Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information for:

Merging Cu-catalysed C-H functionalisation and intramolecular annulations: computational and experimental studies on an expedient construction of complex fused heterocycles

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Contents:

[1] General Experimental Considerations:

All solvents and reagents were purchased from Sigma-Aldrich, Fisher Scientific or Fluorochem and used without further purification. ^{1}H, $^{13}C\{^{1}H\}$ and ^{19}F NMR spectra were recorded on a Bruker AV-400 spectrometer in $CDCl_3$ or d_6-DMSO. High Resolution Mass Spectra (HRMS) were recorded on a Xevo G2-Xs QTof Mass Spectrometer at Sheffield Hallam University.

[2] General Procedure for Copper-Catalyzed Intramolecular Coupling of Benzamide Substrates Bearing Tethered Alkyne:

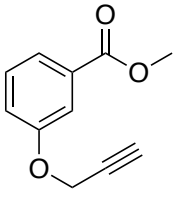
For the initial optimization studies reactions were carried out on a 0.1 mmol scale and for the substrate scoping reactions were carried out on a 0.5 mmol scale. The following represents the general procedure for the 0.5 mmol scale reactions.

To a graduated 15 mL vial equipped with a stirrer bar, under air, was sequentially added benzamide substrate (0.5 mmol), $Cu(OAc)_2$ (18.2 mg, 20 mol %, 0.1 mmol), sodium pivalate hydrate (93.1 mg, 1.5 equiv., 0.75 mmol) and $Mn(OAc)_2.4H_2O$ (245 mg, 2.0 equiv., 1.0 mmol) and trifluoroethanol (5 mL). The vial was sealed with a screw cap containing a Teflon seal. The reaction was then stirred at 80 ^{o}C for 18 hours. The reaction was cooled, the solvent removed under vacuum and analytically pure compounds were obtained after column chromatography: EtOAc:Hexane 70:30.

[3] Synthetic Details and Characterization Data for Tethered Alkyne Starting Materials:

[3.1] Synthetic Details and Characterization Data for Preparation of Terminal Tethered Alkyne (3-(prop-2-yn-1-yloxy)-N-(quinolin-8-yl)benzamide):

(i) Methyl 3-(prop-2-yn-1-yloxy)benzoate

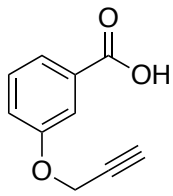


Methyl-3-hydroxybenzoate (10.00 g, 65.7 mmol) was dissolved in 150 mL acetone. To the solution were added potassium carbonate (27.25 g, 197 mmol, 3.0 equiv.) and propargyl bromide (80 wt. % in toluene, 12.70 g, 85.4 mmol, 1.3 equiv.) at 0 ^{o}C. The mixture was then allowed to return to room

temperature and was further stirred at 80 °C overnight. After this period, the acetone was removed under vacuum and to the residue was added 100 mL water. The reaction was then extracted with ethyl acetate (3 x 100 mL). The organic layers were combined, dried over magnesium sulfate and filtered, before the solvent was removed under vacuum to provide an analytically pure colourless oil (12.49 g, 93 %) which was used in the next step without further purification.

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 7.71 (d, 1H, $^{3}J_{HH}$ = 7.8 Hz), 7.67-7.64 (m, 1H), 7.39 (dd, 1H, $^{3}J_{HH}$ = 8.3 and 8.3 Hz), 7.20 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 2.3 Hz), 4.77 (d, 2H, $^{4}J_{HH}$ = 2.3), 3.99, (s, 3H), 2.56 (t, 1H, $^{4}J_{HH}$ = 2.3). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 166.78, 157.48, 131.52, 129.49, 122.88, 120.25, 115.21, 78.10, 75.87, 55.97, 52.25. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{11}H_{10}O_3$+H = 191.0708; obtained = 191.0707 $[M+H]^+$. R_f = 0.75 (EtOAc:Hexane 30:70).

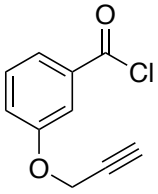
(ii) 3-(prop-2-yn-1-yloxy)benzoic acid



Methyl 3-(prop-2-yn-1-yloxy)benzoate (10.79 g, 56.7 mmol) was dissolved in a mixture of methanol (60 mL) and dioxane (20 mL). To the solution was slowly added NaOH (4 M, 45 mL) at 0 °C. The reaction mixture was allowed to warm to room temperature and stirred for 2 hours. The solvent was removed under vacuum to provide a white residue, to which was added water (100 mL). The pH of the solution was adjusted to around 1 by slow addition of HCl (2 M). The reaction was then extracted with ethyl acetate (3 x 100 mL). The organic layers were combined, dried over magnesium sulfate and filtered, before the solvent was removed under vacuum to provide an analytically pure colourless oil (9.20 g, 92 %) which was used in the next step without further purification.

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 7.80 (d, 1H, $^{3}J_{HH}$ = 7.1 Hz), 7.75-7.71 (m, 1H), 7.44 (dd, 1H, $^{3}J_{HH}$ = 7.7 and 7.7 Hz), 7.26 (dd, 1H, $^{3}J_{HH}$ = 8.0 and $^{4}J_{HH}$ = 2.5 Hz), 4.79 (d, 2H, $^{4}J_{HH}$ = 2.4), 2.58 (t, 1H, $^{4}J_{HH}$ = 2.4). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 171.37, 157.53, 130.57, 129.66, 123.55, 121.23, 115.66, 77.49, 76.00, 56.00. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{10}H_8O_3$+H = 177.0552; obtained = 177.0585 $[M+H]^+$. R_f = 0.25 (EtOAc:Hexane 30:70).

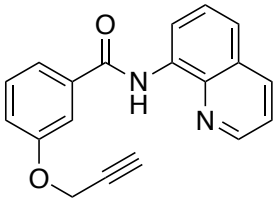
(iii) 3-(prop-2-yn-1-yloxy)benzoyl chloride



3-(prop-2-yn-1-yloxy)benzoic acid (9.10 g, 51.7 mmol) was dissolved in anhydrous dichloromethane (100 mL) under an atmosphere of nitrogen. The solution was cooled to 0 °C in an ice bath and a few drops of DMF were added, before slow addition of oxalyl chloride (9.68 mL, 103.4 mmol, 2.0 equiv.). The mixture was allowed to warm to room temperature, and it was stirred for 2 hours. The solvent was removed under vacuum to provide a colourless oil (9.94 g, yield not calculated due to impurities: the original NMR spectra show trace impurities of starting material, see section 5.) which was used in the next step without further purification.

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 7.81 (d, 1H, $^3J_{HH}$ = 8.4 Hz), 7.73-7.70 (m, 1H), 7.47 (dd, 1H, $^3J_{HH}$ = 7.6 and 7.6 Hz), 7.32 (dd, 1H, $^3J_{HH}$ = 8.0 and $^4J_{HH}$ = 2.0 Hz), 4.79 (d, 2H, $^4J_{HH}$ = 2.0), 2.58 (t, 1H, $^4J_{HH}$ = 2.0). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 167.12, 156.68, 133.49, 128.96, 123.84, 121.59, 115.71, 76.54, 75.35, 55.09. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{10}H_7ClO_2$ = 194.0135; obtained = 194.0129 $[M]^+$. R_f = 0.78 (EtOAc:Hexane 30:70).

(1o) 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide



The crude 3-(prop-2-yn-1-yloxy)benzoyl chloride from the previous step was dissolved in dichloromethane (200 mL). To this solution was added triethylamine (10.4 g, 103 mmol) and thereafter slowly a dichloromethane solution of 8-aminoquinoline (8.94 g, 62.0 mmol in 20 mL). The solution was stirred overnight, and the reaction mixture was thereafter washed sequentially with HCl (100 mL, 1.0 M), NaOH (100 mL, 1.0 M) and brine (100 mL). The organic layer was dried over magnesium sulfate and filtered, before the solvent was removed under vacuum to provide the crude compound. Analytically pure 3-(prop-2-yn-1-yloxy)-N-(quinolin-8-yl)benzamide was obtained as a white powder after column chromatography: EtOAc:Hexane 30:70 (13.4 g, 86 %; yield based on 3-(prop-2-yn-1-yloxy)benzoic acid used).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.76 (br s, 1H), 8.95 (dd, 1H, $^3J_{HH}$ = 7.4 and $^4J_{HH}$ = 1.5 Hz), 8.87 (dd, 1H, $^3J_{HH}$ = 4.1 and $^4J_{HH}$ = 1.6 Hz), 8.21 (dd, 1H, $^3J_{HH}$ = 8.6 and $^4J_{HH}$ = 1.6 Hz), 7.75-7.70 (m, 2H), 7.64-7.54 (m, 2H), 7.52-7.47 (m, 2H), 7.22 (8.95 (ddd, 1H, $^3J_{HH}$ = 8.1 and $^4J_{HH}$ = 2.6 and 0.9 Hz), 4.83 (d, 2H, $^4J_{HH}$ = 2.5 Hz), 2.60 (t, 2H, $^4J_{HH}$ = 2.5 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 164.03, 156.87, 147.26, 137.70, 135.67, 135.39, 133.47, 128.85, 126.96, 126.43, 120.75, 120.68, 119.06, 117.73, 115.58, 112.76, 77.10, 74.98, 55.01. HR-MS (ASAP+, *m*/*z*);

calcd. for $C_{19}H_{14}N_2O_2$+H = 303.1134; obtained = 303.1120 $[M+H]^+$. R_f = 0.47 (EtOAc:Hexane 30:70). mp: 112-113 °C.

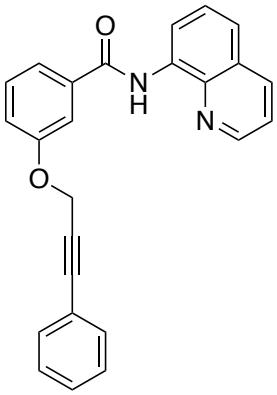
[3.2] Synthetic Details and Characterization Data for Preparation of Internal Tethered Alkyne Substrates:

General procedure for Pd-catalyzed Sonogashira coupling of aryl iodides with 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide

All the derivatives used in the substrate scope were synthesized by Pd-catalyzed Sonogashira coupling of aryl iodides with 3-(prop-2-yn-1-yloxy)-N-(quinolin-8-yl)benzamide using the general procedure:

To a mixture of 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide (302 mg, 1.0 mmol, 1.0 equiv.) in degassed triethylamine (10 mL) were sequentially added $PdCl_2(PPh_3)_2$ (14.0 mg, 2.0 mol %, 0.02 mmol) and CuI (7.6 mg, 4.0 mol %, 0.4 mmol). Thereafter, aryl iodide (1.1 mmol, 1.1 equiv.) was slowly added by syringe and the mixture was stirred overnight. The solvent was removed, and the residue was redissolved in dichloromethane (50 mL). The resulting mixture was extracted with aqueous saturated NH_4Cl solution (50 mL), HCl (50 mL, 0.5 M) and brine (50 mL). The organic layer was dried over magnesium sulfate and filtered, before the solvent was removed under vacuum to provide the crude compound. Analytically pure compounds were obtained after column chromatography: EtOAc:Hexane 30:70.

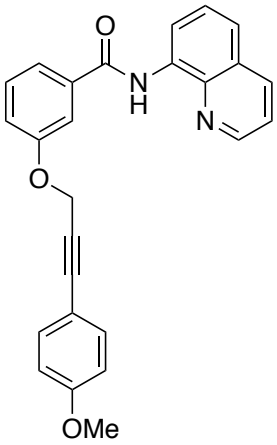
(1a) 3-((3-phenylprop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (351 mg, 93 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and iodobenzene (224 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.76 (br s, 1H), 8.96 (dd, 1H, $^3J_{HH}$ = 7.8 and $^4J_{HH}$ = 1.6 Hz), 8.82 (dd, 1H, $^3J_{HH}$ = 4.5 and $^4J_{HH}$ = 1.8 Hz), 8.20 (dd, 1H, $^3J_{HH}$ = 8.4 and $^4J_{HH}$ = 1.6 Hz), 7.80-7.77 (m, 1H), 7.74-7.71 (m, 1H), 7.65-7.45 (m, 6H), 7.36-7.25 (m, 4H), 5.05 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.17, 158.16, 148.31, 138.73, 136.73, 136.45, 134.54, 131.92, 129.90, 128.77, 128.30, 128.03, 127.48, 122.15, 121.78, 121.70, 120.07, 118.77, 116.68, 113.90, 87.62, 83.42, 56.94. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{18}N_2O_2$+H = 379.1447; obtained = 379.1440 $[M+H]^+$. R_f = 0.47 (EtOAc:Hexane 30:70). mp: 122-123 °C.

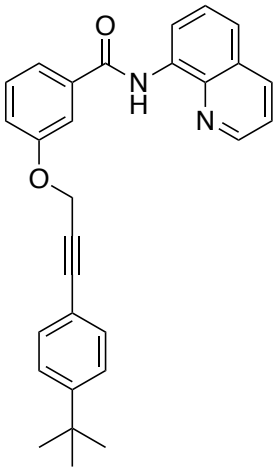
(1b) 3-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (354 mg, 87 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-methoxyiodobenzene (257 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.95 (dd, 1H, $^3J_{HH}$ = 7.5 and $^4J_{HH}$ = 1.2 Hz), 8.83 (dd, 1H, $^3J_{HH}$ = 3.9 and $^4J_{HH}$ = 1.5 Hz), 8.22 (dd, 1H, $^3J_{HH}$ = 8.5 and $^4J_{HH}$ = 1.8 Hz), 7.79-7.77 (m, 1H), 7.74-7.70 (m, 1H), 7.65-7.55 (m, 2H), 7.54-7.47 (m, 2H), 7.44-7.40 (m, 2H), 7.29-7.25 (m, 1H), 6.85-6.80 (m, 2H), 5.04 (s, 2H), 3.81 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.21, 159.96, 158.20, 148.30, 138.71, 136.69, 136.50, 134.54, 133.48, 129.87, 128.03, 127.51, 121.78, 121.70, 120.02, 118.80, 116.75, 114.21, 113.92, 113.89, 87.67, 82.09, 57.06, 55.29. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{20}N_2O_3$+H = 409.1552; obtained = 409.1545 $[M+H]^+$. R_f = 0.45 (EtOAc:Hexane 30:70). mp: 113-114 °C.

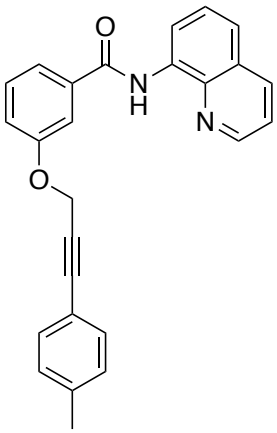
(1c) 3-((3-(4-(*tert*-butyl)phenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (381 mg, 88 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-*tert*-butyliodobenzene (286 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.95 (dd, 1H, $^3J_{HH}$ = 7.3 and $^4J_{HH}$ = 1.3 Hz), 8.81 (dd, 1H, $^3J_{HH}$ = 4.1 and $^4J_{HH}$ = 1.7 Hz), 8.21 (dd, 1H, $^3J_{HH}$ = 8.2 and $^4J_{HH}$ = 1.5 Hz), 7.79-7.76 (m, 1H), 7.74-7.70 (m, 1H), 7.65-7.55 (m, 2H), 7.53-7.46 (m, 2H), 7.44-7.39 (m, 2H), 7.36-7.31 (m, 2H), 7.30-7.25 (m, 1H), 5.05 (s, 2H), 1.31 (s, 9H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.22, 158.18, 152.06, 148.27, 138.69, 136.69, 136.50, 134.54, 131.66, 129.86, 128.02, 127.51, 125.30, 121.77, 121.68, 120.06, 119.11, 118.80, 116.76, 113.94, 87.79, 82.73, 57.03, 34.79, 31.14. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{29}H_{26}N_2O_2$+H = 435.2073; obtained = 435.2071 $[M+H]^+$. R_f = 0.59 (EtOAc:Hexane 30:70). mp: 126-127 °C.

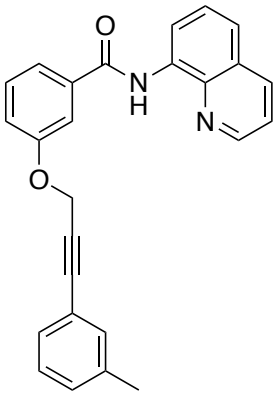
(1d) *N*-(quinolin-8-yl)-3-((3-(*p*-tolyl)prop-2-yn-1-yl)oxy)benzamide



Obtained as a white powder (305 mg, 78 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-methyliodobenzene (239 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.96 (dd, 1H, $^3J_{HH}$ = 7.8 and $^4J_{HH}$ = 1.3 Hz), 8.83 (dd, 1H, $^3J_{HH}$ = 4.5 and $^4J_{HH}$ = 1.6 Hz), 8.22 (dd, 1H, $^3J_{HH}$ = 8.6 and $^4J_{HH}$ = 1.2 Hz), 7.80-7.76 (m, 1H), 7.75-7.70 (m, 1H), 7.65-7.55 (m, 2H), 7.54-7.46 (m, 2H), 7.38 (d, 2H, $^3J_{HH}$ = 8.2 Hz), 7.30-7.25 (m, 1H), 7.12 (d, 2H, $^3J_{HH}$ = 8.2 Hz), 5.04 (s, 2H), 2.35 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.21, 158.19, 148.27, 138.95, 138.68, 136.70, 136.52, 134.53, 131.83, 129.87, 129.05, 128.03, 127.51, 121.78, 121.69, 120.06, 119.06, 118.76, 116.77, 113.93, 87.79, 82.72, 57.02, 21.51. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{20}N_2O_2$+H = 393.1603; obtained = 393.1606 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 30:70). mp: 115-116 °C.

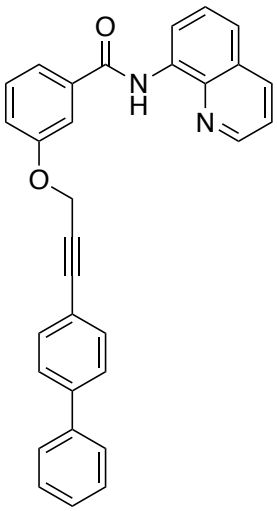
(1e) *N*-(quinolin-8-yl)-3-((3-(*m*-tolyl)prop-2-yn-1-yl)oxy)benzamide



Obtained as a white powder (333 mg, 85 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 3-methyliodobenzene (239 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.96 (dd, 1H, $^{3}J_{HH}$ = 7.7 and $^{4}J_{HH}$ = 1.5 Hz), 8.82 (dd, 1H, $^{3}J_{HH}$ = 4.2 and $^{4}J_{HH}$ = 1.7 Hz), 8.20 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.7 Hz), 7.80-7.76 (m, 1H), 7.73 (d, 1H, $^{3}J_{HH}$ = 8.1 Hz), 7.65-7.54 (m, 2H), 7.54-7.46 (m, 2H), 7.32-7.25 (m, 3H), 7.20 (dd, 1H, $^{3}J_{HH}$ = 7.6 and 7.6 Hz), (d, 1H, $^{3}J_{HH}$ = 7.3 Hz), 5.04 (s, 2H), 2.31 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.19, 158.18, 148.31, 138.74, 138.00, 136.72, 136.44, 134.55, 132.49, 129.89, 129.65, 128.98, 128.19, 128.01, 127.49, 121.94, 121.77, 121.70, 120.06, 118.75, 116.67, 113.93, 87.81, 83.03, 56.96, 21.17. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{20}N_2O_2$+H = 393.1603; obtained = 393.1607 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 30:70). mp: 112-113 °C.

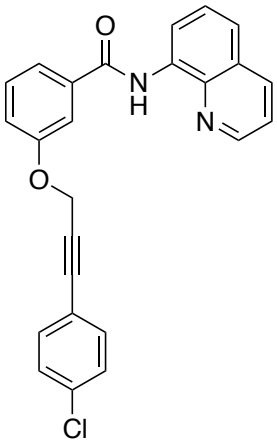
(1f) 3-((3-([1,1'-biphenyl]-4-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (331 mg, 73 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-phenyliodobenzene (308 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.78 (br s, 1H), 8.97 (dd, 1H, $^{3}J_{HH}$ = 7.4 and $^{4}J_{HH}$ = 1.3 Hz), 8.82 (dd, 1H, $^{3}J_{HH}$ = 4.2 and $^{4}J_{HH}$ = 1.3 Hz), 8.21 (dd, 1H, $^{3}J_{HH}$ = 8.5 and $^{4}J_{HH}$ = 1.8 Hz), 7.82-7.78 (m, 1H), 7.76-7.72 (m, 1H), 7.65-7.42 (m, 12H), 7.40-7.34 (m, 1H), 7.31-7.26 (m, 1H), 5.08 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.19, 158.17, 148.32, 141.52, 140.24, 138.75, 136.75, 136.45, 134.55, 132.36, 129.91, 128.87, 128.02, 127.72, 127.49, 127.04, 126.98, 121.78, 121.71, 121.02, 120.09, 118.83, 116.68, 113.91, 87.52, 84.05, 57.00. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{31}H_{22}N_2O_2$+H = 455.1760; obtained = 455.1752 $[M+H]^+$. R_f = 0.59 (EtOAc:Hexane 30:70). mp: 145-146 °C.

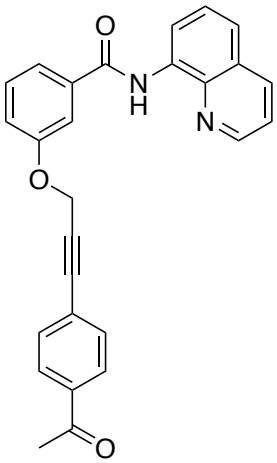
(1g) 3-((3-(4-chlorophenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (387 mg, 94 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-chloroiodobenzene (262 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.96 (dd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.6 Hz), 8.83 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.6 Hz), 8.22 (dd, 1H, $^{3}J_{HH}$ = 8.1 and $^{4}J_{HH}$ = 1.6 Hz), 7.80-7.76 (m, 1H), 7.75-7.71 (m, 1H), 7.66-7.55 (m, 2H), 7.55-7.47 (m, 2H), 7.41 (d, 2H, $^{3}J_{HH}$ = 9.2 Hz), 7.31-7.23 (m, 3H), 5.04 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.15, 158.09, 148.27, 138.69, 136.75, 136.53, 134.87, 134.49, 133.17, 129.91, 128.67, 128.04, 127.51, 121.83, 121.72, 120.62, 120.09, 118.86, 116.75, 113.82, 86.49, 84.43, 56.82. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{17}ClN_2O_2$+H = 413.1057; obtained = 413.1047 $[M+H]^+$. R_f = 0.61 (EtOAc:Hexane 30:70). mp: 135-136 °C.

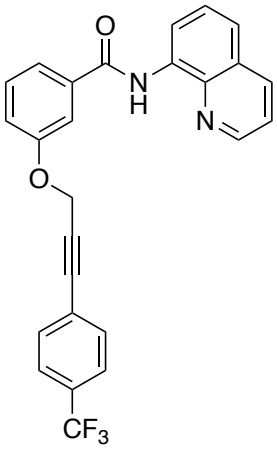
(1h) 3-((3-(4-acetylphenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (264 mg, 63 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-acetyliodobenzene (271 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.78 (br s, 1H), 8.95 (dd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.4 Hz), 8.83 (dd, 1H, $^{3}J_{HH}$ = 4.1 and $^{4}J_{HH}$ = 1.5 Hz), 8.20 (dd, 1H, $^{3}J_{HH}$ = 8.8 and $^{4}J_{HH}$ = 1.7 Hz), 8.07-8.04 (m, 1H), 7.93 (ddd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.4 and 1.4 Hz), 7.81-7.79 (m, 1H), 7.73 (ddd, 1H, $^{3}J_{HH}$ = 7.9 and $^{4}J_{HH}$ = 1.2 and 1.2 Hz), 7.68-7.46 (m, 5H), 7.42 (dd, 1H, $^{3}J_{HH}$ = 8.2 and 8.2 Hz), 7.29-7.25 (m, 1H), 5.06 (s, 2H), 2.59 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 197.28, 165.13, 158.09, 148.33, 138.74, 137.15, 136.76, 136.46, 136.15, 134.51, 131.99, 129.95, 128.72, 128.30, 128.02, 127.48, 122.76, 121.83, 121.73, 120.07, 118.90, 116.65, 113.84, 86.60, 84.53, 56.77, 26.64. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{27}H_{20}N_2O_3$+H = 421.1552; obtained = 421.1549 $[M+H]^+$. R_f = 0.36 (EtOAc:Hexane 30:70). mp: 116-117 °C.

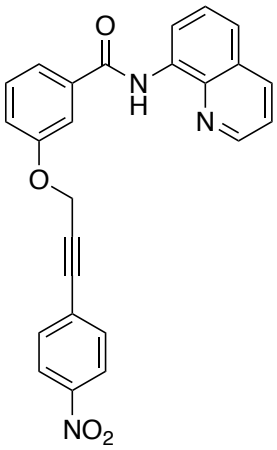
(1i) *N*-(quinolin-8-yl)-3-((3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl)oxy)benzamide



Obtained as a white powder (396 mg, 89 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-trifluoromethyliodobenzene (300 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.95 (dd, 1H, $^{3}J_{HH}$ = 7.3 and $^{4}J_{HH}$ = 1.3 Hz), 8.82 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.6 Hz), 8.22 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.6 Hz), 7.80-7.77 (m, 1H), 7.76-7.71 (m, 1H), 7.65-7.46 (m, 8H), 7.29-7.23 (m, 1H), 5.06 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.13, 158.04, 148.24, 138.64, 136.78, 136.60, 134.45, 132.16, 132.16, 130.50 (q, $^{2}J_{CF}$ = 34.4 Hz), 129.94, 128.05, 127.53, 125.27 (q, $^{3}J_{CF}$ = 2.9 Hz), 124.05 (q, $^{1}J_{CF}$ = 349 Hz), 121.87, 121.71, 120.16, 118.93, 116. 83, 113.81, 86.19, 85.92, 56.73. ^{19}F {^{1}H} NMR ($CDCl_3$, 376 MHz, 298 K); δ 62.90 (s, 3F). HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{17}F_3N_2O_2$+H = 447.1320; obtained = 447.1312 $[M+H]^+$. R_f = 0.58 (EtOAc:Hexane 30:70). mp: 127-128 °C.

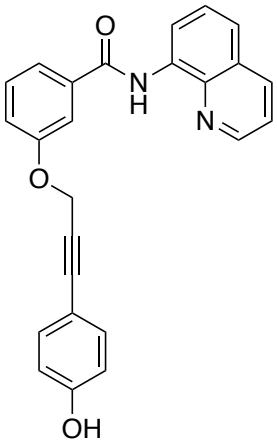
(1j) 3-((3-(4-nitrophenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (397 mg, 94 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-nitroiodobenzene (274 mg).

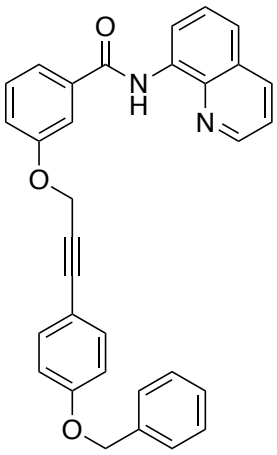
^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.95 (dd, 1H, $^{3}J_{HH}$ = 7.3 and $^{4}J_{HH}$ = 1.6 Hz), 8.84 (dd, 1H, $^{3}J_{HH}$ = 4.7 and $^{4}J_{HH}$ = 1.6 Hz), 8.22 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.6 Hz), 8.18 (d, 1H, $^{3}J_{HH}$ = 8.9 Hz), 7.82-7.78 (m, 1H), 7.74 (d, 1H, $^{3}J_{HH}$ = 7.3 Hz), 7.66-7.47 (m, 6H), 7.26 (dd, 1H, $^{3}J_{HH}$ = 7.8 and $^{4}J_{HH}$ = 2.6 Hz), 5.08 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.05, 157.96, 148.30, 147.42, 138.72, 13683, 136.54, 134.45, 132.69, 129.99, 128.95, 128.04, 127.50, 123.56, 121.90, 121.75, 120.16, 118.99, 116.71, 113.76, 88.73, 85.63, 56.63. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{17}N_3O_4$+H = 424.1297; obtained = 424.1293 $[M+H]^+$. R_f = 0.47 (EtOAc:Hexane 30:70). mp: 169-170 °C.

(1k) 3-((3-(4-hydroxyphenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (315 mg, 80 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-nitroiodobenzene (242 mg). ^{1}H NMR (d$_6$-DMSO, 400 MHz, 298 K); δ 10.65 (br s, 1H), 9.93 (br s, 1H), 8.95 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.9 Hz), 8.73 (dd, 1H, $^{3}J_{HH}$ = 7.4 and $^{4}J_{HH}$ = 1.4 Hz), 8.47 (dd, 1H, $^{3}J_{HH}$ = 8.2 and $^{4}J_{HH}$ = 1.4 Hz), 7.76 (dd, 1H, $^{3}J_{HH}$ = 8.2 and $^{4}J_{HH}$ = 1.4 Hz), 7.70-7.62 (m, 4H), 7.59 (dd, 1H, $^{3}J_{HH}$ = 8.2 and 8.2 Hz), 7.34 (dd, 1H, $^{3}J_{HH}$ = 7.2 and $^{4}J_{HH}$ = 1.4 Hz), 7.30 (d, 2H, $^{3}J_{HH}$ = 9.3 Hz), 6.75 (d, 2H, $^{3}J_{HH}$ = 9.3 Hz), 5.14 (s, 2H). ^{13}C {^{1}H} NMR (d$_6$-DMSO, 100 MHz, 298 K); δ = 164.72, 158.74, 158.21, 149.69, 138.78, 137.26, 136.48, 134.42, 133.72, 130.75, 128.32, 127.51, 122.92, 122.83, 120.00, 119.19, 117.20, 116.15, 114.11, 112.07, 87.88, 82.89, 56.99. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{18}N_2O_3$+H = 395.1396; obtained = 395.1392 $[M+H]^+$. R_f = 0.17 (with tail) (EtOAc:Hexane 30:70). mp: 176-177 °C.

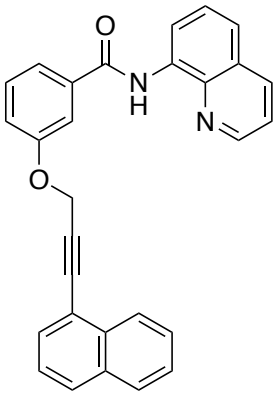
(1l) 3-((3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



Obtained as a white powder (348 mg, 72 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 4-benzyloxyiodobenzene (340 mg).

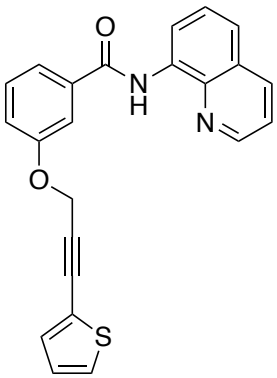
^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.96 (dd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.5 Hz), 8.84 (d, 1H, $^{4}J_{HH}$ = 3.0 Hz), 8.21 (dd, 1H, $^{3}J_{HH}$ = 8.7 and $^{4}J_{HH}$ = 1.5 Hz), 7.80-7.76 (m, 1H), 7.72 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz), 7.65-7.55 (m, 2H), 7.54-7.46 (m, 2H), 7.45-7.31 (m, 7H), 7.28-7.25 (m, 1H), 6.93-6.87 (m, 2H), 5.07 (s, 2H), 5.03 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.21, 159.13, 158.20, 148.32, 138.75, 136.70, 136.50, 136.44, 134.57, 133.49, 129.87, 128.64, 128.11, 128.02, 127.49, 127.47, 121.76, 121.71, 120.01, 118.78, 116.67, 114.83, 114.49, 113.90, 87.59, 82.16, 70.01, 57.04. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{32}H_{24}N_2O_3$+H = 485.1865; obtained = 485.1855 $[M+H]^+$. R_f = 0.53 (EtOAc:Hexane 30:70). mp: 117-118 °C.

(1m) 3-((3-(naphthalen-1-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide



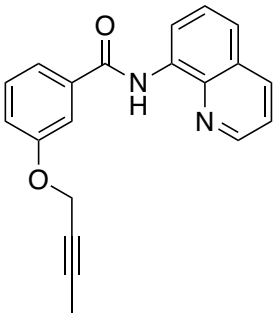
Obtained as a white powder (389 mg, 91 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 1-iodonaphthalene (279 mg). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.79 (br s, 1H), 8.97 (dd, 1H, $^{3}J_{HH}$ = 7.2 and $^{4}J_{HH}$ = 1.1 Hz), 8.79 (dd, 1H, $^{3}J_{HH}$ = 4.1 and $^{4}J_{HH}$ = 1.1 Hz), 8.28 (d, 1H, $^{3}J_{HH}$ = 8.2 Hz), 8.21 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.3 Hz), 7.91-7.87 (m, 1H), 7.86-7070 (m, 2H), 7.76 (d, 1H, $^{3}J_{HH}$ = 7.1 Hz), 7.72 (d, 1H, $^{3}J_{HH}$ = 6.9 Hz), 7.65-7.44 (m, 6H), 7.42 (dd, 1H, $^{3}J_{HH}$ = 7.4 and 7.4 Hz), 7.35 (dd, 1H, $^{3}J_{HH}$ = 8.2 and $^{4}J_{HH}$ = 2.2 Hz), 5.21 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.17, 158.15, 148.25, 138.68, 136.73, 136.51, 134.53, 133.35, 133.05, 130.96, 129.94, 129.27, 128.21, 128.02, 127.52, 126.96, 126.46, 126.09, 125.09, 121.79, 121.69, 120.13, 119.77, 119.03, 116.77, 114.11, 88.25, 85.87, 57.10. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{29}H_{20}N_2O_2$+H = 429.1603; obtained = 429.1594 $[M+H]^+$. R_f = 0.53 (EtOAc:Hexane 30:70). mp: 110-111 °C.

(1n) *N*-(quinolin-8-yl)-3-((3-(thiophen-2-yl)prop-2-yn-1-yl)oxy)benzamide



Obtained as a white powder (326 mg, 85 %) from 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide and 2-iodothiophene (231 mg). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.77 (br s, 1H), 8.96 (dd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.6 Hz), 8.85 (dd, 1H, $^{3}J_{HH}$ = 4.4 and $^{4}J_{HH}$ = 1.6 Hz), 8.22 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.6 Hz), 7.77-7.75 (m, 1H), 7.73 (d, 1H, $^{3}J_{HH}$ = 7.8 Hz), 7.63 (dd, 1H, $^{3}J_{HH}$ = 8.3 and 8.3 Hz), 7.58 (dd, 1H, $^{3}J_{HH}$ = 7.9 and $^{4}J_{HH}$ = 1.4 Hz), 7.53 (d, 1H, $^{3}J_{HH}$ = 7.9 Hz), 7.50 (dd, 1H, $^{3}J_{HH}$ = 4.1 and 3.7 Hz), 7.30-7.23 (m, 2H), 6.98 (dd, 1H, $^{3}J_{HH}$ = 4.8 and 3.7 Hz), 5.06 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.15, 158.09, 148.29, 138.69, 136.74, 136.51, 134.51, 133.05, 129.92, 128.03, 127.84, 127.51, 126.98, 121.96, 121.80, 121.71, 120.13, 118.72, 116.76, 113.89, 87.40, 80.95, 56.98. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{23}H_{16}N_2O_2S$+H = 385.1011; obtained = 385.1012 $[M+H]^+$. R_f = 0.57 (EtOAc:Hexane 30:70). mp: 96-98 °C.

(1p) 3-(but-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide

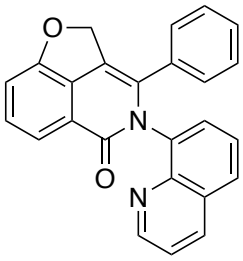


This compound was prepared using the same method to that described above for the preparation of 3-(prop-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide, but using 1/5 scale and 1-bromobut-2-yne replacing propargyl bromide in the first step to yield a white powder (85% over 2 steps).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 10.74 (br s, 1H), 8.95 (d, 1H, $^{3}J_{HH}$ = 7.2 Hz), 8.86 (d, 1H, $^{4}J_{HH}$ = 1.8 Hz), 8.20 (d, 1H, $^{3}J_{HH}$ = 7.7 Hz), 7.75-7.66 (m, 2H), 7.65-7.53 (m, 2H), 7.53-7.44 (m, 2H), 7.20 (d, 1H, $^{3}J_{HH}$ = 8.2 Hz), 4.78 (s, 2H), 1.91 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 165.22, 158.17, 148.30, 138.75, 136.67, 136.43, 134.56, 129.83, 128.01, 127.47, 121.76, 121.72, 119.84, 118.65, 116.61, 113.72, 84.27, 73.63, 56.68, 3.78. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{20}H_{16}N_2O_2$+H = 317.1290; obtained = 317.1280 $[M+H]^+$. R_f = 0.80 (EtOAc:Hexane 50:50). mp: 115-116 °C.

[4] Synthetic Details and Characterization Data for Annulated Products:

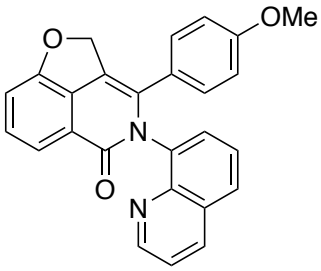
(2a) 3-phenyl-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-phenylprop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (189 mg) was converted to furnish the desired product as an off-white powder (81 %, 152 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.93 (dd, 1H, $^{3}J_{HH}$ = 3.9 and $^{4}J_{HH}$ = 1.5 Hz), 8.11 (dd, 1H, $^{3}J_{HH}$ = 8.5 and $^{4}J_{HH}$ = 1.4 Hz), 7.74 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.5 Hz), 7.70 (d, 1H, $^{3}J_{HH}$ = 7.8 Hz), 7.51 (dd, 1H, $^{3}J_{HH}$ = 7.4 and $^{4}J_{HH}$ = 1.3 Hz), 7.47-7.36 (m, 3H), 7.07-6.95 (m, 6H), 5.57 (d, 1H, $^{2}J_{HH}$ = 14.3 Hz), 5.51 (d, 1H, $^{2}J_{HH}$ = 14.3 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.27, 160.47, 150.94, 144.94, 137.46, 136.15, 135.22, 134.35, 132.60, 131.00, 129.72, 128.84, 128.69, 128.33, 128.31, 127.89, 125.84, 122.84, 121.51, 117.23, 115.62, 109.44, 75.39. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{16}N_2O_2$+H = 377.1290; obtained = 377.1290 $[M+H]^+$. R_f = 0.50 (EtOAc:Hexane 70:30). mp: 140-141 °C.

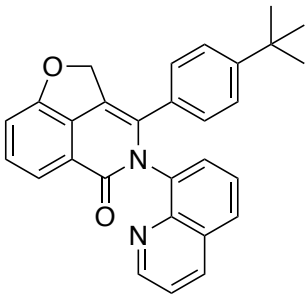
(2b) 3-(4-methoxyphenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-methoxyphenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (204 mg) was converted to furnish the desired product as an off-white powder (76 %, 155 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.92 (dd, 1H, $^{3}J_{HH}$ = 4.2 and $^{4}J_{HH}$ = 1.5 Hz), 8.12 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.5 Hz), 7.76 (dd, 1H, $^{3}J_{HH}$ = 7.8 and $^{4}J_{HH}$ = 1.2 Hz), 7.68 (d, 1H, $^{3}J_{HH}$ = 8.4 Hz), 7.52-7.36 (m, 4H), 7.02 (d, 1H, $^{3}J_{HH}$ = 8.1 Hz), 6.95 (d, 2H, $^{3}J_{HH}$ = 8.4 Hz), 6.51 (d, 2H, $^{3}J_{HH}$ = 8.5 Hz), 5.57 (d, 1H, $^{2}J_{HH}$ = 14.0 Hz), 5.50 (d, 1H, $^{2}J_{HH}$ = 14.0 Hz), 3.65 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.40, 160.41, 159.19, 150.93, 137.59, 136.19, 135.13, 132.66, 130.97, 129.68, 129.52, 128.87, 128.66, 126.90, 126.71, 125.92, 122.70, 121.49, 117.20, 115.56, 113.32, 109.33, 75.45, 55.04. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{18}N_2O_3$+H = 407.1396; obtained = 407.1393 $[M+H]^+$. R_f = 0.44 (EtOAc:Hexane 70:30). mp: 141-142 °C.

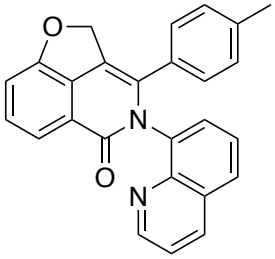
(2c) 3-(4-(*tert*-butyl)phenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-(*tert*-butyl)phenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (217 mg) was converted to furnish the desired product as an off-white powder (83 %, 179 mg).

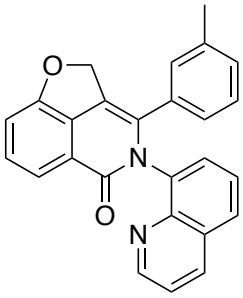
^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.96 (dd, 1H, $^{3}J_{HH}$ = 4.2 and $^{4}J_{HH}$ = 1.4 Hz), 8.13 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.4 Hz), 7.73 (dd, 1H, $^{3}J_{HH}$ = 8.0 and $^{4}J_{HH}$ = 1.5 Hz), 7.69 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.48-7.37 (m, 4H), 7.03 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz), 6.98 (d, 2H, $^{3}J_{HH}$ = 8.5 Hz), 6.92 (d, 2H, $^{3}J_{HH}$ = 8.5 Hz) 5.60 (d, 1H, $^{2}J_{HH}$ = 14.2 Hz), 5.51 (d, 1H, $^{2}J_{HH}$ = 14.2 Hz), 1.13 (s, 9H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.39, 160.43, 151.28, 150.88, 137.51, 136.28, 135.38, 132.69, 131.30, 131.00, 129.56, 128.83, 128.55, 127.95, 125.90, 124.73, 122.76, 121.45, 117.18, 115.63, 109.32, 75.55, 34.46, 30.98, 26.98. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{29}H_{24}N_2O_2$+H = 433.1916; obtained = 433.1911 $[M+H]^+$. R_f = 0.60 (EtOAc:Hexane 70:30). mp: 152-153 °C.

(2d) 4-(quinolin-8-yl)-3-(*p*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



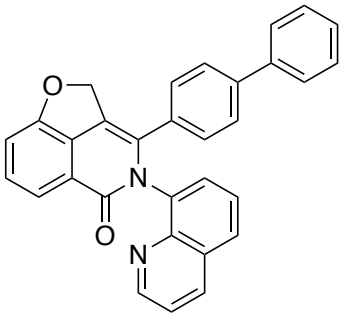
This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. *N*-(quinolin-8-yl)-3-((3-(p-tolyl)prop-2-yn-1-yl)oxy)benzamide (196 mg) was converted to furnish the desired product as an off-white powder (75 %, 146 mg). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.94 (d, 1H, $^{3}J_{HH}$ = 3.0 Hz), 8.13 (d, 1H, $^{3}J_{HH}$ = 7.4 Hz), 7.75 (d, 1H, $^{3}J_{HH}$ = 7.7 Hz), 7.69 (d, 1H, $^{3}J_{HH}$ = 7.7 Hz), 7.53-7.35 (m, 4H), 7.02 (d, 1H, $^{3}J_{HH}$ = 7.4 Hz), 6.92 (d, 2H, $^{3}J_{HH}$ = 8.1 Hz), 6.79 (d, 2H, $^{3}J_{HH}$ = 8.1 Hz) 5.56 (d, 1H, $^{2}J_{HH}$ = 13.3 Hz), 5.49 (d, 1H, $^{2}J_{HH}$ = 13.3 Hz), 2.14 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.38, 160.44, 150.86, 138.19, 137.51, 136.36, 135.35, 132.66, 131.43, 131.05, 129.58, 128.84, 128.84, 128.65, 128.16, 128.16, 125.95, 122.73, 121.50, 117.18, 115.61, 109.36, 75.47, 21.13. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{18}N_2O_2$+H = 391.1447; obtained = 391.1434 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 70:30). mp: 125-126 °C.

(2e) 4-(quinolin-8-yl)-3-(*m*-tolyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. *N*-(quinolin-8-yl)-3-((3-(m-tolyl)prop-2-yn-1-yl)oxy)benzamide (196 mg) was converted to furnish the desired product as an off-white powder (88 %, 171 mg). ^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.95 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.4 Hz), 8.13 (dd, 1H, $^{3}J_{HH}$ = 8.2 and $^{4}J_{HH}$ = 1.8 Hz), 7.75 (dd, 1H, $^{3}J_{HH}$ = 7.3 and $^{4}J_{HH}$ = 1.8 Hz), 7.70 (d, 1H, $^{3}J_{HH}$ = 7.8 Hz), 7.49 (dd, 1H, $^{3}J_{HH}$ = 7.3 and $^{4}J_{HH}$ = 1.5 Hz), 7.47-7.37 (m, 3H), 7.04 (d, 1H, $^{3}J_{HH}$ = 7.3 Hz), 6.91-6.78 (m, 4H), 5.59 (d, 1H, $^{2}J_{HH}$ = 13.5 Hz), 5.51 (d, 1H, $^{2}J_{HH}$ = 13.5 Hz), 2.03 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.32, 160.44, 150.88, 145.05, 137.59, 137.51, 136.15, 135.38, 134.22, 132.63, 130.90, 129.64, 129.02, 129.00, 128.81, 128.63, 127.74, 125.85, 125.35, 122.78, 121.46, 117.21, 115.48, 109.38, 75.44, 21.01. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{26}H_{18}N_2O_2$+H = 391.1447; obtained = 391.1446 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 70:30). mp: 131-132 °C.

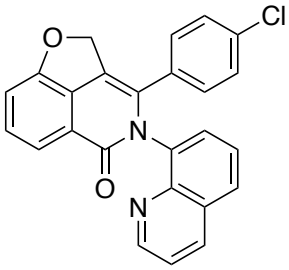
(2f) 3-([1,1'-biphenyl]-4-yl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-([1,1'-biphenyl]-4-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (227 mg) was converted to furnish the desired product as an off-white powder (77 %, 174 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.94 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.8 Hz), 8.11 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.8 Hz), 7.75 (dd, 1H, $^{3}J_{HH}$ = 8.2 and $^{4}J_{HH}$ = 1.2 Hz), 7.71 (d, 1H, $^{3}J_{HH}$ = 7.9 Hz), 7.55 (dd, 1H, $^{3}J_{HH}$ = 7.3 and $^{4}J_{HH}$ = 1.4 Hz), 7.47-7.30 (m, 8H), 7.24 (d, 2H, $^{3}J_{HH}$ = 8.3 Hz), 7.10 (d, 2H, $^{3}J_{HH}$ = 8.2 Hz), 7.04 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz), 5.62 (d, 1H, $^{2}J_{HH}$ = 14.0 Hz), 5.56 (d, 1H, $^{2}J_{HH}$ = 14.0 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.34, 160.49, 150.98, 144.99, 140.76, 139.80, 137.50, 136.22, 135.01, 133.27, 132.62, 131.01, 129.78, 128.89, 128.77, 128.72, 127.66, 126.80, 126.55, 124.47, 125.93, 122.84, 121.64, 117.25, 115.82, 109.48, 75.48. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{31}H_{20}N_2O_2$+H = 453.1603; obtained = 453.1597 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 70:30). mp: 137-138 °C.

