Solvent Effect in Gold(I)-Catalyzed Domino Reaction : Access to Furopyrans.

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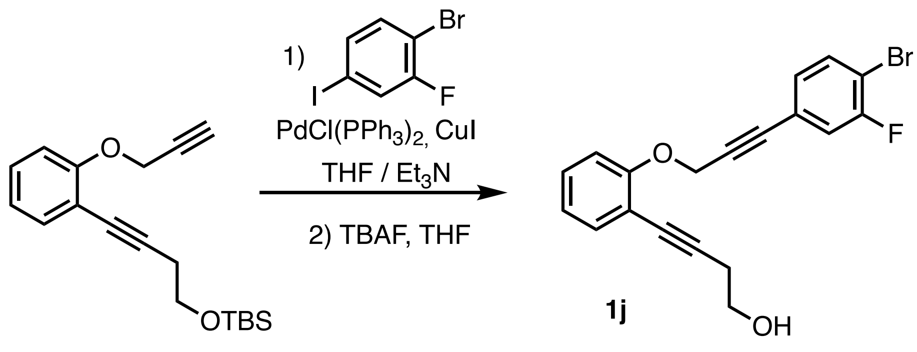
1. General information

All reagents, chemicals and dry solvents were purchased from commercial sources and used without purification. When mentioned that the reaction was conducted in dry media, glassware dried for several hours at 110 °C in an oven was used. Triethylamine (Et_3N) and diisopropylamine (DIPA) were distilled from KOH in an S-tube prior to each experiment in which they were involved. Reactions were monitored by TLC (Thin Layer silica gel Chromatography) using Merck silica gel 60 F254 on aluminum sheets. TLC plates were visualized under UV light and revealed with acidic *p*-anisaldehyde stain or $KMnO_4$ stain. Crude products were purified by flash column chromatography on Merck silica gel Si 60 (40-63 µm). NMR spectra were recorded in $CDCl_3$ or C_6D_6 on a Bruker Avance III BBFO+ probe spectrometer 400 MHz for ^1H analyses and 100 MHz for ^{13}C analyses. Proton chemical shifts are reported in ppm (δ), relatively to residual $CHCl_3$ (δ 7.26 ppm) or C_6H_6 (δ 7.16 ppm). Multiplicities are reported as follows: singlet (s), doublet (d), triplet (t), quartet (q), quintet (quint), broad singlet (bs), broad doublet (bd) combinations or multiplet (m). Coupling constants values J are given in Hz. Carbon chemical shifts are reported in ppm (δ), relatively to the internal standard $CDCl_3$ (δ 77.23 ppm) or C_6H_6 (δ 128.4 ppm). ^1H and ^{13}C NMR signals were assigned mostly on the basis of 2D-NMR (COSY, HSQC, HMBC) experiments. High Resolution Mass Spectral analyses (HRMS) were performed using an Agilent 1200 RRLC HPLC chain and an Agilent 6520 Accurate mass QToF. Infrared spectra (IR) were recorded on a FT IR Thermo Nicollet ATR 380, Diamant Spectrometer. All the microwave experiments have been performed using an Initiator EXP Microwave System from Biotage with IR temperature monitoring. An heating temperature profile reaching as fast as possible 60°C was used.

Except for **1j** and **1n**, all compounds **1** have been already described.[1]

2- Synthesis of 1j and 1n

2.1 Synthesis of **1j**



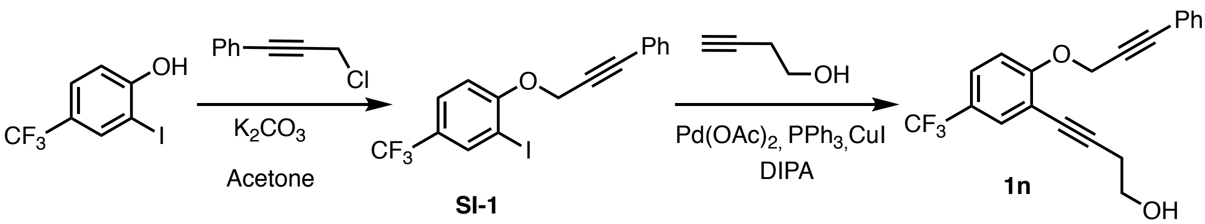
Anhydrous THF (5 mL) and distilled Et_3N (4 mL) are mixed in a 2-necked flask under argon. The 1-bromo-2-fluoro-4-iodobenzene (1.5 eq., 717 mg, 2.38 mmol), $PdCl_2(PPh_3)$ (0,03 eq., 33 mg, 0.048 mmol) and CuI (0,06 eq., 18 mg, 0.095 mmol) were added to the flask and this mixture was degassed with argon for 15 min. The alkyne[1] (1 eq., 500 mg, 1.59 mmol) was dissolved in

[1] Pertschi, R.; Wagner, P.; Ghosh, N.; Gandon, V.; Blond, G. Gold(I)-Catalyzed Synthesis of Furopyrans: Insight into Hetero-Diels–Alder Reactions. *Org. Lett.* **2019**, *21*, 6084–6088. https://doi.org/10.1021/acs.orglett.9b02228

THF (5 mL) degassed with argon for 15 min and added to the 2-necked flask. The mixture was stirred overnight at room temperature (20 °C) and monitored by TLC (9/1 pent/Et_2O). Once the TLC showed complete conversion of the true alkyne, the reaction mixture was filtered through a pad of Celite with CH_2Cl_2 as eluent and concentrated to give the crude product as a dark-brown solid. The latter was purified by flash column chromatography (98/2 pent/Et_2O) to afford the pure TBS protected coupling product.
TBAF (1 eq., 416 mg, 1.6 mmol) was added to a solution of this latter protected product in THF at 0 °C. This mixture was stirred at room temperature until the TLC (9/1 pent/Et2O) showed complete conversion of the starting material. The reaction mixture was dissolved in a saturated aqueous NH_4Cl solution. The aqueous phase was extracted with CH_2Cl_2. The gathered organic layer were dried over $MgSO_4$, filtered and concentrated to afford the crude as a yellowish oil. The latter was purified by flash column chromatography (6/4 pent/Et_2O) to afford **1j** with 57 % (338 mg, 0,906 mmol) as an off white oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.41 (dd, *J* = 7.6, 1.7 Hz, 1H), 7.29 (ddd, *J* = 8.3, 7.5, 1.8 Hz, 1H), 7.18 (dd, *J* = 9.0, 1.8 Hz, 1H), 7.09 (ddd, *J* = 8.3, 1.9, 0.8 Hz, 1H), 7.04 (dd, *J* = 8.4, 1.0 Hz, 1H), 6.96 (td, *J* = 7.5, 1.0 Hz, 1H), 4.96 (s, 2H), 3.83 (t, *J* = 6.1 Hz, 2H), 2.74 (t, *J* = 6.1 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 158.8 (d, *J* = 202.0 Hz), 158.3, 133.6, 133.6, 129.3, 128.8 (d, *J* = 3.6 Hz), 123.3 (d, *J* = 8.6 Hz), 121.7, 119.7 (d, *J* = 23.8 Hz), 113.6, 112.9, 110.2 (d, *J* = 21.0 Hz), 91.4, 85.7, 85.6 (d, *J* = 2.9 Hz), 78.9, 61.1, 57.4, 24.4. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{15}BrFO_2$ 373.0239; Found 373.0224 (Diff.: 2.75 ppm).

2.2 Synthesis of **1n**



2-iodo-1-((3-phenylprop-2-yn-1-yl)oxy)-4-(trifluoromethyl)benzene **SI-1**

2-iodo-4-trifluorophenol (1 eq., 250 mg, 0.87 mmol) and (3-chloroprop-1-yn-1-yl)benzene (1.1 eq., 144 mg, 0,96 mmol) were added to a solution of K_2CO_3 (3.3 eq., 396 mg, 2.87 mmol) in acetone (6 mL) under argon in a sealed tube. This whitish mixture was stirred overnight at 75 °C. The reaction was monitored by TLC. A 10% HCl aqueous solution were added to the reaction mixture. The layers were separated and the aqueous layer was extracted with Et_2O. The organic layers were gathered, dried over $MgSO_4$, filtered and concentrated to afford the crude as a yellowish transparent oil. This crude was purified by flash column chromatography (pentane/Et_2O 8/2) to afford pure **SI-1** (92%, 322 mg, 0.80 mmol) as an colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.61 (d, *J* = 8.6 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 2H), 7.32 (m, *J* = 7.1 Hz, 3H), 7.14 (d, *J* = 8.6 Hz, 1H), 5.06 (s, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.1, 136.9 (q, *J* = 3.7 Hz), 131.9, 129.1, 128.5, 126.9 (q, *J* = 3.8 Hz), 125.2 (q, *J* = 33.1 Hz), 123.3 (q, *J* = 271.9 Hz), 121.9, 112.3, 88.5, 86.3, 82.5, 58.0.

4-(2-((3-phenylprop-2-yn-1-yl)oxy)-5-(trifluoromethyl)phenyl)but-3-yn-1-ol **1n**
In a round bottomed flask under argon, **SI-1** (1 eq., 290 mg, 0.721 mmol), PPh_3 (0.1 eq., 19.6 mg, 0.074 mmol), CuI (0.1 eq., 15.2 mg, 0.08 mmol) and $Pd(OAc)_2$ (0.05 eq., 8.4 mg, 0.04 mmol) were dissolved in DIPA (4 mL). This mixture was degassed with argon. 3-butyn-1-ol (1.2 eq., 55 mg, 0.793 mmol) was added to this flask and the green reaction mixture turns orange; it was stirred at room temperature. The reaction was monitored by TLC, after 3h all the starting material was converted. The reaction mixture was filtered through a pad of Celite with Et_2O as eluent. After solvent evaporation under reduced pressure, purification of the crude by flash column chromatography (pentane/Et_2O 98/2) provided pure **1n** (58 %, 144 mg, 0.418 mmol) as an amorphous white solid.

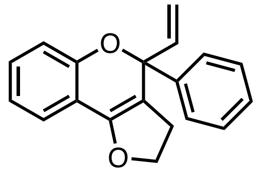
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (s, 1H), 7.47 (d, *J* = 8.7 Hz, 1H), 7.37 (d, *J* = 7.2 Hz, 2H), 7.26 (m, 3H), 7.10 (d, *J* = 8.6 Hz, 1H), 4.97 (s, 2H), 3.78 (t, *J* = 6.2 Hz, 2H), 2.69 (t, *J* = 6.2 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 160.5, 131.9, 130.7 (q, *J* = 3.8 Hz), 129.0, 128.5, 126.2 (q, *J* = 3.9 Hz), 124.0 (q, *J* = 272.6 Hz), 123.7 (q, *J* = 33.0 Hz), 122.0, 114.1, 112.5, 92.9, 88.4, 82.8, 77.5, 61.0, 57.6, 24.2. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}F_3O_2$ 345.1102; Found 345.1095 (Diff.: 0.69 ppm).

3. General procedure for gold(I) catalyzed cascade reactions: preparation of 3a-n

Substrate **1** (1 eq., 50 mg) was placed in a 0.5-2 mL oven dried microwave reactor under argon and dissolved in anhydrous DMF (1 mL). Catalyst **A** (0.05 eq.) was added into the reactor at 20 °C. The reactor was sealed and sonicated until all the reagents were dissolved, and the reactor was placed into the microwave for 20 min at 60 °C. The reaction mixture was filtered through a pad of Celite with AcOEt as eluent. After solvent evaporation under reduced pressure, purification of the crude by flash column chromatography provided the furopyran adduct **3**.

3.1. Synthesis of **3a**

4-phenyl-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene



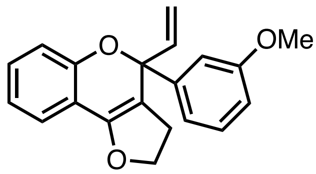
Compound **3a** was prepared following the general procedure using compound **1a** (40 mg, 0.145 mmol, 1 eq.) and catalyst **A** (6 mg, 0.007 mmol, 0.05 eq.) in DMF (1 mL). Purification by chromatography on silica gel (98/2 pentane/ Et_2O) afforded compound **3a** (77 %, 31 mg, 0.112 mmol) as an amorphous white solid.

Scale-up : Substrate **1a** (276 mg, 1 mmol, 1 eq.) was placed in a 2-5 mL microwave reactor and dissolved in anhydrous DMF (5 mL). Catalyst **A** (39 mg, 0,05 mmol, 0.05 eq.) was added into the reactor. Once all the reagents were dissolved, the reactor was placed into the microwave for 20 min at 60 °C. The reaction mixture was filtered through a pad of Celite with CH_2Cl_2 as eluent. After solvent evaporation under reduced pressure, purification by chromatography on silica gel (98/2 pentane/ Et_2O) afforded compound **3a** (71 %, 196 mg, 0.71 mmol) as an amorphous white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.46 (m, 2H), 7.40 – 7.10 (m, 5H), 6.94 – 6.84 (m, 2H), 6.18 (dd, *J* = 17.2, 10.4 Hz, 1H), 5.44 (dd, *J* = 17.2, 1.3 Hz, 1H), 5.40 (dd, *J* = 10.4, 1.3 Hz, 1H), 4.54 (dddd, *J* = 22.8, 10.5, 8.8, 7.8 Hz, 2H), 2.90 – 2.67 (m, 1H), 2.49 (ddd, *J* = 15.1, 10.5, 7.7 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.4, 148.4, 142.5, 138.0, 129.7, 128.4, 128.0, 126.8, 121.1, 120.9, 116.6, 116.0, 116.0, 106.7, 84.8, 70.8, 31.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{17}O_2$ 277.1229; Found 277.1227 (Diff.: -0.89 ppm).

3.2 Synthesis of **3b**

4-(3-methoxyphenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

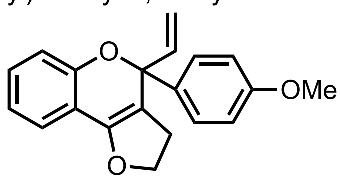


Compound **3b** was prepared following the general procedure using compound **1b** (50 mg, 0.163 mmol, 1 eq.) and catalyst **A** (6 mg, 0.008 mmol, 0.05 eq.) in DMF (0.9 mL). Purification by chromatography on silica gel (90/10 Heptane/AcOEt) afforded compound **3b** (72 %, 36 mg, 0.118 mmol) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (t, *J* = 8.2 Hz, 1H), 7.42 – 7.37 (m, 1H), 7.33 (t, *J* = 7.8 Hz, 1H), 7.29 – 7.22 (m, 2H), 7.13 – 7.00 (m, 3H), 6.33 (dd, *J* = 17.2, 10.5 Hz, 1H), 5.65 – 5.54 (m, 2H), 4.94 – 4.58 (m, 2H), 3.97 (s, 3H), 2.94 (m, 1H), 2.69 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 159.8, 153.4, 148.4, 144.2, 137.9, 129.7, 129.4, 121.1, 120.9, 119.1, 116.6, 116.0, 116.0, 113.2, 112.8, 106.7, 84.8, 70.8, 55.4, 31.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{19}O_3$ 307.1334; Found 307.1330 (Diff.: 0.15 ppm).

3.3 Synthesis of **3c**

4-(4-methoxyphenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

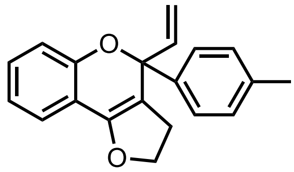


Compound **3c** was prepared following the general procedure using compound **1c** (35 mg, 0.11 mmol, 1 eq.) and catalyst **A** (4 mg, 0.004 mmol, 0.05 eq.) in DMF (0.7 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3c** (29 %, 10 mg, 0.033 mmol) as colorless oil.

^{1}H NMR (400 MHz, C_6D_6) δ 7.51 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.48 – 7.43 (m, 2H), 7.01 – 6.90 (m, 2H), 6.82 – 6.70 (m, 3H), 6.13 (dd, *J* = 17.2, 10.5 Hz, 1H), 5.46 (dd, *J* = 17.2, 1.4 Hz, 1H), 5.21 (dd, *J* = 10.5, 1.5 Hz, 1H), 4.08 (ddd, *J* = 10.1, 8.3, 2.9 Hz, 2H), 3.27 (s, 3H), 2.31 (ddd, *J* = 15.2, 10.2, 8.4 Hz, 1H), 2.17 (ddd, *J* = 15.1, 10.0, 8.2 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 159.9, 154.1, 149.0, 138.8, 135.0, 130.0, 128.7, 121.5, 121.1, 116.6, 116.4, 115.9, 113.9, 107.0, 85.0, 70.5, 54.8, 31.7. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{19}O_3$ 307.1334; Found 307.1326 (Diff.: 0.85 ppm).

3.4 Synthesis of **3d**

4-(*p*-tolyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

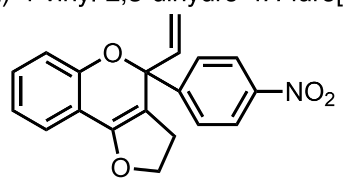


Compound **3d** was prepared following the general procedure using compound **1d** (23 mg, 0.079 mmol, 1 eq.) and catalyst **A** (3 mg, 0.004 mmol, 0.05 eq.) in DMF (0.5 mL). Purification by chromatography on silica gel (99/1 Heptane/AcOEt) afforded compound **3d** (65 %, 15 mg, 0.052 mmol) as colorless oil.

^{1}H NMR (400 MHz, C_6D_6) δ 7.54 – 7.42 (m, 3H), 7.07 – 6.99 (m, 2H), 6.99 – 6.89 (m, 2H), 6.73 (td, *J* = 7.3, 1.4 Hz, 1H), 6.12 (dd, *J* = 17.2, 10.5 Hz, 1H), 5.44 (dd, *J* = 17.2, 1.5 Hz, 1H), 5.20 (dd, *J* = 10.5, 1.5 Hz, 1H), 4.18 – 3.97 (m, 2H), 2.30 (ddd, *J* = 15.1, 10.5, 8.0 Hz, 1H), 2.15 (ddd, *J* = 15.1, 10.4, 7.9 Hz, 1H), 2.09 (s, 3H). ^{13}C NMR (101 MHz, C_6D_6) δ 154.1, 149.0, 140.2, 138.7, 137.5, 130.0, 129.2, 127.2, 121.5, 121.2, 116.7, 116.4, 116.1, 106.9, 85.1, 70.5, 31.8, 21.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{19}O_2$ 291.1385; Found 291.1384 (Diff.: -1.07 ppm).

3.5 Synthesis of **3e**

4-(4-nitrophenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

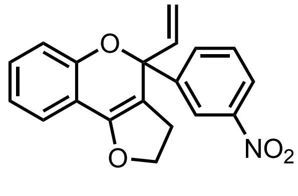


Compound **3e** was prepared following the general procedure using compound **1e** (60 mg, 0.16 mmol, 1 eq.) and catalyst **A** (6 mg, 0.008 mmol, 0.05 eq.) in DMF (1.25 mL). Purification by chromatography on silica gel (9/1 petroleum ether/AcOEt) afforded compound **3e** (63 %, 39 mg, 0.010 mmol) as an orange oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 8.9 Hz, 2H), 7.67 (d, *J* = 8.9 Hz, 2H), 7.23 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.19 (td, *J* = 7.8, 1.7 Hz, 1H), 6.99 – 6.88 (m, 1H), 6.13 (dd, *J* = 17.1, 10.5 Hz, 1H), 5.54 – 5.38 (m, 2H), 4.58 (m, 2H), 2.80 (ddd, *J* = 15.1, 10.7, 8.0 Hz, 1H), 2.46 (ddd, *J* = 15.0, 10.6, 7.6 Hz, 1H).^{13}C NMR (101 MHz, $CDCl_3$) δ 152.9, 149.6, 149.2, 147.6, 137.1, 130.2, 127.7, 123.7, 121.5, 121.4, 118.0, 116.1, 115.8, 105.2, 84.3, 70.9, 31.6. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{16}NO_4$ 322.1079; Found 322.1074 (Diff.: -0.09 ppm).

3.6 Synthesis of **3f**

4-(3-nitrophenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

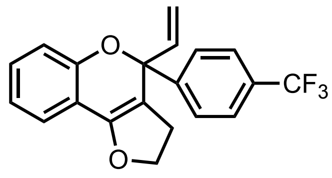


Compound **3f** was prepared following the general procedure using compound **1f** (25 mg, 0.078 mmol, 1 eq.) and catalyst **A** (3 mg, 0.004 mmol, 0.05 eq.) in DMF (0.5 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3f** (66 %, 16 mg, 0.051 mmol) as a yellow oil.

^{1}H NMR (400 MHz, C_6D_6) δ 8.34 (m, 1H), 7.79 – 7.70 (m, 1H), 7.56 – 7.40 (m, 2H), 6.90 (m, 2H), 6.83 – 6.67 (m, 2H), 5.83 (dd, *J* = 17.1, 10.4 Hz, 1H), 5.27 (d, *J* = 17.0 Hz, 1H), 5.10 (d, *J* = 10.5 Hz, 1H), 4.14 – 3.93 (m, 2H), 2.14 (ddd, *J* = 15.0, 10.5, 7.9 Hz, 1H), 1.88 (ddd, *J* = 15.0, 10.5, 7.7 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 153.4, 149.6, 148.6, 144.9, 137.4, 132.6, 130.4, 129.3, 128.7, 128.3, 122.8, 121.8, 121.7, 121.6, 117.4, 105.4, 84.3, 70.6, 31.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{16}NO_4$ 322.1079; Found 322.1067 (Diff.: 2.22 ppm).

3.7 Synthesis of **3g**

4-(4-(trifluoromethyl)phenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

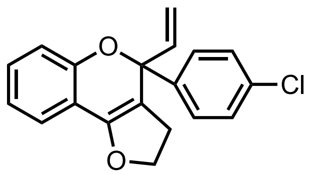


Compound **3g** was prepared following the general procedure using compound **1g** (50 mg, 0.15 mmol, 1 eq.) and catalyst **A** (6 mg, 0.007 mmol, 0.05 eq.) in DMF (1 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3g** (70 %, 35 mg, 0.102 mmol) as colorless oil.

^{1}H NMR (400 MHz, C_6D_6) δ 7.47 (d, *J* = 7.5 Hz, 1H), 7.41 – 7.28 (m, 4H), 7.01 – 6.90 (m, 2H), 6.73 (dt, *J* = 7.4, 4.2 Hz, 1H), 5.91 (dd, *J* = 17.1, 10.4 Hz, 1H), 5.31 (dd, *J* = 17.1, 1.3 Hz, 1H), 5.14 (dd, *J* = 10.5, 1.3 Hz, 1H), 4.19 – 3.90 (m, 2H), 2.44 – 2.06 (m, 1H), 1.88 (ddd, *J* = 15.1, 10.6, 7.7 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 153.3, 148.9, 146.5, 137.4, 129.9, 129.7 (q, *J* = 32.3 Hz), 127.0, 125.1 (q, *J* = 3.8 Hz), 124. 6 (q, *J* = 272.0 Hz), 124.3, 121.3, 121.2, 116.7, 115.9, 105.4, 84.2, 70.2, 31.1. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}F_3O_2$ 345.1102; Found 345.1089 (Diff.: 2.54 ppm).

3.8 Synthesis of **3h**

4-(4-chlorophenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

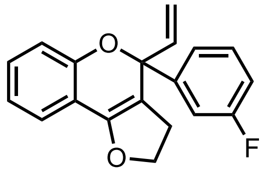


Compound **3h** was prepared following the general procedure using compound **1h** (53 mg, 0.17 mmol, 1 eq.) and catalyst **A** (7 mg, 0.009 mmol, 0.05 eq.) in DMF (1.05 mL). Purification by chromatography on silica gel (98/2 Heptane/AcOEt) afforded compound **3h** (57 %, 30 mg, 0.097 mmol) as an amorphous white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 – 7.41 (m, 2H), 7.39 – 7.31 (m, 2H), 7.21 (dd, *J* = 7.4, 1.7 Hz, 1H), 7.16 (td, *J* = 7.8, 1.7 Hz, 1H), 6.95 – 6.85 (m, 2H), 6.13 (dd, *J* = 17.4, 10.3 Hz, 1H), 5.43 (dd, *J* = 17.4, 1.2 Hz, 1H), 5.40 (dd, *J* = 10.3, 1.2 Hz, 1H), 4.57 (dddd, *J* = 22.6, 10.4, 8.8, 7.8 Hz, 2H), 2.76 (ddd, *J* = 15.1, 10.6, 8.0 Hz, 1H), 2.49 (ddd, *J* = 15.1, 10.5, 7.8 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 153.4, 148.8, 141.1, 137.7, 133.6, 129.8, 128.3, 128.2, 121.2, 121.1, 116.3, 116.1, 115.9, 105.7, 84.2, 70.2, 31.1. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{16}ClO_2$ 311.0839; Found 311.0830 (Diff.: 1.20 ppm).

3.9 Synthesis of **3i**

4-(3-fluorophenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

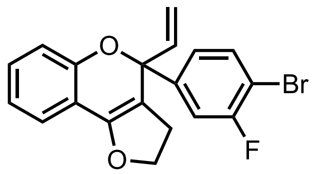


Compound **3i** was prepared following the general procedure using compound **1i** (25 mg, 0.085 mmol, 1 eq.) and catalyst **A** (3 mg, 0.004 mmol, 0.05 eq.) in DMF (0.5 mL). Purification by chromatography on silica gel (98/2 Heptane/AcOEt) afforded compound **3i** (40 %, 10 mg, 0.034 mmol) as a colorless oil.

^1H NMR (400 MHz, C_6D_6) δ 7.46 (dt, *J* = 7.4, 1.2 Hz, 1H), 7.34 (ddd, *J* = 10.1, 2.6, 1.7 Hz, 1H), 7.23 – 7.17 (m, 1H), 6.98 – 6.86 (m, 3H), 6.80 – 6.69 (m, 2H), 5.94 (dd, *J* = 17.1, 10.4 Hz, 1H), 5.34 (dd, *J* = 17.2, 1.3 Hz, 1H), 5.12 (dd, *J* = 10.4, 1.3 Hz, 1H), 4.01 (dddd, *J* = 28.3, 10.6, 8.8, 7.8 Hz, 2H), 2.20 (ddd, *J* = 15.1, 10.7, 8.0 Hz, 1H), 1.98 (ddd, *J* = 15.1, 10.6, 7.6 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 163.4 (d, *J* = 245.7 Hz), 153.7, 149.2, 145.9 (d, *J* = 6.4 Hz), 138.0, 130.2, 130.1 (d, *J* = 8.1 Hz), 122.6 (d, *J* = 3.0 Hz), 121.6, 121.5, 116.8, 116.5, 116.4, 114.8 (d, *J* = 21.0 Hz), 114.2 (d, *J* = 22.2 Hz), 106.0, 84.6, 70.5, 31.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{16}FO_2$ 295.1134; Found 295.1131 (Diff.: -1.53 ppm).

