ELECTRONIC SUPPLEMENTARY INFORMATION

Modular Logic Gates: Cascading Independent Logic Gates via Metal Ion Signals

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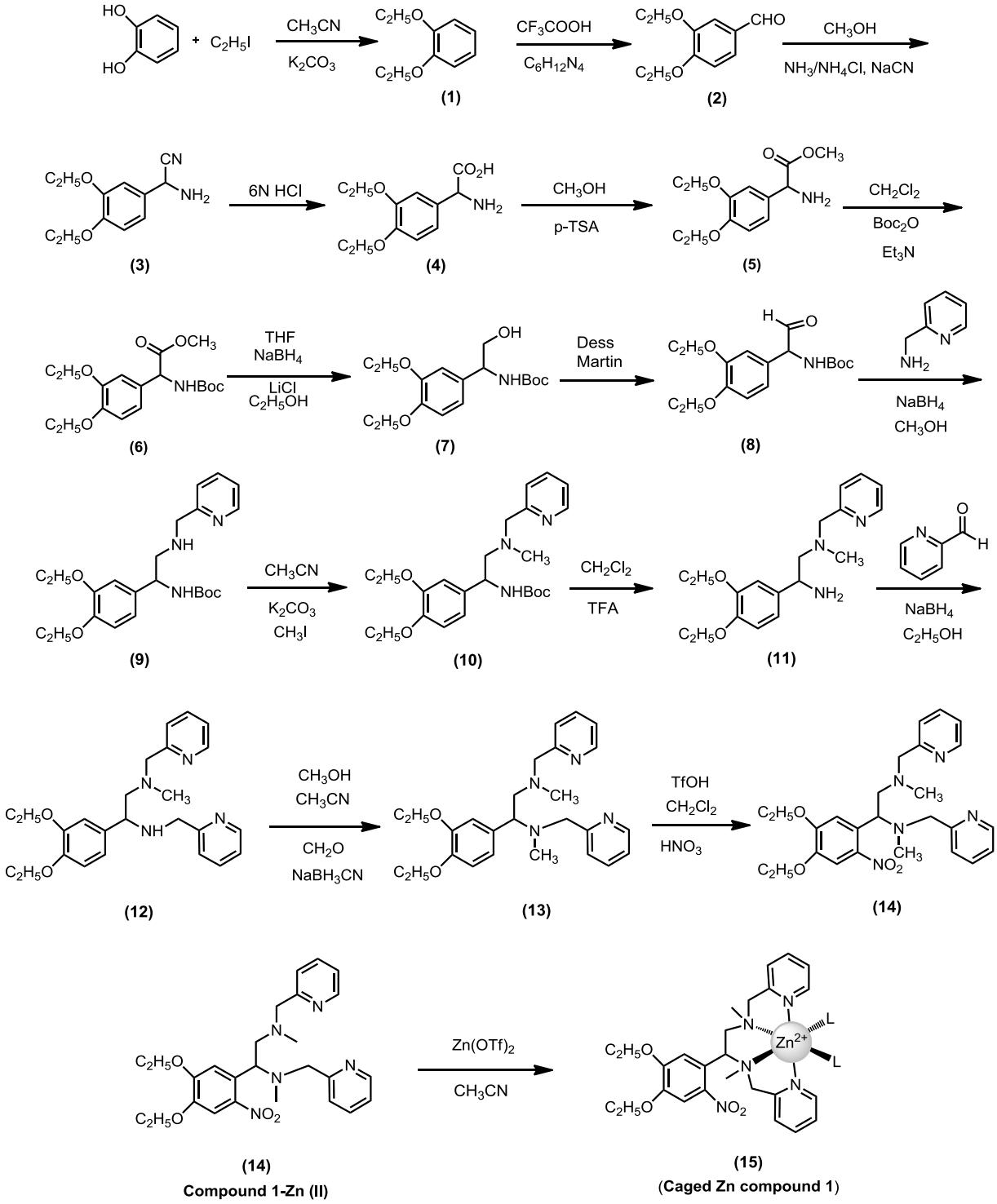
,Methods and Materials

^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker DPX-400 (operating at 400 MHz for ^{1}H NMR and 100 MHz for ^{13}C NMR) in $CDCl_3$ with tetramethylsilane as internal standard. All spectra were recorded at 25 ^{o}C and coupling constants (*J* values) were given in Hz. Chemical shifts were given in parts per million (ppm). Splitting patterns are designated as s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and p (pentet). All the ^{13}C spectra were recorded with simultaneous decoupling of proton nuclei. Mass spectra were recorded on Agilent Technologies 6530 Accurate-Mass Q-TOF LC/MS. Absorption spectra were performed by using a Varian Cary-100 spectrophotometer. Fluorescence measurements were conducted on a Varian Eclipse spectrofluometer. Reactions were monitored by thin layer chromatography using Merck TLC Silica gel 60 F_{254}. Silica gel column chromatography was performed over Merck Silica gel 60 (particle size: 0.040-0.063 mm, 230-400 mesh ASTM). All other reagents and solvents were purchased from Aldrich and used without further purification. Compounds **1**[1], **2**[2], **16**[3] and **17**[4] were synthesized according to literature.

Synthetic Pathway. Numbering of molecules in this document (supporting information) is different from the article text.



Compound 1-Zn (II)

(**Caged Zn compound 1**)

Synthesis of Compound 1[1]

Catechol (10 g, 90 mmol) and ethyl iodide (22 mL, 273 mmol) were dissolved in CH_3CN (150 mL) in a 500 mL round-bottomed flask. K_2CO_3 (37.6 g, 273 mmol) and a few crystals of 18-crown-6 were added. The reaction mixture was refluxed for 18 h and followed by TLC silica gel plates using *n*-hexane- ethyl acetate (8:1) as mobile phase. The reaction mixture was filtered and the CH_3CN was evaporated in vacuo. The crude product was purified by silica gel column chromatography using *n*-hexane- ethyl acetate (8:1) as mobile phase. Fraction containing compound **1** was collected then the solvent was removed under reduced pressure (69.2 mmol, 11.5 g, 76 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 6.92 (s, 4H), 4.12 (q, *J* = 7.0 Hz, 4H), 1.47 (t, *J* = 7.0 Hz, 6H) ppm.
^{13}C NMR (100 MHz, Chloroform-*d*): δ_C 148.9, 121.0, 113.9, 64.6, 14.9 ppm.

Synthesis of Compound 2[2]

Compound **1** (10 g, 60 mmol) were dissolved in trifluoroacetic acid (20 mL) in a 100 mL round-bottomed flask. Hexamethylenetetramine (12.6 g, 90 mmol) was added. The reaction mixture was refluxed for 12 h and followed by TLC silica gel plates using *n*-hexane- ethyl acetate (5:1) as mobile phase. Then, it was extracted with ethyl acetate and water. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by silica gel column chromatography using *n*-hexane- ethyl acetate (5:1) as mobile phase. Fraction containing compound **2** was collected then the solvent was removed under reduced pressure (30 mmol, 5.8 g, 50 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 9.83 (s, 1H), 7.44 – 7.21 (m, 2H), 6.98 (d, *J* = 8.2 Hz, 1H), 4.25 – 4.05 (m, 4H), 1.50 (dt, *J* = 9.0, 7.0 Hz, 6H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*): δ_C δ 190.5, 154.0, 148.8, 129.7, 126.22, 111.5, 110.5, 64.3, 64.2, 14.4, 14.4 ppm.

Synthesis of Compound 3 and 4

Compound **2** (5 g, 25.8 mmol) were dissolved in methanol (15 mL) in a 250 mL round-bottomed flask. Sodium cyanide (1.9 g, 38.6 mmol) and ammonium chloride (2.1 g, 38.6 mmol) in NH_4OH (30 mL, 30%) were added to the reaction mixture in a dropwise manner and the reaction mixture was stirred for 23 h at room temperature. The reaction mixture was filtered and the methanol was evaporated in vacuo. Then, it was extracted with ethyl acetate and water. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. Crude product (**3**) was used in the next step without further purification. Compound **3** in 6 M HCl (60 mL) was refluxed for 4h. The solution was concentrated in vacuo. Filtration of the resulting yellow suspension gave compound **4** as a yellow solid. (4g)

^{1}H NMR (400 MHz, DMSO-d_6): δ_H 8.71 (s,3H), 7.05 (s, 1H), 6.90 (s, 2H),4.87 (s, 1H), 4.00 – 3.85 (m, 4H), 1.23 (q, J = 7.0 Hz, 6H) ppm.
^{13}C NMR (100 MHz, DMSO-d_6): δ_C 170.4, 149.4, 148.6, 125.71, 121.3, 113.7, 113.6, 64.4, 64.3, 55.7, 15.1, 15.1 ppm.

Synthesis of Compound 5

Compound **4** (4 g, 16.7 mmol) and p-toluenesulfonic acid monohydrate (6.4 g, 33.5 mmol) were dissolved in methanol (50 mL) in 250 mL round-bottomed flask and refluxed for 24 h. The solvent was removed, and crude product was dissolved in NH_4OH (30 mL, 30%) and extracted with CH_2Cl_2. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by silica gel column chromatography using CH_2Cl_2:CH_3OH (100:4) as mobile phase. Fraction containing compound **4** was collected then the solvent was removed under reduced pressure (12.3 mmol, 3.1 g, 73 %).

^{1}H NMR (400 MHz, Chloroform-d): δ_H 6.85 – 6.70 (m, 3H), 4.44 (s, 1H), 4.01 – 3.89 (m, 4H), 3.60 (s, 3H), 1.85 (b, 2H), 1.34 (td, J = 7.0, 3.2 Hz, 6H) ppm.

^{13}C NMR (100 MHz, Chloroform-d): δ_C 174.6, 148.9, 148.6, 132.9, 119.2, 113.5, 112.1, 64.6, 64.6, 58.4, 52.3 ppm.

Synthesis of Compound 6 and 7

Compound **5** (3 g, 11.9 mmol) was dissolved in CH_2Cl_2 (60 mL) in 250 mL round-bottomed flask and triethylamine (1.82 mL, 13 mmol) and di-tert-butyl dicarbonate (2.8 g, 13 mmol) were added. The reaction mixture was stirred for 23 h at room temperature and followed by TLC silica gel plates using CH_2Cl_2:CH_3OH (100:4) as mobile phase. Then, it was extracted sequentially with HCl (1M, 20 mL), sat. $NaHCO_3$ (20 mL) and water (20 mL). Organic layer containing compound **6** was dried with Na_2SO_4 and evaporated under reduced pressure. Compound **6** was used in the next step without further purification.

Compound **6** (4 g, 11.3 mmol) was dissolved in THF (30 mL) in 250 mL round-bottomed flask. After reducing the temperature of the reaction mixture to 0 ^oC, $NaBH_4$ (0.86 g, 22.6 mmol), LiCl (0.96 g, 22.6 mmol) and ethanol (20 mL) were added. The reaction mixture was stirred for 23 h at room temperature and followed by TLC silica gel plates using CH_2Cl_2:CH_3OH (100:4) as mobile phase. The solvent mixture was evaporated in vacuo and the product was extracted with CH_2Cl_2 and water. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by silica gel column chromatography using CH_2Cl_2:CH_3OH (100:4) as mobile phase. Fraction containing compound **7** was collected then the solvent was removed under reduced pressure (8 mmol, 2.6 g, 70 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 6.75 – 6.61 (m, 3H), 5.38 (b, 1H), 4.51 (b, 1H), 4.04 – 3.81 (m, 4H), 3.6 (d, *J* = 5.8 Hz, 2H), 3.28 (t, *J* = 5.9 Hz, 1H), 1.28 (t, *J* = 7.0 Hz, 15H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*): δ_H 156.2, 148.8, 148.1, 132.6, 118.9, 113.7, 112.4, 79.7, 66.3, 64.6, 56.4, 28.3, 14.8 ppm.

Synthesis of Compound 8

To a 250 mL round-bottomed flask containing argon-degassed CH_2Cl_2 (120 mL) were added Dess-Martin periodinane (4.9 g, 11.5 mmol) and Compound **7** (2.5 g, 7.7 mmol). The reaction mixture was stirred for 23 h at room temperature and followed by TLC silica gel plates using CH_2Cl_2:CH_3OH (100:4) as mobile phase. The resulting reaction mixture was quenched by adding solution of saturated sodium thiosulfate. Then, it was extracted with CH_2Cl_2. The

crude product was purified by silica gel column chromatography using CH_2Cl_2:CH_3OH (100:4) as mobile phase. Fraction containing compound **8** was collected then the solvent was removed under reduced pressure (7.1 mmol, 2.3 g, 93 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 9.43 (s, 1H), 6.85 – 6.64 (m, 3H), 5.65 (b, 1H), 5.14 (s, 1H), 4.11 – 3.92 (m, 4H), 1.35 (t, *J* = 6.8 Hz, 15H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*): δ_C 195.2, 155.0, 149.4, 149.1, 120.5, 113.8, 112.7, 64.6, 64.5, 64.3, 55.3, 28.3, 14.8, 14.7 ppm.

Synthesis of Compound 9

Compound **8** (2.2 g, 6.8 mmol) and 2-picolylamine (0.9 g, 8.3 mmol) were dissolved in methanol (50 mL) in 100 mL round-bottomed flask and stirred for 6 h at room temperature. After reducing the temperature of the reaction mixture to 0 ^{o}C, $NaBH_4$ (0. 51 g, 13.6 mmol) was added and the resulting mixture was stirred for 18 h at room temperature. The methanol was evaporated in vacuo. Then, crude product was extracted with CH_2Cl_2 and water. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by silica gel column chromatography using CH_2Cl_2:CH_3OH (100:6) as mobile phase. Fraction containing compound **9** was collected then the solvent was removed under reduced pressure (4.1 mmol, 1.7 g, 60 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 8.53 (d, *J* = 4.9 Hz, 1H), 7.63 (td, *J* = 7.7, 1.8 Hz, 1H), 7.24 (d, *J* = 7.8 Hz, 1H), 7.16 (ddd, *J* = 7.6, 5.0, 1.2 Hz, 1H), 6.90 – 6.62 (m, 3H), 5.60 (b, 1H), 4.73 (b, 1H), 4.15 (qd, *J* = 7.0, 1.8 Hz, 1H), 4.08 (q, *J* = 4.0 Hz, 4H), 3.88 (d, *J* = 2.4 Hz, 2H), 2.91 (m, 2H), 1.51 – 1.26 (m, 15H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*): δ_C 159.5, 149.3, 148.8, 147.9, 136.5, 122.2, 121.9, 120.2, 118.5, 113.7, 112.8, 111.9, 64.6, 64.6, 64.5, 54.8, 54.4, 28.4, 11.9, 14.9 ppm.

MS (TOF - ESI): m/z: Calcd: 415.52582 [M^+], Found: 416.26336 [M+H]$^+$, Δ=-21.5 ppm.

Synthesis of Compound 10

Compound **9** (1.6 g, 3.9 mmol) and K_2CO_3 (0.8 g, 5.8 mmol) were dissolved in CH_3CN (40 mL) in a 100 mL round-bottomed flask. Methyl iodide (0.55 g, 3.9 mmol) was added to the reaction mixture in a dropwise manner. The reaction mixture was stirred for 5 h at room temperature and followed by TLC silica gel plates using CH_2Cl_2:CH_3OH (100:6) as mobile phase. It was filtered and the CH_3CN was evaporated in vacuo. The crude product was purified by silica gel column chromatography using CH_2Cl_2:CH_3OH (100:6) as mobile phase. Fraction containing compound **10** was collected then the solvent was removed under reduced pressure (2.6 mmol, 1.1 g, 67 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 8.59 (d, *J* = 2.3 Hz, 1H), 7.66 (td, *J* = 7.7, 1.8 Hz, 1H), 7.32 (d, *J* = 7.9 Hz, 1H), 7.19 (ddd, *J* = 7.5, 4.9, 1.2 Hz, 1H), 6.88 – 6.65 (m, 3H), 5.90 (b, 1H), 4.62 (b, 1H), 4.07 (qd, *J* = 7.0, 1.6 Hz, 4H), 3.80 (d, *J* = 14.2 Hz, 1H), 3.65 (d, *J* = 14.2 Hz, 1H), 2.73 – 2.50 (m, 2H), 2.34 (s, 3H), 1.43 (td, *J* = 7.0, 2.3 Hz, 15H) ppm.

