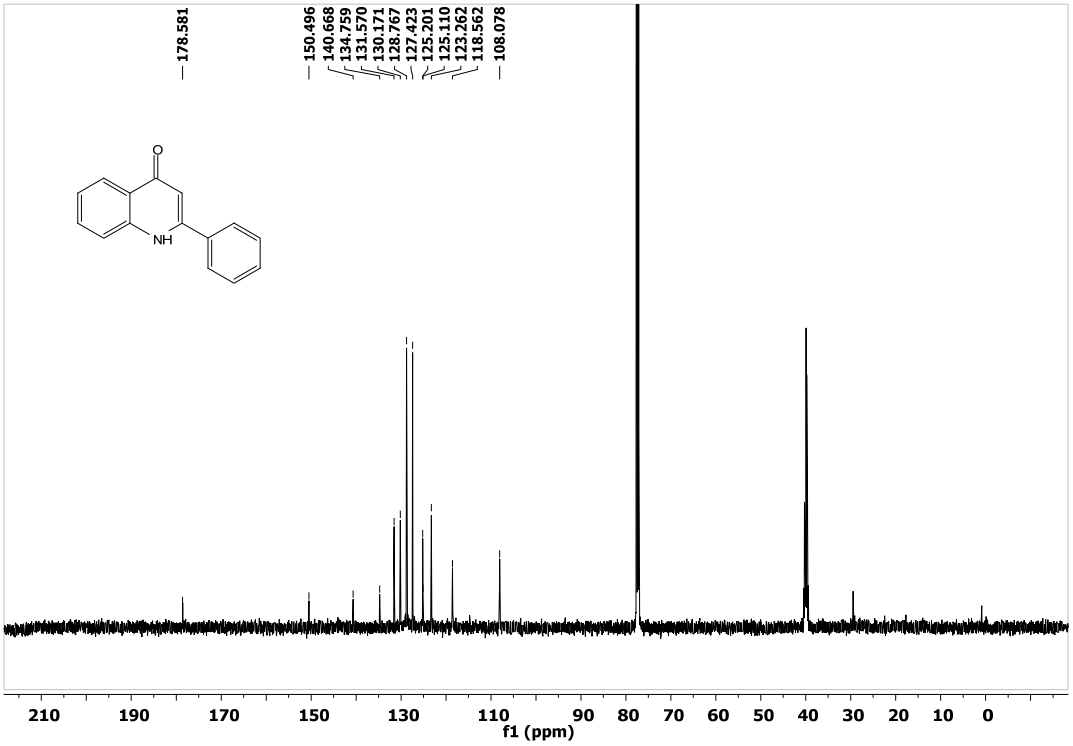
^{13}C NMR (125 MHz, $CDCl_3$ and DMSO-d_6)(**8c**)



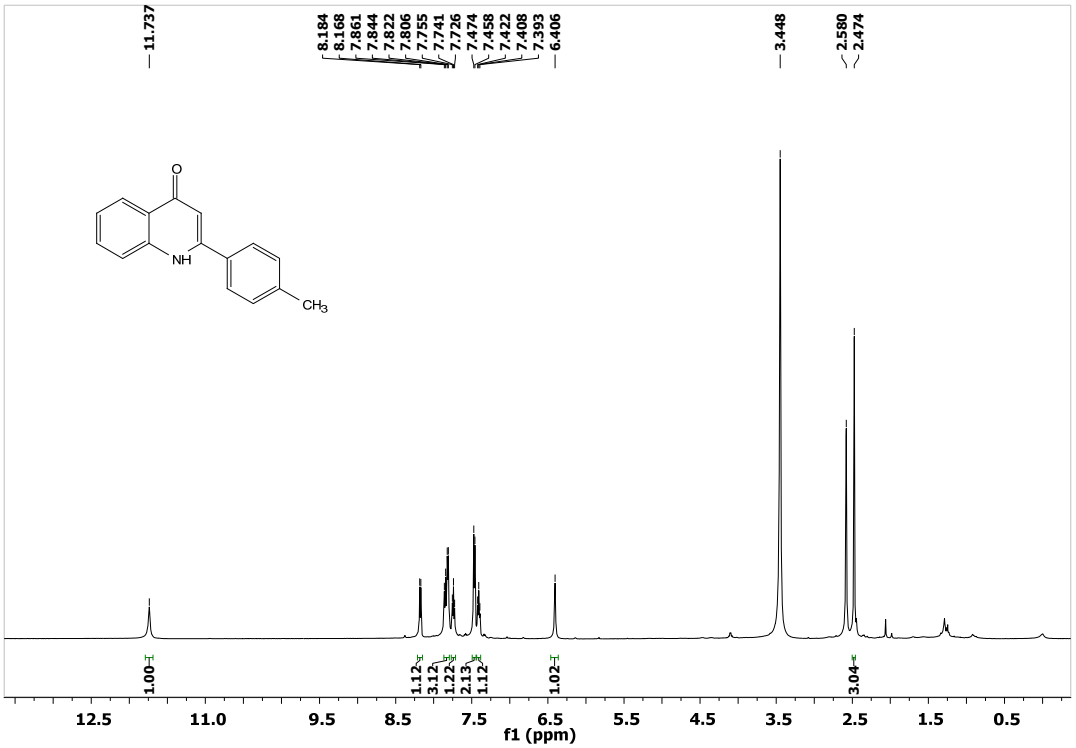
^{1}H NMR (500 MHz, $CDCl_3$ and DMSO-d_6) (**10a**)



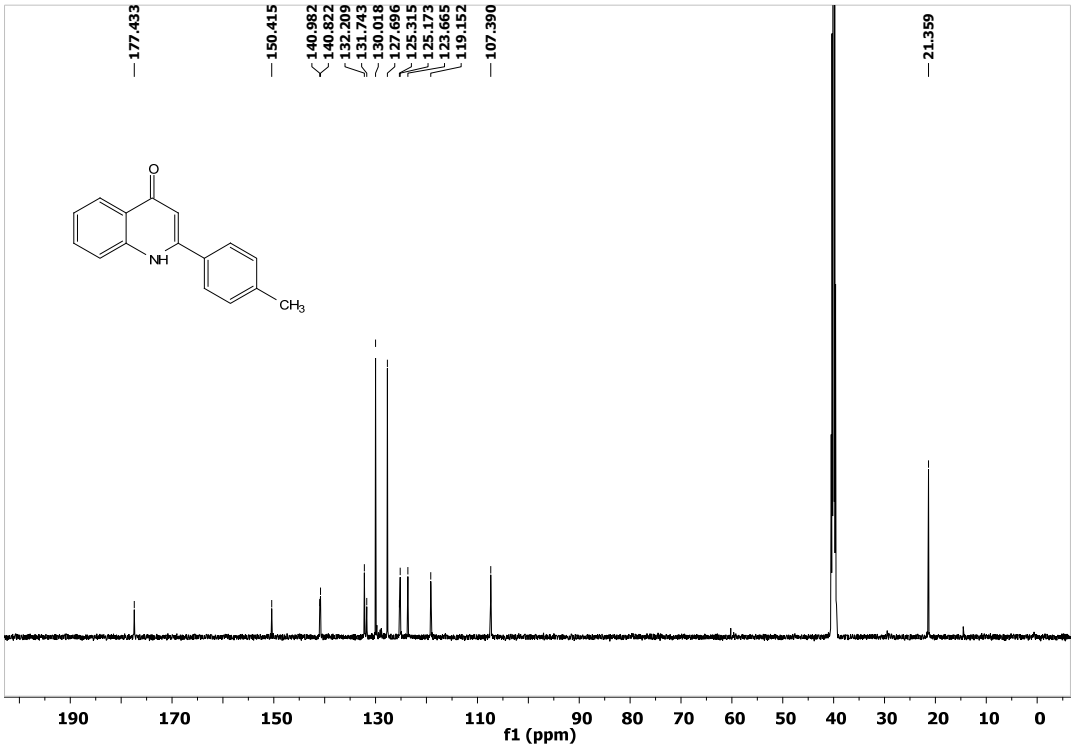
^{13}C NMR (125 MHz, $CDCl_3$ and DMSO-d_6) (**10a**)