3.10 Synthesis of **3j**

4-(4-bromo-3-fluorophenyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

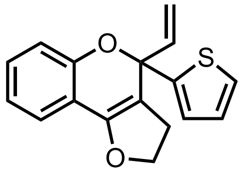


Compound **3j** was prepared following the general procedure using compound **1j** (50 mg, 0.13 mmol, 1 eq.) and catalyst **A** (5 mg, 0.007 mmol, 0.05 eq.) in DMF (1 mL). Purification by chromatography on silica gel (98/2 Heptane/AcOEt) afforded compound **3j** (49 %, 25 mg, 0.066 mmol) as an amorphous white solid.

^1H NMR (400 MHz, C_6D_6) δ 7.52 – 7.42 (m, 1H), 7.25 – 7.17 (m, 2H), 6.90 (m, 3H), 6.73 (m, 1H), 5.82 (dd, *J* = 17.1, 10.4 Hz, 1H), 5.27 (d, *J* = 17.1 Hz, 1H), 5.09 (d, *J* = 10.4 Hz, 1H), 4.18 – 3.93 (m, 2H), 2.12 (ddd, *J* = 15.0, 10.8, 8.0 Hz, 1H), 1.87 (dddd, *J* = 15.0, 10.6, 7.7, 3.5 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 159.1 (d, *J* = 247.4 Hz), 153.2, 149.0, 144.6 (d, *J* = 5.5 Hz), 137.1, 133.2, 129.9, 127.6, 123.5 (d, *J* = 4.0 Hz), 121.3, 121.2, 116.7, 116.0, 115.0 (d, *J* = 23.2 Hz), 108.3 (d, *J* = 20.9 Hz), 105.1, 83.7, 70.2, 31.0. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{16}BrFO_2$ 373.0239; Found 373.0232 (Diff.: 0.21 ppm).

3.11 Synthesis of **3k**

4-(thiophen-2-yl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

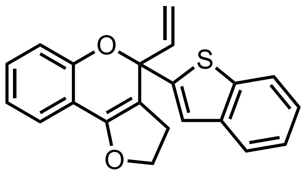


Compound **3k** was prepared following the general procedure using compound **1k** (50 mg, 0.177 mmol, 1 eq.) and catalyst **A** (7 mg, 0.008 mmol, 0.05 eq.) in DMF (0.5 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3k** (62 %, 31 mg, 0.110 mmol) as colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 4.9 Hz, 1H), 7.45 (d, *J* = 7.6 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.29 – 7.25 (m, 1H), 7.20 (p, *J* = 3.0, 2.5 Hz, 1H), 7.17 – 7.08 (m, 2H), 6.50 (ddd, *J* = 17.1, 10.5, 1.8 Hz, 1H), 5.74 (d, *J* = 17.1 Hz, 1H), 5.62 (d, *J* = 10.5 Hz, 1H), 5.05 – 4.71 (m, 2H), 3.18 – 2.86 (m, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 153.0, 148.6, 147.2, 137.9, 129.8, 126.8, 126.5, 125.5, 121.1, 121.1, 116.2, 116.1, 115.8, 106.9, 82.2, 71.0, 31.3. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{17}H_{15}O_2S$ 283.0793; Found 283.0794 (Diff.: -2.33 ppm).

3.12 Synthesis of **3l**

4-(benzo[*b*]thiophen-2-yl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

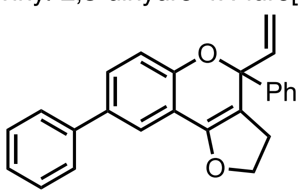


Compound **3l** was prepared following the general procedure using compound **1l** (23 mg, 0.078 mmol, 1 eq.) and catalyst **A** (3 mg, 0.004 mmol, 0.05 eq.) in DMF (0.5 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3l** (58 %, 14 mg, 0.041 mmol) as an amorphous white solid.

^{1}H NMR (400 MHz, C_6D_6) δ 7.55 – 7.40 (m, 3H), 7.15 (s, 1H), 7.10 (ddd, *J* = 8.0, 7.1, 1.1 Hz, 1H), 7.05 – 6.94 (m, 2H), 6.89 (td, *J* = 7.7, 1.7 Hz, 1H), 6.71 (td, *J* = 7.4, 1.2 Hz, 1H), 6.20 (dd, *J* = 17.1, 10.5 Hz, 1H), 5.55 (dd, *J* = 17.1, 1.2 Hz, 1H), 5.21 (dd, *J* = 10.5, 1.2 Hz, 1H), 4.13 – 4.04 (m, 2H), 2.36 – 2.32 (m, 2H).^{13}C NMR (101 MHz, C_6D_6) δ 153.2, 149.0, 148.1, 140.5, 139.5, 137.6, 129.9, 124.4, 124.1, 123.8, 122.4, 121.8, 121.3, 121.2, 116.1, 116.1, 116.0, 106.2, 82.6, 70.4, 30.9. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{21}H_{17}O_2S$ 333.0949; Found 333.0948 (Diff.: -1.38 ppm).

3.13 Synthesis of **3m**

4,8-diphenyl-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

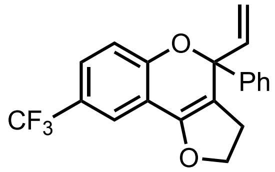


Compound **3m** was prepared following the general procedure using compound **1m** (50 mg, 0.142 mmol, 1 eq.) and catalyst **A** (5 mg, 0.007 mmol, 0.05 eq.) in DMF (1 mL). Purification by chromatography on silica gel (97/3 Heptane/AcOEt) afforded compound **3m** (68 %, 34 mg, 0.10 mmol) as an amorphous white solid.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 – 7.37 (m, 4H), 7.34 (d, *J* = 2.3 Hz, 1H), 7.26 (ddd, *J* = 7.9, 6.6, 3.4 Hz, 4H), 7.22 – 7.10 (m, 3H), 6.84 (d, *J* = 8.4 Hz, 1H), 6.08 (dd, *J* = 17.1, 10.5 Hz, 1H), 5.40 – 5.25 (m, 2H), 4.54 – 4.37 (m, 2H), 2.73 – 2.60 (m, 1H), 2.40 (ddd, *J* = 15.2, 10.5, 7.7 Hz, 1H). ^{13}C NMR (101 MHz, C_6D_6) δ 153.0, 148.3, 142.4, 140.7, 137.9, 134.0, 128.8, 128.5, 128.3, 128.1, 126.9, 126.8, 126.8, 119.7, 116.7, 116.3, 116.1, 107.1, 85.1, 70.9, 31.8. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{25}H_{21}O_2$ 353.1542; Found 353.1536 (Diff.: 0.09 ppm).

3.14 Synthesis of **3n**

4-phenyl-8-(trifluoromethyl)-4-vinyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

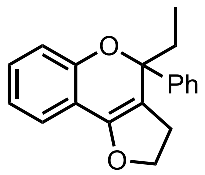


Compound **3n** was prepared following the general procedure using compound **1n** (50 mg, 0.145 mmol, 1 eq.) and catalyst **A** (6 mg, 0.007 mmol, 0.05 eq.) in DMF (1 mL). Purification by chromatography on silica gel (95/5 petroleum ether/Et_2O) afforded compound **3n** (44 %, 22 mg, 0.064 mmol) as a colorless oil.

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 – 7.44 (m, 3H), 7.39 (ddd, *J* = 7.7, 6.7, 1.5 Hz, 3H), 7.36 – 7.29 (m, 1H), 6.94 (d, *J* = 8.5 Hz, 1H), 6.19 (dd, *J* = 17.1, 10.6 Hz, 1H), 5.47 – 5.40 (m, 2H), 4.58 (m, 2H), 2.78 (ddd, *J* = 15.3, 10.7, 8.0 Hz, 1H), 2.52 (ddd, *J* = 15.4, 10.5, 7.8 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 155.9, 147.4, 141.9, 137.6, 128.6, 128.3, 126.8 (q, *J* = 3.9 Hz), 126.7, 124.4 (q, *J* = 271.7 Hz), 123.2 (q, *J* = 33.2 Hz), 118.6 (q, *J* = 3.9 Hz), 117.1, 116.2, 116.0, 108.0, 85.9, 71.0, 31.7. ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.83 (s). HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{20}H_{16}F_3O_2$ 345.1102; Found 345.1105 (Diff.: -1.96 ppm).

4. Synthesis of **12**

4-ethyl-4-phenyl-2,3-dihydro-4*H*-furo[3,2-*c*]chromene

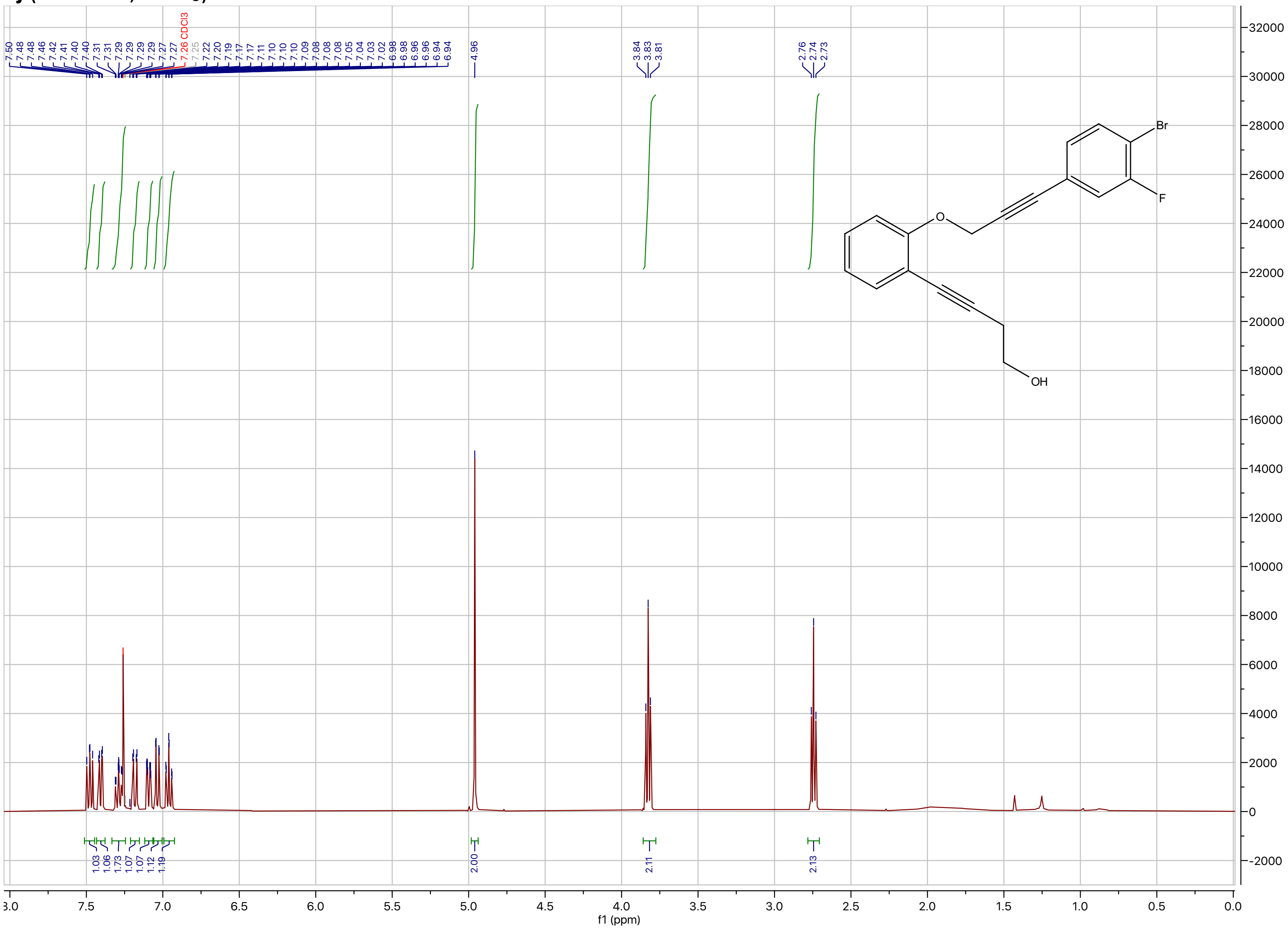


Compound **3a** (30 mg, 0.109 mmol 1 eq.) was placed in a reactor and dissolved in ethyl acetate (3 mL). The mixture was degassed three time with Argon. PtO_2 (3 mg, 0.013 mmol, 0.12 eq.) was added into the reactor. Once all the reagents were dissolved, the reactor was placed under H_2 pressure (1 atm.) for 1 h at room temperature. The reaction mixture was filtered through a pad of Celite with AcOEt as eluent. After solvent evaporation under reduced pressure, product **12** is obtained without any purification (99 %, 30 mg, 0.108 mmol) as amorphous white solid.

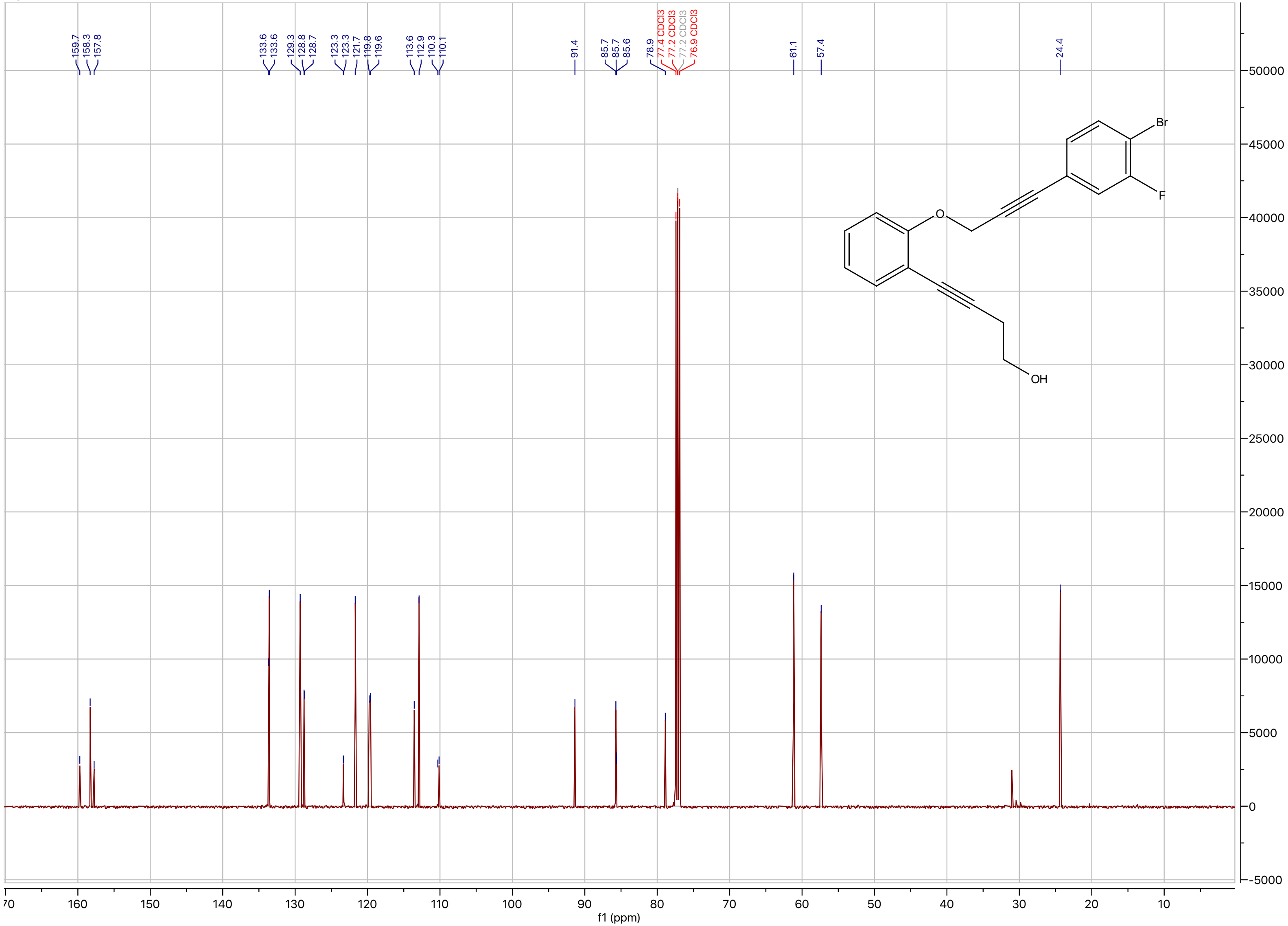
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.34 (m, 2H), 7.31 – 7.23 (m, 2H), 7.21 – 7.14 (m, 1H), 7.08 (t, *J* = 7.7 Hz, 2H), 6.88 – 6.74 (m, 2H), 4.56 – 4.39 (m, 2H), 2.80 (ddd, *J* = 14.9, 10.5, 7.8 Hz, 1H), 2.61 (ddd, *J* = 14.9, 10.5, 7.8 Hz, 1H), 2.28 – 1.99 (m, *J* = 7.2 Hz, 2H), 0.96 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 154.5, 147.9, 144.8, 129.6, 128.4, 127.3, 125.4, 121.0, 120.5, 115.7, 115.4, 107.8, 85.7, 70.5, 32.6, 31.4, 8.5. HRMS (ESI) m/z: $[M+H]^+$ Calcd for $C_{19}H_{19}O_2$ 279.1385; Found 279.1382 (Diff.: -1.11 ppm).

5. ^{1}H and ^{13}C NMR spectra

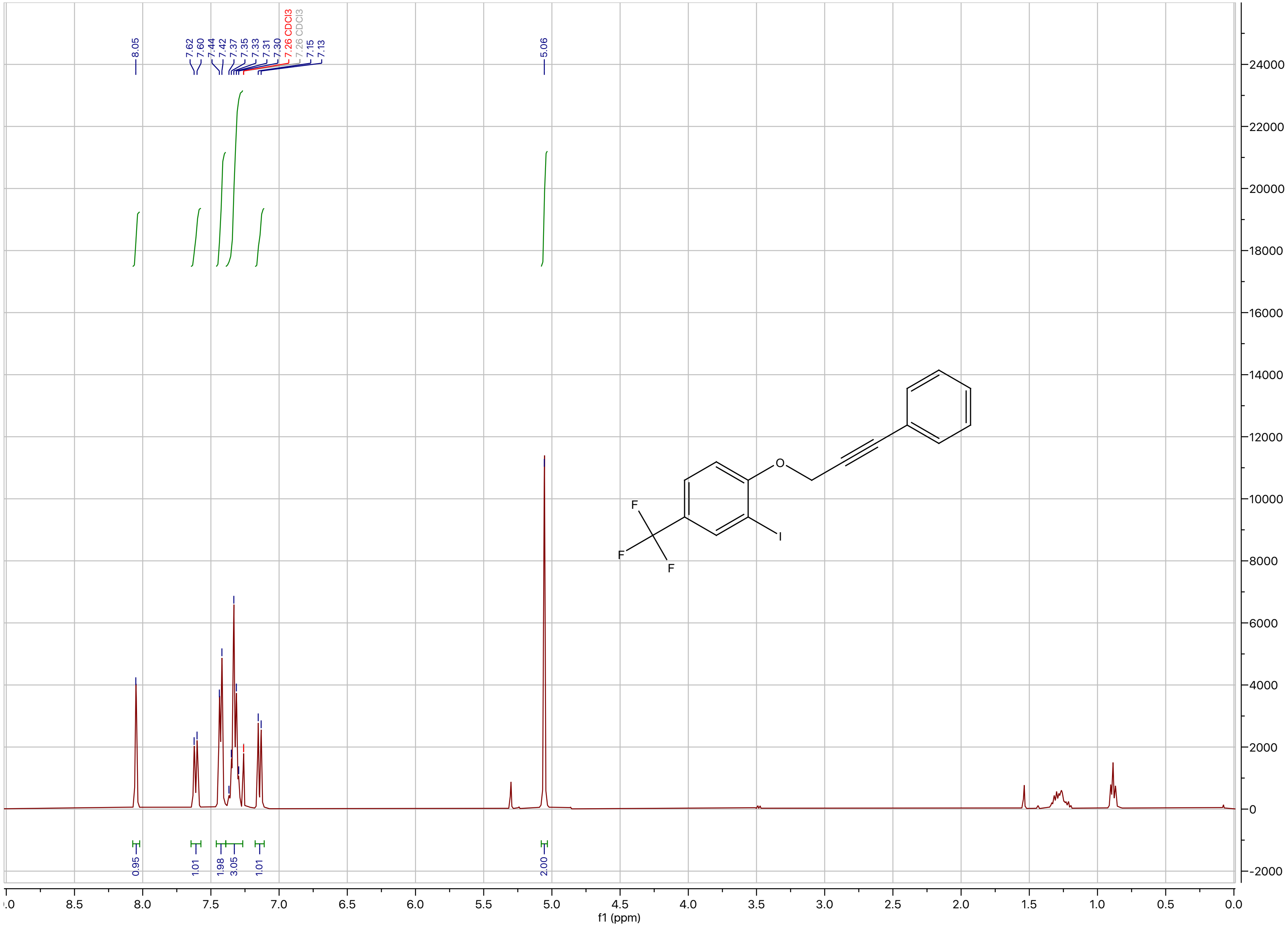
1j (400 MHz, $CDCl_3$)



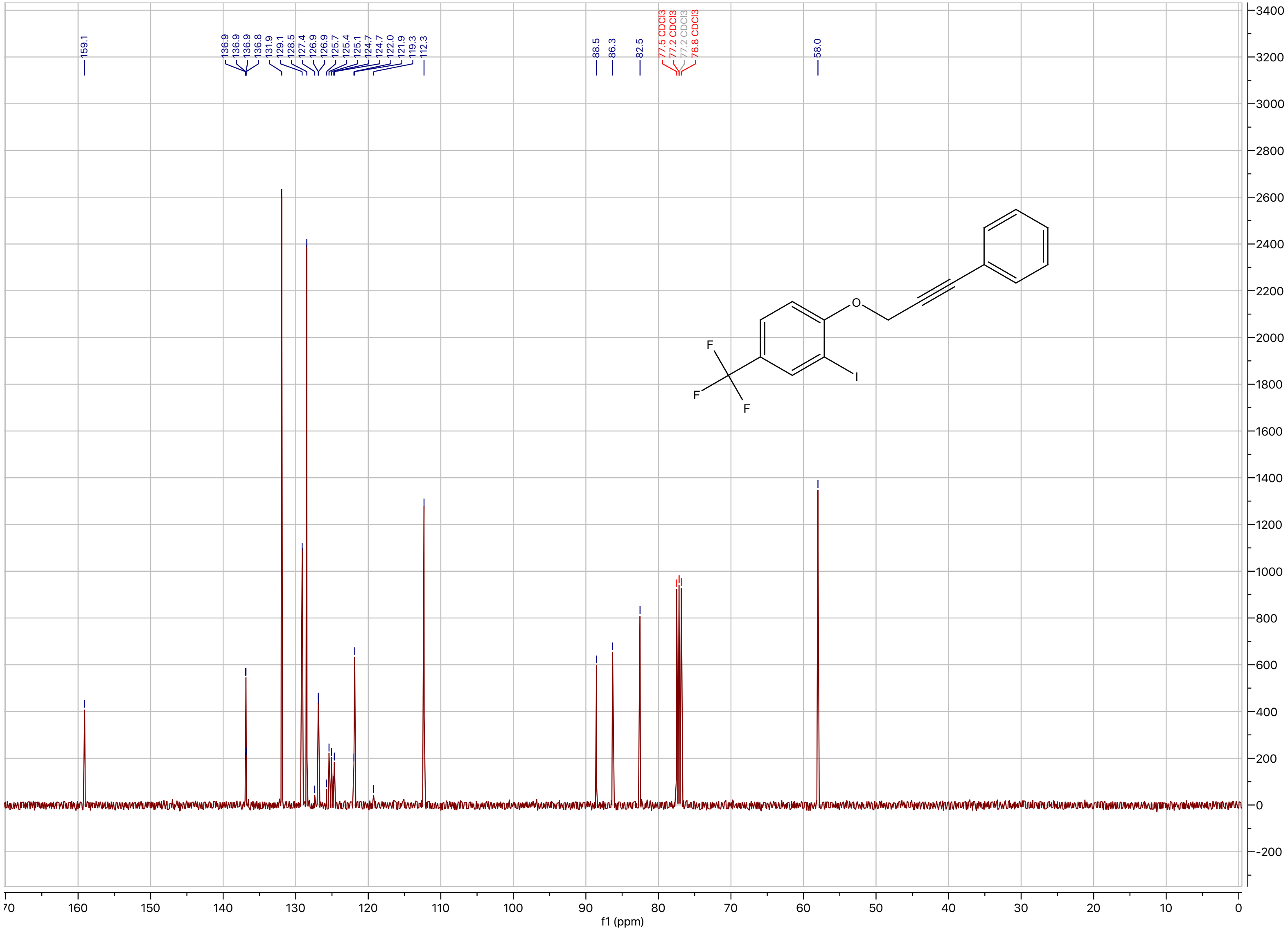
1j (101 MHz, $CDCl_3$)



