Supporting Information

Experimental and Theoretical Investigations into the Unusual Regioselectivity of 4,5-, 5,6-, and 6,7-Indole Aryne Cycloadditions

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I. Experimental Procedures

A. General

^{1}H-NMR (400 MHz) and ^{13}C-NMR (100 MHz) were performed in $CDCl_3$ unless otherwise noted with reference to residual solvent at δ 7.26 ppm and 77.0 ppm, respectively. Melting points when reported are uncorrected. Unless otherwise noted, all commercially obtained starting materials were used as received. Alkyllithiiums were titrated against 2-butanol in anhydrous THF with 1,10-phenanthroline as indicator prior to use. Tetrahydrofuran and diethyl ether were distilled from sodium and benzophenone under nitrogen prior to use. Dichloromethane and toluene were distilled from calcium hydride under nitrogen prior to use. Temperatures of -78 °C were obtained through use of a dry-ice acetone cold bath.

1. General procedure for 4,5-, 5,6-, and 6,7-indolyne generation from *o*-dibromoindoles and trapping with 2-substituted furans: A flame-dried 5 mL round bottom flask was charged with 2 mL Et_2O, 20 mg of the dibromoindole **10**, **13**, or **16** (ref 4) (0.055 mmol) and 5 equiv of the 2-substituted furan (ref 8) (0.275 mmol) under an atmosphere of nitrogen, and the resulting mixture cooled to -78 °C. To this cold solution, 30 μL (2.3M, 0.069 mmol, 1.2 equiv) of n-butyllithium in hexanes solution was added dropwise, and the solution was stirred at -78 °C for 30 min. The cold bath was removed and the solution allowed to warm slowly to room temperature over 1 h. The reaction was quenched with water. The product was extracted with 3 x 5 mL diethyl ether, and the combined organic layers were dried over

magnesium sulfate, filtered and concentrated under reduced pressure. The resulting residues were purified via flash column chromatography using ethyl acetate/hexanes as the eluent. All purified products were obtained as clear or slightly yellow oils or foams.

II. Spectroscopic Data

Compound 14: ^{1}H NMR (400MHz, $CDCl_3$): δ 7.55-7.50 (m, 1H), 7.43-7.37 (m, 1H), 7.36-7.26 (m, 3H), 7.16-7.11 (m, 2H), 7.00 (d, *J* = 7.9 Hz, 1H), 6.96 (d, *J* = 5.5Hz, 1H), 6.93 (s, 1H), 5.72-5.70 (m, 1H), 3.75 (s, 3H), 0.81 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6) δ 27.78, 33.16, 33.49, 81.82, 104.92, 106.02, 114.97, 116.32, 124.21, 127.71, 128.50, 128.81, 133.19, 138.31, 139.34, 142.68, 145.32, 145.76, 147.19; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1780.

Compound 15: ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.49-7.45 (m, 2H), 7.44-7.38 (m, 3H), 7.32-7.27 (m, 1H), 7.14-7.09 (m, 2H), 7.06 (s, 1H), 6.90 (d, *J* = 8.2Hz, 1H), 5.92 (d, *J* = 1.6Hz, 1H), 3.75 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6) δ 27.91, 33.30, 33.66, 81.75, 104.11, 108.48, 115.00, 116.78, 123.54, 127.60, 128.13, 128.81, 132.65, 133.48, 137.01, 139.6, 141.25, 145.82, 148.19; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1781.

Compound 17: ^{1}H NMR (400 MHz, C_6D_6): δ 7.69 (d, *J* = 12.8 Hz, 1 H), 7.56 (d, *J* = 8.4 Hz, 2 H), 7.31 (t, *J* = 7.7 Hz, 2 H), 7.15 (m, 3 H), 6.57 (s, 1 H), 6.12 (m, 1 H), 5.16 (m, 1 H), 3.46 (s, 3 H), 1.48 (s, 9 H); ^{13}C NMR (100 MHz, C_6D_6) δ 27.01, 31.96, 33.11, 81.86, 99.34, 104.74, 110.12, 111.77, 117.67, 122.93, 125.84, 125.93, 129.06, 134.93, 136.59, 142.03, 143.80, 144.21, 144.97; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1782.

Compound 18: ^{1}H NMR (400 MHz, C_6D_6): δ 7.68 (d, *J* = 9.3 Hz, 1 H), 7.60 (d, *J* = 7.1 Hz, 2 H), 7.30 (t, *J* = 7.5 Hz, 2 H), 7.15 (m, 3 H), 6.62 (s, 1 H), 6.27 (d, *J* = 3.7 Hz), 5.29 (m, 1 H), 3.06 (s, 3 H), 1.17 (s, 9 H); ^{13}C NMR (100 MHz, C_6D_6) δ 26.99, 32.08, 33.06, 81.72, 99.50, 102.78, 113.58, 118.22, 123.15, 125.69, 126.02, 128.65, 129.16, 134.68, 136.64, 141.06, 143.13, 143.83, 146.96; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1781.

Compound 19 (R = Me): ^{1}H NMR (CD_3CN, 400 MHz): δ 7.62-7.58 (m, 2H), 7.49 (d, *J* = 7.8 Hz, 1H), 7.44-7.39 (m, 2H), 7.27 (s, 1H), 7.27-7.22 (m, 1H), 7.15-7.11 (m, 2H), 6.94 (d, *J* = 5.4Hz, 1H), 5.68 (d, *J* = 1.9Hz, 1H), 3.96 (s, 3H), 2.14 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN) δ 20.76, 38.16, 82.97, 91.72, 113.93, 116.32, 116.73, 126.59, 128.10, 128.23, 129.59, 130.67, 133.81, 135.59, 136.31, 146.74, 147.21, 148.82; HRMS (EI) *m/e* calcd for $C_{20}H_{17}NO$ 287.1311, found 287.1313.

Compound 19 (R = Et): ^{1}H NMR (C_6D_6, 400 MHz): δ 7.69-7.64 (m, 3H), 7.37-7.31 (m, 2H), 7.21-7.16 (m, 1H), 7.04 (d, *J* = 7.9 Hz, 1H), 6.83 (dd, *J* = 5.5 Hz,, 1.9 Hz, 1H), 6.55 (s, 1H), 6.52 (d, *J* = 5.4 Hz, 1H), 5.56 (d, *J* = 1.8 Hz, 1H), 3.07 (s, 3H), 2.39-2.32 (m, 2H), 1.20 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, CD_3CN) δ 10.19, 26.60, 37.85, 82.87, 96.40, 114.15, 116.46, 116.99, 126.74, 128.27, 128.38, 129.72, 131.03, 134.29, 134.71, 136.42, 146.35, 146.96, 149.30; HRMS (EI) *m/e* calcd for $C_{21}H_{19}NO$ 301.1468, found 301.1467.

Compound 19 (R = *i*-Pr): ^{1}H NMR (CD_3CN, 400 MHz): δ 7.62-7.58 (m, 2H), 7.48 (d, *J* = 7.8 Hz, 1H), 7.44-7.39 (m, 2H), 7.28-7.23 (m, 2H), 7.13 (d, *J* = 7.8 Hz, 1H), 7.09 (dd, *J* = 5.5, 1.8 Hz, 1H), 6.98 (d, *J* = 5.5 Hz, 1H), 5.72 (d, *J* = 1.8 Hz, 1H), 3.93 (s, 3H), 3.27 (septet, *J* = 6.8 Hz, 1H), 1.14 (dd, *J* = 1.8, 6.8 Hz, 6H); ^{13}C NMR (100 MHz, CD_3CN) δ 18.93, 19.06, 30.06, 37.76, 82.64, 100.26, 114.15, 116.44, 117.15, 126.77, 128.29, 128.39, 129.72, 131.29, 134.48, 134.90, 136.39, 146.12, 146.47, 149.32; HRMS (EI) *m/e* calcd for $C_{22}H_{21}NO$ 315.1624, found 315.1624.

Compound 19 (R = *t*-Bu): ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.56-7.51 (m, 3H), 7.43-7.38 (m, 2H), 7.29-7.24 (m, 1H), 7.16-7.12 (m, 2H), 7.03 (d, *J* = 5.5 Hz, 1H), 7.01(s, 1H), 5.17 (d, *J* = 1.8 Hz, 1H), 3.99 (s, 3H), 1.45 (s, 9H); ^{13}C NMR (100 MHz, C_6D_6) δ 29.6, 33.7, 39.1, 82.2, 104.6, 114.1, 116.9, 118.5, 126.4,

128.4, 129.0, 129.7, 131.0, 135.2, 135.6, 136.0, 142.6, 146.4, 149.3; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1779.

Compound 19 (R = Ph): ^{1}H NMR (C_6D_6, 400 MHz): δ 8.03 (d, *J* = 7.9 Hz, 1H), 7.70-7.65 (m, 2H), 7.37-7.31 (m, 4H), 7.21-7.17 (m, 1H), 7.07-6.97 (br, 4H), 6.50 (s, 1H), 5.99 (dd, *J* = 3.6,1.3Hz, 1H), 4.57(d, *J* = 3.7Hz, 1H), 2.60-2.53 (m, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, C_6D_6) δ 30.24, 83.10, 107.37, 114.23, 116.92, 117.87, 126.11, 129.32, 129.38, 129.66, 130.13, 130.45, 131.38, 131.57, 132.18, 135.61, 135.24, 135.89, 142.31, 146.20, 146.92; HRMS (EI) *m/e* calcd for $C_{25}H_{19}NO$ 349.1468, found 349.1470.

Compound 20 (R = Me): ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61-7.54 (m, 3H), 7.43-7.37 (m, 2H), 7.27-7.22 (m, 1H), 7.13-7.08 (m, 3 H), 6.90 (d, *J* = 5.5 Hz, 1H), 6.20 (d, *J* = 1.8 Hz, 1H), 3.93 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, CD_3CN) δ 15.62, 35.15, 81.20, 90.38, 112.93, 116.06, 116.70, 126.47, 126.61, 127.78, 129.61, 129.80, 133.36, 134.74, 136.49, 145.70, 147.76, 148.01; HRMS (EI) *m/e* calcd for $C_{20}H_{17}NO$ 287.1311, found 287.1312.

Compound 20 (R = Et): ^{1}H NMR (C_6D_6, 400 MHz): δ 7.73-7.69 (m, 3H), 7.38-7.32 (m, 2H), 7.21-7.16 (m, 1H), 7.08 (d, *J* = 7.9 Hz, 1H), 6.77 (dd, *J* = 5.4 Hz, 1.8 Hz, 1H), 6.69 (d, *J* = 5.4 Hz 1H), 6.54 (s, 1H), 5.92 (d, *J* = 1.8 Hz, 1H), 2.84 (s, 3H), 2.35 (q, *J* = 7.5 Hz, 2H), 1.28 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, THF-d_8) δ 8.68, 22.40, 34.03, 80.43, 93.53, 109.99, 112.26, 115.20, 125.30, 126.27, 127.05, 128.21, 128.50, 134.61, 136.28, 136.29, 145.05, 145.83, 146.22; HRMS (EI) *m/e* calcd for $C_{21}H_{19}NO$ 301.1468, found 301.1469.

Compound 20 (R = *i*-Pr): ^{1}H NMR (C_6D_6, 400 MHz): δ 7.73-7.68 (m, 3H), 7.38-7.32 (m, 2H), 7.21-7.17 (m, 1H), 7.12 (d, *J* = 0.5 Hz, 1H), 6.76-6.75 (m, 2H), 6.53 (s, 1H), 5.92 (s, 1H), 2.82 (s, 3H), 2.67 (septet, *J* = 6.8 Hz, 1H), 1.36 (dd, *J* = 8.7, 6.8 Hz, 6H); ^{13}C NMR (100 MHz, THF-d_8) δ 18.61, 18.76, 28.32, 35.32, 80.99, 97.93, 114.38, 116.04, 116.92, 126.58, 127.89, 129.74, 129.89, 130.07, 133.42, 135.95, 136.65, 145.72, 146.29, 146.51; HRMS (EI) *m/e* calcd for $C_{22}H_{21}NO$ 315.1624, found 315.1622.

Compound 20 (R = *t*-Bu): ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61-7.57 (m, 2H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.43-7.38 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.28-7.23 (m, 1H), 7.12-7.07 (m, 3H), 6.24 (d, *J* = 1.5 Hz, 1H), 3.93 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, THF-d_8) δ 27.13, 30.63, 34.91, 80.79, 100.45, 115.47, 115.52, 117.32, 126.05, 127.75, 129.15, 129.01, 129.27, 133.61, 136.57, 137.02, 144.72, 145.55, 145.68; HRMS (EI) *m/e* calcd for $C_{23}H_{23}NO$ 329.1781, found 329.1782.

Compound 20 (R = SO_2Ph): ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.61-7.57 (m, 2H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.43-7.38 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.28-7.23 (m, 1H), 7.12-7.07 (m, 3H), 6.24 (d, *J* = 1.5 Hz, 1H), 3.93 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 35.3, 81.0, 116.3, 118.0, 119.2, 121.1, 122.3, 123.5, 123.6, 126.1, 127.1, 128.1, 128.9, 129.0, 129.6, 131.2, 134.1, 138.4, 135.8, 145.3, 148.1; HRMS (EI) *m/e* calcd for $C_{25}H_{19}NO_3S$ 413.1087, found 413.1090.