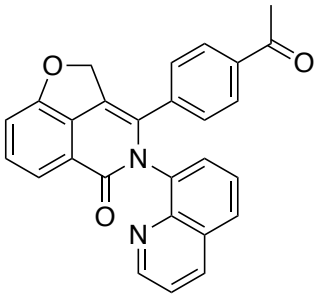
(2g) 3-(4-chlorophenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-chlorophenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (206 mg) was converted to furnish the desired product as an off-white powder (72 %, 147 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.90 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.7 Hz), 8.12 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.7 Hz), 7.77 (dd, 1H, $^{3}J_{HH}$ = 8.4 and $^{4}J_{HH}$ = 1.6 Hz), 7.69 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.53 (dd, 1H, $^{3}J_{HH}$ = 7.2 and $^{4}J_{HH}$ = 1.3 Hz), 7.49-7.36 (m, 3H), 7.04 (d, 1H, $^{3}J_{HH}$ = 7.3 Hz), 7.00 (d, 2H, $^{3}J_{HH}$ = 8.7 Hz), 6.96 (d, 2H, $^{3}J_{HH}$ = 8.7 Hz), 5.53 (d, 1H, $^{2}J_{HH}$ = 13.8 Hz), 5.49 (d, 1H, $^{2}J_{HH}$ = 13.8 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.20, 160.47, 151.00, 144.76, 137.16, 136.29, 134.30, 133.93, 132.80, 132.39, 131.05, 123.00, 129.69, 128.97, 128.93, 128.25, 125.93, 122.92, 121.64, 117.27, 115.97, 109.64, 75.21. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{15}ClN_2O_2$+H = 411.0900; obtained = 411.0897 $[M+H]^+$. R_f = 0.52 (EtOAc:Hexane 70:30). mp: 148-149 °C.

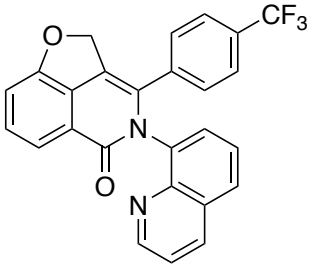
(2h) 3-(4-acetylphenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-acetylphenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (210 mg) was converted to furnish the desired product as an off-white powder (69 %, 144 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.91 (dd, 1H, $^{3}J_{HH}$ = 4.3 and $^{4}J_{HH}$ = 1.7 Hz), 8.12 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.4 Hz), 7.75 (dd, 1H, $^{3}J_{HH}$ = 8.1 and $^{4}J_{HH}$ = 1.1 Hz), 7.70 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.57 (d, 2H, $^{3}J_{HH}$ = 8.3 Hz), 7.54 (dd, 1H, $^{3}J_{HH}$ = 7.6 and $^{4}J_{HH}$ = 1.4 Hz), 7.45 (dd, 1H, $^{3}J_{HH}$ = 8.3 and 8.3 Hz), 7.40 (dd, 1H, $^{3}J_{HH}$ = 8.2 and 4.3 Hz), 7.16 (d, 2H, $^{3}J_{HH}$ = 8.3 Hz), 7.05 (d, 1H, $^{3}J_{HH}$ = 7.6 Hz), 5.54 (d, 1H, $^{2}J_{HH}$ = 14.2 Hz), 5.50 (d, 1H, $^{2}J_{HH}$ = 14.2 Hz), 2.44 (s, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 197.21, 162.11, 160.54, 150.98, 138.95, 137.08, 136.40, 134.02, 132.32, 131.08, 130.24, 129.03, 128.93, 128.55, 128.55, 127.92, 127.92, 125.96, 123.01, 121.67, 117.35, 116.29, 109.79, 75.21, 26.49. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{27}H_{18}N_2O_3$+H = 419.1396; obtained = 419.1389 $[M+H]^+$. R_f = 0.40 (EtOAc:Hexane 70:30). mp: 168-169 °C.

(2i) 4-(quinolin-8-yl)-3-(4-(trifluoromethyl)phenyl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one

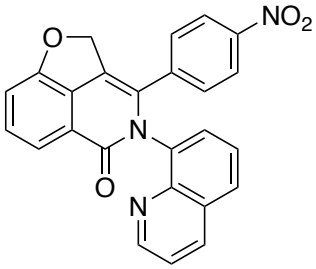


This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. *N*-(quinolin-8-yl)-3-((3-(4-(trifluoromethyl)phenyl)prop-2-yn-1-yl)oxy)benzamide (223 mg) was converted to furnish the desired product as an off-white powder (74 %, 164 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.93 (d, 1H, $^{3}J_{HH}$ = 3.1 Hz), 8.14 (d, 1H, $^{3}J_{HH}$ = 8.0 Hz), 7.80 (d, 1H, $^{3}J_{HH}$ = 8.3 Hz), 7.73 (d, 1H, $^{3}J_{HH}$ = 8.3 Hz), 7.57 (d, 1H, $^{3}J_{HH}$ = 7.2 Hz), 7.48 (dd, 1H, $^{3}J_{HH}$ = 8.0 and 8.0 Hz), 7.42 (dd, 1H, $^{3}J_{HH}$ = 8.0 and 3.3 Hz), 7.28 (d, 1H, $^{3}J_{HH}$ = 8.2 Hz), 7.21 (d, 1H, $^{3}J_{HH}$ = 8.2 Hz), 7.08 (d, 1H, $^{3}J_{HH}$ = 7.7 Hz), 5.56 (d, 1H, $^{2}J_{HH}$ = 14.7 Hz), 5.52 (d, 1H, $^{2}J_{HH}$ = 14.7 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.08, 160.53, 151.02, 144.67, 137.93, 136.98, 136.37, 133.58, 132.27, 131.08, 130.27, 130.20 (q, $^{2}J_{CF}$ = 33.2 Hz), 129.11, 128.94, 128.75, 125.95, 124.95 (q, $^{3}J_{CF}$ = 4.3 Hz), 123.96 (q, $^{1}J_{CF}$ = 271 Hz), 123.06, 121.70, 117.33, 116.33, 109.82, 75.14. ^{19}F {^{1}H} NMR ($CDCl_3$, 376 MHz, 298 K); δ 62.94 (s, 3F). HR-MS (ASAP+, *m*/*z*);

calcd. for $C_{26}H_{15}F_3N_2O_2$+H = 445.1164; obtained = 445.1158 $[M+H]^+$. R_f = 0.58 (EtOAc:Hexane 70:30). mp: 128-129 °C.

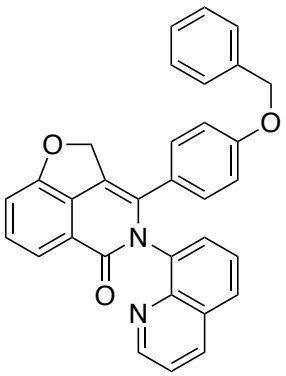
(2j) 3-(4-nitrophenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-nitrophenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (211 mg) was converted to furnish the desired product as a yellow powder (91 %, 192 mg).

^{1}H NMR (d_6-DMSO, 400 MHz, 298 K); δ 8.87 (dd, 1H, $^3J_{HH}$ = 4.2 and $^4J_{HH}$ = 1.5 Hz), 8.36 (dd, 1H, $^3J_{HH}$ = 8.3 and $^4J_{HH}$ = 1.5 Hz), 7.95 (dd, 1H, $^3J_{HH}$ = 8.1 and $^4J_{HH}$ = 1.3 Hz), 7.87 (d, 2H, $^3J_{HH}$ = 8.6 Hz), 7.83 (dd, 1H, $^3J_{HH}$ = 7.4 and $^4J_{HH}$ = 1.2 Hz), 7.61-7.47 (m, 4H), 7.42 (d, 2H, $^3J_{HH}$ = 8.3 Hz), 7.20 (d, 2H, $^3J_{HH}$ = 7.2 Hz), 5.70 (d, 1H, $^2J_{HH}$ = 15.0 Hz), 5.61 (d, 1H, $^2J_{HH}$ = 15.0 Hz). ^{13}C {^{1}H} NMR (d_6-DMSO, 100 MHz, 298 K); δ = 161.31, 160.74, 151.47, 147.20, 144.36, 140.75, 136.89, 136.87, 133.55, 132.24, 132.09, 131.16, 130.31, 129.61, 128.88, 126.40, 123.35, 122.97, 122.43, 116.63, 116.33, 110.27, 75.53. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{25}H_{15}N_3O_4$+H = 422.1141; obtained = 422.1134 $[M+H]^+$. R_f = 0.50 (EtOAc:Hexane 70:30). mp: 173-174 °C.

(2l) 3-(4-(benzyloxy)phenyl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one

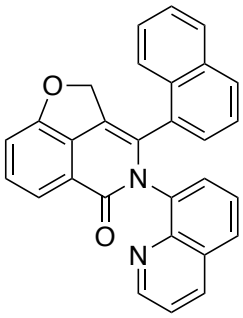


This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(4-(benzyloxy)phenyl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (242 mg) was converted to furnish the desired product as an off-white powder (84 %, 202 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.93 (d, 1H, $^3J_{HH}$ = 3.2 Hz), 8.93 (d, 1H, $^3J_{HH}$ = 7.4 Hz), 7.76 (d, 1H, $^3J_{HH}$ = 7.4 Hz), 7.79 (d, 1H, $^3J_{HH}$ = 8.0 Hz), 7.56-7.29 (m, 9H), 7.02 (d, 1H, $^3J_{HH}$ = 8.0 Hz), 6.96 (d, 2H, $^3J_{HH}$ = 8.0 Hz), 6.59 (d, 2H, $^3J_{HH}$ = 8.0 Hz), 5.57 (d, 1H, $^2J_{HH}$ = 13.7 Hz), 5.51 (d, 1H, $^2J_{HH}$ = 13.7 Hz), 4.88 (s, 2H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.40, 160.42, 158.42, 150.89, 144.88, 137.54, 136.39, 136.28, 135.06, 132.66, 131.04, 129.72, 129.55, 128.88, 128.67, 128.57, 128.09, 127.44, 126.98, 125.96, 122.73, 121.50, 117.20, 115.60, 114.21, 109.36, 75.46, 69.82. HR-MS (ASAP+, *m*/*z*);

calcd. for $C_{32}H_{22}N_2O_3$+H = 483.1709; obtained = 483.1701 $[M+H]^+$. R_f = 0.65 (EtOAc:Hexane 70:30). mp: 145-146 °C.

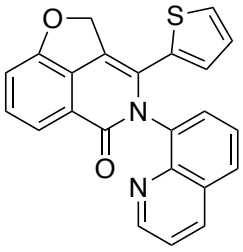
(2m) 3-(naphthalen-1-yl)-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-((3-(naphthalen-1-yl)prop-2-yn-1-yl)oxy)-*N*-(quinolin-8-yl)benzamide (214 mg) was converted to furnish the desired product as an off-white powder (65 %, 138 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K and ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); This product was obtained as an inseparable mixture (after exhaustive attempts) of isomers, in a 30:70 ratio, due to axial chirality of the naphthyl and quinolyl moieties. Original spectra can be seen in section 5. However HR-MS data is consistent with the proposed stricture: HR-MS (ASAP+, *m*/*z*); calcd. for $C_{29}H_{18}N_2O_2$+H = 427.1447; obtained = 427.1444 $[M+H]^+$. R_f = 0.68 (EtOAc:Hexane 70:30). mp: no clear melting point found.

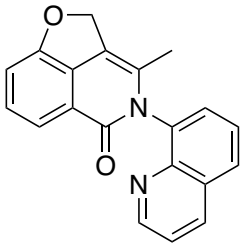
(2n) 4-(quinolin-8-yl)-3-(thiophen-2-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. *N*-(quinolin-8-yl)-3-((3-(thiophen-2-yl)prop-2-yn-1-yl)oxy)benzamide (192 mg) was converted to furnish the desired product as an off-white powder (78 %, 148 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.91 (dd, 1H, $^3J_{HH}$ = 4.3 and $^4J_{HH}$ = 1.7 Hz), 8.18 (dd, 1H, $^3J_{HH}$ = 8.4 and $^4J_{HH}$ = 1.3 Hz), 7.85 (dd, 1H, $^3J_{HH}$ = 8.2 and $^4J_{HH}$ = 1.3 Hz), 7.70 (d, 1H, $^3J_{HH}$ = 8.2 Hz), 7.62 (dd, 1H, $^3J_{HH}$ = 7.3 and $^4J_{HH}$ = 1.5 Hz), 7.54 (dd, 1H, $^3J_{HH}$ = 8.0 and 8.0 Hz), 7.48-7.38 (m, 2H), 7.07-7.02 (m, 2H), 6.66 (dd, 1H, $^3J_{HH}$ = 5.0 and 3.6 Hz), 6.58 (d, 1H, $^3J_{HH}$ = 3.2 Hz), 5.69 (d, 1H, $^2J_{HH}$ = 14.6 Hz), 5.63 (d, 1H, $^2J_{HH}$ = 14.6 Hz). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.31, 160.71, 151.09, 145.33, 137.47, 136.25, 134.83, 132.22, 130.91, 130.19, 129.09, 129.03, 128.61, 128.46, 127.12, 126.42, 126.11, 123.04, 121.67, 117.54, 117.31, 109.65, 75.94. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{23}H_{14}N_2O_2S$ +H = 383.0854; obtained = 383.0846 $[M+H]^+$. R_f = 0.65 (EtOAc:Hexane 70:30). mp: 126-127 °C.

(2p) 3-methyl-4-(quinolin-8-yl)-2,4-dihydro-5*H*-furo[4,3,2-*de*]isoquinolin-5-one



This compound was prepared using the general method for copper-catalyzed intramolecular coupling described above. 3-(but-2-yn-1-yloxy)-*N*-(quinolin-8-yl)benzamide (158 mg) was converted to furnish the desired product as an off-white powder (48 %, 76 mg).

^{1}H NMR ($CDCl_3$, 400 MHz, 298 K); δ 8.92 (dd, 1H, $^{3}J_{HH}$ = 4.2 and $^{4}J_{HH}$ = 1.6 Hz), 8.28 (dd, 1H, $^{3}J_{HH}$ = 8.3 and $^{4}J_{HH}$ = 1.3 Hz), 8.00 (dd, 1H, $^{3}J_{HH}$ = 7.2 and $^{4}J_{HH}$ = 2.2 Hz), 7.76-7.67 (m, 2H), 7.61 (d, 1H, $^{3}J_{HH}$ = 8.2 Hz), 7.47 (dd, 1H, $^{3}J_{HH}$ = 8.4 and 4.2 Hz), 7.34 (dd, 1H, $^{3}J_{HH}$ = 7.5 and 7.5 Hz), 6.98 (d, 1H, $^{3}J_{HH}$ = 7.5 Hz), 5.67 (dq, 1H, $^{2}J_{HH}$ = 13.3 and $^{5}J_{HH}$ = 1.4 Hz), 5.61 (dq, 1H, $^{2}J_{HH}$ = 13.3 and $^{5}J_{HH}$ = 1.4 Hz), 1.82 (m, 3H). ^{13}C {^{1}H} NMR ($CDCl_3$, 100 MHz, 298 K); δ = 162.81, 159.96, 151.42, 144.58, 137.01, 136.52, 132.80, 131.17, 130.30, 129.49, 129.27, 128.72, 126.52, 122.15, 121.88, 117.01, 113.90, 109.01, 74.90, 18.56. HR-MS (ASAP+, *m*/*z*); calcd. for $C_{20}H_{14}N_2O_2$+H = 315.1134; obtained = 315.1130 $[M+H]^+$. R_f = 0.46 (EtOAc:Hexane 70:30). mp: 210-211 °C.

[5] Computational Details:

All DFT calculations undertaken using the ORCA 3.03 computational software.[1] Optimisations were performed at the PBE0/def2-TZVP level of theory,[2,3] with dispersion interactions accounted for with Grimme's D3BJ correction.[4]

Solvation correction was implemented with the COSMO[5] model for trifluoroethanol (ε = 8.55). Graphical visualisation using Gabedit 2.4.8[6] and Avogadro 1.2.0[7] programs. Analytical frequencies were calculated for inclusion of the Zero Point Energy (ZPE) correction and entropic contributions to the free energy term (ΔG_{298K}), as well as confirming all intermediates were true, with no imaginary modes, and all transition states had the correct critical frequency of decomposition (imaginary mode). QTAIM and NCI analysis was performed using the Multiwfn[8] software package.

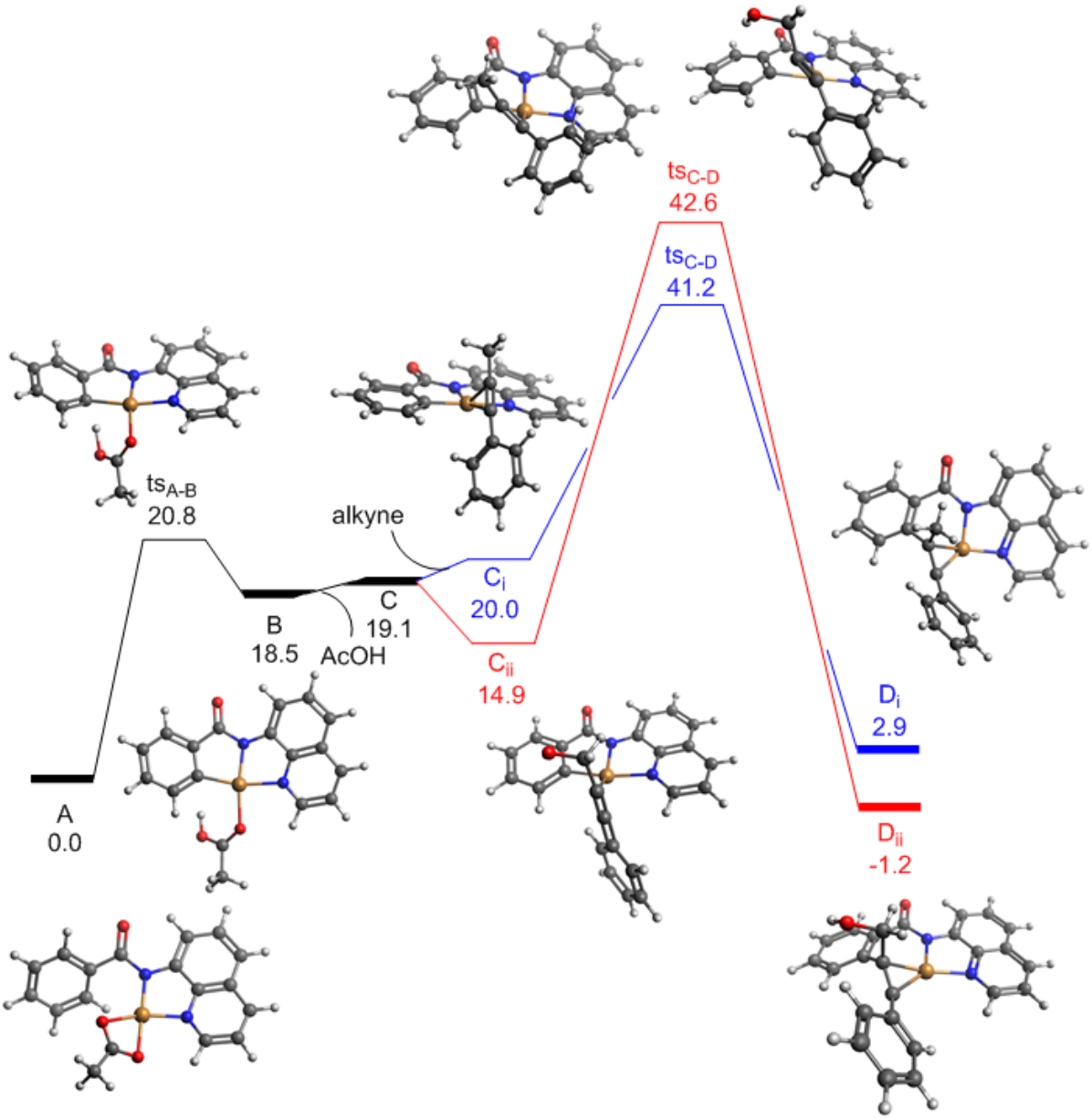


Figure S1: *Intramolecular vs Intermolecular Migratory Insertion Free Energy Surface (ΔG_{298K}), calculated at PBE0/def2-tzvp. Black line represents the initial C-H activation pathway, blue line represents intermolecular migratory insertion of 1-Phenyl-1-propyne and red line represents intermolecular migratory insertion of 3-Phenyl-2-propyn-1-ol.*

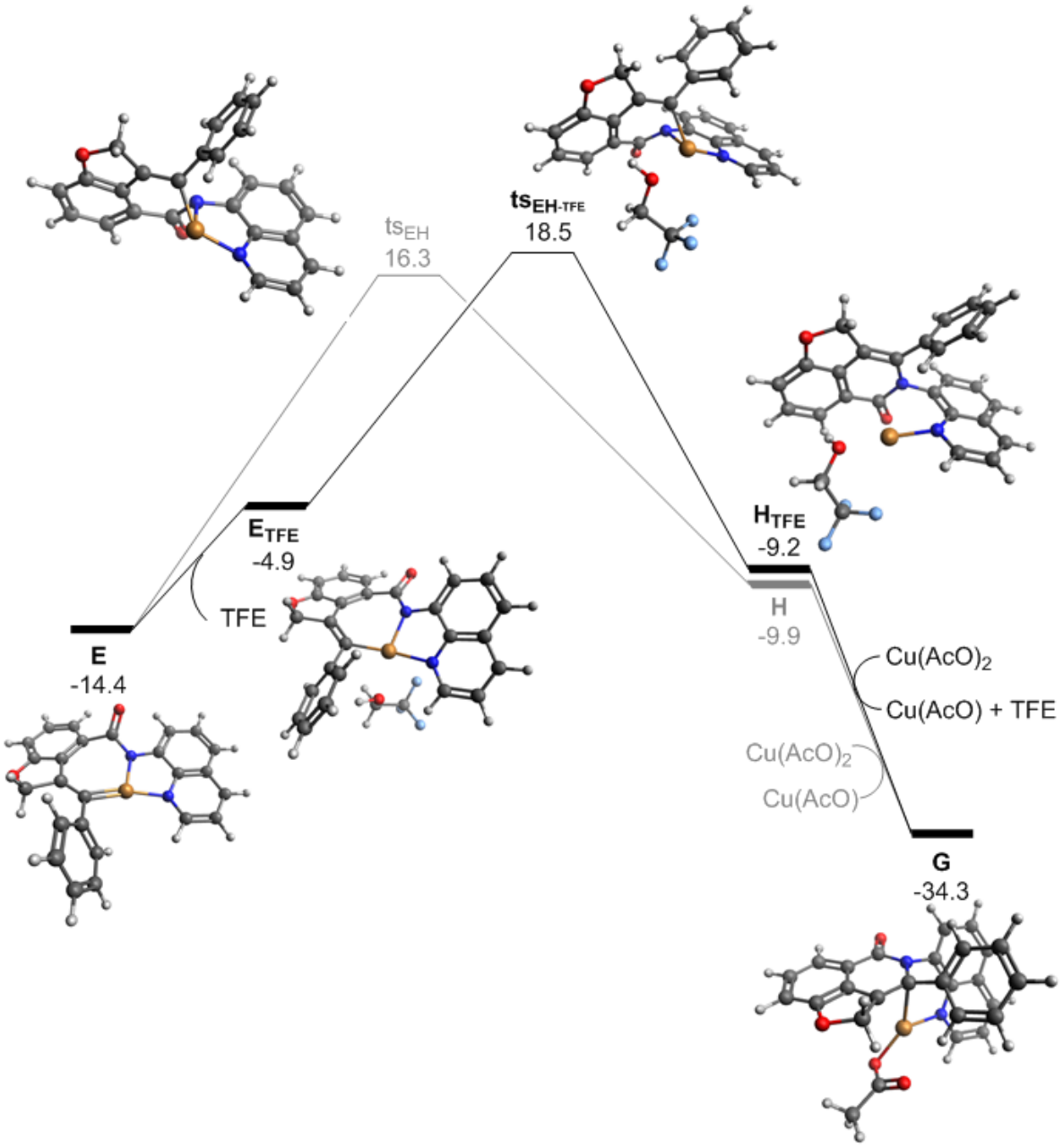


Figure S2: Free Energy Surfaces (ΔG_{298K}), calculated at PBE0/def2-tzvp, for direct Cu(II) - Cu(0) reductive elimination, both with and without explicit solvent (TFE) coordination, followed by Cu(0) to Cu(I) oxidation with $Cu(AcO)_2$.

[6] Original Spectra:

This section contains the original ^{1}H, $^{13}C\{^{1}H\}$ and $^{19}F\{^{1}H\}$ 1D NMR spectra and 2D COSY NMR for each of the compounds described previously in sections 3 and 4.

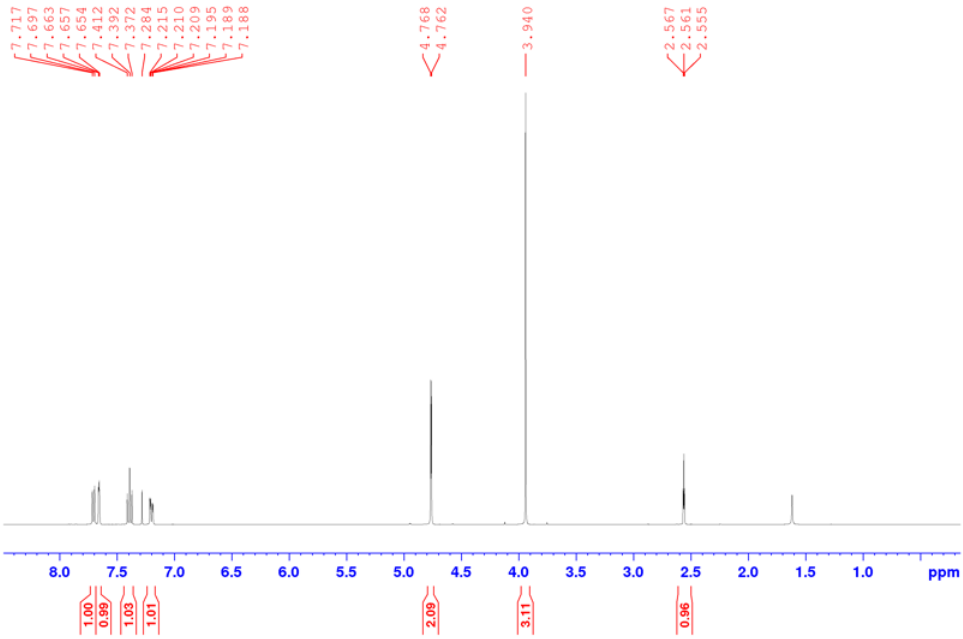


Figure S3: *^{1}H NMR spectrum of compound **i** in $CDCl_3$ at 298 K.*

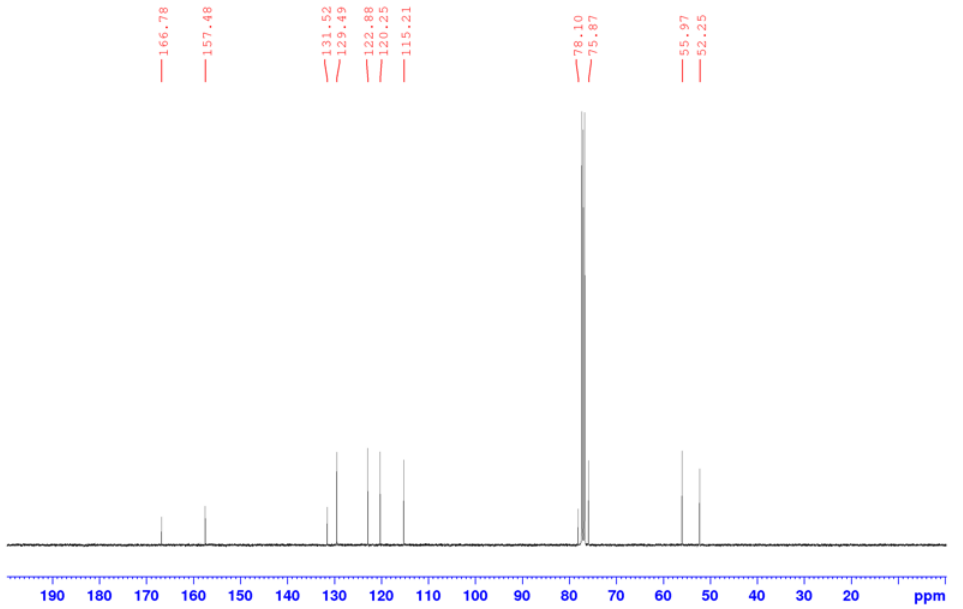


Figure S4: *^{13}C {^{1}H} NMR spectrum of compound **i** in $CDCl_3$ at 298 K.*

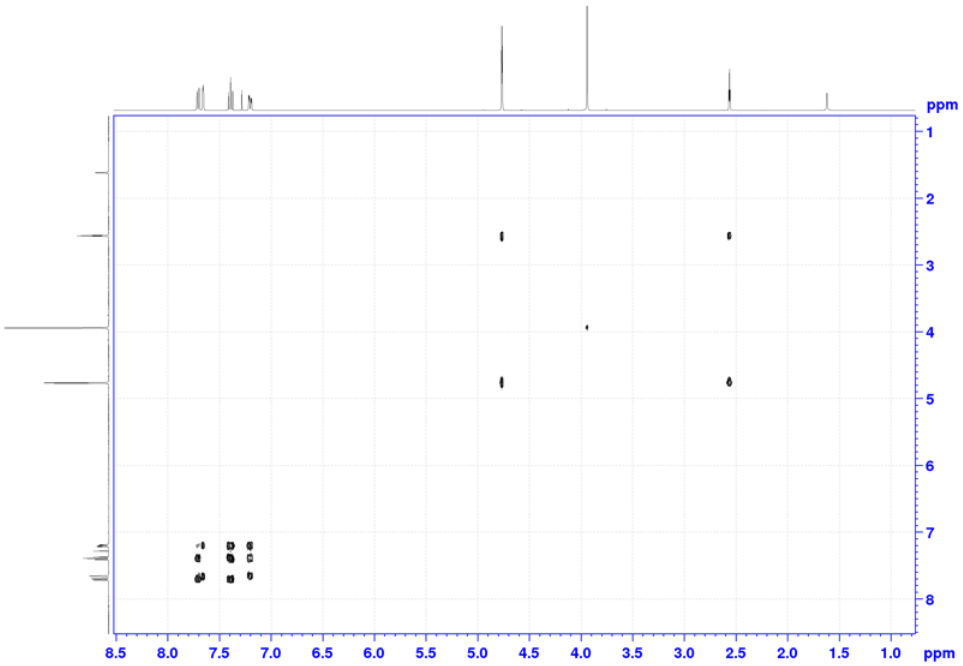


Figure S5: *COSY NMR spectrum of compound* ***i*** *in* $CDCl_3$ *at 298 K.*

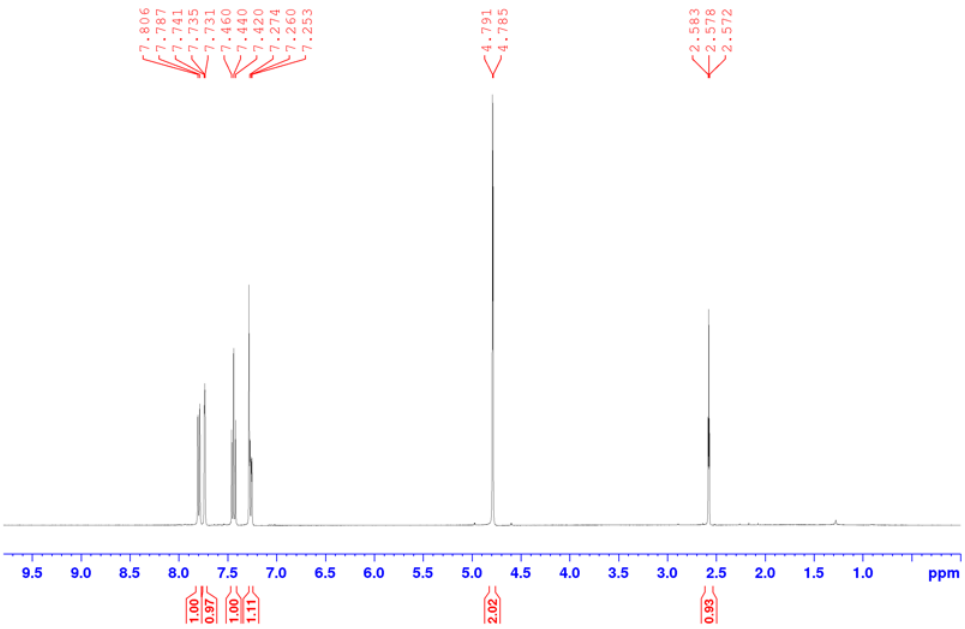


Figure S6: *^{1}H NMR spectrum of compound* ***ii*** *in* $CDCl_3$ *at 298 K.*

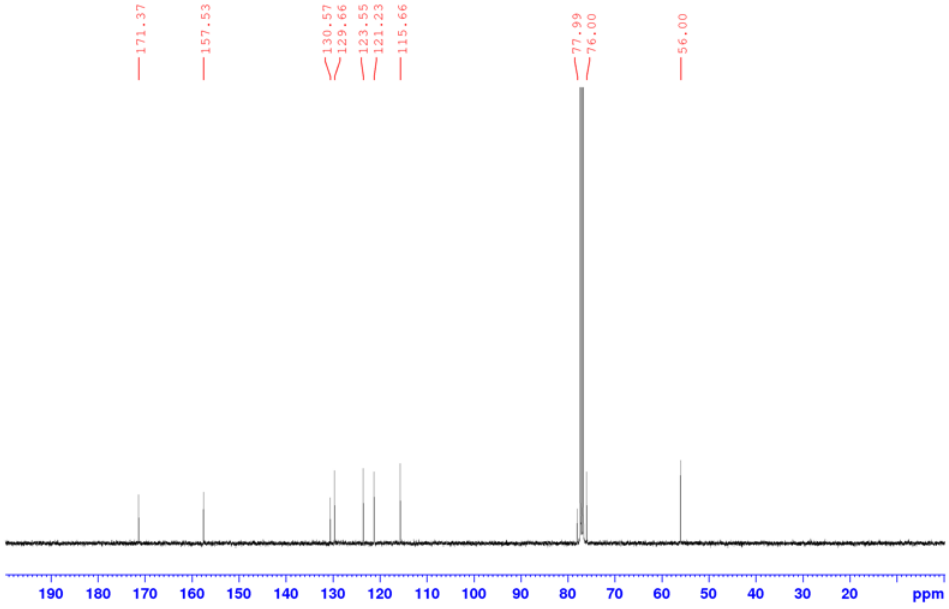


Figure S7: *^{13}C {^{1}H} NMR spectrum of compound **ii** in $CDCl_3$ at 298 K.*

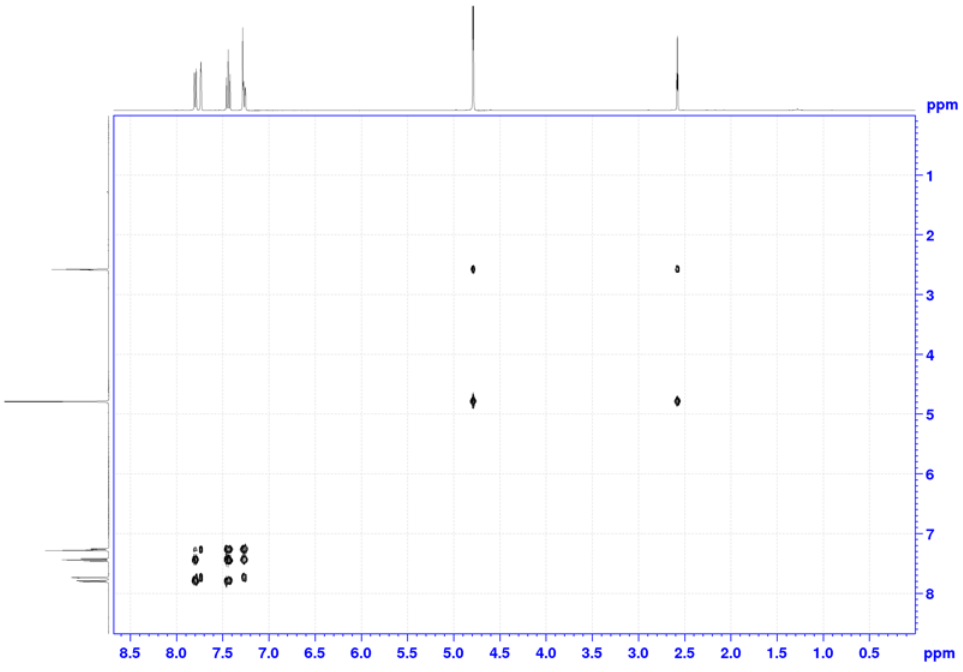


Figure S8: *COSY NMR spectrum of compound **ii** in $CDCl_3$ at 298 K.*

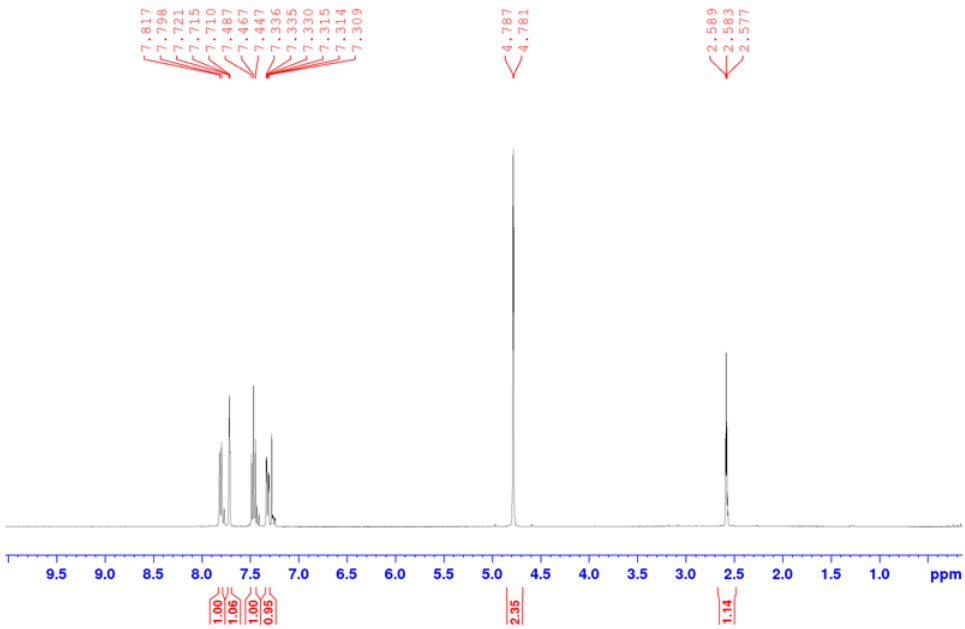


Figure S9: *^{1}H NMR spectrum of compound **iii** in $CDCl_3$ at 298 K. (Contains traces of **ii**)*

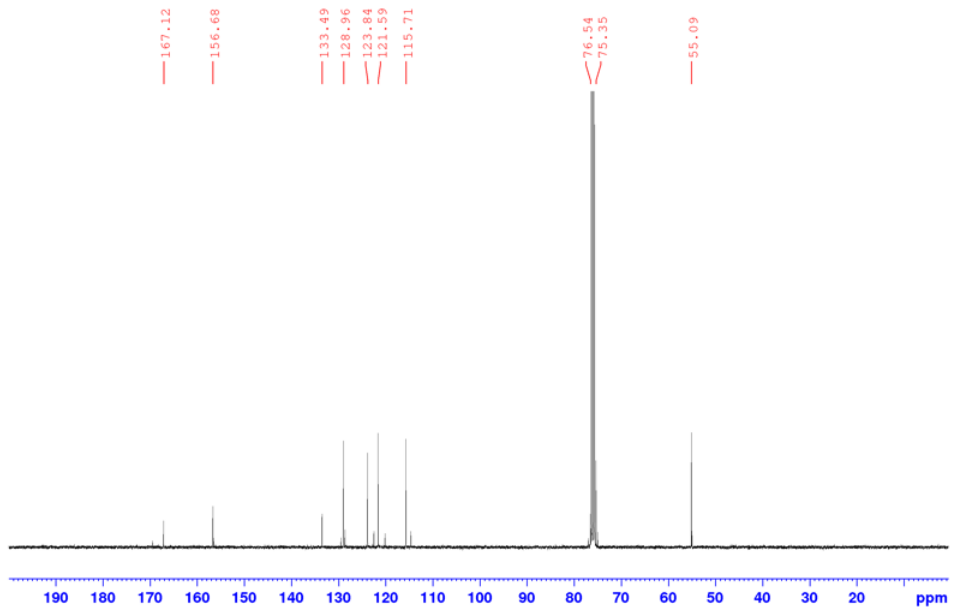


Figure S10: *^{13}C {^{1}H} NMR spectrum of compound **iii** in $CDCl_3$ at 298 K (Contains traces of **ii**).*

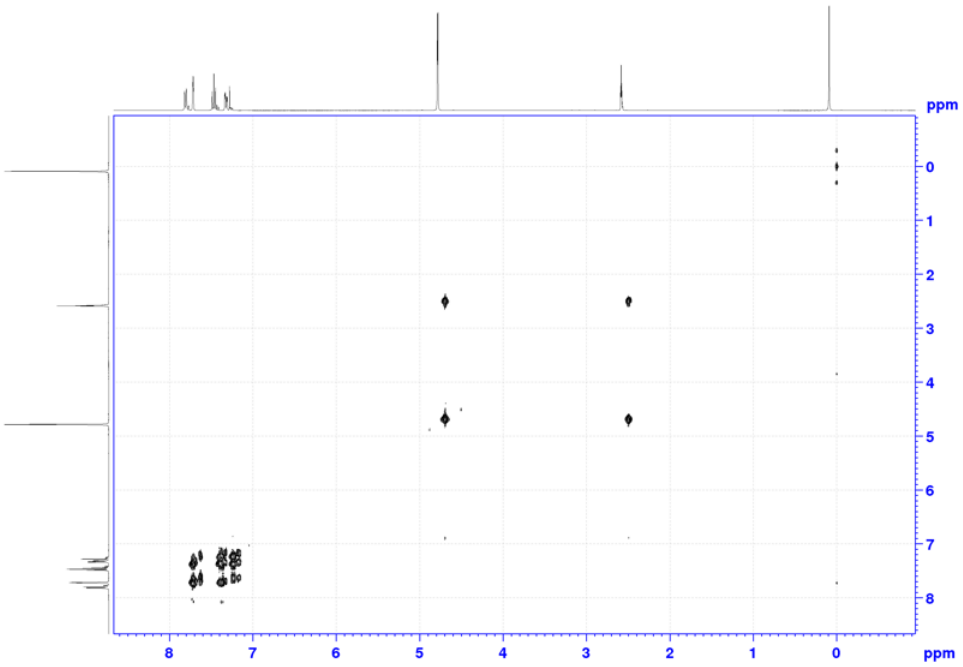


Figure S11: *COSY NMR spectrum of compound* ***iii*** *in* $CDCl_3$ *at 298 K (Contains traces of* ***ii****).*

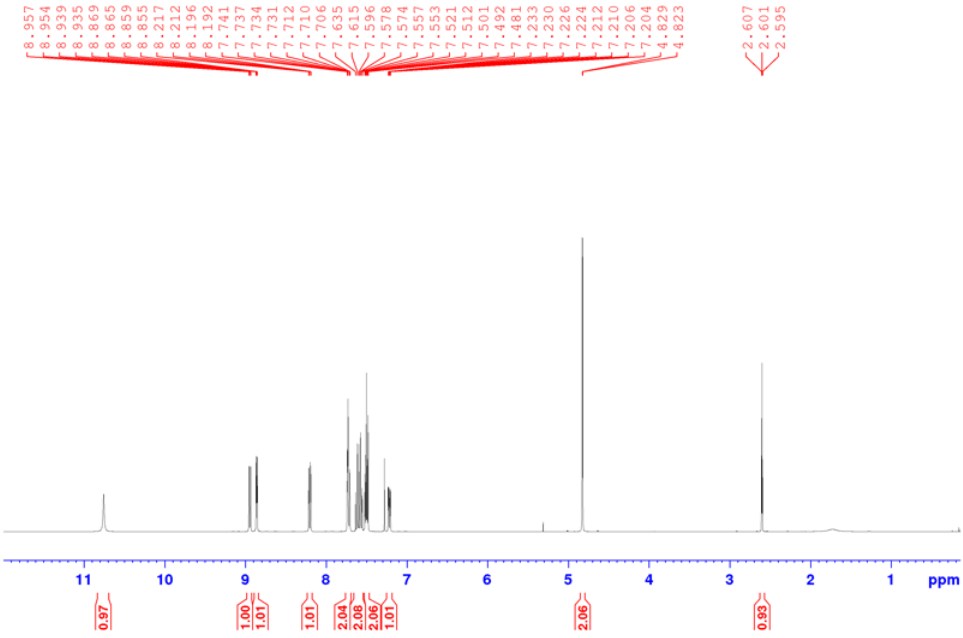


Figure S12: *^{1}H NMR spectrum of compound* ***1o*** *in* $CDCl_3$ *at 298 K.*

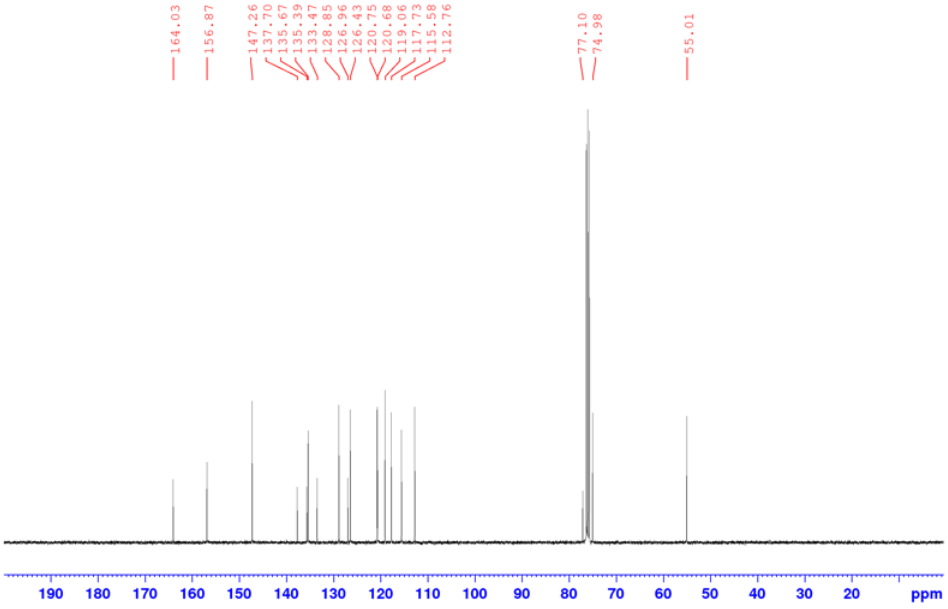


Figure S13: *^{13}C {^{1}H} NMR spectrum of compound* ***1o*** *in $CDCl_3$ at 298 K.*

