

# Supporting Information

## Fundamental Difference between Simple Aarenes and PAHs Found in *o*-PAH-connected porphyrins

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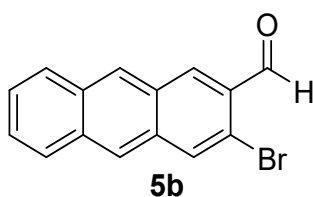
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## 1. General and Synthetic Experiments

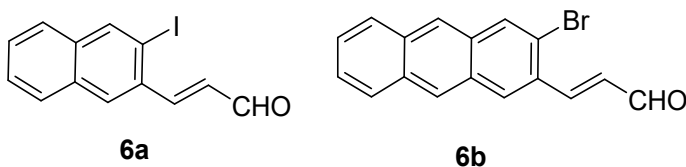
Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. Yields of synthesized compounds were measured after chromatographic purification. UV-vis spectra were recorded on a UV 1800 (Shimadzu) spectrophotometer.  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were measured using JEOL (400 MHz) instruments. Mass spectra were obtained by using a JEOL LMS-HX-110 spectrometer (EI or FAB mode).



### 3-bromoanthracene-2-carbaldehyde (**5b**)

NMO (312 mg, 2.66 mmol) was added to a well-stirred solution of 2-bromo-3-(bromomethyl)anthracene (233 mg, 0.666 mmol) in anhydrous THF (27 mL) under Ar. The reaction mixture was refluxed at 85 °C for 1 h. After the resulting mixture was cooled to room temperature, water was added and the mixture was extracted with DCM. The organic layer was washed with water and dried over  $\text{Na}_2\text{SO}_4$ . The filtrate was evaporated to dryness and purified over silica gel (DCM/hexane, 1/9~1/1) to afford compound **5b** as a yellow powder (159 mg, 84%).

$^1\text{H}$  NMR (400 MHz, Chloroform-*d*)  $\delta$  10.51 (s, 1H), 8.63 (s, 1H), 8.56 (s, 1H), 8.32 (s, 1H), 8.26 (s, 1H), 8.01 (m, 2H), 7.54 (ddt,  $J = 8.2, 6.6, 5.1$  Hz, 2H);  $^{13}\text{C}$  NMR (100 MHz, Chloroform-*d*)  $\delta$  191.97, 133.98, 133.69, 133.50, 132.58, 132.41, 130.14, 129.94, 129.09, 128.73, 128.28, 127.70, 126.58, 125.52, 118.73; HR-EIMS:  $m/z$  calcd for  $\text{C}_{15}\text{H}_9\text{BrO}$   $[\text{M}]^+$ : 283.9837; found: 283.9840.



### (*E*)-3-(3-iodonaphthalen-2-yl)acrylaldehyde (**6a**)

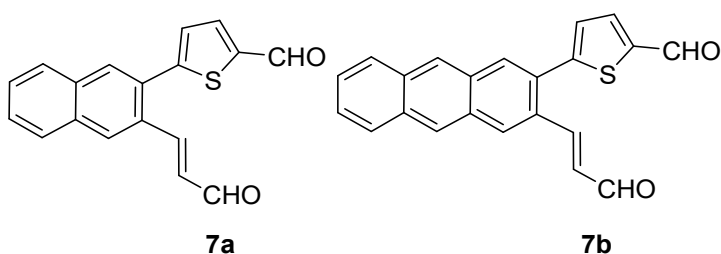
To a 50 mL round bottom flask equipped with a magnetic bar were added toluene (0.7 mL), triphenylphosphoranylideneacetaldehyde (37.4 mg, 0.123 mmol) was added to a well-stirred solution of 3-iodo-2-naphthaldehyde (34.7 mg, 0.123 mmol) in anhydrous toluene (0.7 mL) under Ar. The resulting mixture was stirred at 60 °C for overnight. The reaction mixture was evaporated to dryness and purified over silica gel (EA/hexane, 1/4) to afford compound **6a** as a yellow solid (11.4 mg, 30%).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 9.81 (d, *J* = 7.7 Hz, 1H), 8.45 (s, 1H), 8.10 (s, 1H), 7.88 (d, *J* = 15.7 Hz, 1H), 7.84 (m, 1H), 7.72 (m, 1H), 7.54 (m, 2H), 6.73 (dd, *J* = 15.6, 7.8 Hz, 1H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 193.37, 155.73, 139.50, 135.69, 133.71, 132.64, 130.90, 128.71, 128.47, 127.55, 127.47, 126.68, 96.90; HR-EIMS: *m/z* calcd for C<sub>13</sub>H<sub>9</sub>IO [M]<sup>+</sup>: 307.9698; found: 307.9696.

#### **(*E*)-3-(3-bromoanthracen-2-yl)acrylaldehyde (6b)**

By following the general procedure of **6a**, the reaction of **5b** (76.8 mg, 0.269 mmol) yielded **6b** (34.4 mg, 41% yield).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 9.81 (d, *J* = 7.7 Hz, 1H), 8.42 (s, 1H), 8.29 (m, 3H), 8.02 (d, *J* = 15.7 Hz, 1H), 7.98 (m, 2H), 7.51 (m, 2H), 6.83 (dd, *J* = 15.8, 7.7 Hz, 1H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 193.48, 151.12, 133.21, 132.39, 132.36, 132.11, 130.80, 130.62, 129.72, 128.89, 128.53, 128.28, 128.09, 127.07, 126.45, 125.40, 120.76; HR-EIMS: *m/z* calcd for C<sub>17</sub>H<sub>11</sub>BrO [M]<sup>+</sup>: 309.9993; found: 309.9995.



#### **(*E*)-5-(3-(3-oxoprop-1-en-1-yl)naphthalen-2-yl)thiophene-2-carbaldehyde (7a)**

5-Formyl-2-thiopheneboronic acid (71.0 mg, 0.453 mmol) and Na<sub>2</sub>CO<sub>3</sub> (241 mg, 2.27 mmol) were added to the solution of (*E*)-3-(2-iodophenyl)acrylaldehyde (70.0 mg, 0.227 mmol) in a mixture of 2.4 mL of

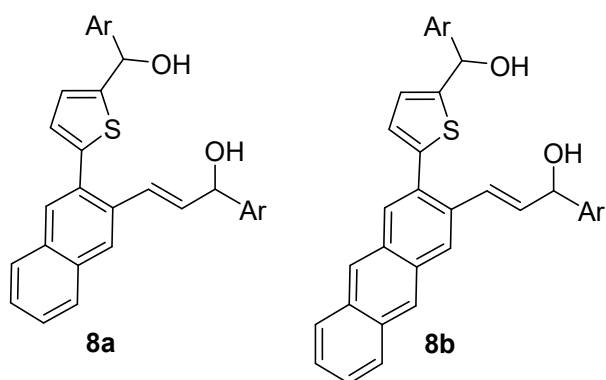
anhydrous DMF and 0.5 mL of H<sub>2</sub>O. The resulting mixture was degassed for 5 min, and then Pd(PPh<sub>3</sub>)<sub>4</sub> (27.0 mg, 0.023 mmol) was added to the solution under Ar. The resulting mixture was heated at 85 °C for 6 h. After cooling the reaction to room temperature, DMF was evaporated. The reaction mixture was extracted with EtOAc. The organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. The residue was purified over silica gel (EA/hexane, 1/3) to afford **7a** as a light green solid (53.0 mg, 80%).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 9.96 (s, 1H), 9.69 (d, *J* = 7.8 Hz, 1H), 8.22 (s, 1H), 8.01 (s, 1H), 7.93 (m, 1H), 7.89 (m, 1H), 7.83 (d, *J* = 3.6 Hz, 1H), 7.79 (d, *J* = 15.8 Hz, 1H), 7.60 (m, 2H), 7.20 (d, *J* = 3.6 Hz, 1H), 6.83 (dd, *J* = 15.8, 7.8 Hz, 1H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 193.38, 182.88, 151.10, 150.55, 144.45, 136.61, 133.87, 133.08, 130.85, 130.76, 130.69, 130.62, 129.40, 128.61, 128.58, 128.30, 128.17, 128.05; HR-EIMS: *m/z* calcd for C<sub>18</sub>H<sub>12</sub>O<sub>2</sub>S [M]<sup>+</sup>: 292.0558; found: 292.0556.

#### **(*E*)-5-(3-(3-oxoprop-1-en-1-yl)anthracen-2-yl)thiophene-2-carbaldehyde (7b)**

By following the general procedure of **7a**, the reaction of **6b** (178 mg, 0.572 mmol) yielded **7b** (159 mg, 81% yield).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 9.97 (s, 1H), 9.69 (d, *J* = 7.7 Hz, 1H), 8.50 (s, 1H), 8.44 (s, 1H), 8.37 (s, 1H), 8.16 (s, 1H), 8.02 (m, 2H), 7.83 (d, *J* = 3.8 Hz, 1H), 7.79 (dd, *J* = 15.8, 0.7 Hz, 1H), 7.53 (m, 2H), 7.23 (d, *J* = 3.8 Hz, 1H), 6.84 (dd, *J* = 15.8, 7.7 Hz, 1H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 193.40, 182.88, 151.31, 150.73, 144.25, 136.70, 133.26, 132.89, 131.08, 131.05, 130.68, 130.49, 130.23, 129.95, 129.23, 129.21, 128.52, 128.41, 127.82, 127.14, 126.94, 126.71; HR-EIMS: *m/z* calcd for C<sub>22</sub>H<sub>14</sub>O<sub>2</sub>S [M]<sup>+</sup>: 342.0715; found: 342.0712.



**(E)-3-(3-(5-(hydroxy(*p*-tolyl)methyl)thiophen-2-yl)naphthalen-2-yl)-1-(*p*-tolyl)prop-2-en-1-ol (**8a**)**

*p*-Tolylmagnesium bromide solution (1.0 mL, 1.03 mmol) was added to a well-stirred solution of **7a** (50.0 mg, 0.171 mmol) in THF (1.8 mL) at -78 °C under Ar. The mixture was stirred at same temperature for 2 h. The reaction mixture was poured into an aqueous saturated solution of NH<sub>4</sub>Cl and extracted with EtOAc. The organic layer was dried over anhydrous Na<sub>2</sub>SO<sub>4</sub> and evaporated to dryness. The residue was purified over silica gel (EA/hexane, 2/3) to afford **8a** as a green foam (60.3 mg, 74%).

<sup>1</sup>H NMR (400 MHz, Acetonitrile-*d*<sub>3</sub>) δ 7.97 (s, 1H), 7.85 (s, 1H), 7.80 (m, 2H), 7.44 (m, 2H), 7.35 (d, *J* = 7.9 Hz, 2H), 7.27 (d, *J* = 8.2 Hz, 2H), 7.18 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 7.9 Hz, 2H), 6.93 (d, *J* = 3.6 Hz, 1H), 6.84 (m, 2H), 6.37 (dd, *J* = 15.6, 6.1 Hz, 1H), 5.98 (d, *J* = 4.0 Hz, 1H), 5.24 (t, *J* = 5.1 Hz, 1H), 4.08 (d, *J* = 4.1 Hz, 1H), 3.48 (d, *J* = 4.1 Hz, 1H), 2.31 (s, 3H), 2.30 (s, 3H); <sup>13</sup>C NMR (100 MHz, Acetonitrile-*d*<sub>3</sub>) δ 150.57, 141.50, 141.13, 140.91, 137.45, 137.02, 135.26, 135.24, 134.07, 132.83, 132.64, 131.67, 129.06, 129.05, 128.79, 128.22, 127.64, 127.37, 126.62, 126.47, 126.41, 126.23, 125.79, 124.57, 73.95, 71.52, 20.23 (one carbon signal overlapped); HR-EIMS: *m/z* calcd for C<sub>32</sub>H<sub>28</sub>O<sub>2</sub>S [M]<sup>+</sup>: 476.1810; found: 476.1813.

**(E)-3-(3-(5-(hydroxy(*p*-tolyl)methyl)thiophen-2-yl)anthracen-2-yl)-1-(*p*-tolyl)prop-2-en-1-ol (**8b**)**

By following the general procedure of **8a**, the reaction of **7b** (94.0 mg, 0.275 mmol) yielded **8b** (108 mg, 75% yield).

<sup>1</sup>H NMR (400 MHz, Acetonitrile-*d*<sub>3</sub>) δ 8.37 (s, 1H), 8.36 (s, 1H), 8.08 (s, 1H), 7.98 (s, 1H), 7.95 (m, 2H), 7.43 (m, 2H), 7.36 (d, *J* = 8.1 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.17 (m, 4H), 6.95 (d, *J* = 3.5 Hz, 1H),

6.86 (m, 2H), 6.40 (dd,  $J = 15.7, 5.7$  Hz, 1H), 5.98 (d,  $J = 3.4$  Hz, 1H), 5.25 (m, 1H), 4.18 (d,  $J = 4.2$  Hz, 1H), 3.58 (d,  $J = 4.2$  Hz, 1H), 2.31 (s, 3H), 2.30 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, Acetonitrile- $d_3$ )  $\delta$  150.56, 141.50, 141.15, 140.89, 137.46, 137.03, 135.36, 135.33, 134.00, 132.17, 132.05, 131.62, 130.89, 130.76, 129.08, 129.05, 128.73, 128.40, 128.11, 127.38, 126.46, 126.43, 126.25, 126.12, 126.03, 125.85, 125.78, 124.62, 73.97, 71.55, 20.25 (one carbon signal overlapped); HR-EIMS:  $m/z$  calcd for  $\text{C}_{36}\text{H}_{30}\text{O}_2\text{S}$   $[\text{M}]^+$ : 526.1967; found: 526.1970.

#### ***o*-naphthalene-connected carbaporphyrin (4a)**

Boron trifluoride diethyl etherate (0.046 mL, 0.370 mmol) was added to the solution of **8a** (220 mg, 0.462 mmol) and 5-(4-methylphenyl)dipyrromethane (109 mg, 0.462 mmol) in distilled dichloromethane (400 mL) under Ar at room temperature. The solution was stirred in the dark under Ar for 1 h. Then, chloranil (342 mg, 1.39 mmol) was added and the reaction mixture was stirred for 1 h. The solvents were removed and the residual was then directly purified by chromatography over silica gel, eluting with DCM/hexane (1/1). The green fraction was collected and the solvent was removed under reduced pressure. The solid was washed with methanol, recrystallized with dichloromethane and washed with hexane which afforded **4a** as a dark green solid (24.8 mg, 8%).

$^1\text{H}$  NMR (400 MHz, Chloroform- $d$ )  $\delta$  9.72 (s, 1H), 8.38 (s, 1H), 8.13 (s, 1H), 7.95 (m, 2H), 7.60 (d,  $J = 8.1$  Hz, 2H), 7.55 (m, 2H), 7.41 (m, 5H), 7.33 (m, 4H), 7.24 (m, 2H), 7.07 (m, 2H), 6.93 (d,  $J = 4.9$  Hz, 1H), 6.86 (d,  $J = 4.9$  Hz, 1H), 6.82 (d,  $J = 3.7$  Hz, 1H), 6.59 (d,  $J = 3.7$  Hz, 1H), 5.30 (d,  $J = 16.4$  Hz, 1H), 2.51 (s, 3H), 2.47 (s, 3H), 2.44 (s, 3H);  $^{13}\text{C}$  NMR (100 MHz, Chloroform- $d$ )  $\delta$  169.62, 160.82, 154.52, 152.24, 147.72, 143.53, 141.58, 140.86, 137.98, 137.56, 137.25, 136.98, 136.52, 136.35, 135.93, 135.13, 134.16, 132.55, 132.47, 132.41, 132.07, 131.87, 131.82, 131.06, 130.41, 130.26, 130.15, 129.85, 129.52, 129.27, 128.73, 128.65, 127.81, 127.68, 126.71, 122.50, 109.08, 21.47, 21.34 (three carbon signals overlapped); HR-FABMS:  $m/z$  calcd for  $\text{C}_{48}\text{H}_{37}\text{N}_2\text{S}$   $[\text{M} + \text{H}]^+$ : 673.2677; found: 673.2674.

#### ***o*-anthracene-connected carbaporphyrin (4b)**

By following the general procedure of **4a**, the reaction of **8b** (77.0 mg, 0.146 mmol) yielded **4b** (9.51 mg, 9% yield).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 10.62 (s, 1H), 8.49 (s, 2H), 8.40 (s, 1H), 8.17 (s, 1H), 8.03 (m, 2H), 7.58 (d, *J* = 8.0 Hz, 2H), 7.50 (m, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.33 (m, 7H), 7.24 (m, 2H), 7.18 (d, *J* = 16.3 Hz, 1H), 6.97 (d, *J* = 5.2 Hz, 1H), 6.89 (d, *J* = 3.6 Hz, 1H), 6.83 (d, *J* = 4.9 Hz, 1H), 6.75 (d, *J* = 4.9 Hz, 1H), 6.67 (d, *J* = 3.6 Hz, 1H), 5.67 (d, *J* = 16.4 Hz, 1H), 2.51 (s, 3H), 2.46 (s, 3H), 2.43 (s, 3H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 162.10, 154.02, 153.11, 147.58, 143.45, 141.81, 137.97, 137.66, 137.57, 137.18, 136.50, 136.38, 136.02, 135.76, 134.29, 132.96, 132.66, 132.20, 131.88, 131.69, 130.84, 130.77, 130.70, 130.46, 130.27, 130.11, 130.01, 129.99, 129.84, 129.55, 129.31, 128.87, 128.76, 128.63, 128.37, 126.41, 126.17, 125.85, 125.80, 121.83, 108.99, 21.49, 21.46, 21.33 (two carbon signals overlapped); HR-FABMS: *m/z* calcd for C<sub>52</sub>H<sub>39</sub>N<sub>2</sub>S [M + H]<sup>+</sup>: 723.2834; found: 723.2830.

#### **Pd complex of *o*-anthracene-connected carbaporphyrin (Pd-4b)**

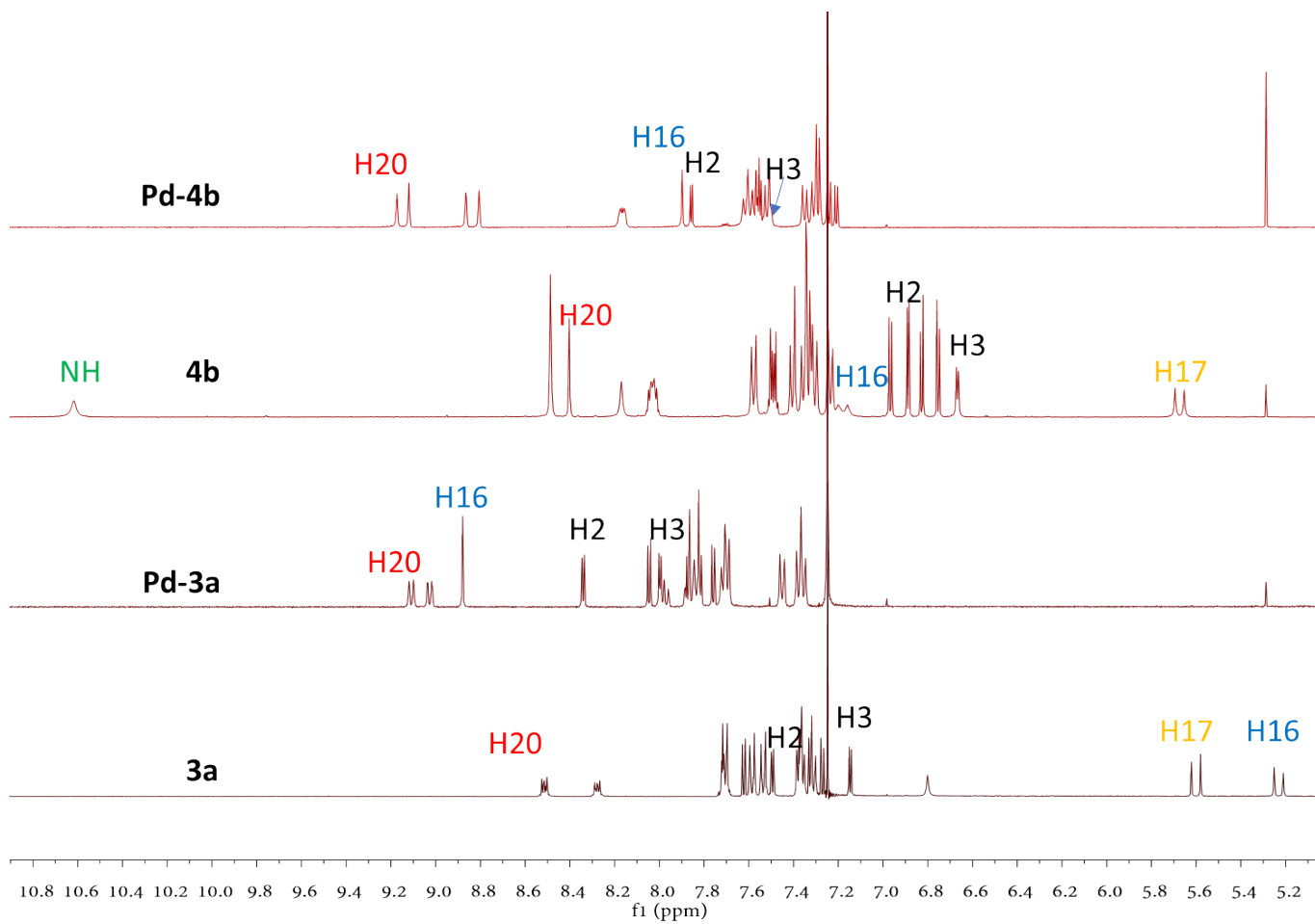
Palladium(II) acetate (9.9 mg, 0.0442 mmol in 0.9 mL of HPLC grade acetonitrile) was added to the solution of **4b** (6.40 mg, 0.00885 mmol) in distilled dichloromethane (9 mL). The mixture was stirred for 12 h. The solution was then purified by column chromatography over silica gel, eluting with dichloromethane. The green fraction was collected and the solvents were removed under reduced pressure. The solid was recrystallized with dichloromethane and washed with hexane, which afforded **Pd-4b** as a dark green solid (3.3 mg, 45%).

<sup>1</sup>H NMR (400 MHz, Chloroform-*d*) δ 9.17 (s, 1H), 9.12 (s, 1H), 8.86 (s, 1H), 8.81 (s, 1H), 8.16 (dt, *J* = 6.3, 2.4 Hz, 2H), 7.90 (s, 1H), 7.86 (d, *J* = 3.9 Hz, 1H), 7.55 (m, 10H), 7.35 (dd, *J* = 8.0 Hz, 2H), 7.29 (m, 5H), 7.25 (m, 1H), 7.21 (d, *J* = 5.0 Hz, 1H), 2.50 (d, *J* = 1.8 Hz, 6H), 2.44 (s, 3H); <sup>13</sup>C NMR (100 MHz, Chloroform-*d*) δ 152.73, 151.30, 149.02, 144.16, 143.18, 140.96, 140.65, 138.51, 138.17, 136.94, 136.85, 136.73, 136.13, 134.86, 133.09, 132.96, 132.72, 132.60, 132.29, 132.01, 131.88, 131.81, 131.32, 130.44, 130.12, 129.48, 129.42, 129.32, 129.12, 128.81, 128.64, 128.41, 128.32, 128.28, 127.07, 125.65,

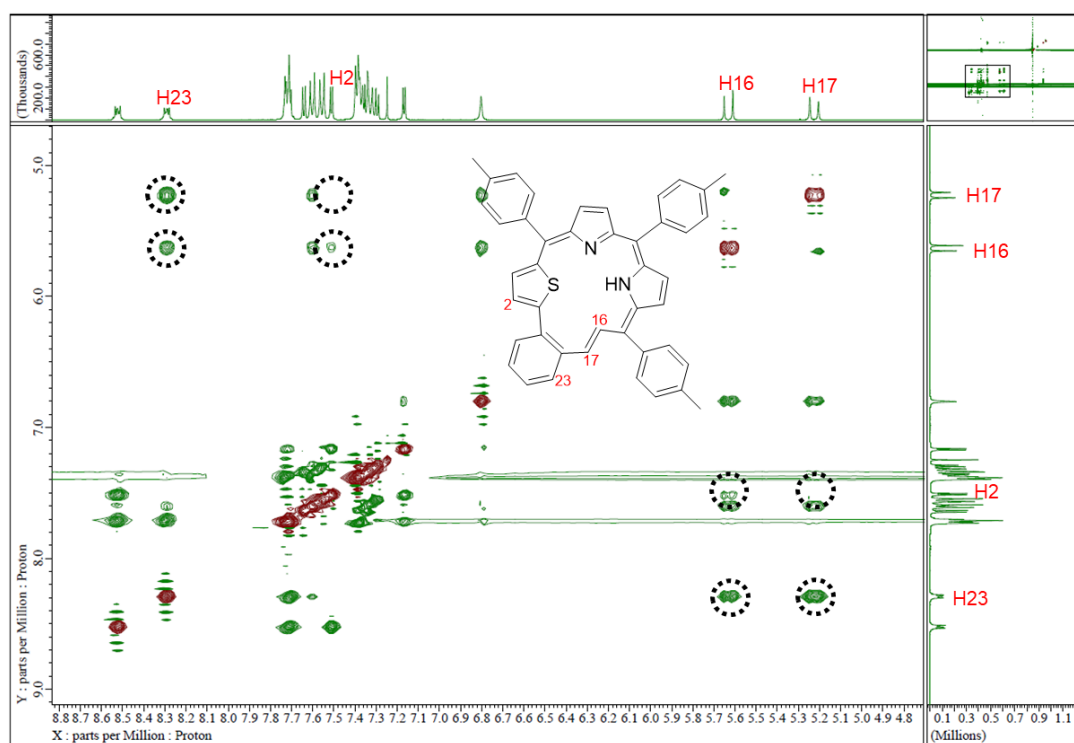
125.60, 125.50, 125.28, 124.85, 123.06, 113.24, 21.48, 21.42, 21.33 (one carbon signal overlapped); HR-FAB: m/z calcd for C<sub>52</sub>H<sub>36</sub>N<sub>2</sub>PdS [M]<sup>+</sup>: 826.1634; found: 826.1637.



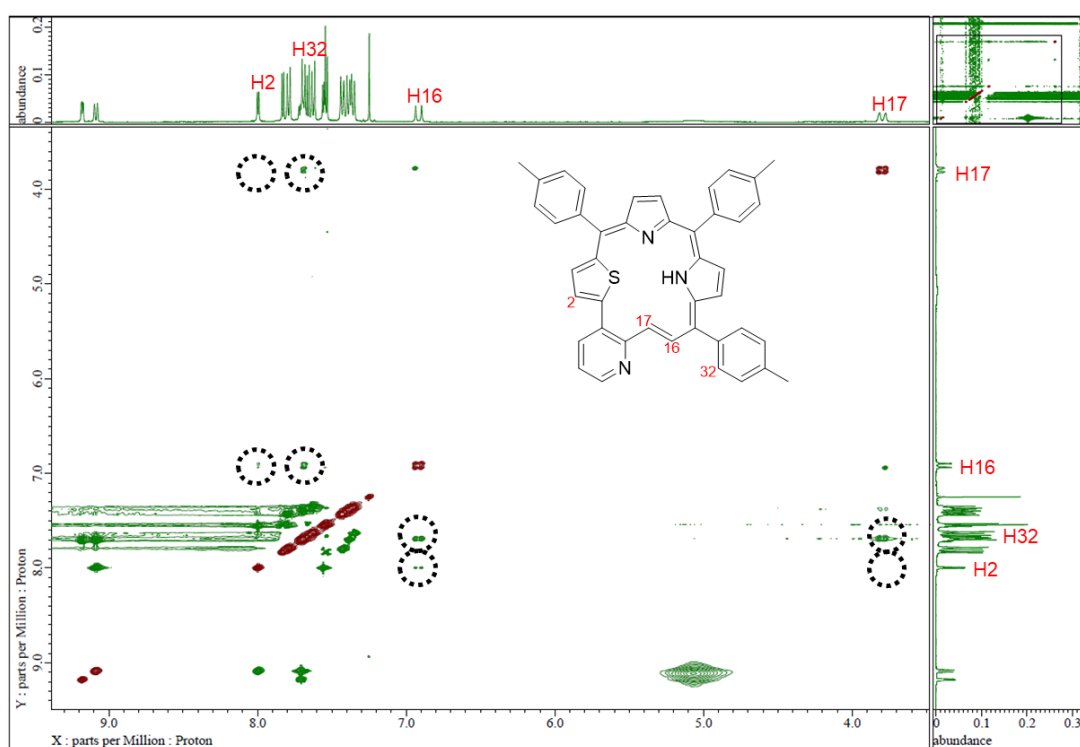
## 2. Stacked $^1\text{H}$ NMR and partial 2D NOESY spectra



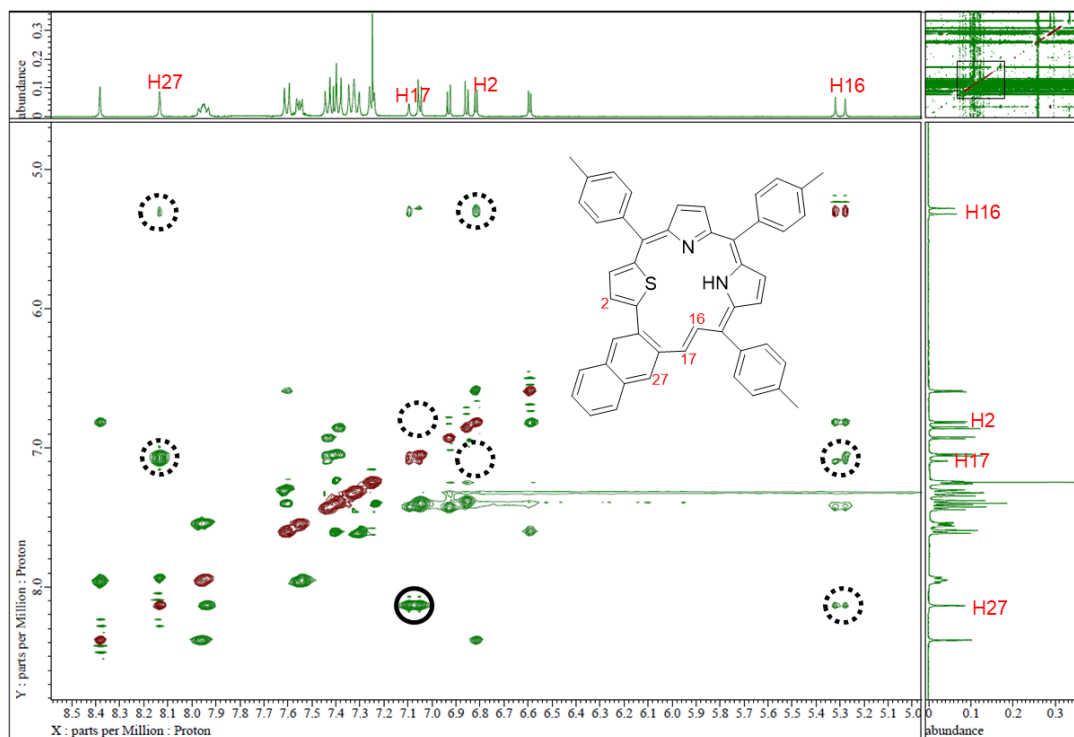
**Figure S1.** Stacked  $^1\text{H}$  NMR spectra of **3a**, **Pd-3a**, **4b**, and **Pd-4b** in  $\text{CDCl}_3$  at 298 K



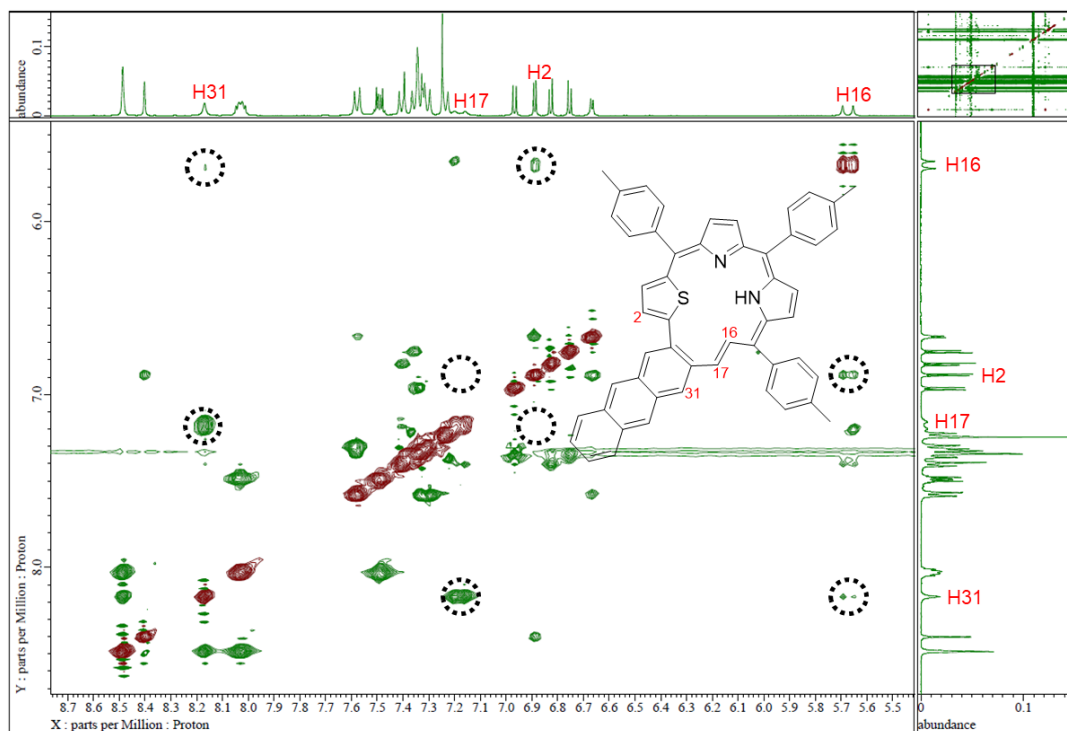
**Figure S2.** Partial 2D NOESY spectrum of **3a** in CDCl<sub>3</sub> at 298 K (400 MHz)



