Electronic Supplementary Material (ESI) for Green Chemistry.

Pyrenediones as Versatile Photocatalysts for Oxygenation Reactions with *in situ* Generation of Hydrogen Peroxide under Visible Light

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I. Materials and Instruments

Chemicals and solvents were purchased from commercial suppliers and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were performed on AV-III400 (400 MHZ) or AMX500 (500 MHz) spectrometer. Chemical shifts were calibrated using residual proteo solvent as an internal reference for ^{1}H NMR ($CHCl_3$: 7.26 ppm) and $CDCl_3$ for ^{13}C NMR at 77.0 ppm). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), dd (doublet of doublet), brs (broad singlet). All Mass spectra were collected on a microTOF-Q II 1026 mass spectrometer. UV-Vis spectra were recorded using a UV-1650 PC Shimadzu spectrophotometer fitted with a quartz cell. Fluorescence measurement was recorded using the Horiba Fluorolog® Spectrofluorometer. Fourier transformation infrared (FTIR) data were measured and analyzed by Bruker OPUS 65 FTIR spectrometer with KBr as the background. The Blue LED strips (2 meter, 18 W) were purchased from InLEDs Pte Ltd (Singapore). Cyclic voltammetry measurement was performed in dry acetonitrile on a CHI 620C electrochemical analyzer with a three-electrode cell, using 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte, AgCl/Ag as reference electrode, gold disk as working electrode, Pt wire as counter electrode, and scan rate at 100 mV s^{-1}.

II. Experiment Procedures for Synthesis of 1,6-PYD and 1,8-PYD

The synthetic method of PYD was optimized based on reported methods.[1] Pyrene (10 g, 49.5 mmol) and $K_2Cr_2O_7$ (15 g, 51.0 mmol) was dissolved in 100 mL 4 M H_2SO_4. Reaction mixtures were heated to 90°C and stirred for 6 hours to afforded mixture of 1,6-PYD (45%) and 1,8-PYD (35%). Isomers 1,6-PYD and 1,8-PYD were separated by silica column with eluent of hexane/ether acetate: 2/1. 1,6-PYD was obtained as yellow powder and 1,8-PYD was obtained as red powder.

III. Mechanistic Study of Photocatalytic *in situ* Generation of PYD in IPA

Table S1. Photophysical data of 1,6-PYD and 1,8-PYD

Photocatalysts	Ground state reduction potential (V *vs* SCE)		Excited state redox potential (V *vs* SCE)	λ_{abs} (nm)
	$E^1_{1/2}$ (P/P^-)	$E^2_{1/2}$ (P/P^-)	$E_{1/2}$ (P^*/P^-)	
1,8-PYD	-0.347	-0.587	2.118	461
1,6-PYD	-0.303	-0.519	2.280	427

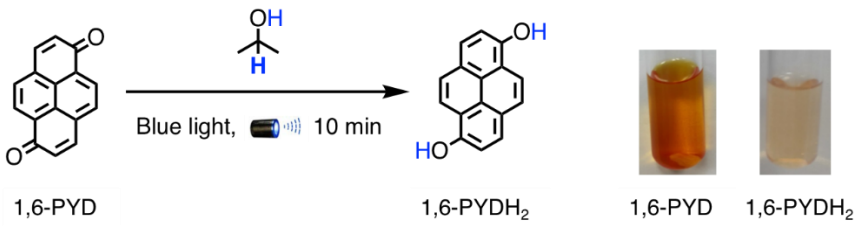


Fig. S1 Colour change of 1,6-PYD upon irradiation by blue light in IPA.

Table S2. Photophysical Properties of Some Common Organophotocatalysts.[2]

Photocatalysts	E^{*}_{red} (P*/P^{-}) V *vs*. SCE	Absorption (nm) λ_{max}
Rose Bengal	0.99	559
Benzophenone	1.55	320-380
DDQ	2.70	330
Anthraquinone	1.67	325
Eosin Y	1.18	539
Acr+-Mes	2.08	425
1,6-PYD	2.28	427
1,8-PYD	2.12	461

General procedures for iodometric detection and quantification of H_2O_2.

The formation of H_2O_2 in the reaction mixture was detected in a typical reaction with KI solution.[3]

1. Potassium iodide solution (1% w/v): Dissolve 1.0 grams KI into 100 mL demineralized water. Store capped in cool place in dark. Yellow-orange tinted KI solution indicates some air oxidation to iodine, which can be removed by adding a 1-2 drops of dilute sodium thiosulfate solution.
2. Ammonium molybdate solution: Dissolve 9 grams ammonium molybdate in 10 mL 6 N NH_4OH. Add 24 grams NH_4NO_3 and dilute to 100 mL.
3. Sulfuric acid solution. Carefully add one part H_2SO_4-98% to four parts demineralized water.
4. Starch indicator.
5. Sodium thiosulfate solution (0.1 N).

To a 250 mL flask 4.0 mL of reaction mixture was added and mixed, with 50 mL of demineralized water, 10 mL of sulfuric acid solution, 10-15 mL of potassium iodide solution, and two drops ammonium molybdate solution. Titrate with 0.1 N sodium thiosulfate to faint yellow colour. Swirl or stir gently during titration. Starch indicator (2.0 mL) was added and titration was continued until the blue colour just disappears.

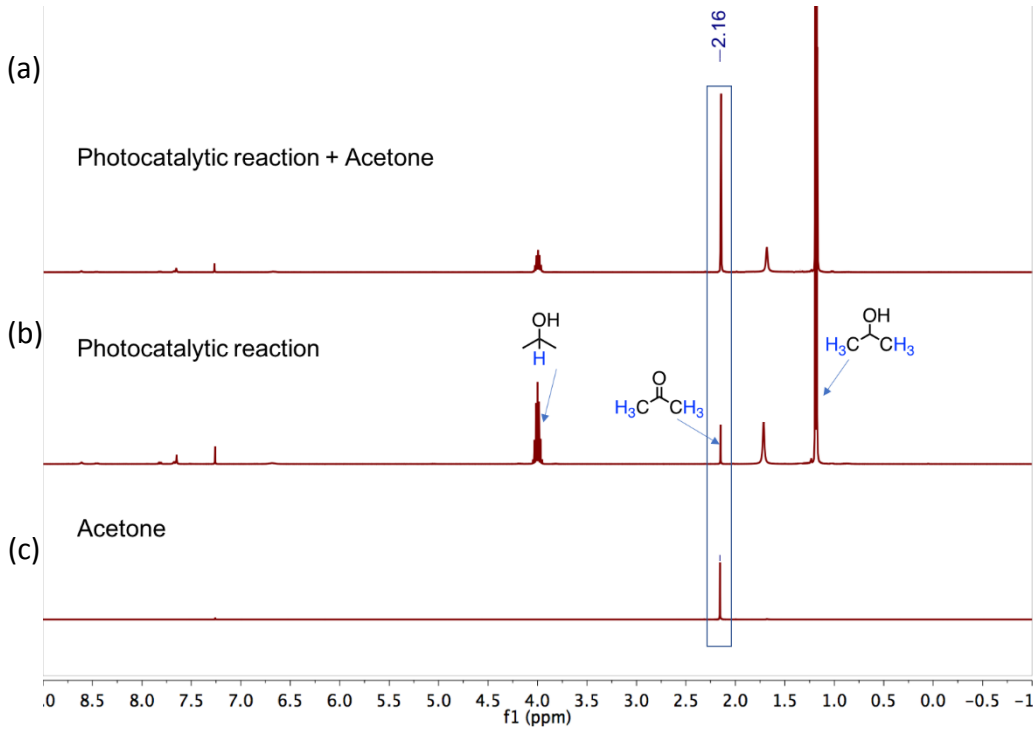


Fig. S2 Detection of acetone by ^{1}H NMR ($CDCl_3$). Reaction condition: 1,6-PYD (0.01 mmol) and IPA (4.0 mL). Irradiation with blue LEDs light under oxygen balloon in room temperature for 24 h.

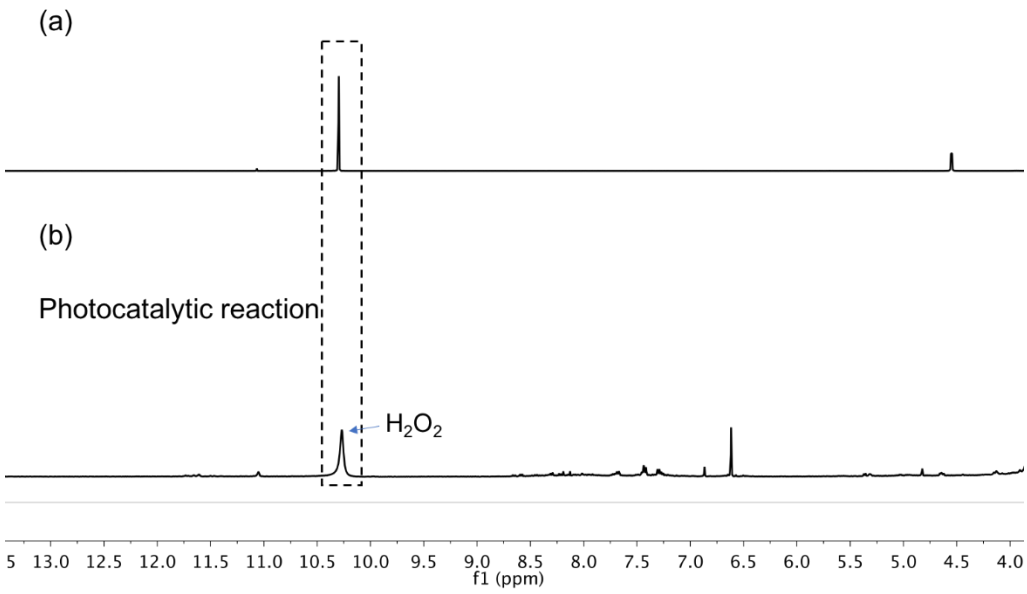
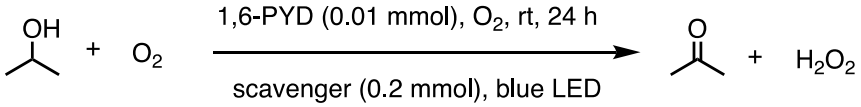


Fig. S3 Detection of hydrogen peroxide by ^{1}H NMR (DMSO-d_6/D_2O (5:1, v/v)). (a) 30% H_2O_2 (1.0 mmol) from commercial supplier. (b) H_2O_2 generated in photocatalytic system. Reaction condition: 1,6-PYD (0.1 mmol) and IPA (10.0 mL). Irradiation with blue LEDs light under oxygen balloon in room temperature for 40 h.

Table S3. Quenching experiment with radical scavengers



Scavengers	H_2O_2 amount (mmol)
NaN_3	0.25
Tempo	0.025
No scavenger	0.27

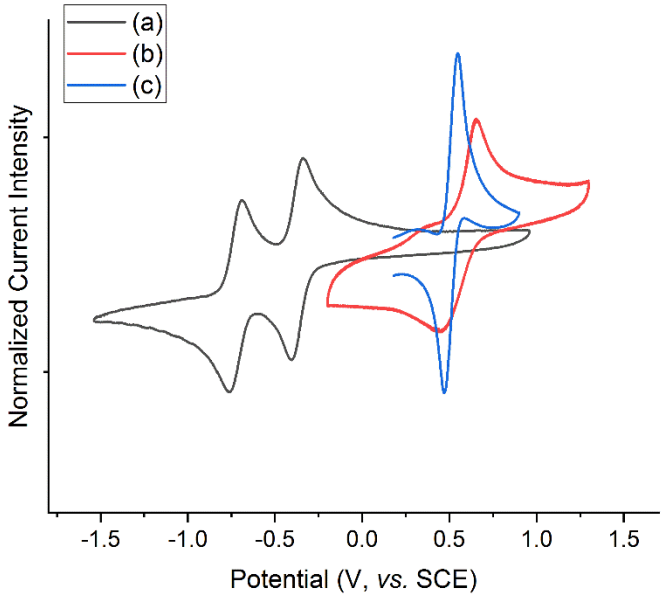


Fig. S4 Cyclic voltammetry in MeCN + 0.1 M Bu_4NPF_6. Scan rate 100 mV s^{-1} (a) 1,6 PYD (b) 1,6-$PYDH_2$ (c) 1,6-PYD + 20 equiv. H_2SO_4.

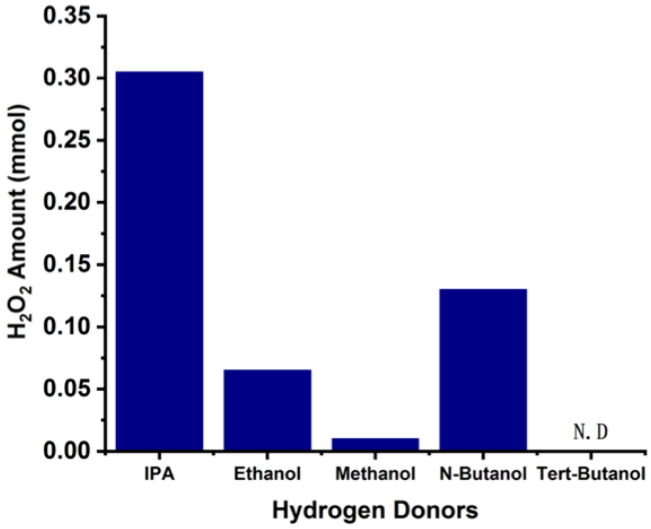


Fig. S5 H_2O_2 amount in different alcohols. Reaction condition: 1,6-PYD (0.01 mmol), Alcohols (4.0 mL). Irradiation by blue LED for 48 h under oxygen balloon in room temperature. H_2O_2 amount was determined by iodometry.

IV. Experiment Procedures for Photocatalytic Reactions

General Procedure for photocatalytic synthesis of epoxides 2a-2k

A test tube (20 mL) with rubber septum and magnetic bar was charged with dicyanide alkene (0.2 mmol), 1,6 pyrenedione (2.32 mg; 5 mol%) and IPA (4.0 mL). The solution was mixed well and bubbled with dry oxygen (balloon) for 10 min. After that, the mixture was irradiated using 2 meters 18 W blue LED strip for 40 h at room temperature under one atm oxygen atmosphere. Finally, the reaction mixture was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/ethyl acetate: 10:1) to afford corresponding epoxides **2a-2k**.

General procedure for photocatalytic synthesis of epoxides 3a-3i:

A test tube (20.0 mL) with rubber septum and magnetic bar was charged with the unsaturated ketone (0.2 mmol), 1,6-PYD (2.32 mg; 5 mol%) and 4.0 mL IPA. 0.4 mmol Na_2CO_3 (0.4 mL was taken from 1N Na_2CO_3 solution) was then added. The solution was mixed well and bubbled with dry oxygen (balloon) for 10 min. After that, the mixture was irradiated using 1 meter 18 W blue LED strip at room temperature under one atm oxygen atmosphere for 18 h. Finally, the reaction mixture was neutralized with H_2SO_4 and extracted with dichloromethane/H_2O. The organic layer was collected and was concentrated by reduced pressure. The crude product was purified by silica gel column chromatography (eluent: hexane/ethyl acetate: 10:1) to afford **3a-3i**.

General procedure for photocatalytic synthesis of phenol and alcohols 5a-5h

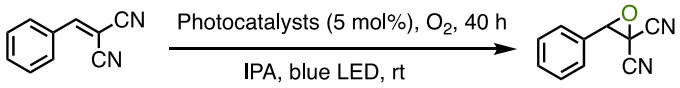
Boronic acid (4a-4h) were obtained from commercial sources and used as received. Boronic acid pinacol esters (**4i**, **4j**) were prepared according to the reported procedure.[4] A test tube (20 mL) with rubber septum and magnetic bar was added with boronic acid or boronic acid pinacol ester (0.2 mmol), 1,6-PYD (4.6 mg; 10 mol%) and IPA (4.0 mL). The solution was mixed well and bubbled with dry oxygen (balloon) for 10 min. The mixture was then irradiated using 2 meters 18 W blue LED strip for 40 h at room temperature under one atm oxygen atmosphere. After completion of the reaction, the mixture was concentrated under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/ethyl acetate: 5:1) to afford corresponding phenol or alcohol **(5a-5h).**

General procedure for photocatalytic synthesis of sulfoxides 7a-7d:

Sulfide compound (**6a-6d**) (0.2 mmol), 1,6-PYD (0.01 mmol, 5 mol%), IPA (4.0 mL) were placed in a 20 mL test tube with rubber septum and magnetic bar. The solution was mixed well and bubbled with dry oxygen (balloon) for 10 min. The mixture was stirred and irradiated using 2 meter 18 W blue LED strip for 24 h at room temperature under one atm oxygen atmosphere. Finally, the reaction mixture was concentrated

under reduced pressure and the crude product was purified by silica gel column chromatography (eluent: hexane/ethyl acetate: 2:1) to afford sulfoxide **(7a-7d)**.

Table S4. Photocatalyst screening[a]

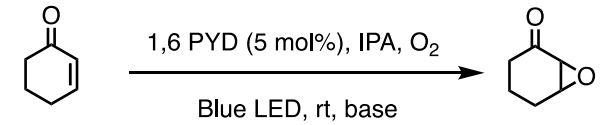


1a **2a**

Photocatalysts	Yields, %
1,6-PYD	93
1,8-PYD	90
Eosin Y	0
Anthraquinone	50
Rose Bengal	20
$Ru(bpy)_3^{2+}$	0

[a]Reaction conditions: **1a** (0.2 mmol) and photocatalyst (0.01 mmol, 5%) in IPA (4.0 mL, 0.05 M) were irradiated using a 20 W blue LED strip (2 meter) at room temperature under oxygen for 40 hours. [b]Yield was determined based on ^{1}H-NMR analysis of the crude product using 1,3,5-trimethoxybenzene as an internal standard.

Table S5. Base screening for epoxidation of unsaturated ketones.

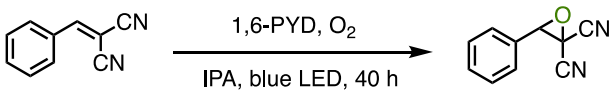


0.2 mmol

Base	Time (h)	Yield[a] (%)
0.5 equiv. Na_2CO_3	24	45
1 equiv. Na_2CO_3	24	55
2 equiv. Na_2CO_3	24	95
2 equiv. NaOH	18	80
2 equiv. KOH	18	80
No base	24	trace

[a]Yield was determined by crude NMR using 1,3,5-trimethoxybenzene as the internal standard.

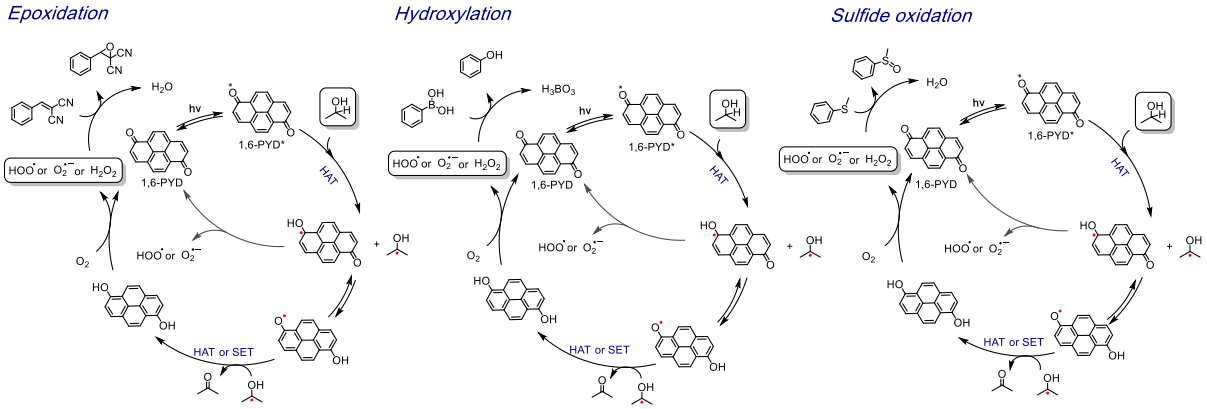
Table S6. Catalyst loading study for epoxidation.



1a
0.2 mmol

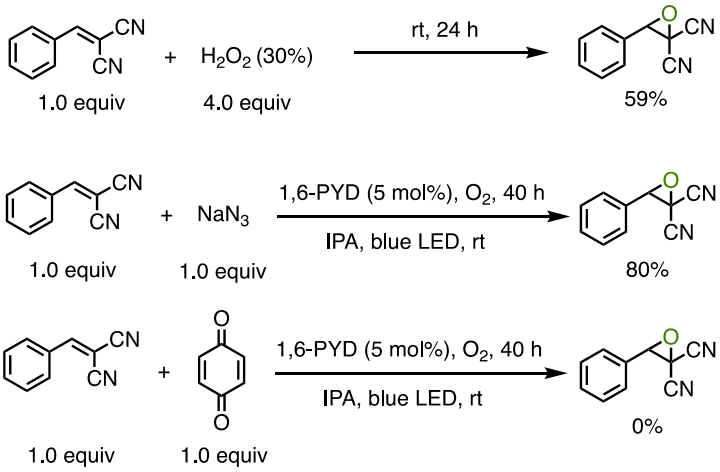
2a

1,6-PYD (%)	Yield (%)
1	45
2.5	55
5	95

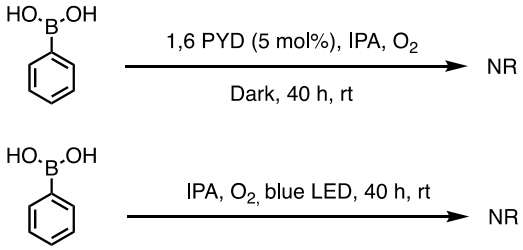


Scheme S1. Proposed mechanisms for three photocatalytic reactions.

V. Control Experiment

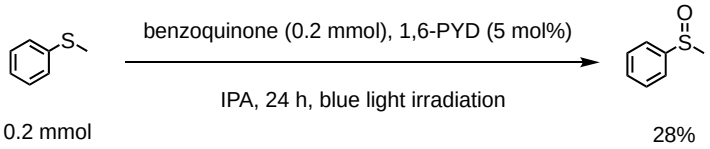


Control experiment for boron hydroxylation



When reaction was carried out in absence of light and photocatalysts, no corresponding product was obtained according to both TLC and NMR analysis. The results showed that light and photocatalysts are essential element for the reaction.

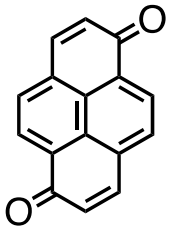
Quenching experiment for sulfide oxidation



When reaction was carried out in absence of benzoquinone, only 28% products was obtained. The results showed that superoxide ion was formed.

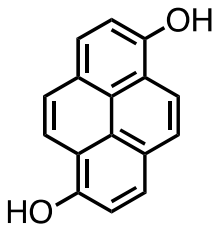
VI. Characterization Data of the Products

1,6-Pyrendione



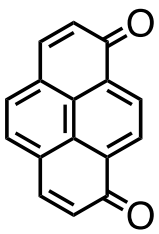
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.49 (d, *J* = 7.4 Hz, 2H), 7.83 (d, *J* = 7.5 Hz, 2H), 7.68 (d, *J* = 9.8 Hz, 2H), 6.70 (d, *J* = 9.8 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 185.51, 141.17, 133.91, 130.90, 130.78, 130.35, 130.18, 127.41. Data were identical to reported literature[1]

1,6-Pyrenediol



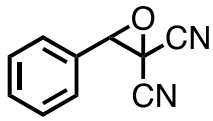
^{1}H NMR (500 MHz, DMSO-d_6) δ 10.34 (s, 2H), 8.06 (d, *J* = 9.1 Hz, 2H), 7.97 (d, *J* = 8.3 Hz, 2H), 7.88 (d, *J* = 9.1 Hz, 2H), 7.52 (d, *J* = 8.2 Hz, 2H). **^{13}C NMR** (126 MHz, DMSO-d_6) δ 151.06, 125.96, 125.59, 124.41, 124.30, 118.61, 117.87, 113.19. **HRMS-ESI** $[M-H]^-$ Calcd for $C_{16}H_9O_2$ 233.0603, found 233.0602. Melting point: 223 °C. FT-IR (KBr, cm^{-1}): ν = 2925, 2855, 1616, 1596, 1558, 1545, 1478, 1429, 1354, 1274, 1251, 1228, 1184, 1114, 833.

1,8-Pyrenedione



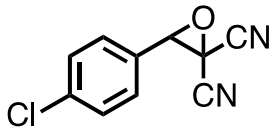
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.64 (s, 2H), 7.67 (s, 2H), 7.68 (d, *J* = 6.3 Hz, 2H), 6.68 (d, *J* = 9.8 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 184.85, 142.81, 132.85, 132.05, 131.11, 129.28, 127.28. Data were identical to reported literature[1]

3-phenyloxirane-2,2-dicarbonitrile (2a)



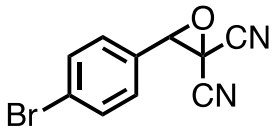
^{1}H NMR (500MHz, $CDCl_3$): δ 7.53-7.42 (m, 5H), 4.71 (s, 1H); **^{13}C NMR** (126 MHz, $CDCl_3$): δ 131.55, 129.30, 127.60, 126.90, 111.71, 110.23, 65.93, 41.80. Data were identical to reported literature.[5]

3-(4-chlorophenyl)oxirane-2,2-dicarbonitrile (2b)



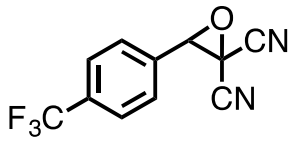
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, J = 8.5 Hz, 2H), 7.37 (d, J = 8.5 Hz, 2H), 4.70 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 137.85, 129.65, 128.25, 126.11, 111.44, 110.05, 65.26, 41.75. Data were identical to reported literature.[5]

3-(4-bromophenyl)oxirane-2,2-dicarbonitrile (2c)



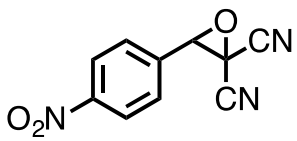
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 (d, J = 8.5 Hz, 2H), 7.30 (d, J = 8.5 Hz, 2H), 4.69 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 132.49, 128.33, 126.55, 126.02, 111.33, 109.94, 65.23, 41.57. Data were identical to reported literature.[6]

3-(4-(trifluoromethyl)phenyl)oxirane-2,2-dicarbonitrile (2d)



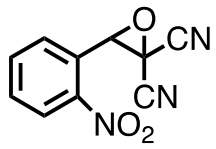
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.78 (d, J = 8.1 Hz, 2H), 7.58 (d, J = 8.1 Hz, 2H), 4.78 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 133.55 (q, *J* = 32.9 Hz), 131.38, 126.24 (q, *J* = 3.8 Hz), 123.38 (d, *J* = 272.7 Hz), 111.08, 109.65, 64.77, 41.52. Data were identical to reported literature.[5]

3-(4-nitrophenyl)oxirane-2,2-dicarbonitrile (2e)



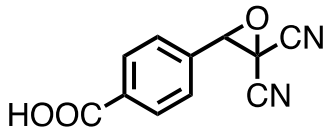
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.37 (d, J = 8.7 Hz, 2H), 7.66 (d, J = 8.8 Hz, 2H), 4.83 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 149.78, 134.04, 128.02, 124.38, 110.79, 109.43, 64.31, 41.50. Data were identical to reported literature.[5]

3-(2-nitrophenyl)oxirane-2,2-dicarbonitrile (2f)



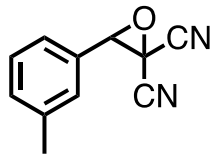
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.38 (d, J = 8.1 Hz, 1H), 7.84 (t, J = 7.6 Hz, 1H), 7.76 (t, J = 7.9 Hz, 1H), 7.64 (d, J = 7.6 Hz, 1H), 5.24 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 135.30, 132.21, 128.59, 125.88, 125.58, 111.00, 109.96, 64.26, 41.47. **HRMS-ESI** $[M-H]^-$ Calcd for $C_{10}H_6N_3O_3$ 215.0409, found 215.0297. Colourless oil. FT-IR (KBr, cm^{-1}): 2925, 2855, 1639, 1461, 1353, 1283, 1243, 1185, 837, 754.

4-(3,3-dicyanooxiran-2-yl)benzoic acid (2g)



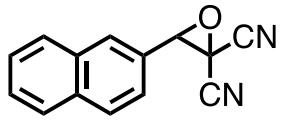
^{1}H NMR (500 MHz, acetone-d_6) δ 8.17 (d, J = 8.3 Hz, 2H), 7.71 (d, J = 8.1 Hz, 2H), 5.40 (s, 1H). **^{13}C NMR** (126 MHz, Acetone-d_6) δ 165.94, 133.73, 132.76, 129.81, 127.29, 112.18, 110.89, 64.96, 42.64. **HRMS-ESI** $[M-H]^-$ Calcd for $C_{11}H_5N_2O_3$ 213.0378, found 213.0301. White solid. Melting point: 214 ^oC. FT-IR (KBr, cm^{-1}): 2929, 2855, 1699, 1619, 1596, 1547, 1499, 1429, 1356 1275, 1183, 1115, 1019, 831.

3-(*m*-tolyl)oxirane-2,2-dicarbonitrile (2h)



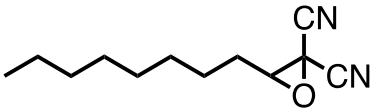
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40 – 7.30 (m, 2H), 7.24 – 7.20 (m, 2H), 4.67 (s, 1H), 2.41 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 139.32, 132.35, 129.18, 127.52, 127.37, 123.97, 111.78, 110.28, 66.03, 41.76, 21.52. **HRMS-ESI** $[M+H]^+$ Calcd for $C_{11}H_9N_2O$ 185.0715, found 185.0785. Colourless oil. FT-IR (KBr, cm^{-1}): 2955, 2926, 2855, 1742, 1634, 1597, 1549, 1498, 1462, 1378, 1354, 1271, 1184, 863, 655.

3-(naphthalen-2-yl)oxirane-2,2-dicarbonitrile (2i)



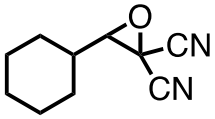
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 – 7.85 (m, 3H), 7.73 – 7.67 (m, 1H), 7.67 – 7.58 (m, 1H), 7.58 – 7.51 (m, 2H), 5.30 (s, 1H). **^{13}C NMR** (126 MHz, CDCl3) δ 133.53, 131.73, 130.82, 129.59, 128.10, 127.09, 125.29, 124.49, 123.91, 121.47, 111.81, 110.15, 64.56, 41.58. Data were identical to reported literature.[6]

3-octyloxirane-2,2-dicarbonitrile (2j)



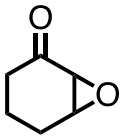
^{1}H NMR (400 MHz, CDCl3) δ 3.64 (dd, *J* = 6.4, 5.6 Hz, 1H), 2.02 – 1.75 (m, 2H), 1.60 (m, 2H), 1.57 – 1.15 (m, 10H), 0.89 (t, 3H). **^{13}C NMR** (126 MHz, CDCl3) δ 111.81, 110.75, 66.04, 38.82, 31.73, 29.31, 29.18, 29.02, 28.97, 25.21, 22.61, 14.06. **HRMS-ESI** $[M+H]^+$ Calcd for $C_{12}H_{19}N_2O$, 207.1497, found 207.1504. Colourless oil. FT-IR (KBr, cm^{-1}): 2956, 2927, 2856, 1752, 1466, 1378, 1261, 1172, 1124, 1087, 723.