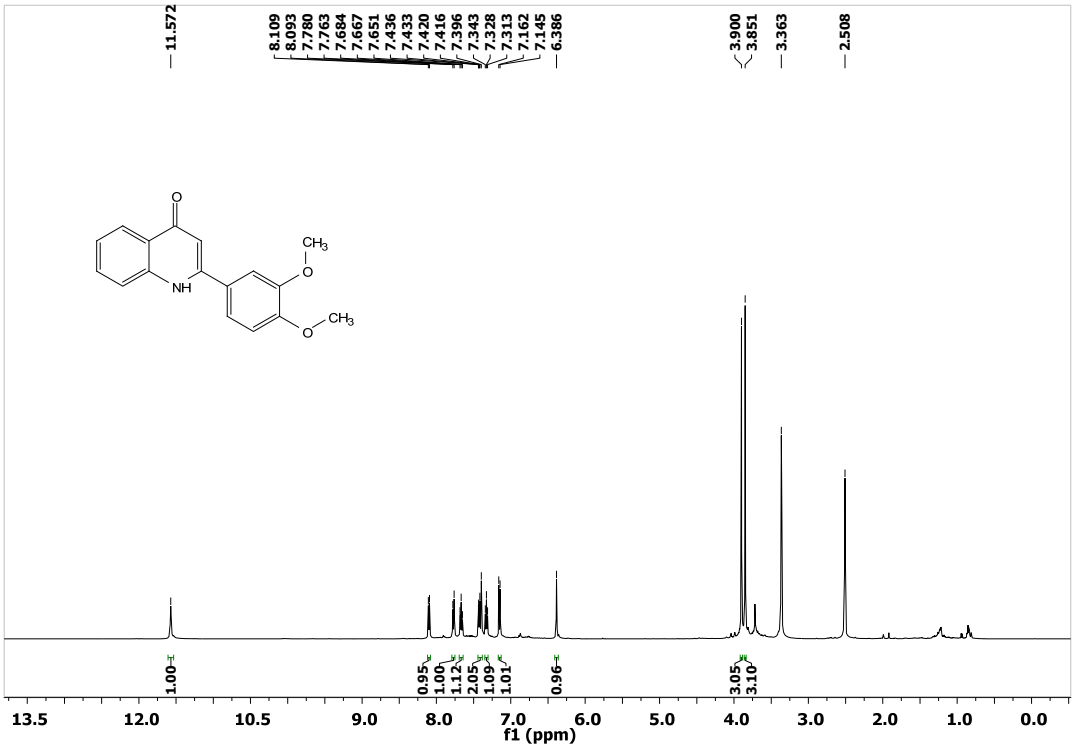
^{1}H NMR (500 MHz, DMSO-d_6) (**10b**)



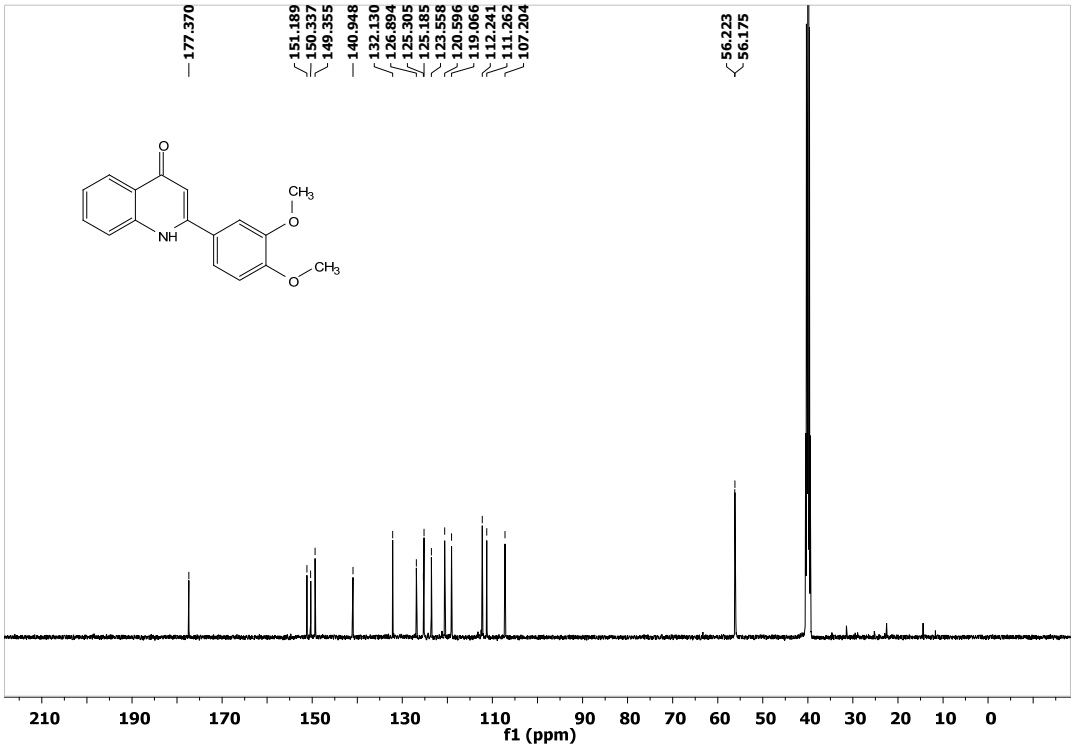
^{13}C NMR (125 MHz, DMSO-d_6) (**10b**)



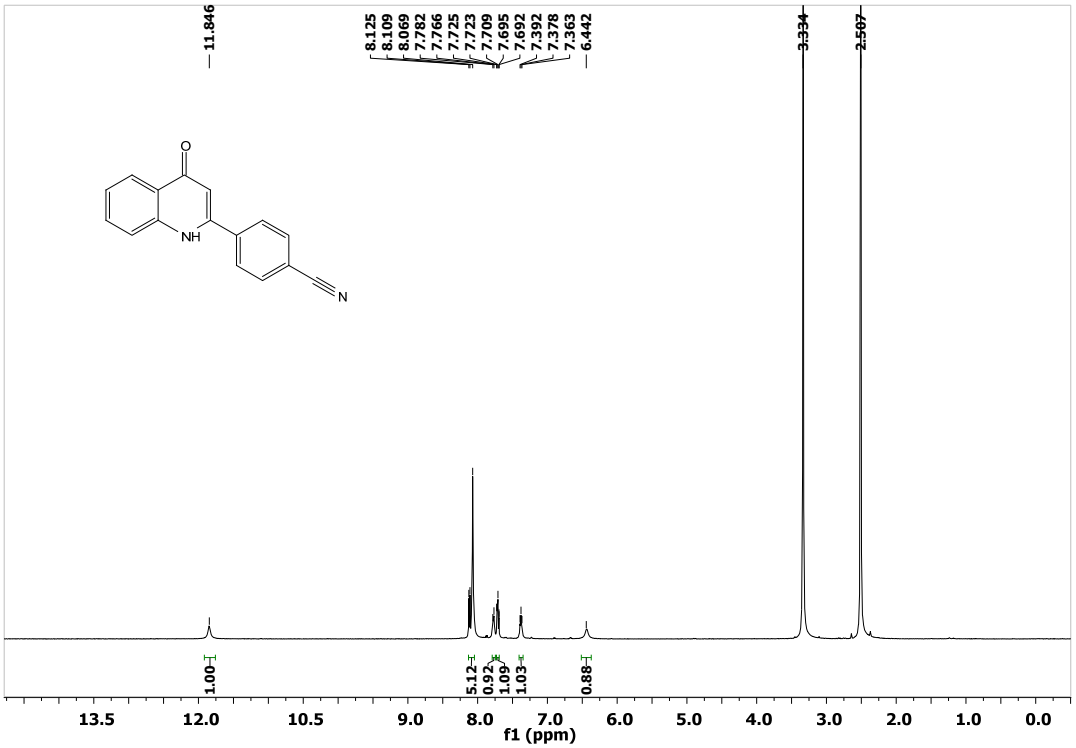
^{1}H NMR (500 MHz, DMSO-d_6) (**10c**)



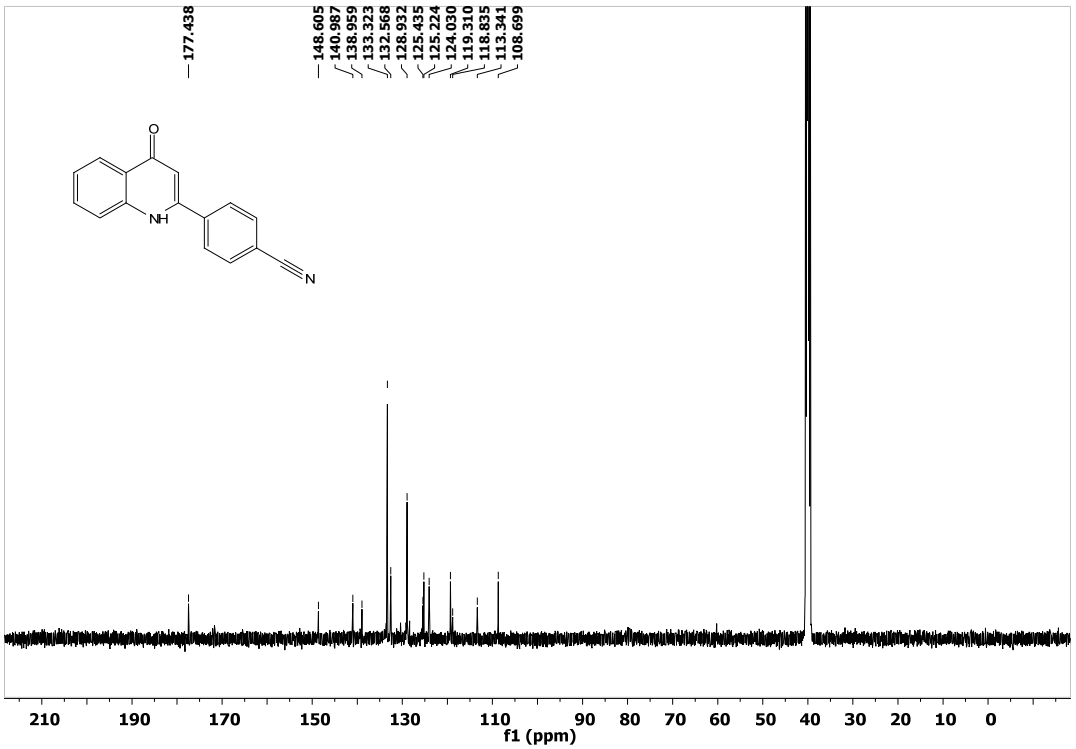
^{13}C NMR (125 MHz, DMSO-d_6) (**10c**)