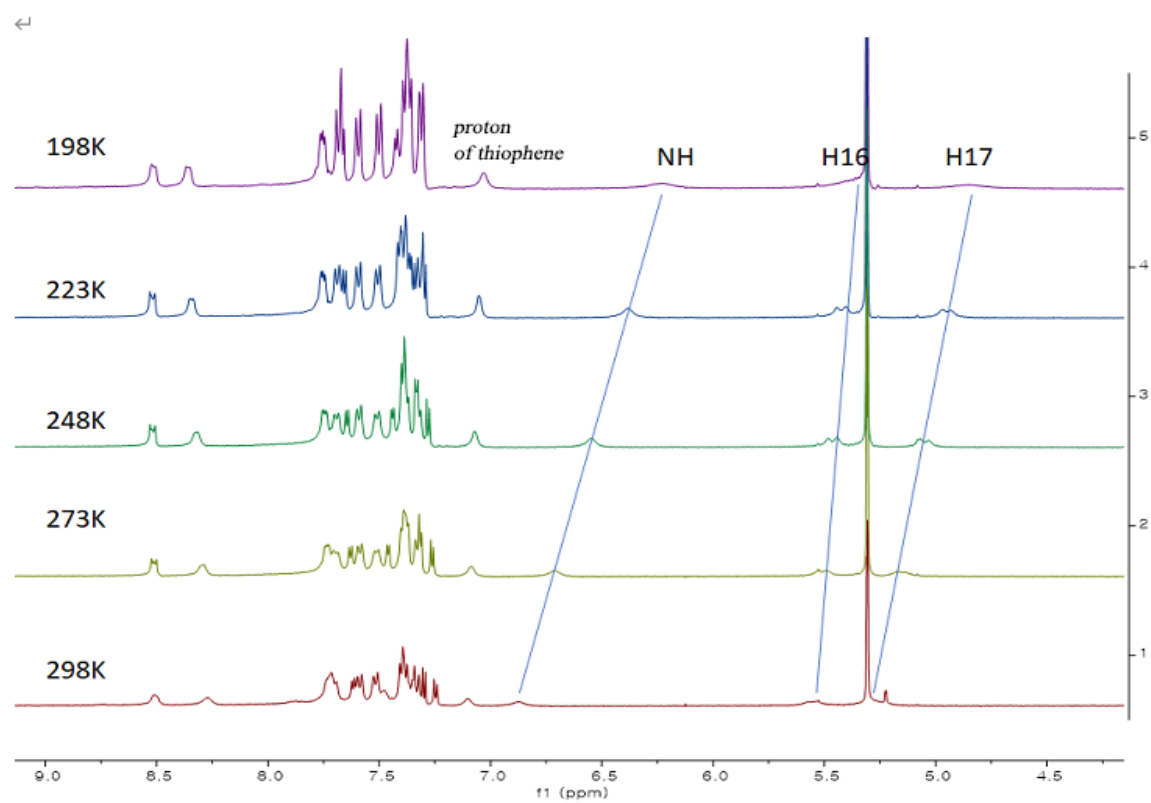
**Figure S3.** Partial 2D NOESY spectrum of **3b** in CDCl<sub>3</sub> at 298 K (400 MHz)



**Figure S4.** Partial 2D NOESY spectrum of **4a** in  $\text{CDCl}_3$  at 298 K (400 MHz)



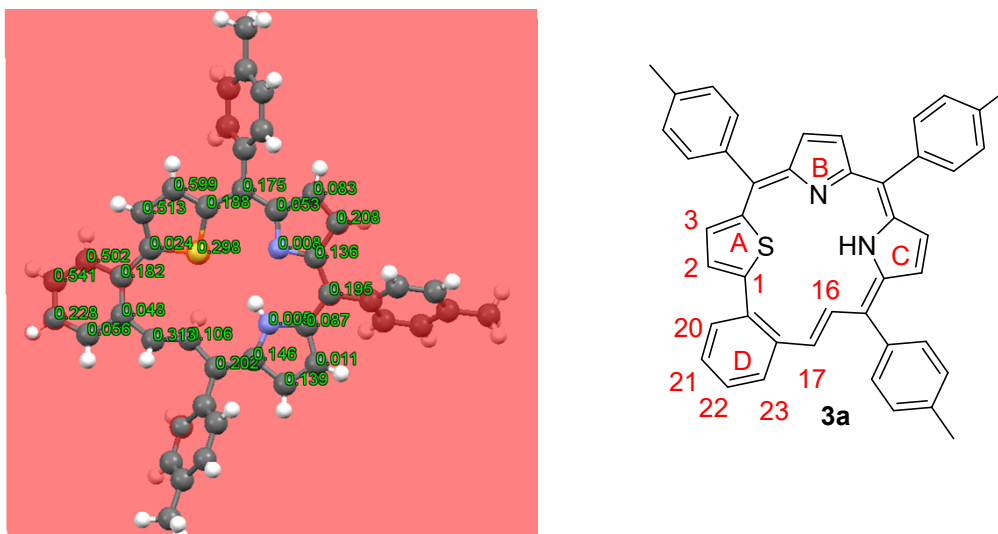
**Figure S5.** Partial 2D NOESY spectrum of **4b** in  $\text{CDCl}_3$  at 298 K (400 MHz)



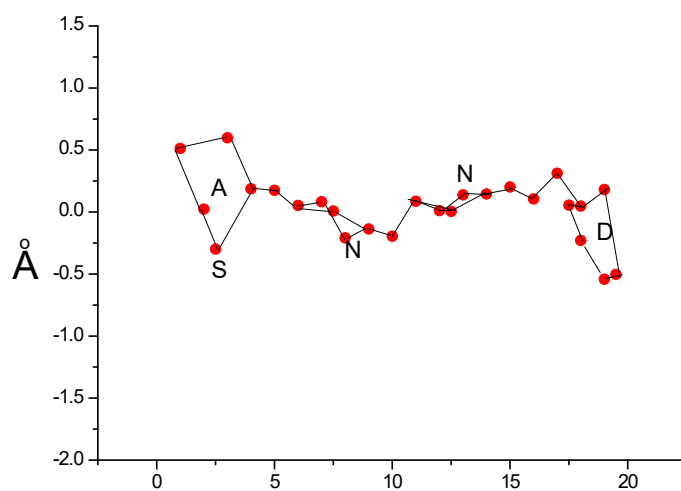
**Figure S6.** Variable temperature <sup>1</sup>H NMR spectra of **3a** in CD<sub>2</sub>Cl<sub>2</sub> (400 MHz)

### 3. Single Crystal X-ray Analyses of 3a, Pd-3a, and 4a

(a)

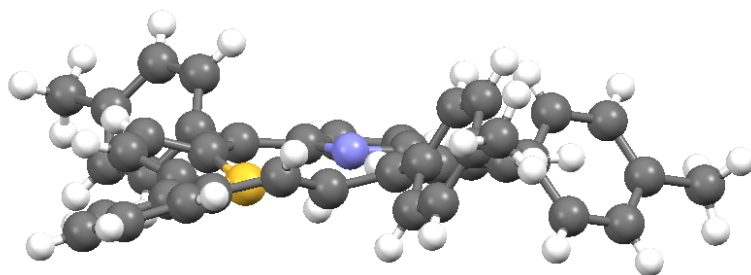


(b)

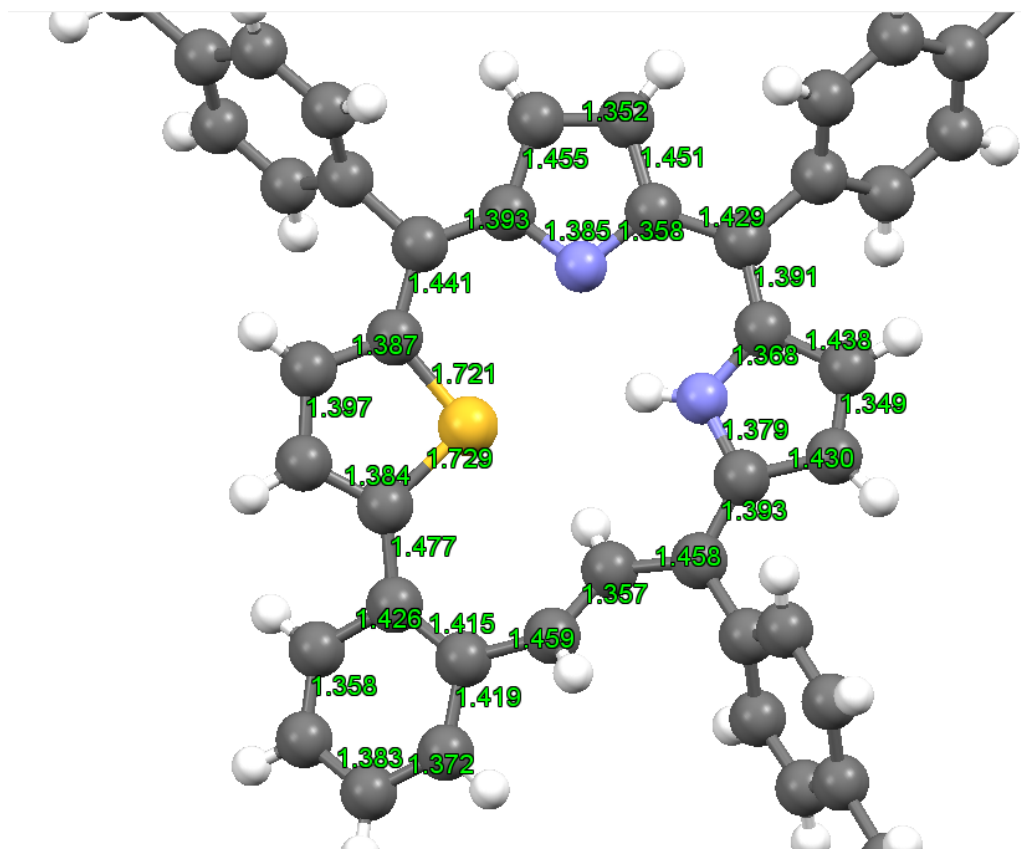


**Figure S7.** (a) Selected distances (Å) between a specific atom and the mean plane (C5, C10, C15, and C19). (b) The mean plane deviation diagram of **3a**. Atoms in red denote the atoms below the mean plane and atoms above the mean plane are highlighted in black.

(a)

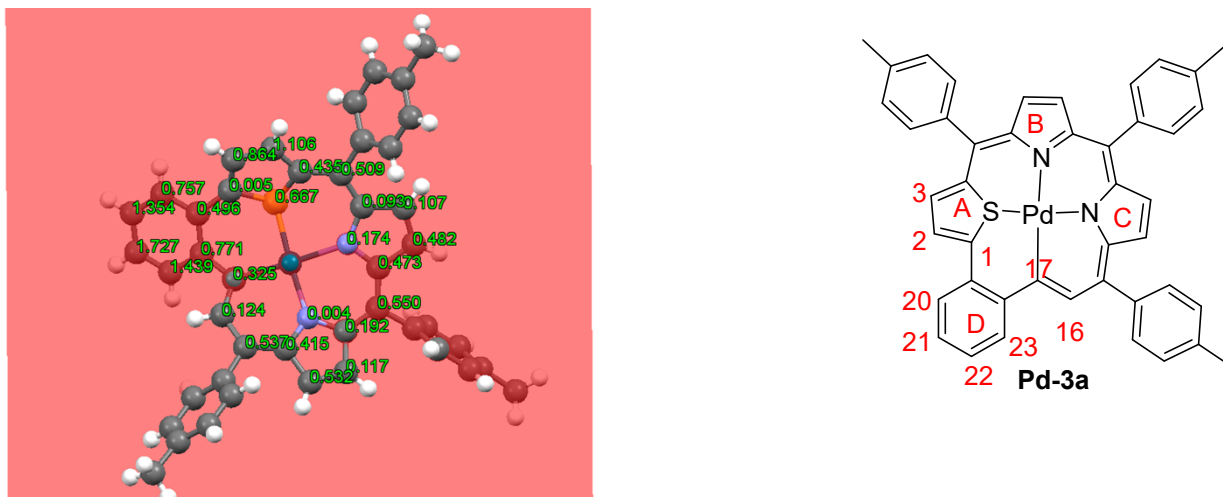


(b)

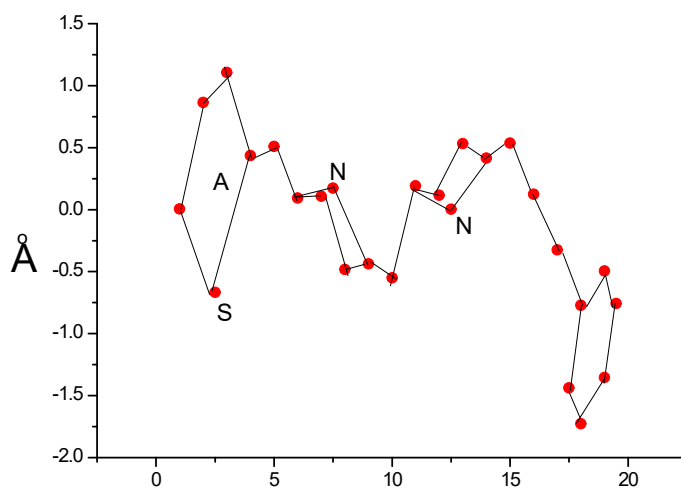


**Figure S8.** (a) Side view and (b) bond lengths (Å) of 3a

(a)

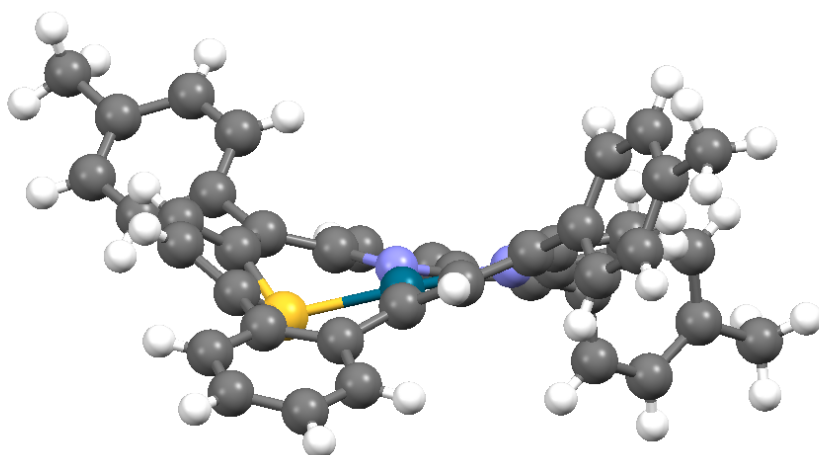


(b)

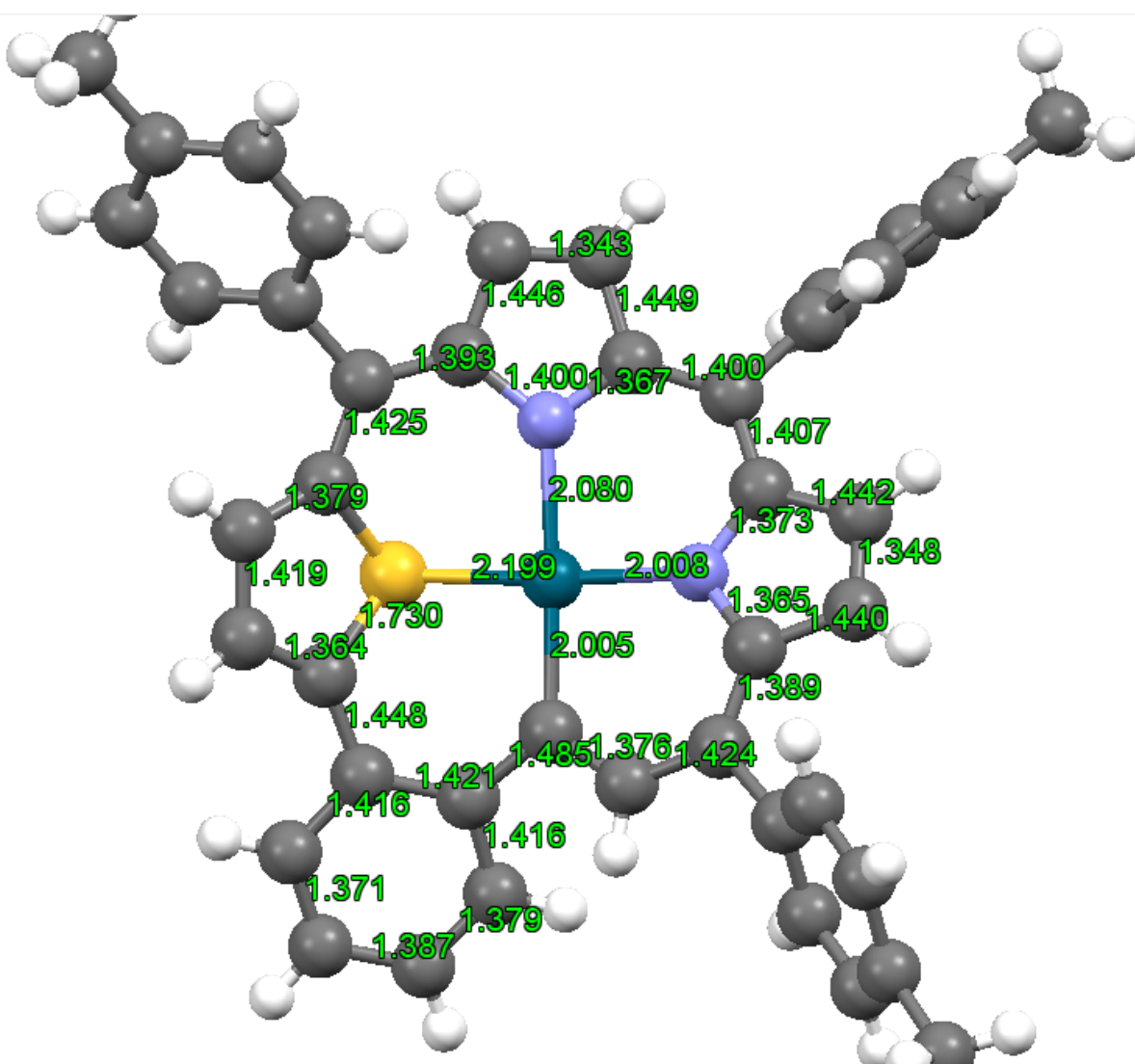


**Figure S9.** (a) Selected distances (Å) between a specific atom and the mean plane (C5, C10, C15, and C19). (b) The mean plane deviation diagram of **Pd-3a**. Atoms in red denote the atoms below the mean plane and atoms above the mean plane are highlighted in black.

(a)



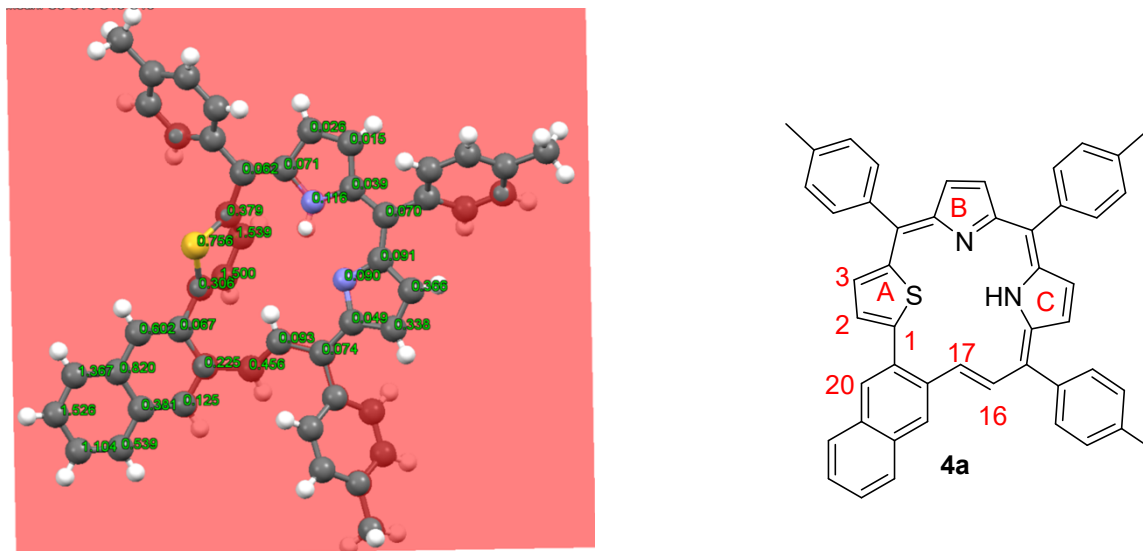
(b)



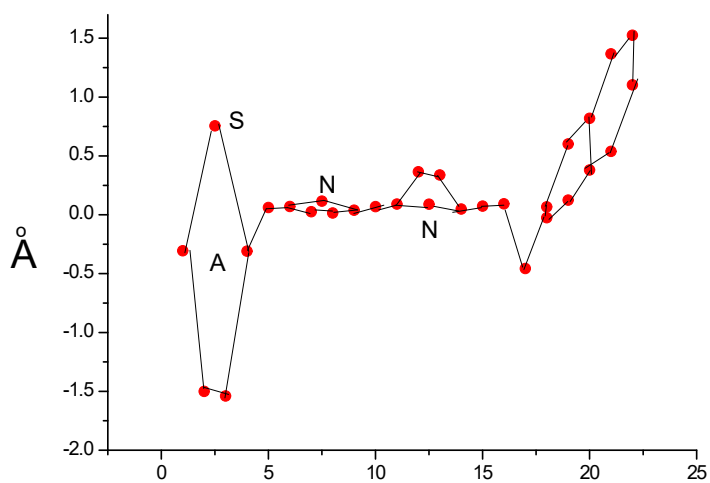
**Figure S10.** (a) Side view and (b) bond lengths (Å) of Pd-3a



(a)

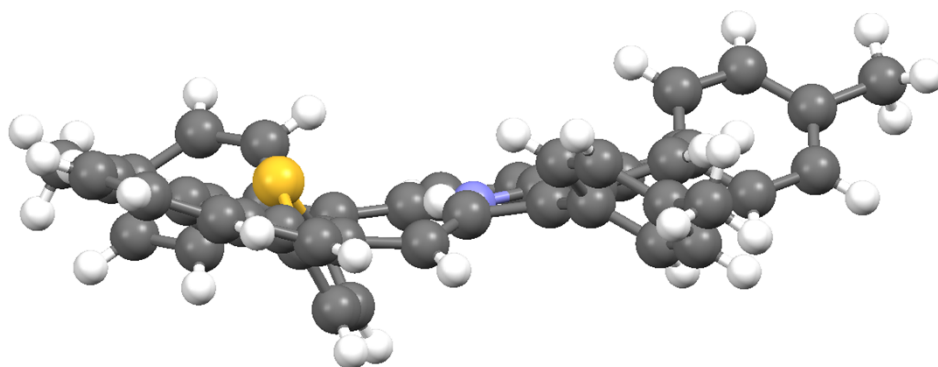


(b)

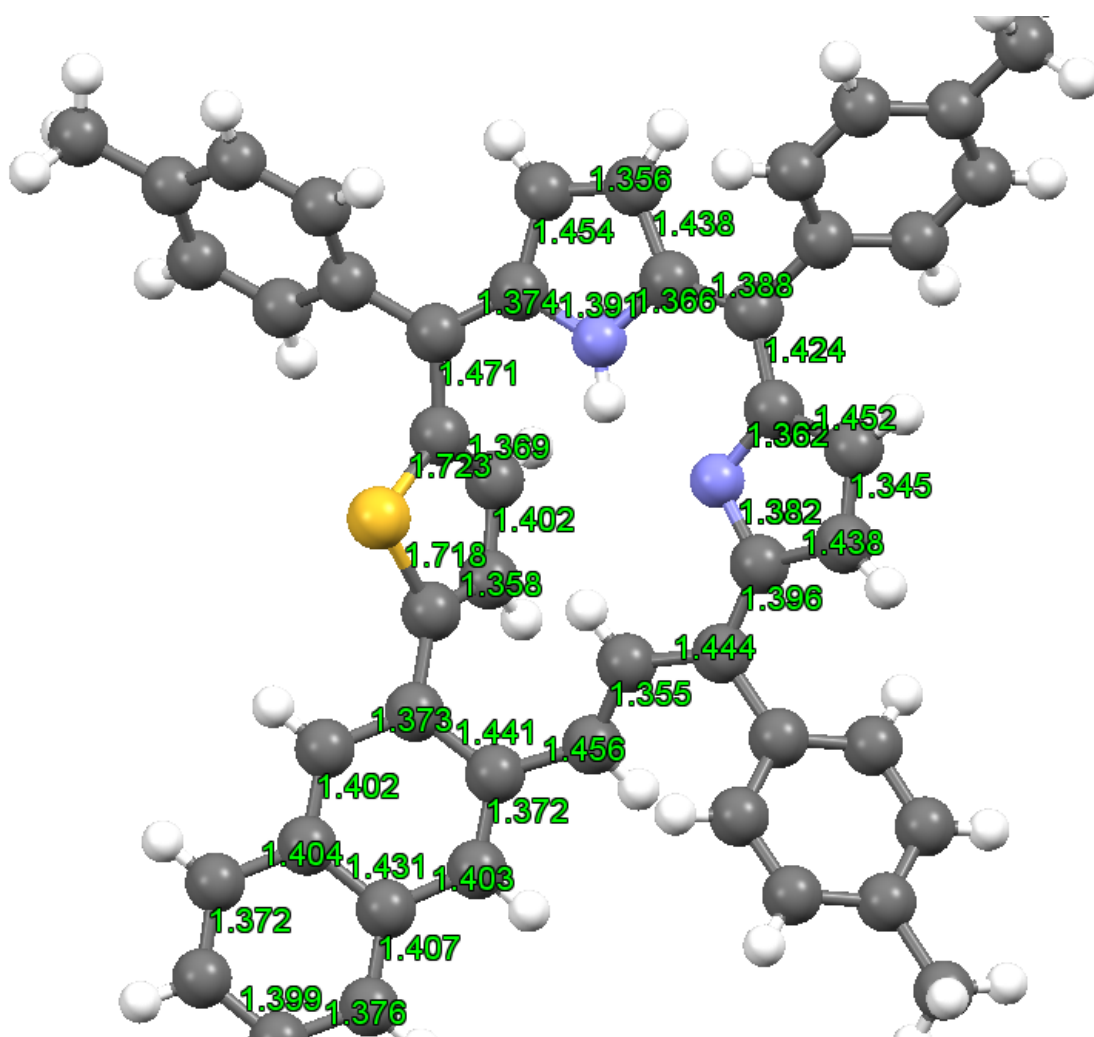


**Figure S11.** (a) Selected distances (Å) between a specific atom and the mean plane (C5, C10, C15, and C19). (b) The mean plane deviation diagram of **4a**. Atoms in red denote the atoms below the mean plane and atoms above the mean plane are highlighted in black.

(a)



(b)



**Figure S12.** (a) Side view and (b) bond lengths (Å) of **4a**

## X-ray structural data of 4a

**Table S1.** Crystal data and structure refinement for **4a**

Empirical formula	C <sub>48</sub> H <sub>36</sub> N <sub>2</sub> S	
Formula weight	672.85	
Temperature	223(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2 <sub>1</sub> /n	
Unit cell dimensions	a = 13.9249(5) Å	a = 90°.
	b = 18.8546(7) Å	b = 117.135(2)°.
	c = 15.0205(6) Å	g = 90°.
Volume	3509.6(2) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.273 Mg/m <sup>3</sup>	
Absorption coefficient	1.100 mm <sup>-1</sup>	
F(000)	1416	
Crystal size	0.080 x 0.075 x 0.035 mm <sup>3</sup>	
Theta range for data collection	3.591 to 71.066°.	
Index ranges	-16 ≤ h ≤ 16, -23 ≤ k ≤ 20, -17 ≤ l ≤ 16	
Reflections collected	26806	
Independent reflections	6438 [R(int) = 0.1092]	
Completeness to theta = 67.679°	97.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7534 and 0.6097	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6438 / 0 / 464	
Goodness-of-fit on F <sup>2</sup>	0.958	
Final R indices [I > 2σ(I)]	R1 = 0.0691, wR2 = 0.1672	
R indices (all data)	R1 = 0.1715, wR2 = 0.2358	
Extinction coefficient	0.0007(2)	
Largest diff. peak and hole	0.248 and -0.321 e.Å <sup>-3</sup>	

## 4. DFT, NICS, and HOMA Calculations

### Calculation Details

All density functional theory (DFT) calculations were performed with a Gaussian 09 program package. Calculations for structural optimizations and frequency calculation were carried out using the density functional theory (DFT) method with Becke's three-parameter hybrid exchange functionals and the Lee-Yang-Parr correlation functional (B3LYP) employing the 631LAN basis set. The 631LAN bases set is composed of 6-31G\*\* for carbon, hydrogen, nitrogen, sulfur and LANL2DZ for palladium metal atoms. Initial structures for ground state were constructed based on the X-ray crystal structures. Ground state geometries were verified by the frequency calculations, where no imaginary frequency was found.

### References

- (1) Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

## NICS (0) Calculations

With the DFT-optimized structures, Nucleus-Independent Chemical Shift (NICS) calculations were carried. The calculated NICS (0) values of all conformations ( $\delta_{i,\text{calc}}$ ) in the center of them were averaged by introducing a normalized Boltzmann factor as follows:

$$p_i = \exp(-\Delta G_i/RT) / \sum \exp(-\Delta G_i/RT)$$

$$\langle \delta_{\text{calc}} \rangle = \sum p_i \cdot \delta_{i,\text{calc}}$$

**Table S2.** Average NICS (0) values ( $\langle \delta_{\text{calc}} \rangle$ ) of **3a**, **3b**, **4a**, and **4b**

		<b>x<sub>1</sub></b>	<b>x<sub>2</sub></b>	<b>x<sub>3</sub></b>	<b>x<sub>4</sub></b>	<b>x<sub>5</sub></b>	<b>x<sub>6</sub></b>	<b>x<sub>7</sub></b>	<b>x<sub>8</sub></b>	$\langle \delta_{\text{calc}} \rangle$
<b>3a</b>	$\delta_i$	-7.19	-6.71	-6.44	-4.76	-9.63	- <sup>a</sup>	- <sup>b</sup>	-8.11	
	$p_i$	0.0415	0.1786	0.6317	0.0068	0.1407			0.0007	
	$p_i \cdot \delta_i$	-0.2986	-1.1977	-4.0707	-0.0325	-1.3543			-0.0054	-6.96
<b>3b</b>	$\delta_i$	-8.53	-7.16	-6.63	-5.36	-11.37	-9.76	- <sup>b</sup>	-8.99	
	$p_i$	0.0275	0.1298	0.3290	0.0039	0.4553	0.0531		0.0014	
	$p_i \cdot \delta_i$	-0.2347	-0.9288	-2.1806	-0.0210	-5.1763	-0.5179		-0.0126	-9.07
<b>4a</b>	$\delta_i$	-3.96	-4.71	-4.46	-1.72	-5.98	- <sup>a</sup>	- <sup>b</sup>	-4.89	
	$p_i$	0.0086	0.1896	0.7587	0.0048	0.0379			0.0003	
	$p_i \cdot \delta_i$	-0.0341	-0.8935	-3.3871	-0.0323	-0.2267			-0.0016	-4.55
<b>4b</b>	$\delta_i$	-2.63	-3.85	-3.55	-0.61	-5.05	- <sup>a</sup>	- <sup>b</sup>	-3.72	
	$p_i$	0.0042	0.1809	0.7905	0.0040	0.0202			0.0002	
	$p_i \cdot \delta_i$	-0.0109	-0.6956	-2.8069	-0.0024	-0.1020			-0.0008	-3.62

<sup>a, b</sup> **3/4x<sub>6</sub>** and **3/4x<sub>7</sub>** are merged to **3/4x<sub>5</sub>** and **3/4x<sub>8</sub>**, respectively except **3b<sub>6</sub>** after the optimization.