MS (TOF - ESI): m/z: Calcd: 429.26276 $[M^+]$, Found: 430.27953 $[M+H]^+$, Δ=-22.1 ppm.

Synthesis of Compound 11

Trifluoroacetic acid (3 mL) was added to a solution of **10** (1.0 g, 2.3 mmol) in CH_2Cl_2 (30 mL) and stirred at for 23 h at room temperature. After removing the solvent, saturated K_2CO_3 was added to the reaction mixture, and the product was extracted into CH_2Cl_2. Organic layer containing compound **11** was dried with Na_2SO_4 and evaporated under reduced pressure. No further purification was required (2.22 mmol, 0.73 g, 95 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 8.54 (b, 1H), 7.66 (t, *J* = 7.7 Hz, 1H), 7.43 (d, *J* = 7.8 Hz, 1H), 7.17 (t, *J* = 6.2 Hz, 1H), 6.95 (s, 1H), 6.91 – 6.75 (m, 2H), 4.08 (q, *J* = 7.0 Hz, 5H), 3.82 (d, *J* = 14.0 Hz, 1H), 3.68 (d, *J* = 14.2 Hz, 1H), 2.79 – 2.42 (m, 2H), 2.34 (s, 3H), 2.13 (b, 2H), 1.44 (t, *J* = 7.0 Hz, 6H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*): δ_C δ 159.4, 149.0, 148.8, 147.9, 136.9, 136.4, 122.9, 121.9, 118.9, 113.6, 112.2, 66.5, 64.7, 64.6, 64.2, 53.0, 42.7, 14.9 ppm.

MS (TOF - ESI): m/z: Calcd: 329.21033 $[M^+]$, Found: 330.22473 $[M+H]^+$, Δ=-21.6 ppm.

Synthesis of Compound 12

Compound **11** (600 mg, 1.8 mmol) and 2-pyridinecarboxaldehyde (0.2 mL, 2.2 mmol) were dissolved in methanol (50 mL) in 100 mL round-bottomed flask and refluxed for 2 h at room temperature. After reducing the temperature of the reaction mixture to 0 ^oC, $NaBH_4$ (140 mg, 3.6 mmol) was added and the resulting mixture was stirred for 18 h at room temperature. The methanol was evaporated in vacuo. Then, crude product was extracted with CH_2Cl_2 and water. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by basic alumina column chromatography using CH_2Cl_2:CH_3OH (100:2) as mobile phase. Fraction containing compound **12** was collected then the solvent was removed under reduced pressure (1.1 mmol, 460 mg, 60 %).

^1H NMR (400 MHz, Chloroform-*d*): δ_H 8.59 – 8.39 (m, 2H), 7.67 (td, *J* = 7.6, 1.8 Hz, 1H), 7.63 – 7.52 (m, 2H), 7.21 – 7.08 (m, 3H), 6.99 (s, 1H), 6.86 – 6.81 (m, 2H), 4.18 – 3.98 (m, 5H), 3.90 – 3.51 (m, 4H), 2.76 (dd, *J* = 12.4, 10.6 Hz, 1H), 2.47 (dd, *J* = 12.4, 3.6 Hz, 1H), 2.25 (s, 3H), 1.44 (td, *J* = 7.0, 4.2 Hz, 6H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*) δ_C 160.2, 159.6, 149.3, 148.9, 148.8, 147.9, 136.4, 136.1, 135.0, 123.0, 122.5, 121.9, 121.7, 120.1, 113.4, 112.6, 65.6, 64.6, 64.5, 63.9, 59.7, 52.7, 42.6, 14.9, 14.9 ppm.

MS (TOF - ESI): m/z: Calcd: 420.25253 $[M^+]$, Found: 421.26430 $[M+H]^+$, Δ=-10.3 ppm.

Synthesis of Compound 13

Compound **12** (400 mg, 0.95 mmol) was dissolved in CH_3CN/CH_3OH (15/15 mL) in a 100 mL round-bottomed flask. Formaldehyde (37% in water, 3.1 mL), $NaBH_3CN$ (180 mg, 2.9 mmol), AcOH (1.2 mL) were added and the reaction mixture was stirred for 18 h at room temperature. After the solvent was removed, saturated $NaHCO_3$ (10 mL) was added, and the product was extracted into CH_2Cl_2. Organic layer was dried with Na_2SO_4 and evaporated in

vacuo. The crude product was purified by basic alumina column chromatography using CH_2Cl_2:CH_3OH (100:4) as mobile phase. Fraction containing compound **13** was collected then the solvent was removed under reduced pressure (0.67 mmol, 290 mg, 70 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 8.60 – 8.39 (m, 2H), 7.62 (td, *J* = 7.5, 1.9 Hz, 1H), 7.56 – 7.41 (m, 2H), 7.20 (d, *J* = 7.8 Hz, 1H), 7.15 – 7.08 (m, 2H), 6.91 – 6.69 (m, 3H), 4.22 – 3.99 (m, 4H), 3.92 (s, 1H), 3.84 – 3.52 (m, 4H), 3.09 – 2.97 (m, 1H), 2.93 – 2.81 (m, 1H), 2.28 (s, 3H), 2.18 (s, 3H), 1.44 (dt, *J* = 8.6, 7.0 Hz, 6H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*) δ_C 160.5, 159.8, 148.9, 148.3, 147.9, 136.3, 136.3, 132.3, 123.1, 122.8, 121.8, 121.7, 121.4, 114.5, 113.0, 66.0, 64.6, 64.5, 60.6, 60.3, 55.9, 43.1, 39.0, 14.9, 14.9 ppm.

MS (TOF - ESI): m/z: Calcd: 434.26818 $[M^+]$, Found: 435.27529 $[M+H]^+$, Δ=0.37 ppm.

Synthesis of Compound 14 (**Compound 1-Zn (II)**)

Trifluoromethanesulfonic acid (0.26 mL, 2.96 mmol) was dissolved in CH_2Cl_2 (10 mL) and anhydrous HNO_3 acid (0.08 mL, 1.48 mmol) was added, which caused a white, crystalline solid to precipitate from the solution. After reducing the temperature of the reaction mixture to 0 ^{o}C, Compound **13** (160 mg, 0.37 mmol) dissolved in CH_2Cl_2 (2 mL) was added in one portion. The reaction mixture was stirred at to 0 ^{o}C, for 2 h and then quickly poured onto 1 g of crushed ice. A saturated solution of $NaHCO_3$ (10 mL) was added, and the crude reaction mixture was extracted with CH_2Cl_2. Organic layer was dried with Na_2SO_4 and evaporated in vacuo. The crude product was purified by basic alumina column chromatography using CH_2Cl_2:CH_3OH (100:1) as mobile phase. Fraction containing compound **14** was collected then the solvent was removed under reduced pressure (0.09 mmol, 44 mg, 25 %).

^{1}H NMR (400 MHz, Chloroform-*d*): δ_H 8.61 – 8.33 (m, 2H), 7.62 (td, *J* = 7.7, 1.9 Hz, 1H), 7.51 (td, *J* = 7.7, 1.9 Hz, 1H), 7.40 (s, 1H), 7.34 (d, *J* = 7.8 Hz, 1H), 7.16 – 7.02 (m, 4H), 4.81 (dd, *J* = 8.6, 5.3 Hz, 1H), 4.21 – 4.11 (m, 2H), 4.10 – 3.96 (m, 2H), 3.86 – 3.51 (m, 4H), 2.98 (dd, *J* = 12.7, 5.3 Hz, 1H), 2.80 (dd, *J* = 12.8, 8.5 Hz, 1H), 2.32 (s, 3H), 2.25 (s, 3H), 1.50 (t, *J* = 7.0 Hz, 3H), 1.44 (t, *J* = 7.0 Hz, 3H) ppm.

^{13}C NMR (100 MHz, Chloroform-*d*) δ_C 159.9, 159.3, 151.8, 148.9, 148.7, 146.8, 143.5, 136.4, 136.2, 131.3, 123.1, 122.4, 121.8, 111.9, 109.129, 64.9, 64.7, 60.8, 60.1, 59.4, 43.2, 39.6, 29.7, 14.6, 14.6 ppm.

MS (TOF - ESI): m/z: Calcd: 479.25325 $[M^+]$, Found: 480.25847 $[M+H]^+$, Δ=4.25 ppm.

Preparation of Compound 15 (Caged Zn compound 1)

Zinc triflate (3.65 mg, 0.01 mmol) and Compound 14 (4.8 mg, 0.01 mmol) were dissolved in CH_3CN (5 mL) and the reaction mixture was stirred for 12 hours at room temperature.

References

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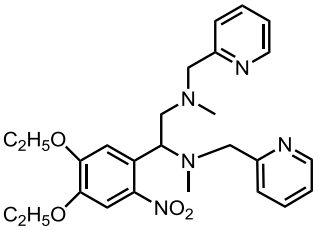
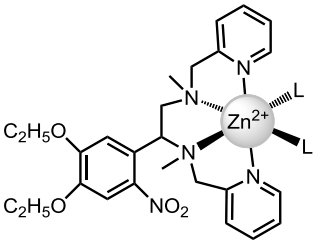
Target Compounds.



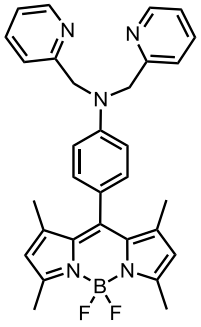
(14)

Compound 1-Zn (II)



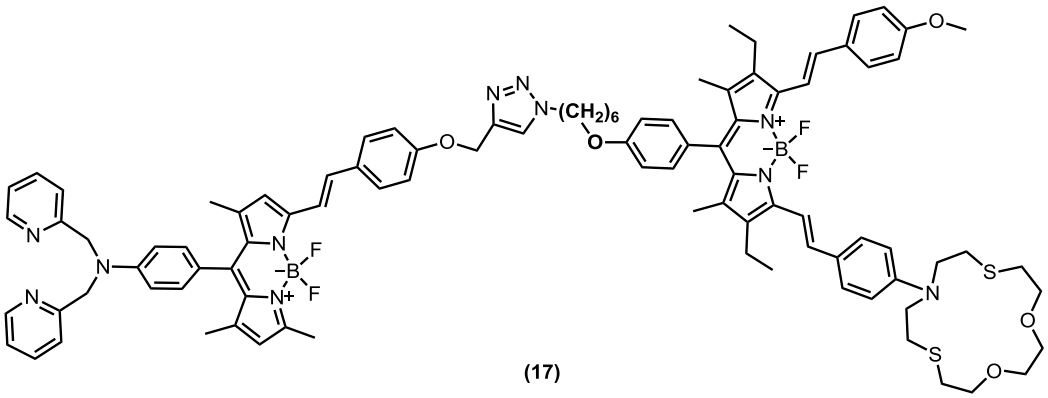
(15)

(Caged Zn compound 1)



(16)

Bodipy dye 2



(17)

Compound 3

Electronic Absorption and Emission Spectra:

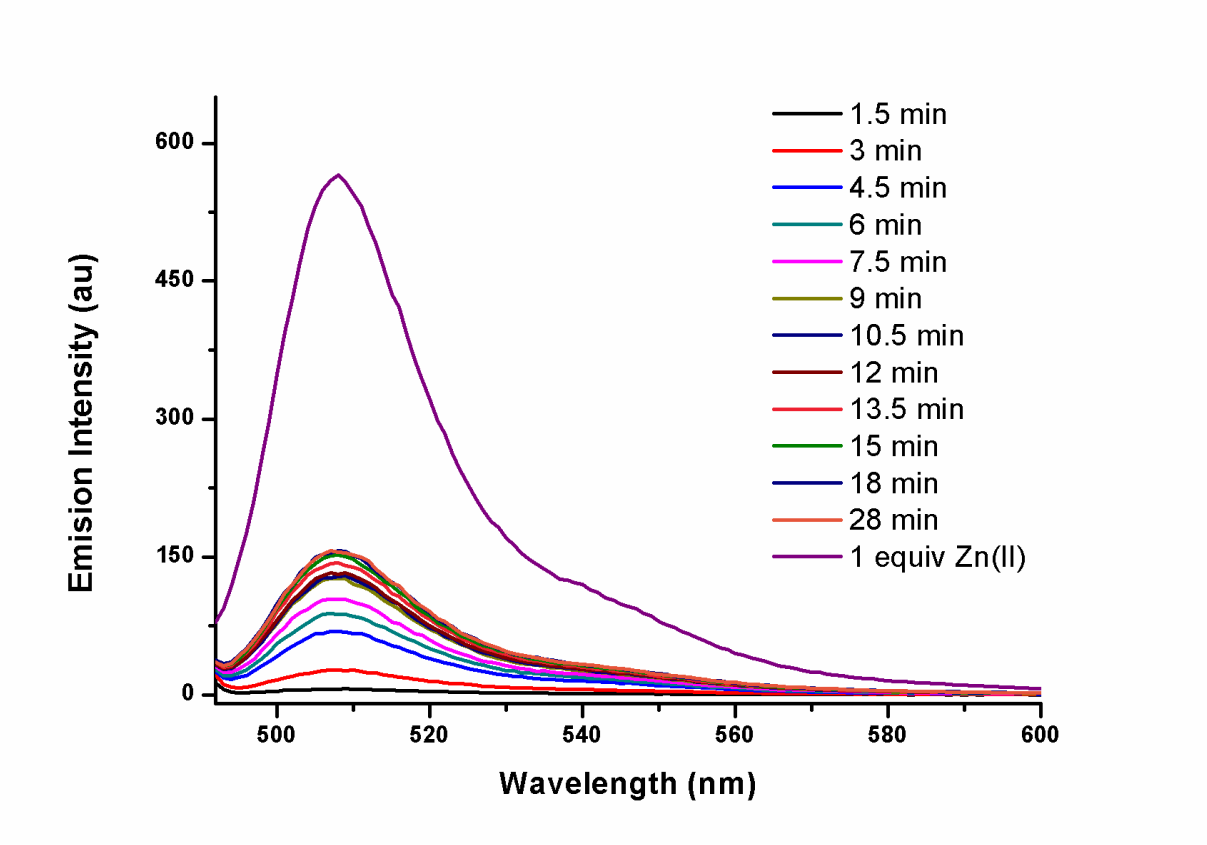


Fıgure 1. Fluorescence response of compound **16 (Bodipy dye 2**) upon uncaging of cage compound **15 (Caged Zn compound 1) (**5 μM each) recorded in acetonitrile. Initially compound **16** exhibits no fluorescence (quenched due to the active PET process), irradiation of the solution at 360 nm (with an optimized slit width of 7 nm) in a cuvette holder of spectrofluorometer, resulted in the complete photolysis of **15** which can be followed by the enhanced emission spectrum of compound **16**. Purple line represents the maximum emission intensity of **16** which was obtained by the addition of 1 equivalent of Zinc(II) triflate cations. (λ_{ex}=480 nm, slit widtsh=5-2.5). The light source of the spectrofluorometer was a 450 W Xe-lamp.