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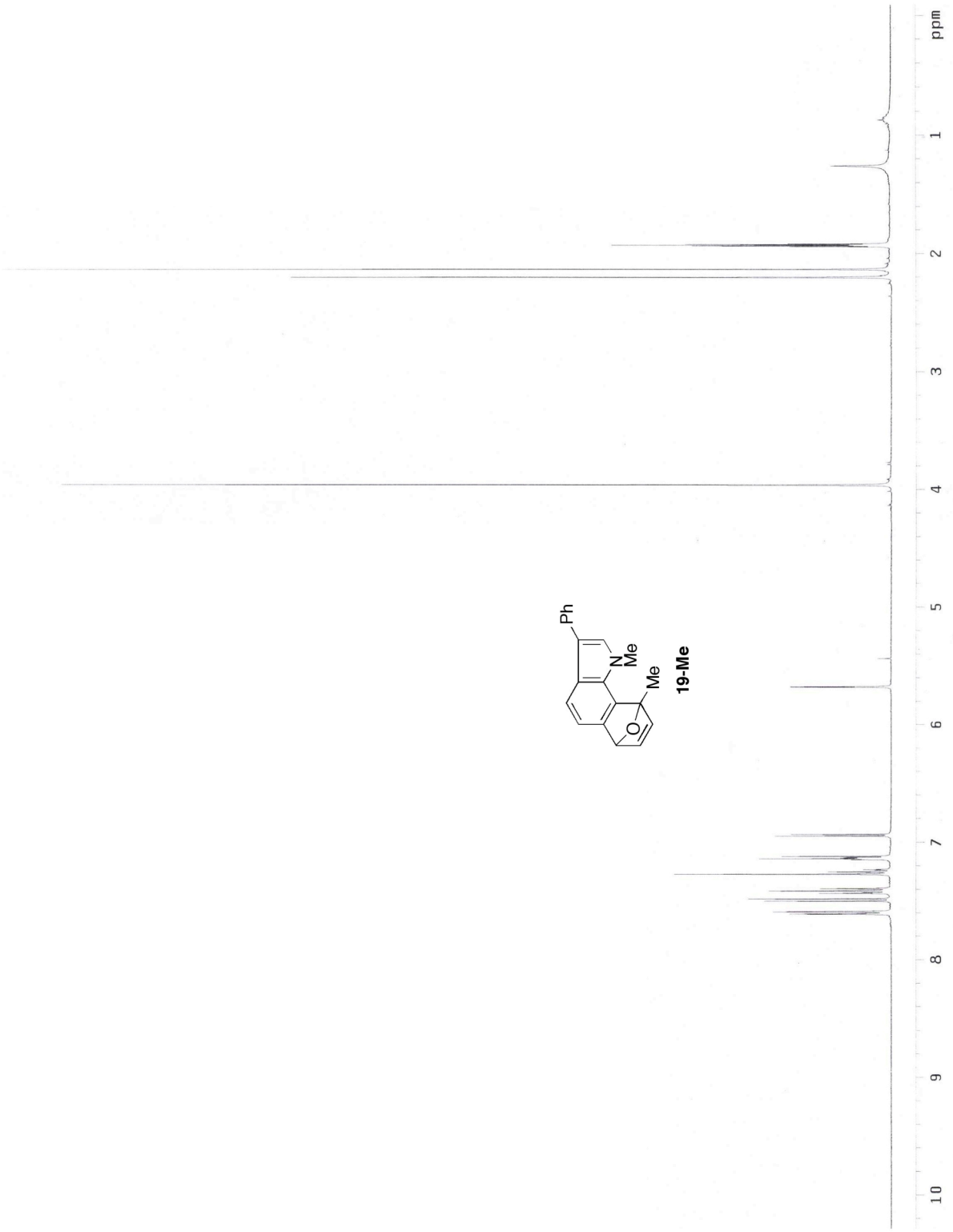
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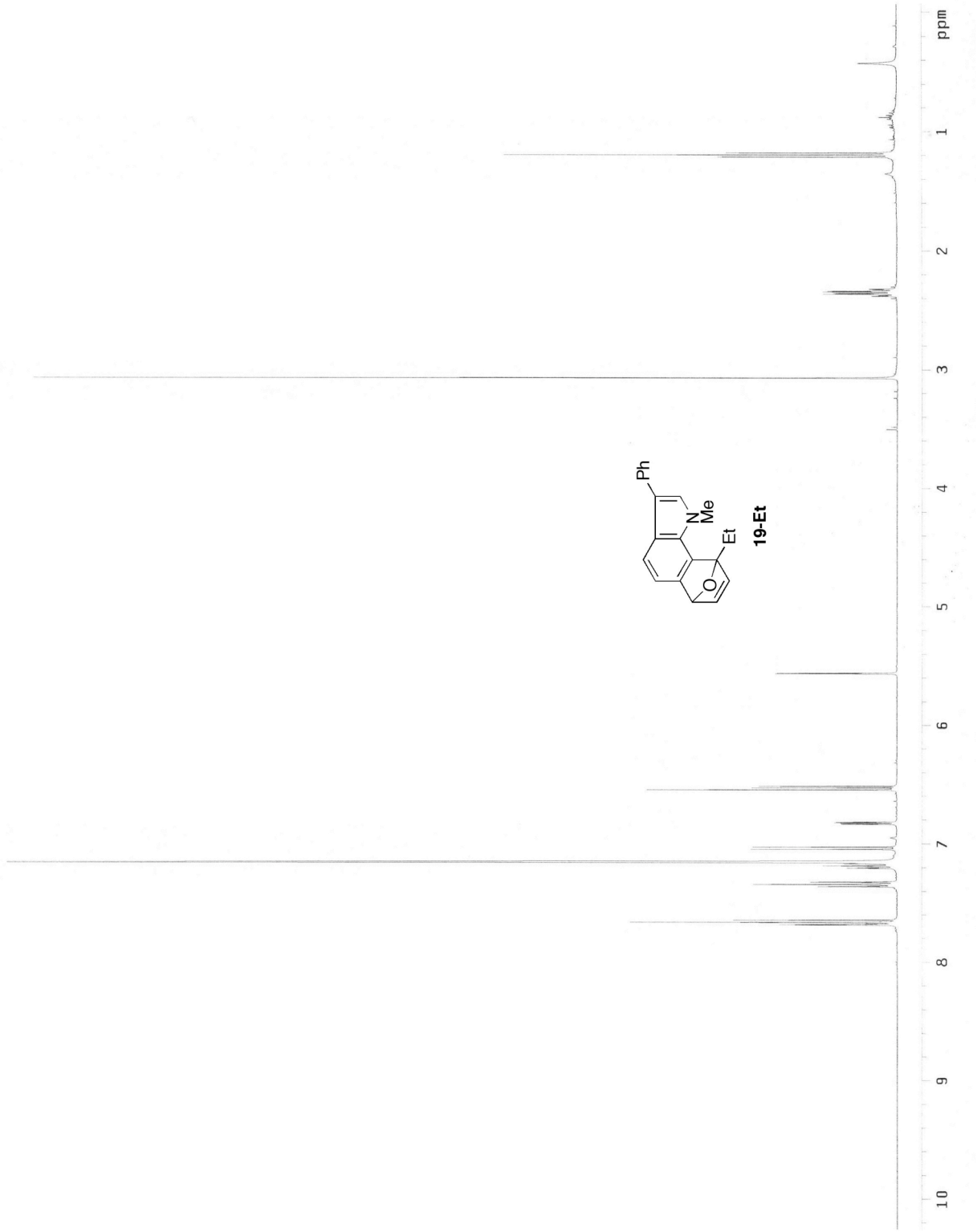
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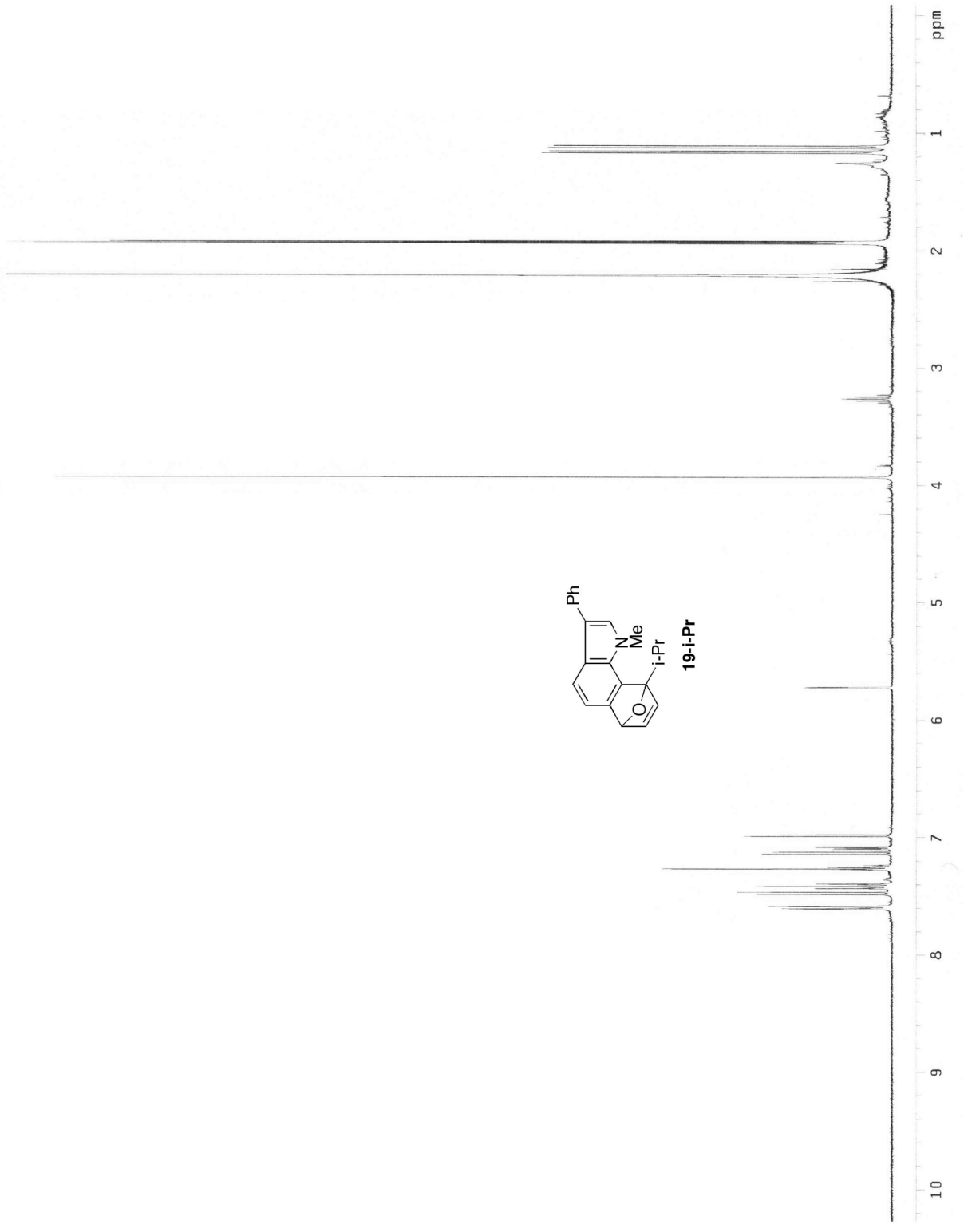
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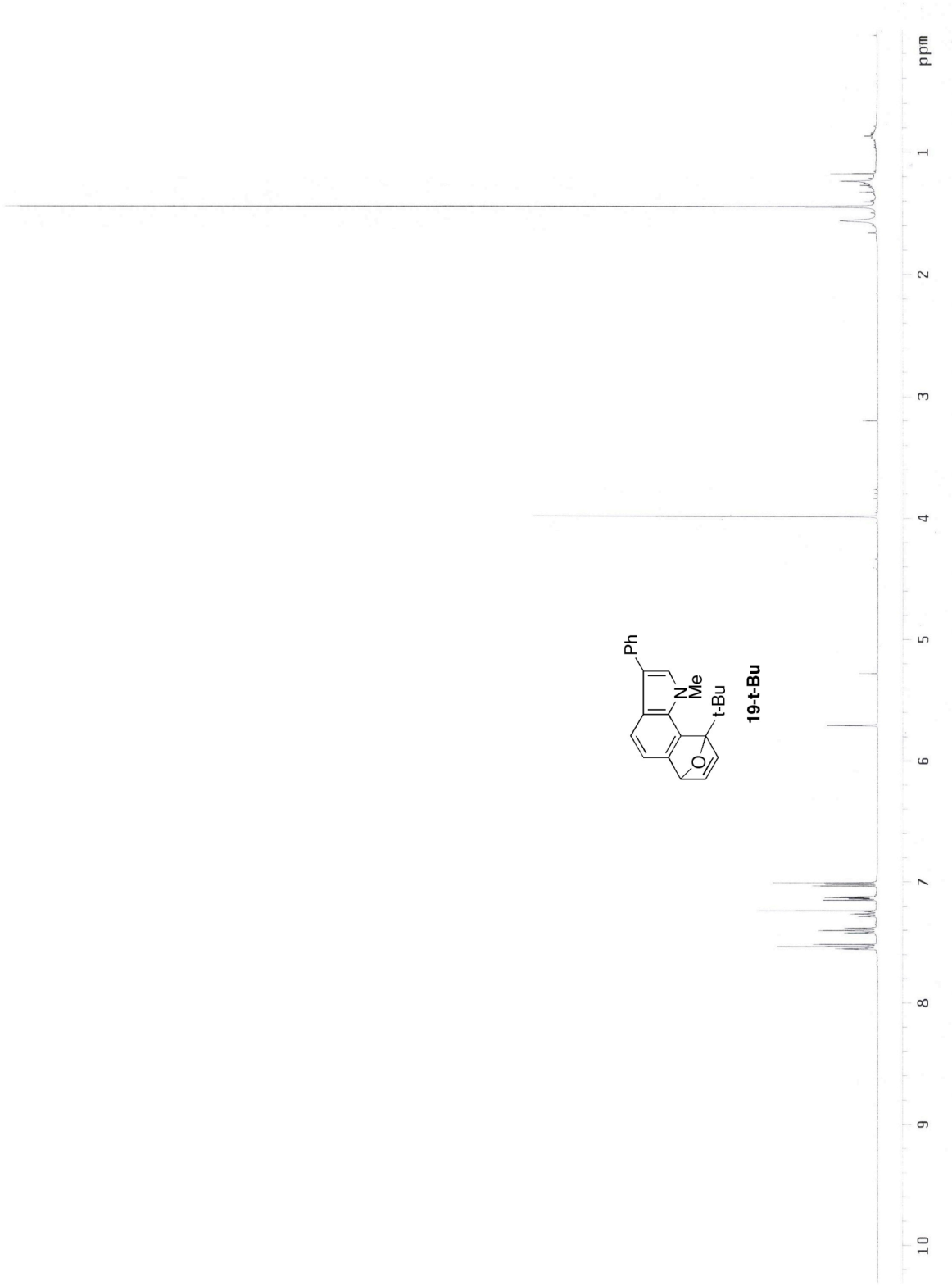
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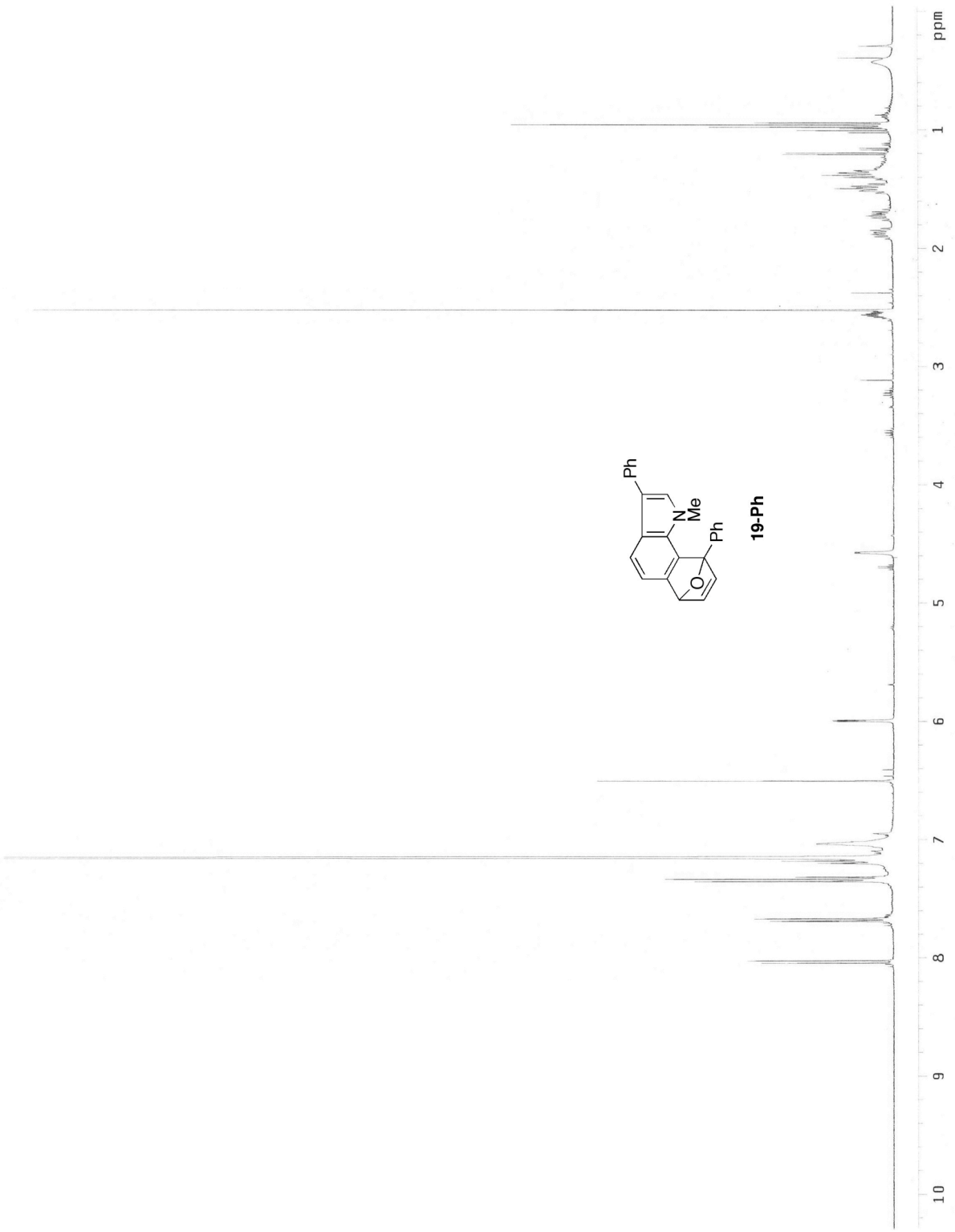
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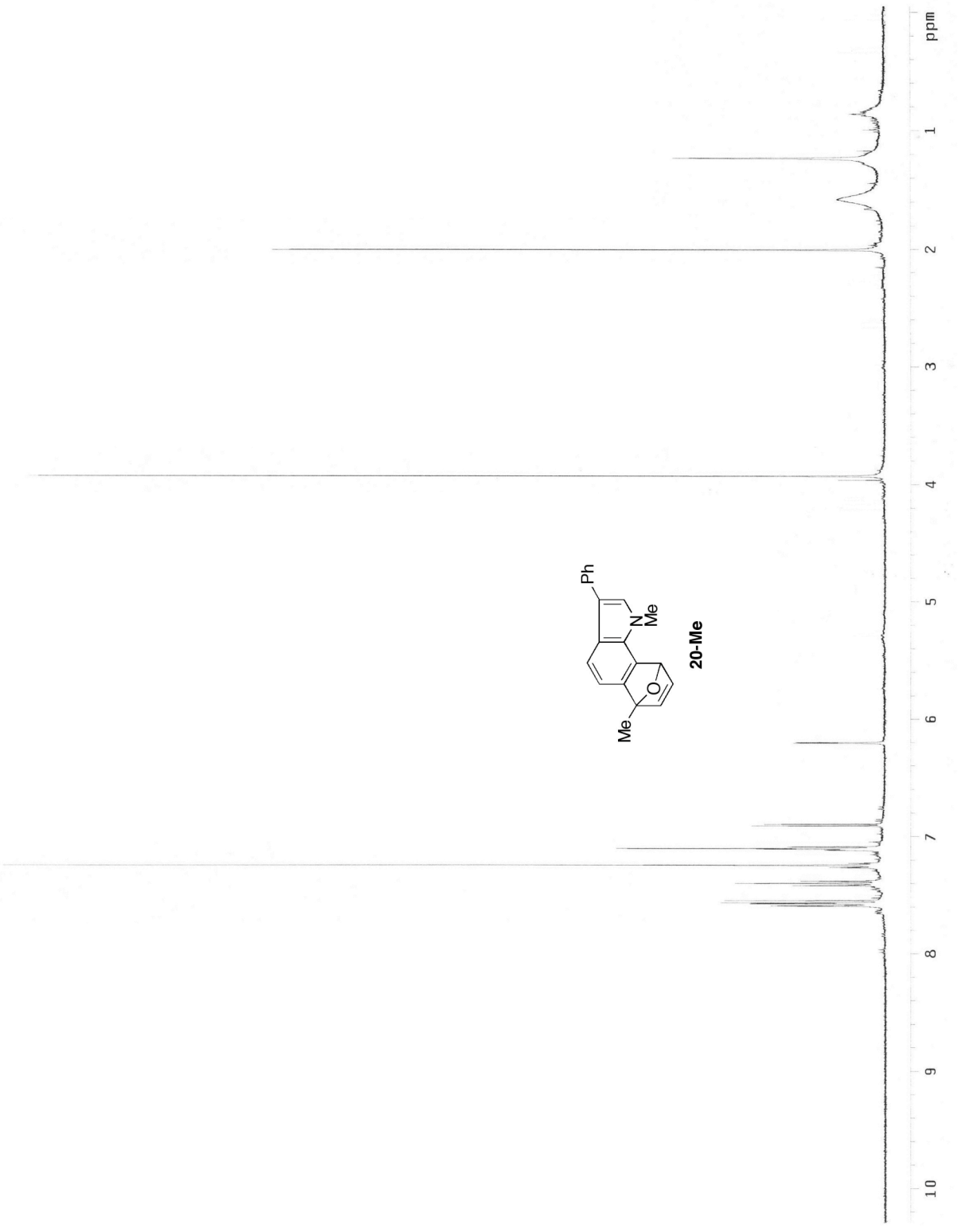
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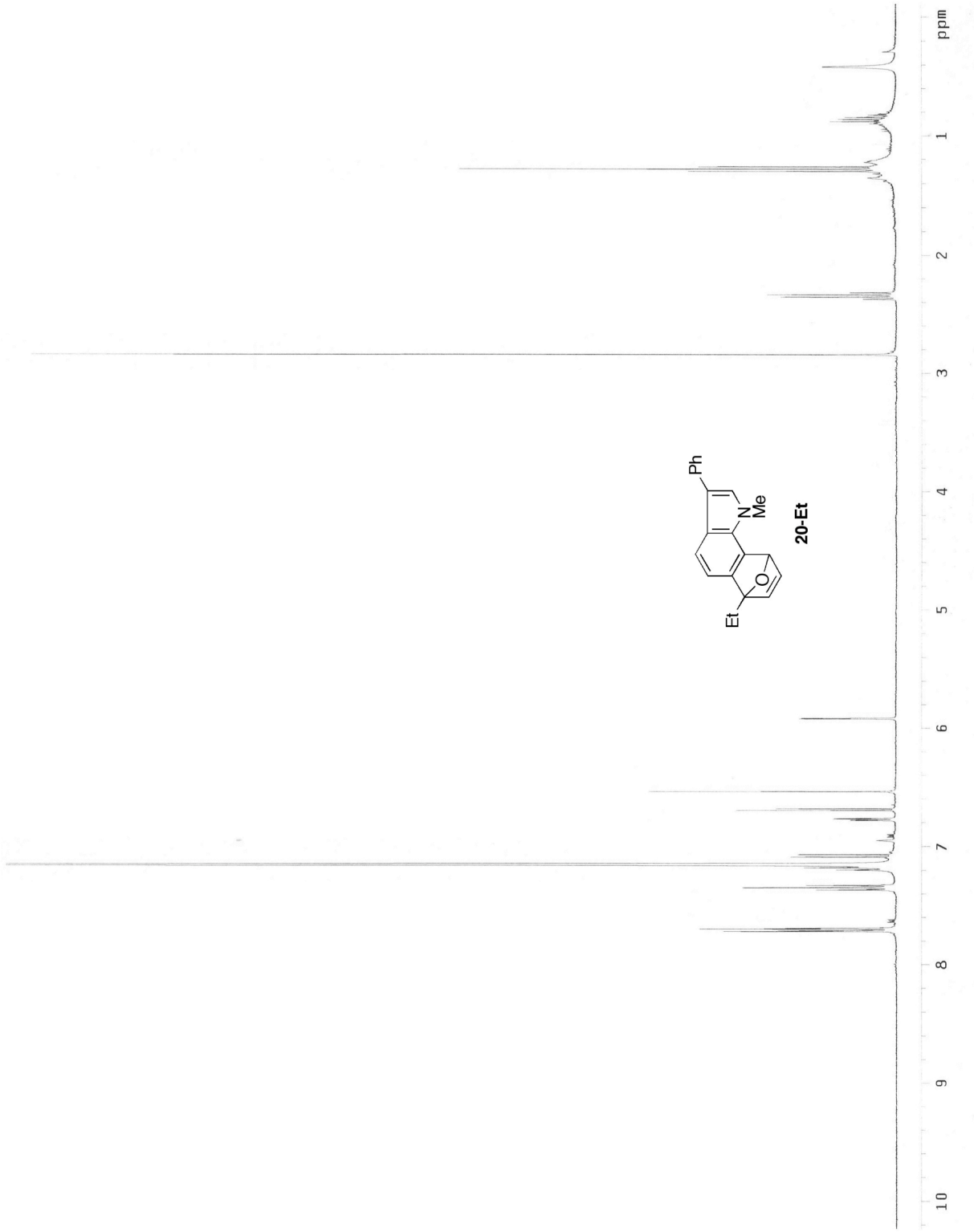
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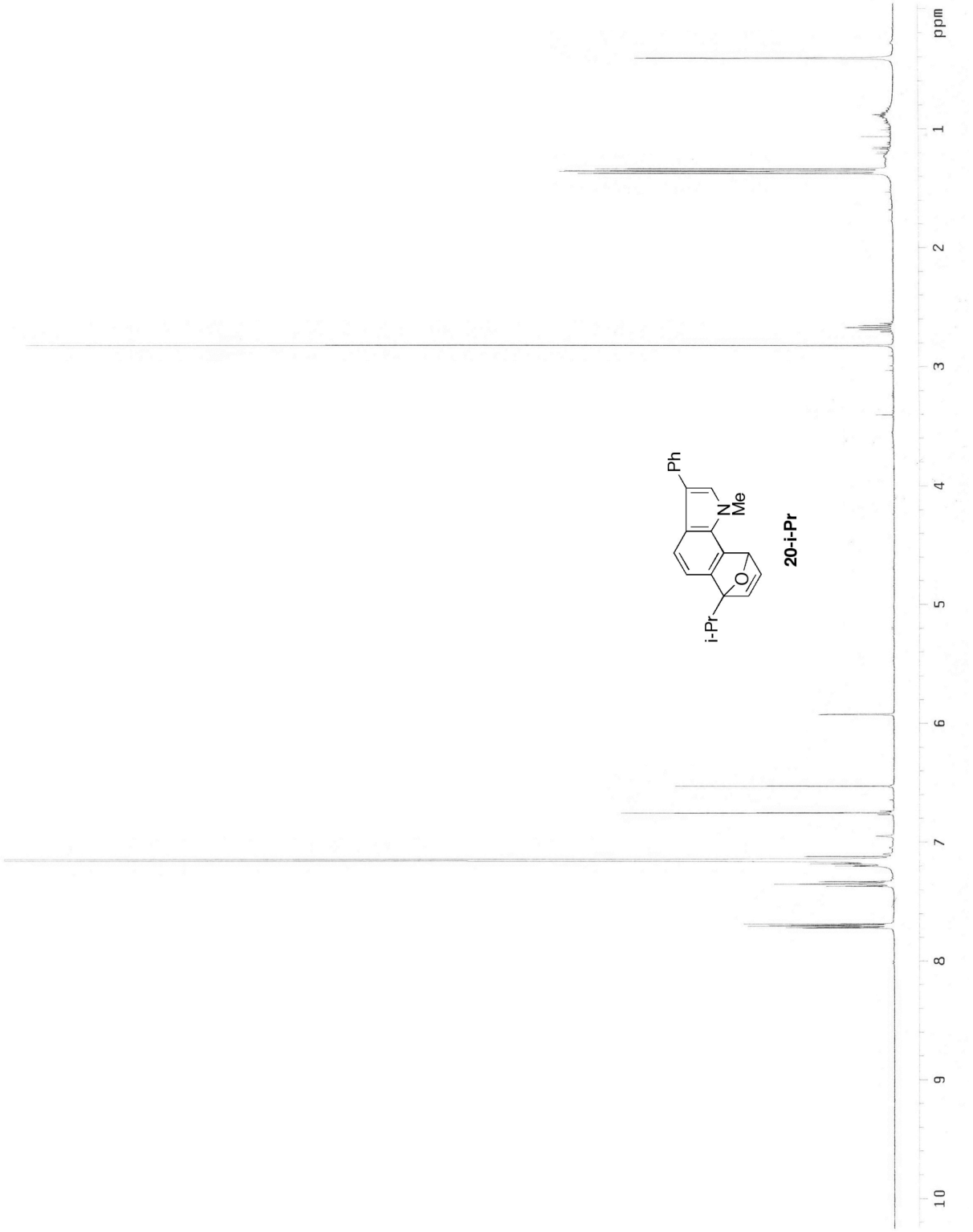
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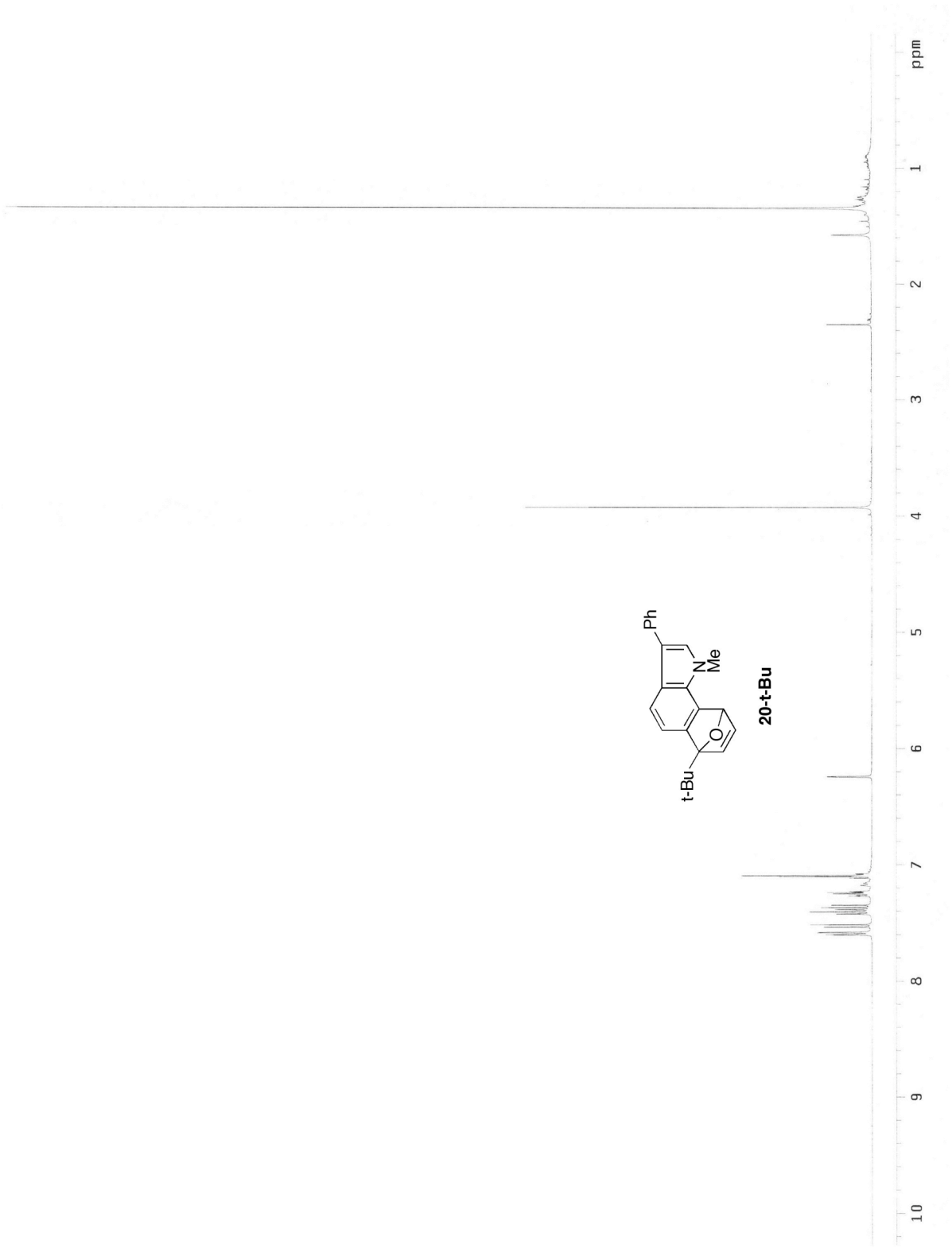
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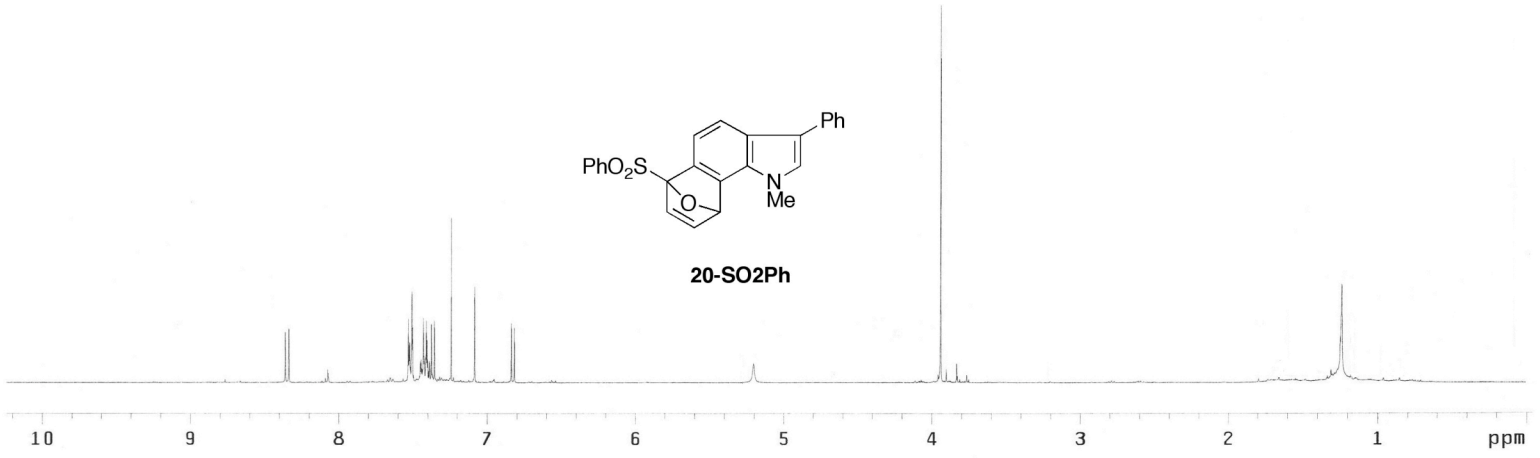
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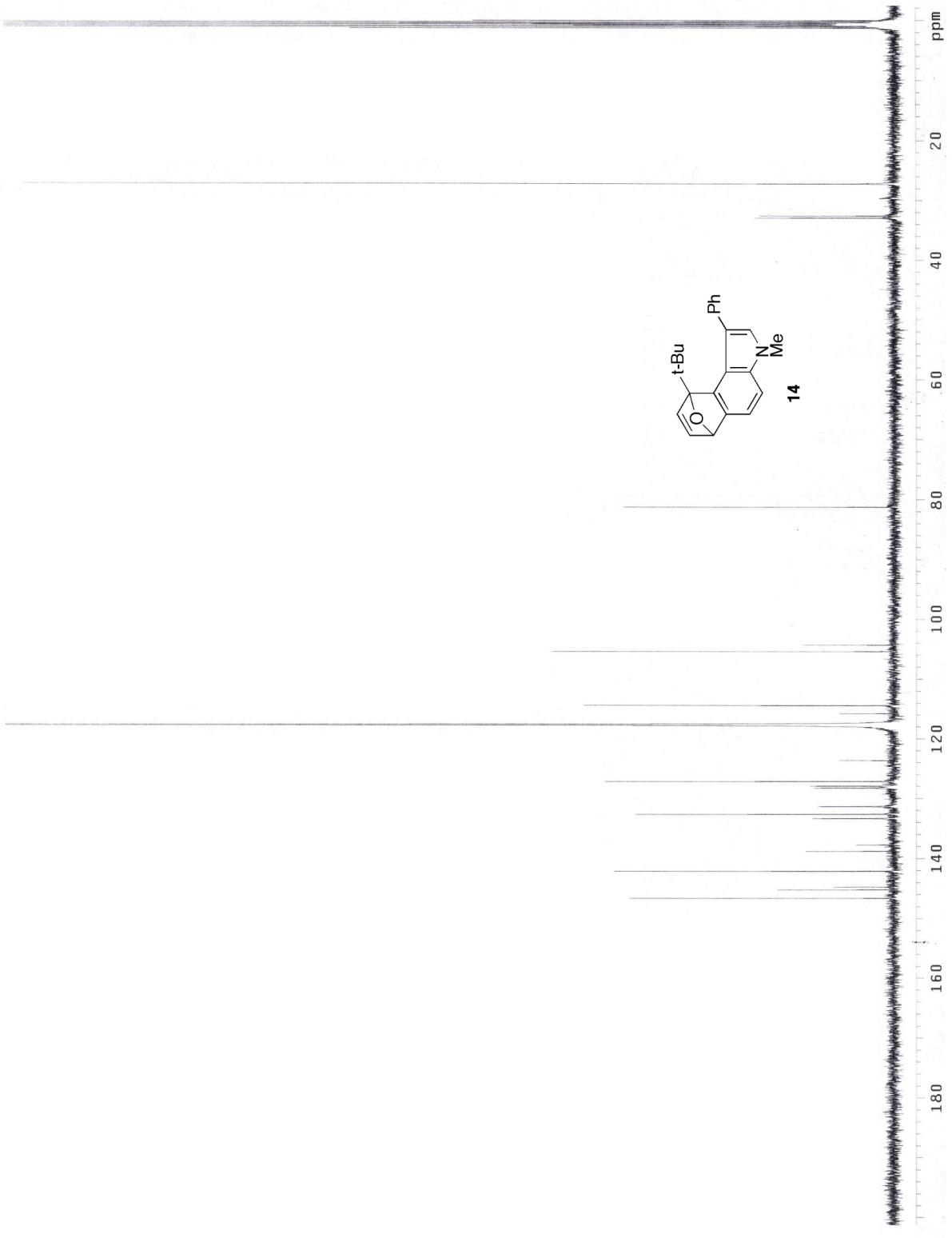