## HOMA Calculations

With the DFT-optimized structures, Harmonic Oscillator Model of Aromaticity (HOMA) calculations were carried. The calculated HOMA values of all conformations ( $h_{i,\text{calc}}$ ) were averaged by introducing a normalized Boltzmann factor as follows:

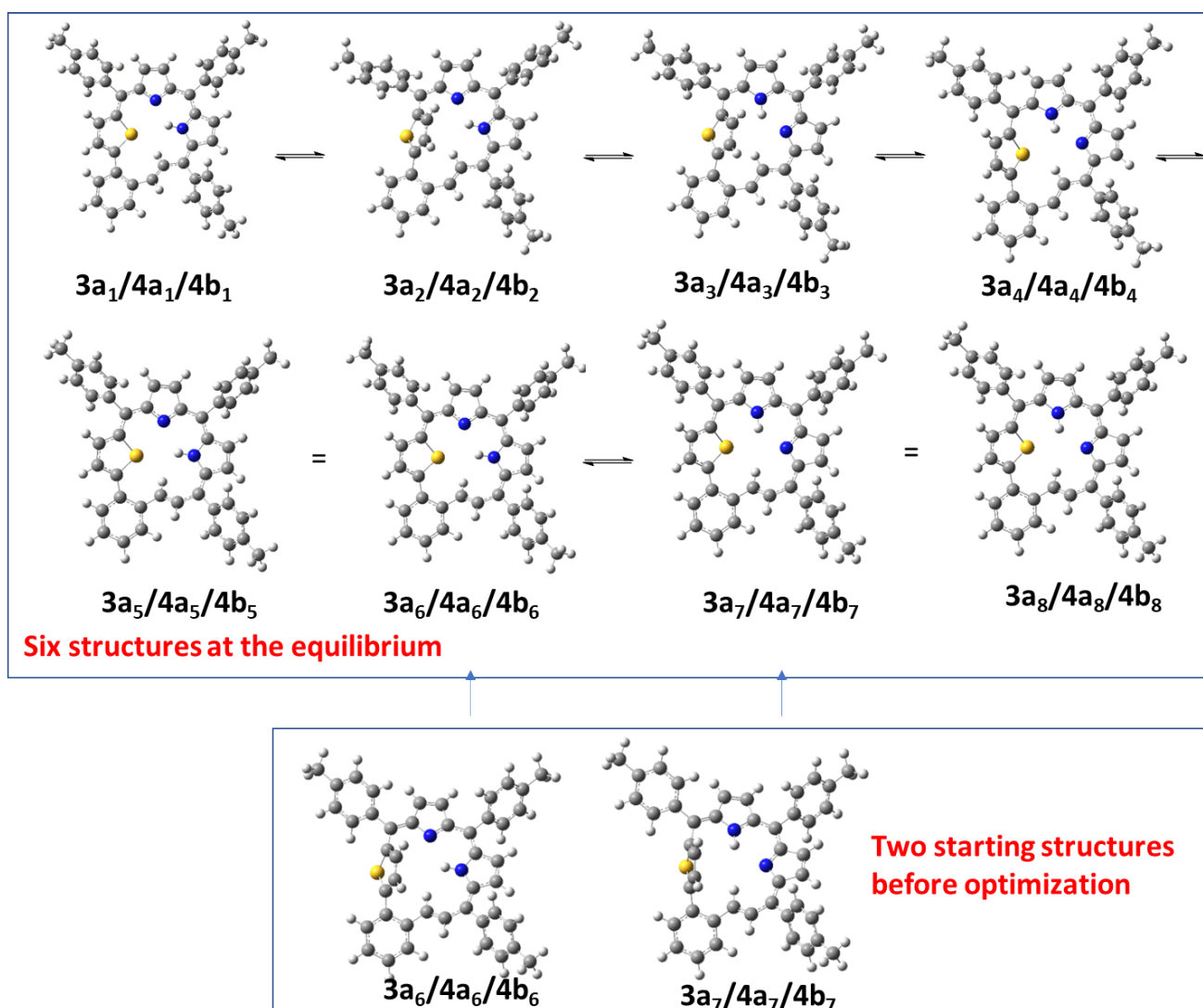
$$p_i = \exp(-\Delta G_i/RT) / \sum \exp(-\Delta G_i/RT)$$

$$\langle h_{\text{calc}} \rangle = \sum p_i \cdot h_{i,\text{calc}}$$

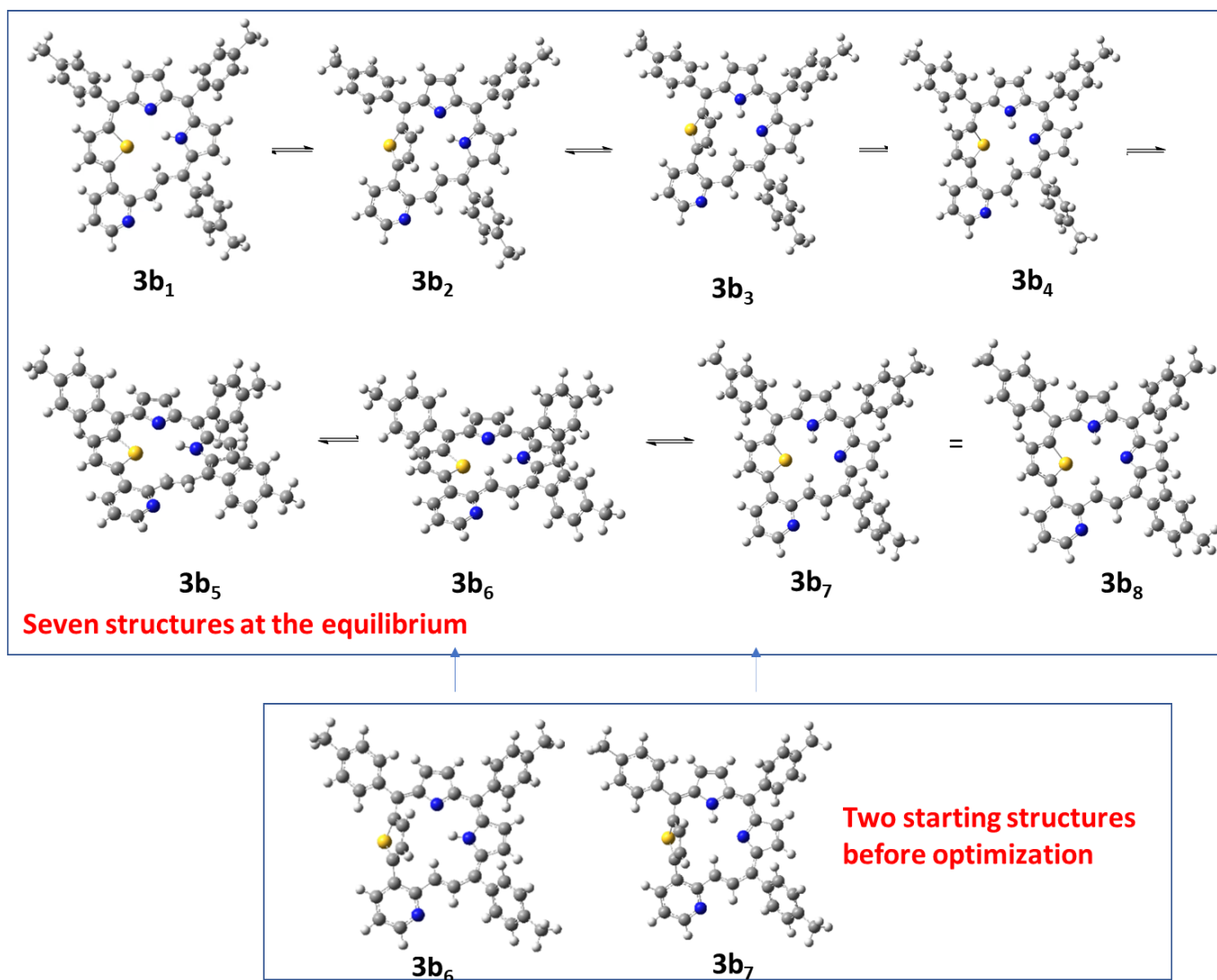
**Table S3.** Average HOMA values ( $\langle h_{\text{calc}} \rangle$ ) of **3a**, **3b**, **4a**, and **4b**

		<b>x<sub>1</sub></b>	<b>x<sub>2</sub></b>	<b>x<sub>3</sub></b>	<b>x<sub>4</sub></b>	<b>x<sub>5</sub></b>	<b>x<sub>6</sub></b>	<b>x<sub>7</sub></b>	<b>x<sub>8</sub></b>	$\langle h_{\text{calc}} \rangle$
<b>3a</b>	$h_i$	0.58	0.55	0.51	0.53	0.63	- <sup>a</sup>	- <sup>b</sup>	0.60	
	$p_i$	0.0415	0.1786	0.6317	0.0068	0.1407			0.0007	
	$p_i \cdot h_i$	0.0241	0.0975	0.3253	0.0036	0.0881			0.0004	0.54
<b>3b</b>	$h_i$	0.60	0.56	0.53	0.55	0.68	0.67	- <sup>b</sup>	0.65	
	$p_i$	0.0275	0.1298	0.329	0.0039	0.4553	0.0531		0.0014	
	$p_i \cdot h_i$	0.0166	0.0727	0.1743	0.0021	0.3112	0.0353		0.0009	0.61
<b>4a</b>	$h_i$	0.49	0.49	0.46	0.43	0.53	- <sup>a</sup>	- <sup>b</sup>	0.50	
	$p_i$	0.0086	0.1896	0.7587	0.0048	0.0379			0.0003	
	$p_i \cdot h_i$	0.0042	0.0926	0.3467	0.0021	0.0202			0.0002	0.47
<b>4b</b>	$h_i$	0.46	0.46	0.43	0.40	0.50	- <sup>a</sup>	- <sup>b</sup>	0.47	
	$p_i$	0.0042	0.1809	0.7905	0.004	0.0202			0.0002	
	$p_i \cdot h_i$	0.0019	0.0835	0.3396	0.0016	0.0100			0.0001	0.44

<sup>a, b</sup> **3/4x<sub>6</sub>** and **3/4x<sub>7</sub>** are merged to **3/4x<sub>5</sub>** and **3/4x<sub>8</sub>**, respectively except **3b<sub>6</sub>** after the optimization.

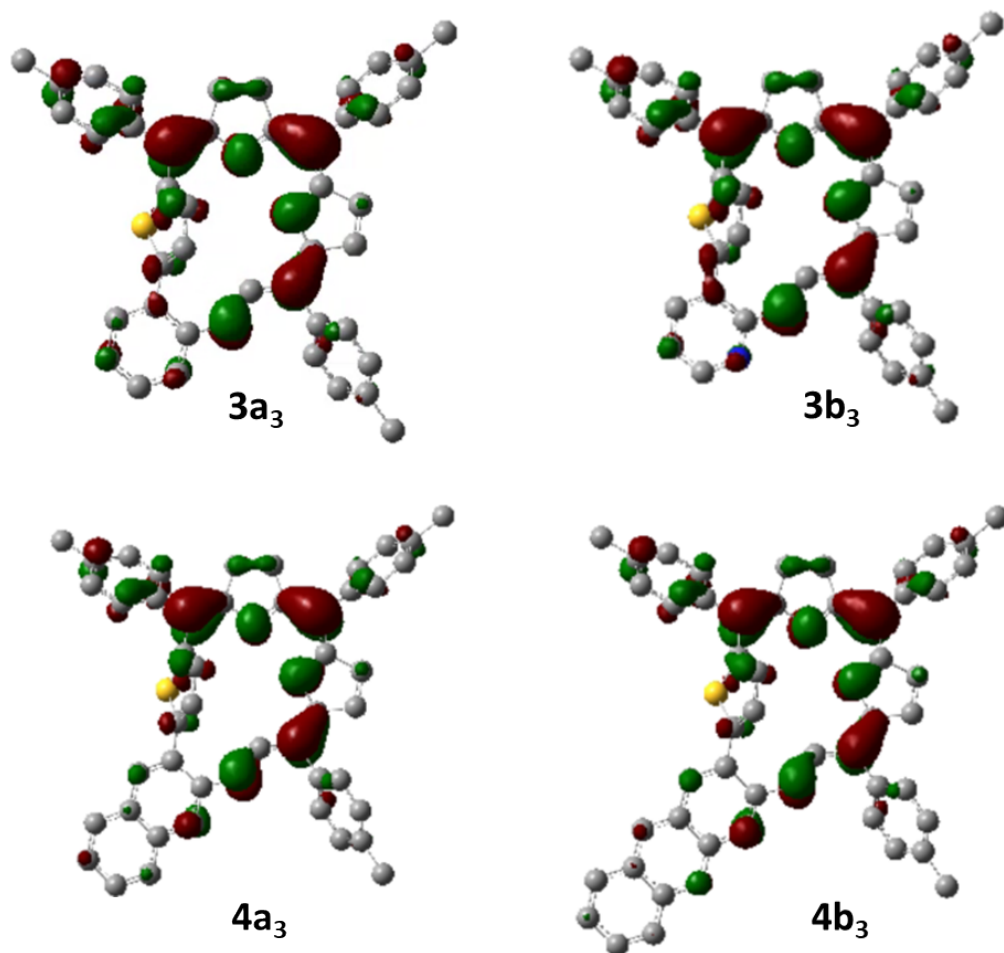


**Figure S13.** Equilibrium structures of **3a/4a/4b** obtained from DFT optimization. The initial set of eight structures was optimized using density functional theory (DFT), resulting in six possible equilibrium structures.

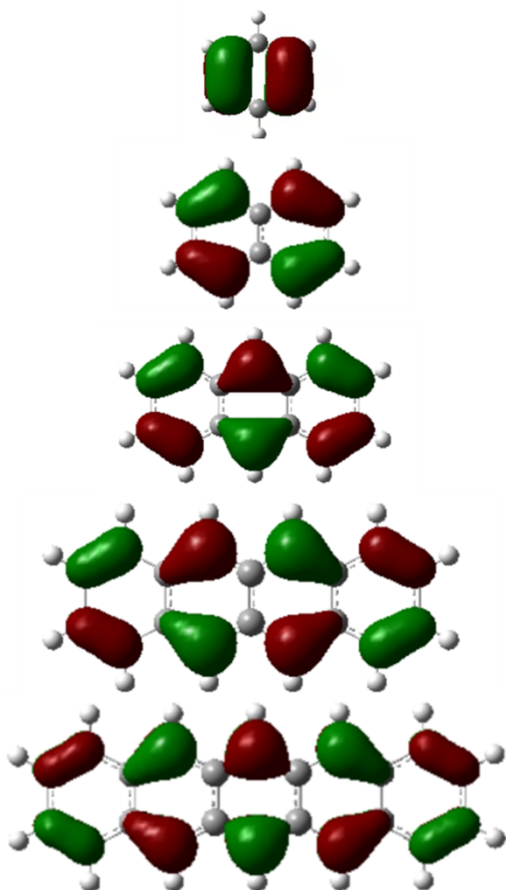


**Figure S14.** Equilibrium structures of **3b** obtained from DFT optimization. The initial set of eight structures was optimized using density functional theory (DFT), resulting in seven possible equilibrium structures.



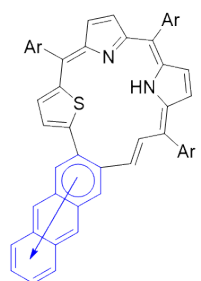
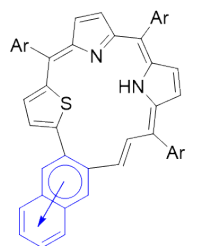
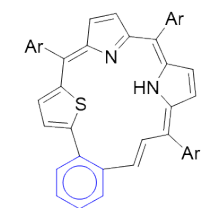


**Figure S15.** DFT-calculated HOMO of **3a<sub>3</sub>**, **3b<sub>3</sub>**, **4a<sub>3</sub>**, and **4b<sub>3</sub>** (isovalue = 0.03 e/Å<sup>3</sup>). Hydrogen atoms are omitted for clarity.

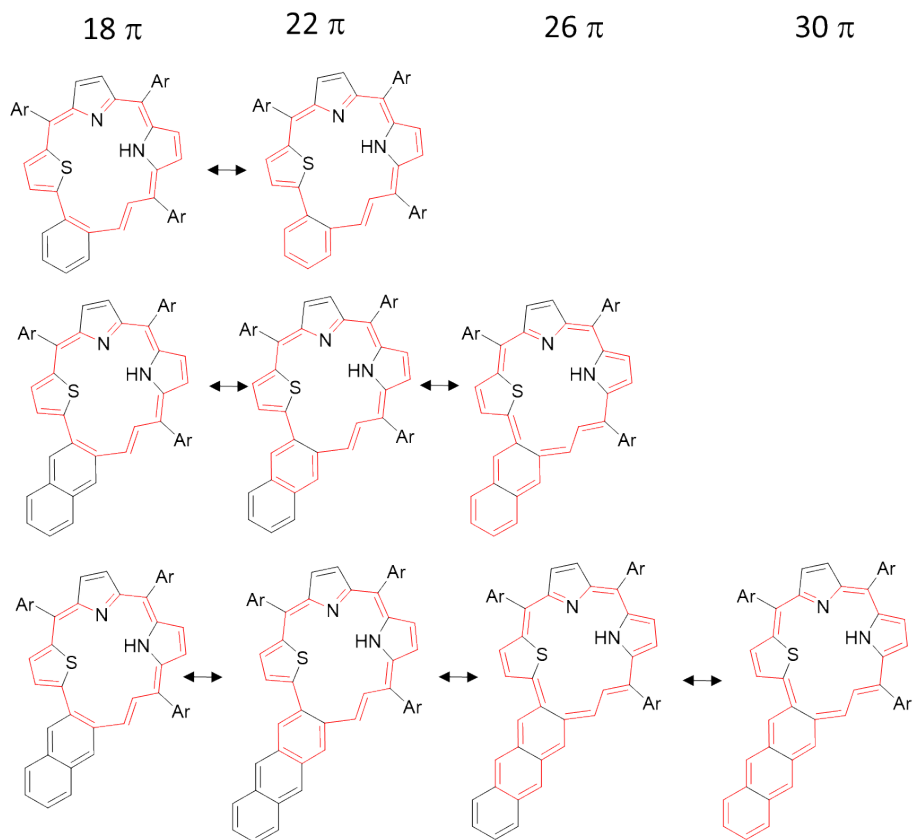


**Figure S16.** Comparison of the highest occupied molecular orbital (HOMO) of benzene and various polycyclic aromatic hydrocarbons (PAHs). This figure illustrates that the electron density of the HOMOs is highest at the centers of the PAH molecules and lowest at their peripheries.

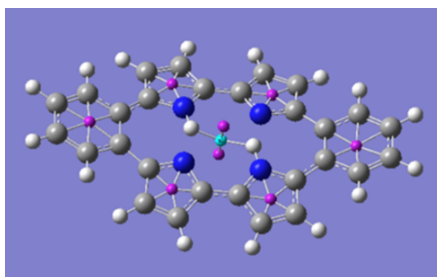
every local  
resonance structure  
(one  $\pi$ -sextet)



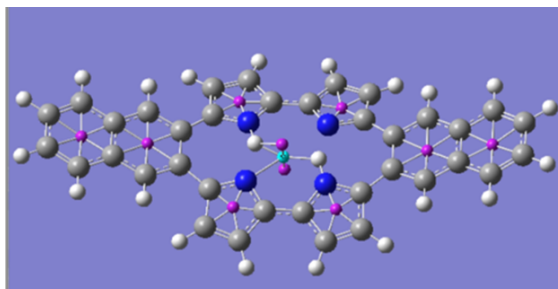
Every global resonance structure (no  $\pi$ -sextet)



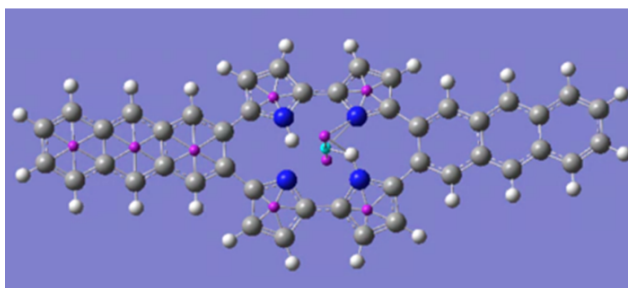
**Figure S17.** Possible global conjugation pathways (red line) of *o*-arene-connected porphyrins and their competing local pathway (blue line) of arenes such as benzene, naphthalene, and anthracene. Three different porphyrinoids have the same number of  $\pi$ -sextet for global and local pathways.



NICS(0) = -10.36

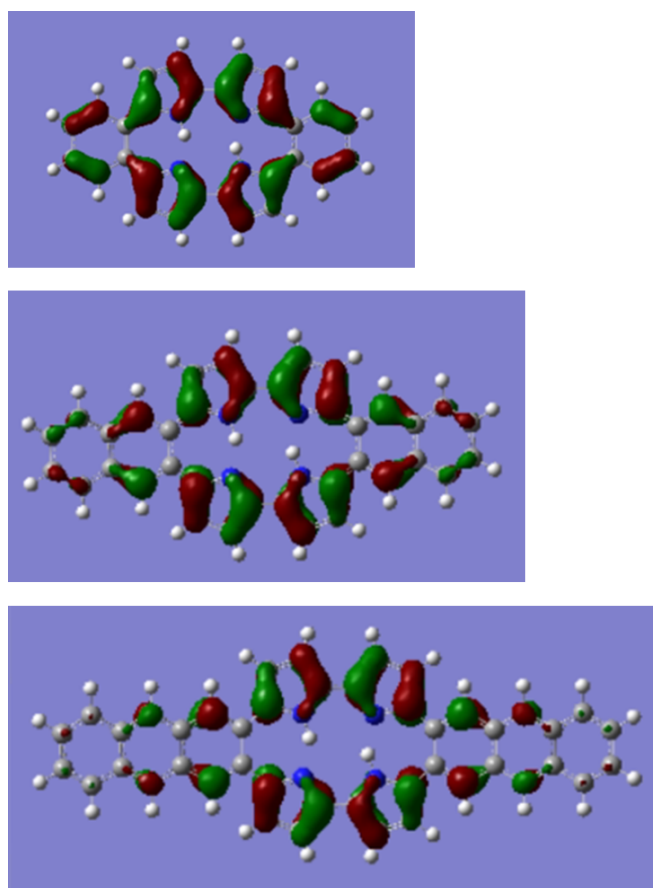


NICS(0) = -7.87



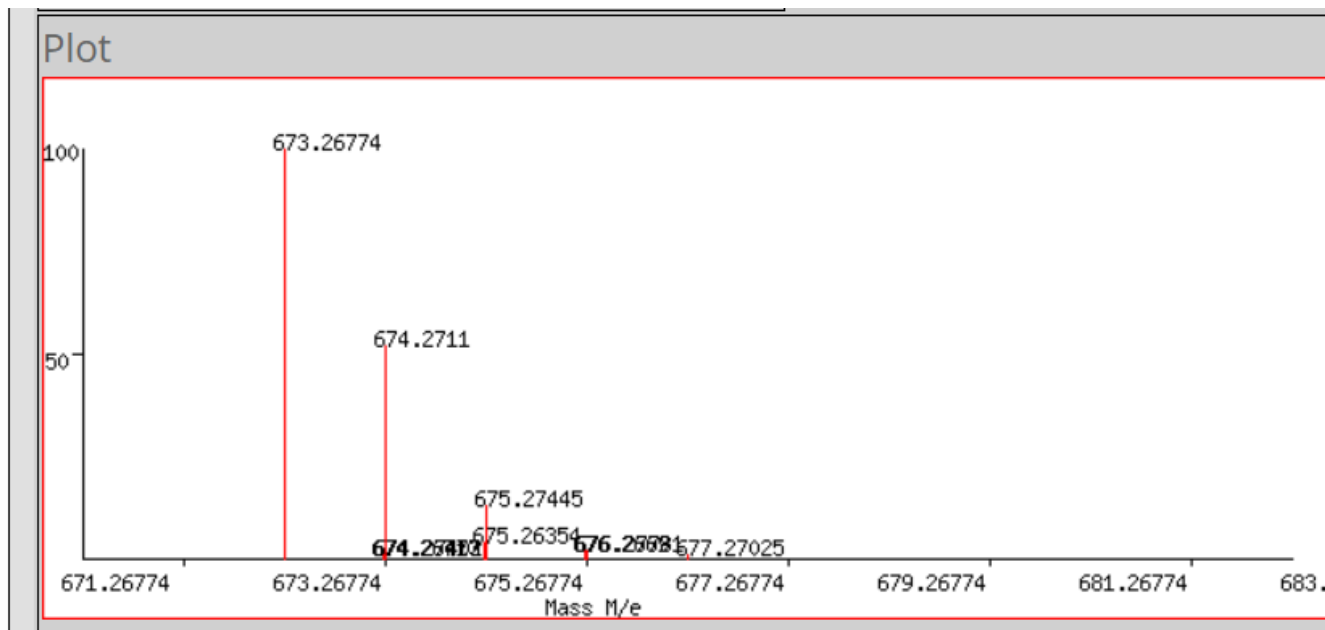
NICS(0) = -6.03

**Figure S18.** NICS (0) values of **9a**, **9b**, and **9c**

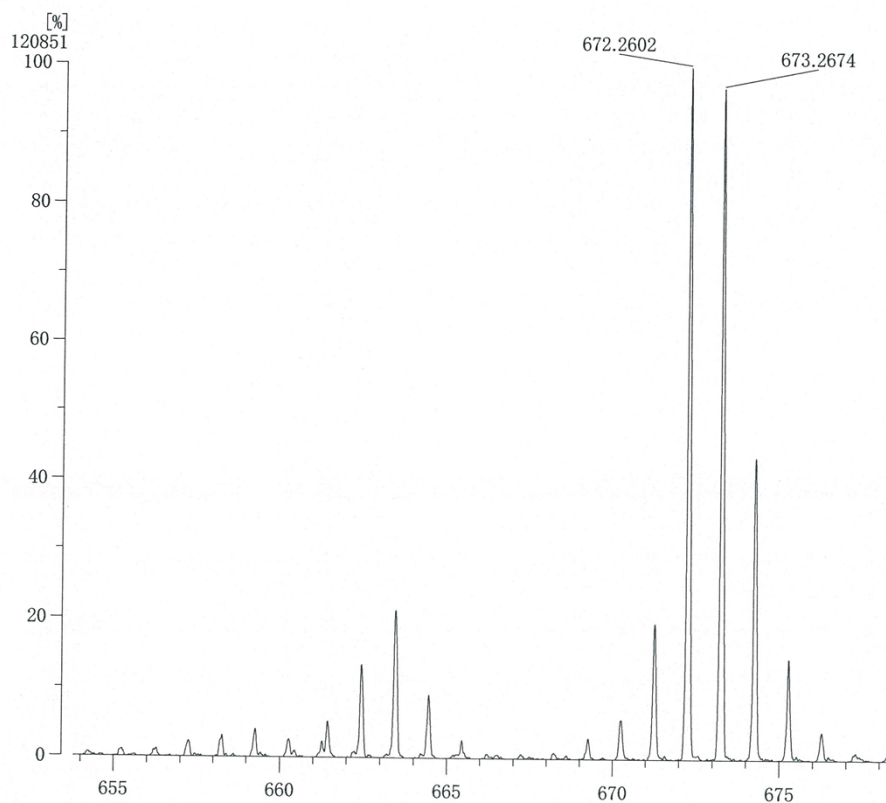


**Figure S19.** DFT-calculated HOMO of **9a**, **9b**, and **9c** (isovalue =  $0.03 \text{ e}/\text{\AA}^3$ )

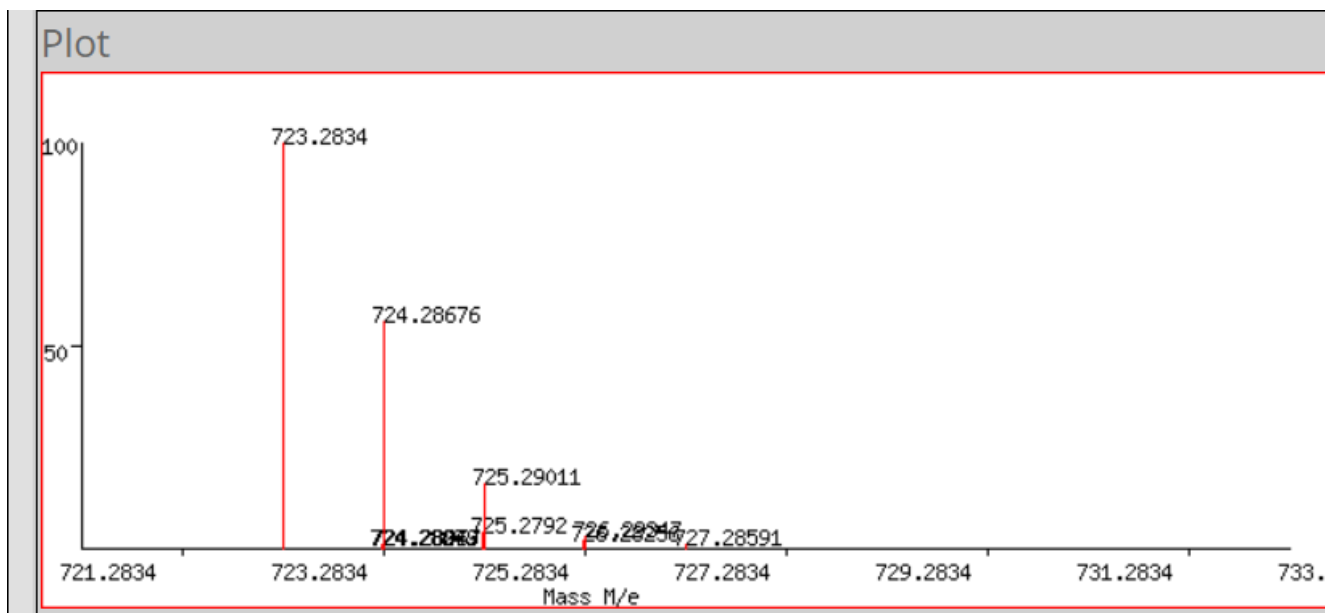
## 5. HR-Mass Data



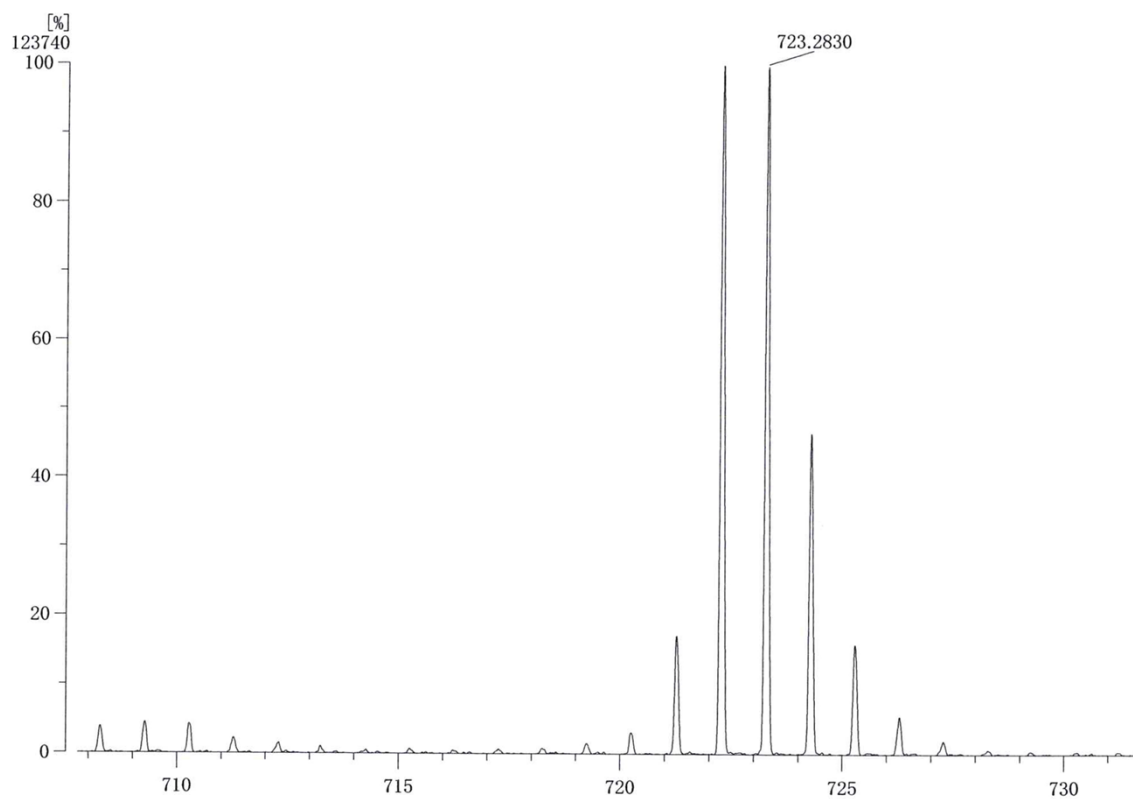
[ Mass Spectrum ]  
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Instrument : MStation  
Sample : -  
Inlet : Direct Ion Mode : FAB+  
Spectrum Type : Normal Ion [EF-Linear]



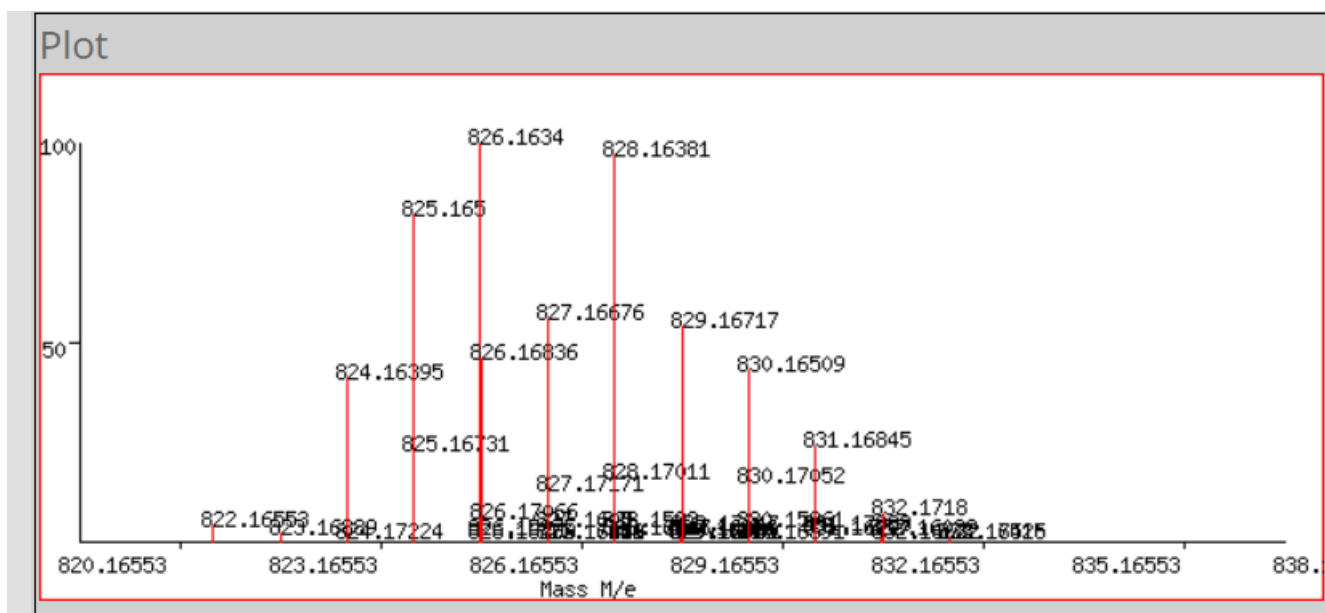
**Figure S20.** Theoretical and observed HRMS data of **4a** (HRMS (FAB):  $m/z$  calcd for  $C_{48}H_{37}N_2S$   $[M + H]^+$ : 673.2677; found: 673.2674)



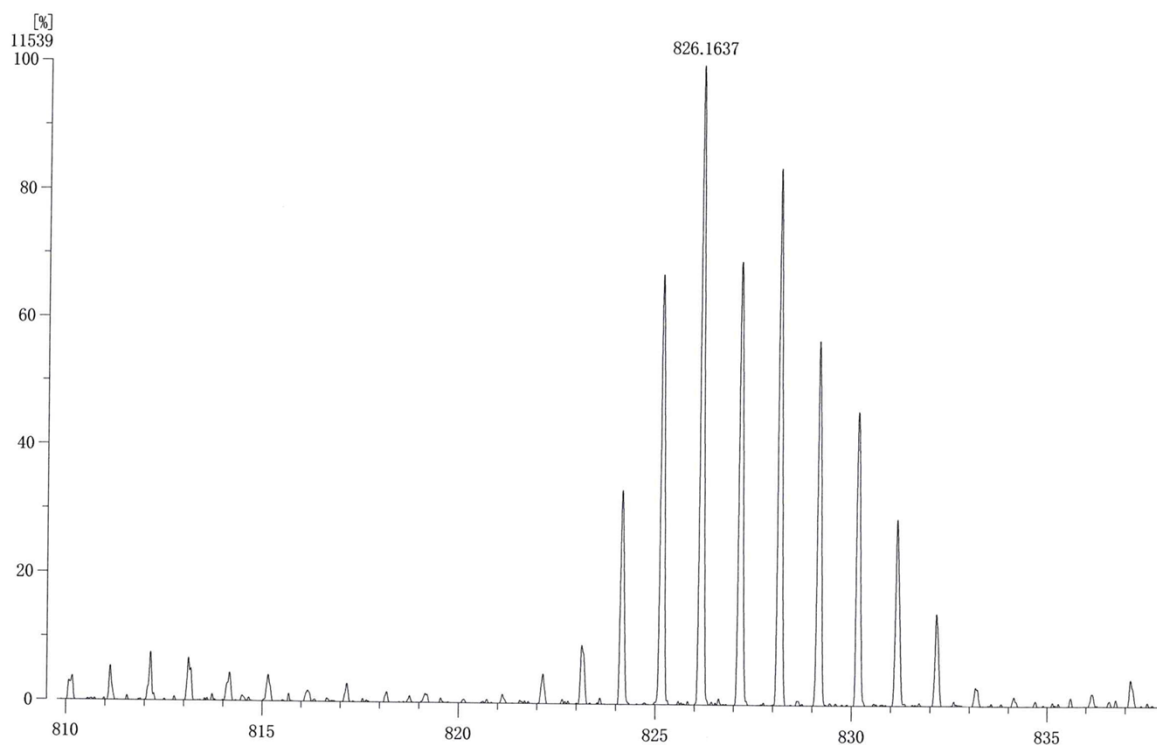
[ Mass Spectrum ]  
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 Instrument : MStation  
 Sample : -  
 Inlet : Direct Ion Mode : FAB+  
 Spectrum Type : Normal Ion [EF-Linear]



**Figure S21.** Theoretical and observed HRMS data of **4b** (HRMS (FAB):  $m/z$  calcd for  $C_{52}H_{39}N_2S [M + H]^+$ : 723.2834; found: 723.2830)



