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Supporting Information

Organocatalyzed Double Dearomatization Reaction of Non-Functionalized Phenols and Propargylic Alcohols: The Important Regulating Effect of Steric Hindrance

Xihong Liu,*[a] Boyan Zhu,[a] Panpan Zhou,[b] Jingying Zhang,[a] Anqi Chu[a] and Rui Wang*[a]

[a] *Key Laboratory of Preclinical Study for New Drugs of Gansu Province, School of Basic Medical Sciences & Research Unit of Peptide Science, Chinese Academy of Medical Sciences, 2019RU066, Lanzhou University, Lanzhou 730000, China.*

[b] *State Key Laboratory of Applied Organic Chemistry, Key Laboratory of Nonferrous Metal Chemistry and Resources Utilization of Gansu Province, College of Chemistry and Chemical Engineering, Lanzhou University, Lanzhou 730000, China.*

Corresponding authors: liuxihong@lzu.edu.cn; wangrui@lzu.edu.cn

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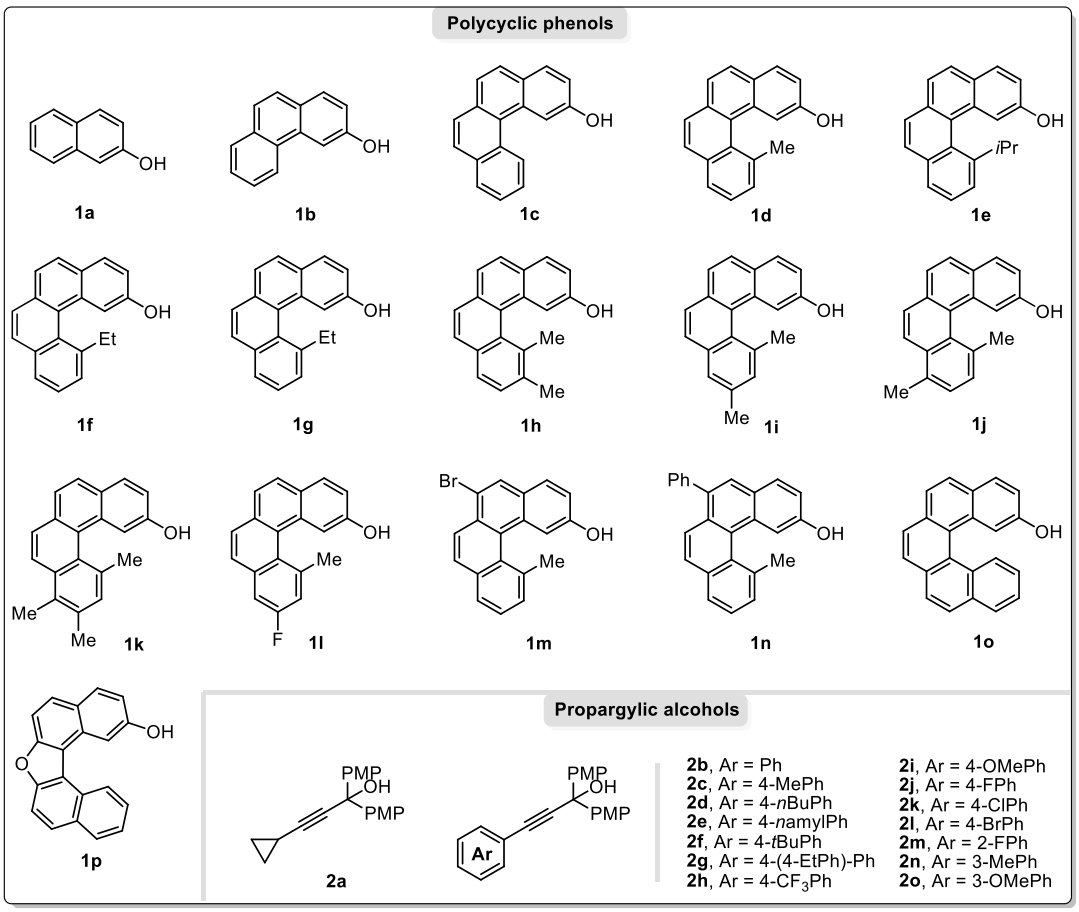
1. General Information

Unless stated otherwise, all reactions were carried out in flame dried glassware. All solvents were dried according to established procedures. Chemicals were purchased from commercial suppliers and used without further purification. Reactions were monitored by thin layer chromatography (TLC), column chromatography purifications were carried out using silica gel. NMR spectra were recorded on a Bruker 300MHz instrument and internally referenced to tetramethylsilane signal or residual protic solvent signals. Data for ^{1}H NMR are recorded as follows: chemical shift, integration, multiplicity (br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet cm = complex multiplet) and coupling constant in Hertz (Hz). Data for ^{13}C NMR are reported in terms of chemical shift (δ, ppm). Melting points were measured on a SCW X-4 and values are uncorrected. High resolution mass spectra (HRMS) were obtained by the ESI ionization sources.

2. Reagents and Substrates

Polycyclic phenols **1c-1p**[1] and propargylic alcohols **2a-2aa**[2] were prepared according to literature methods.



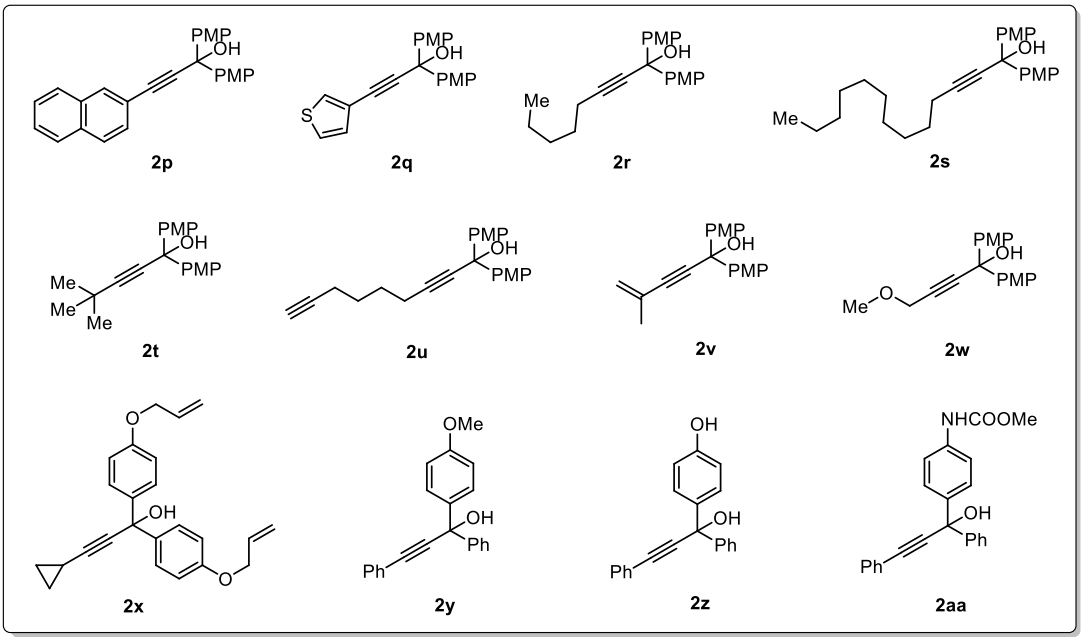
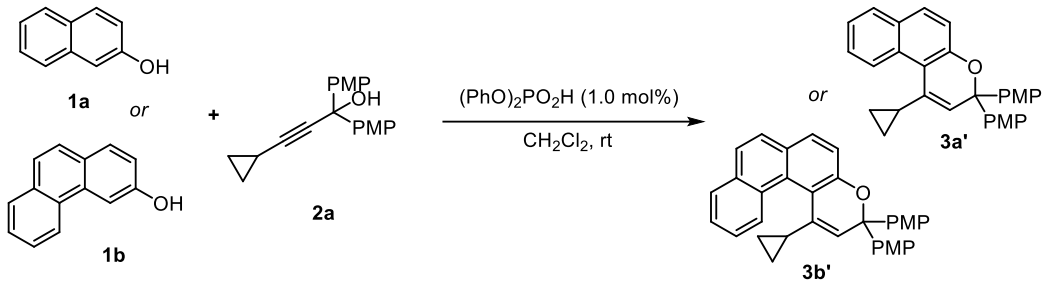
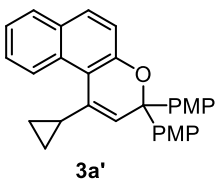


Figure S1. Substrates **1** and **2** employed in this study.

3. General Procedure for [3+3] Cycloaddition Reactions Between Polycyclic Phenols and Propargylic Alcohols

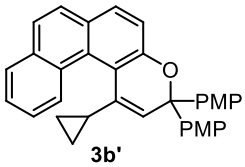


To a mixture of β-naphthol **1a** or phenanthren-3-ol **1b** (0.1 mmol, 1.0 equiv) and propargylic alcohol **2a** (0.12 mmol, 1.2 equiv) in DCM (1.0 mL) was added diphenyl phosphate (0.001 mmol). The resulting solution was stirred at room temperature until the complete consumption of starting material, and the reaction mixture was directly purified by silica gel column chromatography to afford the desired products **3a'** and **3b'**.



Prepared according to the general procedure on a 0.1 mmol scale and purified by flash

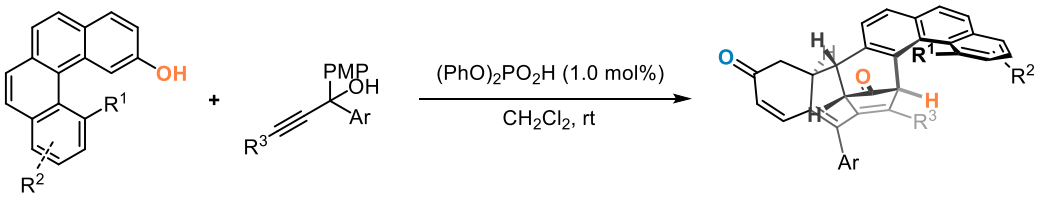
chromatography (petroleum ether/ethyl acetate = 100/1). White solid, m.p. 103-104 ℃, 41.2 mg, 95% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.73 (d, *J* = 8.6 Hz, 1H), 7.64 (dd, *J* = 19.9, 8.4 Hz, 2H), 7.50 – 7.12 (m, 7H), 6.76 (d, *J* = 8.3 Hz, 4H), 5.76 (s, 1H), 3.70 (s, 6H), 2.03 (dd, *J* = 9.6, 4.6 Hz, 1H), 1.04 (d, *J* = 7.8 Hz, 2H), 0.89 (d, *J* = 5.5 Hz, 2H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.72, 151.53, 137.21, 130.61, 130.33, 130.26, 128.74, 128.41, 125.79, 125.64, 123.17, 123.06, 118.82, 118.54, 113.23, 81.62, 55.20, 16.45, 10.08 ppm; **HRMS (ESI)**: $C_{30}H_{27}O_3$ $[M + H]^+$ calcd: 435.1954, found: 435.1933.



3b'

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 100/1). White solid, m.p. 175-176 ℃, 44.5 mg, 92% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.41 (d, *J* = 7.6 Hz, 1H), 7.96 – 7.72 (m, 1H), 7.63 (d, *J* = 8.4 Hz, 1H), 7.61 – 7.42 (m, 6H), 7.41 – 7.23 (m, 3H), 6.87 (d, *J* = 8.3 Hz, 2H), 6.66 (d, *J* = 8.3 Hz, 2H), 5.55 (d, *J* = 2.6 Hz, 1H), 3.77 (s, 3H), 3.56 (s, 3H), 1.64 – 1.38 (m, 1H), 1.05 – 0.84 (m, 2H), 0.48 (ddt, *J* = 29.4, 9.9, 5.0 Hz, 2H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.83, 158.74, 152.87, 141.78, 138.93, 135.18, 132.90, 130.32, 130.00, 129.74, 129.26, 128.21, 128.11, 127.95, 127.40, 126.96, 126.26, 124.68, 124.28, 121.31, 118.58, 117.35, 113.51, 113.01, 82.86, 55.35, 55.01, 14.82, 13.18, 11.43 ppm; **HRMS (ESI)**: $C_{34}H_{29}O_3$ $[M + H]^+$ calcd: 485.2110, found: 485.2098.

4. General Procedure for Double Dearomatization Reactions of Polycyclic Phenols and Propargylic Alcohols

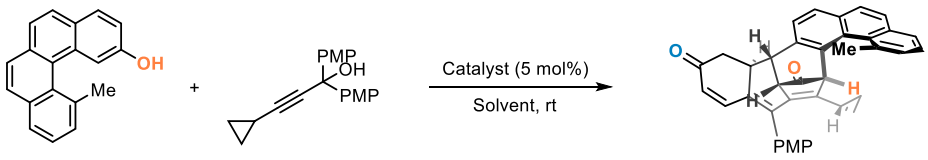


1c-1p **2** **3**

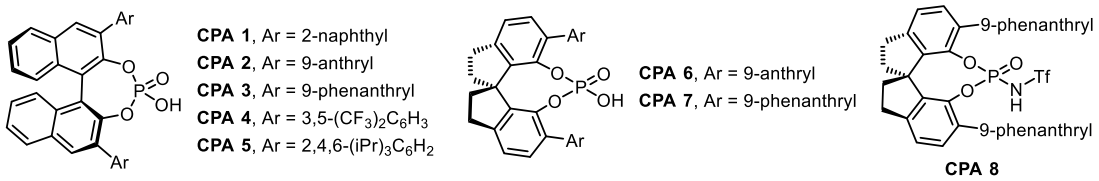
To a mixture of polycyclic phenols **1** (0.1 mmol, 1.0 equiv) and propargylic alcohols **2** (0.12 mmol, 1.2 equiv) in DCM (1.0 mL) was added diphenyl phosphate (0.001 mmol). The resulting solution

was stirred at room temperature for the specified time, the process of which was monitored by TLC. Then the solvent was removed under reduced pressure, and the residue was purified by silica gel column chromatography to afford the desired products **3**.

5. Screening of Chiral Brønsted Acids



1d **2a** **3d**



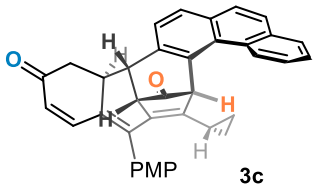
CPA 8

Entry	Catalyst	Solvent	*t* (h)	Yield (%)[a]	ee (%)[b]
1	**CPA 1**	CH_2Cl_2	60	46	0.5
2	**CPA 2**	CH_2Cl_2	60	64	2
3	**CPA 3**	CH_2Cl_2	60	65	0
4	**CPA 4**	CH_2Cl_2	60	37	0
5	**CPA 5**	CH_2Cl_2	60	90	11
6	**CPA 6**	CH_2Cl_2	60	95	26
7	**CPA 7**	CH_2Cl_2	60	86	21
8	**CPA 8**	CH_2Cl_2	60	65	13
9	**CPA 6**	toluene	48	87	49

Reaction conditions: polycyclic phenol **1d** (0.05 mmol, 1.0 equiv.), propargylic alcohol **2a** (0.06 mmol, 1.2 equiv.) and catalyst (5 mol%) in 0.6 mL of solvent. [a] Isolated yield. [b] Enantiomeric excess was determined by chiral HPLC.

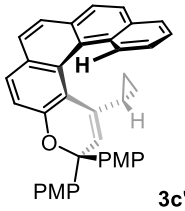
Chiral Brønsted acids were also recruited to catalyze the double dearomatization reaction of polycyclic phenol **1d** and propargylic alcohol **2a**. However, the employment of either chiral phosphoric acids (**CPA 1**-**CPA 7**) or the chiral phosphoric amide **CPA 8** failed to afford a satisfactory outcome with respect to enantioselectivity.

6. Characterization Data



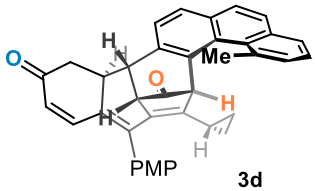
3c

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 4/1 to 2/1). Yellow solid, m.p. 164-165 ℃, 21.3 mg, 41% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.57 – 8.27 (m, 1H), 7.82 (dd, *J* = 7.2, 2.8 Hz, 1H), 7.69 (d, *J* = 8.0 Hz, 1H), 7.55 (dt, *J* = 16.9, 8.6 Hz, 5H), 7.36 (d, *J* = 8.1 Hz, 1H), 7.28 – 7.04 (m, 3H), 6.92 – 6.68 (m, 2H), 5.90 (d, *J* = 10.0 Hz, 1H), 5.16 (s, 1H), 3.74 (s, 3H), 3.66 (d, *J* = 5.6 Hz, 2H), 3.41 (d, *J* = 4.5 Hz, 1H), 3.04 – 2.71 (m, 2H), 0.55 (td, *J* = 8.0, 4.1 Hz, 1H), 0.00 (dtt, *J* = 20.8, 8.2, 4.4 Hz, 2H), -0.34 (dq, *J* = 14.5, 8.0, 6.8 Hz, 1H), -0.95 (dq, *J* = 10.9, 5.5 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 210.00, 198.56, 159.82, 153.64, 144.84, 142.82, 138.52, 136.07, 134.36, 133.41, 131.43, 131.09, 129.75, 129.12, 128.74, 128.30, 128.11, 127.97, 127.73, 127.28, 126.93, 126.46, 125.90, 125.49, 114.17, 55.28, 54.57, 52.90, 49.48, 46.00, 44.82, 29.72, 9.93, 5.62 ppm; **HRMS (ESI):** $C_{37}H_{29}O_3$ $[M + H]^+$ calcd: 521.2110, found: 521.2090.



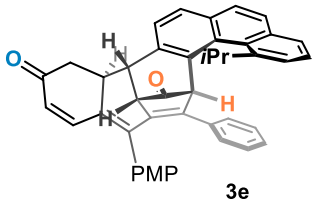
3c'

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 30/1 to 20/1). White solid, m.p. 206-207 ℃, 16.9 mg, 32% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.96 – 7.81 (m, 3H), 7.81 – 7.70 (m, 4H), 7.70 – 7.56 (m, 2H), 7.55 – 7.43 (m, 2H), 7.43 – 7.25 (m, 3H), 6.96 (d, *J* = 7.6 Hz, 2H), 6.86 (d, *J* = 7.0 Hz, 2H), 5.55 (s, 1H), 3.78 (s, 3H), 3.73 (s, 3H), 0.26 (p, *J* = 6.9 Hz, 1H), -0.15 (t, *J* = 6.3 Hz, 3H), -0.30 (td, *J* = 8.8, 8.4, 4.6 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.99, 158.94, 152.85, 141.05, 138.86, 135.68, 132.25, 131.56, 131.34, 130.22, 129.55, 128.83, 128.36, 128.31, 127.60, 127.29, 127.25, 127.22, 126.22, 125.86, 125.50, 125.35, 124.54, 122.27, 118.80, 117.09, 113.48, 113.12, 82.29, 55.33, 55.24, 13.86, 10.46, 9.18 ppm; **HRMS (ESI)**: $C_{38}H_{31}O_3$ $[M + H]^+$ calcd: 535.2267, found: 535.2247.



3d

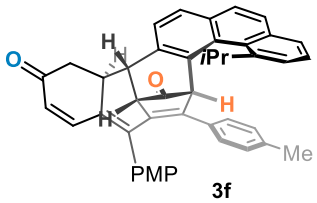
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 219-220 ℃, 45.8 mg, 86% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.82 (d, *J* = 7.7 Hz, 1H), 7.72 (d, *J* = 7.5 Hz, 1H), 7.68 – 7.41 (m, 6H), 7.24 (d, *J* = 1.7 Hz, 2H), 6.90 (d, *J* = 7.0 Hz, 2H), 6.01 (d, *J* = 1.5 Hz, 1H), 4.41 (s, 1H), 3.84 (d, *J* = 1.6 Hz, 4H), 3.73 (t, *J* = 9.9 Hz, 1H), 3.50 (d, *J* = 4.5 Hz, 1H), 2.99 (d, *J* = 9.9 Hz, 3H), 2.77 (s, 3H), 0.47 (hept, *J* = 5.2 Hz, 1H), 0.00 (tq, *J* = 9.1, 5.7 Hz, 1H), -0.22 (dq, *J* = 10.7, 5.6 Hz, 1H), -0.44 (tt, *J* = 7.9, 5.3 Hz, 1H), -1.36 (dq, *J* = 10.6, 5.5 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 208.99, 198.64, 159.72, 153.63, 144.97, 142.92, 136.59, 136.30, 135.22, 134.01, 133.86, 131.64, 131.01, 129.23, 128.95, 128.85, 128.67, 128.23, 127.16, 127.08, 126.66, 125.84, 125.68, 124.95, 114.09, 55.26, 54.38, 53.02, 47.88, 45.92, 45.08, 23.18, 9.65, 5.20 ppm; **HRMS (ESI)**: $C_{38}H_{31}O_3$ $[M + H]^+$ calcd: 535.2267, found: 535.2245.



3e

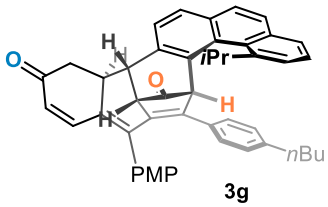
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 168 - 169 ℃, 52.0 mg, 87% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.2 Hz, 1H), 7.56 (dd, *J* = 8.7, 4.2 Hz, 1H), 7.50 (t, *J* = 5.1 Hz, 3H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.31 (d, *J* = 9.0 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 6.74 – 6.56 (m, 3H), 6.37 (t, *J* = 7.6 Hz, 2H), 5.91 (t, *J* = 9.8 Hz, 3H), 5.21 (s, 1H), 3.97 – 3.82 (m, 2H), 3.69 (s, 3H), 3.67 – 3.55 (m, 2H), 3.08 – 2.84 (m, 2H), 1.79 (d, *J* = 6.5 Hz, 3H), 0.50 (d, *J* = 6.5 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.72, 198.41, 159.55, 147.75, 146.79, 144.53, 143.11, 136.17, 135.85, 134.07, 134.02, 133.48, 132.13, 131.82, 130.92, 128.85, 128.29, 127.58, 127.46, 127.29, 127.10, 126.97, 126.88, 126.80, 126.33, 125.44, 125.06, 123.25, 113.82, 56.78, 56.67, 55.24, 48.31, 45.83, 45.48, 32.48, 27.79, 21.85 ppm; **HRMS (ESI)**:

$C_{43}H_{35}O_3$ $[M + H]^+$ calcd: 599.2580, found: 599.2556.



3f

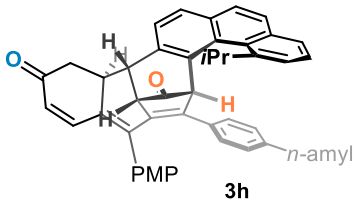
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 161 - 162 ℃, 43.0 mg, 70% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 1H), 7.63 – 7.45 (m, 4H), 7.41 (d, *J* = 8.1 Hz, 1H), 7.30 (dd, *J* = 16.2, 8.8 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.72 (d, *J* = 8.2 Hz, 2H), 6.17 (d, *J* = 7.7 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 5.80 (d, *J* = 7.7 Hz, 2H), 5.20 (s, 1H), 3.97 – 3.84 (m, 2H), 3.71 (s, 3H), 3.63 – 3.49 (m, 2H), 3.07 – 2.85 (m, 2H), 1.90 (s, 3H), 1.78 (d, *J* = 6.3 Hz, 3H), 0.50 (d, *J* = 6.3 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.71, 198.46, 159.57, 147.64, 146.88, 144.52, 143.43, 137.23, 136.19, 136.05, 134.09, 133.53, 133.29, 131.87, 130.91, 129.30, 128.22, 127.61, 127.55, 127.44, 127.33, 127.15, 126.97, 126.94, 126.24, 125.57, 125.10, 123.29, 113.93, 56.93, 56.52, 55.27, 48.41, 45.92, 45.49, 32.51, 27.84, 21.89, 20.90 ppm; **HRMS (ESI)**: $C_{44}H_{37}O_3$ $[M + H]^+$ calcd: 613.2736, found: 613.2715.



3g

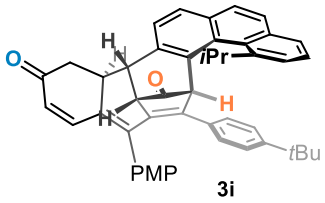
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 125 - 126 ℃, 48.0 mg, 73% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.54 – 7.46 (m, 3H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 8.8 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.5 Hz, 2H), 6.17 (d, *J* = 7.9 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 5.81 (d, *J* = 7.8 Hz, 2H), 5.20 (s, 1H), 3.96 – 3.81 (m, 2H), 3.69 (s, 3H), 3.64 – 3.50 (m, 2H), 3.03 – 2.87 (m, 2H), 2.17 (t, *J* = 7.4 Hz, 2H), 1.79 (d, *J* = 6.5 Hz, 3H), 1.24 (dt, *J* = 15.2, 7.6 Hz, 2H), 1.05 (dq, *J* = 14.2, 7.1 Hz, 2H), 0.82 (t, *J* = 7.2 Hz, 3H), 0.50 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.91, 198.48, 159.54, 147.88, 146.81, 144.62, 143.42, 142.08, 136.33, 135.91, 134.04, 133.37, 133.17, 131.79, 130.96, 129.43, 129.03, 128.25, 127.55, 127.39, 127.29, 127.08, 126.95,

126.88, 126.20, 125.44, 125.05, 123.23, 113.83, 56.78, 55.23, 48.38, 45.87, 45.48, 34.89, 33.14, 32.48, 27.80, 21.86, 13.94 ppm; **HRMS (ESI)**: $C_{47}H_{43}O_3$ $[M + H]^+$ calcd: 655.3206, found: 655.3179.



3h

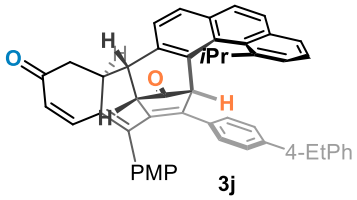
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 112 - 113 ℃, 49.7 mg, 74% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.54 – 7.46 (m, 3H), 7.41 (d, *J* = 8.2 Hz, 1H), 7.29 (d, *J* = 9.3 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 6.17 (d, *J* = 7.9 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 5.81 (d, *J* = 7.9 Hz, 2H), 5.20 (s, 1H), 3.96 – 3.80 (m, 2H), 3.69 (s, 3H), 3.63 – 3.50 (m, 2H), 3.08 – 2.87 (m, 2H), 2.16 (t, *J* = 7.4 Hz, 2H), 1.79 (d, *J* = 6.4 Hz, 3H), 1.33 – 1.14 (m, 4H), 1.02 (dt, *J* = 14.6, 7.4 Hz, 2H), 0.84 (t, *J* = 7.3 Hz, 3H), 0.50 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.87, 198.46, 159.55, 147.85, 146.83, 144.60, 143.42, 142.15, 136.31, 135.93, 134.05, 133.40, 133.19, 131.81, 130.95, 129.44, 129.09, 128.25, 127.55, 127.40, 127.31, 127.10, 126.94, 126.90, 126.21, 125.46, 125.06, 123.24, 113.85, 56.82, 56.73, 55.23, 48.39, 45.88, 45.49, 35.18, 32.48, 31.04, 30.68, 27.81, 22.47, 21.87, 14.05 ppm; **HRMS (ESI)**: $C_{48}H_{45}O_3$ $[M + H]^+$ calcd: 669.3362, found: 669.3342.



3i

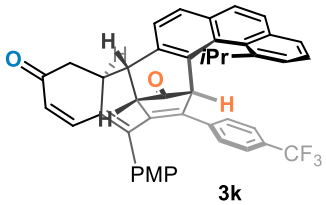
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 138 - 139 ℃, 48.0 mg, 73% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.54 (m, 1H), 7.54 – 7.45 (m, 3H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.28 (t, *J* = 6.0 Hz, 2H), 7.01 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.3 Hz, 2H), 6.35 (d, *J* = 8.1 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 5.82 (d, *J* = 8.1 Hz, 2H), 5.19 (s, 1H), 3.94 – 3.81 (m, 2H), 3.69 (s, 3H), 3.63 – 3.51 (m, 2H), 3.04 – 2.84 (m, 2H),

1.79 (d, *J* = 6.4 Hz, 3H), 0.98 (s, 9H), 0.50 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.91, 198.48, 159.53, 150.16, 147.84, 146.83, 144.66, 143.42, 136.37, 135.87, 134.08, 133.42, 133.26, 131.80, 130.95, 129.29, 129.20, 128.27, 127.55, 127.39, 127.19, 127.12, 126.99, 126.89, 126.23, 125.46, 125.03, 123.71, 123.27, 113.88, 56.83, 56.78, 55.26, 48.34, 45.86, 45.49, 34.10, 32.46, 30.86, 27.83, 21.88 ppm; **HRMS (ESI)**: $C_{47}H_{43}O_3$ $[M + H]^+$ calcd: 655.3206, found: 655.3182.



3j

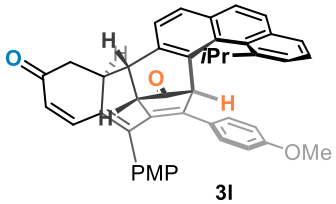
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 181 - 182 °C, 53.8 mg, 77% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.1 Hz, 1H), 7.59 (d, *J* = 4.0 Hz, 1H), 7.55 – 7.47 (m, 3H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.28 (q, *J* = 8.8 Hz, 2H), 7.14 (s, 4H), 7.05 (d, *J* = 8.1 Hz, 2H), 6.71 (d, *J* = 8.3 Hz, 2H), 6.58 (d, *J* = 7.8 Hz, 2H), 6.02 – 5.87 (m, 3H), 5.26 (s, 1H), 3.98 – 3.83 (m, 2H), 3.68 (s, 3H), 3.65 – 3.52 (m, 2H), 3.09 – 2.88 (m, 2H), 2.61 (q, *J* = 7.5 Hz, 2H), 1.80 (d, *J* = 6.3 Hz, 3H), 1.21 (t, *J* = 7.6 Hz, 3H), 0.51 (d, *J* = 6.3 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.65, 198.44, 159.64, 147.36, 146.88, 144.52, 143.58, 143.27, 139.75, 137.63, 136.21, 135.93, 134.12, 134.07, 133.66, 131.92, 130.96, 129.15, 128.26, 128.18, 127.83, 127.60, 127.53, 127.21, 127.01, 126.97, 126.67, 126.38, 125.56, 125.34, 125.17, 123.34, 113.98, 56.93, 56.62, 55.26, 48.40, 45.89, 45.52, 32.55, 28.50, 27.86, 21.90, 15.65 ppm; **HRMS (ESI)**: $C_{51}H_{43}O_3$ $[M + H]^+$ calcd: 703.3206, found: 703.3197.



3k

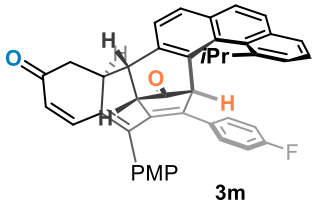
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 146 - 147 °C, 49.5 mg, 74% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.53 (m, 1H),

7.47 (dd, *J* = 13.5, 6.7 Hz, 4H), 7.32 (d, *J* = 8.7 Hz, 2H), 6.95 (d, *J* = 8.4 Hz, 2H), 6.64 (dd, *J* = 20.5, 8.2 Hz, 4H), 5.93 (t, *J* = 8.6 Hz, 3H), 5.18 (s, 1H), 3.96 – 3.80 (m, 2H), 3.69 (s, 3H), 3.67 – 3.57 (m, 2H), 3.08 – 2.87 (m, 2H), 1.78 (d, *J* = 6.5 Hz, 3H), 0.49 (d, *J* = 6.4 Hz, 3H) ppm; **^{19}F NMR** (282 MHz, $CDCl_3$) δ -62.98 ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.11, 198.19, 159.71, 146.71, 146.26, 144.27, 142.12, 136.25, 135.89, 135.48, 134.00, 133.90, 131.87, 130.83, 128.55, 128.24, 127.71, 127.64, 127.46, 127.26, 127.09, 126.80, 126.62, 125.44, 125.18, 123.66, 123.60, 123.32, 113.97, 57.00, 56.35, 55.24, 48.08, 45.66, 45.42, 32.46, 27.73, 21.77 ppm; **HRMS (ESI)**: $C_{44}H_{34}F_3O_3$ $[M + H]^+$ calcd: 667.2454, found: 667.2431.



3l

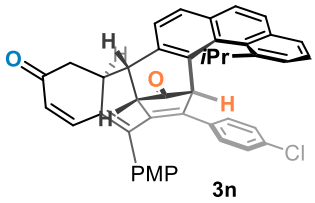
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 204 - 205 ℃, 44.9 mg, 72% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 1H), 7.58 (s, 1H), 7.52 (t, *J* = 4.9 Hz, 3H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.05 (d, *J* = 8.3 Hz, 2H), 6.72 (d, *J* = 8.3 Hz, 2H), 6.02 – 5.78 (m, 5H), 5.21 (s, 1H), 3,97 – 3.83 (m, 2H), 3.70 (s, 3H), 3.65 – 3.55 (m, 2H), 3.46 (s, 3H), 3.10 – 2.85 (m, 2H), 1.79 (d, *J* = 6.4 Hz, 3H), 0.50 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.84, 198.49, 159.59, 158.55, 147.21, 146.89, 144.54, 143.50, 136.26, 136.03, 134.08, 133.41, 132.26, 131.82, 130.93, 129.03, 128.89, 128.16, 127.59, 127.41, 127.12, 126.97, 126.93, 126.15, 125.55, 125.09, 124.65, 123.25, 113.93, 112.28, 56.96, 56.47, 55.25, 54.93, 48.46, 45.91, 45.48, 32.54, 27.82, 21.87 ppm; **HRMS (ESI)**: $C_{44}H_{37}O_4$ $[M + H]^+$ calcd: 629.2686, found: 629.2664.



3m

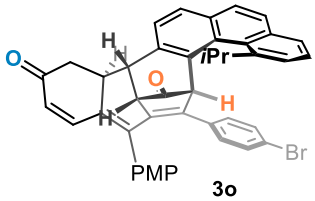
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 162 - 163 ℃,

43.5 mg, 71% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.50 (t, *J* = 4.6 Hz, 3H), 7.43 (d, *J* = 8.2 Hz, 1H), 7.31 (t, *J* = 5.6 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.68 (d, *J* = 8.3 Hz, 2H), 6.07 (t, *J* = 8.5 Hz, 2H), 5.98 – 5.82 (m, 3H), 5.18 (s, 1H), 3,96 – 3.82 (m, 2H), 3.69 (s, 3H), 3.66 – 3.54 (m, 2H), 3.09 – 2.83 (m, 2H), 1.79 (d, *J* = 6.4 Hz, 3H), 0.49 (d, *J* = 6.4 Hz, 3H) ppm; **^{19}F NMR** (282 MHz, $CDCl_3$) δ -113.39 ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.52, 198.32, 159.64, 146.78, 146.60, 144.39, 142.70, 136.08, 135.74, 134.13, 134.00, 133.57, 131.81, 130.88, 129.17, 129.06, 128.57, 128.22, 127.68, 127.52, 127.15, 127.00, 126.76, 126.47, 125.47, 125.14, 123.26, 113.92, 113.89, 113.64, 56.91, 56.56, 55.24, 48.26, 45.77, 45.45, 32.50, 27.76, 21.82 ppm; **HRMS (ESI)**: $C_{43}H_{34}FO_3$ $[M + H]^+$ calcd: 617.2486, found: 617.2461.



3n

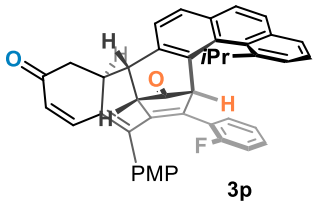
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 169 - 170 °C, 45.4 mg, 72% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.64 – 7.46 (m, 4H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.32 (q, *J* = 8.6 Hz, 2H), 6.99 (d, *J* = 8.1 Hz, 2H), 6.71 (d, *J* = 8.1 Hz, 2H), 6.34 (d, *J* = 8.0 Hz, 2H), 5.94 (d, *J* = 10.2 Hz, 1H), 5.80 (d, *J* = 8.0 Hz, 2H), 5.17 (s, 1H), 3.93 – 3.80 (m, 2H), 3.71 (s, 3H), 3.66 – 3.52 (m, 2H), 3.09 – 2.83 (m, 2H), 1.78 (d, *J* = 6.4 Hz, 3H), 0.49 (d, *J* = 6.3 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.28, 198.27, 159.69, 146.80, 146.34, 144.30, 142.57, 135.95, 135.71, 134.86, 134.04, 133.76, 133.08, 131.88, 130.85, 130.67, 128.71, 128.59, 128.17, 127.65, 127.58, 127.24, 127.05, 127.00, 126.75, 126.59, 125.53, 125.20, 123.31, 113.99, 56.67, 55.28, 48.22, 45.76, 45.44, 32.51, 27.78, 21.82 ppm; **HRMS (ESI)**: $C_{43}H_{33}NaClO_3$ $[M + Na]^+$ calcd: 655.2010, found: 655.1988.



3o

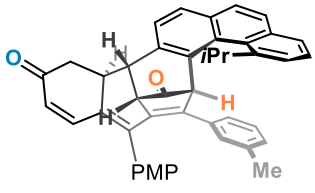
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 172 - 173 °C,

50.6 mg, 75% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.2 Hz, 1H), 7.53 (dt, *J* = 16.0, 8.5 Hz, 4H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.32 (dd, *J* = 16.7, 8.5 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.71 (d, *J* = 8.4 Hz, 2H), 6.48 (d, *J* = 8.2 Hz, 2H), 5.94 (d, *J* = 10.2 Hz, 1H), 5.72 (d, *J* = 8.2 Hz, 2H), 5.16 (s, 1H), 3.94 – 3.79 (m, 2H), 3.70 (d, *J* = 7.7 Hz, 3H), 3.66 – 3.50 (m, 2H), 3.08 – 2.85 (m, 2H), 1.78 (d, *J* = 6.3 Hz, 3H), 0.49 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.24, 198.27, 159.69, 146.79, 146.37, 144.30, 142.55, 135.93, 135.70, 134.96, 134.04, 133.78, 131.89, 131.15, 130.84, 129.95, 128.86, 128.75, 128.17, 127.66, 127.60, 127.26, 127.06, 126.73, 126.62, 125.54, 125.23, 123.33, 121.49, 114.02, 56.63, 55.29, 48.18, 45.76, 45.44, 32.51, 27.79, 21.83 ppm; **HRMS (ESI)**: $C_{43}H_{34}BrO_3$ $[M + H]^+$ calcd: 677.1685, found: 677.1654.



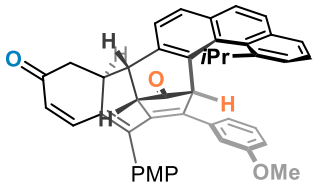
3p

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 148 - 149 °C, 43.5 mg, 71% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.2 Hz, 1H), 7.44 (ddd, *J* = 20.0, 16.1, 8.7 Hz, 4H), 7.30 (s, 1H), 7.22 (d, *J* = 8.5 Hz, 1H), 7.15 (d, *J* = 8.5 Hz, 1H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.68 – 6.38 (m, 3H), 6.14 (t, *J* = 8.2 Hz, 2H), 5.94 (d, *J* = 10.1 Hz, 1H), 5.58 (t, *J* = 7.3 Hz, 1H), 5.20 (s, 1H), 3.90 (d, *J* = 4.5 Hz, 1H), 3.87 – 3.74 (m, 1H), 3.68 (t, *J* = 9.7 Hz, 1H), 3.65 – 3.42 (m, 4H), 2.97 (d, *J* = 9.7 Hz, 2H), 1.79 (d, *J* = 6.5 Hz, 3H), 0.47 (d, *J* = 6.4 Hz, 3H) ppm; ^{19}F NMR (282 MHz, $CDCl_3$) δ -113.44 ppm; ^{13}C NMR (75 MHz, $CDCl_3$) δ 210.32, 198.38, 159.40, 146.50, 144.88, 142.98, 142.39, 136.61, 136.50, 135.42, 133.59, 132.82, 131.62, 131.00, 129.20 ($J_{C\text{-}F}$ = 8.6 Hz), 129.01 ($J_{C\text{-}F}$ = 3.6 Hz), 128.51, 127.66, 127.36, 127.09, 126.99, 126.83, 126.35, 126.31, 124.98, 124.70, 123.13, 122.19 ($J_{C\text{-}F}$ = 3.4 Hz), 119.83 ($J_{C\text{-}F}$ = 15.5 Hz), 113.98 ($J_{C\text{-}F}$ = 22.0 Hz), 113.43, 57.62, 55.14, 55.12, 48.15, 45.54, 45.34, 32.37, 27.66, 21.78 ppm; **HRMS (ESI)**: $C_{43}H_{34}FO_3$ $[M + H]^+$ calcd: 617.2486, found: 617.2466.



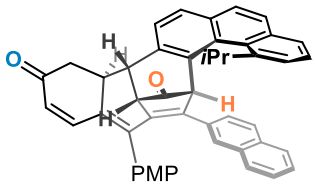
3q

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 140 - 141 ℃, 43.0 mg, 70% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.1 Hz, 1H), 7.62 – 7.40 (m, 5H), 7.35 (q, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.5 Hz, 2H), 6.72 (d, *J* = 8.5 Hz, 2H), 6.46 (d, *J* = 7.5 Hz, 1H), 6.27 (t, *J* = 7.6 Hz, 1H), 5.91 (d, *J* = 10.1 Hz, 1H), 5.68 (d, *J* = 11.5 Hz, 2H), 5.17 (s, 1H), 3.98 – 3.80 (m, 2H), 3.77 – 3.67 (m, 3H), 3.67 – 3.51 (m, 2H), 3.10 – 2.85 (m, 2H), 1.78 (d, *J* = 6.4 Hz, 3H), 1.61 (s, 3H), 0.50 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.45, 198.45, 159.55, 148.09, 146.96, 144.51, 143.30, 136.47, 136.17, 136.06, 134.16, 134.13, 133.66, 132.30, 131.94, 130.88, 129.65, 128.33, 128.18, 128.08, 127.61, 127.54, 127.25, 127.05, 127.00, 126.68, 126.34, 125.64, 125.18, 124.63, 123.40, 113.91, 56.67, 55.27, 48.29, 45.89, 45.44, 32.47, 27.84, 21.91, 20.76 ppm; **HRMS (ESI)**: $C_{44}H_{37}O_3$ $[M + H]^+$ calcd: 613.2736, found: 613.2714.



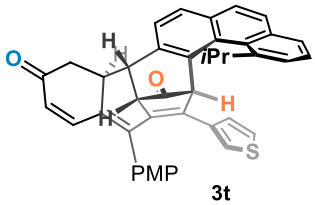
3r

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 213 - 214 ℃, 44.9 mg, 72% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.1 Hz, 1H), 7.55 (s, 1H), 7.46 (dd, *J* = 17.3, 8.0 Hz, 4H), 7.30 (d, *J* = 8.5 Hz, 2H), 6.98 (d, *J* = 8.0 Hz, 2H), 6.66 (d, *J* = 8.1 Hz, 2H), 6.29 (t, *J* = 7.8 Hz, 1H), 6.19 (d, *J* = 8.0 Hz, 1H), 5.93 (d, *J* = 10.1 Hz, 1H), 5.53 (s, 1H), 5.45 (d, *J* = 7.4 Hz, 1H), 5.18 (s, 1H), 3.97 – 3.81 (m, 2H), 3.67 (s, 3H), 3.65 – 3.53 (m, 2H), 3.19 (s, 3H), 3.06 – 2.86 (m, 2H), 1.79 (d, *J* = 6.3 Hz, 3H), 0.48 (d, *J* = 6.2 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.59, 198.38, 159.53, 158.12, 147.76, 146.83, 144.53, 142.99, 136.12, 135.93, 134.44, 134.08, 133.54, 133.45, 131.83, 130.88, 128.64, 128.33, 127.73, 127.60, 127.54, 127.11, 126.87, 126.35, 125.43, 125.11, 123.23, 120.07, 113.86, 113.79, 112.23, 57.02, 56.52, 55.21, 54.79, 48.31, 45.82, 45.48, 32.44, 27.78, 21.94 ppm; **HRMS (ESI)**: $C_{44}H_{37}O_4$ $[M + H]^+$ calcd: 629.2686, found: 629.2664.



3s

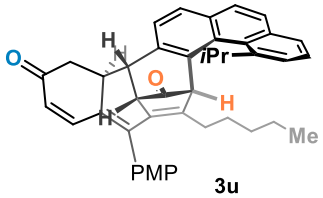
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 165 - 166 ℃, 47.3 mg, 73% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.1 Hz, 1H), 7.64 – 7.56 (m, 1H), 7.56 – 7.46 (m, 3H), 7.42 (d, *J* = 8.2 Hz, 1H), 7.39 – 7.26 (m, 3H), 7.25 – 7.15 (m, 3H), 7.05 (d, *J* = 8.4 Hz, 2H), 6.92 – 6.79 (m, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 6.33 (s, 1H), 6.06 (d, *J* = 8.6 Hz, 1H), 5.93 (d, *J* = 10.1 Hz, 1H), 5.34 (s, 1H), 4.03 – 3.84 (m, 2H), 3.73 – 3.55 (m, 5H), 3.11 – 2.88 (m, 2H), 1.81 (d, *J* = 6.4 Hz, 3H), 0.52 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.29, 198.43, 159.62, 147.57, 147.07, 144.40, 143.27, 136.16, 136.09, 134.88, 134.16, 133.91, 132.10, 132.02, 130.92, 129.85, 129.75, 128.22, 127.65, 127.39, 127.32, 127.09, 127.03, 126.88, 126.48, 126.25, 126.11, 125.74, 125.45, 125.36, 125.03, 123.49, 114.08, 57.01, 56.39, 55.25, 48.41, 45.93, 45.54, 32.59, 27.91, 21.99 ppm; **HRMS (ESI)**: $C_{47}H_{37}O_3$ $[M + H]^+$ calcd: 649.2736, found: 649.2725.



3t

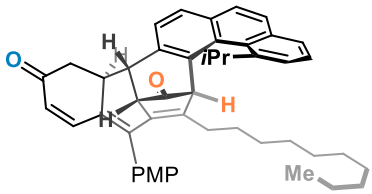
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 173 - 174 ℃, 42.0 mg, 70% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.73 – 7.57 (m, 5H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.16 (d, *J* = 8.3 Hz, 2H), 6.84 (d, *J* = 8.3 Hz, 2H), 6.46 – 6.34 (m, 1H), 5.94 (d, *J* = 10.2 Hz, 1H), 5.53 (s, 1H), 5.47 (d, *J* = 5.0 Hz, 1H), 5.20 (s, 1H), 3.98 – 3.86 (m, 2H), 3.74 (s, *J* = 14.0 Hz, 3H), 3.64 – 3.49 (m, 2H), 3.09 – 2.84 (m, 2H), 1.79 (d, *J* = 6.4 Hz, 3H), 0.52 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.25, 198.38, 159.90, 147.17, 144.22, 143.06, 142.50, 136.17, 135.85, 134.20, 133.92, 133.34, 132.10, 131.96, 131.07, 129.47, 128.00, 127.63, 127.40, 126.97, 126.89, 126.85, 126.43, 125.93, 125.39, 125.10, 124.14, 123.49, 114.44, 56.77, 56.24, 55.37, 48.49, 45.97, 45.44, 32.65, 27.91, 21.90 ppm; **HRMS (ESI)**: $C_{41}H_{33}SO_3$ [M +

H]$^+$ calcd: 605.2144, found: 605.2117.



3u

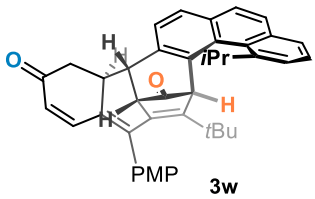
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 122 - 123 ℃, 40.6 mg, 69% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 1H), 7.64 – 7.55 (m, 2H), 7.55 – 7.35 (m, 5H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.80 (d, *J* = 8.4 Hz, 2H), 5.89 (d, *J* = 10.1 Hz, 1H), 4.84 (s, 1H), 3.87 – 3.72 (m, 5H), 3.53 (t, *J* = 9.8 Hz, 1H), 3.41 (d, *J* = 4.5 Hz, 1H), 2.90 (d, *J* = 9.9 Hz, 2H), 1.76 (d, *J* = 6.4 Hz, 3H), 1.11 – 0.95 (m, 1H), 0.65 – 0.45 (m, 9H), 0.39 – 0.24 (m, 1H), 0.24 – 0.04 (m, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 210.77, 198.55, 159.77, 153.01, 147.13, 144.91, 142.68, 136.46, 136.06, 134.05, 133.66, 131.86, 131.73, 130.86, 128.96, 128.38, 128.04, 127.20, 127.10, 126.73, 125.89, 125.72, 125.21, 123.31, 114.00, 55.74, 55.29, 54.26, 48.02, 45.82, 45.13, 32.57, 30.90, 27.72, 26.99, 25.72, 21.86, 21.72, 13.76 ppm; **HRMS (ESI)**: $C_{42}H_{41}O_3$ [M + H]$^+$ calcd: 593.3049, found: 593.3036.



3v

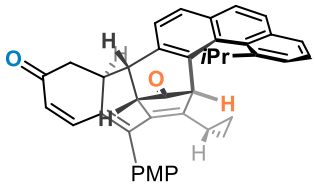
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 73 - 74 ℃, 49.0 mg, 74% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.2 Hz, 1H), 7.62 – 7.56 (m, 2H), 7.55 – 7.50 (m, 1H), 7.48 (d, *J* = 5.9 Hz, 1H), 7.46 – 7.34 (m, 3H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.80 (d, *J* = 8.2 Hz, 2H), 5.89 (d, *J* = 10.1 Hz, 1H), 4.83 (s, 1H), 3.86 – 3.70 (m, 5H), 3.53 (t, *J* = 9.8 Hz, 1H), 3.41 (d, *J* = 4.4 Hz, 1H), 2.90 (d, *J* = 9.9 Hz, 2H), 1.76 (d, *J* = 6.4 Hz, 3H), 1.35 – 1.13 (m, 8H), 1.03 (dt, *J* = 13.5, 6.6 Hz, 3H), 0.97 – 0.80 (m, 6H), 0.62 – 0.40 (m, 6H), 0.30 (dt, *J* = 16.2, 8.4 Hz, 1H), 0.14 (dt, *J* = 31.4, 7.1 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 210.73, 198.54, 159.77, 153.01, 147.13, 144.90, 142.70, 136.47, 136.07, 134.04, 133.69, 131.86, 131.73, 130.87, 128.93,

128.40, 128.04, 127.20, 127.09, 126.75, 125.88, 125.73, 125.23, 123.31, 113.99, 55.79, 55.25, 54.26, 48.02, 45.82, 45.14, 32.56, 31.94, 29.48, 29.30, 29.28, 28.71, 27.72, 27.11, 26.10, 22.74, 21.87, 14.20 ppm; **HRMS (ESI)**: $C_{47}H_{51}O_3$ $[M + H]^+$ calcd: 663.3832, found: 663.3806.



3w

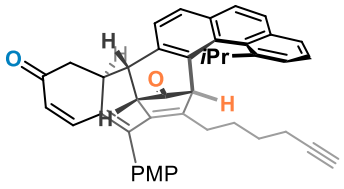
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 192 - 193 ℃, 38.9 mg, 67% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.74 (d, *J* = 8.1 Hz, 1H), 7.61 (d, *J* = 7.5 Hz, 2H), 7.56 – 7.48 (m, 2H), 7.44 (t, *J* = 7.0 Hz, 3H), 7.08 (d, *J* = 7.6 Hz, 2H), 6.84 (d, *J* = 7.8 Hz, 2H), 5.92 (d, *J* = 10.2 Hz, 1H), 4.80 (s, 1H), 4.03 – 3.60 (m, 5H), 3.56 – 3.26 (m, 2H), 3.17 – 2.80 (m, 2H), 1.76 (d, *J* = 6.4 Hz, 3H), 0.49 (d, *J* = 6.6 Hz, 3H), -0.09 (s, 9H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.62, 198.51, 159.53, 158.15, 147.18, 144.59, 143.97, 137.30, 135.67, 134.05, 133.38, 133.24, 132.02, 131.03, 130.26, 128.39, 127.49, 127.40, 127.19, 127.11, 127.01, 126.10, 125.91, 125.33, 123.34, 113.83, 58.18, 55.30, 54.53, 48.60, 46.19, 45.23, 33.97, 32.33, 29.44, 27.92, 22.18 ppm; **HRMS (ESI)**: $C_{41}H_{39}O_3$ $[M + H]^+$ calcd: 579.2893, found: 579.2874.



3x

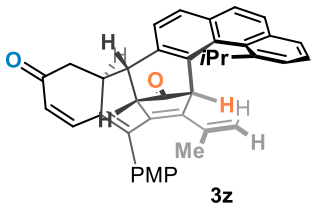
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 222 - 223 ℃, 37.0 mg, 66% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.1 Hz, 1H), 7.78 – 7.60 (m, 4H), 7.54 (dd, *J* = 17.0, 8.6 Hz, 3H), 7.27 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 6.00 (d, *J* = 10.1 Hz, 1H), 4.53 (s, 1H), 3.95 – 3.76 (m, 5H), 3.69 (t, *J* = 9.8 Hz, 1H), 3.51 (d, *J* = 4.5 Hz, 1H), 3.01 (d, *J* = 10.0 Hz, 2H), 1.81 (d, *J* = 6.4 Hz, 3H), 0.55 (d, *J* = 6.4 Hz, 3H), 0.52 – 0.39 (m, 1H), 0.07 – -0.08 (m, 1H), -0.19 – -0.36 (m, 1H), -0.39 – -0.55 (m, 1H), -1.42 (dq, *J* = 10.4, 5.2 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.43, 198.65, 159.72, 153.56, 147.13, 144.93, 142.97,

136.40, 136.04, 134.06, 133.70, 131.80, 131.69, 131.00, 129.00, 128.14, 128.08, 127.37, 127.32, 127.05, 126.68, 125.94, 125.76, 125.43, 123.34, 114.09, 55.25, 54.40, 52.41, 48.07, 46.00, 45.27, 32.52, 27.78, 21.99, 9.66, 5.27, 5.10 ppm; **HRMS (ESI)**: $C_{40}H_{35}O_3$ $[M + H]^+$ calcd: 563.2580, found: 563.2558.



3y

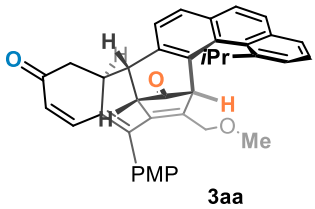
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 127 - 128 °C, 41.8 mg, 70% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.2 Hz, 1H), 7.46 – 7.19 (m, 7H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.64 (d, *J* = 8.4 Hz, 2H), 5.72 (d, *J* = 10.1 Hz, 1H), 4.65 (s, 1H), 3.69 – 3.53 (m, 5H), 3.35 (t, *J* = 9.8 Hz, 1H), 3.24 (d, *J* = 4.4 Hz, 1H), 2.73 (d, *J* = 9.8 Hz, 2H), 1.64 – 1.53 (m, 4H), 1.21 (t, *J* = 7.2 Hz, 2H), 0.95 – 0.80 (m, 1H), 0.46 – 0.34 (m, 2H), 0.31 (d, *J* = 6.4 Hz, 3H), 0.25 – 0.13 (m, 1H), -0.00 (dtd, *J* = 20.9, 14.0, 6.9 Hz, 2H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 210.48, 198.49, 159.81, 151.99, 147.15, 144.80, 142.39, 136.34, 136.05, 134.23, 134.00, 132.05, 131.73, 130.82, 128.82, 128.35, 128.10, 127.29, 127.10, 126.67, 126.03, 125.78, 125.25, 123.39, 114.10, 84.18, 68.00, 55.67, 55.30, 54.25, 47.96, 45.79, 45.13, 32.57, 27.71, 27.61, 26.55, 25.31, 21.86, 17.55 ppm; **HRMS (ESI)**: $C_{43}H_{39}O_3$ $[M + H]^+$ calcd: 603.2893, found: 603.2867.



3z

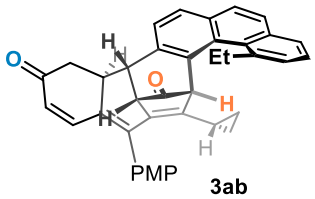
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 166 - 167 °C, 37.0 mg, 66% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.2 Hz, 1H), 7.55 (dd, *J* = 18.0, 7.7 Hz, 4H), 7.41 (q, *J* = 8.5 Hz, 3H), 7.05 (d, *J* = 8.3 Hz, 2H), 6.78 (d, *J* = 8.3 Hz, 2H), 5.93 (d, *J* = 10.2 Hz, 1H), 5.01 (s, 1H), 3.94 (s, 1H), 3.89 – 3.81 (m, 2H), 3.75 (s, 3H), 3.61 – 3.43 (m, 3H), 3.05 – 2.82 (m, 2H), 1.77 (d, *J* = 6.4 Hz, 3H), 0.61 (s, 3H), 0.49 (d, *J* = 6.4 Hz, 3H) ppm; **^{13}C**

NMR (75 MHz, $CDCl_3$) δ 209.94, 198.40, 159.50, 149.29, 146.96, 144.38, 143.35, 136.19, 136.01, 134.06, 133.89, 133.01, 131.79, 131.12, 129.12, 128.28, 127.48, 127.41, 127.14, 127.05, 126.97, 126.14, 125.74, 125.24, 123.26, 117.67, 113.70, 56.64, 55.24, 55.18, 48.52, 45.87, 45.30, 32.52, 27.80, 21.92, 21.18 ppm; **HRMS (ESI)**: $C_{40}H_{35}O_3$ $[M + H]^+$ calcd: 563.2580, found: 563.2554.



3aa

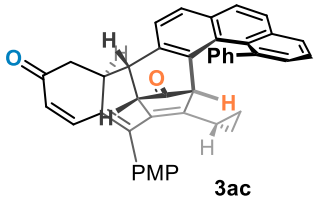
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 151 - 152 °C, 37.5 mg, 66% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.74 (d, *J* = 8.2 Hz, 1H), 7.63 – 7.56 (m, 2H), 7.50 (dd, *J* = 15.8, 6.6 Hz, 3H), 7.40 (dd, *J* = 8.3, 3.9 Hz, 2H), 7.09 (d, *J* = 8.2 Hz, 2H), 6.81 (d, *J* = 8.2 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 5.02 (s, 1H), 3.93 – 3.79 (m, 3H), 3.76 (s, 3H), 3.59 – 3.49 (m, 1H), 3.47 (d, *J* = 4.5 Hz, 1H), 2.97 – 2.82 (m, 3H), 2.34 (d, *J* = 12.9 Hz, 1H), 2.05 (s, 3H), 1.76 (d, *J* = 6.4 Hz, 3H), 0.48 (d, *J* = 6.3 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 210.09, 198.36, 159.92, 148.07, 147.12, 144.55, 141.35, 136.35, 136.15, 135.57, 133.95, 132.68, 131.71, 130.82, 128.67, 128.24, 127.81, 127.36, 127.24, 127.01, 126.51, 125.51, 125.07, 123.40, 114.18, 65.67, 57.77, 55.29, 54.58, 54.46, 47.83, 45.64, 45.20, 32.54, 29.72, 27.80, 21.81 ppm; **HRMS (ESI)**: $C_{39}H_{35}O_4$ $[M + H]^+$ calcd: 567.2529, found: 567.2506.



3ab

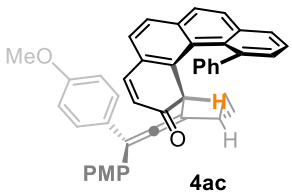
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 237 - 238 °C, 48.2 mg, 88% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 8.1 Hz, 1H), 7.74 (d, *J* = 7.1 Hz, 1H), 7.69 – 7.44 (m, 6H), 7.27 (d, *J* = 7.6 Hz, 2H), 6.92 (d, *J* = 7.4 Hz, 2H), 6.01 (d, *J* = 10.0 Hz, 1H), 4.47 (s, 1H), 4.00 – 3.82 (m, 4H), 3.73 (t, *J* = 9.9 Hz, 1H), 3.48 (dd, *J* = 21.1, 6.1 Hz, 2H), 3.15 (dq, *J* = 15.2, 7.6 Hz, 1H), 3.01 (d, *J* = 9.9 Hz, 2H), 1.09 – 0.84 (m, 3H), 0.47 (td, *J* =

8.3, 4.3 Hz, 1H), -0.00 (hept, *J* = 5.2 Hz, 1H), -0.26 (dt, *J* = 10.7, 5.2 Hz, 1H), -0.45 (qd, *J* = 8.6, 8.1, 5.5 Hz, 1H), -1.41 (dq, *J* = 10.7, 5.5 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.16, 198.65, 159.72, 153.66, 144.99, 142.94, 142.18, 136.44, 136.25, 133.81, 133.72, 131.67, 131.63, 131.00, 128.96, 128.29, 128.18, 127.70, 127.11, 127.03, 125.81, 125.05, 114.08, 55.26, 54.34, 53.00, 47.88, 45.94, 45.10, 28.87, 17.66, 9.62, 5.22, 5.13 ppm; **HRMS (ESI)**: $C_{39}H_{33}O_3$ $[M + H]^+$ calcd: 549.2423, found: 549.2407.



3ac

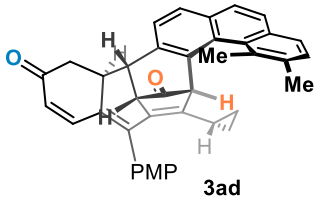
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 4/1 to 2/1). Yellow solid, m.p. 194 - 195 ℃, 24.6 mg, 41% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.45 – 6.03 (m, 17H), 5.85 (d, *J* = 10.1 Hz, 1H), 4.58 (s, 1H), 3.74 (d, *J* = 1.7 Hz, 3H), 3.47 (dd, *J* = 15.9, 5.6 Hz, 2H), 3.05 (d, *J* = 4.6 Hz, 1H), 2.94 – 2.63 (m, 2H), 0.34 (td, *J* = 7.6, 3.8 Hz, 1H), 0.07 – -0.15 (m, 1H), -0.21 (dt, *J* = 10.2, 5.5 Hz, 1H), -0.50 (dt, *J* = 11.7, 6.2 Hz, 1H), -1.32 (dq, *J* = 11.0, 5.6 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 206.43, 198.63, 159.69, 153.85, 144.92, 143.00, 142.35, 140.83, 136.99, 136.46, 135.15, 133.77, 131.82, 131.60, 130.93, 130.22, 129.04, 128.95, 128.81, 128.34, 127.74, 127.47, 127.09, 126.83, 126.75, 126.46, 125.63, 114.04, 55.23, 53.71, 51.70, 47.23, 45.83, 45.23, 9.66, 5.30, 5.18 ppm; **HRMS (ESI)**: $C_{43}H_{33}O_3$ $[M + H]^+$ calcd: 597.2423, found: 597.2401.



4ac

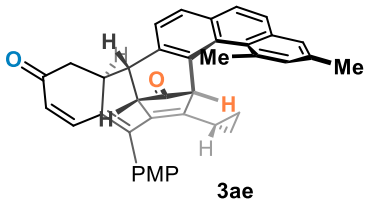
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 7/1). Yellow solid, m.p. 100 - 101 ℃, 32.6 mg, 53% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.08 – 6.99 (m, 13H), 6.77 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.4 Hz, 2H), 6.59 (d, *J* = 8.2 Hz, 2H), 6.27 (d, *J* = 8.2 Hz, 2H), 5.71 (d, *J* = 9.7 Hz, 1H), 5.36 (s, 1H), 3.82 (s, 3H), 3.76 (s, 3H), 1.06 (tt, *J* = 9.1, 5.5 Hz, 1H), 0.27 (d, *J* = 8.2 Hz, 2H), -0.11 (dt, *J* = 8.3, 4.6 Hz, 1H), -0.48 (dt, *J* = 10.4, 4.3 Hz, 1H) ppm; **^{13}C NMR** (75 MHz,

$CDCl_3$) δ 200.89, 198.10, 158.57, 158.38, 145.97, 143.42, 140.53, 140.44, 134.84, 134.73, 129.86, 129.28, 128.73, 128.59, 128.55, 128.49, 128.32, 128.21, 128.04, 127.76, 127.40, 127.23, 127.11, 126.86, 126.40, 126.22, 122.63, 113.33, 113.30, 112.42, 112.19, 57.77, 55.33, 55.26, 12.42, 7.08, 6.28 ppm; **HRMS (ESI)**: $C_{44}H_{35}O_3$ $[M + H]^+$ calcd: 611.2580, found: 611.2560.



3ad

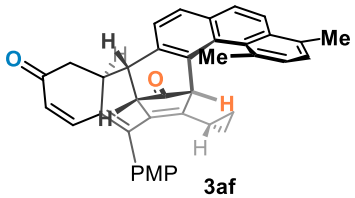
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 176 - 177 °C, 50.4 mg, 92% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.1 Hz, 1H), 7.66 (t, *J* = 9.3 Hz, 2H), 7.60 – 7.39 (m, 4H), 7.26 (d, *J* = 8.2 Hz, 2H), 6.91 (d, *J* = 8.2 Hz, 2H), 6.00 (d, *J* = 10.1 Hz, 1H), 4.38 (s, 1H), 4.10 – 3.80 (m, 4H), 3.73 (t, *J* = 9.9 Hz, 1H), 3.51 (d, *J* = 4.3 Hz, 1H), 3.00 (d, *J* = 9.9 Hz, 2H), 2.66 (s, 3H), 2.56 (s, 3H), 0.57 – 0.39 (m, 1H), 0.08 – -0.09 (m, 1H), -0.27 (td, *J* = 10.1, 5.2 Hz, 1H), -0.35 – -0.54 (m, 1H), -1.38 (dq, *J* = 10.3, 5.1 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.16, 198.65, 159.72, 153.59, 144.97, 142.93, 136.38, 136.16, 136.01, 133.90, 133.39, 132.27, 131.86, 131.62, 130.99, 129.44, 129.16, 128.99, 128.66, 128.00, 127.09, 126.93, 125.82, 124.86, 124.80, 114.08, 55.25, 54.40, 52.98, 47.90, 45.93, 45.08, 21.32, 20.74, 9.64, 5.20 ppm; **HRMS (ESI)**: $C_{39}H_{33}O_3$ $[M + H]^+$ calcd: 549.2423, found: 549.2409.



3ae

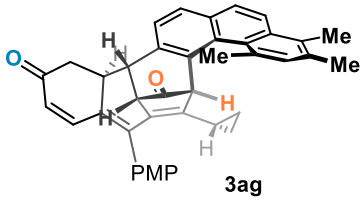
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 228 - 229 °C, 39.9 mg, 73% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.1 Hz, 1H), 7.62 (d, *J* = 10.1 Hz, 1H), 7.55 – 7.39 (m, 4H), 7.31 (s, 1H), 7.24 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.3 Hz, 2H), 5.98 (d, *J* = 10.1 Hz, 1H), 4.37 (s, 1H), 3.83 (s, 4H), 3.72 (t, *J* = 9.9 Hz, 1H), 3.48 (d, *J* = 4.3 Hz, 1H), 2.97 (d, *J* = 10.0 Hz, 2H), 2.72 (s, 3H), 2.57 (s, 3H), 0.58 – 0.38 (m, 1H), 0.06 – -0.08 (m, 1H), -0.21 (td, *J* = 10.2, 5.3 Hz, 1H), -0.35 – -0.53 (m, 1H), -1.31 (dq, *J* = 10.5, 5.3 Hz, 1H) ppm; **^{13}C NMR**

(75 MHz, $CDCl_3$) δ 209.07, 198.67, 159.72, 153.69, 144.99, 142.96, 136.50, 136.41, 136.04, 135.03, 134.25, 133.80, 131.63, 131.40, 131.01, 130.60, 129.01, 128.87, 127.77, 127.30, 127.15, 126.96, 125.82, 125.66, 124.88, 114.08, 55.25, 54.43, 53.11, 47.92, 45.90, 45.04, 23.04, 21.26, 9.71, 5.23 ppm; **HRMS (ESI)**: $C_{39}H_{33}O_3$ $[M + H]^+$ calcd: 549.2423, found: 549.2400.



3af

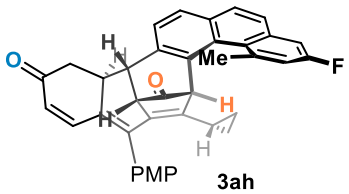
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 194 - 195 °C, 50.9 mg, 93% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.82 (t, *J* = 9.3 Hz, 2H), 7.64 (d, *J* = 10.1 Hz, 1H), 7.53 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.40 (q, *J* = 7.6 Hz, 2H), 7.32 – 7.17 (m, 2H), 7.03 – 6.67 (m, 2H), 6.00 (d, *J* = 10.0 Hz, 1H), 4.41 (s, 1H), 3.84 (d, *J* = 1.5 Hz, 4H), 3.73 (t, *J* = 9.8 Hz, 1H), 3.49 (d, *J* = 4.5 Hz, 1H), 2.99 (d, *J* = 9.9 Hz, 2H), 2.74 (d, *J* = 13.7 Hz, 6H), 0.46 (dq, *J* = 8.9, 5.5, 4.5 Hz, 1H), -0.00 (tq, *J* = 8.2, 5.2 Hz, 1H), -0.22 (dq, *J* = 10.5, 5.3 Hz, 1H), -0.46 (td, *J* = 9.1, 4.4 Hz, 1H), -1.37 (dq, *J* = 10.6, 5.4 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.16, 198.75, 159.70, 153.78, 145.06, 142.98, 136.47, 136.38, 133.74, 132.92, 132.69, 131.62, 131.30, 131.02, 130.98, 129.36, 129.03, 128.96, 128.24, 128.13, 128.04, 127.03, 125.79, 125.44, 123.00, 114.07, 55.27, 54.37, 52.97, 47.87, 45.92, 45.06, 22.96, 19.57, 9.67, 5.28, 5.18 ppm; **HRMS (ESI)**: $C_{39}H_{33}O_3$ $[M + H]^+$ calcd: 549.2423, found: 549.2411.



3ag

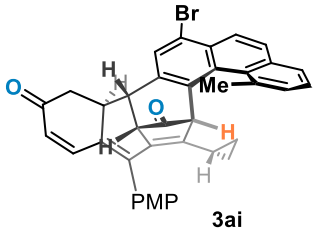
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 182 - 183 °C, 43.4 mg, 77% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.83 (dd, *J* = 13.0, 8.6 Hz, 2H), 7.64 (d, *J* = 10.1 Hz, 1H), 7.57 – 7.43 (m, 2H), 7.33 – 7.19 (m, 3H), 6.91 (d, *J* = 8.2 Hz, 2H), 6.00 (d, *J* = 10.1 Hz, 1H), 4.39 (s, 1H), 3.85 (s, 4H), 3.74 (t, *J* = 9.8 Hz, 1H), 3.49 (d, *J* = 4.4 Hz, 1H), 2.99 (d, *J* = 10.0 Hz, 2H), 2.69 (d, *J* = 7.3 Hz, 6H), 2.57 (s, 3H), 0.56 – 0.40 (m, 1H), 0.07 – -0.09 (m, 1H), -0.21 (td, *J* = 10.2, 5.2 Hz, 1H), -0.34 – -0.55 (m, 1H), -1.20 – -1.42 (m, 1H) ppm; **^{13}C NMR** (75

MHz, $CDCl_3$) δ 209.18, 198.70, 159.70, 153.80, 145.01, 142.99, 136.34, 136.17, 134.65, 133.71, 132.96, 132.11, 131.65, 131.01, 130.94, 130.87, 129.20, 129.04, 128.67, 127.89, 127.73, 126.84, 125.78, 125.23, 123.15, 114.07, 55.25, 54.42, 53.07, 47.92, 45.91, 45.04, 22.74, 20.59, 14.82, 9.70, 5.30, 5.23 ppm; **HRMS (ESI)**: $C_{40}H_{35}O_3$ $[M + H]^+$ calcd: 563.2580, found: 563.2560.



3ah

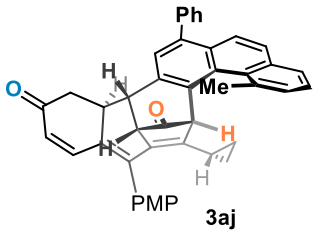
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 167 - 168 °C, 49.6 mg, 89% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.75 (d, *J* = 8.1 Hz, 1H), 7.57 (d, *J* = 10.1 Hz, 1H), 7.44 (q, *J* = 8.8, 6.5 Hz, 3H), 7.38 – 7.06 (m, 5H), 6.83 (d, *J* = 8.2 Hz, 2H), 5.92 (d, *J* = 10.1 Hz, 1H), 4.23 (s, 1H), 3.77 (s, 4H), 3.65 (t, *J* = 9.9 Hz, 1H), 3.43 (d, *J* = 4.4 Hz, 1H), 2.91 (d, *J* = 9.9 Hz, 2H), 2.70 (s, 3H), 0.41 (q, *J* = 6.9 Hz, 1H), -0.02 (p, *J* = 7.2 Hz, 1H), -0.26 (dq, *J* = 10.8, 5.3 Hz, 1H), -0.48 (p, *J* = 8.1 Hz, 1H), -1.43 (dq, *J* = 10.9, 5.5 Hz, 1H) ppm; **^{19}F NMR** (282 MHz, $CDCl_3$) δ -115.15 ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 208.85, 198.66, 160.80 ($J_{C\text{-}F}$ = 247.8 Hz), 159.74, 153.44, 144.99, 142.87, 138.23 ($J_{C\text{-}F}$ = 7.9 Hz), 137.10, 136.07, 135.40 ($J_{C\text{-}F}$ = 9.1 Hz), 133.91, 131.61, 131.17, 131.01, 128.86, 128.63, 128.21, 127.39, 127.10, 126.49 ($J_{C\text{-}F}$ = 3.6 Hz), 126.02, 125.88, 116.84 ($J_{C\text{-}F}$ = 22.3 Hz), 114.10, 109.59 ($J_{C\text{-}F}$ = 20.8 Hz), 55.27, 54.31, 52.98, 47.90, 45.88, 45.03, 23.39, 9.66, 5.29, 5.23 ppm; **HRMS (ESI)**: $C_{38}H_{30}FO_3$ $[M + H]^+$ calcd: 553.2173, found: 553.2149.



3ai

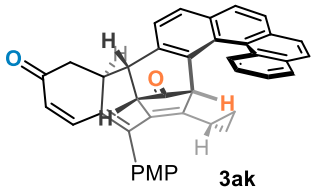
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 186 - 187 °C, 41.1 mg, 67% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.8 Hz, 1H), 7.73 (d, *J* = 8.5 Hz, 2H), 7.68 – 7.53 (m, 3H), 7.49 (d, *J* = 7.1 Hz, 1H), 7.25 (d, *J* = 8.3 Hz, 2H), 6.89 (d, *J* = 8.3 Hz,

2H), 5.99 (d, *J* = 10.1 Hz, 1H), 4.31 (s, 1H), 3.83 (s, 3H), 3.79 (d, *J* = 4.2 Hz, 1H), 3.66 (t, *J* = 9.8 Hz, 1H), 3.47 (d, *J* = 4.1 Hz, 1H), 2.96 (d, *J* = 9.9 Hz, 2H), 2.72 (s, 3H), 0.45 (dd, *J* = 11.4, 6.6 Hz, 1H), 0.05 – -0.08 (m, 1H), -0.27 (dd, *J* = 9.3, 5.0 Hz, 1H), -0.35 – -0.52 (m, 1H), -1.33 – -1.52 (m, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 208.16, 198.36, 159.78, 153.58, 144.88, 142.72, 137.33, 136.03, 135.62, 133.93, 133.84, 132.00, 131.61, 131.00, 130.70, 130.29, 129.28, 128.87, 128.79, 128.58, 127.31, 126.02, 124.96, 124.36, 121.96, 114.14, 55.26, 54.09, 52.96, 47.40, 45.78, 45.04, 22.97, 9.62, 5.27 ppm; **HRMS (ESI)**: $C_{38}H_{30}BrO_3$ $[M + H]^+$ calcd: 613.1372, found: 613.1357.



3aj

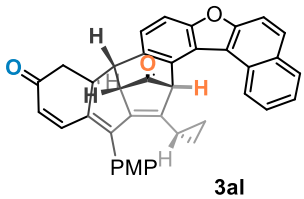
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 173 - 174 ℃, 50.3 mg, 82% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.61 (dd, *J* = 8.9, 6.0 Hz, 2H), 7.56 – 7.35 (m, 11H), 7.23 (d, *J* = 9.3 Hz, 2H), 7.02 – 6.71 (m, 2H), 5.94 (d, *J* = 10.0 Hz, 1H), 4.33 (s, 1H), 3.80 (d, *J* = 4.9 Hz, 1H), 3.77 (s, 3H), 3.68 (t, *J* = 9.9 Hz, 1H), 3.43 (d, *J* = 4.6 Hz, 1H), 2.89 (d, *J* = 10.6 Hz, 2H), 2.72 (s, 3H), 0.46 (tt, *J* = 8.6, 5.3 Hz, 1H), -0.04 (ddd, *J* = 14.3, 6.6, 2.9 Hz, 1H), -0.27 (dq, *J* = 10.5, 5.4 Hz, 1H), -0.36 – -0.58 (m, 1H), -1.37 (dq, *J* = 10.7, 5.5 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.07, 198.63, 159.78, 153.77, 145.02, 143.02, 139.85, 139.32, 136.03, 135.47, 135.38, 133.85, 133.81, 131.66, 131.08, 130.67, 129.66, 129.50, 129.27, 129.07, 128.97, 128.80, 128.56, 127.83, 126.80, 126.71, 125.91, 124.55, 124.13, 114.12, 55.28, 54.30, 52.90, 47.91, 45.97, 45.34, 23.10, 9.76, 5.33 ppm; **HRMS (ESI)**: $C_{44}H_{35}O_3$ $[M + H]^+$ calcd: 611.2580, found: 611.2562.



3ak

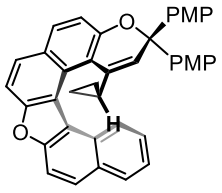
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 221 - 222 ℃,

51.3 mg, 90% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.47 (d, *J* = 8.3 Hz, 1H), 8.26 – 7.99 (m, 5H), 7.96 (d, *J* = 12.9 Hz, 2H), 7.87 – 7.64 (m, 3H), 7.35 (d, *J* = 8.3 Hz, 2H), 7.00 (d, *J* = 8.3 Hz, 2H), 6.15 (d, *J* = 10.1 Hz, 1H), 4.58 (s, 1H), 4.07 (d, *J* = 4.4 Hz, 1H), 3.96 (s, 3H), 3.93 – 3.84 (m, 1H), 3.66 (d, *J* = 4.4 Hz, 1H), 3.17 (d, *J* = 9.8 Hz, 2H), 0.65 – 0.42 (m, 1H), -0.01 (dd, *J* = 11.3, 6.4 Hz, 1H), -0.23 – -0.59 (m, 2H), -1.17 – -1.44 (m, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.45, 198.60, 159.71, 153.36, 144.95, 142.87, 137.31, 136.79, 134.29, 132.10, 131.77, 131.37, 130.98, 130.59, 129.83, 128.95, 128.01, 127.93, 127.86, 127.42, 127.16, 126.89, 126.70, 126.28, 125.98, 125.75, 114.06, 55.23, 54.47, 52.64, 48.58, 45.99, 45.10, 9.47, 5.11, 5.06 ppm; **HRMS (ESI)**: $C_{41}H_{31}O_3$ $[M + H]^+$ calcd: 571.2267, found: 571.2252.



3al

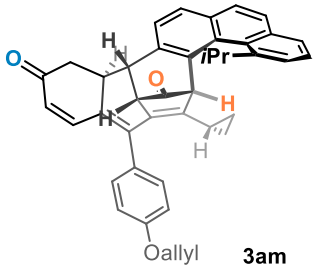
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 7/1 to 2/1). Yellow solid, m.p. 224 - 225 ℃, 33.7 mg, 60% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.59 (d, *J* = 8.5 Hz, 1H), 7.98 (dd, *J* = 20.5, 8.5 Hz, 2H), 7.70 (d, *J* = 8.7 Hz, 2H), 7.66 – 7.43 (m, 3H), 7.43 – 7.13 (m, 2H), 6.87 (d, *J* = 8.4 Hz, 2H), 5.94 (d, *J* = 10.1 Hz, 1H), 5.04 (s, 1H), 3.79 (s, 3H), 3.73 – 3.54 (m, 2H), 3.44 (d, *J* = 4.7 Hz, 1H), 3.03 – 2.78 (m, 2H), 0.68 (p, *J* = 6.7 Hz, 1H), 0.08 (q, *J* = 7.5 Hz, 2H), -0.12 – -0.33 (m, 1H), -0.45 (td, *J* = 7.8, 3.8 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 208.82, 198.55, 159.82, 155.53, 154.30, 152.87, 144.87, 142.78, 134.83, 133.69, 133.30, 131.51, 131.14, 131.11, 130.10, 129.73, 129.16, 128.01, 127.10, 125.95, 125.63, 124.45, 123.55, 116.95, 114.18, 112.57, 111.32, 55.28, 54.58, 53.91, 48.72, 46.02, 45.17, 10.01, 6.07, 5.76 ppm; **HRMS (ESI)**: $C_{39}H_{29}O_4$ $[M + H]^+$ calcd: 561.2060, found: 561.2056.



3al'

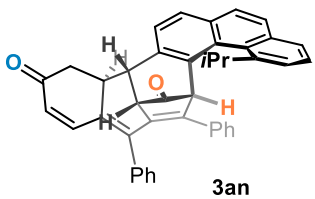
Prepared according to the general procedure on a 0.1 mmol scale and purified by flash

chromatography (petroleum ether/ethyl acetate = 20/1 to 10/1). White solid, m.p. 194 - 195 ℃, 20.3 mg, 35% yield; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.04 (d, *J* = 8.5 Hz, 1H), 7.99 – 7.53 (m, 8H), 7.53 – 7.16 (m, 5H), 7.03 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.5 Hz, 2H), 5.47 (s, 1H), 3.78 (s, 6H), 0.26 – -0.13 (m, 4H), -0.32 (t, *J* = 9.3 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 159.03, 158.87, 155.46, 153.50, 152.87, 140.88, 139.30, 135.36, 132.12, 130.37, 129.95, 128.97, 128.74, 128.24, 127.71, 127.16, 126.70, 125.22, 124.07, 121.62, 119.34, 119.19, 116.45, 116.15, 113.54, 113.42, 112.18, 110.28, 81.98, 55.32, 13.29, 11.31, 10.33 ppm; **HRMS (ESI)**: $C_{40}H_{31}O_4$ $[M + H]^+$ calcd: 575.2216, found: 575.2189.



3am

Prepared according to the general procedure on a 0.1 mmol scale and purified by flash chromatography (petroleum ether/ethyl acetate = 10/1 to 4/1). Yellow solid, m.p. 146 - 147 ℃, 43.2 mg, 74% yield; **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.84 (d, *J* = 8.1 Hz, 1H), 7.77 – 7.45 (m, 7H), 7.26 (d, *J* = 8.3 Hz, 2H), 6.93 (d, *J* = 8.3 Hz, 2H), 6.16 – 6.04 (m, 1H), 6.00 (d, *J* = 10.1 Hz, 1H), 5.41 (dd, *J* = 34.0, 13.8 Hz, 2H), 4.63 – 4.50 (m, 3H), 3.91 – 3.77 (m, 2H), 3.68 (t, *J* = 9.9 Hz, 1H), 3.50 (d, *J* = 4.5 Hz, 1H), 3.01 (d, *J* = 10.0 Hz, 2H), 1.81 (d, *J* = 6.4 Hz, 3H), 0.55 (d, *J* = 6.4 Hz, 3H), 0.47 (dd, *J* = 11.3, 6.8 Hz, 1H), 0.07 – -0.09 (m, 1H), -0.27 (td, *J* = 10.2, 5.2 Hz, 1H), -0.38 – -0.57 (m, 1H), -1.41 (td, *J* = 10.4, 5.4 Hz, 1H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.42, 198.66, 158.75, 153.57, 147.14, 144.92, 142.94, 136.39, 136.03, 134.06, 133.70, 132.82, 131.80, 131.70, 131.00, 129.16, 128.13, 128.08, 127.37, 127.32, 127.05, 126.68, 125.94, 125.78, 125.42, 123.33, 118.00, 114.82, 68.77, 54.40, 52.41, 48.06, 45.99, 45.27, 32.52, 27.78, 21.98, 9.65, 5.27, 5.11 ppm; **HRMS (ESI)**: $C_{42}H_{37}O_3$ $[M + H]^+$ calcd: 589.2736, found: 589.2715.