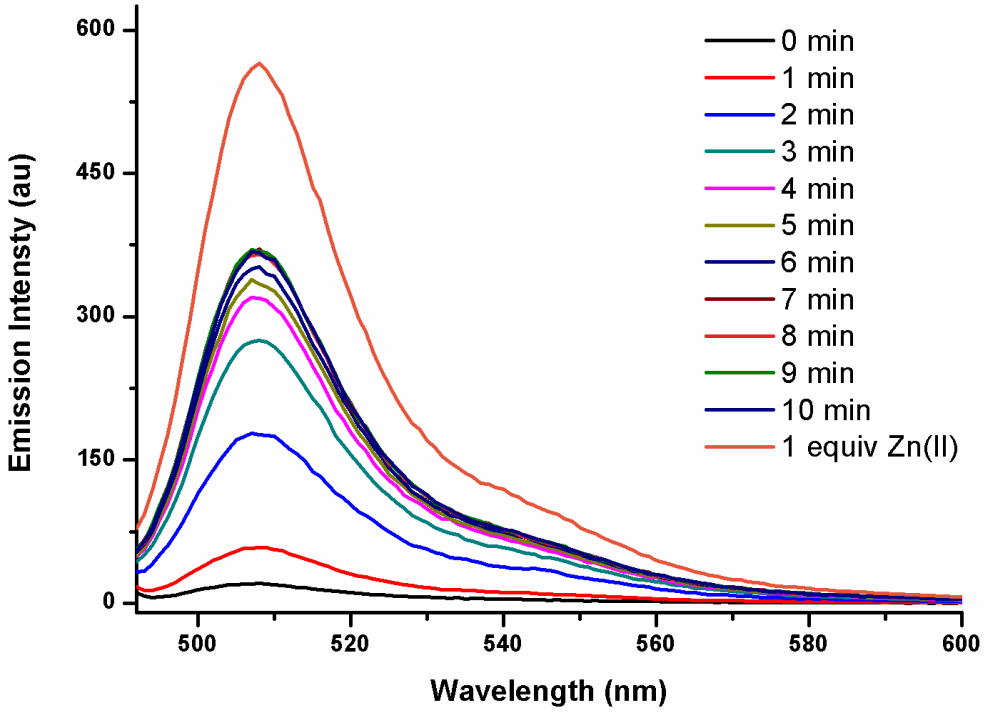


Fıgure 2. Fluorescence response of compound **16 (Bodipy dye 2**) upon uncaging of 2 equivalents of compound **15 (Caged Zn compound 1),** recorded in acetonitrile. Again orange line represents the maximum emission intensity of **16** which was obtained by the addition of 1 equivalent of Zinc(II) triflate cations. (λex=480 nm, slit width=5-2.5).

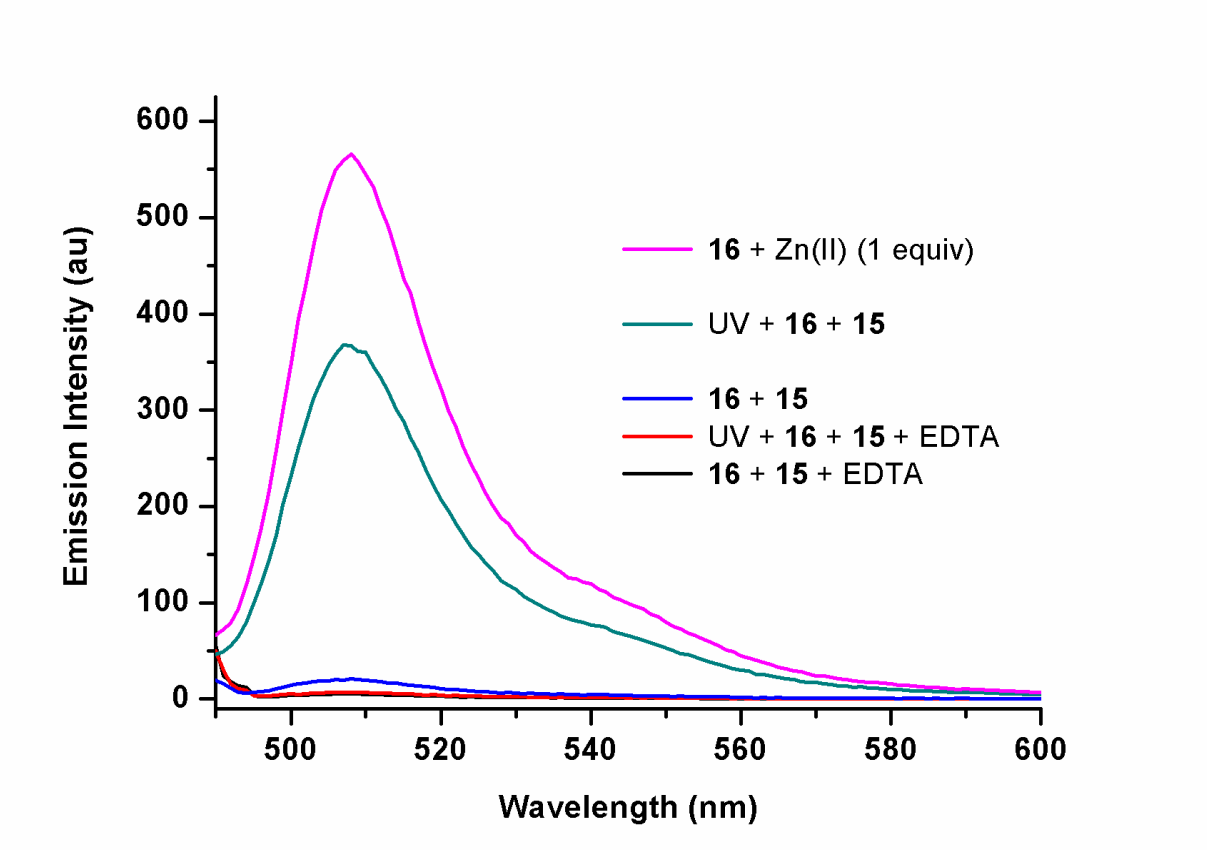


Fıgure 3. Fluorescence response of compound **16 (Bodipy dye 2**) upon uncaging of 2 equivalents of compound **15 (Caged Zn compound 1)** in the presence of **EDTA** (1 equiv) in acetonitrile solution. (λex=480 nm, slit width=5-2.5).

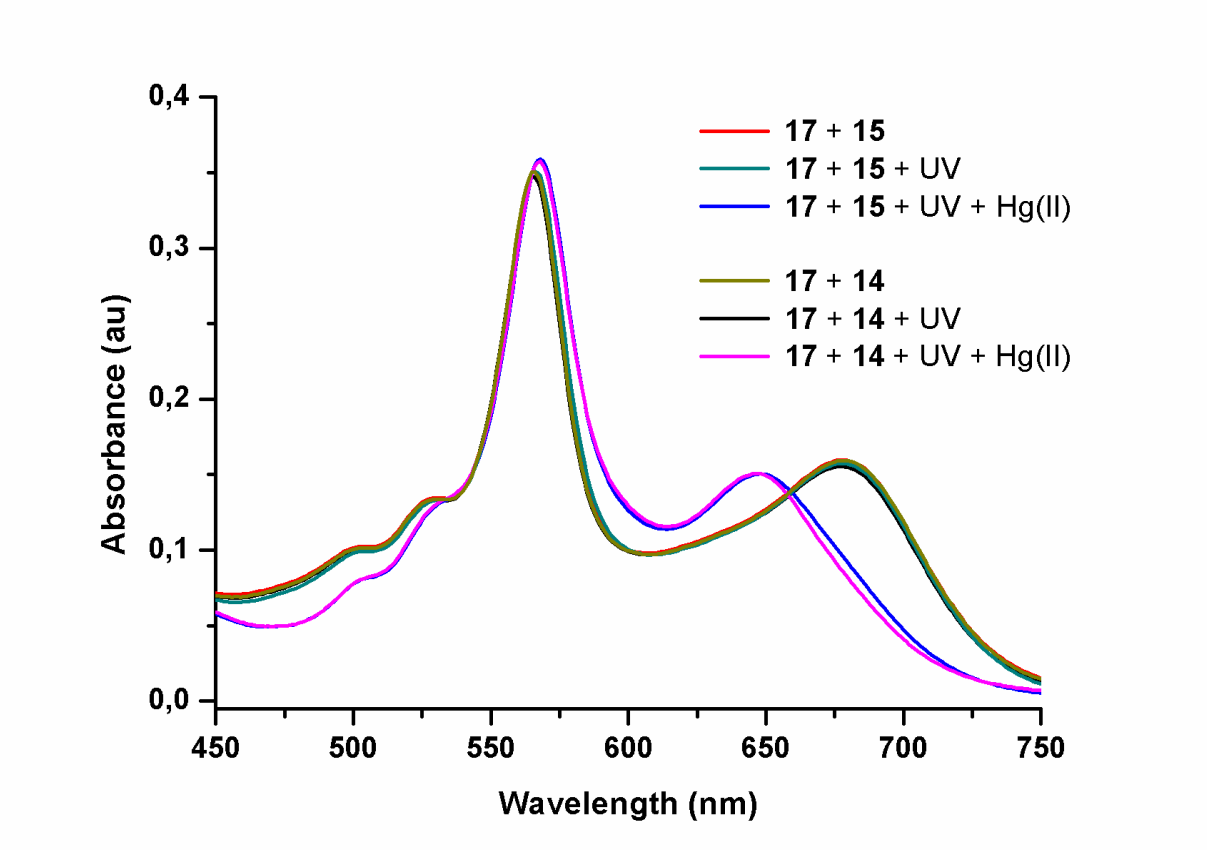


Figure 4. Absorbance spectra of Compound **17 (Compund 3)** (3.0 µM) recorded in acetonitrile, in the presence of compound **15 (Caged Zn compound 1)** and Hg(II) cations (3.0 µM, 18.0 µM, respectively).

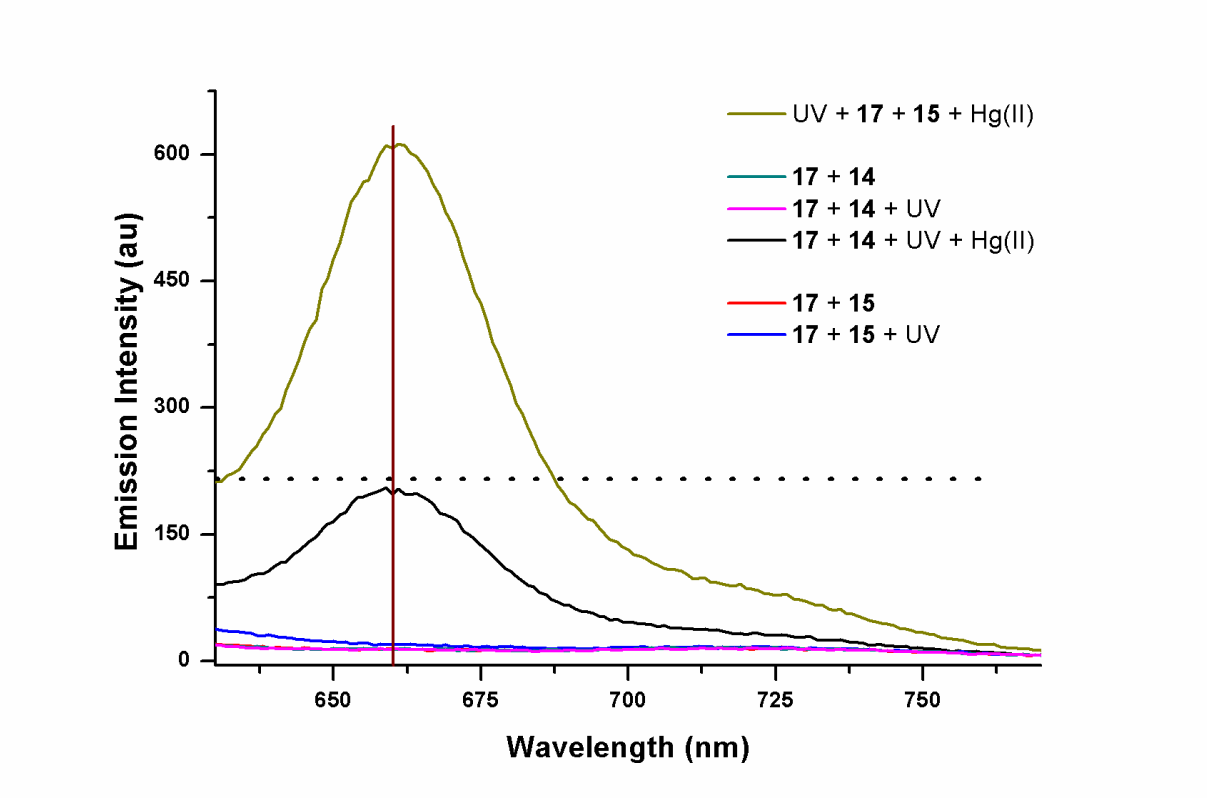


Fıgure 5. Emission spectra of Compound **17 (Compund 3)** (3.0 µM) in acetonitrile in the presence of compound **15 (Caged Zn compound 1)** and Hg(II) cations (3.0 µM, 18.0 µM, respectively). λex=560 nm, slit width=5-2.5

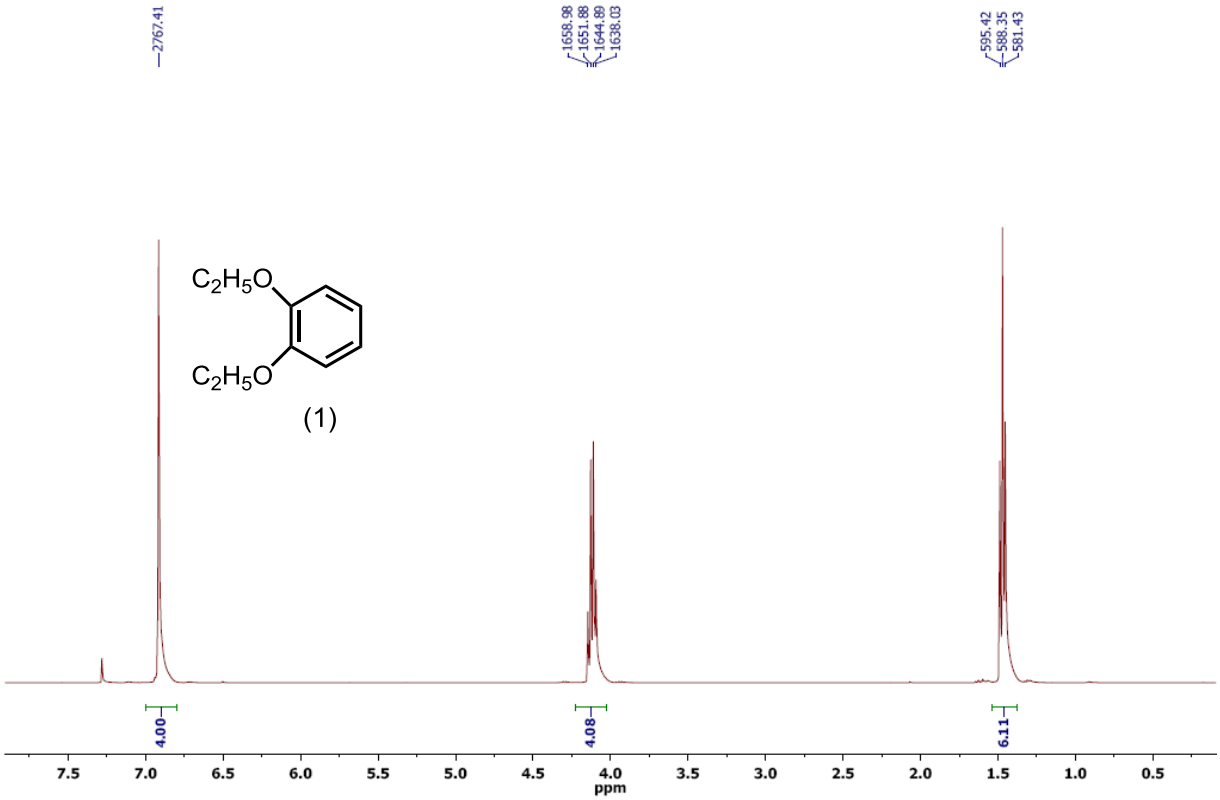


Figure 1: ^{1}H NMR spectrum of compound **1** (400 MHz, $CDCl_3$)

