Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Synthesis of diarylalkanes through intramolecular/intermolecular addition sequence by auto-tandem catalysis with strong Brønsted base

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Contents

General Information

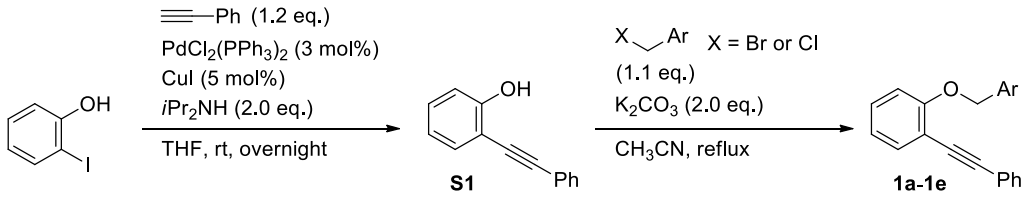
Unless otherwise noted, the reactions were carried out with dried glassware under argon atmosphere. ^{1}H NMR spectra were recorded on a JEOL JNM-ECA600 (600 MHz) spectrometer. Chemical shifts are reported in ppm from the solvent resonance or tetramethylsilane (TMS) as the internal standard ($CDCl_3$: 7.26 ppm, TMS: 0.00 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR spectra were recorded on a JEOL JNM-ECA600 (150 MHz) spectrometer with complete proton decoupling. Chemical shifts are reported in ppm from the solvent resonance as the internal standard ($CDCl_3$: 77.0 ppm). Analytical thin layer chromatography (TLC) was performed on Merck precoated TLC plates (silica gel 60 GF_{254}, 0.25 mm). Flash column chromatography was performed on silica gel 60N (spherical, neutral, 40-50 μm; Kanto Chemical Co., Inc.). High resolution mass spectra analysis was performed on a Bruker Daltonics solariX 9.4T FT-ICR-MS spectrometer and a JEOL JMS-T100GCV Time-of-Flight Mass Spectrometer at the Research and Analytical Center for Giant Molecules, Graduate School of Science, Tohoku University.

Materials: Unless otherwise noted, materials were purchased from Wako Pure Chemical Industries, Ltd., Tokyo Chemical Industry Co., LTD., Aldrich Inc., and other commercial suppliers and were used without purification. Dichloromethane, diethyl ether, tetrahydrofuran and toluene were supplied from Kanto Chemical Co., Inc. as “Dehydrated solvent system”. Other solvents were purchased from commercial suppliers as dehydrated solvents, and used under argon atmosphere.

Experimental Procedure

Substrate Synthesis[1]

Preparation of 1a-1e



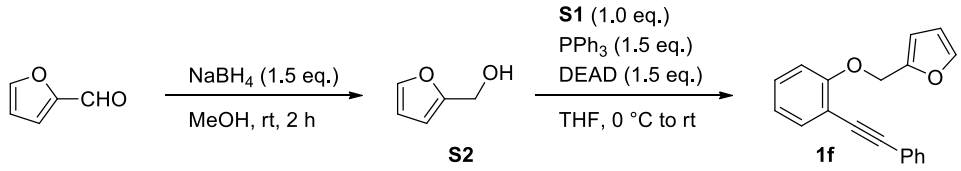
*Synthesis of **S1***[2]

To a mixture of $PdCl_2(PPh_3)_2$ (0.21 g, 0.30 mmol), CuI (38 mg, 0.50 mmol) and 2-iodophenol (2.2 g, 10 mmol) in THF (35 mL) was added phenylacetylene (1.3 mL, 12 mmol) at room temperature. After the 2-iodophenol was completely consumed, the reaction was quenched with sat. aq. NH_4Cl. The product was extracted with AcOEt, and the combined organic layer was dried over Na_2SO_4. The solvent was removed under reduced pressure and the residue was purified by silica gel column chromatography (Hexane/AcOEt = 10 : 1) to afford **S1** (1.8 g, 9.0 mmol, 90%) as a brown solid.

*Synthesis of **1** from **S1***[3]

Benzyl halide (2.0 mmol) was added to a mixture of **S1** (0.35 g, 1.8 mmol) and K_2CO_3 (0.28 g, 3.6 mmol) in acetonitrile (10 mL). The resulting mixture was heated at reflux until **S1** was consumed. After cooled to room temperature, the reaction was quenched with H_2O, and the product was extracted with AcOEt. The combined organic layer was dried over Na_2SO_4, filtered and evaporated to afford a crude mixture which was purified by silica gel column chromatography.

Preparation of 1f



*Synthesis of **S2***[4]

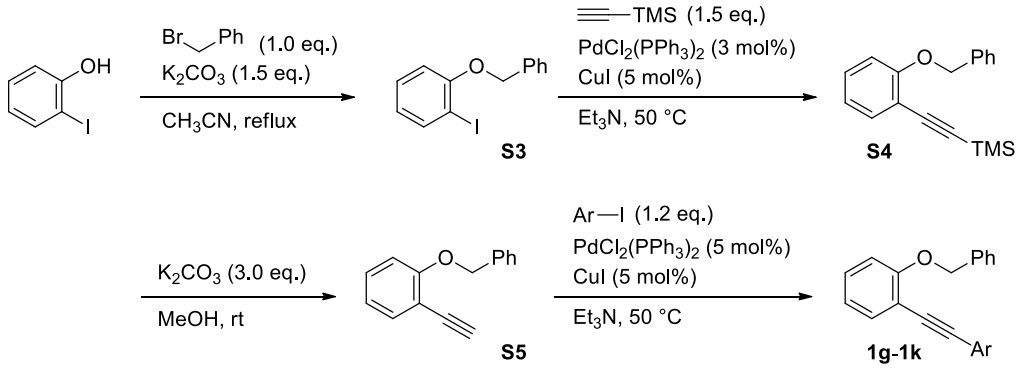
Sodium borohydride (0.57 g, 15 mmol) was added portion-wise to a solution of furfural (0.82 mL, 10 mmol) in methanol (25 mL) at 0 °C. The resulting mixture was stirred at room temperature for 2 h. The solvent was evaporated and the residue was dissolved in diethyl ether. The product was extracted with diethyl ether. The combined organic layer was dried over Na_2SO_4 and concentrated under reduced pressure to provide **S2**, which was used in the next step without further purification.

*Synthesis of **1f** from **S1** and **S2***[5]

Diethyl azodicarboxylate (0.60 mL, 3.5 mmol) was added to a solution of **S2** (0.23 g, 2.3 mmol), **S1** (0.45 g, 2.3

mmol), and PPh_3 (0.90 g, 3.5 mmol) in THF (10 mL) at 0 °C over 5 min. The mixture was allowed to warm to room temperature and stirred until the disappearance of **S1** and **S2** according to TLC. The product was extracted with AcOEt, and the combined organic layer was washed with brine, dried over Na_2SO_4, filtered and concentrated. The residue was purified by silica gel column chromatography (Hexane/AcOEt = 50 : 1) to give **1f** (0.27 g, 0.99 mmol, 43%) as a colorless oil.

Preparation of 1g-1k



*Synthesis of **S3***

Benzyl bromide (1.2 mL, 10 mmol) was added to a mixture of the 2-iodophenol (2.2 g, 10 mmol) and K_2CO_3 (2.1 g, 15 mmol) in acetonitrile (35 mL). The resulting mixture was heated at reflux until 2-iodophenol was consumed. After cooled to room temperature, the reaction was quenched with H_2O and the product was extracted with AcOEt. The combined organic layer was dried over Na_2SO_4, filtered and evaporated. The residue was purified by silica gel column chromatography (Hexane/AcOEt = 100 : 1) to afford **S3** (2.9 g, 9.4 mmol, 94%) as a colorless oil.

*Synthesis of **S4***

To a mixture of $PdCl_2(PPh_3)_2$ (0.21 g, 0.30 mmol), CuI (35 mg, 0.50 mmol) and **S3** (2.0 g, 9.0 mmol) in triethylamine (25 mL) was added trimethylsilylacetylene (1.0 mL, 13.5 mmol). The reaction mixture was stirred at 50°C. After **S3** was completely consumed, sat. aq. NH_4Cl was added to quench the reaction. The product was extracted with AcOEt, and the combine organic layer was dried over Na_2SO_4 and evaporated. The residue was then purified by silica gel column chromatography (Hexane/AcOEt = 50 : 1) to provide **S4** (2.2 g, 7.8 mmol, 87%) as a white solid.

*Synthesis of **S5***

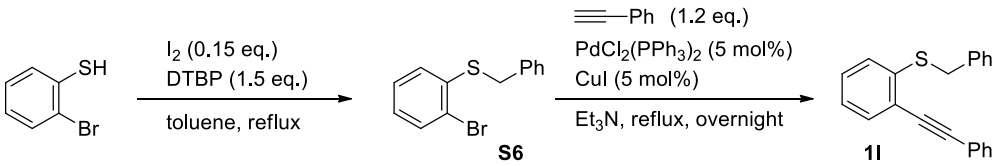
A mixture of **S4** (2.0 g, 7.0 mmol) and K_2CO_3 (2.9 g, 21 mmol) in methanol (25 ml) was stirred at room temperature until **S4** was completely consumed. The reaction was quenched with H_2O and the product was extracted with AcOEt. The combined organic layer was dried over Na_2SO_4 and concentrated. The crude mixture was purified by silica gel column chromatography (Hexane/AcOEt = 50 : 1) to provide **S5** (1.4 g, 6.7 mmol, 95%) as a yellow solid.

*Synthesis of **1** from **S5***

A mixture of $PdCl_2(PPh_3)_2$ (63 mg, 0.090 mmol), CuI (18 mg, 0.090 mmol), **S5** (0.35 g, 1.7 mmol) and aryl iodide (2.0 mmol) in triethylamine (10 mL) was stirred at 50 °C. After **S5** was completely consumed, sat. aq. NH_4Cl was

added to the solution to quench the reaction. The product was extracted with AcOEt, and the combined organic layer was dried over Na_2SO_4 and evaporated to provide a crude mixture which was purified by silica gel column chromatography.

Preparation of 1l



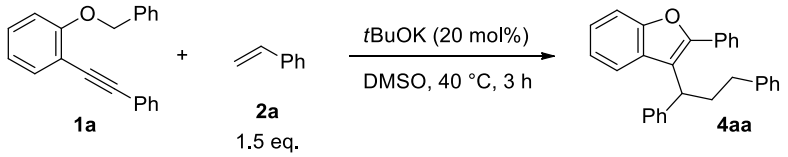
*Synthesis of **S6***[6]

2-Bromobenzenethiol (0.48 mL, 8.0 mmol) was added to a solution of I_2 (0.15 g, 1.2 mmol) in toluene (50 mL) under N_2 atmosphere. Then di-*tert*-butyl peroxide (7.4 mL, 40 mmol) was added to the mixture. The solution was heated at reflux for 20 h. After the completion of the reaction, the reaction was quenched with H_2O and the product was extracted with AcOEt. The combined organic layers was dried over Na_2SO_4 and concentrated under reduce pressure. The purification of the crude mixture by silica gel column chromatography (Hexane/AcOEt = 100 : 1) provided **S6** (1.7 g, 6.0 mmol, 75%) as a white solid.

*Preparation of **1l** from **S6***

A mixture of $PdCl_2(PPh_3)_2$ (0.16 g, 0.23 mmol), CuI (45 mg, 0.23 mmol), **S6** (1.3 g, 4.5 mmol) and phenylacetylene (0.6 mL, 5.4 mmol) in triethylamine (20 mL) was heated at reflux overnight. After cooled to room temperature, sat. aq. NH_4Cl was added to the solution to quench the reaction. The product was extracted with AcOEt, and the combined organic layer was dried over Na_2SO_4 and evaporated. The residue was purified by silica gel column chromatography (Hexane/AcOEt = 100 : 1) to afford **1l** (0.62 g, 2.1 mmol, 46 %) as a yellow solid.

General Procedure for Synthesis of Diarylalkanes through Intramolecular/Intermolecular Addition Sequence Catalyzed by Brønsted Base.

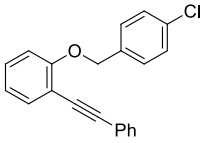


The reaction of **1a** with **2b** is representative (Table 1, entry 5).

A DMSO solution (2.0 mL) of **1a** (57 mg, 0.20 mmol) and styrene (**2a**, 35 μL, 0.30 mmol) was added a solution of potassium *tert*-butoxide in THF (1.0 M, 40 μL, 0.040 mmol). The reaction mixture was stirred at 40 °C for 3 h. The reaction was quenched by sat. aq. NH_4Cl, and the product was extracted with AcOEt. The combined organic layer was dried over Na_2SO_4 and evaporated. The crude mixture was purified by silica gel column chromatography (Hexane/AcOEt = 100 : 1) to provide **4aa** (71 mg, 0.18 mmol, 91%) as a white solid.

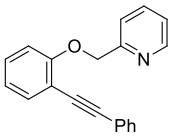
Analytical Data

1-(4-Chlorobenzyloxy)-2-(phenylethynyl)benzene (1b):



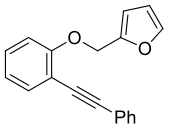
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49-7.53 (m, 3H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.31-7.36 (m, 5H), 7.28 (ddd, *J* = 8.4, 7.2, 2.4 Hz, 1H), 6.97 (ddd, *J* = 7.2, 7.2, 0.6 Hz, 1H), 6.92 (d, *J* = 8.4 Hz, 1H), 5.16 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 135.6, 133.5, 133.4, 131.5, 129.6, 128.7, 128.3, 128.3, 128.2, 123.6, 121.2, 113.5, 112.9, 93.8, 85.7, 69.8; IR (ATR): 3060, 3032, 2866, 2216, 1898, 1593, 1496, 1447, 1277, 1240, 1219, 1013, 808 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{21}H_{15}ClO$ 318.0811, Found 318.0810; Mp. 67.7-68.7 °C.

2-(Phenylethynyl)-1-(2-pyridylmethoxy)benzene (1e):



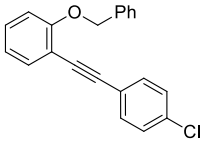
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.59 (d, *J* = 4.2 Hz, 1H), 7.79 (d, *J* = 7.8 Hz, 1H), 7.71 (ddd, *J* = 7.8, 7.2, 1.8 Hz, 1H), 7.56 (dd, *J* = 8.4, 1.8 Hz, 2H), 7.54 (dd, *J* = 7.8, 1.8 Hz, 1H), 7.32-7.38 (m, 3H), 7.29 (ddd, *J* = 8.4, 7.2, 1.8 Hz, 1H), 7.22 (dd, *J* = 7.2, 4.2 Hz, 1H), 6.98 (dd, *J* = 7.2, 7.2 Hz, 1H), 6.96 (d, *J* = 8.4 Hz, 1H), 5.32 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.8, 157.4, 149.0, 136.9, 133.4, 131.6, 129.8, 128.3, 128.2, 123.7, 122.5, 121.10, 121.05, 113.2, 112.5, 93.7, 85.8, 70.9; IR (ATR): 3377, 3061, 3017, 2943, 2216, 1591, 1573, 1497, 1482, 1280, 1242, 1219, 1108, 1049 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{20}H_{15}NO$ 285.1154, Found 285.1152; Mp. 42.7-43.7 °C.

1-(2-Furylmethoxy)-2-(phenylethynyl)benzene (1f):



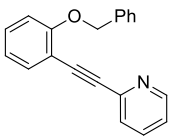
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.49-7.53 (m, 3H), 7.44 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.30-7.35 (m, 3H), 7.28 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.02 (d, *J* = 8.4 Hz, 1H), 6.98 (ddd, *J* = 7.2, 7.2, 0.6 Hz, 1H), 6.45 (d, *J* = 3.0 Hz, 1H), 6.38 (dd, *J* = 3.0, 1.8 Hz, 1H), 5.14 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.0, 150.4, 142.9, 133.5, 131.6, 129.6, 128.2, 128.1, 123.7, 121.5, 114.02, 113.95, 110.5, 109.8, 93.7, 85.7, 63.9; IR (ATR): 3059, 3032, 2920, 2408, 2217, 1592, 1495, 1482, 1444, 1279, 1234, 1219, 1103, 917, 884 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{19}H_{14}O_2$ 274.0994, Found 274.0993.

1-Benzyloxy-2-(4-chlorophenyl)ethynylbenzene (1g):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 2H), 7.50 (d, *J* = 7.8, 1.8 Hz, 1H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.38 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 8.4 Hz, 2H), 7.29 (ddd, *J* = 7.8, 7.2, 1.8 Hz, 1H), 6.96 (dd, *J* = 7.2, 7.2 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 1H), 5.20 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.3, 137.0, 134.0, 133.3, 132.8, 129.9, 128.6, 128.5, 127.8, 126.9, 122.2, 121.0, 113.1, 112.8, 92.6, 86.9, 70.5; IR (ATR): 3065, 3032, 2903, 2860, 2217, 1945, 1894, 1597, 1571, 1498, 1219, 1086, 823 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{21}H_{15}ClO$ 318.0811, Found 318.0810; Mp. 101.4-102.4 °C.

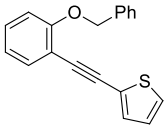
1-Benzyloxy-2-(2-pyridylethynyl)benzene (1j):



Light yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 4.8, 0.6 Hz, 1H), 7.60-7.63 (m, 1H), 7.58 (dd, *J* = 7.2, 1.8 Hz, 1H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.46 (d, *J* = 7.8 Hz, 1H), 7.36 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.25-7.31 (m, 2H), 7.19 (dd, *J* = 7.2, 5.4 Hz, 1H), 6.94 (ddd, *J* = 7.8, 7.8, 0.6 H, 1H),

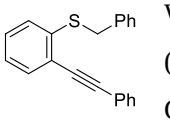
6.92 (d, J = 8.4 Hz, 1H), 5.20 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.7, 150.0, 143.8, 137.0, 136.0, 133.8, 130.4, 128.5, 127.7, 127.2, 126.9, 122.5, 120.9, 112.8, 112.4, 92.9, 86.0, 70.4; IR (ATR): 3396, 3062, 3032, 2913, 2219, 1580, 1491, 1445, 1380, 1277, 1088 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{20}H_{15}NO$ 285.1154, Found 285.1152.

1-Benzyloxy-2-(2-thienylethynyl)benzene (1k):



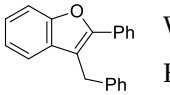
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.53 (d, J = 7.8 Hz, 2H), 7.49 (dd, J = 7.8, 1.8 Hz, 1H), 7.39 (dd, J = 7.8, 7.2 Hz, 2H), 7.31 (t, J = 7.2 Hz, 1H), 7.25-7.28 (m, 3H), 7.01 (dd, J = 5.4, 3.6 Hz, 1H), 6.95 (dd, J = 7.8, 7.8 Hz, 1H), 6.94 (d, J = 8.4 Hz, 1H), 5.20 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.1, 137.0, 133.0, 131.6, 129.8, 128.5, 127.7, 127.09, 127.06, 126.8, 123.8, 121.0, 113.2, 112.9, 89.7, 86.8, 70.4; IR (ATR): 3089, 3067, 3032, 2869, 2205, 1595, 1485, 1445, 1273, 1219, 1023 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{19}H_{14}OS$ 290.0765, Found 290.0764; Mp. 66.4-67.4 °C.

1-Benzylthio-2-(phenylethynyl)benzene (1l):



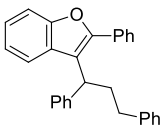
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56-7.58 (m, 2H), 7.51 (d, J = 7.8 Hz, 1H), 7.31-7.37 (m, 5H), 7.19-7.30 (m, 5H), 7.14 (ddd, J = 7.8, 7.8, 1.2 Hz, 1H), 4.22 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 139.5, 136.9, 132.6, 131.7, 128.9, 128.6, 128.5, 128.4, 128.3, 127.9, 127.2, 125.5, 123.24, 123.18, 95.5, 87.3, 37.6; IR (ATR): 3059, 3028, 2917, 1597, 1579, 1490, 1457, 1440, 1236, 1088 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{21}H_{16}S$ 300.0973, Found 300.0972; Mp. 69.1-70.1 °C.

3-Benzyl-2-phenylbenzofuran (3a):



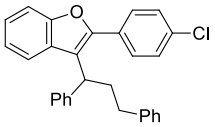
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (dd, J = 7.8, 1.2 Hz, 2H), 7.53 (ddd, J = 7.8, 1.2, 0.6 Hz, 1H), 7.44 (ddd, J = 7.8, 7.2, 1.2 Hz, 2H), 7.34-7.38 (m, 2H), 7.26-7.31 (m, 5H), 7.21 (td, J = 7.2, 1.8 Hz, 1H), 7.15-7.19 (m, 1H), 4.31 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.1, 152.1, 139.3, 130.9, 130.5, 128.7, 128.6, 128.4, 128.2, 126.9, 126.3, 124.4, 122.6, 120.0, 113.8, 111.1, 30.1; IR (ATR): 3083, 3061, 3026, 2900, 1946, 1602, 1493, 1455, 1218, 1059, 1027, 741 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{21}H_{16}O$ 284.1201, Found 284.1200; Mp. 81.7-82.7 °C.

3-(1,3-Diphenylprop-1-yl)-2-phenylbenzofuran (4aa):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65-7.68 (m, 3H), 7.58 (d, J = 8.4 Hz, 1H), 7.39-7.47 (m, 5H), 7.31-7.35 (m, 3H), 7.22-7.25 (m, 2H), 7.17-7.19 (m, 2H), 7.13-7.15 (m, 1H), 7.02 (d, J = 7.2 Hz, 2H), 4.52 (dd, J = 9.0, 5.4 Hz, 1H), 2.51-2.71 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.6, 143.8, 141.7, 131.0, 128.9, 128.6, 128.5 (2C), 128.4, 128.2, 127.9, 127.7, 126.3, 125.7, 124.2, 122.5, 121.6, 117.3, 111.4, 40.9, 36.6, 34.2; IR (ATR): 3059, 3025, 2921, 1601, 1493, 1455, 1236, 1088 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{24}O$ 388.1827, Found 388.1825; Mp. 84.0-85.0 °C.

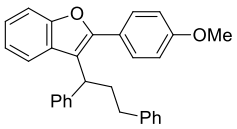
2-(4-Chlorophenyl)-3-(1,3-diphenylprop-1-yl)benzofuran (4ba):



Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, J = 7.8 Hz, 1H), 7.53 (d, J = 8.4 Hz, 1H), 7.50 (d, J = 8.4 Hz, 2H), 7.36 (d, J = 8.4 Hz, 2H), 7.35-7.37 (m, 2H), 7.27-7.32 (m, 3H), 7.18-7.22 (m, 2H), 7.10-7.17 (m, 3H), 6.97 (d, J = 8.4 Hz, 2H), 4.38-4.41 (m, 1H), 2.55-2.64 (m, 3H), 2.48-2.51 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 151.3, 143.5, 141.4, 134.5, 129.4, 129.1, 128.9,

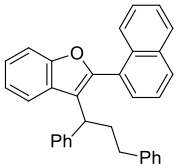
128.8, 128.6, 128.4, 128.3, 127.6, 126.4, 125.8, 124.5, 122.6, 121.6, 117.9, 111.5, 40.8, 36.4, 34.1; IR (ATR): 3083, 3059, 3025, 2942, 2861, 1601, 1583, 1488, 1451, 1092, 1013, 832 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{23}ClO$ 422.1437, Found 422.1437.

3-(1,3-Diphenylprop-1-yl)-2-(4-methoxyphenyl)benzofuran (4ca):



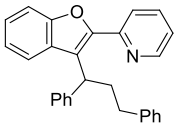
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 9.0 Hz, 2H), 7.51 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.26-7.30 (m, 3H), 7.17-7.21 (m, 2H), 7.15 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 2H), 7.10-7.12 (m, 1H), 6.98 (d, *J* = 7.2 Hz, 2H), 6.93 (d, *J* = 9.0 Hz, 2H), 4.42 (dd, J = 9.6, 6.0 Hz, 1H), 3.86 (s, 3H), 2.47-2.66 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 159.8, 154.4, 152.7, 144.0, 141.8, 129.3, 129.1, 128.53, 128.45, 128.2, 127.7, 126.3, 125.7, 123.8, 123.5, 122.4, 121.3, 116.1, 114.1, 111.3, 55.4, 41.0, 36.6, 34.3; IR (ATR): 3059, 3024, 2932, 2861, 2836, 1612, 1507, 1453, 1251, 1176, 1095, 834 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{30}H_{26}O_2$ 418.1933, Found 418.1931.

3-(1,3-Diphenylprop-1-yl)-2-(1-naphthyl)benzofuran (4da):



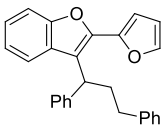
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 7.2, 2.4 Hz, 1H), 7.92 (d, *J* = 8.4 Hz, 1H), 7.86 (d, *J* = 8.4 Hz, 1H), 7.71 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 1H), 7.52 (ddd, *J* = 8.4, 7.2, 1.2 Hz, 1H), 7.42-7.47 (m, 3H), 7.34 (ddd, *J* = 7.2, 7.2, 1.2 Hz, 1H), 7.29 (d, *J* = 7.2 Hz, 2H), 7.22-7.27 (m, 3H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.06-7.09 (m, 3H), 6.90 (dd, *J* = 7.8, 2.4 Hz, 2H), 4.14 (dd, *J* = 9.0, 5.4 Hz, 1H), 2.53-2.61 (m, 2H), 2.41-2.48 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.9, 152.5, 143.8, 141.8, 133.8, 132.7, 129.9, 129.1, 128.4, 128.3 (3C), 128.2, 128.1, 127.7, 126.7, 126.23, 126.19, 126.1, 125.7, 125.0, 124.2, 122.6, 121.4, 119.9, 111.6, 41.3, 36.3, 34.4; IR (ATR): 3059, 3025, 2922, 2863, 2407, 2361, 1944, 1494, 1452, 1217, 1087, 894 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{33}H_{26}O$ 438.1984, Found 438.1982.