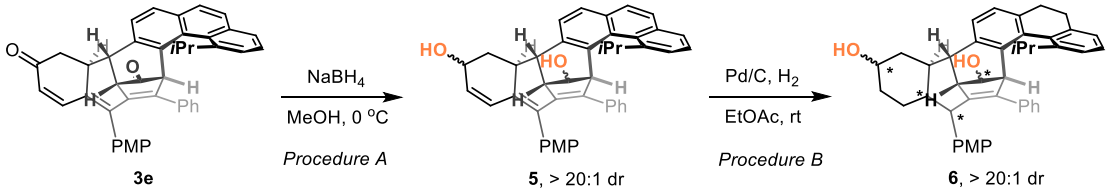


3an

Yellow solid, m.p. 225 - 226 ℃; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 8.0 Hz, 1H),

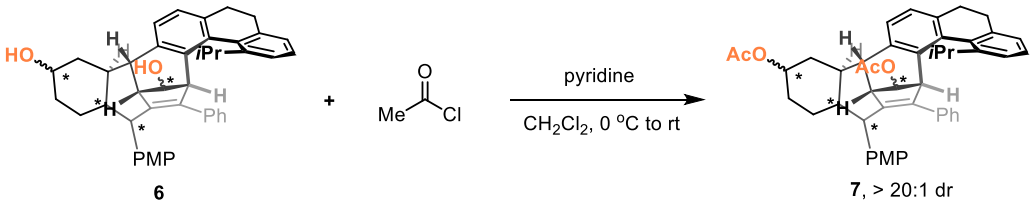
7.63 – 7.38 (m, 5H), 7.38 – 7.27 (m, 2H), 7.15 (dd, *J* = 4.4, 2.3 Hz, 3H), 7.11 – 6.98 (m, 2H), 6.62 (t, *J* = 7.4 Hz, 1H), 6.45 – 6.27 (m, 2H), 5.93 (d, *J* = 10.2 Hz, 1H), 5.81 (d, *J* = 7.7 Hz, 2H), 5.18 (s, 1H), 3.88 (dd, *J* = 14.5, 5.9 Hz, 2H), 3.63 (t, *J* = 7.9 Hz, 2H), 3.00 (q, *J* = 7.3, 5.7 Hz, 2H), 1.78 (d, *J* = 6.5 Hz, 3H), 0.50 (d, *J* = 6.5 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 209.60, 198.46, 148.14, 146.80, 144.38, 143.28, 136.91, 136.17, 135.74, 134.14, 134.02, 134.00, 132.24, 131.88, 129.57, 128.45, 128.33, 128.26, 127.67, 127.54, 127.32, 127.27, 127.19, 127.06, 126.85, 126.81, 125.53, 125.10, 123.34, 56.95, 56.50, 48.19, 45.77, 45.41, 32.48, 27.86, 21.89 ppm; **HRMS (ESI)**: $C_{42}H_{33}O_2$ $[M + H]^+$ calcd: 569.2474, found: 569.2457.

7. General Procedures for the Transformations of Double Dearomatization Product 3e



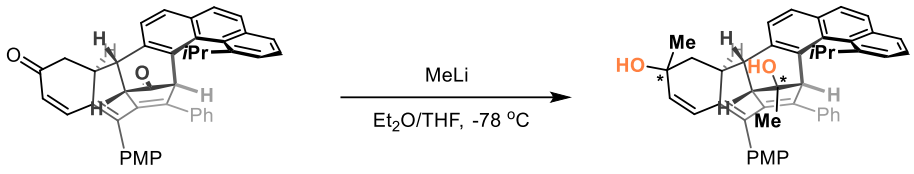
Procedure A: To a solution of polycyclic diketone **3e** (0.1 mmol, 1.0 equiv) in methanol (1.0 mL) was added $NaBH_4$ (0.5 mmol, 5.0 equiv) slowly at 0 °C. The resulting reaction mixture was then stirred for 1 h. After the complete consumption of **3e** (monitored by TLC), the reaction was quenched by water and the aqueous layer was extracted with EtOAc for three times. The combined organic layers were washed with brine, dried, and concentrated. The resulting residue was then purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 4:1 to 2:1) to afford polycyclic diol **5** in 83% yield. White solid, m.p. 174-175 °C; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.72 – 7.34 (m, 5H), 7.23 (s, 1H), 7.17 (s, 2H), 6.99 (d, *J* = 9.0 Hz, 2H), 6.63 (d, *J* = 7.7 Hz, 2H), 6.58 – 6.41 (m, 2H), 6.28 (t, *J* = 7.3 Hz, 2H), 6.02 (d, *J* = 8.3 Hz, 2H), 5.71 (d, *J* = 10.3 Hz, 1H), 5.11 (s, 2H), 4.73 (t, *J* = 7.7 Hz, 1H), 4.04 (p, *J* = 6.5 Hz, 1H), 3.63 (s, 3H), 3.58 (d, *J* = 5.0 Hz, 1H), 3.10 (d, *J* = 5.0 Hz, 1H), 3.01 – 2.83 (m, 1H), 2.66 (t, *J* = 6.8 Hz, 2H), 1.98 (q, *J* = 11.9 Hz, 1H), 1.75 (d, *J* = 6.7 Hz, 3H), 0.57 (d, *J* = 6.5 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.46, 146.97, 143.54, 138.29, 135.79, 135.76, 134.10, 134.03, 133.56, 133.15, 132.98, 131.94, 130.75, 130.08, 129.48, 127.79, 127.61, 127.33, 127.09, 126.59, 126.50, 126.42, 126.15, 126.06, 125.77, 125.01, 123.06, 113.40, 71.62, 69.02, 55.12, 52.15, 51.07, 43.72, 42.14, 39.88, 32.12, 28.06, 21.31 ppm; **HRMS (ESI)**: $C_{43}H_{39}O_3$ $[M + H]^+$ calcd: 603.2893, found: 603.2897.

Procedure B: To a solution of polycyclic diol **5** (0.074 mmol, 1.0 equiv) in ethyl acetate (1.0 mL) was added 10% palladium on carbon catalyst (0.015 mmol, 0.2 equiv) and the resulting reaction mixture was stirred at hydrogen atmosphere for 40 h until the complete consumption of the start material. Then the mixture was filtrated with celite and evaporated to give a residue, which was purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 3:1 to 1:1) to afford polycyclic diol **6** in 75% yield. White solid, m.p. 127-128 ℃; **^{1}H NMR** (300 MHz, DMSO-d_6) δ 8.23 (s, 1H), 7.21 (d, *J* = 7.8 Hz, 1H), 7.00 (dd, *J* = 18.9, 7.7 Hz, 2H), 6.80 (t, *J* = 7.5 Hz, 1H), 6.65 (t, *J* = 7.2 Hz, 1H), 6.55 (d, *J* = 7.3 Hz, 1H), 6.43 (t, *J* = 7.6 Hz, 2H), 6.34 – 6.07 (m, 4H), 5.65 (d, *J* = 7.5 Hz, 2H), 5.06 (d, *J* = 3.8 Hz, 1H), 4.53 (d, *J* = 4.5 Hz, 2H), 3.75 (s, 1H), 3.51 (q, *J* = 6.9, 6.2 Hz, 2H), 3.43 (s, 3H), 3.30 – 3.20 (m, 1H), 3.10 (dd, *J* = 11.9, 6.1 Hz, 1H), 2.88 (d, *J* = 12.5 Hz, 1H), 2.49 (d, *J* = 5.3 Hz, 1H), 2.35 (d, *J* = 13.2 Hz, 1H), 2.17 – 1.85 (m, 4H), 1.58 (t, *J* = 12.0 Hz, 3H), 1.43 (d, *J* = 12.1 Hz, 1H), 1.26 (d, *J* = 6.4 Hz, 3H), 0.86 – 0.64 (m, 2H), 0.44 (d, *J* = 6.6 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, DMSO) δ 156.90, 146.01, 142.08, 140.12, 138.61, 138.32, 136.40, 135.52, 134.31, 132.44, 130.39, 130.24, 130.04, 126.50, 125.45, 125.11, 124.49, 123.80, 123.22, 112.59, 79.65, 72.15, 69.60, 55.09, 51.40, 47.26, 43.24, 43.10, 41.51, 37.43, 31.31, 31.04, 29.40, 29.07, 27.61, 21.83 ppm; **HRMS (ESI)**: $C_{43}H_{45}O_3$ $[M + H]^+$ calcd: 609.3362, found: 609.3374.



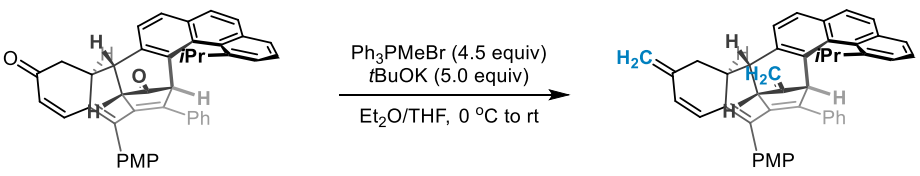
To a solution of polycyclic diol **6** (0.063 mmol, 1.0 equiv) and pyridine (0.38 mmol, 6.0 equiv) in DCM (1.0 mL) was added acetyl chloride (0.38 mmol, 6.0 equiv) at 0 °C. The reaction mixture was then stirred at room temperature for 2 days. After the complete conversion of diol **6**, the reaction mixture was concentrated under vacuo and the residue was purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 30:1 to 15:1) to give diacetate **7** in 75% yield. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.38 – 7.13 (m, 2H), 7.07 (d, *J* = 7.8 Hz, 1H), 6.95 (t, *J* = 7.5 Hz, 1H), 6.79 (t, *J* = 7.3 Hz, 1H), 6.73 – 6.51 (m, 3H), 6.36 (d, *J* = 8.2 Hz, 2H), 6.26 (d, *J* = 8.3 Hz, 2H), 5.77 (s, 2H), 5.62 (t, *J* = 4.9 Hz, 1H), 5.11 (td, *J* = 11.3, 10.7, 5.1 Hz, 1H), 3.77 (t, *J* = 5.6 Hz, 1H), 3.60 (s, 3H), 3.42 (td, *J* = 13.8, 12.9, 6.3 Hz, 2H), 3.31 – 3.15 (m, 2H), 3.15 – 2.92

(m, 2H), 2.59 – 2.13 (m, 4H), 2.11 (s, 3H), 2.03 (s, 3H), 1.92 – 1.55 (m, 5H), 1.29 (d, *J* = 6.8 Hz, 3H), 0.67 (d, *J* = 6.6 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 171.13, 170.74, 157.12, 145.12, 142.43, 139.66, 138.41, 136.65, 135.62, 135.11, 133.68, 133.47, 131.97, 130.64, 130.00, 129.82, 126.68, 126.50, 125.36, 125.07, 124.91, 123.87, 122.68, 112.40, 74.57, 73.02, 54.95, 50.68, 45.17, 43.15, 42.75, 40.57, 40.18, 38.03, 33.04, 31.25, 30.96, 29.49, 29.02, 27.25, 21.44, 21.30, 21.25 ppm; **HRMS (ESI)**: $C_{47}H_{48}NaO_5$ $[M + Na]^+$ calcd: 715.3394, found: 715.3373.



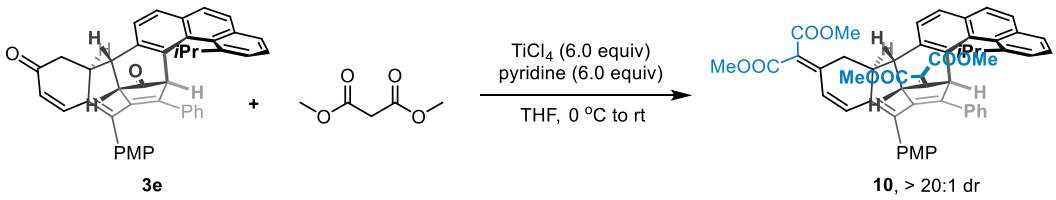
3e **8**, > 20:1 dr

A solution of 1.3 M MeLi (0.4 mmol, 0.31 mL) in ether was added dropwise to a stirred solution of **3e** (0.1 mmol, 1.0 equiv) in a mixed solution of Et_2O (1.0 mL) and THF (0.5 mL) at -78 °C under Ar. After stirred for 1 h at the same temperature, the reaction mixture was quenched by saturated NH_4Cl aqueous solution. The aqueous layer was extracted with EtOAc for three times, and the combined organic layers were washed with brine, dried, and concentrated. The resulting residue was then purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 4:1 to 3:1) to give dimethylated **8** in 79% yield. White solid, m.p. 127-128 °C; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.62 (d, *J* = 8.2 Hz, 1H), 7.57 – 7.34 (m, 4H), 7.16 (t, *J* = 6.6 Hz, 2H), 6.97 (d, *J* = 8.3 Hz, 2H), 6.63 (d, *J* = 8.3 Hz, 2H), 6.56 – 6.40 (m, 2H), 6.29 (t, *J* = 7.6 Hz, 2H), 6.03 (d, *J* = 7.7 Hz, 2H), 5.63 (d, *J* = 10.2 Hz, 1H), 4.96 (s, 1H), 4.13 (p, *J* = 6.6 Hz, 1H), 3.64 (s, 4H), 3.06 – 2.78 (m, 2H), 2.63 (s, 1H), 2.44 (dd, *J* = 12.1, 3.7 Hz, 1H), 2.15 (t, *J* = 13.2 Hz, 1H), 1.95 (s, 4H), 1.75 (d, *J* = 6.6 Hz, 3H), 1.56 (s, 3H), 0.51 (d, *J* = 6.5 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.44, 146.89, 144.56, 138.17, 136.47, 135.81, 135.72, 135.57, 134.10, 133.88, 133.12, 131.91, 130.63, 129.85, 129.36, 127.77, 127.67, 127.12, 126.73, 126.42, 126.07, 125.65, 125.21, 125.03, 122.48, 113.38, 71.39, 58.13, 57.13, 55.11, 47.94, 44.04, 41.43, 32.01, 27.77, 27.34, 25.47, 21.76 ppm; **HRMS (ESI)**: $C_{45}H_{42}NaO_3$ $[M + Na]^+$ calcd: 653.3026, found: 653.3009.



3e **9**, > 20:1 dr

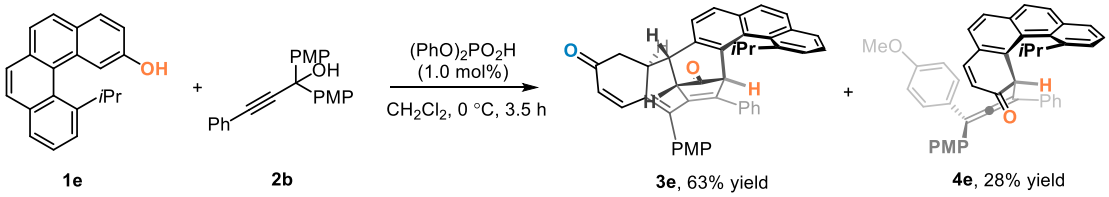
Potassium *tert*-butanolate (0.5 mmol, 5.0 equiv) was added to a solution of methyltriphenylphosphonium bromide (0.45 mmol, 4.5 equiv) in Et_2O (1.0 mL) under Ar and the resulting mixture was stirred at 0 °C for 1 h. Subsequently, a solution of **3e** (0.1 mmol, 1.0 equiv) in THF (1.0 mL) was added dropwise to the reaction mixture, which was then stirred for 5 days at room temperature. Then the reaction mixture was quenched by saturated NH_4Cl aqueous solution. The aqueous layer was extracted with EtOAc for three times, and the combined organic layers were washed with brine, dried, and concentrated. The resulting residue was then purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 200:1) to give **9** in 66% yield. White solid, m.p. 160-161 °C; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.64 – 7.34 (m, 5H), 7.13 (q, *J* = 8.5 Hz, 2H), 6.99 (d, *J* = 8.3 Hz, 2H), 6.70 – 6.44 (m, 4H), 6.30 (t, *J* = 7.6 Hz, 2H), 6.12 (d, *J* = 9.9 Hz, 1H), 5.98 (d, *J* = 7.7 Hz, 2H), 5.37 (s, 1H), 5.28 (s, 1H), 5.17 (s, 1H), 5.01 (d, *J* = 4.7 Hz, 2H), 4.11 (dq, *J* = 14.2, 7.0 Hz, 1H), 3.61 (s, 5H), 3.10 – 2.72 (m, 3H), 1.72 (d, *J* = 6.7 Hz, 3H), 0.44 (d, *J* = 6.5 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 158.35, 153.21, 145.88, 145.81, 143.63, 138.86, 137.95, 137.15, 135.97, 134.26, 134.03, 133.07, 131.13, 130.97, 129.99, 128.69, 128.49, 127.96, 127.70, 127.47, 127.35, 126.34, 126.30, 126.02, 125.96, 125.78, 125.57, 124.98, 121.64, 113.20, 112.48, 99.88, 55.08, 54.69, 54.12, 47.14, 44.68, 39.60, 31.93, 27.45, 21.80 ppm; **HRMS (ESI)**: $C_{45}H_{38}NaO$ $[M + Na]^+$ calcd: 617.2815, found: 617.2814.



A solution of $TiCl_4$ (0.6 mmol, 6.0 equiv) in DCM (0.6 mL) was added dropwise to a stirred solution of polycyclic diketone **3e** (0.1 mmol, 1.0 equiv), dimethyl malonate (0.2 mmol, 2.0 equiv) and pyridine (0.6 mmol, 6.0 equiv) in THF (0.4 mL) at 0 °C. The resulting reaction mixture was stirred at room temperature for 16 h, the process of which was monitored TLC. Then the reaction mixture was quenched by water. The aqueous layer was extracted with EtOAc for three times, and the combined organic layers were washed with brine, dried, and concentrated. The resulting residue was then purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 20:1 to 10:1) to give the desired product **10** in 42% yield. Yellow solid, m.p. 251-252 °C; **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 7.57 (d, *J* = 8.1 Hz, 1H), 7.50 – 7.22 (m, 5H), 7.02 (q, *J* = 8.8 Hz, 3H), 6.92 (d, *J* = 8.2 Hz, 2H), 6.66 (d, *J* = 10.2 Hz, 1H), 6.54 (dd, *J* = 15.6, 7.8 Hz, 3H), 6.35

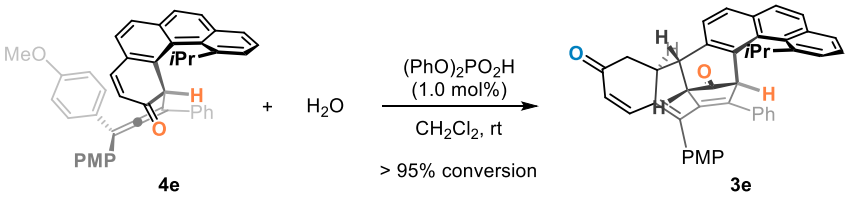
(t, *J* = 7.5 Hz, 2H), 6.04 (s, 1H), 5.89 (d, *J* = 7.6 Hz, 2H), 3.99 (s, 3H), 3.97 (s, 3H), 3.89 (s, 3H), 3.82 (d, *J* = 6.2 Hz, 4H), 3.64 (d, *J* = 4.6 Hz, 1H), 3.59 (s, 4H), 3.46 (q, *J* = 4.7, 2.9 Hz, 1H), 3.32 (dd, *J* = 14.8, 4.3 Hz, 1H), 2.85 (t, *J* = 15.3 Hz, 1H), 1.28 (d, *J* = 8.3 Hz, 3H), 0.15 (d, *J* = 6.3 Hz, 3H) ppm; **^{13}C NMR** (75 MHz, $CDCl_3$) δ 166.66, 166.26, 166.07, 166.01, 164.41, 159.05, 151.20, 149.02, 144.60, 140.10, 136.85, 136.64, 136.49, 133.89, 133.65, 133.37, 131.50, 131.14, 130.57, 129.45, 128.30, 128.13, 127.72, 127.43, 126.75, 126.54, 126.38, 126.30, 126.14, 124.41, 124.28, 123.96, 121.55, 121.02, 116.86, 113.27, 55.07, 54.78, 53.84, 52.49, 52.36, 45.17, 43.89, 35.45, 31.11, 25.19, 20.80 ppm; **HRMS (ESI)**: $C_{53}H_{47}O_9$ $[M + H]^+$ calcd: 827.3214, found: 827.3202.

8. Control Experiments



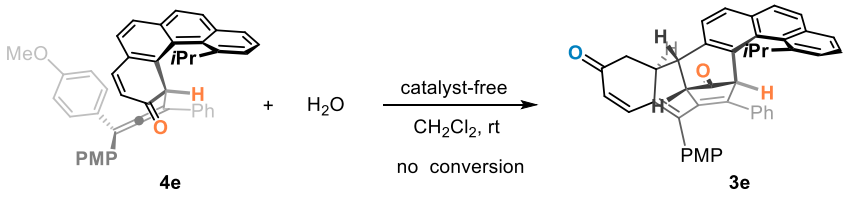
1e **2b** **3e**, 63% yield **4e**, 28% yield

To a solution of 2-[4]helicenol **1e** (0.2 mmol) and propargylic alcohol **2b** (0.24 mmol) in DCM (2.0 mL) was added diphenyl phosphate (0.002 mmol) at 0 °C. After stirred at the same temperature for 3.5 h, the resulting reaction mixture was directly purified by silica gel column chromatography (eluting with hexane/ethyl acetate = 20:1 to 10:1 to 4:1) to give the double dearomatization product **3e** and allene intermediate **4e** in 63% and 28% yield, respectively.



4e **3e**

To a solution of **4e** (0.028 mmol) and diphenyl phosphate (0.00028 mmol) in DCM (0.28 mL) was added water (0.028 mmol). When the resulting reaction mixture was stirred at room temperature for 6 h, a complete conversion of **4e** to **3e** was observed by NMR analysis.



4e **3e**

When the solution of **4e** (0.028 mmol) and water (0.028 mmol) in DCM was stirred at room

temperature for 24 h, there was no formation of **3e** was detected. Which indicated that diphenyl phosphate plays an indispensable role in the intramolecular dearomative Diels-Alder reaction/ dearomative polyene cyclization and subsequent formal demethylation sequence.

9. The Computed Reaction Free Energy Profiles for the Dearomatization and [3+3] Cycloaddition Pathways

9.1 Computational details

All theoretical callculations were performed using Gaussian 16 C.01 software package.[3] Geometry optimizations, vibrational frequency calculations and intrinsic reaction coordinate (IRC) [4,5] calculations were carried out at M06-2X[6]-D3[7]/Def2-SVP[8]/SMD(CH_2Cl_2)[9] level of theory. All optimized structures of reactants, catalyst, intermediates (denoted as **Int**s), and products have no imaginary frequency, while each optimized transition state (denoted as **TS**) structure has only one imaginary frequency. The optimized structures were drawn using CYLview software.[10]

9.2 Possible reaction pathways

We proposed three possible reaction pathways, denoted as **path a**, **b** and **c**. **Path a** will lead to dearomatized product **3e**, while **path b** and **path c** will lead to [3+3] cyclization product **3e'**. **Int 1** exists in two possible conformations, denoted as **Int 1$_{C1}$** and **Int 1$_{C2}$**. Notably, **Int 1$_{C2}$** has a higher Gibbs free energy than **Int 1$_{C1}$** by 2.7 kcal/mol. The optimized structures of **Int 1$_{C1}$**, **Int 1$_{C2}$**, **3e**, **3e'**, diphenyl phosphorous acid (**DPA**) and corresponding anion (**DPA-anion**), H_2O and MeOH were displayed in **Figure S2**.

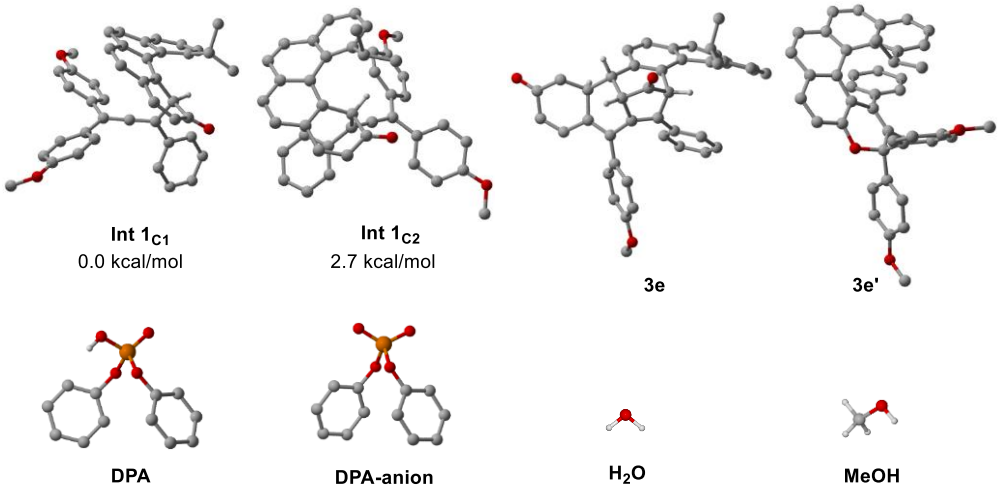


Figure S2. Optimized structures of **Int 1$_{C1}$**, **Int 1$_{C2}$**, **3e**, **3e'**, diphenyl phosphorous acid (**DPA**) and corresponding anion (**DPA-anion**), H_2O and MeOH, and relative Gibbs free energies of **Int 1$_{C1}$** and **Int 1$_{C2}$**. Some H atoms are omitted for clarity.

9.2.1 Relative free energy profile of **path a**

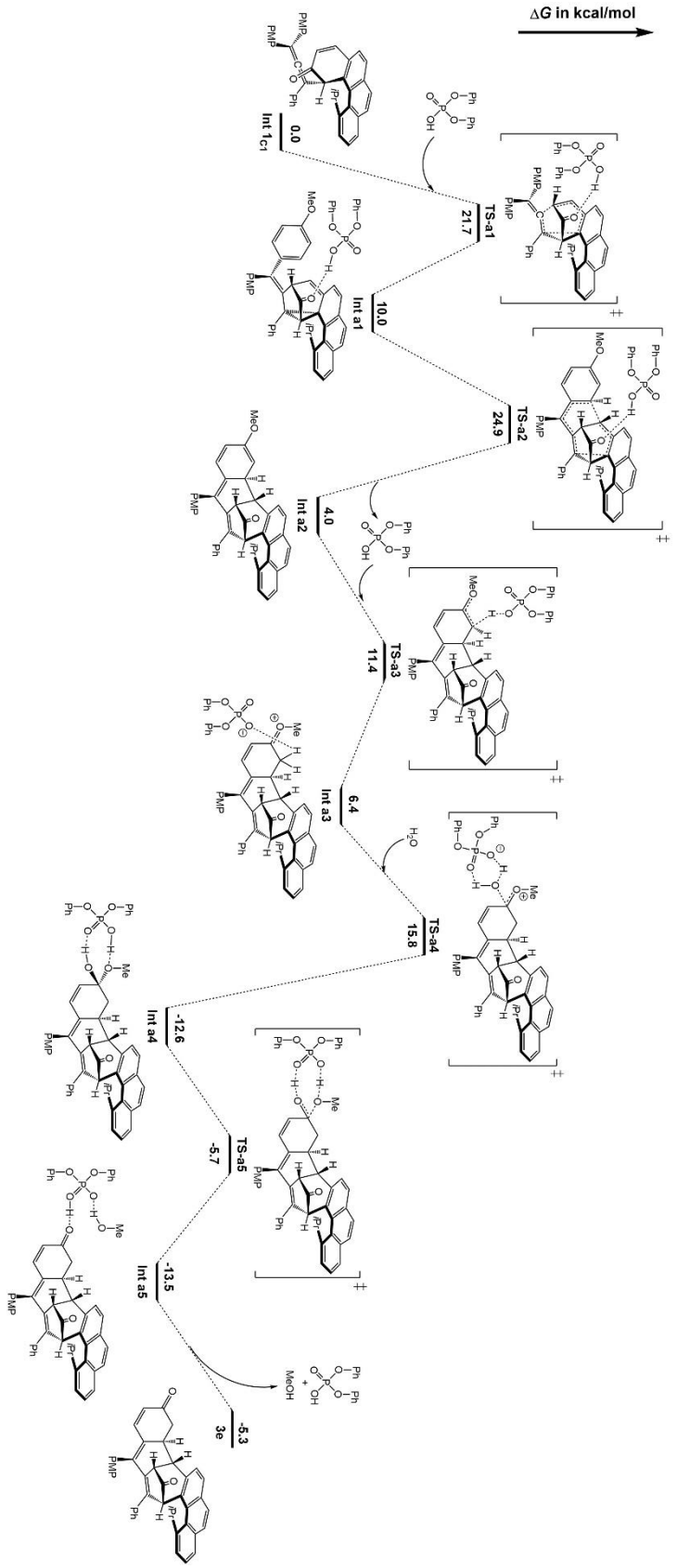


Figure S3. Potential free energy diagram of **path a**. Some intra- and intermolecular interactions were omitted. The Gibbs free energy of **Int 1$_{C1}$** and **DPA** were set to 0.0 kcal/mol as reference.

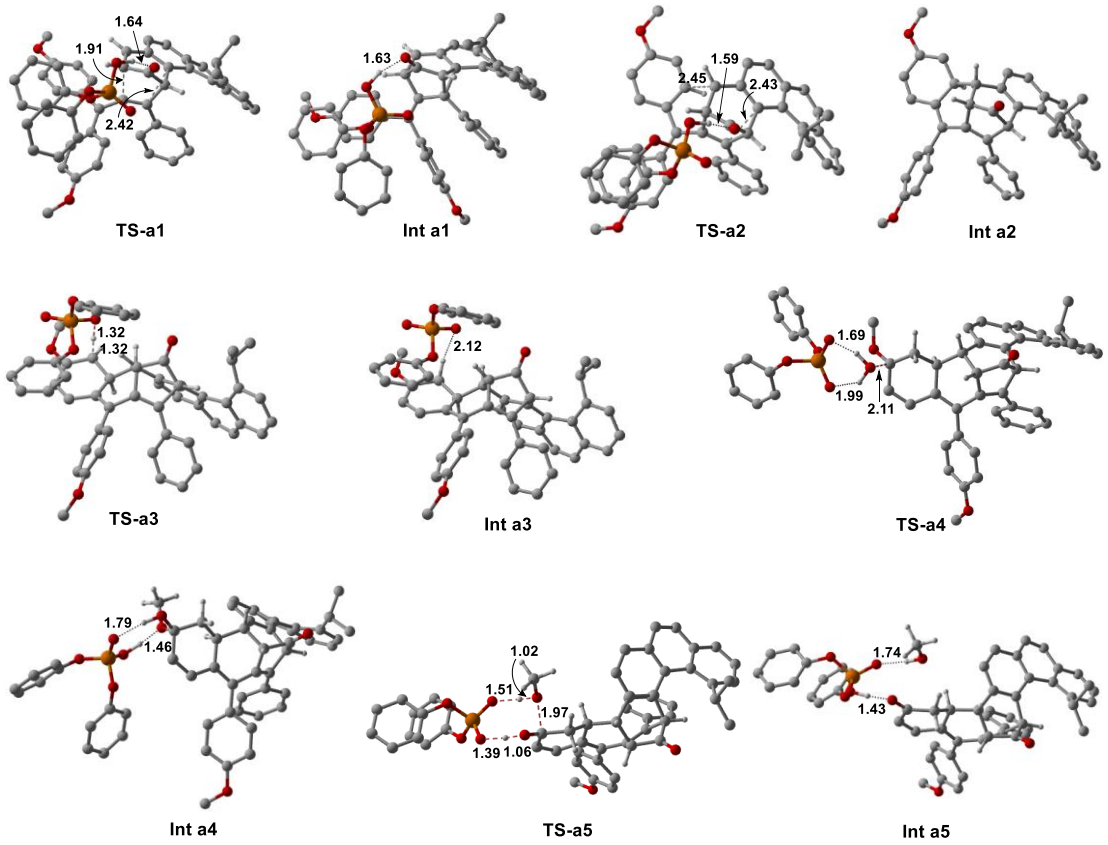


Figure S4. Optimized structures of **path a**. Some H atoms and intermolecular interactions are omitted for clarity. Distances are in Å.

Starting from **Int 1$_{C1}$**, an intramolecular Diels-Alder reaction occurred with the assistance of **DPA**. The reaction journeyed through transition state **TS-a1** to generate intermediate **Int a1**, in which the naphthalen-2(1*H*)-one moiety acts as the diene, while the C=C bond of the allene serves as the dienophile. This reaction unfolded in a concerted but asynchronous manner, necessitating a free energy uphill of 21.7 kcal/mol from the reactant to transition state **TS-a1**. Subsequently, a polyene cyclization reaction took place via **TS-a2** to generate **Int a2**, and the **DPA** was temporarily detached. From **Int a1** to **TS-a2**, there is a 14.9 kcal/mol free energy barrier. Next, **Int a2** was acidified by **DPA** via **TS-a3** to form ion-pair **Int a3**. From **Int a2** to **TS-a3**, a 7.4 kcal/mol activation free energy is needed. Afterwards hydrolysis reaction occurred via **TS-a4** to generate hemiketal **Int a4**. In **Int a3→TS-a4** procedure, there is a rise in the Gibbs free energy by 9.4 kcal/mol. Following this, in the **TS-a4** to **Int a4** transition, there is an irreversible release of Gibbs free energy, amounting to 28.4 kcal/mol. Then, the hemiketal decomposition reaction took place via **TS-a5** to produce hydrogen-bond complex **Int a5**, with a mere energy input of 6.9 kcal/mol being necessary for the process. Finally, **3e** and by-product **MeOH** were released with 8.2 kcal/mol free energy uphill, and **DPA** will join another catalytic cycle. The potential free energy

diagram and the optimized structures of **path a** are shown in **Figures S3** and **S4**, respectively.

9.2.2 Relative free energy profile of **path b**

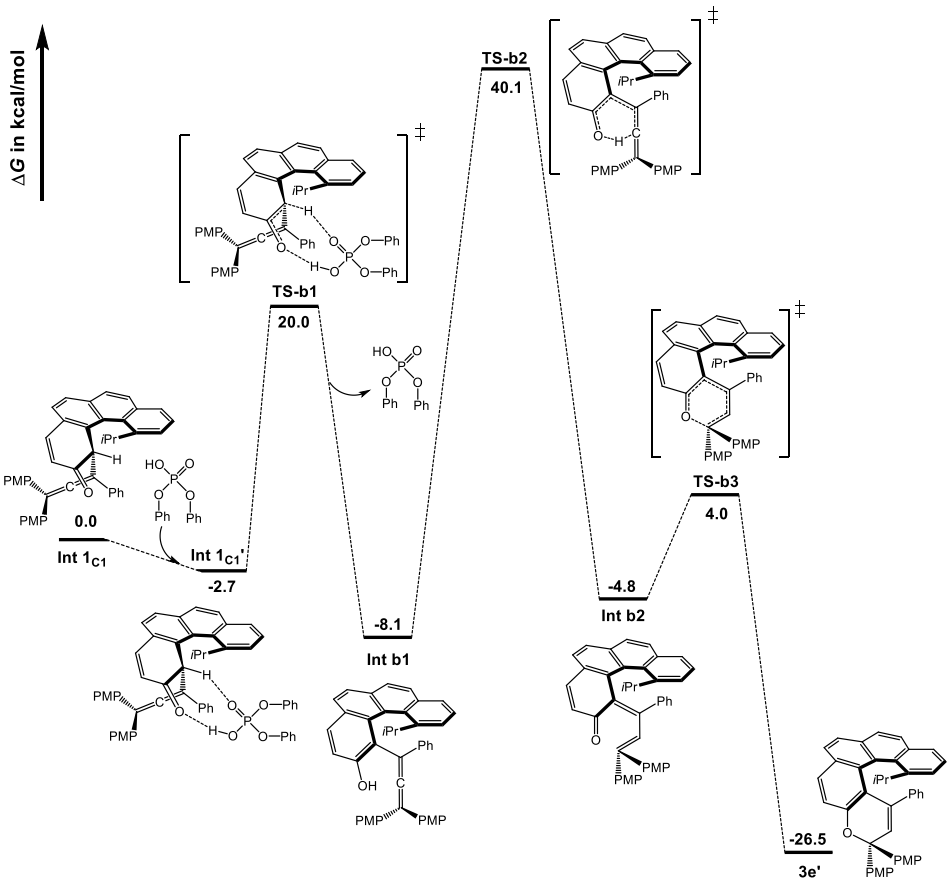


Figure S5. Potential free energy diagram of **path b**. Some intra- and intermolecular interactions were omitted. The Gibbs free energies of **Int 1$_{C1}$** and **DPA** were set to 0.0 kcal/mol as reference.

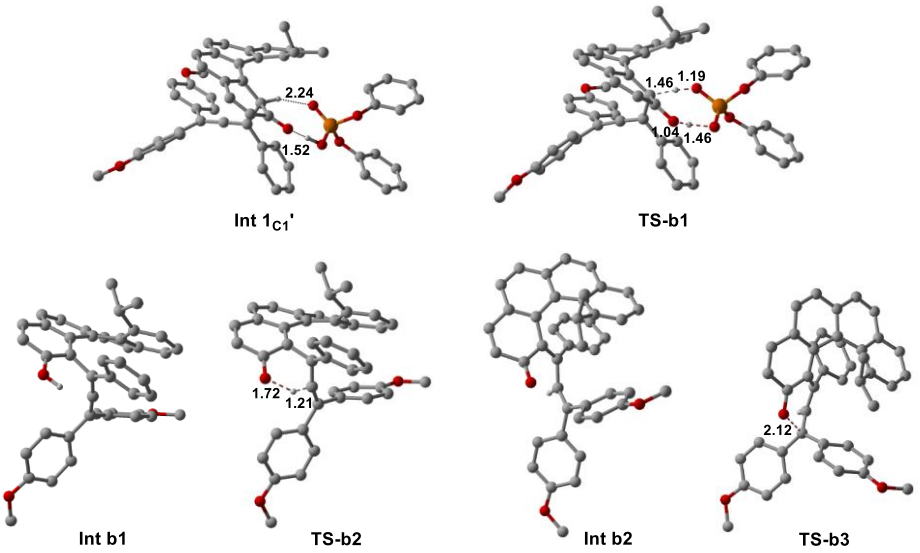


Figure S6. Optimized structures of **path b**. Some H atoms and intermolecular interactions are omitted for clarity. Distances are in Å.

In pathway b, initially, **DPA** interacted with **Int 1$_{C1}$** via hydrogen bonds, leading to the formation of **Int 1$_{C1}$'** and resulting in a free energy release of 2.7 kcal/mol. Afterwards **Int 1$_{C1}$** and **DPA** exchanged their protons via **TS-b1** to generate **Int b1**, which has larger π-conjugated system than **Int 1$_{C1}$**. From **Int 1$_{C1}$'** to **TS-b1**, a 22.7 kcal/mol free energy barrier should be overcome. The **TS-b1→Int b1** procedure is 28.1 kcal/mol exothermic, and **DPA** was released to join another catalytic cycle. Next, the intramolecular proton transfer between phenol moiety and allene moiety took place via 6-membered ring transition state **TS-b2** to form **Int b2**. From **Int b1** to **TS-b2**, the activation free energy is 48.2 kcal/mol, which is too high to overcome. Finally, **Int b2** went through an intramolecular oxa-6π electrocyclization via **TS-b3** to produce **3e'** with only 8.8 kcal/mol free energy barrier. The potential free energy diagram and the optimized structures of **path b** are shown in **Figures S5** and **S6**, respectively.

9.2.3 Relative free energy profile of **path c**

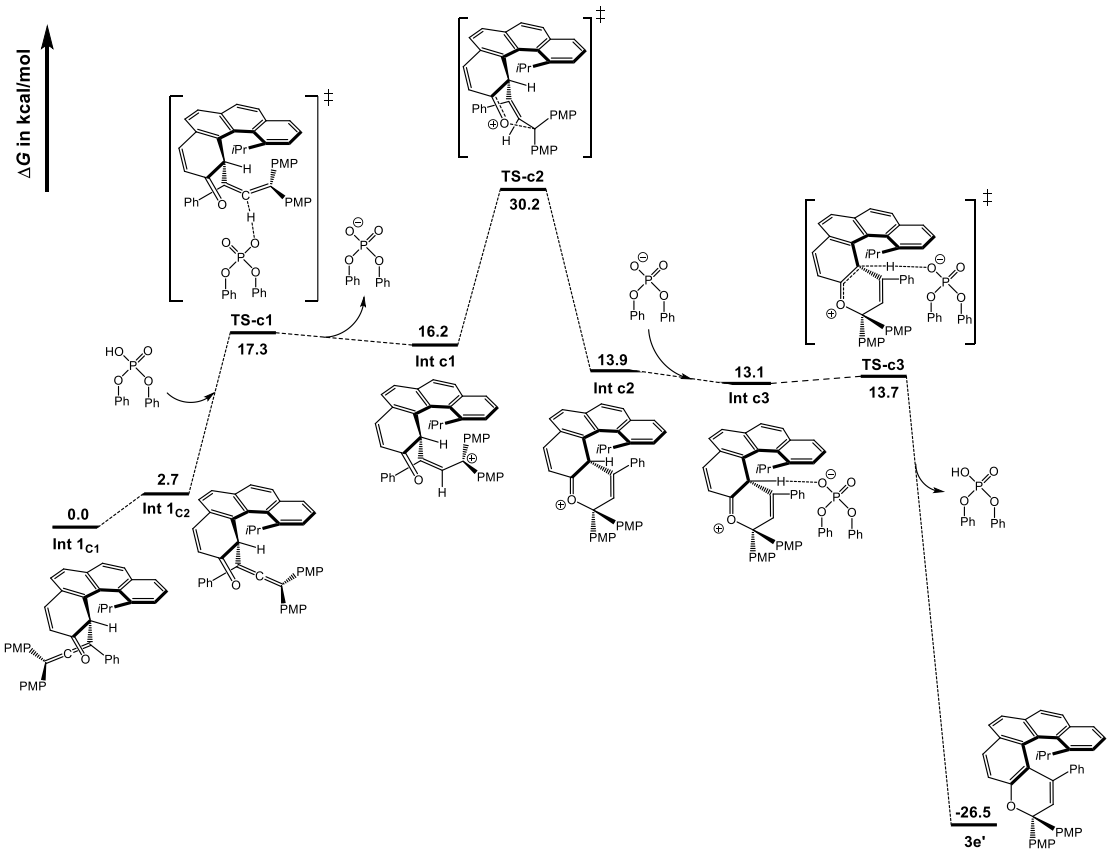


Figure S7. Potential free energy diagram of **path b**. Some intra- and intermolecular interactions were omitted. The Gibbs free energies of **A$_{C1}$** and **DPA** were set to 0.0 kcal/mol as reference.

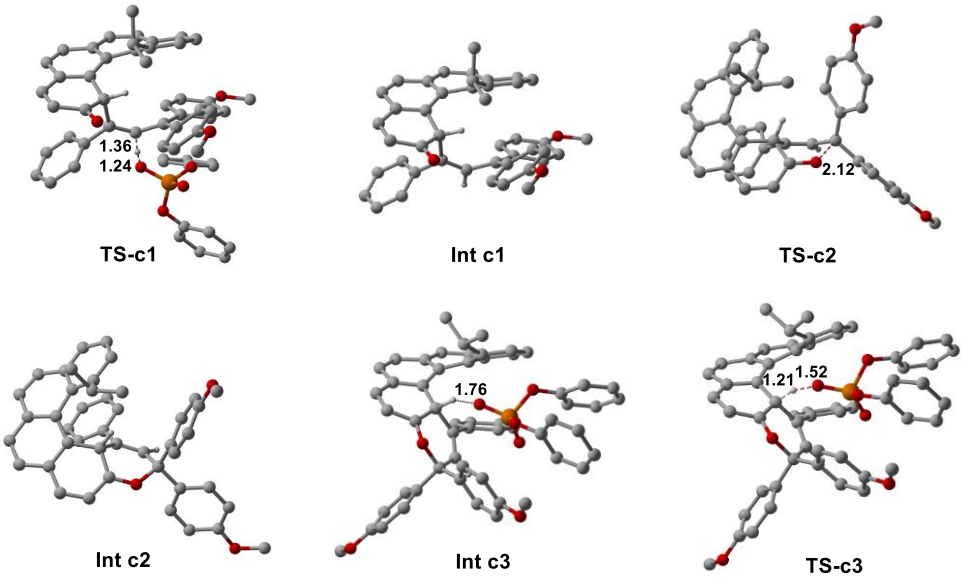


Figure S8. Optimized structures of **path c**. Some H atoms and intermolecular interactions are omitted for clarity. Distances are in Å.

In **path c**, **Int 1$_{C1}$** firstly changed its conformation to **Int 1$_{C2}$** with 2.7 kcal/mol free energy rise. Then intermolecular proton-transfer reaction between **DPA** and central C atom of allene occurred via **TS-c1** to form **Int c1** and **DPA-anion**. From **Int 1$_{C2}$** to **TS-c1**, a 14.6 kcal/mol free energy uphill is required. Afterwards the O atom of ketene moiety attacked carbocation via **TS-c2** with boat-conformation to generate **Int c2**. The **Int c1→TS-c2** procedure needed 14.0 kcal/mol activation free energy. Subsequently, **Int c2** combined with **DPA-anion** to form ion-pair **Int c3** with 0.8 kcal/mol free energy release. Finally, the proton transfer reaction took place via **TS-c3** to generate **DPA** and **3e'**. From **Int c3** to **TS-c3**, there is only 0.6 kcal/mol free energy barrier. The potential free energy diagram and the optimized structures of **path b** are shown in **Figures S7** and **S8**, respectively.

9.2.4 Conclusions

According to Murdoch's study,[11] the calculated activation Gibbs free energies of the three reaction pathways are as follows: ΔG_{act}(**path a**) = G(**TS-a2**) - G(**Int 1$_{C1}$**) = 24.9 kcal/mol, ΔG_{act}(**path b**) = G(**TS-b2**) - G(**Int b1**) = 48.2 kcal/mol, ΔG_{act}(**path c**) = G(**TS-c2**) - G(**Int 1$_{C1}$**) = 30.2 kcal/mol. **path a** is less exothermic, but it has the lowest activation Gibbs free energy among three pathways, therefore **3e** is the main product.

9.3 Calculated Original Data

Table S1. Calculated Gibbs free energies (denoted as Gs, in a.u.) of all optimized structures, and imaginary frequencies (denoted as ν_is, in cm^{-1}) of all transition state structures.

	G	ν_i		*G*	ν_i
Int 1_{C1}	-1921.234225		**Int a4**	-3102.678132	
Int 1_{C2}	-1921.229931		**TS-a5**	-3102.667042	-230.7
3e	-1882.021947		**Int a5**	-3102.679615	
3e'	-1921.276505		**Int 1_{C1}'**	-3026.335873	
DPA	-1105.097413		**TS-b1**	-3026.299813	-1312.0
DPA-anion	-1104.645771		**Int b1**	-1921.247135	
H_2O	-76.326399		**TS-b2**	-1921.170271	-500.9
MeOH	-115.547081		**Int b2**	-1921.241795	
TS-a1	-3026.297026	-412.8	**TS-b3**	-1921.227787	-354.7
Int a1	-3026.315723		**TS-c1**	-3026.304053	-1392.6
TS-a2	-3026.291884	-194.6	**Int c1**	-1921.660045	
Int a2	-1921.227788		**TS-c2**	-1921.637773	-224.2
TS-a3	-3026.313514	-1261.8	**Int c2**	-1921.663791	
Int a3	-3026.321425		**Int c3**	-3026.310732	
TS-a4	-3102.632797	-230.1	**TS-c3**	-3026.309812	-175.4

9.4 Cartesian Coordinates

Int 1_{C1}

C	-4.67974100	1.64103400	0.74537100
C	-3.71984500	2.51323900	0.27662400
C	-2.71726600	2.05452700	-0.60525600
C	-2.63614300	0.67461100	-0.94313800
C	-3.75457600	-0.16200900	-0.62783800
C	-4.72191700	0.32982600	0.24272700
C	-1.84435500	3.00264200	-1.25347700
C	-1.45153100	0.23716600	-1.68885800
C	-0.72005400	1.20395500	-2.43196700
C	-0.96676900	2.60467300	-2.20742600
C	0.32591700	0.79561000	-3.29262000
H	0.84775900	1.55322000	-3.88060300
C	0.69080400	-0.52913500	-3.36818400
C	0.11163700	-1.46466900	-2.48153600
C	-0.90581000	-1.07118600	-1.60705500
H	-1.96019800	4.06067500	-1.00656800
H	-5.45032600	1.98316600	1.43810300
H	-3.73606500	3.56985200	0.55233300
H	-5.57599600	-0.30055700	0.49833600
H	-0.36773100	3.33124900	-2.76015700
H	1.47898700	-0.85620700	-4.04924800
C	-4.08119100	-1.43913100	-1.40718900
C	-5.09258200	-1.07784000	-2.50464800
C	-4.61869200	-2.59143500	-0.55555600

H	-3.17922100	-1.78951700	-1.92329500
H	-4.70930000	-0.27332800	-3.14956600
H	-5.30096700	-1.95541300	-3.13527400
H	-6.04258700	-0.73849800	-2.06352400
H	-3.91625100	-2.90192000	0.23206100
H	-5.57608600	-2.33086400	-0.08035500
H	-4.80050000	-3.46790400	-1.19506600
C	0.60969500	-2.84065100	-2.44942400
C	0.15119200	-3.77708100	-1.59573100
H	1.37652200	-3.10158500	-3.18429800
H	0.49398400	-4.81252700	-1.62615000
C	-1.17148200	-1.95257700	-0.40901600
H	-2.19366100	-1.87339800	-0.03943500
C	-0.89906300	-3.43837400	-0.62169800
O	-1.48644000	-4.27773500	0.02832500
C	-0.26850900	-1.49387000	0.75836500
C	-0.53531400	-2.05831400	2.11551900
C	-1.84354500	-2.23654600	2.58785700
C	0.53743200	-2.38937400	2.95592300
C	-2.06947200	-2.72428800	3.87403700
H	-2.69698300	-1.97535500	1.95930600
C	0.30941800	-2.87891700	4.24060600
H	1.55847500	-2.26664900	2.58768600
C	-0.99568300	-3.04880000	4.70408900
H	-3.09373400	-2.84950700	4.22958400
H	1.15656300	-3.13469600	4.87952600
H	-1.17592100	-3.43554500	5.70860900
C	1.63473900	0.30669400	0.45459800
C	3.04248400	-0.07282100	0.13681800
C	4.12415300	0.69674000	0.57742800
C	3.32414900	-1.25177800	-0.57676900
C	5.44394200	0.32134700	0.31715300
H	3.94456900	1.60832200	1.15005100
C	4.62764800	-1.63832000	-0.84230800
H	2.49666000	-1.87043000	-0.92942100
C	5.70388000	-0.85141200	-0.40063200
H	6.25679900	0.94796000	0.68209200
H	4.84407600	-2.55011100	-1.40102200
C	1.26143500	1.74190800	0.63914400
C	0.28099800	2.11281600	1.56433700
C	1.85490000	2.75508300	-0.13497600
C	-0.10747500	3.44342900	1.72699700
H	-0.19016600	1.34347000	2.18074900
C	1.47988600	4.08189400	0.01553000

H	2.61357500	2.49652300	-0.87653300
C	0.49129000	4.43863200	0.94583100
H	-0.87456500	3.68753700	2.46110100
H	1.93218900	4.86877600	-0.59009900
O	6.93848700	-1.29434300	-0.70937900
O	0.17736200	5.74854700	1.01585900
C	8.04800700	-0.53159900	-0.29184900
H	8.08914600	-0.44883100	0.80610900
H	8.94137600	-1.05871200	-0.64548800
H	8.02866900	0.47947500	-0.72963200
C	-0.80109300	6.15441400	1.94539200
H	-0.89727500	7.24150600	1.84509700
H	-1.77637800	5.68601700	1.73497000
H	-0.50108700	5.91193400	2.97754000
C	0.70189700	-0.62175600	0.58347700

Int 1$_{C2}$

C	-1.84199100	3.67863200	1.65352100
C	-2.63571300	3.57385500	0.52995600
C	-3.14728900	2.31777800	0.14011400
C	-2.78010800	1.13781800	0.84953400
C	-2.12282000	1.28969600	2.11224500
C	-1.63740000	2.54747500	2.45823900
C	-4.14700600	2.25026500	-0.89831400
C	-3.21708900	-0.14431800	0.28352700
C	-4.33111700	-0.15121200	-0.60197100
C	-4.79042500	1.08862900	-1.17234300
C	-4.90222000	-1.37675000	-1.01619600
H	-5.78003900	-1.35368200	-1.66484600
C	-4.34813700	-2.57357000	-0.62274900
C	-3.12194600	-2.57677700	0.07738600
C	-2.52623600	-1.37101100	0.46617000
H	-4.42975100	3.17937300	-1.39757400
H	-1.43128400	4.64338900	1.95625500
H	-2.90563000	4.45644500	-0.05391500
H	-1.12589000	2.67244200	3.41459200
H	-5.61557200	1.05492300	-1.88658700
H	-4.80278300	-3.52395600	-0.90902100
C	-2.15120100	0.22564900	3.21212200
C	-3.27405800	0.57975400	4.19724500
C	-0.82508600	0.06014600	3.95992300
H	-2.42237100	-0.74254300	2.77583700
H	-4.24291000	0.66270900	3.68280600
H	-3.36067400	-0.19773400	4.97147400
H	-3.06882000	1.53937700	4.69624600

H	0.02170700	-0.14075600	3.28659100
H	-0.58362300	0.95731900	4.54914000
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C	-1.27950700	-3.93660200	1.02470700
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H	-0.83931300	-4.89553900	1.30342600
C	-1.05578000	-1.40490500	0.80930300
H	-0.75232700	-0.61912400	1.49835200
C	-0.54432100	-2.71912200	1.39703700
O	0.45887000	-2.73571700	2.07904000
C	-0.22822400	-1.15292400	-0.47762500
C	-0.66211300	-1.76626200	-1.77390400
C	-0.24072400	-3.04946500	-2.14084900
C	-1.52451100	-1.05859900	-2.62173700
C	-0.68739900	-3.62285500	-3.33232500
H	0.43432800	-3.60188300	-1.48276800
C	-1.97209900	-1.63379800	-3.81010900
H	-1.84495900	-0.05238100	-2.34045400
C	-1.55839300	-2.91928100	-4.16462600
H	-0.35347000	-4.62416900	-3.61015400
H	-2.64603400	-1.07458900	-4.46178600
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C	1.97392100	0.28129000	-0.31426000
C	1.97388100	1.75096300	-0.56133000
C	3.12149600	2.40158000	-1.02587100
C	0.80579200	2.51708800	-0.39130800
C	3.12345600	3.76708800	-1.31913900
H	4.04112000	1.83450200	-1.18023600
C	0.79302100	3.87178900	-0.68081500
H	-0.10595700	2.03937300	-0.02031300
C	1.95261000	4.51252100	-1.14769300
H	4.03921100	4.23136400	-1.68284200
H	-0.11105700	4.46706100	-0.54685900
C	3.24278400	-0.42876300	0.02798100
C	3.53018500	-1.68573800	-0.51002600
C	4.15550900	0.12411400	0.94327800
C	4.68368300	-2.38734400	-0.15572400
H	2.83801100	-2.12678100	-1.23101600
C	5.30446000	-0.56158600	1.30693800
H	3.95314700	1.10150000	1.38629700
C	5.58008600	-1.82542300	0.76064100
H	4.87356300	-3.36254500	-0.60234600
H	6.01050700	-0.14044800	2.02418900

O	1.84799400	5.83260000	-1.39918900
O	6.71985500	-2.41932400	1.16774300
C	2.98630100	6.51634900	-1.87195700
H	3.32845100	6.10900500	-2.83692400
H	2.68904500	7.56221100	-2.00961700
H	3.81416200	6.46957800	-1.14613500
C	7.02903400	-3.69624100	0.65786400
H	7.97533200	-3.99780600	1.12122500
H	6.25053400	-4.43215700	0.91619200
H	7.15543000	-3.67325800	-0.43663600
C	0.85986600	-0.42574600	-0.40135400

3e

C	5.30637400	-2.60744800	0.09176900
C	4.91518100	-2.40540400	-1.21492300
C	4.13836700	-1.27705200	-1.55528700
C	3.67138600	-0.39283600	-0.54097100
C	4.25992200	-0.49733500	0.75906200
C	5.02574100	-1.62156200	1.05158600
C	3.91757700	-0.95980900	-2.94497600
C	2.67873900	0.61487600	-0.93886600
C	2.62692900	0.99156900	-2.30886500
C	3.29683300	0.19003900	-3.30140400
C	1.80868800	2.06782700	-2.70867400
H	1.83369300	2.38987000	-3.75163800
C	0.95412300	2.66917900	-1.81063100
C	0.80122100	2.14986800	-0.51024500
C	1.66093300	1.12423500	-0.07947200
H	4.33470000	-1.63233100	-3.69733800
H	5.89578000	-3.48374100	0.36670400
H	5.22043200	-3.09167400	-2.00752500
H	5.46834200	-1.71895500	2.04430100
H	3.20818300	0.48501400	-4.34892000
H	0.33521100	3.50937800	-2.13214000
C	4.29670200	0.66899800	1.74617600
C	5.60064100	1.44779400	1.52213000
C	4.17157500	0.25365100	3.21281300
H	3.48039700	1.36546200	1.52511500
H	5.68174900	1.79846200	0.48254000
H	5.63929000	2.32526800	2.18548200
H	6.47508400	0.81434400	1.73788600
H	3.28507700	-0.37285700	3.39215300
H	5.05868000	-0.30232300	3.55197100
H	4.07857900	1.14794300	3.84411000

C	-0.30084400	2.73925600	0.38403500
C	-0.50703400	1.87212000	1.64192900
H	0.05414400	3.73556600	0.69524200
H	-1.15557900	2.37449100	2.37166000
C	1.28417500	0.38462200	1.22094500
H	2.06534100	-0.27749600	1.59207000
C	0.83990800	1.46681100	2.18430100
O	1.43076500	1.91912800	3.12744500
C	-0.02747800	-0.29920400	0.86740700
C	0.00315300	-1.55966900	0.10026900
C	-0.69636500	-1.69712900	-1.10808300
C	0.82078700	-2.61570200	0.53414100
C	-0.60253700	-2.87424300	-1.84882700
H	-1.29428700	-0.86327500	-1.48019400
C	0.91095000	-3.79239300	-0.20589700
H	1.38707800	-2.51387600	1.46292100
C	0.19657500	-3.92560900	-1.39791400
H	-1.14782200	-2.96515900	-2.78995300
H	1.54647100	-4.60647400	0.14689400
H	0.27158600	-4.84500100	-1.98120500
C	-2.39270000	0.62991500	0.52120800
C	-3.24621100	-0.58013400	0.57966200
C	-3.98788700	-1.02215900	-0.52262200
C	-3.24561200	-1.38348400	1.73459900
C	-4.72417700	-2.20569200	-0.48377600
H	-3.96457500	-0.45037600	-1.45270800
C	-3.97761500	-2.55846600	1.79249100
H	-2.65749600	-1.07639100	2.60187400
C	-4.72556900	-2.98214100	0.68228700
H	-5.27644200	-2.51940400	-1.36866700
H	-3.98252700	-3.17860800	2.68987700
C	-2.72757500	1.83843600	-0.02706100
C	-1.69043400	2.93174400	-0.29598300
C	-4.08866800	2.15996200	-0.44115000
C	-2.26603400	4.31476300	0.02257000
H	-1.54238600	2.89853800	-1.38866700
C	-4.48772700	3.40512900	-0.78263700
H	-4.82844100	1.35822400	-0.43888800
C	-3.59365900	4.57111000	-0.65761300
H	-2.43893800	4.40613500	1.11074300
H	-5.51368000	3.60648200	-1.09760400
O	-5.39809300	-4.13959400	0.81881200
O	-3.92991100	5.68195600	-1.01479100
C	-6.14649400	-4.61591300	-0.27730300

H	-5.50201300	-4.80780700	-1.15008100
H	-6.60597600	-5.55761000	0.04349300
H	-6.93966500	-3.90584400	-0.56114100
C	-1.03908600	0.57321600	1.08374400
H	-1.56872200	5.11167000	-0.26975300

3e'

C	-3.31854500	1.43632600	-3.08385600
C	-4.31157800	0.57673100	-2.67912000
C	-4.33119500	0.09896100	-1.34768400
C	-3.27760300	0.42988300	-0.44360400
C	-2.37080100	1.48430500	-0.81745800
C	-2.39641100	1.92160700	-2.13605900
C	-5.46937000	-0.64104300	-0.88402100
C	-3.28011600	-0.24049700	0.84940500
C	-4.51255700	-0.72462100	1.33934500
C	-5.60439600	-0.93709700	0.43647800
C	-4.67060100	-1.01260200	2.73291200
H	-5.65684500	-1.31214100	3.09283500
C	-3.62405400	-0.85516100	3.58944400
C	-2.30745600	-0.62607200	3.07687800
C	-2.10627700	-0.46248900	1.67540400
H	-6.26199000	-0.87404400	-1.59809400
H	-3.28435000	1.80606100	-4.11015400
H	-5.10822000	0.26886100	-3.35981700
H	-1.71221400	2.70738700	-2.45263600
H	-6.51996800	-1.38692800	0.82575000
H	-3.74816000	-0.98913700	4.66587400
C	-1.56637800	2.28026200	0.21393600
C	-2.50088000	2.86942000	1.28249400
C	-0.74809200	3.41705100	-0.39360200
H	-0.85080400	1.61942300	0.71882100
H	-3.07282500	2.10253300	1.82155600
H	-1.91360100	3.43390900	2.02243700
H	-3.21855600	3.56347600	0.81623800
H	-0.04021000	3.05824300	-1.15275500
H	-1.39519300	4.18034900	-0.85426700
H	-0.16670000	3.90900000	0.39969200
C	-1.19322700	-0.66062100	3.95170400
C	0.08635600	-0.61292300	3.46036400
H	-1.37138700	-0.74051900	5.02588700
H	0.96114600	-0.63215900	4.11133100
C	-0.77583500	-0.63050400	1.15952800
C	0.28846500	-0.62946000	2.06361800

O	1.57536500	-0.74149700	1.66974000
C	-0.41766400	-0.98582800	-0.23467400
C	-1.36462600	-1.70179800	-1.13853100
C	-2.21916700	-2.69524800	-0.63549800
C	-1.36316400	-1.44950200	-2.51593800
C	-3.06779100	-3.39748800	-1.48828500
H	-2.21743100	-2.91895500	0.43310800
C	-2.20781300	-2.15825500	-3.37015900
H	-0.71147900	-0.66986000	-2.91635100
C	-3.06976700	-3.12802800	-2.85892600
H	-3.72963500	-4.16343900	-1.07954700
H	-2.20222400	-1.93828600	-4.43951500
H	-3.73901800	-3.67544000	-3.52506400
C	1.94593700	-0.38412900	0.32951600
C	2.16737400	1.12240200	0.22995300
C	2.39921100	1.70371300	-1.01820800
C	2.25283400	1.92993500	1.36982900
C	2.72229900	3.05481500	-1.14362600
H	2.34751900	1.08962200	-1.92096900
C	2.55820800	3.28200300	1.25960700
H	2.09176100	1.49496500	2.35705400
C	2.79766200	3.85585100	0.00349200
H	2.89998100	3.47286600	-2.13374500
H	2.61784500	3.92025600	2.14251500
C	3.24263900	-1.16445000	0.08526500
C	4.49653600	-0.56415600	0.00438200
C	3.17078500	-2.56543900	0.00194500
C	5.65833500	-1.32452300	-0.17013000
H	4.59360400	0.51979700	0.07720900
C	4.31043000	-3.33306300	-0.17009100
H	2.19990000	-3.06084000	0.07833300
C	5.57004200	-2.71601200	-0.26075900
H	6.62036600	-0.81763800	-0.23145100
H	4.25729700	-4.42065400	-0.23716800
O	3.08233700	5.17420100	-0.01181500
O	6.62699800	-3.53394800	-0.43216000
C	3.29924900	5.79777500	-1.25667700
H	2.40992800	5.72415700	-1.90356800
H	3.50309200	6.85400100	-1.04698800
H	4.16454700	5.36168600	-1.78155700
C	7.91090400	-2.95849400	-0.51927400
H	8.61694700	-3.78602400	-0.65244100
H	7.98827300	-2.27604500	-1.38103200
H	8.16827400	-2.40908600	0.40056300

C	0.86749300	-0.86555200	-0.61898900
H	1.18635900	-1.22136400	-1.60019600

DPA

P	-0.19670500	1.95246800	0.01868500
O	-0.86588200	0.92510200	-1.02598500
O	0.49786800	3.03828400	-0.67808600
O	-1.32863800	2.43531600	1.02133600
H	-1.62235400	1.77118900	1.67016900
O	0.66282200	0.99828400	0.99759800
C	-1.58348800	-0.19513700	-0.63381900
C	-2.87148100	-0.05008600	-0.12176100
C	-1.00470400	-1.45074100	-0.80572200
C	-3.58376600	-1.19256300	0.24486500
H	-3.30819700	0.94544100	-0.02848200
C	-1.72967300	-2.58340300	-0.43830700
H	0.00018700	-1.52501600	-1.22490400
C	-3.01537800	-2.45733000	0.09119300
H	-4.59343200	-1.08924500	0.64556300
H	-1.28420300	-3.57092100	-0.56897200
H	-3.57762100	-3.34722400	0.37766500
C	1.64399800	0.12426900	0.56057000
C	1.80255900	-1.05086400	1.29229700
C	2.43651400	0.40251300	-0.55148500
C	2.76851500	-1.97159200	0.89402800
H	1.15986100	-1.22990500	2.15529100
C	3.39329400	-0.53573500	-0.94321500
H	2.30914700	1.33873900	-1.09745400
C	3.56234900	-1.72048800	-0.22752900
H	2.89678600	-2.89466900	1.46168800
H	4.01444100	-0.32812400	-1.81604500
H	4.31416900	-2.44622900	-0.54038800

DPA-anion

P	-0.28512000	2.20804400	-0.16896700
O	-0.78588500	0.98190000	-1.19364900
O	0.69149400	3.00466500	-0.96000000
O	-1.44383300	2.79052600	0.56061700
O	0.50429600	1.24995500	0.95462500
C	-1.38438500	-0.15984900	-0.76244500
C	-2.27994200	-0.18976000	0.31401600
C	-1.06588700	-1.34332200	-1.43961200
C	-2.83801400	-1.40692400	0.70618500
H	-2.51355600	0.74389300	0.82667600

C	-1.63726900	-2.54977700	-1.04275300
H	-0.35812300	-1.29282200	-2.26899100
C	-2.52368500	-2.58997200	0.03591300
H	-3.53177600	-1.42613700	1.54941500
H	-1.37990500	-3.46724900	-1.57586000
H	-2.96582100	-3.53639600	0.35121700
C	1.38397900	0.26822400	0.62389800
C	1.37893100	-0.88676500	1.41554300
C	2.26676500	0.36942700	-0.45866000
C	2.25017500	-1.93426800	1.12742900
H	0.67365800	-0.94381800	2.24661600
C	3.12852800	-0.69119100	-0.74058200
H	2.25311900	1.27710400	-1.06272200
C	3.12794500	-1.84490900	0.04472000
H	2.23606500	-2.83144100	1.74956500
H	3.81185400	-0.60939800	-1.58854900
H	3.80573200	-2.66859600	-0.18502000

H_2O

O	0.00000000	0.00000000	0.12032000
H	0.00000000	0.75555900	-0.48127900
H	0.00000000	-0.75555900	-0.48127900

MeOH

O	-0.74320700	0.12365700	0.00000400
H	-1.13063500	-0.76068600	0.00001400
C	0.65363700	-0.01938700	0.00000100
H	1.02887600	-0.55041700	-0.89334900
H	1.09654300	0.98690200	-0.00099500
H	1.02905100	-0.54873200	0.89428900

TS-a1

C	-6.62333800	-3.15481100	0.92151600
C	-7.05503100	-1.89333100	1.27163700
C	-6.47489500	-0.75466300	0.66927900
C	-5.38114400	-0.89962100	-0.23086800
C	-5.10030900	-2.20577200	-0.74501300
C	-5.69561400	-3.29910300	-0.12491400
C	-7.05457200	0.54490500	0.88886800
C	-4.67559600	0.32321900	-0.62396000
C	-5.37508700	1.55942200	-0.53528700
C	-6.59392600	1.63351800	0.21995000
C	-4.81356700	2.73288600	-1.10182400
H	-5.39571500	3.65616800	-1.07314000

C	-3.55748800	2.71488200	-1.65121700
C	-2.75010000	1.54957800	-1.54221000
C	-3.30284300	0.37271200	-0.98677700
H	-7.92097100	0.61639900	1.54954200
H	-7.05360200	-4.04014000	1.39256700
H	-7.86126000	-1.75342700	1.99471900
H	-5.47991500	-4.30323200	-0.49433500
H	-7.08939200	2.60223700	0.31016600
H	-3.12885000	3.61338100	-2.10026800
C	-4.39441700	-2.43918300	-2.08157800
C	-5.46506700	-2.52944300	-3.17847200
C	-3.49980500	-3.68002500	-2.11209600
H	-3.77754500	-1.56803400	-2.32976900
H	-6.08489200	-1.62102900	-3.20658200
H	-4.99137400	-2.65430500	-4.16409100
H	-6.12869500	-3.39053700	-3.00394400
H	-2.77248200	-3.69348400	-1.28684900
H	-4.09451500	-4.60418300	-2.05875600
H	-2.93389000	-3.70697700	-3.05390500
C	-1.35505900	1.61606400	-1.88697800
C	-0.48536400	0.56328800	-1.56446300
H	-0.96691700	2.52832200	-2.34081500
H	0.54205700	0.59897700	-1.93512900
C	-2.30573200	-0.72277200	-0.60408100
H	-2.74324100	-1.70836000	-0.44685500
C	-1.18643000	-0.75867800	-1.60373700
O	-0.89457200	-1.69617300	-2.31736700
C	-1.57724200	-0.16684100	0.61766000
C	-2.21079200	-0.19237700	1.95613800
C	-3.17595300	-1.16177500	2.27486600
C	-1.85478800	0.74332300	2.94434600
C	-3.76379100	-1.19437600	3.54000200
H	-3.46770900	-1.91065100	1.53715500
C	-2.44660500	0.71094800	4.20290400
H	-1.11310300	1.51096200	2.71621000
C	-3.40477800	-0.25881300	4.50849900
H	-4.50746400	-1.96117000	3.76504400
H	-2.15937500	1.45195900	4.95103400
H	-3.86708300	-0.28351400	5.49670800
C	0.65319500	1.14264300	0.87100900
C	1.61042700	0.43013800	1.73627100
C	2.46159400	1.12102500	2.61256000
C	1.67730500	-0.98062000	1.74469200
C	3.37207000	0.45472100	3.43503100

H	2.41195000	2.20915600	2.67271400
C	2.57091400	-1.65338500	2.55753700
H	1.04860600	-1.55444800	1.06242200
C	3.44174100	-0.94279500	3.40273400
H	4.01253900	1.03472100	4.09838900
H	2.62769600	-2.74326400	2.54863500
C	0.82196700	2.54979500	0.49012800
C	-0.31300900	3.35220800	0.27538500
C	2.08839700	3.13465900	0.24444200
C	-0.21142600	4.68213800	-0.14517300
H	-1.30089200	2.94174600	0.49402700
C	2.19970000	4.44059700	-0.18979100
H	2.99300300	2.53743300	0.36661700
C	1.04926300	5.23246500	-0.38537400
H	-1.11880100	5.27073600	-0.27610200
H	3.17491000	4.88348100	-0.39853400
O	4.29529900	-1.67922500	4.14099800
O	1.26018200	6.49476900	-0.79866900
C	5.20597200	-1.00696400	4.98108200
H	4.68336200	-0.41506000	5.74944400
H	5.80856100	-1.77947400	5.47210600
H	5.86996600	-0.34404600	4.40293100
C	0.14111800	7.32610500	-1.01271000
H	0.52983700	8.29403800	-1.34843300
H	-0.52223400	6.91339600	-1.78975200
H	-0.43466800	7.46974500	-0.08443100
C	-0.43294900	0.48805400	0.34014700
P	2.26230900	-2.15450900	-1.80960500
O	2.49815200	-0.79562900	-0.97418600
O	1.56439700	-3.14145900	-0.96755400
O	1.56938500	-1.75095500	-3.16870700
H	0.57764200	-1.73950800	-3.03043500
O	3.73026000	-2.53313900	-2.35591600
C	3.45449900	0.17215200	-1.20553800
C	3.45651100	0.91423200	-2.38363000
C	4.39256300	0.39715600	-0.19802100
C	4.42402300	1.90805200	-2.54915600
H	2.71440800	0.70967900	-3.15745300
C	5.35205500	1.39049000	-0.37735300
H	4.35058500	-0.21057100	0.70841800
C	5.36950800	2.14835800	-1.55191300
H	4.43406900	2.49743600	-3.46745600
H	6.08986900	1.57232100	0.40614300
H	6.12249200	2.92575600	-1.68997700

C	4.82793500	-2.58750600	-1.51180000
C	6.03316200	-2.10058500	-2.01299200
C	4.72480400	-3.07905600	-0.21159000
C	7.15234200	-2.08515000	-1.18410400
H	6.06860000	-1.72053500	-3.03501200
C	5.85162900	-3.04270100	0.61161200
H	3.77172100	-3.46855900	0.14980800
C	7.06289100	-2.54438100	0.13251000
H	8.09830400	-1.69840300	-1.56684700
H	5.77271800	-3.40518000	1.63822200
H	7.93900600	-2.51786700	0.78201100

Int a1

C	-6.13593800	2.03597200	1.31065200
C	-6.37623500	1.51514000	0.06360800
C	-5.79370400	0.27653100	-0.31904100
C	-4.86419700	-0.36686000	0.55781900
C	-4.83356000	0.06023000	1.93519000
C	-5.42363100	1.26585500	2.26141100
C	-6.16885800	-0.36319400	-1.53553800
C	-4.08797900	-1.44638900	0.00678200
C	-4.60198800	-2.15046600	-1.08322200
C	-5.67568000	-1.60447800	-1.84033800
C	-4.04406400	-3.45874400	-1.42732600
H	-4.56939800	-4.04242700	-2.18666100
C	-2.97368900	-3.97123600	-0.78830500
C	-2.17209000	-3.13134100	0.08914200
C	-2.66398900	-1.74283600	0.36699400
H	-6.90323200	0.12528000	-2.17933700
H	-6.56870500	2.99355100	1.60509200
H	-7.03164700	2.02546500	-0.64547400
H	-5.41018800	1.60318500	3.29994300
H	-6.03863200	-2.15593900	-2.71010800
H	-2.60963700	-4.97681600	-1.00766900
C	-4.46567400	-0.91101000	3.05749500
C	-5.75129300	-1.60954700	3.52413800
C	-3.75582400	-0.26614900	4.24922000
H	-3.81914800	-1.69925500	2.65264700
H	-6.25798300	-2.11126800	2.68651700
H	-5.51869200	-2.36653000	4.28869400
H	-6.45247700	-0.88214000	3.96149600
H	-2.85879300	0.29877200	3.95424900
H	-4.42494900	0.42030300	4.78936900
H	-3.44149700	-1.04356800	4.96094600

C	-0.88948100	-3.41824100	0.39710800
C	-0.03541500	-2.23158700	0.80655900
H	-0.43099800	-4.38057700	0.16360500
H	1.00380500	-2.48852900	1.03826700
C	-1.94268800	-0.90492700	1.39604800
H	-2.47029900	-0.17073600	1.99293000
C	-0.77194900	-1.58968100	1.97004300
O	-0.45424400	-1.61941300	3.14268900
C	-1.59845300	-0.61695100	-0.04533900
C	-2.18124600	0.58549800	-0.71428400
C	-2.35747300	1.77511000	-0.00270700
C	-2.61233900	0.51012900	-2.04362200
C	-2.95410000	2.87980600	-0.61282900
H	-2.00714300	1.83569400	1.03000300
C	-3.19304000	1.61741200	-2.65830200
H	-2.48505100	-0.42394200	-2.59652000
C	-3.36934800	2.80472800	-1.94210400
H	-3.09078400	3.80312500	-0.04659100
H	-3.51843000	1.55163200	-3.69863300
H	-3.83270700	3.66899500	-2.42165500
C	0.67935700	-0.87302600	-1.25219600
C	0.51378800	0.33323700	-2.11558800
C	0.40786600	0.22642500	-3.50274300
C	0.50043600	1.61196300	-1.53891400
C	0.22761000	1.35431300	-4.30636200
H	0.44158400	-0.76015900	-3.97165900
C	0.33470600	2.74360200	-2.32398800
H	0.59897500	1.69504800	-0.45363700
C	0.18012700	2.62245000	-3.71403000
H	0.12245900	1.23318400	-5.38382800
H	0.30776400	3.74172600	-1.88301000
C	1.94644700	-1.62415400	-1.47273400
C	2.05340100	-3.01189700	-1.31917300
C	3.10235300	-0.93579300	-1.89664300
C	3.25902100	-3.68972400	-1.51554400
H	1.16795800	-3.59651600	-1.07148300
C	4.30261100	-1.59219200	-2.10924600
H	3.05961900	0.14532200	-2.03998300
C	4.39978900	-2.97662400	-1.90111800
H	3.28943800	-4.77045700	-1.38171300
H	5.19681300	-1.04813700	-2.41797900
O	-0.00290100	3.77137000	-4.39830000
O	5.61113400	-3.53158800	-2.10158200
C	-0.19256300	3.69754300	-5.79181000

H	-1.08389500	3.10045000	-6.04535200
H	-0.33804800	4.72531700	-6.14389300
H	0.68620800	3.26558800	-6.29762400
C	5.76419300	-4.91071700	-1.85729000
H	6.81695200	-5.14838300	-2.04799300
H	5.52089300	-5.16164100	-0.81184800
H	5.13207100	-5.51319100	-2.52938600
C	-0.22912300	-1.18912000	-0.29878500
P	1.81343800	0.58504800	2.30200800
O	2.68869200	0.27562600	0.98870000
O	0.44853500	0.99890900	1.91819900
O	1.95234200	-0.65568600	3.26412300
H	1.09899900	-1.16651900	3.34802600
O	2.70576300	1.65625300	3.10888800
C	3.99785700	-0.17936700	1.00684300
C	4.28292000	-1.48187600	1.40945700
C	4.99283400	0.67002000	0.52914900
C	5.59638300	-1.94208500	1.31851000
H	3.48017900	-2.12419800	1.77258400
C	6.30178900	0.19718000	0.44464900
H	4.72557700	1.67964400	0.21139600
C	6.60578500	-1.10856000	0.83418300
H	5.82792600	-2.96486600	1.62161800
H	7.08635200	0.85326900	0.06394400
H	7.62972900	-1.47734900	0.75838500
C	3.18297900	2.81965800	2.53018500
C	4.47271000	3.21313400	2.88094900
C	2.41061600	3.56922600	1.64386600
C	5.00236100	4.37466000	2.32348700
H	5.04416900	2.59663200	3.57613300
C	2.96008300	4.72386000	1.08415200
H	1.39361100	3.25409200	1.40460300
C	4.25188300	5.12916600	1.41875000
H	6.01250500	4.68712100	2.59338300
H	2.36389100	5.31171300	0.38414300
H	4.67295300	6.03408400	0.97858200

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C	-6.09021700	-3.30202700	2.30788900
C	-6.79179600	-2.16423900	1.97079600
C	-6.35650100	-1.35600500	0.89650400
C	-5.13830500	-1.65801000	0.22283600
C	-4.55658700	-2.94907400	0.43213600
C	-5.01851900	-3.71537300	1.49681700

C	-7.19806400	-0.29352900	0.41142600
C	-4.62337900	-0.64706900	-0.70556000
C	-5.55251800	0.26438800	-1.27913300
C	-6.86056000	0.40272400	-0.70556200
C	-5.14545400	1.10508000	-2.34858700
H	-5.89325900	1.74347700	-2.82369800
C	-3.83885700	1.13667000	-2.75913000
C	-2.84156700	0.42552200	-2.03207800
C	-3.24463700	-0.44895700	-0.98989100
H	-8.14872900	-0.11727000	0.91870600
H	-6.41032100	-3.92461800	3.14501800
H	-7.70292200	-1.88536900	2.50413700
H	-4.57424500	-4.69584900	1.67809700
H	-7.53991600	1.14095900	-1.13636700
H	-3.52864200	1.77728900	-3.58742600
C	-3.65133100	-3.62636600	-0.59810900
C	-4.53240700	-4.47419100	-1.52654000
C	-2.54153000	-4.48706400	0.00898800
H	-3.18420100	-2.86533000	-1.23362600
H	-5.30433800	-3.86007000	-2.01352200
H	-3.91856600	-4.94226200	-2.31105700
H	-5.03720300	-5.27320600	-0.96169300
H	-1.94331200	-3.93825300	0.75192400
H	-2.95225600	-5.38251200	0.49916200
H	-1.85840400	-4.82757000	-0.78178100
C	-1.45195600	0.69267600	-2.29141000
C	-0.45636900	0.15266200	-1.35325400
H	-1.14562400	1.05153500	-3.27248200
H	0.57611900	0.20512800	-1.71357400
C	-2.12826500	-1.00415500	-0.10055200
H	-2.39827000	-1.88361000	0.48146600
C	-0.91617600	-1.22914500	-0.96344500
O	-0.41664100	-2.29156500	-1.27082000
C	-1.64141100	0.18404800	0.72687400
C	-2.31226500	0.58368700	1.97647900
C	-3.09893500	-0.33681000	2.69112100
C	-2.19154300	1.89058500	2.48478000
C	-3.73318700	0.03350300	3.87641600
H	-3.21792900	-1.35863500	2.32825300
C	-2.82698300	2.25689900	3.66718500
H	-1.60835300	2.63232800	1.93764200
C	-3.59948100	1.32995400	4.37089800
H	-4.33612600	-0.70094800	4.41356900
H	-2.72286400	3.27770500	4.03903900

H	-4.09776400	1.61988200	5.29752900
C	0.11614100	2.03445500	0.23542600
C	1.05722600	2.14360400	1.35231700
C	1.54599900	3.38683600	1.78847400
C	1.47965200	0.99544100	2.05916100
C	2.45228900	3.49159700	2.84235100
H	1.19583600	4.30283500	1.30973300
C	2.36912300	1.08665700	3.11340700
H	1.11942700	0.01181800	1.75048500
C	2.88285400	2.33488900	3.50467300
H	2.80502300	4.47645300	3.14569900
H	2.70772800	0.19561800	3.64400000
C	0.01107400	2.96866800	-0.83254400
C	-1.21070700	3.01775200	-1.57369100
C	1.10016300	3.78058500	-1.29408200
C	-1.34402100	3.87005800	-2.69960800
H	-2.11780000	2.67066500	-1.08304400
C	0.97476500	4.55435900	-2.41285600
H	2.05854800	3.73363300	-0.77532100
C	-0.26111100	4.61018400	-3.13022900
H	-2.31023800	3.93782900	-3.19881100
H	1.81237600	5.13903900	-2.79632200
O	3.77424100	2.32546600	4.51264200
O	-0.26437200	5.43269700	-4.19286500
C	4.35570600	3.54831900	4.90596500
H	3.59737700	4.25118500	5.28616900
H	5.06299900	3.31473200	5.70966400
H	4.89914200	4.01932400	4.07071100
C	-1.44724800	5.53237900	-4.95417900
H	-1.23521400	6.22615800	-5.77529900
H	-1.73719600	4.55379700	-5.36973900
H	-2.27878600	5.92848300	-4.34951700
C	-0.67287600	0.85709000	0.05127400
P	3.00378100	-2.79212900	-1.29893000
O	3.20274200	-2.03780700	0.11899300
O	2.69249100	-4.21135900	-1.07165000
O	1.98467300	-1.95301600	-2.15926200
H	1.02693600	-2.16131700	-1.92540700
O	4.35618600	-2.43769700	-2.10462200
C	3.87490500	-0.84603800	0.31337100
C	3.64317100	0.27009600	-0.48808900
C	4.78784900	-0.80480200	1.36635300
C	4.34113000	1.44899800	-0.21699800
H	2.92950500	0.21699900	-1.31228300

C	5.47253100	0.37920400	1.62865400
H	4.94572700	-1.70402400	1.96372600
C	5.25042300	1.51011300	0.83910200
H	4.16847500	2.32644800	-0.84296000
H	6.18227400	0.41834000	2.45691000
H	5.78724700	2.43742200	1.04590300
C	5.61075200	-2.61720000	-1.54842100
C	6.54799500	-1.60851700	-1.76352500
C	5.92096900	-3.75110800	-0.79960600
C	7.81830800	-1.73435200	-1.20665700
H	6.26227900	-0.73537300	-2.35203000
C	7.19554300	-3.85792000	-0.24048100
H	5.17048100	-4.53048100	-0.65765400
C	8.14378200	-2.85479500	-0.43856300
H	8.55554700	-0.94594400	-1.36723200
H	7.44517000	-4.73948900	0.35236000
H	9.13744000	-2.94636900	0.00221300

Int a2

C	5.69107400	-2.38911900	-0.09017200
C	5.40501200	-1.95695500	-1.36785400
C	4.56313100	-0.84118400	-1.56673200
C	3.92508400	-0.21438600	-0.45784900
C	4.40324500	-0.53285600	0.85284100
C	5.23746200	-1.63601000	1.00506700
C	4.44459400	-0.26685600	-2.88420700
C	2.88361500	0.77742900	-0.75837400
C	2.92333200	1.41623000	-2.02778300
C	3.75398300	0.88248200	-3.07701400
C	2.04900400	2.48908500	-2.30243200
H	2.13657100	3.00779200	-3.25921900
C	1.07003400	2.84176100	-1.40087900
C	0.85645500	2.07242500	-0.23915800
C	1.75160200	1.03628400	0.07194000
H	4.99010100	-0.74138400	-3.70246800
H	6.32978200	-3.25871900	0.07326100
H	5.84335500	-2.44638300	-2.24004000
H	5.59695900	-1.89567700	2.00236300
H	3.73512000	1.37531000	-4.05114500
H	0.39747500	3.67356500	-1.62411300
C	4.25531600	0.41704900	2.04040300
C	5.50458400	1.30751600	2.10264800
C	4.03742400	-0.28623400	3.38067400
H	3.40742200	1.08943500	1.87236400