3-cyclohexyloxirane-2,2-dicarbonitrile (2k)



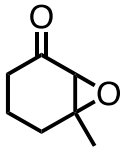
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.38 (d, *J* = 8.9 Hz, 1H), 1.96 – 1.72 (m, 5H), 1.37 – 1.18 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 112.01, 110.94, 69.58, 38.85, 38.58, 29.84, 29.58, 28.01, 25.72, 24.89. Data were identical to reported literature.[5]

7-oxabicyclo[4.1.0]heptan-2-one (3a)



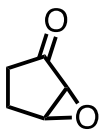
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.71 – 3.44 (m, 1H), 3.22 (d, *J* = 3.9 Hz, 1H), 2.60 – 2.45 (m, 1H), 2.36 – 2.20 (m, 1H), 2.13 – 2.01 (m, 1H), 1.96 – 1.88 (m, 2H), 1.73 – 1.59 (m, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 206.11, 56.10, 55.28, 36.51, 23.01, 17.19. Data were identical to reported literature.[7]

6-methyl-7-oxabicyclo[4.1.0]heptan-2-one (3b)



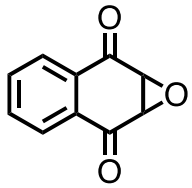
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.06 (s, 1H), 2.53 – 2.42 (m, 1H), 2.12 – 1.78 (m, 4H), 1.67 – 1.52 (m, 1H), 1.43 (s, 3H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 206.88, 62.51, 62.04, 35.76, 28.46, 22.29, 17.24. **HRMS-ESI** $[M-H]^-$ Calcd for $C_7H_9O_2$,129.0603, found 129.0615. Data were identical to reported literature.[8]

6-oxabicyclo[3.1.0]hexan-2-one (3c)



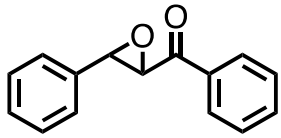
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.90 (m, 1H), 3.31 (d, *J* = 2.5 Hz, 1H), 2.45 – 2.20 (m, 2H), 2.20 – 1.87 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 210.17, 57.97, 54.95, 30.63, 23.29. Data were identical to reported literature.[7]

1a,7a-dihydronaphtho[2,3-*b*]oxirene-2,7-dione (3d)



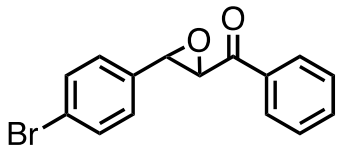
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00-7.97 (m, 2H), 7.78-7.75 (m, 2H), 4.02 (s, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 190.79, 185.11, 138.77, 134.80, 134.02, 132.02, 131.89, 127.31, 126.50, 55.42. Data were identical to reported literature.[7]

Phenyl(3-phenyloxiran-2-yl)methanone (3e)



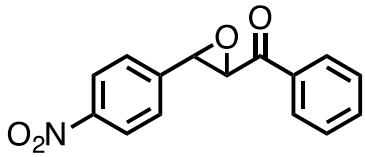
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 7.86 (m, 2H), 7.70 – 7.57 (m, 1H), 7.49 (m, 2H), 7.39 (m, 5H), 4.30 (d, *J* = 1.8 Hz, 1H), 4.08 (d, *J* = 1.9 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 193.25, 135.66, 134.13, 129.21, 129.04, 128.93, 128.52, 125.96, 61.21, 59.53. Data were identical to reported literature.[9]

(3-(4-bromophenyl)oxiran-2-yl)(phenyl)methanone (3f)



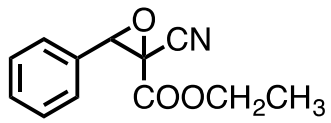
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.3, 2H), 7.66 – 7.60 (m, 1H), 7.57 – 7.47 (m, 4H), 7.25 (d, *J* = 8.1 Hz, 2H), 4.24 (d, *J* = 1.9 Hz, 1H), 4.05 (d, *J* = 1.8 Hz, 1H). **^{13}C NMR** (126 MHz, CDCl3) δ 192.85, 135.55, 134.76, 134.26, 132.15, 129.09, 128.52, 127.56, 123.25, 61.08, 58.87. Data were identical to reported literature.[9]

(3-(4-nitrophenyl)oxiran-2-yl)(phenyl)methanone (3g)



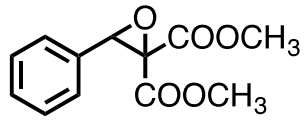
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.8 Hz, 2H), 8.01 (d, *J* = 7.1 Hz, 2H), 7.70 – 7.62 (m, 1H), 7.64 – 7.41 (m, 4H), 4.27 (d, *J* = 1.8 Hz, 1H), 4.21 (d, *J* = 1.8 Hz, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 192.21, 148.51, 142.90, 135.37, 134.48, 129.17, 128.57, 126.78, 124.22, 61.02, 58.14. Data were identical to reported literature.[10]

Ethyl 2-cyano-3-phenyloxirane-2-carboxylate (3h)



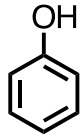
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 – 7.42 (m, 5H), 4.52 (s, 1H), 4.45 – 4.33 (m, 2H), 1.40 (t, 3H, *J* = 7.2 Hz). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 162.84, 130.55, 129.93, 128.93, 126.90, 113.05, 64.60, 64.30, 53.45, 14.14. Data were identical to reported literature.[11]

Dimethyl 3-phenyloxirane-2,2-dicarboxylate (3i)



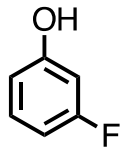
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.27 (m, 5H), 4.57 (s, 1H), 3.88 (s, 3H), 3.57 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 165.94, 164.11, 132.01, 129.32, 128.59, 126.21, 63.24, 62.45, 53.70, 52.75. Data were identical to reported literature.[12]

Phenol (5a)[13]



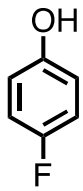
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23 – 7.19 (m, 2H), 6.91 – 6.87 (m, 1H), 6.83-6.81 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 155.61, 129.81, 120.93, 115.44. Data were identical to reported literature.[13]

3-Fluorophenol (5b)



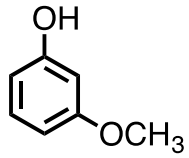
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20-7.14 (m, 1H), 6.65 – 6.55 (m, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 163.77 (d, *J* = 244.4 Hz), 158.10 (d, *J* = 11.8 Hz), 130.32 (d, *J* = 10.4 Hz), 111.40 (d, *J* = 2.8 Hz), 106.86 (d, *J* = 21.3 Hz), 103.29 (d, *J* = 24.2 Hz). Data were identical to reported literature.[13]

4-Fluorophenol (5c)



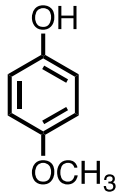
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.92-6.82 (m, 2H), 6.80-6.70 (m, 2H). **^{13}C NMR** (126 MHz, CDCl3) δ 156.89 (d, *J* = 236.4 Hz), 152.58 (d, *J* = 2.1 Hz), 116.31 (d, *J* = 7.8 Hz), 115.77 (d, *J* = 23.1 Hz). Data were identical to reported literature.[13]

3-methoxyphenol (5d)



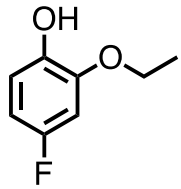
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.17-7.11 (m, 1H), 6.61 – 6.48 (m, 1H), 6.45 – 6.42 (m, 2H), 3.78 (s, 3H**).** **^{13}C NMR** (126 MHz, $CDCl_3$) δ 161.06, 156.98, 130.26, 107.99, 106.49, 101.73, 55.42. Data were identical to reported literature.[14]

4-methoxyphenol (5e)



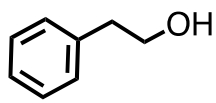
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.81-6.75 (m, 4H), 3.76 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 153.77, 149.70, 116.20, 115.00, 55.96. Data were identical to reported literature.[15]

2-ethoxy-4-fluorophenol (5f)



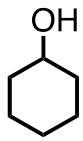
^{1}H NMR (400 MHz, $CDCl_3$) δ 6.83 (dd, *J* = 8.7, 5.5 Hz, 1H), 6.68 – 6.41 (m, 2H), 4.09 (q, *J* = 7.0 Hz, 2H), 1.46 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 156.72 (d, *J* = 237.4 Hz), 146.17 (d, *J* = 10.2 Hz), 141.99 (d, *J* = 3.0 Hz), 114.28 (d, *J* = 9.6 Hz), 106.82 (d, *J* = 22.6 Hz), 100.20 (d, *J* = 27.5 Hz), 64.91, 14.85. **HRMS-ESI** $[M-H]^-$ Calcd for $C_8H_8FO_2$ 155.0508, found 155.0510. Data were identical to reported literature.[15]

2-phenylethan-1-ol (5g)



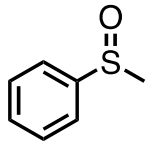
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 – 7.28 (m, 2H), 7.24 (m, 3H), 3.87 (t, *J* = 6.6 Hz, 2H), 2.88 (t, *J* = 6.6 Hz, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 138.62, 129.15, 128.70, 126.59, 63.78, 39.32. Data were identical to reported literature.[16]

Cyclohexanol (5h)



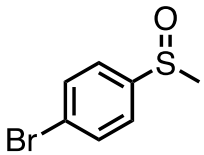
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.94 – 1.84 (m, 2H), 1.72 (m, 2H), 1.59 – 1.49 (m, 1H), 1.35 – 1.23 (m, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 70.40, 35.62, 25.57, 24.25. Data were identical to reported literature.[17]

(Methylsulfinyl)benzene (7a)



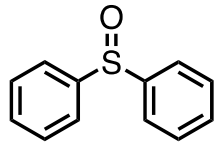
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.55 – 7.41 (m, 3H), 2.72 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.47, 131.19, 129.46, 123.61, 43.90. Data were identical to reported literature.[18]

1-Bromo-4-(methylsulfinyl)benzene (7b)



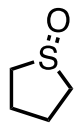
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.6 Hz, 2H), 2.70 (s, 3H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 144.64, 132.62, 125.55, 125.22, 43.90. Data were identical to reported literature.[18]

Sulfinyldibenzene (7c)



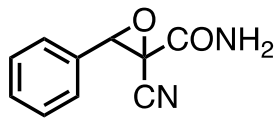
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 7.8 Hz, 4H), 7.45 (d, *J* = 7.2 Hz, 6H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 145.73, 131.19, 129.46, 124.93. Data were identical to reported literature.[19]

Tetrahydrothiophene 1-oxide (7d)

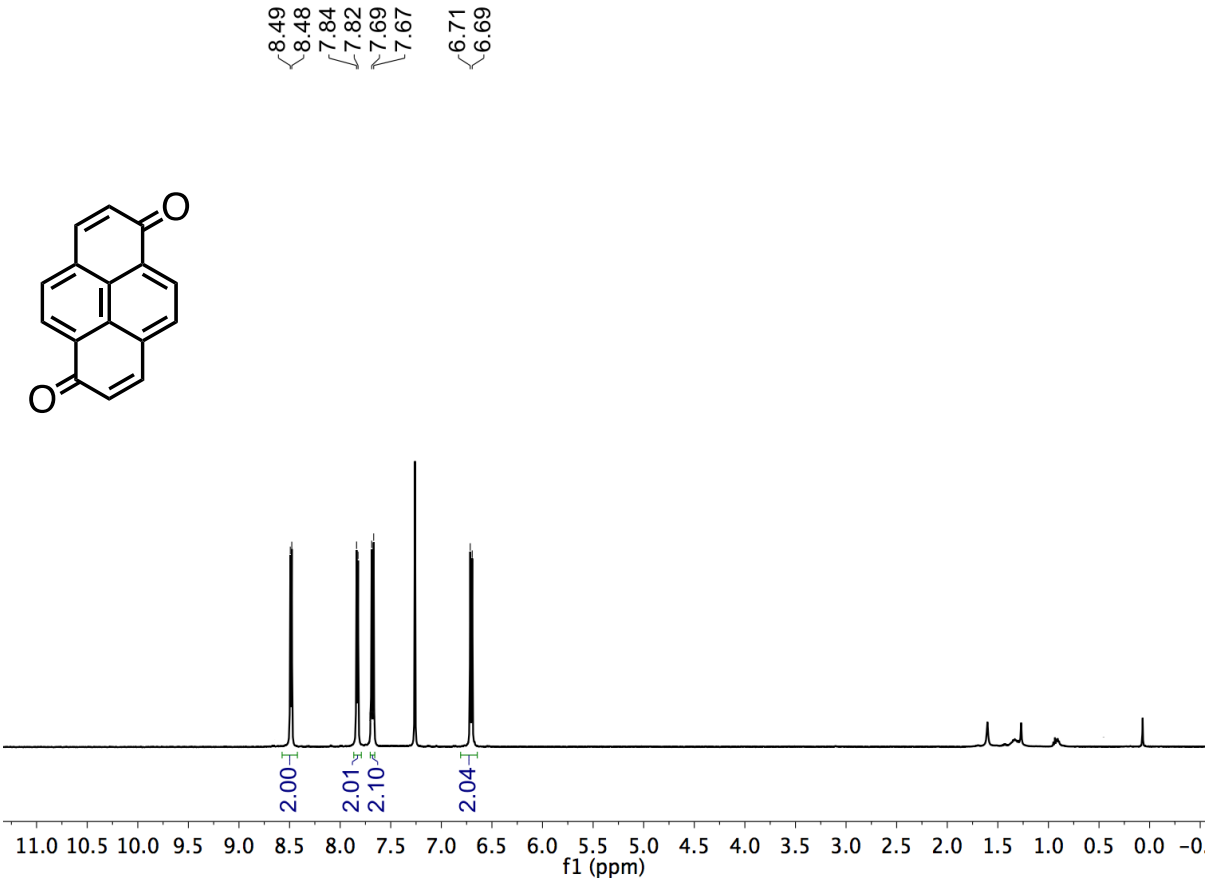


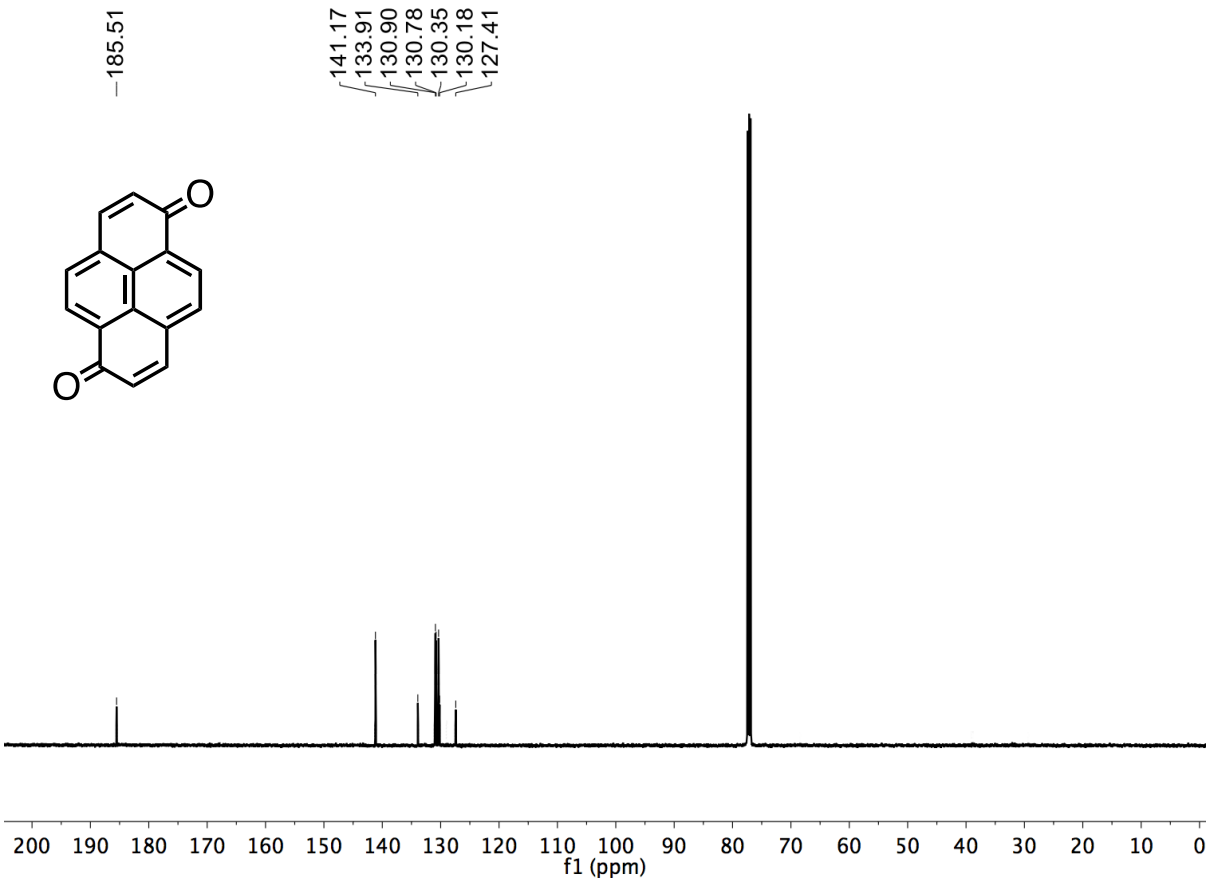
^{1}H NMR (500 MHz, $CDCl_3$) δ 2.82-2.75 (m, 4H), 2.47-2.33 (m,2H), 2.20-1.90 (m, 2H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 54,40, 25.60. Data were identical to reported literature.[20]

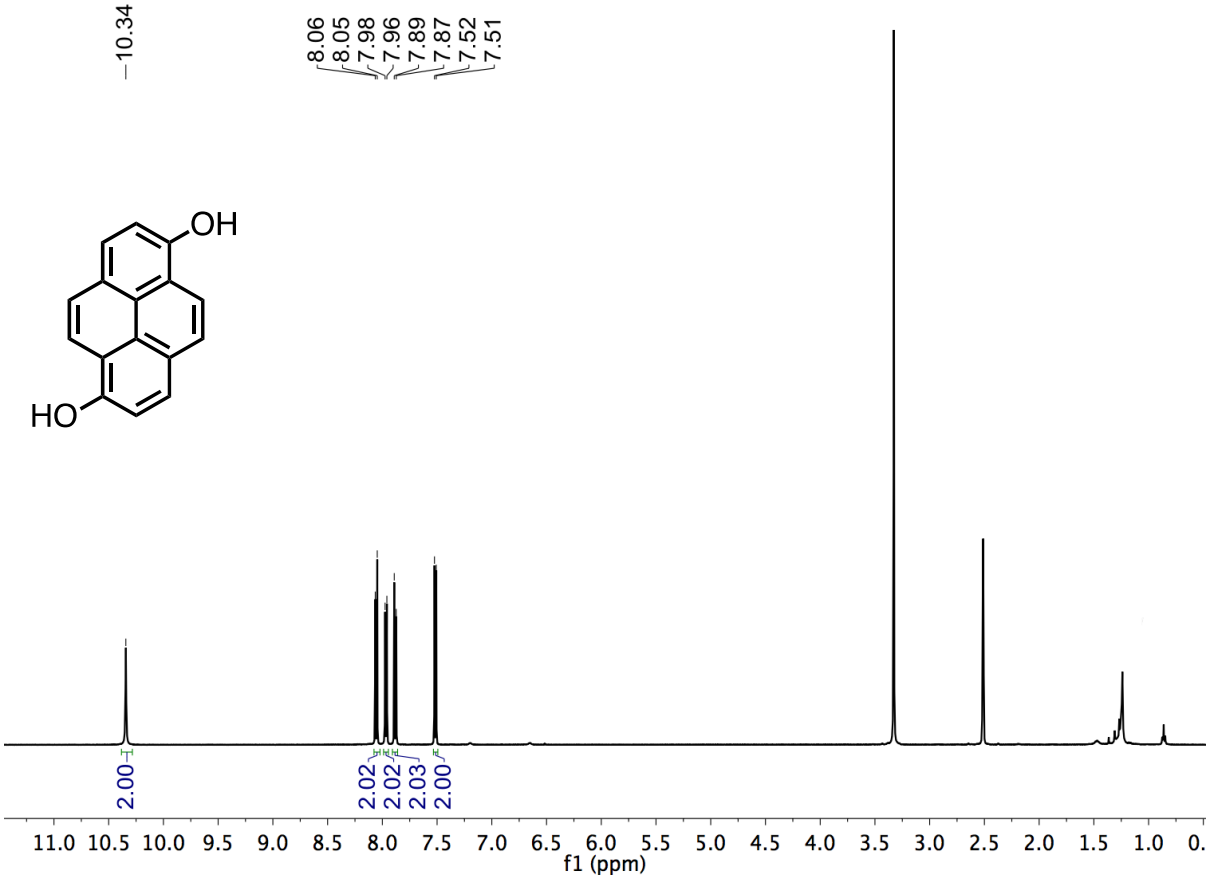
2-Cyano-3-phenyloxirane-2-carboxamide (2a')

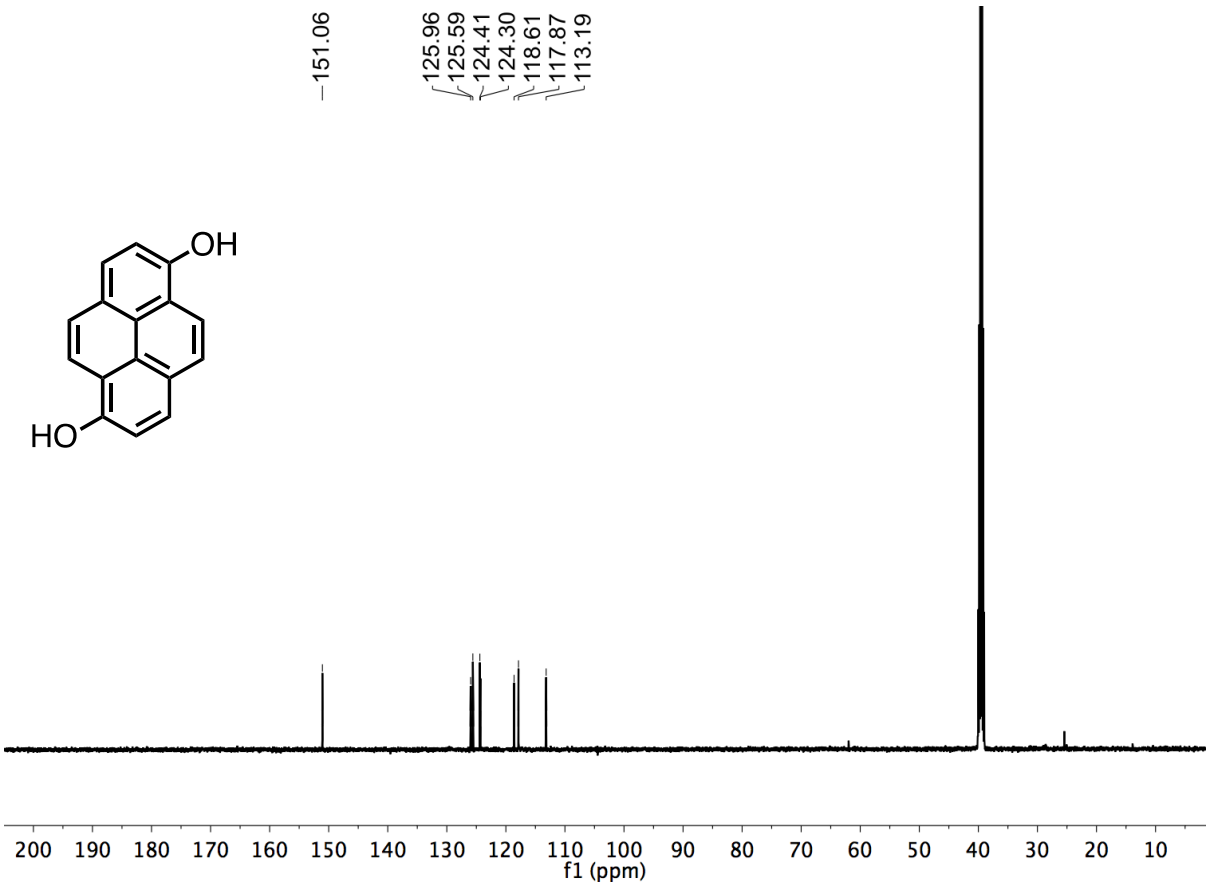


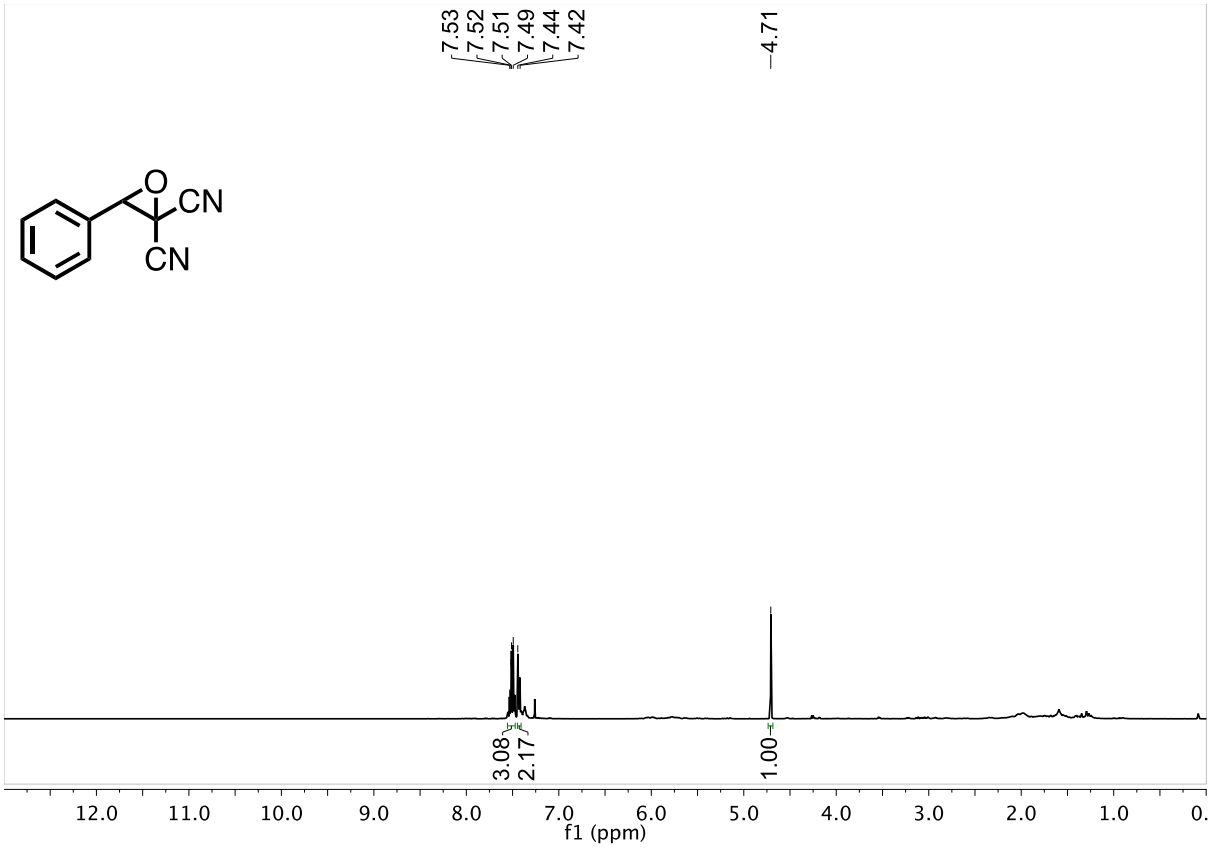
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.16 (m, 5H), 6.57 (br, 1H), 6.44 (br, 1H), 4.41 (s, 1H). **^{13}C NMR** (126 MHz, $CDCl_3$) δ 164.70, 130.62, 129.73, 128.96, 126.76, 113.12, 64.84, 55.25. **HRMS-ESI** $[M-H]^-$ Calcd for $C_{10}H_7N_2O_2$ 187.0508, found 187.0960. Data were identical to reported literature.[21]

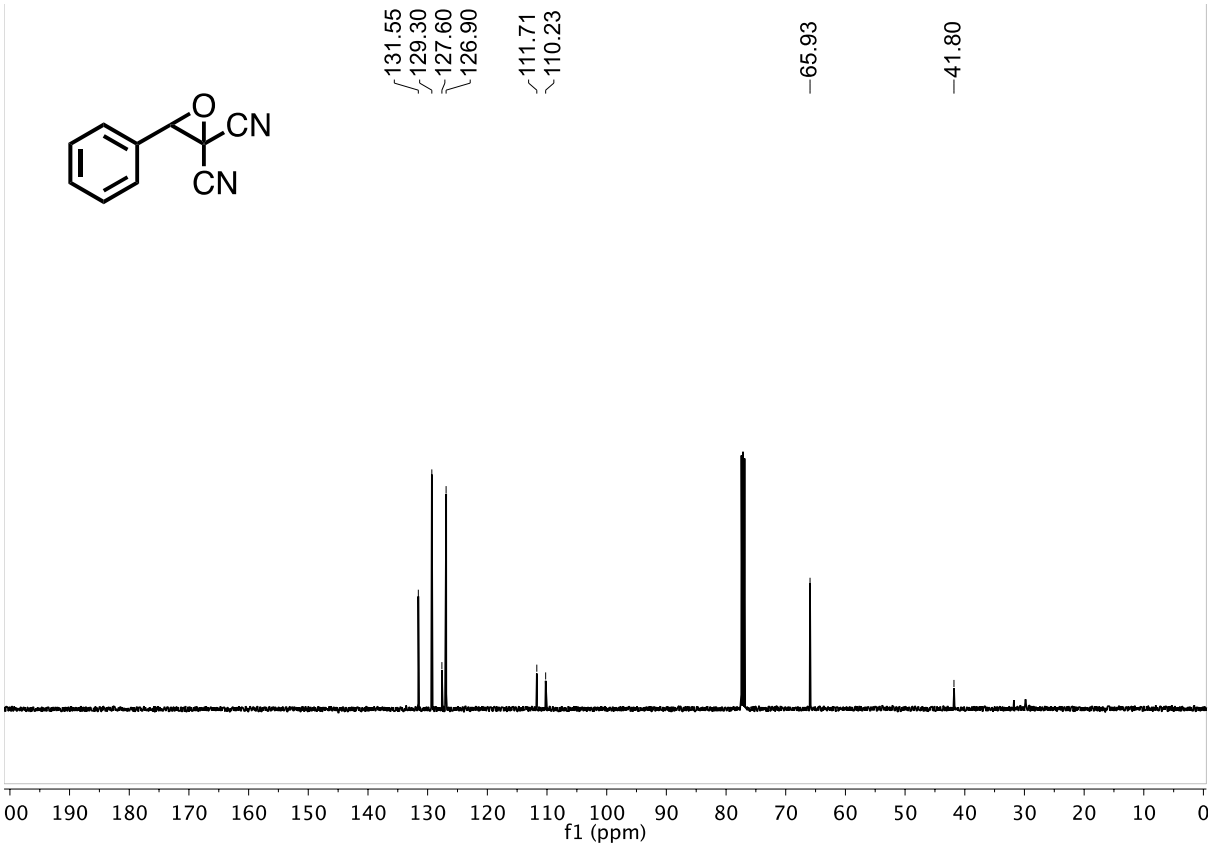


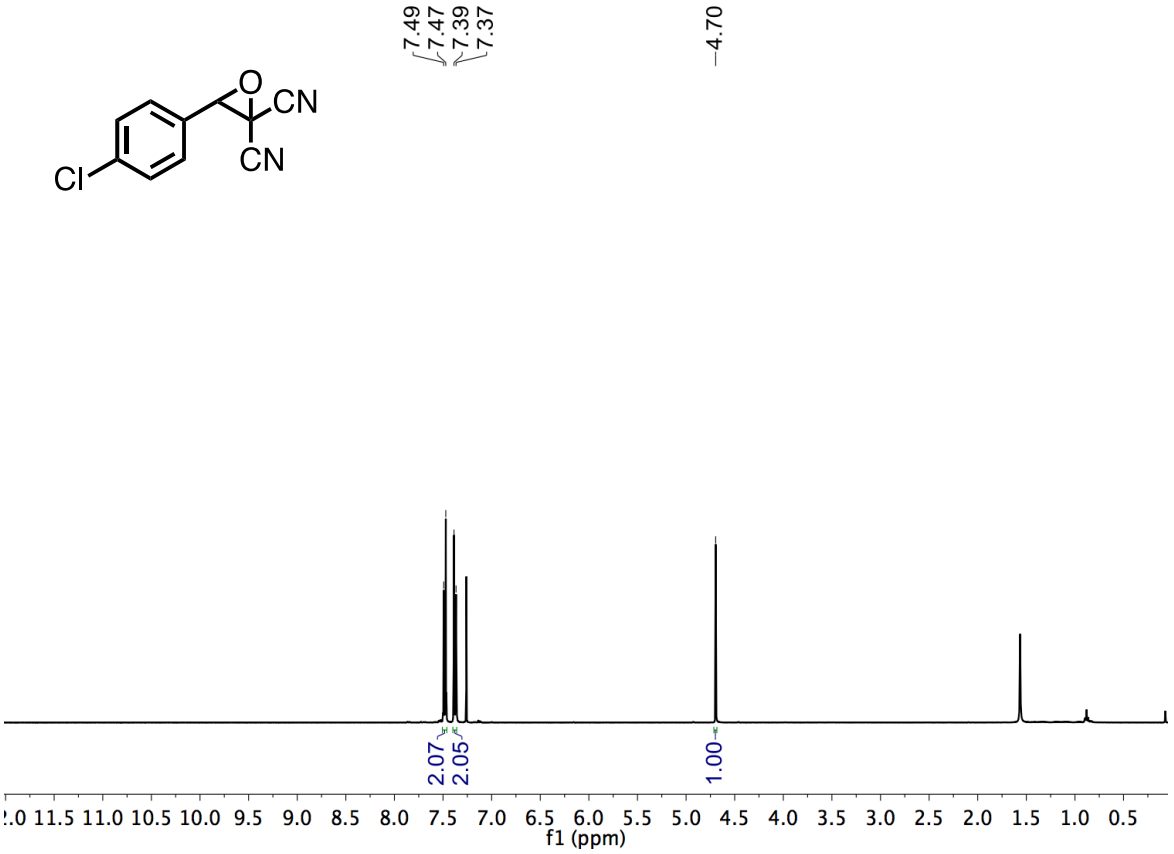

185.51
141.17
133.91
130.90
130.78
130.35
130.18
127.41
O
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