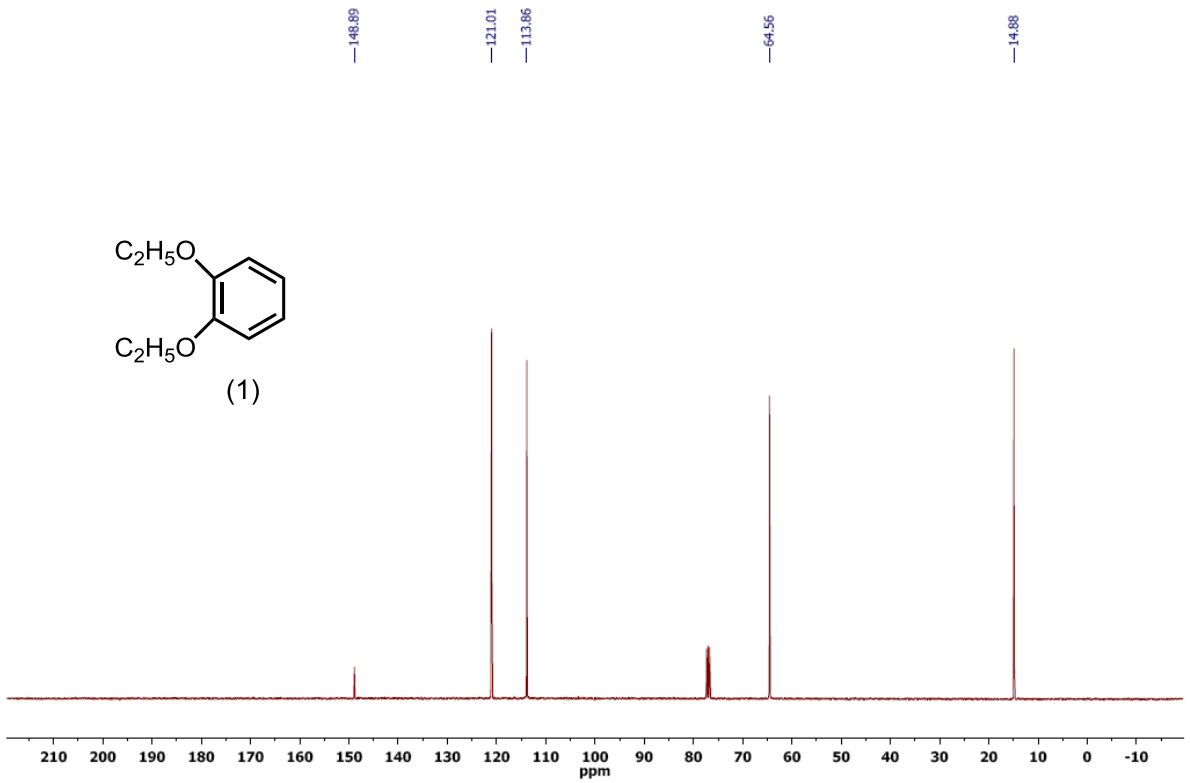


Figure 2: ^{13}C NMR spectrum of compound **1** (100 MHz, $CDCl_3$)

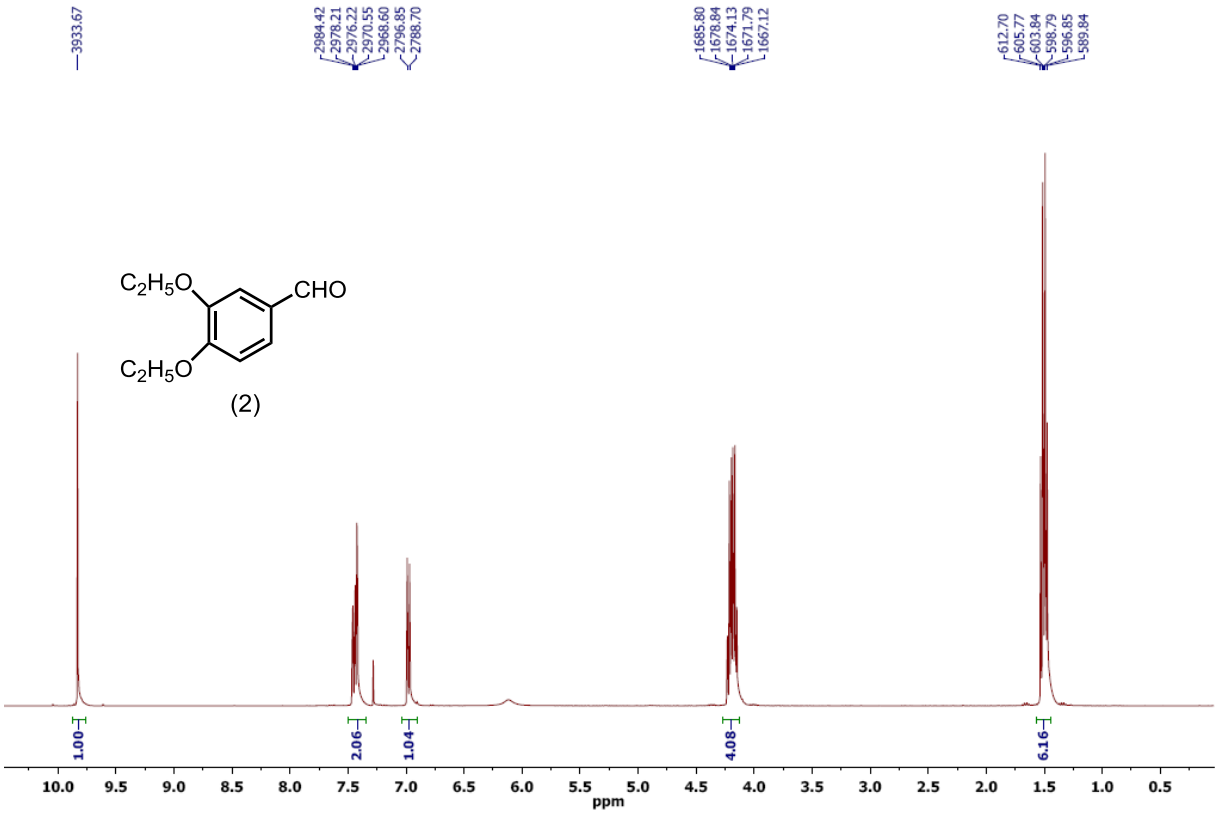


Figure 3: ^{1}H NMR spectrum of compound **2** (400 MHz, $CDCl_3$)

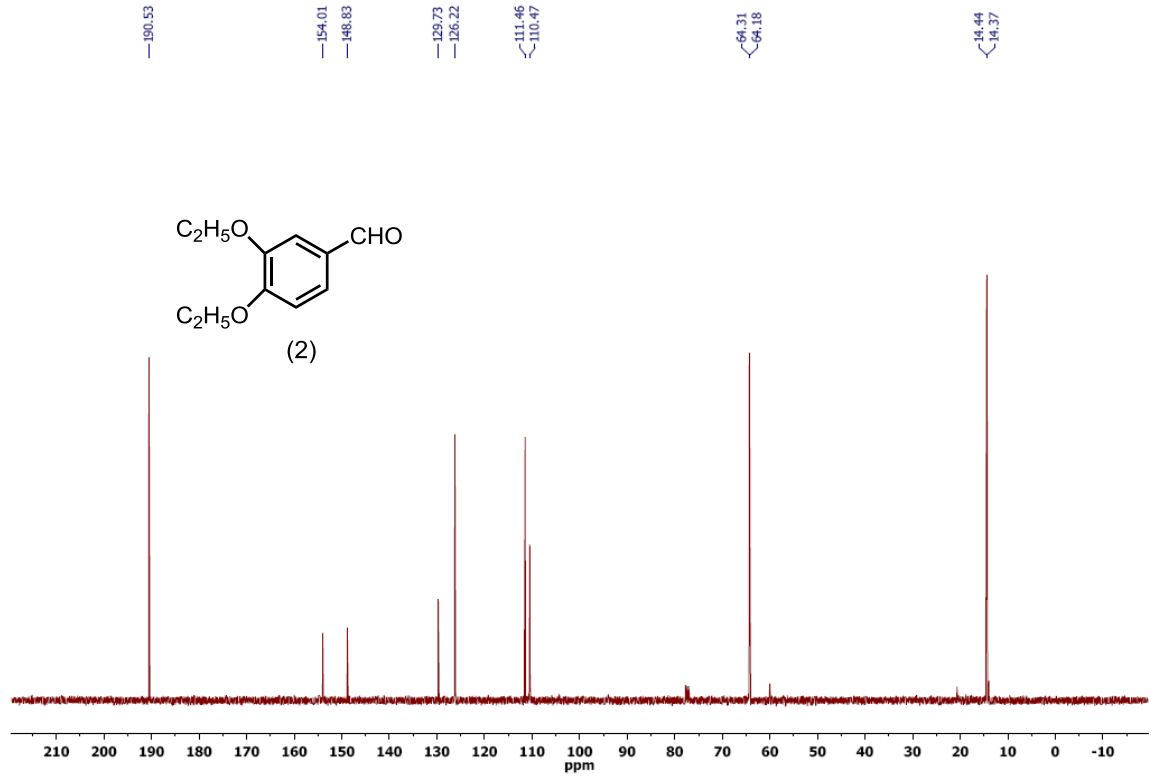


Figure 4: ^{13}C NMR spectrum of compound **2** (100 MHz, $CDCl_3$)

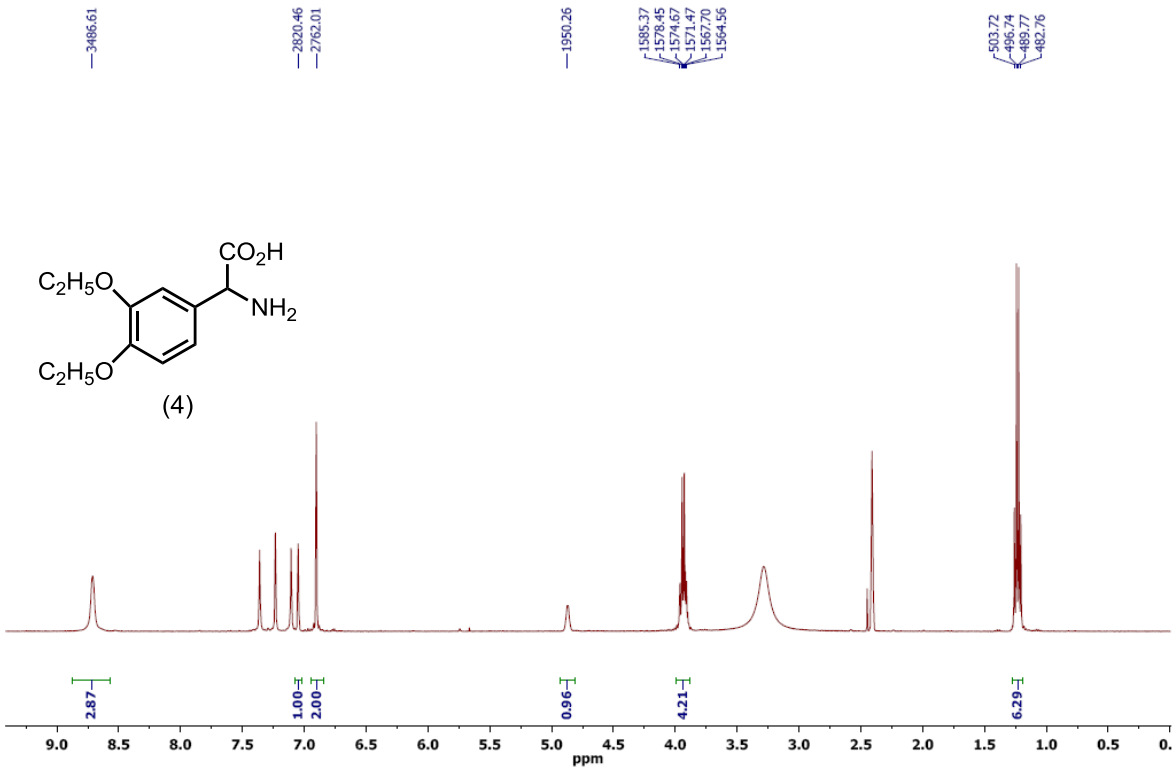


Figure 5: ^{1}H NMR spectrum of compound **4** (400 MHz, $CDCl_3$)

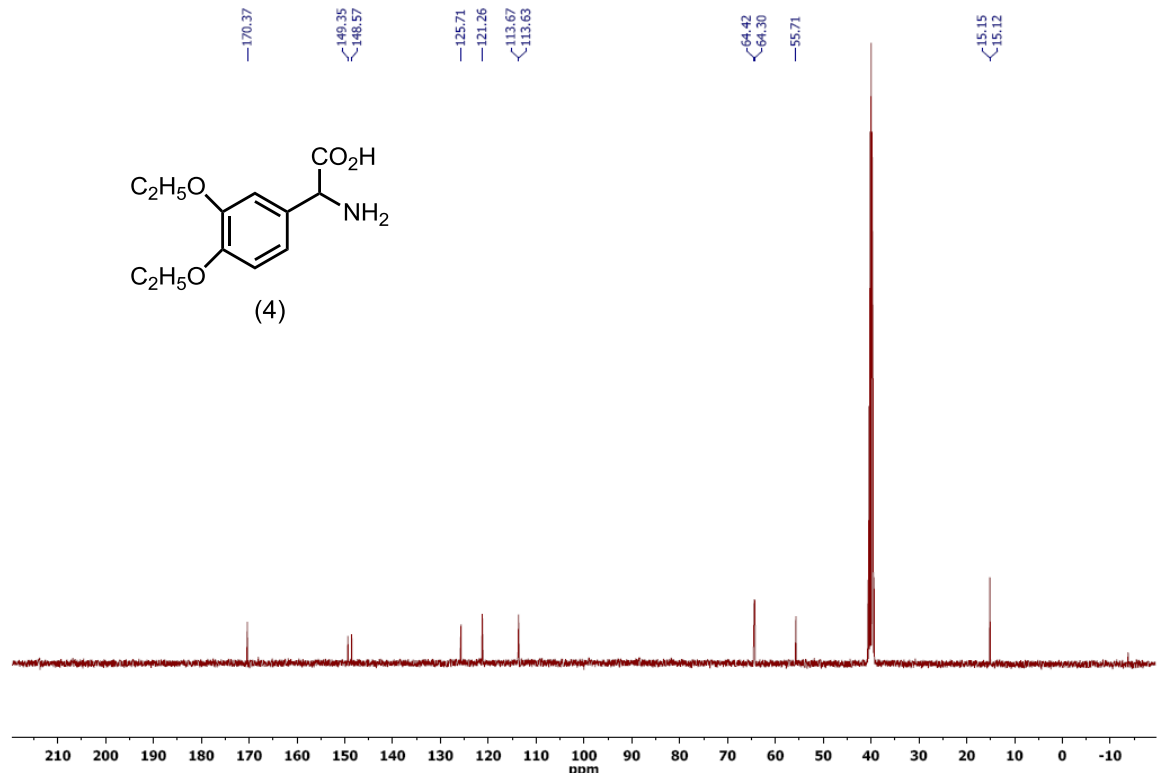


Figure 6: ^{13}C NMR spectrum of compound **4** (100 MHz, $CDCl_3$)

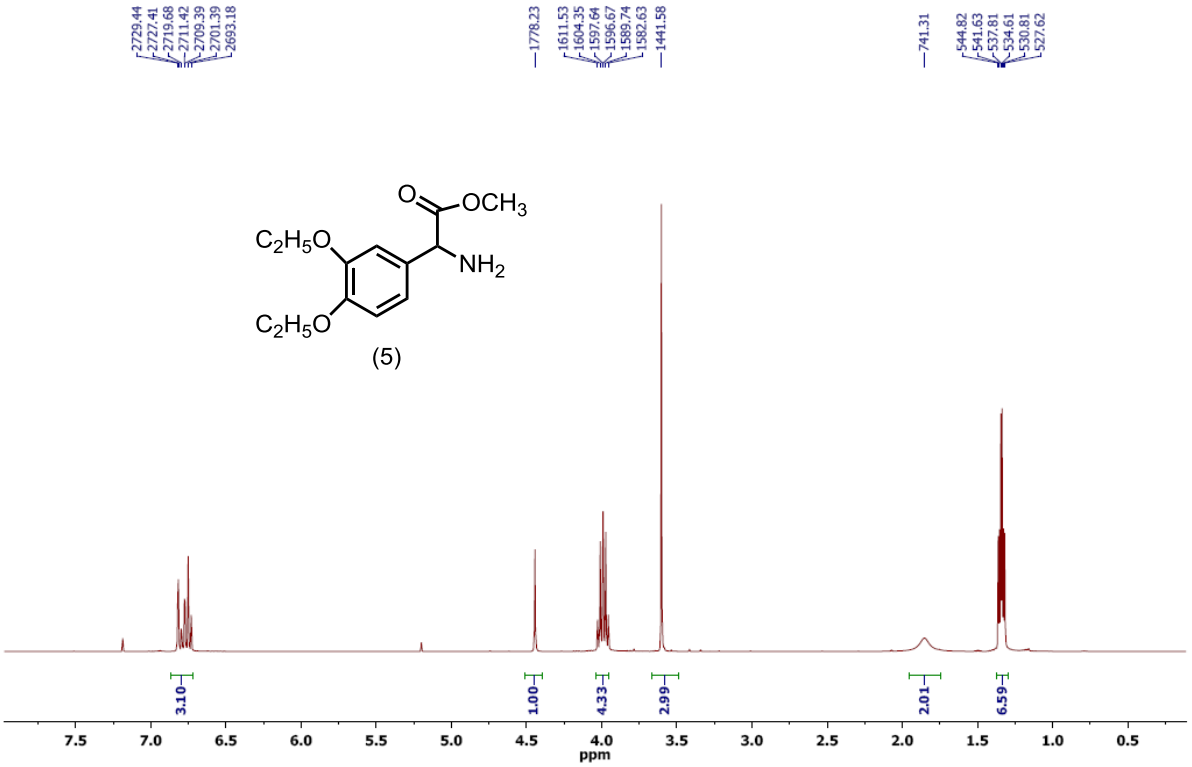


Figure 7: ^{1}H NMR spectrum of compound **5** (400 MHz, $CDCl_3$)