H	5.64779900	1.85959700	1.16187900
H	5.41059500	2.03890000	2.91983100
H	6.40666900	0.70273800	2.28422500
H	3.19679900	-0.99538000	3.34396200
H	4.93617200	-0.83682700	3.69705600
H	3.80942600	0.45731200	4.15640600
C	-0.37902800	2.39866800	0.60908800
C	-0.57091200	1.36793900	1.73386200
H	-0.20614700	3.38732100	1.06164600
H	-1.27513000	1.72809300	2.49424000
C	1.32555100	0.06055600	1.18321000
H	2.11928000	-0.61415200	1.50120800
C	0.76859300	0.94914300	2.28120400
O	1.27689400	1.25955400	3.32476300
C	0.06866200	-0.62820800	0.66337000
C	0.17299600	-1.76827700	-0.26527600
C	-0.69277400	-1.89739700	-1.36384900
C	1.18814900	-2.72517000	-0.09511200
C	-0.56969000	-2.97038500	-2.24354200
H	-1.45126100	-1.13469900	-1.54300900
C	1.31071100	-3.79701700	-0.97703700
H	1.88557700	-2.63576900	0.74064300
C	0.42869900	-3.92656200	-2.05065500
H	-1.25063500	-3.05236300	-3.09264400
H	2.10277500	-4.53246300	-0.82546000
H	0.52663000	-4.76460500	-2.74292200
C	-2.38917200	0.17765800	0.49641900
C	-3.23166200	-1.03983800	0.53175200
C	-4.09388700	-1.38065100	-0.51816800
C	-3.12164000	-1.94340500	1.60523000
C	-4.84329500	-2.55726700	-0.50126500
H	-4.16277900	-0.72823800	-1.39133700
C	-3.86274500	-3.11403000	1.63995700
H	-2.44143400	-1.71699700	2.42908000
C	-4.73515900	-3.43195300	0.58704900
H	-5.49307900	-2.78767500	-1.34466600
H	-3.78226900	-3.80974600	2.47641000
C	-2.77119100	1.41999400	0.06440500
C	-1.70792700	2.48699000	-0.23953000
C	-4.15708500	1.78039700	-0.19773200
C	-2.24175100	3.89532100	-0.28019400
H	-1.40766100	2.23579100	-1.27561600
C	-4.53130000	3.05526300	-0.43196600
H	-4.92285100	1.01016300	-0.10362500

C	-3.55843200	4.14491600	-0.42656100
H	-1.50974300	4.70348900	-0.26027900
H	-5.58132200	3.32480800	-0.55793800
O	-5.41408400	-4.59025400	0.69837000
O	-4.12955000	5.36370000	-0.54280100
C	-6.28970900	-4.95817600	-0.34305200
H	-5.75099100	-5.08387100	-1.29601200
H	-6.73478700	-5.91697700	-0.05382600
H	-7.09156400	-4.21424100	-0.47644500
C	-3.27804500	6.48306900	-0.51451300
H	-3.91258200	7.36974700	-0.62552500
H	-2.73106300	6.54436200	0.44096600
H	-2.54834500	6.45147700	-1.34076500
C	-1.00806300	0.12547200	0.98993000

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C	-7.28293700	-0.08441500	1.68403400
C	-7.36143500	0.28560900	0.35812800
C	-6.36514400	-0.12740400	-0.55278700
C	-5.22381400	-0.84542900	-0.09374700
C	-5.26983300	-1.39952300	1.22485300
C	-6.27231800	-0.97120800	2.08946100
C	-6.56583200	0.07837400	-1.96613500
C	-4.12321900	-1.03239400	-1.04892500
C	-4.42912400	-0.96737500	-2.43599800
C	-5.69383900	-0.43000400	-2.86948100
C	-3.44453200	-1.30381100	-3.38827700
H	-3.71592500	-1.31331600	-4.44584000
C	-2.15132000	-1.56819300	-2.99448200
C	-1.76447000	-1.40002900	-1.65045600
C	-2.74706800	-1.12467300	-0.68461300
H	-7.47814500	0.58567100	-2.28656000
H	-8.04103400	0.24137400	2.39816200
H	-8.20219700	0.87453300	-0.01418900
H	-6.30900700	-1.37694700	3.10196300
H	-5.88530800	-0.36098900	-3.94222800
H	-1.40054800	-1.83833900	-3.74062200
C	-4.43922100	-2.61294300	1.64136100
C	-5.27177200	-3.87652300	1.38152700
C	-3.96545400	-2.57893200	3.09486300
H	-3.55329000	-2.69195000	1.00201100
H	-5.57947800	-3.94115400	0.32728400
H	-4.68539600	-4.77562400	1.62478200
H	-6.18057200	-3.87949700	2.00322700

H	-3.42060100	-1.65240800	3.33080700
H	-4.80889600	-2.66906000	3.79584900
H	-3.28490700	-3.42075200	3.28196800
C	-0.27618400	-1.53169400	-1.30564900
C	0.00558600	-1.07583200	0.13756900
H	-0.02885200	-2.60288900	-1.38228300
H	1.02285200	-1.35600600	0.43906600
C	-2.25725900	-0.66645800	0.70398500
H	-3.04500700	-0.62611400	1.45542900
C	-1.09251200	-1.58289200	1.03256600
O	-1.06526600	-2.51535500	1.79178100
C	-1.56211100	0.65936800	0.42834800
C	-2.35643800	1.89261000	0.27692900
C	-2.17435500	2.74670400	-0.82211200
C	-3.36090600	2.19615900	1.21020100
C	-2.95276500	3.89334500	-0.96406400
H	-1.43334700	2.49448800	-1.58233900
C	-4.13865100	3.34333400	1.06628400
H	-3.52763100	1.53228300	2.06146400
C	-3.93298800	4.19753700	-0.01816100
H	-2.80086700	4.54623800	-1.82535800
H	-4.91146800	3.56834500	1.80321200
H	-4.54445700	5.09429500	-0.13223000
C	0.71928100	1.20164400	-0.63219800
C	0.99768200	2.58779100	-0.20592300
C	1.25089400	3.61525100	-1.12421700
C	0.91589700	2.93307900	1.15736000
C	1.45300100	4.93190500	-0.71373000
H	1.25258100	3.39596000	-2.19371100
C	1.11768600	4.23520400	1.58184900
H	0.69206300	2.15935200	1.89452900
C	1.39475100	5.24927600	0.64970800
H	1.63414800	5.70166400	-1.46254400
H	1.06169000	4.50108400	2.63831000
C	1.31541800	0.52431000	-1.66993200
C	0.70137600	-0.75443200	-2.25495200
C	2.53988200	0.98629800	-2.27702500
C	1.75115600	-1.70885700	-2.81041300
H	0.10485600	-0.38512900	-3.10849900
C	3.29064000	0.22362000	-3.11674500
H	2.94145700	1.95204300	-1.96619700
C	2.91699700	-1.14061500	-3.37264900
H	1.32787600	-2.54714100	-3.37949700
H	4.25056300	0.56804100	-3.50148600

O	1.57255400	6.48593600	1.14565600
O	3.79237600	-1.82223600	-4.05807900
C	1.84079800	7.54053600	0.24778500
H	1.00994000	7.68439900	-0.46120700
H	1.95612300	8.44561200	0.85456400
H	2.77098400	7.36110000	-0.31437000
C	3.64686700	-3.23478900	-4.18983700
H	4.55452500	-3.58511100	-4.68998800
H	3.56709200	-3.68961800	-3.19343400
H	2.76569100	-3.47729000	-4.80055100
C	-0.27469700	0.40765600	0.09210800
P	3.91057800	-2.47729400	-0.32297400
O	4.33964800	-3.03297500	1.14471600
O	5.06279600	-2.55360400	-1.25094400
O	2.57667800	-3.11450800	-0.73778700
H	2.20181700	-2.42841400	-1.79830400
O	3.44134200	-0.94612300	0.02011300
C	3.65512500	-2.70773800	2.29682400
C	2.28284900	-2.92899700	2.42213600
C	4.39114600	-2.15218100	3.34338500
C	1.64548700	-2.57437100	3.61212600
H	1.72424500	-3.36271400	1.59148100
C	3.74435400	-1.81281800	4.53050900
H	5.46102900	-1.98758600	3.20611700
C	2.37010600	-2.01840900	4.66731100
H	0.57017900	-2.73640400	3.69957500
H	4.31906100	-1.37764700	5.35000800
H	1.86477300	-1.74606000	5.59518000
C	4.25475500	0.09299100	0.39413100
C	3.76652900	0.94211000	1.38855300
C	5.48610600	0.33795800	-0.21828500
C	4.51033300	2.05849400	1.76519900
H	2.80440200	0.71117300	1.85023700
C	6.22397900	1.45498200	0.17653200
H	5.84354500	-0.34468400	-0.98933800
C	5.74163300	2.31921100	1.16039300
H	4.12456000	2.72629600	2.53782100
H	7.18661700	1.65171000	-0.29913700
H	6.32388600	3.19302200	1.45646900

Int a3

C	7.22242100	-0.33532700	-1.65695900
C	7.30964200	0.05241600	-0.33673700
C	6.29856600	-0.31482500	0.57760700

C	5.13609200	-1.00293400	0.12596700
C	5.16798700	-1.57943800	-1.18347200
C	6.18539300	-1.19624100	-2.05164300
C	6.50224700	-0.09474000	1.98825100
C	4.02716100	-1.13827600	1.07985300
C	4.33073200	-1.06140400	2.46653700
C	5.61144800	-0.56052500	2.89633800
C	3.33191700	-1.34831800	3.42069300
H	3.60012500	-1.35151400	4.47909400
C	2.03168400	-1.57258400	3.02658200
C	1.65435200	-1.41164600	1.67861700
C	2.64921700	-1.18893400	0.71206300
H	7.43000100	0.38683100	2.30402400
H	7.99222600	-0.04494200	-2.37380600
H	8.16806500	0.61973100	0.02873400
H	6.21201400	-1.61871600	-3.05758100
H	5.80219600	-0.48241700	3.96857800
H	1.26857000	-1.80321900	3.77353600
C	4.30024600	-2.77258000	-1.58282000
C	5.09138700	-4.05746800	-1.29911000
C	3.83254600	-2.74776500	-3.03857800
H	3.41050300	-2.81329000	-0.94485200
H	5.39261000	-4.11480700	-0.24259600
H	4.47757600	-4.94115100	-1.53063700
H	6.00201200	-4.09883500	-1.91675700
H	3.32305500	-1.80635800	-3.29394000
H	4.67459400	-2.88148000	-3.73427700
H	3.12234200	-3.56745600	-3.21319800
C	0.16255600	-1.48264900	1.33395000
C	-0.09557300	-1.04308000	-0.11948000
H	-0.14656600	-2.53648700	1.42149300
H	-1.12049700	-1.29492800	-0.41428500
C	2.18459600	-0.73949600	-0.68854000
H	2.97692200	-0.74243900	-1.43579000
C	0.98146900	-1.60809300	-1.00758900
O	0.91311000	-2.53785100	-1.76648500
C	1.54867200	0.61952600	-0.44177600
C	2.39915400	1.81759200	-0.32115800
C	2.29794500	2.68062600	0.78084700
C	3.37905700	2.07014400	-1.29471600
C	3.13529400	3.78878300	0.88815300
H	1.57431100	2.46505700	1.56900100
C	4.21328400	3.18059500	-1.18632200
H	3.48075600	1.39682700	-2.14884000

C	4.09049600	4.04439000	-0.09709600
H	3.04954500	4.44945100	1.75256000
H	4.96559700	3.36859200	-1.95407500
H	4.74768300	4.91129700	-0.00990500
C	-0.69052600	1.28439700	0.60618600
C	-0.88104600	2.67972200	0.19455600
C	-1.08063400	3.70688200	1.12905400
C	-0.76873200	3.03391000	-1.16600800
C	-1.19349700	5.03724400	0.73581100
H	-1.10183900	3.47069800	2.19488500
C	-0.88922600	4.34998600	-1.57220000
H	-0.59305400	2.25523200	-1.91112400
C	-1.10529100	5.36704800	-0.62453500
H	-1.32898500	5.80852700	1.49242600
H	-0.81456300	4.62743700	-2.62429600
C	-1.33702000	0.64329400	1.65079600
C	-0.77186600	-0.63691200	2.26913300
C	-2.54345700	1.16424100	2.19121100
C	-1.84032000	-1.54663300	2.89203800
H	-0.15536800	-0.25971800	3.10123400
C	-3.35705800	0.47338100	3.06527600
H	-2.90838700	2.12252000	1.81637900
C	-3.07878400	-0.87418600	3.34671200
H	-1.40457600	-2.07633500	3.75574600
H	-4.31032700	0.88412900	3.39648800
O	-1.19916700	6.61584200	-1.10231700
O	-3.98806400	-1.53234400	3.98562400
C	-1.40320300	7.67763400	-0.19335000
H	-0.56799800	7.75773600	0.52012600
H	-1.45508900	8.59351800	-0.79214400
H	-2.34638700	7.55251000	0.36127600
C	-3.89301500	-2.95119200	4.18029000
H	-4.76300700	-3.21932000	4.78652600
H	-3.94802300	-3.44285000	3.20073700
H	-2.96865900	-3.20282300	4.71545100
C	0.24725100	0.42843600	-0.10936400
P	-3.76419200	-2.68734000	0.23063300
O	-4.38412600	-2.86701000	-1.29043500
O	-4.89447100	-2.85875100	1.18839600
O	-2.46418600	-3.41154500	0.38686600
H	-2.13513900	-2.34961300	2.19091900
O	-3.32112400	-1.08171800	0.14332800
C	-3.73360900	-2.42982700	-2.41300200
C	-2.35661900	-2.59295900	-2.59789400

C	-4.50748400	-1.79795200	-3.39078700
C	-1.76161500	-2.10008400	-3.76044100
H	-1.76369300	-3.09006900	-1.82935100
C	-3.90234600	-1.32121700	-4.55157400
H	-5.57793100	-1.67940200	-3.21392200
C	-2.52564400	-1.46412500	-4.73987100
H	-0.68468600	-2.22393300	-3.89085400
H	-4.51141200	-0.82609900	-5.31030400
H	-2.05246000	-1.08368900	-5.64648400
C	-4.15171300	-0.06716600	-0.23508100
C	-3.63041700	0.88850200	-1.11226600
C	-5.45503200	0.05658600	0.25555300
C	-4.40699300	1.98358500	-1.48531100
H	-2.61612000	0.75025200	-1.49331100
C	-6.22621700	1.15229700	-0.13518700
H	-5.83703100	-0.70768600	0.93327300
C	-5.70855300	2.12065900	-0.99712700
H	-3.99308800	2.72993000	-2.16651000
H	-7.24455000	1.25031800	0.24614100
H	-6.31811500	2.97630900	-1.29157700

TS-a4

C	8.84595200	-1.71862700	0.99644900
C	8.10379100	-1.83182600	2.15295100
C	6.72002300	-2.10215600	2.08283700
C	6.06335300	-2.16539900	0.82065300
C	6.87743900	-2.26465400	-0.35178100
C	8.23767400	-1.99518400	-0.23884700
C	5.99743500	-2.43008200	3.28737900
C	4.59520300	-2.21052300	0.83261100
C	3.95554300	-2.69343000	2.00687600
C	4.70377300	-2.82779400	3.23091900
C	2.56303100	-2.91534600	2.00516900
H	2.09806700	-3.35384500	2.89041600
C	1.79629400	-2.54166600	0.92358200
C	2.37002900	-1.83097600	-0.14878100
C	3.76457700	-1.66276700	-0.18981400
H	6.54519100	-2.42423600	4.23194900
H	9.91318900	-1.49523500	1.04034700
H	8.57275100	-1.74313700	3.13504200
H	8.86592600	-2.05114700	-1.12953000
H	4.17564800	-3.16771500	4.12405000
H	0.72099300	-2.73371300	0.93057000
C	6.37798100	-2.89458400	-1.65129900

C	6.70128500	-4.39504000	-1.61176000
C	6.95465000	-2.26039400	-2.91730400
H	5.28662500	-2.81710000	-1.70478600
H	6.24902600	-4.87728200	-0.73242400
H	6.31421400	-4.89209000	-2.51430100
H	7.78933100	-4.55833700	-1.56865800
H	6.80706200	-1.17015500	-2.93917700
H	8.03205700	-2.46246300	-3.01329000
H	6.45694300	-2.68069500	-3.80189200
C	1.43507700	-1.28042700	-1.23608100
C	2.18980700	-0.32499600	-2.18002200
H	1.08988100	-2.15114000	-1.81722400
H	1.59096200	-0.08215300	-3.06747700
C	4.32593700	-0.65274600	-1.21206200
H	5.41032800	-0.68581900	-1.31106200
C	3.54737700	-0.90686600	-2.48848000
O	3.90783400	-1.46445200	-3.48884600
C	3.76548300	0.68269600	-0.74823300
C	4.42430700	1.40470800	0.35647400
C	3.70571700	1.82347700	1.48627400
C	5.81217900	1.61511300	0.31826600
C	4.35492500	2.46822400	2.53751700
H	2.63592300	1.61713900	1.54963800
C	6.45869700	2.26220000	1.36895800
H	6.38717400	1.27626800	-0.54677900
C	5.73075000	2.69403500	2.47903100
H	3.78418900	2.78493500	3.41224700
H	7.53659300	2.42616100	1.32243100
H	6.23819300	3.19672200	3.30417400
C	1.40442600	1.67928800	-0.87304700
C	1.61754800	3.12393400	-0.63569300
C	1.07497200	3.78212900	0.47531400
C	2.47480900	3.85393000	-1.47966200
C	1.34787900	5.12387600	0.73562000
H	0.45508600	3.22768200	1.18319300
C	2.74961700	5.18989400	-1.23917300
H	2.93053100	3.35979600	-2.34008400
C	2.18792800	5.83972300	-0.12778600
H	0.91718700	5.59399200	1.61861400
H	3.40788000	5.75953700	-1.89640700
C	0.22551300	0.99523800	-0.73538600
C	0.17202300	-0.53527700	-0.70352000
C	-1.05022200	1.66628800	-0.54912900
C	-1.08434500	-1.04238100	-1.43086600

H	0.05284300	-0.78501500	0.36465900
C	-2.23949900	1.02198500	-0.53857300
H	-1.05307700	2.74824000	-0.41442100
C	-2.29591700	-0.40228900	-0.82366400
H	-1.04206200	-0.74558900	-2.48728700
H	-3.19299000	1.51874200	-0.34848200
O	2.51567400	7.13279700	0.03874800
O	-3.18355500	-1.05562000	-0.15495000
C	1.99281400	7.82295000	1.15263300
H	2.32093200	7.36343500	2.09859100
H	2.38106600	8.84601700	1.09632100
H	0.89189700	7.85260000	1.12574000
C	-3.32508000	-2.47842200	-0.26351400
H	-4.26131000	-2.71682200	0.24911000
H	-3.39374900	-2.77596100	-1.31642800
H	-2.48009800	-2.96973900	0.23655100
C	2.53596600	0.84572800	-1.29039800
H	-1.14209200	-2.13558100	-1.38268800
O	-3.35650700	-0.21246700	-2.63771700
H	-4.10522700	-0.86401000	-2.54388000
H	-3.84839300	0.59872700	-2.39717500
P	-6.04903200	-0.27903900	-1.07137600
O	-6.08982800	-0.68129900	0.52611100
O	-5.34471600	1.03981900	-1.16774500
O	-5.57109100	-1.43367000	-1.91167600
O	-7.66033400	-0.14598900	-1.37432700
C	-6.94481300	-1.61222300	1.05321600
C	-7.28305600	-2.78786600	0.37651400
C	-7.47882200	-1.34001900	2.31528100
C	-8.17183700	-3.68326200	0.97370100
H	-6.85822400	-2.97928600	-0.60998700
C	-8.35962700	-2.24587500	2.90117300
H	-7.20071800	-0.40895300	2.81173500
C	-8.71368900	-3.41955800	2.23183700
H	-8.44168400	-4.59853400	0.44330200
H	-8.77902400	-2.02785300	3.88508000
H	-9.40930700	-4.12463800	2.68921800
C	-8.52760100	0.52646100	-0.55314500
C	-9.78203900	-0.05140000	-0.34336500
C	-8.18874300	1.73457500	0.06149100
C	-10.70035900	0.58031100	0.49181500
H	-10.01192800	-0.99867400	-0.83393400
C	-9.11606400	2.35221400	0.90182900
H	-7.20491100	2.16832600	-0.12175200

C	-10.36999800	1.78189200	1.12247000
H	-11.67850800	0.12476400	0.65682500
H	-8.85106500	3.29375900	1.38671100
H	-11.08810500	2.27183200	1.78170900

Int a4

C	8.47981400	0.44272500	1.82649300
C	7.66979300	-0.01357300	2.84483500
C	6.52713800	-0.78801700	2.54833900
C	6.14753000	-1.02027400	1.19535900
C	7.10853400	-0.73343800	0.17460300
C	8.22474400	0.02676600	0.50939300
C	5.81281100	-1.44040500	3.61799600
C	4.82604600	-1.61964900	0.96534300
C	4.25117500	-2.38114100	2.01921800
C	4.79816800	-2.29689000	3.34952400
C	3.06725900	-3.11350200	1.79049200
H	2.67721600	-3.74802900	2.58892300
C	2.39002800	-2.98992700	0.59808600
C	2.80359600	-2.05233100	-0.36829200
C	4.01462500	-1.36667600	-0.18131400
H	6.16449800	-1.28513000	4.64000500
H	9.35744000	1.05330100	2.04525600
H	7.91039400	0.18859200	3.89059800
H	8.95676000	0.26380200	-0.26464300
H	4.31298200	-2.86706300	4.14428000
H	1.47755100	-3.56402600	0.42414600
C	7.10093100	-1.43089000	-1.18509100
C	7.98016500	-2.68570200	-1.08563700
C	7.56464100	-0.54869000	-2.34481600
H	6.08914700	-1.78233400	-1.41435500
H	7.62818200	-3.35663900	-0.28798800
H	7.96043800	-3.24083500	-2.03587400
H	9.02466500	-2.41422900	-0.86708700
H	7.00434700	0.39705000	-2.39636100
H	8.63556600	-0.30836500	-2.26442200
H	7.41118500	-1.07659100	-3.29585300
C	1.88399700	-1.82431800	-1.57616800
C	2.38733600	-0.64998900	-2.43607500
H	1.92510400	-2.74515700	-2.18074200
H	1.89865900	-0.63155200	-3.41847100
C	4.29631000	-0.17757400	-1.11713000
H	5.31464000	0.20127500	-1.04757800
C	3.89320800	-0.66982100	-2.49519100

O	4.59938500	-1.01371900	-3.40416300
C	3.20614900	0.83983800	-0.80506100
C	3.34057200	1.73992800	0.35501500
C	2.25134700	2.02225000	1.19601900
C	4.59401700	2.28999900	0.67350800
C	2.40440700	2.85805200	2.29997800
H	1.28365300	1.56065700	0.99724500
C	4.74572400	3.12360100	1.77948200
H	5.46063500	2.06993700	0.04641700
C	3.65006800	3.41530800	2.59305800
H	1.54692300	3.06411600	2.94311500
H	5.72682100	3.54385300	2.00767100
H	3.76914300	4.06620100	3.46097200
C	0.70216300	0.91762200	-1.45965400
C	0.30417800	2.34293400	-1.41737900
C	-0.72610800	2.80057700	-0.58593300
C	1.01647400	3.30046200	-2.16343700
C	-1.06606500	4.15100200	-0.51247700
H	-1.26020300	2.09077000	0.04920300
C	0.68901900	4.64568600	-2.10496500
H	1.84040000	2.97782300	-2.80344500
C	-0.35931600	5.08492700	-1.28033300
H	-1.86951000	4.46381600	0.15308300
H	1.23595100	5.38701700	-2.68916600
C	-0.14349500	-0.15618000	-1.44392200
C	0.38186800	-1.57568900	-1.19491000
C	-1.58499900	-0.01612800	-1.64193800
C	-0.52868500	-2.63017400	-1.82753800
H	0.29587000	-1.70610300	-0.10261900
C	-2.43877100	-1.05178400	-1.63445400
H	-1.96780900	0.97748400	-1.88236200
C	-1.97253800	-2.46459100	-1.37624500
H	-0.51577000	-2.55000200	-2.92548500
H	-3.49230700	-0.90592300	-1.88394600
O	-0.60861300	6.40787200	-1.27770200
O	-2.05198600	-2.64232100	0.06650100
C	-1.64380700	6.89345900	-0.45252700
H	-1.44185900	6.68333000	0.61012300
H	-1.68112300	7.97827300	-0.60308000
H	-2.61687600	6.45686800	-0.72919600
C	-1.75889200	-3.94014800	0.57068900
H	-2.22555400	-4.01229800	1.56134700
H	-2.17641000	-4.71438900	-0.08612800
H	-0.67378500	-4.08007400	0.67823500

C	2.12149700	0.55522100	-1.56307700
H	-0.17891200	-3.64077300	-1.56767300
O	-2.75926700	-3.39886700	-2.00877600
H	-3.69040100	-3.22264800	-1.75483200
P	-5.25291200	-1.66515700	0.18712000
O	-5.50234400	-0.20275600	-0.44631700
O	-5.16962800	-2.65510200	-0.91482600
O	-4.03617000	-1.59244300	1.16153200
H	-3.18046300	-1.99199600	0.73617000
O	-6.46574800	-1.84596700	1.22554500
C	-5.63522000	0.95517600	0.30515900
C	-4.55101300	1.46191400	1.01912400
C	-6.86154800	1.61556100	0.27790900
C	-4.70925100	2.65298300	1.72788000
H	-3.60279900	0.92401700	1.01420300
C	-7.00378300	2.80707700	0.98791500
H	-7.68523700	1.18944000	-0.29787600
C	-5.93138800	3.32656900	1.71501700
H	-3.86659300	3.05523900	2.29310100
H	-7.96094400	3.33071000	0.97113900
H	-6.04797400	4.25825700	2.27047000
C	-7.79170600	-1.62022000	0.89585100
C	-8.59392500	-1.05404500	1.88421500
C	-8.30311000	-1.94596800	-0.35916200
C	-9.93475200	-0.80038000	1.60514000
H	-8.15195000	-0.81188800	2.85158900
C	-9.64644200	-1.67644400	-0.62611000
H	-7.65875100	-2.40340900	-1.11173900
C	-10.46372000	-1.10503600	0.34888200
H	-10.56829900	-0.35543100	2.37418100
H	-10.05386200	-1.92349700	-1.60783600
H	-11.51292600	-0.89991300	0.13201300

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C	8.75725700	-0.37029700	1.75938800
C	7.89099200	-0.60118500	2.80694000
C	6.62588700	-1.17929600	2.56582000
C	6.19579700	-1.43964000	1.23298100
C	7.18016900	-1.39912500	0.19507300
C	8.41681300	-0.82638200	0.47557000
C	5.81973100	-1.61247000	3.68041200
C	4.78748300	-1.81487600	1.04610500
C	4.09836600	-2.37899000	2.15456700
C	4.66602400	-2.29194200	3.47596100

C	2.80044000	-2.90318000	1.98162600
H	2.31166600	-3.39057900	2.82753900
C	2.14155300	-2.75689400	0.78135500
C	2.70631000	-1.99039300	-0.25667000
C	4.02092200	-1.51484700	-0.11962600
H	6.20519200	-1.44595900	4.68837700
H	9.73154300	0.08920700	1.93407100
H	8.17528800	-0.36991900	3.83555900
H	9.16995400	-0.77675200	-0.31283800
H	4.09589900	-2.70471000	4.31065100
H	1.13809900	-3.17037800	0.65778400
C	7.03416800	-2.17565600	-1.11299300
C	7.68692000	-3.55311700	-0.92899800
C	7.62566700	-1.46681000	-2.33214100
H	5.97396200	-2.36296000	-1.31489500
H	7.23664300	-4.09799700	-0.08600300
H	7.55942200	-4.15970200	-1.83855600
H	8.76537600	-3.45047000	-0.73206700
H	7.23630900	-0.44398800	-2.44693800
H	8.72301900	-1.41108700	-2.27155700
H	7.36951800	-2.02283100	-3.24429200
C	1.84045400	-1.70954400	-1.49333700
C	2.51132600	-0.67065100	-2.41121400
H	1.75999100	-2.66339100	-2.04043600
H	2.01690700	-0.62096800	-3.38997000
C	4.49347200	-0.45414500	-1.13367000
H	5.56166100	-0.24706600	-1.08389500
C	3.99237500	-0.94528900	-2.47883100
O	4.61424600	-1.45653600	-3.37021200
C	3.59191000	0.74318700	-0.86889600
C	3.89180100	1.65656900	0.24953200
C	2.90835800	2.01216700	1.18562600
C	5.20104100	2.13213700	0.42963300
C	3.21921300	2.85115100	2.25397500
H	1.90041800	1.60585900	1.08798600
C	5.50964600	2.97077100	1.49840400
H	5.98257900	1.84952800	-0.27938500
C	4.51827500	3.33661000	2.41042800
H	2.44415000	3.11635100	2.97518900
H	6.53036200	3.33696100	1.62121100
H	4.76093500	3.99052200	3.24985400
C	1.12258300	1.18528800	-1.44241800
C	0.97723100	2.65443900	-1.35382800
C	0.09909900	3.26005100	-0.44561000

C	1.80465100	3.49133300	-2.12598600
C	0.01842500	4.64597400	-0.31866200
H	-0.51386400	2.63750800	0.20980200
C	1.73141100	4.87003500	-2.01677400
H	2.51499100	3.04638000	-2.82574900
C	0.83546200	5.46240800	-1.11149300
H	-0.66841300	5.07563900	0.40924400
H	2.36594400	5.52023400	-2.62049800
C	0.11038600	0.26286700	-1.39681600
C	0.39020900	-1.22546800	-1.16952700
C	-1.28695100	0.64632100	-1.52057800
C	-0.64373000	-2.09938800	-1.87714200
H	0.22002400	-1.36549400	-0.09101200
C	-2.31311700	-0.22918500	-1.58921900
H	-1.51351600	1.70768200	-1.63160000
C	-2.05516300	-1.67381900	-1.60790300
H	-0.52078800	-2.03675800	-2.97354000
H	-3.33789300	0.11253300	-1.73860800
O	0.83528600	6.80634900	-1.06185500
O	-2.03372100	-1.97196000	0.33425600
C	-0.03841500	7.44709100	-0.15854000
H	0.18497300	7.16609500	0.88299000
H	0.12007200	8.52430500	-0.28196800
H	-1.09080500	7.20895400	-0.38096900
C	-2.14347600	-3.33873100	0.68215800
H	-2.63000400	-3.43507400	1.66367700
H	-2.74118000	-3.88856200	-0.06393600
H	-1.13912200	-3.77970200	0.74142900
C	2.45821200	0.59877600	-1.59394600
H	-0.52722700	-3.15687600	-1.59977300
O	-2.97310000	-2.48445100	-1.99763200
H	-3.95000600	-2.10072600	-1.82432500
P	-5.45532400	-1.09761200	-0.06113100
O	-6.12714300	0.37277700	-0.25578100
O	-5.19359700	-1.59442900	-1.46661500
O	-4.31560300	-1.07562300	0.91758700
H	-2.90876700	-1.52731800	0.60260800
O	-6.65790900	-1.92841600	0.65042500
C	-6.85722300	1.01135100	0.72297100
C	-6.46486700	1.00194500	2.06179300
C	-8.01893100	1.66899400	0.31735000
C	-7.26498500	1.65059700	3.00379100
H	-5.54835100	0.48655900	2.35228800
C	-8.80308900	2.31828900	1.26780700

H	-8.29560600	1.64863600	-0.73790300
C	-8.43257600	2.30682900	2.61444800
H	-6.96598700	1.64165300	4.05344500
H	-9.71462300	2.82979800	0.95377300
H	-9.05227100	2.81019200	3.35792900
C	-7.97728400	-1.85231500	0.25886700
C	-8.93369100	-1.77283700	1.27131900
C	-8.34952700	-1.84950600	-1.08553300
C	-10.28139900	-1.68081100	0.93160200
H	-8.60310000	-1.77228600	2.31111200
C	-9.70324000	-1.74917800	-1.41053900
H	-7.58320700	-1.91909100	-1.85868700
C	-10.67079000	-1.66289300	-0.40954000
H	-11.03122100	-1.61405700	1.72184400
H	-9.99974000	-1.74135900	-2.46090500
H	-11.72652600	-1.58397100	-0.67292700

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C	8.37782500	-0.03432600	1.97360600
C	7.44500600	-0.15349800	2.98204700
C	6.19931400	-0.76635900	2.72602300
C	5.85936400	-1.18062500	1.40650200
C	6.90850800	-1.24554400	0.43539900
C	8.12287900	-0.63334700	0.72919400
C	5.31942700	-1.07459400	3.82655500
C	4.46806300	-1.58924400	1.17100400
C	3.70417900	-2.02610400	2.28786200
C	4.18167500	-1.78139400	3.62523600
C	2.41694700	-2.56598500	2.08982000
H	1.86569300	-2.94365000	2.95342100
C	1.83701300	-2.56535600	0.83959900
C	2.48033200	-1.92999400	-0.24165500
C	3.78309800	-1.43094400	-0.06969300
H	5.63544200	-0.78943600	4.83209700
H	9.33773700	0.45081500	2.15839900
H	7.66065300	0.19581600	3.99393700
H	8.92524500	-0.66308900	-0.01009000
H	3.55581300	-2.09786500	4.46211800
H	0.83064900	-2.97286500	0.71124800
C	6.84623700	-2.15784000	-0.78922000
C	7.47736200	-3.50691700	-0.41647100
C	7.52126600	-1.58144700	-2.03430200
H	5.80118300	-2.36723800	-1.04189300
H	6.96910700	-3.95946700	0.44790600

H	7.40707600	-4.20740800	-1.26256900
H	8.54101000	-3.38251600	-0.16021000
H	7.14219000	-0.57924800	-2.28411700
H	8.61210700	-1.51411900	-1.90605000
H	7.32632900	-2.23326500	-2.89692700
C	1.71818700	-1.80504200	-1.56950800
C	2.41709600	-0.80654200	-2.51452600
H	1.73710500	-2.80488000	-2.03411900
H	1.98026600	-0.83749400	-3.52135900
C	4.31486200	-0.45864600	-1.14541200
H	5.37515300	-0.22809900	-1.04559800
C	3.90231900	-1.05938700	-2.47362100
O	4.58205600	-1.63587900	-3.27919200
C	3.38068600	0.73514400	-1.01928500
C	3.60764600	1.71173500	0.06375200
C	2.60491800	2.01260300	0.99746100
C	4.87899000	2.28574500	0.22381900
C	2.85910700	2.89356200	2.04721800
H	1.63013200	1.52888200	0.91391900
C	5.12984500	3.16895300	1.27161900
H	5.67525600	2.04043800	-0.48289800
C	4.11897100	3.47793100	2.18342300
H	2.07116200	3.11419800	2.76948900
H	6.12090800	3.61277500	1.38014300
H	4.31720800	4.16493500	3.00796500
C	0.92954400	1.05685600	-1.68723900
C	0.74132700	2.52109800	-1.59621600
C	-0.15341800	3.09863600	-0.68592200
C	1.54990800	3.38276400	-2.36050400
C	-0.26675900	4.48085300	-0.54827800
H	-0.75060000	2.45758900	-0.03389100
C	1.44371000	4.75862100	-2.24110300
H	2.27309600	2.95987800	-3.06079000
C	0.53254100	5.32266100	-1.33305200
H	-0.96386500	4.88792900	0.18285700
H	2.06440900	5.42817600	-2.83794700
C	-0.05963600	0.10644100	-1.65959300
C	0.23193100	-1.37504000	-1.43443900
C	-1.46515900	0.44151300	-1.77761700
C	-0.68083900	-2.25253700	-2.29169100
H	-0.08737300	-1.56055600	-0.39825300
C	-2.44774100	-0.48501800	-1.91579100
H	-1.74824900	1.49485300	-1.79347100
C	-2.12777100	-1.89218000	-2.12294400

H	-0.44595300	-2.12853600	-3.36573900
H	-3.49109700	-0.17584100	-2.00118600
O	0.50068800	6.66548600	-1.27241300
O	-1.57681200	-3.04989600	0.50012900
C	-0.38553800	7.27830100	-0.36172100
H	-0.15300500	6.99345600	0.67676800
H	-0.25210600	8.35986900	-0.47631100
H	-1.43269100	7.01766200	-0.58375500
C	-1.99718300	-4.37744300	0.32325500
H	-2.59835400	-4.74197200	1.17501900
H	-2.59158300	-4.50688200	-0.59862300
H	-1.10607000	-5.01844800	0.24592900
C	2.28666100	0.51044200	-1.78561500
H	-0.55812300	-3.31381600	-2.03883200
O	-3.00549200	-2.75021600	-2.26995800
H	-4.33258000	-2.38651200	-1.88916400
P	-5.20732600	-1.53910800	-0.05680400
O	-5.50206600	0.03734400	-0.27104600
O	-5.26853700	-2.08769000	-1.51286900
O	-3.99039300	-1.84621200	0.73020600
H	-2.38157600	-2.51288500	0.62937600
O	-6.51588900	-2.06202500	0.71851100
C	-5.90275400	0.87691700	0.75418600
C	-5.33478200	0.80344400	2.02472600
C	-6.90697700	1.79672000	0.45728100
C	-5.80542400	1.66208800	3.01987600
H	-4.54170900	0.08163400	2.22572200
C	-7.35968900	2.65185300	1.45899300
H	-7.32639000	1.81800500	-0.54974300
C	-6.81550300	2.58302300	2.74373900
H	-5.37165100	1.60738700	4.01976000
H	-8.14964300	3.37067700	1.23520300
H	-7.17792900	3.24902300	3.52804000
C	-7.79764500	-1.57689800	0.52092500
C	-8.53146100	-1.24878100	1.65889000
C	-8.32754700	-1.42098000	-0.75788600
C	-9.82133400	-0.74414200	1.51034500
H	-8.07546600	-1.38229300	2.64096900
C	-9.61852600	-0.90726500	-0.89084600
H	-7.73434400	-1.69418100	-1.63193200
C	-10.36576100	-0.56612800	0.23656900
H	-10.40060100	-0.48089200	2.39689000
H	-10.04060000	-0.77678400	-1.88872300
H	-11.37374300	-0.16457600	0.12347400

Int1$_{C1}$'

C	-1.27367500	4.10954300	0.31502600
C	0.06639100	4.29947700	0.58026000
C	1.03329500	3.57453300	-0.14848400
C	0.62794000	2.57590300	-1.07637100
C	-0.74131000	2.54412300	-1.49205600
C	-1.65929400	3.28364300	-0.75419200
C	2.42511700	3.94590900	-0.06306300
C	1.68123400	1.74804500	-1.66730100
C	3.00224600	2.27191300	-1.72217200
C	3.34350300	3.40531400	-0.90230900
C	3.99336000	1.62121900	-2.49477300
H	4.98918900	2.06467400	-2.55451600
C	3.70155000	0.44916000	-3.15299200
C	2.46415300	-0.19213400	-2.91434500
C	1.49098900	0.41351300	-2.11032700
H	2.70397600	4.74098000	0.63262900
H	-2.03299800	4.65543800	0.87778900
H	0.39926200	5.03179800	1.31896000
H	-2.71336600	3.24920100	-1.02763900
H	4.37551100	3.76110800	-0.91476600
H	4.44274400	-0.04023000	-3.78788300
C	-1.16442200	1.95226200	-2.84028800
C	-0.50391100	2.76452200	-3.96586000
C	-2.67520800	1.91427700	-3.06198800
H	-0.80749400	0.92037200	-2.93636700
H	0.59337900	2.75355200	-3.89561900
H	-0.78665400	2.35332400	-4.94669700
H	-0.83811100	3.81310700	-3.92562400
H	-3.18212700	1.36907400	-2.25592200
H	-3.10088500	2.92771600	-3.12777900
H	-2.89050800	1.40642500	-4.01358300
C	2.21599600	-1.51435600	-3.47363800
C	1.10503100	-2.23692000	-3.21208900
H	2.97172700	-1.91201700	-4.15681000
H	0.90806200	-3.20096600	-3.68242600
C	0.45342500	-0.49027700	-1.47908200
H	-0.48022100	0.01190500	-1.18704900
C	0.10234700	-1.72250600	-2.28792300
O	-0.95176400	-2.32738100	-2.10751500
C	1.04763200	-1.03859100	-0.14657100
C	0.14478600	-1.83563000	0.74571900
C	-0.64460500	-1.19116900	1.70522900

C	0.10301900	-3.23163700	0.64341100
C	-1.46282000	-1.93694300	2.55342800
H	-0.62801300	-0.10139100	1.76836000
C	-0.72128100	-3.97389400	1.48819600
H	0.72515200	-3.73444100	-0.10094100
C	-1.50444000	-3.32741300	2.44488400
H	-2.07766000	-1.42737700	3.29680900
H	-0.74771000	-5.06156700	1.40101500
H	-2.14929500	-3.90799000	3.10740800
C	3.50120200	-0.54627300	0.67484400
C	4.62552100	-1.48230000	0.38526100
C	5.69500300	-1.63308300	1.27409200
C	4.61201900	-2.29123300	-0.76525500
C	6.72547000	-2.54424500	1.03309500
H	5.72822800	-1.03988600	2.18943500
C	5.62619300	-3.20021200	-1.01887200
H	3.78421500	-2.19763400	-1.47047600
C	6.69898500	-3.33323900	-0.12212400
H	7.53661400	-2.63217700	1.75484000
H	5.61600000	-3.82277900	-1.91480200
C	3.72606500	0.68887600	1.48409100
C	2.71493500	1.19738100	2.30544100
C	4.93227200	1.40725400	1.40384300
C	2.87931000	2.38130700	3.02463900
H	1.77200100	0.65219800	2.38886100
C	5.11271900	2.58397300	2.11614400
H	5.73703400	1.04734800	0.75963800
C	4.08454800	3.08697000	2.92787300
H	2.06414800	2.74055600	3.65176100
H	6.04424500	3.14794200	2.04735600
O	7.64709700	-4.23347800	-0.44836600
O	4.33530100	4.24809700	3.56653600
C	8.74317800	-4.39770800	0.42281100
H	8.41793300	-4.73838200	1.41899800
H	9.38744600	-5.16270400	-0.02523700
H	9.31536700	-3.46204600	0.53017100
C	3.32736600	4.79069600	4.38884700
H	3.72881400	5.72233600	4.80351000
H	2.41525300	5.01632400	3.81248500
H	3.07112900	4.10880600	5.21564600
C	2.28384800	-0.80311500	0.22409600
P	-3.44145000	-0.79321300	-0.14948200
O	-4.08883500	-0.89478600	1.32250500
O	-2.47962600	0.32400100	-0.23483500

O	-2.92950000	-2.22010400	-0.52755300
H	-2.09284100	-2.21651800	-1.10954500
O	-4.75247300	-0.64544900	-1.09475300
C	-5.25074700	-1.57930000	1.62849100
C	-5.46106600	-2.88969700	1.20321600
C	-6.20245800	-0.90061100	2.38800100
C	-6.66140100	-3.51925300	1.53704300
H	-4.69713400	-3.40215700	0.61730300
C	-7.39239300	-1.54466700	2.71888000
H	-5.99973900	0.12592600	2.69716000
C	-7.62776700	-2.85287100	2.29022100
H	-6.83634000	-4.54358700	1.20372500
H	-8.14314200	-1.01662000	3.30915600
H	-8.56328600	-3.35278200	2.54522800
C	-5.75295100	0.27315500	-0.84383300
C	-7.05901000	-0.13085700	-1.11683200
C	-5.47976100	1.54248600	-0.33284800
C	-8.10932800	0.74953200	-0.86813700
H	-7.23078700	-1.13476000	-1.50800600
C	-6.54395700	2.41067600	-0.08323800
H	-4.44898500	1.83874900	-0.12828200
C	-7.85661300	2.02043800	-0.34689800
H	-9.13358100	0.43594400	-1.07669000
H	-6.33765200	3.40320400	0.32112500
H	-8.68216000	2.70519700	-0.14795900

TS-b1

C	-1.66992500	4.02035400	0.15136600
C	-0.35319000	4.18388700	0.52388100
C	0.65879300	3.46218800	-0.14758300
C	0.31268600	2.45581500	-1.09316600
C	-1.02496800	2.44022700	-1.60686900
C	-1.98129200	3.20965000	-0.95528900
C	2.03431600	3.86877500	-0.01387000
C	1.40282900	1.67603600	-1.67506200
C	2.68265900	2.28311700	-1.73510600
C	2.97872100	3.38775300	-0.86322400
C	3.66905400	1.78137600	-2.62863800
H	4.62907700	2.29646900	-2.69638700
C	3.38255200	0.70493100	-3.42455400
C	2.20181800	-0.05008900	-3.17973100
C	1.27433300	0.35018100	-2.20009100
H	2.27481700	4.65493400	0.70560300
H	-2.46156500	4.58135000	0.65160900

H	-0.06680800	4.90958300	1.28830200
H	-3.00429000	3.22053100	-1.33065500
H	3.99430000	3.78859100	-0.86349800
H	4.08352100	0.35642100	-4.18548400
C	-1.35194400	1.82784700	-2.97052500
C	-0.64505900	2.63913500	-4.06785100
C	-2.84361900	1.74172200	-3.28149300
H	-0.96545700	0.80384100	-3.01637400
H	0.44489100	2.67010500	-3.92464200
H	-0.84615400	2.19752800	-5.05569600
H	-1.01685200	3.67586600	-4.07548400
H	-3.37960900	1.17384100	-2.51066700
H	-3.30440300	2.73732000	-3.37286500
H	-2.98561900	1.22679000	-4.24305200
C	1.96823600	-1.27513000	-3.89158500
C	0.93942400	-2.10881100	-3.57919600
H	2.63884500	-1.52316600	-4.71840700
H	0.74255000	-3.02540900	-4.13515600
C	0.36597300	-0.67615100	-1.59603200
H	-0.97566000	-0.28010100	-1.18681400
C	0.17387300	-1.87222200	-2.39339000
O	-0.61846000	-2.84105800	-2.06425100
C	0.88306300	-1.04686500	-0.18422400
C	0.12634800	-1.93286000	0.76313200
C	-0.68320000	-1.37268300	1.75596000
C	0.29873200	-3.32356900	0.72204400
C	-1.33501200	-2.19237300	2.67780800
H	-0.81873200	-0.28935400	1.78872100
C	-0.35538100	-4.14025200	1.64128600
H	0.95138000	-3.76185000	-0.03563700
C	-1.17704600	-3.57607800	2.61979800
H	-1.97489700	-1.74479500	3.44091400
H	-0.21745900	-5.22212800	1.59866800
H	-1.69108900	-4.21603800	3.33943700
C	3.25947000	-0.35493300	0.72133800
C	4.43182700	-1.23240100	0.43266200
C	5.44636200	-1.42651800	1.37561000
C	4.52226400	-1.93398300	-0.78275100
C	6.51818800	-2.28770800	1.13123700
H	5.40049400	-0.90713700	2.33475000
C	5.57970100	-2.79201700	-1.04056700
H	3.74466000	-1.79235200	-1.53715500
C	6.59123700	-2.97733300	-0.08440200
H	7.28315000	-2.41468700	1.89630700

H	5.65195400	-3.33210700	-1.98578400
C	3.41236700	0.86346500	1.56658000
C	2.34947500	1.31889400	2.35283800
C	4.59792100	1.61908700	1.56024600
C	2.44037400	2.49271800	3.10080000
H	1.42301200	0.74058000	2.38017300
C	4.70561400	2.78722300	2.30105300
H	5.44336700	1.29749500	0.94854700
C	3.62370700	3.24051700	3.07139400
H	1.58657800	2.81191900	3.69742500
H	5.62021700	3.38212500	2.28827500
O	7.58487800	-3.82558300	-0.41740200
O	3.80465900	4.39750300	3.74092100
C	8.61663900	-4.04859300	0.51645700
H	8.22633500	-4.48082900	1.45196100
H	9.30920700	-4.76106000	0.05397000
H	9.15898700	-3.11754700	0.74771600
C	2.73740900	4.89637200	4.51425600
H	3.08563900	5.83446900	4.96125200
H	1.85069200	5.10110800	3.89204900
H	2.45924100	4.19546200	5.31764300
C	2.07452700	-0.67201500	0.22508000
P	-3.08033400	-1.13385700	-0.41821300
O	-3.54198300	-0.82585600	1.09540800
O	-2.05786000	-0.03945500	-0.74559100
O	-2.63893300	-2.54420300	-0.66820800
H	-1.37047900	-2.67918200	-1.36901500
O	-4.44737200	-0.89027600	-1.24964400
C	-4.60653400	-1.45015300	1.71854900
C	-4.86148300	-2.81153200	1.55716800
C	-5.40970400	-0.65260900	2.53307000
C	-5.95619900	-3.37135800	2.21853400
H	-4.21120400	-3.41670300	0.92427500
C	-6.49425600	-1.22832700	3.19021700
H	-5.17513800	0.40818100	2.63220500
C	-6.77375800	-2.58760700	3.03188200
H	-6.16462100	-4.43538400	2.09461500
H	-7.12774900	-0.60763000	3.82606700
H	-7.62694500	-3.03472900	3.54391900
C	-5.41857500	0.03570900	-0.92045700
C	-6.74339100	-0.33590800	-1.13737300
C	-5.09465600	1.28612200	-0.39470900
C	-7.76100700	0.56180500	-0.81934800
H	-6.95612600	-1.32602300	-1.54253300

C	-6.12343600	2.17350000	-0.07953100
H	-4.05005100	1.55325800	-0.22314400
C	-7.45601400	1.81655800	-0.28873500
H	-8.80069000	0.27398000	-0.98370400
H	-5.87478700	3.15199200	0.33572700
H	-8.25600700	2.51444200	-0.03800300

Int b1

C	-3.11189600	2.17218000	1.94663900
C	-2.44814100	2.92296600	1.00759900
C	-2.05588100	2.33761900	-0.22048400
C	-2.25788500	0.94589700	-0.45640600
C	-3.13482200	0.23559400	0.43871000
C	-3.49970900	0.85578000	1.62556300
C	-1.55765800	3.18088300	-1.26809200
C	-1.69741100	0.38550100	-1.67978100
C	-1.48038500	1.27140600	-2.75792100
C	-1.39290300	2.68271500	-2.52179900
C	-1.35014500	0.76960000	-4.09277400
H	-1.27232100	1.48755000	-4.91161900
C	-1.37261200	-0.57018300	-4.32800700
C	-1.28973500	-1.48769300	-3.23244100
C	-1.33323900	-1.01092800	-1.89025900
H	-1.41120400	4.24294000	-1.05722600
H	-3.41405600	2.60835900	2.90027100
H	-2.23729100	3.98156400	1.17325200
H	-4.14901700	0.33301100	2.32660400
H	-1.13979700	3.33321600	-3.36150600
H	-1.34138400	-0.96760200	-5.34444000
C	-3.85287400	-1.04756700	0.01813500
C	-4.68547800	-0.79330300	-1.24927200
C	-4.77002100	-1.62187200	1.09707000
H	-3.11462500	-1.82158700	-0.22303400
H	-4.07274500	-0.46648400	-2.10046500
H	-5.20992100	-1.71433600	-1.54545900
H	-5.44283400	-0.01682900	-1.05702100
H	-4.24770100	-1.78180000	2.04980300
H	-5.63079100	-0.96040000	1.28324000
H	-5.16330400	-2.59312400	0.76156400
C	-1.01633600	-2.85432100	-3.49053400
C	-0.63781200	-3.69855000	-2.48019300
H	-1.05036600	-3.20974600	-4.52232200
H	-0.36629500	-4.73860100	-2.66451000
C	-0.86067300	-1.88206400	-0.85203700

C	-0.47769800	-3.18324300	-1.17443500
O	0.12256000	-4.01550600	-0.29342800
C	-0.47527300	-1.38823200	0.52038400
C	-1.10259500	-1.90495700	1.77430100
C	-0.89577300	-1.22734100	2.98804400
C	-1.86643800	-3.08090300	1.78920700
C	-1.42349400	-1.71681000	4.17746900
H	-0.32511700	-0.29619400	2.98440100
C	-2.38328600	-3.57954500	2.98693700
H	-2.06957000	-3.61778900	0.86072700
C	-2.16557400	-2.90210700	4.18393600
H	-1.25732000	-1.16958800	5.10703300
H	-2.97022700	-4.49963300	2.97505000
H	-2.57614000	-3.28870000	5.11816300
C	1.65731700	0.15583400	0.42719000
C	2.99799000	-0.48436400	0.29524300
C	4.16671800	0.22087300	0.59617700
C	3.12383000	-1.82084600	-0.12824700
C	5.42683700	-0.37286800	0.49040200
H	4.10234800	1.25833100	0.92950100
C	4.36562000	-2.42259500	-0.23752300
H	2.22880000	-2.39537500	-0.37764700
C	5.53298100	-1.70316200	0.07113000
H	6.31272000	0.21046400	0.73836700
H	4.46437700	-3.45671100	-0.57067800
C	1.55368300	1.64693000	0.40752100
C	0.97645200	2.34817600	1.46479800
C	2.05270400	2.37587800	-0.68718400
C	0.88278200	3.74311400	1.44861700
H	0.58898700	1.79795600	2.32509900
C	1.95914700	3.75743800	-0.72123600
H	2.51131200	1.84458900	-1.52428300
C	1.36676700	4.45383300	0.34664100
H	0.42441300	4.25595200	2.29327300
H	2.32920900	4.32971600	-1.57326900
O	6.69800400	-2.36524200	-0.06658300
O	1.30381700	5.79551600	0.22236900
C	7.89595200	-1.68394000	0.22984000
H	7.92296700	-1.35684600	1.28169100
H	8.71176500	-2.39432700	0.05428300
H	8.03321800	-0.80803100	-0.42455100
C	0.71368300	6.53666900	1.26543700
H	0.76112700	7.59031500	0.96771700
H	-0.34068400	6.25182800	1.41496900

H	1.26013900	6.40428900	2.21312300
C	0.56976400	-0.58121400	0.54571900
H	0.27741600	-3.57619200	0.55651800

TS-b2

C	2.77805800	2.61819100	-1.45304400
C	2.22130300	3.13770500	-0.30645800
C	1.97477000	2.29892800	0.80305600
C	2.20254400	0.89225800	0.71646300
C	2.99850600	0.41923000	-0.38429700
C	3.21539500	1.28170400	-1.45467000
C	1.63225900	2.89276800	2.06454900
C	1.78616400	0.06999000	1.85109200
C	1.70131300	0.70540600	3.11293200
C	1.61819600	2.13748600	3.19206400
C	1.66526400	-0.06372400	4.31433500
H	1.68751200	0.46118700	5.27103900
C	1.61737500	-1.42639200	4.25254400
C	1.41163800	-2.07922700	3.00502000
C	1.40971600	-1.33414500	1.78942300
H	1.47636500	3.97327500	2.10158700
H	2.96443700	3.25201900	-2.32189400
H	1.99057800	4.20195100	-0.21625300
H	3.79561700	0.93710700	-2.30991800
H	1.47962400	2.59124600	4.17553800
H	1.62930400	-2.03206600	5.16144300
C	3.82752000	-0.86144800	-0.28144600
C	4.80360400	-0.75019400	0.90147700
C	4.62040500	-1.17924300	-1.54828500
H	3.17205200	-1.71645800	-0.07505100
H	4.28408100	-0.61994700	1.86093300
H	5.41519600	-1.66254100	0.96989500
H	5.48201700	0.10586700	0.75967200
H	3.98869000	-1.18754700	-2.44743300
H	5.42866400	-0.44758800	-1.70530500
H	5.08394900	-2.17222300	-1.45213500
C	1.06342800	-3.46241900	2.98621500
C	0.54074900	-4.05622600	1.87617100
H	1.15746200	-4.02718300	3.91720600
H	0.19457800	-5.09115000	1.88348900
C	0.93882600	-1.99247100	0.61433400
C	0.29976700	-3.28839300	0.67983200
O	-0.50946200	-3.67049000	-0.21751500
C	0.56050500	-1.34892300	-0.65391900

C	1.17088400	-1.73466400	-1.93027400
C	0.95241300	-0.94065000	-3.06904500
C	1.92048200	-2.91914100	-2.04001200
C	1.49406900	-1.31284600	-4.29372300
H	0.37237200	-0.02188800	-2.97293100
C	2.41438100	-3.31394400	-3.27786000
H	2.09324100	-3.53569300	-1.15693200
C	2.21220400	-2.50760700	-4.40068800
H	1.34362100	-0.68222800	-5.17075600
H	2.97163900	-4.24732400	-3.36670100
H	2.61754000	-2.81203200	-5.36734900
C	-1.74714400	-0.02054000	-0.45233800
C	-3.16198700	-0.44767800	-0.28811900
C	-4.20666100	0.45600400	-0.51136300
C	-3.49839100	-1.76081300	0.09796700
C	-5.54405300	0.07953800	-0.37652000
H	-3.97967500	1.48208900	-0.80619800
C	-4.82015200	-2.14772900	0.23476300
H	-2.71292800	-2.49295900	0.30291900
C	-5.85927000	-1.23118700	-0.00208700
H	-6.32529200	0.81483900	-0.56418300
H	-5.08099200	-3.16223300	0.53928500
C	-1.44297000	1.43965200	-0.38751400
C	-1.07399800	2.14958700	-1.53010900
C	-1.60245500	2.14067600	0.81925500
C	-0.83764800	3.52564400	-1.48448600
H	-0.98975700	1.62820100	-2.48562600
C	-1.35938900	3.50376100	0.88076900
H	-1.90940100	1.60355800	1.71972500
C	-0.95678300	4.20407400	-0.26783800
H	-0.54505400	4.04743300	-2.39494200
H	-1.45645300	4.05327600	1.81830300
O	-7.11276300	-1.69290100	0.16040700
O	-0.69201900	5.51718300	-0.10491100
C	-8.18847500	-0.80593400	-0.05090200
H	-8.20322900	-0.43203500	-1.08717200
H	-9.10525300	-1.37573400	0.13811300
H	-8.14548200	0.04944100	0.64222400
C	-0.31289000	6.26839900	-1.23596000
H	-0.15069600	7.29560200	-0.89014900
H	0.62058100	5.88645800	-1.68058300
H	-1.10406000	6.26613500	-2.00307900
C	-0.77465000	-0.91298600	-0.64618900
H	-1.01584100	-2.09605400	-0.68132300

Int b2

C	2.65798400	2.45716200	2.31871400
C	3.59507800	1.48084800	2.59169300
C	3.90727400	0.51178800	1.61267500
C	3.19201000	0.49497800	0.38664700
C	2.39895500	1.62753900	0.03248600
C	2.11516300	2.55952700	1.02400900
C	5.01797200	-0.39176700	1.79350700
C	3.39427000	-0.64840700	-0.49413700
C	4.60165500	-1.38503200	-0.38450400
C	5.41785900	-1.21543500	0.79028100
C	4.92456700	-2.35241100	-1.36524500
H	5.87173400	-2.88961900	-1.28676100
C	4.05628800	-2.59994900	-2.40530300
C	2.76831600	-2.01710200	-2.40699300
C	2.39346300	-1.13137600	-1.38176500
H	5.57998700	-0.33481300	2.72839100
H	2.39999200	3.20092700	3.07484800
H	4.12192700	1.45714000	3.54802400
H	1.50396300	3.42993000	0.77516500
H	6.31838500	-1.82530000	0.88717400
H	4.32073400	-3.29820200	-3.20191800
C	2.12706800	1.98942200	-1.42681200
C	3.21795600	2.97257800	-1.87680400
C	0.74239900	2.56410500	-1.70104200
H	2.24241900	1.09394100	-2.04712600
H	4.22406000	2.55332000	-1.72610500
H	3.09994700	3.20989500	-2.94516500
H	3.15201700	3.91320000	-1.30758100
H	-0.04983700	1.87444700	-1.38151300
H	0.59610400	3.53058500	-1.19428100
H	0.62214800	2.74091400	-2.78109400
C	1.81797000	-2.32972900	-3.46775500
C	0.59133400	-1.77502600	-3.52387800
H	2.16031700	-2.99393700	-4.26550400
H	-0.08734800	-1.94113300	-4.36243300
C	0.93417300	-0.89359300	-1.20366300
C	0.10255100	-0.88493000	-2.45193700
O	-0.94537800	-0.27818800	-2.56321600
C	0.30313900	-1.11064400	-0.00405800
C	1.04058000	-1.55784900	1.22422400
C	1.91139500	-2.65777200	1.19831200
C	0.80039000	-0.92064300	2.44764000

C	2.55470200	-3.07815600	2.36050800
H	2.08518000	-3.18767700	0.25932500
C	1.45338300	-1.33301200	3.60912200
H	0.10513400	-0.08251800	2.48853100
C	2.33728400	-2.41006800	3.56763900
H	3.23012500	-3.93496300	2.32249700
H	1.26624900	-0.80992700	4.54855600
H	2.84798400	-2.73798800	4.47484000
C	-2.21210300	-0.43450800	0.03756500
C	-2.12158400	1.04400800	-0.10103400
C	-1.53776200	1.82600600	0.89506200
C	-2.73519000	1.70199000	-1.18338300
C	-1.53773600	3.22372000	0.82782100
H	-1.09349100	1.34588500	1.76711000
C	-2.72370000	3.08282900	-1.27741800
H	-3.20402400	1.10906700	-1.97017700
C	-2.11947000	3.85804200	-0.27129400
H	-1.07801900	3.79632400	1.63257500
H	-3.17668300	3.59733300	-2.12632300
C	-3.59200100	-0.99005300	0.12681200
C	-4.63826100	-0.24874200	0.69019200
C	-3.89315500	-2.27641100	-0.36006300
C	-5.93041100	-0.76418800	0.79793500
H	-4.44243000	0.75644300	1.06876700
C	-5.17212300	-2.80135800	-0.26522800
H	-3.11148500	-2.86388100	-0.84567900
C	-6.20494900	-2.05112700	0.32001900
H	-6.71093400	-0.15585000	1.25307300
H	-5.40664400	-3.79336800	-0.65413700
O	-2.14427100	5.19514100	-0.44999600
O	-7.41768200	-2.63551600	0.36944400
C	-1.54367500	6.01023900	0.52931400
H	-0.46792900	5.79157000	0.63183100
H	-1.66723400	7.04662200	0.19489600
H	-2.03038200	5.88744200	1.51037900
C	-8.48941300	-1.91229200	0.93157500
H	-9.37075800	-2.56081200	0.87033700
H	-8.29748900	-1.66419000	1.98784200
H	-8.68541800	-0.98347400	0.37191700
C	-1.15935700	-1.27239100	0.16508300
H	-1.39540500	-2.29368600	0.49075100

TS-b3

C	2.92359600	2.57907300	2.15088400

C	3.91139400	1.62895000	2.28106400
C	4.07410500	0.64207800	1.28104900
C	3.15864900	0.57267300	0.19589500
C	2.30003300	1.69646200	-0.05050500
C	2.17204300	2.64252600	0.95944900
C	5.22283000	-0.22522900	1.29890800
C	3.24897500	-0.58767800	-0.68061500
C	4.49548400	-1.25196100	-0.77575500
C	5.48302400	-1.04655600	0.24801800
C	4.73178800	-2.16864700	-1.83619800
H	5.71753200	-2.62932700	-1.92512900
C	3.73827700	-2.44008400	-2.73996000
C	2.41838800	-1.96570000	-2.51389900
C	2.13584600	-1.13465600	-1.40661100
H	5.92399200	-0.13701900	2.13165700
H	2.77745100	3.33730700	2.92224000
H	4.59382200	1.63502100	3.13385600
H	1.51008300	3.49648100	0.81384400
H	6.41028200	-1.62095500	0.19573600
H	3.92105800	-3.09090500	-3.59753100
C	1.74760700	1.98720900	-1.44892400
C	2.89853500	2.06131800	-2.46557800
C	0.94153000	3.27903100	-1.53687900
H	1.07543300	1.17563400	-1.75500600
H	3.47416200	1.12854200	-2.52986400
H	2.49795900	2.27973300	-3.46686200
H	3.59266200	2.87257500	-2.19321500
H	0.09564200	3.28120100	-0.84020700
H	1.56688200	4.16193900	-1.32816700
H	0.53891500	3.38859200	-2.55455200
C	1.34329100	-2.39689000	-3.36814500
C	0.05993200	-2.04113900	-3.12619600
H	1.59218400	-3.01481000	-4.23434500
H	-0.75802900	-2.33293500	-3.78663800
C	0.74199000	-0.96746800	-0.98843200
C	-0.30333700	-1.21979500	-1.97852600
O	-1.49533600	-0.86430700	-1.85763600
C	0.34191300	-1.04335000	0.37649000
C	1.27917100	-1.47465400	1.46128800
C	2.15660300	-2.55990000	1.32285400
C	1.22522900	-0.80252800	2.68956400
C	2.97783000	-2.94157900	2.38102900
H	2.19001600	-3.11208300	0.38133400
C	2.05339600	-1.17957200	3.74721100

H	0.53971800	0.04026700	2.80361100
C	2.93579500	-2.24752600	3.59342800
H	3.65452900	-3.78957000	2.25984600
H	2.00913200	-0.63362300	4.69135800
H	3.58599900	-2.54647300	4.41764900
C	-2.07104800	-0.38745900	0.12808000
C	-2.03218600	1.07959300	-0.12717900
C	-1.60985000	1.91906100	0.90753900
C	-2.62683400	1.66624000	-1.26043300
C	-1.78650800	3.30454200	0.84454300
H	-1.16912000	1.48000300	1.80463500
C	-2.78400500	3.03868600	-1.34760600
H	-2.96449400	1.02399400	-2.07415800
C	-2.37519700	3.87167000	-0.28951200
H	-1.45641200	3.92257900	1.67849800
H	-3.23049200	3.50272400	-2.22834200
C	-3.41576700	-0.99934400	0.22929400
C	-4.57990900	-0.23930700	0.40271300
C	-3.54605400	-2.40149500	0.16042800
C	-5.83248100	-0.84080900	0.51966600
H	-4.51485500	0.84748900	0.47310300
C	-4.78195600	-3.01204800	0.26702500
H	-2.65628800	-3.01157200	-0.00731600
C	-5.94084300	-2.23547400	0.44968000
H	-6.71209900	-0.21598400	0.66755700
H	-4.88837000	-4.09563700	0.20038500
O	-2.57289800	5.19218700	-0.45899400
O	-7.09959900	-2.90789500	0.54123000
C	-2.12803800	6.07094300	0.54992400
H	-1.03933900	5.98777000	0.70126800
H	-2.36719700	7.08490500	0.21008500
H	-2.64166600	5.88005400	1.50577600
C	-8.29542200	-2.17640400	0.70566300
H	-9.10719800	-2.91129900	0.74519300
H	-8.28565300	-1.59785400	1.64299600
H	-8.46617800	-1.49345000	-0.14149800
C	-1.00812400	-1.04046700	0.77279500
H	-1.26555400	-1.72721300	1.58422600

TS-c1

C	-2.01851600	-0.18825800	-4.14024100
C	-1.55882100	-1.46255400	-3.88628000
C	-2.00264300	-2.15868800	-2.74136500
C	-2.85423200	-1.52358700	-1.79250700

C	-3.47715600	-0.28974200	-2.17281000
C	-3.01477400	0.35739500	-3.31364600
C	-1.65931100	-3.54950900	-2.58523200
C	-3.13300000	-2.25127400	-0.54900200
C	-2.95314100	-3.66394000	-0.53490900
C	-2.19607600	-4.29229600	-1.58553900
C	-3.44663100	-4.43332100	0.54548500
H	-3.32713800	-5.51792700	0.51376500
C	-4.07579400	-3.82244800	1.60586600
C	-4.07634800	-2.41291800	1.69758300
C	-3.51732200	-1.63767300	0.67489500
H	-1.01846900	-4.00705200	-3.34215000
H	-1.67226600	0.36463900	-5.01543100
H	-0.86726300	-1.96036200	-4.56948500
H	-3.47846200	1.30152400	-3.60782000
H	-2.01805200	-5.36758200	-1.52248000
H	-4.51665600	-4.40987400	2.41363000
C	-4.78717900	0.22341500	-1.56762300
C	-5.93679500	-0.16473200	-2.50821900
C	-4.81148700	1.73149200	-1.30018600
H	-4.98120700	-0.29614100	-0.62210400
H	-5.95603900	-1.25020200	-2.68590600
H	-6.90266300	0.13010200	-2.07053600
H	-5.83353900	0.33920800	-3.48156300
H	-3.98804900	2.06431400	-0.64946300
H	-4.75748300	2.30471000	-2.23834900
H	-5.75543800	2.00425000	-0.80479800
C	-4.69008600	-1.75222300	2.84976800
C	-4.73273100	-0.41361700	3.00143600
H	-5.17588000	-2.39999500	3.58465500
H	-5.25652600	0.06300200	3.83163000
C	-3.15101000	-0.20674300	1.00733600
H	-3.11253200	0.43824800	0.12931400
C	-4.05109500	0.46794700	2.04207400
O	-4.11392100	1.67910100	2.10319900
C	-1.71538000	-0.18696100	1.58343900
C	-1.50180000	-0.71896200	2.96415600
C	-1.61768800	0.12524900	4.07575000
C	-1.20393200	-2.07250900	3.15912700
C	-1.44855400	-0.38097900	5.36378800
H	-1.84881500	1.18272900	3.92681900
C	-1.03840400	-2.57812100	4.44904500
H	-1.10743000	-2.73105300	2.29204800
C	-1.16515800	-1.73456000	5.55294200

H	-1.53786600	0.28558600	6.22335700
H	-0.80663700	-3.63532600	4.59040300
H	-1.03558100	-2.13033200	6.56179800
C	-0.49192100	0.91656200	-0.35648300
C	0.39573500	0.30112200	-1.33613500
C	1.15356500	1.05400500	-2.25333700
C	0.63080300	-1.09433400	-1.27649000
C	2.06997800	0.45280900	-3.10583400
H	1.07278800	2.14056100	-2.26362100
C	1.53825200	-1.70460500	-2.11317800
H	0.07174200	-1.70010500	-0.55955500
C	2.27203800	-0.93499100	-3.03770000
H	2.65256100	1.07161400	-3.78648100
H	1.72072700	-2.77922200	-2.07035400
C	-1.05625300	2.25180500	-0.52835100
C	-1.44298700	3.00886000	0.59419500
C	-1.32592700	2.78787100	-1.81029300
C	-2.06142200	4.24430300	0.46309400
H	-1.22171600	2.63061600	1.59234300
C	-1.95766300	4.00692900	-1.95343400
H	-1.08531700	2.21072200	-2.70161200
C	-2.33225600	4.75075500	-0.81818000
H	-2.33065400	4.80316800	1.35780900
H	-2.19416800	4.40908500	-2.93932400
O	3.14799100	-1.60209700	-3.79297300
O	-2.93568500	5.92039900	-1.04871700
C	3.94496100	-0.88554200	-4.71453200
H	4.56723100	-0.13521500	-4.20319000
H	4.59321600	-1.62214400	-5.20149400
H	3.32224200	-0.38845200	-5.47447600
C	-3.35261400	6.70386800	0.05295000
H	-3.82603400	7.59841400	-0.36586500
H	-4.08275200	6.16035900	0.67213600
H	-2.49472300	7.00329600	0.67441900
C	-0.67897100	0.24315100	0.85731400
P	2.70325300	0.76540800	1.12360500
O	3.45855400	0.26979000	-0.23655700
O	2.17614400	2.12812300	0.88667800
O	1.73892200	-0.32933600	1.61262500
H	0.56889000	-0.04712700	1.32684200
O	3.92186400	0.66806500	2.20850900
C	4.29152300	-0.81079000	-0.35351500
C	4.10054900	-1.99431900	0.36303300
C	5.35422100	-0.68181500	-1.25040000

C	4.99461300	-3.04948500	0.17428000
H	3.25998100	-2.08038400	1.05269300
C	6.23259700	-1.74684300	-1.43484400
H	5.47838800	0.26436000	-1.78014800
C	6.05818600	-2.93462000	-0.72138500
H	4.84998300	-3.97505300	0.73465900
H	7.06344900	-1.64419100	-2.13542800
H	6.74920900	-3.76686700	-0.86265800
C	5.17893300	1.15858600	1.94197400
C	6.26522900	0.37214000	2.32768700
C	5.37175500	2.38729500	1.30758600
C	7.55939100	0.81975900	2.07163500
H	6.07581400	-0.58544100	2.81525000
C	6.67355500	2.81870900	1.05024600
H	4.50451400	2.98405400	1.02088700
C	7.76874600	2.04128200	1.42803800
H	8.40971200	0.20442200	2.37089800
H	6.82866100	3.77690800	0.55093700
H	8.78320200	2.38658900	1.22336800

Int c1

C	-3.02915800	-0.39732200	2.23152600
C	-2.68620400	-1.71539500	2.01230900
C	-1.32815000	-2.08102600	1.89586900
C	-0.31214800	-1.08345700	1.89639800
C	-0.66476000	0.24039300	2.31470900
C	-2.01403100	0.55110900	2.44239600
C	-0.96466700	-3.47627000	1.89001800
C	1.05885300	-1.52328600	1.62640700
C	1.39128300	-2.88716600	1.85792000
C	0.33448400	-3.85769500	1.98056400
C	2.74785300	-3.28944500	1.88365200
H	2.98198800	-4.33217200	2.10647800
C	3.74931400	-2.37670300	1.64216500
C	3.41645200	-1.08095500	1.18744600
C	2.07743900	-0.68967300	1.09228400
H	-1.76843800	-4.21557600	1.90691100
H	-4.07665400	-0.10372600	2.32251300
H	-3.44835500	-2.49596300	1.96166100
H	-2.29481000	1.55567300	2.76713100
H	0.60822800	-4.90875700	2.09102000
H	4.80045900	-2.66141800	1.71697300
C	0.34266700	1.24011900	2.88962600
C	0.24777400	1.18998300	4.42090100

C	0.16325000	2.67758300	2.39600000
H	1.35999500	0.91956500	2.63634000
H	0.40439100	0.16774400	4.79566800
H	1.01060300	1.84302600	4.87102400
H	-0.74132000	1.53167900	4.76283700
H	0.24771300	2.76488800	1.30238500
H	-0.81302600	3.08815000	2.69589900
H	0.93943300	3.31942400	2.83912700
C	4.47336600	-0.14131600	0.81587400
C	4.23260700	1.09736400	0.34227800
H	5.50294400	-0.47038400	0.97995700
H	5.03422000	1.80712300	0.13260400
C	1.74617900	0.49812400	0.19922500
H	0.83830900	1.01670600	0.50954000
C	2.85864500	1.54902600	0.08785400
O	2.59234100	2.68060300	-0.26014900
C	1.48899800	-0.08505800	-1.19476500
C	2.63082900	-0.74618100	-1.90023000
C	3.45793400	0.01030700	-2.73991900
C	2.87697200	-2.11378300	-1.73876300
C	4.52521900	-0.59494900	-3.40205900
H	3.26756400	1.07880800	-2.86910600
C	3.94660500	-2.71600500	-2.40137000
H	2.23510900	-2.70343100	-1.07858400
C	4.77325700	-1.95751100	-3.23066800
H	5.16516800	0.00194300	-4.05392000
H	4.13384600	-3.78272800	-2.26679600
H	5.61038400	-2.42983300	-3.74743000
C	-1.00619900	0.42034800	-1.38237700
C	-2.12793700	-0.47977700	-1.43779400
C	-3.45645500	-0.04009100	-1.66190000
C	-1.90829700	-1.88048800	-1.31885800
C	-4.51586100	-0.92755600	-1.70644300
H	-3.65319600	1.01189000	-1.86858000
C	-2.95302900	-2.77204000	-1.35514200
H	-0.89654500	-2.25340600	-1.14851600
C	-4.27510600	-2.30535100	-1.53209800
H	-5.51988200	-0.55494900	-1.90241700
H	-2.79214400	-3.84371000	-1.23320000
C	-1.12645900	1.80351900	-1.04865300
C	-0.14917400	2.73311300	-1.49801400
C	-2.22069700	2.31378400	-0.28450900
C	-0.25891000	4.08464900	-1.24050600
H	0.68891700	2.38070200	-2.09759200

C	-2.33228400	3.65263400	-0.01344200
H	-2.94751900	1.62425600	0.14065800
C	-1.35439300	4.55944600	-0.49191100
H	0.50434300	4.76529900	-1.61305000
H	-3.14701400	4.04580300	0.59524800
O	-5.22517600	-3.22823200	-1.53970800
O	-1.54253900	5.83009600	-0.18459700
C	-6.58061800	-2.83551200	-1.69467700
H	-6.73761900	-2.34765600	-2.66787200
H	-7.17245700	-3.75507700	-1.64669300
H	-6.88527800	-2.15764400	-0.88370900
C	-0.58942300	6.80105700	-0.59573100
H	-0.95308200	7.76220700	-0.21929300
H	0.39780300	6.58335200	-0.16299300
H	-0.51915300	6.83623700	-1.69254700
C	0.28195800	-0.13681500	-1.80085400
H	0.23020600	-0.73815100	-2.71448100

TS-c2

C	-3.19639300	2.87691200	-1.92906700
C	-3.94550700	1.75992800	-2.24111300
C	-3.96978800	0.65973900	-1.35809300
C	-3.13463700	0.65281600	-0.20595700
C	-2.51430100	1.87628700	0.19903900
C	-2.54435400	2.94842400	-0.68721900
C	-4.93739400	-0.39467000	-1.54281400
C	-3.09722000	-0.57945600	0.57997800
C	-4.20004500	-1.47167000	0.50406200
C	-5.12369900	-1.34677600	-0.59302500
C	-4.32063500	-2.52590800	1.44227000
H	-5.20228300	-3.16822400	1.40077900
C	-3.34334100	-2.72923100	2.38840200
C	-2.13141600	-2.00405600	2.29997900
C	-1.97722700	-1.00037200	1.33957100
H	-5.58099600	-0.35115400	-2.42403100
H	-3.17541400	3.73490300	-2.60336100
H	-4.56115400	1.72912100	-3.14232600
H	-2.08803600	3.89494100	-0.39004100
H	-5.92938000	-2.07872700	-0.67725000
H	-3.44983800	-3.50037900	3.15356800
C	-2.09942300	2.15593400	1.64788200
C	-3.25109100	2.91377100	2.32453600
C	-0.79140600	2.93239000	1.81788500
H	-1.99681900	1.20639600	2.18724800

H	-4.19734300	2.35991200	2.23701200
H	-3.03473500	3.06202300	3.39320200
H	-3.39042600	3.90297400	1.86168600
H	0.08308800	2.39031800	1.42715700
H	-0.82831100	3.91220700	1.31699700
H	-0.61555100	3.11759800	2.88792100
C	-1.02783500	-2.31014400	3.19552300
C	0.19983600	-1.74601000	3.10101000
H	-1.22577800	-3.02707600	3.99698400
H	1.00428100	-1.97212800	3.80043600
C	-0.57734600	-0.57546900	0.95755900
H	-0.50687100	0.50888100	0.80174100
C	0.50950400	-0.89199100	1.97407500
O	1.64970500	-0.48473000	1.76068700
C	-0.11363400	-1.21714700	-0.36494300
C	-1.00519500	-2.17925500	-1.07118800
C	-1.30396900	-3.42779800	-0.50948000
C	-1.56507200	-1.82585300	-2.30398600
C	-2.16351100	-4.30358800	-1.16861700
H	-0.85409100	-3.71371200	0.44367500
C	-2.42968700	-2.70428300	-2.95957200
H	-1.33366900	-0.85239600	-2.74267200
C	-2.73413000	-3.94029800	-2.39099200
H	-2.38826900	-5.27569200	-0.72632200
H	-2.86963100	-2.41620700	-3.91596200
H	-3.41330600	-4.62510900	-2.90154600
C	2.12437600	-0.07778600	-0.26109800
C	1.90831600	1.35845700	-0.33345700
C	2.77640900	2.28619200	0.28249600
C	0.85851300	1.87046400	-1.13708900
C	2.58301700	3.65072700	0.16114600
H	3.61635100	1.94110400	0.88173900
C	0.69262400	3.22726200	-1.31216300
H	0.18372800	1.18766800	-1.65482900
C	1.53151700	4.13606600	-0.64146600
H	3.25871100	4.33376100	0.67323600
H	-0.09617200	3.62006500	-1.95321800
C	3.49302200	-0.63762900	-0.14596200
C	4.00770000	-1.38976800	-1.21252900
C	4.32724800	-0.41407200	0.97007500
C	5.31240500	-1.87819900	-1.19701700
H	3.40853300	-1.57394600	-2.10415000
C	5.61276000	-0.91819300	1.00590100
H	3.94228600	0.11356000	1.84075300

C	6.12683800	-1.64767200	-0.08210300
H	5.67840000	-2.43598900	-2.05757000
H	6.24917800	-0.76871100	1.87882700
O	1.26819900	5.42618100	-0.82122800
O	7.38647400	-2.08399900	0.03539800
C	2.07717900	6.39669100	-0.17647500
H	3.12392600	6.31692400	-0.50563200
H	1.67599000	7.37265900	-0.46826400
H	2.02187800	6.28945700	0.91726200
C	7.94943400	-2.82954900	-1.02576100
H	8.97140000	-3.07967900	-0.72114600
H	7.38525400	-3.75850600	-1.20236700
H	7.98147800	-2.23806000	-1.95399000
C	1.11899600	-0.97600200	-0.84885900
H	1.44993400	-1.57367000	-1.70248700

Int c2

C	-3.12702700	1.96266900	-2.72152900
C	-4.05594800	0.95091000	-2.57970900
C	-4.16096000	0.26135300	-1.35304400
C	-3.25550900	0.55497300	-0.29997000
C	-2.49332000	1.75785400	-0.36978400
C	-2.40041900	2.40128800	-1.59969100
C	-5.25241300	-0.64803800	-1.10979200
C	-3.24239800	-0.35169100	0.84552800
C	-4.42281900	-1.09922000	1.12295700
C	-5.44557100	-1.19682600	0.11829700
C	-4.53410500	-1.84404800	2.32351300
H	-5.47328100	-2.35629600	2.53938100
C	-3.47123000	-1.92667200	3.18474100
C	-2.21638400	-1.39467600	2.79283800
C	-2.07767500	-0.67726900	1.58867800
H	-5.96819700	-0.81819200	-1.91701100
H	-3.02125400	2.48620300	-3.67300800
H	-4.73105600	0.68607700	-3.39589500
H	-1.80679300	3.31382400	-1.68362200
H	-6.32710700	-1.80224200	0.33555100
H	-3.54670500	-2.45966100	4.13377500
C	-2.08995900	2.50286000	0.90194500
C	-3.26230300	3.41494800	1.29366500
C	-0.80264700	3.31304100	0.78965300
H	-1.97527800	1.78608000	1.72528800
H	-4.18974000	2.83969100	1.43025100
H	-3.03751800	3.93908600	2.23480000

H	-3.43914800	4.16960000	0.51199000
H	0.04124600	2.69399800	0.45814100
H	-0.90819900	4.14913500	0.08171800
H	-0.54712900	3.74502000	1.76868200
C	-1.07725500	-1.60615800	3.63557300
C	0.20288400	-1.25721100	3.29329200
H	-1.25386600	-2.08546600	4.60220500
H	1.05617200	-1.44674000	3.94264900
C	-0.68209700	-0.42584000	1.05706000
H	-0.53288200	0.65760500	0.87543100
C	0.42557500	-0.76242800	1.99818300
O	1.64916200	-0.64346900	1.61525900
C	-0.31592700	-1.08326800	-0.30112000
C	-1.30649900	-1.75418000	-1.18023200
C	-2.15203300	-2.76792200	-0.70641100
C	-1.34845900	-1.40820500	-2.53782600
C	-3.02583200	-3.41535600	-1.57696100
H	-2.11963500	-3.05973600	0.34595600
C	-2.22343100	-2.05872600	-3.40658200
H	-0.70194200	-0.60913300	-2.90706700
C	-3.06754700	-3.05982400	-2.92715000
H	-3.67844800	-4.20396400	-1.19806300
H	-2.25157900	-1.77354800	-4.45962500
H	-3.75765100	-3.56602300	-3.60431600
C	2.01603300	-0.36746700	0.20931700
C	2.10515100	1.13917000	0.02904500
C	2.56493400	1.95143800	1.06647500
C	1.83835000	1.71942700	-1.21911700
C	2.73798600	3.32372700	0.88411100
H	2.79861900	1.51436700	2.03936300
C	2.01850900	3.08017700	-1.41728000
H	1.49066000	1.10237900	-2.04982500
C	2.46216900	3.89715900	-0.36486100
H	3.08594000	3.93211700	1.71793400
H	1.81110500	3.54246900	-2.38325400
C	3.35719200	-1.06899900	0.03754900
C	4.50816700	-0.40817400	-0.38251000
C	3.42615700	-2.44987700	0.28986300
C	5.71346600	-1.09616500	-0.55410200
H	4.48489200	0.66242900	-0.59014200
C	4.61361900	-3.14202400	0.13282900
H	2.53276200	-2.98883400	0.61620000
C	5.77267500	-2.46869800	-0.29480200
H	6.59328400	-0.54806300	-0.88764000