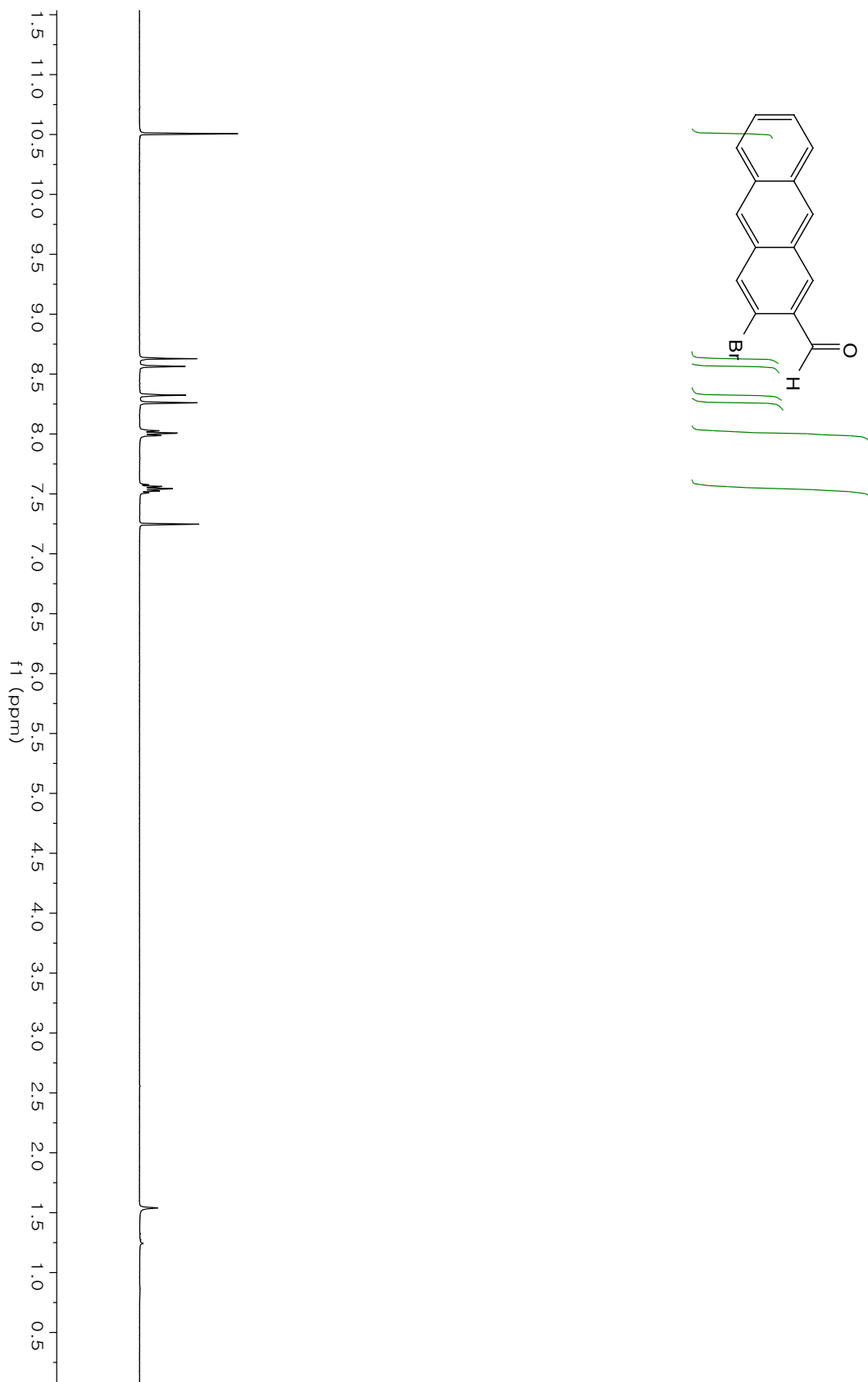
[ Mass Spectrum ]  
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 Instrument : MStation  
 Sample : -  
 Inlet : Direct Ion Mode : FAB+  
 Spectrum Type : Normal Ion [EF-Linear]



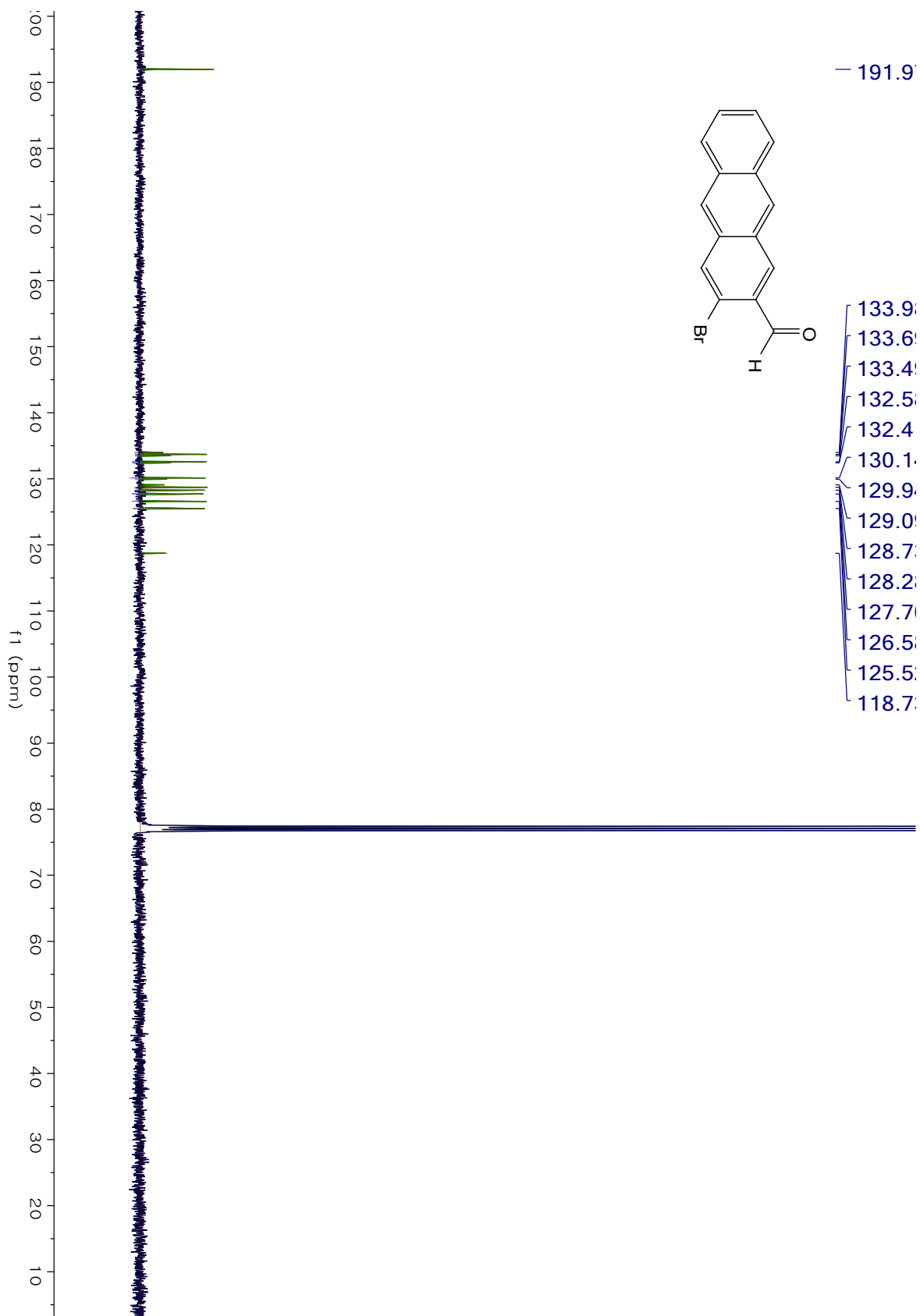
**Figure S22.** Theoretical and observed HRMS data of **Pd-4b** (HRMS (FAB): m/z calcd for  $[M]^+$   $C_{52}H_{36}N_2PdS$ : 826.1634; found: 826.1637)



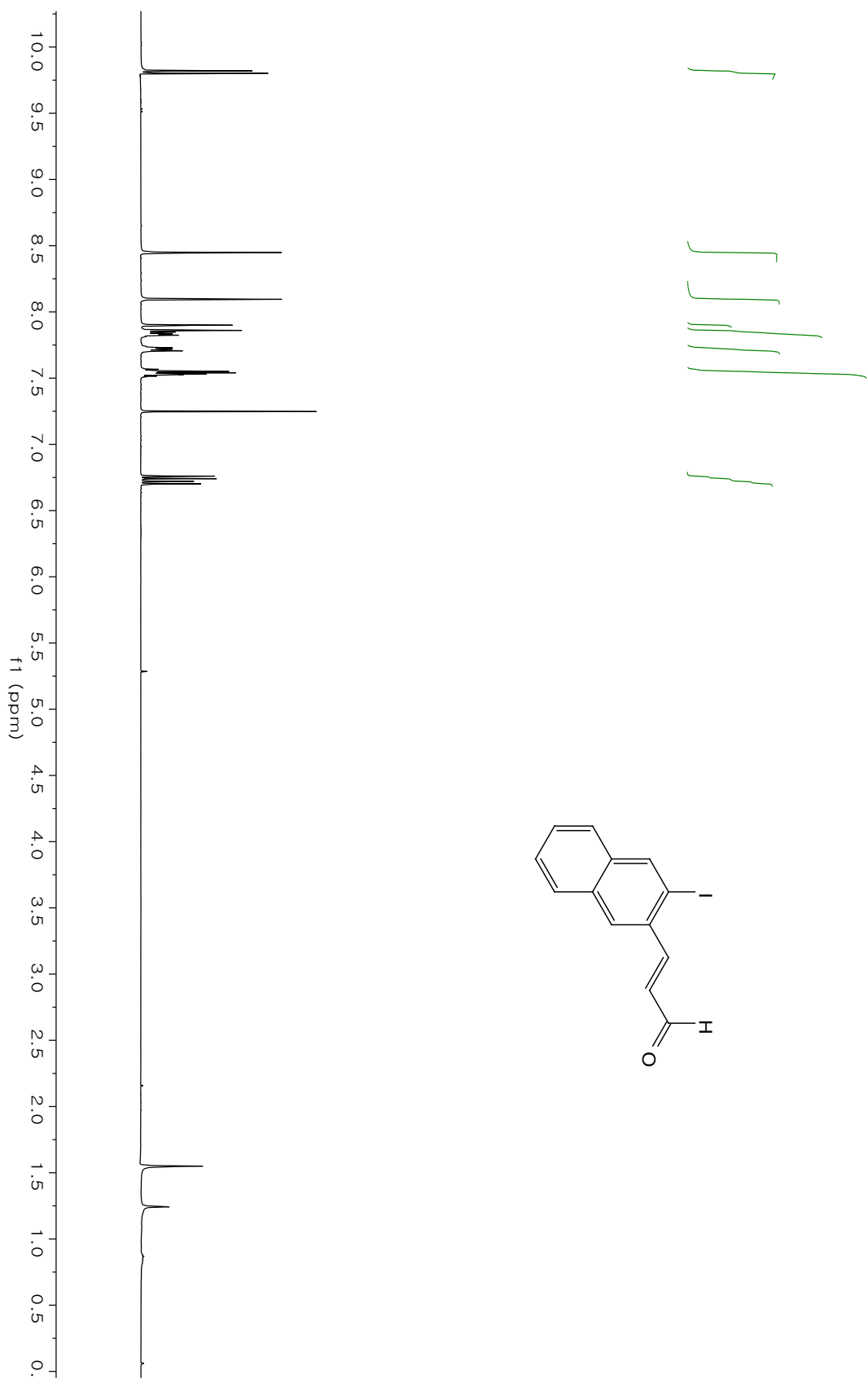
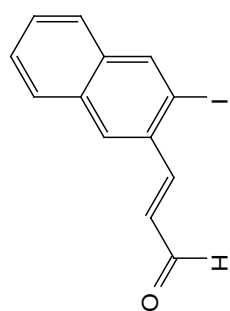
## 6. NMR Spectra



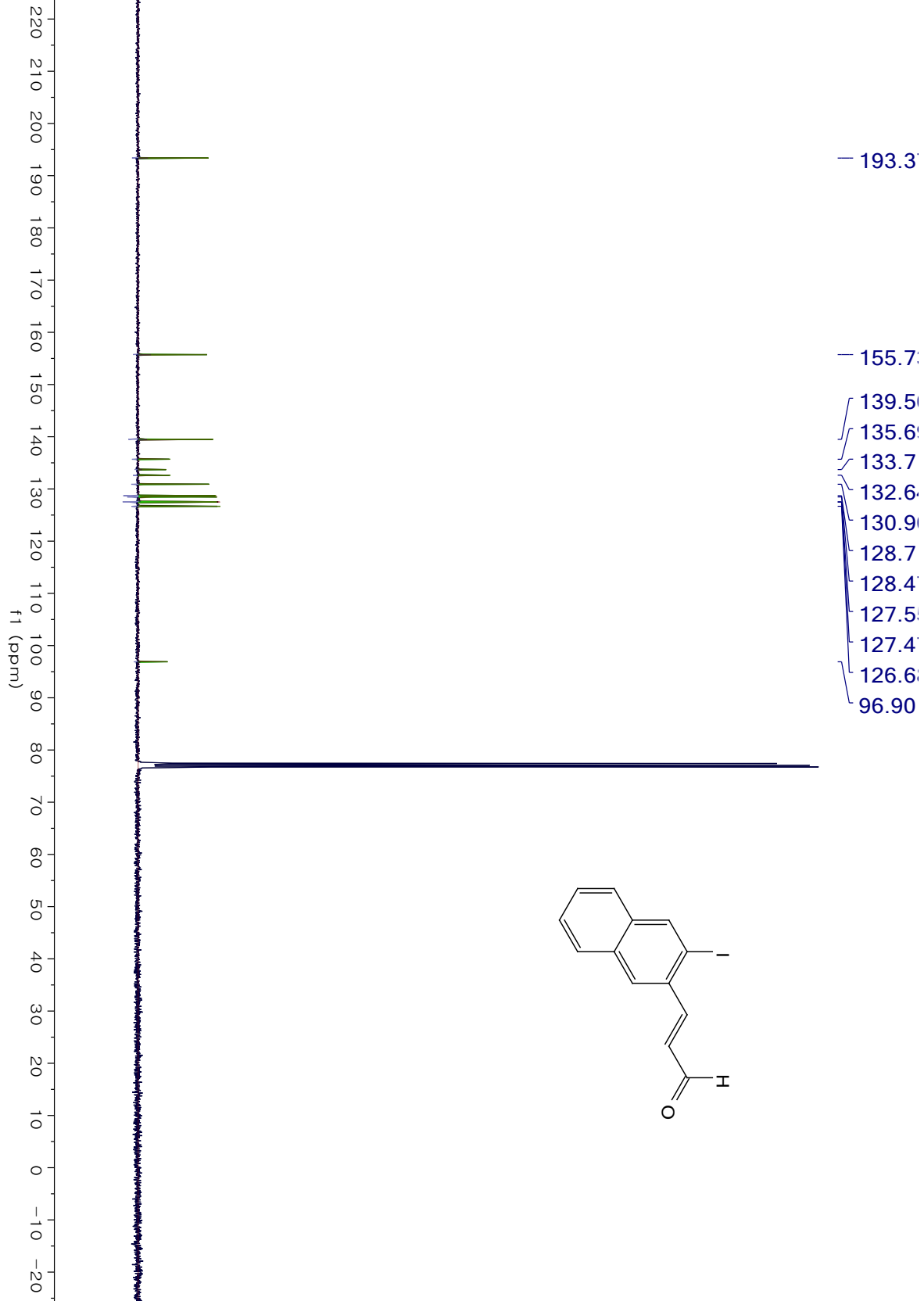
**Figure S23.**  $^1\text{H}$  NMR spectrum of **5b** recorded in  $\text{CDCl}_3$



**Figure S24.**  $^{13}\text{C}$  NMR spectrum of **5b** recorded in  $\text{CDCl}_3$

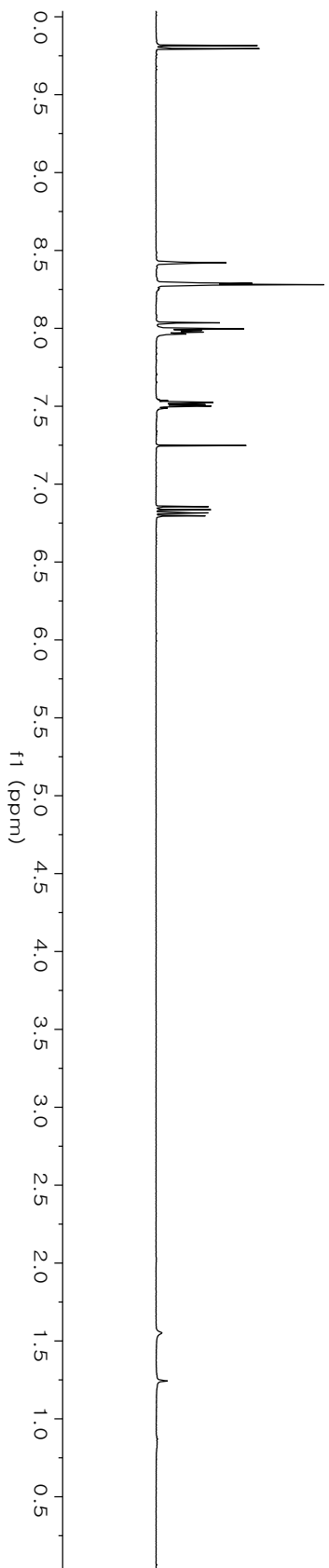
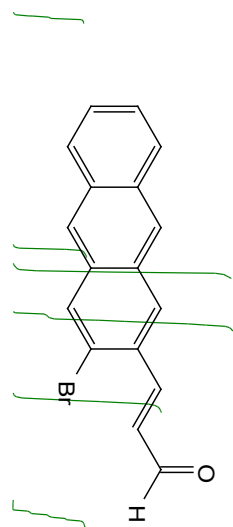


**Figure S25.**  $^1\text{H}$  NMR spectrum of **6a** recorded in  $\text{CDCl}_3$

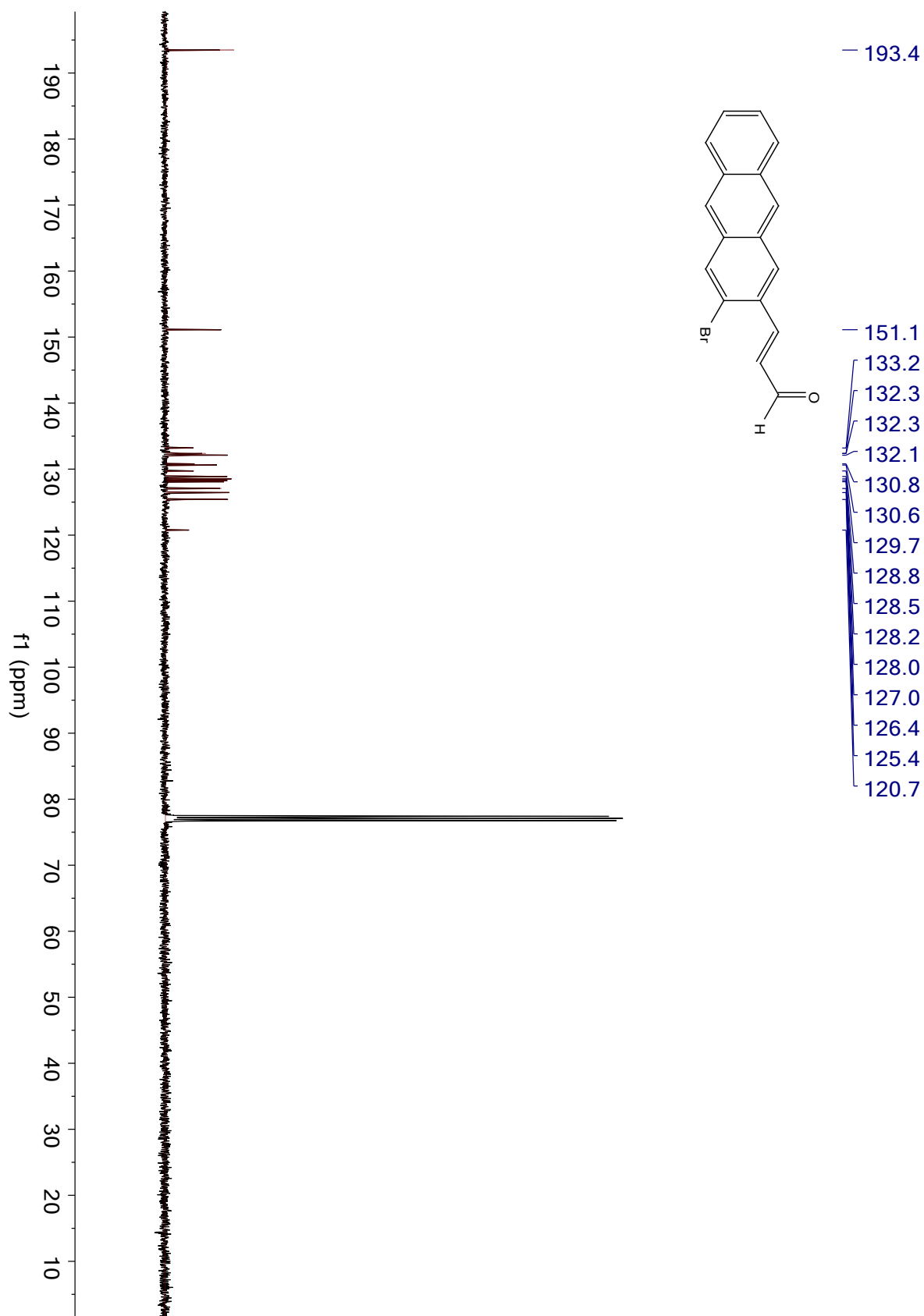


**Figure S26.**  $^{13}\text{C}$  NMR spectrum of **6a** recorded in  $\text{CDCl}_3$

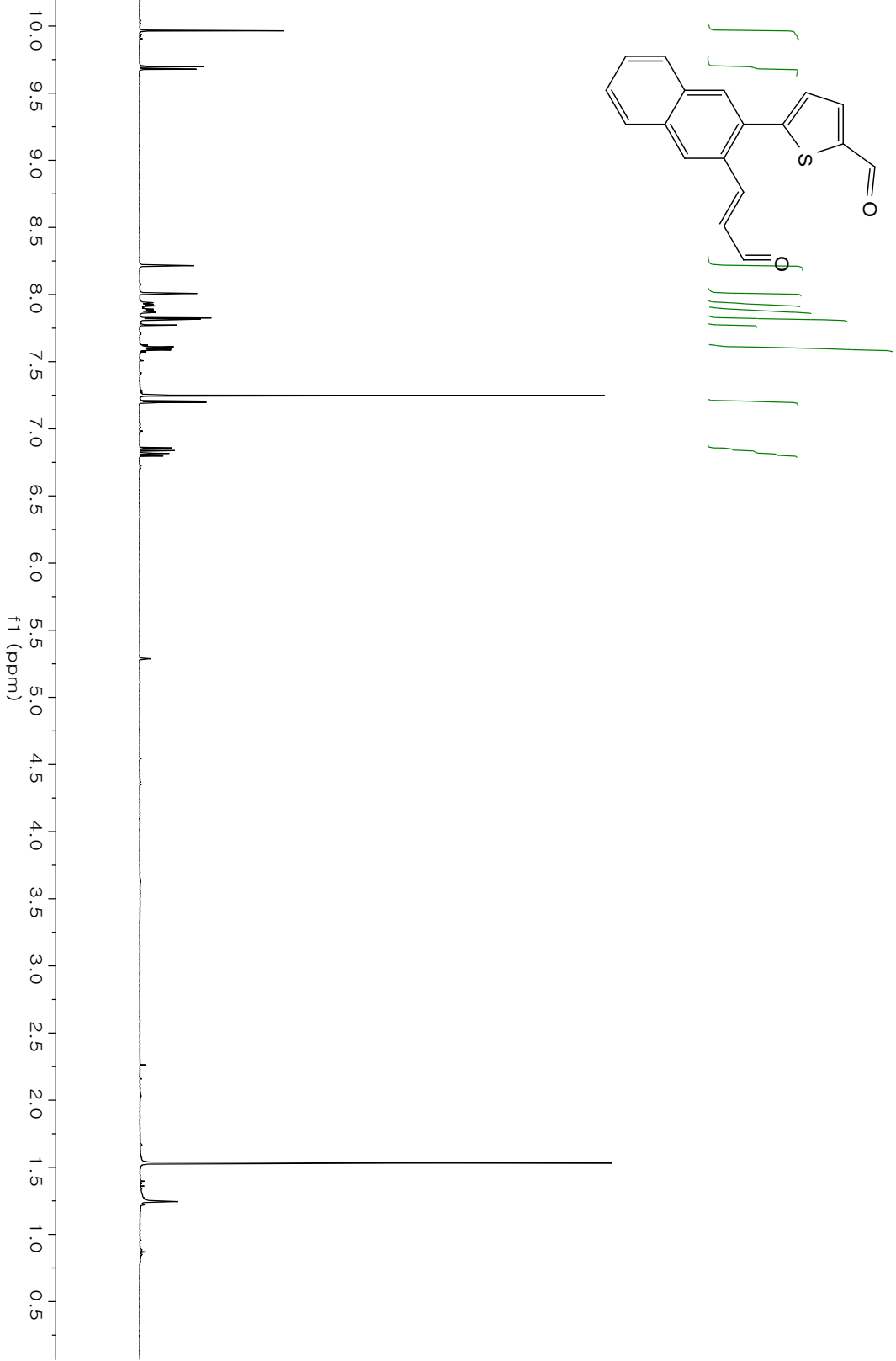




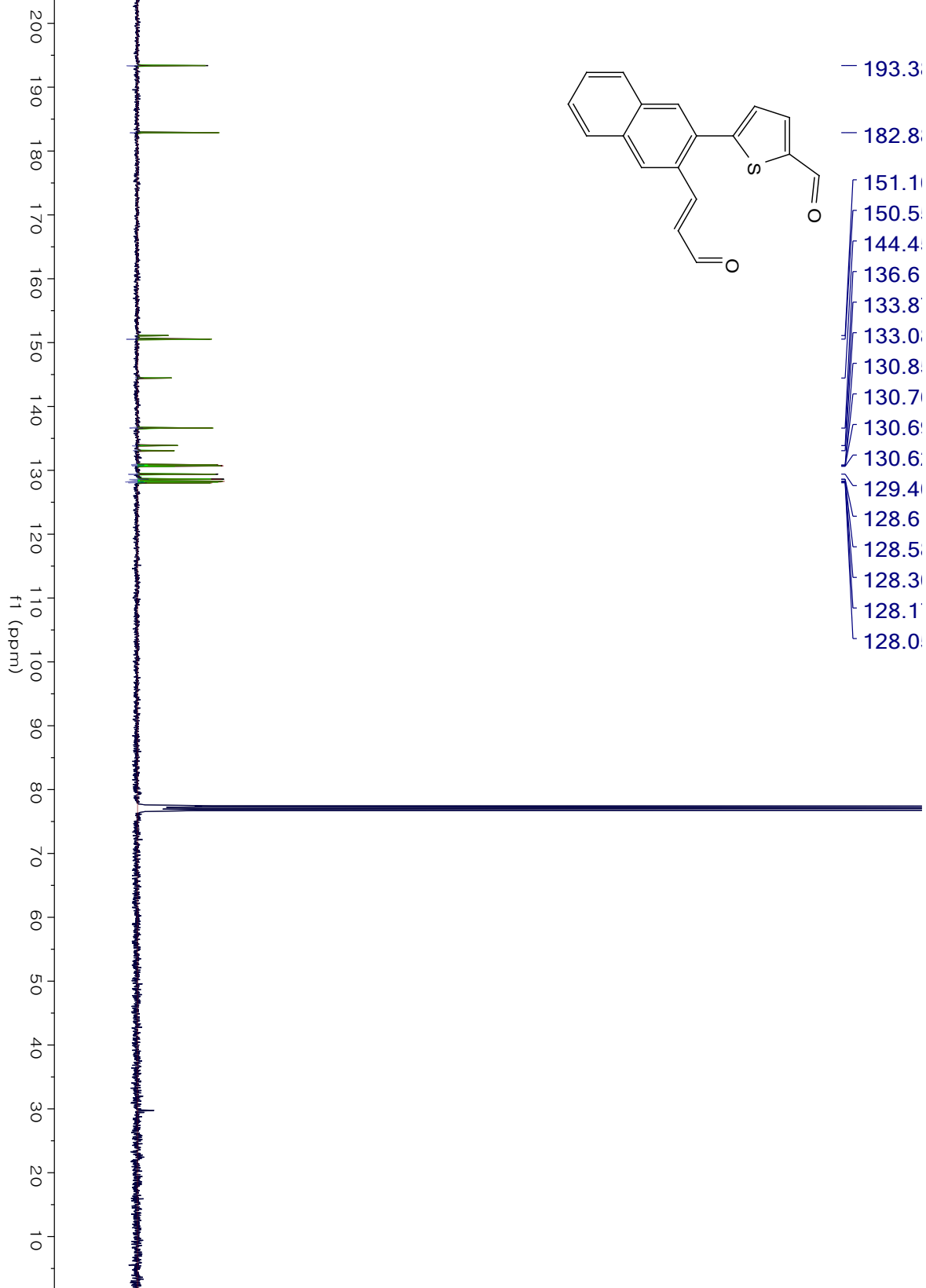
**Figure S27.**  $^1\text{H}$  NMR spectrum of **6b** recorded in  $\text{CDCl}_3$



