Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Visible Light Induced Boryl Radical and the Application in Reduction of Unsaturated X=O (X=C, N, S) Bonds

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1. General information

Chromatography and Instrumentation

All NMR spectra were recorder at 25 °C. Chemical shifts (δ) are given in parts per million (ppm) and referenced to $CDCl_3$ (1H: 7.26 ppm, 13C: 77.16) or DMSO-d6 (1H: 2.50 ppm, 13C: 39.52). Coupling constants (J) are given in Hertz (Hz) and refer to apparent multiplicities (s = singlet, br. s = broad singlet, d = doublet, t = triplet, q = quartet, quin = quintet, sex = sextet, h = heptet, m = multiplet, dd = doublet of doublets, etc.). The 1H NMR spectra are reported as follows: chemical shift (multiplicity, coupling constants, number of protons)

Femtosecond transient absorption (fs-TA) experiments

The fs-TA measurements were performed based on a femtosecond Ti: Sapphire regenerative amplifier laser system (Coherent, Astrella-Tunable-F-1k) and femtosecond transient absorption spectrometer system (Ultrafast Systems, Helios Fire). The laser probe pulse was produced with ~4% of the amplified 800 nm laser pulses to generate a white-light continuum (320 800 nm) in a CaF2 crystal and then this probe beam was split into two parts before traversing the sample. One probe laser beam goes through the sample while the other probe laser beam goes to the reference spectrometer to monitor the fluctuations in the probe beam intensity. The instrument response function was determined to be ca. 120 fs. At each temporal delay, data were averaged for 2 s and collected by the acquisition system. For the experiments described in this study, the sample solution was excited by a 365 nm pump beam with a power of 0.2 mW (from TOPAS). The sample solutions were excited in a 2 mm path-length cuvette. The data were stored as three-dimensional (3D) wavelength-time-absorbance matrices that were exported for use with the fitting software. Chirp correction was done for all the data shown here. The kinetics of all fs-TA spectra were fitted by single-wavelength fitting via Surface Xplorer software; all the error values were shown with 90% confidence intervals.

2. Spectroscopy Study

Spectroscopy study of boryl radical

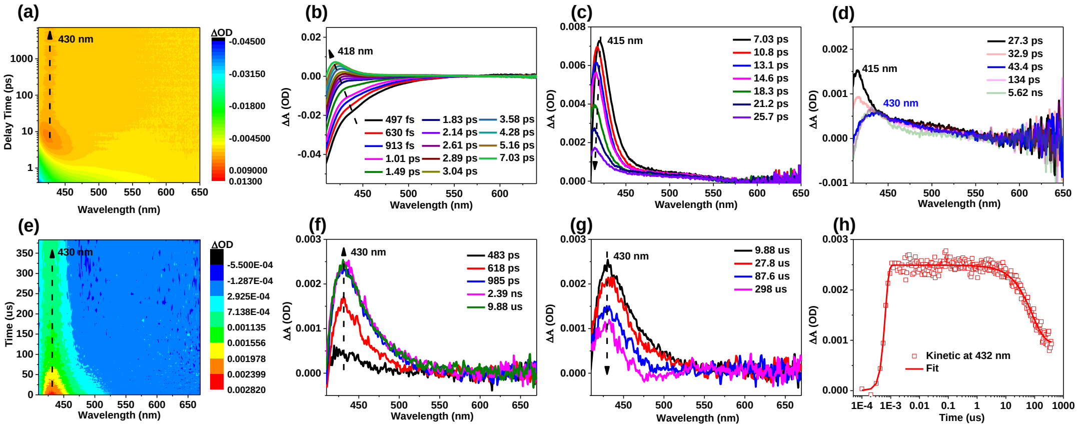


Figure S1. The transient spectra of mechanism study of boryl radical generation. (a)-(d) The fs-TA spectra of B_2cat_2, 4-cyanopyridine in DMF under 400 nm irradiation; (e)-(g) The ns-TA spectra of B2cat2 and 4-cyanopyridine in DMF under 400 nm irradiation; (h) The excited state kinetics and fitting results at 432 nm.

Spectroscopy study of reductive hydrogeneration of aromatic ketone

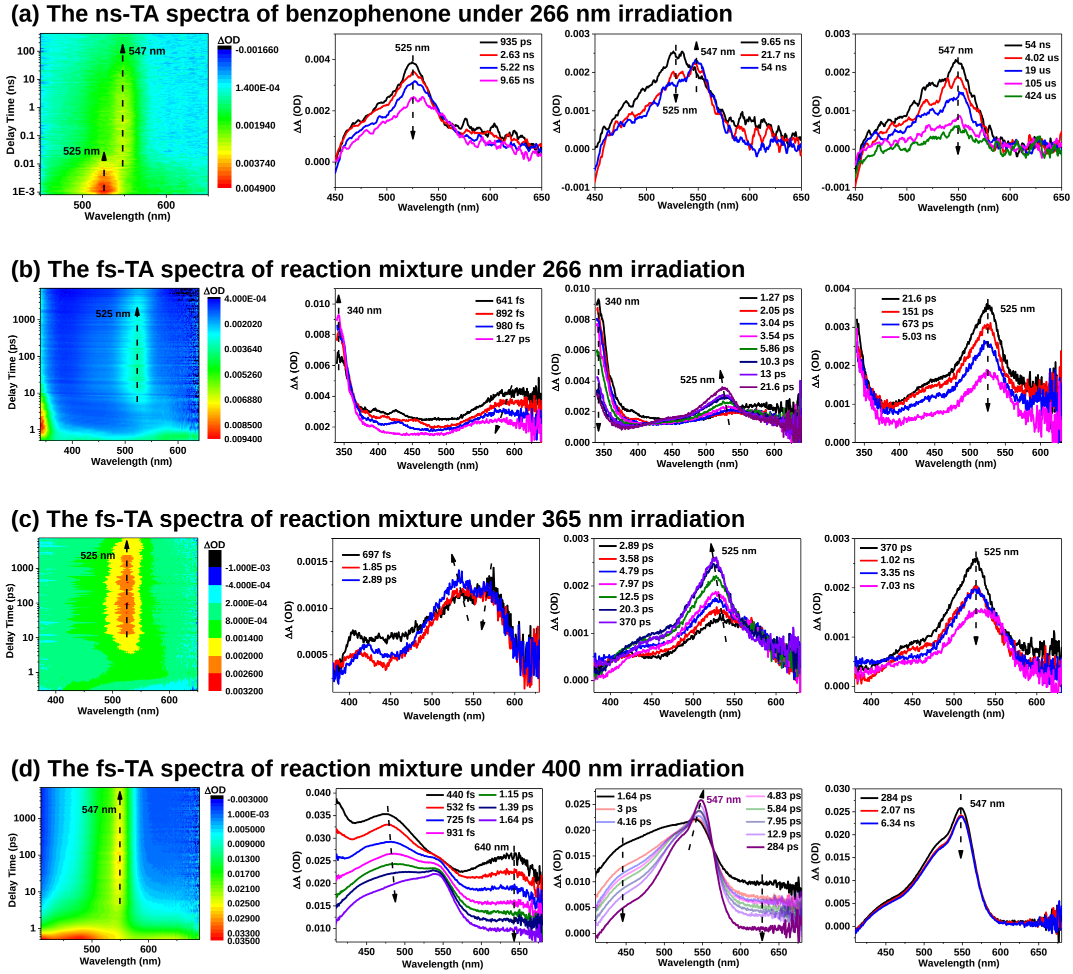


Figure S2. The transient spectra of mechanism study of reductive hydrogeneration of aromatic ketone to aromatic pinacol. (a) The ns-TA spectra of benzophenone in THF/isopropanol under 266 nm irradiation; (b) The fs-TA spectra of benzophenone, B_2cat_2 and 4-cyanopyridine in THF/H_2O under 266 nm irradiation; (c) The fs-TA spectra of benzophenone, B_2cat_2 and 4-cyanopyridine in THF/H_2O solution under 365 nm irradiation; (d) The fs-TA spectra of benzophenone, B_2cat_2 and 4-cyanopyridine in THF/H_2O under 400 nm irradiation.

Computational Results

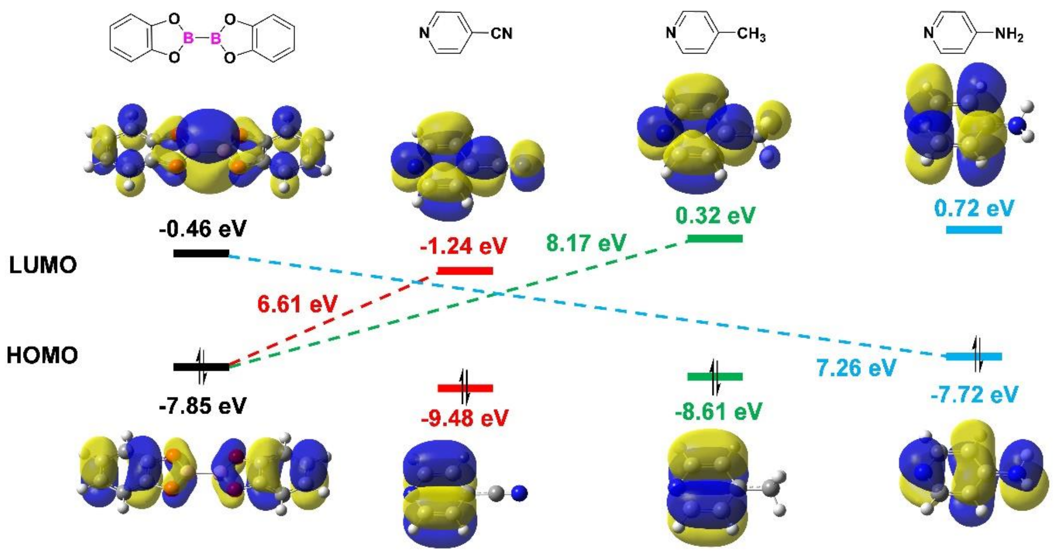
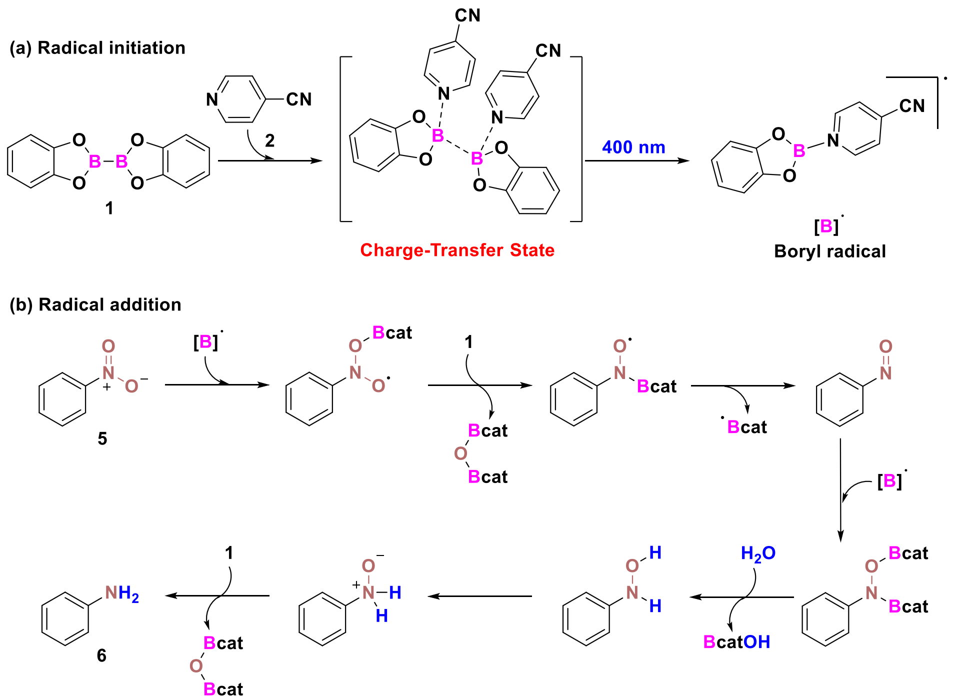


Figure S3. Frontier molecular orbital analysis for B2cat2, 4-cyanopyridine Energy profile for mechanism of reductive deoxygenation of sulfoxides to sulfides (solvent correction with M062x/6-311++G(d,p) in THF based on optimized geometry with M062x/6-311G(d)).



Scheme S1. Proposed mechanism of reductive hydrogeneration of nitroaromatic compounds to aromatic arylamines.

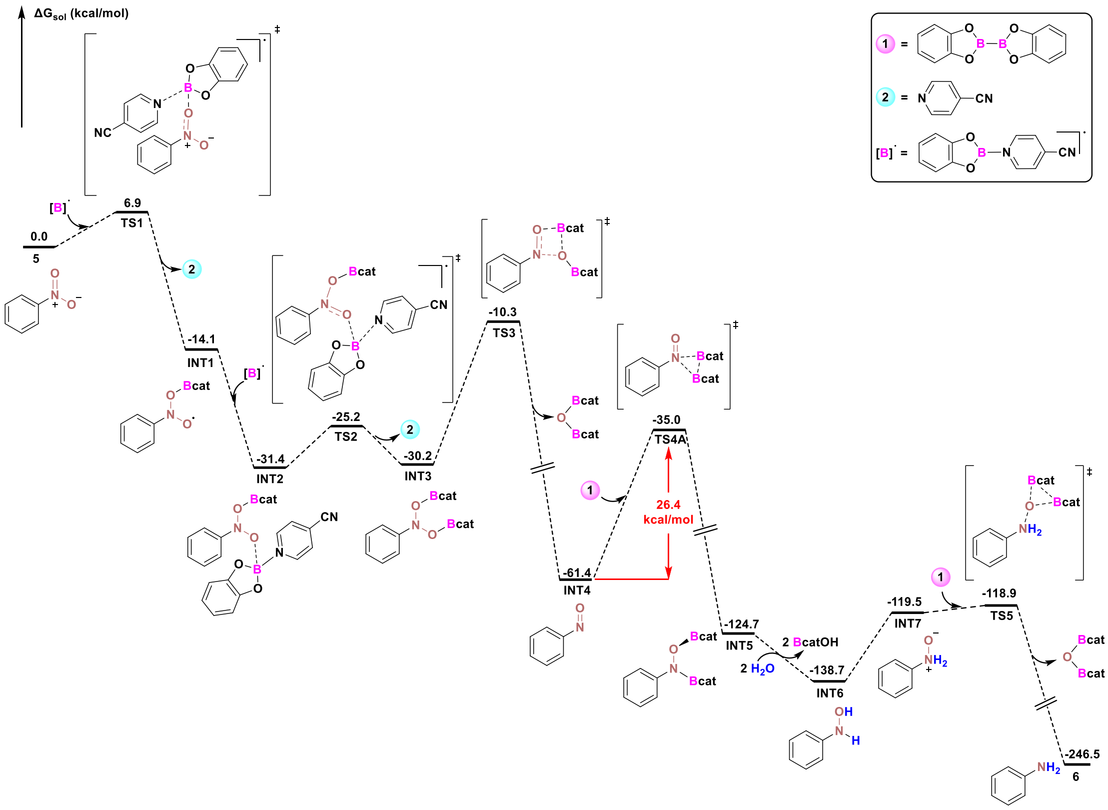


Figure S4. Energy profile for unfavorable pathway of reductive hydrogeneration of nitroaromatic compounds to aromatic arylamines (solvent correction with M062x/6-311++G(d,p) in THF based on optimized geometry with M062x/6-311G(d)).

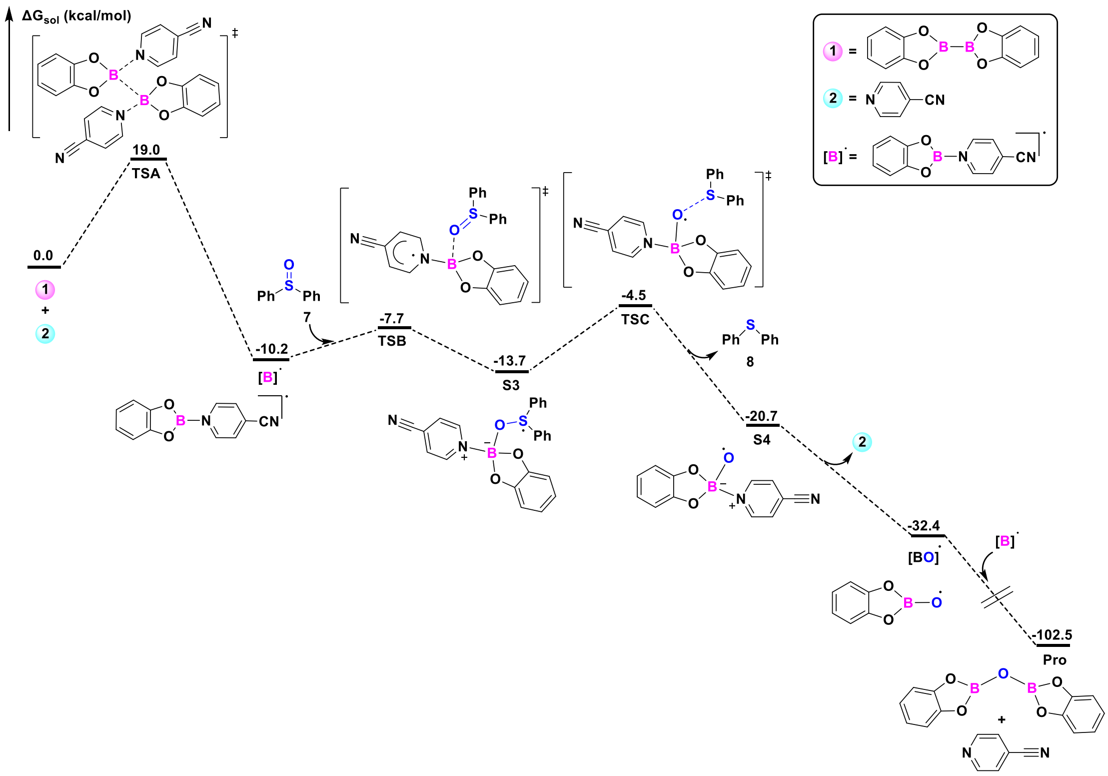
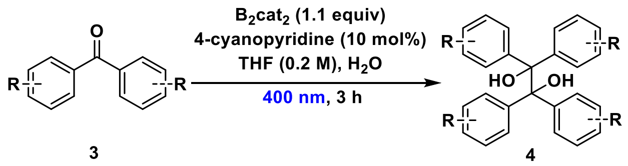


Figure S5. Energy profile for reductive deoxygenation of sulfoxides to sulfides by boryl radical (solvent correction with M062x/6-311++G(d,p) in THF based on optimized geometry with M062x/6-311G(d)).

3. Experimental procedure

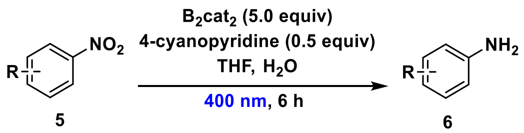
General Procedures

1) General Procedure 1 (GP1): Conversion of aromatic Ketone to aromatic Pinacol



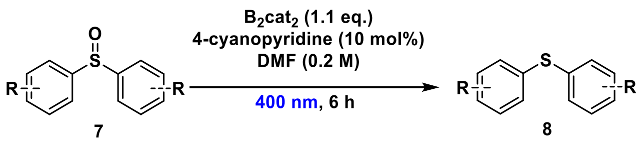
Aromatic ketone (1.0 eq., 0.4 mmol), B_2cat_2 (104 mg, 1.1eq., 0.44 mmol) and 4-cyanopyridine (4 mg, 10 mol%) are carefully weighed into a flame-dried 15 mL tube containing a small magnetic stirrer bar. THF (2.0 mL, 0.2 M) and H_2O (0.1 mL) are added in the glovebox. The tube is tightly sealed and stirred under blue LED irradiation for 3 hours. Irradiation is stopped and the reaction mixture is extracted with ethyl acetate (30 + 15 mL), washed with brine (30 mL), dried over $MgSO_4$, and concentrated under reduced pressure. The crude product is purified by flash column chromatography on silica gel (hexane: ethyl acetate = 30:1 ~ 10:1).

2) General Procedure 2 (GP2): Reduction of nitroaromatic compound to arylamines



Nitroaromatic compound (1.0 eq., 0.2 mmol), B_2cat_2 (237.4 mg, 5.0 eq., 1 mmol) and 4-cyanopyridine (10.4 mg, 0.5 eq., 0.1 mmol) are carefully weighed into a flame-dried 15mL tube containing a small magnetic stirrer bar. THF (3.0 mL) and H_2O (0.2 mL) are added in the glovebox. The tube is tightly sealed and stirred under blue LED irradiation for 0.5 hour. Irradiation is stopped and the reaction mixture is extracted with ethyl acetate (30 + 15 mL), washed with brine (30 mL), dried over MgSO4, and concentrated under reduced pressure. The crude product is purified by flash column chromatography on silica gel (hexane: ethyl acetate = 30:1~8:1).

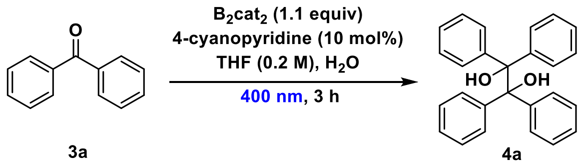
3) General Procedure 3 (GP3): Reductive deoxygenation of sulfoxides to sulfides



Sulfoxides (1.0 eq., 0.4 mmol), B_2cat_2 (104 mg, 1.1 eq., 4.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) are carefully weighed into a flame-dried 15mL tube containing a small magnetic stirrer bar. DMF (2.0 mL) are added in the glovebox. The tube is tightly sealed and stirred under blue LED irradiation for 6 hours. Irradiation is stopped and the reaction mixture is extracted with ethyl acetate (30 + 15 mL), washed with brine (30 mL), dried over MgSO4, and concentrated under reduced pressure. The crude product is purified by flash column chromatography on silica gel (hexane: ethyl acetate = 100:1).

Generation of aromatic pinacol

(1) Conversion of aromatic ketone **3a** to aromatic pinacol **4a**.

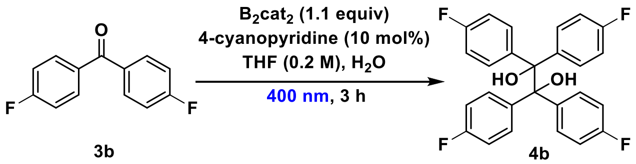


According to GP1, the reaction is carried out with **3a** (73 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.44 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2M), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **4a** (65 mg, 90% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.32-7.30 (d, 8H), 7.20 (s, 12H), 3.06 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 144.17, 128.60, 127.30, 126.95, 83.02.

(2) Conversion of Aromatic ketone **3b** to aromatic pinacol **4b**.

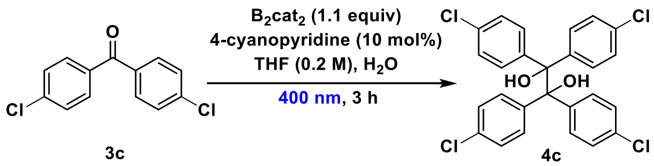


According to GP1, the reaction is carried out with **3b** (88 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 8:1) give the desired product **4b** (81 mg, 94% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.26-7.22 (m, 8H), 6.90-6.85 (t, 8H), 2.86 (s, 1.86H).

^{13}C NMR (125 MHz, $CDCl_3$) d 163.04, 160.57, 139.66, 139.62, 130.32, 130.25, 114.42, 114.21.

(3) Conversion of aromatic ketone **3c** to aromatic pinacol **4c**.

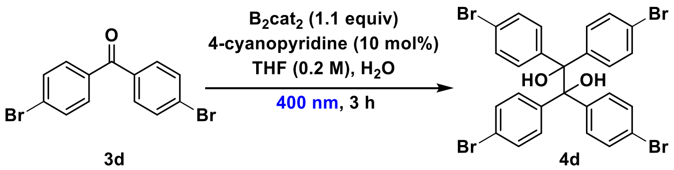


According to GP1, the reaction is carried out with **3c** (100 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4c** (82 mg, 80% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.23-7.21 (d, 8H), 7.18-7.16 (d, 8H), 2.89 (s, 1.75H).

^{13}C NMR (125 MHz, $CDCl_3$) d 142.01, 133.49, 129.86, 127.74, 82.49.

(4) Conversion of aromatic ketone **3d** to aromatic pinacol **4d**.

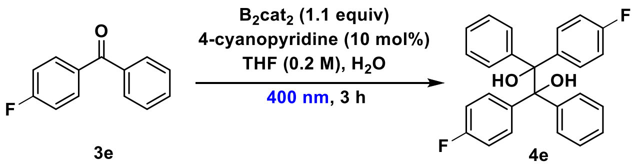


According to GP1, the reaction is carried out with **3d** (136 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4d** (110 mg, 81% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.33-7.31 (d, 7.98H), 7.16-7.14 (d, 8.01H), 2.88 (s, 1.80H).

^{13}C NMR (125 MHz, $CDCl_3$) d 142.43, 130.72, 130.18, 121.82, 82.51.

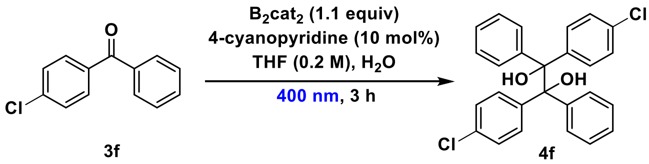
(5) Conversion of aromatic ketone **3e** to aromatic pinacol **4e**.



According to GP1, the reaction is carried out with **3e** (80.4 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.44 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **4e** (70 mg, 85% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.43-7.39 (m, 2.12H), 7.31-7.28 (m, 4.06H), 7.24-7.19 (m, 6H), 7.17-7.15 (m, 2.02H), 6.90-6.85 (m, 3.95 H), 2.99-2.97 (d, 1.84H).

(6) Conversion of aromatic ketone **3f** to aromatic pinacol **4f**.

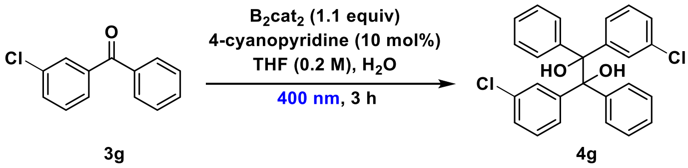


According to GP1, the reaction is carried out with **3f** (87 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4f** (70 mg, 79% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.43-7.41 (d, 1.92H), 7.27-7.20 (dd, 10H), 7.17-7.14 (m, 4.1H) 7.10-7.08 (d, 1.8 H) 2.98-2.96 (d, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 143.50, 143.19, 142.70, 133.01, 132.82, 130.13, 130.09, 128.34, 128.27, 127.62, 127.56, 127.51, 127.41, 127.37, 82.74, 82.70.

(7) Conversion of aromatic ketone **3g** to aromatic pinacol **4g**.

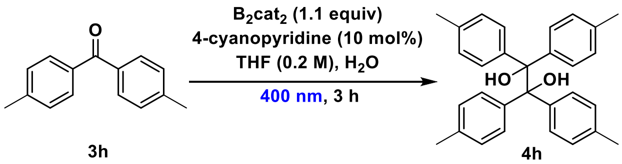


According to GP1, the reaction is carried out with **3g** (87 mg, 0.40 mmol), B_2cat_2 (94 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O is dropped into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4g** (72 mg, 80% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.50-7.49 (t, 1.04H), 7.44-7.42 (d, 1.12H), 7.35 (t, 0.9H), 7.31-7.28 (m, 2.94H), 7.24-7.23 (m, 4.90H), 7.21-7.20 (m, 2.06H), 7.17-7.13 (m, 5.16H), 3.02-3.00 (d, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 146.20, 146.15, 143.14, 142.93, 133.54, 133.49, 128.90, 128.85, 128.48, 128.43, 128.31, 127.67, 127.64, 127.52, 127.27, 127.17, 126.88, 126.83, 82.83, 82.78

(8) Conversion of aromatic ketone **3h** to aromatic pinacol **4h**.

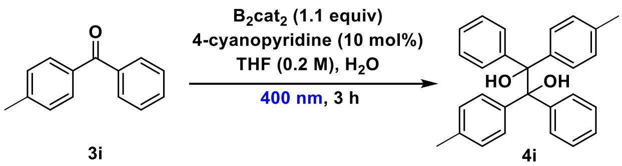


According to GP1, the reaction is carried out with **3h** (84 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4h** (68 mg, 80% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.18-7.16 (d, 8H), 7.00-6.98 (d, 7.98H), 2.98 (s, 1.75H), 2.30 (11.96 H).

^{13}C NMR (125 MHz, $CDCl_3$) d 141.53, 136.30, 128.48, 127.96, 82.84, 20.97.

(9) Conversion of aromatic ketone **3i** to aromatic pinacol **4i**

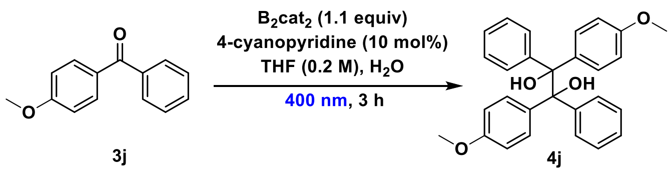


According to GP1, the reaction is carried out with **3i** (79 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4i** (72 mg, 92% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.45-7.40 (m, 4H), 7.26-7.22 (m, 10H), 7.08-7.04 (t, 4H), 3.12 (s, 1.81H), 2.37-2.36 (d, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) d 144.59, 144.57, 141.39, 141.34, 136.62, 136.53, 128.73, 128.68, 128.64, 128.59, 128.13, 128.10, 127.30, 127.28, 126.88, 126.81, 83.04, 21.16.

(10) Conversion of aromatic ketone **3j** to aromatic pinacol **4j**.

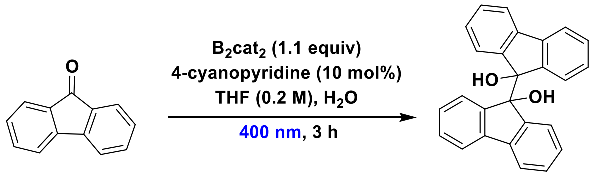


According to GP1, the reaction is carried out with **3j** (85 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4j** (65 mg, 75% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.35-7.30 (m, 4H), 7.22-7.18 (m, 10H), 6.76-6.70 (t, 4H), 3.78-3.77 (d, 6.10H), 2.99 (s, 1.87H).

^{13}C NMR (125 MHz, $CDCl_3$) d 158.38, 158.32, 144.54, 136.58, 129.92, 129.85, 128.61, 128.54, 127.25, 126.83, 126.77, 112.57, 82.59, 55.13, 55.12.

(11) Conversion of aromatic ketone **3k** to aromatic pinacol **4k**.



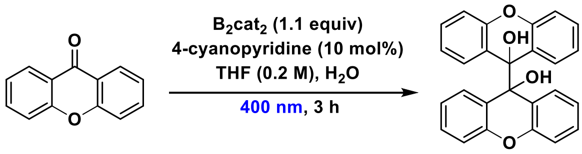
3k 4k

According to GP1, the reaction is carried out with **3k** (72 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4k** (56 mg, 77% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.39-7.07 (m, 15.93H), 3.22 (s, 2.0H).

^{13}C NMR (125 MHz, $CDCl_3$) d 145.19, 140.63, 129.15, 127.09, 125.21, 119.27, 86.48.

(12) Conversion of aromatic ketone **3l** to aromatic pinacol **4l**.



3l 4l

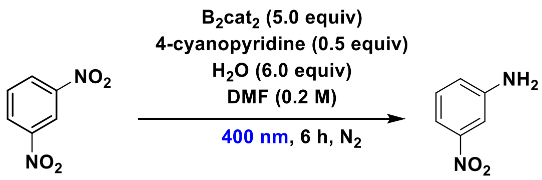
According to GP1, the reaction is carried out with **3l** (79 mg, 0.40 mmol), B_2cat_2 (104 mg, 0.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in THF (2 mL, 0.2 M) and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **4l** (64 mg, 81% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.30-7.26 (m, 4.03H), 7.12-7.10 (d, 4.02H), 7.00-6.96 (t, 4.10H), 6.85-6.83 (d, 4.0H), 3.33 (s, 1.81H).

^{13}C NMR (125 MHz, $CDCl_3$) d 151.90, 129.23, 127.40, 122.71, 122.10, 115.22, 75.43.

Optimization of the reaction condition.

Table S1. Optimization of the reaction condition of reductive hydrogeneration of nitrobenzene. [a]



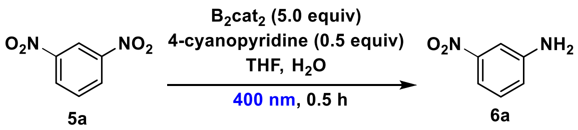
Entry	Variation from standard condition	yield (%)[b]
1	none	80
2	$B(OH)_3$	N.D.
3	B_2pin_2	Trace
4	1.0 eq B_2cat_2 and 0.1 eq 4-cyanopyridine	20
5	2.5 eq B_2cat_2 and 0.25 eq 4-cyanopyridine	60
6	1.0 eq B_2cat_2 and 1.0 eq 4-cyanopyridine	Trace
7 [c]	No light	50
8	no B_2cat_2	N.D.
9	no 4-cyanopyridine	20
10	no H_2O	65

11	blue LED (450 nm)	N.D.
12	UV (365 nm)	70
13	MeOH	65
14	DCM	45
15	ACN	70
16	THF	95
17	THF, 30 min irradiation	94

[a] Reaction conditions: 1 (0.2 mmol, 1 equiv), B_2cat_2 (1 mmol, 5 eqiuv), 4-cyanopyridine (0.5 equiv), DMF (1 mL), H_2O (0.1 mL), 6 h, r. t., blue LEDs (400 nm). [b] The yield was determined by HPLC. [c] no light, 80 °C.

Generation of arylamine

(1) Conversion of nitroaromatic compound **5a** to arylamine **6a**.

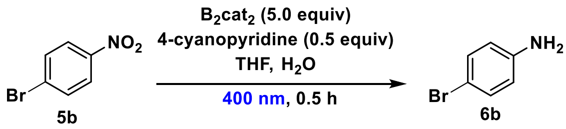


According to GP2, the reaction is carried out with **5a** (33.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6a** (26.2 mg, 95% yield) as a yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.60-7.57 (dd, 0.91H), 7.51-7.49 (t, 0.90H), 7.31-7.26 (t, 0.94H), 6.97-6.95 (dd, 0.94H), 4.04 (s, 1.92H).

^{13}C NMR (125 MHz, $CDCl_3$) d 149.26, 147.47, 129.92, 120.63 113.13, 109.02.

(2) Conversion of nitroaromatic compound **5b** to arylamine **6b**.

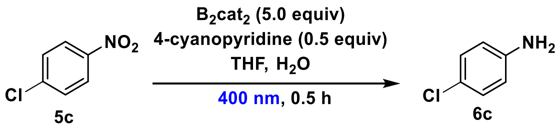


According to GP2, the reaction is carried out with **5b** (40.4 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6b** (33.1 mg, 96% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.27-7.23 (m, 2.02H), 6.60-6.59 (m, 2.04H), 3.68 (s, 1.89H).

^{13}C NMR (125 MHz, $CDCl_3$) d 145.41, 132.02, 116.0, 110.22.

Conversion of nitroaromatic compound 5c to arylamine 6c.

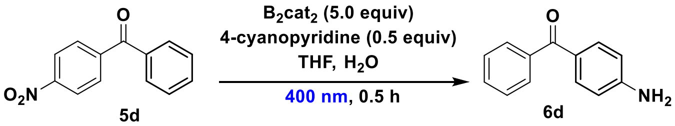


According to GP2, the reaction is carried out with **5c** (31.4 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6c** (24.5 mg, 96% yield) as a white powder.