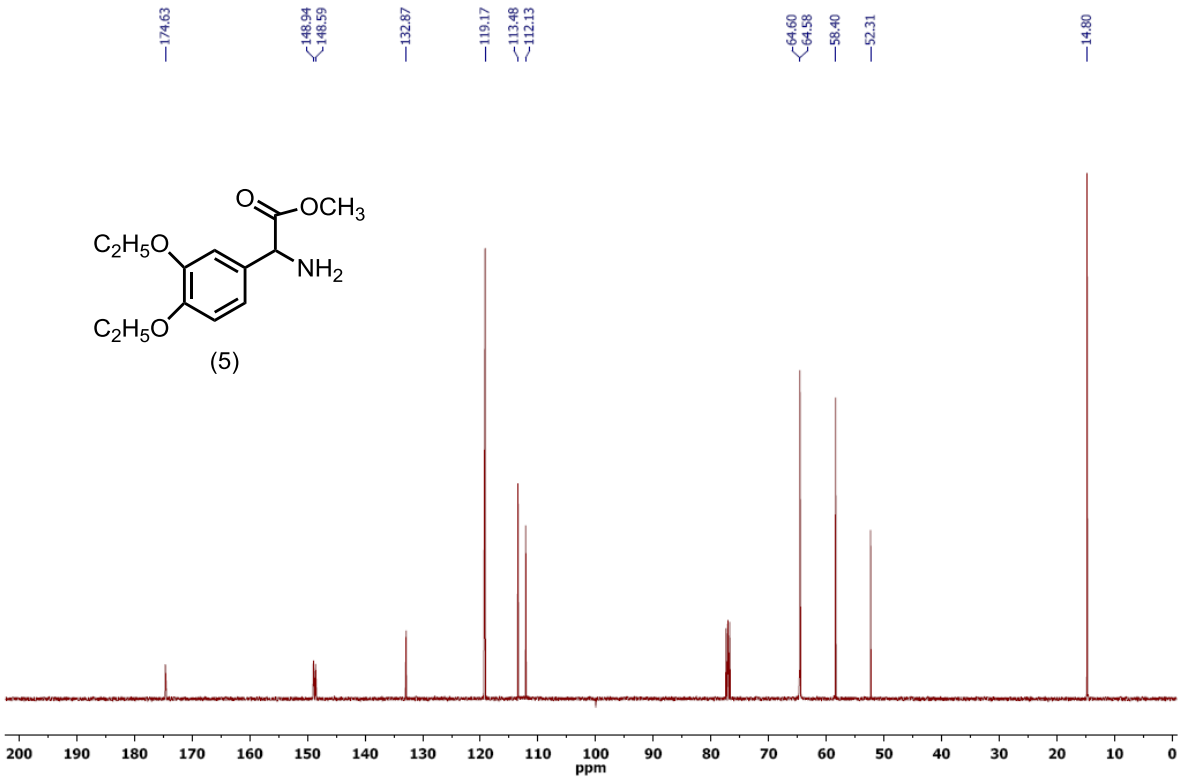


Figure 8: ^{13}C NMR spectrum of compound **5** (100 MHz, $CDCl_3$)

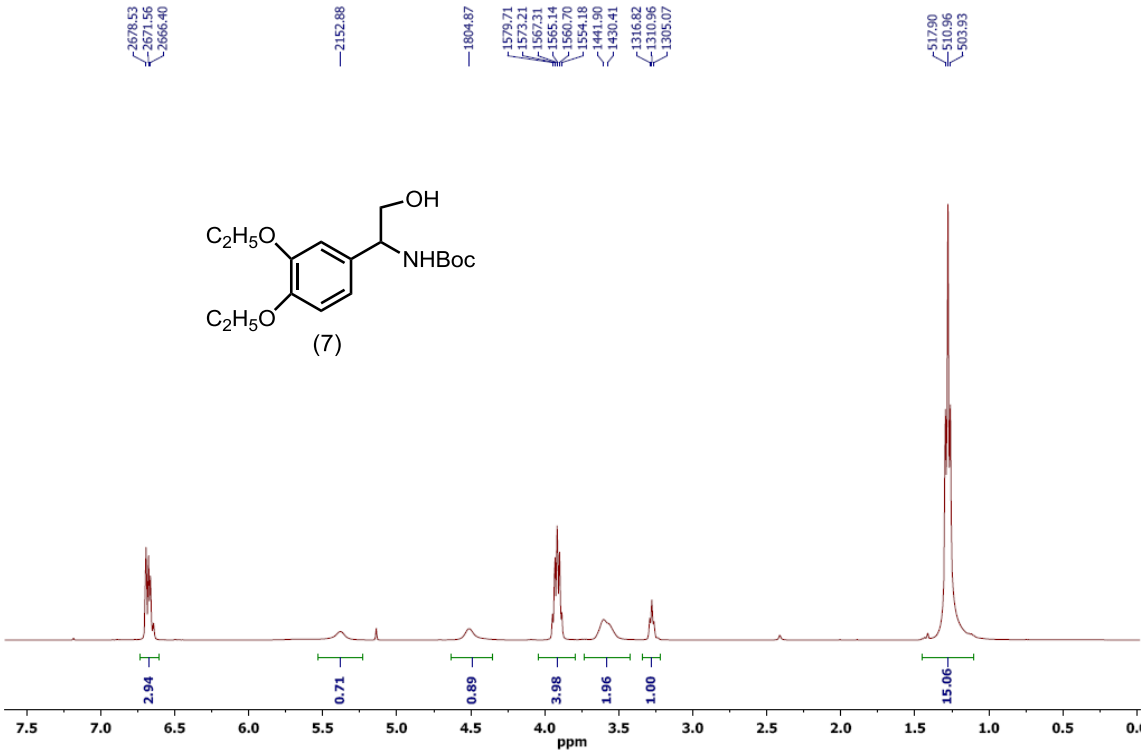


Figure 9: ^{1}H NMR spectrum of compound **7** (400 MHz, $CDCl_3$)

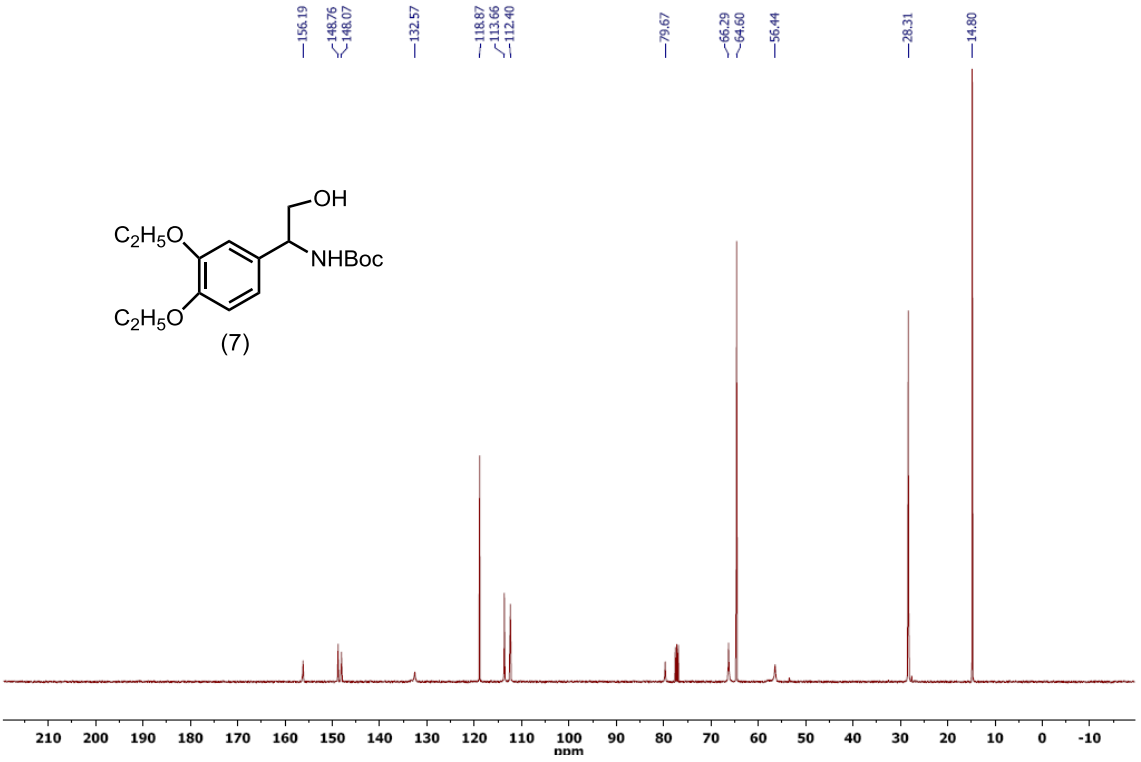


Figure 10: ^{13}C NMR spectrum of compound **7** (100 MHz, $CDCl_3$)

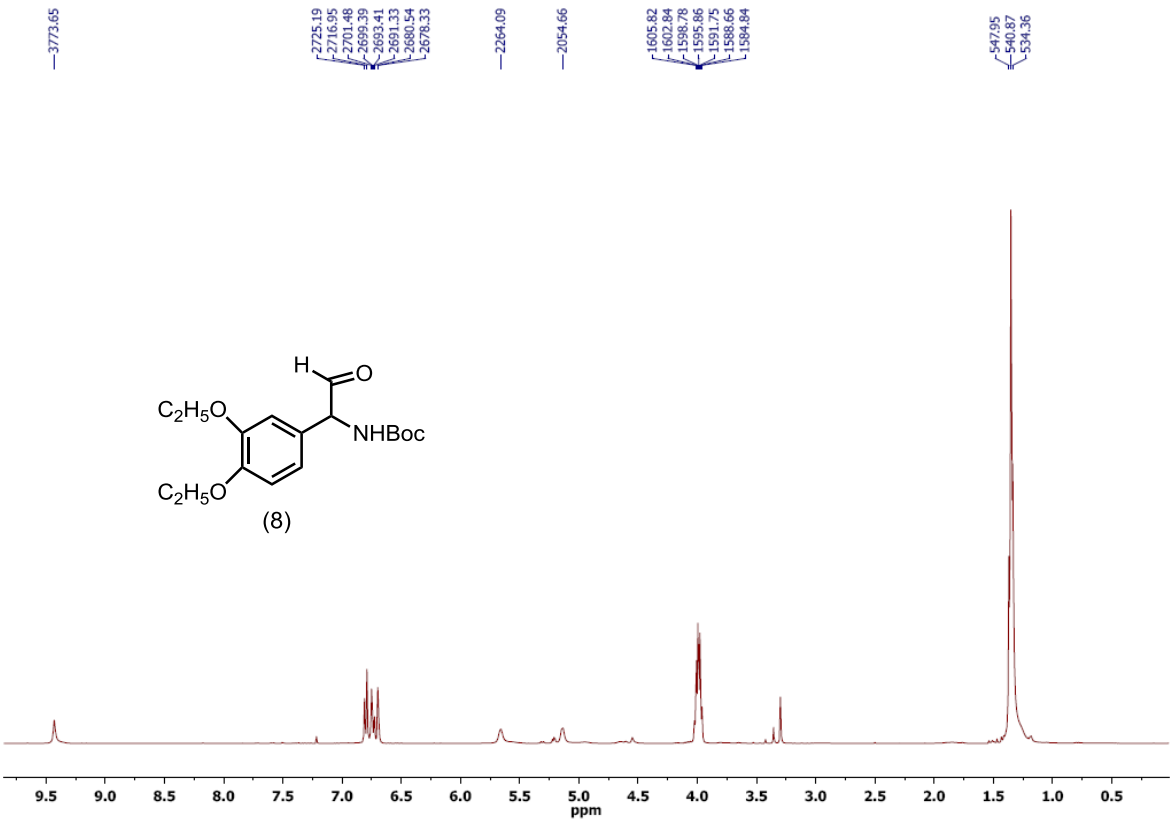


Figure 11: ^{1}H NMR spectrum of compound **8** (400 MHz, $CDCl_3$)

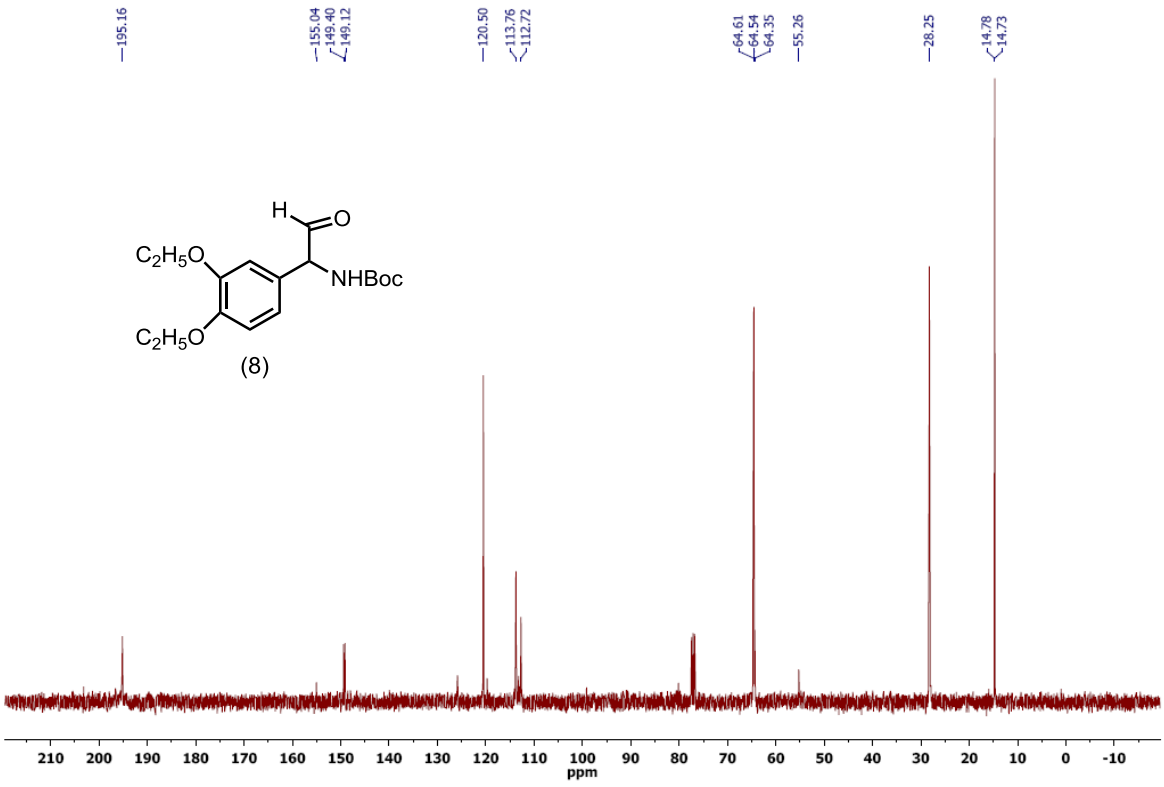


Figure 12: ^{13}C NMR spectrum of compound **8** (100 MHz, $CDCl_3$)