H	4.67652500	-4.21293400	0.33012300
O	2.58960200	5.20601900	-0.63952200
O	6.88063800	-3.21766300	-0.42768400
C	3.02184100	6.07305300	0.38717200
H	4.02689100	5.79979400	0.74560400
H	3.05500900	7.07837200	-0.04701800
H	2.31916400	6.06830300	1.23574600
C	8.06832700	-2.59322800	-0.86560600
H	8.83429800	-3.37550700	-0.90891600
H	7.94329300	-2.15352100	-1.86789500
H	8.39166500	-1.80920100	-0.16261300
C	0.96716600	-1.00679600	-0.66661800
H	1.30806700	-1.44694100	-1.60483500

Int c3

C	0.75279600	-4.68526300	0.60659700
C	-0.45576900	-5.03061200	1.17430200
C	-1.64871500	-4.48365500	0.65612900
C	-1.59082400	-3.49574300	-0.36282700
C	-0.37512400	-3.33230300	-1.09908100
C	0.77597800	-3.90101500	-0.56139900
C	-2.92525300	-5.02907300	1.04121800
C	-2.84540400	-2.84645400	-0.72854700
C	-4.05421100	-3.57369300	-0.53393400
C	-4.06090000	-4.68184100	0.37959200
C	-5.24548600	-3.16949000	-1.19019100
H	-6.14331500	-3.77883700	-1.07309000
C	-5.24200300	-2.05571400	-1.98819900
C	-4.11257500	-1.19578800	-1.97124700
C	-2.95983800	-1.51929700	-1.22350300
H	-2.94079000	-5.80695400	1.80817500
H	1.68667800	-5.09149100	0.99939200
H	-0.51309500	-5.75206900	1.99213400
H	1.72476900	-3.77282700	-1.07881200
H	-5.00878500	-5.18608500	0.57588300
H	-6.11248300	-1.77527000	-2.58341800
C	-0.37972900	-2.85156500	-2.55566100
C	-1.27434700	-3.78113900	-3.39331200
C	1.00929200	-2.80400400	-3.18734800
H	-0.79078400	-1.83787800	-2.63071400
H	-2.31969000	-3.78611100	-3.05328500
H	-1.26337400	-3.46176700	-4.44647000
H	-0.89790700	-4.81533100	-3.34859200
H	1.69488300	-2.18339500	-2.60020500

H	1.43470700	-3.81517300	-3.28897600
H	0.93179900	-2.37612400	-4.19792200
C	-4.11681300	-0.00042600	-2.75661500
C	-3.12732300	0.94616900	-2.69618200
H	-4.96522100	0.16033500	-3.42748000
H	-3.15950500	1.86490000	-3.28020500
C	-1.98051900	-0.41698000	-0.89962700
H	-0.91357300	-0.65367900	-1.21565500
C	-2.18941000	0.83443400	-1.65348500
O	-1.51538100	1.90784400	-1.37942800
C	-1.72238200	-0.08739500	0.58614000
C	-1.80716500	-1.10710600	1.66736400
C	-3.03918000	-1.62690700	2.08602400
C	-0.63815100	-1.45723500	2.35670700
C	-3.09827300	-2.49390500	3.17612200
H	-3.95562600	-1.33729100	1.56560300
C	-0.70283800	-2.33075500	3.44339900
H	0.31014500	-1.01659600	2.03256900
C	-1.93035200	-2.85178500	3.85383600
H	-4.06266700	-2.88951200	3.50064200
H	0.21222800	-2.60062600	3.97514000
H	-1.98008500	-3.53209400	4.70618500
C	-1.21446800	2.31439700	-0.00409800
C	0.17287000	2.93325100	0.00936300
C	0.97693400	3.00476200	-1.11983400
C	0.64133800	3.48475700	1.21226000
C	2.23686300	3.61228500	-1.06640600
H	0.64332800	2.55629600	-2.05517300
C	1.89045200	4.07569800	1.28102500
H	0.01626700	3.45367300	2.10817200
C	2.70743800	4.13533800	0.13838400
H	2.85594400	3.62479400	-1.96253500
H	2.26876200	4.49419600	2.21470300
C	-2.28987200	3.36218000	0.31520000
C	-3.44450700	3.03637400	1.02542500
C	-2.16540800	4.66496600	-0.19538200
C	-4.45454000	3.97760900	1.24450400
H	-3.57537900	2.03064400	1.42865300
C	-3.16133400	5.60586600	0.00443200
H	-1.27173800	4.94367700	-0.75731800
C	-4.31703800	5.27137200	0.73141500
H	-5.33713900	3.68912700	1.81384900
H	-3.06981400	6.61924500	-0.38884700
O	3.91995800	4.70432400	0.30157800

O	-5.22960600	6.24781600	0.88466300
C	4.78565600	4.76169600	-0.80839700
H	4.35662600	5.37331200	-1.61951800
H	5.71343800	5.23014700	-0.45919900
H	5.01277500	3.75469400	-1.19533200
C	-6.40274200	5.96357700	1.61431300
H	-6.99904800	6.88293300	1.61793900
H	-6.98494300	5.15721100	1.14023700
H	-6.16999700	5.67979200	2.65307100
C	-1.31195000	1.13832900	0.91785500
H	-1.07982000	1.35737300	1.96214700
P	1.97365400	-0.16600000	-0.43892000
O	3.06203400	0.76041600	-1.27217000
O	1.88110800	0.23224200	0.99617500
O	0.79652800	-0.26150500	-1.36086100
O	2.77995900	-1.61607100	-0.54678500
C	4.32138300	1.05801500	-0.84784900
C	4.60195500	1.45638300	0.46439500
C	5.34506500	0.99991700	-1.79987100
C	5.91290700	1.77849600	0.81350500
H	3.78572000	1.50449100	1.18448900
C	6.65042300	1.32941800	-1.43793800
H	5.09502300	0.68912900	-2.81564700
C	6.94158300	1.71731300	-0.12853000
H	6.12860600	2.08880900	1.83783900
H	7.44513300	1.27913100	-2.18491700
H	7.96377200	1.97287000	0.15503200
C	3.65295000	-2.06844500	0.40186000
C	3.21239700	-2.39814000	1.68667200
C	4.99383900	-2.24281200	0.04994800
C	4.12347900	-2.89442400	2.61813600
H	2.16006300	-2.26071600	1.93391900
C	5.89646900	-2.74050400	0.98884600
H	5.31113500	-1.97605600	-0.95957700
C	5.46649200	-3.06558800	2.27648400
H	3.77785500	-3.14947600	3.62193800
H	6.94398800	-2.87098400	0.71077600
H	6.17483700	-3.45223400	3.01087200

TS-c3

C	0.84660500	-4.70382700	0.65943900
C	-0.36605200	-5.04209100	1.22275400
C	-1.55563000	-4.49763800	0.69204900
C	-1.48626100	-3.51170700	-0.32780000

C	-0.26559500	-3.35352000	-1.05748600
C	0.87977800	-3.92641800	-0.51369900
C	-2.83696800	-5.04739800	1.05446300
C	-2.73476900	-2.87618200	-0.72671200
C	-3.93516000	-3.62058500	-0.57106000
C	-3.95700100	-4.71686100	0.35751500
C	-5.09880800	-3.25414100	-1.29815500
H	-5.99204700	-3.87535000	-1.21159700
C	-5.06567700	-2.16937100	-2.13374900
C	-3.95509700	-1.28403200	-2.08133500
C	-2.84406400	-1.55675000	-1.25365100
H	-2.86614200	-5.81881600	1.82751400
H	1.77668700	-5.11177300	1.05951500
H	-0.42946100	-5.76010700	2.04320900
H	1.83115000	-3.81020700	-1.02998200
H	-4.90451400	-5.23050900	0.53061300
H	-5.90528700	-1.92447500	-2.78635200
C	-0.26970100	-2.88026900	-2.51649200
C	-1.14846100	-3.82516500	-3.35391700
C	1.11988000	-2.81789200	-3.14558900
H	-0.69513000	-1.87295000	-2.59252300
H	-2.19595200	-3.84015500	-3.02077000
H	-1.13447700	-3.51157200	-4.40885000
H	-0.76088300	-4.85491700	-3.30123400
H	1.80084500	-2.19052000	-2.56034700
H	1.55738300	-3.82428200	-3.24375000
H	1.03958200	-2.39433900	-4.15776100
C	-3.94277900	-0.10459700	-2.89147100
C	-2.99061800	0.86983800	-2.77211000
H	-4.74382100	0.01587200	-3.62578400
H	-3.00195400	1.77841400	-3.37263500
C	-1.92678500	-0.42306200	-0.89005600
H	-0.76365200	-0.57411700	-1.16896200
C	-2.12462900	0.80005200	-1.65857300
O	-1.50671900	1.90627800	-1.36263900
C	-1.69337200	-0.09719300	0.59341700
C	-1.79933500	-1.11118500	1.67881400
C	-3.03923800	-1.64454900	2.05546200
C	-0.65419700	-1.43769400	2.41741000
C	-3.12868000	-2.50253500	3.15043100
H	-3.93881900	-1.37219600	1.49785600
C	-0.74838500	-2.30334200	3.50840900
H	0.29887500	-0.98642300	2.12580100
C	-1.98310000	-2.83896400	3.87565000

H	-4.09949200	-2.90868700	3.44099700
H	0.14915800	-2.55516000	4.07746600
H	-2.05628200	-3.51307900	4.73120300
C	-1.23385300	2.31771800	0.01359500
C	0.14493300	2.95664400	0.03910500
C	0.92952700	3.08950900	-1.09823400
C	0.62424500	3.46867800	1.25548200
C	2.18166400	3.71266600	-1.04042600
H	0.58508500	2.68313200	-2.04887500
C	1.86467000	4.07693500	1.32827400
H	0.01549900	3.39236300	2.15963000
C	2.66412400	4.19243200	0.17721000
H	2.78472200	3.77219600	-1.94563400
H	2.25165900	4.46315700	2.27229500
C	-2.33108900	3.34490400	0.32708400
C	-3.53471900	2.95576300	0.91511600
C	-2.18527200	4.68483500	-0.06681000
C	-4.57211300	3.86719300	1.12665700
H	-3.68125200	1.91893900	1.22421500
C	-3.20718600	5.59970500	0.12927200
H	-1.25588200	5.01673900	-0.53310700
C	-4.41176500	5.19986300	0.73167800
H	-5.49298900	3.52696600	1.59841600
H	-3.09836600	6.64213300	-0.17331100
O	3.87444900	4.76427300	0.34561000
O	-5.34720700	6.15395100	0.88934500
C	4.72966800	4.85437600	-0.77034500
H	4.29536300	5.49288300	-1.55751200
H	5.66270100	5.30794800	-0.41560000
H	4.94888400	3.85909300	-1.19117900
C	-6.57531300	5.80018300	1.48586800
H	-7.18379800	6.71115800	1.51254200
H	-7.10114700	5.03187400	0.89668500
H	-6.43115900	5.43197600	2.51420200
C	-1.32193800	1.13893400	0.93637500
H	-1.12783500	1.36393300	1.98683600
P	1.90935700	-0.14967700	-0.40892100
O	2.92929400	0.81640900	-1.26833400
O	1.79970500	0.25473300	1.02010500
O	0.72155500	-0.29950600	-1.32745700
O	2.76376200	-1.56181700	-0.52114000
C	4.20334700	1.11785400	-0.88043300
C	4.51751600	1.50715200	0.42622200
C	5.19829300	1.06507100	-1.86105300

C	5.83782700	1.82400300	0.74310700
H	3.72130600	1.55174200	1.16890800
C	6.51356200	1.39027000	-1.53144900
H	4.92055100	0.76103700	-2.87159400
C	6.84011400	1.76697600	-0.22719900
H	6.08162900	2.12601800	1.76350700
H	7.28795700	1.34425300	-2.29962900
H	7.87021300	2.01787900	0.03065200
C	3.64427300	-2.00002800	0.43096400
C	3.20751200	-2.34138800	1.71321100
C	4.98793700	-2.14546600	0.07854400
C	4.12808300	-2.82062400	2.64452900
H	2.15225300	-2.22785400	1.96016400
C	5.89942400	-2.62657900	1.01740300
H	5.30063600	-1.86933900	-0.92987200
C	5.47448400	-2.96304900	2.30380700
H	3.78657500	-3.08534700	3.64714400
H	6.94962600	-2.73499700	0.74019000
H	6.18979600	-3.33667200	3.03814000

10. Computational Investigation on the Intramolecular Noncovalent Interactions of Dearomatized Allene Intermediates

To enhance our understanding of the stabilization mechanisms of dearomatized intermediates, we conducted computational investigations into the intramolecular noncovalent interactions present in **Int-H** and **Int-*i*Pr**. The optimized structures of **Int-H** and **Int-*i*Pr** are shown in Fig. S9. Quantum theory of atoms in molecules (QTAIM)[12-14] analyses were applied to analyze the weak noncovalent interactions formed in **Int-H** and **Int-*i*Pr**, and the bond critical points (BCPs) for the intramolecular noncovalent interactions in **Int-H** and **Int-*i*Pr** were plotted in Fig. S10. The corresponding distances between interacting atoms for the intramolecular noncovalent interactions, the electron density, and its Laplacian value at the bond critical points for the intramolecular

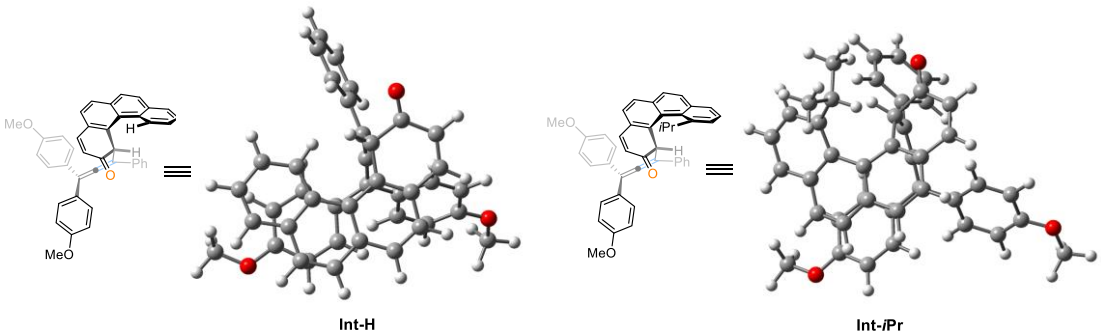

Figure S9. The optimized structures of **Int-H** and **Int-*i*Pr**.

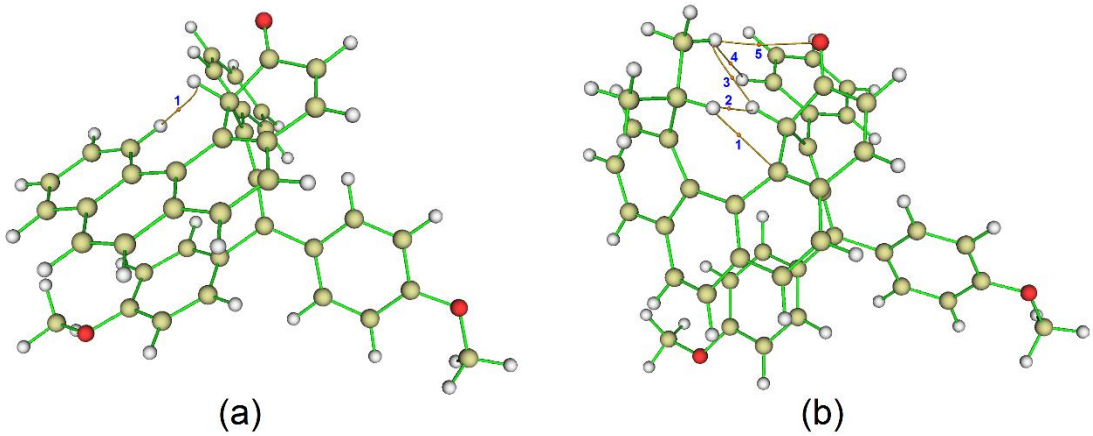

Figure S10. The bond critical points for the intramolecular noncovalent interactions in (a) **Int-H** and (b) **Int-*i*Pr.**

noncovalent interactions in **Int-H** and **Int-*i*Pr** are outlined in Table S2. In Fig. S10 it can be clearly seen that there are intramolecular C-H---H-C close contact, C-H---O and C-H---π interaction formed between alkyl C-H group and H atom of benzene ring, between alkyl C-H group and O atom of the carbonyl group, between alkyl C-H group and π ring of benzene in **Int-*i*Pr**, while there is only one intramolecular C-H---H-C close contact in **Int-H**. Clearly, the existences of more types of intramolecular noncovalent interactions in **Int-*i*Pr** should contribute to its stability. Therefore, after the H atom of **Int-H** is substituted by alkyl group to form **Int-*i*Pr**, **Int-*i*Pr** possessing the alkyl group is more stable than **Int-H**.

Table S2. Numbers of bond critical points (BCPs No.) and the corresponding distances between atoms (d, in Å), classifications of the intramolecular interactions, electron density (ρ, in a.u.) and its Laplacian value ($\nabla^2\rho$, in a.u.) at the BCPs of **Int-H** and **Int-*i*Pr**.

	BCPs No.	Classification	d	ρ	$\nabla^2\rho$
Int-H	1	C-H…H-C	1.7999	0.0209	0.0746
Int-*i*Pr	1	C-H…π	2.4050	0.0139	0.0481
	2	C-H…H-C	2.1280	0.0147	0.0659
	3	C-H…H-C	2.0244	0.0121	0.0416
	4	C-H…H-C	2.3089	0.0058	0.0206
	5	C-H…O	2.7992	0.0056	0.0205

Cartesian Coordinates

Int-H

C	-4.87672600	-0.26717000	-0.28868600
C	-4.52368900	-1.29783900	0.55532400
C	-3.31726100	-1.26609500	1.29303100
C	-2.42007500	-0.15681900	1.19764000
C	-2.81584800	0.86679600	0.29603100

C	-3.99984000	0.81992800	-0.41823200
C	-3.01284300	-2.39807000	2.12046800
C	-1.17289100	-0.17212800	1.99433600
C	-0.91116300	-1.35964000	2.75142800
C	-1.84950400	-2.44611000	2.80540400
C	0.28735600	-1.52321600	3.48001200
H	0.44517000	-2.45841500	4.01996000
C	1.22758500	-0.52855500	3.50588600
C	0.97786600	0.68243200	2.82903900
C	-0.19802600	0.87986800	2.08839600
H	-3.72946800	-3.22091200	2.16096000
H	-5.81055200	-0.30063500	-0.85249600
H	-5.17004200	-2.17101900	0.66891500
H	-4.23716700	1.64224000	-1.09568500
H	-1.59086400	-3.31137500	3.41848300
H	2.16127700	-0.64799200	4.05829900
C	1.99981700	1.72555800	2.94741000
C	1.83656300	2.98436000	2.50764900
H	2.92040000	1.44143100	3.46440000
H	2.57814100	3.76901500	2.66434000
C	-0.30883700	2.20686600	1.35779700
H	-1.33259900	2.59147000	1.42640700
C	0.55760500	3.35066300	1.89278100
O	0.20331200	4.50251700	1.75701800
C	0.08092900	2.03977700	-0.13077000
C	-0.22300400	3.12040400	-1.11347500
C	-1.21762800	4.08054800	-0.87651700
C	0.46286000	3.15714100	-2.33958700
C	-1.53001600	5.03371100	-1.84687500
H	-1.74911000	4.10278200	0.07451400
C	0.15215700	4.11046800	-3.30421900
H	1.25417900	2.42828800	-2.52836000
C	-0.85005700	5.05308700	-3.06310600
H	-2.31034200	5.76910800	-1.64338300
H	0.70030300	4.12136000	-4.24795400
H	-1.09307900	5.80304100	-3.81771200
C	1.05884800	-0.30461900	-0.82131800
C	2.49182100	-0.69846800	-0.78276000
C	2.95283700	-1.82719300	-1.46585300
C	3.42920600	0.07012200	-0.06732800
C	4.30067400	-2.19366200	-1.44512700
H	2.25180600	-2.43836600	-2.03722900
C	4.76831700	-0.27957200	-0.03869200
H	3.09027300	0.95407300	0.47886400

C	5.21844100	-1.41952800	-0.72730300
H	4.62032900	-3.07989300	-1.99185600
H	5.49600900	0.31197300	0.51884300
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C	-1.06296900	-0.97049800	-1.99452600
C	-0.05050100	-2.54101600	-0.47853000
C	-2.14943500	-1.82747600	-2.17970300
H	-1.04463800	-0.01147900	-2.51768100
C	-1.12643600	-3.39937900	-0.64781000
H	0.75978000	-2.82042500	0.19904700
C	-2.19555100	-3.04083400	-1.48503100
H	-2.95775600	-1.52994000	-2.84677100
H	-1.17799300	-4.35199100	-0.11829800
O	6.53505000	-1.69092200	-0.64056000
O	-3.22103700	-3.91484800	-1.55410000
C	7.03059600	-2.82717600	-1.31219500
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H	8.10734000	-2.86459100	-1.11162600
H	6.56145400	-3.75147700	-0.93817200
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H	-5.00567000	-4.44706200	-2.33151800
H	-4.79165800	-2.67911500	-2.14157700
H	-3.95211200	-3.54929600	-3.46806200
C	0.64511900	0.91046900	-0.51122900
H	-2.19138100	1.72453900	0.10333400

Int-*i*Pr

C	-4.68173800	1.63889400	0.74561800
C	-3.72209400	2.51190000	0.27782100
C	-2.71889300	2.05425500	-0.60392900
C	-2.63692200	0.67460700	-0.94264100
C	-3.75507100	-0.16276400	-0.62838700
C	-4.72303000	0.32799200	0.24209600
C	-1.84621100	3.00322900	-1.25121100
C	-1.45176600	0.23821900	-1.68810300
C	-0.72044000	1.20583500	-2.43028300
C	-0.96798300	2.60629300	-2.20500400
C	0.32612900	0.79854500	-3.29070500
H	0.84785100	1.55678100	-3.87798800
C	0.69174800	-0.52596900	-3.36686900
C	0.11264500	-1.46233600	-2.48105500
C	-0.90544400	-1.06991400	-1.60684700
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H	-5.45279900	1.98017500	1.43824100
H	-3.73893000	3.56831700	0.55423400

H	-5.57689900	-0.30299200	0.49692600
H	-0.36909800	3.33351800	-2.75705300
H	1.48045300	-0.85223000	-4.04771900
C	-4.08065700	-1.43955900	-1.40870100
C	-5.09182400	-1.07810300	-2.50630500
C	-4.61782700	-2.59272200	-0.55803900
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H	-4.70875500	-0.27292200	-3.15051500
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H	-6.04220300	-0.73961800	-2.06532700
H	-3.91539300	-2.90350300	0.22946300
H	-5.57541600	-2.33292000	-0.08280800
H	-4.79914500	-3.46877800	-1.19825300
C	0.61144600	-2.83806800	-2.44948100
C	0.15303400	-3.77523400	-1.59654300
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H	0.49642700	-4.81047200	-1.62732300
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C	-0.89793900	-3.43764300	-0.62289000
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C	-0.53618100	-2.05840900	2.11529600
C	-1.84465400	-2.23688400	2.58686200
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C	0.30745600	-2.87956200	4.24059300
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C	1.63500900	0.30648600	0.45508300
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C	4.62729700	-1.63944900	-0.84186000
H	2.49626400	-1.87115500	-0.92854300
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H	6.25722100	0.94682900	0.68172900
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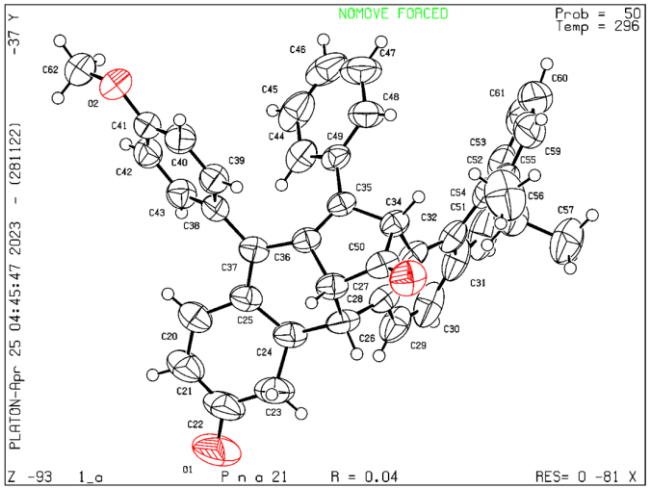
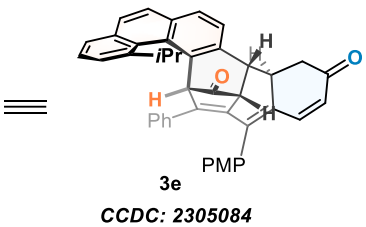
11. X-Ray Structure of 3e





3e

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h, k, lmax	14,16,35	14, 16, 35
Nref	8773 [4480]	8060
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Correction method = # Reported T Limits: Tmin = 0.674 Tmax = 0.746 AbsCorr = MULTI - SCAN

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12. Supplementary References

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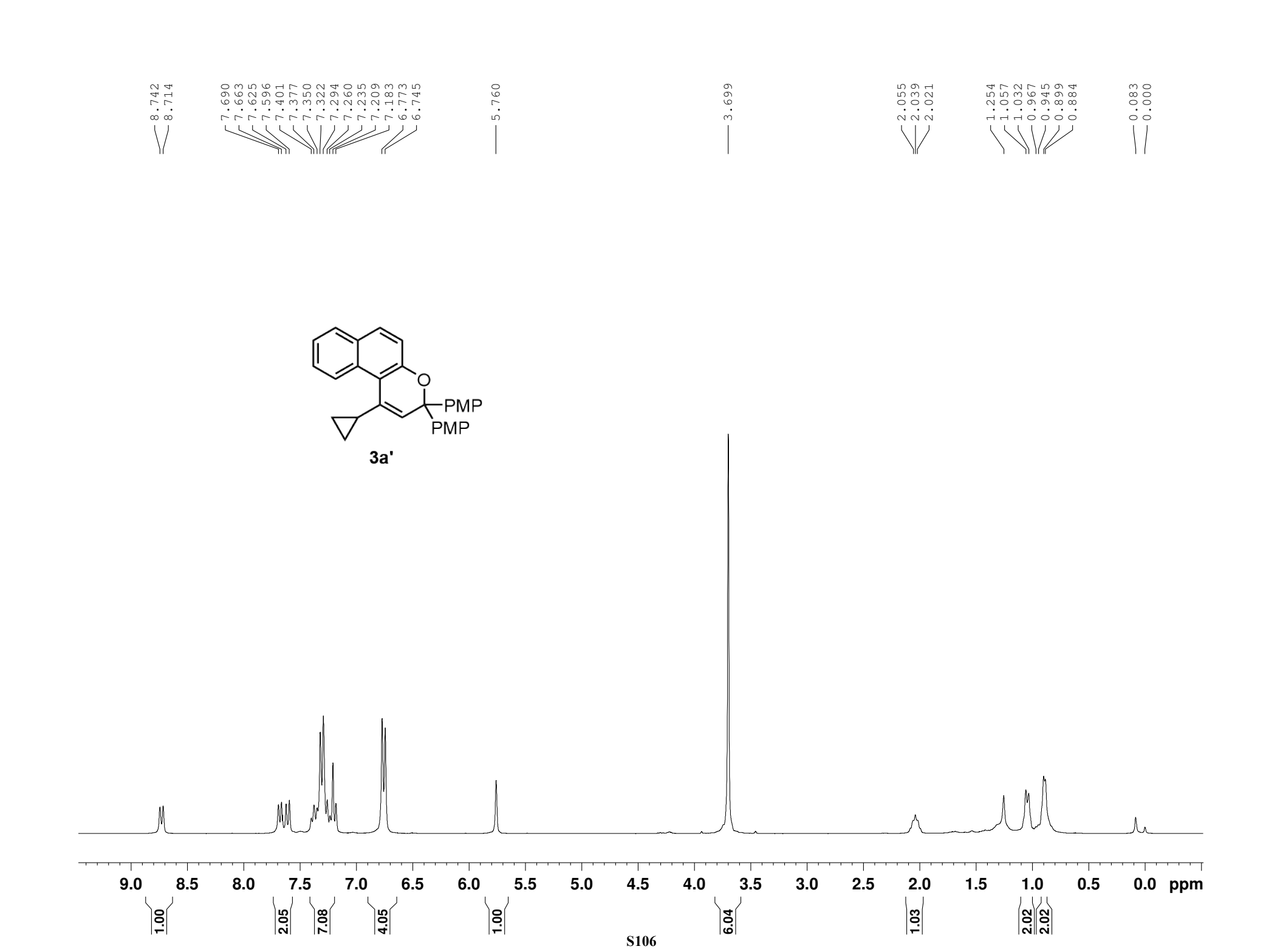
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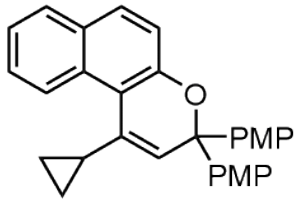

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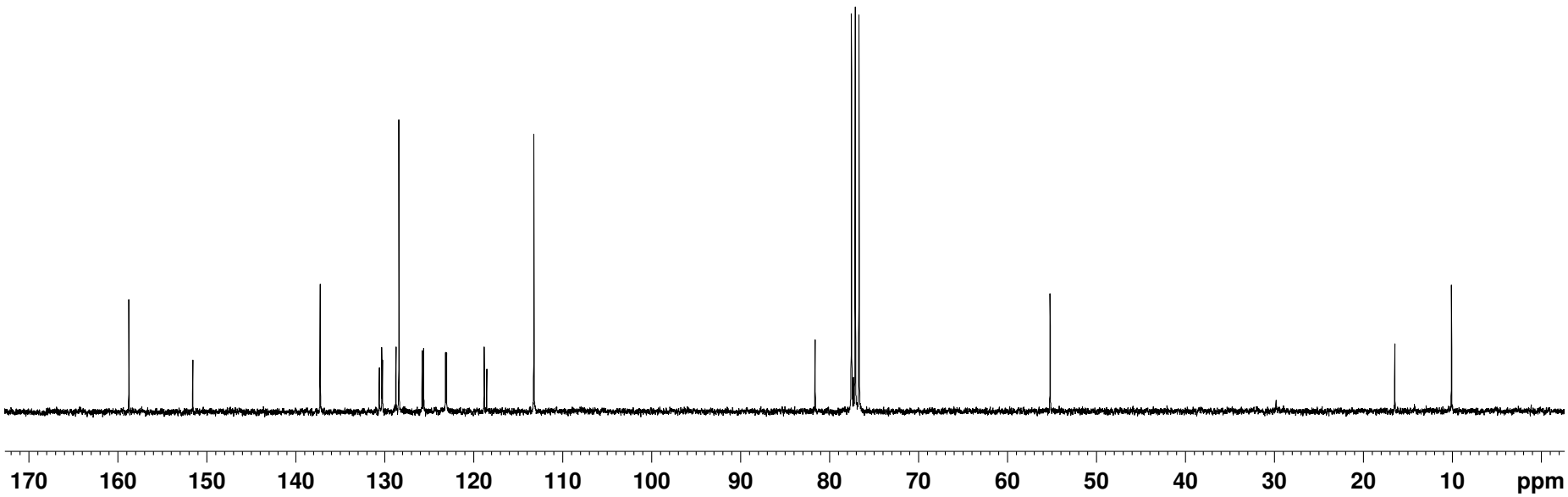

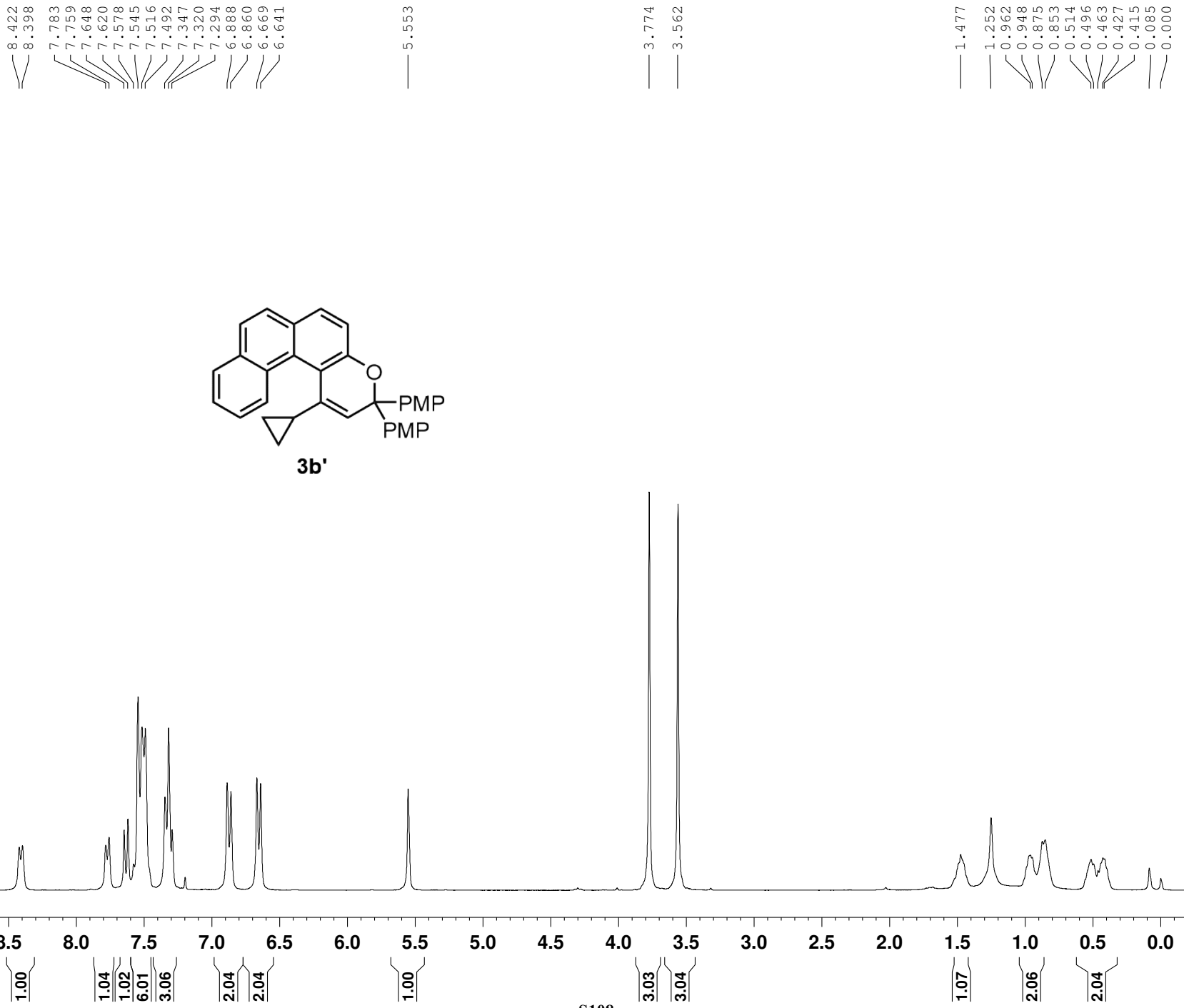
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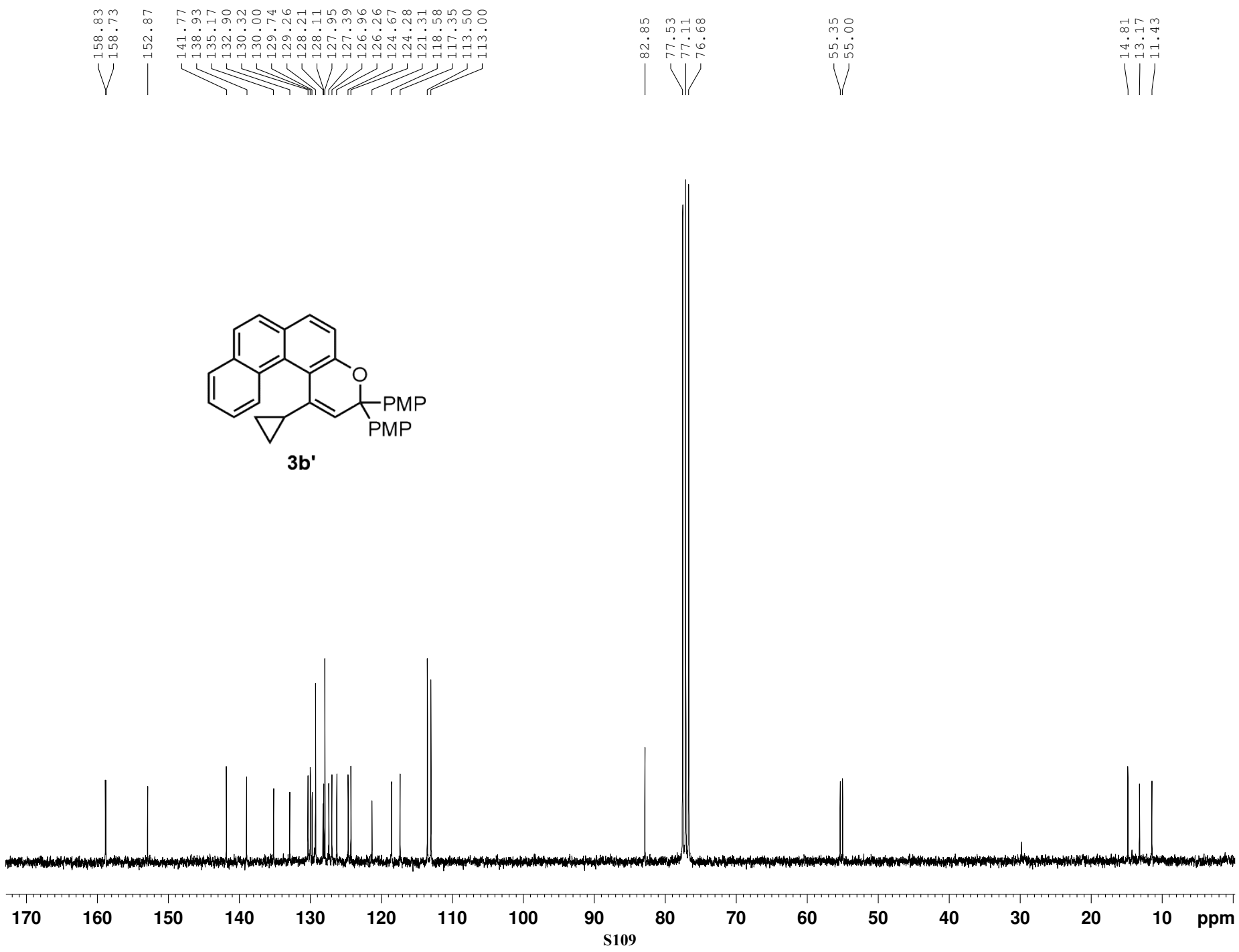
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55.00
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O
PMP
PMP
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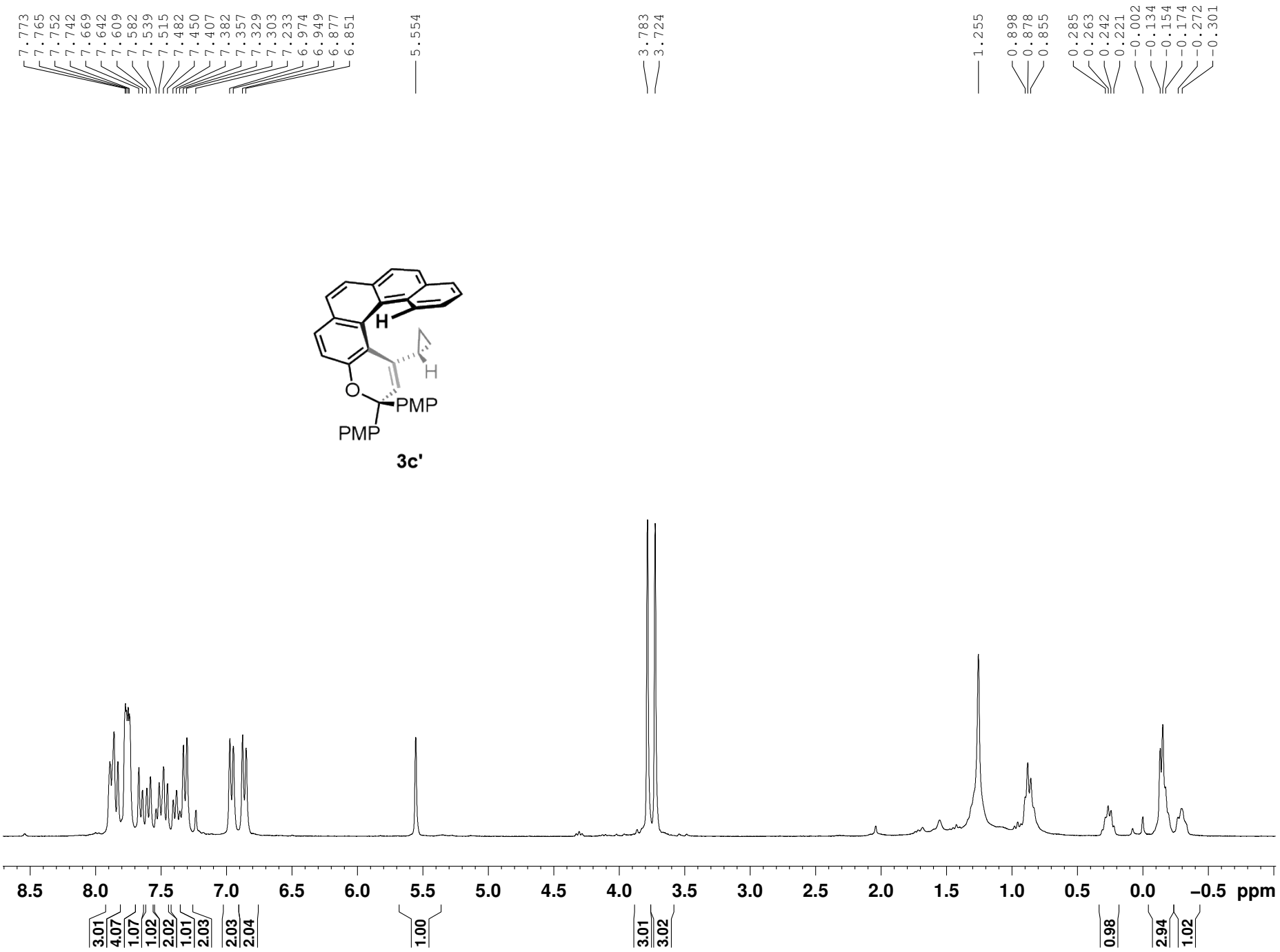
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7.407
7.382
7.357
7.329
7.303
7.233
6.974
6.949
6.877
6.851
5.554
3.783
3.724
1.255
0.898
0.878
0.855
0.285
0.263
0.242
0.221
-0.002
-0.134
-0.154
-0.174
-0.272
-0.301
H
H
O
PMP
PMP
3c'
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7.0
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6.0
5.5
5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
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1.07
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2.04
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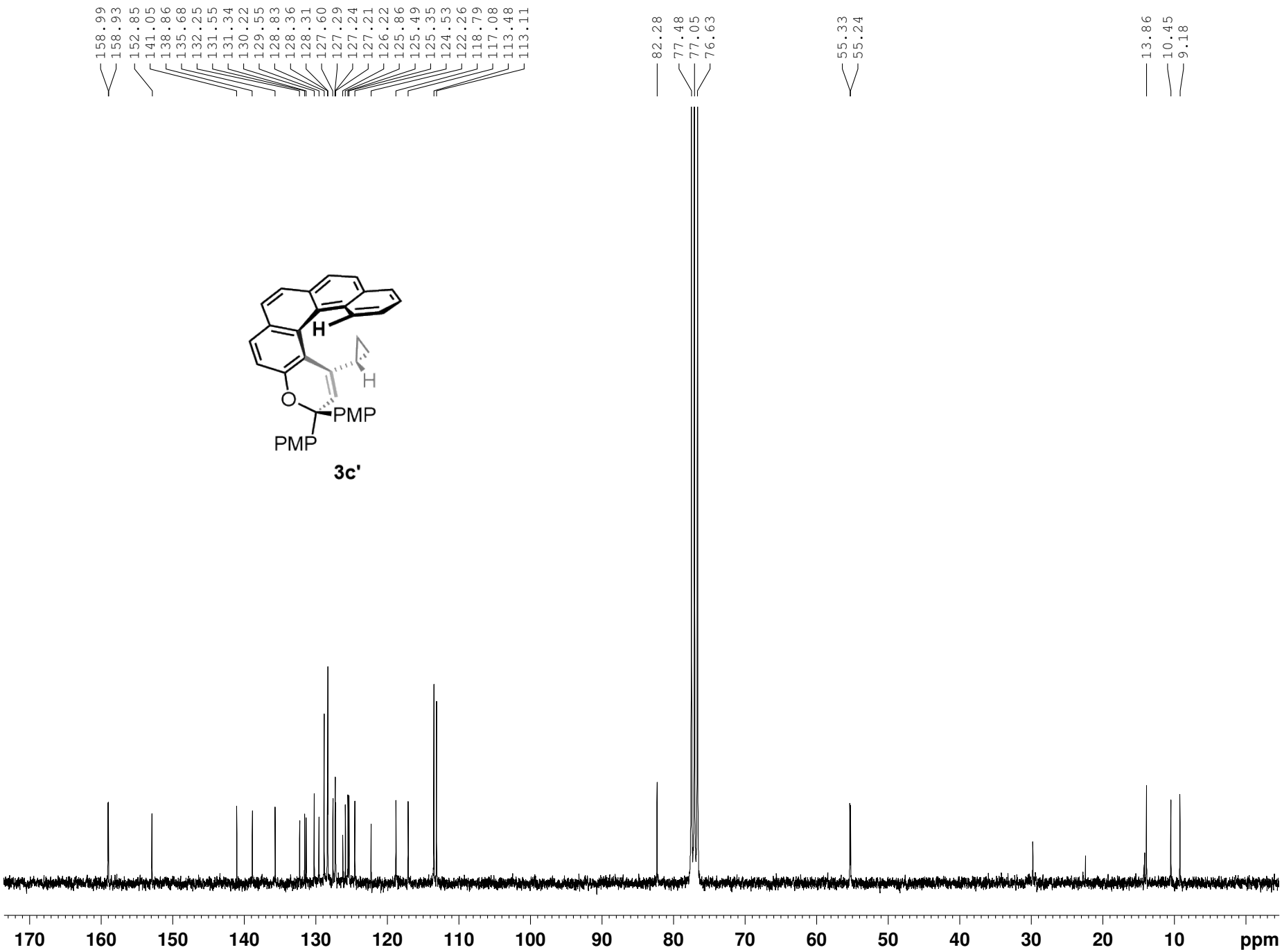
1.02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127.24
127.21
126.22
125.86
125.49
125.35
124.53
122.26
118.79
117.08
113.48
113.11
82.28
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77.05
76.63
55.33
55.24
13.86
10.45
9.18
H
H
O
PMP
PMP
3c'
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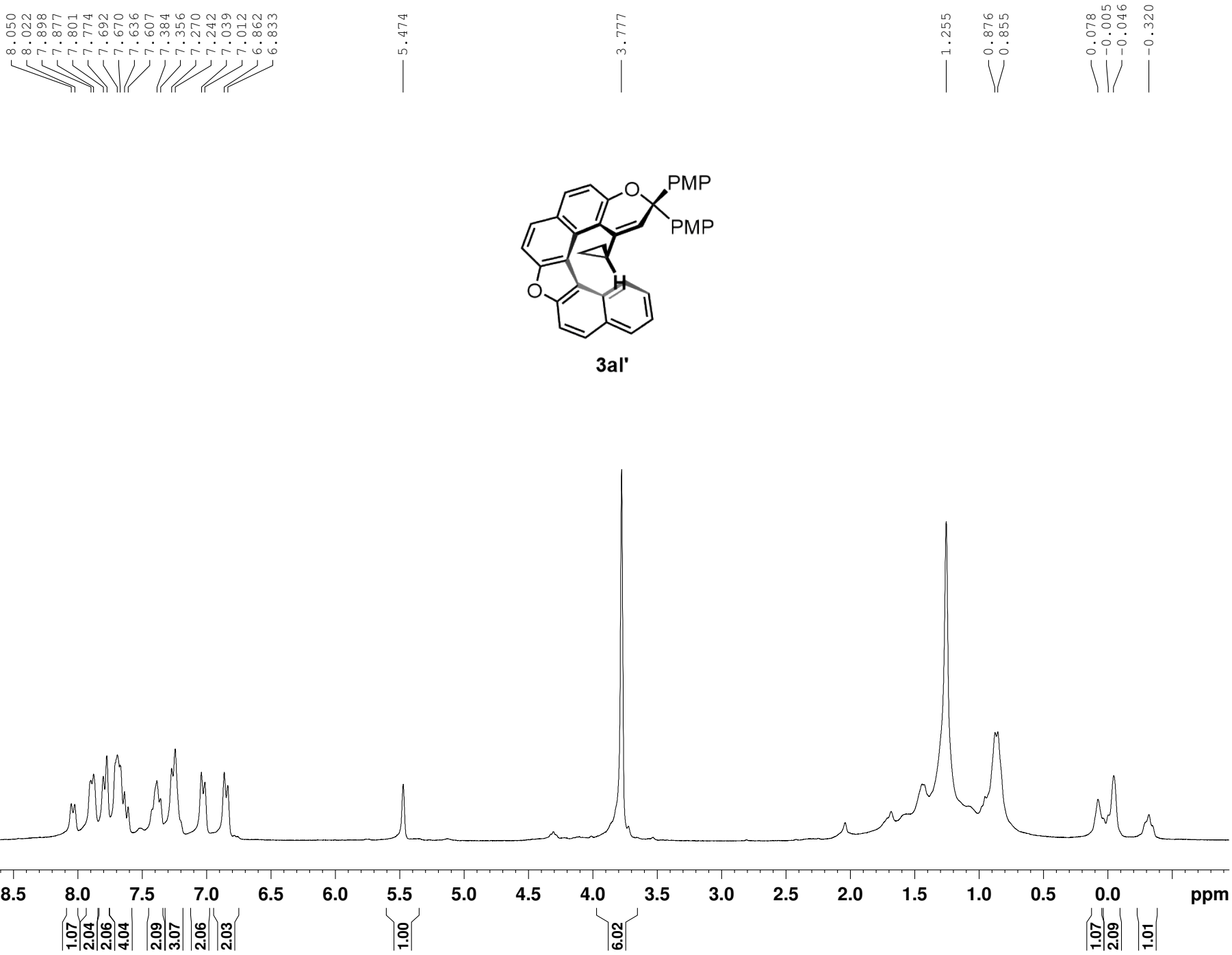
ppm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7.242
7.039
7.012
6.862
6.833
5.474
3.777
1.255
0.876
0.855
0.078
0.005
0.046
0.320
PMP
PMP
O
O
H
3al'
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
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4.04
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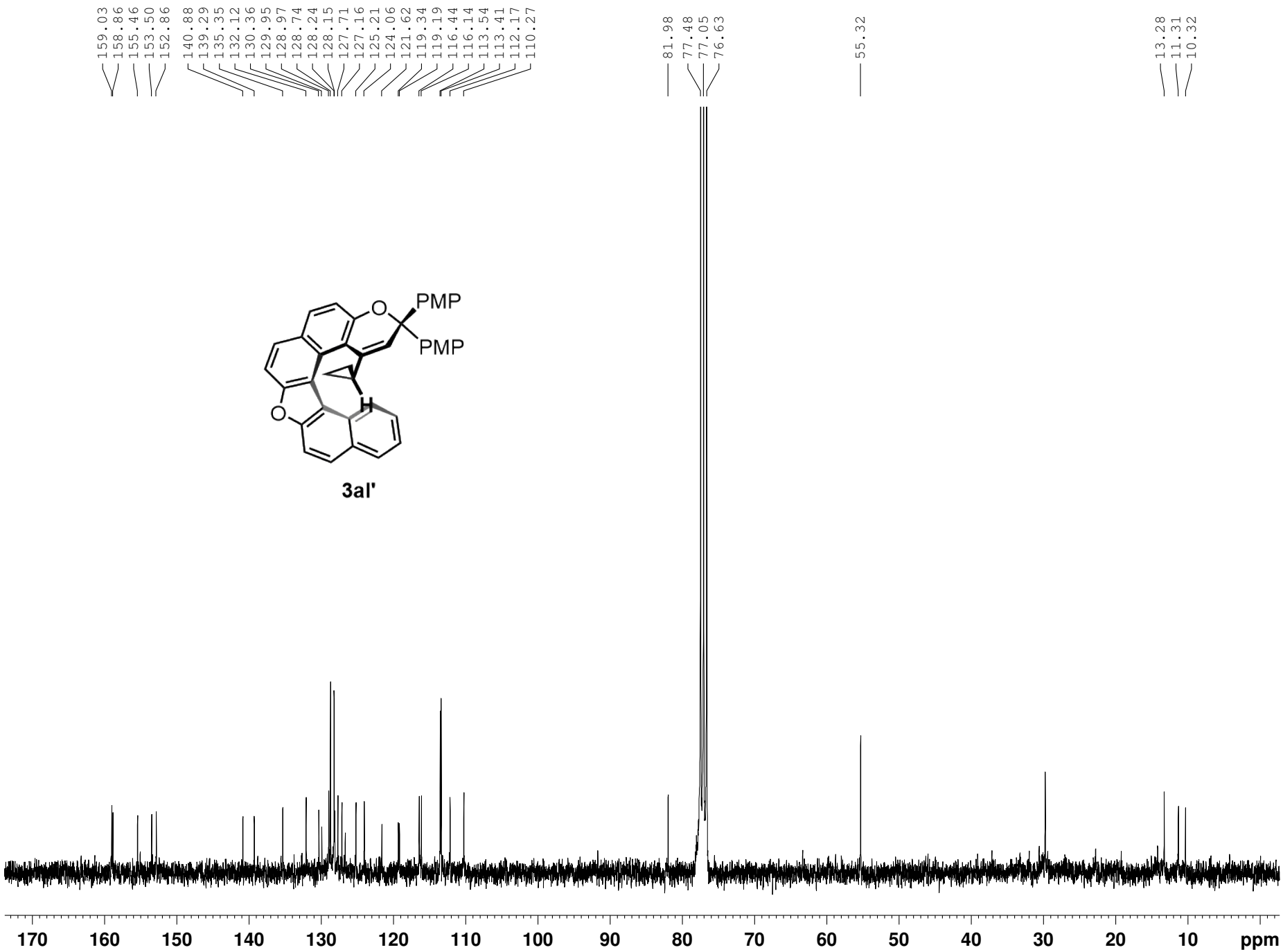
3.07
2.06
2.03
1.00
6.02
1.07
2.09
1.01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55.32
13.28
11.31
10.32
PMP
PMP
O
O
H
3al'
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120
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40
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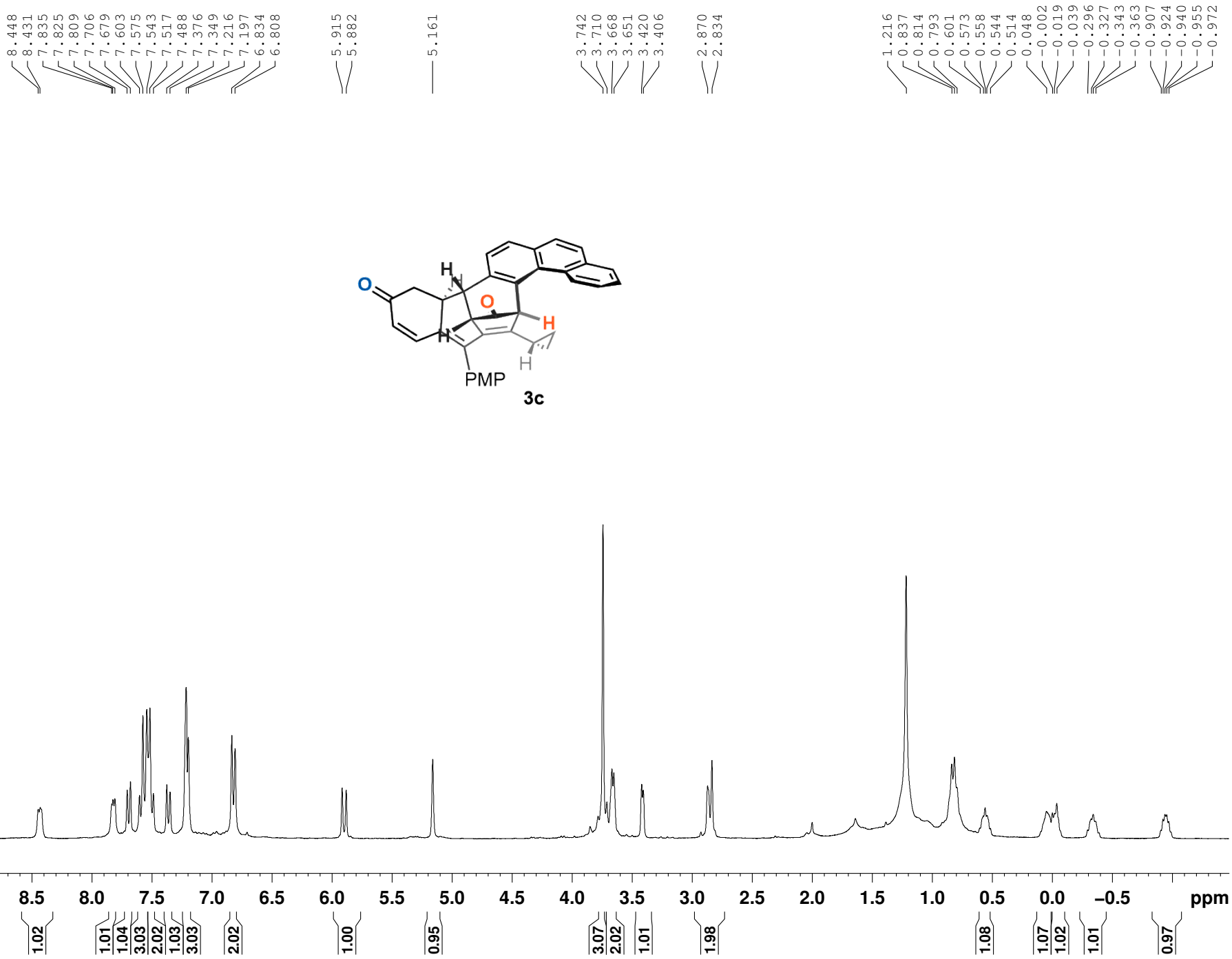
ppm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7.376
7.349
7.216
7.197
6.834
6.808
5.915
5.882
5.161
3.742
3.710
3.668
3.651
3.420
3.406
2.870
2.834
1.216
0.837
0.814
0.793
0.601
0.573
0.558
0.544
0.514
0.048
-0.002
-0.019
-0.039
-0.296
-0.327
-0.343
-0.363
-0.907
-0.924
-0.940
-0.955
-0.972
O
H
O
H
H
H
PMP
3c
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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
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0.0
−0.5
ppm
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1.01
1.04
3.03
2.02
1.03
3.03
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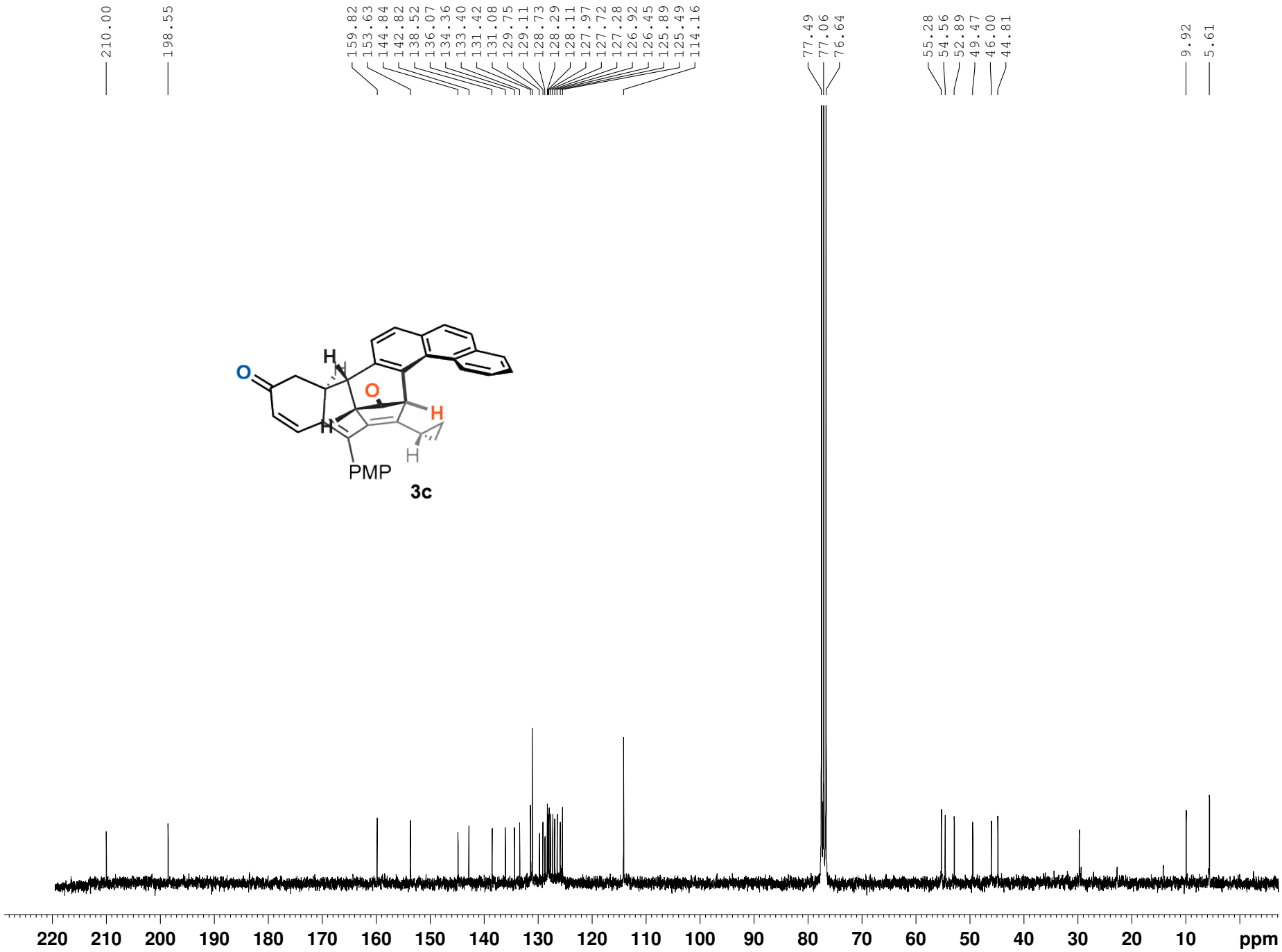
1.98
1.08
1.07
1.02
1.01
0.97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131.42
131.08
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128.73
128.29
128.11
127.97
127.72
127.28
126.92
126.45
125.89
125.49
114.16
77.49
77.06
76.64
55.28
54.56
52.89
49.47
46.00
44.81
9.92
5.61
O
H
O
H
H
H
PMP
220
210
200
190
180
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140
130
120
110
100
90
80
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60
50
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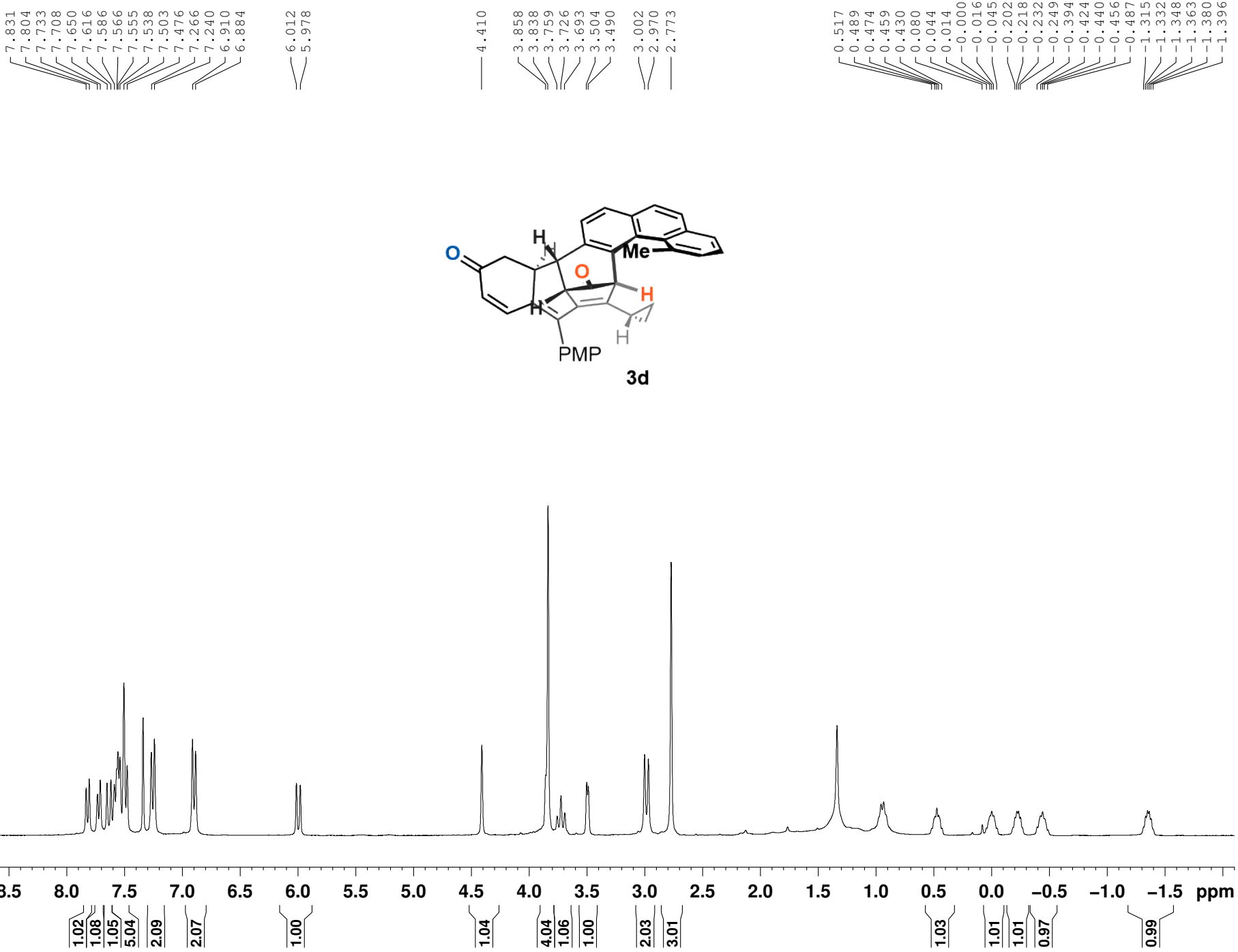
30
20
10
ppm

3c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7.555
7.538
7.503
7.476
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7.240
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6.012
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3.759
3.726
3.693
3.504
3.490
3.002
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0.474
0.459
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0.080
0.044
0.014
-0.000
-0.016
-0.045
-0.202
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-0.249
-0.394
-0.424
-0.440
-0.456
-0.487
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-1.332
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-1.363
-1.380
-1.396
O
H
H
Me
O
H
H
H
PMP
3d
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6.5
6.0
5.5
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4.5
4.0
3.5
3.0
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2.0
1.5
1.0
0.5
0.0
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−1.0
−1.5
ppm
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1.08
1.05
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2.09
2.07
1.00
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4.04
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1.00
2.03
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1.03
1.01
1.01
0.97
0.99

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131.63
131.00
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128.95
128.85
128.67
128.22
127.15
127.08
126.65
125.84
125.68
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45.07
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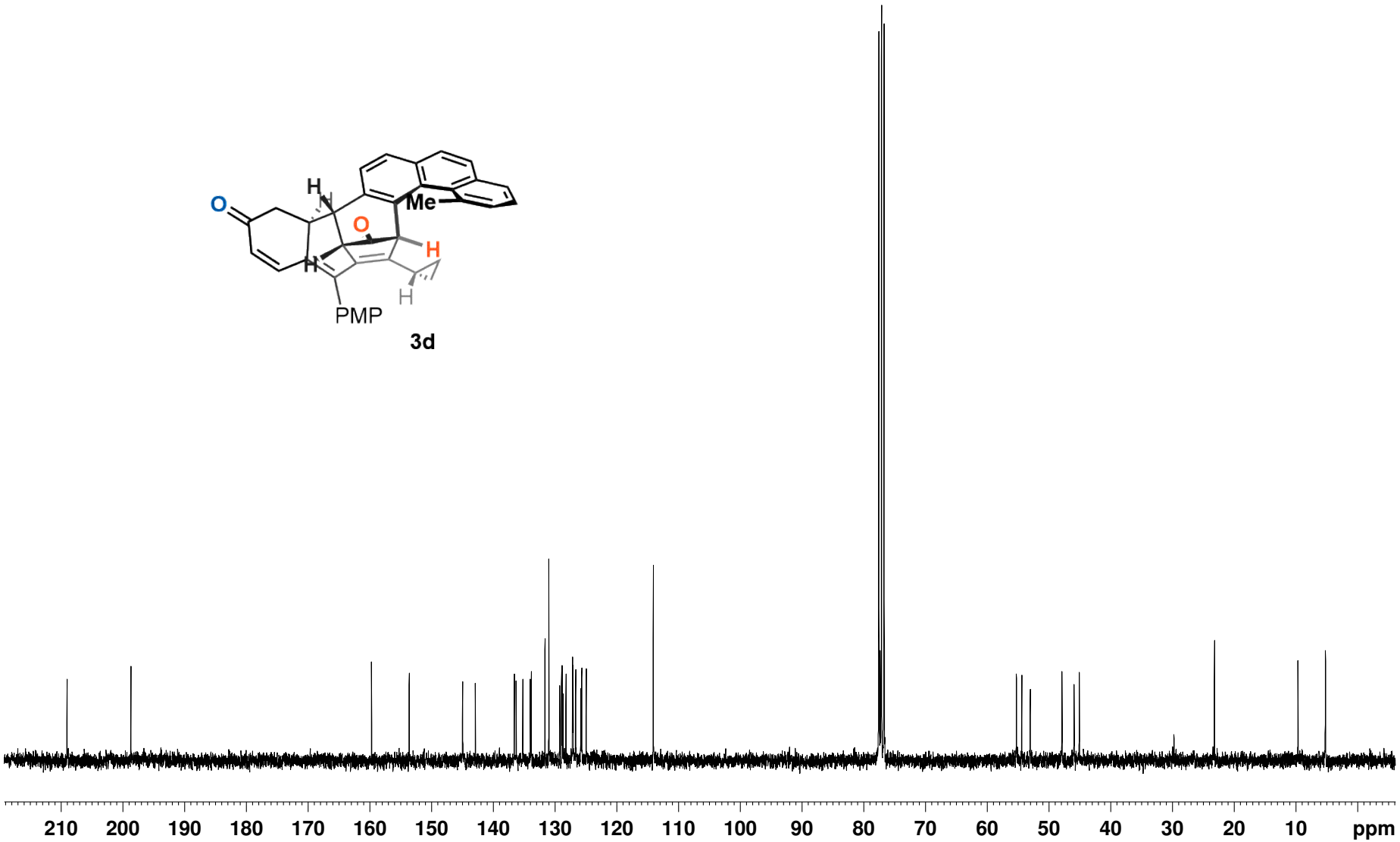
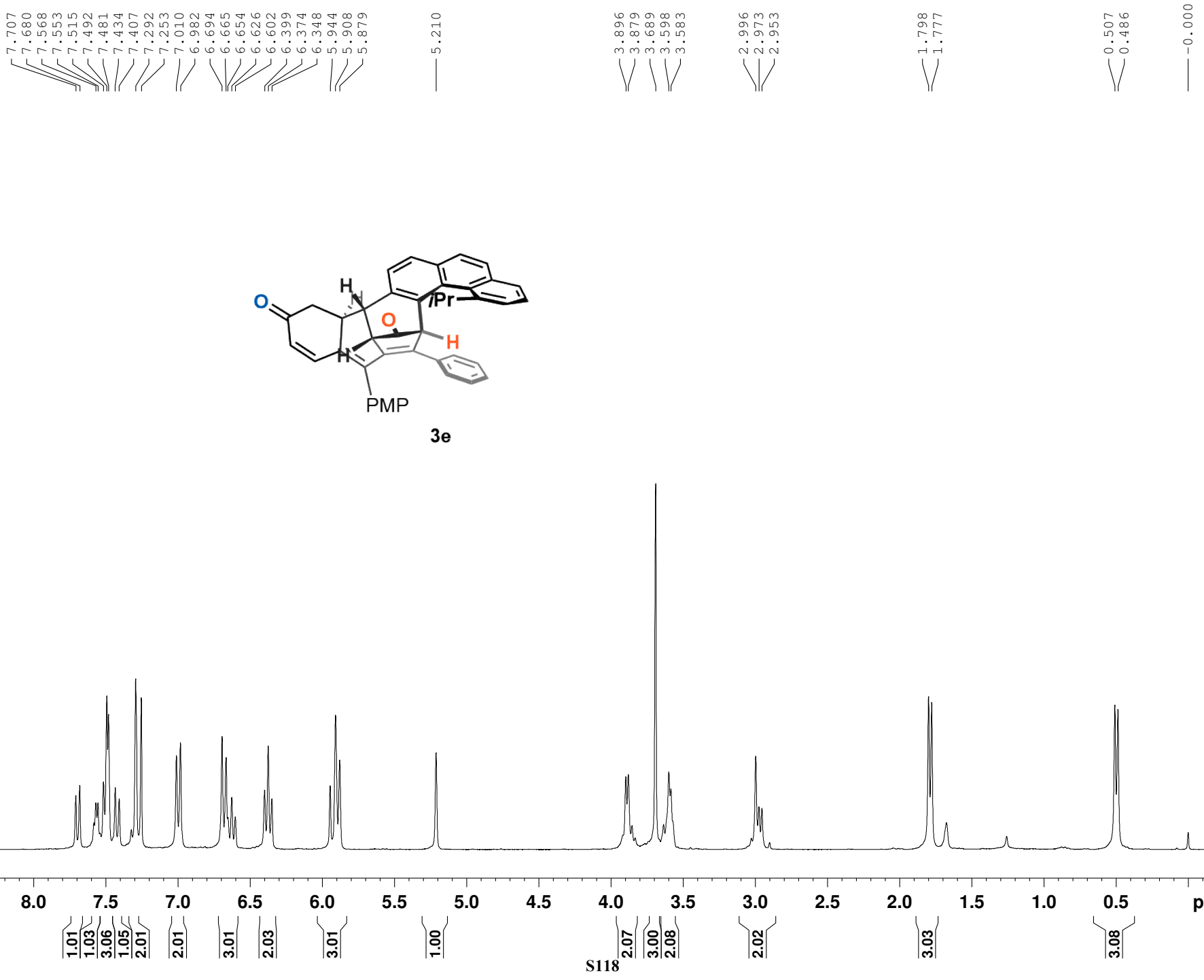
9.65
5.21

3d

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7.253
7.010
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6.694
6.665
6.654
6.626
6.602
6.399
6.374
6.348
5.944
5.908
5.879
5.210
3.896
3.879
3.689
3.598
3.583
2.996
2.973
2.953
1.798
1.777
0.507
0.486
-0.000
O
H
H
O
iPr
H
PMP
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
ppm
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1.03
3.06
1.05
2.01
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3.01
2.03
3.01
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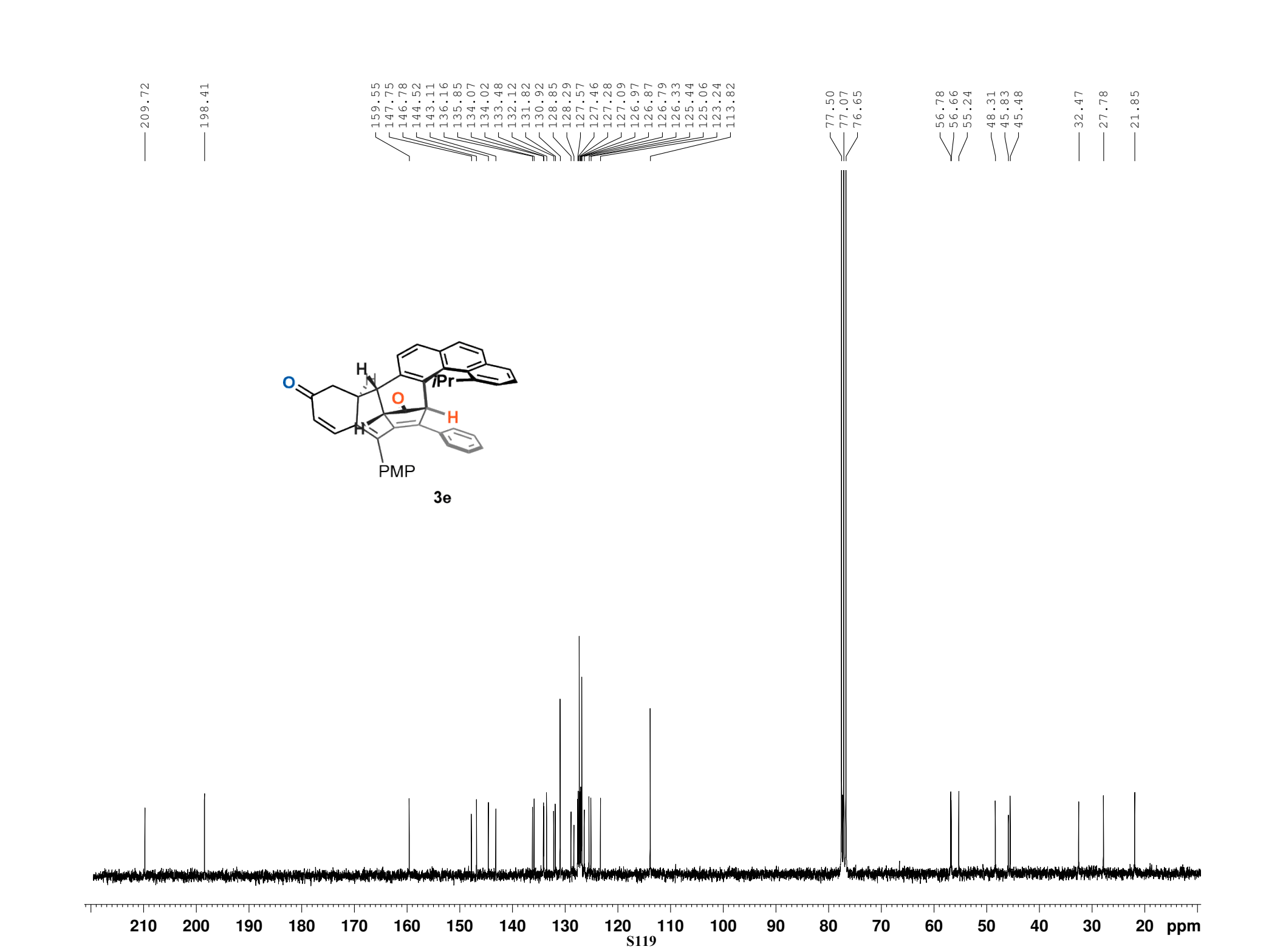
2.08
2.02
3.03
3.08

3e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130.92
128.85
128.29
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127.46
127.28
127.09
126.97
126.87
126.79
126.33
125.44
125.06
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77.50
77.07
76.65
56.78
56.66
55.24
48.31
45.83
45.48
32.47
27.78
21.85
O
H
iPr
O
H
H
PMP
3e
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200
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150
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120
110
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90
80
70
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50
40
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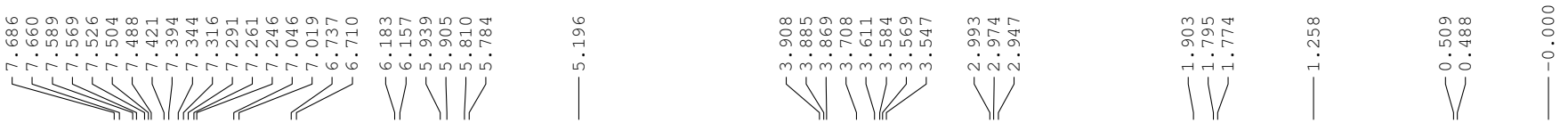
20
ppm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7.261
7.246
7.046
7.019
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6.710
6.183
6.157
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5.905
5.810
5.784
5.196
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3.885
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3.708
3.611
3.584
3.569
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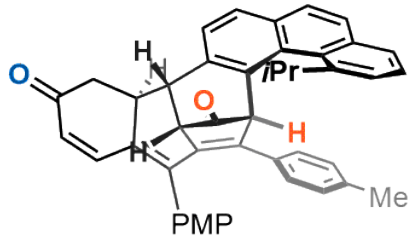
0.000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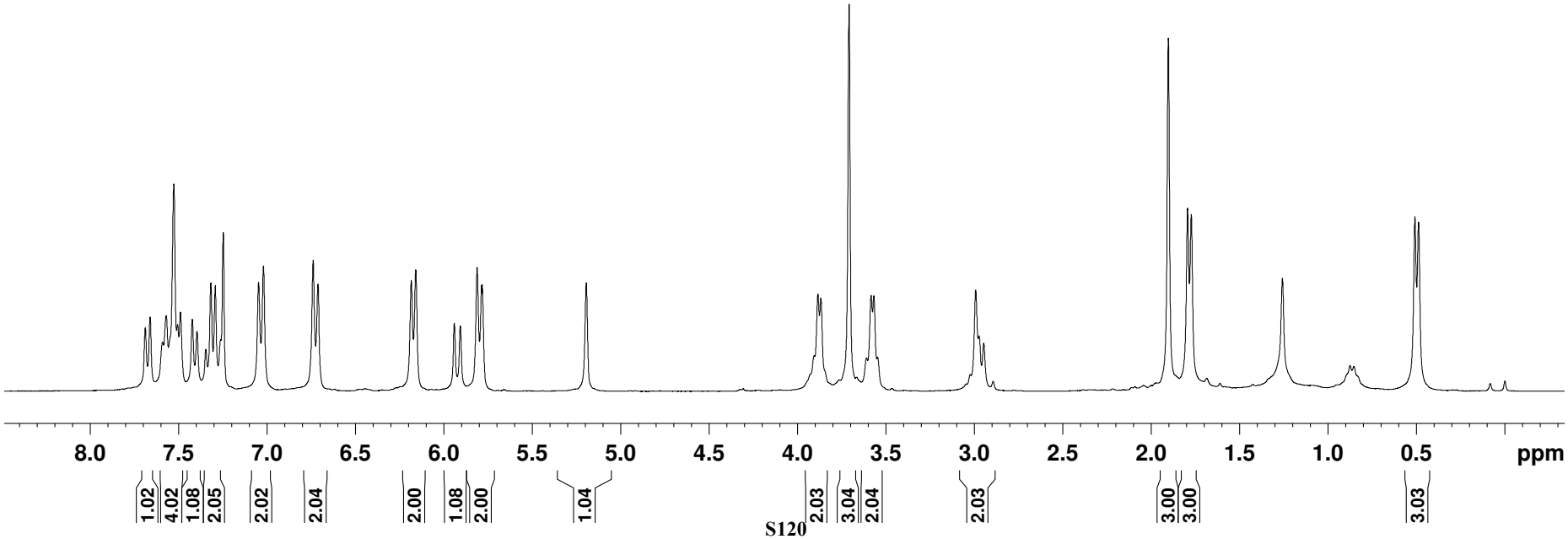
H
N
iPr
O
H
H
Me
PMP

3f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ppm
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2.02
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2.00
1.08
2.00
1.04
2.03
3.04
2.04
2.03
3.00
3.00
3.03

