Supporting Information

Catalytic Rearrangement Reaction of *p*-Hydroxybenzyl Alcohols with *o*-Alkynylnaphthols for Synthesis of Naphthopyrans

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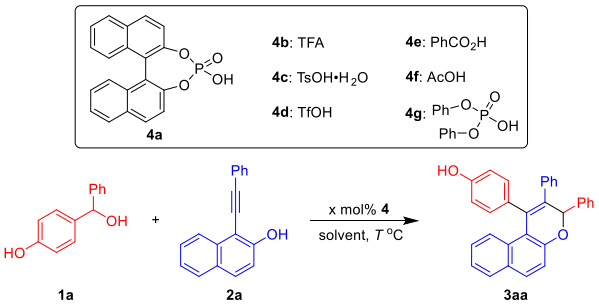
Contents:

1. General information

^{1}H and ^{13}C NMR spectra were measured respectively at 400 and 100 MHz, respectively. The solvent used for NMR spectroscopy were $CDCl_3$, using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a HRMS/MS instrument. Enantiomeric excesses (*ee*) were determined by chiral high-performance liquid chromatography (chiral HPLC). The chiral columns used for the determination of Enantiomeric ratios by chiral HPLC were Chiralpak columns. Optical rotation values were measured with instruments operating at λ = 589 nm, corresponding to the sodium D line at the temperatures indicated. The X-ray source used for the single crystal X-ray diffraction analysis of compounds **3aa** was GaKα (λ = 1.34139), and the thermal ellipsoid was drawn at the 30% probability level. Analytical grade solvents for the column chromatography were distilled before use. All starting materials commercially available were used directly. Substrates **1** and **2** were synthesized according to the literature methods

2. Condition optimizations for catalytic rearrangement reaction

Table S1 Screening of catalysts and optimization of reaction conditions[a]



entry	**Cat.**	solvent	**1a**: **2a**	yield (%)[b]
1	**4a**	DCM	1:1.2	62
2	**4b**	DCM	1:1.2	34
3	**4c**	DCM	1:1.2	45
4	**4d**	DCM	1:1.2	trace
5	**4e**	DCM	1:1.2	trace
6	**4f**	DCM	1:1.2	trace
7	**4g**	DCM	1:1.2	7
8	**4a**	toluene	1:1.2	45
9	**4a**	EtOAc	1:1.2	trace
10	**4a**	THF	1:1.2	trace
11	**4a**	acetone	1:1.2	trace
12	**4a**	MeCN	1:1.2	24
13	**4a**	DCM	1.5: 1	64
14	**4a**	DCM	1.2: 1	59

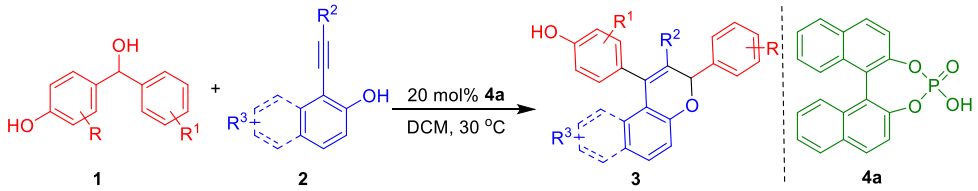
15	**4a**	DCM	1:1.2	65
16	**4a**	DCM	1:1.5	71
17[c]	**4a**	DCM	1:1.5	50
18[d]	**4a**	DCM	1:1.5	73
19[e]	**4a**	DCM	1:1.5	73
20[d, f]	**4a**	DCM	1:1.5	59
21[d, g]	**4a**	DCM	1:1.5	80
22[d,h]	**4a**	DCM	1:1.5	51
23[d,g,i]	**4a**	DCM	1:1.5	57
24[d,g,j]	**4a**	DCM	1:1.5	76
25[d,g,k]	**4a**	DCM	1:1.5	71
26[d,g,k]	**4a**	MeOH	1:1.5	trace
27[d,g,k]	**4a**	EtOH	1:1.5	trace
28[d,g,k]	**4a**	*i*PrOH	1:1.5	trace

[a]Unless otherwise indicated, the reaction was carried out at 0.1 mmol scale and catalyzed by 20 mol% **Cat.** in a solvent (1.0 mL) at 20 °C for 12 h. [b]Isolated yield. [c]Performed in 0.5 mL of DCM. [d]Performed in 2.0 mL of DCM. [e]Performed in 3.0 mL of DCM. [f]Performed at 0 °C, [g]Performed at 30 °C, [h]Performed at 50 °C, [i]Catalyzed by 5 mol% **4a**, [j]Catalyzed by 10 mol% **4a**, [k]Catalyzed by 30 mol% **4a**.

3. Synthetic procedures and characterization data of products 3

General synthetic procedure for substrates 1 and 2: Substrates **1** and **2** are known compounds, and the synthetic procedure for these substrates was followed by the literature methods.[1-2]

General procedure for the synthesis of products 3:



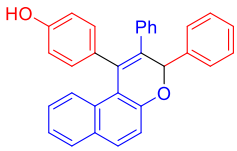
p-Hydroxybenzyl alcohols **1** (0.1 mmol), *o*-alkynylnaphthols **2** (0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, dichloromethane (DCM, 2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA) to afford pure products **3**.

Synthetic procedures and characterization data of products 3:

[1]Y. F. Wong, Z. Wang, J. Sun, *Org. Biomol. Chem.* **2016**, *14*, 5751-5754.

[2]L.-W. Zeng, J.-M. Li, S.-L. Cui, *Angew. Chem. Int. Ed.* **2022**, *61*, e202205037.

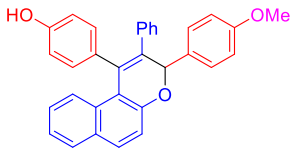
4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3aa):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3aa** in 80% yield (34.1 mg); yellow solid; m.p. 96 – 98 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.60 (m, 4H), 7.34 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 7.19 – 7.08 (m, 6H), 7.07 – 6.82 (m, 5H), 6.68 (d, *J* = 8.0 Hz, 2H), 5.98 (s, 1H), 5.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 151.5, 139.4, 138.2, 133.5, 132.5, 132.0, 130.9, 130.6, 130.5, 129.4, 129.3, 128.9, 128.6, 128.5, 128.5, 127.9, 126.6, 126.3, 125.0, 123.0, 119.1, 118.3, 115.5, 79.8; IR (KBr): 3420, 2819, 1590, 1385, 1351, 1275, 1121, 749, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{22}O_2\text{-}H)^-$ requires m/z 425.1547, found m/z 425.1542.

p-Hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **7c** (6.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (1 mL) was added to the reaction mixture, which was stirred at 25 ^{o}C for 24 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel to afford pure chiral product **3aa** in 45% yield (19.2 mg); The enantiomeric excess: 7%, determined by HPLC (Daicel Chiralpak ID, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, T = 30 ^{o}C, 254 nm): t_R = 3.656 (major), t_R = 4.259 (minor).

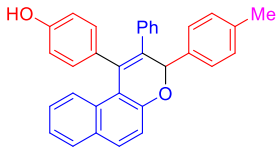
4-(3-(4-methoxyphenyl)-2-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ba):



Following the general procedure, *p*-hydroxybenzyl alcohol **1b** (23.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 3:1) to afford pure product **3ba** in 87% yield (39.7 mg); yellow solid; m.p. 81 – 83 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.50 (m, 4H), 7.21 – 7.06 (m, 6H), 7.05 – 6.84 (m, 5H), 6.80 (d, *J* = 7.6 Hz, 2H), 6.68 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 5.16 (s,

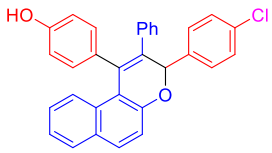
1H), 3.72 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 154.7, 151.4, 139.5, 133.3, 132.5, 132.0, 130.8, 130.6, 130.4, 130.3, 130.0, 129.7, 129.2, 128.5, 127.8, 126.6, 126.2, 125.0, 123.0, 119.1, 118.4, 115.4, 113.9, 79.4, 55.2; IR (KBr): 3444, 1589, 1508, 1385, 1351, 1261, 1121, 764, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_3\text{-}H)^-$ requires m/z 455.1652, found m/z 455.1653.

4-(2-phenyl-3-(*p*-tolyl)-3*H*-benzo[*f*]chromen-1-yl)phenol (3ca):



Following the general procedure, *p*-hydroxybenzyl alcohol **1c** (21.4 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ca** in 73% yield (32.3 mg); yellow solid; m.p. 112 – 114 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 – 7.60 (m, 2H), 7.56 (d, *J* = 7.6 Hz, 2H), 7.19 – 7.06 (m, 8H), 7.05 – 6.75 (m, 5H), 6.68 (d, *J* = 8.0 Hz, 2H), 5.94 (s, 1H), 4.95 (s, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 151.5, 139.5, 138.4, 135.1, 133.4, 132.6, 132.0, 130.8, 130.5, 130.4, 129.5, 129.3, 129.2, 128.9, 128.5, 127.8, 126.6, 126.3, 124.9, 122.9, 119.1, 118.4, 115.4, 79.6, 21.2; IR (KBr): 3346, 1589, 1510, 1385, 1351, 1262, 1120, 749, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_2\text{-}H)^-$ requires m/z 439.1703, found m/z 439.1705.

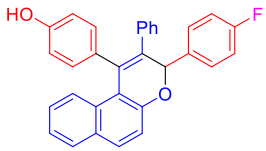
4-(3-(4-chlorophenyl)-2-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3da):



Following the general procedure, *p*-hydroxybenzyl alcohol **1d** (23.5 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3da** in 80% yield (37.1 mg); yellow solid; m.p. 113 – 115 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.58 (m, 4H), 7.26 – 7.21 (m, 2H), 7.20 – 7.15 (m, 1H), 7.14 – 7.06 (m, 5H), 7.05 – 6.80 (m, 5H), 6.69 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 4.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.8, 151.2, 139.2, 136.8, 134.4, 133.8, 132.3, 131.9, 131.1, 130.6, 130.4, 130.2, 129.2, 129.0, 128.7, 128.5, 128.0, 126.8, 126.2, 125.2, 123.2, 119.0,

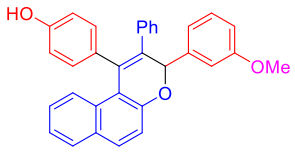
118.2, 115.5, 79.0; IR (KBr): 3446, 1588, 1510, 1458, 1350, 1261, 1012, 750, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}ClO_2\text{-}H)^-$ requires m/z 459.1157, found m/z 459.1158.

4-(3-(4-fluorophenyl)-2-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ea):



Following the general procedure, *p*-hydroxybenzyl alcohol **1e** (21.8 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ea** in 68% yield (30.1 mg); yellow solid; m.p. 72 – 74 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 4H), 7.21 – 7.08 (m, 6H), 7.06 – 6.80 (m, 7H), 6.68 (d, *J* = 8.0 Hz, 2H), 5.94 (s, 1H), 4.99 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8 (d, *J* = 245.9 Hz), 154.8, 151.3, 139.2, 134.0, 133.9, 133.7 (d, *J* = 28.6 Hz), 132.4, 131.9, 131.0, 130.7 (d, *J* = 8.4 Hz), 130.4, 129.4, 129.2, 128.5, 127.9, 126.7, 126.2, 125.1, 123.1, 119.0, 118.2, 115.5, 115.4 (d, *J* = 21.3 Hz), 79.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.19 (s); IR (KBr): 3447, 2089, 1589, 1506, 1459, 1386, 1222, 749, 579 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1453.

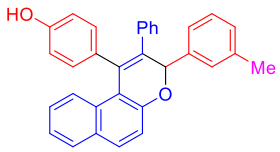
4-(3-(3-methoxyphenyl)-2-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3fa):



Following the general procedure, *p*-hydroxybenzyl alcohol **1f** (23.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 3:1) to afford pure product **3fa** in 71% yield (32.5 mg); yellow solid; m.p. 69 – 71 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.60 (m, 2H), 7.31 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 7.21 – 7.07 (m, 7H), 7.06 – 6.82 (m, 5H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.68 (d, *J* = 7.6 Hz, 2H), 5.95 (s, 1H), 4.92 (s, 1H), 3.71 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 154.7, 151.5, 139.8, 139.4, 133.6, 132.5, 132.0, 130.9, 130.6, 130.5, 129.4, 129.3, 129.2, 128.5, 127.9, 126.6, 126.3, 125.0, 123.0, 121.3, 119.1, 118.3, 115.5, 114.5, 114.1, 79.6, 55.2; IR (KBr): 3420, 1589,

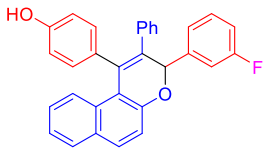
1510, 1458, 1351, 1260, 1122, 749, 618, 526 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_3\text{-}H)^-$ requires m/z 455.1652, found m/z 455.1653.

4-(2-phenyl-3-(*m*-tolyl)-3*H*-benzo[*f*]chromen-1-yl)phenol (3ga):



Following the general procedure, *p*-hydroxybenzyl alcohol **1g** (21.5 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ga** in 58% yield (25.7 mg); yellow solid; m.p. 71 – 73 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.68 – 7.60 (m, 2H), 7.52 – 7.43 (m, 2H), 7.20 – 7.07 (m, 7H), 7.07 – 6.84 (m, 6H), 6.68 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 4.83 (s, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 151.5, 139.4, 138.1, 138.0, 133.4, 132.6, 132.0, 130.8, 130.5, 130.5, 129.8, 129.4, 129.3, 128.4, 128.2, 127.8, 126.6, 126.3, 125.7, 124.9, 122.9, 119.1, 118.3, 115.4, 79.8, 21.5; IR (KBr): 3446, 2115, 1651, 1584, 1510, 1385, 1350, 1122, 749, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_2\text{-}H)^-$ requires m/z 425.1547, found m/z 425.1542.

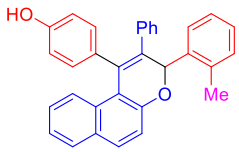
4-(3-(3-fluorophenyl)-2-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ha):



Following the general procedure, *p*-hydroxybenzyl alcohol **1h** (21.8 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ha** in 66% yield (29.3 mg); yellow solid; m.p. 68 – 70 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 2H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.40 (d, *J* = 9.6 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.25 – 7.10 (m, 6H), 7.09 – 6.76 (m, 6H), 6.74 – 6.61 (m, 2H), 5.97 (s, 1H), 4.89 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.9 (d, *J* = 244.9 Hz), 154.8, 151.3, 141.1 (d, *J* = 6.3 Hz), 139.2, 133.9, 132.3, 132.0, 131.1, 130.5 (d, *J* = 17.2 Hz), 129.9 (d, *J* = 7.9 Hz), 129.2, 128.8, 128.5, 128.0, 126.8, 126.3, 125.1, 124.4 (d, *J* = 2.7 Hz), 123.2, 119.0, 118.2, 115.9, 115.7 (d, *J* = 4.6 Hz), 115.5, 79.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.93 (s);

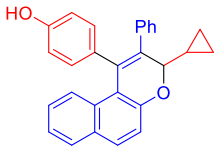
IR (KBr): 3455, 2089, 1651, 1580, 1386, 1275, 1124, 750, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1453.

4-(2-phenyl-3-(*o*-tolyl)-3*H*-benzo[*f*]chromen-1-yl)phenol (3ia):



Following the general procedure, *p*-hydroxybenzyl alcohol **1i** (21.5 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ia** in 77% yield (33.9 mg); yellow solid; m.p. 75 – 77 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.75 (d, *J* = 7.6 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.24 – 7.13 (m, 4H), 7.13 – 6.93 (m, 8H), 6.93 – 6.87 (m, 2H), 6.69 (d, *J* = 8.0 Hz, 2H), 6.18 (s, 1H), 4.80 (s, 1H), 2.65 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 151.5, 139.6, 138.6, 134.9, 133.9, 132.6, 132.0, 131.0, 130.8, 130.6, 130.4, 129.1, 129.0, 128.7, 128.5, 127.9, 126.6, 126.2, 125.6, 125.0, 122.9, 119.0, 118.1, 115.4, 19.7; IR (KBr): 3445, 1651, 1589, 1511, 1386, 1261, 1171, 765, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_2\text{-}H)^-$ requires m/z 439.1703, found m/z 439.1702.

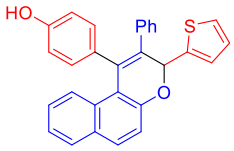
4-(3-cyclopropyl-2-phenyl-3H-benzo[*f*]chromen-1-yl)phenol (3ja):



Following the general procedure, *p*-hydroxybenzyl alcohols **1j** (16.6 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ja** in 78% yield (30.5 mg); white solid; m.p. 140 – 142 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.71 (m, 2H), 7.33 (d, *J* = 8.8 Hz, 1H), 7.26 – 7.07 (m, 7H), 7.06 – 6.99 (m, 1H), 6.91 – 6.69 (m, 2H), 6.57 (d, *J* = 8.0 Hz, 2H), 5.08 (s, 1H), 4.04 (d, *J* = 9.6 Hz, 1H), 1.52 – 1.38 (m, 1H), 0.82 – 0.68 (m, 1H), 0.68 – 0.58 (m, 1H), 0.58 – 0.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 152.7, 139.5, 133.9, 132.5, 131.8, 131.7, 130.6, 130.5, 130.0, 128.5, 127.8, 126.5, 126.3, 125.2, 123.1, 118.9, 118.3, 115.1,

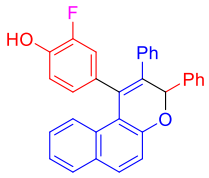
84.0, 13.9, 5.6, 3.4; IR: 3416, 3055, 1618, 1510, 1432, 1384, 1223, 1025, 814, 599 cm^{-1}; ESI FTMS exact mass calcd for $(C_{28}H_{22}O_2+H)^+$ requires m/z 391.1693, found m/z 391.1682.

4-(2-phenyl-3-(thiophen-2-yl)-3H-benzo[*f*]chromen-1-yl)phenol (3ka):



Following the general procedure, *p*-hydroxybenzyl alcohols **1k** (20.6 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ka** in 82% yield (35.4 mg); yellow solid; m.p. 145 – 147 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.64 (m, 2H), 7.37 – 7.30 (m, 1H), 7.24 – 7.10 (m, 7H), 7.09 – 6.76 (m, 6H), 6.73 – 6.60 (m, 2H), 6.20 (s, 1H), 5.03 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 151.0, 142.1, 139.0, 133.0, 132.3, 132.0, 131.1, 130.7, 130.5, 130.1, 129.2, 128.6, 128.4, 128.0, 127.1, 126.9, 126.7, 126.4, 125.1, 123.2, 119.1, 118.4, 115.5, 75.2; IR: 3413, 3055, 1616, 1510, 1431, 1386, 1225, 1006, 835, 592 cm^{-1}; ESI FTMS exact mass calcd for $(C_{29}H_{20}O_2S-H)^-$ requires m/z 433.1257, found m/z 433.1247.

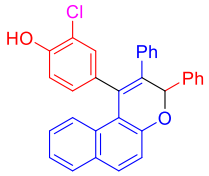
4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)-2-fluorophenol (3la):



Following the general procedure, *p*-hydroxybenzyl alcohol **1l** (21.8 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3la** in 71% yield (31.5 mg); yellow solid; m.p. 64 – 66 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.57 (m, 4H), 7.35 – 7.26 (m, 2H), 7.26 – 7.22 (m, 1H), 7.21 – 7.06 (m, 6H), 7.06 – 7.00 (m, 1H), 6.96 – 6.89 (m, 2H), 6.89 – 6.64 (m, 3H), 5.96 (s, 1H), 5.23 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 151.0 (d, *J* = 236.8 Hz), 142.7 (d, *J* = 14.2 Hz), 139.0, 137.9, 133.0 (d, *J* = 6.4 Hz), 132.6, 131.1, 130.5, 130.3 (d, *J* = 3.2 Hz), 129.2, 128.8, 128.6, 128.6, 128.5, 128.0, 127.3, 126.9, 126.0, 125.2, 123.1, 118.6, 118.3, 117.7 (d, *J* = 19.8 Hz), 117.2, 79.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -140.55 (s); IR (KBr): 3447, 2088, 1589, 1515,

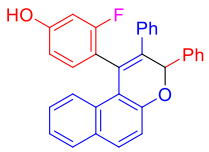
1350, 1276, 1118, 815, 749, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1453.

2-chloro-4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ma):



Following the general procedure, *p*-hydroxybenzyl alcohol **1m** (23.5 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ma** in 64% yield (29.3 mg); yellow solid; m.p. 71 – 73 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.60 (m, 4H), 7.33 – 7.26 (m, 2H), 7.26 – 7.21 (m, 1H), 7.20 – 7.11 (m, 5H), 7.10 – 6.99 (m, 3H), 6.98 – 6.78 (m, 4H), 5.96 (s, 1H), 5.57 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 150.4, 138.9, 137.9, 133.4, 132.3, 131.1, 130.8, 130.5, 130.4, 130.2, 129.2, 128.8, 128.6, 128.6, 128.5, 128.0, 126.9, 126.0, 125.3, 123.2, 119.9, 118.5, 118.3, 116.2, 79.8; IR (KBr): 3447, 2089, 1589, 1497, 1386, 1351, 1277, 1123, 1049, 748, 698 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}ClO_2\text{-}H)^-$ requires m/z 459.1157, found m/z 459.1162.

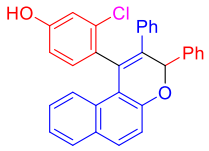
4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)-3-fluorophenol (3na):



Following the general procedure, *p*-hydroxybenzyl alcohol **1n** (21.8 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^oC for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3na** in 91% yield (40.6 mg); yellow solid; 67:33 dr; m.p. 87 – 89 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.60 (m, 4H), 7.34 – 7.28 (m, 2H), 7.26 – 7.23 (m, 1H), 7.22 – 7.09 (m, 6H), 7.08 – 6.95 (m, 3H), 6.92 – 6.28 (m, 3H), 6.08 – 5.98 (m, 1H), 5.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9 (d, *J* = 246.6 Hz), 160.3 (d, *J* = 245.1 Hz), 156.8, 156.7, 156.5, 151.3, 150.8, 139.4, 138.9, 138.1, 137.8, 133.5 (d, *J* = 5.4 Hz), 132.3 (d, *J* = 5.2 Hz), 131.6, 131.4, 130.9, 130.7, 130.5, 130.3, 130.1, 129.1, 129.0, 128.9, 128.8, 128.7, 128.6, 128.5, 128.4, 128.2, 127.9, 127.9, 127.0, 126.9 (d, *J* = 20.4 Hz), 125.6, 125.4 (d, *J* = 7.8 Hz), 124.1, 123.2, 120.3 (d, *J* =

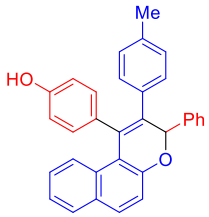
15.5 Hz), 120.2 (d, *J* = 16.0 Hz), 118.7, 118.5, 118.3, 111.8 (d, *J* = 2.8 Hz), 103.9 (d, *J* = 25.5 Hz), 103.6 (d, *J* = 24.7 Hz), 79.6, 79.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -109.76 (s), -110.68 (s); IR (KBr): 3443, 2089, 1588, 1508, 1459, 1386, 1275, 1112, 1012, 749, 619 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1452.

3-chloro-4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3oa):



Following the general procedure, *p*-hydroxybenzyl alcohol **1o** (23.5 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3oa** in 87% yield (40.6 mg); yellow solid; 60:40 dr; m.p. 65 – 67 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 – 7.61 (m, 4H), 7.39 – 7.26 (m, 3H), 7.25 – 7.04 (m, 7H), 7.04 – 6.74 (m, 4H), 6.70 – 6.56 (m, 1H), 6.05 (s, 1H), 5.08 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.6, 155.5, 151.1, 150.8, 139.3, 138.9, 138.1, 137.8, 134.9, 134.4, 133.9, 132.9, 131.8, 131.7, 131.5, 131.4, 131.2, 131.0, 130.9, 130.7, 130.5, 130.2, 130.1, 129.3, 128.9, 128.7, 128.6, 128.6, 128.5, 128.4, 128.3, 127.9, 127.8, 127.0, 125.7, 125.6, 125.2, 123.9, 123.1, 123.1, 119.1, 118.6, 118.3, 117.1, 116.8, 114.7, 114.6, 80.1, 79.2; IR (KBr): 3446, 1651, 1586, 1496, 1386, 1279, 748, 698, 557 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}ClO_2\text{-}H)^-$ requires m/z 459.1157, found m/z 459.1157.

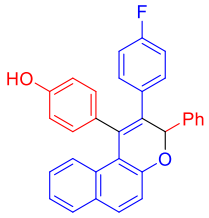
4-(3-phenyl-2-(*p*-tolyl)-3*H*-benzo[*f*]chromen-1-yl)phenol (3ab):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2b** (38.7 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ab** in 67% yield (29.4 mg); yellow solid; m.p. 74 – 76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 – 7.58 (m, 4H), 7.32 – 7.26 (m, 2H), 7.26 – 7.21 (m, 1H), 7.18 – 7.09 (m, 3H), 7.07 – 6.85 (m, 5H), 6.85 – 6.79 (m, 2H), 6.74 – 6.65

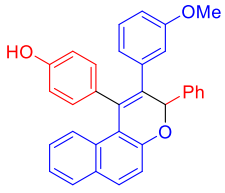
(m, 2H), 5.96 (s, 1H), 4.94 (s, 1H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 151.3, 138.3, 136.5, 136.3, 133.1, 132.8, 132.0, 130.7, 130.6, 130.4, 129.3, 129.1, 128.8, 128.6, 128.5, 128.5, 128.4, 126.3, 124.9, 123.0, 119.2, 118.3, 115.5, 79.8, 21.2; IR (KBr): 3444, 2089, 1651, 1584, 1508, 1386, 1264, 1222, 1012, 748, 545 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_2\text{-}H)^-$ requires m/z 439.1703, found m/z 439.1703.

4-(2-(4-fluorophenyl)-3-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ac):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2c** (39.3 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ac** in 65% yield (28.8 mg); yellow solid; m.p. 70 – 72 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.58 (m, 4H), 7.33 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 7.19 – 7.08 (m, 3H), 7.07 – 6.82 (m, 5H), 6.82 – 6.75 (m, 2H), 6.69 (d, *J* = 8.0 Hz, 2H), 5.93 (s, 1H), 5.00 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3 (d, *J* = 245.3 Hz), 154.8, 151.5, 137.9, 135.4 (d, *J* = 3.4 Hz), 133.8, 132.3, 131.9, 131.0 (d, *J* = 2.4 Hz), 130.9, 130.6, 130.4, 128.8, 128.7, 128.5, 128.5, 128.3, 126.2, 125.1, 123.1, 118.9, 118.3, 115.6, 114.8 (d, *J* = 21.1 Hz), 79.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.82 (s); IR (KBr): 3447, 2088, 1590, 1506, 1458, 1385, 1224, 1159, 1014, 748, 544 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1453.

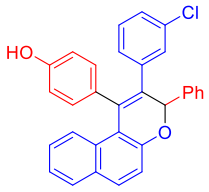
4-(2-(3-methoxyphenyl)-3-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ad):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2d** (41.1 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 3:1) to afford pure product **3ad** in 74% yield (33.6 mg); yellow solid; m.p. 101 – 103 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 – 7.60 (m, 4H),

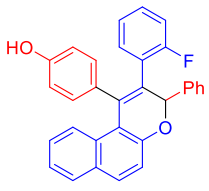
7.36 – 7.26 (m, 2H), 7.25 – 7.21 (m, 1H), 7.19 – 7.11 (m, 3H), 7.09 – 6.81 (m, 4H), 6.74 – 6.63 (m, 3H), 6.55 (d, *J* = 7.6 Hz, 1H), 6.47 (s, 1H), 5.98 (s, 1H), 5.05 (s, 1H), 3.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 154.8, 151.5, 140.7, 138.1, 133.7, 132.6, 131.9, 131.0, 130.6, 130.5, 129.2, 128.9, 128.8, 128.6, 128.5, 128.4, 126.3, 125.0, 123.0, 121.7, 119.0, 118.3, 115.5, 114.8, 112.9, 79.7, 55.0; IR (KBr): 3421, 1590, 1510, 1351, 1264, 1228, 1170, 1050, 749, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_3\text{-H})^-$ requires m/z 455.1652, found m/z 455.1652.

4-(2-(3-chlorophenyl)-3-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ae):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2e** (41.8 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ae** in 72% yield (33.3 mg); yellow solid; m.p. 62 – 64 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 – 7.61 (m, 4H), 7.33 – 7.27 (m, 2H), 7.26 – 7.22 (m, 1H), 7.19 – 7.07 (m, 4H), 7.06 – 6.83 (m, 5H), 6.80 (d, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 2H), 5.94 (s, 1H), 5.05 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 151.7, 141.2, 137.8, 134.6, 133.7, 132.0, 131.9, 131.3, 130.6, 130.5, 129.3, 129.1, 128.8, 128.5, 127.8, 127.7, 126.8, 126.2, 125.2, 123.1, 118.8, 118.3, 115.6, 79.4; IR (KBr): 3443, 1589, 1510, 1386, 1262, 1171, 1013, 815, 748, 617 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}ClO_2\text{-H})^-$ requires m/z 459.1157, found m/z 459.1157.

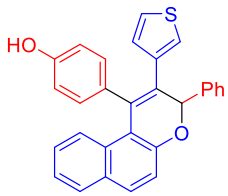
4-(2-(2-fluorophenyl)-3-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3af):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2f** (39.3 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3af** in 75% yield (33.4 mg); yellow solid; m.p. 106 – 108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.60 – 7.51

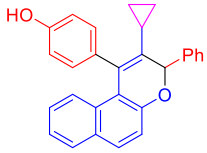
(m, 2H), 7.25 – 7.17 (m, 5H), 7.17 – 7.13 (m, 1H), 7.08 – 7.00 (m, 2H), 6.99 – 6.85 (m, 3H), 6.85 – 6.76 (m, 2H), 6.60 (d, *J* = 8.0 Hz, 2H), 5.92 (s, 1H), 4.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1 (d, *J* = 242.7 Hz), 154.6, 153.0, 137.7, 135.8, 132.4, 131.9, 131.3, 131.1, 130.5 (d, *J* = 3.4 Hz), 128.8, 128.7, 128.5, 128.4, 128.1, 126.9 (d, *J* = 16.7 Hz), 126.2, 125.9, 125.3, 123.5 (d, *J* = 3.3 Hz), 123.2, 118.5, 118.1, 115.3, 115.1, 80.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.04 (s); IR (KBr): 3445, 2089, 1589, 1511, 1386, 1227, 1103, 1009, 749, 599 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}FO_2\text{-}H)^-$ requires m/z 443.1453, found m/z 443.1454.

4-(3-phenyl-2-(thiophen-2-yl)-3*H*-benzo[*f*]chromen-1-yl)phenol (3ag):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2g** (37.5 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ag** in 68% yield (29.1 mg); yellow solid; m.p.122 – 124 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.66 (m, 2H), 7.65 – 7.57 (m, 2H), 7.33 – 7.27 (m, 2H), 7.26 – 7.23 (m, 1H), 7.23 – 7.08 (m, 4H), 7.07 – 6.86 (m, 3H), 6.85 – 6.66 (m, 3H), 6.43 (d, *J* = 4.8 Hz, 1H), 6.04 (s, 1H), 4.83 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.0, 151.1, 140.0, 138.2, 133.1, 133.0, 131.7, 130.8, 130.6, 130.4, 128.5, 128.5, 128.4, 126.2, 125.0, 124.7, 123.9, 123.8, 123.0, 118.6, 118.3, 115.8, 79.1; IR (KBr): 3444, 2089, 1589, 1561, 1386, 1224, 1010, 814, 747, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{29}H_{20}O_2S\text{-}H)^-$ requires m/z 431.1111, found m/z 431.1110.

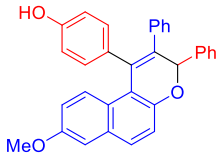
4-(2-cyclopropyl-3-phenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ah):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2h** (31.2 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 10:1) to afford pure product **3ah** in 78% yield (30.4 mg); yellow solid; m.p.

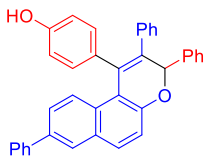
61– 63 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 8.0 Hz, 1H), 7.59 – 7.53 (m, 3H), 7.34 – 7.18 (m, 4H), 7.17 – 6.93 (m, 5H), 6.93 – 6.57 (m, 2H), 5.45 (s, 1H), 5.05 (s, 1H), 2.10 – 1.99 (m, 1H), 0.79 – 0.62 (m, 3H), 0.54 – 0.46 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 150.7, 138.6, 132.9, 132.4, 131.6, 130.5, 130.1, 129.7, 128.4, 128.2, 128.2, 128.0, 126.0, 124.9, 122.8, 119.1, 118.3, 115.5, 73.9, 13.1, 7.0, 6.0; IR (KBr): 3443, 2819, 2148, 1589, 1511, 1351, 1262, 1122, 751, 618 cm^{-1}; ESI FTMS exact mass calcd for $(C_{28}H_{22}O_2\text{-}H)^-$ requires m/z 389.1547, found m/z 389.1549.

4-(8-methoxy-2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3ai):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2i** (41.1 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 3:1) to afford pure product **3ai** in 55% yield (24.9 mg); yellow solid; m.p. 74 – 76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 2H), 7.59 – 7.49 (m, 2H), 7.36 – 7.26 (m, 3H), 7.21 – 7.03 (m, 4H), 7.02 – 6.84 (m, 4H), 6.81 (d, *J* = 9.2 Hz, 1H), 6.74 – 6.67 (m, 2H), 6.51 (s, 1H), 5.96 (s, 1H), 5.01 (s, 1H), 3.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.7, 154.7, 152.1, 139.3, 138.2, 133.5, 132.7, 132.1, 131.7, 130.6, 129.8, 129.4, 129.3, 128.8, 128.6, 128.5, 127.8, 126.6, 125.8, 118.2, 115.8, 115.7, 115.5, 105.8, 79.7, 54.5; IR (KBr): 3420, 2824, 1593, 1511, 1351, 1232, 1134, 1026, 699, 617 cm^{-1}; ESI FTMS exact mass calcd for $C_{32}H_{24}O_3\text{-}H)^-$ requires m/z 455.1652, found m/z 455.1651.

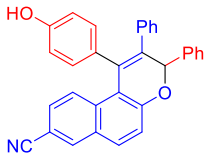
4-(2,3,8-triphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3aj):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2j** (48.1 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3aj** in 83% yield (41.9 mg); yellow solid; m.p. 74 – 76 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.63 (m, 4H), 7.48 – 7.43 (m, 2H), 7.39 – 7.26 (m, 5H),

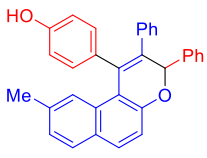
7.25 – 7.21 (m, 1H), 7.21 – 6.87 (m, 10H), 6.79 (d, *J* = 7.6 Hz, 2H), 6.02 (s, 1H), 5.02 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 151.8, 141.1, 139.3, 138.1, 137.2, 133.6, 132.9, 130.6, 130.5, 129.7, 129.4, 129.3, 129.0, 128.9, 128.6, 128.5, 127.9, 127.4, 127.2, 126.7, 125.1, 122.4, 119.3, 118.4, 115.6, 79.7; IR (KBr): 3440, 2927, 2088, 1590, 1510, 1385, 1263, 1171, 1054, 699 cm^{-1}; ESI FTMS exact mass calcd for $(C_{37}H_{26}O_2\text{-}H)^-$ requires m/z 501.1860, found m/z 501.1860.

1-(4-hydroxyphenyl)-2,3-diphenyl-3H-benzo[*f*]chromene-8-carbonitrile (3ak):



Following the general procedure, *p*-hydroxybenzyl alcohols **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2k** (40.4 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3ak** in 54% yield (24.3 mg); white solid; m.p. 132 – 134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.69 – 7.61 (m, 3H), 7.36 – 7.27 (m, 3H), 7.24 – 7.17 (m, 2H), 7.15 – 7.08 (m, 4H), 7.07 – 6.75 (m, 4H), 6.75 – 6.68 (m, 2H), 6.03 (s, 1H), 5.38 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.1, 153.9, 138.8, 137.5, 134.4, 132.7, 132.1, 131.8, 131.7, 131.1, 130.3, 129.4, 129.2, 128.9, 128.8, 128.6, 128.0, 127.1, 127.0, 125.6, 120.2, 119.5, 119.4, 115.8, 106.2, 80.0; IR: 3413, 3059, 2228, 1616, 1512, 1466, 1387, 1239, 1013, 834, 699 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{21}NO_2\text{+}H)^+$ requires m/z 452.1645, found m/z 452.1643.