**Figure S28.**  $^{13}\text{C}$  NMR spectrum of **6b** recorded in  $\text{CDCl}_3$

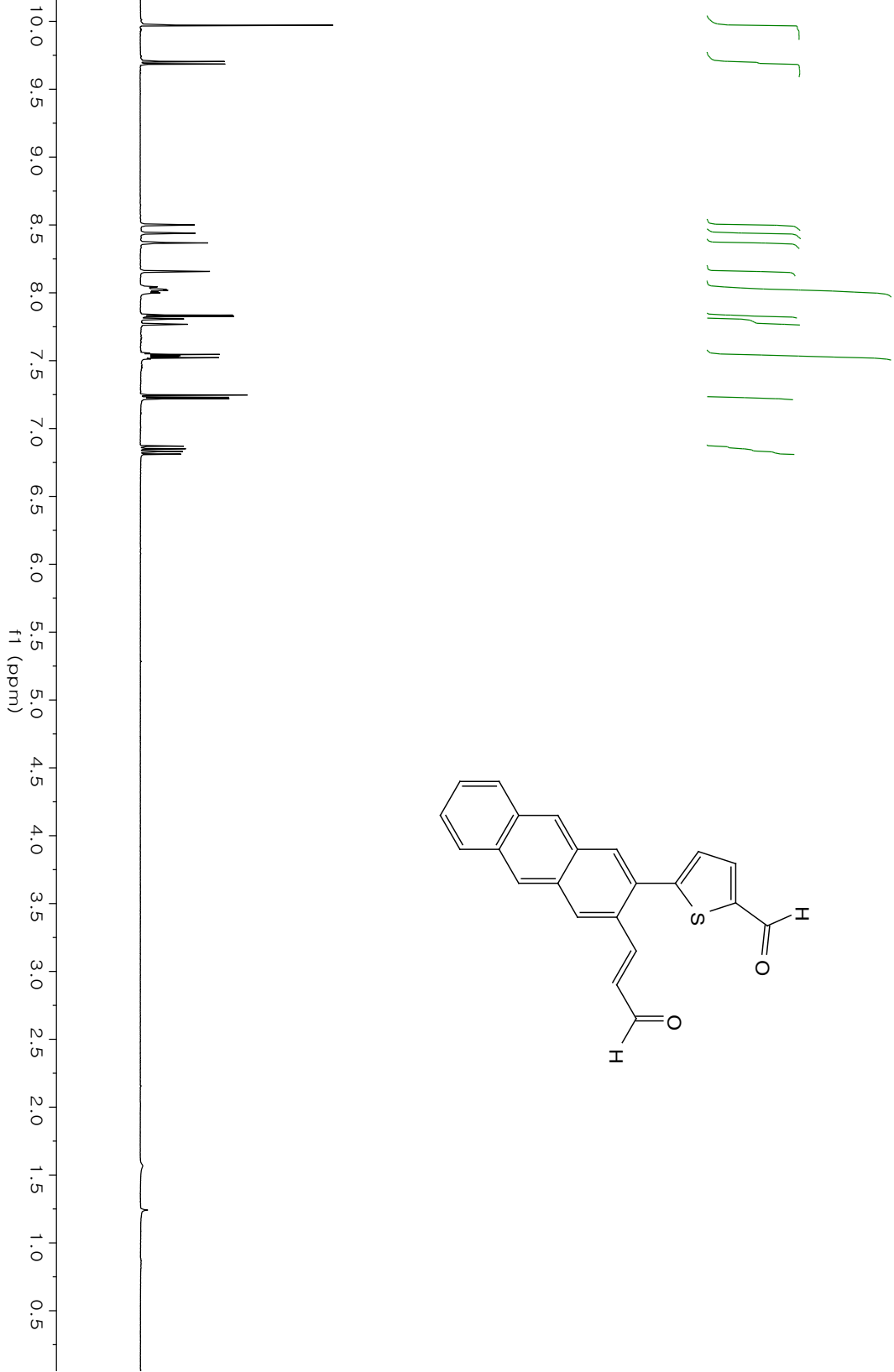


**Figure S29.**  $^1\text{H}$  NMR spectrum of **7a** recorded in  $\text{CDCl}_3$

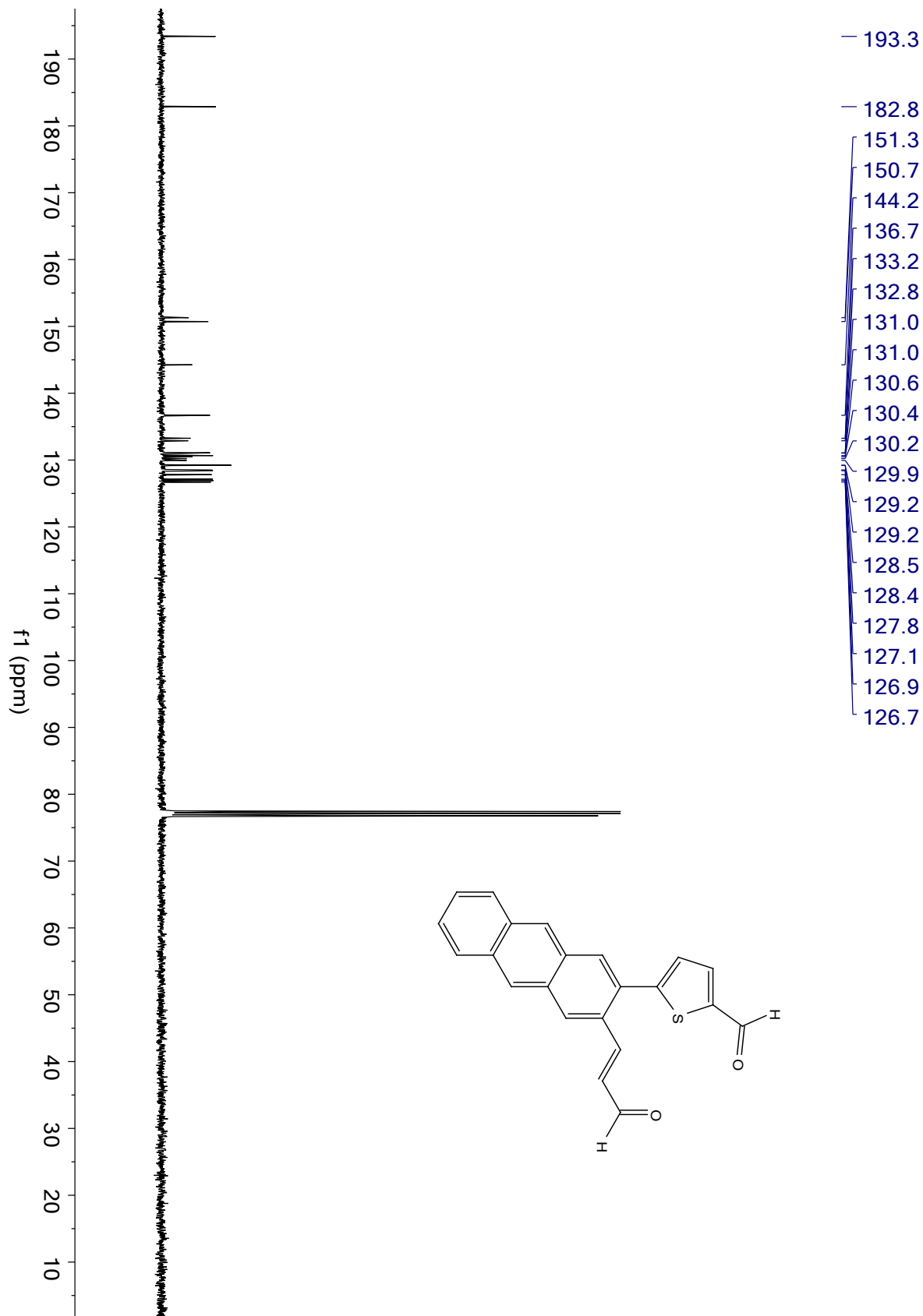


**Figure S30.**  $^{13}\text{C}$  NMR spectrum of **7a** recorded in  $\text{CDCl}_3$

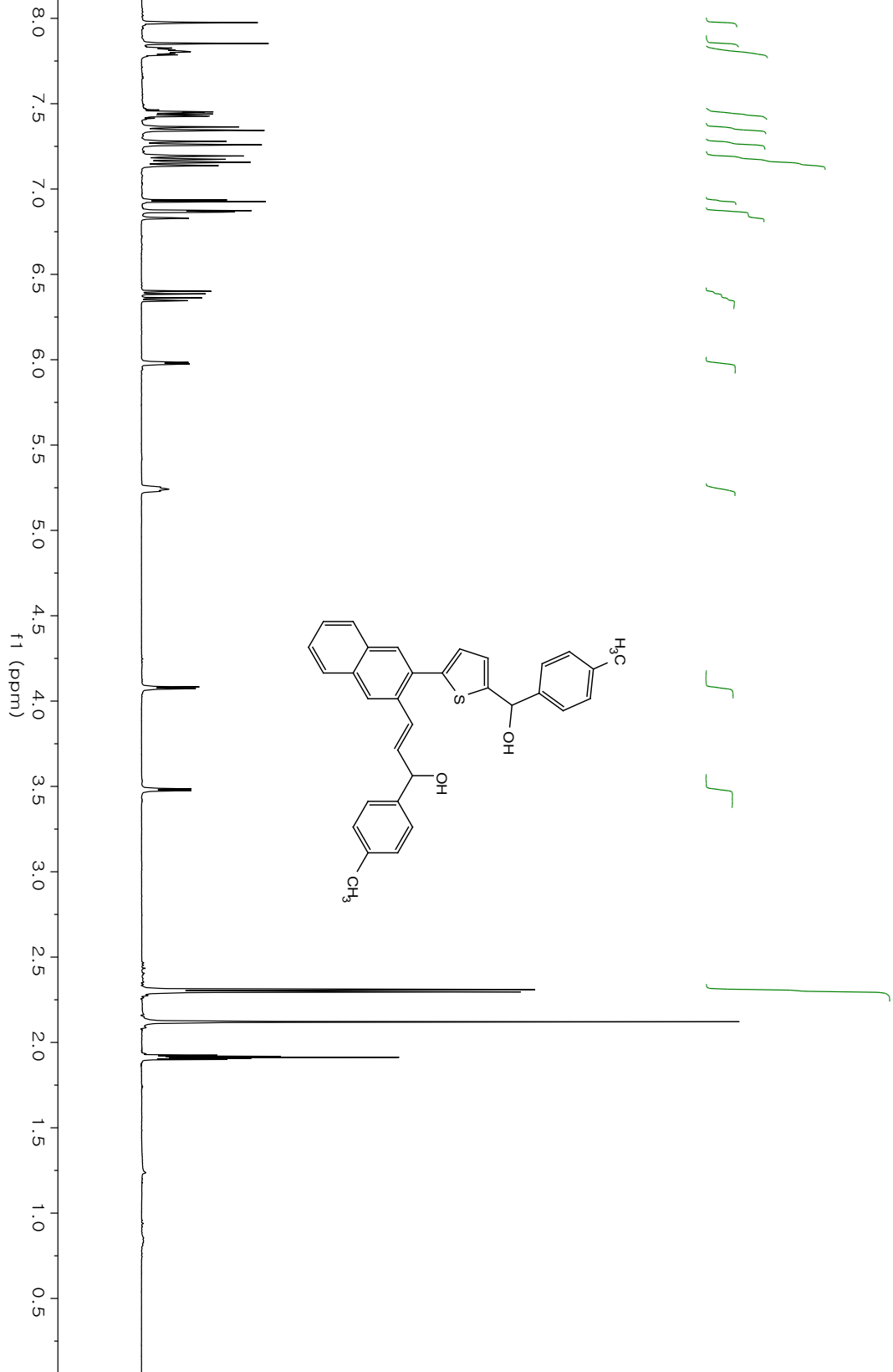




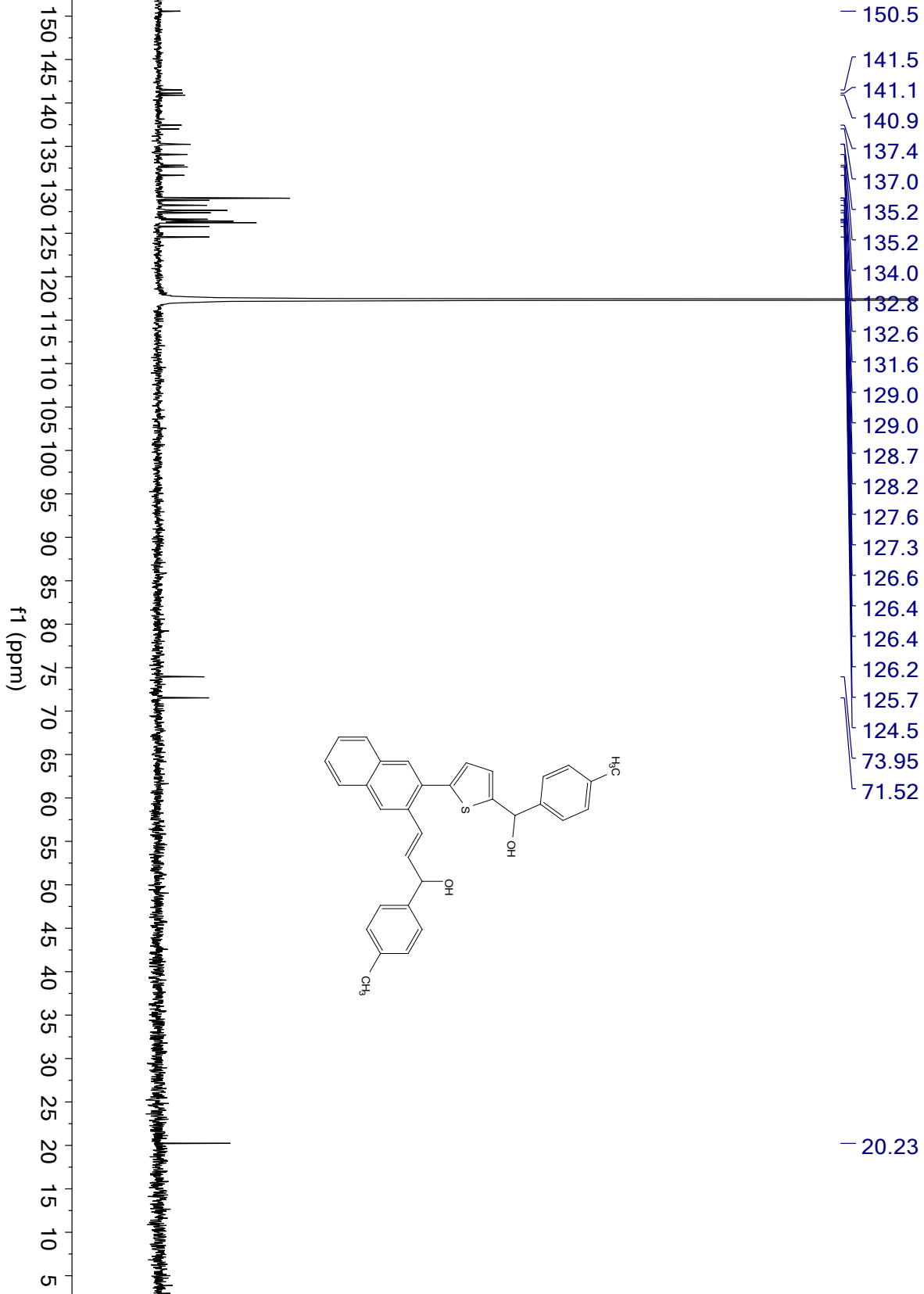
**Figure S31.**  $^1\text{H}$  NMR spectrum of **7b** recorded in  $\text{CDCl}_3$



**Figure S32.**  $^{13}\text{C}$  NMR spectrum of **7b** recorded in  $\text{CDCl}_3$

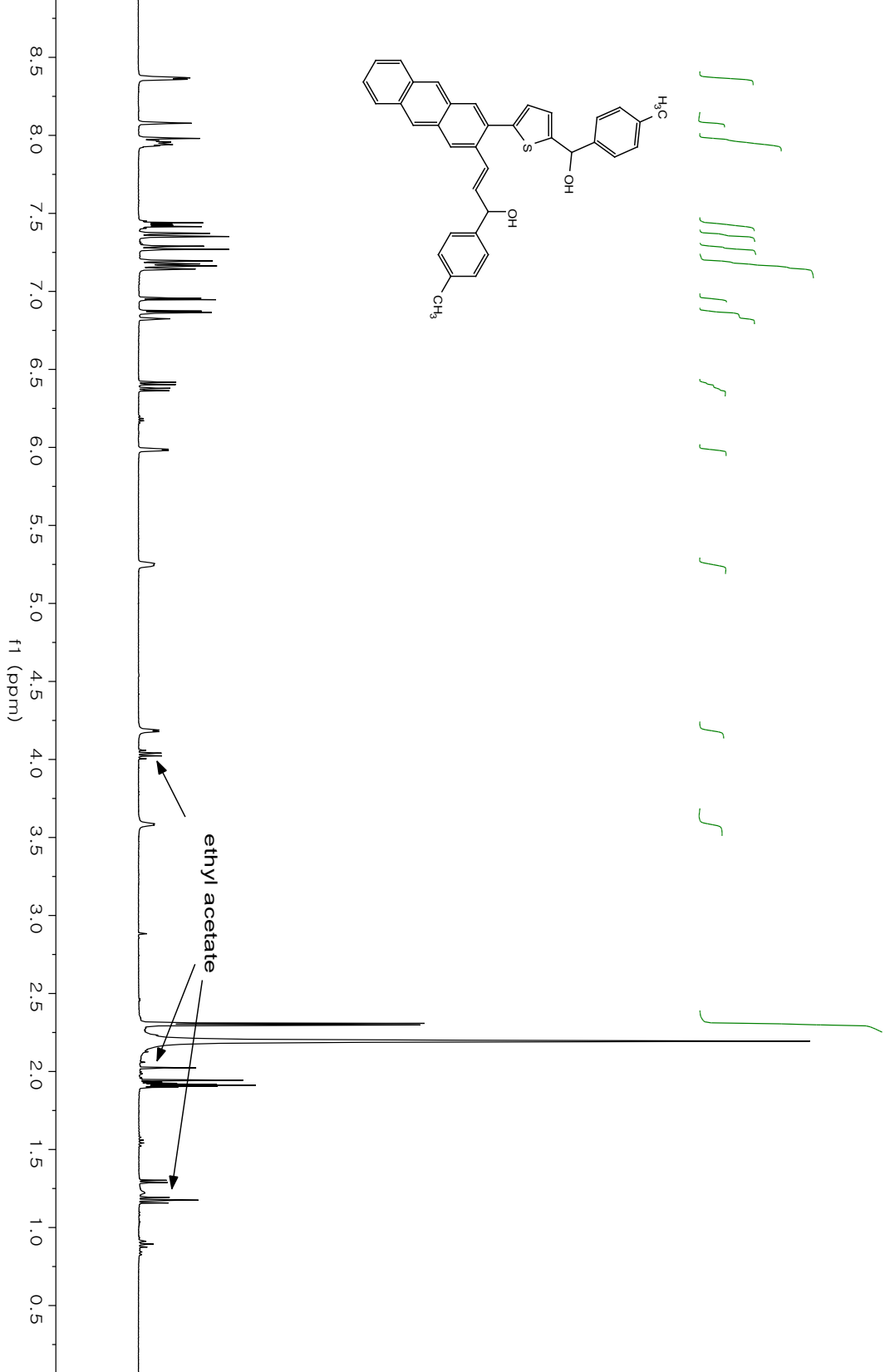


**Figure S33.**  $^1\text{H}$  NMR spectrum of **8a** recorded in  $\text{CD}_3\text{CN}$

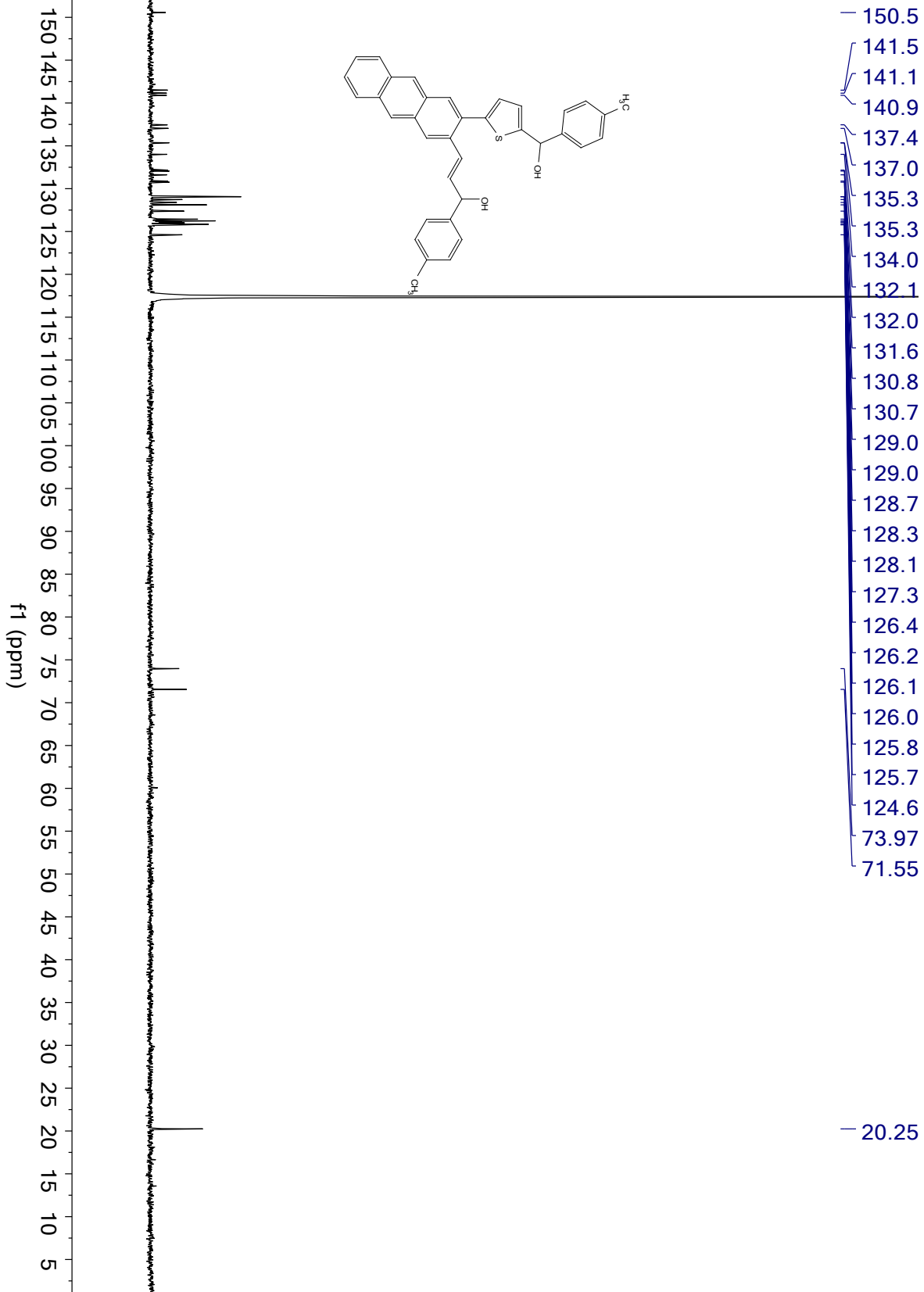


**Figure S34.**  $^{13}\text{C}$  NMR spectrum of **8a** recorded in  $\text{CD}_3\text{CN}$

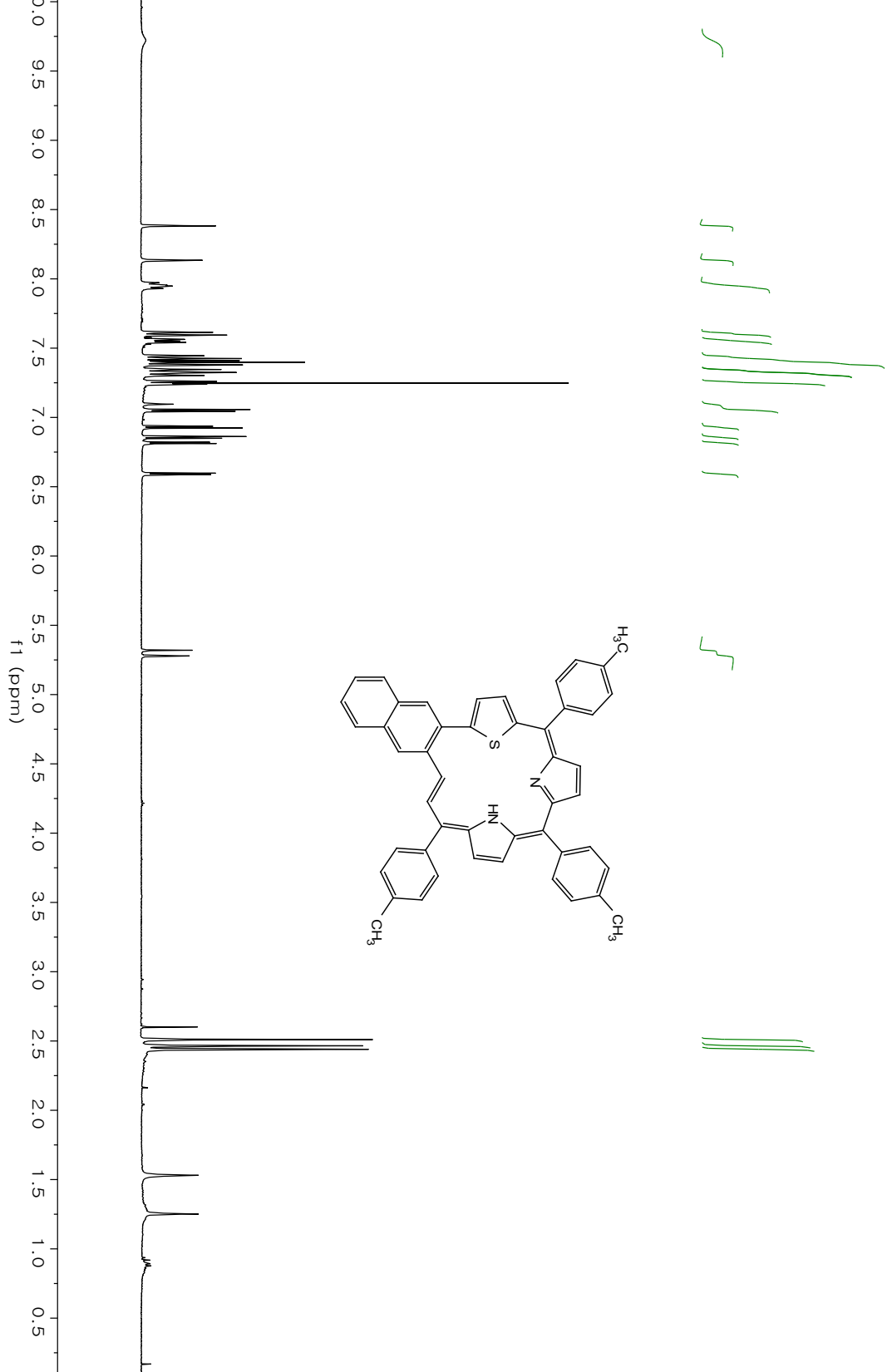




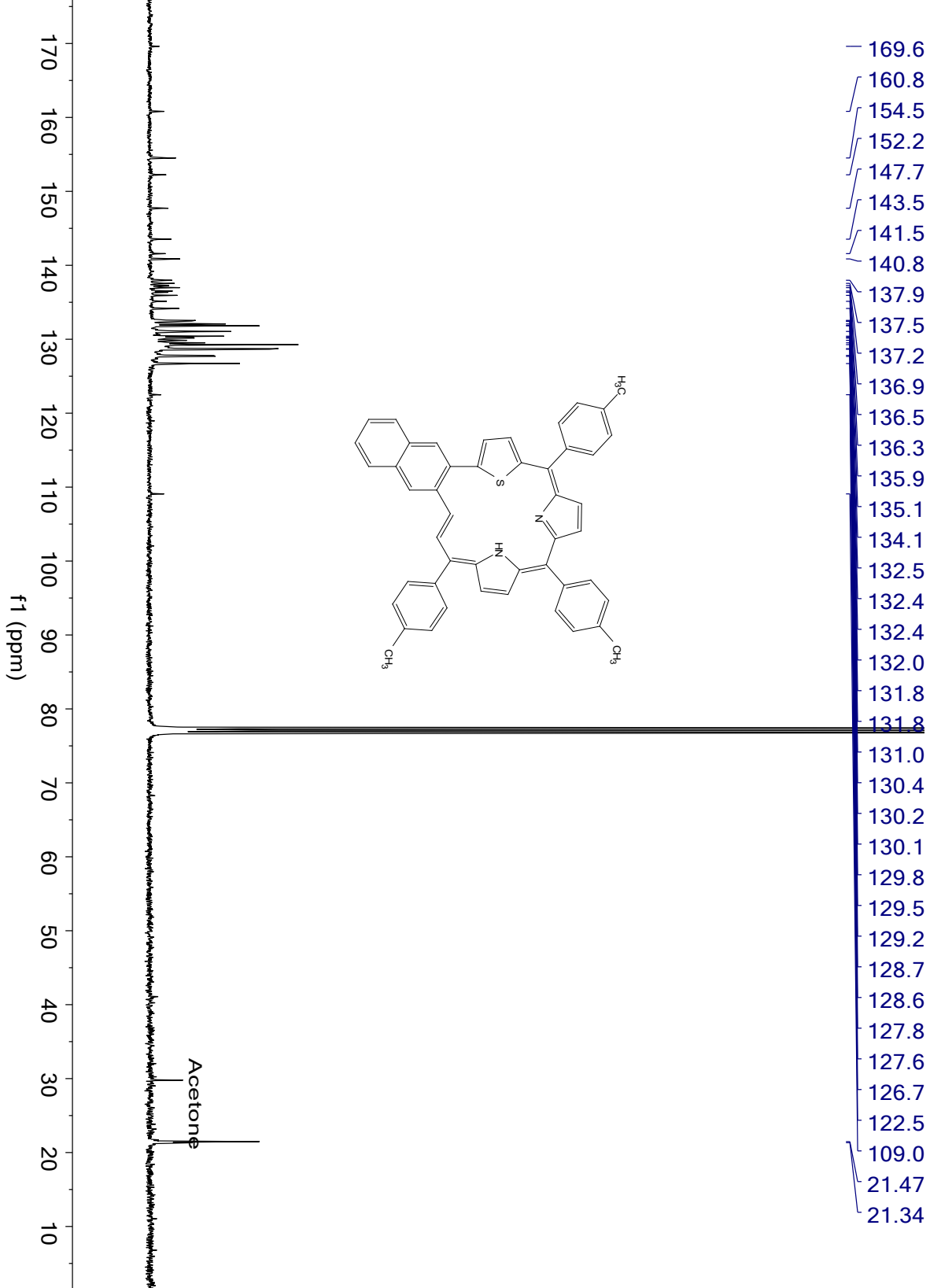
**Figure S35.**  $^1\text{H}$  NMR spectrum of **8b** recorded in  $\text{CD}_3\text{CN}$



**Figure S36.**  $^{13}\text{C}$  NMR spectrum of **8b** recorded in  $\text{CD}_3\text{CN}$

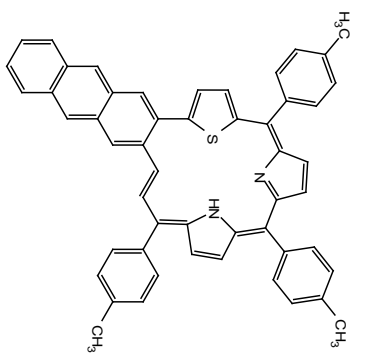
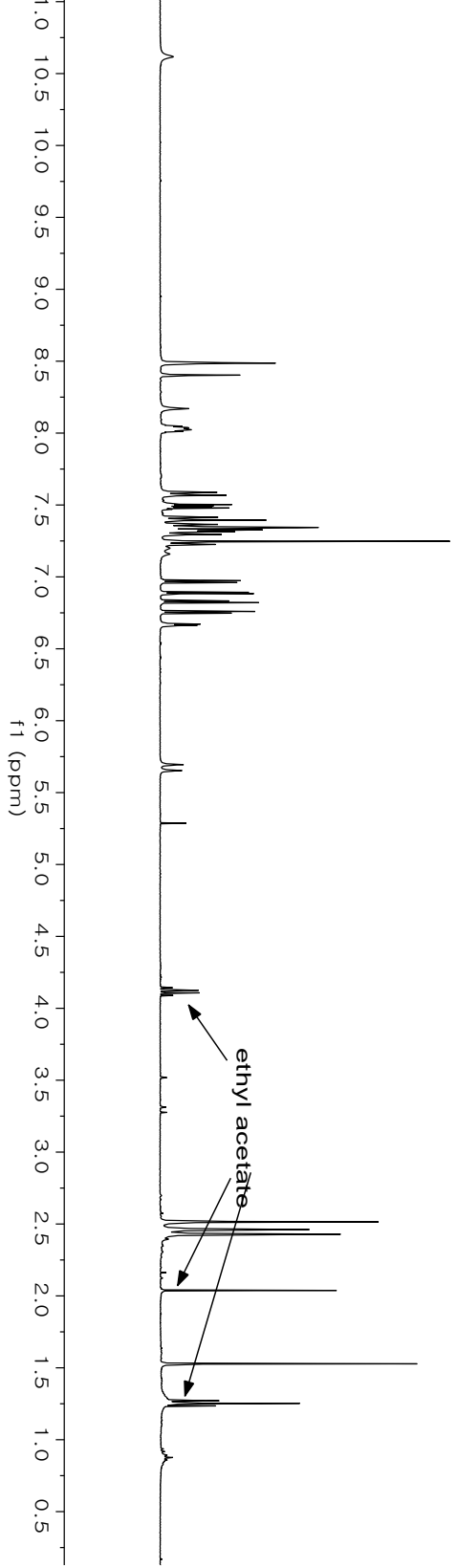


**Figure S37.**  $^1\text{H}$  NMR spectrum of **4a** recorded in  $\text{CDCl}_3$



**Figure S38.**  $^{13}\text{C}$  NMR spectrum of **4a** recorded in  $\text{CDCl}_3$

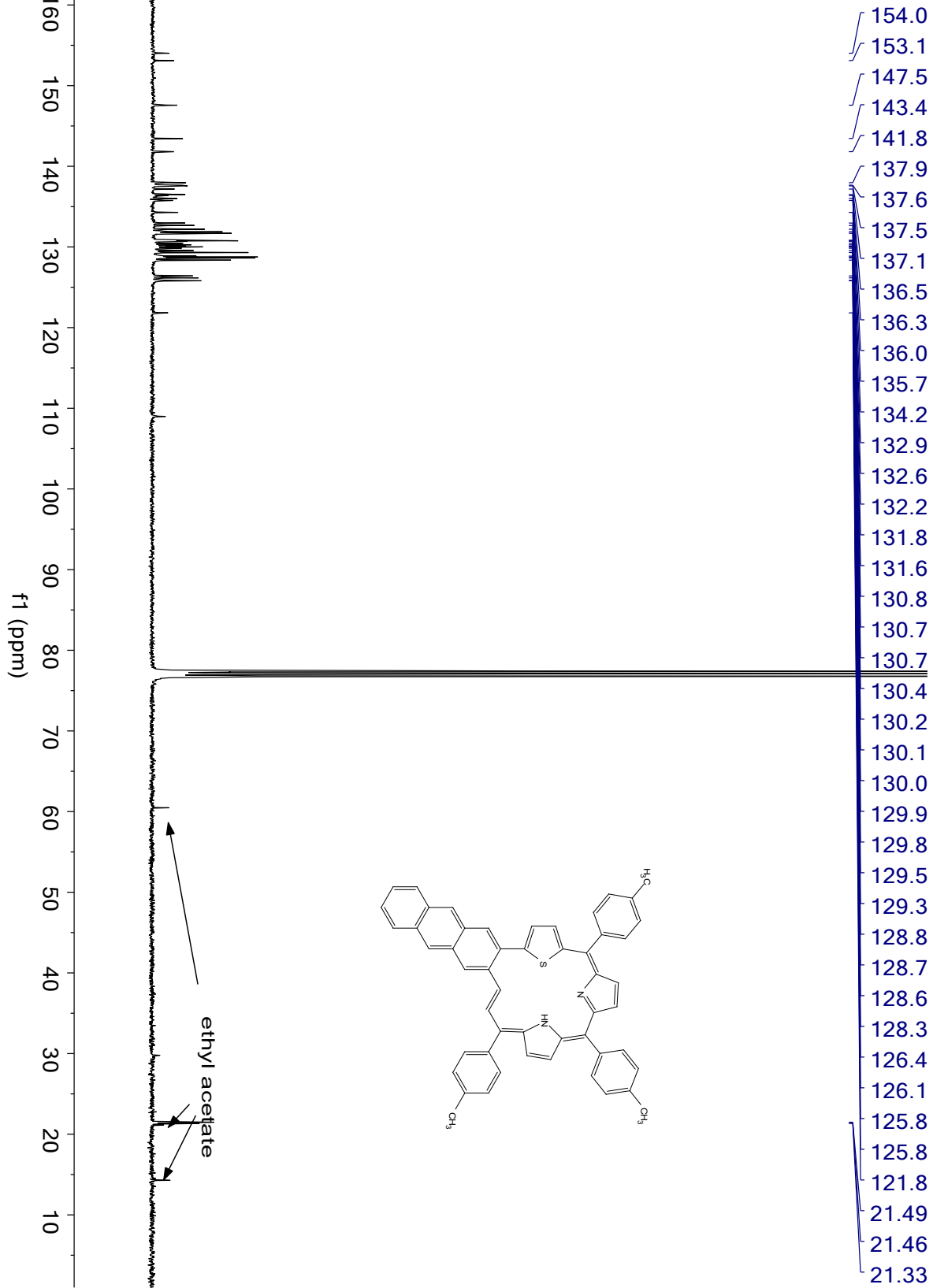




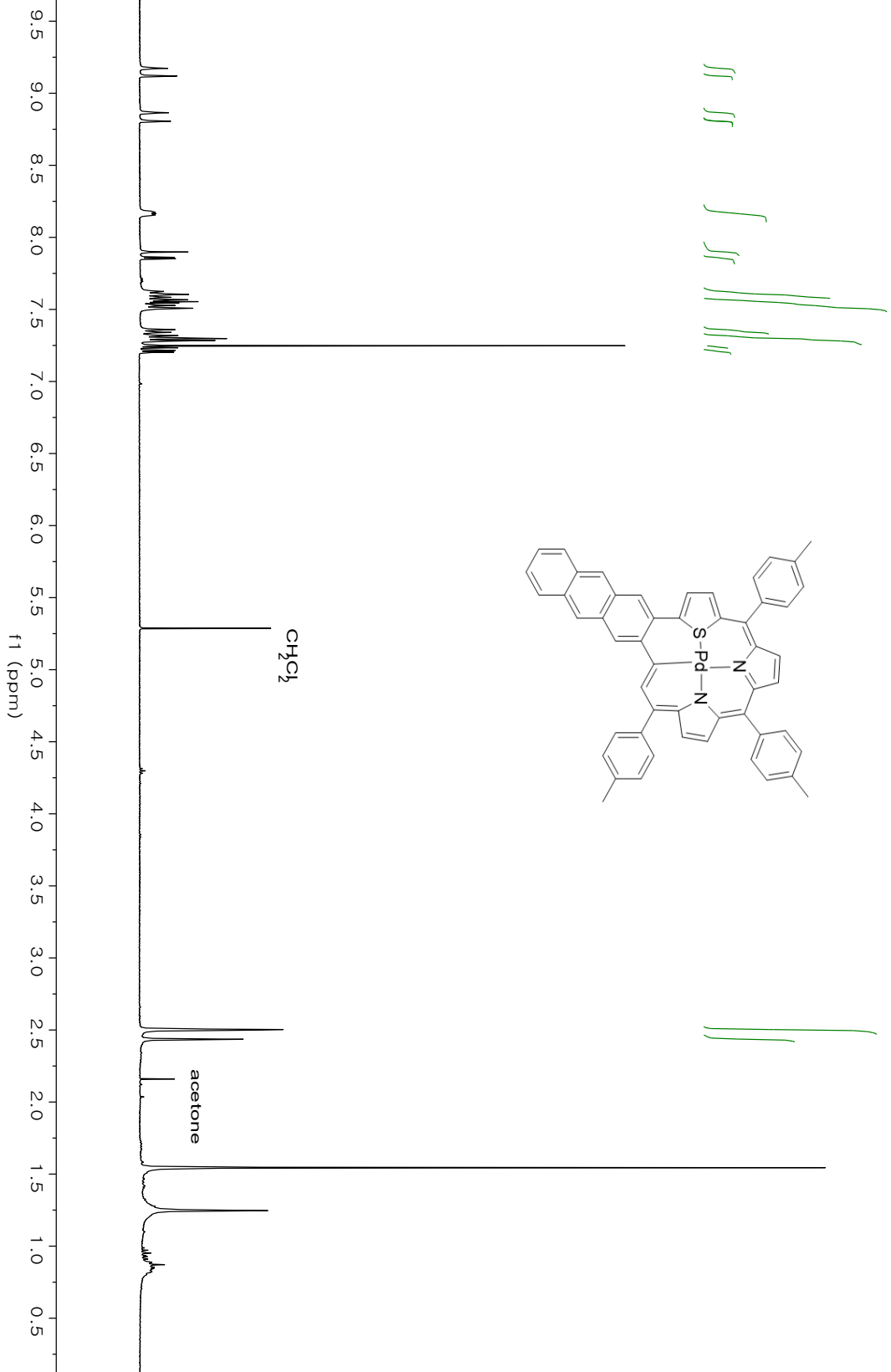
Handwritten notes in green ink, including a large vertical line and several horizontal lines, likely indicating integration or peak assignments.

Handwritten notes in green ink, consisting of three vertical lines.