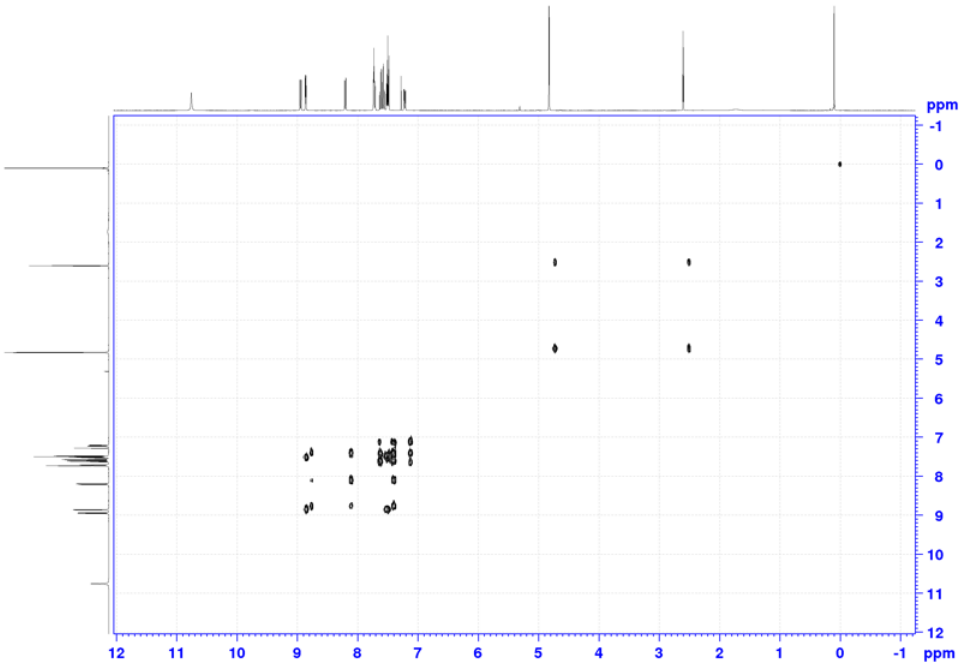


Figure S14: *COSY NMR spectrum of compound* ***1o*** *in $CDCl_3$ at 298 K.*

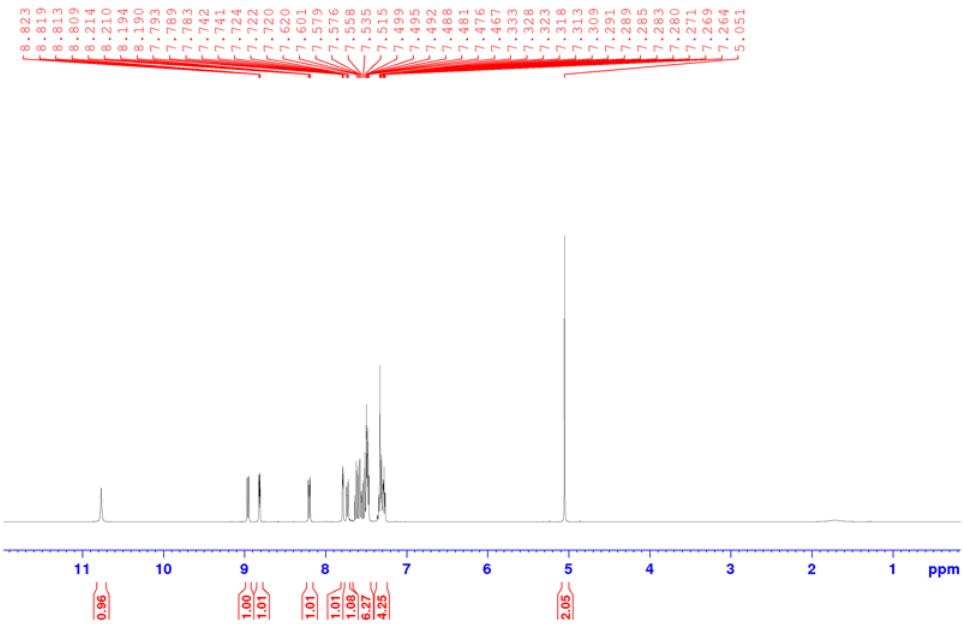


Figure S15: *^{1}H NMR spectrum of compound **1a** in $CDCl_3$ at 298 K.*

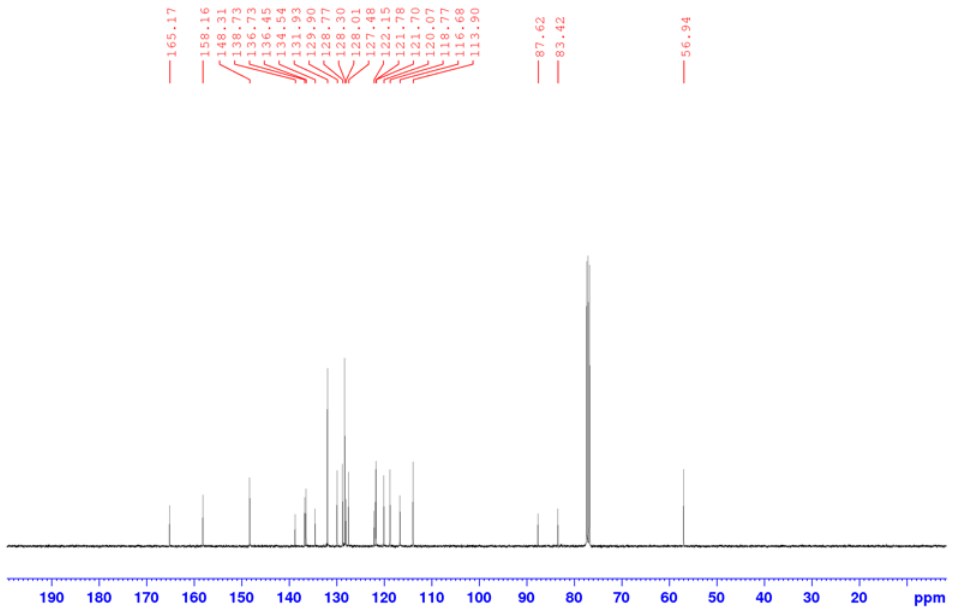


Figure S16: *^{13}C {^{1}H} NMR spectrum of compound **1a** in $CDCl_3$ at 298 K.*

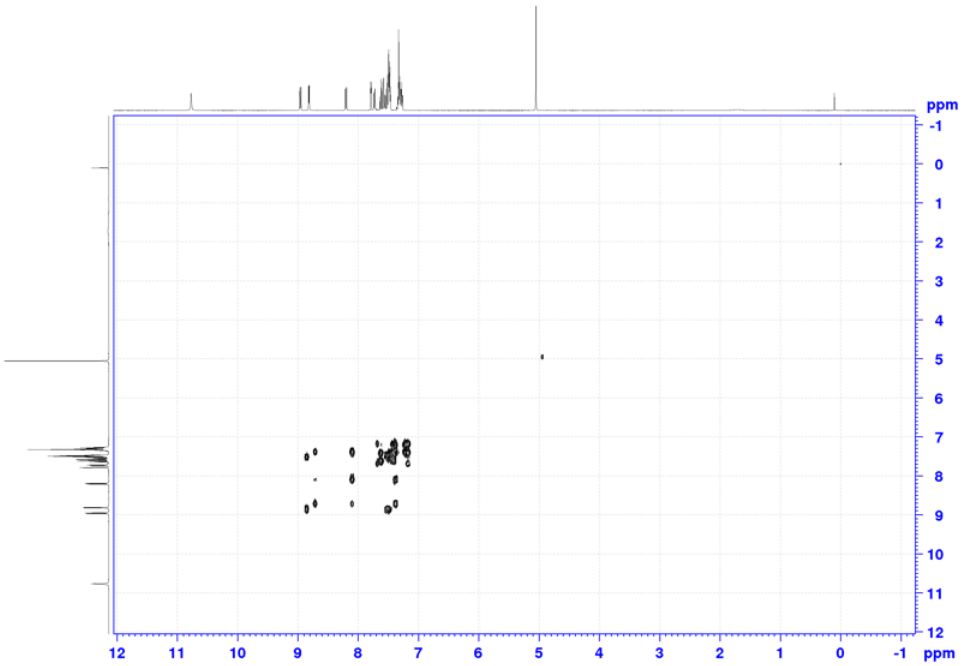


Figure S17: *COSY NMR spectrum of compound* ***1a*** *in* $CDCl_3$ *at 298 K.*

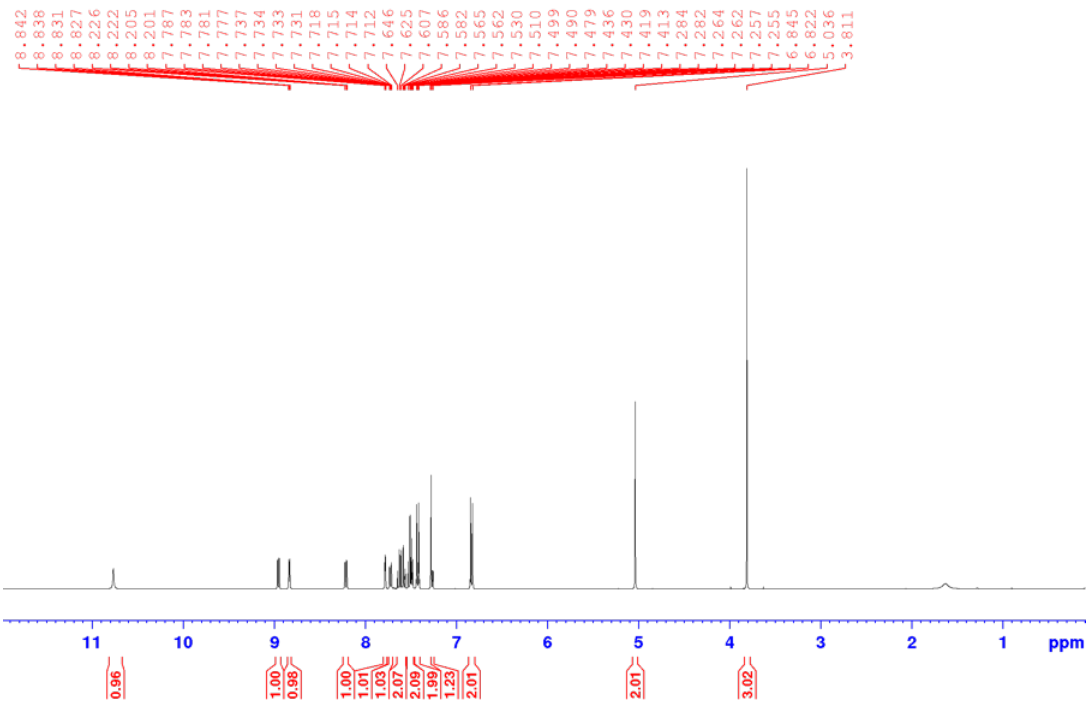


Figure S18: ^{1}*H NMR spectrum of compound* ***1b*** *in* $CDCl_3$ *at 298 K.*

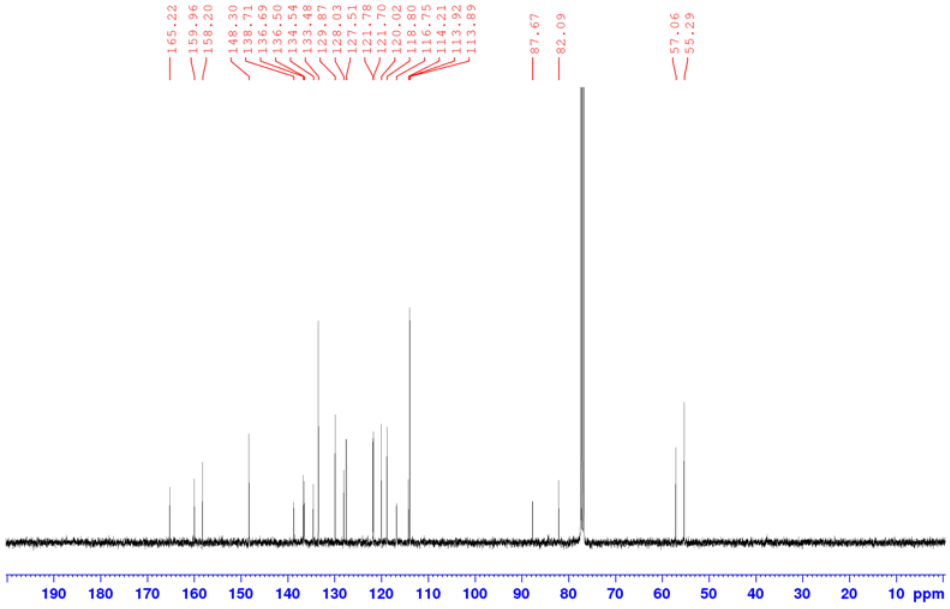


Figure S19: *^{13}C {^{1}H} NMR spectrum of compound* ***1b*** *in $CDCl_3$ at 298 K.*

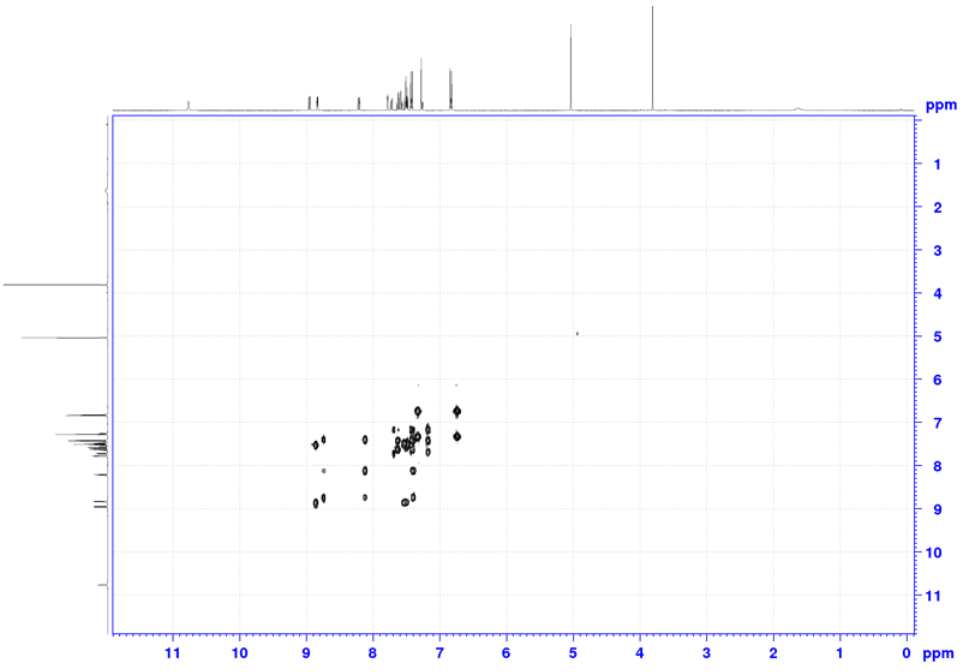


Figure S20: *COSY NMR spectrum of compound* ***1b*** *in $CDCl_3$ at 298 K.*

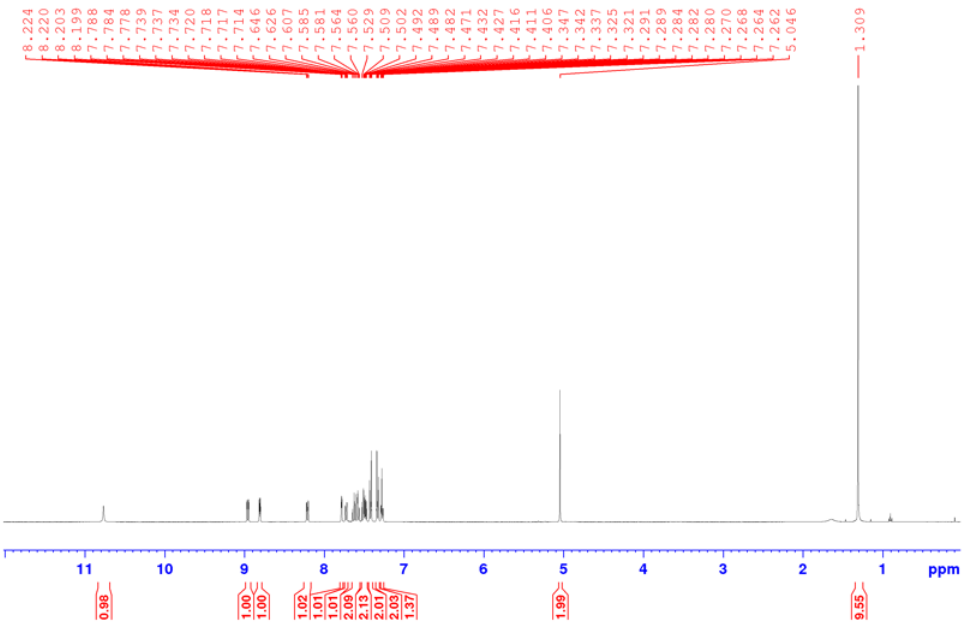


Figure S21: *^{1}H NMR spectrum of compound **1c** in $CDCl_3$ at 298 K.*

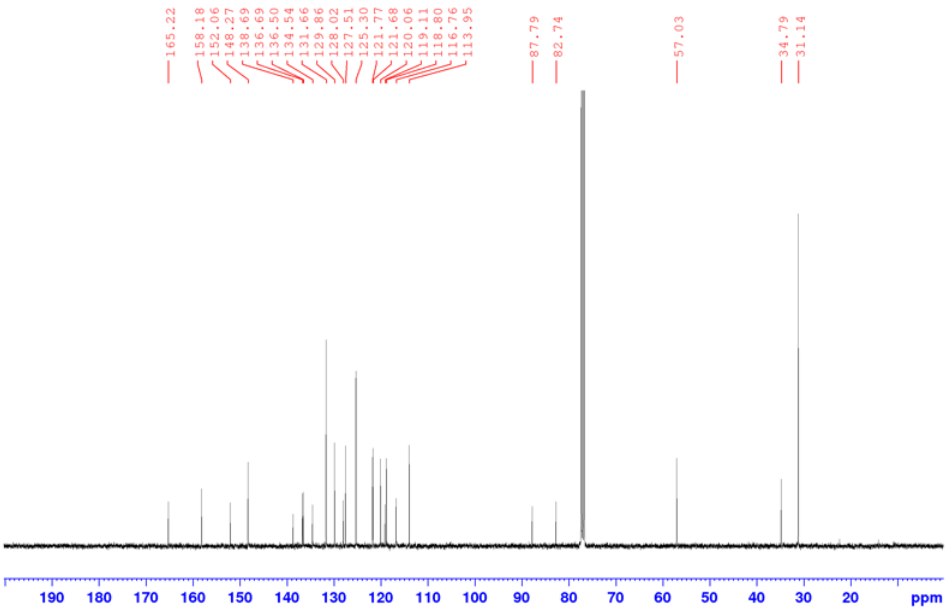


Figure S22: *^{13}C {^{1}H} NMR spectrum of compound **1c** in $CDCl_3$ at 298 K.*

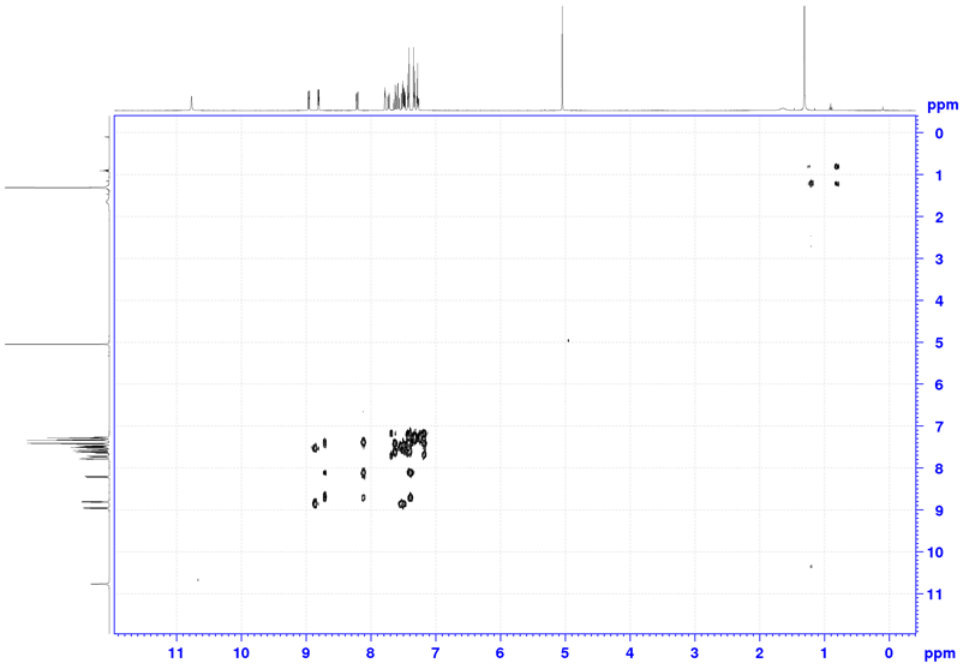


Figure S23: *COSY NMR spectrum of compound* ***1c*** *in* $CDCl_3$ *at 298 K.*

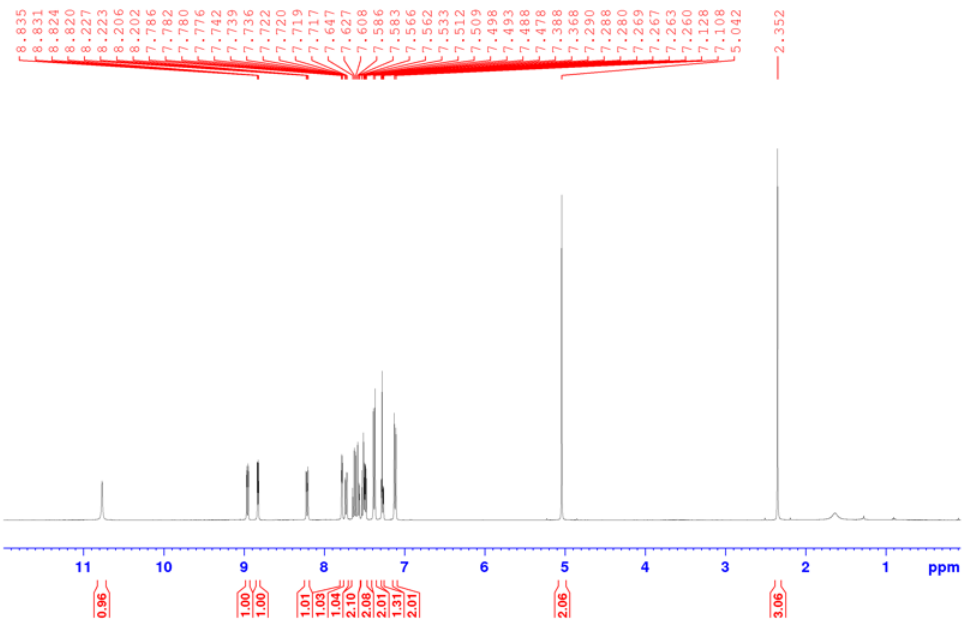


Figure S24: ^{1}*H NMR spectrum of compound* ***1d*** *in* $CDCl_3$ *at 298 K.*

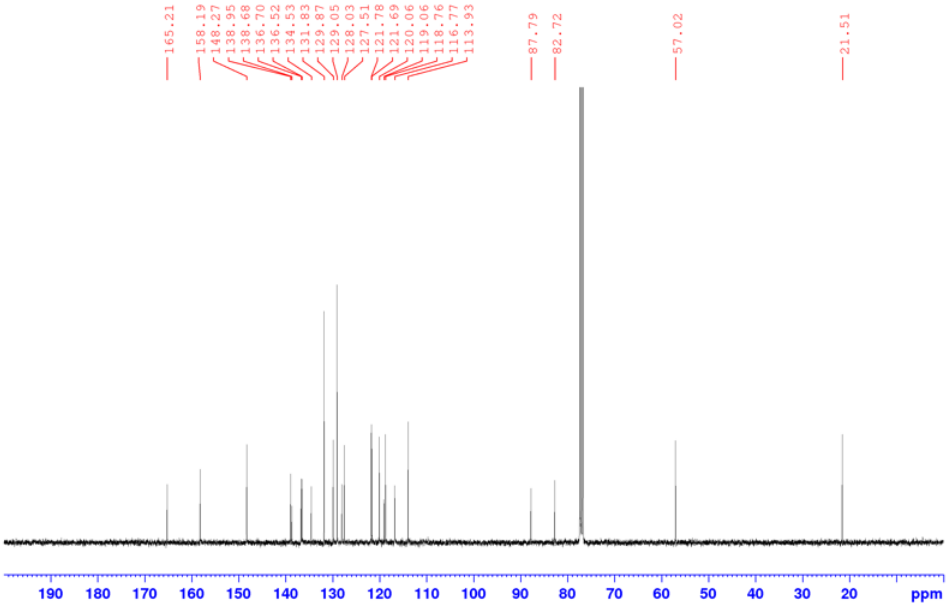


Figure S25: *^{13}C {^{1}H} NMR spectrum of compound **1d** in $CDCl_3$ at 298 K.*

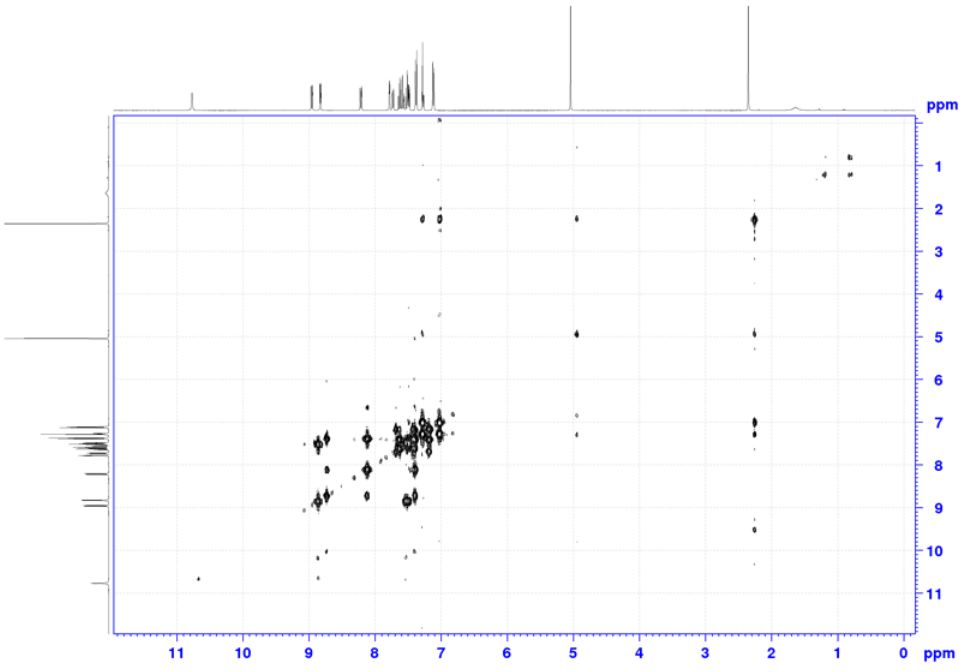


Figure S26: *COSY NMR spectrum of compound **1d** in $CDCl_3$ at 298 K.*

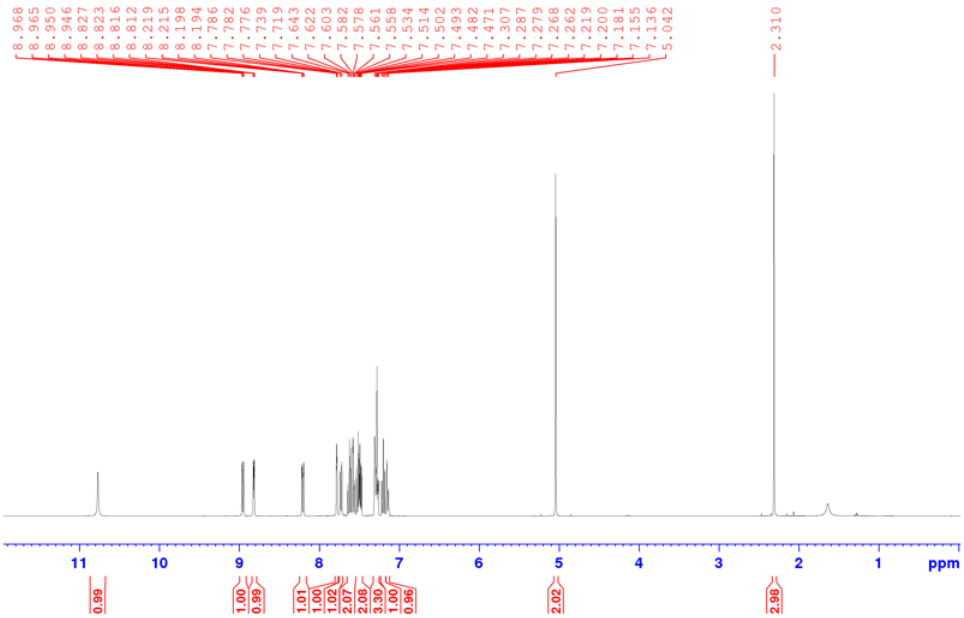


Figure S27: *^{1}H NMR spectrum of compound **1e** in $CDCl_3$ at 298 K.*

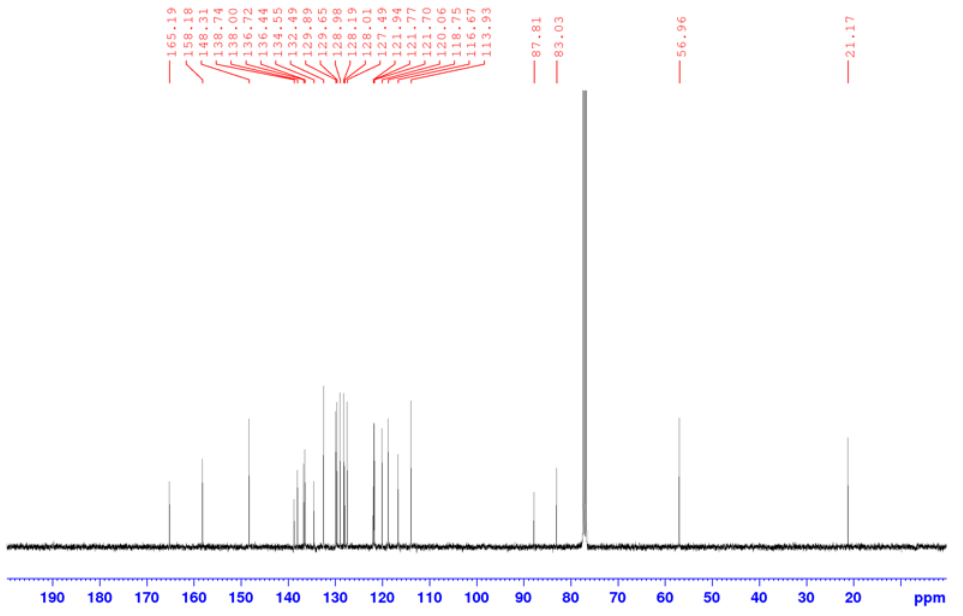


Figure S28: *^{13}C {^{1}H} NMR spectrum of compound **1e** in $CDCl_3$ at 298 K.*

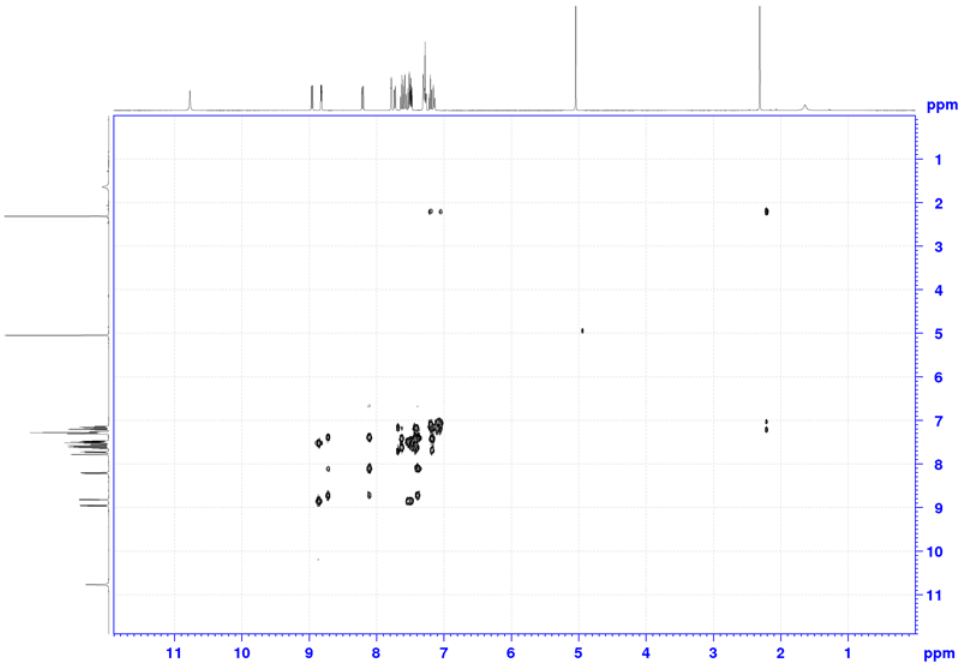


Figure S29: *COSY NMR spectrum of compound* ***1e*** *in* $CDCl_3$ *at 298 K.*

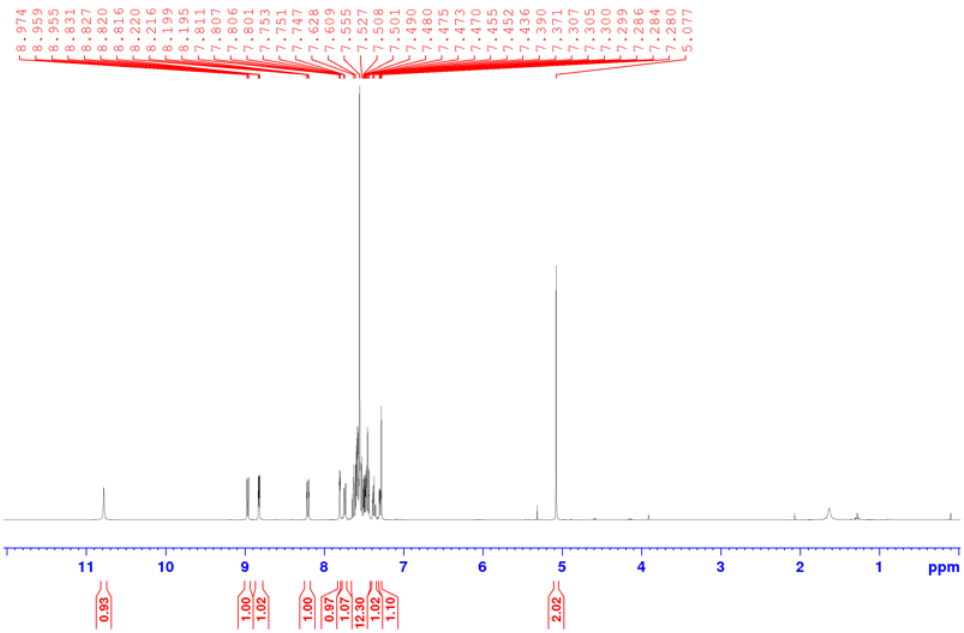


Figure S30: *^{1}H NMR spectrum of compound* ***1f*** *in* $CDCl_3$ *at 298 K.*

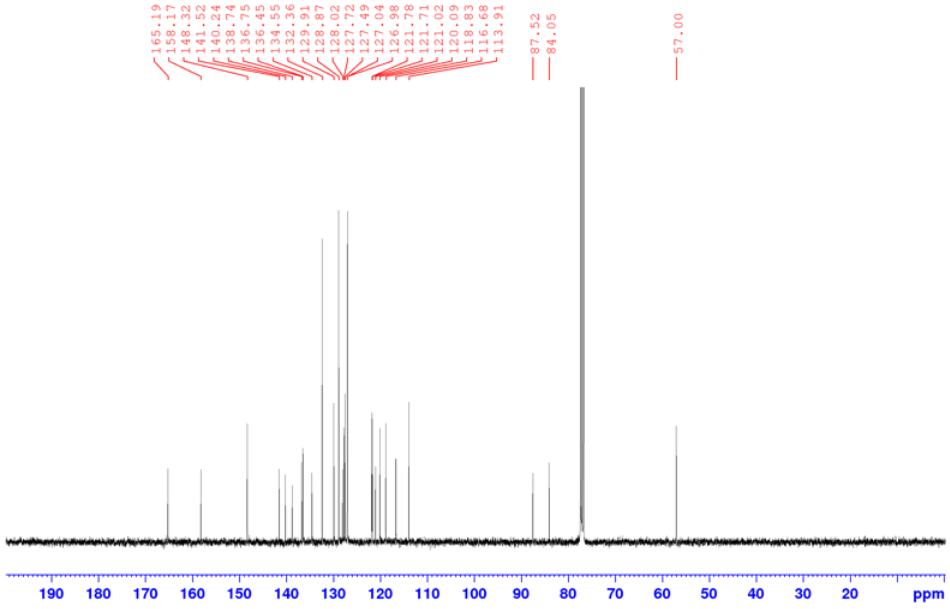


Figure S31: *^{13}C {^{1}H} NMR spectrum of compound **1f** in $CDCl_3$ at 298 K.*

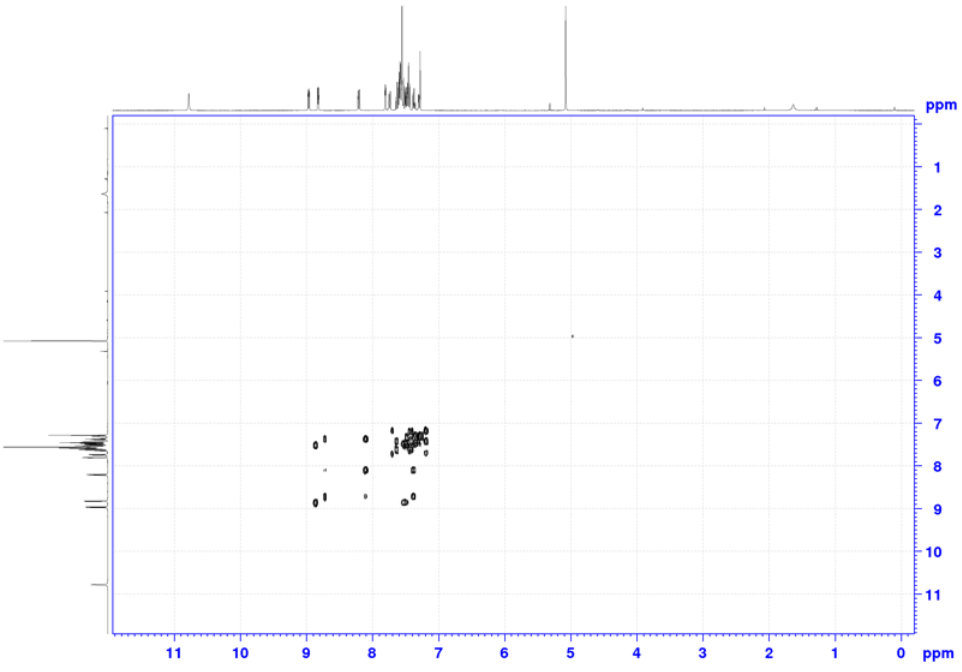


Figure S32: *COSY NMR spectrum of compound **1f** in $CDCl_3$ at 298 K.*

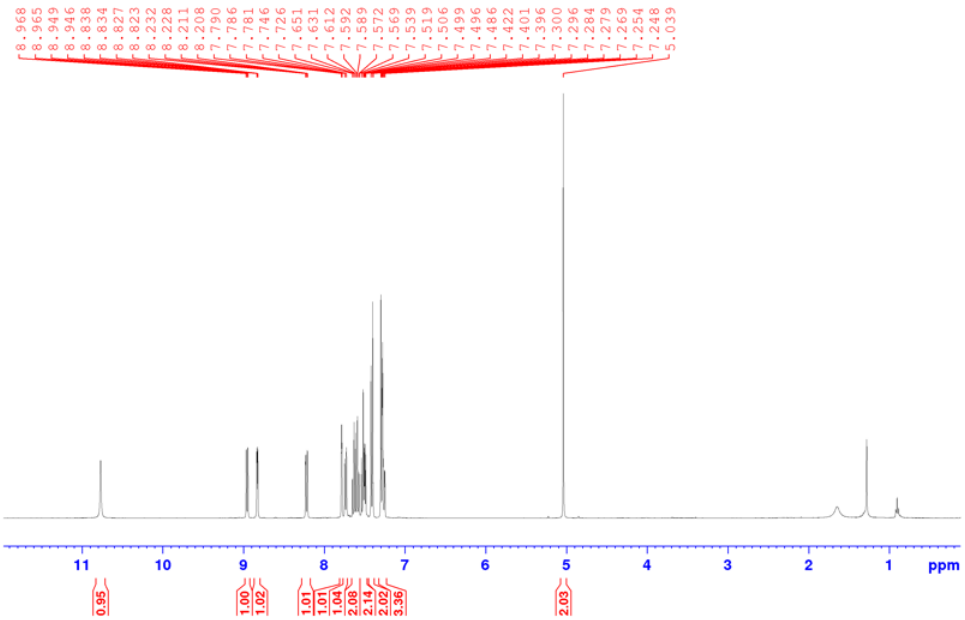


Figure S33: *^{1}H NMR spectrum of compound **1g** in $CDCl_3$ at 298 K.*

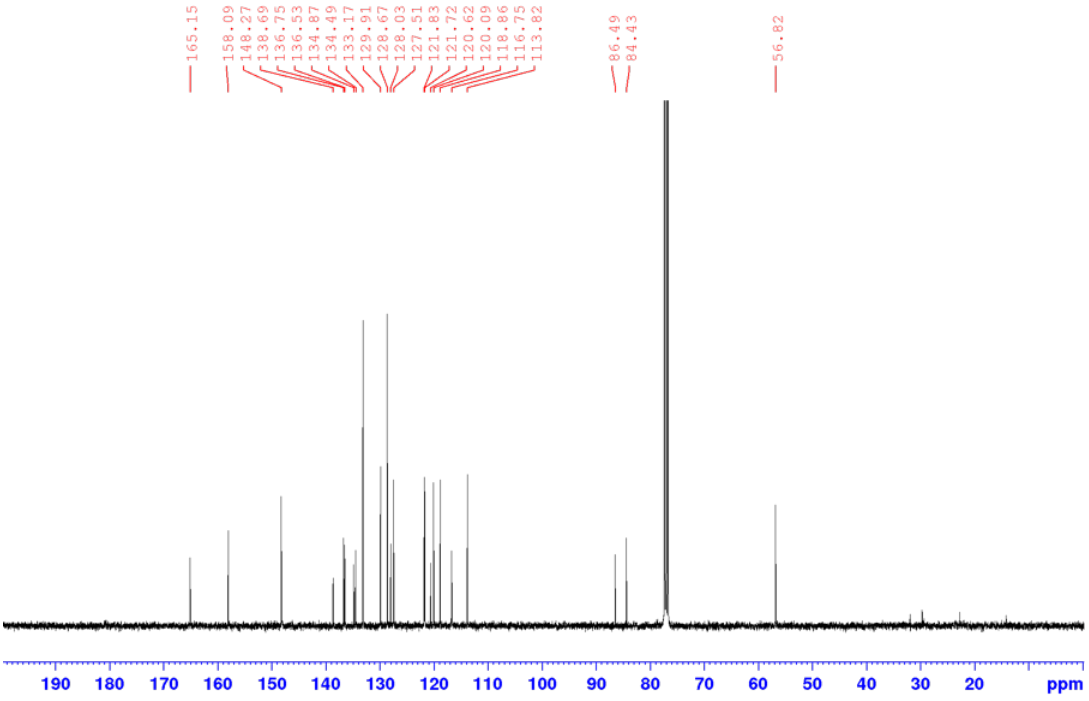


Figure S34: *$^{13}C\ \{^{1}H\}$ NMR spectrum of compound **1g** in $CDCl_3$ at 298 K.*

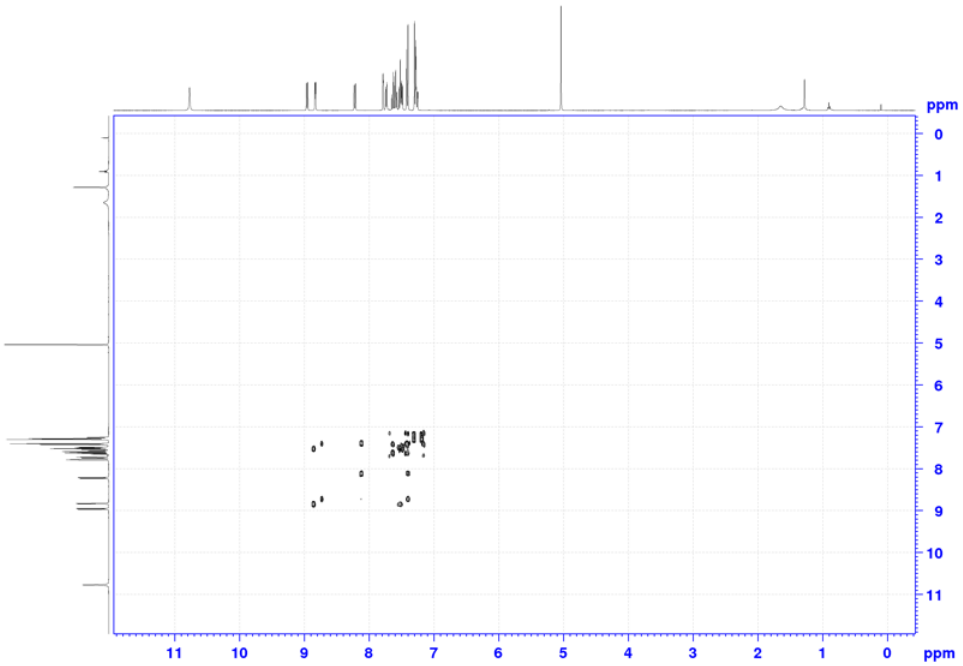


Figure S35: *COSY NMR spectrum of compound* ***1g*** *in* $CDCl_3$ *at 298 K.*

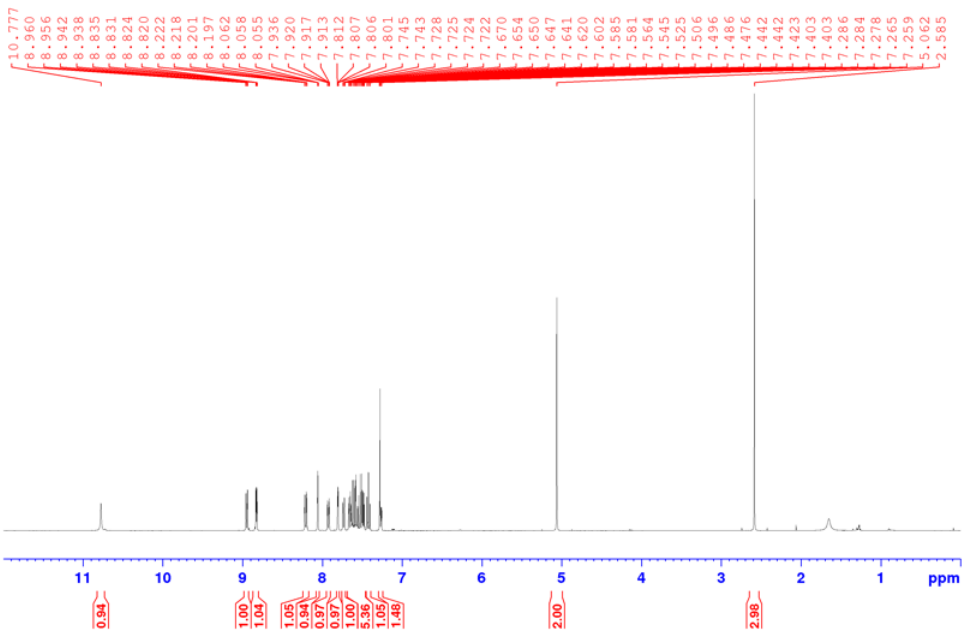


Figure S36: *^{1}H NMR spectrum of compound* ***1h*** *in* $CDCl_3$ *at 298 K.*

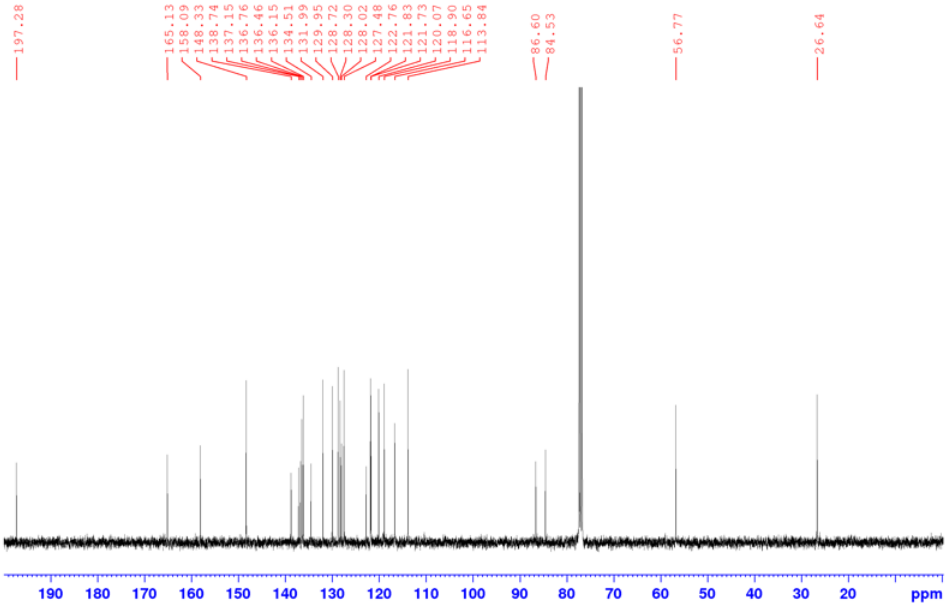


Figure S37: *^{13}C {^{1}H} NMR spectrum of compound* ***1h*** *in $CDCl_3$ at 298 K.*