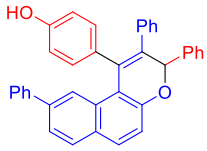
4-(9-methyl-2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3al):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2l** (38.7 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3al** in 67% yield (30.2 mg); yellow solid; m.p. 95 – 97 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.66 (m, 2H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.43 (s, 1H), 7.34 – 7.27 (m, 2H), 7.26 – 7.20 (m, 1H), 7.16 – 7.08 (m, 4H), 7.08 – 6.88 (m, 5H), 6.86 (d, *J* =

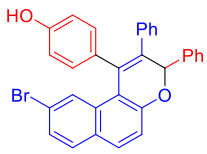
8.8 Hz, 1H), 6.73 – 6.64 (m, 2H), 5.97 (s, 1H), 4.91 (s, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 150.9, 139.4, 138.2, 133.6, 132.6, 132.4, 132.0, 130.8, 130.2, 129.4, 129.3, 128.9, 128.5, 128.4, 127.8, 127.5, 127.2, 126.6, 126.1, 119.0, 118.3, 115.4, 79.7, 21.1; IR (KBr): 3446, 2089, 1651, 1575, 1510, 1385, 1263, 1098, 749, 699 cm^{-1}; ESI FTMS exact mass calcd for $(C_{32}H_{24}O_2\text{-}H)^-$ requires m/z 439.1703, found m/z 439.1703.

4-(2,3,9-triphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3am):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2m** (48.1 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3am** in 80% yield (40.0 mg); yellow solid; m.p. 98 – 100 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.74 – 7.67 (m, 3H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.45 – 7.39 (m, 2H), 7.36 – 7.26 (m, 5H), 7.21 – 7.15 (m, 2H), 7.15 – 7.09 (m, 3H), 7.09 – 6.84 (m, 4H), 6.71 (d, *J* = 8.0 Hz, 2H), 6.01 (s, 1H), 4.96 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.8, 151.6, 140.7, 139.4, 138.2, 135.5, 133.5, 132.5, 132.0, 131.2, 130.9, 129.6, 129.5, 129.3, 128.9, 128.8, 128.6, 128.5, 127.9, 127.1, 126.8, 126.7, 126.2, 124.6, 119.1, 118.8, 115.5, 79.8; IR (KBr): 3420, 1590, 1510, 1351, 1261, 1170, 836, 758, 697 cm^{-1}; ESI FTMS exact mass calcd for $(C_{37}H_{26}O_2\text{-}H)^-$ requires m/z 501.1860, found m/z 501.1858.

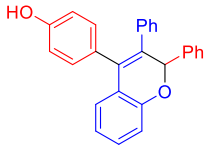
4-(9-bromo-2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenol (3an):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2n** (48.5 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 5:1) to afford pure product **3an** in 68% yield (34.3 mg); yellow solid; m.p. 69 – 71 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.65 (d, *J* = 7.2 Hz, 2H), 7.52 (d, *J* = 8.8 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.26 – 7.21 (m, 1H), 7.18 – 7.08 (m, 4H), 7.07 – 7.04 (m, 1H), 7.03 – 6.77 (m,

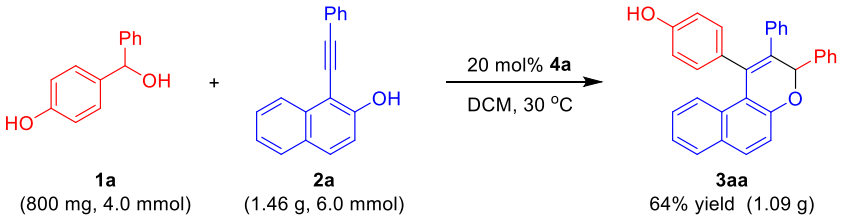
5H), 6.69 (d, *J* = 7.6 Hz, 2H), 5.98 (s, 1H), 4.95 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 151.7, 139.1, 137.9, 133.1, 132.2, 131.9, 131.8, 130.3, 129.9, 129.8, 129.2, 128.9, 128.8, 128.7, 128.5, 128.2, 127.9, 126.8, 119.4, 119.4, 116.8, 115.6, 79.8; IR (KBr): 3447, 1651, 1585, 1510, 1385, 1350, 1236, 1171, 1015, 698, 530 cm^{-1}; ESI FTMS exact mass calcd for $(C_{31}H_{21}BrO_2\text{-}H)^-$ requires m/z 503.0652, found m/z 503.0652.

4-(2,3-diphenyl-2*H*-chromen-4-yl)phenol (3ao):



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2o** (29.1 mg, 0.15 mmol), catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Then, DCM (2 mL) was added to the reaction mixture, which was stirred at 30 ^{o}C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 10:1) to afford pure product **3ao** in 36% yield (13.5 mg); yellow solid; m.p. 63 – 65^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.52 (m, 2H), 7.37 – 7.29 (m, 3H), 7.13 – 7.03 (m, 6H), 6.94 – 6.87 (m, 3H), 6.83 – 6.73 (m, 4H), 6.00 (s, 1H), 4.81 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.7, 151.8, 138.9, 138.7, 133.4, 132.2, 130.7, 129.6, 129.3, 129.0, 128.6, 128.5, 127.8, 126.8, 126.4, 125.3, 121.1, 116.7, 115.3, 79.9; IR (KBr): 3445, 2924, 2089, 1646, 1586, 1510, 1386, 1227, 1016, 738, 611 cm^{-1}; ESI FTMS exact mass calcd for $(C_{27}H_{20}O_2\text{-}H)^-$ requires m/z 375.1390, found m/z 375.1400.

4. Procedure for gram-scale reaction

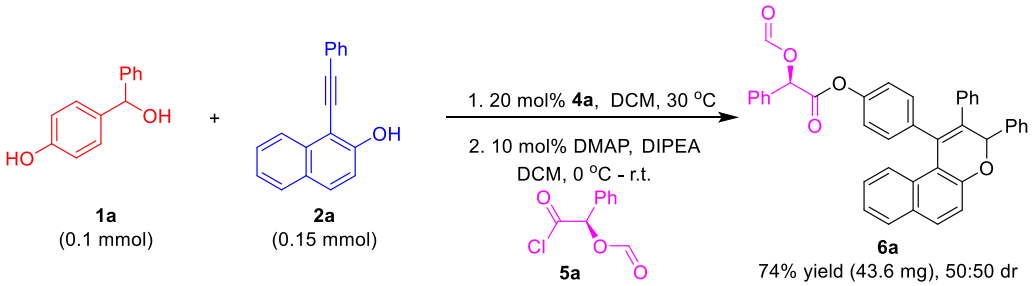


1a (800 mg, 4.0 mmol) **2a** (1.46 g, 6.0 mmol) **3aa** 64% yield (1.09 g)

p-Hydroxybenzyl alcohol **1a** (800 mg, 4.0 mmol), *o*-alkynylnaphthol **2a** (1.46 g, 6.0 mmol), catalyst **4a** (278.4 mg, 0.8 mmol) were added to a reaction tube. Then, DCM (80 mL) was added to the reaction mixture, which was stirred at 30 °C for 36 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was purified through flash column chromatography on silica gel (PE:EA = 10:1) to afford pure product **3aa** (1.09 g, 64%).

5. Synthetic procedures and characterization data of compounds 6.

Synthetic procedure and characterization data of compound 6:

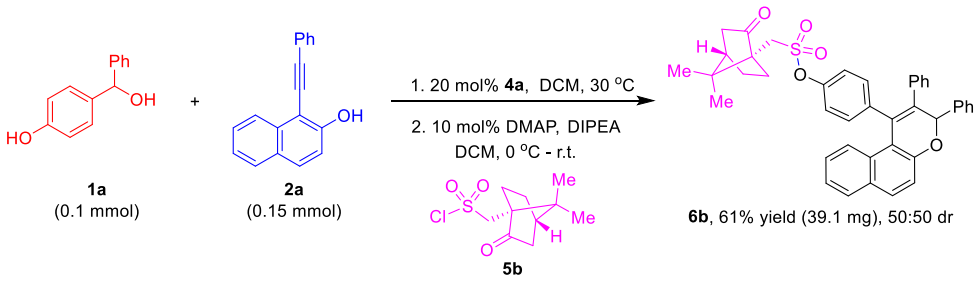


1a (0.1 mmol) **2a** (0.15 mmol) **6a** 74% yield (43.6 mg), 50:50 dr

Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), and catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Dichloromethane (DCM, 2 mL) was then added, and the reaction mixture was stirred at 30 °C for 36 h. Upon completion of the reaction as monitored by TLC, 4-dimethylaminopyridine (DMAP, 3.6 mg, 0.03 mmol) and *i*-Pr_2NEt (DIPEA, 52.2 uL, 0.3 mmol) were directly added to the mixture. Subsequently, (*R*)-(-)-*O*-formylmandeloyl chloride (36.4 μL, 0.24 mmol) was added dropwise at 0 °C, and the mixture was stirred at room temperature for an additional 6 h. After confirming reaction completion by TLC analysis, the mixture was diluted by DCM and quenched with hydrochloric acid (1 M). The resultant mixture was extracted by DCM, and the organic layer was washed successively by saturated $NaHCO_3$ aqueous solution and saturated NaCl aqueous solution. Subsequently, the resultant organic layer was dried by anhydrous Na_2SO_4 and concentrated in vacuo to give a residue, which was further purified by preparative

thin layer chromatography (PE:DCM = 2:1) to afford pure products **6a** (43.6 mg, 74% yield, 50:50 dr).

4-(2,3-diphenyl-3*H*-benzo[*f*]chromen-1-yl)phenyl (2*R*)-2-(formyloxy)-2-phenylacetate (6a): 74% yield (43.6 mg); white solid; 50:50 dr; m.p. 72 – 74 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.81 – 7.51 (m, 7H), 7.50 – 7.41 (m, 3H), 7.30 – 7.27 (m, 2H), 7.18 – 7.08 (m, 7H), 7.02 – 6.98 (m, 2H), 6.93 – 6.87 (m, 4H), 6.28 (s, 1H), 5.98 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 159.9, 151.6, 149.3, 138.9, 138.2, 137.9, 133.0, 132.8, 131.7, 131.1, 130.5, 130.50, 130.2, 129.8, 129.3, 129.1, 128.9, 128.7, 128.6, 128.5, 128.0, 127.8, 127.0, 126.8, 126.1, 125.3, 123.2, 121.2, 121.1, 118.7, 118.3, 115.5, 79.8, 74.0; IR (KBr): 3446, 2089, 1775, 1730, 1585, 1386, 1275, 1141, 1017, 749, 698, 593 cm^{-1}; ESI FTMS exact mass calcd for $(C_{40}H_{28}O_5+Na)^+$ requires m/z 611.1829, found m/z 611.1803.



Following the general procedure, *p*-hydroxybenzyl alcohol **1a** (20.0 mg, 0.10 mmol), *o*-alkynylnaphthol **2a** (33.6 mg, 0.15 mmol), and catalyst **4a** (7.0 mg, 0.02 mmol) were added to a reaction tube. Dichloromethane (DCM, 2 mL) was then added, and the reaction mixture was stirred at 30 °C for 36 h. Upon completion of the reaction as monitored by TLC, 4-dimethylaminopyridine (DMAP, 3.6 mg, 0.03 mmol) and *i*-Pr_2NEt (DIPEA, 52.2 uL, 0.3 mmol) were directly added to the mixture. Subsequently, *L*-(−)-10-camphorsulfonyl chloride (60.2 mg, 0.24 mmol) was added dropwise at 0 °C, and the mixture was stirred at room temperature for an additional 6 h. After confirming reaction completion by TLC analysis, the mixture was diluted by DCM and quenched with hydrochloric acid (1 M). The resultant mixture was extracted by DCM, and the organic layer was washed successively by saturated $NaHCO_3$ aqueous solution and saturated NaCl aqueous solution. Subsequently, the resultant organic layer was dried by anhydrous Na_2SO_4 and concentrated in vacuo to give a residue, which was further purified by preparative thin layer chromatography (PE:DCM = 2:1) to afford pure products **6b** (39.1 mg, 61% yield,

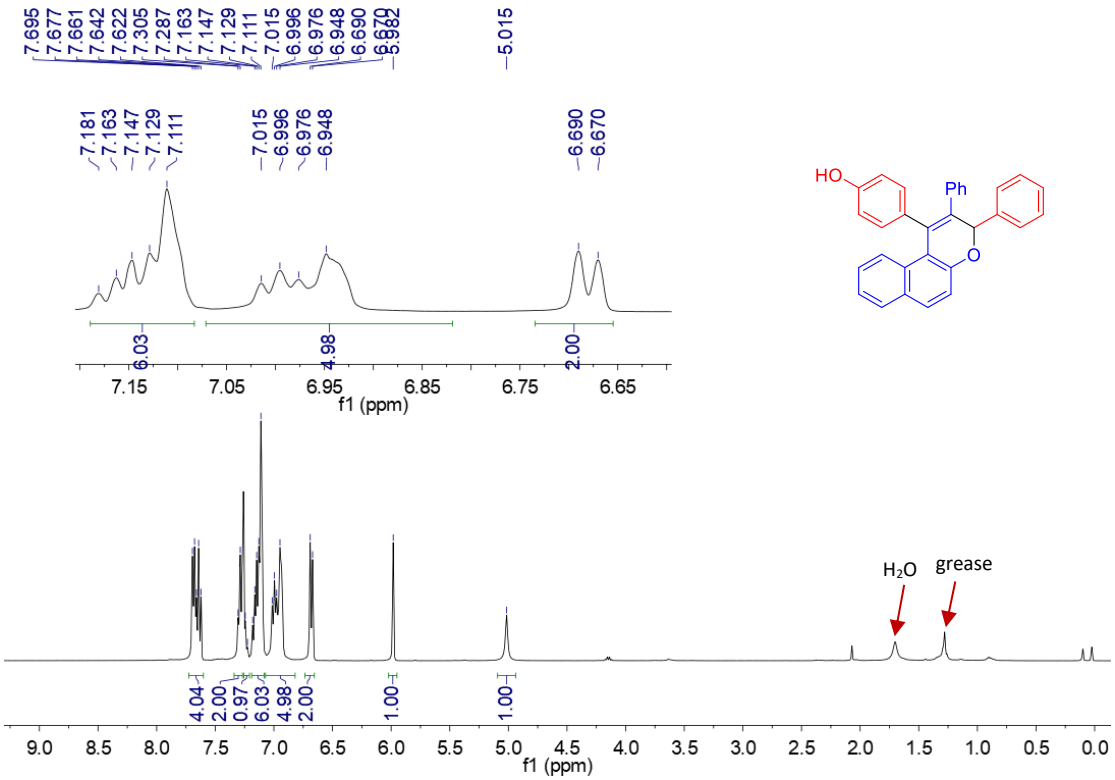
50:50 dr).

4-(2,3-diphenyl-3H-benzo[*f*]chromen-1-yl)phenyl ((1R,4S)-7,7-dimethyl-2-oxobicyclo[2.2.1]heptan-1-yl)methanesulfonate (6b):

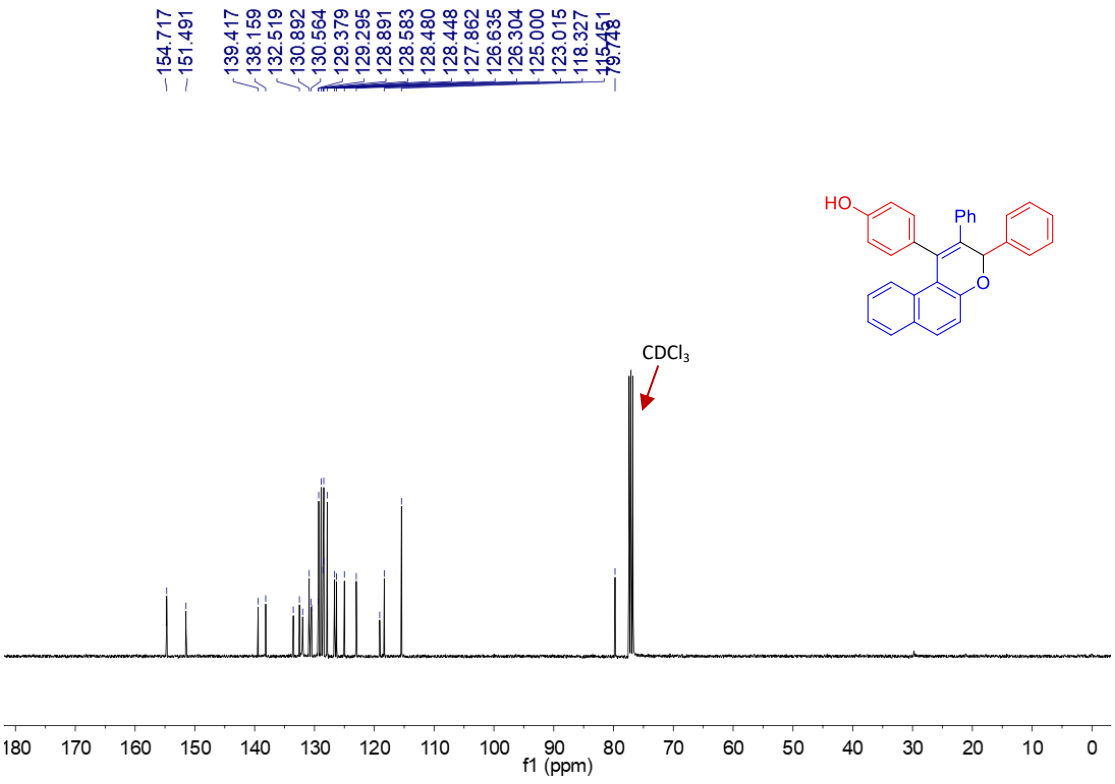
61% yield (39.1 mg); white solid; 50:50 dr; m.p. 68 – 70 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 – 7.61 (m, 4H), 7.35 – 7.26 (m, 3H), 7.25 – 7.06 (m, 9H), 7.05 – 6.96 (m, 2H), 6.95 – 6.87 (m, 2H), 6.00 (s, 1H), 3.81 (d, *J* = 14.8 Hz, 1H), 3.18 (d, *J* = 14.8 Hz, 1H), 2.62 – 2.52 (m, 1H), 2.44 (d, *J* = 18.4 Hz, 1H), 2.19 – 2.05 (m, 2H), 1.99 (d, *J* = 19.2 Hz, 1H), 1.78 – 1.70 (m, 1H), 1.48 (t, *J* = 11.2 Hz, 1H), 1.18 (s, 3H), 0.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 213.9, 151.7, 148.4, 139.3, 139.3, 138.7, 137.9, 132.8, 132.2, 131.2, 130.7, 130.6, 130.1, 129.3, 128.8, 128.7, 128.6, 128.5, 128.0, 127.1, 126.0, 125.3, 123.2, 122.0, 121.9, 118.5, 118.3, 79.8, 58.1, 48.0, 47.3, 42.9, 42.5, 26.9, 25.2, 20.0, 19.8; IR (KBr): 2957, 1748, 1501, 1374, 1275, 1149, 1016, 865, 749, 568 cm^{-1}; ESI FTMS exact mass calcd for $(C_{41}H_{36}O_5S\text{-}H)^-$ requires m/z 639.2210, found m/z 639.2208.

6. NMR spectra of products 3 and 6

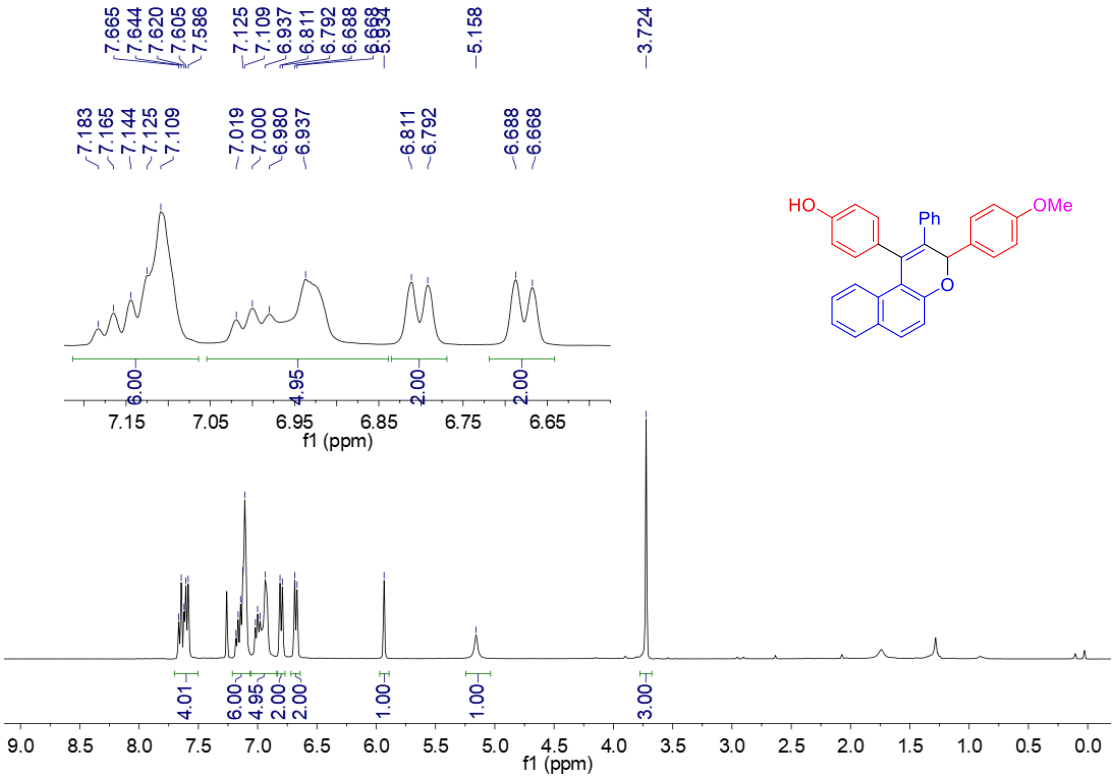
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aa**:



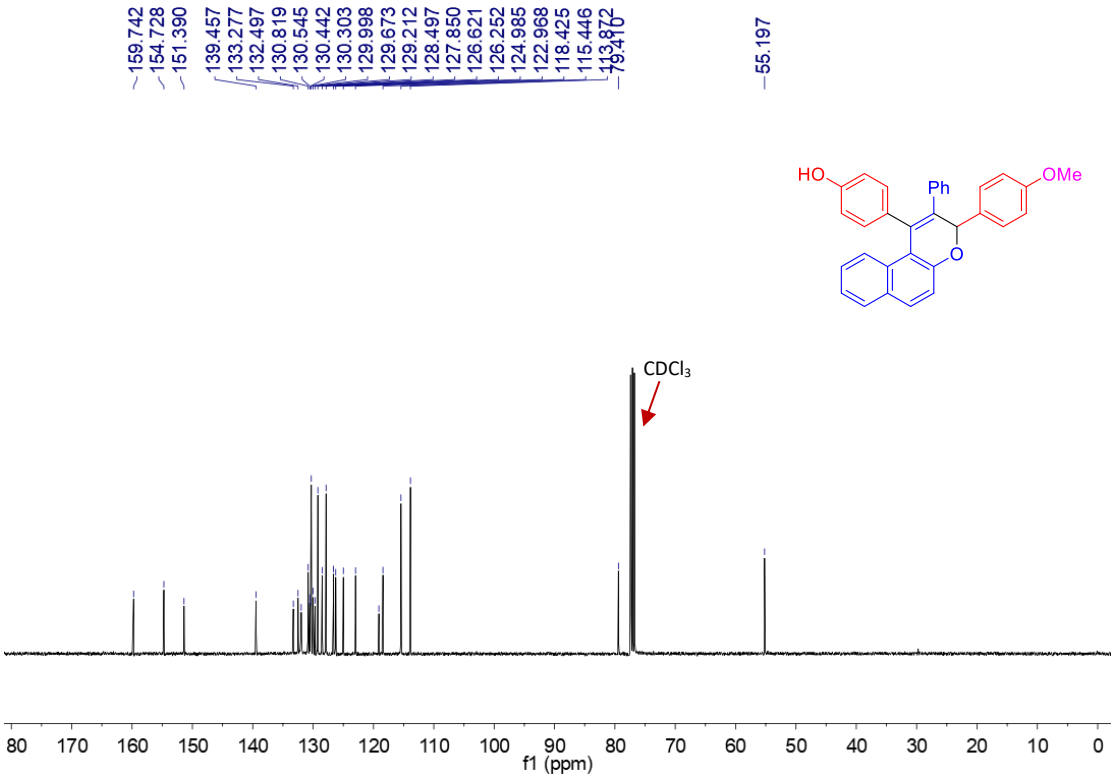
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aa**:



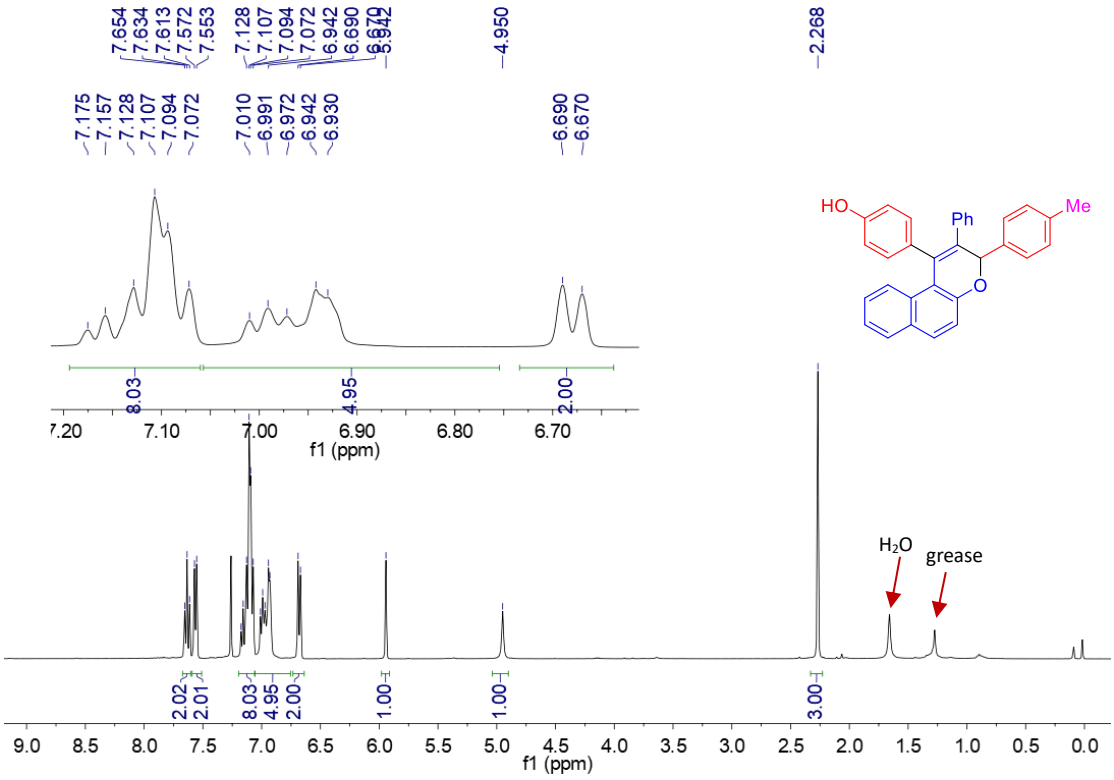
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ba**:



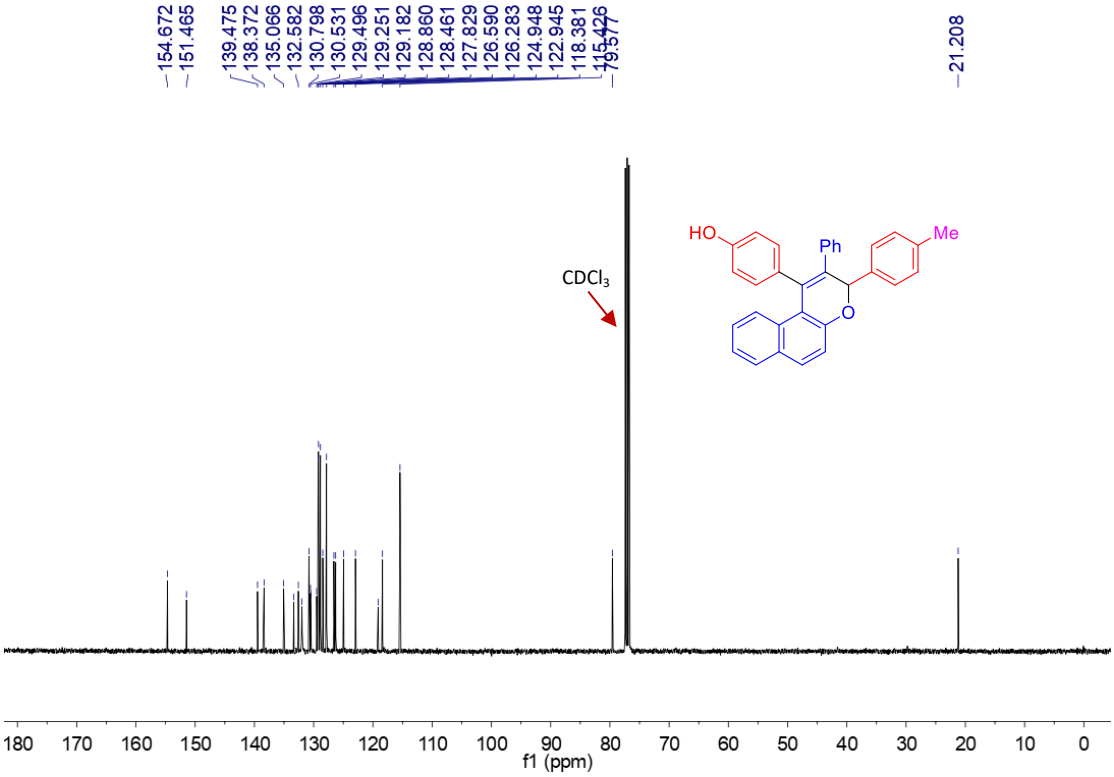
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ba**:



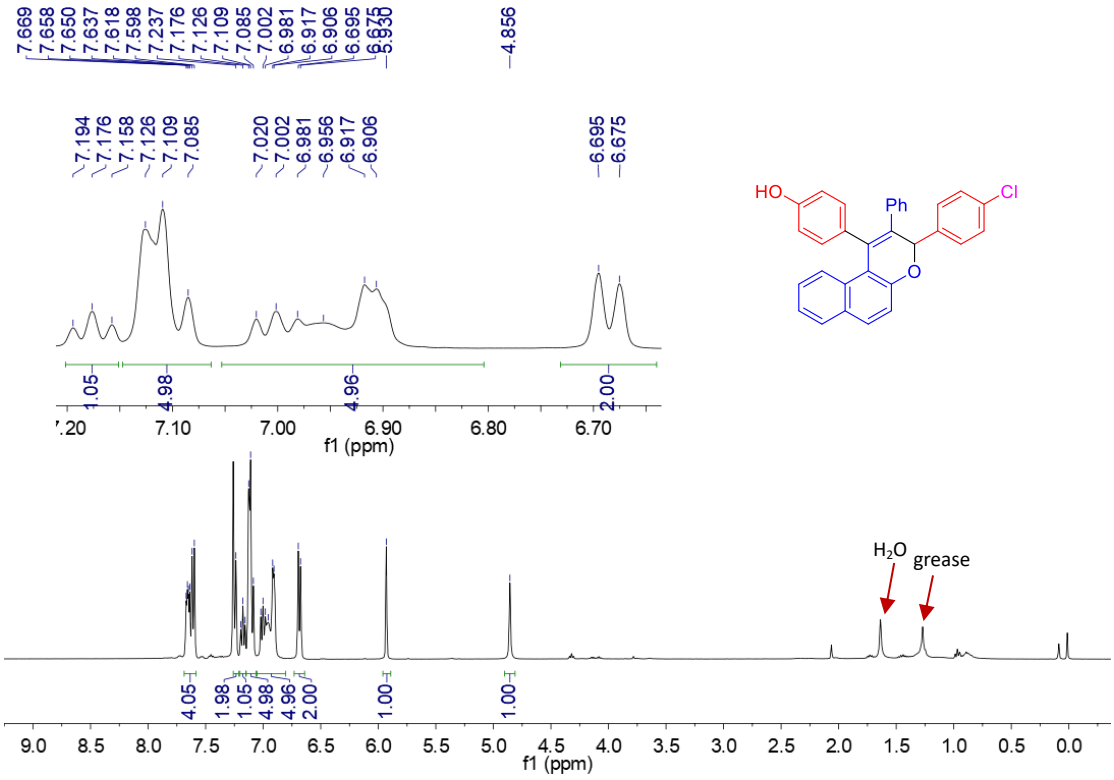
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ca**:



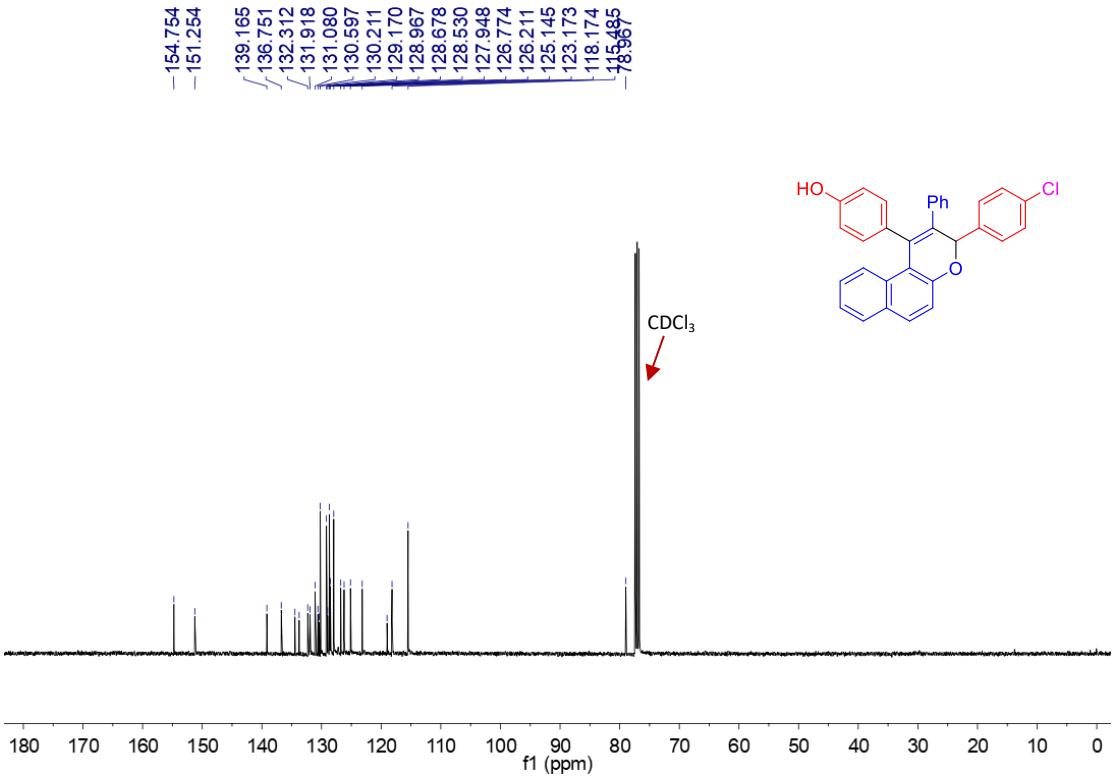
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ca**:



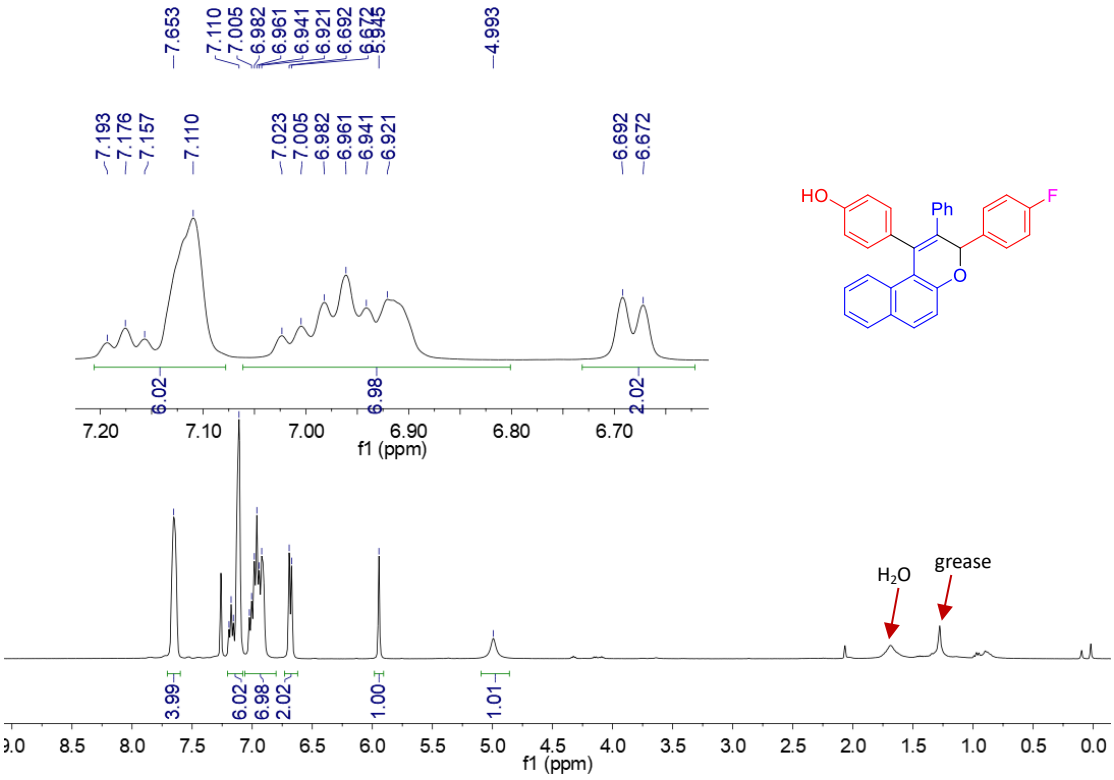
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3da**:



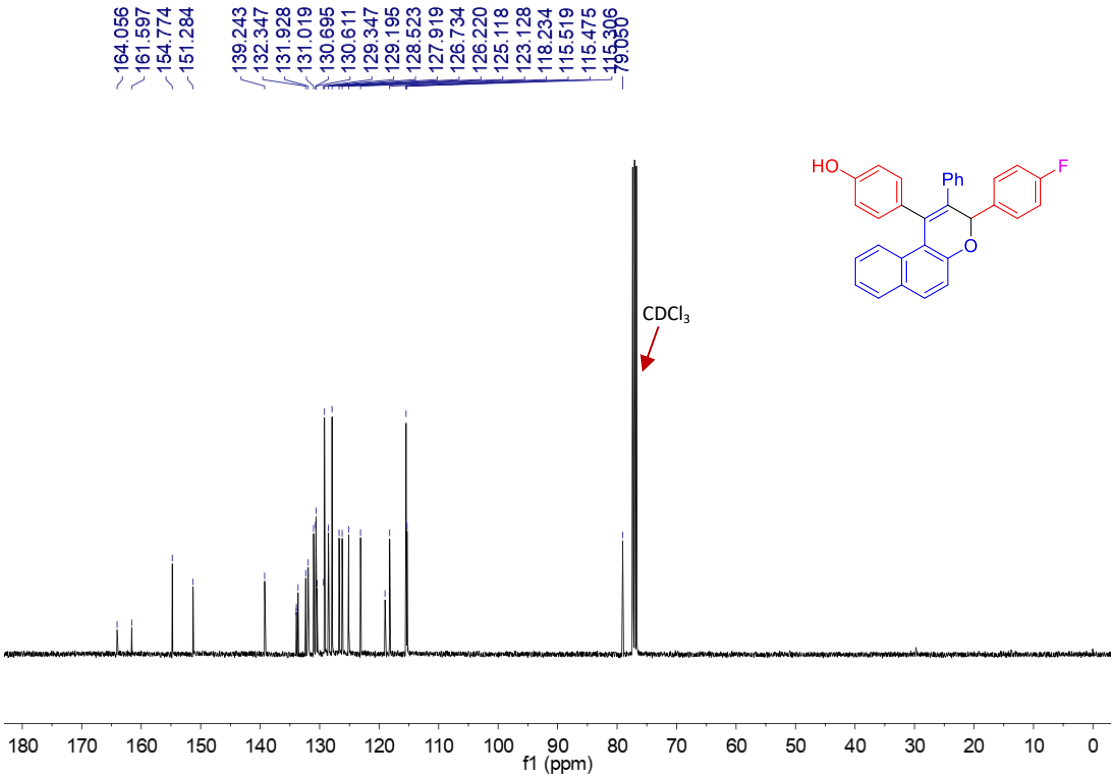
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3da**:



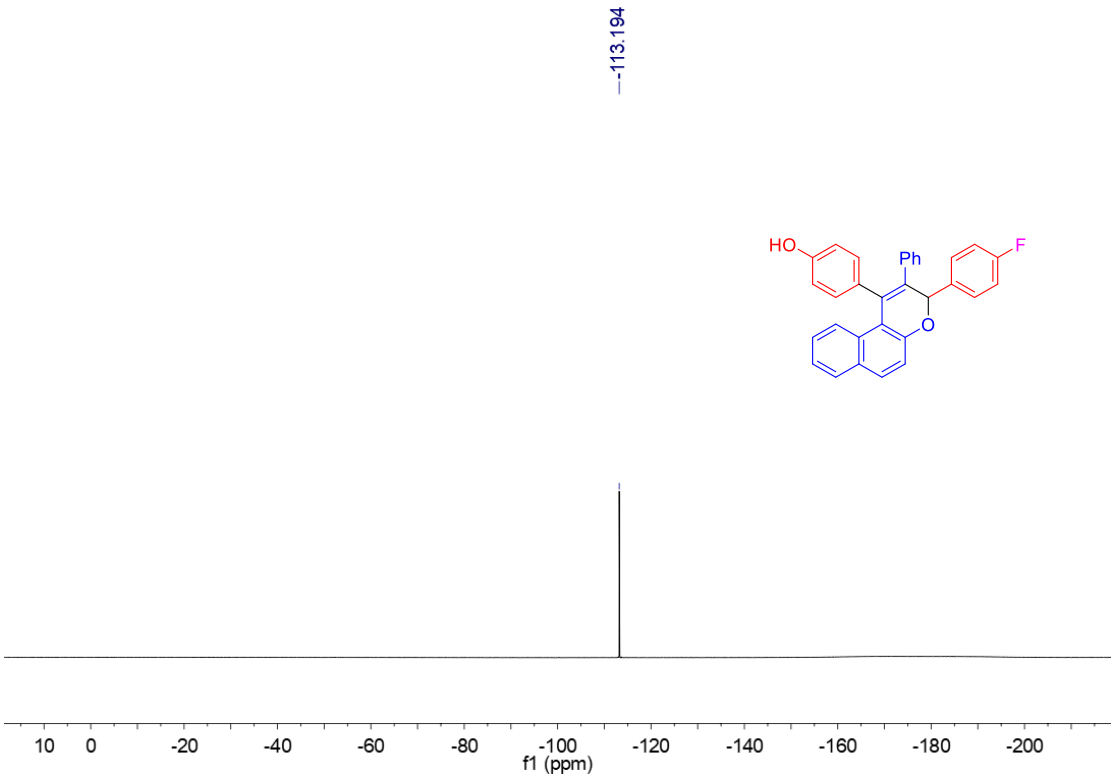
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ea**:



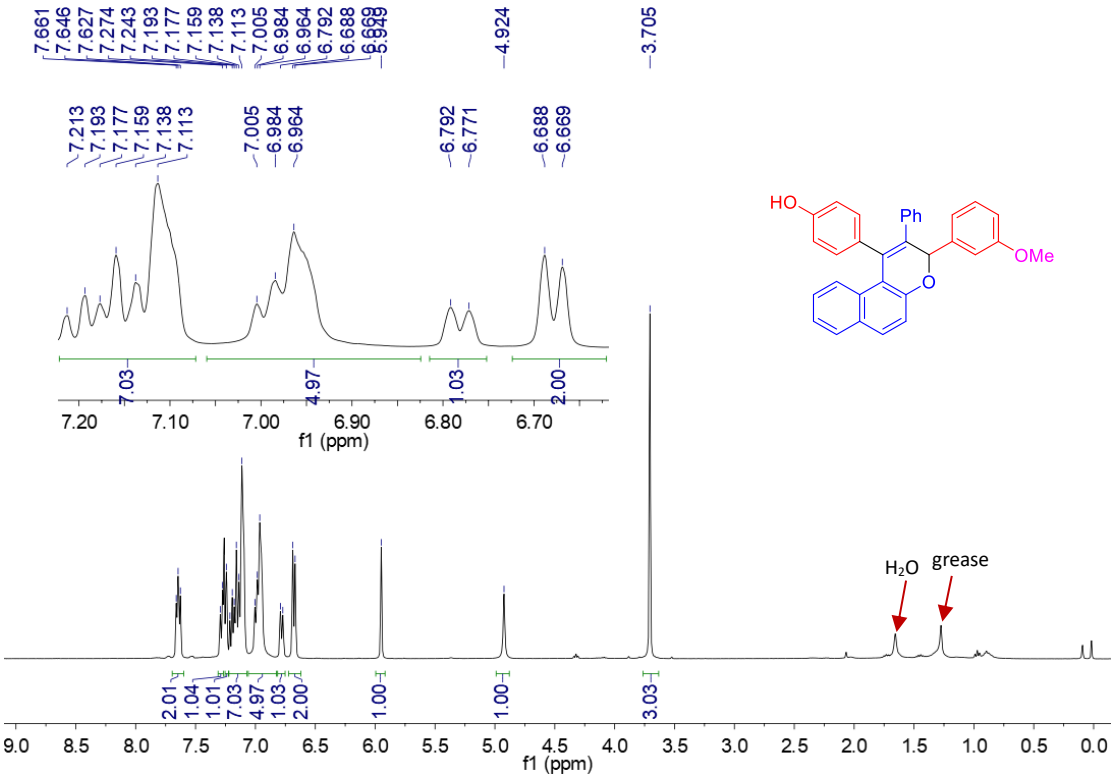
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ea**:



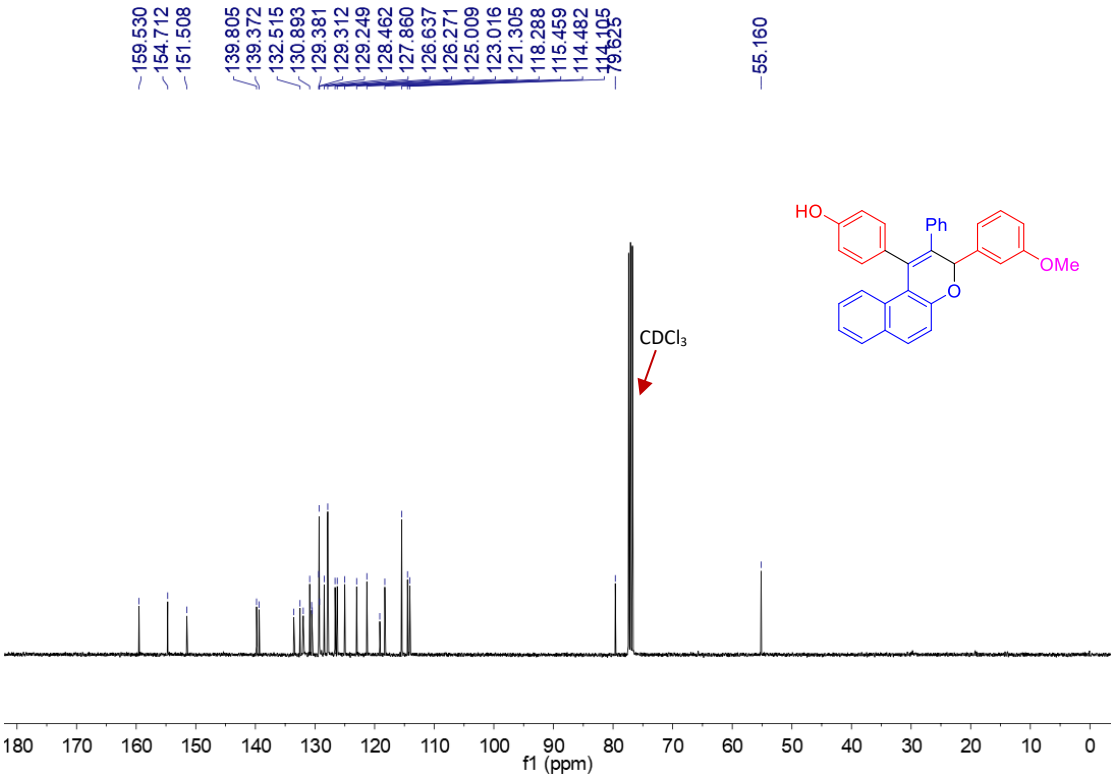
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3ea**:



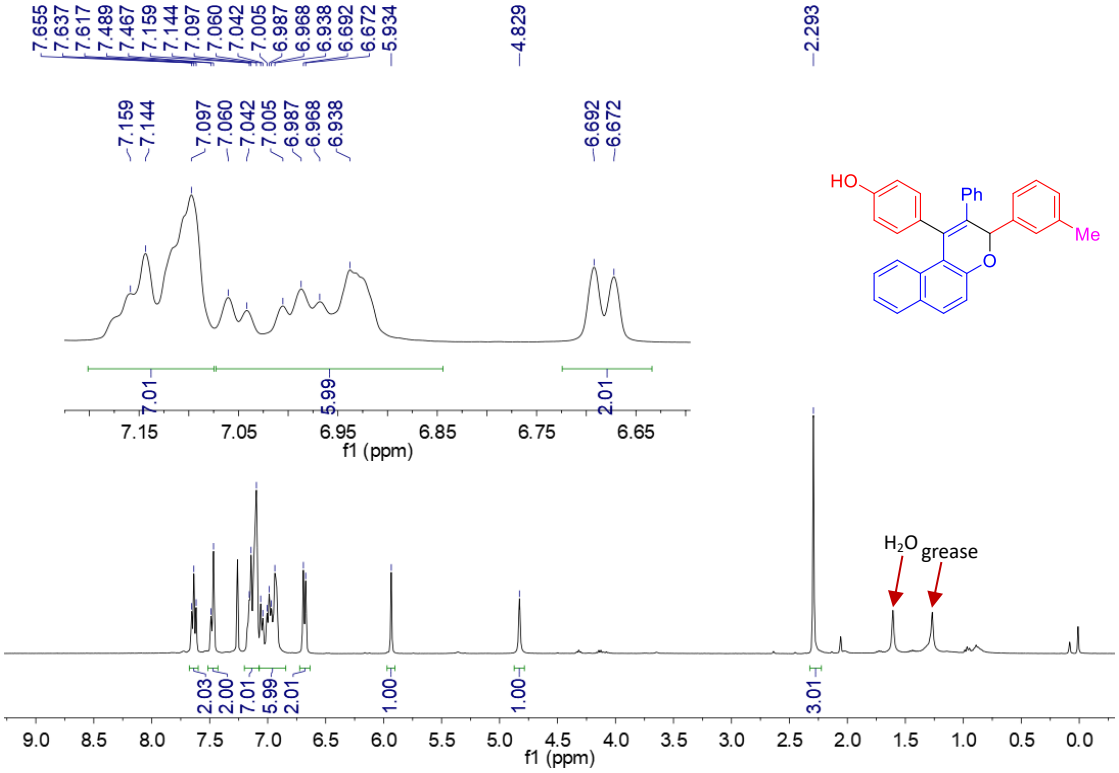
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3fa**:



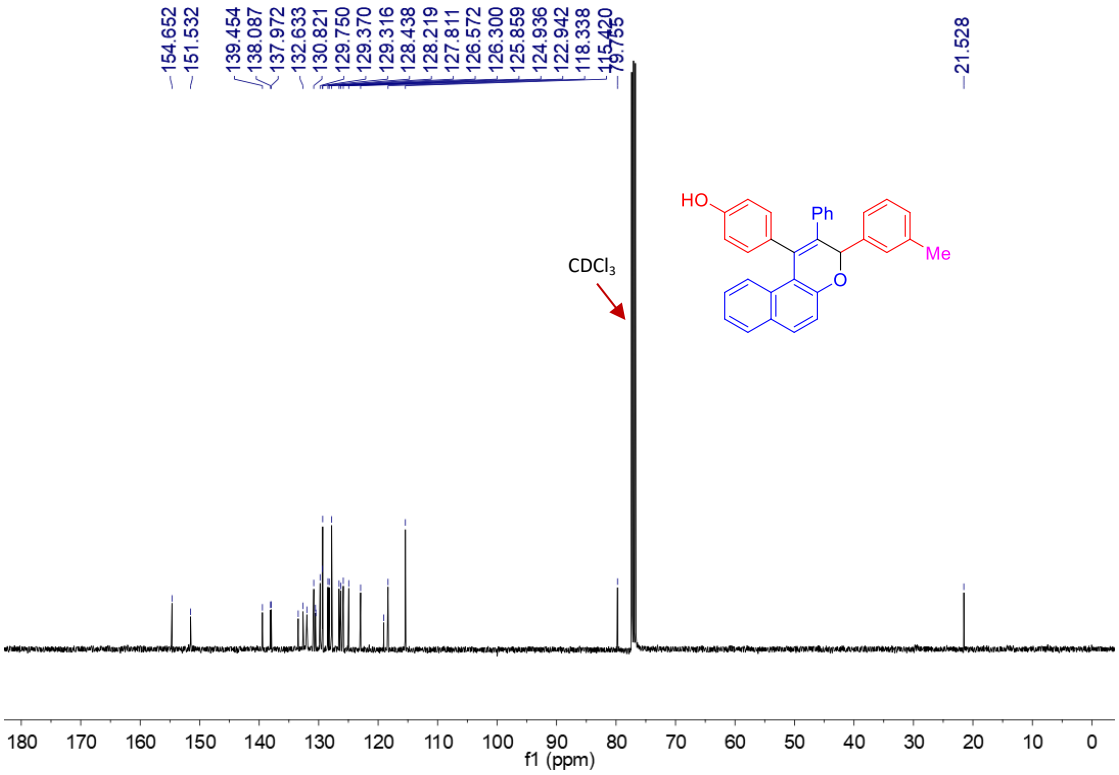
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3fa**:



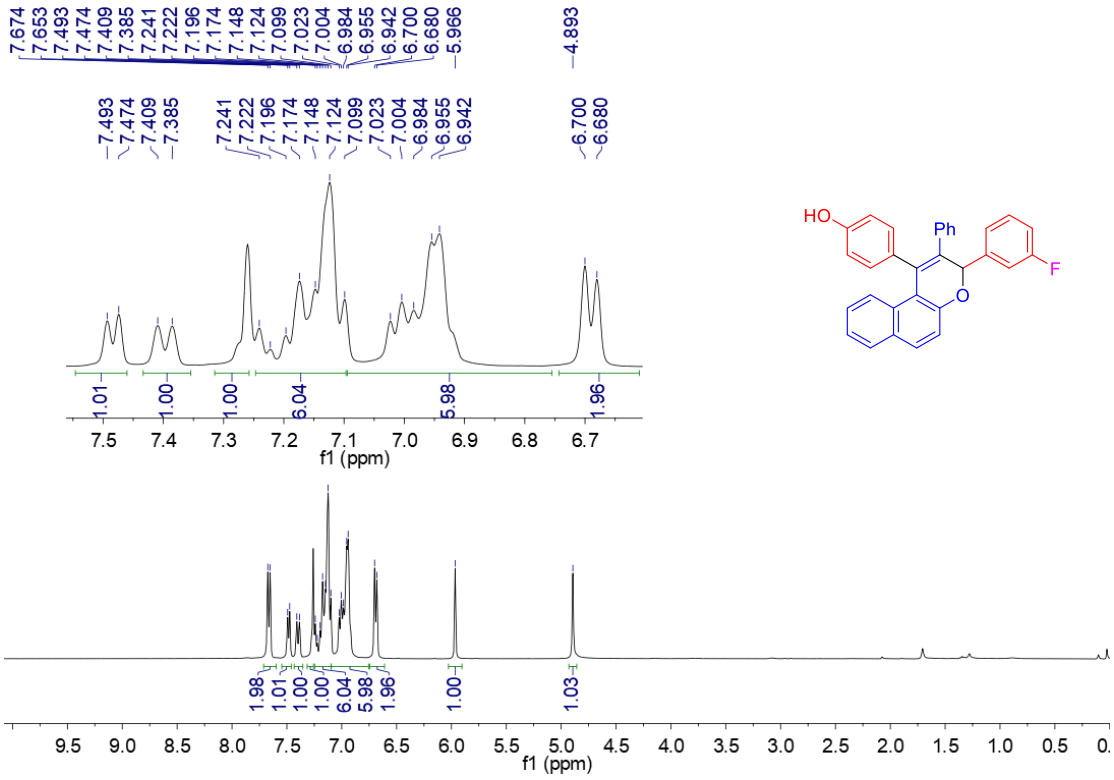
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ga**:



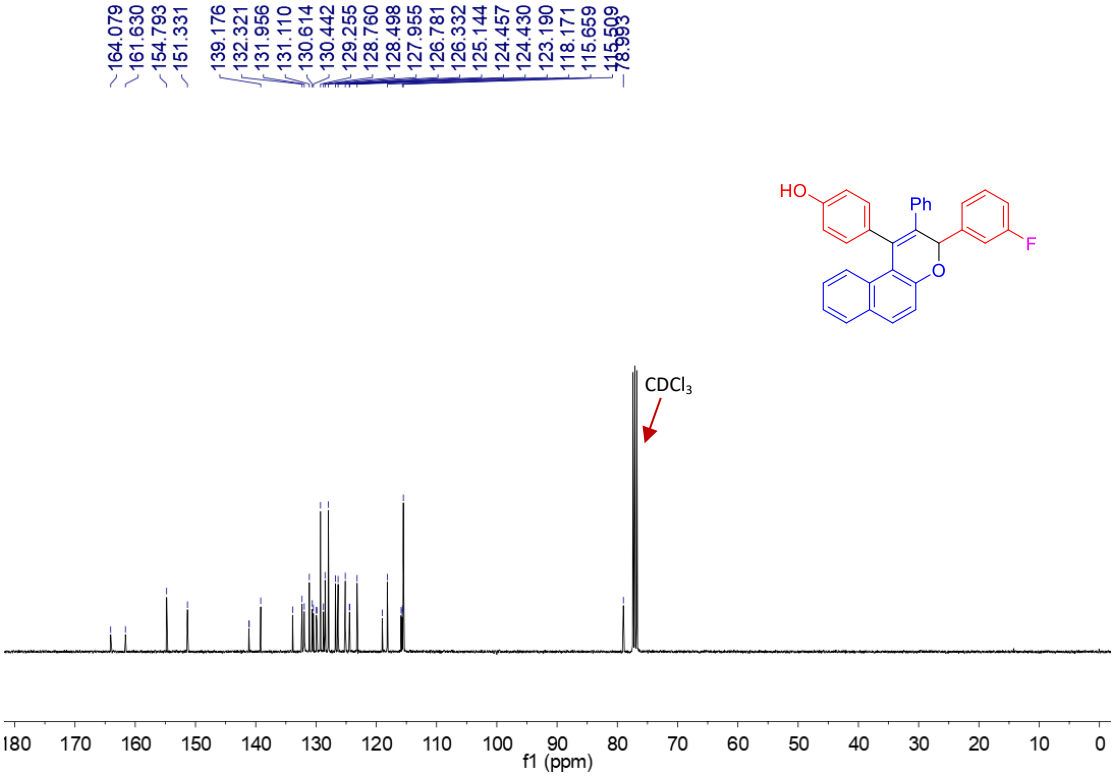
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ga**:



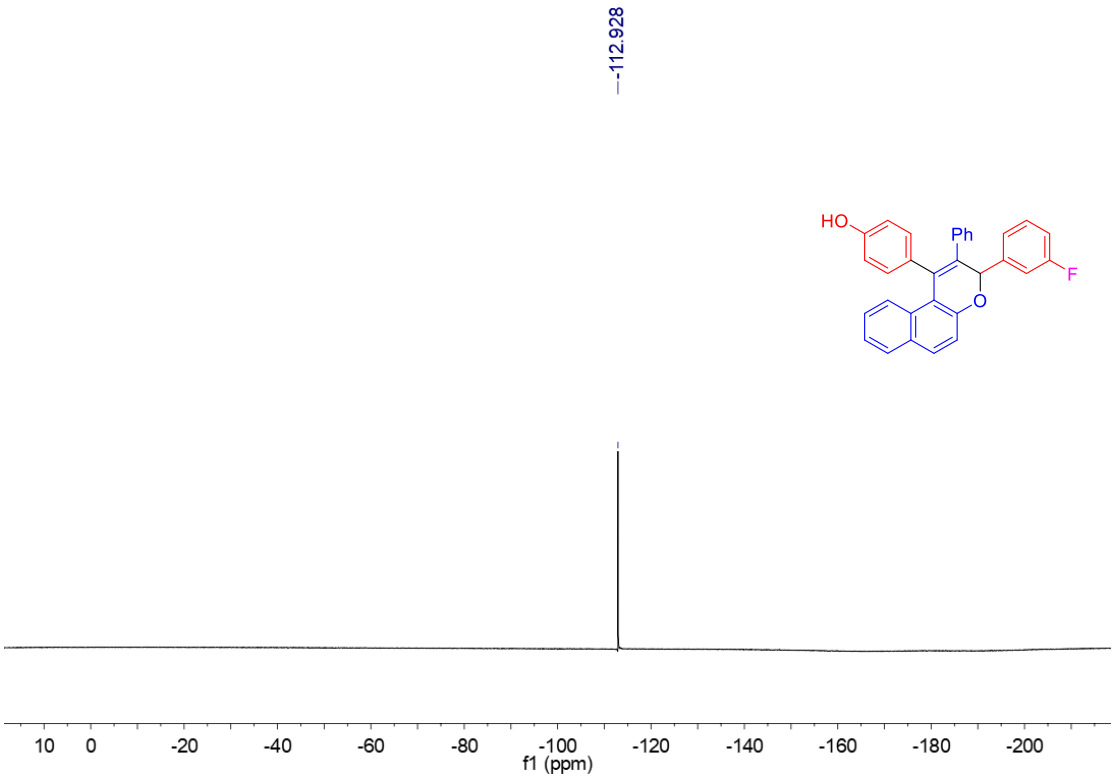
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ha**:



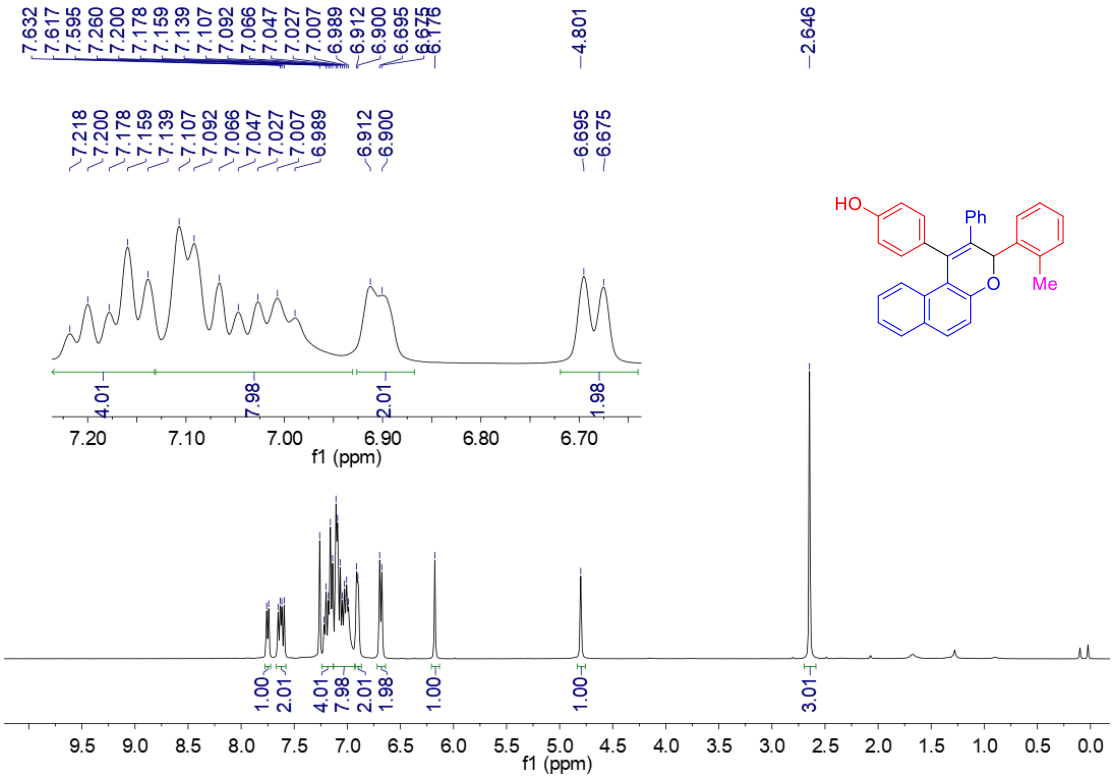
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ha**:



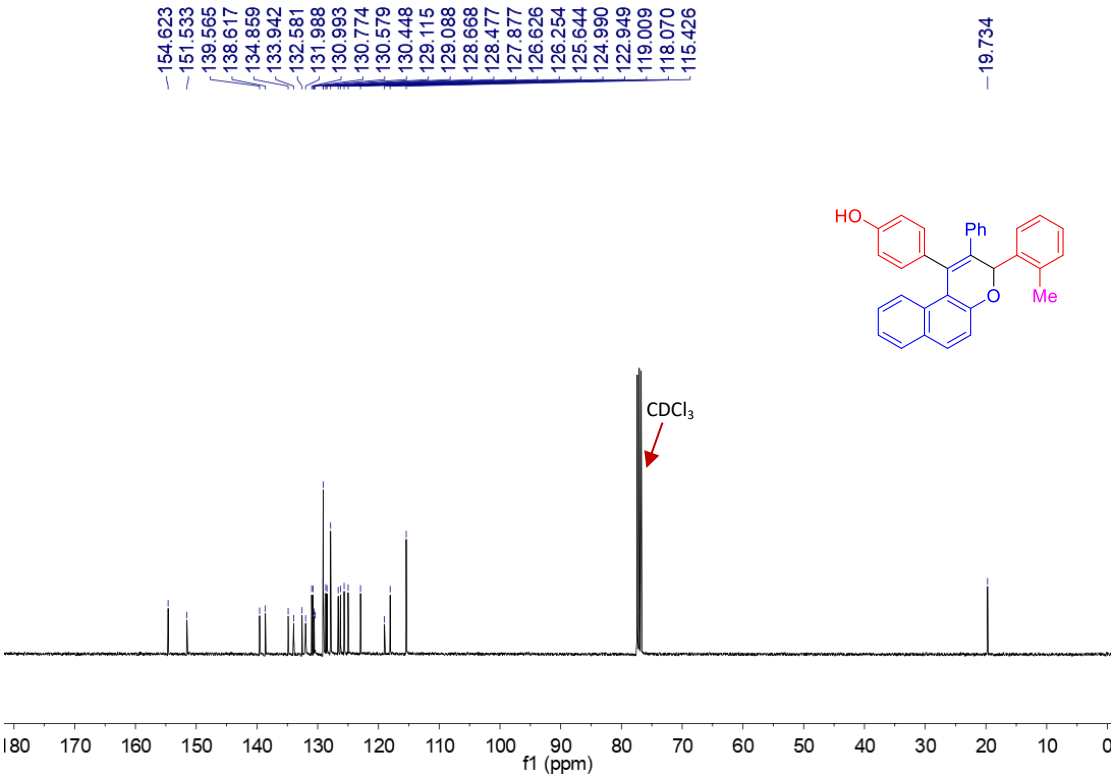
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3ha**:



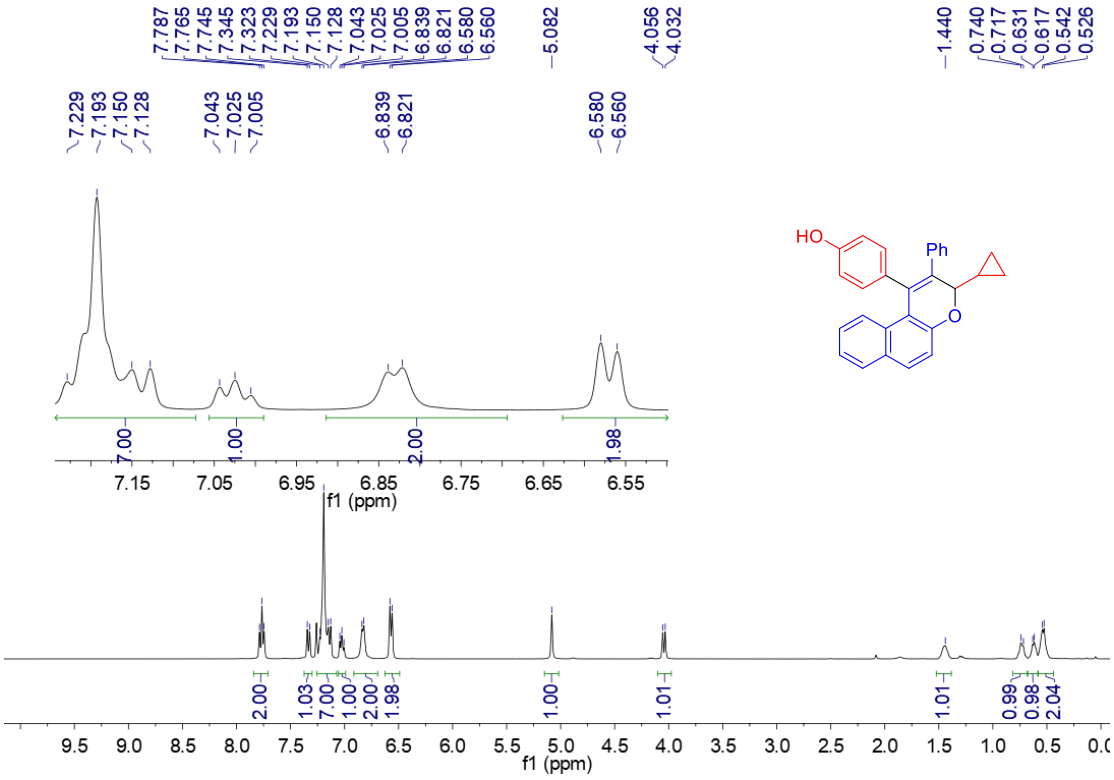
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ia**:



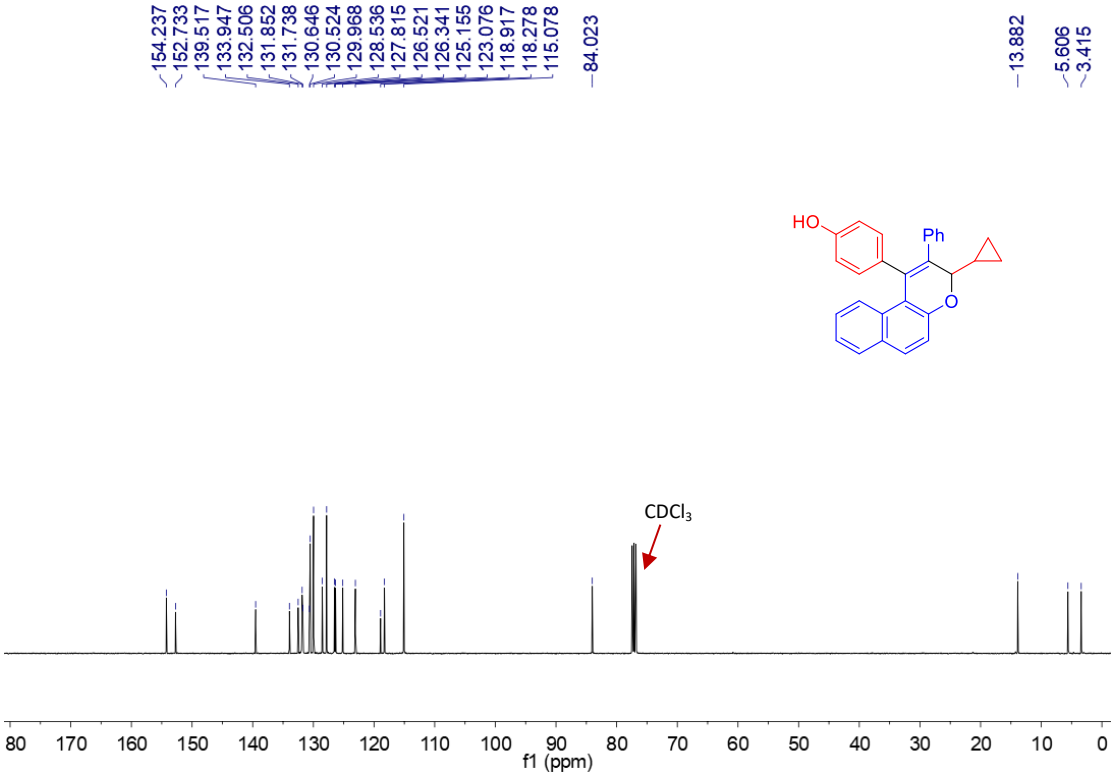
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ia**:



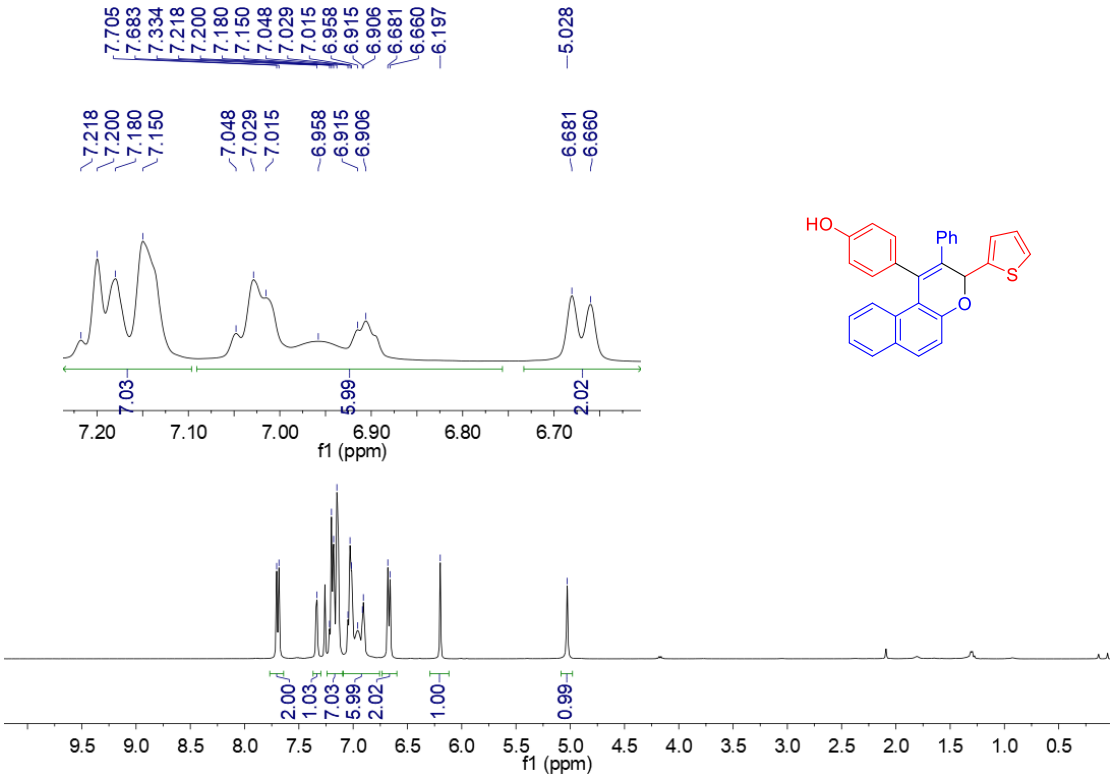
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ja**:



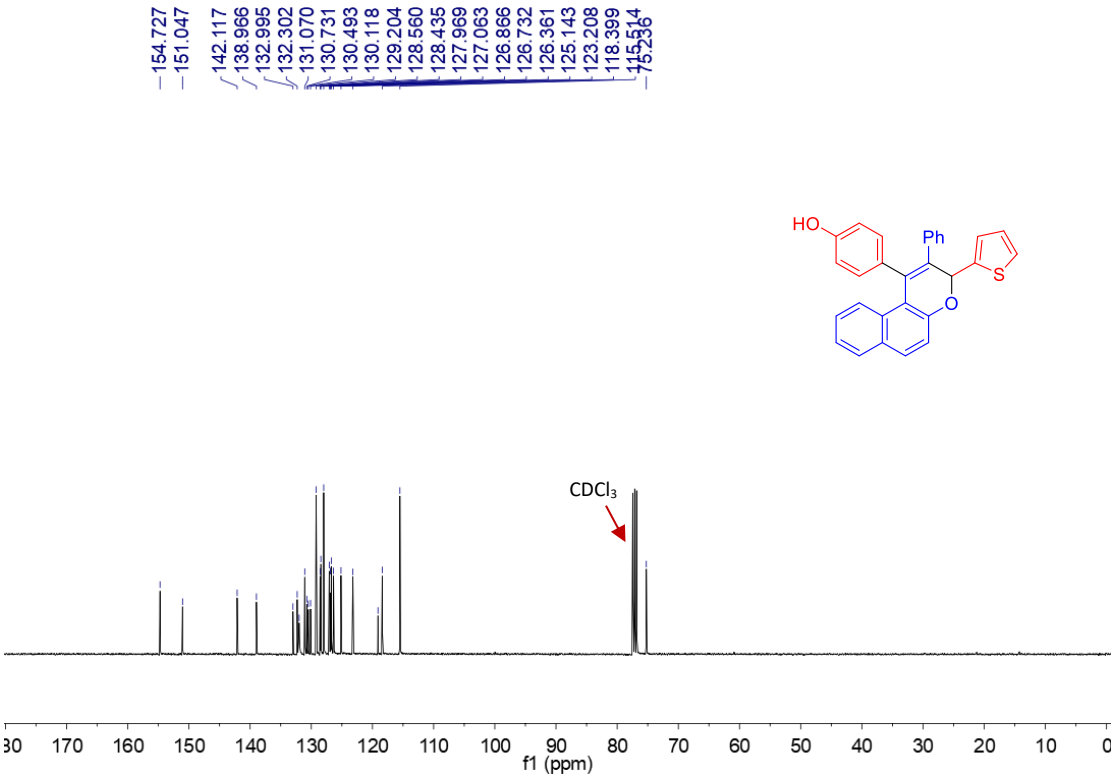
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ja**:



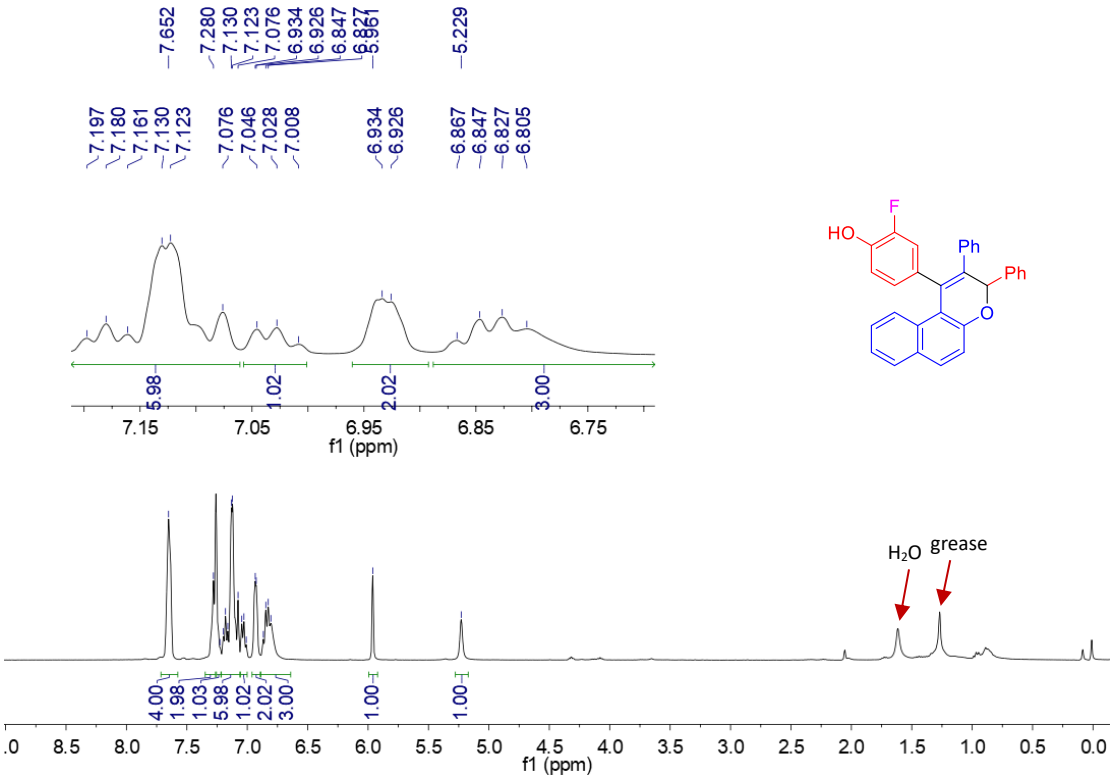
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ka**:



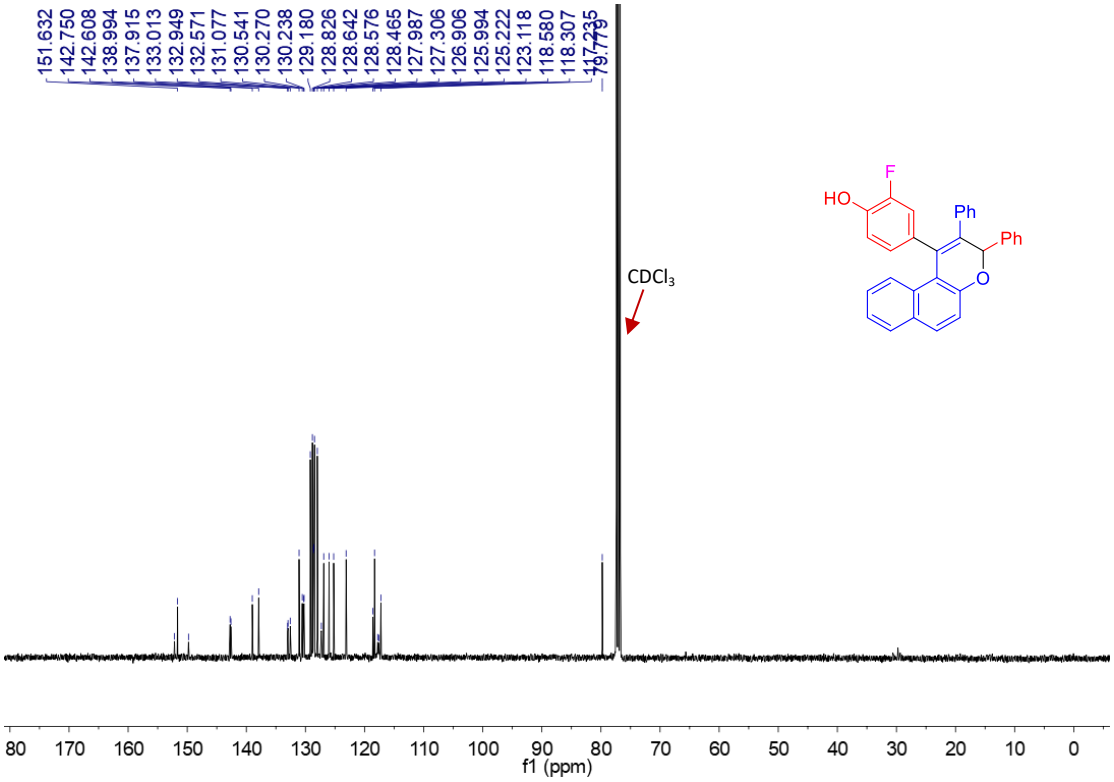
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ka**:



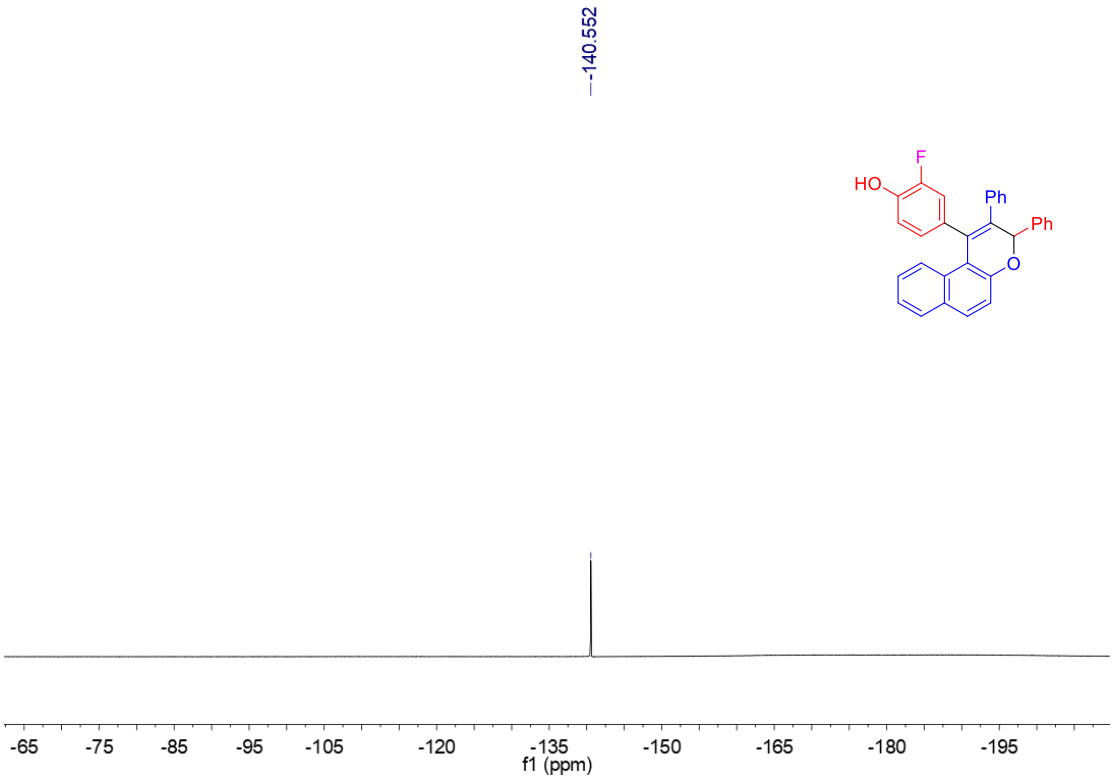
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3la**:



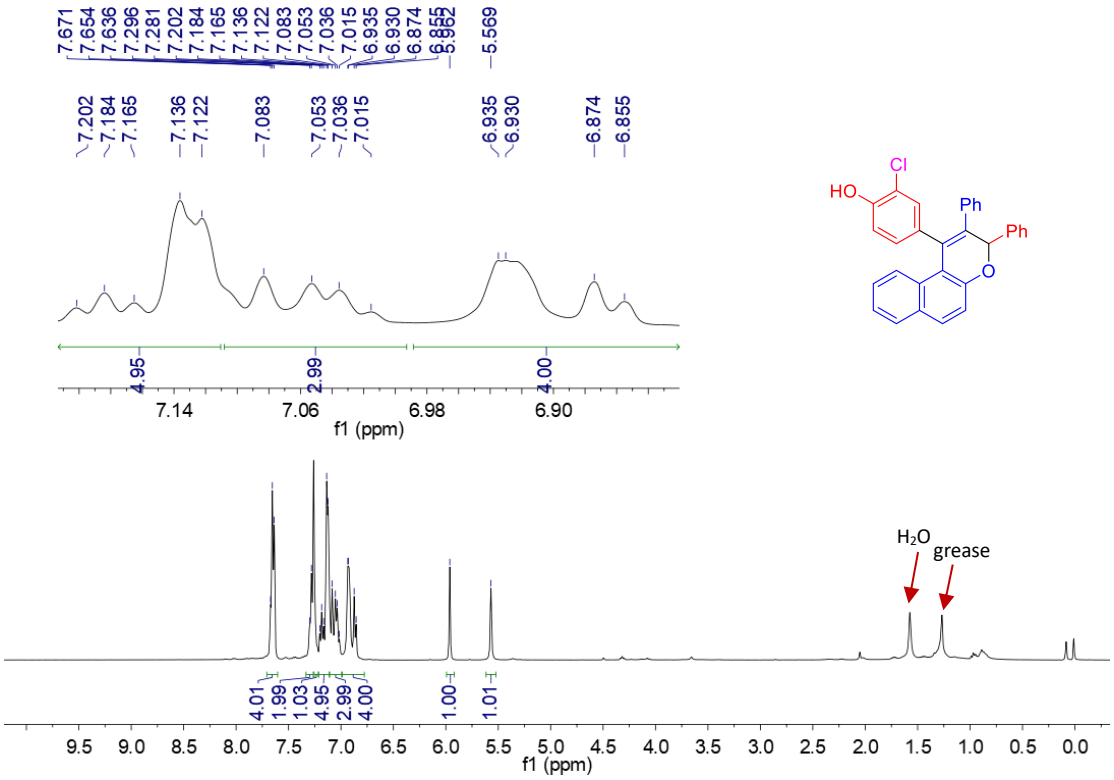
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3la**:



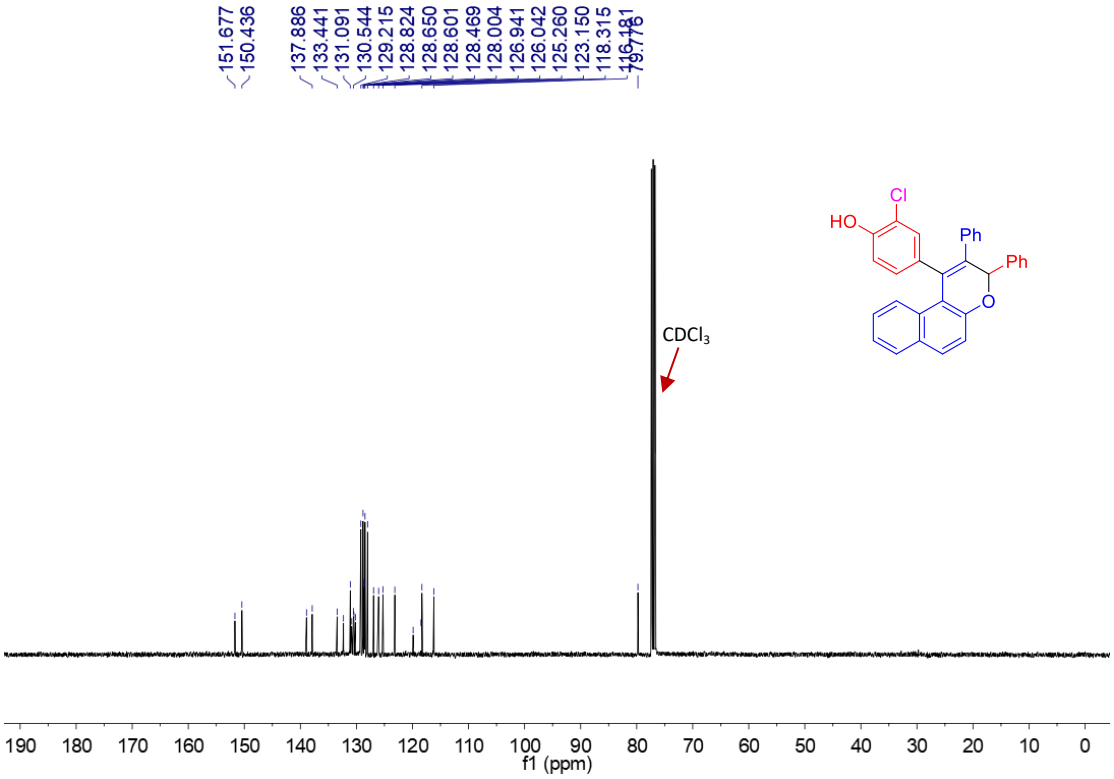
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3la**:



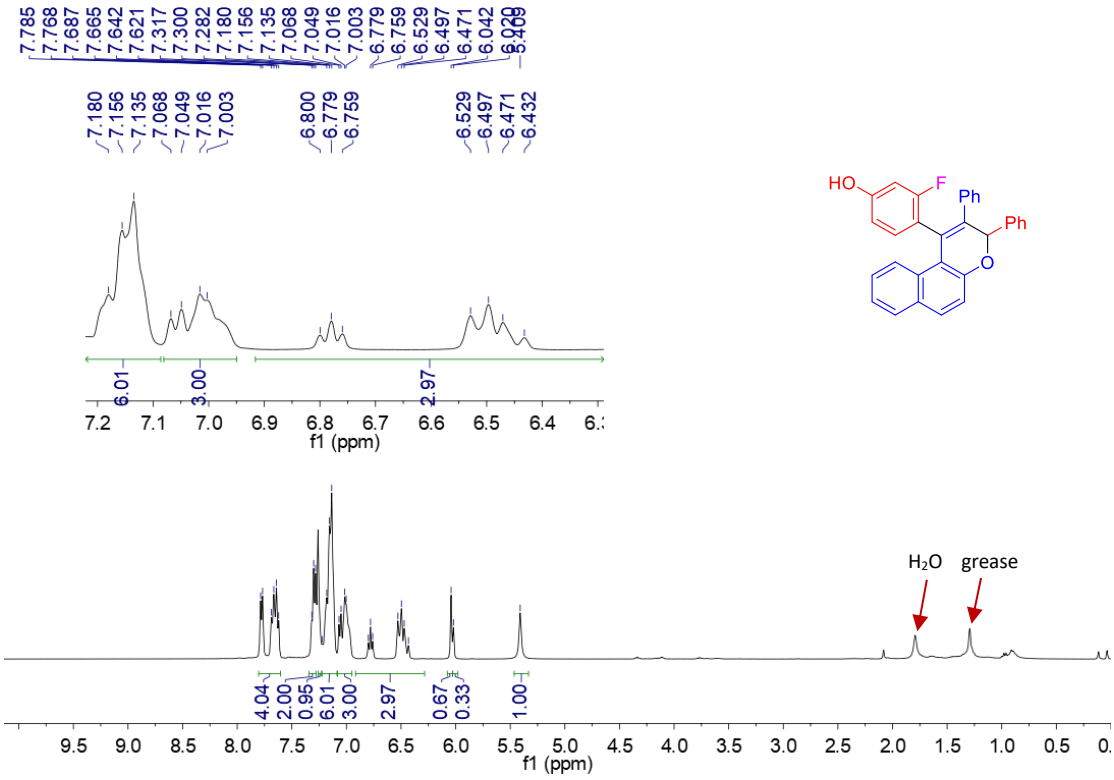
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ma**:



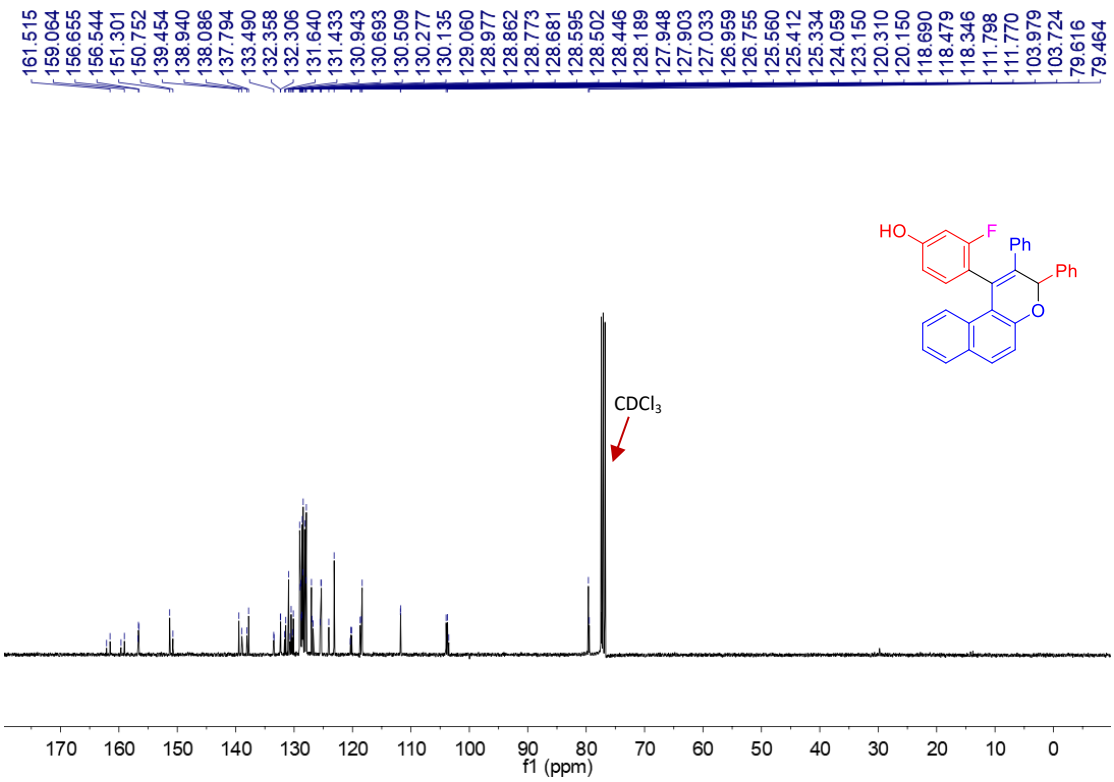
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ma**:



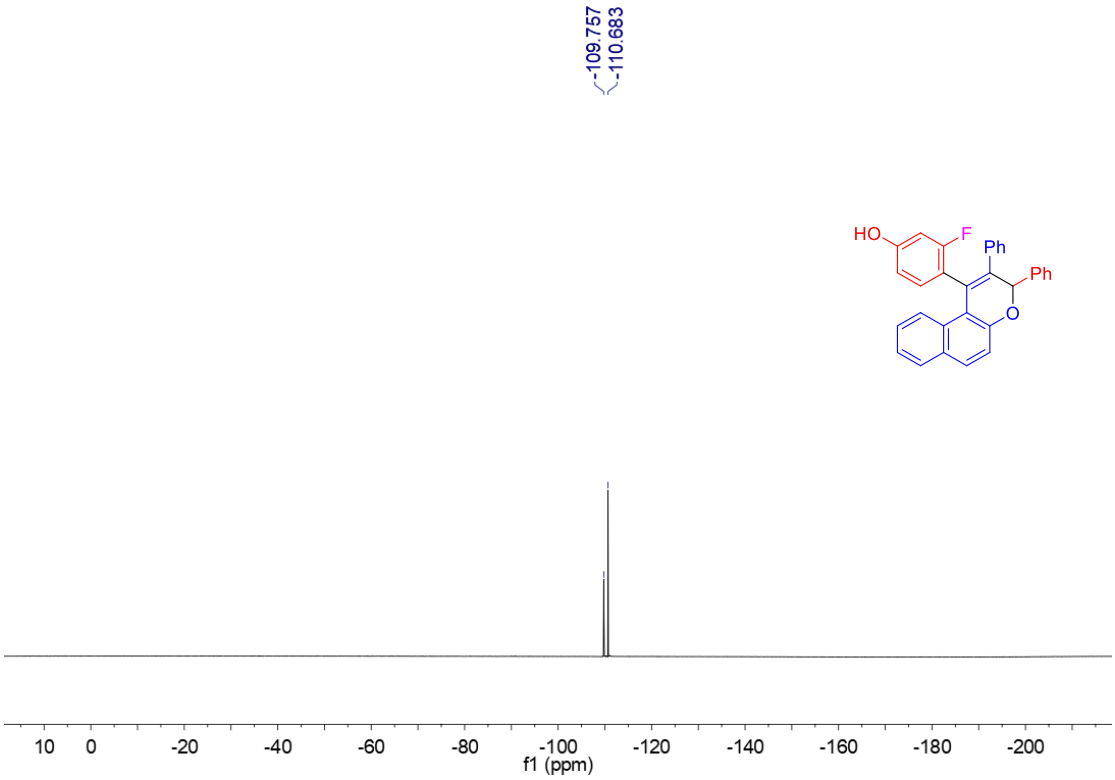
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3na**: (67:33 dr)



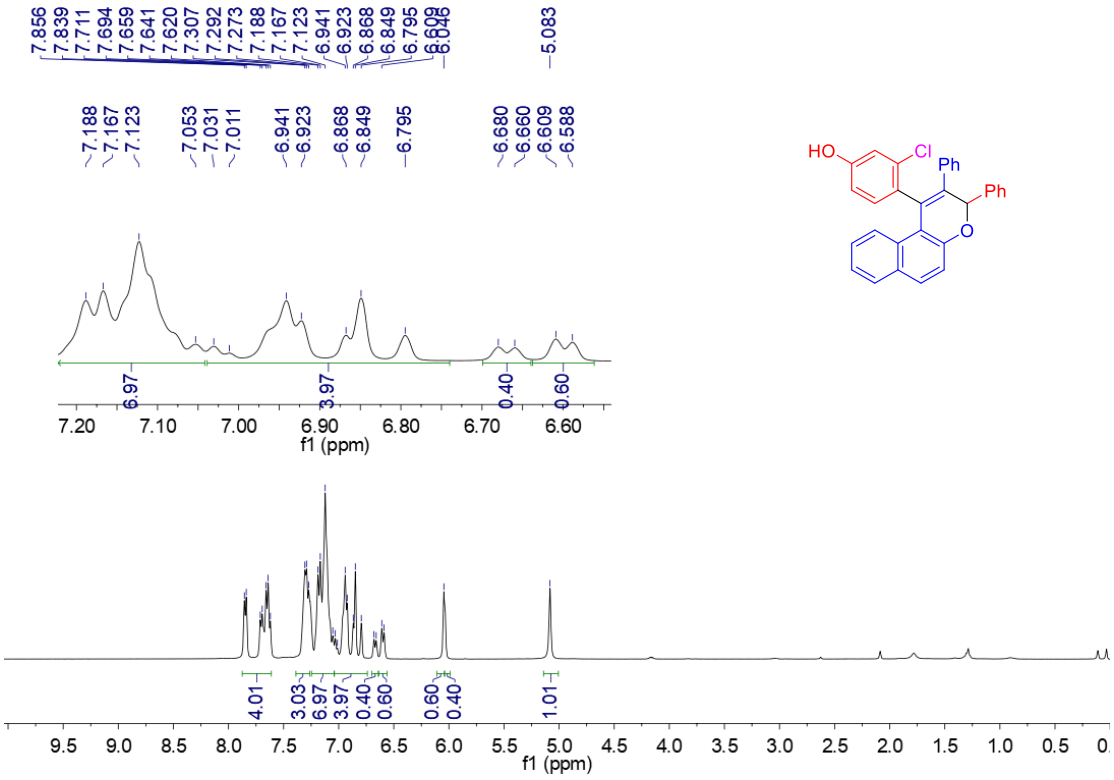
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3na**: (67:33 dr)



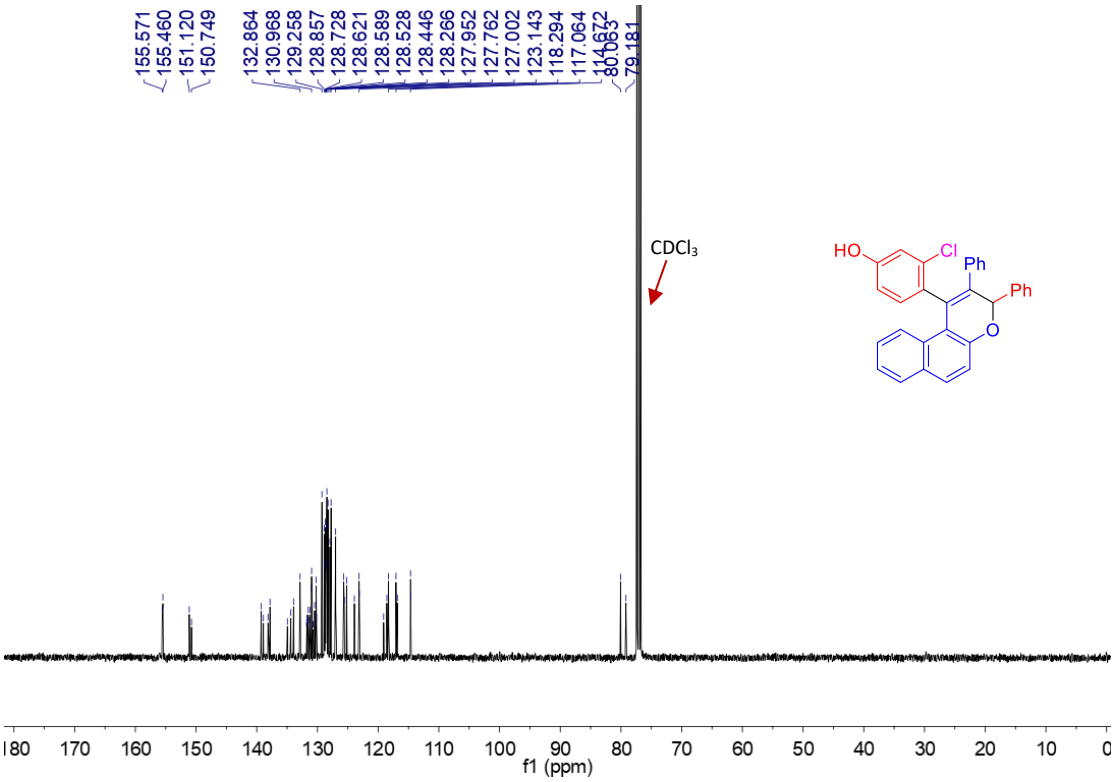
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3na**: (67:33 dr)



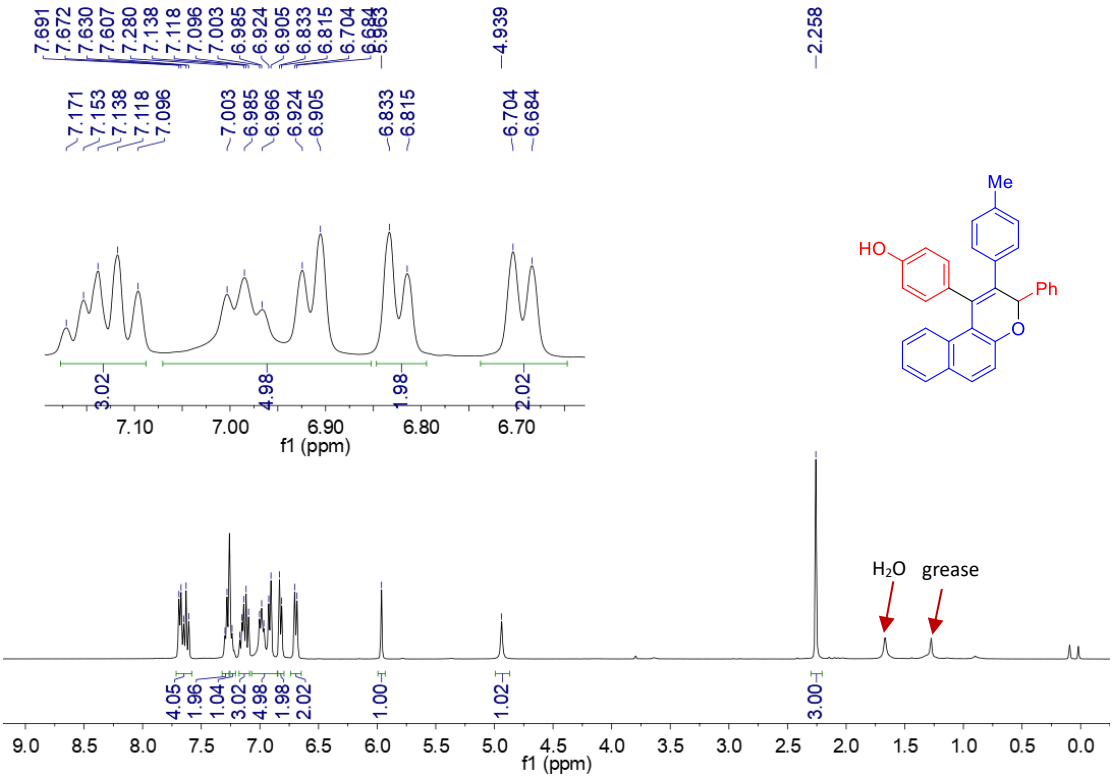
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3oa**: (60:40 dr)



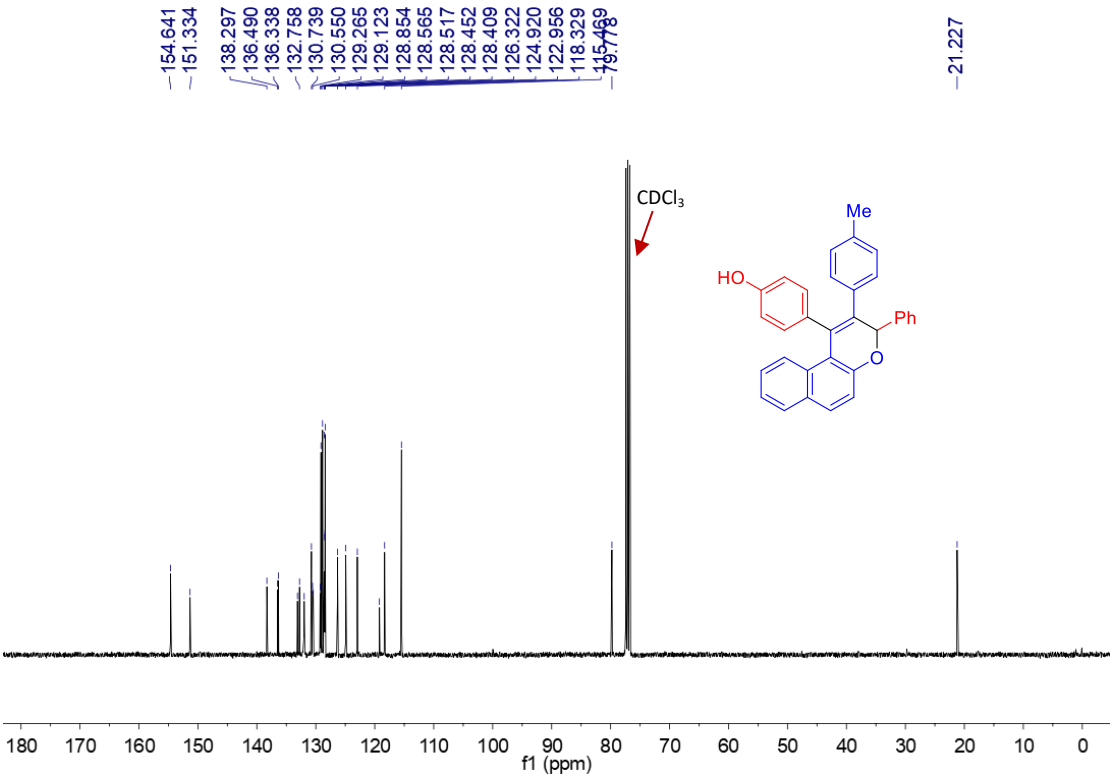
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3oa**: (60:40 dr)