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136.19
136.04
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126.97
126.93
126.24
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77.10
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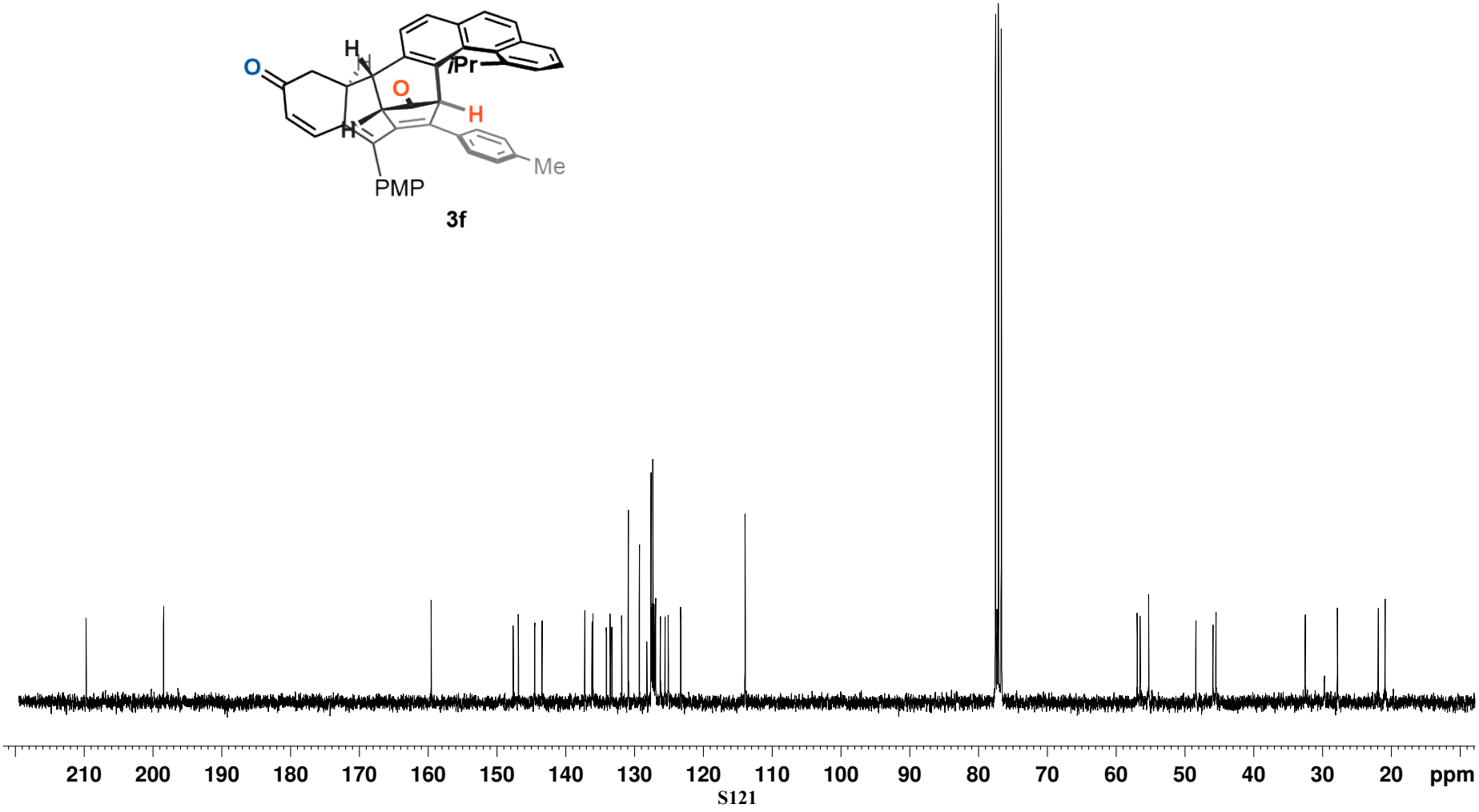
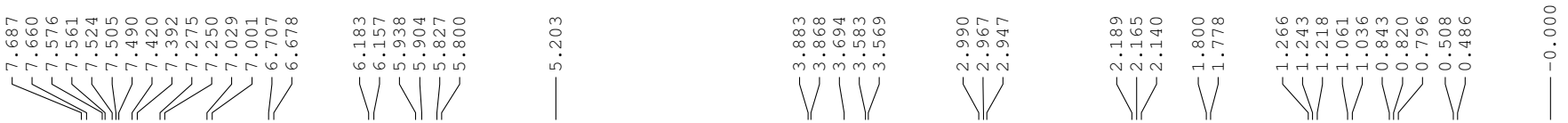
3f

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7.420
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7.275
7.250
7.029
7.001
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3.694
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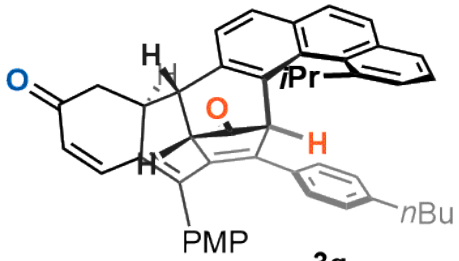
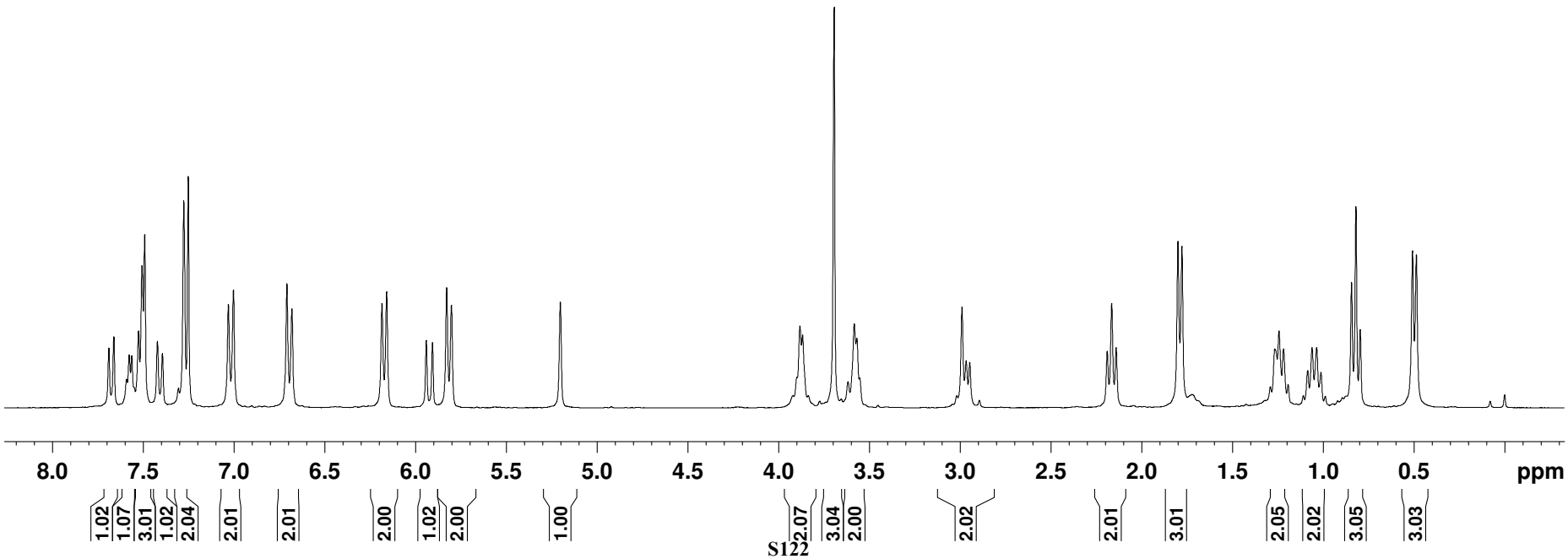

O
H
H
O
iPr
H
nBu
PMP

3g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0.5
ppm
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3.01
1.02
2.04
2.01
2.01
2.00
1.02
2.00
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2.07
3.04
2.00
2.02
2.01
3.01
2.05
2.02
3.05
3.03

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125.05
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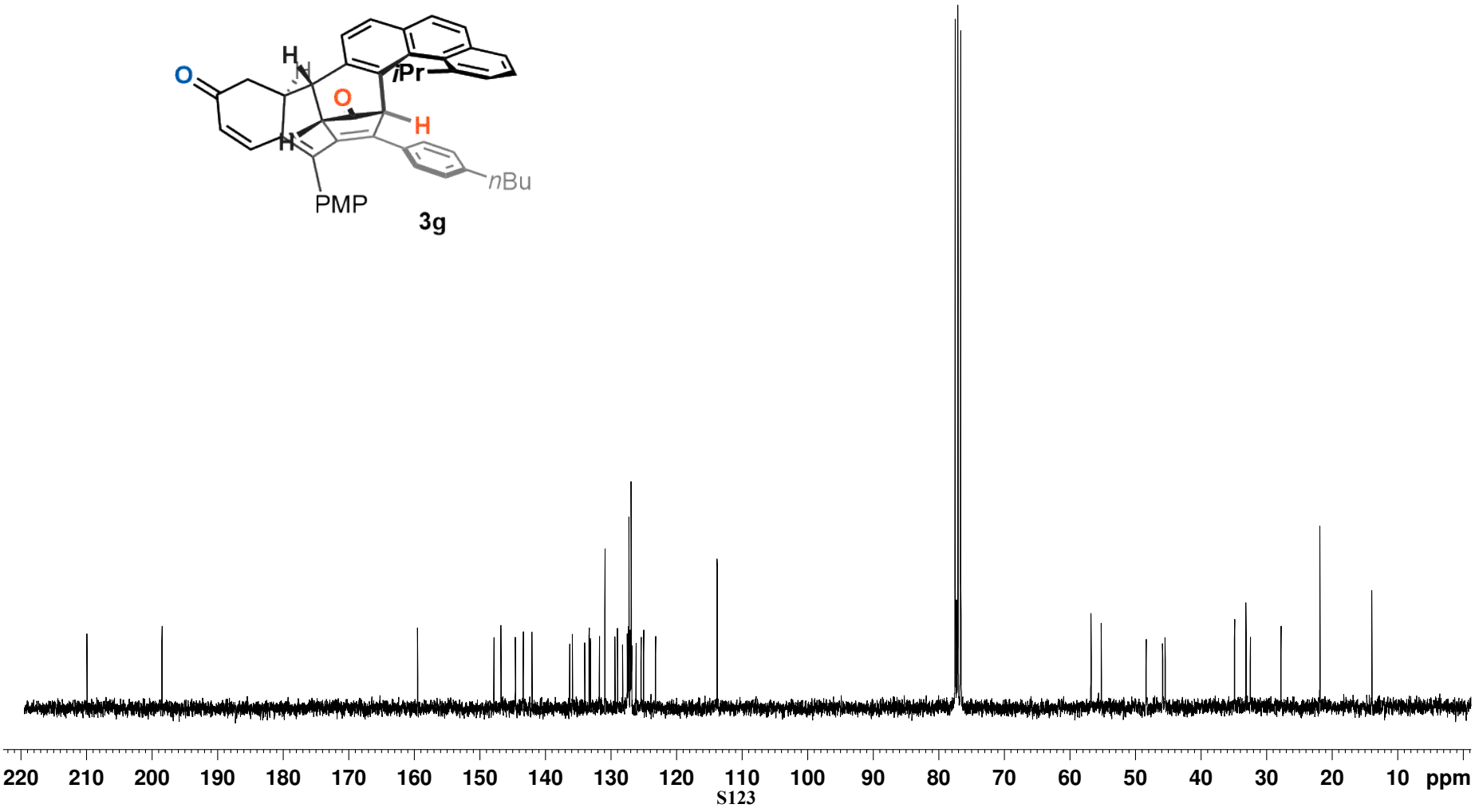
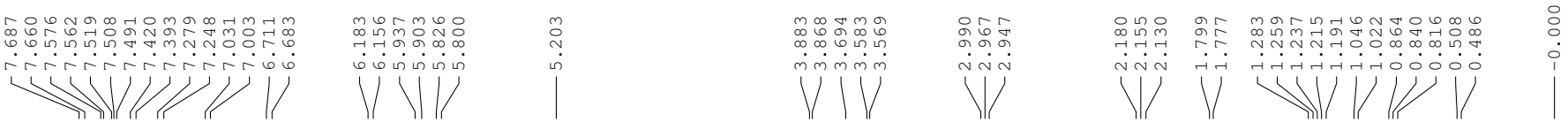
3g

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3.583
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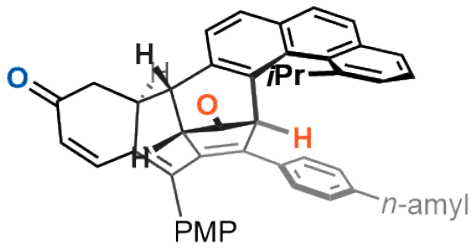
O
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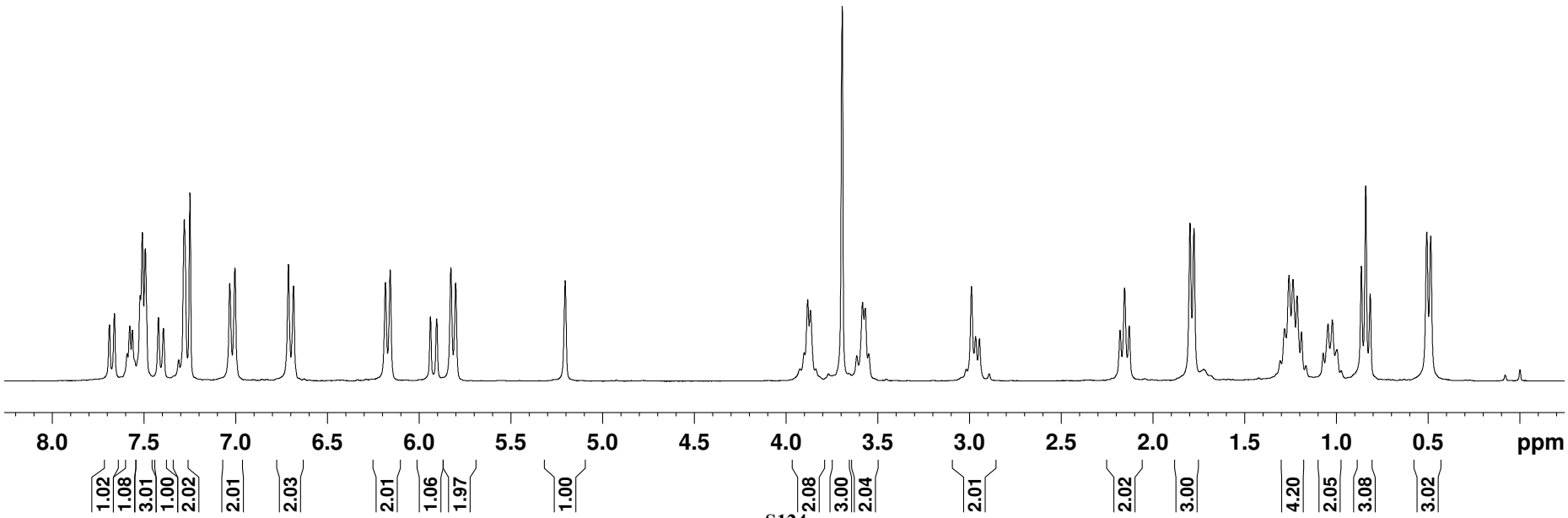
N
iPr
O
H
H
n-amyl
PMP

3h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1.0
0.5
ppm
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1.08
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1.00
2.02
2.01
2.03
2.01
1.06
1.97
1.00
2.08
3.00
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2.01
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3.02

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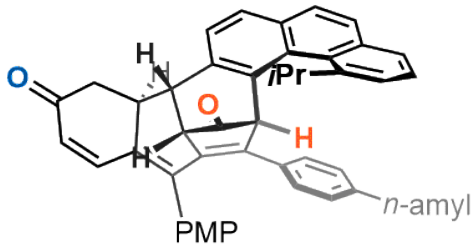

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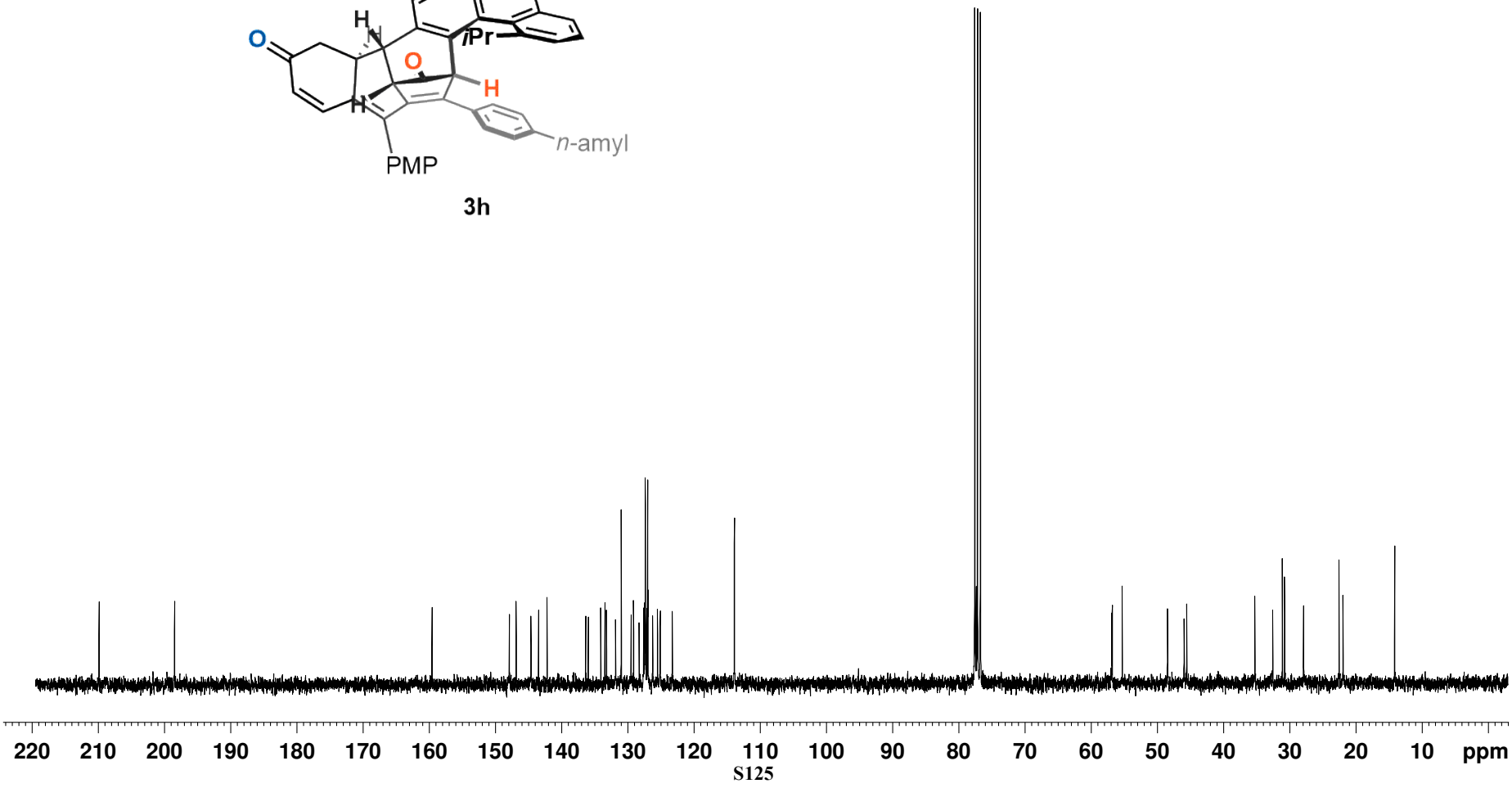

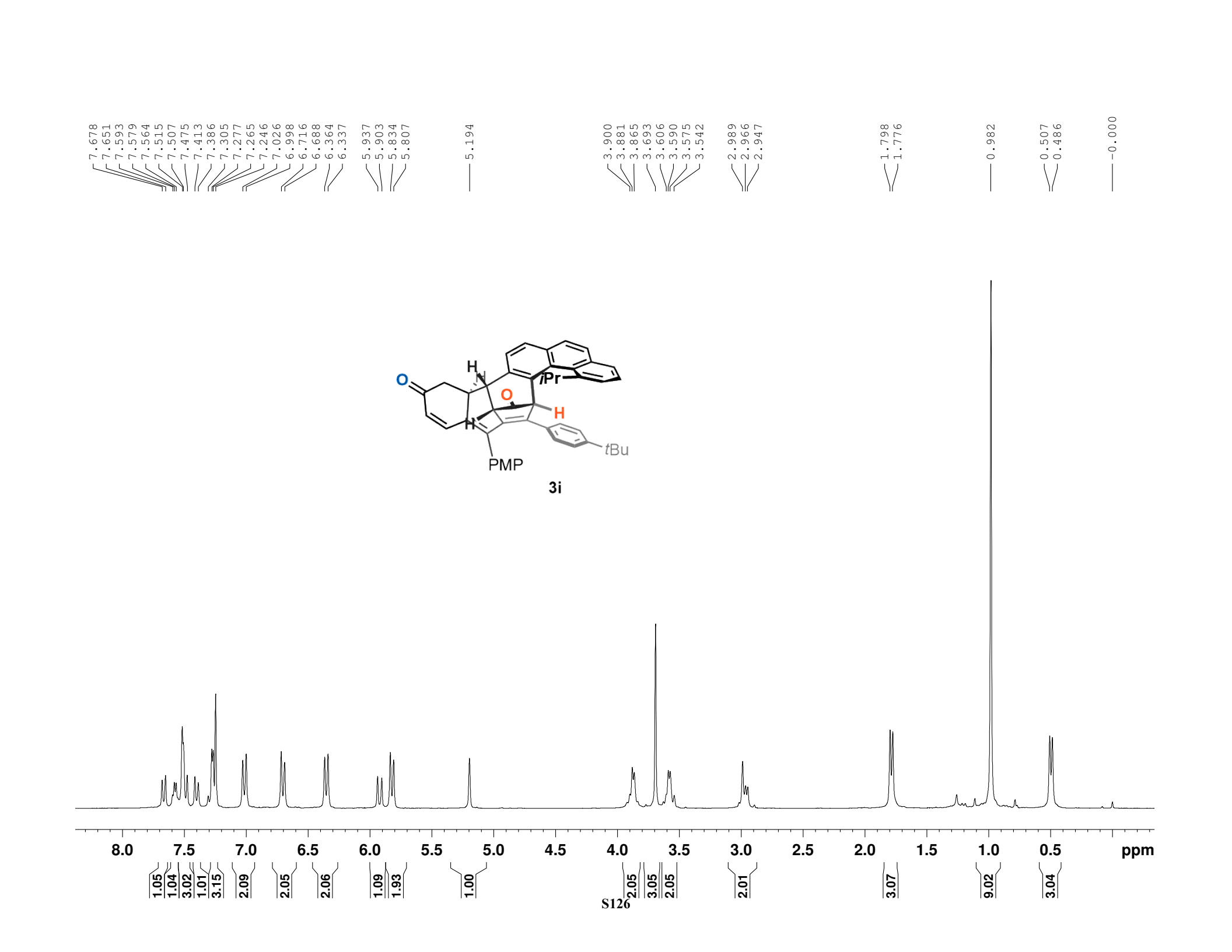
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H
O
H
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tBu
PMP
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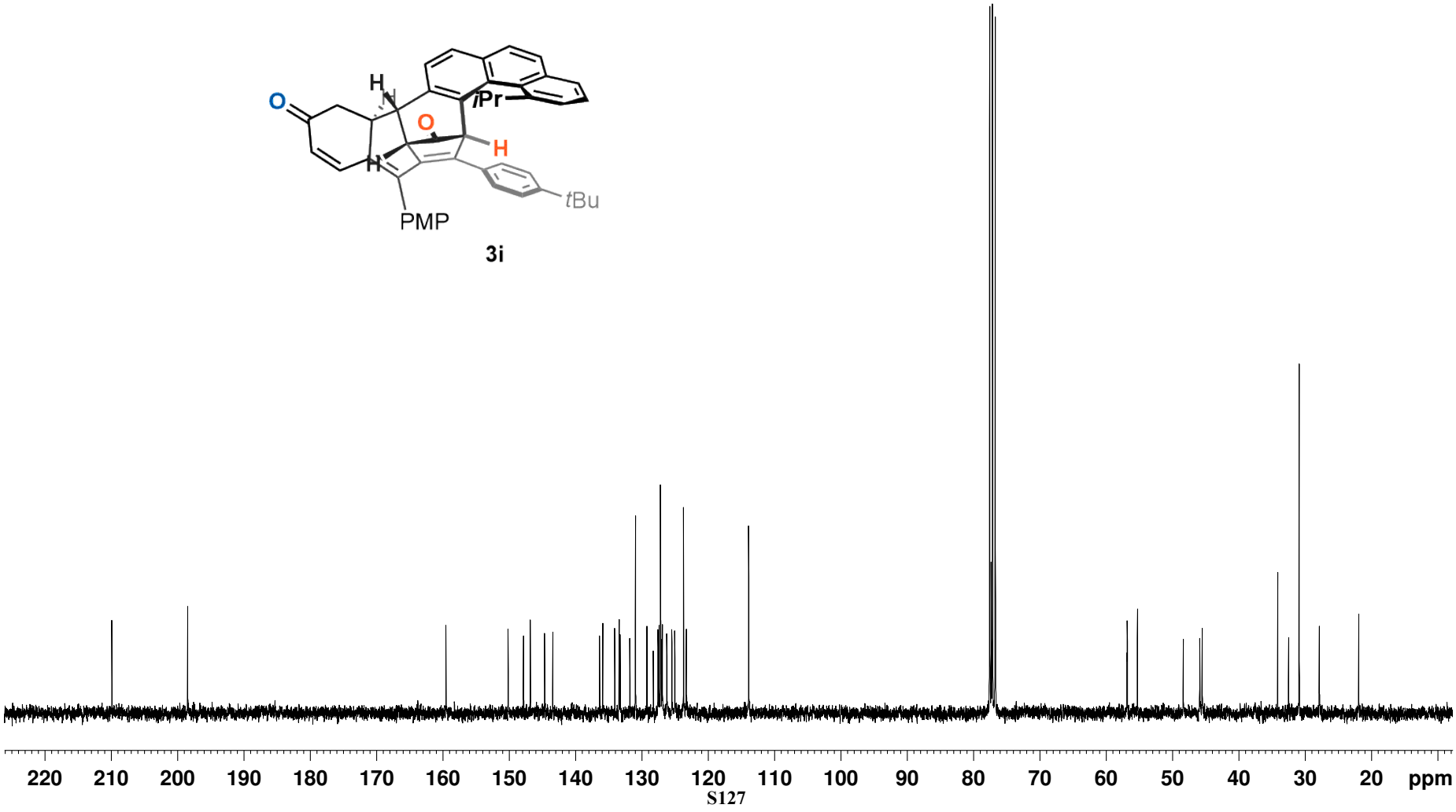

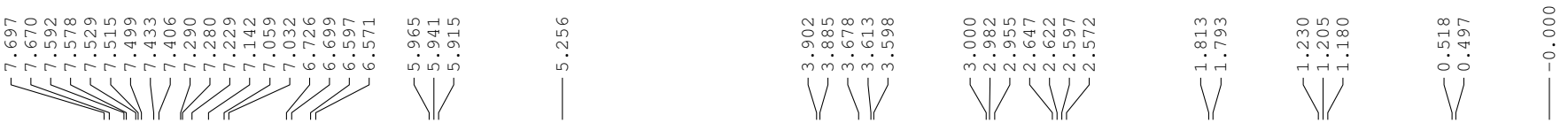
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3.598
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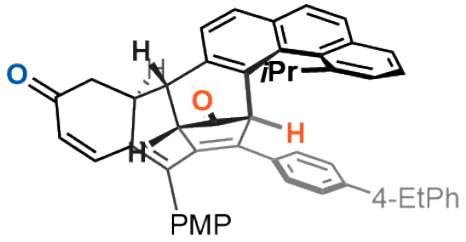
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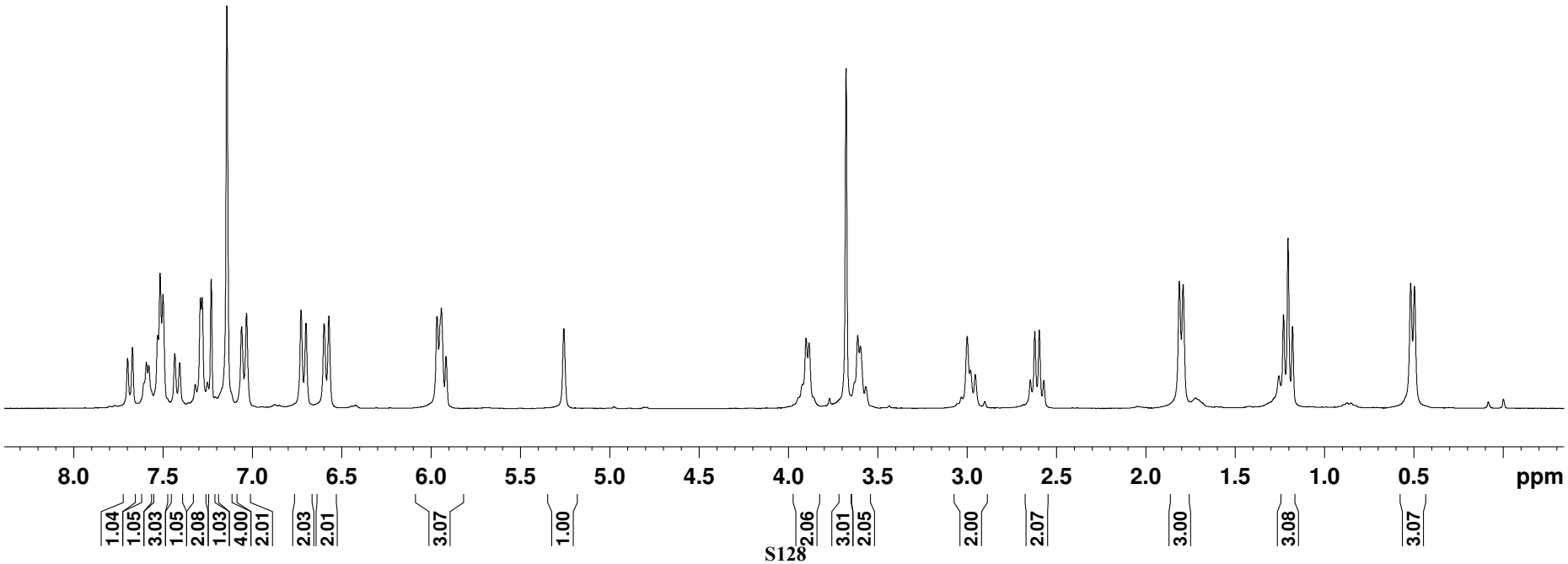
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3.08
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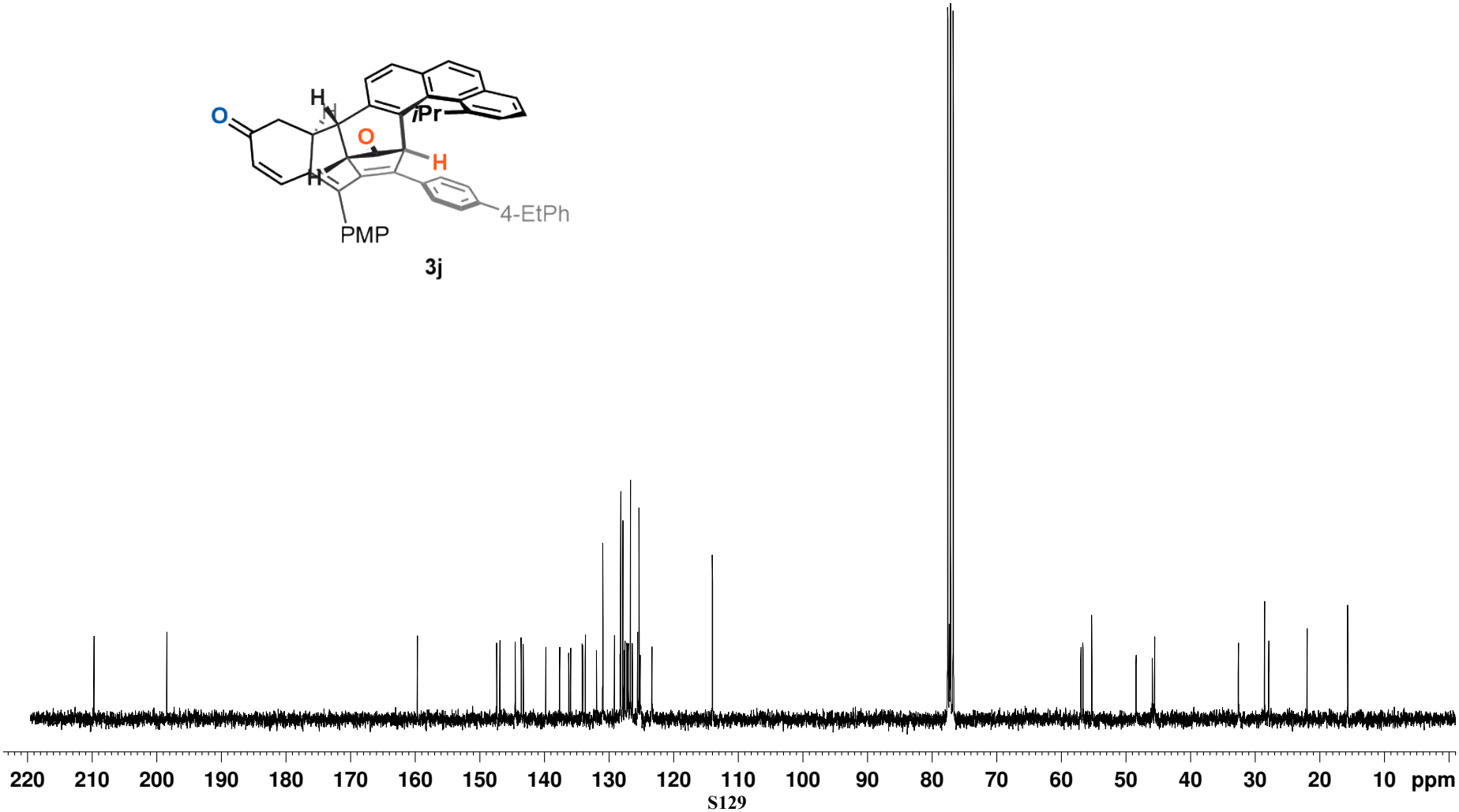
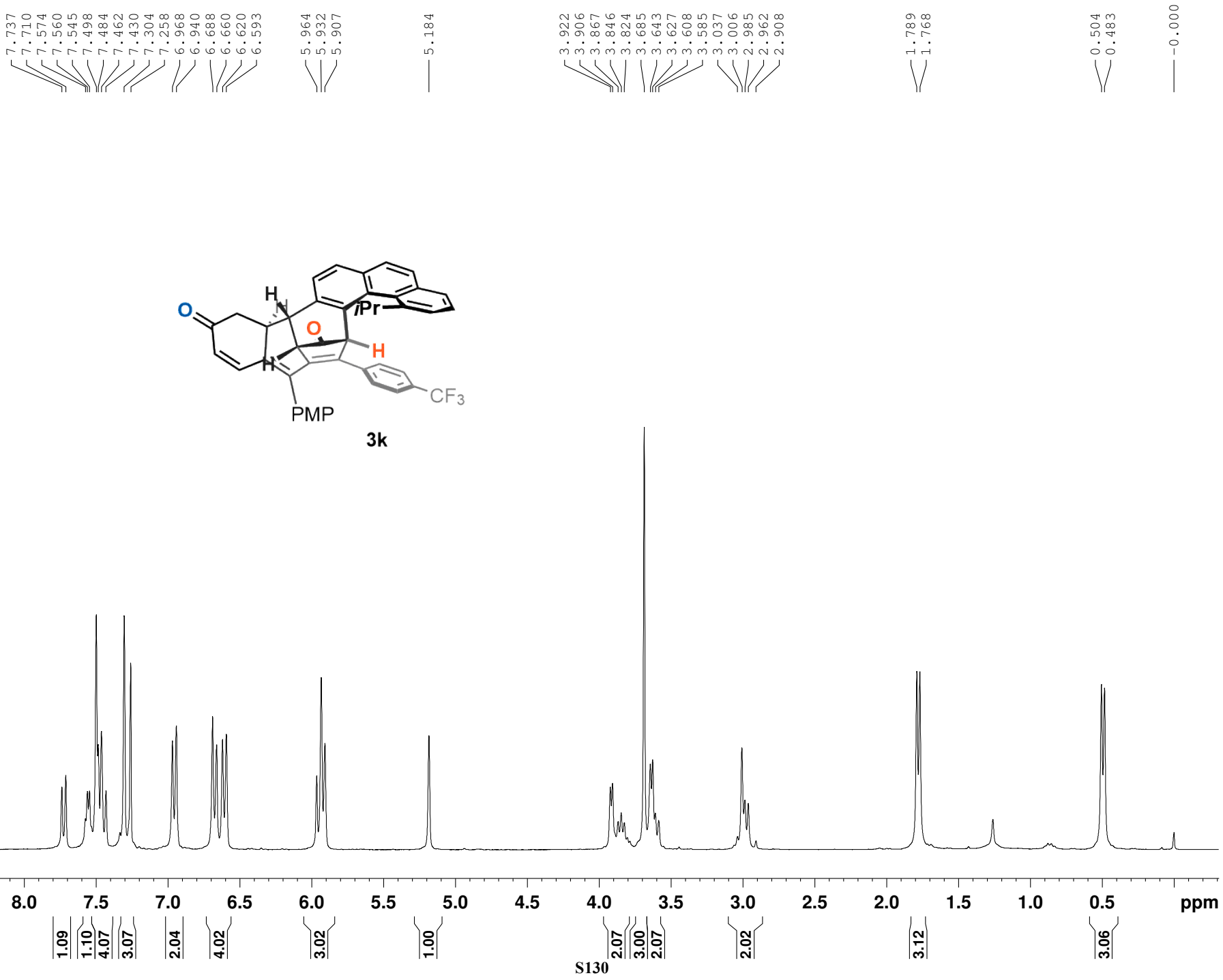
3j

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H
O
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H
H
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PMP
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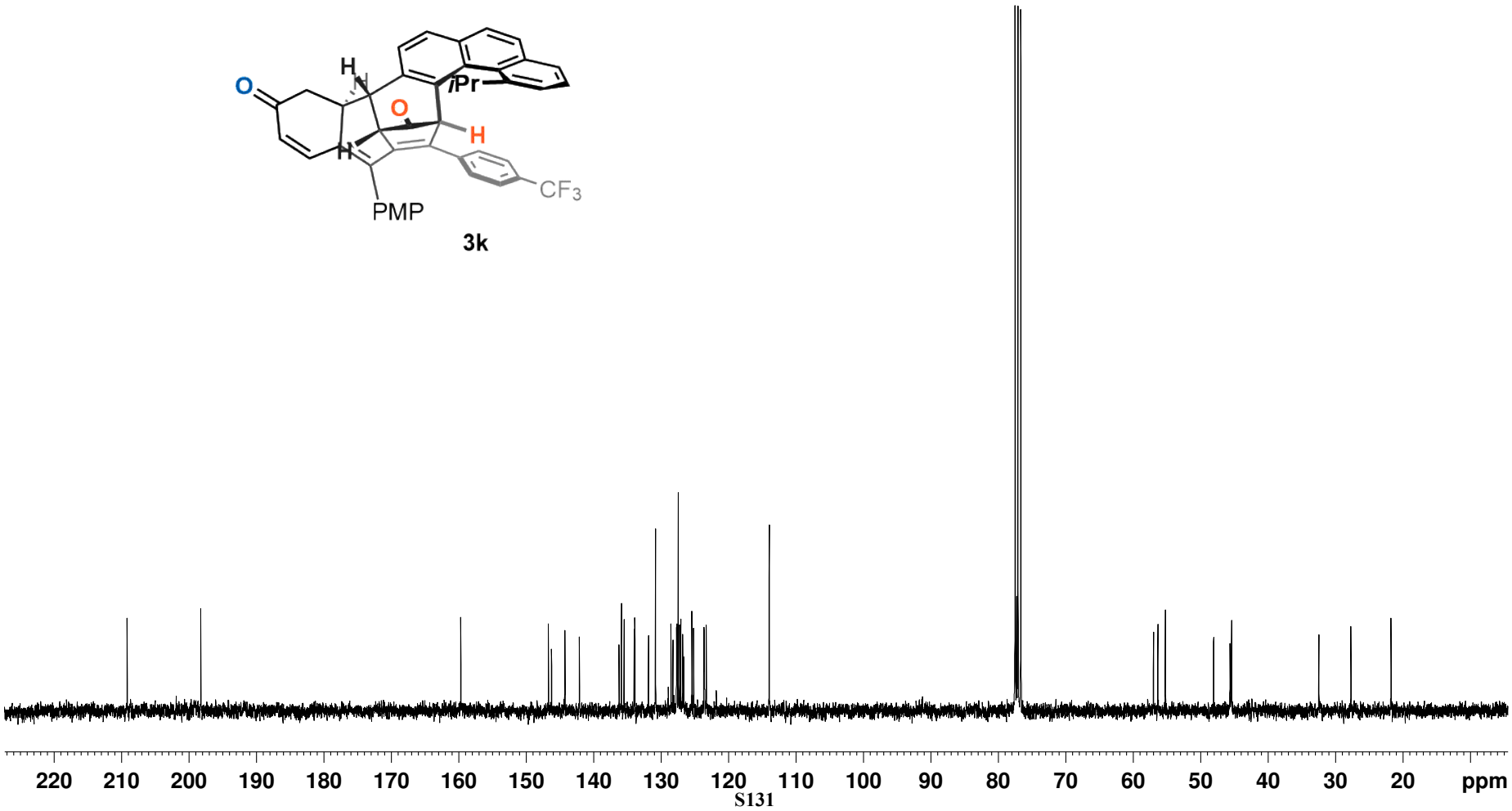

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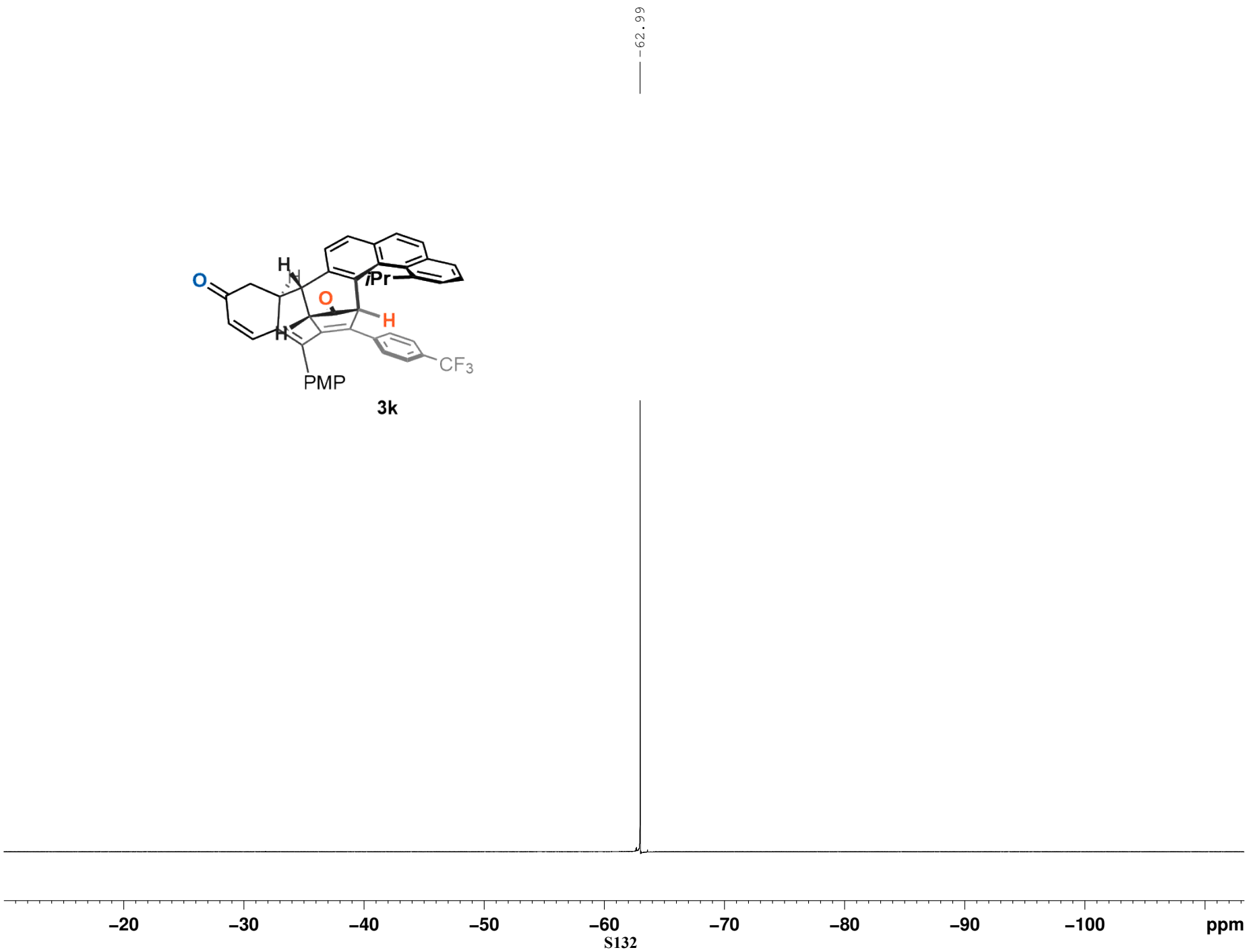

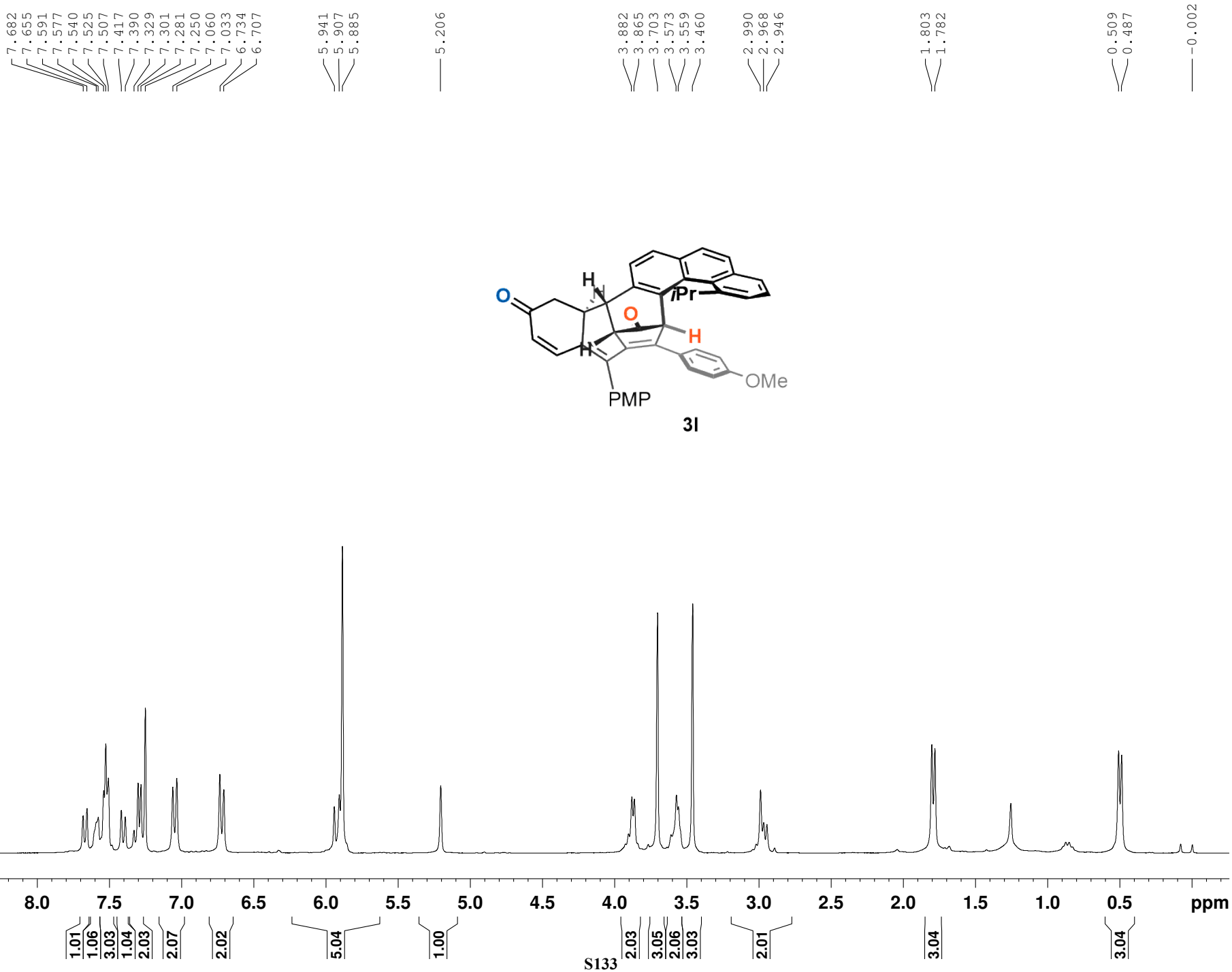
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6.707
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3.865
3.703
3.573
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2.968
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H
N
iPr
O
H
H
OMe
PMP
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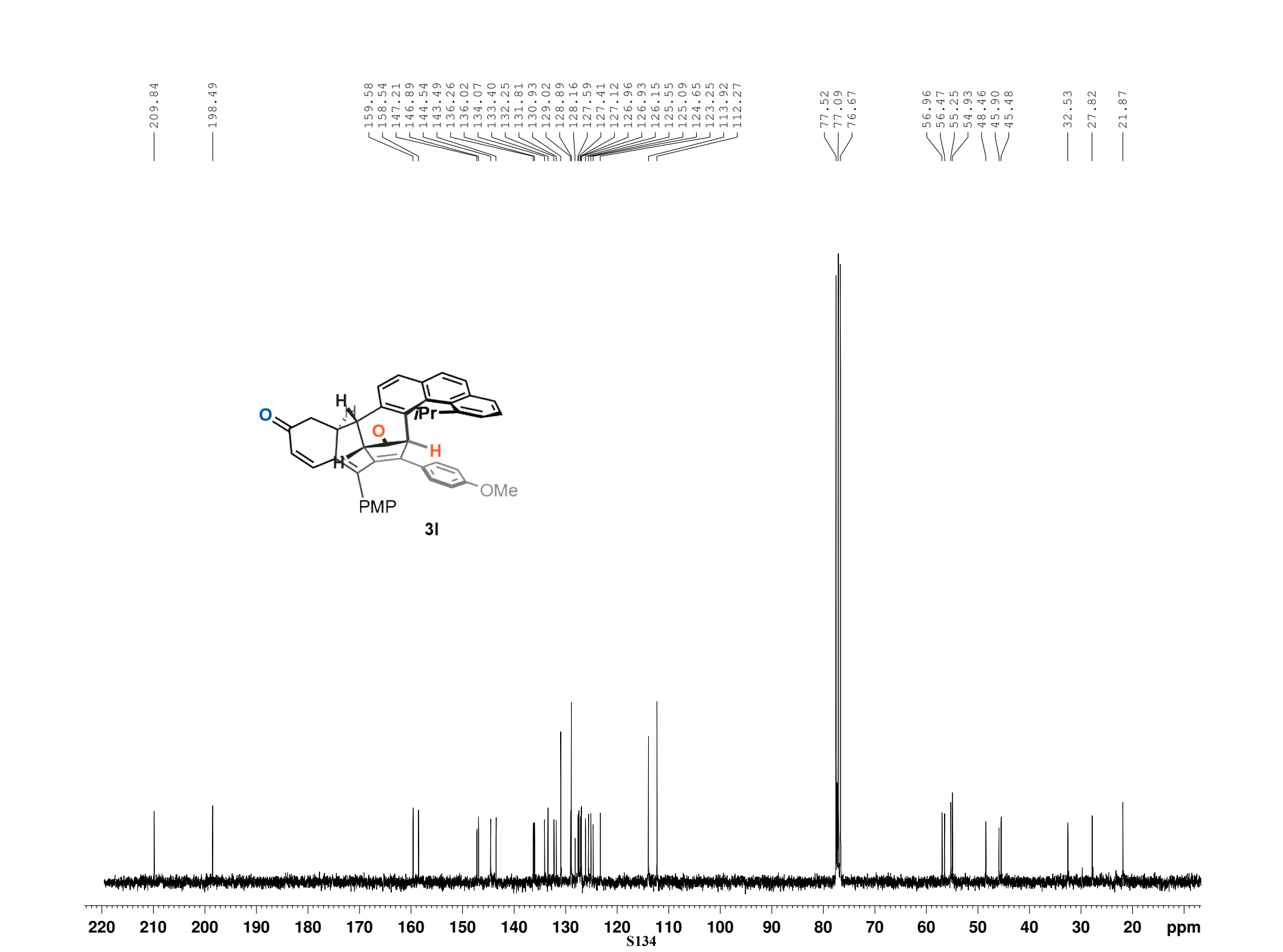
3.04
3.04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77.09
76.67
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21.87
O
H
H
iPr
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H
H
OMe
PMP
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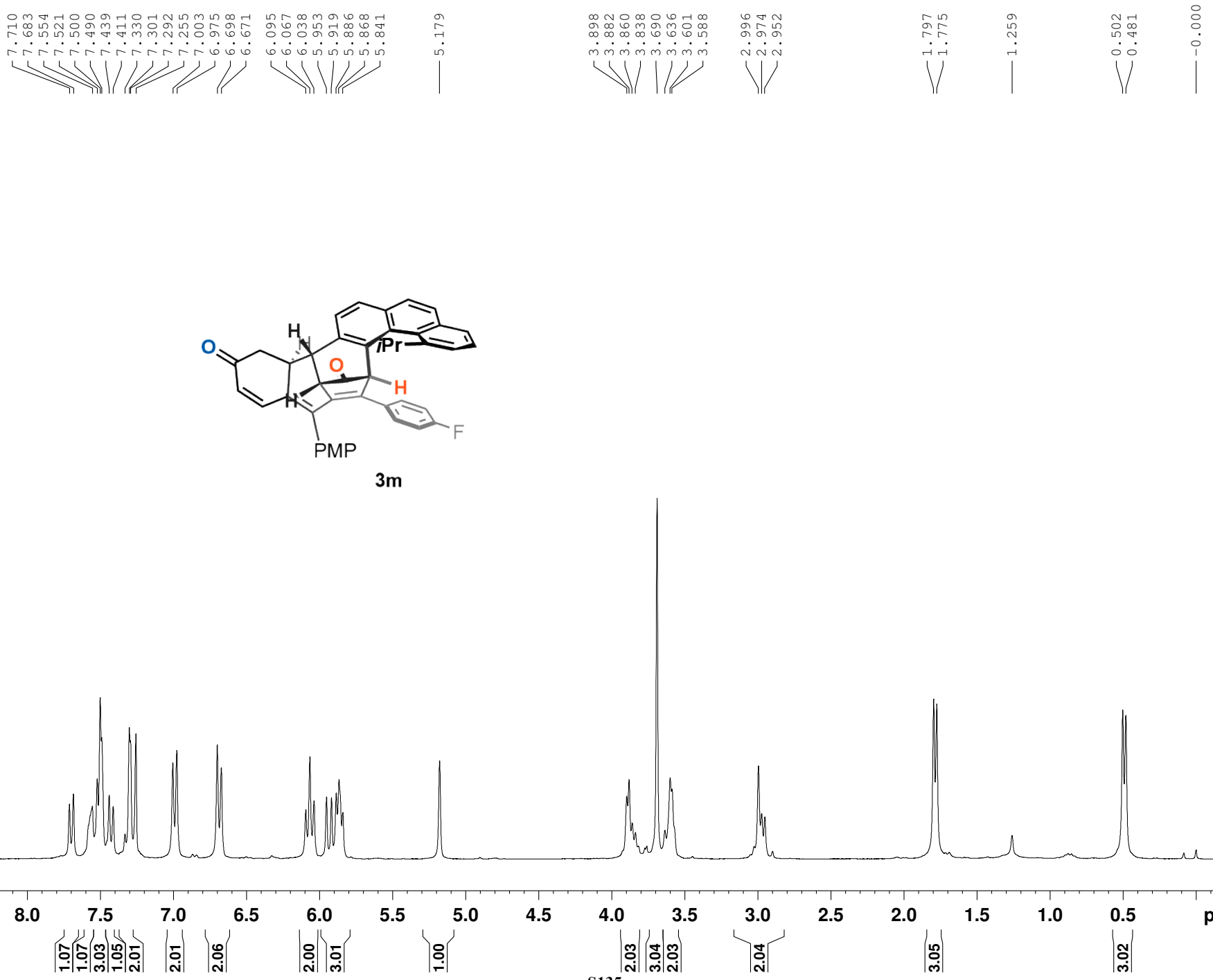
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H
iPr
O
H
H
F
PMP
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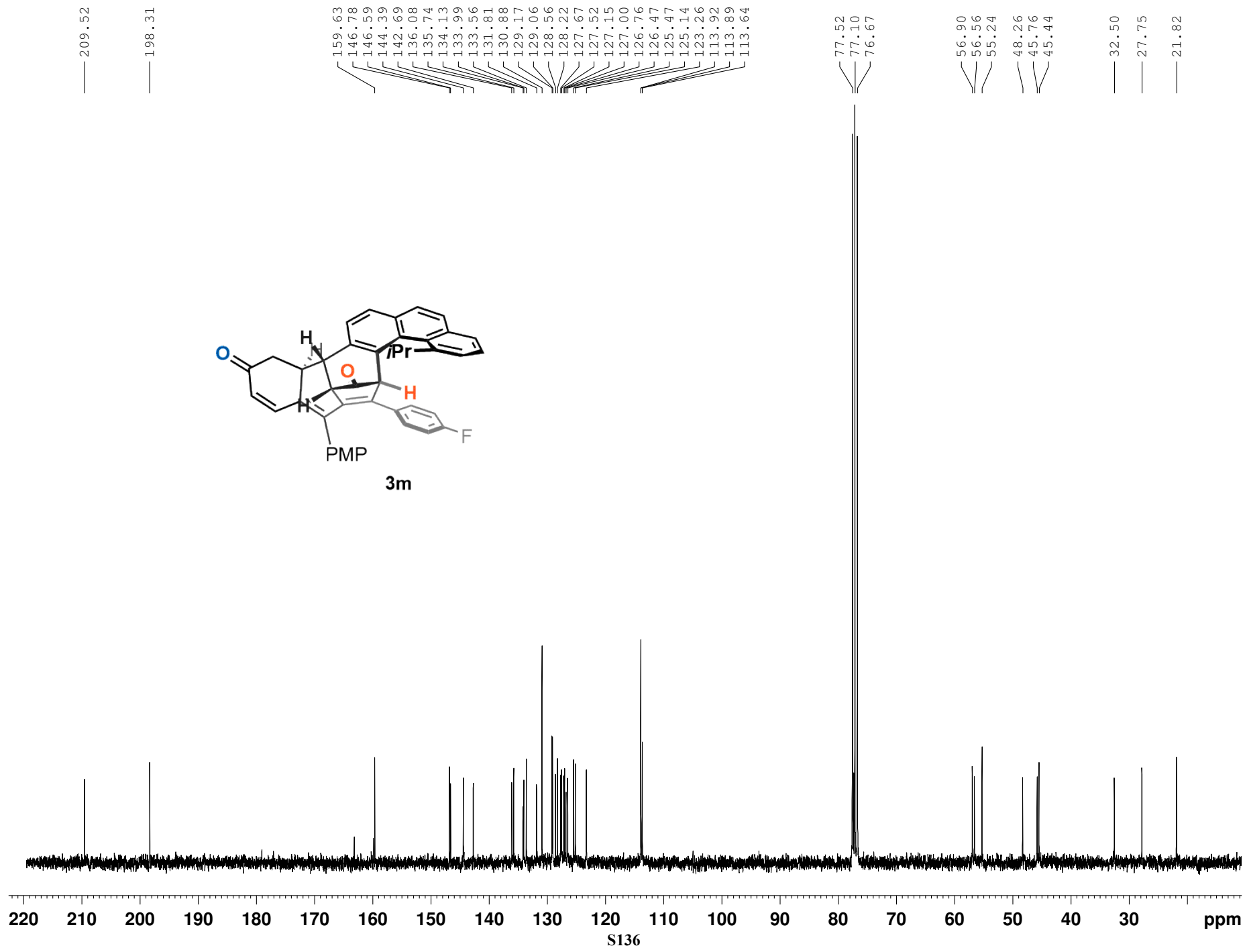
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77.10
76.67
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56.56
55.24
48.26
45.76
45.44
32.50
27.75
21.82
O
H
H
iPr
O
H
H
F
PMP
3m
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210
200
190
180
170
160
150
140
130
120
110
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60
50
40
30
ppm

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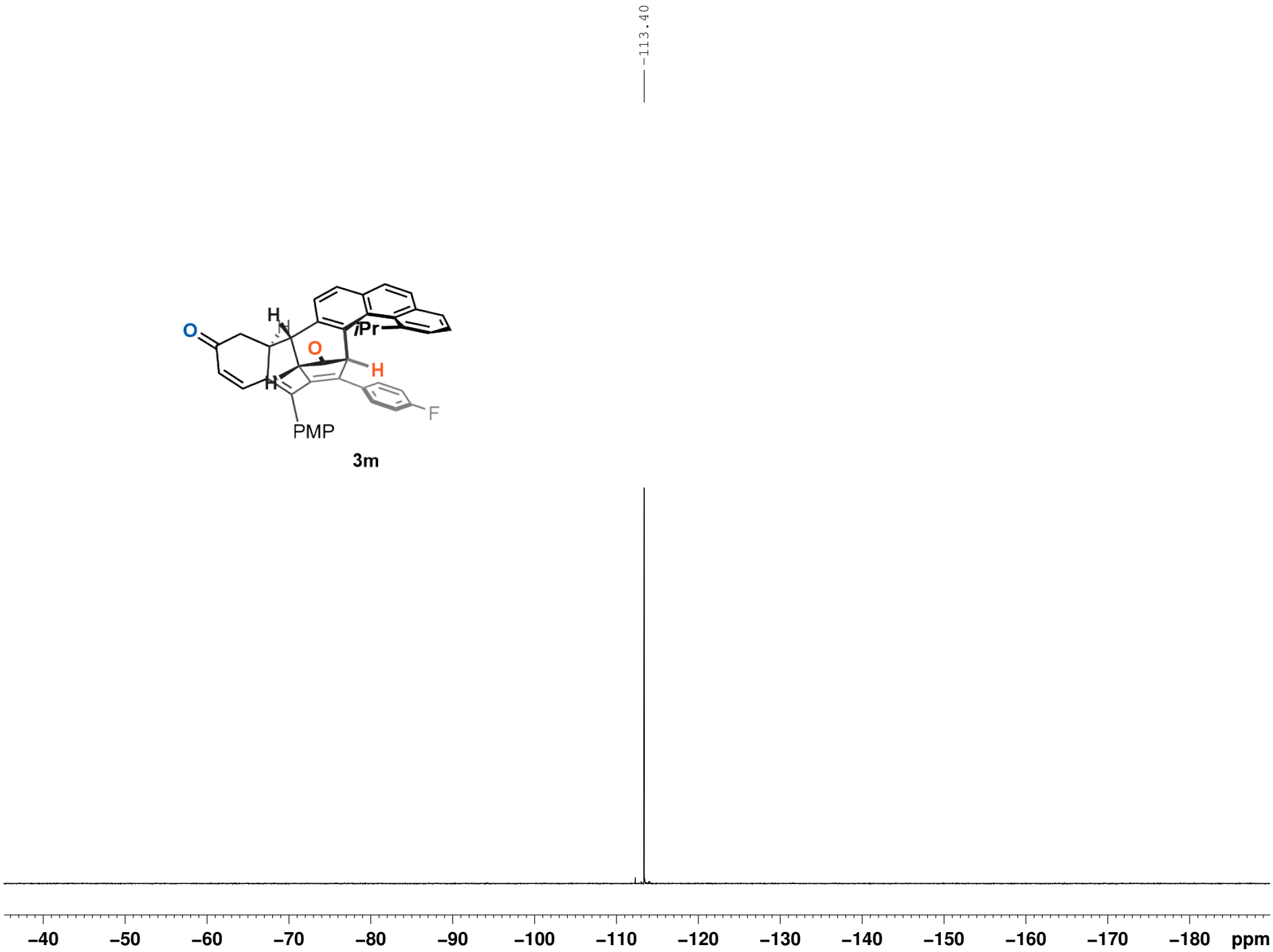
H
O
iPr
H
H
F
PMP

3m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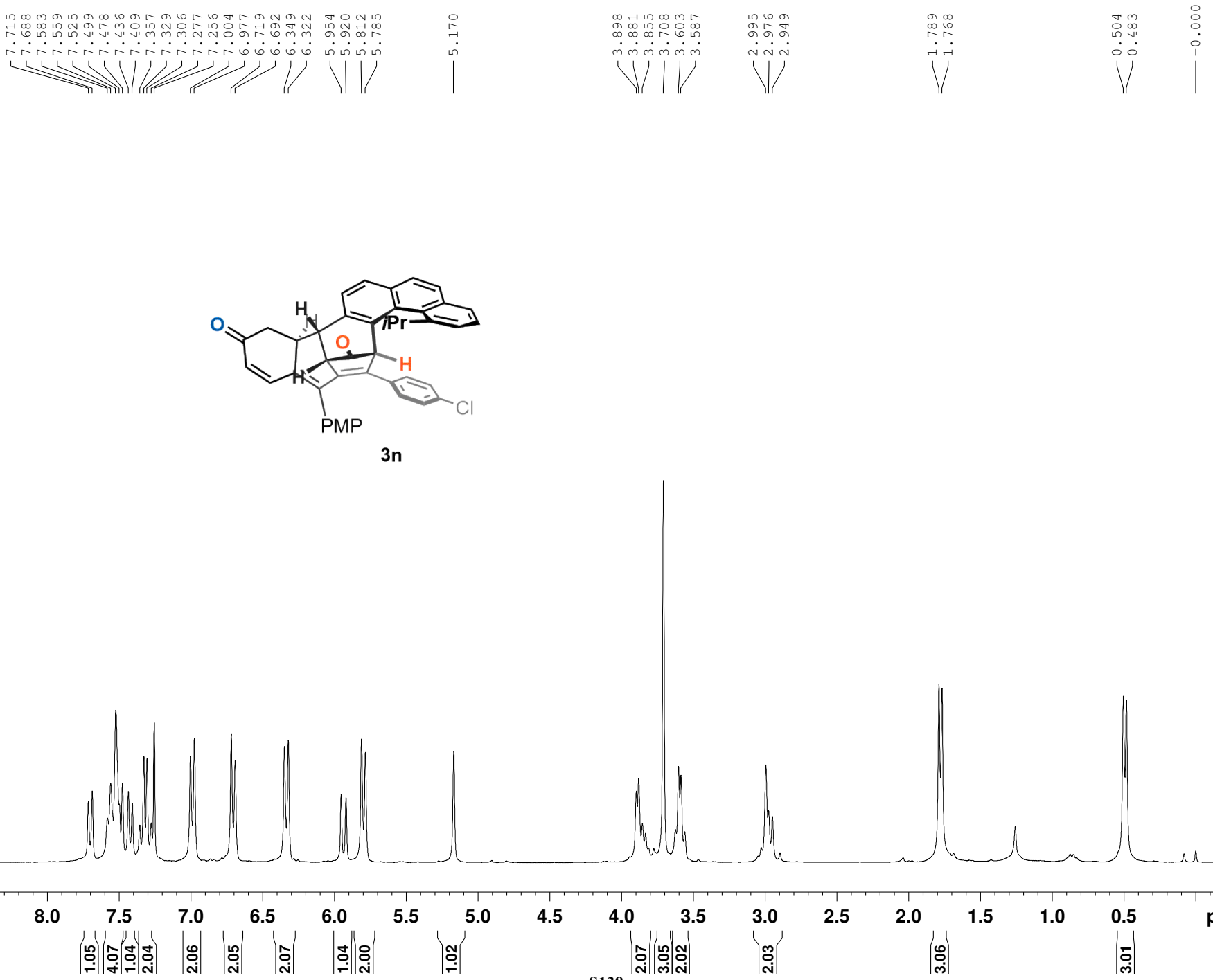
-180
ppm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H
iPr
O
H
H
Cl
PMP
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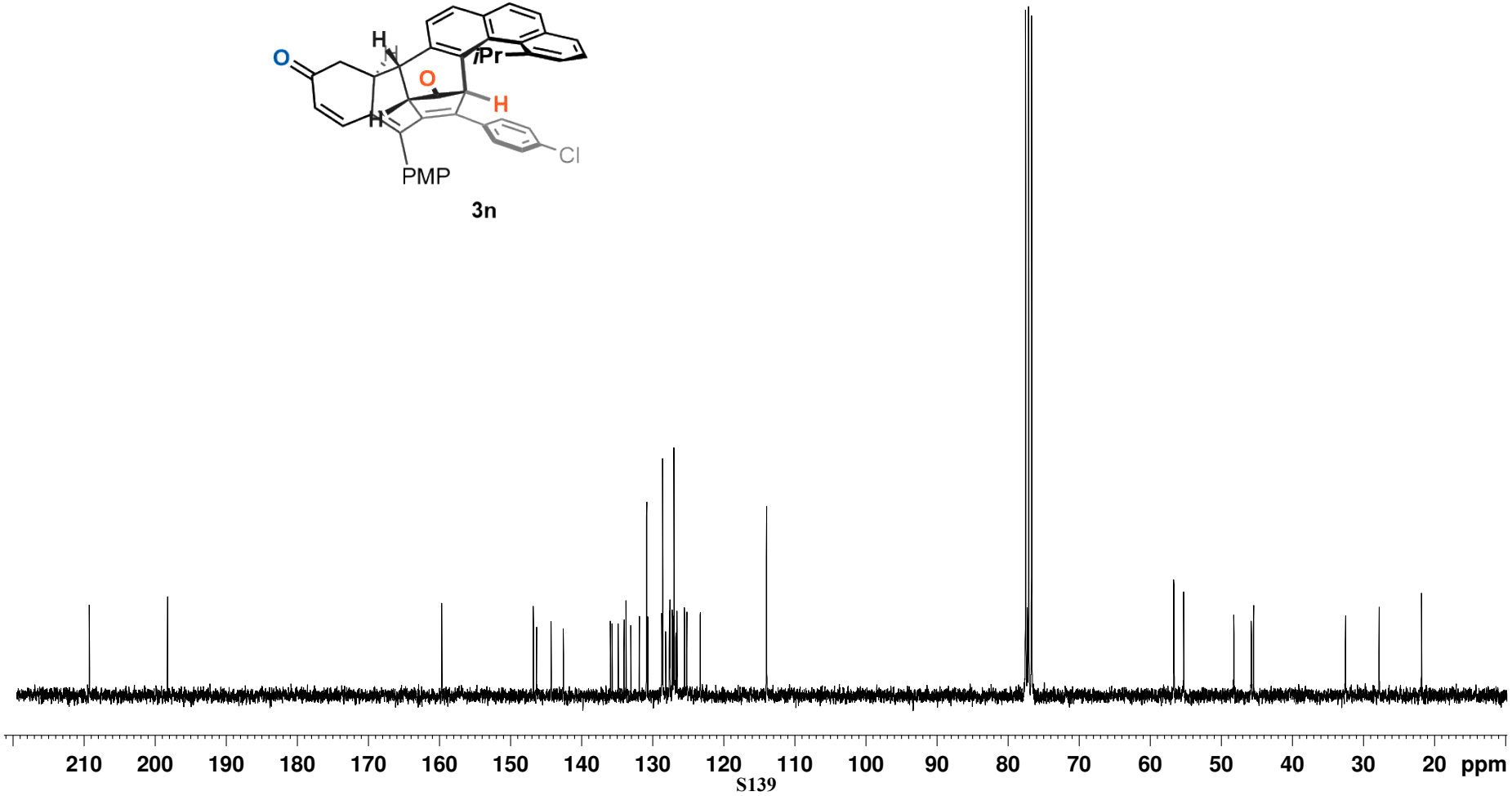

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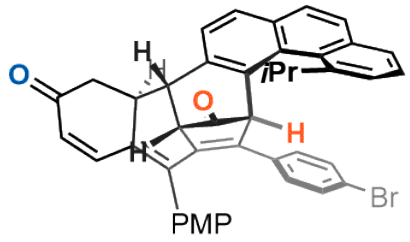

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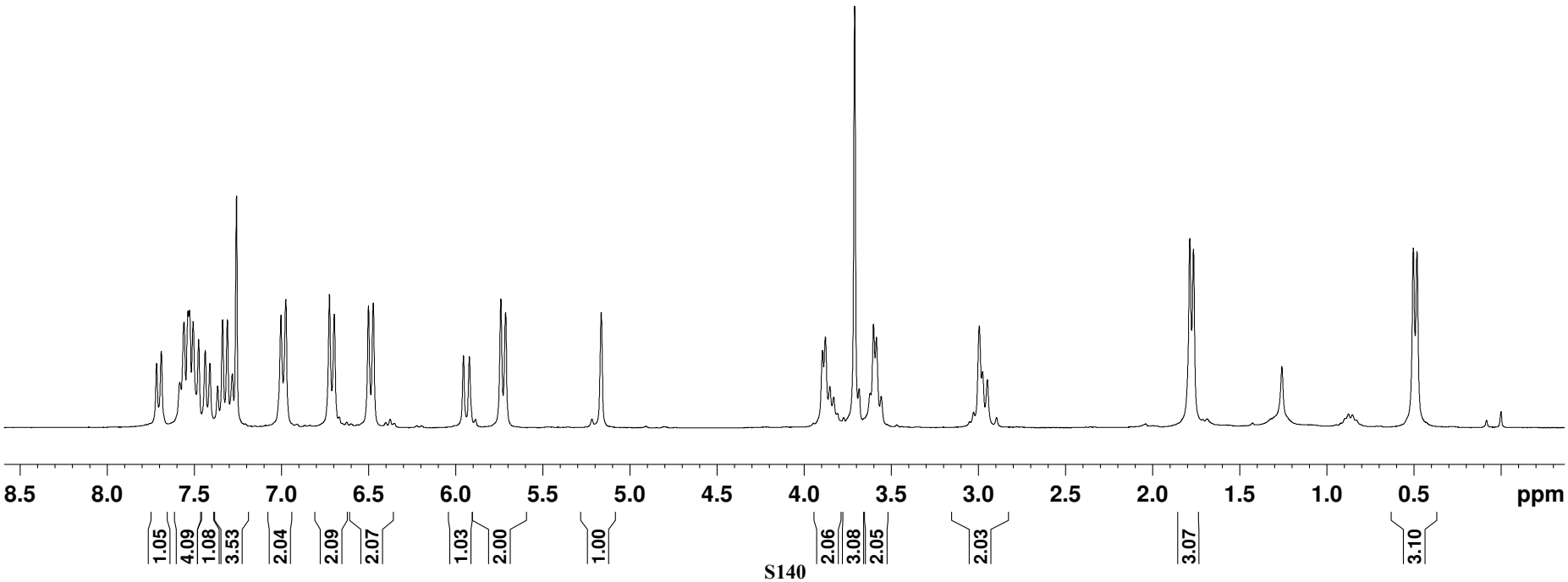

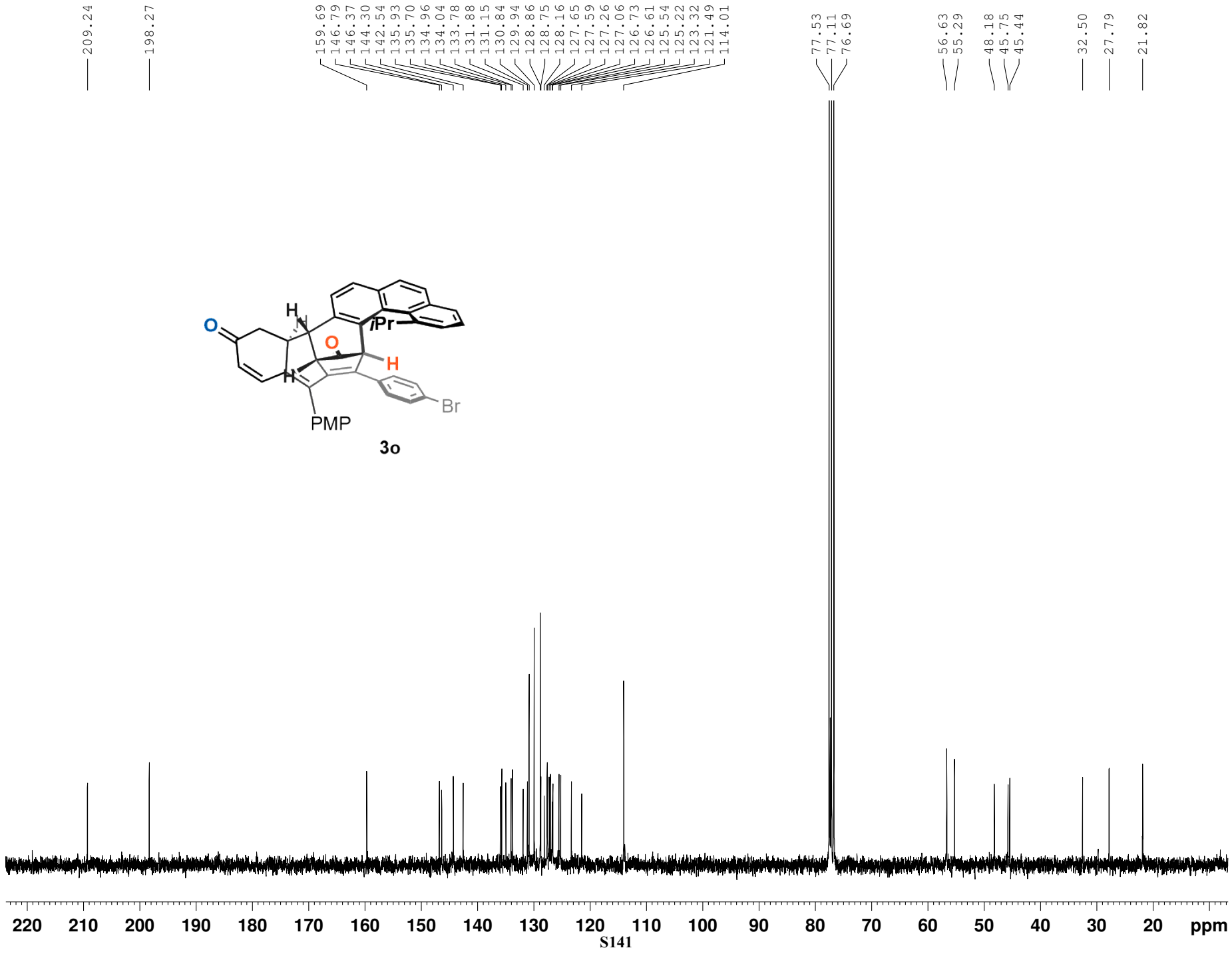
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129.94
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128.75
128.16
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127.59
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127.06
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125.54
125.22
123.32
121.49
114.01
77.53
77.11
76.69
56.63
55.29
48.18
45.75
45.44
32.50
27.79
21.82
O
H
H
O
iPr
H
Br
PMP
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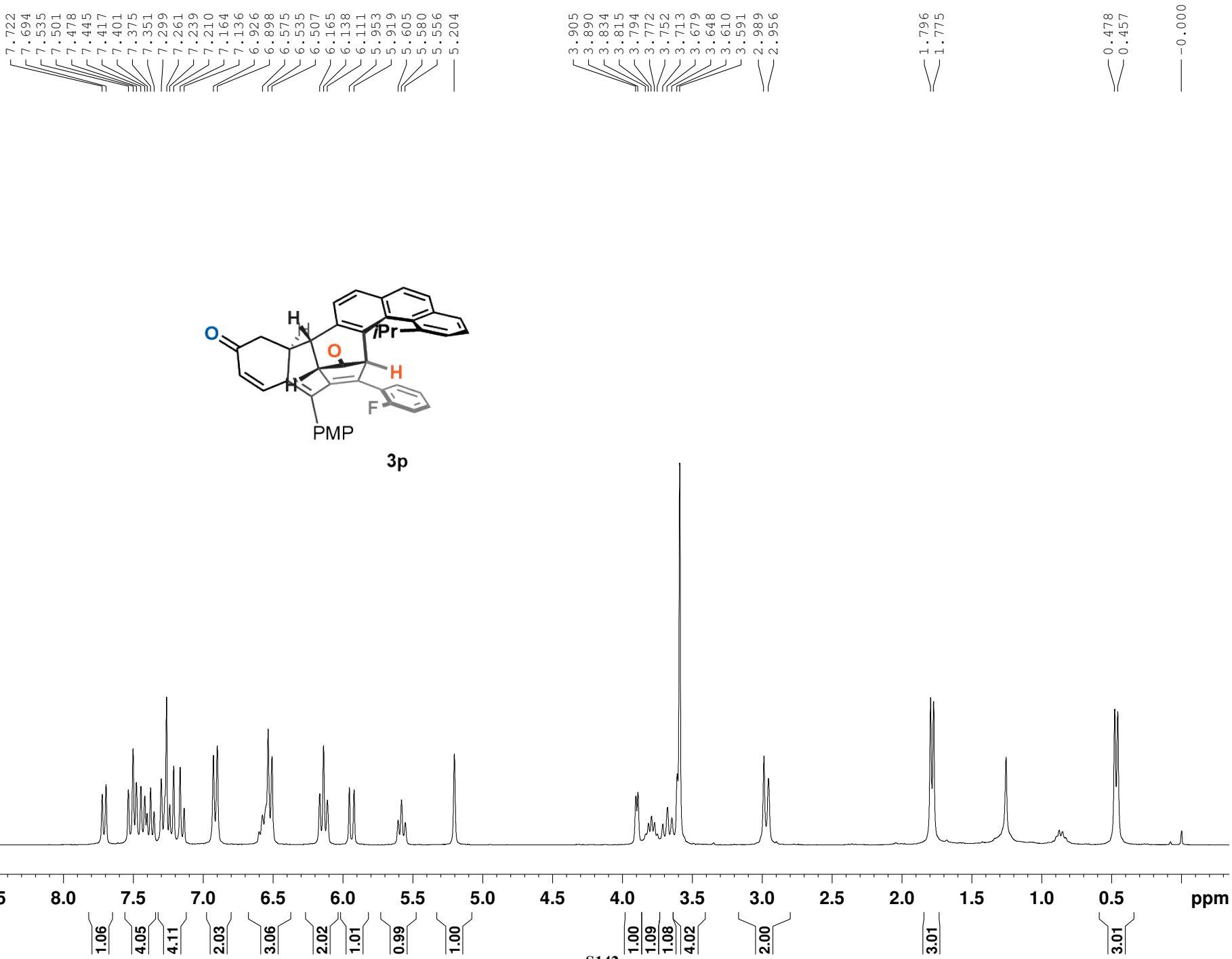
20
ppm

3o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PMP
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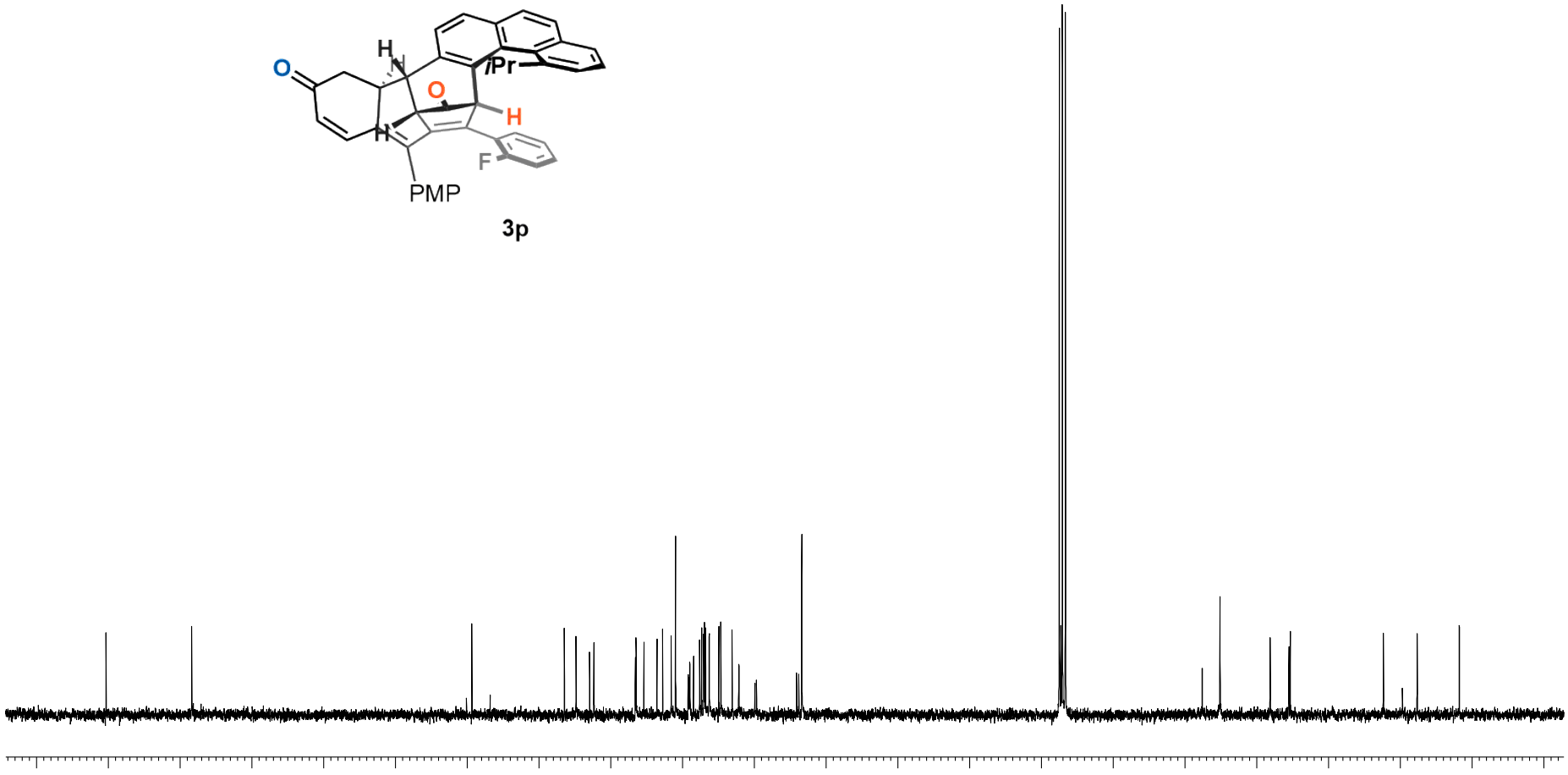
21.78