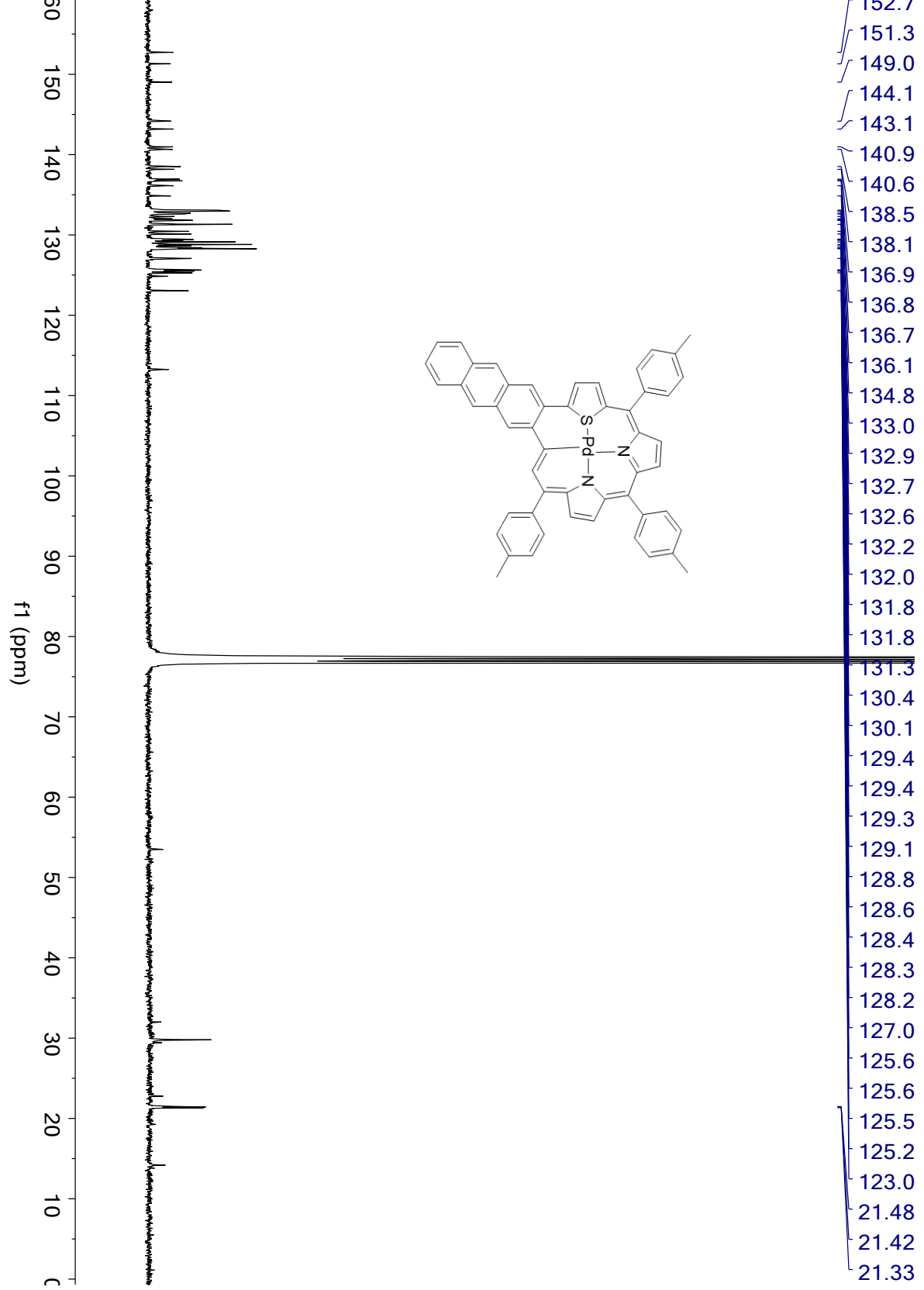
**Figure S39.**  $^1\text{H}$  NMR spectrum of **4b** recorded in  $\text{CDCl}_3$



**Figure S40.**  $^{13}\text{C}$  NMR spectrum of **4b** recorded in  $\text{CDCl}_3$



**Figure S41.**  $^1\text{H}$  NMR spectrum of **Pd-4b** recorded in  $\text{CDCl}_3$



**Figure S42.**  $^{13}\text{C}$  NMR spectrum of **Pd-4b** recorded in  $\text{CDCl}_3$



## 7. Cartesian Coordinates of DFT-optimized Structures

**Table S4.** Cartesian coordinates (in Angstrom) of DFT-optimized structures without an imaginary structure

<b>3a<sub>1</sub></b>				<b>3a<sub>2</sub></b>			
C	-1.9169	-2.356761	0.082002	C	-2.534708	8.581746	-0.633328
C	-1.960223	-3.719462	0.392061	H	-3.540724	8.742193	-0.233789
H	-2.846188	-4.195779	0.791152	H	-2.512652	8.954691	-1.661249
C	-0.758141	-4.397746	0.161264	H	-1.850377	9.205837	-0.044991
H	-0.625196	-5.449587	0.382412	C	-4.357354	-1.965396	0.403652
C	0.276974	-3.599258	-0.327313	C	-5.120537	-1.533258	1.500992
C	1.597657	-4.118058	-0.698568	H	-4.700909	-0.800998	2.183571
C	1.573444	-5.450847	-1.194419	C	-6.399201	-2.039744	1.728475
H	0.60883	-5.896048	-1.408038	H	-6.964965	-1.689063	2.587998
C	2.715067	-6.192604	-1.435129	C	-6.965628	-2.993688	0.872824
H	2.631916	-7.201802	-1.826618	C	-6.204508	-3.421963	-0.224257
C	3.968784	-5.629842	-1.164631	H	-6.623572	-4.150868	-0.913421
H	4.880242	-6.196854	-1.326573	C	-4.923643	-2.924871	-0.453303
C	4.031738	-4.328814	-0.704226	H	-4.360999	-3.266385	-1.316612
H	5.004342	-3.885165	-0.511847	C	-8.339099	-3.561862	1.137998
C	2.886908	-3.508367	-0.50944	H	-8.280159	-4.458555	1.767544
C	3.234064	-2.15219	-0.0963	H	-8.838419	-3.85105	0.208639
H	4.15867	-2.107871	0.474736	H	-8.976194	-2.841391	1.65907
C	2.671416	-0.952682	-0.41491	N	0.976976	1.414566	-0.272109
H	1.79266	-0.930473	-1.045947	H	0.346267	0.620671	-0.155658
C	3.18504	0.338694	-0.034106	N	-1.634974	0.622368	-0.08823
C	2.353733	1.454675	-0.103907	S	-0.299319	-1.951035	-0.471055
C	2.702602	2.855218	-0.062871				
H	3.712772	3.227397	0.021502				
C	1.56111	3.592665	-0.197528				
H	1.47905	4.668795	-0.220902				
C	0.443433	2.683529	-0.29812				
C	-0.927436	2.967338	-0.327247				
C	-1.91665	1.938086	-0.23975				
C	-3.361937	2.149722	-0.283271				
H	-3.858897	3.097695	-0.430057				
C	-3.935687	0.929774	-0.119413				
H	-4.98955	0.692253	-0.117011				
C	-2.844273	-0.031021	0.005109				
C	-2.993264	-1.413475	0.155475				
C	4.589198	0.509607	0.417428				
C	5.660911	-0.020519	-0.326271				
H	5.45359	-0.560832	-1.244721				
C	6.978221	0.162156	0.082777				
H	7.784627	-0.24553	-0.521923				
C	7.285956	0.871357	1.254119				
C	6.221182	1.396699	1.996549				
H	6.427271	1.947789	2.910676				
C	4.899061	1.218889	1.590871				
H	4.092991	1.622209	2.195846				
C	8.715923	1.036777	1.708733				
H	9.061807	0.150289	2.254925				
H	8.826843	1.895399	2.376749				
H	9.391732	1.174768	0.859089				
C	-1.349904	4.394921	-0.407176				
C	-0.948061	5.207883	-1.480108				
H	-0.340997	4.779503	-2.272245				
C	-1.334301	6.545757	-1.554963				
H	-1.013068	7.14559	-2.402957				
C	-2.138754	7.125978	-0.565887				
C	-2.545757	6.314056	0.502265				
H	-3.170107	6.735657	1.286356				
C	-2.158026	4.978149	0.584209				
H	-2.476126	4.378072	1.431391				

H	4.746731	-1.049027	-1.99137
C	6.665032	-0.494202	-1.19872
H	7.207479	-0.945096	-2.026218
C	7.378736	0.143173	0.172002
C	6.645772	0.713416	-0.875285
H	7.171541	1.203859	1.69065
C	5.251448	0.657489	0.896472
H	4.708138	1.097793	1.727235
C	8.886156	0.223209	-0.210562
H	9.330243	-0.733447	-0.504204
H	9.296564	0.504031	0.76314
H	9.224004	0.9705	-0.939024
C	-0.913704	4.637398	-0.015109
C	-1.732833	5.201454	-1.008125
H	-2.193711	4.554127	-1.748234
C	-1.950431	6.577247	-1.066515
H	-2.588187	6.982111	-1.848556
C	-1.355767	7.447972	-0.143533
C	-0.54035	6.886999	0.848624
H	-0.075681	7.534606	1.588286
C	-0.324362	5.511429	0.914673
H	0.294403	5.102796	1.708125
C	-1.565412	8.941067	-0.228911
H	-1.563195	9.402793	0.763116
H	-2.513793	9.184947	-0.716201
H	-0.767845	9.420424	-0.810389
C	-4.426287	-1.611047	0.100013
C	-5.301587	-1.102144	-0.880463
H	-4.997739	-0.244323	-1.470518
C	-6.528047	-1.710603	-1.131957
H	-7.175802	-1.301426	-1.90302
C	-6.933125	-2.853362	-0.428162
C	-6.054447	-3.37436	0.534124
H	-6.338833	-4.263712	1.09085
C	-4.828176	-2.772434	0.792052
H	-4.174147	-3.188494	1.551972
C	-8.274377	-3.495204	-0.684757
H	-9.029944	-3.120557	0.017328
H	-8.22864	-4.581187	-0.56003
H	-8.634308	-3.280393	-1.694864
N	0.980361	1.350803	0.035281
H	0.232777	0.661565	0.158638
N	-1.649689	0.939815	0.246421
S	-1.454772	-3.140155	-0.300893

**3a<sub>3</sub>**

C	-2.091362	-1.709808	0.693341
C	-1.176896	-1.58335	1.722725
H	-1.291	-0.844583	2.507496
C	-0.096547	-2.491242	1.64802
H	0.716571	-2.522457	2.363208
C	-0.147308	-3.320011	0.549272
C	0.845376	-4.303919	0.103399
C	0.426772	-5.620393	-0.160273
H	-0.62782	-5.858346	-0.057884
C	1.329996	-6.622806	-0.495477
H	0.976915	-7.632966	-0.677908
C	2.694771	-6.323433	-0.560727
H	3.416705	-7.09852	-0.799122
C	3.124325	-5.025238	-0.326548
H	4.182938	-4.792935	-0.403375
C	2.22735	-3.969412	-0.033551
C	2.831644	-2.639587	0.042833
H	3.910897	-2.679838	0.168483
C	2.287647	-1.39523	-0.112109
H	1.220909	-1.273598	-0.246474
C	3.044111	-0.170704	-0.092065
C	2.399749	1.069872	-0.074987

C	3.049755	2.368084	-0.238002
H	4.107928	2.528119	-0.386336
C	2.066369	3.302558	-0.216034
H	2.167972	4.371132	-0.340122
C	0.808589	2.578659	-0.021502
C	-0.489101	3.187078	0.037304
C	-1.650397	2.414666	0.150011
C	-3.042378	2.812283	0.213163
H	-3.3893	3.834938	0.216189
C	-3.808389	1.684602	0.28161
H	-4.883663	1.634305	0.367405
C	-2.929782	0.531932	0.295123
C	-3.209042	-0.825682	0.378092
C	4.534228	-0.205994	-0.091086
C	5.246721	-0.836363	-1.12776
H	4.699677	-1.303718	-1.940924
C	6.638613	-0.852182	-1.13427
H	7.161846	-1.337498	-1.954607
C	7.37791	-0.24993	-0.104653
C	6.669159	0.367908	0.932459
H	7.214837	0.833466	1.749286
C	5.274108	0.393383	0.940393
H	4.748674	0.871352	1.761463
C	8.88766	-0.255285	-0.129695
H	9.279905	-1.238593	-0.408847
H	9.304549	0.013063	0.844769
H	9.273322	0.463601	-0.862956
C	-0.618089	4.669719	-0.041501
C	-1.373579	5.28439	-1.053925
H	-1.851135	4.667364	-1.809317
C	-1.506981	6.671521	-1.11296
H	-2.098748	7.115636	-1.909709
C	-0.884702	7.50211	-0.172504
C	-0.128613	6.890402	0.837459
H	0.356693	7.507564	1.589772
C	0.002028	5.504722	0.904526
H	0.578191	5.058373	1.709629
C	-1.000949	9.005462	-0.257079
H	-1.007418	9.462838	0.737011
H	-1.91449	9.307526	-0.777254
H	-0.1552	9.438114	-0.806143
C	-4.547247	-1.382459	0.122163
C	-5.423949	-0.828494	-0.832047
H	-5.095228	0.012118	-1.433845
C	-6.687557	-1.372119	-1.047606
H	-7.335644	-0.92716	-1.798427
C	-7.129499	-2.49626	-0.336712
C	-6.248976	-3.064953	0.596503
H	-6.559871	-3.942794	1.157543
C	-4.987805	-2.525092	0.821917
H	-4.333202	-2.978045	1.560106
C	-8.507772	-3.070084	-0.556649
H	-9.216055	-2.693071	0.191941
H	-8.504672	-4.161354	-0.47561
H	-8.900582	-2.801063	-1.541207
N	1.033373	1.247902	0.052031
H	-0.752367	0.549134	0.188982
N	-1.644981	1.047765	0.228855
S	-1.60004	-3.015481	-0.380811

**3a<sub>4</sub>**

C	-2.033857	-2.229878	0.106939
C	-1.972327	-3.380041	0.882362
H	-2.758523	-3.651324	1.576249
C	-0.77767	-4.111028	0.727915
H	-0.552144	-5.012393	1.28608
C	0.125391	-3.55712	-0.164919
C	1.388188	-4.19701	-0.57634

C	1.245935	-5.564285	-0.911649
H	0.24381	-5.979123	-0.923467
C	2.317892	-6.377358	-1.248477
H	2.149001	-7.416814	-1.512127
C	3.606926	-5.836862	-1.249782
H	4.465797	-6.44829	-1.508952
C	3.779684	-4.50634	-0.911887
H	4.784959	-4.095345	-0.90319
C	2.709203	-3.632593	-0.578034
C	3.162562	-2.291269	-0.218814
H	4.231038	-2.264424	-0.021514
C	2.516562	-1.092706	-0.152442
H	1.462654	-1.022554	-0.368381
C	3.130243	0.169725	0.16023
C	2.345834	1.32458	0.166662
C	2.823605	2.697736	0.298837
H	3.850534	2.995009	0.455993
C	1.739118	3.501666	0.155912
H	1.707468	4.581205	0.191677
C	0.59077	2.616037	-0.055082
C	-0.76775	3.041443	-0.222973
C	-1.82021	2.120444	-0.262251
C	-3.2359	2.344884	-0.449446
H	-3.683536	3.308251	-0.642109
C	-3.875095	1.143531	-0.358765
H	-4.932512	0.960375	-0.475138
C	-2.889958	0.10858	-0.121283
C	-3.10232	-1.252695	0.068347
C	4.587555	0.274903	0.451923
C	5.553138	-0.09387	-0.501854
H	5.231335	-0.45764	-1.473003
C	6.913105	0.022278	-0.225599
H	7.636609	-0.261829	-0.985957
C	7.365858	0.503327	1.01209
C	6.404081	0.864601	1.963161
H	6.724593	1.233592	2.934151
C	5.040197	0.755996	1.690236
H	4.314792	1.034944	2.448412
C	8.842369	0.644097	1.295579
H	9.401758	-0.229185	0.94491
H	9.034238	0.764199	2.365218
H	9.261247	1.519829	0.784843
C	-1.075805	4.494604	-0.33409
C	-0.489522	5.283955	-1.339534
H	0.186292	4.819971	-2.051783
C	-0.77816	6.642649	-1.448217
H	-0.315579	7.223284	-2.242733
C	-1.663499	7.271653	-0.561333
C	-2.251607	6.486184	0.438144
H	-2.940858	6.94568	1.142432
C	-1.961659	5.127001	0.554444
H	-2.416836	4.548098	1.352472
C	-1.951369	8.750436	-0.665951
H	-2.92419	9.000211	-0.232785
H	-1.944867	9.086159	-1.70739
H	-1.195569	9.339929	-0.131889
C	-4.479053	-1.756513	0.305353
C	-5.350764	-1.128222	1.213072
H	-5.003696	-0.267492	1.775458
C	-6.642543	-1.609821	1.419975
H	-7.290319	-1.104354	2.131699
C	-7.11492	-2.740066	0.741368
C	-6.242624	-3.374326	-0.15699
H	-6.583677	-4.249703	-0.704196
C	-4.952139	-2.900259	-0.36722
H	-4.302748	-3.406076	-1.074687
C	-8.502575	-3.280281	0.988188
H	-8.478487	-4.127198	1.685223
H	-8.961577	-3.639862	0.061964

H	-9.157417	-2.518991	1.420911
N	0.97732	1.325453	-0.035859
H	-0.72592	0.388766	0.039046
N	-1.666559	0.762588	-0.105105
S	-0.577147	-2.117488	-0.874845

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**3a<sub>g</sub>**

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C	-2.619962	-1.974641	0.068142
C	-3.010846	-3.30989	0.225459
H	-3.98505	-3.587952	0.60646
C	-2.024357	-4.239352	-0.117269
H	-2.171862	-5.307079	-0.013811
C	-0.821482	-3.668897	-0.54177
C	0.403973	-4.371835	-0.891786
C	0.310728	-5.767037	-1.131287
H	-0.670049	-6.22688	-1.169049
C	1.425172	-6.560201	-1.331434
H	1.305581	-7.622515	-1.521135
C	2.702342	-5.981923	-1.301745
H	3.586877	-6.588854	-1.468777
C	2.825258	-4.618099	-1.100751
H	3.80975	-4.16441	-1.139887
C	1.706555	-3.770051	-0.915457
C	1.954542	-2.334485	-0.769084
H	1.314386	-1.646855	-1.308825
C	3.016223	-1.842456	-0.063374
H	3.648279	-2.580824	0.425247
C	3.474792	-0.491796	0.112683
C	2.752641	0.692042	-0.083212
C	3.333407	2.005856	-0.216276
H	4.394945	2.19839	-0.224116
C	2.333228	2.917667	-0.374761
H	2.437374	3.983047	-0.509811
C	1.072897	2.224596	-0.322861
C	-0.196404	2.814027	-0.322577
C	-1.419917	2.107132	-0.13599
C	-2.742996	2.727666	-0.129474
H	-2.951405	3.776588	-0.281705
C	-3.634761	1.726676	0.08732
H	-4.711832	1.799184	0.128823
C	-2.858348	0.49632	0.183521
C	-3.396206	-0.795984	0.268196
C	4.887902	-0.369532	0.573547
C	5.904859	-1.135006	-0.025769
H	5.661706	-1.777582	-0.866967
C	7.223033	-1.057704	0.417555
H	7.987307	-1.650894	-0.078393
C	7.583671	-0.221921	1.483441
C	6.571647	0.537204	2.087171
H	6.817847	1.188195	2.922443
C	5.252046	0.463699	1.647481
H	4.486795	1.044064	2.153025
C	9.006474	-0.163337	1.984694
H	9.162379	-0.865059	2.813684
H	9.259499	0.834607	2.355053
H	9.718732	-0.426875	1.197613
C	-0.258646	4.299761	-0.499373
C	0.103766	4.899041	-1.715486
H	0.426263	4.272068	-2.541759
C	0.040311	6.282678	-1.88098
H	0.319812	6.718349	-2.837121
C	-0.386495	7.119163	-0.841424
C	-0.753161	6.519289	0.371323
H	-1.090273	7.142858	1.195749
C	-0.689378	5.137189	0.541944
H	-0.973492	4.698633	1.49404
C	-0.427346	8.619215	-1.011993
H	-1.241652	9.065762	-0.433552

H	-0.560495	8.898745	-2.061038
H	0.505865	9.082246	-0.667563
C	-4.851886	-0.9583	0.542294
C	-5.434892	-0.376473	1.680599
H	-4.809502	0.179591	2.371959
C	-6.797855	-0.514949	1.937728
H	-7.220097	-0.056995	2.828665
C	-7.631001	-1.235688	1.072204
C	-7.049177	-1.811884	-0.066301
H	-7.673592	-2.363846	-0.764397
C	-5.686949	-1.682691	-0.326038
H	-5.266333	-2.127058	-1.222652
C	-9.101381	-1.408917	1.367556
H	-9.283986	-2.330872	1.933692
H	-9.689122	-1.473074	0.447086
H	-9.489915	-0.578947	1.964577
N	1.377106	0.877695	-0.193241
H	0.645284	0.201544	0.003727
N	-1.516089	0.771272	0.054054
S	-0.954954	-1.925444	-0.498455

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**3a<sub>g</sub>**

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C	-2.643465	-1.987092	0.027466
C	-2.931885	-3.300983	0.402921
H	-3.811877	-3.561454	0.977331
C	-1.946313	-4.229722	0.029021
H	-1.992202	-5.278046	0.299294
C	-0.857937	-3.674749	-0.639965
C	0.36583	-4.339823	-1.066585
C	0.281529	-5.724284	-1.347292
H	-0.696272	-6.194172	-1.34511
C	1.398652	-6.486809	-1.642868
H	1.28975	-7.543716	-1.866096
C	2.66057	-5.87913	-1.672532
H	3.54477	-6.457456	-1.922531
C	2.771589	-4.522555	-1.41349
H	3.745023	-4.04925	-1.483119
C	1.653499	-3.707085	-1.1156
C	1.895882	-2.284896	-0.851129
H	1.219677	-1.534683	-1.236986
C	2.982217	-1.855643	-0.14457
H	3.641782	-2.628522	0.243865
C	3.418156	-0.518219	0.159343
C	2.700823	0.682538	0.013497
C	3.360927	1.988947	0.015211
H	4.423185	2.156442	0.111619
C	2.396147	2.916358	-0.189669
H	2.511734	3.988037	-0.255113
C	1.135433	2.184463	-0.279561
C	-0.130949	2.841476	-0.363721
C	-1.360607	2.187355	-0.225454
C	-2.690406	2.740114	-0.267241
H	-2.917445	3.777212	-0.460853
C	-3.581388	1.729546	-0.041834
H	-4.65838	1.801851	-0.036538
C	-2.854124	0.494459	0.11348
C	-3.396246	-0.789017	0.244058
C	4.805355	-0.444457	0.703937
C	5.861916	-1.14033	0.086829
H	5.67262	-1.694342	-0.828024
C	7.152623	-1.100237	0.606426
H	7.950063	-1.632738	0.093865
C	7.444494	-0.379544	1.773996
C	6.393305	0.305891	2.396182
H	6.586289	0.867048	3.307101
C	5.100549	0.274758	1.875939
H	4.302131	0.798692	2.391376
C	8.83849	-0.369113	2.353399

H	9.017116	-1.259254	2.969544
H	9.000887	0.505538	2.989463
H	9.598474	-0.36523	1.566012
C	-0.156815	4.321666	-0.569288
C	0.375426	4.893912	-1.737124
H	0.805205	4.247404	-2.496606
C	0.345104	6.272152	-1.940554
H	0.757321	6.684002	-2.858515
C	-0.216284	7.135319	-0.988951
C	-0.749072	6.565255	0.174304
H	-1.189651	7.208975	0.931698
C	-0.717899	5.186549	0.383828
H	-1.125702	4.773908	1.301912
C	-0.221178	8.630677	-1.200164
H	-1.036862	9.109695	-0.650965
H	-0.327034	8.884812	-2.259158
H	0.715802	9.08278	-0.851442
C	-4.831131	-0.922804	0.611484
C	-5.366384	-0.226547	1.70923
H	-4.715409	0.403141	2.30749
C	-6.712862	-0.34739	2.048276
H	-7.096983	0.200958	2.904677
C	-7.576513	-1.168926	1.312516
C	-7.042009	-1.865409	0.218117
H	-7.691313	-2.500472	-0.379357
C	-5.697968	-1.751253	-0.124836
H	-5.314811	-2.291788	-0.984564
C	-9.027625	-1.322848	1.698705
H	-9.175972	-2.206711	2.331637
H	-9.664502	-1.447071	0.817675
H	-9.385973	-0.455889	2.260724
N	1.340649	0.844022	-0.179259
H	-0.683677	0.254067	0.108462
N	-1.511404	0.837151	-0.005601
S	-1.117453	-1.967962	-0.844948

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**3b<sub>1</sub>**

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C	-1.964723	-2.341356	0.07105
C	-2.049807	-3.719212	0.302172
H	-2.961305	-4.196342	0.637217
C	-0.856562	-4.411476	0.079038
H	-0.759443	-5.476832	0.247587
C	0.217352	-3.611035	-0.319474
C	1.540246	-4.140145	-0.649714
C	1.533124	-5.471068	-1.150568
H	0.582425	-5.920655	-1.411867
C	2.692698	-6.194337	-1.32715
H	2.673161	-7.204441	-1.721985
C	3.898459	-5.582151	-0.958306
H	4.839717	-6.126495	-1.015936
N	3.965581	-4.331782	-0.536013
C	2.841504	-3.559651	-0.440751
C	3.219201	-2.201532	-0.073763
H	4.171383	-2.186263	0.447414
C	2.661372	-0.999907	-0.397368
H	1.763713	-0.9764	-1.000829
C	3.200928	0.288304	-0.054036
C	2.381487	1.41519	-0.126126
C	2.749646	2.810604	-0.103742
H	3.766049	3.169712	-0.042226
C	1.615021	3.562337	-0.219111
H	1.546426	4.639217	-0.248214
C	0.484853	2.667363	-0.292046
C	-0.882849	2.969316	-0.301284
C	-1.8864	1.956531	-0.205297
C	-3.327892	2.194096	-0.238603
H	-3.807994	3.152291	-0.37398
C	-3.921982	0.982975	-0.085277

H	-4.979682	0.76352	-0.07987
C	-2.846507	0.002167	0.024449
C	-3.022211	-1.38038	0.151441
C	4.614415	0.448477	0.371325
C	5.665945	-0.115739	-0.377263
H	5.43595	-0.678879	-1.276155
C	6.991103	0.053614	0.008054
H	7.780803	-0.385364	-0.596806
C	7.328238	0.784654	1.158677
C	6.284231	1.339502	1.907431
H	6.513007	1.901583	2.809247
C	4.952636	1.175396	1.525062
H	4.162712	1.599892	2.136793
C	8.770957	0.95704	1.568191
H	9.253084	-0.011722	1.74155
H	8.858766	1.544703	2.485648
H	9.347665	1.464888	0.786665
C	-1.285798	4.403209	-0.374789
C	-0.894753	5.208812	-1.456927
H	-0.310654	4.771197	-2.261164
C	-1.263486	6.552024	-1.524892
H	-0.951865	7.146691	-2.380016
C	-2.038002	7.14436	-0.519283
C	-2.433888	6.339367	0.558316
H	-3.035198	6.770595	1.355027
C	-2.064266	4.997993	0.633159
H	-2.373323	4.402765	1.487115
C	-2.414447	8.605549	-0.579593
H	-3.413945	8.77891	-0.169196
H	-2.397866	8.980369	-1.606871
H	-1.715504	9.218504	0.003168
C	-4.400848	-1.908966	0.374044
C	-5.155093	-1.502216	1.486938
H	-4.719434	-0.807657	2.198389
C	-6.446415	-1.985334	1.692186
H	-7.005437	-1.654875	2.564027
C	-7.034346	-2.889994	0.798155
C	-6.282022	-3.292013	-0.314538
H	-6.717548	-3.981628	-1.033245
C	-4.988728	-2.817416	-0.522314
H	-4.433621	-3.136649	-1.398988
C	-8.422121	-3.433697	1.038977
H	-8.388457	-4.343257	1.65167
H	-8.918217	-3.693919	0.099474
H	-9.048941	-2.710047	1.568155
N	1.00213	1.391884	-0.266243
H	0.363774	0.606045	-0.142114
N	-1.626809	0.634035	-0.064918
S	-0.316759	-1.942871	-0.388011

### 3b<sub>2</sub>

C	-1.985522	-1.81302	0.728178
C	-1.056883	-1.600407	1.732459
H	-1.190342	-0.828742	2.479996
C	0.05748	-2.461058	1.674745
H	0.88659	-2.425698	2.371174
C	0.026751	-3.333305	0.605452
C	1.066658	-4.262836	0.165959
C	0.740276	-5.6033	-0.099626
H	-0.294787	-5.920888	-0.013761
C	1.732766	-6.519286	-0.413837
H	1.501303	-7.561476	-0.604754
C	3.055722	-6.063254	-0.426912
H	3.87374	-6.757589	-0.612251
N	3.397478	-4.79542	-0.224992
C	2.432384	-3.866315	0.015642
C	2.97496	-2.510387	0.054981
H	4.056372	-2.523789	0.148072

C	2.365634	-1.296782	-0.114358
H	1.290098	-1.260485	-0.24228
C	3.049425	-0.033678	-0.125819
C	2.350153	1.174438	-0.107627
C	2.887495	2.508063	-0.277419
H	3.932461	2.723123	-0.441939
C	1.860161	3.404094	-0.23775
H	1.923023	4.474696	-0.36233
C	0.630604	2.674689	-0.025666
C	-0.680214	3.159772	0.060701
C	-1.794889	2.268713	0.197166
C	-3.211942	2.633318	0.277957
H	-3.61027	3.638001	0.295409
C	-3.908402	1.466967	0.335345
H	-4.977633	1.342532	0.433147
C	-2.919477	0.391872	0.330643
C	-3.132122	-0.985346	0.395206
C	4.540175	0.018971	-0.144661
C	5.271148	-0.570264	-1.191921
H	4.739267	-1.069236	-1.996257
C	6.661329	-0.506597	-1.219393
H	7.198814	-0.960274	-2.048509
C	7.38071	0.137617	-0.201144
C	6.653635	0.721065	0.843032
H	7.183716	1.224901	1.647366
C	5.259757	0.66285	0.873922
H	4.720935	1.115214	1.701165
C	8.889923	0.177182	-0.225457
H	9.315485	-0.790373	0.067669
H	9.281633	0.930899	0.462976
H	9.267346	0.402266	-1.228167
C	-0.91027	4.630012	-0.008289
C	-1.730202	5.193458	-1.000848
H	-2.192643	4.545976	-1.739821
C	-1.946087	6.569418	-1.06023
H	-2.584132	6.974379	-1.841926
C	-1.349557	7.44014	-0.138404
C	-0.53361	6.879313	0.853404
H	-0.067478	7.527066	1.591947
C	-0.318522	5.503666	0.920144
H	0.30105	5.09497	1.712909
C	-1.557899	8.933306	-0.224683
H	-1.555196	9.395605	0.767046
H	-2.50599	9.177699	-0.712216
H	-0.759762	9.411297	-0.806449
C	-4.429854	-1.611617	0.096526
C	-5.299992	-1.096834	-0.885488
H	-4.992497	-0.236594	-1.470072
C	-6.525824	-1.702856	-1.145264
H	-7.169712	-1.289611	-1.917332
C	-6.935274	-2.84828	-0.448239
C	-6.061768	-3.374677	0.515849
H	-6.350012	-4.265894	1.067504
C	-4.835986	-2.775467	0.781935
H	-4.186369	-3.195257	1.543579
C	-8.27609	-3.487223	-0.713569
H	-9.034305	-3.11329	-0.013999
H	-8.232666	-4.573597	-0.591751
H	-8.630677	-3.268665	-1.724735
N	0.982815	1.342868	0.041059
H	0.236336	0.653403	0.16747
N	-1.650695	0.933912	0.257625
S	-1.46259	-3.144807	-0.296285

### 3b<sub>3</sub>

C	-2.095418	-1.717553	0.700174
C	-1.181047	-1.58759	1.730224
H	-1.29695	-0.847852	2.513666

C	-0.100429	-2.493583	1.658137
H	0.713128	-2.52193	2.372926
C	-0.151092	-3.32482	0.560433
C	0.845844	-4.299355	0.115367
C	0.455852	-5.617885	-0.171892
H	-0.594109	-5.885434	-0.098334
C	1.405131	-6.575822	-0.495368
H	1.124334	-7.6024	-0.704031
C	2.748439	-6.184647	-0.497498
H	3.532685	-6.91391	-0.693526
N	3.14956	-4.938034	-0.271829
C	2.22897	-3.969556	-0.017672
C	2.838099	-2.640752	0.048491
H	3.917247	-2.713468	0.141869
C	2.29175	-1.396898	-0.099468
H	1.22259	-1.274539	-0.212591
C	3.047002	-0.172159	-0.097046
C	2.397513	1.06651	-0.081266
C	3.044027	2.366134	-0.255413
H	4.100441	2.526923	-0.414317
C	2.059656	3.298402	-0.227888
H	2.157484	4.366652	-0.357303
C	0.804438	2.572348	-0.020021
C	-0.491908	3.179435	0.045326
C	-1.653509	2.406502	0.16282
C	-3.044927	2.8043	0.227451
H	-3.391726	3.82694	-0.232122
C	-3.810964	1.676225	0.29394
H	-4.886217	1.625331	0.379503
C	-2.93214	0.524402	0.305674
C	-3.211512	-0.834071	0.382917
C	4.536625	-0.20548	-0.105988
C	5.243148	-0.847587	-1.139371
H	4.692284	-1.324781	-1.944029
C	6.63482	-0.859243	-1.155661
H	7.153456	-1.350613	-1.97522
C	7.379683	-0.244669	-0.137485
C	6.676894	0.389791	0.893635
H	7.227152	0.872494	1.697352
C	5.28201	0.411414	0.91124
H	4.761254	0.903716	1.72684
C	8.888889	-0.287594	-0.148826
H	9.258434	-1.279848	0.137462
H	9.314903	0.436965	0.55039
H	9.286711	-0.073419	-1.146102
C	-0.62217	4.662088	-0.033072
C	-1.380385	5.276257	-1.043656
H	-1.859435	4.659292	-1.1798144
C	-1.514181	6.663326	-1.102093
H	-2.107773	7.107479	-1.897414
C	-0.890123	7.493818	-0.162674
C	-0.131522	6.88228	0.845484
H	0.355275	7.499442	1.596779
C	-0.000009	5.496653	0.911839
H	0.57831	5.050214	1.715342
C	-1.007252	8.997097	-0.246557
H	-1.011635	9.454158	0.747663
H	-1.922034	9.298878	-0.764671
H	-0.162832	9.430035	-0.797391
C	-4.547611	-1.390289	0.115929
C	-5.417242	-0.832856	-0.842659
H	-5.084272	0.009919	-1.439039
C	-6.679079	-1.376011	-1.069068
H	-7.321904	-0.9288	-1.822993
C	-7.125834	-2.502455	-0.364794
C	-6.252236	-3.074114	0.573187
H	-6.567427	-3.953412	1.12944
C	-4.99281	-2.534996	0.809335
H	-4.343939	-2.989719	1.551477

C	-8.502327	-3.07572	-0.596289
H	-9.214586	-2.704383	0.151313
H	-8.498797	-4.167502	-0.522721
H	-8.890074	-2.800032	-1.580959
N	1.032621	1.241784	0.056618
H	-0.754561	0.541941	0.196873
N	-1.647298	1.040149	0.240982
S	-1.604373	-3.02583	-0.370744