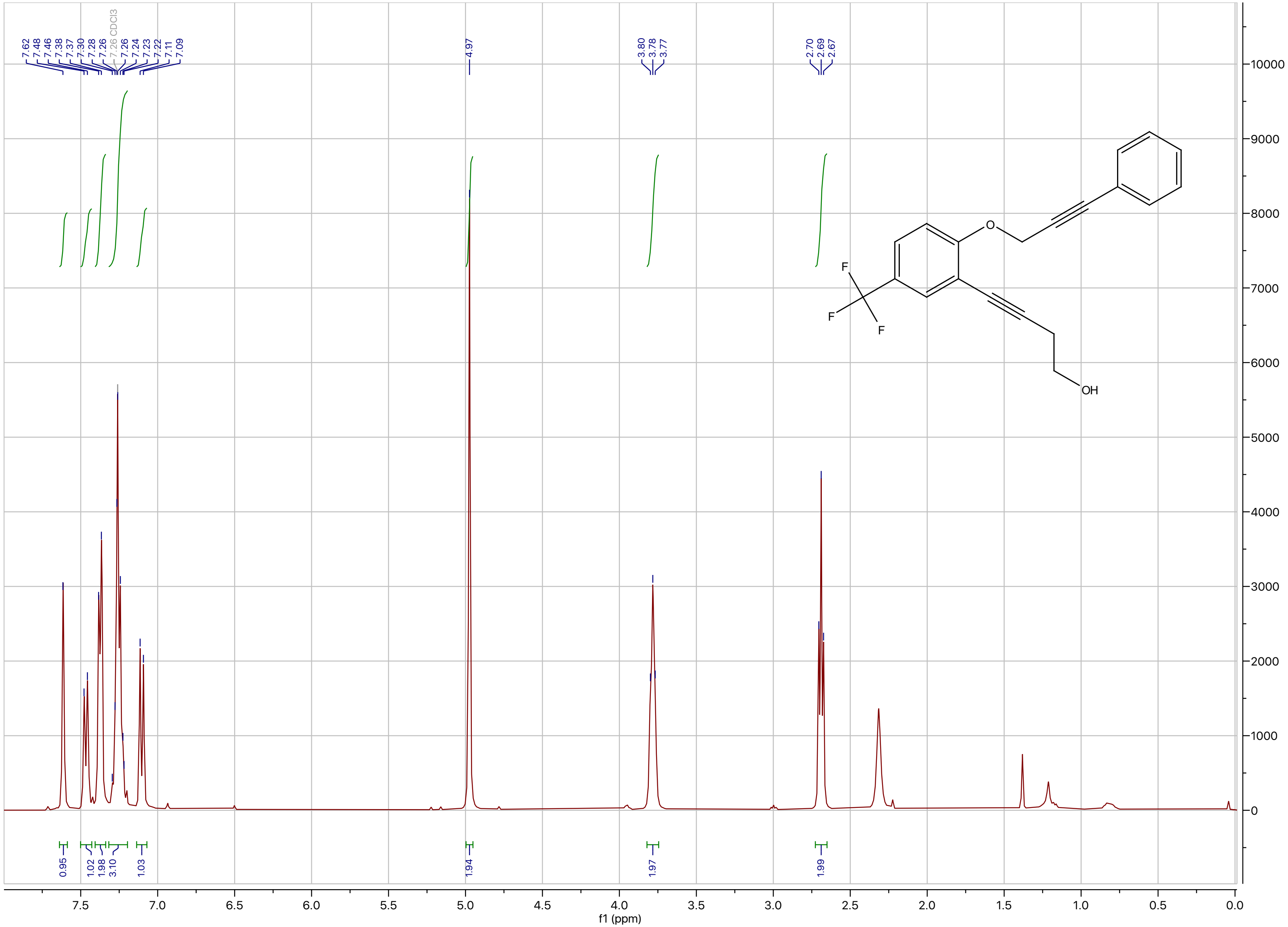
SI-1 (400 MHz, $CDCl_3$)



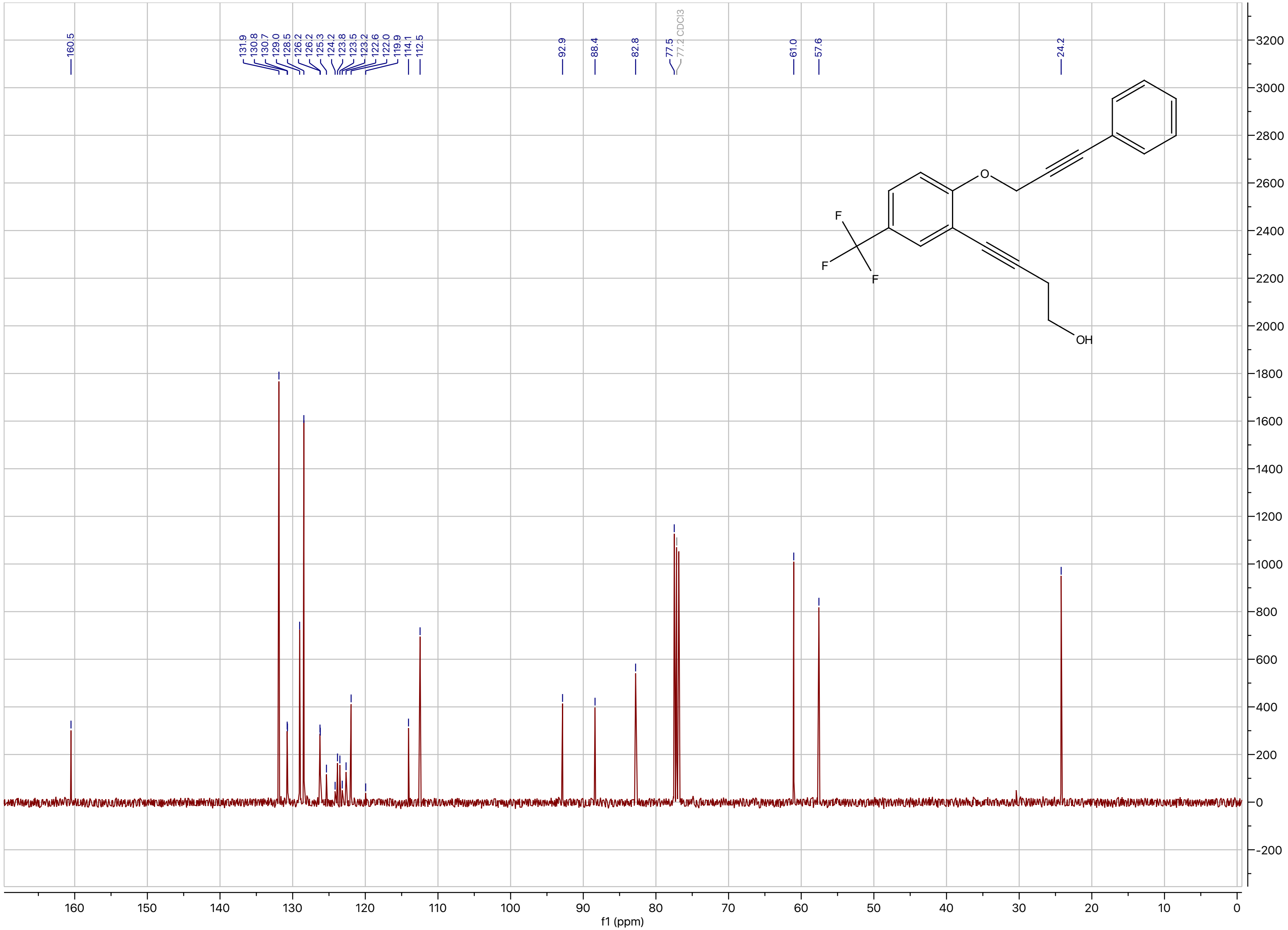
SI-1 (101 MHz, $CDCl_3$)



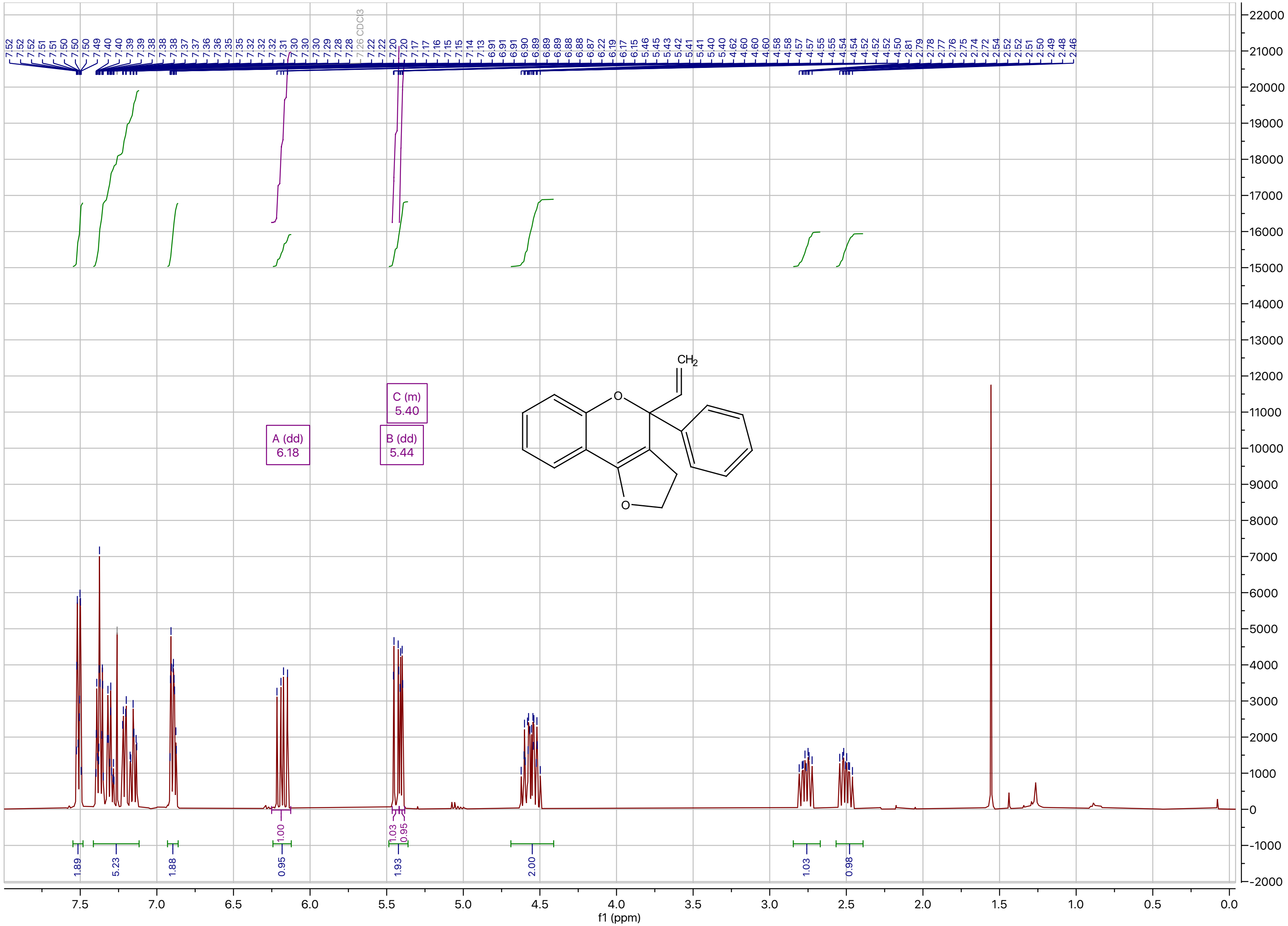
1n (400 MHz, $CDCl_3$)



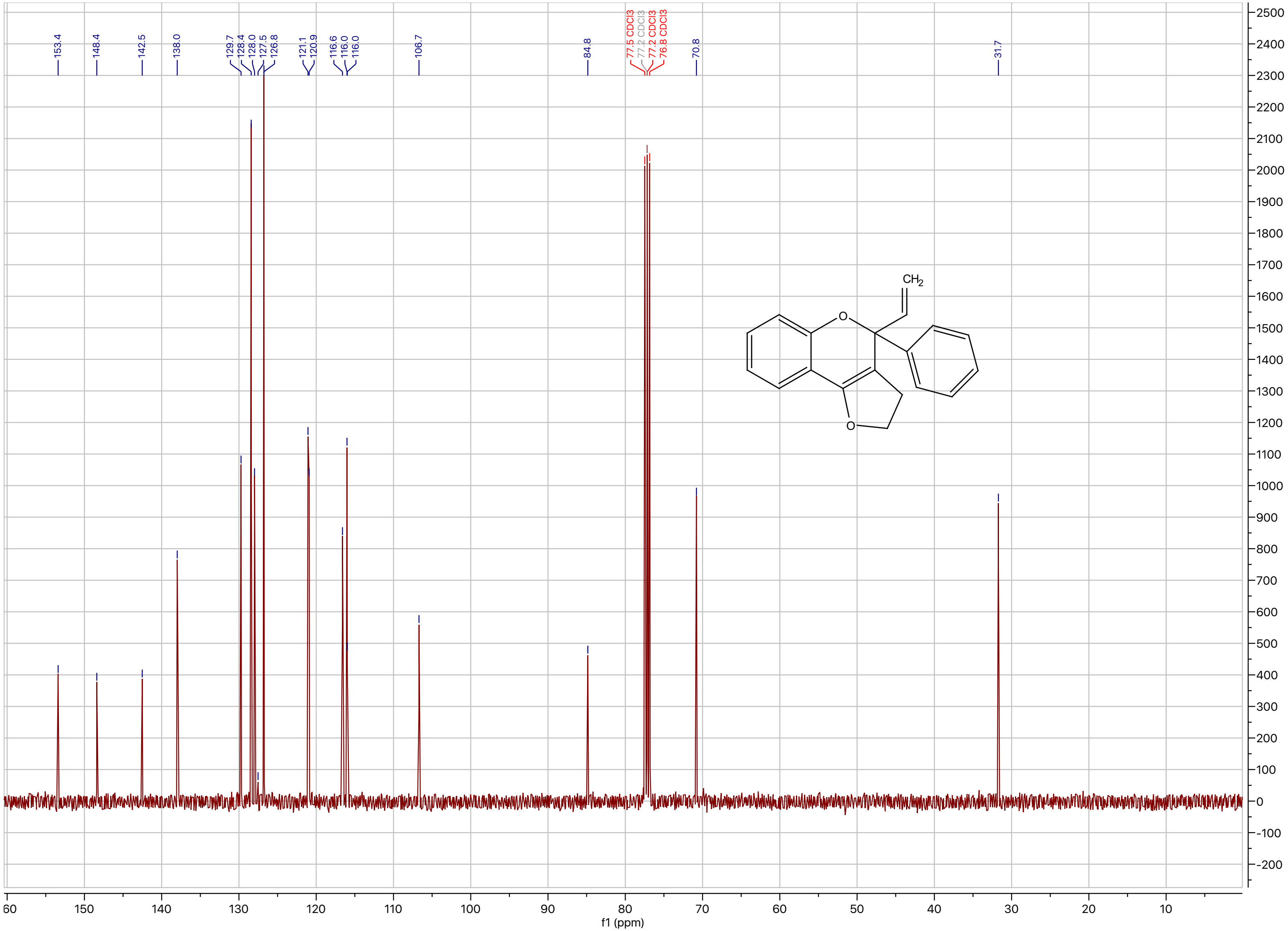
1n (101 MHz, $CDCl_3$)



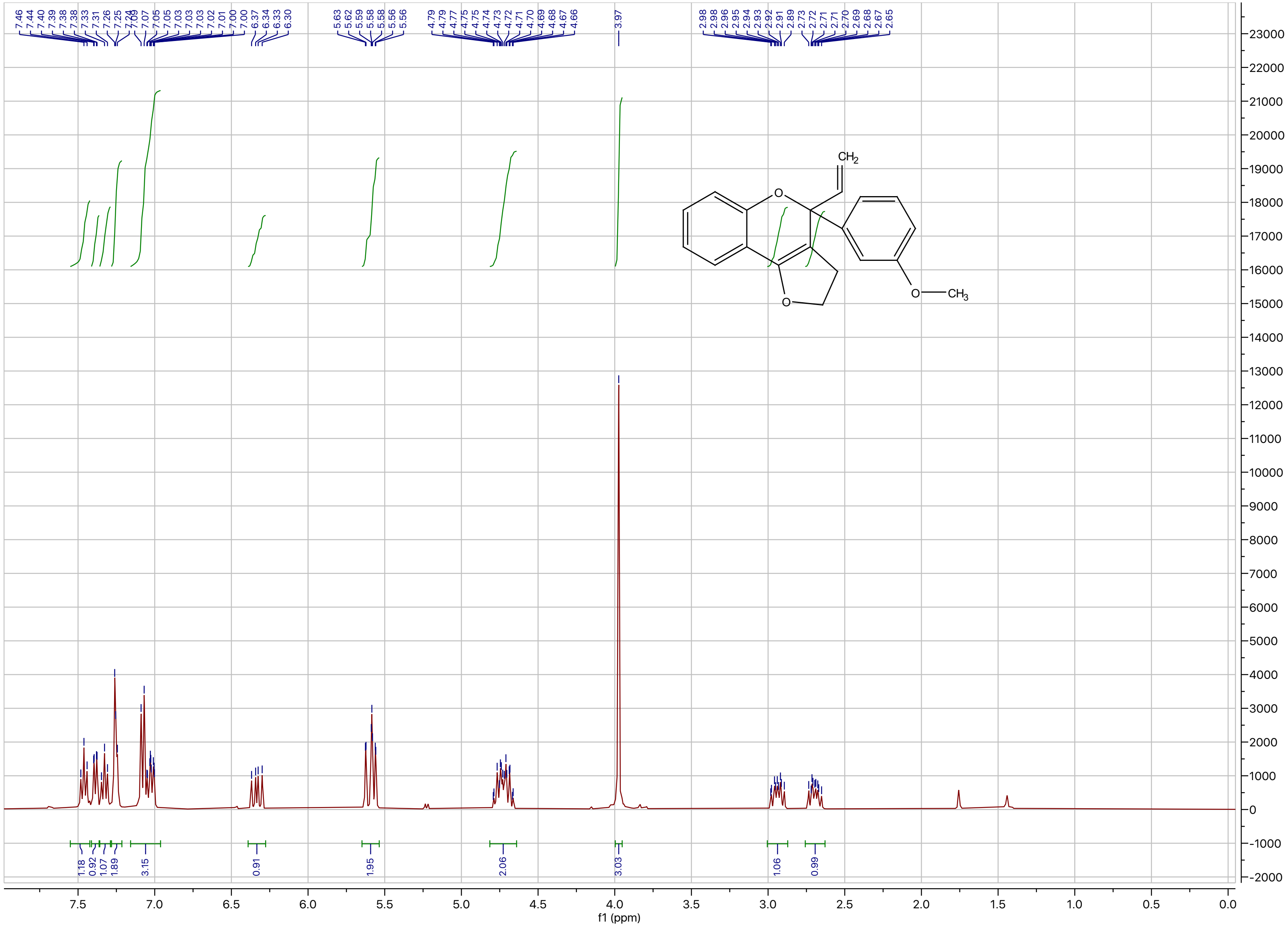
3a (400 MHz, $CDCl_3$)



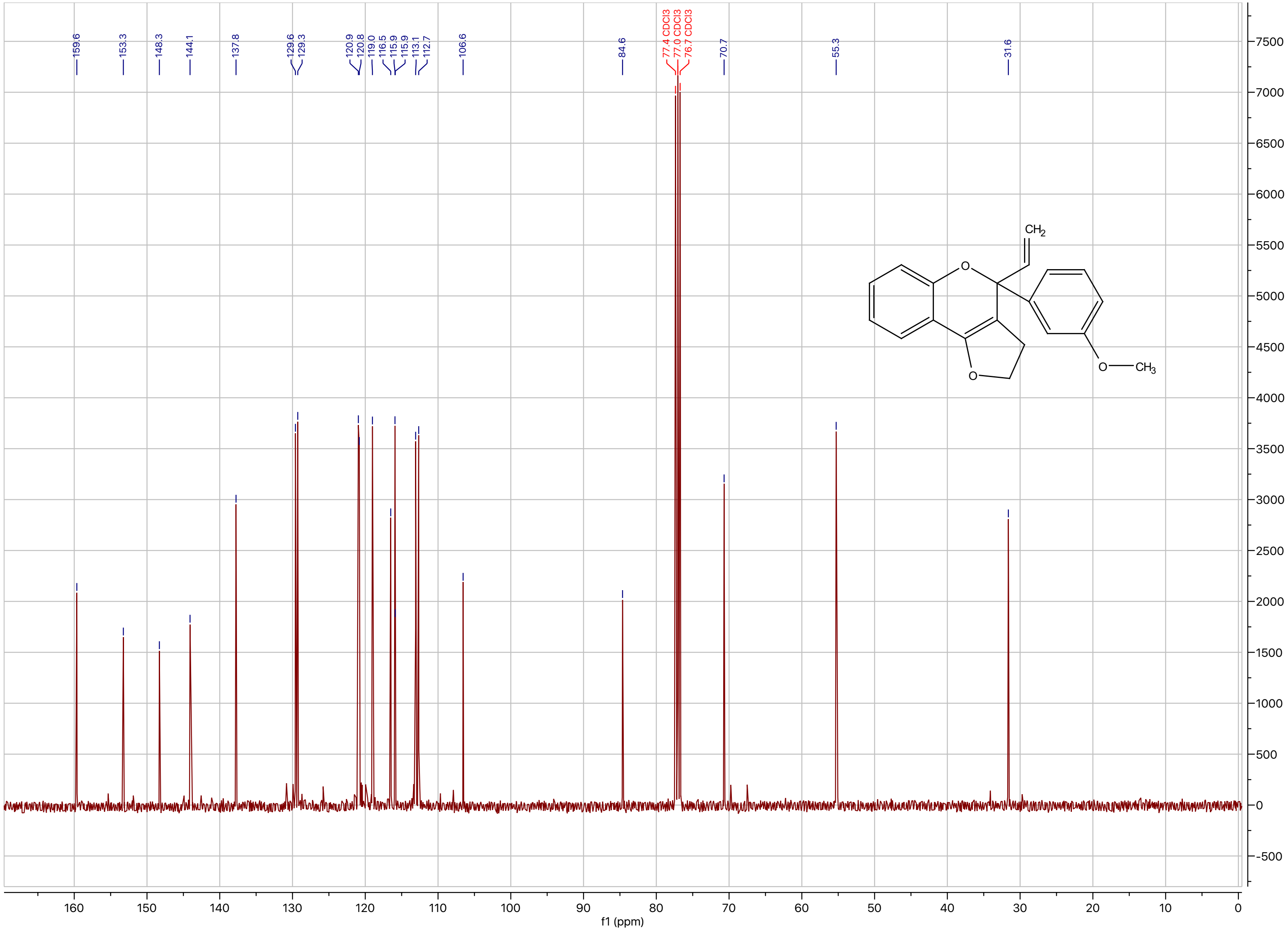
3a (101 MHz, $CDCl_3$)



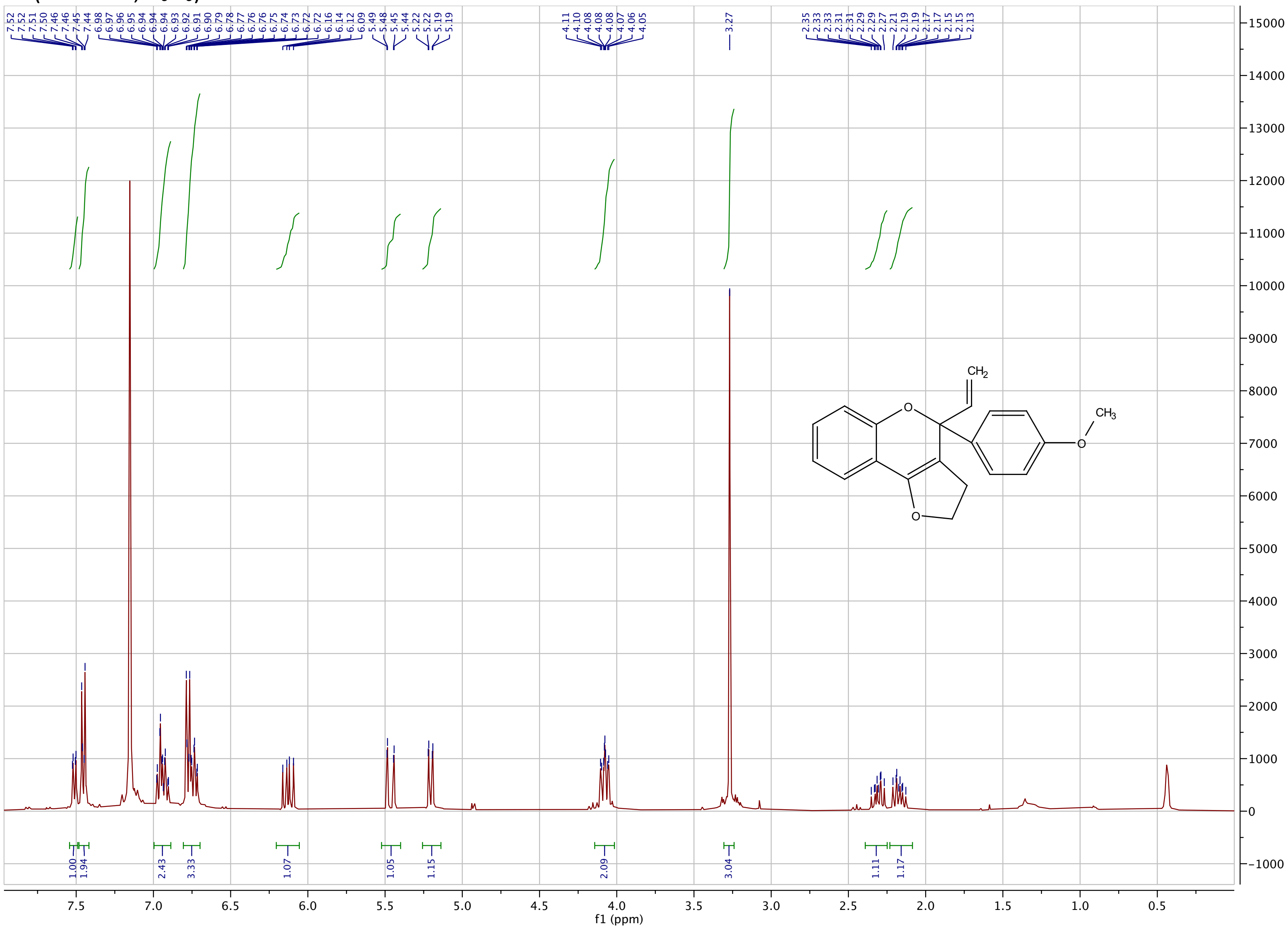
3b (400 MHz, $CDCl_3$)