3-(1,3-Diphenylprop-1-yl)-2-(2-pyridyl)benzofuran (4ea):



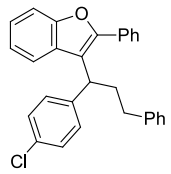
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.63 (ddd, *J* = 4.8, 1.8, 0.6 Hz, 1H), 7.91 (dt, *J* = 8.4, 1.2 Hz, 1H), 7.76 (ddd, *J* = 7.8, 7.8, 1.8 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.50-7.53 (m, 3H), 7.24-7.31 (m, 3H), 7.21 (ddd, *J* = 7.2, 4.8, 1.2 Hz, 1H), 7.12-7.18 (m, 4H), 7.10 (tt, *J* = 7.2, 1.8 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 5.87 (dd, *J* = 6.0, 6.0 Hz, 1H), 2.60-2.70 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.4, 151.2, 149.6, 149.2, 144.0, 142.3, 136.3, 128.8, 128.4, 128.2, 128.1, 127.9, 126.0, 125.6, 125.0, 122.5, 122.24, 122.19 (2C), 121.3, 111.5, 39.4, 35.3, 34.2; IR (ATR): 3084, 3058, 3024, 2922, 2862, 1945, 1596, 1494, 1453, 1423, 1218, 1088, 889 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{28}H_{23}NO$ 389.1780, Found 389.1779.

3-(1,3-Diphenylprop-1-yl)-2-(2-furyl)benzofuran (4fa):



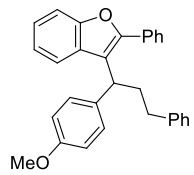
Light red oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.49 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.47 (d, *J* = 7.8 Hz, 1H), 7.43 (d, *J* = 7.2 Hz, 2H), 7.24-7.29 (m, 3H), 7.12-7.21 (m, 5H), 7.07 (d, *J* = 8.4 Hz, 2H), 6.75 (dd, *J* = 3.6, 0.6 Hz, 1H), 6.52 (dd, *J* = 3.0, 1.8 Hz, 1H), 4.86 (dd, *J* = 9.6, 5.4 Hz, 1H), 2.56-2.69 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 146.6, 144.0, 143.5, 142.8, 141.9, 128.5, 128.4, 128.3, 128.2, 127.7, 126.2, 125.7, 124.5, 122.7, 121.4, 117.8, 111.4, 111.3, 109.1, 39.9, 35.4, 34.2; IR (ATR): 3083, 3059, 3025, 2924, 2861, 1600, 1494, 1444, 1345, 1262, 1161, 1008, 884 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{27}H_{22}O_2$ 378.1620, Found 378.1618.

3-(1-(4-Chlorophenyl)-3-phenylprop-1-yl)-2-phenylbenzofuran (4ga):



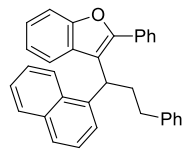
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56-7.58 (m, 3H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.37-7.43 (m, 3H), 7.28-7.32 (m, 3H), 7.24-7.26 (m, 2H), 7.19 (ddd, *J* = 7.8, 7.8, 0.6 Hz, 1H), 7.09-7.16 (m, 3H), 6.96 (d, *J* = 7.2 Hz, 2H), 4.43 (dd, *J* = 9.6, 5.4 Hz, 1H), 2.55-2.65 (m, 2H), 2.45-2.53 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.7, 142.3, 141.4, 132.0, 130.8, 129.2, 128.7 (3C), 128.6, 128.4, 128.3, 127.9, 125.8, 124.3, 122.6, 121.3, 116.7, 111.5, 40.3, 36.5, 34.1; IR (ATR): 3060, 3025, 2942, 2861, 2408, 1897, 1490, 1454, 1218, 1092, 1013, 746 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{23}ClO$ 422.1437, Found 422.1435.

3-(1-(4-Methoxyphenyl)-3-phenylprop-1-yl)-2-phenylbenzofuran (4ha):



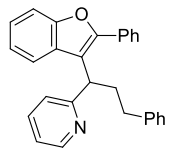
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60-7.62 (m, 3H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.36-7.43 (m, 3H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.27-7.30 (m, 1H), 7.18 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.14 (dd, *J* =7.8, 7.2 Hz, 2H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.97 (d, *J* = 7.2 Hz, 2H), 6.83 (d, *J* = 8.4 Hz, 2H), 4.42 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.76 (s, 3H), 2.46-2.64 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 158.0, 154.5, 152.4, 141.8, 135.8, 131.0, 128.9, 128.61, 128.59, 128.5, 128.4, 128.2, 127.9, 125.7, 124.2, 122.4, 121.6, 117.6, 113.9, 111.4, 55.2, 40.0, 36.7, 34.2; IR (ATR): 3059, 3025, 2948, 2860, 2833, 2339, 1609, 1509, 1454, 1218, 1178, 1033, 823 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{30}H_{26}O_2$ 418.1933, Found 418.1931.

3-(1-(1-Naphthyl)-3-phenylprop-1-yl)-2-phenylbenzofuran (4ia):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.73 (d, *J* = 7.8 Hz, 1H), 7.72 (d, *J* = 7.2 Hz, 1H), 7.56 (d, *J* = 7.8 Hz, 2H), 7.48 (d, *J* = 7.2 Hz, 2H), 7.43 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.39 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.24-7.35 (m, 6H), 7.11-7.14 (m, 3H), 6.95-6.98 (m, 2H), 5.11 (dd, *J* = 9.6, 4.2 Hz, 1H), 2.70-2.81 (m, 2H), 2.55-2.62 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.6, 152.6, 141.4, 139.6, 134.2, 131.1, 130.9, 129.6, 129.1, 128.7, 128.6, 128.5, 128.2, 127.9, 127.3, 126.0, 125.9, 125.5, 125.4, 124.8, 124.2, 123.2, 122.6, 121.8, 117.1, 111.6, 37.2, 36.6, 34.3; IR (ATR): 3058, 3032, 2925, 2857, 2408, 1598, 1493, 1454, 1219, 1026 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{33}H_{26}O$ 438.1984, Found 438.1983; Mp. 134.4-135.4 °C.

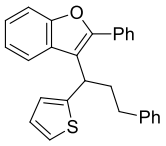
2-Phenyl-3-(3-phenyl-1-(2-pyridyl)prop-1-yl)benzofuran (4ja):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.64 (d, *J* = 4.2 Hz, 1H), 7.74 (d, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.51 (ddd, *J* = 7.8, 7.8, 1.8 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.42 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.37 (tt, *J* = 7.2, 1.2 Hz, 1H), 7.27 (ddd, *J* = 8.4, 7.8, 1.2 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.17 (d, *J* = 7.8, 7.2 Hz, 1H), 7.15 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.08-7.12 (m, 2H), 7.00 (d, *J* = 7.2 Hz, 2H), 4.63 (dd, *J* = 7.8, 6.6 Hz, 1H), 2.86-2.95 (m, 1H), 2.55-2.64 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 162.5, 154.5, 152.5, 149.2, 141.8, 136.5, 130.9, 128.70, 128.65, 128.5 (2C), 128.2, 127.9, 125.7, 124.2, 122.8, 122.4, 121.9, 121.4, 116.9, 111.3, 43.4, 34.9, 34.1; IR (ATR): 3060, 3025, 2930, 2858, 1588, 1568, 1494, 1455, 1348, 1091, 889 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{28}H_{23}NO$ 389.1780, Found 389.1779; Mp. 82.7-83.7 °C.

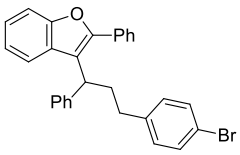
2-Phenyl-3-(3-phenyl-1-(2-thienyl)prop-1-yl)benzofuran (4ka):

White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69-7.72 (m, 2H), 7.62 (d, *J* = 7.2 Hz, 1H), 7.57 (d, *J* = 7.2 Hz, 1H),



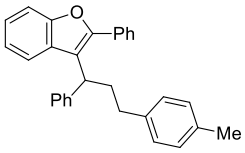
7.45-7.49 (m, 2H), 7.43 (tt, *J* = 7.2, 1.8 Hz, 1H), 7.33 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 7.19-7.24 (m, 2H), 7.11-7.18 (m, 3H), 6.99 (dd, *J* = 7.2, 1.2 Hz, 2H), 6.95-6.97 (m, 2H), 4.70 (dd, *J* = 9.6, 4.8 Hz, 1H), 2.69-2.77 (m, 1H), 2.59-2.66 (m, 2H), 2.49-2.54 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.6, 152.6, 148.0, 141.2, 130.7, 128.7 (2C), 128.4, 128.2, 128.1, 127.9, 126.7, 125.8, 124.3, 124.1, 123.6, 122.4, 121.4, 117.1, 111.4, 37.3, 36.8, 33.8; IR (ATR): 3060, 3025, 2942, 2858, 2340, 1601, 1493, 1454, 1219, 1062, 745 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{27}H_{22}OS$ 394.1391, Found 394.1390; Mp. 95.0-96.0 °C.

3-(1-(4-Bromophenyl)-3-phenylprop-3-yl)-2-phenylbenzofuran (4ab):



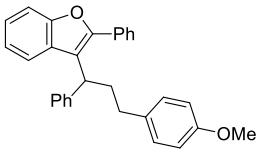
White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.8 Hz, 1H), 7.57-7.60 (m, 2H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.39-7.43 (m, 3H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.28-7.32 (m, 3H), 7.22 (d, *J* =8.4 Hz, 2H), 7.18-7.23 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 4.42 (dd, *J* = 9.6, 4.8 Hz, 1H), 2.58-2.64 (m, 1H), 2.46-2.57 (m, 2H), 2.40-2.45 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.6, 143.6, 140.5, 131.2, 130.8, 130.2, 128.8, 128.64 (2C), 128.61, 127.8, 127.6, 126.4, 124.3, 122.5, 121.5, 119.5, 117.0, 111.5, 40.6, 36.4, 33.5; IR (ATR): 3058, 3032, 2942, 2861, 2408, 1893, 1599, 1487, 1454, 1218, 1071, 1010, 744 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{23}BrO$ 466.0932, Found 466.0930; Mp. 102.0-103.0 °C.

3-(1-(4-Methylphenyl)-3-phenylprop-3-yl)-2-phenylbenzofuran (4ac):



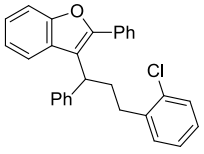
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.8 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 2H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.35-7.42 (m, 5H), 7.26-7.30 (m, 3H), 7.19 (d, *J* = 7.2 Hz, 1H), 7.17 (d, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 7.8 Hz, 2H), 6.86 (d, *J* = 7.8 Hz, 2H), 4.47 (dd, *J* = 9.6, 5.4 Hz, 1H), 2.42-2.65 (m, 4H), 2.26 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.5, 143.9, 138.6, 135.1, 131.0, 128.9 (2C), 128.6, 128.52, 128.49, 128.3, 127.9, 127.7, 126.3, 124.2, 122.5, 121.6, 117.4, 111.4, 40.9, 36.7, 33.8, 21.0; IR (ATR): 3083, 3056, 3023, 2922, 2860, 1893, 1492, 1454, 1218, 1099, 889, 745 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{30}H_{26}O$ 402.1984, Found 400.1983.

3-(1-(4-Methoxyphenyl)-3-phenylprop-3-yl)-2-phenylbenzofuran (4ad):



Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.59-7.63 (m, 3H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.36-7.41 (m, 5H), 7.26-7.30 (m, 3H), 7.17-7.20 (m, 2H), 6.87 (d, *J* = 9.0 Hz, 2H), 6.67 (d, *J* = 9.0 Hz, 2H), 4.45 (dd, *J* = 9.0, 6.0 Hz, 1H), 3.72 (s, 3H), 2.41-2.63 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 157.7, 154.5, 152.5, 143.9, 133.7, 131.0, 129.3, 128.9, 128.6, 128.52, 128.49, 127.9, 127.7, 126.3, 124.2, 122.5, 121.6, 117.3, 113.6, 111.4, 55.2, 40.7, 36.8, 33.2; IR (ATR): 3058, 3031, 3000, 2934, 2860, 2833, 2408, 1611, 1510, 1455, 1245, 1219, 1035, 832 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{30}H_{26}O_2$ 418.1933, Found 418.1930.

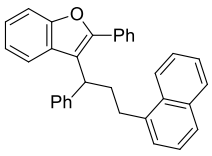
3-(1-(2-Chlorophenyl)-3-phenylprop-3-yl)-2-phenylbenzofuran (4ae):



Light yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.2, 1.2 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.43 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.38-7.42 (m, 3H), 7.27-7.32 (m, 3H), 7.25 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.20 (t, *J* = 7.8 Hz, 1H), 7.18 (ddd, *J* = 7.8, 7.2, 0.6 Hz,

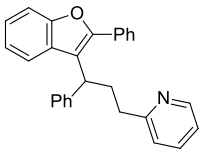
1H), 7.04 (ddd, *J* = 7.8, 7.2, 1.8 Hz, 1H), 6.97 (ddd, *J* = 7.8, 7.2, 1.2 Hz, 1H), 6.89 (dd, *J* = 7.2, 1.2 Hz, 1H), 4.49 (dd, *J* = 9.0, 6.6 Hz, 1H), 2.54-2.71 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.6, 143.6, 139.3, 133.8, 130.9, 130.5, 129.4, 128.9, 128.62, 128.58, 128.56, 128.0, 127.7, 127.3, 126.6, 126.3, 124.2, 122.4, 121.7, 117.2, 111.4, 41.2, 34.5, 32.3; IR (ATR): 3059, 3032, 2925, 2408, 1600, 1492, 1455, 1219, 1089, 889, 745 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{23}ClO$ 422.1437, Found 422.1436.

3-(1-(1-Naphthyl)-3-phenylprop-3-yl)-2-phenylbenzofuran (4af):



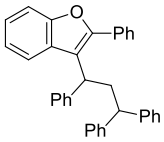
Green oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.62-7.66 (m, 4H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.38-7.45 (m, 6H), 7.26-7.34 (m, 4H), 7.18-7.22 (m, 3H), 7.05 (d, *J* = 7.2 Hz, 1H), 4.58 (dd, *J* = 10.2, 6.0 Hz, 1H), 3.05 (ddd, *J* = 13.8, 10.2, 5.4 Hz, 1H), 2.93 (ddd, *J* = 13.8, 9.6, 6.0 Hz, 1H), 2.73-2.81 (m, 1H), 2.62-2.70 (m, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.6, 152.9, 143.6, 137.8, 133.8, 131.6, 130.9, 128.8, 128.7, 128.62, 128.58, 128.5, 127.9, 127.7, 126.6, 126.3, 126.2, 125.6, 125.4, 125.3, 124.3, 123.7, 122.5, 121.7, 117.4, 111.5, 41.4, 35.8, 31.5; IR (ATR): 3058, 3033, 2949, 2869, 2408, 1806, 1596, 1492, 1454, 1218, 1087, 745 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{33}H_{26}O$ 438.1984, Found 438.1983.

2-Phenyl-3-(3-phenyl-1-(2-pyridyl)prop-3-yl)benzofuran (4ag):



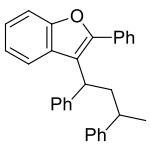
Light yellow oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.43 (dd, *J* = 4.8, 0.6 Hz, 1H), 7.63 (dd, *J* = 7.8, 1.2 Hz, 2H), 7.61 (d, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 1H), 7.33-7.43 (m, 6H), 7.26-7.31 (m, 3H), 7.20 (dd, *J* = 7.8, 7.2 Hz, 1H), 7.13 (ddd, *J* = 7.2, 7.2, 1.2 Hz, 1H), 6.99 (ddd, *J* = 7.2, 4.8, 1.2 Hz, 1H), 6.78 (d, *J* = 7.8 Hz, 1H), 4.48 (dd, *J* = 9.0, 5.4 Hz, 1H), 2.64-2.81 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 161.1, 154.5, 152.6, 149.0, 143.6, 136.2, 130.9, 128.8, 128.6, 128.5 (2C), 127.9, 127.7, 126.3, 124.2, 123.1, 122.5, 121.6, 121.0, 117.1, 111.4, 40.9, 36.5, 34.4; IR (ATR): 3058, 2928, 1590, 1492, 1455, 1218, 1091, 1027, 889, 744 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{28}H_{23}NO$ 389.1780, Found 389.1778.

2-Phenyl-3-(1,1,3-triphenylprop-3-yl)benzofuran (4ah):



Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 1H), 7.22-7.35 (m, 10H), 7.15-7.20 (m, 4H), 7.03-7.13 (m, 8H), 4.40 (t, *J* = 7.8 Hz, 1H), 3.82 (t, *J* = 7.8 Hz, 1H), 3.03 (dd, *J* = 7.8, 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 152.6, 144.9, 143.5, 143.1, 130.7, 128.8, 128.6, 128.39 (2C), 128.36, 128.3, 128.1, 127.7, 127.6 (2C), 126.3, 126.2, 126.1, 124.2, 122.5, 121.6, 116.9, 111.4, 49.0, 40.7, 39.1; IR (ATR): 3083, 3059, 3025, 2923, 2408, 1599, 1493, 1454, 1219, 1088, 889 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{35}H_{28}O$ 464.2140, Found 464.2138.

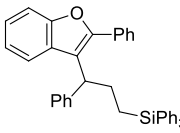
3-(1,3-Diphenylbut-1-yl)-2-phenylbenzofuran (4ai):



White solid, a mixture of diasteromers (dr = 60:40); ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 0.4H), 7.60 (d, *J* = 8.4 Hz, 0.6H), 7.56 (d, *J* = 8.4 Hz, 0.4H), 7.49 (d, *J* = 8.4 Hz, 0.6H), 7.14-7.48 (m, 14H), 6.97-7.04 (m, 2.2H), 6.83-6.87 (m, 0.8H), 4.48 (dd, *J* = 8.4, 7.8 Hz, 0.6H), 4.19 (dd, *J* = 11.4, 4.2 Hz, 0.4H), 2.63-2.74 (m, 1H), 2.45-2.57 (m, 1.6H), 2.39 (ddd, *J* = 13.8, 10.8, 4.2 Hz, 0.4H), 1.16 (d, *J* = 7.2 Hz, 1.8H), 1.15 (d, *J* = 7.2 Hz, 1.2 H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 154.4, 152.9, 151.8, 147.0,

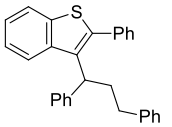
145.8, 144.3, 143.5, 130.9, 130.8, 129.2, 128.9, 128.52 (2C), 128.47, 128.4 (2C), 128.34, 128.32, 128.2, 127.79, 127.77, 127.6, 127.5, 127.01, 126.99, 126.3, 126.1, 126.0, 125.8, 124.1 (2C), 122.5, 122.4, 121.6, 121.5, 117.9, 116.6, 111.5, 111.3, 43.8, 43.5, 39.4, 39.3, 38.1, 37.7, 23.4, 21.0; IR (ATR): 3082, 3059, 3025, 2957, 2925, 2867, 1947, 1887, 1600, 1454, 1218, 1026, 745 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{30}H_{26}O$ 402.1984, Found 402.1981; Mp. 140.7-141.2 °C.

2-Phenyl-3-(1-(triphenylsilyl)-3-phenylprop-3-yl)benzofuran (4aj):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.67 (dd, *J* = 7.8, 1.8 Hz, 2H), 7.51 (d, *J* = 8.4 Hz, 1H), 7.44 (dd, *J* = 7.8, 7.2 Hz, 2H), 7.34-7.41 (m, 11H), 7.28 (dd, *J* = 7.2, 7.2 Hz, 9H), 7.22-7.25 (m, 2H), 7.16 (t, *J* = 7.2 Hz, 1H), 7.10 (ddd, *J* = 7.8, 7.2, 0.6 Hz, 1H), 4.41 (dd, *J* = 8.4, 5.4 Hz, 1H), 2.42-2.51 (m, 1H), 2.32-2.40 (m, 1H), 1.23-1.34 (m, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 154.5, 153.0, 144.0, 135.6, 134.8, 131.0, 129.4, 128.8, 128.59, 128.55, 128.5, 128.1, 127.8, 127.7, 126.2, 124.1, 122.4, 121.8, 117.2, 111.3, 45.2, 29.4, 11.9; IR (ATR): 3067, 3022, 2928, 2408, 1588, 1492, 1455, 1428, 1255, 1219, 1110, 1028 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{41}H_{34}OSi$ 570.2379, Found 570.2377; Mp. 154.1-155.1 °C.

3-(1,3-Diphenylprop-1-yl)-2-phenylbenzothiophene (4la):



White solid; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84 (d, *J* = 7.8 Hz, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.44-7.47 (m, 2H), 7.37-7.40 (m, 3H), 7.32 (d, *J* = 7.2 Hz, 2H), 7.24-7.30 (m, 3H), 7.15-7.22 (m, 4H), 7.10 (t, *J* = 7.2 Hz, 1H), 6.95 (d, *J* = 7.2 Hz, 2H), 4.58 (dd, *J* = 8.4, 6.0 Hz, 1H), 2.52-2.63 (m, 2H), 2.40 (t, *J* = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 143.3, 142.0, 140.6, 139.6, 138.9, 134.7, 133.3, 130.0, 128.5, 128.4, 128.3, 128.23, 128.20, 127.6, 126.1, 125.7, 124.0, 123.9, 123.8, 122.3, 42.6, 35.0, 34.3; IR (ATR): 3058, 3024, 2923, 2861, 1599, 1494, 1444, 1432, 1219, 1088, 890 cm^{-1}; HRMS (FD+) *m/z*: [M] Calcd for $C_{29}H_{24}S$ 404.1599, Found 404.1597; Mp. 136.7-137.7 °C.