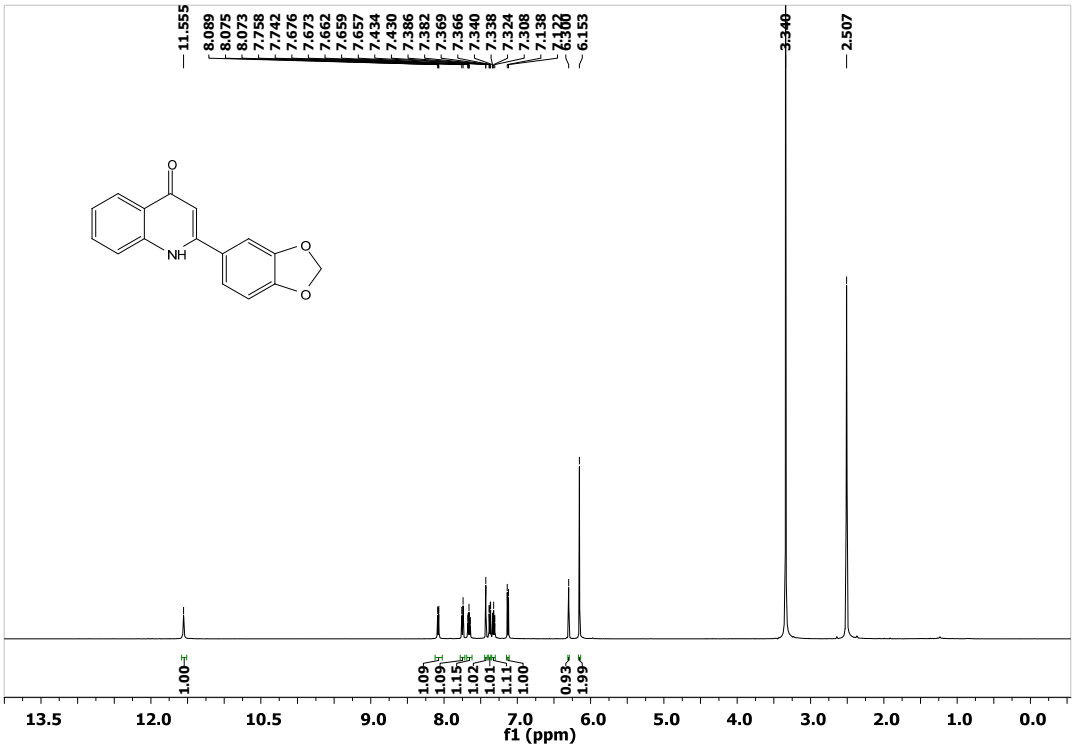
^{1}H NMR (500 MHz, DMSO-d_6) (**10d**)



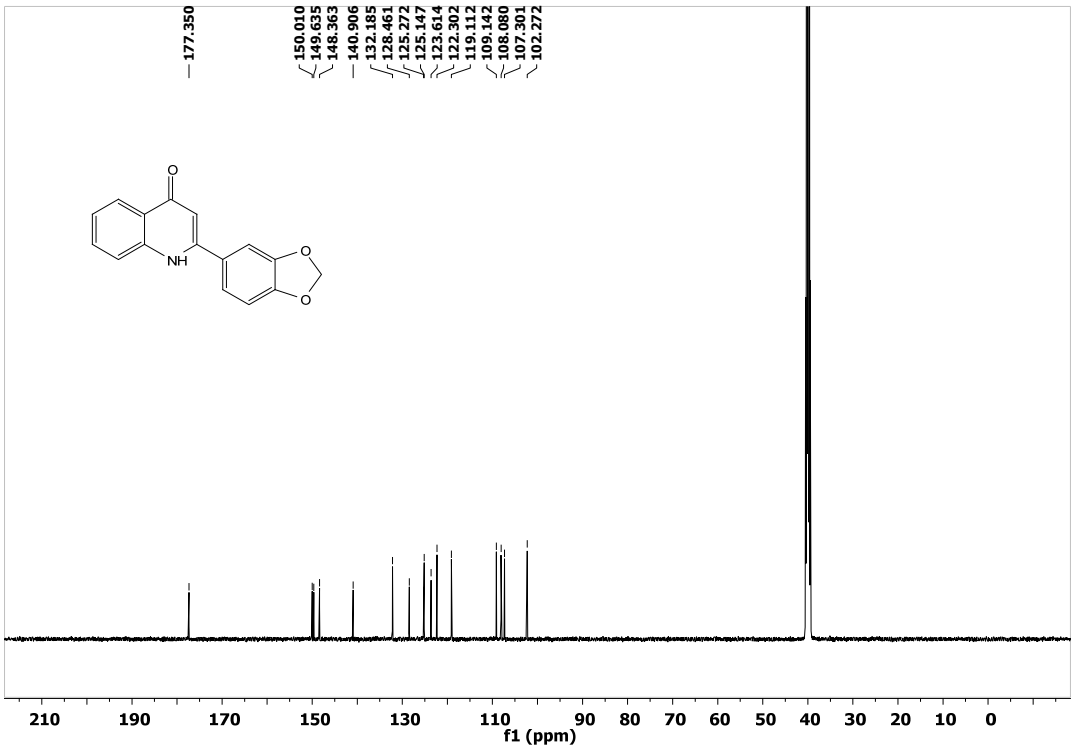
^{13}C NMR (125 MHz, DMSO-d_6) (**10d**)



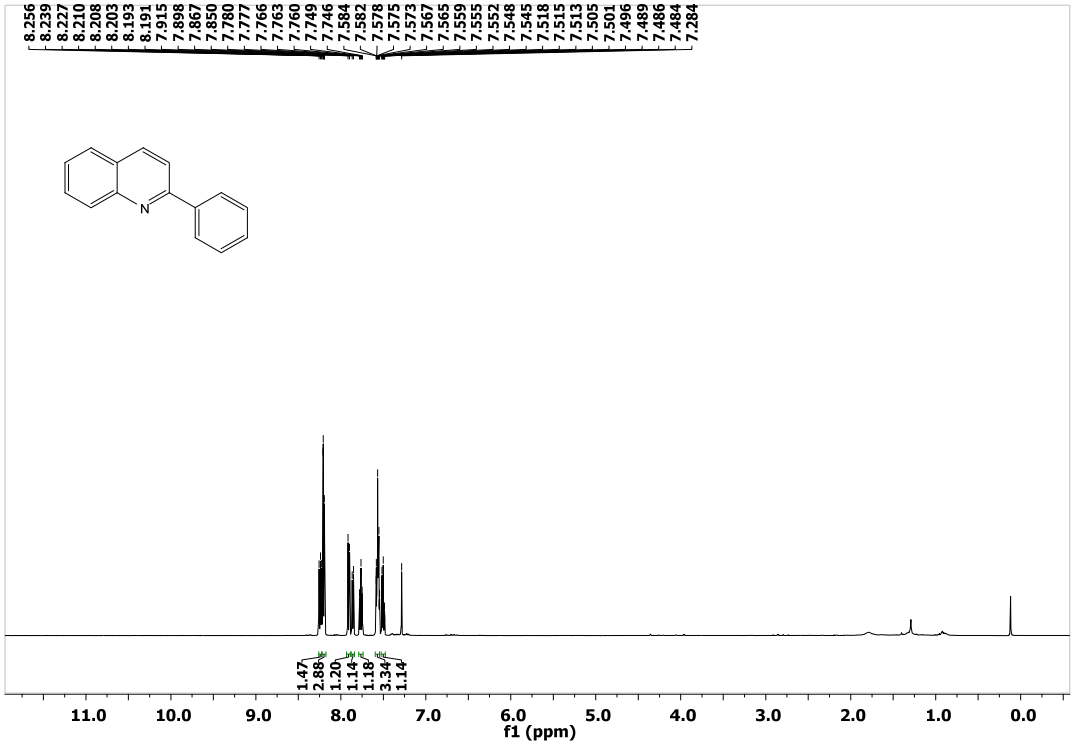
^{1}H NMR (500 MHz, DMSO-d_6) (**10f**)