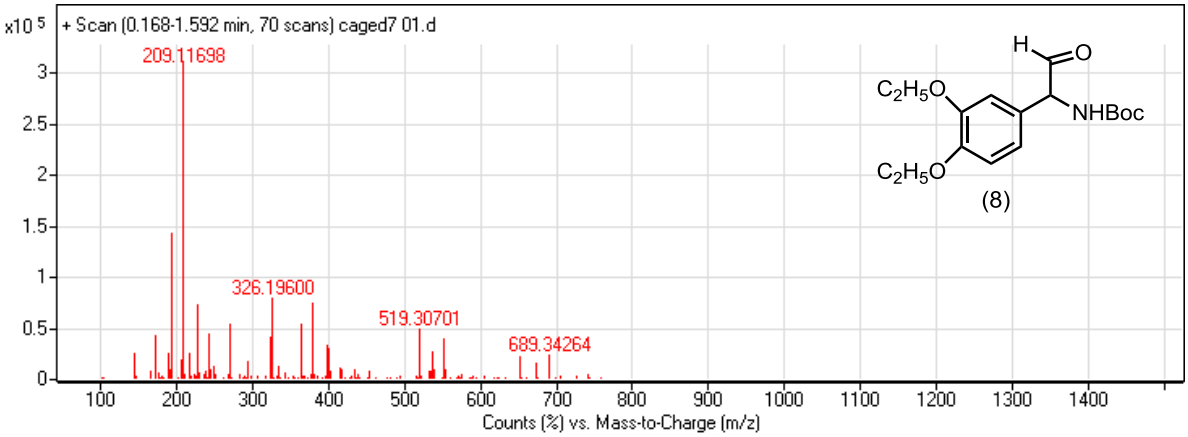


Figure 13: Mass spectrum of compound **8**

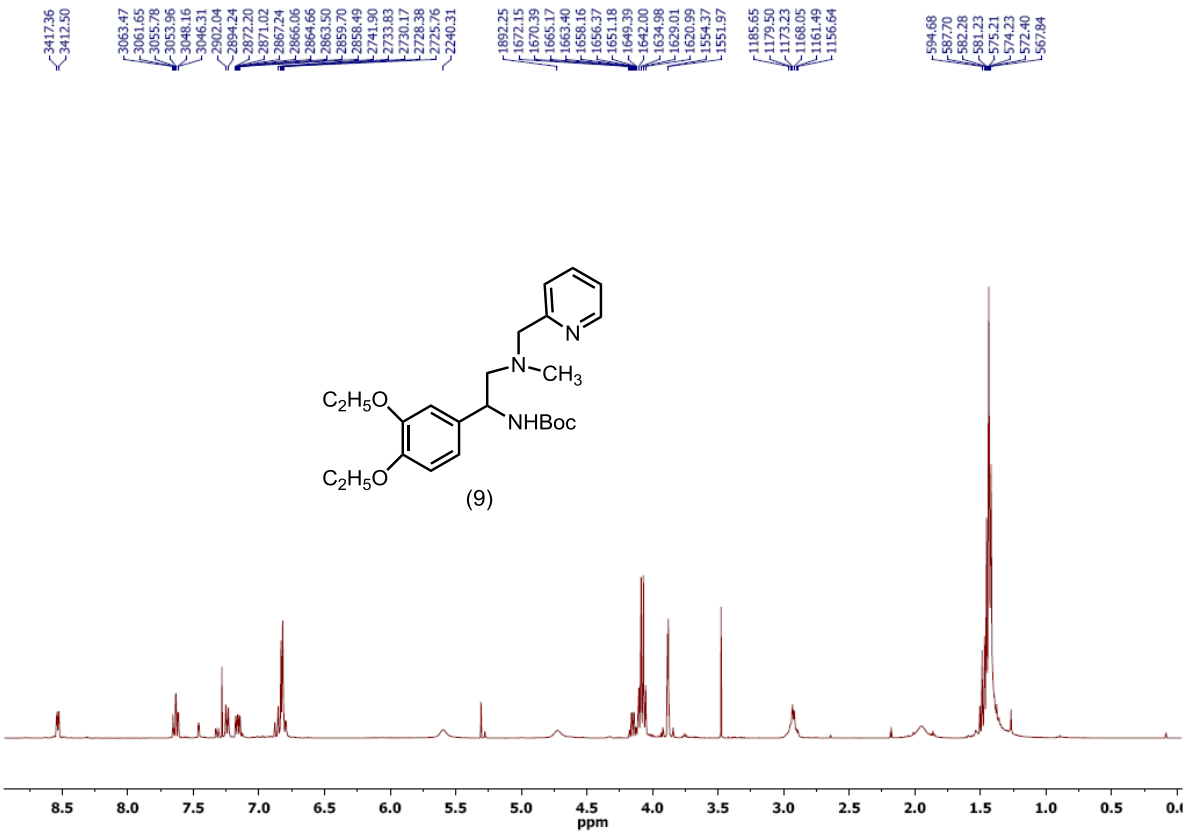


Figure 14: ^{1}H NMR spectrum of compound **9** (400 MHz, $CDCl_3$)

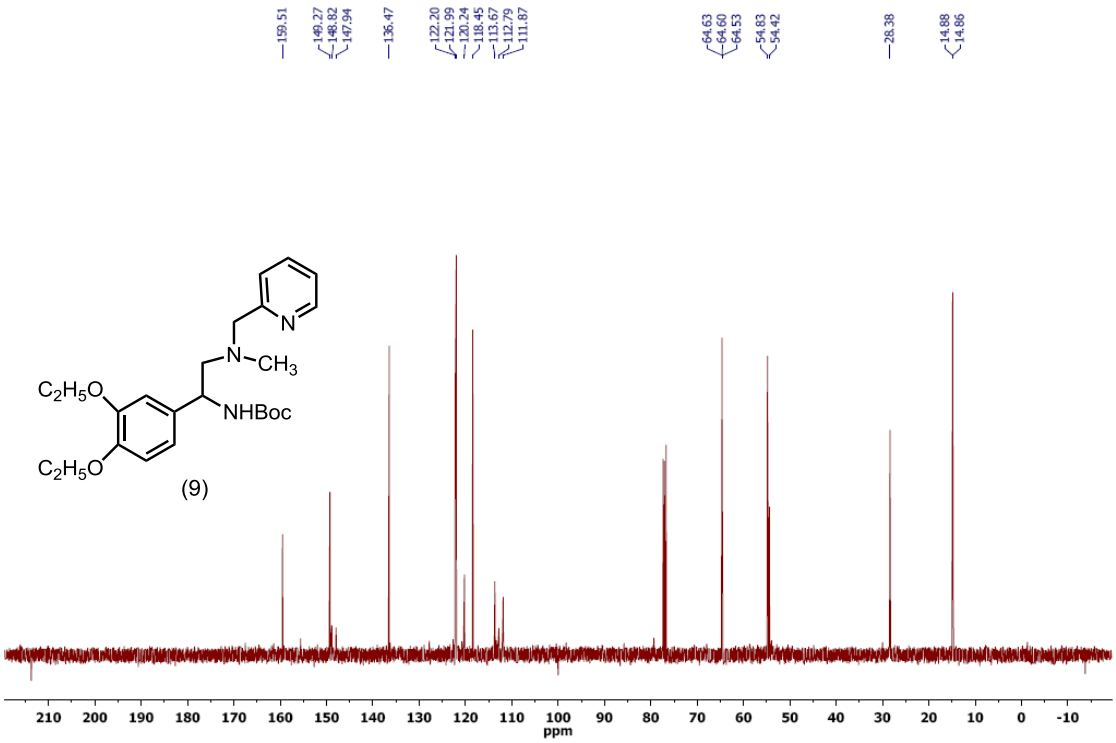


Figure 15: ^{13}C NMR spectrum of compound **9** (100 MHz, $CDCl_3$)

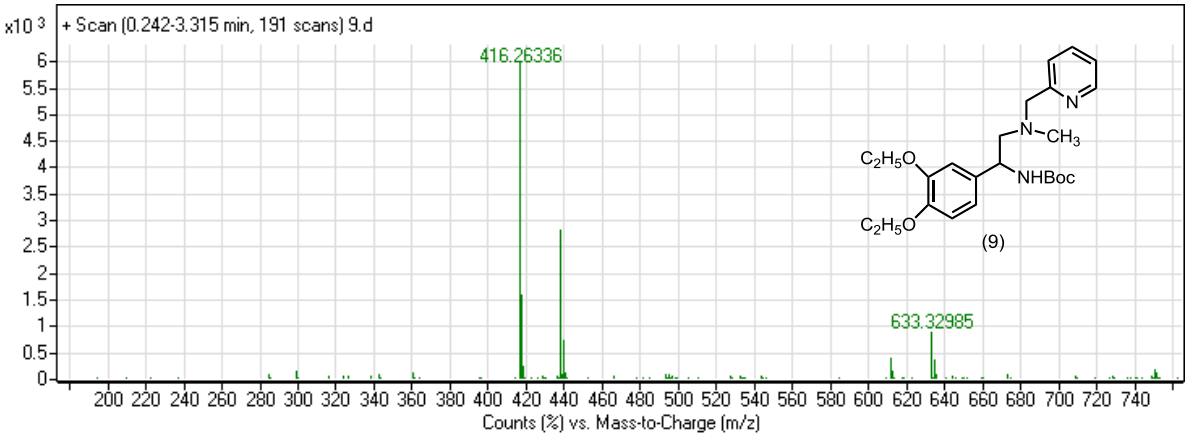


Figure 16: Mass spectrum of compound **9**

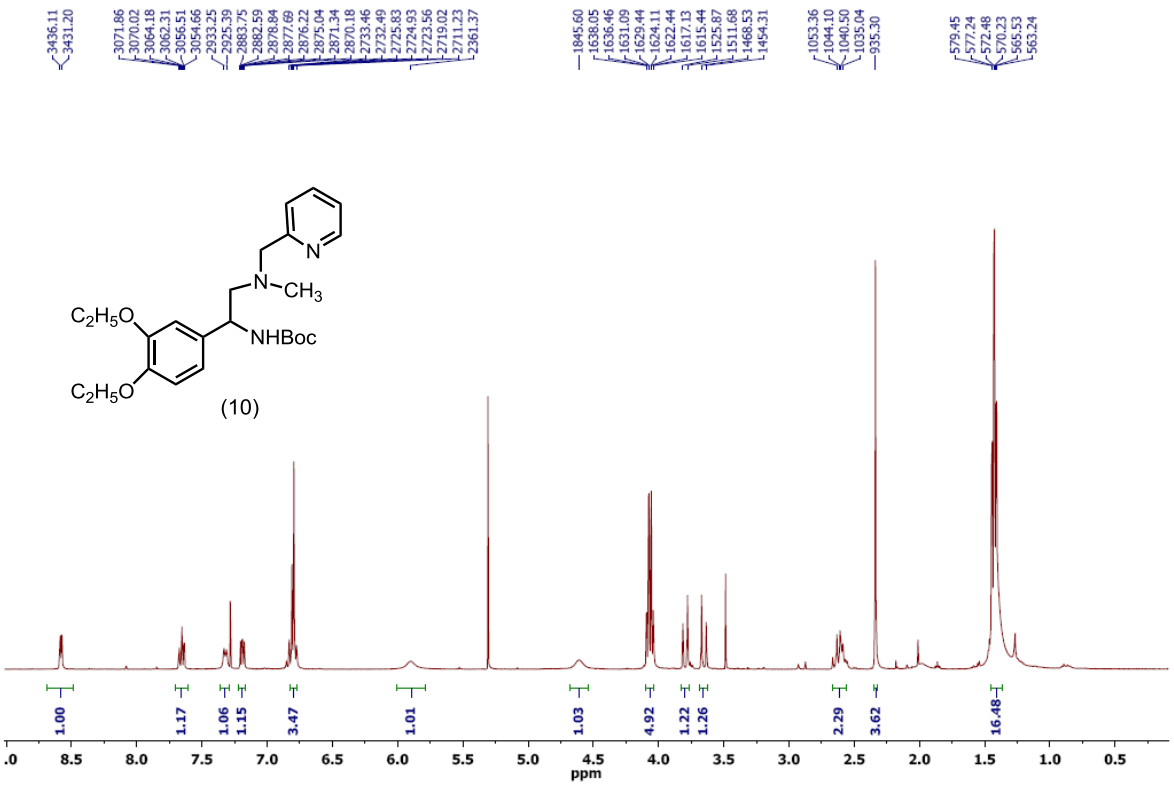


Figure 17: ^{1}H NMR spectrum of compound **10** (400 MHz, $CDCl_3$)

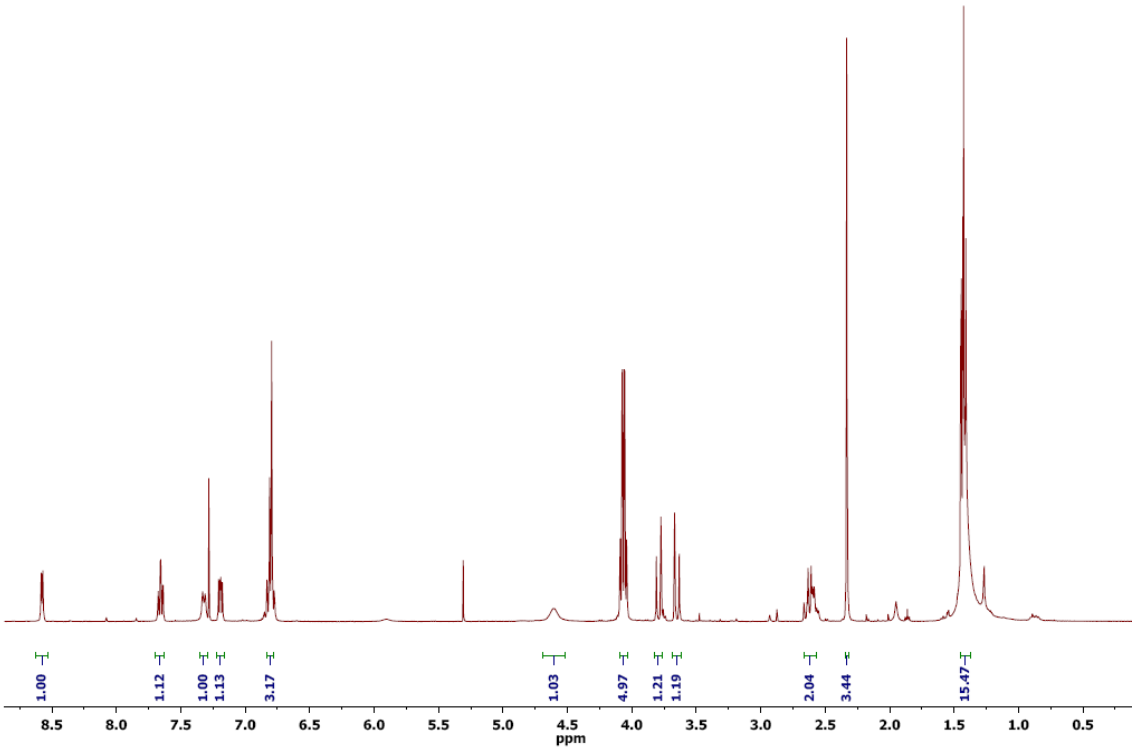


Figure 18: ^{1}H NMR spectrum of compound **10** (400 MHz, $CDCl_3$)

Figure 19: ^{13}C NMR spectrum of compound **10** (100 MHz, $CDCl_3$)