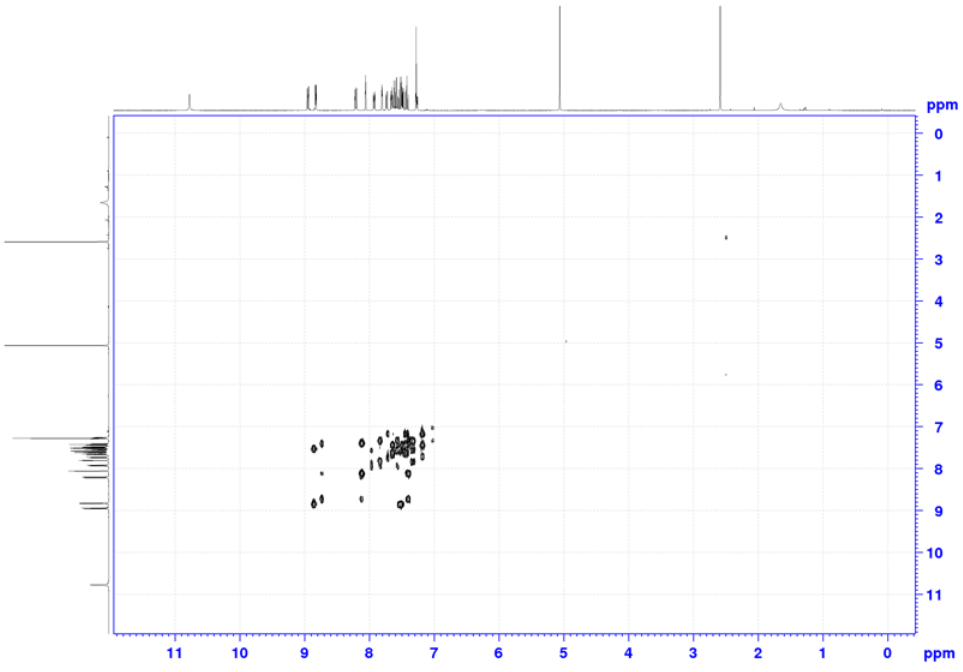


Figure S38: *COSY NMR spectrum of compound* ***1h*** *in $CDCl_3$ at 298 K.*

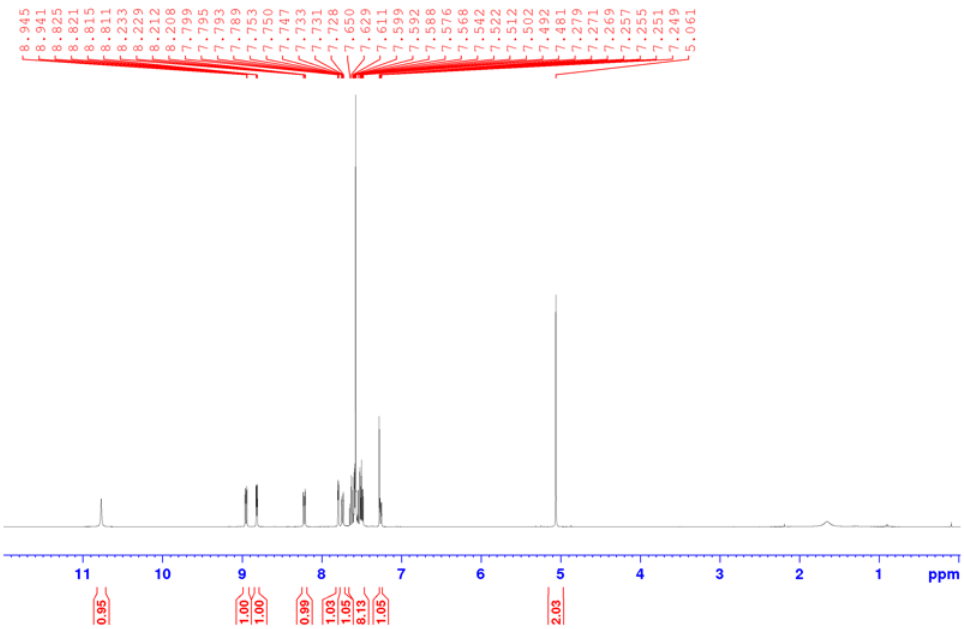


Figure S39: *^{1}H NMR spectrum of compound **1i** in $CDCl_3$ at 298 K.*

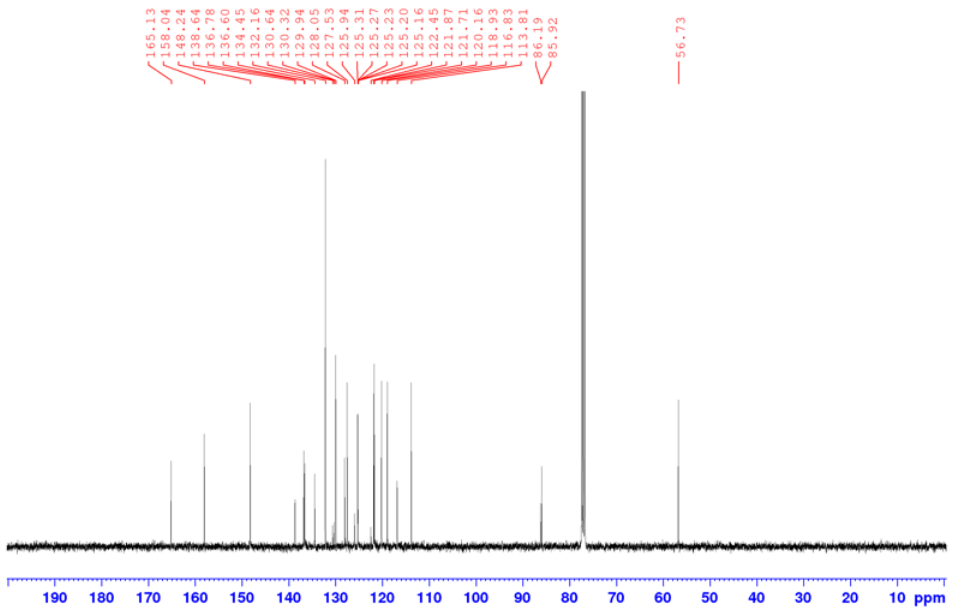


Figure S40: *^{13}C {^{1}H} NMR spectrum of compound **1i** in $CDCl_3$ at 298 K.*

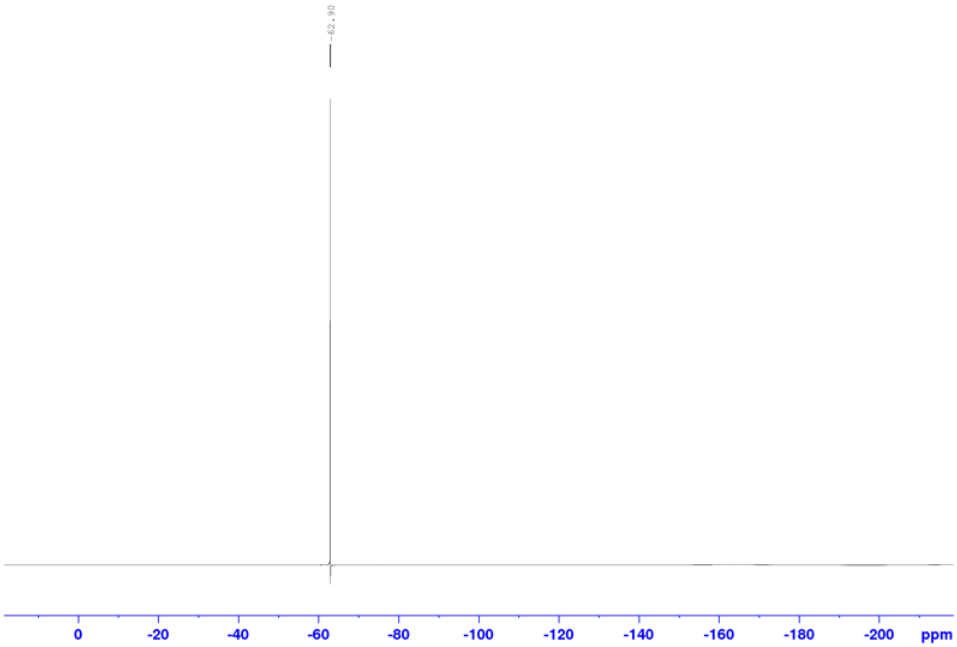


Figure S41: *^{19}F {^{1}H} NMR spectrum of compound* ***1i*** *in $CDCl_3$ at 298 K.*

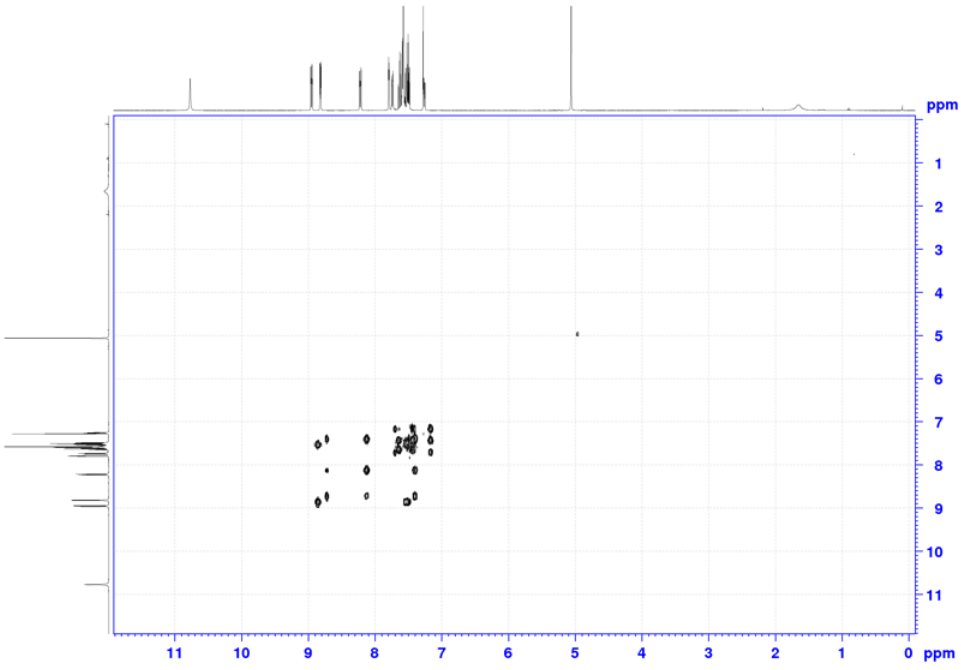


Figure S42: *COSY NMR spectrum of compound* ***1i*** *in $CDCl_3$ at 298 K.*

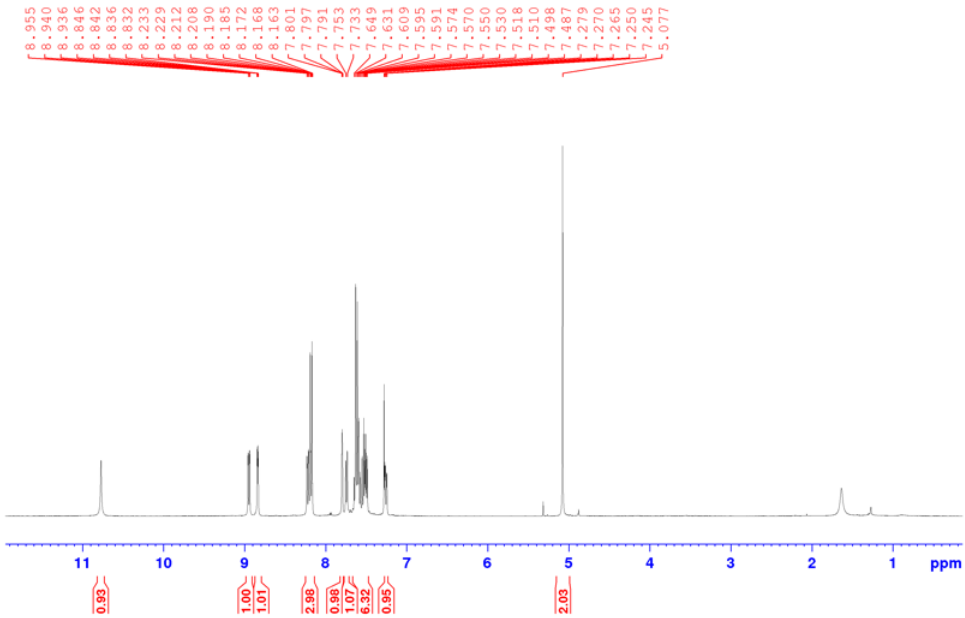


Figure S43: *^{1}H NMR spectrum of compound **1j** in $CDCl_3$ at 298 K.*

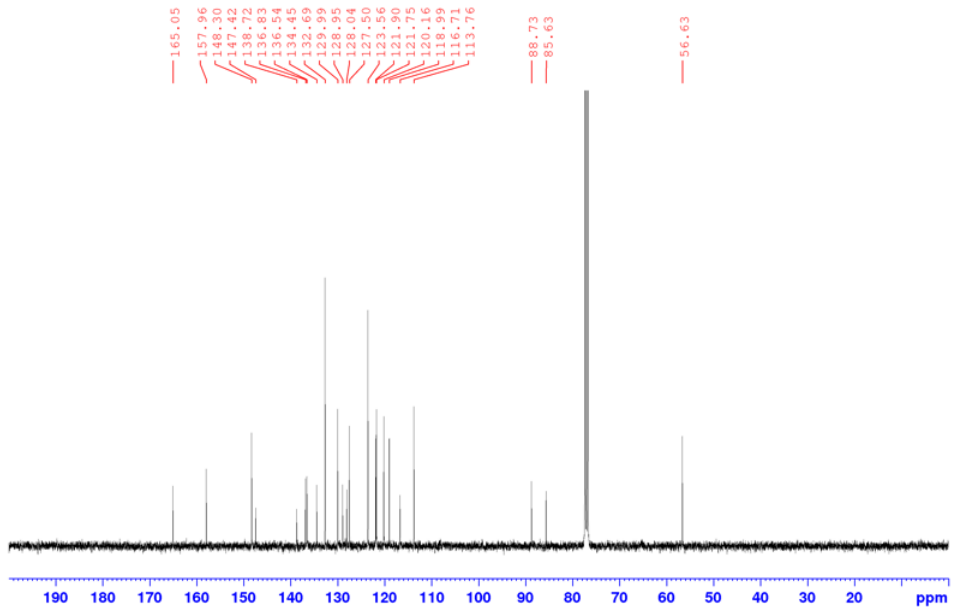


Figure S44: *^{13}C {^{1}H} NMR spectrum of compound **1j** in $CDCl_3$ at 298 K.*

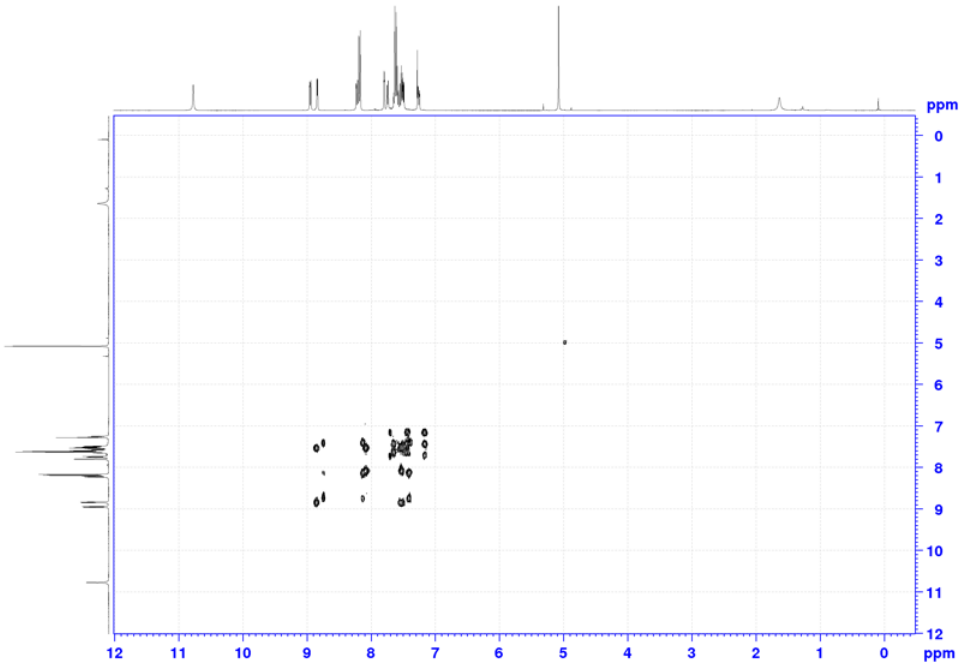


Figure S45: *COSY NMR spectrum of compound* ***1j*** *in* $CDCl_3$ *at 298 K.*

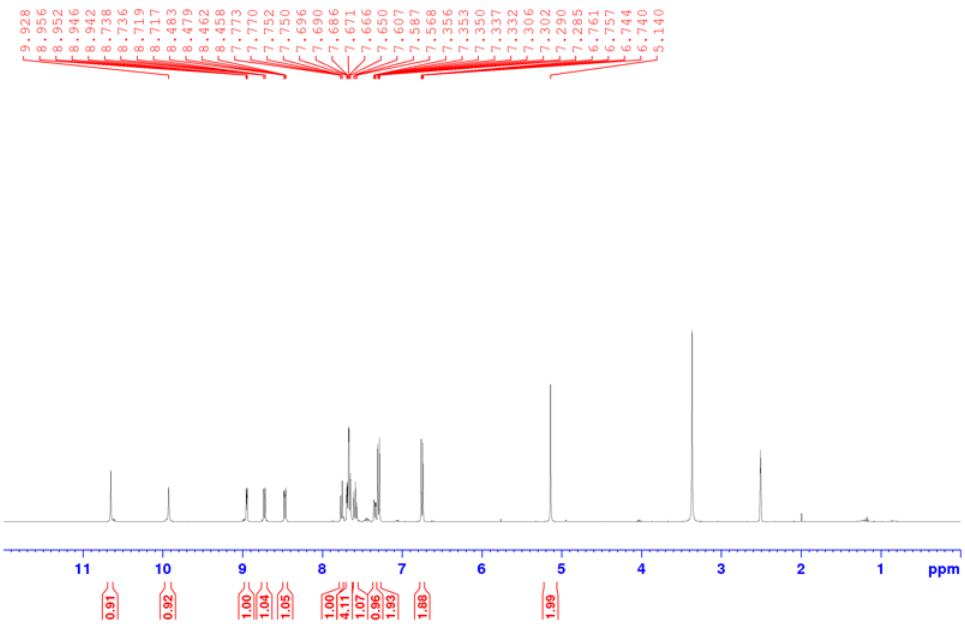


Figure S46: *^{1}H NMR spectrum of compound* ***1k*** *in* d_6-DMSO *at 298 K.*

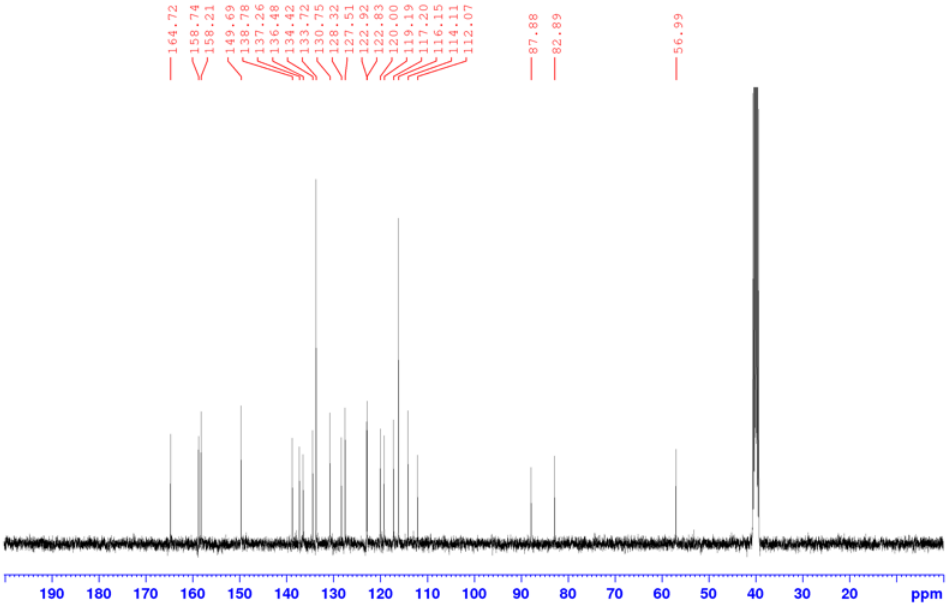


Figure S47: *^{13}C {^{1}H} NMR spectrum of compound* ***1k*** *in* d_6-DMSO *at 298 K.*

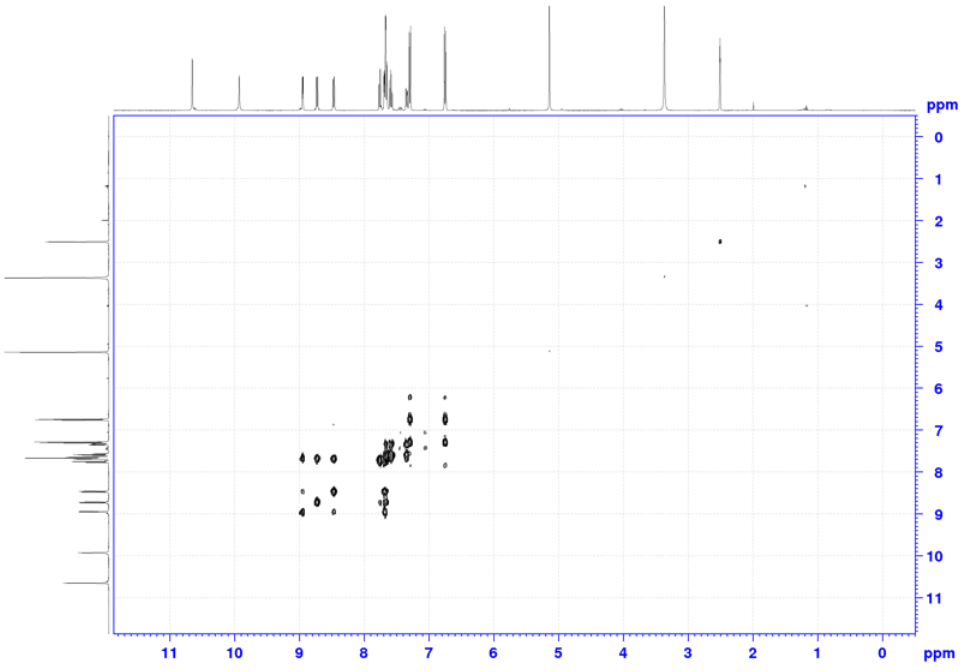


Figure S48: *COSY NMR spectrum of compound* ***1k*** *in* d_6-DMSO *at 298 K.*

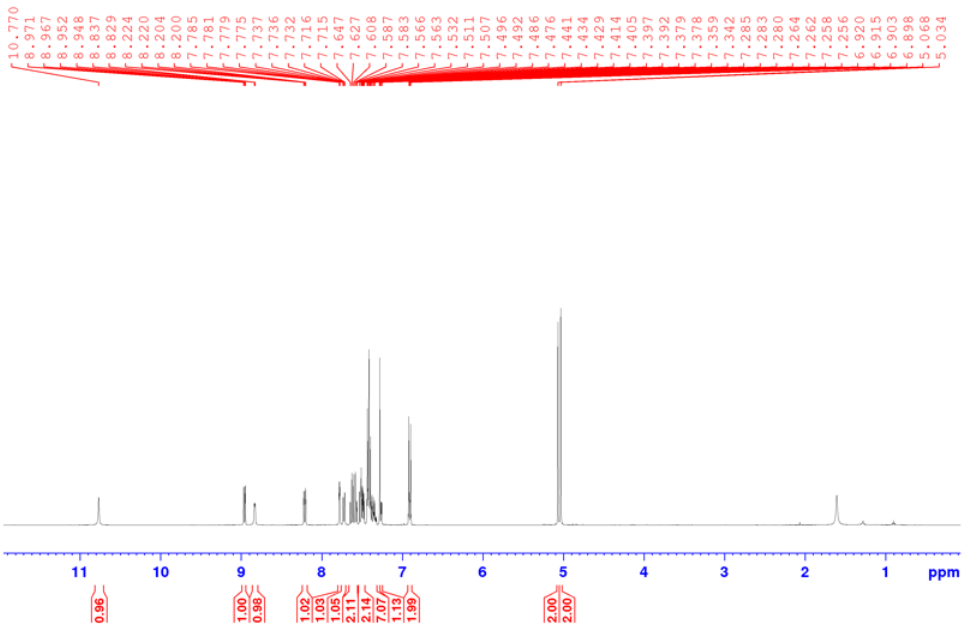


Figure S49: *^{1}H NMR spectrum of compound **1l** in $CDCl_3$ at 298 K.*

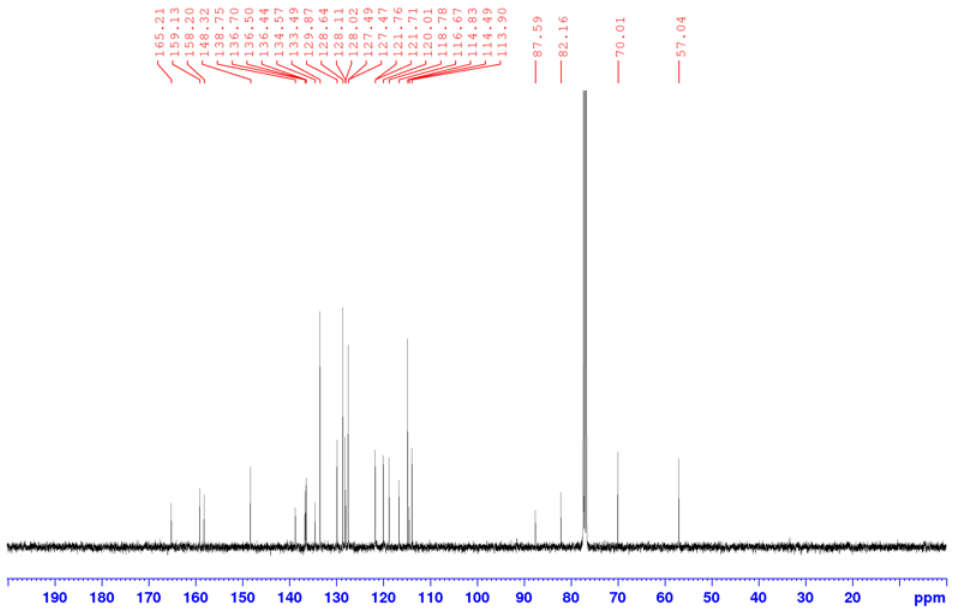


Figure S50: *^{13}C {^{1}H} NMR spectrum of compound **1l** in $CDCl_3$ at 298 K.*

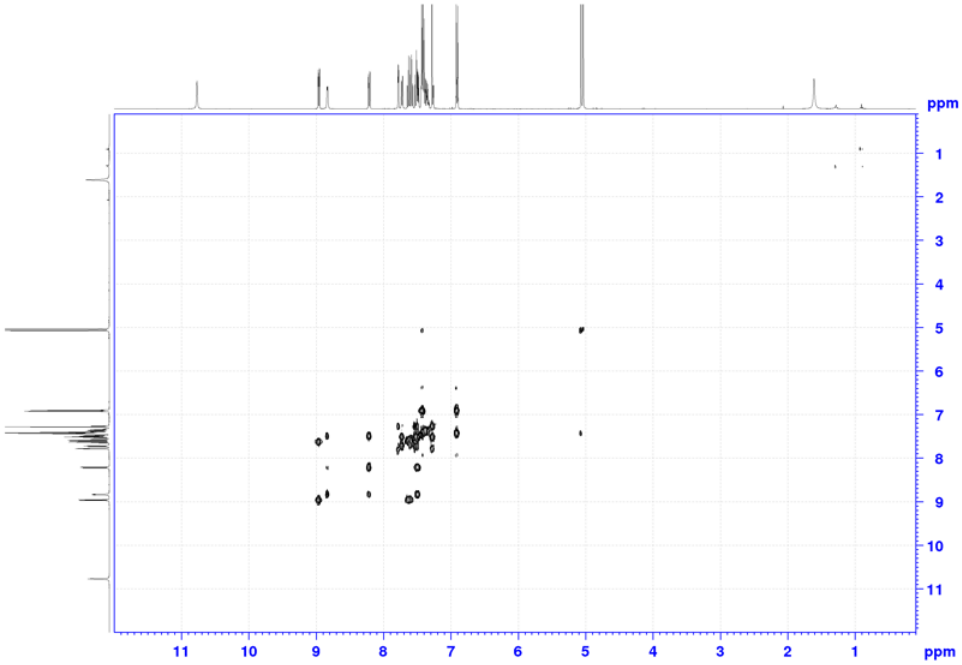


Figure S51: *COSY NMR spectrum of compound* ***1l*** *in* $CDCl_3$ *at 298 K.*

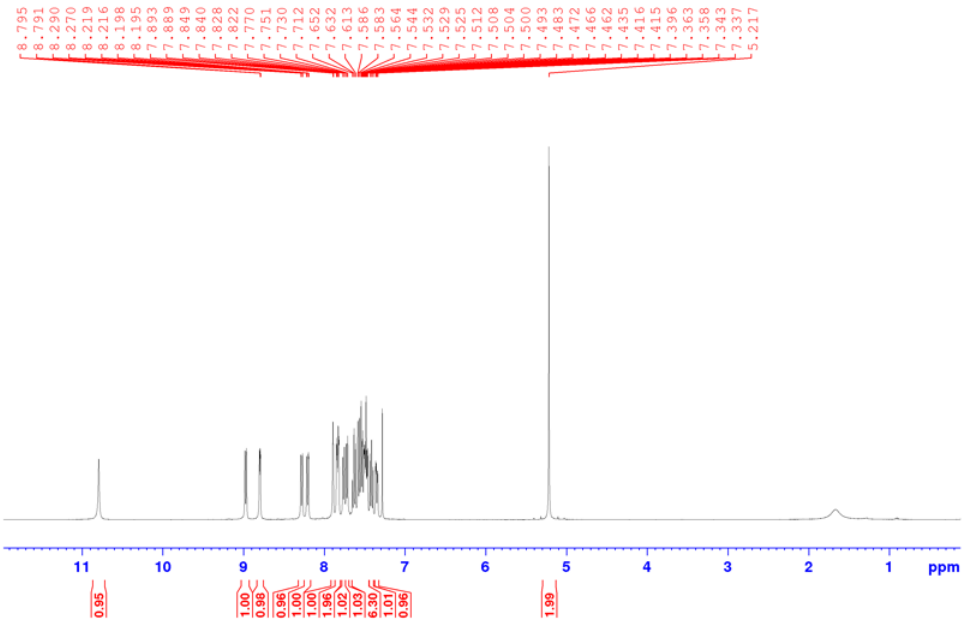


Figure S52: *^{1}H NMR spectrum of compound* ***1m*** *in* $CDCl_3$ *at 298 K.*

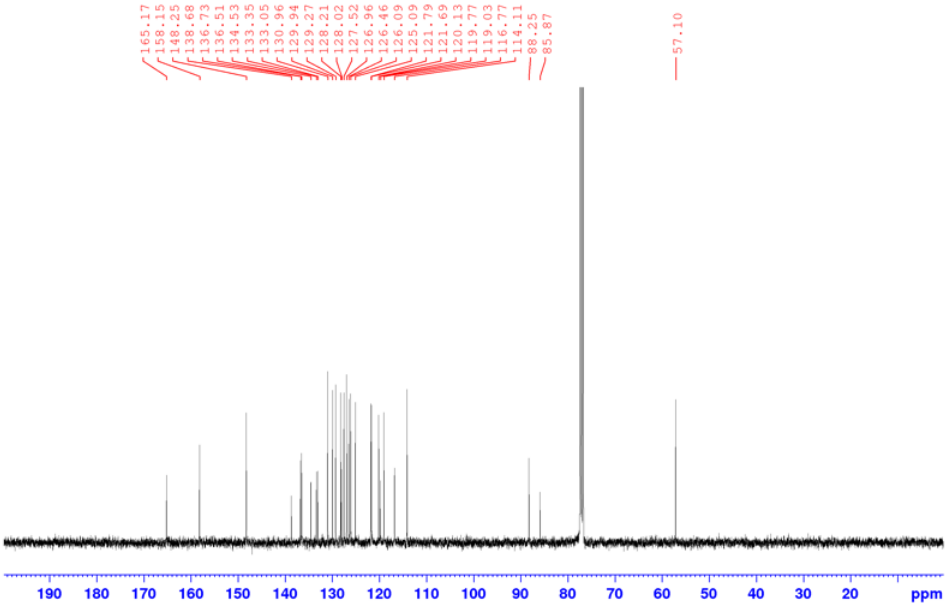


Figure S53: *^{13}C {^{1}H} NMR spectrum of compound* ***1m*** *in $CDCl_3$ at 298 K.*

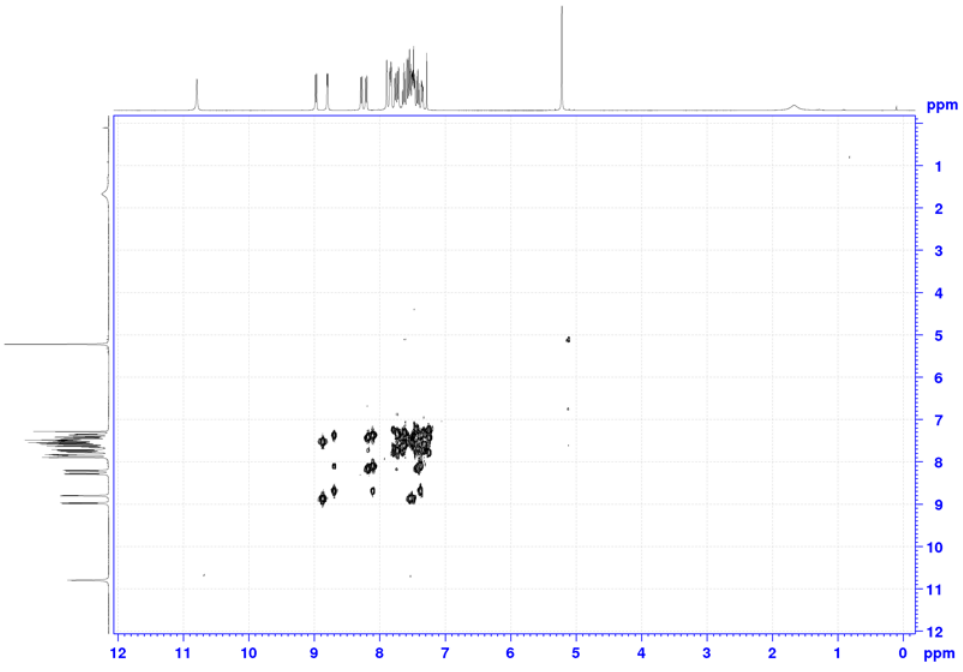


Figure S54: *COSY NMR spectrum of compound* ***1m*** *in $CDCl_3$ at 298 K.*

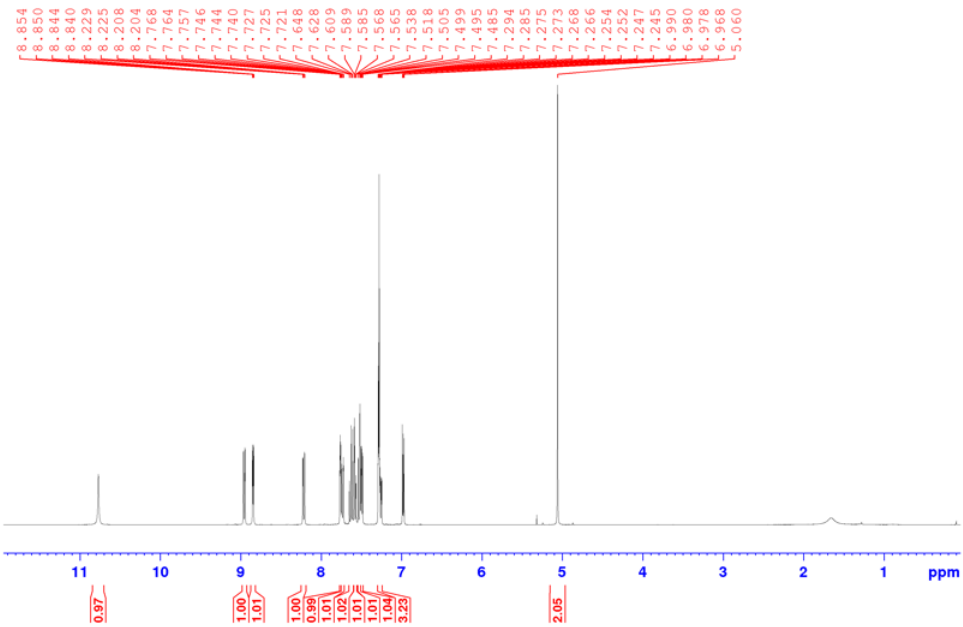


Figure S55: *^{1}H NMR spectrum of compound **1n** in $CDCl_3$ at 298 K.*

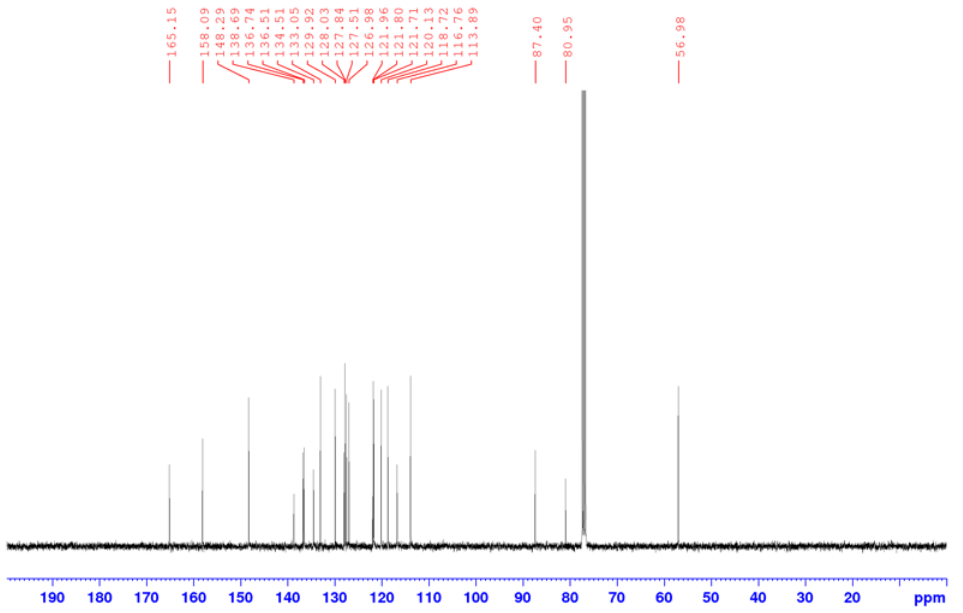


Figure S56: *^{13}C {^{1}H} NMR spectrum of compound **1n** in $CDCl_3$ at 298 K.*

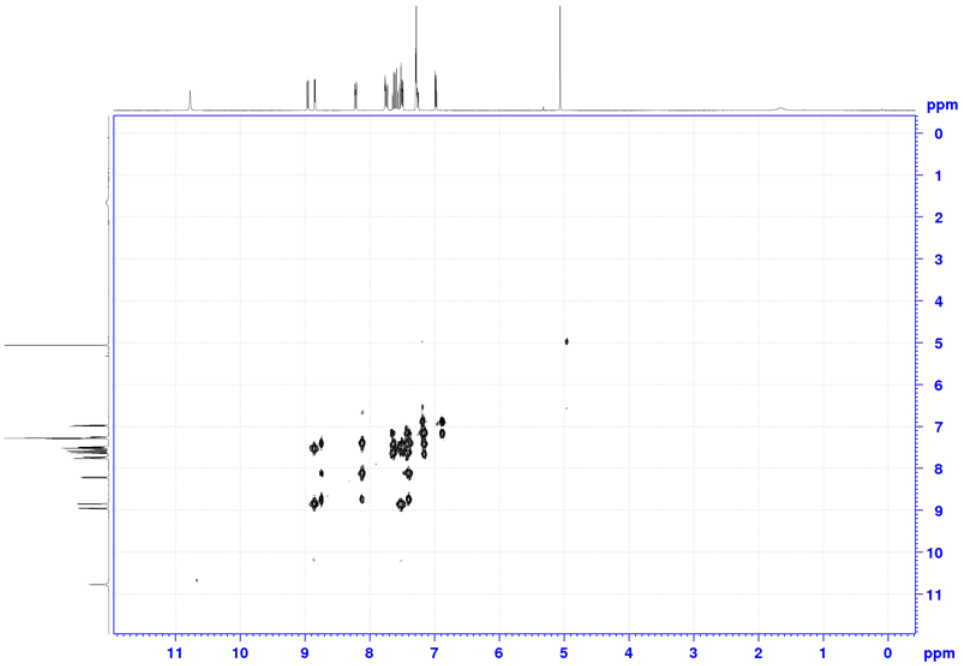


Figure S57: *COSY NMR spectrum of compound* ***1n*** *in* $CDCl_3$ *at 298 K.*

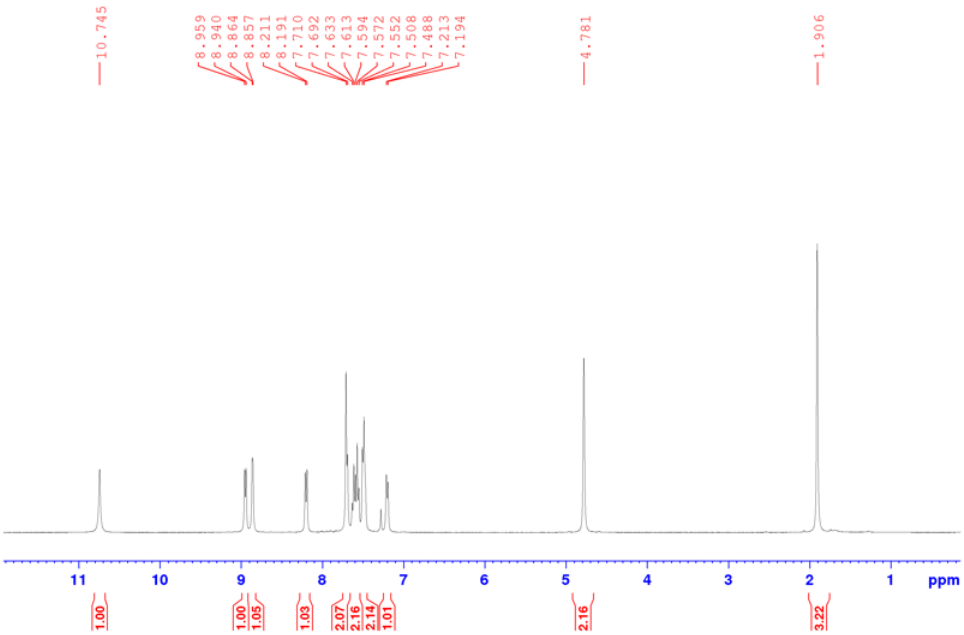


Figure S58: ^1H *NMR spectrum of compound* ***1p*** *in* $CDCl_3$ *at 298 K.*

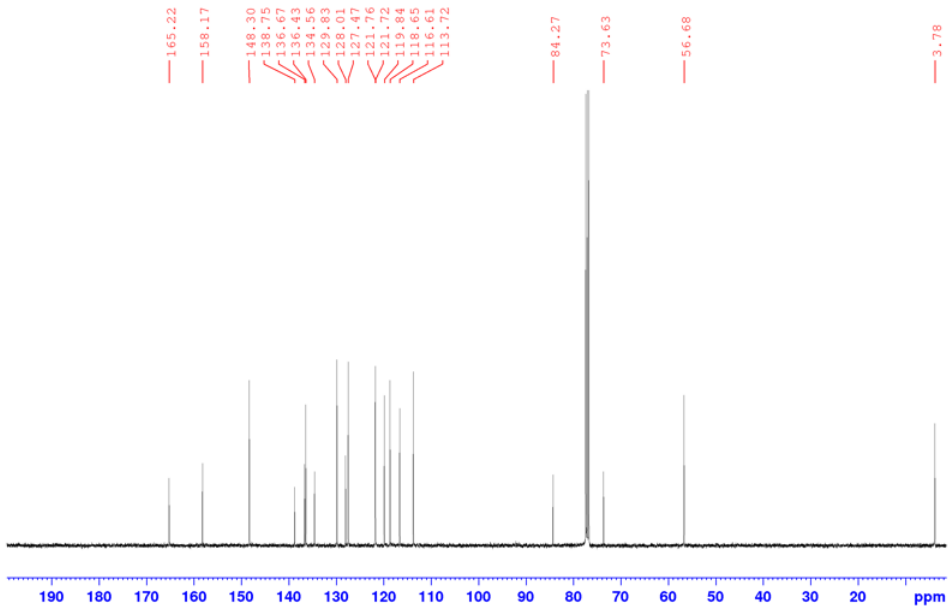


Figure S59: *^{13}C {^{1}H} NMR spectrum of compound **1p** in $CDCl_3$ at 298 K.*