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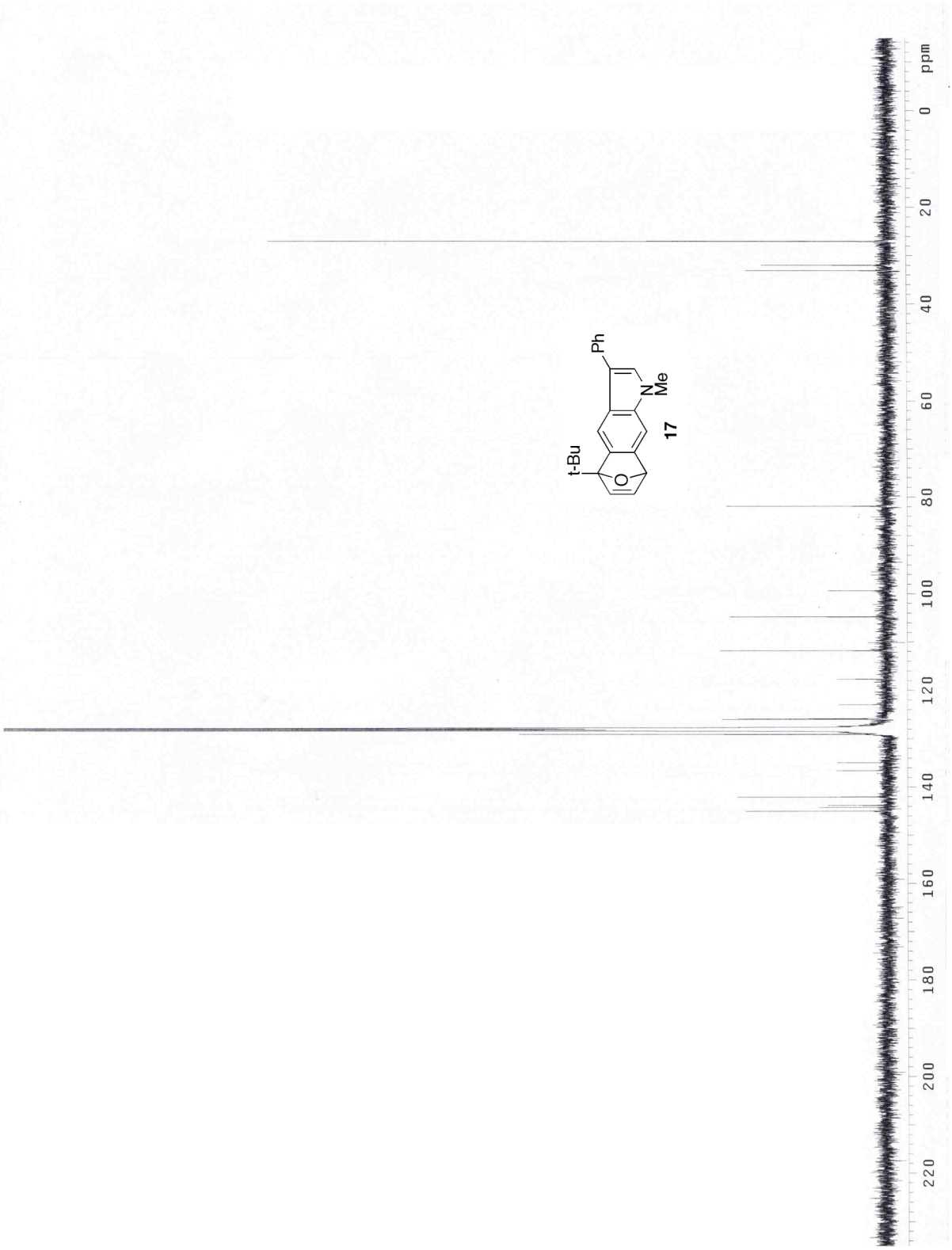
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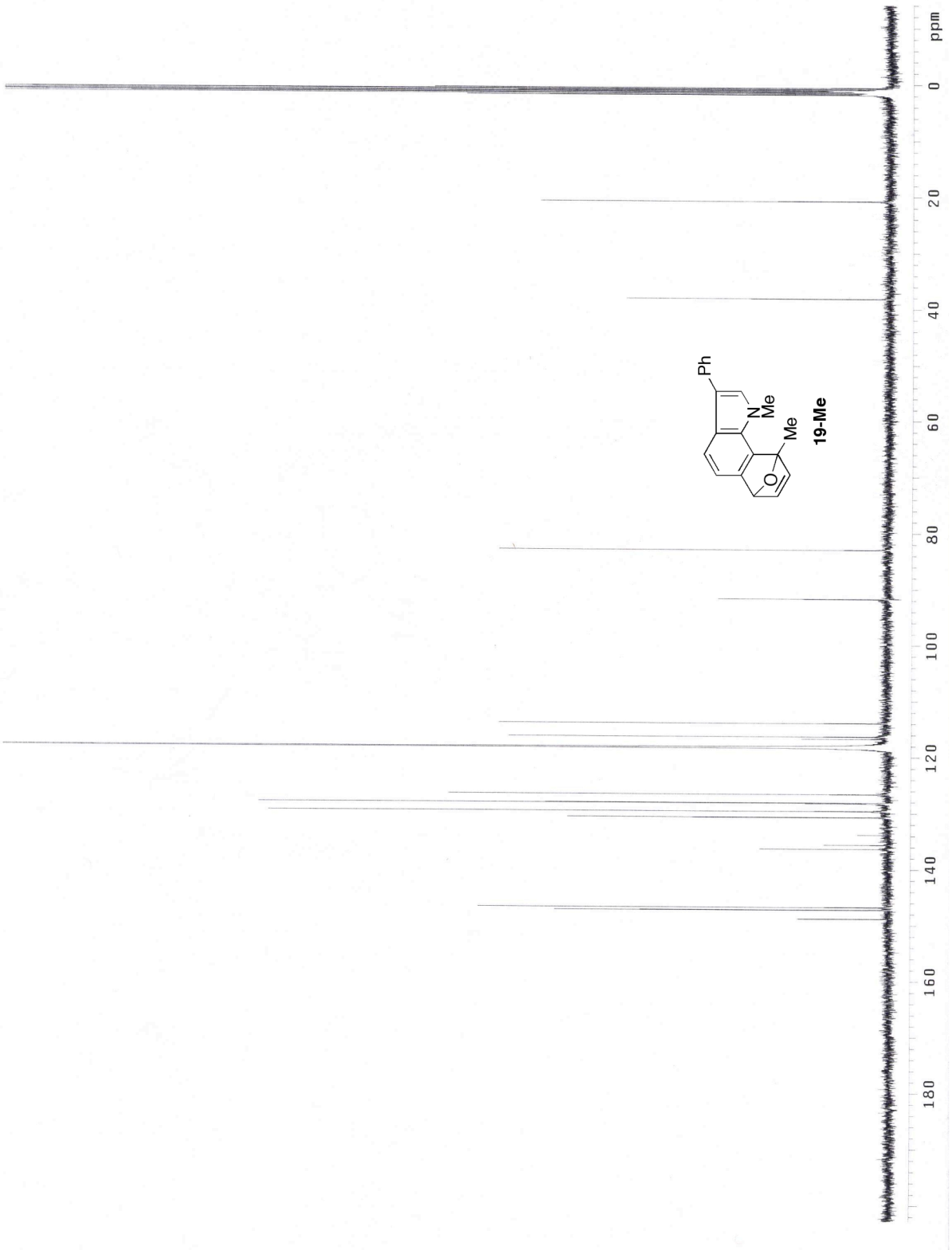
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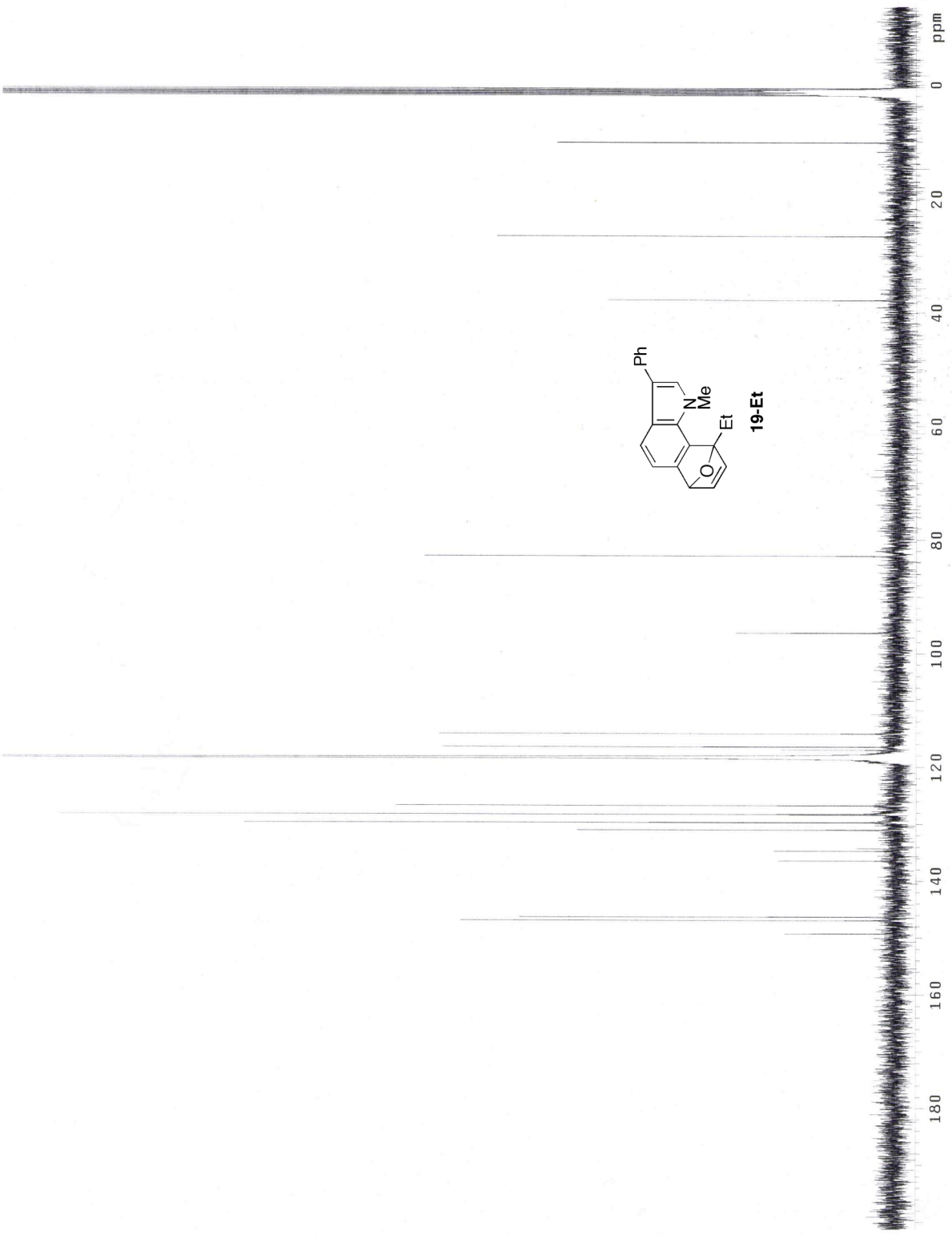
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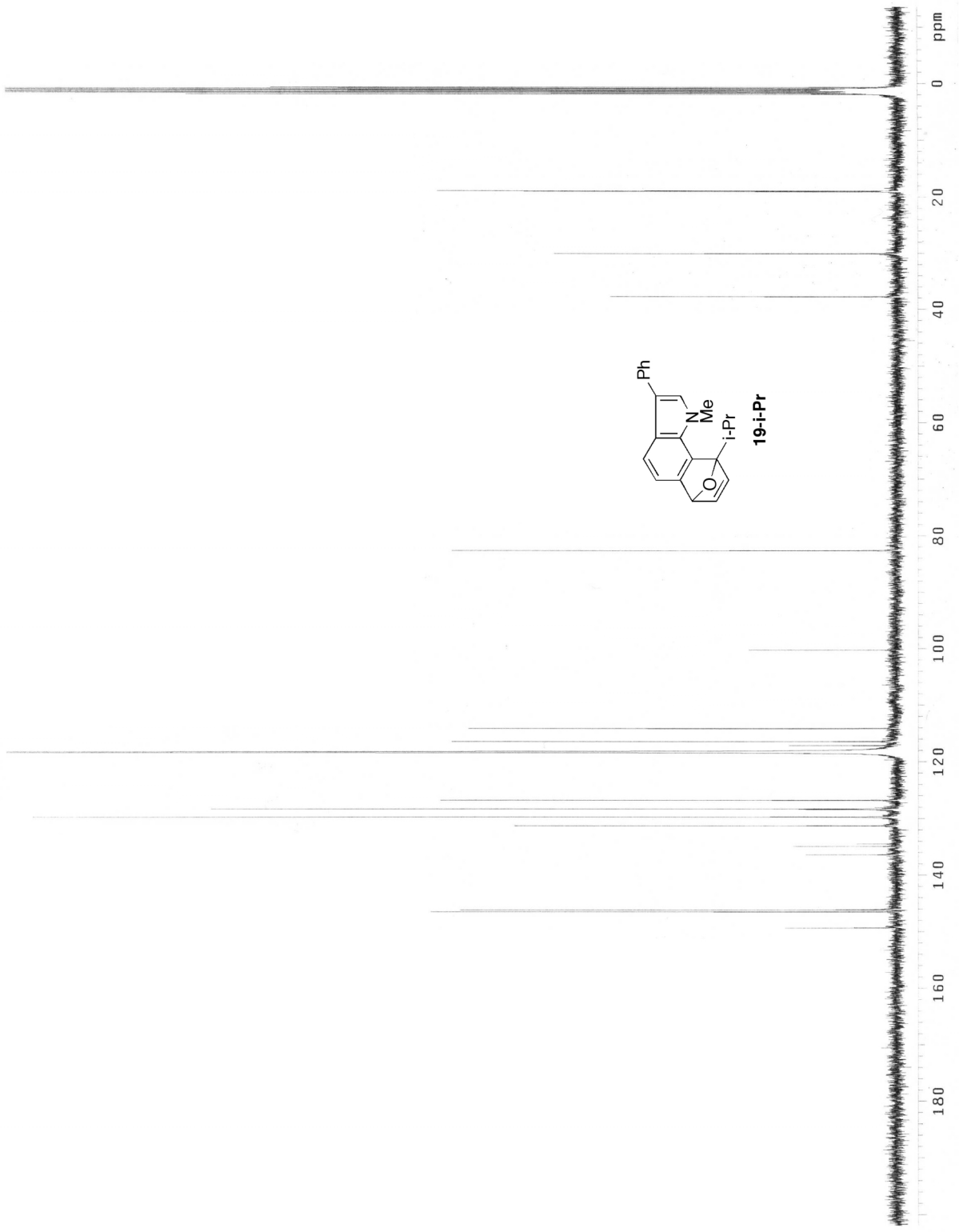
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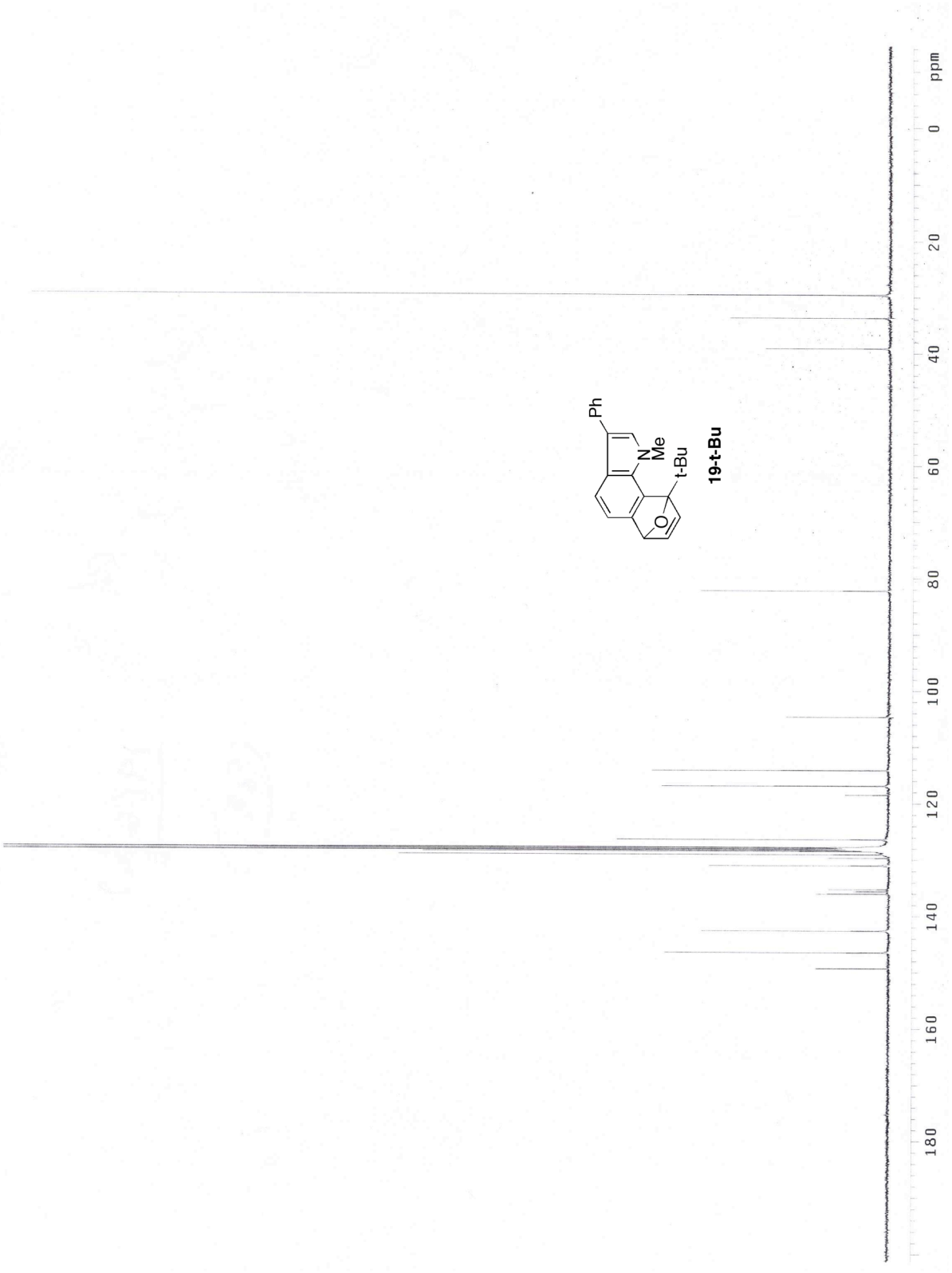
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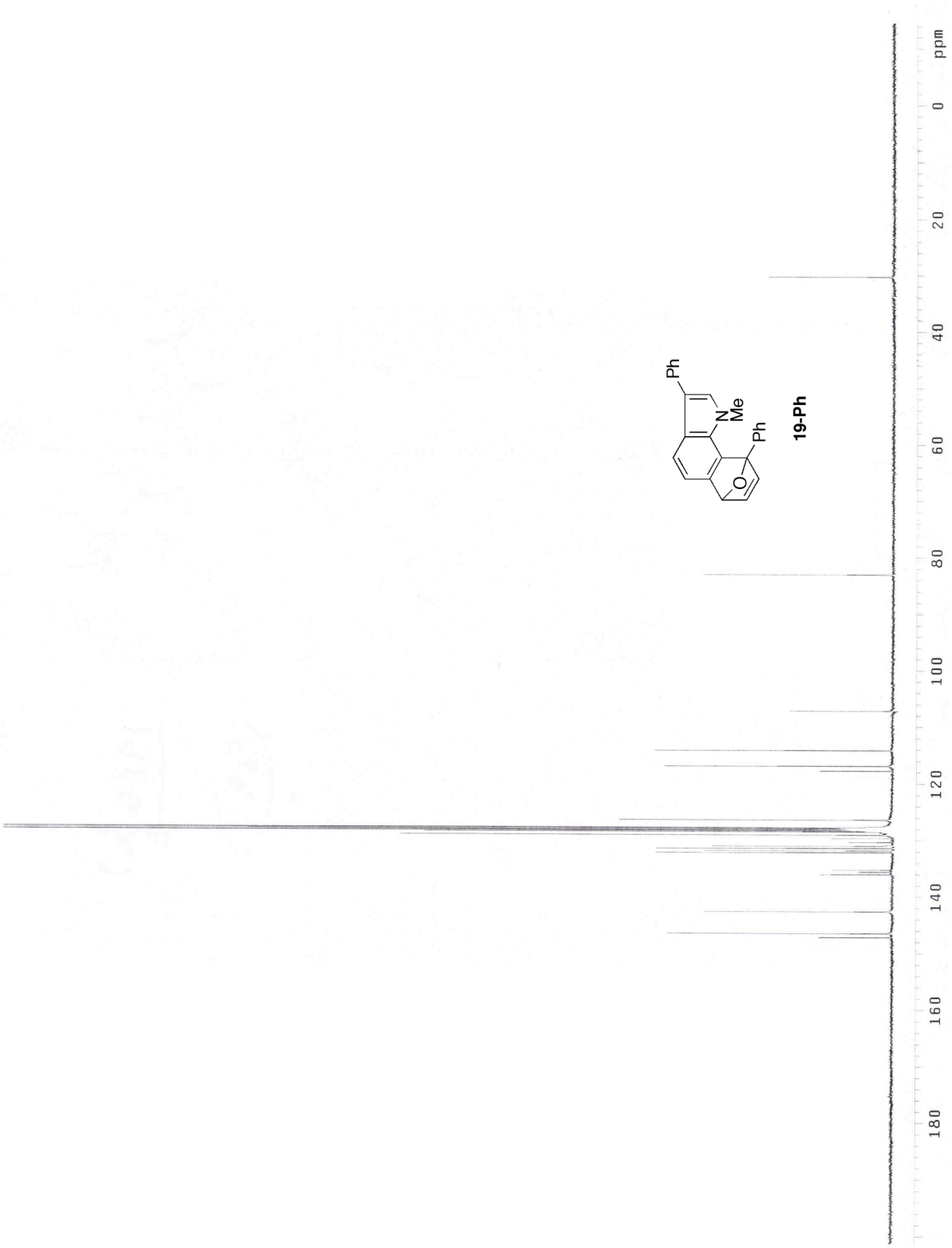
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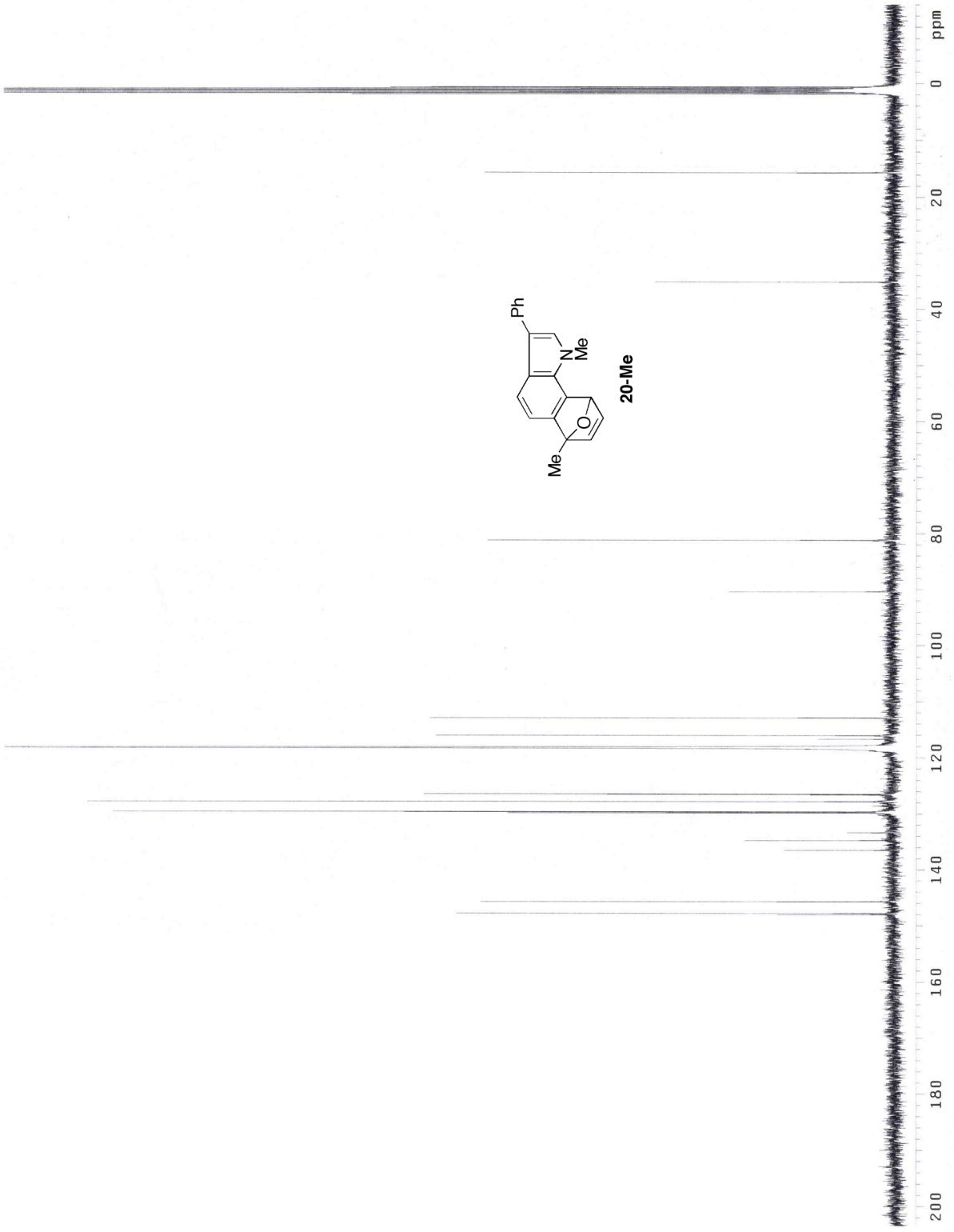
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Me
O
Me
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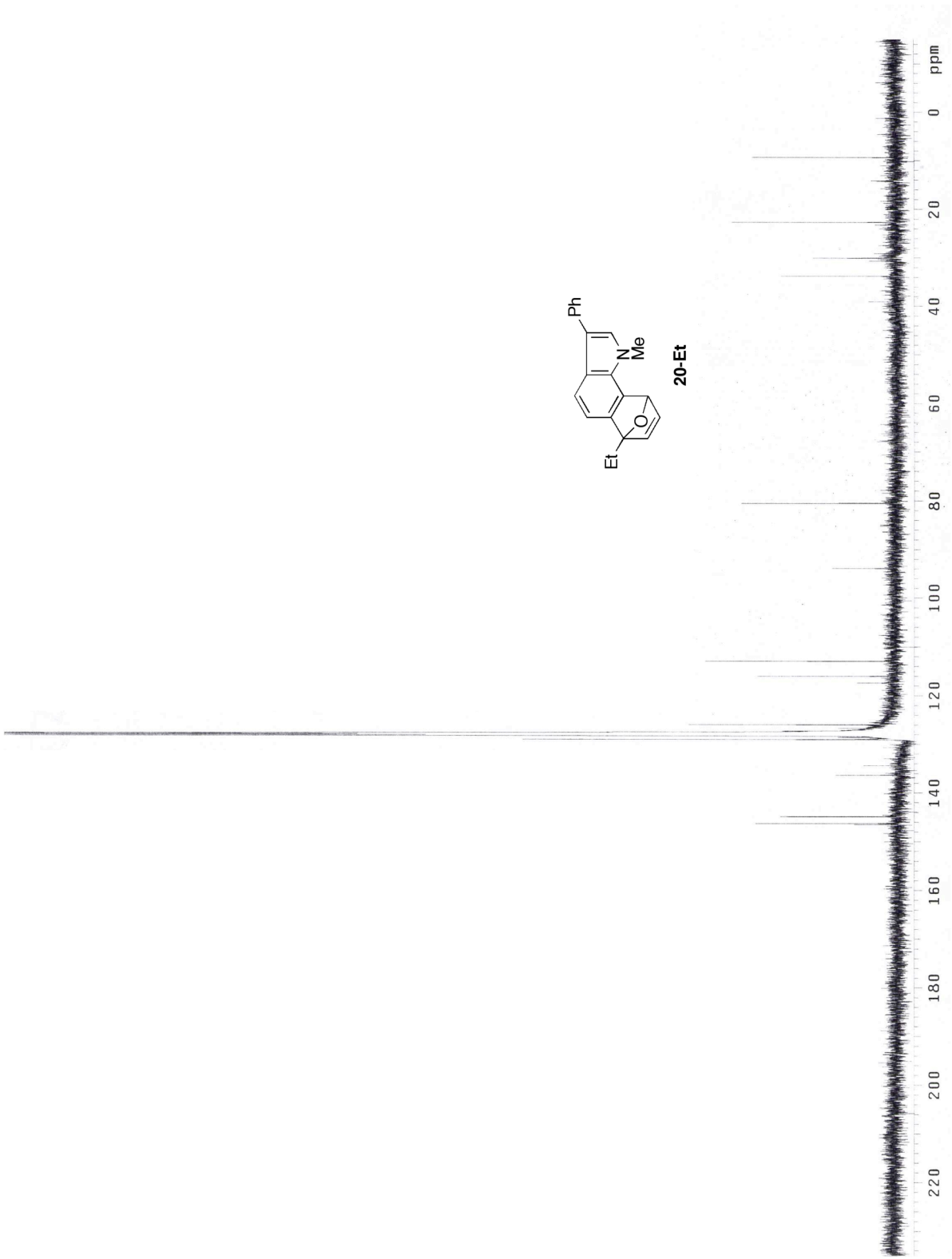
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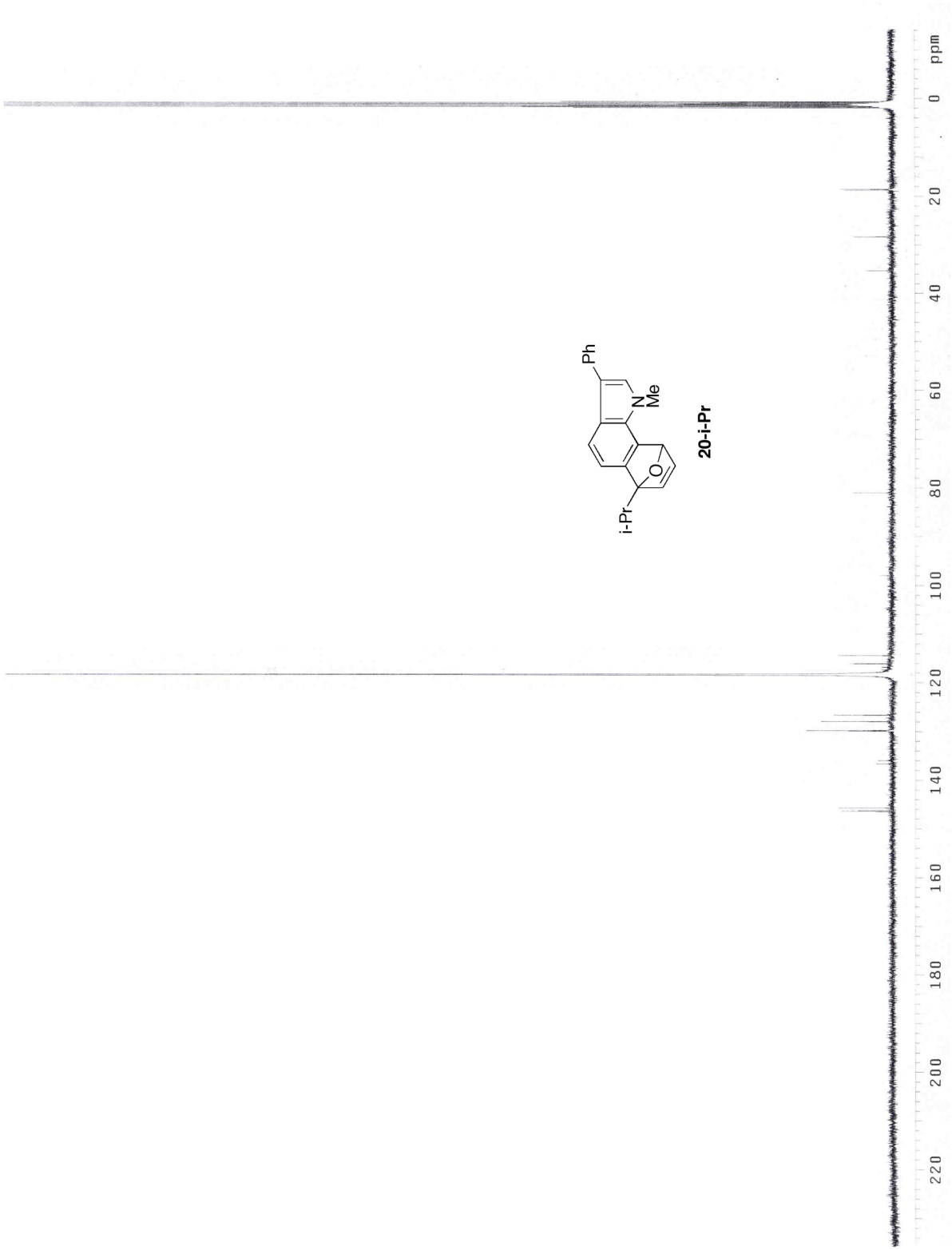
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O
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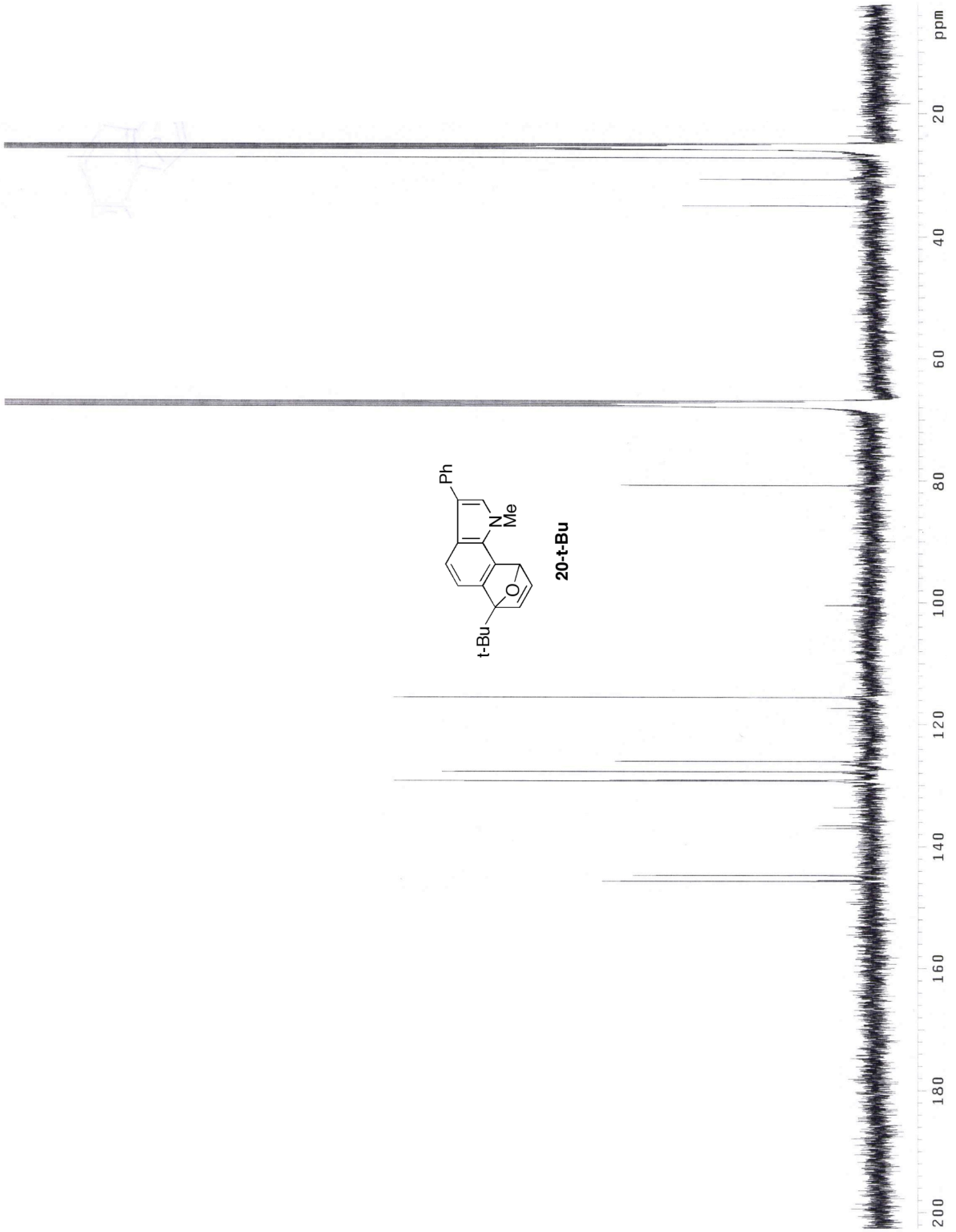
