Supplementary Information for

Synthesis and Functions of Binaphthyl Derivatives with Comprehensive Introduction of Phenylethynyl Groups

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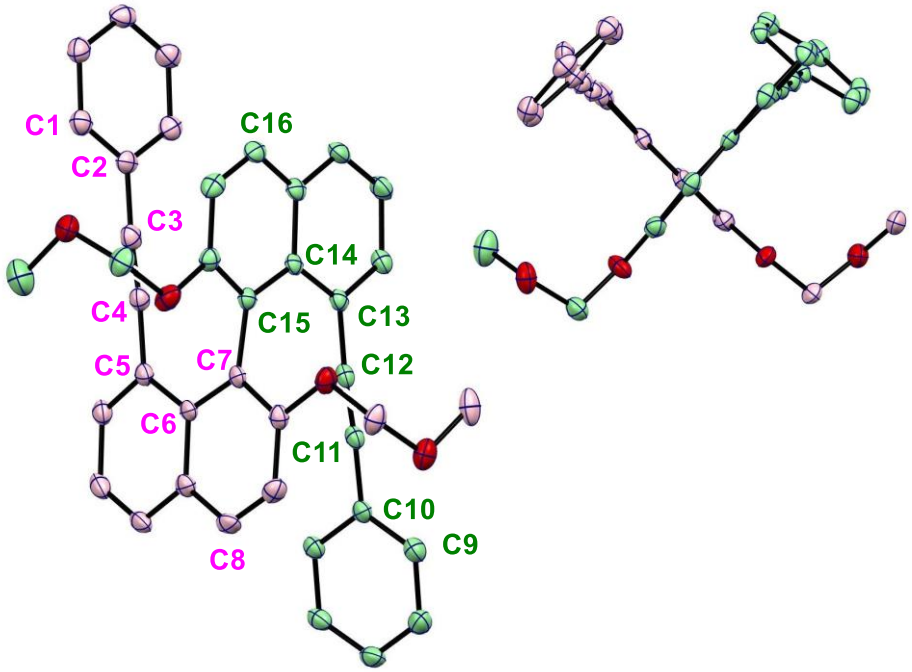
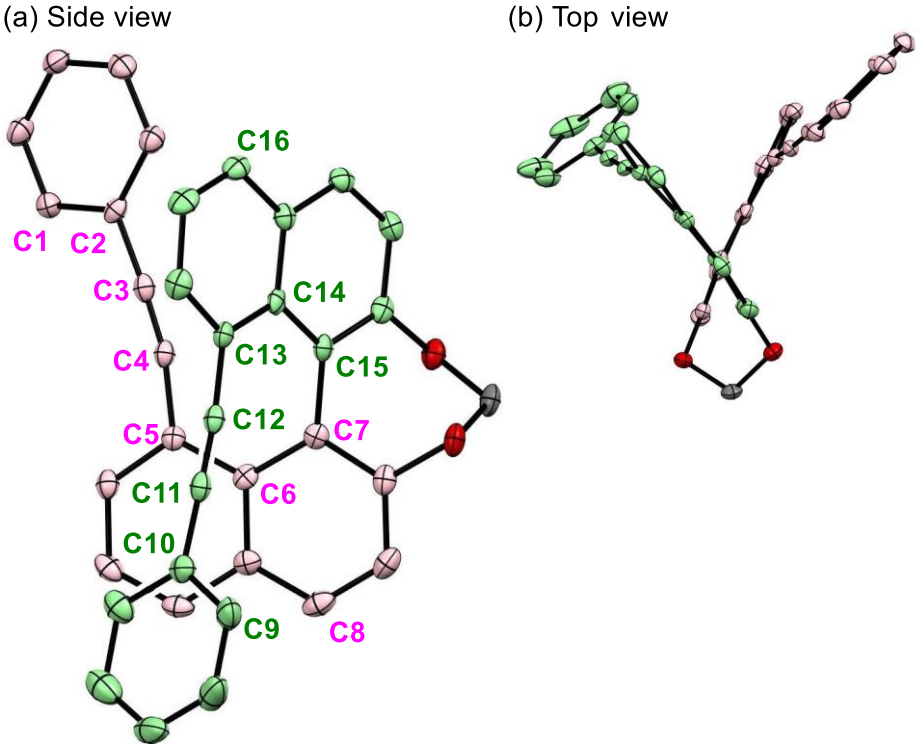
1.1. Crystal structure of of **8-PE-MOM** (crystallised from $CHCl_3/CH_3OH$ = 2/1).

(a) Side view (b) Top view



1.2. Crystal structure of **8-PE** (crystallised from *n*-hexane/*i*-PrOH = 9/1).

(a) Side view (b) Top view



2. Crystal data of of 8-PE-MOM and 8-PE

2.1. **Table S1.** Crystal data and structure refinement for **8-PE-MOM**.

Identification code	MS1382fr1_a	
Empirical formula	C40 H30 O4	
Formula weight	574.64	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$ (#14)	
Unit cell dimensions	a = 14.0381(5) Å	α= 90°.
	b = 21.0795(8) Å	β= 98.450(3)°.
	c = 10.0691(3) Å	γ = 90°.
Volume	2947.26(18) $Å^3$	
Z	4	
Density (calculated)	1.295 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	1208	
Crystal size	0.100 x 0.080 x 0.060 mm^3	
Theta range for data collection	2.262 to 29.185°.	
Index ranges	-19<=h<=19, -28<=k<=28, -13<=l<=13	
Reflections collected	54774	
Independent reflections	7620 [R(int) = 0.1244]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7620 / 0 / 399	
Goodness-of-fit on F^2	1.049	
Final R indices [I>2sigma(I)]	R1 = 0.0618, wR2 = 0.1432	
R indices (all data)	R1 = 0.1011, wR2 = 0.1584	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.356 and -0.277 $e.Å^{-3}$	

2.2. Table S2. Crystal data and structure refinement for **8-PE**.

Identification code	MS1533a	
Empirical formula	C37 H22 O2	
Formula weight	498.54	
Temperature	103(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$ (#4)	
Unit cell dimensions	a = 13.0329(10) Å	α= 90°.
	b = 8.1371(4) Å	β= 118.013(10)°.
	c = 13.5899(10) Å	γ = 90°.
Volume	1272.36(18) $Å^3$	
Z	2	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	0.079 mm^{-1}	
F(000)	520	
Crystal size	0.150 x 0.120 x 0.030 mm^3	
Theta range for data collection	2.973 to 29.177°.	
Index ranges	-17<=h<=17, -11<=k<=10, -18<=l<=18	
Reflections collected	23273	
Independent reflections	6333 [R(int) = 0.0733]	
Completeness to theta = 25.242°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6333 / 1 / 352	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1006	
R indices (all data)	R1 = 0.0931, wR2 = 0.1122	
Absolute structure parameter	0.6(10)	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.224 and -0.229 $e.Å^{-3}$	

3. Experimental procedures

3.1. General procedure for introduction of phenylethynyl groups using Sonogashira reaction.

The synthesis of **4,6-PE** is typical. An oven-dried 50-mL double-necked flask was charged with compound (*S*)-**7** (1.0 g, 1.6 mmol), CuI (8.6 mg, 0.045 mmol), $PdCl_2(PPh_3)_2$ (25 mg, 0.036 mmol), NEt_3 (2.3 mL, 16 mmol), Ethynylbenzene (894 μL, 8.14 mmol) and DMF (10 mL). After the mixture was stirred at 80 ˚C in a oil bath for 12 h. The reaction mixture was filtered by Cerite and washed with AcOEt. Then, the filtrate was washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by GPC column chromatography to afford compound **4,6-PE** as a yellow powder (581 mg, 67%).
m.p.: 238~239 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.71 (s, 2H), 7.79 (s, 2H), 7.74 (d, *J* = 7.8 Hz, 4H), 7.61 (d, *J* = 4.6 Hz, 4H), 7.46 (m, *J* = 6.4 Hz, 10H), 7.38 (d, *J* = 5.9 Hz, 6H), 5.73 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.5, 132.0, 131.9, 131.5, 130.2, 129.6, 129.0, 128.7, 128.6, 128.5, 127.2, 126.7, 125.8, 123.5, 123.2, 123.0, 121.0, 103.2, 96.5, 90.8, 89.7, 86.6, 1 peak overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{53}H_{30}O_2Na$ 721.21380; found: 721.21363, $[\alpha]^{25}_D$; +279.0 ($CHCl_3$, c=0.096 g/dL)

12: 15% yield; yellow powder; m.p.: 267~269 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.68 (d, *J* = 1.8 Hz, 2H), 7.76 (s, 2H), 7.72-7.69 (m, 4H), 7.46-7.43 (m, 8H), 7.33 (d, *J* = 9.1 Hz, 2H), 5.70 (s, 2H) ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.1, 133.0, 131.9, 130.6, 130.4, 129.1, 128.7, 126.6, 126.0, 122.9, 122.7, 120.7, 103.2, 96.6, 90.8, 89.7, 86.2, HRMS (FAB) m/z; $[M]^+$: calcd for $C_{37}H_{20}Br_2O_2$ 653.98301; found: 653.9815, $[\alpha]^{25}_D$; +14.7 ($CHCl_3$, c=0.0135 g/dL)

3-PE: 17% yield; yellow powder; m.p.: 108~110 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.68 (d, *J* = 1.8 Hz, 2H), 7.76 (s, 2H), 7.72-7.69 (m, 4H), 7.46-7.43 (m, 8H), 7.33 (d, *J* = 9.1 Hz, 2H), 5.70 (s, 2H) ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 150.6, 134.0, 131.9, 131.3, 128.5, 128.4, 126.9, 126.6, 125.8, 123.3, 116.7, 103.0, 93.7, 85.1, 3 peaks overlapped, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{37}H_{22}O_2$ 498.16143; found: 498.1624, $[\alpha]^{25}_D$; +492.5 ($CHCl_3$, c=0.0115 g/dL)

17: 98% yield; yellow amorphous; ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.10 (s, 2H), 7.94 (d, *J* = 8.7 Hz, 2H), 7.61 (d, *J* = 9.1 Hz, 2H), 7.55 (d, *J* = 6.4 Hz, 4H), 7.35 (d, *J* = 5.9 Hz, 8H), 7.12 (d, *J* = 8.7 Hz, 2H), 5.13 (d, *J* = 6.9 Hz, 2H), 5.00 (d, *J* = 6.4 Hz, 2H), 3.17 (s, 6H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 153.5, 133.6, 131.8, 129.7, 129.5, 129.1, 128.5, 128.4, 125.7, 123.5, 120.8, 118.9, 117.6, 95.0, 90.1, 89.6, 56.1, 3 peaks overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for

$C_{40}H_{30}O_4Na$ 597.20363; found 597.20544, $[\alpha]^{25}_D$; +87.9 ($CHCl_3$, c=0.025 g/dL)

3,6-PE: 45% yield; yellow powder; m.p: 139~140 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.21 (s, 2H), 8.12 (s, 2H), 7.62-7.58 (m, 8H), 7.45-7.37 (m, 18H), 5.91 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.3, 133.7, 131.9, 131.8, 131.6, 131.1, 131.0, 129.6, 128.8, 128.5, 126.8, 126.4, 123.1, 120.8, 117.6, 103.1, 94.3, 90.6, 89.2, 84.7, 3 peaks overlapped, HRMS (ESI) m/z: $[M+Na]^+$ calcd for $C_{53}H_{30}O_2Na$ 721.21380; found: 721.21546, $[\alpha]^{25}_D$; +368.8 ($CHCl_3$, c=0.085 g/dL)

5,6-PE; 42% yield; yellow powder; m.p: 158~160 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.67 (d, *J* = 9.6 Hz, 2H), 7.76-7.73 (m, 4H), 7.62 (m, 6H), 7.48-7.42 (m, 10H), 7.39-7.36 (m, 8H), 5.76 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.4, 131.9, 131.8, 131.5, 131.4, 129.4, 128.84, 128.79, 128.6, 128.5, 126.8, 126.2, 124.4, 123.8, 123.43, 123.36, 122.4, 103.3, 99.6, 94.9, 89.2, 86.8, 1 peak overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{53}H_{30}O_2Na$ 721.21380; found: 721.21528, $[\alpha]^{25}_D$; +158.9 ($CHCl_3$, c=0.0235 g/dL)

5-PE; 28% yield; yellow powder; m.p: 177~179 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.66 (d, *J* = 8.7 Hz, 2H), 7.75 (d, *J* = 6.9 Hz, 2H), 7.71 (dd, *J* = 7.5, 1.6 Hz, 4H), 7.62 (d, *J* = 8.7 Hz, 2H), 7.50 (d, *J* = 8.7 Hz, 2H), 7.46-7.41 (m, 6H), 7.30 (dd, *J* = 8.5, 7.1 Hz, 2H), 5.74 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.8, 132.2, 131.8, 131.7, 129.8, 129.1, 128.9, 128.6, 127.6, 126.4, 125.9, 125.7, 123.4, 121.9, 121.6, 103.3, 94.7, 87.6, 1 peak overlapped, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{37}H_{22}O_2$ 498.16143; found: 498.1624, $[\alpha]^{25}_D$; +156.9 ($CHCl_3$, c=0.0405 g/dL)

6,7-PE; 38% yield; yellow powder; m.p: 209~211 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.21 (s, 2H), 7.97 (d, *J* = 8.7 Hz, 2H), 7.72 (s, 2H), 7.60 (s, 4H), 7.49 (m, 6H), 7.34 (m, 6H), 7.25 (s, 2H), 5.69 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.5, 132.4, 131.9, 131.8, 131.4, 131.0, 130.5, 129.7, 128.54, 128.48, 128.44, 128.3, 125.6, 123.5, 123.3, 123.2, 122.4, 122.2, 103.2, 93.9, 93.4, 88.5, 88.4, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{53}H_{30}O_2Na$ 721.21380; found: 721.21383, $[\alpha]^{25}_D$; +934.1 ($CHCl_3$, c=0.011 g/dL)

3,4,6-PE; 43% yield; yellow powder; m.p: 184~186 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ8.74 (s, 2H), 7.80-7.78 (m, 4H), 7.67-7.61 (m, 8H), 7.51-7.43 (m, 10H), 7.41-7.38 (m, 12H), 5.93 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.1, 132.0, 132.0, 131.9, 131.2, 130.7, 130.4, 130.1, 129.1, 129.0, 128.7, 128.7, 128.6, 128.5, 127.2, 126.5, 126.1, 123.2, 123.1, 121.6, 120.9, 101.3, 99.1, 91.1, 89.5, 86.3, 84.5, 2 peaks overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{69}H_{38}O_2Na$ 921.27640, found: 921.27977, $[\alpha]^{25}_D$; +126.6 ($CHCl_3$, c=0.0525 g/dL)

3.2. General procedure for removal of protecting groups of binaphthol.

The synthesis of Compound **10** is typical. To a mixture of compound (*S*)-**9** (93 mg, 0.13 mmol) in dichloromethane (1.0 mL) was added with ice-bath cooling. After 15 minutes, 1 M BBr_3 in dichloromethane (283 μL, 0.283 mmol) was added and the reaction mixture was stirred for 1.5 h at room temperature. The reaction mixture was poured into water. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was washed with Hexane to afford compound (*S*)-**10** as a white powder (89 mg, quant.).
m.p: 271~273 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.32 (d, *J* = 1.8 Hz, 2H), 8.03 (s, 2H), 7.39 (dd, *J* = 8.9, 2.1 Hz, 2H), 6.91 (d, *J* = 9.1 Hz, 2H), 5.09 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.6, 135.1, 135.1, 131.9, 131.7, 130.4, 126.4, 120.4, 111.3, 101.4, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{20}H_{10}Br_2I_2O_2$ 693.71315, $[\alpha]^{25}_D$; –10.7 ($CHCl_3$, c=0.0665 g/dL)

32; 76% yield; yellow powder; m.p: more over 300 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.44 (s, 2H), 7.85 (d, *J* = 9.1 Hz, 2H), 7.39-7.36 (m, 2H), 7.32 (s, 2H), 5.17 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 154.0, 140.1, 134.0, 130.8, 129.6, 128.9, 127.1, 119.4, 109.2, 96.2, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{20}H_{10}Br_2I_2O_2$ 693.71315, $[\alpha]^{25}_D$; +103.5 ($CHCl_3$, c=0.0185 g/dL)

3.3. General procedure for one-carbon cross-linking of binaphthol hydroxyl groups.

The synthesis of Compound **7** is typical. To a mixture of compound (*S*)-**6** (200 mg, 0.332 mmol), K_2CO_3 (276 mg, 2.00 mmol), CH_2Br_2 (116 μL, 1.66 mmol) in DMF (2.0 mL) was added and the reaction mixture was stirred for 1.5 h at 80 °C. The reaction mixture was poured into water. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was washed with Hexane to afford compound (*S*)-**7** as a white powder (129 mg, 63%).
m.p: 232~234 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.52 (s, 2H), 7.83 (s, 2H), 7.44 (dd, J=9.2 Hz, 2H), 7.27 (d, J=8.7 Hz, 2H), 5.68 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.1, 131.7, 131.1, 130.8, 130.1, 128.6, 126.4, 125.3, 123.1, 121.3, 103.4, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{21}H_{10}Br_4O_2$ 609.74088; found: 609.7415, $[\alpha]^{25}_D$; +71.0 ($CHCl_3$, c=0.024 g/dL)

11; 76% yield; yellow powder; m.p: 168~170 °C ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.39 (d, *J* = 1.8 Hz, 2H), 8.11 (s, 2H), 7.39 (dd, *J* = 9.1, 1.8 Hz, 2H), 7.21 (d, *J* = 8.7 Hz, 2H), 5.66 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.2, 135.0, 134.1, 133.7, 130.7, 130.4, 128.8, 126.2, 121.7, 103.4, 99.2, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{21}H_{10}Br_2I_2O_2$ 705.71315; found:705.7139, $[\alpha]^{25}_D$; The specific rotation could not be measured due to the compound's extreme insolubility.

20; 69% yield; yellow powder; m.p: 150~152 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.48 (s, 2H), 8.03 (d, *J* = 1.4 Hz, 2H), 7.58-7.55 (m, 4H), 7.43-7.35 (m, 10H), 5.70 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 171.3, 150.3, 139.6, 132.8, 131.8, 131.1, 130.7, 129.5, 128.7, 128.5, 126.8, 126.3, 123.0, 121.1, 102.2, 90.9, 90.8, 89.0, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{37}H_{20}I_2O_2$ 772.94450; found: 772.94713, $[\alpha]^{25}_D$; +227.4 ($CHCl_3$, c=0.017 g/dL)

23; 65% yield; yellow powder; m.p: 239~241 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.52 (d, *J* = 9.1 Hz, 2H), 7.57 (d, *J* = 9.1 Hz, 2H), 7.46 (d, *J* = 9.1 Hz, 2H), 7.20 (d, *J* = 9.1 Hz, 2H), 5.68 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.2, 136.7, 132.3, 132.2, 131.8, 130.6, 127.4, 125.9, 123.4, 103.1, 100.4, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{21}H_{10}Br_4O_2Na$ 772.94450; found: 772.94713, $[\alpha]^{25}_D$; +167.4 ($CHCl_3$, c=0.0145 g/dL)

26; 60% yield; yellow powder; m.p: > 300 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.46 (d, *J* = 9.1 Hz, 2H), 7.75 (d, *J* = 7.3 Hz, 2H), 7.59 (d, *J* = 9.1 Hz, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 7.13 (t, *J* = 8.5 Hz, 2H), 5.70 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) The ^{13}C-NMR of compound **26** did not yield meaningful signals even after accumulating data for 11,024 scans, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{21}H_{12}Br_2O_2$, 453.91986; found 453.9203, $[\alpha]^{25}_D$; The specific rotation of **26** could not be measured due to the compound's extreme insolubility.

33; 79% yield; yellow powder; m.p: 266~267 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.50 (s, 2H), 7.86 (d, *J* = 8.7 Hz, 2H), 7.75 (s, 2H), 7.48 (d, *J* = 8.7 Hz, 2H), 5.67 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.6, 140.2, 132.3, 131.9, 129.8, 129.3, 127.6, 124.5, 122.5, 103.4, 97.8, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{21}H_{10}Br_2I_2O_2Na$ 728.70292; found 728.70607, $[\alpha]^{25}_D$; +318.5 ($CHCl_3$, c=0.096 g/dL)

37; 76% yield; yellow powder; m.p: 136~138 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.95 (d, *J* = 8.7 Hz, 2H), 7.87 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.57 (dd, *J* = 7.3, 1.4 Hz, 2H), 7.45 (d, *J* = 8.7 Hz, 2H), 7.35 (dd, *J* = 8.2, 7.3 Hz, 2H), 5.68 (s, 2H), -0.15 (s, 18H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.0, 136.3, 134.5, 131.6, 131.4, 130.1, 127.4, 124.2, 120.5, 119.4, 104.3, 102.7, 99.5, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{31}H_{30}O_2Si_2Na$ 513.16765; found 513.16688

40; 59% yield; yellow powder; m.p: > 300 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.62 (s, 2H), 7.43 (dd, *J* = 8.9, 2.1 Hz, 2H), 7.19 (d, *J* = 9.1 Hz, 2H), 5.71 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 148.3, 132.6, 131.2, 131.0, 129.8, 128.5, 126.5, 126.2, 122.5, 122.3, 102.4, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{20}H_8Br_6O_2$ 753.56246; found 765.5626, $[\alpha]^{25}_D$; +12.5 ($CHCl_3$, c=0.015 g/dL)

3.4. General procedure for iodination of aromatic rings.

The synthesis of Compound **9** is typical. To a mixture of compound (*S*)-**8** (4.53 g, 9.59 mmol), DIH (4.73 g, 12.5 mmol), TfOH (1.69 mL, 19.2 mmol) in 1,4-dioxane (36 mL) was added and the reaction mixture was stirred for 5 h at room temperature. The reaction mixture was poured into sat. Na_2SO_3 aq. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO2, *n*-hexane : toluene = 6:1) to afford compound (*S*)-**9** as a white powder (4.84 g, 70%).
m.p: 244~246 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.28 (d, *J* = 1.8 Hz, 2H), 8.01 (s, 2H), 7.28 (dd, *J* = 9.1, 1.8 Hz, 2H), 6.88 (d, *J* = 8.7 Hz, 2H), 3.75 (s, 6H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 154.9, 134.4, 132.3, 131.5, 130.8, 127.4, 126.4, 119.8, 119.4, 99.1, 56.9, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{22}H_{14}Br_2I_2O_2$ 721.74445; found: 721.7446, $[\alpha]^{25}_D$; –25.6 ($CHCl_3$, c=0.076 g/dL)

31; 88% yield; yellow powder; m.p: 235~236 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.42 (s, 2H), 7.85 (d, *J* = 9.1 Hz, 2H), 7.45 (d, *J* = 9.1 Hz, 2H), 7.32 (s, 2H), 3.77 (s, 6H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 155.9, 139.7, 134.4, 129.3, 129.0, 128.1, 127.5, 117.1, 114.8, 95.3, 56.6, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{22}H_{14}Br_2I_2O_2$ 721.74445, found 721.7459, $[\alpha]^{25}_D$; +67.5 ($CHCl_3$, c=0.2155 g/dL)

3.5. Synthesis of 4-PE.

An oven-dried 10 mL double-necked flask was charged with compound (*S*)-**12** (11.3 mg, 0.0172 mmol) was added THF (0.7 mL) at -78 °C. After 15 minutes, *n*-BuLi (23.8 μL, 0.0379 mmol) was added dropwise. After the mixture was stirred at -78 °C for 30 minutes. The reaction mixture was poured into excess 1 M HCl aq., and the organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane : ethyl acetate = 5:1) to afford compound **4-PE** as a yellow powder (7.2 mg, 84%).
m.p: 100~102 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.56 (d, *J* = 7.8 Hz, 2H), 7.77 (s, 2H), 7.72-7.69 (m, 4H), 7.59-7.52 (m, 4H), 7.46-7.34 (m, 8H), 5.71 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 150.8, 132.2, 131.9, 131.8, 128.8, 128.7, 128.6, 128.6, 127.3, 127.1, 126.9, 126.8, 126.1, 125.0, 123.4, 123.1, 95.8, 87.1, 1 peak overlapped, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{37}H_{22}O_2$ 498.16143; found 498.1606, $[\alpha]^{25}_D$; +14.7 ($CHCl_3$, c=0.0135 g/dL)

3.6. Synthesis of 18.

An oven-dried 30 mL double-necked flask was charged with compound (*S*)-**17** (393 mg, 0.683 mmol) was added THF (4.0 mL) at -78 °C. After 15 minutes, *n*-BuLi (1.29 mL, 2.05 mmol) was

added dropwise. After the mixture was stirred at room temperature for 2 h. The mixture was cooled at -78 °C for 10 minutes. I_2 in THF (3.0 mL) was added. After the mixture was stirred at room temperature for 2 h. The reaction mixture was poured into excess sat. Na_2SO_3 aq., and the organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane : ethyl acetate : Chloroform = 24:2:1) to afford compound **18** as a yellow amorphous (476 mg, 84%).

^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.56 (d, *J* = 7.8 Hz, 2H), 7.77 (s, 2H), 7.72-7.69 (m, 4H), 7.59-7.52 (m, 4H), 7.46-7.34 (m, 8H), 5.71 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 153.1, 140.0, 133.2, 131.9, 131.8, 130.1, 129.9, 128.6, 128.5, 126.7, 126.2, 123.0, 120.9, 99.7, 93.5, 90.7, 89.1, 56.6, 2 peaks overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{40}H_{28}I_2O_4Na$ 848.99693; found 848.99882, $[\alpha]^{25}_D$; +38.2 ($CHCl_3$, c=0.236 g/dL)

3.7. Synthesis of 19.

Compound (*S*)-**18** (322 mg, 0.390 mmol) was solved in 4 M HCl in 1,4-dioxane (2.0 mL) and the reaction mixture was stirred for 3 h. The reaction mixture was poured into water. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a compound (*S*)-**19** as a white amorphous (287 mg, quantum yield).

m.p: 146~148 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.48 (s, 2H), 7.99 (s, 2H), 7.57-7.54 (m, 4H), 7.43-7.35 (m, 8H), 7.03 (d, *J* = 8.7 Hz, 2H), 5.51 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 150.8, 140.23, 140.16, 132.7, 131.8, 130.7, 130.3, 128.5, 124.7, 124.6, 123.1, 119.8, 112.8, 90.3, 89.2, 87.9, 2 peaks overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{36}H_{20}I_2O_2Na$ 760.94450; found; 760.94397, $[\alpha]^{25}_D$; +19.0 ($CHCl_3$, c=0.005 g/dL)

3.8. Synthesis of 24

To a mixture of compound (*S*)-**1-Tf** (1.57 g, 2.85 mmol) in AcOH (10 mL), Br_2 (1.75 mL, 34.2 mmol) was added at room temperature and the reaction mixture was stirred for 14 h at 100 °C. The reaction mixture was poured into sat. Na_2SO_3 aq.. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane : toluene = 5:1) to afford compound (*S*)-**24** as a yellow oil (877 mg, 43%).

^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.64 (d, *J* = 9.6 Hz, 2H), 7.90 (dd, *J* = 7.3, 0.9 Hz, 2H), 7.74 (d, *J* = 9.6 Hz, 2H), 7.28-7.24 (m, 2H), 7.20-7.18 (m, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 146.1, 134.3, 132.0, 131.7, 131.1, 128.6, 126.7, 123.6, 123.4, 120.7, 31.7, 22.8, 14.2, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{22}H_{10}Br_2F_6O_6S_2$ 705.81843, found: 705.8184. $[\alpha]^{25}_D$; +9.8 ($CHCl_3$, c=0.151 g/dL)

3.9. Synthesis of 36

To a mixture of compound **35** (20.0 mg, 0.0832 mmol) in dichloromethane (1.0 mL), Cu-TMEDA (1.2 mg, 2.49×10^{-3} mmol) was added at room temperature and the reaction mixture was stirred for 1 h. The reaction mixture was poured into 1 M HCl aq. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane : AcOEt = 6:1) to afford compound **36** as a yellow powder (19 mg, 96%).

m.p; 100~102 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.94 (d, *J* = 9.1 Hz, 2H), 7.82 (dd, *J* = 8.0, 1.1 Hz, 2H), 7.66 (dd, *J* = 7.3, 1.4 Hz, 2H), 7.30-7.25 (m, 4H), 4.99 (s, 2H), –0.27 (s, 18H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 154.6, 137.2, 133.5, 132.7, 130.1, 129.7, 123.3, 119.1, 117.8, 112.6, 103.8, 99.3, –0.1, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{30}H_{30}O_2Si_2Na$ 501.16765; found: 501.16678.

3.10. Synthesis of 38

To a mixture of compound **37** (47.0 mg, 0.0958 mmol) in THF (1.0 mL), 1 M TBAF (383 μL, 0.383 mmol) was added at room temperature and the reaction mixture was stirred for 30 minutes. The reaction mixture was poured into H_2O. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a compound **38** as a yellow powder (32.7 mg, quantum yield).

m.p; 176~178 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.95 (d, *J* = 8.7 Hz, 2H), 7.90 (dd, *J* = 8.2, 0.9 Hz, 2H), 7.55-7.53 (m, 2H), 7.45 (d, *J* = 8.7 Hz, 2H), 7.35 (dd, *J* = 8.2, 7.3 Hz, 2H), 5.69 (s, 2H), 2.12 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.1, 135.6, 135.0, 131.7, 130.9, 130.0, 127.5, 124.3, 120.6, 118.1, 102.5, 82.6, 80.5, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{25}H_{14}O_2Na$ 369.08860; found: 369.08999.

3.11. Synthesis of 8-PE

An oven-dried 10-mL double-necked flask was charged with compound **38** (52.0 mg, 0.150 mmol), CuI (1.4 mg, 0.0075 mmol), Pd $(PPh_3)_4$ (8.7 mg, 0.0075 mmol), Iodobenzene (40.2 μL, 0.360 mmol) and DMF:NEt_3 =2:1 (1.5 mL). After the mixture was stirred at 80 ˚C in a oil bath for 4 h. T The reaction mixture was poured into H_2O. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by GPC column chromatography to afford compound **8-PE** as a yellow powder (57.8 mg, 77%). A portion of the synthesized racemic **8-PE** was optically resolved using a chiral column chromatography. The stereo configuration was determined by CD measurements and theoretical calculations (see, Page S42).