References

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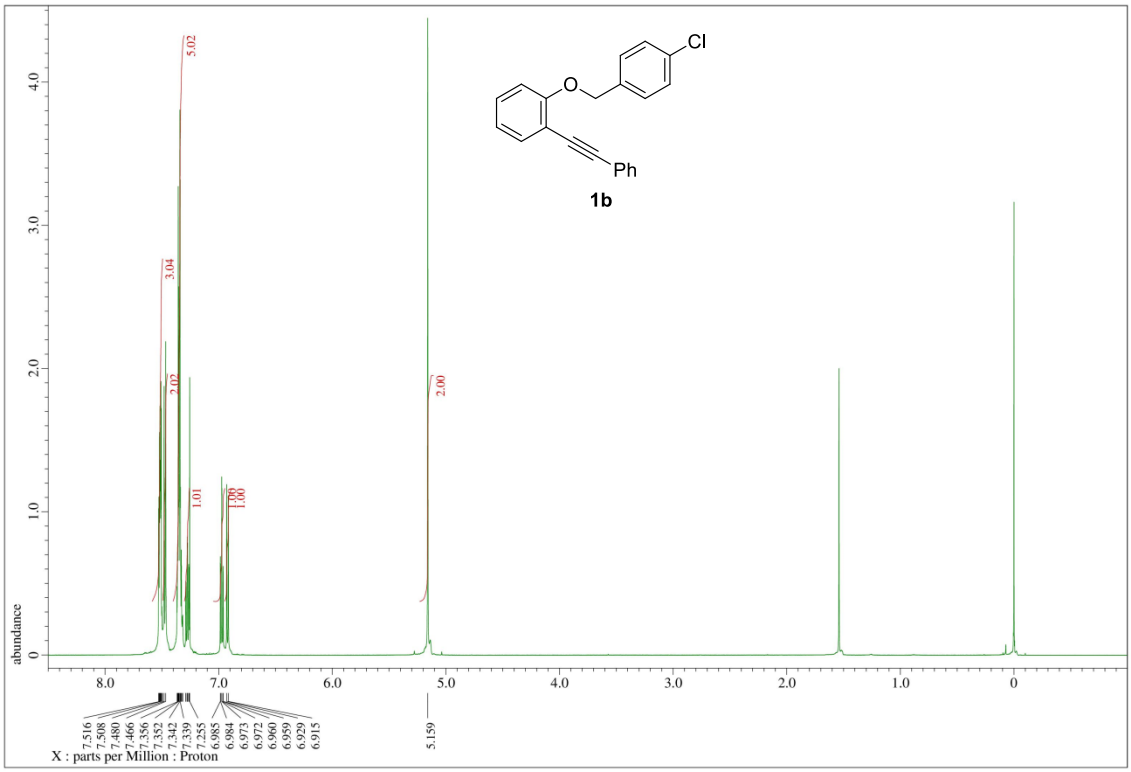
S6. J. Yuan, X. Ma, H. Yi, C. Liu and A. Lei, *Chem. Commun.*, 2014, **50**, 14386-14389.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2.00
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5.0
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1.0
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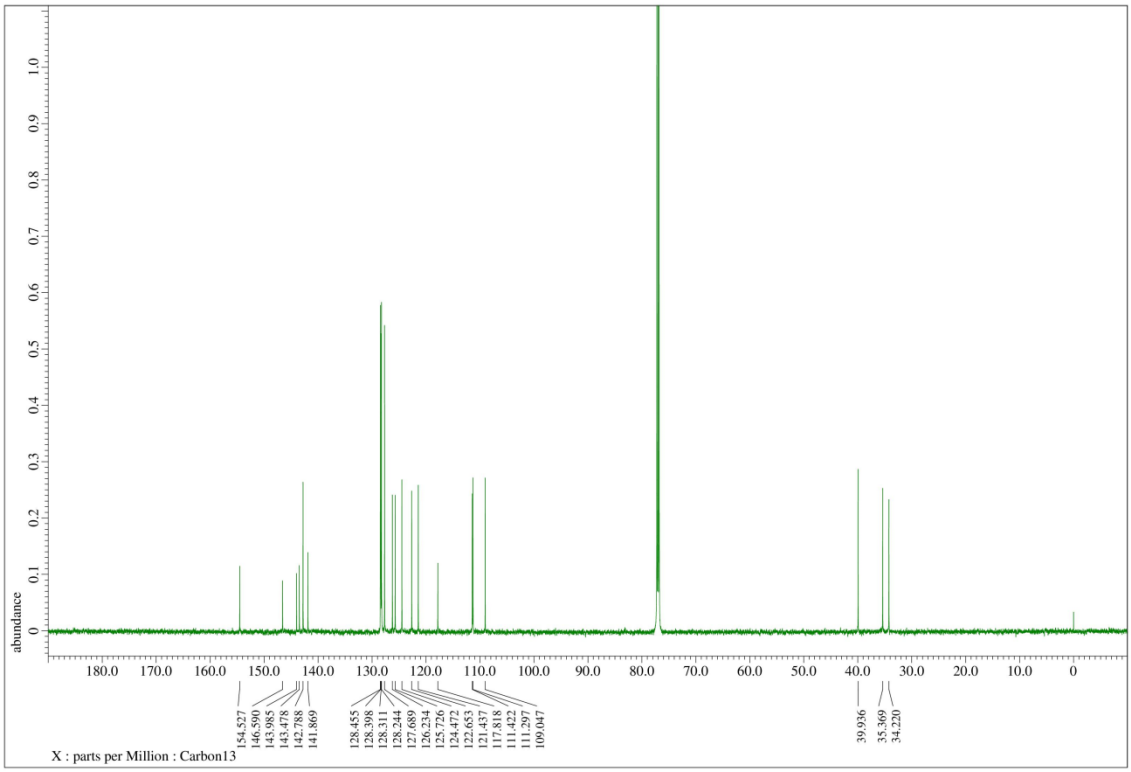
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40.0
30.0
20.0
10.0
0
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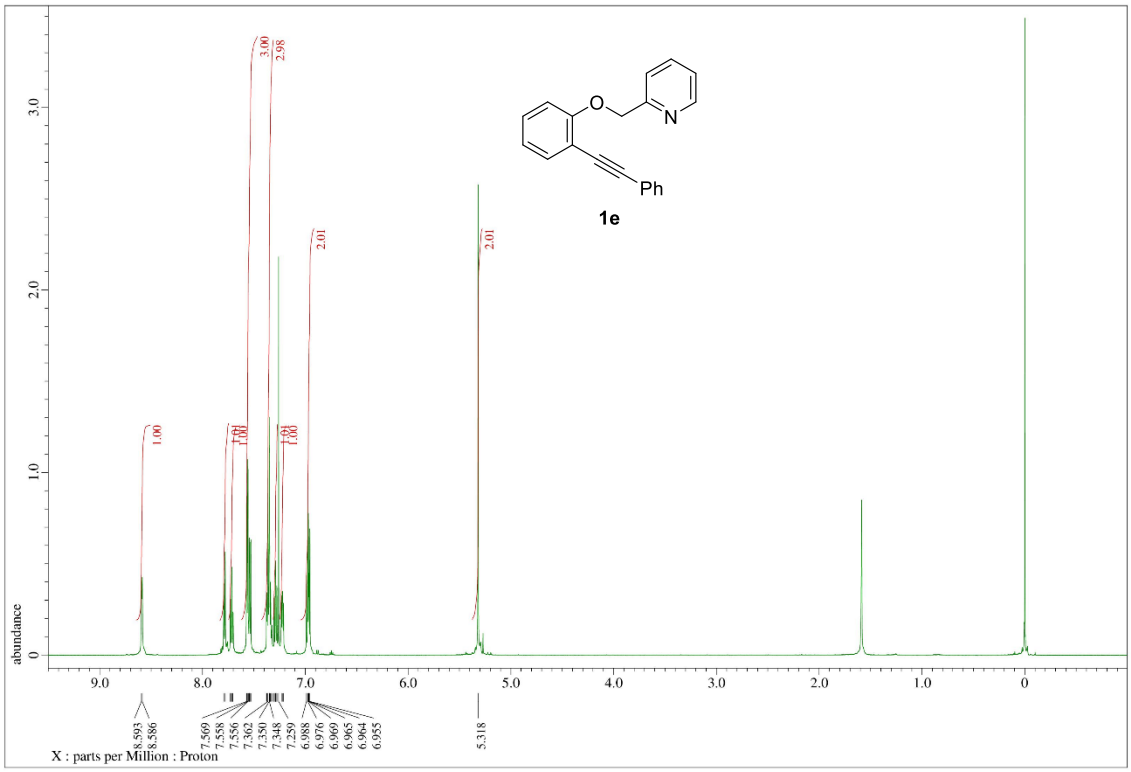
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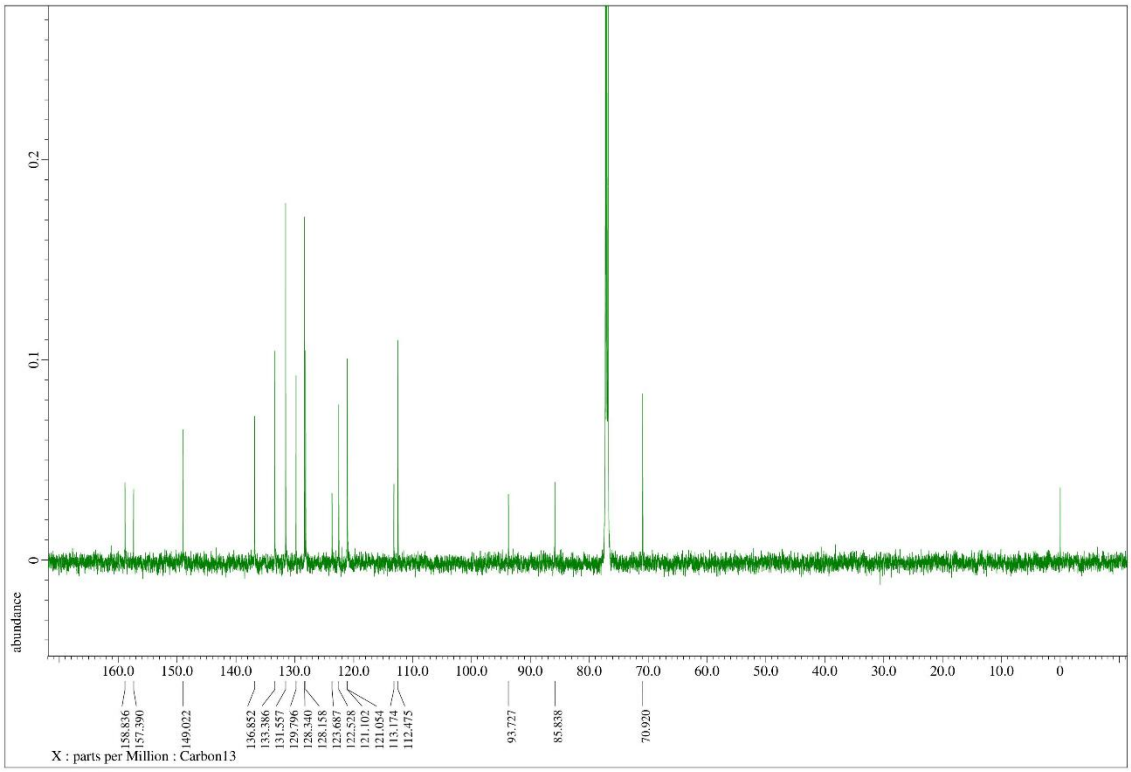
abundance
X : parts per Million : Proton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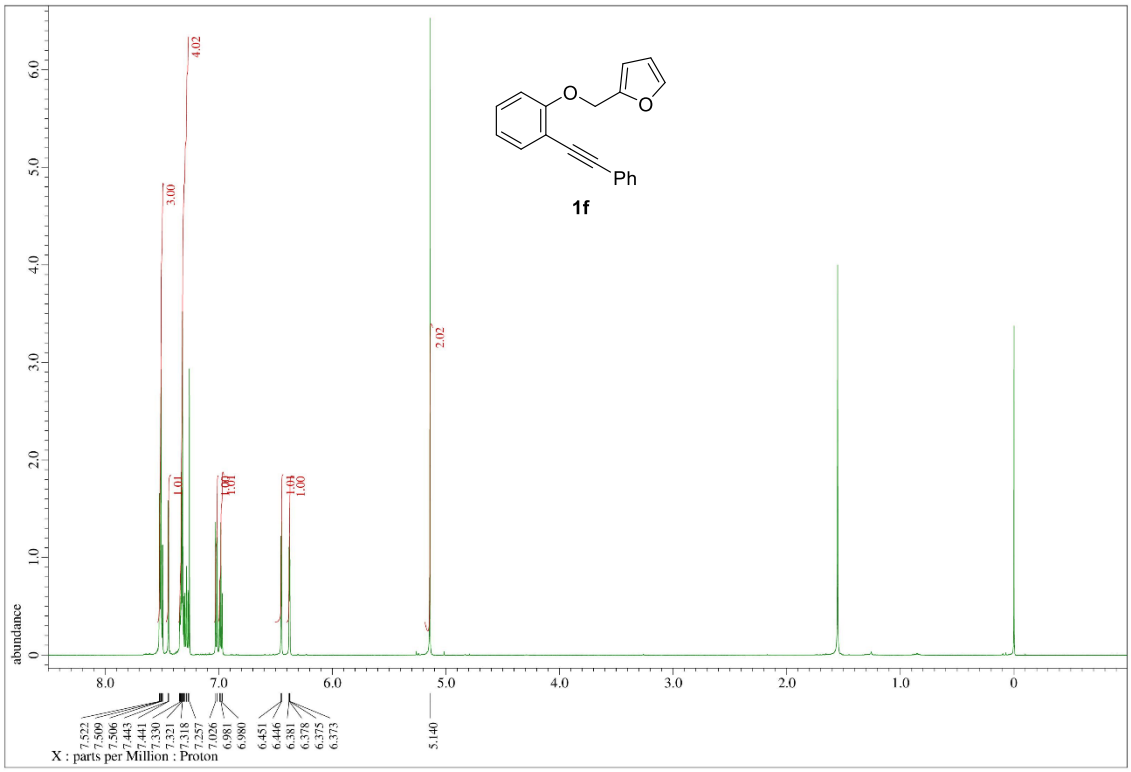
X : parts per Million : Carbon13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2.0
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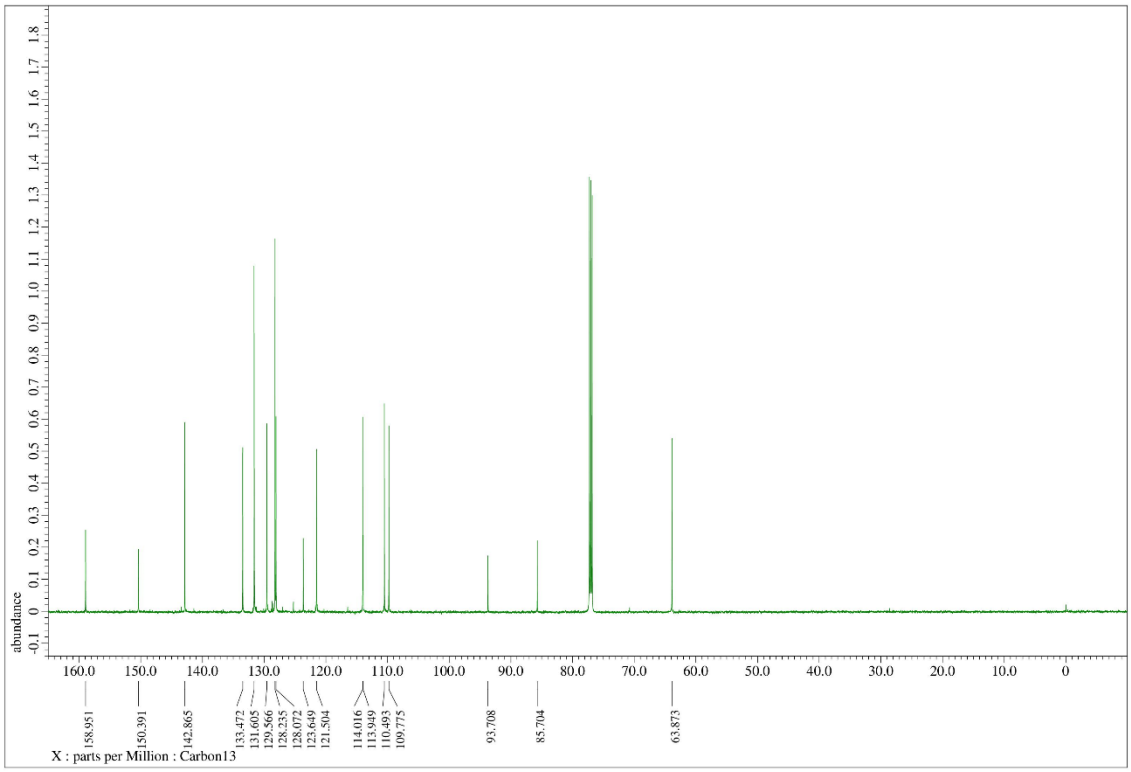
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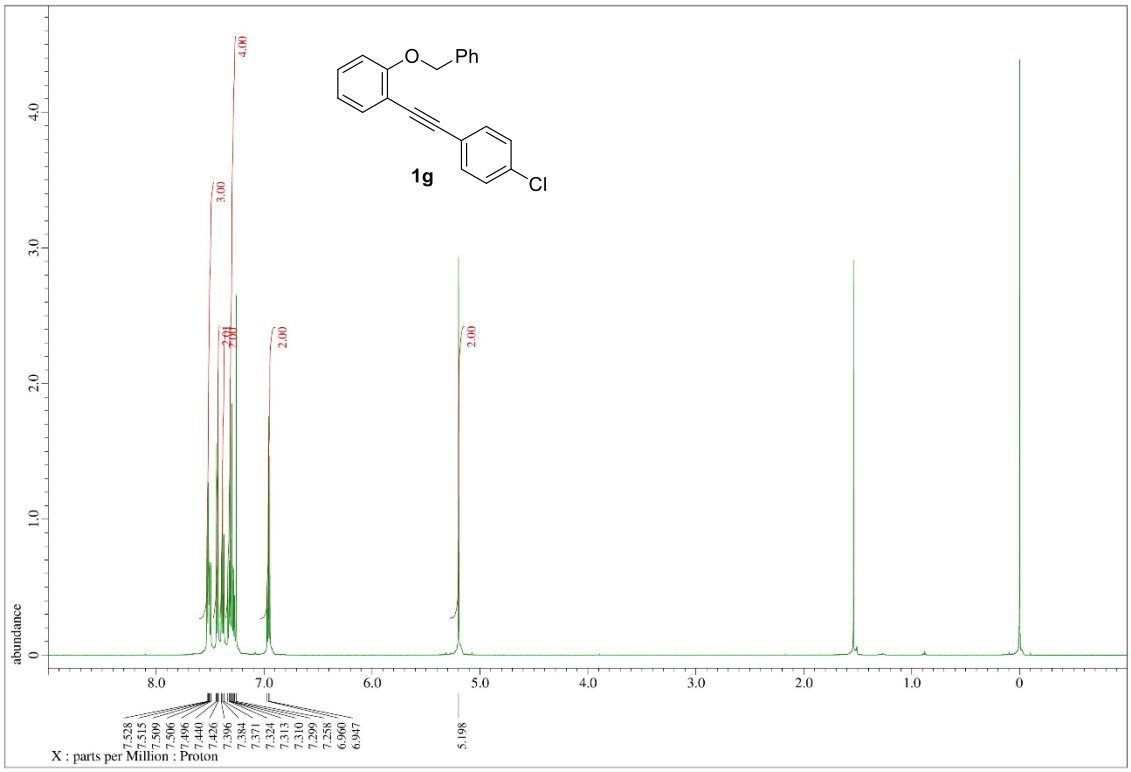
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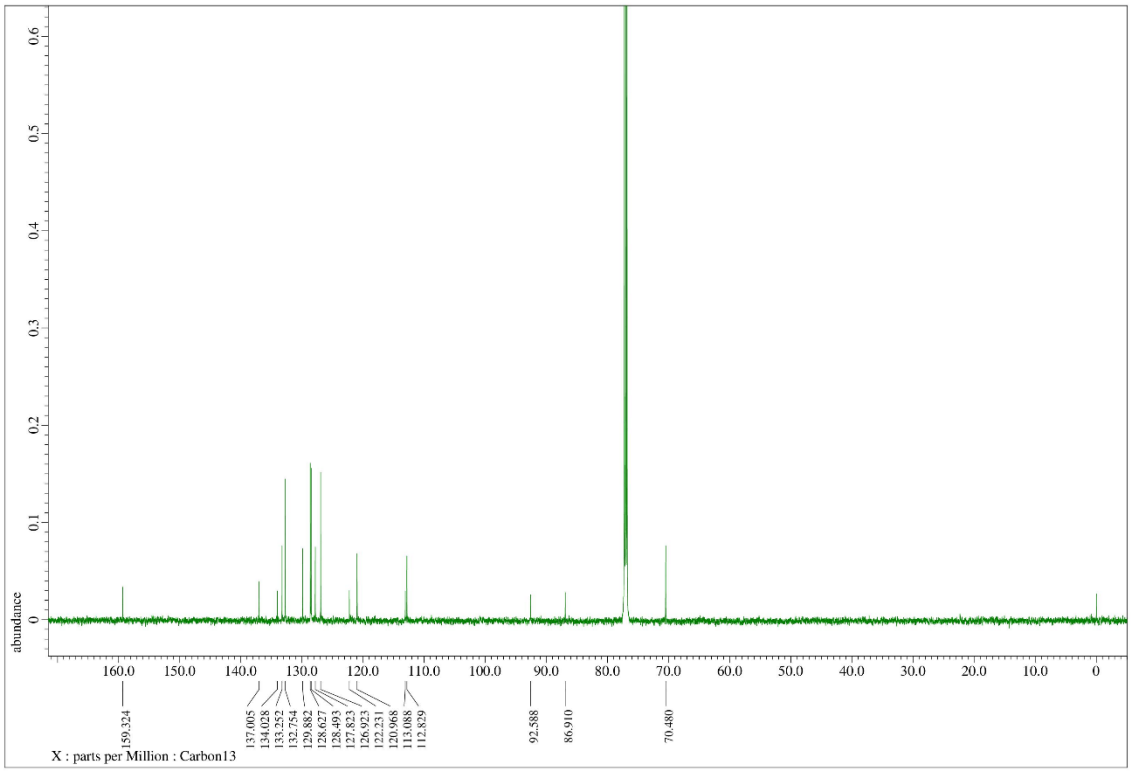