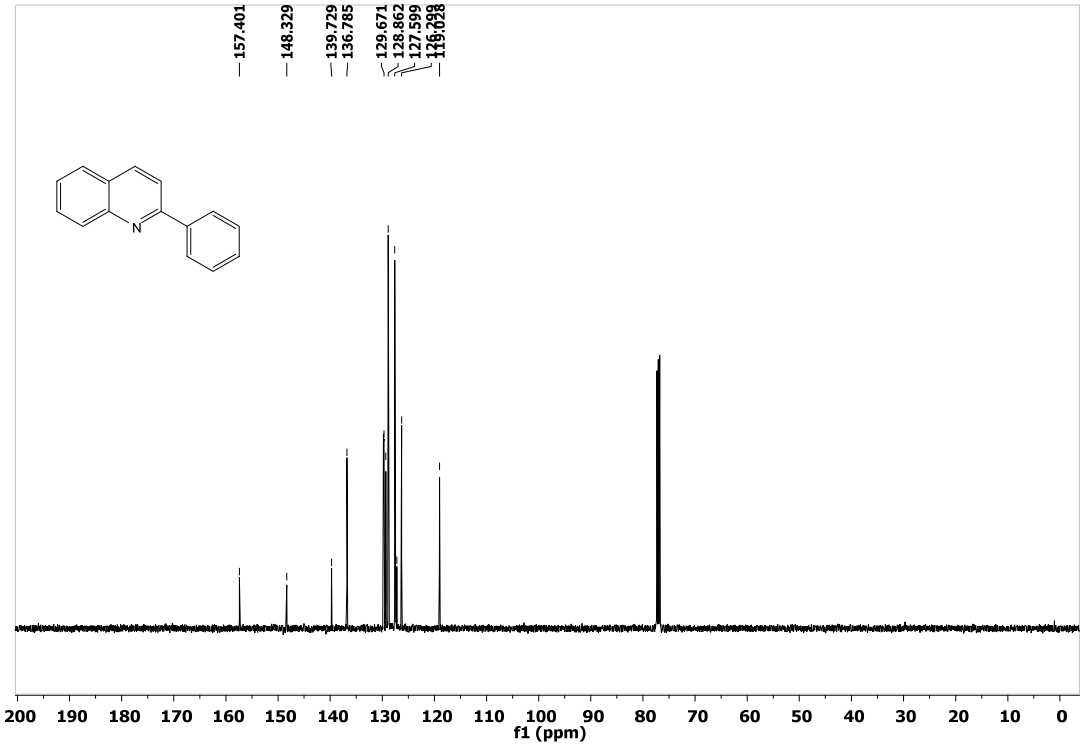
^{13}C NMR (125 MHz, DMSO-d_6) (**10f**)



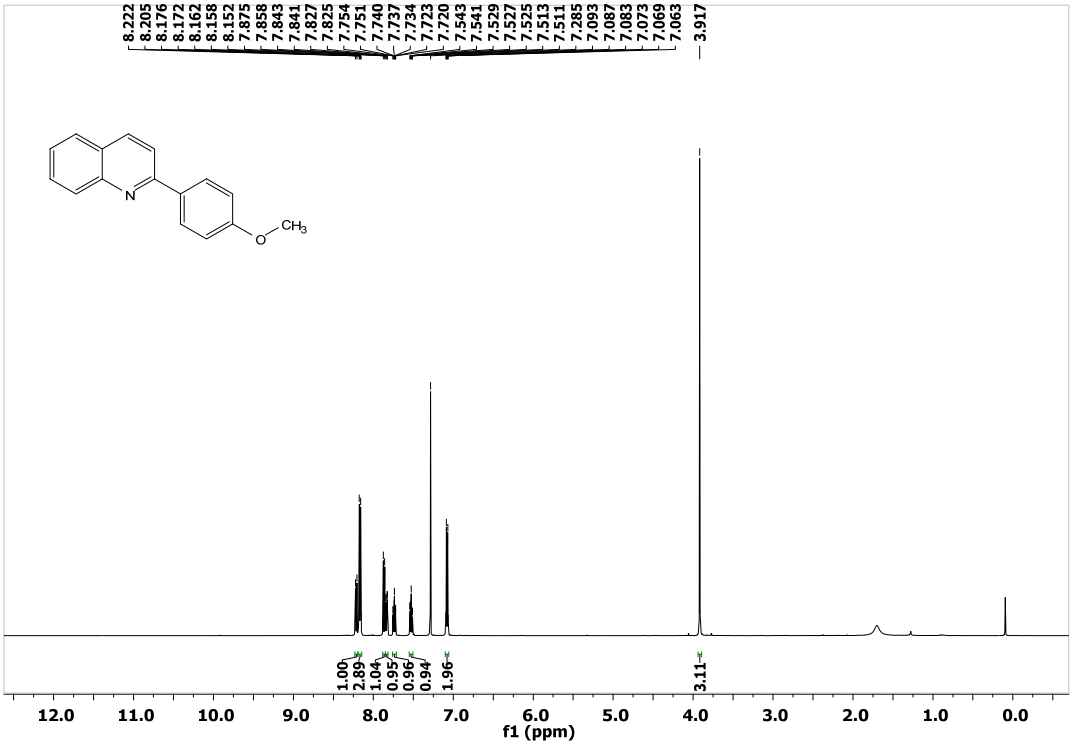
^{1}H NMR (500 MHz, $CDCl_3$) (**12a**)



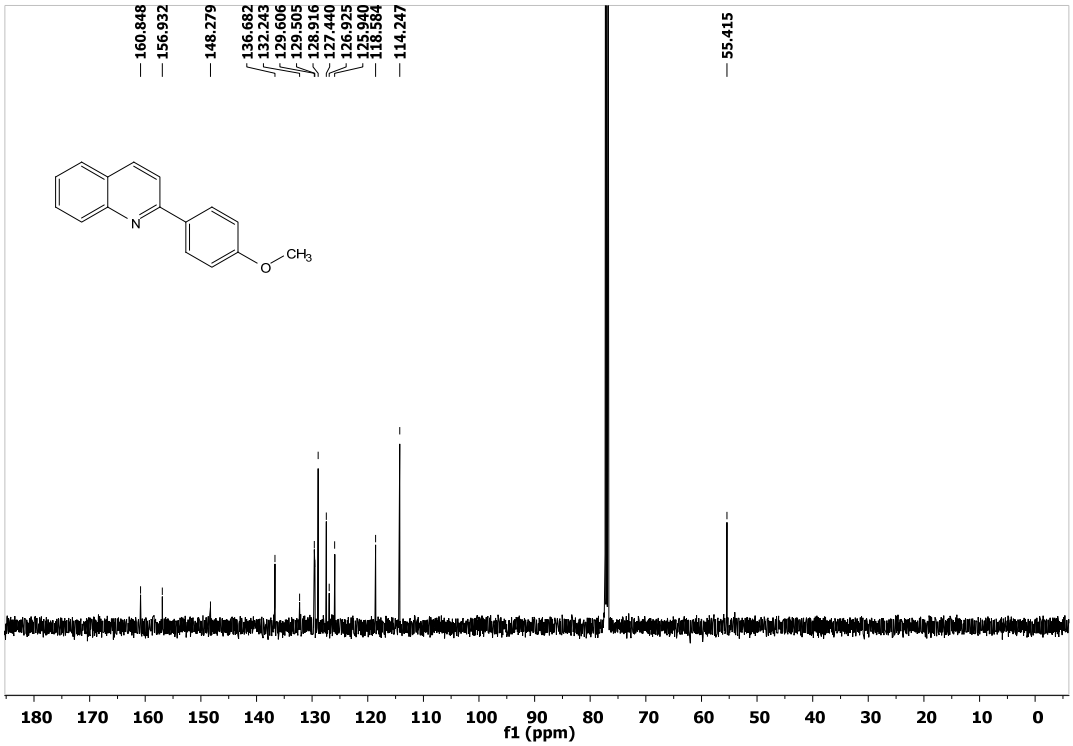
^{13}C NMR (125 MHz, $CDCl_3$) (**12a**)