^{1}H NMR (400 MHz, CDCl$_3$) d 7.13-7.10 (d, 1.98H), 6.64-6.61 (d, 2.01H), 3.67 (s, 2H).

^{13}C NMR (125 MHz, CDCl$_3$) d 144.94, 129.12, 123.18, 116.22.

Conversion of nitroaromatic compound **5d** to arylamine **6d**.

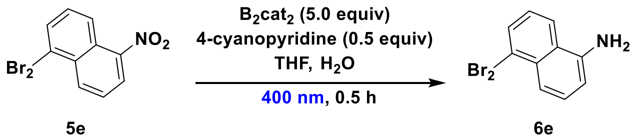


According to GP2, the reaction is carried out with **5d** (45.4 mg, 0.2 mmol), B$_2$cat$_2$ (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6d** (35.5 mg, 90% yield) as a white powder.

^{1}H NMR (400 MHz, CDCl$_3$) d 7.75-7.73 (d, 3.92H), 7.56-7.53 (t, 1.04H), 7.49-7.45 (t, 1.97H), 6.70-6.68 (d, 2H), 4.21 (s, 1.70H).

^{13}C NMR (125 MHz, CDCl$_3$) d 195.44, 151.05, 138.86, 132.98, 131.45, 129.54, 128.09, 127.34, 113.65

Conversion of nitroaromatic compound **5e** to arylamine **6e**.

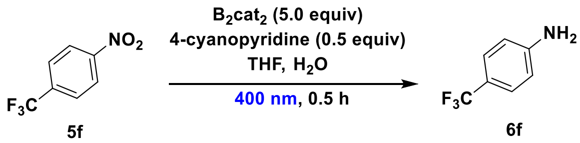


According to GP2, the reaction is carried out with **5e** (50.4 mg, 0.2 mmol), B$_2$cat$_2$ (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6e** (36.4 mg, 82% yield) as a dark brown powder.

^{1}H NMR (400 MHz, CDCl$_3$) d 7.83-7.78 (q, 1.91H), 7.74-7.72 (d, 0.91H), 7.43-7.39 (t, 0.96H), 7.31-7.28 (t, 1.29H), 6.87-6.85 (d, 0.95H), 4.20 (s, 2H).

^{13}C NMR (125 MHz, CDCl$_3$) d 142.42, 132.94, 130.13, 127.75, 124.89, 124.77, 123.67, 120.74, 118.18, 110.70.

Conversion of nitroaromatic compound **5f** to arylamine **6f**.

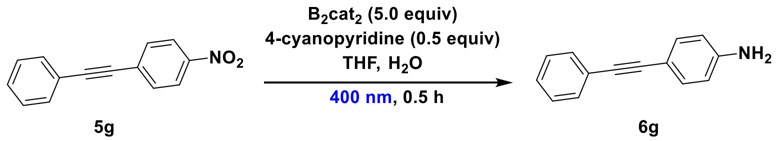


According to GP2, the reaction is carried out with **5f** (38.2 mg, 0.2 mmol), B$_2$cat$_2$ (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6f** (30.6 mg, 95% yield) as a pure yellow oil.

^{1}H NMR (400 MHz, CDCl$_3$) d 7.07-7.05 (d, 1.90H), 6.68-6.66 (d, 1.92H), 3.83 (s, 2H).

^{13}C NMR (125 MHz, CDCl$_3$) d 146.45, 141.61, 122.19, 120.38, 117.19, 115.49.

Conversion of nitroaromatic compound **5g** to arylamine **6g**.

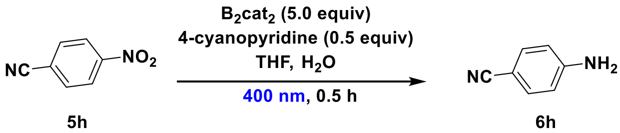


According to GP2, the reaction is carried out with **5g** (44.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6g** (36.7 mg, 94% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.55-7.52 (dd, 1.98H), 7.39-7.34 (m, 5H), 6.67-6.65 (d, 2.02H), 3.84 (s, 1.97H).

^{13}C NMR (125 MHz, $CDCl_3$) d 146.69, 132.99, 131.38, 128.31, 127.70, 123.92, 114.778, 112.60, 90.17, 87.36.

Conversion of nitroaromatic compound **5h** to arylamine **6h**.

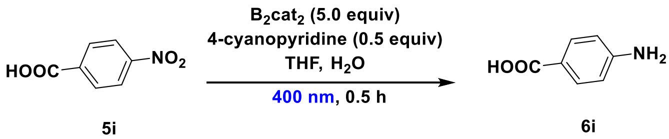


According to GP2, the reaction is carried out with **5h** (44.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6h** (36.7 mg, 94% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.43-7.41 (d, 2H), 6.66-6.64 (d, 2.05H), 4.16 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 150.37, 132.83, 120.11, 114.45, 100.27.

Conversion of nitroaromatic compound **5i** to arylamine **6i**.

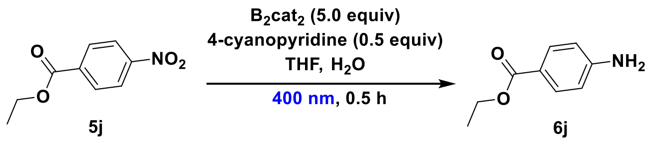


According to GP2, the reaction is carried out with **5i** (33.4 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6i** (26.3 mg, 96% yield) as a white powder.

^{1}H NMR (400 MHz, DMSO-d^6) d 11.97 (s, 0.92H), 7.62-7.59 (d, 1.98H), 6.54-6.52 (d, 2H), 5.88 (s, 1.94H).

^{13}C NMR (125 MHz, DMSO-d^6) d 167.94, 153.59, 131.66, 117.39, 113.02.

Conversion of nitroaromatic compound **5j** to arylamine **6j**.

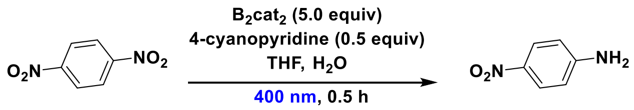


According to GP2, the reaction is carried out with **5j** (39.0 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6j** (30.4 mg, 92% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.88-7.86 (d, 1.82H), 6.66-6.64 (d, 1.89H), 4.35-4.30 (q, 2H), 4.09 (s, 1.89H), 1.39-1.36 (t, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) d 166.73, 150.75, 131.55, 120.10, 113.78, 60.31, 14.42.

Conversion of nitroaromatic compound **5k** to arylamine **6k**.



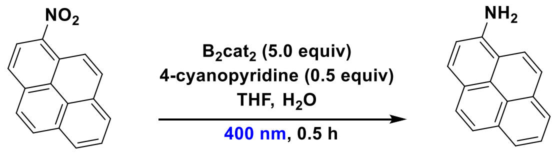
5k 6k

According to GP2, the reaction is carried out with **5k** (33.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6k** (27.0 mg, 96% yield) as a yellow powder.

^{1}H NMR (400 MHz, DMSO-d^{6}) d 7.93-7.91 (d, 1.99H), 6.72 (s, 2H), 6.58-6.56 (d, 2.11H).

^{13}C NMR (125 MHz, DMSO-d^{6}) d 156.15, 136.10, 126.83, 112.82.

Conversion of nitroaromatic compound **5l** to arylamine **6l**.



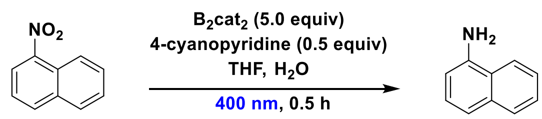
5l 6l

According to GP2, the reaction is carried out with **5l** (49.4 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 30:1) give the desired product **6l** (35.6 mg, 82% yield) as a yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 8.10-8.06 (t, 2.02H), 8.02-8.00 (d, 1.99H), 7.95-7.93 (m, 2.96H), 7.86-7.84 (d, 0.99H), 7.40-7.38 (d, 0.98H), 4.49 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 140.91, 132.22, 131.67, 127.63, 126.04, 125.99, 125.51, 124.30, 124.12, 123.75, 123.55, 120.16, 116.88, 113.97.

Conversion of nitroaromatic compound **5m** to arylamine **6m**.



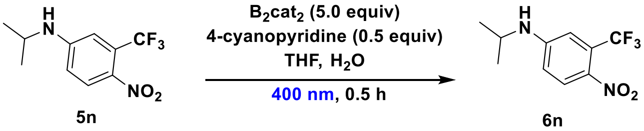
5m 6m

According to GP2, the reaction is carried out with **5m** (34.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 20:1) give the desired product **6m** (25.7 mg, 89% yield) as a white powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.87-7.83 (m, 1.99H), 7.52-7.46 (m, 1.96H), 7.35-7.31 (m, 1.97H), 6.83-6.80 (dd, 0.96H), 4.16 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) d 142.08, 134.42, 128.58, 126.36, 125.8, 124.88, 123.68, 120.81, 119.01, 109.72

Conversion of nitroaromatic compound **5n** to arylamine **6n**.



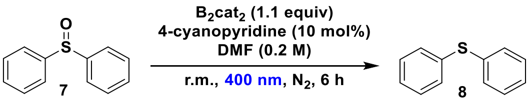
According to GP2, the reaction is carried out with **5n** (49.6 mg, 0.2 mmol), B_2cat_2 (237.4 mg, 1 mmol) and 4-cyanopyridine (10.4 mg, 0.1 mmol) in THF (3 mL), and 0.1 mL H_2O are added into the tube. Purification by flash column chromatography (hexane: ethyl acetate = 12:1) give the desired product **6n** (32.7 mg, 75% yield) as a pare yellow powder.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.57-7.56 (d, 0.98H), 7.49-7.46 (dd, 1.01H), 7.26 (s, 0.94H), 6.72-6.89 (d, 1H), 4.09 (s, 1.93H), 2.51-2.47 (m, 1H), 1.25-1.24 (d, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) d 175.40, 141.23, 128.61, 125.92, 123.20, 119.02, 118.97, 117.68, 36.34, 19.57.

Optimization of the reaction conditions for generation of sulfides.

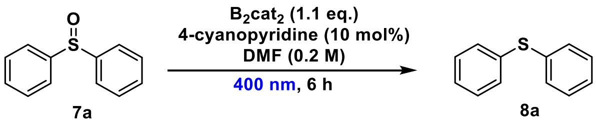
Table S2. Optimization of the reaction condition of reductive hydrogeneration of sulfoxide. [a]



Entry	Variation from standard condition	yield (%) [b]
1	None	90
2	no 4-cyanopyridine	70
3	no 4-cyanopyridine,12h	88
4	DCM (0.2 M)	90
5	THF (0.2 M)	80
6	MeOH (0.2 M)	82

[a] Reaction conditions: 7 (0.2 mmol, 1 equiv), B_2cat_2 (0.22 mmol, 1.2 eqiuv), 4-cyanopyridine (0.11 mmol), DMF (1 mL), 6 h, r. t., blue LEDs (400 nm). [b] The yield was determined by HPLC. [c]

Conversion of sulfoxide **7a** to sulfide **8a**.

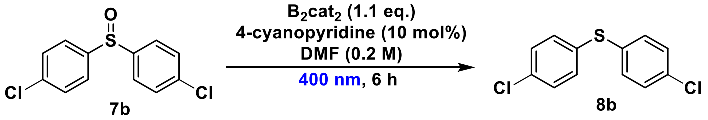


According to GP3, the reaction is carried out with **7a** (80.5 mg, 0.4 mmol), B_2cat_2 (104 mg, 4.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in DMF (2 mL). Purification by flash column chromatography (hexane: ethyl acetate = 100:1) give the desired product **8a** (66.9 mg, 90% yield) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.38-7.25 (m, 10H).

^{13}C NMR (125 MHz, $CDCl_3$) d 135.79, 131.05, 129.20, 127.05.

Conversion of sulfoxide **7b** to sulfide **8b**.

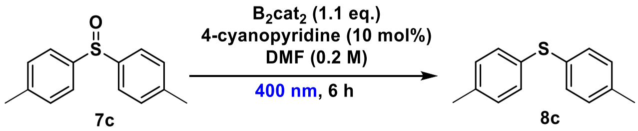


According to GP3, the reaction is carried out with **7a** (108.4 mg, 0.4 mmol), B_2cat_2 (104 mg, 4.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in DMF (2 mL). Purification by flash column chromatography (hexane: ethyl acetate = 100:1) give the desired product **8a** (81.6 mg, 80% yield) as white solid.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.31-7.25 (m, 8H).

^{13}C NMR (125 MHz, $CDCl_3$) d 133.94, 133.48, 132.31, 129.50.

Conversion of sulfoxide **7c** to sulfide **8c**.



According to GP3, the reaction is carried out with **7a** (92.2 mg, 0.4 mmol), B_2cat_2 (104 mg, 4.4 mmol) and 4-cyanopyridine (4 mg, 10 mol%) in DMF (2 mL). Purification by flash column chromatography (hexane: ethyl acetate = 100:1) give the desired product **8c** (76.2 mg, 89% yield) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) d 7.27-7.25 (d, 4.07H), 7.14-7.12 (d, 3.81H), 2.35 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$) d 136.91, 132.67, 131.07, 129.92, 21.08.

5. Computational Results

Computational Details

All the calculations were carried out via density functional theory (DFT) calculation using Gaussian 16[1] with the M062x[2] functional. Geometric structures of all species in this work were optimized in gas phase. In addition, free energy corrections were considered at a concentration of 1 M and a temperature of 298.15 K. Frequency calculation were performed to determine all the stationary points (no imaginary frequency) and transition state structures (only one imaginary frequency). The 6-311G(d)[3] basis set was used for all atoms. In addition, the intrinsic reaction coordinate (IRC) calculation[4] were applied to confirm the connection of each transition state to its corresponding appropriate intermediates, reactants, or products. Base on the gas phase optimized geometries, solvent effects were computed by using the SMD[5] model at the same level of theory while 6-311++G(d,p) basis set for all atoms. Tetrahydrofuran (ε =7.52) was used as the solvent, and Bondi atomic radii[6] was used for the SMD calculation. All 3D molecular structures were drawn by using the CYLview (Version) program[7].

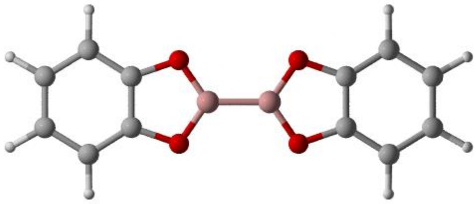
Table S2. The gas phase relative electronic energies (ΔEgas), gas phase relative free energies (ΔGgas) and solvation corrected relative electronic energies (ΔEsol) in kcal/mol calculated for species involved in **Figure S4**.

Species	ΔEgas	ΔGgas	ΔEsol
5	0.0	0.0	0.0

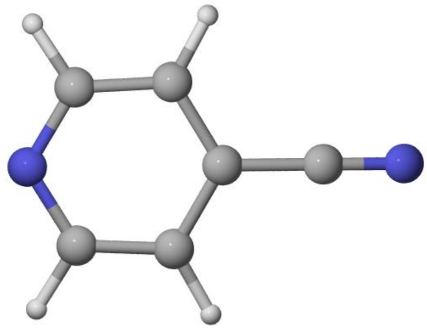
TS1	-12.8	0.4	-6.3
INT1	-16.5	-18.0	-12.6
INT2	-51.5	-33.3	-49.6
TS2	-47.4	-30.3	-42.2
INT3	-34.6	-32.4	-32.4
TS3	-11.0	-10.3	-10.9
INT4	-47.3	-60.4	-48.3
TS4A	-36.2	-35.1	-36.1
INT5	-130.7	-128.2	-127.2
INT6	-151.4	-149.5	-140.6
INT7	-125.5	-123.4	-121.6
TS5	-144.2	-128.4	-134.6
6	-262.6	-260.5	-249.1

Table S3. The gas phase relative electronic energies (ΔEgas), gas phase relative free energies (ΔGgas) and solvation corrected relative electronic energies (ΔEsol) in kcal/mol calculated for species involved in **Figure 3**.

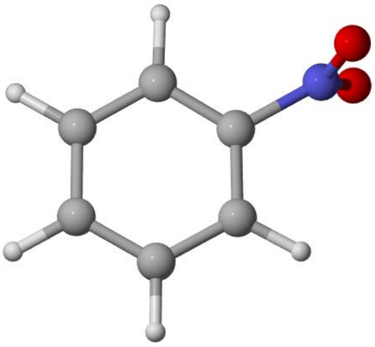
Species	ΔEgas	ΔGgas	ΔEsol
5	0.0	0.0	0.0
TS1	-12.8	0.4	-6.3
INT1	-16.5	-18.0	-12.6
INT2	-51.5	-33.3	-49.6
TS2	-47.4	-30.3	-42.2
INT3	-34.6	-32.4	-32.4
TS3	-11.0	-10.3	-10.9
INT4	-47.3	-60.4	-48.3
TS4B	-57.6	-56.9	-55.5
INT4-B	-64.3	-77.0	-64.7
TS4-B-oss	-80.3	-77.3	-75.9
TS4-B-ts	-81.2	-78.2	-76.5
INT5	-105.3	-116.2	-103.5
INT6	-126.0	-137.6	-116.9
INT7	-100.1	-111.5	-97.9
TS5	-118.8	-116.5	-111.0
6	-237.2	-248.6	-225.4



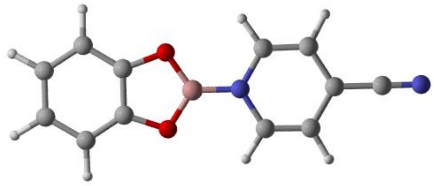
1



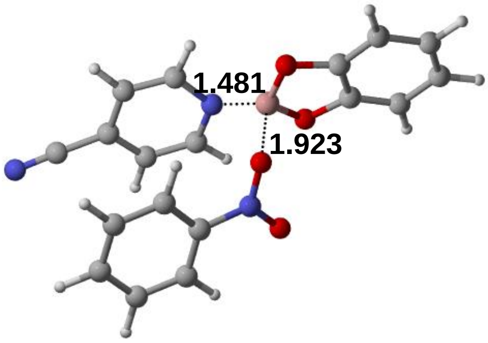
2



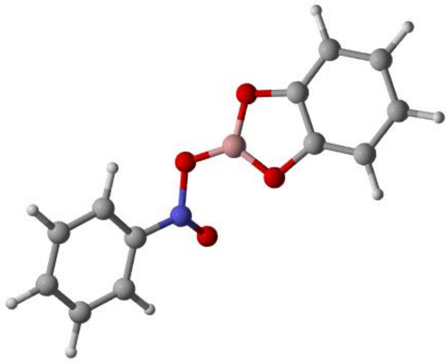
5



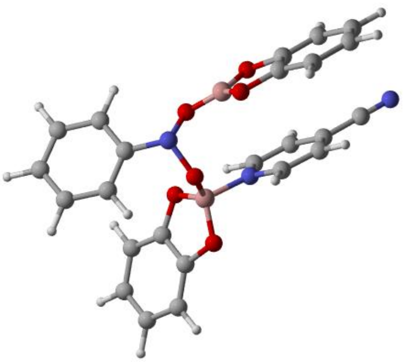
[B]$^{\cdot}$



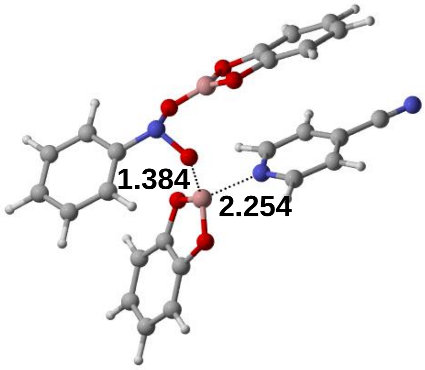
TS1



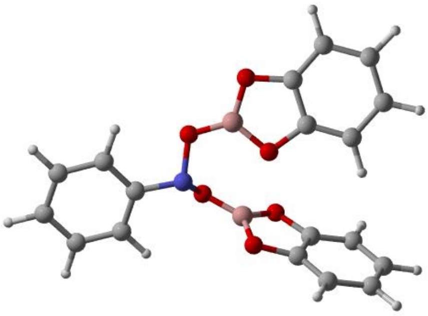
INT1



INT2



TS2



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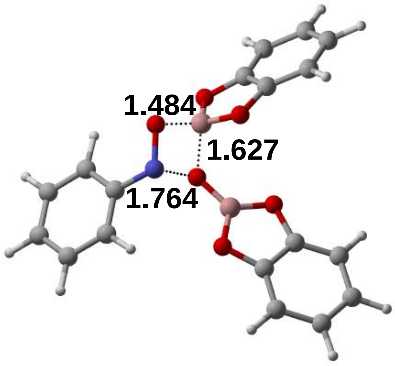

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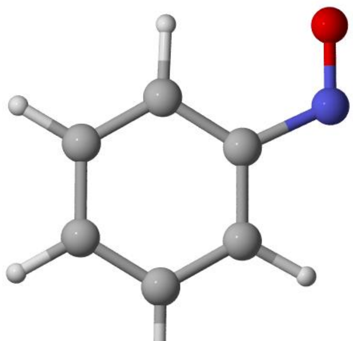

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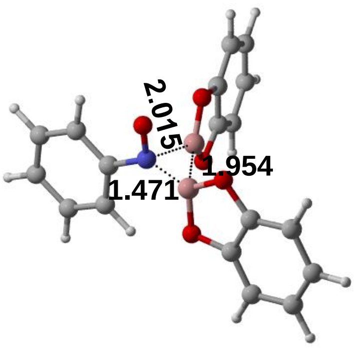

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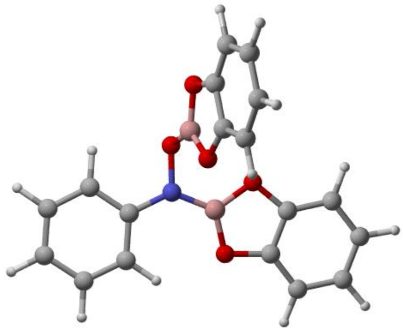

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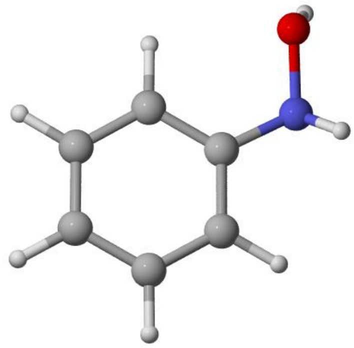

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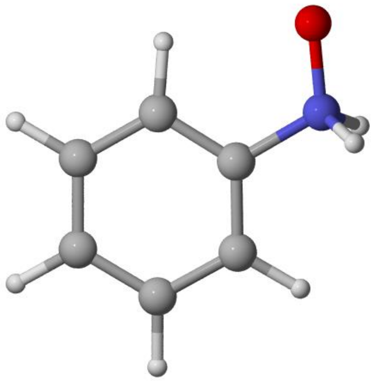

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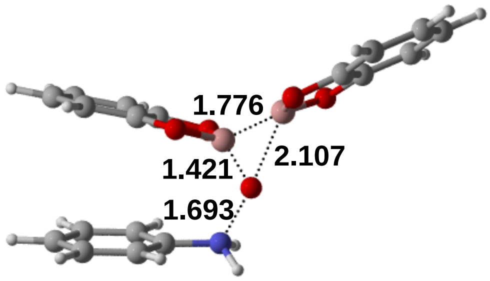

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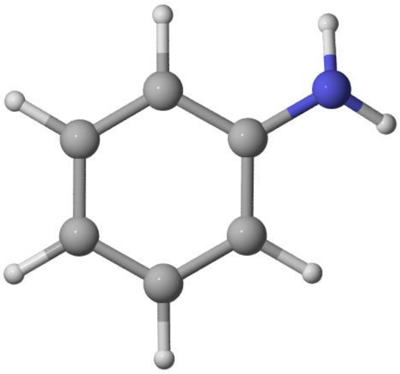

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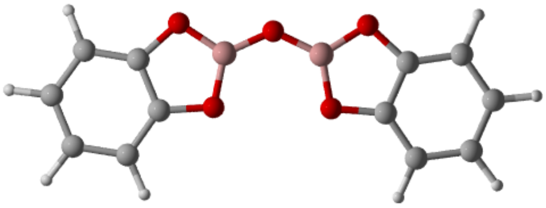
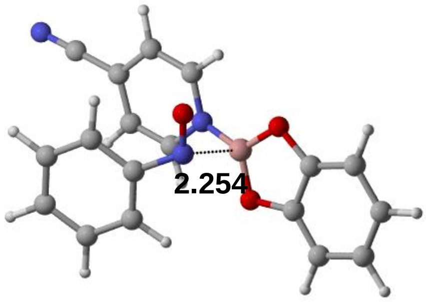
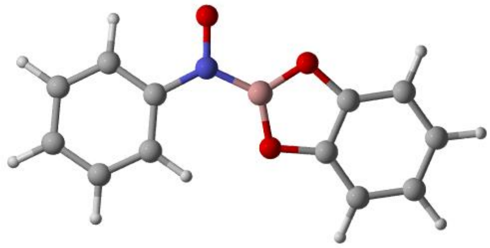


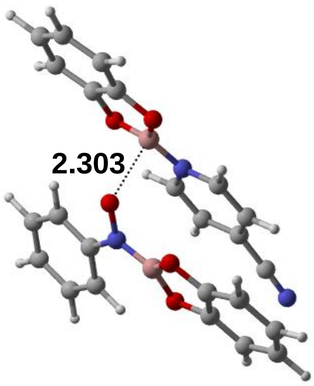
Bcat-O-Bcat



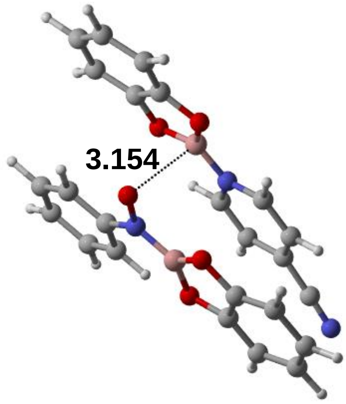
TS4B



INT4-B



TS4-B-oss



TS4-B-ts

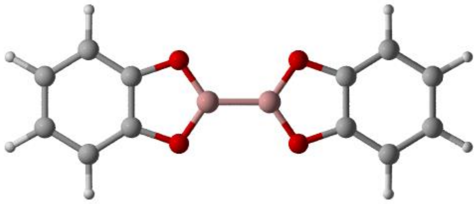
Figure S6. Optimized structures of all species involved in Figure S4 and Figure 3 with M062x/6-311G(d). 3D geometric structures of relative transition states are given in Angstrom (Å).

Table S4. The gas phase relative electronic energies (ΔEgas), gas phase relative free energies (ΔGgas) and solvation corrected relative electronic energies (ΔEsol) in kcal/mol calculated for species involved in **Figure S5**.

Species	**ΔEgas**	**ΔGgas**	**ΔEsol**
1 + 2	0	0	0
TSA	-19.1	12.0	-12.0
[B]·	-25.4	-11.9	-23.7
TSB	-10.0	16.9	-34.6
S3	-13.3	14.1	-41.2
TSC	-6.2	20.6	-31.3
S4	-30.3	-18.2	-32.7
[BO]·	-20.4	-22.9	-30.0
Pro	-103.1	-103.6	-102.0

Table S5. The gas phase relative electronic energies (ΔEgas), gas phase relative free energies (ΔGgas) and solvation corrected relative electronic energies (ΔEsol) in kcal/mol calculated for species involved in **Figure 4**.

Species	ΔEgas	ΔGgas	ΔEsol
1	0	0	0
TSB-1	17.0	30.5	-10.0
S3-1	14.9	28.8	-12.9
TSC-1	32.5	46.3	6.5
BOB	-103.1	-103.6	-102.0



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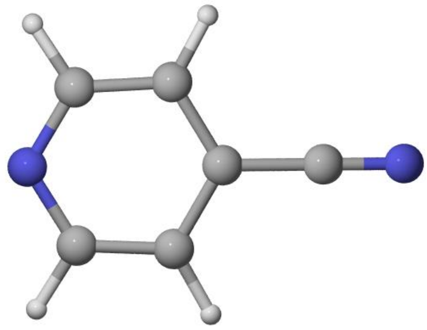

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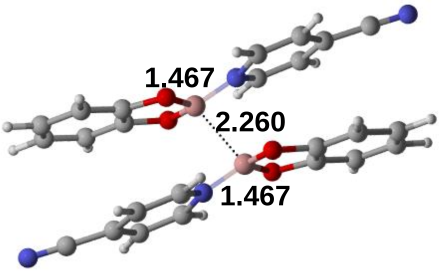
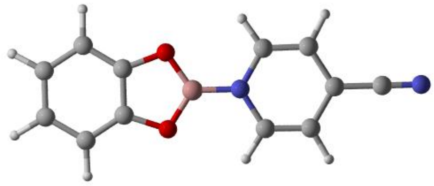
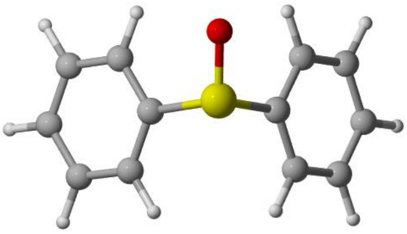


TSA



[B]$^{\cdot}$



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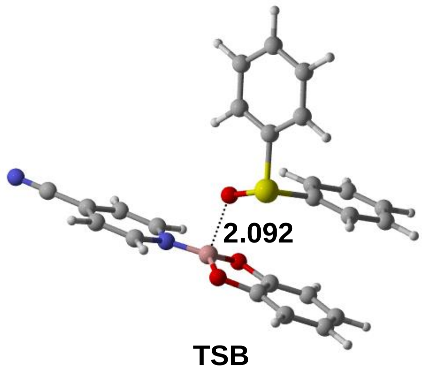
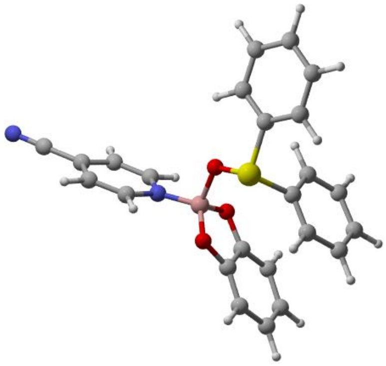
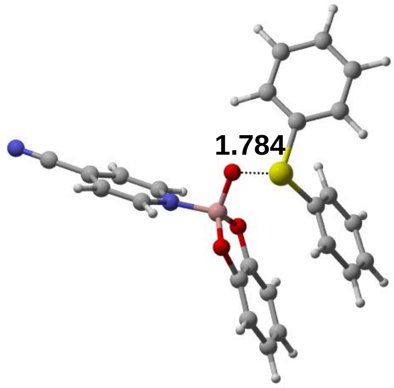


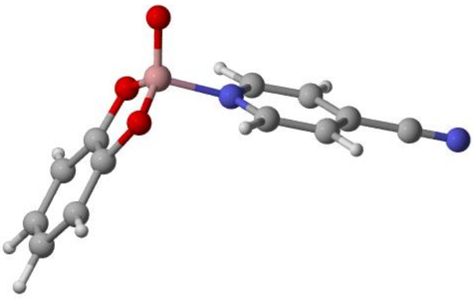
TSB



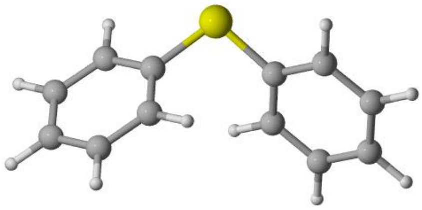
S3



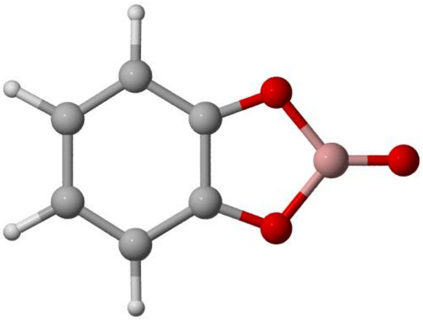
TSC



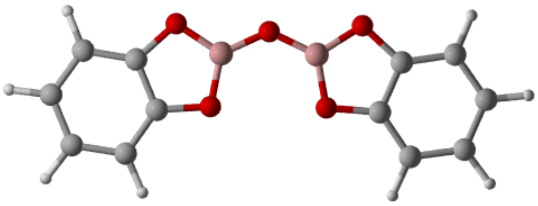
S4



8



[BO]$^{\cdot}$



Bcat-O-Bcat

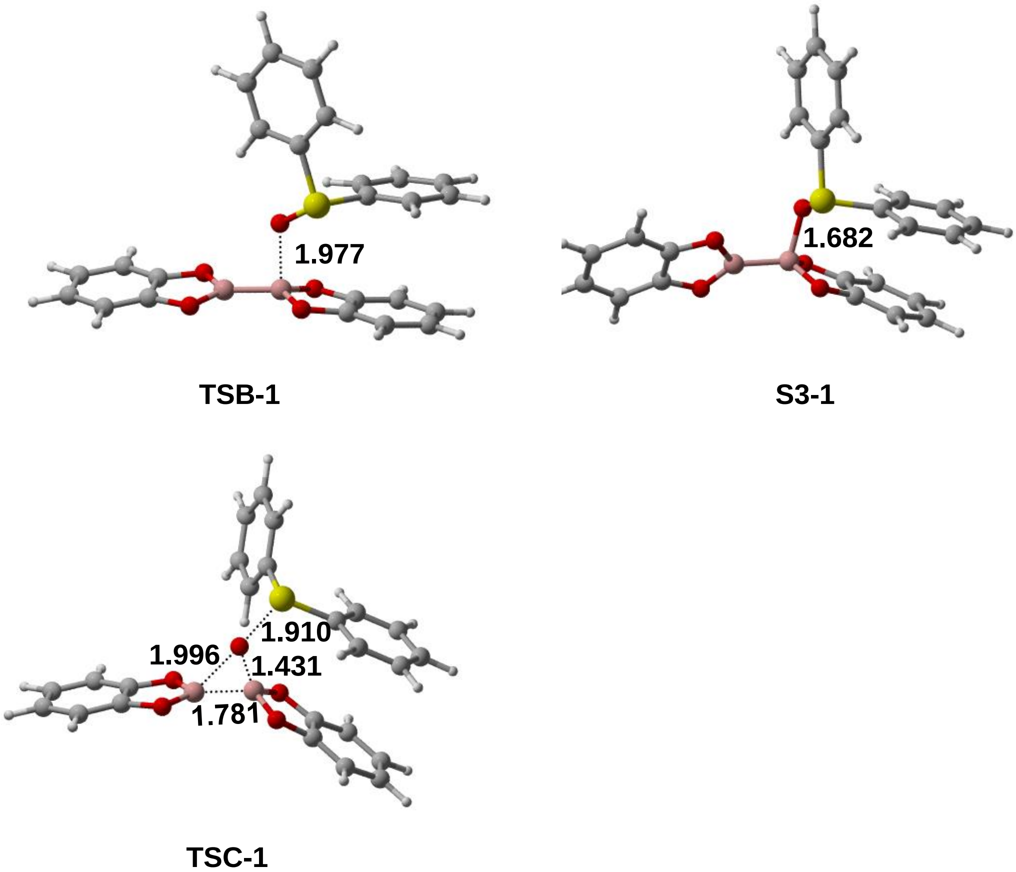


Figure S7. Optimized structures of some species involved in Figure S5 and Figure 4 with M062x/6-311G(d). 3D geometric structures of relative transition states are given in Angstrom (Å).