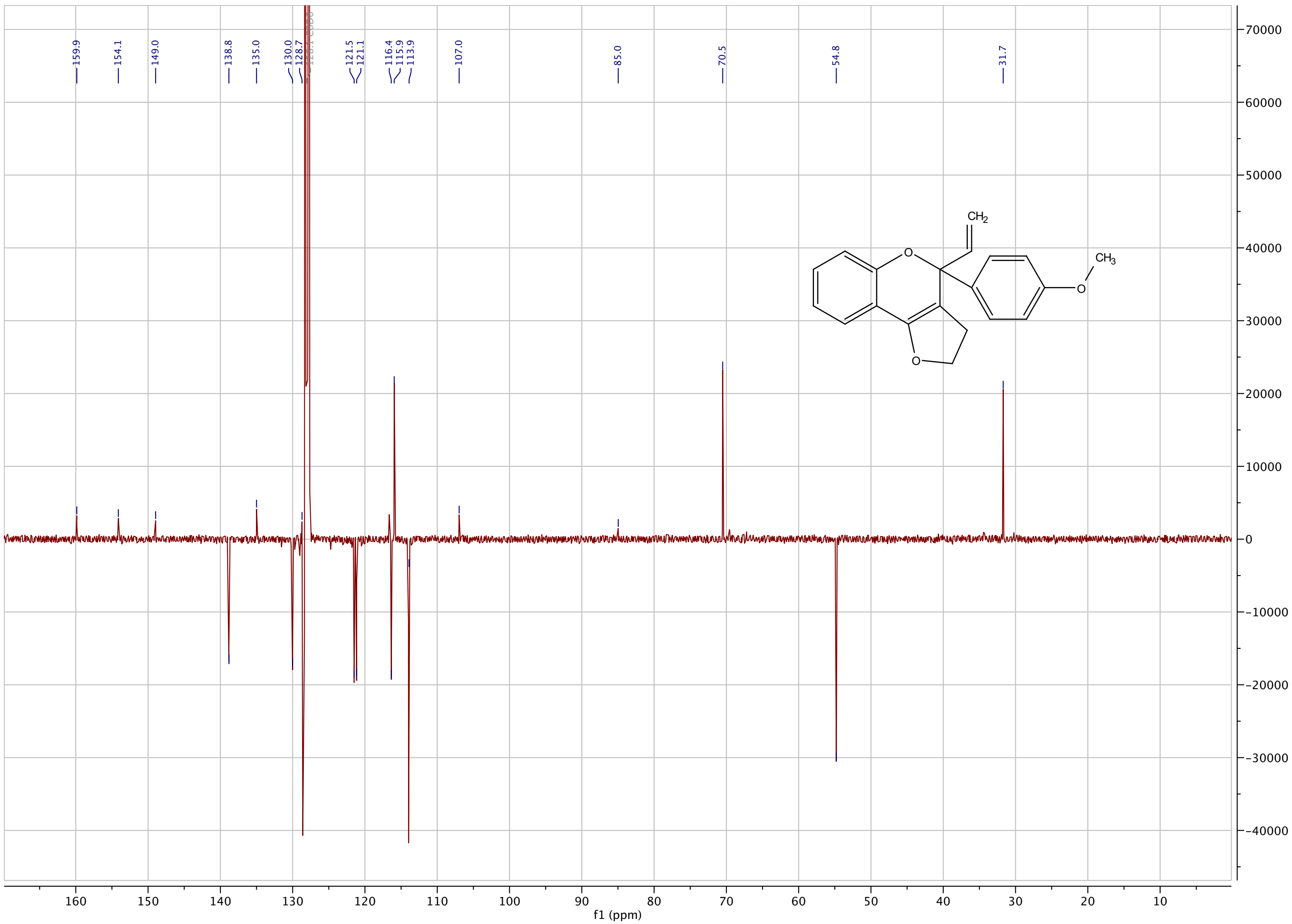
3b (101 MHz, $CDCl_3$)



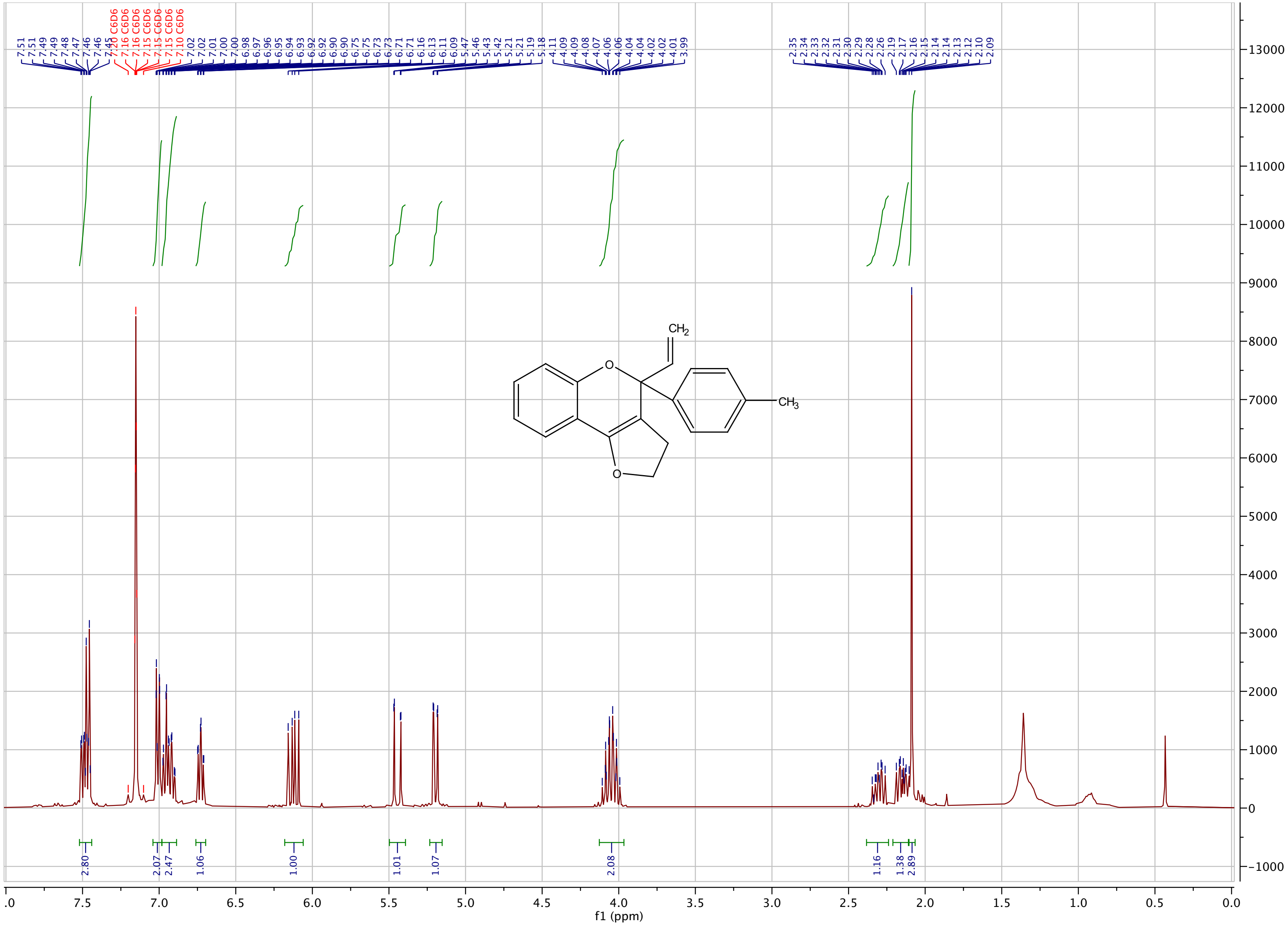
3c (400 MHz, C_6D_6)



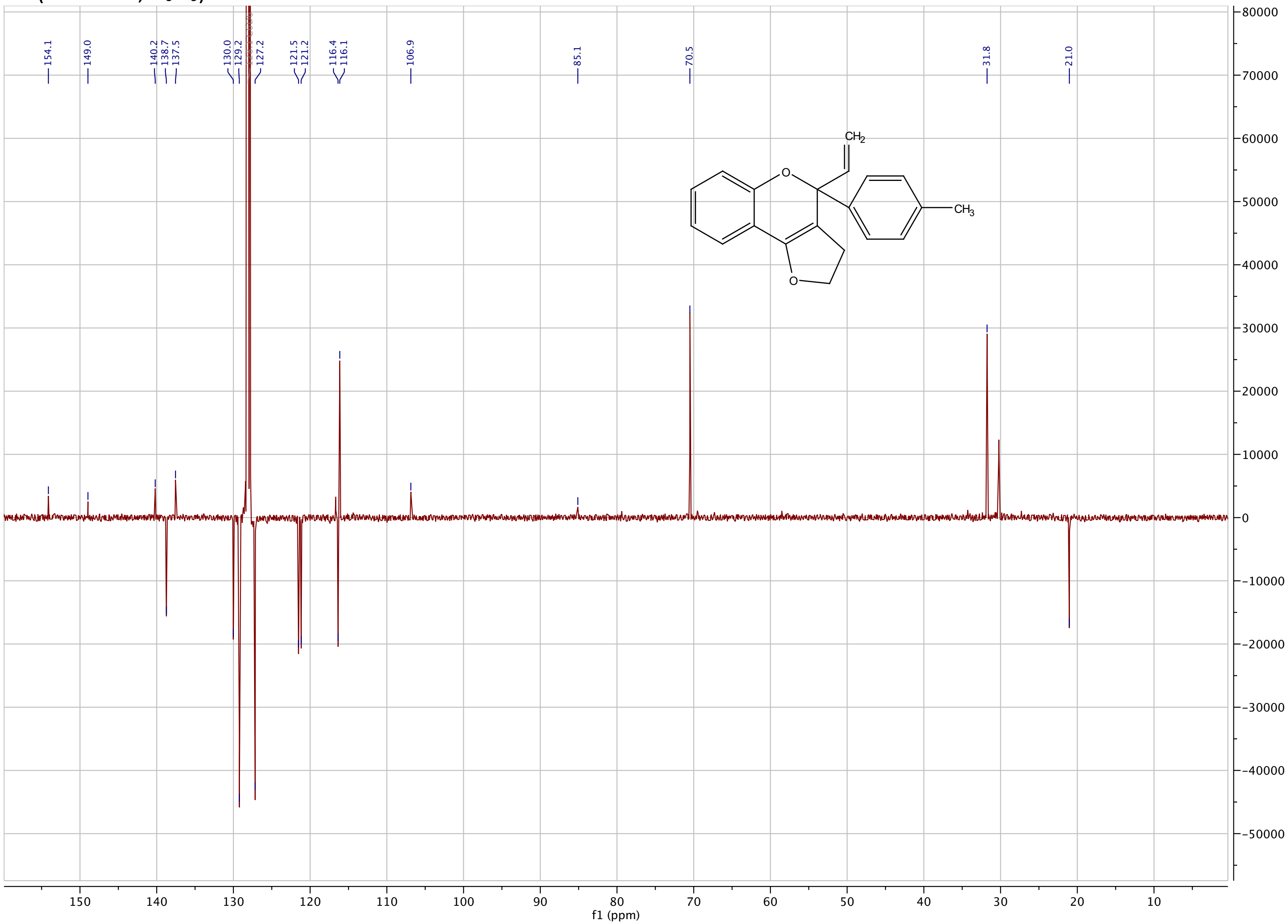
3c (101 MHz, C_6D_6)



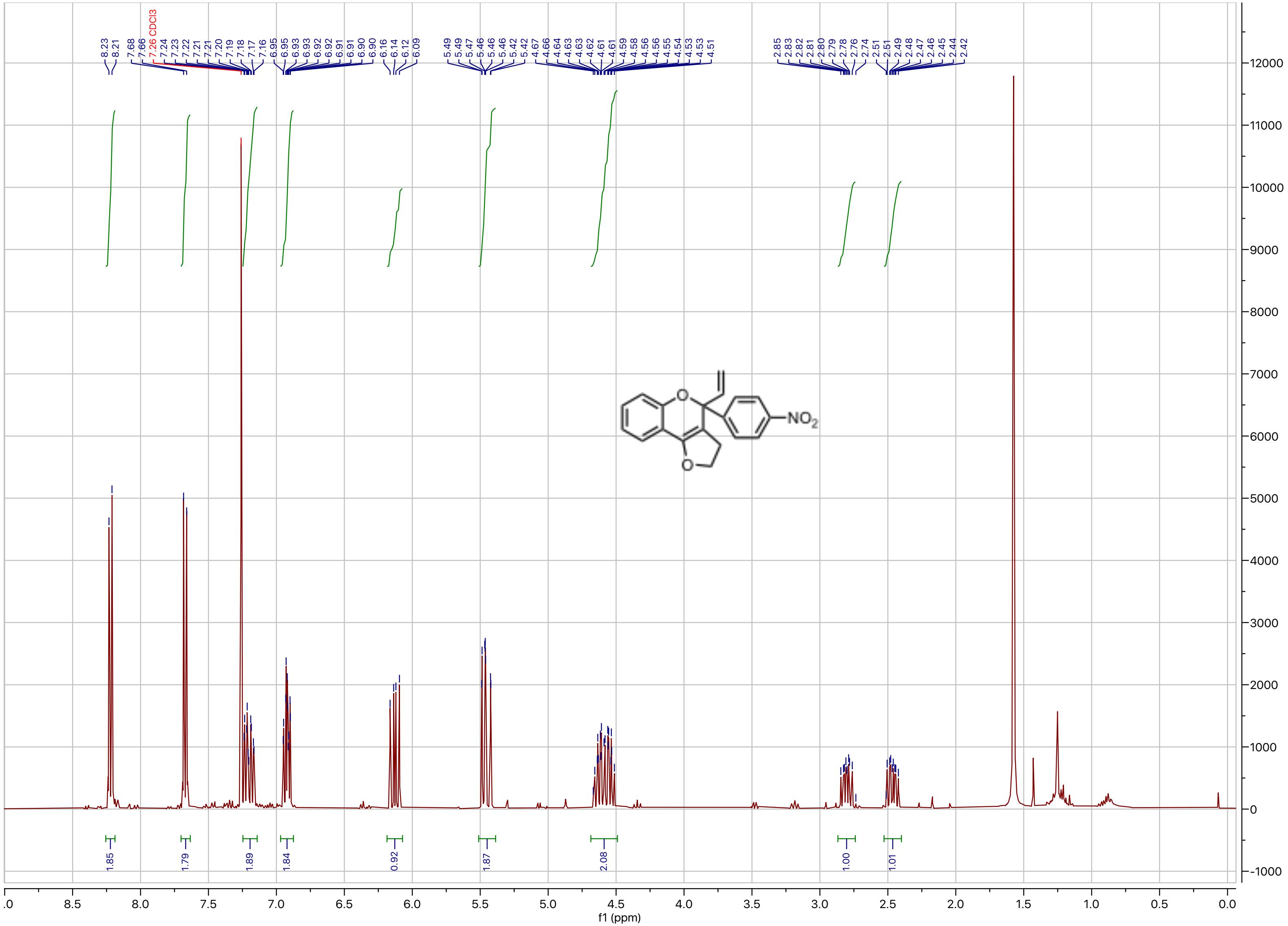
3d (400 MHz, C_6D_6)



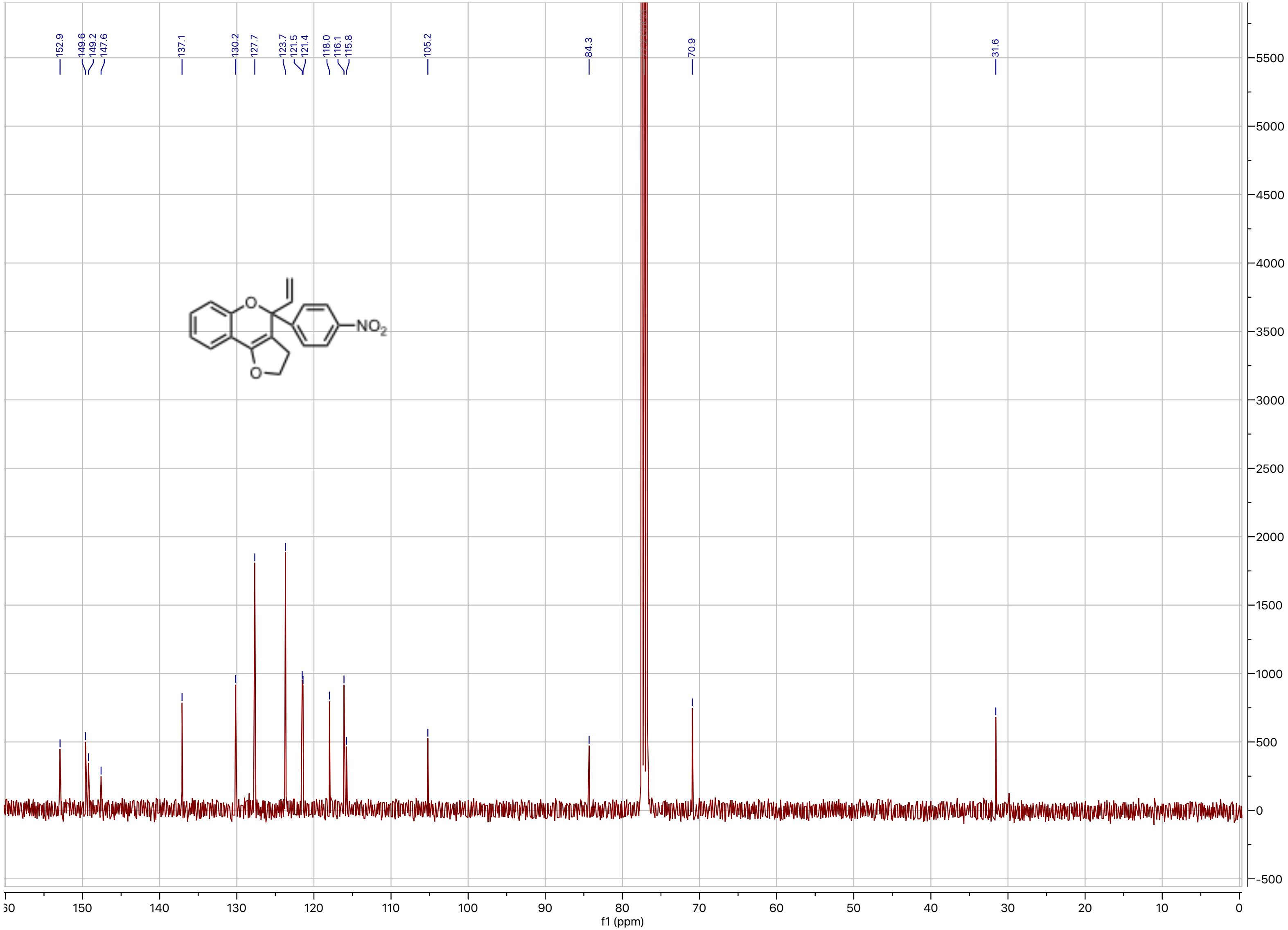
3d (101 MHz, C_6D_6)



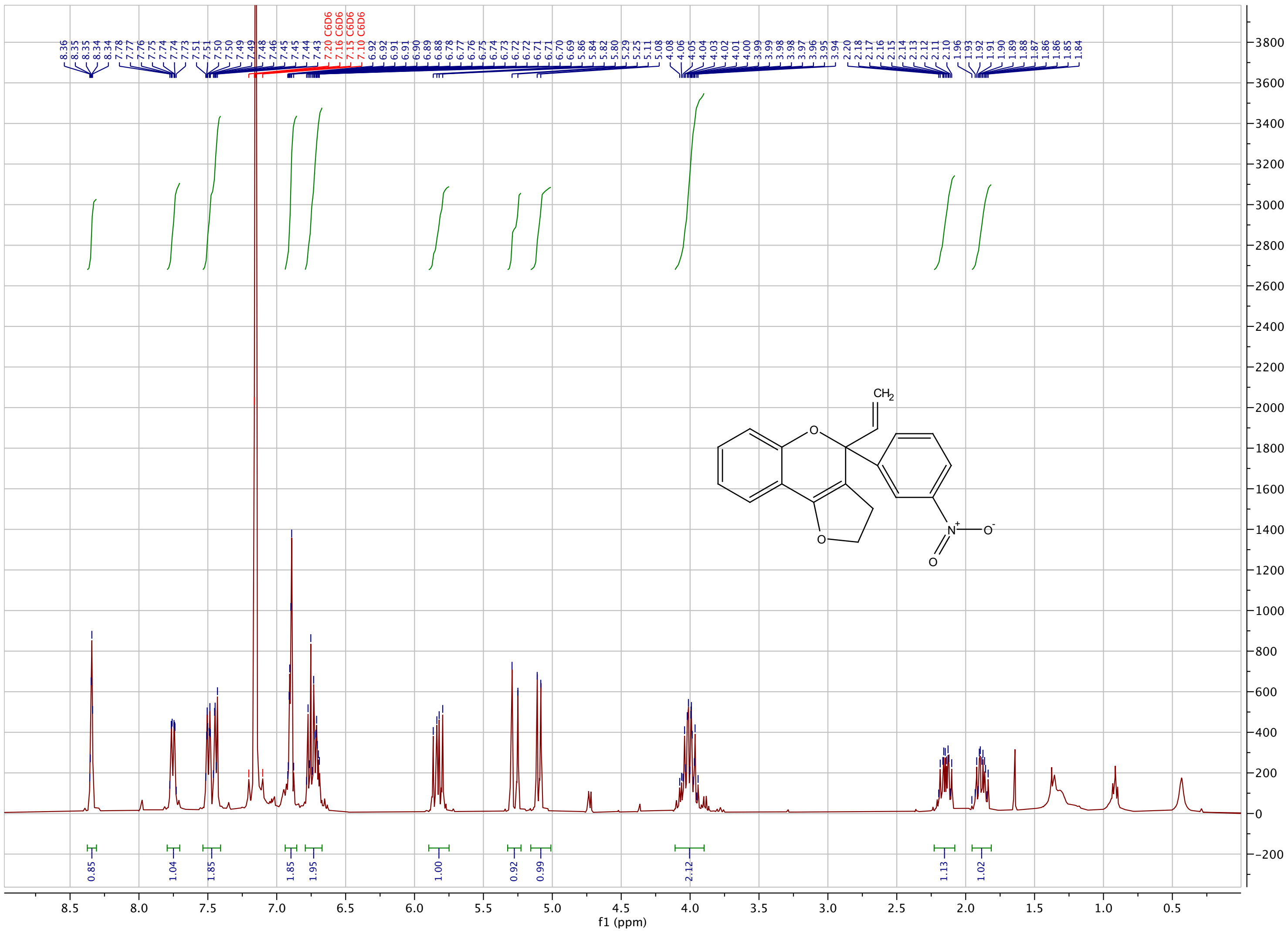
3e (400 MHz, $CDCl_3$)



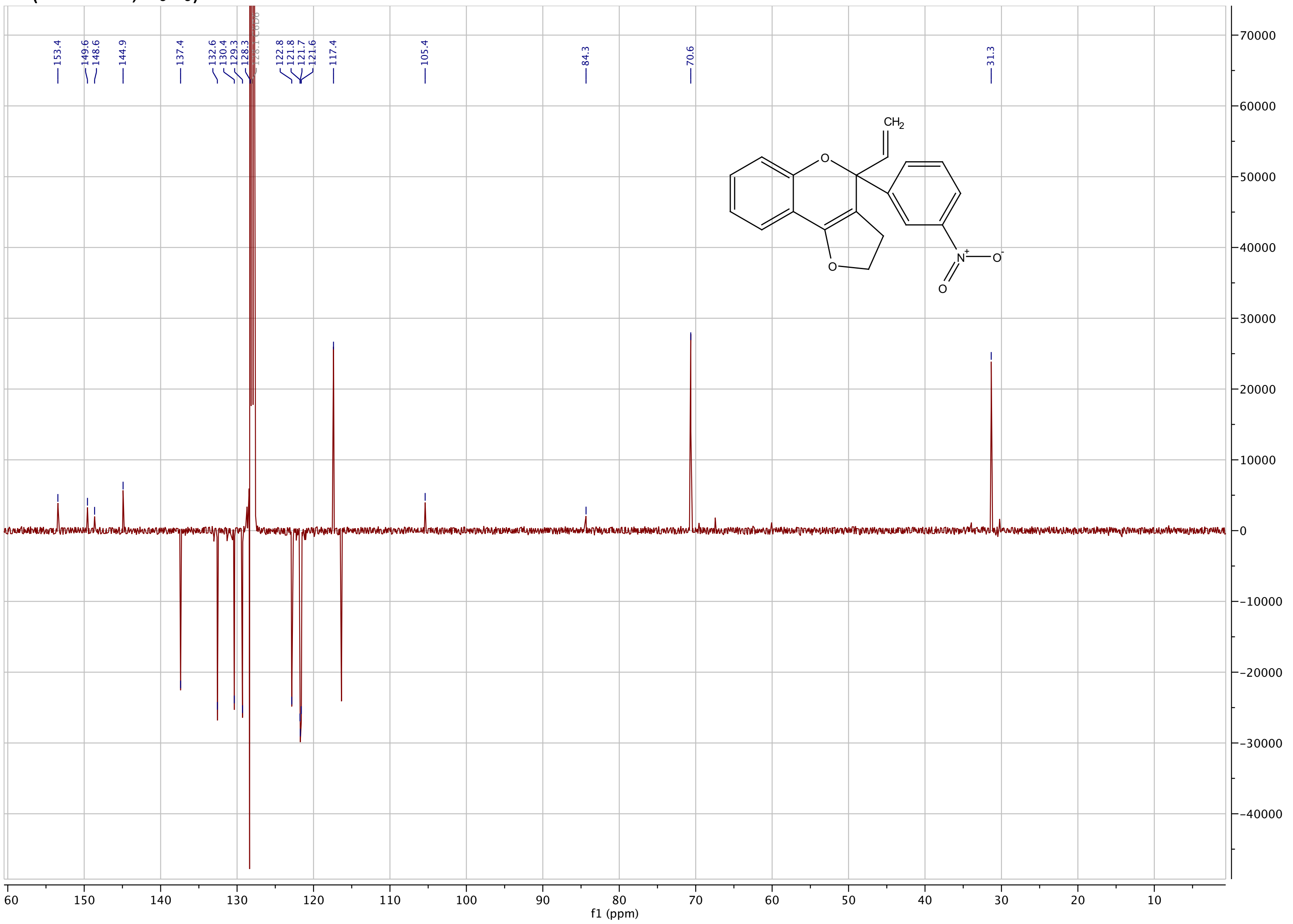
3e (101 MHz, $CDCl_3$)