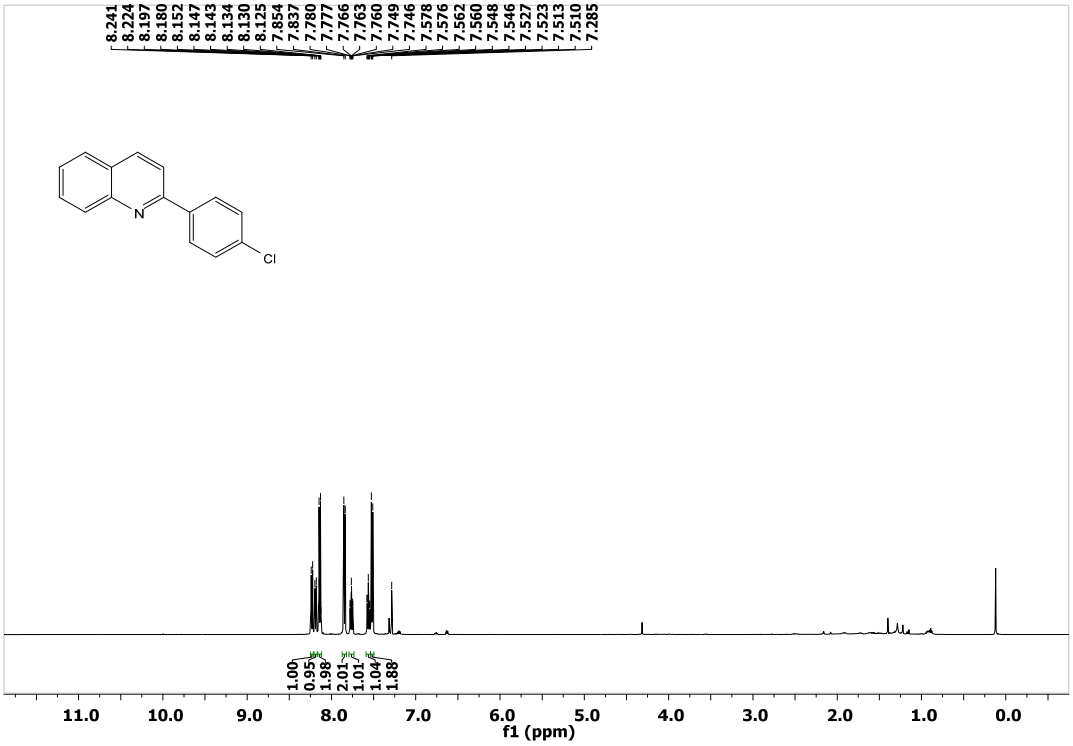
^{1}H NMR (500 MHz, $CDCl_3$) (**12c**)



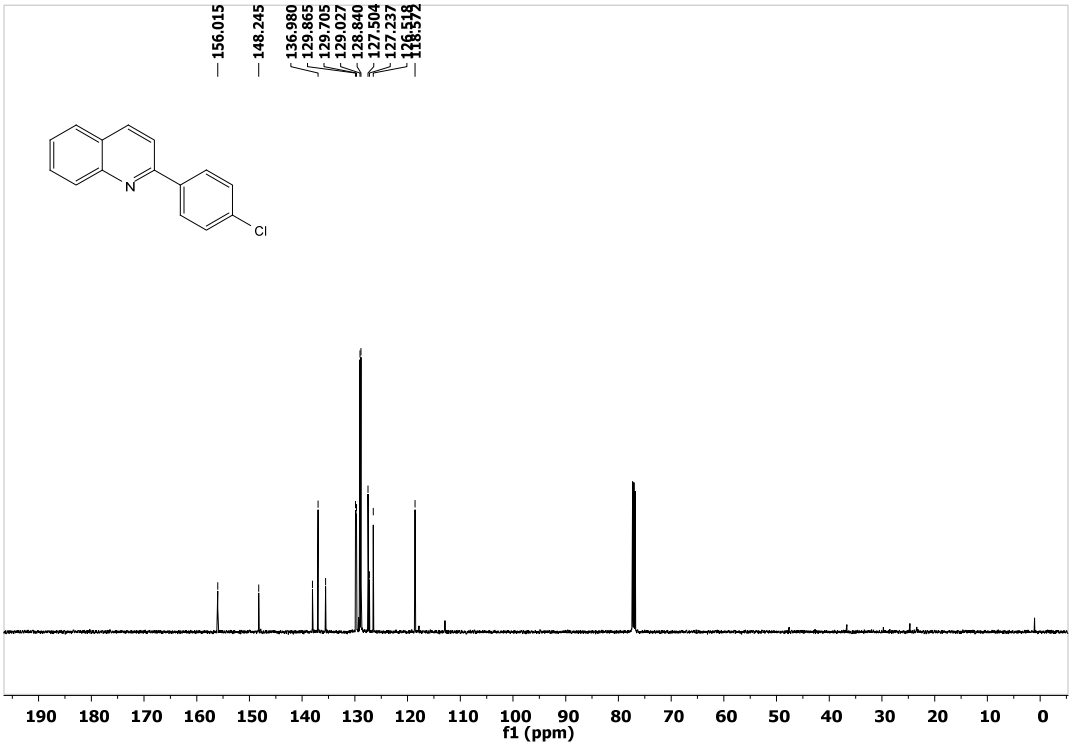
^{13}C NMR (125 MHz, $CDCl_3$) (**12c**)



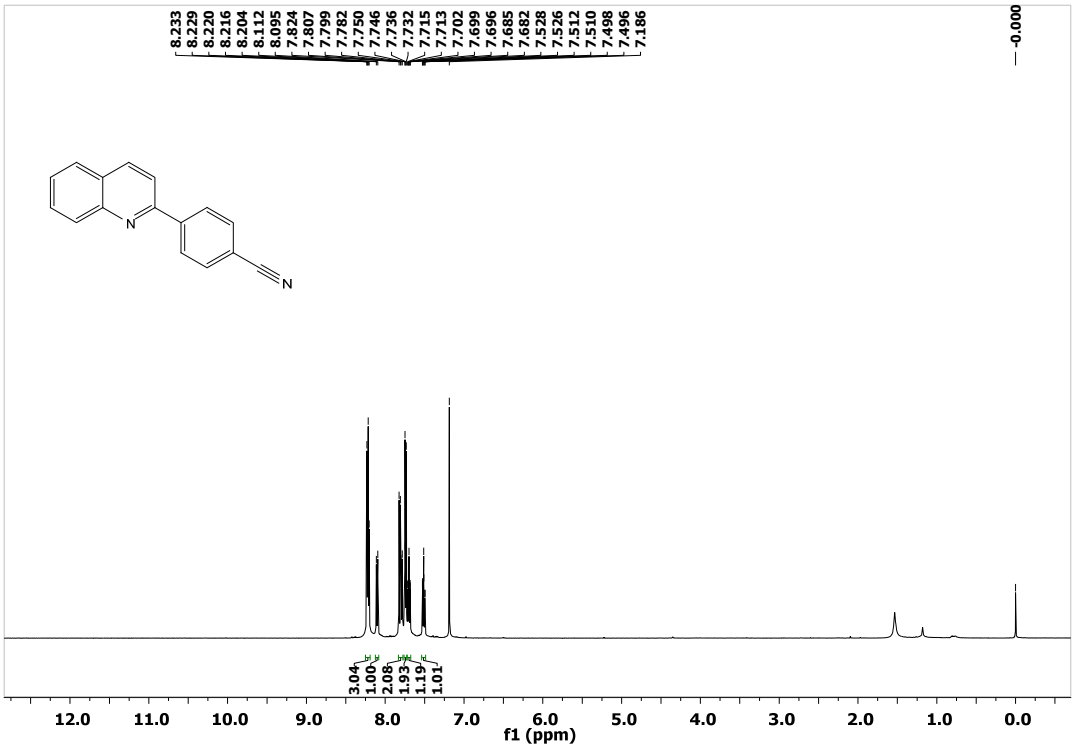
^{1}H NMR (500 MHz, $CDCl_3$) (**12b**)