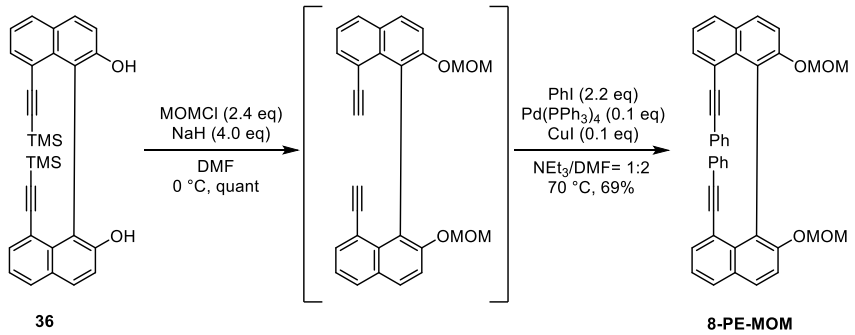
m.p.: 180~181 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 7.61-7.59 (m, 4H), 7.57 (dd, *J* = 8.2, 1.4 Hz, 2H), 7.39 (d, *J* = 8.7 Hz, 2H), 7.29 (dd, *J* = 8.2, 7.3 Hz, 2H), 7.21-7.17 (m, 2H), 7.15-7.11 (m, 4H), 6.78 (m, 4H), 5.71 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 151.0, 134.7, 134.0, 132.1, 131.8, 131.5, 130.0, 127.5, 127.4, 127.3, 124.2, 123.4, 120.3, 119.3, 102.7, 94.5, 89.5, 2 peaks overlapped, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{37}H_{22}O_2Na$ 521.15120, found: 521.15019. $[\alpha]^{25}_D$; (*R*)-**8PE**; –422.0455 ($CHCl_3$, c=0.011 g/dL), (*S*)-**8PE**; +420.4 ($CHCl_3$, c=0.012 g/dL)

3.12. Synthesis of (*S*)-39;

To a mixture of compound (*S*)-**6** (184 mg, 0.264 mmol) in dichloromethane (1.5 mL), Br_2 (134 μL, 2.64 mmol) was added at 0 °C and the reaction mixture was stirred for 14 h at room temperature. The reaction mixture was poured into sat. Na_2SO_3 aq.×. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO2, *n*-hexane : AcOEt = 5:1) to afford compound (*S*)-**39** as a yellow solid (60.5 mg, 28%).

m.p.; 153~155 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) δ 8.51 (s, 2H), 7.40 (d, *J* = 8.7 Hz, 2H), 6.95 (d, *J* = 9.1 Hz, 2H), 5.77 (s, 2H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 152.8, 132.7, 131.7, 130.0, 129.3, 126.4, 124.5, 123.2, 119.7, 111.2, HRMS (FAB) m/z; $[M]^+$ calcd for $C_{20}H_8Br_6O_2$ 753.56191; found: 753.5540. $[\alpha]^{25}_D$; –8.0 ($CHCl_3$, c=0.0075 g/dL)

3.13. Synthesis of 8-PE-MOM



Scheme S1. Synthesis of **8-PE-MOM**

To a mixture of compound **36** (105 mg, 0.219 mmol) was added DMF (1.5 mL) at 0 °C. After 15 minutes, NaH (38.6 mg, 0.965 mmol) MOMCl (39.6 mL, 0.526 mmol) was added. After the mixture was stirred at 0 °C for 1 h. The reaction mixture was poured into H_2O. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue as a yellow solid (98 mg, quantum yield). The residue was used the next reaction without purification. An oven-dried 10-mL double-necked flask was charged with the residue (98 mg, 0.219 mmol), CuI (4.1 mg, 0.0219 mmol), $Pd(PPh_3)_4$ (25.2 mg, 0.02189 mmol), Iodobenzene (53.4 μL, 0.479 mmol) and DMF:NEt_3 =2:1 (1.5 mL). After the mixture was stirred at 70 ˚C in a oil bath for 10 h. The reaction mixture was poured into H_2O. The organic layer was separated and washed with water and brine, and dried over sodium sulfate and evaporated to give a residue. The residue was purified by column chromatography (SiO_2, *n*-hexane : AcOEt = 3:1) to afford compound **8-PE-MOM** as a yellow powder (86.1 mg, 69%).

m.p.; 103~104 °C, ^{1}H-NMR (400 MHz, CHLOROFORM-D) 1H-NMR (400 MHz, CHLOROFORM-D) δ 7.68-7.66 (m, 4H), 7.56 (d, J = 9.1 Hz, 2H), 7.37 (d, J = 9.1 Hz, 2H), 7.29 (dd, J = 7.8 Hz, J = 7.8 Hz, 2H), 7.11 (d, J = 7.8 Hz, 2H), 7.04 (dd, J = 7.8 Hz, J = 6.9 Hz, 4H), 6.56-6.54 (m, 4H), 5.01 (d, J = 6.4 Hz, 2H), 4.97 (d, J = 6.9 Hz, 2H), 3.15 (s, 6H), ^{13}C-NMR (101 MHz, CHLOROFORM-D) δ 154.0, 134.8, 134.1, 131.2, 130.7, 130.5, 129.6, 127.4, 127.2, 123.8, 123.0, 123.0, 120.2, 117.0, 95.0, 94.4, 90.1, 55.8, HRMS (ESI) m/z; $[M+Na]^+$ calcd for $C_{40}H_{30}O_4Na$ 597.20363, found: 597.20184

4. Computational data

4.1. Compound 6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.158893 A.U

C	0.959	2.85211	1.99077
C	0.2084	1.62899	1.9226
C	0.33944	0.66316	2.97695
C	1.09108	1.01261	4.0926
C	1.83205	2.21205	4.16578
C	1.7842	3.10467	3.12118
C	0.84798	3.80329	0.94547
C	0	3.59911	-0.13575
C	-0.78022	2.4023	-0.1736
C	-0.67541	1.45687	0.81788
C	-0.33944	-0.66316	2.97695
C	-0.2084	-1.62899	1.9226
C	-0.959	-2.85211	1.99077
C	-1.7842	-3.10467	3.12118
C	-1.83205	-2.21205	4.16578
C	-1.09108	-1.01261	4.0926
C	0.67541	-1.45687	0.81788
C	0.78022	-2.4023	-0.1736
C	0	-3.59911	-0.13575
C	-0.84798	-3.80329	0.94547
O	1.17766	0.13016	5.1569
O	-1.17766	-0.13016	5.1569
C	0	0	5.93558
C	-0.11053	4.56069	-1.18161
C	0.11053	-4.56069	-1.18161
C	-0.21387	5.37204	-2.08434
C	-0.33275	6.3249	-3.13886
C	0.4325	7.50998	-3.12594

C	0.31227	8.43813	-4.15868
C	-0.56901	8.20463	-5.21938
C	-1.33226	7.03279	-5.24162
C	-1.2185	6.09892	-4.21339
C	0.21387	-5.37204	-2.08434
C	0.33275	-6.3249	-3.13886
C	1.2185	-6.09892	-4.21339
C	1.33226	-7.03279	-5.24162
C	0.56901	-8.20463	-5.21938
C	-0.31227	-8.43813	-4.15868
C	-0.4325	-7.50998	-3.12594
H	2.43324	2.39839	5.04975
H	2.35825	4.02626	3.15916
H	1.43179	4.71713	1.00398
H	-1.4666	2.25113	-1.00031
H	-1.28937	0.56568	0.76473
H	-2.35825	-4.02626	3.15916
H	-2.43324	-2.39839	5.04975
H	1.28937	-0.56568	0.76473
H	1.4666	-2.25113	-1.00031
H	-1.43179	-4.71713	1.00398
H	-0.17166	0.88882	6.55238
H	0.17166	-0.88882	6.55238
H	1.11562	7.68965	-2.30197
H	0.90767	9.34629	-4.13587
H	-0.66026	8.93015	-6.0223
H	-2.0183	6.84583	-6.06269
H	-1.81008	5.18919	-4.22917
H	1.81008	-5.18919	-4.22917
H	2.0183	-6.84583	-6.06269
H	0.66026	-8.93015	-6.0223
H	-0.90767	-9.34629	-4.13587
H	-1.11562	-7.68965	-2.30197

4.2. Compound 4,6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -2187.437091 A.U

C	-1.1418	3.3918	-1.13945
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C	-1.09548	1.15962	-0.17274
C	-0.31651	1.61369	0.93023
C	0	3.01276	0.99103
C	-0.40866	3.86578	-0.05889
C	0.10728	0.73571	1.98305
C	0.7047	1.30685	3.1025
C	1.02042	2.67115	3.18018
C	0.70751	3.53033	2.13504
C	-0.10728	-0.73571	1.98305
C	0.31651	-1.61369	0.93023
C	0	-3.01276	0.99103
C	-0.70751	-3.53033	2.13504
C	-1.02042	-2.67115	3.18018
C	-0.7047	-1.30685	3.1025
C	1.09548	-1.15962	-0.17274
C	1.49587	-2.01029	-1.17126
C	1.1418	-3.3918	-1.13945
C	0.40866	-3.86578	-0.05889
C	-1.55108	4.26089	-2.18932
C	1.55108	-4.26089	-2.18932
C	1.06409	4.9031	2.22235
C	-1.06409	-4.9031	2.22235
O	1.07261	0.49951	4.16425
O	-1.07261	-0.49951	4.16425
C	1.38015	6.07503	2.3172
C	-1.90724	4.99102	-3.09525
C	1.90724	-4.99102	-3.09525
C	-1.38015	-6.07503	2.3172

C	-2.32253	5.84916	-4.15371
C	2.32253	-5.84916	-4.15371
C	1.75662	7.443	2.43988
C	-1.75662	-7.443	2.43988
C	-3.06979	5.34242	-5.23626
C	-3.47341	6.18456	-6.26809
C	-3.14208	7.5414	-6.24175
C	-2.40184	8.05399	-5.17366
C	-1.99367	7.21978	-4.1372
C	1.99367	-7.21978	-4.1372
C	2.40184	-8.05399	-5.17366
C	3.14208	-7.5414	-6.24175
C	3.47341	-6.18456	-6.26809
C	3.06979	-5.34242	-5.23626
C	2.44737	7.89347	3.58342
C	2.81453	9.23042	3.70172
C	2.50228	10.13974	2.68818
C	1.81819	9.70375	1.55089
C	1.44653	8.36883	1.42313
C	-2.44737	-7.89347	3.58342
C	-2.81453	-9.23042	3.70172
C	-2.50228	-10.13974	2.68818
C	-1.81819	-9.70375	1.55089
C	-1.44653	-8.36883	1.42313
C	0	0	4.93989
H	-2.0953	1.64106	-1.99662
H	-1.38885	0.11797	-0.21344
H	-0.1507	4.91702	-0.00493
H	1.52658	3.03909	4.06519
H	-1.52658	-3.03909	4.06519
H	1.38885	-0.11797	-0.21344
H	2.0953	-1.64106	-1.99662
H	0.1507	-4.91702	-0.00493
H	-3.32553	4.28809	-5.25359
H	-4.04877	5.78117	-7.09617
H	-3.45885	8.19537	-7.04866

H	-2.14182	9.10816	-5.14856
H	-1.41875	7.61443	-3.30592
H	1.41875	-7.61443	-3.30592
H	2.14182	-9.10816	-5.14856
H	3.45885	-8.19537	-7.04866
H	4.04877	-5.78117	-7.09617
H	3.32553	-4.28809	-5.25359
H	2.6885	7.18422	4.36834
H	3.34638	9.56469	4.58757
H	2.79052	11.18223	2.78405
H	1.57344	10.40706	0.76047
H	0.91516	8.02762	0.54077
H	-2.6885	-7.18422	4.36834
H	-3.34638	-9.56469	4.58757
H	-2.79052	-11.18223	2.78405
H	-1.57344	-10.40706	0.76047
H	-0.91516	-8.02762	0.54077
H	0.44763	-0.7847	5.56058
H	-0.44763	0.7847	5.56058

4.3. Compound 4-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.157423 A.U

C	-1.61955	3.18357	-3.01295
C	-1.7747	1.78014	-3.05811
C	-1.25333	0.98882	-2.05999
C	-0.54808	1.55293	-0.95996
C	-0.43509	2.98237	-0.89635
C	-0.96829	3.76722	-1.95073
C	0	0.74346	0.09439
C	0.5088	1.39355	1.21291
C	0.6246	2.78941	1.29192

C	0.19043	3.59418	0.24702
C	0	-0.74346	0.09439
C	0.54808	-1.55293	-0.95996
C	0.43509	-2.98237	-0.89635
C	-0.19043	-3.59418	0.24702
C	-0.6246	-2.78941	1.29192
C	-0.5088	-1.39355	1.21291
C	1.25333	-0.98882	-2.05999
C	1.7747	-1.78014	-3.05811
C	1.61955	-3.18357	-3.01295
C	0.96829	-3.76722	-1.95073
O	0.99024	0.64729	2.2751
O	-0.99024	-0.64729	2.2751
C	0	0	3.0505
C	0.34574	5.00481	0.33599
C	-0.34574	-5.00481	0.33599
C	0.48978	6.20988	0.43246
C	-0.48978	-6.20988	0.43246
C	0.66618	7.61756	0.55894
C	-0.66618	-7.61756	0.55894
C	-0.22613	-8.49282	-0.45466
C	-0.40245	-9.86693	-0.3231
C	-1.01754	-10.39334	0.81532
C	-1.45747	-9.53498	1.82589
C	-1.28579	-8.15949	1.70358
C	0.22613	8.49282	-0.45466
C	0.40245	9.86693	-0.3231
C	1.01754	10.39334	0.81532
C	1.45747	9.53498	1.82589
C	1.28579	8.15949	1.70358
H	-2.02758	3.80074	-3.80774
H	-2.31487	1.32198	-3.88133
H	-1.3902	-0.08476	-2.09915
H	-0.86251	4.84517	-1.89188
H	1.07288	3.22582	2.17706
H	-1.07288	-3.22582	2.17706

H	1.3902	0.08476	-2.09915
H	2.31487	-1.32198	-3.88133
H	2.02758	-3.80074	-3.80774
H	0.86251	-4.84517	-1.89188
H	-0.55507	0.71274	3.6715
H	0.55507	-0.71274	3.6715
H	0.25137	-8.0819	-1.33814
H	-0.05878	-10.53005	-1.11149
H	-1.15331	-11.46611	0.91431
H	-1.93641	-9.93928	2.71276
H	-1.6266	-7.48989	2.48638
H	-0.25137	8.0819	-1.33814
H	0.05878	10.53005	-1.11149
H	1.15331	11.46611	0.91431
H	1.93641	9.93928	2.71276
H	1.6266	7.48989	2.48638

4.4. Compound 3-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.155243 A.U

C	-2.65518	2.41783	-4.83143
C	-2.30121	1.04924	-4.88752
C	-1.52811	0.4816	-3.89868
C	-1.06455	1.24958	-2.79594
C	-1.46427	2.62659	-2.7182
C	-2.24775	3.18492	-3.76607
C	-0.26011	0.69956	-1.73929
C	0	1.48081	-0.62551
C	-0.40201	2.84855	-0.52983
C	-1.10236	3.40106	-1.59213
C	0.26011	-0.69956	-1.73929
C	1.06455	-1.24958	-2.79594

C	1.46427	-2.62659	-2.7182
C	1.10236	-3.40106	-1.59213
C	0.40201	-2.84855	-0.52983
C	0	-1.48081	-0.62551
C	1.52811	-0.4816	-3.89868
C	2.30121	-1.04924	-4.88752
C	2.65518	-2.41783	-4.83143
C	2.24775	-3.18492	-3.76607
O	0.71342	0.94121	0.42505
O	-0.71342	-0.94121	0.42505
C	0	0	1.20658
C	-0.08282	3.61118	0.62729
C	0.08282	-3.61118	0.62729
C	0.17883	4.27461	1.61248
C	-0.17883	-4.27461	1.61248
C	0.49625	5.04285	2.76929
C	-0.49625	-5.04285	2.76929
C	1.31595	4.50354	3.78142
C	1.62458	5.25534	4.91115
C	1.1252	6.55232	5.0534
C	0.31249	7.09631	4.0559
C	-0.00201	6.35231	2.9225
C	0.00201	-6.35231	2.9225
C	-0.31249	-7.09631	4.0559
C	-1.1252	-6.55232	5.0534
C	-1.62458	-5.25534	4.91115
C	-1.31595	-4.50354	3.78142
H	-3.25899	2.85395	-5.62148
H	-2.64783	0.4378	-5.71536
H	-1.27615	-0.57051	-3.9514
H	-2.53076	4.23194	-3.6985
H	-1.40571	4.44211	-1.54344
H	1.40571	-4.44211	-1.54344
H	1.27615	0.57051	-3.9514
H	2.64783	-0.4378	-5.71536
H	3.25899	-2.85395	-5.62148

H	2.53076	-4.23194	-3.6985
H	0.76163	-0.48684	1.82502
H	-0.76163	0.48684	1.82502
H	1.7037	3.49693	3.66466
H	2.25788	4.82868	5.6834
H	1.36846	7.13592	5.93624
H	-0.07773	8.10428	4.16187
H	-0.63326	6.77155	2.14585
H	0.63326	-6.77155	2.14585
H	0.07773	-8.10428	4.16187
H	-1.36846	-7.13592	5.93624
H	-2.25788	-4.82868	5.6834
H	-1.7037	-3.49693	3.66466

4.5. Compound 3,6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -2187.434208 A.U

C	2.44836	3.45303	-1.01083
C	2.4914	2.0846	-1.41824
C	1.50191	1.20555	-1.05365
C	0.39638	1.61873	-0.25904
C	0.3213	3.00356	0.1132
C	1.3649	3.8872	-0.26019
C	-0.65918	0.73286	0.141
C	-1.77384	1.26643	0.76892
C	-1.86825	2.64415	1.13567
C	-0.80554	3.47936	0.82475
C	-0.65901	-0.73296	-0.1409
C	0.39674	-1.61858	0.25918
C	0.32201	-3.00343	-0.11307
C	-0.80468	-3.47949	-0.82467
C	-1.86759	-2.64453	-1.13562

C	-1.77352	-1.26679	-0.76886
C	1.50215	-1.20514	1.05385
C	2.49182	-2.08396	1.41848
C	2.44912	-3.4524	1.01106
C	1.3658	-3.88682	0.26036
O	-2.82396	0.43554	1.09779
O	-2.82382	-0.43615	-1.09777
C	-3.60575	-0.00037	-0.00001
C	-3.02539	3.13055	1.80402
C	-3.02458	-3.1312	-1.80402
C	-4.01051	3.5619	2.3719
C	-4.00958	-3.56278	-2.37194
C	-5.16728	4.05439	3.04168
C	-5.16619	-4.05554	-3.0418
C	-6.17545	3.16734	3.47029
C	-7.30505	3.65048	4.12396
C	-7.45072	5.0194	4.36182
C	-6.45703	5.90677	3.94155
C	-5.32373	5.4334	3.28693
C	-5.32234	-5.43459	-3.28701
C	-6.45549	-5.90821	-3.94169
C	-7.44933	-5.02107	-4.36206
C	-7.30396	-3.65211	-4.12426
C	-6.17451	-3.16871	-3.47052
C	3.49157	4.34555	-1.3866
C	3.49253	-4.34468	1.38687
C	4.39065	5.09724	-1.71355
C	4.39177	-5.09618	1.71383
C	5.44051	5.98197	-2.09405
C	5.44181	-5.98078	2.09413
C	5.41519	-7.33499	1.70391
C	6.44323	-8.19523	2.07804
C	7.51242	-7.72519	2.84442
C	7.54859	-6.38486	3.23645
C	6.52529	-5.51689	2.86725
C	6.52432	5.51802	-2.86668

C	7.54745	6.38611	-3.23607
C	7.51079	7.72662	-2.84471
C	6.44127	8.19672	-2.07881
C	5.4134	7.33636	-1.70451
H	3.32146	1.74853	-2.03048
H	1.55625	0.17673	-1.38791
H	1.30248	4.9287	0.03943
H	-0.85304	4.52648	1.10589
H	-0.85193	-4.52662	-1.10582
H	1.55622	-0.17631	1.38812
H	3.32178	-1.7477	2.03076
H	1.30364	-4.92834	-0.03927
H	-4.22385	-0.81139	0.39931
H	-4.22397	0.81053	-0.39938
H	-6.05585	2.10485	3.28577
H	-8.07441	2.95688	4.45021
H	-8.33345	5.39253	4.8724
H	-6.56589	6.97167	4.12471
H	-4.54992	6.11963	2.95875
H	-4.54841	-6.12064	-2.95875
H	-6.56412	-6.97315	-4.12481
H	-8.33195	-5.3944	-4.8727
H	-8.07344	-2.95868	-4.45059
H	-6.05514	-2.10619	-3.28604
H	4.58314	-7.69668	1.10875
H	6.41054	-9.23639	1.77081
H	8.31269	-8.3994	3.13448
H	8.37761	-6.01464	3.83237
H	6.55018	-4.47527	3.17015
H	6.54959	4.47626	-3.16906
H	8.37673	6.01584	-3.8316
H	8.31093	8.40093	-3.13491
H	6.4082	9.23803	-1.77211
H	4.5811	7.6981	-1.10973

4.6. Compound 5,6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -2187.435098 A.U

C	-1.13558	3.38215	-0.40055
C	-1.4933	2.00477	-0.41273
C	-1.0987	1.15315	0.58647
C	-0.31543	1.6115	1.68395
C	0.00731	3.00753	1.75008
C	-0.39591	3.88734	0.68445
C	0.11092	0.73692	2.73916
C	0.71245	1.30317	3.8561
C	1.02527	2.6744	3.92804
C	0.70035	3.50535	2.88269
C	-0.11092	-0.73692	2.73916
C	0.31543	-1.6115	1.68395
C	-0.00731	-3.00753	1.75008
C	-0.70035	-3.50535	2.88269
C	-1.02527	-2.6744	3.92804
C	-0.71245	-1.30317	3.8561
C	1.0987	-1.15315	0.58647
C	1.4933	-2.00477	-0.41273
C	1.13558	-3.38215	-0.40055
C	0.39591	-3.88734	0.68445
C	-0.06811	5.26793	0.73343
C	0.06811	-5.26793	0.73343
O	1.07564	0.49481	4.91853
O	-1.07564	-0.49481	4.91853
C	0	0	5.69317
C	0.19841	6.45537	0.76409
C	-0.19841	-6.45537	0.76409
C	0.48156	7.8511	0.77322
C	-0.48156	-7.8511	0.77322
C	0.27538	-8.73396	-0.0246

C	0	-10.0981	-0.01861
C	-1.02873	-10.60671	0.77823
C	-1.78332	-9.74085	1.57334
C	-1.51568	-8.375	1.57464
C	1.51568	8.375	1.57464
C	1.78332	9.74085	1.57334
C	1.02873	10.60671	0.77823
C	0	10.0981	-0.01861
C	-0.27538	8.73396	-0.0246
C	-1.53359	4.21579	-1.4789
C	1.53359	-4.21579	-1.4789
C	-1.87746	4.89949	-2.42504
C	1.87746	-4.89949	-2.42504
C	-2.26058	5.72045	-3.52372
C	2.26058	-5.72045	-3.52372
C	-1.65821	6.98066	-3.71736
C	-2.03398	7.7816	-4.79166
C	-3.01176	7.34512	-5.68907
C	-3.6134	6.09756	-5.50712
C	-3.24402	5.28873	-4.43643
C	3.24402	-5.28873	-4.43643
C	3.6134	-6.09756	-5.50712
C	3.01176	-7.34512	-5.68907
C	2.03398	-7.7816	-4.79166
C	1.65821	-6.98066	-3.71736
H	-2.09245	1.63713	-1.23881
H	-1.3988	0.11342	0.5491
H	1.52932	3.04561	4.81415
H	0.94478	4.56077	2.92186
H	-0.94478	-4.56077	2.92186
H	-1.52932	-3.04561	4.81415
H	1.3988	-0.11342	0.5491
H	2.09245	-1.63713	-1.23881
H	-0.44378	0.78674	6.31424
H	0.44378	-0.78674	6.31424
H	1.07837	-8.33502	-0.63576

H	0.5916	-10.76778	-0.63587
H	-1.24056	-11.67171	0.78025
H	-2.58381	-10.13158	2.19461
H	-2.10255	-7.70022	2.18928
H	2.10255	7.70022	2.18928
H	2.58381	10.13158	2.19461
H	1.24056	11.67171	0.78025
H	-0.5916	10.76778	-0.63587
H	-1.07837	8.33502	-0.63576
H	-0.89425	7.31263	-3.02185
H	-1.5611	8.74933	-4.93105
H	-3.3024	7.97308	-6.52594
H	-4.37325	5.75359	-6.20265
H	-3.70957	4.31935	-4.29187
H	3.70957	-4.31935	-4.29187
H	4.37325	-5.75359	-6.20265
H	3.3024	-7.97308	-6.52594
H	1.5611	-8.74933	-4.93105
H	0.89425	-7.31263	-3.02185

4.7. Compound 5-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.157478 A.U

C	-0.46929	3.5333	-1.97971
C	-1.08258	2.26762	-2.01543
C	-0.85641	1.34544	-1.01757
C	0	1.6448	0.07789
C	0.5896	2.95163	0.14922
C	0.3543	3.89053	-0.91839
C	0.2514	0.70152	1.13381
C	0.95164	1.13946	2.24942
C	1.52675	2.42367	2.32331

C	1.36926	3.30313	1.27924
C	-0.2514	-0.70152	1.13381
C	0	-1.6448	0.07789
C	-0.5896	-2.95163	0.14922
C	-1.36926	-3.30313	1.27924
C	-1.52675	-2.42367	2.32331
C	-0.95164	-1.13946	2.24942
C	0.85641	-1.34544	-1.01757
C	1.08258	-2.26762	-2.01543
C	0.46929	-3.5333	-1.97971
C	-0.3543	-3.89053	-0.91839
O	1.15153	0.27511	3.31202
O	-1.15153	-0.27511	3.31202
C	0	0	4.0864
C	0.94555	5.18536	-0.89286
C	-0.94555	-5.18536	-0.89286
C	1.44277	6.29656	-0.89485
C	-1.44277	-6.29656	-0.89485
C	2.01602	7.60072	-0.9121
C	-2.01602	-7.60072	-0.9121
C	1.72287	8.49567	-1.96129
C	2.28329	9.76934	-1.97736
C	3.14265	10.17498	-0.95342
C	3.43996	9.29627	0.09098
C	2.88456	8.02043	0.11569
C	-2.88456	-8.02043	0.11569
C	-3.43996	-9.29627	0.09098
C	-3.14265	-10.17498	-0.95342
C	-2.28329	-9.76934	-1.97736
C	-1.72287	-8.49567	-1.96129
H	-0.64616	4.24872	-2.77566
H	-1.74605	2.01993	-2.83846
H	-1.34737	0.381	-1.05483
H	2.09499	2.68679	3.20931
H	1.81613	4.29037	1.31755
H	-1.81613	-4.29037	1.31755

H	-2.09499	-2.68679	3.20931
H	1.34737	-0.381	-1.05483
H	1.74605	-2.01993	-2.83846
H	0.64616	-4.24872	-2.77566
H	0.28165	-0.85822	4.70772
H	-0.28165	0.85822	4.70772
H	1.05475	8.17777	-2.75494
H	2.04879	10.44856	-2.79169
H	3.57798	11.16961	-0.9693
H	4.10759	9.60646	0.88941
H	3.11512	7.33645	0.92594
H	-3.11512	-7.33645	0.92594
H	-4.10759	-9.60646	0.88941
H	-3.57798	-11.16961	-0.9693
H	-2.04879	-10.44856	-2.79169
H	-1.05475	-8.17777	-2.75494

4.8. Compound 7-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.158666 A.U

C	0	3.59767	-0.04695
C	0.7844	2.40617	-0.11652
C	0.66905	1.45328	0.88931
C	-0.20772	1.63297	1.98927
C	-0.95432	2.85765	2.06831
C	-0.83586	3.80917	1.01796
C	-0.33692	0.66416	3.04523
C	-1.08571	1.01317	4.16146
C	-1.81745	2.2164	4.24193
C	-1.77024	3.11066	3.1995
C	0.33692	-0.66416	3.04523
C	0.20772	-1.63297	1.98927

C	0.95432	-2.85765	2.06831
C	1.77024	-3.11066	3.1995
C	1.81745	-2.2164	4.24193
C	1.08571	-1.01317	4.16146
C	-0.66905	-1.45328	0.88931
C	-0.7844	-2.40617	-0.11652
C	0	-3.59767	-0.04695
C	0.83586	-3.80917	1.01796
C	1.68037	2.20878	-1.20502
C	-1.68037	-2.20878	-1.20502
C	2.44216	2.05147	-2.14054
C	-2.44216	-2.05147	-2.14054
C	3.33872	1.85453	-3.2298
C	-3.33872	-1.85453	-3.2298
C	-4.1029	-0.67361	-3.32231
C	-4.97901	-0.48431	-4.3868
C	-5.10989	-1.46275	-5.37531
C	-4.35684	-2.6365	-5.29349
C	-3.47815	-2.83513	-4.23268
C	4.1029	0.67361	-3.32231
C	4.97901	0.48431	-4.3868
C	5.10989	1.46275	-5.37531
C	4.35684	2.6365	-5.29349
C	3.47815	2.83513	-4.23268
O	-1.17642	0.12953	5.22346
O	1.17642	-0.12953	5.22346
C	0	0	5.99807
H	0.08899	4.33252	-0.83981
H	1.27688	0.55962	0.83195
H	-1.41669	4.72545	1.08209
H	-2.4122	2.40181	5.13007
H	-2.33738	4.03626	3.24268
H	2.33738	-4.03626	3.24268
H	2.4122	-2.40181	5.13007
H	-1.27688	-0.55962	0.83195
H	-0.08899	-4.33252	-0.83981

H	1.41669	-4.72545	1.08209
H	-3.99749	0.0844	-2.5532
H	-5.56183	0.4302	-4.44618
H	-5.79435	-1.3114	-6.20465
H	-4.45477	-3.40004	-6.05965
H	-2.89163	-3.74561	-4.16603
H	3.99749	-0.0844	-2.5532
H	5.56183	-0.4302	-4.44618
H	5.79435	1.3114	-6.20465
H	4.45477	3.40004	-6.05965
H	2.89163	3.74561	-4.16603
H	-0.17281	-0.88651	6.61955
H	0.17281	0.88651	6.61955

4.9. Compound 7,6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -2187.434996 A.U

C	0.06123	3.60283	0.95779
C	-0.74683	2.40587	0.90212
C	-0.64182	1.46234	1.91393
C	0.23181	1.62765	3.01821
C	0.99096	2.84441	3.09626
C	0.89382	3.79125	2.04864
C	0.34523	0.65984	4.07456
C	1.09689	1.00143	5.19214
C	1.8429	2.19654	5.27216
C	1.80849	3.09055	4.22999
C	-0.34523	-0.65984	4.07456
C	-0.23181	-1.62765	3.01821
C	-0.99096	-2.84441	3.09626
C	-1.80849	-3.09055	4.22999
C	-1.8429	-2.19654	5.27216

C	-1.09689	-1.00143	5.19214
C	0.64182	-1.46234	1.91393
C	0.74683	-2.40587	0.90212
C	-0.06123	-3.60283	0.95779
C	-0.89382	-3.79125	2.04864
O	1.17745	0.11826	6.25413
O	-1.17745	-0.11826	6.25413
C	0	0	7.02928
C	0	4.56742	-0.08433
C	-1.65489	2.20339	-0.17268
C	1.65489	-2.20339	-0.17268
C	0	-4.56742	-0.08433
C	-0.0424	5.38694	-0.98213
C	-2.43764	2.03166	-1.08755
C	2.43764	-2.03166	-1.08755
C	0.0424	-5.38694	-0.98213
C	-0.10163	6.3304	-2.04766
C	-3.35307	1.84649	-2.16306
C	3.35307	-1.84649	-2.16306
C	0.10163	-6.3304	-2.04766
C	0.42231	7.62921	-1.89078
C	0.35846	8.54456	-2.93736
C	-0.22458	8.18449	-4.15465
C	-0.74505	6.89874	-4.32131
C	-0.68658	5.9763	-3.28077
C	-3.77533	2.94642	-2.93745
C	-4.66832	2.76367	-3.98927
C	-5.1548	1.4885	-4.28768
C	-4.74339	0.39253	-3.52541
C	-3.85132	0.56475	-2.47096
C	3.85132	-0.56475	-2.47096
C	4.74339	-0.39253	-3.52541
C	5.1548	-1.4885	-4.28768
C	4.66832	-2.76367	-3.98927
C	3.77533	-2.94642	-2.93745
C	0.68658	-5.9763	-3.28077

C	0.74505	-6.89874	-4.32131
C	0.22458	-8.18449	-4.15465
C	-0.35846	-8.54456	-2.93736
C	-0.42231	-7.62921	-1.89078
H	-1.26544	0.57962	1.85684
H	1.48713	4.69851	2.10759
H	2.43865	2.37537	6.16092
H	2.38622	4.00937	4.27268
H	-2.38622	-4.00937	4.27268
H	-2.43865	-2.37537	6.16092
H	1.26544	-0.57962	1.85684
H	-1.48713	-4.69851	2.10759
H	0.16419	-0.8882	7.65046
H	-0.16419	0.8882	7.65046
H	0.87361	7.9059	-0.94357
H	0.76496	9.54271	-2.80323
H	-0.27226	8.90137	-4.96889
H	-1.19666	6.6132	-5.26687
H	-1.08382	4.97449	-3.40769
H	-3.39995	3.93586	-2.69711
H	-4.98783	3.61911	-4.57728
H	-5.85124	1.34974	-5.10925
H	-5.1187	-0.60063	-3.75385
H	-3.52751	-0.28439	-1.87825
H	3.52751	0.28439	-1.87825
H	5.1187	0.60063	-3.75385
H	5.85124	-1.34974	-5.10925
H	4.98783	-3.61911	-4.57728
H	3.39995	-3.93586	-2.69711
H	1.08382	-4.97449	-3.40769
H	1.19666	-6.6132	-5.26687
H	0.27226	-8.90137	-4.96889
H	-0.76496	-9.54271	-2.80323
H	-0.87361	-7.9059	-0.94357

4.10. Compound 8-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -1573.137762 A.U

C	-3.4496	-1.19491	-1.68209
C	-2.67994	-0.02106	-1.70659
C	-1.75742	0.28403	-0.70418
C	-1.53965	-0.65275	0.37296
C	-2.41117	-1.79698	0.42969
C	-3.33584	-2.0534	-0.61465
C	-0.54824	-0.50622	1.40381
C	-0.62242	-1.34234	2.51229
C	-1.51509	-2.42779	2.59633
C	-2.36376	-2.67225	1.54689
C	0.54824	0.50622	1.40381
C	0.62242	1.34234	2.51229
C	1.51509	2.42779	2.59633
C	2.36376	2.67225	1.54689
C	2.41117	1.79698	0.42969
C	1.53965	0.65275	0.37296
C	3.33584	2.0534	-0.61465
C	3.4496	1.19491	-1.68209
C	2.67994	0.02106	-1.70659
C	1.75742	-0.28403	-0.70418
C	-1.17724	1.58515	-0.78524
C	1.17724	-1.58515	-0.78524
C	-0.85596	2.74274	-0.98433
C	0.85596	-2.74274	-0.98433
C	-0.48235	4.09743	-1.2188
C	0.48235	-4.09743	-1.2188
C	0	4.91189	-0.17422
C	0.34678	6.23764	-0.41894
C	0.22214	6.77695	-1.70151
C	-0.25555	5.97901	-2.74385

C	-0.6069	4.65303	-2.50897
C	0	-4.91189	-0.17422
C	-0.34678	-6.23764	-0.41894
C	-0.22214	-6.77695	-1.70151
C	0.25555	-5.97901	-2.74385
C	0.6069	-4.65303	-2.50897
O	-0.25727	1.15358	3.56508
O	0.25727	-1.15358	3.56508
C	0	0	4.34216
H	-4.15368	-1.39509	-2.48367
H	-2.82105	0.69932	-2.50518
H	-3.95781	-2.94156	-0.54711
H	-1.48987	-3.05739	3.47952
H	-3.03588	-3.52527	1.56701
H	1.48987	3.05739	3.47952
H	3.03588	3.52527	1.56701
H	3.95781	2.94156	-0.54711
H	4.15368	1.39509	-2.48367
H	2.82105	-0.69932	-2.50518
H	0.09898	4.48882	0.81901
H	0.71512	6.85444	0.39591
H	0.49411	7.81179	-1.8873
H	-0.35564	6.39185	-3.74351
H	-0.97877	4.03133	-3.31691
H	-0.09898	-4.48882	0.81901
H	-0.71512	-6.85444	0.39591
H	-0.49411	-7.81179	-1.8873
H	0.35564	-6.39185	-3.74351
H	0.97877	-4.03133	-3.31691
H	-0.89496	-0.12357	4.96342
H	0.89496	0.12357	4.96342

4.11. Compound 3,4,6-PE

Method: B3LYP/6-31+G (d,p) level of theory,

Key word: opt freq b3lyp/6-31g(d,p) geom=connectivity

imaginary frequencies: 0,

Sum of electronic and zero-point Energies: -2801.710889 A.U

C	-1.14865	3.38253	-2.71144
C	-1.5103	2.00337	-2.73724
C	-1.10717	1.15439	-1.73734
C	-0.32143	1.61034	-0.64245
C	0	3.00662	-0.5827
C	-0.40806	3.85734	-1.63625
C	0.11198	0.73657	0.40992
C	0.71789	1.29594	1.52376
C	1.03413	2.67988	1.62481
C	0.71071	3.53157	0.55279
C	-0.11198	-0.73657	0.40992
C	0.32143	-1.61034	-0.64245
C	0	-3.00662	-0.5827
C	-0.71071	-3.53157	0.55279
C	-1.03413	-2.67988	1.62481
C	-0.71789	-1.29594	1.52376
C	1.10717	-1.15439	-1.73734
C	1.5103	-2.00337	-2.73724
C	1.14865	-3.38253	-2.71144
C	0.40806	-3.85734	-1.63625
C	-1.5565	4.25004	-3.7633
C	1.5565	-4.25004	-3.7633
C	1.06469	4.90266	0.614
C	-1.06469	-4.90266	0.614
O	1.07953	0.47749	2.57288
O	-1.07953	-0.47749	2.57288
C	1.38569	6.0756	0.67415
C	-1.91059	4.9788	-4.67106
C	1.91059	-4.9788	-4.67106
C	-1.38569	-6.0756	0.67415
C	-2.32292	5.83543	-5.73194
C	2.32292	-5.83543	-5.73194
C	1.78418	7.43871	0.77211
C	-1.78418	-7.43871	0.77211

C	-3.11385	5.33918	-6.78795
C	-3.51426	6.17984	-7.82224
C	-3.13619	7.52466	-7.82467
C	-2.35224	8.0267	-6.78309
C	-1.94702	7.19393	-5.74433
C	1.94702	-7.19393	-5.74433
C	2.35224	-8.0267	-6.78309
C	3.13619	-7.52466	-7.82467
C	3.51426	-6.17984	-7.82224
C	3.11385	-5.33918	-6.78795
C	2.75779	7.82727	1.71567
C	3.14803	9.15936	1.81381
C	2.57921	10.12437	0.97877
C	1.61504	9.74934	0.04003
C	1.21823	8.41971	-0.06687
C	-1.21823	-8.41971	-0.06687
C	-1.61504	-9.74934	0.04003
C	-2.57921	-10.12437	0.97877
C	-3.14803	-9.15936	1.81381
C	-2.75779	-7.82727	1.71567
C	0	0	3.3558
C	1.66536	3.16701	2.79827
C	2.18961	3.58819	3.81176
C	2.80453	4.08504	4.99608
C	3.45237	3.20729	5.88863
C	4.05245	3.69787	7.04456
C	4.01698	5.06457	7.3321
C	3.37556	5.94263	6.45495
C	2.77301	5.46232	5.29589
C	-1.66536	-3.16701	2.79827
C	-2.18961	-3.58819	3.81176
C	-2.80453	-4.08504	4.99608
C	-2.77301	-5.46232	5.29589
C	-3.37556	-5.94263	6.45495
C	-4.01698	-5.06457	7.3321
C	-4.05245	-3.69787	7.04456