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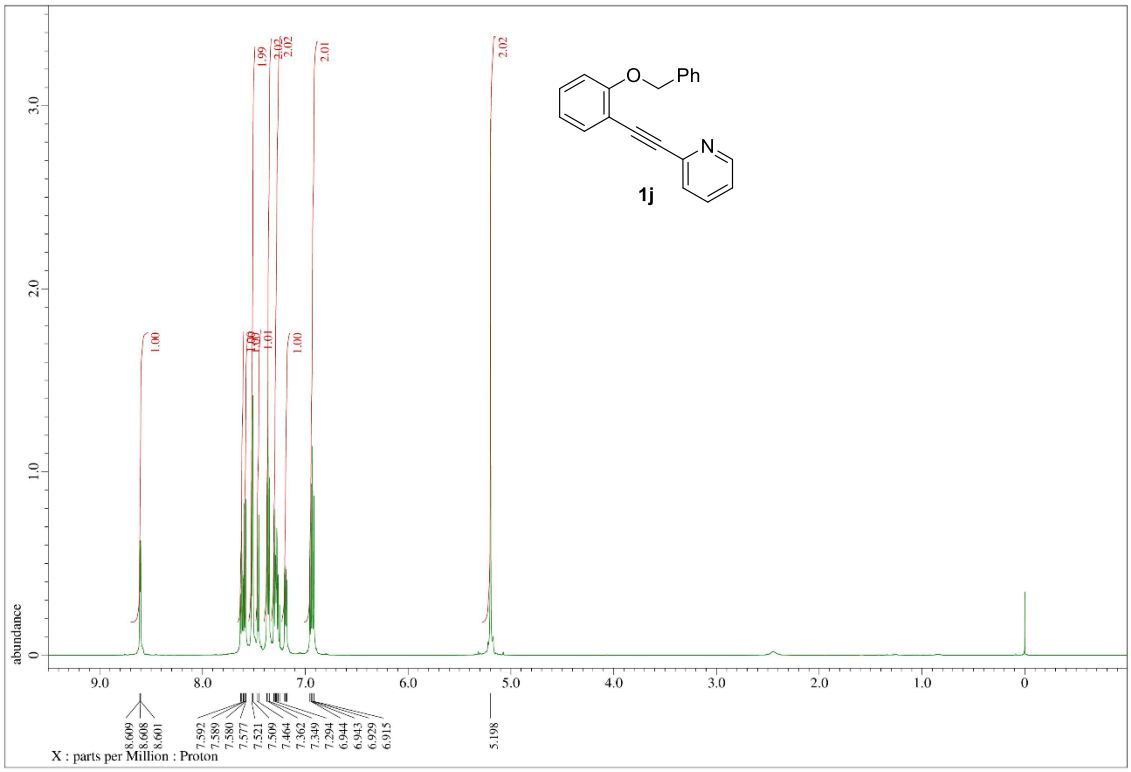
X : parts per Million : Carbon13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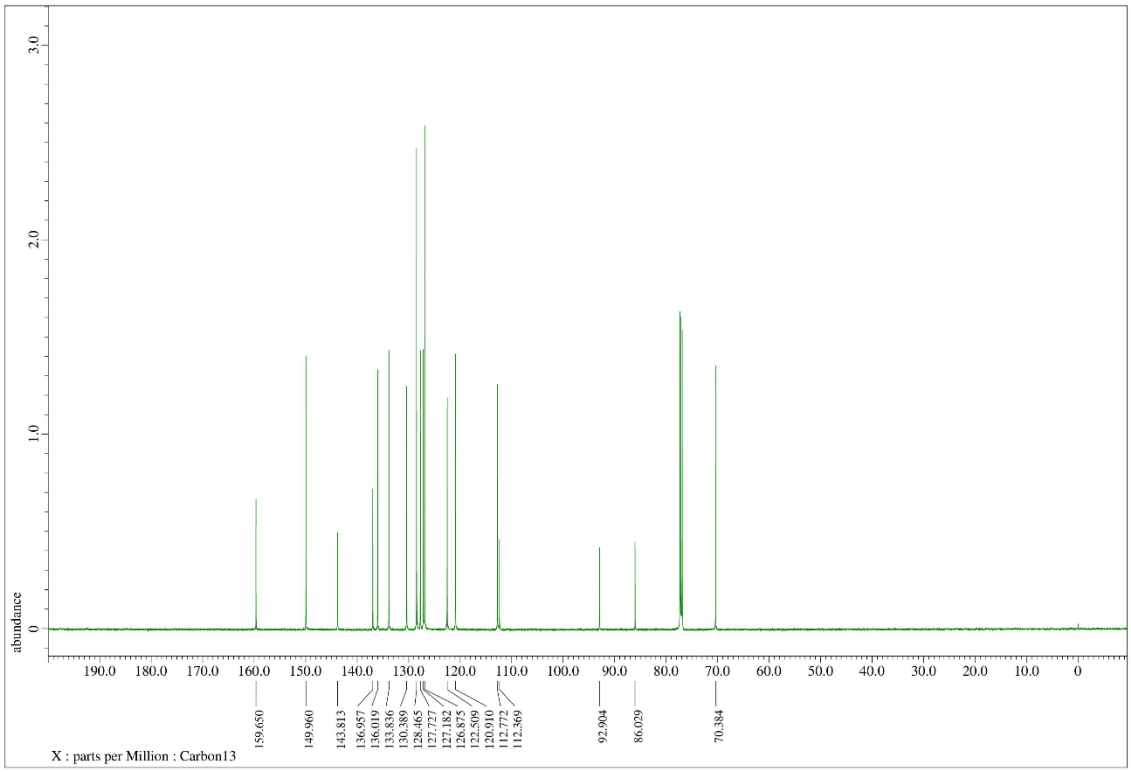
abundance
X : parts per Million : Proton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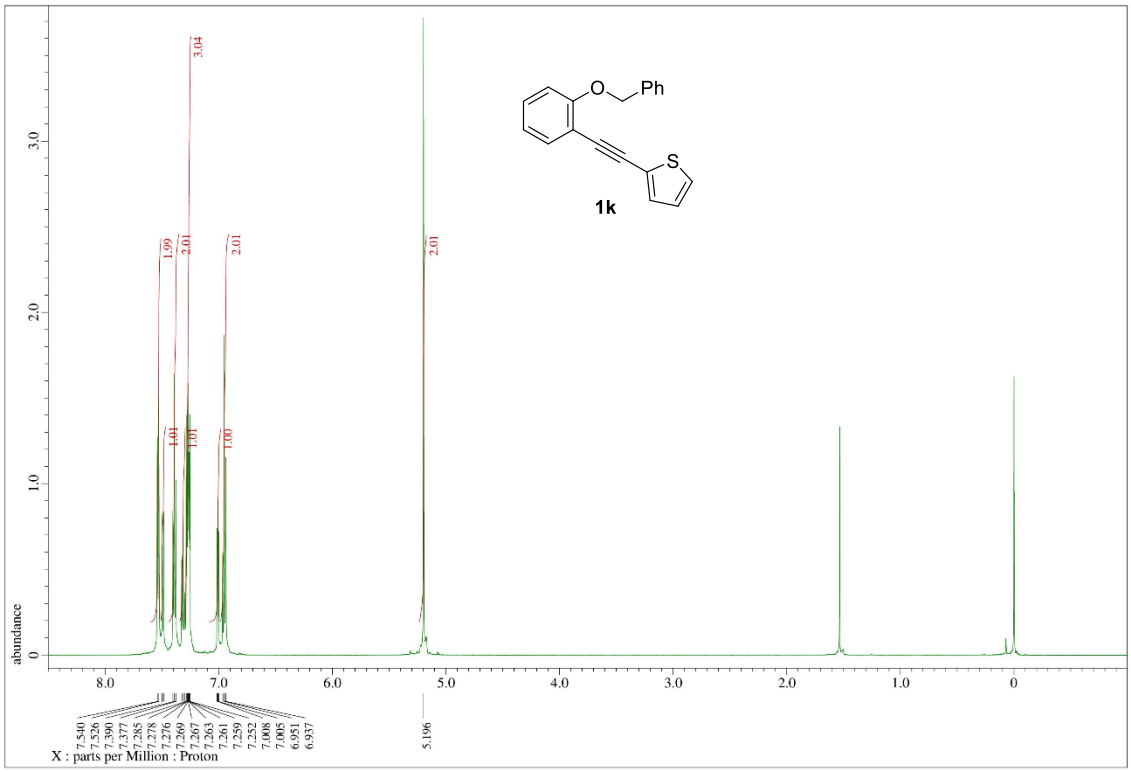
X : parts per Million : Carbon13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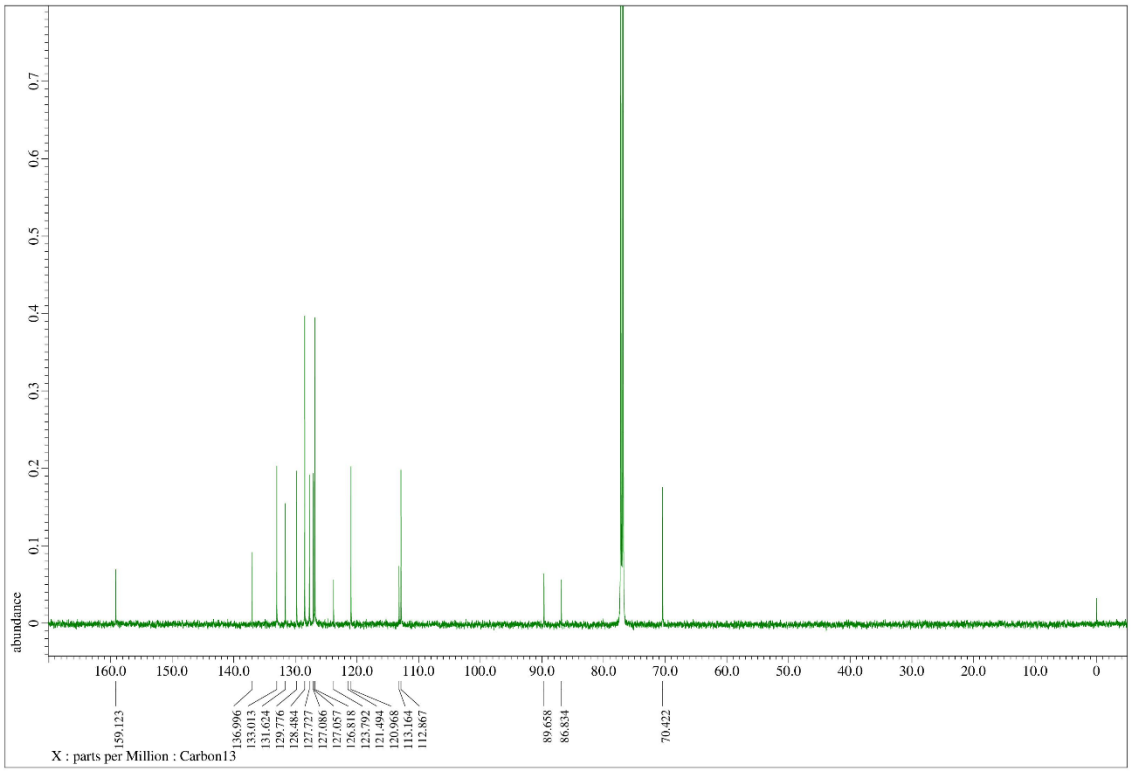
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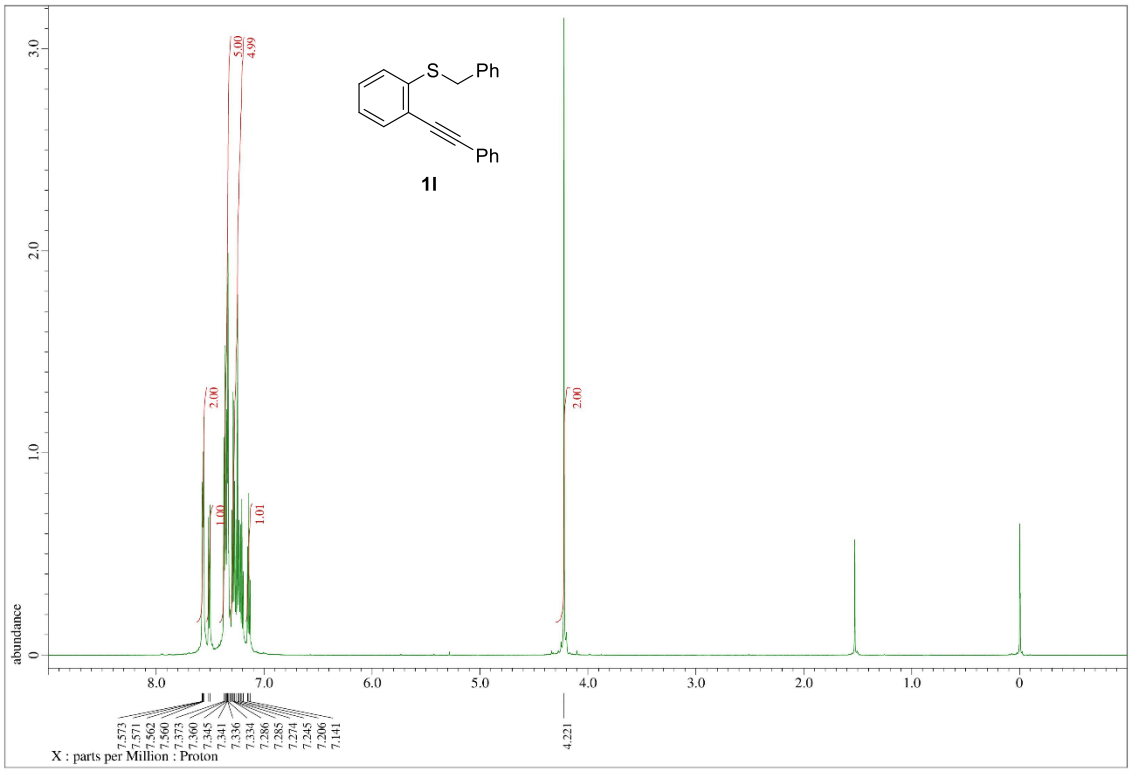
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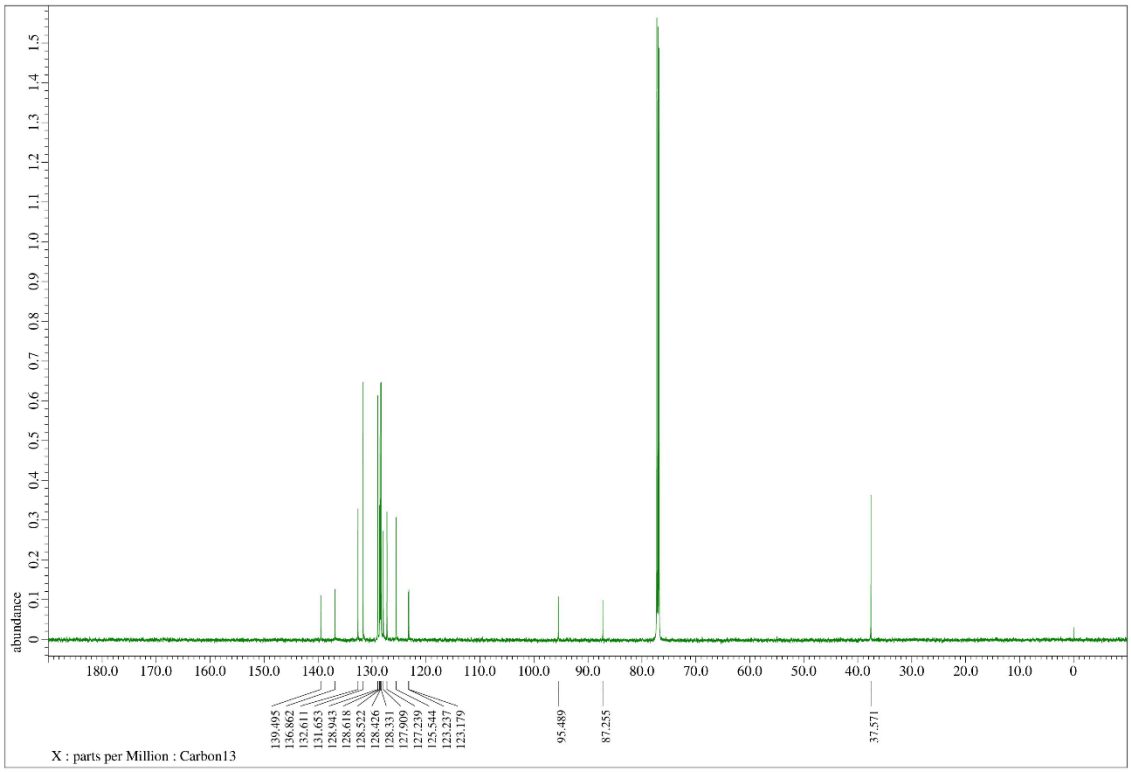
abundance
X : parts per Million : Proton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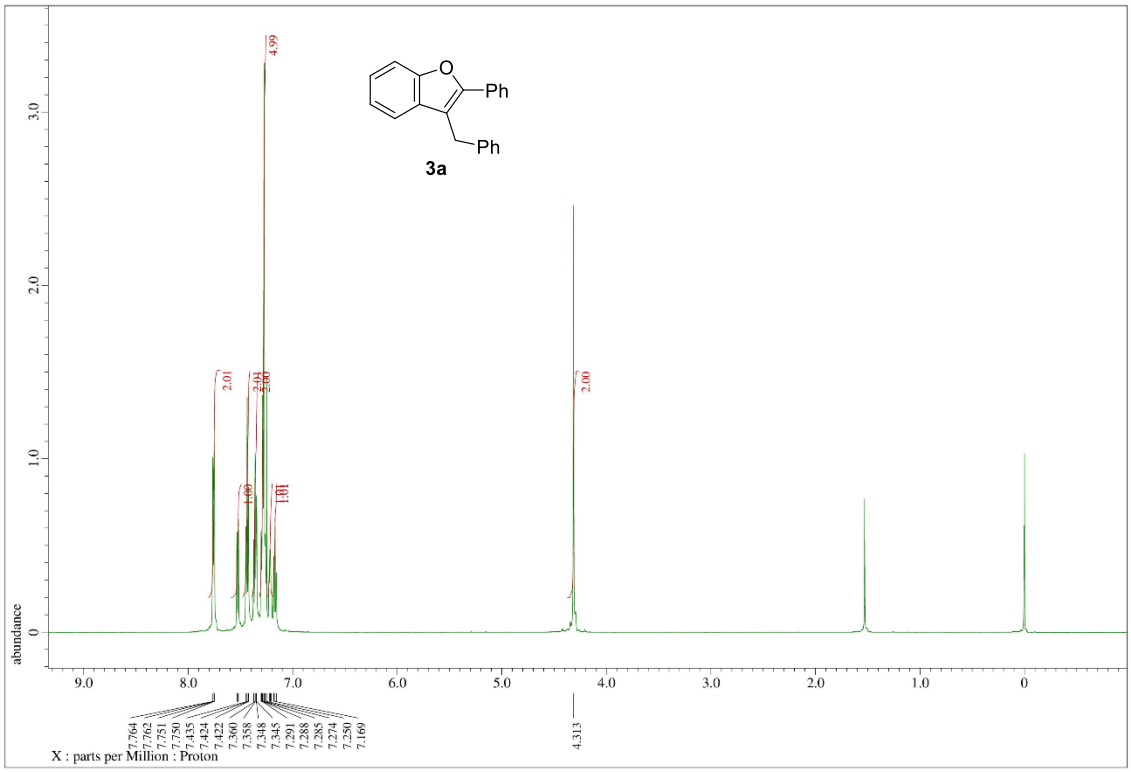
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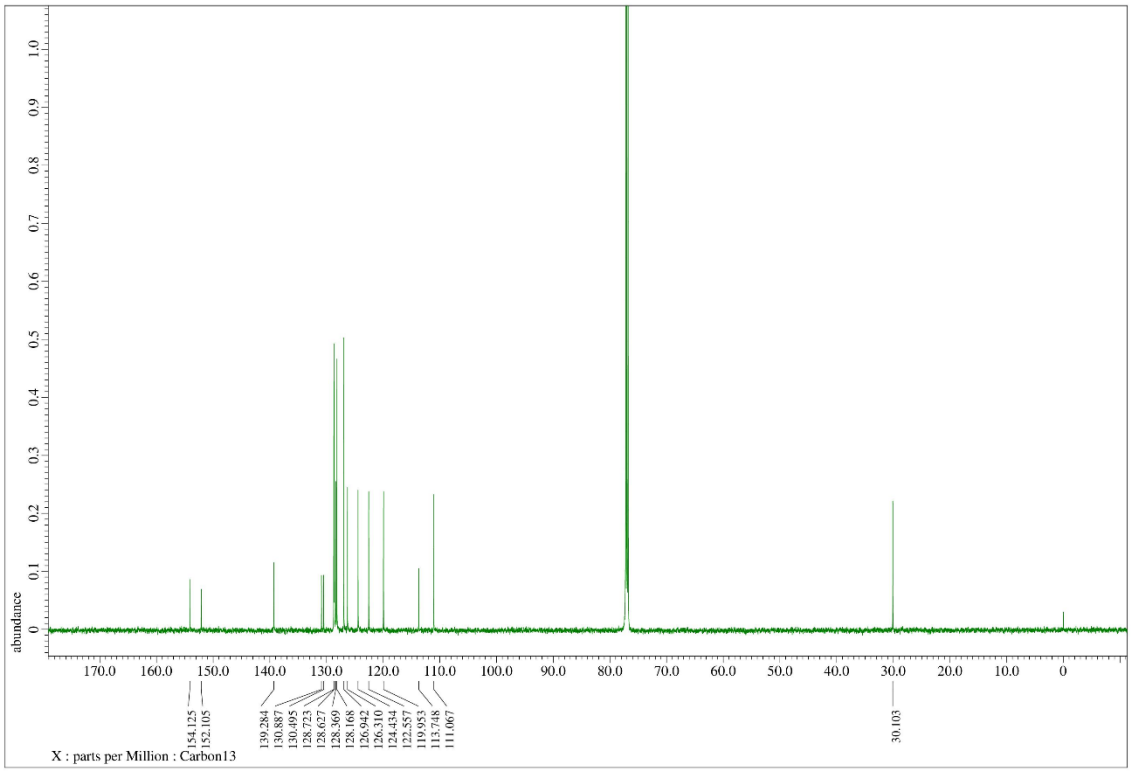
X : parts per Million : Proton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50.0
40.0
30.0
20.0
10.0
0
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152.105
139.284
130.887
130.495
128.723
128.627
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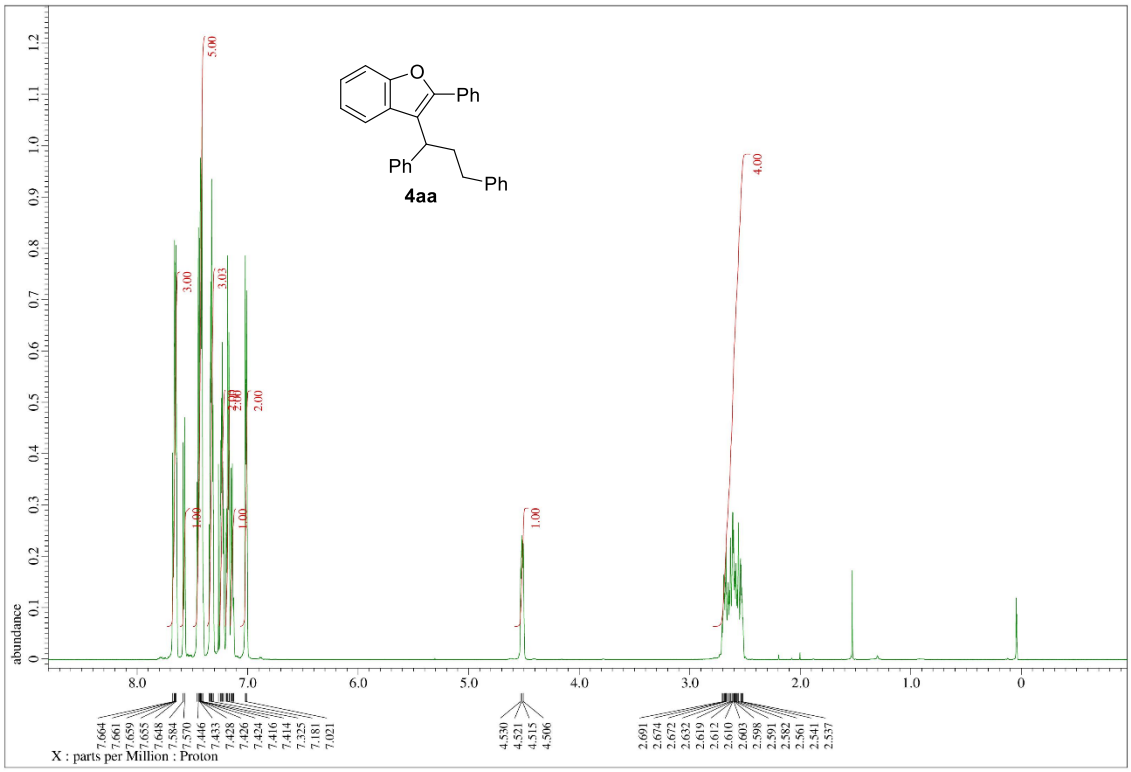
O
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abundance