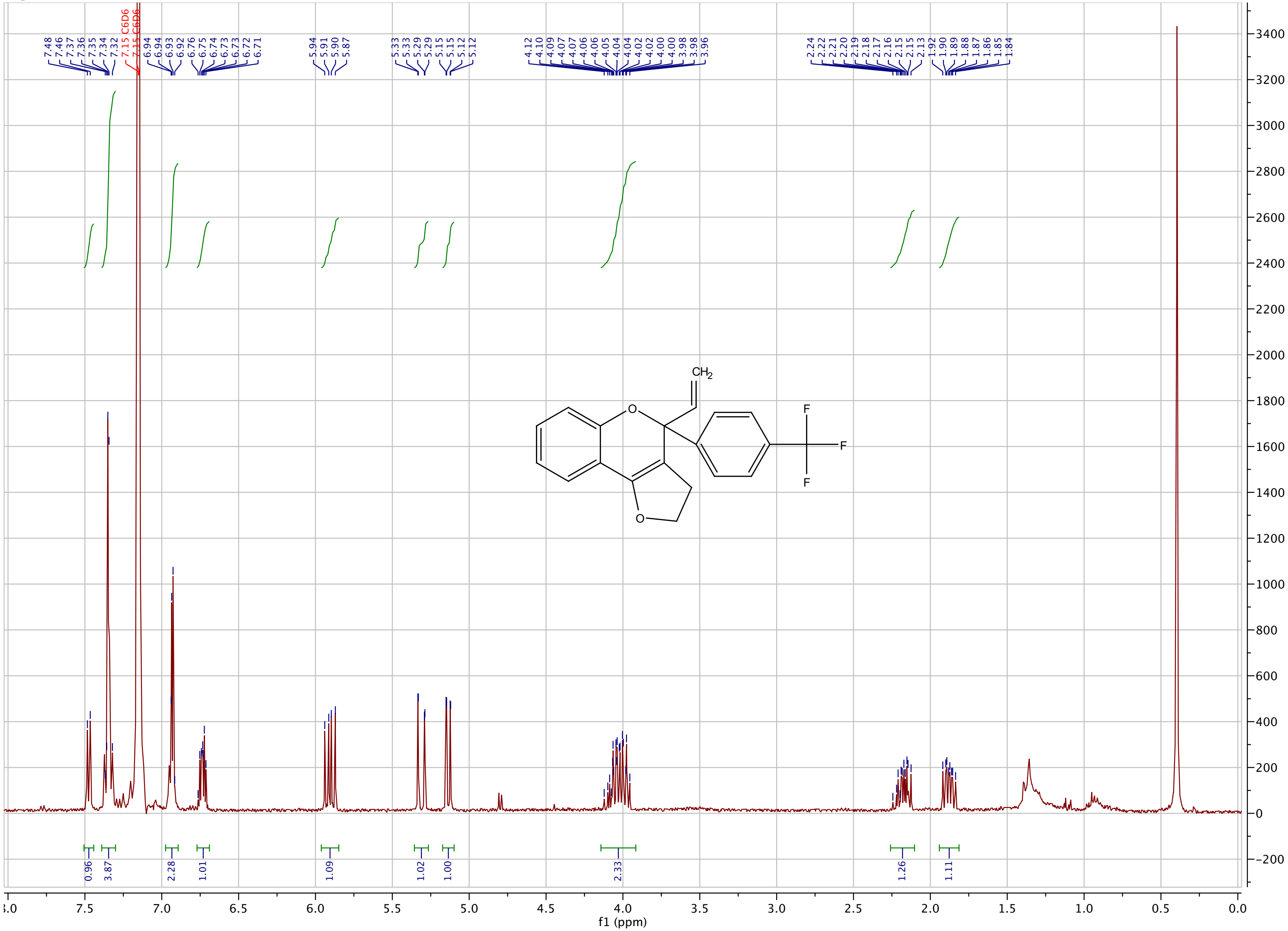
3f (400 MHz, C_6D_6)



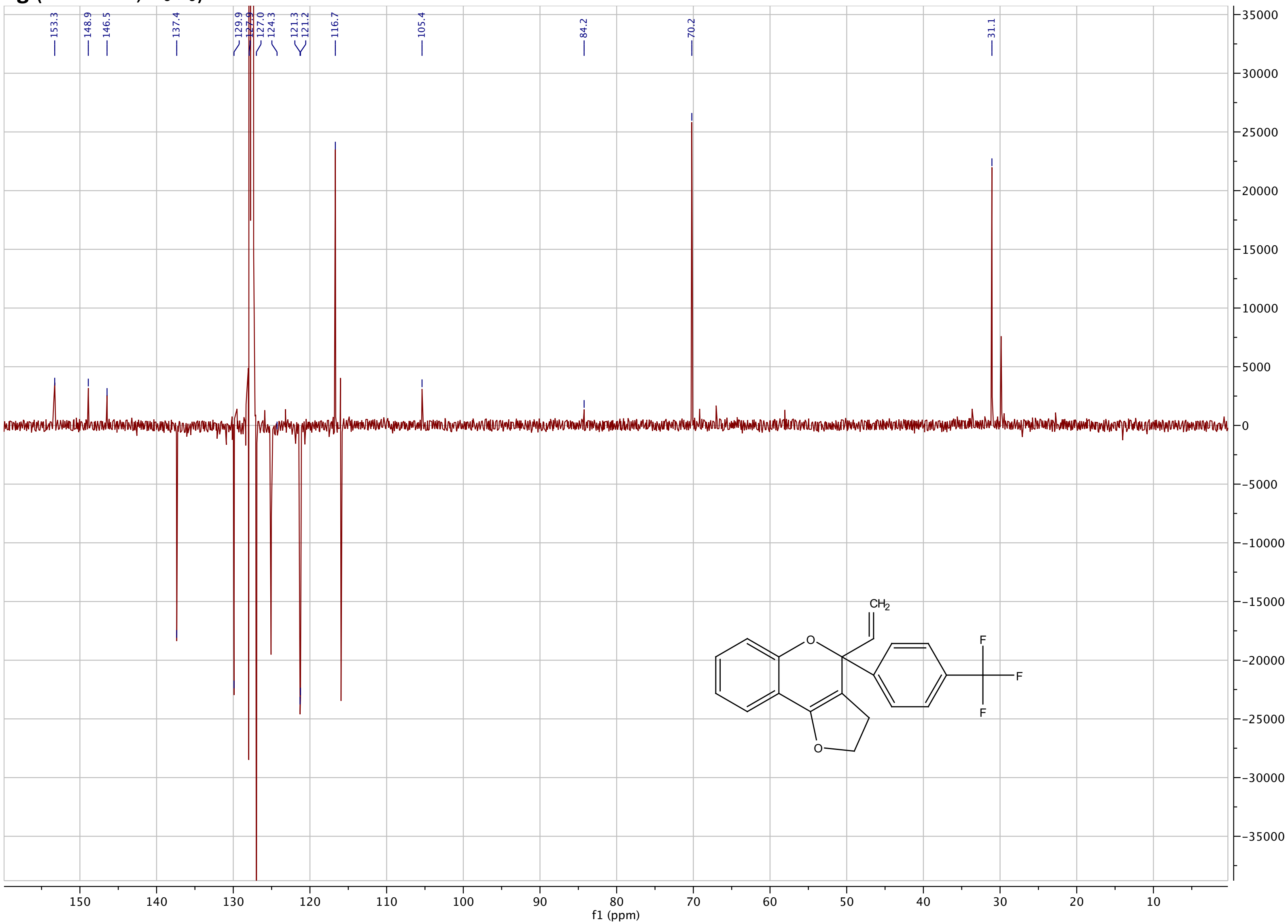
3f (101 MHz, C_6D_6)



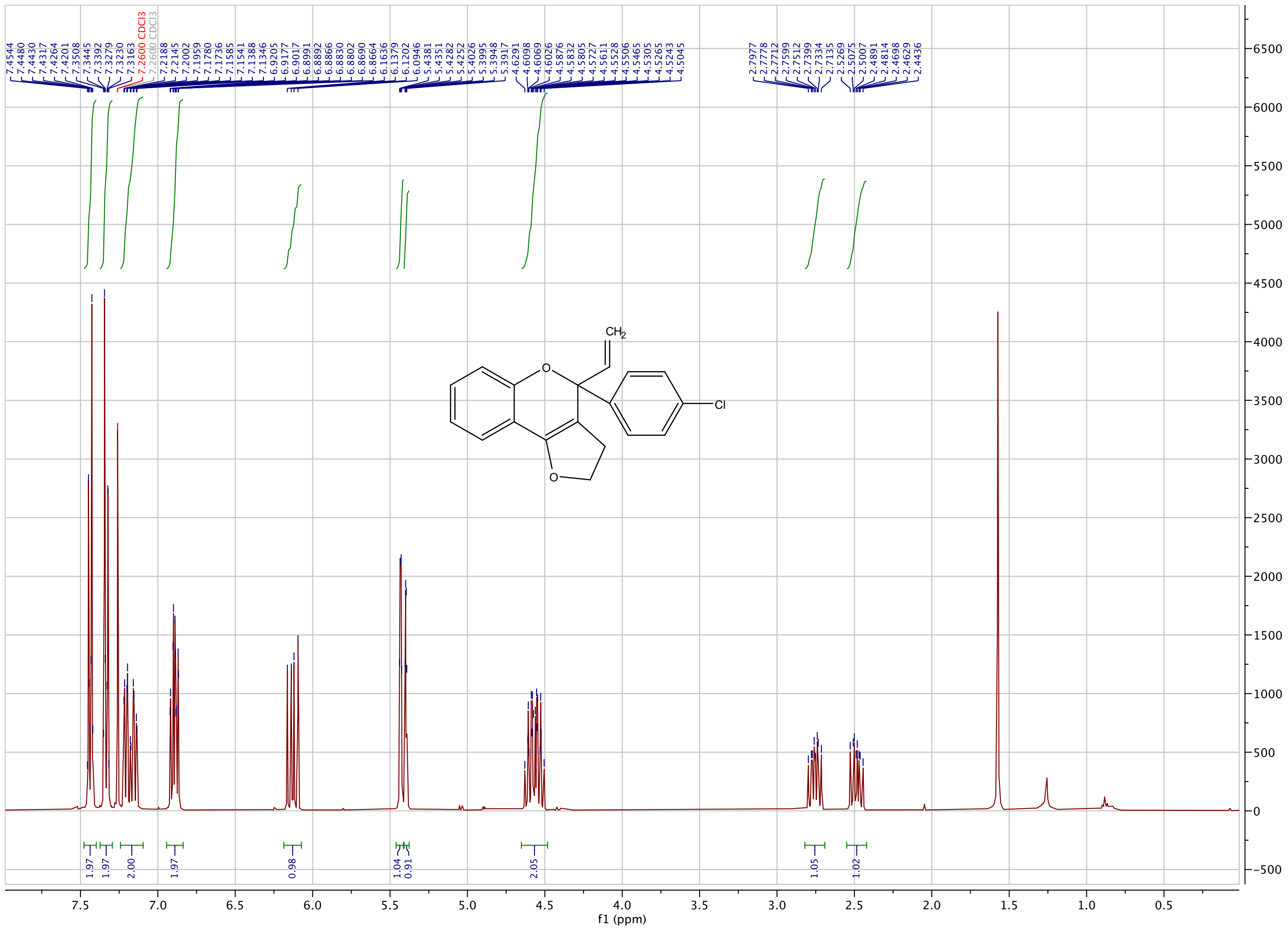
3g (400 MHz, C_6D_6)



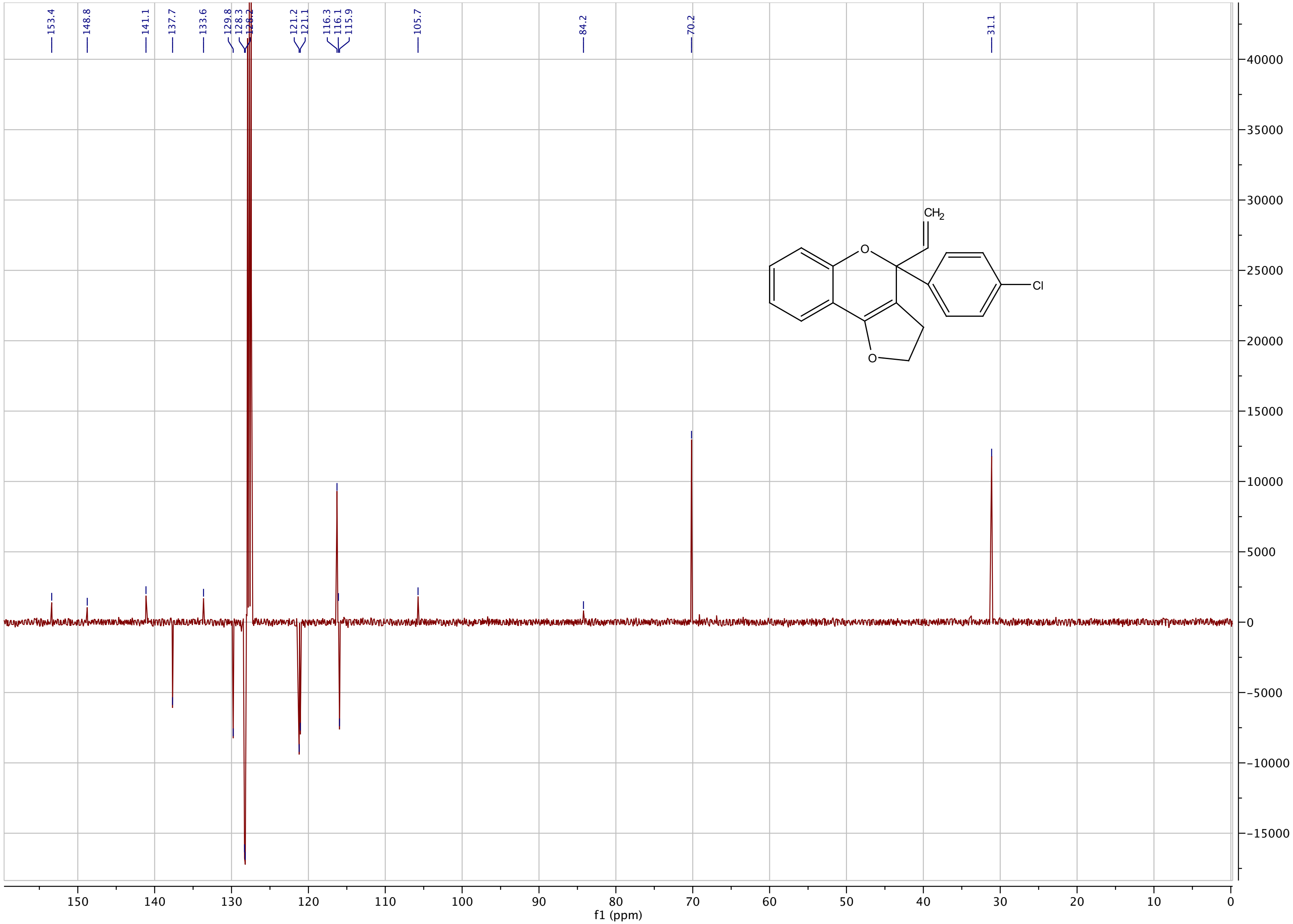
3g (101 MHz, C_6D_6)



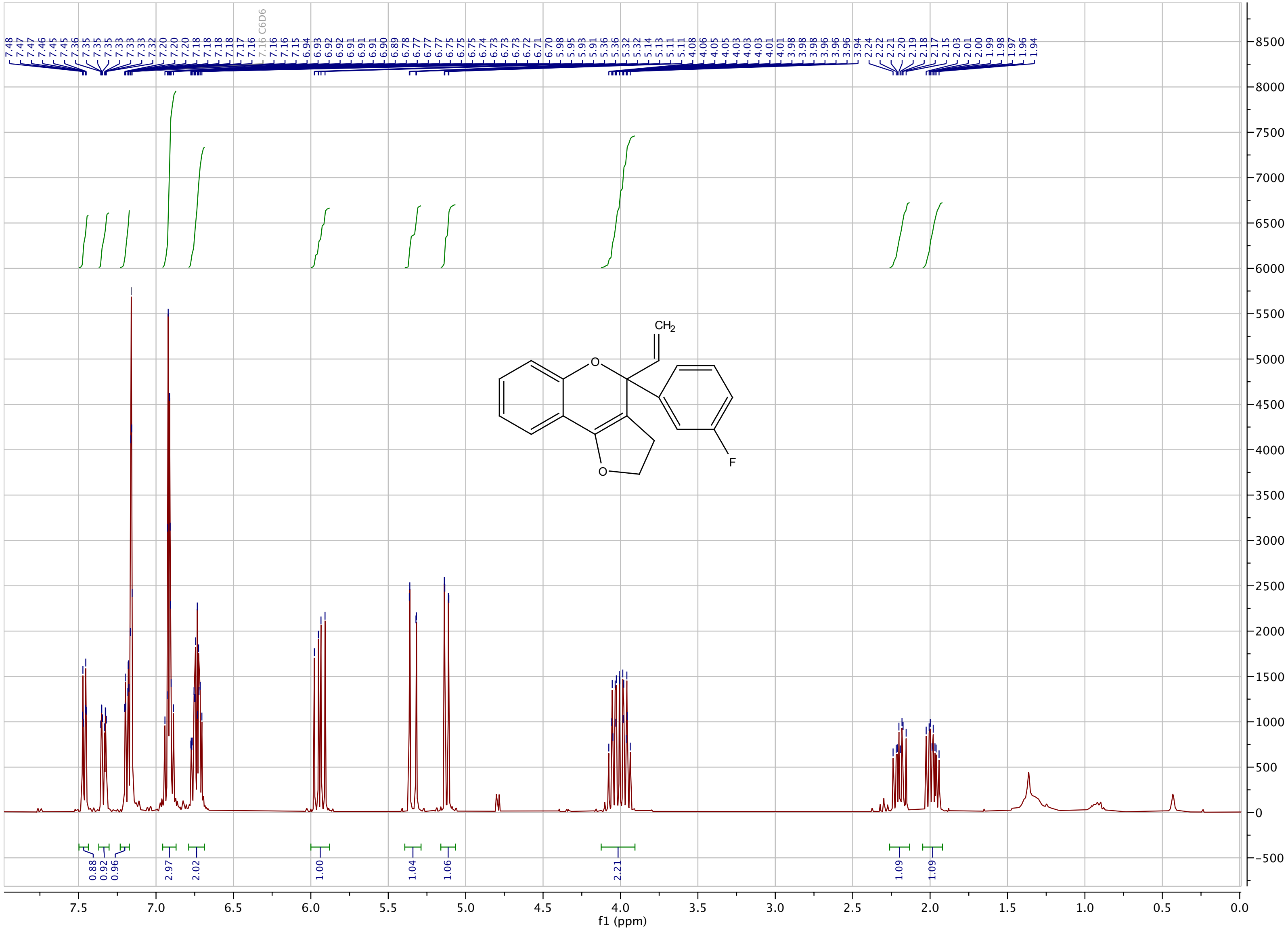
3h (400 MHz, $CDCl_3$)



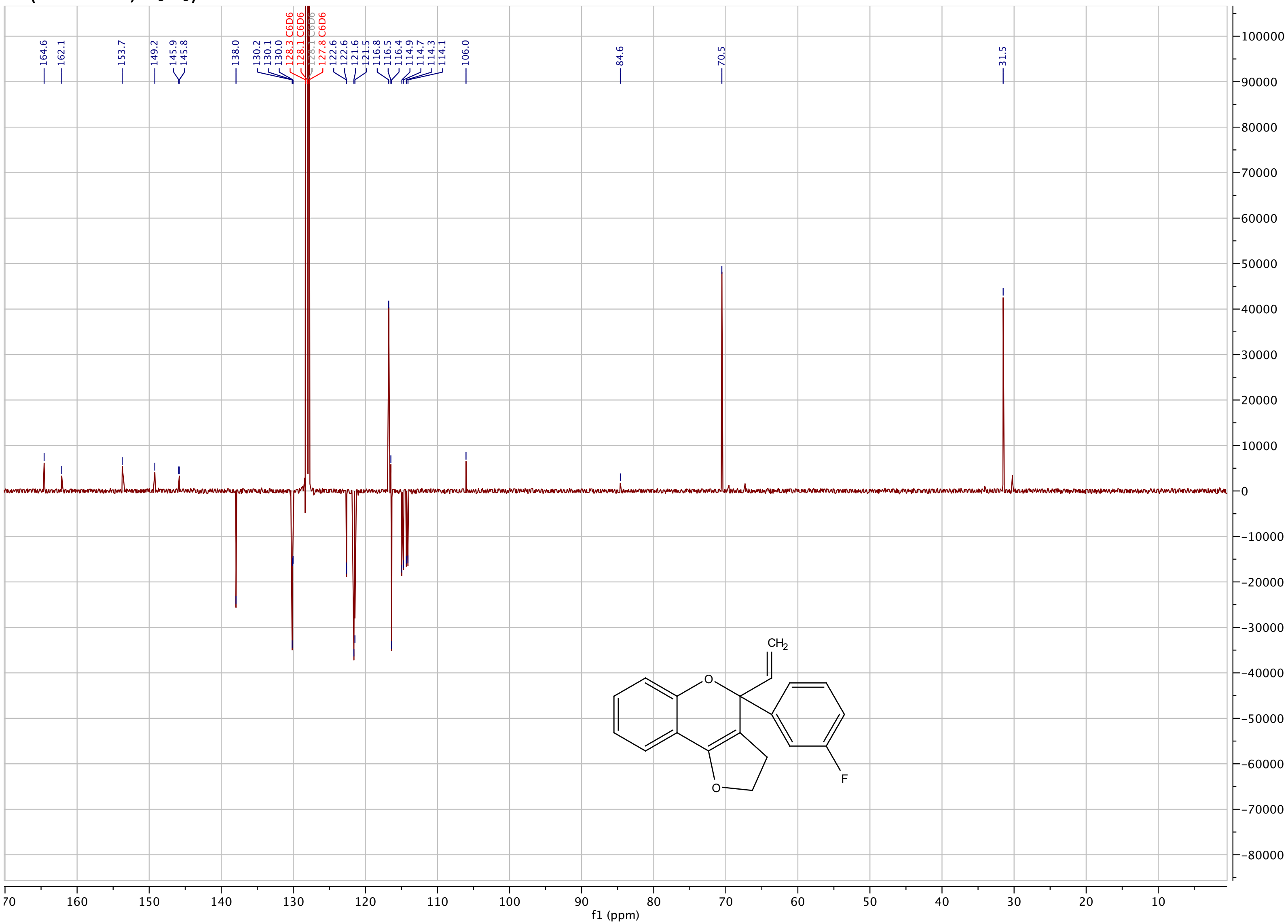
3h (101 MHz, $CDCl_3$)



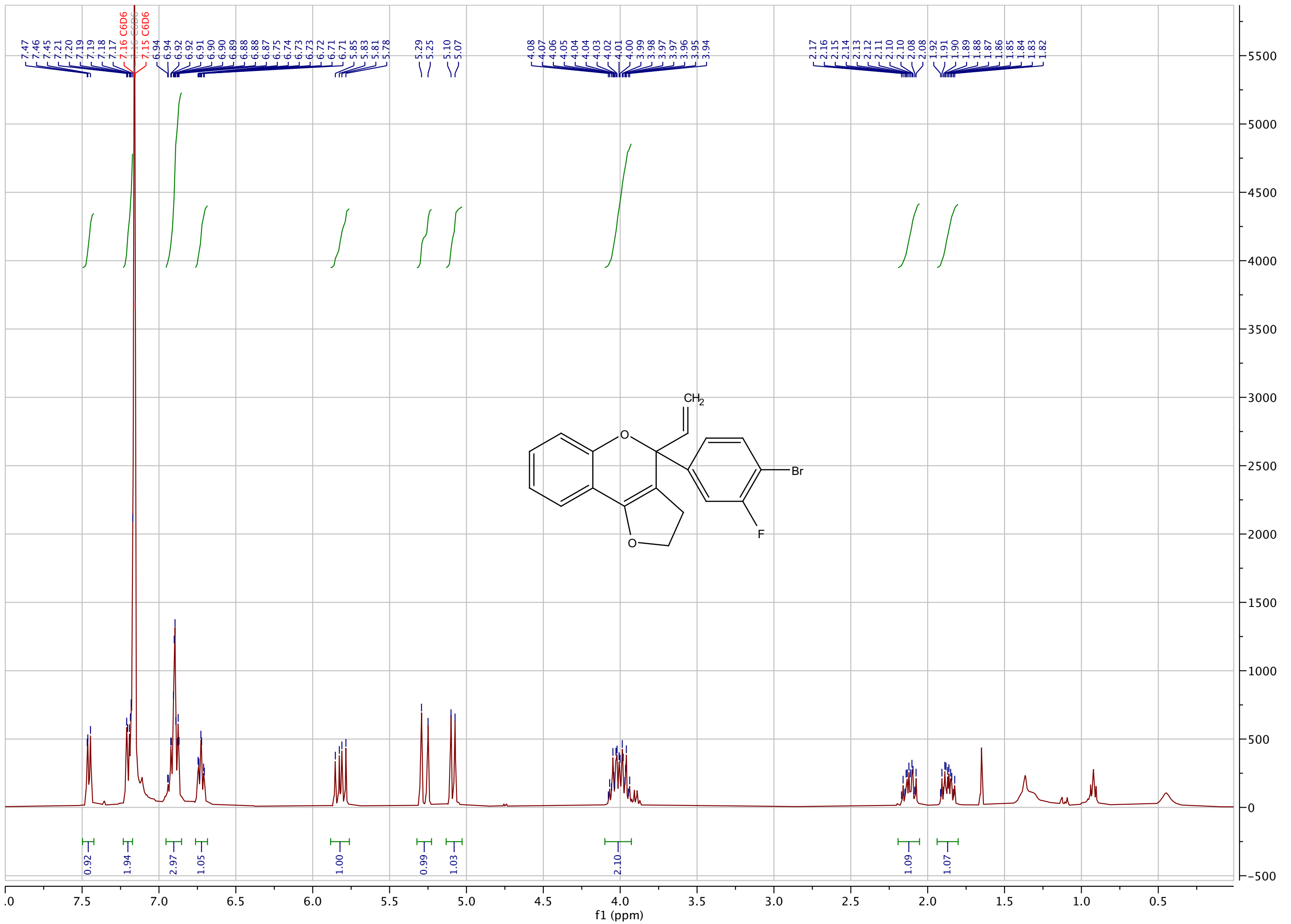
3i (400 MHz, C_6D_6)