C	-3.45237	-3.20729	5.88863
H	-2.11486	1.63374	-3.55857
H	-1.4027	0.11315	-1.77305
H	-0.14385	4.90703	-1.58919
H	1.4027	-0.11315	-1.77305
H	2.11486	-1.63374	-3.55857
H	0.14385	-4.90703	-1.58919
H	-3.40583	4.29417	-6.78291
H	-4.12364	5.78471	-8.6297
H	-3.45049	8.17748	-8.63348
H	-2.05545	9.07142	-6.78069
H	-1.33755	7.58017	-4.93396
H	1.33755	-7.58017	-4.93396
H	2.05545	-9.07142	-6.78069
H	3.45049	-8.17748	-8.63348
H	4.12364	-5.78471	-8.6297
H	3.40583	-4.29417	-6.78291
H	3.2013	7.07278	2.35712
H	3.90038	9.44602	2.54265
H	2.88632	11.16284	1.0585
H	1.17066	10.49621	-0.61116
H	0.46813	8.12585	-0.79379
H	-0.46813	-8.12585	-0.79379
H	-1.17066	-10.49621	-0.61116
H	-2.88632	-11.16284	1.0585
H	-3.90038	-9.44602	2.54265
H	-3.2013	-7.07278	2.35712
H	-0.42998	0.79517	3.97358
H	0.42998	-0.79517	3.97358
H	3.47892	2.14716	5.65916
H	4.55016	3.01201	7.72375
H	4.48619	5.44322	8.23523
H	3.34317	7.00539	6.67629
H	2.26792	6.13956	4.61483
H	-2.26792	-6.13956	4.61483
H	-3.34317	-7.00539	6.67629

H	-4.48619	-5.44322	8.23523
H	-4.55016	-3.01201	7.72375
H	-3.47892	-2.14716	5.65916

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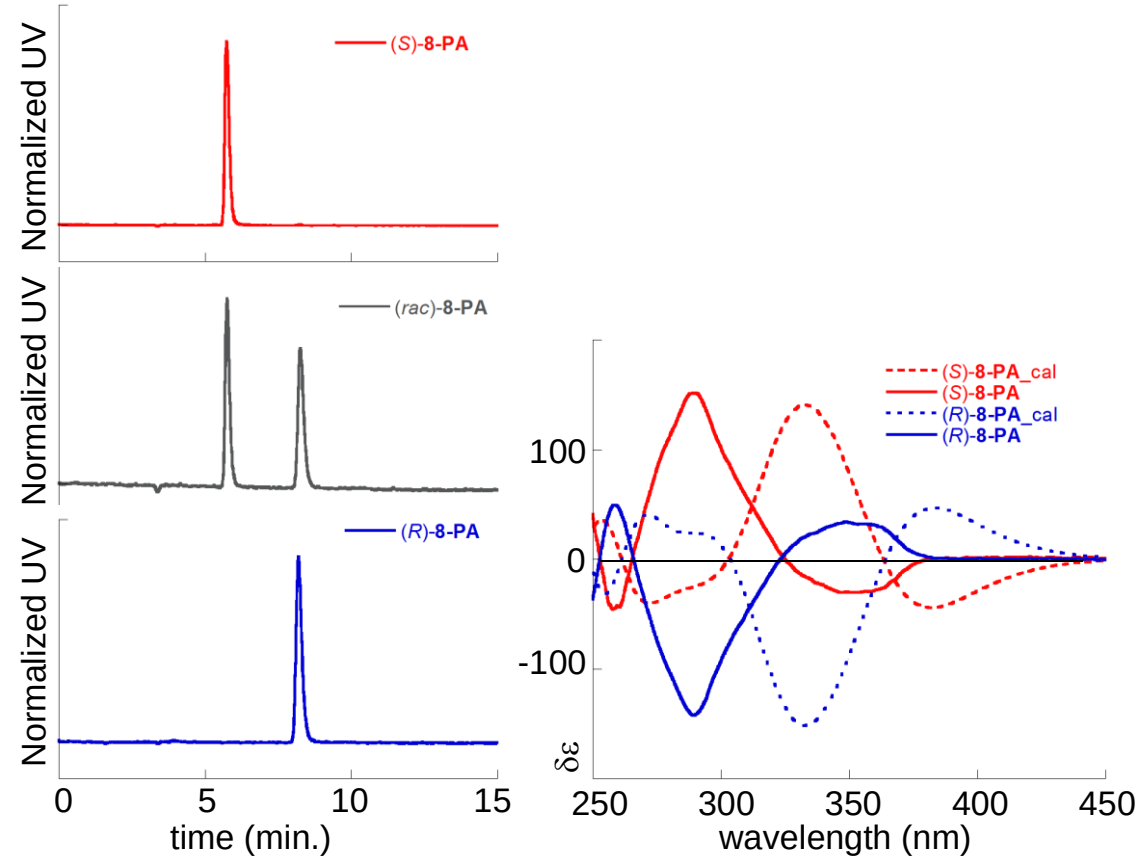
5. Optical resolution of 8-PE



Conditions; Hexane:IPA=90:10, 1.0 ml/min., 30 °C, CHIRALPAK IB, 3.4 MPa

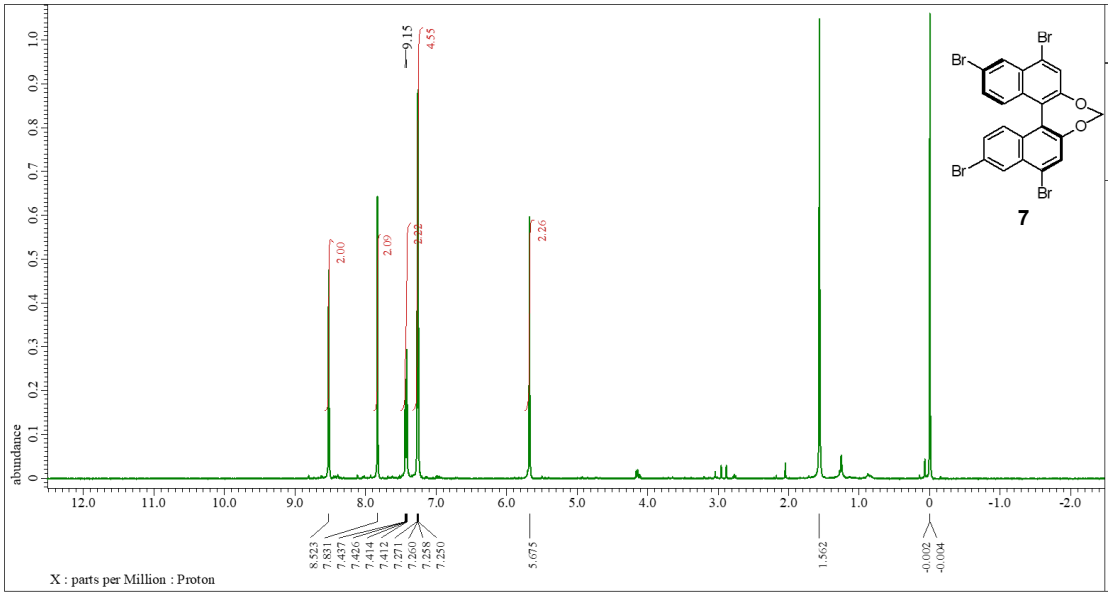
Conditions; $CHCl_3$, 1.0×10^{-5} M, 25 °C
DFT calculation at the B3LYP/6-31G+(d,p)

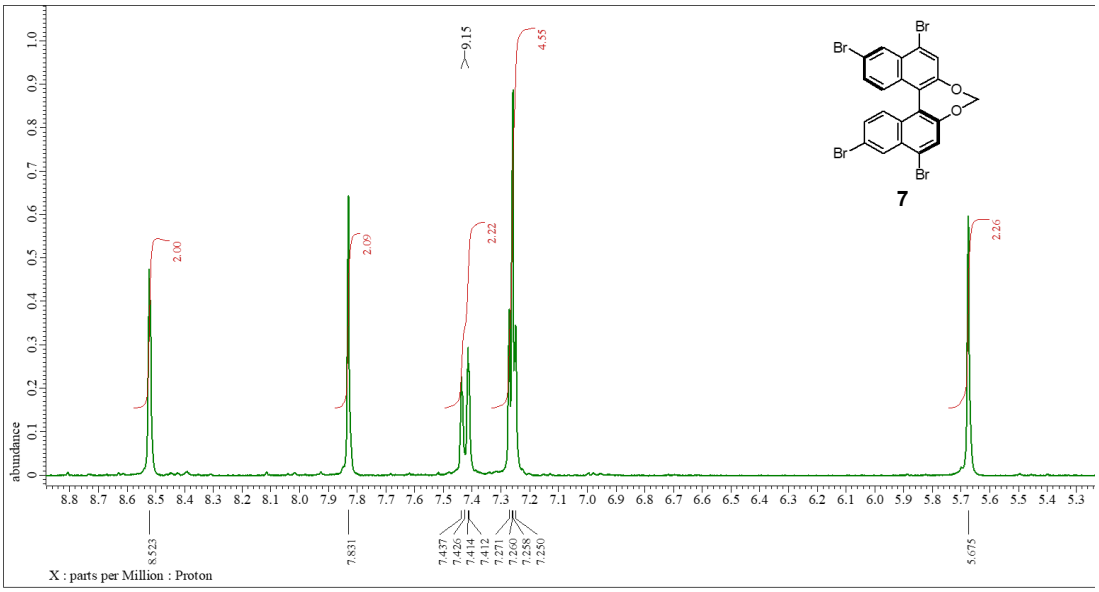
Figure S1. Optical resolution of **8-PE**

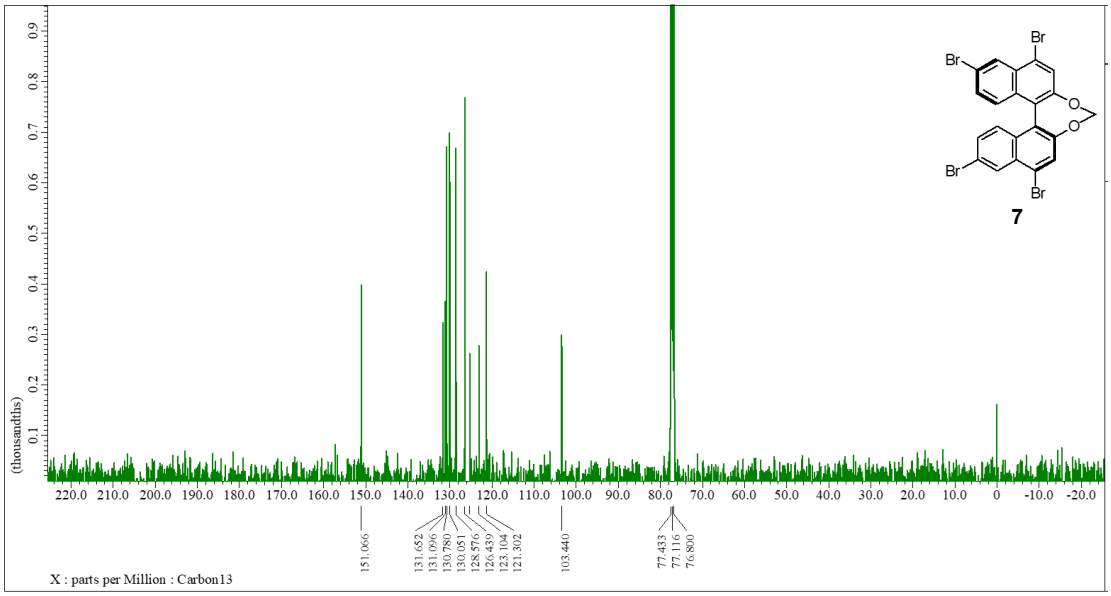
Conditions; CHIRALPAK IB (*n*-hexane/*iso*-propanol =90/10, flow rate = 1.0 mL/min, λ = 254 nm, pressure = 3.4 MPa, temp.= 303 K), (*S*)-**8-PE** (fraction 1, tR=5.8 min.), and (*R*)-**8-PE** (fraction 2, tR=8.3 min.), 100%ee.

6. ^{1}H and ^{13}C NMR spectra for all new compounds

Conditions: ^{1}H (400 MHz) and ^{13}C NMR (100 MHz), $CDCl_3$.



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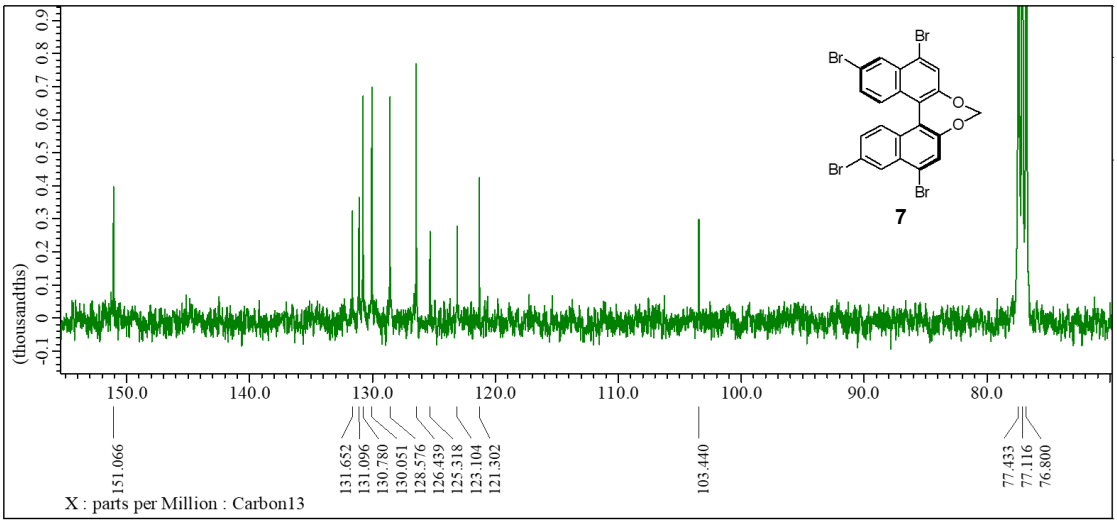
0.7
0.6
0.5
0.4
0.3
0.2
0.1
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
151.066
131.652
131.096
130.780
130.051
128.576
126.439
123.104
121.302
103.440
77.433
77.116
76.800
X : parts per Million : Carbon13
Br
Br
Br
Br
O
O
7


(thousandths)
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0.5
0.4
0.3
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0.1
0
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150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0
151.066
131.652
131.096
130.780
130.051
128.576
126.439
125.318
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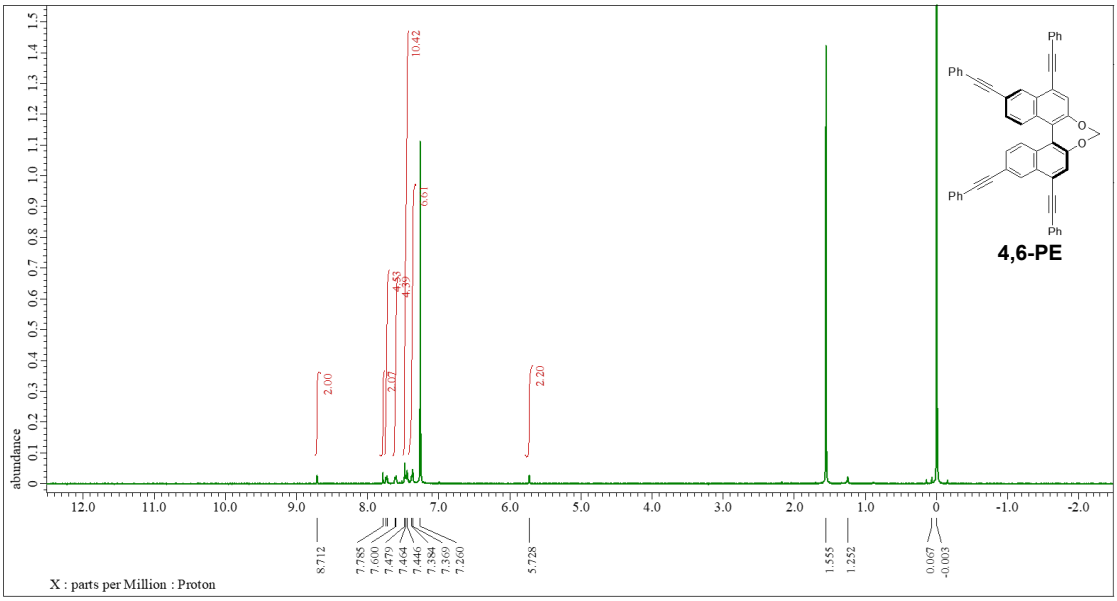
Br
Br
Br
O
O
7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4.53
4.39
2.20
2.00
2.07
Ph
Ph
Ph
Ph
O
O
4,6-PE
8.712
7.785
7.600
7.479
7.464
7.446
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5.728
1.555
1.252
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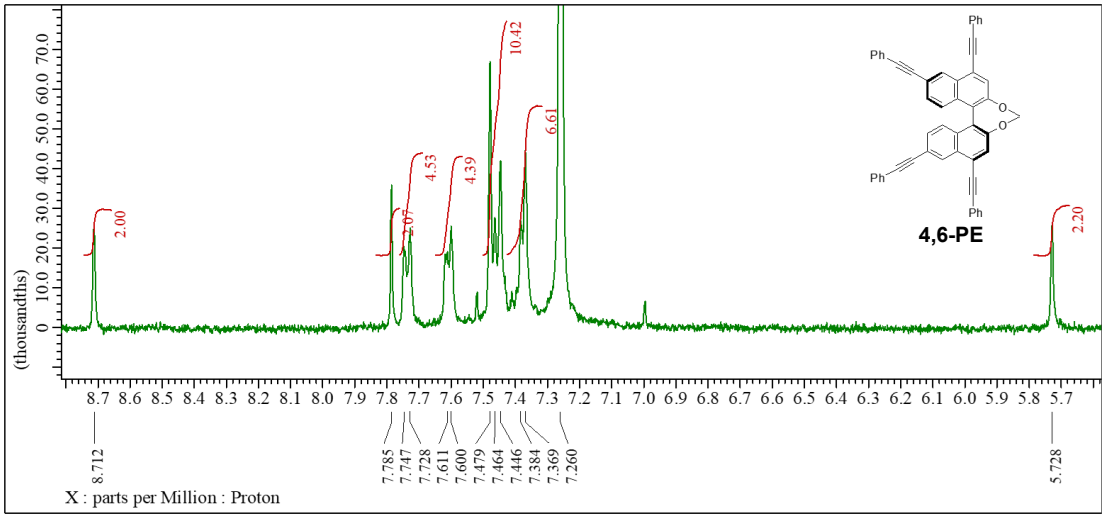
X : parts per Million : Proton


(thousandths)
10.42
6.61
4.53
4.39
2.20
2.00
2.07
Ph
Ph
Ph
Ph
O
O
4,6-PE
8.712
7.785
7.747
7.728
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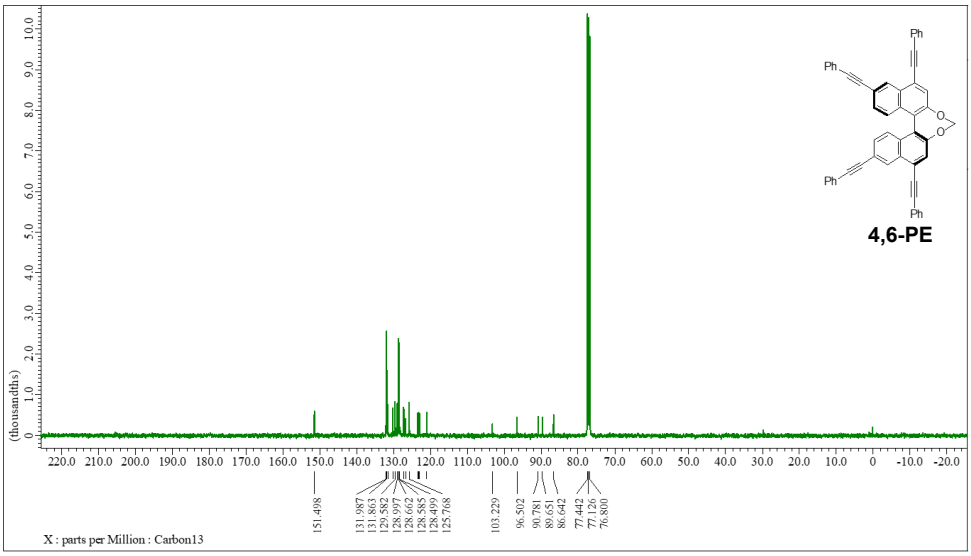
7.600
7.479
7.464
7.446
7.384
7.369
7.260
5.728
X : parts per Million : Proton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Ph
Ph
Ph
O
O
4,6-PE
(thousandths)
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8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
151.498
131.987
131.863
129.582
128.997
128.662
128.585
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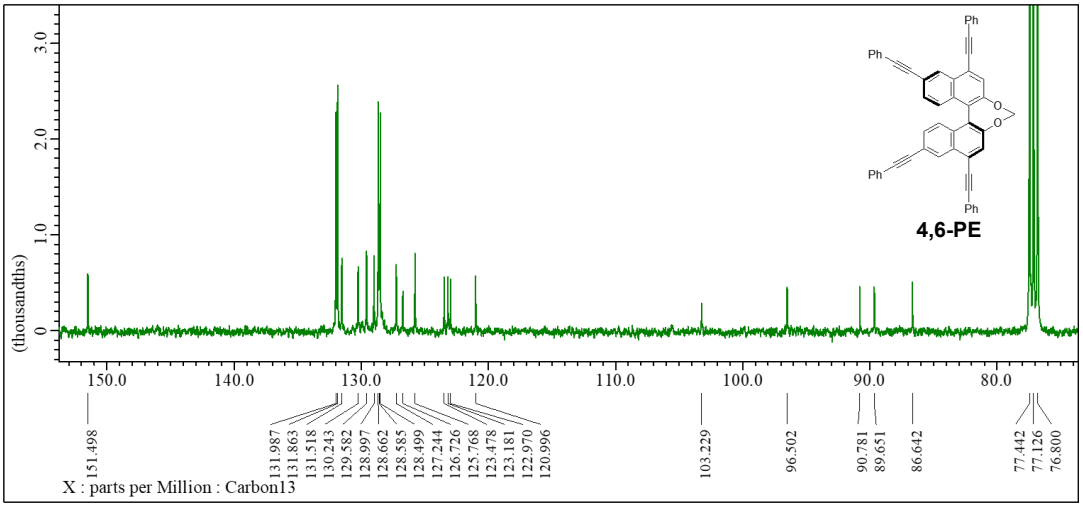
X : parts per Million : Carbon13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Ph
Ph
Ph
O
O
4,6-PE
(thousandths)
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2.0
1.0
0
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131.863
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130.243
129.582
128.997
128.662
128.585
128.499
127.244
126.726
125.768
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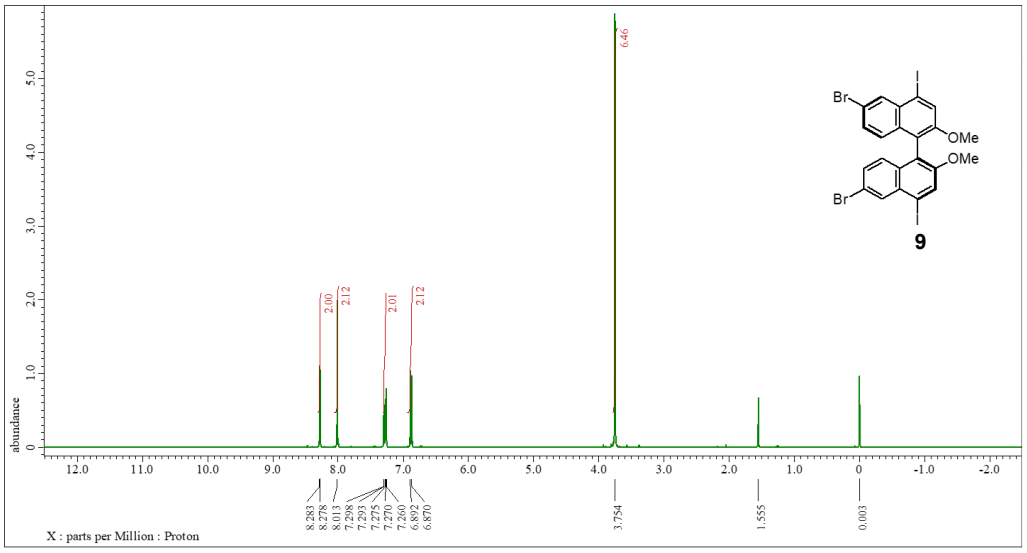
76.800
X : parts per Million : Carbon13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2.01
2.12
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OMe
OMe
Br
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8.278
8.013
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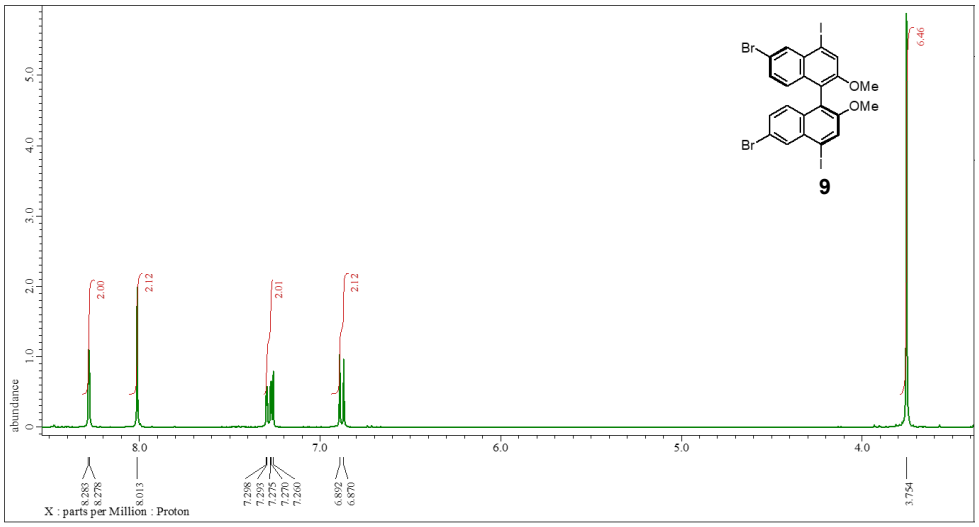
7.293
7.275
7.270
7.260
6.892
6.870
3.754
1.555
0.003
X : parts per Million : Proton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2.00
2.12
2.01
2.12
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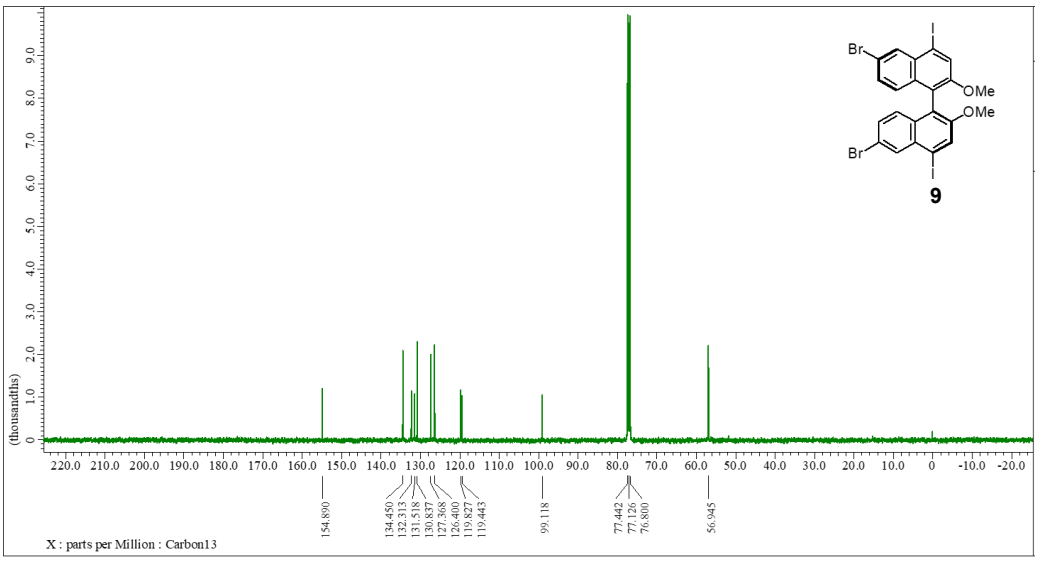
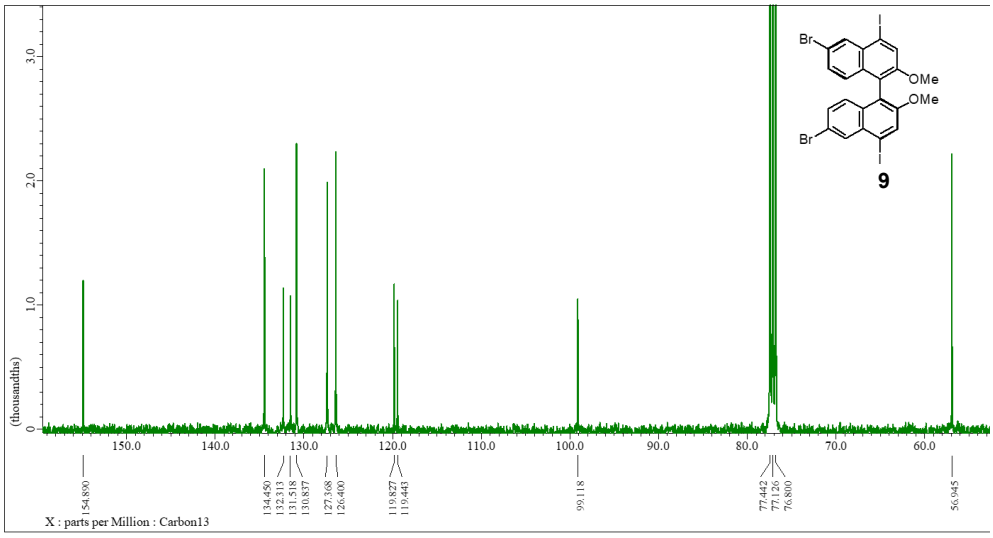
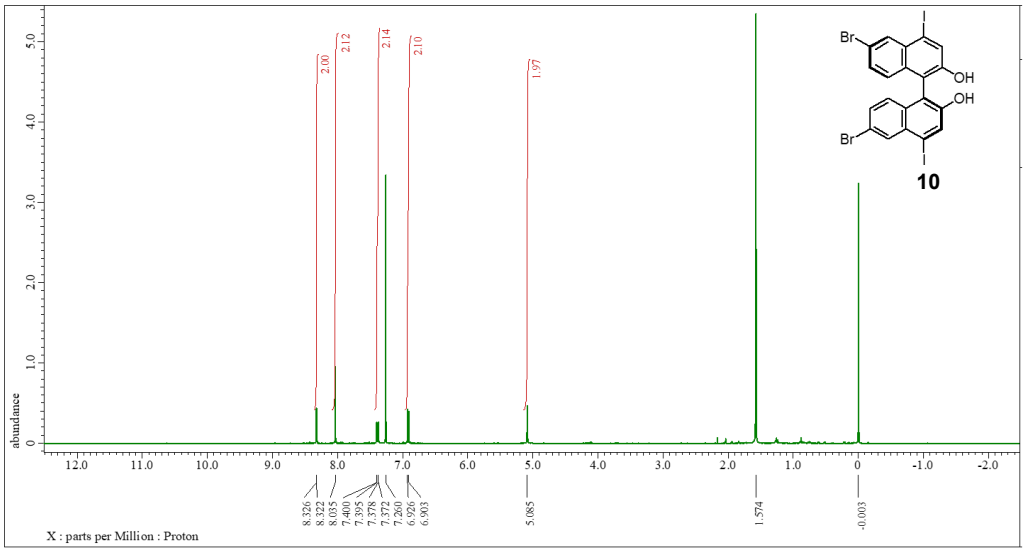
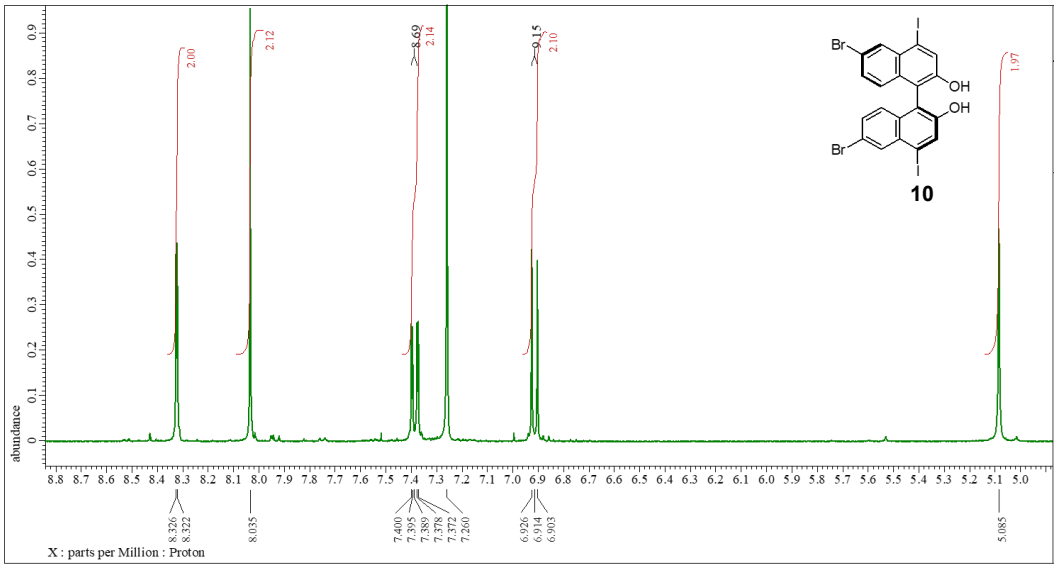
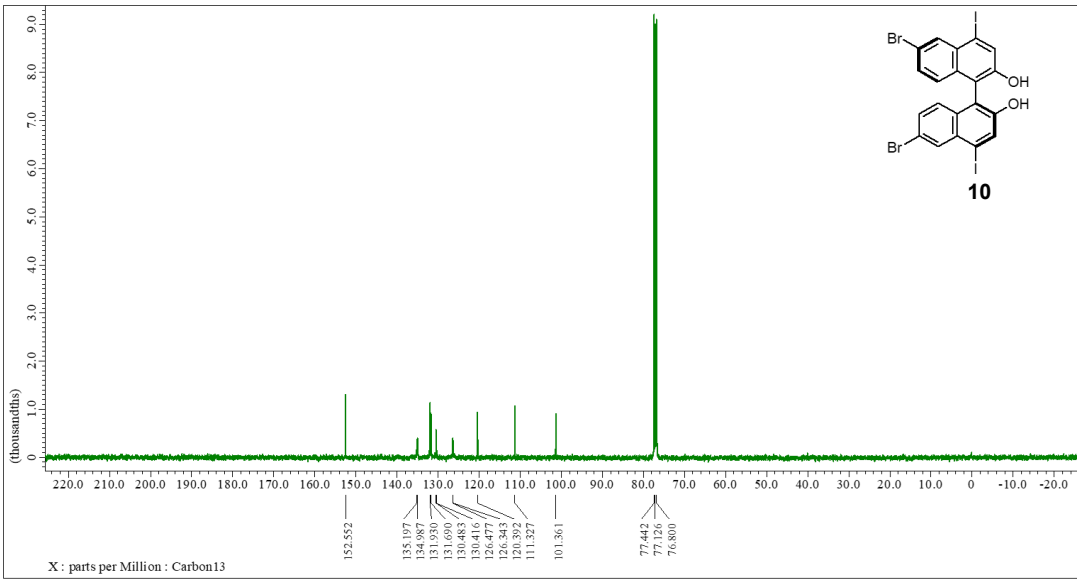
OMe
OMe
Br
9
8.283
8.278
8.013
7.298
7.293
7.275
7.270
7.260
6.892
6.870
3.754
X : parts per Million : Proton