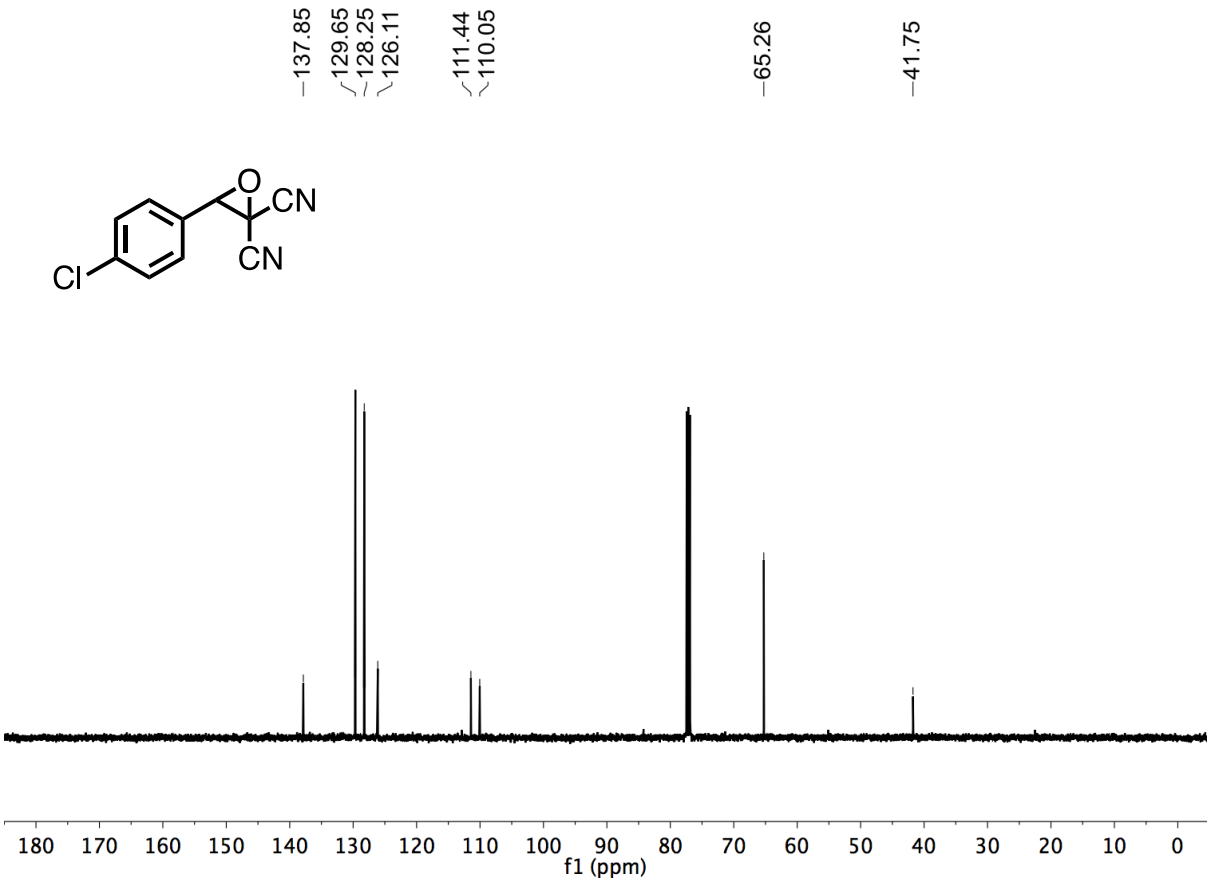

10.34
8.06
8.05
7.98
7.96
7.89
7.87
7.52
7.51
OH
HO
2.00
2.02
2.02
2.03
2.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.
f1 (ppm)

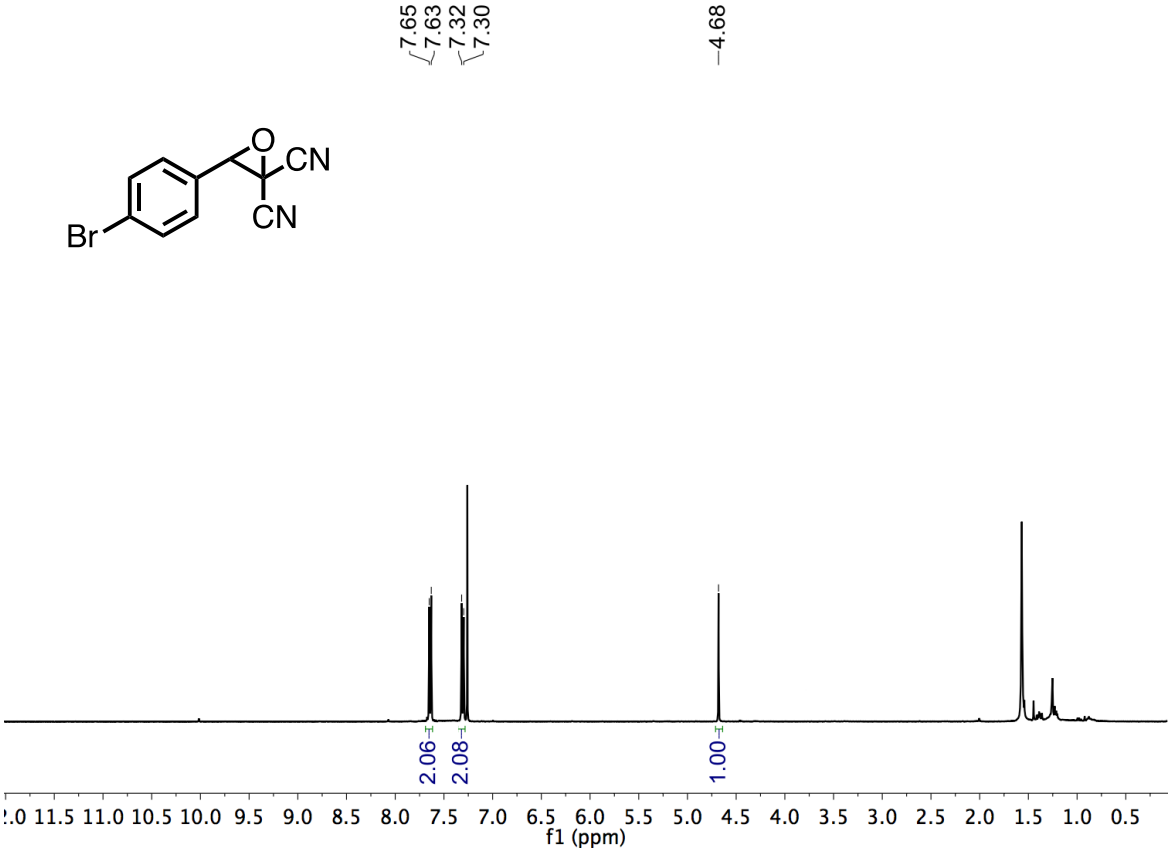

151.06
125.96
125.59
124.41
124.30
118.61
117.87
113.19
OH
HO
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

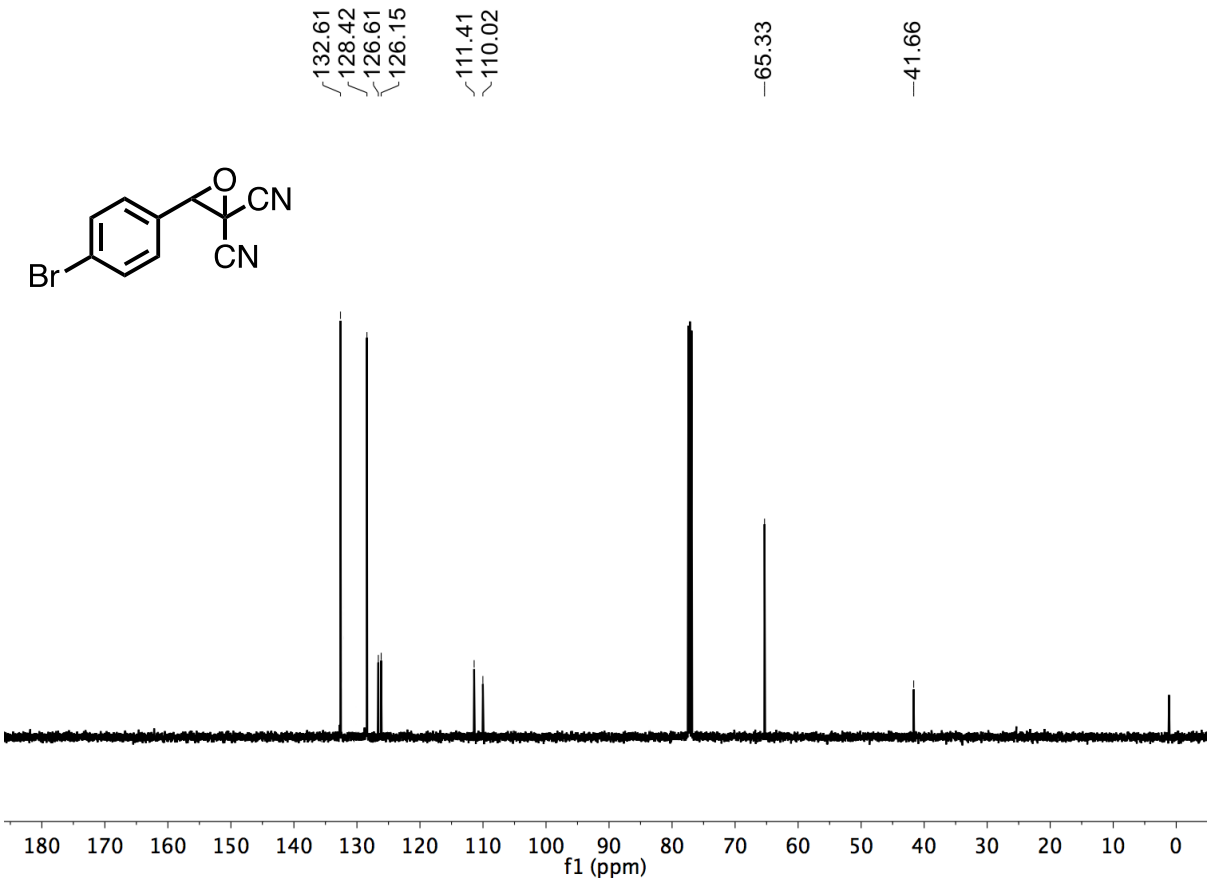

7.53
7.52
7.51
7.49
7.44
7.42
4.71
O
CN
CN
3.08
2.17
1.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.
f1 (ppm)

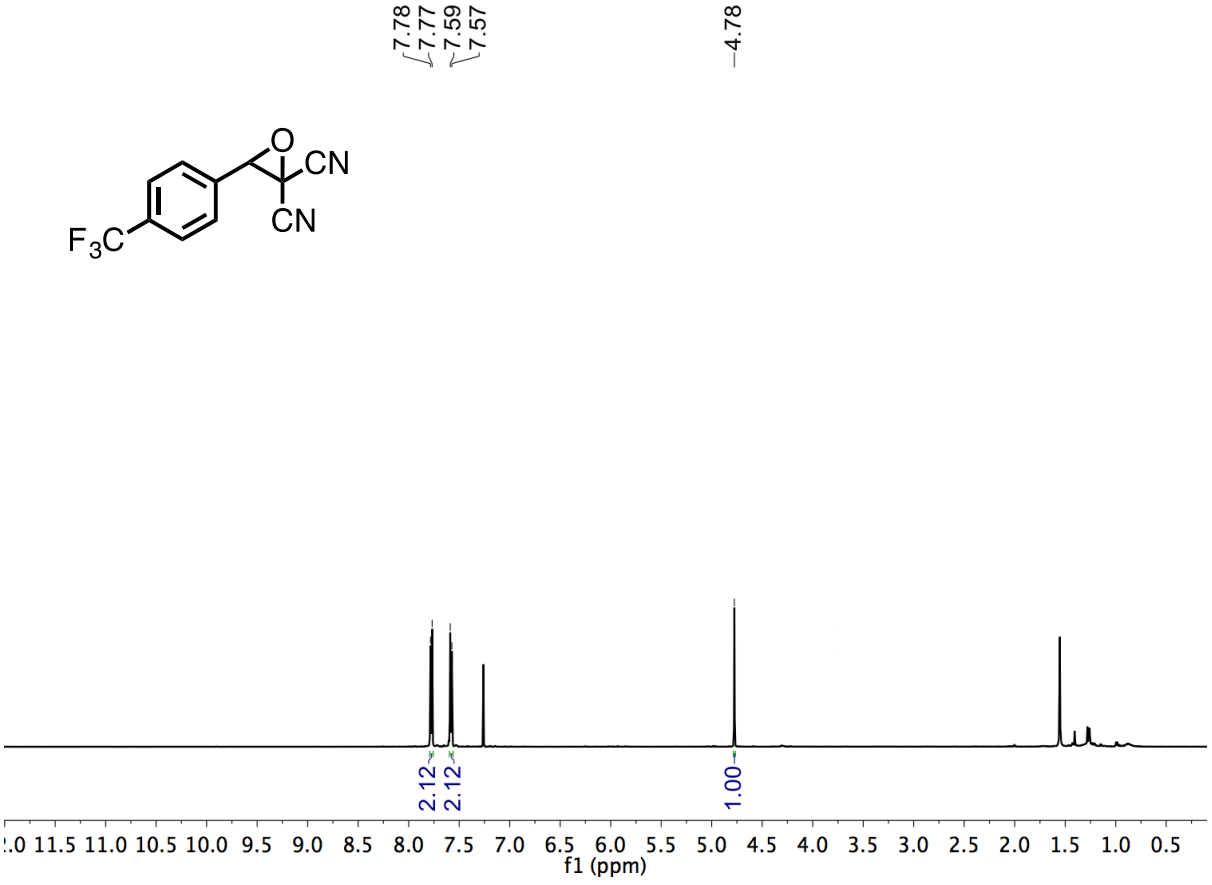

131.55
129.30
127.60
126.90
111.71
110.23
65.93
41.80
O
CN
CN
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

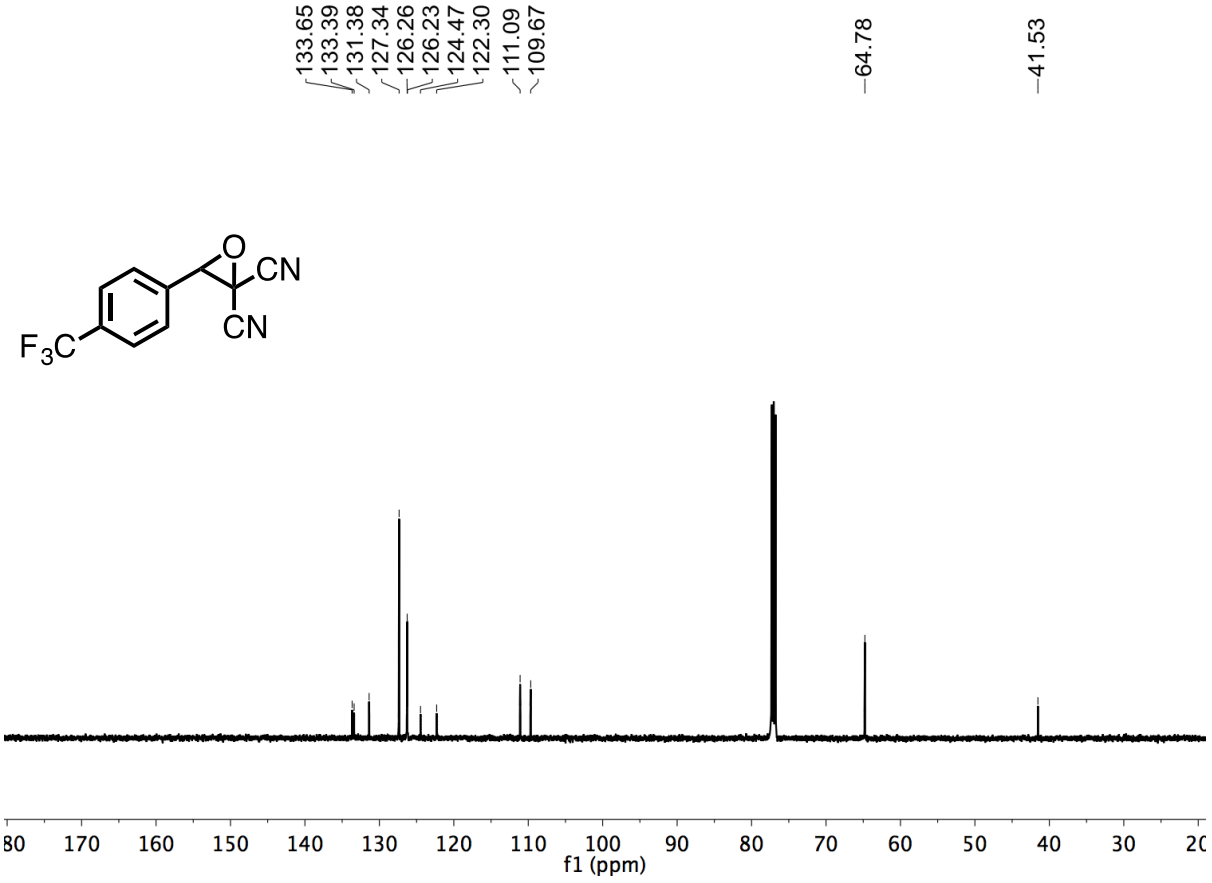

7.49
7.47
7.39
7.37
4.70
O
CN
CN
Cl
2.07
2.05
1.00
.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

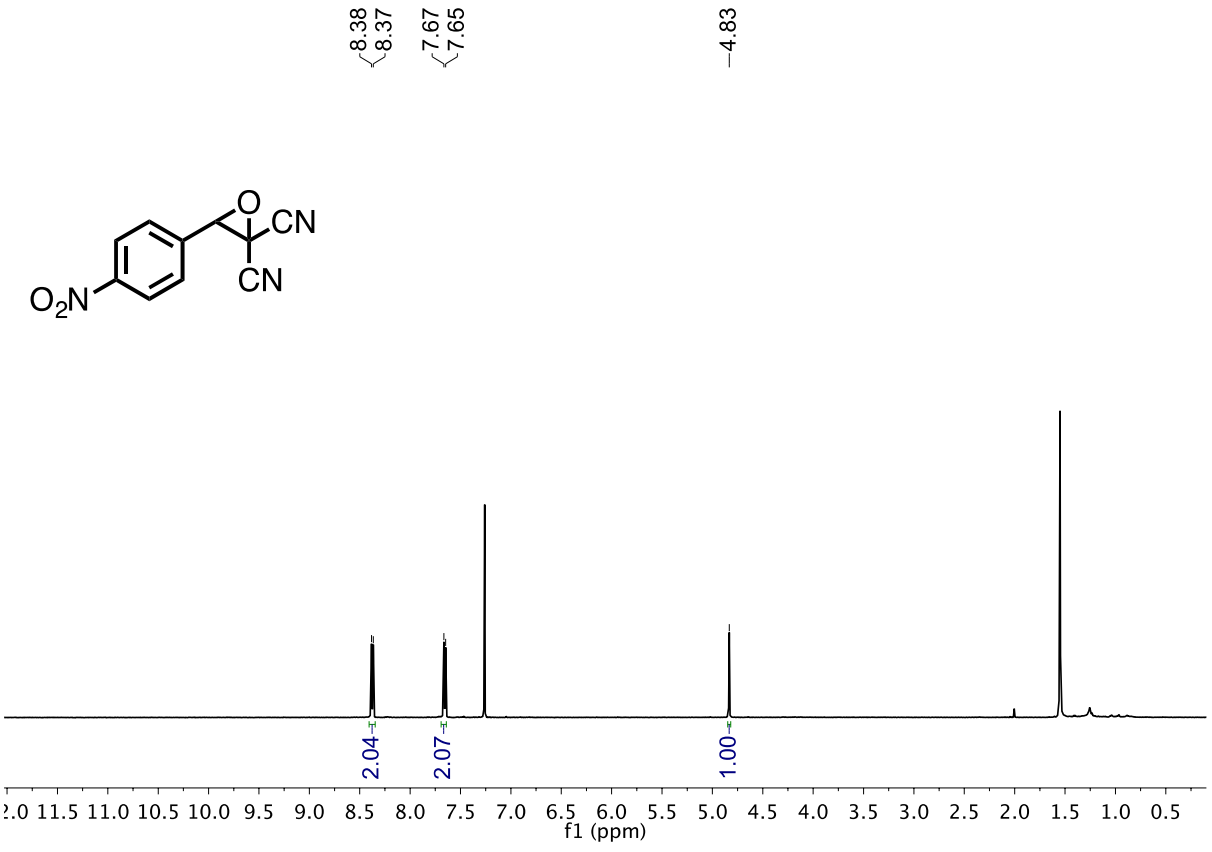

137.85
129.65
128.25
126.11
111.44
110.05
65.26
41.75
O
CN
CN
Cl
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

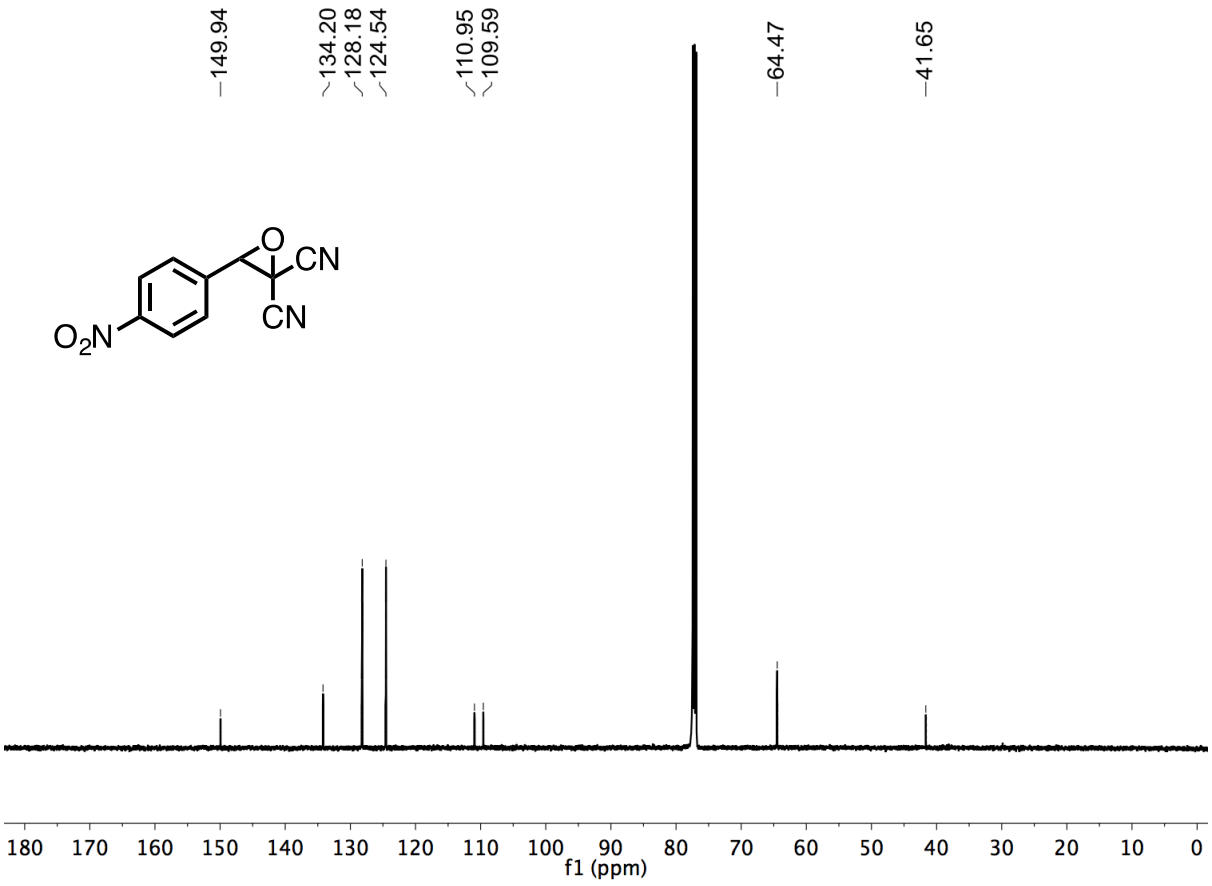

7.65
7.63
7.32
7.30
4.68
O
CN
CN
Br
2.06
2.08
1.00
f1 (ppm)


132.61
128.42
126.61
126.15
111.41
110.02
65.33
41.66
O
CN
CN
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

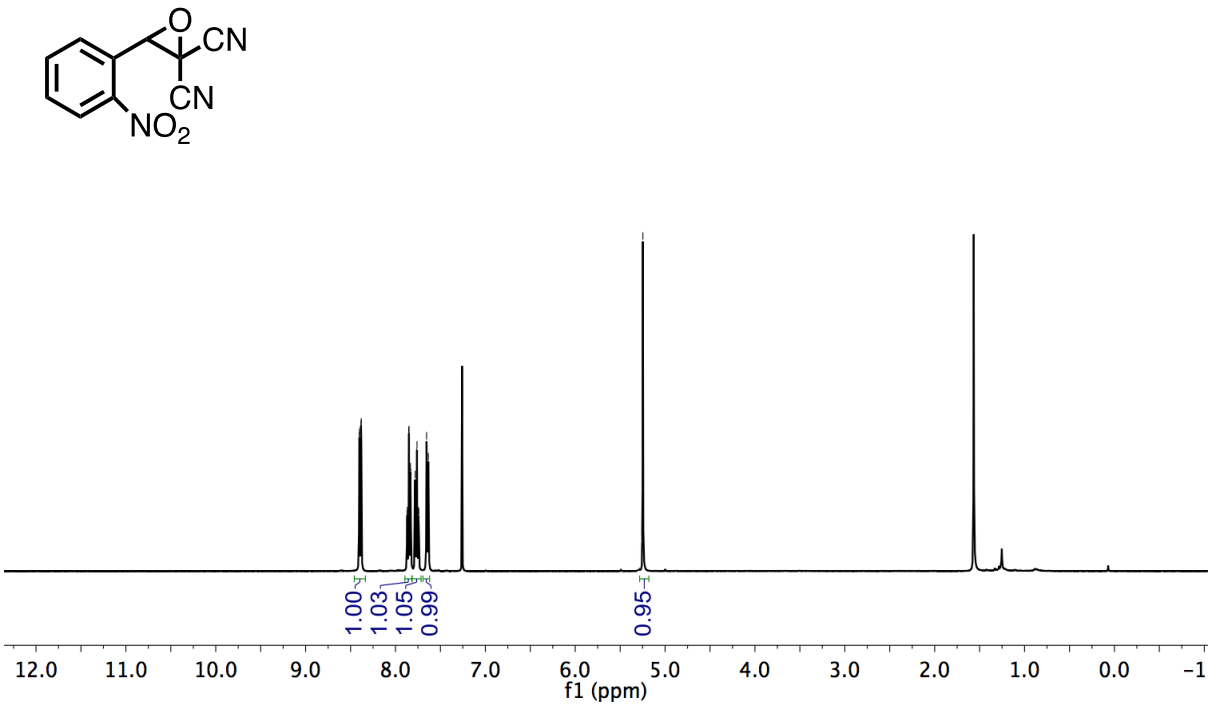

7.78
7.77
7.59
7.57
4.78
O
CN
CN
F3C
2.12
2.12
1.00
f1 (ppm)

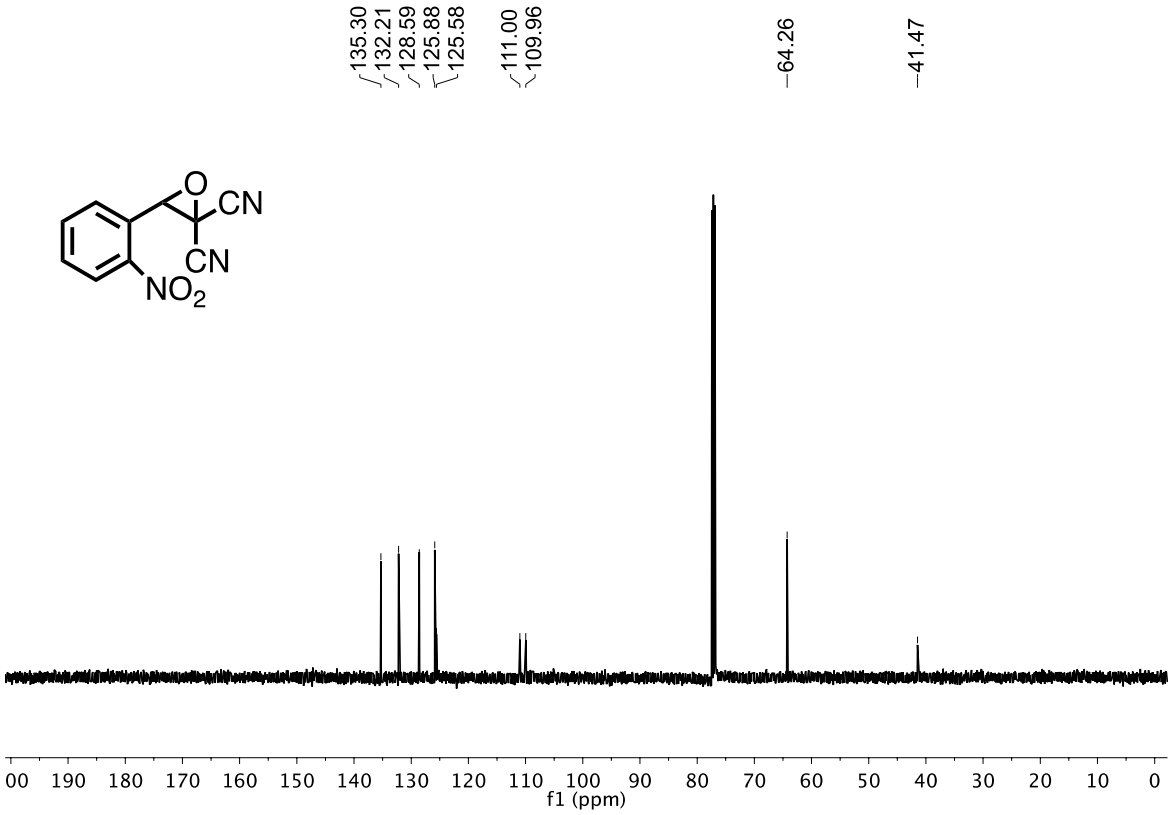

133.65
133.39
131.38
127.34
126.26
126.23
124.47
122.30
111.09
109.67
64.78
41.53
O
CN
CN
F3C
80 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20
f1 (ppm)

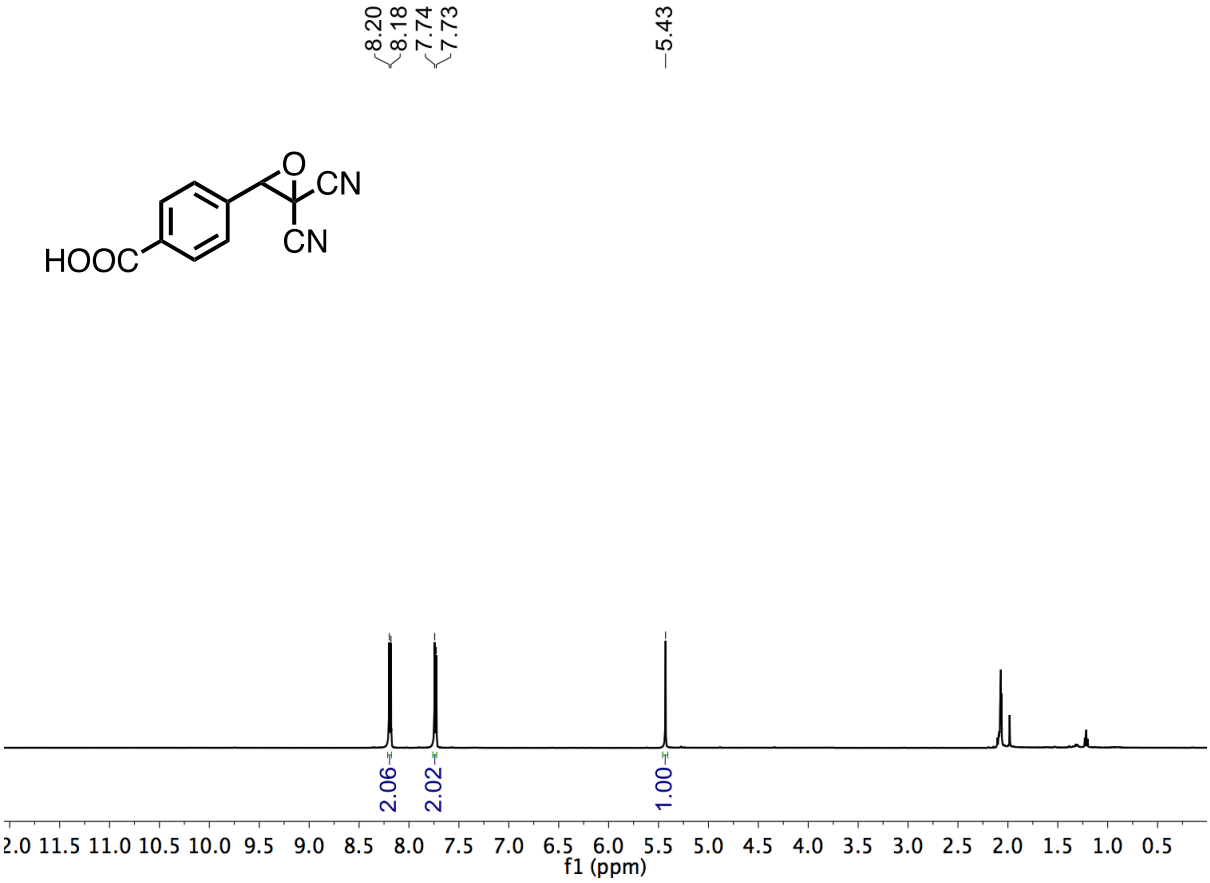

8.38
8.37
7.67
7.65
4.83
O
CN
CN
O2N
2.04
2.07
1.00
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