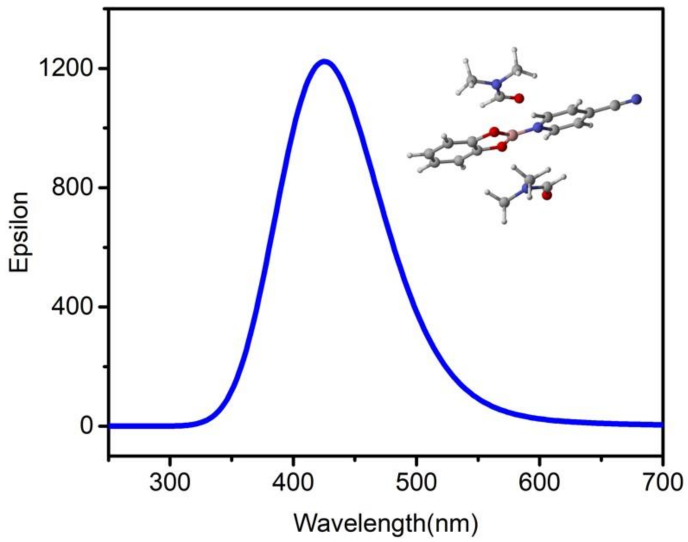


Figure S8. The calculated UV-Vis absorption of boryl radical in DMF proposed in Figure 1f.

Cartesian coordinates for the complexes calculated in this study: [gas phase results optimized at the level of M062x/6-311G(d)

Cartesian coordinates in Firgure S4

1

0 1

C	-4.09412900	-1.42716300	-0.00163300
C	-2.92493200	-0.69468100	-0.00076600
C	-2.92520500	0.69480600	0.00078800
C	-4.09468200	1.42683900	0.00156000
C	-5.28466300	0.69729300	0.00068700
C	-5.28439300	-0.69807300	-0.00087100
H	-4.07808300	-2.50957300	-0.00283300
H	-4.07904600	2.50925600	0.00277100
H	-6.22931700	1.22770700	0.00124000
H	-6.22884200	-1.22885300	-0.00150800
O	-1.62799000	1.13878100	0.00136000
O	-1.62755100	-1.13815600	-0.00118600
B	-0.84126700	0.00047000	0.00005600
C	4.09412800	-1.42716200	0.00156100
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C	5.28439300	-0.69807700	0.00068200
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O	1.62755100	-1.13815900	0.00136100
B	0.84126400	0.00046300	0.00006800

2

0 1

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C	-1.50011600	1.13881100	-0.00000200
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H	0.40601500	2.15136600	-0.00001500
H	-2.08647100	2.05215200	-0.00000500
C	2.03271600	0.00000700	-0.00000300
N	3.18194800	-0.00000200	0.00000200

5

0 1

C	1.80757600	1.20742800	-0.00029000
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C	-0.24113400	-0.00063300	-0.00000200
C	0.41816800	-1.21633700	0.00028300
C	1.80856800	-1.20668900	0.00028800
C	2.49994600	0.00031000	0.00000300
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H	-0.14478900	2.14186700	-0.00049900
H	-0.14290700	-2.14313900	0.00049300
H	2.34995800	-2.14509900	0.00051900
H	3.58346700	0.00061900	0.00000500
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O	-2.26466600	0.00081900	1.07796000
O	-2.26466800	-0.00065300	-1.07795700

[B]•

0 2

C	3.66521000	-1.42623200	0.00010600
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C	3.66535900	1.42613300	-0.00000500
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C	4.85772300	-0.69637000	0.00013000
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H	5.80118000	-1.22850500	0.00019200
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TS1

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INT1

0 2

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C	2.85468100	-1.14642400	0.35941600
C	2.64849500	0.11698800	-0.19352600
H	3.44931900	2.06064000	-0.60850000
H	5.64451000	1.54154200	0.44146700
H	6.04422400	-0.69633100	1.43457400
H	4.25380700	-2.40863300	1.36823100
H	2.07394300	-1.89266100	0.31959900
N	1.40926700	0.47217000	-0.76580900
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O	1.18825600	1.50750900	-1.39932100

INT2

0 1

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C	3.81504514	-2.38070774	-1.76861306
C	5.14868499	-2.29105942	-1.35199844
C	5.47939059	-1.97519983	-0.03671008

H	4.73779728	-1.48102292	1.94941876
H	3.54212724	-2.62122121	-2.78843288
H	5.93908654	-2.47151568	-2.07048037
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O	2.03520697	-1.56519504	1.20724263
B	1.01052076	-1.71983076	0.28085992
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C	1.04373539	1.59760556	1.22037800
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C	2.36583444	1.73214873	1.61128739
H	0.20701356	1.73188924	1.89329206
C	3.36327869	1.49061285	0.67165360
H	3.77553054	0.91341184	-1.37256226
H	2.61031466	1.99869360	2.63040727
O	-1.20455694	2.14992680	-1.34642453
O	-1.65568980	1.14907204	0.72207435
C	-2.56551268	2.13708596	0.46610364
C	-3.63087426	2.53073249	1.24292145
C	-4.42190302	3.58245264	0.75972058
C	-4.13866321	4.19289229	-0.45522266
C	-3.05729289	3.77633972	-1.24401876
C	-2.28540957	2.74075156	-0.76369167
H	-3.84561100	2.03102059	2.17974046
H	-5.27068890	3.91836820	1.34369074
H	-4.76745274	5.00257485	-0.80685130
H	-2.83294769	4.23658490	-2.19848260
N	0.72365488	1.25116733	-0.02770091
C	4.74748540	1.57729753	1.05057802
N	5.85178225	1.64023072	1.36129509

TS2

0 1

C	4.05568700	-1.38370900	1.28801900
C	2.81620400	-1.68981100	0.77148800
C	2.63713000	-2.02394400	-0.56867300
C	3.68979600	-2.07079100	-1.45551800
C	4.95285000	-1.75041300	-0.94529000
C	5.13164900	-1.41205100	0.39426600
H	4.17875900	-1.11320200	2.32954500
H	3.53354000	-2.32864400	-2.49562300
H	5.80992200	-1.76531900	-1.60783200
H	6.12136700	-1.15567900	0.75208200
O	1.29826900	-2.20382900	-0.81740600
O	1.59435900	-1.66294900	1.39816900
B	0.68431000	-1.91756300	0.38533900
C	-3.81898600	-1.79291800	-1.03957400
C	-5.14569100	-2.01790100	-0.69786000
C	-5.47547800	-2.55824200	0.54046500
C	-4.46388700	-2.87377400	1.43943400
C	-3.13048700	-2.65193600	1.11530400
C	-2.81667200	-2.10595100	-0.12423200
H	-3.55706600	-1.38127700	-2.00574700
H	-5.92520900	-1.76803300	-1.40834200
H	-6.51265000	-2.73167200	0.80189400
H	-4.70930500	-3.29245600	2.40879400
H	-2.34380900	-2.88530900	1.81849900
N	-1.44458900	-1.96376000	-0.53838400
O	-0.64847400	-1.80539300	0.62151200
O	-1.27474500	-0.82889400	-1.34213400
B	-1.47788300	0.42742900	-0.79865900
C	1.56019000	0.89354500	-1.26335300
C	1.03500100	1.30357200	0.93691300
C	2.88344200	1.27127800	-1.07762100
H	1.19917700	0.54956300	-2.22757900
C	2.33028300	1.70623400	1.22625100
H	0.26369800	1.27434500	1.69979900
C	3.27099400	1.67724700	0.19703800
H	3.59682600	1.22574400	-1.88975700
H	2.60754400	2.01492000	2.22569100
O	-1.60341800	1.50967900	-1.67279300
O	-1.98011500	0.71428200	0.46906300
C	-2.25199200	2.05862900	0.42044700
C	-2.68545500	2.88210500	1.43583000
C	-2.87867000	4.23086900	1.11613700
C	-2.64251600	4.70999000	-0.16850100
C	-2.20344700	3.86347600	-1.19266400
C	-2.01562200	2.53796400	-0.86824200
H	-2.87249100	2.49173700	2.42857400
H	-3.22050700	4.91268600	1.88565100
H	-2.80224800	5.75983700	-0.38353100
H	-2.01868300	4.22290800	-2.19720600
N	0.66303200	0.90161900	-0.27856700
C	4.64064700	2.02772500	0.46068600
N	5.73615500	2.29788100	0.67922600

INT3

0 1

C	2.64056300	3.82896500	-0.09263100
C	1.63176900	2.89340900	-0.04094200
C	1.89552600	1.54796200	0.19333400
C	3.16852300	1.06171300	0.38301400
C	4.20038500	2.00448300	0.33048400
C	3.94202400	3.35348800	0.09937900
H	2.42807900	4.87444400	-0.27558100
H	3.34815100	0.00695200	0.56023100
H	5.22253500	1.67514900	0.47234700
H	4.76766300	4.05405900	0.06556100
O	0.70394900	0.85683500	0.19364100
O	0.27452700	3.07499400	-0.19887300
B	-0.26292300	1.81469000	-0.05973000
C	-3.91058700	-1.17037300	-0.13470400
C	-5.28608100	-1.32843600	-0.04253000
C	-6.10266900	-0.24413000	0.26271300
C	-5.53132500	1.00368900	0.47670100
C	-4.15467500	1.17929900	0.38643500
C	-3.35256400	0.08762700	0.07476700
H	-3.27332300	-2.01239800	-0.37004600
H	-5.72007100	-2.30703600	-0.21183200
H	-7.17629400	-0.37260800	0.33316500
H	-6.15810200	1.85596300	0.71249500
H	-3.70966500	2.15081500	0.54624300
N	-1.91825300	0.20255500	0.08129000
O	-1.59016700	1.55211400	-0.19641500
O	-1.39775600	-0.54328000	-1.00294800
C	1.99190900	-2.91903700	1.47932100
C	1.21380100	-2.34050600	0.50078000
C	1.67467100	-2.17612300	-0.80440100
C	2.93035200	-2.58754700	-1.19314800
C	3.72959900	-3.17623900	-0.20734800
C	3.27124200	-3.33759200	1.09803200
H	1.62363200	-3.03386800	2.49080200
H	3.27496700	-2.44705300	-2.20974500
H	4.72644900	-3.51183500	-0.46708200
H	3.91791500	-3.79651100	1.83625600
O	0.71174700	-1.53993900	-1.54700400
O	-0.05334700	-1.82614800	0.60221900
B	-0.28719200	-1.26158600	-0.63473700

TS3

0 1

C	3.34557400	-2.93754300	1.08772900
C	2.32021200	-2.33112900	0.39846100
C	2.56401000	-1.46956400	-0.67323100
C	3.84337800	-1.18252300	-1.09262000
C	4.89468900	-1.79347000	-0.39661900
C	4.65174900	-2.65170900	0.66893200
H	3.14019400	-3.60399500	1.91624300
H	4.01746100	-0.51301700	-1.92578700
H	5.91580300	-1.59146800	-0.69822800
H	5.48556200	-3.10976200	1.18783700
O	1.37891600	-1.01782500	-1.17829500
O	0.97245200	-2.44201400	0.60322900
B	0.37265300	-1.59031700	-0.34790000
C	-3.76040500	-0.12103200	-0.57163300
C	-5.04214800	-0.23747200	-0.05631200
C	-5.40402400	-1.39267200	0.63277400
C	-4.49207700	-2.43316600	0.81739100
C	-3.20545700	-2.32692400	0.31700200
C	-2.85829000	-1.16867200	-0.38266800
H	-3.42954300	0.75943700	-1.10983400
H	-5.75868400	0.56326800	-0.19207800
H	-6.40794600	-1.48563900	1.03147500
H	-4.79002500	-3.32403300	1.35689900
H	-2.47183500	-3.11229700	0.44242900
N	-1.59061300	-0.97354200	-0.97150600
O	-0.86372100	-2.10789000	-0.98502400
O	-0.51933700	-0.39582800	0.30487000
C	-0.66710600	4.36571600	-0.38602300
C	-0.29674800	3.07770600	-0.07119100
C	0.94539200	2.78030200	0.48106500
C	1.87918100	3.75687400	0.74544700
C	1.51554000	5.06949800	0.43023900
C	0.27235500	5.36716800	-0.12227100
H	-1.63624900	4.58282100	-0.81683500
H	2.84201500	3.50836300	1.17296700
H	2.21895800	5.87126100	0.61970900
H	0.02564000	6.39608700	-0.35459800
O	1.03596200	1.42436500	0.68970800

O	-1.01432900	1.91086700	-0.22034600
B	-0.16696800	0.92472400	0.24757600

INT4

0 1

C	1.26809700	1.33185700	0.00003300
C	-0.09622900	1.09401400	-0.00002100
C	-0.54978700	-0.22361200	0.00002200
C	0.33406100	-1.29485800	-0.00010300
C	1.70253600	-1.05090900	-0.00014300
C	2.16458300	0.26085700	0.00005400
H	1.64180300	2.34917400	0.00032800
H	-0.82071400	1.89933000	-0.00005400
H	-0.07151200	-2.30038200	0.00004300
H	2.40451000	-1.87616600	-0.00029900
H	3.23123300	0.45517700	0.00012300
N	-1.95410300	-0.57972500	0.00051400
O	-2.70577200	0.35335500	-0.00034900

TS4A

0 1

C	-3.92201400	0.07474600	-1.57946900
C	-2.96510100	0.21509100	-0.59934200
C	-3.12305600	-0.33570000	0.67141700
C	-4.24997700	-1.04976400	1.01578100
C	-5.23140500	-1.19582200	0.02963800
C	-5.07156300	-0.64663800	-1.23872600
H	-3.78344100	0.50756500	-2.56217400
H	-4.35928500	-1.47072200	2.00714200
H	-6.13355800	-1.74928400	0.26115700
H	-5.85074900	-0.77872500	-1.97978600
O	-2.03073300	-0.05118900	1.44395400
O	-1.76397400	0.87436200	-0.67043900
B	-1.15819900	0.63290100	0.58346300
C	2.07109300	2.61700000	0.99052400
C	2.99148400	3.38409000	0.28909500
C	2.77592500	3.68791400	-1.05088700
C	1.63367900	3.22025700	-1.69318800
C	0.70313100	2.44730600	-1.01088500
C	0.93773200	2.15793700	0.33112100
H	2.19738800	2.37463000	2.03670600
H	3.87800400	3.74800400	0.79494300
H	3.49516400	4.28968300	-1.59417800
H	1.46082400	3.45630800	-2.73652300
H	-0.17859200	2.07651200	-1.51413200
N	-0.02233400	1.38763700	1.13558300
O	0.17650500	1.36001500	2.37428400
C	2.85893500	-2.89278700	1.10127400
C	1.96253400	-1.96422800	0.61809800
C	1.70482700	-1.82373400	-0.74096200
C	2.32890300	-2.60281900	-1.69082600
C	3.24178900	-3.54592500	-1.21423700
C	3.50052600	-3.68729900	0.14906600
H	3.04709200	-2.99127300	2.16252000
H	2.11581100	-2.48292000	-2.74517700
H	3.75986700	-4.18219200	-1.92151300
H	4.21525800	-4.43156500	0.47875200
O	0.76755500	-0.82564100	-0.91574600
O	1.19730100	-1.05729600	1.31686500
B	0.48513200	-0.40074800	0.35791600

INT5

0 1

C	4.79827700	0.65285200	0.67317300
C	3.48518200	0.26319800	0.53555800
C	2.79148900	0.41818700	-0.66134800
C	3.37614100	0.97095200	-1.77806200
C	4.71009000	1.37155900	-1.65124600
C	5.40426300	1.21633300	-0.45440000
H	5.32496900	0.52591700	1.61034500
H	2.82329100	1.08439300	-2.70176900
H	5.21158300	1.81210600	-2.50445100
H	6.43687600	1.53796000	-0.39238100
O	1.50947900	-0.05840900	-0.50590800
O	2.65553100	-0.31195100	1.47059300
B	1.46216700	-0.48857800	0.80430800
C	-0.41507700	-3.51607800	0.67664600
C	-0.76859200	-4.79128300	0.25024200
C	-1.80518300	-4.97890800	-0.65370300
C	-2.49115000	-3.86769400	-1.13412900
C	-2.15082700	-2.58637500	-0.72664200
C	-1.10695300	-2.40769300	0.18751800
H	0.38258800	-3.38128300	1.39343800
H	-0.22347200	-5.64430800	0.63830500
H	-2.07603600	-5.97541000	-0.98125100
H	-3.30125700	-3.99408600	-1.84350800
H	-2.68802900	-1.73242900	-1.11569900
N	-0.76025800	-1.10891300	0.60691900
O	0.38028900	-1.04862900	1.41667000
C	-1.66289700	3.65138300	0.75991800
C	-1.72663900	2.29647700	0.52321000
C	-2.76228300	1.72622400	-0.21033300
C	-3.78393300	2.48012700	-0.74167900
C	-3.73009300	3.85828800	-0.50865200
C	-2.69414000	4.42990200	0.22454800
H	-0.85132300	4.08146400	1.33278300
H	-4.58367400	2.02112000	-1.30884400
H	-4.51305300	4.49156100	-0.90794800
H	-2.68397000	5.50111000	0.38573400
O	-2.56986600	0.36448900	-0.28683600
O	-0.85953300	1.31145300	0.92846600
B	-1.39615200	0.13936700	0.41553700

INT6

0 1

C	-1.32445600	1.34712500	-0.00854000
C	0.03580400	1.05923000	-0.05108900
C	0.45780300	-0.26731700	-0.05298900
C	-0.48693600	-1.29594200	-0.01066600
C	-1.83970100	-0.99521900	0.03261800
C	-2.26910400	0.32946000	0.03253500
H	-1.64440200	2.38327600	-0.00263100
H	0.77344000	1.84960000	-0.06608600
H	-0.15574500	-2.33006000	-0.02176600
H	-2.56327200	-1.80206500	0.06686100
H	-3.32664200	0.56238700	0.06689900
N	1.82305100	-0.61956000	-0.17454400
O	2.68346900	0.42577100	0.20992600
H	3.19983700	0.60691300	-0.58130400
H	2.04721100	-1.40332200	0.42920900

INT7

0 1

C	1.31623800	-1.35117000	-0.00007300
C	-0.04673600	-1.06824600	-0.00013900
C	-0.43889300	0.25332300	-0.00006800
C	0.46815300	1.30175700	0.00001500
C	1.82646300	1.00789600	0.00014900
C	2.24873500	-0.31932000	0.00005400
H	1.64955600	-2.38242300	-0.00011700
H	-0.82867700	-1.81687600	-0.00022200
H	0.12631700	2.33354600	0.00007100
H	2.55265100	1.81224700	0.00026400
H	3.30850900	-0.54657200	0.00011100
N	-1.90118400	0.53700000	-0.00026700
O	-2.69933700	-0.54772700	0.00043900
H	-2.07458800	1.13929900	0.81845100
H	-2.07454200	1.13815000	-0.81983600

TS5

0 1

C	3.77012600	2.04765200	1.20433700
C	2.57723300	2.38651700	0.58718300
C	2.27864900	1.83094500	-0.65412600
C	3.13775200	0.92345200	-1.26315100
C	4.33307900	0.59361500	-0.63492300
C	4.65153800	1.15617100	0.59304600
H	4.00822600	2.46968200	2.17335500
H	1.86460300	3.04482900	1.07237000
H	2.86253000	0.45979600	-2.20483900
H	4.99375600	-0.13058200	-1.09505400
H	5.57473500	0.88255600	1.08968500
N	1.03316300	2.14412600	-1.27864700
O	-0.34241200	1.34369500	-0.70252600
H	0.72993200	3.10171900	-1.14239600
H	1.00051700	1.88945400	-2.26013300
C	-6.36912100	-0.36051900	-0.35228400
C	-6.26848100	0.09127000	0.96288200
C	-5.02979900	0.37876300	1.54145200
C	-3.91832800	0.19518200	0.74560800
C	-4.01866000	-0.25549000	-0.56665000
C	-5.23559300	-0.54513200	-1.14781200
H	-7.34679200	-0.57508700	-0.76730800
H	-7.16938900	0.22082100	1.55084100
H	-4.93547700	0.72696600	2.56226900
H	-5.29797200	-0.89815200	-2.16943900
B	-0.12132300	0.02354200	-0.22568100
B	-1.89225400	0.05104300	-0.09623900
O	-2.59795800	0.39512300	1.04728500
O	-2.76227700	-0.34253700	-1.10367200
O	0.60545300	-0.14740700	1.02808300
O	0.49498700	-0.89763500	-1.18313900
C	3.52060200	-2.37916800	1.14194400
C	3.44556100	-2.84168700	-0.16738500
C	2.42819500	-2.40989300	-1.02963700
C	1.51258900	-1.50525500	-0.53120700
C	1.58609900	-1.04193300	0.79070900
C	2.58041300	-1.47032000	1.64513400
H	4.31417500	-2.73441000	1.78965000
H	4.17905600	-3.55442200	-0.52711600
H	2.35488300	-2.76257100	-2.05192800
H	2.62948500	-1.09733400	2.66121700

6

0 1

C	1.16735000	-1.19782600	0.00363100
C	-0.22042100	-1.20305100	-0.00591900
C	-0.93473100	-0.00001900	-0.00878500
C	-0.22055000	1.20297700	-0.00594700
C	1.16732000	1.19784600	0.00367600
C	1.87450100	0.00008100	0.00901200
H	1.70038900	-2.14238900	0.00700700
H	-0.76171700	-2.14427300	-0.01725600
H	-0.76185000	2.14419300	-0.01746800
H	1.70015800	2.14252100	0.00718400
H	2.95771700	0.00002000	0.01713900
N	-2.32896300	-0.00002500	-0.07755800
H	-2.76643100	-0.83350300	0.28620200
H	-2.76634100	0.83355600	0.28609200

Cartesian coordinates in Firgure 3

TS4B

0 2

C	4.09087600	0.87891800	1.23439500
C	3.02877200	0.13582500	0.77083900
C	3.18077000	-0.82978600	-0.22272900
C	4.40338500	-1.09236100	-0.79876700
C	5.48975700	-0.34136500	-0.33838500
C	5.33780100	0.62135400	0.65503600
H	3.95863300	1.62314600	2.00964200
H	4.50613200	-1.84315200	-1.57173500
H	6.46954200	-0.51413100	-0.76706300
H	6.20087900	1.18521100	0.98776600
O	1.96864700	-1.42387400	-0.47713400
O	1.71061700	0.18251500	1.16736800
B	1.07941700	-0.70776700	0.30632400
C	-1.08822200	-0.50475700	1.46463500
C	-2.43495900	-0.68185200	1.50485900
C	-3.07157400	-1.51122600	0.54826600
C	-2.25852300	-2.15396200	-0.41613100
C	-0.91111800	-1.95713000	-0.42183600
N	-0.30639100	-1.11244200	0.49423700
H	-0.55357300	0.12139300	2.16471900
H	-3.01407200	-0.18158200	2.26976000
H	-2.69972800	-2.81130000	-1.15393600
H	-0.24667100	-2.41675700	-1.13961000
C	-4.48095900	-1.66739400	0.54042200
N	-5.62939000	-1.78327000	0.52858200
C	-3.15210700	1.96512000	-0.92846200
C	-2.09539400	1.24230800	-1.45972700
C	-0.81679200	1.42707800	-0.93306700
C	-0.58552600	2.31804500	0.11264900
C	-1.64697200	3.05459900	0.62326200
C	-2.92773100	2.87200500	0.10813400
H	-4.15491400	1.81973900	-1.31318200
H	-2.23511000	0.52329100	-2.25749700
H	0.41999700	2.41404600	0.50742800
H	-1.47987600	3.76177400	1.42727600
H	-3.75863500	3.43511000	0.51777600
N	0.28981500	0.61306600	-1.34007100
O	0.11363500	-0.04013400	-2.34680300

INT4-B

0 2

C	3.82525900	-1.01999200	-0.03154600
C	2.49552500	-0.65873900	-0.02524000
C	2.09589800	0.67097200	0.03720600
C	2.99915900	1.70879100	0.09681700
C	4.35113400	1.35490700	0.09096800
C	4.75382500	0.02228800	0.02826600
H	4.12257400	-2.05957300	-0.08020200
H	2.67144500	2.73929400	0.14639000
H	5.10063800	2.13560100	0.13689900
H	5.81116100	-0.21330800	0.02593000
O	0.71842000	0.72275200	0.02824300
O	1.38591200	-1.46488400	-0.07453600
B	0.31973800	-0.59833500	-0.03892200
C	-3.46259100	-0.92613800	0.16560200
C	-4.63518400	-0.18653700	0.19670700
C	-4.60432700	1.19557200	0.03643600
C	-3.38553900	1.83427600	-0.15904200
C	-2.20057400	1.10916900	-0.19443300
C	-2.24427600	-0.27531800	-0.02782900
H	-3.46861300	-2.00064200	0.28453700
H	-5.57995300	-0.69566400	0.34857000
H	-5.52320900	1.76938700	0.06218100
H	-3.35009000	2.90963700	-0.29017300
H	-1.26090400	1.61887900	-0.35165900
N	-1.05526800	-1.07038900	-0.06044400
O	-1.18742000	-2.34470700	-0.07223600

TS4-B-oss

0 1

C	4.51770100	0.20171400	-0.72124300
C	3.21712700	-0.00931500	-1.12323100
C	2.78165100	-1.23051200	-1.62706700
C	3.63461500	-2.30393900	-1.77166300
C	4.96007100	-2.10267300	-1.37685100
C	5.38992200	-0.88118500	-0.86049700
H	4.83044100	1.14434600	-0.29138300
H	3.28342800	-3.24946500	-2.16490300
H	5.66724200	-2.91824800	-1.46904300
H	6.42125200	-0.76749600	-0.54998500
O	1.43693900	-1.16456800	-1.88606000
O	2.14490900	0.85534200	-1.06114600
B	1.06738400	0.09866200	-1.47706300
C	-2.21625800	2.02280400	-1.30636800
C	-2.73368200	3.30513300	-1.18569200
C	-1.88857900	4.40717900	-1.10276100
C	-0.51112700	4.21649200	-1.14758400
C	0.02644800	2.94203600	-1.26817700
C	-0.83271000	1.84272700	-1.34088100
H	-2.86181100	1.15790300	-1.37283700
H	-3.80876900	3.44174200	-1.15929000
H	-2.29872000	5.40567900	-1.00858200
H	0.15775500	5.06741000	-1.08873500
H	1.09904100	2.80726500	-1.29153900
N	-0.32416500	0.51733400	-1.45535000
O	-1.17337500	-0.45636400	-1.51465300
C	-4.09757000	-3.76602500	-0.94178000
C	-3.40509900	-2.72868600	-0.35971900
C	-4.02441400	-1.52619300	-0.02578400
C	-5.36269500	-1.30515400	-0.26038200
C	-6.07671500	-2.35185600	-0.85343600
C	-5.45854500	-3.55344500	-1.18596000
H	-3.60312000	-4.69413000	-1.19853100
H	-5.83055200	-0.36593700	0.00670100
H	-7.13255100	-2.22120500	-1.05765800
H	-6.04109100	-4.34265300	-1.64569800
O	-3.10143100	-0.67913200	0.54203800
O	-2.07622800	-2.67064900	-0.01144800
B	-1.90918500	-1.38242300	0.46088400
C	0.46348100	-1.68697900	1.04403600
C	1.66536200	-1.19841700	1.45112800
C	1.77446100	0.14252300	1.91149800
C	0.59937300	0.92974200	1.91077500
C	-0.58604400	0.40000300	1.50169700
N	-0.68883100	-0.91688200	1.08271300
H	0.33609800	-2.68847000	0.65672500
H	2.54093300	-1.83393300	1.40316500
H	0.63311300	1.96722200	2.21688800
H	-1.50407500	0.97123600	1.47045100
C	3.02848200	0.69632900	2.26577800
N	4.05514200	1.15257900	2.53437300

TS4-B-ts

0 3

C	4.27522400	0.34909200	-0.98715400
C	2.99034700	-0.07204300	-1.24504800
C	2.67339400	-1.40755100	-1.46174100
C	3.63296100	-2.39643300	-1.44064900
C	4.94355900	-1.98471900	-1.18049000
C	5.25674300	-0.64493200	-0.95512800
H	4.50386000	1.38705800	-0.78231500
H	3.37293500	-3.43422800	-1.60581500
H	5.73219700	-2.72673700	-1.14709000
H	6.27877600	-0.36336500	-0.73377800
O	1.31474100	-1.53318100	-1.62437900
O	1.82750900	0.66985800	-1.26104400
B	0.82874200	-0.25673600	-1.47283500
C	-2.61637000	1.36791400	-1.60391700
C	-3.27703000	2.57301000	-1.42018600
C	-2.57874800	3.70962000	-1.02222500
C	-1.20618000	3.63277100	-0.81573100
C	-0.52634800	2.43326900	-0.99361700
C	-1.24066000	1.29947000	-1.38245100
H	-3.14762600	0.47360000	-1.90094600
H	-4.34638200	2.62232700	-1.59239200
H	-3.09955800	4.64940400	-0.88080300
H	-0.65152400	4.51351000	-0.51271900
H	0.53991600	2.38511400	-0.82344000
N	-0.60032500	0.02919300	-1.53498100
O	-1.34978700	-0.99405900	-1.72856800
C	-3.81894000	-2.78577700	0.36120100
C	-2.97130400	-1.79050100	0.79171400
C	-3.41012800	-0.48576400	0.99321800
C	-4.71727200	-0.11031700	0.77870300
C	-5.58905300	-1.11271700	0.34310100
C	-5.14918500	-2.41866100	0.13829300
H	-3.46109300	-3.79368300	0.19597800
H	-5.03743500	0.91204000	0.93556000
H	-6.62774500	-0.86621100	0.15868300
H	-5.85193200	-3.16836400	-0.20465200
O	-2.34898200	0.29301700	1.39797800
O	-1.62605700	-1.86676200	1.07596600

B	-1.27547800	-0.57341100	1.39614300
C	1.13170500	-1.06024900	1.56140100
C	2.41495800	-0.66177000	1.72968300
C	2.71846600	0.70044200	2.02007600
C	1.62464700	1.60584200	2.13924800
C	0.35216500	1.17806700	1.96431800
N	0.06670700	-0.15729800	1.66832100
H	0.85187000	-2.07756700	1.32407600
H	3.21391200	-1.38524800	1.61880500
H	1.80387500	2.64955200	2.36334200
H	-0.50773000	1.83055100	2.02650900
C	4.05498200	1.14130000	2.13660900
N	5.15081400	1.50465000	2.20515400

Cartesian coordinates in Firgure S5

TSA

0 1

C	3.58870300	-1.65245100	-1.42023800
C	2.42760600	-1.48468700	-0.69682600
C	2.42774900	-1.48463000	0.69671600
C	3.58899600	-1.65233500	1.41990200
C	4.77400000	-1.82682600	0.69500000
C	4.77385600	-1.82687900	-0.69556500
H	3.57462700	-1.64041000	-2.50343600
H	3.57514400	-1.64020500	2.50310200
H	5.70897100	-1.94892100	1.22804500
H	5.70871700	-1.94901700	-1.22879200
O	1.15980500	-1.25458800	1.16840800
O	1.15956600	-1.25468000	-1.16827300
B	0.37926400	-1.06437700	0.00014100
B	-0.37926000	1.06434500	0.00002000
C	-3.58874100	1.65239400	-1.42031300
C	-2.42762800	1.48464500	-0.69692200
C	-2.42772000	1.48476100	0.69661700
C	-3.58893000	1.65263000	1.41982700
C	-4.77394600	1.82711900	0.69494700
C	-4.77385300	1.82700200	-0.69561900
H	-3.57470500	1.64021400	-2.50351000
H	-3.57503800	1.64062800	2.50302700
H	-5.70888900	1.94934300	1.22801100
H	-5.70872500	1.94914400	-1.22882800
O	-1.15977600	1.25469500	1.16828600
O	-1.15962200	1.25448800	-1.16838400
C	1.72082700	1.57857300	1.18538800
C	3.08534000	1.65635500	1.20598400
C	3.80570000	1.64109900	0.00010600
C	3.08540900	1.65620700	-1.20581300
C	1.72089300	1.57843900	-1.18528400
H	1.11204700	1.56132200	2.07774000
H	3.60244500	1.70919000	2.15507600
H	3.60256800	1.70892600	-2.15488300
H	1.11216100	1.56108600	-2.07766600
C	5.23078700	1.61127800	0.00014800
N	6.38201100	1.56766300	0.00018300
N	1.03367800	1.46031100	0.00004000
C	-1.72088500	-1.57845000	1.18556300
C	-3.08540000	-1.65621200	1.20611300
C	-3.80570600	-1.64116100	0.00019900
C	-3.08536700	-1.65645100	-1.20568800
C	-1.72084900	-1.57868800	-1.18511000
H	-1.11214500	-1.56103600	2.07793900
H	-3.60254800	-1.70888700	2.15519100
H	-3.60248500	-1.70931100	-2.15477200
H	-1.11207700	-1.56145100	-2.07746900
C	-5.23079400	-1.61139700	0.00017700
N	-6.38202100	-1.56782900	0.00016100
N	-1.03368900	-1.46039900	0.00022500

[B]•

0 2

C	3.66521000	-1.42623200	0.00010600
C	2.49826000	-0.69566100	0.00002200
C	2.49830300	0.69571900	-0.00003200
C	3.66535900	1.42613300	-0.00000500
C	4.85778200	0.69612900	0.00007400
C	4.85772300	-0.69637000	0.00013000
H	3.64984700	-2.50858100	0.00015400
H	3.65019500	2.50848600	-0.00004800
H	5.80128300	1.22818800	0.00009300
H	5.80118000	-1.22850500	0.00019200
O	1.19760500	1.15001500	-0.00010700
O	1.19750000	-1.14984600	0.00000800
B	0.43132300	0.00014000	-0.00004700
C	-1.71274300	-1.20126300	-0.00017400
C	-3.06550000	-1.21676700	-0.00021000
C	-3.80684500	0.00000700	-0.00011900
C	-3.06558500	1.21681400	-0.00006900
C	-1.71281800	1.20135100	-0.00002900
N	-0.99513100	0.00008300	-0.00005000
H	-1.10970200	-2.09823800	-0.00021600
H	-3.58213600	-2.16769500	-0.00034600
H	-3.58224500	2.16772700	-0.00009000
H	-1.10986100	2.09838900	0.00001100
C	-5.21959500	-0.00007700	0.00014600
N	-6.37534400	-0.00015900	0.00037100

7

0 1

C	3.00768000	-0.05535800	1.36773400
C	1.96283900	0.69514500	0.84225100
C	1.35293300	0.26735200	-0.32541600
C	1.77482200	-0.87477600	-0.99203700
C	2.81669100	-1.62108700	-0.45642700
C	3.43029200	-1.21270500	0.72336600
H	3.49529900	0.26712400	2.28148200
H	1.61955400	1.61292200	1.30800300
H	1.30328900	-1.18071000	-1.92107900
H	3.15570400	-2.51722300	-0.96492700
H	4.24749100	-1.79454200	1.13615900
S	0.00001200	1.27570400	-0.99565300
C	-1.35297600	0.26755400	-0.32530900
C	-1.77566900	-0.87397800	-0.99242900
C	-1.96209200	0.69485100	0.84296200
C	-2.81752000	-1.62025000	-0.45670700
H	-1.30480700	-1.17944700	-1.92196600
C	-3.00691600	-0.05558800	1.36854300
H	-1.61824400	1.61223600	1.30907200
C	-3.43030300	-1.21238700	0.72368200
H	-3.15716900	-2.51592400	-0.96559600
H	-3.49392600	0.26650100	2.28275500
H	-4.24748900	-1.79417900	1.13656500
O	0.00017800	2.55241700	-0.20891100