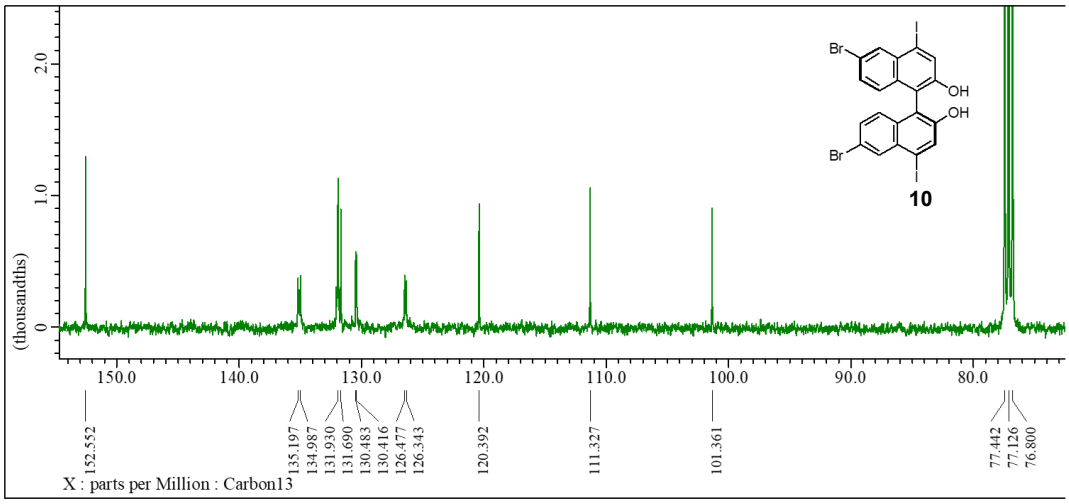

(thousandths)
X : parts per Million : Carbon13
154.890
134.450
132.313
131.518
130.837
127.368
126.400
119.827
119.443
99.118
77.442
77.126
76.800
56.945
Br
OMe
OMe
Br
9

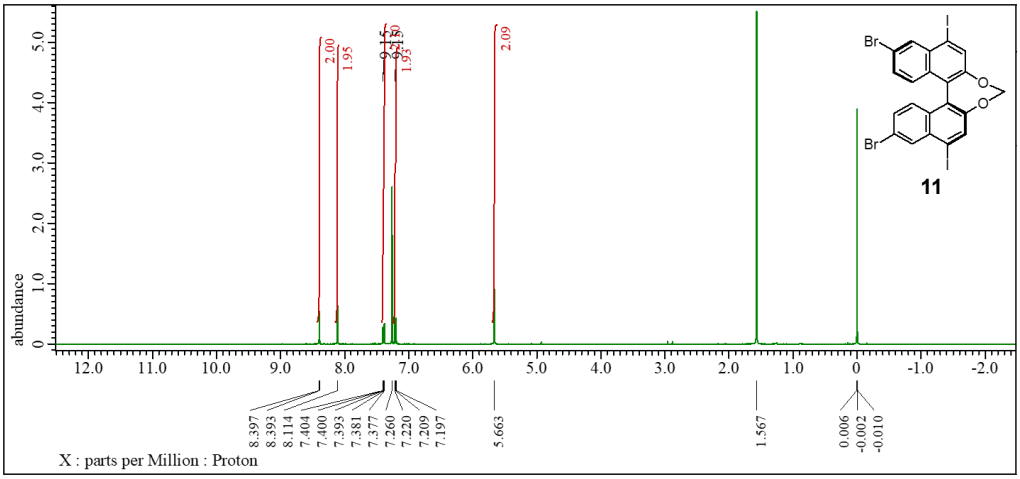

(thousandths)
X : parts per Million : Carbon13
154.890
134.450
132.313
131.518
130.837
127.368
126.400
119.827
119.443
99.118
77.442
77.126
76.800
56.945
Br
OMe
OMe
Br
9

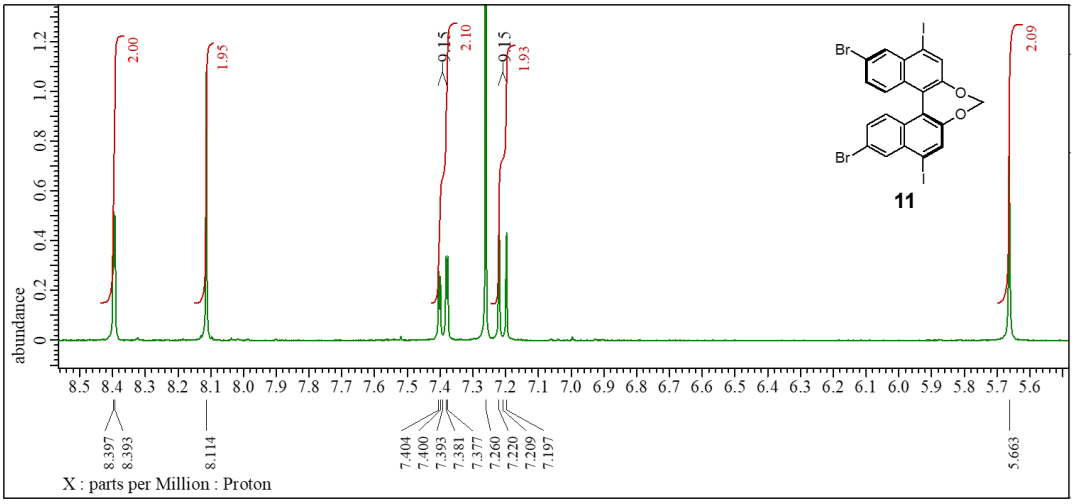

abundance
X : parts per Million : Proton
2.00
2.12
2.14
2.10
1.97
8.326
8.322
8.035
7.400
7.395
7.378
7.372
7.260
6.926
6.903
5.085
1.574
-0.003
Br
OH
OH
Br
10

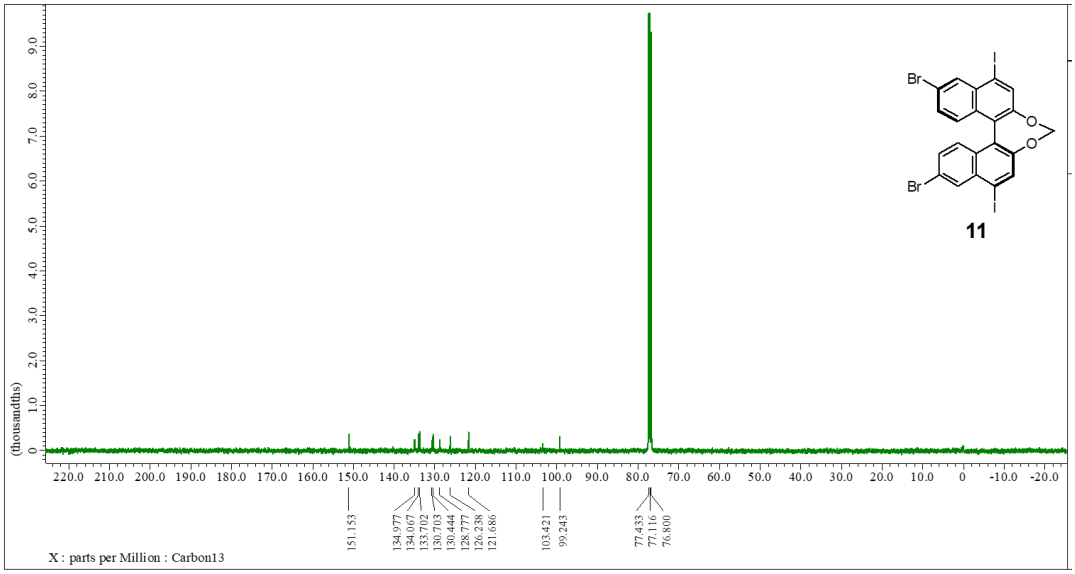

abundance
X : parts per Million : Proton
2.00
2.12
8.69
2.14
9.15
2.10
1.97
8.326
8.322
8.035
7.400
7.395
7.389
7.378
7.372
7.260
6.926
6.914
6.903
5.085
Br
OH
OH
Br
10

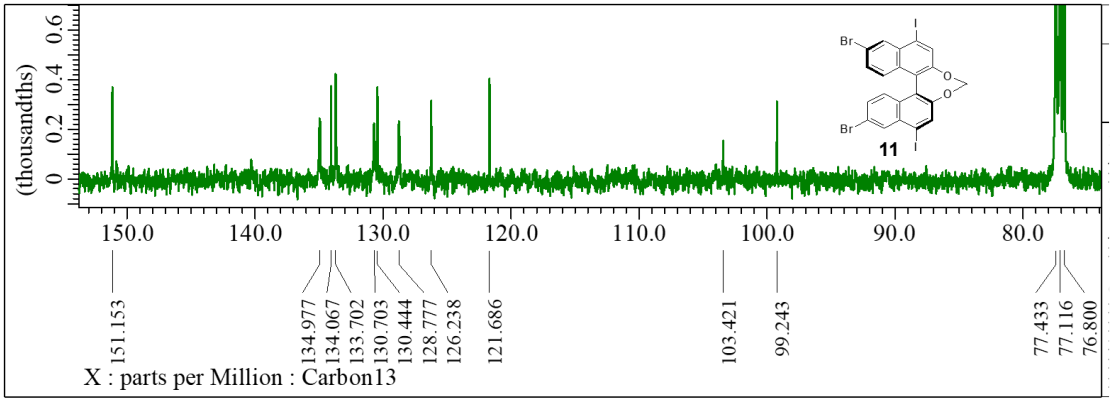

Br
OH
OH
Br
10
(thousandths)
X : parts per Million : Carbon13
152.552
135.197
134.987
131.930
131.690
130.483
130.416
126.477
126.343
120.392
111.327
101.361
77.442
77.126
76.800

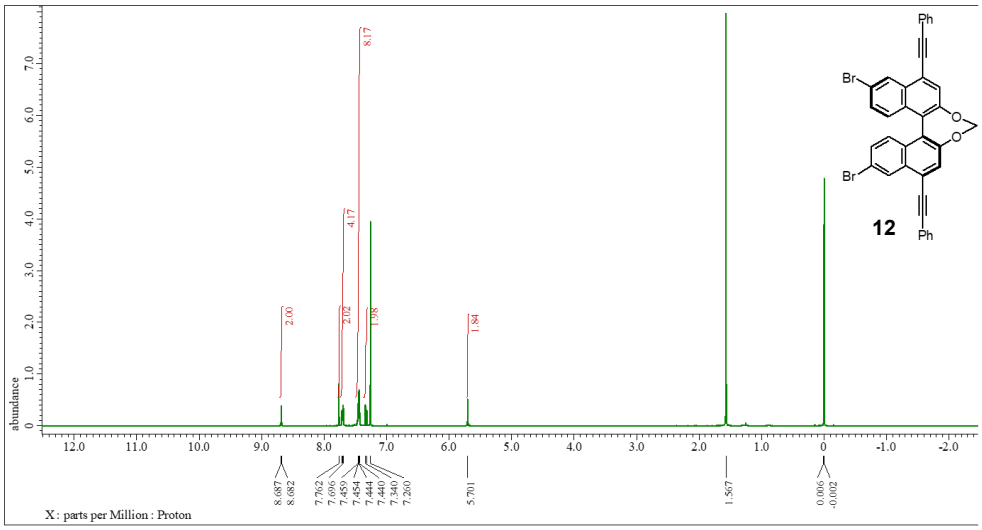

Br
OH
OH
Br
10
(thousandths)
X : parts per Million : Carbon13
152.552
135.197
134.987
131.930
131.690
130.483
130.416
126.477
126.343
120.392
111.327
101.361
77.442
77.126
76.800

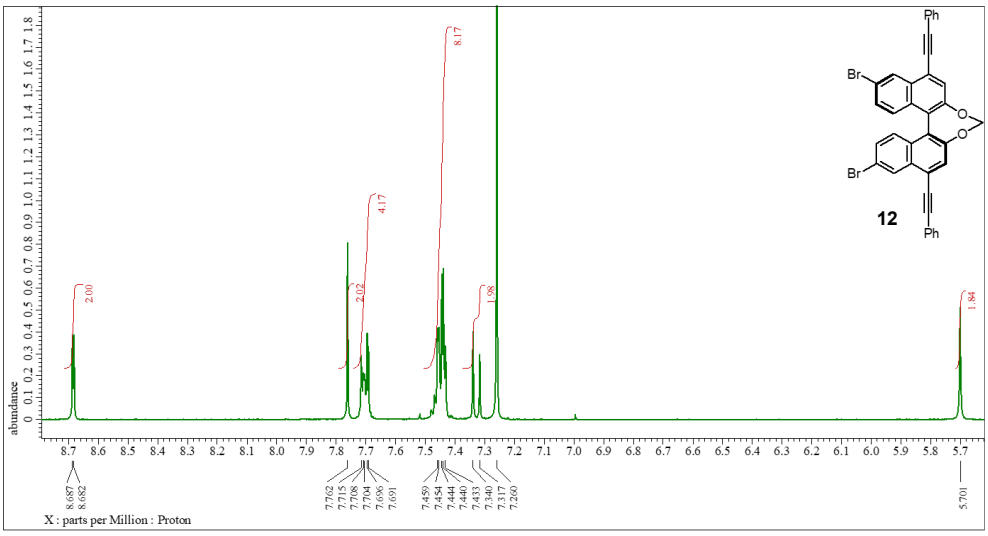

abundance
X : parts per Million : Proton
11

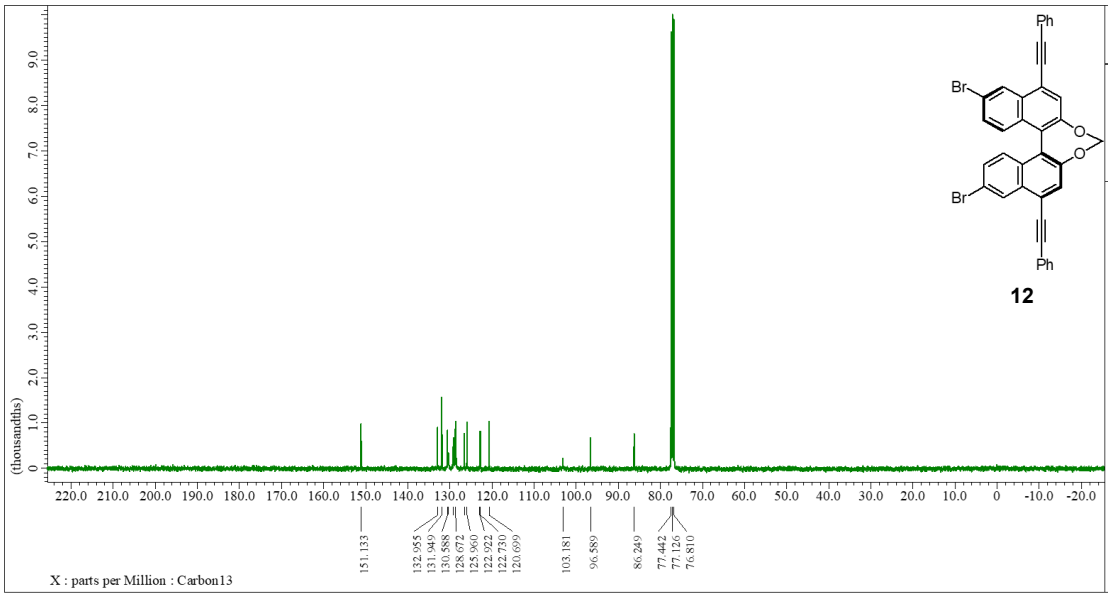

abundance
X : parts per Million : Proton
11

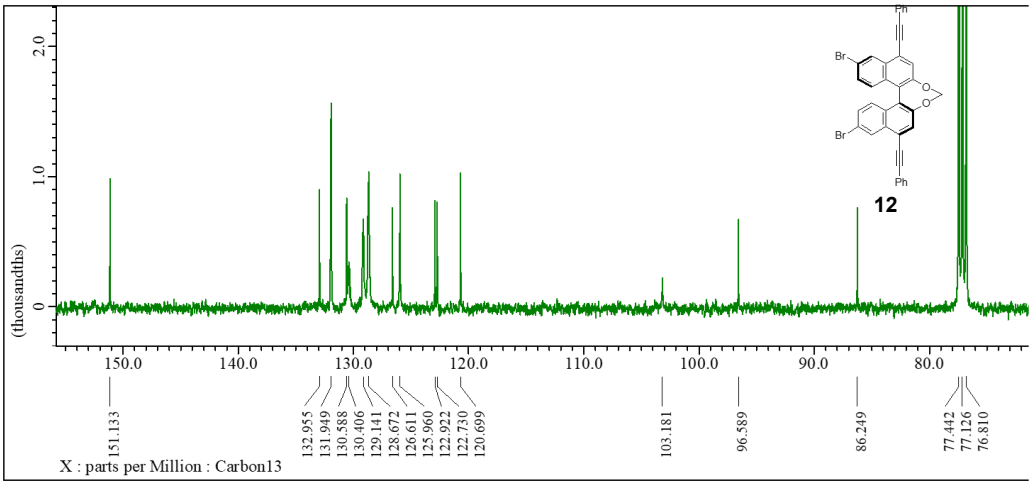

(thousandths)
X : parts per Million : Carbon13
151.153
134.977
134.067
133.702
130.703
130.444
128.777
126.238
121.686
103.421
99.243
77.433
77.116
76.800
Br
Br
O
O
11

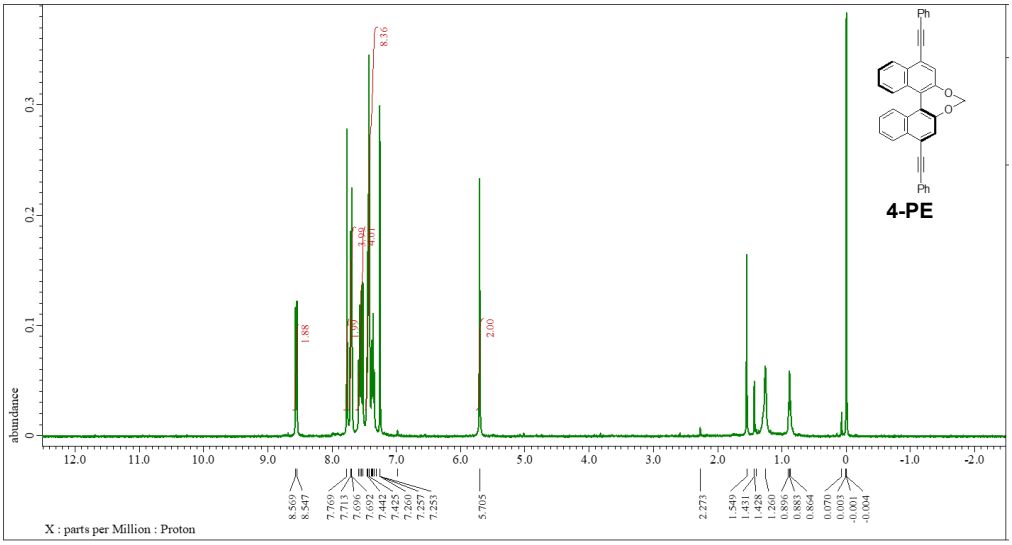

(thousandths)
X : parts per Million : Carbon13
151.153
134.977
134.067
133.702
130.703
130.444
128.777
126.238
121.686
103.421
99.243
77.433
77.116
76.800
Br
Br
O
O
11

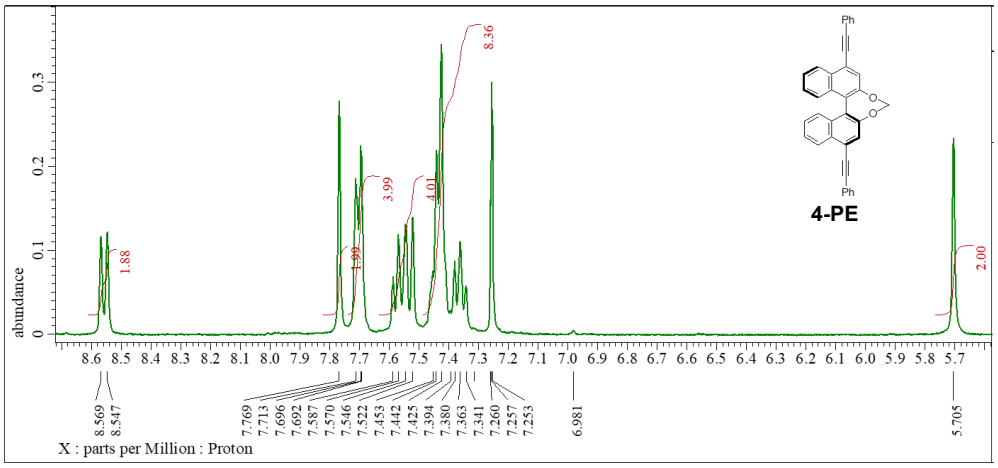

Ph
Br
O
O
Br
Ph
12
abundance
X : parts per Million : Proton

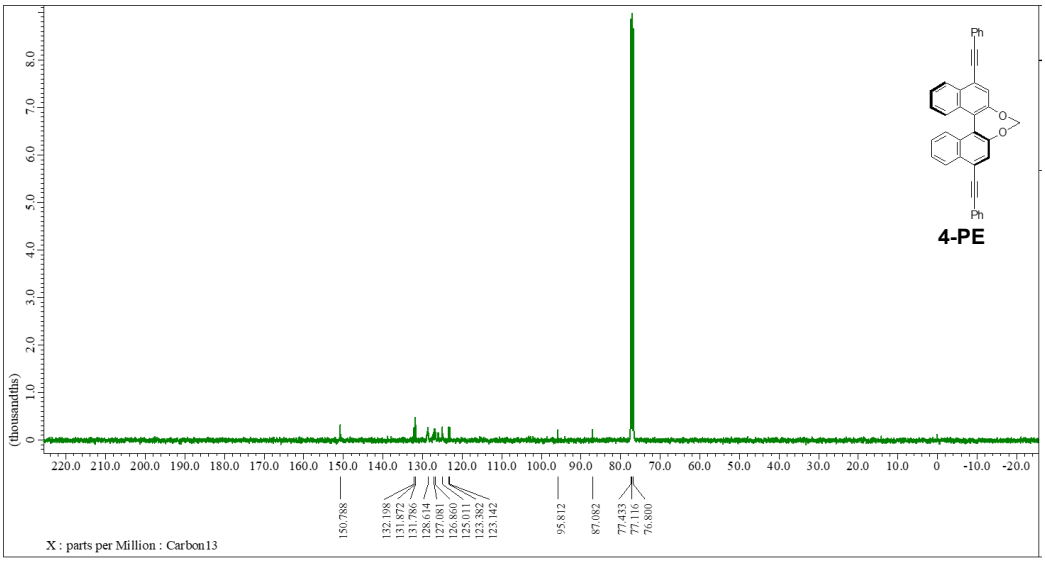

Ph
Br
O
O
Br
Ph
12
abundance
X : parts per Million : Proton

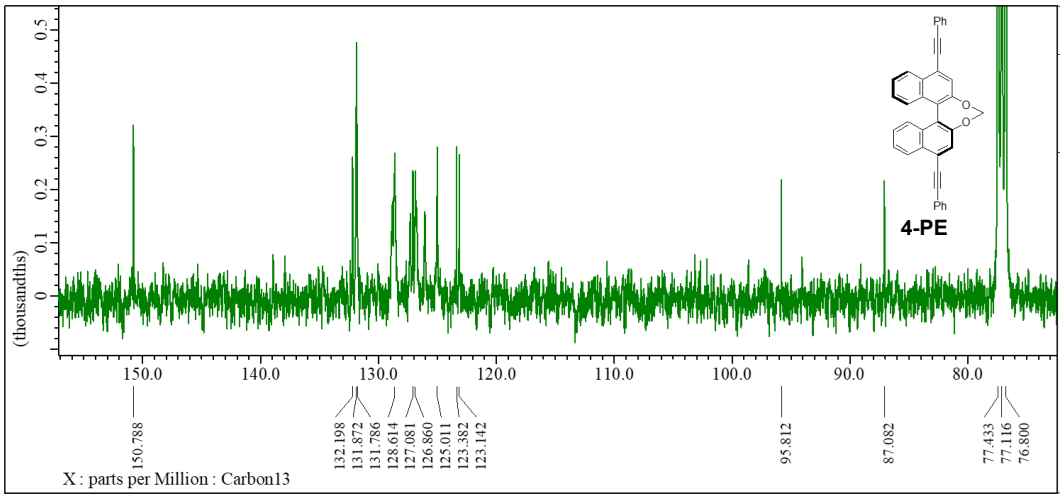

Ph
Br
Br
Ph
12
(thousandths)
X : parts per Million : Carbon13
151.133
132.955
131.949
130.588
128.672
125.960
122.922
122.730
120.699
103.181
96.589
86.249
77.442
77.126
76.810

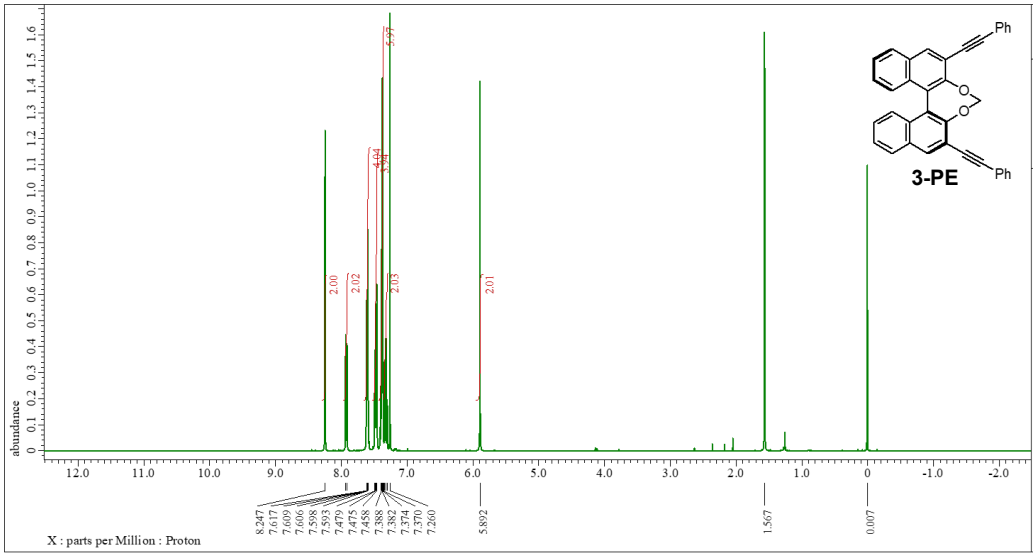

Ph
Br
Br
Ph
12
(thousandths)
X : parts per Million : Carbon13
151.133
132.955
131.949
130.588
130.406
129.141
128.672
126.611
125.960
122.922
122.730
120.699
103.181
96.589
86.249
77.442
77.126
76.810

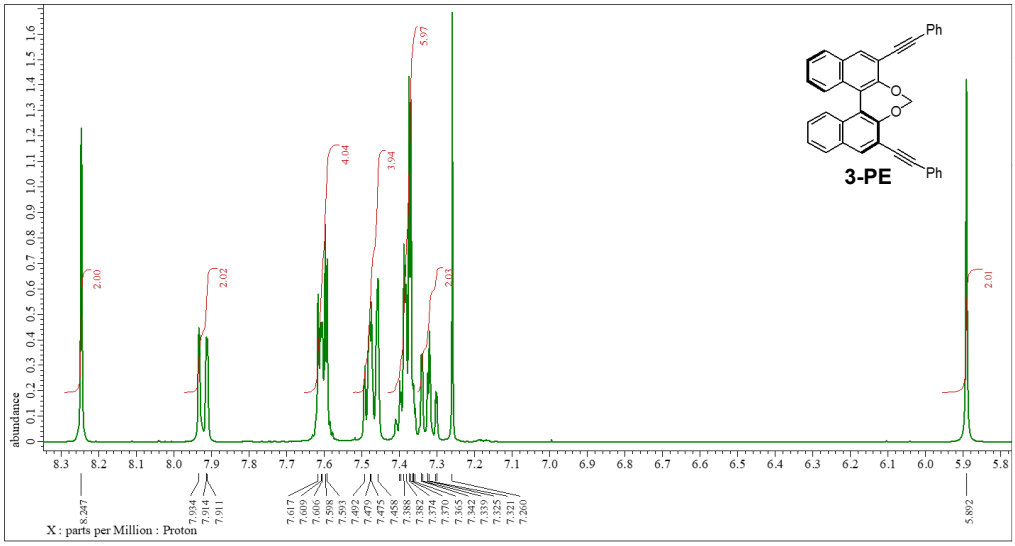

Ph
Ph
4-PE
abundance
X : parts per Million : Proton

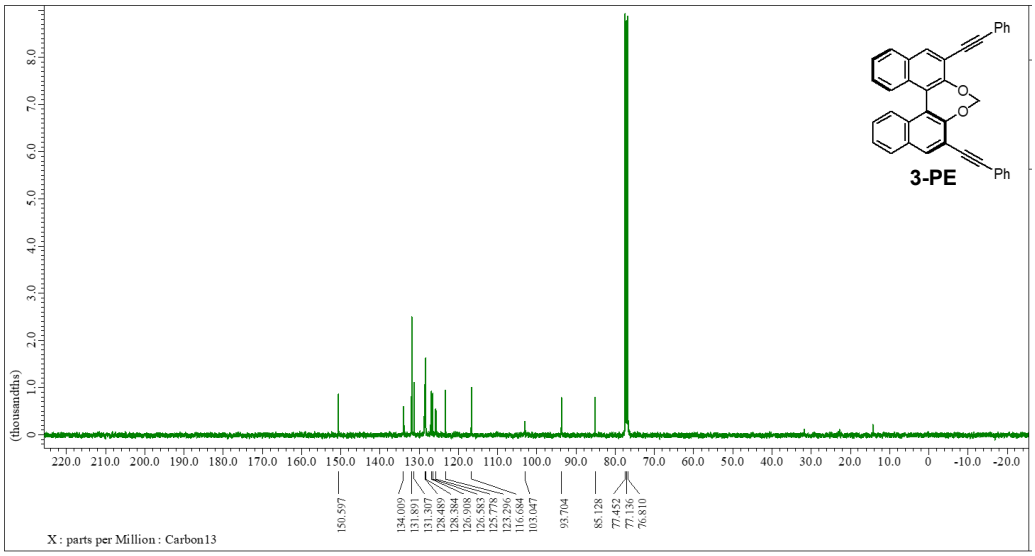

Ph
Ph
4-PE
abundance
X : parts per Million : Proton

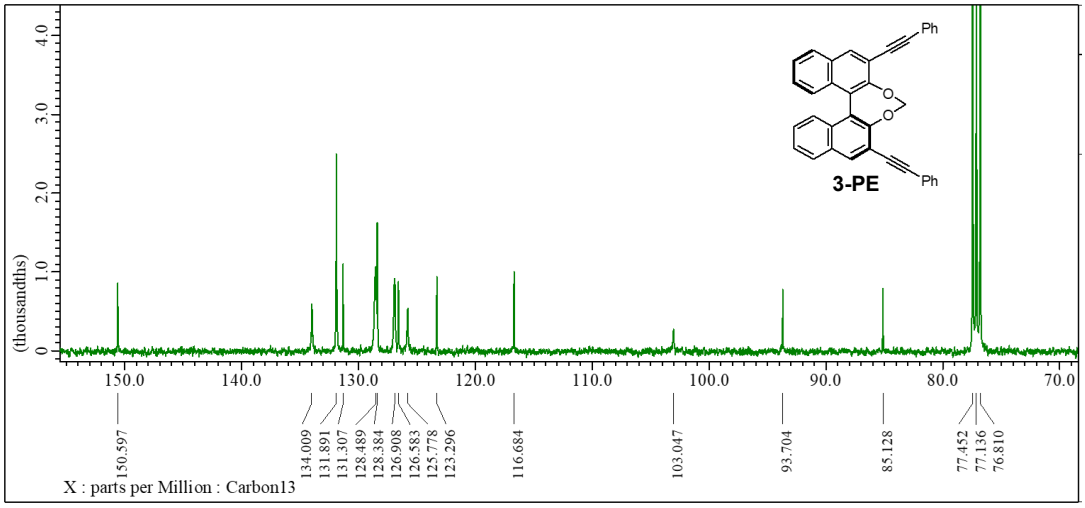

Ph
O
O
Ph
4-PE
(thousandths)
X : parts per Million : Carbon13
150.788
132.198
131.872
131.786
128.614
127.081
126.860
125.011
123.382
123.142
95.812
87.082
77.433
77.116
76.800

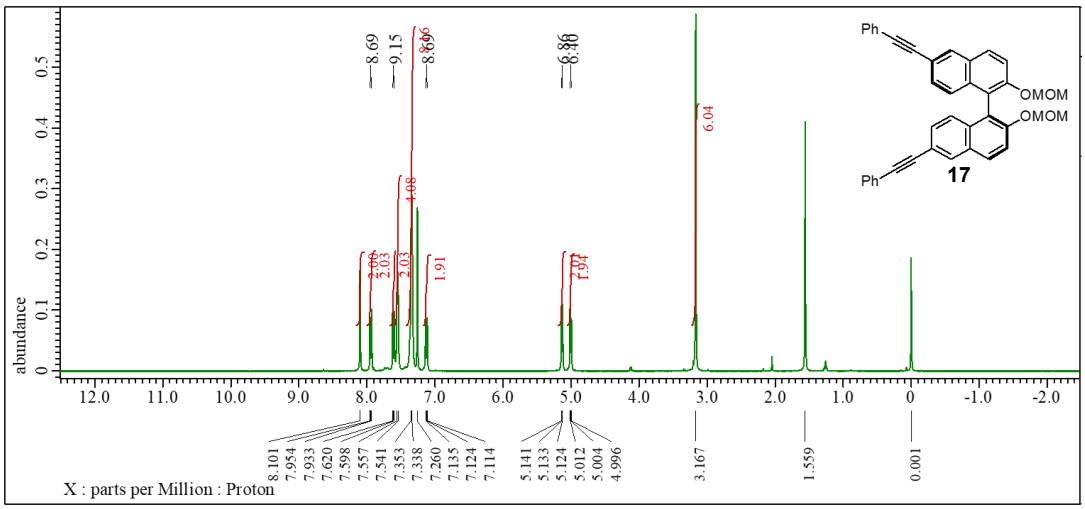

Ph
O
O
Ph
4-PE
(thousandths)
X : parts per Million : Carbon13
150.788
132.198
131.872
131.786
128.614
127.081
126.860
125.011
123.382
123.142
95.812
87.082
77.433
77.116
76.800