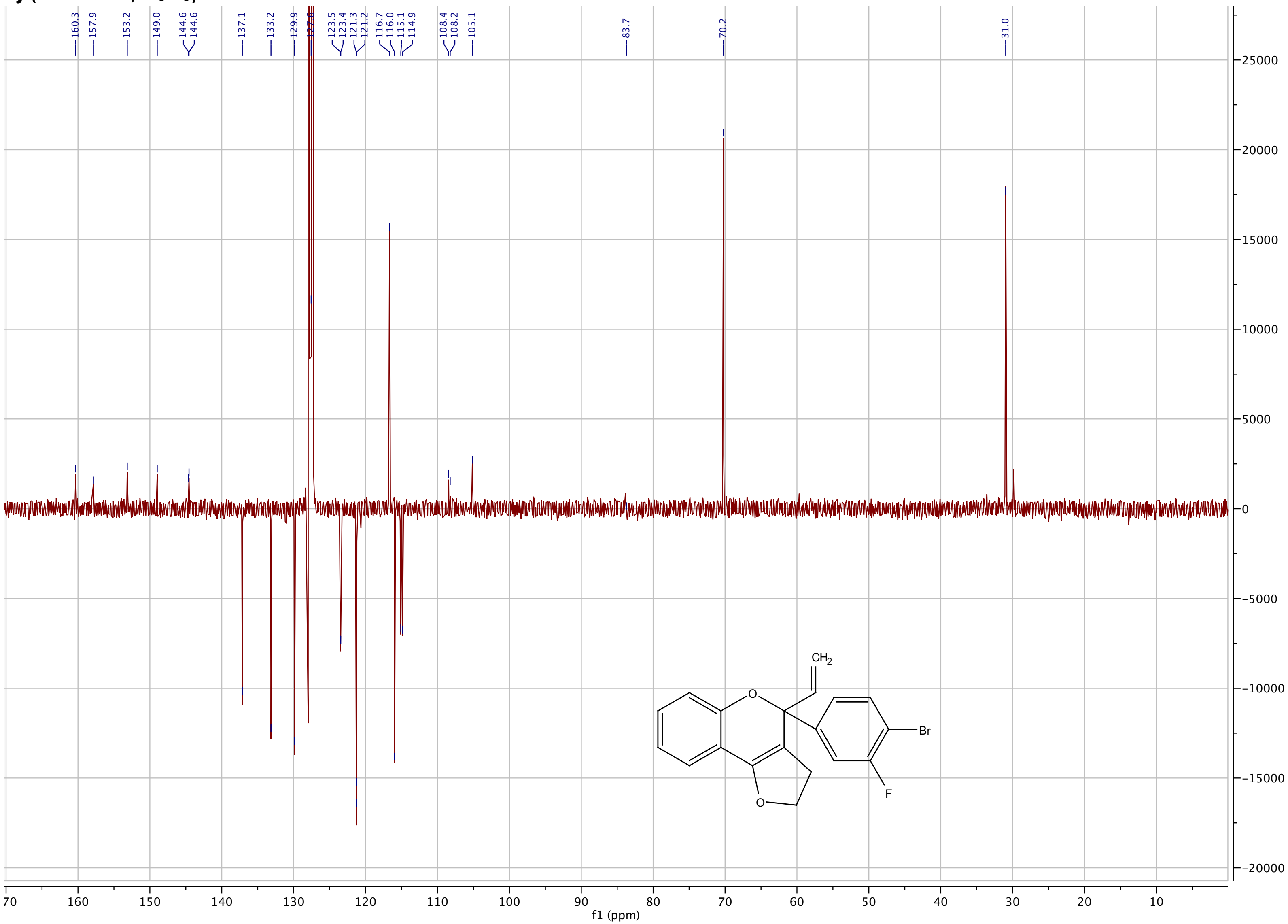
3i (101 MHz, C_6D_6)



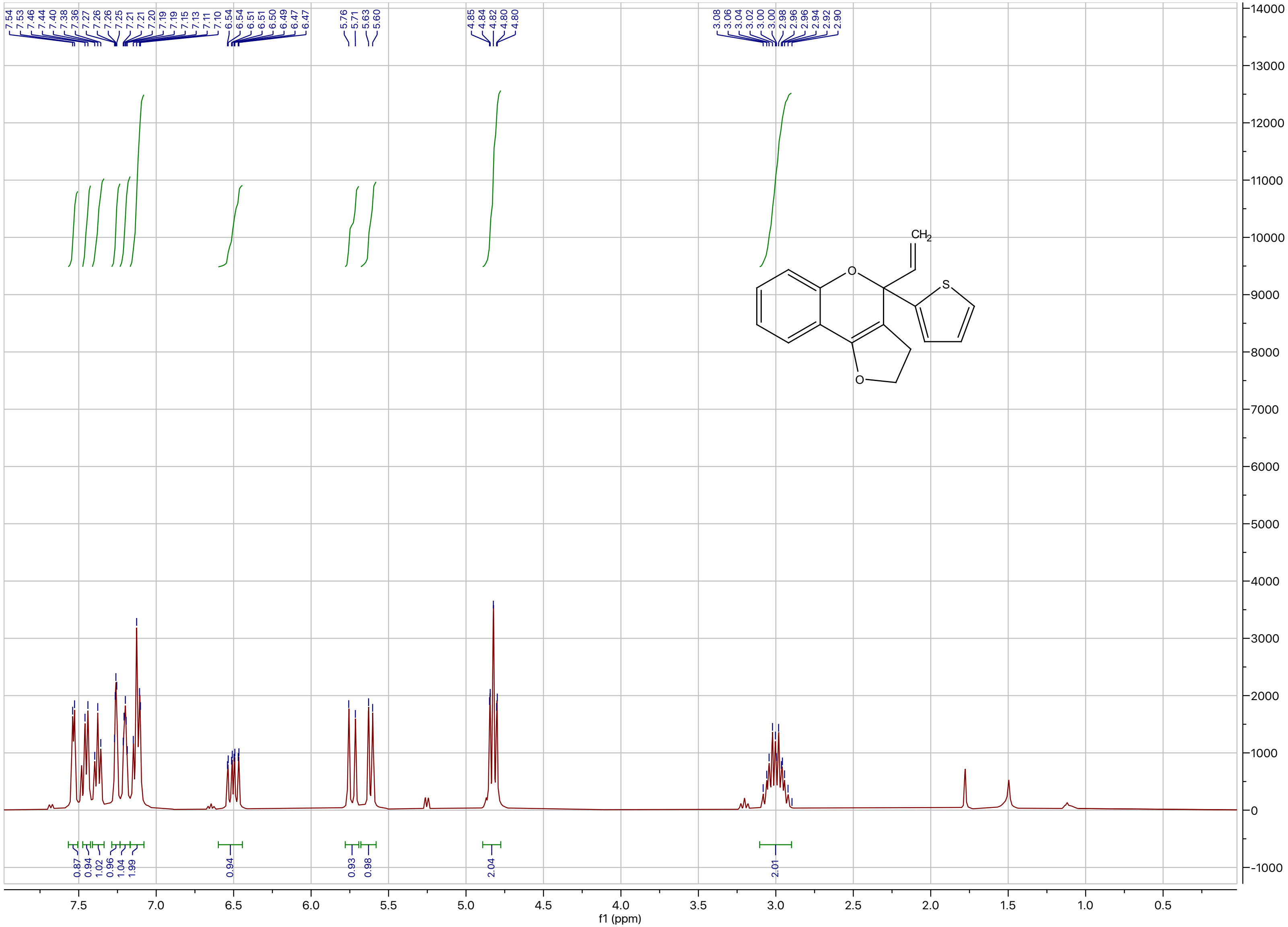
3j (400 MHz, C_6D_6)



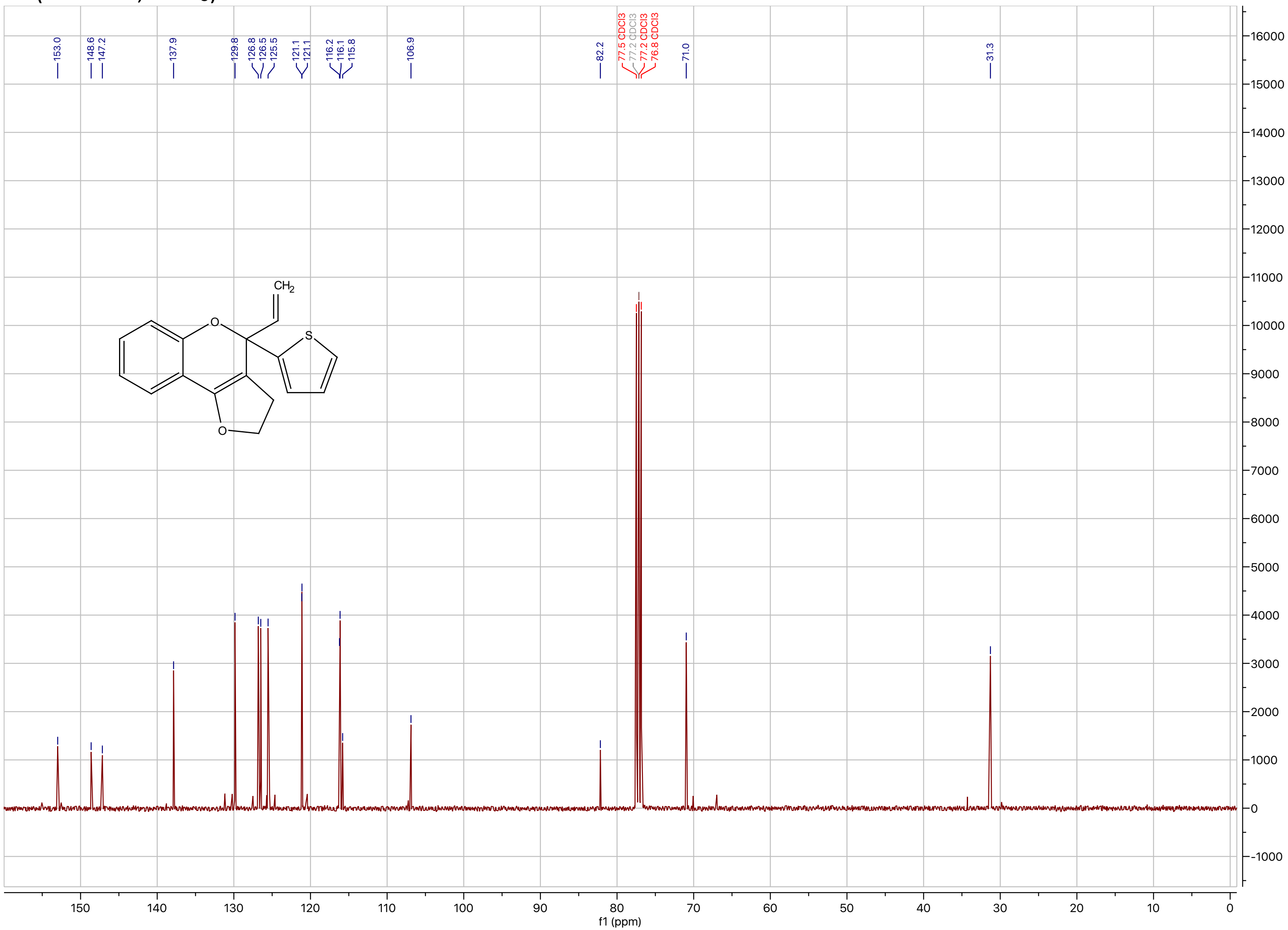
3j (101 MHz, C_6D_6)



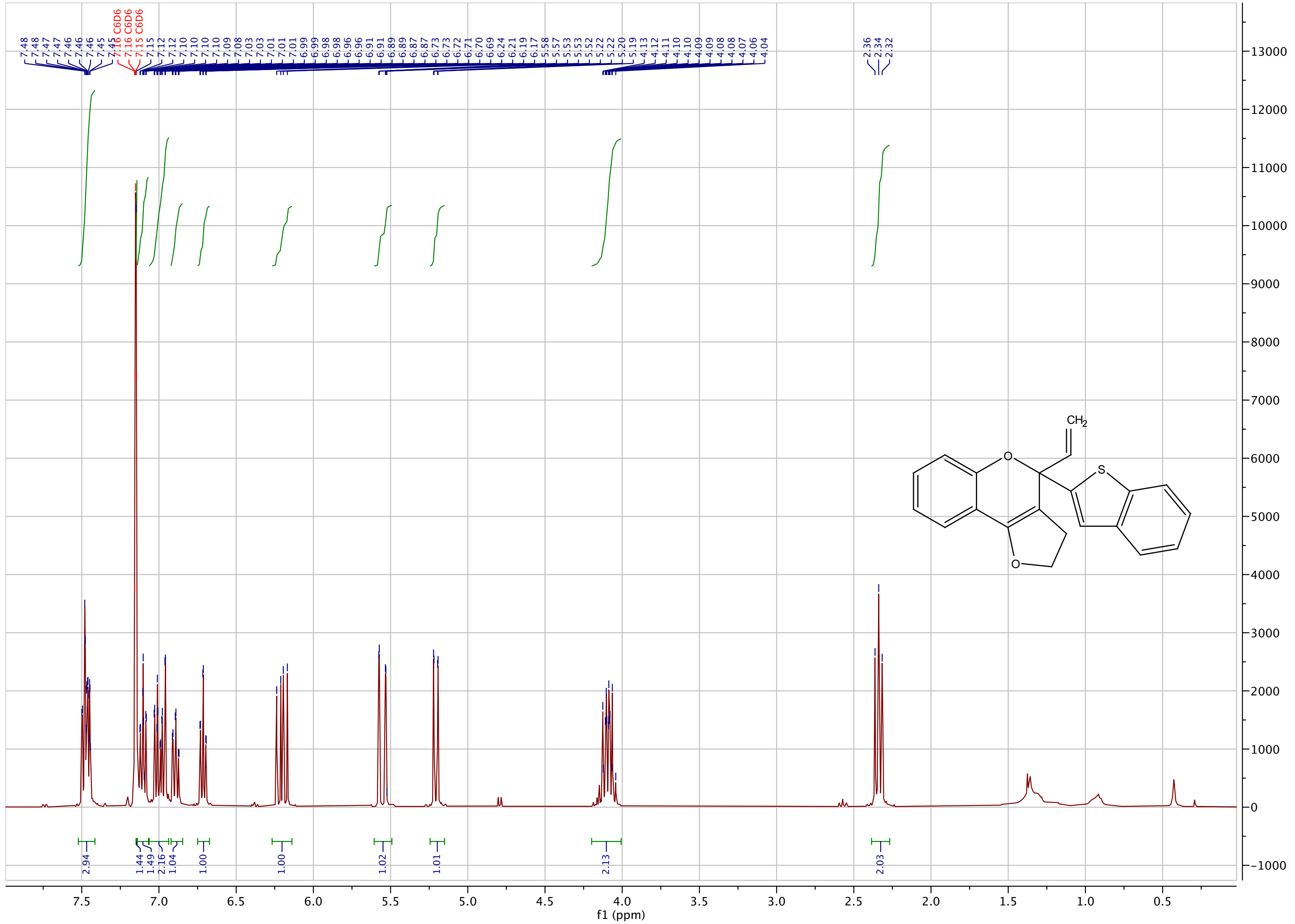
3k (400 MHz, $CDCl_3$)



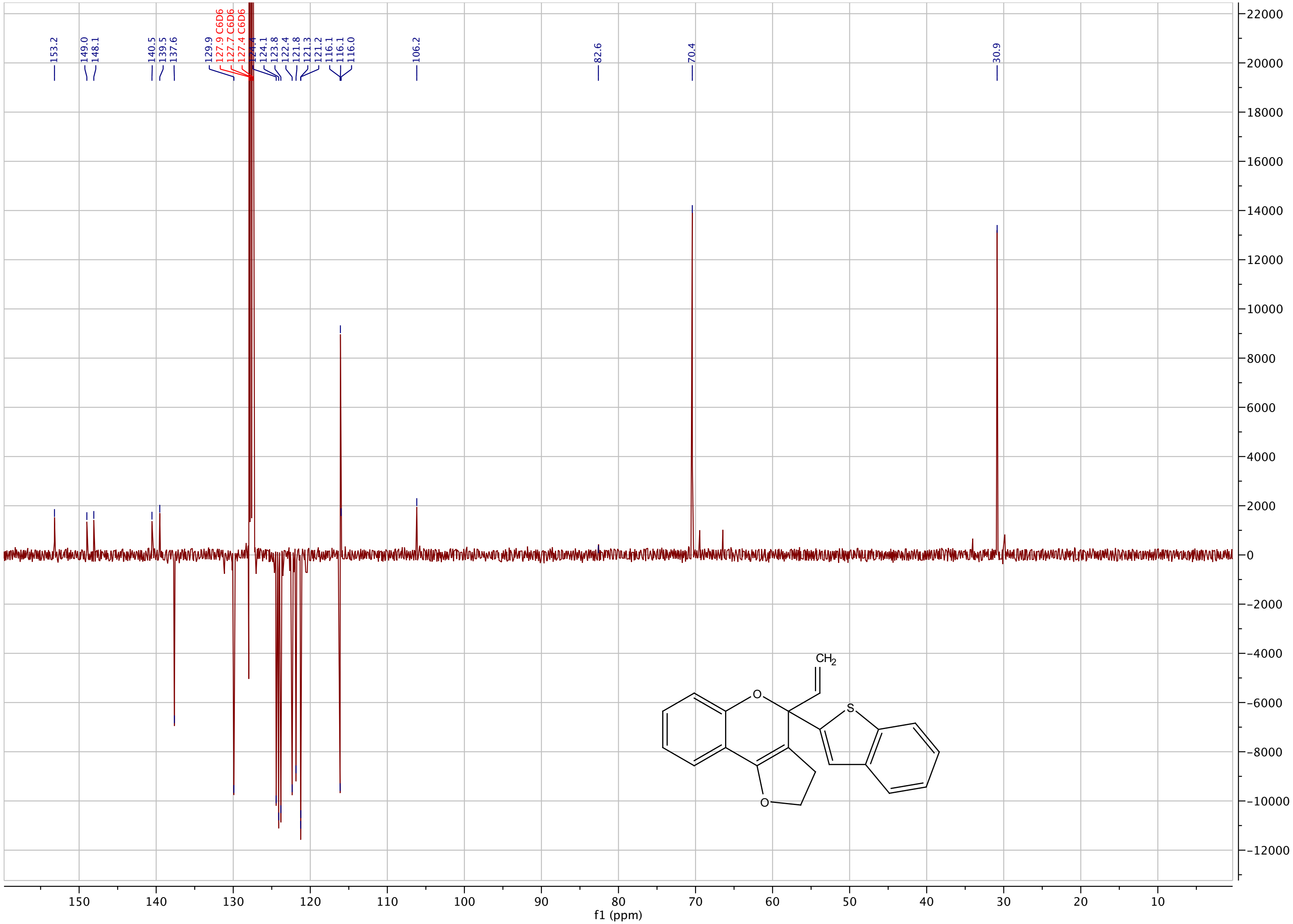
3k (101 MHz, $CDCl_3$)



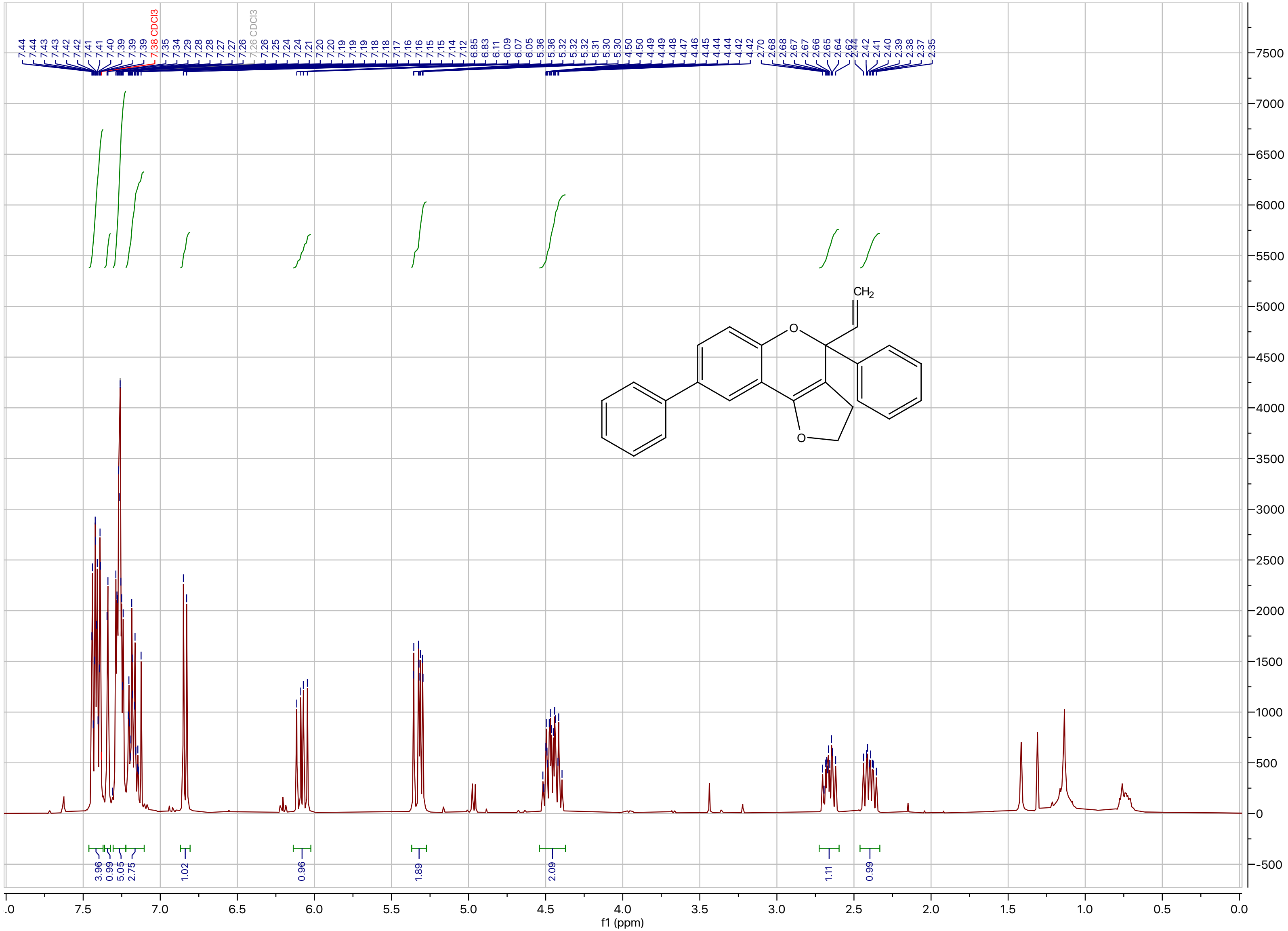
3l (400 MHz, C_6D_6)



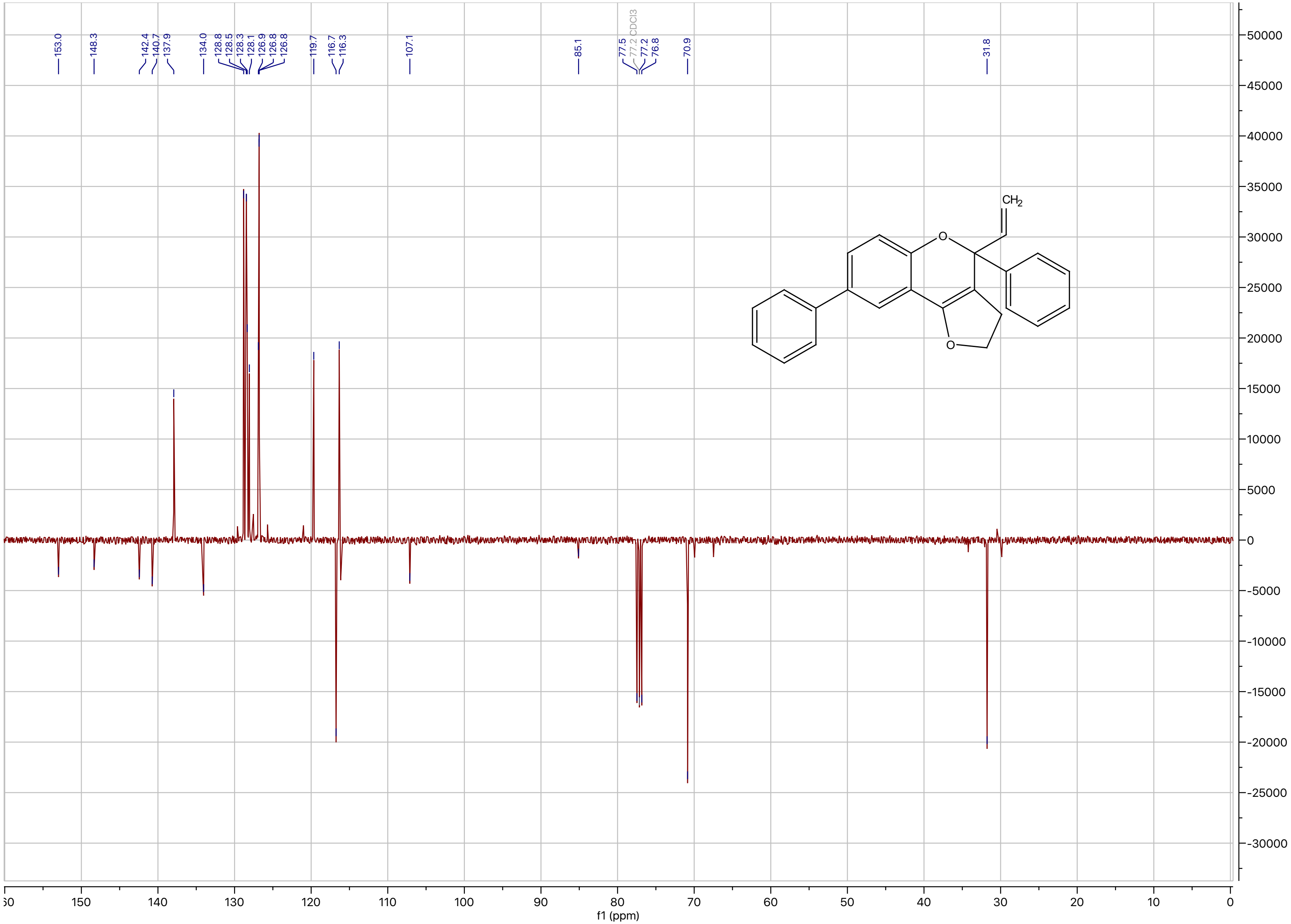
3l (101 MHz, C_6D_6)