TSB

0 2

C	1.63262700	2.79557200	-2.02504100
C	0.62706800	2.39594900	-1.17041100
C	0.74529600	2.52471800	0.21487700
C	1.86947400	3.06651400	0.79929000
C	2.89219500	3.48121700	-0.05969500
C	2.77864800	3.34722700	-1.44062500
H	1.52526400	2.69051400	-3.09761200
H	1.95077600	3.15253600	1.87564400
H	3.79359400	3.90977500	0.36272700
H	3.58880800	3.68087700	-2.07841300
O	-0.37471500	2.02713500	0.82009100
O	-0.57970900	1.82669100	-1.47880600
C	-3.28305500	0.73539000	-1.15482800
C	-4.55357500	0.29156800	-1.00804100
C	-5.15187000	0.21877800	0.28524600
C	-4.35253500	0.62844200	1.39381200
C	-3.08557700	1.06691100	1.20452500
N	-2.52109900	1.14629600	-0.06497400
H	-2.78904100	0.80336100	-2.11408300
H	-5.11371000	-0.01077800	-1.88340300
H	-4.75614100	0.59179400	2.39741800
H	-2.44483300	1.38734300	2.01410400
B	-1.12927600	1.49071400	-0.23222500
C	-6.47180600	-0.24718700	0.46170500
N	-7.55342400	-0.63138900	0.60741700
C	2.90578600	0.08148500	2.55597400
C	1.91650400	-0.33999600	1.68025300
C	2.19778000	-0.34982600	0.31930800
C	3.41742200	0.06911900	-0.18906200
C	4.40537100	0.48060000	0.70238200
C	4.14926300	0.48425800	2.06751000
H	2.70956000	0.09955200	3.62178200
H	0.93113200	-0.63310700	2.02563000
H	3.58538800	0.10312500	-1.26054400
H	5.36367300	0.81828700	0.32543400
H	4.91712200	0.81318900	2.75843500
S	0.90736500	-0.85520100	-0.82684400
O	-0.41121500	-0.47229200	-0.15265400
C	1.00626500	-2.63914600	-0.56657900
C	2.12165500	-3.33537500	-1.01757500
C	-0.06082500	-3.27186000	0.05037000
C	2.17001900	-4.70979000	-0.82887600
H	2.94348800	-2.81422600	-1.49872100
C	0.00092500	-4.65157500	0.22981900
H	-0.91369900	-2.68506300	0.37097300
C	1.11026300	-5.36614700	-0.20602800
H	3.03302200	-5.26972700	-1.16938500
H	-0.82382200	-5.16558400	0.70934900
H	1.15082600	-6.43990700	-0.06471700

S3

0 2

C	-1.07237900	-3.38363000	-1.57432800
C	-0.39963000	-2.42278900	-0.85180800
C	-0.48366200	-2.36228300	0.54505500
C	-1.25338800	-3.25703600	1.25488800
C	-1.94453900	-4.23722700	0.52745700
C	-1.85567800	-4.30041200	-0.85684600

H	-0.98997600	-3.42140400	-2.65418600
H	-1.31367800	-3.19605900	2.33498700
H	-2.54850200	-4.96351300	1.05932400
H	-2.38787800	-5.07681700	-1.39429800
O	0.24475800	-1.31994600	1.01885900
O	0.36610900	-1.40004500	-1.31992100
C	3.11887800	-0.29869400	-1.15648900
C	4.44598700	-0.03225200	-1.08936200
C	5.12248300	-0.03815400	0.16857000
C	4.33591000	-0.35774200	1.31809800
C	3.01084000	-0.61799300	1.19540800
N	2.36589200	-0.59172200	-0.02973500
H	2.57619800	-0.31974700	-2.09257700
H	4.99326700	0.17879000	-1.99931700
H	4.79699300	-0.40046000	2.29659700
H	2.38356100	-0.87329100	2.03821000
B	0.86968800	-0.69637400	-0.13537500
C	6.49732600	0.25241000	0.26968000
N	7.62685500	0.49468700	0.35347100
C	-3.32342200	-0.36044800	1.92191700
C	-2.37541900	0.40184400	1.25996300
C	-2.23261600	0.22819700	-0.11412100
C	-2.98547600	-0.69407400	-0.83091300
C	-3.93908300	-1.44724900	-0.15282600
C	-4.10244500	-1.27825100	1.21528300
H	-3.45021400	-0.24990700	2.99213900
H	-1.74372500	1.10469700	1.79155300
H	-2.81404100	-0.83779200	-1.89175200
H	-4.52382800	-2.18354600	-0.68963100
H	-4.83300900	-1.87860400	1.74521900
S	-0.96000200	1.09462600	-1.00955700
O	0.39570900	0.79478100	-0.25050200
C	-1.23898300	2.77889800	-0.45636400
C	-2.44782600	3.37595400	-0.79996700
C	-0.24897700	3.45260500	0.24310800
C	-2.67228500	4.68970000	-0.41483800
H	-3.20602300	2.82229200	-1.34438200
C	-0.49265100	4.77141300	0.61959400
H	0.68104200	2.95436300	0.48429900
C	-1.69510000	5.38589600	0.29367600
H	-3.60981600	5.16986100	-0.66789600
H	0.26665300	5.31523400	1.16860100
H	-1.87442600	6.41257200	0.59023500

TSC

0 2

C	-0.66326600	-3.61300800	-1.31465600
C	-0.17712100	-2.47309100	-0.71212900
C	-0.32174900	-2.25497800	0.66493600
C	-0.96336100	-3.16995700	1.47011200
C	-1.46519200	-4.33081200	0.86381500
C	-1.31765900	-4.54860900	-0.49946400
H	-0.54402600	-3.76691700	-2.38079200
H	-1.07946900	-2.98258200	2.53110500
H	-1.97048500	-5.07117000	1.47359100
H	-1.70580100	-5.45845000	-0.94299300
O	0.20633600	-1.05563500	1.01373000
O	0.42860000	-1.40738500	-1.29727700
C	3.12527000	-0.29476900	-1.15343900
C	4.46539800	-0.02815400	-1.07564900
C	5.06021100	0.17532800	0.18660900
C	4.24110500	0.07037700	1.32987700
C	2.90731100	-0.20217900	1.18169800
N	2.34214500	-0.36754200	-0.04325900
H	2.61406000	-0.46973300	-2.09070900
H	5.06071200	0.01540300	-1.97811300
H	4.66004600	0.19160300	2.32004500
H	2.22959000	-0.30866500	2.01767800
B	0.78186200	-0.48409500	-0.20626800
C	6.44847500	0.46402400	0.30383100
N	7.57340100	0.70002400	0.39918500
C	-3.43978100	-0.59606200	1.65612900
C	-2.59123300	0.29644900	1.02304200
C	-2.32406300	0.12366500	-0.34055100
C	-2.85683300	-0.96159600	-1.04637700
C	-3.69947600	-1.84866800	-0.39364500
C	-3.99701600	-1.66432300	0.95299600
H	-3.65370600	-0.47053900	2.71124700
H	-2.12545000	1.10762200	1.56973100
H	-2.59989600	-1.10803000	-2.08973700
H	-4.10283100	-2.69723700	-0.93249600
H	-4.64566300	-2.36685800	1.46299000
S	-1.18828100	1.13734900	-1.20336800
O	0.42335600	0.89121800	-0.48001600
C	-1.45466400	2.74719700	-0.46197600
C	-2.75752000	3.24219700	-0.42841200
C	-0.37812600	3.51171800	-0.02802000
C	-2.98265000	4.51885000	0.06632900
H	-3.58440100	2.63039700	-0.77130600
C	-0.62121400	4.79395200	0.45814300
H	0.62046200	3.09919100	-0.05695000
C	-1.91480300	5.29696100	0.50726800
H	-3.99370900	4.90679400	0.10418800
H	0.21073800	5.39682700	0.80287000
H	-2.09437700	6.29522400	0.88910100

S4

0 2

C	-3.08115300	-0.76231000	-1.41805500
C	-2.23549000	0.05257500	-0.69909400
C	-2.23545800	0.05363900	0.69906600
C	-3.08110300	-0.76013200	1.41930900
C	-3.94559500	-1.59276100	0.69541200
C	-3.94561800	-1.59382800	-0.69285000
H	-3.07532900	-0.74725100	-2.50111400
H	-3.07523300	-0.74341500	2.50234200
H	-4.62659800	-2.24263000	1.23218200
H	-4.62663900	-2.24452600	-1.22859300
O	-1.31302100	0.94289000	1.17663700
O	-1.31309300	0.94110900	-1.17806600
C	1.48111800	0.39177000	-1.16024800
C	2.74622400	-0.16705100	-1.20549700
C	3.38740300	-0.44758500	0.00028300
C	2.74685800	-0.16375400	1.20563400
C	1.48173600	0.39494300	1.15951700
N	0.87967900	0.66419000	-0.00057500
H	0.90783300	0.62485000	-2.04912000
H	3.22013500	-0.38385100	-2.15328500
H	3.22126500	-0.37795900	2.15376400
H	0.90893500	0.63046300	2.04806100
B	-0.65690200	1.45346700	-0.00112000
C	4.70119500	-1.03117500	0.00073700
N	5.75112700	-1.49717800	0.00110200
O	-0.38716300	2.84124000	-0.00202000

8

0 1

C	3.59502000	0.05157500	-0.67468000
C	2.47878100	-0.77472100	-0.75237500
C	1.38243400	-0.54245700	0.07374000
C	1.40425600	0.52513400	0.97127500
C	2.51112700	1.35916900	1.02670600
C	3.61200800	1.12215700	0.20888200
H	4.44695000	-0.13714500	-1.31944300
H	2.45482400	-1.59673200	-1.45972200
H	0.55126100	0.70359900	1.61690600
H	2.51905600	2.19244400	1.72158100
H	4.47881200	1.77225700	0.26106500
S	0.00020700	-1.67071000	0.00019200
C	-1.38236700	-0.54290900	-0.07365300
C	-2.47747500	-0.77346700	0.75456800
C	-1.40557200	0.52274500	-0.97346200
C	-3.59388300	0.05260600	0.67674900
H	-2.45240700	-1.59397200	1.46361800
C	-2.51256100	1.35660200	-1.02905900
H	-0.55351900	0.69983000	-1.62071600
C	-3.61221700	1.12127500	-0.20909200
H	-4.44486600	-0.13477100	1.32315200
H	-2.52157900	2.18837800	-1.72571400
H	-4.47914100	1.77120700	-0.26140400

[BO]·

0 2

C	-1.28329300	1.44706600	0.00000900
C	-0.08172800	0.72062000	0.00012900
C	-0.08172500	-0.72061700	0.00012400
C	-1.28329200	-1.44706800	0.00001700
C	-2.44477800	-0.71476200	-0.00010900
C	-2.44477900	0.71475400	-0.00011400
H	-1.26968600	2.52896700	0.00007700
H	-1.26967400	-2.52896900	0.00009300
H	-3.39898100	-1.22771900	-0.00020700
H	-3.39898100	1.22771100	-0.00022000
O	1.13357800	-1.16481100	0.00011100
O	1.13357800	1.16482000	0.00012400
B	2.07744300	0.00002100	-0.00003200
O	3.31630400	-0.00001500	-0.00022600

Bcat-O-Bcat

0 1

C	4.76299000	-0.88891200	0.00032300
C	3.40237100	-0.67610300	0.00015200
C	2.85620900	0.60395300	-0.00019300
C	3.64297100	1.73408700	-0.00037800
C	5.02645700	1.53147600	-0.00019900
C	5.57327000	0.25054600	0.00014200
H	5.17353500	-1.89056700	0.00058400
H	3.20286300	2.72307100	-0.00064500
H	5.68538000	2.39136300	-0.00032400
H	6.65008000	0.13181600	0.00027400
O	1.48474700	0.50734400	-0.00030500
O	2.38603500	-1.59990000	0.00026800
B	1.22612300	-0.85037500	-0.00002700
O	0.00000500	-1.42340600	-0.00005200
C	-4.76299100	-0.88891300	-0.00028000

C	-3.40237700	-0.67609700	-0.00013100
C	-2.85620400	0.60395400	0.00018500
C	-3.64297000	1.73408500	0.00036500
C	-5.02645800	1.53147400	0.00021500
C	-5.57327300	0.25054600	-0.00010000
H	-5.17353400	-1.89056900	-0.00052000
H	-3.20286700	2.72307100	0.00060600
H	-5.68537600	2.39136300	0.00034700
H	-6.65008300	0.13181600	-0.00020900
O	-1.48475000	0.50734300	0.00027600
O	-2.38602800	-1.59990500	-0.00025100
B	-1.22613000	-0.85037400	-0.00001400

Cartesian coordinates in Firgure 4

TSB-1

0 1

C	5.69029600	-0.34751500	-1.13918100
C	4.47873300	-0.59742900	-0.52906900
C	4.30620900	-0.46817800	0.84488300
C	5.33715800	-0.08312200	1.67656000
C	6.56943100	0.17389400	1.07004400
C	6.74206400	0.04479100	-0.30723600
H	5.80962500	-0.45395800	-2.21004300
H	5.18882200	0.01008400	2.74508200
H	7.40809000	0.47861500	1.68488500
H	7.71235200	0.25124500	-0.74324200
O	3.01247500	-0.77990400	1.16107600
O	3.29548700	-0.99266700	-1.08968900
B	2.38753000	-1.09857600	-0.04109900
B	0.75748900	-1.48951000	-0.20524000
C	-2.06128800	-2.78857100	-1.97050400
C	-1.03979300	-2.39997700	-1.12746000
C	-1.14830100	-2.51633000	0.26026100
C	-2.28186100	-3.03039100	0.85542700
C	-3.32107500	-3.43027400	0.00876300
C	-3.21533200	-3.31089100	-1.37442200
H	-1.95921200	-2.69511700	-3.04497700
H	-2.35589100	-3.10755300	1.93327100
H	-4.22799700	-3.83705800	0.44161100
H	-4.03704500	-3.63364400	-2.00347700
O	-0.01880700	-2.03856700	0.84764100
O	0.16813400	-1.85459100	-1.44542700
C	-3.17494400	0.05296400	2.52811400
C	-2.14883100	0.41381000	1.66793900
C	-2.40221000	0.41079900	0.30169800
C	-3.62654100	0.03341500	-0.22752200
C	-4.65004800	-0.31726300	0.64892300
C	-4.42408100	-0.30335000	2.01931900
H	-3.00075700	0.04161800	3.59776300
H	-1.15634300	0.65854900	2.02960200
H	-3.77029100	-0.02083000	-1.30153400
H	-5.61161600	-0.62637500	0.25637100
H	-5.21947600	-0.58809700	2.69865200
S	-1.07106100	0.83814400	-0.82795000
O	0.21690400	0.40954600	-0.10484400
C	-1.08607600	2.62715900	-0.59688800
C	-2.13506400	3.36714800	-1.13005100
C	-0.03439200	3.21972200	0.08330400
C	-2.13179900	4.74512700	-0.96172100
H	-2.94535600	2.87679600	-1.66048700
C	-0.04333400	4.60323500	0.24073700
H	0.76672100	2.60039900	0.46897900
C	-1.08644600	5.36156200	-0.27741200
H	-2.94286400	5.33858800	-1.36696200
H	0.77059600	5.08619600	0.76863100
H	-1.08588300	6.43812800	-0.15232700

S3-1

0 1

C	5.06436500	0.89335800	-0.95464300
C	4.10920500	0.02214800	-0.47404100
C	4.44790400	-1.20696000	0.08177200
C	5.75841800	-1.62430900	0.18476200
C	6.73535500	-0.75038700	-0.29917100
C	6.39608000	0.48116600	-0.85664600
H	4.78679400	1.84739300	-1.38522000
H	6.00628000	-2.58410700	0.62022300
H	7.77839300	-1.03789500	-0.23943300
H	7.18006300	1.13371500	-1.22238800
O	3.30581200	-1.85161700	0.46943200
O	2.74865100	0.16224500	-0.43757900
B	2.24909500	-1.00876600	0.14691000
B	0.58224400	-1.26237200	0.36146300
C	-2.34675200	-2.84330600	-1.00617600
C	-1.24238700	-2.37405000	-0.32782300
C	-1.09832000	-2.54888000	1.05397100
C	-2.07278200	-3.18327200	1.79762200
C	-3.20449000	-3.65386900	1.11731100
C	-3.33727200	-3.49142600	-0.25690000
H	-2.43980000	-2.69906600	-2.07619600
H	-1.95205000	-3.31274800	2.86650900
H	-3.98341500	-4.16226900	1.67439700
H	-4.22030500	-3.86992500	-0.75953900
O	0.07448800	-2.01669400	1.47799800
O	-0.18038300	-1.68253300	-0.82179700
C	-4.23505800	-0.23015000	0.38324400
C	-2.92425100	0.21050700	0.48859300
C	-2.26516100	0.60390400	-0.67029800
C	-2.86007600	0.54970800	-1.92140900
C	-4.18283200	0.12303200	-2.00842700
C	-4.86277900	-0.26581800	-0.86057400
H	-4.75901000	-0.56844500	1.26884200
H	-2.40024700	0.21482100	1.43792700
H	-2.29844500	0.81025600	-2.81243800
H	-4.66947800	0.07214700	-2.97527600
H	-5.88413000	-0.62086900	-0.93586100
S	-0.53984600	1.07113900	-0.56558300
O	-0.01161600	0.28016300	0.67260600
C	-0.70164400	2.71622300	0.13937500
C	-1.26430100	3.71254000	-0.65099500
C	-0.23990400	2.96328200	1.42280600
C	-1.37673300	4.99360200	-0.12960600
H	-1.61922200	3.49209000	-1.65276900
C	-0.35795100	4.25496800	1.92952100
H	0.19935900	2.15926100	1.99905700
C	-0.92342000	5.26381200	1.15959600
H	-1.81676400	5.78109100	-0.72972500
H	-0.00345700	4.46824100	2.93101100
H	-1.01064400	6.26630100	1.56189500

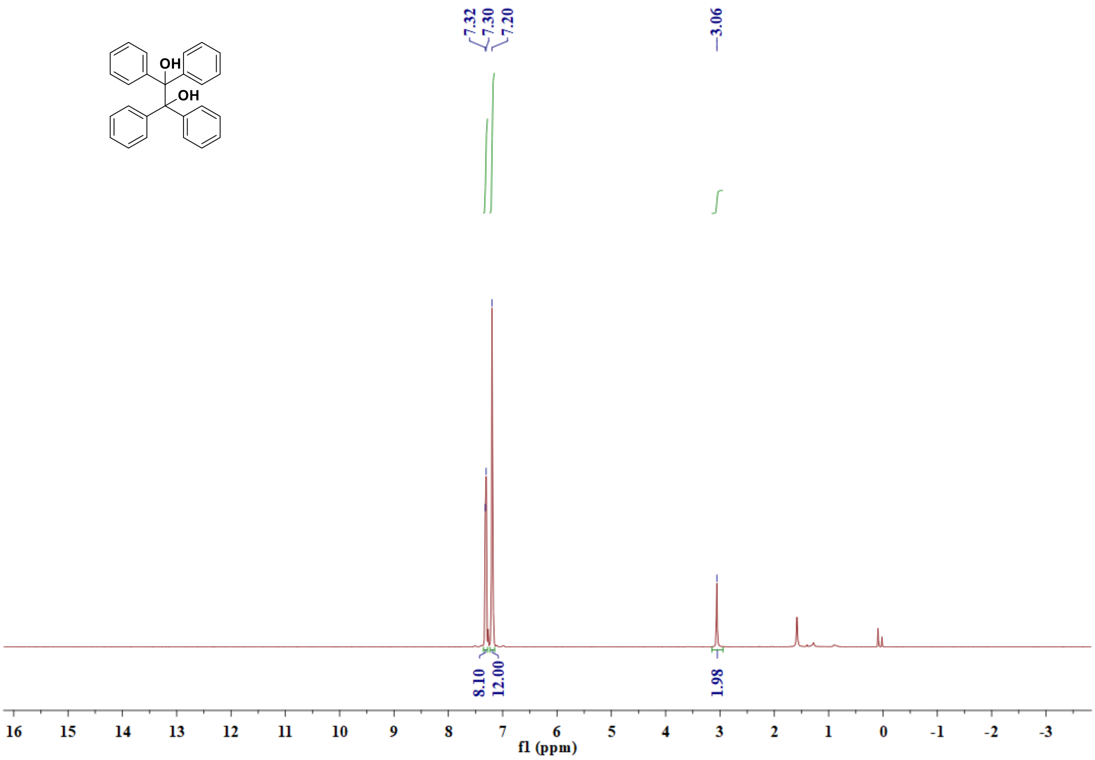
TSB-1

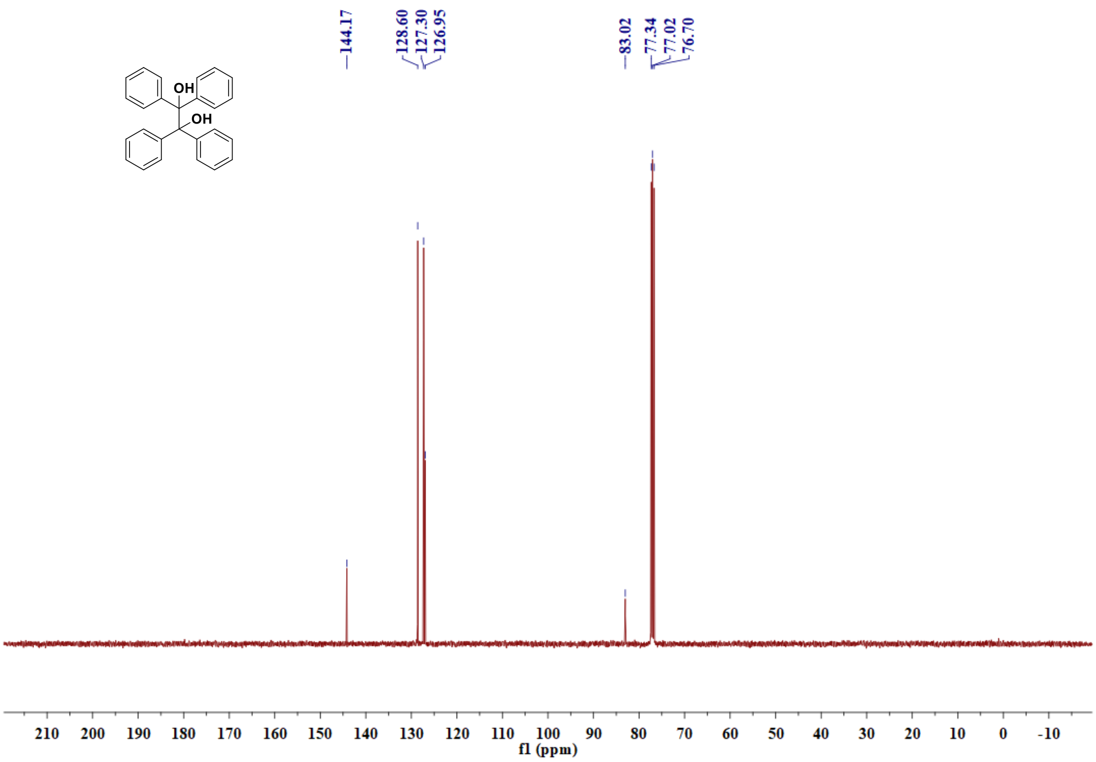
0 1

C	5.31306300	-1.74633500	-1.07270900
C	4.08751300	-1.34875400	-0.58138100
C	3.97196200	-0.57214500	0.56771900
C	5.07641700	-0.15689900	1.28146000
C	6.32418000	-0.55154000	0.79172300
C	6.43979600	-1.32866000	-0.35960200
H	5.38680100	-2.35194200	-1.96709900
H	4.97149900	0.44402000	2.17602400
H	7.21988000	-0.24733000	1.32021300
H	7.42375200	-1.61729100	-0.70970100
O	2.64564000	-0.33843400	0.81493100
O	2.83586000	-1.61286900	-1.07032700
B	1.95325400	-0.99267200	-0.20064800
B	0.17351100	-1.02314700	-0.26157700
C	-2.47569100	-3.46516100	-0.34364800
C	-1.53022600	-2.48180500	-0.12993400
C	-1.54400800	-1.69402600	1.03014600
C	-2.51073800	-1.85827200	1.99976700
C	-3.48385400	-2.84060500	1.77979600
C	-3.46459200	-3.62974600	0.63362900
H	-2.44689600	-4.07227800	-1.24069300
H	-2.51269800	-1.23686100	2.88730700
H	-4.25873300	-2.99500200	2.52209300
H	-4.22348900	-4.39176200	0.49660600
O	-0.52456900	-0.80637300	0.99869400
O	-0.51729200	-2.10217400	-0.93854100
C	-4.13763400	0.92291800	0.70362900
C	-2.91487800	1.40699600	0.26235200
C	-2.34865900	0.85923400	-0.88926300
C	-2.99026200	-0.16438300	-1.58569000
C	-4.20942000	-0.64328900	-1.12264100
C	-4.78635100	-0.10100500	0.01801900
H	-4.58035600	1.34256700	1.59956800
H	-2.41009800	2.19362500	0.80841900
H	-2.52429600	-0.60593600	-2.46031900
H	-4.69364500	-1.45820900	-1.64665300
H	-5.73044000	-0.48693200	0.38340700
S	-0.79707900	1.40481600	-1.56942300
O	0.52611300	0.15140500	-0.99875400
C	-0.31981500	2.73338100	-0.48449800
C	-0.57626600	4.03485400	-0.90684100
C	0.28973400	2.46795900	0.73971600
C	-0.22464300	5.09549700	-0.07976600
H	-1.04396200	4.21547800	-1.86807100
C	0.63352700	3.54021500	1.55426200
H	0.48510700	1.44723300	1.04372900
C	0.37823500	4.84709200	1.14857300
H	-0.41784000	6.11271300	-0.39901600
H	1.10900300	3.34883400	2.50889200
H	0.65549200	5.67555500	1.79022700