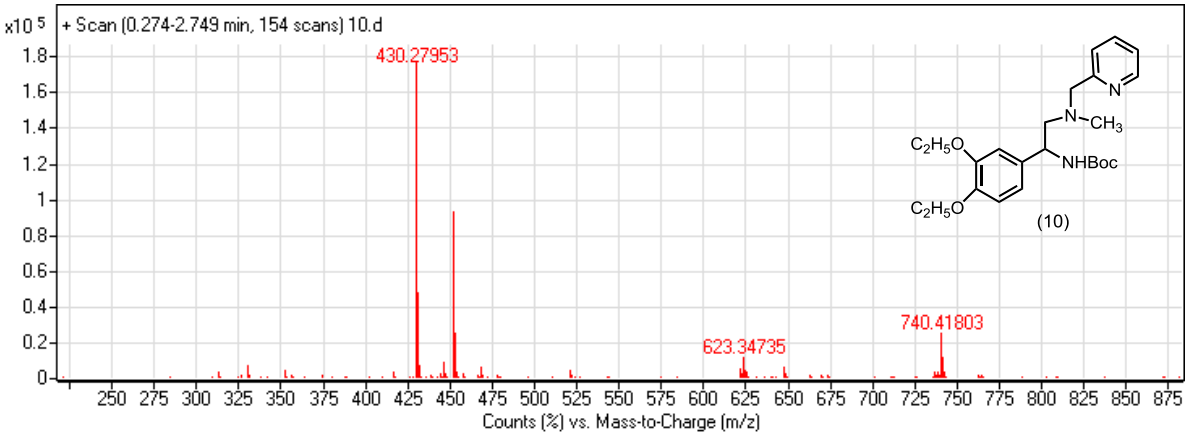


Figure 20: Mass spectrum of compound **10**

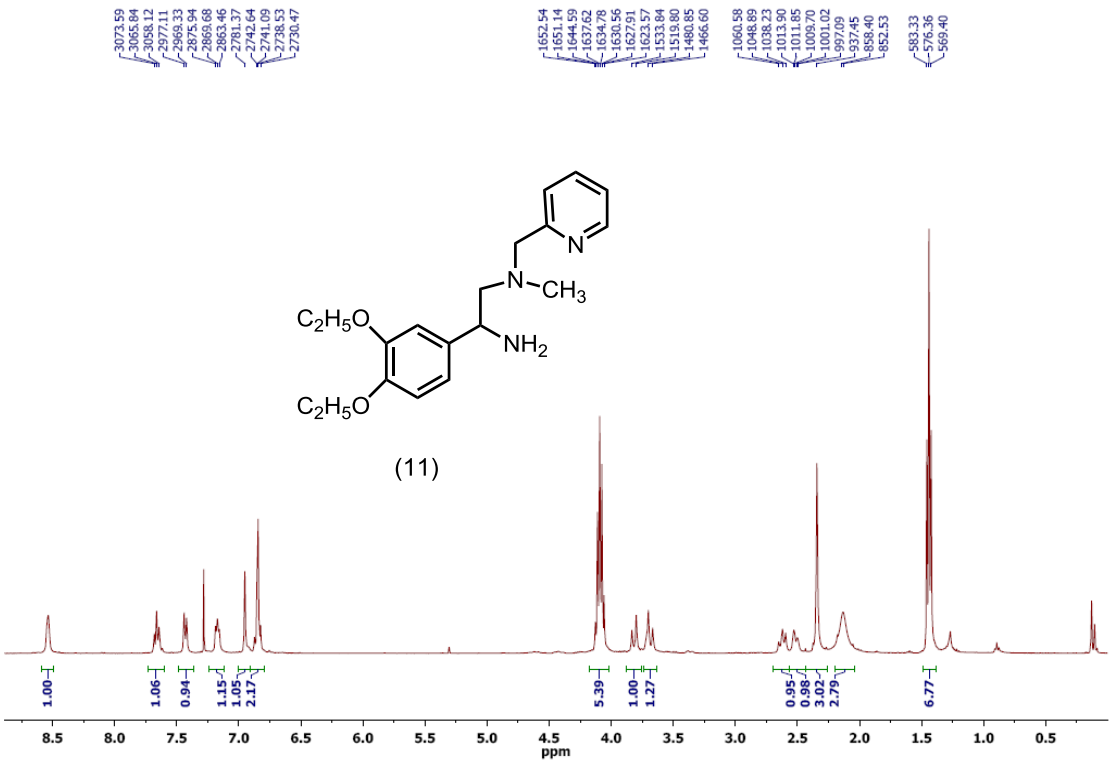


Figure 21: ^{1}H NMR spectrum of compound **11** (400 MHz, $CDCl_3$)

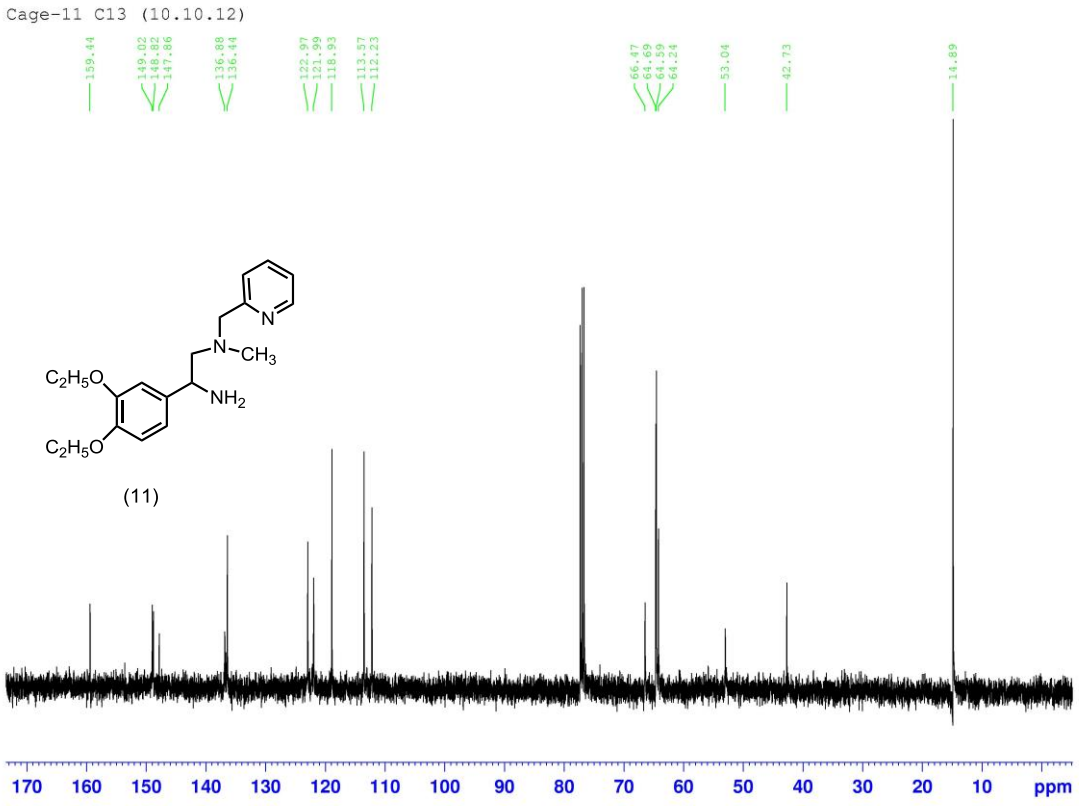


Figure 22: ^{13}C NMR spectrum of compound **11** (100 MHz, $CDCl_3$)

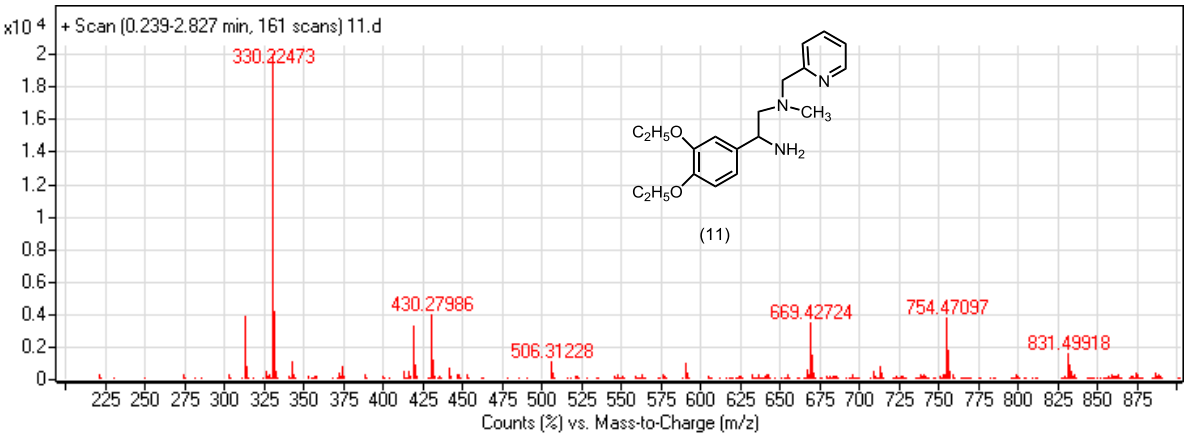


Figure 23: Mass spectrum of compound **11**

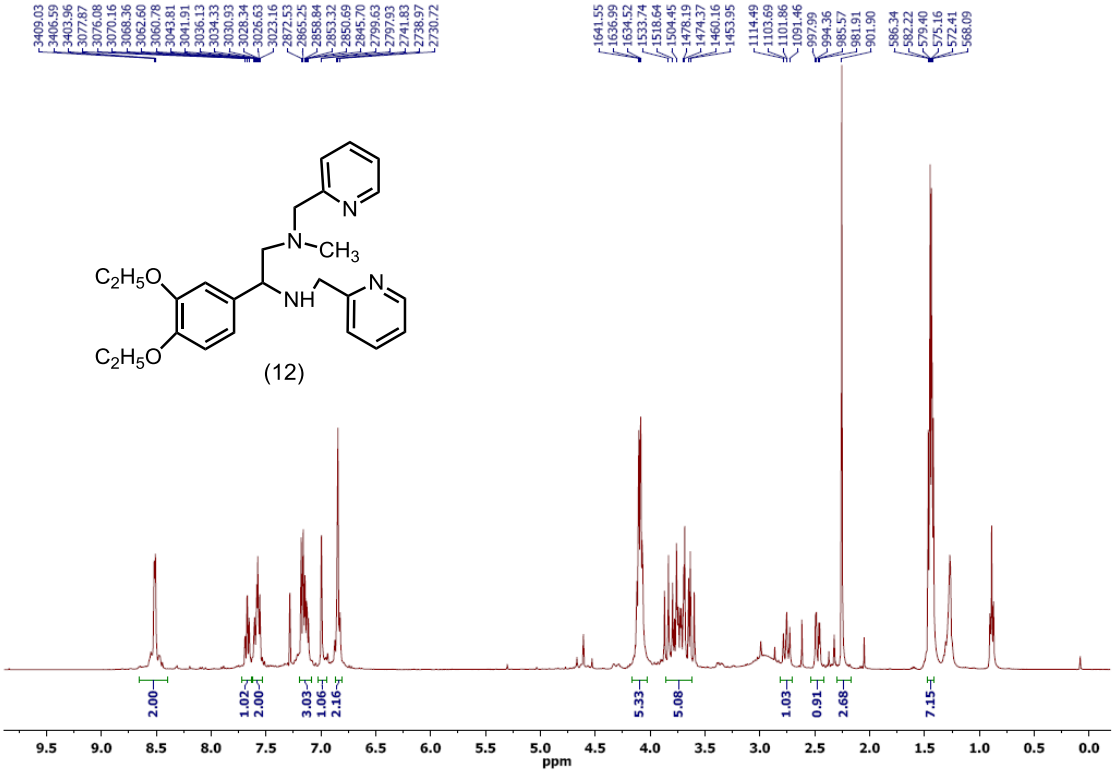


Figure 24: ^{1}H NMR spectrum of compound **12** (400 MHz, $CDCl_3$)

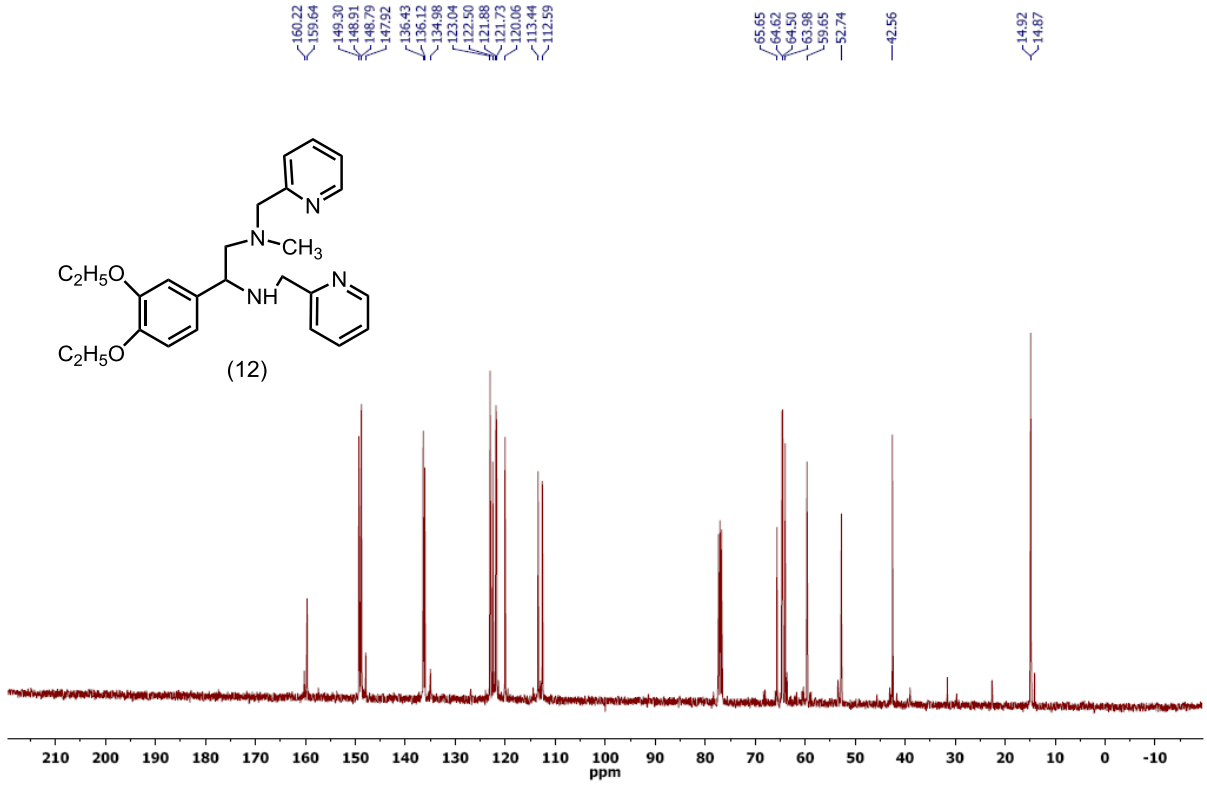


Figure 25: ^{13}C NMR spectrum of compound **12** (100 MHz, $CDCl_3$)