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ppm
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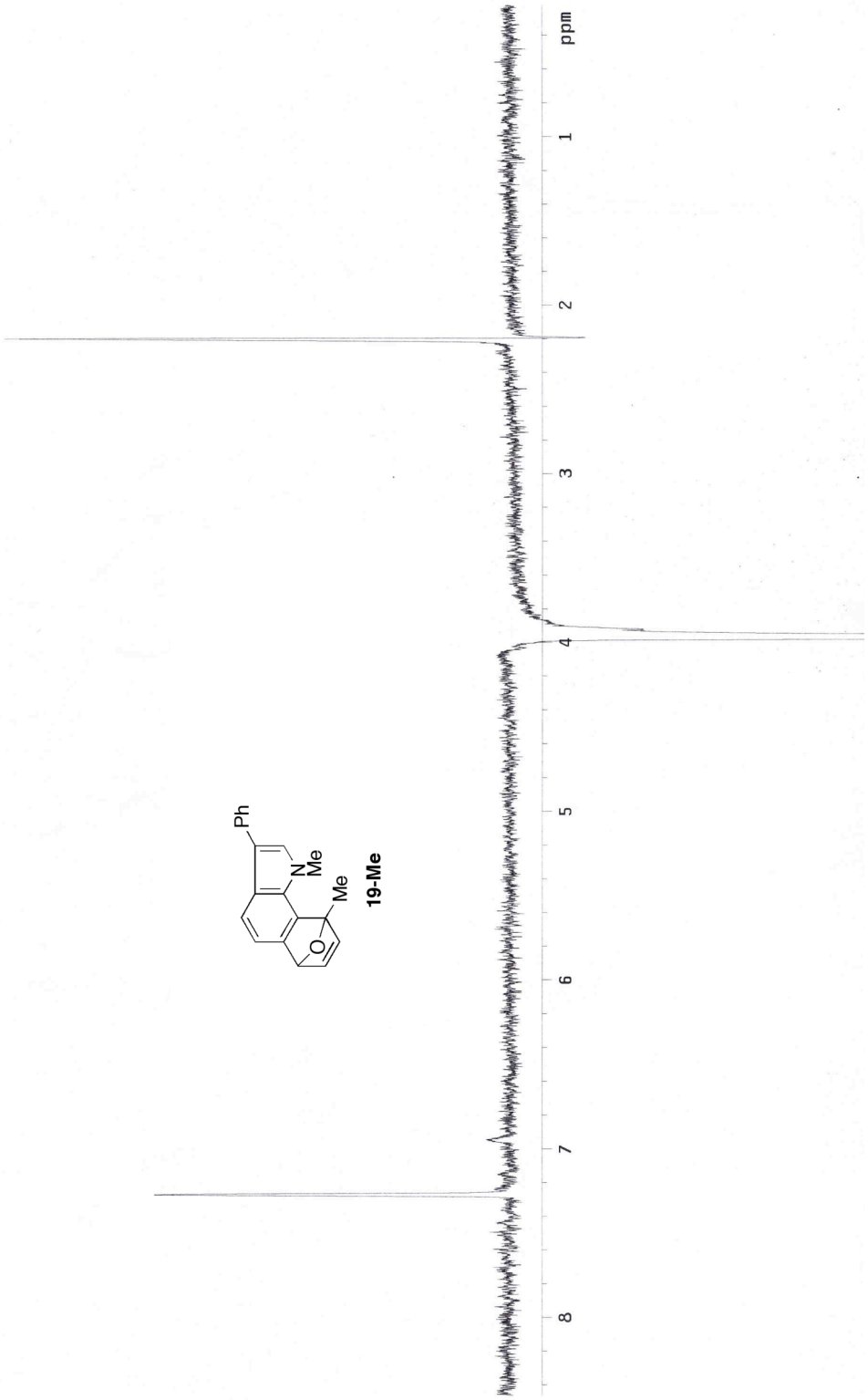
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O
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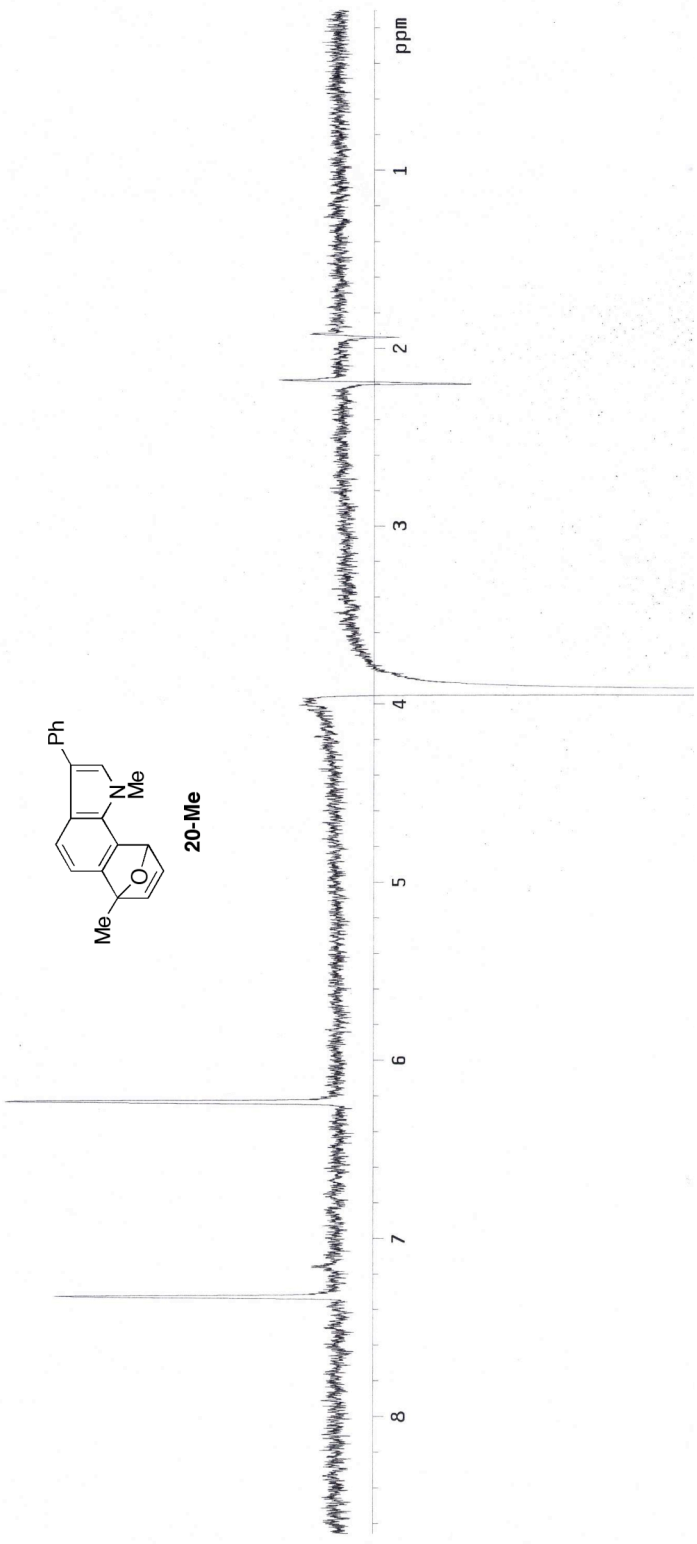
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O
Me
20-Me
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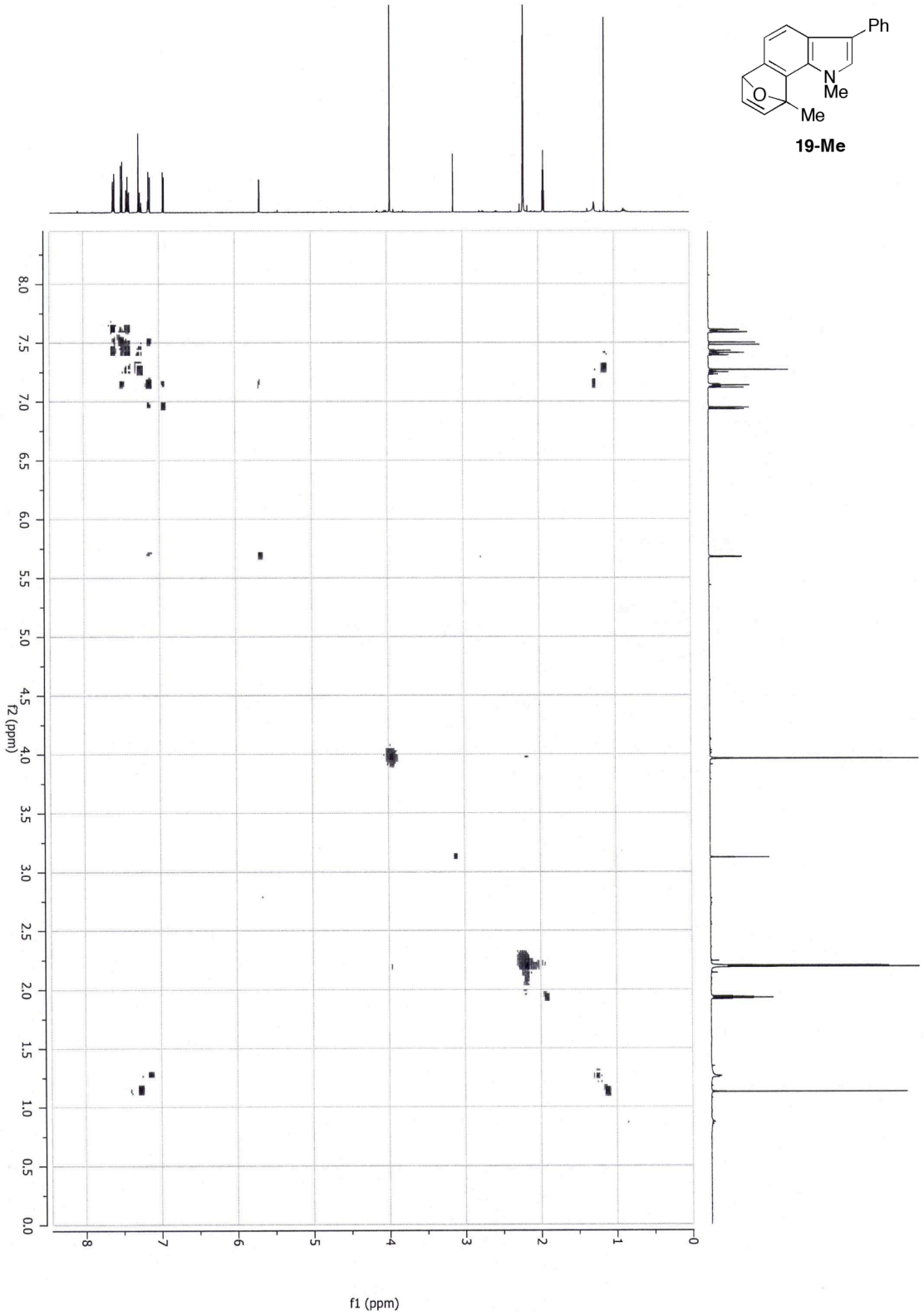
4
3
2
1
ppm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Me
O
Me
19-Me
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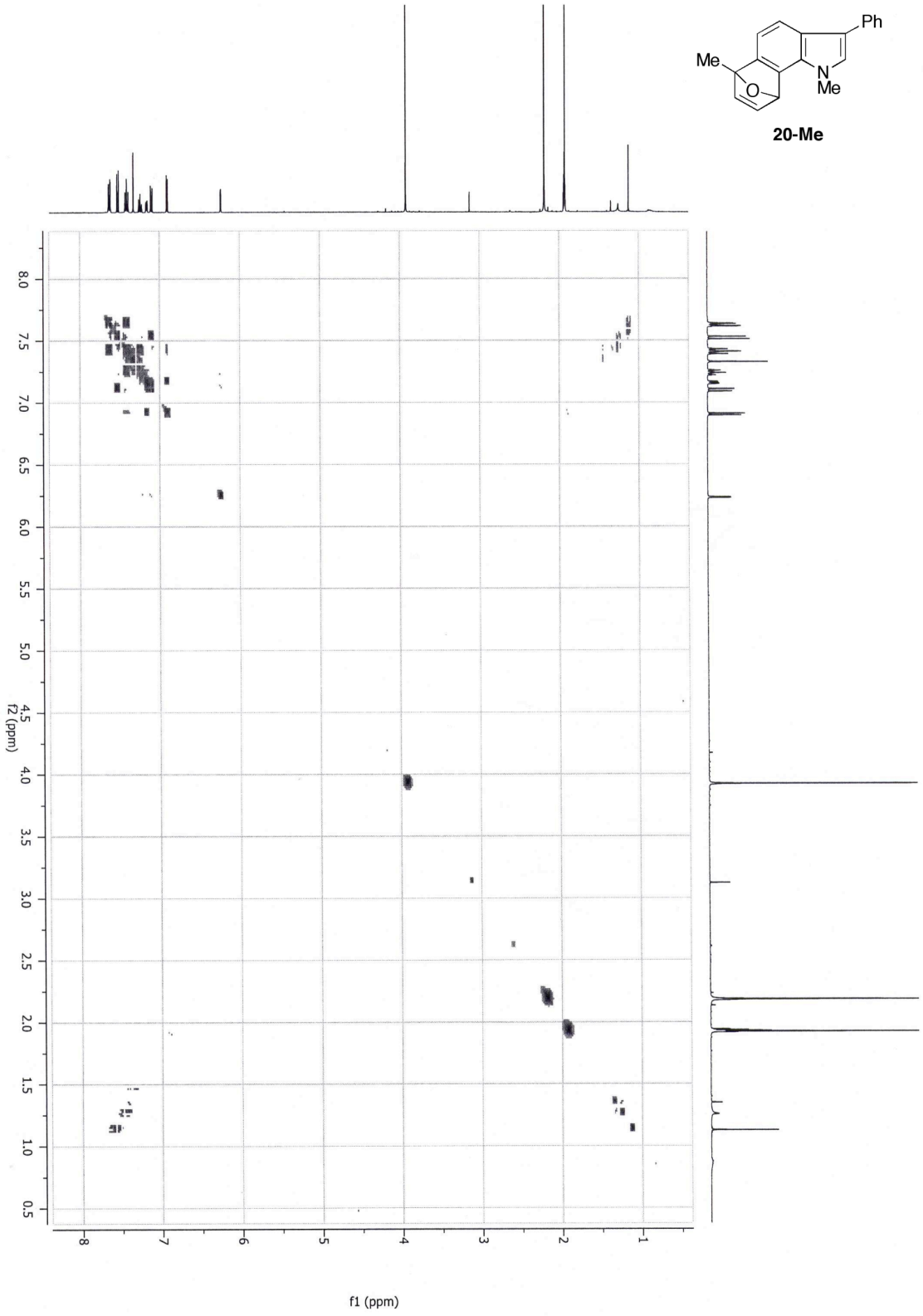
f1 (ppm)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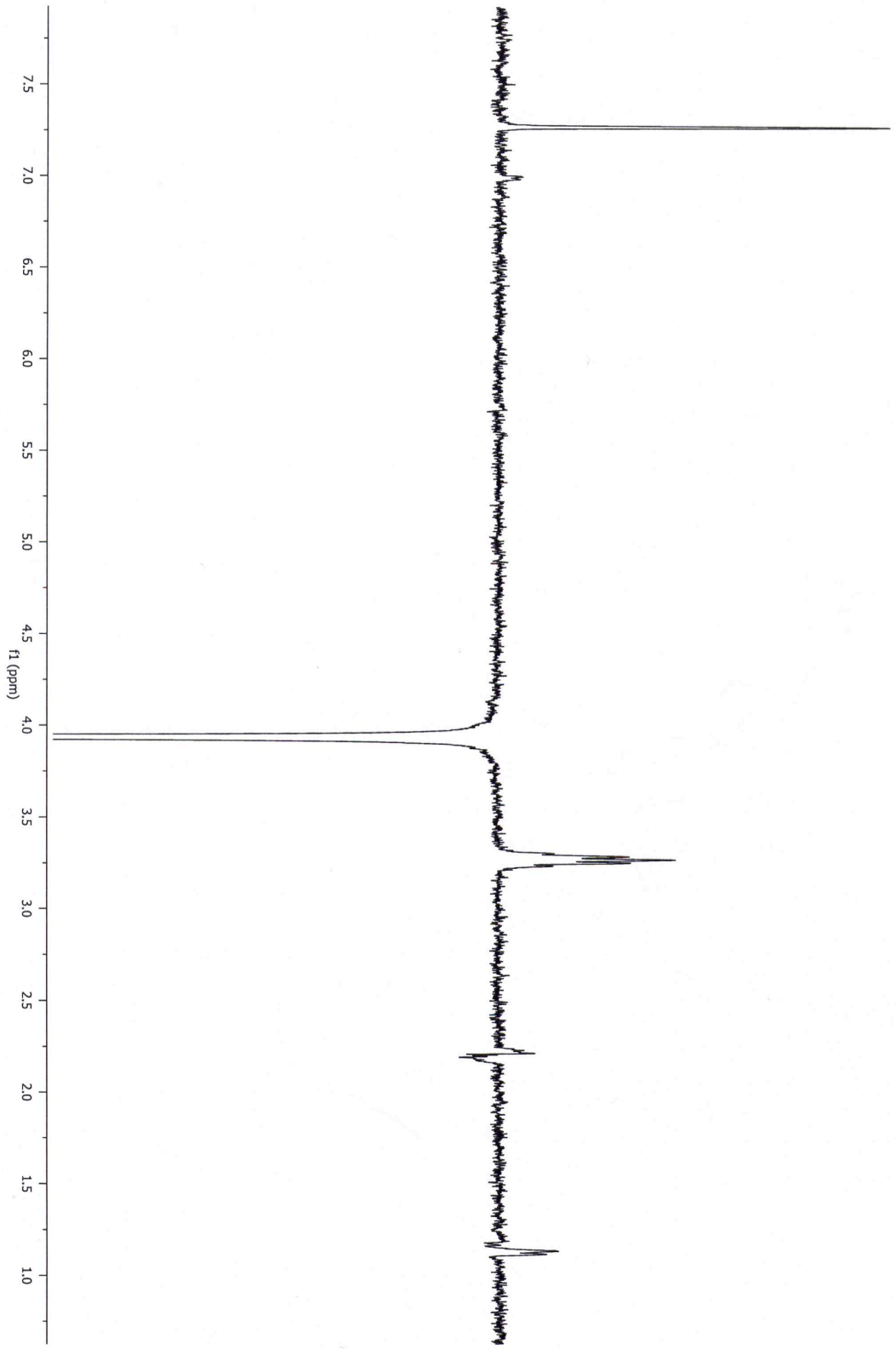
Me
O
20-Me
f2 (ppm)
f1 (ppm)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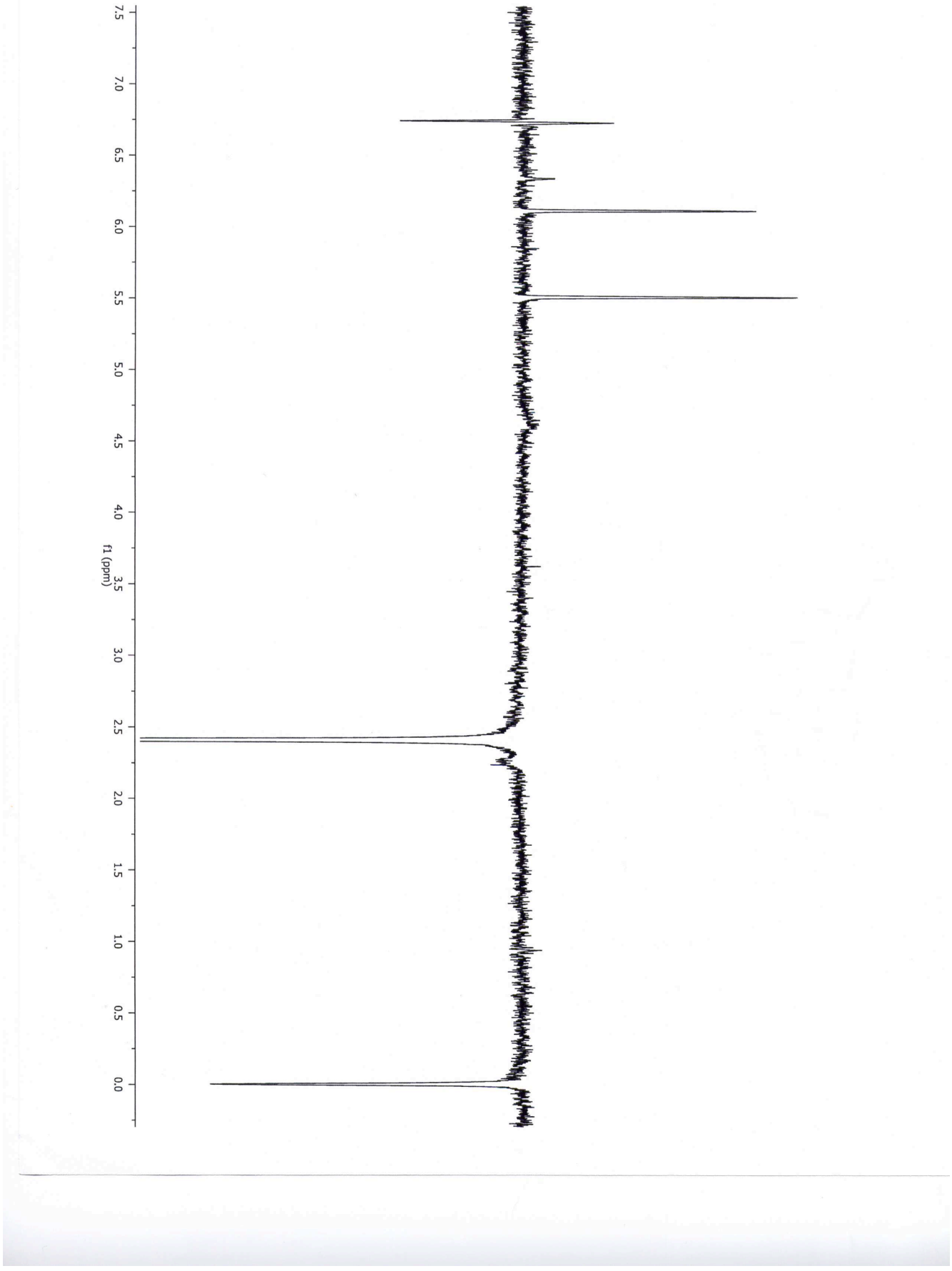
2.0
1.5
1.0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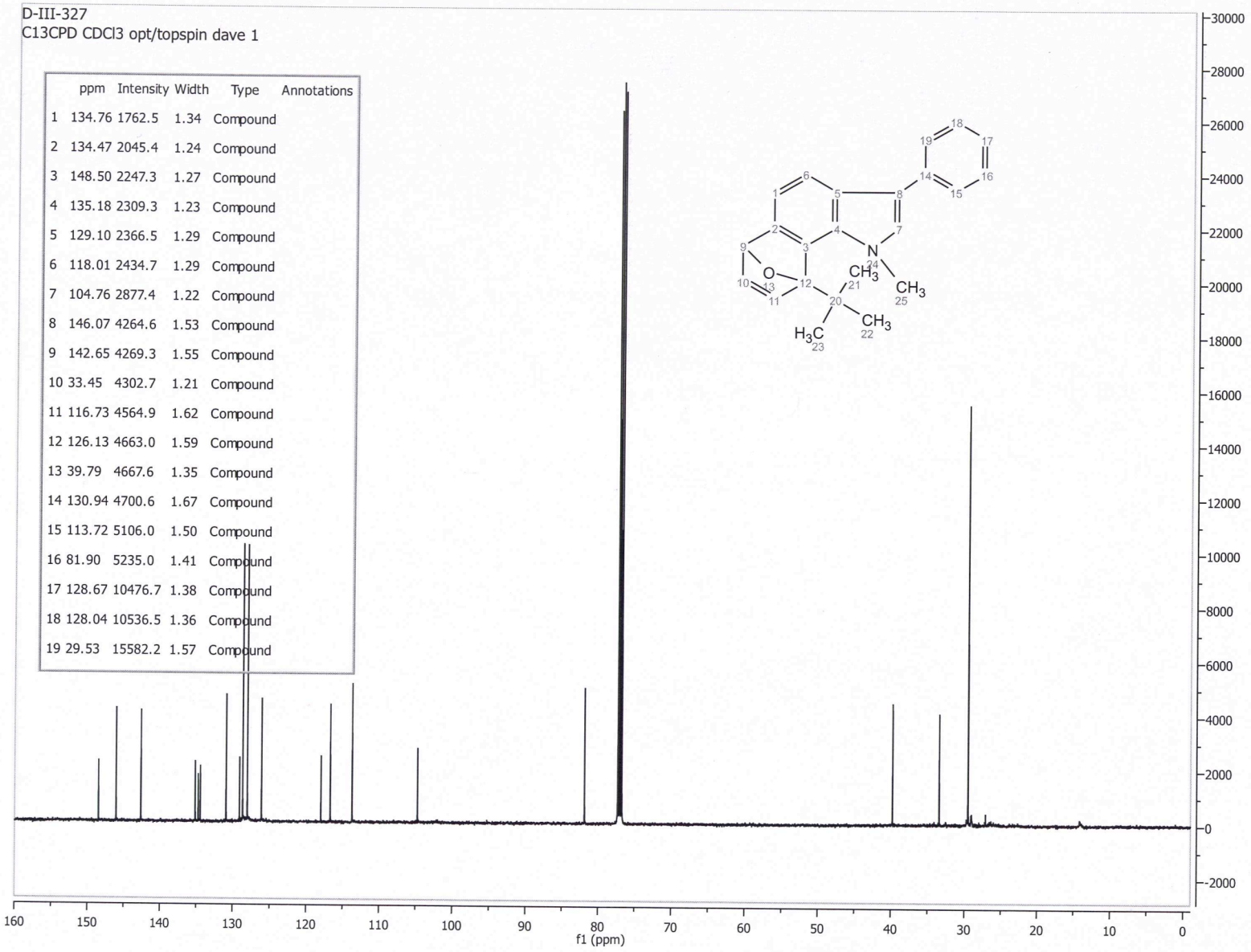
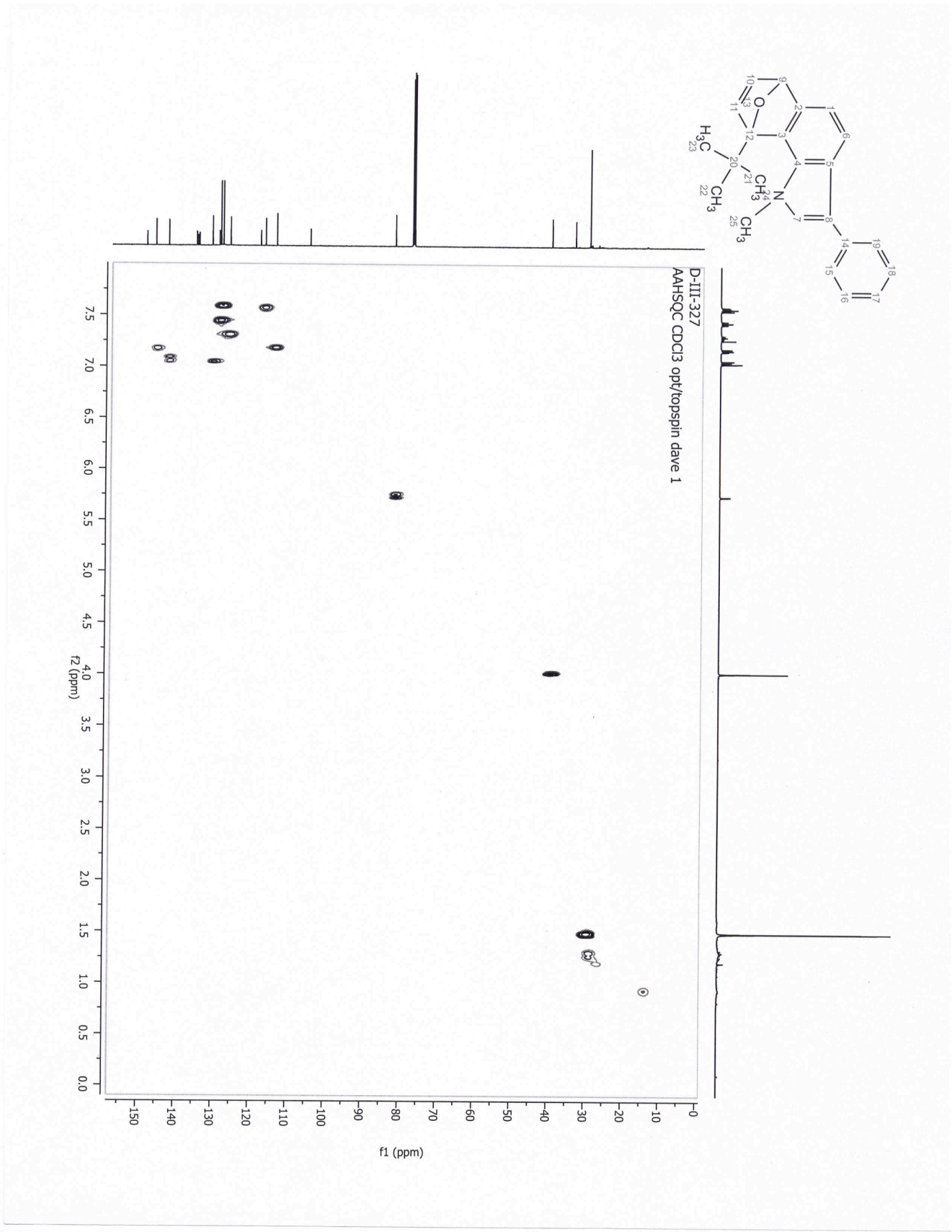
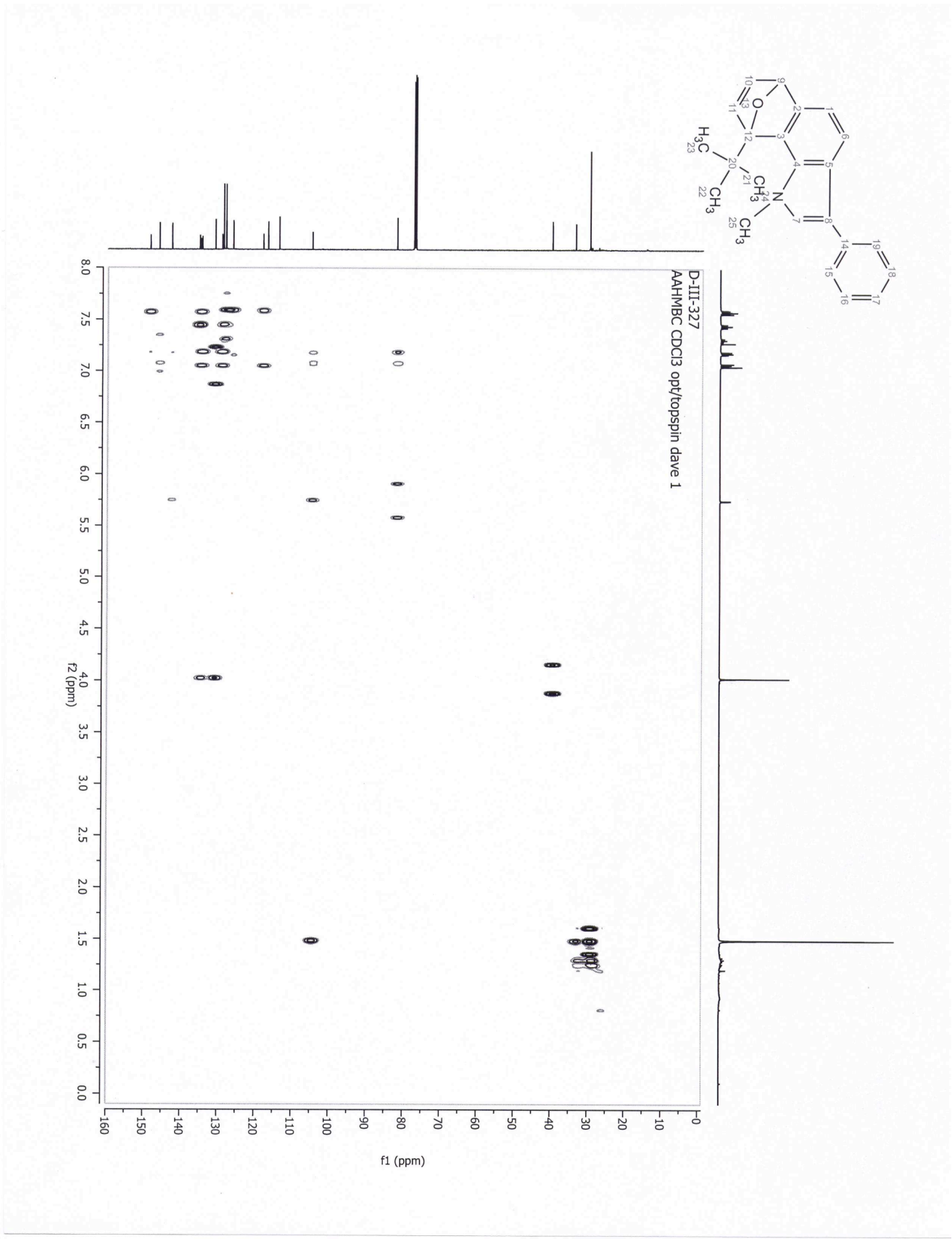
0.0
f1 (ppm)