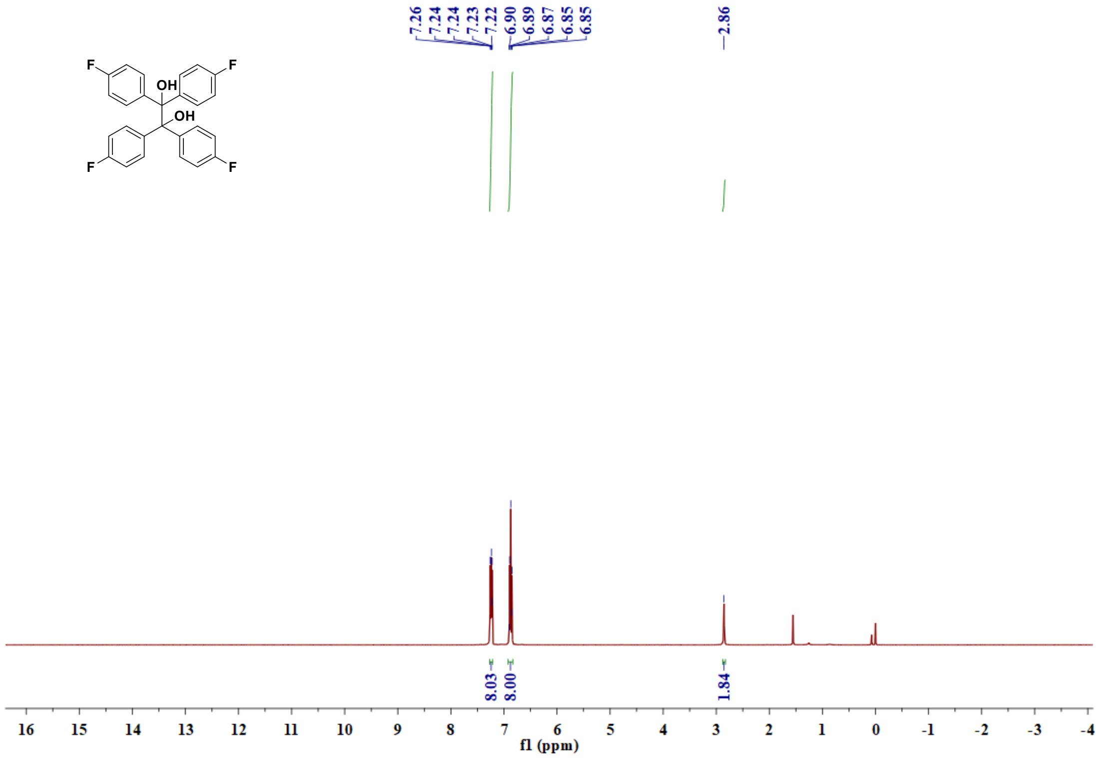
NMR spectra

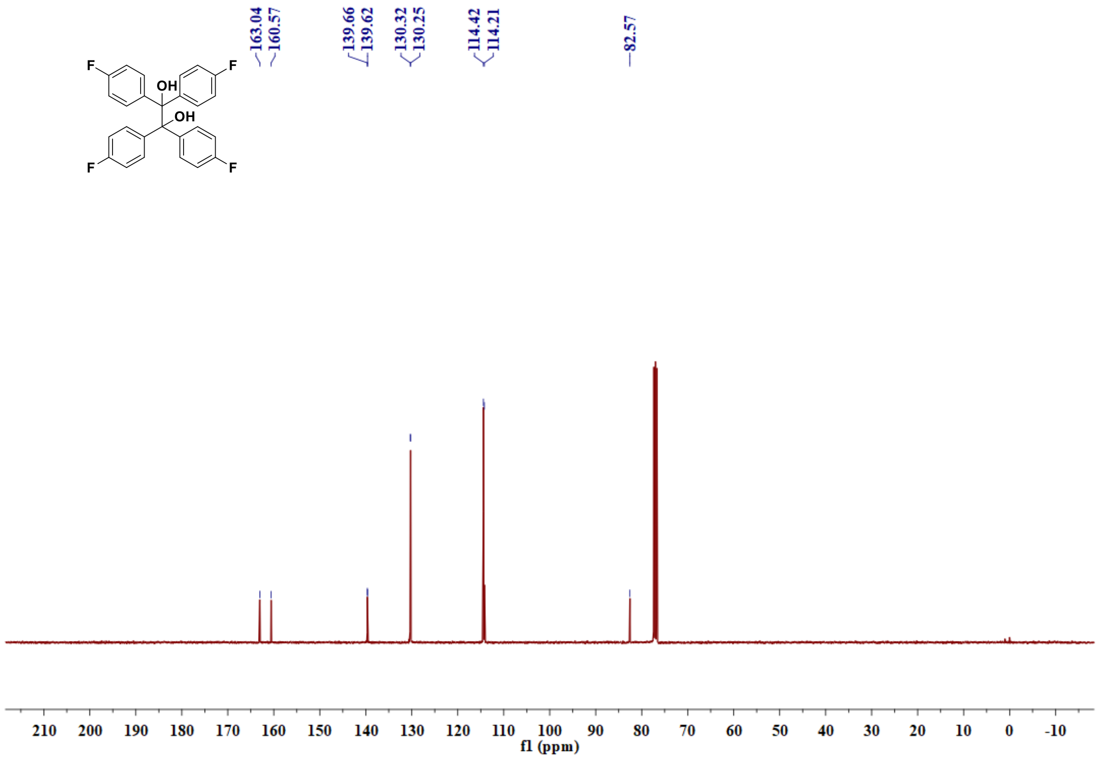
Aromatic pinacol 4a





Aromatic pinacol 4b





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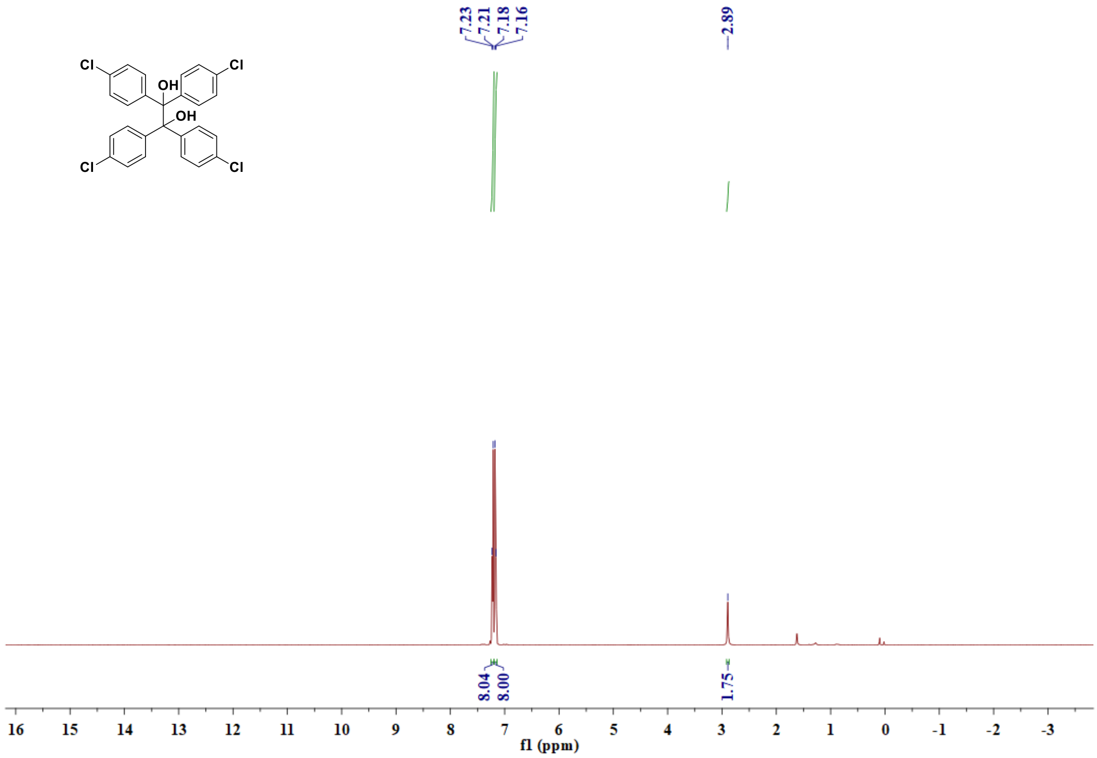
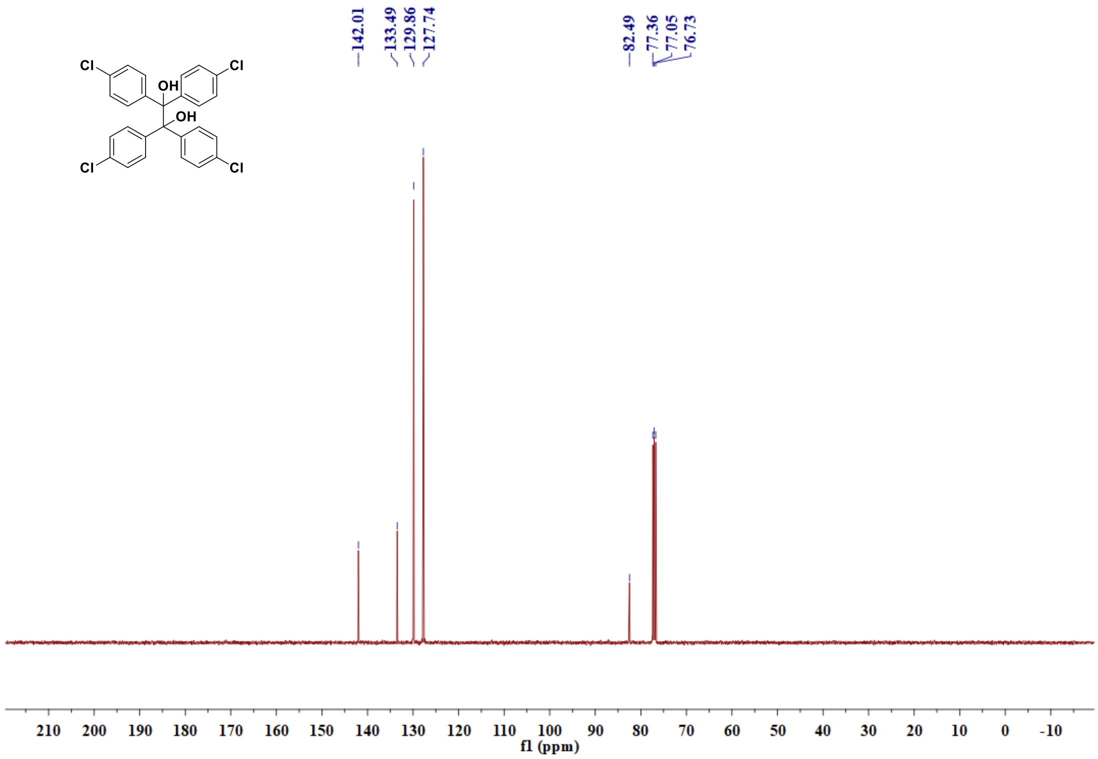
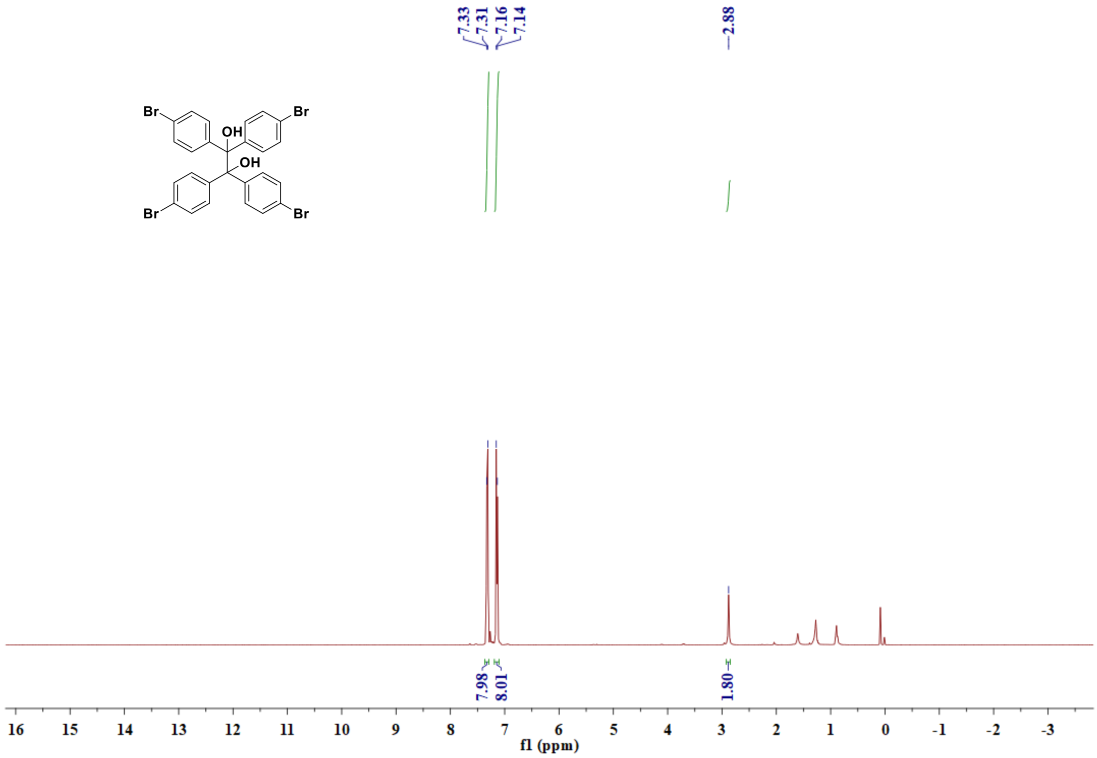
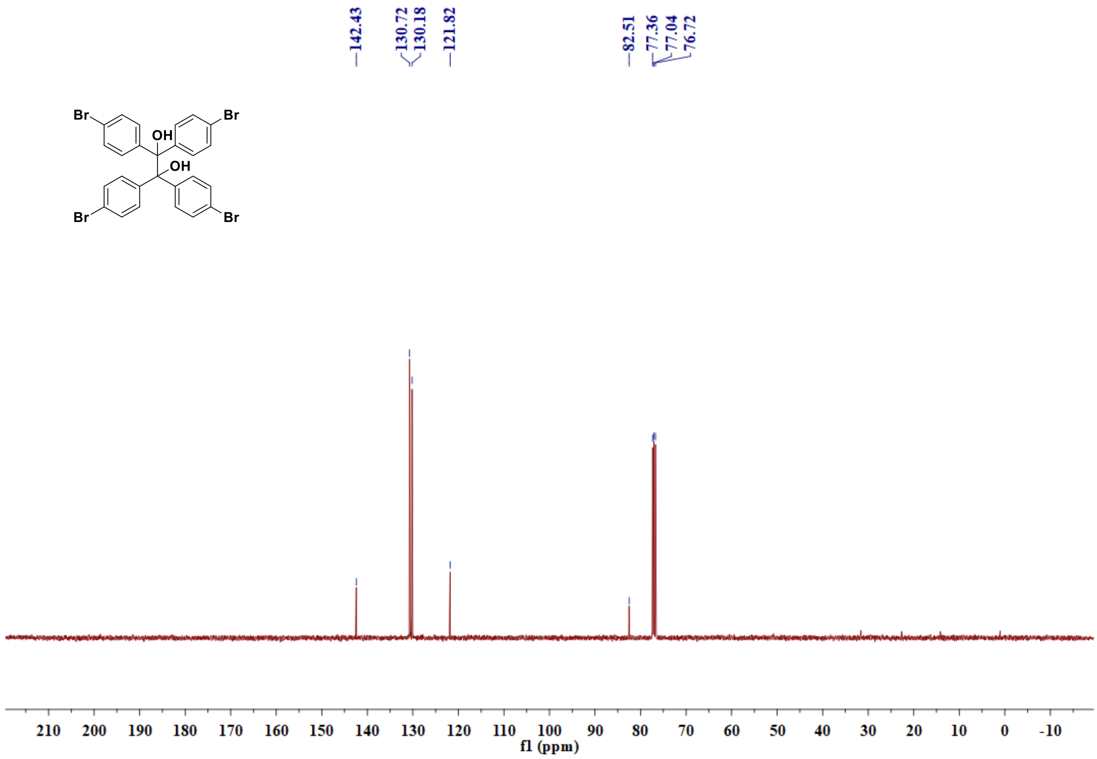


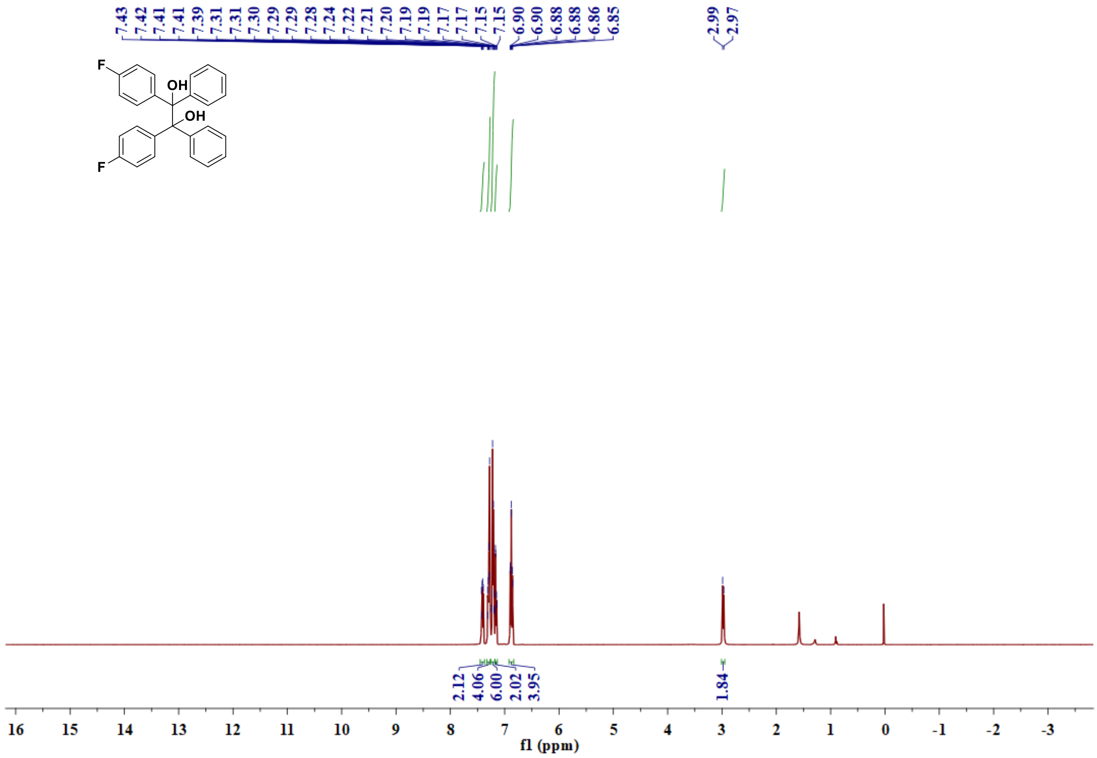


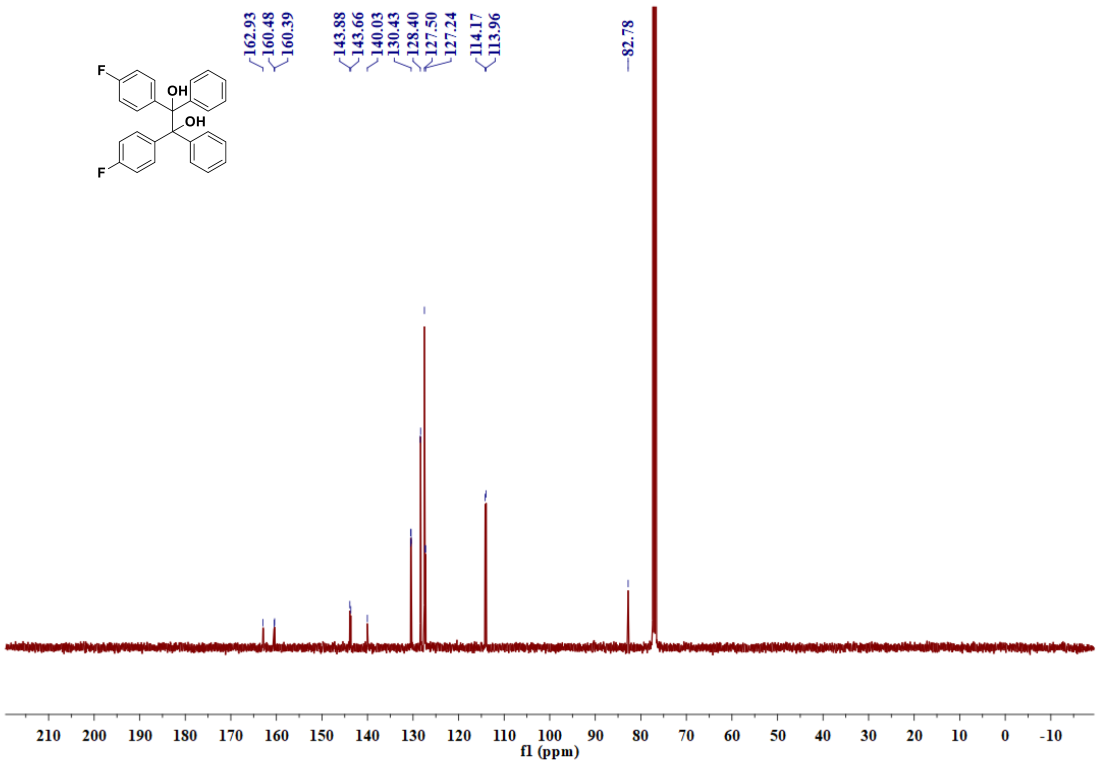
Aromatic pinacol 4d





Arylamine 4e





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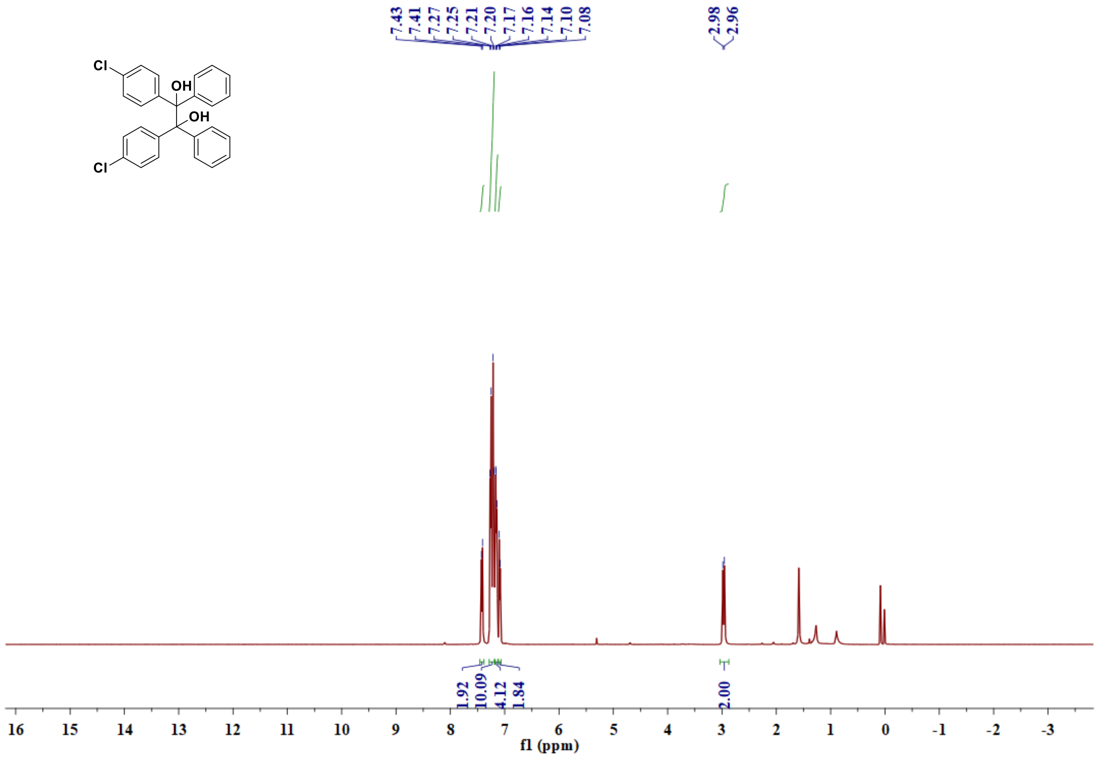

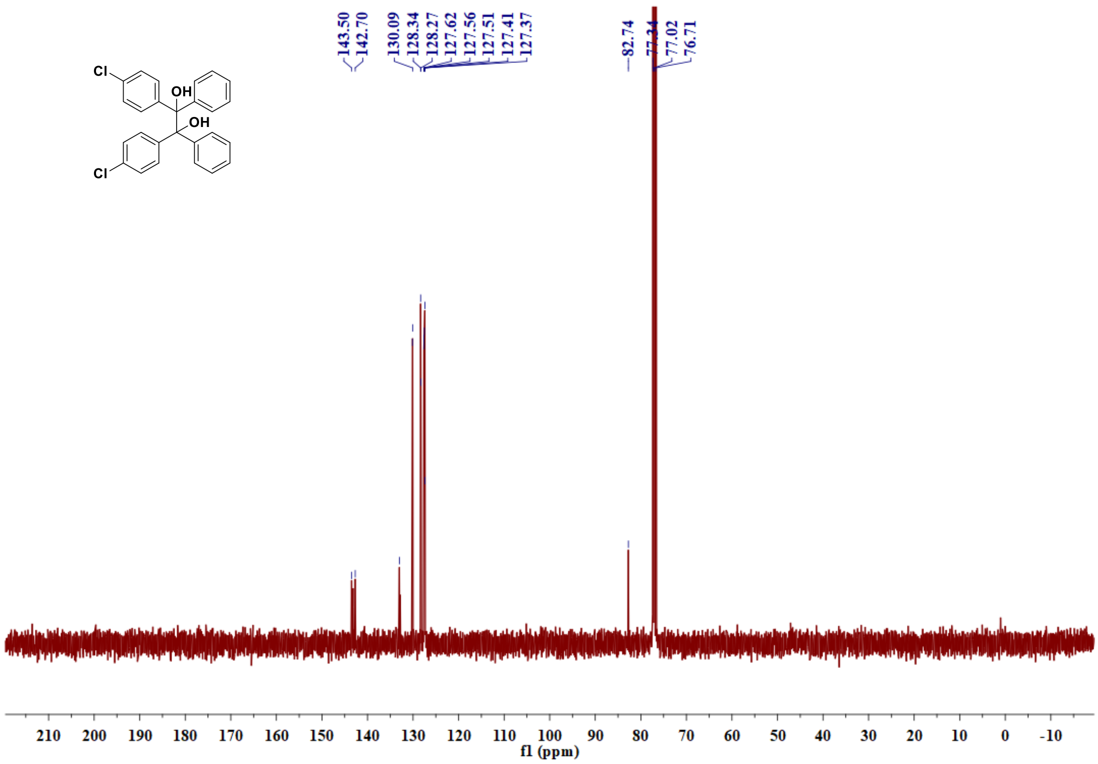

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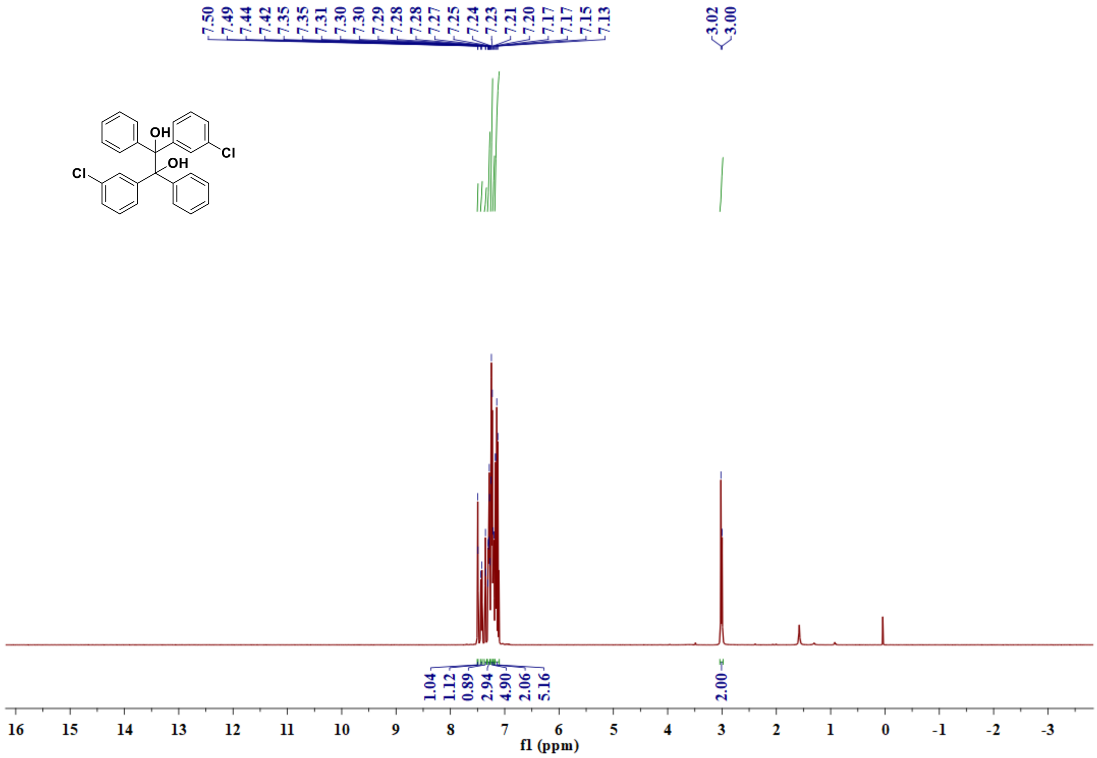
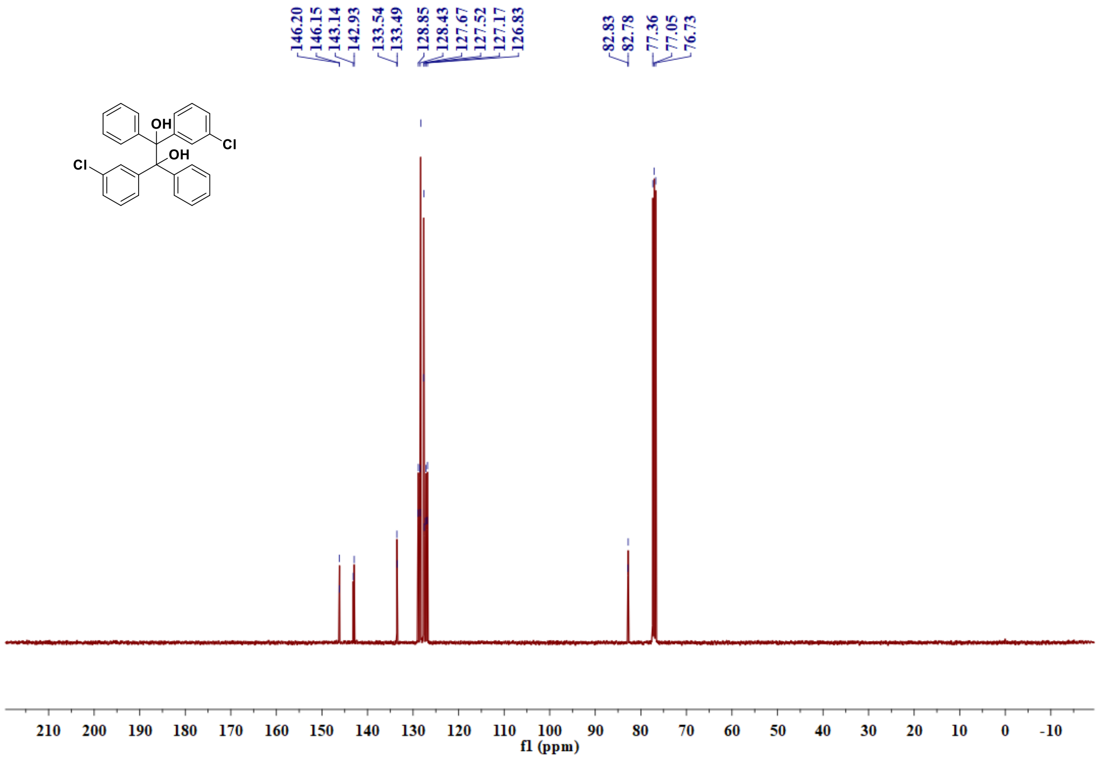
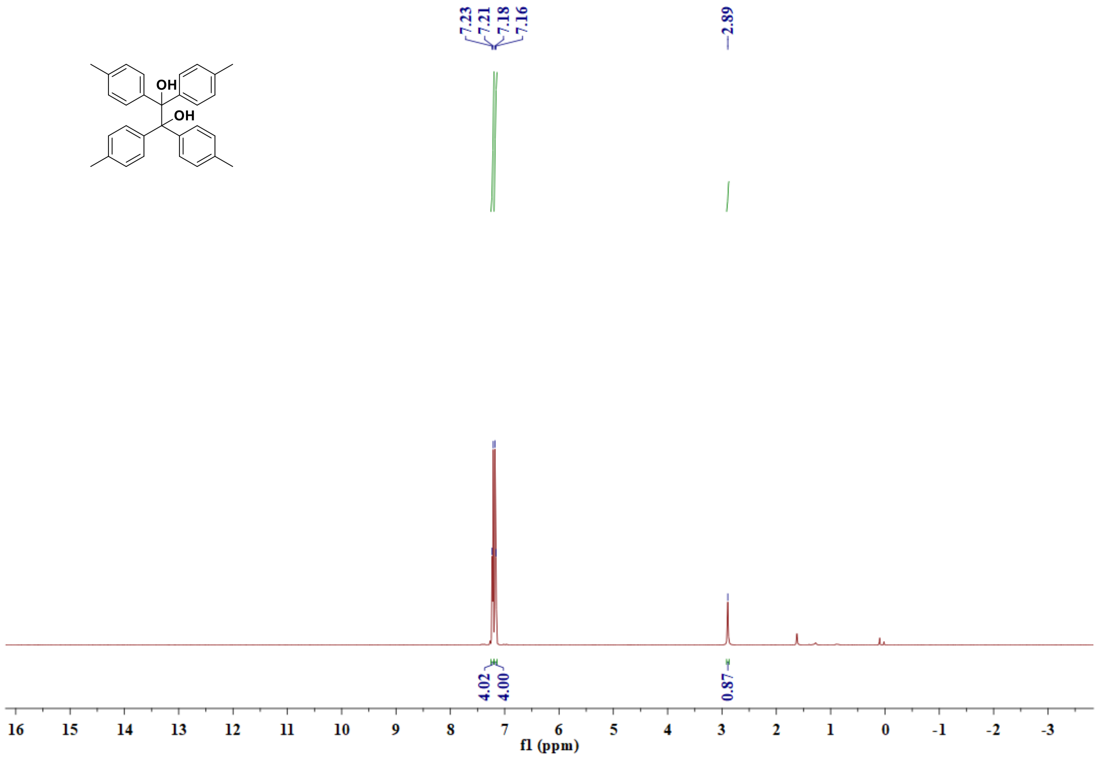
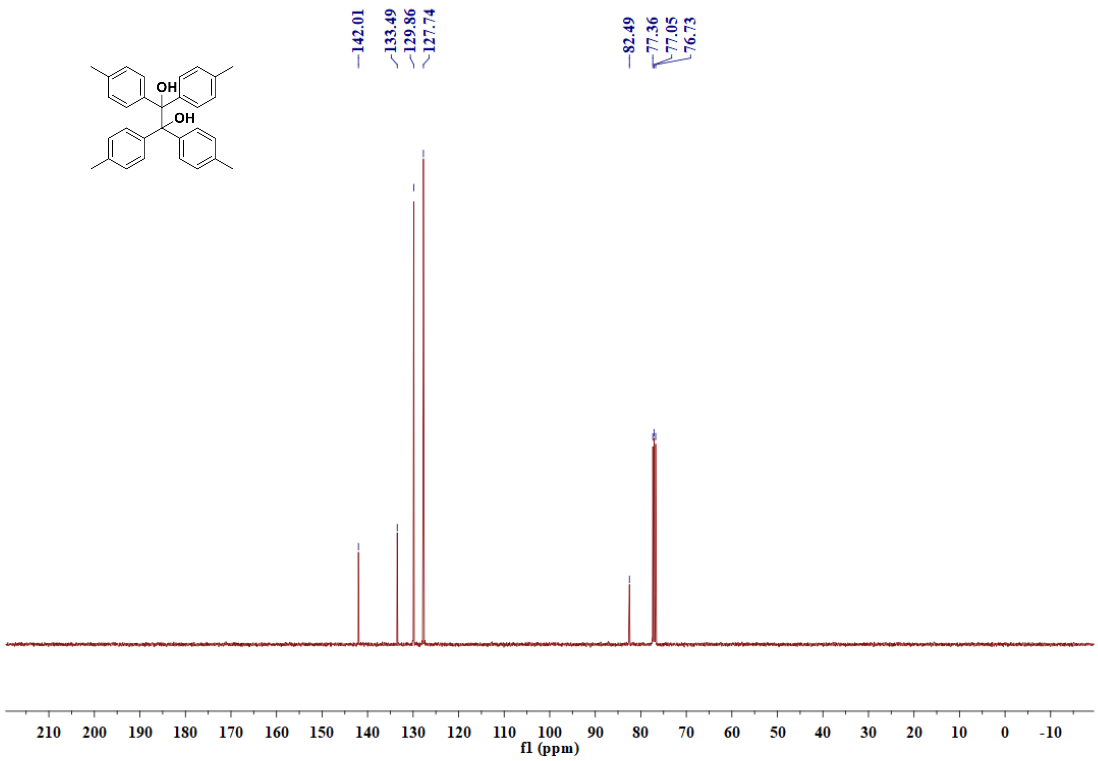




Aromatic ketone 4h





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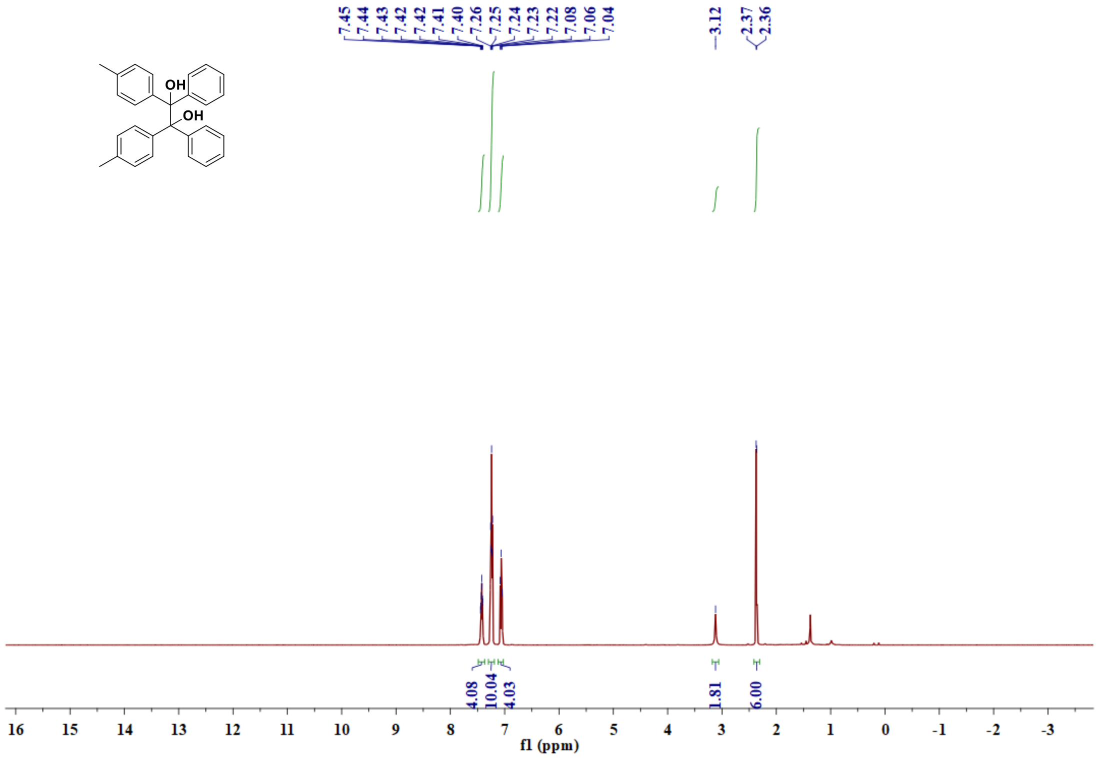

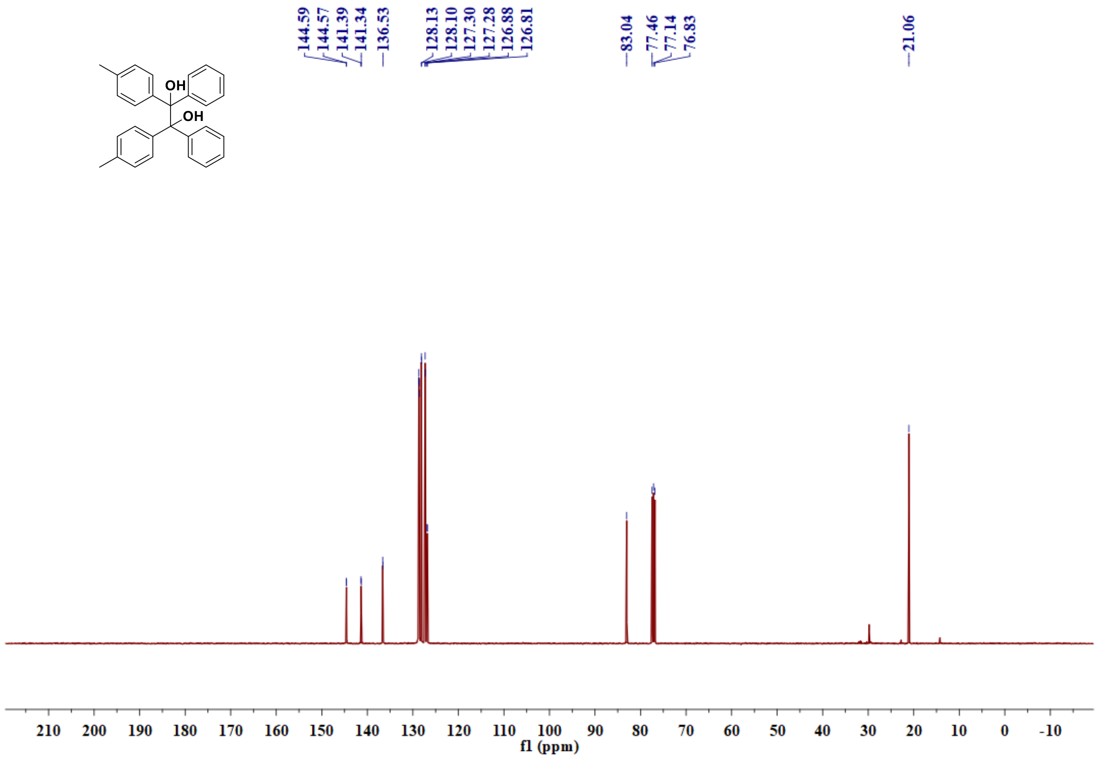

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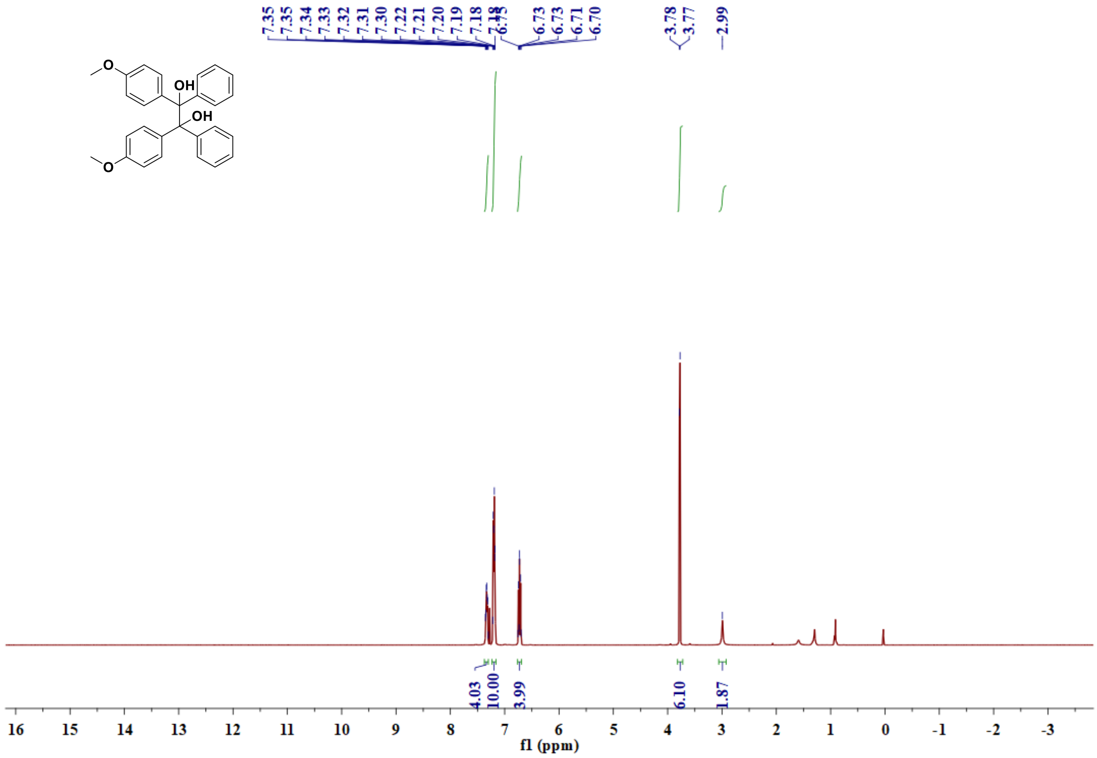