3p



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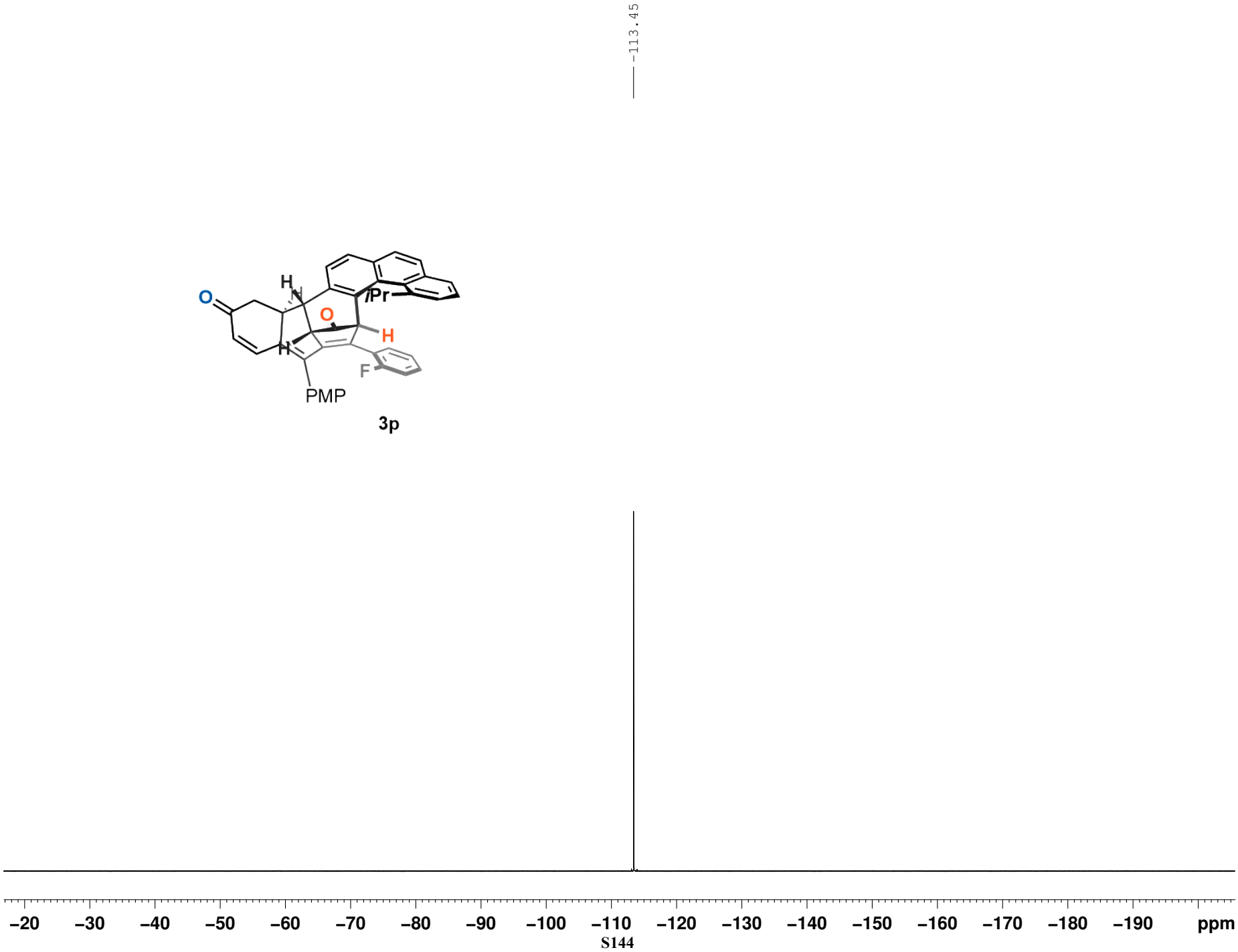
O
iPr
H
H
F
PMP

3p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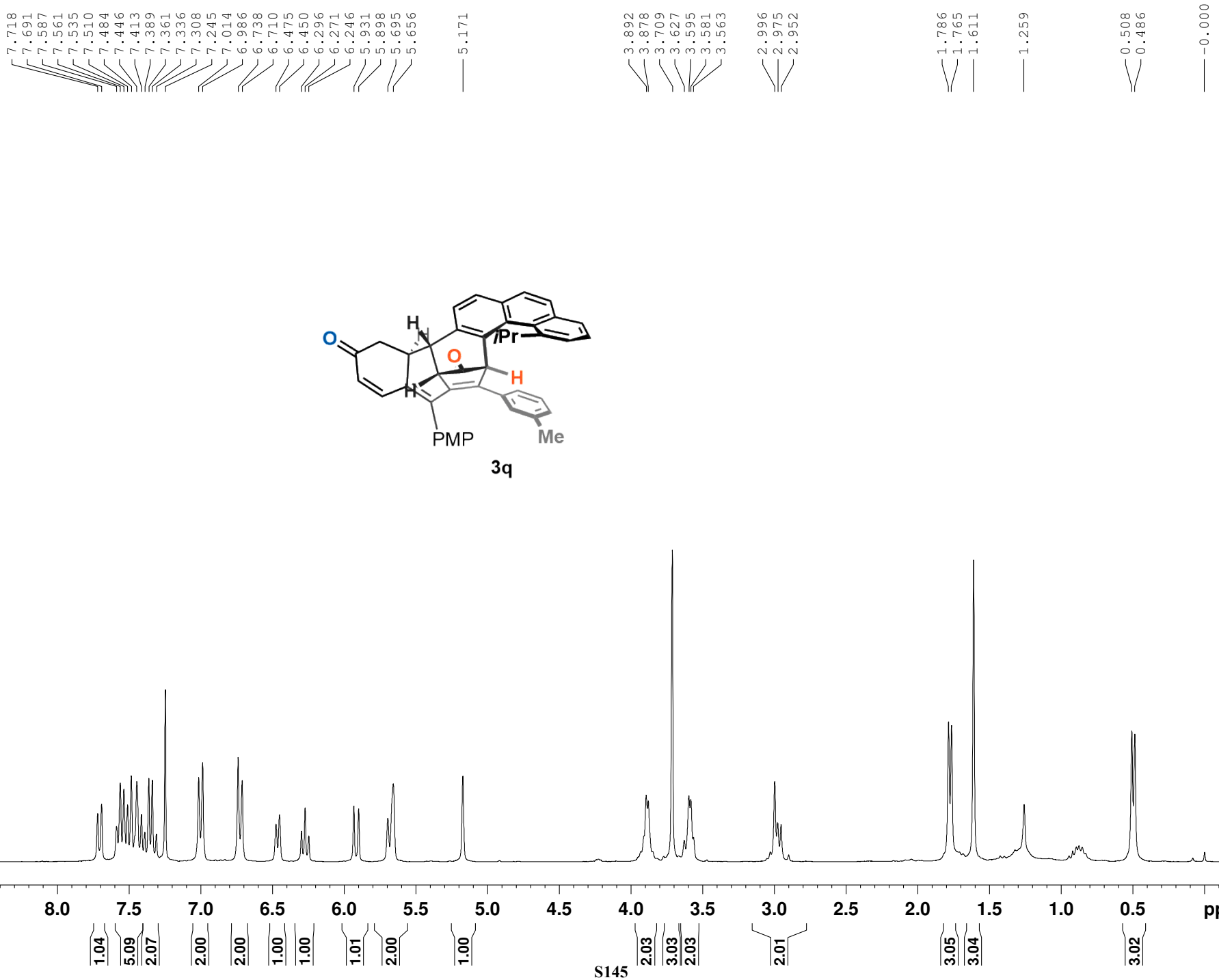
ppm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7.014
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6.475
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6.271
6.246
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3.581
3.563
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2.975
2.952
1.786
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1.611
1.259
0.508
0.486
-0.000
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H
H
O
iPr
H
PMP
Me
3q
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7.5
7.0
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6.0
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2.00
1.00
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3.03
2.03
2.01
3.05
3.04
3.02

209.45
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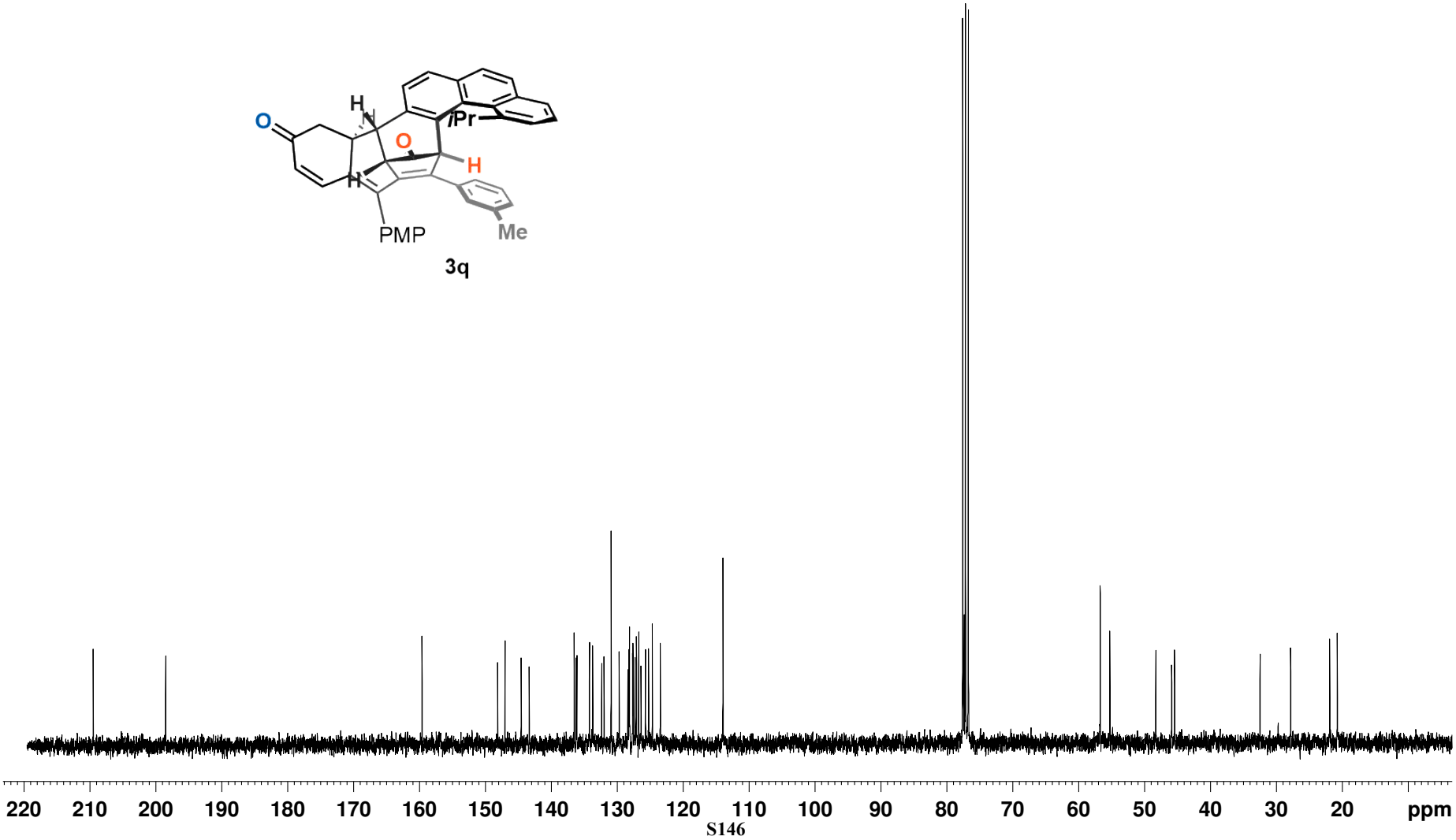
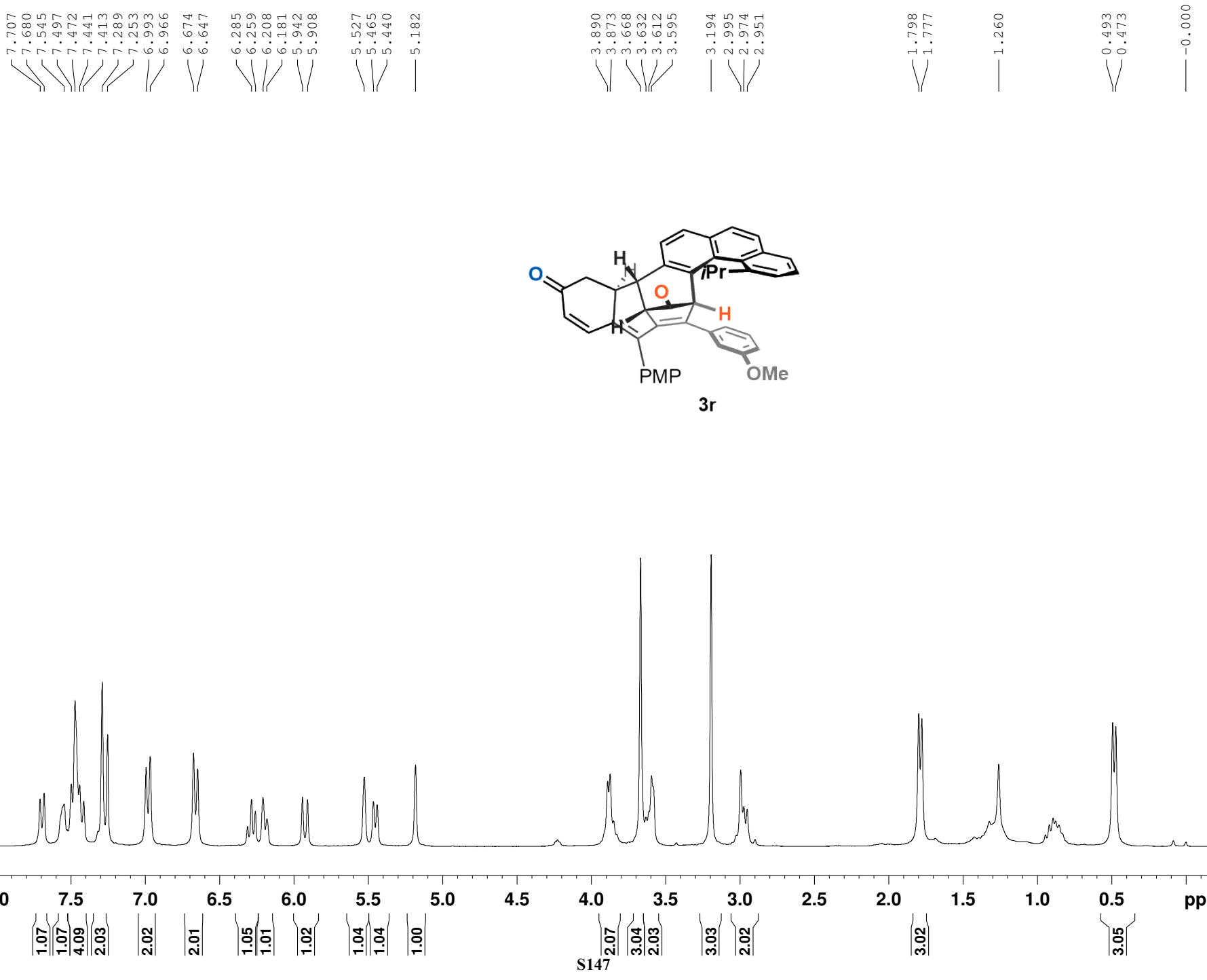
3q

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6.674
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6.285
6.259
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6.181
5.942
5.908
5.527
5.465
5.440
5.182
3.890
3.873
3.668
3.632
3.612
3.595
3.194
2.995
2.974
2.951
1.798
1.777
1.260
0.493
0.473
-0.000
O
H
H
iPr
O
H
PMP
OMe
3r
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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
ppm
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1.07
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2.02
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1.05
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1.02
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3.04
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3.02
3.05

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125.11
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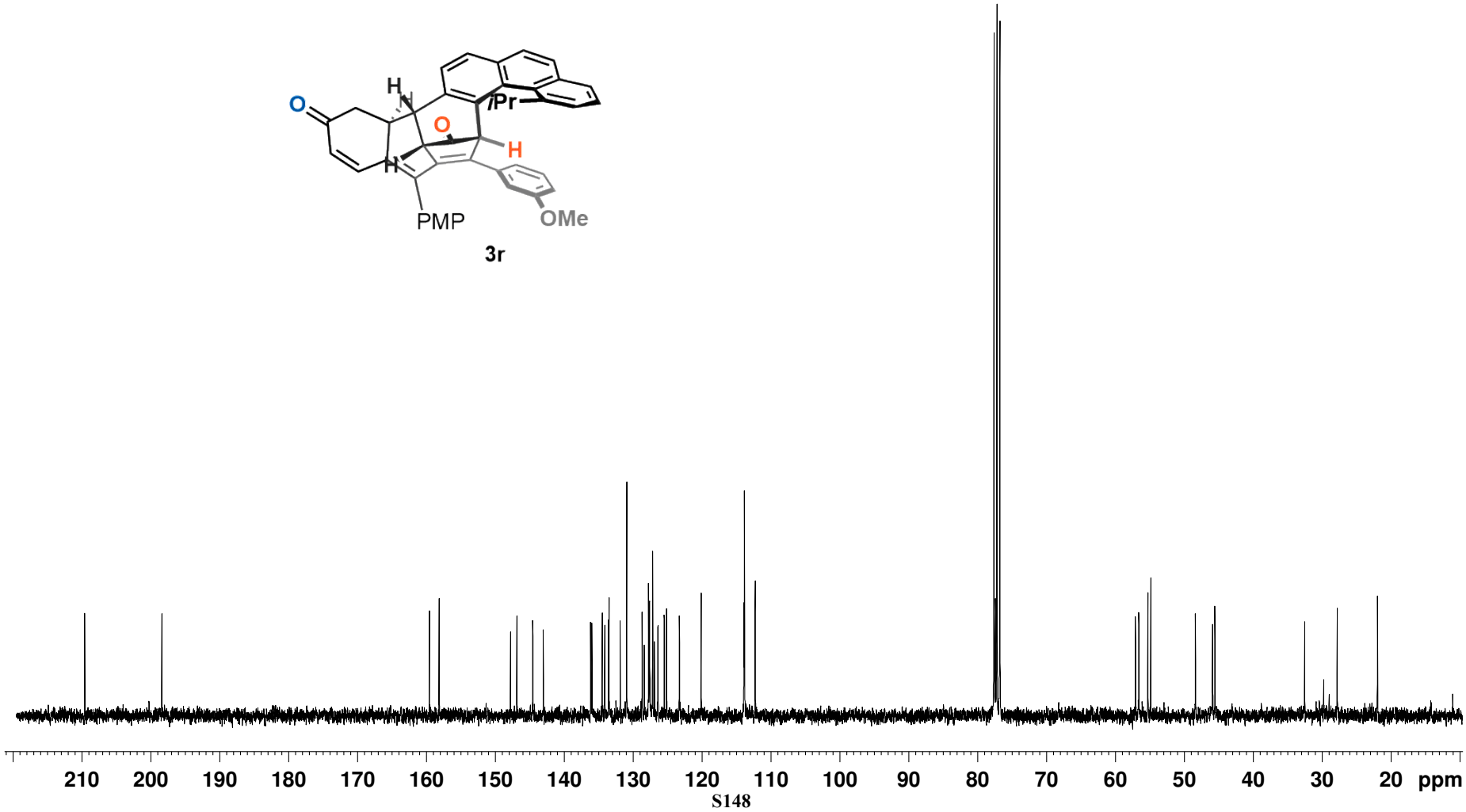
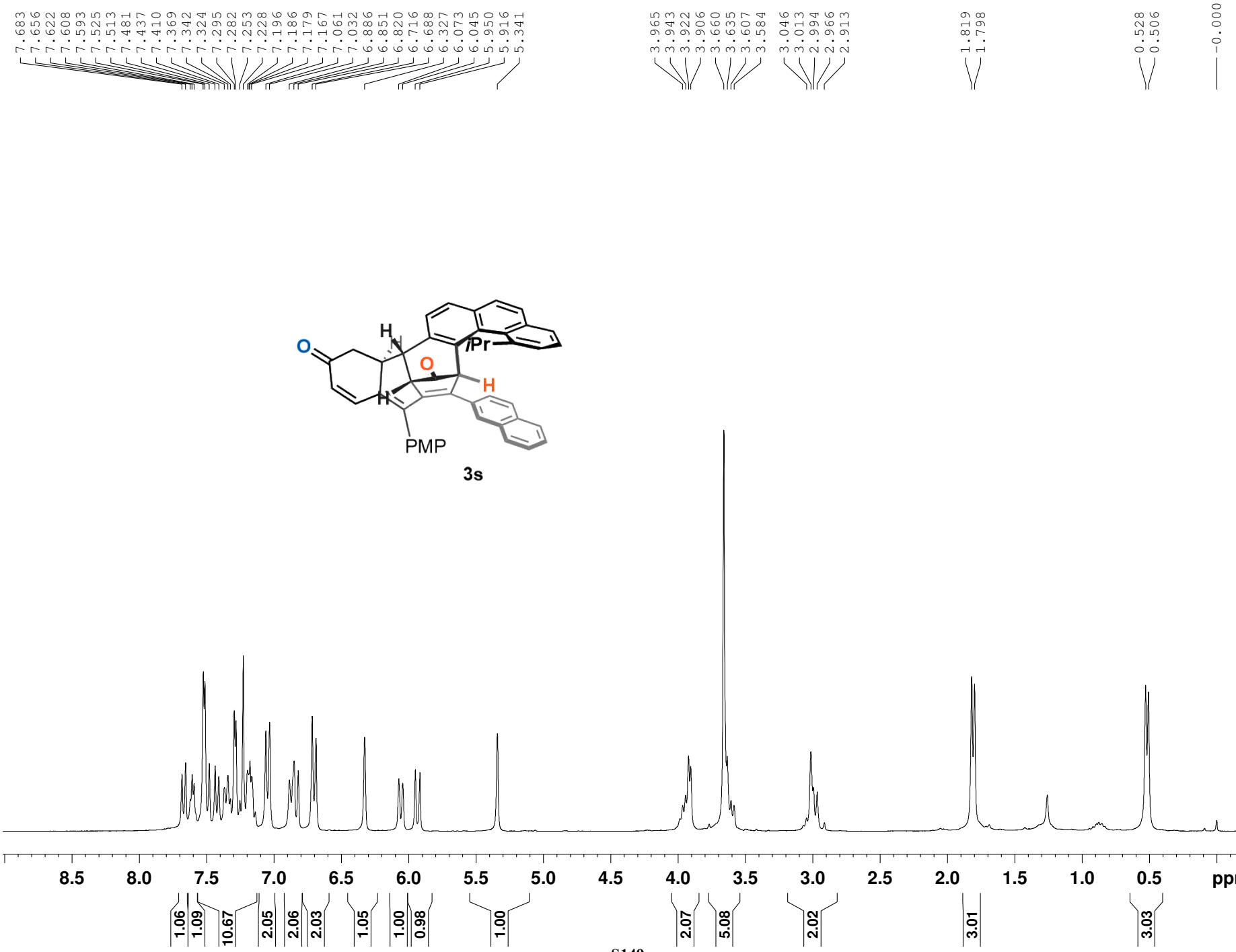
3r

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7.324
7.295
7.282
7.253
7.228
7.196
7.186
7.179
7.167
7.061
7.032
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6.851
6.820
6.716
6.688
6.327
6.073
6.045
5.950
5.916
5.341
3.965
3.943
3.922
3.906
3.660
3.635
3.607
3.584
3.046
3.013
2.994
2.966
2.913
1.819
1.798
0.528
0.506
-0.000
O
H
H
O
iPr
H
H
PMP
3s
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
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1.0
0.5
ppm
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2.07
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2.02
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3.03

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134.16
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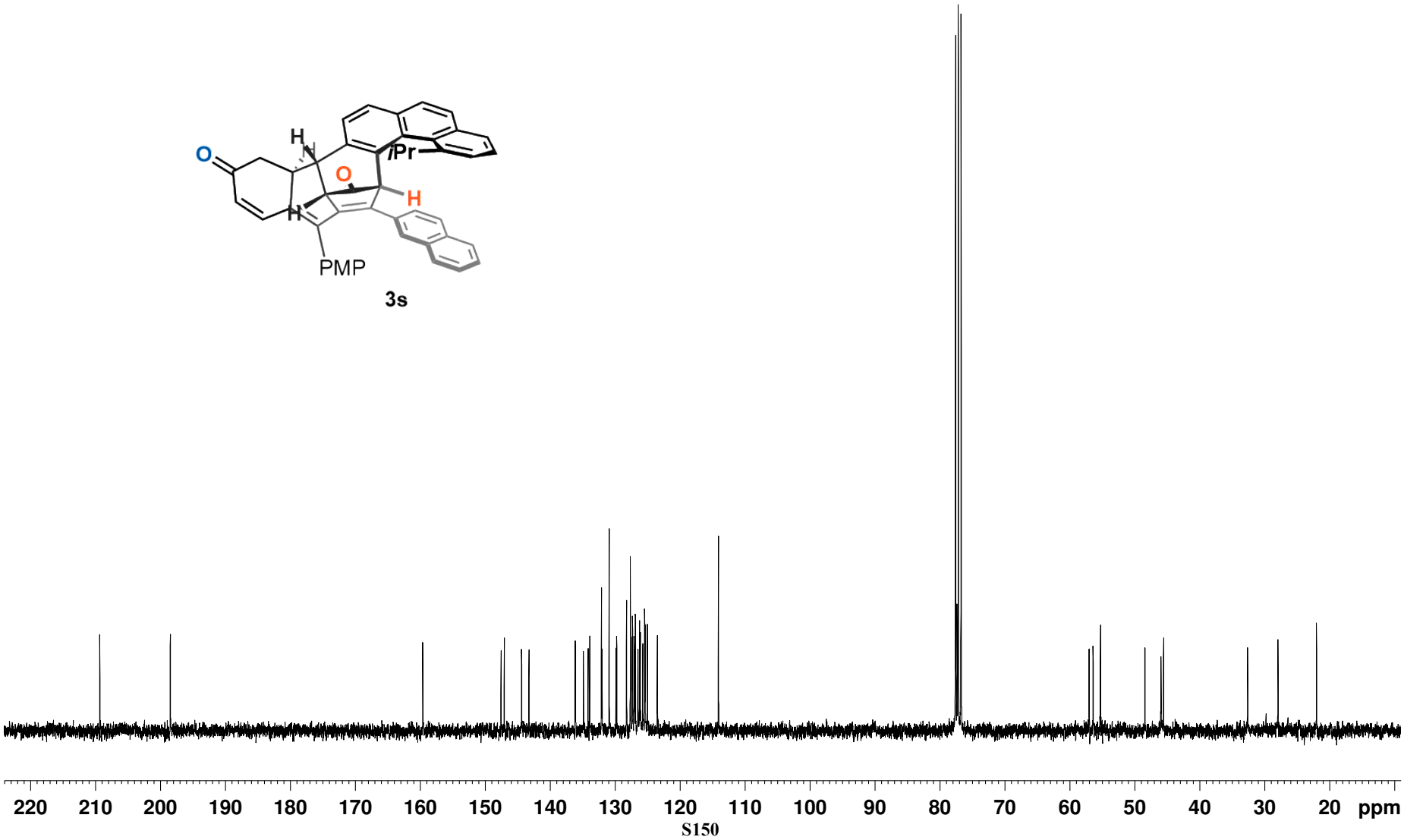

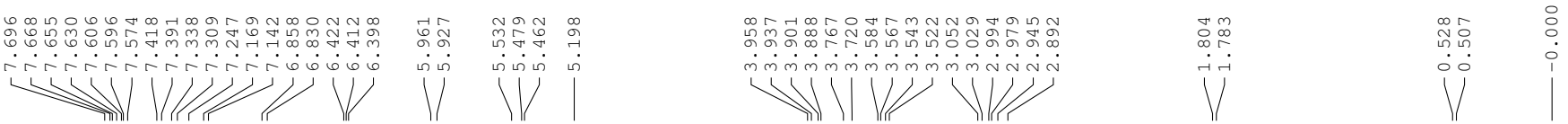
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7.169
7.142
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6.830
6.422
6.412
6.398
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5.927
5.532
5.479
5.462
5.198
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3.937
3.901
3.888
3.767
3.720
3.584
3.567
3.543
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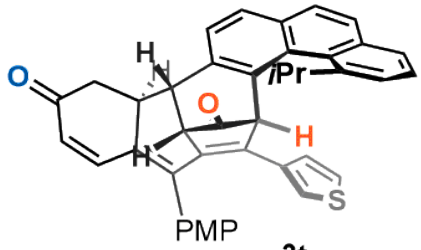
-0.000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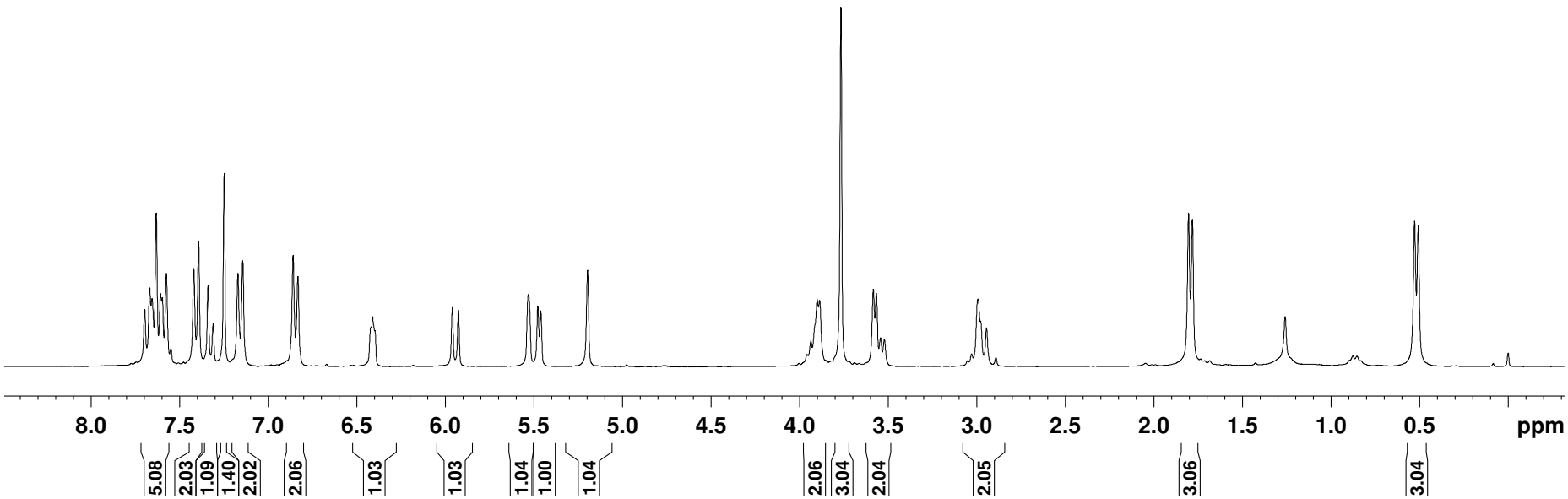
H
N
iPr
O
H
H
S
PMP

3t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1.0
0.5
ppm
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2.03
1.09
1.40
2.02
2.06
1.03
1.03
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1.00
1.04
2.06
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2.05
3.06
3.04

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125.93
125.39
125.09
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123.48
114.43
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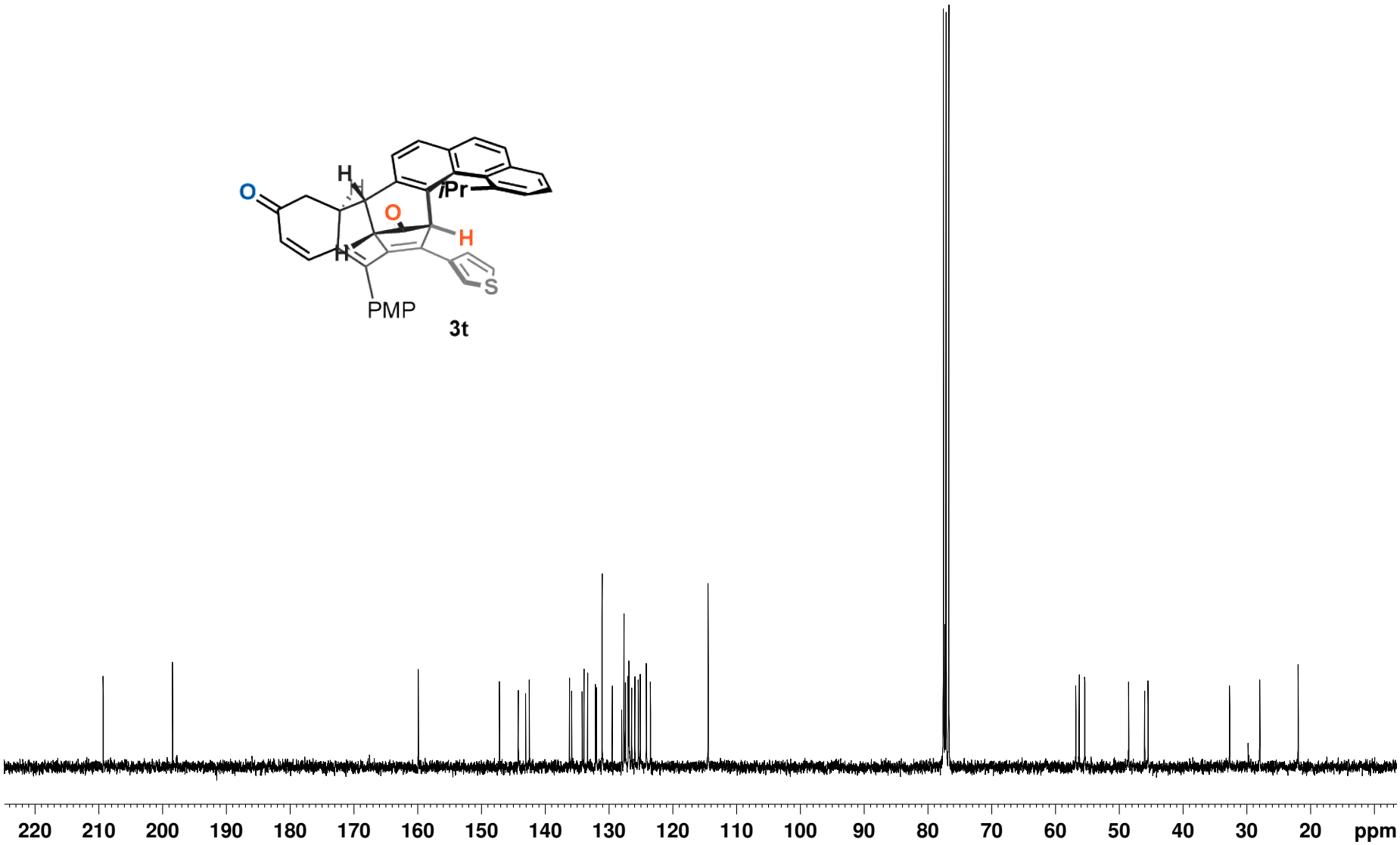
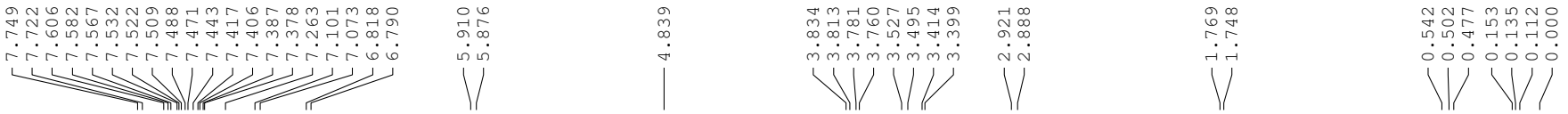
3t

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7.073
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6.790
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3.834
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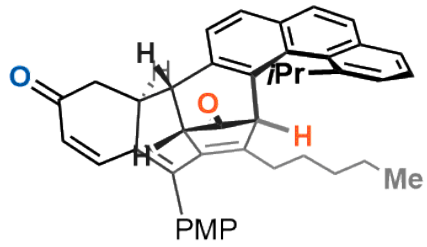
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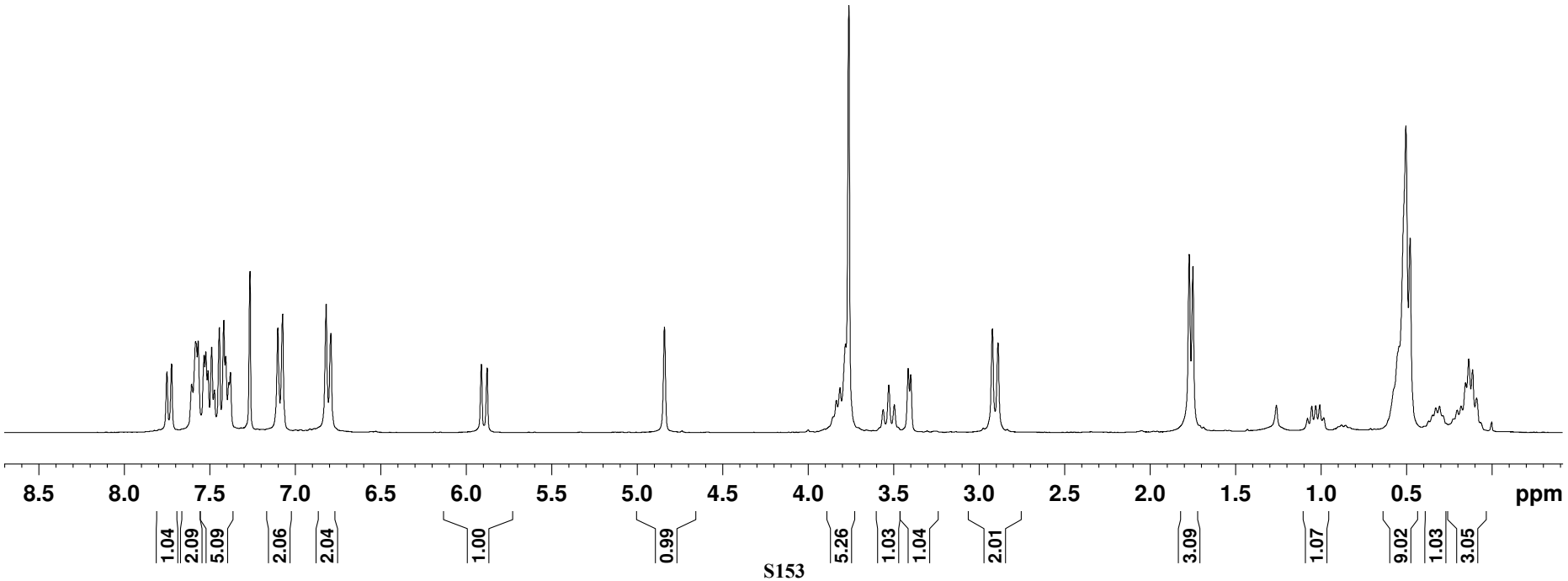
N
iPr
O
H
H
Me
PMP

3u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ppm
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5.09
2.06
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3.09
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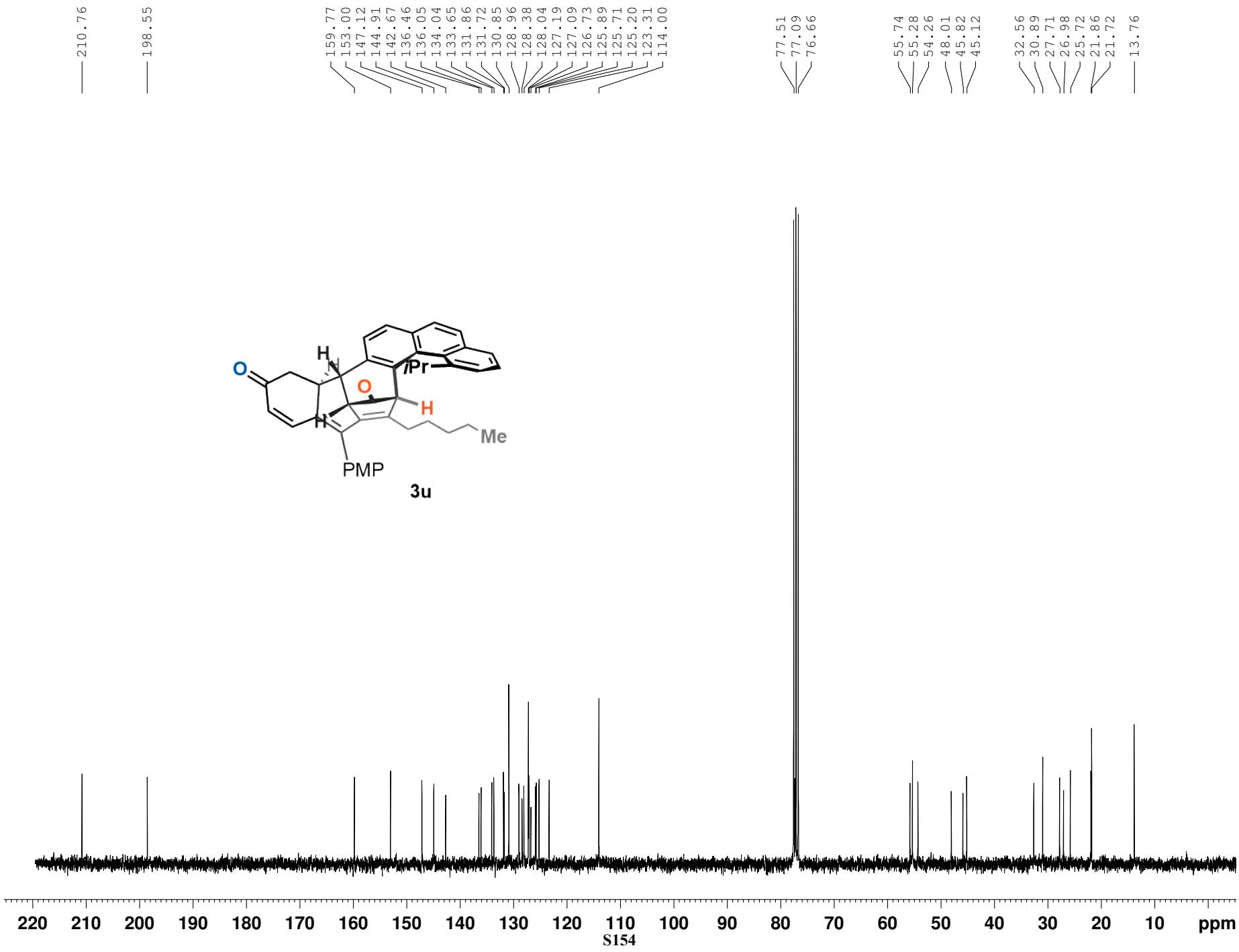
3.05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127.09
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77.09
76.66
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55.28
54.26
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45.12
32.56
30.89
27.71
26.98
25.72
21.86
21.72
13.76
O
H
H
O
iPr
H
H
Me
PMP
3u
220
210
200
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140
130
120
110
100
90
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70
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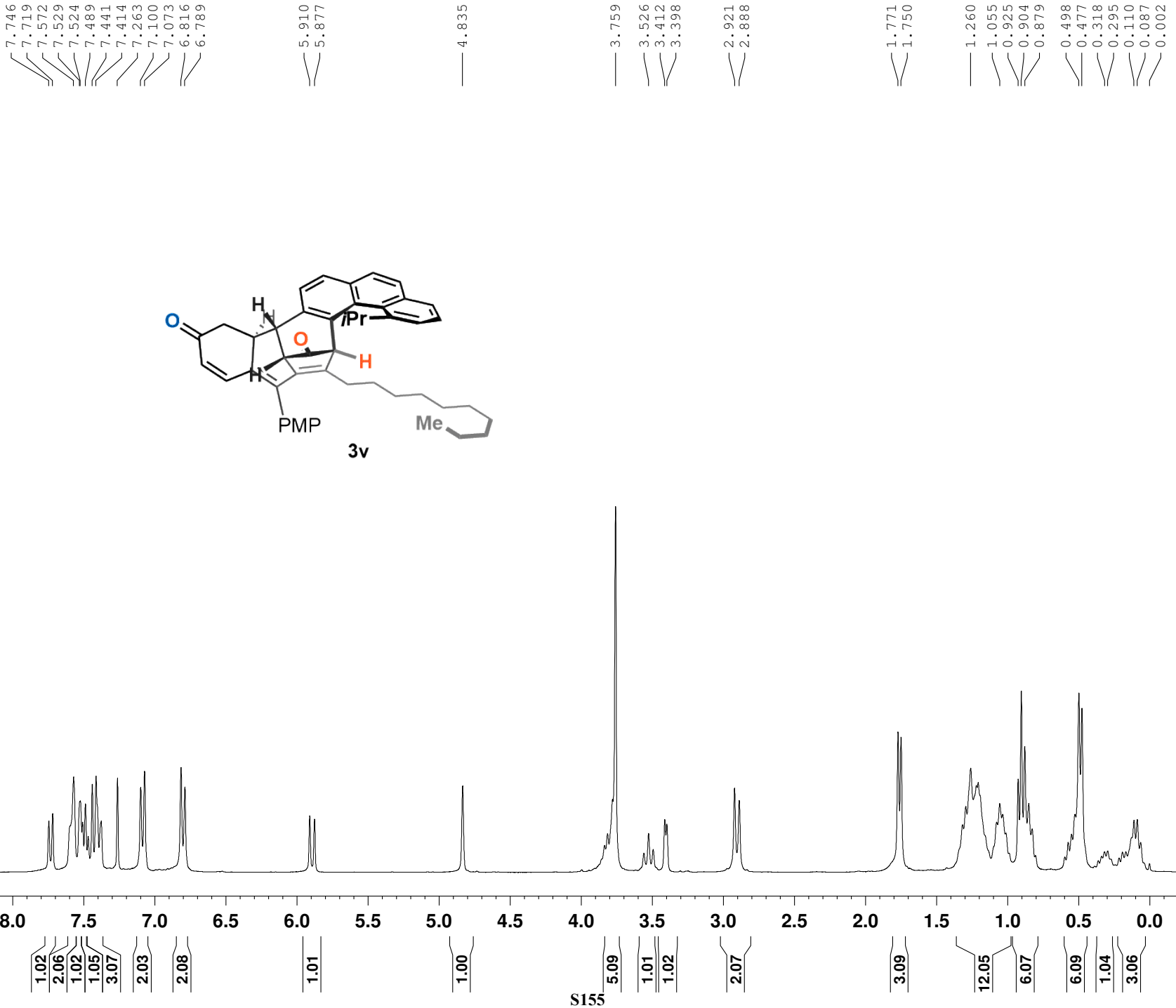
50
40
30
20
10
ppm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0.087
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H
H
O
H
iPr
H
PMP
Me
3v
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4.0
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2.0
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1.0
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0.0
ppm
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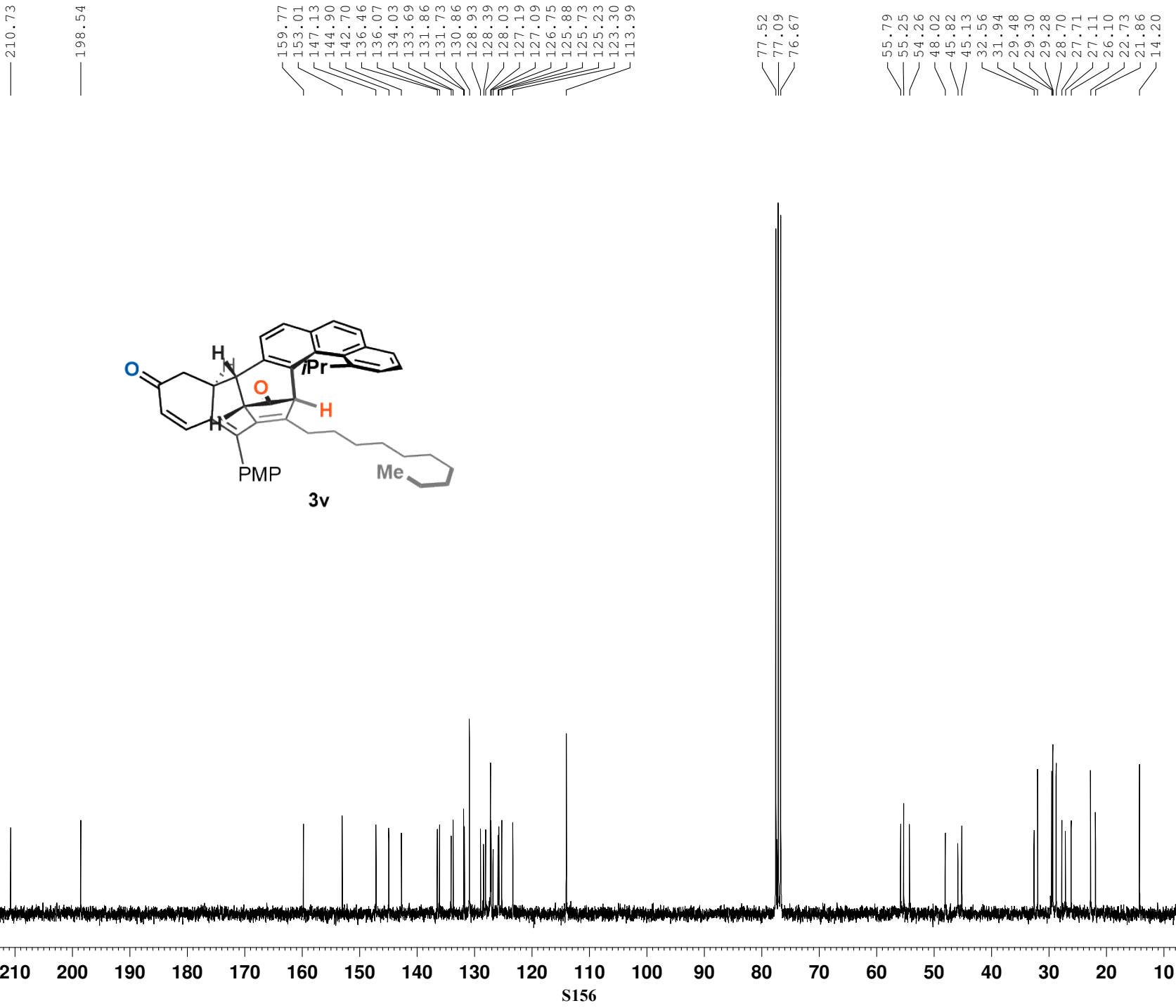
3.06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H
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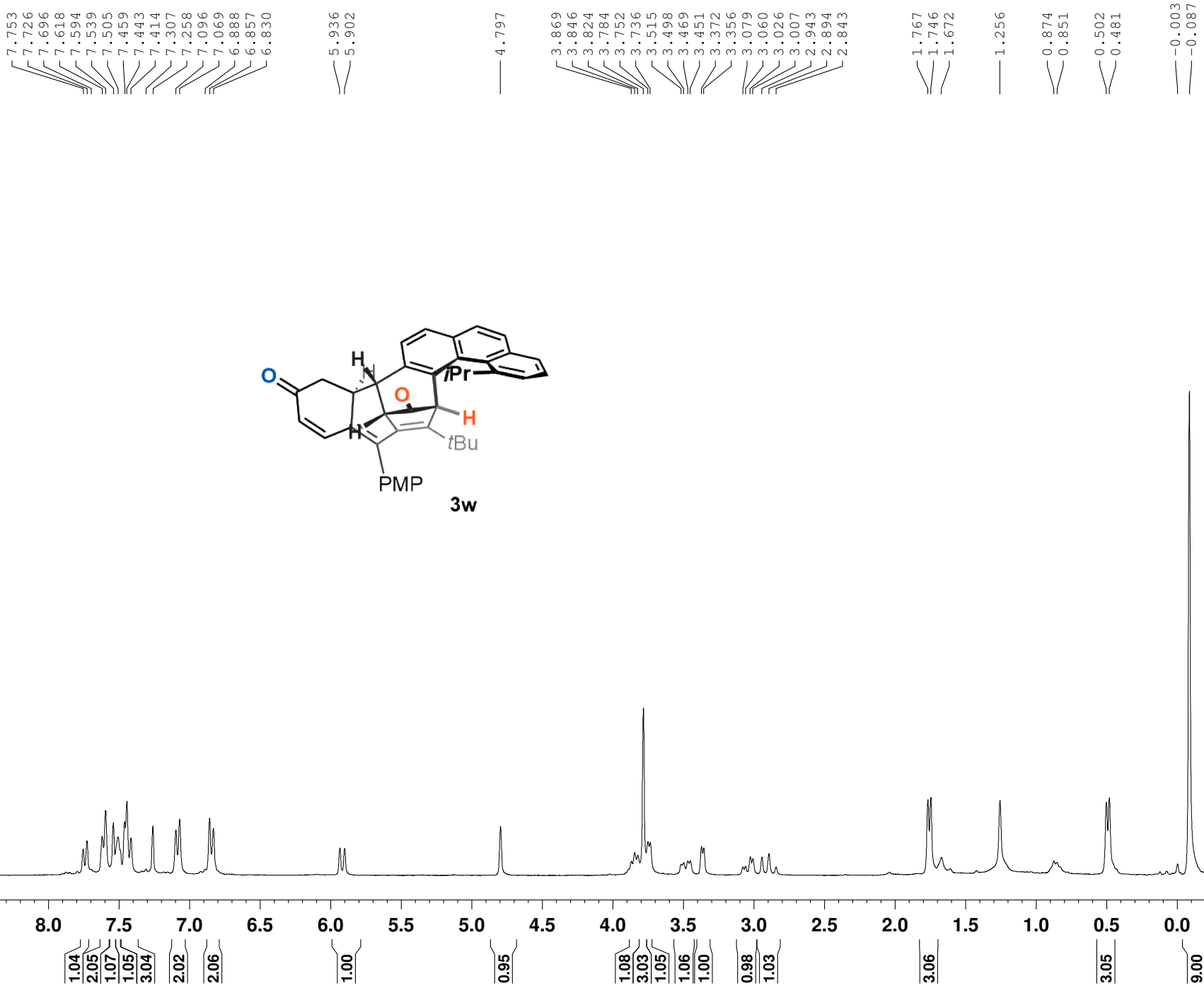
10
ppm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0.481
-0.003
-0.087
O
H
iPr
O
H
H
tBu
PMP
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5.0
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4.0
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3.0
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1.0
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ppm
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2.05
1.07
1.05
3.04
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1.06
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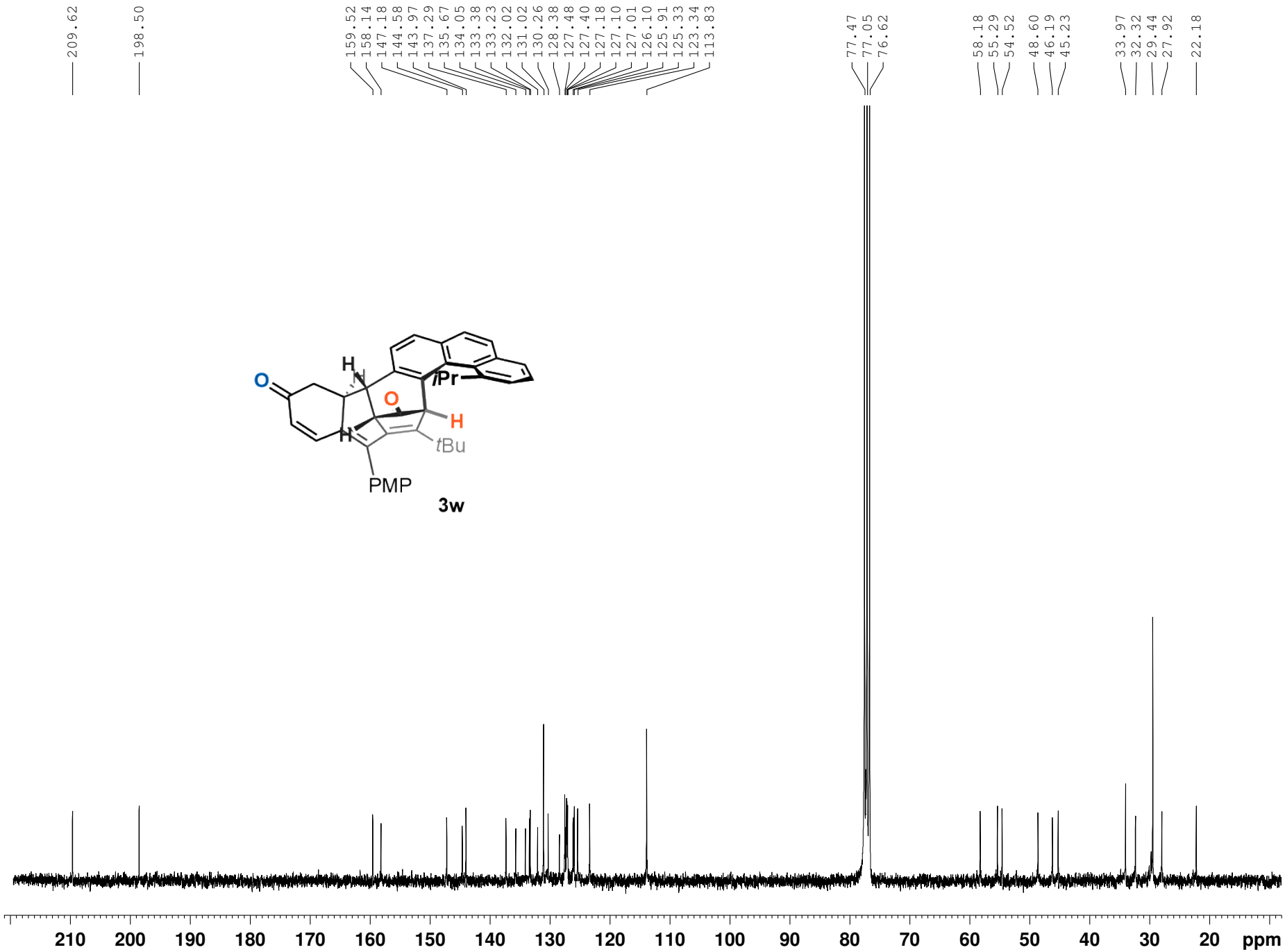
3.06
3.05
9.00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131.02
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127.18
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125.33
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77.05
76.62
58.18
55.29
54.52
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46.19
45.23
33.97
32.32
29.44
27.92
22.18
O
H
N
iPr
O
H
H
tBu
PMP
3w
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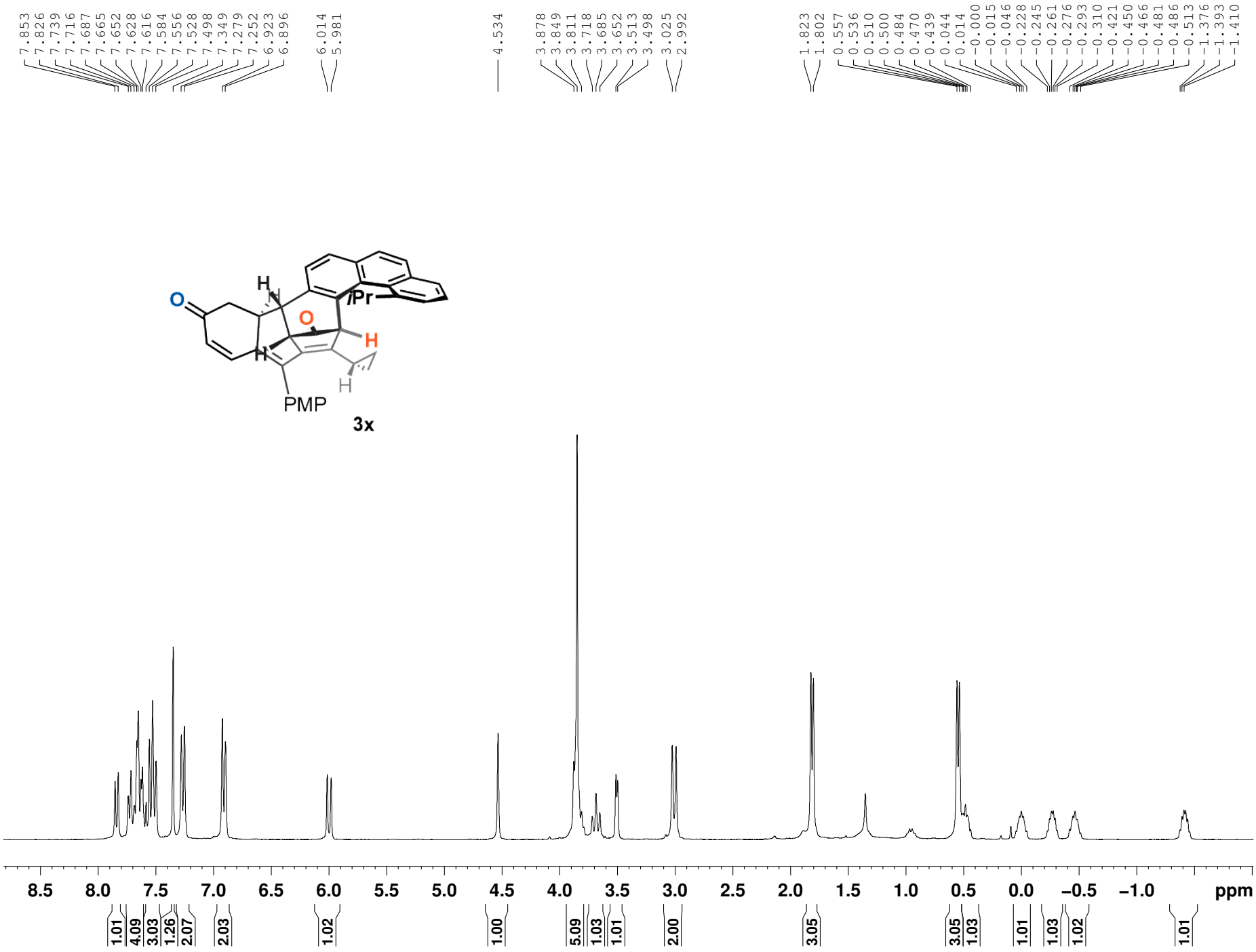
20
ppm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-0.450
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-0.481
-0.486
-0.513
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H
H
O
iPr
H
H
PMP
3x
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2.03
1.02
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3.05
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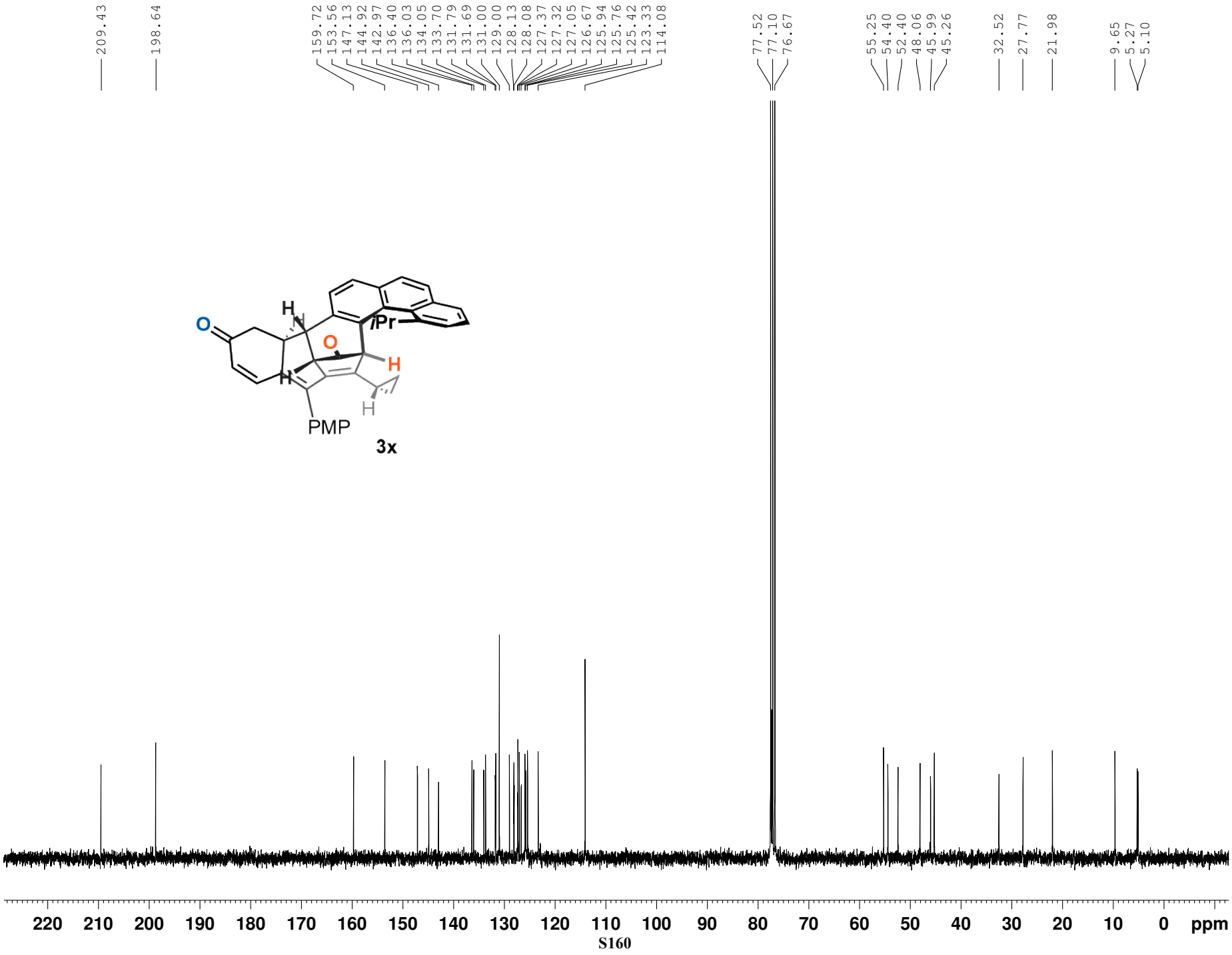
1.01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32.52
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9.65
5.27
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O
H
H
O
iPr
H
H
PMP
3x
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200
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180
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110
100
90
80
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60
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30
20
10
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5.705
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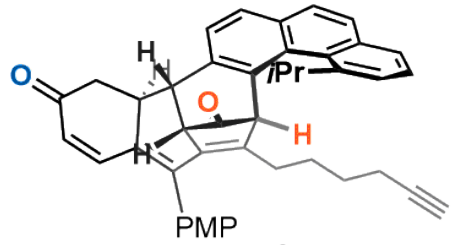

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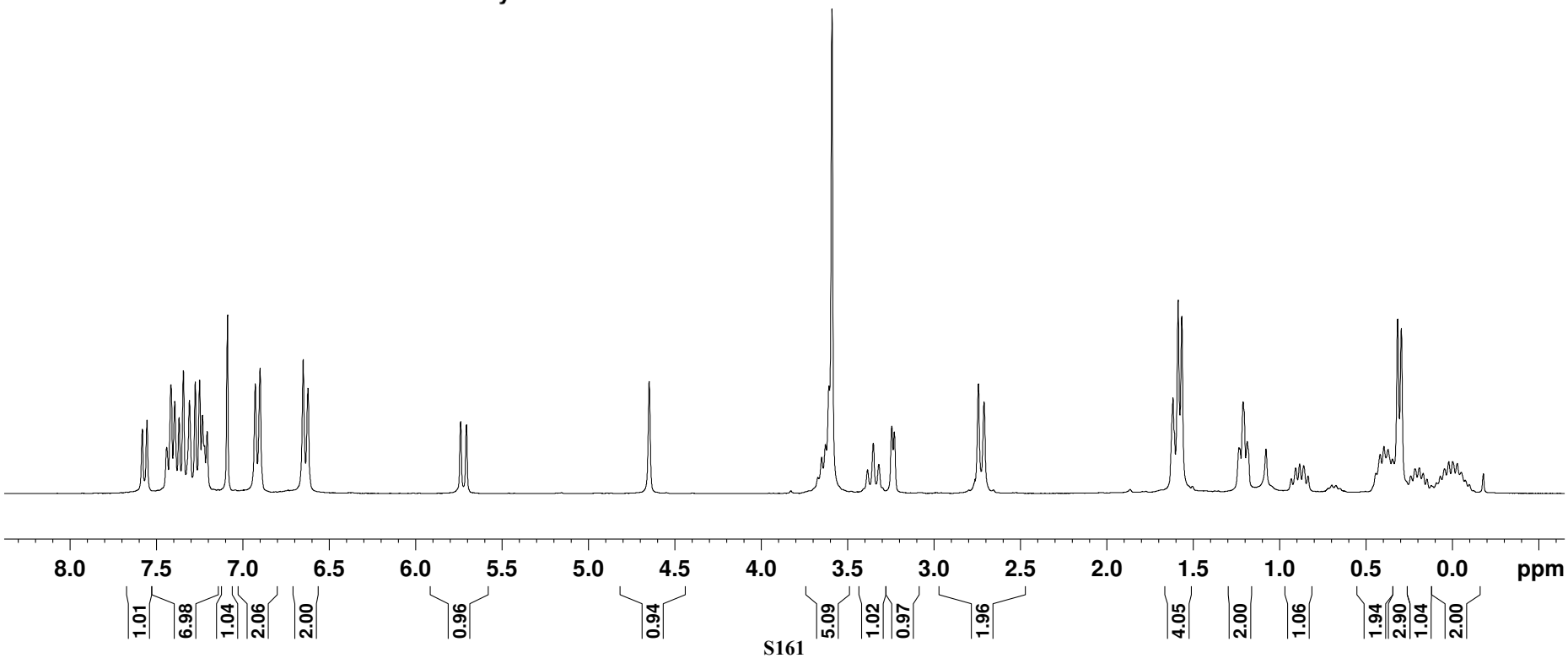

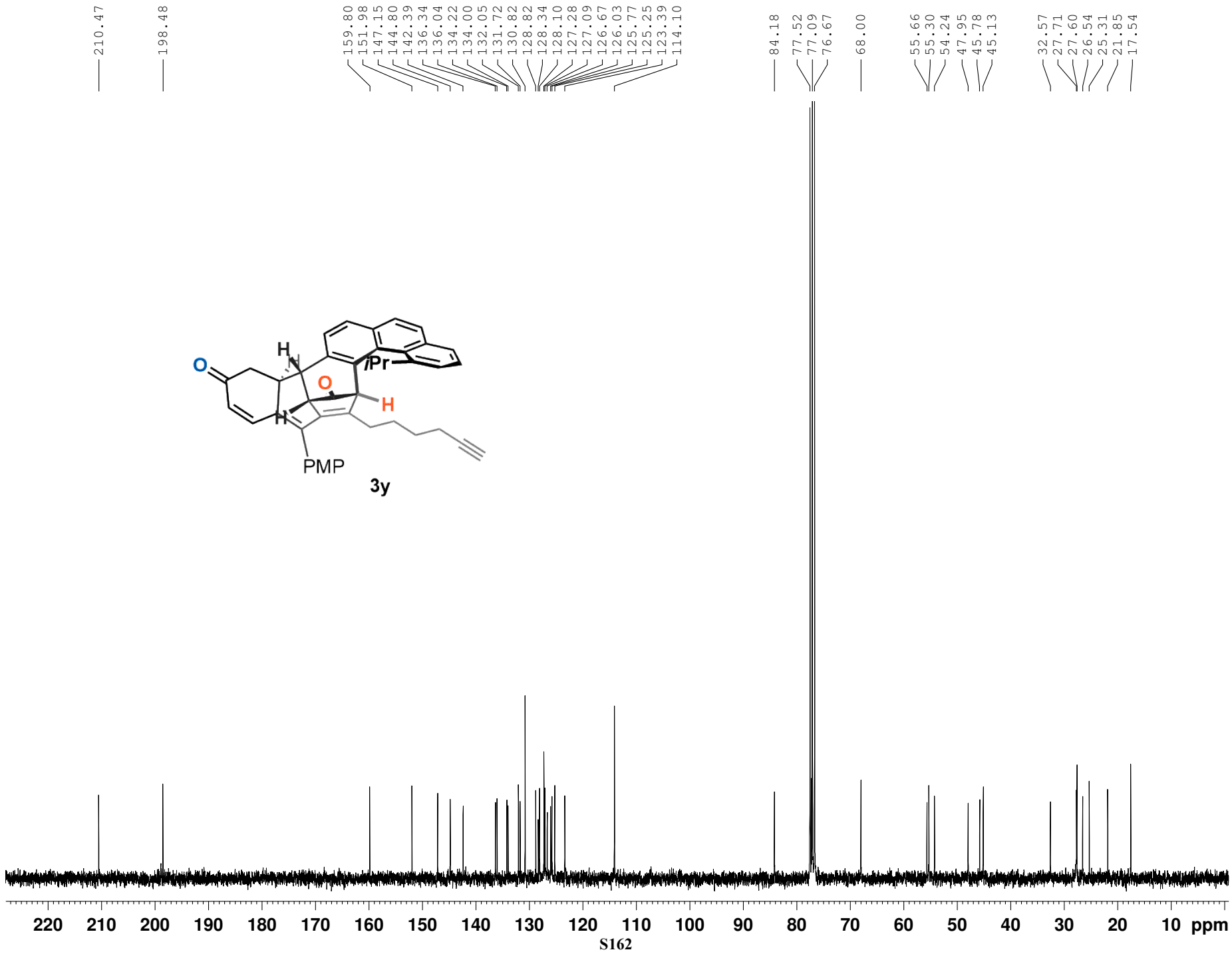
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76.67
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55.30
54.24
47.95
45.78
45.13
32.57
27.71
27.60
26.54
25.31
21.85
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H
H
iPr
O
H
H
PMP
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220
210
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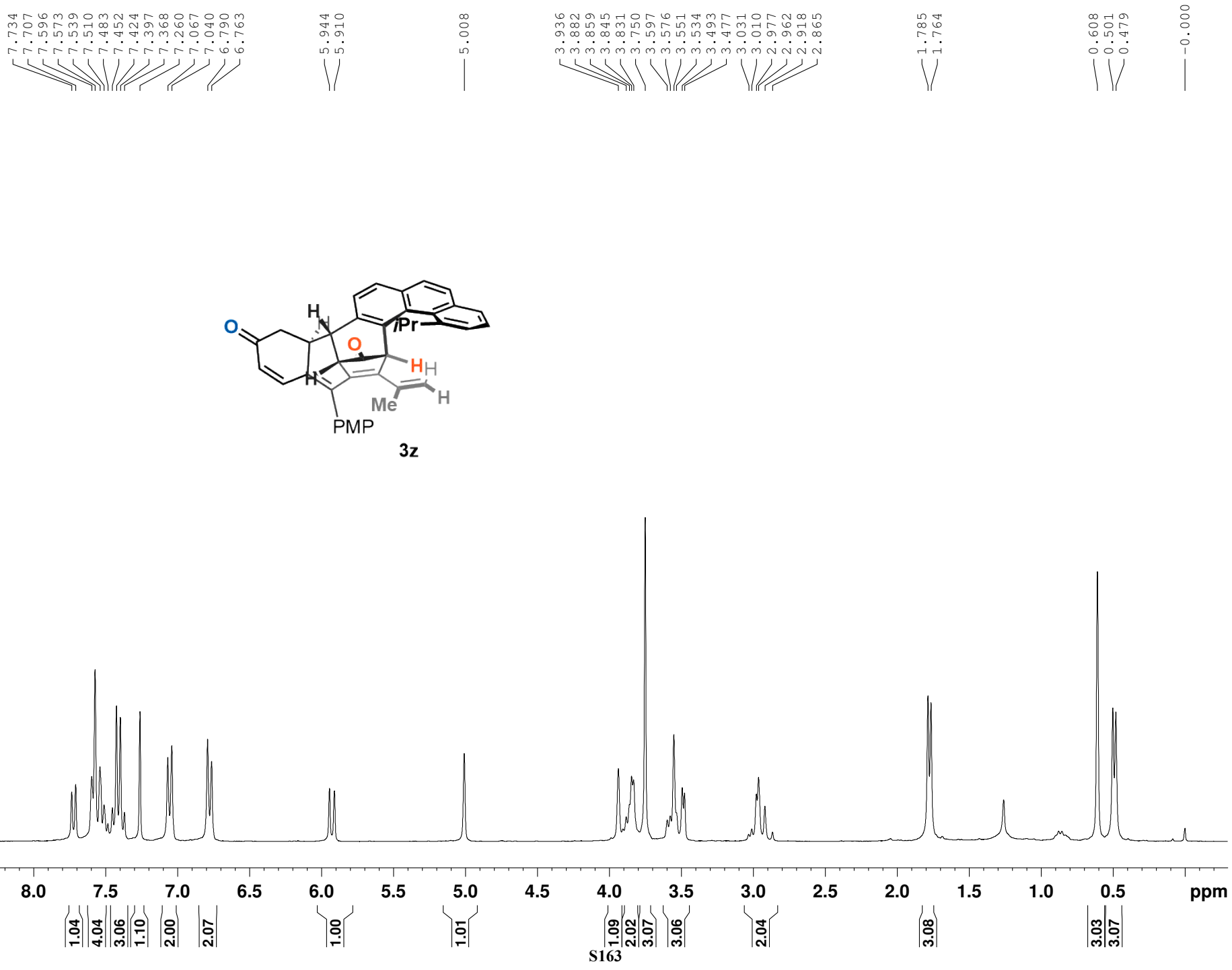
ppm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5.008
3.936
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3.845
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3.750
3.597
3.576
3.551
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H
N
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O
H
H
H
Me
H
PMP
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3.06
2.04
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125.24
123.25
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113.70
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77.09
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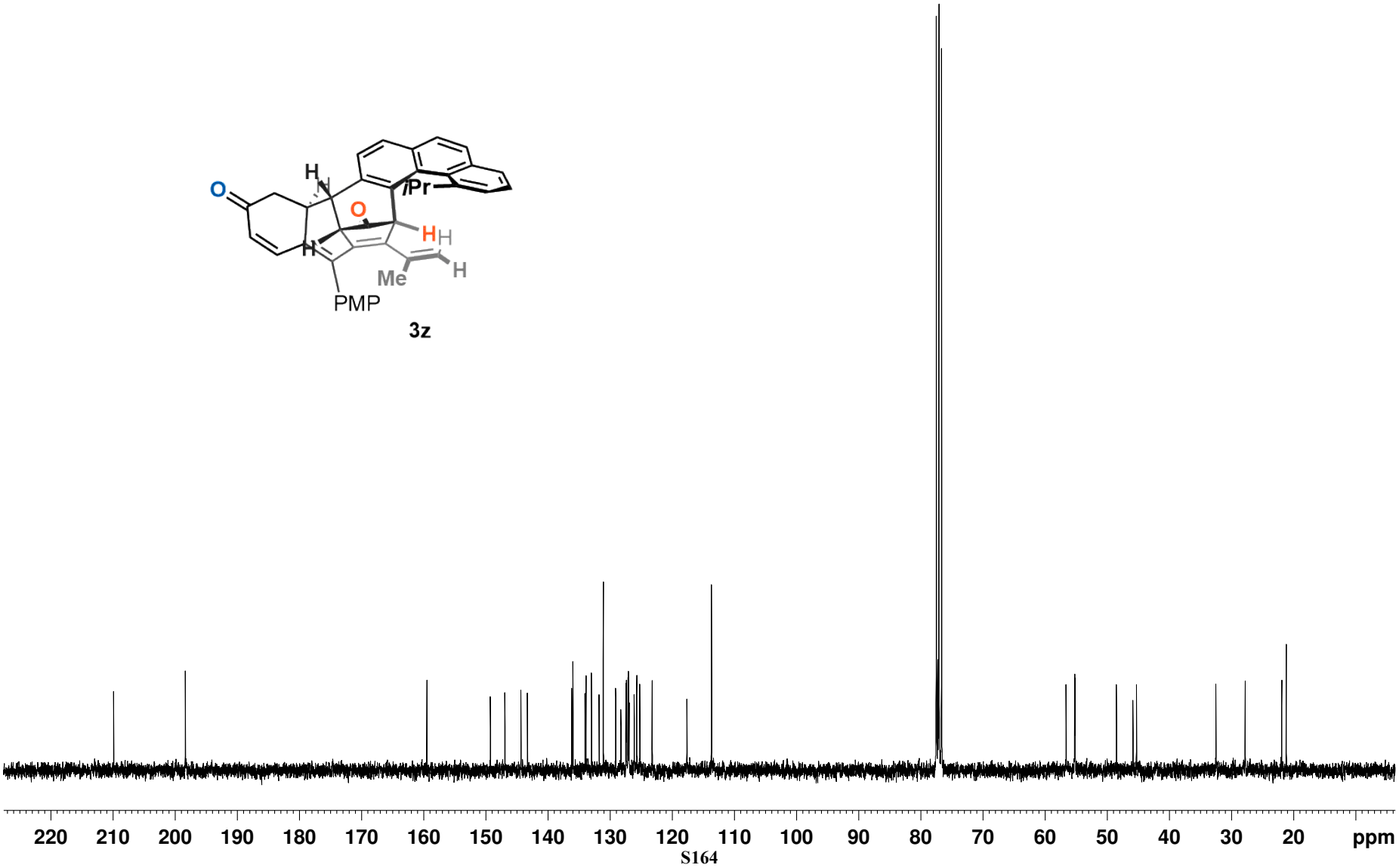
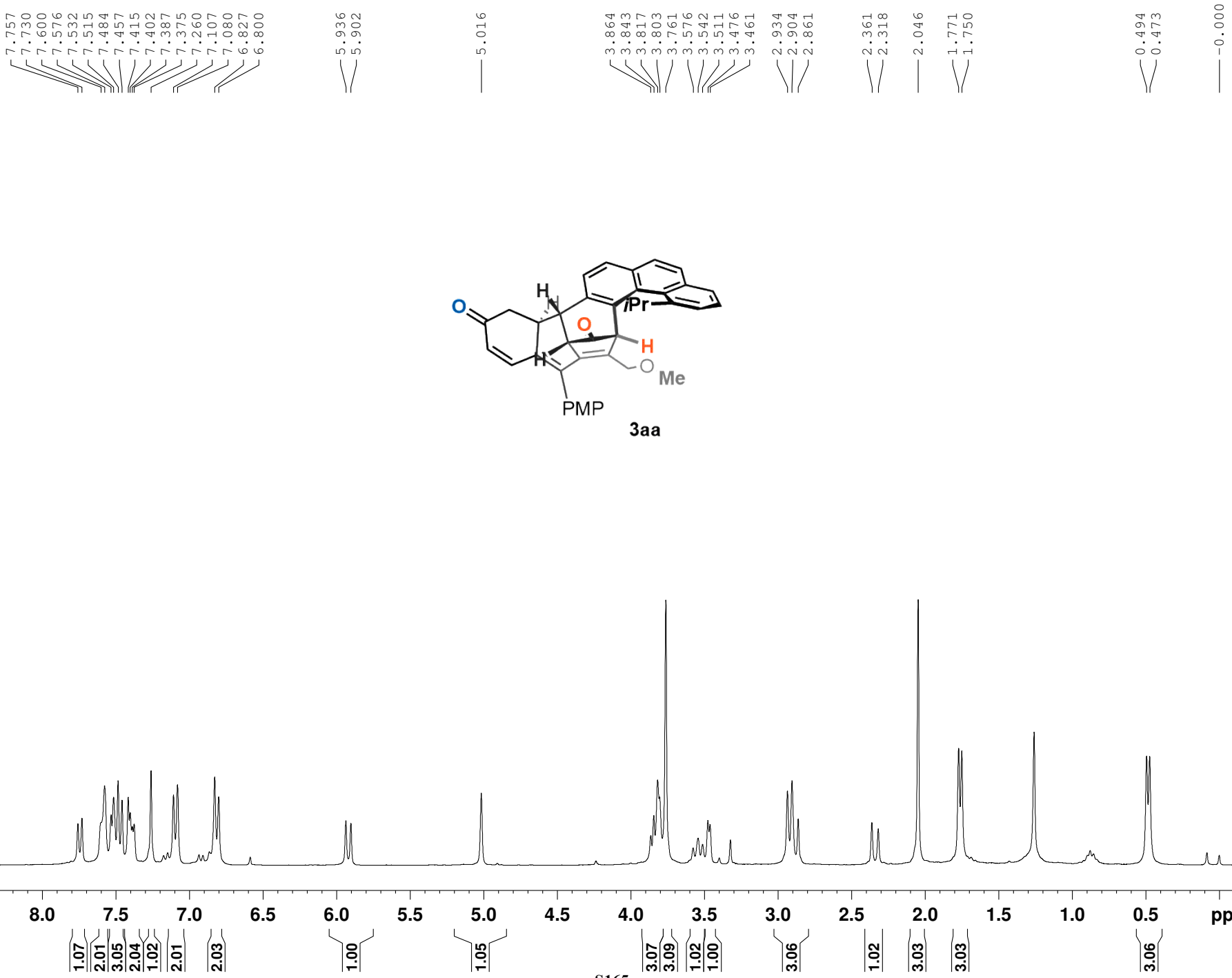
21.18