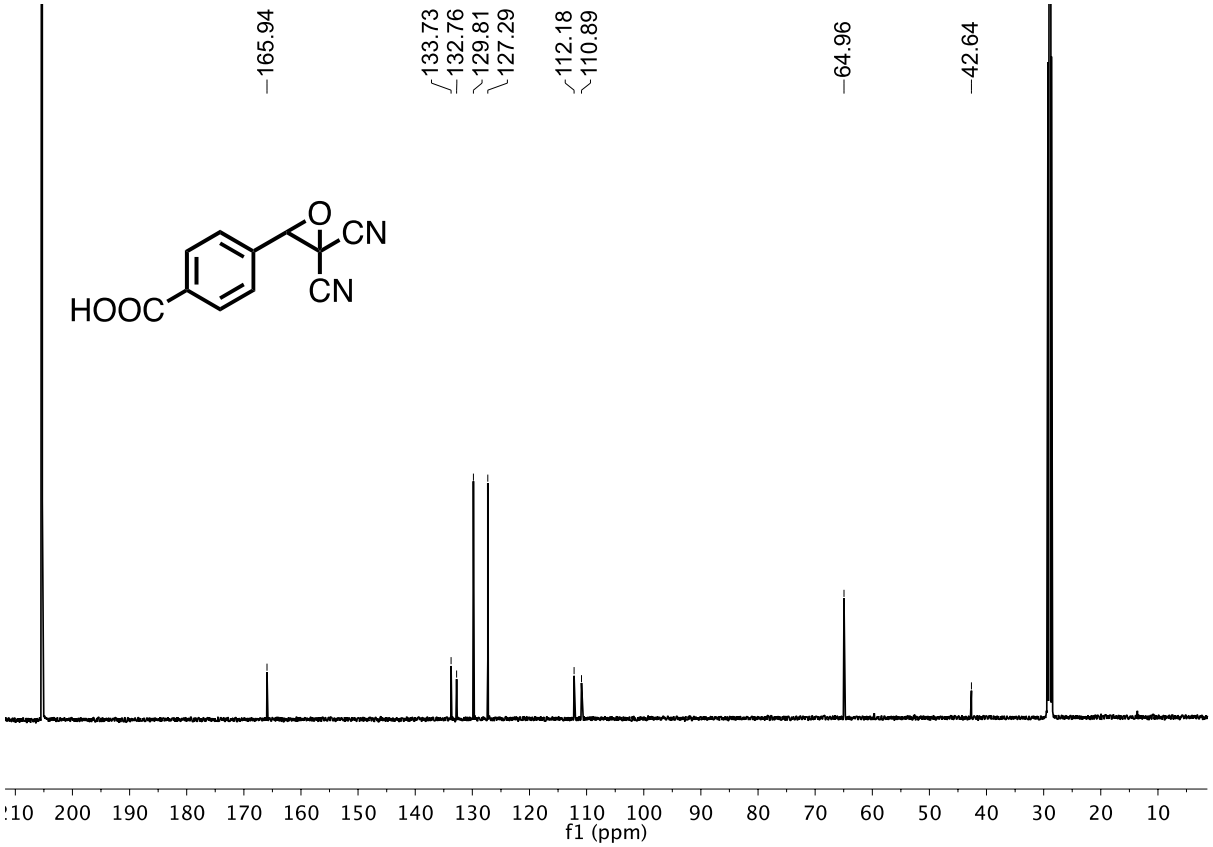

149.94
134.20
128.18
124.54
110.95
109.59
64.47
41.65
O
CN
CN
O2N
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

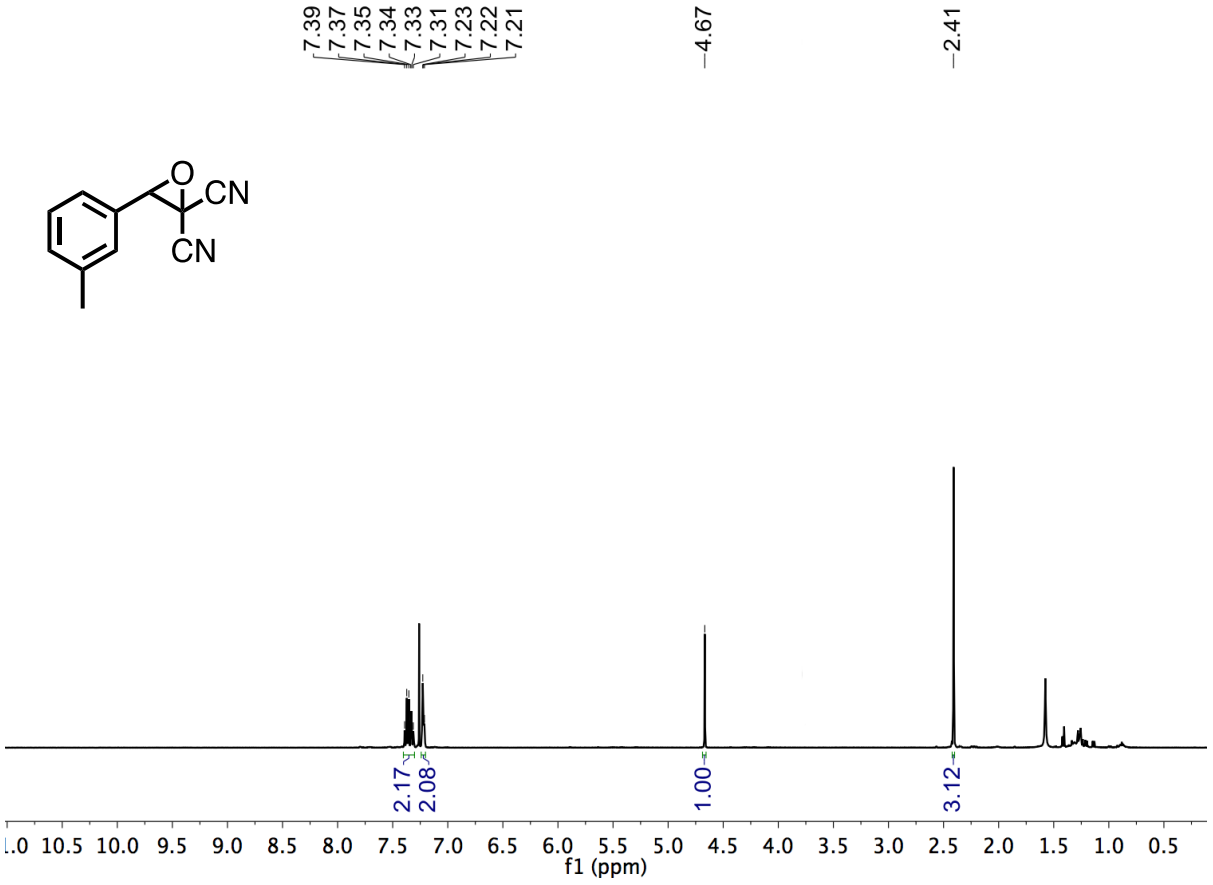

8.40
8.40
8.38
8.38
7.87
7.87
7.85
7.85
7.83
7.83
7.78
7.78
7.76
7.76
7.74
7.74
7.66
7.65
7.65
7.64
7.63
7.63
5.25

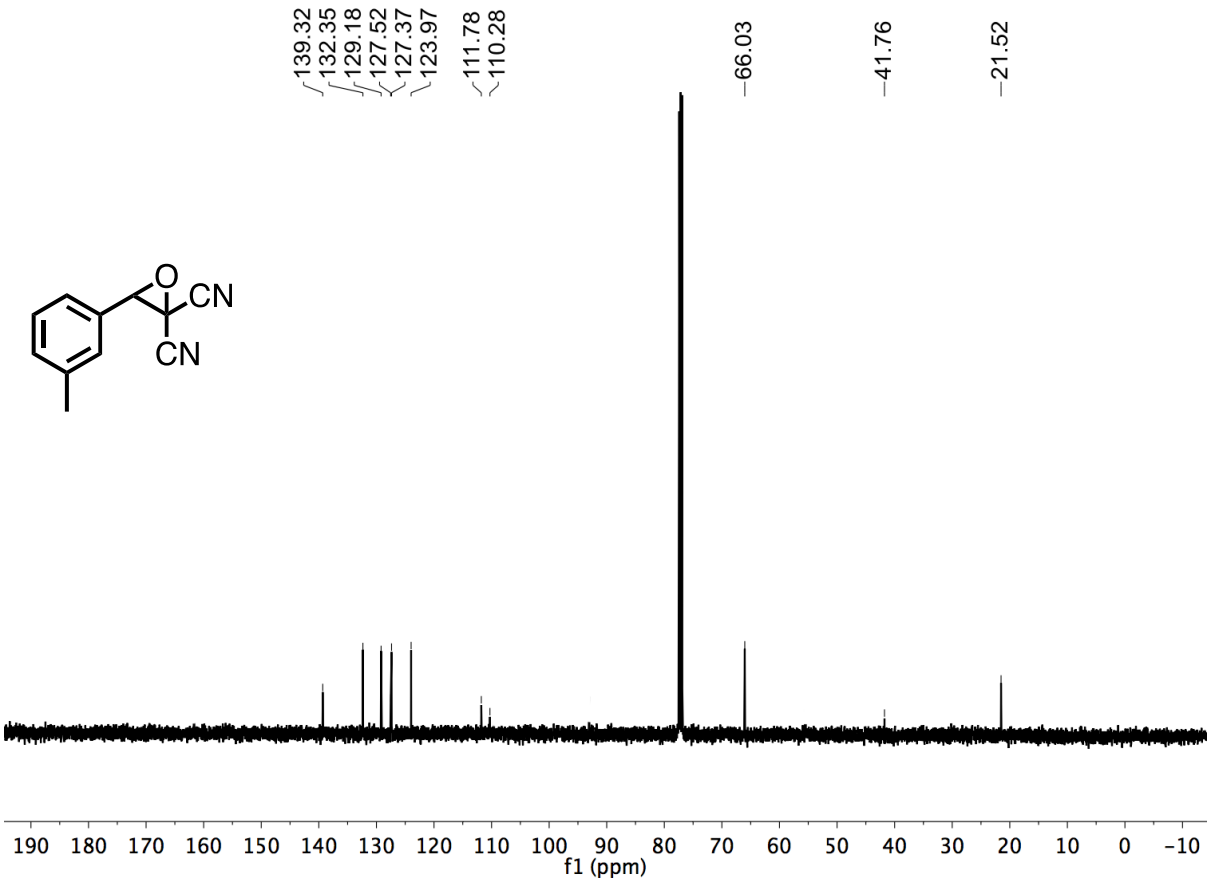

O
CN
CN
NO2
1.00
1.03
1.05
0.99
0.95
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1
f1 (ppm)

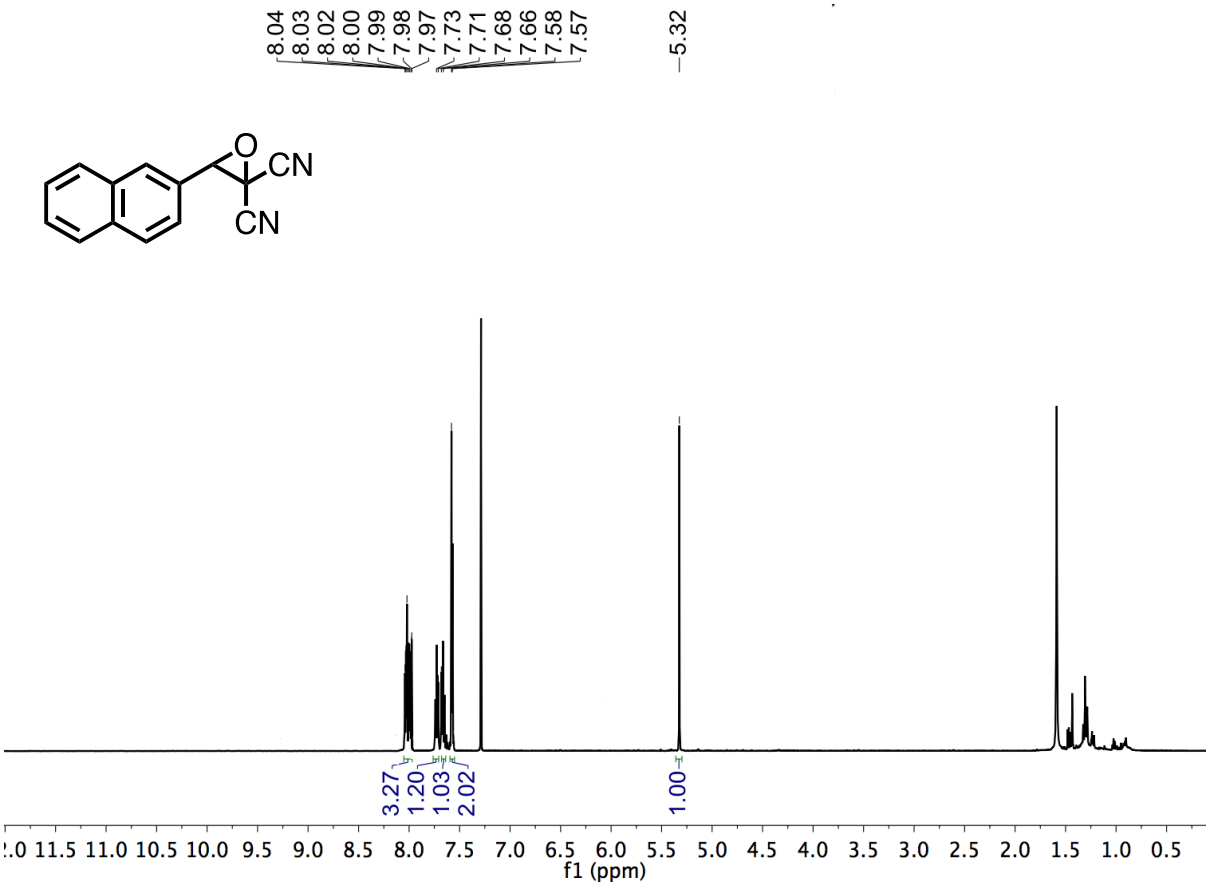

135.30
132.21
128.59
125.88
125.58
111.00
109.96
64.26
41.47
O
CN
CN
NO2
00 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

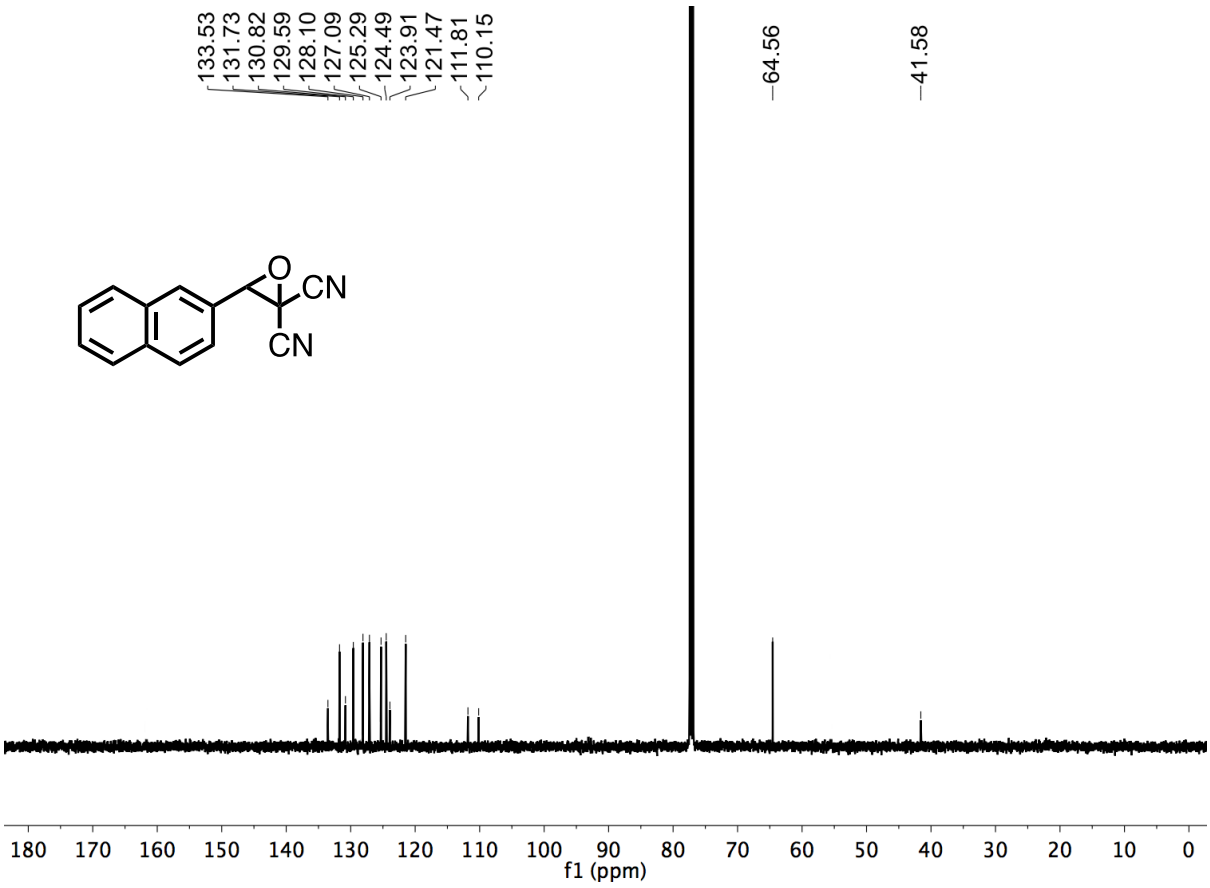

8.20
8.18
7.74
7.73
5.43
O
CN
CN
HOOC
2.06
2.02
1.00
2.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5
f1 (ppm)

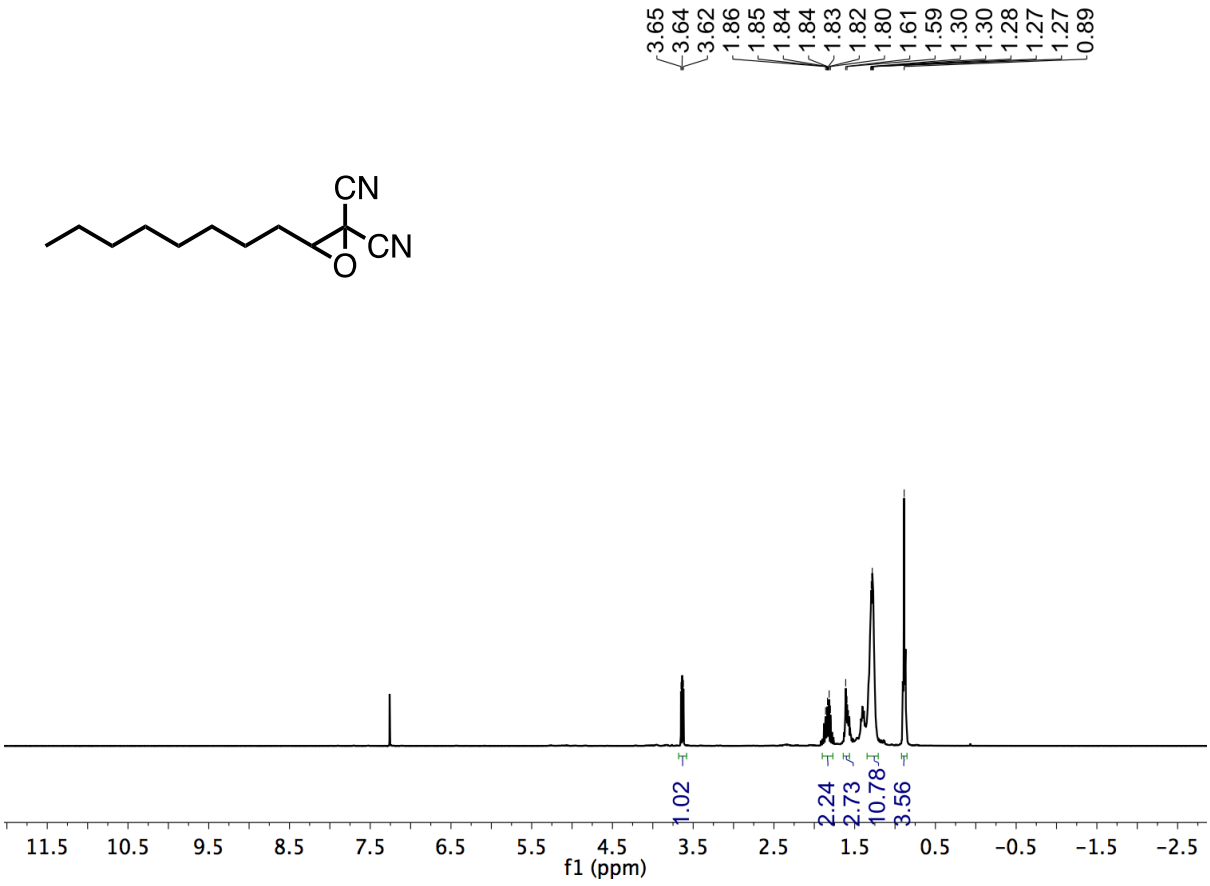

165.94
133.73
132.76
129.81
127.29
112.18
110.89
64.96
42.64
O
CN
CN
HOOC
f1 (ppm)

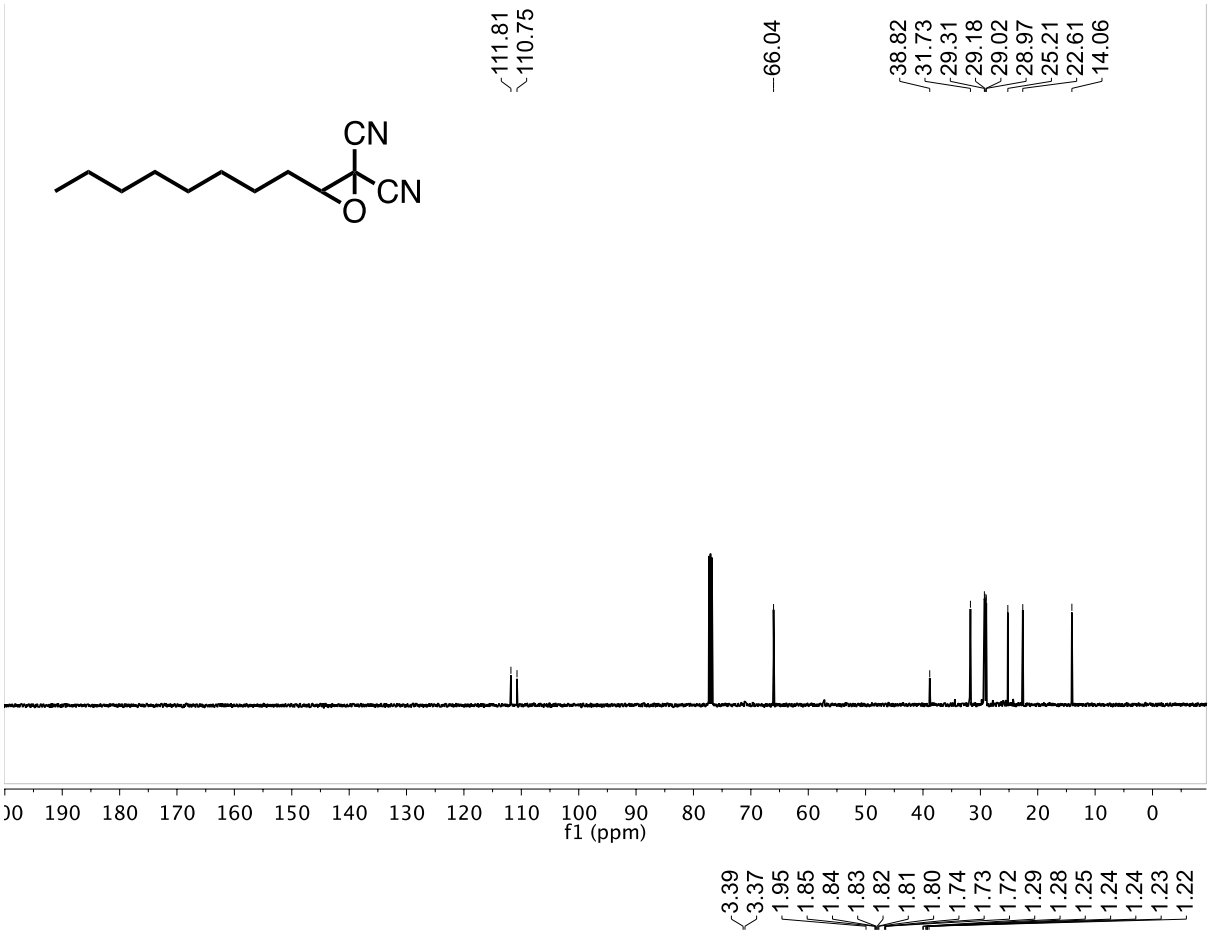

7.39
7.37
7.35
7.34
7.33
7.31
7.23
7.22
7.21
4.67
2.41
O
CN
CN
2.17
2.08
1.00
3.12
f1 (ppm)

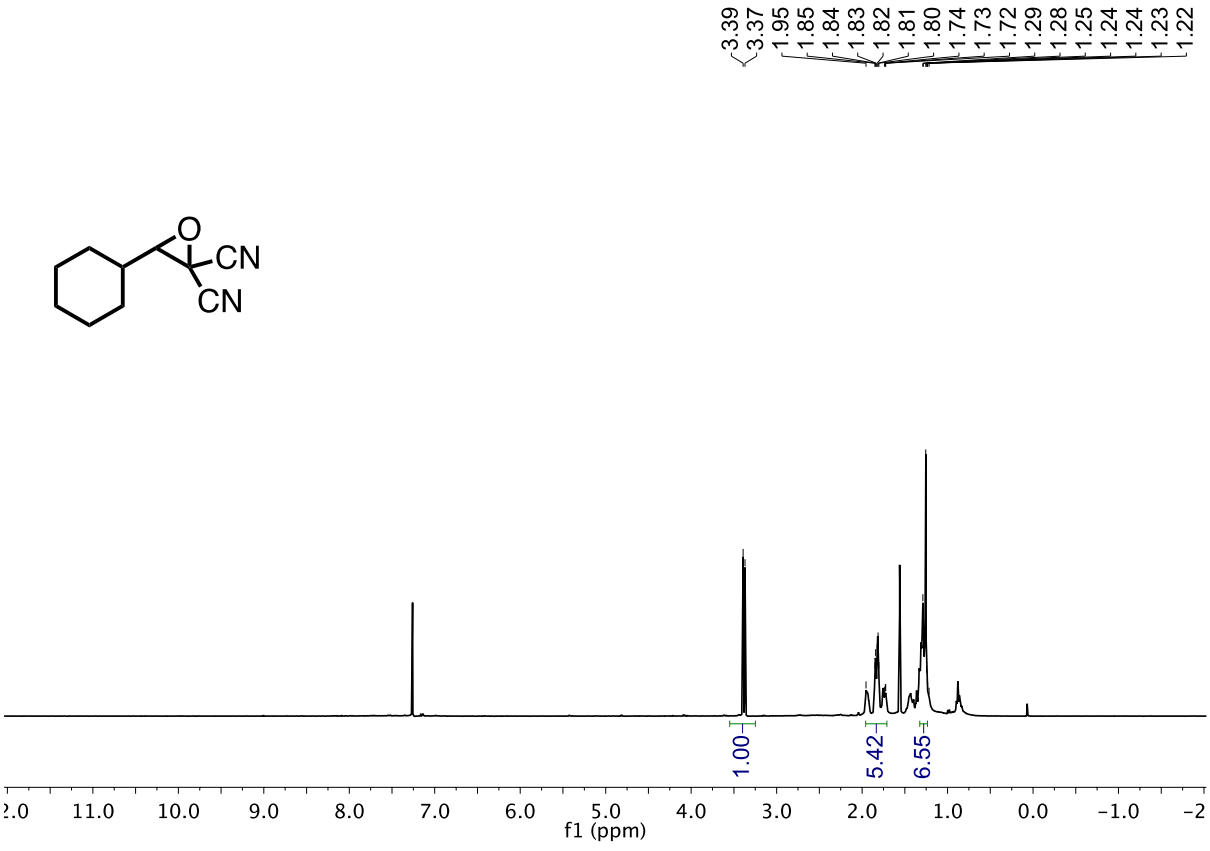

139.32
132.35
129.18
127.52
127.37
123.97
111.78
110.28
66.03
41.76
21.52
O
CN
CN
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

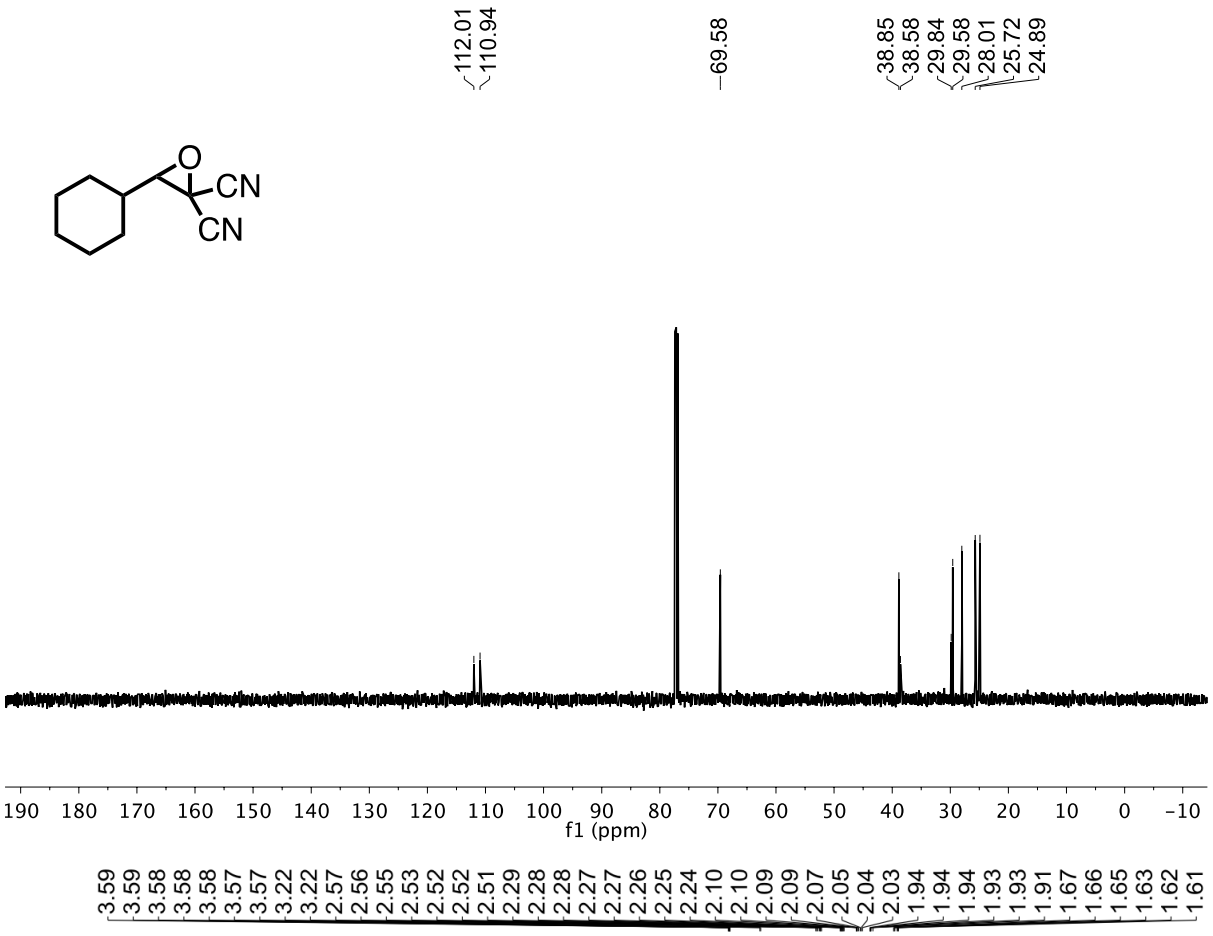

8.04
8.03
8.02
8.00
7.99
7.98
7.97
7.73
7.71
7.68
7.66
7.58
7.57
5.32
O
CN
CN
3.27
1.20
1.03
2.02
1.00
f1 (ppm)


133.53
131.73
130.82
129.59
128.10
127.09
125.29
124.49
123.91
121.47
111.81
110.15
64.56
41.58
O
CN
CN
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


3.65
3.64
3.62
1.86
1.85
1.84
1.84
1.83
1.82
1.80
1.61
1.59
1.30
1.30
1.28
1.27
1.27
0.89
CN
CN
O
1.02
2.24
2.73
10.78
3.56
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5 -1.5 -2.5
f1 (ppm)


111.81
110.75
66.04
38.82
31.73
29.31
29.18
29.02
28.97
25.21
22.61
14.06
CN
CN
O
f1 (ppm)


3.39
3.37
1.95
1.85
1.84
1.83
1.82
1.81
1.80
1.74
1.73
1.72
1.29
1.28
1.25
1.24
1.24
1.23
1.22
O
CN
CN
1.00
5.42
6.55
f1 (ppm)