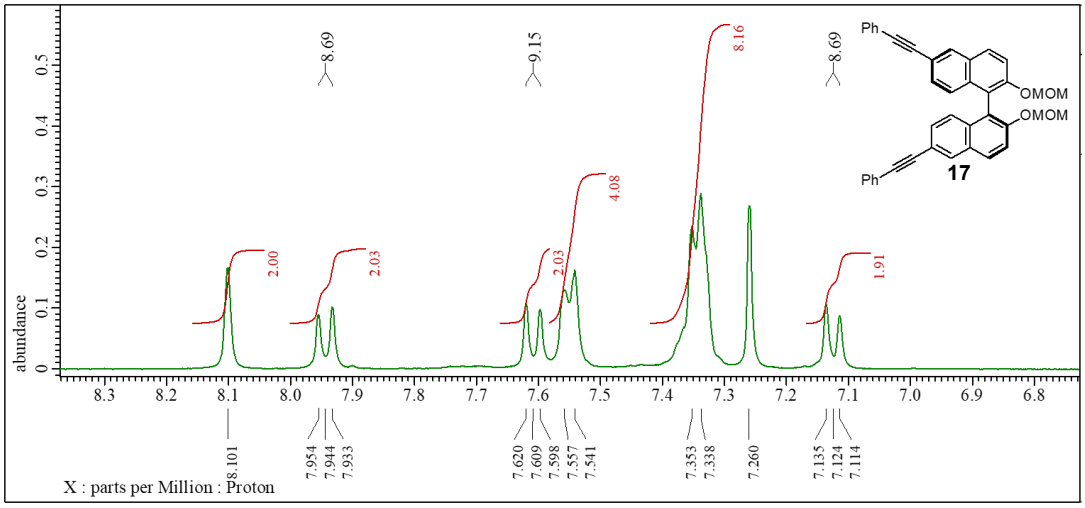

Ph
Ph
3-PE
abundance
X : parts per Million : Proton

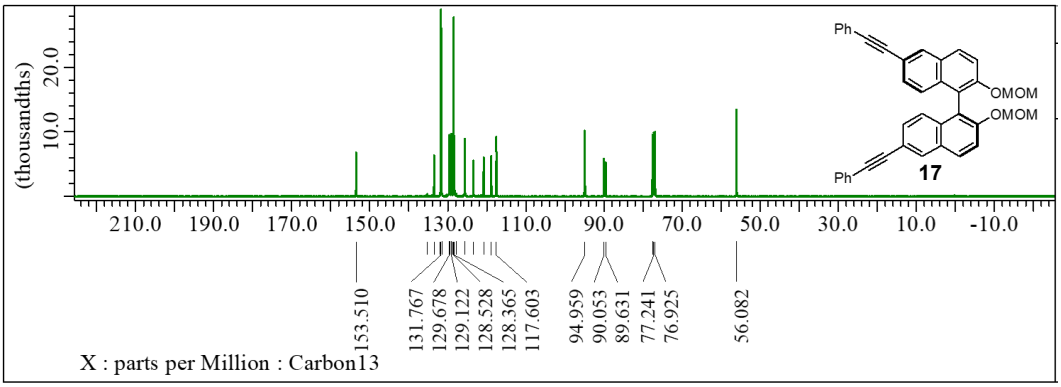

Ph
Ph
3-PE
abundance
X : parts per Million : Proton

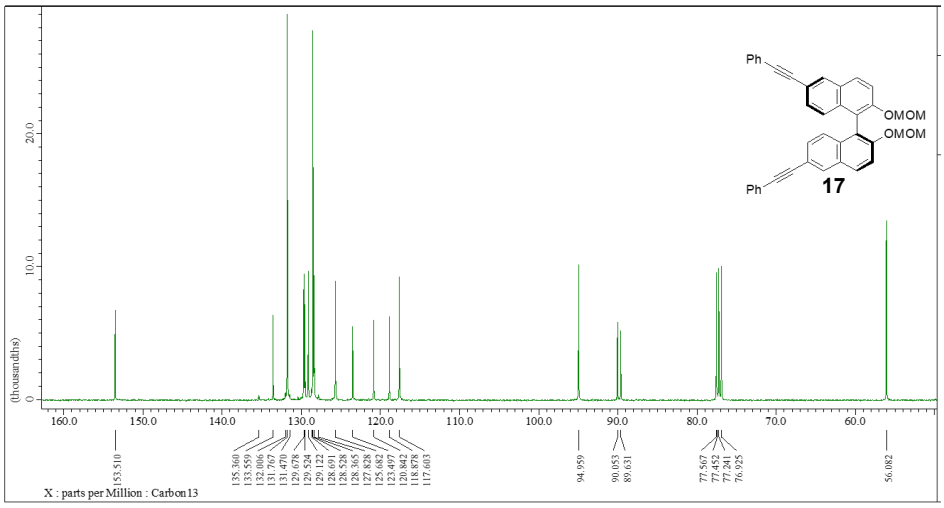

Ph
O
O
Ph
3-PE
(thousandths)
X : parts per Million : Carbon13


Ph
O
O
Ph
3-PE
(thousandths)
150.597
134.009
131.891
131.307
128.489
128.384
126.908
126.583
125.778
123.296
116.684
103.047
93.704
85.128
77.452
77.136
76.810
X : parts per Million : Carbon13


abundance
X : parts per Million : Proton
Ph
OMOM
OMOM
Ph
17


abundance
X : parts per Million : Proton
Ph
OMOM
OMOM
Ph
17


(thousandths)
10.0
20.0
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
-10.0
153.510
131.767
129.678
129.122
128.528
128.365
117.603
94.959
90.053
89.631
77.241
76.925
56.082
X : parts per Million : Carbon13
Ph
OMOM
OMOM
Ph
17


(thousandths)
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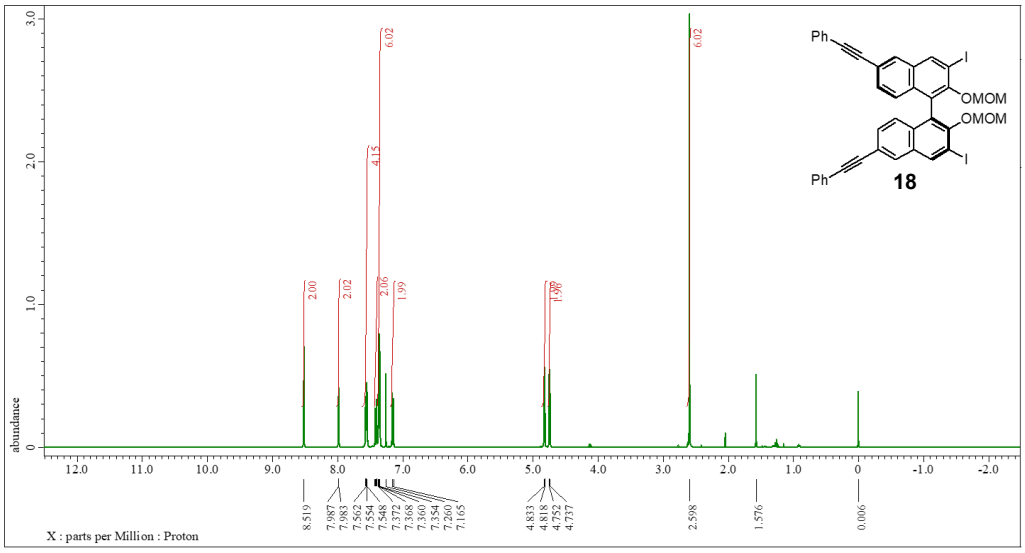
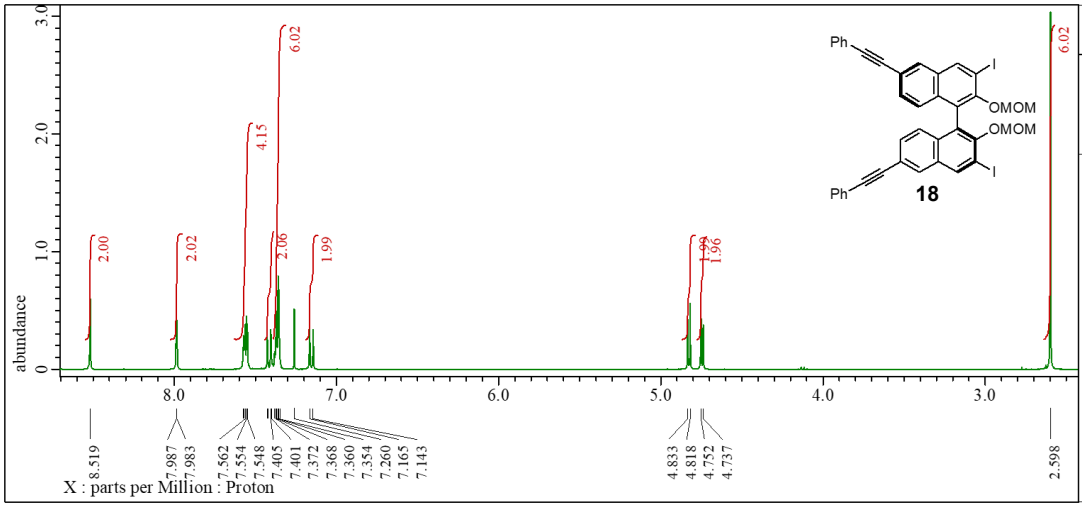
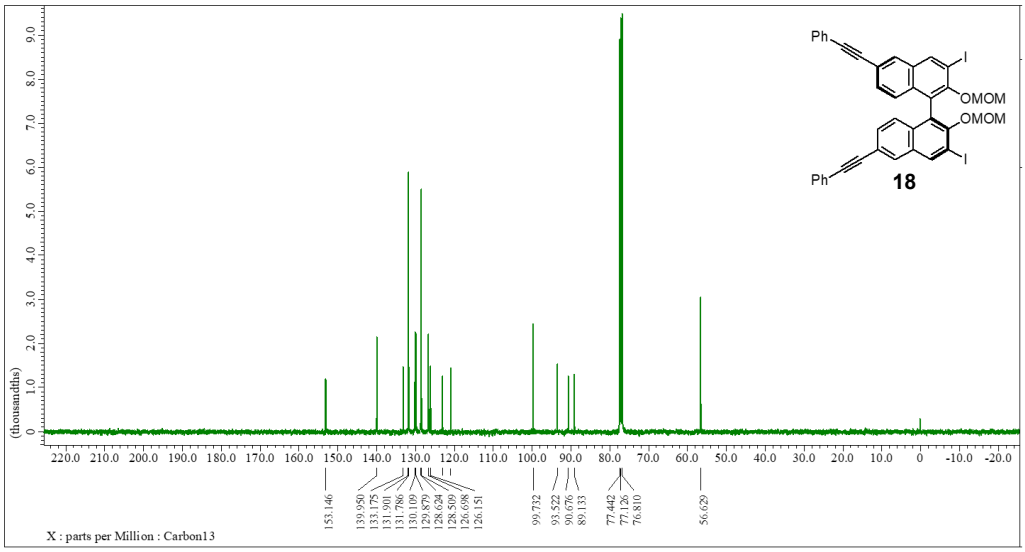
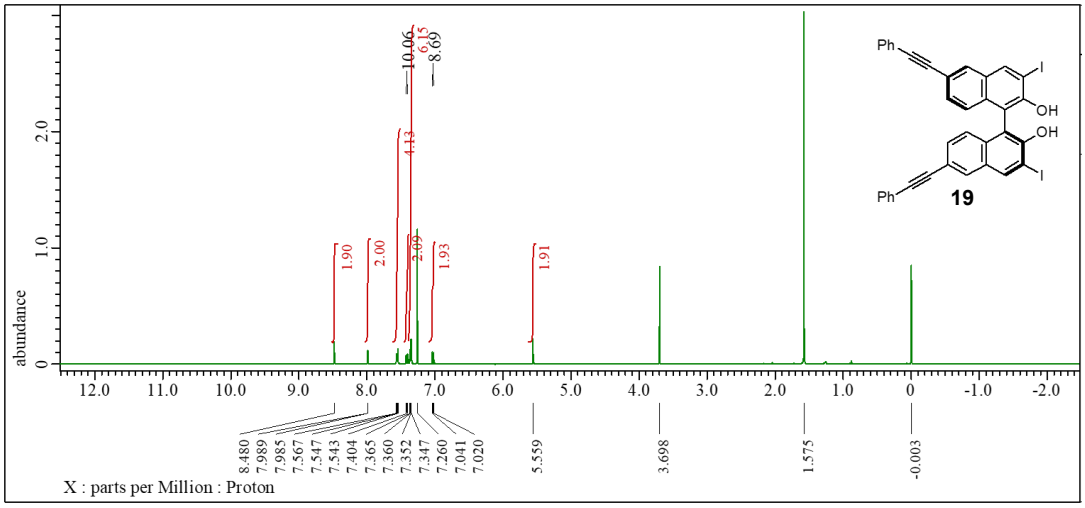
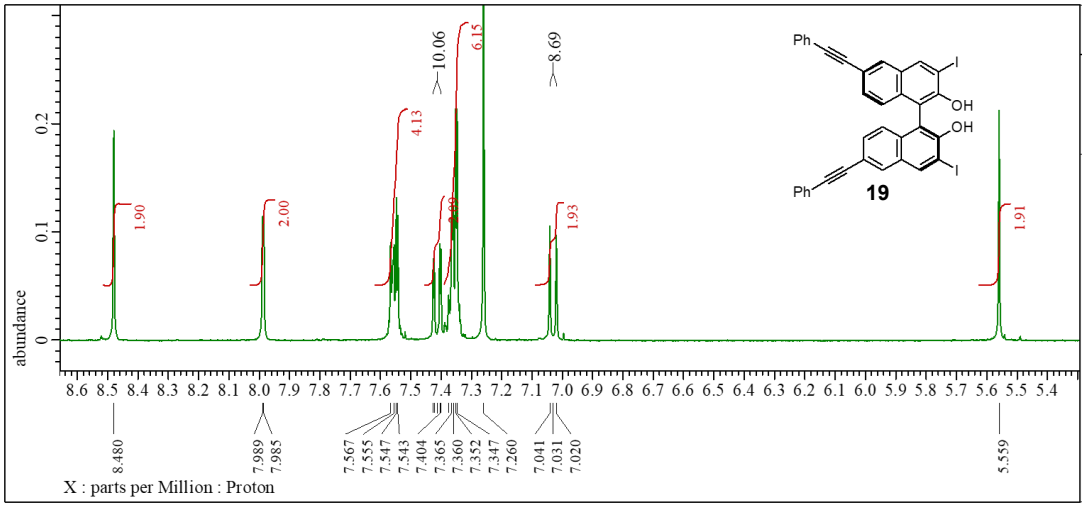
20.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
153.510
135.360
133.559
132.006
131.767
131.470
129.678
129.384
129.122
128.691
128.528
128.365
127.828
125.682
123.497
120.842
118.878
117.603
94.959
90.053
89.631
77.567
77.452
77.241
76.925
56.082
X : parts per Million : Carbon13
Ph
OMOM
OMOM
Ph
17

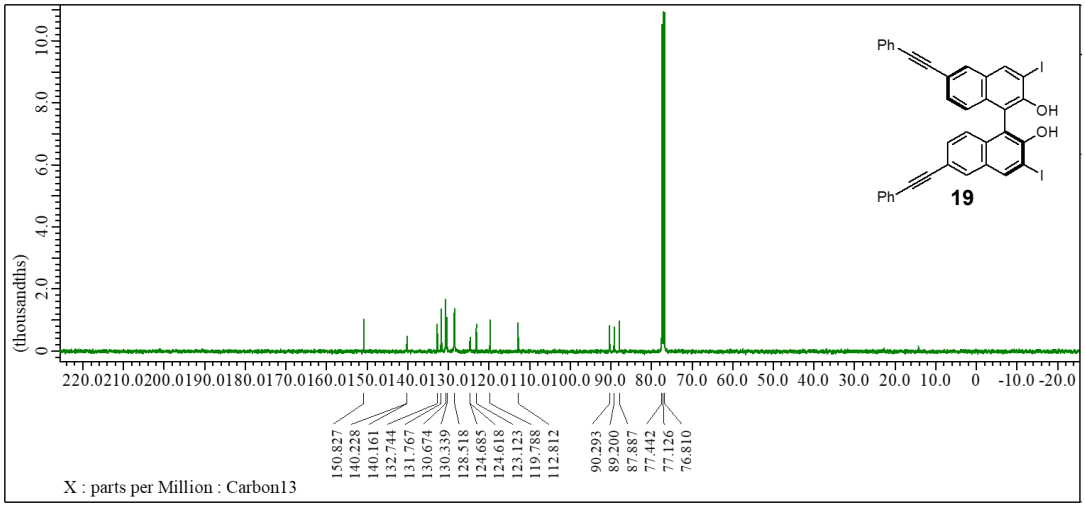

abundance
X : parts per Million : Proton
Ph
I
OMOM
OMOM
I
Ph
18

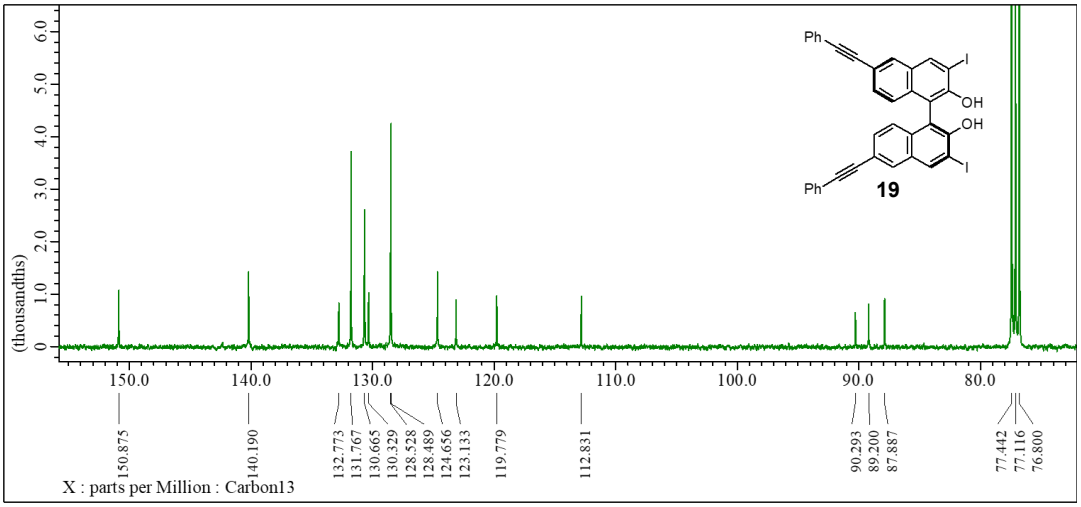

abundance
X : parts per Million : Proton
Ph
I
OMOM
OMOM
I
Ph
18

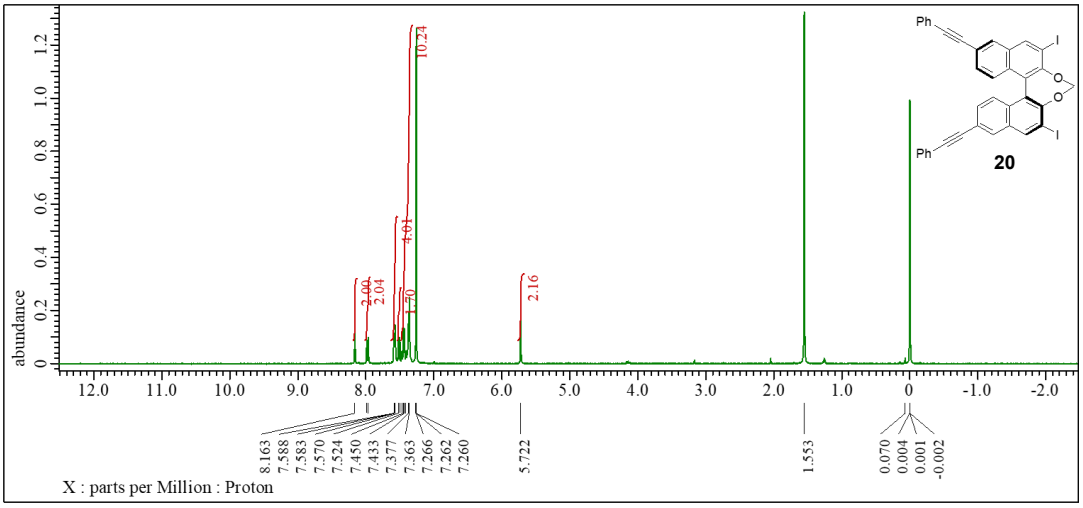

Ph
I
OMOM
OMOM
I
Ph
18
(thousandths)
X : parts per Million : Carbon13

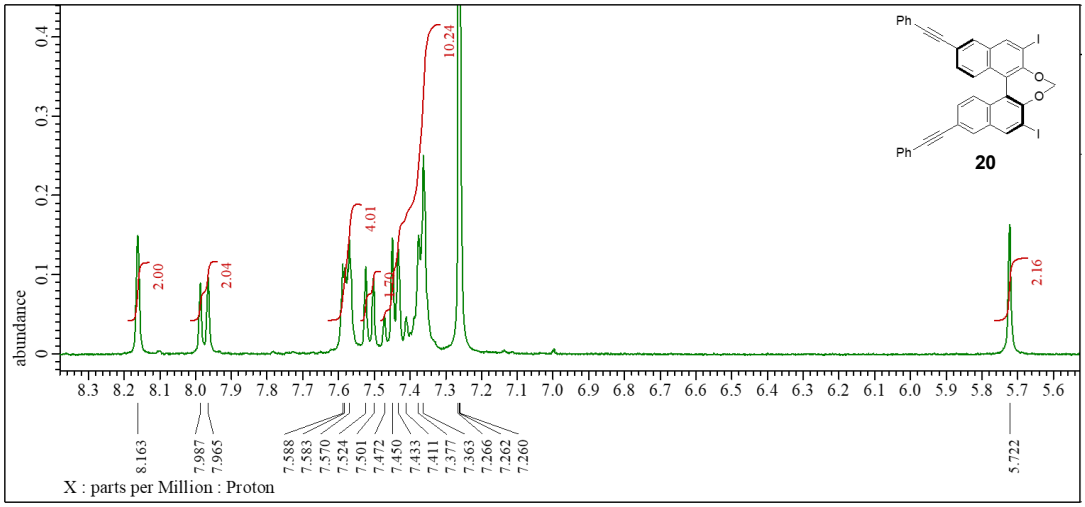

Ph
I
OH
OH
I
Ph
19
abundance
X : parts per Million : Proton

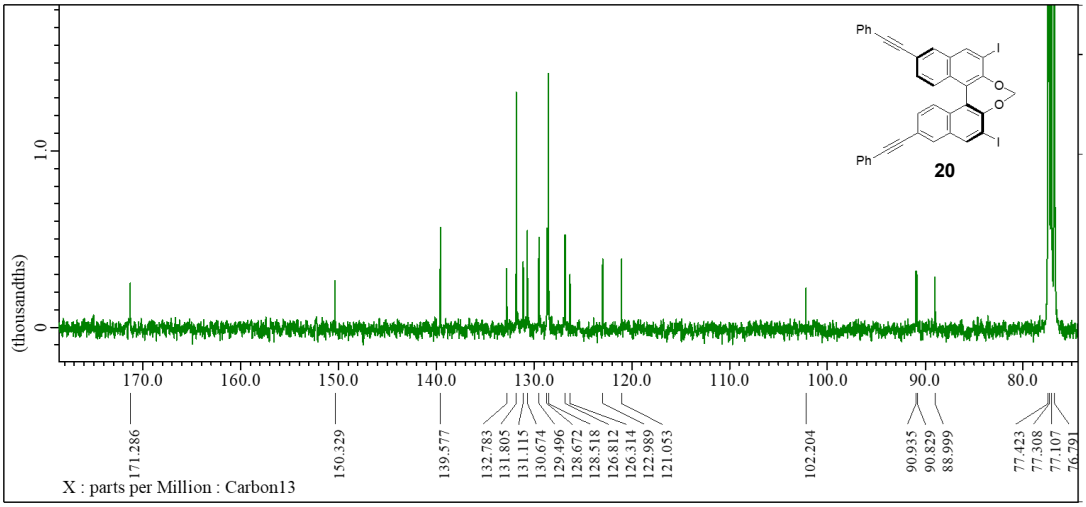

abundance
X : parts per Million : Proton
19

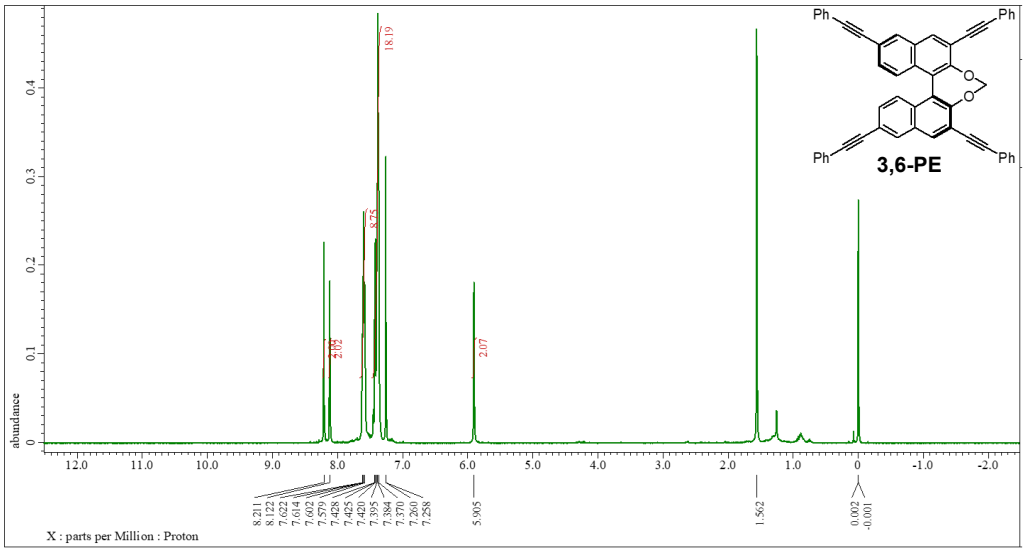

(thousandths)
X : parts per Million : Carbon13
19

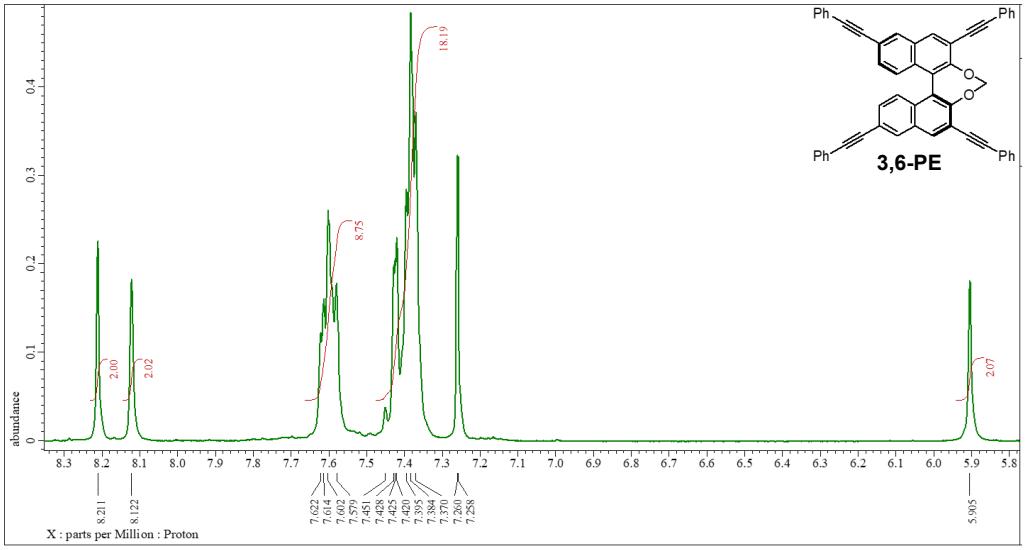

Ph
I
OH
OH
I
Ph
19
(thousandths)
6.0
5.0
4.0
3.0
2.0
1.0
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
150.875
140.190
132.773
131.767
130.665
130.329
128.528
128.489
124.656
123.133
119.779
112.831
90.293
89.200
87.887
77.442
77.116
76.800
X : parts per Million : Carbon13


Ph
I
O
O
I
Ph
20
abundance
1.2
1.0
0.8
0.6
0.4
0.2
0
10.24
4.01
3.00
2.04
1.30
2.16
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.163
7.588
7.583
7.570
7.524
7.450
7.433
7.377
7.363
7.266
7.262
7.260
5.722
1.553
0.070
0.004
0.001
-0.002
X : parts per Million : Proton


abundance
0
0.1
0.2
0.3
0.4
10.24
4.01
2.00
2.04
1.70
2.16
8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6
8.163
7.987
7.965
7.588
7.583
7.570
7.524
7.501
7.472
7.450
7.433
7.411
7.377
7.363
7.266
7.262
7.260
5.722
X : parts per Million : Proton
Ph
I
O
O
I
Ph
20


(thousandths)
0
1.0
170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0
171.286
150.329
139.577
132.783
131.805
131.115
130.674
129.496
128.672
128.518
126.812
126.314
122.989
121.053
102.204
90.935
90.829
88.999
77.423
77.308
77.107
76.791
X : parts per Million : Carbon13
Ph
I
O
O
I
Ph
20


Ph
Ph
Ph
Ph
3,6-PE
abundance
18.19
8.75
2.00
2.02
2.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.211
8.122
7.622
7.614
7.602
7.579
7.428
7.425
7.420
7.395
7.384
7.370
7.260
7.258
5.905
1.562
0.002
-0.001
X : parts per Million : Proton


Ph
Ph
Ph
Ph
3,6-PE
abundance
18.19
8.75
2.00
2.02
2.07
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
6.2
6.1
6.0
5.9
5.8
8.211
8.122
7.622
7.614
7.602
7.579
7.451
7.428
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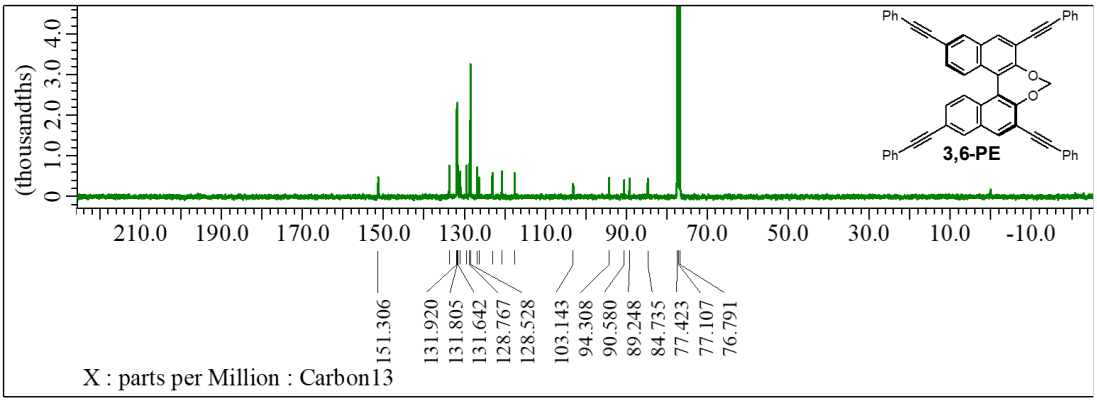
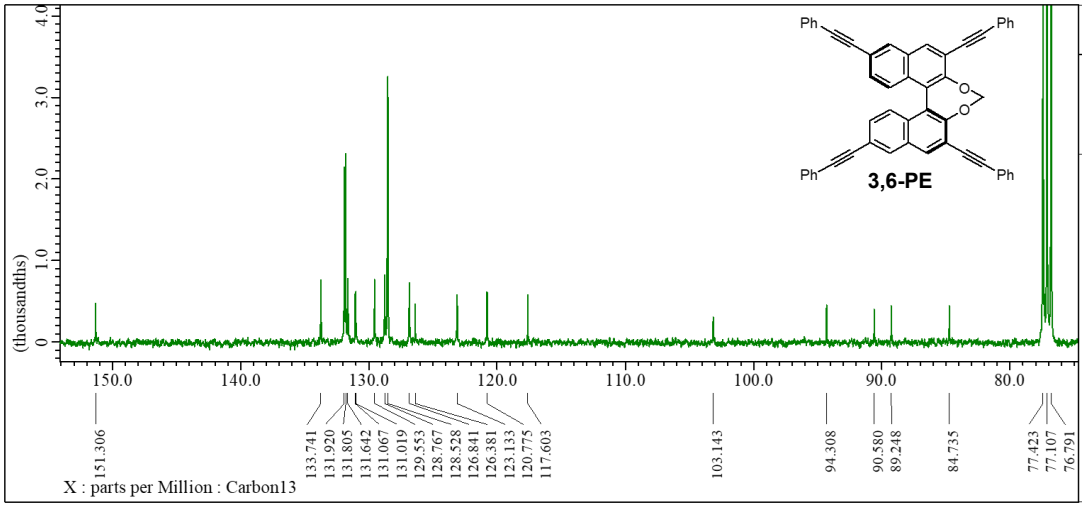
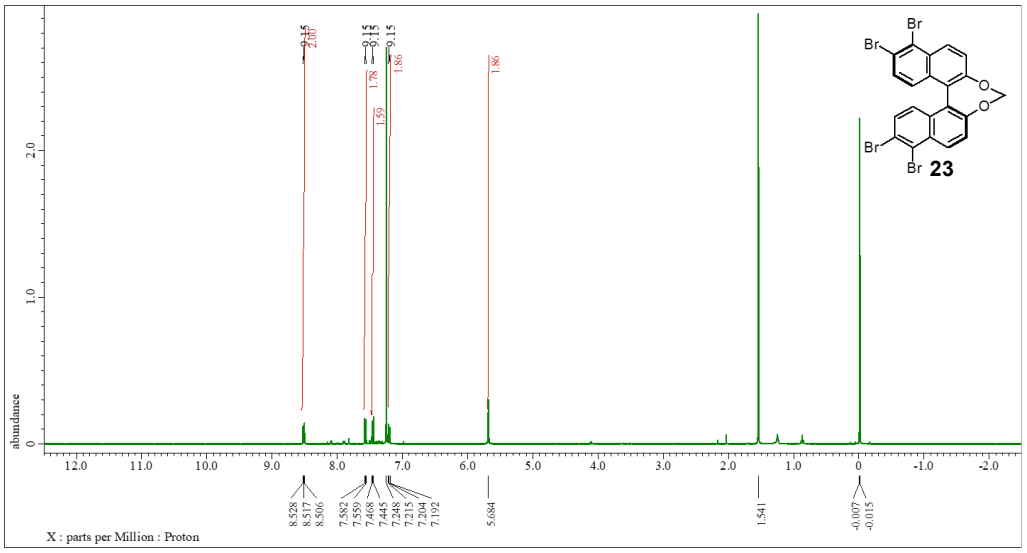
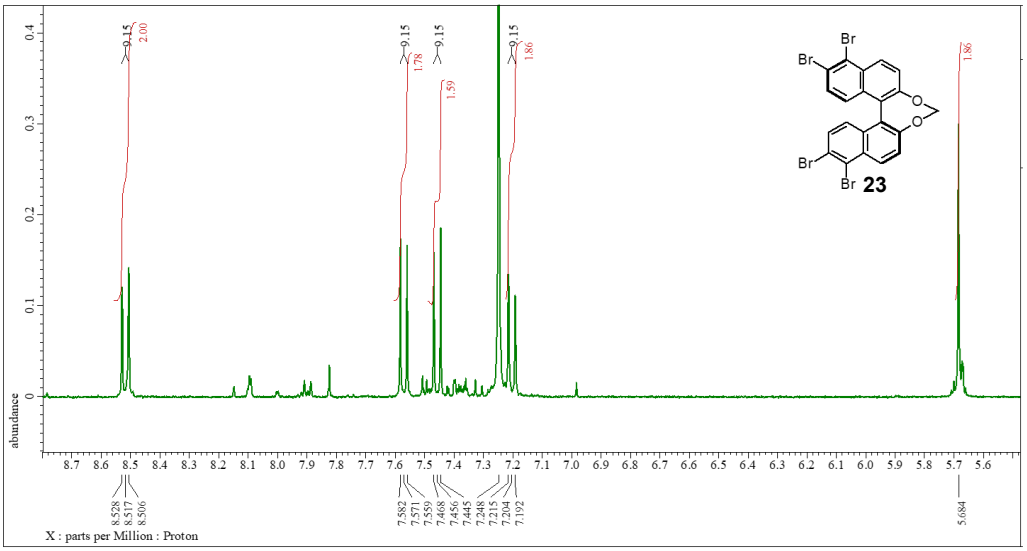
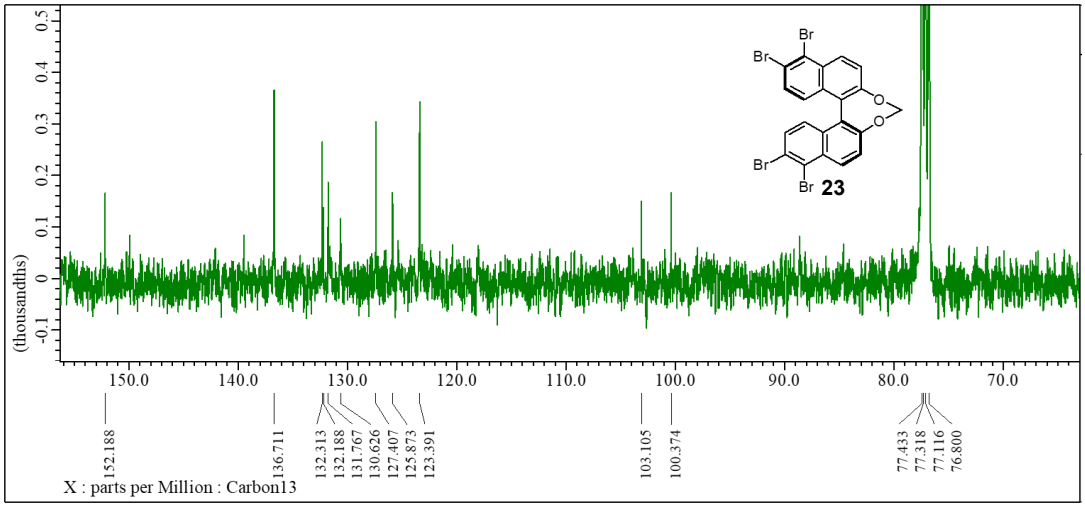
7.420
7.395
7.384
7.370
7.260
7.258
5.905
X : parts per Million : Proton