	ppm	Intensity	Width	Type	Annotations
1	134.76	1762.5	1.34	Compound	
2	134.47	2045.4	1.24	Compound	
3	148.50	2247.3	1.27	Compound	
4	135.18	2309.3	1.23	Compound	
5	129.10	2366.5	1.29	Compound	
6	118.01	2434.7	1.29	Compound	
7	104.76	2877.4	1.22	Compound	
8	146.07	4264.6	1.53	Compound	
9	142.65	4269.3	1.55	Compound	
10	33.45	4302.7	1.21	Compound	
11	116.73	4564.9	1.62	Compound	
12	126.13	4663.0	1.59	Compound	
13	39.79	4667.6	1.35	Compound	
14	130.94	4700.6	1.67	Compound	
15	113.72	5106.0	1.50	Compound	
16	81.90	5235.0	1.41	Compound	
17	128.67	10476.7	1.38	Compound	
18	128.04	10536.5	1.36	Compound	
19	29.53	15582.2	1.57	Compound	


D-III-327
AAHSQC CDCl3 opt/topspin dave 1
f1 (ppm)
f2 (ppm)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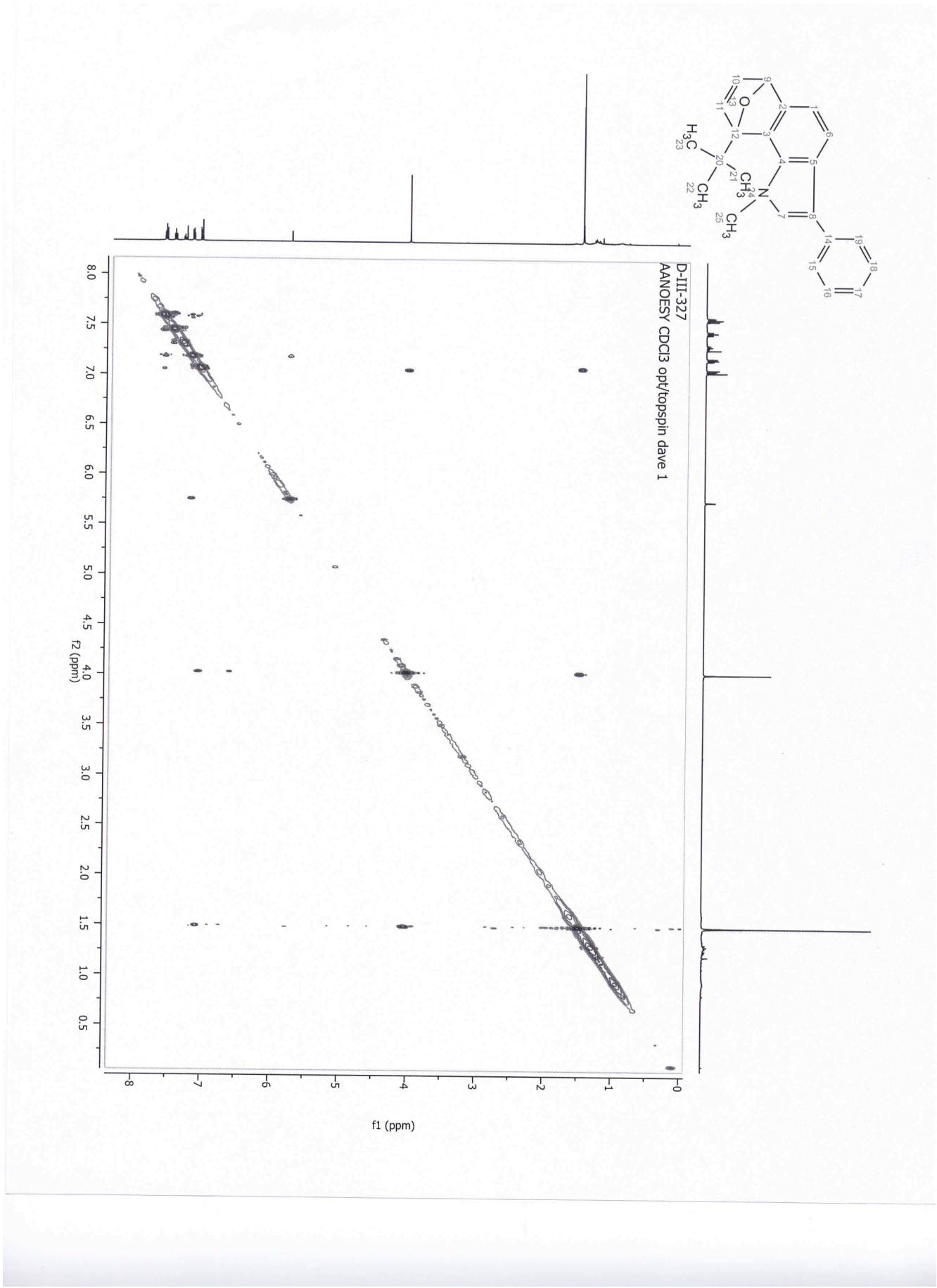
f1 (ppm)
f2 (ppm)