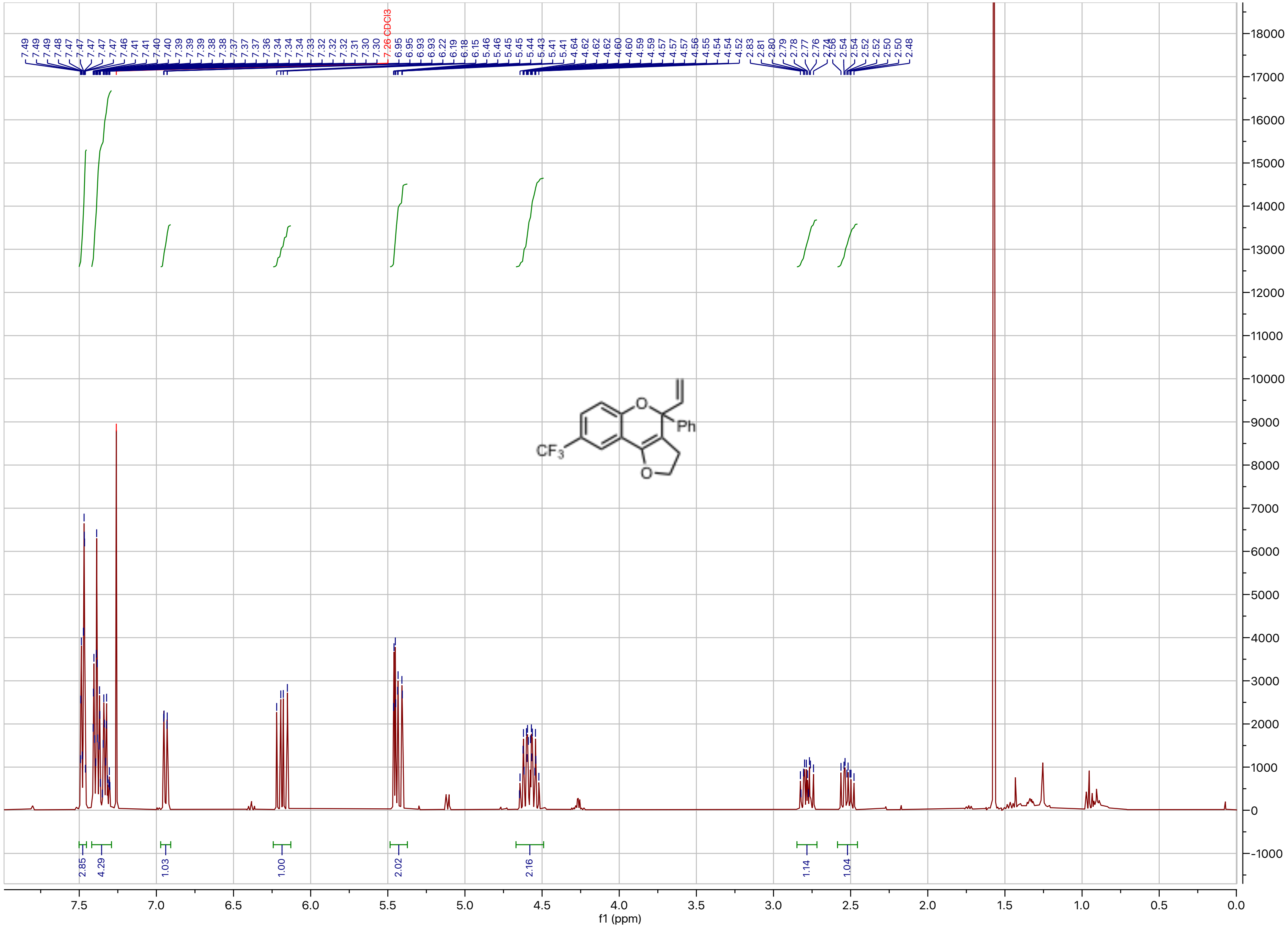
3m (400 MHz, $CDCl_3$)



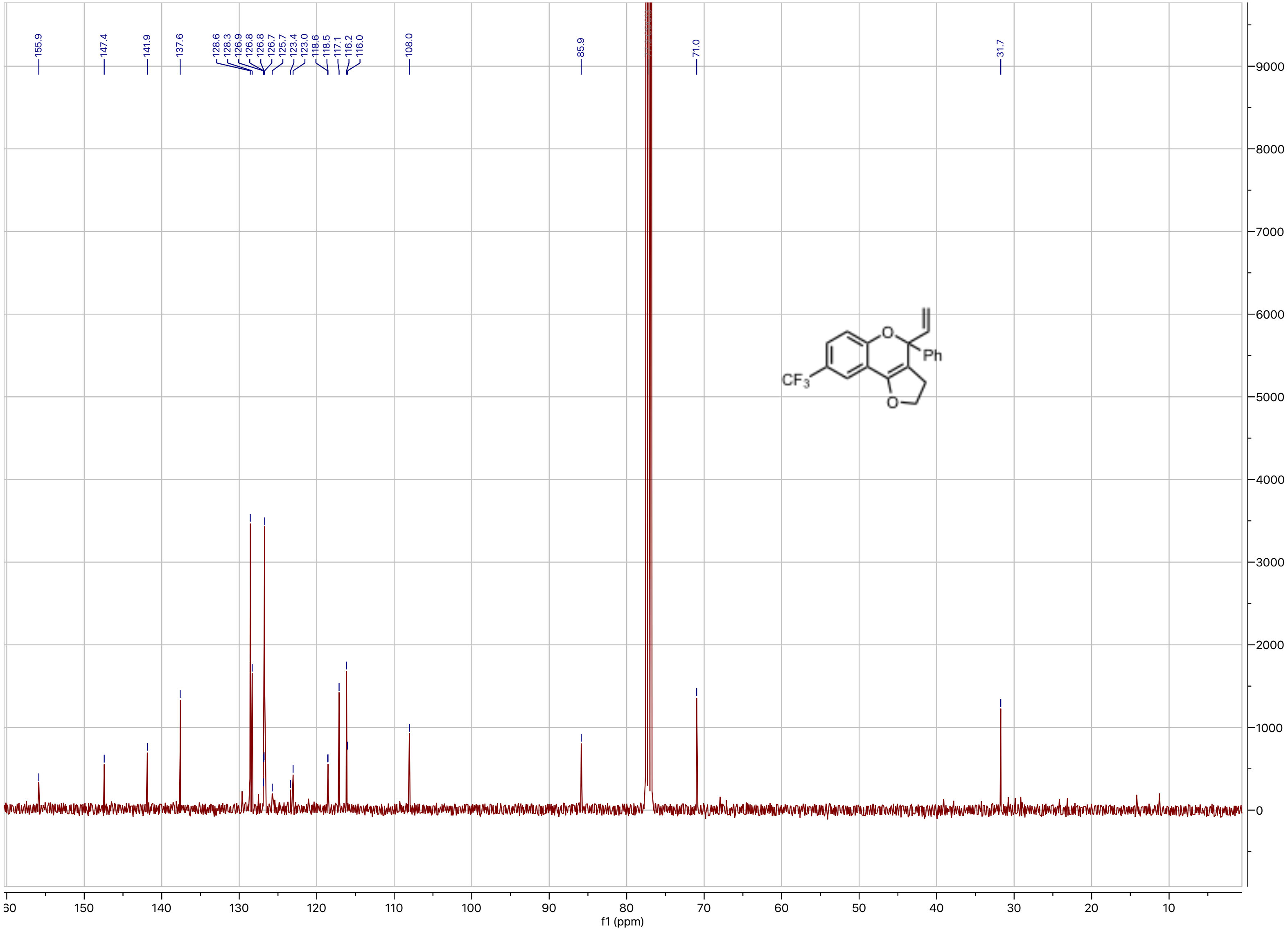
3m (101 MHz, $CDCl_3$)



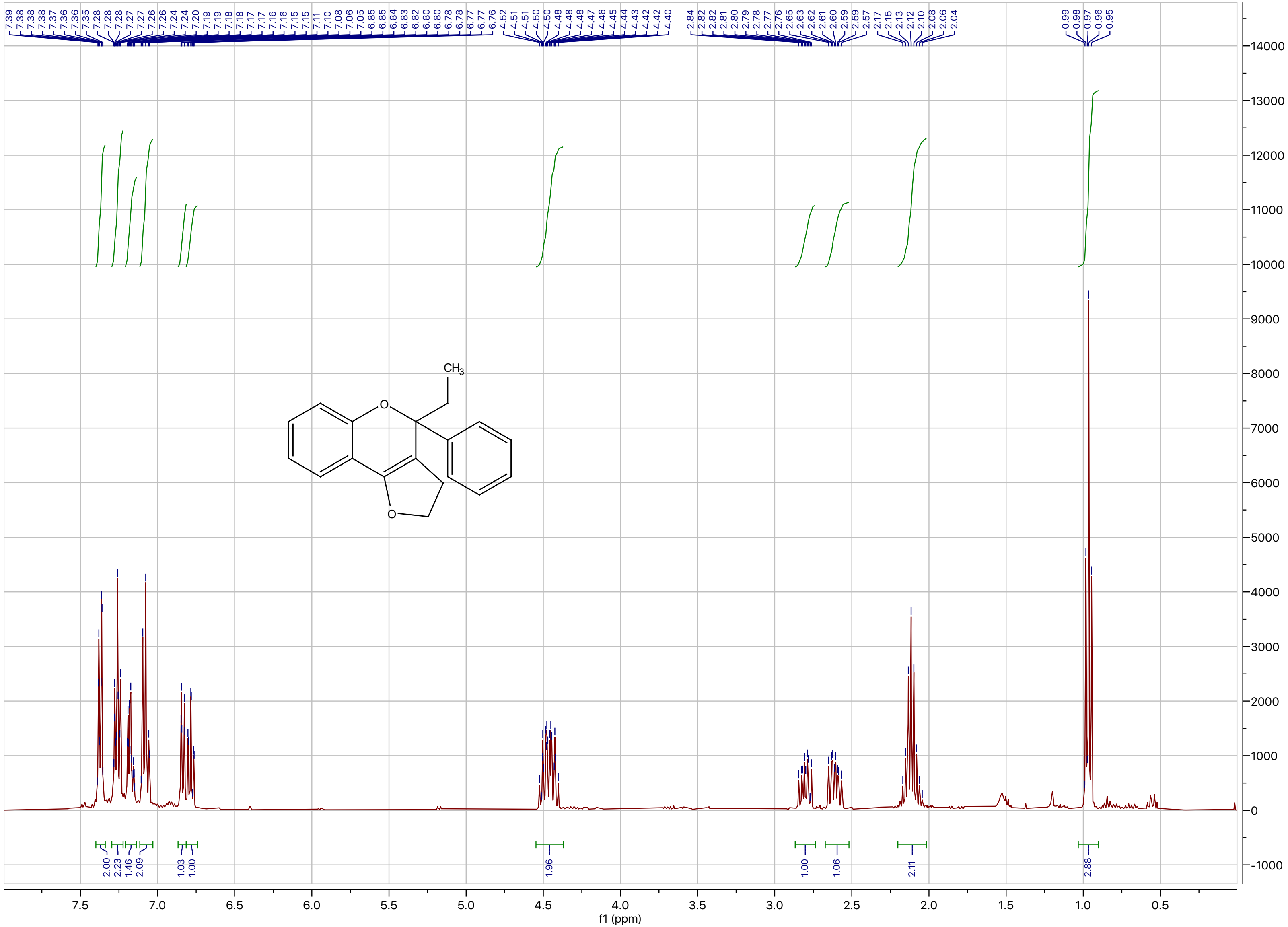
3n (400 MHz, $CDCl_3$)



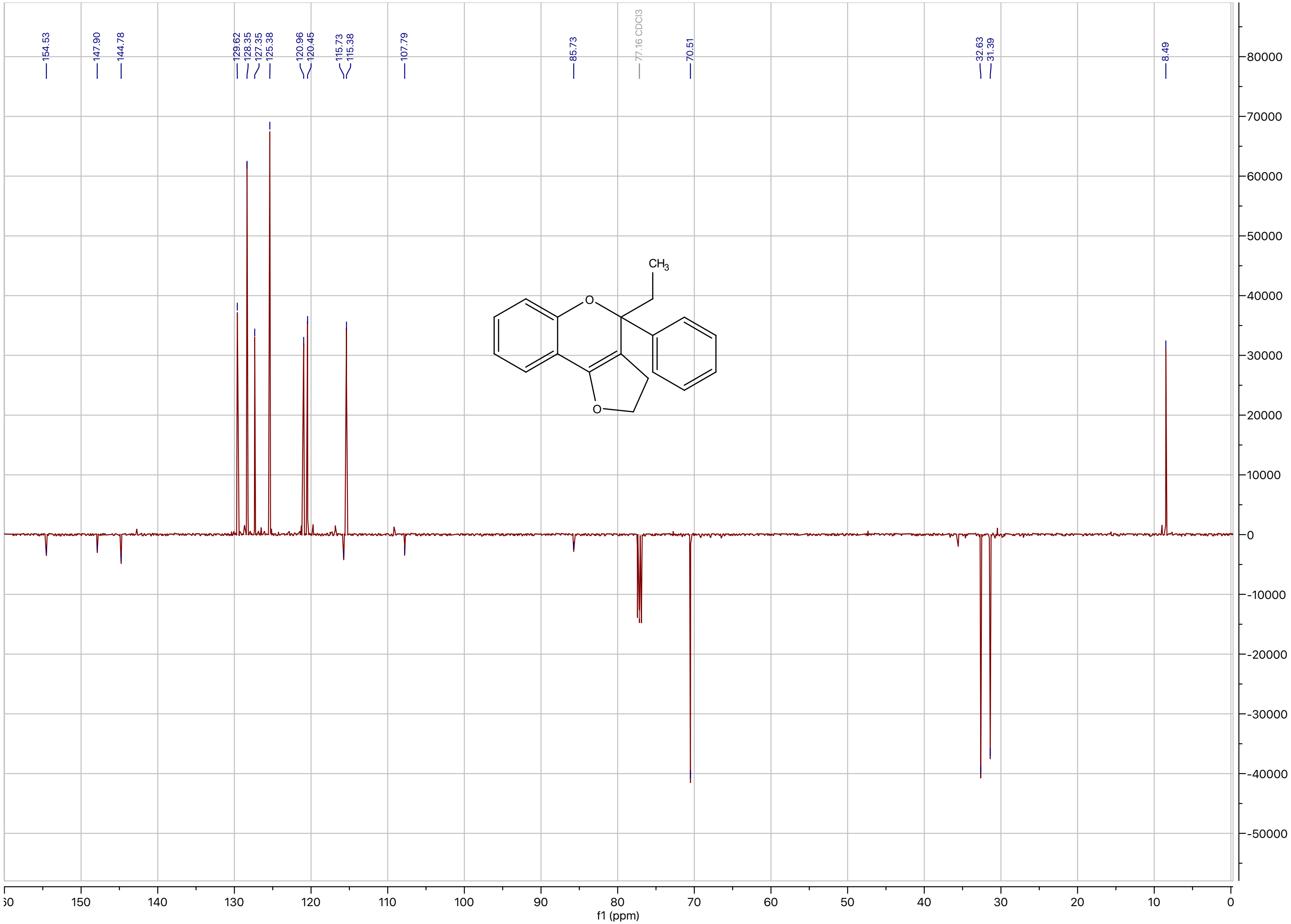
3n (101 MHz, $CDCl_3$)



12 (400 MHz, $CDCl_3$)



12 (101 MHz, $CDCl_3$)

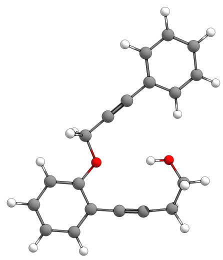


6. Computations details

Computational Details. DFT computations were carried out using the Gaussian 09 software package.[2] All structures were optimized at the B3LYP[3] level of density functional theory (DFT). The effective-core potential of Hay and Wadt with a double-ξ valence basis set (LANL2DZ) was used to describe Au.[4] The other atoms were described by the 6-31G(d,p) basis set. Thermal corrections to the Gibbs free energy were obtained at the same level of theory.[5] Single-point energy calculations were carried out at the M06 level with the quadruple-ζ valence def2-QZVP basis set on Au and the 6-311+G(2d,p) basis set on other elements. This level was also chosen to obtain the solvation energy in dioxane using the CPCM model. The values presented herein are Gibbs free energies (ΔG_{298}, kcal/mol). Compound **1a** was used as model substrate and (2-biphenyl)dimethylphosphine as model ligand (L).

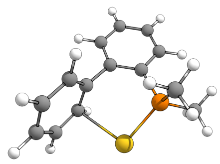
Table S1. Geometry, Energy (Hartree) and Cartesian coordinates (x,y,z) of the computed species.

1a



E(RM06) = -883.570747924
E(RM06 CPCM) = -883.5811303
Thermal correction to Gibbs Free Energy= 0.203843

LAu$^+$



E(RM06) = -1019.15893713
E(RM06 CPCM) = -1019.229938
Thermal correction to Gibbs Free Energy= 0.245742

O	0.782083	2.241517	0.41035	Au	-1.301241	-0.775318	-0.340088
C	-2.725746	1.51366	0.001861	P	0.760782	-1.410716	0.487396
C	-2.086008	2.544128	0.012134	C	1.963691	-0.103964	0.038595
C	-1.172507	3.684032	0.021649	C	0.721148	-1.556446	2.315444
C	-3.436951	0.278318	-0.003732	C	1.365022	-3.018358	-0.147181
C	-4.838509	0.228296	-0.022698	C	3.302772	-0.484707	-0.15895

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

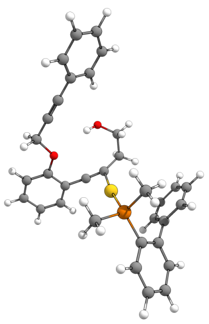
[3] (a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652. (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785-789. (c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys*. **1980**, *58*, 1200-1211. (d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem*. **1994**, *98*, 11623-11627.

[4] P. J. Hay, W. R. Wadt, *J. Chem. Phys*. **1985**, *82*, 299-310.

[5] Y. Zhao, D. G. Truhlar, The M06 Suite of Density Functionals for Main Group Thermochemistry, Thermochemical Kinetics, Noncovalent Interactions, Excited States, and Transition Elements. *Theor. Chem. Acc.* **2008**, *120*, 215-241.

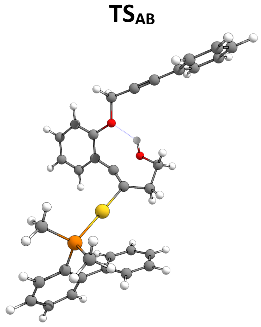
C	-2.712508	-0.941596	0.011248	C	1.598915	1.263495	-0.086004
C	-5.515882	-0.990009	-0.026342	H	0.044672	-2.365599	2.601553
H	-5.38697	1.164432	-0.034129	H	1.727938	-1.765245	2.690153
C	-4.790307	-2.178939	-0.010802	H	0.359725	-0.620426	2.744674
H	-6.600755	-1.008459	-0.040868	H	2.303762	-3.303992	0.335545
C	-3.392416	-2.161361	0.008103	H	0.61047	-3.777233	0.072474
H	-5.306383	-3.134362	-0.012763	H	1.506927	-2.963257	-1.228349
H	-2.849541	-3.098669	0.02122	H	3.599129	-1.524783	-0.074981
O	-1.353234	-0.812072	0.027759	C	4.277966	0.462075	-0.466448
C	-0.556667	-2.002651	0.029139	C	2.597458	2.194539	-0.397905
H	0.2197	1.455209	0.326345	C	0.194731	1.75463	0.096128
C	0.242286	3.251262	-0.421312	H	5.306015	0.147552	-0.613414
H	-1.113273	4.107443	1.032498	C	3.923695	1.804473	-0.586296
H	-1.533704	4.481643	-0.641228	H	4.675359	2.54908	-0.828293
C	0.846363	-1.613457	0.020827	H	2.322827	3.240282	-0.494933
C	2.012221	-1.282853	0.013678	C	-0.263134	2.191772	1.34365
C	3.384632	-0.882004	0.004856	C	-0.705693	1.757029	-0.995158
C	4.407425	-1.840951	-0.11879	H	0.425106	2.225968	2.18346
C	3.721439	0.480848	0.119341	C	-1.597173	2.583326	1.521497
H	-0.793221	-2.613023	-0.854858	C	-2.047545	2.135564	-0.811977
H	-0.786474	-2.606157	0.919765	H	-0.342741	1.507042	-1.9887
C	5.741531	-1.443041	-0.127281	H	-1.930301	2.923417	2.497035
H	4.145216	-2.890396	-0.206859	C	-2.494448	2.53893	0.455993
C	6.072044	-0.09076	-0.014205	H	-3.527042	2.84205	0.596013
H	6.524575	-2.189559	-0.222493	H	-2.719965	2.161856	-1.664542
H	0.919186	4.108198	-0.347988				
H	0.209233	2.934582	-1.474327				
C	5.060393	0.864452	0.108606				
H	2.927747	1.216236	0.216164				
H	5.315162	1.916479	0.19814				
H	7.113716	0.2166	-0.021186				

A



E(RM06) = -1902.79118906
E(RM06 CPCM) = -1902.849944
Thermal correction to Gibbs Free Energy= 0.469659

TS_{AB}



E(RM06) = -1902.77516453
E(RM06 CPCM) = -1902.828694
Thermal correction to Gibbs Free Energy= 0.471304
Frequency -183.6014

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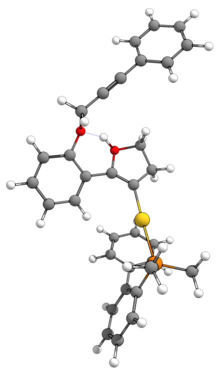
C	0.575638	1.842915	-1.428027	C	1.056995	0.854769	-0.962968
C	0.426641	0.678919	-1.848634	C	0.435493	-0.256351	-0.750714
C	0.826261	-0.396687	-2.796076	C	0.984085	-1.519843	-1.371314

Au	-0.838584	0.191814	-0.095893	Au	-1.301726	-0.212245	0.402331
C	0.817545	3.133497	-0.910509	C	1.240353	2.269454	-0.938117
C	0.000714	4.233911	-1.249157	C	0.186393	3.122693	-1.320674
C	1.948559	3.32925	-0.064337	C	2.462462	2.841503	-0.49444
C	0.293224	5.50093	-0.767431	C	0.316323	4.502892	-1.215624
H	-0.852885	4.068079	-1.8981	H	-0.73398	2.675881	-1.681101
C	1.408792	5.67966	0.059774	C	1.517465	5.04615	-0.755284
H	-0.33228	6.345866	-1.032856	H	-0.506035	5.150901	-1.49844
C	2.234036	4.611702	0.414517	C	2.593266	4.227243	-0.401919
H	1.643966	6.669982	0.437903	H	1.630163	6.123037	-0.676647
H	3.087173	4.785994	1.058439	H	3.515579	4.678234	-0.057841
O	2.663839	2.218231	0.21274	O	3.456177	1.948802	-0.207003
C	3.914156	2.338873	0.937388	C	4.74882	2.44186	0.242141
H	3.143126	0.156598	-1.324998	H	3.311707	0.546911	-1.457605
C	2.060684	-1.169833	-2.275288	C	2.479061	-1.263983	-1.637598
H	1.076313	0.070643	-3.75503	H	0.438272	-1.72024	-2.300749
H	0.001477	-1.096147	-2.961508	H	0.848274	-2.393566	-0.729204
C	4.542264	1.030212	0.945392	C	5.644064	1.308905	0.376497
C	5.07807	-0.057393	0.909159	C	6.418731	0.381726	0.485877
C	5.714673	-1.335678	0.851071	C	7.331747	-0.709073	0.618242
C	6.370275	-1.85987	1.981351	C	7.412114	-1.426048	1.828082
C	5.694329	-2.074631	-0.348383	C	8.163062	-1.074841	-0.458468
H	3.712262	2.69422	1.956365	H	4.611824	2.963133	1.197696
H	4.548833	3.079998	0.433307	H	5.133418	3.159625	-0.493685
P	-2.071999	-0.624168	1.728167	P	-3.207044	-0.203577	1.809118
C	6.999116	-3.099965	1.907799	C	8.306362	-2.485658	1.953108
H	6.386339	-1.287577	2.903326	H	6.774684	-1.140957	2.658797
C	6.977198	-3.829641	0.716345	C	9.127066	-2.842739	0.879937
H	7.508539	-3.497318	2.780388	H	8.366032	-3.032452	2.889124
H	2.30432	-1.938852	-3.014831	H	2.849978	-1.861798	-2.474067
H	1.805358	-1.679019	-1.334098	H	3.073266	-1.475596	-0.74365
C	6.323296	-3.31577	-0.40663	C	9.053702	-2.136272	-0.32347
H	5.180444	-1.664841	-1.212653	H	8.104808	-0.519106	-1.38881
H	6.308493	-3.882109	-1.333042	H	9.693757	-2.411433	-1.156063
H	7.470559	-4.795477	0.663081	H	9.824552	-3.668553	0.982165
C	-3.895765	-0.575131	1.557319	C	-4.851869	-0.027699	1.005827
C	-1.567955	-2.342497	2.152045	C	-3.288256	-1.689895	2.897881
C	-1.647162	0.328431	3.243365	C	-3.077598	1.180846	3.018823
C	-4.663977	-0.102169	2.635758	C	-5.853456	0.680377	1.694197
C	-4.542565	-0.957991	0.357076	C	-5.125556	-0.524122	-0.292805
H	-0.510992	-2.337071	2.432375	H	-2.399607	-1.708883	3.53485
H	-2.167273	-2.718191	2.986173	H	-4.184708	-1.656735	3.523505
H	-1.697489	-2.990586	1.28523	H	-3.301455	-2.598242	2.294217
H	-2.078619	-0.125502	4.139424	H	-3.81876	1.1065	3.818627
H	-0.558676	0.329611	3.33943	H	-2.079635	1.141455	3.462623
H	-1.989895	1.361183	3.151701	H	-3.190631	2.137519	2.504105
H	-4.186863	0.1997	3.560934	H	-5.663994	1.067448	2.689206
C	-6.050559	-0.001798	2.541067	C	-7.100859	0.914374	1.120669