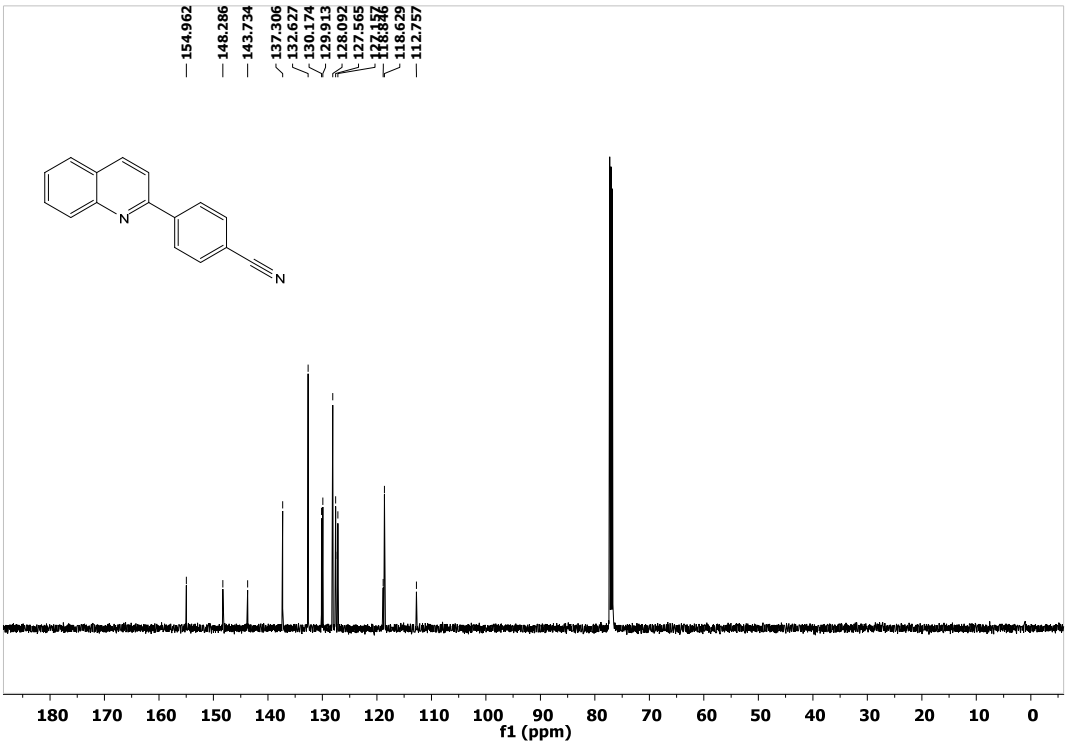
^{13}C NMR (125 MHz, $CDCl_3$) (**12b**)



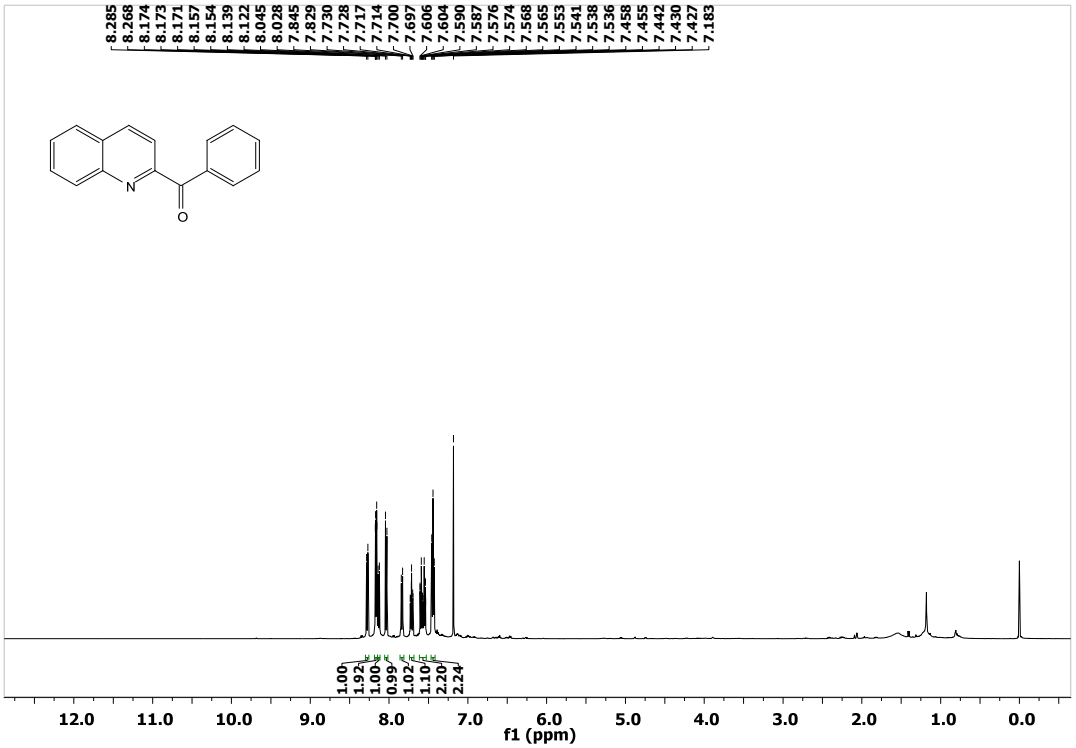
^{1}H NMR (500 MHz, $CDCl_3$) (**12d**)



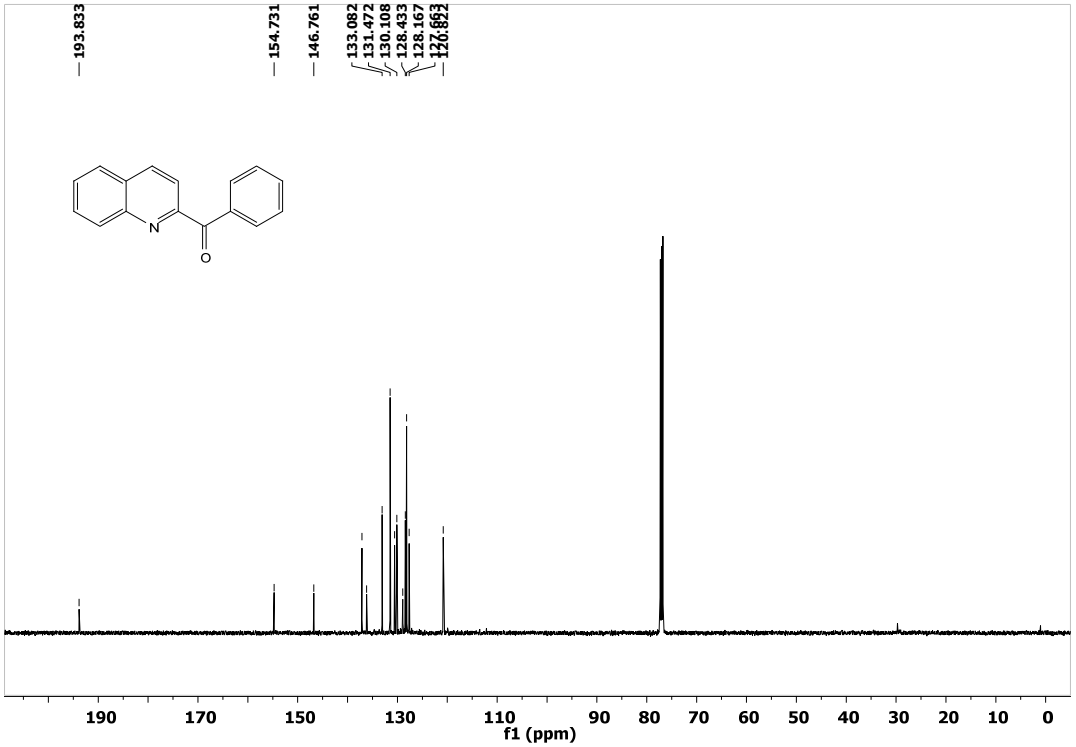
^{13}C NMR (125 MHz, $CDCl_3$) (**12d**)



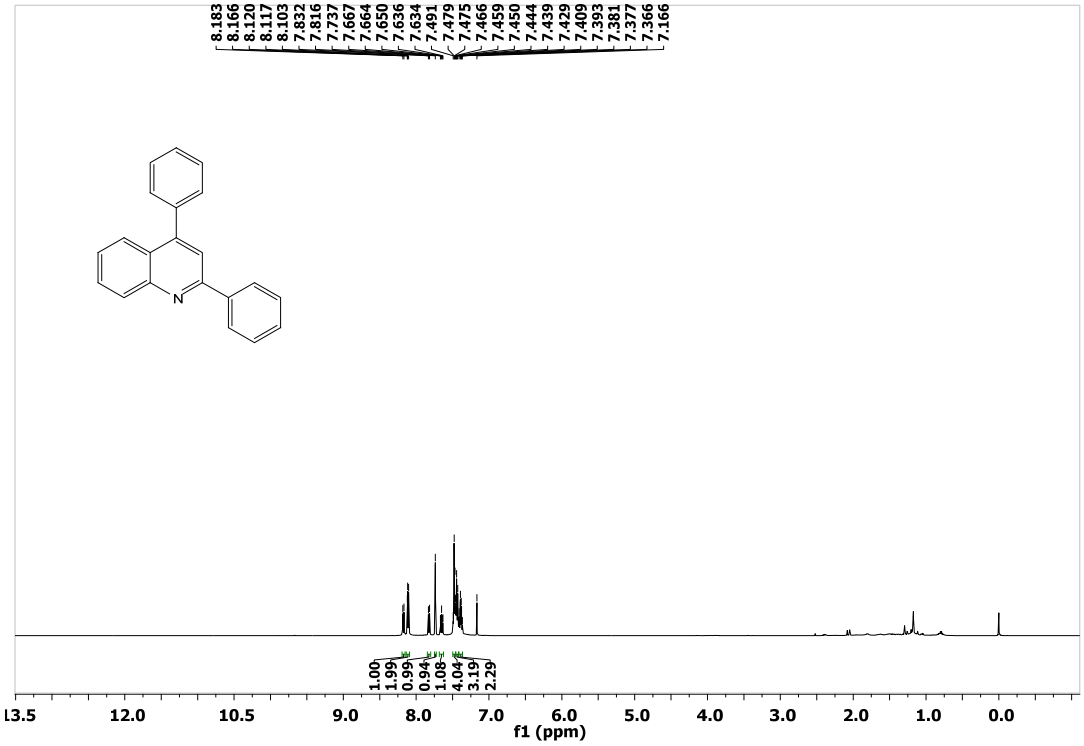
^{1}H NMR (500 MHz, $CDCl_3$) (**12f**)