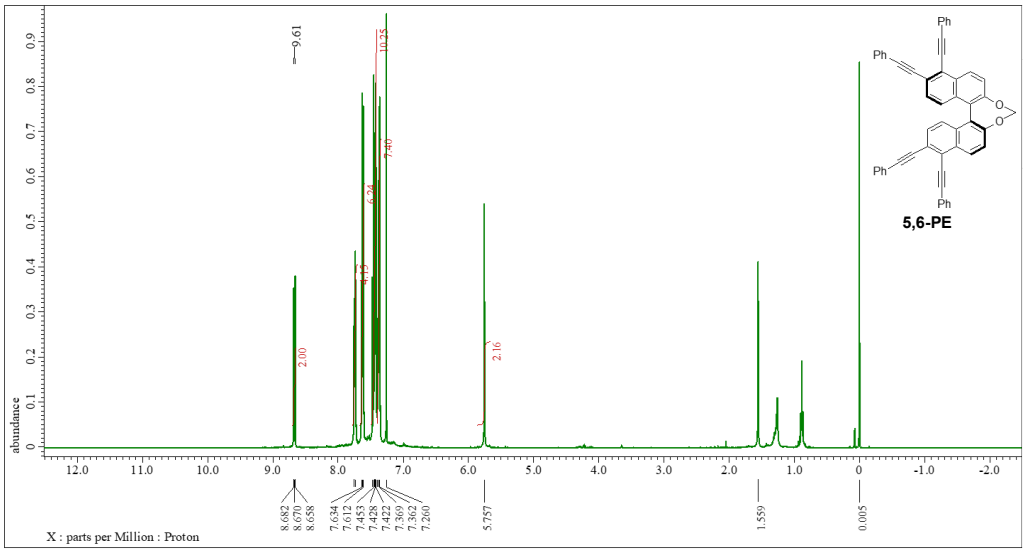

(thousandths)
0 1.0 2.0 3.0 4.0
210.0 190.0 170.0 150.0 130.0 110.0 90.0 70.0 50.0 30.0 10.0 -10.0
151.306
131.920
131.805
131.642
128.767
128.528
103.143
94.308
90.580
89.248
84.735
77.423
77.107
76.791
X : parts per Million : Carbon13
Ph
Ph
Ph
Ph
O
O
3,6-PE

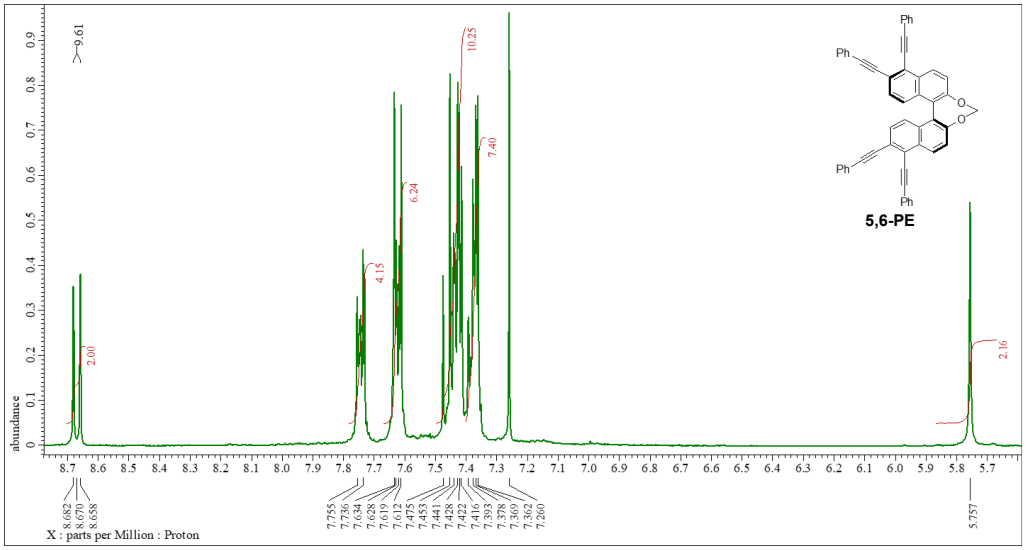

(thousandths)
0 1.0 2.0 3.0 4.0
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0
151.306
133.741
131.920
131.805
131.642
131.067
131.019
129.553
128.767
128.528
126.841
126.381
123.133
120.775
117.603
103.143
94.308
90.580
89.248
84.735
77.423
77.107
76.791
X : parts per Million : Carbon13
Ph
Ph
Ph
Ph
O
O
3,6-PE

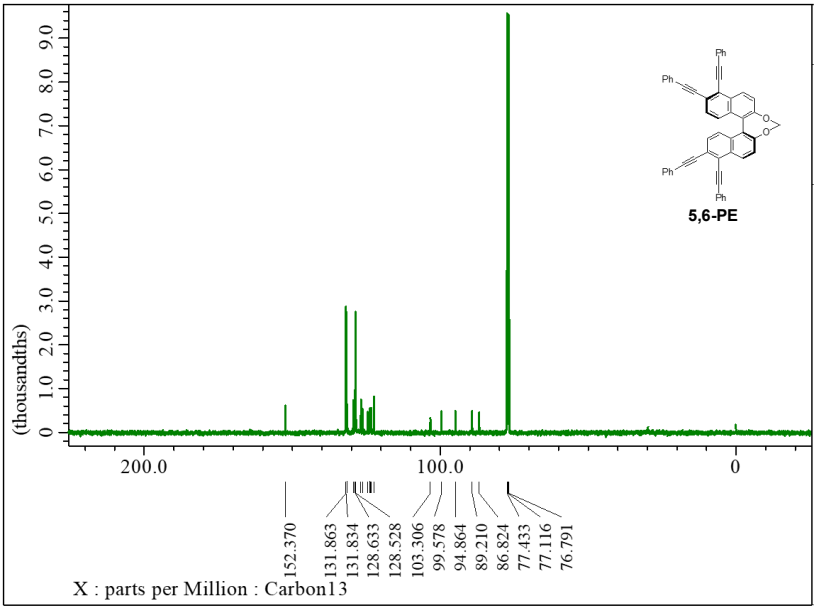

Br
Br
Br
Br
23
abundance
X : parts per Million : Proton

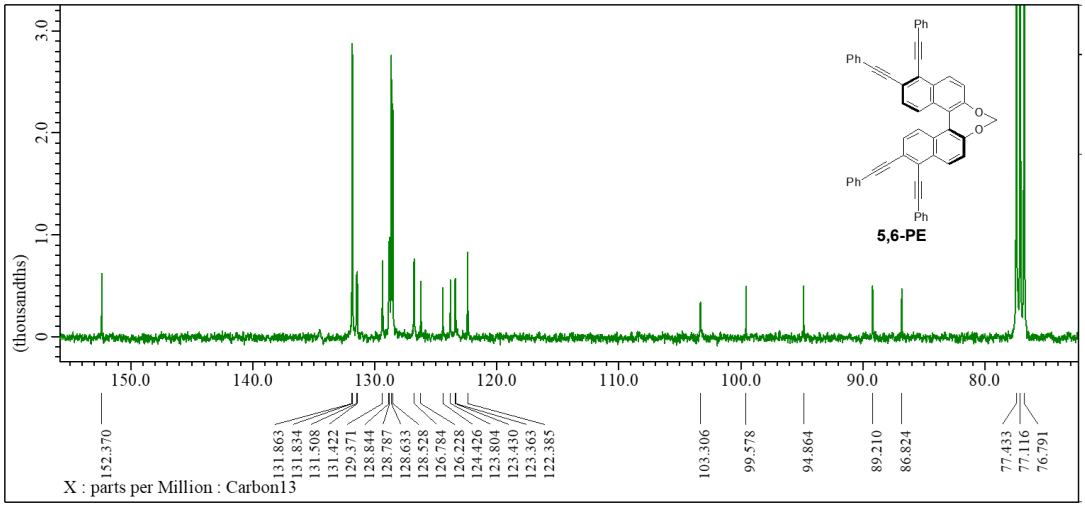

Br
Br
Br
Br
23
abundance
X : parts per Million : Proton

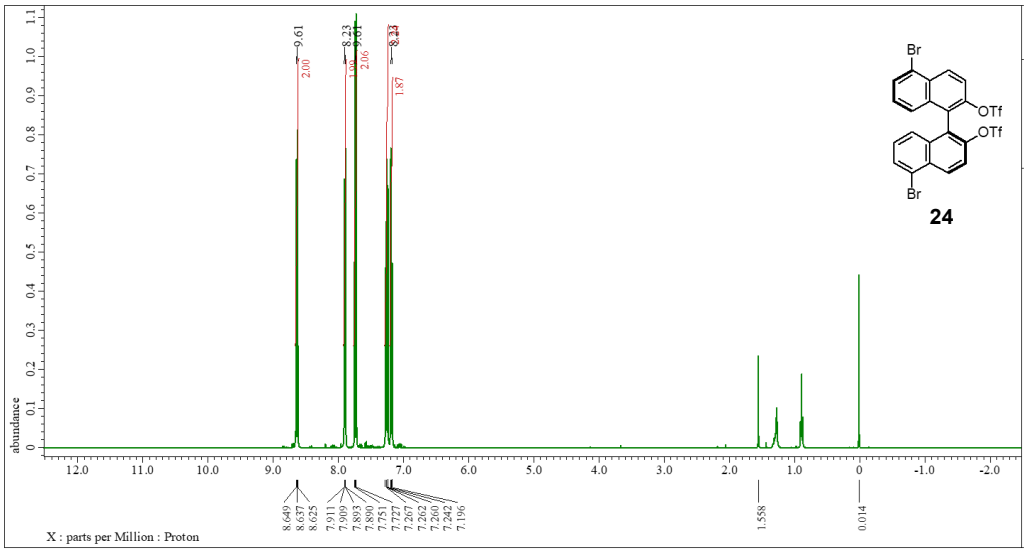

Br
Br
O
O
Br
Br
23
(thousandths)
0.5
0.4
0.3
0.2
0.1
0
-0.1
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
152.188
136.711
132.313
132.188
131.767
130.626
127.407
125.873
123.391
103.105
100.374
77.433
77.318
77.116
76.800
X : parts per Million : Carbon13

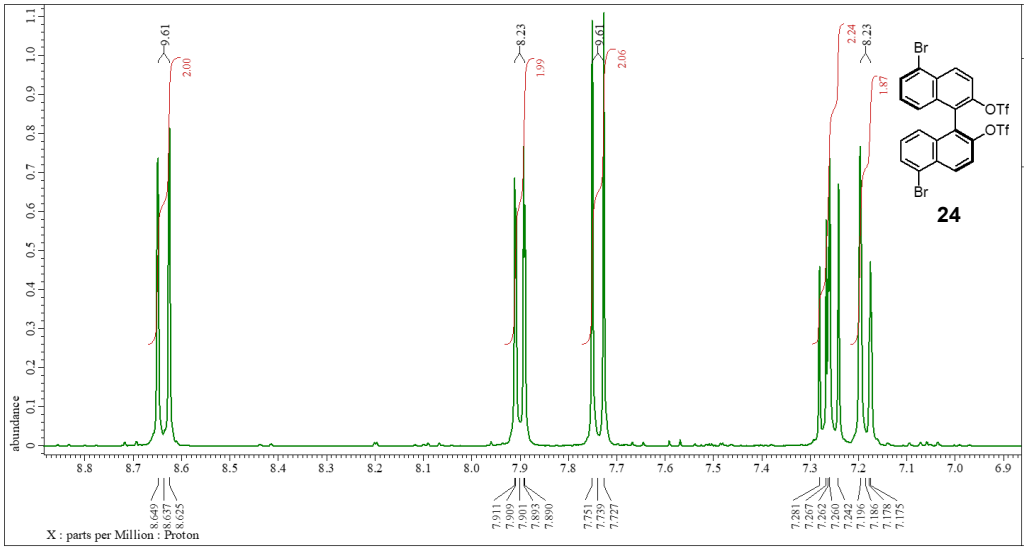

9.61
10.25
7.40
6.24
4.15
2.00
2.16
abundance
X : parts per Million : Proton
5,6-PE

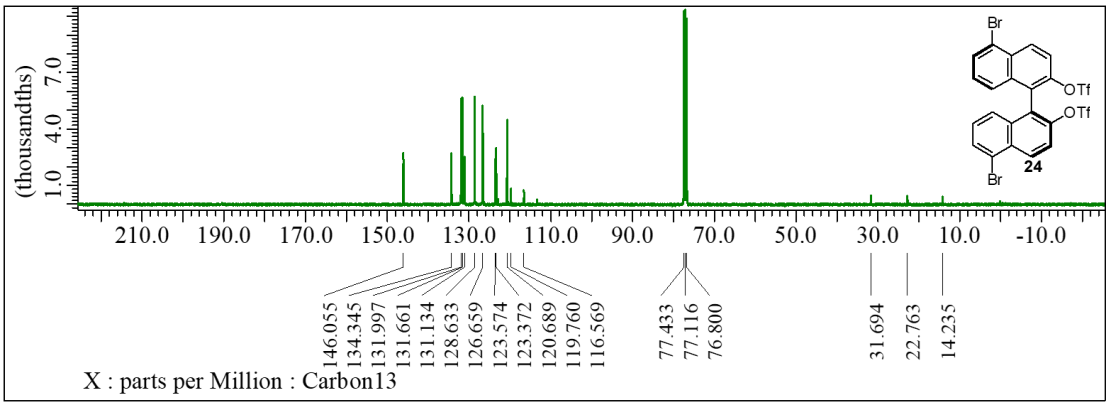

9.61
10.25
7.40
6.24
4.15
2.00
2.16
abundance
X : parts per Million : Proton
5,6-PE

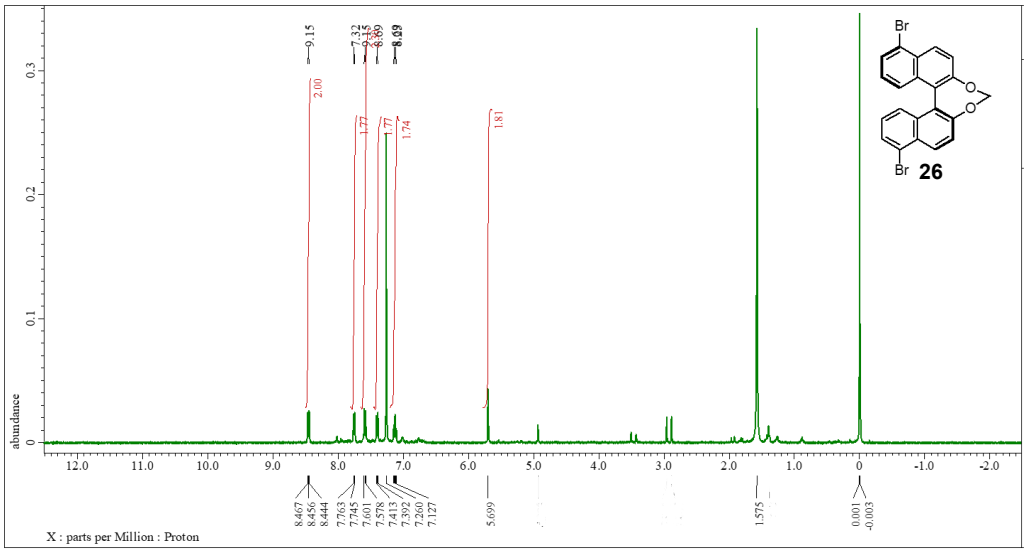

(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
200.0
100.0
0
152.370
131.863
131.834
128.633
128.528
103.306
99.578
94.864
89.210
86.824
77.433
77.116
76.791
X : parts per Million : Carbon13
Ph
Ph
Ph
Ph
O
O
5,6-PE

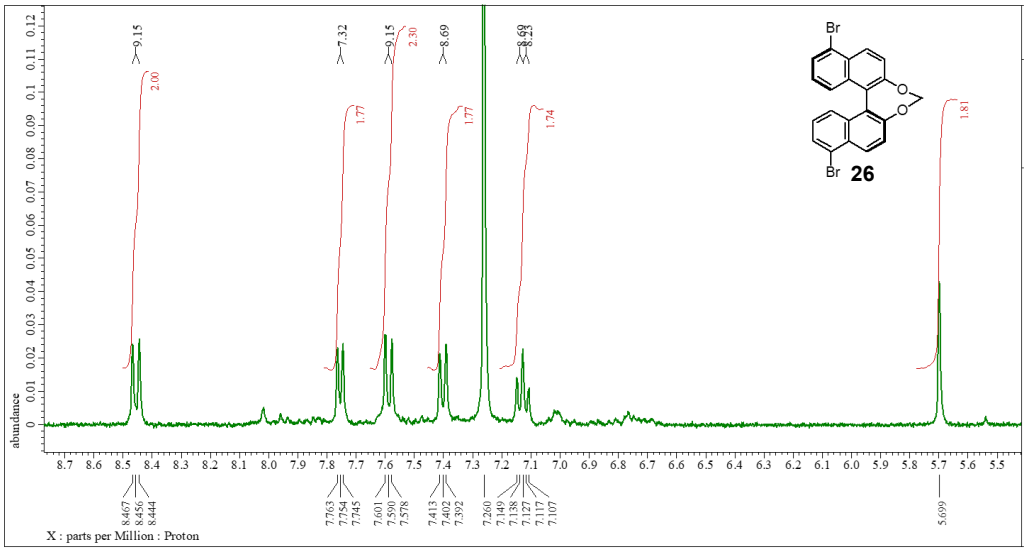

(thousandths)
0
1.0
2.0
3.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
152.370
131.863
131.834
131.508
131.422
129.371
128.844
128.787
128.633
128.528
126.784
126.228
124.426
123.804
123.430
123.363
122.385
103.306
99.578
94.864
89.210
86.824
77.433
77.116
76.791
X : parts per Million : Carbon13
Ph
Ph
Ph
Ph
O
O
5,6-PE

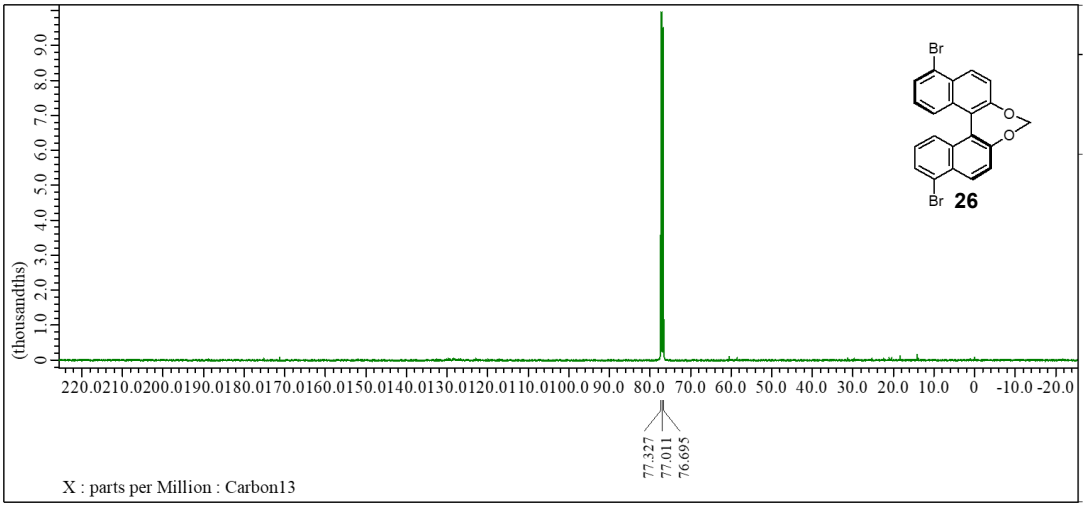

9.61
8.23
2.00
2.06
1.87
Br
OTf
OTf
Br
24
abundance
X : parts per Million : Proton

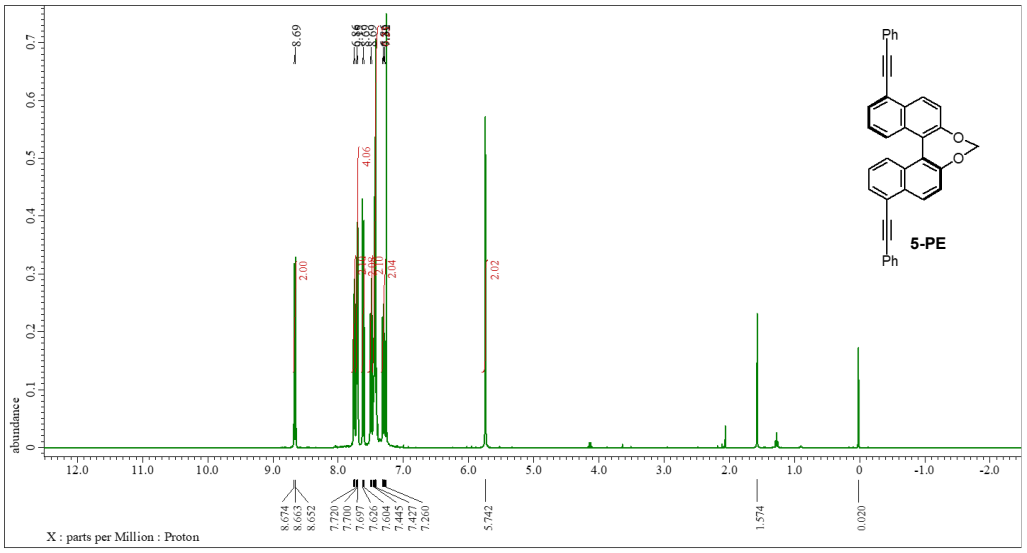

9.61
8.23
2.00
1.99
2.06
2.24
1.87
Br
OTf
OTf
Br
24
abundance
X : parts per Million : Proton

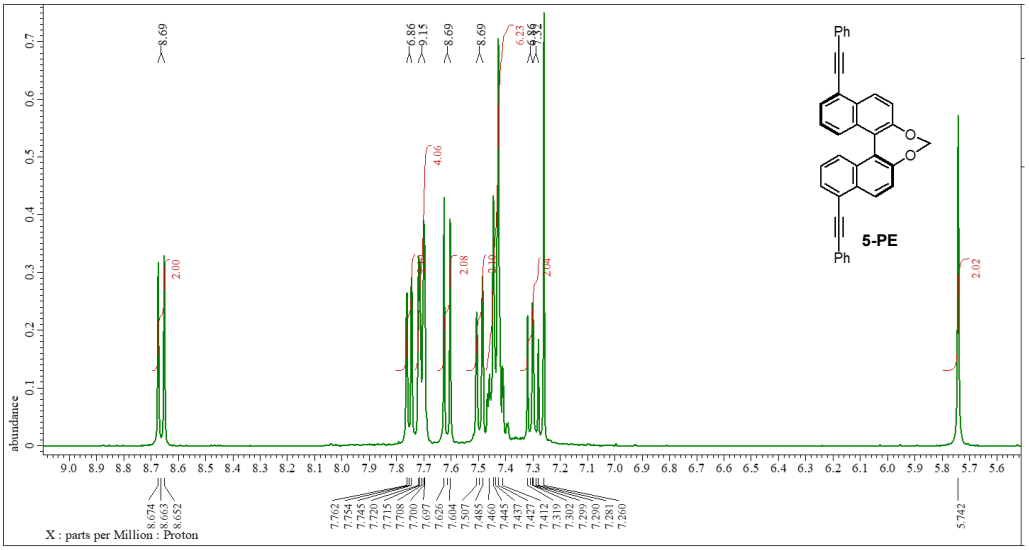

(thousandths)
1.0
4.0
7.0
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
-10.0
146.055
134.345
131.997
131.661
131.134
128.633
126.659
123.574
123.372
120.689
119.760
116.569
77.433
77.116
76.800
31.694
22.763
14.235
X : parts per Million : Carbon13
Br
OTf
OTf
Br
24

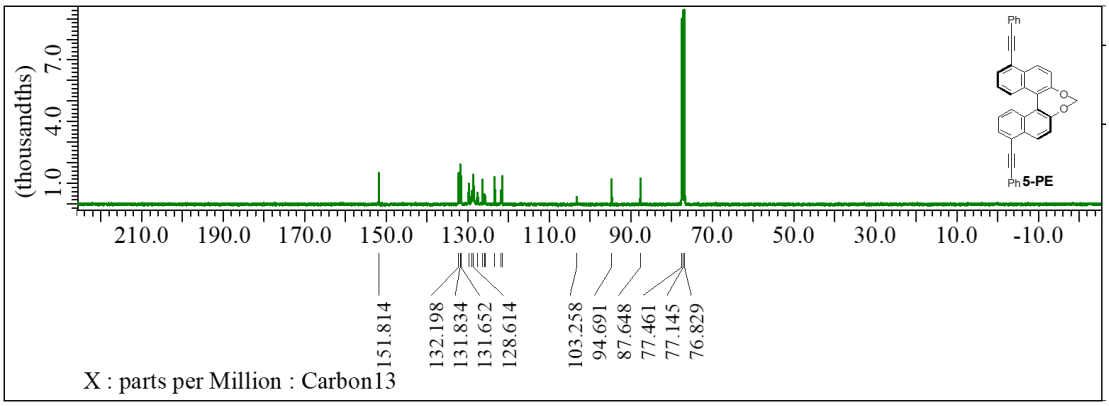

Br
Br
26
abundance
X : parts per Million : Proton

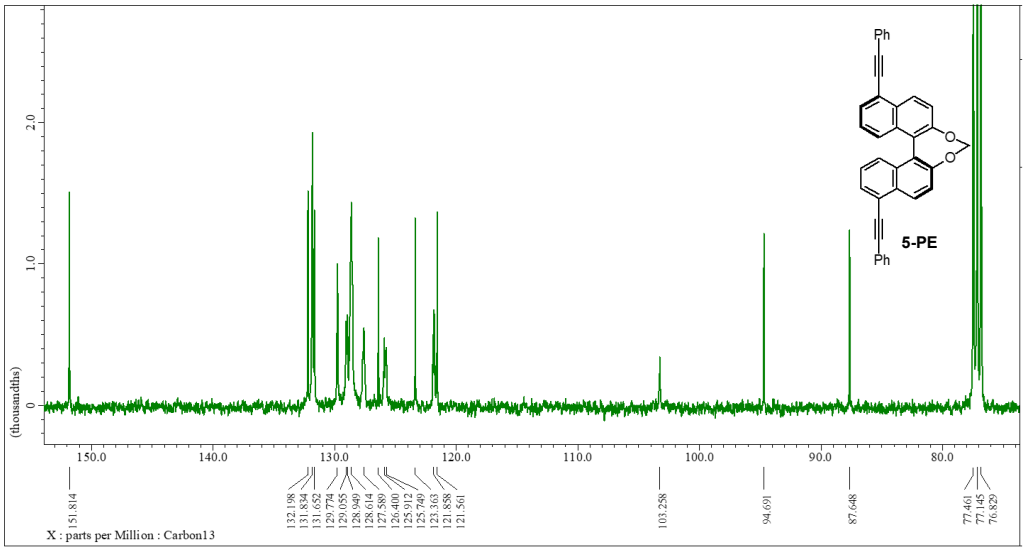

Br
Br
26
abundance
X : parts per Million : Proton

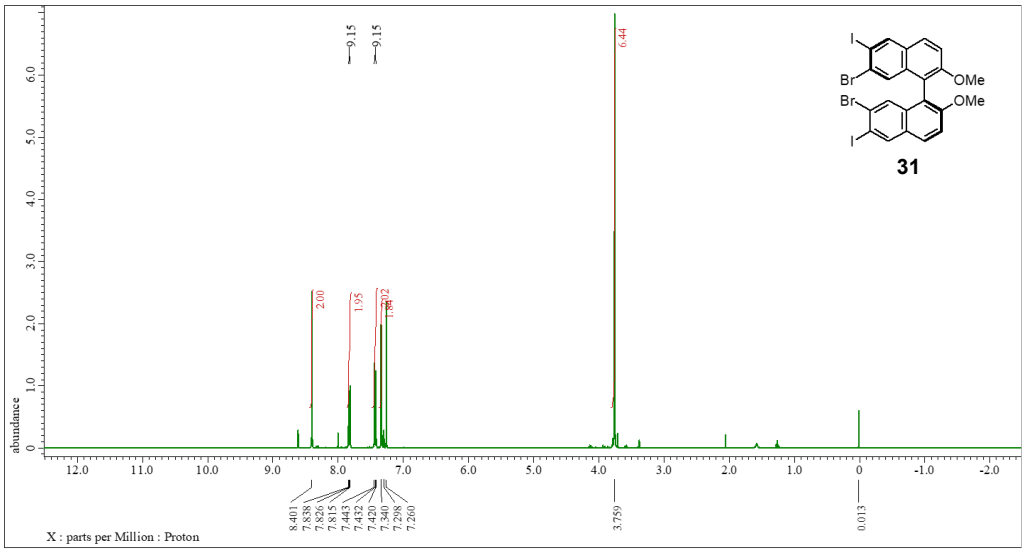

Br
O
O
Br
26
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0
220.0210.0200.0190.0180.0170.0160.0150.0140.0130.0120.0110.0100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
77.327
77.011
76.695
X : parts per Million : Carbon13

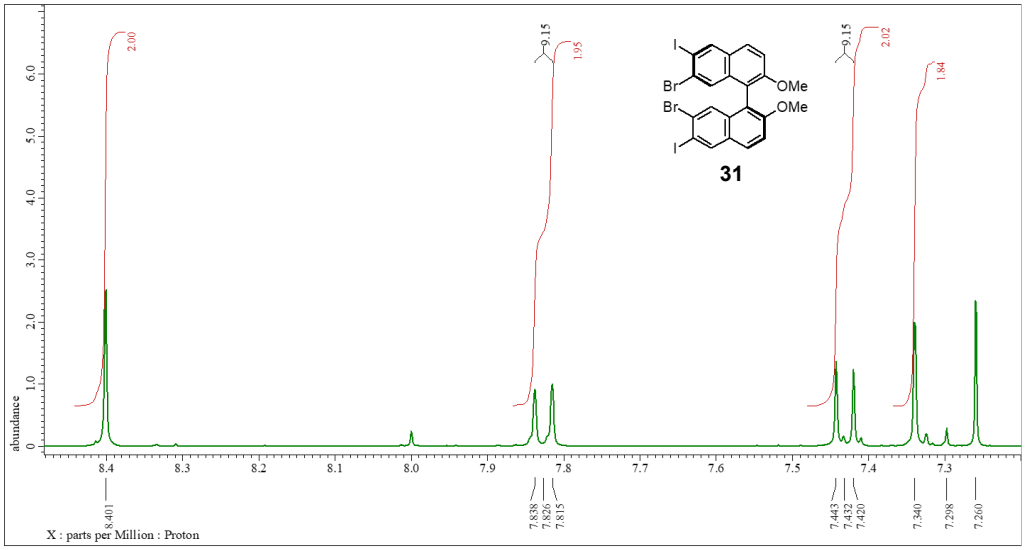

5-PE
X : parts per Million : Proton

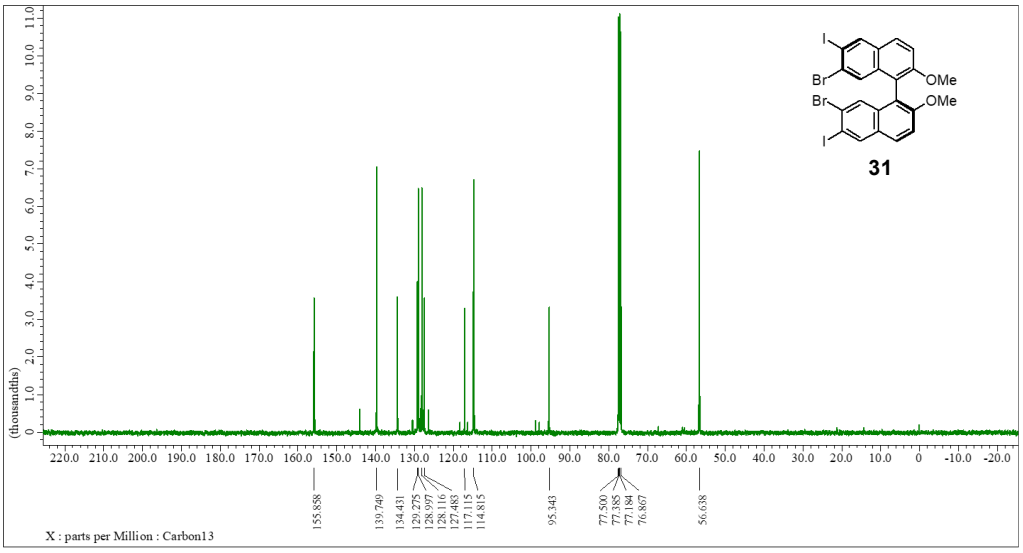

5-PE
X : parts per Million : Proton

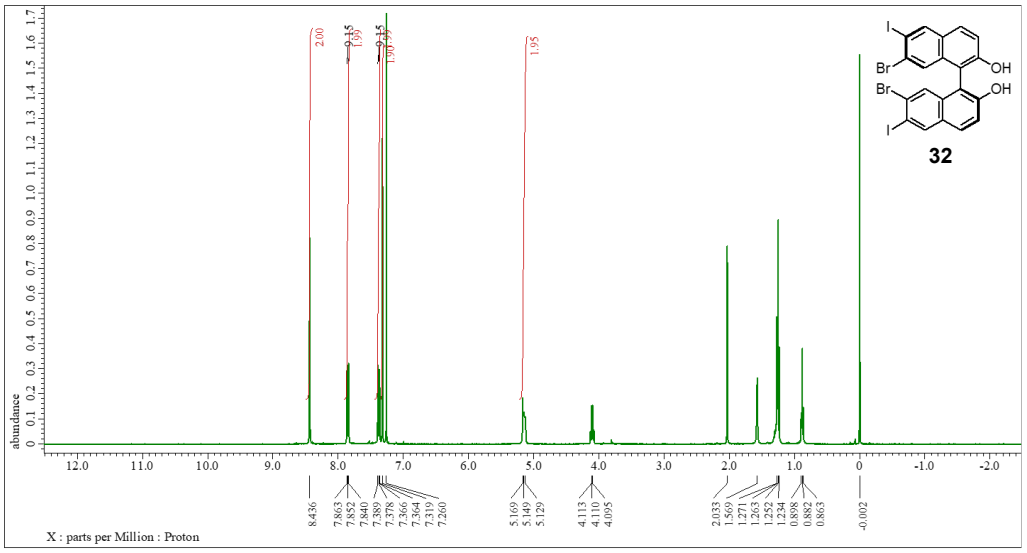

(thousandths)
1.0
4.0
7.0
210.0
190.0
170.0
150.0
130.0
110.0
90.0
70.0
50.0
30.0
10.0
-10.0
151.814
132.198
131.834
131.652
128.614
103.258
94.691
87.648
77.461
77.145
76.829
X : parts per Million : Carbon13
Ph
Ph
5-PE