**3b<sub>4</sub>**

C	-2.066844	-2.220184	0.096797
C	-2.039126	-3.377489	0.865229
H	-2.845338	-3.64345	1.537635
C	-0.849896	-4.118993	0.738361
H	-0.648504	-5.023035	1.301455
C	0.083363	-3.568527	-0.127723
C	1.348558	-4.218573	-0.500048
C	1.227439	-5.599408	-0.779936
H	0.236154	-6.039611	-0.77184
C	2.325019	-6.380155	-1.090763
H	2.222796	-7.435421	-1.319542
C	3.573757	-5.750915	-1.111316
H	4.474075	-6.31336	-1.354081
N	3.740484	-4.466265	-0.838615
C	2.67413	-3.665879	-0.536305
C	3.146314	-2.320654	-0.22246
H	4.227901	-2.320807	-0.135316
C	2.502545	-1.126228	-0.09088
H	1.434056	-1.057012	-0.217027
C	3.136369	0.135404	0.177046
C	2.359643	1.2959	0.192789
C	2.85293	2.665757	0.311784
H	3.884607	2.952656	0.455891
C	1.774972	3.479135	0.180811
H	1.753593	4.558941	0.21395
C	0.615564	2.60332	-0.015336
C	-0.736546	3.042169	-0.186404
C	-1.798476	2.131704	-0.241596
C	-3.208406	2.372776	-0.445683
H	-3.643221	3.342448	-0.635852
C	-3.860812	1.176892	-0.375336
H	-4.918097	1.00515	-0.508594
C	-2.889529	0.13074	-0.132955
C	-3.120445	-1.229925	0.045079
C	4.60415	0.234184	0.415992
C	5.533548	-0.129095	-0.574618
H	5.177187	-0.484289	-1.536695
C	6.902657	-0.021018	-0.34454
H	7.597893	-0.302558	-1.131635
C	7.400189	0.446551	0.881017
C	6.473987	0.803339	1.86813
H	6.829799	1.162655	2.830433
C	5.100866	0.702259	1.642006
H	4.40359	0.977296	2.427643
C	8.886598	0.574141	1.115025
H	9.420865	-0.323279	0.78625
H	9.111966	0.735222	2.172612
H	9.3046	1.419369	0.554821
C	-1.031816	4.498642	-0.292731
C	-0.44121	5.28621	-1.296797
H	0.229168	4.81931	-2.012238
C	-0.719333	6.647543	-1.400029
H	-0.253849	7.227279	-2.193447
C	-1.597727	7.280318	-0.508964
C	-2.190387	6.49611	0.488852
H	-2.874782	6.958545	1.195888
C	-1.911391	5.134208	0.599562
H	-2.37033	4.555721	1.395763

C	-1.873937	8.761682	-0.607741
H	-2.844402	9.017518	-0.17288
H	-1.865364	9.10127	-1.647879
H	-1.113011	9.342843	-0.071881
C	-4.506973	-1.717551	0.259336
C	-5.381666	-1.086721	1.162126
H	-5.03074	-0.236284	1.737602
C	-6.682141	-1.553524	1.347464
H	-7.332464	-1.047056	2.056053
C	-7.160356	-2.670233	0.650837
C	-6.285001	-3.306899	-0.242954
H	-6.630436	-4.171889	-0.803703
C	-4.985844	-2.847906	-0.431504
H	-4.334072	-3.354712	-1.136086
C	-8.558442	-3.193909	0.872744
H	-8.552499	-4.065073	1.539523
H	-9.019033	-3.512935	-0.067528
H	-9.201861	-2.436537	1.32863
N	0.989439	1.308545	0.008705
H	-0.725084	0.387685	0.060301
N	-1.660228	0.771719	-0.092703
S	-0.584423	-2.116612	-0.846633

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**3b<sub>s</sub>**

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C	-2.723842	-1.941195	0.026375
C	-3.177012	-3.269601	0.057925
H	-4.199599	-3.527267	0.301031
C	-2.192275	-4.216589	-0.220442
H	-2.394975	-5.280122	-0.206138
C	-0.921631	-3.674671	-0.458329
C	0.311448	-4.405772	-0.663979
C	0.234418	-5.813596	-0.834619
H	-0.735115	-6.284594	-0.947634
C	1.368856	-6.592882	-0.854108
H	1.313079	-7.667611	-0.989504
C	2.609074	-5.952853	-0.677746
H	3.52844	-6.535537	-0.641898
N	2.736853	-4.643101	-0.572361
C	1.635201	-3.841596	-0.614553
C	1.911622	-2.41706	-0.587329
H	1.196812	-1.747357	-1.042835
C	3.077834	-1.910802	-0.072384
H	3.779285	-2.655941	0.290833
C	3.534562	-0.56354	0.035625
C	2.795923	0.624509	-0.118213
C	3.374762	1.932657	-0.283296
H	4.434569	2.119163	-0.356276
C	2.372598	2.853462	-0.369981
H	2.476586	3.918695	-0.504666
C	1.114586	2.169431	-0.252763
C	-0.147873	2.776394	-0.208153
C	-1.388666	2.102495	-0.033824
C	-2.690112	2.767582	-0.023658
H	-2.860031	3.828167	-0.137404
C	-3.618995	1.789671	0.131872
H	-4.693641	1.897017	0.156373
C	-2.884996	0.531444	0.19676
C	-3.46991	-0.746483	0.214036
C	4.982005	-0.425934	0.378624
C	5.951476	-1.17935	-0.308247
H	5.642162	-1.827394	-1.123024
C	7.300104	-1.095656	0.027683
H	8.024491	-1.685511	-0.528536
C	7.74063	-0.263054	1.06663
C	6.775223	0.476132	1.762479
H	7.082476	1.113351	2.587972
C	5.424229	0.397474	1.429043
H	4.698143	0.961621	2.005911

C	9.206806	-0.154902	1.40967
H	9.719009	-1.113876	1.285573
H	9.352572	0.179177	2.440805
H	9.712693	0.568014	0.75743
C	-0.18264	4.268661	-0.352472
C	0.112574	4.883687	-1.578324
H	0.36673	4.266985	-2.43557
C	0.070067	6.271458	-1.712351
H	0.296127	6.720738	-2.676218
C	-0.267514	7.094964	-0.630292
C	-0.567577	6.47829	0.592115
H	-0.836088	7.091682	1.448704
C	-0.525269	5.09155	0.731294
H	-0.758964	4.638886	1.690501
C	-0.284176	8.598745	-0.768924
H	-1.032338	9.052676	-0.112366
H	-0.501808	8.903222	-1.796719
H	0.687746	9.031281	-0.500378
C	-4.945221	-0.865742	0.397329
C	-5.568488	-0.340734	1.541238
H	-4.963396	0.143477	2.301461
C	-6.947736	-0.444155	1.71611
H	-7.402358	-0.032151	2.613466
C	-7.756491	-1.071276	0.759364
C	-7.133643	-1.588761	-0.385468
H	-7.737466	-2.066592	-1.152918
C	-5.755411	-1.493996	-0.563874
H	-5.302094	-1.890246	-1.467208
C	-9.246173	-1.208018	0.963091
H	-9.494225	-2.171282	1.426097
H	-9.78559	-1.158592	0.012505
H	-9.634316	-0.422756	1.617858
N	1.418225	0.819231	-0.14035
H	0.696393	0.140493	0.075458
N	-1.534006	0.763338	0.108769
S	-1.004556	-1.929152	-0.334293

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**3b<sub>e</sub>**

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C	-2.807089	-1.909426	0.011143
C	-3.261566	-3.197064	0.333006
H	-4.292398	-3.399657	0.593265
C	-2.26334	-4.174281	0.325
H	-2.456704	-5.205065	0.595796
C	-0.992532	-3.692888	-0.010135
C	0.236441	-4.456981	-0.114481
C	0.126406	-5.864911	-0.24711
H	-0.857046	-6.320975	-0.254824
C	1.242103	-6.655149	-0.412985
H	1.161061	-7.730661	-0.526775
C	2.496005	-6.018384	-0.462892
H	3.401159	-6.603264	-0.621042
N	2.653532	-4.715806	-0.325882
C	1.569761	-3.911816	-0.127234
C	1.862875	-2.509789	0.077295
H	1.058543	-1.880136	0.420141
C	3.112822	-1.968194	-0.062935
H	3.902804	-2.676744	-0.294895
C	3.552211	-0.619034	0.094316
C	2.805839	0.569921	0.1252
C	3.3943	1.888047	0.168424
H	4.454624	2.07291	0.230724
C	2.40669	2.821707	0.100956
H	2.522828	3.894091	0.108981
C	1.141862	2.143358	0.000661
C	-0.107809	2.765022	-0.105472
C	-1.373171	2.107936	-0.14882
C	-2.65212	2.802226	-0.296622
H	-2.785148	3.867062	-0.419283

C	-3.61417	1.845195	-0.257326
H	-4.681655	1.978325	-0.355879
C	-2.922514	0.571585	-0.095083
C	-3.540031	-0.686486	-0.010023
C	5.045783	-0.481744	0.181314
C	5.867578	-0.905335	-0.875212
H	5.413473	-1.295634	-1.781706
C	7.255645	-0.823072	-0.782056
H	7.865533	-1.154119	-1.619078
C	7.87885	-0.319327	0.368081
C	7.058621	0.092112	1.426334
H	7.512505	0.471454	2.338574
C	5.668844	0.011569	1.338172
H	5.05831	0.320342	2.181676
C	9.38235	-0.205449	0.453678
H	9.876617	-1.007455	-0.10272
H	9.727711	-0.246528	1.490705
H	9.732212	0.744804	0.031089
C	-0.109454	4.263911	-0.16485
C	0.37825	4.945825	-1.289917
H	0.760786	4.376896	-2.132351
C	0.36454	6.339486	-1.345477
H	0.74151	6.841096	-2.233335
C	-0.134006	7.103154	-0.281813
C	-0.625351	6.420411	0.839389
H	-1.021222	6.986564	1.678934
C	-0.613579	5.02747	0.899279
H	-0.997772	4.522844	1.780958
C	-0.120193	8.612576	-0.331261
H	-0.950486	9.039287	0.239128
H	-0.187816	8.979254	-1.359593
H	0.807135	9.013523	0.096679
C	-5.023196	-0.77327	0.096057
C	-5.721868	-0.081222	1.10056
H	-5.167746	0.5133	1.819863
C	-7.109601	-0.162003	1.19254
H	-7.622637	0.38129	1.982137
C	-7.854408	-0.934327	0.290399
C	-7.157105	-1.623758	-0.711123
H	-7.709382	-2.220526	-1.43251
C	-5.768921	-1.551713	-0.805722
H	-5.255876	-2.085238	-1.599847
C	-9.355564	-1.03977	0.410922
H	-9.639548	-1.809532	1.139296
H	-9.815033	-1.309333	-0.544139
H	-9.796894	-0.097476	0.749197
N	1.43128	0.785216	0.030189
H	0.689204	0.099273	-0.026278
N	-1.561139	0.773979	-0.051188
S	-1.089719	-1.972525	-0.319362

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**3b<sub>g</sub>**

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C	-2.819282	-1.943852	-0.037636
C	-3.16226	-3.205099	0.458869
H	-4.090449	-3.389273	0.984832
C	-2.160043	-4.172158	0.291823
H	-2.239688	-5.17675	0.690231
C	-1.006985	-3.704023	-0.338076
C	0.233239	-4.424285	-0.558701
C	0.147545	-5.829621	-0.712256
H	-0.831519	-6.296896	-0.727612
C	1.280407	-6.59714	-0.876755
H	1.222216	-7.67176	-1.011151
C	2.521383	-5.93555	-0.888616
H	3.441548	-6.501303	-1.028649
N	2.650611	-4.629959	-0.744079
C	1.550107	-3.842068	-0.574408
C	1.819361	-2.430867	-0.36935

H	1.004068	-1.72797	-0.322825
C	3.081994	-1.94402	-0.166923
H	3.876162	-2.684094	-0.166457
C	3.512184	-0.602259	0.081991
C	2.765356	0.594785	0.053159
C	3.425783	1.902671	0.079045
H	4.490113	2.06931	0.14094
C	2.455022	2.835991	-0.037385
H	2.568706	3.909256	-0.062409
C	1.191969	2.107041	-0.126547
C	-0.059756	2.785768	-0.222013
C	-1.318686	2.173883	-0.194641
C	-2.612825	2.794184	-0.311005
H	-2.773731	3.849545	-0.468351
C	-3.565951	1.820913	-0.208957
H	-4.635206	1.948237	-0.282365
C	-2.913677	0.547182	-0.043027
C	-3.530266	-0.706057	0.061933
C	4.973188	-0.503145	0.396943
C	5.93795	-1.059468	-0.461464
H	5.620802	-1.523072	-1.391181
C	7.294734	-1.000008	-0.153524
H	8.017148	-1.422897	-0.847438
C	7.746262	-0.400351	1.031206
C	6.785749	0.144599	1.892312
H	7.10402	0.610344	2.821743
C	5.4265	0.094572	1.584765
H	4.703272	0.512356	2.278206
C	9.215592	-0.370968	1.377984
H	9.532585	-1.314624	1.83944
H	9.443202	0.43069	2.086287
H	9.834064	-0.225213	0.486958
C	-0.049048	4.279156	-0.345014
C	0.454482	4.90546	-1.496381
H	0.840347	4.295226	-2.307695
C	0.453843	6.294341	-1.616016
H	0.84307	6.751075	-2.522681
C	-0.047524	7.111519	-0.593267
C	-0.554113	6.485876	0.553248
H	-0.951128	7.093366	1.362849
C	-0.554054	5.096531	0.677811
H	-0.945319	4.637468	1.581096
C	-0.018311	8.616689	-0.713227
H	-0.82598	9.079773	-0.138904
H	-0.112773	8.936613	-1.755134
H	0.926353	9.025314	-0.333107
C	-4.992157	-0.771584	0.324988
C	-5.585854	-0.025688	1.358044
H	-4.962384	0.600431	1.988343
C	-6.957561	-0.0951	1.595127
H	-7.387764	0.490628	2.403415
C	-7.789015	-0.913052	0.819265
C	-7.195783	-1.661248	-0.208848
H	-7.817722	-2.296424	-0.834588
C	-5.826736	-1.598365	-0.450054
H	-5.39602	-2.178611	-1.26004
C	-9.269861	-1.009704	1.095187
H	-9.500755	-1.893328	1.703089
H	-9.843901	-1.098312	0.167777
H	-9.633059	-0.13413	1.64023
N	1.398063	0.760781	-0.075879
H	-0.772627	0.186946	0.087465
N	-1.550094	0.825855	-0.050297
S	-1.245945	-2.041345	-0.805512

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**4a<sub>1</sub>**

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C	0.423675	2.814343	0.304138
C	-0.447521	3.785088	0.796945



H	-0.096826	4.691342	1.273522
C	-1.806505	3.465061	0.644437
H	-2.609301	4.098723	1.001711
C	-2.04435	2.239446	0.032042
C	-3.389261	1.748808	-0.315952
C	-4.264408	2.745272	-0.756119
H	-3.863208	3.734412	-0.950359
C	-5.643107	2.544725	-0.967957
C	-6.189196	1.252539	-0.690686
C	-5.308097	0.240439	-0.266021
H	-5.723992	-0.745711	-0.075744
C	-3.928004	0.409536	-0.120933
C	-3.230271	-0.824776	0.251205
H	-3.836706	-1.488147	0.863697
C	-2.027954	-1.310279	-0.156395
H	-1.414959	-0.716371	-0.821756
C	-1.493422	-2.613292	0.170582
C	-0.135217	-2.858416	0.003011
C	0.565281	-4.122909	-0.029674
H	0.086247	-5.085011	0.075281
C	1.887593	-3.883046	-0.263581
H	2.675742	-4.614268	-0.361184
C	2.08155	-2.452718	-0.354777
C	3.274634	-1.731353	-0.465038
C	3.309236	-0.304071	-0.347134
C	4.507836	0.526128	-0.462745
H	5.501022	0.174253	-0.701369
C	4.116337	1.804381	-0.22581
H	4.72685	2.695366	-0.246939
C	2.676843	1.762116	0.014098
C	1.861455	2.864021	0.274109
C	-2.372555	-3.704326	0.660668
C	-3.567678	-4.031793	-0.009916
H	-3.847954	-3.474303	-0.898243
C	-4.379303	-5.069574	0.435264
H	-5.289577	-5.304837	-0.111077
C	-4.041719	-5.82359	1.570741
C	-2.859956	-5.49333	2.243915
H	-2.578748	-6.049612	3.134453
C	-2.040325	-4.454815	1.80117
H	-1.140266	-4.207751	2.355525
C	-4.923525	-6.956648	2.037208
H	-5.970447	-6.643623	2.111171
H	-4.610776	-7.329553	3.016085
H	-4.890849	-7.798332	1.33492
C	4.544359	-2.488059	-0.660205
C	4.718835	-3.333169	-1.768973
H	3.922621	-3.415675	-2.503008
C	5.902768	-4.046948	-1.952221
H	6.009725	-4.686218	-2.825175
C	6.961092	-3.944437	-1.040191
C	6.790796	-3.097186	0.063715
H	7.594318	-2.997691	0.789512
C	5.607282	-2.386648	0.25426
H	5.498328	-1.749926	1.127061
C	8.232946	-4.737433	-1.225308
H	9.104561	-4.187696	-0.857389
H	8.402561	-4.980825	-2.278124
H	8.192626	-5.685437	-0.674209
C	2.493998	4.186166	0.543525
C	3.460035	4.332153	1.553272
H	3.730063	3.472112	2.157727
C	4.062392	5.565772	1.796466
H	4.803361	5.648766	2.587517
C	3.726408	6.699017	1.045055
C	2.761972	6.552867	0.036751
H	2.490106	7.412195	-0.571156
C	2.151163	5.325711	-0.206355
H	1.415697	5.239388	-1.000099

C	4.359189	8.040371	1.326822
H	3.73075	8.640368	1.99683
H	4.494599	8.619133	0.408127
H	5.334834	7.929235	1.808149
N	0.832475	-1.887406	-0.223667
H	0.763442	-0.879497	-0.078168
N	2.226604	0.460644	-0.087117
S	-0.514631	1.474854	-0.335901
C	-7.584863	1.036176	-0.873437
C	-8.395651	2.05513	-1.314749
H	-9.459071	1.884048	-1.45242
C	-7.851818	3.337679	-1.596564
H	-8.506639	4.130311	-1.945866
C	-6.508167	3.577478	-1.428292
H	-6.090023	4.557871	-1.640207
H	-7.996374	0.053015	-0.661641

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C	-0.025067	2.488289	0.793811
C	-0.250141	1.579079	1.809443
H	0.509043	1.341765	2.544138
C	-1.534945	0.99226	1.779994
H	-1.877099	0.249369	2.490462
C	-2.310744	1.417078	0.723191
C	-3.640678	0.941433	0.319649
C	-4.653408	1.865197	0.117437
H	-4.429512	2.922272	0.23343
C	-5.98544	1.487261	-0.17505
C	-6.294105	0.090273	-0.24138
C	-5.249777	-0.841395	-0.059798
H	-5.487534	-1.898715	-0.147234
C	-3.923233	-0.472876	0.171078
C	-2.956583	-1.570106	0.193957
H	-3.429796	-2.538756	0.333749
C	-1.606882	-1.586479	-0.021804
H	-1.084793	-0.651214	-0.186533
C	-0.801605	-2.7813	-0.042869
C	0.590009	-2.72624	-0.063296
C	1.516083	-3.823286	-0.256928
H	1.215776	-4.849229	-0.40778
C	2.7871	-3.3308	-0.260234
H	3.701125	-3.885115	-0.411571
C	2.720394	-1.900839	-0.051969
C	3.761474	-0.965976	-0.000456
C	3.490364	0.435053	0.145113
C	4.471906	1.523486	0.197561
H	5.546856	1.411312	0.178589
C	3.763137	2.679875	0.283872
H	4.151464	3.68468	0.373247
C	2.352009	2.301172	0.323573
C	1.23521	3.124899	0.433
C	-1.448172	-4.125979	-0.039234
C	-2.335661	-4.504455	-1.06329
H	-2.550005	-3.804997	-1.865765
C	-2.929704	-5.763194	-1.068377
H	-3.604724	-6.030358	-1.877868
C	-2.669337	-6.694919	-0.051523
C	-1.793221	-6.31569	0.972045
H	-1.580879	-7.012268	1.779196
C	-1.192632	-5.055843	0.98035
H	-0.526093	-4.782767	1.792954
C	-3.303592	-8.065001	-0.075779
H	-4.368072	-8.008379	-0.325584
H	-3.207546	-8.567234	0.890644
H	-2.831041	-8.70645	-0.829696
C	5.168156	-1.442127	-0.115662
C	6.016233	-0.970643	-1.132645
H	5.632824	-0.257536	-1.856372

C	7.334046	-1.413227	-1.235071
H	7.963229	-1.02934	-2.034506
C	7.859588	-2.349308	-0.334153
C	7.016154	-2.819637	0.681117
H	7.398253	-3.535803	1.404681
C	5.699361	-2.37517	0.791571
H	5.076788	-2.739968	1.603202
C	9.277533	-2.851771	-0.467151
H	9.704341	-3.107274	0.50733
H	9.924158	-2.105272	-0.937562
H	9.321292	-3.756201	-1.086993
C	1.272188	4.570663	0.160509
C	2.098193	5.121397	-0.840448
H	2.698455	4.460893	-1.456679
C	2.118757	6.492416	-1.078324
H	2.756264	6.885673	-1.866609
C	1.315773	7.372843	-0.339207
C	0.477622	6.825107	0.643804
H	-0.16108	7.483119	1.227518
C	0.450203	5.456374	0.887313
H	-0.198746	5.060222	1.66205
C	1.361347	8.861224	-0.583119
H	2.112201	9.341632	0.05693
H	0.399203	9.33282	-0.363014
H	1.626141	9.088583	-1.61975
N	1.380992	-1.592339	0.054725
H	1.122851	-0.610445	0.190627
N	2.244115	0.923782	0.248628
S	-1.463079	2.631598	-0.20896
C	-7.635928	-0.30635	-0.503301
C	-8.620977	0.636103	-0.6899
H	-9.641598	0.32394	-0.890003
C	-8.313695	2.019916	-0.62239
H	-9.102167	2.751342	-0.77183
C	-7.025646	2.435573	-0.369044
H	-6.787702	3.494457	-0.314387
H	-7.868355	-1.366607	-0.555541

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**4a<sub>3</sub>**

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C	-0.014233	2.515286	0.765352
C	-0.262013	1.646613	1.809949
H	0.472916	1.447269	2.581265
C	-1.543486	1.046925	1.76884
H	-1.899022	0.331548	2.500627
C	-2.295177	1.42965	0.681733
C	-3.623974	0.949413	0.276225
C	-4.631296	1.871705	0.046372
H	-4.404638	2.930308	0.140544
C	-5.962488	1.491753	-0.24999
C	-6.276216	0.095174	-0.289402
C	-5.236582	-0.835918	-0.078143
H	-5.4769	-1.894119	-0.144785
C	-3.911638	-0.465691	0.156684
C	-2.948535	-1.565765	0.203183
H	-3.428533	-2.53064	0.346101
C	-1.597426	-1.587419	0.00411
H	-1.047063	-0.668762	-0.1492
C	-0.800644	-2.788969	-0.004367
C	0.593735	-2.725293	-0.037136
C	1.493037	-3.859697	-0.234623
H	1.188947	-4.886811	-0.375384
C	2.753729	-3.359302	-0.256315
H	3.67576	-3.899775	-0.415069
C	2.631564	-1.913835	-0.053715
C	3.731816	-0.991459	-0.029575
C	3.522878	0.385112	0.095802
C	4.472269	1.480707	0.135995
H	5.545356	1.36367	0.103873

C	3.776031	2.649354	0.235836
H	4.186566	3.644849	0.316668
C	2.360016	2.338586	0.292145
C	1.251965	3.162094	0.42025
C	-1.458188	-4.126533	0.019035
C	-2.36278	-4.510092	-0.988013
H	-2.581492	-3.81995	-1.797258
C	-2.958173	-5.768432	-0.974931
H	-3.639995	-6.043612	-1.775905
C	-2.688686	-6.690165	0.048147
C	-1.7924	-6.30679	1.053073
H	-1.564854	-6.99991	1.859003
C	-1.186504	-5.050208	1.040792
H	-0.499437	-4.775148	1.835061
C	-3.362177	-8.041405	0.07156
H	-4.393475	-7.96334	0.4374
H	-2.834095	-8.740007	0.726264
H	-3.409481	-8.481332	-0.929647
C	5.127314	-1.498347	-0.159129
C	5.966629	-1.068498	-1.200388
H	5.581795	-0.371754	-1.939275
C	7.277541	-1.532594	-1.308972
H	7.900578	-1.179731	-2.127268
C	7.801413	-2.451506	-0.391087
C	6.964636	-2.882853	0.648062
H	7.346188	-3.586264	1.384354
C	5.656782	-2.416703	0.764698
H	5.039145	-2.754118	1.591778
C	9.209428	-2.980188	-0.52797
H	9.666542	-3.15816	0.450238
H	9.846447	-2.283442	-1.080285
H	9.223853	-3.934499	-1.069307
C	1.302059	4.614755	0.191159
C	2.148314	5.197052	-0.773443
H	2.75843	4.558359	-1.403263
C	2.179123	6.576378	-0.963089
H	2.836353	6.993322	-1.721967
C	1.361561	7.434384	-0.215466
C	0.499012	6.855024	0.728438
H	-0.153666	7.494077	1.318133
C	0.465869	5.479864	0.927927
H	-0.201884	5.060263	1.673973
C	1.409814	8.930272	-0.408774
H	1.994298	9.412333	0.384886
H	0.407924	9.370279	-0.381025
H	1.872517	9.195345	-1.363356
N	1.334258	-1.558952	0.065408
H	1.454528	0.358075	0.207135
N	2.284154	0.956076	0.217703
S	-1.424556	2.602259	-0.283732
C	-7.616704	-0.302826	-0.554591
C	-8.596665	0.638887	-0.770163
H	-9.616628	0.32627	-0.972631
C	-8.284439	2.022424	-0.729774
H	-9.068696	2.753331	-0.90213
C	-6.997109	2.439247	-0.473882
H	-6.755933	3.498211	-0.440042
H	-7.852341	-1.363158	-0.586141

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**4a<sub>4</sub>**

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C	0.327253	2.761902	0.359285
C	-0.495763	3.32359	1.317818
H	-0.116993	3.980899	2.091421
C	-1.847881	2.916952	1.221935
H	-2.62259	3.238287	1.908713
C	-2.104474	2.037333	0.19066
C	-3.452874	1.571815	-0.206884
C	-4.346509	2.594202	-0.499896

H	-3.977668	3.615387	-0.497825
C	-5.708435	2.378767	-0.814322
C	-6.193488	1.034507	-0.812549
C	-5.28947	0.000642	-0.496682
H	-5.67158	-1.016815	-0.483875
C	-3.935321	0.200247	-0.208123
C	-3.210803	-1.030068	0.10743
H	-3.883561	-1.857066	0.318868
C	-1.881044	-1.321987	0.1077
H	-1.14946	-0.563821	-0.125576
C	-1.319587	-2.625536	0.361044
C	0.058545	-2.807943	0.277333
C	0.770529	-4.081134	0.342182
H	0.31887	-5.046715	0.519427
C	2.078969	-3.806581	0.108955
H	2.904672	-4.502901	0.076278
C	2.170569	-2.356556	-0.089247
C	3.381831	-1.625178	-0.336925
C	3.394596	-0.228253	-0.343891
C	4.48957	0.685343	-0.597826
H	5.486275	0.382162	-0.881228
C	4.031836	1.958257	-0.437683
H	4.590164	2.871336	-0.578774
C	2.62532	1.906674	-0.085057
C	1.76397	2.953201	0.205269
C	-2.190766	-3.792211	0.680754
C	-3.139223	-4.271982	-0.239488
H	-3.235879	-3.788897	-1.207208
C	-3.933725	-5.375862	0.061849
H	-4.647696	-5.734827	-0.675433
C	-3.822997	-6.037772	1.293334
C	-2.878	-5.559089	2.209242
H	-2.766802	-6.05404	3.170718
C	-2.075207	-4.458078	1.910947
H	-1.352185	-4.104518	2.639763
C	-4.709578	-7.21429	1.625248
H	-5.693894	-6.88106	1.977013
H	-4.273349	-7.833367	2.414046
H	-4.878488	-7.847058	0.748489
C	4.654462	-2.36308	-0.567838
C	4.763714	-3.313137	-1.599227
H	3.908553	-3.499067	-2.24224
C	5.954774	-4.000458	-1.822677
H	6.008725	-4.721753	-2.634587
C	7.088407	-3.768848	-1.030613
C	6.983007	-2.820734	-0.005105
H	7.843731	-2.621091	0.628589
C	5.790648	-2.13556	0.227189
H	5.733161	-1.422174	1.043928
C	8.369114	-4.535401	-1.260463
H	9.238126	-3.981784	-0.893445
H	8.523183	-4.746965	-2.322996
H	8.352862	-5.500256	-0.738197
C	2.28817	4.319217	0.44016
C	3.437734	4.551755	1.218157
H	3.942328	3.713344	1.686975
C	3.919529	5.843656	1.421843
H	4.807466	5.988918	2.032033
C	3.272519	6.957248	0.87169
C	2.117537	6.728648	0.107335
H	1.596025	7.572672	-0.337401
C	1.630229	5.442861	-0.099046
H	0.738713	5.296816	-0.700678
C	3.776394	8.358473	1.118308
H	3.225306	8.838768	1.936571
H	3.650609	8.989287	0.23289
H	4.835081	8.360495	1.392076
N	0.958829	-1.78423	0.026234
H	1.402586	0.105492	0.116364

N	2.298071	0.557556	-0.079043
S	-0.633267	1.752867	-0.718799
C	-7.561782	0.793238	-1.122781
C	-8.403806	1.83956	-1.421333
H	-9.446271	1.648537	-1.657703
C	-7.920132	3.174164	-1.423801
H	-8.598176	3.98825	-1.661514
C	-6.601788	3.438324	-1.126989
H	-6.228454	4.458823	-1.12784
H	-7.92885	-0.229494	-1.120525

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C	-1.327892	-2.823044	0.284706
C	-0.784958	-4.061873	0.632862
H	-1.371338	-4.841243	1.102405
C	0.585473	-4.182639	0.360923
H	1.15889	-5.065616	0.615818
C	1.153603	-3.044546	-0.205974
C	2.558105	-2.845655	-0.554156
C	3.347243	-3.980153	-0.742926
H	2.875662	-4.957565	-0.739653
C	4.740463	-3.923358	-0.946465
C	5.377174	-2.640925	-0.962521
C	4.572521	-1.49163	-0.804184
H	5.050576	-0.519495	-0.875666
C	3.194262	-1.542063	-0.624108
C	2.467918	-0.263382	-0.525142
H	1.604536	-0.114173	-1.164392
C	2.918709	0.764366	0.245294
H	3.814605	0.566111	0.830633
C	2.433942	2.120258	0.364027
C	1.156214	2.590692	0.059652
C	0.798766	3.977326	-0.136037
H	1.505339	4.792241	-0.105503
C	-0.531985	4.056173	-0.410671
H	-1.104159	4.94734	-0.617425
C	-1.086461	2.725563	-0.369856
C	-2.438994	2.387718	-0.4666
C	-2.956095	1.072241	-0.259925
C	-4.371658	0.713632	-0.33764
H	-5.181945	1.38206	-0.589921
C	-4.448578	-0.609988	-0.044903
H	-5.330941	-1.23321	-0.032089
C	-3.080775	-1.064085	0.177753
C	-2.689335	-2.391842	0.378388
C	3.433469	3.098395	0.87732
C	4.752438	3.101994	0.385618
H	5.024703	2.417067	-0.412025
C	5.706604	3.984075	0.885283
H	6.714085	3.966282	0.476944
C	5.391016	4.897907	1.90122
C	4.082684	4.887866	2.402495
H	3.813234	5.569181	3.205666
C	3.123775	4.007307	1.905714
H	2.127832	4.002281	2.337036
C	6.421651	5.869942	2.422628
H	7.422507	5.427742	2.428146
H	6.185859	6.19474	3.439976
H	6.469321	6.769243	1.795735
C	-3.403263	3.492296	-0.76684
C	-3.381544	4.152181	-2.005801
H	-2.659825	3.84608	-2.757638
C	-4.280456	5.180165	-2.288669
H	-4.244268	5.66744	-3.259985
C	-5.235542	5.588358	-1.348235
C	-5.260813	4.925599	-0.113527
H	-5.991901	5.219325	0.635757
C	-4.361987	3.89939	0.174588

H	-4.398964	3.407829	1.142337
C	-6.189021	6.721253	-1.645536
H	-7.130576	6.605268	-1.100827
H	-6.417702	6.781613	-2.713647
H	-5.760147	7.687173	-1.350518
C	-3.72351	-3.421181	0.672052
C	-4.638766	-3.240755	1.723144
H	-4.57161	-2.348513	2.337456
C	-5.616538	-4.196606	1.994235
H	-6.307472	-4.032042	2.817136
C	-5.720927	-5.366058	1.230248
C	-4.8095	-5.544046	0.178877
H	-4.87611	-6.434999	-0.440494
C	-3.825998	-4.597084	-0.09303
H	-3.142888	-4.755082	-0.921571
C	-6.761434	-6.414362	1.54219
H	-6.350563	-7.196247	2.193119
H	-7.117409	-6.906731	0.632218
H	-7.623788	-5.981988	2.057362
N	-0.02164	1.870508	-0.132786
H	-0.18827	0.891857	0.084134
N	-2.204185	-0.006693	0.044897
S	-0.0597	-1.802514	-0.382003
C	6.78299	-2.569785	-1.169797
C	7.523386	-3.715704	-1.34635
H	8.596438	-3.652552	-1.500169
C	6.892382	-4.988357	-1.330985
H	7.490477	-5.88339	-1.473671
C	5.5346	-5.090164	-1.138791
H	5.049412	-6.062463	-1.12777
H	7.262221	-1.594513	-1.184927

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**4a<sub>g</sub>**

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C	-1.245431	-2.879079	0.299845
C	-0.615143	-3.975196	0.882425
H	-1.13415	-4.662467	1.538857
C	0.762684	-4.059081	0.597133
H	1.413503	-4.812534	1.025385
C	1.237925	-3.037188	-0.212402
C	2.618299	-2.782492	-0.621081
C	3.446174	-3.882798	-0.819282
H	3.015308	-4.878289	-0.768091
C	4.824899	-3.764315	-1.097304
C	5.392157	-2.452674	-1.181371
C	4.54486	-1.337831	-0.990402
H	4.974798	-0.346128	-1.092796
C	3.184028	-1.448298	-0.724923
C	2.413371	-0.204611	-0.539051
H	1.466676	-0.072041	-1.04694
C	2.884969	0.816402	0.225903
H	3.83431	0.642859	0.728552
C	2.340082	2.138077	0.445007
C	1.042386	2.585477	0.165705
C	0.698337	4.006249	0.08445
H	1.386561	4.827843	0.215934
C	-0.61162	4.073806	-0.250146
H	-1.209681	4.959206	-0.407505
C	-1.086618	2.693665	-0.333605
C	-2.465927	2.36038	-0.528963
C	-2.978324	1.071075	-0.362086
C	-4.341574	0.613148	-0.489639
H	-5.169756	1.234353	-0.794568
C	-4.378693	-0.714701	-0.179267
H	-5.240442	-1.364348	-0.204201
C	-3.037873	-1.161172	0.11821
C	-2.621322	-2.466771	0.378232
C	3.307659	3.100159	1.044448
C	4.62196	3.20652	0.551688