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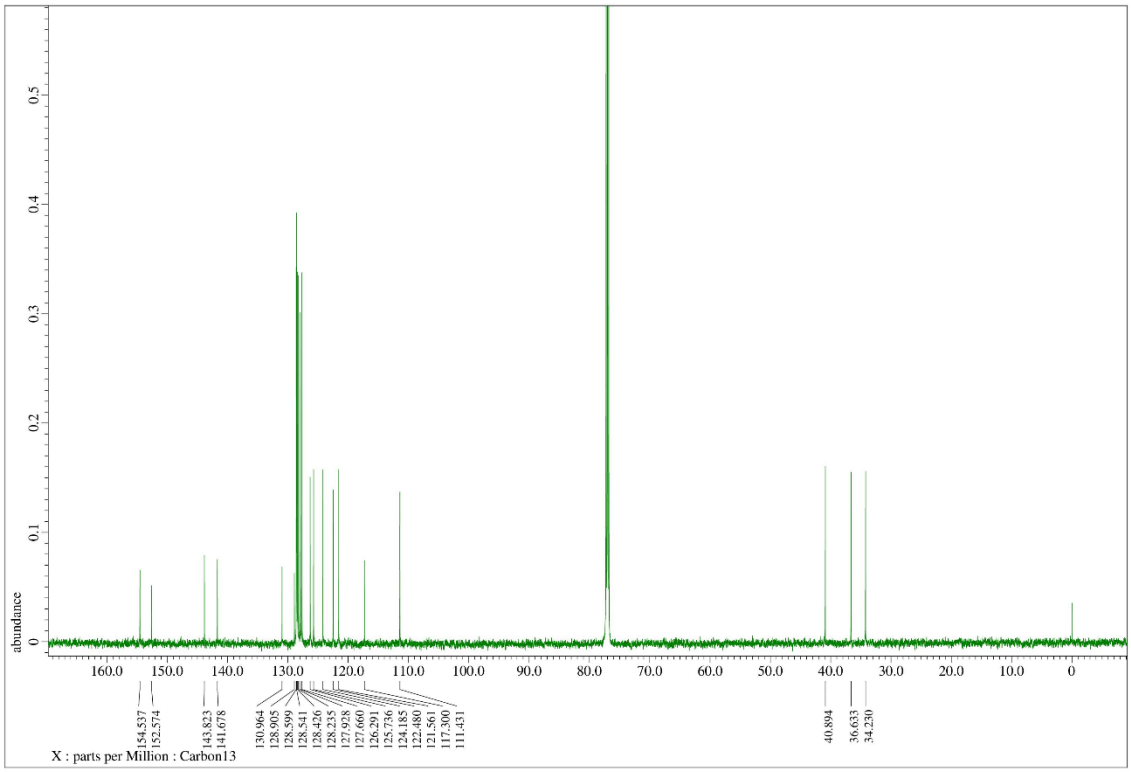
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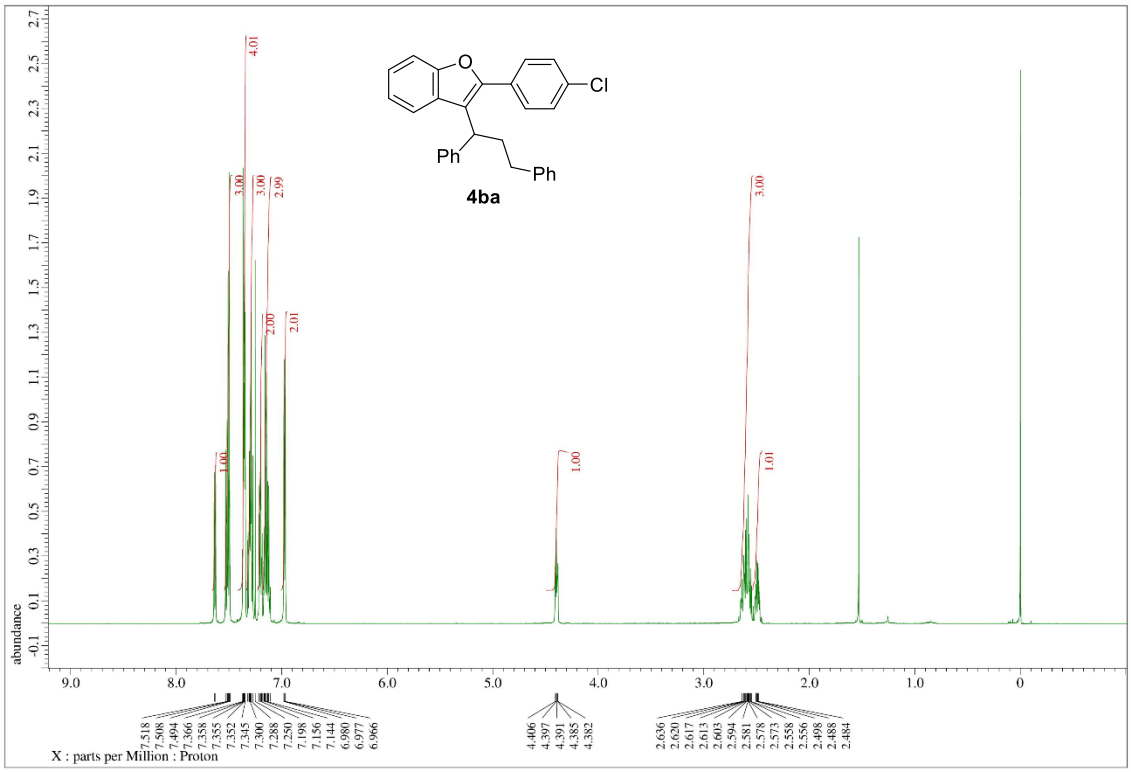
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1.01
abundance
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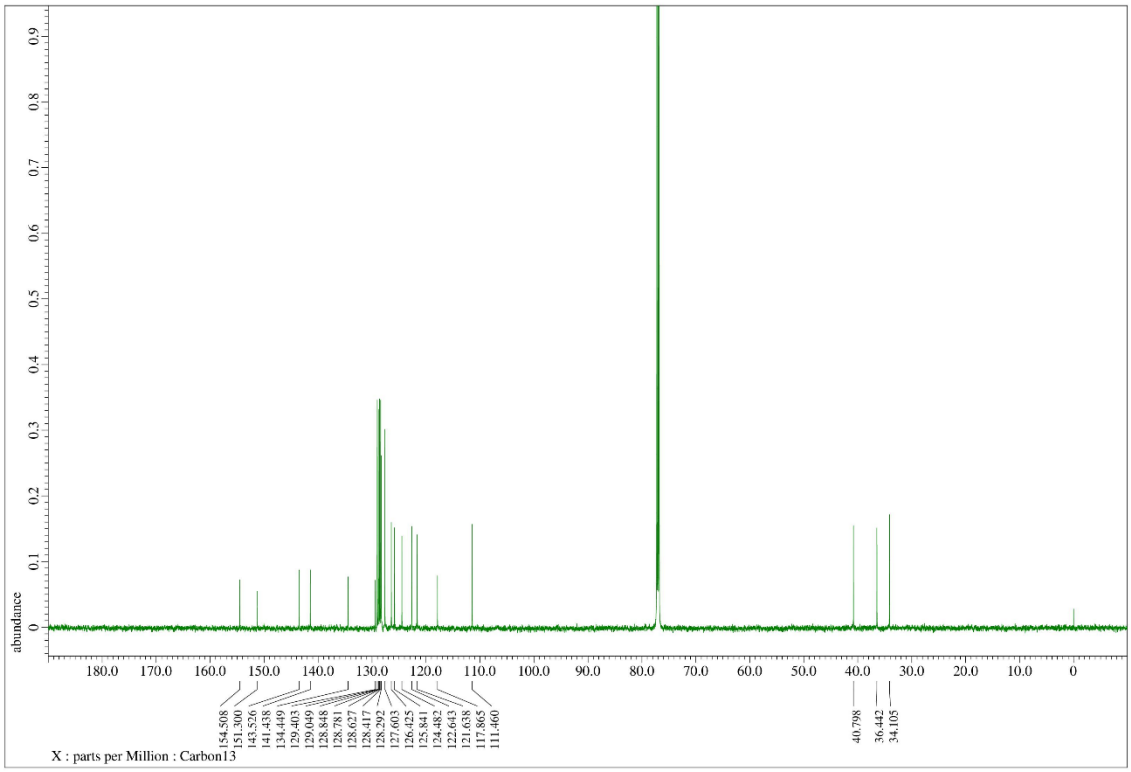
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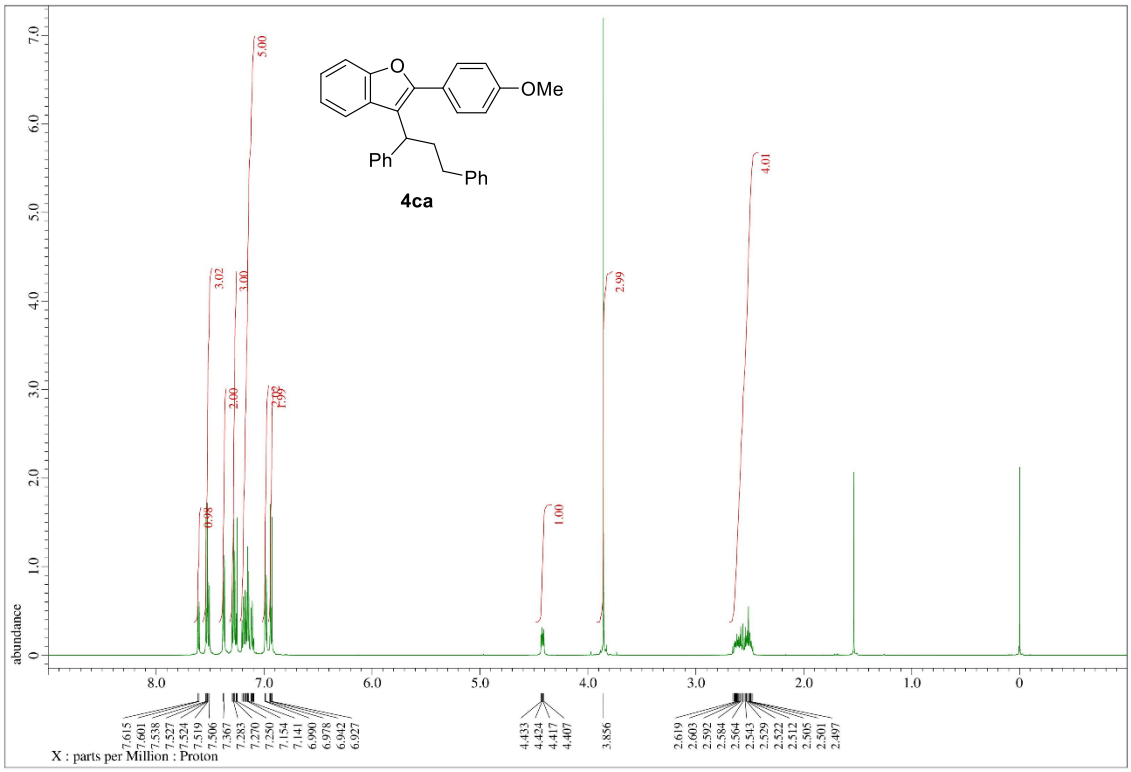
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4ca
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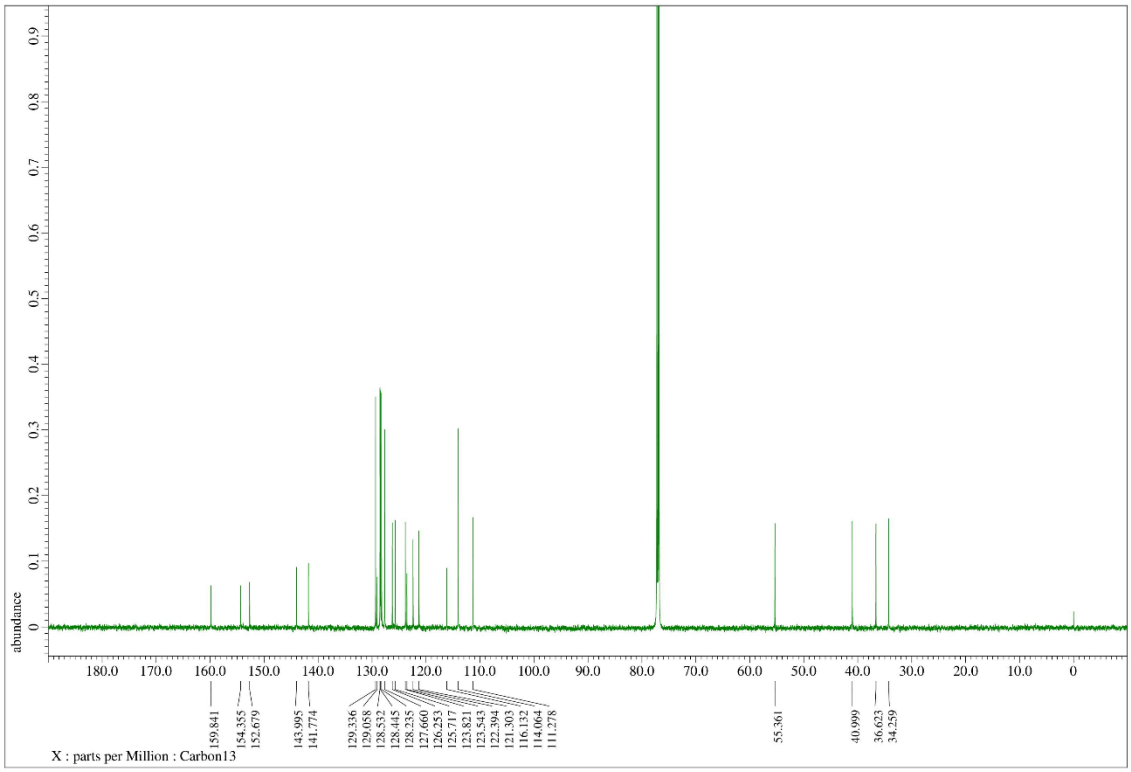
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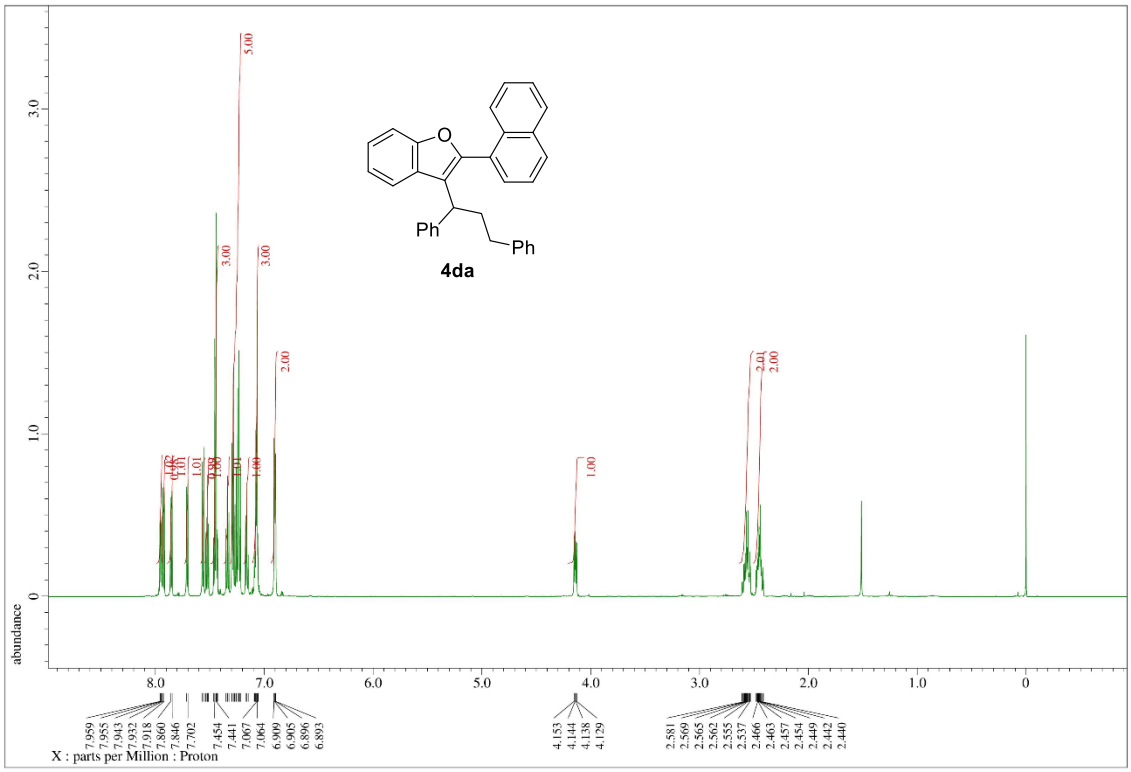
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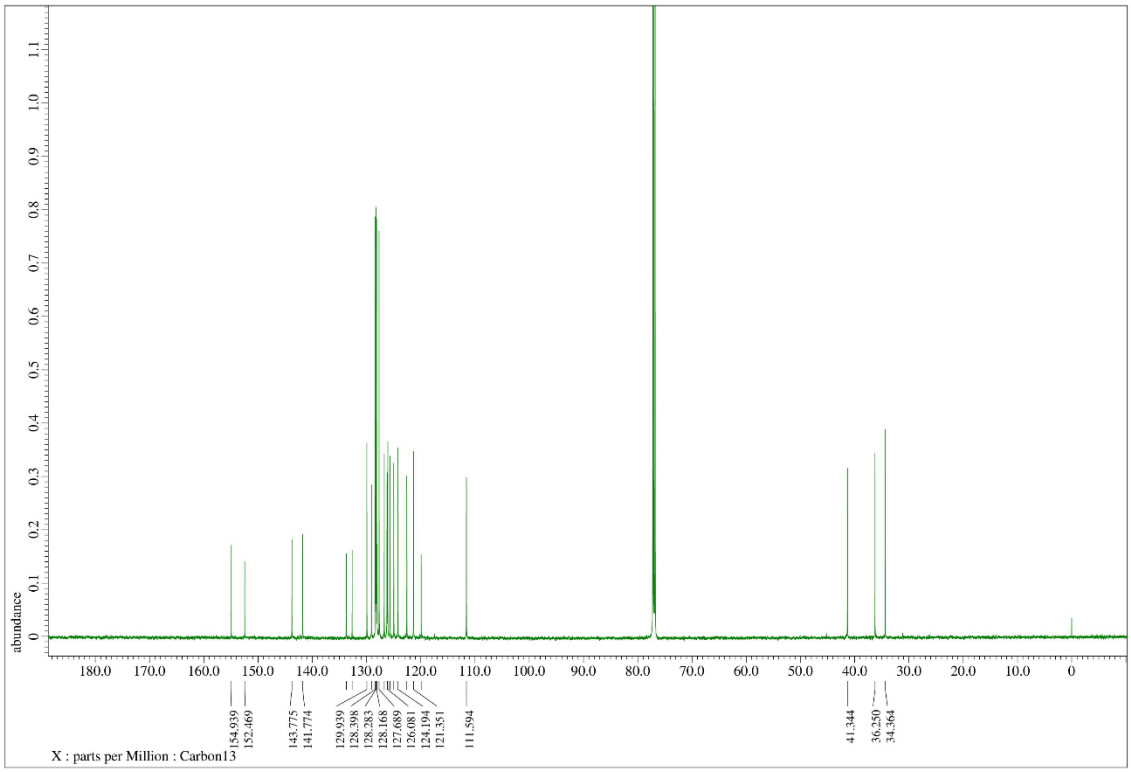
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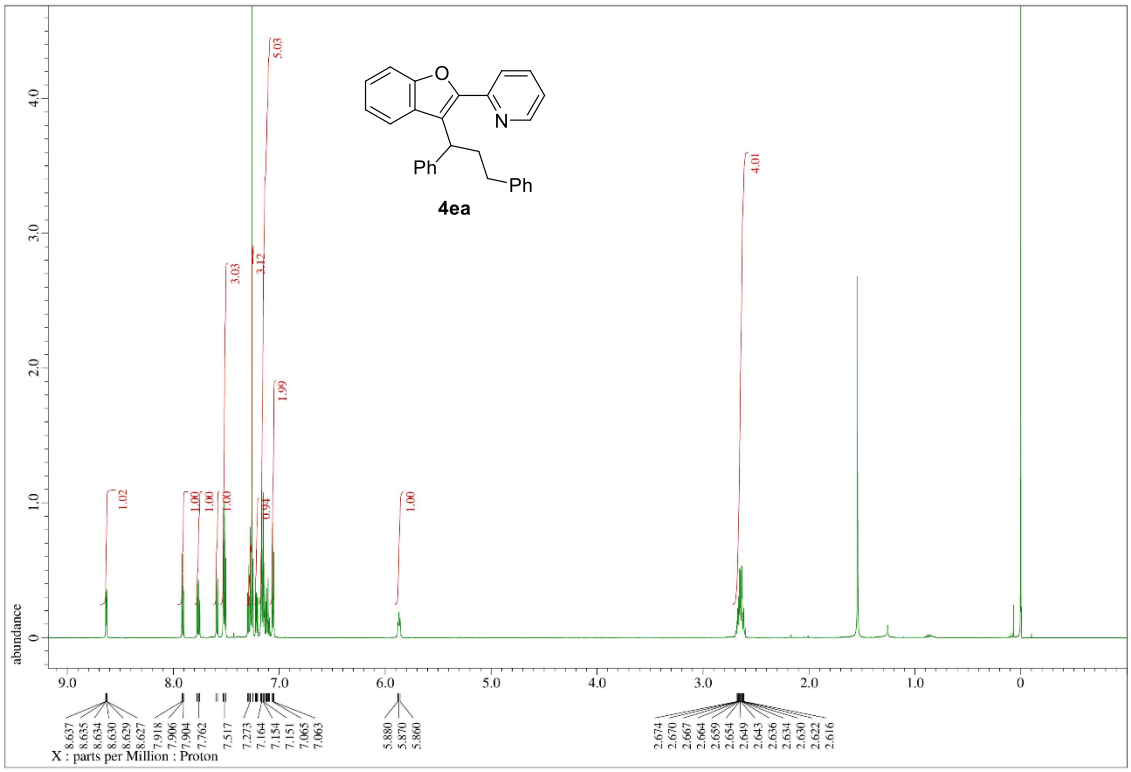
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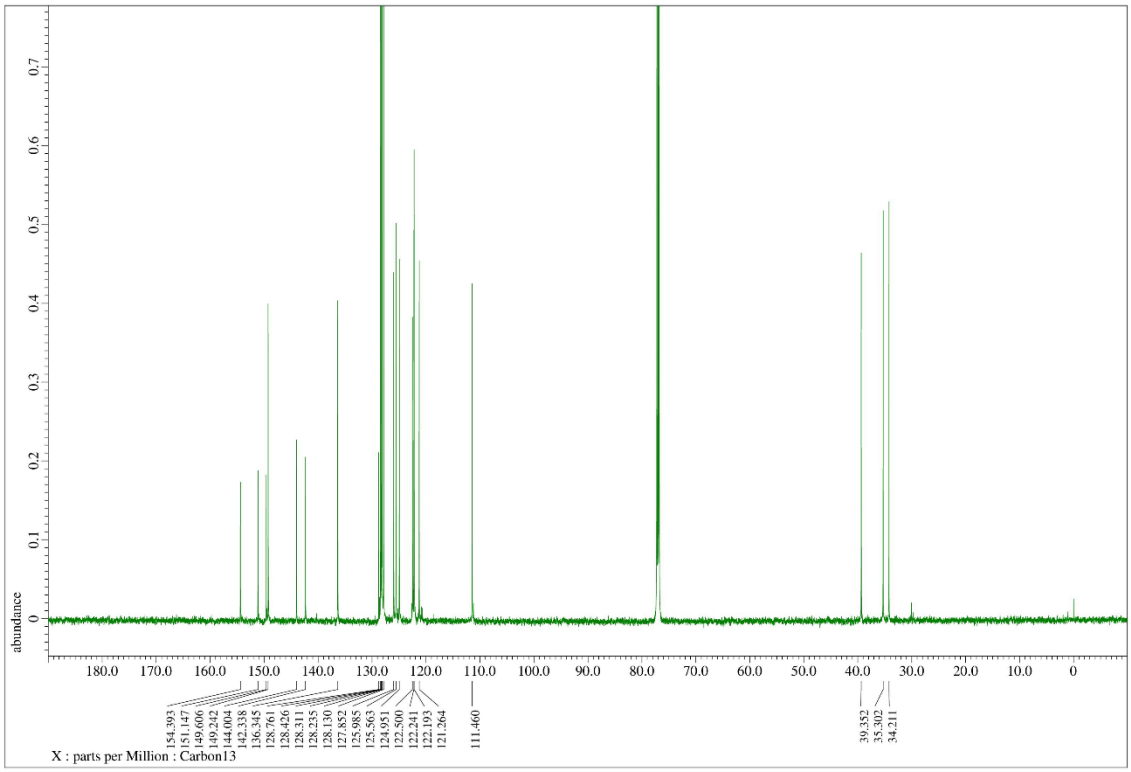
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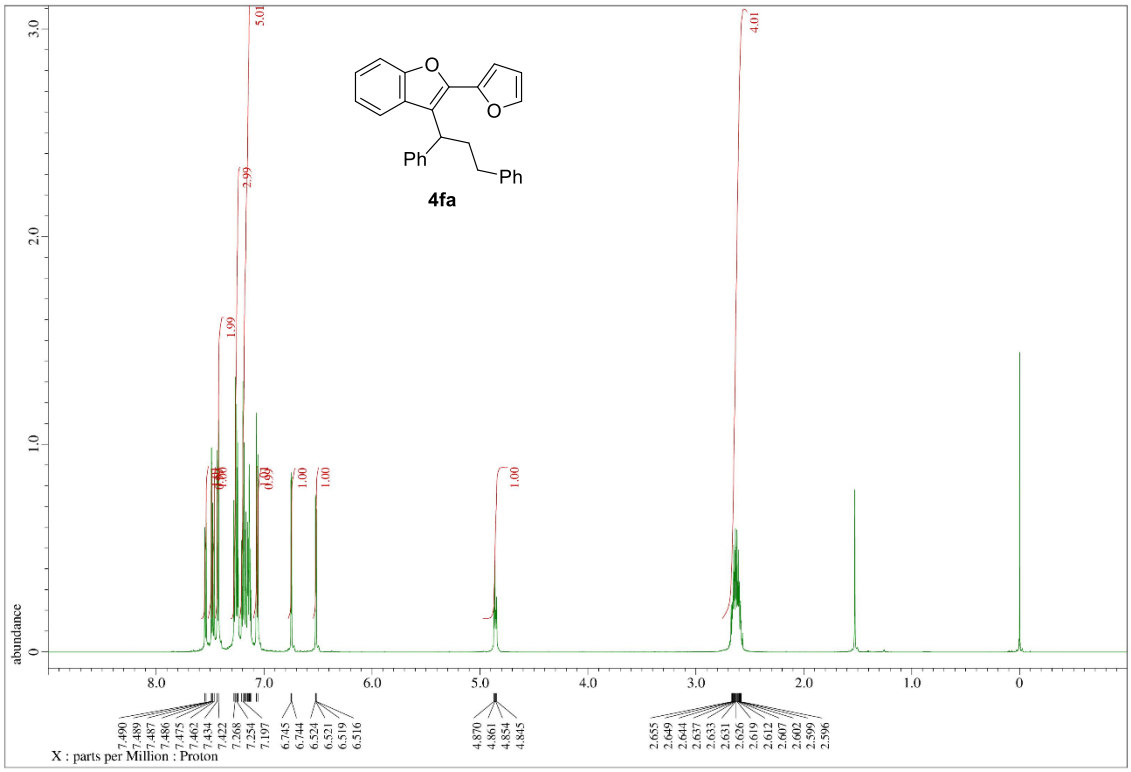
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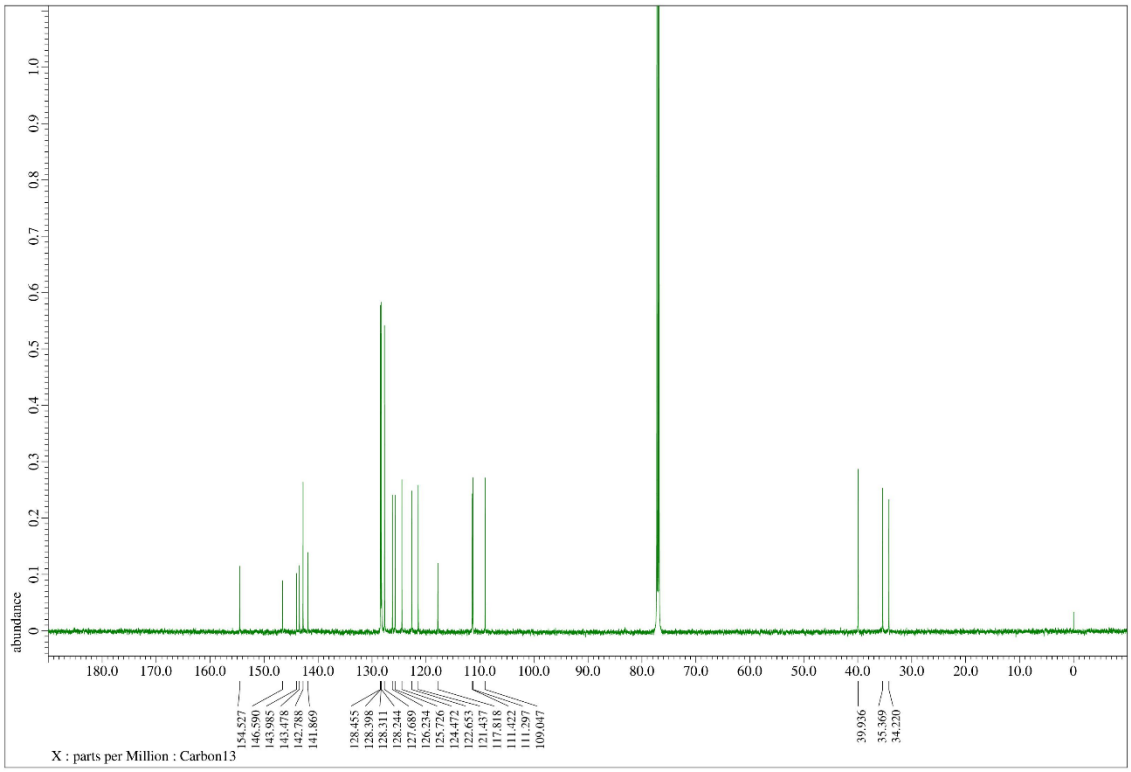
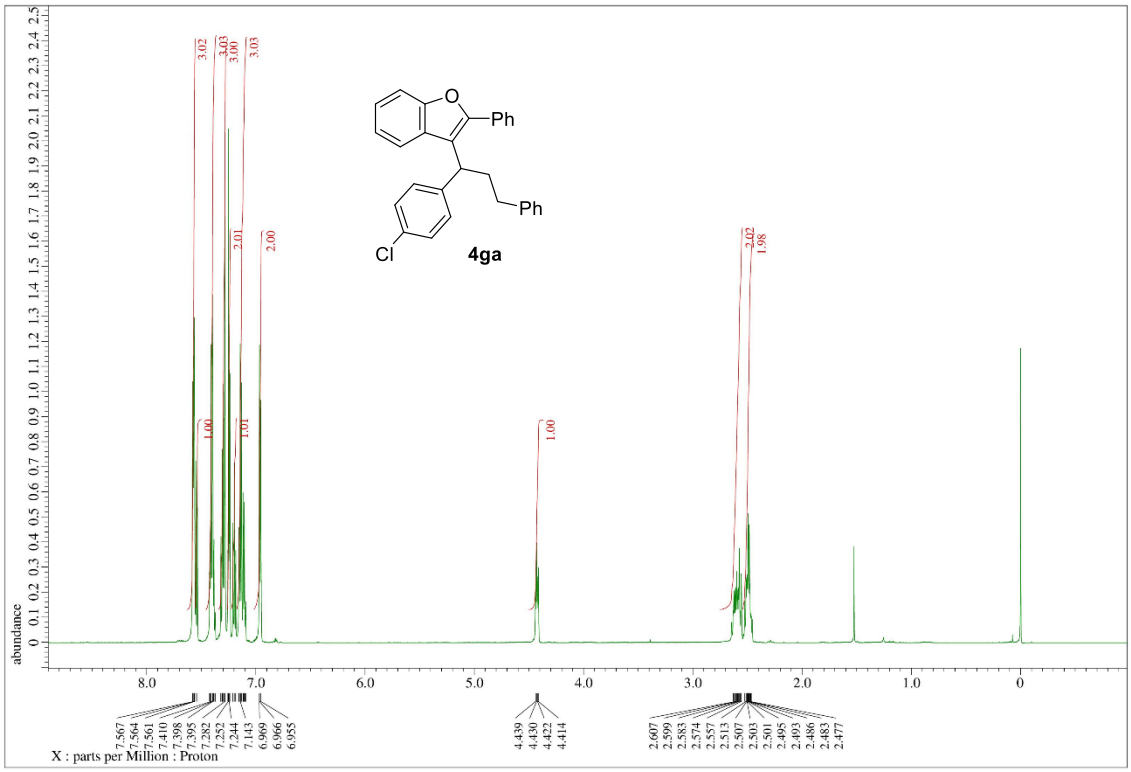
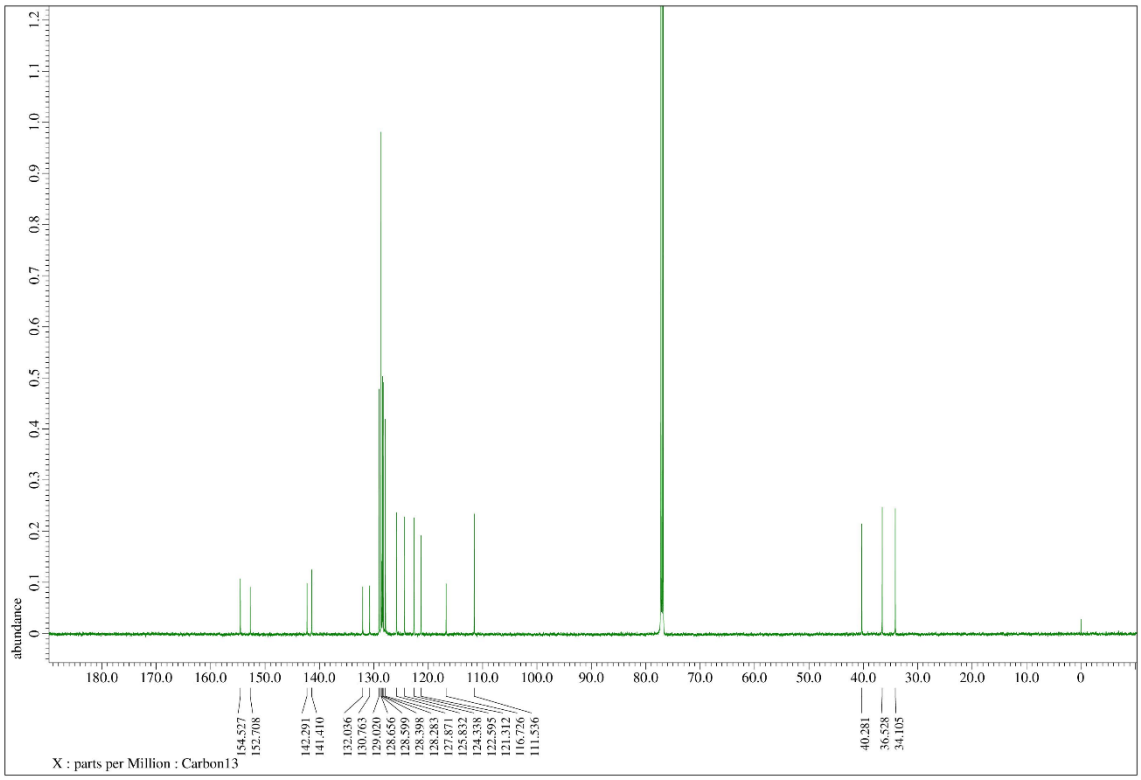