D-III-327
AANOESY CDCl3 opt/topspin dave 1
f1 (ppm)
f2 (ppm)

Furan: E[M06-2X/6-311+G(2df,p)]= -230.00340 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	1.086883	0.346665
2	6	0	0.000000	0.716420	-0.952848
3	6	0	0.000000	-0.716420	-0.952848
4	6	0	0.000000	-1.086883	0.346665
5	8	0	0.000000	0.000000	1.150067
6	1	0	0.000000	2.041866	0.842669
7	1	0	0.000000	1.373450	-1.805839
8	1	0	0.000000	-1.373450	-1.805839
9	1	0	0.000000	-2.041866	0.842669

Me-Furan: E[M06-2X/6-311+G(2df,p)]= -269.31631 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.388716	-0.728538	-0.000013
2	6	0	-1.541657	0.612161	-0.000014
3	6	0	-0.215813	1.158103	0.000026
4	6	0	0.633596	0.103907	0.000016
5	8	0	-0.073267	-1.053611	0.000003
6	1	0	-2.080197	-1.553013	-0.000067
7	1	0	-2.475065	1.149159	0.000176
8	1	0	0.066842	2.197653	-0.000212
9	6	0	2.111686	-0.016742	0.000007
10	1	0	2.560365	0.975015	-0.000178
11	1	0	2.459740	-0.556763	-0.882475
12	1	0	2.459874	-0.556499	0.882595

Et-Furan: E[M06-2X/6-311+G(2df,p)]= -308.62115 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.026503	-0.422831	0.000037
2	6	0	-1.807571	0.908392	0.000067
3	6	0	-0.382607	1.072772	-0.000019
4	6	0	0.146454	-0.174276	-0.000111
5	8	0	-0.849779	-1.094728	-0.000078
6	1	0	-2.916858	-1.027208	0.000039
7	1	0	-2.558653	1.680121	0.000077
8	1	0	0.169429	1.997706	-0.000150
9	6	0	1.538856	-0.696229	0.000087
10	6	0	2.572381	0.422658	-0.000023
11	1	0	2.462374	1.054185	0.882931
12	1	0	2.462463	1.053976	-0.883114
13	1	0	1.675720	-1.338927	-0.874645
14	1	0	1.675575	-1.338545	0.875126
15	1	0	3.582124	0.013607	0.000122

iPr-Furan: E[M06-2X/6-311+G(2df,p)]= -347.92780 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.193844	-0.621087	-0.098703
2	6	0	-2.229141	0.674330	0.276712
3	6	0	-0.869824	1.130397	0.243136
4	6	0	-0.119152	0.073207	-0.151086
5	8	0	-0.920857	-1.002141	-0.360916
6	1	0	-2.949997	-1.376429	-0.224478
7	1	0	-3.106231	1.239187	0.543821
8	1	0	-0.505600	2.116310	0.478509
9	6	0	1.341604	-0.129830	-0.374811
10	6	0	2.100884	1.178318	-0.182794
11	6	0	1.885484	-1.226712	0.545874
12	1	0	1.991652	1.535762	0.843938
13	1	0	3.163979	1.029127	-0.374750
14	1	0	1.736337	1.955200	-0.856379
15	1	0	2.940522	-1.410864	0.335617
16	1	0	1.790869	-0.921484	1.590393
17	1	0	1.338297	-2.159647	0.411945
18	1	0	1.470965	-0.461773	-1.411254

tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -387.23206 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.672492	2.369566	0.000000
2	6	0	-0.672392	2.487991	0.000000
3	6	0	-1.183479	1.150591	0.000000
4	6	0	-0.107553	0.323977	0.000000
5	8	0	1.029042	1.063627	0.000000
6	1	0	1.480303	3.080409	0.000000
7	1	0	-1.234506	3.406620	0.000000
8	1	0	-2.218129	0.848888	0.000000
9	6	0	0.018161	-1.175994	0.000000
10	6	0	-0.672392	-1.736604	1.251461
11	6	0	-0.672392	-1.736604	-1.251461
12	6	0	1.490184	-1.592277	0.000000
13	1	0	-0.200991	-1.354408	2.158633
14	1	0	-1.727375	-1.457269	1.273666
15	1	0	-0.606505	-2.827235	1.259269
16	1	0	-0.200991	-1.354408	-2.158633
17	1	0	-0.606505	-2.827235	-1.259269
18	1	0	-1.727375	-1.457269	-1.273666
19	1	0	1.556835	-2.681937	0.000000
20	1	0	2.008562	-1.214527	-0.882301
21	1	0	2.008562	-1.214527	0.882301

21: E[M06-2X/6-311+G(2df,p)]= -401.75014 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.278989	-1.139979	0.000000
2	6	0	0.000000	0.264734	0.000000
3	6	0	0.984080	1.272076	0.000000
4	6	0	2.335669	0.937476	0.000000
5	6	0	2.504428	-0.444977	0.000000
6	6	0	1.656476	-1.336883	0.000000
7	6	0	-0.966780	-1.822877	0.000000
8	6	0	-1.930717	-0.853932	0.000000
9	1	0	0.694504	2.316398	0.000000
10	1	0	3.113936	1.686171	0.000000
11	1	0	-1.133376	-2.886114	0.000000
12	1	0	-3.004870	-0.954257	0.000000
13	7	0	-1.366232	0.394847	0.000000
14	6	0	-2.078741	1.650524	0.000000
15	1	0	-3.148069	1.449817	0.000000
16	1	0	-1.829466	2.233541	0.888658
17	1	0	-1.829466	2.233541	-0.888658

22: E[M06-2X/6-311+G(2df,p)]= -401.74652 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408965	-0.996811	0.000000
2	6	0	0.000000	0.377356	0.000000
3	6	0	0.888803	1.474188	0.000000
4	6	0	2.171928	0.987383	0.000000
5	6	0	2.528739	-0.201583	0.000000
6	6	0	1.779293	-1.347271	0.000000
7	6	0	-0.795056	-1.774464	0.000000
8	6	0	-1.835213	-0.897094	0.000000
9	1	0	0.565637	2.506444	0.000000
10	1	0	2.125946	-2.371129	0.000000
11	1	0	-0.873022	-2.848634	0.000000
12	1	0	-2.898102	-1.084834	0.000000
13	7	0	-1.372053	0.397072	0.000000
14	6	0	-2.173089	1.595908	0.000000
15	1	0	-3.225080	1.318174	0.000000
16	1	0	-1.968616	2.197407	0.888489
17	1	0	-1.968616	2.197407	-0.888489

23: E[M06-2X/6-311+G(2df,p)]= -401.75143 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.138949	-0.973210	0.000000
2	6	0	0.000000	0.447098	0.000000
3	6	0	1.183561	1.180415	0.000000
4	6	0	2.241950	0.543730	0.000000
5	6	0	2.582759	-0.797939	0.000000
6	6	0	1.418417	-1.565681	0.000000
7	6	0	-1.196309	-1.489982	0.000000
8	6	0	-2.040234	-0.418670	0.000000
9	1	0	3.572058	-1.227708	0.000000
10	1	0	1.510361	-2.645671	0.000000
11	1	0	-1.496098	-2.524819	0.000000
12	1	0	-3.118426	-0.388857	0.000000
13	7	0	-1.326252	0.757621	0.000000
14	6	0	-1.859513	2.099934	0.000000
15	1	0	-2.946165	2.047654	0.000000
16	1	0	-1.527721	2.640942	0.887234
17	1	0	-1.527721	2.640942	-0.887234

27,O: E[M06-2X/6-311+G(2df,p)]= -382.30617 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.466039	-0.763004	0.000000
2	6	0	0.000000	0.569902	0.000000
3	6	0	1.343822	0.963149	0.000000
4	6	0	2.343748	-0.008532	0.000000
5	6	0	1.785949	-1.280684	0.000000
6	6	0	0.608914	-1.643850	0.000000
7	6	0	-1.897801	-0.682494	0.000000
8	6	0	-2.178839	0.636788	0.000000
9	1	0	1.594840	2.015901	0.000000
10	1	0	3.394130	0.241207	0.000000
11	1	0	-2.610201	-1.489129	0.000000
12	1	0	-3.112375	1.173836	0.000000
13	8	0	-1.063116	1.413817	0.000000

28,O: E[M06-2X/6-311+G(2df,p)]= -382.30462 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.256284	-0.726106	0.000000
2	6	0	0.000000	0.669869	0.000000
3	6	0	-1.266998	1.265770	0.000000
4	6	0	-2.197094	0.252144	0.000000
5	6	0	-1.984907	-0.968887	0.000000
6	6	0	-0.799035	-1.660234	0.000000
7	6	0	1.694695	-0.837323	0.000000
8	6	0	2.167745	0.421727	0.000000
9	1	0	-1.420973	2.335204	0.000000
10	1	0	-0.650111	-2.730409	0.000000
11	1	0	2.285776	-1.737543	0.000000
12	1	0	3.169882	0.817294	0.000000
13	8	0	1.173910	1.351712	0.000000

29,O: E[M06-2X/6-311+G(2df,p)]= -382.30728 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.676840	0.000000
2	6	0	-0.391119	-0.679644	0.000000
3	6	0	0.612189	-1.626959	0.000000
4	6	0	1.771258	-1.193857	0.000000
5	6	0	2.359381	0.053105	0.000000
6	6	0	1.360477	1.030914	0.000000
7	6	0	-1.242300	1.409211	0.000000
8	6	0	-2.220686	0.483934	0.000000
9	1	0	3.412204	0.287933	0.000000
10	1	0	1.652007	2.074262	0.000000
11	1	0	-1.382381	2.477200	0.000000
12	1	0	-3.294300	0.565634	0.000000
13	8	0	-1.735341	-0.790787	0.000000

27,S: E[M06-2X/6-311+G(2df,p)]= -705.28893 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.207575	-0.945526	0.000000
2	6	0	0.000000	0.464698	0.000000
3	6	0	1.042190	1.411147	0.000000
4	6	0	2.376844	1.014052	0.000000
5	6	0	2.468350	-0.372349	0.000000
6	6	0	1.572471	-1.215732	0.000000
7	6	0	-1.013422	-1.685199	0.000000
8	6	0	-2.092900	-0.871401	0.000000
9	1	0	0.804077	2.468211	0.000000
10	1	0	3.191111	1.723289	0.000000
11	1	0	-1.065618	-2.763584	0.000000
12	1	0	-3.131322	-1.163874	0.000000
13	16	0	-1.697806	0.808614	0.000000

28,S: E[M06-2X/6-311+G(2df,p)]= -705.28474 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.319496	-0.813911	0.000000
2	6	0	0.000000	0.573993	0.000000
3	6	0	0.966631	1.601425	0.000000
4	6	0	2.213748	1.034744	0.000000
5	6	0	2.499583	-0.172741	0.000000
6	6	0	1.666518	-1.255903	0.000000
7	6	0	-0.868032	-1.625528	0.000000
8	6	0	-2.002855	-0.898654	0.000000
9	1	0	0.710163	2.651656	0.000000
10	1	0	1.931676	-2.304120	0.000000
11	1	0	-0.848563	-2.706368	0.000000
12	1	0	-3.017753	-1.265266	0.000000
13	16	0	-1.721629	0.810222	0.000000

29,S: E[M06-2X/6-311+G(2df,p)]= -705.28785 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.138828	-0.760618	0.000000
2	6	0	0.000000	0.656558	0.000000
3	6	0	1.210897	1.327877	0.000000
4	6	0	2.287206	0.728326	0.000000
5	6	0	2.592221	-0.623124	0.000000
6	6	0	1.415287	-1.366876	0.000000
7	6	0	-1.150752	-1.392592	0.000000
8	6	0	-2.170016	-0.506603	0.000000
9	1	0	3.572351	-1.075186	0.000000
10	1	0	1.480334	-2.448962	0.000000
11	1	0	-1.294938	-2.463949	0.000000
12	1	0	-3.226260	-0.725528	0.000000
13	16	0	-1.654594	1.145996	0.000000

TS for **21 → 24** with Furan: E[M06-2X/6-311+G(2df,p)]= -631.75594 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.902528	-0.768261	-0.056686
2	6	0	-1.787548	0.351528	-0.003352
3	6	0	-1.357068	1.688480	0.000304
4	6	0	0.006391	1.964854	-0.049931
5	6	0	0.780389	0.812655	-0.100961
6	6	0	0.442006	-0.395552	-0.097758
7	6	0	-1.714372	-1.941093	-0.041244
8	6	0	-3.009842	-1.514813	0.019179
9	1	0	-2.073831	2.500243	0.040865
10	1	0	0.378138	2.981098	-0.053987
11	1	0	-1.384695	-2.965683	-0.071903
12	1	0	-3.924031	-2.087307	0.048042
13	7	0	-3.067281	-0.143580	0.043914
14	6	0	-4.263990	0.658189	0.107946
15	1	0	-5.130425	0.000231	0.134594
16	1	0	-4.265565	1.278363	1.006939
17	1	0	-4.341555	1.306432	-0.767592
18	6	0	2.978604	-1.274467	-0.300569
19	6	0	3.226523	-0.883254	0.990362
20	6	0	3.328487	0.514003	0.954950
21	6	0	3.109288	0.878522	-0.355184
22	8	0	3.049801	-0.224062	-1.131638
23	1	0	2.871722	-2.241951	-0.759643
24	1	0	3.258339	-1.527967	1.852004
25	1	0	3.458335	1.189895	1.783553
26	1	0	3.208083	1.819450	-0.869509

TS for **21 → 24a** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -788.99060 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.502760	-0.509586	0.201346
2	6	0	2.706739	0.216602	-0.048398
3	6	0	0.448638	1.522447	-0.103505
4	6	0	0.367760	0.301095	0.152416
5	6	0	1.873279	-1.868457	0.426940
6	6	0	3.233318	-1.921433	0.313797
7	1	0	1.223191	-2.699303	0.644933
8	1	0	3.901535	-2.762664	0.414290
9	7	0	3.744178	-0.679603	0.031602
10	6	0	5.136326	-0.353983	-0.157199
11	1	0	5.731656	-1.256302	-0.031971
12	1	0	5.307026	0.044039	-1.159788
13	1	0	5.461537	0.386773	0.576376
14	6	0	-1.864596	2.306642	-0.299093
15	6	0	-2.028409	2.252235	1.059960
16	6	0	-2.341807	0.914789	1.359225
17	6	0	-2.372546	0.241900	0.161943
18	8	0	-2.191961	1.116452	-0.848268
19	1	0	-1.704282	3.121494	-0.984142
20	1	0	-1.860360	3.062939	1.749156
21	1	0	-2.465522	0.474098	2.333914
22	6	0	-2.759720	-1.160838	-0.202755
23	6	0	-4.250627	-1.167517	-0.581547
24	1	0	-4.864941	-0.822700	0.252271
25	1	0	-4.433862	-0.515075	-1.437073
26	1	0	-4.562871	-2.179881	-0.848063
27	6	0	-2.528351	-2.068790	1.005003
28	1	0	-2.780397	-3.098675	0.744527
29	1	0	-1.482411	-2.031723	1.317113
30	1	0	-3.153384	-1.775141	1.850933
31	6	0	1.557532	2.318991	-0.358786
32	1	0	1.546938	3.379330	-0.572930
33	6	0	2.746300	1.594331	-0.322000
34	1	0	3.690237	2.093679	-0.506723
35	6	0	-1.932806	-1.657995	-1.392394
36	1	0	-0.872346	-1.698121	-1.139890
37	1	0	-2.267115	-2.659201	-1.673421
38	1	0	-2.050920	-1.000571	-2.254305