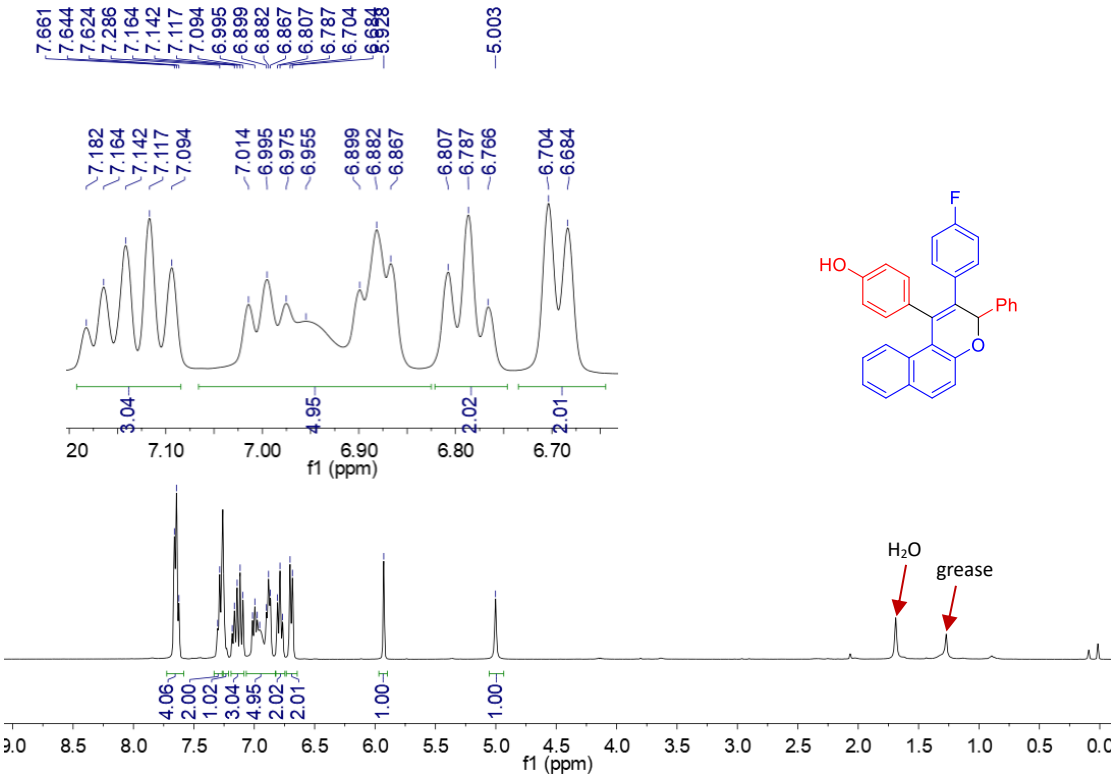
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ab**:



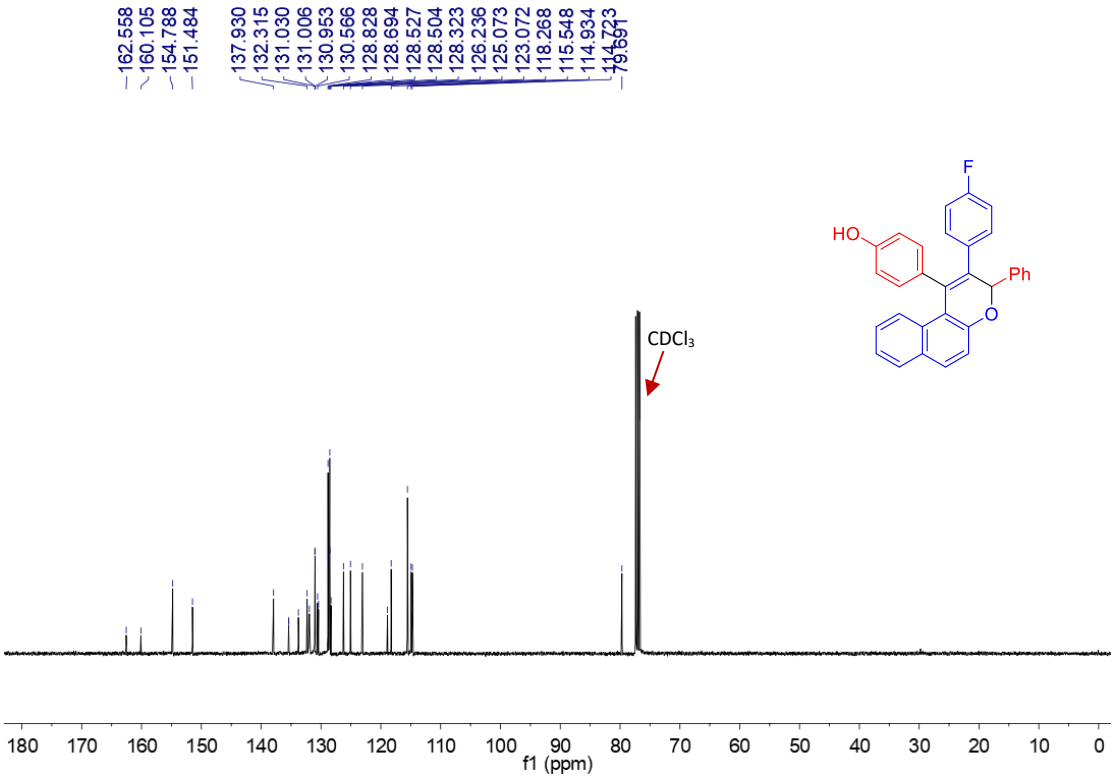
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ab**:



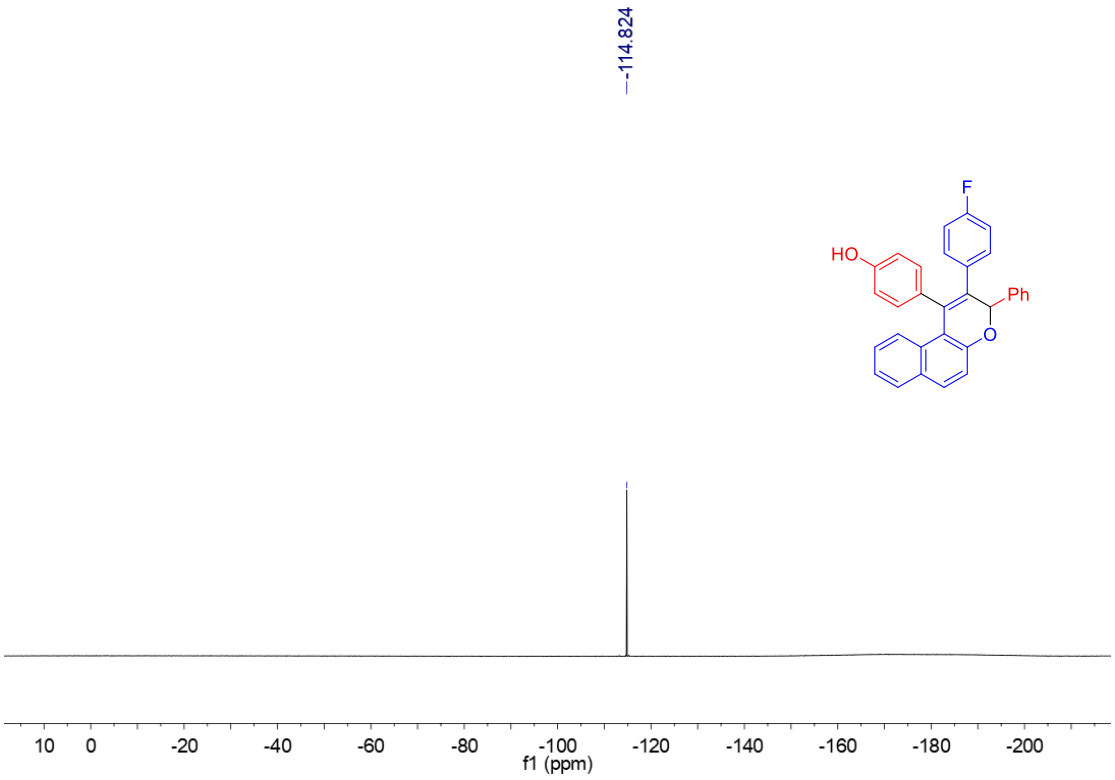
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ac**:



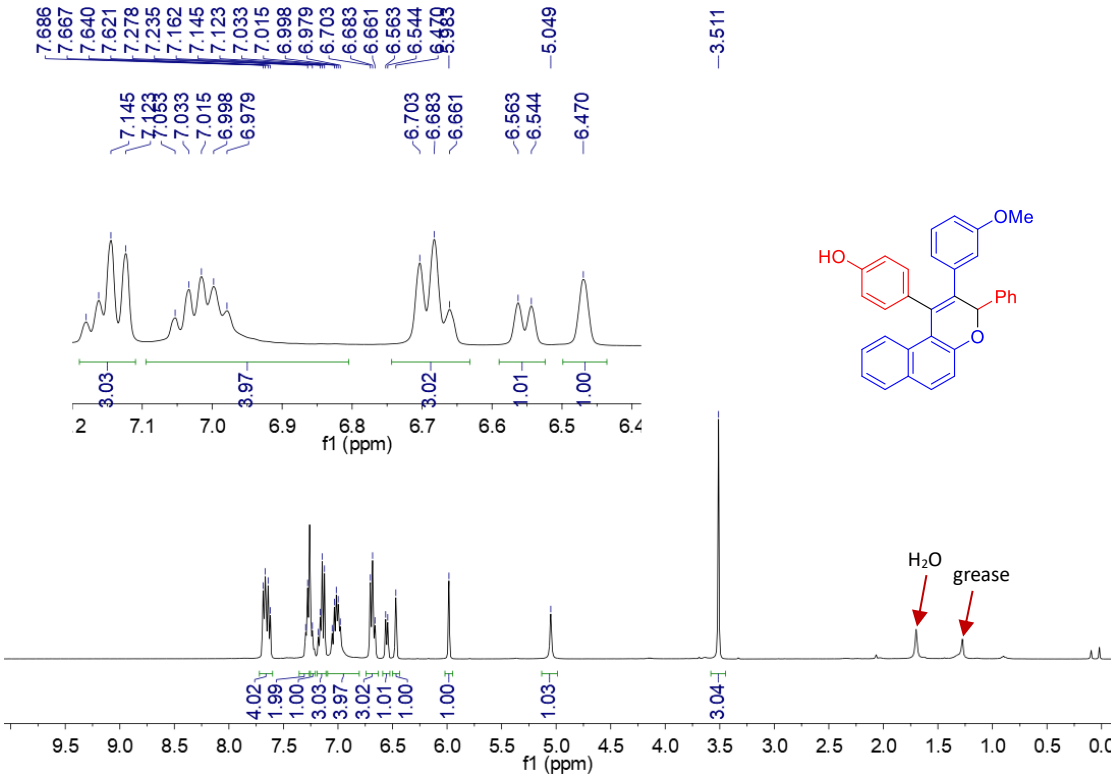
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ac**:



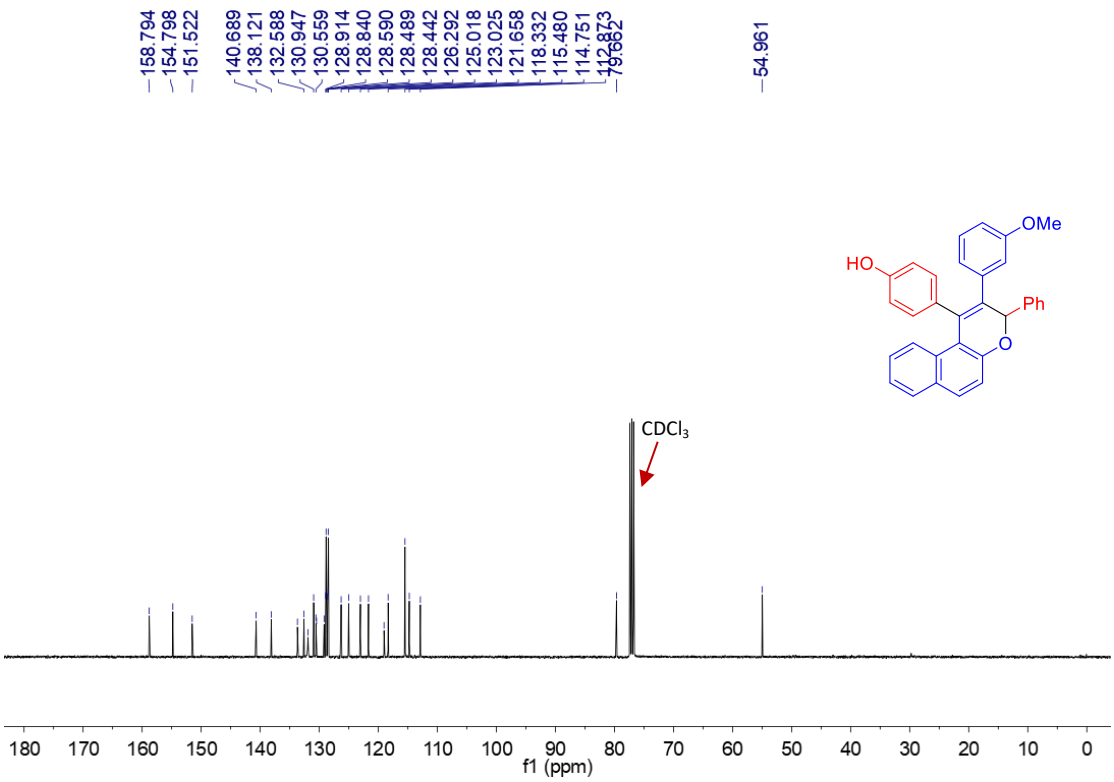
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3ac**:



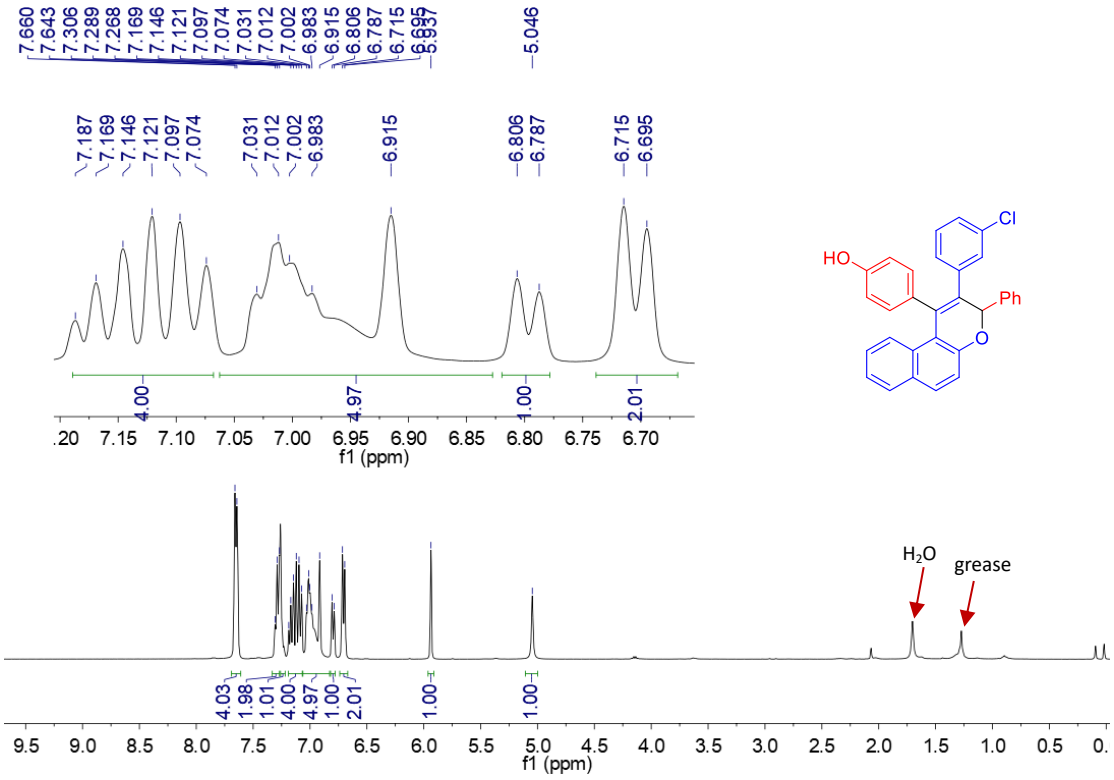
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ad**:



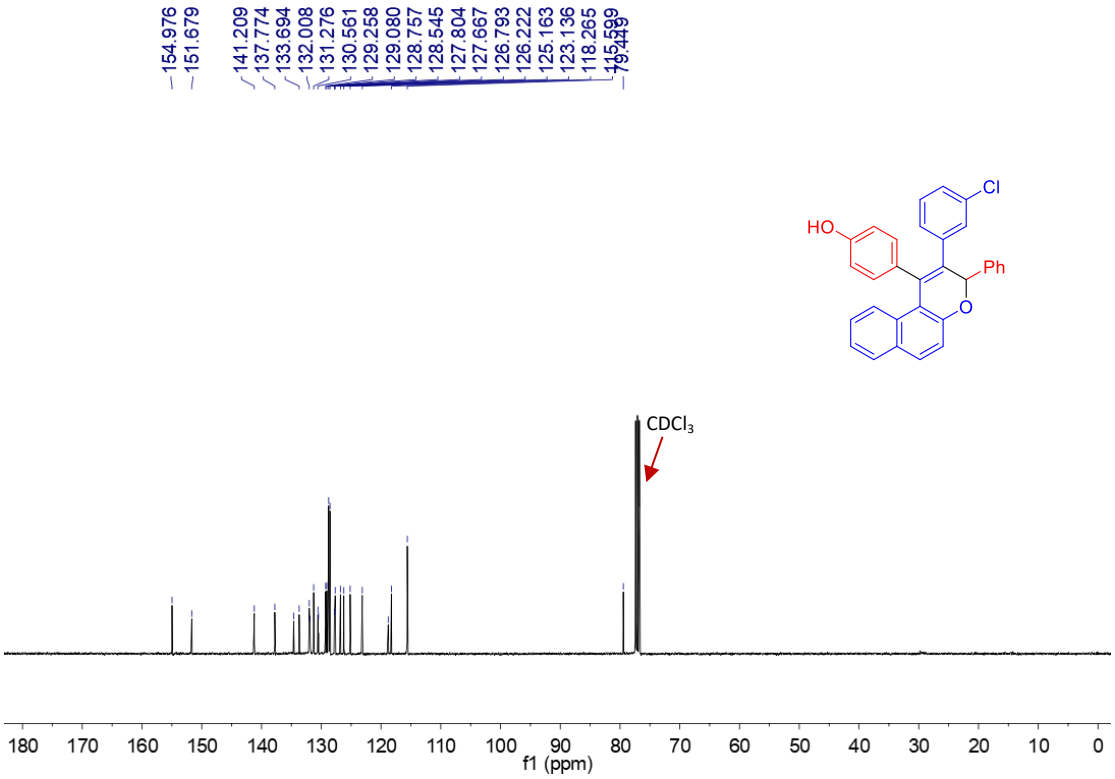
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ad**:



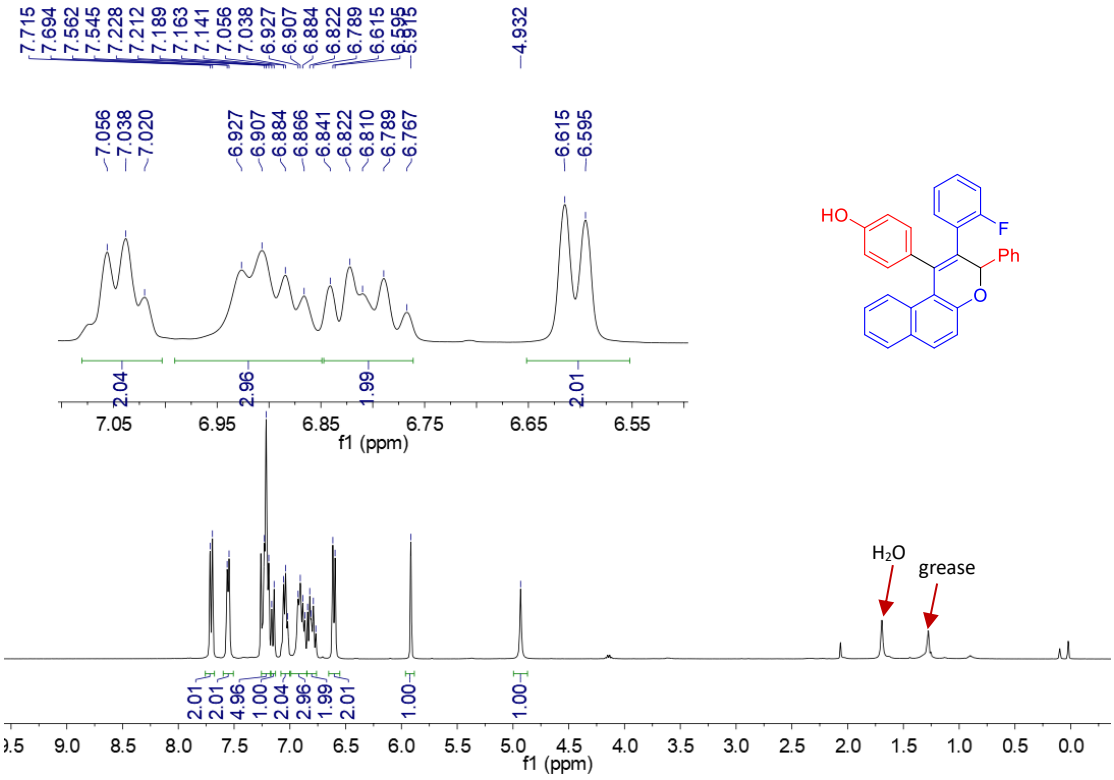
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ae**:



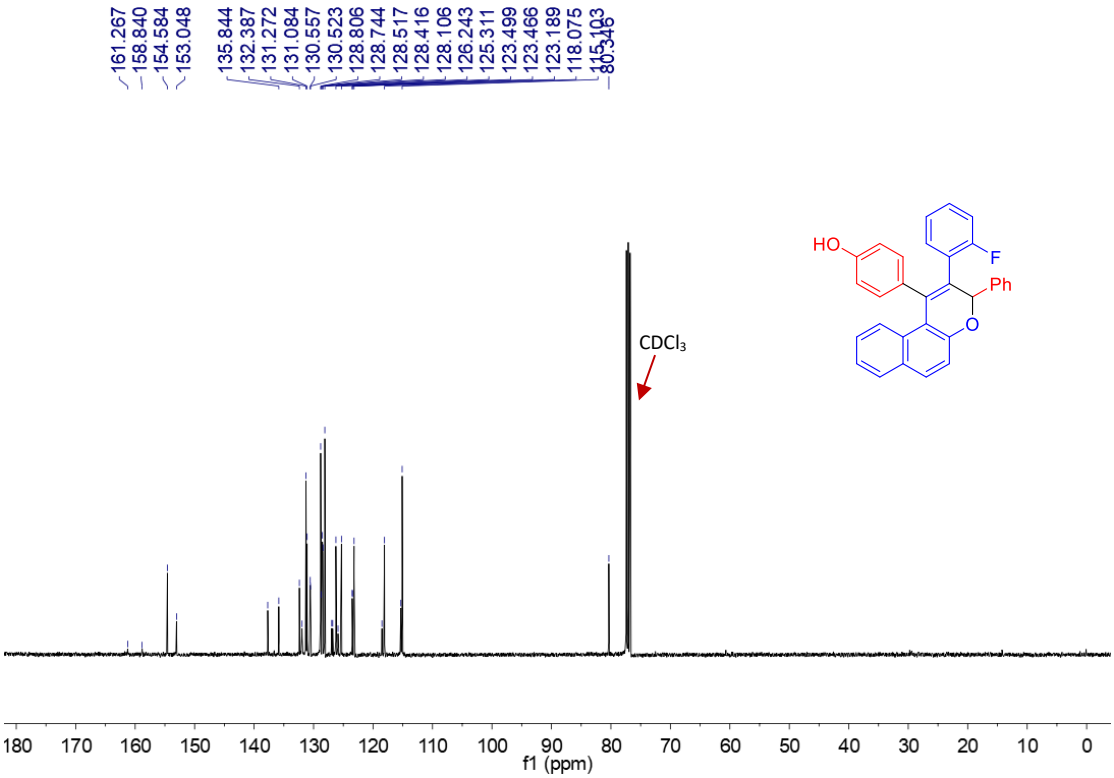
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ae**:



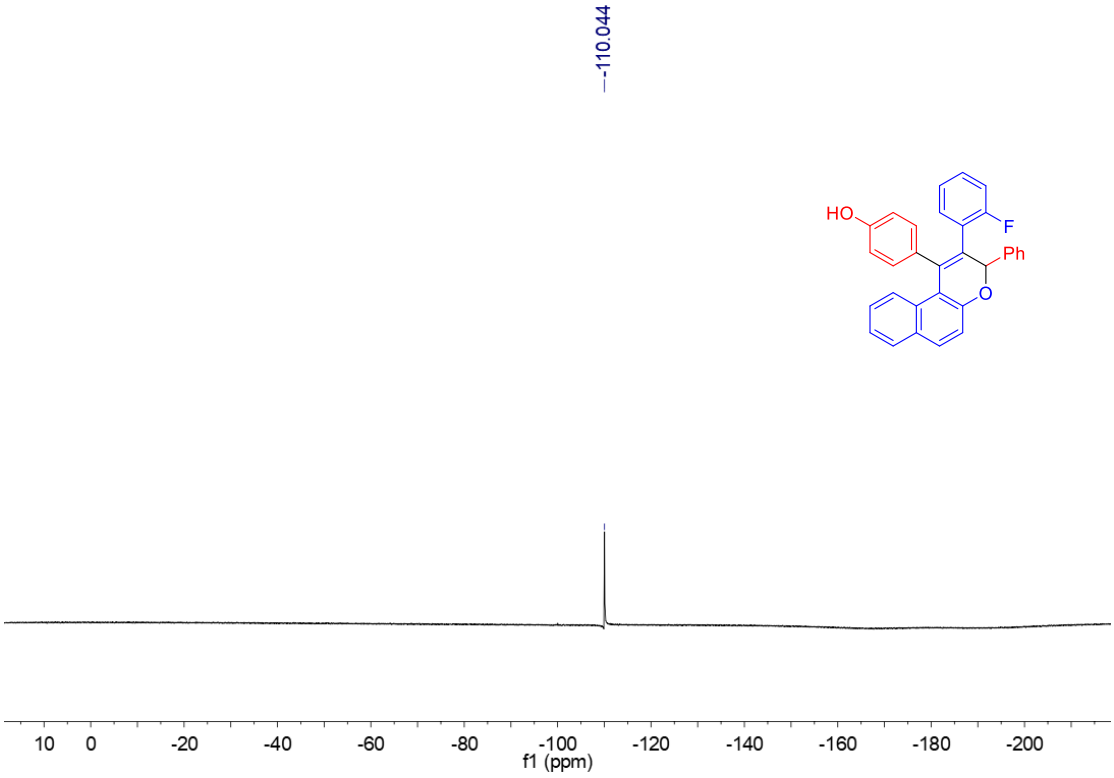
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3af**:



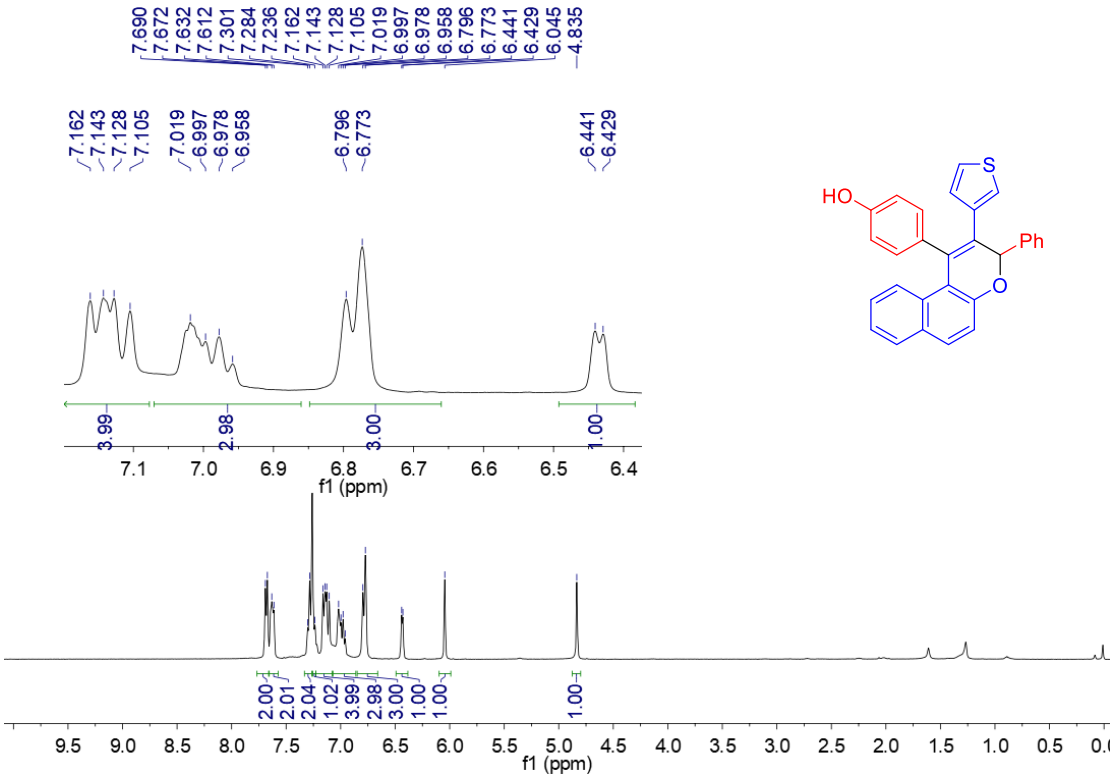
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3af**:



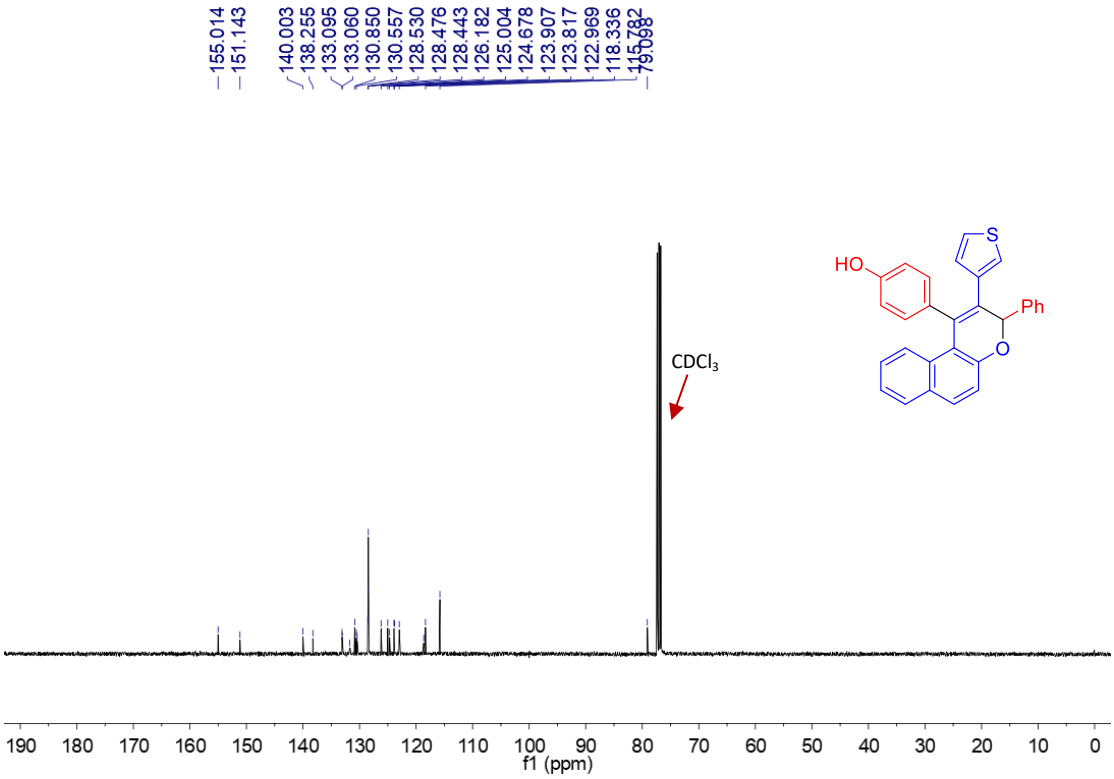
^{19}F NMR (376 MHz, $CDCl_3$) of compound **3af**:



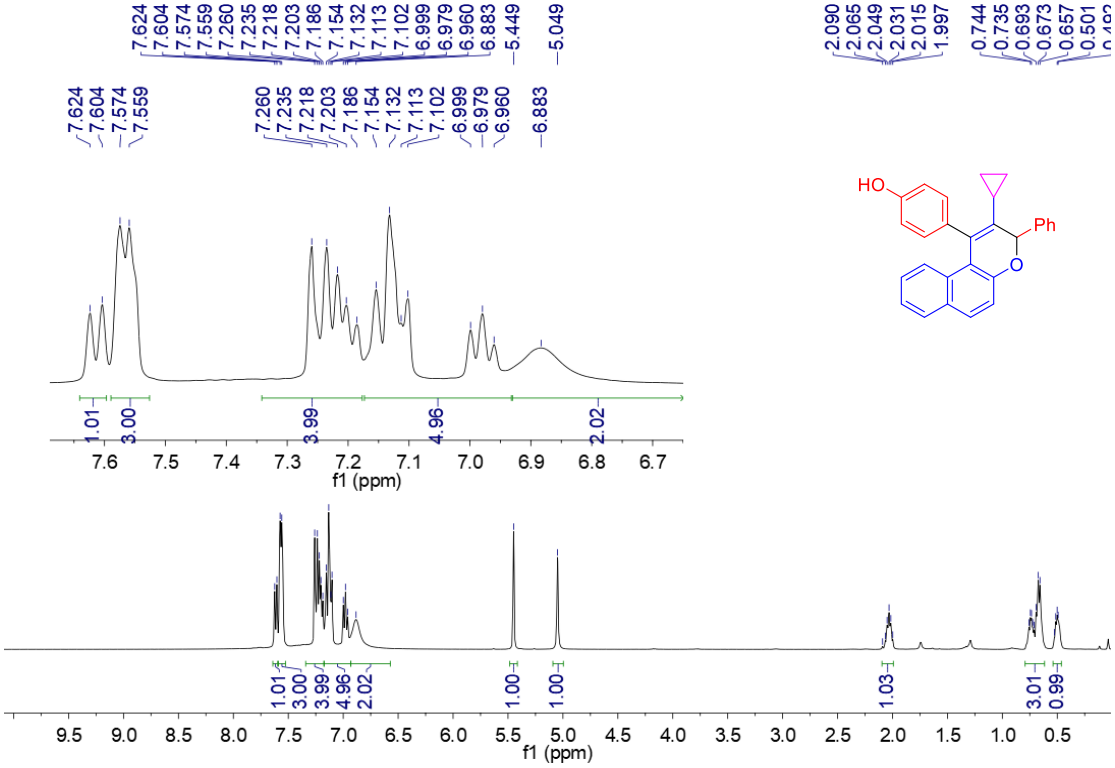
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ag**:



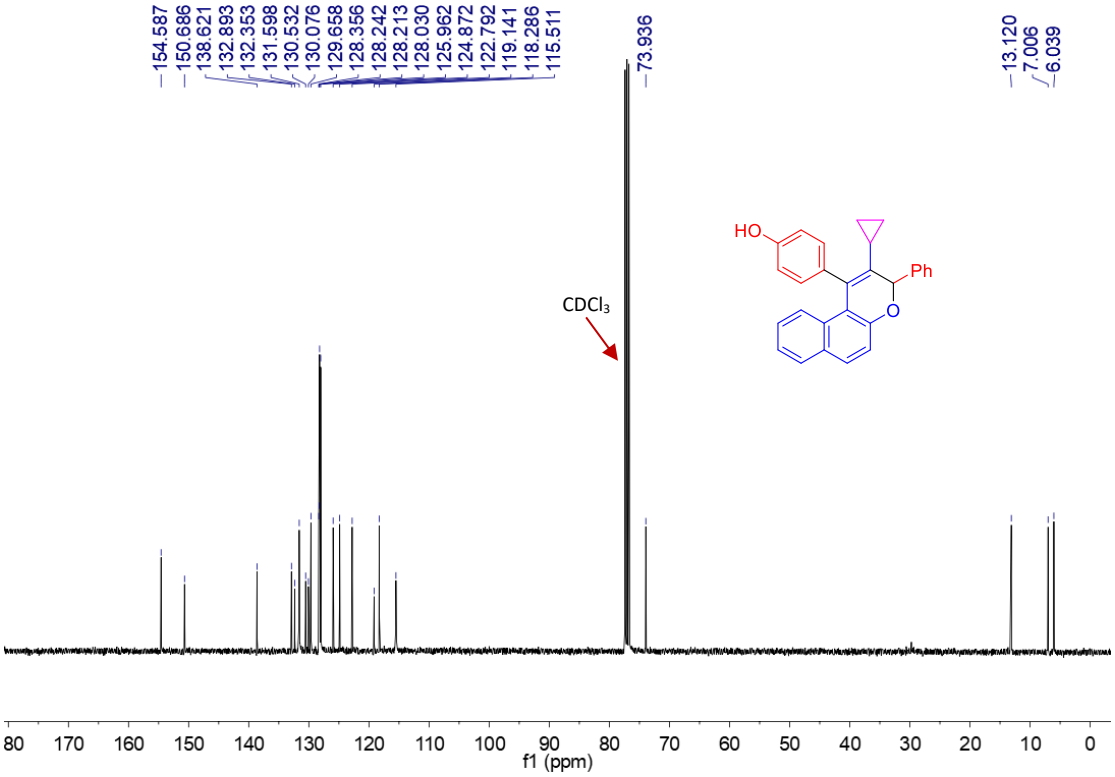
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ag**:



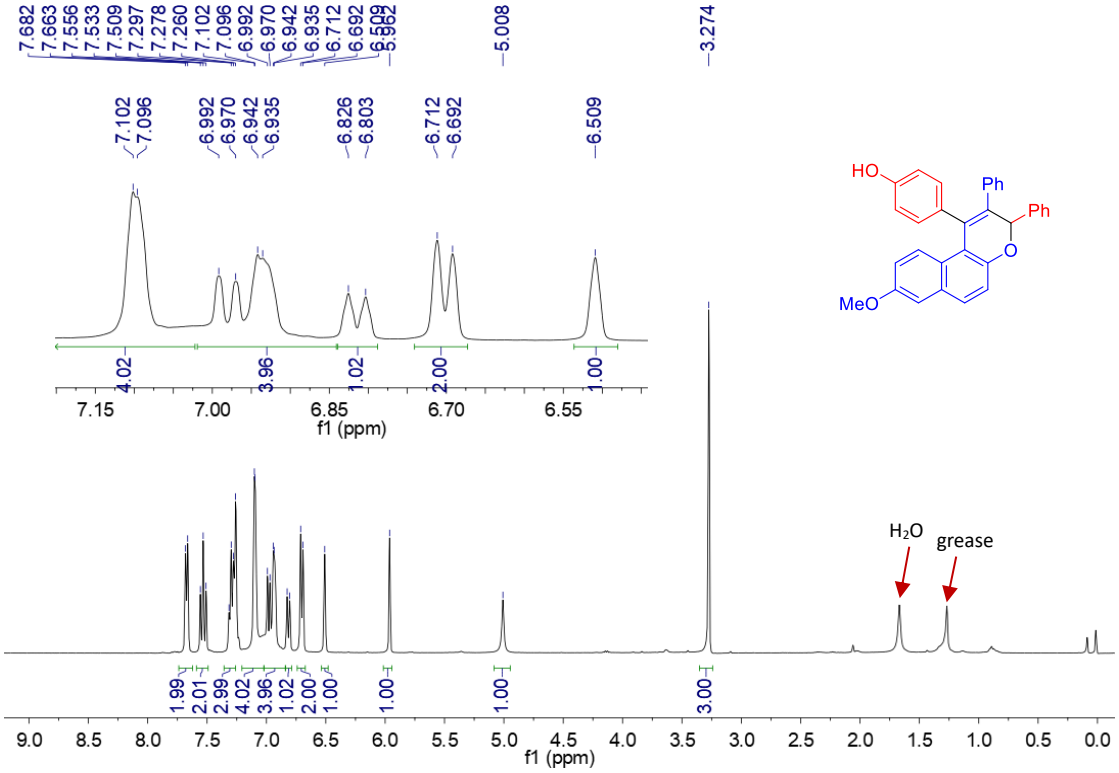
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ah**:



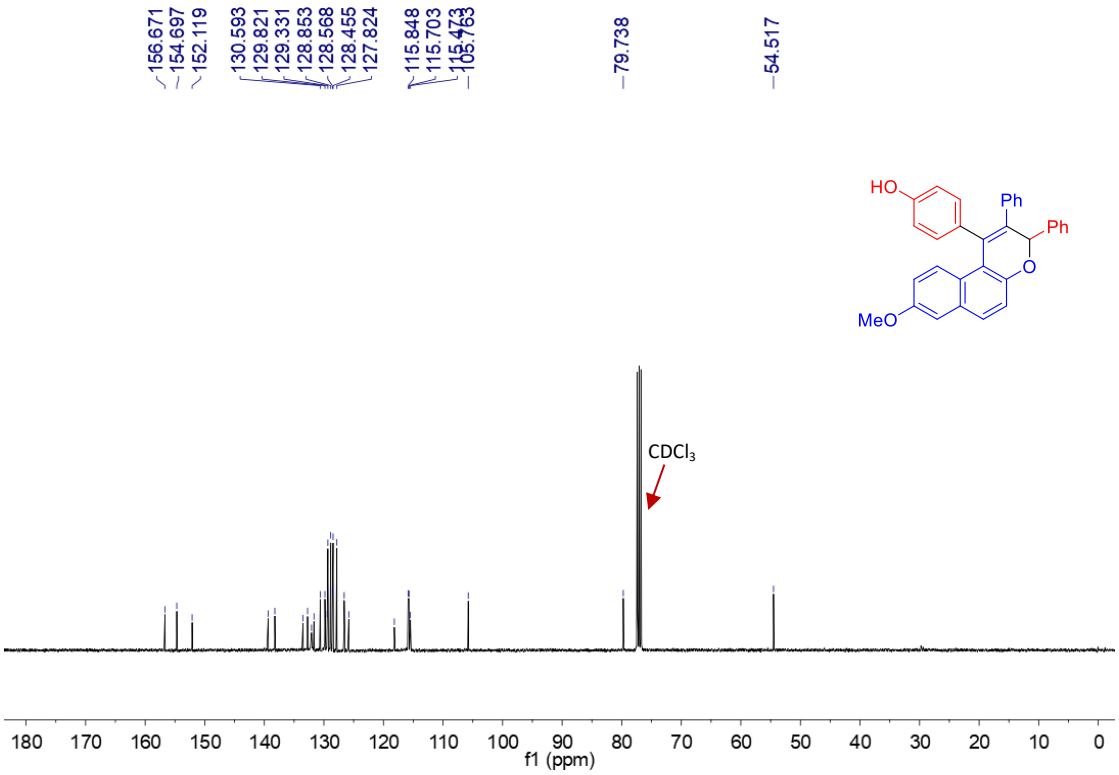
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ah**:



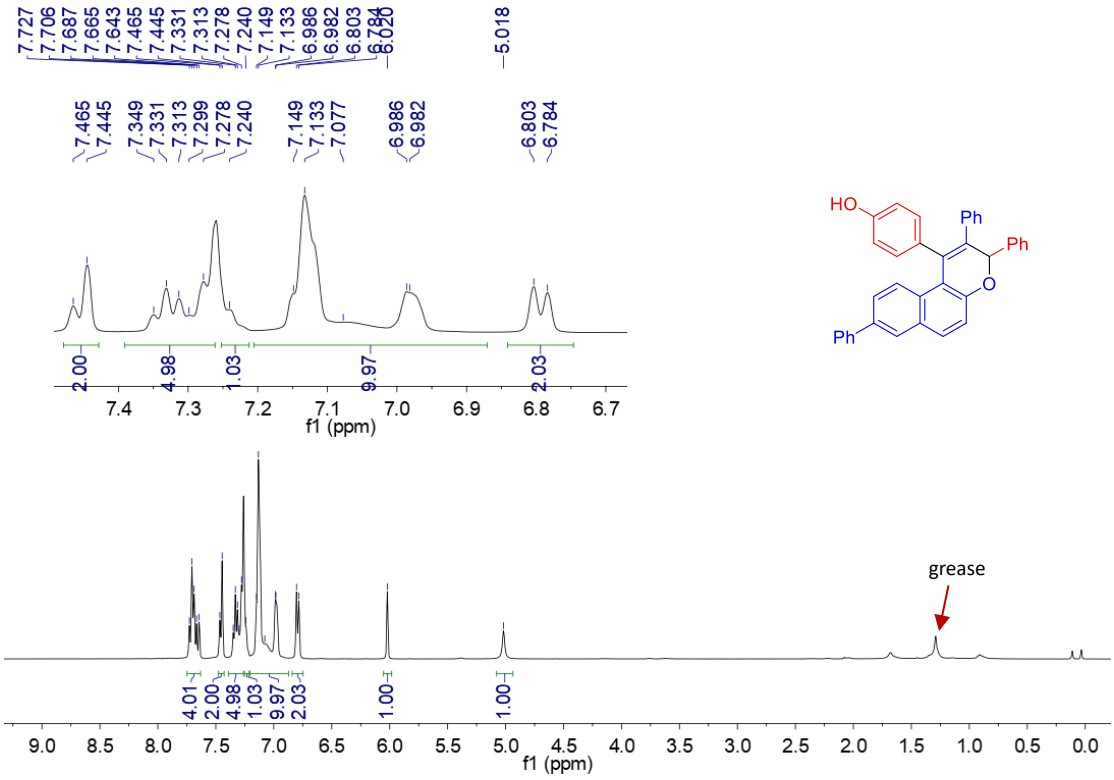
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ai**:



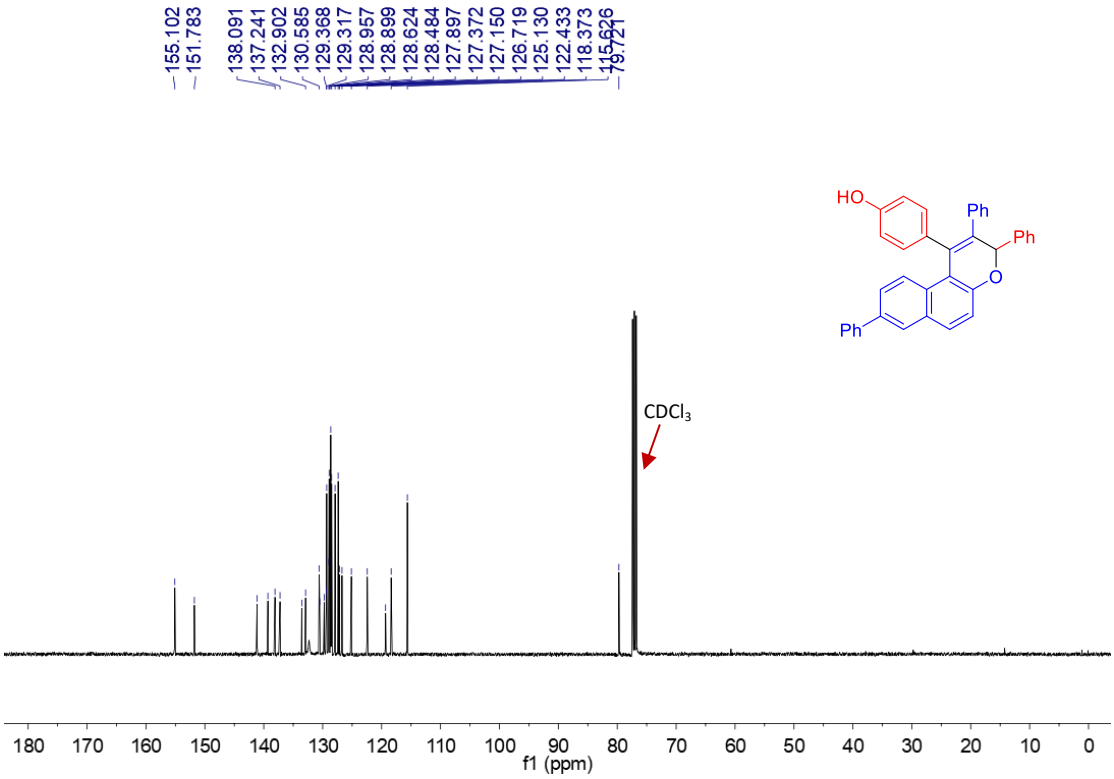
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ai**:



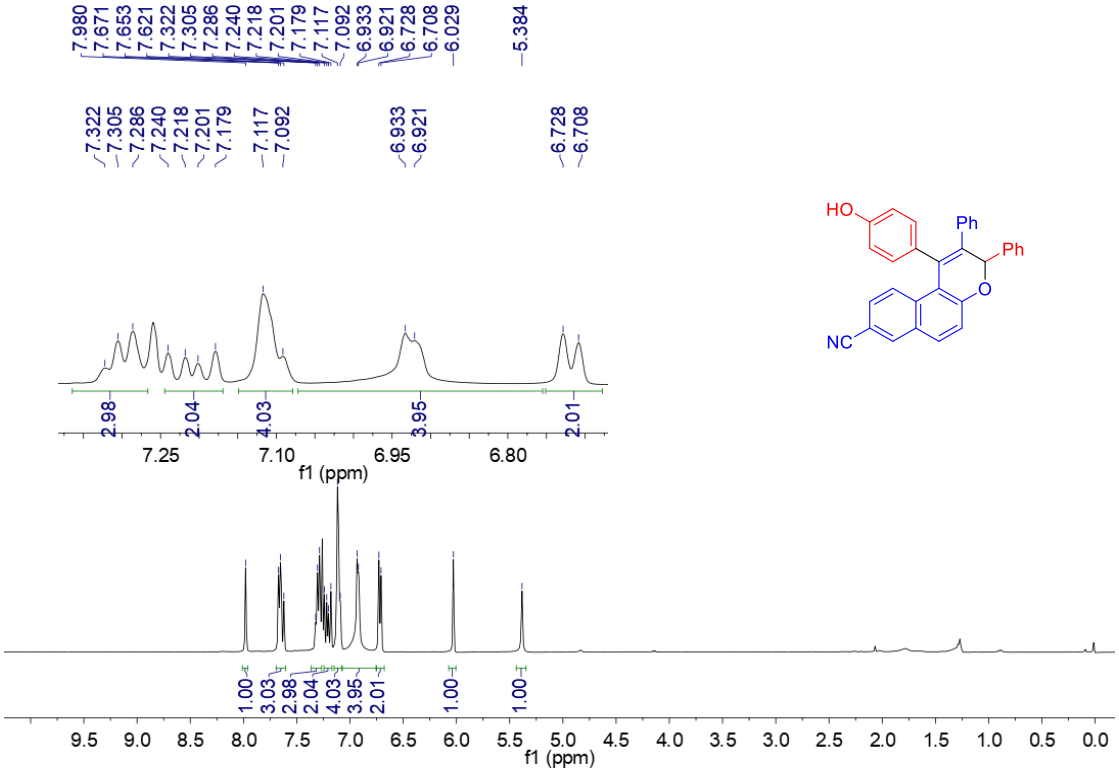
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3aj**:



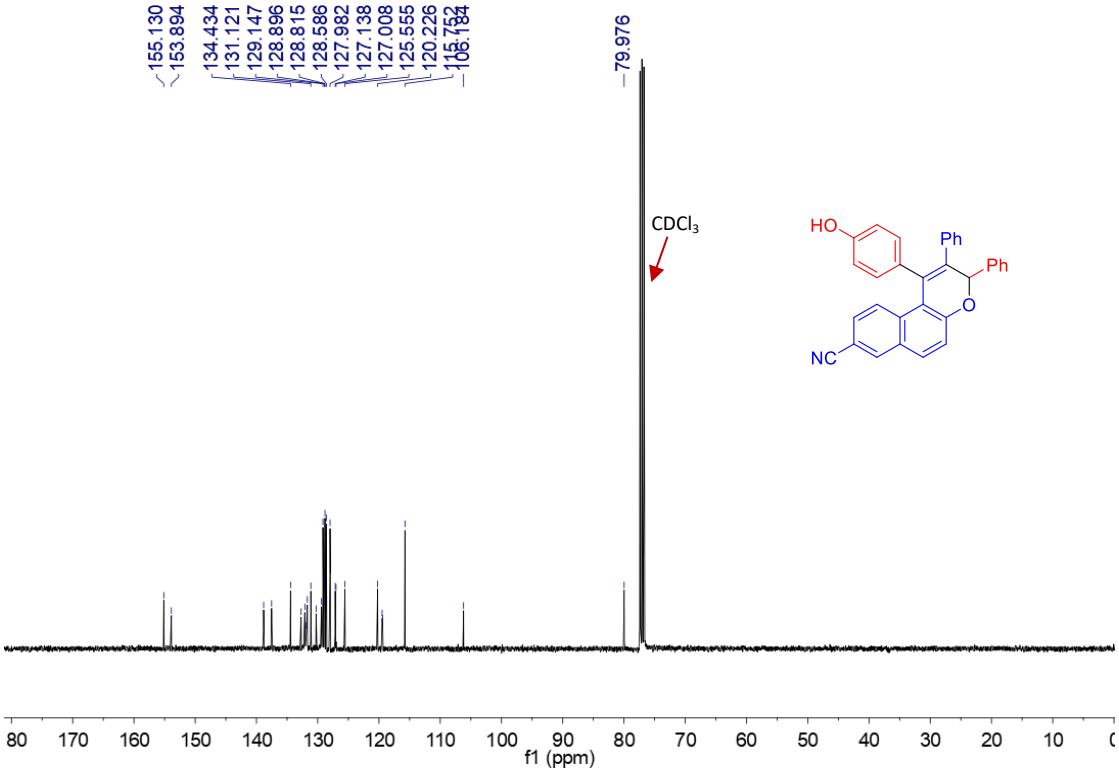
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3aj**:



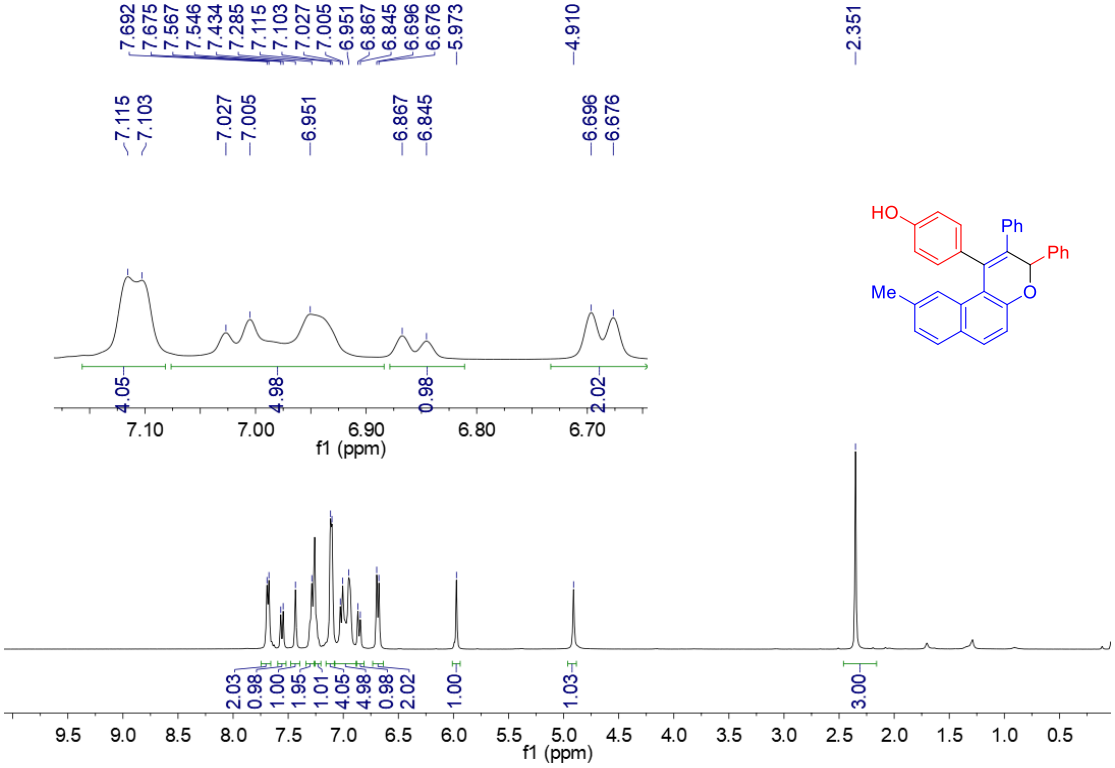
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ak**:



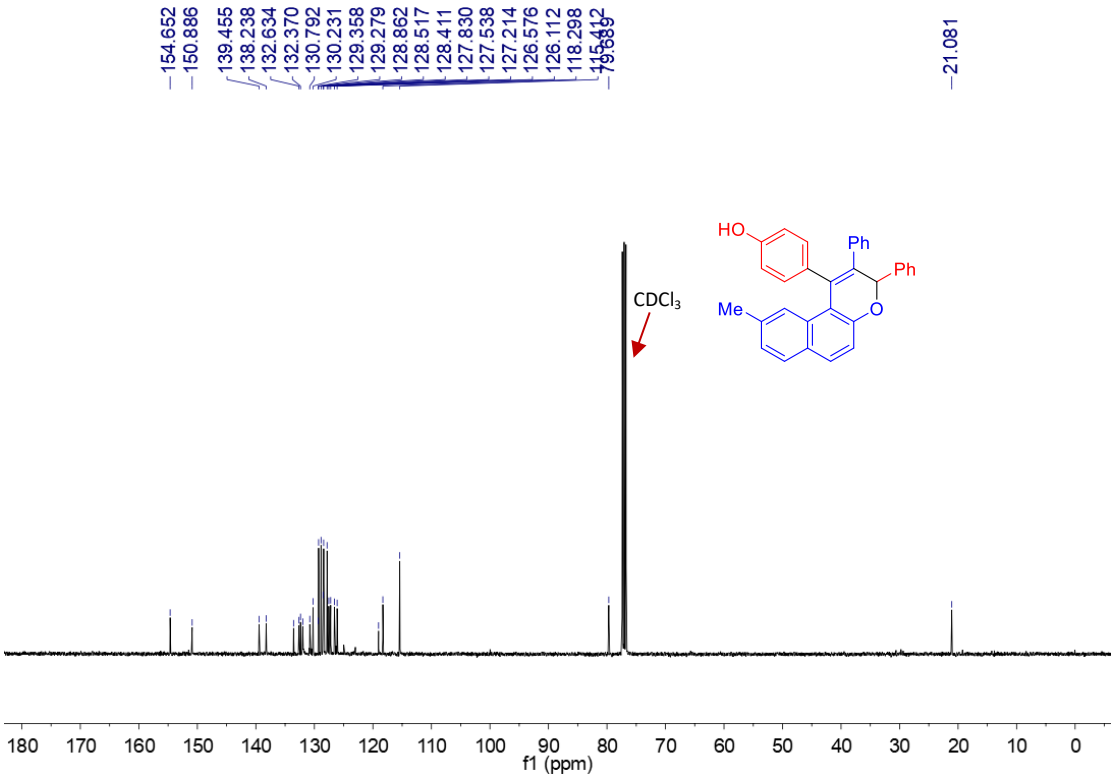
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ak**:



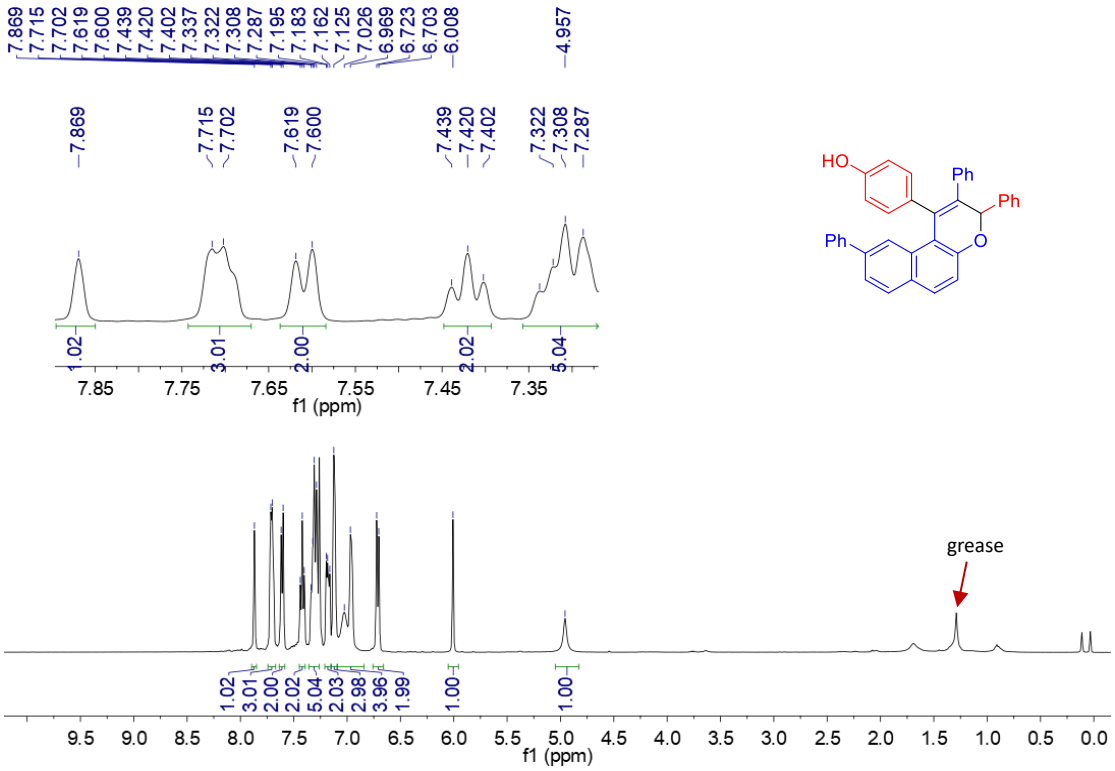
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3al**:



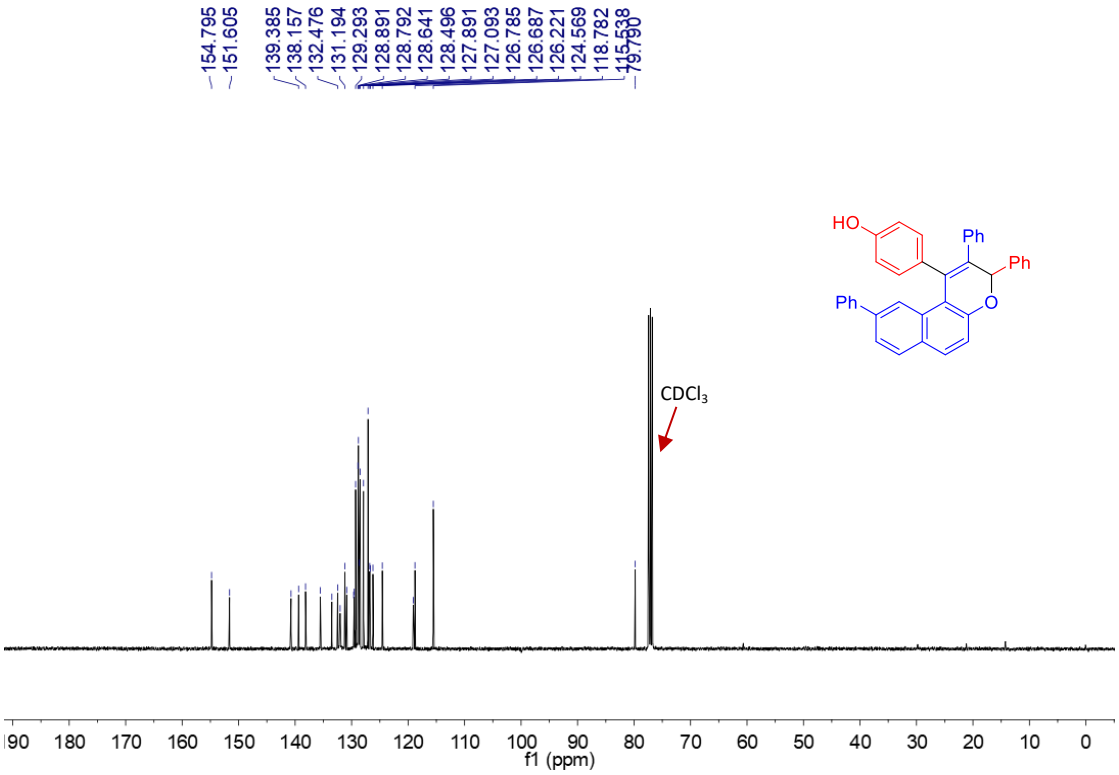
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3al**:



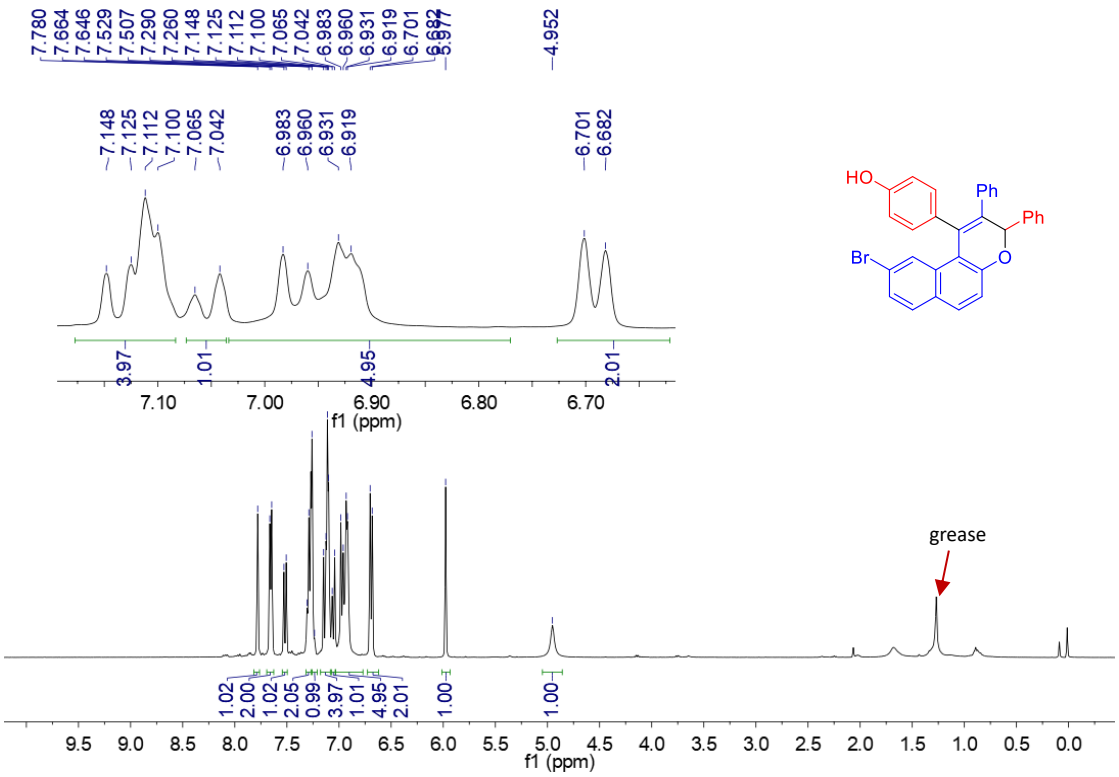
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3am**:



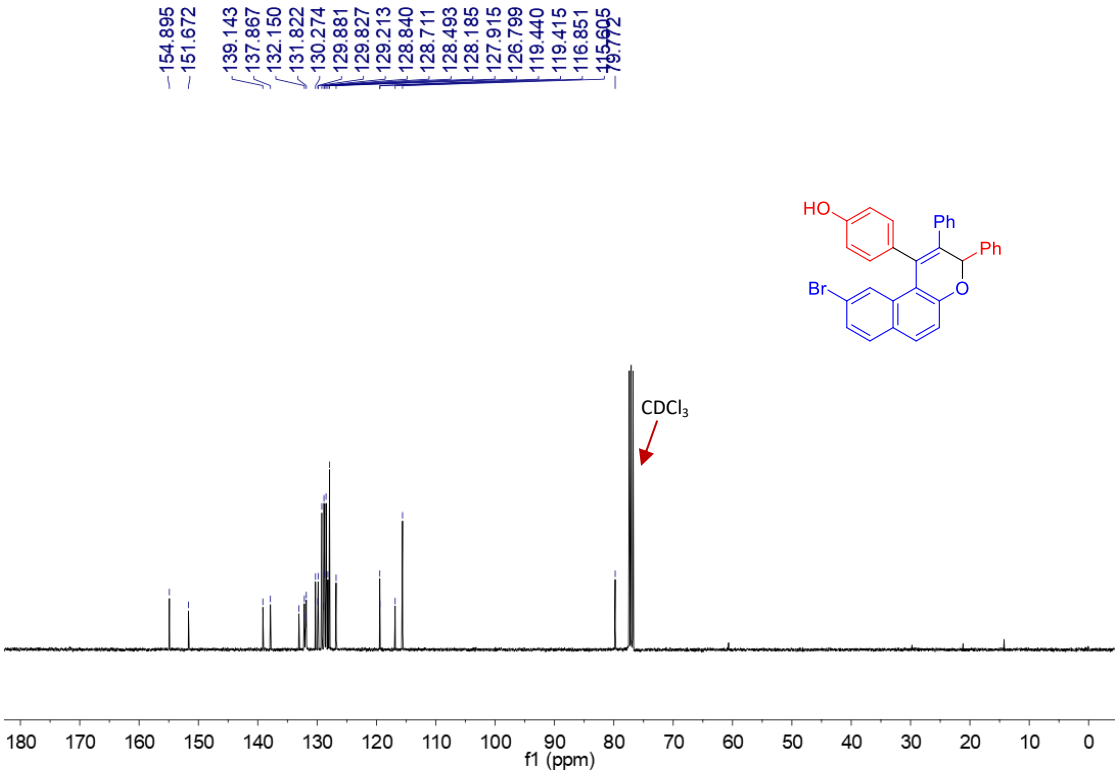
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3am**:



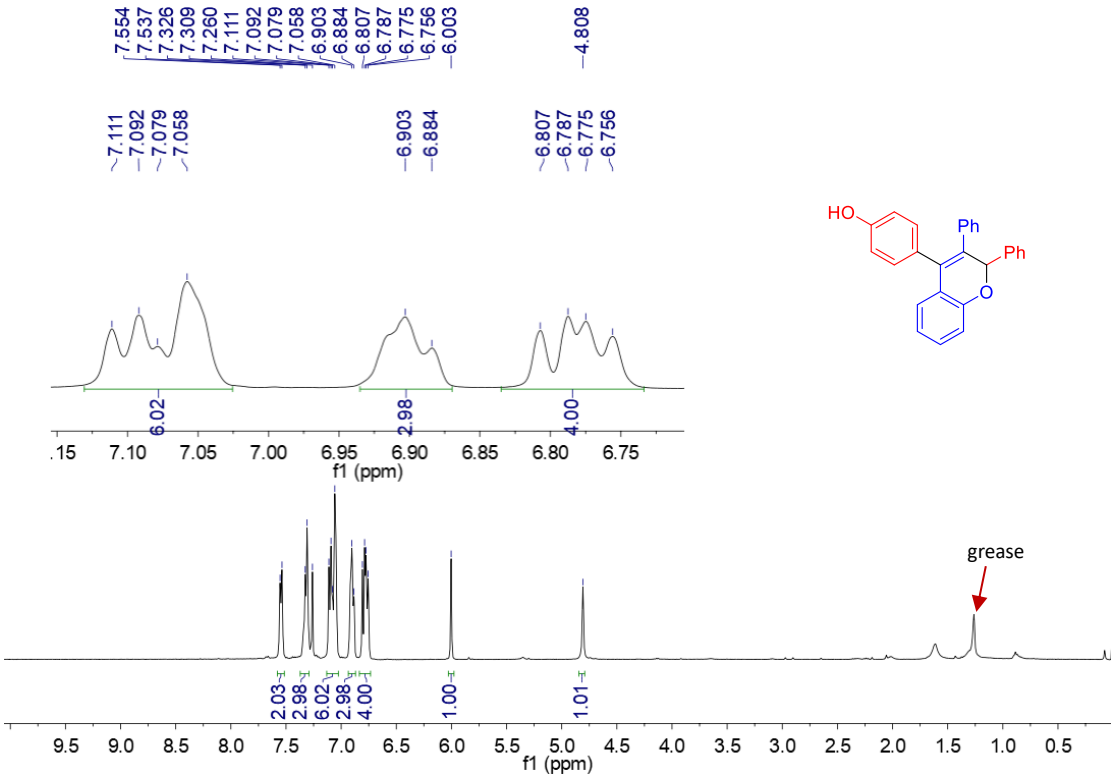
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3an**:



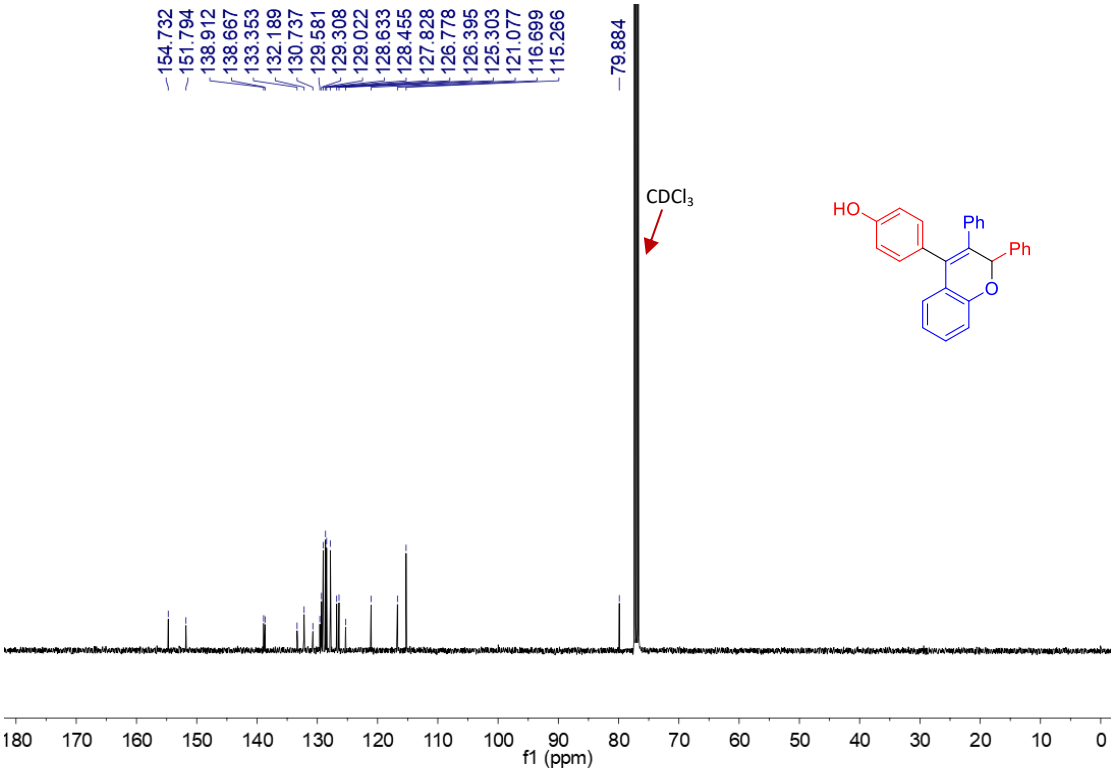
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3an**:



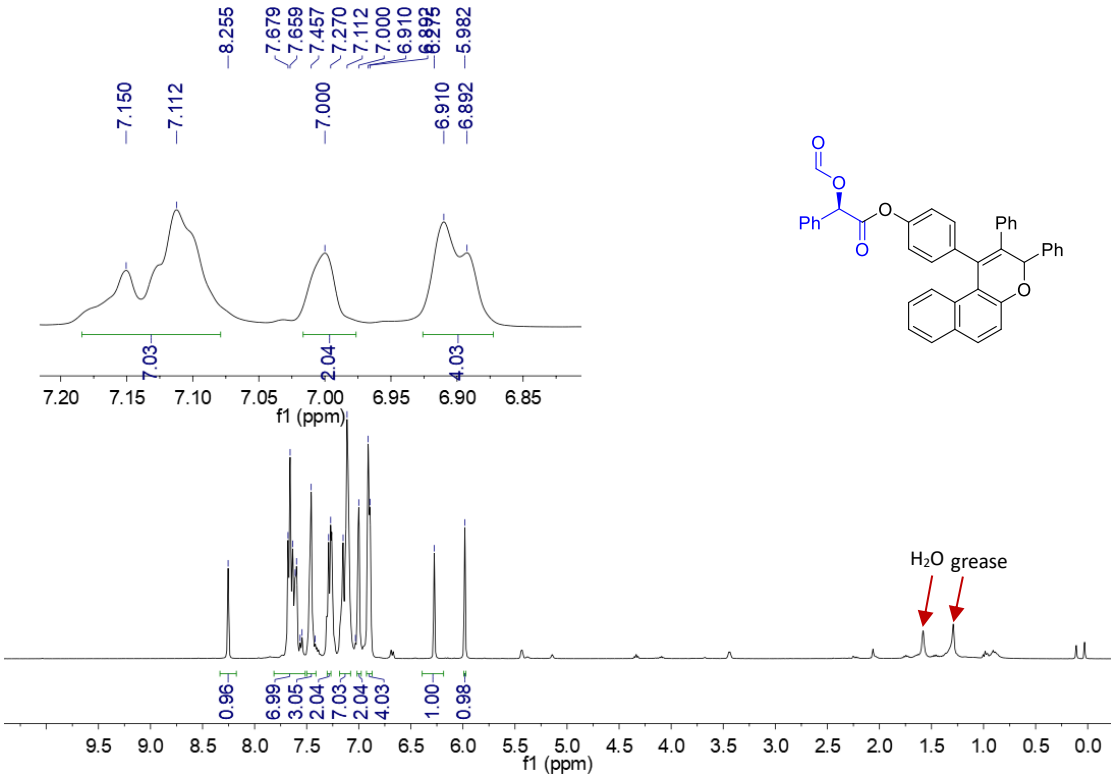
^{1}H NMR (400 MHz, $CDCl_3$) of compound **3ao**:



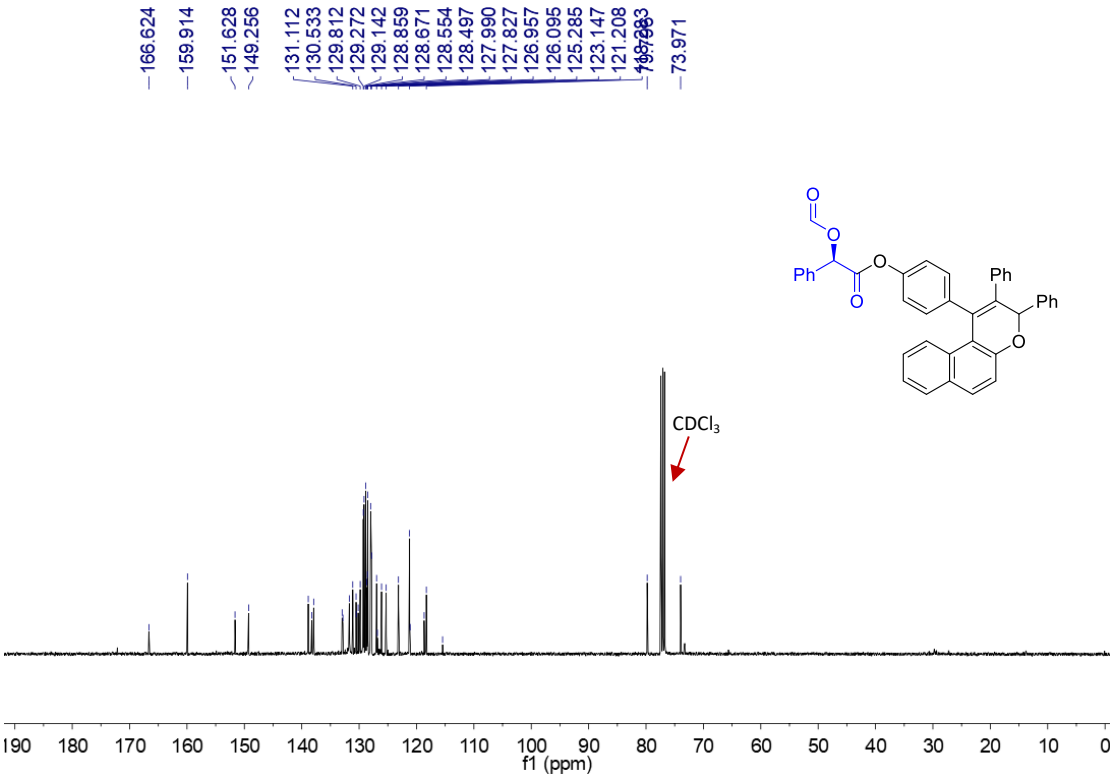
^{13}C NMR (100 MHz, $CDCl_3$) of compound **3ao**:



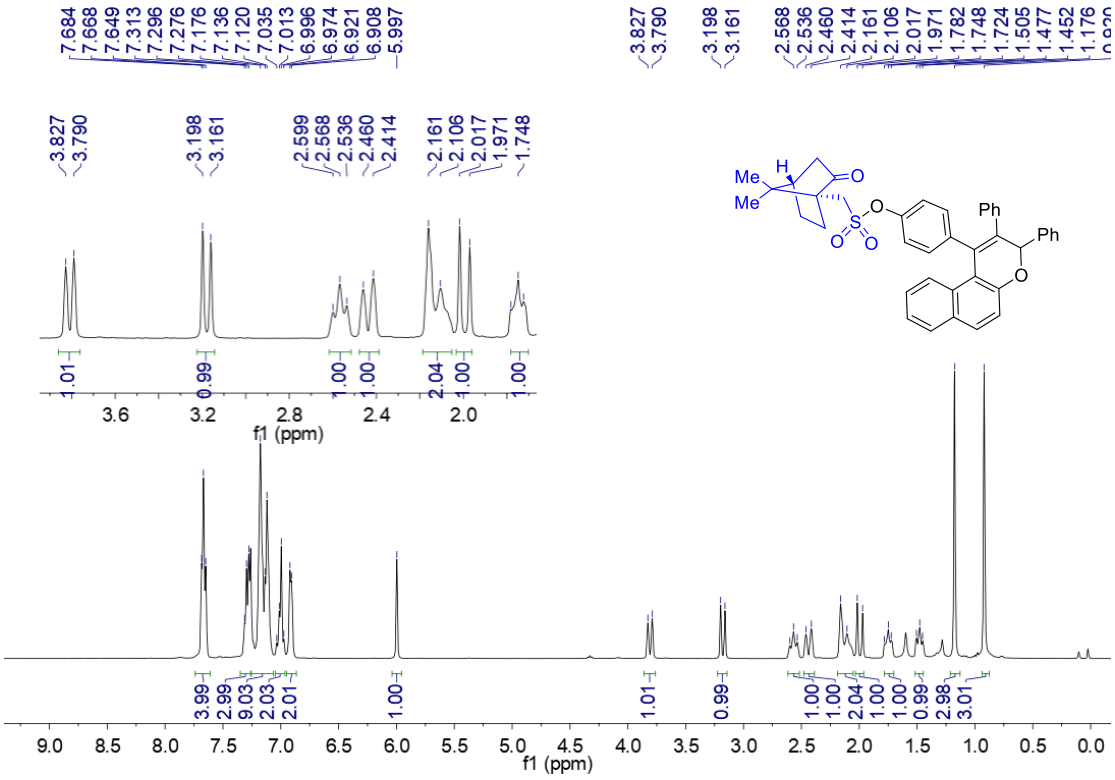
^{1}H NMR (400 MHz, $CDCl_3$) of compound **6a**: 50:50 dr



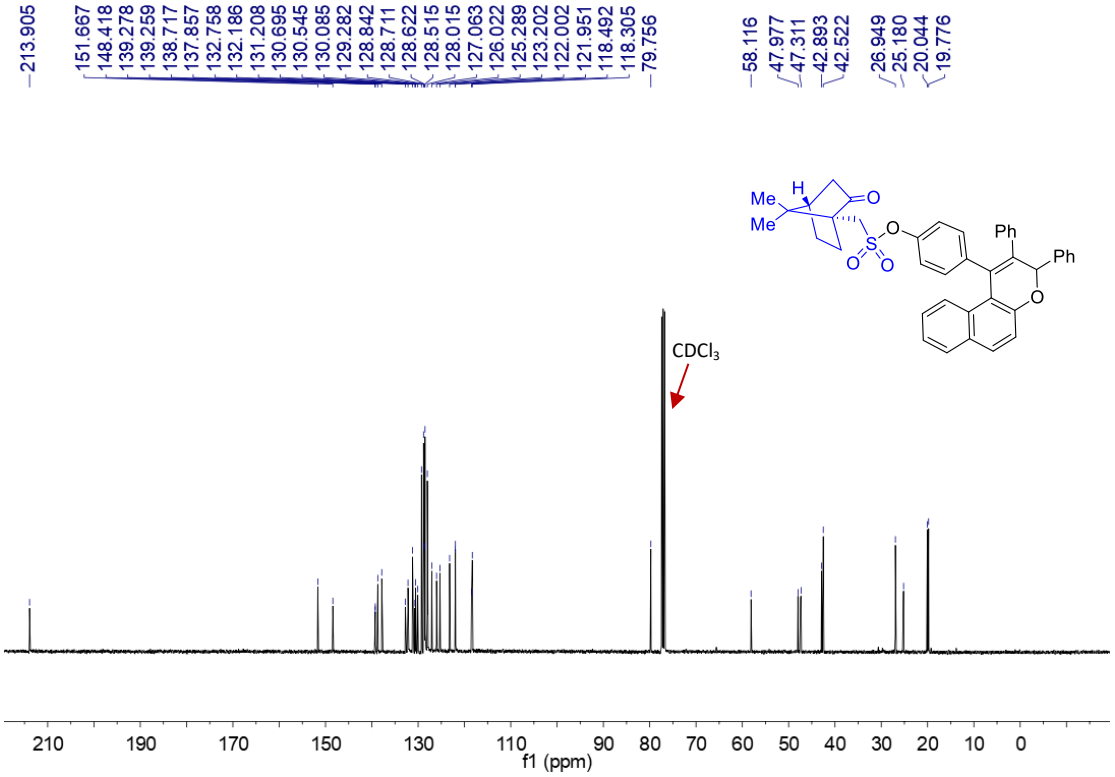
^{13}C NMR (100 MHz, $CDCl_3$) of compound **6a**: 50:50 dr



^{1}H NMR (400 MHz, $CDCl_3$) of compound **6b**: 50:50 dr

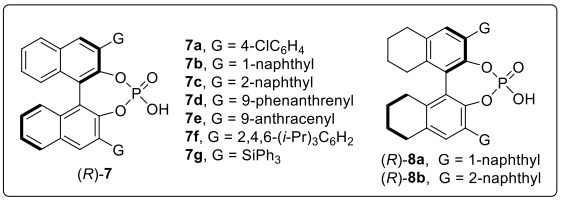


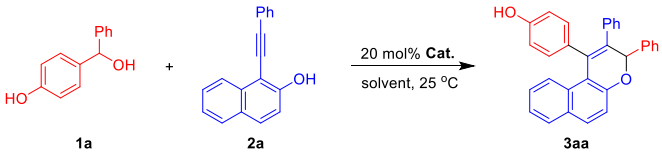
^{13}C NMR (100 MHz, $CDCl_3$) of compound **6b**: 50:50 dr



7. Investigation on the catalytic asymmetric version of the reaction

Table S2 Investigation on the catalytic asymmetric version of the reaction[a]





entry	**Cat.**	solvent	addition	**1a**:**2a**	yield (%)[b]	ee (%)[c]
1	**7a**	DCM	-	1:1.2	53	2
2	**7b**	DCM	-	1:1.2	42	7
3	**7c**	DCM	-	1:1.2	45	7
4	**7d**	DCM	-	1:1.2	37	1
5	**7e**	DCM	-	1:1.2	41	1
6	**7f**	DCM	-	1:1.2	12	0
7	**7g**	DCM	-	1:1.2	23	4
8	**8a**	DCM	-	1:1.2	trace	-
9	**8b**	DCM	-	1:1.2	37	3
10	**7c**	toluene	-	1:1.2	38	5
11	**7c**	MeCN	-	1:1.2	trace	-
12	**7c**	EtOAc	-	1:1.2	9	3
13	**7c**	THF	-	1:1.2	trace	-
14	**7c**	acetone	-	1:1.2	trace	-
15	**7c**	DCE	-	1:1.2	51	4
16	**7c**	$CHCl_3$	-	1:1.2	49	4
17	**7c**	DCM	3Å	1:1.2	47	3
18	**7c**	DCM	4Å	1:1.2	56	3
19	**7c**	DCM	5Å	1:1.2	53	2
20	**7c**	DCM	Na_2SO_4	1:1.2	41	2
21	**7c**	DCM	$MgSO_4$	1:1.2	54	2
22	**7c**	DCM	-	1:1.5	71	5
23	**7c**	DCM	-	1:2	70	4
24	**7c**	DCM	-	1.2:1	56	3
25	**7c**	DCM	-	1.5:1	53	2
26	**7c**	DCM	-	2:1	53	3
27[d]	**7c**	DCM	-	1:1.5	42	2
28[e]	**7c**	DCM	-	1:1.5	53	1
29[f]	**7c**	DCM	-	1:1.5	31	3
30[g]	**7c**	DCM	-	1:1.5	61	3

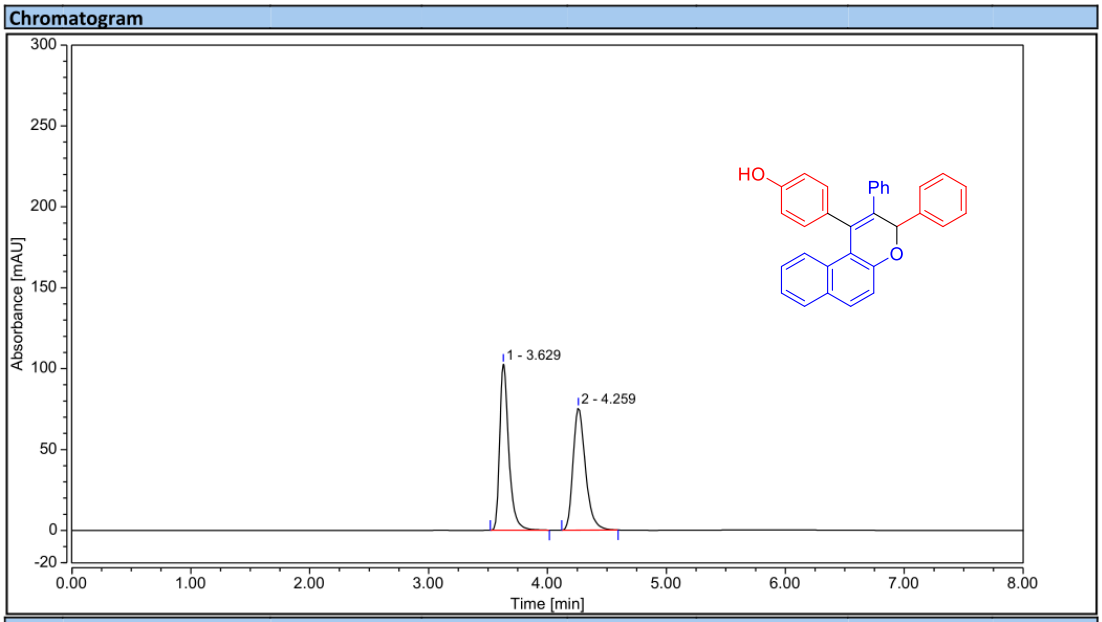
[a]Unless otherwise indicated, the reaction was carried out at 0.1 mmol scale and catalyzed by 20 mol% **Cat.** in

DCM (1.0 mL) at 25 ^{o}C for 24 h, and the molar ratio of **1a**:**2a** was 1.2:1. [b]Isolated yield. [c]The enantiomeric excess (ee) was determined by HPLC, [d]Catalyzed by 5 mol% **7c**, [e]Catalyzed by 10 mol% **7c**, [f]erformed at 0 ^{o}C, [g]erformed at 50 ^{o}C.

8. HPLC traces of product 3aa

3aa

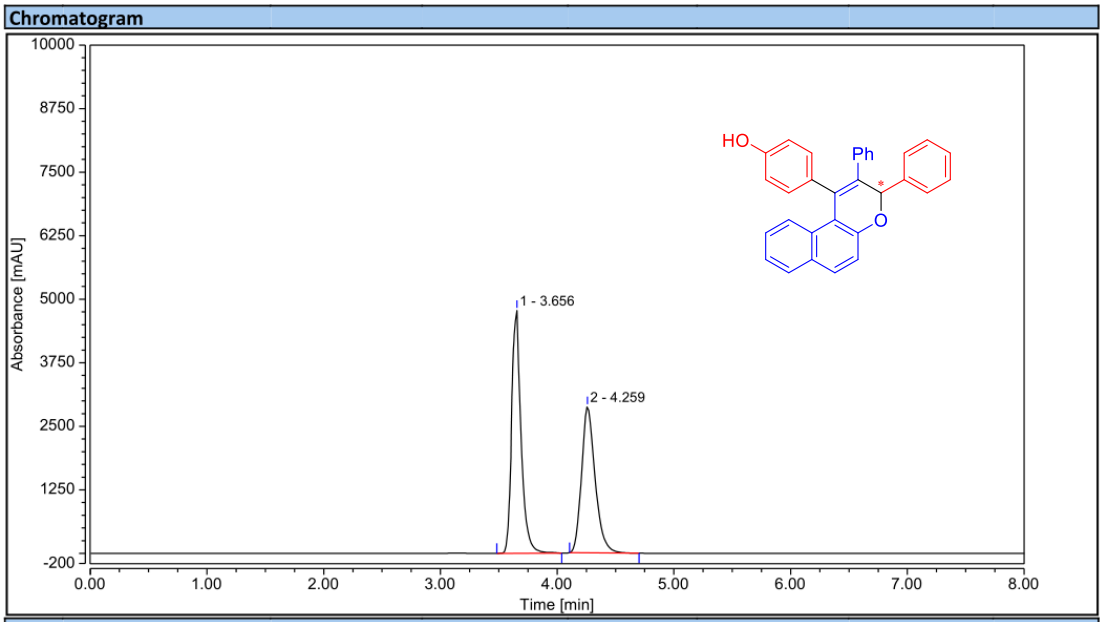
Racemic:



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.629	9.097	102.688	49.94	57.61	n.a.
2		4.259	9.117	75.544	50.06	42.39	n.a.
Total:			**18.214**	**178.231**	**100.00**	**100.00**	

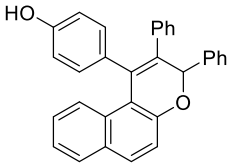
Enantioselective:



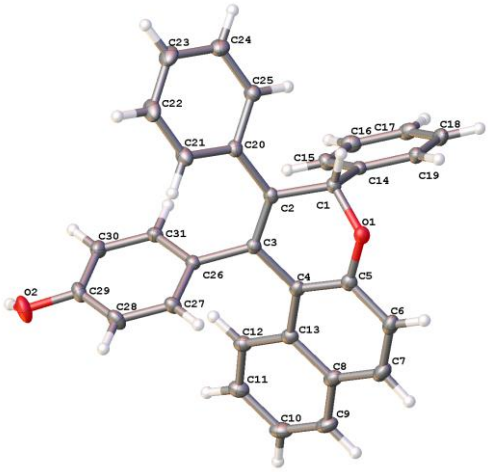
Integration Results

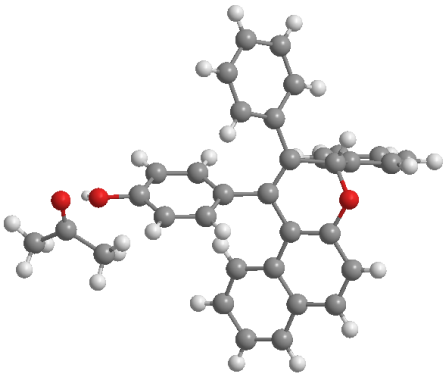
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.656	443.445	4778.248	53.38	62.43	n.a.
2		4.259	387.319	2875.203	46.62	37.57	n.a.
Total:			**830.764**	**7653.451**	**100.00**	**100.00**	

9. X-ray single crystal data for products 3aa



3aa





(with acetone)

The single-crystal of **3aa** was grown from the mixed solution of *n*-hexane and acetone (V/V = 2:1).

The X-ray source used for the single crystal X-ray diffraction analysis was GaKα (λ = 1.34139), and the thermal ellipsoid was drawn at the 30% probability level.

Identification code	240102sf	
Empirical formula	C34 H28 O3	
Formula weight	484.56	
Temperature	173.00 K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 10.44920(10) Å	α= 90 °.

	b = 18.0226(3) Å	β= 105.5920(10) °.
	c = 14.2881(2) Å	γ = 90 °.
Volume	2591.74(6) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/m^3	
Absorption coefficient	0.392 mm^{-1}	
F(000)	1024	
Crystal size	0.17 x 0.17 x 0.05 mm^3	
Theta range for data collection	3.515 to 54.964 °.	
Index ranges	-12<=h<=12, -21<=k<=21, -17<=l<=17	
Reflections collected	33732	
Independent reflections	4924 [R(int) = 0.0490]	
Completeness to theta = 53.594 °	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7508 and 0.6165	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4924 / 0 / 337	
Goodness-of-fit on F^2	1.046	
Final R indices [I>2sigma(I)]	R1 = 0.0374, wR2 = 0.0948	
R indices (all data)	R1 = 0.0441, wR2 = 0.0998	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.220 and -0.205 $e.Å^{-3}$	

10. Theoretical calculations on the reaction pathway

Computational studies Computational details:

All calculations were performed using Gaussian 16, Revision A.03 package.[3] All of the reactants, intermediates, transition states, products were optimized by the DFT with the B3LYP-D3(BJ) functional. [4] For geometry optimizations and frequency calculations, BS-I basis set system was employed. In BS-I, we employed 6-31G(d) basis sets for H, C, O, P. All the stationary structures were characterized with no imaginary frequency and the transition state structures (TSs) were characterized with a single imaginary frequency. Intrinsic reaction coordinate (IRC) calculations were performed on the TSs. The solvent effect of dichloromethane was evaluated through the SMD method,[5] in which a better basis system BS-II was used. In BS-II, we employed 6-311++G(2d,2p) basis sets for H, C, O, P. All reported energies are free energies at a concentration of 1 M and a temperature of 298.15 K.

[3] Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2016**.

[4] S. Grimme, *J. Comp. Chem.* **2006**, *27*, 1787.

[5] A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B.*, **2009**, *113*, 6378.

Cartesian coordinates of the optimized structures:

4a

E = -1412.389764 a.u.

0 1

C	-3.51493400	-7.41742400	1.26239200
C	-2.15787100	-7.33463300	1.05582400
C	-1.52431200	-6.07975600	0.85548900
C	-2.30961600	-4.88088000	0.90021900
C	-3.71313200	-5.00621600	1.08651700
C	-4.29828700	-6.23967800	1.26363400
H	0.45299500	-6.90869300	0.55310700
H	-3.98908500	-8.38329800	1.40961300
H	-1.54620700	-8.23277700	1.02986500
C	-0.13370500	-5.99488400	0.58365500
C	-1.66536200	-3.60933700	0.71669000
H	-4.32729300	-4.11433500	1.07923500
H	-5.37370400	-6.30912200	1.39911700
C	-0.32010200	-3.60908600	0.39011000
C	0.45737300	-4.78233700	0.33004000
C	-2.40138200	-2.32349700	0.81894400
C	-2.35267700	-1.42014200	-0.22835900
C	-3.14032700	-1.94782300	1.99263400
C	-3.06487600	-0.20520400	-0.23480500
C	-3.88262800	-0.72089100	1.99138700
C	-3.13502700	-2.72704800	3.18126100
C	-3.83693200	0.12404300	0.85155200
C	-4.62773300	-0.35787200	3.14439600
C	-3.85738200	-2.33912200	4.28707800
H	-2.54423000	-3.63407200	3.21406900
H	-4.40125200	1.05221000	0.86214200
C	-4.62349900	-1.15019000	4.26836500
H	-5.19327300	0.57009300	3.12355900
H	-3.83290500	-2.94910700	5.18542000
H	-5.19319400	-0.85938800	5.14602100
O	0.33837900	-2.40267600	0.13712200
O	-1.58891300	-1.71872800	-1.36225400
P	0.02230400	-1.59125800	-1.23130900
O	0.44587300	-2.57512200	-2.43474200
H	1.15151800	-2.15735900	-2.95570000
O	0.63660100	-0.25343600	-1.25262900
H	-2.98292700	0.43937700	-1.10260000
H	1.51033000	-4.69332300	0.08762700

I1

E = -1989.059482 a.u.

0 1

C	-2.24354000	-9.95908700	1.62637500
C	-1.06326600	-9.25428300	1.66705100
C	-1.05730200	-7.84765200	1.86065500
C	-2.30106300	-7.15859800	2.04649200
C	-3.50259000	-7.91436300	1.96902200
C	-3.47411100	-9.27573700	1.76617300
H	1.09178600	-7.63983500	1.69930000
H	-2.23524600	-11.03424700	1.47255700
H	-0.11078300	-9.76221800	1.53831400
C	0.15483700	-7.10895400	1.84360100
C	-2.29373200	-5.73802900	2.26077200
H	-4.45264100	-7.40304300	2.06300500
H	-4.40683100	-9.82926800	1.70602600
C	-1.08123200	-5.07447600	2.17022400
C	0.14378000	-5.74251300	1.97099700
C	-3.53510800	-4.96537300	2.52290800
C	-3.84815000	-3.87871500	1.72277000
C	-4.41735000	-5.27152900	3.61465200
C	-5.03241200	-3.12985600	1.87560300
C	-5.63209700	-4.52508100	3.76792400
C	-4.11661300	-6.26676100	4.58418400
C	-5.91940500	-3.46567900	2.86779000
C	-6.51251800	-4.84071500	4.83637000
C	-4.98582800	-6.53886900	5.61646600
H	-3.18269500	-6.80980400	4.50810300
H	-6.84151900	-2.90490100	2.99319000
C	-6.20372300	-5.83009100	5.74033400
H	-7.43417600	-4.27216800	4.93164000
H	-4.73020500	-7.30113300	6.34693600
H	-6.88320000	-6.05898500	6.55619300
O	-1.03637600	-3.69024500	2.30712200
O	-2.98997500	-3.50797300	0.69029900
P	-1.59805900	-2.76115600	1.08511500
O	-0.75756400	-3.10070400	-0.20214000
H	0.02491200	-2.47734500	-0.36331500
O	-1.68903900	-1.35052900	1.52043100
H	-5.20976800	-2.30279200	1.19740900
H	1.05152800	-5.15137900	1.92416700
C	0.69011900	0.38835500	0.34256800
C	1.58816200	-0.45146900	-0.44558800
C	2.83376300	0.15750000	-0.91701800

C	3.11990700	1.45919700	-0.68500800
C	2.19999500	2.31203100	0.04810600
C	1.00252900	1.68361600	0.58084100
H	-0.21608400	-0.06341500	0.73851800
H	3.52283600	-0.49651300	-1.44183100
H	4.06931800	1.87215200	-1.00595400
H	0.32868400	2.30388900	1.16731500
O	1.34978800	-1.65043500	-0.70409700
C	2.40828600	3.64507300	0.28943300
H	1.71162600	4.11909400	0.98062500
C	3.44189000	4.52830200	-0.23105500
C	3.99675100	4.39254300	-1.52014700
C	3.87556900	5.60157800	0.57382600
C	4.98130500	5.27062000	-1.96329900
H	3.61742600	3.62822600	-2.18884500
C	4.86887200	6.46932400	0.13321400
H	3.43695800	5.73359100	1.55927600
C	5.42946700	6.30323000	-1.13599500
H	5.38988100	5.15846700	-2.96320100
H	5.20146900	7.28010800	0.77445600
H	6.19761800	6.98655600	-1.48569300

2a

E = -768.374240 a.u.

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C	-3.56902700	-7.13201600	1.88205100
C	-2.28973800	-7.22600600	1.38817600
C	-1.64550200	-6.10130800	0.81216600
C	-2.34785400	-4.85663200	0.75021000
C	-3.68513000	-4.76962600	1.26947300
C	-4.27251300	-5.90717200	1.82593600
H	0.19738600	-7.13111100	0.35031700
H	-4.05387900	-8.00138400	2.32198700
H	-1.75653800	-8.17159000	1.43546600
C	-0.32530400	-6.17925700	0.29709800
C	-1.69563400	-3.73814200	0.17273500
C	-0.41318800	-3.84576400	-0.31868200
C	0.28251200	-5.07647300	-0.25797600
H	1.29315200	-5.14669100	-0.64933000
H	0.07003000	-2.97736900	-0.75761500
H	-2.22970900	-2.79498100	0.12654000
O	-5.54087400	-5.79816000	2.31111900
H	-5.81586700	-6.65898900	2.66281400
C	-4.40775300	-3.55249300	1.22300300

C	-5.01701600	-2.50105800	1.17661600
C	-5.75605600	-1.28773400	1.13753700
C	-5.19503700	-0.11805000	0.58752900
C	-7.06760700	-1.23762900	1.65138800
C	-5.92740100	1.06480500	0.55422100
H	-4.18521900	-0.15322400	0.19100300
C	-7.79199400	-0.05021600	1.61359300
H	-7.49961300	-2.13848300	2.07499100
C	-7.22679800	1.10443800	1.06601000
H	-5.48325900	1.95968300	0.12739900
H	-8.80205200	-0.02448000	2.01285600
H	-7.79544900	2.02946700	1.03834500

I2

E = -2757.492674 a.u.

0 1

C	0.17882500	-12.63854500	4.85102400
C	0.86293300	-11.88972600	3.92222100
C	0.31320700	-10.68875800	3.40130400
C	-0.96299000	-10.23594600	3.87344400
C	-1.65461400	-11.05079500	4.81107000
C	-1.09894900	-12.21697900	5.28711000
H	1.95386900	-10.29945300	2.04404300
H	0.60812800	-13.55783500	5.23881800
H	1.83603200	-12.21198700	3.55995800
C	0.99023900	-9.94490100	2.39986600
C	-1.50922100	-9.00924400	3.36209400
H	-2.63897300	-10.74800700	5.14573700
H	-1.65129600	-12.82293000	5.99974900
C	-0.82140100	-8.36309400	2.34655600
C	0.42499100	-8.81508900	1.86423800
C	-2.79757300	-8.45475400	3.85253400
C	-3.81078800	-8.16394300	2.95228800
C	-3.02901000	-8.16630300	5.23980200
C	-5.08007300	-7.69939500	3.35657800
C	-4.32524900	-7.72205600	5.66150700
C	-1.99783600	-8.24314400	6.21452100
C	-5.34030500	-7.51176100	4.69138500
C	-4.55271100	-7.44634700	7.03615400
C	-2.24404400	-7.94647700	7.53560200
H	-0.99887300	-8.51862400	5.90038800
H	-6.31807600	-7.16870500	5.01860600
C	-3.53773500	-7.56006200	7.95848700
H	-5.54510700	-7.12459600	7.34210800

H	-1.43336400	-7.99349000	8.25636800
H	-3.72191700	-7.33893900	9.00601000
O	-1.33069000	-7.20101400	1.79414400
O	-3.60344300	-8.35393200	1.59343700
P	-2.65916300	-7.26213900	0.81637000
O	-2.30016100	-7.91912700	-0.50543900
O	-3.23412700	-5.87246900	0.83663500
H	-5.82322200	-7.50739900	2.59080900
H	0.90270900	-8.25458600	1.06890400
C	-0.79445300	-5.25617000	-1.25355100
C	0.21479700	-6.26084700	-1.41437100
C	1.57534100	-5.85678300	-1.62588600
C	1.91484200	-4.53970900	-1.55382200
C	0.93650200	-3.53166700	-1.23183600
C	-0.43733200	-3.94692000	-1.14250600
H	-1.83305500	-5.55239000	-1.19161100
H	2.30930400	-6.63384100	-1.80955200
H	2.94896900	-4.23074000	-1.66797000
H	-1.20762800	-3.19667600	-1.01857700
O	-0.05033800	-7.52699300	-1.39597200
C	1.36815300	-2.23668400	-1.01199900
C	0.64586100	-1.13389400	-0.42961800
C	-0.39294000	-1.31620900	0.51165300
C	1.06428900	0.17932300	-0.74418500
C	-1.01254600	-0.20853100	1.08136600
H	-0.65801700	-2.30935300	0.85480900
C	0.42437100	1.27701400	-0.18829000
H	1.89115400	0.31904100	-1.43467200
C	-0.61810000	1.08375800	0.72743200
H	-1.79204300	-0.36004100	1.82134700
H	0.74127700	2.28195100	-0.44994400
H	-1.10527700	1.94273800	1.17979400
C	-2.50086700	-4.77623200	3.88030200
C	-2.43224800	-4.86472800	5.24692600
C	-1.26996200	-4.46329200	5.95761200
C	-0.15090100	-3.95986600	5.22579400
C	-0.23342000	-3.87009900	3.79372000
C	-1.40163300	-4.26905300	3.13882500
H	-2.04847200	-4.95528000	7.90660000
H	-3.38433100	-5.09993900	3.34121300
H	-3.27471400	-5.25485800	5.80735600
C	-1.19029900	-4.56163100	7.36956200
C	1.00989200	-3.57578600	5.94396900
C	1.05820100	-3.68420200	7.31754400

C	-0.05011100	-4.18104200	8.04201500
H	0.00209600	-4.26202100	9.12412700
H	1.95787300	-3.38587400	7.84924500
H	1.86288100	-3.19651200	5.39048100
O	-1.47512900	-4.13568200	1.79818000
C	0.88050600	-3.41024200	3.04188000
C	1.86267100	-3.02122000	2.43841900
C	2.98627400	-2.57107000	1.68921700
C	3.83663700	-3.49319900	1.04681100
C	3.24803100	-1.19477600	1.54137300
C	4.90044200	-3.04959900	0.26498600
H	3.63755900	-4.55361700	1.16139300
C	4.31102200	-0.75730200	0.75541600
H	2.59095100	-0.48197100	2.02781600
C	5.13797000	-1.68042900	0.10911900
H	5.54854300	-3.77284500	-0.22281900
H	4.49370100	0.30792200	0.64464100
H	5.96751700	-1.33659000	-0.50201700
H	-1.06281000	-7.73009000	-1.04843700
H	-2.20404100	-4.71863200	1.43735600
H	2.39950200	-2.01795100	-1.28578600

TS1

E = -2757.474879 a.u.