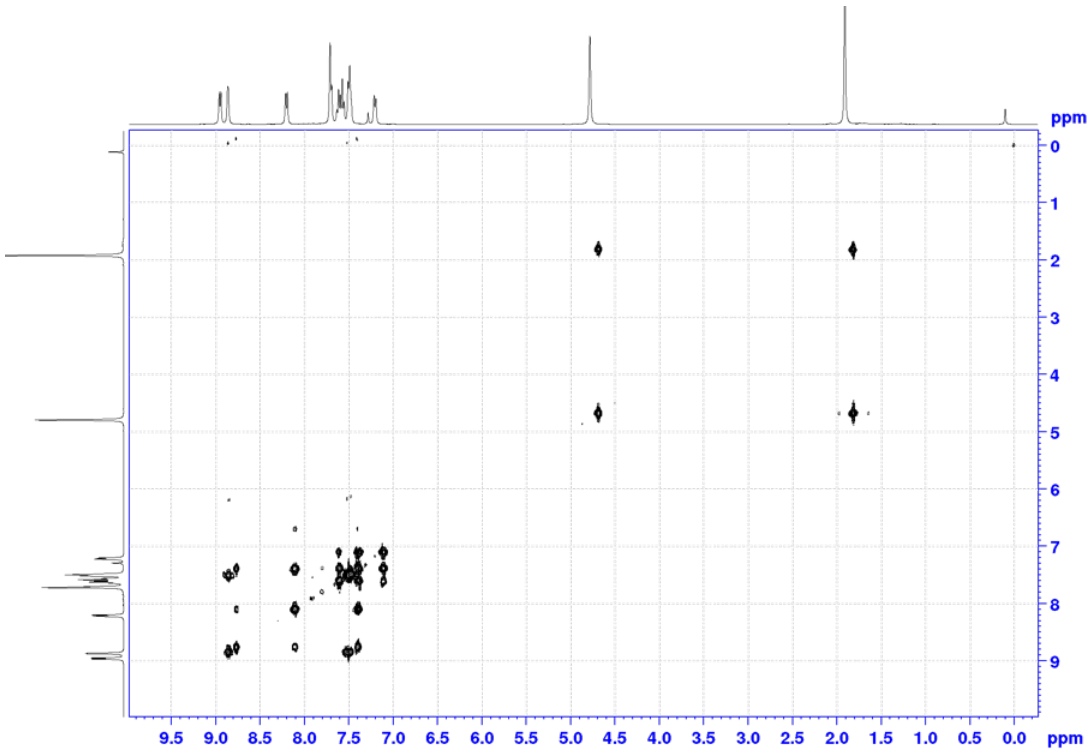


Figure S60: *COSY NMR spectrum of compound **1p** in $CDCl_3$ at 298 K.*

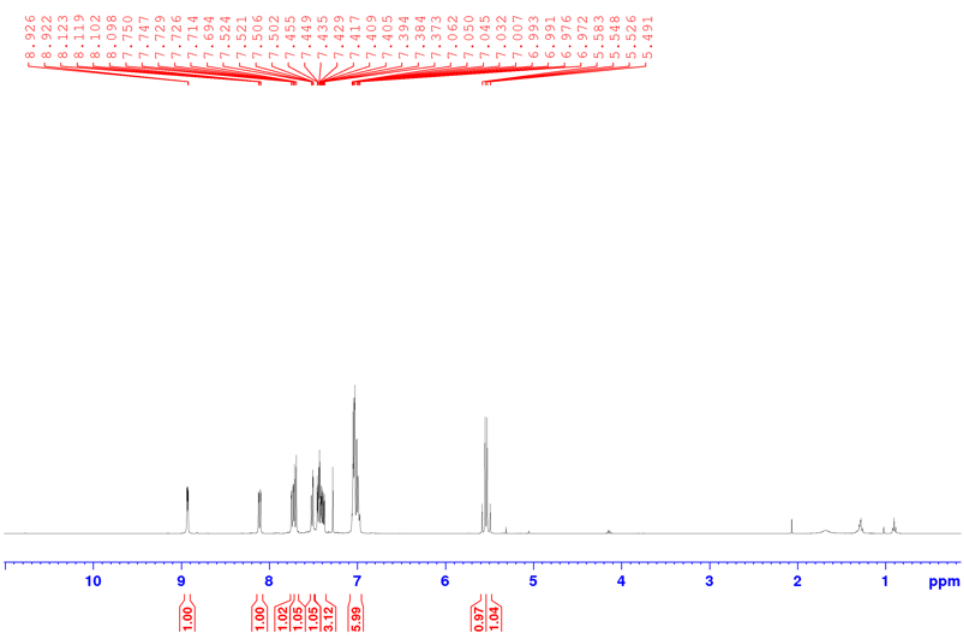


Figure S61: *^{1}H NMR spectrum of compound **2a** in $CDCl_3$ at 298 K.*

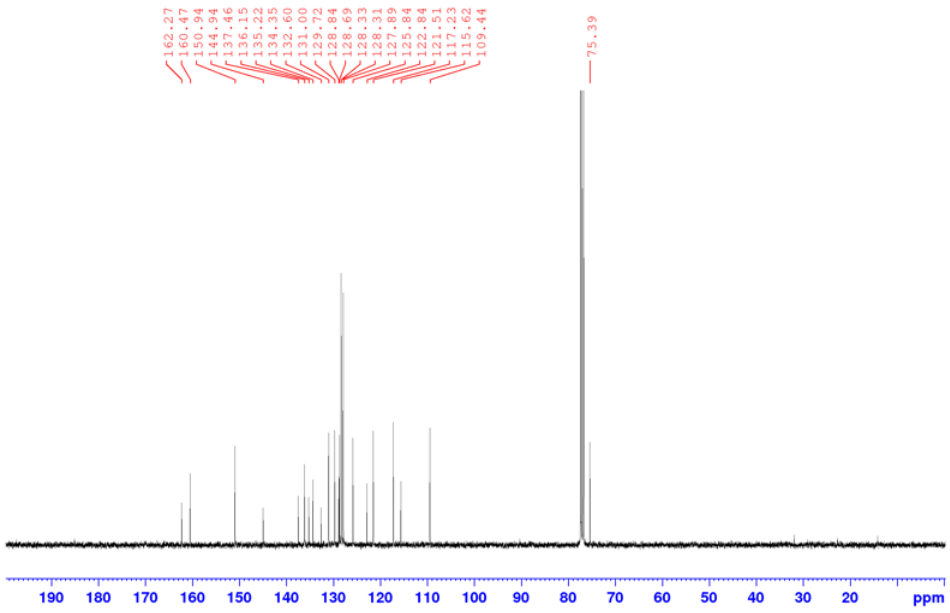


Figure S62: *^{13}C {^{1}H} NMR spectrum of compound **2a** in $CDCl_3$ at 298 K.*

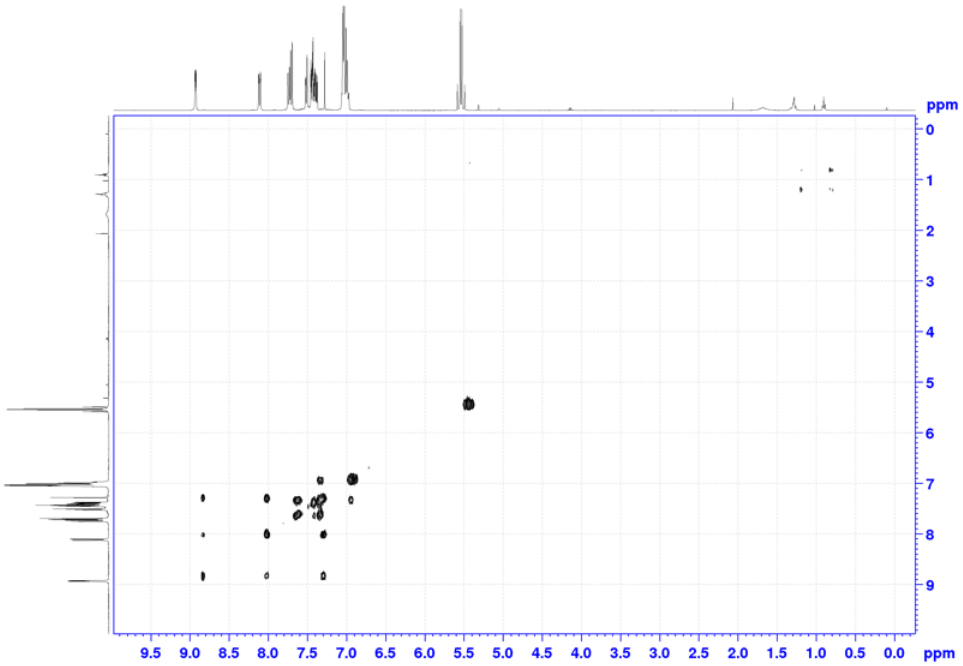


Figure S63: *COSY NMR spectrum of compound* ***2a*** *in $CDCl_3$ at 298 K.*

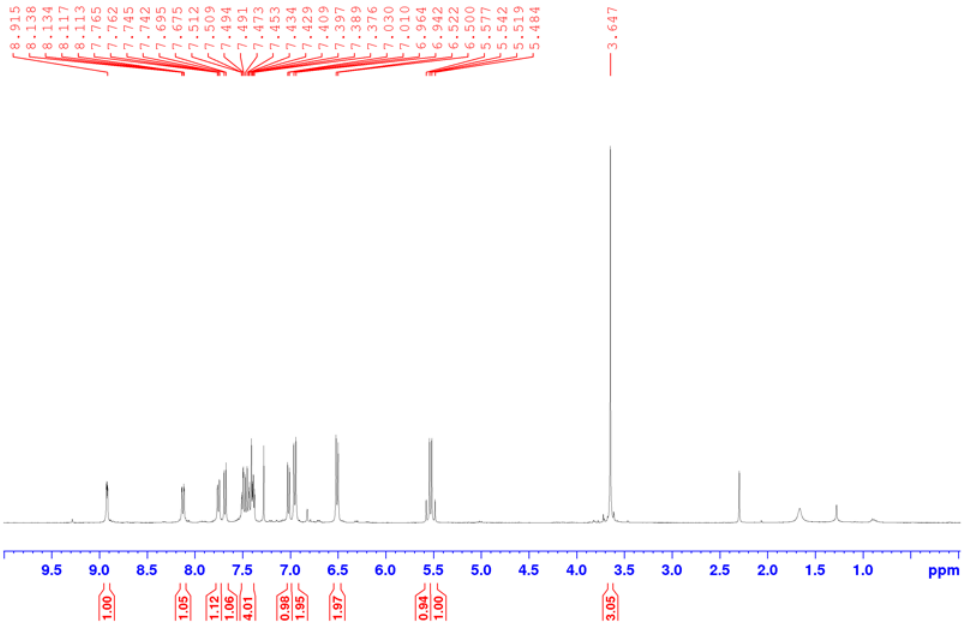


Figure S64: *^{1}H NMR spectrum of compound* ***2b*** *in $CDCl_3$ at 298 K.*

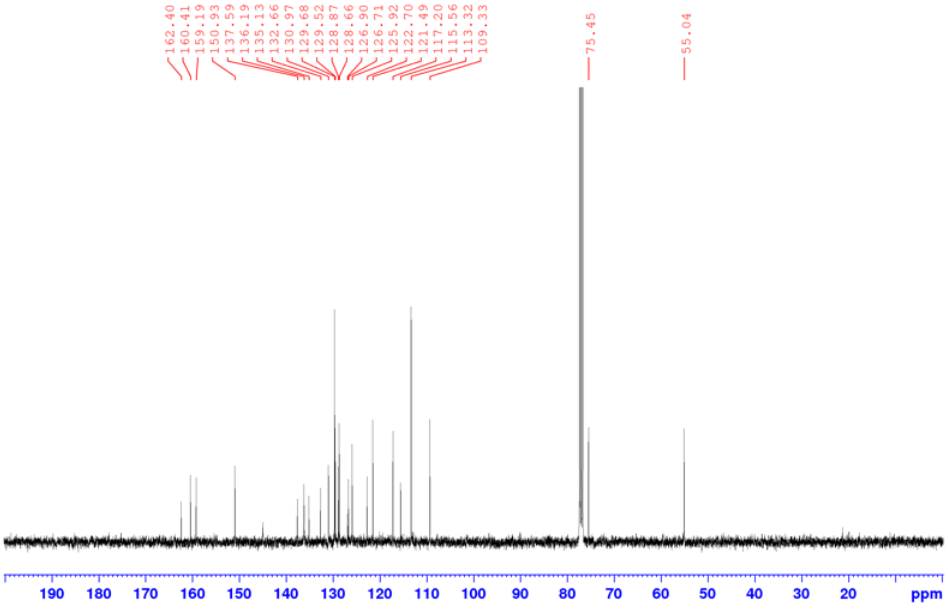


Figure S65: *^{13}C {^{1}H} NMR spectrum of compound* ***2b*** *in $CDCl_3$ at 298 K.*

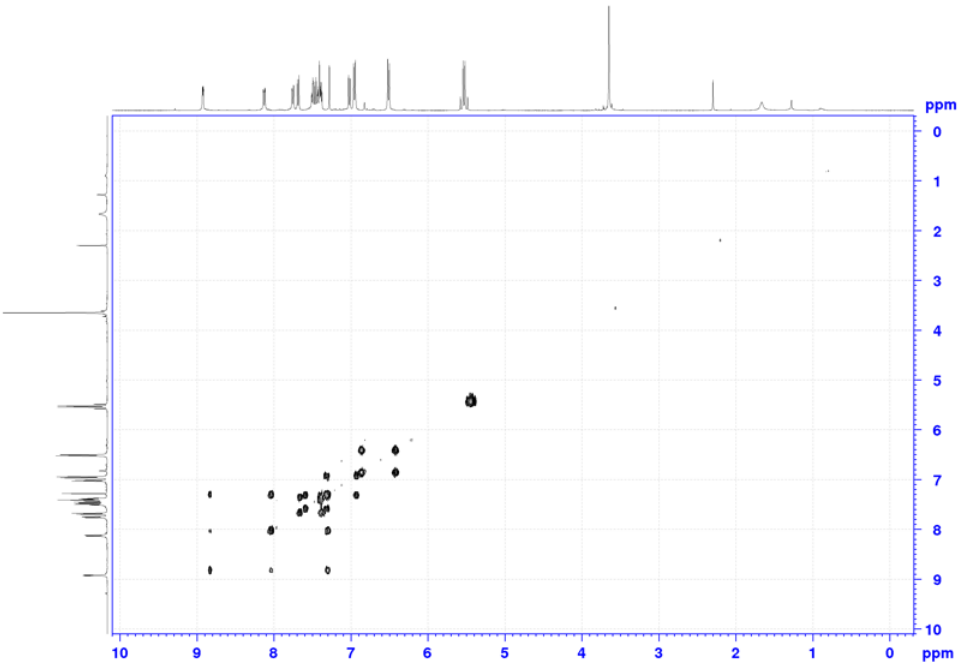


Figure S66: *COSY NMR spectrum of compound* ***2b*** *in $CDCl_3$ at 298 K.*

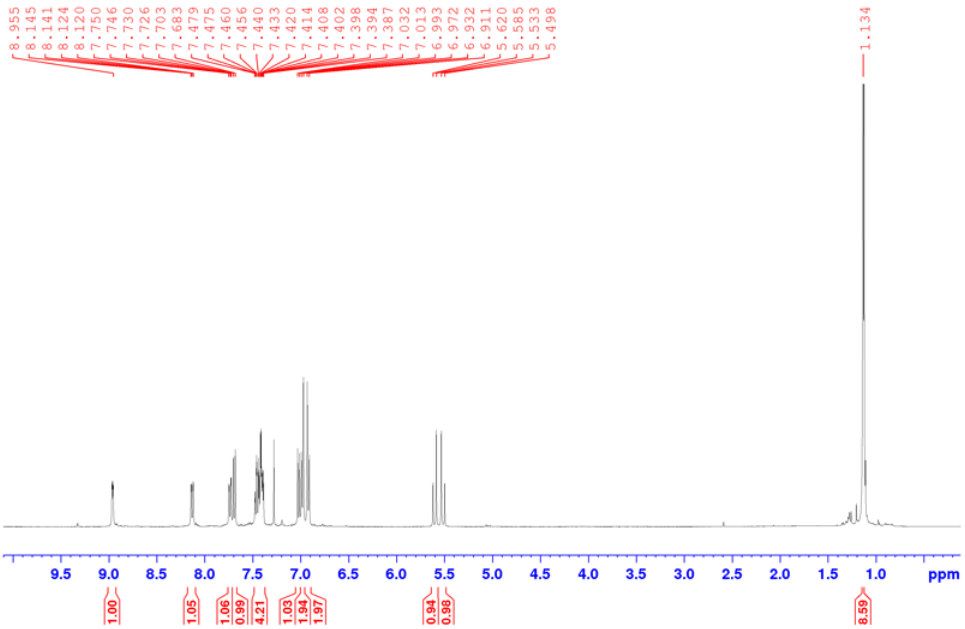


Figure S67: *^{1}H NMR spectrum of compound **2c** in $CDCl_3$ at 298 K.*

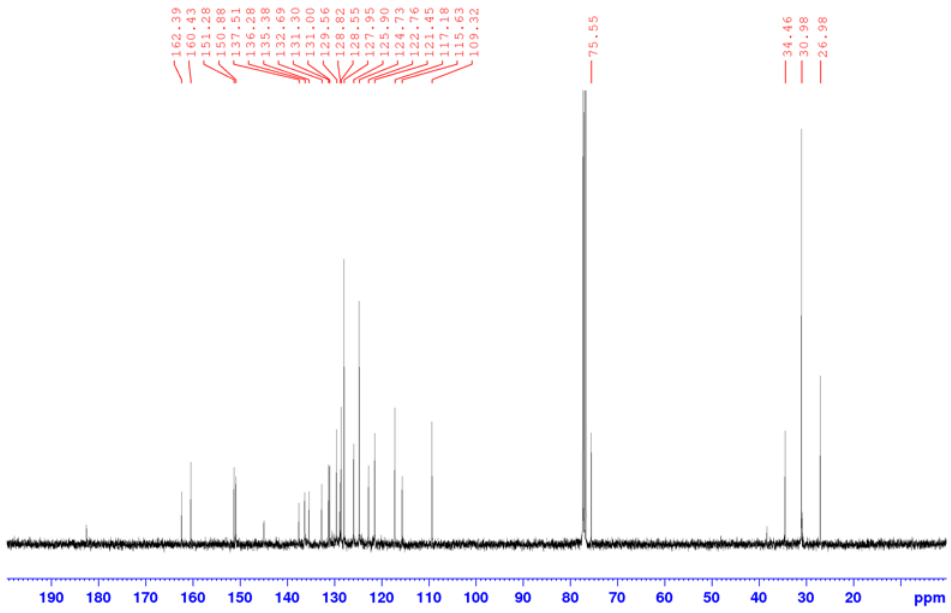


Figure S68: *^{13}C {^{1}H} NMR spectrum of compound **2c** in $CDCl_3$ at 298 K.*

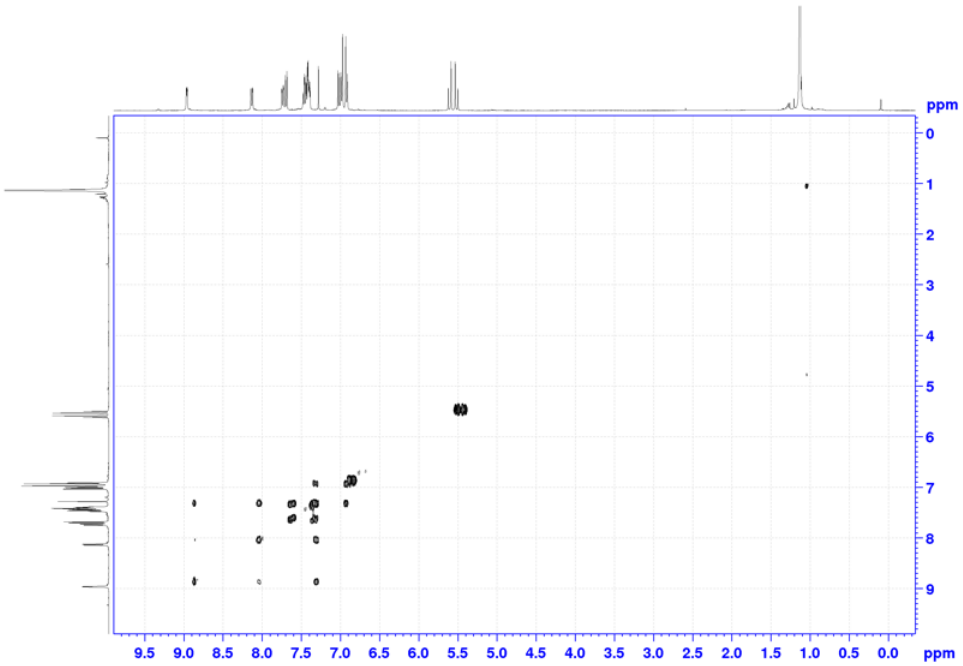


Figure S69: *COSY NMR spectrum of compound* ***2c*** *in $CDCl_3$ at 298 K.*

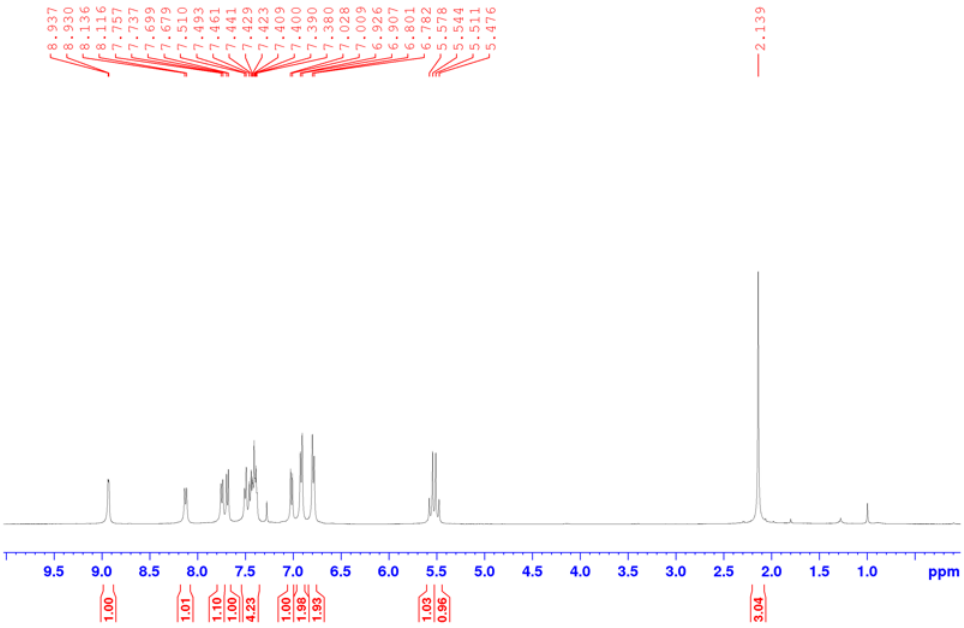


Figure S70: *^1H NMR spectrum of compound* ***2d*** *in $CDCl_3$ at 298 K.*

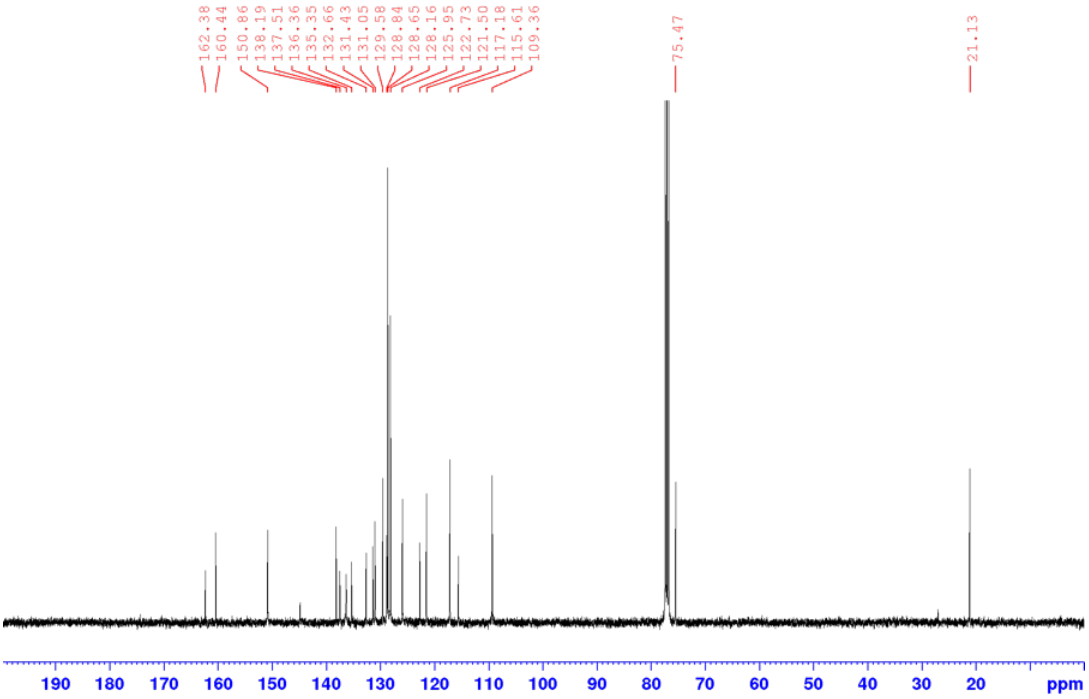


Figure S71: *^{13}C {^{1}H} NMR spectrum of compound **2d** in $CDCl_3$ at 298 K.*

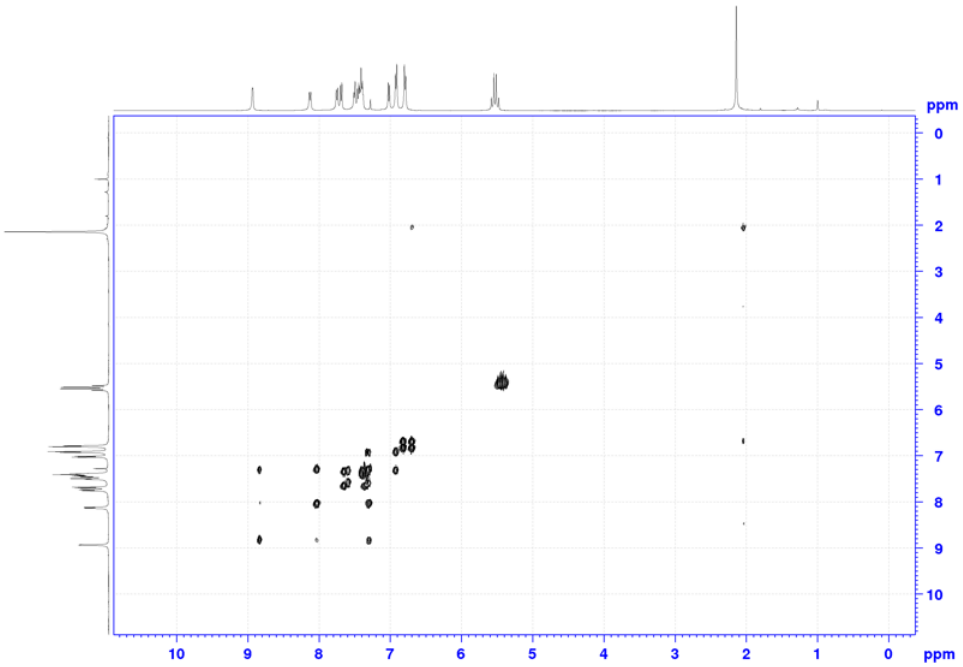


Figure S72: *COSY NMR spectrum of compound **2d** in $CDCl_3$ at 298 K.*

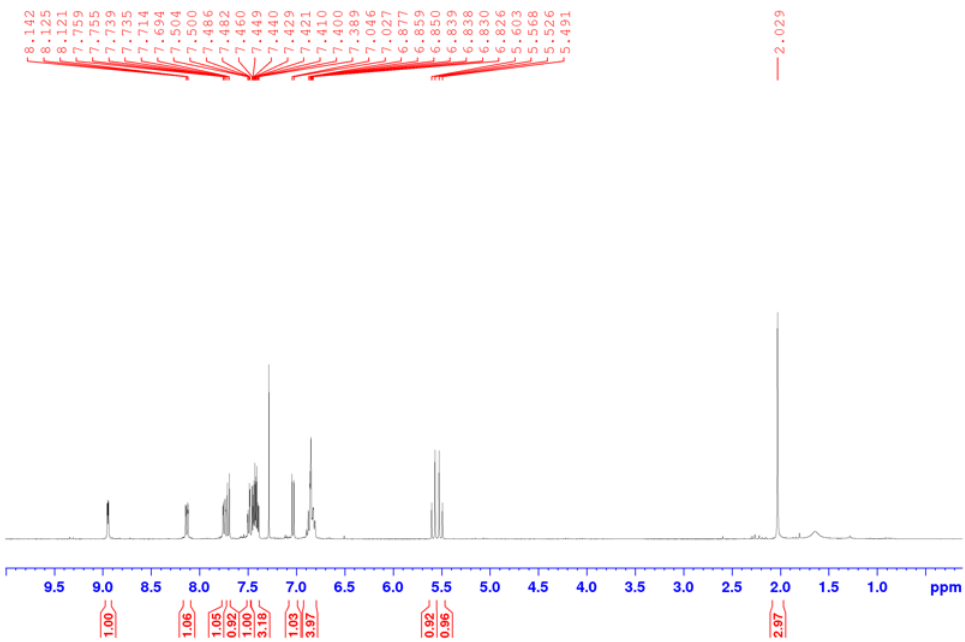


Figure S73: *^{1}H NMR spectrum of compound **2e** in $CDCl_3$ at 298 K.*

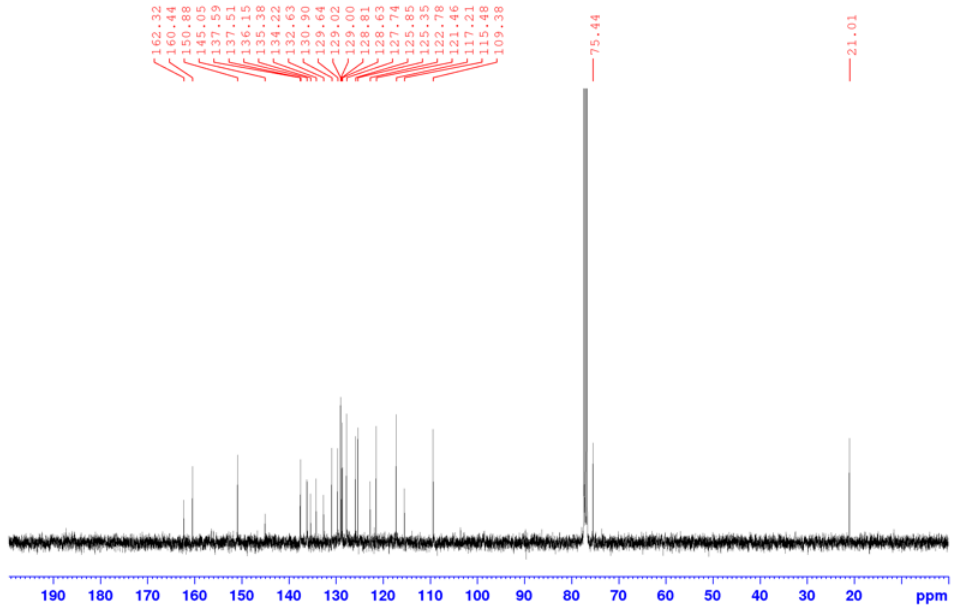


Figure S74: *$^{13}C\{^{1}H\}$ NMR spectrum of compound **2e** in $CDCl_3$ at 298 K.*

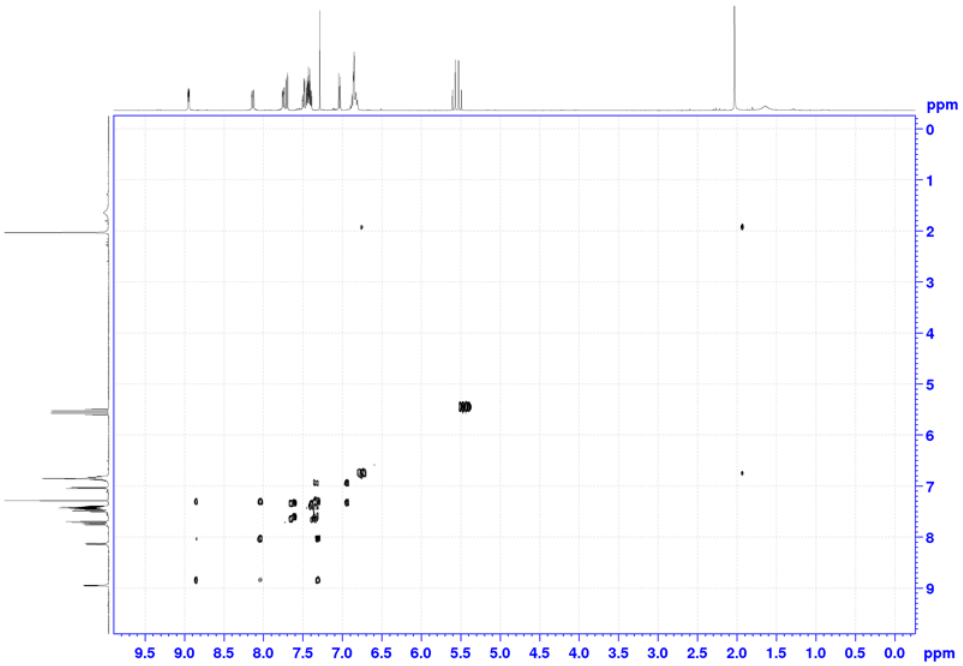


Figure S75: *COSY NMR spectrum of compound* ***2e*** *in* $CDCl_3$ *at 298 K.*

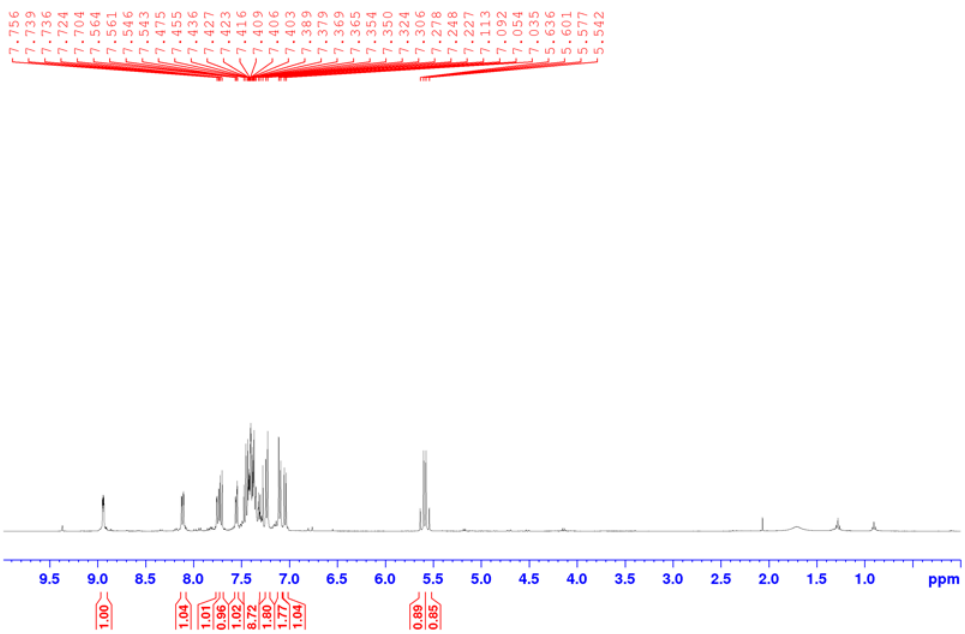


Figure S76: *^{1}H NMR spectrum of compound* ***2f*** *in* $CDCl_3$ *at 298 K.*

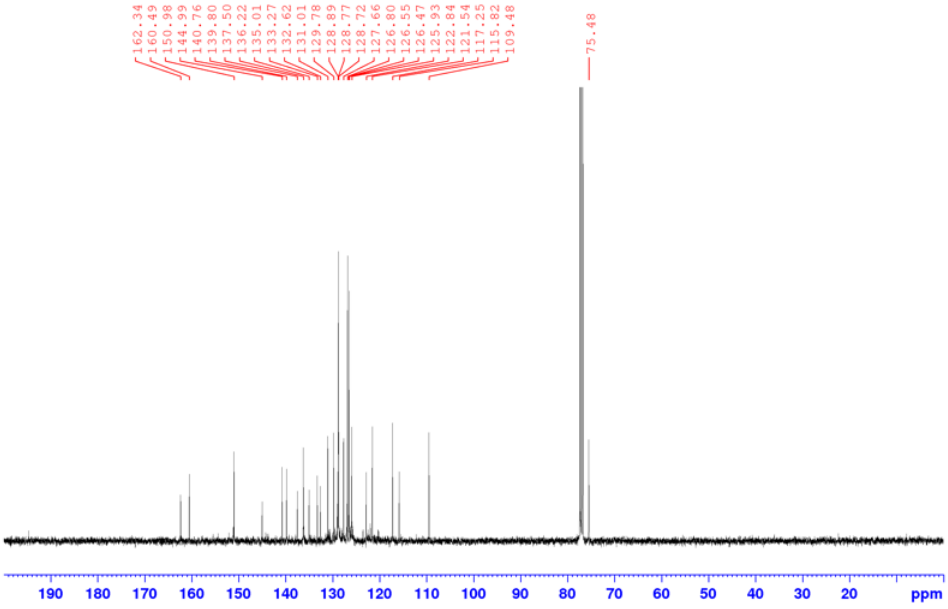


Figure S77: *^{13}C {^{1}H} NMR spectrum of compound **2f** in $CDCl_3$ at 298 K.*

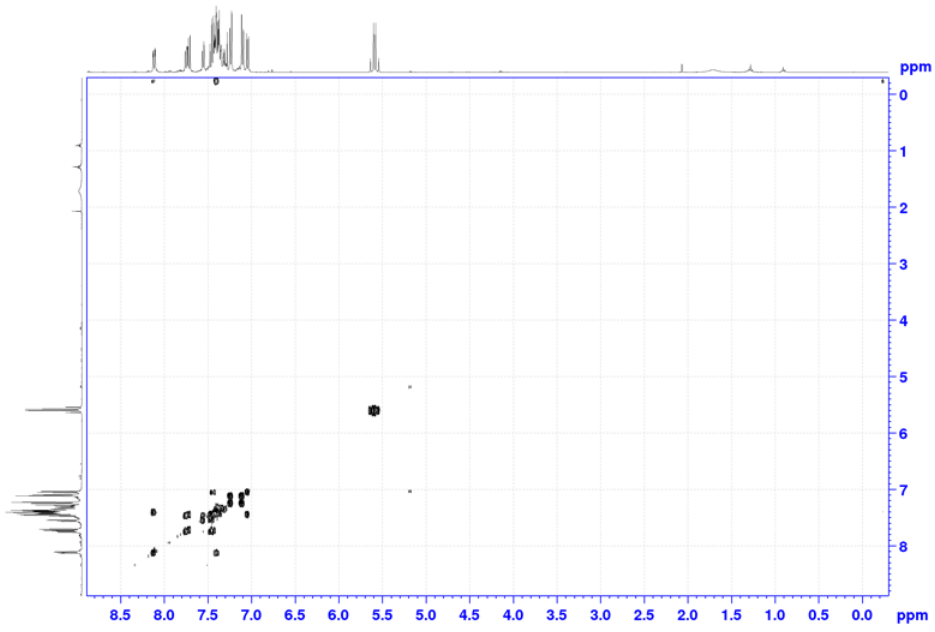


Figure S78: *COSY NMR spectrum of compound **2f** in $CDCl_3$ at 298 K.*

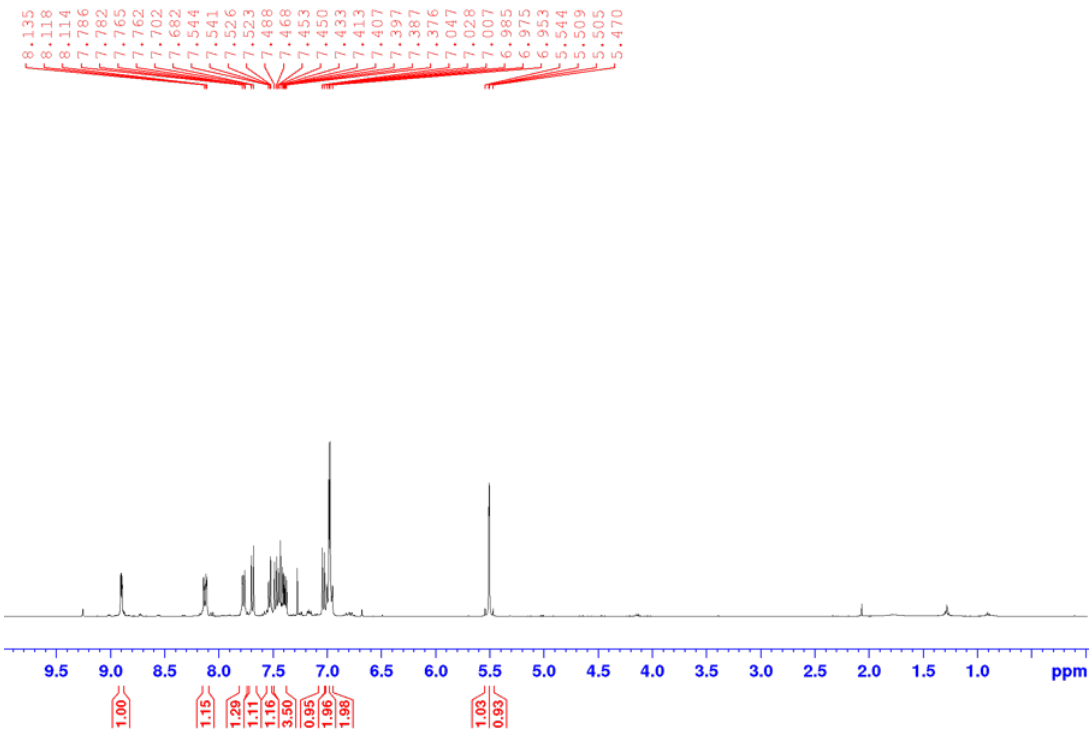


Figure S79: *^{1}H NMR spectrum of compound **2g** in $CDCl_3$ at 298 K.*

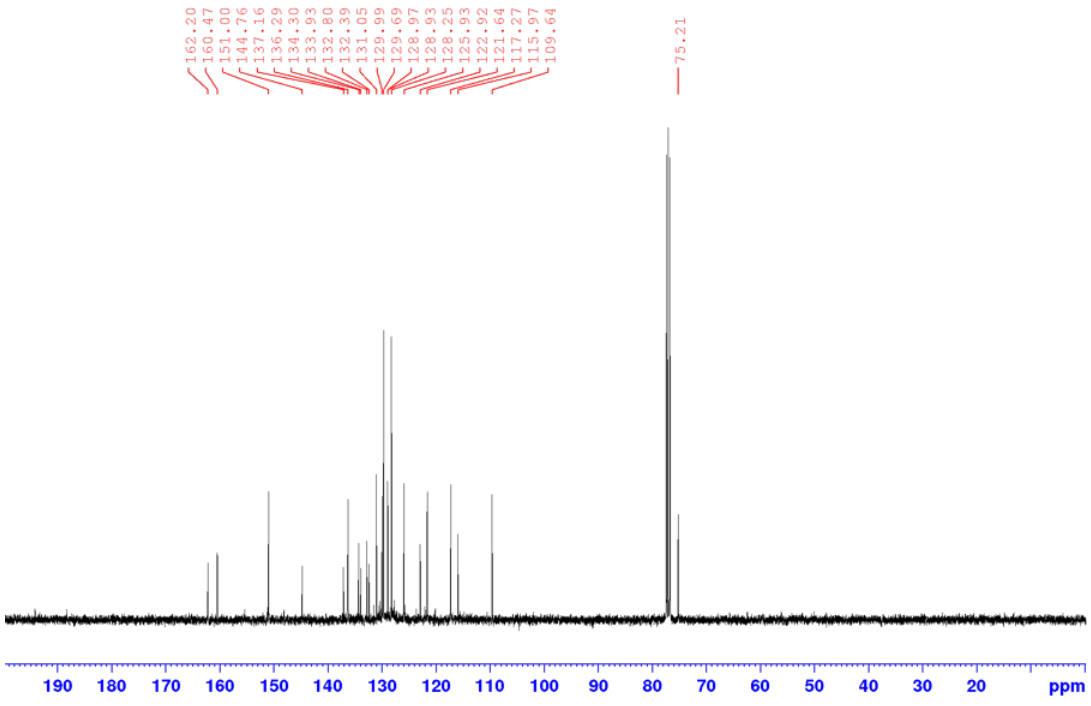


Figure S80: *^{13}C {^{1}H} NMR spectrum of compound **2g** in $CDCl_3$ at 298 K.*

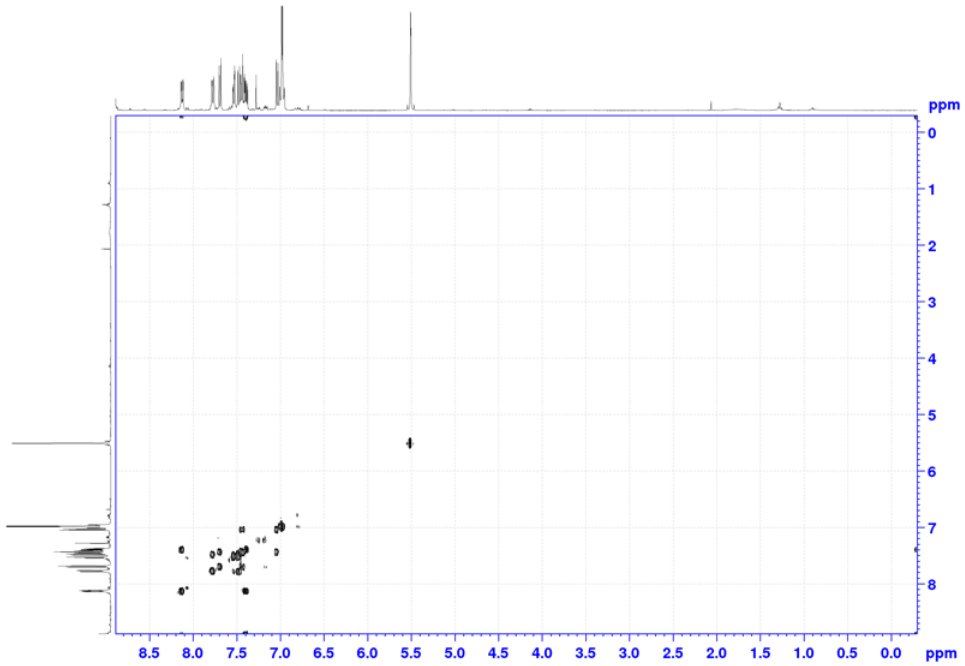


Figure S81: *COSY NMR spectrum of compound* ***2g*** *in* $CDCl_3$ *at 298 K.*

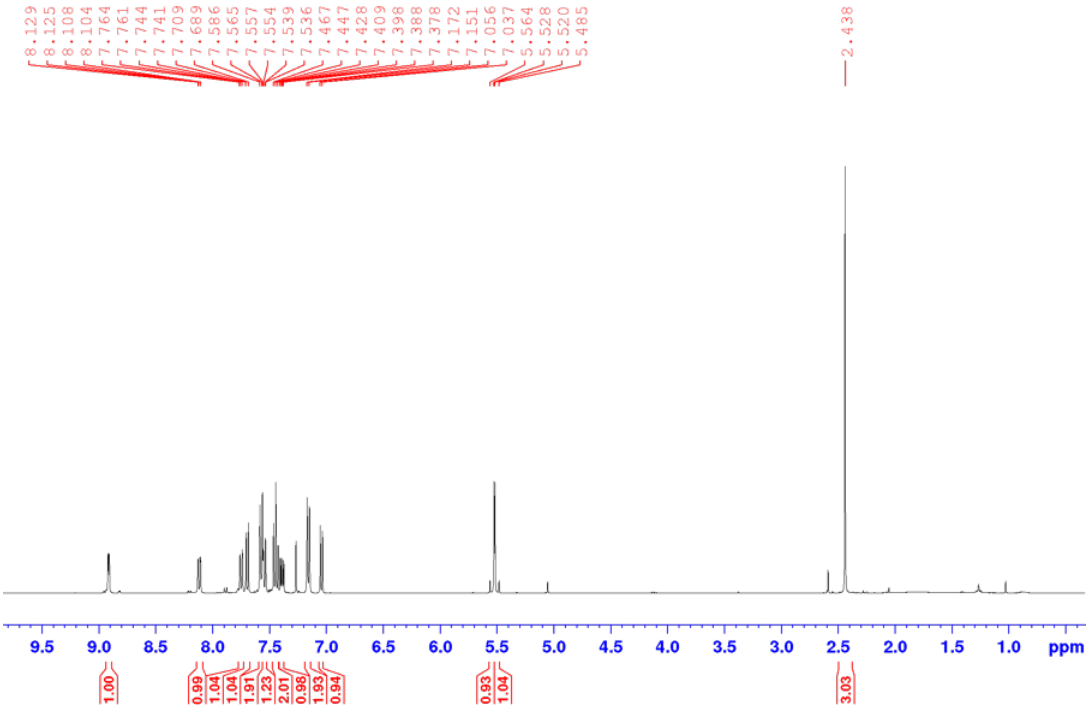


Figure S82: *^{1}H NMR spectrum of compound* ***2h*** *in* $CDCl_3$ *at 298 K.*

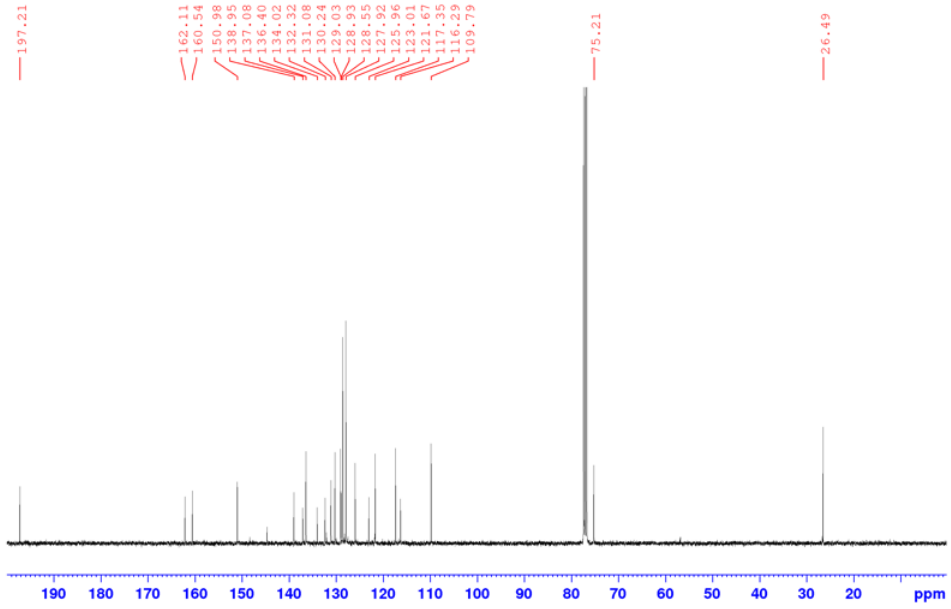


Figure S83: *^{13}C {^{1}H} NMR spectrum of compound* ***2h*** *in $CDCl_3$ at 298 K.*