TS for **21 → 24b** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -788.98956 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.029785	0.721482	-0.138451
2	6	0	2.719173	-0.513391	0.062507
3	6	0	2.077736	-1.728237	0.356729
4	6	0	0.690711	-1.763335	0.467332
5	6	0	0.075980	-0.524411	0.272188
6	6	0	0.659868	0.548533	0.003542
7	6	0	3.014250	1.712595	-0.421159
8	6	0	4.222179	1.076200	-0.382031
9	1	0	2.656280	-2.633819	0.498842
10	1	0	0.176490	-2.690719	0.688331
11	1	0	2.855358	2.757996	-0.624574
12	1	0	5.213879	1.470956	-0.539655
13	7	0	4.059363	-0.254627	-0.093150
14	6	0	5.109746	-1.235906	0.025346
15	1	0	6.068924	-0.750542	-0.143897
16	1	0	5.110901	-1.680059	1.022932
17	1	0	4.981194	-2.029398	-0.713849
18	6	0	-1.158060	2.191599	-0.251314
19	6	0	-1.383149	2.199127	1.101528
20	6	0	-2.168376	1.067339	1.367960
21	6	0	-2.394155	0.450045	0.157880
22	8	0	-1.881666	1.210319	-0.831177
23	1	0	-0.683750	2.892741	-0.916262
24	1	0	-0.953768	2.888814	1.808842
25	1	0	-2.479979	0.698837	2.330785
26	6	0	-3.278129	-0.695202	-0.241784
27	6	0	-4.667001	-0.134055	-0.591691
28	1	0	-4.599267	0.574048	-1.419470
29	1	0	-5.333973	-0.946911	-0.888250
30	1	0	-5.105549	0.379834	0.265645
31	6	0	-3.394934	-1.666057	0.933344
32	1	0	-4.019706	-2.514995	0.648791
33	1	0	-2.410337	-2.037525	1.224636
34	1	0	-3.854882	-1.188760	1.801079
35	6	0	-2.703808	-1.419981	-1.462190
36	1	0	-1.724808	-1.845018	-1.237516
37	1	0	-3.379671	-2.225434	-1.757735
38	1	0	-2.590454	-0.738281	-2.305630

TS for **22** → **25** with Furan: E[M06-2X/6-311+G(2df,p)]= -631.75330 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.448783	1.108919	-0.014856
2	6	0	-1.684061	-0.299342	-0.018709
3	6	0	-0.661507	-1.268762	-0.067932
4	6	0	0.580159	-0.678076	-0.106638
5	6	0	0.766073	0.573074	-0.108819
6	6	0	-0.126645	1.606391	-0.062783
7	6	0	-2.736549	1.735429	0.045137
8	6	0	-3.662340	0.737238	0.075680
9	1	0	-0.872312	-2.331986	-0.069206
10	1	0	0.096790	2.666069	-0.067164
11	1	0	-2.945428	2.792043	0.063543
12	1	0	-4.739300	0.793239	0.121176
13	7	0	-3.043792	-0.489131	0.038441
14	6	0	-3.690150	-1.776882	0.051711
15	1	0	-4.767844	-1.631983	0.095125
16	1	0	-3.447633	-2.340997	-0.851773
17	1	0	-3.378254	-2.357851	0.922710
18	6	0	3.243529	-1.218557	-0.289577
19	6	0	3.422733	-0.789160	0.998473
20	6	0	3.345035	0.611747	0.951003
21	6	0	3.101333	0.934249	-0.363252
22	8	0	3.177369	-0.173866	-1.129152
23	1	0	3.262698	-2.195085	-0.741476
24	1	0	3.532215	-1.416865	1.866278
25	1	0	3.381471	1.305453	1.774161
26	1	0	3.072231	1.875192	-0.885873

TS for **22** → **25a** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -788.98675 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.227488	-1.138967	0.252892
2	6	0	2.713682	0.163919	-0.071995
3	6	0	1.882434	1.286953	-0.267151
4	6	0	0.574265	0.921459	-0.088353
5	6	0	0.117299	-0.217470	0.201042
6	6	0	0.840270	-1.367352	0.397451
7	6	0	3.381409	-1.983055	0.364990
8	6	0	4.470183	-1.204797	0.116343
9	1	0	2.265494	2.267238	-0.523608
10	1	0	0.445722	-2.349350	0.632465
11	1	0	3.396544	-3.034208	0.600235
12	1	0	5.518104	-1.463114	0.102501
13	7	0	4.082855	0.087837	-0.147647
14	6	0	4.948389	1.197007	-0.457548
15	1	0	5.981318	0.854737	-0.444873
16	1	0	4.724093	1.599116	-1.448341
17	1	0	4.834209	1.995100	0.279759
18	6	0	-1.517488	2.329808	-0.269629
19	6	0	-1.681869	2.287290	1.088458
20	6	0	-2.284687	1.048143	1.365527
21	6	0	-2.469204	0.420086	0.155835
22	8	0	-2.100341	1.254089	-0.838947
23	1	0	-1.334126	3.025913	1.791059
24	1	0	-2.505407	0.629248	2.332867
25	6	0	-3.197974	-0.833637	-0.231478
26	6	0	-3.152884	-1.815540	0.939390
27	1	0	-3.654480	-1.409305	1.820127
28	1	0	-3.660771	-2.741578	0.662967
29	1	0	-2.120471	-2.049422	1.207114
30	6	0	-4.658522	-0.465380	-0.543665
31	1	0	-4.708437	0.246860	-1.369139
32	1	0	-5.216152	-1.360781	-0.827928
33	1	0	-5.140861	-0.017516	0.327090
34	6	0	-2.561844	-1.468976	-1.471057
35	1	0	-1.530178	-1.762256	-1.273619
36	1	0	-3.131873	-2.355317	-1.757973
37	1	0	-2.560768	-0.773622	-2.311014
38	1	0	-1.164901	3.093743	-0.940890

TS for **22** → **25b** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -788.98730 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.746712	-1.015808	-0.207966
2	6	0	2.562155	0.375222	0.058872
3	6	0	1.303350	0.979986	0.252721
4	6	0	0.286893	0.055649	0.160950
5	6	0	0.481195	-1.166574	-0.084315
6	6	0	1.628401	-1.876975	-0.291825
7	6	0	4.159480	-1.220310	-0.337718
8	6	0	4.754177	-0.009394	-0.152475
9	1	0	1.195876	2.040881	0.451364
10	1	0	1.719464	-2.935496	-0.500340
11	1	0	4.665902	-2.148952	-0.541455
12	1	0	5.799722	0.258133	-0.171159
13	7	0	3.806841	0.956554	0.087086
14	6	0	4.050359	2.356451	0.326428
15	1	0	5.122520	2.540142	0.294641
16	1	0	3.565934	2.969993	-0.436656
17	1	0	3.672074	2.652732	1.307502
18	6	0	-2.539956	-0.297042	0.174434
19	6	0	-2.388987	-0.967502	1.360422
20	6	0	-1.859619	-2.233789	1.041346
21	6	0	-1.698792	-2.244068	-0.317296
22	8	0	-2.207189	-1.110313	-0.848582
23	1	0	-2.583778	-0.568540	2.341323
24	1	0	-1.561237	-3.016401	1.718832
25	1	0	-1.406267	-3.010016	-1.014994
26	6	0	-3.144160	1.030297	-0.174487
27	6	0	-4.599502	0.799162	-0.615675
28	1	0	-5.066068	1.752348	-0.874698
29	1	0	-4.638380	0.148491	-1.490943
30	1	0	-5.178929	0.335153	0.184599
31	6	0	-3.114324	1.929919	1.060641
32	1	0	-2.089141	2.067256	1.411143
33	1	0	-3.532881	2.907546	0.813809
34	1	0	-3.706619	1.508327	1.875451
35	6	0	-2.367101	1.690427	-1.317756
36	1	0	-2.847321	2.633719	-1.587443
37	1	0	-1.336619	1.888505	-1.020483
38	1	0	-2.346326	1.048900	-2.199247

TS for **23** → **26** with Furan: E[M06-2X/6-311+G(2df,p)]= -631.75974 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.931655	-1.103771	0.024792
2	6	0	1.283304	0.164329	-0.012910
3	6	0	-0.108468	0.228893	-0.059201
4	6	0	-0.674024	-0.899900	-0.091326
5	6	0	-0.226485	-2.212021	-0.052135
6	6	0	1.160897	-2.281417	0.006821
7	6	0	3.335697	-0.833449	0.086345
8	6	0	3.478509	0.523627	0.082786
9	1	0	-0.849690	-3.095361	-0.078242
10	1	0	1.644892	-3.250651	0.033874
11	1	0	4.139487	-1.549496	0.136613
12	1	0	4.375080	1.122968	0.118444
13	7	0	2.249876	1.135104	0.032211
14	6	0	1.999306	2.552030	-0.064258
15	1	0	2.756296	3.097659	0.498013
16	1	0	2.010110	2.889980	-1.103106
17	1	0	1.018086	2.759481	0.361127
18	6	0	-2.703929	1.460891	-0.223315
19	6	0	-2.964022	0.979878	1.028731
20	6	0	-3.103380	-0.411198	0.881822
21	6	0	-2.888125	-0.678635	-0.451680
22	8	0	-2.768773	0.481161	-1.134618
23	1	0	-2.538233	2.454522	-0.602655
24	1	0	-2.988450	1.554221	1.938686
25	1	0	-3.264728	-1.146106	1.652891
26	1	0	-3.027411	-1.567791	-1.043013

TS for **23 → 26a** with Me-Furan: E[M06-2X/6-311+G(2df,p)]= -671.07348 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.024658	-1.204534	0.106200
2	6	0	1.518920	0.122785	0.000260
3	6	0	0.144238	0.343105	0.036096
4	6	0	-0.554531	-0.707461	0.134765
5	6	0	-0.243166	-2.054841	0.257439
6	6	0	1.128491	-2.281357	0.237813
7	6	0	3.450955	-1.094587	0.056850
8	6	0	3.742005	0.232304	-0.072801
9	1	0	-0.954616	-2.864668	0.344431
10	1	0	1.502499	-3.295113	0.321298
11	1	0	4.172489	-1.892682	0.118670
12	1	0	4.699442	0.724723	-0.144887
13	7	0	2.587748	0.975862	-0.098961
14	6	0	2.487605	2.400126	-0.300469
15	1	0	3.346110	2.895649	0.151519
16	1	0	2.445859	2.651848	-1.362863
17	1	0	1.575933	2.754704	0.179237
18	6	0	-2.152864	1.867543	-0.154559
19	6	0	-2.442088	1.540887	1.141799
20	6	0	-2.820228	0.191194	1.115589
21	6	0	-2.726181	-0.225886	-0.201168
22	8	0	-2.447807	0.850393	-0.978010
23	1	0	-1.837274	2.784344	-0.621947
24	1	0	-2.312509	2.176159	2.001088
25	1	0	-3.065152	-0.445190	1.950608
26	6	0	-3.228826	-1.441187	-0.894733
27	1	0	-3.300568	-2.263890	-0.184712
28	1	0	-2.556578	-1.729402	-1.702323
29	1	0	-4.221337	-1.259206	-1.311790

TS for **23 → 26b** with Me-Furan: E[M06-2X/6-311+G(2df,p)]= -671.07390 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.332546	-0.982981	-0.044976
2	6	0	1.495461	0.168179	0.024320
3	6	0	0.109774	0.005568	0.017128
4	6	0	-0.257416	-1.189753	-0.068402
5	6	0	0.370854	-2.420403	-0.136698
6	6	0	1.754731	-2.265026	-0.122076
7	6	0	3.678769	-0.497264	-0.008517
8	6	0	3.608509	0.862619	0.076809
9	1	0	-0.108551	-3.386447	-0.201235
10	1	0	2.385834	-3.144538	-0.173921
11	1	0	4.585856	-1.078527	-0.032670
12	1	0	4.401416	1.592664	0.126575
13	7	0	2.297744	1.274515	0.105748
14	6	0	1.822251	2.635965	0.112943
15	1	0	2.528220	3.267206	0.651085
16	1	0	1.698044	3.020776	-0.902109
17	1	0	0.858007	2.665717	0.619913
18	6	0	-2.759609	0.868961	-0.027132
19	6	0	-2.894372	0.245023	1.176760
20	6	0	-2.853777	-1.145659	0.912403
21	6	0	-2.686822	-1.267448	-0.436842
22	8	0	-2.698687	-0.046981	-1.016095
23	1	0	-2.965426	0.732220	2.134545
24	1	0	-2.895738	-1.956203	1.620825
25	1	0	-2.674343	-2.113087	-1.102911
26	6	0	-2.738853	2.295048	-0.433074
27	1	0	-1.865689	2.500079	-1.052736
28	1	0	-3.632694	2.549677	-1.006660
29	1	0	-2.701940	2.927745	0.451953

TS for **23** → **26a** with Et-Furan: E[M06-2X/6-311+G(2df,p)]= -710.37823 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.274471	-1.287827	0.115812
2	6	0	1.859659	0.066788	-0.031375
3	6	0	0.509815	0.390458	0.083644
4	6	0	-0.251581	-0.597451	0.289637
5	6	0	-0.032321	-1.956578	0.467692
6	6	0	1.314978	-2.285750	0.368444
7	6	0	3.697739	-1.289319	-0.035805
8	6	0	4.073909	0.003081	-0.259952
9	1	0	-0.792296	-2.704228	0.648571
10	1	0	1.620569	-3.319155	0.483661
11	1	0	4.362193	-2.135823	0.021979
12	1	0	5.056851	0.416774	-0.424398
13	7	0	2.977407	0.829954	-0.250743
14	6	0	2.967508	2.245394	-0.525941
15	1	0	3.876907	2.702041	-0.136680
16	1	0	2.896370	2.444028	-1.597954
17	1	0	2.104245	2.687594	-0.029880
18	6	0	-1.702202	2.080904	-0.037358
19	6	0	-1.917671	1.841490	1.290921
20	6	0	-2.389026	0.521693	1.365384
21	6	0	-2.418383	0.032867	0.071534
22	8	0	-2.118099	1.044484	-0.781109
23	1	0	-1.356780	2.946812	-0.575441
24	1	0	-1.685986	2.509433	2.102694
25	1	0	-2.618087	-0.051719	2.249267
26	6	0	-3.061713	-1.173664	-0.520094
27	6	0	-4.480518	-0.882795	-1.013700
28	1	0	-5.114098	-0.543761	-0.193017
29	1	0	-4.467538	-0.103606	-1.776108
30	1	0	-4.927115	-1.777869	-1.447474
31	1	0	-3.079083	-1.951165	0.246025
32	1	0	-2.441191	-1.540668	-1.340234

TS for **23 → 26b** with Et-Furan: E[M06-2X/6-311+G(2df,p)]= -710.37834 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.769371	-0.682530	-0.164307
2	6	0	1.746273	0.289854	0.031466
3	6	0	0.414331	-0.122187	0.069725
4	6	0	0.259035	-1.354707	-0.095246
5	6	0	1.092490	-2.442339	-0.287776
6	6	0	2.425235	-2.039427	-0.318933
7	6	0	4.007716	0.035738	-0.145223
8	6	0	3.701639	1.350748	0.051395
9	1	0	0.790491	-3.472595	-0.408823
10	1	0	3.198954	-2.783746	-0.466925
11	1	0	5.001034	-0.367815	-0.253519
12	1	0	4.353635	2.207194	0.125947
13	7	0	2.342138	1.514826	0.167603
14	6	0	1.633208	2.763272	0.303964
15	1	0	2.235267	3.465898	0.878817
16	1	0	1.403668	3.200684	-0.670617
17	1	0	0.699192	2.576336	0.833400
18	6	0	-2.540801	0.232064	0.220075
19	6	0	-2.505154	-0.486871	1.377942
20	6	0	-2.250162	-1.829250	1.007425
21	6	0	-2.140822	-1.829656	-0.353521
22	8	0	-2.388469	-0.593169	-0.837599
23	1	0	-2.600415	-0.084152	2.372321
24	1	0	-2.116476	-2.681201	1.653150
25	1	0	-2.025851	-2.614660	-1.081251
26	6	0	-2.795713	1.665056	-0.080039
27	1	0	-1.993802	2.034059	-0.723626
28	1	0	-2.739679	2.217693	0.859219
29	6	0	-4.152439	1.886964	-0.753492
30	1	0	-4.305917	2.944137	-0.971742
31	1	0	-4.208782	1.332815	-1.690635
32	1	0	-4.963771	1.546546	-0.108875

TS for **23** → **26a** with iPr-Furan: E[M06-2X/6-311+G(2df,p)]= -749.68483 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.397185	-1.381735	0.019881
2	6	0	2.074091	0.005167	-0.000241
3	6	0	0.743701	0.385699	0.132915
4	6	0	-0.093777	-0.550035	0.253715
5	6	0	0.045106	-1.932101	0.290543
6	6	0	1.371423	-2.333572	0.166158
7	6	0	3.819134	-1.460404	-0.130377
8	6	0	4.279744	-0.180269	-0.231896
9	1	0	-0.757127	-2.651215	0.383924
10	1	0	1.609149	-3.391016	0.176495
11	1	0	4.427358	-2.349774	-0.151320
12	1	0	5.288399	0.182635	-0.354931
13	7	0	3.238145	0.712072	-0.146790
14	6	0	3.317165	2.144592	-0.289879
15	1	0	3.187511	2.450102	-1.330975
16	1	0	2.529417	2.600254	0.309677
17	1	0	4.284821	2.494417	0.067520
18	6	0	-1.148241	2.258299	-0.116670
19	6	0	-1.451821	2.118794	1.212081
20	6	0	-2.144034	0.906333	1.317785
21	6	0	-2.210270	0.370183	0.042686
22	8	0	-1.723593	1.283380	-0.836272
23	1	0	-0.657721	3.038330	-0.673312
24	1	0	-1.137823	2.774294	2.006447
25	1	0	-2.490746	0.423057	2.216310
26	6	0	-3.017689	-0.757054	-0.521340
27	6	0	-4.174643	-0.216160	-1.367061
28	1	0	-4.843885	0.388847	-0.751013
29	1	0	-3.808599	0.403051	-2.185433
30	1	0	-4.749314	-1.042713	-1.788518
31	1	0	-2.361848	-1.344902	-1.170821
32	6	0	-3.535605	-1.646826	0.604709
33	1	0	-4.027395	-2.528226	0.191976
34	1	0	-2.731397	-1.977438	1.263793
35	1	0	-4.267879	-1.106707	1.209845

TS for **23** → **26b** with iPr-Furan: E[M06-2X/6-311+G(2df,p)]= -749.68597 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.006829	-0.550702	-0.085989
2	6	0	1.883085	0.321840	-0.004728
3	6	0	0.598729	-0.222181	0.027585
4	6	0	0.578863	-1.473398	-0.043093
5	6	0	1.524164	-2.480482	-0.119588
6	6	0	2.809259	-1.944128	-0.139275
7	6	0	4.163978	0.292125	-0.089515
8	6	0	3.718497	1.579542	-0.015720
9	1	0	1.332713	-3.542637	-0.167488
10	1	0	3.660041	-2.612646	-0.200961
11	1	0	5.196602	-0.013056	-0.132392
12	1	0	4.276802	2.502628	0.004712
13	7	0	2.345822	1.609718	0.044183
14	6	0	1.511712	2.786182	0.040960
15	1	0	1.974591	3.570080	0.639702
16	1	0	1.349113	3.157647	-0.973582
17	1	0	0.548052	2.525652	0.477492
18	6	0	-2.369144	-0.168874	0.068767
19	6	0	-2.310592	-0.820465	1.265350
20	6	0	-1.914153	-2.149350	0.976684
21	6	0	-1.754603	-2.209524	-0.377419
22	8	0	-2.099112	-1.029775	-0.936384
23	1	0	-2.474900	-0.382106	2.234959
24	1	0	-1.725583	-2.949904	1.672594
25	1	0	-1.533918	-3.015296	-1.056509
26	6	0	-2.725947	1.225607	-0.321129
27	1	0	-1.924260	1.584324	-0.974800
28	6	0	-4.039731	1.248535	-1.109281
29	1	0	-4.266384	2.263928	-1.438990
30	1	0	-3.981522	0.605374	-1.987331
31	1	0	-4.862654	0.899043	-0.481712
32	6	0	-2.800707	2.120815	0.910122
33	1	0	-1.866179	2.096749	1.473333
34	1	0	-3.005400	3.151252	0.617287
35	1	0	-3.606418	1.795881	1.573082

TS for **23** → **26a** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -788.99131 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.634435	-1.354696	0.133351
2	6	0	2.236538	0.002462	-0.033385
3	6	0	0.885842	0.298997	0.076764
4	6	0	0.085883	-0.644472	0.303797
5	6	0	0.316082	-2.004683	0.488770
6	6	0	1.663525	-2.339232	0.394229
7	6	0	4.058506	-1.369336	-0.022098
8	6	0	4.446294	-0.084754	-0.266855
9	1	0	-0.436862	-2.757524	0.678303
10	1	0	1.962554	-3.373182	0.522917
11	1	0	4.715204	-2.221227	0.043224
12	1	0	5.431997	0.318236	-0.439844
13	7	0	3.355626	0.752784	-0.270215
14	6	0	3.349454	2.169592	-0.536728
15	1	0	2.937809	2.381706	-1.526190
16	1	0	2.743876	2.681858	0.212229
17	1	0	4.369060	2.547434	-0.486901
18	6	0	-0.797095	2.233235	0.006187
19	6	0	-1.039296	2.094086	1.348620
20	6	0	-1.868365	0.972502	1.471443
21	6	0	-2.098467	0.502022	0.190886
22	8	0	-1.547434	1.363398	-0.694425
23	1	0	-0.264464	2.973442	-0.565745
24	1	0	-0.591359	2.675366	2.136821
25	1	0	-2.214179	0.508271	2.380086
26	6	0	-3.106457	-0.472742	-0.350546
27	6	0	-4.370161	0.319237	-0.728937
28	1	0	-4.772012	0.847759	0.137557
29	1	0	-4.148458	1.051175	-1.507186
30	1	0	-5.135908	-0.362602	-1.105701
31	6	0	-3.451103	-1.491189	0.735616
32	1	0	-4.147466	-2.231235	0.336991
33	1	0	-2.557797	-2.010690	1.085728
34	1	0	-3.927573	-1.011123	1.592894
35	6	0	-2.570130	-1.183003	-1.596953
36	1	0	-1.710444	-1.808880	-1.358023
37	1	0	-3.354644	-1.813120	-2.021528
38	1	0	-2.262149	-0.460480	-2.353697

TS for **27,O → 30,O** with Furan: E[M06-2X/6-311+G(2df,p)]= -612.31417 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.360903	-0.632902	-0.038350
2	6	0	2.126975	0.547809	0.026196
3	6	0	-0.436853	0.774064	-0.085835
4	6	0	-0.015280	-0.408874	-0.086575
5	6	0	2.313871	-1.710871	-0.020340
6	6	0	3.524572	-1.123472	0.051083
7	1	0	2.119455	-2.769175	-0.056920
8	1	0	4.522367	-1.527625	0.086970
9	6	0	-2.758449	0.765910	-0.394699
10	6	0	-2.974557	0.431246	0.921279
11	6	0	-2.881855	-0.969542	0.986903
12	6	0	-2.643207	-1.388250	-0.292807
13	8	0	-2.681367	-0.353660	-1.144914
14	1	0	-2.849047	1.695031	-0.931585
15	1	0	-3.108838	1.124946	1.734419
16	1	0	-2.925086	-1.595139	1.861860
17	6	0	0.217939	1.993171	-0.023171
18	1	0	-0.249428	2.968850	-0.024763
19	6	0	1.602482	1.841178	0.035523
20	1	0	2.260471	2.698723	0.085586
21	8	0	3.448292	0.235113	0.082442
22	1	0	-2.524552	-2.364033	-0.731039

TS for **27,O → 30a,O** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -769.54842 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.936181	-0.623430	0.163535
2	6	0	3.119476	0.097034	-0.095417
3	6	0	0.901720	1.398733	-0.098750
4	6	0	0.797446	0.180385	0.144428
5	6	0	2.347675	-1.985893	0.367861
6	6	0	3.688162	-1.982516	0.223783
7	1	0	1.732417	-2.841207	0.590814
8	1	0	4.422612	-2.767716	0.288756
9	6	0	-1.473597	2.318028	-0.315409
10	6	0	-1.595567	2.284068	1.042212
11	6	0	-2.004627	0.969094	1.364123
12	6	0	-2.118705	0.295646	0.179969
13	8	0	-1.859599	1.136729	-0.844685
14	1	0	-1.247320	3.104328	-1.015064
15	1	0	-1.367575	3.090211	1.719419
16	1	0	-2.153053	0.552860	2.345968
17	6	0	1.997580	2.203476	-0.363125
18	1	0	1.983636	3.266075	-0.561976
19	6	0	3.183297	1.468411	-0.354309
20	1	0	4.136883	1.943025	-0.545390
21	8	0	4.184187	-0.746634	-0.053713
22	6	0	-2.596297	-1.081145	-0.172722
23	6	0	-1.719379	-1.689956	-1.272325
24	1	0	-2.119310	-2.665051	-1.559378
25	1	0	-1.698572	-1.051213	-2.155862
26	1	0	-0.693609	-1.818434	-0.924409
27	6	0	-2.546865	-1.960427	1.076093
28	1	0	-3.205608	-1.578453	1.858801
29	1	0	-2.873579	-2.971822	0.826930
30	1	0	-1.530173	-2.011077	1.472168
31	6	0	-4.044864	-0.976504	-0.679059
32	1	0	-4.421492	-1.968575	-0.938173
33	1	0	-4.693688	-0.548097	0.087083
34	1	0	-4.098085	-0.345631	-1.567835