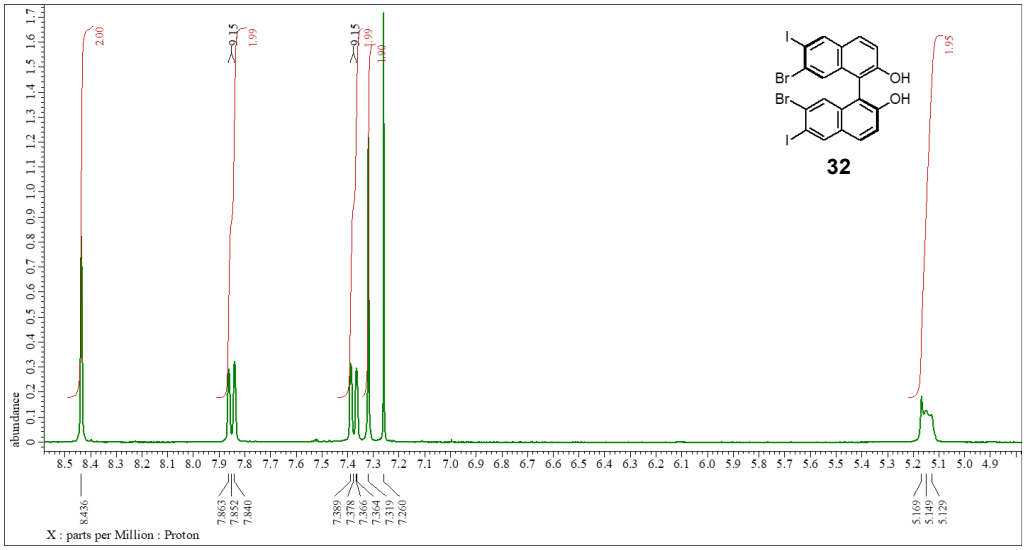

(thousandths)
2.0
1.0
0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
151.814
132.198
131.834
131.652
129.774
129.055
128.949
128.614
127.589
126.400
125.912
125.749
123.363
121.838
121.561
103.258
94.691
87.648
77.461
77.145
76.829
X : parts per Million : Carbon13
Ph
Ph
5-PE

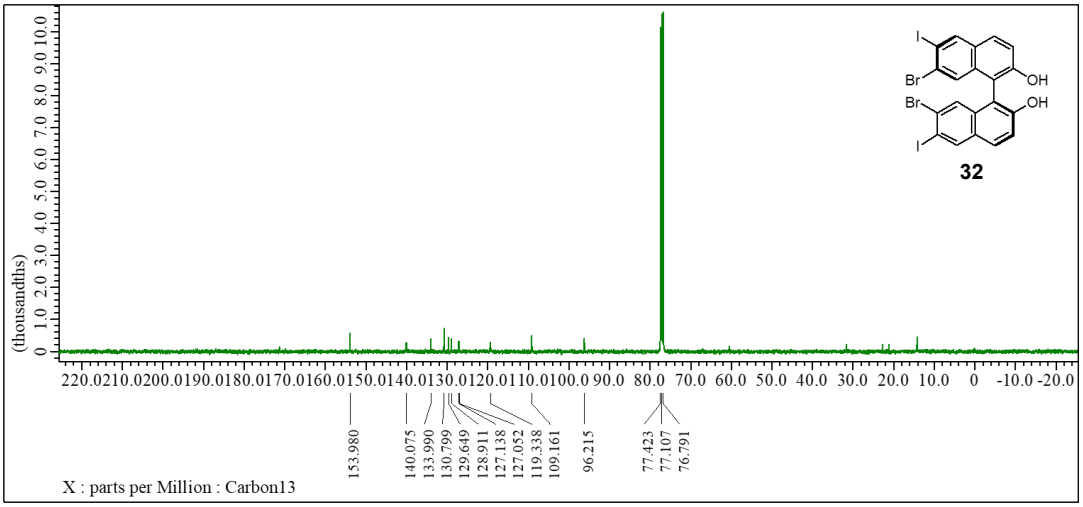

9.15
9.15
6.44
2.00
1.95
2.02
1.84
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.401
7.838
7.826
7.815
7.443
7.432
7.420
7.340
7.298
7.260
3.759
0.013
X : parts per Million : Proton
I
Br
OMe
Br
OMe
I
31

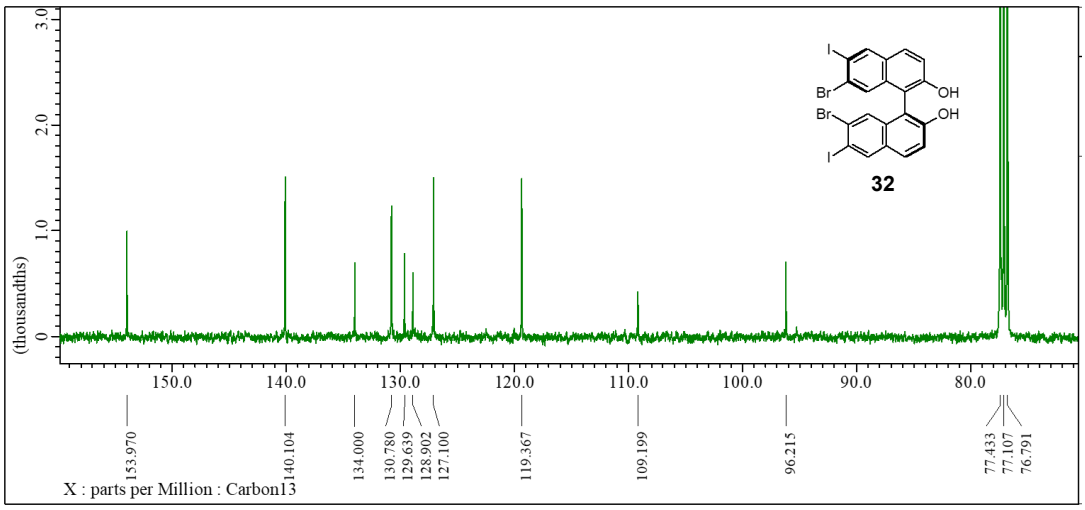

2.00
9.15
1.95
9.15
2.02
1.84
abundance
8.4
8.3
8.2
8.1
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
8.401
7.838
7.826
7.815
7.443
7.432
7.420
7.340
7.298
7.260
X : parts per Million : Proton
I
Br
OMe
Br
OMe
I
31

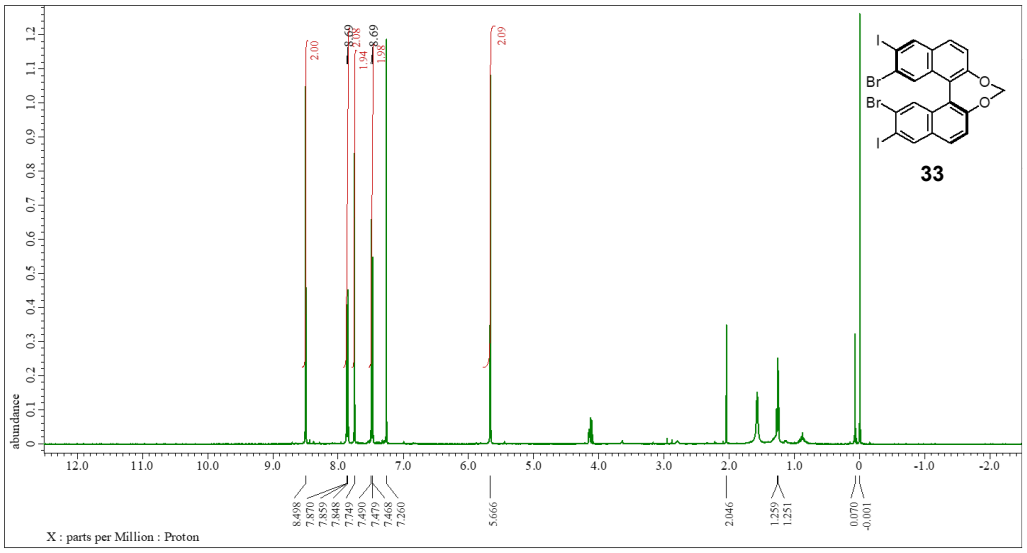

I
Br
OMe
Br
OMe
I
31
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
155.858
139.749
134.431
129.275
128.977
128.116
127.483
117.115
114.815
95.343
77.500
77.385
77.184
76.867
56.638
X : parts per Million : Carbon13

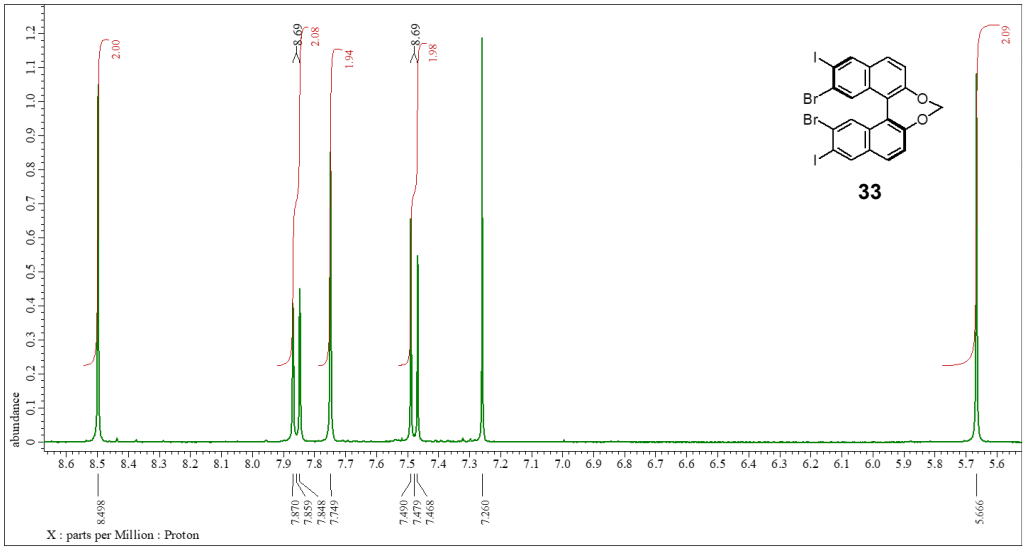

32
abundance
X : parts per Million : Proton

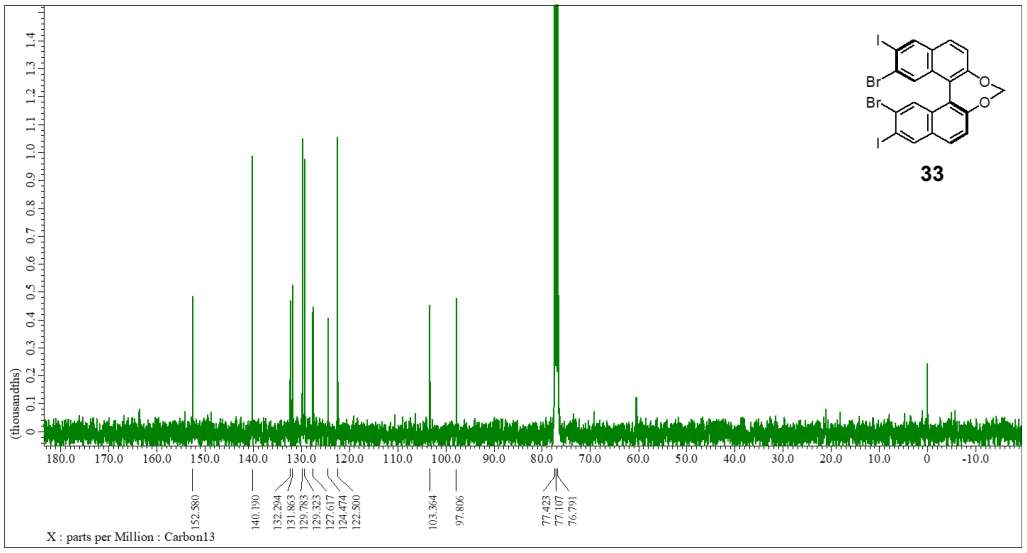

32
abundance
X : parts per Million : Proton

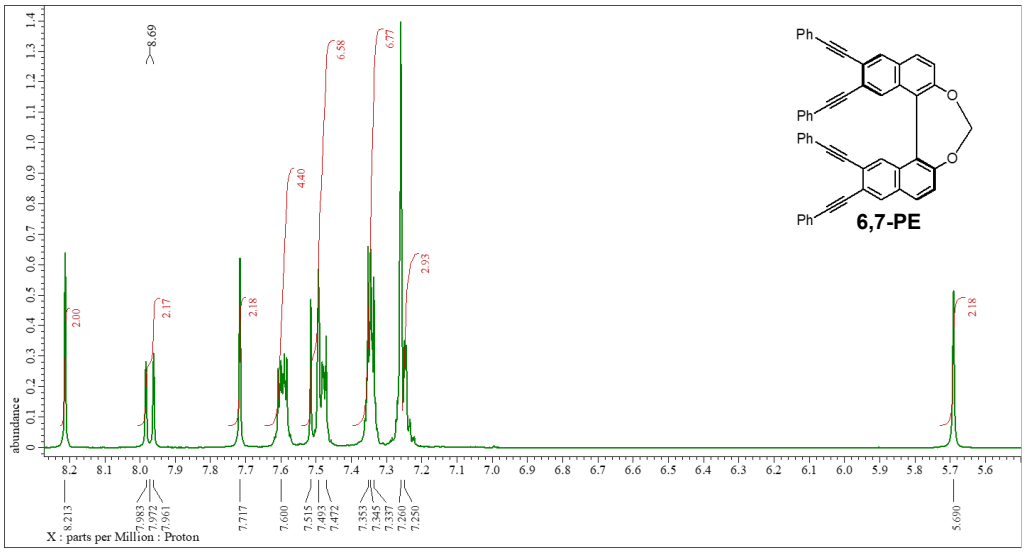

(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
153.980
140.075
133.990
130.799
129.649
128.911
127.138
127.052
119.338
109.161
96.215
77.423
77.107
76.791
X : parts per Million : Carbon13
I
Br
OH
Br
OH
I
32

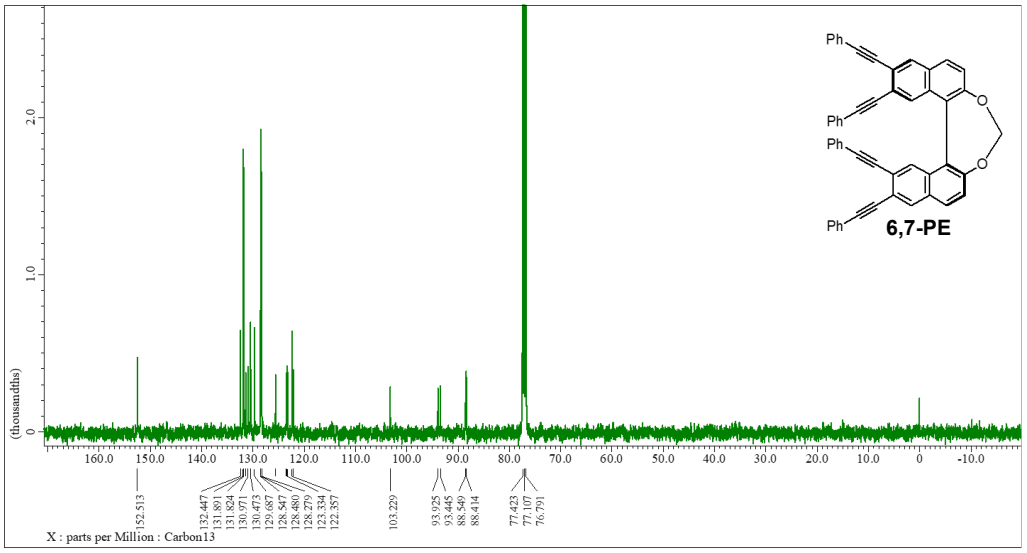

(thousandths)
0 1.0 2.0 3.0
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0
153.970
140.104
134.000
130.780
129.639
128.902
127.100
119.367
109.199
96.215
77.433
77.107
76.791
X : parts per Million : Carbon13
I
Br
OH
Br
OH
I
32

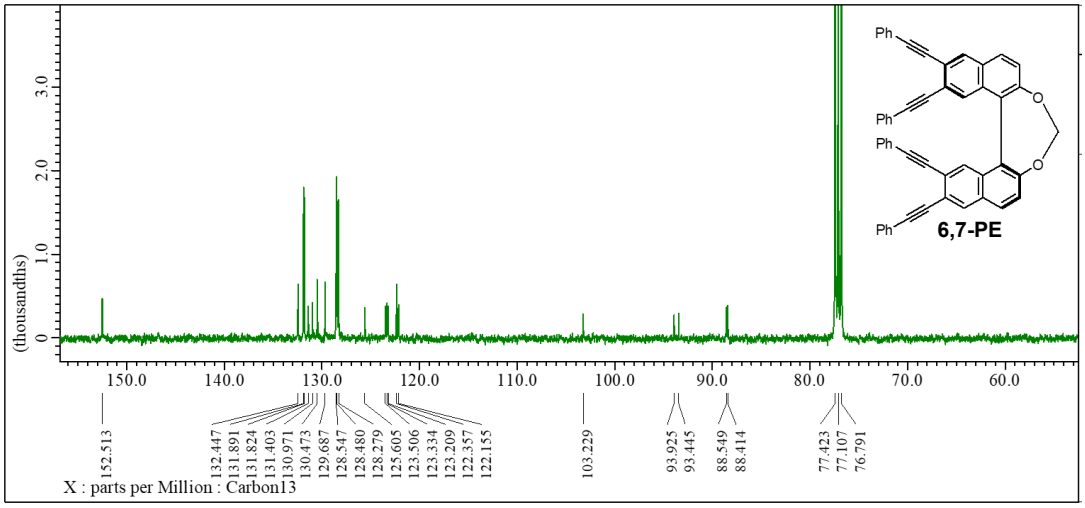

abundance
X : parts per Million : Proton
33

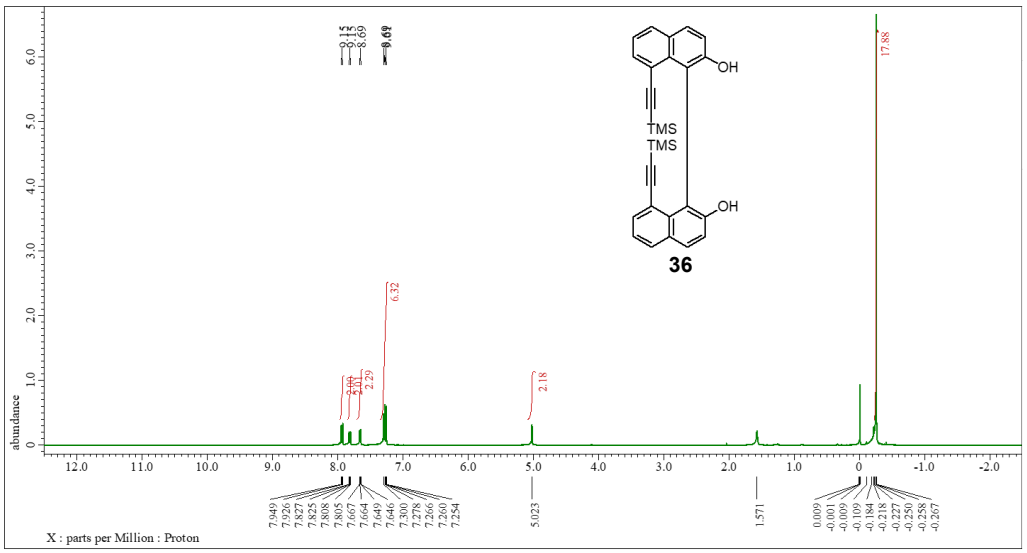

abundance
X : parts per Million : Proton
33

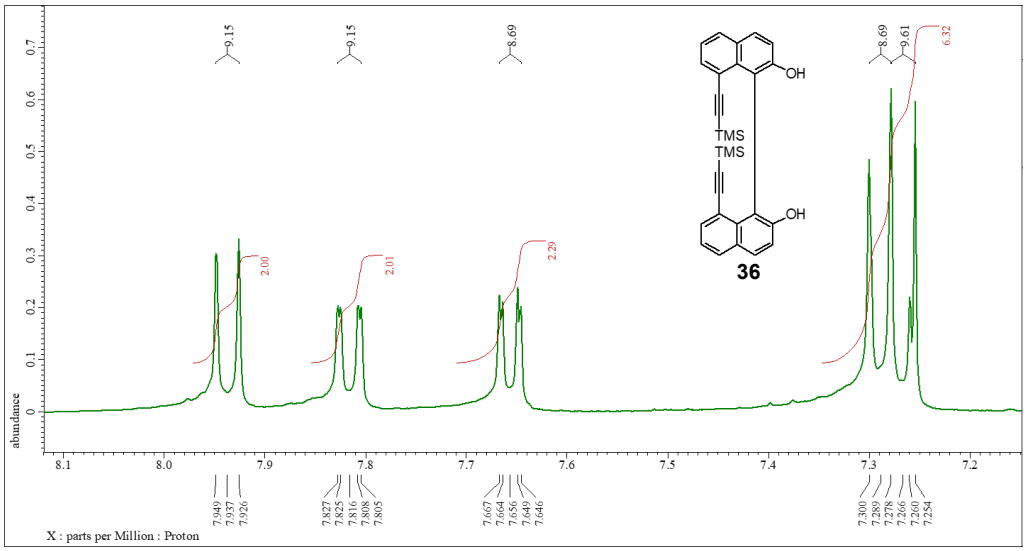

I
Br
Br
I
O
O
33
(thousandths)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
152.580
140.190
132.294
131.863
129.783
129.323
127.617
124.474
122.500
103.364
97.806
77.423
77.107
76.791
X : parts per Million : Carbon13

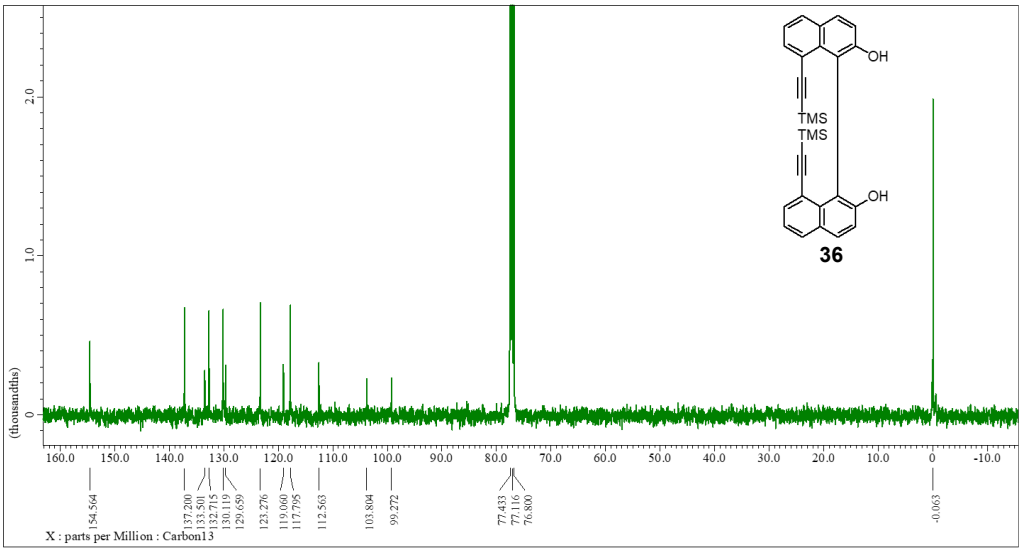

abundance
8.69
6.58
6.77
4.40
2.93
2.00
2.17
2.18
2.18
Ph
Ph
Ph
Ph
O
O
6,7-PE
8.213
7.983
7.972
7.961
7.717
7.600
7.515
7.493
7.472
7.353
7.345
7.337
7.260
7.250
5.690
X : parts per Million : Proton

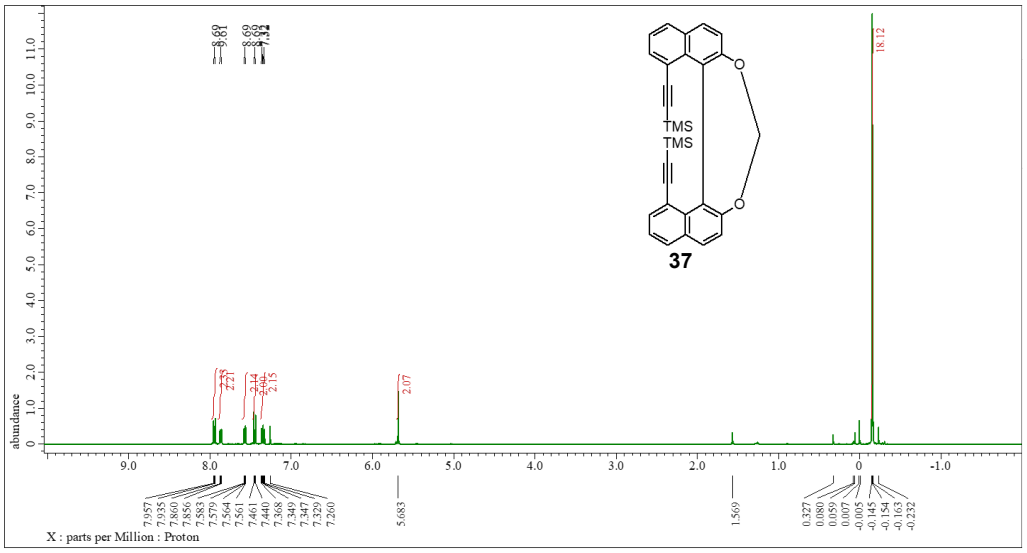

Ph
Ph
Ph
Ph
O
O
6,7-PE
(thousandths)
2.0
1.0
0
160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0
152.513
132.447
131.891
131.824
130.971
130.473
129.687
128.547
128.480
128.279
123.334
122.357
103.229
93.925
93.445
88.549
88.414
77.423
77.107
76.791
X : parts per Million : Carbon13

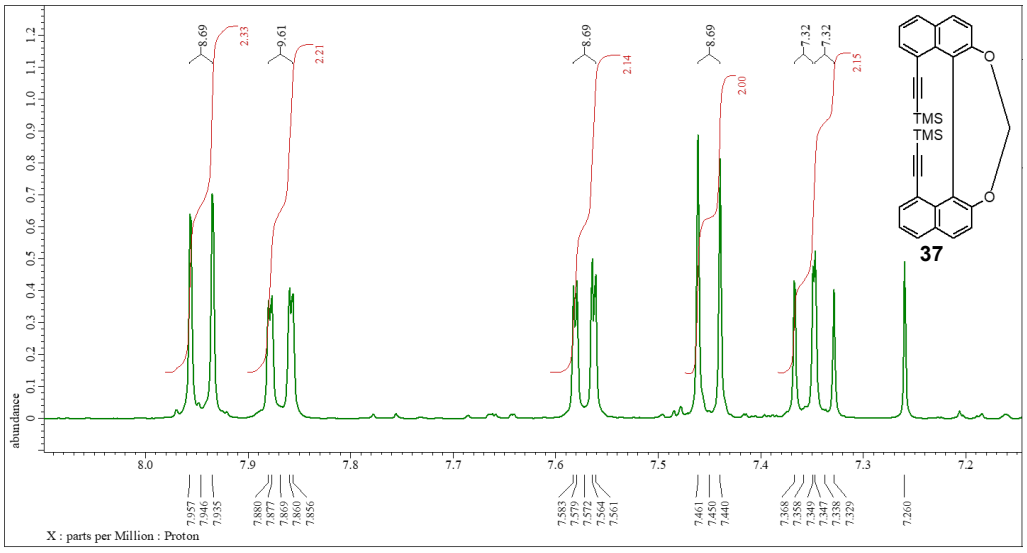

Ph
Ph
Ph
Ph
O
O
6,7-PE
(thousandths)
3.0
2.0
1.0
0
150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0
152.513
132.447
131.891
131.824
131.403
130.971
130.473
129.687
128.547
128.480
128.279
125.605
123.506
123.334
123.209
122.357
122.155
103.229
93.925
93.445
88.549
88.414
77.423
77.107
76.791
X : parts per Million : Carbon13

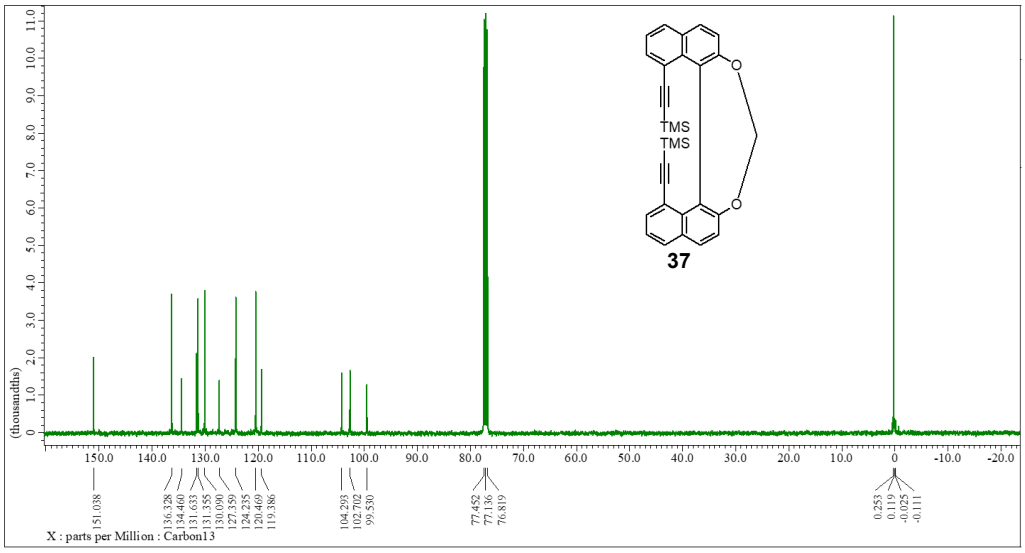

OH
TMS
TMS
OH
36
abundance
X : parts per Million : Proton

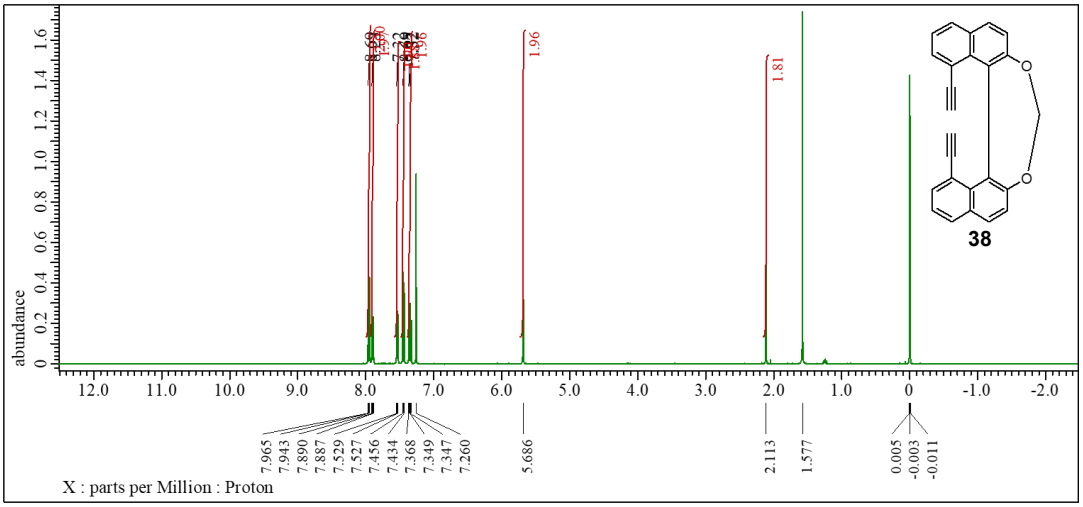

OH
TMS
TMS
OH
36
abundance
X : parts per Million : Proton

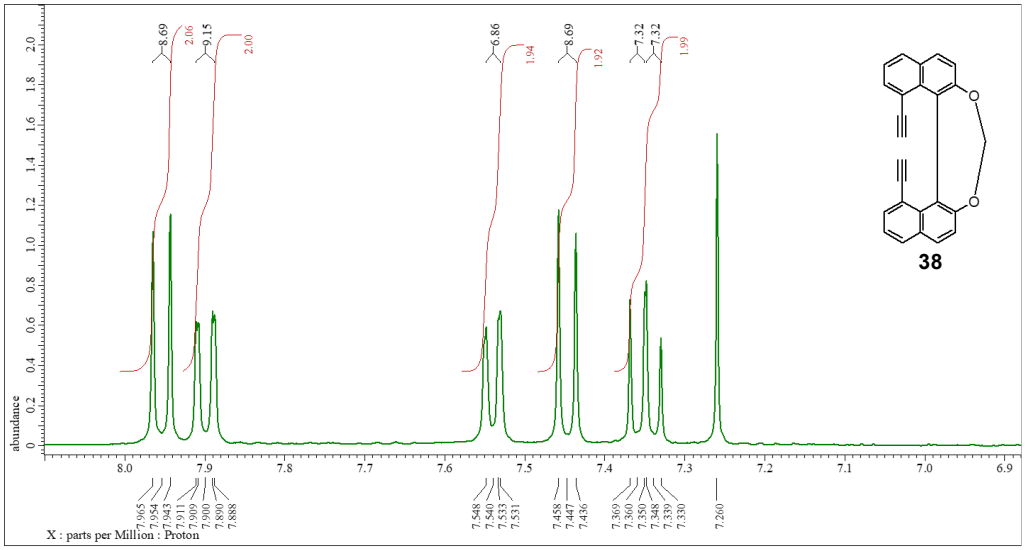

OH
TMS
TMS
OH
36
(thousandths)
2.0
1.0
0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
154.564
137.200
133.501
132.715
130.119
129.659
123.276
119.060
117.795
112.563
103.804
99.272
77.433
77.116
76.800
-0.063
X : parts per Million : Carbon13