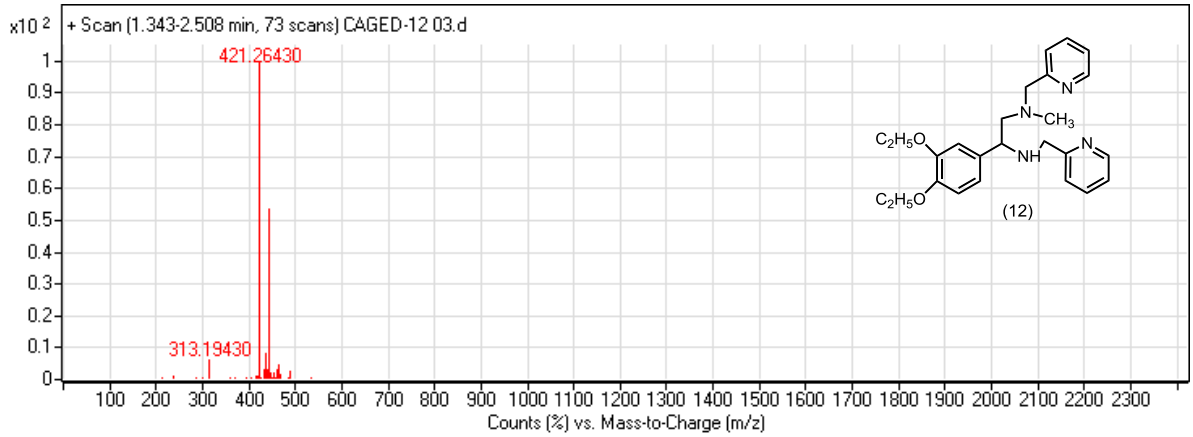


Figure 26: Mass spectrum of compound **12**

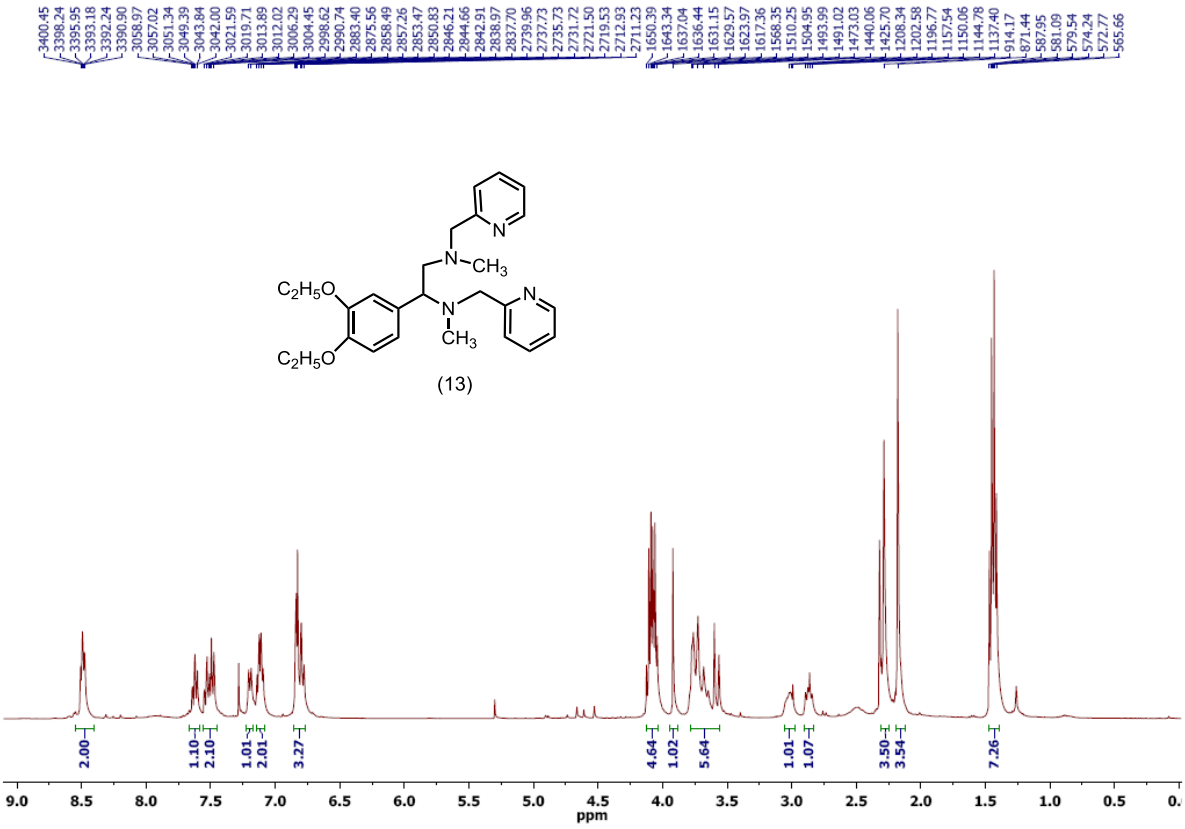


Figure 27: ^{1}H NMR spectrum of compound **13** (400 MHz, $CDCl_3$)

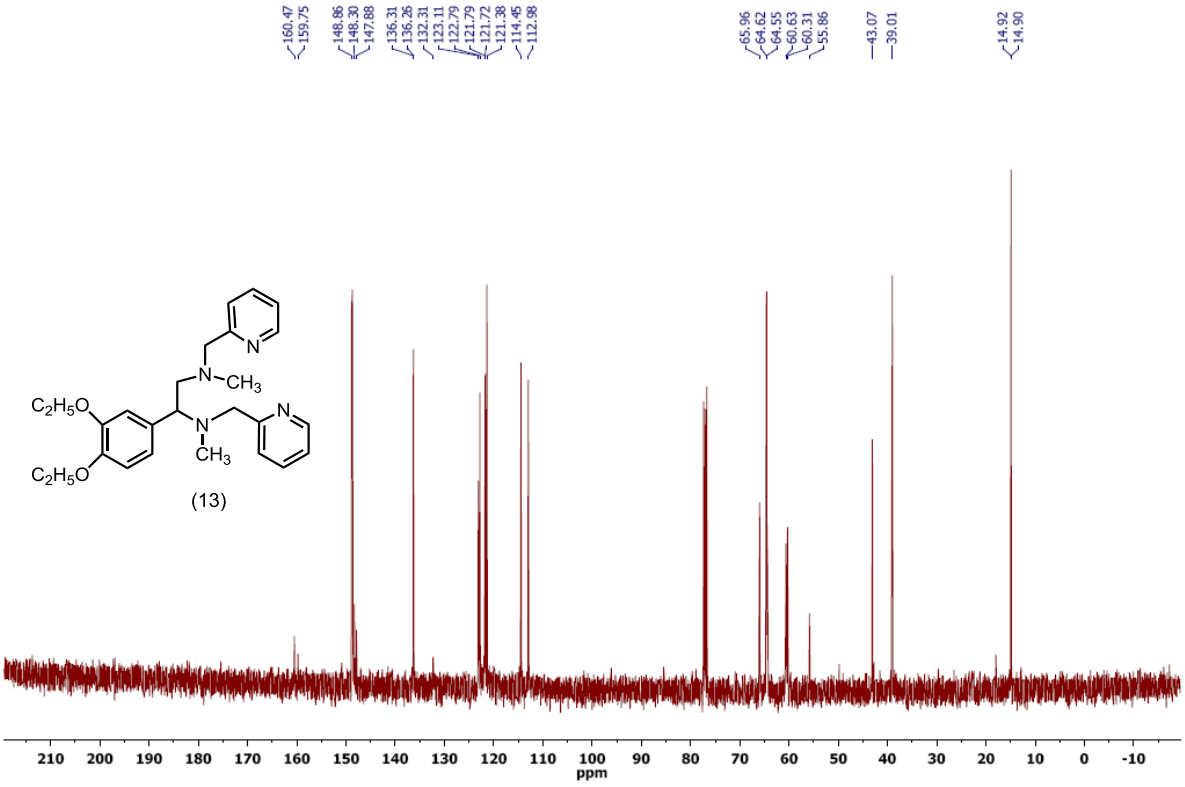


Figure 28: ^{13}C NMR spectrum of compound **13** (100 MHz, $CDCl_3$)

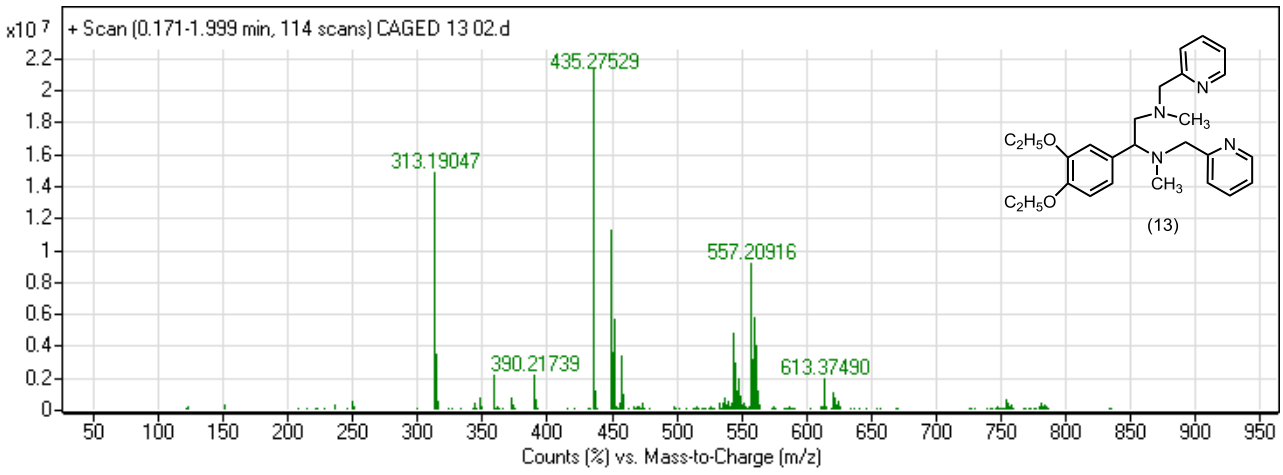


Figure 29: Mass spectrum of compound **13**

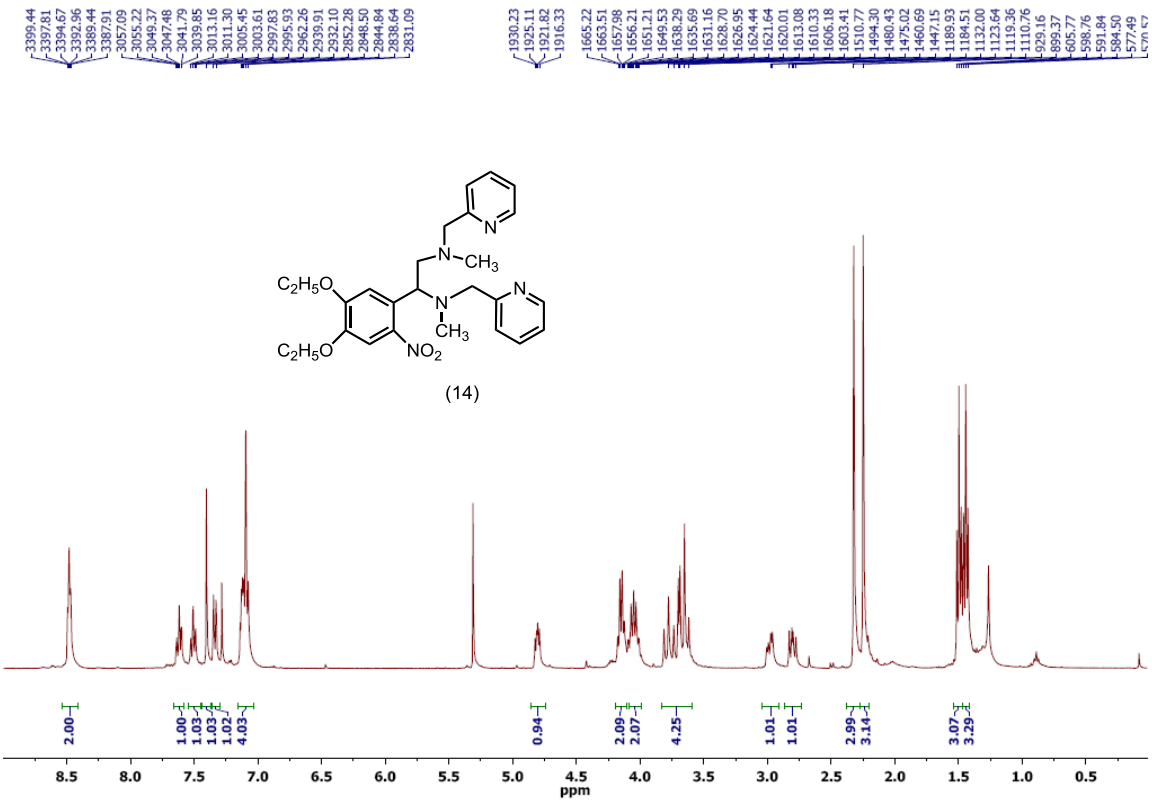


Figure 30: ^{1}H NMR spectrum of compound **14** (400 MHz, $CDCl_3$)

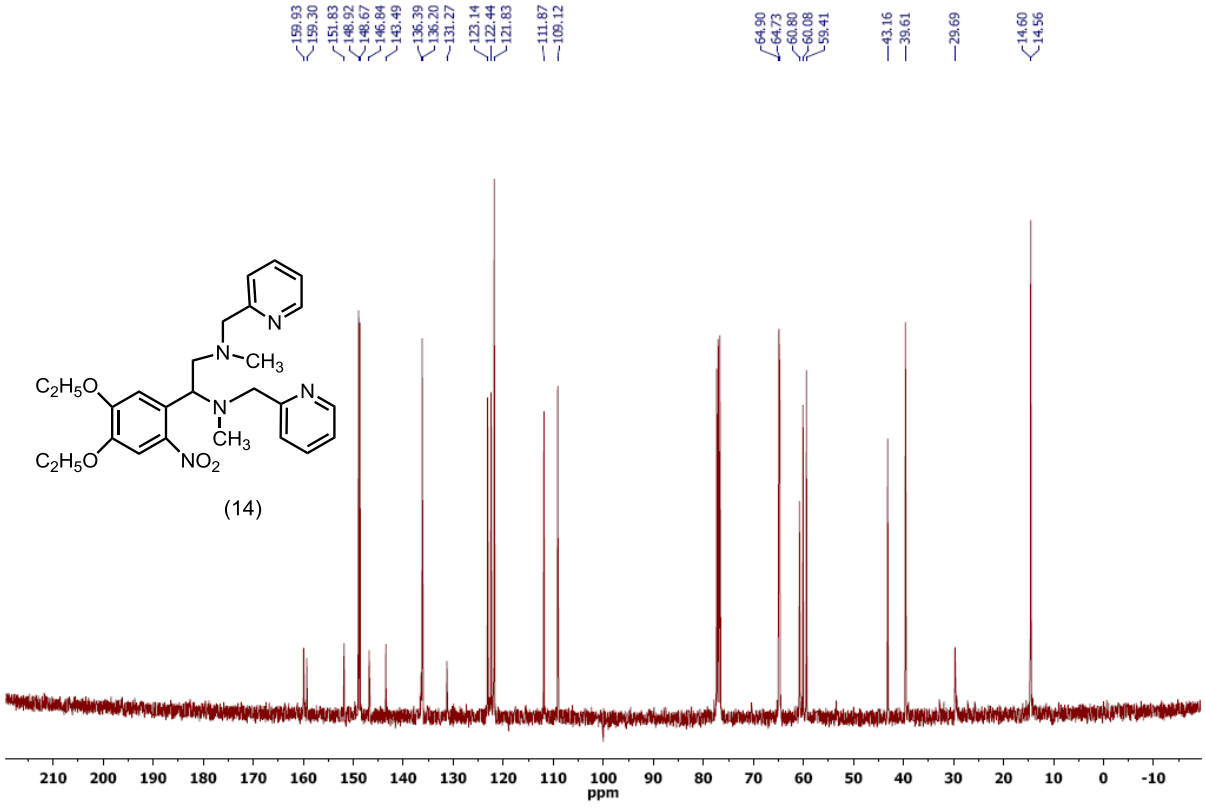


Figure 31: ^{13}C NMR spectrum of compound **14** (100 MHz, $CDCl_3$)

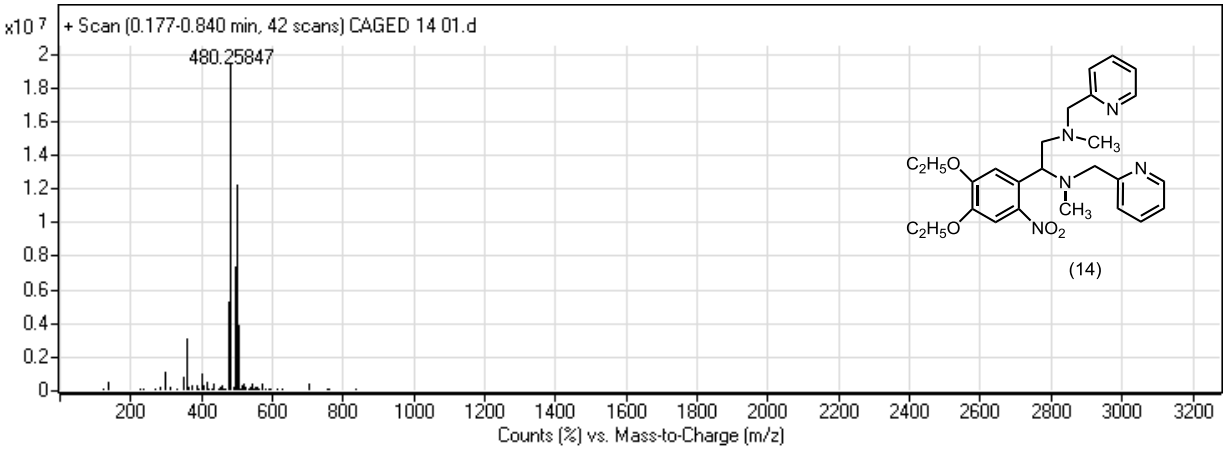


Figure 32: Mass spectrum of compound **14**