112.01
110.94
69.58
38.85
38.58
29.84
29.58
28.01
25.72
24.89
O
CN
CN
f1 (ppm)
3.59
3.59
3.58
3.58
3.58
3.57
3.57
3.22
3.22
2.57
2.56
2.55
2.53
2.52
2.52
2.51
2.29
2.28
2.28
2.27
2.27
2.26
2.25
2.24
2.10
2.10
2.09
2.09
2.07
2.05
2.04
2.03
1.94
1.94
1.94
1.93
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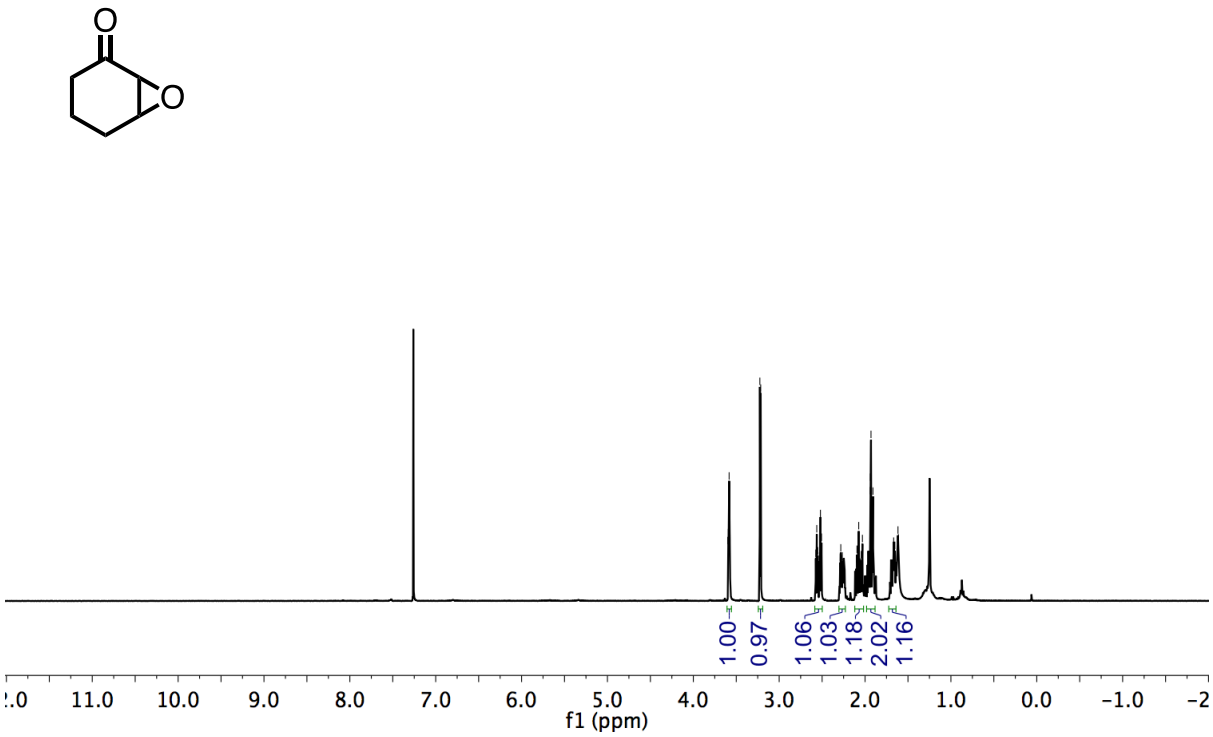
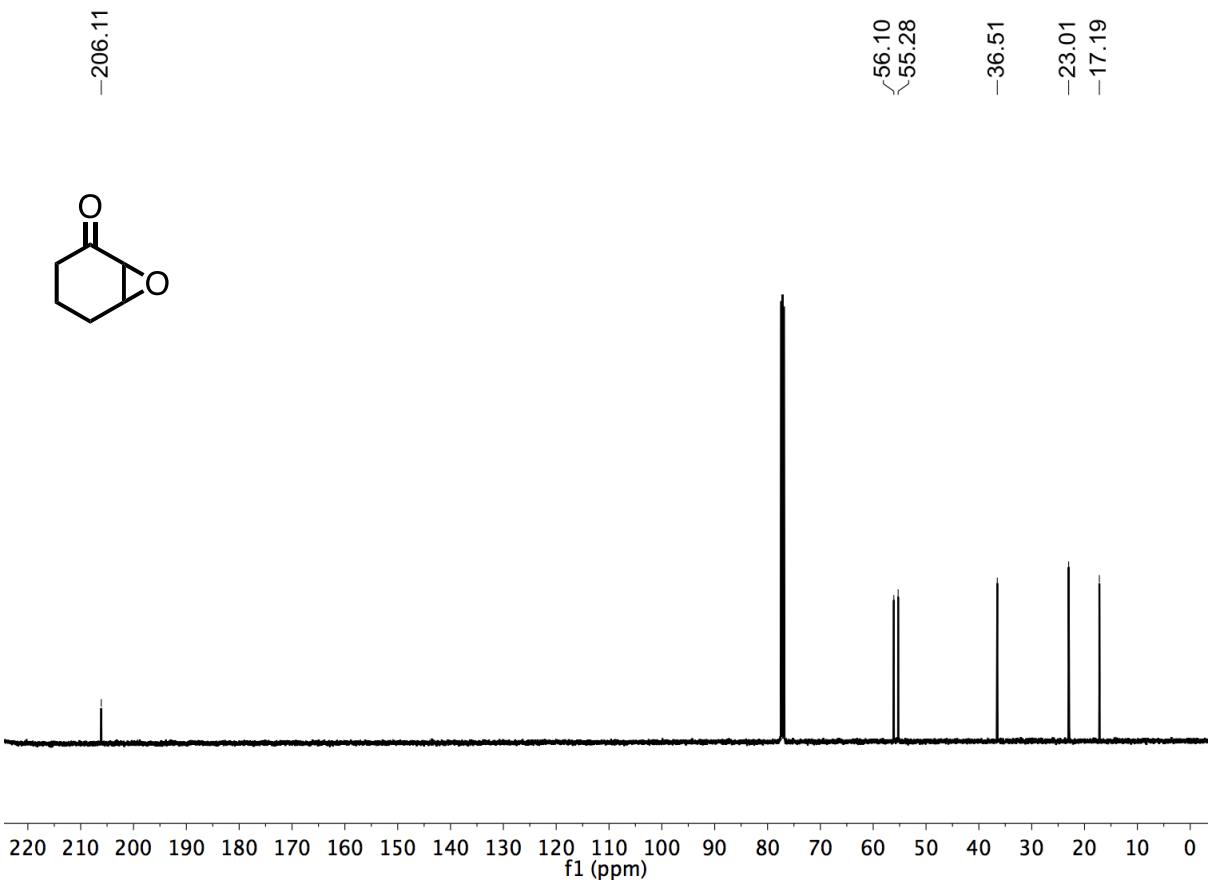
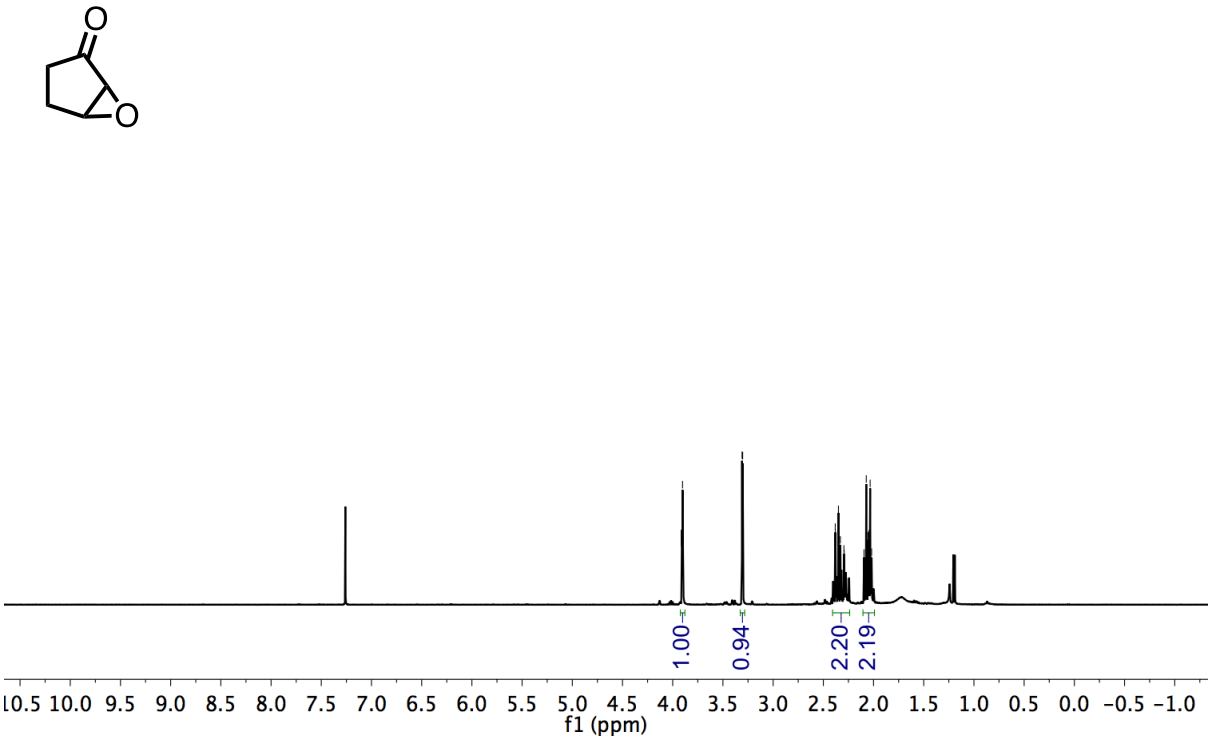
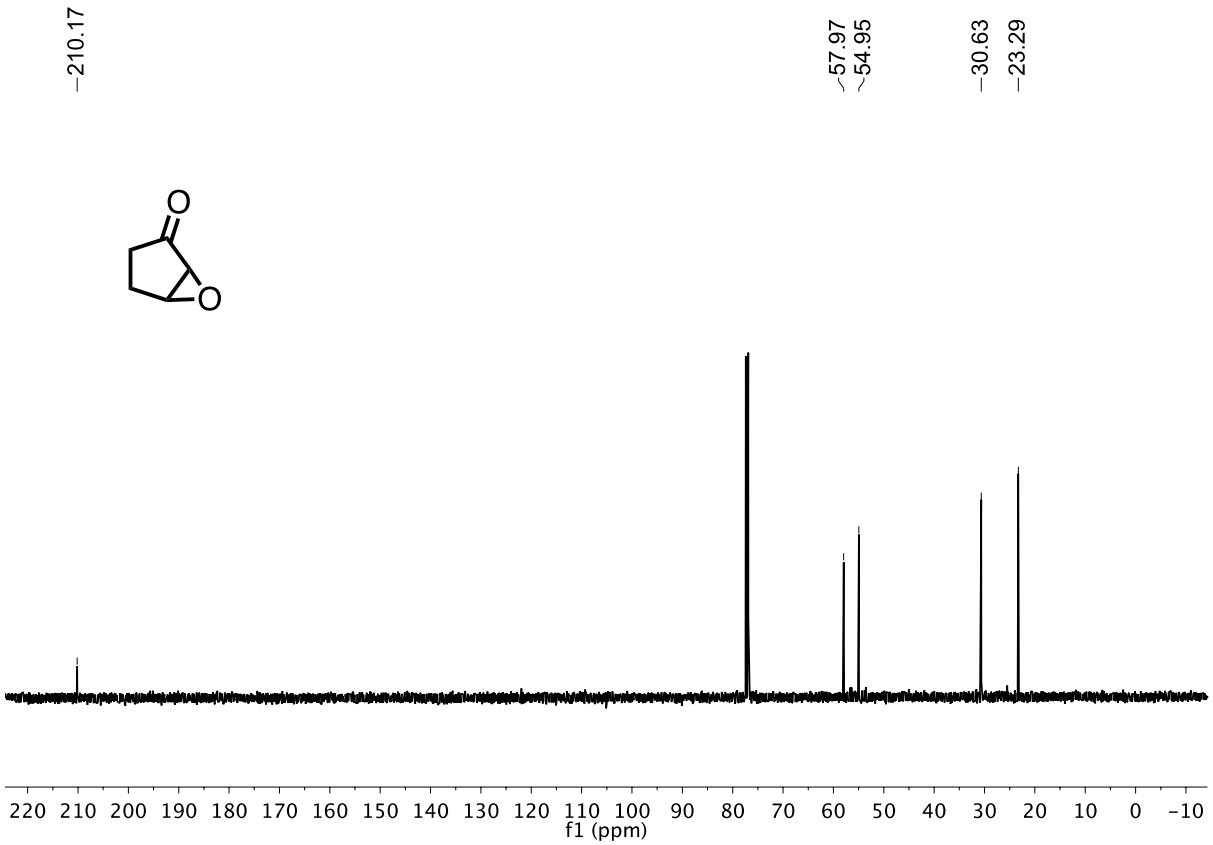
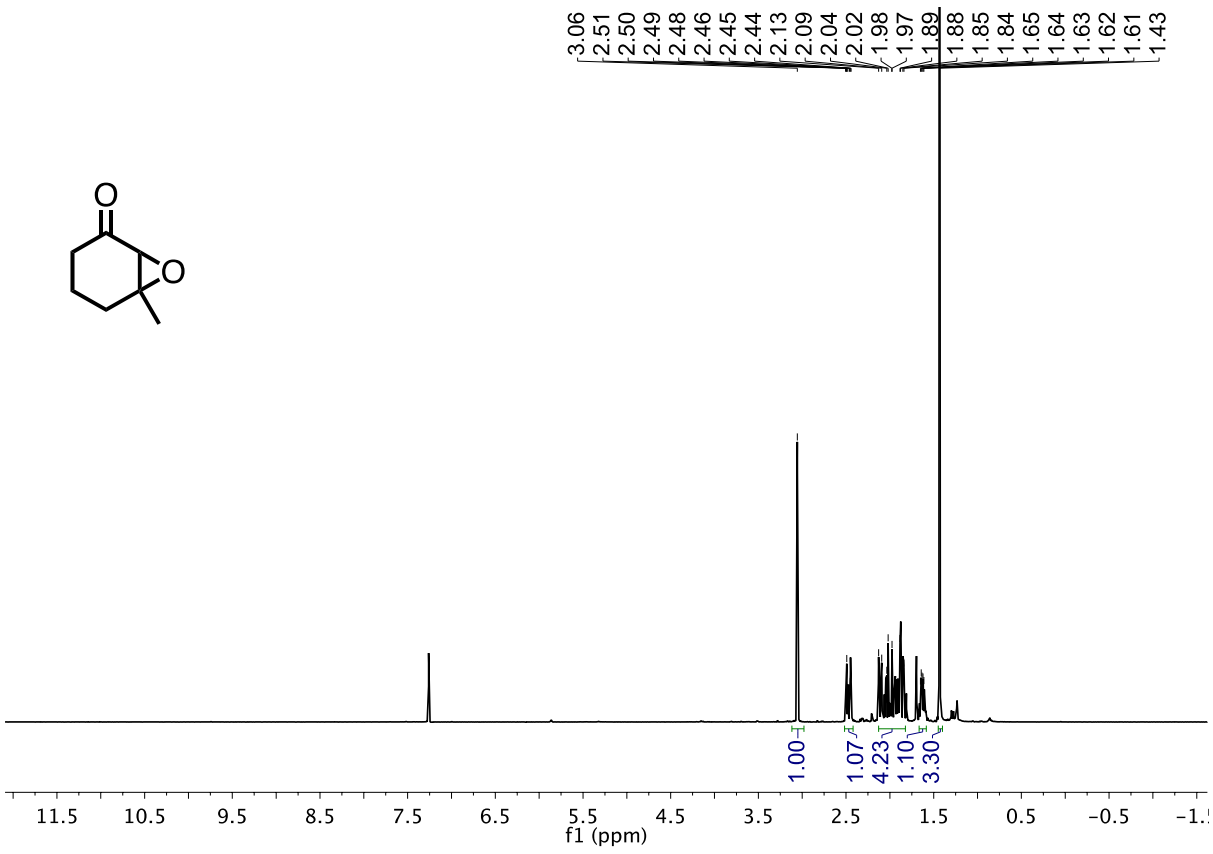
1.67
1.66
1.65
1.63
1.62
1.61

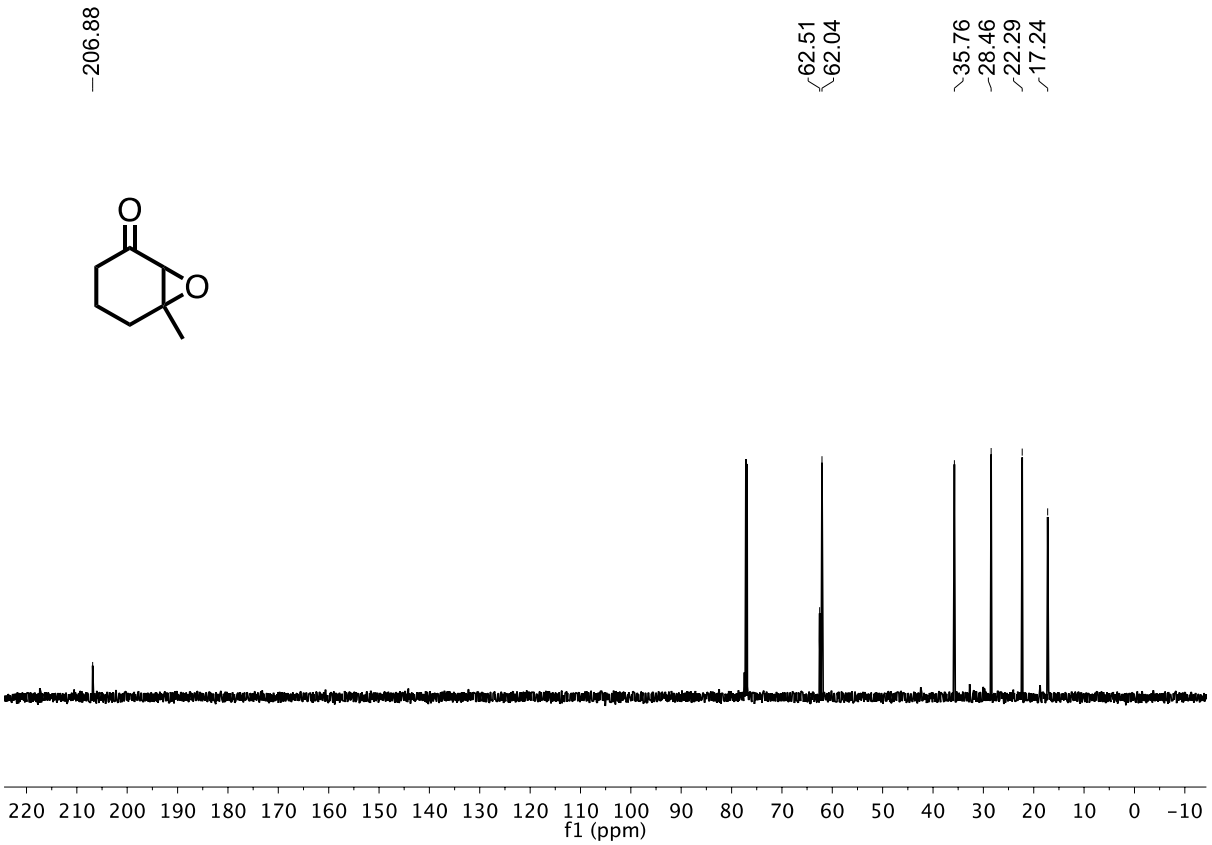

O
O
1.00
0.97
1.06
1.03
1.18
2.02
1.16
f1 (ppm)

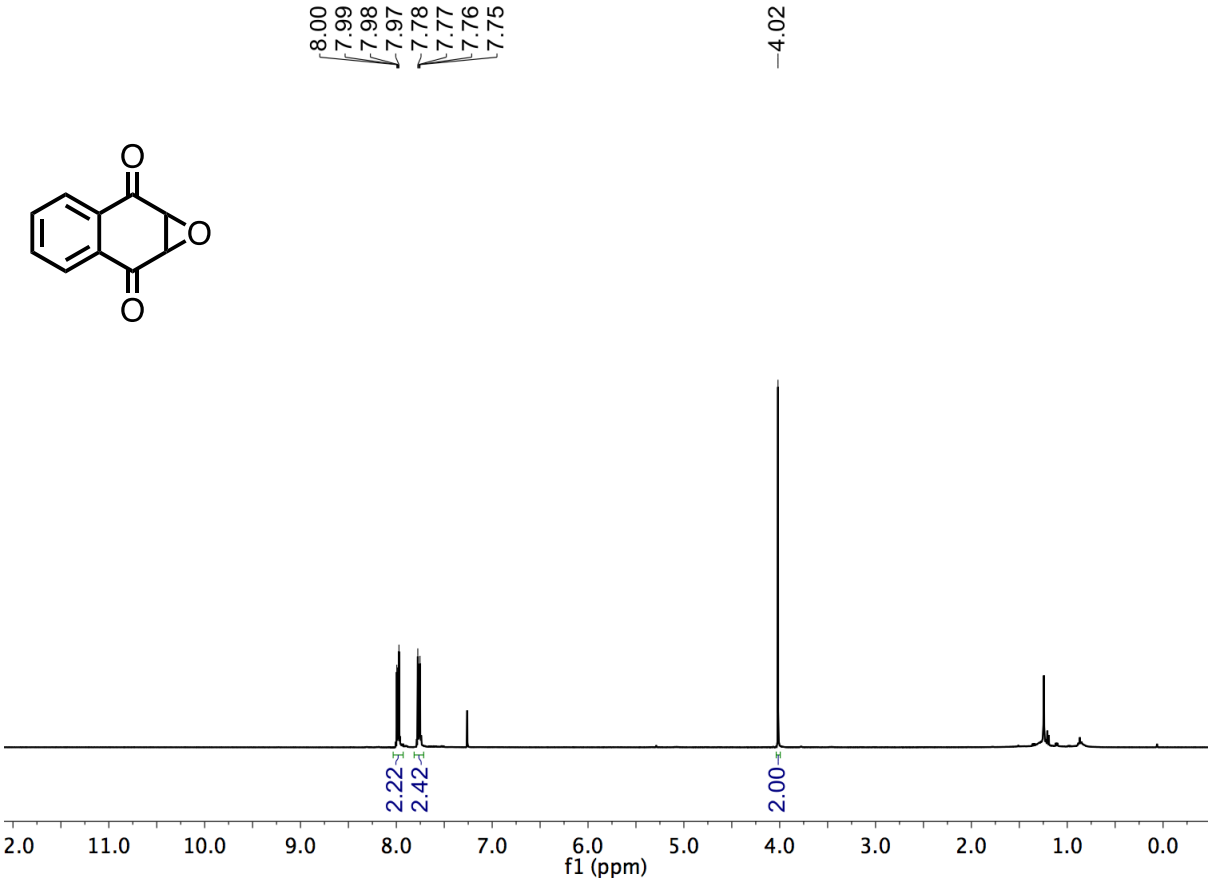

206.11
56.10
55.28
36.51
23.01
17.19
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
3.91 3.91 3.90 3.90 3.90 3.90 3.31 3.30 2.38 2.38 2.35 2.35 2.33 2.29 2.29 2.09 2.07 2.06 2.05 2.05 2.05 2.04 2.04 2.03 2.02

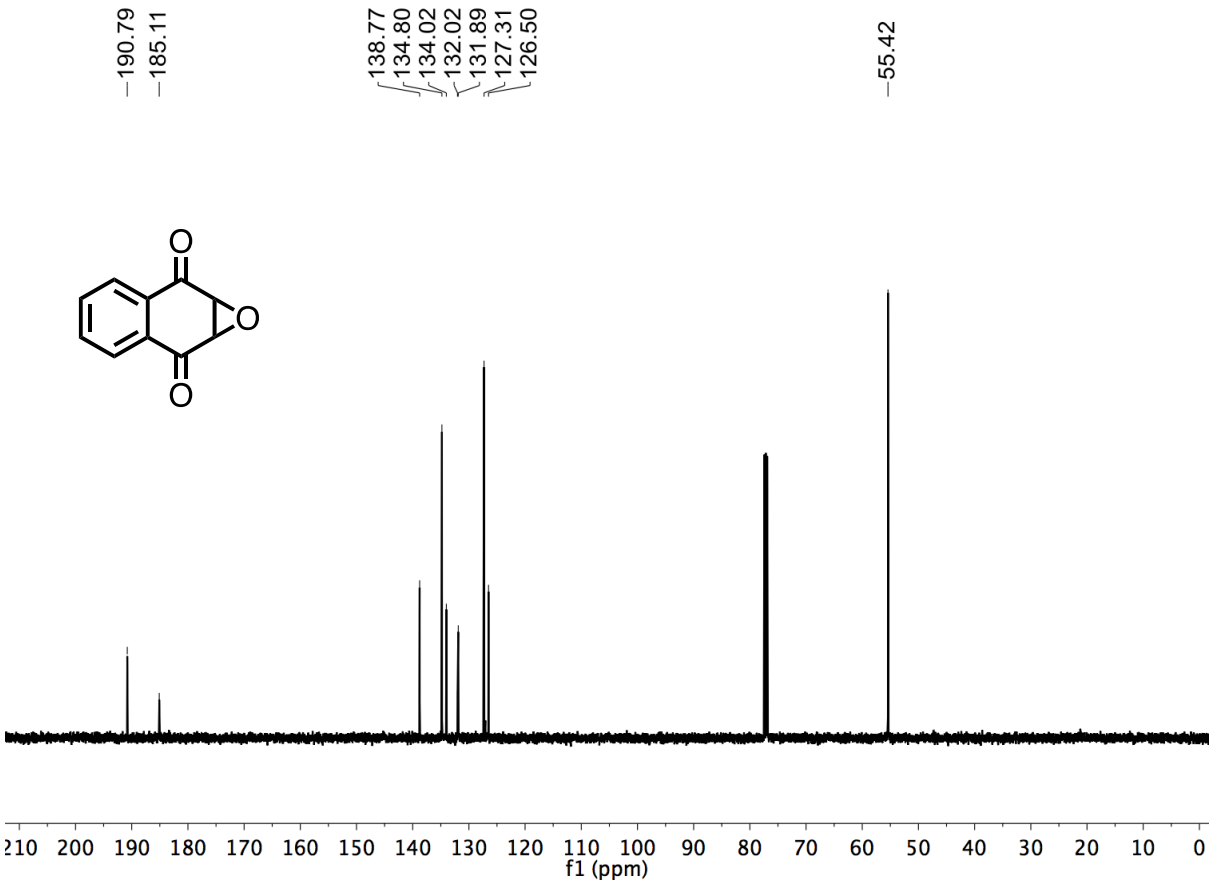

O
O
1.00
0.94
2.20
2.19
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

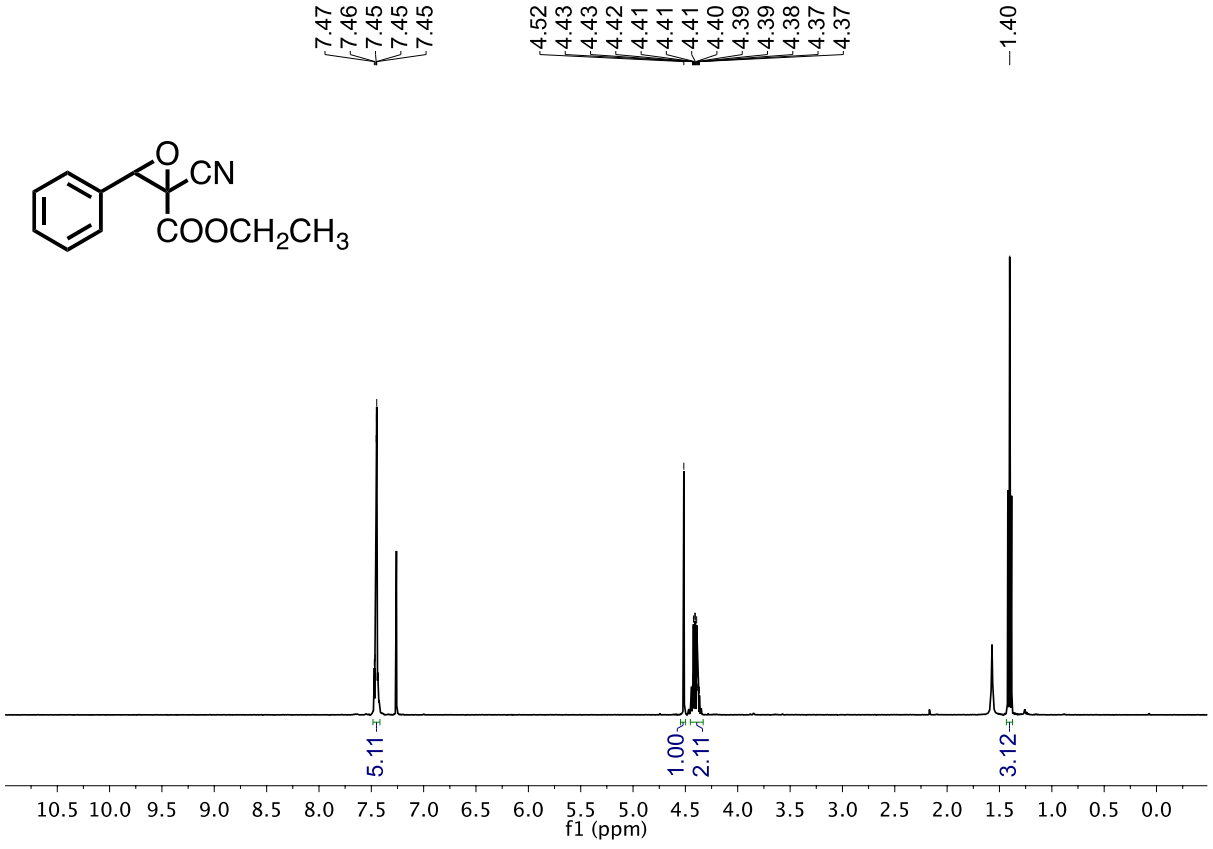

210.17
57.97
54.95
30.63
23.29
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

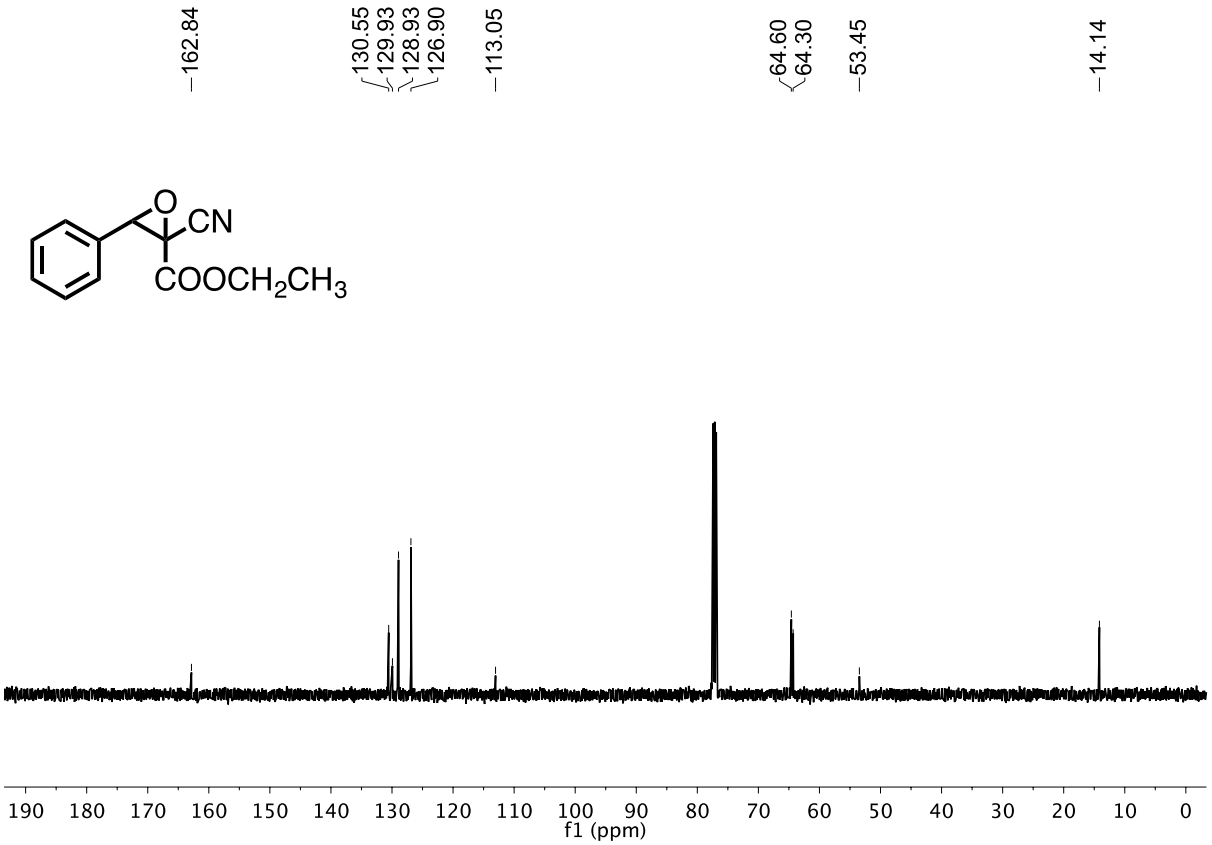

3.06
2.51
2.50
2.49
2.48
2.46
2.45
2.44
2.13
2.09
2.04
2.02
1.98
1.97
1.89
1.88
1.85
1.84
1.65
1.64
1.63
1.62
1.61
1.43
O
O
1.00
1.07
4.23
1.10
3.30
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