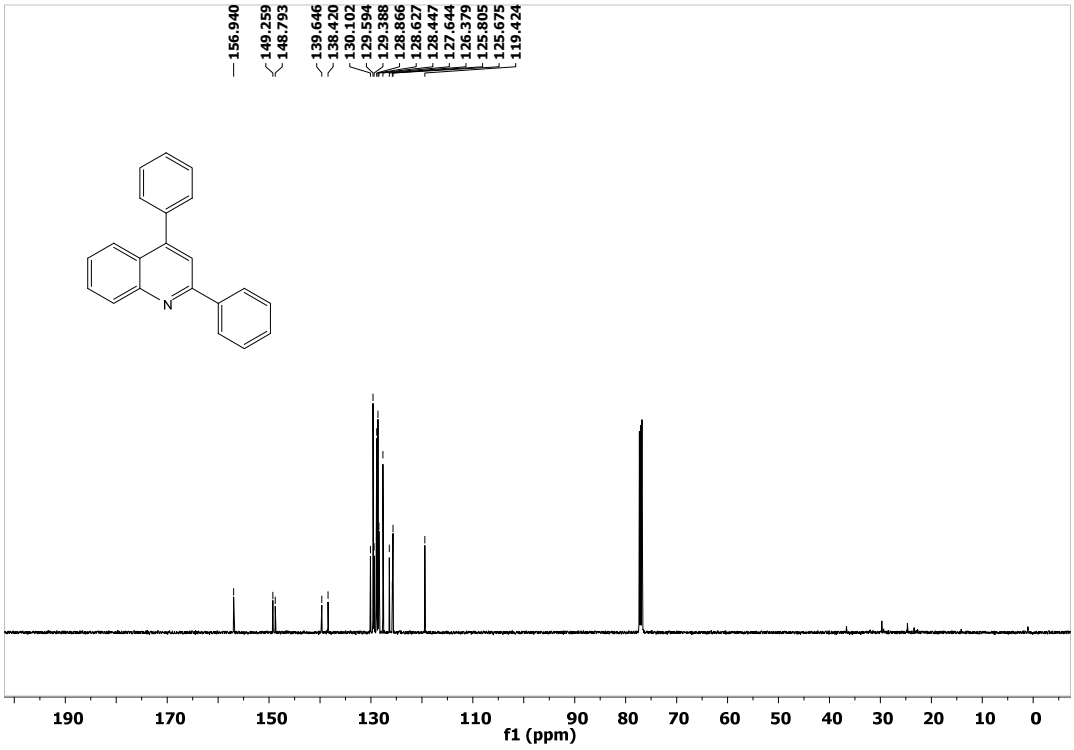
^{13}C NMR (125 MHz, $CDCl_3$) (**12f**)



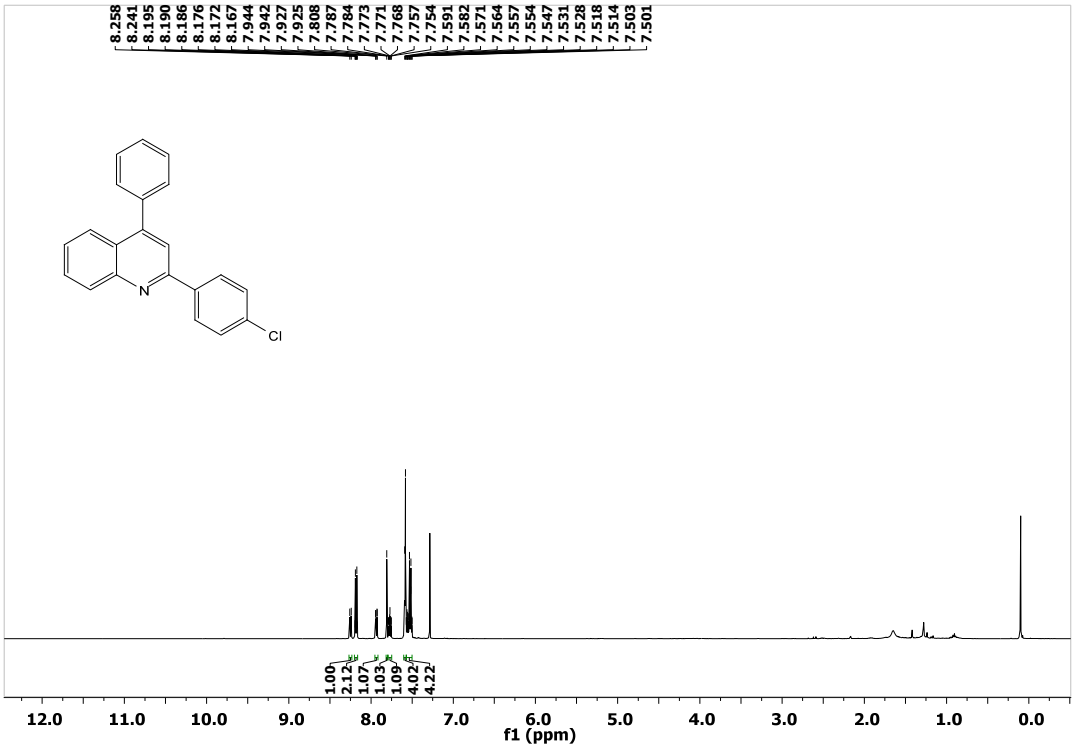
^{1}H NMR (500 MHz, $CDCl_3$) (**14a**)



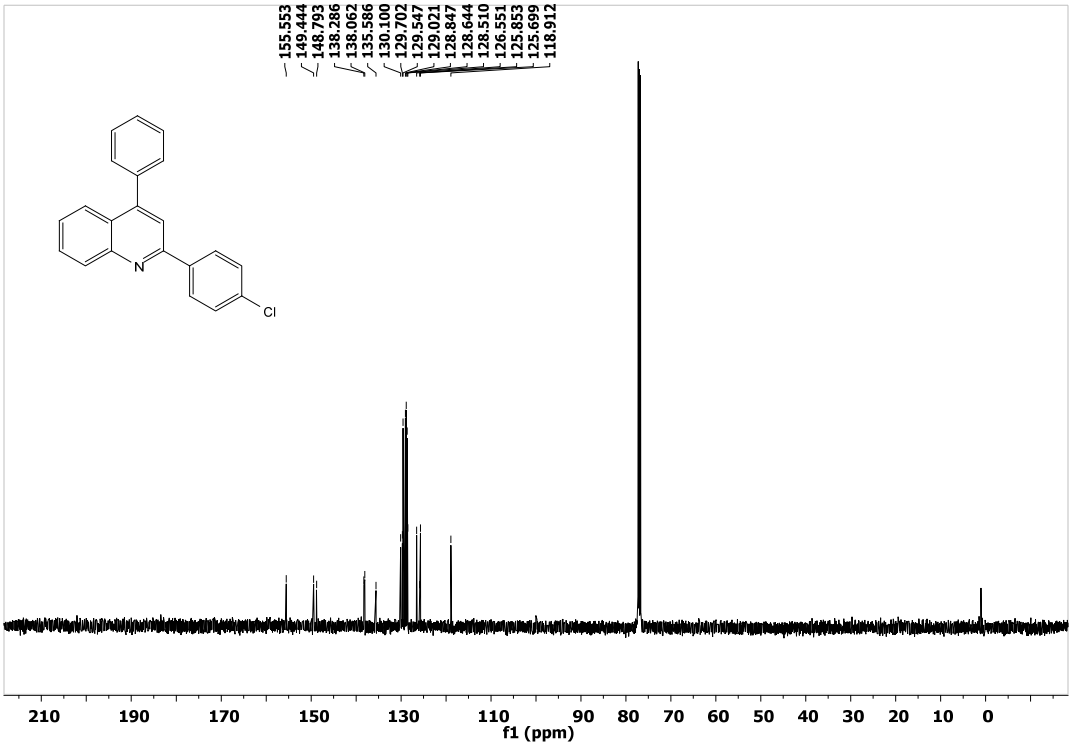
^{13}C NMR (125 MHz, $CDCl_3$) (**14a**)