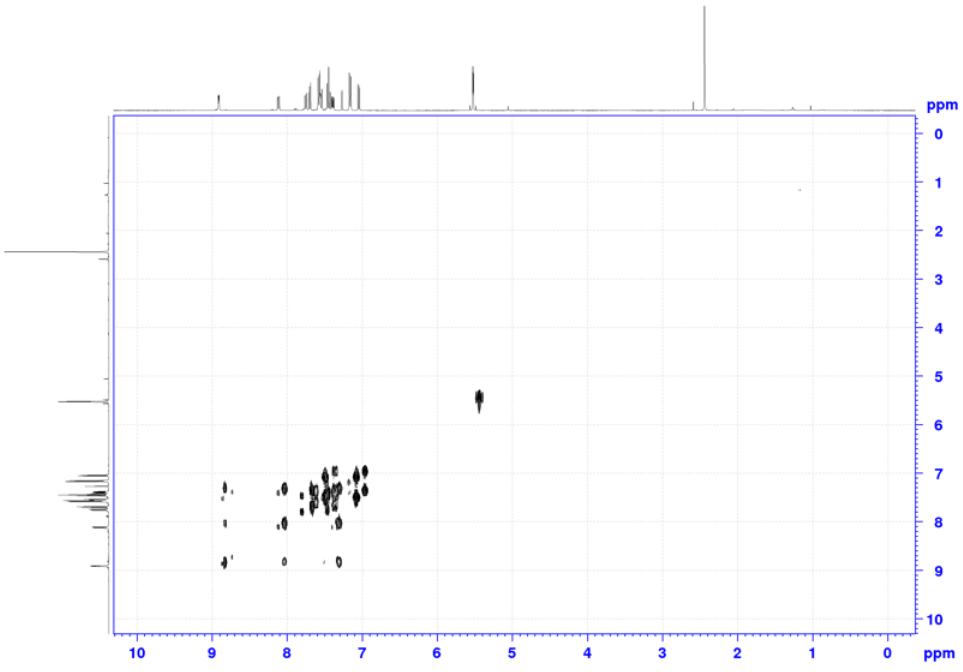


Figure S84: *COSY NMR spectrum of compound* ***2h*** *in $CDCl_3$ at 298 K.*

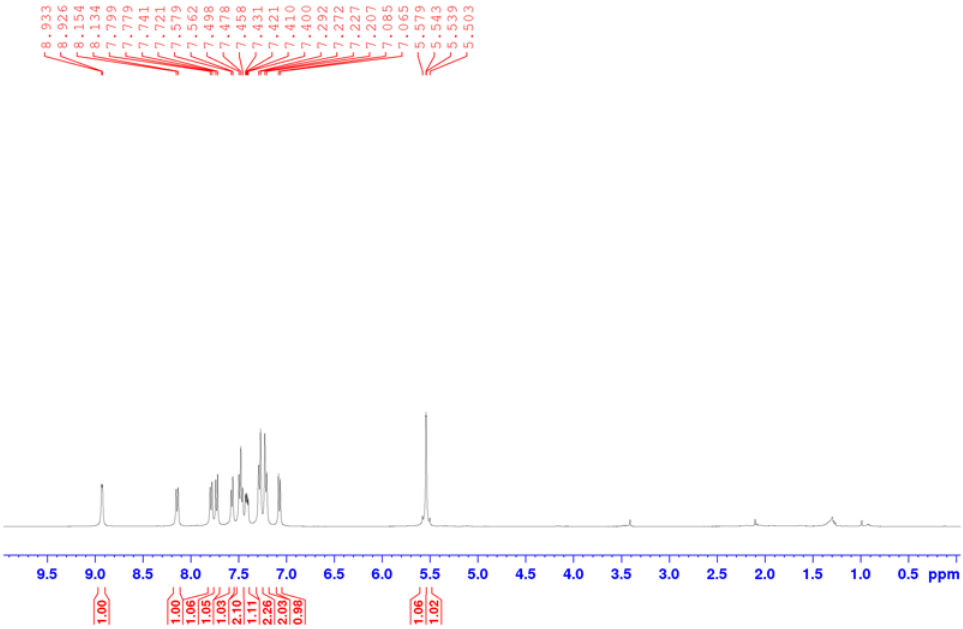


Figure S85: *^{1}H NMR spectrum of compound **2i** in $CDCl_3$ at 298 K.*

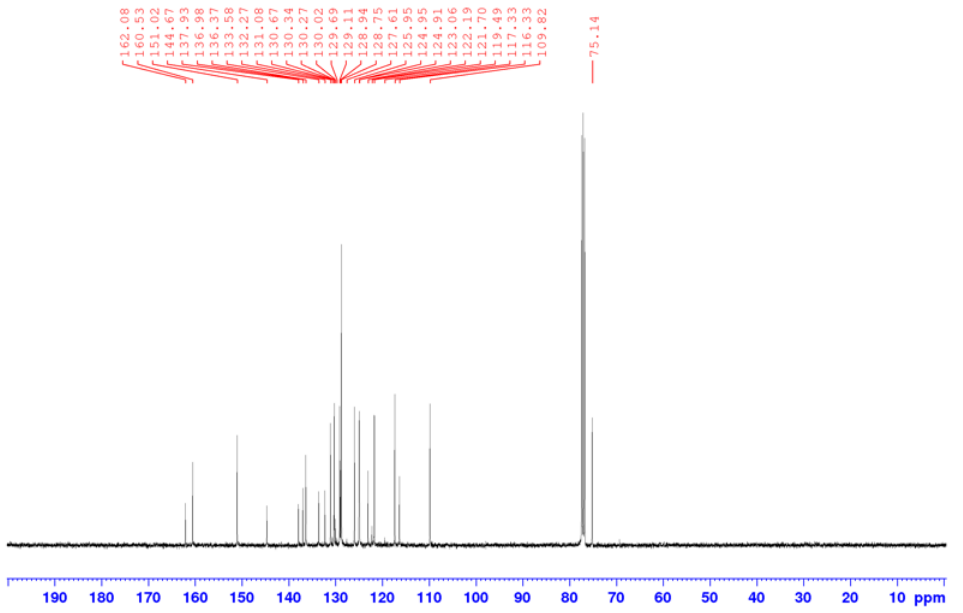


Figure S86: *^{13}C {^{1}H} NMR spectrum of compound **2i** in $CDCl_3$ at 298 K.*

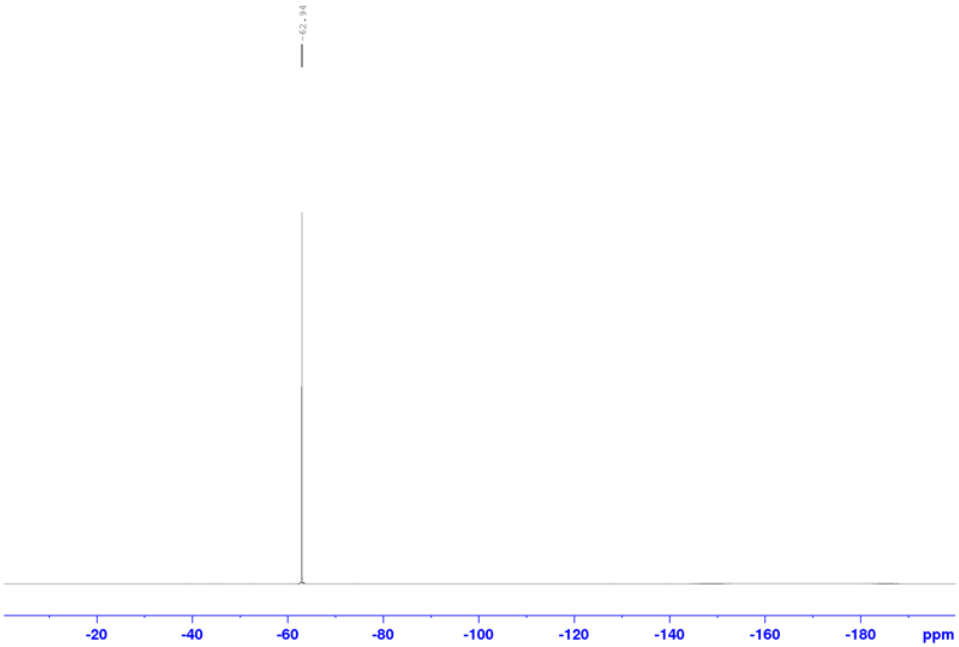


Figure S87: *^{19}F {^{1}H} NMR spectrum of compound **2i** in $CDCl_3$ at 298 K.*

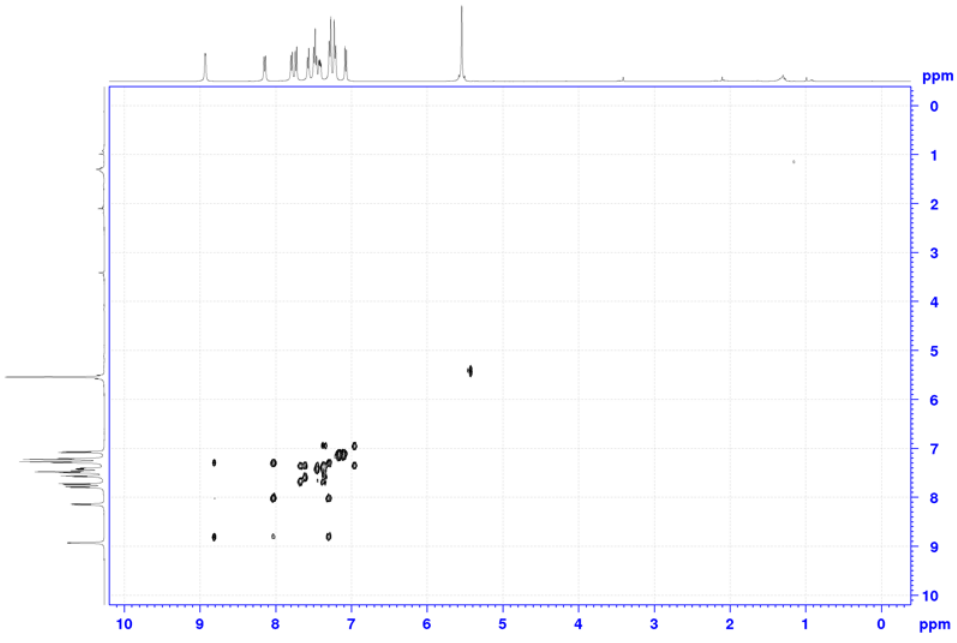


Figure S88: *COSY NMR spectrum of compound **2i** in $CDCl_3$ at 298 K.*

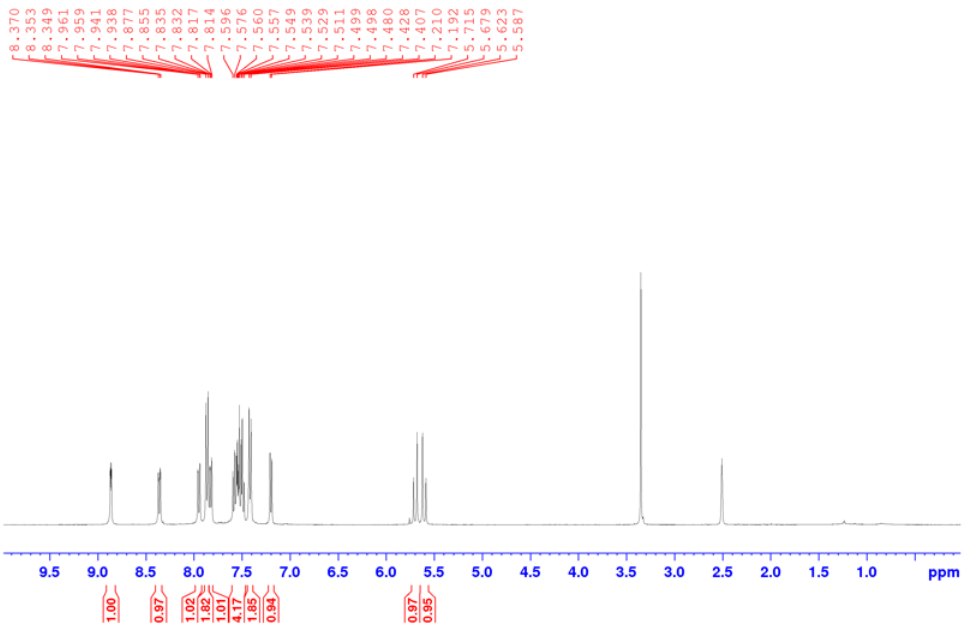


Figure S89: *^{1}H NMR spectrum of compound* ***2j*** *in* d_6-DMSO *at 298 K.*

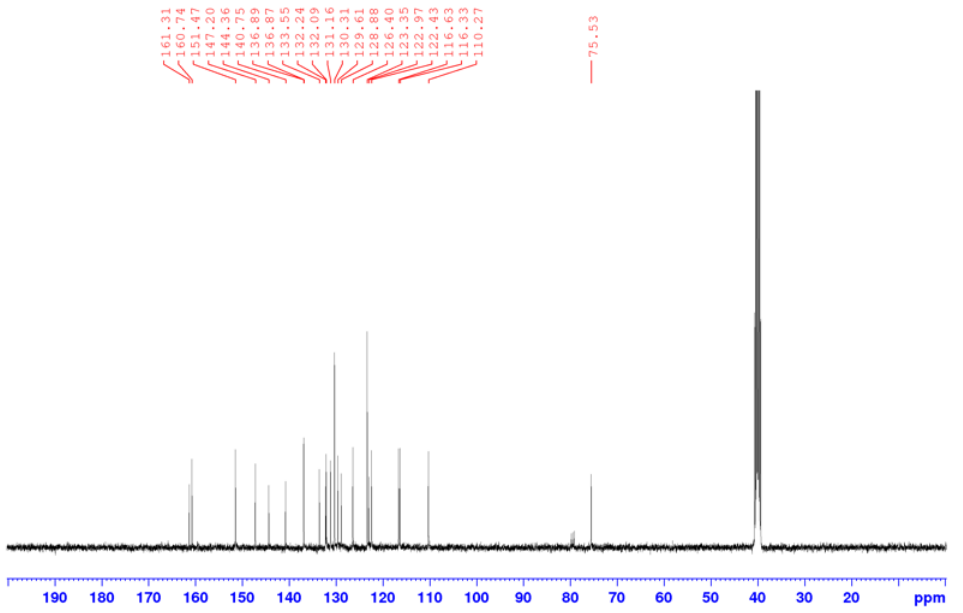


Figure S90: *^{13}C {^{1}H} NMR spectrum of compound* ***2j*** *in* d_6-DMSO *at 298 K.*

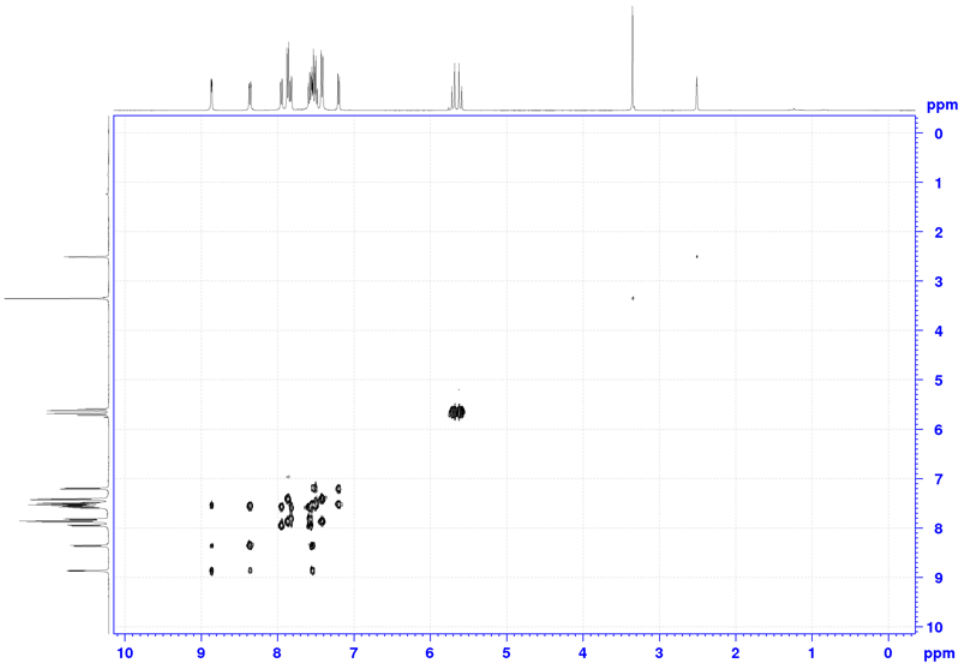


Figure S91: *COSY NMR spectrum of compound* ***2j*** *in* d_6-DMSO *at 298 K.*

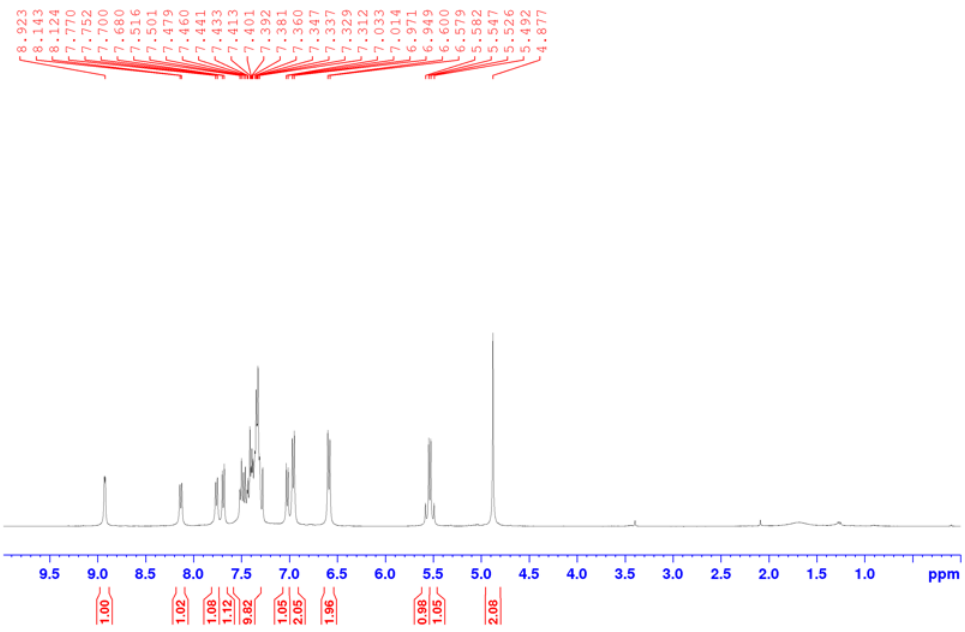


Figure S92: *^{1}H NMR spectrum of compound* ***2l*** *in $CDCl_3$ at 298 K.*

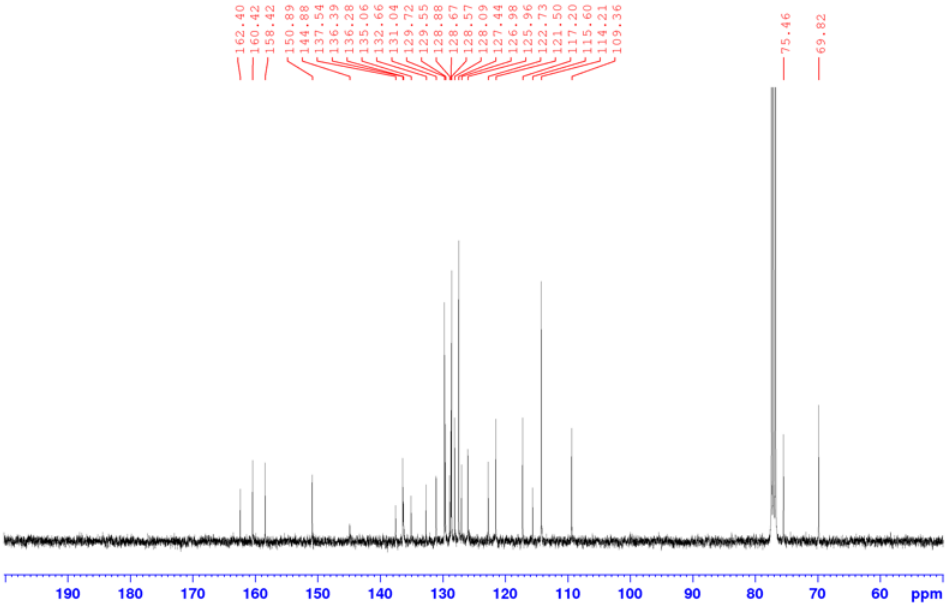


Figure S93: *^{13}C {^{1}H} NMR spectrum of compound **2l** in $CDCl_3$ at 298 K.*

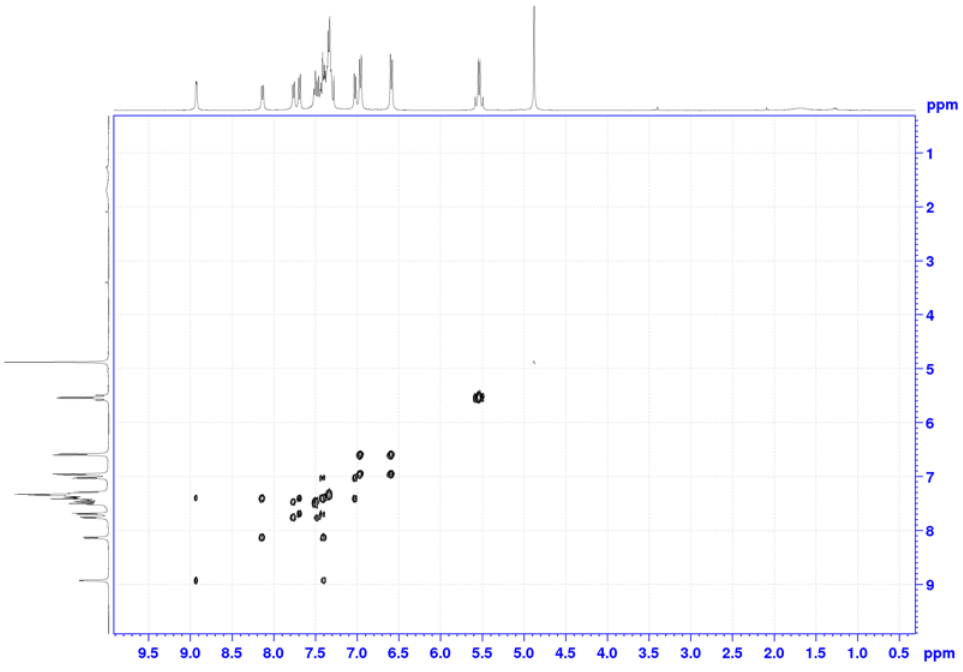


Figure S94: *COSY NMR spectrum of compound **2l** in $CDCl_3$ at 298 K.*

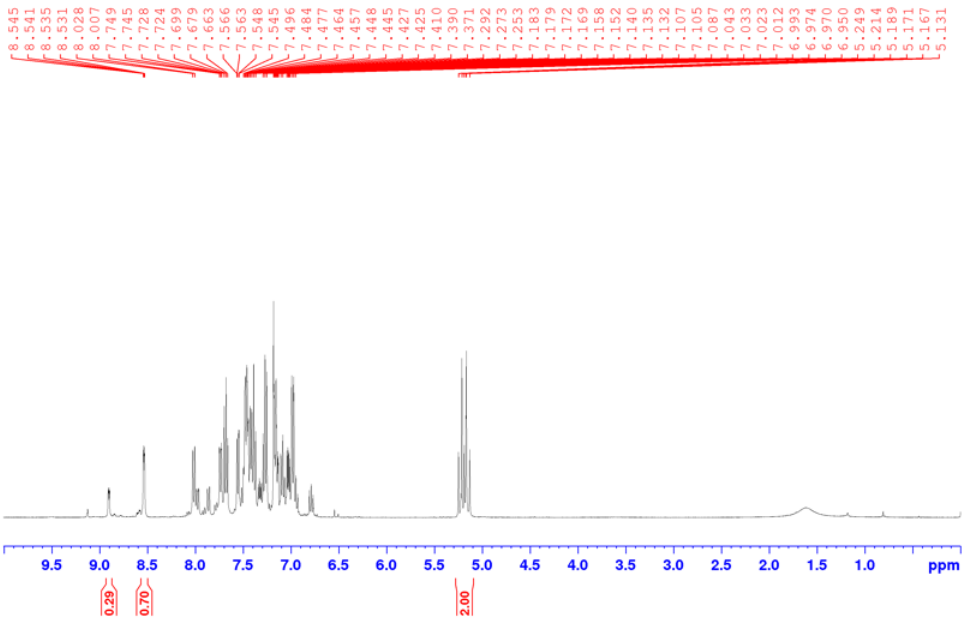


Figure S95: *^{1}H NMR spectrum of compound **2m** in $CDCl_3$ at 298 K.*

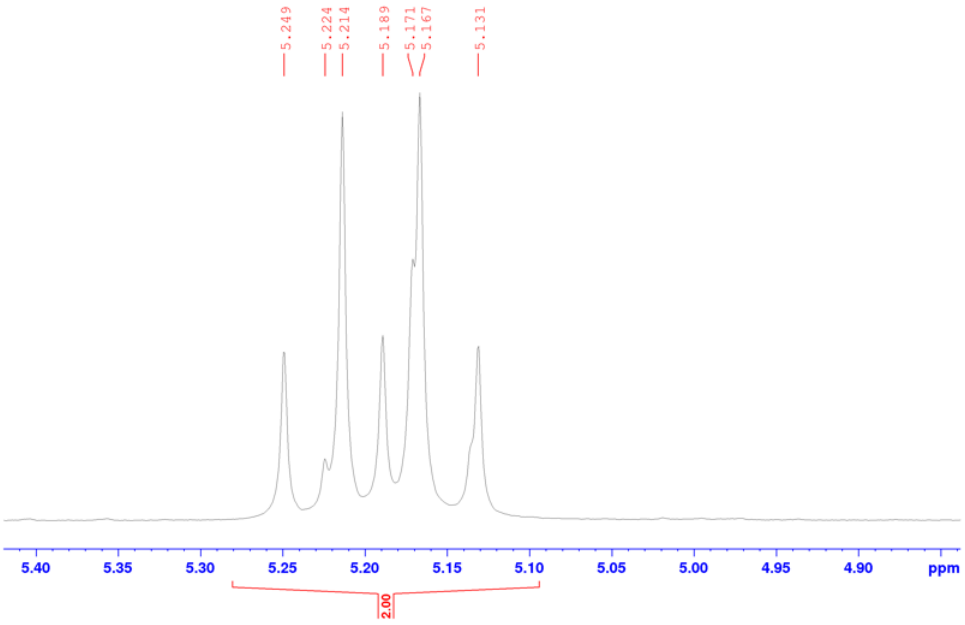


Figure S96: *^{1}H NMR spectrum of compound **2m** in $CDCl_3$ at 298 K.*

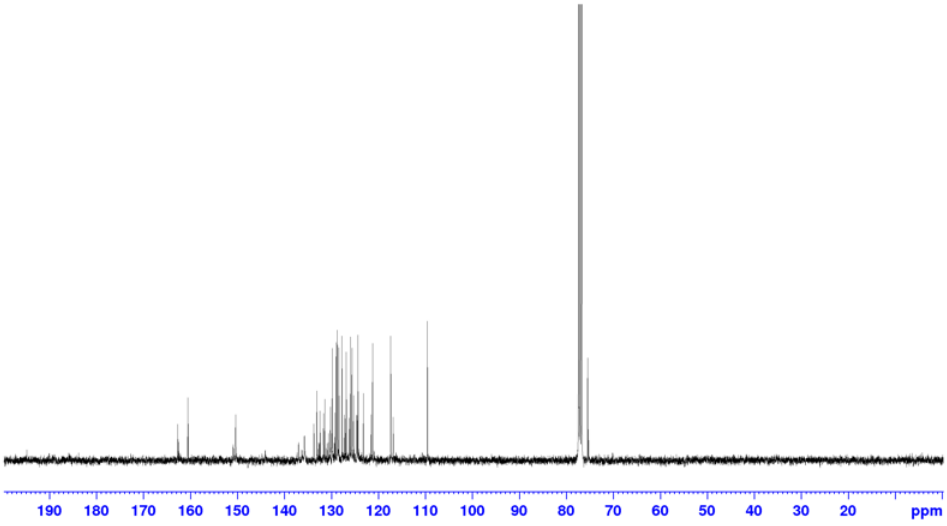


Figure S97: *^{13}C {^{1}H} NMR spectrum of compound* ***2m*** *in $CDCl_3$ at 298 K.*

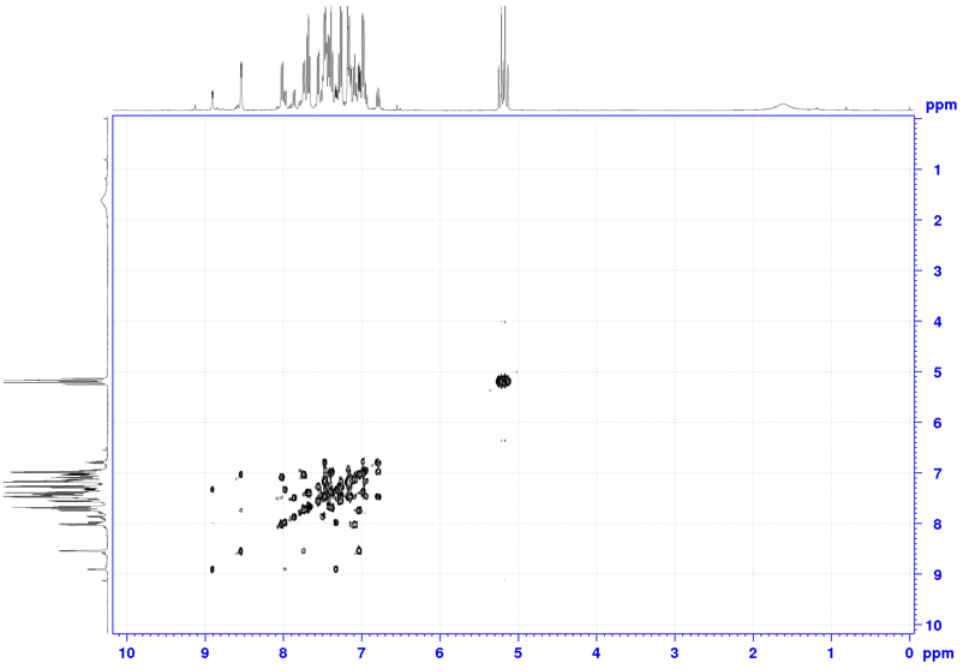


Figure S98: *COSY NMR spectrum of compound* ***2m*** *in $CDCl_3$ at 298 K.*

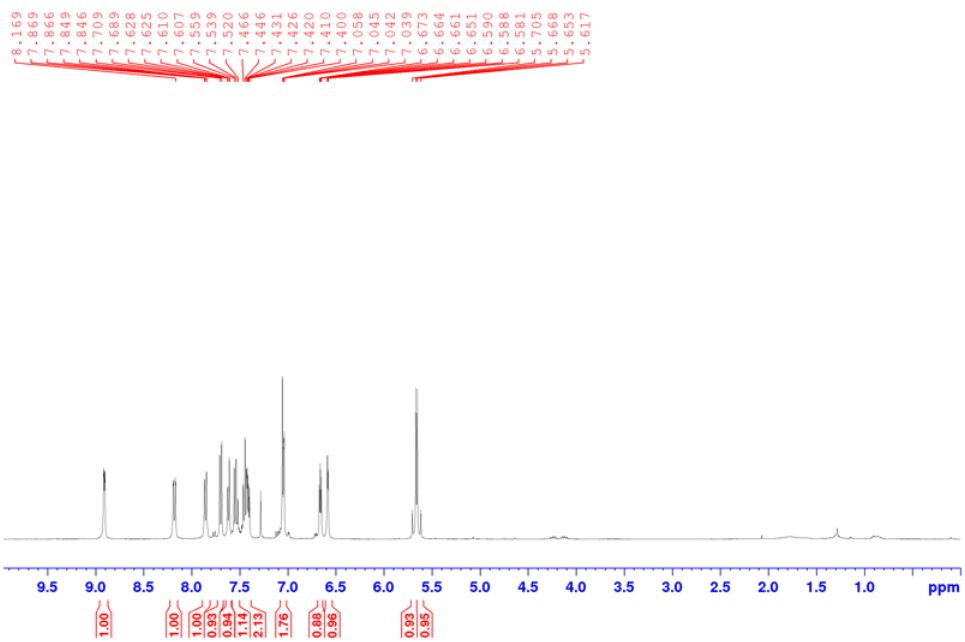


Figure S99: *^{1}H NMR spectrum of compound **2n** in $CDCl_3$ at 298 K.*

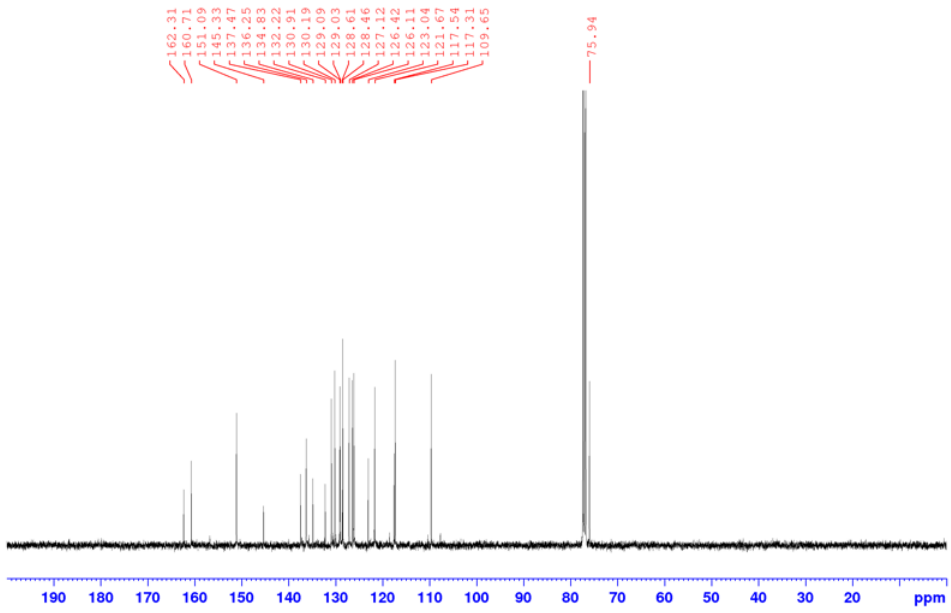


Figure S100: *^{13}C {^{1}H} NMR spectrum of compound **2n** in $CDCl_3$ at 298 K.*

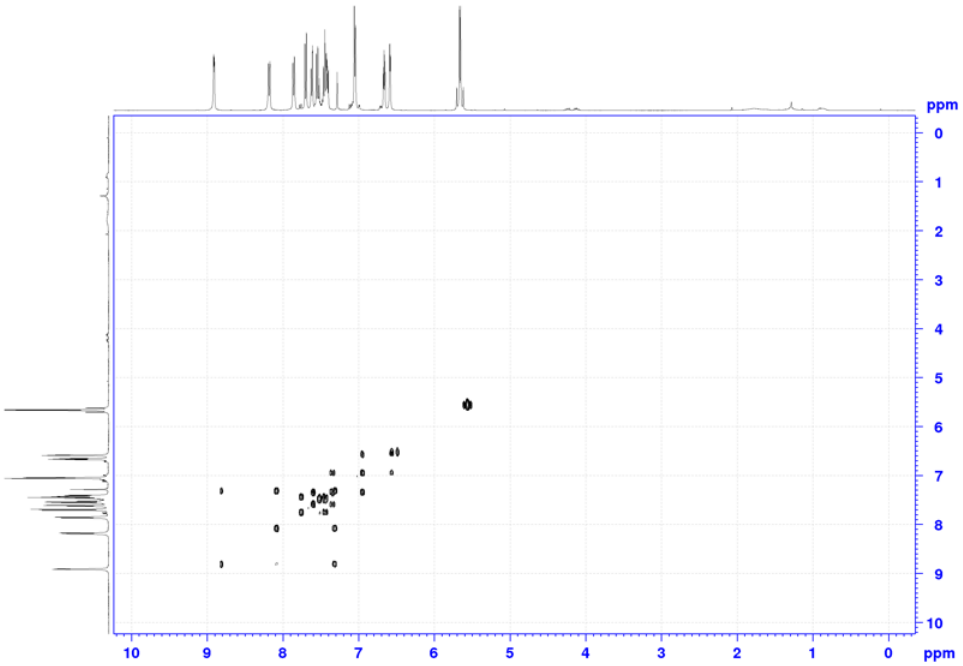


Figure S101: *COSY NMR spectrum of compound* ***2n*** *in* $CDCl_3$ *at 298 K.*

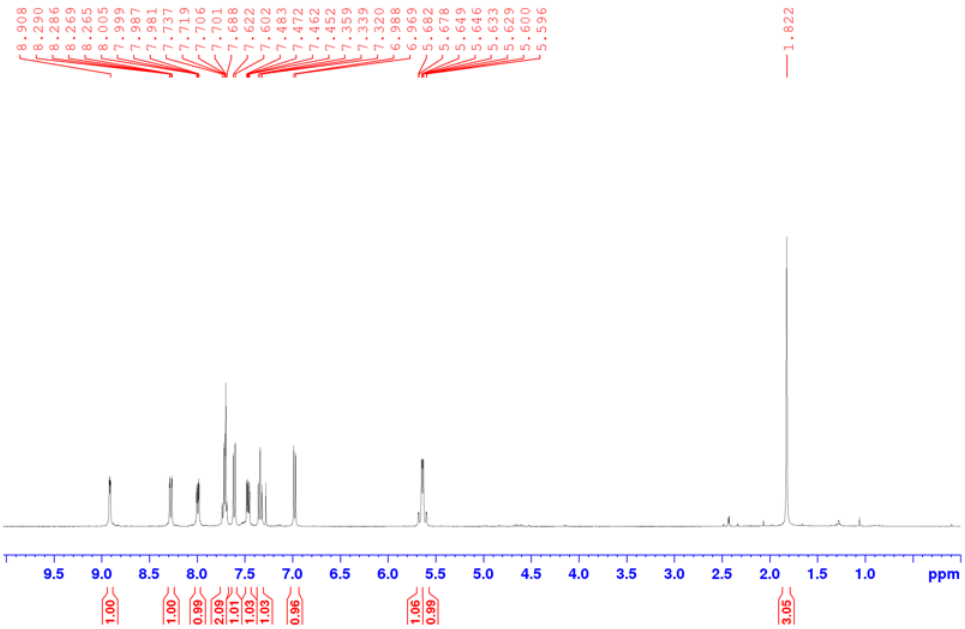


Figure S102*:* ^1H *NMR spectrum of compound* ***2p*** *in* $CDCl_3$ *at 298 K.*

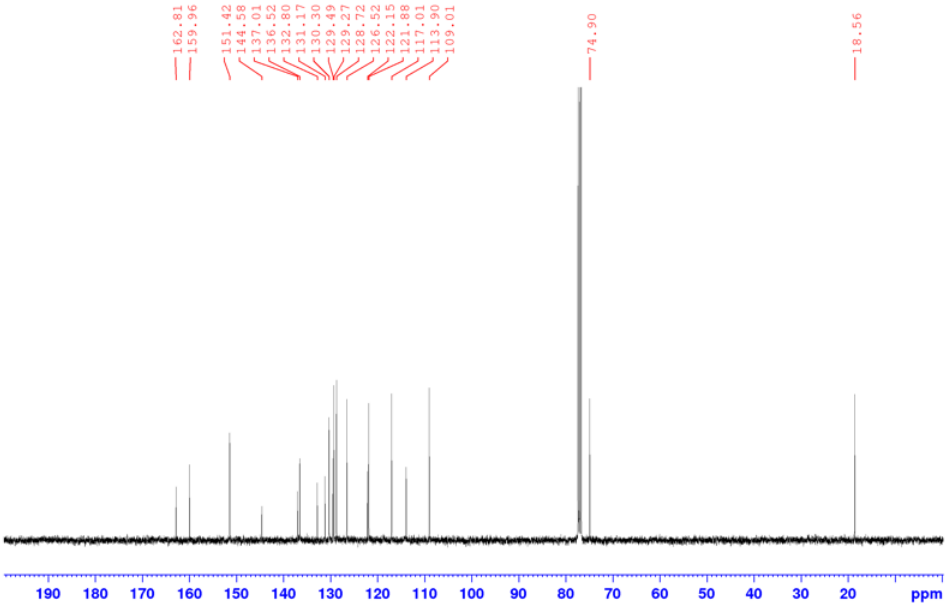


Figure S103: *^{13}C {^{1}H} NMR spectrum of compound* ***2p*** *in $CDCl_3$ at 298 K.*

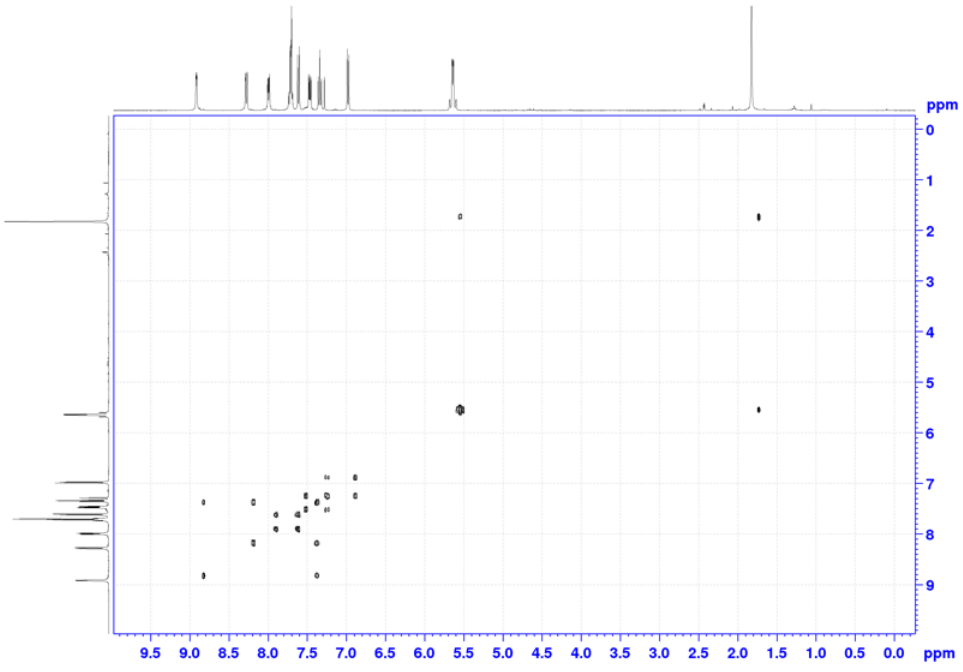


Figure S104: *COSY NMR spectrum of compound* ***2p*** *in $CDCl_3$ at 298 K.*

[7] Structure Coordinates from Computational Study:

Structure Coordinates

Cu(AcO)

C	2.50933686635251	-1.64223063596847	-1.56411691514006
O	1.70184869222216	-1.93291022430620	-2.49166972128398
O	2.13383281604602	-1.03286708446876	-0.52414185277730
Cu	0.26021397950846	-0.97271995552303	-1.37958252713689
C	3.95049463471364	-2.04615159521123	-1.69071302765958
H	4.56868724036999	-1.49805558530093	-0.98424216548521
H	4.29625780024634	-1.88130293551538	-2.71127264774117
H	4.03202490900506	-3.11462496647735	-1.47357295612496

$Cu(AcO)_2$

C	2.50895792048560	-1.68386755752670	-1.55132915800473
O	1.66030451578597	-1.96050727926118	-2.45211296027883
O	2.09534442397231	-1.06928754969619	-0.52447230391653
Cu	0.34527235342112	-0.91337586340387	-1.41700921095301
C	3.94645729516147	-2.04665329096367	-1.69125656833390
H	4.54799253211264	-1.47869565151063	-0.98518304952652
H	4.27690073106124	-1.85601092049497	-2.71284707375144
H	4.07146716646382	-3.11246486991414	-1.48510148858419
C	-1.69945673468762	0.14801883193868	-1.38468217981353
O	-0.85286104116666	0.31425833880740	-0.45794142172367
O	-1.39636040805441	-0.65667349316127	-2.31533059844420
C	-3.00667869749271	0.86146139394527	-1.37261703733354
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TFE

C	0.48075933126383	-0.59632083953210	-0.42241083905197
F	1.33398067801528	-0.95479473855884	0.55381258623068
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C	-0.64984470259147	0.25844847329980	0.11611446740470
H	-1.16420794033466	-0.33078433124931	0.88537769540939
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O	-0.21783648342866	1.50238565858896	0.57392464756912
H	0.37820162471070	1.37741598093379	1.31745536661848

AcOH

C	-0.53641046129509	0.10868583410063	-0.20728986260227
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O	-1.06536356616577	-0.94784158441634	0.43966998763340
H	-2.00674536933645	-0.96146885497118	0.21605561524205
C	0.92947855119091	0.23096626492270	0.06053481095968
H	1.43069567658622	-0.68645014900809	-0.25476831660435
H	1.10739682217660	0.34610955690419	1.13160366077755

H	1.33549592581304	1.08046515854192	-0.48002263509000

AcO

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H	1.16493084444664	0.40322720722317	1.12063502470831
H	1.32011794158585	1.06584740235233	-0.52845200161361

A

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C	2.61078686138022	-3.39189246902562	0.29566751890386
Cu	-0.69768592739387	-1.53780150350602	1.91290442995248
H	0.54232615646608	-3.87760254137480	3.50071699909345
H	2.57039187116682	-5.29781469381036	3.11367830335213
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O	-4.93657849441950	-2.97006732301775	1.20594810483692
C	-4.12016246194438	-3.59627996405905	2.17829802312407
H	-3.64035521171931	-2.83687257904242	2.80983125505830
H	-4.80767084110870	-4.16928146938834	2.80447336003868
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C	1.14372819238982	-7.11568654443031	-0.44309602264310
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H	2.00400746576552	-7.61686336817635	-0.87131320879605
H	1.13727349838260	-5.53408797643739	-1.89893456121071
H	-0.82516087550994	-4.40246555906238	-0.92277695224115
H	-2.37875360222108	-2.54464103168311	0.53338154439215
C	-1.92449855929476	-0.61606594494877	3.68130939810549
O	-1.76951496139044	0.02745030372082	2.61300150325100
O	-1.36570214870326	-1.75483235107231	3.78631357993834
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H	-3.19109819069037	-0.85509654677827	5.38554429304914
H	-3.50036605579566	0.61371142420300	4.39972026256253
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Ai