abundance
X : parts per Million : Carbon13


O
Ph
Ph
Cl
4ga
abundance
X : parts per Million : Proton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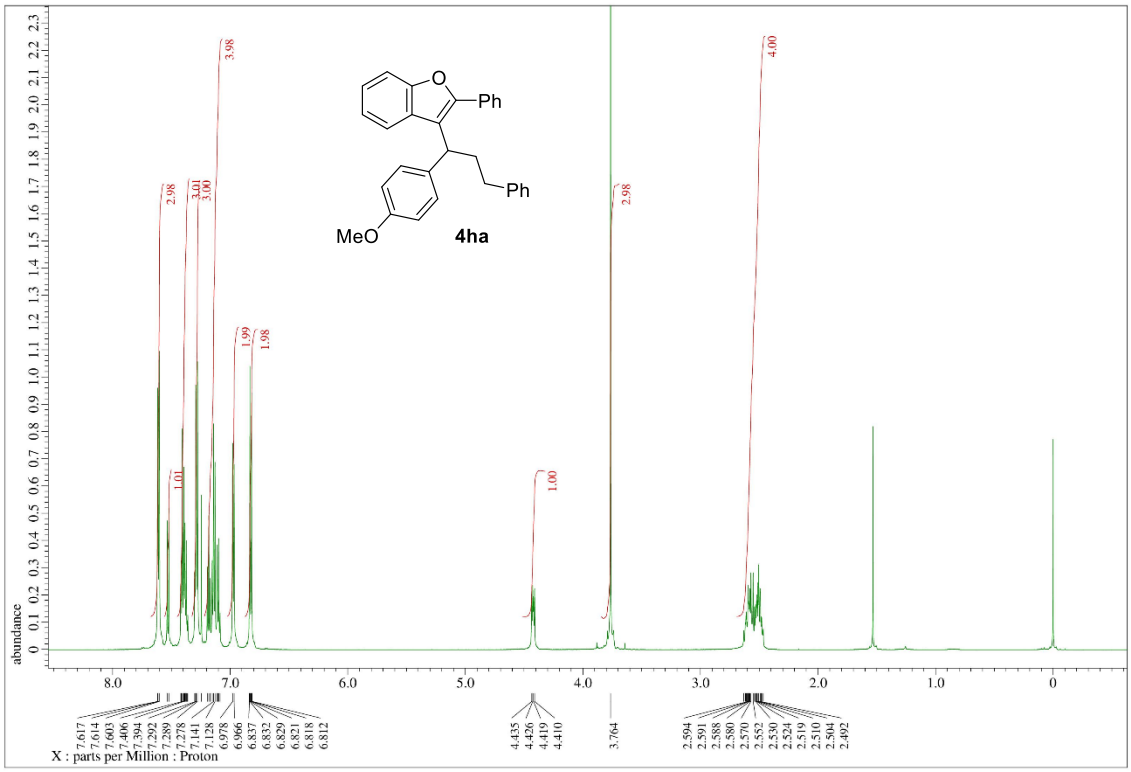
O
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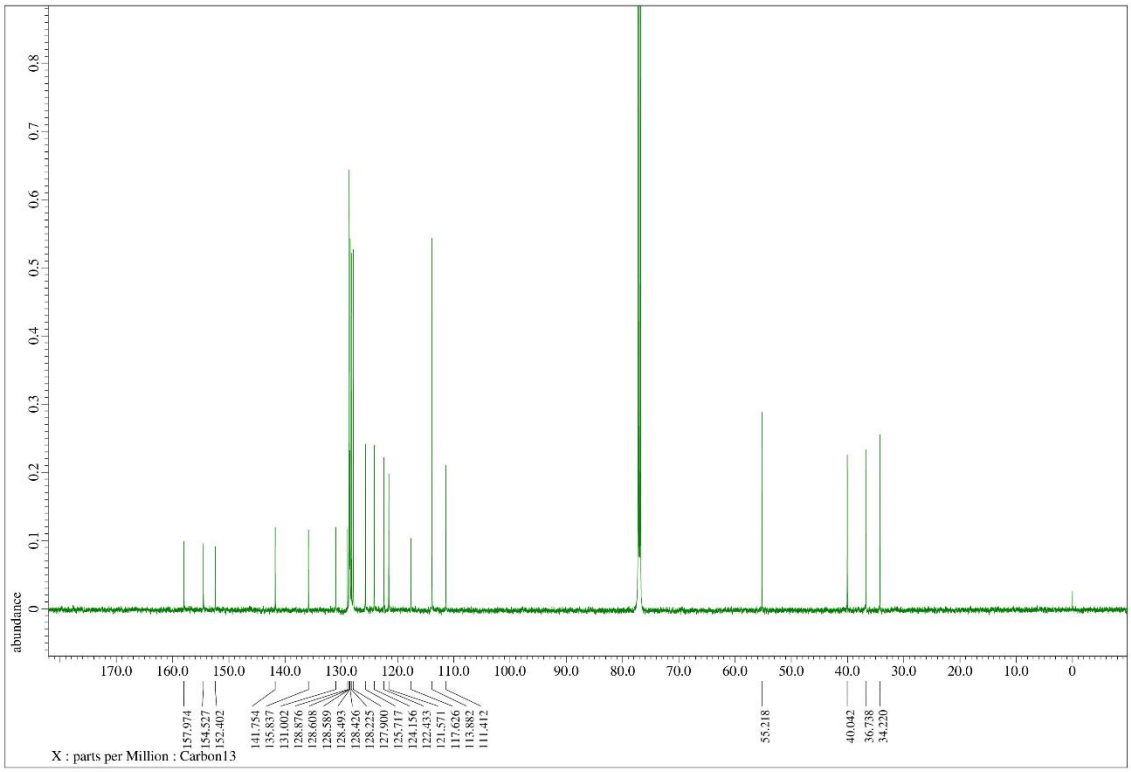
Ph
MeO
4ha
abundance
X : parts per Million : Proton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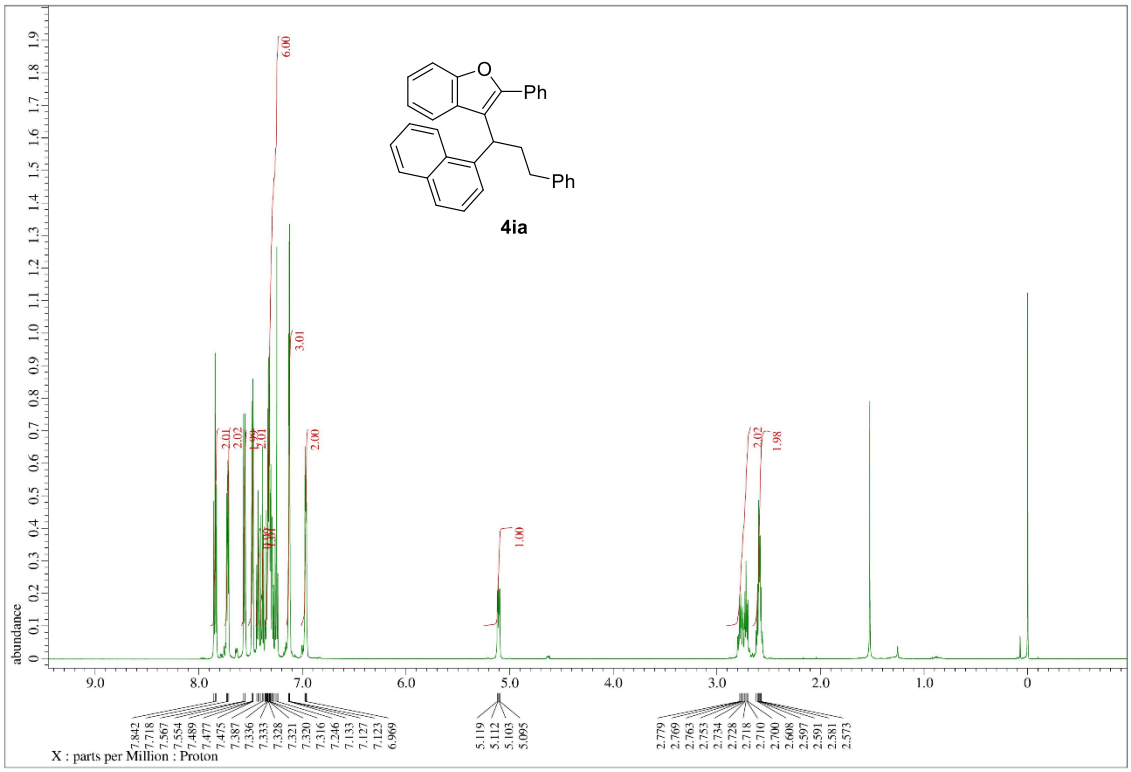
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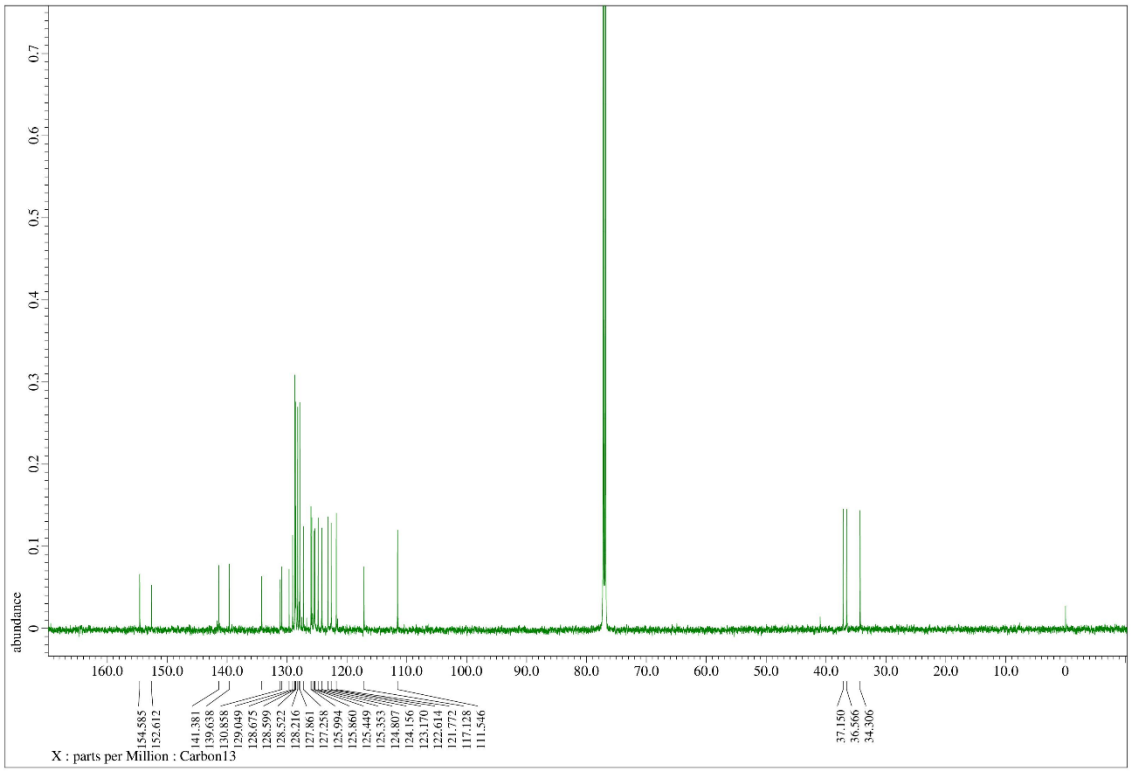
Ph
Ph
4ia
abundance
X : parts per Million : Proton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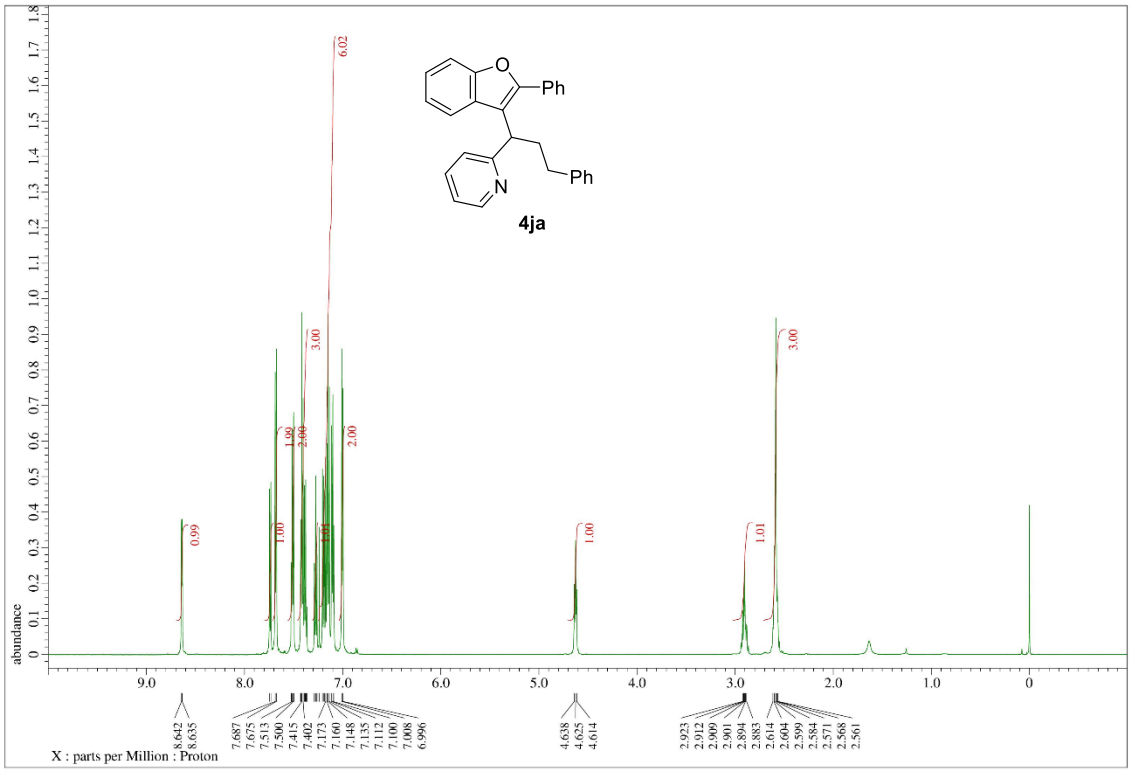
X : parts per Million : Carbon13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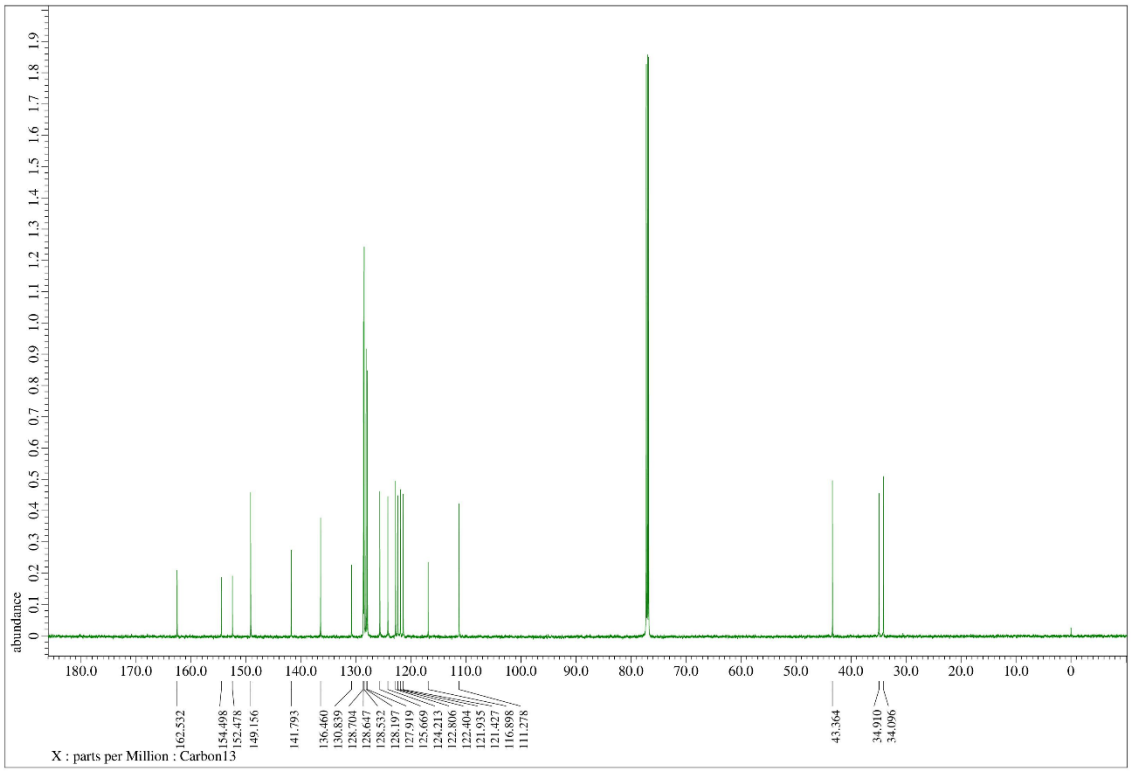
Ph
N
4ja
abundance
X : parts per Million : Proton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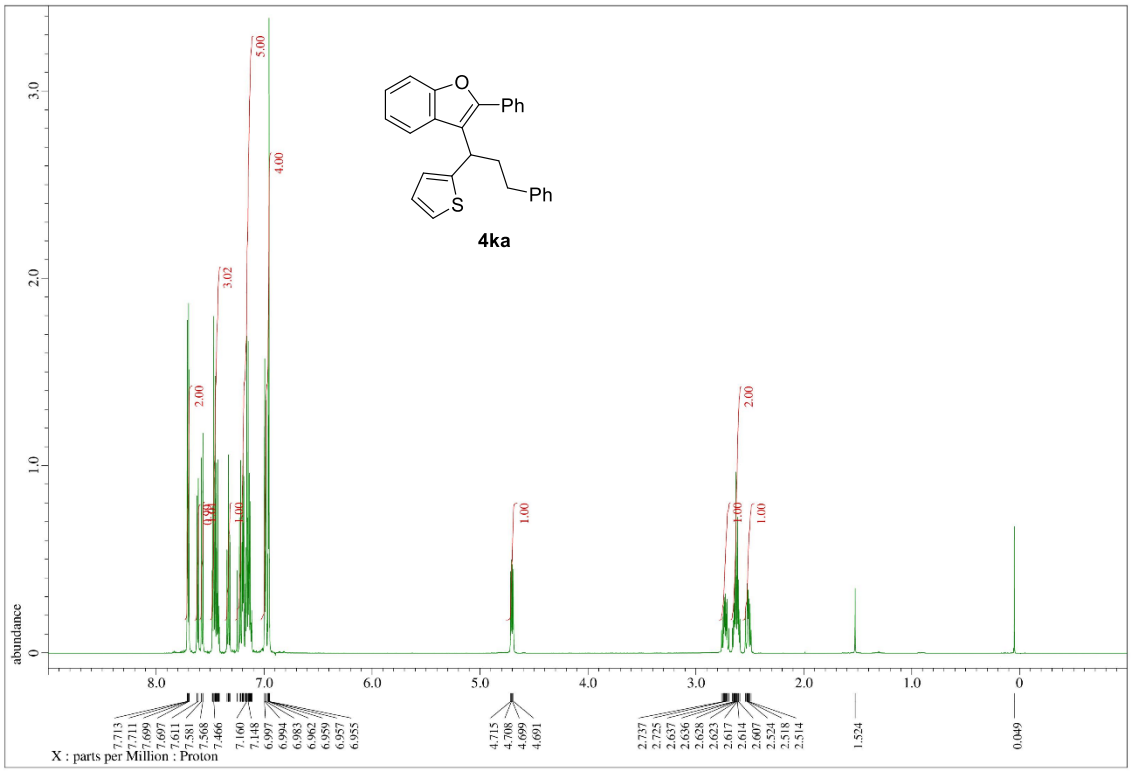
X : parts per Million : Carbon13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S
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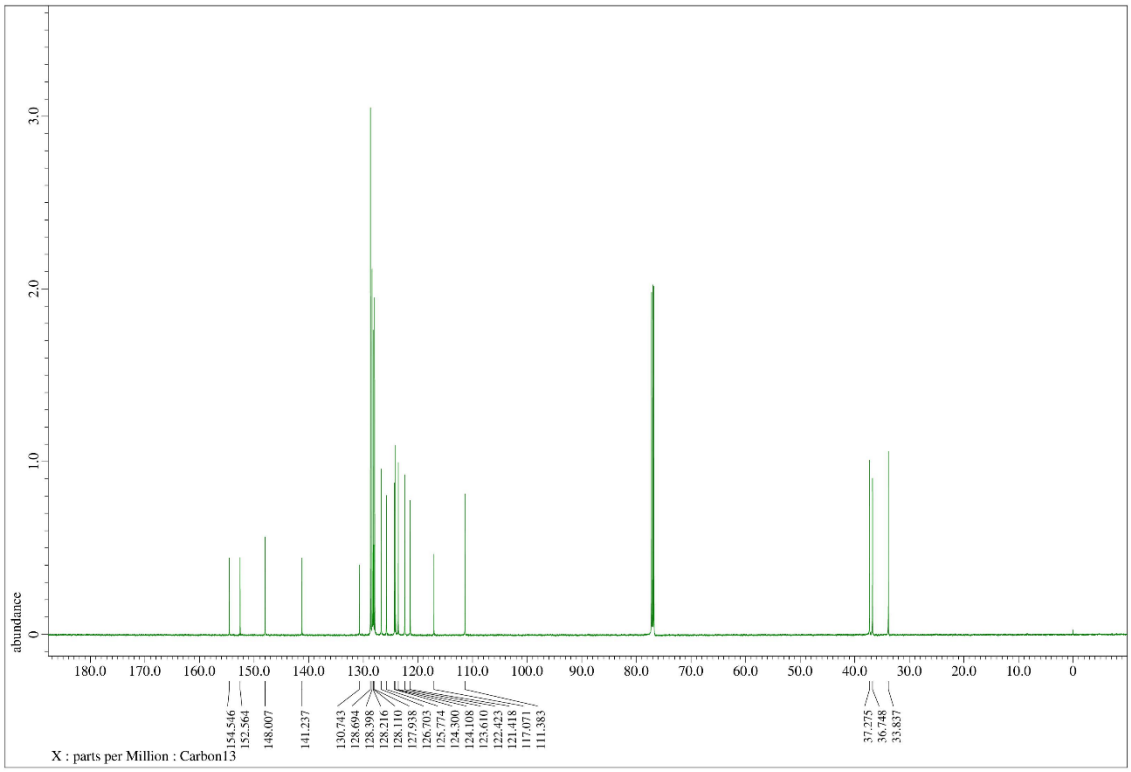
abundance
X : parts per Million : Proton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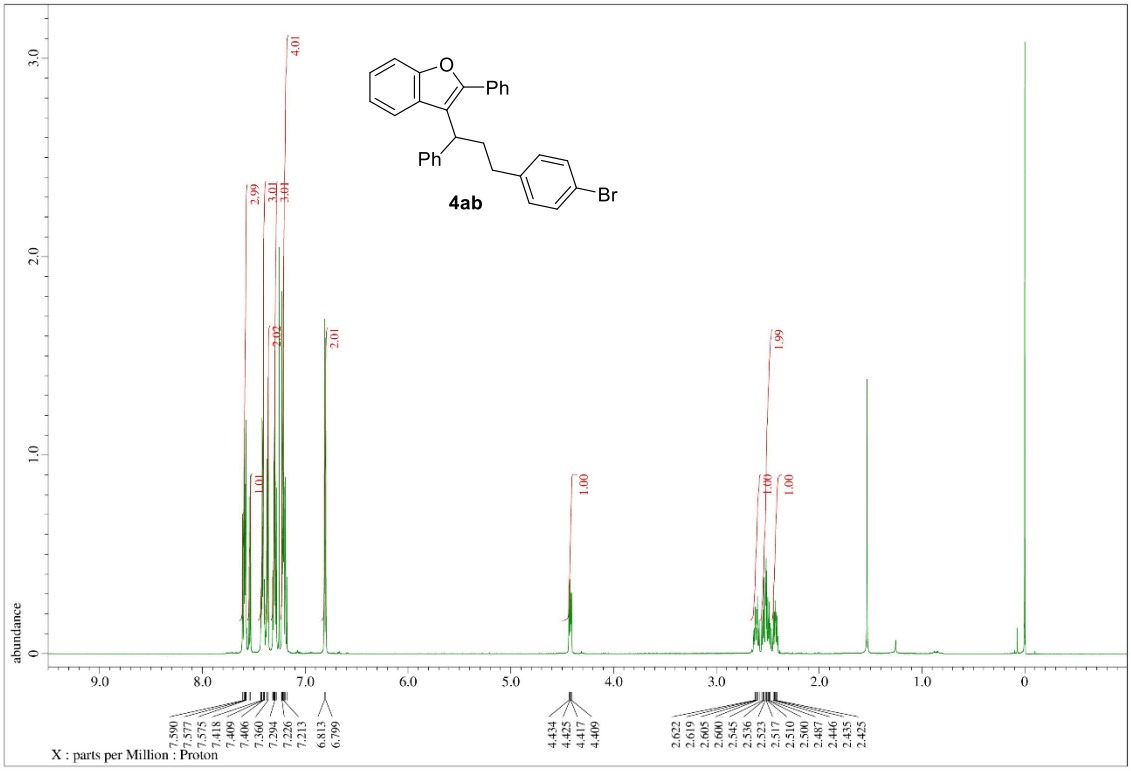
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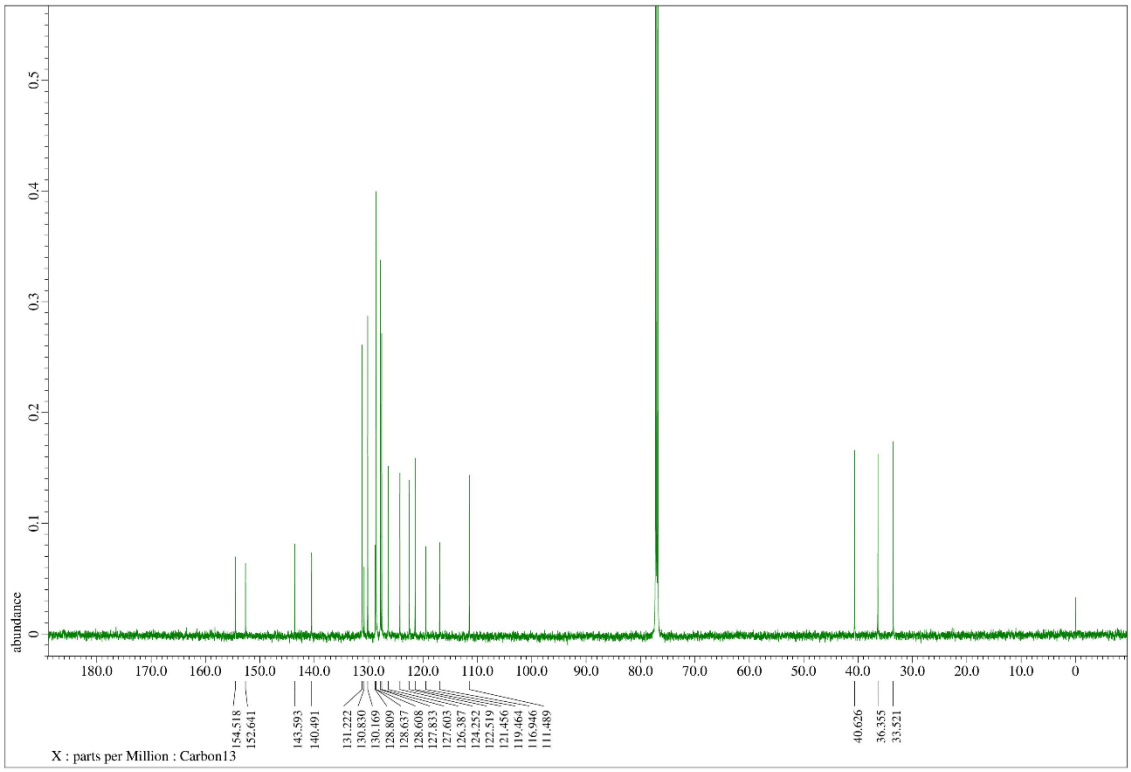
abundance
X : parts per Million : Proton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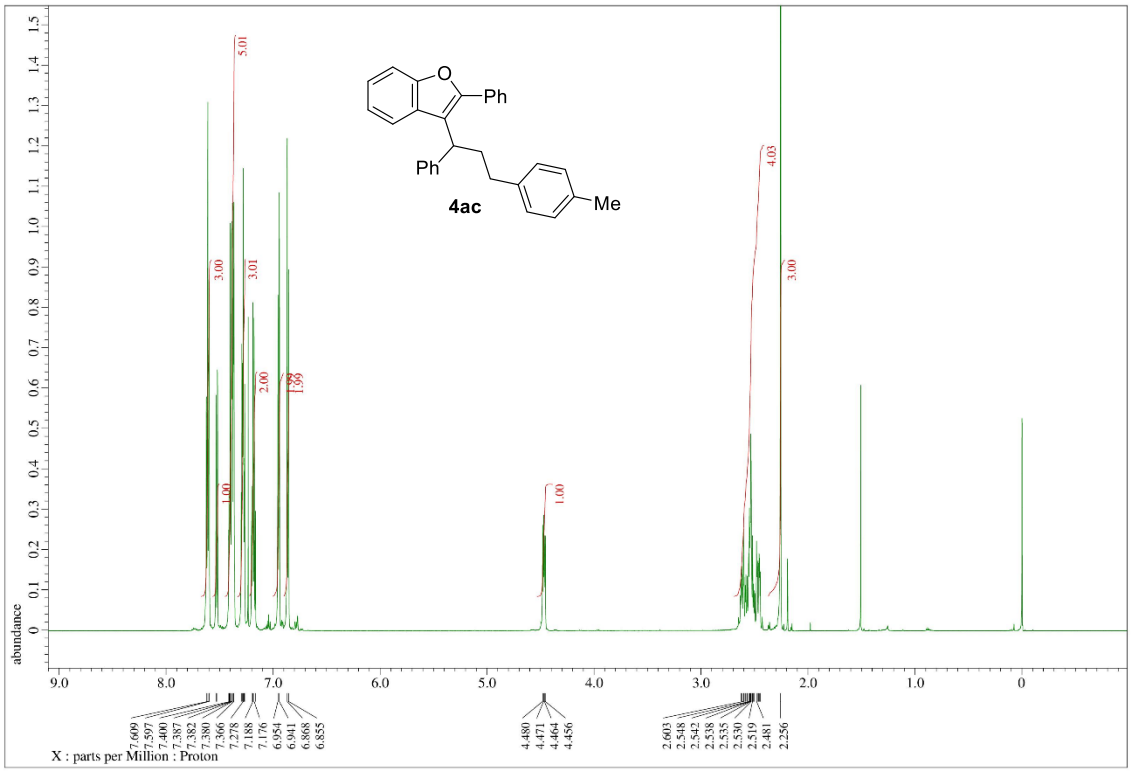
O
Ph
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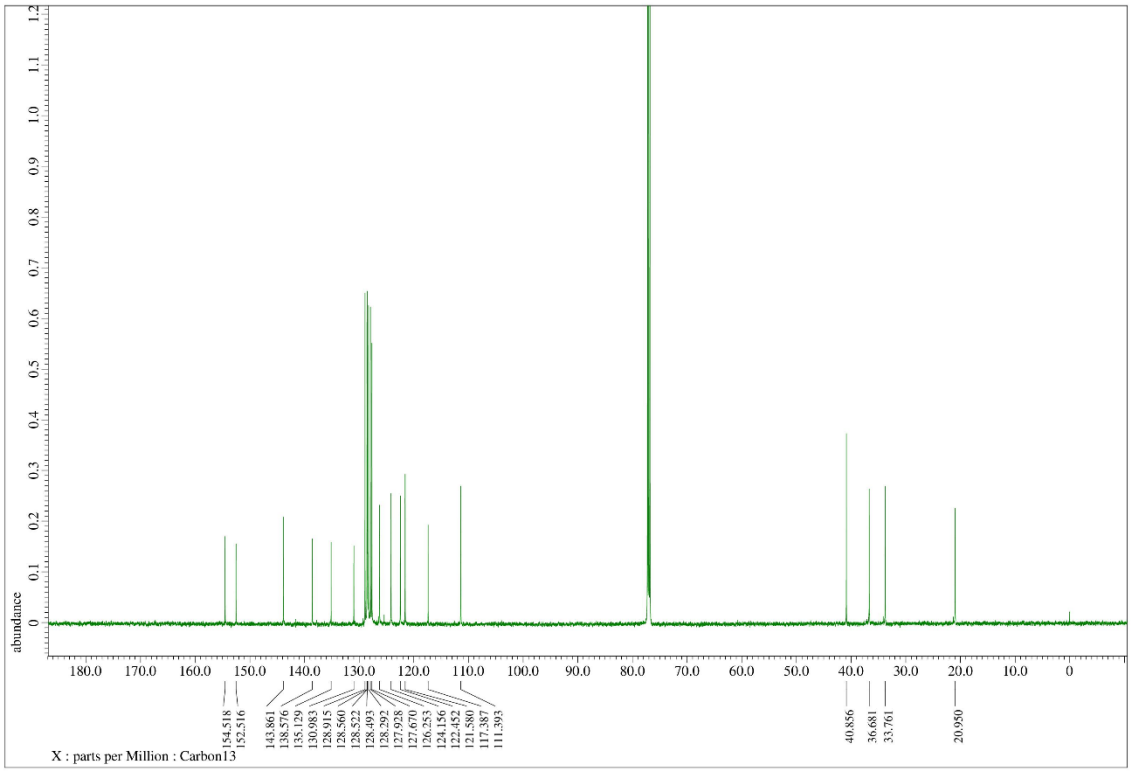
1.00
abundance