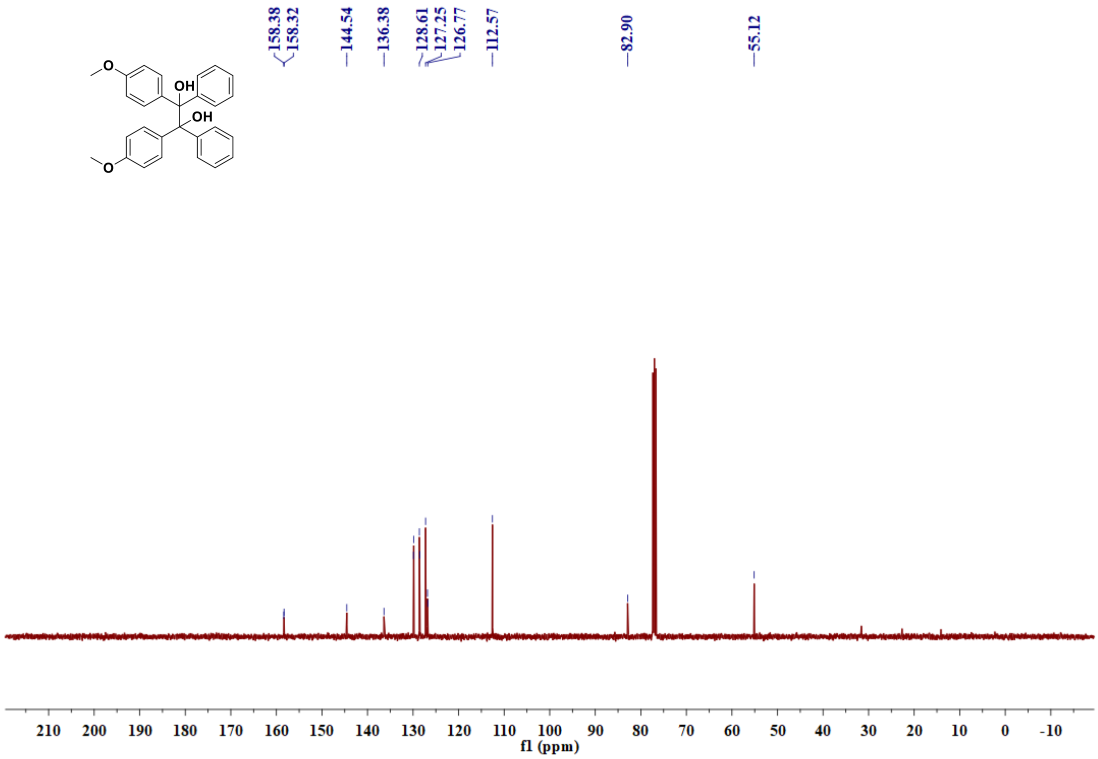

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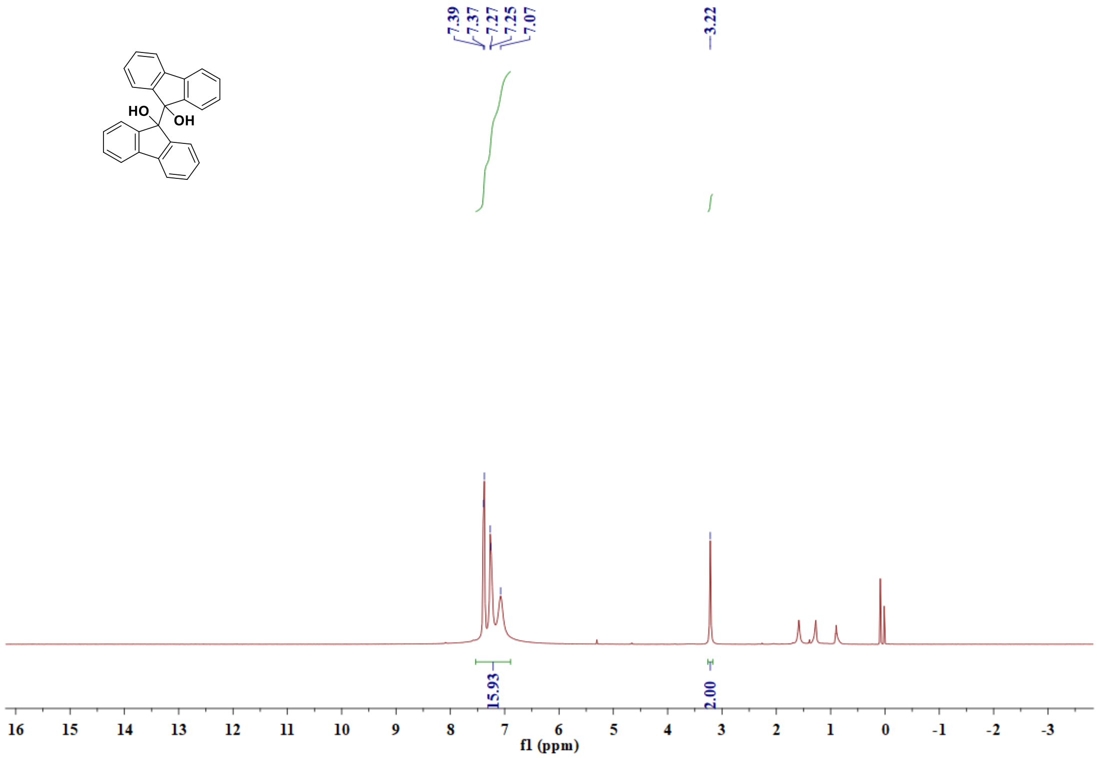

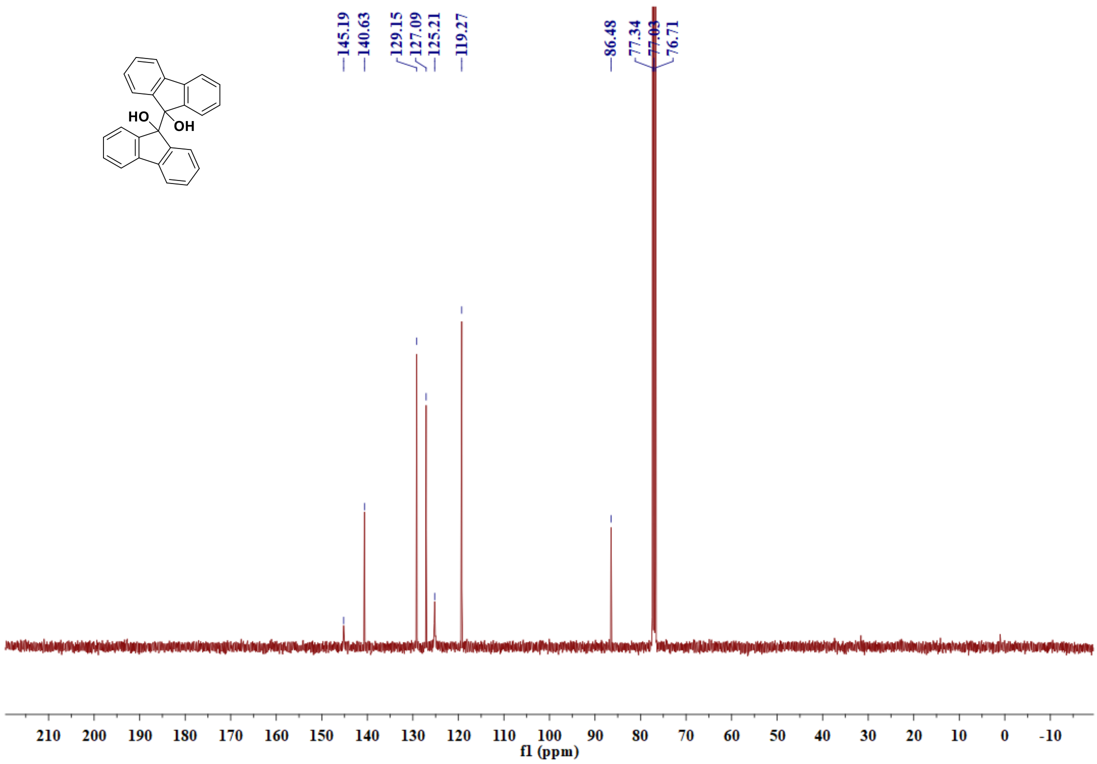

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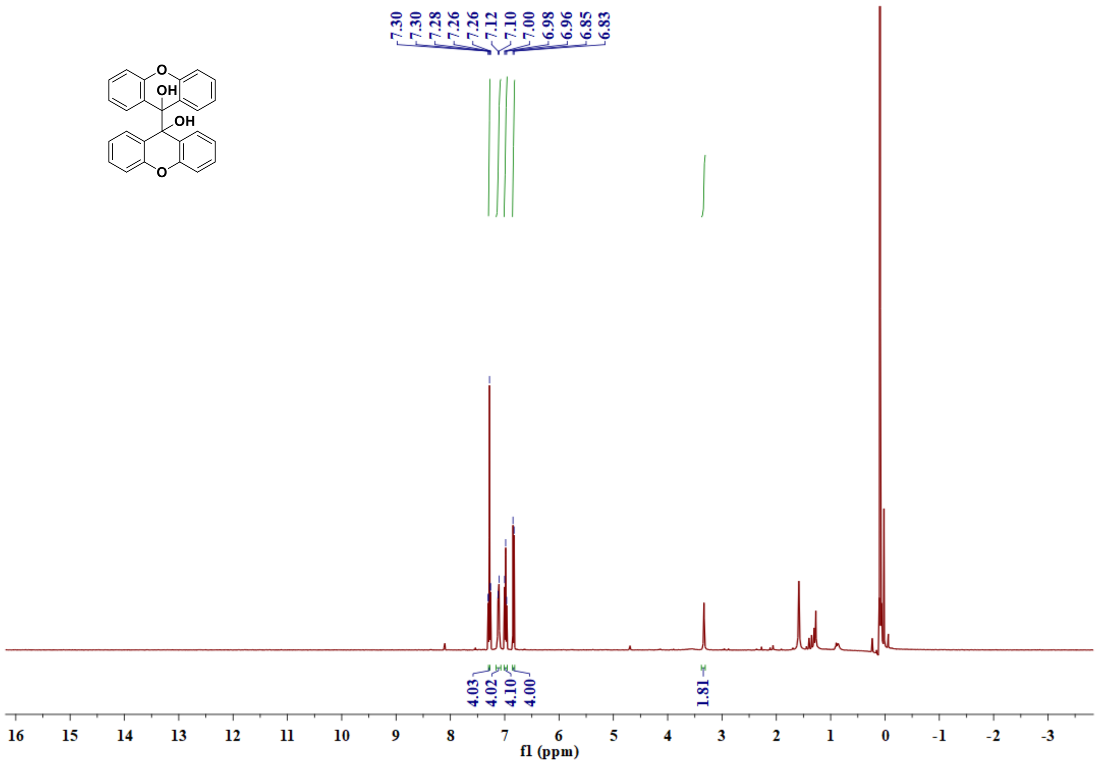

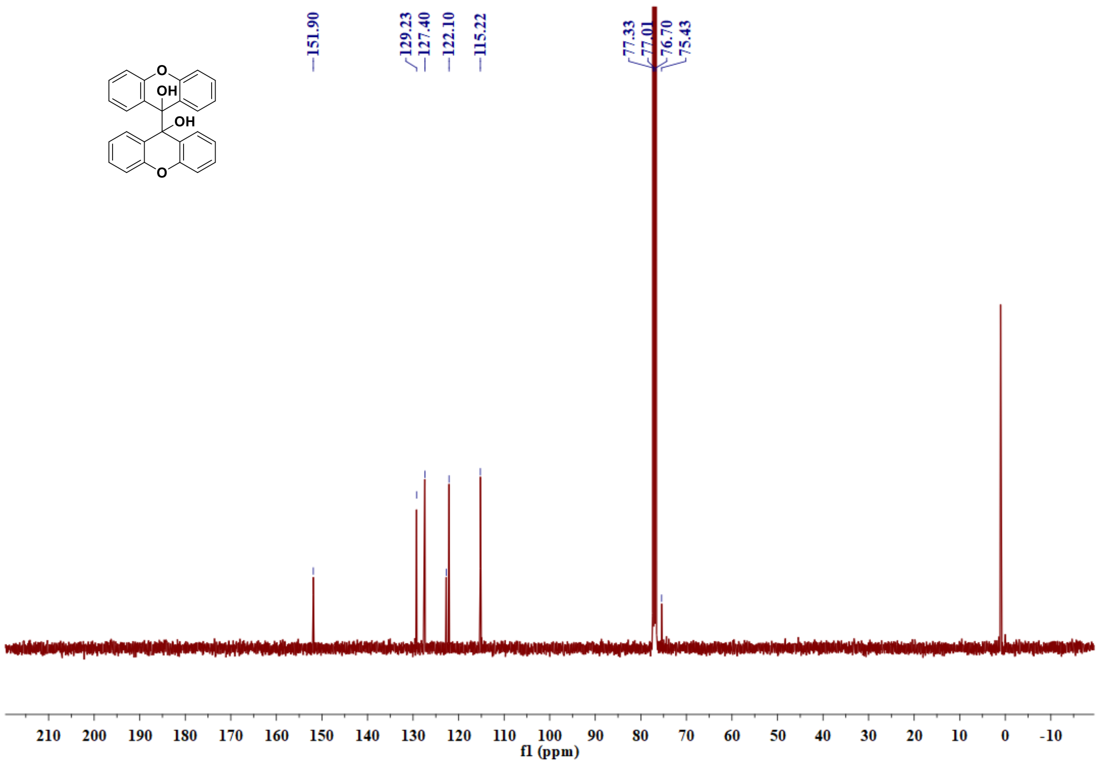

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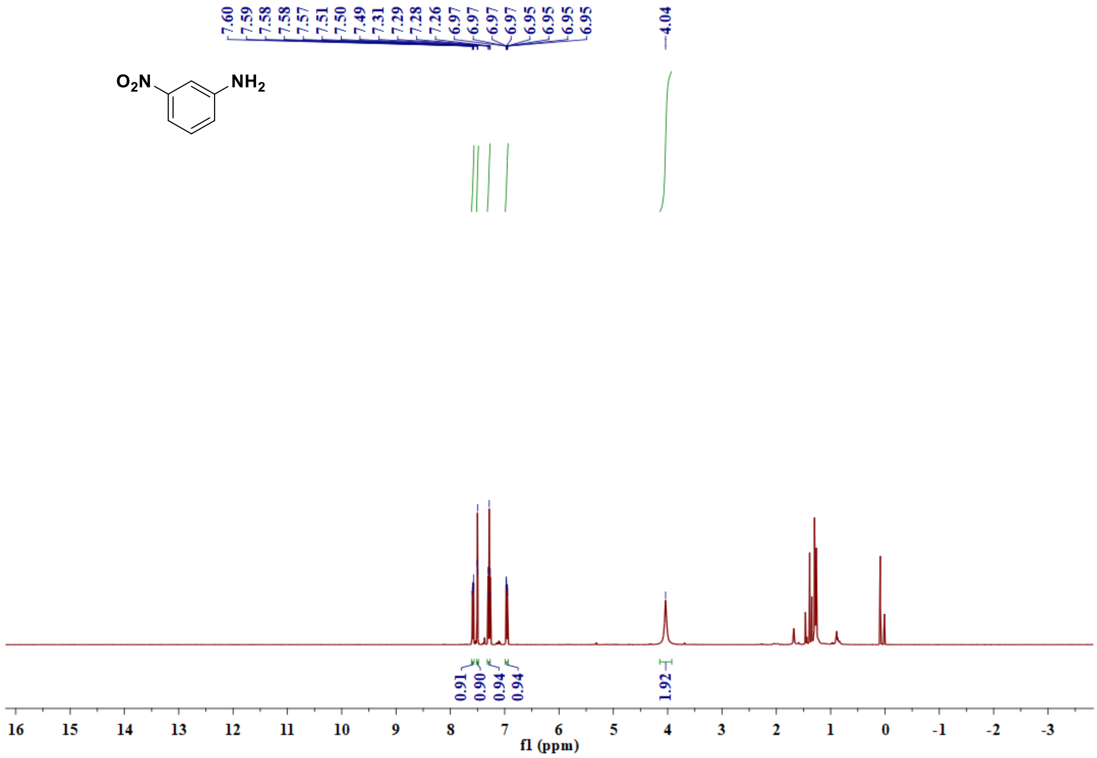

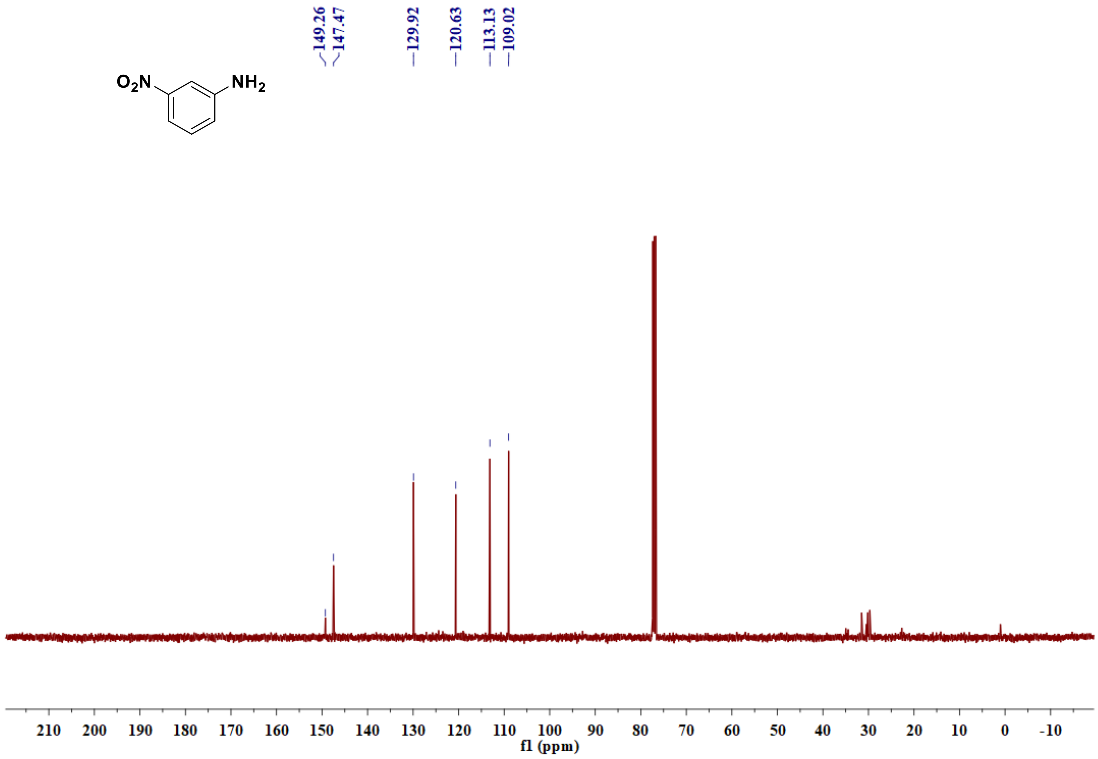

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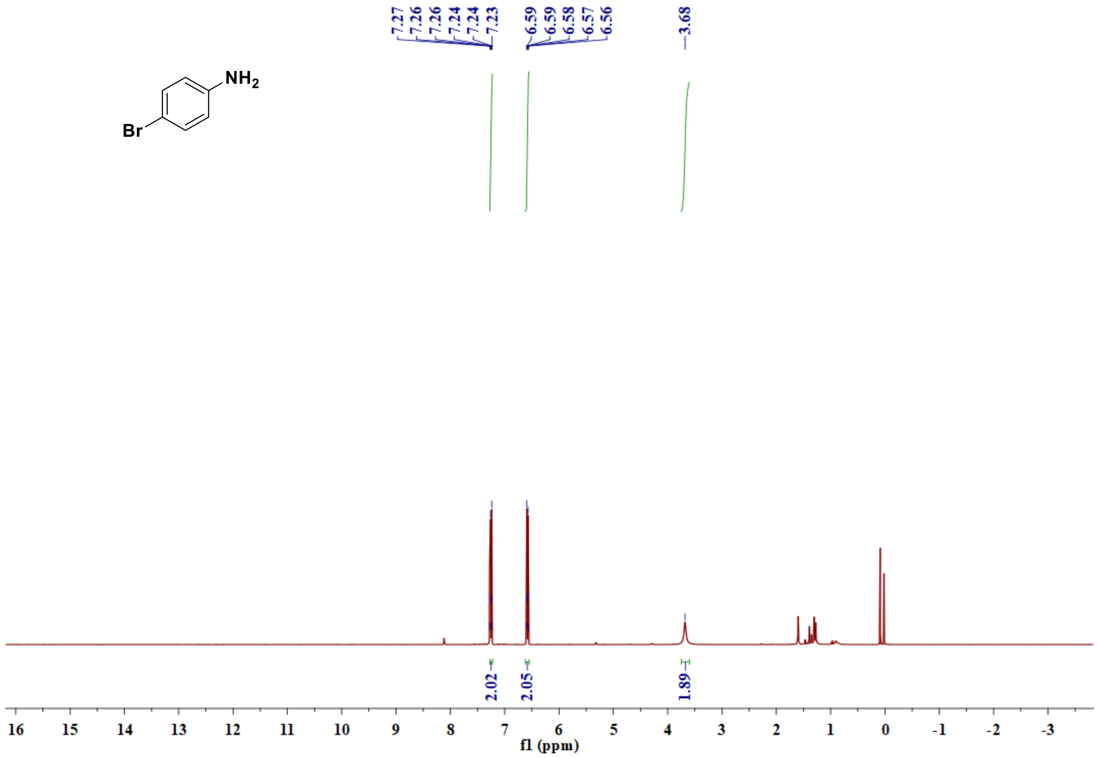

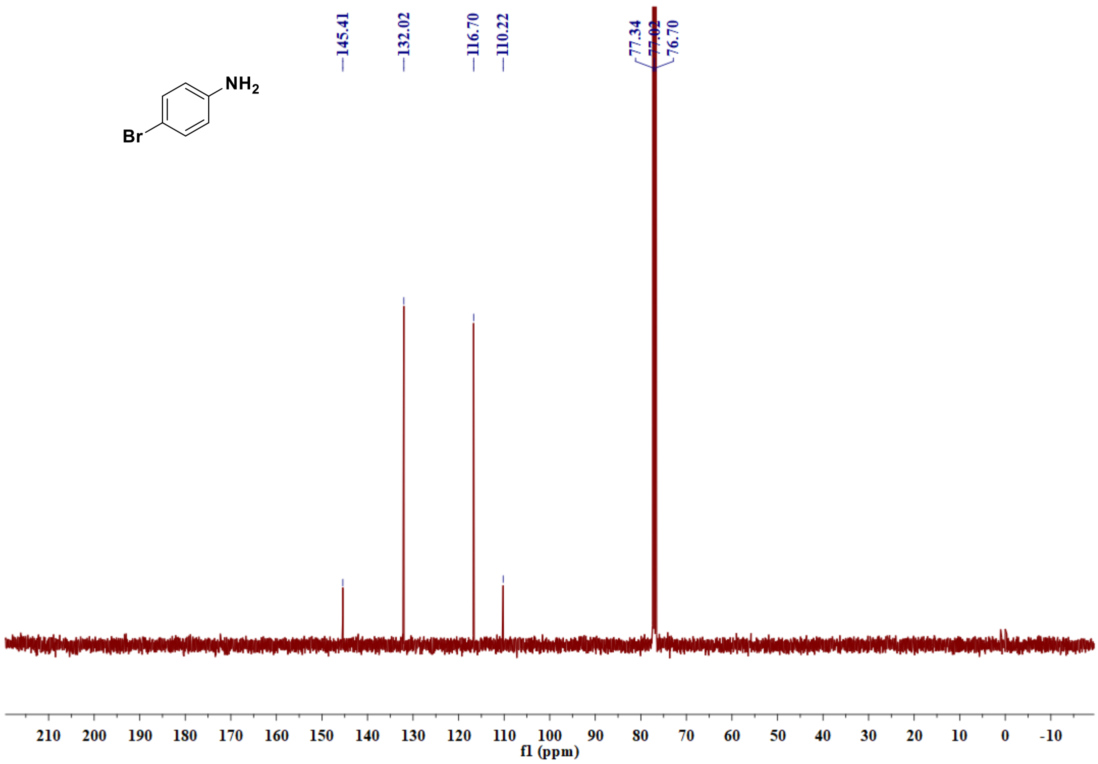

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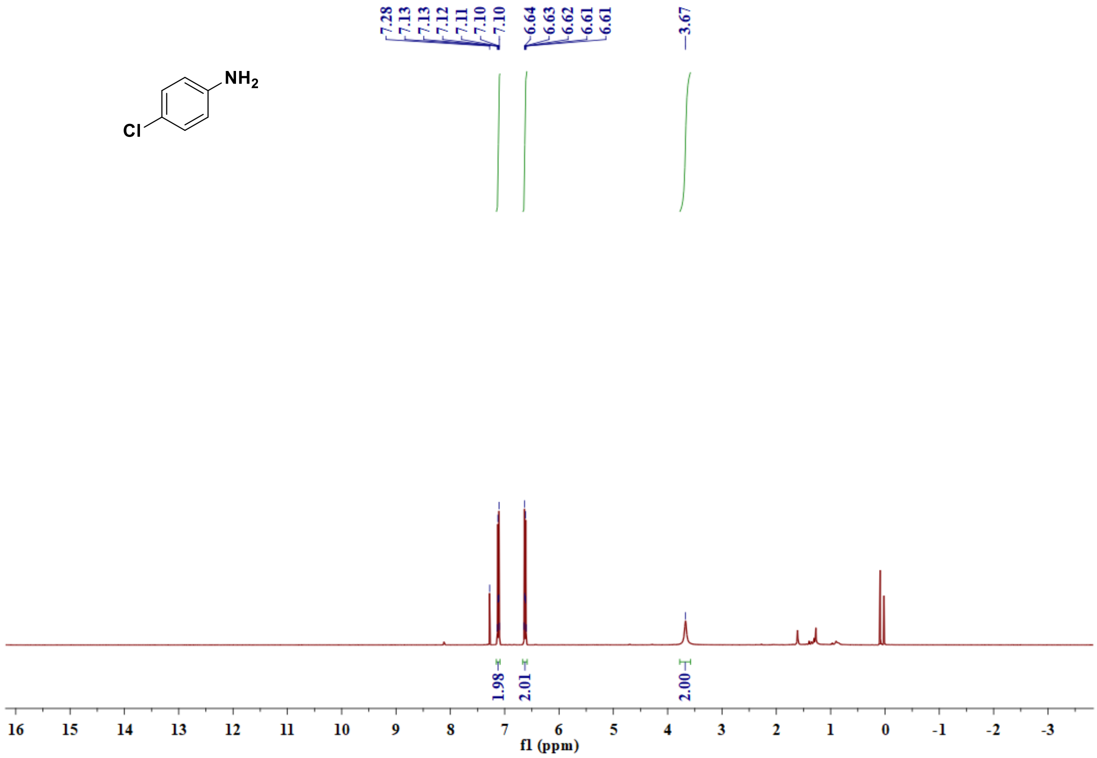

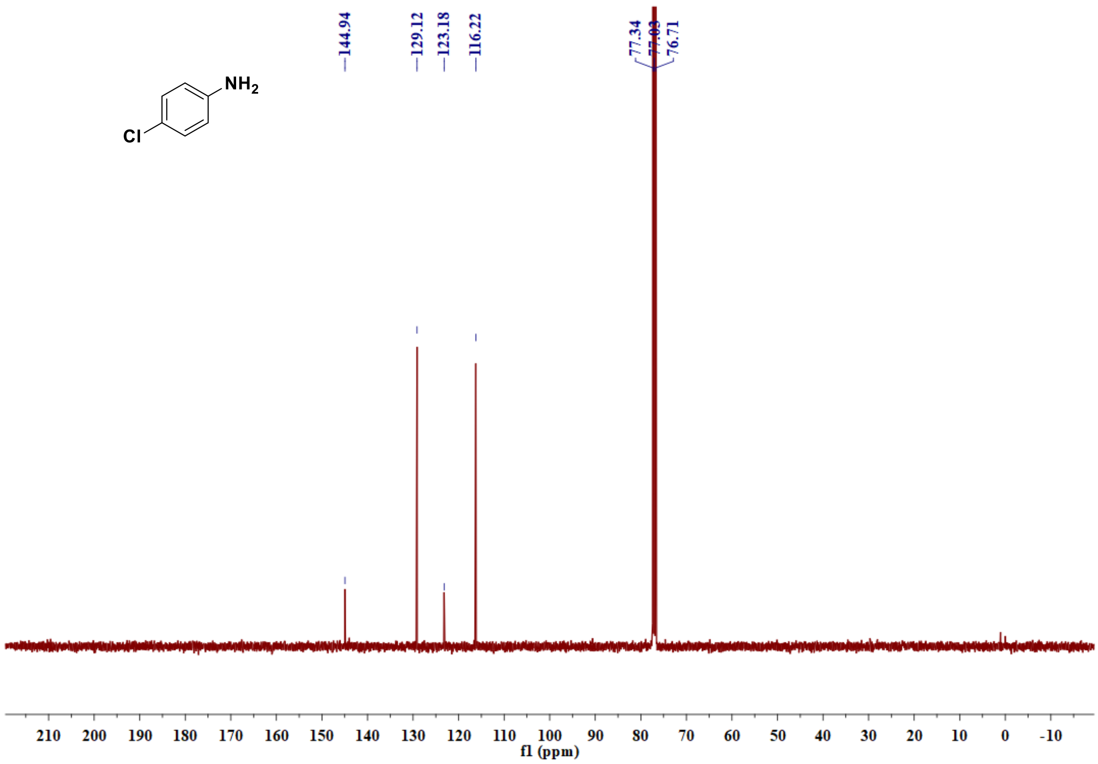

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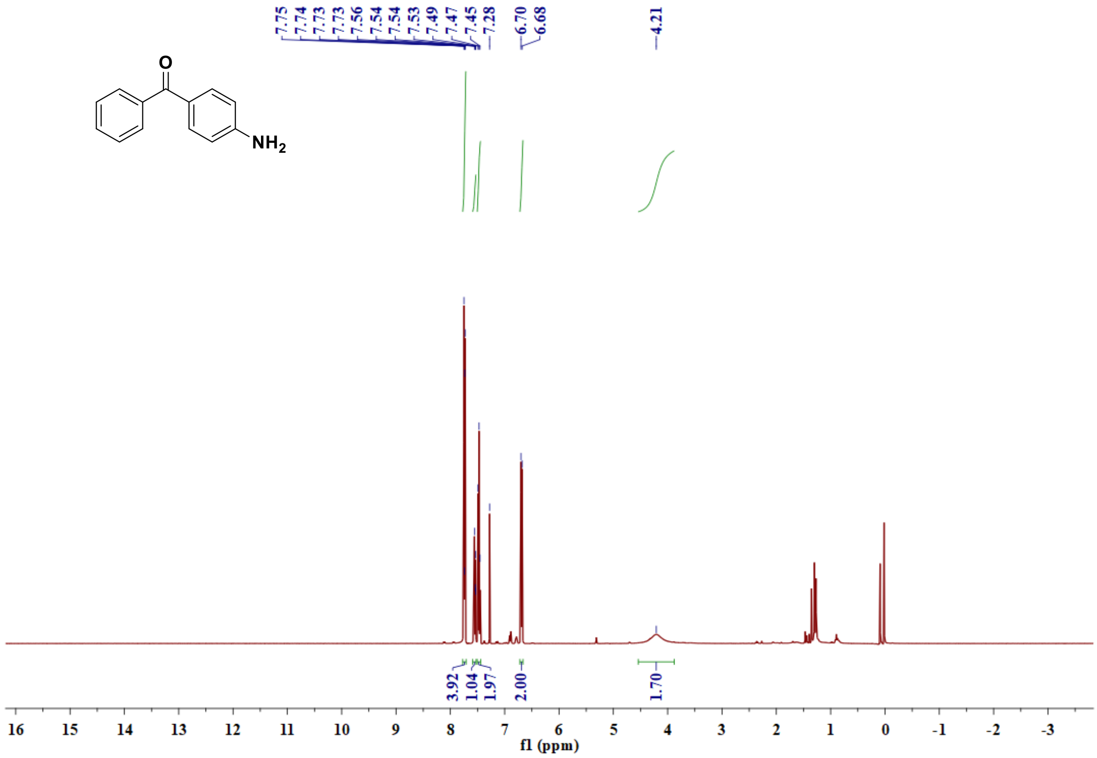