C	0.81590396469085	-1.17067710370243	-0.82951961039396
C	1.48070077835898	-0.31869570440489	-1.71191851798372
C	2.76522674931948	-0.64361841432700	-2.19802577124865
C	3.43680338810167	-1.78868216342023	-1.82517551366554
H	4.38961698124232	-4.16208177609936	-0.79563296944758
C	3.40657625171447	-3.86426095595612	-0.41933634695685
C	2.74264570660415	-4.64778935784800	0.50147727990597
C	1.47265923847353	-4.24122956797663	0.95060375929150
N	0.90668527775327	-3.14061233222288	0.49560454104295
C	1.53053206676238	-2.34121707339814	-0.40478681683452
C	2.82400527231333	-2.66652553165025	-0.89942701342376
Cu	-0.82548666099378	-2.38164748678960	1.05136741190996
H	0.89563486470571	-4.81604562918749	1.68181883278098
H	3.18269837001972	-5.56850761554825	0.88802991961847
H	3.23818702758684	0.05167425180441	-2.89717840948310
H	0.98469800613886	0.59721045401736	-2.02633116199933
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C	-1.34200764605779	-0.09799218685573	-0.76472945845242
O	-1.01718489942879	0.96117555178096	-1.27753572819353
C	-2.80270950206890	-0.42012457398083	-0.60721118324347
C	-3.30344745427481	-1.72370978394985	-0.74678848893457
C	-4.67643887991788	-1.93774004497945	-0.73409601297811
C	-5.57004940574437	-0.87477605393165	-0.57992266547005
C	-5.06879398743491	0.42500257232251	-0.43896076066334
C	-3.68757154360977	0.64178259704953	-0.46511979527531
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H	-5.07436191377628	-2.94655654048746	-0.87378975638332
H	-6.64349727655478	-1.07338065023387	-0.58306979435763
H	4.42687098073003	-2.02421635254466	-2.22084769474330
C	-8.24241637203786	3.90944106460002	-0.32288406765919
C	-7.78683421055803	2.78401931509062	-0.33223159650439
O	-5.82504518355317	1.53559735919674	-0.29654321978002
C	-7.22189939001376	1.44396924461370	-0.41031905743821
H	-7.50542788826328	0.98350916180144	-1.37836596160929
H	-7.64466282196905	0.80311466038143	0.38883053929555
C	-8.73942104741056	5.24919009117641	-0.31927477273615
C	-10.11703471732471	5.51241083635063	-0.41223757150183
C	-10.58288943597098	6.82366589940498	-0.41450544809279
C	-9.68825606931776	7.88938926636335	-0.32448849583801

C	-8.31947988970761	7.63728565871007	-0.23194362065701
C	-7.84445329413506	6.33007313911892	-0.22943995653802
H	-10.81553079428512	4.67632193660408	-0.48569126542590
H	-11.65600300940960	7.01805391334088	-0.48997135583192
H	-10.06032813584415	8.91724260042743	-0.32663369097321
H	-7.61358482590772	8.46818667892447	-0.15971697981159
H	-6.77339582618810	6.12747501522939	-0.15675377162660
H	-3.31018095495443	1.66345233635621	-0.39924175347688
C	-2.27175311072347	-3.07617172942971	2.77514993823635
O	-2.36588494941634	-1.90544313040386	2.32682030488727
O	-1.33537070639008	-3.81501162591603	2.33288780092510
C	-3.25505303339048	-3.62628209600858	3.75691952990671
H	-3.99823772962653	-4.21553501658634	3.19553601359764
H	-3.77740861110497	-2.81960917064555	4.28531478618355
H	-2.75307522415918	-4.30419183975476	4.46003366436303

$A_{Cu(III)}$

C	1.64790246001059	-3.85787147540525	-0.69626533057375
C	1.83810917259623	-5.22813623769051	-0.62235951450624
C	3.13633315510141	-5.75886335162678	-0.52655207026243
C	4.25825779616884	-4.97514580069972	-0.48869635961423
H	6.18413919771277	-3.01555942520907	-0.40368226340696
C	5.16540028295724	-2.64961307022589	-0.46817990720139
C	4.90761554748339	-1.30360528111792	-0.47962340337790
C	3.58327999041589	-0.85925647339294	-0.54019692568705
N	2.58335062194990	-1.70890537134285	-0.60141730760796
C	2.80240888529156	-3.04674780975535	-0.61332918716425
C	4.10816165550869	-3.57442154609160	-0.52987719786875
Cu	0.72365102644752	-1.32127111112062	-0.45790750814970
H	3.33021362497742	0.19076013274707	-0.51649904253774
H	5.70468107757501	-0.57422321852593	-0.42844209814220
H	3.23614683985626	-6.83703480000677	-0.47523714007483
H	0.98746173976037	-5.88745143272510	-0.64464969464562
N	0.48272534068644	-3.14110957987976	-0.93056063893591
C	-0.72860049631427	-3.79753893855590	-1.03498439648388
O	-0.88208306324622	-4.94940259168326	-0.67075965030763
C	-1.85557218462956	-3.10688315626362	-1.71666713382112
C	-3.14053747573819	-3.40761225594633	-1.26625897789904
C	-4.23079419980953	-2.89095176778003	-1.93133094394865
C	-4.06118617042371	-2.13024412738694	-3.08355541260532
C	-2.77896670443343	-1.88454893443296	-3.56409495771891
C	-1.66904112213021	-2.33305397139515	-2.84932001181771
H	-3.25788613012175	-4.04976797746577	-0.40337516662439
H	-5.23231903109011	-3.09565737692018	-1.57035282731464
H	-4.93091353910942	-1.74295077379681	-3.59664667907543
H	5.24817300379123	-5.40640783707353	-0.40189238717530
C	-2.93600125611187	-0.73308405942742	-8.13987839722777
C	-3.18419140769189	-0.85235870246271	-6.96758429483381
O	-2.52341309640287	-1.24531291075909	-4.73339354568872
C	-3.62443862250157	-1.06120025939155	-5.60215162171790
H	-4.26339709724164	-1.95301101669220	-5.58337019249960
H	-4.23382178617310	-0.21141616317034	-5.26756330824273
C	-2.68371821092884	-0.64643317705097	-9.53773248807936
C	-2.59207827785183	-1.81551260013429	-10.30019997459121

C	-2.41417718612332	-1.74507586191586	-11.67032754920005
C	-2.31855303847954	-0.51117874821144	-12.29856851986349
C	-2.38890770468563	0.65417713200114	-11.54724645539338
C	-2.56691815757593	0.59178226817721	-10.17570984756484
H	-2.67238160749209	-2.77428204598520	-9.80318116524744
H	-2.34933102671483	-2.65728294635415	-12.25175233237147
H	-2.18178987013244	-0.45741710154348	-13.37239610052006
H	-2.30476914314016	1.61846914734691	-12.03466810974169
H	-2.62836779025713	1.49731181828985	-9.58470540068823
H	-0.67826693200664	-2.10391666891808	-3.22309005793247
C	0.99566700427240	1.18248744832867	-1.03507262291800
O	0.81407882300977	0.74328263014925	-2.15638180642933
O	1.07021401759083	0.43296700913161	0.02994636550647
C	1.17044675427251	2.64605800083458	-0.72809245039594
H	0.21859069963098	3.03700776601082	-0.36061440343735
H	1.45742166809352	3.18130615767410	-1.63119549184630
H	1.90741824701149	2.79513448917859	0.06058929511361
C	-1.12128270890855	-1.36808562574500	1.23443450025227
O	-0.15944641305755	-1.75636471946729	1.87401744901067
O	-1.04420668981301	-1.05423692659998	-0.03010215787916
C	-2.50832846059735	-1.23157966382913	1.80220326763976
H	-3.20749002025700	-0.84569244212363	1.06369333458418
H	-2.47451423856662	-0.57539298670625	2.67237663925064
H	-2.83537977241451	-2.21712467986530	2.13888557750178

ts_{A-B}

C	1.04409131778988	-2.44331354492827	-2.64967816025854
C	1.31429475551646	-2.13406671187388	-3.97157471019912
C	2.61243111547305	-1.76793988789940	-4.36301216182267
C	3.65620950936308	-1.69209066280154	-3.47724547626540
H	5.42313733684163	-1.65731235328226	-1.38588377944640
C	4.41058068414512	-1.93712049137818	-1.11532889776656
C	4.09243430820859	-2.23894867709831	0.18279342174475
C	2.77617182486813	-2.60111180527030	0.49378723774148
N	1.83670151096136	-2.65256345376315	-0.42352303606806
C	2.12061834802388	-2.35343040971814	-1.71567033349715
C	3.42366991678343	-1.98331467323063	-2.11836370177700
Cu	-0.05989754323303	-3.29086093837769	-0.23663994202646
H	2.47855736519083	-2.87246843747072	1.50029883082026
H	4.83678570065653	-2.20755731334031	0.96768865878172
H	2.78516802258540	-1.53677314979924	-5.40821932588034
H	0.51200256881354	-2.19477172150454	-4.69206834238683
N	-0.14141944910494	-2.82912743687662	-2.08984913595571
C	-1.31272019340760	-3.02301435893899	-2.74778767301934
O	-1.50401287395446	-2.90658004239448	-3.94722745267142
C	-2.41331085807239	-3.33501234724427	-1.77601312675395
C	-3.71393854841856	-3.03611032374997	-2.15120692615063
C	-4.71890269496590	-3.08343577821887	-1.20084020520627
C	-4.43803765685316	-3.44402117765810	0.10804898157702
C	-3.13979077207076	-3.81928275709583	0.45199049894797
C	-2.09514367568487	-3.78122232045366	-0.48306044256253
H	-3.90472553210678	-2.71659555946284	-3.16836465653131
H	-5.73259271553452	-2.80695089506403	-1.46843356561845
H	-5.23231625302277	-3.42507563256710	0.84261570335177

H	4.65001828324086	-1.40742216744401	-3.80182243817821
C	-3.15641701920863	-6.24527259010215	4.50872109152192
C	-3.40257600551266	-5.45269543857854	3.63580873975273
O	-2.81082170733641	-4.26461485477082	1.69166057614300
C	-3.86377003355578	-4.56551832796492	2.58480220854798
H	-4.27275547631566	-3.64418321361375	3.02006839333501
H	-4.67740385150516	-5.06850079796575	2.04814534217374
C	-2.93082165709479	-7.21294965714154	5.52735484598449
C	-2.94285490259695	-8.57502339976306	5.20999500251245
C	-2.80578633145285	-9.52466659809884	6.20676425553248
C	-2.64868156128970	-9.13156210849289	7.52829302023944
C	-2.61395048277694	-7.78170038201694	7.84932266174440
C	-2.74777990466909	-6.82568368817956	6.85777517607612
H	-3.07749496431678	-8.87547002955154	4.17796471009551
H	-2.82836128891361	-10.57759254010714	5.95105814523029
H	-2.55146227361684	-9.87722907279023	8.30837130195152
H	-2.48544711676012	-7.47086292276922	8.87955007544714
H	-2.72930466452539	-5.77109065511603	7.10456618831911
C	-0.08091343629074	-5.42270793069781	1.37814658520473
O	0.29521262490853	-4.22668952685869	1.45789743542774
O	-0.73297947592247	-5.87643338032469	0.38715232415712
H	-1.27525340947481	-4.89222124537071	-0.14978244768821
C	0.24572494680934	-6.36728108013757	2.48692842019492
H	0.69805230097548	-7.27022297832162	2.07497487137622
H	-0.68756786575877	-6.65519895478721	2.97605179001588
H	0.90926575416897	-5.90046559757352	3.21060644378163

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C	3.04043300000000	2.97609600000000	-4.80992700000000
C	4.06215500000000	2.79442700000000	-3.90202500000000
H	5.76973900000000	2.24819100000000	-1.80865200000000
C	4.73342100000000	1.94130400000000	-1.64192100000000
C	4.36171400000000	1.33145900000000	-0.46262200000000
C	3.01760700000000	0.95009700000000	-0.28559500000000
N	2.10693300000000	1.17716200000000	-1.21065000000000
C	2.44151600000000	1.77695400000000	-2.38368700000000
C	3.77688500000000	2.18181100000000	-2.65707800000000
Cu	0.13825900000000	0.67246000000000	-1.19501600000000
H	2.67474500000000	0.43761200000000	0.61812000000000
H	5.08620800000000	1.13415000000000	0.32932800000000
H	3.25920300000000	3.45043400000000	-5.76996700000000
H	0.92098800000000	2.72270400000000	-5.28150900000000
N	0.15879600000000	1.54153800000000	-2.90745600000000
C	-1.00720500000000	1.60248900000000	-3.60964200000000
O	-1.12485000000000	1.80698700000000	-4.80786500000000
C	-2.19108300000000	1.46494700000000	-2.69124700000000
C	-1.95984400000000	0.45158300000000	-1.76467900000000
C	-3.08922300000000	0.12341700000000	-0.90103200000000
C	-4.31649500000000	0.76841500000000	-1.03367900000000
C	-4.47019400000000	1.77346300000000	-1.99382300000000
C	-3.40775000000000	2.17583500000000	-2.82055900000000
H	-2.96130300000000	-0.66120300000000	-0.15028600000000

H	-5.16360500000000	0.52675100000000	-0.38710800000000
H	5.08041400000000	3.11854300000000	-4.12758100000000
C	-8.03626800000000	4.82928200000000	-2.84027400000000
C	-7.01426100000000	4.17511100000000	-2.90701400000000
O	-5.66877700000000	2.43865700000000	-2.04142900000000
C	-5.76175500000000	3.44190500000000	-3.03224900000000
H	-4.91827800000000	4.15203800000000	-2.93598200000000
H	-5.69807400000000	2.99294400000000	-4.04258200000000
C	-9.22105500000000	5.62905800000000	-2.79450300000000
C	-9.93061500000000	5.90540100000000	-3.97708900000000
C	-11.05561800000000	6.72329100000000	-3.94985900000000
C	-11.49665000000000	7.27395600000000	-2.74553400000000
C	-10.80947200000000	6.99333100000000	-1.56442400000000
C	-9.68182600000000	6.17859700000000	-1.58456900000000
H	-9.58193300000000	5.47851200000000	-4.91954300000000
H	-11.58923300000000	6.93022300000000	-4.88095500000000
H	-12.37741400000000	7.92000200000000	-2.72326000000000
H	-11.15251000000000	7.41385700000000	-0.61573400000000
H	-9.14335200000000	5.96855000000000	-0.65847900000000
C	-0.14769300000000	-1.76611200000000	-0.06331800000000
O	0.36244800000000	-0.65928400000000	0.25699000000000
O	-0.88032100000000	-1.91582400000000	-1.08609100000000
H	-1.26773800000000	-0.77449300000000	-1.41781000000000
C	0.11453600000000	-2.97527800000000	0.78257600000000
H	0.50525800000000	-3.78431800000000	0.14918000000000
H	-0.84408200000000	-3.31624100000000	1.20117000000000
H	0.81826000000000	-2.74436900000000	1.58980700000000
H	-3.52260600000000	2.91590700000000	-3.51271200000000

B

C	0.73988024243163	-1.80507242639540	-2.56517258334238
C	0.88793188126216	-1.68711481689689	-3.94006461147879
C	1.69228458197403	-0.66723489248753	-4.48268095868886
C	2.36474100729826	0.23924030916990	-3.70259122286539
H	3.51747172650908	1.83479330930514	-1.79124033445979
C	2.87955209948632	1.05070307528598	-1.40247055941263
C	2.69321418126897	0.91437920454630	-0.05031302202411
C	1.86114408067262	-0.13052376604092	0.41392625714270
N	1.25767286102111	-0.96570784192909	-0.39543079906497
C	1.42117547659784	-0.85446008436243	-1.73836782564934
C	2.24229766622995	0.15644673886728	-2.30037228541586
Cu	0.10019641388704	-2.57101236217864	0.04957505921640
H	1.68497663050237	-0.28140031745810	1.47207828478988
H	3.17395194337311	1.58737348810442	0.65951693728991
H	1.78385072202902	-0.58802718583436	-5.56028234054388
H	0.37542012291676	-2.36334567123641	-4.57498445597979
N	0.01923965526175	-2.70742432388802	-1.86569651525025
C	-0.72722711220667	-3.71151115419075	-2.37076145494188
O	-0.86619074366420	-3.99235087570180	-3.55240640366232
C	-1.39399976998574	-4.48399495260836	-1.26076297480601
C	-2.26881079676049	-5.52314563240794	-1.54899272123902
C	-2.88669227151195	-6.23210076679853	-0.51311761798518
C	-2.63341622475167	-5.88344993574986	0.79917027029048
C	-1.76280327834079	-4.82316867029785	1.05599391576349

C	-1.11682147568649	-4.09915530761579	0.06022025902661
H	-2.45431725308964	-5.76675463847084	-2.58545414237149
H	-3.56704279600042	-7.04820816141612	-0.72426790497873
H	-3.10192501029459	-6.41167232461714	1.62713741828742
H	2.98685189055651	1.04075075296987	-4.14317385210165
C	-2.26488932445304	-3.15692560322940	5.48780100885614
C	-2.22316571244527	-3.28710022075115	4.28452544425023
O	-1.55161770852440	-4.53529685359093	2.40786036027452
C	-2.23471802045265	-3.37517057668540	2.83882487260950
H	-1.76359065623368	-2.49244198670295	2.39282739067702
H	-3.26364193865299	-3.43295207090153	2.48018073433490
C	-2.27443385620943	-2.98961812456439	6.91329940598460
C	-2.95550991316842	-1.91805808355306	7.49661259357228
C	-2.94531243919714	-1.75224958505176	8.87966896476380
C	-2.26496368935852	-2.64319220949250	9.69855584275460
C	-1.59348448161342	-3.71794873818653	9.12852353568407
C	-1.59514134707015	-3.89076380065164	7.74549489839299
H	-3.49708799882793	-1.22267768237425	6.84979844244657
H	-3.46328340196466	-0.92183903324282	9.31714310788333
H	-2.25018473303706	-2.50357418467719	10.77847374838340
H	-1.05522243228418	-4.42109789457813	9.76647294798154
H	-1.07774446089873	-4.72129380157729	7.29689313545157
C	1.47121807190109	-3.37414825588932	2.56659178219769
O	0.83683845230654	-2.51091946963792	2.00239270027664
O	0.94778327060841	-4.45275244963276	3.04177081107971
H	-0.03894738932270	-4.46060978442151	2.81411301864942
C	2.91470009375693	-3.22826052082110	2.76893887373283
H	3.39986451966305	-4.18369933079792	2.58999130775763
H	3.11156657108188	-2.92255357718965	3.76827877649681
H	3.30003307341207	-2.46362393146597	2.11240947996310

C

C	1.03554450798501	-0.10658736264048	-2.03989298847212
C	1.17221487113276	0.56332599318461	-3.24647556463838
C	2.42664917290677	1.03504735784536	-3.65834213916357
C	3.55951901200412	0.87341460803671	-2.90269702777711
H	5.52641317793004	0.41243485247799	-1.07304350272509
C	4.55005970721686	0.03794236147449	-0.78383087496802
C	4.36719222448471	-0.58870699661388	0.42007248017823
C	3.09131684928166	-1.06079609799918	0.74932738847281
N	2.05526796534893	-0.91240424640809	-0.04559173270880
C	2.20790212653240	-0.27767764702987	-1.23834842884900
C	3.46406733706082	0.21888790542597	-1.65952731333122
Cu	0.12043909131790	-1.49452780987666	0.21523616419833
H	2.91396401573136	-1.57774278087299	1.68589725263309
H	5.18523279116639	-0.72843018368954	1.11471684010373
H	2.49275932272651	1.54834071989444	-4.61102150621114
H	0.29220370920342	0.71454082382669	-3.85387096420415
N	-0.09053536963113	-0.62670216232311	-1.48441896252412
C	-1.36570552807985	-0.48885203768178	-1.94707988946125
O	-1.68685980533980	0.02252519690285	-3.00759017571665
C	-2.34073280007226	-1.05501152794645	-0.96181069961649
C	-3.69669829857264	-1.06515797163445	-1.24454602024241
C	-4.57451593099226	-1.61469327120218	-0.32042678418666

C	-4.09564033036483	-2.14592264810661	0.86485421841894
C	-2.72795845021464	-2.11792981146997	1.13131544176315
C	-1.82667385085049	-1.58061563073797	0.23136164953258
H	-4.04090128136273	-0.64026293107551	-2.18043692398925
H	-5.63864865041281	-1.63508956087722	-0.52696160395998
H	-4.76554728566211	-2.57925590943501	1.59943072427246
H	4.51865233867625	1.25017440068010	-3.23794172489007
C	0.86944535168261	-3.50135260622452	1.39600924079969
C	0.01413726007756	-2.87269761610612	1.99238018115725
O	-2.35747014031273	-2.67942939876687	2.33413729826762
C	-1.08682939781949	-2.36040365157551	2.82131723125819
H	-0.97820819826611	-1.27513945750149	2.94314252849019
H	-1.02037531536740	-2.82798250187391	3.80708364520810
C	1.83714719816212	-4.22824177726351	0.64812572738026
C	2.95218438770298	-4.79291725052874	1.27476863828233
C	3.87743961871154	-5.50053265879475	0.52816345678105
C	3.70527355629718	-5.64917281719493	-0.84073665882565
C	2.59889215804260	-5.09131049481275	-1.46825345262991
C	1.67045593691036	-4.37829317108267	-0.73222817110949
H	3.08389823660728	-4.67320707685274	2.34334533925358
H	4.73738537182380	-5.94068635555899	1.01853953490733
H	4.43379634166468	-6.20259158945250	-1.42084725409916
H	2.45627044871528	-5.21383646179037	-2.53522418814344
H	0.80950154621737	-3.93008574674786	-1.21555442891576

$ts_{C\text{-}D}$

C	1.15706633003260	-0.10636290413751	-1.45861271642426
C	1.33108743414008	0.95077750966232	-2.35858877776059
C	2.43962342212986	1.81379262582873	-2.27243754726080
C	3.41533864664742	1.66681777390479	-1.30988233273200
H	5.11181042992895	1.04034932882290	0.73312453494004
C	4.25823091261623	0.36382381934556	0.63646459119781
C	4.11040440864159	-0.70302153667775	1.49492576758233
C	3.00235279232382	-1.55116150897348	1.32498766592785
N	2.09138209375525	-1.34743295588974	0.39040434470180
C	2.19468736687666	-0.29124975440546	-0.46601370188559
C	3.30645300673994	0.60279651917624	-0.38376044753311
Cu	0.45236906860328	-2.40014892031919	-0.03701233796260
H	2.85998423921693	-2.42222298900182	1.97107240901303
H	4.83137763134396	-0.90723466270267	2.28824069935346
H	2.51952059780396	2.62868324788187	-2.99682130698769
H	0.58009827814438	1.08668663764642	-3.13370308354414
N	0.09253752392752	-0.97015980429036	-1.38877714911842
C	-0.88341803527064	-1.01396625004735	-2.32890026001835
O	-0.92387830199812	-0.38051717929330	-3.37885714483812
C	-2.09444141662511	-1.85368860578090	-1.96119084009121
C	-3.29996209694263	-1.45800307861913	-2.55496489962342
C	-4.52479039458660	-2.00268078268440	-2.16637328921500
C	-4.60597869077639	-2.94301092438694	-1.13816966754326
C	-3.40958211309190	-3.35037213658670	-0.56220933754380
C	-2.16470225451500	-2.87629879773480	-1.00256801580222
H	-3.23938105761392	-0.67588334256901	-3.31344690199938
H	-5.44001245347664	-1.65499478402372	-2.65227272257348
H	-5.55332396552726	-3.35091945603874	-0.78129936827334

H	4.26952559647624	2.34472266571349	-1.25460268748316
C	0.04390226804000	-4.22172447831600	-0.63924115114521
C	-1.16267199664468	-3.71011223610730	-0.26048270220692
O	-3.32815567072074	-4.23388491288012	0.45966187329885
C	-1.97310855608003	-4.28833873283372	0.89156802685788
H	-1.86882726071192	-3.68834924682238	1.81385446483226
H	-1.70457781448059	-5.33001902444225	1.11371166772288
C	0.77886901224601	-4.36754054630172	-1.86058208272965
C	2.18996960487321	-4.38298995875279	-1.86589076435456
C	2.88921175227464	-4.47377050150042	-3.06135465833274
C	2.20132607345736	-4.55796938934545	-4.27359996045400
C	0.80413827375027	-4.57248863080444	-4.28201937567502
C	0.09540999497553	-4.48977626116548	-3.09183835991712
H	2.72166115672392	-4.31235367087925	-0.91450594831862
H	3.98162070971493	-4.47577132243279	-3.05186790625405
H	2.75625748058118	-4.61626337827272	-5.21258511977509
H	0.26216316937815	-4.64166712769949	-5.22780328867682
H	-0.99645719630170	-4.48744733526312	-3.09605019137437

D

C	1.15706633003260	-0.10636290413751	-1.45861271642426
C	1.33108743414008	0.95077750966232	-2.35858877776059
C	2.43962342212986	1.81379262582873	-2.27243754726080
C	3.41533864664742	1.66681777390479	-1.30988233273200
H	5.11181042992895	1.04034932882290	0.73312453494004
C	4.25823091261623	0.36382381934556	0.63646459119781
C	4.11040440864159	-0.70302153667775	1.49492576758233
C	3.00235279232382	-1.55116150897348	1.32498766592785
N	2.09138209375525	-1.34743295588974	0.39040434470180
C	2.19468736687666	-0.29124975440546	-0.46601370188559
C	3.30645300673994	0.60279651917624	-0.38376044753311
Cu	0.45236906860328	-2.40014892031919	-0.03701233796260
H	2.85998423921693	-2.42222298900182	1.97107240901303
H	4.83137763134396	-0.90723466270267	2.28824069935346
H	2.51952059780396	2.62868324788187	-2.99682130698769
H	0.58009827814438	1.08668663764642	-3.13370308354414
N	0.09253752392752	-0.97015980429036	-1.38877714911842
C	-0.88341803527064	-1.01396625004735	-2.32890026001835
O	-0.92387830199812	-0.38051717929330	-3.37885714483812
C	-2.09444141662511	-1.85368860578090	-1.96119084009121
C	-3.29996209694263	-1.45800307861913	-2.55496489962342
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C	-4.60597869077639	-2.94301092438694	-1.13816966754326
C	-3.40958211309190	-3.35037213658670	-0.56220933754380
C	-2.16470225451500	-2.87629879773480	-1.00256801580222
H	-3.23938105761392	-0.67588334256901	-3.31344690199938
H	-5.44001245347664	-1.65499478402372	-2.65227272257348
H	-5.55332396552726	-3.35091945603874	-0.78129936827334
H	4.26952559647624	2.34472266571349	-1.25460268748316
C	0.04390226804000	-4.22172447831600	-0.63924115114521
C	-1.16267199664468	-3.71011223610730	-0.26048270220692
O	-3.32815567072074	-4.23388491288012	0.45966187329885
C	-1.97310855608003	-4.28833873283372	0.89156802685788
H	-1.86882726071192	-3.68834924682238	1.81385446483226

H	-1.70457781448059	-5.33001902444225	1.11371166772288
C	0.77886901224601	-4.36754054630172	-1.86058208272965
C	2.18996960487321	-4.38298995875279	-1.86589076435456
C	2.88921175227464	-4.47377050150042	-3.06135465833274
C	2.20132607345736	-4.55796938934545	-4.27359996045400
C	0.80413827375027	-4.57248863080444	-4.28201937567502
C	0.09540999497553	-4.48977626116548	-3.09183835991712
H	2.72166115672392	-4.31235367087925	-0.91450594831862
H	3.98162070971493	-4.47577132243279	-3.05186790625405
H	2.75625748058118	-4.61626337827272	-5.21258511977509
H	0.26216316937815	-4.64166712769949	-5.22780328867682
H	-0.99645719630170	-4.48744733526312	-3.09605019137437

E

C	1.11577407117260	0.41291695576198	-1.91953446874995
C	0.98122759766444	1.39390707778707	-2.89499744188786
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C	3.37540289053068	1.52875112792102	-3.28864970880956
H	5.71787710753085	0.46106046371588	-2.44469725763460
C	4.84290544805213	0.04576203012838	-1.95507839784461
C	4.96813152986637	-0.92808912886631	-0.99886696588995
C	3.81106438660233	-1.43225387892624	-0.39761941059005
N	2.61059213047914	-0.99477681297548	-0.71489081136279
C	2.45069411386184	-0.02468814318782	-1.65023289269539
C	3.57318707079649	0.53043029397894	-2.31817083267348
Cu	0.87992379797570	-1.47221070358099	0.05556412112405
H	3.86584684564949	-2.20554483076976	0.36123516445302
H	5.93414807102433	-1.31398507328663	-0.70000036218266
H	1.92025254189448	2.69431414402111	-4.30803635998845
H	-0.00167120235232	1.77039448837136	-3.12785274303828
N	0.10290099890566	-0.23896776392713	-1.23329639702053
C	-1.16681223876937	0.27270830617392	-1.24689704709451
O	-1.42295042858366	1.42083221615941	-1.57814028993046
C	-2.34915034791769	-0.62408310590180	-0.97187044253459
C	-3.42257098303884	-0.37265065789675	-1.83452776821015
C	-4.63857091987547	-1.02216811480697	-1.70837742507420
C	-4.86448820783978	-1.92247175026323	-0.67694027504377
C	-3.81812402476917	-2.15204808036206	0.18780161575813
C	-2.55158115535507	-1.56260823469270	0.04630055565915
H	-3.29124777434337	0.38087181705567	-2.59839893985744
H	-5.43590493394300	-0.79571123582228	-2.40671549170228
H	-5.81785134133480	-2.41358623531359	-0.52993161606396
H	4.22865062069548	1.96362250722431	-3.79525904533501
C	-0.40458940435709	-2.18293736733474	1.22456762036202
C	-1.73289084450359	-2.13306532757371	1.10733834905012
O	-3.91819850488582	-2.97703626328090	1.25443677252136
C	-2.71526998122684	-2.84362893983261	2.01064977028354
H	-2.94356667558244	-2.24883713558894	2.90354886616230
H	-2.37756373312434	-3.83150841003483	2.32749915489035
C	0.29627591660604	-2.83776957582012	2.32835594172654
C	0.02089808077306	-2.51752964535969	3.66472420389124
C	0.69128930442834	-3.14167401794571	4.70134582249308
C	1.66802818996040	-4.09402766591608	4.43354844966914
C	1.96928869803500	-4.41361431037893	3.11705736001035

C	1.29694667367231	-3.79012331712161	2.07763736322192
H	-0.72926771968140	-1.76503501644069	3.87721016917821
H	0.44854403102644	-2.88106546158122	5.72569228747023
H	2.19060890698173	-4.58446608437475	5.24606202354204
H	2.72439248590882	-5.16027127374031	2.89938643984469
H	1.51486613850398	-4.06779188520900	1.04948080958531

F

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C	3.50979239488177	1.23986322045220	1.85496293016067
C	4.51455502378950	0.59969821409907	1.17828103255794
H	6.17456581790992	-0.91080648351304	-0.39903491258274
C	5.11607227218429	-1.07031378776589	-0.57584350056422
C	4.69156548013949	-1.97064689830901	-1.51808030758491
C	3.31503148348035	-2.15295761311672	-1.71370337127850
N	2.42494988434292	-1.48163633274732	-1.02511277244742
C	2.81419652495253	-0.58451251835231	-0.08877144036563
C	4.18007525245787	-0.33939769230668	0.18187942880045
Cu	0.44572567230174	-1.78871978447323	-0.77370821289189
H	2.93085033530473	-2.86613535723992	-2.43448738094998
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C	-1.81657680294506	0.54312618236900	-0.37531462279391
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C	-3.88374828240687	1.51620401404520	-1.18177885534249
C	-4.60519659637229	0.36098958265352	-0.89096150226804
C	-3.89847598759977	-0.68994273022349	-0.35018744769429
C	-2.51599117424067	-0.64007594082172	-0.16974287861737
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H	-4.40484980056010	2.36952249675641	-1.59947399393408
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H	5.55611506269745	0.80000340348062	1.40231837711755
C	-0.93490781662538	-2.49945293137559	0.33950750076484
C	-2.12296779347040	-1.92556216570241	0.36461966580381
O	-4.44245496517085	-1.85478555026044	0.07794908573246
C	-3.42659837981374	-2.56877481078973	0.79284464272822
H	-3.61000822311707	-2.44489959835313	1.86769521156938
H	-3.49055842696097	-3.62294575913943	0.52571036441588
C	-0.37876381455552	-3.60440971321519	1.09296970752656
C	-0.06759750654069	-3.38735709414730	2.44357234751096
C	0.46642310746255	-4.40306304003534	3.21468728852490
C	0.69614741581772	-5.65256779619669	2.65307202723449
C	0.39765483617270	-5.87728128171287	1.31627423694870
C	-0.12106281820683	-4.86186013830885	0.53224280014444
H	-0.24697762332179	-2.40649714740571	2.86845626732120
H	0.71031123098019	-4.21936165246474	4.25476869818362
H	1.11192946046053	-6.45040468281073	3.25733750549901
H	0.58075828061725	-6.85126730696558	0.87752938439757
H	-0.32963400431782	-5.01995918537821	-0.51635802360504

C	0.12168862086617	-2.75601058886804	-3.05171301018367
O	-0.12822838350027	-1.55772033781679	-3.13886957199129
O	0.38745221690044	-3.31785731326291	-1.91514752766387
C	0.15268840222989	-3.65964773431823	-4.25394396179879
H	0.82226281285859	-4.50405134898229	-4.09284332740266
H	0.45021502791587	-3.08991776894617	-5.13297907264613
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C	4.12779074342198	-0.16297360495963	1.57354929082340
H	5.71636602574107	-2.11370060572084	0.52355182464378
C	4.71011164957713	-2.09001558415632	0.11843858339850
C	4.32471229472970	-2.97718972388670	-0.84886317762482
C	3.01130311793223	-2.90599687383735	-1.33768785235553
N	2.13932116460083	-2.03820599143040	-0.89411890510782
C	2.48994825930256	-1.15294768495666	0.06275625246592
C	3.79840636215712	-1.12986666824722	0.60411753968476
Cu	0.03998911888838	-1.71746816677214	-1.30131242441853
H	2.66386778683552	-3.58938129770699	-2.10696532009969
H	5.00821779342093	-3.72072973067565	-1.23868695596117
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H	1.14078737931241	1.42055534035807	1.81263868322515
N	0.21987692484351	-0.32472910900888	-0.01750165805873
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O	-0.23618935938032	1.92170820497597	-0.01034883681848
C	-2.00916073734232	0.47011254785660	-0.54266084343228
C	-2.83627273420547	1.46308708458102	-1.06444695118572
C	-4.19461264542201	1.23225112894586	-1.22123154597539
C	-4.80506440324170	0.04725284986670	-0.80216107186120
C	-3.98392992140212	-0.91358304985687	-0.25565594518494
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C	-0.74200234784057	-2.21529258016586	0.39146492246845
C	-2.03777845051556	-1.90547295926322	0.40961925828679
O	-4.37370404266184	-2.08960742995975	0.28862210879416
C	-3.22584389694189	-2.69942123913077	0.90337264666411
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H	-3.19187971464344	-3.74568294626443	0.59882782628228
C	0.08582038436920	-3.09543023999380	1.18730773179310
C	0.44587523563995	-2.71195628377826	2.48266491665914
C	1.30197045488839	-3.49949766543796	3.23365002371017
C	1.80112980642225	-4.67895611848203	2.70088176648590
C	1.43612776671109	-5.07670752643716	1.42044548575583
C	0.59700359182082	-4.28490706776356	0.65822533350304
H	0.06502245922060	-1.77867042228612	2.87966745855065
H	1.59616784120489	-3.18057137052341	4.22689918315115
H	2.47381824960719	-5.29457692737575	3.28707053164233
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C	-0.07574019972390	-2.29409581652999	-3.59701239512200
O	0.27269994557447	-1.13052727377183	-3.28672133104680
O	-0.41816593961829	-3.11913024644216	-2.69180115965988
C	-0.10344136317839	-2.70945529467741	-5.03526478378435
H	0.16951729412286	-3.75971186549992	-5.14252038004588
H	0.56000464206187	-2.07787756030387	-5.62245624458847
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H	5.43668032227846	-2.03714434897244	-2.58892612303444
C	4.44254726633406	-1.92103708987039	-2.17048164884049
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C	2.08791548503759	-2.24975219284859	-2.21426441140174
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C	2.98009174761569	-1.09968639990262	-0.41930962467998
C	4.28791152417033	-1.22031161874584	-0.95890316282542
Cu	0.05324189541396	-1.77675693664768	-0.28209461417376
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H	3.74866679523445	0.74592128460866	2.31941881200681
N	1.54677679121921	-0.34475413360766	1.42877993978656
C	0.94088341369245	0.93922693500163	1.49343158490983
O	1.60491766372298	1.93965906011886	1.33092861649497
C	-0.50383777923264	0.92958054416903	1.72888950420682
C	-1.32332692040027	2.05943878234145	1.81880362939186
C	-2.67991884662200	1.88714936845170	2.04124606380396
C	-3.27660147752073	0.62573890927039	2.22129367804655
C	-2.45392121997771	-0.47449293536699	2.14792798224883
C	-1.10892951939354	-0.29976014334551	1.85859991277540
H	-0.89298090611494	3.04595765987720	1.70991220551999
H	-3.31554251941929	2.76293658086136	2.09746105862966
H	-4.33596835403614	0.53302994621828	2.42451595521497
H	6.37410872426613	-0.75421848084508	-0.71755427653719
C	0.89208278099597	-1.59674887831499	1.62002097920343
C	-0.47386589897509	-1.56701244694694	1.80391191046629
O	-2.75230156338743	-1.78025012656019	2.32416806912407
C	-1.51856020073282	-2.54760682727830	2.28258756645190
H	-1.30760852368660	-2.90954749549522	3.29505444510557
H	-1.67304517074729	-3.39047157738819	1.61173610664533
C	1.72392127677914	-2.78378474884502	1.91351006733069
C	2.84545543014569	-2.69627788790506	2.73784345122076
C	3.60930320184081	-3.82027611347119	3.00470743247058
C	3.26272261394644	-5.04674786987314	2.45697401804659
C	2.13634407648913	-5.14380730923483	1.65233854574567
C	1.37037722739467	-4.02292935013635	1.37918312815610
H	3.12272868485888	-1.74388172533219	3.17091114612230
H	4.47962670379860	-3.73666069459291	3.64461418058199
H	3.86409659862779	-5.92437172579902	2.66341280402736

H	1.85076608275297	-6.09536575120554	1.21868395620730
H	0.50761153529988	-4.10434719239035	0.72277045690679
C	-2.05799958563899	-2.91479711825311	-1.04624111786806
O	-1.64697926553863	-1.73538441879947	-1.29009310452857
O	-1.32465903038468	-3.80575234155951	-0.57389683857374
C	-3.51845798619873	-3.18713374927218	-1.28710977616893
H	-3.74145340276633	-4.24820446817403	-1.19239543653258
H	-3.82334555527982	-2.81036268330308	-2.26456997046337
H	-4.09154097039867	-2.63447976377474	-0.53872240000802

Intermolecular migratory insertion

Alkyne (1-Phenyl-1-propyne***)***

C	-2.57981641691998	-4.77575178075089	2.07462030674781
C	-3.49357298934755	-3.99772520016603	1.97678904481806
H	-4.94518972436978	-3.02159881266160	0.81191236051884
C	-4.58727163157165	-3.05987158225151	1.84419279410261
H	-4.27286420715828	-2.05304224829614	2.13282522832206
H	-5.42898784483474	-3.34716501808050	2.47895192408244
C	-1.50972379457699	-5.70539624698265	2.19106675792719
C	-1.06366609308221	-6.12053403091654	3.44869556119638
C	-0.02369758076350	-7.02751125394818	3.55688641489582
C	0.58663274719106	-7.53554088036938	2.41775462407453
C	0.15026938043817	-7.12767428619490	1.16546430003903
C	-0.88756556036974	-6.21927210274055	1.04926167610155
H	-1.54374940333846	-5.71877354129259	4.33319576664781
H	0.31638965715096	-7.34275829188747	4.53707213712908
H	1.40033544053342	-8.24524232320733	2.50719910543534
H	0.62231118999916	-7.52131107105168	0.27270082977584
H	-1.23288816897989	-5.89307332920206	0.07539016818560

C_{inter}

C	0.90560969814199	0.48926989872813	-1.78082781448491
C	0.92337700974697	1.65058129895715	-2.54033790935127
C	2.14056344945136	2.24061038363728	-2.91127182160312
C	3.35387191319056	1.70969207851739	-2.55449301586565
H	5.52649973217420	0.33422246788977	-1.65290255454454
C	4.57386611730573	-0.09871883264169	-1.36522261444124
C	4.51974626214581	-1.23935731895330	-0.60842197256988
C	3.26895123753953	-1.76366324335441	-0.26222902312400
N	2.14009777799174	-1.20581227806366	-0.64372291566871
C	2.16612593371879	-0.07258377613388	-1.39595799238621
C	3.38662730932755	0.53063113657895	-1.78439883079407
Cu	0.21209699204644	-1.75431568800536	-0.25556946277257
H	3.18949423945929	-2.65840132175459	0.34490678211584
H	5.41894282309423	-1.73802361020791	-0.27000378578292
H	2.11141711578139	3.14949739418075	-3.50171439000323
H	-0.02054622242834	2.08623027531617	-2.83414808562727
N	-0.17167198769031	-0.21217480811283	-1.34274513558339
C	-1.48907265063161	0.06819024321830	-1.55936666254679
O	-1.93058155105289	1.04981733052561	-2.13646574321884
C	-2.34546114885399	-1.01261479192632	-0.97585493283144

C	-3.72477530701633	-0.98097923928122	-1.12855201960370
C	-4.49481422694212	-2.00258786177117	-0.59264939328700
C	-3.88432902502962	-3.03473368708797	0.10854771084211
C	-2.50049033530837	-3.05299782667203	0.26920980455397
C	-1.71219614381580	-2.04947658988413	-0.27809417151546
H	-4.17134118052365	-0.15863685137977	-1.67739390737772
H	-5.57140329318321	-1.99561691210391	-0.72193130795071
H	-4.48822596361895	-3.82932040182822	0.53497496435238
H	4.28455191748747	2.17718361358189	-2.85408491399840
C	0.89364250450115	-3.26134571535495	1.59503811033523
C	0.72686323974059	-2.14542762607724	2.03983283909555
H	-0.54129963715697	-0.55065135316123	2.54197205769831
C	0.51810925666169	-0.81580680915562	2.58277385442562
H	1.07526902328735	-0.07148878173234	2.00825262307645
H	0.85730054325915	-0.77112552046274	3.62047784208854
C	1.15261905594867	-4.59539821683565	1.16062146465173
C	2.04614067525949	-5.39131006086241	1.88418207268675
C	2.30826362500430	-6.68681762614449	1.47739758751000
C	1.68630136264677	-7.20507312971404	0.34930604374168
C	0.79894331106740	-6.41973105826863	-0.37308193647386
C	0.52891493991470	-5.12234408585874	0.02584963238049
H	2.52576998104871	-4.98231195950817	2.76509022969933
H	2.99815208209160	-7.29812523601740	2.04691213487482
H	1.90414228807419	-8.21642054188215	0.02610327708708
H	0.30996568482908	-6.81987328240768	-1.25325819395879
H	-0.16650373193022	-4.50698080613444	-0.53424344290952
H	-2.04957369675549	-3.86457427239109	0.83400991905933

$ts_{C\text{-}D\_inter}$

C	0.98386348930710	0.50213010830733	-1.36170785141245
C	1.18092987359290	1.81419900135921	-1.76142820818161
C	2.45823197113093	2.26063926410150	-2.13049275724680
C	3.55207560226845	1.43431046506825	-2.13908472303243
H	5.43284600830427	-0.53874519059012	-2.08063940781686
C	4.43687085748242	-0.86263162652756	-1.79786087388855
C	4.19105940741404	-2.16895782616875	-1.47095164011199
C	2.89056406692120	-2.54563187634341	-1.11288603723723
N	1.89578720589944	-1.68621358162664	-1.07374630627003
C	2.11054129583679	-0.38233869323037	-1.39909874728655
C	3.39130019560798	0.08010694325753	-1.78331862284546
Cu	0.00279202107974	-1.93940158620460	-0.40227594193176
H	2.65924082662910	-3.56996827189720	-0.84283764939197
H	4.97730626388162	-2.91252745270023	-1.48369464129021
H	2.57383334592561	3.29801585857233	-2.42480860539735
H	0.33298526363867	2.48343991401677	-1.76976806845126
N	-0.17425578723550	-0.09131601992170	-0.96067509743815
C	-1.41221315905162	0.45310573635683	-0.98985979622142
O	-1.71256273621843	1.60189050200049	-1.28003738635561
C	-2.44834453105072	-0.60532275952964	-0.72298947832894
C	-3.77106689400514	-0.34759223308349	-1.05317333114633
C	-4.70808635248521	-1.37222739396068	-1.05132472884719
C	-4.31707203393682	-2.66785173701895	-0.74876265071031
C	-3.00021479276412	-2.92896698613161	-0.38275522182659
C	-2.07294099104050	-1.90041697615493	-0.34554235669021

H	-4.03013749369688	0.65983707636788	-1.36203828460975
H	-5.73687319027939	-1.16472389266603	-1.32303746400267
H	-5.03779809104407	-3.47753337974715	-0.78597466720080
H	4.53075468724710	1.79824789366094	-2.42903229906359
C	0.05625379635187	-3.39075672897038	1.01658466227906
C	-0.89270123650037	-2.60853871522665	1.30362032400947
H	-2.73834334871498	-2.28043928849887	2.31317991462693
C	-1.68283581292834	-2.01594865852548	2.39114486194294
H	-1.59619856702645	-0.92778300442838	2.38297628319558
H	-1.28065419826278	-2.39706305962465	3.33452403165547
C	0.96142488110422	-4.37668662759247	1.52488929510367
C	2.16449518631264	-4.01200987826636	2.14114676680956
C	2.98667961248464	-4.97906438353844	2.69256166846259
C	2.63622975839729	-6.32137710939887	2.63584885388040
C	1.45684971675578	-6.69157589067086	2.00401505637874
C	0.63006590565492	-5.73368634640350	1.44568367676819
H	2.43462279470214	-2.96378568527126	2.20367058809479
H	3.90313694005326	-4.67822127368111	3.18725786924695
H	3.27633166016943	-7.07152894933378	3.08352073746773
H	1.16987243417294	-7.73576866245929	1.95151784041582
H	-0.28986486318638	-6.02351225268654	0.95188965333322
H	-2.70749398889873	-3.93468176498908	-0.09879223943707

D_{inter}

C	0.83641903992463	0.22123070643487	-1.42357562636679
C	0.96355904291097	1.52949302019145	-1.86477243721742
C	2.21755867558013	2.05326807053570	-2.21090264003510
C	3.36270909942444	1.30438499230484	-2.16296044641720
H	5.37187484669920	-0.50734240371574	-1.98617578672845
C	4.40190195533139	-0.89191238981091	-1.68953979555513
C	4.25672800897159	-2.18875735529826	-1.27839475202669
C	2.98893587935386	-2.62897760100165	-0.88221014517719
N	1.92585083571301	-1.85488623627499	-0.90344796872102
C	2.03281088671026	-0.57223521050463	-1.35320477454951
C	3.28506041017322	-0.03790086645113	-1.74385938430084
Cu	0.09578376891961	-2.08808048983747	-0.14305884471717
H	2.84339914890281	-3.64426702944715	-0.53195628841751
H	5.09679555855217	-2.86983499865636	-1.23835496514495
H	2.26968533851464	3.08599825857701	-2.53734105997336
H	0.07305498601452	2.13579685144232	-1.93235704425257
N	-0.30868505062080	-0.43459214785927	-1.05621328379793
C	-1.55762517721900	0.07479661011352	-1.16087167512802
O	-1.86133147800826	1.21043534283350	-1.50773386830897
C	-2.65562873234090	-0.94089313479307	-0.91494138995491
C	-3.77872725270030	-0.81271332324922	-1.72334809558328
C	-4.80023235831517	-1.74871332518074	-1.68723871379444
C	-4.71568691252217	-2.82869070066941	-0.82238155933543
C	-3.62141396733841	-2.94873156413736	0.02109519251430
C	-2.59089995827418	-2.01482263571358	-0.00974579687042
H	-3.82128361744504	0.03625189315226	-2.39468880054224
H	-5.65951705382581	-1.63389208294220	-2.33733528762681
H	-5.50663973163774	-3.56893672780610	-0.78851617445510
H	4.32340712652152	1.71956462447085	-2.44421687134415
C	-0.72140431253819	-3.22454880175257	1.20968791888936