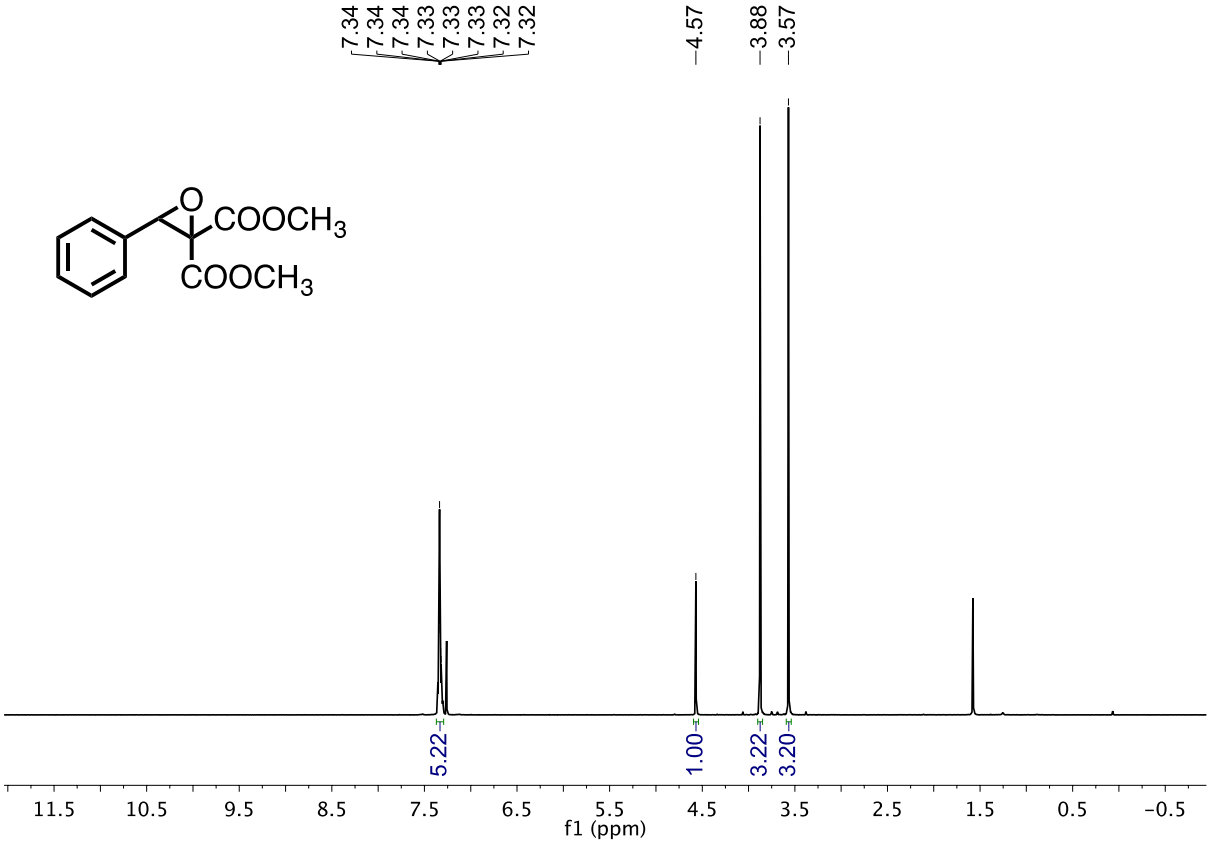

206.88
62.51
62.04
35.76
28.46
22.29
17.24
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

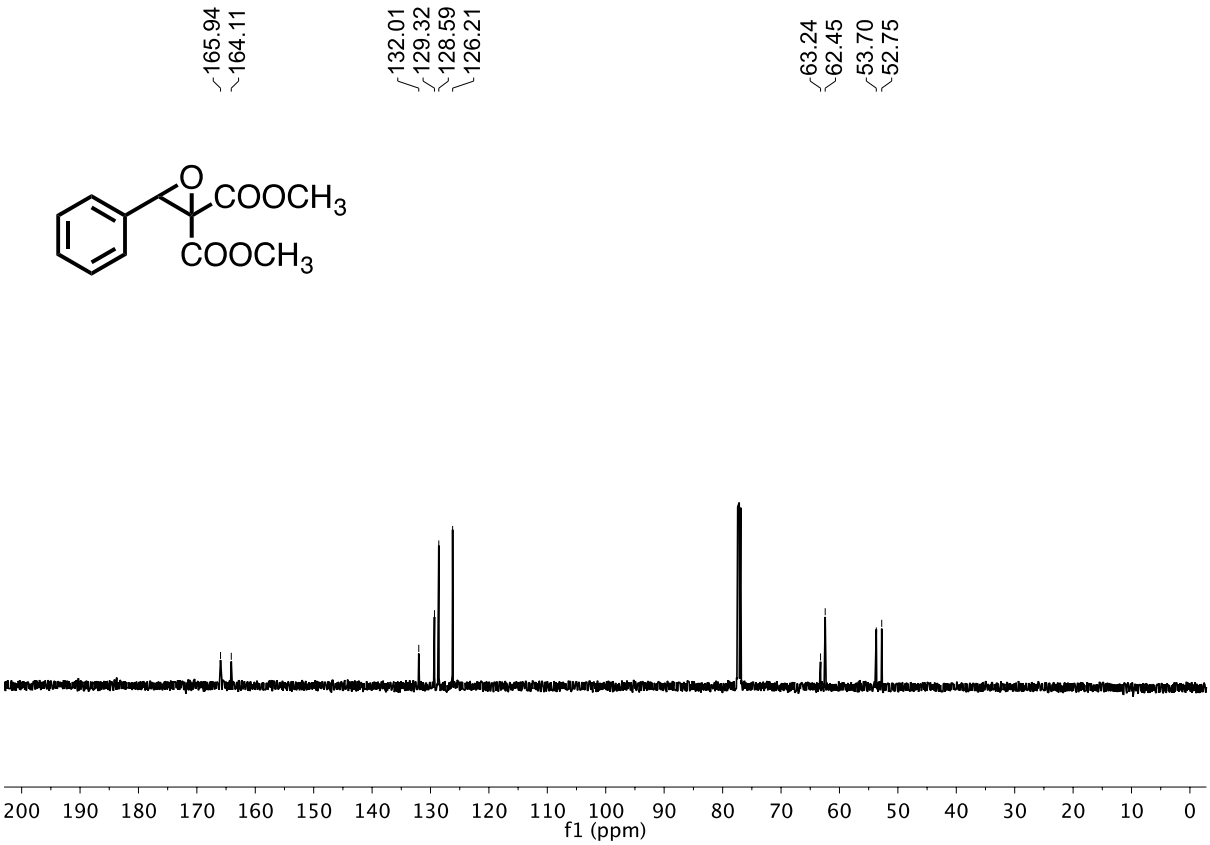

8.00
7.99
7.98
7.97
7.78
7.77
7.76
7.75
4.02
O
O
O
2.22
2.42
2.00
2.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

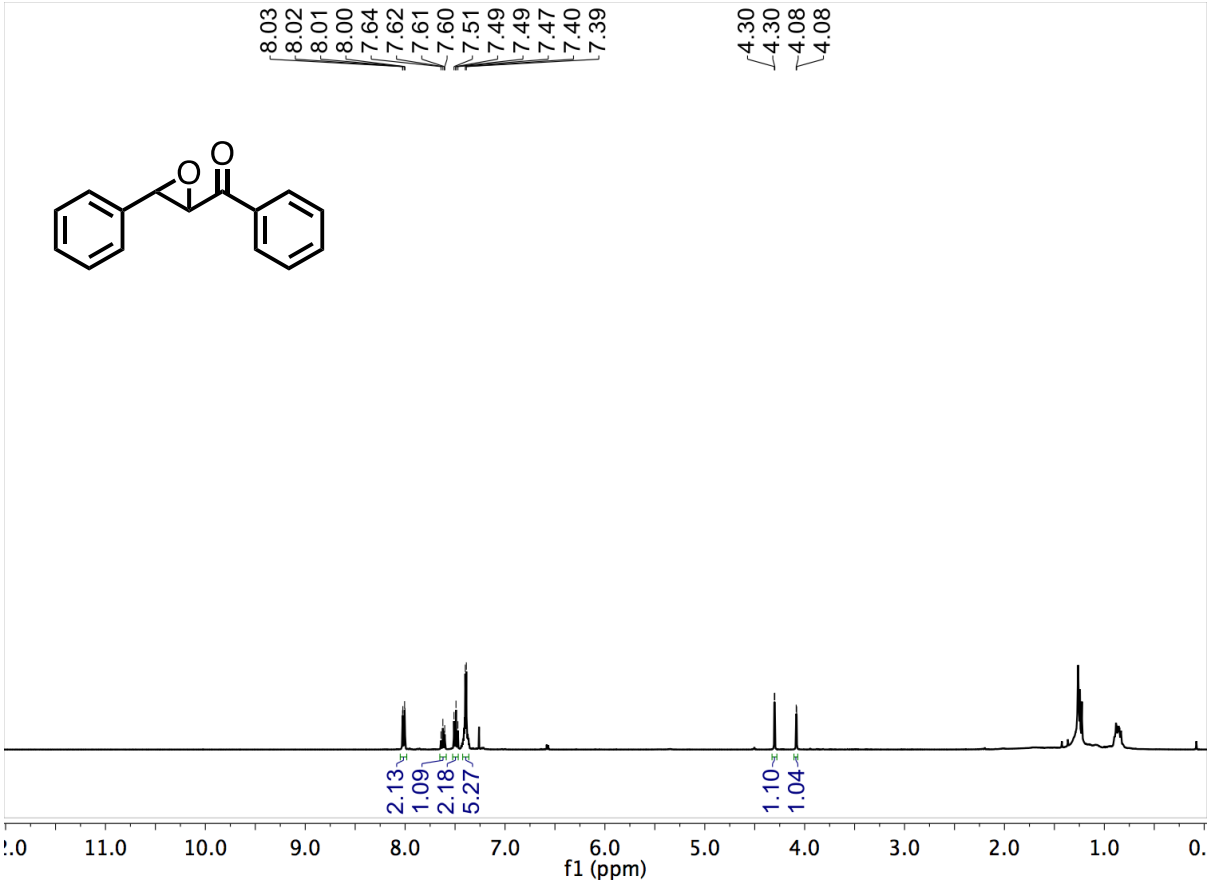

190.79
185.11
138.77
134.80
134.02
132.02
131.89
127.31
126.50
55.42
O
O
O
f1 (ppm)

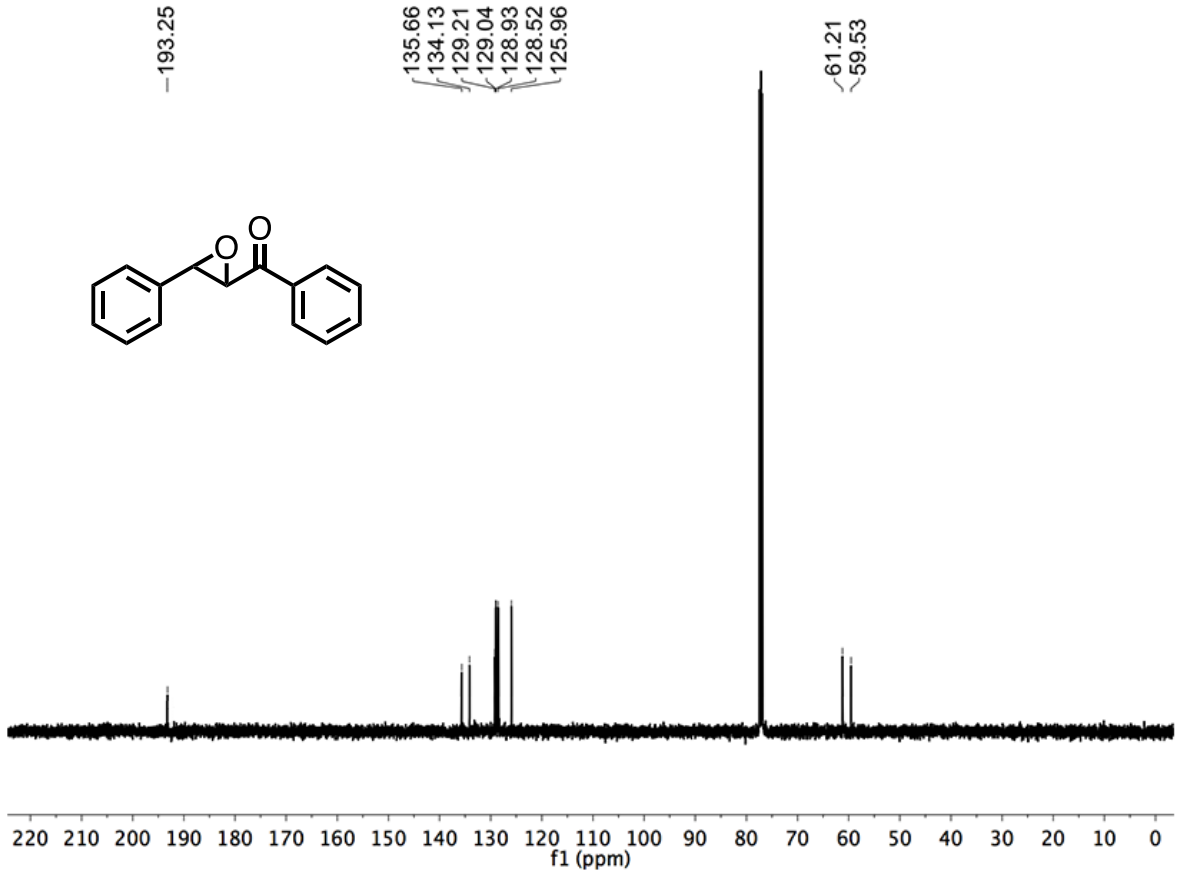

7.47
7.46
7.45
7.45
7.45
4.52
4.43
4.43
4.42
4.41
4.41
4.41
4.40
4.39
4.39
4.38
4.37
4.37
1.40
O
CN
COOCH2CH3
5.11
1.00
2.11
3.12
f1 (ppm)

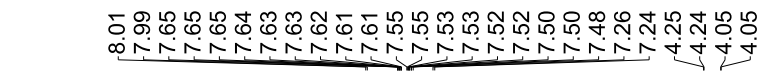

162.84
130.55
129.93
128.93
126.90
113.05
64.60
64.30
53.45
14.14
O
CN
COOCH2CH3
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

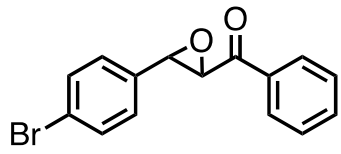

7.34
7.34
7.34
7.33
7.33
7.33
7.32
7.32
4.57
3.88
3.57
O
COOCH3
COOCH3
5.22
1.00
3.22
3.20
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

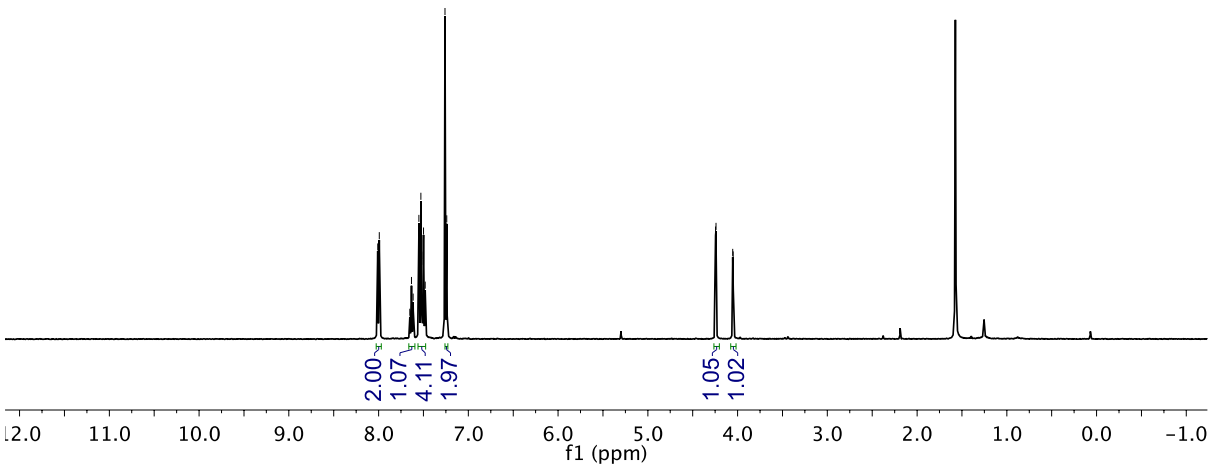

165.94
164.11
132.01
129.32
128.59
126.21
63.24
62.45
53.70
52.75
O
COOCH3
COOCH3
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

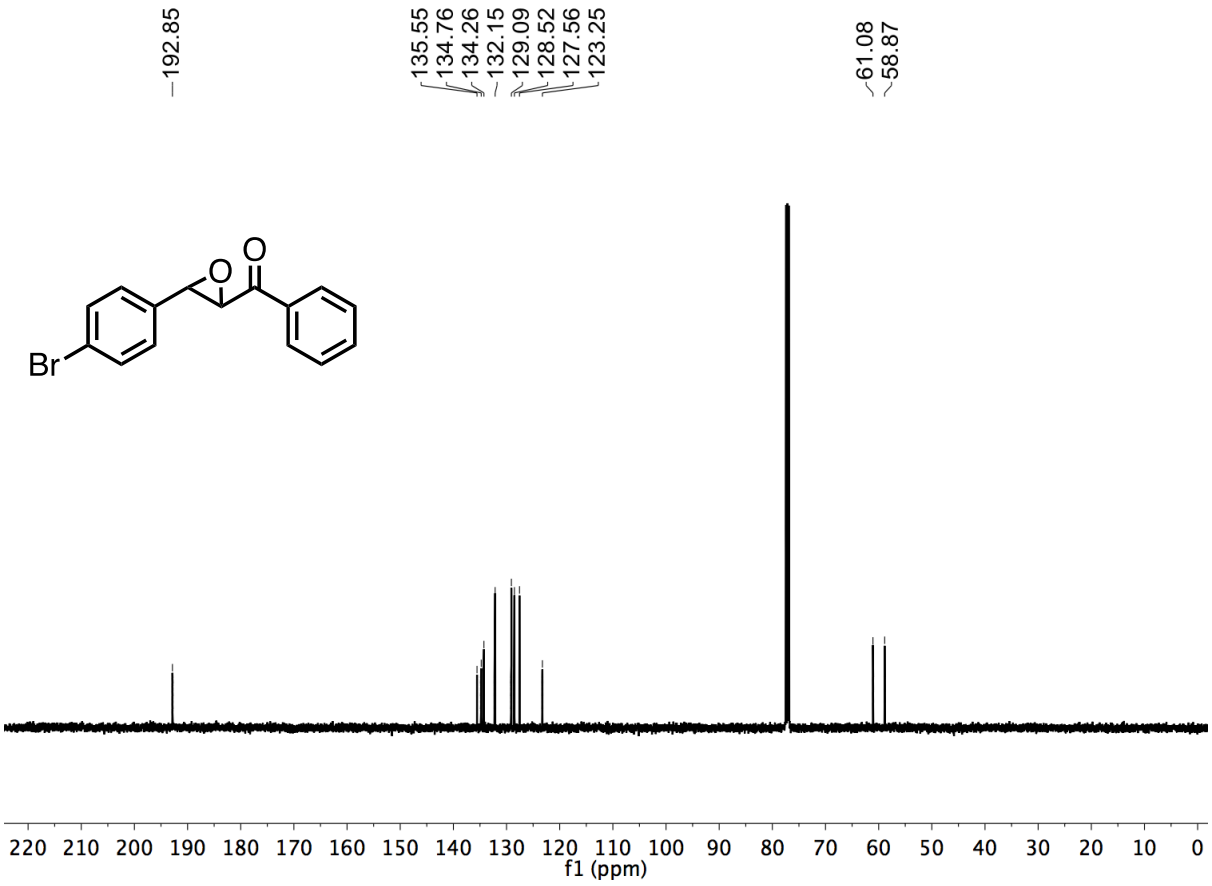

8.03
8.02
8.01
8.00
7.64
7.62
7.61
7.60
7.51
7.49
7.49
7.47
7.40
7.39
4.30
4.30
4.08
4.08
O
O
2.13
1.09
2.18
5.27
1.10
1.04
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.
f1 (ppm)

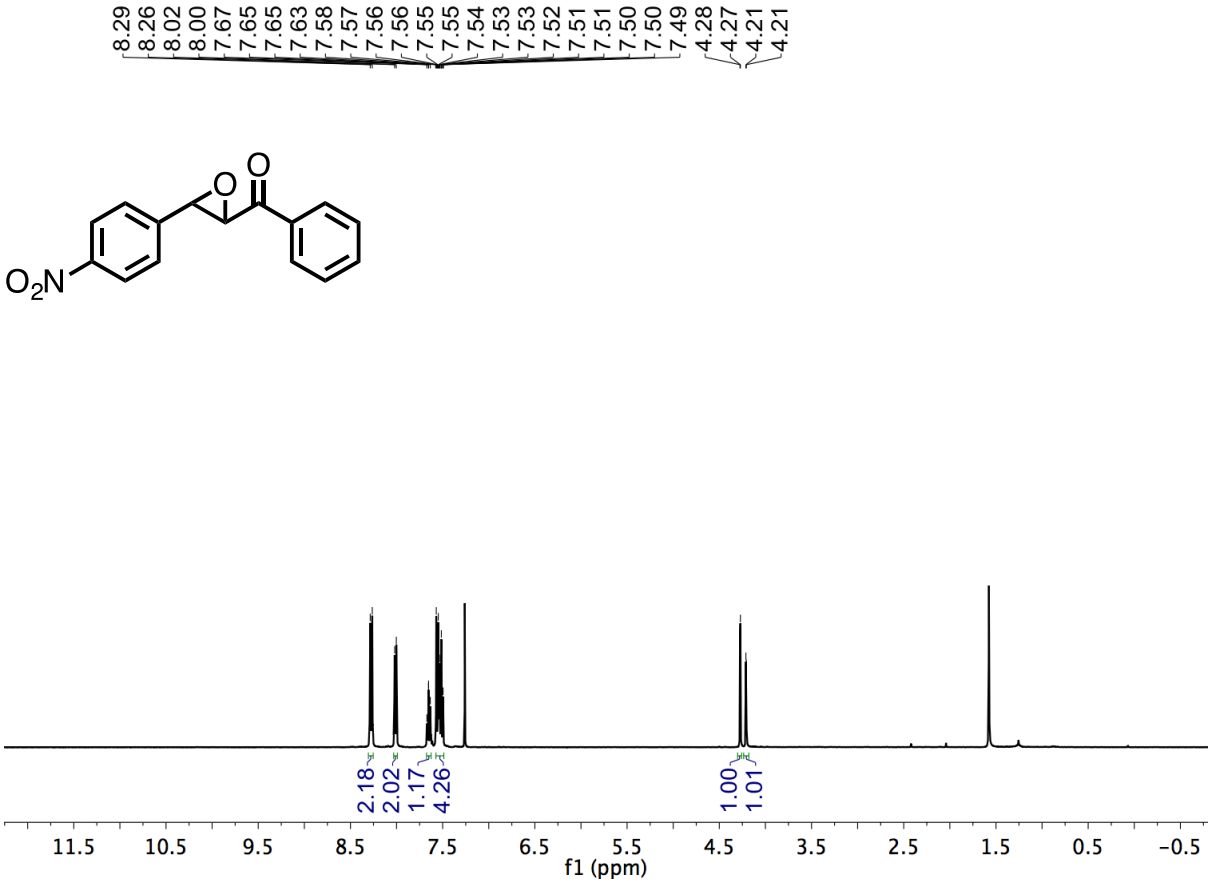

193.25
135.66
134.13
129.21
129.04
128.93
128.52
125.96
61.21
59.53
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

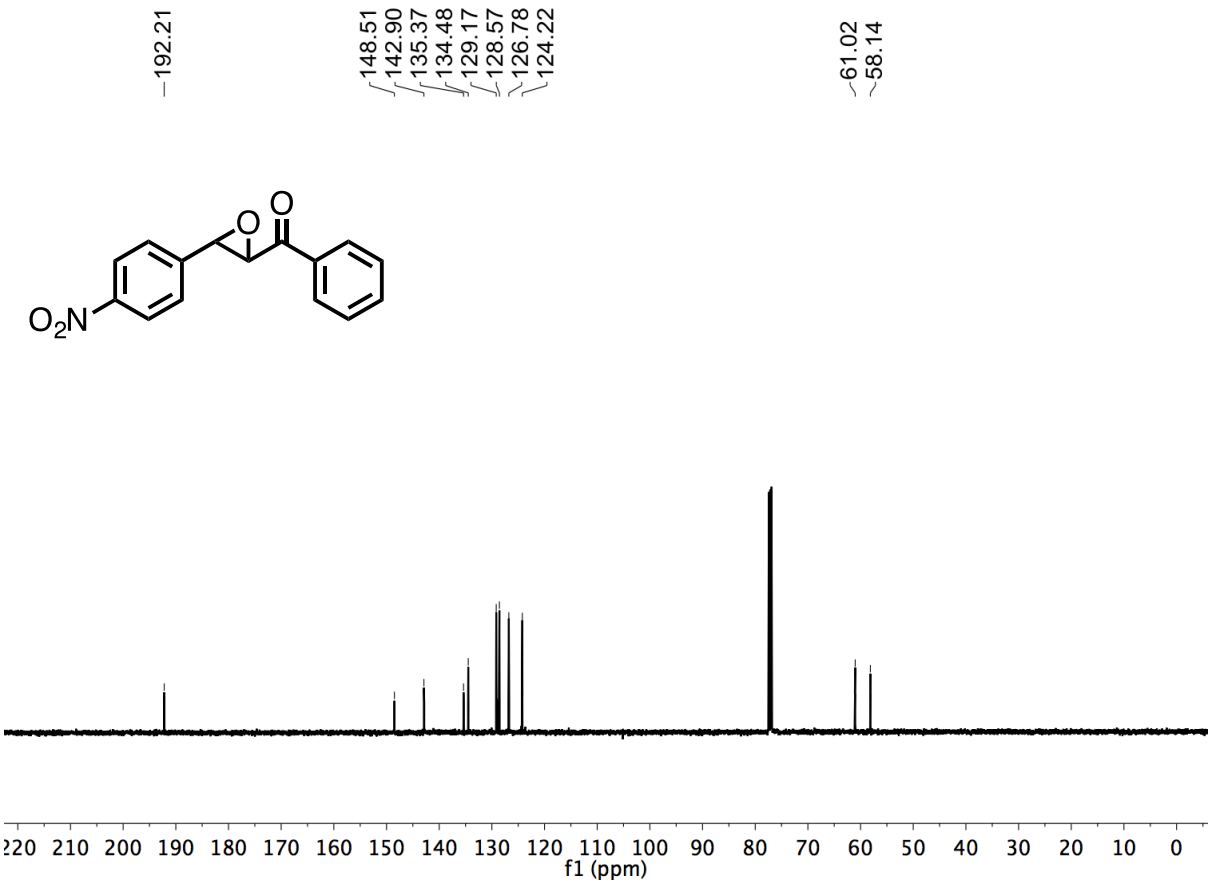

8.01
7.99
7.65
7.65
7.65
7.64
7.63
7.63
7.62
7.61
7.61
7.55
7.55
7.53
7.53
7.52
7.52
7.50
7.50
7.48
7.26
7.24
4.25
4.24
4.05
4.05


O
O
Br

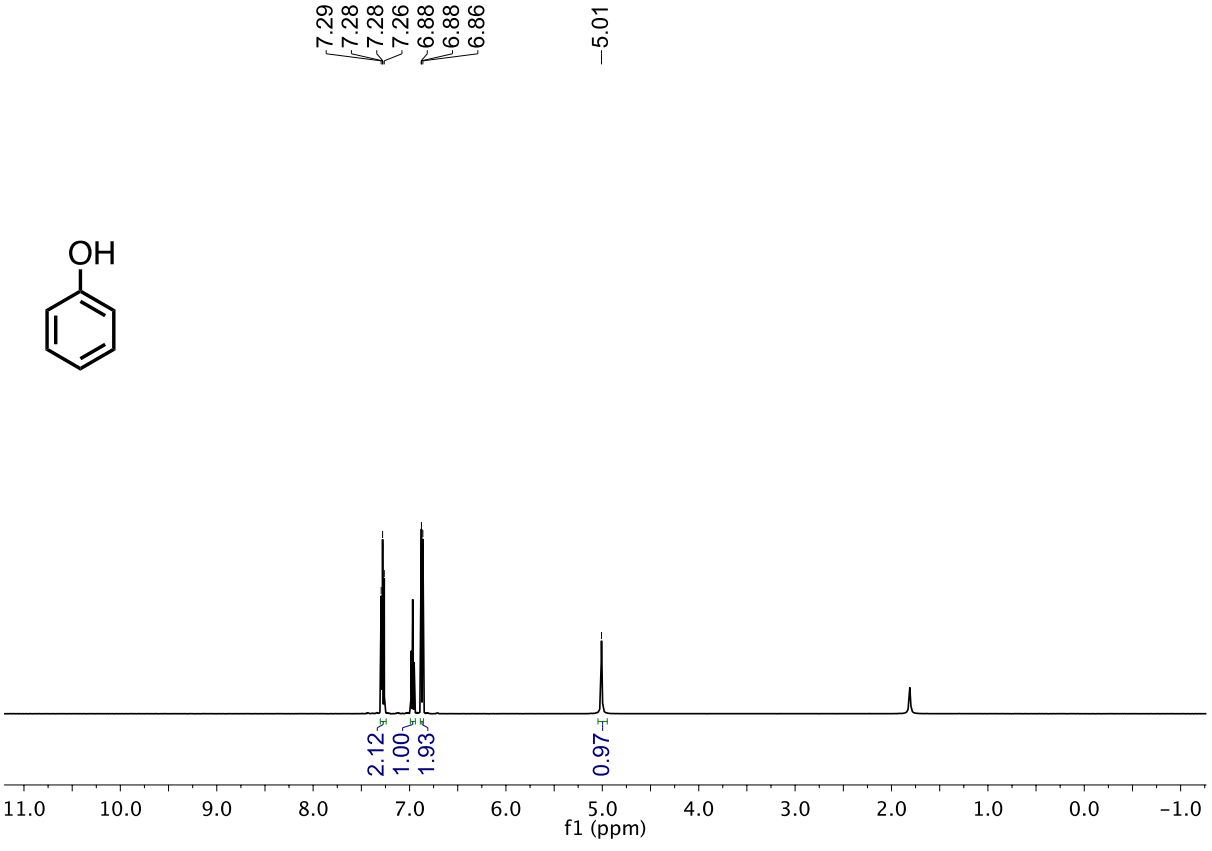

2.00
1.07
4.11
1.97
1.05
1.02
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0
f1 (ppm)

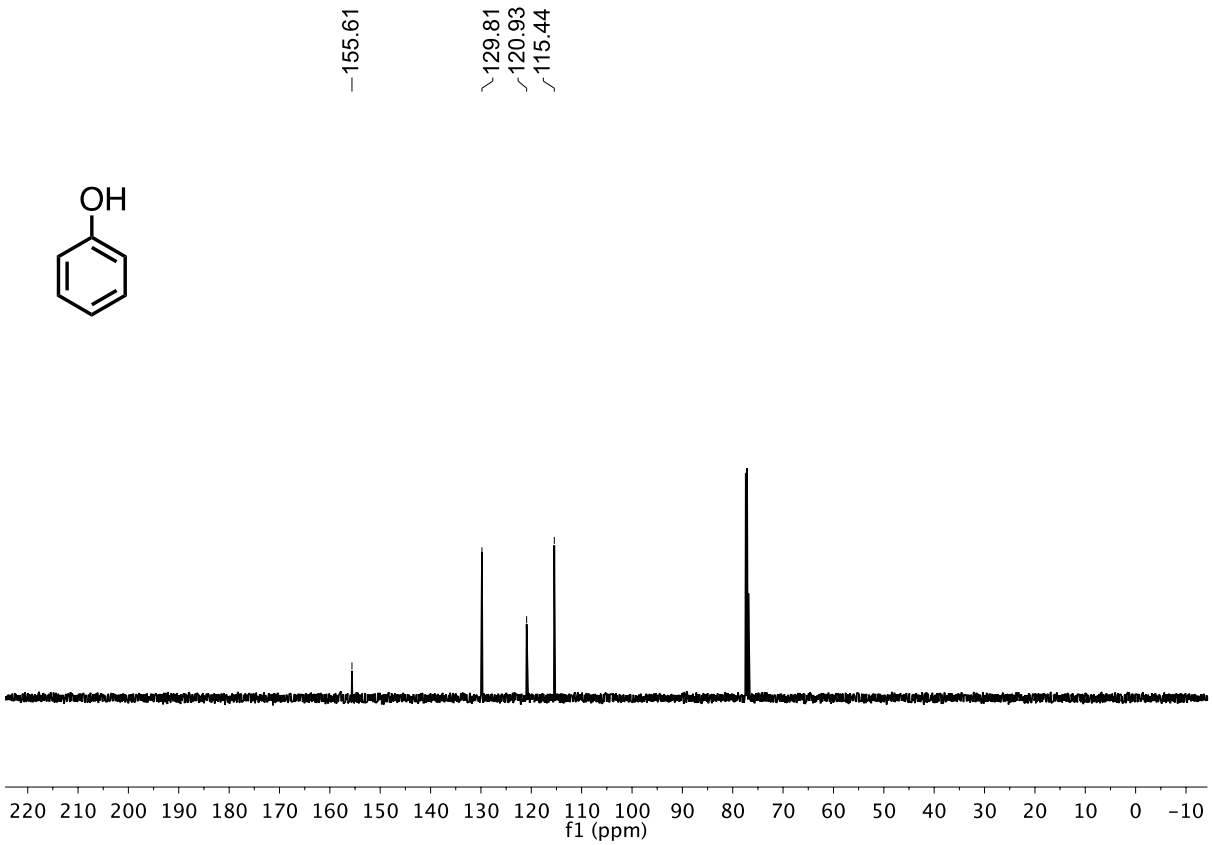

192.85
135.55
134.76
134.26
132.15
129.09
128.52
127.56
123.25
61.08
58.87
Br
O
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