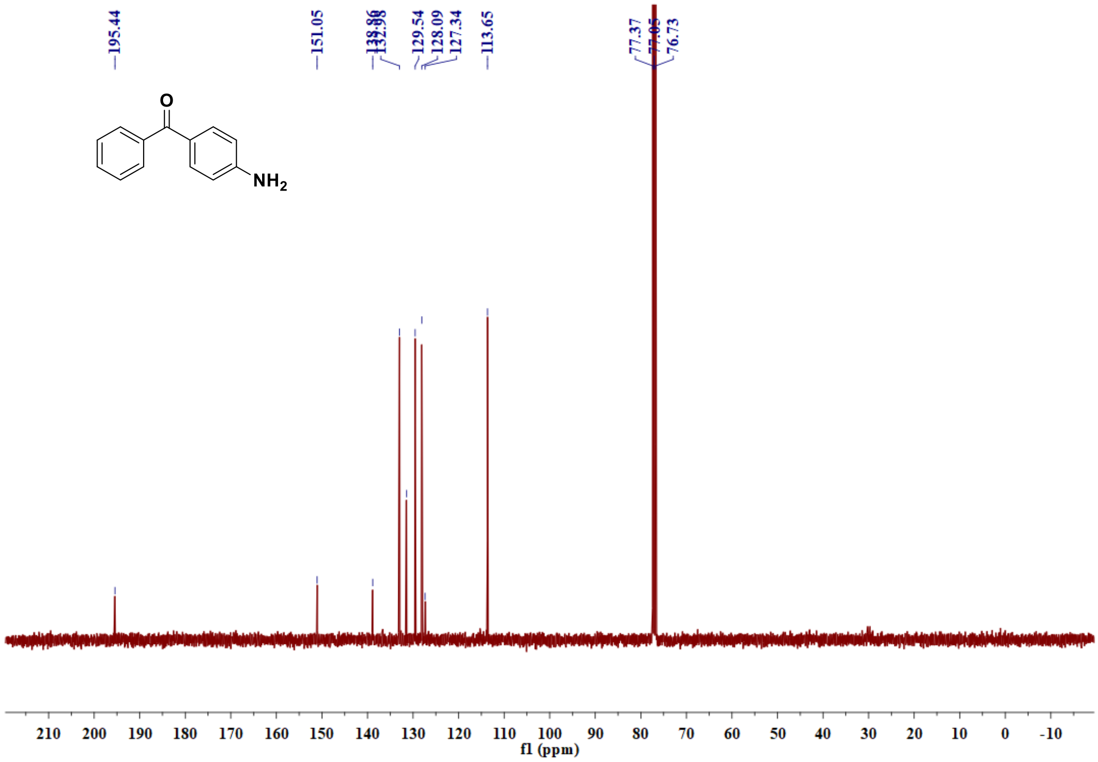

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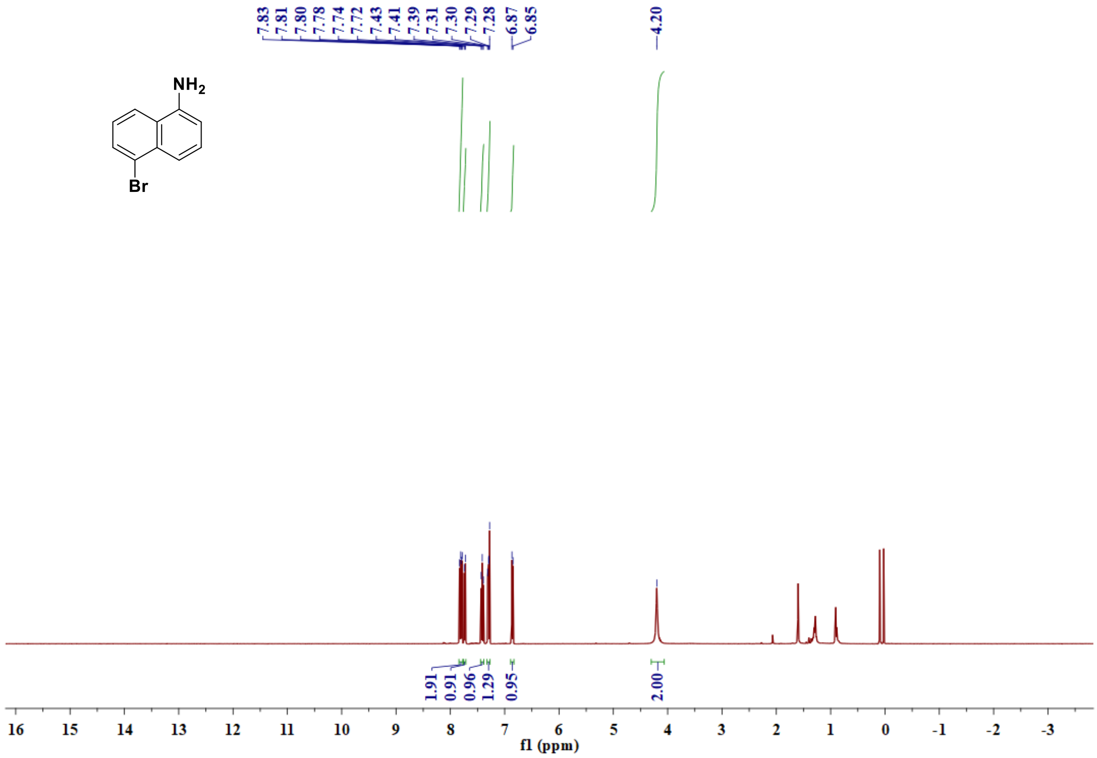

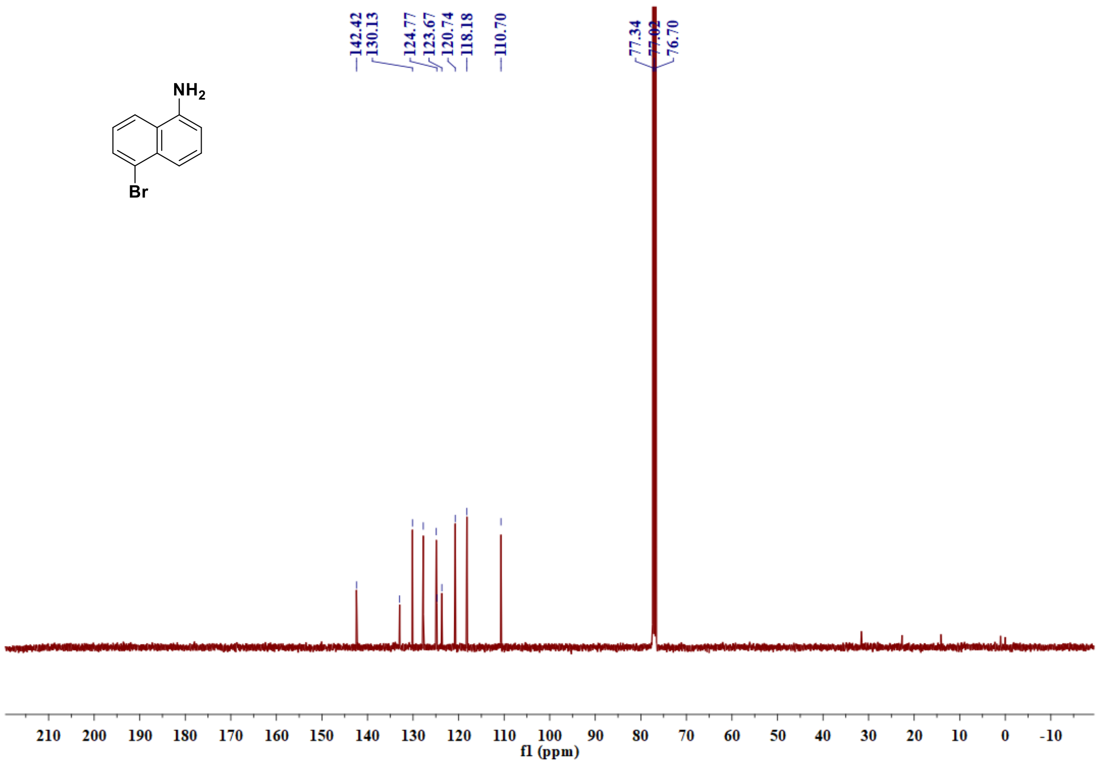

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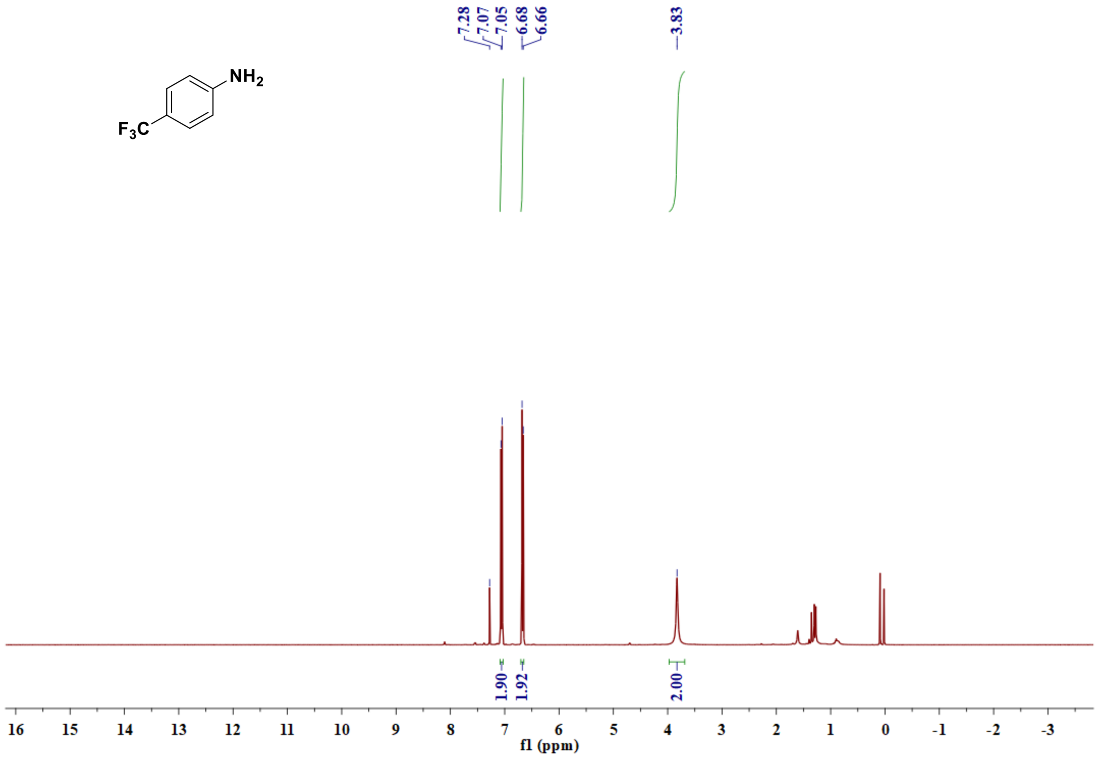

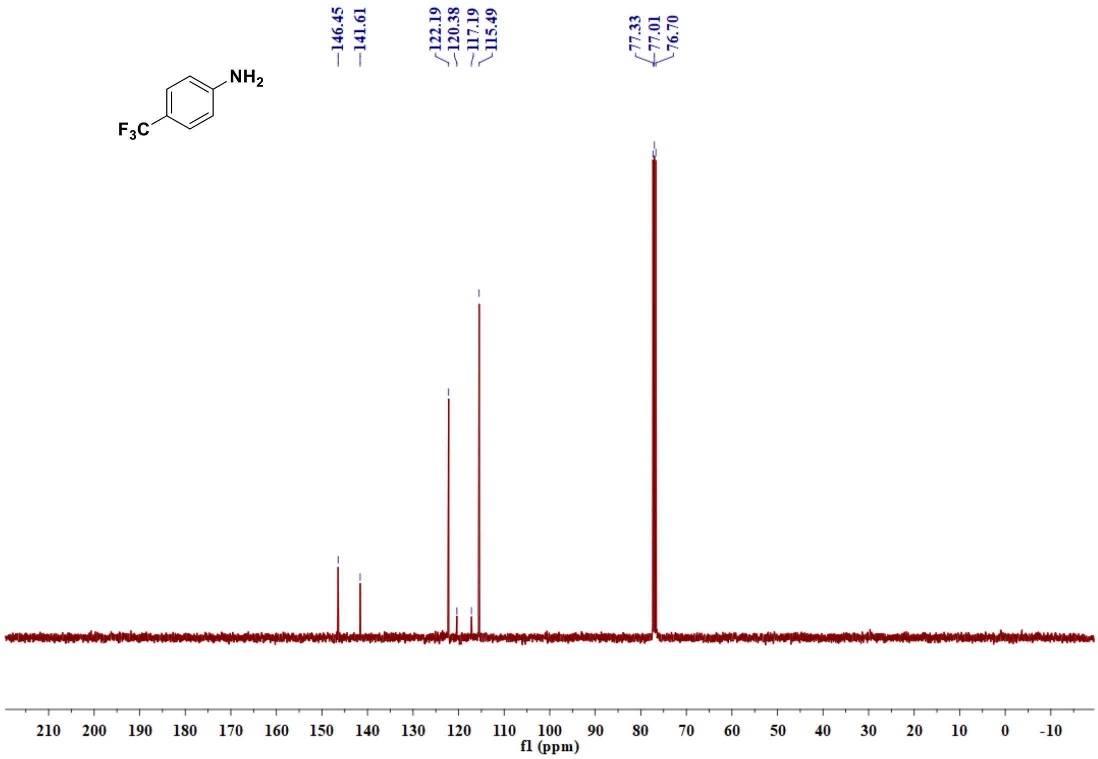

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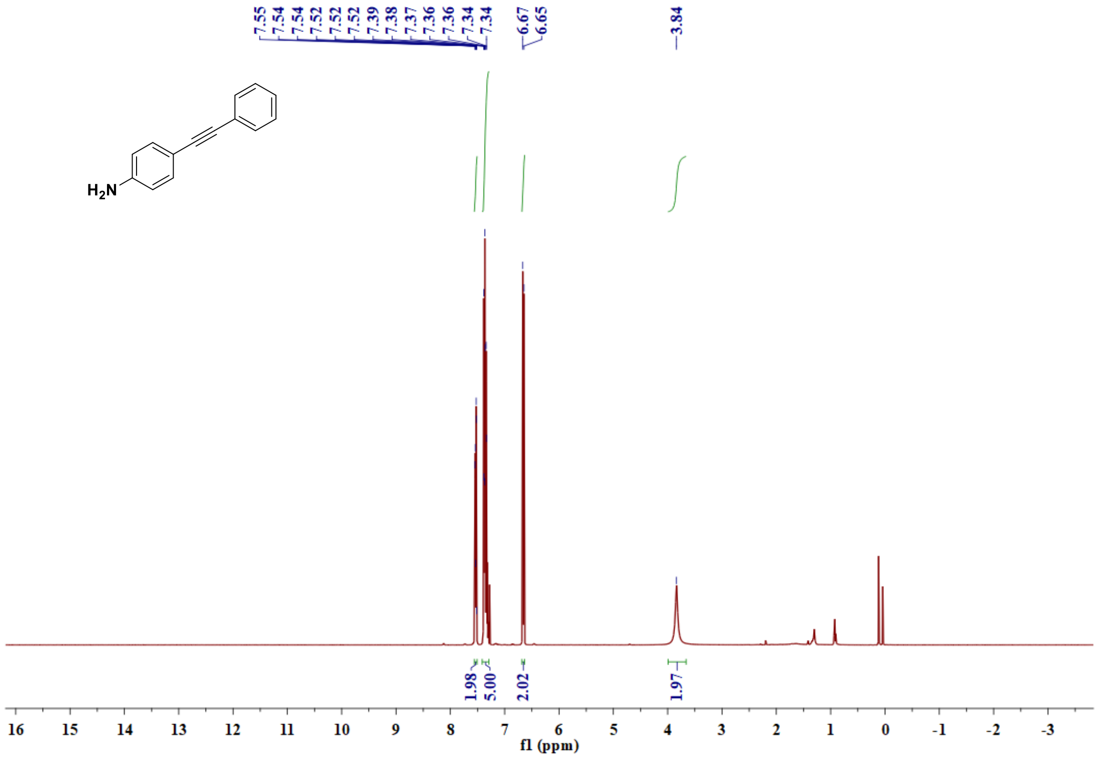

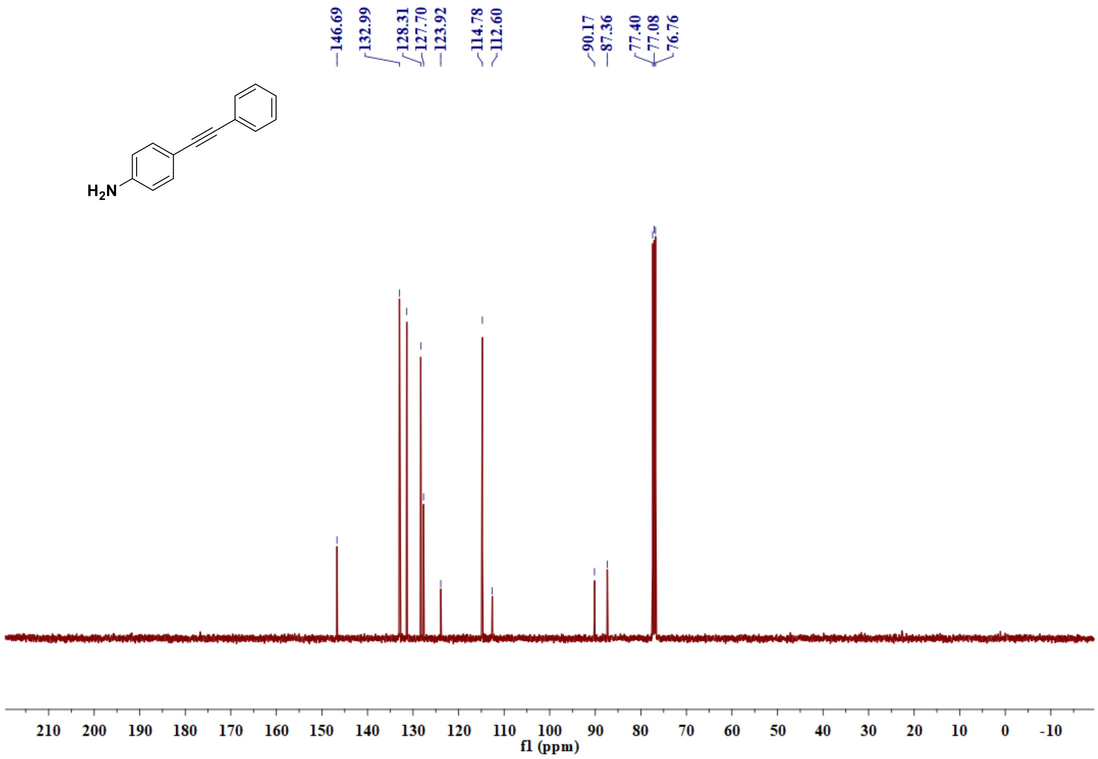

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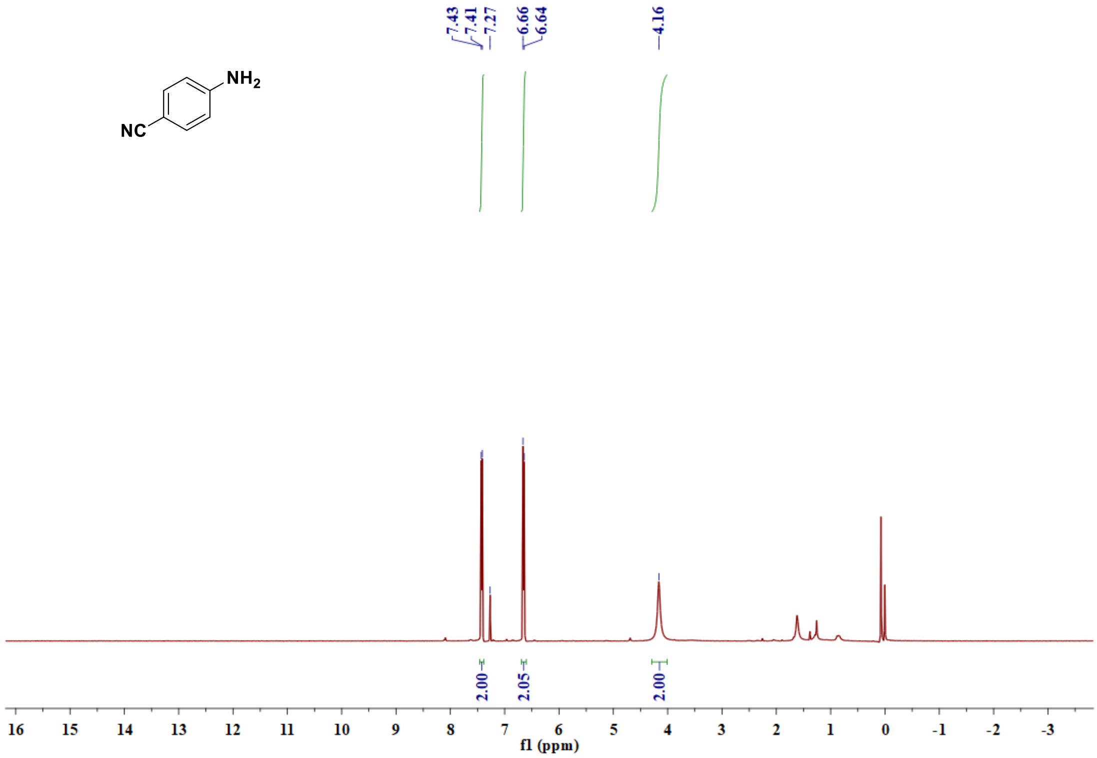

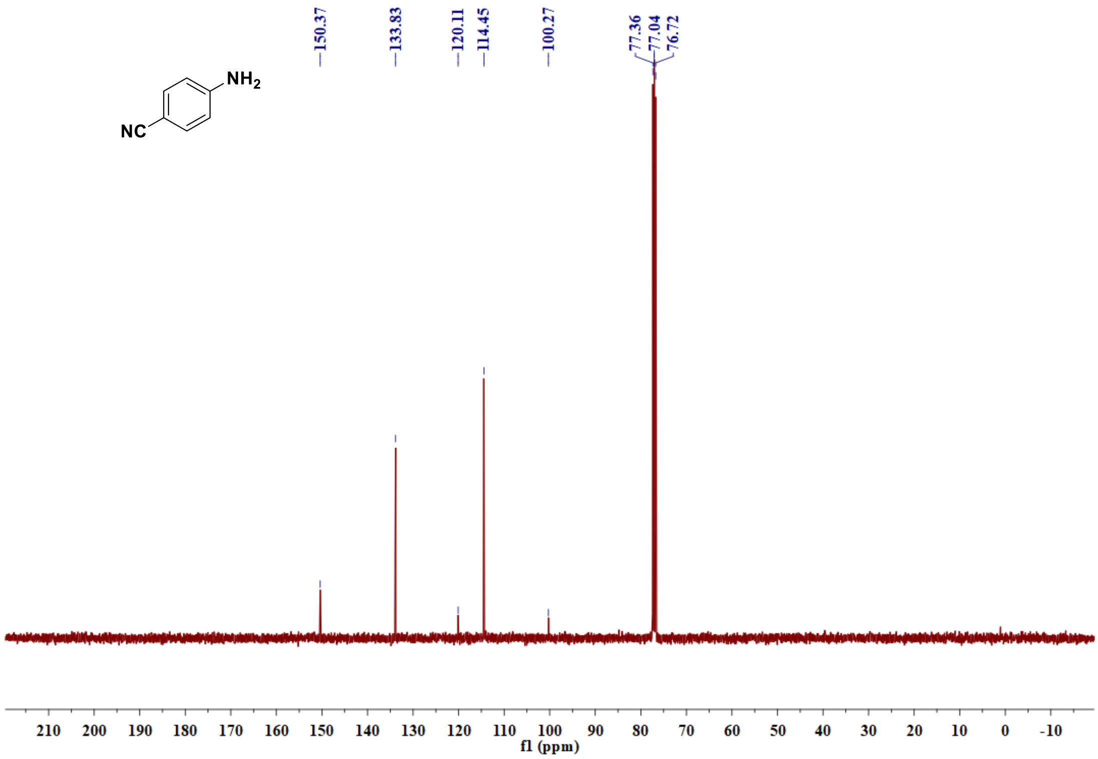

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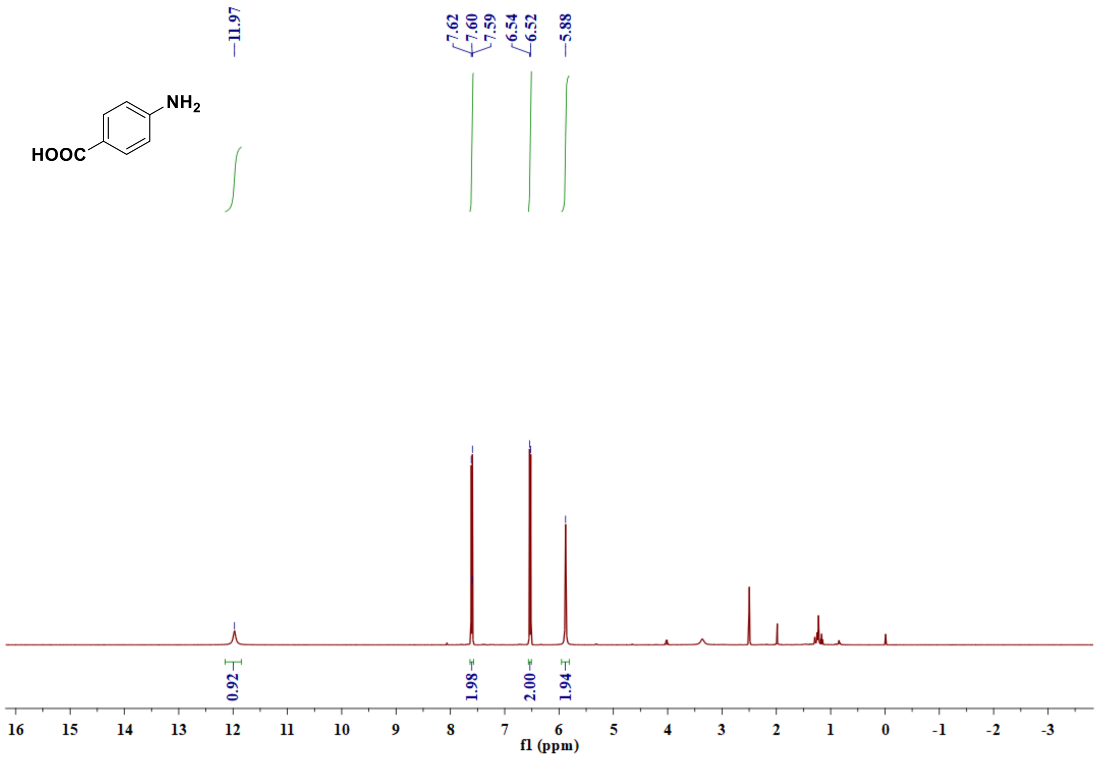

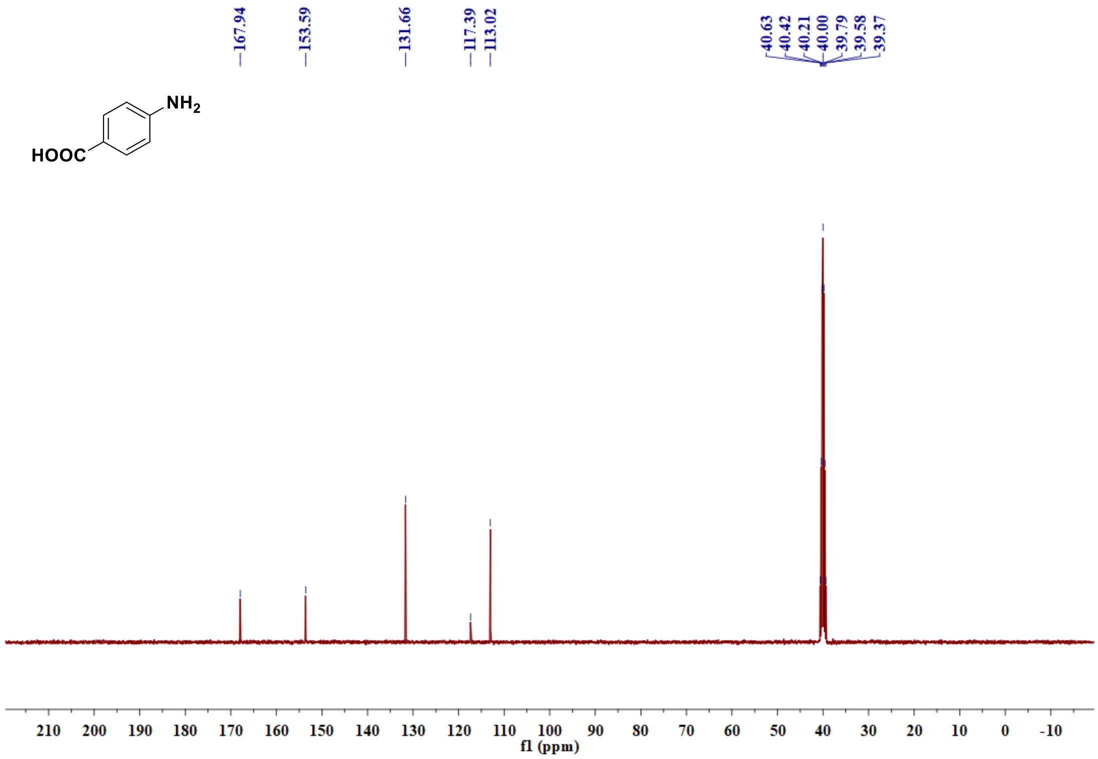

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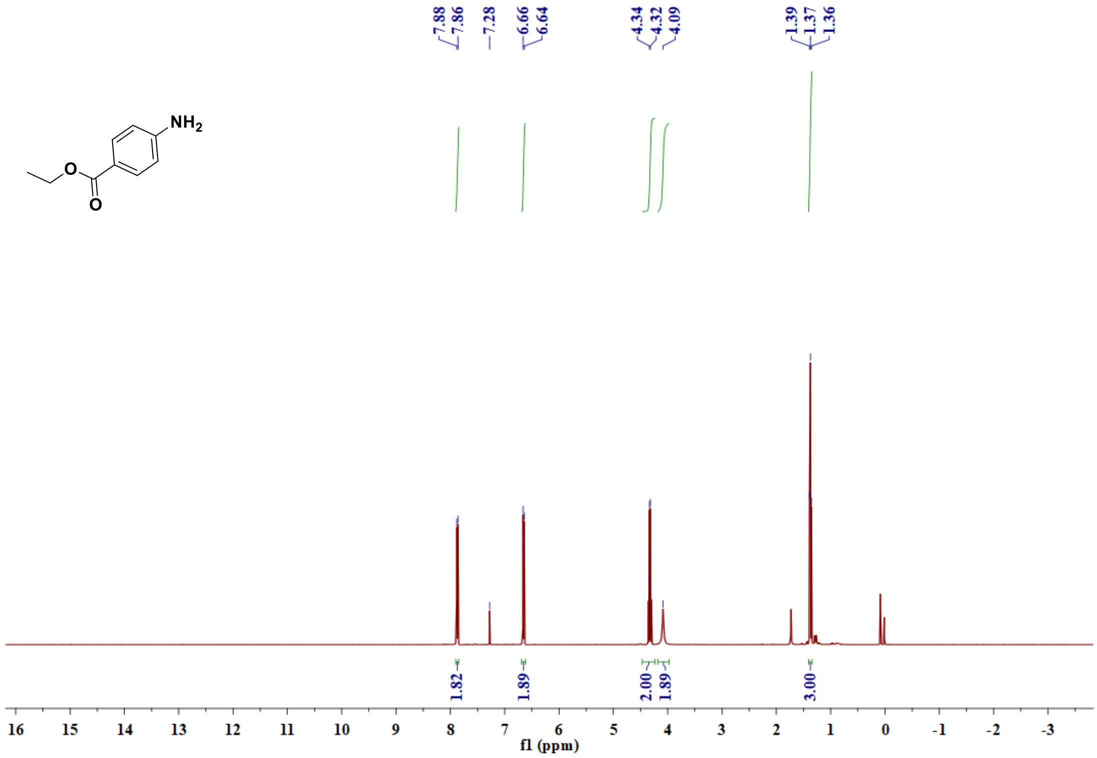

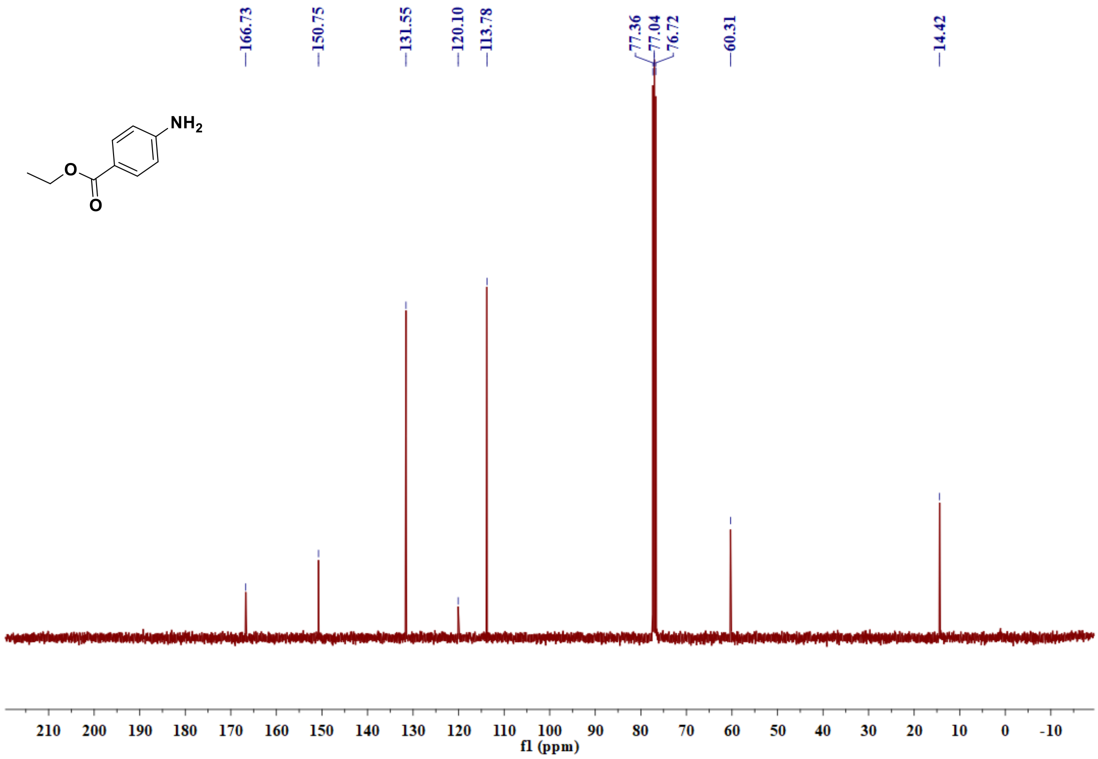

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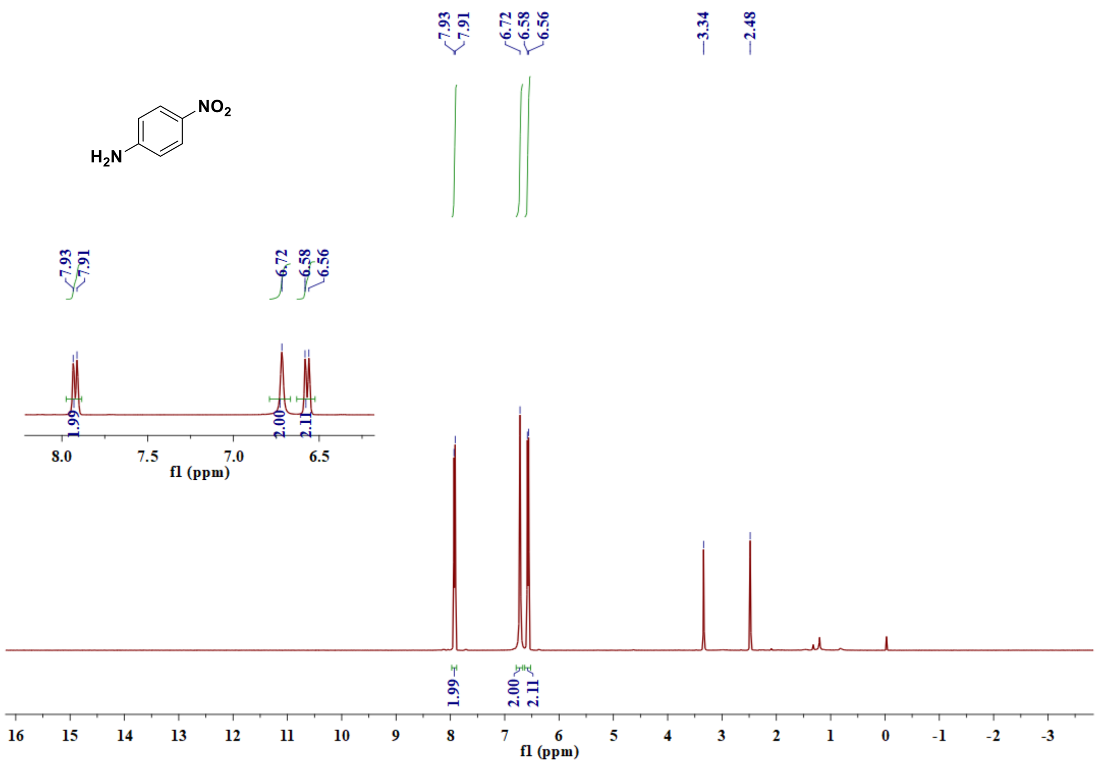