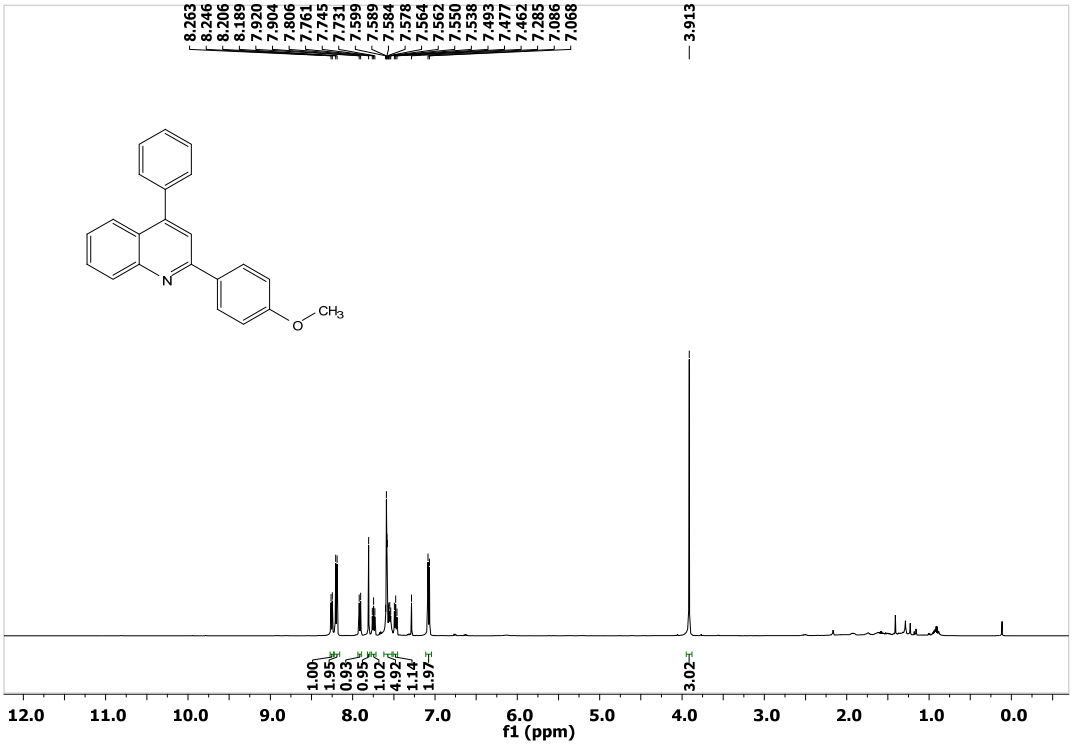
^{1}H NMR (500 MHz, $CDCl_3$) (**14b**)



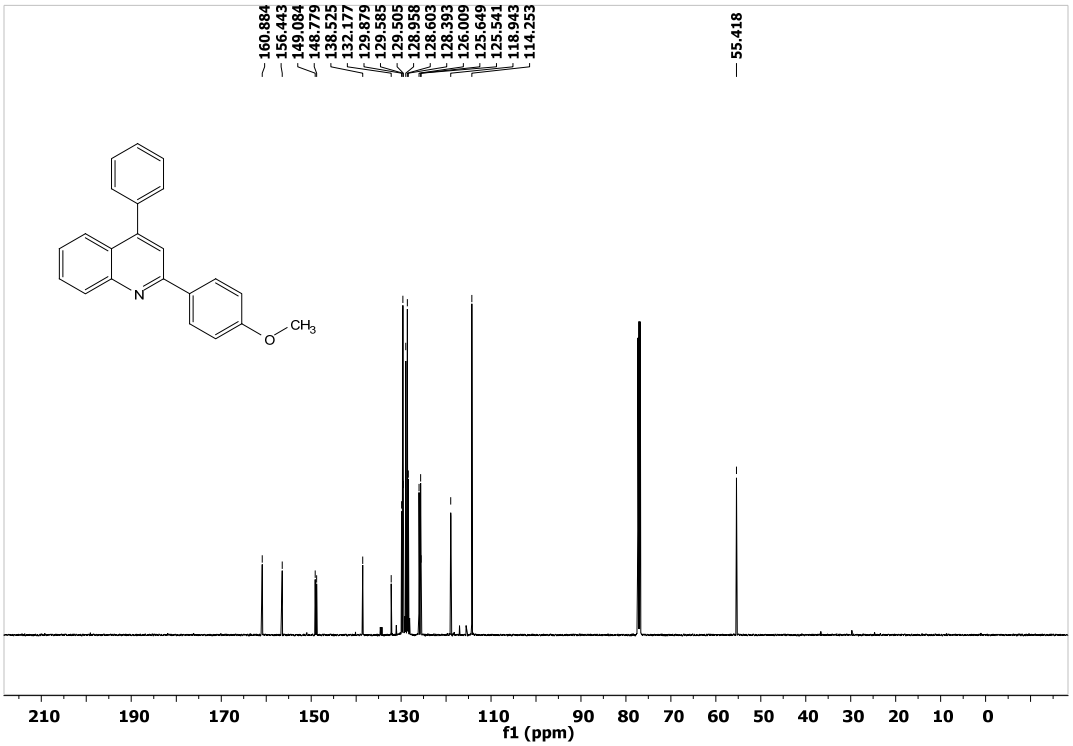
^{13}C NMR (125 MHz, $CDCl_3$) (**14b**)



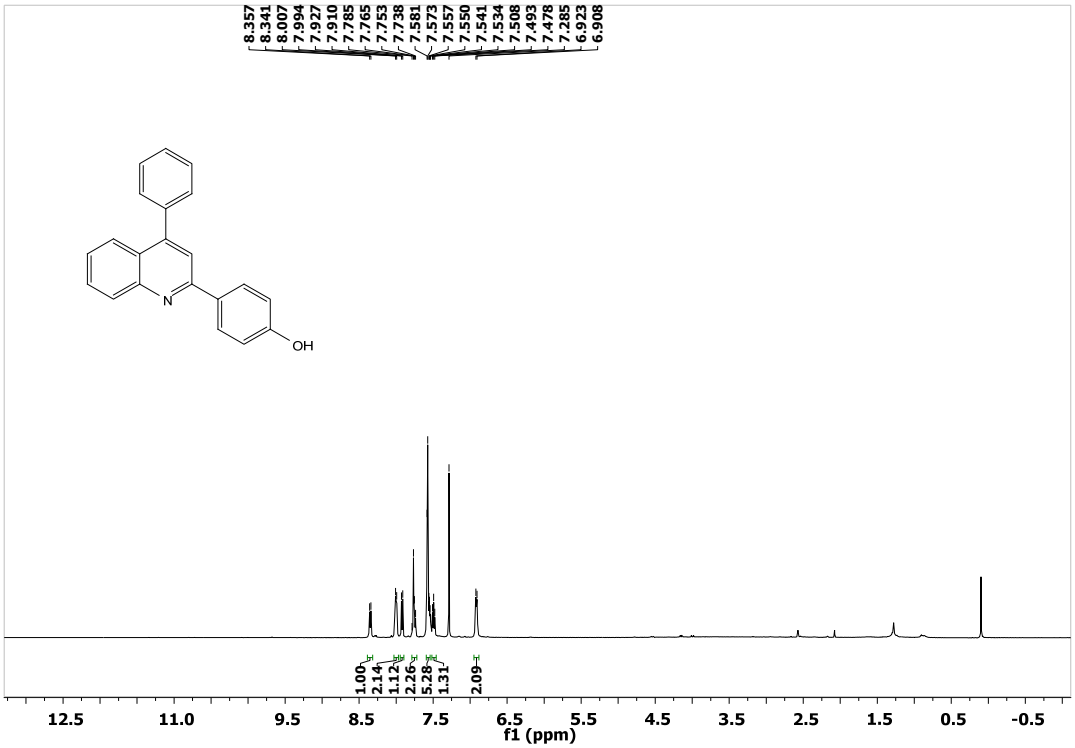
^{1}H NMR (500 MHz, $CDCl_3$) (**14c**)



^{13}C NMR (125 MHz, $CDCl_3$) (**14c**)



^{1}H NMR (500 MHz, $CDCl_3$) (**14d**)



^{13}C NMR (125 MHz, $CDCl_3$) (**14d**)