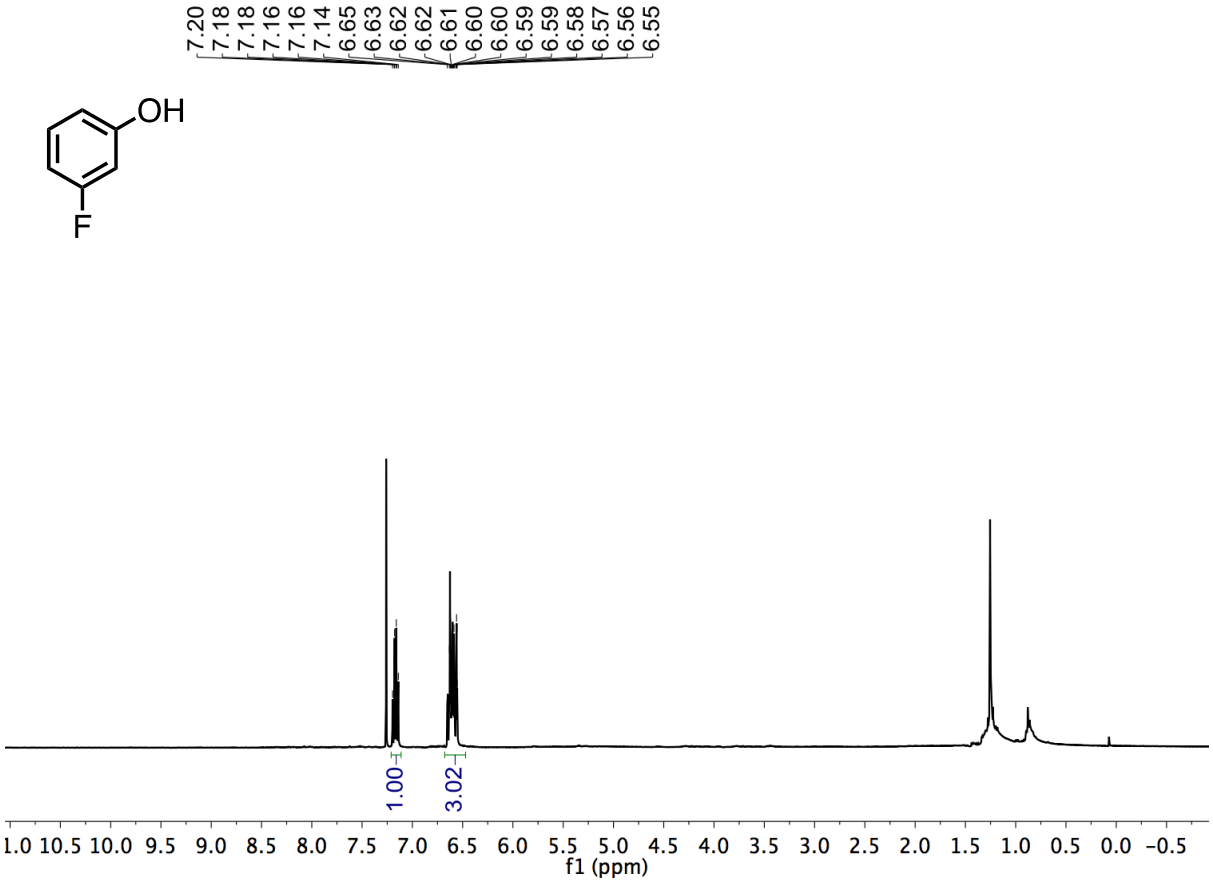

8.29
8.26
8.02
8.00
7.67
7.65
7.65
7.63
7.58
7.57
7.56
7.56
7.55
7.55
7.54
7.53
7.53
7.52
7.51
7.51
7.50
7.50
7.49
4.28
4.27
4.21
4.21
O
O
O2N
2.18
2.02
1.17
4.26
1.00
1.01
11.5 10.5 9.5 8.5 7.5 6.5 5.5 4.5 3.5 2.5 1.5 0.5 -0.5
f1 (ppm)

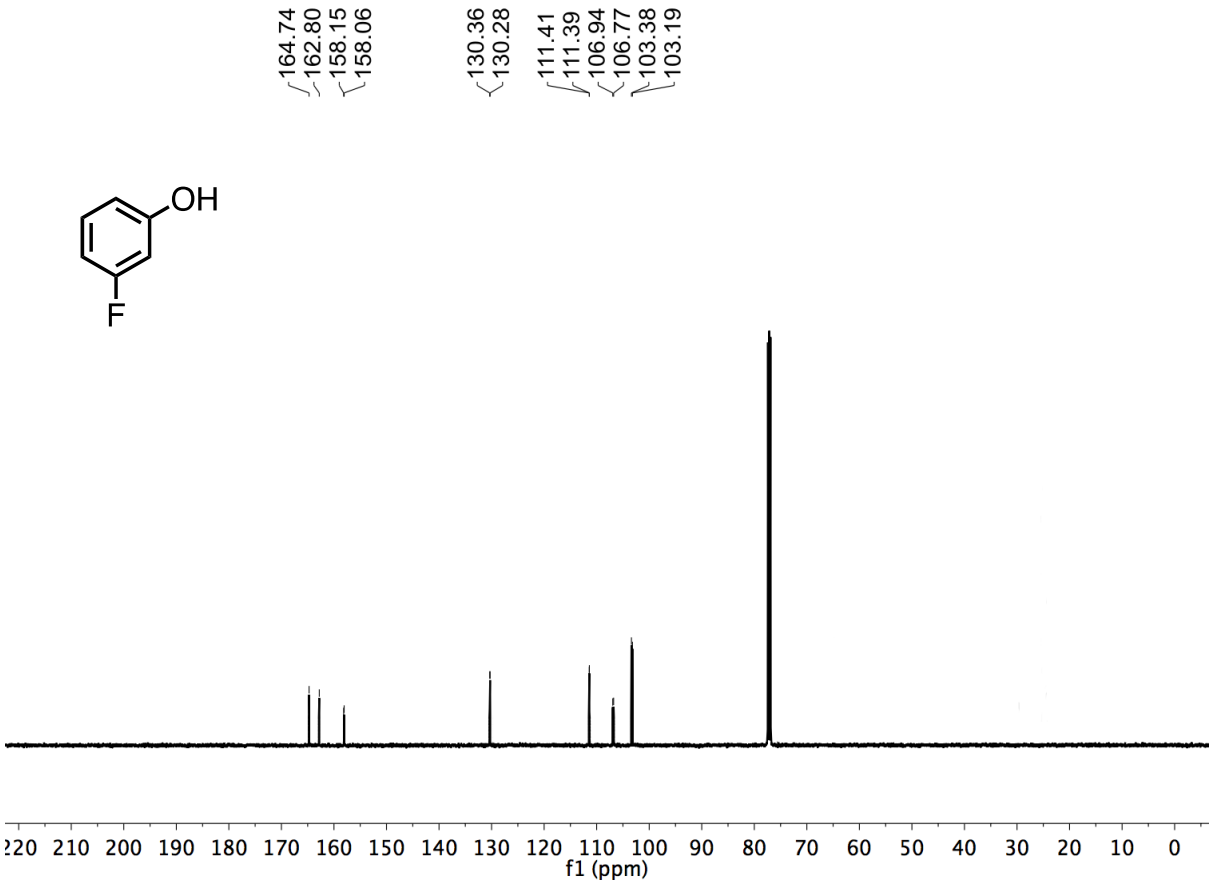


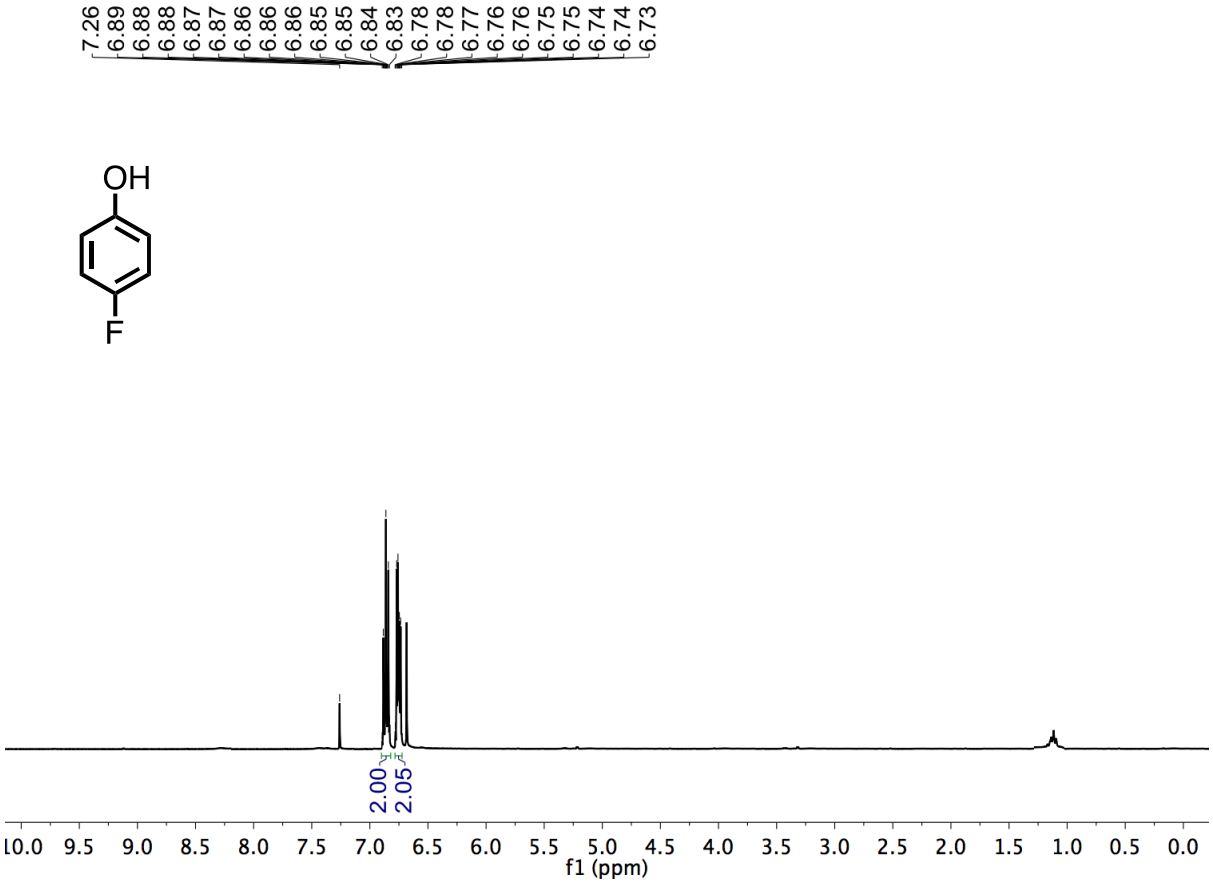
^{1}H NMR of 5a-5i

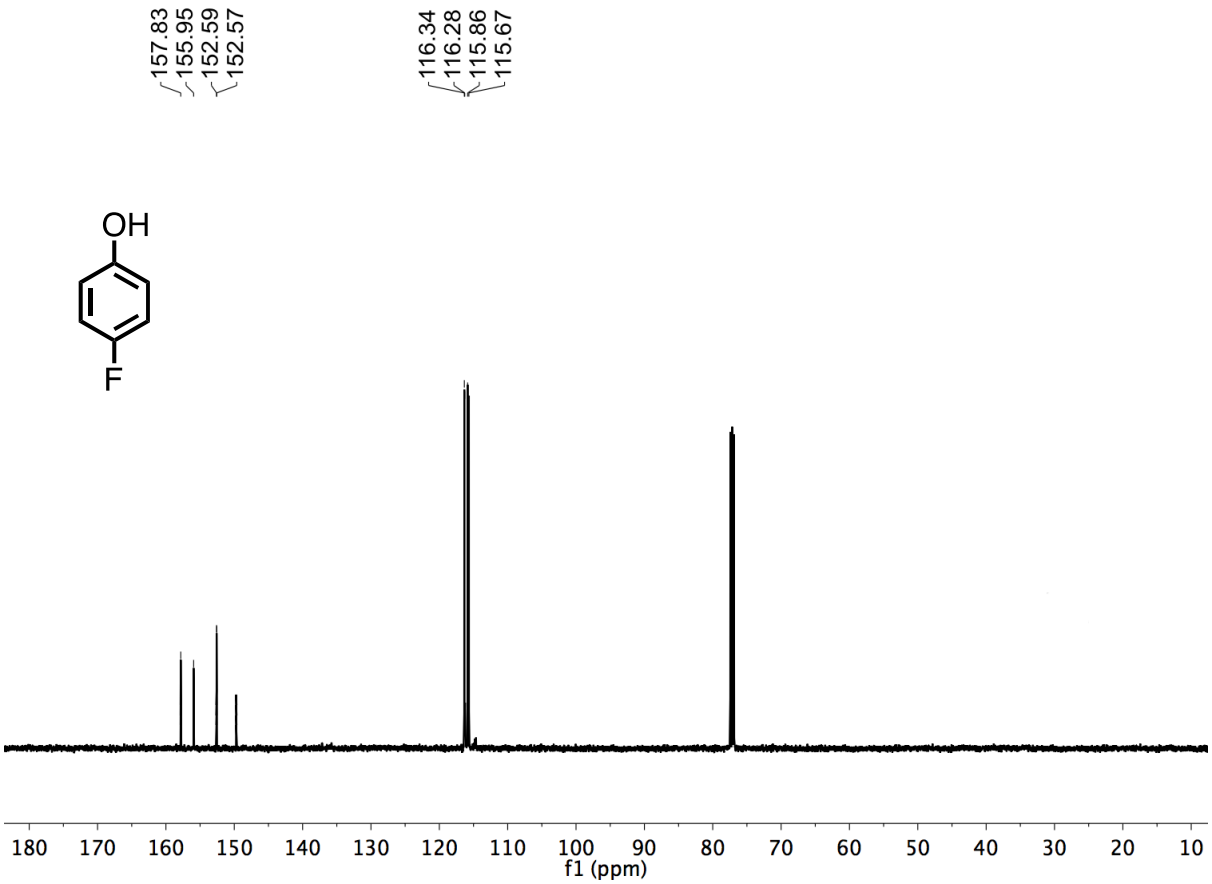


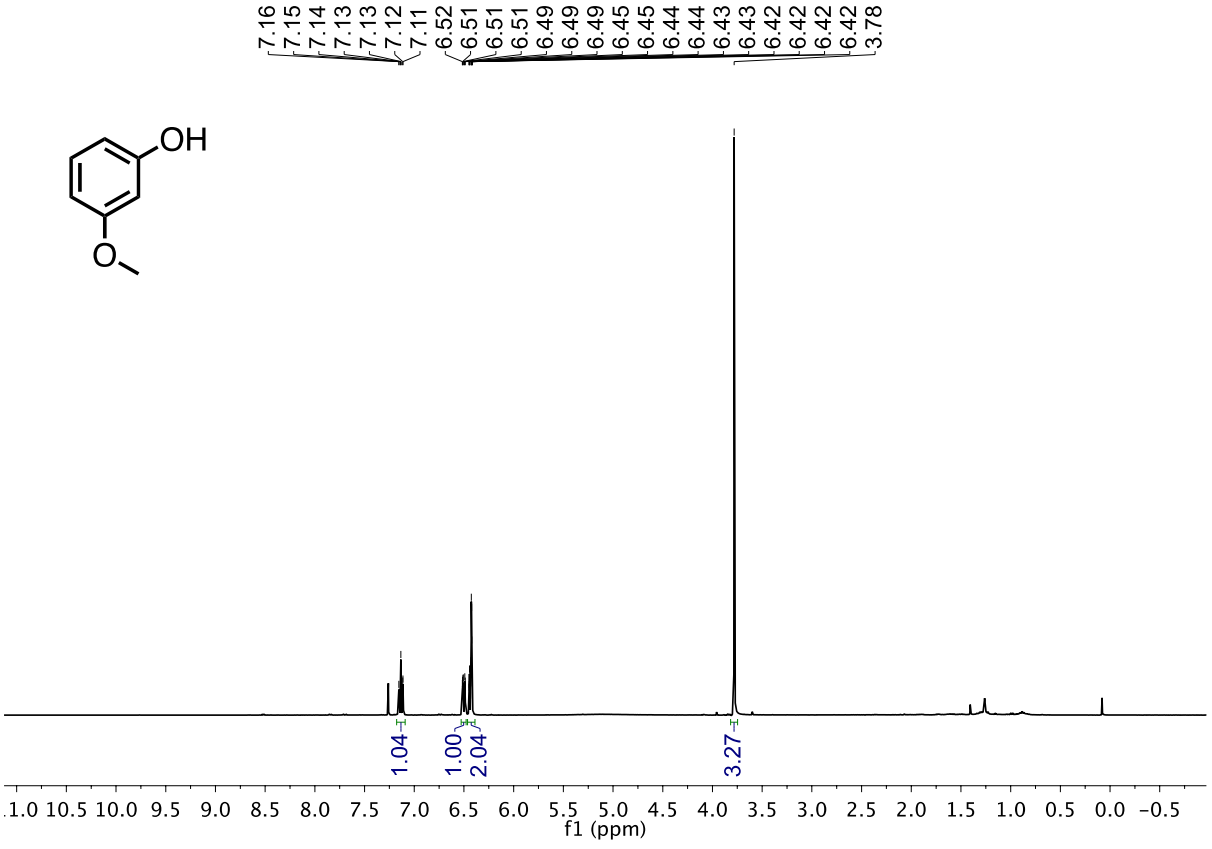

155.61
129.81
120.93
115.44
OH
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

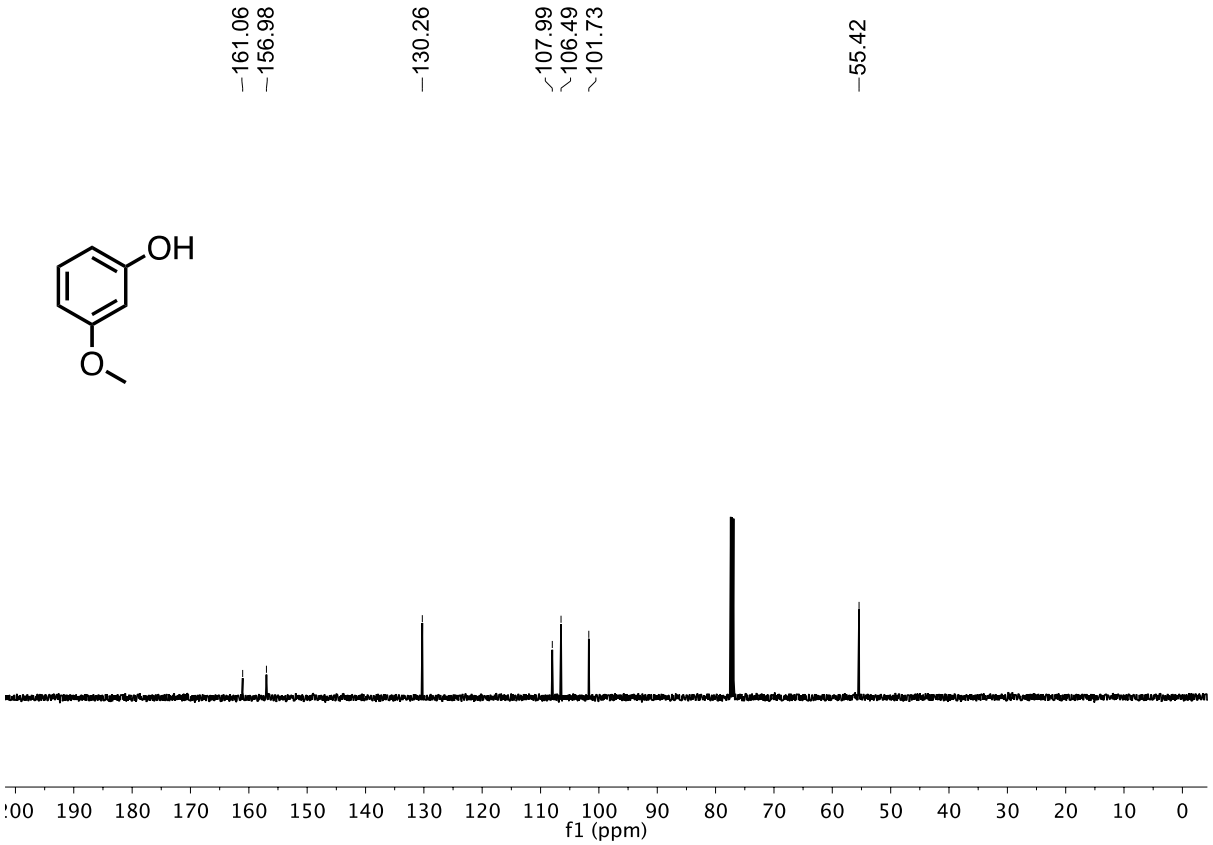

7.20
7.18
7.18
7.16
7.16
7.14
6.65
6.63
6.62
6.62
6.61
6.60
6.60
6.59
6.59
6.58
6.57
6.56
6.55
OH
F
1.00
3.02
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

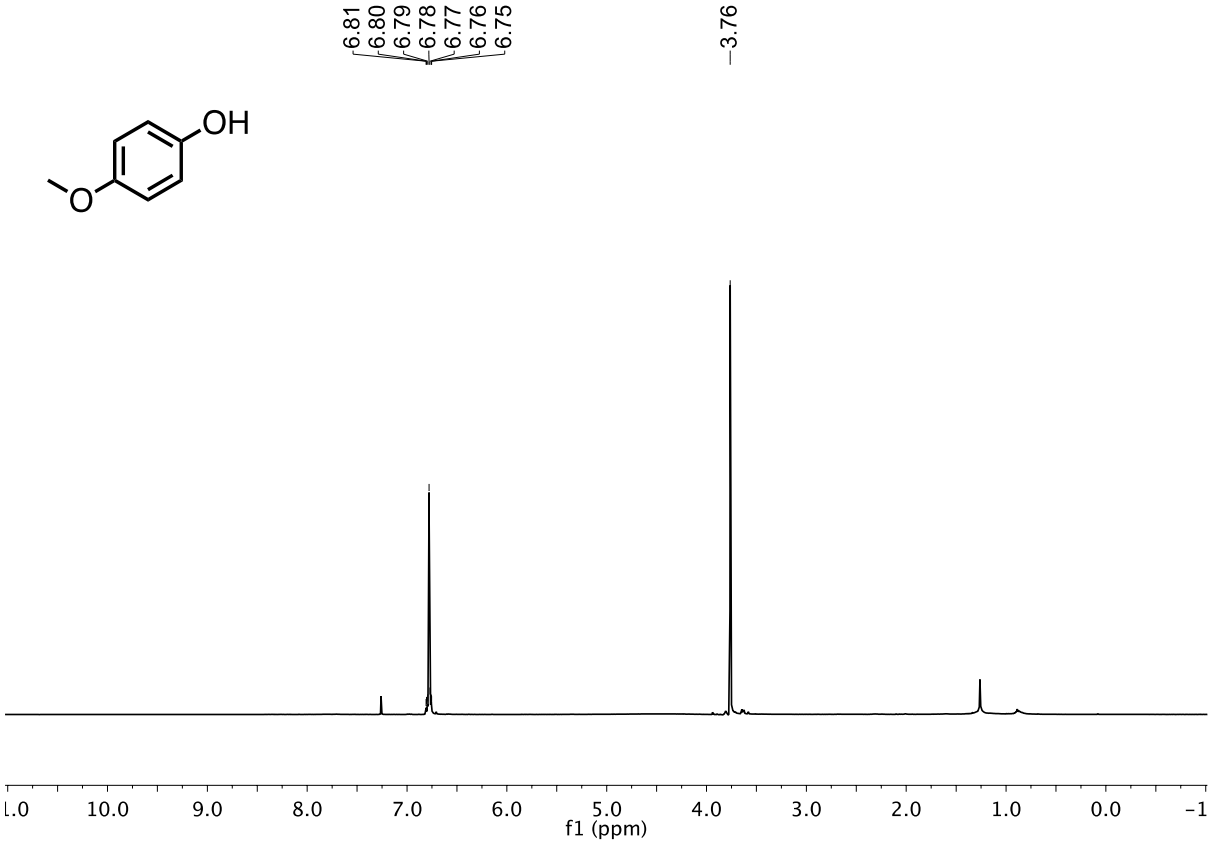

164.74
162.80
158.15
158.06
130.36
130.28
111.41
111.39
106.94
106.77
103.38
103.19
OH
F
f1 (ppm)

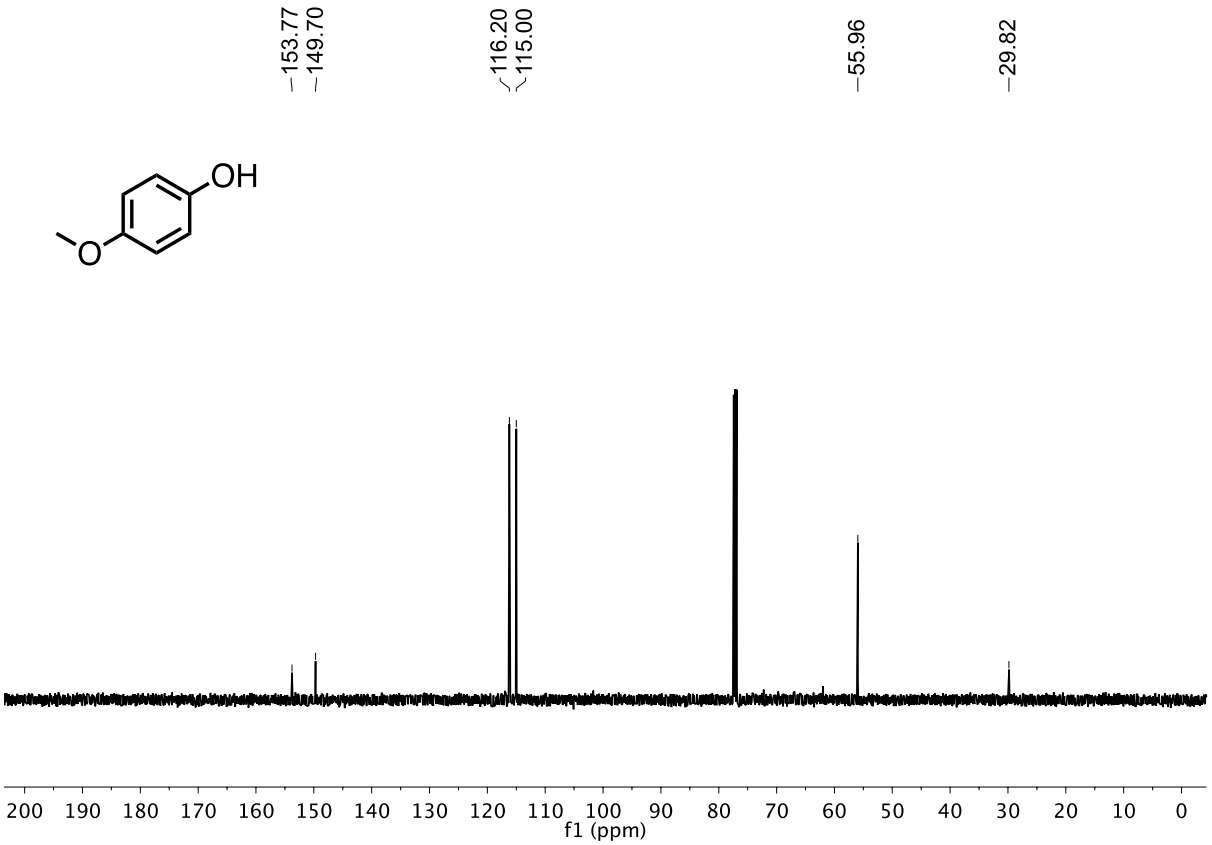

7.26
6.89
6.88
6.88
6.87
6.87
6.86
6.86
6.86
6.85
6.85
6.84
6.83
6.78
6.78
6.77
6.76
6.76
6.75
6.75
6.74
6.74
6.73
OH
F
2.00
2.05
f1 (ppm)

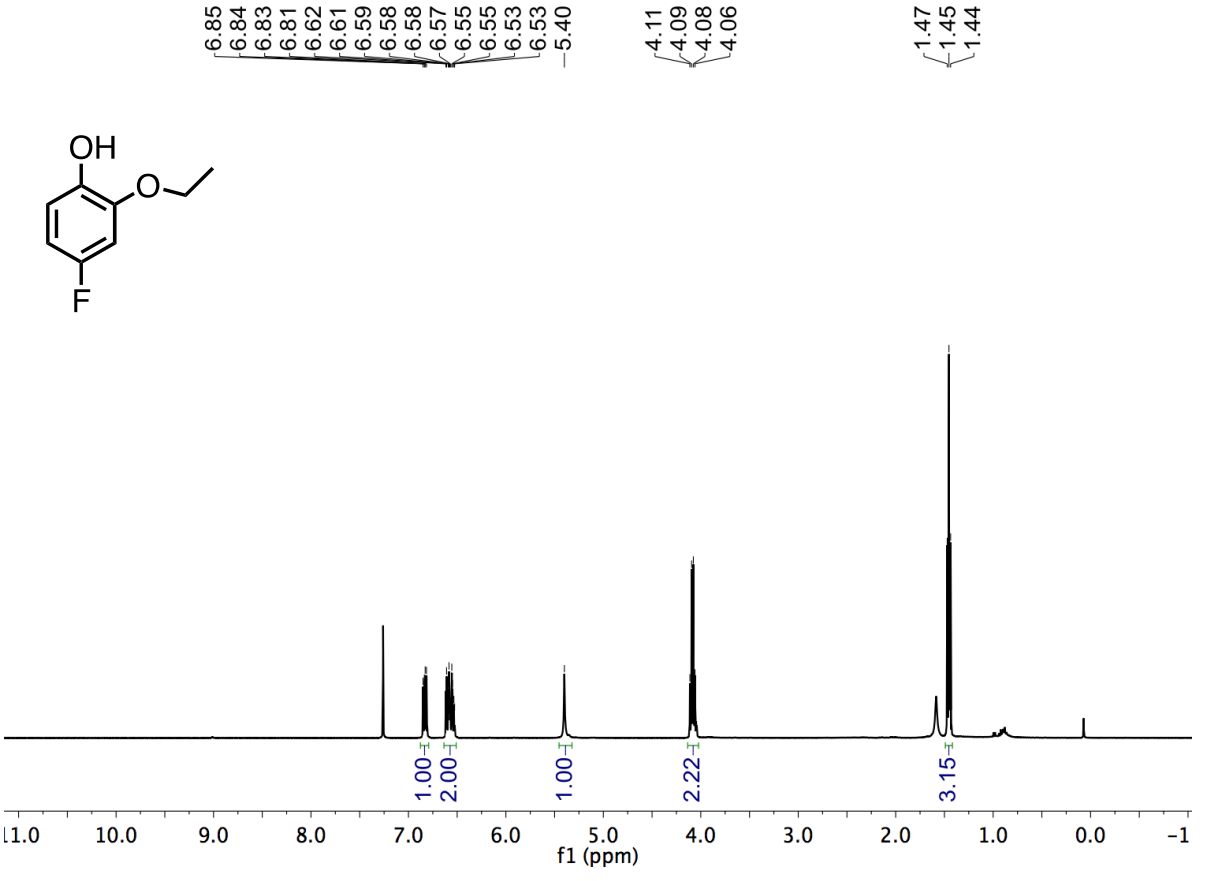

157.83
155.95
152.59
152.57
116.34
116.28
115.86
115.67
OH
F
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

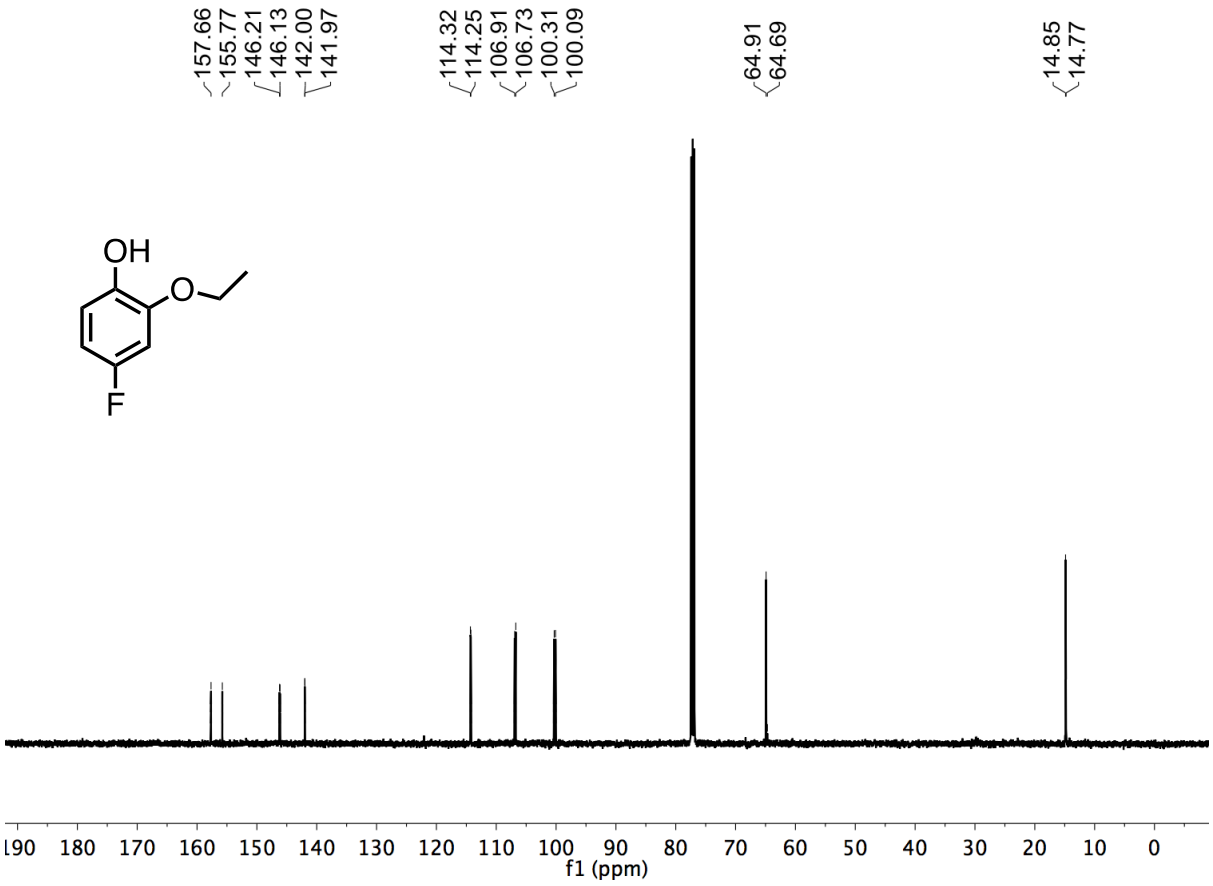

7.16
7.15
7.14
7.13
7.13
7.12
7.11
6.52
6.51
6.51
6.51
6.49
6.49
6.49
6.45
6.45
6.44
6.44
6.43
6.43
6.42
6.42
6.42
6.42
3.78
OH
O
1.04
1.00
2.04
3.27
.1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