X : parts per Million : Proton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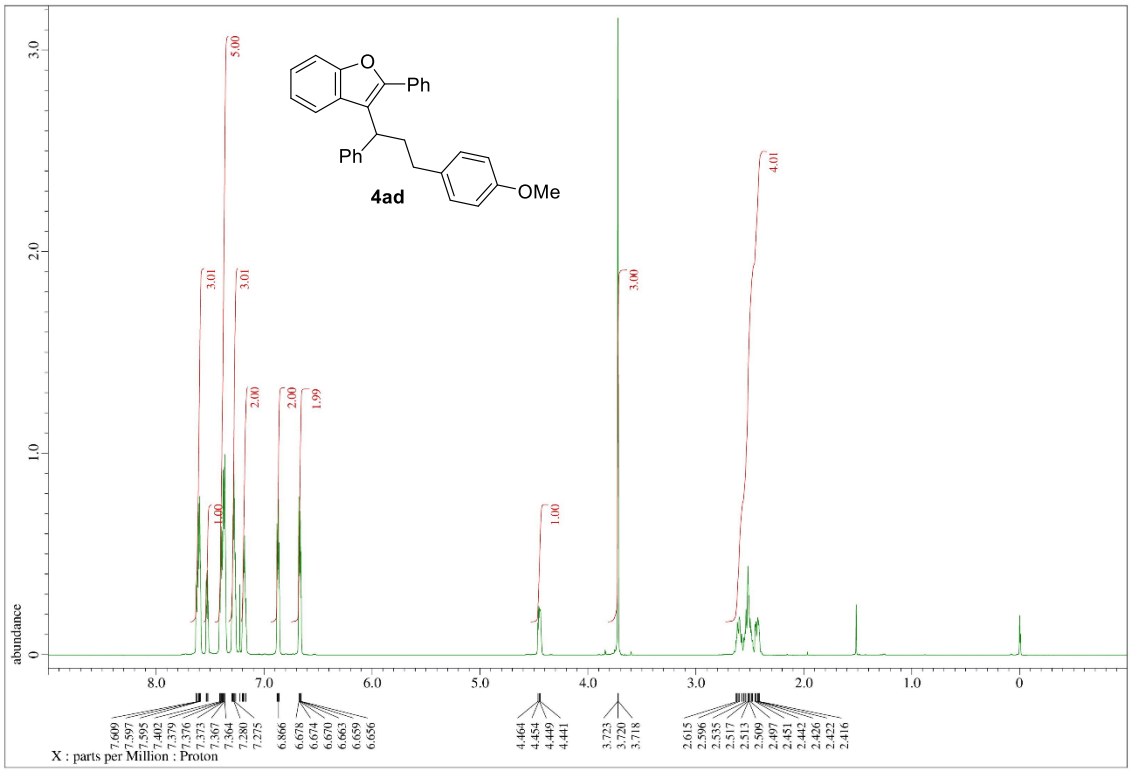
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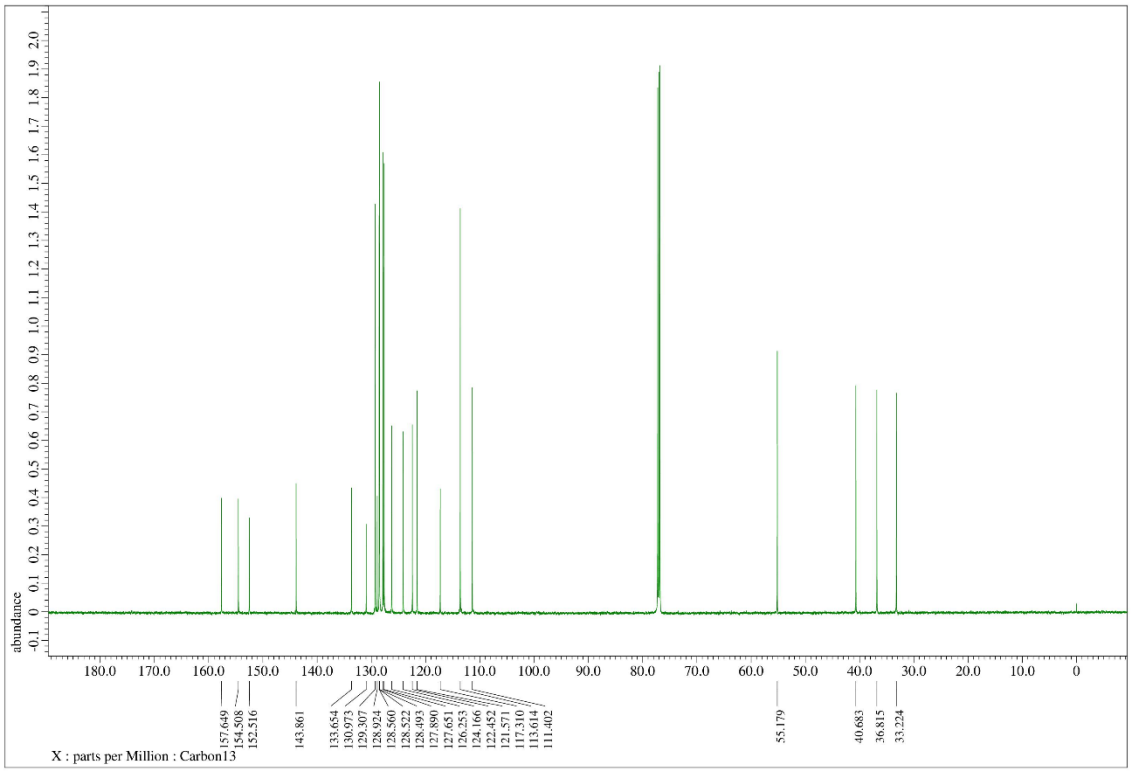
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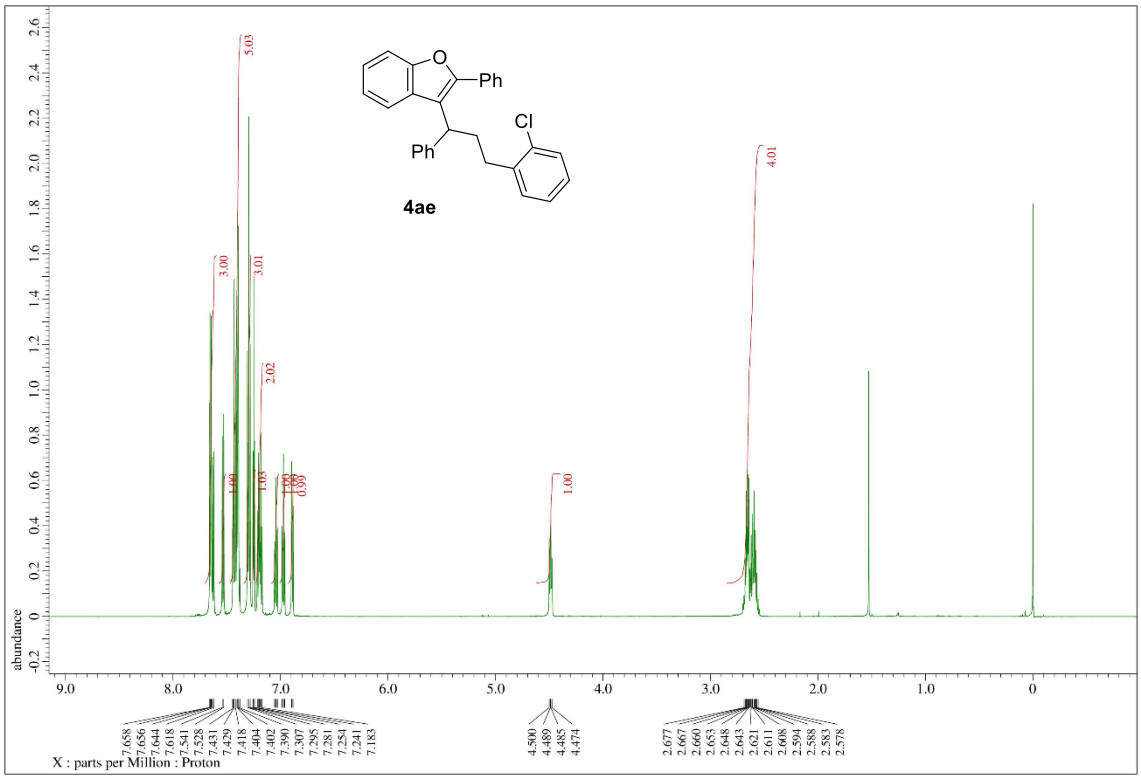
X : parts per Million : Carbon13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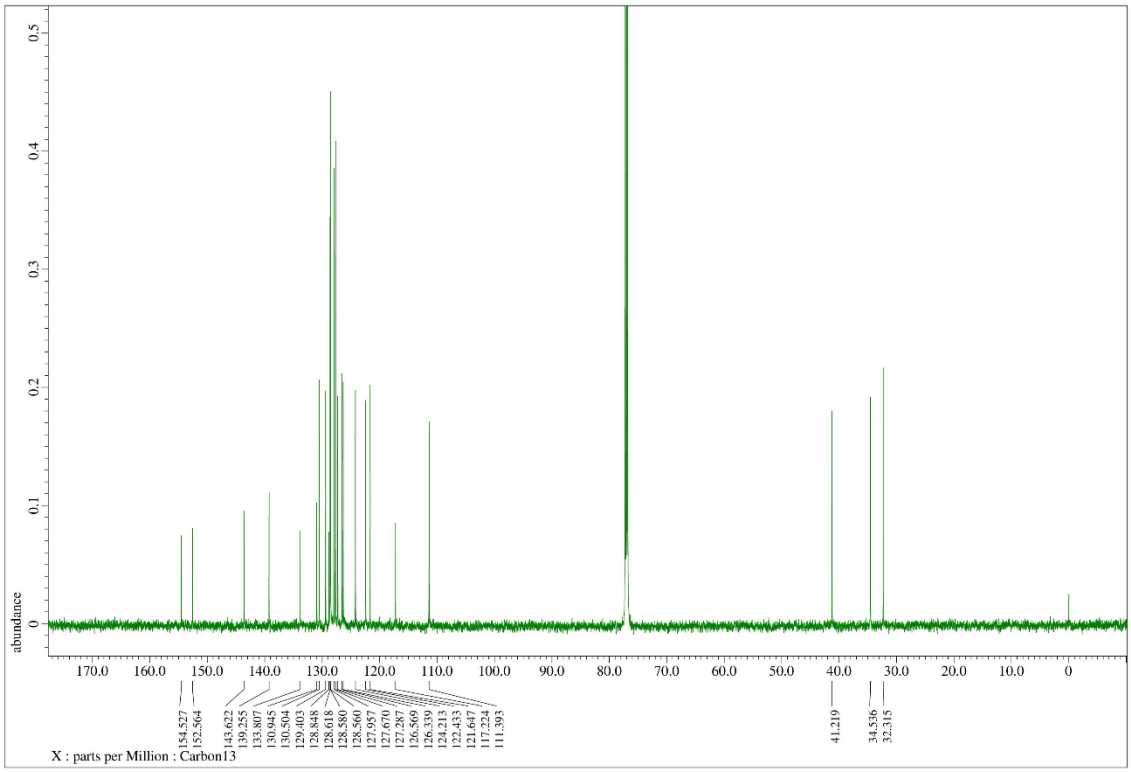
3.01
2.02
1.00
4.01
abundance
X : parts per Million : Proton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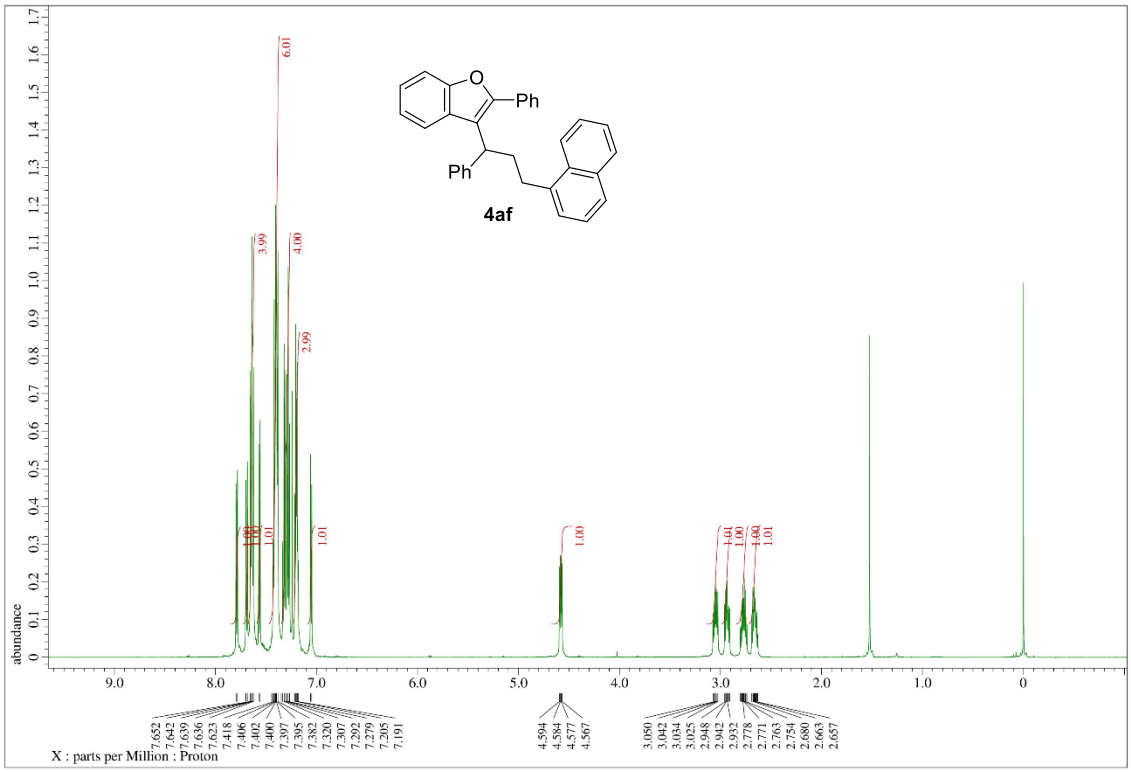
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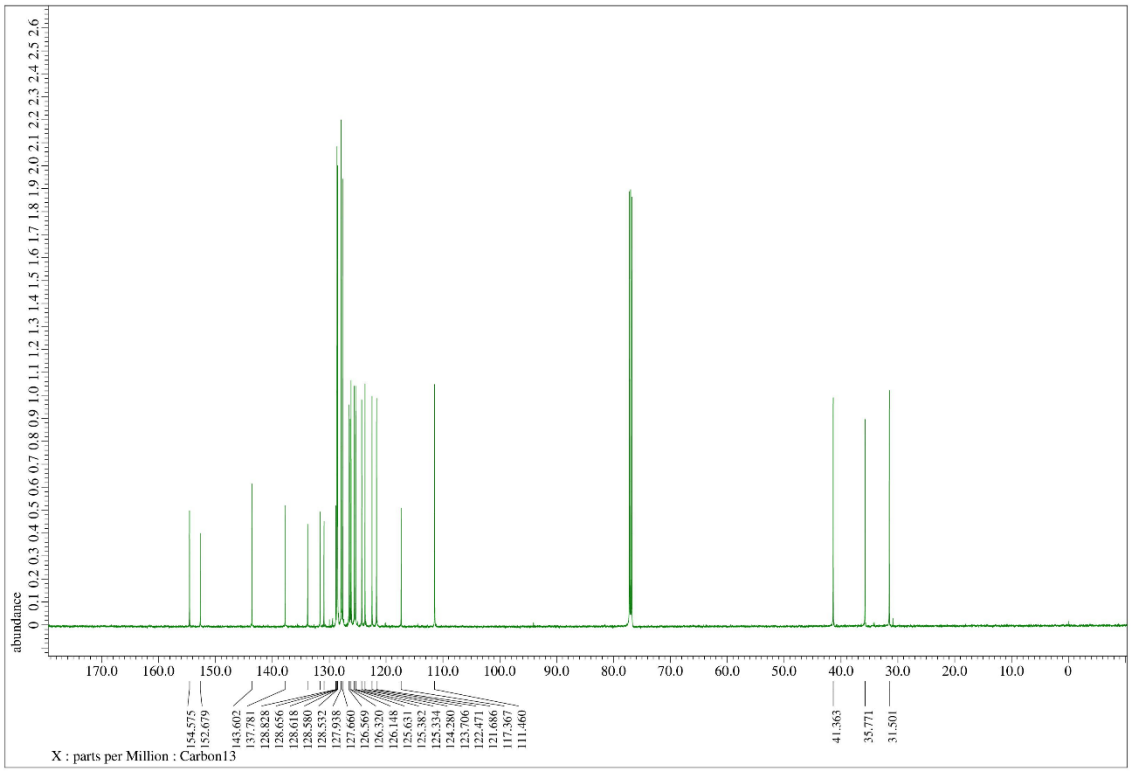
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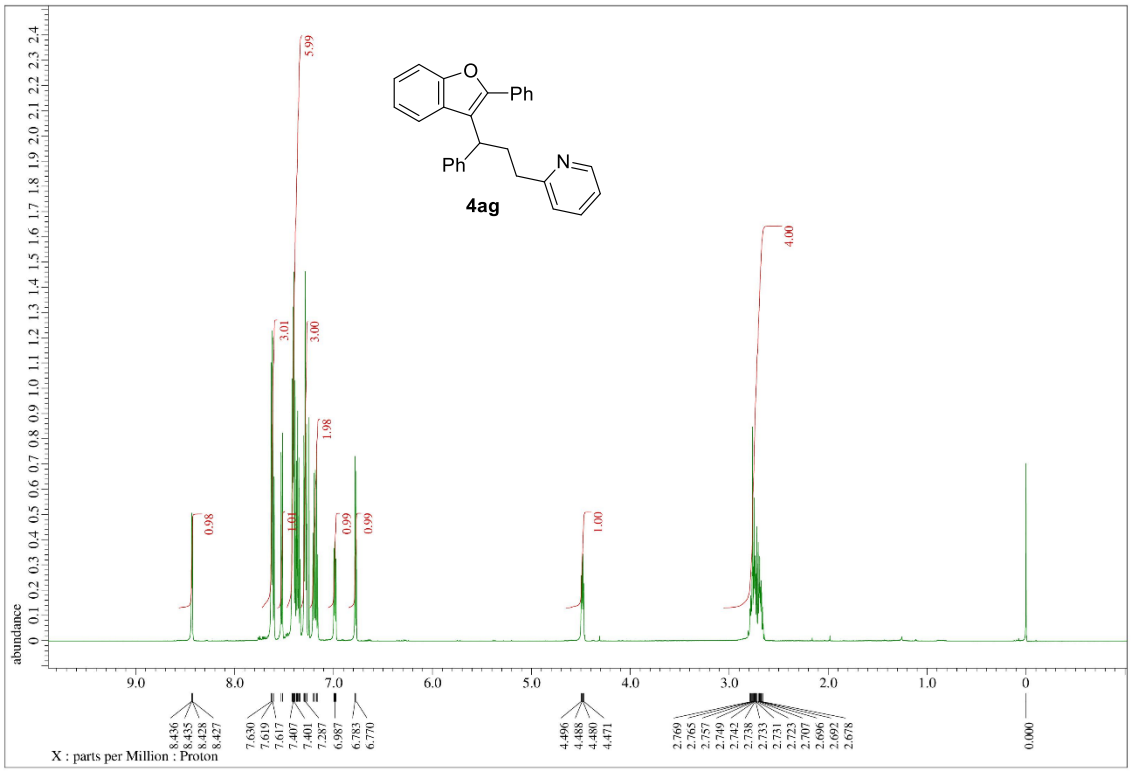
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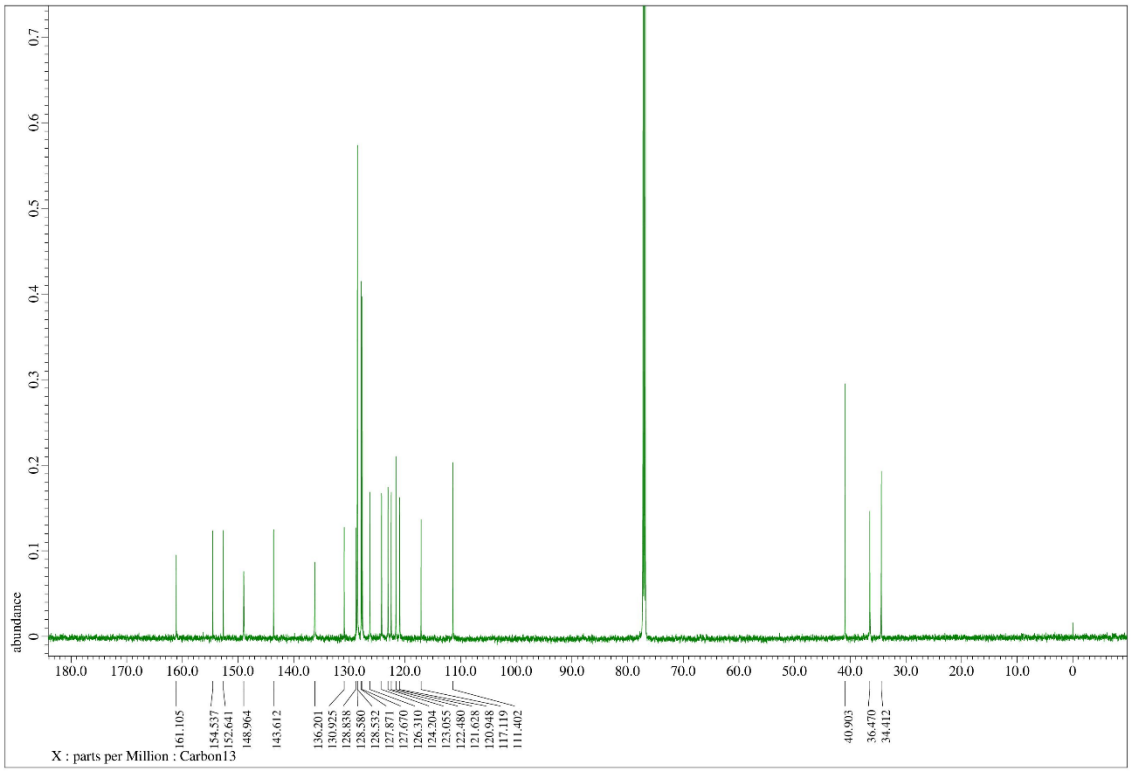
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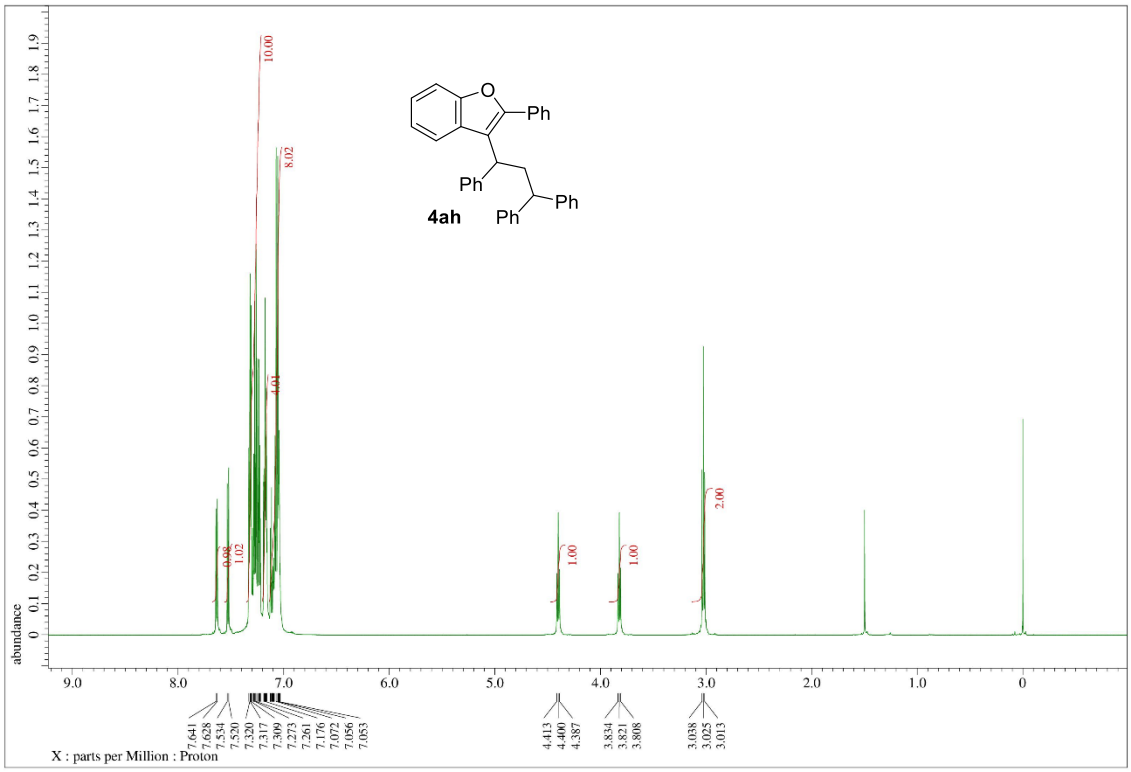
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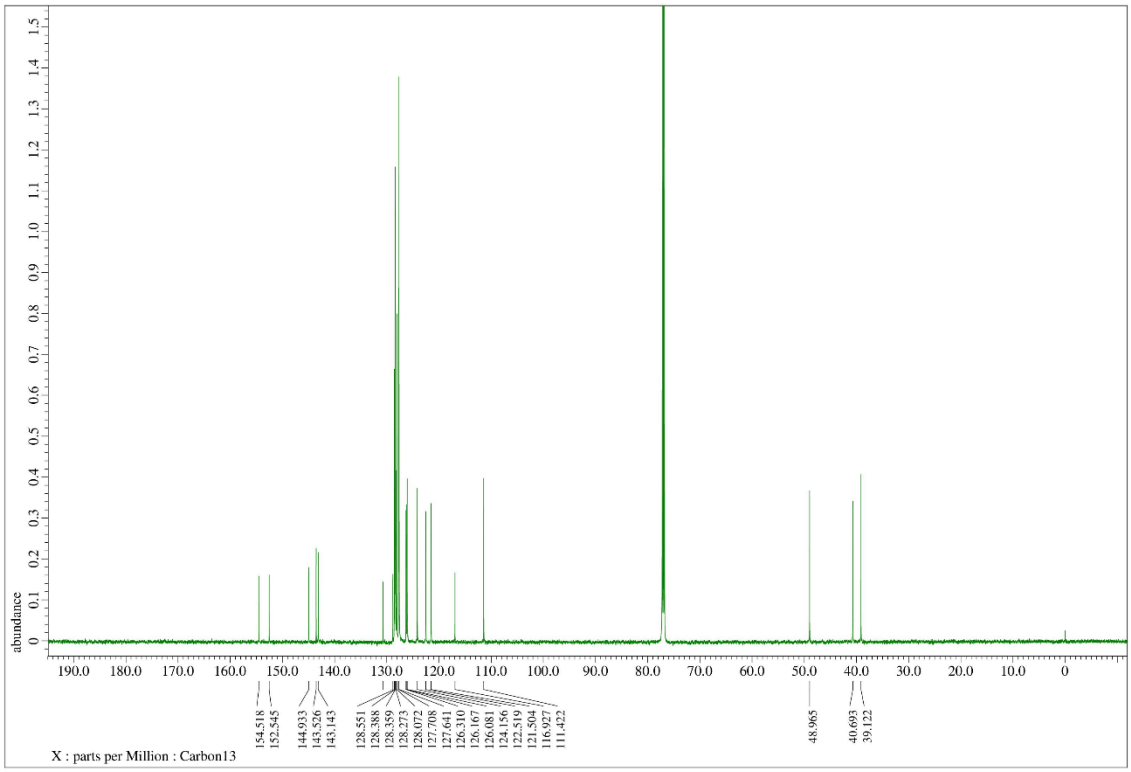
abundance
X : parts per Million : Proton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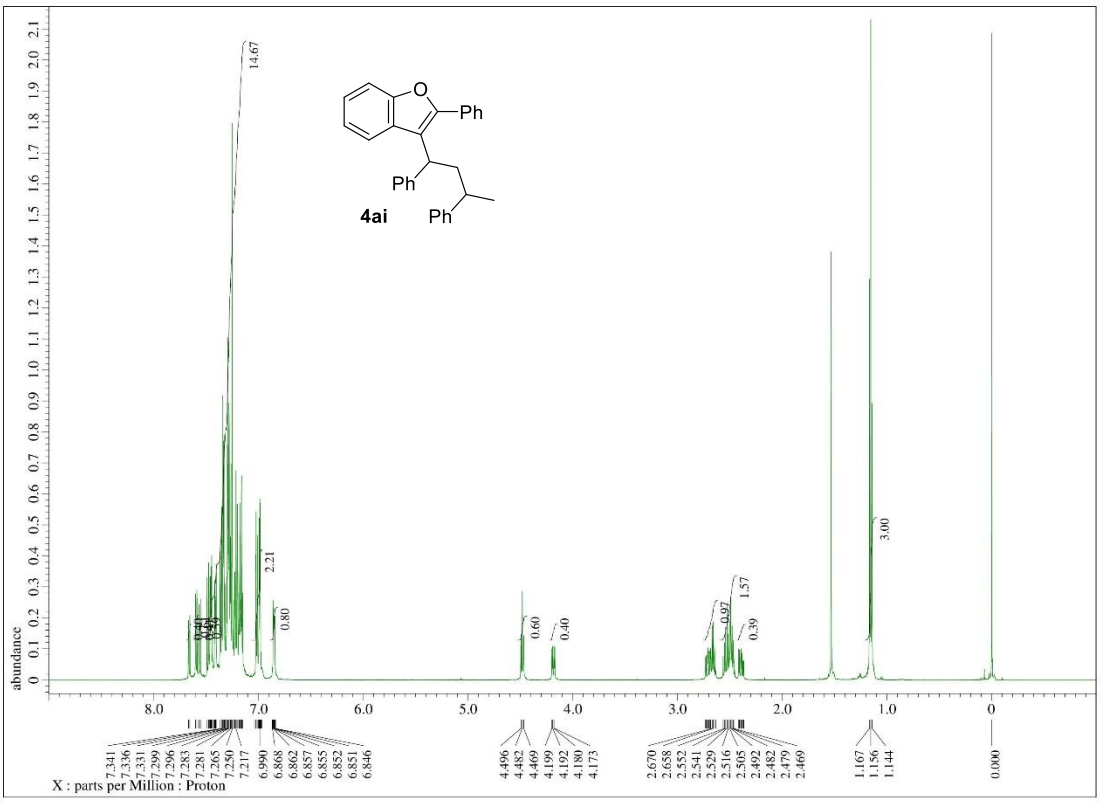
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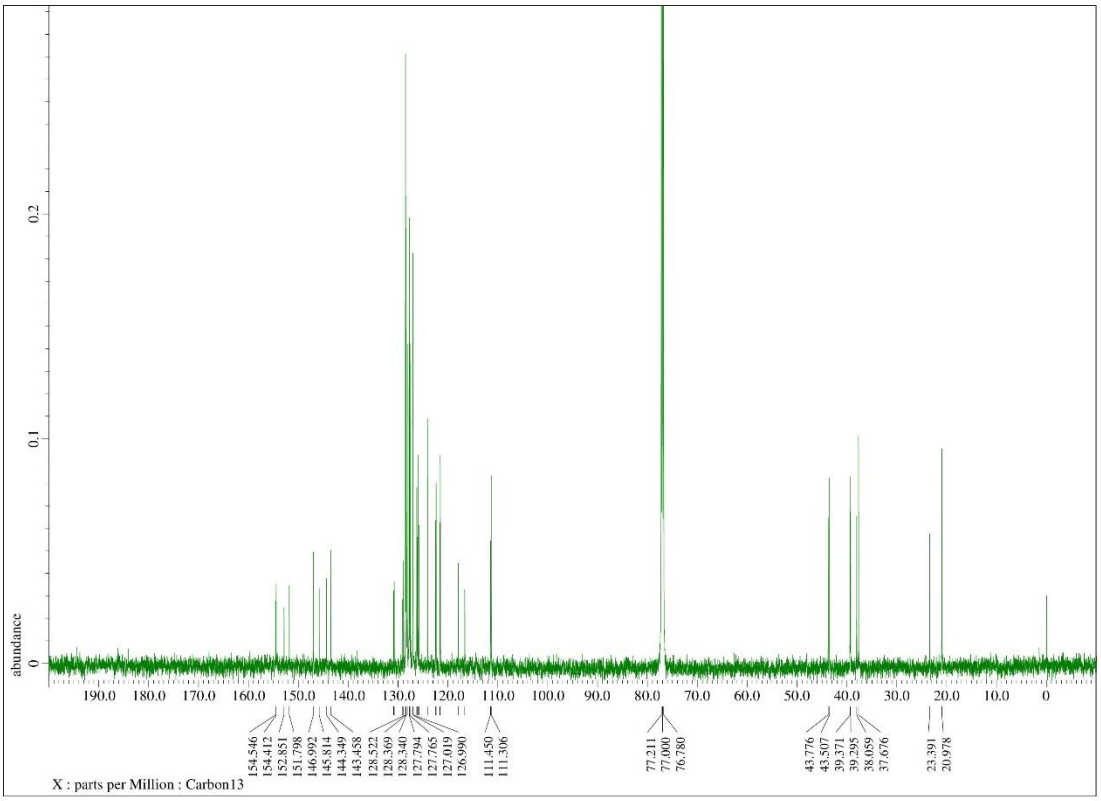
X : parts per Million : Proton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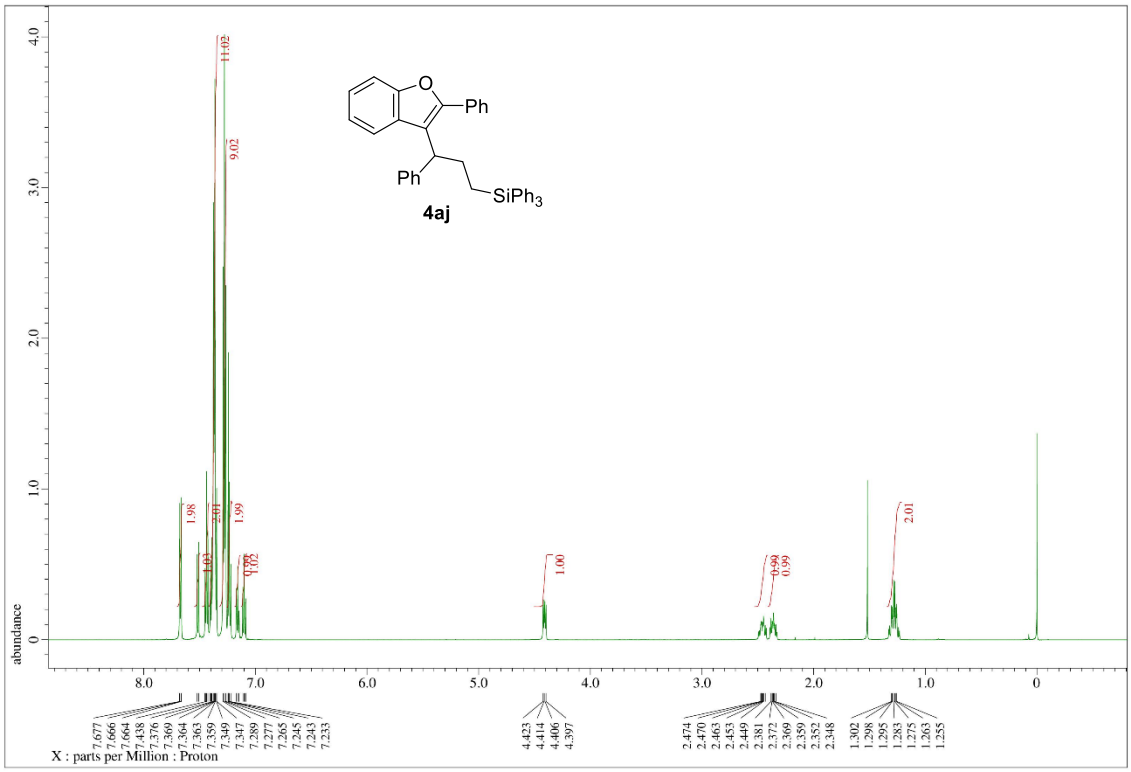
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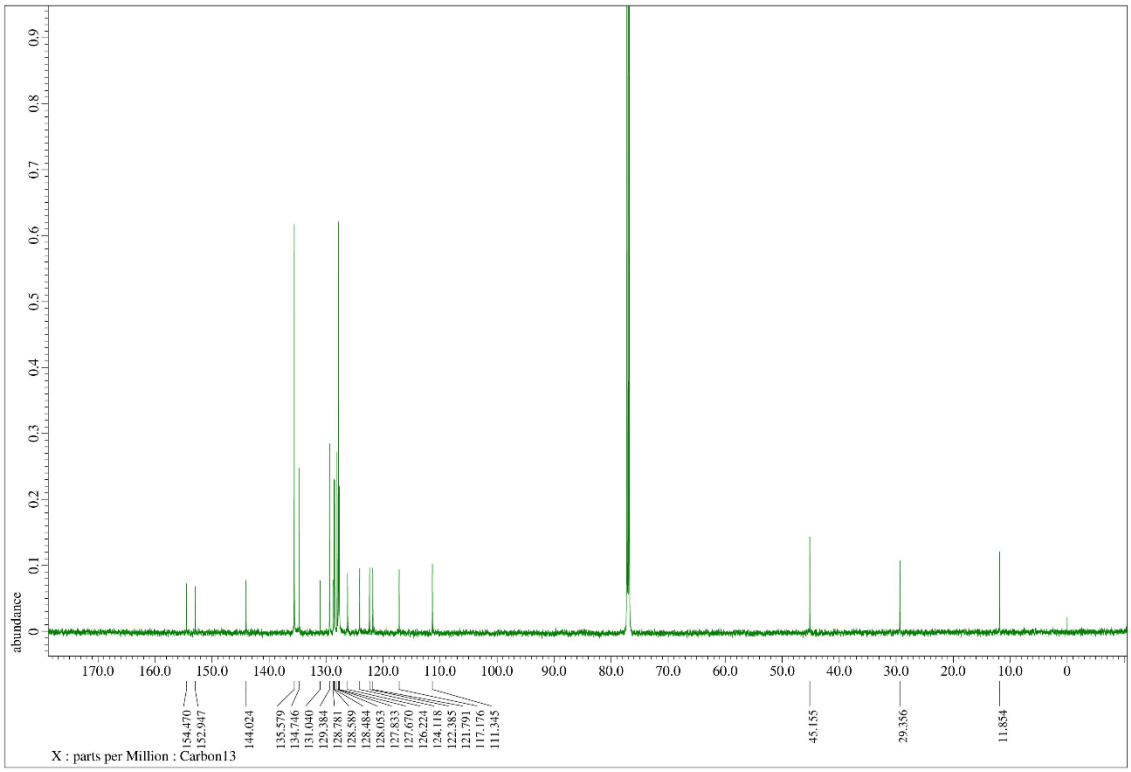
X : parts per Million : Proton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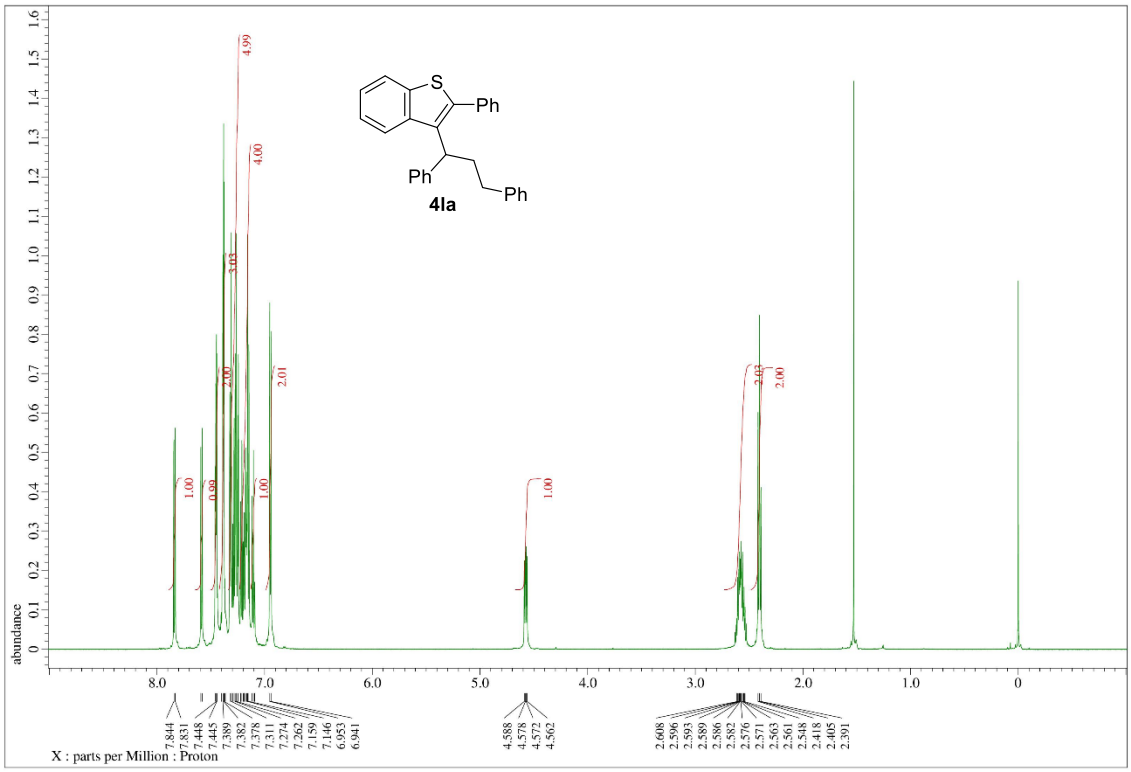
X : parts per Million : Carbon13