H	4.917522	2.61537	-0.310198
C	5.538193	4.084289	1.12435
H	6.539231	4.156891	0.706389
C	5.191392	4.881434	2.225048
C	3.887487	4.769762	2.725218
H	3.59135	5.367716	3.583511
C	2.96441	3.897827	2.151475
H	1.968623	3.815852	2.574693
C	6.198658	5.804159	2.867633
H	6.906199	6.198369	2.132149
H	6.785134	5.278407	3.631615
H	5.709567	6.649993	3.359286
C	-3.423417	3.452651	-0.878364
C	-3.276635	4.179325	-2.072832
H	-2.46065	3.933128	-2.745923
C	-4.167218	5.195818	-2.410521
H	-4.031612	5.734047	-3.345566
C	-5.240885	5.529854	-1.572211
C	-5.389241	4.805167	-0.383275
H	-6.210457	5.042877	0.28841
C	-4.497062	3.789019	-0.038984
H	-4.627214	3.254863	0.897619
C	-6.18819	6.649922	-1.931173
H	-7.132577	6.565029	-1.386289
H	-6.412081	6.656331	-3.002563
H	-5.755704	7.628206	-1.687094
C	-3.634674	-3.489412	0.743396
C	-4.609214	-3.232035	1.723827
H	-4.604635	-2.276979	2.239512
C	-5.564716	-4.190937	2.056352
H	-6.302664	-3.963053	2.821282
C	-5.58318	-5.444946	1.433039
C	-4.607483	-5.704452	0.458127
H	-4.604044	-6.665065	-0.050945
C	-3.649985	-4.752877	0.122191
H	-2.91561	-4.977417	-0.64474
C	-6.598238	-6.495105	1.814078
H	-6.17401	-7.214716	2.525387
H	-6.930436	-7.064734	0.940613
H	-7.477937	-6.049024	2.286135
N	-0.07871	1.816035	-0.106923
H	-1.23875	0.074823	0.179052
N	-2.23401	-0.032192	-0.012144
S	-0.072906	-1.986206	-0.659034
C	6.778145	-2.317737	-1.472318
C	7.565155	-3.430114	-1.66389
H	8.622933	-3.317662	-1.881963
C	7.002495	-4.730935	-1.580178
H	7.636207	-5.598893	-1.735754
C	5.66425	-4.894535	-1.306073
H	5.230535	-5.888949	-1.243364
H	7.205631	-1.320828	-1.53852

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**4b<sub>1</sub>**

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C	0.563845	2.741448	0.457392
C	-0.456965	3.479608	1.051917
H	-0.275683	4.419445	1.557195
C	-1.725301	2.879567	0.960054
H	-2.619762	3.308695	1.395677
C	-1.736819	1.660785	0.29364
C	-2.969597	0.91049	-0.011391
C	-4.041919	1.707571	-0.390057
H	-3.861705	2.760279	-0.581069
C	-5.371237	1.233346	-0.536588
C	-5.62967	-0.152563	-0.245549
C	-4.528664	-0.96746	0.116577
H	-4.725172	-2.018668	0.311269
C	-3.213671	-0.52175	0.188656

C	-2.250886	-1.584391	0.495412
H	-2.667231	-2.368851	1.123091
C	-0.997626	-1.795096	0.014484
H	-0.562777	-1.073313	0.664599
C	-0.179262	-2.958384	0.279383
C	1.187102	-2.906886	0.031
C	2.134594	-3.994526	-0.074547
H	1.875225	-5.037369	0.031861
C	3.359734	-3.47817	-0.377939
H	4.275934	-4.025506	-0.540547
C	3.243745	-2.037338	-0.442162
C	4.250681	-1.080435	-0.600772
C	3.992961	0.321163	-0.44641
C	4.981553	1.387479	-0.609083
H	6.009151	1.256512	-0.915793
C	4.347024	2.550633	-0.313379
H	4.754431	3.550649	-0.34595
C	2.966458	2.202235	0.010233
C	1.955437	3.100169	0.349189
C	-0.776402	-4.21653	0.793216
C	-1.911852	-4.786621	0.184693
H	-2.35436	-4.296806	-0.677122
C	-2.455237	-5.978039	0.653754
H	-3.322407	-6.40103	0.152299
C	-1.899509	-6.649695	1.754367
C	-0.773804	-6.082505	2.363015
H	-0.324123	-6.576014	3.220902
C	-0.222815	-4.889219	1.896067
H	0.638696	-4.462529	2.400229
C	-2.51338	-7.928189	2.271576
H	-3.442088	-7.728075	2.819973
H	-1.835547	-8.45056	2.951897
H	-2.766131	-8.609519	1.452589
C	5.636558	-1.549466	-0.887385
C	5.91724	-2.323291	-2.026137
H	5.113067	-2.562733	-2.715758
C	7.211203	-2.767627	-2.295453
H	7.395966	-3.357587	-3.189932
C	8.27853	-2.455544	-1.44331
C	8.001423	-1.678422	-0.311003
H	8.808661	-1.41989	0.371109
C	6.708639	-1.237299	-0.033555
H	6.522661	-0.649636	0.860459
C	9.674633	-2.95935	-1.72208
H	10.433032	-2.260607	-1.356586
H	9.838466	-3.111062	-2.792955
H	9.855121	-3.921509	-1.226312
C	2.305905	4.520956	0.626348
C	3.293073	4.851929	1.569096
H	3.790129	4.058465	2.117831
C	3.627499	6.182554	1.82044
H	4.391234	6.408409	2.560164
C	2.993186	7.231147	1.143809
C	2.006975	6.900305	0.201317
H	1.505234	7.693222	-0.347875
C	1.663239	5.575633	-0.048881
H	0.903209	5.348138	-0.789684
C	3.339037	8.672806	1.428396
H	2.543383	9.164707	2.001076
H	3.46584	9.243084	0.502318
H	4.262327	8.75553	2.007887
N	1.913889	-1.750068	-0.225794
H	1.644937	-0.782053	-0.045818
N	2.793781	0.835712	-0.10173
S	-0.1092	1.2613	-0.205675
C	-6.939785	-0.645208	-0.3494
C	-8.000731	0.1827	-0.732745
C	-7.739149	1.575753	-1.03185
C	-6.43159	2.064034	-0.927046

H	-6.235028	3.110546	-1.147166
H	-7.133652	-1.692311	-0.129738
C	-10.362921	0.532971	-1.219786
C	-9.343795	-0.300233	-0.841725
H	-9.538327	-1.345444	-0.616813
H	-11.377242	0.153253	-1.297822
C	-10.104862	1.905693	-1.514907
H	-10.926632	2.549701	-1.813336
C	-8.834367	2.409289	-1.423778
H	-8.636076	3.453961	-1.648016

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**4b<sub>2</sub>**

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C	0.447119	2.42475	0.847212
C	0.347262	1.502355	1.869681
H	1.144785	1.353261	2.586872
C	-0.865918	0.776277	1.871194
H	-1.107558	0.003873	2.591364
C	-1.707682	1.109096	0.832663
C	-2.990187	0.493247	0.464946
C	-4.094368	1.298332	0.284959
H	-3.983873	2.374158	0.39021
C	-5.395397	0.778618	0.02912
C	-5.555226	-0.654585	-0.0129
C	-4.40175	-1.466297	0.148984
H	-4.526301	-2.54382	0.07546
C	-3.12342	-0.954509	0.334024
C	-2.039206	-1.934659	0.333065
H	-2.395497	-2.948632	0.496917
C	-0.704845	-1.801361	0.068288
H	-0.297405	-0.815676	-0.123417
C	0.228562	-2.899195	0.02216
C	1.603076	-2.688547	-0.050118
C	2.638533	-3.675974	-0.278736
H	2.449534	-4.729453	-0.419972
C	3.845312	-3.044787	-0.328512
H	4.809432	-3.494006	-0.5138
C	3.627163	-1.630281	-0.115797
C	4.559987	-0.586744	-0.095367
C	4.141612	0.775909	0.068726
C	5.001448	1.964034	0.103568
H	6.081097	1.968523	0.050814
C	4.175538	3.035826	0.226981
H	4.455995	4.075582	0.31875
C	2.814939	2.506335	0.304309
C	1.620397	3.201516	0.460147
C	-0.262916	-4.3074	0.054779
C	-1.142565	-4.791105	-0.930388
H	-1.465399	-4.127243	-1.726733
C	-1.585614	-6.110914	-0.910831
H	-2.25318	-6.460031	-1.694867
C	-1.179076	-7.000482	0.09528
C	-0.306109	-6.518643	1.078108
H	0.025529	-7.183916	1.871422
C	0.142918	-5.197828	1.061652
H	0.811987	-4.847699	1.841984
C	-1.688535	-8.421521	0.12778
H	-2.682904	-8.474604	0.588344
H	-1.025776	-9.07082	0.706573
H	-1.778615	-8.836996	-0.88065
C	6.006169	-0.905004	-0.256537
C	6.76546	-0.341255	-1.296638
H	6.283815	0.327033	-2.004245
C	8.119991	-0.636566	-1.441713
H	8.678712	-0.184984	-2.257895
C	8.772272	-1.511539	-0.562287
C	8.017702	-2.072982	0.476226
H	8.498599	-2.744292	1.183637
C	6.664273	-1.77541	0.629436

H	6.110566	-2.20674	1.458109
C	10.231495	-1.85668	-0.742107
H	10.709981	-2.081533	0.215738
H	10.781627	-1.037467	-1.214309
H	10.353894	-2.740499	-1.380842
C	1.489861	4.64736	0.22016
C	2.224714	5.310135	-0.783763
H	2.879148	4.73609	-1.430706
C	2.0866	6.680152	-0.986807
H	2.658008	7.159993	-1.777276
C	1.207698	7.447957	-0.209616
C	0.458737	6.786861	0.775815
H	-0.236436	7.354855	1.388843
C	0.59055	5.418807	0.985199
H	0.007624	4.934898	1.762557
C	1.079898	8.937118	-0.415932
H	1.758219	9.485707	0.24974
H	0.065249	9.285429	-0.201359
H	1.330635	9.222088	-1.441607
N	2.266361	-1.472515	0.03812
H	1.90515	-0.525806	0.187735
N	2.854277	1.12522	0.21562
S	-1.018931	2.403147	-0.12314
C	-6.831973	-1.19367	-0.231385
C	-7.952636	-0.373105	-0.409501
C	-7.790532	1.064127	-0.364453
C	-6.514664	1.601077	-0.144152
H	-6.392063	2.680843	-0.107485
H	-6.953378	-2.273648	-0.266424
C	-10.339169	-0.080075	-0.806623
C	-9.260406	-0.907467	-0.635833
H	-9.380766	-1.986952	-0.669427
H	-11.326112	-0.499467	-0.977548
C	-10.178894	1.336793	-0.761911
H	-11.045929	1.975826	-0.899643
C	-8.943348	1.889883	-0.547442
H	-8.819057	2.968945	-0.513484

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**4b<sub>3</sub>**

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C	0.447452	2.456699	0.82937
C	0.326857	1.575455	1.884531
H	1.099794	1.466774	2.636589
C	-0.879098	0.832274	1.879841
H	-1.131807	0.087231	2.624663
C	-1.697294	1.120045	0.812096
C	-2.977821	0.495564	0.447744
C	-4.081069	1.296171	0.247509
H	-3.971774	2.3738	0.333281
C	-5.380366	0.770801	-0.008348
C	-5.539222	-0.662753	-0.027927
C	-4.386183	-1.470574	0.156685
H	-4.508983	-2.549324	0.101004
C	-3.110504	-0.953357	0.342673
C	-2.026071	-1.933424	0.357974
H	-2.386494	-2.945949	0.521175
C	-0.689874	-1.800844	0.107659
H	-0.254624	-0.826416	-0.07007
C	0.237752	-2.904859	0.067873
C	1.613097	-2.683869	-0.019511
C	2.627358	-3.709049	-0.253987
H	2.436996	-4.764445	-0.38499
C	3.821053	-3.068471	-0.323486
H	4.792052	-3.500723	-0.517967
C	3.542912	-1.645617	-0.11357
C	4.531872	-0.603686	-0.127407
C	4.172999	0.739615	0.012095
C	4.995445	1.934658	0.02582
H	6.072879	1.93764	-0.046874

C	4.178163	3.017404	0.162345
H	4.478615	4.051859	0.237185
C	2.807873	2.550613	0.268429
C	1.622462	3.244582	0.448982
C	-0.262363	-4.308193	0.115282
C	-1.159228	-4.795062	-0.852707
H	-1.49018	-4.136799	-1.650285
C	-1.605062	-6.113764	-0.817958
H	-2.284072	-6.466517	-1.590396
C	-1.188068	-6.996712	0.189367
C	-0.299028	-6.510858	1.156069
H	0.04171	-7.171538	1.949341
C	0.15705	-5.193269	1.121808
H	0.841068	-4.840141	1.887353
C	-1.702316	-8.415384	0.240863
H	-2.680928	-8.4633	0.734641
H	-1.023604	-9.066687	0.798591
H	-1.827604	-8.83177	-0.763314
C	5.970429	-0.949361	-0.306591
C	6.72102	-0.42616	-1.372489
H	6.235676	0.223461	-2.094904
C	8.071901	-0.738784	-1.525442
H	8.624494	-0.317239	-2.361577
C	8.725716	-1.593713	-0.62933
C	7.97772	-2.118179	0.434383
H	8.460576	-2.774878	1.15412
C	6.630166	-1.803004	0.595361
H	6.081315	-2.20865	1.440086
C	10.179076	-1.960384	-0.814289
H	10.687332	-2.077372	0.147797
H	10.713267	-1.200632	-1.391937
H	10.282582	-2.911389	-1.351668
C	1.502079	4.697259	0.248492
C	2.241446	5.388838	-0.732472
H	2.894714	4.834979	-1.398373
C	2.109892	6.765347	-0.893714
H	2.687199	7.266082	-1.666951
C	1.229081	7.513008	-0.099637
C	0.472403	6.823277	0.859673
H	-0.226833	7.373359	1.484539
C	0.601278	5.449365	1.030648
H	0.010972	4.944462	1.789065
C	1.106663	9.00829	-0.261853
H	1.782208	9.536186	0.423198
H	0.091565	9.353059	-0.043353
H	1.363583	9.32301	-1.277365
N	2.219884	-1.440185	0.055694
H	2.126472	0.481112	0.203712
N	2.883558	1.168181	0.183443
S	-0.989131	2.374232	-0.183043
C	-6.81329	-1.207362	-0.246667
C	-7.933526	-0.391057	-0.446428
C	-7.772737	1.046716	-0.423958
C	-6.498921	1.588926	-0.203361
H	-6.377869	2.669261	-0.183778
H	-6.933064	-2.2879	-0.264651
C	-10.317065	-0.10739	-0.865937
C	-9.23884	-0.930749	-0.673521
H	-9.3578	-2.010749	-0.690184
H	-11.302356	-0.530427	-1.03721
C	-10.158184	1.310063	-0.843388
H	-11.024736	1.945866	-0.998012
C	-8.924824	1.868138	-0.62899
H	-8.801911	2.947716	-0.611965

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**4b<sub>4</sub>**

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C	0.501149	2.685407	0.511112
C	-0.347778	3.026968	1.545931

H	-0.058054	3.720595	2.326344
C	-1.592677	2.351691	1.512992
H	-2.367104	2.480491	2.260515
C	-1.736181	1.479759	0.455286
C	-2.986978	0.761556	0.113226
C	-4.072867	1.581878	-0.12174
H	-3.917604	2.656487	-0.122106
C	-5.388858	1.099762	-0.373165
C	-5.595419	-0.324604	-0.358221
C	-4.477878	-1.156351	-0.096304
H	-4.647398	-2.229663	-0.074808
C	-3.184813	-0.688641	0.120722
C	-2.204957	-1.742684	0.372448
H	-2.678537	-2.695648	0.593285
C	-0.845082	-1.748816	0.300799
H	-0.301027	-0.849582	0.055607
C	-0.013992	-2.912933	0.484992
C	1.36457	-2.808422	0.319998
C	2.322457	-3.910365	0.309151
H	2.088001	-4.950329	0.485771
C	3.531005	-3.371234	0.008362
H	4.477303	-3.883453	-0.090723
C	3.314173	-1.93039	-0.156261
C	4.335042	-0.964833	-0.457552
C	4.06397	0.404649	-0.433262
C	4.932885	1.525929	-0.730038
H	5.951135	1.435327	-1.077437
C	4.236808	2.676512	-0.51531
H	4.587451	3.686079	-0.667815
C	2.893761	2.334843	-0.083086
C	1.855465	3.177527	0.277487
C	-0.607474	-4.239938	0.816461
C	-1.491286	-4.887328	-0.06419
H	-1.744448	-4.415473	-1.008796
C	-2.02932	-6.133549	0.249717
H	-2.703823	-6.614741	-0.454281
C	-1.713095	-6.780452	1.453041
C	-0.837197	-6.131745	2.33261
H	-0.580084	-6.604753	3.27705
C	-0.290974	-4.886664	2.021505
H	0.379583	-4.40086	2.723882
C	-2.27839	-8.143117	1.775255
H	-3.29683	-8.255088	1.391026
H	-2.298608	-8.322996	2.853816
H	-1.673181	-8.938631	1.322872
C	5.713112	-1.426541	-0.782511
C	5.945271	-2.318633	-1.845286
H	5.105598	-2.663645	-2.441315
C	7.233059	-2.747517	-2.15786
H	7.378821	-3.429977	-2.991863
C	8.345154	-2.305036	-1.426829
C	8.116795	-1.41446	-0.370614
H	8.958185	-1.055584	0.217177
C	6.828154	-0.987214	-0.04963
H	6.680653	-0.313152	0.788963
C	9.735908	-2.79366	-1.755009
H	10.500623	-2.118397	-1.361047
H	9.883732	-2.882436	-2.835892
H	9.92034	-3.785077	-1.322711
C	2.096203	4.620537	0.509497
C	3.222368	5.083218	1.216225
H	3.921233	4.365493	1.633072
C	3.436922	6.445717	1.415457
H	4.31439	6.769834	1.969375
C	2.535557	7.402885	0.932576
C	1.403871	6.943012	0.241193
H	0.688866	7.662659	-0.149865
C	1.182442	5.585117	0.039577
H	0.302145	5.259752	-0.505654

C	2.752043	8.876624	1.17651
H	2.196508	9.217505	2.059248
H	2.407428	9.476292	0.328476
H	3.808061	9.102726	1.348771
N	2.021662	-1.618614	0.045237
H	2.077607	0.320665	0.14994
N	2.849018	0.947221	-0.087861
S	-0.305404	1.538869	-0.556284
C	-6.880338	-0.834574	-0.598551
C	-7.965043	0.013181	-0.853498
C	-7.755475	1.445271	-0.867787
C	-6.470417	1.950861	-0.626453
H	-6.311634	3.026447	-0.636721
H	-7.036668	-1.910488	-0.587996
C	-10.324908	0.364568	-1.349352
C	-9.281711	-0.488583	-1.102653
H	-9.437379	-1.563972	-1.091967
H	-11.319097	-0.029871	-1.536703
C	-10.117996	1.776073	-1.362714
H	-10.95755	2.435763	-1.560242
C	-8.872656	2.298446	-1.129084
H	-8.713225	3.373313	-1.139355

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**4b<sub>s</sub>**

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C	0.906271	2.993415	0.400276
C	-0.035222	3.921018	0.848745
H	0.247083	4.840888	1.344606
C	-1.366934	3.529963	0.641206
H	-2.212658	4.11789	0.977033
C	-1.502534	2.29012	0.023992
C	-2.750252	1.596102	-0.286541
C	-3.902505	2.35779	-0.413241
H	-3.826564	3.440159	-0.391104
C	-5.193296	1.79248	-0.574795
C	-5.309413	0.356164	-0.613647
C	-4.118071	-0.414441	-0.519522
H	-4.203493	-1.49319	-0.607024
C	-2.85987	0.141588	-0.38067
C	-1.703129	-0.775045	-0.342406
H	-0.88941	-0.602759	-1.039205
C	-1.693032	-1.884722	0.443414
H	-2.55918	-2.022175	1.088
C	-0.737346	-2.969572	0.507884
C	0.601594	-2.935438	0.122396
C	1.433839	-4.091401	-0.127049
H	1.082187	-5.110189	-0.075396
C	2.678917	-3.671733	-0.480307
H	3.525467	-4.28772	-0.741526
C	2.704388	-2.229582	-0.438136
C	3.826946	-1.413906	-0.599319
C	3.828848	-0.001651	-0.377197
C	5.002352	0.860996	-0.511722
H	5.986031	0.548116	-0.830114
C	4.600299	2.111816	-0.169417
H	5.187371	3.018758	-0.174852
C	3.177604	2.019091	0.13743
C	2.335123	3.099117	0.414441
C	-1.276496	-4.246006	1.053226
C	-2.534702	-4.727214	0.644599
H	-3.092367	-4.183767	-0.11253
C	-3.065722	-5.900158	1.174384
H	-4.036416	-6.248239	0.829816
C	-2.370283	-6.642991	2.139318
C	-1.124281	-6.158908	2.559656
H	-0.570771	-6.699499	3.323375
C	-0.588358	-4.985672	2.032933
H	0.363649	-4.619366	2.403612
C	-2.936972	-7.92845	2.691883

H	-4.029516	-7.89642	2.73997
H	-2.556228	-8.13367	3.696468
H	-2.66566	-8.783454	2.059875
C	5.112323	-2.077571	-0.981888
C	5.258864	-2.704488	-2.228964
H	4.428113	-2.695738	-2.928681
C	6.457279	-3.322576	-2.587281
H	6.542533	-3.793725	-3.563405
C	7.554775	-3.337109	-1.717393
C	7.41048	-2.705663	-0.473748
H	8.245366	-2.699546	0.222896
C	6.213947	-2.090466	-0.110306
H	6.1273	-1.616523	0.863046
C	8.843709	-4.028365	-2.093931
H	9.715141	-3.480528	-1.722252
H	8.94129	-4.128511	-3.178573
H	8.891171	-5.037778	-1.666582
C	2.928242	4.43049	0.713702
C	3.908588	4.571185	1.710916
H	4.215691	3.699321	2.279695
C	4.476624	5.813659	1.987585
H	5.228957	5.892201	2.768264
C	4.091908	6.961557	1.283041
C	3.115054	6.820325	0.286042
H	2.806733	7.691275	-0.286902
C	2.537993	5.584054	0.009558
H	1.793971	5.502217	-0.776452
C	4.687272	8.311591	1.602006
H	4.050727	8.868249	2.301129
H	4.790691	8.925328	0.702045
H	5.673082	8.214818	2.065371
N	1.416063	-1.829941	-0.12066
H	1.224666	-0.859446	0.113213
N	2.749854	0.712807	0.004283
S	0.07188	1.60317	-0.281606
C	-6.574155	-0.226793	-0.77138
C	-7.730769	0.554343	-0.885181
C	-7.615096	1.997029	-0.846532
C	-6.35068	2.577428	-0.695936
H	-6.263022	3.660892	-0.66812
H	-6.659434	-1.31033	-0.804185
C	-10.143996	0.764758	-1.151484
C	-9.029767	-0.024611	-1.040731
H	-9.114452	-1.107677	-1.069139
H	-11.123807	0.311713	-1.269269
C	-10.03027	2.187038	-1.113324
H	-10.925279	2.795442	-1.202612
C	-8.805636	2.782567	-0.96556
H	-8.717162	3.865291	-0.936289

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**4b<sub>8</sub>**

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C	0.88867	3.01865	0.435595
C	-0.042978	3.808295	1.102408
H	0.246818	4.615739	1.76328
C	-1.380396	3.413217	0.89265
H	-2.223527	3.87895	1.389665
C	-1.522171	2.314124	0.05873
C	-2.752233	1.607042	-0.295329
C	-3.912745	2.350801	-0.41695
H	-3.852614	3.433002	-0.352237
C	-5.188603	1.764366	-0.631077
C	-5.268954	0.32846	-0.731048
C	-4.065888	-0.423045	-0.619778
H	-4.1295	-1.500886	-0.733166
C	-2.82407	0.151419	-0.418613
C	-1.654954	-0.74423	-0.312823
H	-0.76513	-0.544458	-0.89699
C	-1.684171	-1.857438	0.466362

H	-2.592784	-2.016694	1.043455
C	-0.704092	-2.913748	0.610975
C	0.643922	-2.882475	0.23726
C	1.453292	-4.093726	0.089905
H	1.104623	-5.104604	0.239745
C	2.677615	-3.698186	-0.330831
H	3.533157	-4.318284	-0.5544
C	2.63684	-2.238171	-0.401062
C	3.798061	-1.442419	-0.671096
C	3.839928	-0.058688	-0.485131
C	4.9469	0.850421	-0.671703
H	5.916766	0.564589	-1.049224
C	4.541403	2.100375	-0.30717
H	5.11989	3.010633	-0.352946
C	3.151601	2.043878	0.084015
C	2.325385	3.114467	0.421041
C	-1.238124	-4.155365	1.237991
C	-2.471863	-4.698305	0.831615
H	-3.018188	-4.230795	0.017675
C	-2.990384	-5.840869	1.434049
H	-3.939716	-6.241832	1.087466
C	-2.309914	-6.485582	2.47761
C	-1.091304	-5.936885	2.897532
H	-0.55105	-6.40077	3.718972
C	-0.564391	-4.79695	2.293439
H	0.368144	-4.378539	2.657682
C	-2.864649	-7.737906	3.112072
H	-3.958085	-7.71848	3.147158
H	-2.491793	-7.868556	4.13192
H	-2.575369	-8.629927	2.542288
C	5.047743	-2.127285	-1.118439
C	5.078704	-2.847958	-2.32444
H	4.182388	-2.897597	-2.935828
C	6.24249	-3.483342	-2.753638
H	6.236277	-4.025606	-3.696087
C	7.422557	-3.426437	-1.998968
C	7.393283	-2.707026	-0.797267
H	8.292049	-2.646325	-0.188291
C	6.229596	-2.073504	-0.361675
H	6.232289	-1.53709	0.582658
C	8.674003	-4.139926	-2.452368
H	9.575005	-3.640435	-2.084434
H	8.732804	-4.189803	-3.543665
H	8.69892	-5.171411	-2.079001
C	2.939159	4.419911	0.774015
C	4.006006	4.499893	1.686403
H	4.370574	3.592976	2.15821
C	4.585319	5.726159	2.008746
H	5.406015	5.755243	2.720915
C	4.121575	6.920229	1.442789
C	3.053396	6.841616	0.535641
H	2.679212	7.750765	0.071486
C	2.46908	5.621731	0.21078
H	1.65172	5.590597	-0.502572
C	4.727704	8.25171	1.814544
H	4.120822	8.764227	2.571323
H	4.790302	8.917569	0.948218
H	5.733125	8.132513	2.227486
N	1.406888	-1.768407	-0.082951
H	1.902691	0.255041	0.191931
N	2.783715	0.707742	-0.048619
S	0.040228	1.798622	-0.504042
C	-6.514962	-0.275196	-0.948477
C	-7.68621	0.484134	-1.063381
C	-7.60552	1.925822	-0.96303
C	-6.358894	2.527467	-0.752755
H	-6.297161	3.610563	-0.67915
H	-6.574208	-1.358155	-1.02628
C	-10.095535	0.651477	-1.387946



C	-8.966467	-0.116872	-1.278309
H	-9.024921	-1.19946	-1.352804
H	-11.06098	0.181945	-1.551026
C	-10.01606	2.072917	-1.289314
H	-10.922237	2.664511	-1.378854
C	-8.809829	2.688991	-1.083665
H	-8.747415	3.771297	-1.008221

**9a**

N	1.477353	-1.316956	0.002858
H	-1.18395	0.303918	0.09876
H	1.183995	-0.303838	0.098872
N	-1.477362	1.317003	0.002658
C	-1.586969	-3.51545	-0.467407
H	-1.283085	-4.526147	-0.703341
C	-0.713304	-2.396257	-0.217756
C	0.696969	-2.419065	-0.211346
C	1.577804	-3.524356	-0.404155
H	1.271977	-4.541602	-0.602565
C	2.865846	-3.051366	-0.294771
H	3.764763	-3.63541	-0.417761
C	2.800814	-1.640051	-0.038901
C	3.903721	-0.728694	0.150909
C	2.753226	1.611896	-0.057267
C	2.859561	3.031942	-0.367072
H	3.765945	3.593926	-0.535759
C	1.586961	3.51538	-0.467489
H	1.28307	4.526066	-0.703455
C	0.713299	2.396197	-0.217825
C	-0.696969	2.419144	-0.211219
C	-1.577806	3.524461	-0.403864
H	-1.271991	4.541769	-0.601971
C	-2.865847	3.051405	-0.294797
H	-3.764752	3.63549	-0.417675
C	-2.800816	1.640059	-0.039082
C	-3.881919	-0.725796	0.143601
C	-2.753245	-1.611952	-0.057256
C	-2.859576	-3.031987	-0.367102
H	-3.765958	-3.593965	-0.535823
N	-1.442567	-1.273906	0.020785
N	1.442544	1.273822	0.020732
C	-3.903709	0.728691	0.150831
C	-5.134724	-1.385386	0.340713
H	-5.138973	-2.466057	0.382951
C	-5.167193	1.364849	0.348531
H	-5.19341	2.445849	0.391527
C	5.167208	-1.364852	0.348603
H	5.193405	-2.445852	0.391664
C	3.881936	0.725786	0.143491
C	5.134741	1.385389	0.340599
H	5.139014	2.466063	0.382706
C	6.326139	0.727411	0.524079
H	7.239542	1.292281	0.682837
C	6.343744	-0.679927	0.526508
H	7.270432	-1.222629	0.685226
C	-6.326135	-0.727404	0.524096
H	-7.239541	-1.292264	0.682868
C	-6.343733	0.679934	0.526449
H	-7.270422	1.222649	0.685116

**9b**

N	-1.471	1.329483	-0.212447
H	1.178908	-0.321249	-0.091744
H	-1.178729	0.321644	-0.0918
N	1.470962	-1.329391	-0.211945
C	1.604612	3.482747	-0.809608
H	1.307804	4.480234	-1.103587

C	0.723073	2.38766	-0.494158
C	-0.687034	2.419428	-0.483669
C	-1.565977	3.515053	-0.725167
H	-1.258872	4.520837	-0.97363
C	-2.856499	3.049349	-0.589
H	-3.758158	3.623363	-0.739088
C	-2.791357	1.655381	-0.266057
C	-3.89869	0.753884	-0.019087
C	-2.754519	-1.596928	-0.29622
C	-2.874533	-2.993263	-0.68793
H	-3.788892	-3.52981	-0.894591
C	-1.60462	-3.482812	-0.809586
H	-1.30783	-4.480218	-1.103859
C	-0.723064	-2.387795	-0.493798
C	0.68703	-2.419352	-0.483422
C	1.565983	-3.514871	-0.725434
H	1.258848	-4.520592	-0.974119
C	2.856486	-3.049188	-0.589296
H	3.758162	-3.623092	-0.739704
C	2.791317	-1.655298	-0.265985
C	3.881914	0.715118	-0.035673
C	2.754525	1.596849	-0.29651
C	2.874537	2.993246	-0.687841
H	3.788899	3.529867	-0.894286
N	1.445303	1.271667	-0.193905
N	-1.445304	-1.271904	-0.193325
C	3.898746	-0.753873	-0.01925
C	5.104378	1.368047	0.21013
H	5.110164	2.450385	0.247172
C	6.315656	0.717874	0.45907
C	6.328139	-0.716524	0.473712
C	5.126641	-1.389102	0.239649
H	5.146287	-2.471039	0.295933
C	-6.31566	-0.717895	0.45905
C	-6.328115	0.716495	0.473787
C	-5.126603	1.389076	0.239786
H	-5.146284	2.471013	0.296031
C	-3.881865	-0.715148	-0.035456
C	-5.104368	-1.368062	0.210146
H	-5.110175	-2.450406	0.247066
C	8.704889	-0.687751	0.980373
H	9.635183	-1.210286	1.182193
C	7.555381	-1.395429	0.744048
H	7.560605	-2.482141	0.757153
C	8.692879	0.738655	0.966329
H	9.614253	1.280582	1.157603
C	7.531686	1.422011	0.71614
H	7.518637	2.50867	0.707612
C	-8.692926	-0.73868	0.966124
H	-9.61432	-1.280615	1.157287
C	-8.704907	0.687745	0.980266
H	-9.635205	1.210286	1.182051
C	-7.555366	1.395416	0.744072
H	-7.560582	2.482127	0.757247
C	-7.531724	-1.422037	0.71597
H	-7.51869	-2.508695	0.707364

**9c**

N	1.466662	-1.336569	-0.482144
H	-1.175519	0.330963	-0.352026
H	1.175518	-0.330959	-0.352027
N	-1.466663	1.336574	-0.482144
C	-1.615366	-3.466703	-1.130884
H	-1.322506	-4.458331	-1.447715
C	-0.729425	-2.383532	-0.78925
C	0.680654	-2.420315	-0.777028
C	1.558161	-3.511808	-1.038109
H	1.249921	-4.512051	-1.306678

C	2.850092	-3.050227	-0.890933	C	3.881911	0.70806	-0.290311
H	3.752668	-3.620336	-1.051063	C	5.092304	1.358188	-0.024505
C	2.785566	-1.664394	-0.540504	H	5.099275	2.44081	0.008754
C	3.894986	-0.768721	-0.269029	C	-8.696183	0.719822	0.830735
C	2.756417	1.588025	-0.576571	C	-7.515701	1.412273	0.567419
C	2.883621	2.973388	-1.000648	H	-7.519544	2.499588	0.586568
H	3.801826	3.498087	-1.221011	C	-8.688179	-0.732587	0.809517
C	1.615365	3.46671	-1.130876	C	-7.500309	-1.404046	0.526257
H	1.322505	4.458338	-1.447705	H	-7.492211	-2.491404	0.513674
C	0.729424	2.383537	-0.789246	C	8.688165	0.73257	0.809511
C	-0.680655	2.42032	-0.777024	C	8.696196	-0.719839	0.830739
C	-1.558162	3.511814	-1.038104	C	7.515695	-1.412272	0.56742
H	-1.249921	4.512057	-1.306671	H	7.519529	-2.499588	0.586567
C	-2.850093	3.050232	-0.890931	C	7.500316	1.404048	0.526256
H	-3.752668	3.620342	-1.05106	H	7.492226	2.491405	0.513675
C	-2.785567	1.664399	-0.540504	C	-11.06241	-0.74268	1.361538
C	-3.881913	-0.708055	-0.290314	H	-11.981697	-1.282465	1.568391
C	-2.756418	-1.58802	-0.576574	C	-11.070285	0.687298	1.38248
C	-2.883622	-2.973382	-1.000655	H	-11.995464	1.210594	1.604898
H	-3.801827	-3.498079	-1.22102	C	-9.927242	1.391798	1.12595
N	-1.447434	-1.270053	-0.464151	H	-9.931624	2.478459	1.141733
N	1.447432	1.270058	-0.464149	C	11.070253	-0.687323	1.38247
C	-3.894987	0.768727	-0.269032	H	11.995408	-1.210664	1.604881
C	-5.092304	-1.358182	-0.024506	C	11.062448	0.742656	1.361543
H	-5.099273	-2.440804	0.008754	H	11.981761	1.282395	1.568403
C	-6.30735	-0.706309	0.253181	C	9.91171	1.426554	1.084714
C	-6.315714	0.735379	0.274547	H	9.903907	2.513182	1.068669
C	-5.106681	1.405526	0.016708	C	-9.91163	-1.426551	1.084699
H	-5.121199	2.487395	0.078315	H	-9.90384	-2.513177	1.068656
C	6.307348	0.706315	0.253181	C	9.927169	-1.391798	1.125932
C	6.315714	-0.735374	0.27455	H	9.931565	-2.478457	1.141717
C	5.106679	-1.40552	0.01671				
H	5.121196	-2.487389	0.078318				