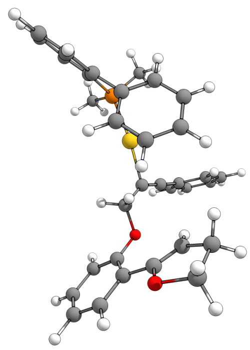
C	-5.937731	-0.837898	0.28194	C	-6.384137	-0.25974	-0.857792
C	-3.827102	-1.493451	-0.843743	C	-4.170397	-1.334962	-1.105073
H	-6.623251	0.364326	3.38714	H	-7.85616	1.462025	1.675361
C	-6.688969	-0.366218	1.357357	C	-7.363275	0.449748	-0.166971
H	-7.76808	-0.287191	1.269524	H	-8.328346	0.630933	-0.630022
H	-6.434267	-1.13141	-0.637752	H	-6.594722	-0.642032	-1.851778
C	-3.413857	-2.834046	-0.897865	C	-3.777731	-2.620175	-0.697624
C	-3.652425	-0.685693	-1.980085	C	-3.728829	-0.861219	-2.35187
H	-3.595906	-3.48499	-0.04742	H	-4.163313	-3.027552	0.232065
C	-2.823423	-3.350956	-2.053157	C	-2.953744	-3.405097	-1.506695
C	-3.066278	-1.20474	-3.136633	C	-2.905182	-1.645569	-3.160649
H	-3.993288	0.345429	-1.958198	H	-4.039757	0.124069	-2.687053
H	-2.524503	-4.394448	-2.08475	H	-2.677862	-4.404862	-1.184499
C	-2.648142	-2.537612	-3.174783	C	-2.514339	-2.919187	-2.739842
H	-2.209789	-2.946092	-4.080498	H	-1.89082	-3.537779	-3.378673
H	-2.952723	-0.572451	-4.012338	H	-2.581173	-1.266744	-4.125625

B



E(RM06) = -1902.77844192
E(RM06 CPCM) = -1902.832125
Thermal correction to Gibbs Free Energy= 0.47144

C



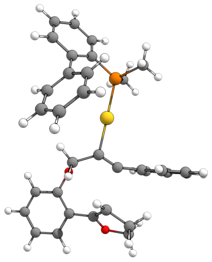
E(RM06) = -1902.81607774
E(RM06 CPCM) = -1902.874469
Thermal correction to Gibbs Free Energy= 0.471295

C	-0.651224	-0.320932	0.605505	C	4.100115	-0.589139	1.55402
C	-6.101152	0.437407	-0.665225	C	0.887997	2.242138	-0.168511
C	-1.271229	0.854451	0.67028	C	4.586495	-1.472278	0.661312
C	-1.081596	2.232167	0.215653	C	4.690341	-1.440762	-0.804468
C	0.20283	2.781845	0.063076	C	5.550241	-2.349525	-1.449184
C	0.371487	4.0769	-0.420737	C	5.717353	-2.336122	-2.831679
C	-0.739453	4.86282	-0.736744	C	5.027968	-1.406933	-3.61208
C	-2.02666	4.350944	-0.56848	C	4.160751	-0.503477	-2.997787
H	-0.608564	5.877948	-1.097204	H	5.16248	-1.382791	-4.689
H	1.371836	4.481423	-0.534232	H	6.39323	-3.046233	-3.29771
H	1.062156	2.17945	0.337222	H	6.091615	-3.062445	-0.839103
C	-2.184765	3.048584	-0.107782	C	3.991488	-0.522581	-1.614988
O	-3.46683	2.513242	0.091183	O	3.119026	0.412107	-1.0578
H	-2.900345	4.957761	-0.783033	H	3.614633	0.235237	-3.576457
O	-2.55658	0.719036	1.464063	O	5.119846	-2.600608	1.244904
C	-1.473942	-1.365618	1.350647	C	4.289827	-1.134779	2.950086
H	-3.234613	1.327531	0.975358	H	3.669118	0.368912	1.309574
C	-5.287876	1.318639	-0.856578	C	0.906795	1.041425	-0.513137

C	-7.063013	-0.597394	-0.453933	C	0.834161	3.601423	0.209184
C	-4.330321	2.379422	-1.095623	C	1.789384	-0.084887	-0.92126
Au	1.145042	-0.743492	-0.294437	Au	-1.256872	0.741199	-0.430497
H	-3.691744	2.165717	-1.960334	H	1.740314	-0.872087	-0.158086
H	-4.828747	3.341025	-1.255779	H	1.434382	-0.50757	-1.870366
C	-6.828468	-1.897865	-0.943446	C	0.909532	3.963029	1.574714
C	-7.772175	-2.900582	-0.73899	C	0.900948	5.304542	1.933933
H	-5.912616	-2.106077	-1.488039	H	0.97805	3.184929	2.327577
C	-2.857504	-0.728643	1.528995	C	5.190096	-2.359803	2.671951
H	-3.335596	-0.899102	2.492603	H	4.873996	-3.273959	3.179002
H	-3.543536	-0.953743	0.708934	H	6.236671	-2.157637	2.927341
H	-1.005011	-1.590155	2.31651	H	3.335019	-1.418081	3.418698
H	-1.546295	-2.307489	0.801297	H	4.773016	-0.423786	3.629206
C	-8.257971	-0.323836	0.240053	C	0.752785	4.607332	-0.782368
C	-9.195363	-1.333843	0.438975	C	0.747533	5.944975	-0.408535
H	-8.440324	0.678649	0.612533	H	0.704123	4.320677	-1.827643
C	-8.954871	-2.621337	-0.048598	C	0.820269	6.292398	0.945444
H	-10.11576	-1.116391	0.971588	H	0.690754	6.719223	-1.166544
H	-9.689689	-3.405286	0.106651	H	0.816757	7.339685	1.232043
H	-7.588286	-3.899858	-1.121679	H	0.961261	5.586069	2.980088
P	3.156255	-1.309078	-1.440881	P	-3.555111	0.259145	-0.563344
C	4.710932	-0.452622	-0.94799	C	-4.003277	-1.513229	-0.42552
C	3.527144	-3.116877	-1.408205	C	-4.544044	1.204971	0.669365
C	2.94857	-0.974542	-3.242965	C	-4.211768	0.849901	-2.177642
C	5.683708	-0.221982	-1.937027	C	-5.07506	-1.985711	-1.204714
C	4.936637	0.027646	0.365948	C	-3.281267	-2.421599	0.387545
H	5.53078	-0.585364	-2.947196	H	-5.63817	-1.306531	-1.834972
C	6.852591	0.481963	-1.65685	C	-5.432201	-3.331765	-1.198903
H	7.586619	0.644222	-2.439906	H	-6.264185	-3.671777	-1.807139
C	7.063476	0.979594	-0.372262	C	-4.708714	-4.232223	-0.418719
C	6.114797	0.749929	0.621253	C	-3.648614	-3.776214	0.361589
H	7.966416	1.536481	-0.140095	H	-4.971216	-5.285522	-0.411513
H	6.289323	1.115782	1.628321	H	-3.096872	-4.473697	0.984055
C	4.009465	-0.195658	1.515235	C	-2.156115	-2.028767	1.287557
C	3.764806	-1.484252	2.016531	C	-2.380176	-1.237624	2.425795
C	3.435006	0.902051	2.178056	C	-0.862676	-2.529763	1.058943
H	4.250687	-2.339113	1.555591	H	-3.387703	-0.903378	2.654798
C	2.952734	-1.672604	3.137225	C	-1.334474	-0.93307	3.299817
H	2.79004	-2.675381	3.52119	H	-1.52926	-0.33391	4.184353
C	2.3765	-0.574097	3.77786	C	-0.050908	-1.423201	3.053689
H	1.757831	-0.718884	4.65867	H	0.759059	-1.197802	3.740723
C	2.621486	0.714027	3.296746	C	0.181995	-2.227103	1.934944
H	2.189655	1.574688	3.799136	H	1.174633	-2.627192	1.749832
H	3.634182	1.905956	1.813683	H	-0.682804	-3.164225	0.195667
H	2.685942	-3.659811	-1.848474	H	-4.412839	2.274213	0.482279
H	4.437125	-3.331916	-1.975703	H	-5.602731	0.94527	0.579474
H	3.657098	-3.455197	-0.378901	H	-4.200142	0.981209	1.679429
H	3.754677	-1.399817	-3.846505	H	-5.303265	0.806362	-2.214845

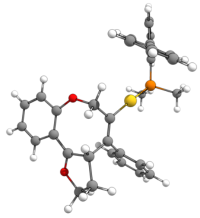
H	2.002632	-1.425743	-3.557206	H	-3.898731	1.888632	-2.308476
H	2.891694	0.102278	-3.4168	H	-3.793295	0.254809	-2.992082

TS_{CD}



E(RM06) = -1902.79717349
E(RM06 CPCM) = -883.6073239
Thermal correction to Gibbs Free Energy= 0.246486
Frequency -207.9203

D

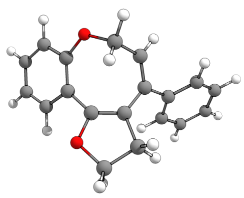


E(RM06) = -1902.83705245
E(RM06 CPCM) = -1902.891218
Thermal correction to Gibbs Free Energy= 0.482255

C	3.94613	0.074691	1.071311	C	3.70052	-4.172752	-2.236306
C	1.825918	0.916791	0.286762	C	4.878892	-3.40146	-2.300907
C	4.622891	-0.582438	0.060921	C	4.989261	-2.297151	-1.498469
C	4.511018	-1.951108	-0.461857	C	3.966082	-1.894856	-0.56781
C	5.699955	-2.702579	-0.561721	C	2.768953	-2.702468	-0.510035
C	5.681043	-4.021745	-0.997969	C	2.684859	-3.820612	-1.375663
C	4.470669	-4.61262	-1.371473	C	4.271013	-0.708396	0.169428
C	3.289397	-3.876816	-1.312939	C	3.625712	-0.070741	1.364837
H	4.449086	-5.639364	-1.723419	C	2.295723	0.525263	0.836785
H	6.6066	-4.585232	-1.053281	C	1.18421	-0.244284	0.8001
H	6.636566	-2.235271	-0.278361	C	1.276697	-1.672366	1.272541
C	3.301214	-2.553477	-0.867486	C	2.122053	3.017467	1.175943
O	2.143478	-1.821477	-0.988239	C	5.562085	1.160792	0.616348
H	2.346167	-4.298345	-1.644239	C	4.708321	0.915442	1.856416
O	5.680008	0.103394	-0.406616	C	2.337355	1.927881	0.315992
C	4.813174	1.243298	1.499758	C	2.598504	2.182858	-1.040763
H	3.331531	-0.462855	1.778706	C	2.651482	3.492702	-1.522212
C	1.044319	-0.096369	0.200767	C	2.440918	4.567854	-0.655505
C	2.100068	2.317072	0.180172	C	2.170632	4.326883	0.693136
C	1.368228	-1.567265	0.191551	H	3.58715	-5.051942	-2.863293
Au	-0.954323	0.519085	-0.16321	H	5.685587	-3.675947	-2.971123
H	1.926548	-1.84304	1.095257	H	5.889893	-1.698905	-1.539131
H	0.462588	-2.177119	0.15878	H	1.770228	-4.399448	-1.320629
C	1.957165	3.168387	1.297173	H	3.422469	-0.819023	2.128167
C	2.184998	4.53619	1.166052	H	1.959118	-1.84494	2.113952
H	1.650273	2.747873	2.249561	H	0.300628	-2.054729	1.565864
C	5.773096	1.375092	0.306287	H	6.639292	1.160017	0.785293
H	6.820897	1.519929	0.573319	H	5.271547	2.041774	0.042743
H	5.467113	2.155998	-0.394628	H	5.300956	0.448809	2.647643
H	5.347573	0.99466	2.425667	H	4.28145	1.840865	2.243253
H	4.264972	2.171311	1.682032	H	2.74313	1.350523	-1.72417
C	2.494686	2.862869	-1.061348	H	2.851581	3.672321	-2.574534
C	2.72813	4.228875	-1.178925	H	2.482798	5.586193	-1.029878
H	2.604641	2.20529	-1.917643	H	1.995494	5.157475	1.370506

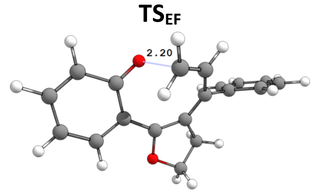
C	2.573171	5.066529	-0.067741	H	1.89504	2.83378	2.222609
H	3.024921	4.645302	-2.136424	O	5.28511	0.004295	-0.252832
H	2.754206	6.132611	-0.165116	O	1.641914	-2.586029	0.196892
H	2.062461	5.188594	2.024847	Au	-0.634551	0.424811	0.087135
P	-3.156314	1.195019	-0.695631	P	-2.660615	1.309477	-0.826309
C	-4.464448	-0.095349	-0.703049	C	-4.12316	0.207533	-1.02958
C	-3.755885	2.576221	0.369233	C	-4.959332	0.404771	-2.14317
C	-3.159963	1.941781	-2.37989	H	-4.765974	1.218312	-2.833329
C	-5.50781	0.03155	-1.63813	H	-6.669542	-0.255885	-3.266711
C	-4.434834	-1.227247	0.149219	C	-6.040992	-0.434391	-2.399889
H	-5.549301	0.889753	-2.299421	C	-6.300216	-1.502636	-1.543251
C	-6.502377	-0.936436	-1.751666	C	-5.486965	-1.70709	-0.431653
H	-7.296506	-0.811904	-2.480928	H	-7.13575	-2.169443	-1.733003
C	-6.461573	-2.062683	-0.931588	H	-5.700242	-2.524677	0.250052
C	-5.439287	-2.198646	0.003996	C	-4.40105	-0.863365	-0.143991
H	-7.225865	-2.829353	-1.012986	C	-3.627671	-1.152651	1.10011
H	-5.418954	-3.064466	0.658536	C	-3.607388	-0.248295	2.173462
C	-3.412327	-1.458474	1.211773	H	-4.151573	0.687652	2.093851
C	-3.303172	-0.602398	2.319361	C	-2.947719	-0.563713	3.362628
C	-2.603666	-2.607092	1.168854	H	-2.955127	0.143716	4.1865
H	-3.966633	0.253076	2.401763	C	-2.307789	-1.79631	3.503069
C	-2.397576	-0.874828	3.346623	H	-1.81129	-2.049952	4.435054
H	-2.340284	-0.21084	4.204027	C	-2.332986	-2.711881	2.447552
C	-1.592257	-2.013487	3.287508	H	-1.85763	-3.682828	2.556535
H	-0.901027	-2.234918	4.095184	C	-2.986817	-2.392858	1.256294
C	-1.700492	-2.880678	2.197323	H	-3.007826	-3.108283	0.439322
H	-1.093863	-3.780851	2.154974	C	-3.259736	2.816763	0.057789
H	-2.69179	-3.287564	0.326783	H	-2.469256	3.572116	0.034375
H	-3.085382	3.431244	0.246723	H	-4.158932	3.213817	-0.42154
H	-4.771788	2.864744	0.084528	H	-3.47935	2.581607	1.099943
H	-3.746236	2.274695	1.417409	C	-2.299108	1.971611	-2.51035
H	-4.102135	2.445187	-2.610661	H	-3.110358	2.588337	-2.905476
H	-2.351915	2.676486	-2.419631	H	-1.397943	2.585326	-2.433147
H	-2.963748	1.170316	-3.127646	H	-2.097063	1.147779	-3.198479

E



E(RM06) = -883.649955562
E(RM06 CPCM) = -883.6579542
Thermal correction to Gibbs Free Energy= 0.256951

TS_{EF}

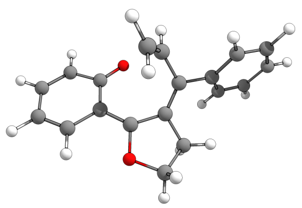


E(RM06) = -883.611811442
E(RM06 CPCM) = -883.6231194
Thermal correction to Gibbs Free Energy= 0.253471
Frequency -235.7489

C	-4.194974	1.074341	-1.527582	O	-1.469039	-1.883695	0.547307
C	-3.880965	-0.250166	-1.846277	C	-0.512307	-2.018545	-1.425559
C	-2.854768	-0.87858	-1.160169	C	-2.477143	-1.122222	0.423562
C	-2.092628	-0.23588	-0.155815	C	-2.362377	0.28516	0.062286
C	-2.436236	1.100748	0.165324	C	-3.572041	1.055746	-0.015112

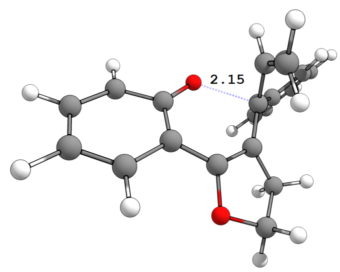
C	-3.484195	1.727993	-0.535275	C	-4.804393	0.504755	0.221853
C	-1.02594	-1.076813	0.437055	C	-4.921439	-0.872927	0.552826
C	0.291625	-0.878352	0.688517	C	-3.803371	-1.655696	0.627503
C	1.025238	0.386833	0.619812	H	-5.903611	-1.299925	0.739859
C	0.502822	1.513473	1.153243	H	-5.694963	1.121414	0.14867
C	-0.778737	1.545665	1.92634	H	-3.500122	2.102892	-0.275756
C	3.415824	1.176436	0.452414	C	-1.127404	0.970406	-0.170499
C	-0.23843	-3.17833	0.877148	H	-3.854311	-2.711285	0.874774
C	0.891036	-2.183508	1.188967	C	0.280746	0.686517	-0.192074
C	2.359395	0.394958	-0.043267	O	-1.320725	2.324583	-0.297748
C	2.585302	-0.376838	-1.19522	C	1.087246	-0.44681	-0.398285
C	3.820624	-0.354925	-1.840129	C	0.968104	2.055943	-0.043649
C	4.858964	0.43402	-1.34128	C	0.726948	-1.70281	-0.950263
C	4.651715	1.198813	-0.191924	C	2.536675	-0.33804	-0.033006
H	-4.99392	1.594523	-2.048021	H	1.46587	-2.493712	-0.861043
H	-4.429573	-0.78328	-2.61601	H	-1.215271	-1.25051	-1.720689
H	-2.608587	-1.90918	-1.38773	H	-0.740521	-3.03019	-1.743026
H	-3.71644	2.750149	-0.25629	C	3.535864	-0.639092	-0.97232
H	1.016792	2.461089	1.014249	C	4.885161	-0.577397	-0.624053
H	-0.964664	0.590347	2.426157	H	3.247807	-0.910871	-1.983693
H	-0.748278	2.333527	2.683707	C	-0.084363	2.978352	-0.62408
H	-0.465444	-3.870742	1.690741	H	-0.005666	3.061021	-1.716659
H	-0.034093	-3.757695	-0.03194	H	-0.117473	3.978716	-0.188377
H	1.110962	-2.127009	2.264589	H	1.919858	2.11347	-0.572601
H	1.826257	-2.447736	0.686582	H	1.154723	2.300213	1.009307
H	1.772846	-0.978021	-1.593101	C	2.926446	0.006191	1.271463
H	3.971539	-0.950619	-2.735907	C	4.27415	0.055281	1.623412
H	5.823193	0.448496	-1.840845	H	2.162359	0.209591	2.015705
H	5.457586	1.80606	0.210408	C	5.258607	-0.230881	0.675167
H	3.268071	1.751946	1.361152	H	4.555803	0.310347	2.640933
O	-1.422947	-2.381162	0.63462	H	6.308765	-0.189153	0.948718
O	-1.924588	1.912264	1.133002	H	5.644212	-0.802701	-1.367629

F



E(RM06) = -883.625691507
E(RM06 CPCM) = -883.6383646
Thermal correction to Gibbs Free Energy= 0.252049

TS$_{FG}$

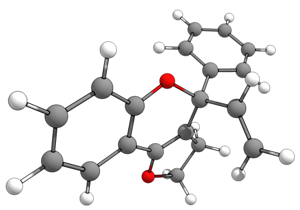


E(RM06) = -883.615806259
E(RM06 CPCM) = -883.6273191
Thermal correction to Gibbs Free Energy= 0.25283
Frequency -213.2367

O	-1.110502	-1.738517	0.863732	O	0.417247	-1.600845	0.005227
C	-0.109527	-1.168081	-2.361446	C	-0.805144	0.048532	0.633527
C	-2.194023	-1.18132	0.612962	C	1.650471	-1.288105	-0.157708

C	-2.319873	0.184015	0.038998	C	2.205326	0.048217	0.019756
C	-3.635402	0.717908	-0.214514	C	2.58063	-2.304265	-0.559034
C	-4.765678	0.004999	0.050683	C	3.604943	0.255708	-0.081865
C	-4.665596	-1.305865	0.624221	C	1.308789	1.151104	-0.010883
C	-3.455171	-1.859975	0.903417	C	4.468241	-0.779896	-0.358321
H	-5.577453	-1.859893	0.835698	H	3.981103	1.263816	0.061897
H	-5.743021	0.423368	-0.168101	C	3.935456	-2.066725	-0.60787
H	-3.707214	1.71193	-0.641027	H	5.538797	-0.610352	-0.407415
C	-1.22299	1.027178	-0.131415	H	4.609187	-2.887063	-0.84416
H	-3.362259	-2.852448	1.332813	H	2.171739	-3.291885	-0.744735
C	0.221198	0.850088	0.004743	C	-0.082806	1.114586	0.060447
O	-1.488717	2.34946	-0.327107	O	1.768165	2.35436	-0.447746
C	0.985021	-0.222393	-0.353049	C	-0.598182	2.346134	-0.670111
C	0.745919	2.226875	0.389648	C	0.631433	3.256407	-0.528237
C	0.460543	-1.339505	-1.163726	C	-0.492667	-0.443397	1.990987
C	2.430762	-0.291631	-0.025765	C	0.089798	0.291264	2.944996
H	0.643261	-2.338826	-0.780077	H	0.388042	1.319722	2.770396
H	-0.266732	-0.17975	-2.783159	H	0.285826	-0.123193	3.928758
H	-0.441548	-2.015032	-2.953856	C	-2.164186	-0.259008	0.119191
C	3.347425	-0.80911	-0.959097	H	-1.489271	2.785279	-0.213813
C	4.704559	-0.890303	-0.656124	H	-0.824838	2.152812	-1.726438
H	2.985484	-1.134914	-1.928994	H	-0.809304	-1.461238	2.197188
C	-0.256579	3.107189	-0.35483	C	-3.255106	-0.405057	0.991199
H	0.034852	3.265982	-1.400306	C	-2.376128	-0.409645	-1.261529
H	-0.462618	4.070932	0.114	C	-4.530007	-0.670745	0.492979
H	1.777609	2.396998	0.079371	H	-3.103341	-0.28845	2.05969
H	0.67526	2.408682	1.469315	C	-4.728782	-0.813275	-0.88077
C	2.915057	0.112325	1.231598	H	-5.366754	-0.769302	1.178181
C	4.271219	0.021041	1.537105	H	0.594321	3.844216	0.397323
H	2.214398	0.46322	1.982102	H	0.808574	3.922768	-1.373583
C	5.171926	-0.474721	0.592396	C	-3.646759	-0.687265	-1.756497
H	4.623526	0.326633	2.517966	H	-1.525413	-0.347886	-1.931802
H	6.229042	-0.545426	0.830981	H	-3.793643	-0.815718	-2.824807
H	5.398411	-1.2813	-1.394563	H	-5.720252	-1.02906	-1.26807

G



E(RM06) = -883.650642072
E(RM06 CPCM) = -883.6581416
Thermal correction to Gibbs Free Energy= 0.254003

O	0.292475	-1.30132	0.262897
C	-0.556967	-0.161715	0.641709
C	1.635557	-1.132478	0.067845
C	2.191286	0.11102	-0.299679

C	2.450087	-2.259788	0.167218
C	3.562929	0.207651	-0.556795
C	1.240395	1.196525	-0.40442
C	4.37763	-0.91802	-0.451375
H	3.973552	1.170579	-0.842336
C	3.816967	-2.146871	-0.091968
H	5.44181	-0.839785	-0.649678
H	4.447545	-3.027149	-0.007642
H	2.001137	-3.207485	0.444617
C	-0.033922	1.099791	0.003727
O	1.582077	2.389163	-0.975458
C	-0.75668	2.380325	-0.342585
C	0.43274	3.266248	-0.800288
C	-0.550534	-0.138363	2.165017
C	-0.047148	0.830794	2.926459
H	0.394319	1.723703	2.494141
H	-0.05119	0.75544	4.009539
C	-1.955424	-0.496078	0.104608
H	-1.288461	2.830454	0.503392
H	-1.497467	2.228022	-1.138619
H	-0.975025	-1.0318	2.619848
C	-3.095953	0.006662	0.741805
C	-2.108735	-1.250523	-1.06433
C	-4.367603	-0.241651	0.222107
H	-2.989163	0.589748	1.651704
C	-4.513831	-0.999219	-0.939647
H	-5.242577	0.153712	0.730175
H	0.698157	4.011749	-0.04204
H	0.260755	3.776788	-1.750244
C	-3.379826	-1.503563	-1.579263
H	-1.228735	-1.646594	-1.557573
H	-3.484081	-2.097081	-2.483161
H	-5.502805	-1.197522	-1.342511