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C	-1.86540500	-13.27831500	5.12046900
C	-0.87924600	-12.76872000	4.30795800
C	-0.98563800	-11.46464000	3.75682600
C	-2.12693000	-10.65828500	4.07605800
C	-3.14040200	-11.22746800	4.89504300
C	-3.01237100	-12.50026400	5.40413400
H	0.85877100	-11.57281300	2.62968200
H	-1.77469700	-14.27964800	5.53152600
H	-0.00308800	-13.36360700	4.06187600
C	-0.00064800	-10.95308900	2.87194100
C	-2.22405100	-9.33133900	3.53784900
H	-4.03020100	-10.64729800	5.10884100
H	-3.80397200	-12.91401300	6.02250300
C	-1.26140800	-8.91668000	2.62672200
C	-0.14274200	-9.71413100	2.29856700
C	-3.32968400	-8.40776000	3.89683800
C	-4.08602300	-7.82906900	2.88802500
C	-3.59069700	-8.01254900	5.25327100
C	-5.13759100	-6.92502300	3.15254000

C	-4.66024900	-7.09704300	5.52609700
C	-2.78908200	-8.44668800	6.34650500
C	-5.42973300	-6.58211400	4.44908600
C	-4.90771800	-6.69462400	6.86521500
C	-3.04675700	-8.02433900	7.63199400
H	-1.96338900	-9.12147800	6.15623200
H	-6.23670000	-5.88744800	4.66598300
C	-4.12282400	-7.14658500	7.90050800
H	-5.72860500	-6.00732000	7.05405100
H	-2.41722900	-8.36962700	8.44733900
H	-4.31980300	-6.82572000	8.91922000
O	-1.34125500	-7.66165900	2.05693300
O	-3.79636500	-8.12037400	1.56677100
P	-2.50916400	-7.30016300	0.93067200
O	-2.16093700	-7.93516200	-0.38397400
O	-2.75669400	-5.81583100	1.06997400
H	-5.68058200	-6.51247900	2.30998300
H	0.56451200	-9.32620400	1.57579300
C	0.01641300	-5.80711400	-0.90108500
C	0.80308500	-6.81377000	-0.30509800
C	1.97076800	-6.45260800	0.39837500
C	2.31412000	-5.12064700	0.52661600
C	1.52569200	-4.09417500	-0.04943900
C	0.37502000	-4.48273300	-0.77307700
H	-0.87284100	-6.09048000	-1.45023000
H	2.56678700	-7.23496900	0.85597700
H	3.19347600	-4.84756800	1.10496600
H	-0.22719500	-3.73378700	-1.26942900
O	0.48047000	-8.10701600	-0.40160500
C	1.92480900	-2.71289900	0.09119900
C	1.20693800	-1.60942200	-0.56725400
C	-0.18659900	-1.45281500	-0.43550300
C	1.93689400	-0.63320600	-1.26287400
C	-0.82926600	-0.37151600	-1.02979100
H	-0.74378400	-2.15153900	0.18021800
C	1.28981400	0.44700300	-1.85784000
H	3.01667000	-0.72564000	-1.33316200
C	-0.09536600	0.57740300	-1.74762200
H	-1.90375300	-0.25912200	-0.91877200
H	1.86757200	1.19113000	-2.39781900
H	-0.60012700	1.42382000	-2.20426300
C	-1.23251400	-5.48597800	3.87301500
C	-0.48707800	-6.08438600	4.85050700
C	0.88038500	-5.74450000	5.08583400

C	1.46876400	-4.69131500	4.33296600
C	0.65721700	-4.00637600	3.33496200
C	-0.66285800	-4.47890100	3.04932300
H	1.18187500	-7.22175400	6.62606900
H	-2.25431700	-5.78698700	3.68852500
H	-0.94417700	-6.85291800	5.46618300
C	1.64869800	-6.42071800	6.05924300
C	2.80878500	-4.34222800	4.58811100
C	3.54711300	-5.02884500	5.53779700
C	2.96794300	-6.07449400	6.28145500
H	3.55554600	-6.60243200	7.02617800
H	4.58382300	-4.75461300	5.71115900
H	3.25863800	-3.53032800	4.02553700
O	-1.31924700	-3.97927700	2.02609500
C	1.14178900	-2.89513300	2.69781100
C	1.66613800	-1.96848100	2.04323200
C	2.03855900	-0.56942700	2.02391600
C	3.39284100	-0.20856800	1.94043100
C	1.05622700	0.43320500	2.00854500
C	3.75694400	1.13289600	1.84653700
H	4.15302000	-0.98448000	1.95017500
C	1.42692000	1.77109800	1.90480400
H	0.01112400	0.15039000	2.05796400
C	2.77532200	2.12550400	1.82235800
H	4.80746600	1.40267900	1.78799300
H	0.65954500	2.53938000	1.88572300
H	3.05983800	3.17035000	1.73973500
H	-0.51225200	-8.17839400	-0.55291600
H	-1.99092100	-4.68285700	1.66174800
H	2.99898400	-2.55654900	0.17653500

I3

E = -2757.514004 a.u.

0 1

C	-0.28396400	-12.19737000	5.43600900
C	0.49513100	-11.38714300	4.64301200
C	-0.04522900	-10.22787500	4.02688200
C	-1.41477000	-9.88074000	4.26727800
C	-2.19871300	-10.75657600	5.06597200
C	-1.64883900	-11.88348600	5.63454900
H	1.77908400	-9.68020800	2.99501000
H	0.13945300	-13.08589200	5.89508800
H	1.53845300	-11.63068300	4.45942500
C	0.73710900	-9.42168500	3.15906600

C	-1.95630000	-8.68762000	3.67555100
H	-3.24808800	-10.53181500	5.21664900
H	-2.27109100	-12.54156300	6.23409700
C	-1.16473300	-8.02044500	2.75203000
C	0.17949900	-8.35598300	2.50060500
C	-3.29053000	-8.14802800	4.05116200
C	-4.20998100	-7.80546700	3.07379100
C	-3.63915700	-7.86348700	5.41969200
C	-5.46722100	-7.23540400	3.35589700
C	-4.91970500	-7.28933900	5.71645600
C	-2.74347400	-8.07534200	6.50499200
C	-5.81984100	-6.99377300	4.65927800
C	-5.25976600	-6.99330000	7.06358100
C	-3.09952200	-7.76724200	7.79922100
H	-1.76070200	-8.47864900	6.30451400
H	-6.78580600	-6.55721100	4.89662700
C	-4.37415200	-7.22749700	8.08878100
H	-6.23838000	-6.56565600	7.26555300
H	-2.39161200	-7.93933000	8.60508100
H	-4.64512800	-6.99318600	9.11384100
O	-1.66105900	-6.90814700	2.06944400
O	-3.91711000	-8.04693600	1.73394600
P	-2.85779900	-7.08288500	0.97775100
O	-2.48929300	-7.69362500	-0.32065900
O	-3.50912500	-5.64648800	0.96500400
H	-6.12329100	-7.00038200	2.52556200
H	0.74294700	-7.74588600	1.80727700
C	-0.21413800	-5.67228200	-0.92327400
C	0.61401700	-6.77859400	-0.67837800
C	1.93904200	-6.56328400	-0.27317100
C	2.40187500	-5.26488300	-0.06958500
C	1.56601100	-4.15963400	-0.25983000
C	0.25860400	-4.38582300	-0.70352300
H	-1.22752800	-5.83035000	-1.27207900
H	2.58344700	-7.42265500	-0.11474100
H	3.42716000	-5.10990200	0.26135800
H	-0.40699700	-3.54683600	-0.86938000
O	0.18252600	-8.05538800	-0.81254100
C	2.02929100	-2.76079500	0.12735700
C	1.54230400	-1.69500500	-0.84382700
C	0.31604000	-1.04594100	-0.66250000
C	2.31356600	-1.38449700	-1.96878000
C	-0.12912100	-0.10439200	-1.59073100
H	-0.29073000	-1.28157000	0.20674100

C	1.87198500	-0.44147200	-2.89617300
H	3.26395500	-1.89132600	-2.11978100
C	0.64751200	0.20270400	-2.70874200
H	-1.08364400	0.39105600	-1.43710300
H	2.48355400	-0.20987800	-3.76383000
H	0.30206500	0.93902700	-3.42879600
C	-2.01013000	-4.66193800	4.03808500
C	-1.35712200	-5.35486500	5.00161300
C	0.04694600	-5.69805200	4.90738000
C	0.82484100	-5.15523000	3.85837600
C	0.18023500	-4.20901500	2.92917500
C	-1.30686200	-4.17026300	2.86363100
H	0.03438000	-6.99824500	6.62121600
H	-3.08344300	-4.50572400	4.07739300
H	-1.90720700	-5.73520100	5.85602900
C	0.63831300	-6.59214400	5.81551400
C	2.16780500	-5.52716500	3.73436100
C	2.73160200	-6.43264600	4.62808300
C	1.96800000	-6.96706400	5.67350500
H	2.41108000	-7.67475000	6.36738200
H	3.76917200	-6.73028500	4.50724600
H	2.75205400	-5.12222500	2.91479000
O	-1.90167000	-3.74095400	1.85680100
C	0.87723000	-3.35702800	2.19322900
C	1.59570300	-2.45657000	1.56685200
C	1.98139000	-1.18172100	2.22855400
C	2.92960200	-0.32715500	1.64705600
C	1.41569200	-0.81560400	3.46184800
C	3.30530800	0.85485800	2.28506700
H	3.36691300	-0.57075100	0.68651000
C	1.79059000	0.36392500	4.09548900
H	0.67412000	-1.46356100	3.91917800
C	2.73989700	1.20620200	3.50995300
H	4.03952900	1.50375900	1.81629100
H	1.33830200	0.62927800	5.04687800
H	3.03074800	2.12927700	4.00293800
H	-0.80237600	-8.05198900	-0.81142400
H	-2.95026900	-4.87448400	1.29080300
H	3.12744700	-2.75308900	0.11359100

TS2

E = -2757.482480 a.u.

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C	-0.32276800	-12.88638100	-1.45045000

C	0.21293200	-11.71160400	-1.92491800
C	-0.17958800	-10.45815000	-1.38622800
C	-1.12687500	-10.42076400	-0.31099700
C	-1.68038900	-11.65186600	0.13544900
C	-1.28917600	-12.85021800	-0.41788100
H	1.05945200	-9.27390800	-2.70930700
H	-0.01904600	-13.83879700	-1.87517100
H	0.93966200	-11.72211100	-2.73352000
C	0.33069300	-9.23905000	-1.90391000
C	-1.50784200	-9.15707000	0.25312100
H	-2.43042600	-11.63612900	0.91738900
H	-1.73305500	-13.77626000	-0.06363200
C	-1.04960000	-7.99951600	-0.36290500
C	-0.11371400	-8.03489100	-1.41971500
C	-2.36044700	-9.04795700	1.46440600
C	-3.48678600	-8.24044500	1.44022200
C	-2.00061300	-9.66883300	2.70997000
C	-4.31088900	-8.04685300	2.56966500
C	-2.83919900	-9.48070400	3.85874800
C	-0.80224500	-10.41654700	2.87812400
C	-3.99968700	-8.66884700	3.75247300
C	-2.47351100	-10.07618600	5.09541700
C	-0.47182900	-10.97321800	4.09411700
H	-0.13247000	-10.53206200	2.03633000
H	-4.62616800	-8.53049100	4.62946700
C	-1.31746300	-10.81172000	5.21652300
H	-3.12621600	-9.92791800	5.95205500
H	0.45059600	-11.53927800	4.19177100
H	-1.04785500	-11.25888800	6.16880600
O	-1.44412600	-6.76004700	0.08897400
O	-3.83940600	-7.59429600	0.27070000
P	-3.00816700	-6.22764500	-0.11741700
O	-3.28377100	-5.97306800	-1.57721500
O	-3.20563800	-5.15678300	0.92424700
H	-5.17266200	-7.39713900	2.46720000
H	0.24159800	-7.09164100	-1.81747600
C	-0.88317100	-5.82225100	2.85097700
C	-0.10070500	-6.90663800	3.13323000
C	1.19601000	-7.06463600	2.56057300
C	1.72531800	-6.03179100	1.73142200
C	0.94690900	-4.80773900	1.55757600
C	-0.39058900	-4.77774200	2.02566300
H	1.52644900	-9.00400800	3.43146900
H	-1.90164600	-5.75404900	3.21368100

H	-0.48182400	-7.69583600	3.77223600
C	1.94966100	-8.23905600	2.78857000
C	2.98644000	-6.23998300	1.13416600
C	3.69094400	-7.41158400	1.34794300
C	3.17992700	-8.41742700	2.18924500
H	3.74742500	-9.32739300	2.35882200
H	4.65114800	-7.55185400	0.85975200
H	3.40394600	-5.47824400	0.48806900
O	-1.17572200	-3.77258300	1.66613000
C	1.51974700	-3.72269100	0.89650000
C	2.64813100	-3.04309800	0.66736400
C	0.98529000	-2.84269300	-0.91371400
C	2.47577600	-2.45412200	-0.71152000
C	3.82675000	-2.94689500	1.53536900
C	5.02618100	-2.42162300	1.02563900
C	3.79426600	-3.39825700	2.86698900
C	6.16613300	-2.36040700	1.82472500
H	5.06379500	-2.05575700	0.00534600
C	4.93272400	-3.32853600	3.66220400
H	2.87191800	-3.80031500	3.27187300
C	6.12404300	-2.81196800	3.14437700
H	7.08663900	-1.95421300	1.41560800
H	4.89188800	-3.67967200	4.68912600
H	7.01209800	-2.75995400	3.76746800
C	2.77360900	-0.97930100	-0.88524100
C	2.70430700	-0.08320200	0.18785400
C	3.08707900	-0.48844100	-2.15769000
C	2.94029800	1.27753400	-0.00962600
H	2.47465200	-0.45397300	1.18209500
C	3.32263600	0.87128000	-2.35795300
H	3.14118900	-1.17786300	-2.99703500
C	3.24933400	1.75882600	-1.28267300
H	2.88559700	1.96054100	0.83321900
H	3.56527100	1.23665200	-3.35174300
H	3.43514400	2.81791300	-1.43576100
H	3.08249300	-3.01223400	-1.43823100
C	-0.03319300	-1.87087300	-0.65868700
C	0.61130700	-4.00782800	-1.64378800
C	-1.33121100	-2.07901600	-1.03621800
C	-0.70428300	-4.26475300	-1.95472000
C	-1.70306400	-3.29738800	-1.65878100
O	-2.97575800	-3.47868200	-1.94173800
H	-3.18560700	-4.48212000	-1.96131100
H	-2.09597500	-4.16704900	1.48332400

H	0.24145200	-0.95159600	-0.15430100
H	-2.11183300	-1.35743400	-0.82304100
H	-1.00274800	-5.18707800	-2.43724900
H	1.38108500	-4.73199900	-1.90013100

I4

E = -2757.506807 a.u.

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C	-0.73541900	-12.88839100	-1.49395800
C	-0.14887700	-11.76247200	-2.02280000
C	-0.43117400	-10.47493000	-1.49516800
C	-1.31799500	-10.35363500	-0.37550200
C	-1.92738300	-11.53491700	0.12786700
C	-1.64340900	-12.76724000	-0.41597100
H	0.80978400	-9.40527000	-2.91067500
H	-0.51592200	-13.86747200	-1.90943400
H	0.53412900	-11.83797600	-2.86500800
C	0.12975800	-9.30458200	-2.06943400
C	-1.58792100	-9.05419300	0.17336200
H	-2.63266300	-11.45506600	0.94626600
H	-2.12693900	-13.65454300	-0.01767600
C	-1.07551900	-7.95120400	-0.49031400
C	-0.20498400	-8.06200500	-1.59283300
C	-2.39259000	-8.86315500	1.40648200
C	-3.47025800	-7.99593600	1.40171600
C	-2.04029000	-9.48641600	2.65246500
C	-4.26974300	-7.74901000	2.53520900
C	-2.85215300	-9.24919700	3.81059600
C	-0.87366300	-10.28352700	2.80564000
C	-3.97293300	-8.38249700	3.71621000
C	-2.49639600	-9.85217200	5.04634200
C	-0.55303400	-10.84764000	4.02016200
H	-0.21559000	-10.42445400	1.95846000
H	-4.57929700	-8.20853300	4.60059700
C	-1.37440700	-10.64066300	5.15297900
H	-3.12602300	-9.66608300	5.91251700
H	0.34716000	-11.44891800	4.11052800
H	-1.11004200	-11.09258700	6.10435800
O	-1.36976100	-6.66576400	-0.04732200
O	-3.80712500	-7.32321900	0.22439100
P	-2.87486400	-6.06070800	-0.18012000
O	-3.23490800	-5.94000400	-1.70772800
O	-2.99491200	-4.84948600	0.67045300
H	-5.10064100	-7.05892300	2.44169400

H	0.18803000	-7.15309400	-2.03088600
C	-0.72616700	-5.77817600	2.95741700
C	-0.00044100	-6.88990700	3.29296600
C	1.31132700	-7.08304800	2.78354900
C	1.88948500	-6.08368100	1.93412500
C	1.14296100	-4.88545100	1.64651000
C	-0.15742200	-4.77558900	2.13197300
H	1.58685500	-8.99462600	3.73805400
H	-1.73952300	-5.63774500	3.31929200
H	-0.42510200	-7.64558600	3.94500400
C	2.04448500	-8.25936000	3.08325200
C	3.16836400	-6.35112900	1.37765800
C	3.84914100	-7.51306600	1.67239400
C	3.29269900	-8.47517500	2.54404500
H	3.84359600	-9.38204900	2.77656700
H	4.82486300	-7.68849900	1.22767300
H	3.61177700	-5.63025900	0.70341000
O	-0.87217300	-3.65766300	1.84261800
C	1.68393100	-3.83253400	0.78721300
C	2.87321200	-3.18911000	0.65345000
C	1.06685000	-3.21064600	-0.50227800
C	2.53282100	-2.53343800	-0.67194000
C	4.10484800	-3.10095000	1.42469700
C	5.23797200	-2.48870100	0.85953200
C	4.19092400	-3.59922500	2.73872800
C	6.42650500	-2.39131500	1.57922100
H	5.17875800	-2.08276700	-0.14566400
C	5.37889000	-3.49663300	3.45506500
H	3.32094400	-4.06154300	3.19076700
C	6.50207700	-2.89647000	2.87860700
H	7.29308900	-1.91759100	1.12665500
H	5.42963000	-3.88667600	4.46765200
H	7.42840300	-2.81971000	3.44081900
C	2.59389000	-1.03779300	-0.82221400
C	2.65771300	-0.19321400	0.29304300
C	2.54793800	-0.46704100	-2.10018900
C	2.67267400	1.19235000	0.13227500
H	2.70299300	-0.62578000	1.28757100
C	2.55868500	0.91727500	-2.26334600
H	2.49668900	-1.11631800	-2.97121000
C	2.62134500	1.75188400	-1.14541100
H	2.72662500	1.83468800	1.00676000
H	2.51996300	1.34442100	-3.26152200
H	2.63321300	2.83088900	-1.27012800

H	3.04096600	-3.00403800	-1.52312000
C	-0.01217700	-2.20450500	-0.31324000
C	0.75861700	-4.23319200	-1.53483100
C	-1.16417000	-2.21393200	-1.00909300
C	-0.42577400	-4.30238600	-2.16444000
C	-1.49012900	-3.32890000	-1.88472300
O	-2.64143200	-3.48557900	-2.34288300
H	-3.09040600	-5.00629900	-2.07864700
H	-1.77380900	-3.94277300	1.55656600
H	0.17574900	-1.43228500	0.42385200
H	-1.94417000	-1.47815600	-0.84382000
H	-0.65555800	-5.08314100	-2.88315800
H	1.53594400	-4.97035400	-1.72870900

TS3

E = -2757.486282 a.u.

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C	-1.22203600	-12.98490900	-1.80318300
C	-0.70130400	-11.86284600	-2.40449900
C	-0.90228800	-10.57350500	-1.84491500
C	-1.63910700	-10.44571800	-0.62177300
C	-2.18412200	-11.62345500	-0.04111500
C	-1.97987200	-12.85789000	-0.61497600
H	0.15083600	-9.50943400	-3.40816400
H	-1.06533300	-13.96552600	-2.24313400
H	-0.13344100	-11.94340300	-3.32812300
C	-0.40841300	-9.40580800	-2.48216800
C	-1.82625700	-9.14638800	-0.04605000
H	-2.77498300	-11.53709100	0.86303300
H	-2.41077800	-13.74263800	-0.15495300
C	-1.37483900	-8.03828100	-0.74692300
C	-0.65618700	-8.16201500	-1.95618500
C	-2.50193100	-8.93509400	1.25740100
C	-3.57414600	-8.06056100	1.32975100
C	-2.01374100	-9.51774300	2.47442300
C	-4.24780700	-7.78565800	2.53891300
C	-2.69169900	-9.23897000	3.70649200
C	-0.82994800	-10.30386900	2.52331900
C	-3.82392300	-8.38069400	3.70144700
C	-2.18882000	-9.78829600	4.91578000
C	-0.36349800	-10.81456400	3.71415100
H	-0.27878300	-10.48206100	1.60884200
H	-4.33107500	-8.17550100	4.64031000
C	-1.05132600	-10.56332800	4.92490300

H	-2.71673200	-9.57143900	5.84103300
H	0.54701200	-11.40705000	3.72413300
H	-0.67452000	-10.97236200	5.85788400
O	-1.57160200	-6.77343300	-0.23428500
O	-3.99468800	-7.39800100	0.18348000
P	-3.08729200	-6.08419000	-0.22344200
O	-3.47690000	-5.67999600	-1.62838200
O	-3.07348800	-5.07466900	0.89046000
H	-5.07854000	-7.08970600	2.51673100
H	-0.30943900	-7.26168500	-2.45030100
C	-0.52776600	-6.15827700	2.83915600
C	0.32059800	-7.12832900	3.29493200
C	1.70888200	-7.09588800	2.98537900
C	2.23212100	-6.02423100	2.18992200
C	1.33962300	-4.97938500	1.74632400
C	-0.02442800	-5.07206800	2.07560800
H	2.13466700	-8.93553700	4.01885400
H	-1.59119400	-6.19191400	3.04982900
H	-0.06008700	-7.94772400	3.89505600
C	2.56504500	-8.13557700	3.42202500
C	3.60254400	-6.08784300	1.83016500
C	4.41332300	-7.11638200	2.26740500
C	3.90036400	-8.14762500	3.08137300
H	4.54943900	-8.94991400	3.42000400
H	5.45921600	-7.13135600	1.97299700
H	4.02207500	-5.32435100	1.19022800
O	-0.84872500	-4.08064800	1.70819900
C	1.75882600	-3.89636100	0.85932300
C	2.87586900	-3.12568100	0.69962800
C	0.88261800	-3.46950500	-0.28339300
C	2.68239900	-2.55088700	-0.66059700
C	4.00808300	-2.83763700	1.58051000
C	5.21456700	-2.33485900	1.06283000
C	3.90794400	-3.05541400	2.96699300
C	6.28860700	-2.05728000	1.90500500
H	5.30854400	-2.16505400	-0.00566500
C	4.98460000	-2.78238700	3.80459700
H	2.98017300	-3.43958400	3.37692500
C	6.17860500	-2.28134600	3.27885200
H	7.21407000	-1.67072900	1.48761300
H	4.89141200	-2.95909600	4.87223200
H	7.01741100	-2.06881200	3.93532500
C	2.79832800	-1.13385100	-0.98633000
C	2.79253500	-0.14557700	0.01803600

C	2.89243900	-0.73383600	-2.33217000
C	2.89320600	1.19877900	-0.31844900
H	2.72073700	-0.44648000	1.05791500
C	2.98742000	0.61321800	-2.66731700
H	2.88653700	-1.49172800	-3.11138700
C	2.98906700	1.58226400	-1.66078800
H	2.89556400	1.95231100	0.46337100
H	3.05947700	0.90931800	-3.70951100
H	3.06297000	2.63421500	-1.92043200
H	2.88677700	-3.21274500	-1.50001000
C	0.06839700	-2.28482700	-0.16449000
C	0.42209800	-4.48455400	-1.19895000
C	-1.10596100	-2.13432400	-0.84893200
C	-0.76421600	-4.36322500	-1.85105800
C	-1.61404400	-3.23844200	-1.58254200
O	-2.86000400	-3.23496500	-1.97409800
H	-3.20265900	-4.21855500	-1.99679800
H	-1.77025800	-4.44007500	1.50522000
H	0.39228700	-1.52016600	0.53211900
H	-1.74385600	-1.26924300	-0.70803800
H	-1.14973000	-5.14858300	-2.48789700
H	1.01388900	-5.38931900	-1.30087400

I5

E = -2757.528935 a.u.

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C	-1.61751400	-13.34420900	-1.43894000
C	-1.25574600	-12.25433900	-2.19610800
C	-1.39291000	-10.93471400	-1.69047400
C	-1.89534300	-10.74073400	-0.36186700
C	-2.28208300	-11.88792900	0.38357600
C	-2.14535900	-13.15374000	-0.13989900
H	-0.67808300	-9.95552000	-3.48369000
H	-1.51212100	-14.34870000	-1.83847600
H	-0.86659000	-12.38495600	-3.20285000
C	-1.06211500	-9.80203600	-2.47875400
C	-2.01656600	-9.40999200	0.15585700
H	-2.69811900	-11.75305900	1.37508700
H	-2.45283400	-14.01459000	0.44705400
C	-1.73919600	-8.34129000	-0.68350600
C	-1.24801100	-8.53075200	-1.99429400
C	-2.44408000	-9.12406000	1.54699100
C	-3.51427100	-8.27001700	1.76217600
C	-1.71150700	-9.60195600	2.68499300

C	-3.95427300	-7.92126100	3.05745000
C	-2.14968100	-9.24353400	4.00229900
C	-0.51371500	-10.35876900	2.56002900
C	-3.29420500	-8.41544400	4.15509400
C	-1.40417200	-9.68606300	5.12703300
C	0.19179100	-10.76418900	3.67160600
H	-0.14704100	-10.60231100	1.57085900
H	-3.61946800	-8.14979600	5.15730700
C	-0.25861600	-10.43286200	4.97151900
H	-1.75288900	-9.41020900	6.11907900
H	1.10574900	-11.33854000	3.54777400
H	0.30434500	-10.76043700	5.84074400
O	-1.87379800	-7.05100200	-0.21951000
O	-4.15761300	-7.69481000	0.67567800
P	-3.37957500	-6.37666200	0.05135600
O	-4.03254700	-6.00888800	-1.25055000
O	-3.16182300	-5.36366700	1.14949400
H	-4.79668900	-7.24530400	3.14745100
H	-1.02223500	-7.65933800	-2.59837500
C	-0.13512400	-6.32474300	2.31374200
C	0.91911700	-7.12929700	2.63765600
C	2.23887700	-6.86692600	2.15681000
C	2.46421900	-5.74551900	1.30044400
C	1.35171300	-4.89542800	0.94820300
C	0.06547800	-5.17820400	1.49332000
H	3.11185200	-8.57404500	3.13548500
H	-1.13458700	-6.52065200	2.68464300
H	0.76187600	-7.99316400	3.27596800
C	3.31110300	-7.72456100	2.48724600
C	3.76197000	-5.56958900	0.76810500
C	4.79838500	-6.41693300	1.11614200
C	4.57977700	-7.50016200	1.98809900
H	5.39871000	-8.16352700	2.24941100
H	5.78815700	-6.25021000	0.70038800
H	3.94215000	-4.76691700	0.06279000
O	-0.90380400	-4.29360700	1.33885300
C	1.47063600	-3.72752800	0.09652900
C	2.46360900	-2.69379500	0.32285800
C	0.44621700	-3.58026300	-0.88975400
C	2.83831800	-1.91029000	-0.73991100
C	3.00487500	-2.54695400	1.70041800
C	4.38598700	-2.52347000	1.93922500
C	2.12286700	-2.46189000	2.78723100
C	4.87633500	-2.40674600	3.23698300

H	5.07226100	-2.60003300	1.10186800
C	2.61492100	-2.33858500	4.08597600
H	1.05181000	-2.49541200	2.61010800
C	3.99175400	-2.31196100	4.31407300
H	5.94869200	-2.39891000	3.40942400
H	1.92171900	-2.26913600	4.91912000
H	4.37463700	-2.22379200	5.32671800
C	3.64957100	-0.70213100	-0.77255700
C	3.81006200	0.16486000	0.32931300
C	4.25466500	-0.34736200	-1.99564800
C	4.56752900	1.32379600	0.20899600
H	3.32543000	-0.06592300	1.26929600
C	5.02580300	0.80503900	-2.10806200
H	4.11765400	-0.99451100	-2.85812000
C	5.18696000	1.64407800	-1.00352100
H	4.67329000	1.98511700	1.06391700
H	5.49267000	1.05382000	-3.05641800
H	5.78186200	2.54875500	-1.08865700
H	2.48707800	-2.24046000	-1.71518800
C	-0.24302000	-2.34535000	-1.08052000
C	-0.12749700	-4.75400100	-1.45373400
C	-1.52286000	-2.32762800	-1.59045200
C	-1.37526100	-4.72985200	-2.01574900
C	-2.15122000	-3.54768600	-1.94277600
O	-3.45567600	-3.57243300	-2.17030600
H	-3.79347800	-4.50218700	-1.96348200
H	-1.84139800	-4.72085900	1.37399100
H	0.18183500	-1.43704000	-0.66787100
H	-2.11361200	-1.41814300	-1.60213400
H	-1.83667000	-5.62436000	-2.40878000
H	0.42009100	-5.68745900	-1.38878300

TS4

E = -2757.499879 a.u.

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C	8.17248700	2.91227500	4.02420600
C	6.98294900	3.02417400	4.67130700
C	6.10097800	1.90234500	4.83034300
C	6.42689200	0.68248600	4.17313400
C	7.64240200	0.57876300	3.38268200
C	8.65655300	1.62778900	3.54331700
H	4.70252200	2.93328300	6.10648900
H	8.86938800	3.74102500	3.95649000
H	6.69816400	3.97103500	5.12654400

C	4.93980300	1.98788300	5.62586500
C	5.58266500	-0.43022300	4.39714700
C	4.45057200	-0.32605300	5.18857200
C	4.11081400	0.89505100	5.79617800
H	3.21204300	0.97537300	6.39935000
H	3.81830900	-1.19593300	5.33654100
H	5.84028700	-1.38588700	3.95507000
O	9.88083200	1.52575200	3.25967900
C	7.78934600	-0.33468300	2.30663700
C	9.08613000	-0.65140600	1.81796100
C	6.60563800	-0.81841200	1.56292300
C	10.16759200	-0.53311000	2.69649200
C	9.36583700	-0.89103500	0.38234500
C	8.70339400	-0.18185900	-0.63448400
C	10.34051000	-1.83136700	0.00846100
C	9.00190700	-0.41068300	-1.97432700
H	7.95715300	0.55806400	-0.36711700
C	10.64680100	-2.05514800	-1.33331000
H	10.84367100	-2.40577400	0.78189900
C	9.97525800	-1.34800800	-2.33087900
H	8.47923300	0.15026800	-2.74413600
H	11.40120100	-2.79070500	-1.59870500
H	10.20541400	-1.52594100	-3.37746600
C	10.19443300	-0.98003700	4.09549900
C	9.27609500	-1.92131600	4.59057200
C	11.20213000	-0.50399800	4.95136200
C	9.34114100	-2.34506500	5.91420200
H	8.51921700	-2.32264500	3.92600600
C	11.26494600	-0.92614700	6.27578500
H	11.91103200	0.22577300	4.57334400
C	10.33158700	-1.84473600	6.76307800
H	8.62184600	-3.07038600	6.28332500
H	12.04125300	-0.53961400	6.92990200
H	10.38274400	-2.17763300	7.79586100
H	11.14672400	-0.38418900	2.24739600
C	5.55248800	0.04105100	1.22354100
C	6.51687300	-2.16019300	1.15100900
C	4.43408600	-0.42069900	0.53330800
C	5.39120200	-2.64624200	0.50109500
C	4.32140700	-1.78696900	0.20112300
O	3.23638400	-2.30484800	-0.40507500
H	5.62679900	1.09053400	1.49000600
H	3.67034900	0.27593500	0.20308700
H	5.30813300	-3.69155800	0.22305700

H	7.33947200	-2.83274100	1.37483300
H	2.45349700	-1.72796800	-0.24173800
C	1.68654900	5.56582800	6.36623000
C	2.67654900	5.21688000	5.47724800
C	2.41313900	4.32774800	4.40214100
C	1.08676900	3.81136900	4.22691100
C	0.09282700	4.17953900	5.17307300
C	0.38578900	5.03096900	6.21477700
H	4.44836800	4.31383700	3.65642100
H	1.90180800	6.24082800	7.18921800
H	3.68452600	5.60845200	5.58914000
C	3.44748500	3.91648700	3.52234600
C	0.81773500	2.91582500	3.13528200
H	-0.90515700	3.77001300	5.07358600
H	-0.38860900	5.28983300	6.93091000
C	1.89686100	2.48613000	2.38390100
C	3.20295300	2.98252300	2.54871800
C	-0.55508700	2.45399200	2.79840900
C	-0.84170500	1.10504000	2.67591100
C	-1.61705400	3.38588900	2.52422600
C	-2.13027700	0.60846900	2.39901700
C	-2.93671300	2.89161200	2.25805500
C	-1.40626200	4.79048300	2.46648900
C	-3.16484300	1.49143300	2.21702900
C	-3.98913600	3.81175700	2.00926900
C	-2.44609100	5.65514100	2.20848400
H	-0.40830600	5.18167700	2.61809800
H	-4.16767600	1.12701000	2.01347800
C	-3.75525900	5.16663100	1.99088900
H	-4.98481900	3.41913400	1.82020000
H	-2.25644600	6.72366100	2.16450900
H	-4.56701600	5.86075200	1.79462200
O	1.70691800	1.52688300	1.38342900
O	0.15864700	0.14995300	2.88674100
P	1.37163600	0.00324700	1.83764800
O	2.48797000	-0.45960000	2.87435400
H	3.35695000	-0.61255900	2.44350900
O	1.15821600	-0.82902100	0.62970800
H	-2.26944800	-0.46518800	2.34189500
H	3.98818000	2.61460400	1.89928300

3aa

E = -1345.109786 a.u.

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C	4.61129500	-1.02204200	4.17428200
C	3.77481100	-1.19187900	5.24740800
C	2.74073200	-2.16573300	5.21895800
C	2.52467800	-2.93767200	4.02764800
C	3.33409200	-2.66950700	2.86627400
C	4.40847900	-1.78944200	3.00849700
H	2.11815000	-1.79526600	7.25149700
H	5.44020300	-0.32245200	4.19182600
H	3.92012500	-0.61003900	6.15372100
C	1.94124100	-2.40201200	6.36672000
C	1.54568100	-3.96717700	4.08517800
C	0.79619000	-4.18222300	5.22183600
C	0.97839100	-3.38456900	6.37294300
H	0.37542700	-3.55986900	7.25914700
H	0.06108600	-4.98221500	5.23186600
H	1.39488800	-4.60713900	3.22741600
O	5.29841500	-1.59953300	1.99586000
C	3.07859700	-3.17548700	1.50368300
C	4.10717200	-3.17416800	0.61146900
C	1.69921400	-3.55190600	1.10008700
C	5.46131300	-2.75851400	1.14245600
C	4.02103200	-3.48627400	-0.83068800
C	2.99018100	-2.98550000	-1.64560700
C	5.02613500	-4.26409900	-1.43234000
C	2.95651700	-3.27202500	-3.00725100
H	2.21873700	-2.36480700	-1.20467400
C	4.98814800	-4.55467700	-2.79567900
H	5.83240400	-4.65965000	-0.82092100
C	3.95161900	-4.06213200	-3.58890900
H	2.15337000	-2.87039900	-3.61903500
H	5.77008700	-5.16686200	-3.23662300
H	3.92204600	-4.28480500	-4.65178900
C	6.24671400	-3.83504700	1.88273100
C	5.75703100	-5.12940600	2.06885400
C	7.50768700	-3.50365800	2.39591100
C	6.51580900	-6.08163900	2.75333300
H	4.77669300	-5.38839300	1.68335600
C	8.26414500	-4.44941500	3.08284400
H	7.88436800	-2.49301600	2.26396200
C	7.76905100	-5.74451500	3.26215100
H	6.12165500	-7.08425200	2.89397700
H	9.23968400	-4.17972100	3.47794000
H	8.35858800	-6.48420400	3.79655800
H	6.07037900	-2.37508200	0.32072400

C	0.62453800	-2.67631300	1.32263200
C	1.43550900	-4.77957200	0.48073300
C	-0.66692300	-3.00504700	0.92970400
C	0.14423500	-5.12569400	0.09103200
C	-0.91213000	-4.23617200	0.31134000
O	-2.19979700	-4.51515500	-0.05062300
H	0.80996900	-1.72612300	1.81355300
H	-1.49710400	-2.32671500	1.09643700
H	-0.04217600	-6.08604000	-0.38584700
H	2.25260200	-5.46979500	0.29742900
H	-2.22568900	-5.39059900	-0.46717500