S
Ph
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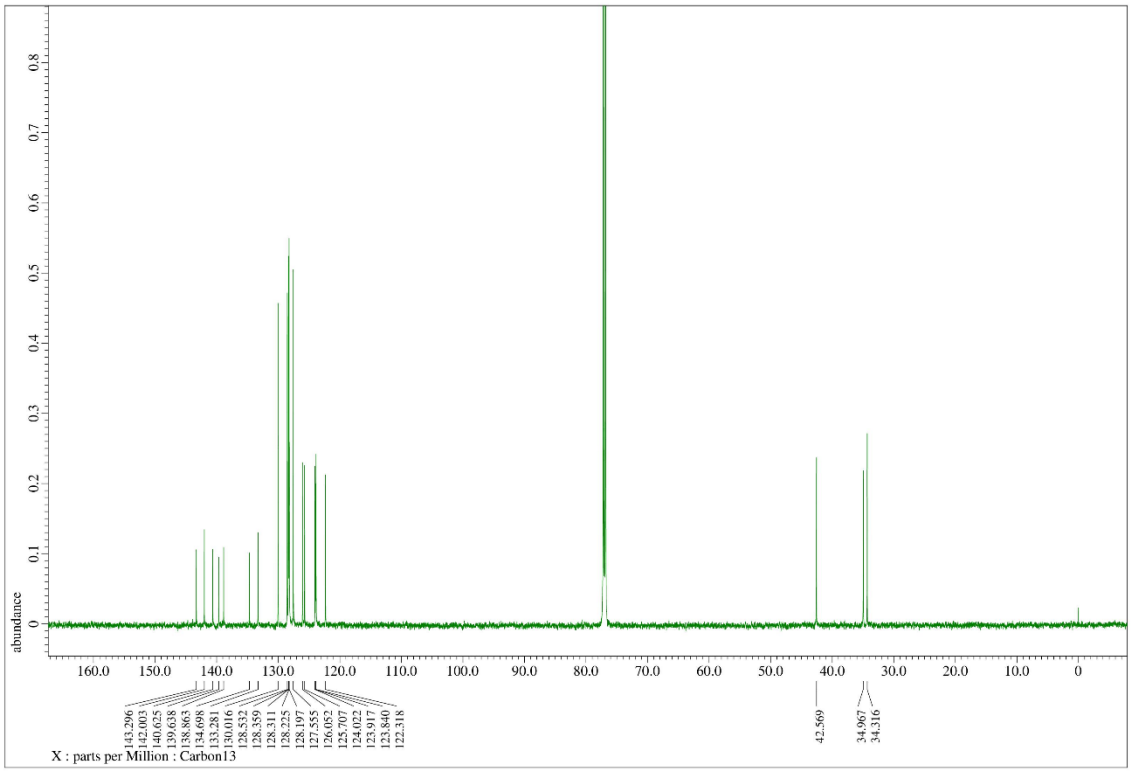
abundance
X : parts per Million : Proton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X : parts per Million : Carbon13