TS for **27,O → 30b,O** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -769.54719 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.430843	0.457699	-0.160583
2	6	0	-2.966383	-0.822384	0.088738
3	6	0	-0.375083	-0.541795	0.263730
4	6	0	-1.049165	0.469432	-0.032076
5	6	0	-3.557007	1.298698	-0.462434
6	6	0	-4.638141	0.498290	-0.373244
7	1	0	-3.559006	2.346761	-0.708711
8	1	0	-5.688989	0.688501	-0.513575
9	6	0	2.021720	0.514858	0.156023
10	6	0	1.760408	1.103656	1.372927
11	6	0	0.966257	2.233006	1.112939
12	6	0	0.776992	2.254365	-0.242264
13	8	0	1.509612	1.285301	-0.827360
14	1	0	2.062986	0.722938	2.334004
15	1	0	0.517904	2.905244	1.825041
16	6	0	-0.831329	-1.833245	0.510816
17	1	0	-0.212400	-2.687833	0.752977
18	6	0	-2.217076	-1.953751	0.415800
19	1	0	-2.711382	-2.900672	0.590167
20	8	0	-4.319142	-0.781550	-0.043174
21	6	0	2.951360	-0.590751	-0.252942
22	6	0	3.128119	-1.552557	0.921819
23	1	0	3.781486	-2.376213	0.627926
24	1	0	3.583757	-1.054230	1.779886
25	1	0	2.166629	-1.965290	1.233773
26	6	0	2.401056	-1.342019	-1.468692
27	1	0	1.455607	-1.831732	-1.233112
28	1	0	2.230534	-0.662707	-2.304435
29	1	0	3.120425	-2.101324	-1.782731
30	6	0	4.308500	0.035229	-0.617694
31	1	0	4.728734	0.574775	0.232991
32	1	0	5.011220	-0.746519	-0.914935
33	1	0	4.199944	0.733788	-1.449071
34	1	0	0.292484	2.952124	-0.903100

TS for **28,O → 31,O** with Furan: E[M06-2X/6-311+G(2df,p)]= -612.31265 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.875239	0.737326	-0.016460
2	6	0	-1.926388	-0.675253	-0.002292
3	6	0	-0.814638	-1.522077	-0.047749
4	6	0	0.342011	-0.774647	-0.102667
5	6	0	0.380370	0.485583	-0.120232
6	6	0	-0.636073	1.403956	-0.081005
7	6	0	-3.252900	1.161054	0.048084
8	6	0	-3.988236	0.035393	0.095364
9	1	0	-0.910245	-2.600034	-0.035836
10	1	0	-0.547420	2.482614	-0.099947
11	1	0	-3.633766	2.168515	0.057681
12	1	0	-5.051213	-0.131639	0.149660
13	6	0	3.043736	-1.044536	-0.280108
14	6	0	3.174332	-0.590426	1.004507
15	6	0	2.972650	0.798837	0.944165
16	6	0	2.715658	1.087850	-0.373565
17	8	0	2.883119	-0.016661	-1.128463
18	1	0	3.152873	-2.018745	-0.724275
19	1	0	3.337162	-1.198262	1.878094
20	1	0	2.946709	1.500244	1.761153
21	1	0	2.598871	2.016856	-0.905155
22	8	0	-3.221202	-1.088077	0.067259

TS for **28,O → 31a,O** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -769.54622 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.633839	-0.859798	0.195896
2	6	0	3.004694	0.449660	-0.187312
3	6	0	2.113295	1.503805	-0.414594
4	6	0	0.836804	1.047736	-0.194159
5	6	0	0.471170	-0.104605	0.149845
6	6	0	1.278154	-1.194775	0.379640
7	6	0	3.879901	-1.579289	0.308518
8	6	0	4.850147	-0.699881	0.001314
9	1	0	2.437076	2.490572	-0.717287
10	1	0	0.960262	-2.191115	0.662566
11	1	0	4.022647	-2.611488	0.581236
12	1	0	5.922375	-0.793026	-0.047095
13	6	0	-1.398505	2.310858	-0.368790
14	6	0	-1.505126	2.307211	0.993539
15	6	0	-2.007181	1.037724	1.338721
16	6	0	-2.191393	0.353931	0.161948
17	8	0	-1.907108	1.168647	-0.876134
18	1	0	-1.192030	3.097322	1.655220
19	1	0	-2.167484	0.644478	2.328451
20	6	0	-2.832998	-0.965252	-0.154708
21	6	0	-2.691670	-1.889490	1.054784
22	1	0	-3.202589	-1.482538	1.929744
23	1	0	-3.136252	-2.860846	0.829895
24	1	0	-1.639540	-2.037237	1.307307
25	6	0	-4.322885	-0.718769	-0.447830
26	1	0	-4.442360	-0.048866	-1.301088
27	1	0	-4.818255	-1.664057	-0.681053
28	1	0	-4.819183	-0.269899	0.414448
29	6	0	-2.177225	-1.606017	-1.381373
30	1	0	-1.123705	-1.818606	-1.195702
31	1	0	-2.687835	-2.541641	-1.619225
32	1	0	-2.241552	-0.948746	-2.248993
33	1	0	-1.118932	3.067675	-1.081235
34	8	0	4.357262	0.532569	-0.302593

TS for **28,O → 31b,O** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -769.54662 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.101517	0.528688	-0.177760
2	6	0	-2.767908	-0.806891	0.148219
3	6	0	-1.469996	-1.288916	0.345076
4	6	0	-0.559989	-0.264397	0.184363
5	6	0	-0.873580	0.914773	-0.112743
6	6	0	-2.091990	1.499844	-0.330490
7	6	0	-4.540797	0.539973	-0.276806
8	6	0	-4.943173	-0.717035	-0.015968
9	1	0	-1.269677	-2.324430	0.590121
10	1	0	-2.294299	2.531507	-0.586708
11	1	0	-5.179466	1.375333	-0.509880
12	1	0	-5.920160	-1.169615	0.022111
13	6	0	2.278253	0.384444	0.155905
14	6	0	2.053443	1.093249	1.304222
15	6	0	1.403332	2.287444	0.919944
16	6	0	1.258579	2.217514	-0.435363
17	8	0	1.857955	1.103028	-0.907450
18	1	0	2.288502	0.769239	2.303761
19	1	0	1.034295	3.074292	1.556467
20	1	0	0.885020	2.908152	-1.171890
21	6	0	3.010261	-0.892296	-0.130397
22	6	0	4.400775	-0.538234	-0.684327
23	1	0	4.960677	-1.451986	-0.895660
24	1	0	4.313433	0.033329	-1.609740
25	1	0	4.965763	0.056103	0.036132
26	6	0	3.156932	-1.684283	1.168110
27	1	0	2.177754	-1.908294	1.596887
28	1	0	3.671219	-2.626152	0.968098
29	1	0	3.742051	-1.132778	1.907011
30	6	0	2.250725	-1.727394	-1.166666
31	1	0	2.829804	-2.620775	-1.410758
32	1	0	1.277840	-2.033209	-0.780173
33	1	0	2.087122	-1.160034	-2.083435
34	8	0	-3.901704	-1.552975	0.244417

TS for **29,O → 32,O** with Furan: E[M06-2X/6-311+G(2df,p)]= -612.31764 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.238455	0.617631	0.027498
2	6	0	-1.441087	-0.545114	-0.026084
3	6	0	-0.066430	-0.428781	-0.067828
4	6	0	0.341044	0.755447	-0.065298
5	6	0	-0.245113	2.002035	-0.015689
6	6	0	-1.635787	1.886116	0.031962
7	6	0	-3.595826	0.135082	0.070410
8	6	0	-3.511182	-1.208939	0.039354
9	1	0	0.260911	2.956405	-0.015579
10	1	0	-2.242553	2.782562	0.072645
11	1	0	-4.505449	0.710319	0.117283
12	1	0	-4.264075	-1.978980	0.051443
13	6	0	2.759659	-1.407275	-0.195635
14	6	0	2.961368	-0.871029	1.036460
15	6	0	3.010382	0.532010	0.844070
16	6	0	2.829943	0.735942	-0.493793
17	8	0	2.735395	-0.444808	-1.135825
18	1	0	2.653127	-2.418374	-0.548267
19	1	0	3.024230	-1.412118	1.964803
20	1	0	3.131386	1.297958	1.591807
21	8	0	-2.225808	-1.651790	-0.018365
22	1	0	2.854621	1.616251	-1.113185

TS for **29,O → 32a,O** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -769.54982 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.963137	-0.904628	0.130339
2	6	0	2.428606	0.366825	-0.160734
3	6	0	1.072060	0.563069	-0.043859
4	6	0	0.387327	-0.432523	0.306477
5	6	0	0.738194	-1.734231	0.623041
6	6	0	2.112870	-1.950154	0.521257
7	6	0	4.383188	-0.765027	-0.077020
8	6	0	4.578217	0.511493	-0.459709
9	1	0	0.062991	-2.526944	0.913689
10	1	0	2.516670	-2.929961	0.746575
11	1	0	5.149204	-1.513291	0.041181
12	1	0	5.468721	1.057728	-0.721574
13	6	0	-0.866480	2.332920	-0.168447
14	6	0	-1.036183	2.237690	1.184237
15	6	0	-1.732342	1.036146	1.398714
16	6	0	-1.960505	0.479758	0.156859
17	8	0	-1.517852	1.333300	-0.793049
18	1	0	-0.419060	3.080622	-0.799899
19	1	0	-0.631524	2.909399	1.922078
20	1	0	-2.001027	0.592337	2.343008
21	6	0	-2.857942	-0.635104	-0.300424
22	6	0	-4.197386	-0.012790	-0.731879
23	1	0	-4.654065	0.537311	0.092997
24	1	0	-4.052424	0.674587	-1.566621
25	1	0	-4.886293	-0.799056	-1.048557
26	6	0	-3.095993	-1.597015	0.862841
27	1	0	-3.713227	-2.432573	0.527759
28	1	0	-2.154401	-1.995821	1.244046
29	1	0	-3.617735	-1.103475	1.685338
30	8	0	3.419015	1.223001	-0.520184
31	6	0	-2.246460	-1.379625	-1.491496
32	1	0	-1.331789	-1.900275	-1.207663
33	1	0	-2.962304	-2.113467	-1.867938
34	1	0	-2.004903	-0.688353	-2.299726

TS for **27,S → 30,S** with Furan: E[M06-2X/6-311+G(2df,p)]= -935.29632 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.039485	-0.578742	-0.054563
2	6	0	1.824422	0.605320	0.012256
3	6	0	-0.775282	0.848361	-0.098329
4	6	0	-0.332767	-0.324783	-0.101084
5	6	0	1.846932	-1.762075	-0.050636
6	6	0	3.166593	-1.482680	0.016933
7	1	0	1.442223	-2.762600	-0.096706
8	1	0	3.985637	-2.184639	0.034483
9	6	0	-3.107322	0.747926	-0.364884
10	6	0	-3.295947	0.376517	0.946699
11	6	0	-3.113642	-1.014314	0.986306
12	6	0	-2.853639	-1.394944	-0.303411
13	8	0	-2.974049	-0.351356	-1.136683
14	1	0	-3.260619	1.679340	-0.883205
15	1	0	-3.466502	1.045899	1.773259
16	1	0	-3.110493	-1.657175	1.849843
17	6	0	-0.110100	2.062328	-0.035674
18	1	0	-0.565136	3.043904	-0.035478
19	6	0	1.270280	1.895343	0.021384
20	1	0	1.916781	2.763147	0.071795
21	1	0	-2.686302	-2.354981	-0.760191
22	16	0	3.511421	0.210525	0.080605

TS for **27,S → 30a,S** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -1092.53091 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.668246	-0.415323	0.150680
2	6	0	2.824945	0.373782	-0.099494
3	6	0	0.501881	1.558500	-0.112138
4	6	0	0.490204	0.333659	0.125452
5	6	0	1.989463	-1.792997	0.373472
6	6	0	3.317827	-2.027413	0.296219
7	1	0	1.252548	-2.555734	0.581358
8	1	0	3.825788	-2.970655	0.423305
9	6	0	-1.872892	2.293460	-0.277151
10	6	0	-1.995772	2.226132	1.082257
11	6	0	-2.297117	0.880709	1.379384
12	6	0	-2.359548	0.220375	0.180703
13	8	0	-2.183820	1.099420	-0.827618
14	1	0	-1.724098	3.111204	-0.961392
15	1	0	-1.824251	3.034148	1.773779
16	1	0	-2.404397	0.434351	2.353357
17	6	0	1.553767	2.422866	-0.367351
18	1	0	1.485220	3.483895	-0.565001
19	6	0	2.775411	1.754904	-0.352206
20	1	0	3.690455	2.304142	-0.538745
21	6	0	-2.735956	-1.182272	-0.192554
22	6	0	-1.859207	-1.687489	-1.343041
23	1	0	-2.185252	-2.687530	-1.637306
24	1	0	-1.933547	-1.031030	-2.210522
25	1	0	-0.811380	-1.732499	-1.043091
26	6	0	-2.562531	-2.085189	1.028208
27	1	0	-3.221652	-1.782899	1.844673
28	1	0	-2.809296	-3.114832	0.762365
29	1	0	-1.531150	-2.054808	1.386509
30	6	0	-4.208481	-1.185441	-0.637449
31	1	0	-4.512344	-2.198334	-0.911059
32	1	0	-4.857700	-0.833393	0.166301
33	1	0	-4.350922	-0.537940	-1.504217
34	16	0	4.250069	-0.612064	-0.044332

TS for **27,S → 30b,S** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -1092.52984 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.122828	0.495457	-0.116455
2	6	0	-2.718746	-0.778292	0.099974
3	6	0	-0.079813	-0.599036	0.272143
4	6	0	-0.741895	0.426761	0.008191
5	6	0	-3.090374	1.509996	-0.403654
6	6	0	-4.351739	1.025738	-0.399816
7	1	0	-2.840527	2.542815	-0.598766
8	1	0	-5.263333	1.572810	-0.582999
9	6	0	2.333548	0.506218	0.159695
10	6	0	2.072841	1.086923	1.379818
11	6	0	1.243190	2.192984	1.130789
12	6	0	1.032770	2.207993	-0.222127
13	8	0	1.786597	1.260080	-0.816765
14	1	0	2.398049	0.714916	2.336807
15	1	0	0.787013	2.853492	1.849036
16	6	0	-0.590140	-1.877885	0.482311
17	1	0	-0.008319	-2.765242	0.698386
18	6	0	-1.977696	-1.935369	0.390335
19	1	0	-2.489740	-2.877885	0.544320
20	6	0	3.271567	-0.587771	-0.259973
21	6	0	3.458095	-1.557526	0.906872
22	1	0	4.121607	-2.370832	0.606872
23	1	0	3.906533	-1.061653	1.770124
24	1	0	2.500165	-1.983416	1.212470
25	6	0	2.721981	-1.334949	-1.478472
26	1	0	1.776698	-1.825501	-1.243265
27	1	0	2.550891	-0.653564	-2.312339
28	1	0	3.441701	-2.093030	-1.794597
29	6	0	4.622687	0.051051	-0.624629
30	1	0	5.043151	0.585055	0.229410
31	1	0	5.329414	-0.722801	-0.932794
32	1	0	4.505566	0.757061	-1.448574
33	1	0	0.527711	2.897186	-0.876829
34	16	0	-4.442503	-0.665238	-0.054573

TS for **28,S → 31,S** with Furan: E[M06-2X/6-311+G(2df,p)]= -935.29296 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.549119	0.861810	-0.024537
2	6	0	-1.659695	-0.553731	-0.021291
3	6	0	-0.547182	-1.416624	-0.072933
4	6	0	0.630840	-0.713125	-0.118754
5	6	0	0.715427	0.545347	-0.124521
6	6	0	-0.277109	1.481150	-0.081034
7	6	0	-2.840305	1.492185	0.035970
8	6	0	-3.856578	0.607688	0.083042
9	1	0	-0.659987	-2.493770	-0.072624
10	1	0	-0.167330	2.558618	-0.090403
11	1	0	-2.978969	2.564541	0.043002
12	1	0	-4.912788	0.823022	0.132255
13	6	0	3.309914	-1.108179	-0.286853
14	6	0	3.456083	-0.678958	1.004316
15	6	0	3.334046	0.720864	0.961471
16	6	0	3.106358	1.041168	-0.353509
17	8	0	3.211430	-0.061154	-1.121948
18	1	0	3.368220	-2.080715	-0.744076
19	1	0	3.579457	-1.306197	1.870665
20	1	0	3.343195	1.411768	1.787666
21	1	0	3.040452	1.981702	-0.873235
22	16	0	-3.327486	-1.040457	0.057133

TS for **28,S → 31a,S** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -1092.52669 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.345406	-0.886282	0.203481
2	6	0	2.741969	0.431988	-0.146476
3	6	0	1.826974	1.483031	-0.359327
4	6	0	0.549136	1.033819	-0.169263
5	6	0	0.169143	-0.123083	0.144076
6	6	0	0.975658	-1.209617	0.357706
7	6	0	3.483098	-1.752865	0.358966
8	6	0	4.657037	-1.128141	0.139495
9	1	0	2.142512	2.480680	-0.636486
10	1	0	0.661146	-2.215020	0.613822
11	1	0	3.401852	-2.798018	0.624127
12	1	0	5.647740	-1.552660	0.191010
13	6	0	-1.700774	2.326121	-0.321939
14	6	0	-1.801441	2.290462	1.039260
15	6	0	-2.313909	1.016253	1.356486
16	6	0	-2.507130	0.362557	0.165549
17	8	0	-2.212779	1.196842	-0.854472
18	1	0	-1.483141	3.063407	1.718506
19	1	0	-2.476890	0.602420	2.337328
20	6	0	-3.153845	-0.946449	-0.181216
21	6	0	-3.018617	-1.897570	1.007975
22	1	0	-3.528991	-1.507428	1.890877
23	1	0	-3.467339	-2.861701	0.761330
24	1	0	-1.967478	-2.055563	1.258642
25	6	0	-4.642073	-0.687493	-0.471878
26	1	0	-4.757049	0.001619	-1.310333
27	1	0	-5.140772	-1.625346	-0.726982
28	1	0	-5.138371	-0.255778	0.399106
29	6	0	-2.498187	-1.563142	-1.420339
30	1	0	-1.445856	-1.784327	-1.237542
31	1	0	-3.012021	-2.491364	-1.679250
32	1	0	-2.558287	-0.887089	-2.273700
33	1	0	-1.413460	3.095241	-1.017913
34	16	0	4.472749	0.544915	-0.268257

TS for **28,S → 31b,S** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -1092.52688 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.784663	0.775365	-0.199273
2	6	0	-2.511384	-0.583646	0.111997
3	6	0	-1.208864	-1.089346	0.294140
4	6	0	-0.265466	-0.102139	0.143849
5	6	0	-0.526577	1.094373	-0.136987
6	6	0	-1.727449	1.707268	-0.342808
7	6	0	-4.196962	1.012750	-0.330970
8	6	0	-4.938278	-0.095005	-0.129845
9	1	0	-1.026745	-2.132489	0.524257
10	1	0	-1.908344	2.746153	-0.588236
11	1	0	-4.617926	1.980494	-0.566322
12	1	0	-6.013010	-0.182404	-0.171062
13	6	0	2.563000	0.328104	0.171778
14	6	0	2.375876	1.002610	1.348090
15	6	0	1.849542	2.268536	1.007936
16	6	0	1.734248	2.274571	-0.351585
17	8	0	2.239178	1.131648	-0.864008
18	1	0	2.554469	0.612894	2.335859
19	1	0	1.538400	3.056122	1.673725
20	1	0	1.439588	3.027821	-1.061927
21	6	0	3.187140	-0.995050	-0.157860
22	6	0	4.643491	-0.749021	-0.587642
23	1	0	5.125563	-1.698708	-0.830321
24	1	0	4.682274	-0.108601	-1.470409
25	1	0	5.208360	-0.267425	0.212586
26	6	0	3.158084	-1.882512	1.086032
27	1	0	2.132251	-2.031729	1.430026
28	1	0	3.591734	-2.856819	0.852947
29	1	0	3.737252	-1.444729	1.901674
30	6	0	2.431510	-1.677690	-1.302489
31	1	0	2.932758	-2.612270	-1.563542
32	1	0	1.403692	-1.899420	-1.012599
33	1	0	2.403357	-1.042237	-2.188150
34	16	0	-3.987286	-1.495928	0.230461

TS for **29,S → 32,S** with Furan: E[M06-2X/6-311+G(2df,p)]= -935.29696 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.907459	0.922616	0.027695
2	6	0	-1.202807	-0.309811	-0.036531
3	6	0	0.181997	-0.239549	-0.086969
4	6	0	0.710906	0.896733	-0.090324
5	6	0	0.185873	2.175174	-0.031321
6	6	0	-1.203142	2.144180	0.028534
7	6	0	-3.325855	0.706552	0.087834
8	6	0	-3.657273	-0.602580	0.067387
9	1	0	0.745073	3.100674	-0.035995
10	1	0	-1.755760	3.075486	0.076372
11	1	0	-4.054403	1.503724	0.142122
12	1	0	-4.649936	-1.023932	0.098914
13	6	0	2.761154	-1.473873	-0.259410
14	6	0	3.021375	-1.042470	1.008951
15	6	0	3.231313	0.346874	0.906882
16	6	0	3.062470	0.660469	-0.418128
17	8	0	2.877349	-0.465605	-1.137387
18	1	0	2.556242	-2.445878	-0.673602
19	1	0	3.009562	-1.645648	1.900432
20	1	0	3.422982	1.047507	1.702399
21	1	0	3.222410	1.565231	-0.979643
22	16	0	-2.291641	-1.659889	-0.022469

TS for **29,S → 32a,S** with tBu-Furan: E[M06-2X/6-311+G(2df,p)]= -1092.52985 E_h

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.713112	1.122529	0.138021
2	6	0	-2.211819	-0.190710	-0.073143
3	6	0	-0.840678	-0.313877	0.029404
4	6	0	-0.101055	0.661389	0.281085
5	6	0	-0.455297	1.987684	0.495883
6	6	0	-1.829889	2.185677	0.417100
7	6	0	-4.144649	1.149042	0.018373
8	6	0	-4.671137	-0.061325	-0.265880
9	1	0	0.223862	2.804806	0.701107
10	1	0	-2.234708	3.179242	0.573726
11	1	0	-4.741414	2.042466	0.140320
12	1	0	-5.712779	-0.303827	-0.406768
13	6	0	0.913927	-2.234786	-0.100803
14	6	0	1.115596	-2.137054	1.247323
15	6	0	1.960678	-1.027542	1.430767
16	6	0	2.235208	-0.527450	0.178522
17	8	0	1.671758	-1.328930	-0.751166
18	1	0	0.383251	-2.942807	-0.713653
19	1	0	0.648511	-2.745750	2.003099
20	1	0	2.293653	-0.604925	2.363938
21	6	0	3.209892	0.505411	-0.308360
22	6	0	4.520049	-0.210869	-0.678592
23	1	0	4.933953	-0.734538	0.185013
24	1	0	4.350399	-0.938416	-1.474017
25	1	0	5.255566	0.516759	-1.029081
26	6	0	3.473374	1.509774	0.813247
27	1	0	4.159441	2.282577	0.461584
28	1	0	2.545749	1.988648	1.133149
29	1	0	3.928843	1.027749	1.680665
30	6	0	2.665606	1.227647	-1.544544
31	1	0	1.758550	1.784919	-1.307962
32	1	0	3.417538	1.926190	-1.917713
33	1	0	2.429431	0.519283	-2.339190
34	16	0	-3.485880	-1.315261	-0.407207