3z

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7.080
6.827
6.800
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5.902
5.016
3.864
3.843
3.817
3.803
3.761
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3.542
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3.476
3.461
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2.904
2.861
2.361
2.318
2.046
1.771
1.750
0.494
0.473
-0.000
O
H
N
iPr
O
H
H
O
Me
PMP
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5.5
5.0
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4.0
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3.0
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1.0
0.5
ppm
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2.01
3.05
2.04
1.02
2.01
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3.07
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1.02
1.00
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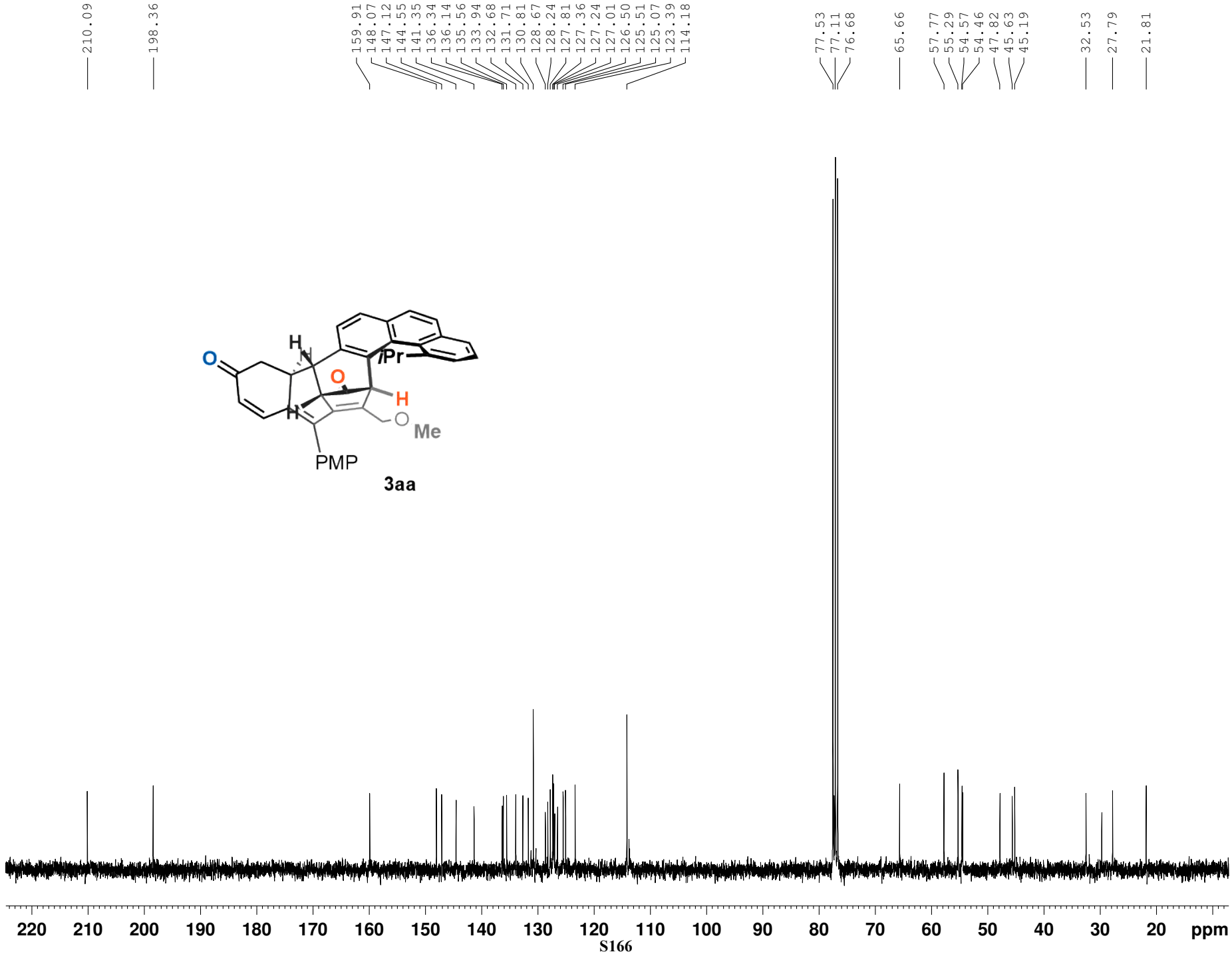
1.02
3.03
3.03
3.06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127.36
127.24
127.01
126.50
125.51
125.07
123.39
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77.11
76.68
65.66
57.77
55.29
54.57
54.46
47.82
45.63
45.19
32.53
27.79
21.81
O
H
N
iPr
O
H
H
O
Me
PMP
3aa
220
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160
150
140
130
120
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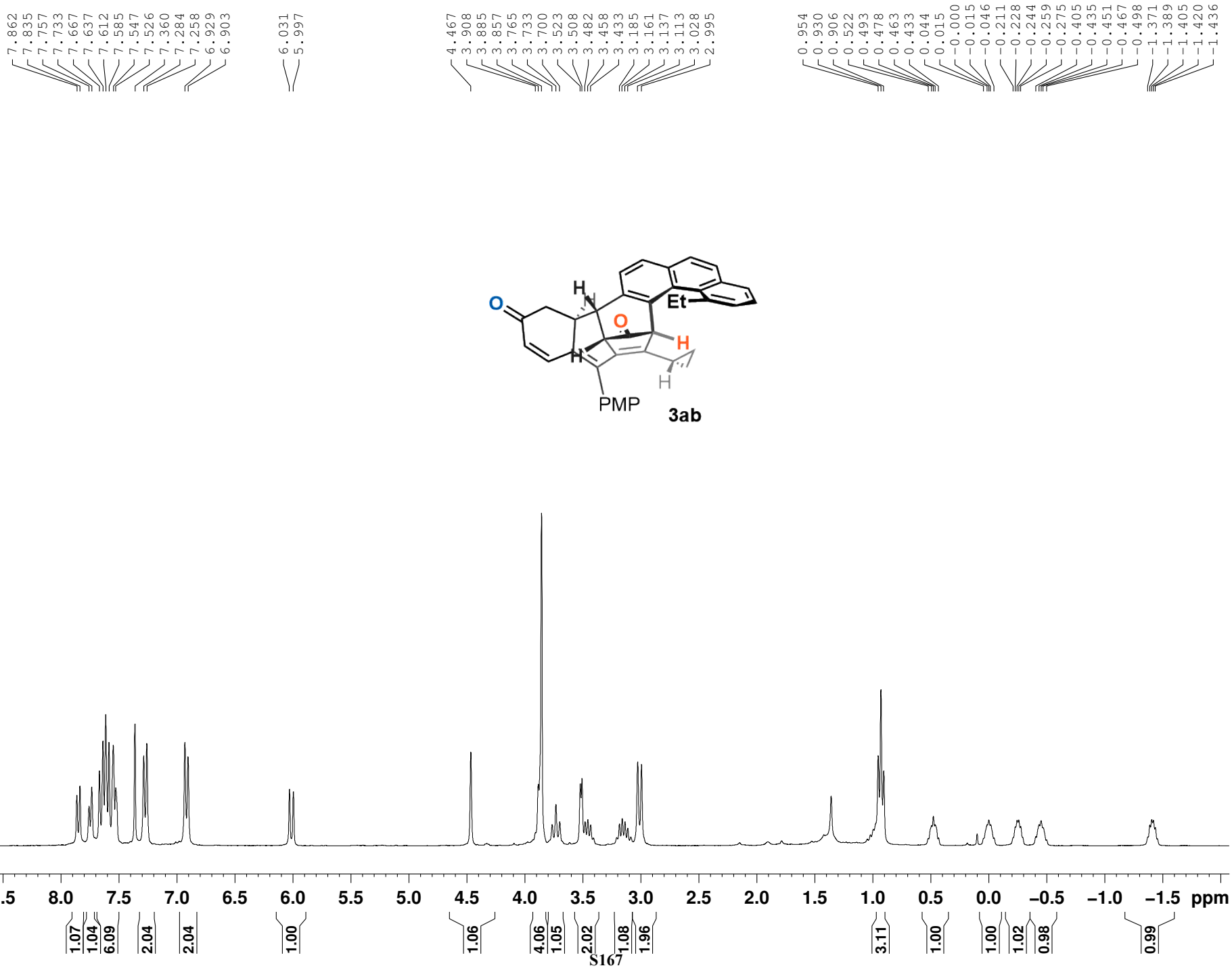
80
70
60
50
40
30
20
ppm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7.526
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6.031
5.997
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3.908
3.885
3.857
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3.733
3.700
3.523
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3.458
3.433
3.185
3.161
3.137
3.113
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0.493
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0.463
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-0.000
-0.015
-0.046
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-0.228
-0.244
-0.259
-0.275
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-0.435
-0.451
-0.467
-0.498
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-1.389
-1.405
-1.420
-1.436
O
H
H
Et
O
H
H
PMP
3ab
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7.5
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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
−1.5
ppm
1.07
1.04
6.09
2.04
2.04
1.00
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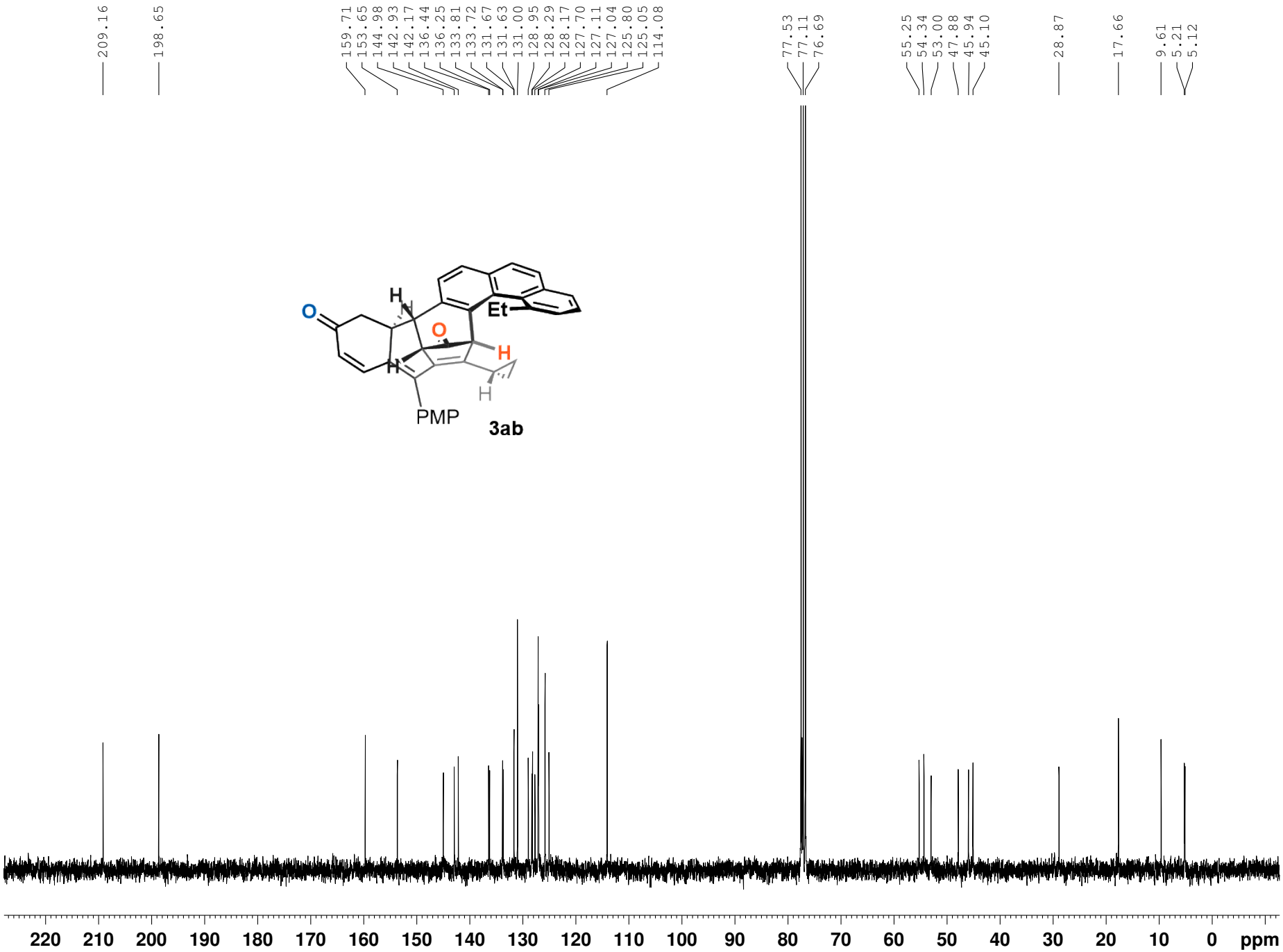
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128.17
127.70
127.11
127.04
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77.11
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53.00
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45.10
28.87
17.66
9.61
5.21
5.12
O
H
N
Et
O
H
H
H
PMP
3ab
220
210
200
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20
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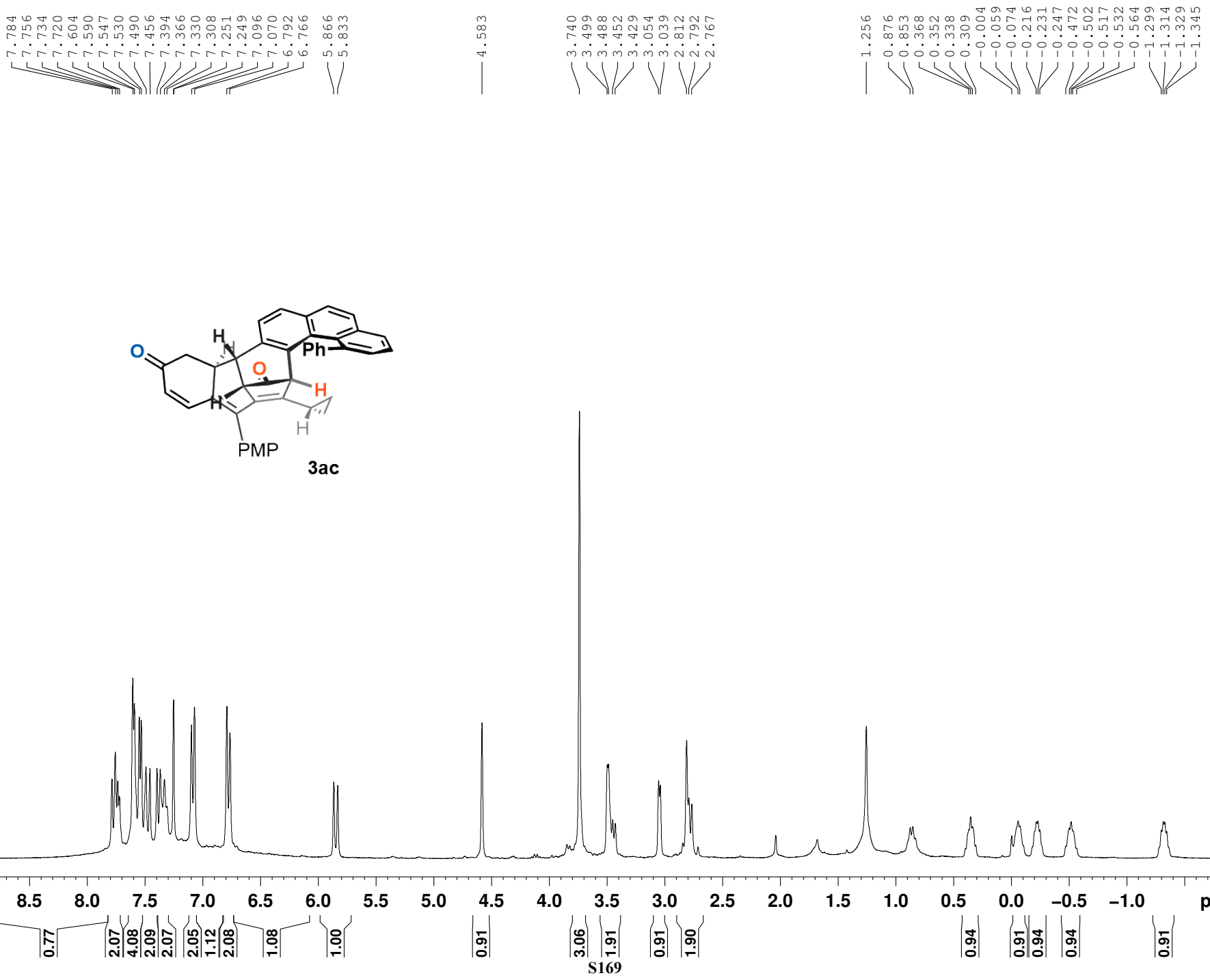
ppm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3.452
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0.309
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-0.517
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-1.329
-1.345
O
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H
O
Ph
H
H
PMP
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−0.5
−1.0
ppm
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2.08
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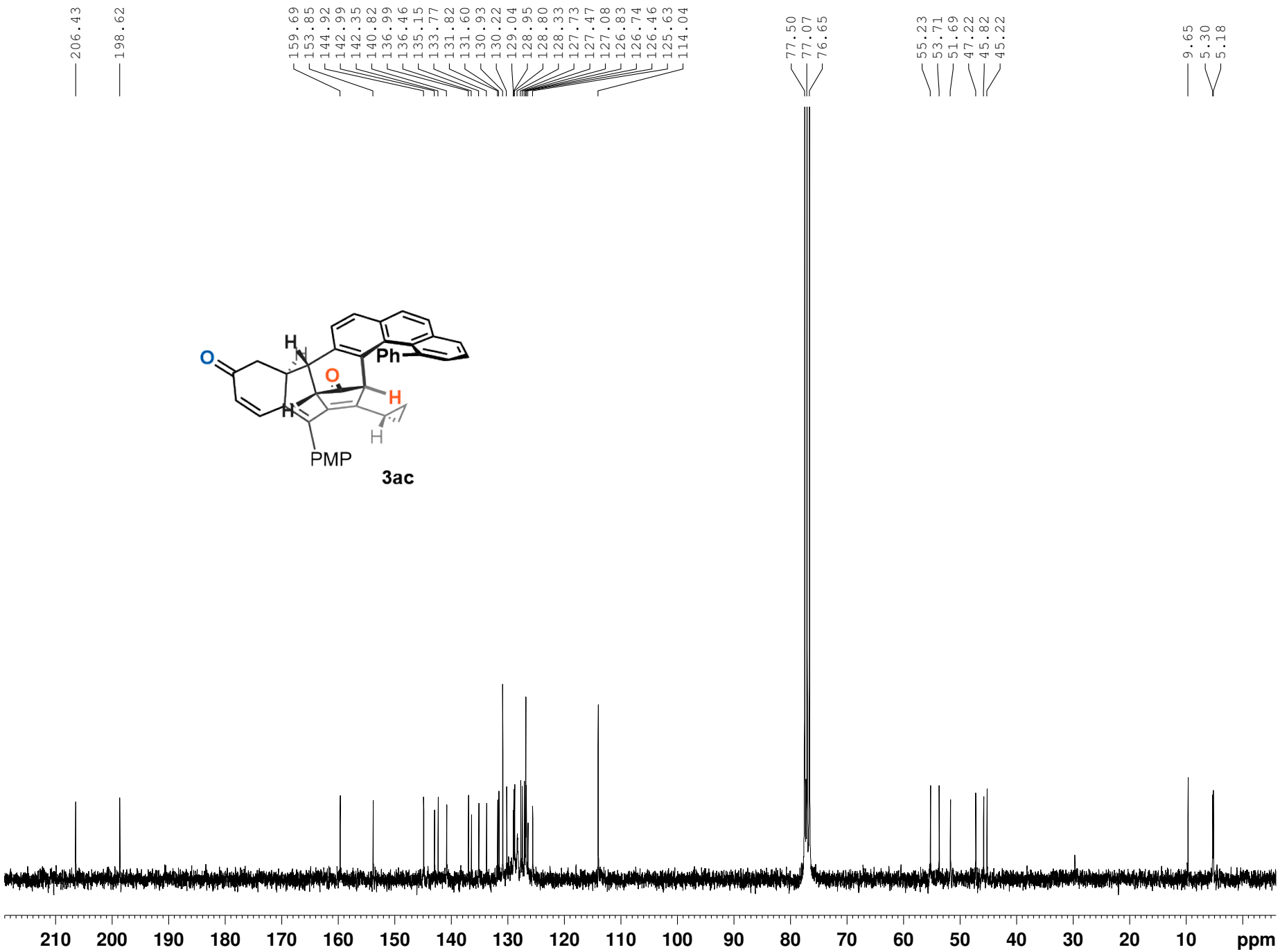
0.94
0.91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114.04
77.50
77.07
76.65
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51.69
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45.22
9.65
5.30
5.18
O
H
N
Ph
O
H
H
H
PMP
3ac
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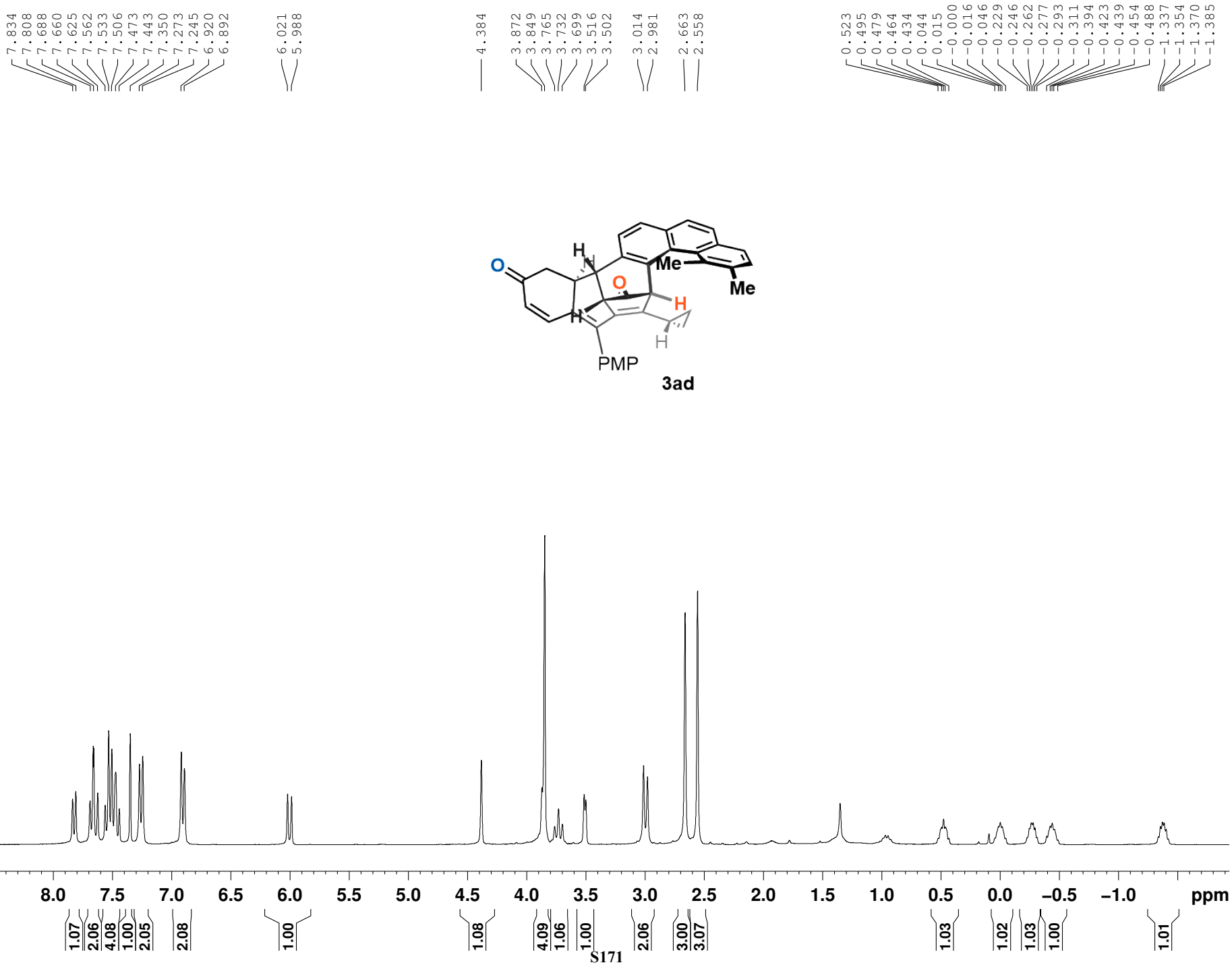
10
ppm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7.245
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6.892
6.021
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3.765
3.732
3.699
3.516
3.502
3.014
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0.015
-0.000
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-0.394
-0.423
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H
Me
Me
O
H
H
H
PMP
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−1.0
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2.05
2.08
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1.08
4.09
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1.00
2.06
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3.07
1.03
1.02
1.03
1.00
1.01

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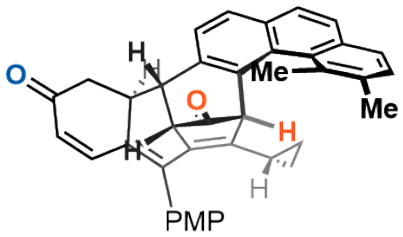

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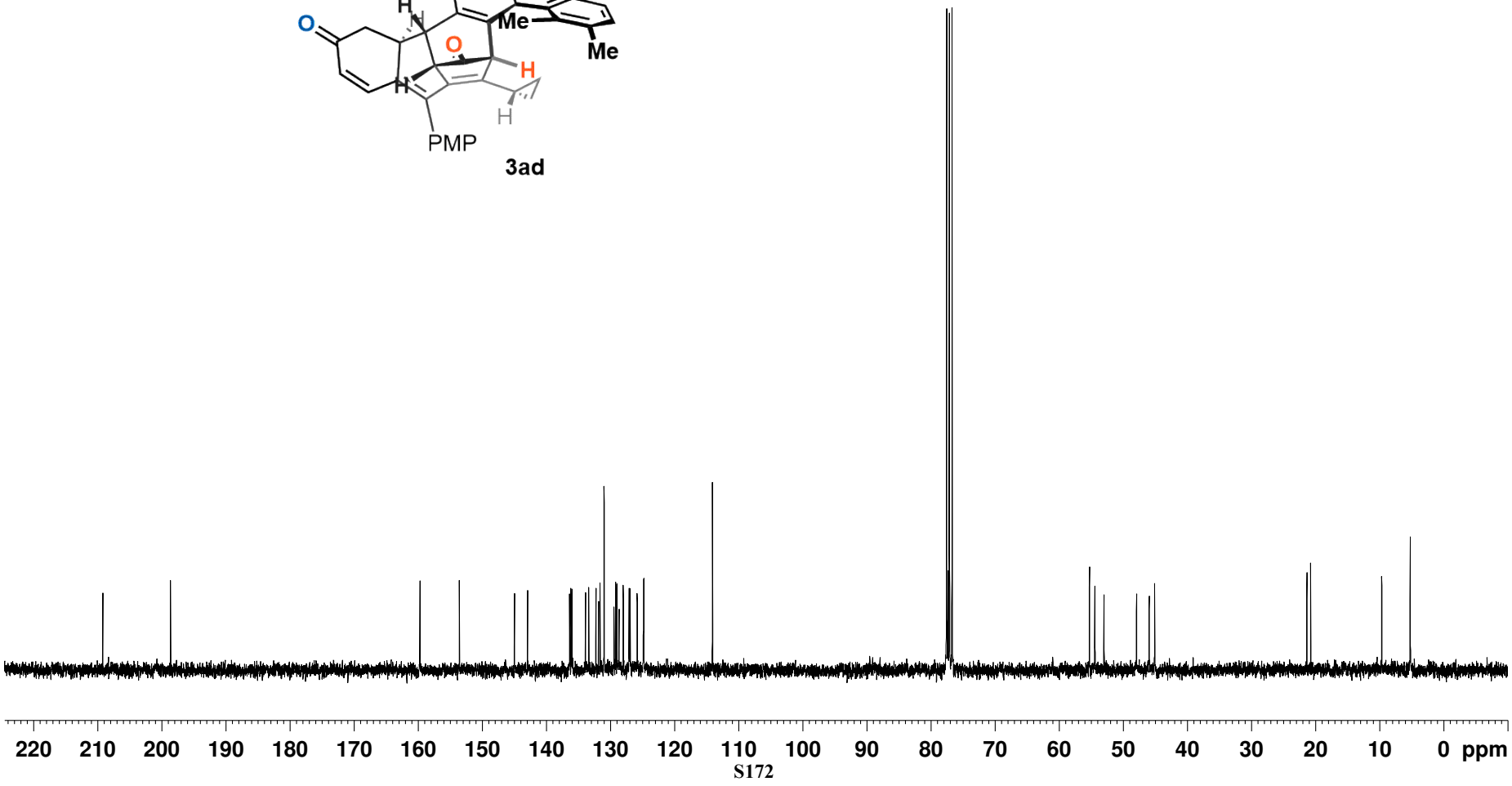

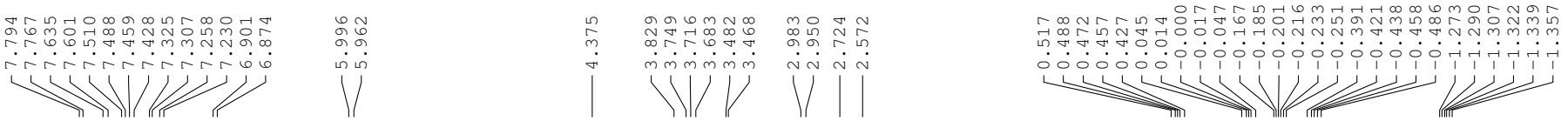
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3.683
3.482
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2.983
2.950
2.724
2.572
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0.488
0.472
0.457
0.427
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-0.017
-0.047
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-0.185
-0.201
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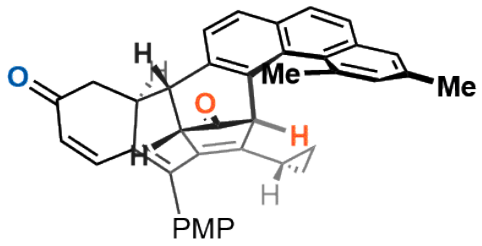
O
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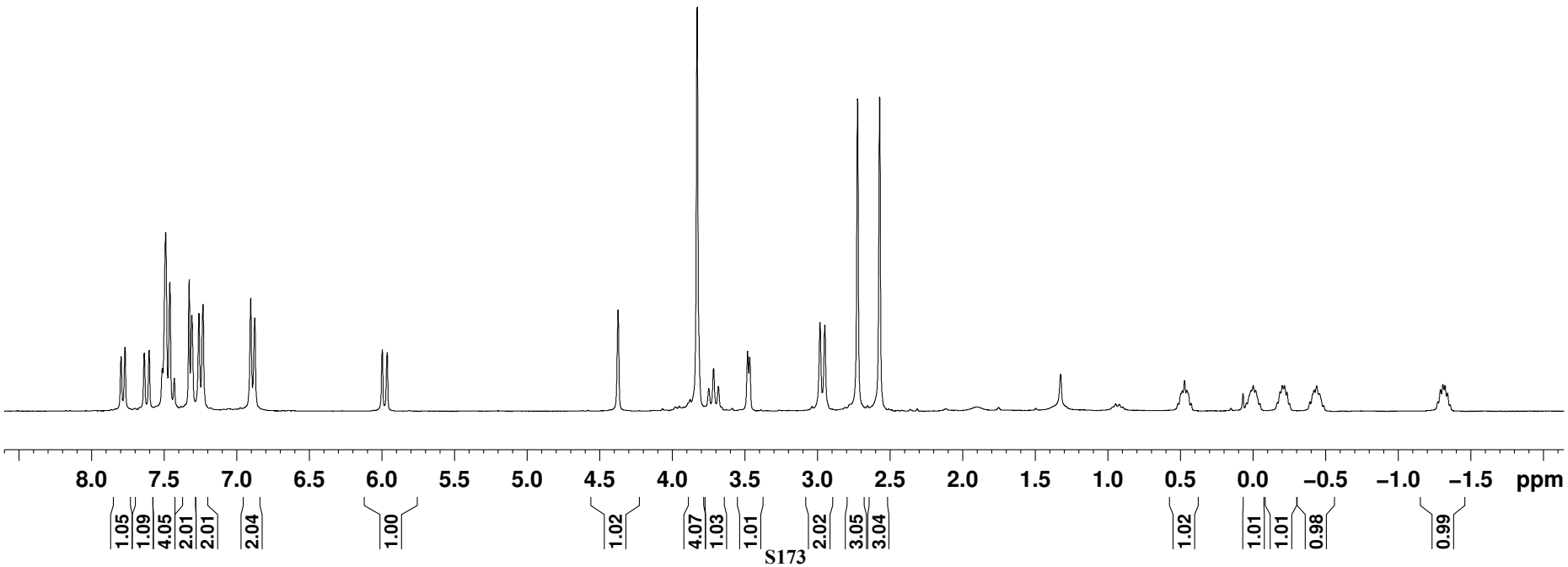
H
Me
Me
O
H
H
H
PMP

3ae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2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ppm
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1.09
4.05
2.01
2.01
2.04
1.00
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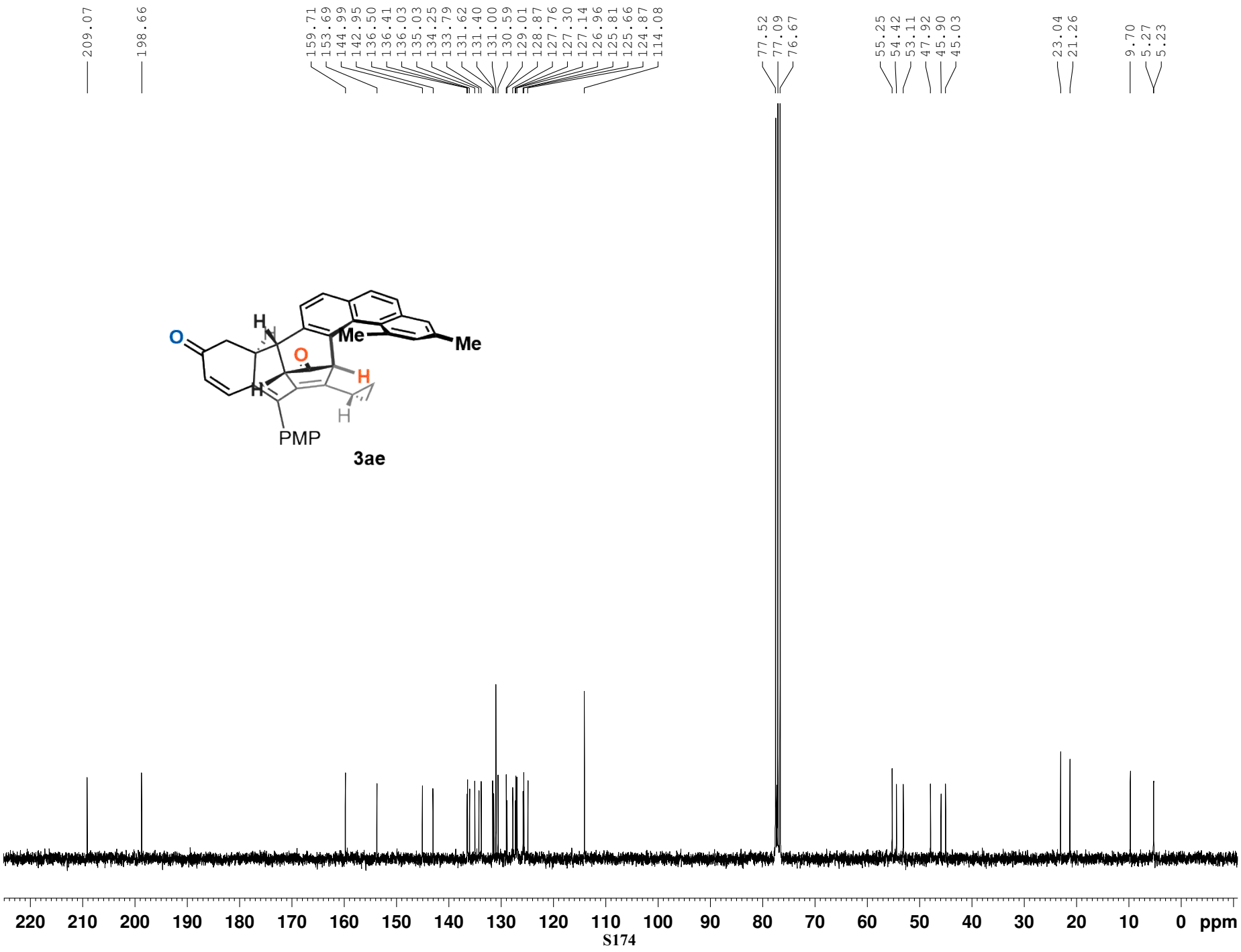
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125.81
125.66
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77.09
76.67
55.25
54.42
53.11
47.92
45.90
45.03
23.04
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5.27
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O
H
N
Me
Me
O
H
H
H
PMP
3ae
220
210
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150
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120
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100
90
80
70
60
50
40
30
20
10
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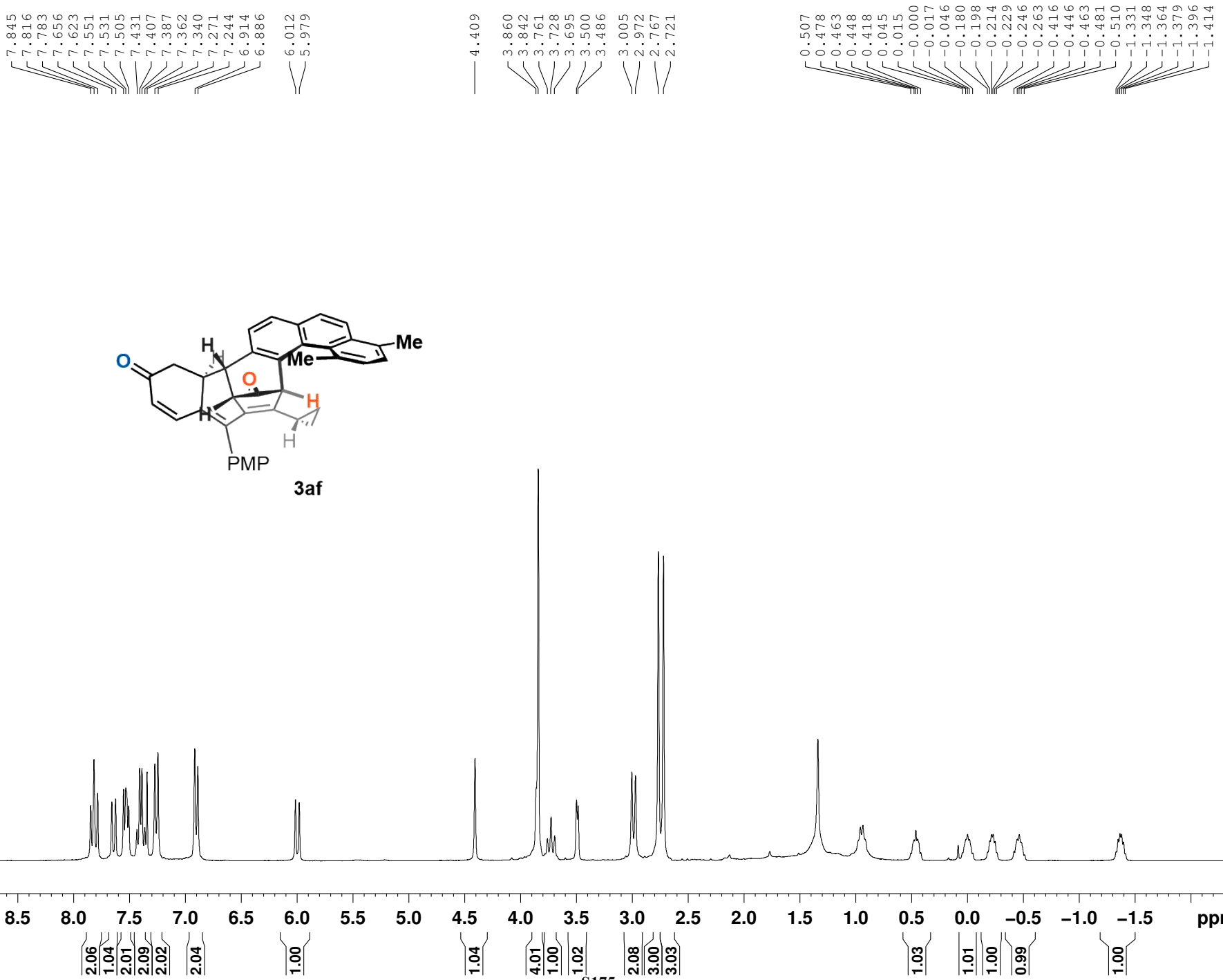
ppm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7.362
7.340
7.271
7.244
6.914
6.886
6.012
5.979
4.409
3.860
3.842
3.761
3.728
3.695
3.500
3.486
3.005
2.972
2.767
2.721
0.507
0.478
0.463
0.448
0.418
0.045
0.015
0.000
-0.017
-0.046
-0.180
-0.198
-0.214
-0.229
-0.246
-0.263
-0.416
-0.446
-0.463
-0.481
-0.510
-1.331
-1.348
-1.364
-1.379
-1.396
-1.414
O
H
H
Me
Me
O
H
H
H
PMP
3af
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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
−1.5
ppm
2.06
1.04
2.01
2.09
2.02
2.04
1.00
1.04
4.01
1.00
1.02
2.08
3.00
3.03
1.03
1.01
1.00
0.99
1.00

209.15
198.74
159.69
153.77
145.05
142.98
136.46
136.38
133.73
132.92
132.69
131.62
131.29
131.02
130.98
129.35
129.03
128.95
128.23
128.13
128.03
127.03
125.78
125.43
122.99
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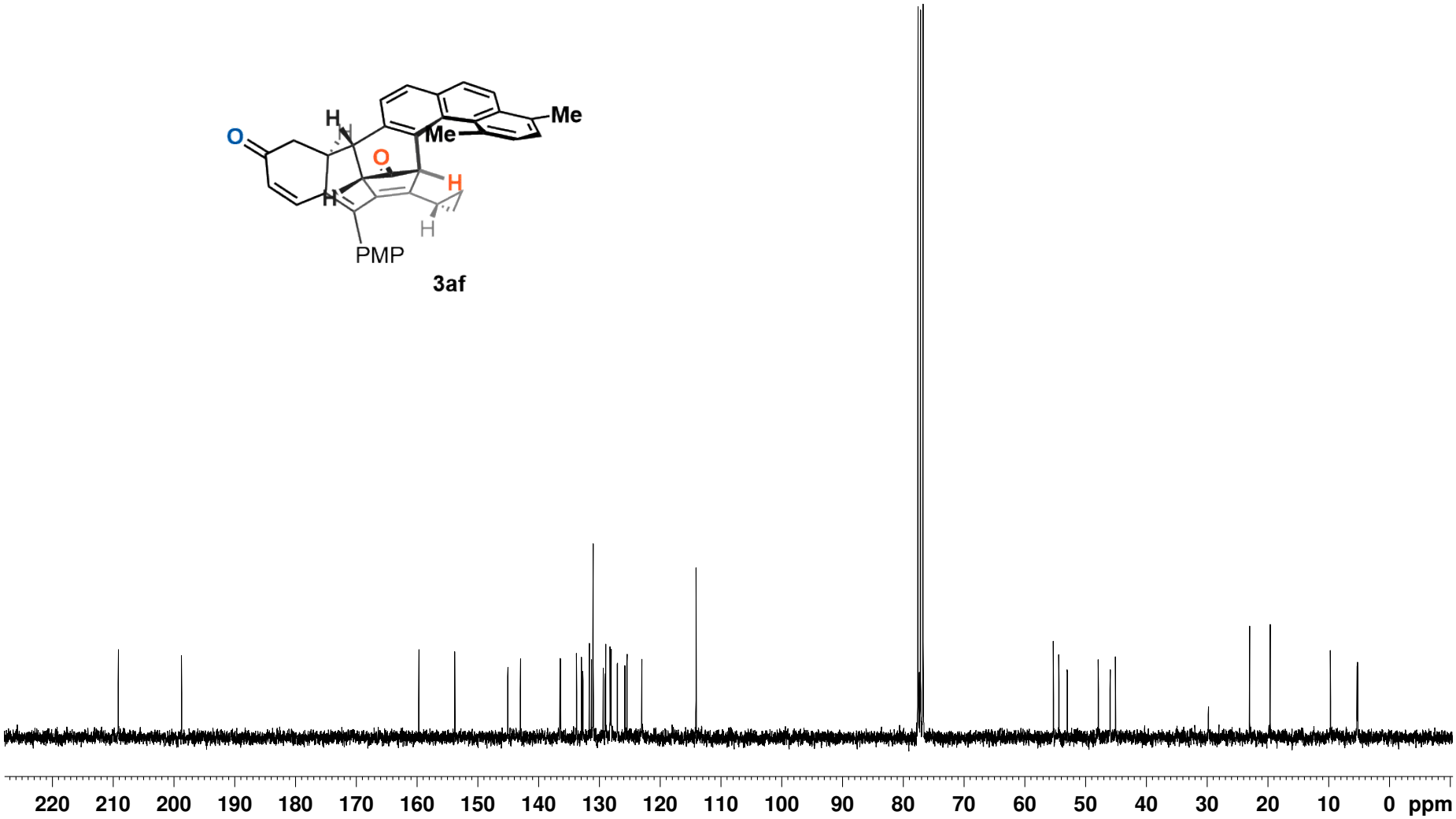

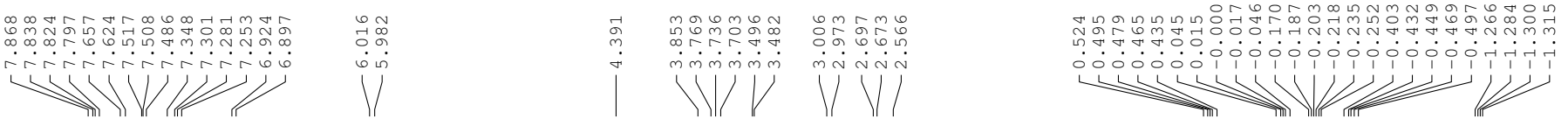
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7.348
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6.897
6.016
5.982
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3.703
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3.482
3.006
2.973
2.697
2.673
2.566
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0.495
0.479
0.465
0.435
0.045
0.015
-0.000
-0.017
-0.046
-0.170
-0.187
-0.203
-0.218
-0.235
-0.252
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-0.432
-0.449
-0.469
-0.497
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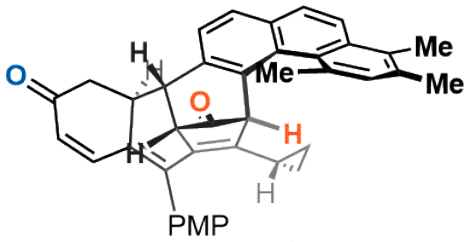
-1.284
-1.300
-1.315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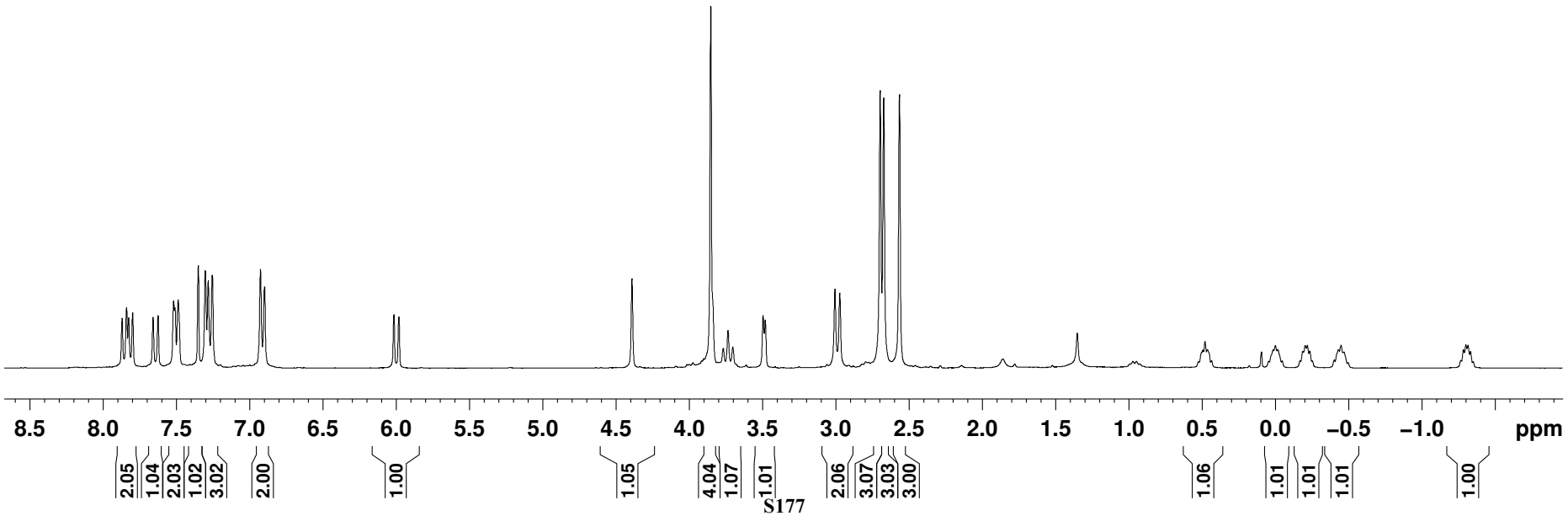
N
Me
Me
Me
O
H
H
H
PMP

3ag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6.0
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5.0
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4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
ppm
2.05
1.04
2.03
1.02
3.02
2.00
1.00
1.05
4.04
1.07
1.01
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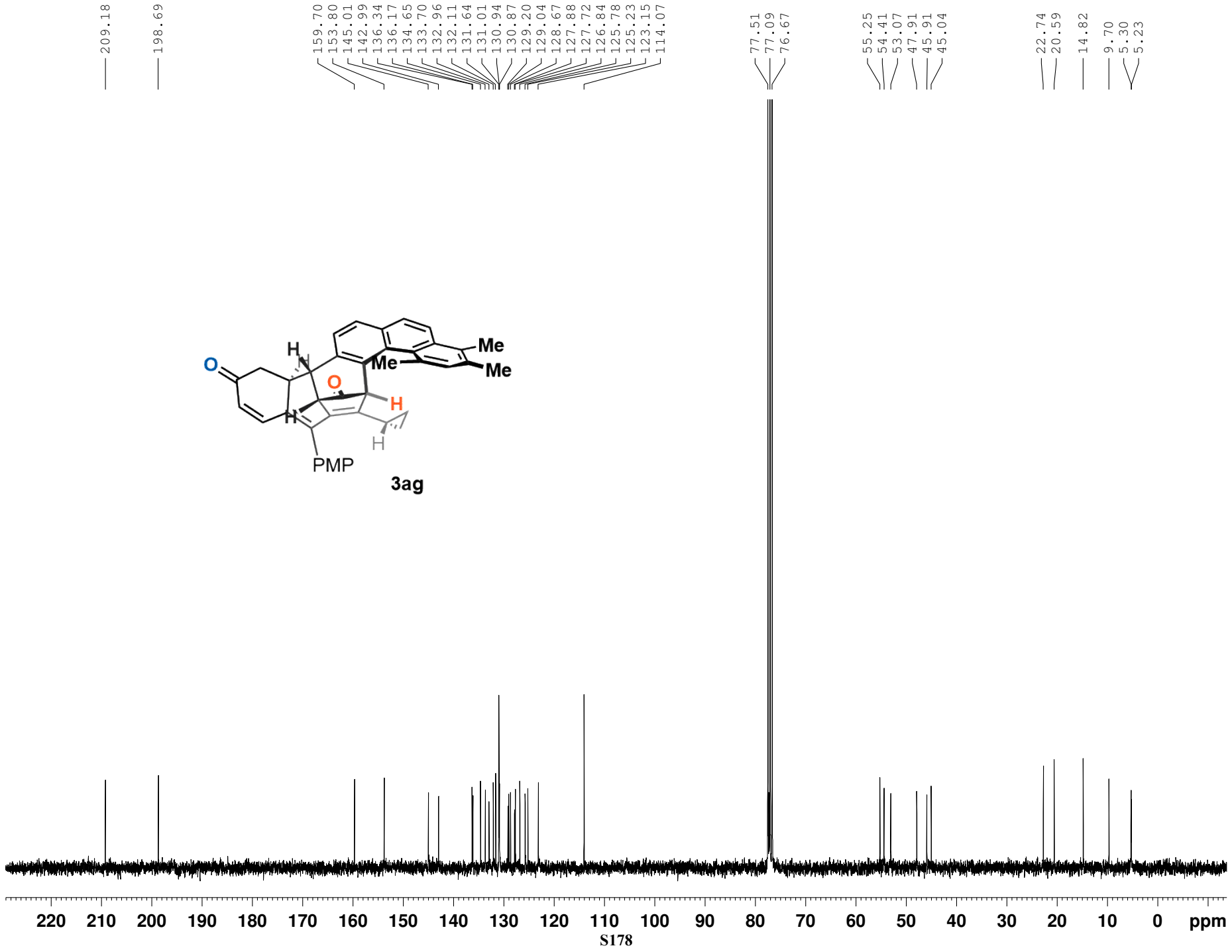
3.00
1.06
1.01
1.01
1.01
1.00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132.96
132.11
131.64
131.01
130.94
130.87
129.20
129.04
128.67
127.88
127.72
126.84
125.78
125.23
123.15
114.07
77.51
77.09
76.67
55.25
54.41
53.07
47.91
45.91
45.04
22.74
20.59
14.82
9.70
5.30
5.23
O
H
H
Me
Me
Me
O
H
H
H
PMP
3ag
220
210
200
190
180
170
160
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140
130
120
110
100
90
80
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60
50
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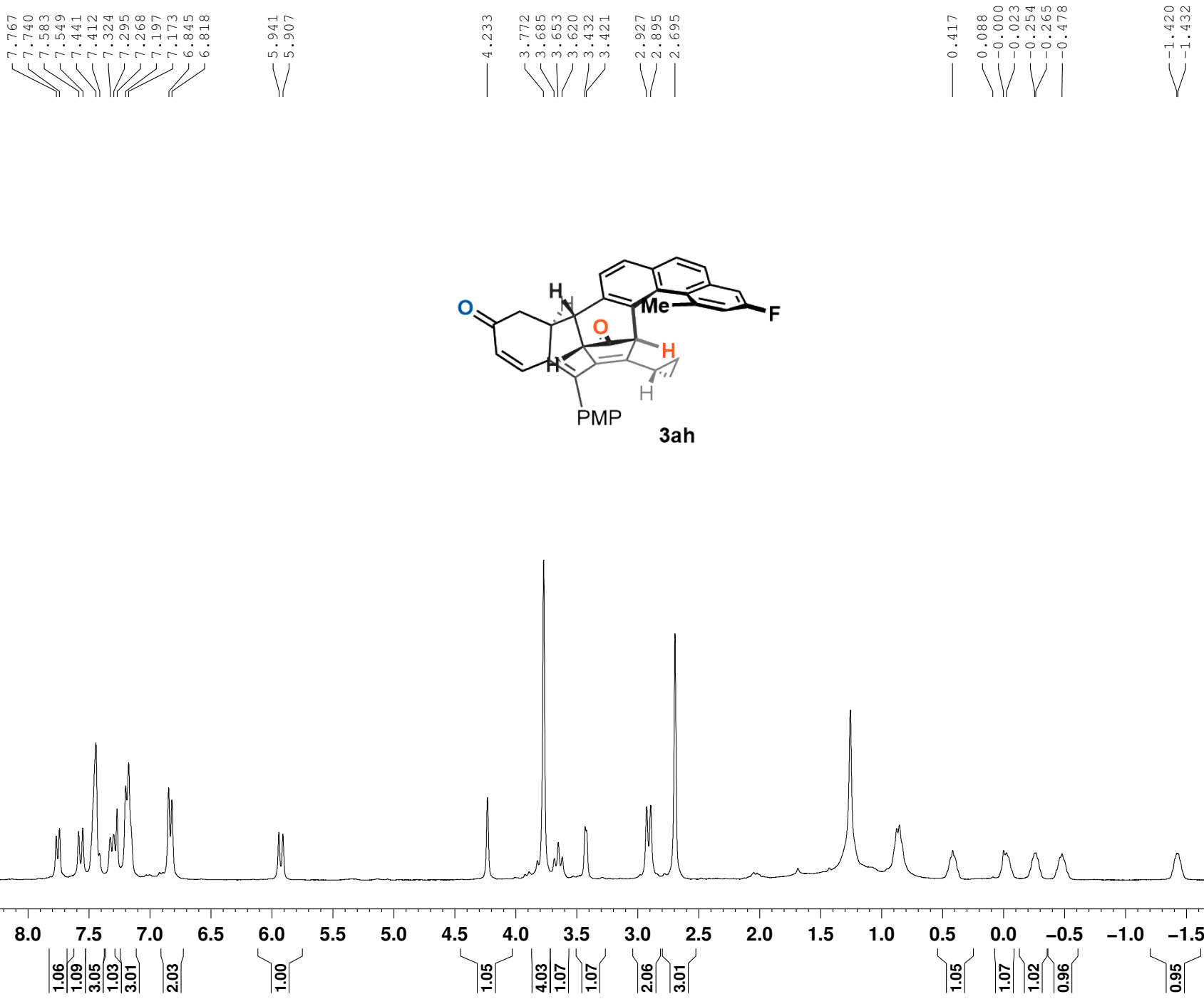
30
20
10
0
ppm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7.173
6.845
6.818
5.941
5.907
4.233
3.772
3.685
3.653
3.620
3.432
3.421
2.927
2.895
2.695
0.417
0.088
0.000
-0.023
-0.254
-0.265
-0.478
-1.420
-1.432
O
H
H
Me
F
O
H
H
H
PMP
3ah
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ppm
1.06
1.09
3.05
1.03
3.01
2.03
1.00
1.05
4.03
1.07
1.07
2.06
3.01
1.05
1.07
1.02
0.96
0.95

208.84
198.65
159.74
153.44
144.99
142.87
138.28
138.17
137.10
136.06
135.45
135.34
133.90
131.61
131.16
131.01
128.86
128.63
128.20
127.38
127.10
126.51
126.00
125.87
116.98
116.68
114.10
109.72
109.44
77.54
77.11
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54.31
52.98
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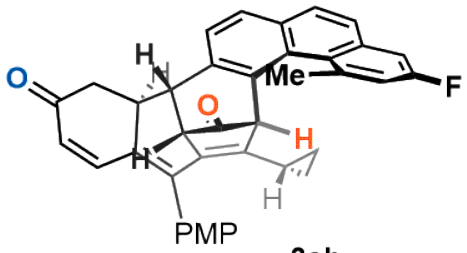
5.22

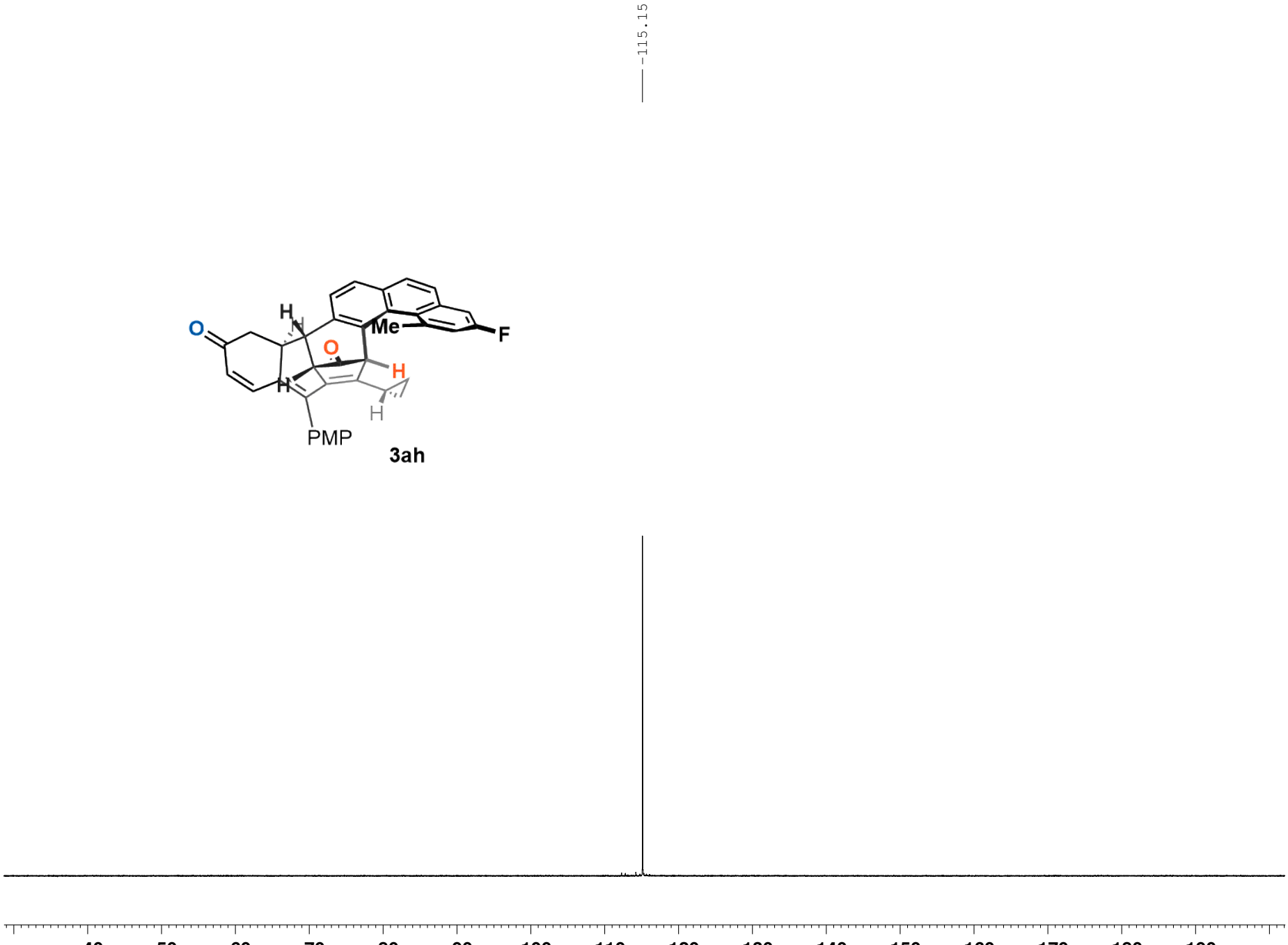


3ah

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

O
H
H
O
Me
F
H
H
H
PMP

3ah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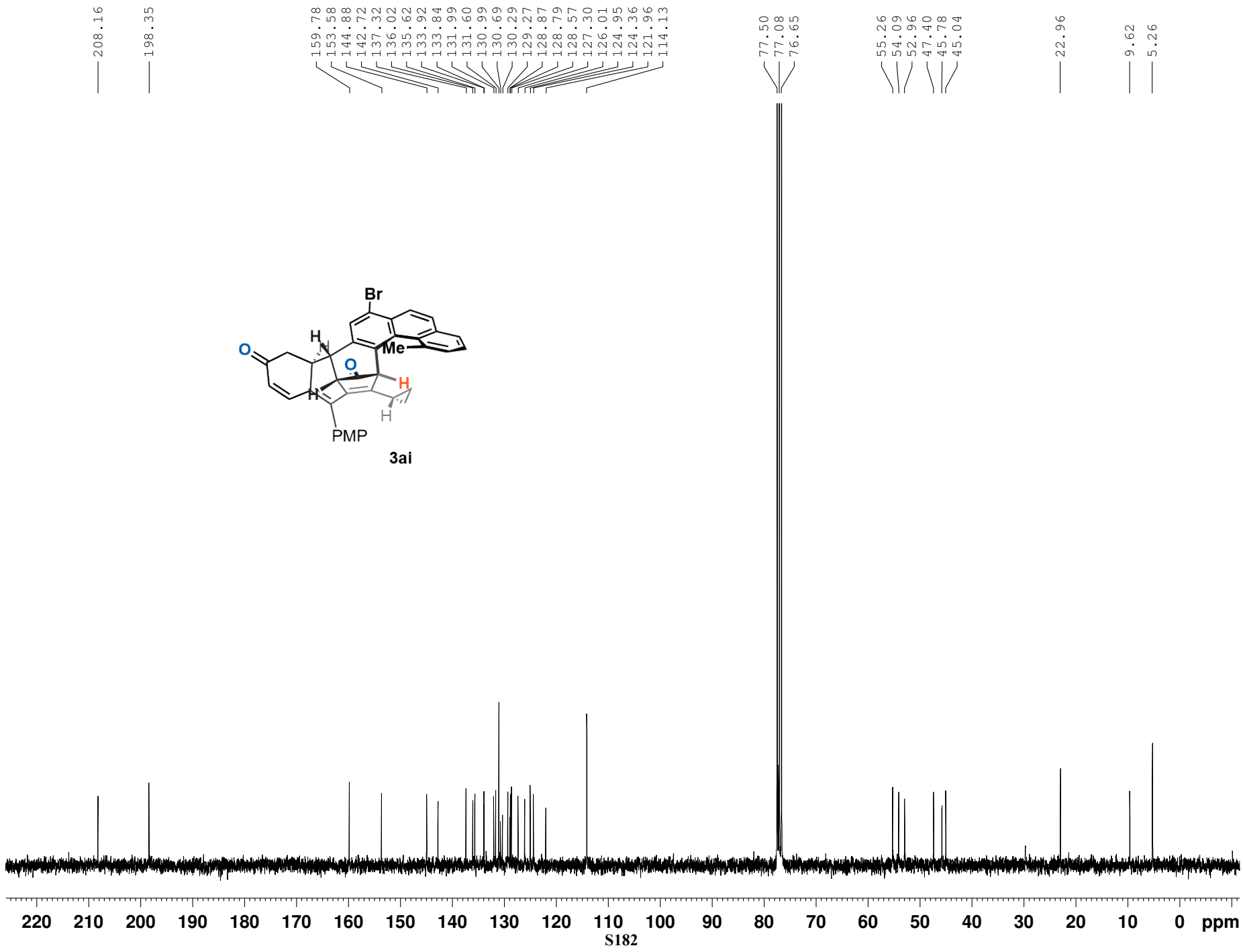
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
ppm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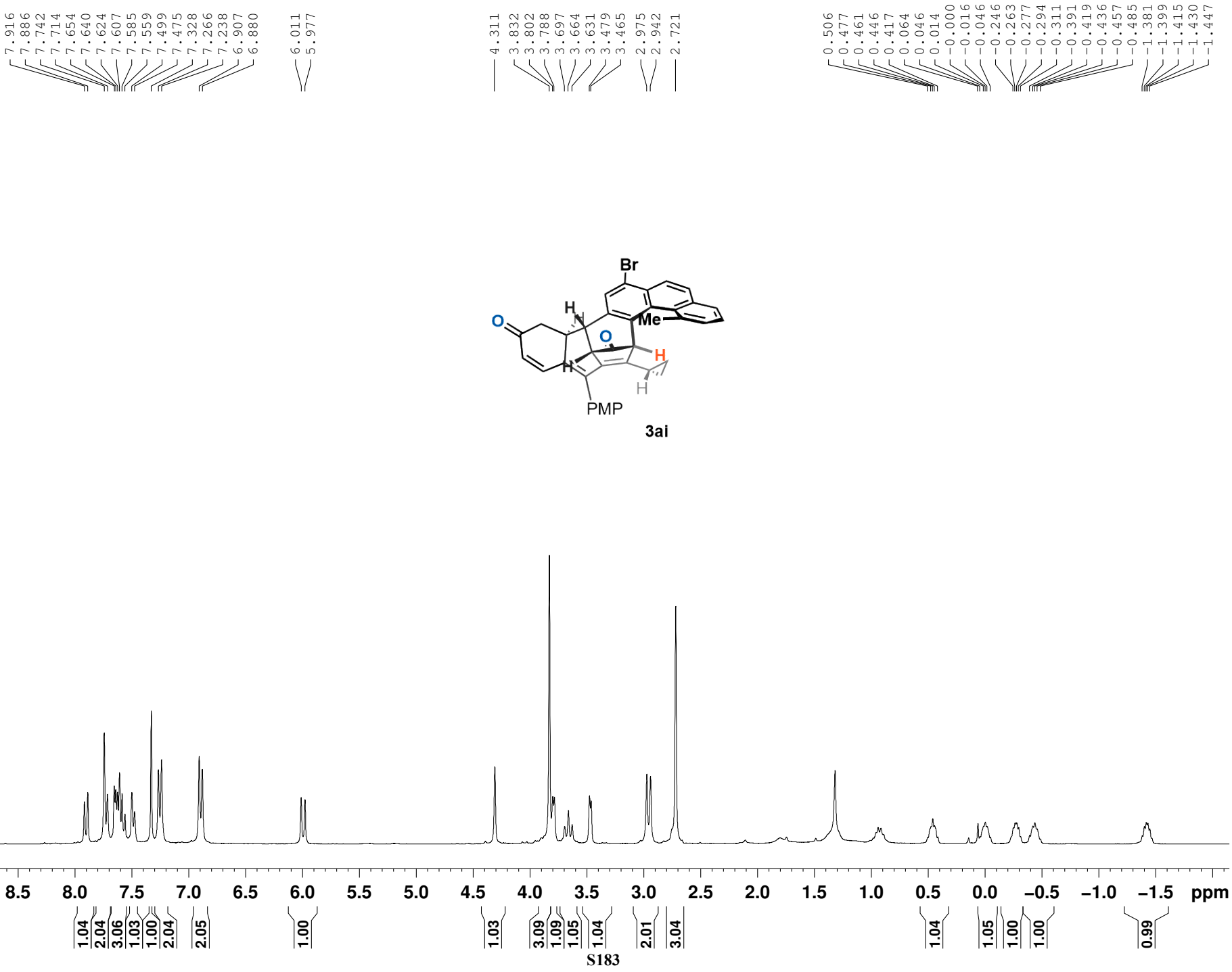
144.88
142.72
137.32
136.02
135.62
133.92
133.84
131.99
131.60
130.99
130.69
130.29
129.27
128.87
128.79
128.57
127.30
126.01
124.95
124.36
121.96
114.13
77.50
77.08
76.65
55.26
54.09
52.96
47.40
45.78
45.04
22.96
9.62
5.26
Br
O
H
H
Me
O
H
H
PMP
3ai
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.475
7.328
7.266
7.238
6.907
6.880
6.011
5.977
4.311
3.832
3.802
3.788
3.697
3.664
3.631
3.479
3.465
2.975
2.942
2.721
0.506
0.477
0.461
0.446
0.417
0.064
0.046
0.014
-0.000
-0.016
-0.046
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-0.263
-0.277
-0.294
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-0.419
-0.436
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-0.485
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-1.399
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-1.430
-1.447
Br
Me
O
O
H
H
H
H
PMP
3ai
8.5
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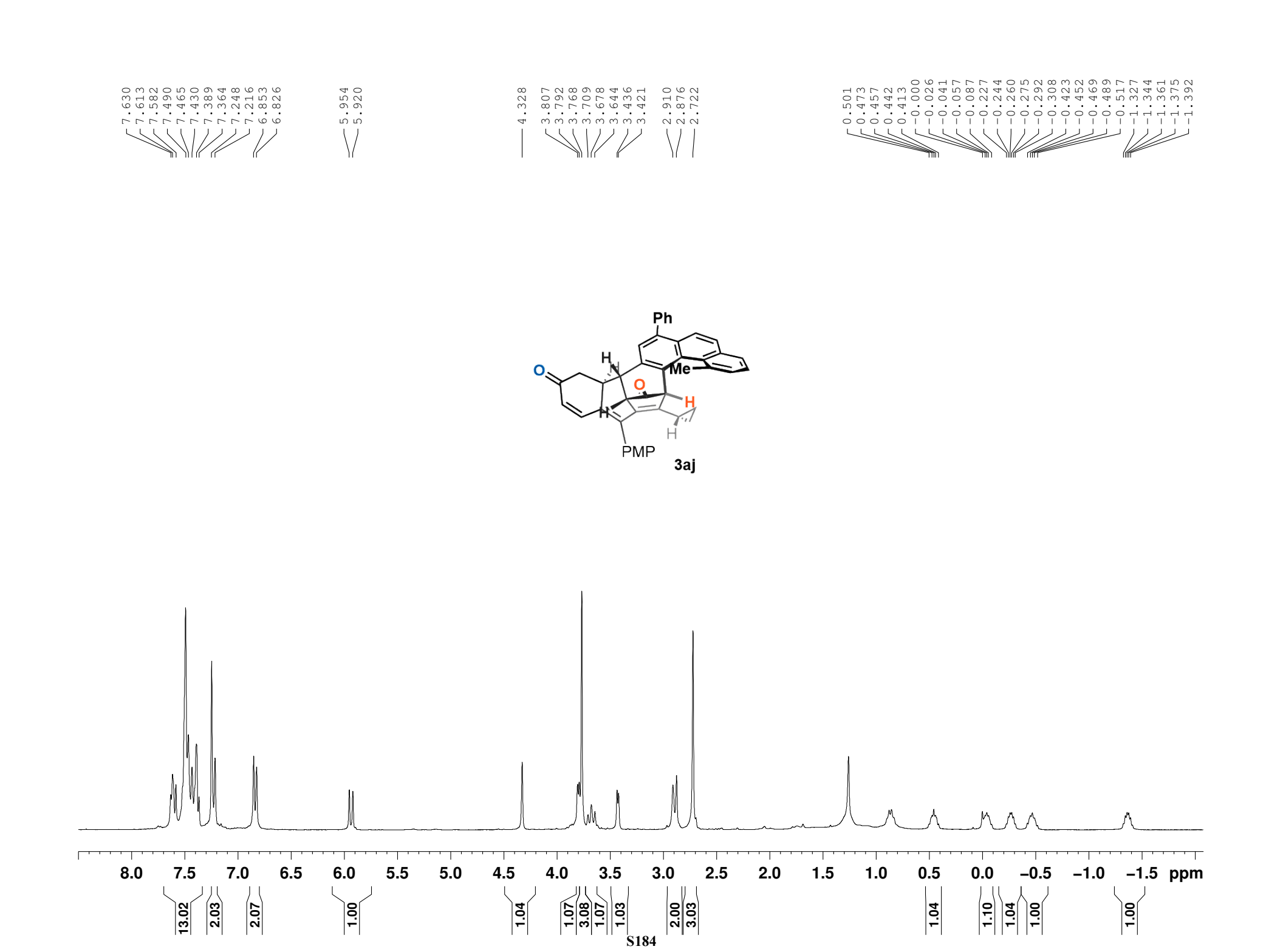
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ppm
1.04
2.04
3.06
1.03
1.00
2.04
2.05
1.00
1.03
3.09
1.09
1.05
1.04
2.01
3.04
1.04
1.05
1.00
1.00
0.99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7.430
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7.364
7.248
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6.826
5.954
5.920
4.328
3.807
3.792
3.768
3.709
3.678
3.644
3.436
3.421
2.910
2.876
2.722
0.501
0.473
0.457
0.442
0.413
-0.000
-0.026
-0.041
-0.057
-0.087
-0.227
-0.244
-0.260
-0.275
-0.292
-0.308
-0.423
-0.452
-0.469
-0.489
-0.517
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-1.344
-1.361
-1.375
-1.392
Ph
Me
O
O
H
H
H
H
PMP
3aj
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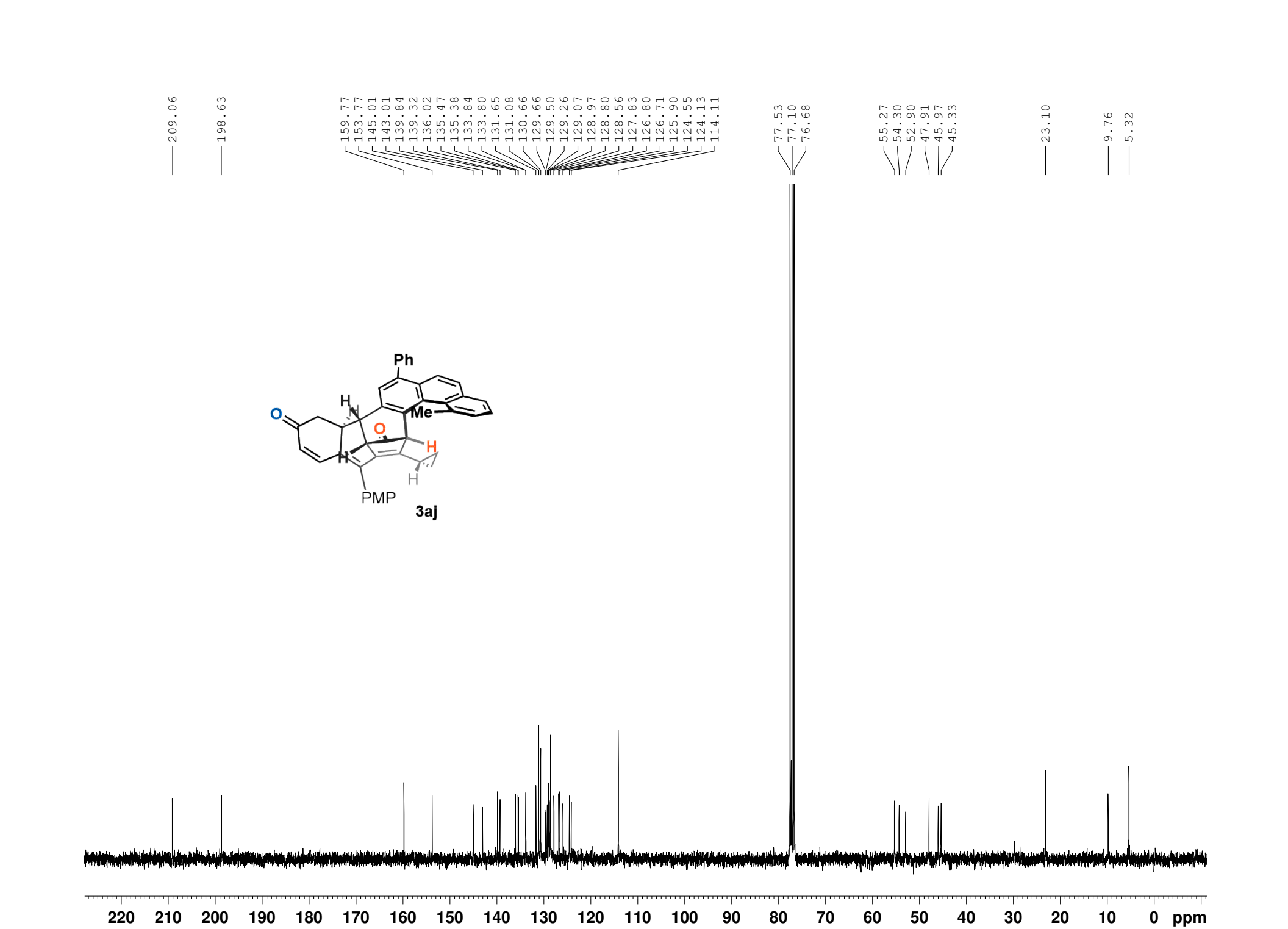
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
ppm
13.02
2.03
2.07
1.00
1.04
1.07
3.08
1.07
1.03
2.00
3.03
1.04
1.10
1.04
1.00
1.00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131.08
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129.66
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129.26
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128.56
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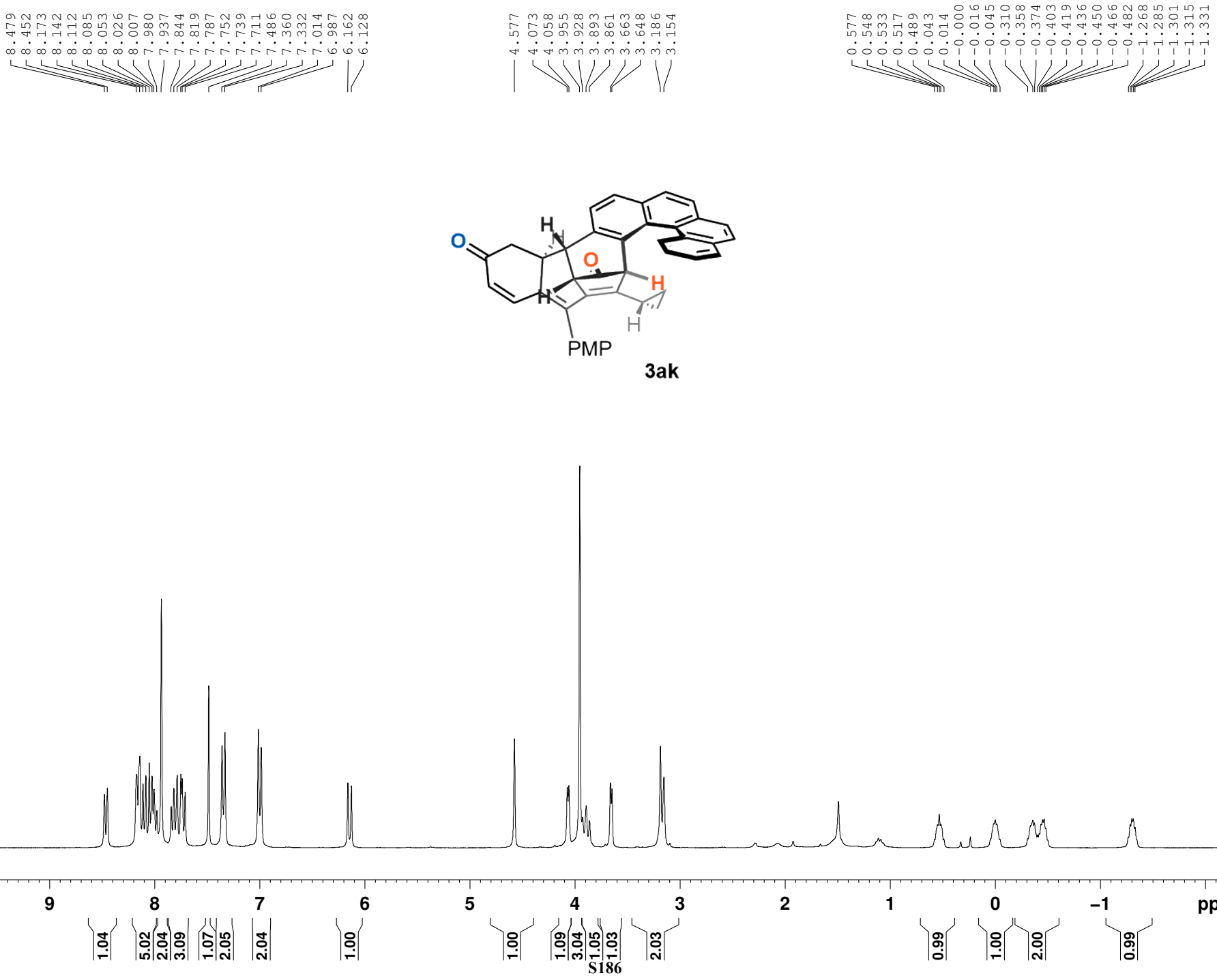
126.80
126.71
125.90
124.55
124.13
114.11
77.53
77.10
76.68
55.27
54.30
52.90
47.91
45.97
45.33
23.10
9.76
5.32
Ph
H
Me
O
O
H
H
H
PMP
3aj
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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8.026
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7.844
7.819
7.787
7.752
7.739
7.711
7.486
7.360
7.332
7.014
6.987
6.162
6.128
4.577
4.073
4.058
3.955
3.928
3.893
3.861
3.663
3.648
3.186
3.154
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0.548
0.533
0.517
0.489
0.043
0.014
-0.000
-0.016
-0.045
-0.310
-0.358
-0.374
-0.403
-0.419
-0.436
-0.450
-0.466
-0.482
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-1.285
-1.301
-1.315
-1.331
O
H
O
H
H
H
PMP
3ak
9
8
7
6
5
4
3
2
1
0
−1
ppm
1.04
5.02
2.04
3.09
1.07
2.05
2.04
1.00
1.00
1.09
3.04
1.05
1.03
2.03
0.99
1.00
2.00
0.99