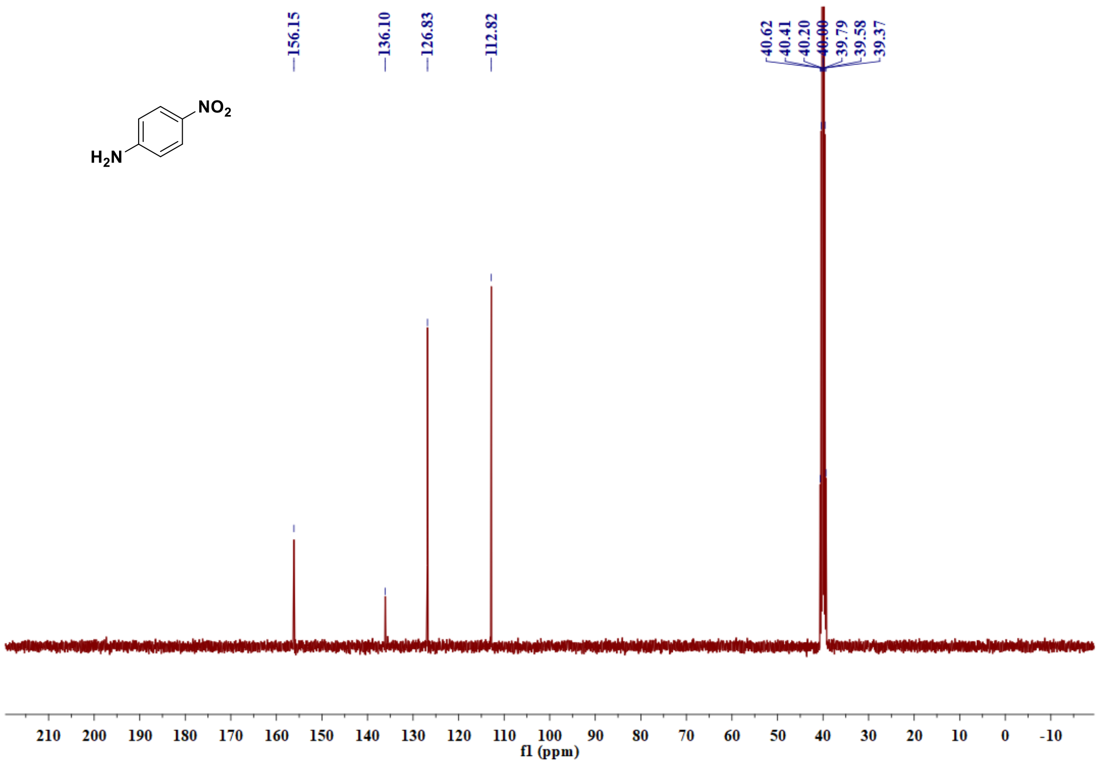

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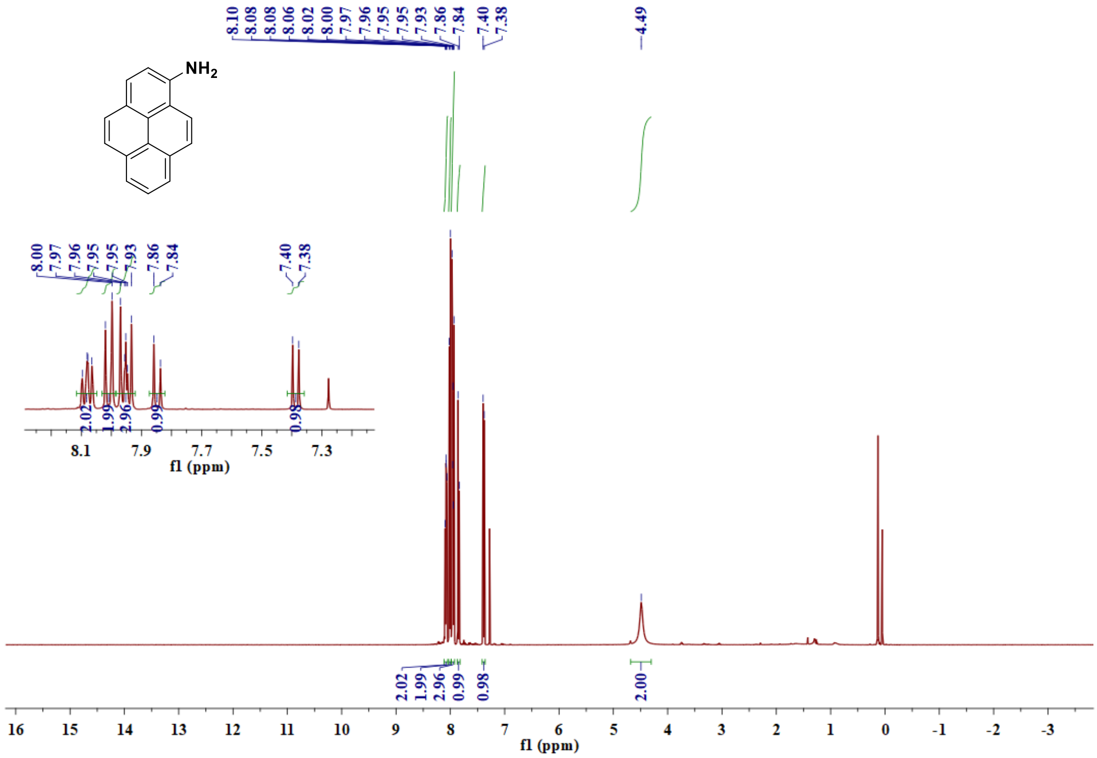

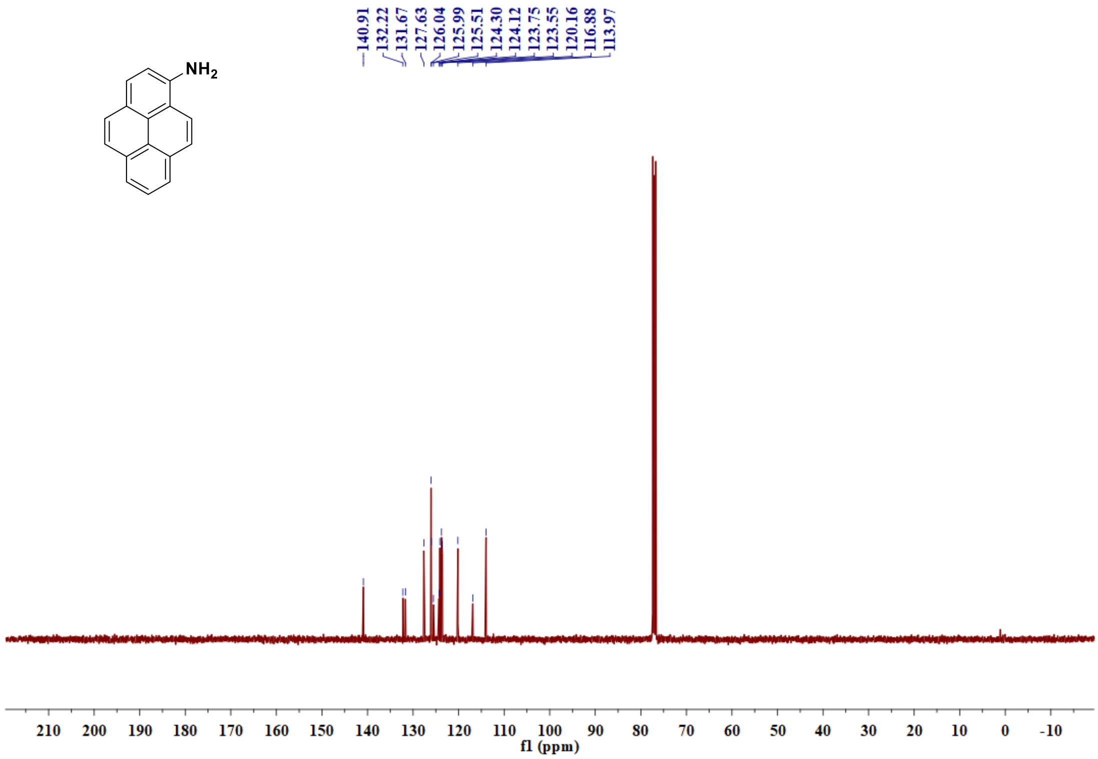

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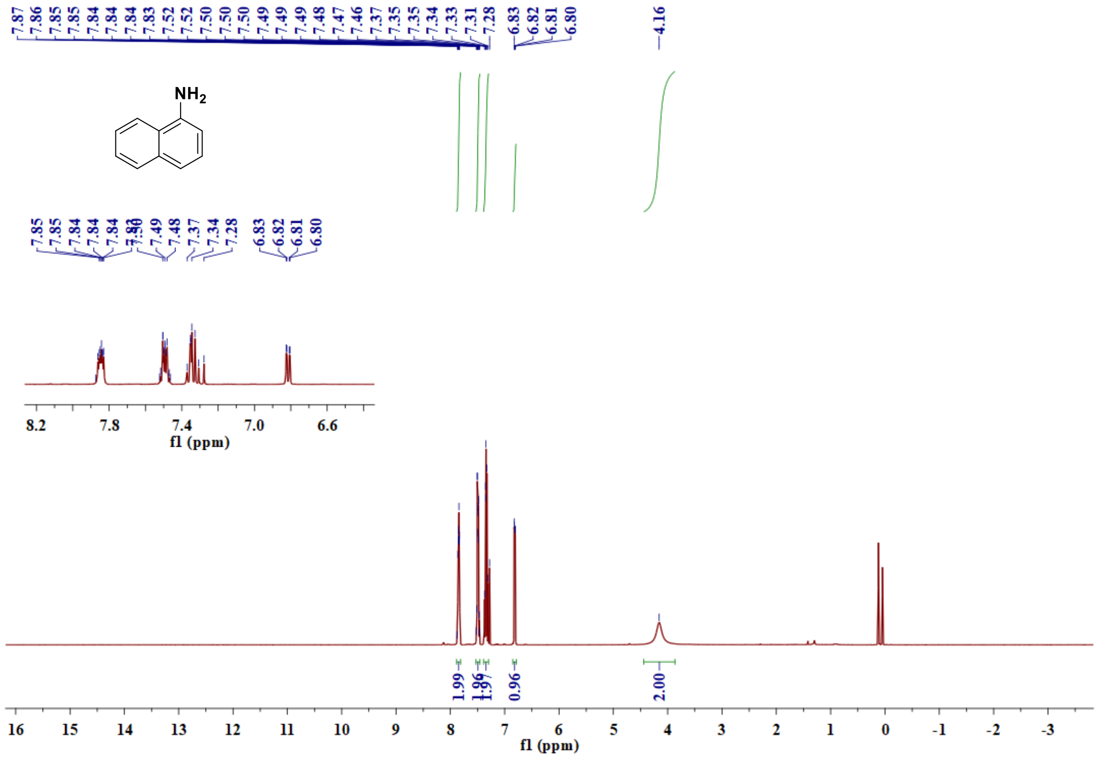

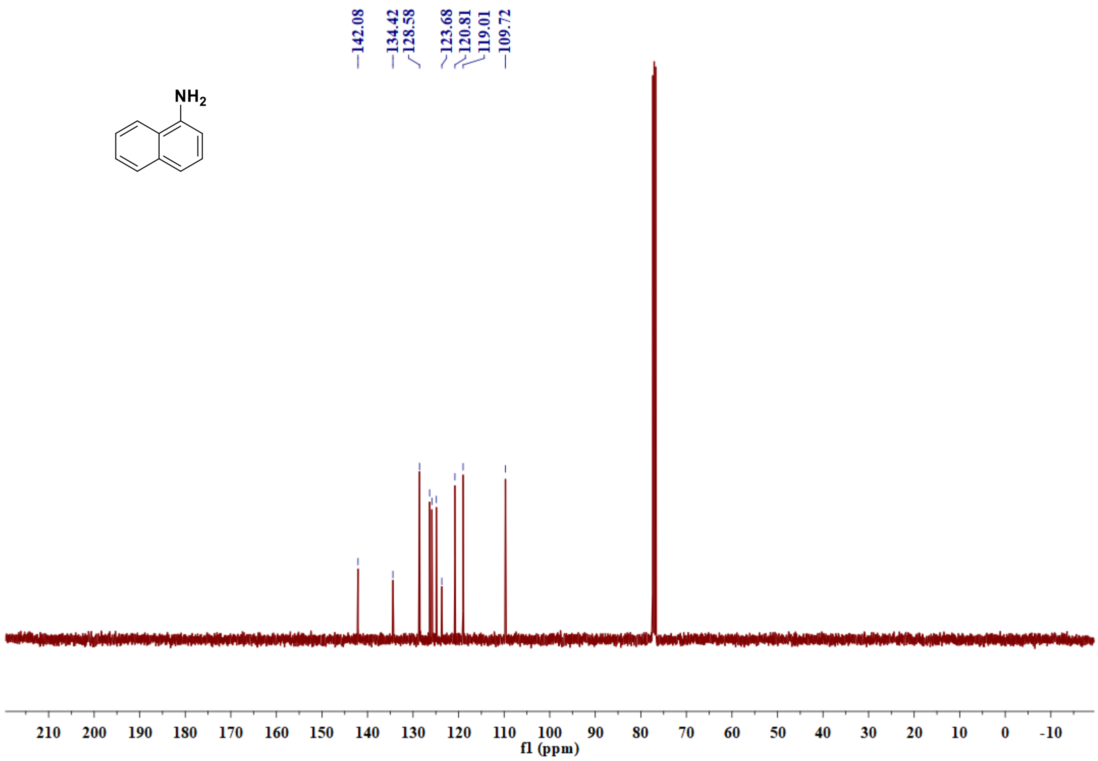

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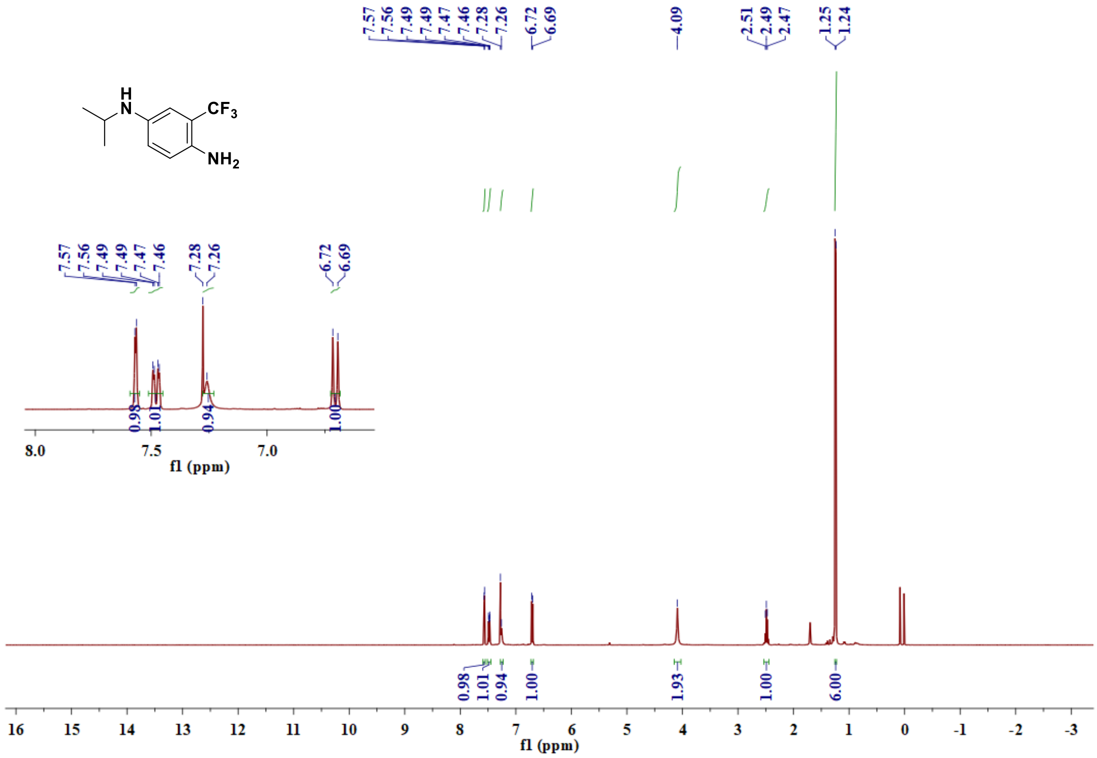

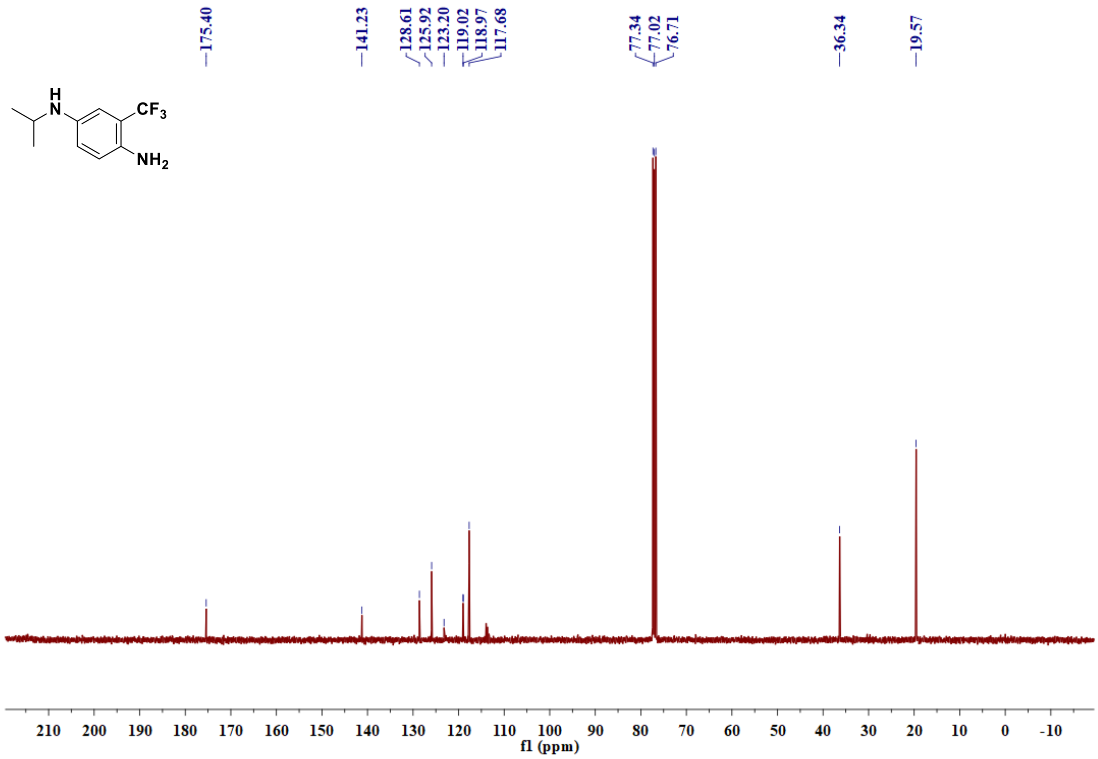

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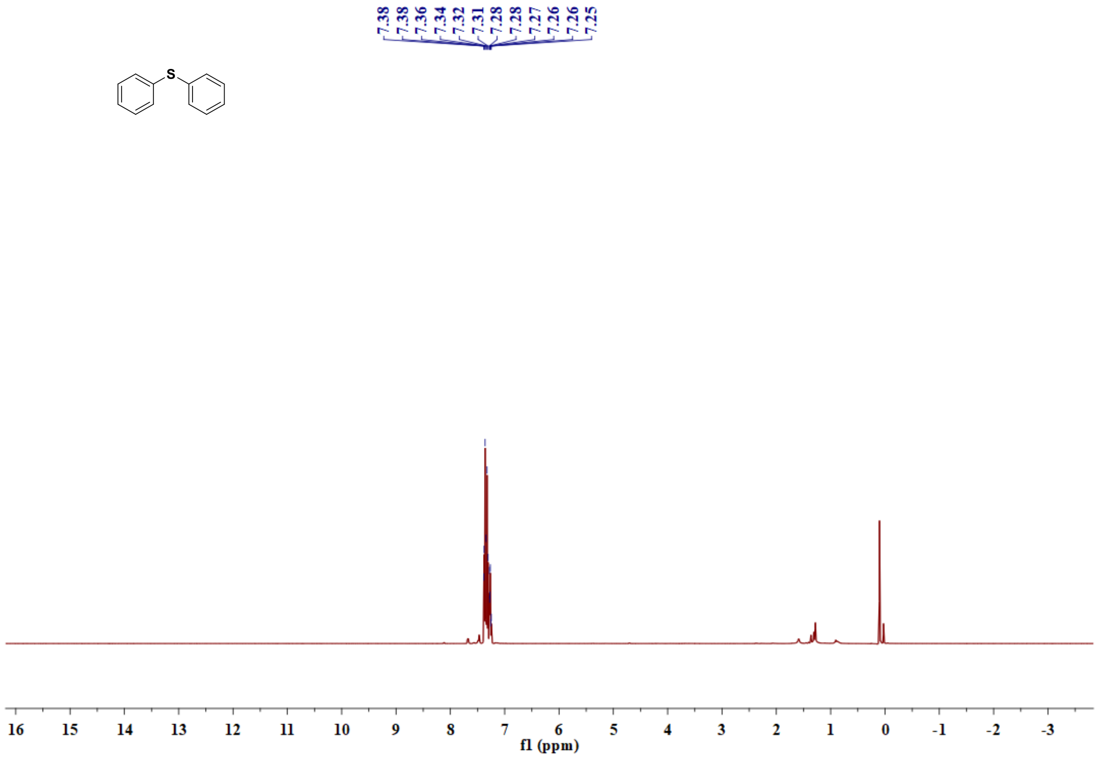
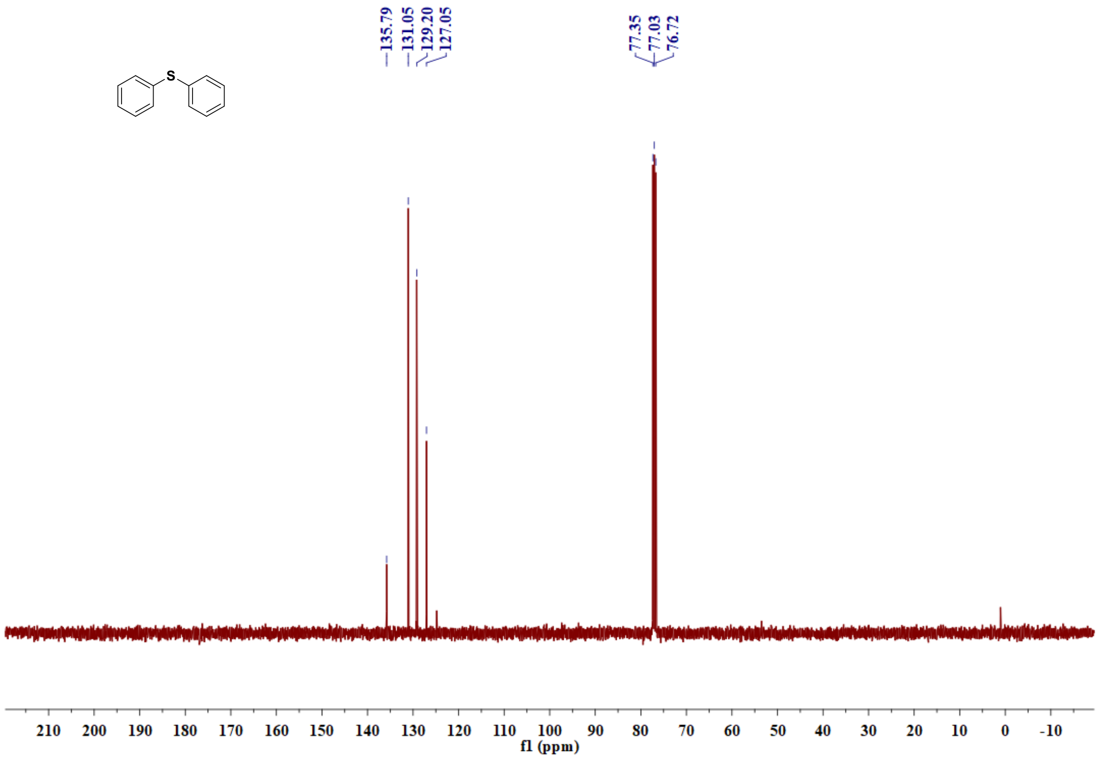
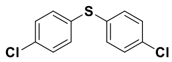
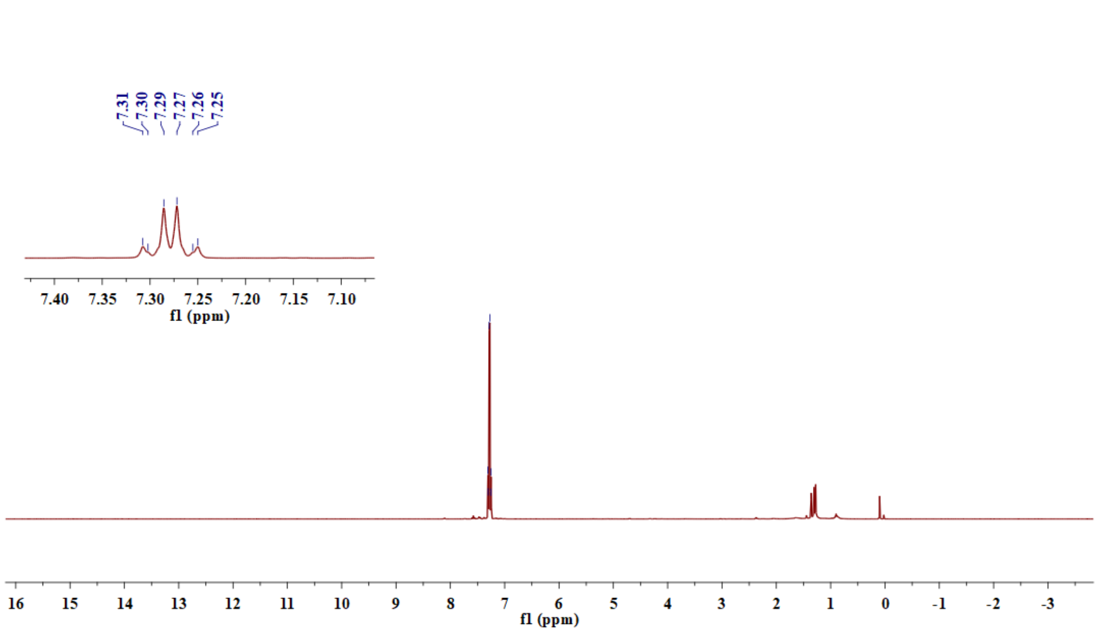
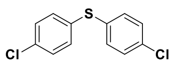

S
7.38
7.38
7.36
7.34
7.32
7.31
7.28
7.28
7.27
7.26
7.26
7.25
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

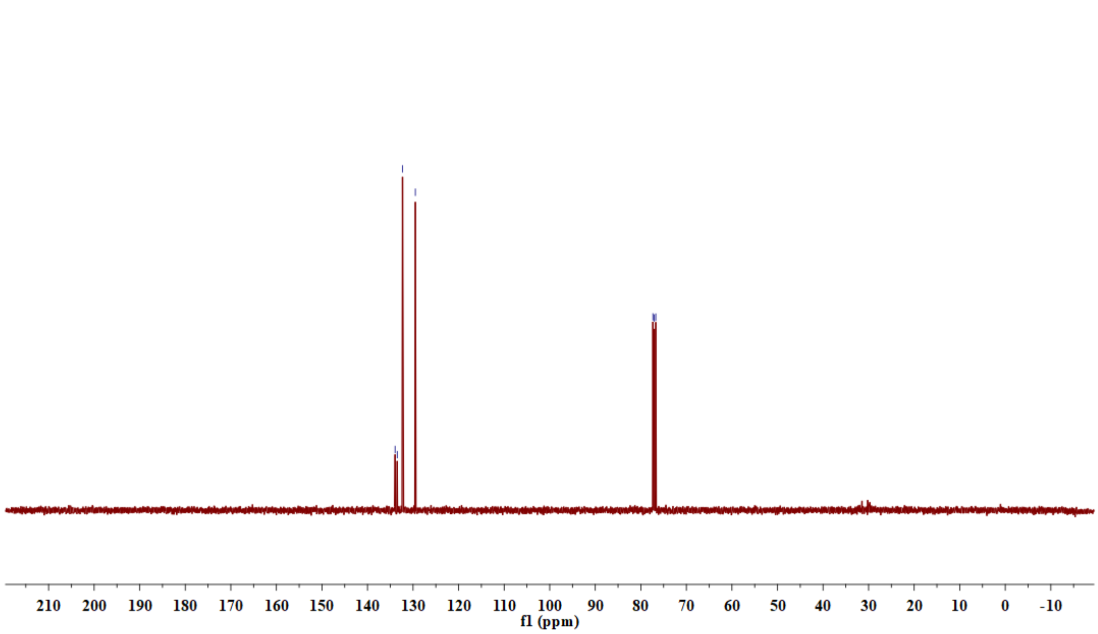

S
135.79
131.05
129.20
127.05
77.35
77.03
76.72
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

Sulfide 8b

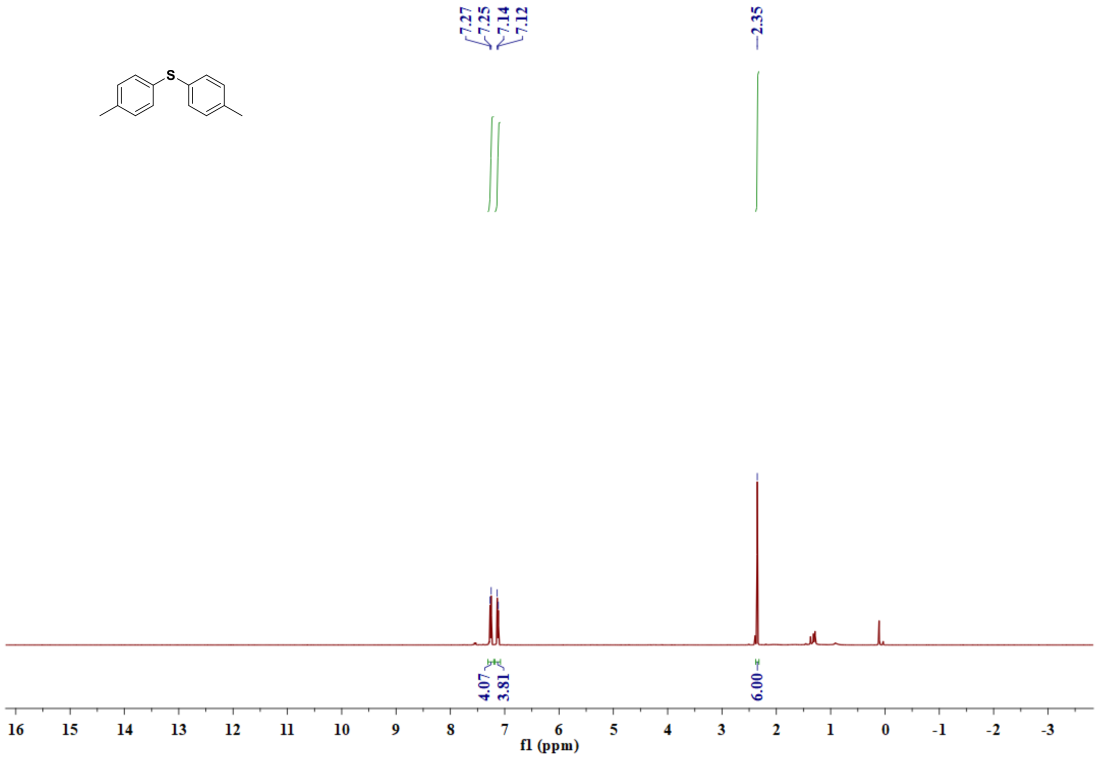


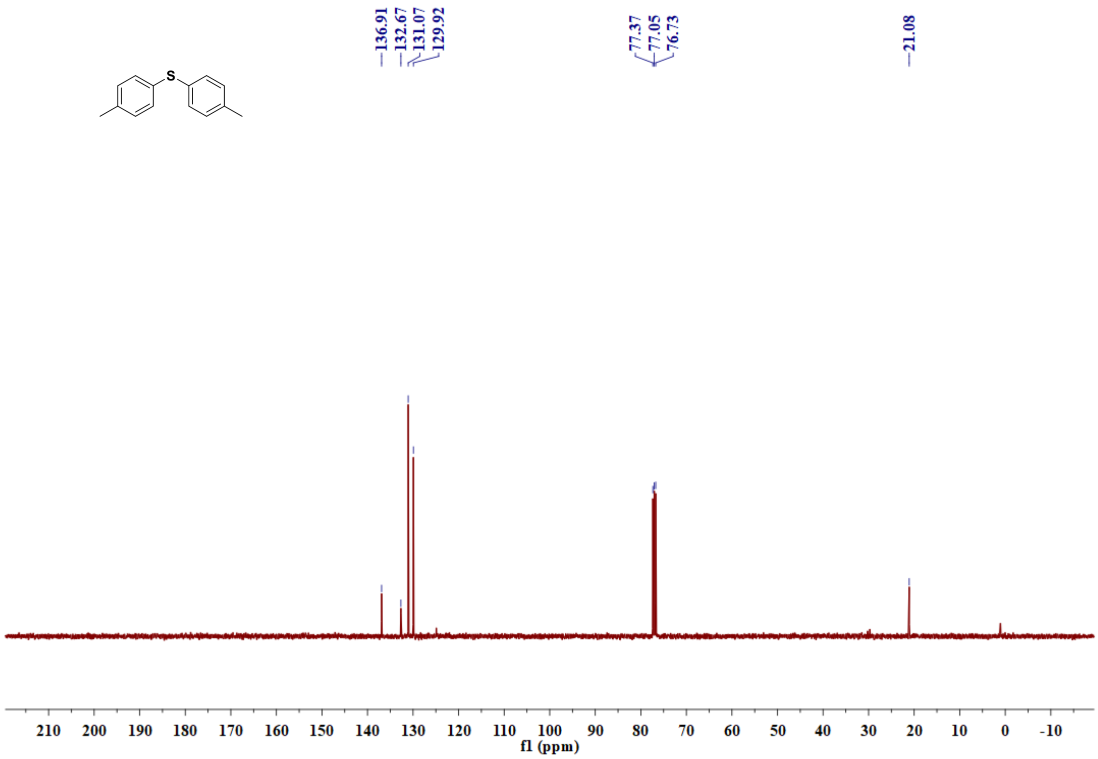

7.31
7.30
7.29
7.27
7.26
7.25
f1 (ppm)
f1 (ppm)




133.94
133.48
132.31
129.50
77.35
77.04
76.72
f1 (ppm)

Sulfide 8c


7.27
7.25
7.14
7.12
2.35
S
4.07
3.81
6.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


136.91
132.67
131.07
129.92
77.37
77.05
76.73
21.08
S
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

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