C	-1.50579469186347	-2.11140715109432	1.01335955246900
H	-2.41668740062444	-1.08041184675658	2.64391756420557
C	-1.51612691598347	-0.98588617953168	2.02816152752532
H	-1.56134712067068	-0.01443981052253	1.53403416255019
H	-0.64359835927344	-1.02256931453768	2.68003597810117
C	-0.16085865950464	-3.87745324946975	2.33722169163617
C	-0.85113555396190	-3.92434985488188	3.56521234125688
C	-0.27597651993211	-4.50450635059411	4.67866559005087
C	0.98810588422021	-5.07620654530953	4.59687229978553
C	1.66655431327526	-5.07920937168983	3.38280058957661
C	1.09935802113064	-4.49782323582663	2.26790313949529
H	-1.83535259461812	-3.47654891753393	3.63162345264095
H	-0.81296092894983	-4.50814655732354	5.62043256694336
H	1.44153808881984	-5.52360285271106	5.47369490846754
H	2.64669554017189	-5.53624677966248	3.31263001490445
H	1.62287522388390	-4.50131840775771	1.31951289855827
H	-3.56163733155164	-3.76865991975124	0.72815308677180

Alkyne (3-Phenyl-2-propyn-1-ol***)***

H	-5.87847130832230	-2.51948499947059	0.45962868848635
C	-2.57559668734383	-4.75859513556673	2.06087094693876
C	-3.49965726849060	-3.97998508272831	1.95098269751743
O	-5.20059237868580	-3.19654901566963	0.54999281205522
C	-4.61835630711423	-3.05808035735590	1.81710006524489
H	-4.23997423216198	-2.02959864244549	1.99558059768165
H	-5.34240143910950	-3.27280111843465	2.63014549736402
C	-1.50081665253952	-5.68891768322491	2.18273969855440
C	-1.07850952535505	-6.12514913393464	3.44985485630829
C	-0.04322767778914	-7.04712956177113	3.56440587281534
C	0.58214432679537	-7.54748927722181	2.42194994916723
C	0.17093254050711	-7.11583190132526	1.16051171746199
C	-0.86127564391535	-6.19114987299215	1.03643207343410
H	-1.57999022354120	-5.73043318703599	4.33619031752838
H	0.27968637889100	-7.38498870433956	4.55242434583610
H	1.39321541536104	-8.27303913304289	2.51743815722342
H	0.66272969002959	-7.50504071325395	0.26570369946325
H	-1.19143800721562	-5.84315448018640	0.05505300691916

C_{inter}

C	0.97105349796961	0.30402241246427	-1.86190351064779
C	1.03527782864789	1.38984985532850	-2.73563884756369
C	2.27973346929098	1.89544844002769	-3.15884416660462
C	3.47697481585495	1.35918297465561	-2.73143751789834
H	5.60401818016984	0.02892050828287	-1.62718056739231
C	4.62631856252909	-0.34983055734774	-1.31542932597944
C	4.52106859207550	-1.40100781043778	-0.43087639674517
C	3.24079001867577	-1.85796995136015	-0.06719641218413
N	2.13637400720593	-1.31527948856614	-0.54257129498210
C	2.21091328868868	-0.26437520345771	-1.40682399695042
C	3.46189408259209	0.26319399220597	-1.83549691233010
Cu	0.16864640138874	-1.78648636514967	-0.15143550938941
H	3.12211325013121	-2.69430102574513	0.62692150866744

H	5.40268076640640	-1.88659112255045	-0.00899941713470
H	2.28799987326818	2.74738468823212	-3.84363262075924
H	0.09944577767530	1.83389121406164	-3.07141109796273
N	-0.13827330741236	-0.30936828920853	-1.36601880105016
C	-1.43888204416449	0.05432972006914	-1.56765670262599
O	-1.82893084893749	1.01792736678507	-2.20768197883432
C	-2.36308091466607	-0.90585036223463	-0.87881589442728
C	-3.74455850999207	-0.74911966592350	-0.97924724038080
C	-4.58455281386479	-1.66316188760955	-0.34445878047389
C	-4.03952458998315	-2.72867270866116	0.37399476540548
C	-2.64954855758449	-2.87751972814888	0.47428867909838
C	-1.79243017310790	-1.96411688704183	-0.14651566652918
H	-4.13389518814487	0.09414878274523	-1.55600756874551
H	-5.66906407392693	-1.54277606277153	-0.40752244220130
H	-4.69944370756661	-3.44515313996575	0.87053097195069
H	4.43203646628904	1.76995512215035	-3.06626496263383
C	0.72562001828571	-3.28902412227843	1.66510739154351
C	0.32579645272242	-2.24972435757020	2.17185835204399
O	-1.64793702695283	-1.09978541809916	2.89023731728560
C	-0.26853193419276	-1.03570256856449	2.76432053577921
H	0.07280856962547	-0.16373910563619	2.16853791832969
H	0.15936212069911	-0.90321243789079	3.77193475486822
C	1.21744822402508	-4.50925036664291	1.10371627940114
C	2.31025132640384	-5.16941974407660	1.69086097654785
C	2.80299958627931	-6.33864780352082	1.12250290904762
C	2.21241779256414	-6.86277414159847	-0.02795202053449
C	1.12085276724759	-6.21710058996621	-0.60894453793759
C	0.62142532577056	-5.04542065426368	-0.05064286070041
H	2.76593395969522	-4.75016222387599	2.59037102050104
H	3.65051967487547	-6.84986608045280	1.58457364475483
H	2.60845154478299	-7.77695305876816	-0.47623103483262
H	0.65011901686654	-6.63151973631639	-1.50313829780999
H	-0.23365043332447	-4.53179254842542	-0.49968038829232
H	-2.24523814835627	-3.70755644456621	1.06401235522900
H	-2.02488098652510	-1.25147941831538	2.00841439208018

ts$_{C\text{-}D_inter}$

C	0.93422051427292	0.22589566505335	-1.53593856750066
C	1.00163593692738	1.40431634788842	-2.27619276989844
C	2.24428004043465	1.92499884363966	-2.68485458587851
C	3.43727437911371	1.31396687390127	-2.36128760279747
H	5.56407636323365	-0.17318340143799	-1.49350754201823
C	4.58919601028325	-0.56781689100713	-1.19302608494381
C	4.48989084852273	-1.71449972984423	-0.43723390697851
C	3.21157991853728	-2.18984952200082	-0.08697404924727
N	2.10520414186338	-1.57282288732161	-0.45192465719028
C	2.17255931740691	-0.42732519200142	-1.18912169363414
C	3.42103373905571	0.12244163056327	-1.59595731540423
Cu	0.14894316226079	-1.95810300885530	0.03555003268431
H	3.09361818239622	-3.10164149211460	0.50634351484757
H	5.37475073463039	-2.26079050296307	-0.10636710106362
H	2.25508015723515	2.84952305568322	-3.26764106763855
H	0.06693126491362	1.90503857048413	-2.52563866405163
N	-0.18012934482560	-0.41041405198601	-1.08022352444781

C	-1.46617205802010	-0.01101076850048	-1.20033524492888
O	-1.88904428798362	1.00558209650471	-1.73179775386484
C	-2.39669941989697	-1.06923607523386	-0.64625295650060
C	-3.72892347532834	-1.04387171354450	-1.06206121437797
C	-4.58998181021331	-2.09880610774873	-0.75854101788550
C	-4.11397365597232	-3.19866434123910	-0.04781491791902
C	-2.79590756186609	-3.21188918170818	0.41527530239654
C	-1.92877090804256	-2.15154645274405	0.13863496614689
H	-4.05001149112514	-0.18661643938369	-1.65998633261728
H	-5.62880780745703	-2.06865914750924	-1.09549852796188
H	-4.77826371065414	-4.03359569766612	0.18795558014233
H	4.39275306759340	1.73769192132257	-2.67840983472393
C	0.02668214015838	-2.96630202624091	2.03604772239566
C	-0.85946354520678	-2.06477334187722	1.79672978287821
O	-2.85955565635386	-0.87557084946069	2.56493691483687
C	-1.47365613064891	-0.87495801277979	2.49248745678544
H	-1.07784880867965	0.03212660773867	1.99425338732258
H	-1.08671432241090	-0.87964568192100	3.52250229438355
C	0.77473809445467	-4.15377146496560	1.71445723841072
C	1.91625890785267	-4.51262530576406	2.45738405340864
C	2.66434199148292	-5.63523397820437	2.11034201918351
C	2.28959441147429	-6.42444961845595	1.02217078197664
C	1.15336129178498	-6.09001210265956	0.28402404402329
C	0.40202049182996	-4.97050300530085	0.62295518869178
H	2.20840300331116	-3.89224705007539	3.30681321590147
H	3.54667518776470	-5.90129355075762	2.69730719854809
H	2.88089692219136	-7.30102853018359	0.74799393552678
H	0.84937854422574	-6.70498963193229	-0.56614807557232
H	-0.48138822527555	-4.70784204897528	0.03675188570552
H	-2.46236906276842	-4.03500033101558	1.05292088212547
H	-3.20856848248277	-0.75483547739942	1.67315361072352

D_{inter}

C	0.86624256157278	0.21376831895121	-1.67192946164117
C	0.88460333724363	1.33129931249060	-2.50893572441744
C	2.09280942788742	1.84872262102128	-3.01394972802456
C	3.31488805725775	1.30072749097515	-2.69333487120565
H	5.50867861700558	-0.03886965913050	-1.79126760137768
C	4.56065821022707	-0.44746813416870	-1.42974223756795
C	4.53274503154933	-1.53882766834239	-0.58957282773001
C	3.28568220712543	-2.03623197587566	-0.17134291591863
N	2.14690854677690	-1.48416107005449	-0.54375849137855
C	2.13983561635728	-0.38117466828916	-1.34647759354407
C	3.35705066856385	0.17112764588732	-1.84147842640827
Cu	0.27989461637045	-1.91090523853143	-0.00561879911798
H	3.21739115957665	-2.91050134353461	0.48230134799590
H	5.44822346744554	-2.02499192075807	-0.24863878117382
H	2.04677661466940	2.72322224150505	-3.66806674498865
H	-0.06573747750543	1.79758828297743	-2.75727672800853
N	-0.23268576635317	-0.41443179694837	-1.13186469061343
C	-1.50457928101722	0.01471375437075	-1.34155075604031
O	-1.82409910458189	1.04616605888822	-1.92234646731523
C	-2.60911738122827	-0.93093872744675	-0.89812563917560
C	-3.82362181452632	-0.77317043195679	-1.57548735655915

C	-4.89503252752707	-1.63470884388523	-1.36023228161430
C	-4.77111510828823	-2.68237114957297	-0.44942232288773
C	-3.58298654194717	-2.83428039467341	0.26319284800530
C	-2.50409675850893	-1.96281221737018	0.06159726343145
H	-3.89035649683964	0.05243115530066	-2.28688880559615
H	-5.82899475869163	-1.48358166617632	-1.90690554169745
H	-5.60216051038078	-3.37015352408452	-0.27477862106185
H	4.24577417070939	1.72512445149685	-3.07555795101664
C	-0.59627469780671	-3.18578228889280	1.21857604148320
C	-1.36394443554059	-2.05767865930575	1.02343448584206
O	-2.50654808941096	-1.12239016893622	2.92109658744826
C	-1.39639004727871	-0.95318940835197	2.08506288720950
H	-1.39754383813609	0.03124730417324	1.58012469098042
H	-0.50152435939544	-1.01238717063193	2.72104457777869
C	-0.16373148170555	-4.01553210152802	2.28683993614134
C	-0.85976736047121	-4.00526290490595	3.52265599504429
C	-0.45119519065467	-4.83027353038514	4.56209640482175
C	0.62574348789148	-5.70636681946071	4.39457057107397
C	1.30957669337285	-5.74127699172945	3.17515327690402
C	0.92721454548202	-4.90434710197590	2.13689212516701
H	-1.70332723360825	-3.32040770876241	3.64715238855562
H	-0.98187546716412	-4.79123141305804	5.51658672913939
H	0.93430349434813	-6.36037765631821	5.21344289836677
H	2.14745583430853	-6.42851508258736	3.03593295095564
H	1.44951501918352	-4.93720208867776	1.17771512297081
H	-3.48063291628786	-3.62613900572397	1.00974049847472
H	-3.29964674006906	-1.08179110600661	2.37079773829069

Direct reductive elimination Cu(II) to Cu(0)

$ts_{E\text{-}H}$

C	2.66199935539060	0.42681576896716	1.08734366986573
C	3.23845871766889	0.94013602647281	2.24107779032656
C	4.58021174148283	1.36036050830123	2.27607738942351
C	5.36693379619972	1.29419965749528	1.14729204714601
H	6.60862610340470	1.07096067536585	-1.26402622758847
C	5.58038274371997	0.69970853001745	-1.25663217280386
C	5.01192426502170	0.17521121268706	-2.39360424235909
C	3.69341804718906	-0.30775720301169	-2.32548921375924
N	2.96416798249920	-0.24364407026777	-1.22559547571620
C	3.48395819341530	0.31170460637215	-0.08600426532980
C	4.83330462685326	0.77568744928886	-0.05555753380380
Cu	1.33760025881550	-1.19388823100606	-0.69008418197645
H	3.22406885419074	-0.76641453110234	-3.20010231579430
H	5.56370102887717	0.11550037997471	-3.33296251653489
H	4.99139681238532	1.76893717821639	3.20237762213310
H	2.60732323104497	1.04838239952731	3.12496818675073
N	1.31005452487921	0.07590744499276	1.04044659905933
C	0.39585997411696	1.10785551641100	0.92093945451454
O	0.73091840505635	2.28077751944891	0.84003301935987
C	-1.03863735407924	0.71140403709137	0.94931986330410
C	-2.05473632772294	1.67683592896268	0.91694568222704
C	-3.38332650104251	1.31062580654025	1.13157994960704
C	-3.75814193841497	-0.01195303141234	1.44426704524129

C	-2.74895904357381	-0.95598744706562	1.49715927424224
C	-1.42086737992727	-0.61357072868783	1.18848160436028
H	-1.77018573634069	2.71714812547359	0.74704451757150
H	-4.15965763640923	2.07871007798902	1.09054376060687
H	-4.79336570370331	-0.27801352325821	1.66446354880767
H	6.40098382715923	1.64624252764595	1.16111610979743
C	0.71974423128031	-1.84503250818418	1.01605093642528
C	-0.62158661366113	-1.76818486416334	1.35851061239592
O	-2.85502376172826	-2.25264971888123	1.86168995916327
C	-1.54569789120039	-2.83140787244620	1.89945080089049
H	-1.31425716905425	-3.13558659777709	2.93808873940971
H	-1.55294081088499	-3.74534680608091	1.28265329366425
C	1.67337876095492	-2.71219367098293	1.72625042309698
C	2.07121926247631	-2.39994380236042	3.03817084564951
C	2.99790376334301	-3.19425203750697	3.70722642917508
C	3.51765819464382	-4.33442315172044	3.09332747113035
C	3.11280254837876	-4.66955571307923	1.79989425578842
C	2.21822887480193	-3.85281391331181	1.11385806190708
H	1.64869318123161	-1.51406848437052	3.51796099290334
H	3.32035919134245	-2.91790315118798	4.71488352476651
H	4.23839041468434	-4.96245614061080	3.62244001553805
H	3.51513372681657	-5.56221007701501	1.31437728704104
H	1.91359722841830	-4.09460610175093	0.09118136237594

H

C	2.85283682230361	-0.54099493625236	0.78080150347196
C	3.95614755016180	0.01412481181017	1.38327479442278
C	5.21394072891183	0.03093116669141	0.77009171852762
C	5.37538551175165	-0.50281806429479	-0.47515743296377
H	5.37360298918976	-1.52318655059835	-2.93383098392473
C	4.39622302677408	-1.54053033167979	-2.46384464405186
C	3.30175149593231	-2.01229276251638	-3.13188100895759
C	2.07826606611100	-2.01890819576635	-2.46287565035090
N	1.91975537934841	-1.59366672253830	-1.22412807336351
C	2.98430009025546	-1.08609728664687	-0.53356869054826
C	4.26709776268917	-1.04959811165634	-1.15289561753422
Cu	0.20184924654538	-1.82976127113401	-0.33101602118583
H	1.18779028188633	-2.39314919897308	-2.95575149748413
H	3.36318480852504	-2.38227379858305	-4.14655637898234
H	6.05343000318685	0.47354639618936	1.29221059041438
H	3.82671200664913	0.45736318521146	2.36120363539466
N	1.60415065971216	-0.47500918969813	1.45462511907555
C	1.02509915481231	0.81793635582137	1.53833019474505
O	1.70598110662388	1.81256346739179	1.41054646755754
C	-0.42897057183707	0.82677286707606	1.70520433830574
C	-1.20742182449415	1.97981029825089	1.86842847701500
C	-2.57628783389314	1.85769783251782	2.01768097402184
C	-3.21988396229777	0.60481941139115	2.06920703936310
C	-2.43924604558121	-0.51298348791731	1.91082393649353
C	-1.07873921117373	-0.38819702535944	1.65406623820817
H	-0.72433111229203	2.94824040267202	1.88342588385018
H	-3.17646574770752	2.75107431163506	2.14184225331637
H	-4.28265612259403	0.53034865575165	2.26371334377515
H	6.34053299619503	-0.50586028535057	-0.96763744459051

C	0.93086320297082	-1.70988485532951	1.72394707129459
C	-0.49070801286312	-1.69414595372537	1.53475824802823
O	-2.79511096708080	-1.82019013375525	1.99874573244976
C	-1.57610932146073	-2.59593315404047	2.10133470366791
H	-1.39655942434176	-2.82375690093212	3.16273976416629
H	-1.74820200540881	-3.52697685467122	1.56748779497176
C	1.69841817667552	-2.85253348957875	2.14262893297369
C	2.89878645166346	-2.73957782239551	2.86936050800221
C	3.59943378161910	-3.86307007184887	3.26059246037463
C	3.14093435041514	-5.13808326788883	2.94553814442737
C	1.95454794400267	-5.26949523462068	2.23453880741353
C	1.24472522063977	-4.15114855521020	1.84233748186842
H	3.26314098980233	-1.76130386779564	3.15069642793956
H	4.51442345357291	-3.74447086262222	3.83003080313370
H	3.69512209246668	-6.01425265166076	3.25922663507973
H	1.57973328324805	-6.25311309226951	1.97353636119031
H	0.33486852838425	-4.27471217510012	1.26659205899732

Inclusion of Explict TFE solvent

E_{TFE}

C	1.88825818985023	0.43251311155828	-1.93137214546102
C	2.21394674970030	1.32740992788817	-2.95531668052499
C	3.47709354190439	1.94728281155130	-3.02036959835600
C	4.46392493430177	1.70836179440005	-2.09083460790415
H	6.10745526592634	0.97863285202398	-0.03222558985568
C	5.11520550148269	0.52098925830278	0.00256336135695
C	4.77410823078665	-0.34110703888788	1.02121777265266
C	3.48228002934645	-0.89542128467219	1.03070824610732
N	2.59868116772653	-0.61684867562666	0.09271281416785
C	2.90278277308989	0.21359424394580	-0.93618750910002
C	4.18606214619796	0.83017995840510	-1.01847548420778
Cu	0.63844888823980	-1.05189321616226	0.03538197267777
H	3.15854936906834	-1.58623758851014	1.81306094708035
H	5.47945518218134	-0.59587821023858	1.81351245273535
H	3.67458137627016	2.63054455140670	-3.85030567770781
H	1.48356642542731	1.52148826883458	-3.73419632535984
N	0.69377325754853	-0.25602024484709	-1.75929182673880
C	-0.13517036927413	-0.42927674729436	-2.83417702760379
O	0.17301777199307	-0.08745898815517	-3.97080551675419
C	-1.50398688557769	-1.06980677387474	-2.69975699269285
C	-2.00796710135320	-1.54847875969565	-3.92445474257032
C	-3.32722754295343	-1.95869526645762	-4.08270032960325
C	-4.23673703041190	-1.86172802577793	-3.03045148294681
C	-3.74596803626254	-1.39686349780286	-1.82111703412006
C	-2.39222038408989	-1.05891283839451	-1.60708470244499
H	-1.33130735492186	-1.53693965585562	-4.77827722895948
H	-3.66543710641396	-2.33264319618234	-5.05232893645744
H	-5.28735123893810	-2.13687516139583	-3.13507475950708
H	5.44566606121194	2.17977631924220	-2.16882046901151
C	-1.19653837951231	-0.83825660710615	0.61913123426710
C	-2.28333648021644	-0.81753360824407	-0.16587015384102
O	-4.52044072836047	-1.24321121561050	-0.72616096394183
C	-3.71658700140486	-0.70016485965711	0.31263182137267

H	-4.00264800302560	0.35551420143850	0.47908824867757
H	-3.91523687066728	-1.25211963877599	1.24134705599643
C	-1.23181556146080	-0.77450433969884	2.08576278059026
C	-0.59662575040805	0.27783656839481	2.77870214110891
C	-0.50509947362686	0.27449628231329	4.16716257633200
C	-1.03214414220423	-0.78541753079060	4.90847618103155
C	-1.65730397733406	-1.84141006491595	4.24678902524888
C	-1.75186069015918	-1.84288204084566	2.85365007804284
H	-0.17004065502791	1.10165664528589	2.20046385644301
H	-0.01065669584468	1.10402699204811	4.67910593430767
H	-0.95023098832212	-0.78898906460684	5.99752978277734
H	-2.07613116850994	-2.67322011297904	4.81896797653449
H	-2.24422629650919	-2.67362222394243	2.33855080440462
C	2.06975091805051	-4.35066126572115	0.47544895069281
F	3.16068841187386	-4.24622346476309	1.23497300269053
F	1.97005808963626	-5.61459117717512	0.07027610362748
F	2.25010182002392	-3.58009477236309	-0.59620459174563
C	0.81975178687748	-3.95299485137574	1.23018264699545
H	0.72173027982856	-4.62878487498001	2.09521935229066
H	-0.04323543719307	-4.10767043432340	0.55852719236880
O	0.95229918565930	-2.61617487887183	1.63010171002381
H	0.22410999578021	-2.38361759046147	2.23710935481324

$ts_{E\text{-}H\_TFE}$

C	3.06698143296735	-0.97533307084210	0.81848566399918
C	3.64859782200801	-0.33763755232845	-0.25845033421250
C	4.95426382319192	0.16120978911495	-0.18982656774029
C	5.69417026782200	0.04011491068304	0.95650551161716
H	6.86852402771841	-0.38221921188578	3.35798689563874
C	5.85112207530590	-0.75311057895918	3.29205180970088
C	5.25961334028898	-1.37922841467644	4.35368349966774
C	3.94037275454438	-1.82760839783902	4.21945431193981
N	3.24125788752694	-1.69055252293360	3.11115109882245
C	3.81304950211535	-1.08791655564544	2.02827451765509
C	5.13787534960741	-0.58363503091283	2.08859792485864
Cu	1.32268211759095	-2.03663954429653	2.80878155819155
H	3.44342047685096	-2.32523501981609	5.04430855949154
H	5.78667795980194	-1.53786913815986	5.28566543718443
H	5.38505169623106	0.63814867542624	-1.06263760859334
H	3.08301640521106	-0.25559264147010	-1.17708248342116
N	1.78603615210291	-1.50471141674876	0.77253342225375
C	1.44247415942282	-2.41555678330960	-0.19424698198831
O	2.22120837085466	-2.85668472792868	-1.02804000810000
C	0.02380906476558	-2.84658860906977	-0.16815797401922
C	-0.43358109445433	-3.91744906208309	-0.94145572186889
C	-1.78763258139976	-4.19936270859964	-1.02174786199838
C	-2.75954439562225	-3.39002419338561	-0.40402945666479
C	-2.30720743688061	-2.31423989241395	0.32255709680829
C	-0.93600645886347	-2.08591107183948	0.50448671978053
H	0.29321782036149	-4.50078237644316	-1.49268617639858
H	-2.11796467776239	-5.04589198656697	-1.61139654117514
H	-3.81613541546369	-3.59446957252421	-0.52355878383772
H	6.70853432702577	0.41905910598514	1.00929387136288
C	0.41850386660527	-0.53726679634548	1.85628029209639

C	-0.77330991905325	-0.91753928500512	1.28494724985962
O	-3.04842664967887	-1.35994081953933	0.93159822562760
C	-2.15447807405414	-0.32990049679793	1.41746947908549
H	-2.30750084314751	0.56913209286590	0.80671736910627
H	-2.43324339930562	-0.09746691804346	2.44760636176549
C	0.81204920606725	0.84730599890132	2.08504885442062
C	0.84225251739485	1.74298289366662	1.01006749877585
C	1.24715255061131	3.05250033019486	1.19284570940398
C	1.61385500406728	3.49490566141862	2.45682835002461
C	1.59549237655514	2.61606883747457	3.53182914211247
C	1.21793337380609	1.29764581046482	3.34242376164894
H	0.55955281987194	1.38344793034423	0.02701961527163
H	1.27971661211782	3.73190543052916	0.34878192041748
H	1.93232966886551	4.52078813476159	2.60147777973476
H	1.89604845640636	2.95877033957152	4.51522634469010
H	1.22818869152770	0.59371182504231	4.16752050375086
C	0.34651717180355	-5.05266741109610	2.61846214237988
H	-0.48402830105770	-5.74227139035188	2.79409365142045
H	0.70236321711851	-5.16057549276331	1.58944652891354
C	1.47168107862149	-5.45148866386345	3.53994415485002
F	2.55499501448538	-4.68835738970924	3.35989297503504
F	1.81866259216423	-6.71855626843695	3.29724240129921
F	1.12237547341014	-5.35532303507690	4.82667674764093
O	-0.03199890032947	-3.72393099176033	2.90958146626839
H	-0.61523737774262	-3.41964572697696	2.19525107544610

H_{TFE}

C	3.19083591944566	-0.82018148475909	0.51415123104490
C	3.90305981472036	-0.24092191333555	-0.53168585960132
C	5.21508134151096	0.14264300130618	-0.33567161171910
C	5.80675394529923	-0.05161394062095	0.90236407239880
H	6.72454057723559	-0.52120295217847	3.40684792627481
C	5.71077004242933	-0.86098169219703	3.23364519311322
C	4.96455868784521	-1.46787672951524	4.24229215575684
C	3.68660323469087	-1.87897715128080	3.98490476606366
N	3.07441415507565	-1.72284882412007	2.76595501878307
C	3.76784918119940	-1.08549339238952	1.76339610358836
C	5.11992758127246	-0.65786233186957	1.96469339761299
Cu	1.59038029460999	-2.83411855995538	2.53714185650261
H	3.09113567131725	-2.35697896284852	4.75282779001620
H	5.38187142366823	-1.62898150976033	5.22883142033645
H	5.77542906520483	0.59662984066550	-1.14406004617374
H	3.40988517118707	-0.09439426943972	-1.48452338111883
N	1.81209097409929	-1.15107451370501	0.30360158429242
C	1.55863300567146	-2.39601290628553	-0.32132749055765
O	2.46182054214176	-3.06283418048906	-0.77823825590919
C	0.15513000437666	-2.81202693156037	-0.28543739605610
C	-0.33412348629319	-4.09164062115732	-0.61571946416731
C	-1.67504012714856	-4.37410578065079	-0.40068140262497
C	-2.59152181402597	-3.43706902759019	0.12924947426737
C	-2.09871808215298	-2.19302226395345	0.44152318171198
C	-0.74944071910940	-1.91284048963336	0.23684569838175
H	0.33979098614745	-4.83128617961433	-1.02992514267467
H	-2.04776472671435	-5.35867628036472	-0.66013201746142

H	-3.62512491425285	-3.70905715460774	0.30017214446887
H	6.83009961492548	0.26643532356977	1.07192352232416
C	0.85513848573870	-0.28307218010330	0.82238265856304
C	-0.44679204031315	-0.64724238428746	0.76620133111552
O	-2.72485827858221	-1.14471624358370	1.01812888804319
C	-1.76233109861444	-0.06333553078056	1.19747154233468
H	-2.08636780126168	0.77343057328344	0.57244128657934
H	-1.80209724807110	0.24481913042406	2.24365210921224
C	1.33281379426014	0.95806775322767	1.46765890485044
C	1.82749763441386	2.02059860035126	0.71664439060057
C	2.28890291538459	3.16198886563982	1.34874853630562
C	2.26006532466672	3.25227482340092	2.73394524995286
C	1.75715479835151	2.20240266091333	3.48585897823747
C	1.29242100973264	1.05870232883888	2.85516187218390
H	1.86877269049853	1.94044847574713	-0.36280537869421
H	2.68617691883088	3.97837892415511	0.75743325015784
H	2.63767241171867	4.14037955209262	3.22683834248344
H	1.73949929378333	2.26768426249123	4.56726249177456
H	0.94075031575179	0.21608641728052	3.43777383090301
C	-0.06734602069923	-5.30398266066353	3.08021760812654
H	-0.41300258953647	-5.06945349454092	4.08745133832106
H	-0.80699083358754	-5.93194918739652	2.58031579593006
C	1.23026295542160	-6.08228385377409	3.18002874538781
F	1.71976237822454	-6.36316733227817	1.97125680546858
F	1.03119187998125	-7.23142510046769	3.82919611272462
F	2.15137132960900	-5.38265524309489	3.85081089332939
O	0.10257046449854	-4.09683702542148	2.36955107865631
H	-0.11011705457730	-4.23221125311301	1.42324086857796

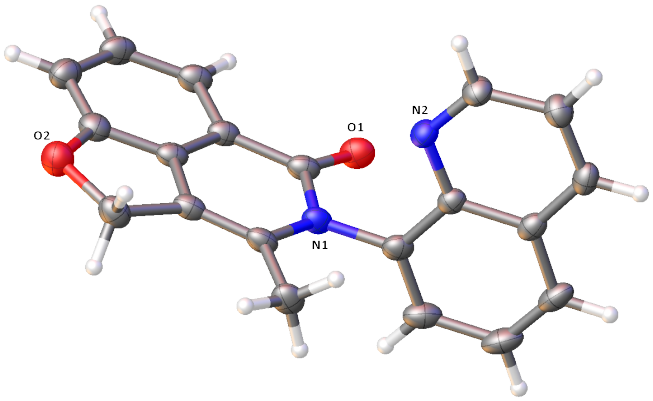
Inclusion of Mn(II)(OAc)$_2$

ts$_{C\text{-}D(Mn)}$

C	-0.78290036024193	1.20772023500363	-2.24084490916617
C	-0.99168964138857	1.18321802589211	-3.61012510204146
C	-0.00865433482635	1.66511513565032	-4.48747119976462
C	1.17838155104073	2.18781617167053	-4.04398402500357
H	3.36831133520494	3.17893471211781	-2.74717460458962
C	2.60048567846859	2.78327303508933	-2.09084741736430
C	2.75578645623922	2.81970796905575	-0.73130392602303
C	1.73773100968096	2.30432695358968	0.07889020445644
N	0.64350848453284	1.77032370225872	-0.41942642532741
C	0.45762744124037	1.73408277673010	-1.76623816125525
C	1.43234934994798	2.23831906686749	-2.65844045941362
Cu	-0.96599814196990	0.97038522756231	0.54627401505074
H	1.81878101603124	2.33328288407591	1.16001553845997
H	3.64286077728580	3.23397411881217	-0.27163441255837
H	-0.21513207403608	1.63425555099054	-5.55181702534974
H	-1.92799248596638	0.79597570241432	-3.98328135808817
N	-1.63420112260000	0.80744580596344	-1.25300772845132
C	-2.88217475642239	0.29917000641507	-1.42441354929397
O	-3.47798623331635	0.13781592954710	-2.47908396638562
C	-3.46714808358780	-0.06717078564951	-0.09680081758572
C	-4.82918092852681	-0.27161692806354	0.06915291619849
C	-5.33338236244593	-0.52075144974513	1.33996995595391

C	-4.48164637154384	-0.63996839434952	2.43220881563027
C	-3.12074112574638	-0.48752143999434	2.22477818770569
C	-2.59684901006133	-0.14081135226408	0.99593724597827
H	-5.47841216522319	-0.20216732163287	-0.79599261072189
H	-6.39981933727858	-0.65267952954041	1.48288317713163
H	-4.85790508862715	-0.88315950609480	3.41920279141714
H	1.91788863839368	2.57415628104503	-4.73580693843021
C	0.01592715363941	-1.76579909146217	0.49821058640414
C	-0.77096579598942	-1.33770670437743	1.39400922031080
O	-2.23269354106392	-0.74663556994789	3.24461784149540
C	-1.21959036064397	-1.60652450385025	2.79399245913784
H	-0.38274366971082	-1.52245914491104	3.49046877282148
H	-1.58653469207691	-2.64179093011891	2.82185017035767
C	0.17275116902828	-1.94064299450484	-0.91479168714432
C	1.40398879567393	-1.79044414414426	-1.55843819282089
C	1.48760035044755	-1.91549037044650	-2.93447747037278
C	0.35553801026006	-2.20505967091729	-3.68169709459475
C	-0.86844987781427	-2.37728460291331	-3.04746858563980
C	-0.96170504126263	-2.25394797124354	-1.67544403673810
H	2.29175115160567	-1.55614739692894	-0.98078562661365
H	2.44293179066421	-1.78262539540624	-3.42753404808074
H	0.42494381211240	-2.29460186179092	-4.75926947311999
H	-1.76133919130816	-2.58576728500000	-3.62408065062330
H	-1.91569350752339	-2.37418822792347	-1.17756501316430
C	4.00272159170511	-1.16841852397693	1.74714109107774
O	3.52557600785652	-0.30518951459244	0.94427324458379
O	3.22457439727500	-1.87377667049268	2.44490463751408
C	5.48360391654013	-1.29813411129144	1.89724868367388
H	5.79583861772359	-0.62912602276224	2.70313554566704
H	5.99266460443227	-0.98740757567226	0.98668539870779
H	5.75504971786995	-2.31305529318078	2.18273314291501
C	0.04526347715467	1.33451649021503	3.28207928288300
O	-0.60291511501526	1.79278031760519	2.32057373260338
O	1.02944030087277	0.53923839694630	3.16959007426574
C	-0.37600767590128	1.69875325295975	4.67335734142214
H	0.42949712942145	1.52588748374383	5.38405602667060
H	-1.21480264708965	1.04314023516393	4.92276869695063
H	-0.73746344468196	2.72524837110810	4.71732545165973
Mn	1.61504445154129	-0.69709255330354	1.70447526662216

[8] X-Ray Crystallography Data:



A suitable crystal of **2p** was selected and data collected following a standard method.[9] The crystal (0.200×0.160×0.050 mm^3) was mounted on a MITIGEN holder in perfluoroether oil on a Rigaku FRE+ diffractometer equipped with VHF Varimax confocal mirrors, an AFC12 goniometer and HyPix 6000 detector. The crystal was kept at a steady T = 100(2) K during data collection. The structure was solved with the ShelXT[10] structure solution program using the Intrinsic Phasing solution method and by using Olex2[11] as the graphical interface. The model was refined with version 2018/3 of ShelXL[12] using Least Squares minimisation.

Crystal Data. $C_{20}H_{14}N_2O_2$, M_r = 314.33, monoclinic, $P2_1/c$ (No. 14), a = 9.9390(2) Å, b = 7.7806(2) Å, c = 19.4608(4) Å, β = 94.236(2)˚, α = γ = 90˚, V = 1500.82(6) Å^3, T = 100(2) K, Z = 4, Z' = 1, μ(Mo K$_\alpha$) = 0.091 mm^{-1}, 23520 reflections measured, 3878 unique (R_{int} = 0.0228) which were used in all calculations. The final wR_2 was 0.1314 (all data) and R_1 was 0.0488 (I > 2(I)).

Compound	**2p**
Formula	$C_{20}H_{14}N_2O_2$
$D_{calc.}$/ g cm^{-3}	1.391
μ/mm^{-1}	0.091
Formula Weight	314.33
Colour	yellow
Shape	block
Size/mm^3	0.200×0.160×0.050
T/K	100(2)
Crystal System	monoclinic
Space Group	$P2_1/c$
a/Å	9.9390(2)
b/Å	7.7806(2)
c/Å	19.4608(4)
α/˚	90
β/˚	94.236(2)
γ/˚	90
V/Å^3	1500.82(6)
Z	4
Z'	1
Wavelength/Å	0.71075
Radiation type	Mo K$_\alpha$
Θ_{min}/˚	2.055
Θ_{max}/˚	28.698
Measured Refl's.	23520
Ind't Refl's	3878
Refl's with I > 2(I)	3485
R_{int}	0.0228
Parameters	218
Restraints	0
Largest Peak	0.413
Deepest Hole	-0.231
GooF	1.037
wR_2 (all data)	0.1314
wR_2	0.1287
R_1 (all data)	0.0534
R_1	0.0488

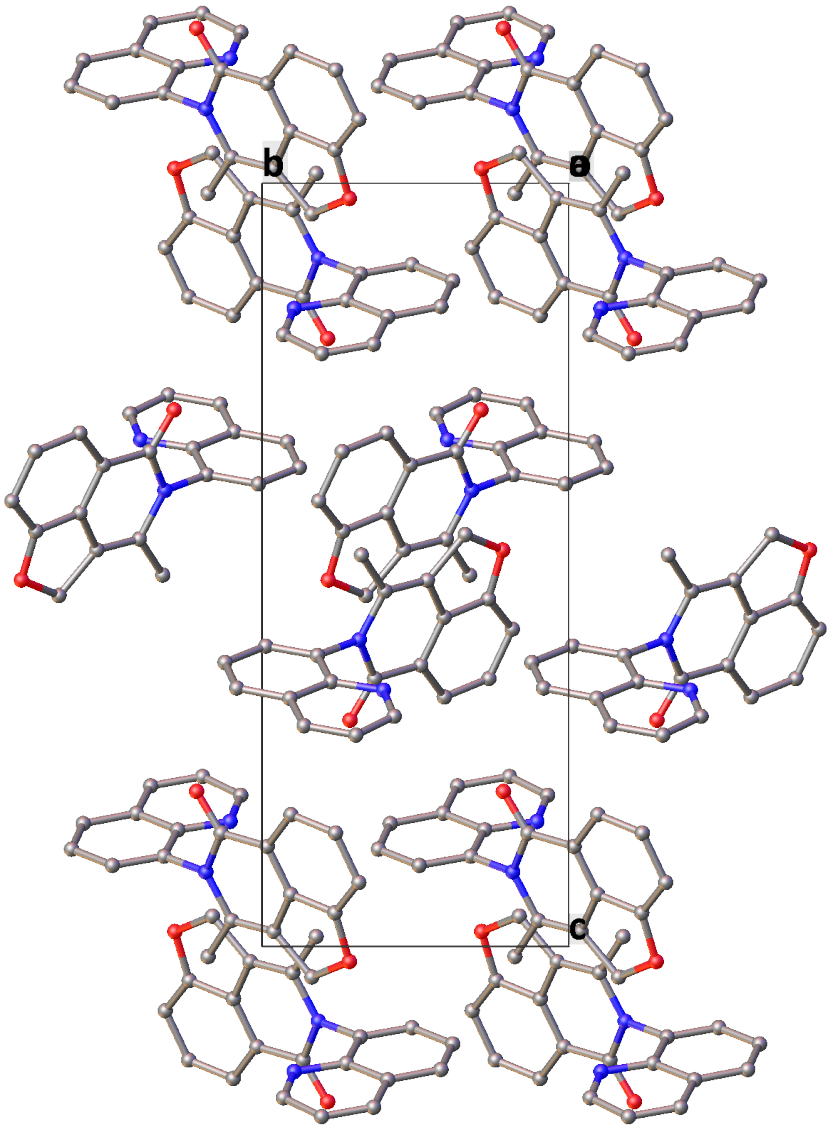


Figure S105: Packing diagram of **2p**.

Table S1*: Bond Lengths in Å for* ***2p****.*

Atom	Atom	Length/Å
O1	C1	1.2314(17)
O2	C6	1.3782(17)
O2	C9	1.4759(18)
N1	C1	1.4079(16)
N1	C10	1.4148(17)
N1	C12	1.4396(18)
N2	C17	1.3721(17)
N2	C18	1.3158(18)
C1	C2	1.460(2)
C2	C3	1.4123(17)
C2	C7	1.3801(18)
C3	C4	1.385(2)
C4	C5	1.415(2)
C5	C6	1.374(2)

Atom	Atom	Length/Å
C6	C7	1.383(2)
C7	C8	1.4158(17)
C8	C9	1.507(2)
C8	C10	1.338(2)
C10	C11	1.4937(17)
C12	C13	1.368(2)
C12	C17	1.4192(18)
C13	C14	1.410(2)
C14	C15	1.365(2)
C15	C16	1.4191(19)
C16	C17	1.4177(18)
C16	C20	1.414(2)
C18	C19	1.411(2)
C19	C20	1.361(2)

***Table S2**: Bond Angles in ° for **2p**.*

Atom	Atom	Atom	Angle/°
C6	O2	C9	108.14(11)
C1	N1	C10	126.42(12)
C1	N1	C12	114.46(11)
C10	N1	C12	118.65(10)
C18	N2	C17	116.62(12)
O1	C1	N1	120.34(13)
O1	C1	C2	124.77(12)
N1	C1	C2	114.89(11)
C3	C2	C1	126.48(12)
C7	C2	C1	116.59(11)
C7	C2	C3	116.91(13)
C4	C3	C2	118.84(13)
C3	C4	C5	123.55(13)
C6	C5	C4	116.40(14)
O2	C6	C7	110.89(12)
C5	C6	O2	128.65(14)
C5	C6	C7	120.45(13)
C2	C7	C6	123.84(12)
C2	C7	C8	125.92(13)
C6	C7	C8	110.24(12)
C7	C8	C9	105.88(12)
C10	C8	C7	118.69(12)
C10	C8	C9	135.42(12)
O2	C9	C8	104.85(11)
N1	C10	C11	117.78(12)
C8	C10	N1	117.48(11)
C8	C10	C11	124.71(12)
C13	C12	N1	120.84(13)
C13	C12	C17	121.13(13)
C17	C12	N1	118.02(12)
C12	C13	C14	120.50(14)
C15	C14	C13	119.97(14)
C14	C15	C16	120.79(14)
C17	C16	C15	119.53(13)
C20	C16	C15	122.93(13)
C20	C16	C17	117.53(12)
N2	C17	C12	118.92(12)
N2	C17	C16	122.99(12)
C16	C17	C12	118.09(12)
N2	C18	C19	124.70(13)
C20	C19	C18	118.91(13)
C19	C20	C16	119.23(13)

***Table S3**: Torsion Angles in ° for **2p**.*

Atom	Atom	Atom	Atom	Angle/°
O1	C1	C2	C3	0.4(2)
O1	C1	C2	C7	-177.92(12)
O2	C6	C7	C2	-179.95(12)
O2	C6	C7	C8	-0.34(16)
N1	C1	C2	C3	179.56(12)
N1	C1	C2	C7	1.22(17)
N1	C12	C13	C14	178.84(12)
N1	C12	C17	N2	1.33(17)
N1	C12	C17	C16	-178.47(11)
N2	C18	C19	C20	-0.4(2)
C1	N1	C10	C8	0.98(19)
C1	N1	C10	C11	179.05(12)
C1	N1	C12	C13	-91.18(15)
C1	N1	C12	C17	87.41(14)
C1	C2	C3	C4	-178.56(12)
C1	C2	C7	C6	179.43(12)
C1	C2	C7	C8	-0.12(19)
C2	C3	C4	C5	-0.2(2)
C2	C7	C8	C9	-179.76(12)
C2	C7	C8	C10	-0.7(2)
C3	C2	C7	C6	0.9(2)
C3	C2	C7	C8	-178.63(12)
C3	C4	C5	C6	0.0(2)
C4	C5	C6	O2	179.21(13)
C4	C5	C6	C7	0.7(2)
C5	C6	C7	C2	-1.2(2)
C5	C6	C7	C8	178.41(12)
C6	O2	C9	C8	0.49(14)
C6	C7	C8	C9	0.63(15)
C6	C7	C8	C10	179.70(12)
C7	C2	C3	C4	-0.22(19)
C7	C8	C9	O2	-0.67(14)
C7	C8	C10	N1	0.29(18)

Atom	Atom	Atom	Atom	Angle/°
C7	C8	C10	C11	-177.64(12)
C9	O2	C6	C5	-178.73(14)
C9	O2	C6	C7	-0.12(15)
C9	C8	C10	N1	179.01(14)
C9	C8	C10	C11	1.1(2)
C10	N1	C1	O1	177.45(12)
C10	N1	C1	C2	-1.73(19)
C10	N1	C12	C13	96.19(16)
C10	N1	C12	C17	-85.22(15)
C10	C8	C9	O2	-179.51(14)
C12	N1	C1	O1	5.48(18)
C12	N1	C1	C2	-173.70(11)
C12	N1	C10	C8	172.64(12)
C12	N1	C10	C11	-9.28(18)
C12	C13	C14	C15	-0.5(2)
C13	C12	C17	N2	179.92(12)
C13	C12	C17	C16	0.12(19)
C13	C14	C15	C16	0.3(2)
C14	C15	C16	C17	0.1(2)
C14	C15	C16	C20	-178.48(13)
C15	C16	C17	N2	179.88(12)
C15	C16	C17	C12	-0.34(18)
C15	C16	C20	C19	178.40(13)
C17	N2	C18	C19	-1.2(2)
C17	C12	C13	C14	0.3(2)
C17	C16	C20	C19	-0.25(19)
C18	N2	C17	C12	-177.67(12)
C18	N2	C17	C16	2.12(18)
C18	C19	C20	C16	1.1(2)
C20	C16	C17	N2	-1.43(18)
C20	C16	C17	C12	178.36(11)

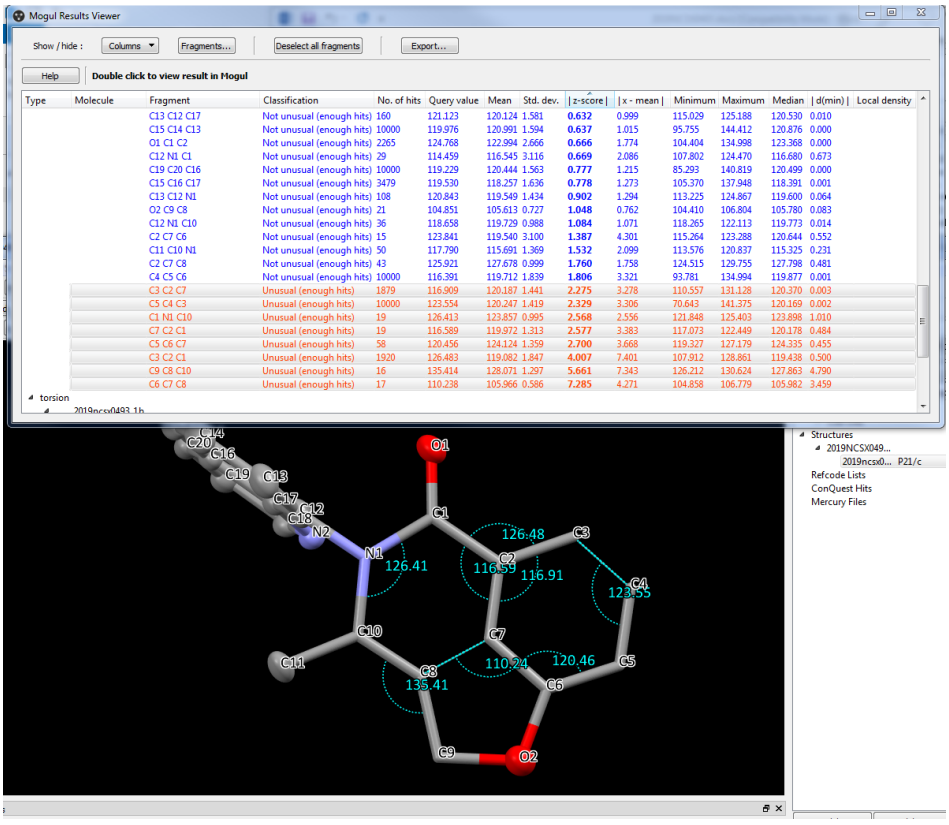


Figure S106: Significant distortions from idealized geometries **2p** obtained using Mogul.[13]

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