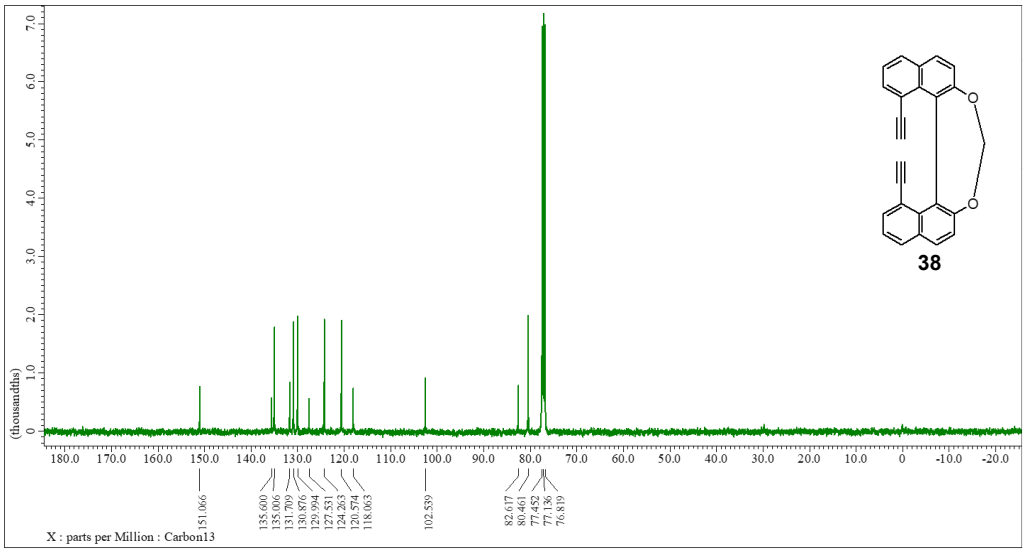

TMS
TMS
37
abundance
X : parts per Million : Proton

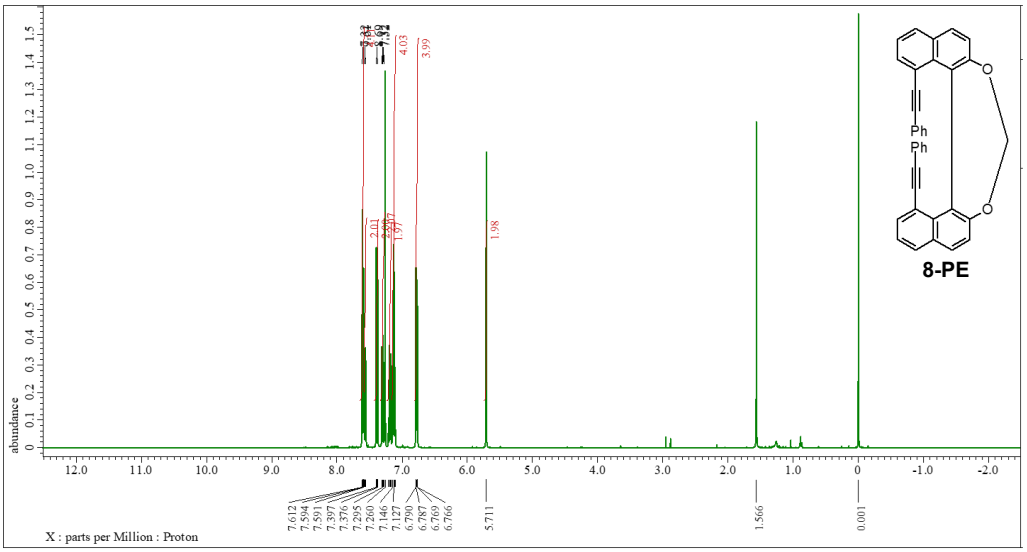

TMS
TMS
37
abundance
X : parts per Million : Proton

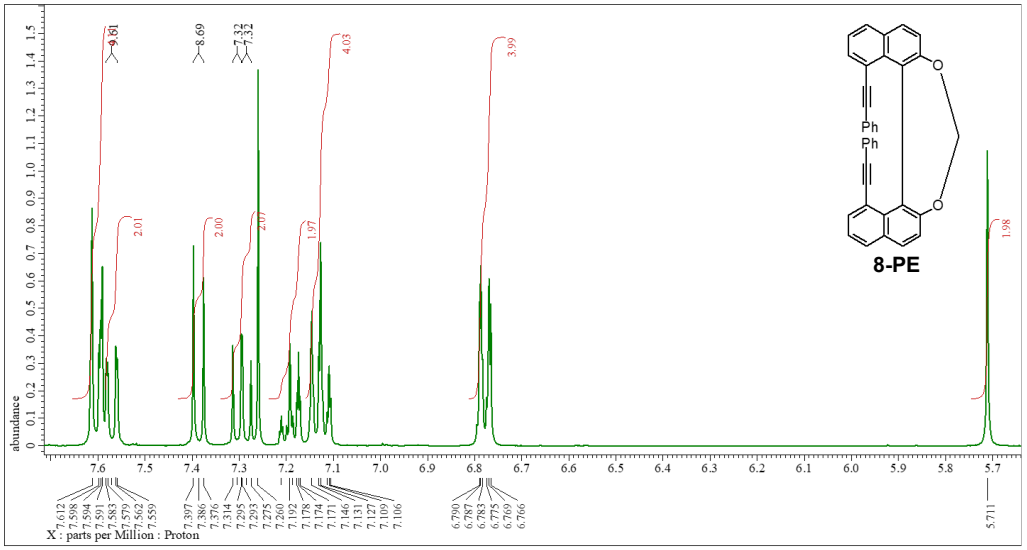

TMS
TMS
O
O
37
(thousandths)
X : parts per Million : Carbon13
151.038
136.328
134.460
131.653
131.355
130.090
127.359
124.235
120.469
119.386
104.293
102.702
99.530
77.452
77.136
76.819
0.253
0.119
-0.025
-0.111

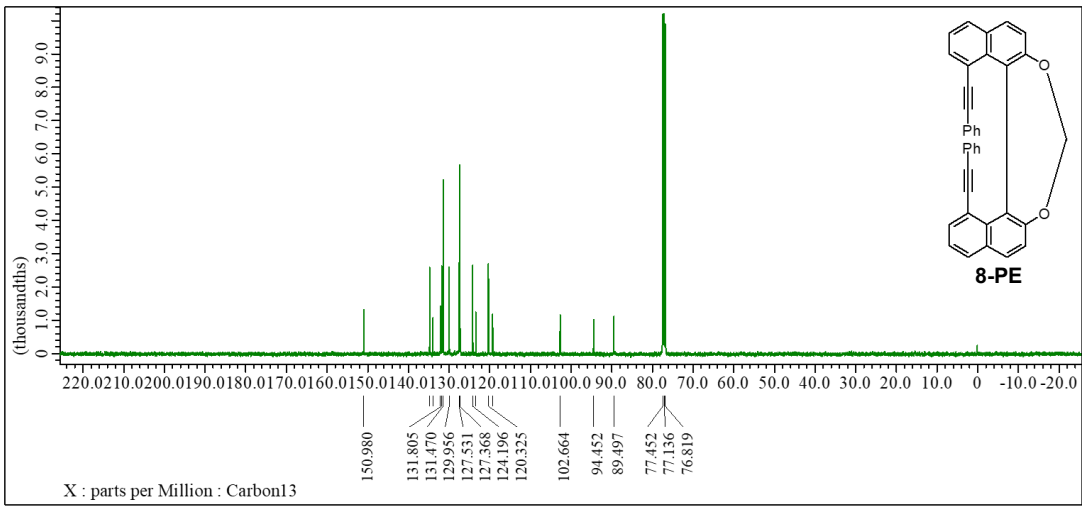

abundance
1.96
1.81
38
7.965
7.943
7.890
7.887
7.529
7.527
7.456
7.434
7.368
7.349
7.347
7.260
5.686
2.113
1.577
0.005
-0.003
-0.011
X : parts per Million : Proton

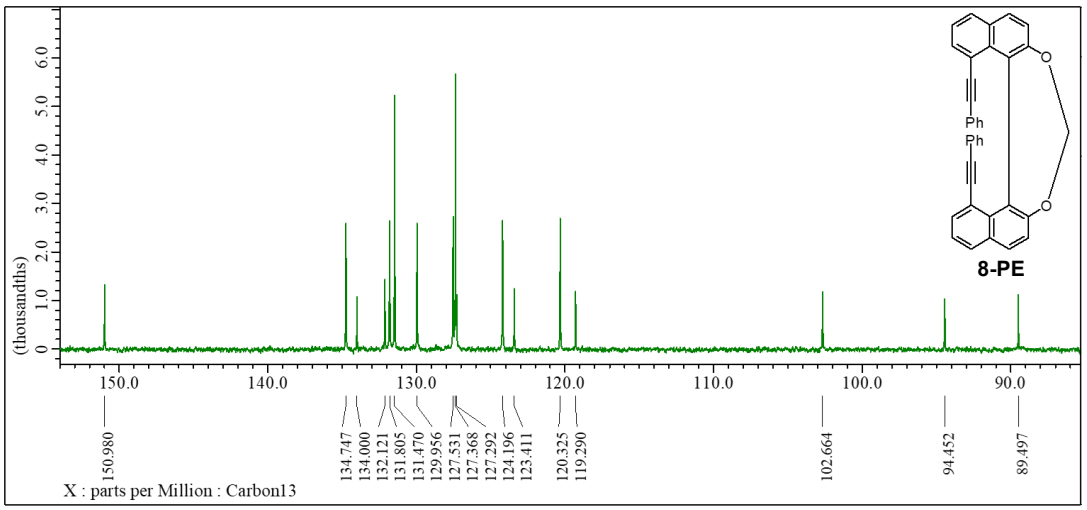

abundance
8.69
2.06
9.15
2.00
6.86
1.94
8.69
1.92
7.32
7.32
1.99
38
7.965
7.954
7.943
7.911
7.909
7.900
7.890
7.888
7.548
7.540
7.533
7.531
7.458
7.447
7.436
7.369
7.360
7.350
7.348
7.339
7.330
7.260
X : parts per Million : Proton

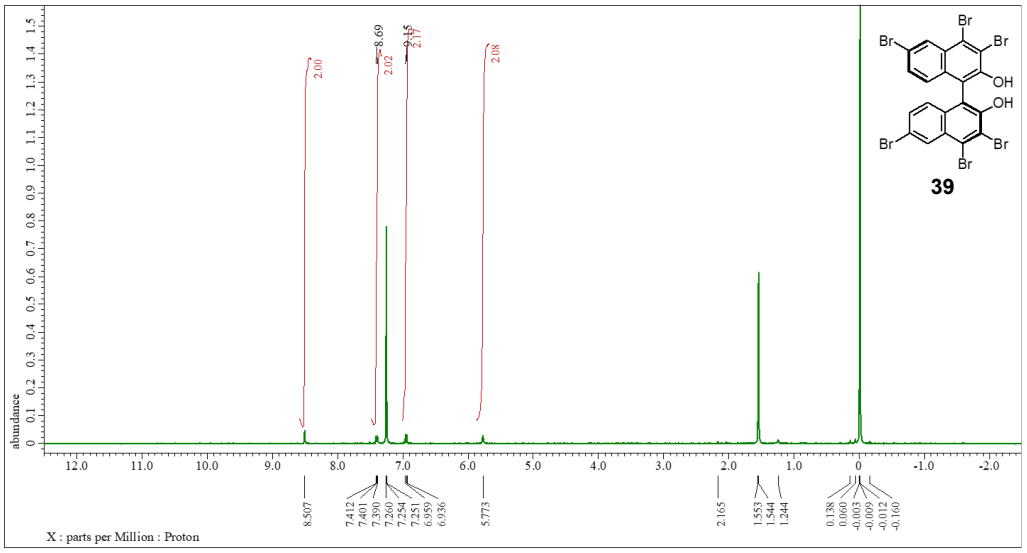

(thousandths)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
151.066
135.600
135.006
131.709
130.876
129.994
127.531
124.263
120.574
118.063
102.539
82.617
80.461
77.452
77.136
76.819
X : parts per Million : Carbon13
O
O
38

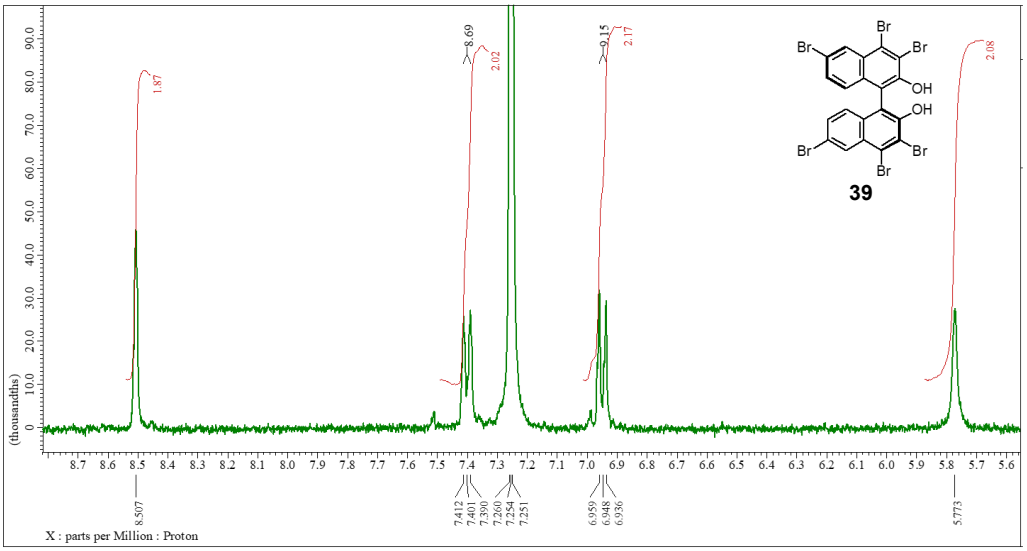

abundance
X : parts per Million : Proton
8-PE

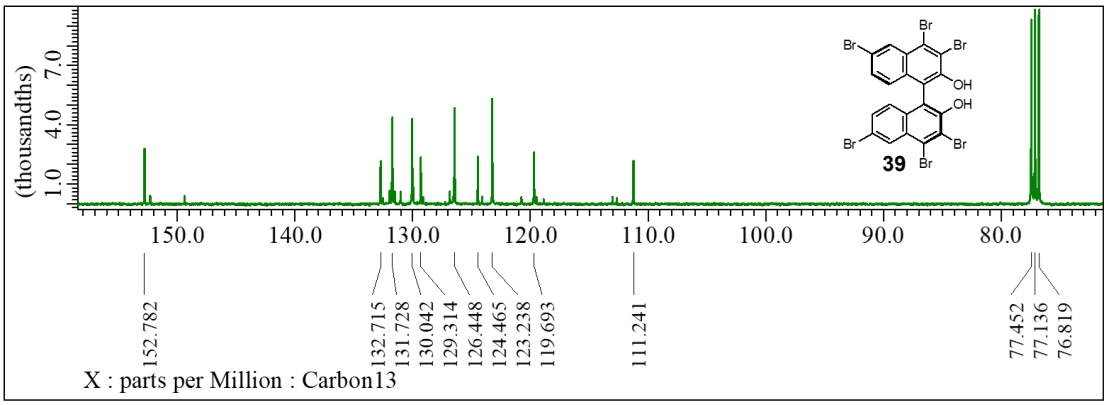

abundance
X : parts per Million : Proton
8-PE

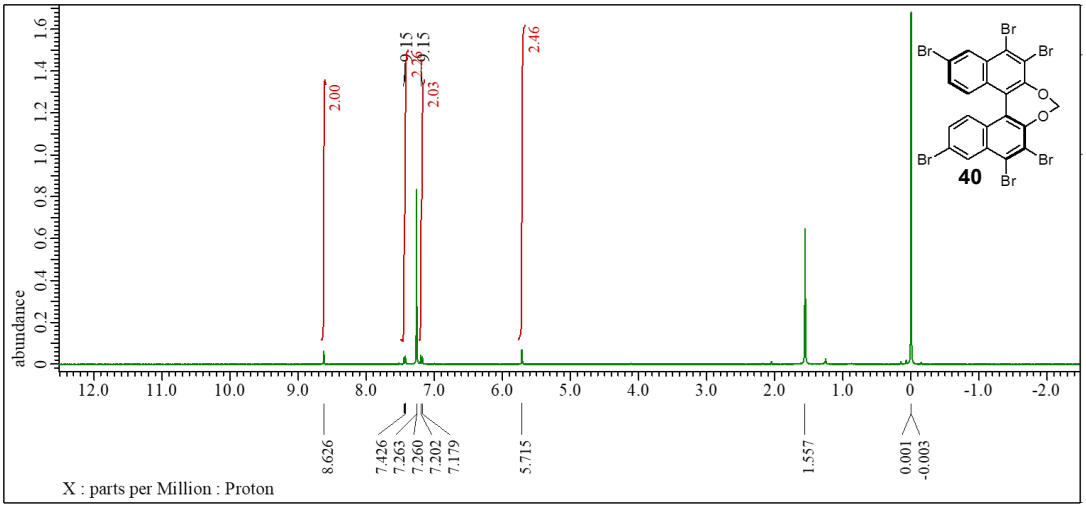

(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
150.980
131.805
131.470
129.956
127.531
127.368
124.196
120.325
102.664
94.452
89.497
77.452
77.136
76.819
X : parts per Million : Carbon13
Ph
Ph
O
O
8-PE

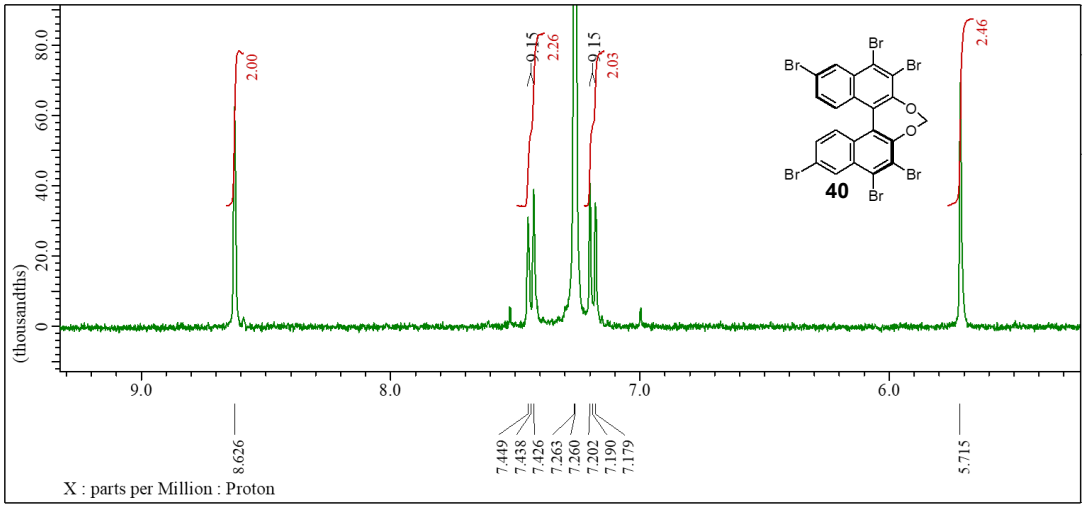

(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0
150.0 140.0 130.0 120.0 110.0 100.0 90.0
150.980
134.747
134.000
132.121
131.805
131.470
129.956
127.531
127.368
127.292
124.196
123.411
120.325
119.290
102.664
94.452
89.497
X : parts per Million : Carbon13
Ph
Ph
O
O
8-PE

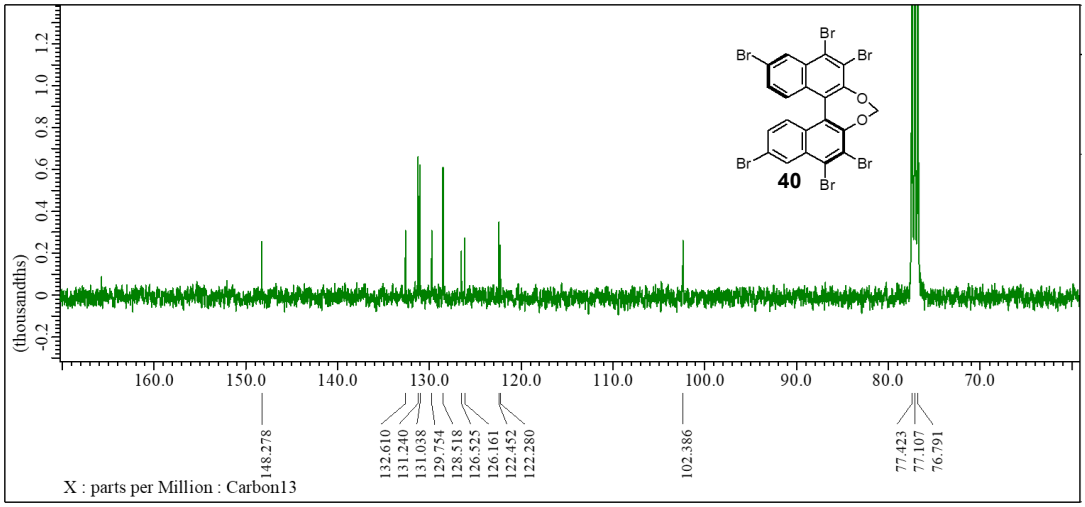

abundance
X : parts per Million : Proton
39

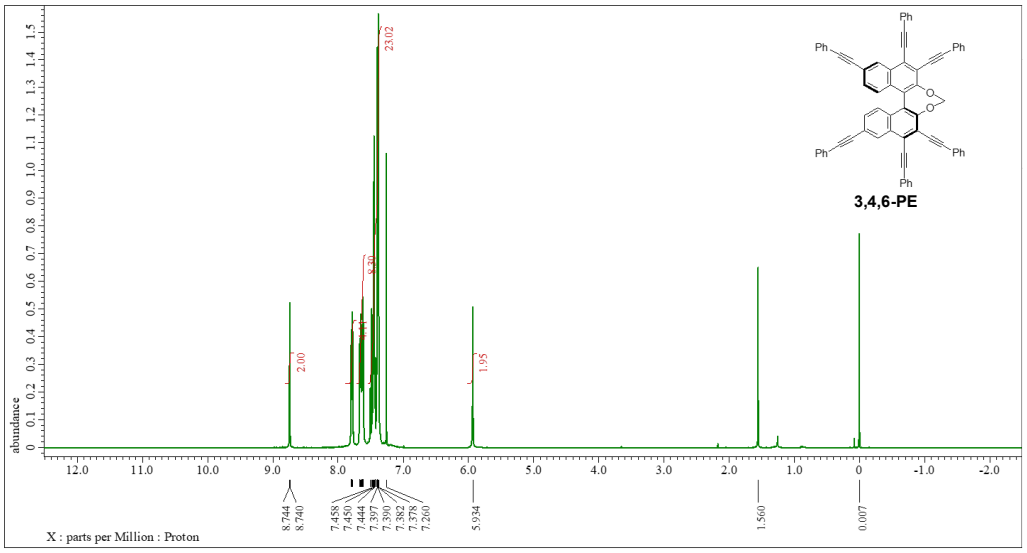

(thousandths)
X : parts per Million : Proton
39

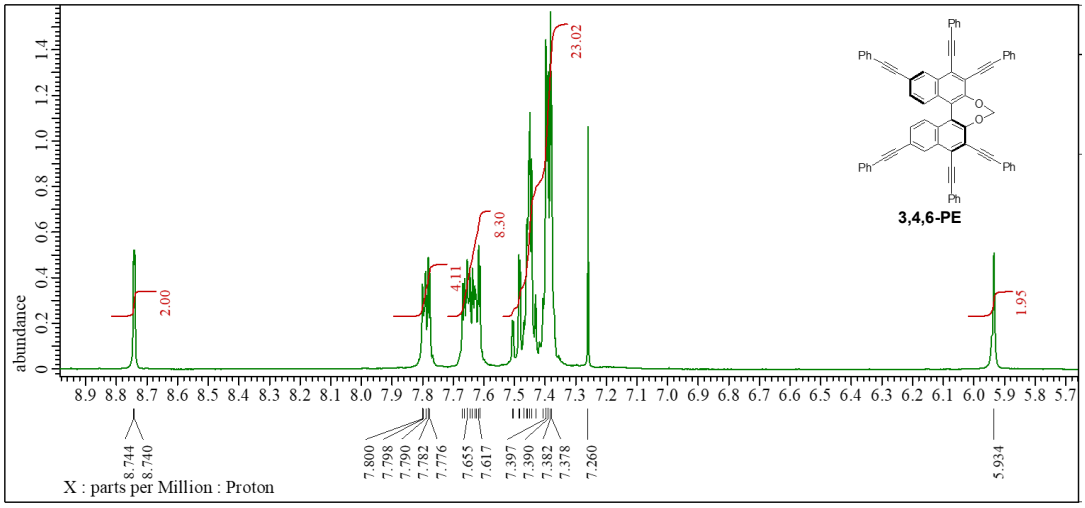

(thousandths)
1.0
4.0
7.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
152.782
132.715
131.728
130.042
129.314
126.448
124.465
123.238
119.693
111.241
77.452
77.136
76.819
X : parts per Million : Carbon13
Br
Br
Br
OH
OH
Br
Br
Br
39

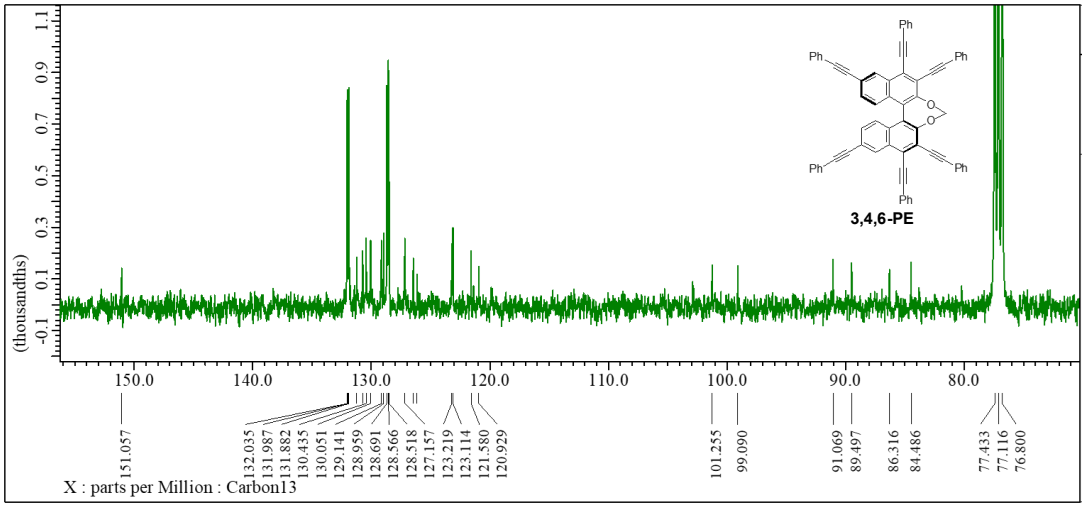

abundance
2.00
9.15
2.26
9.15
2.03
2.46
Br
Br
Br
Br
O
O
Br
Br
40
Br
8.626
7.426
7.263
7.260
7.202
7.179
5.715
1.557
0.001
-0.003
X : parts per Million : Proton

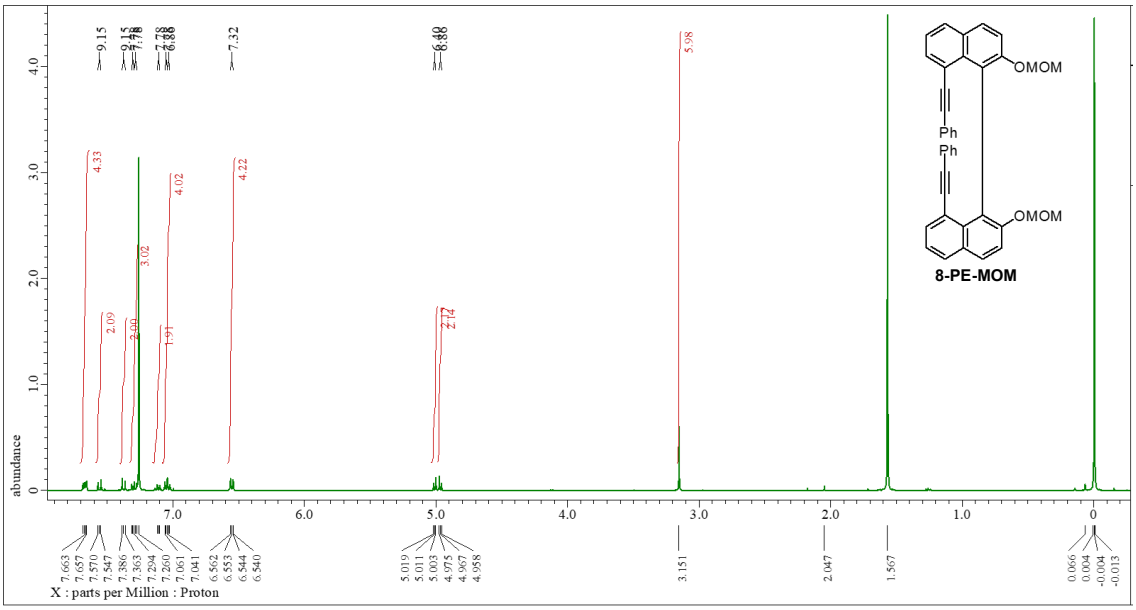

(thousandths)
2.00
9.15
2.26
9.15
2.03
2.46
Br
Br
Br
Br
O
O
Br
Br
40
Br
8.626
7.449
7.438
7.426
7.263
7.260
7.202
7.190
7.179
5.715
X : parts per Million : Proton

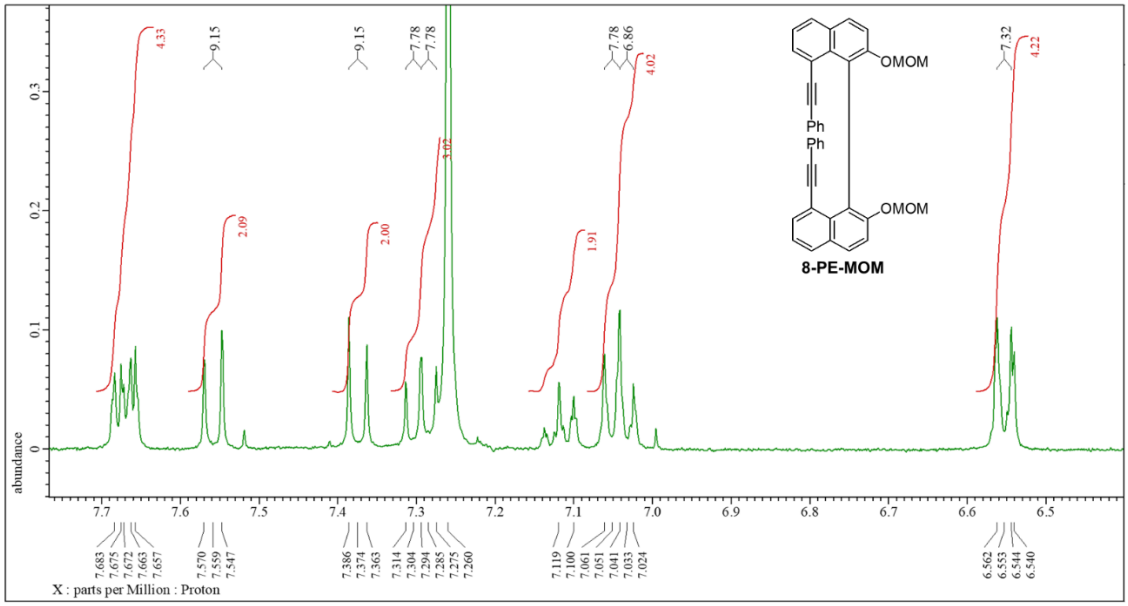

Br
Br
Br
O
O
Br
Br
Br
40
(thousandths)
-0.2
0
0.2
0.4
0.6
0.8
1.0
1.2
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
148.278
132.610
131.240
131.038
129.754
128.518
126.525
126.161
122.452
122.280
102.386
77.423
77.107
76.791
X : parts per Million : Carbon13

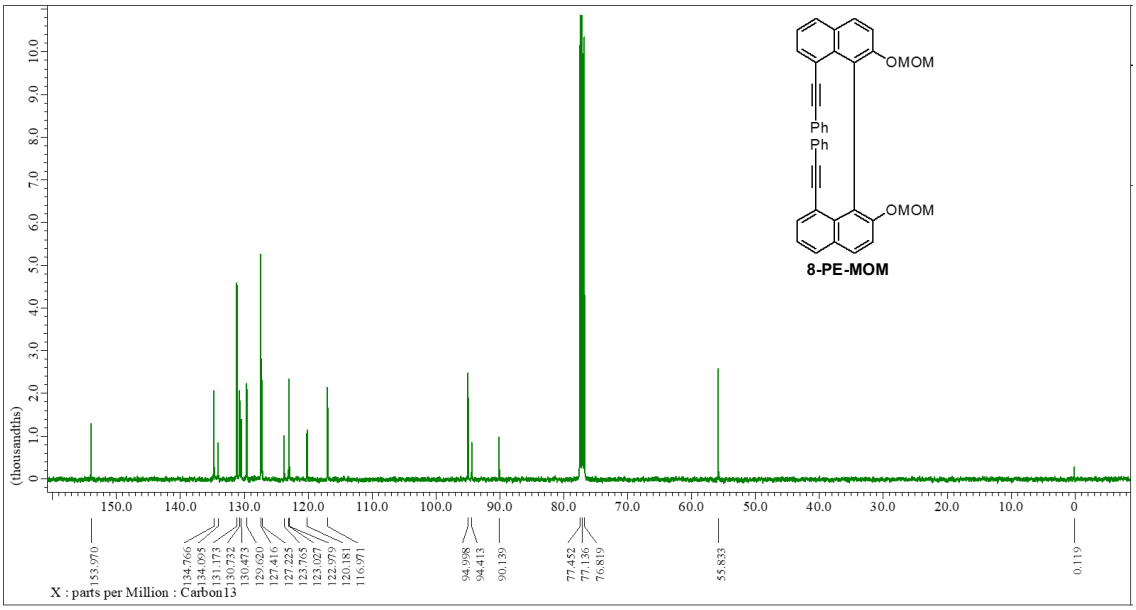

abundance
23.02
8.30
4.11
2.00
1.95
3,4,6-PE
8.744
8.740
7.458
7.444
7.397
7.390
7.382
7.378
7.260
5.934
1.560
0.007
X : parts per Million : Proton


abundance
23.02
8.30
4.11
2.00
1.95
3,4,6-PE
8.744
8.740
7.800
7.798
7.790
7.782
7.776
7.655
7.617
7.397
7.390
7.382
7.378
7.260
5.934
X : parts per Million : Proton


Ph
Ph
Ph
Ph
Ph
Ph
O
O
3,4,6-PE
(thousandths)
-0.1
0.1
0.3
0.5
0.7
0.9
1.1
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
151.057
132.035
131.987
131.882
130.435
130.051
129.141
128.959
128.691
128.566
128.518
127.157
123.219
123.114
121.580
120.929
101.255
99.090
91.069
89.497
86.316
84.486
77.433
77.116
76.800
X : parts per Million : Carbon13


OMOM
Ph
Ph
OMOM
8-PE-MOM
abundance
X : parts per Million : Proton


OMOM
Ph
Ph
OMOM
8-PE-MOM
abundance
X : parts per Million : Proton


OMOM
Ph
Ph
OMOM
8-PE-MOM
(thousandths)
X : parts per Million : Carbon13
153.970
134.766
134.095
131.173
130.732
130.473
129.620
127.416
127.225
123.765
123.027
122.979
120.181
116.971
94.998
94.413
90.139
77.452
77.136
76.819
55.833
0.119