209.45
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134.28
132.10
131.77
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128.95
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127.16
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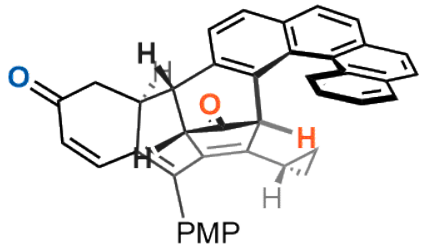
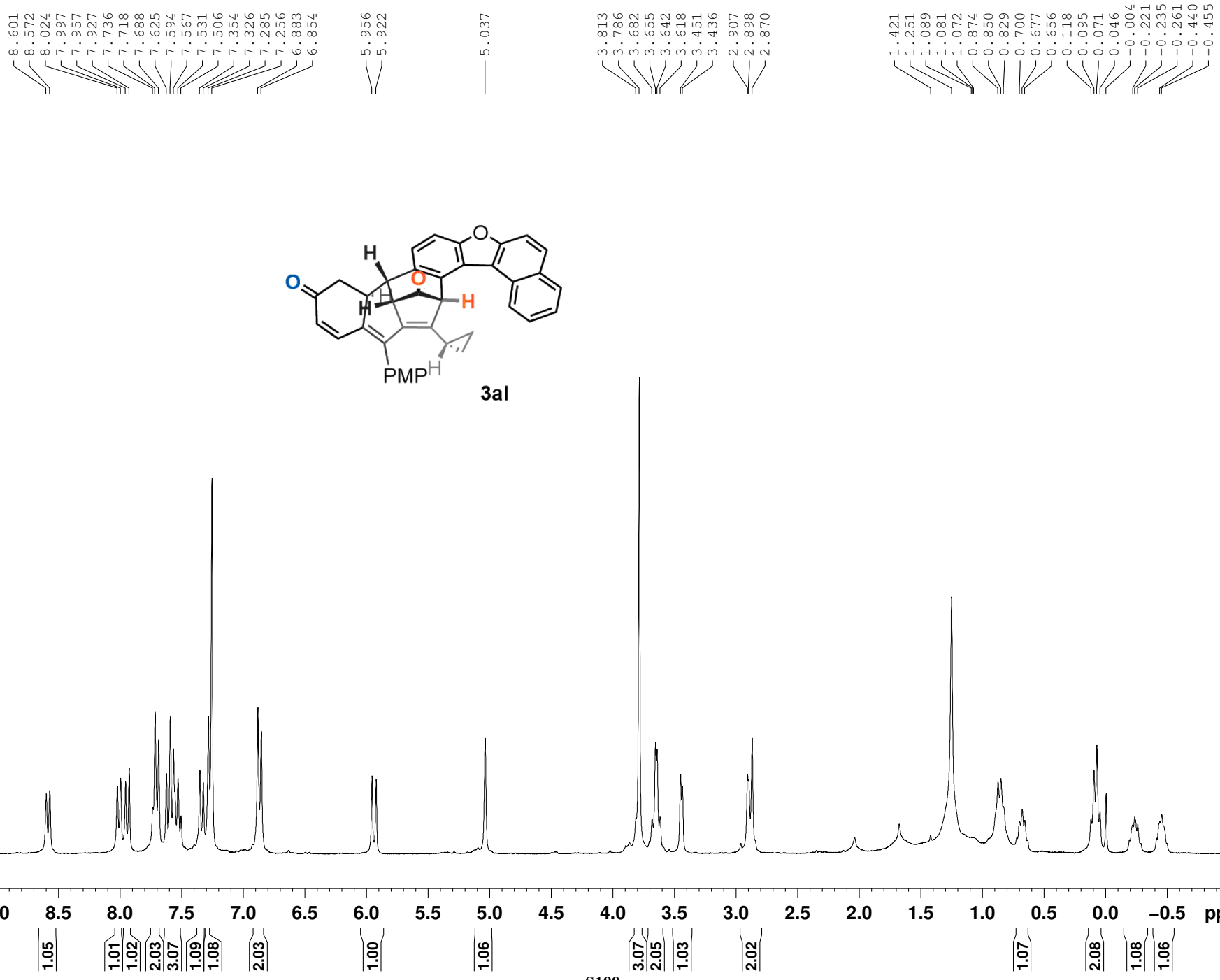
5.06



3ak

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm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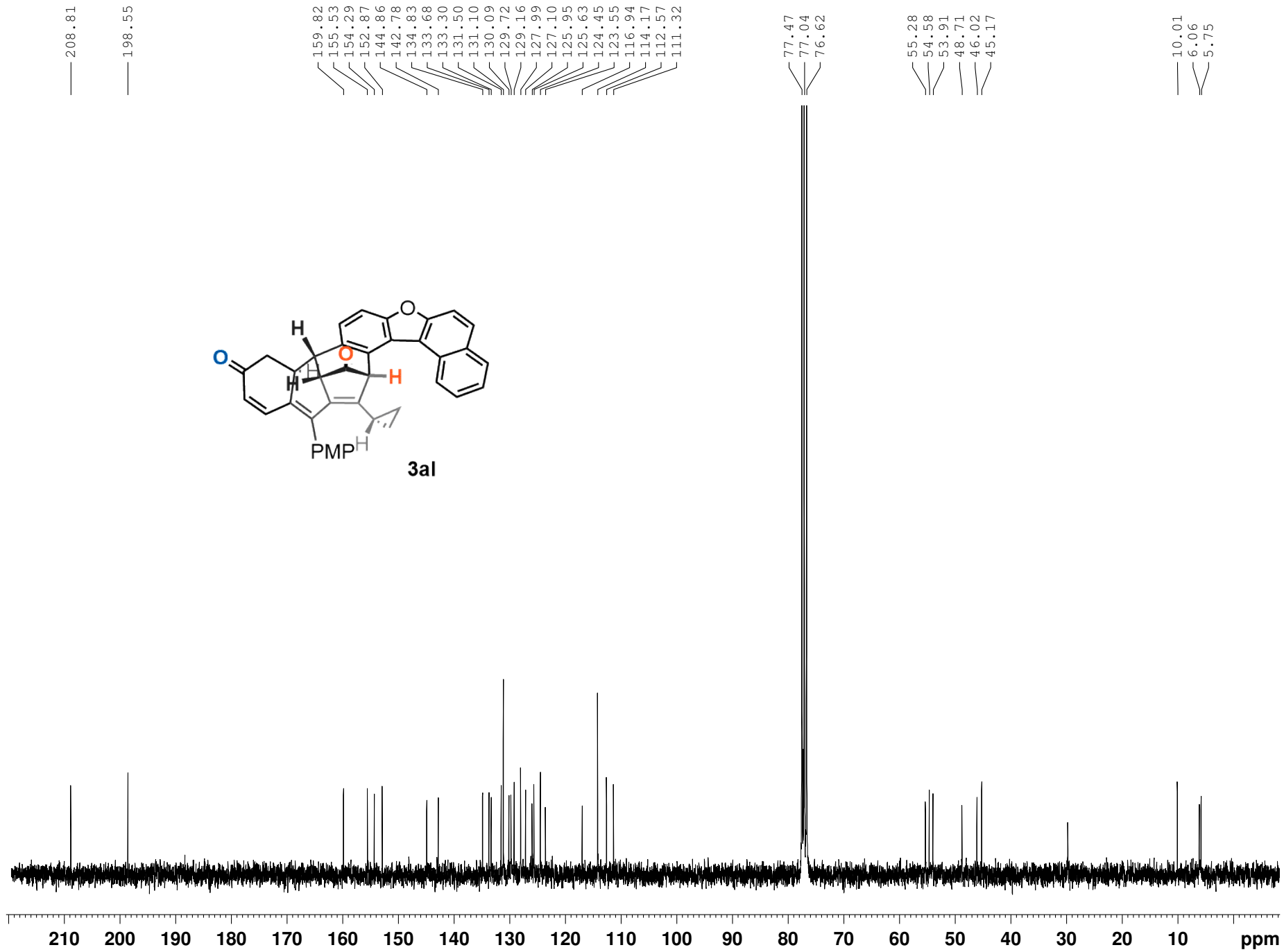
7.567
7.531
7.506
7.354
7.326
7.285
7.256
6.883
6.854
5.956
5.922
5.037
3.813
3.786
3.682
3.655
3.642
3.618
3.451
3.436
2.907
2.898
2.870
1.421
1.251
1.089
1.081
1.072
0.874
0.850
0.829
0.700
0.677
0.656
0.118
0.095
0.071
0.046
-0.004
-0.221
-0.235
-0.261
-0.440
-0.455
O
H
O
H
H
H
PMP
3aI
9.0
8.5
8.0
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
ppm
1.05
1.01
1.02
2.03
3.07
1.09
1.08
2.03
1.00
1.06
3.07
2.05
1.03
2.02
1.07
2.08
1.08
1.06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133.68
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131.50
131.10
130.09
129.72
129.16
127.99
127.10
125.95
125.63
124.45
123.55
116.94
114.17
112.57
111.32
77.47
77.04
76.62
55.28
54.58
53.91
48.71
46.02
45.17
10.01
6.06
5.75
O
H
O
H
H
O
PMP
H
3al
210
200
190
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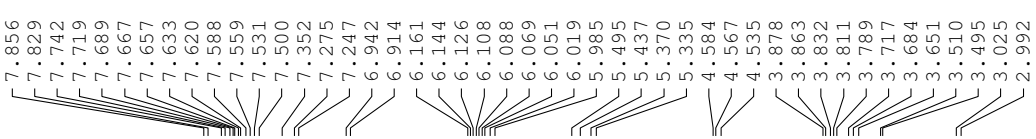
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.559
7.531
7.500
7.352
7.275
7.247
6.942
6.914
6.161
6.144
6.126
6.108
6.088
6.069
6.051
6.019
5.985
5.495
5.437
5.370
5.335
4.584
4.567
4.535
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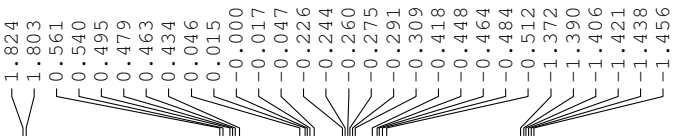
2.992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0.495
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0.463
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0.046
0.015
-0.000
-0.017
-0.047
-0.226
-0.244
-0.260
-0.275
-0.291
-0.309
-0.418
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-1.390
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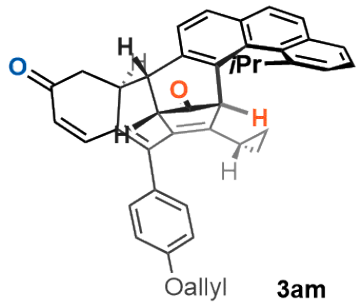
-1.421
-1.438
-1.456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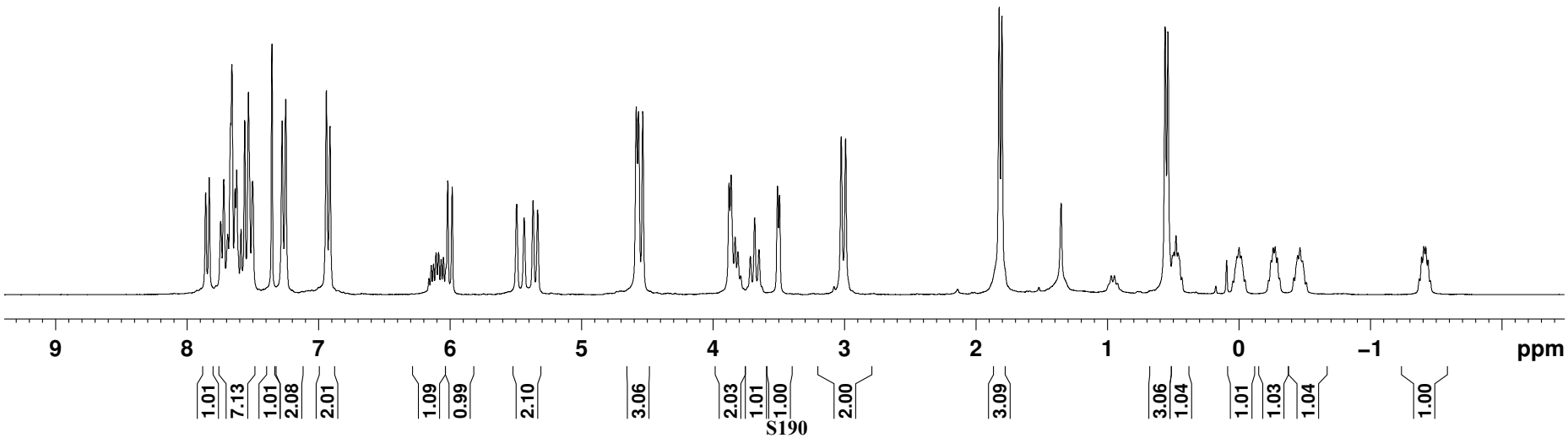
iPr
O
H
H
H
Oallyl

3am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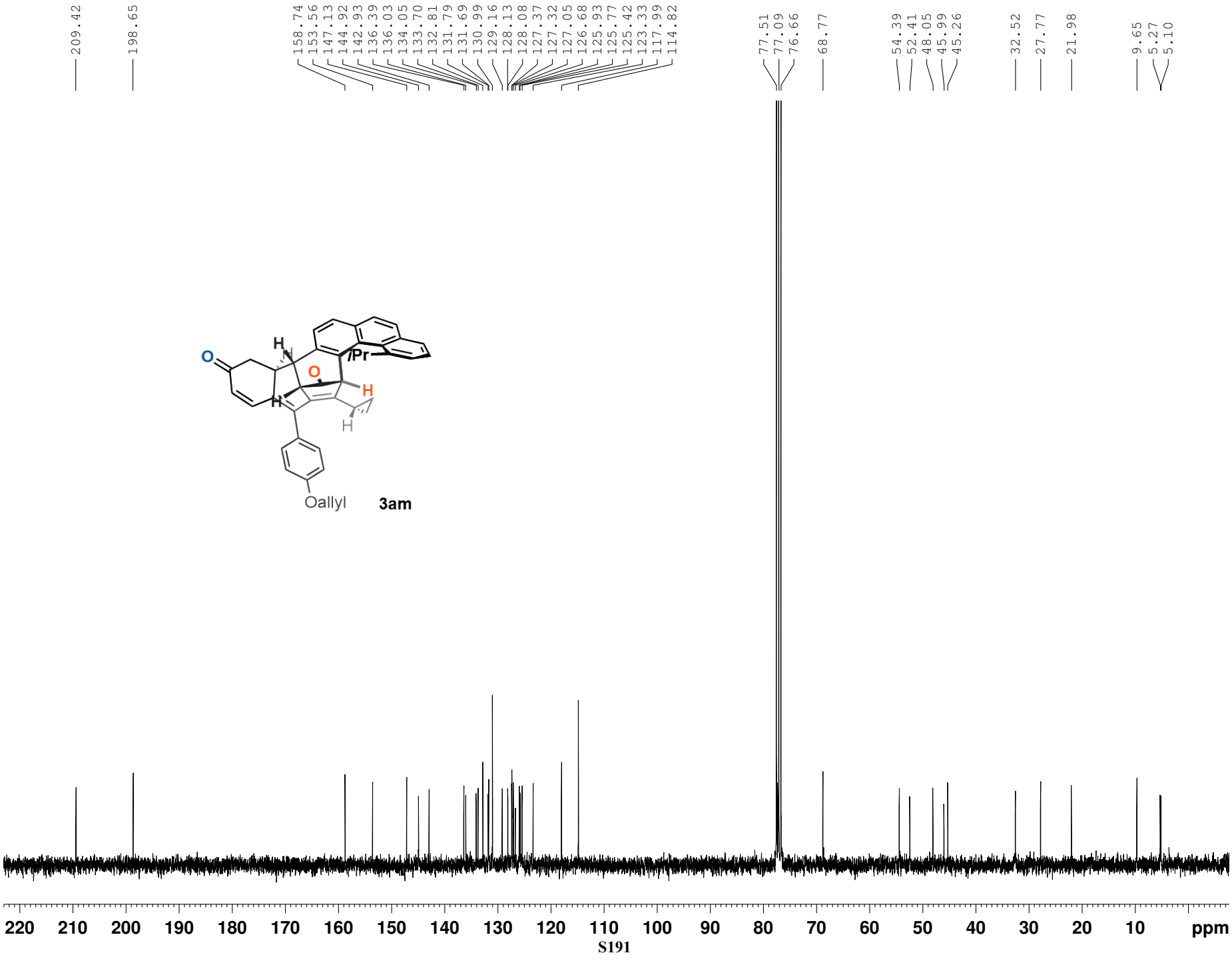
1.03
1.04
1.00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127.37
127.32
127.05
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125.93
125.77
125.42
123.33
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77.51
77.09
76.66
68.77
54.39
52.41
48.05
45.99
45.26
32.52
27.77
21.98
9.65
5.27
5.10
O
H
iPr
O
H
H
Oallyl
3am
220
210
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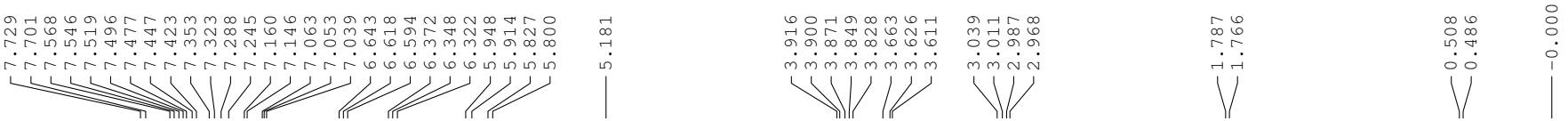
ppm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7.245
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7.146
7.063
7.053
7.039
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6.594
6.372
6.348
6.322
5.948
5.914
5.827
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5.181
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3.900
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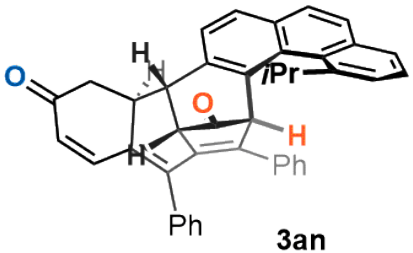
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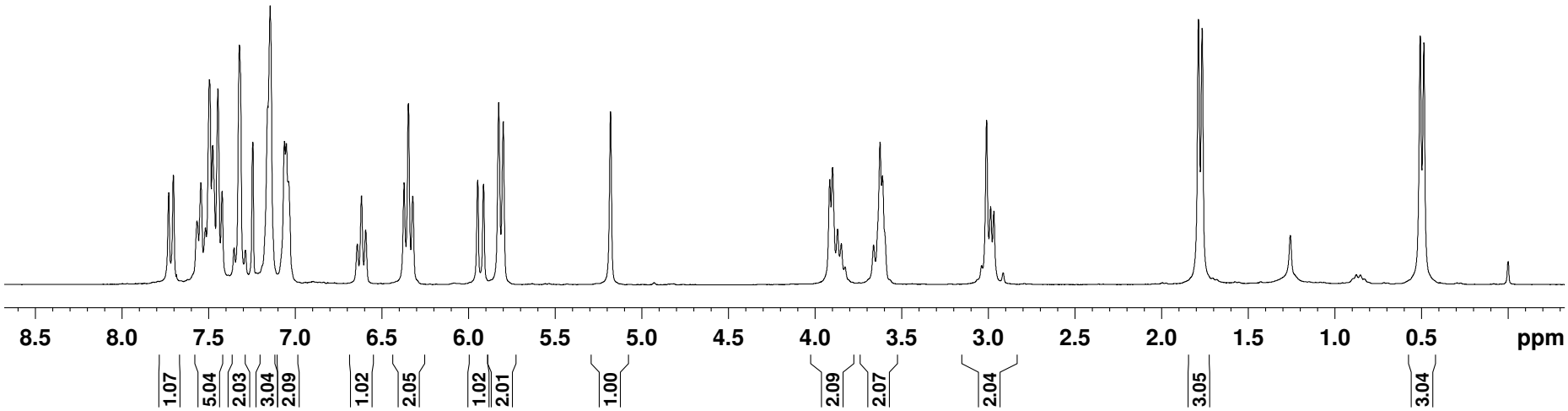
H
O
iPr
H
Ph
H
Ph

3an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ppm
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2.03
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2.05
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2.09
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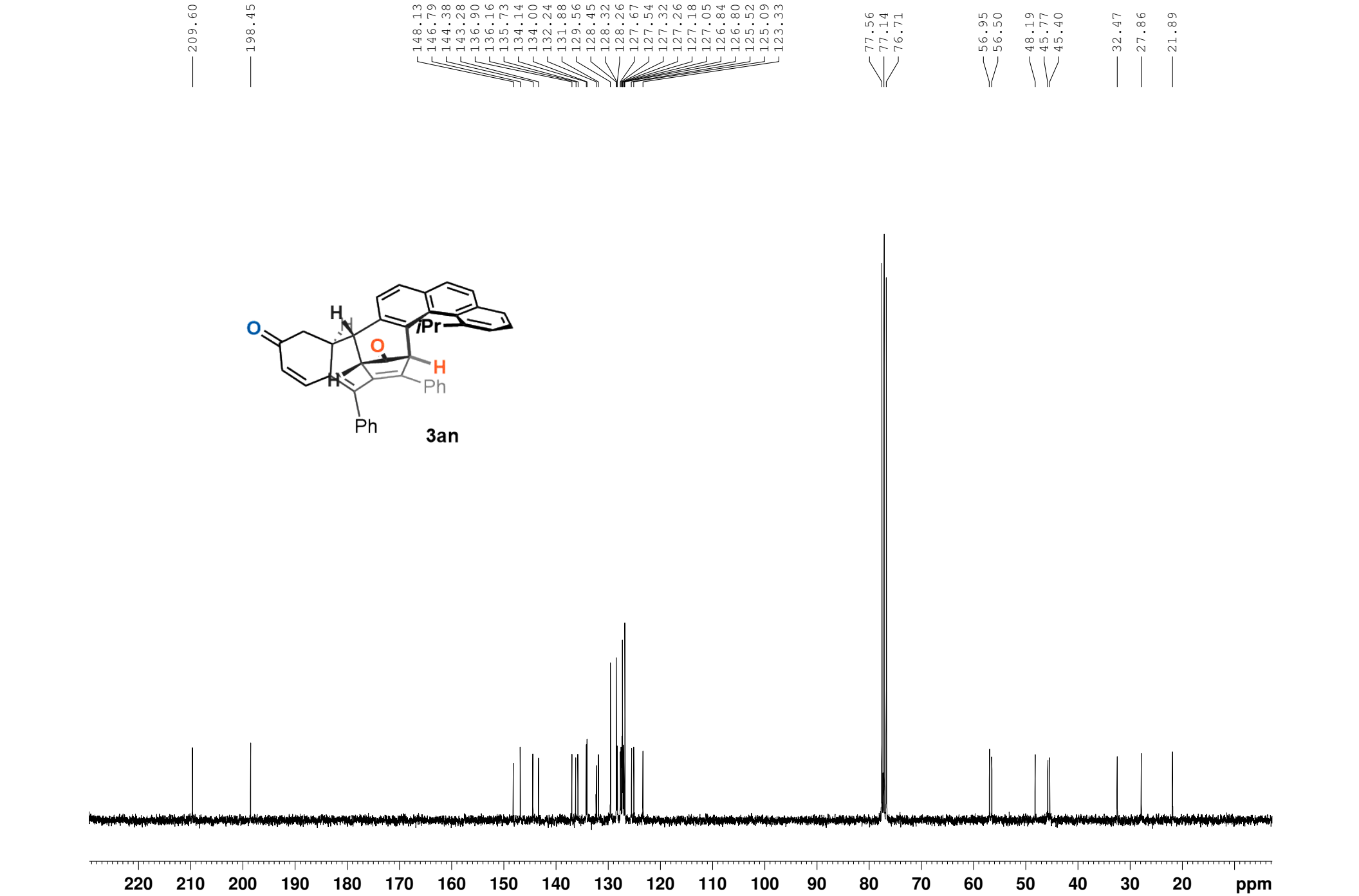
2.04
3.05
3.04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127.26
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125.09
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56.50
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45.77
45.40
32.47
27.86
21.89
O
H
N
iPr
O
H
H
Ph
Ph
3an
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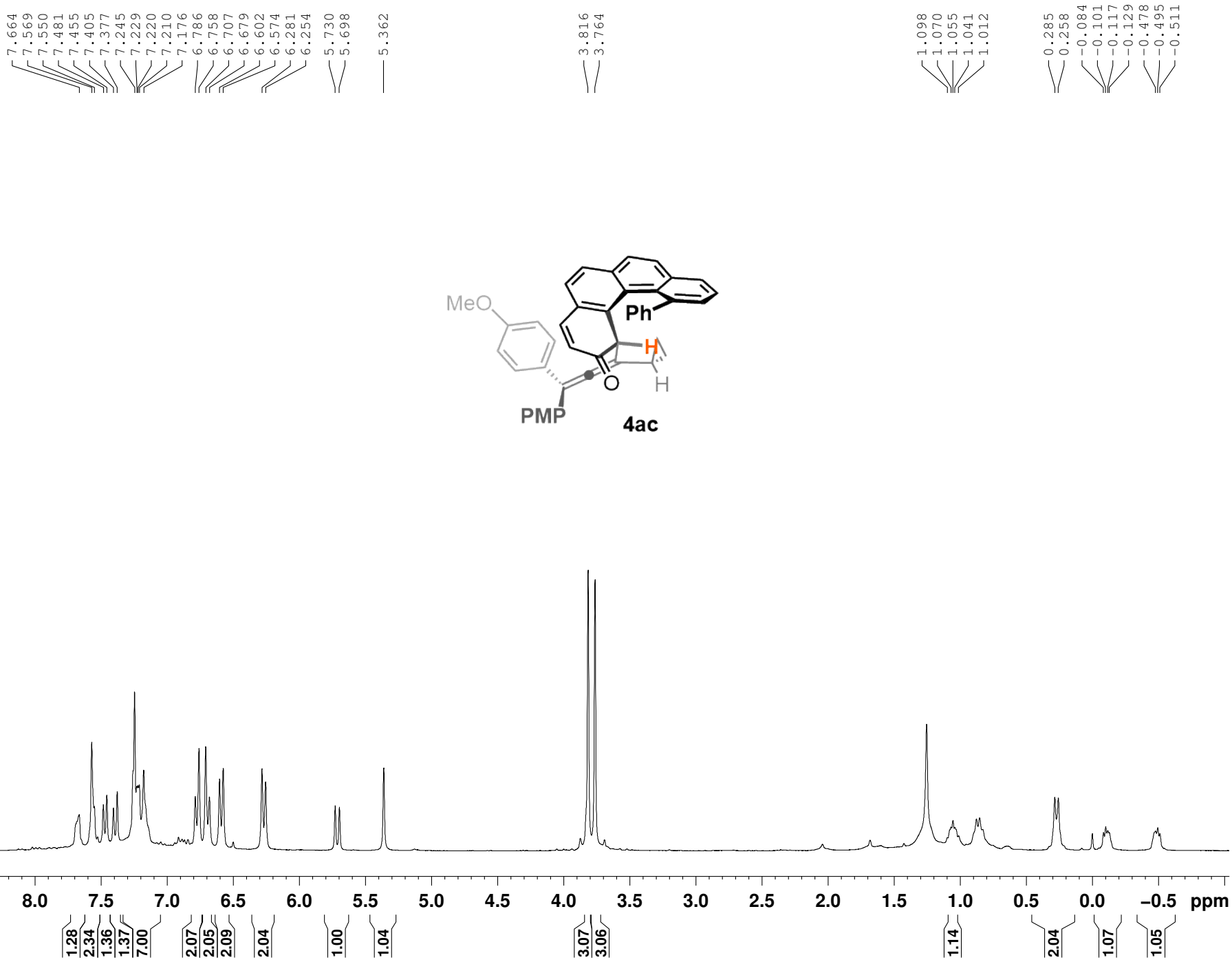
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7.245
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7.176
6.786
6.758
6.707
6.679
6.602
6.574
6.281
6.254
5.730
5.698
5.362
3.816
3.764
1.098
1.070
1.055
1.041
1.012
0.285
0.258
-0.084
-0.101
-0.117
-0.129
-0.478
-0.495
-0.511
MeO
Ph
H
O
H
PMP
4ac
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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
ppm
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2.34
1.36
1.37
7.00
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2.05
2.09
2.04
1.00
1.04
3.07
3.06
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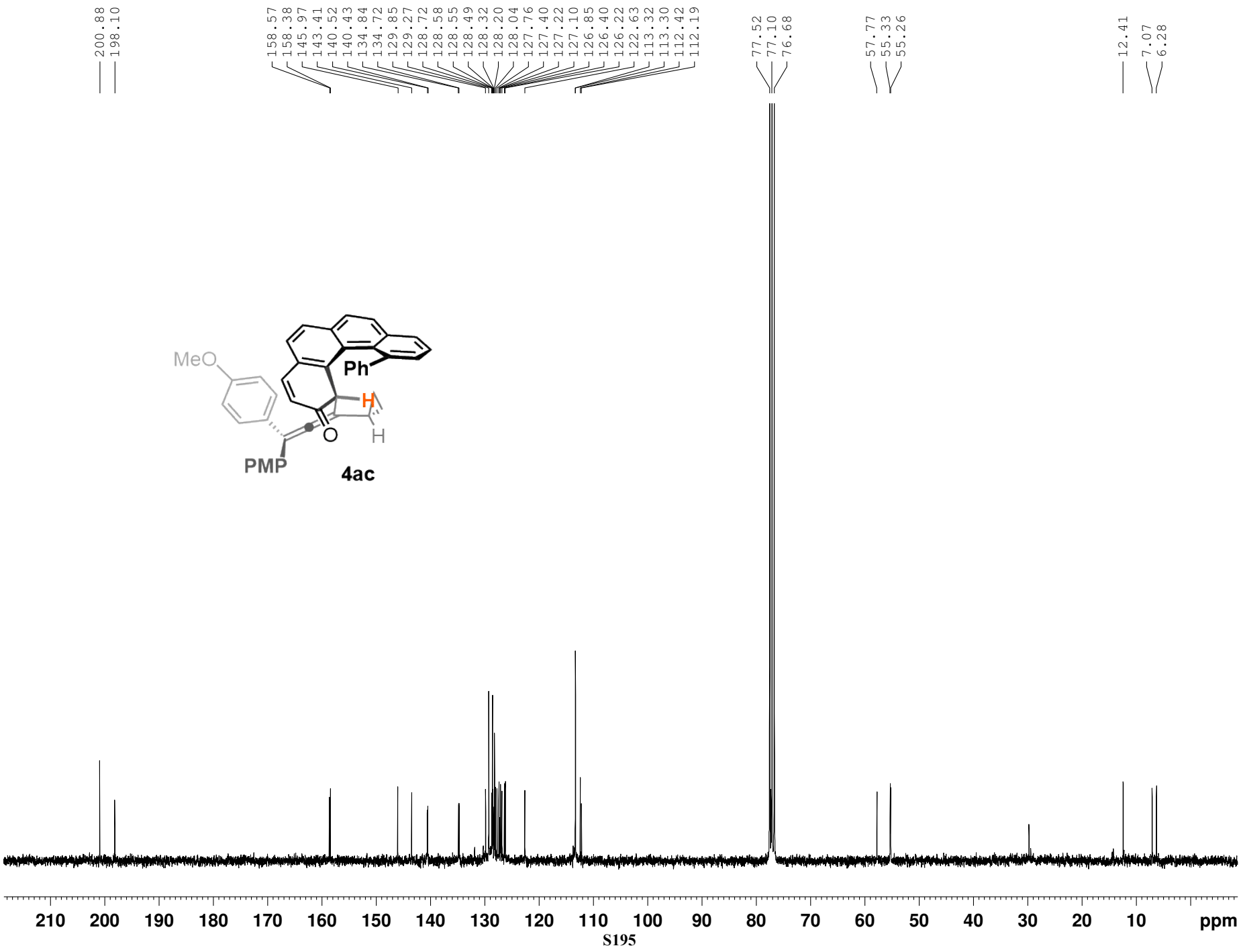
2.04
1.07
1.05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128.58
128.55
128.49
128.32
128.20
128.04
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127.22
127.10
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126.40
126.22
122.63
113.32
113.30
112.42
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77.52
77.10
76.68
57.77
55.33
55.26
12.41
7.07
6.28
MeO
Ph
H
O
H
PMP
4ac
210
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150
140
130
120
110
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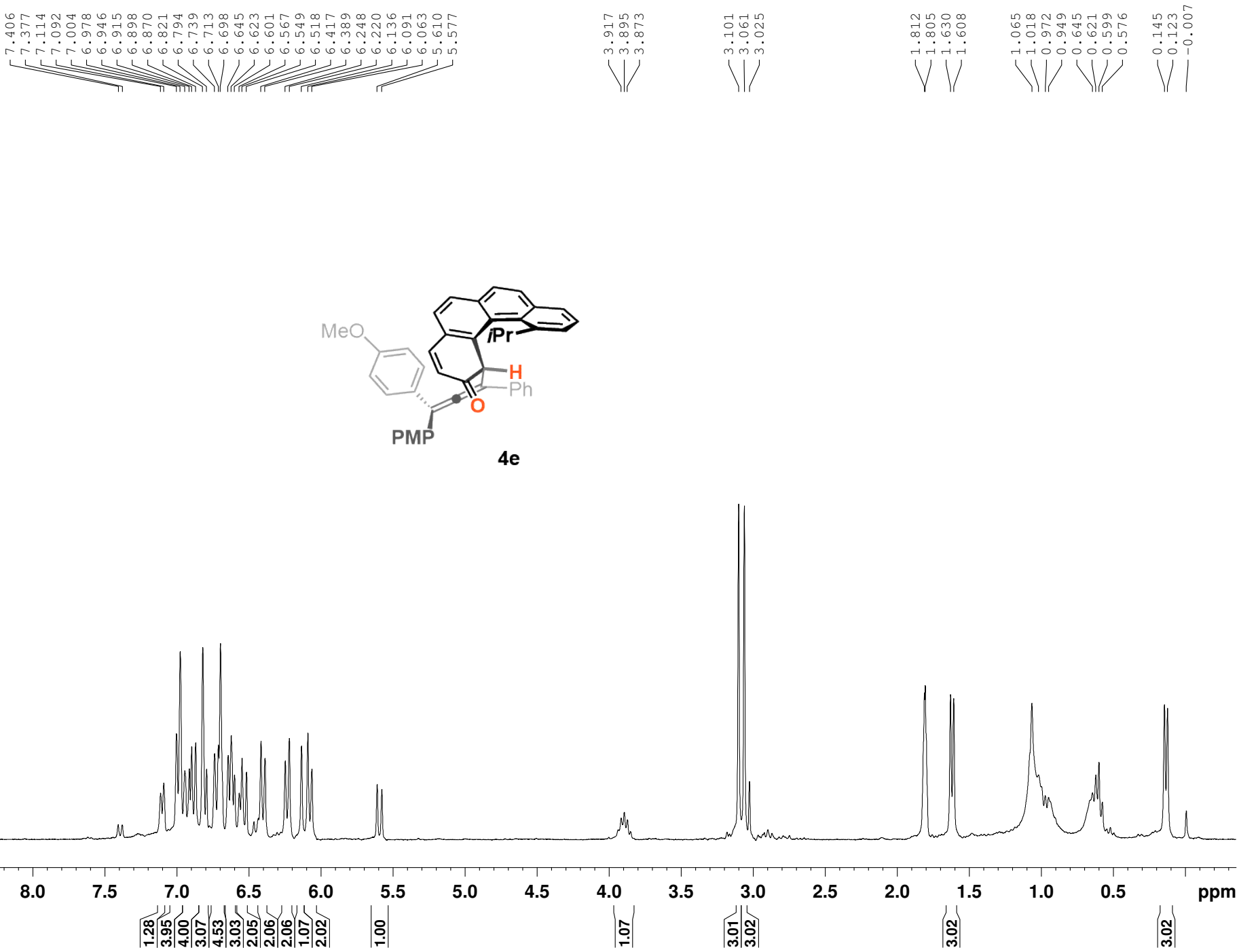
ppm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6.915
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6.821
6.794
6.739
6.713
6.698
6.645
6.623
6.601
6.567
6.549
6.518
6.417
6.389
6.248
6.220
6.136
6.091
6.063
5.610
5.577
3.917
3.895
3.873
3.101
3.061
3.025
1.812
1.805
1.630
1.608
1.065
1.018
0.972
0.949
0.645
0.621
0.599
0.576
0.145
0.123
-0.007
MeO
iPr
H
Ph
O
PMP
4e
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5.0
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4.0
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0.5
ppm
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3.07
4.53
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2.06
2.06
1.07
2.02
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1.07
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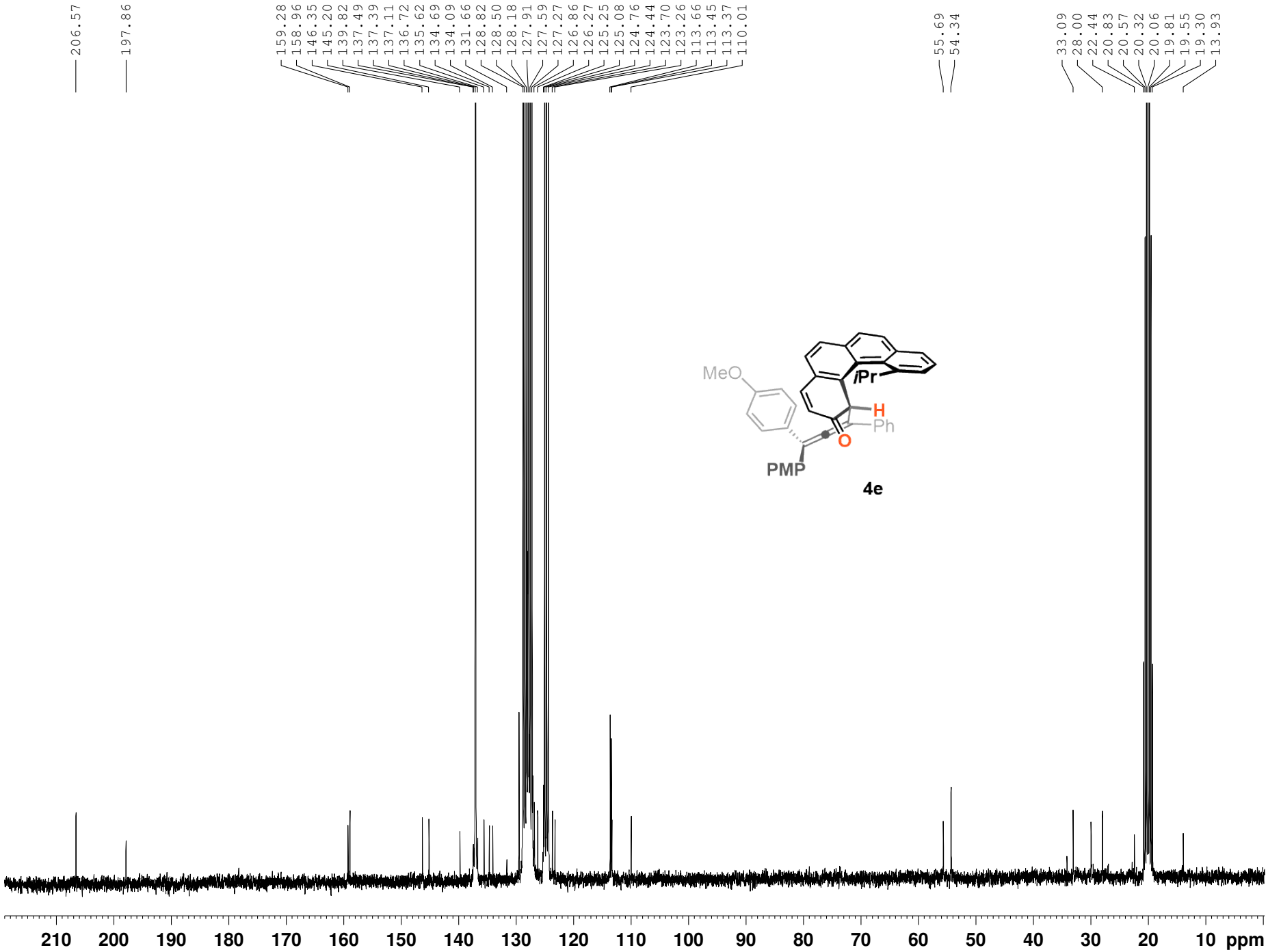
3.02
3.02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128.50
128.18
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127.59
127.27
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126.27
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125.08
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124.44
123.70
123.26
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113.45
113.37
110.01
55.69
54.34
33.09
28.00
22.44
20.83
20.57
20.32
20.06
19.81
19.55
19.30
13.93
MeO
iPr
H
Ph
O
PMP
4e
210
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30
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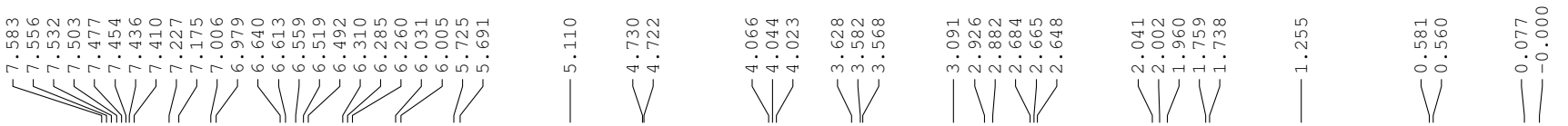
10
ppm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6.640
6.613
6.559
6.519
6.492
6.310
6.285
6.260
6.031
6.005
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5.691
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4.722
4.066
4.044
4.023
3.628
3.582
3.568
3.091
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2.882
2.684
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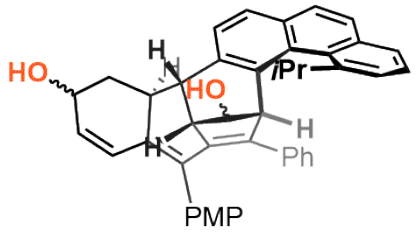
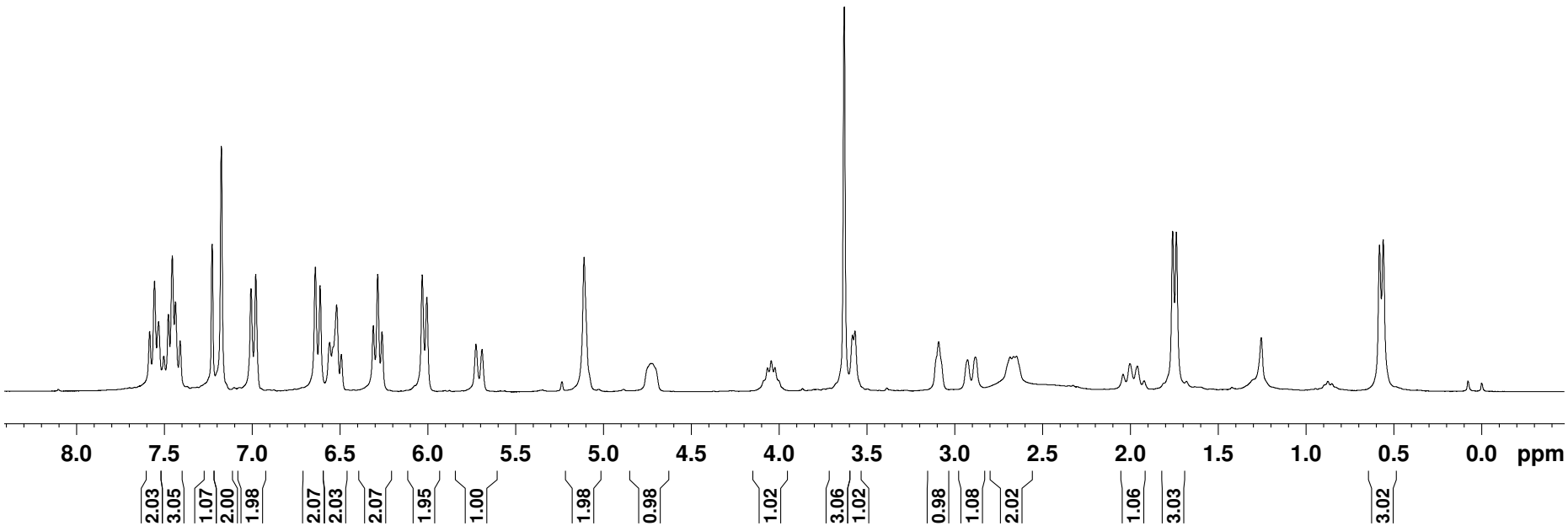

HO
H
H
HO
iPr
H
H
Ph
PMP

5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1.0
0.5
0.0
ppm
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1.07
2.00
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2.03
2.07
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1.06
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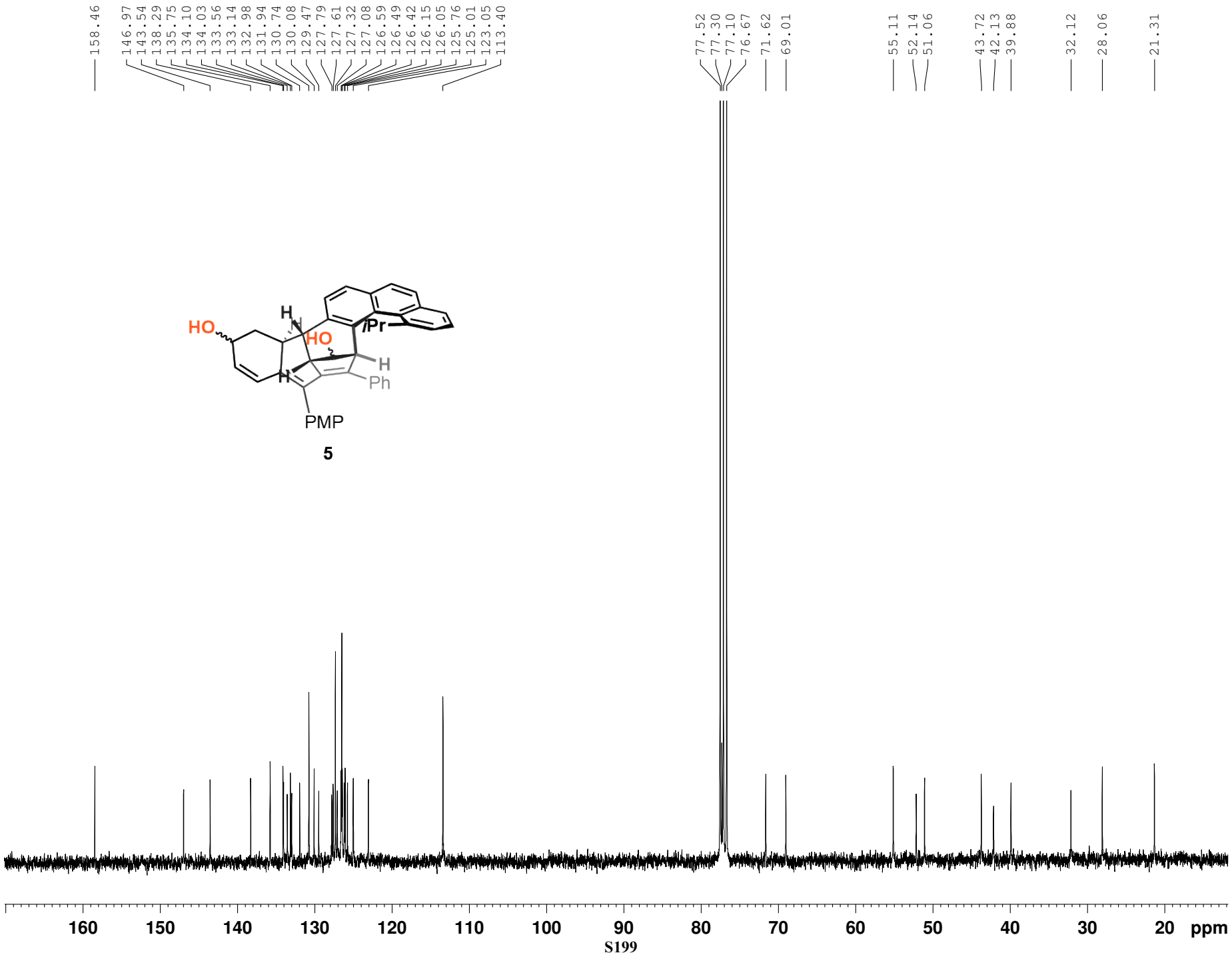
3.02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125.01
123.05
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77.10
76.67
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69.01
55.11
52.14
51.06
43.72
42.13
39.88
32.12
28.06
21.31
HO
HO
iPr
H
H
H
Ph
PMP
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70
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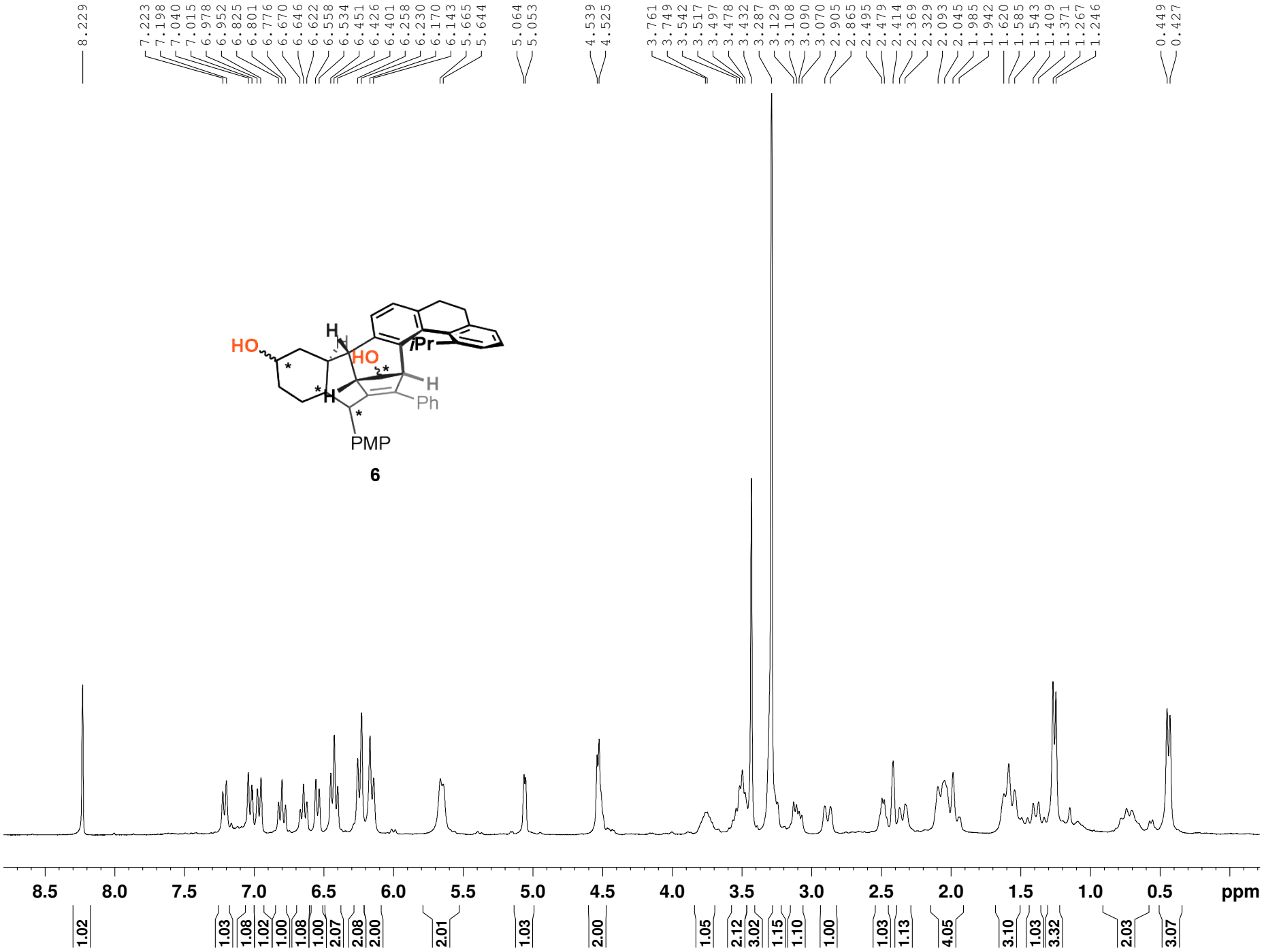
ppm

5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6.534
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6.426
6.401
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6.230
6.170
6.143
5.665
5.644
5.064
5.053
4.539
4.525
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3.542
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3.432
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3.129
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3.070
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2.865
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2.329
2.093
2.045
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1.942
1.620
1.585
1.543
1.409
1.371
1.267
1.246
0.449
0.427
HO
H
H
HO
iPr
H
Ph
PMP
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6.0
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1.08
1.02
1.00
1.08
1.00
2.07
2.08
2.00
2.01
1.03
2.00
1.05
2.12
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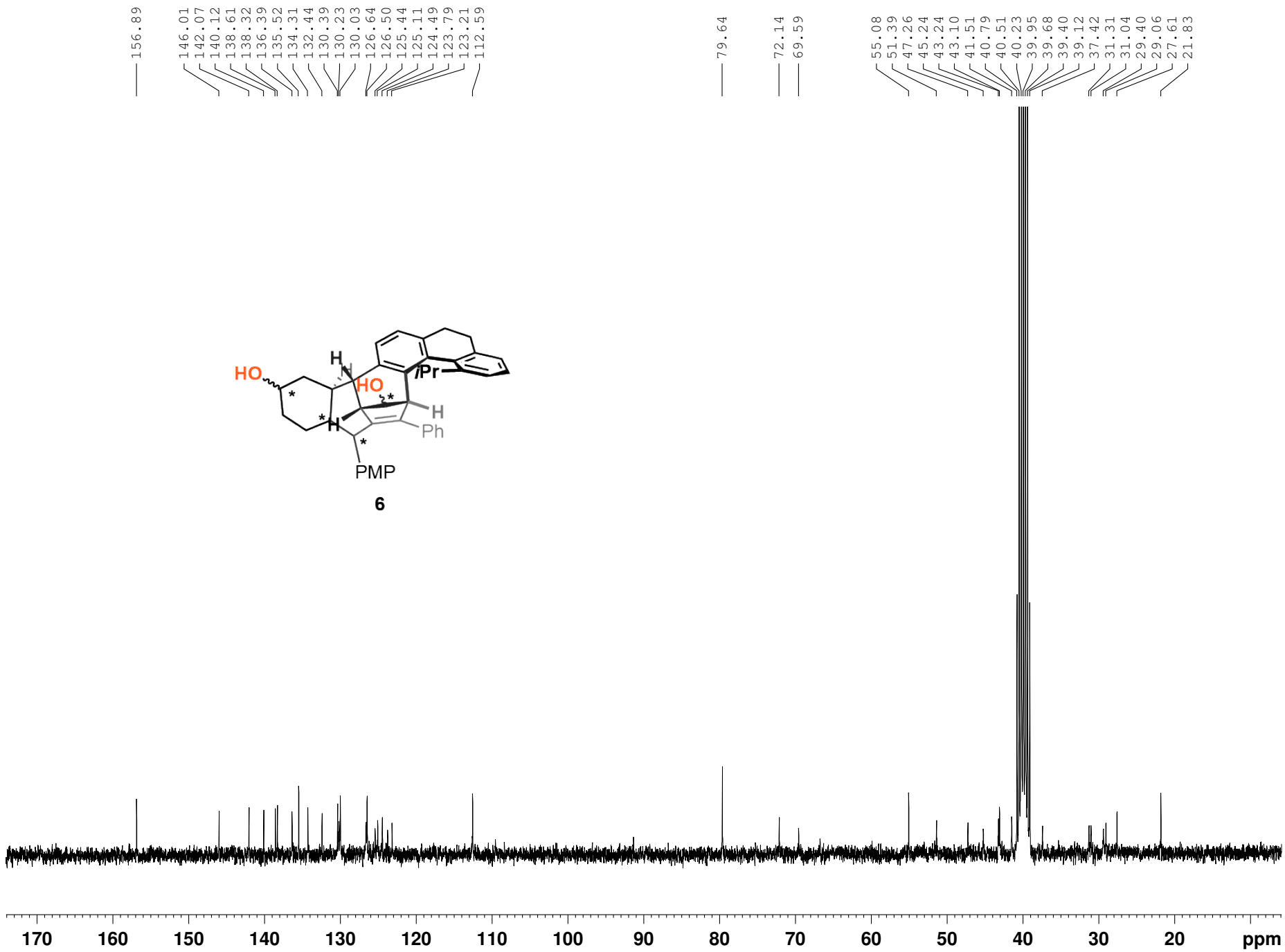
3.32
2.03
3.07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123.79
123.21
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69.59
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45.24
43.24
43.10
41.51
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40.23
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39.12
37.42
31.31
31.04
29.40
29.06
27.61
21.83
HO
HO
iPr
H
H
H
Ph
PMP
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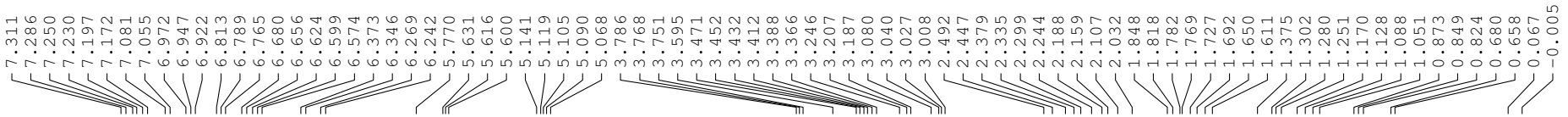
ppm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6.656
6.624
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6.574
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3.432
3.412
3.388
3.366
3.246
3.207
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2.188
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0.680
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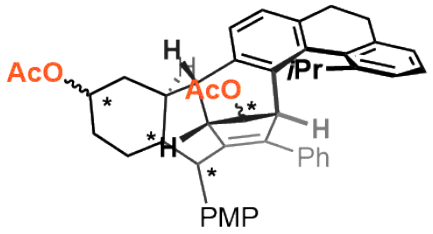
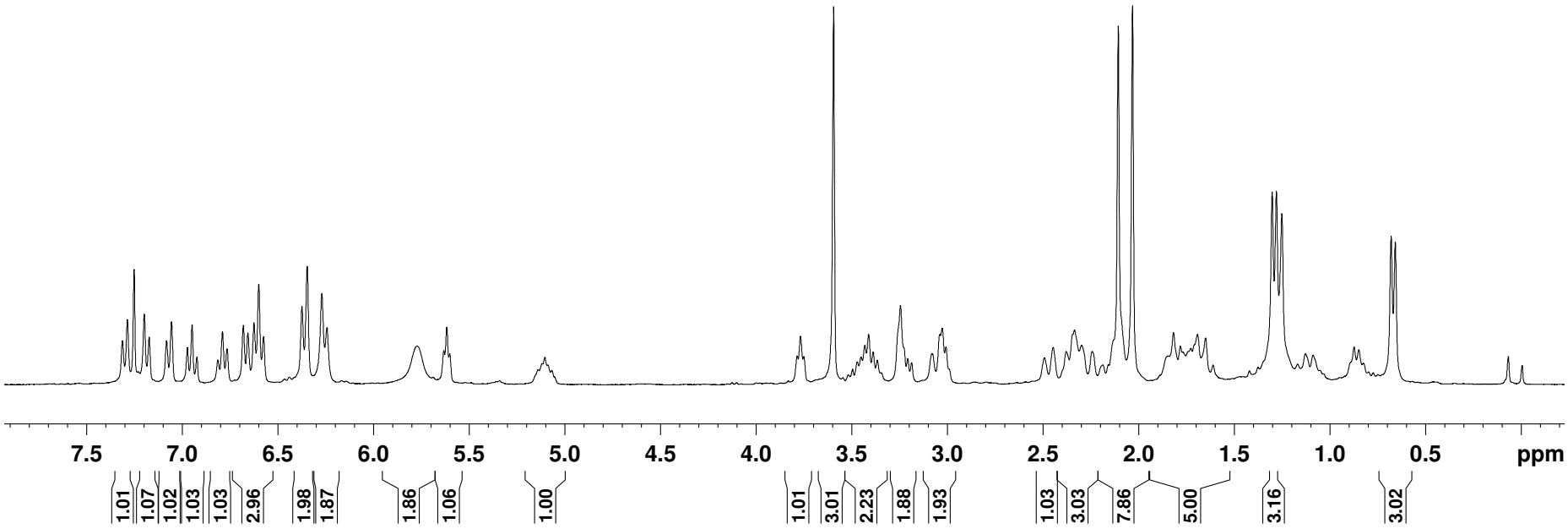

AcO
H
AcO
iPr
H
Ph
PMP

7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1.0
0.5
ppm
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1.07
1.02
1.03
1.03
2.96
1.98
1.87
1.86
1.06
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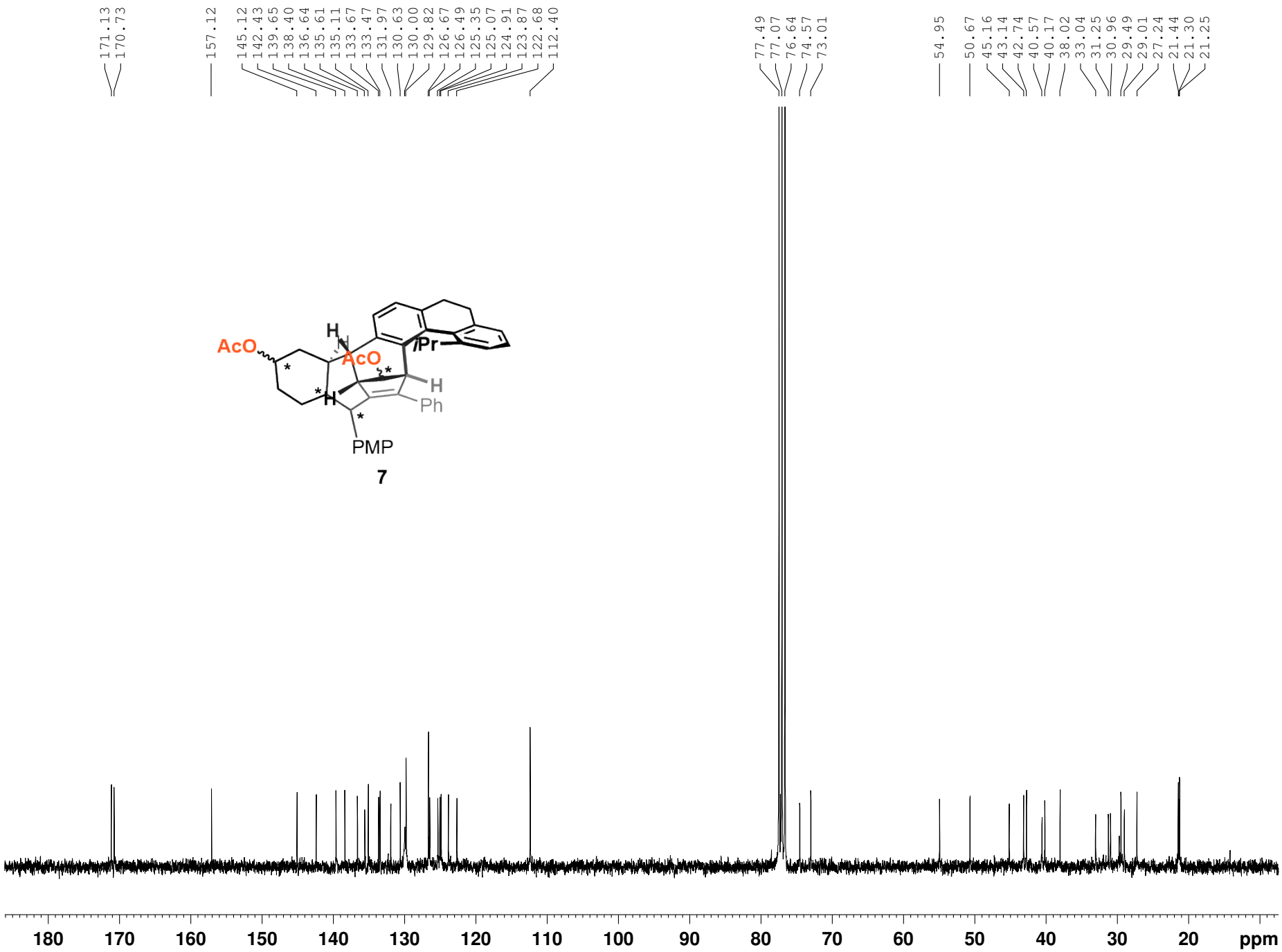
3.02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40.17
38.02
33.04
31.25
30.96
29.49
29.01
27.24
21.44
21.30
21.25
AcO
AcO
iPr
H
H
H
Ph
PMP
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180
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160
150
140
130
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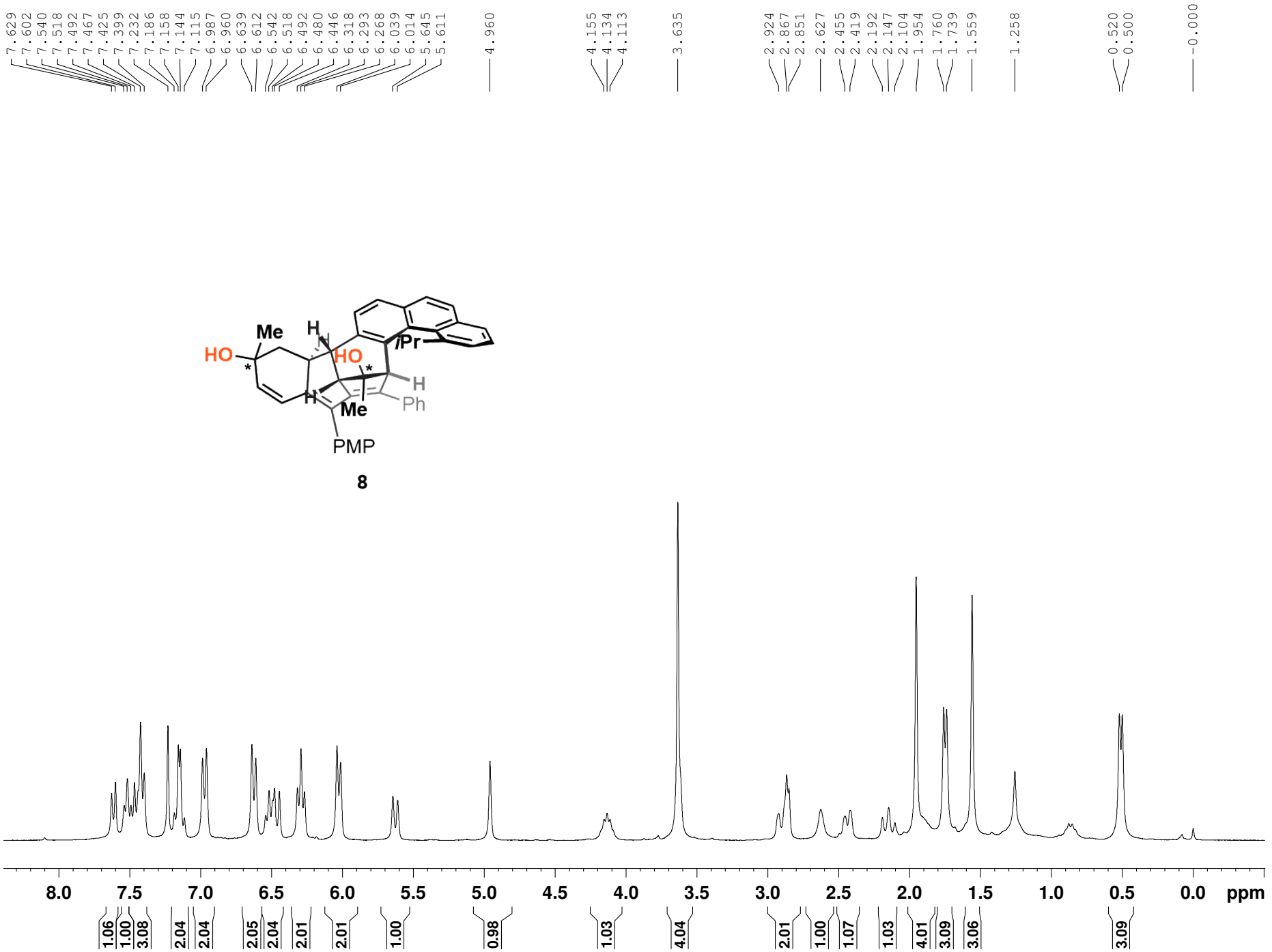
110
100
90
80
70
60
50
40
30
20
ppm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1.559
1.258
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0.500
-0.000
Me
H
HO
HO
iPr
H
Ph
H
Me
PMP
8
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7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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0.0
ppm
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2.04
2.04
2.05
2.04
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2.01
1.00
0.98
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4.04
2.01
1.00
1.07
1.03
4.01
3.09
3.06
3.09

158.44
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135.81
135.71
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134.09
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77.09
76.66
76.40
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41.43

32.01

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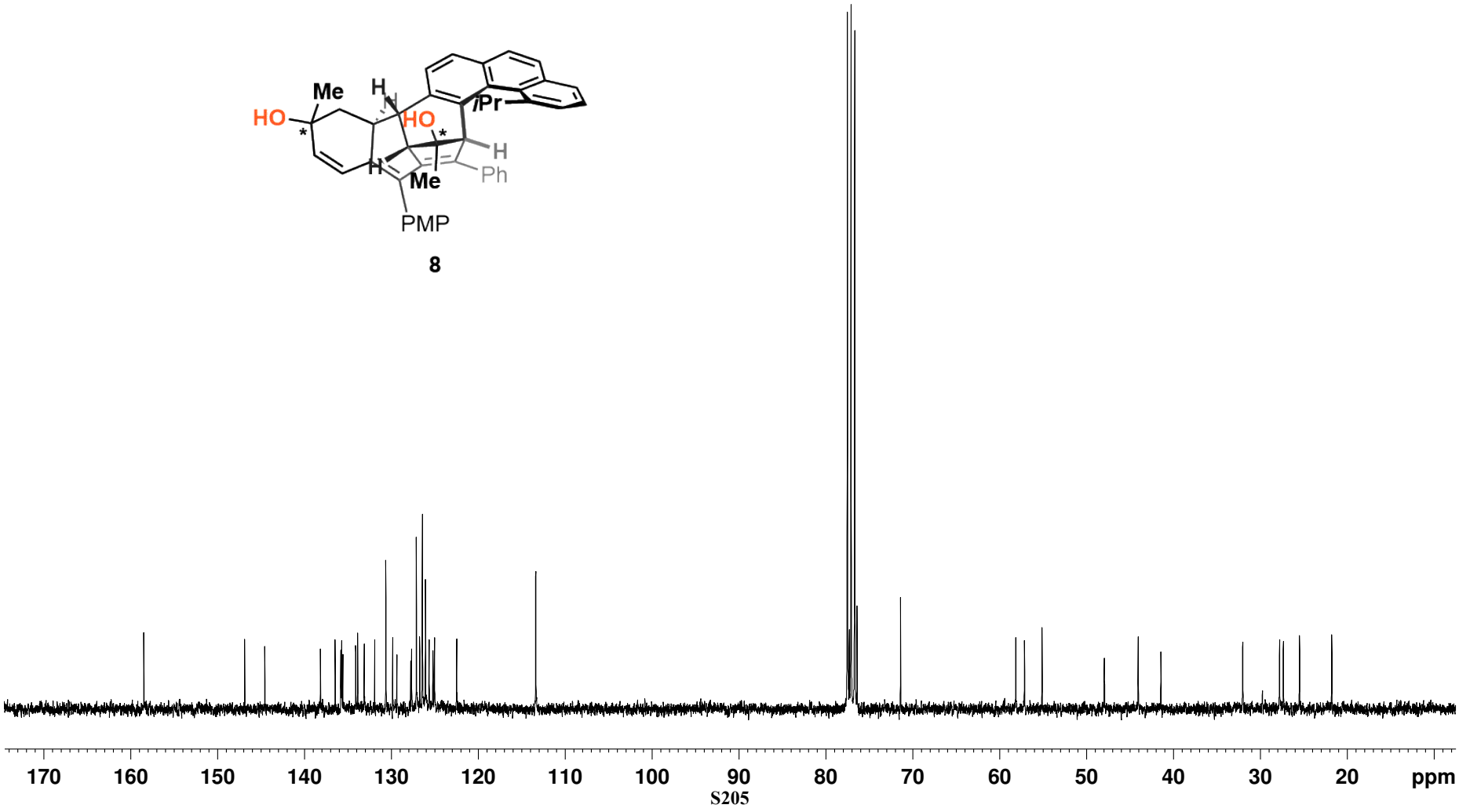
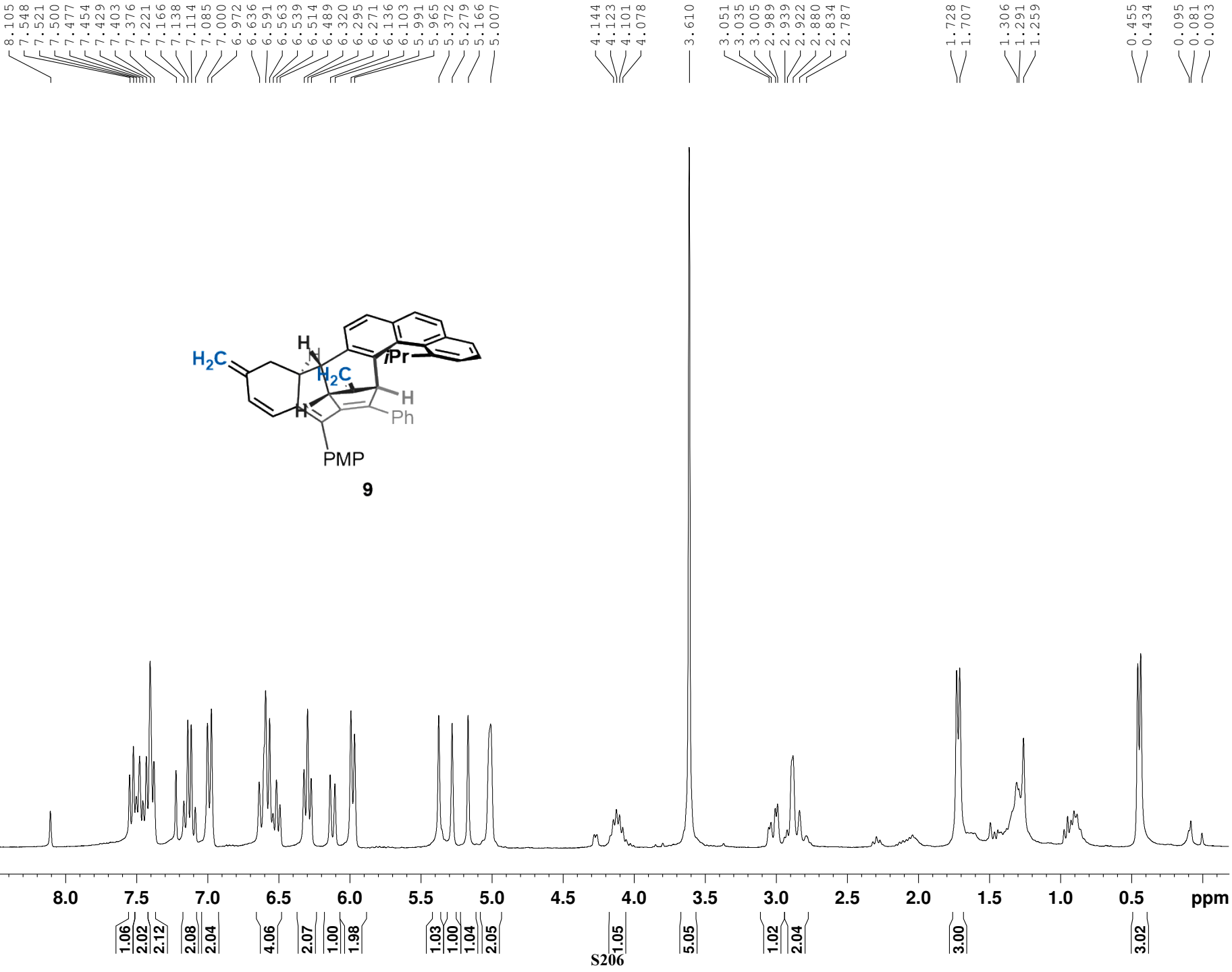
21.76

8

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H
H2C
iPr
H
H
Ph
PMP
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6.5
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1.0
0.5
ppm
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2.08
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5.05
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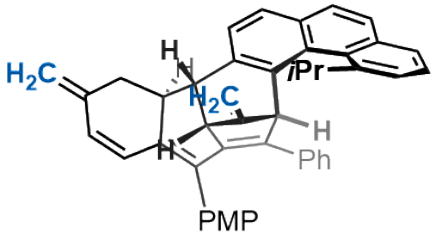

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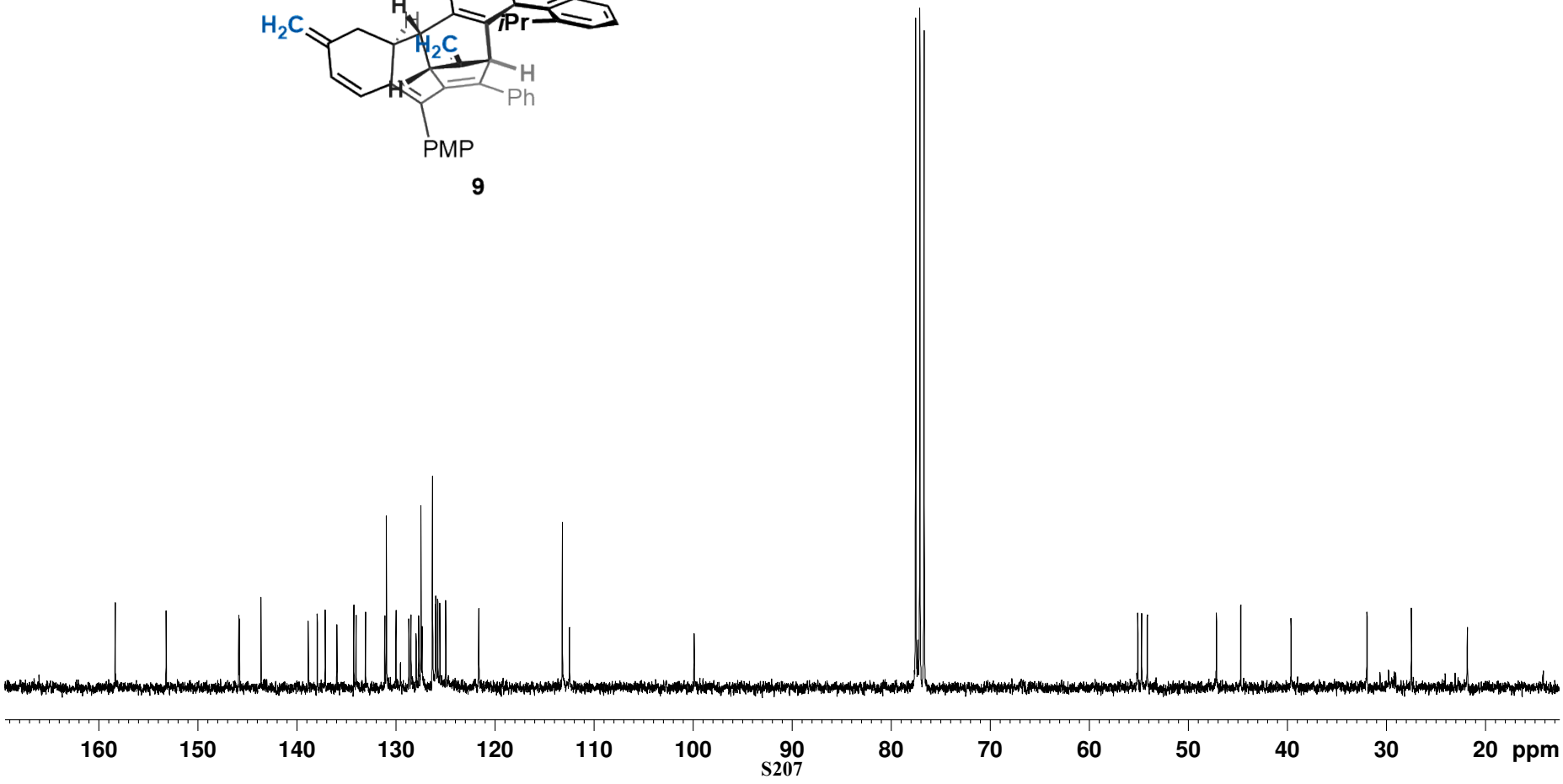

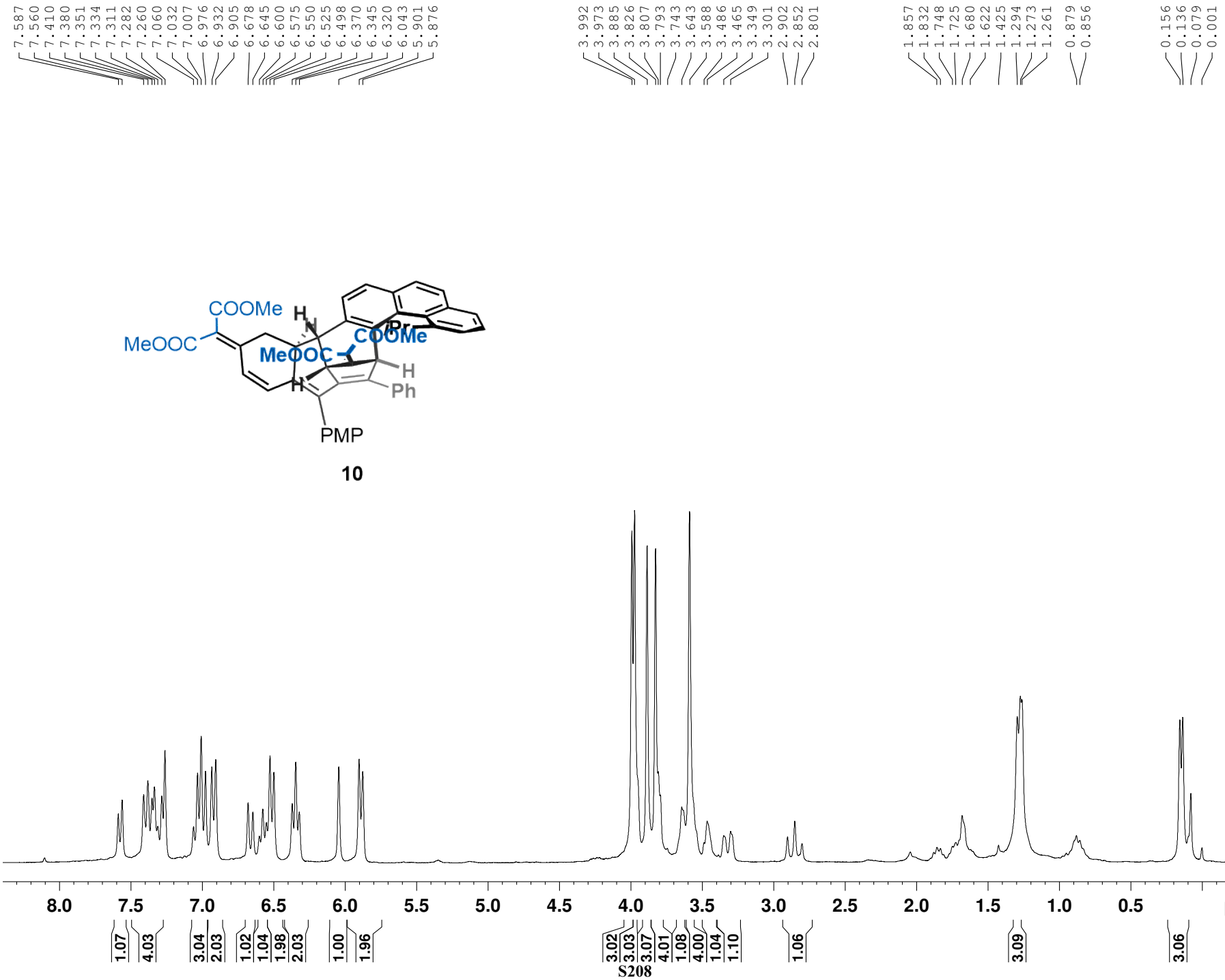
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6.905
6.678
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6.320
6.043
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3.973
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3.826
3.807
3.793
3.743
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3.588
3.486
3.465
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2.801
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COOMe
MeOOC
H
H
iPr
COOMe
MeOOC
H
H
Ph
PMP
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0.5
ppm
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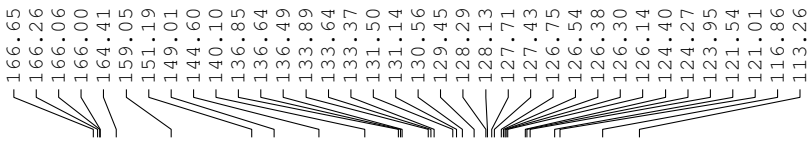
3.06



10

```
NAME                230313
EXPNO                    6
PROCNO                   1
Date_             20230313
Time                 14.19
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     2335
DS                        4
SWH              18028.846 Hz
FIDRES            0.275098 Hz
AQ                1.8175818 sec
RG                      203
DW                 27.733 usec
DE                  6.50 usec
TE                  290.9 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                  11.00 usec
PL1                 -1.00 dB
PL1W           36.99864960 W
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                  0.00 dB
PL12                15.78 dB
PL13                17.00 dB
PL2W           11.55467796 W
PL12W           0.30532184 W
PL13W           0.23054613 W
SFO2           300.1312005 MHz
SI                    32768
SF              75.4677490 MHz
WDW                     EM
SSB                      0
LB                  1.00 Hz
GB                       0
PC                    1.40
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