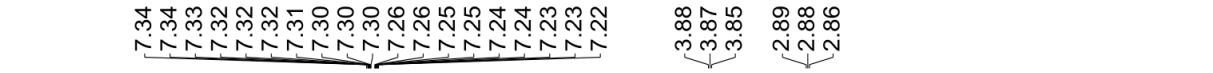

161.06
156.98
130.26
107.99
106.49
101.73
55.42
OH
O
f1 (ppm)

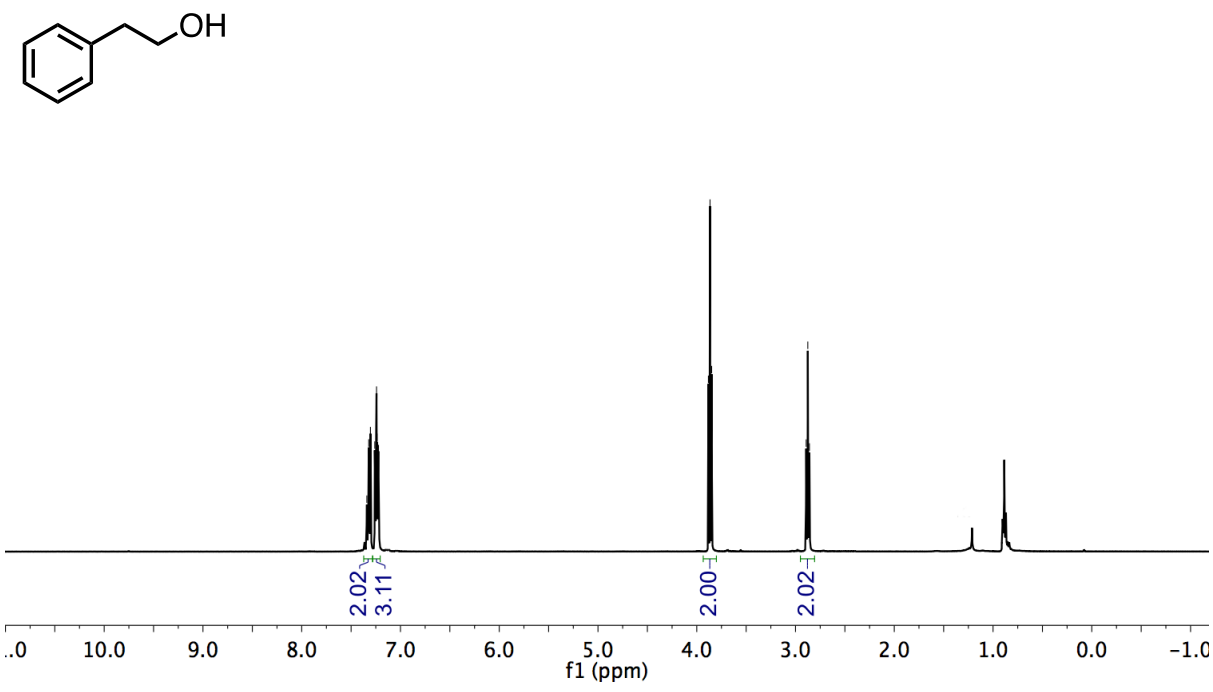

6.81
6.80
6.79
6.78
6.77
6.76
6.75
3.76
OH
O
f1 (ppm)

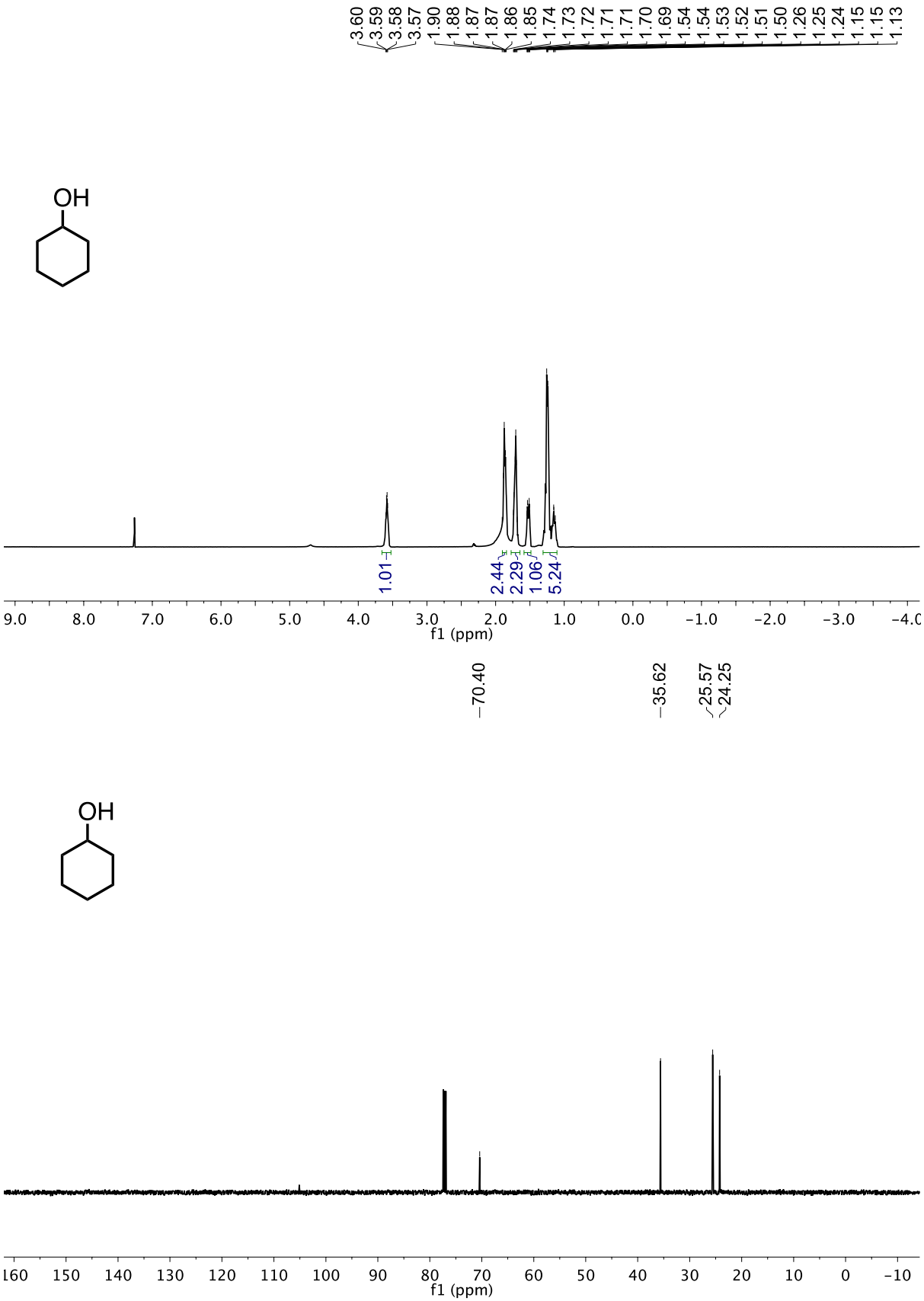

153.77
149.70
116.20
115.00
55.96
29.82
OH
O
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


6.85
6.84
6.83
6.81
6.62
6.61
6.59
6.58
6.58
6.57
6.55
6.55
6.53
6.53
5.40
4.11
4.09
4.08
4.06
1.47
1.45
1.44
OH
O
F
1.00
2.00
1.00
2.22
3.15
11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1
f1 (ppm)

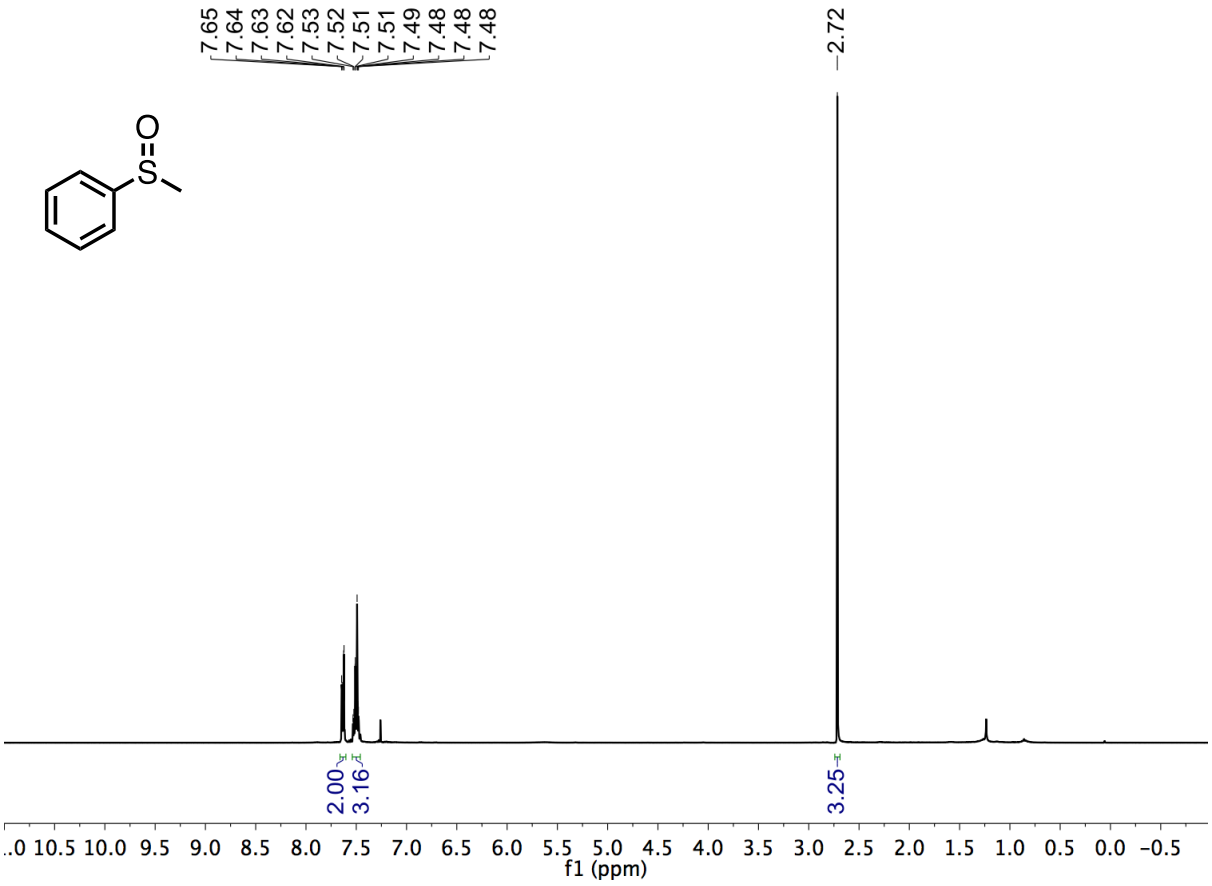

157.66
155.77
146.21
146.13
142.00
141.97
114.32
114.25
106.91
106.73
100.31
100.09
64.91
64.69
14.85
14.77
OH
O
F
f1 (ppm)

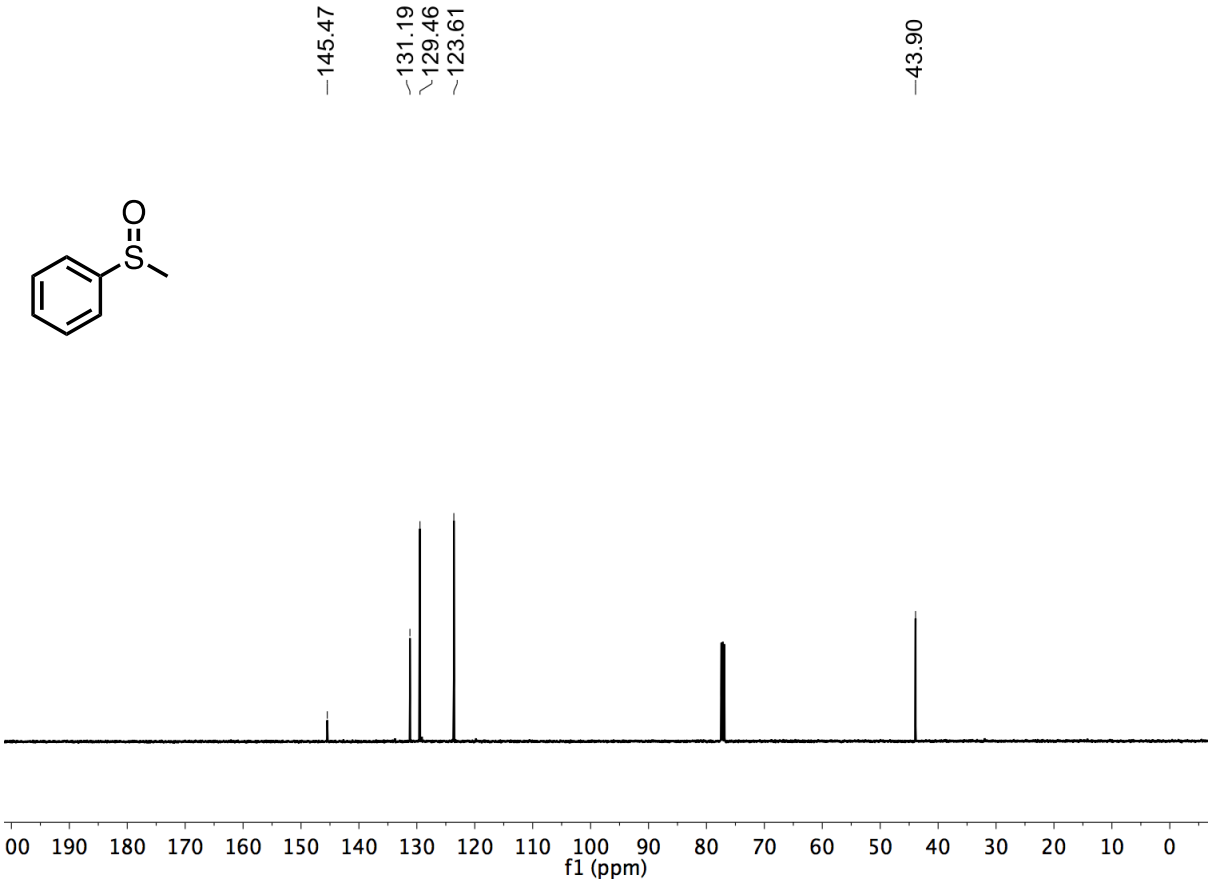

7.34
7.34
7.33
7.32
7.32
7.32
7.31
7.30
7.30
7.30
7.26
7.26
7.25
7.25
7.24
7.24
7.23
7.23
7.22
3.88
3.87
3.85
2.89
2.88
2.86

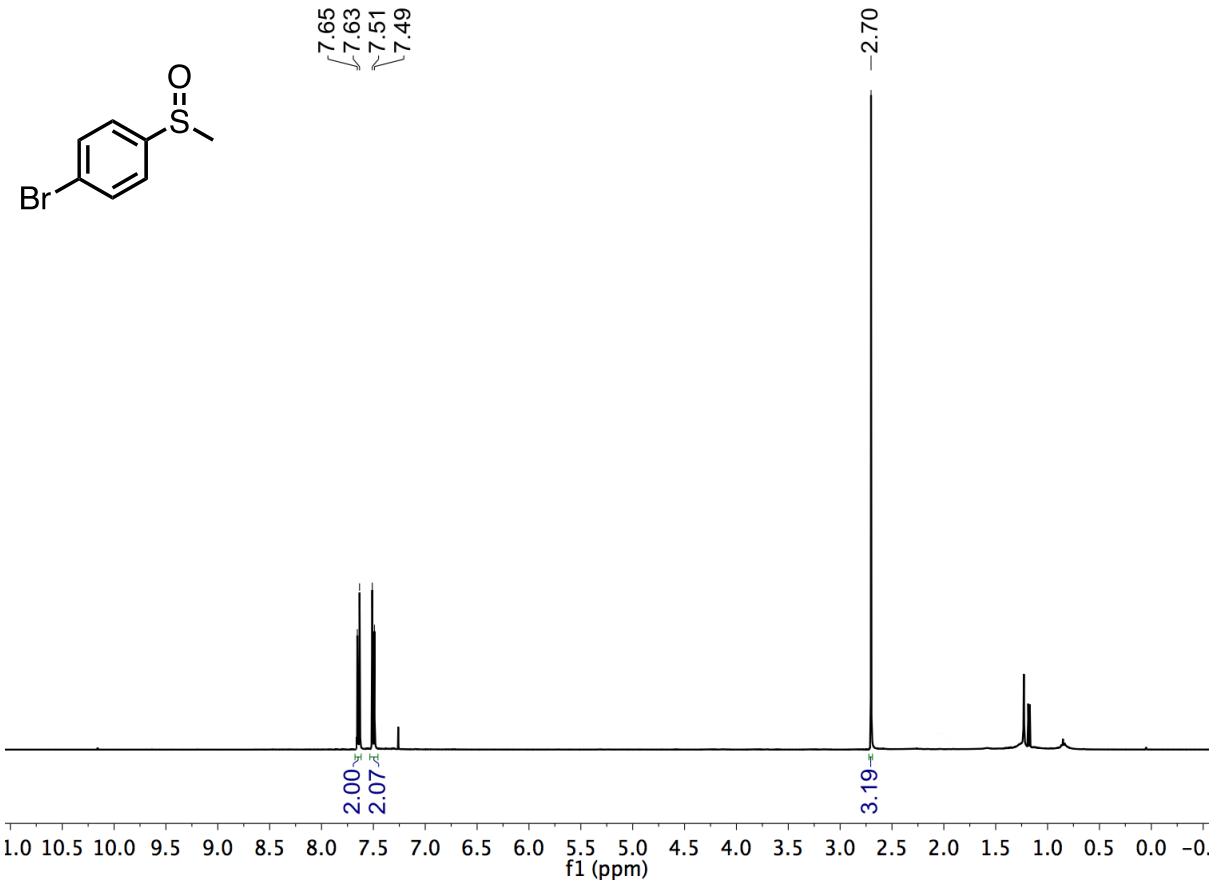

OH
2.02
3.11
2.00
2.02
f1 (ppm)

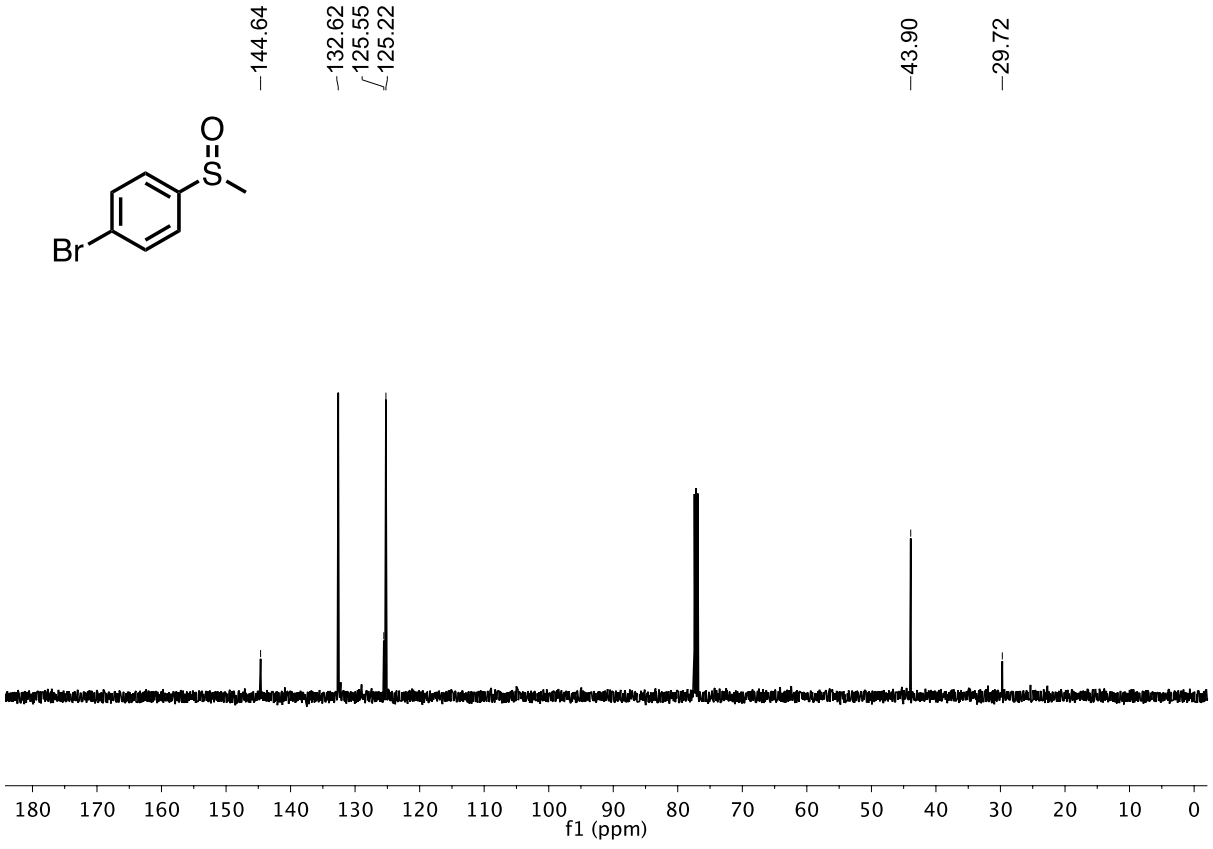


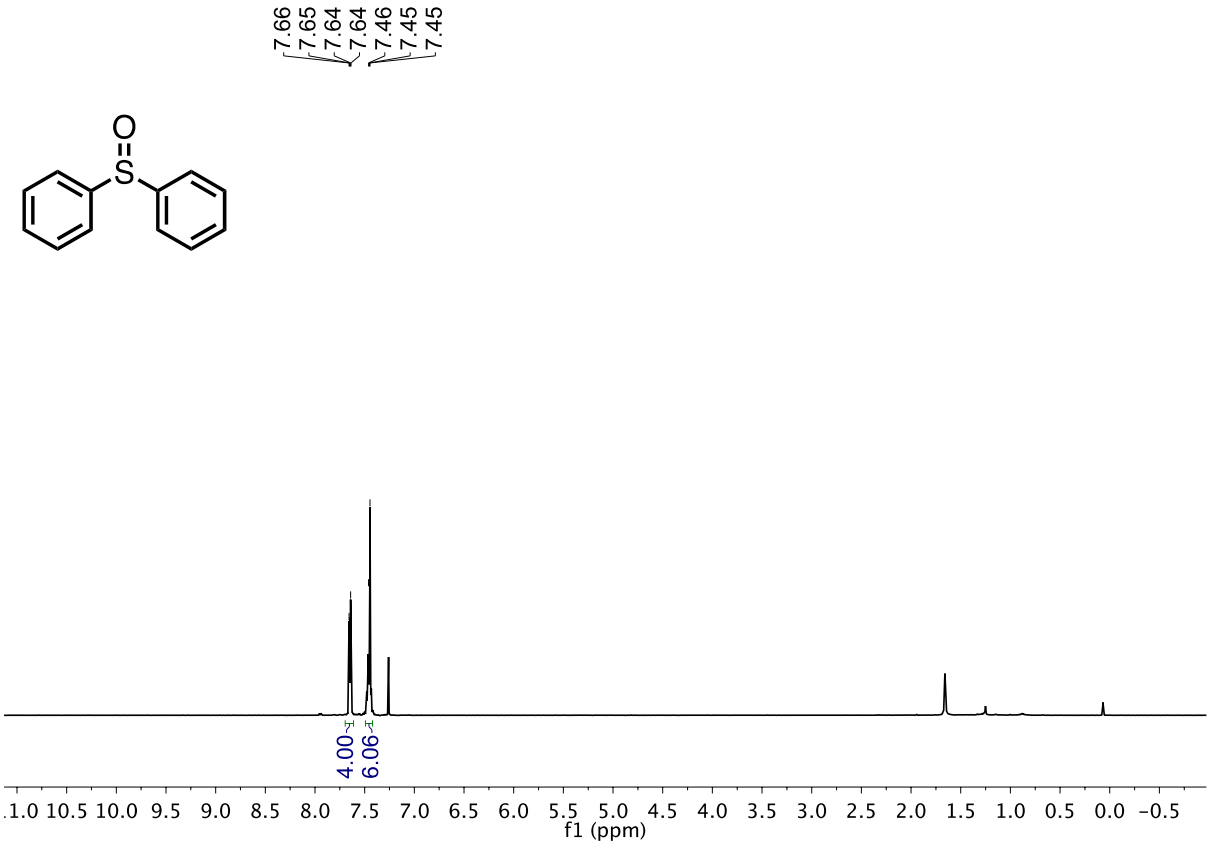
^{1}H NMR of 7a-7c

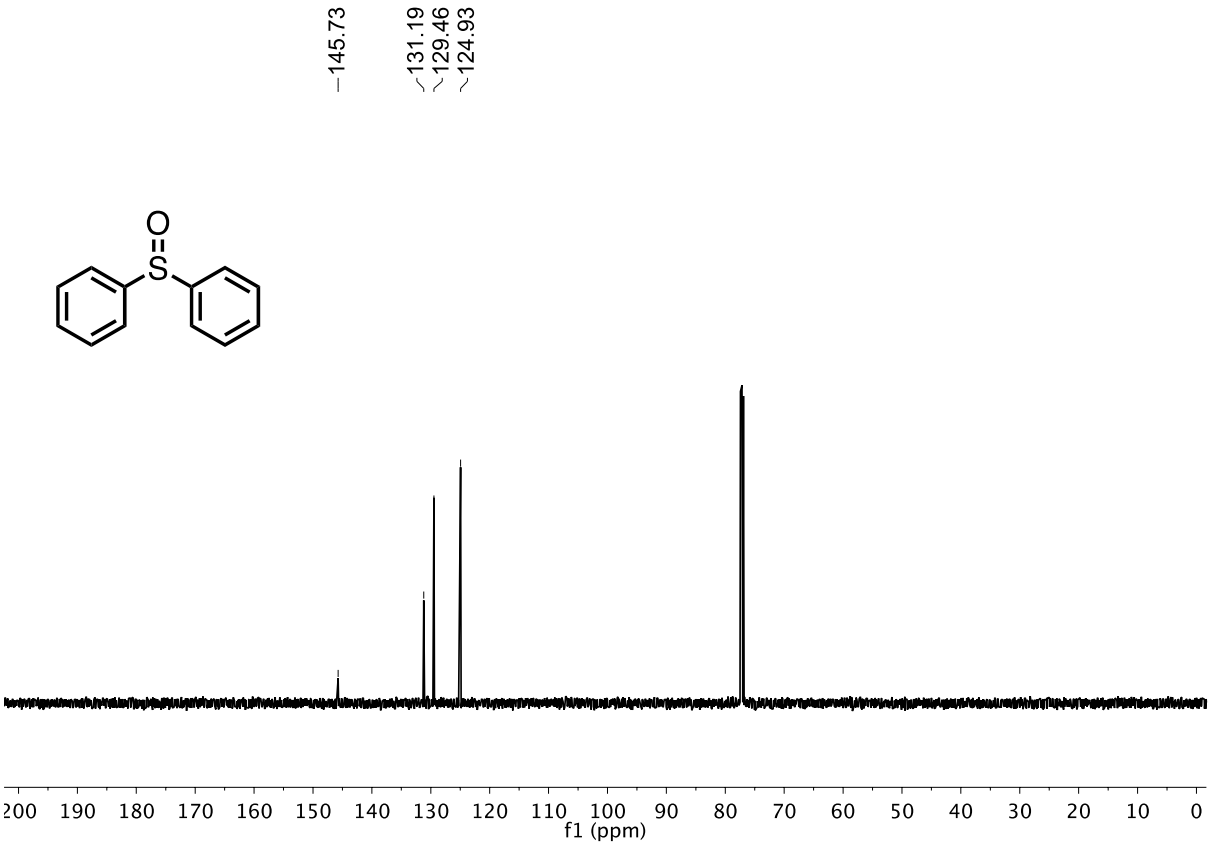

7.65
7.64
7.63
7.62
7.53
7.52
7.51
7.51
7.49
7.48
7.48
7.48
2.72
2.00
3.16
3.25
f1 (ppm)

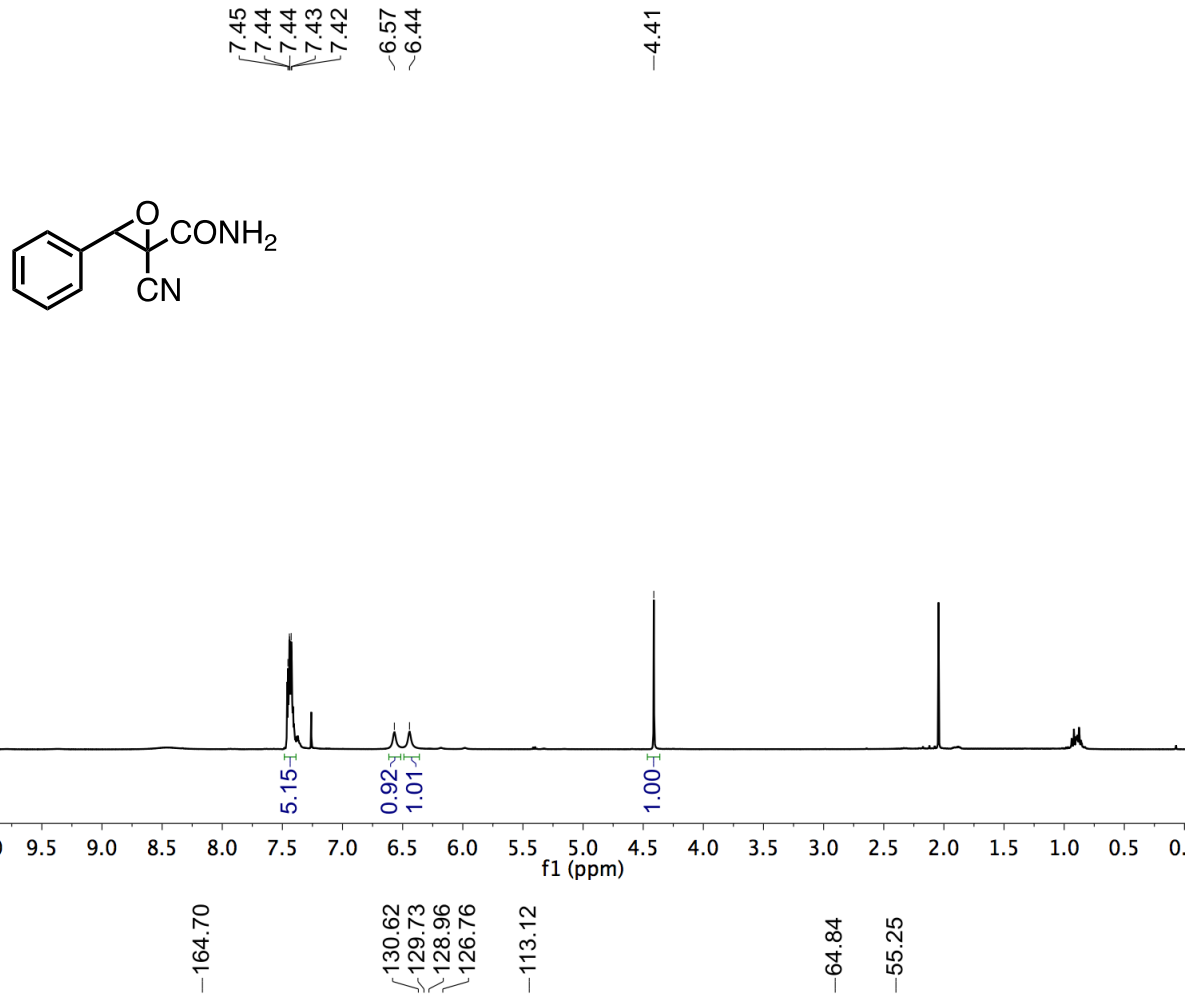

145.47
131.19
129.46
123.61
43.90
f1 (ppm)


7.65
7.63
7.51
7.49
2.70
O
S
Br
2.00
2.07
3.19
f1 (ppm)


144.64
132.62
125.55
125.22
43.90
29.72
O
S
Br
f1 (ppm)


7.66
7.65
7.64
7.64
7.46
7.45
7.45
O
S
4.00
6.06
f1 (ppm)


145.73
131.19
129.46
124.93
O
S
f1 (ppm)


7.45
7.44
7.44
7.43
7.42
6.57
6.44
4.41
O
CONH2
CN
5.15
0.92
1.01
1.00
f1 (ppm)
164.70
130.62
129.73
128.96
126.76
113.12
64.84
55.25
O
CONH2
CN
f1 (ppm)

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