Supporting Information

Asymmetric Induction via a Helically Chiral Anion: Enantioselective PCCP Brønsted Acid-Catalyzed Inverse Electron-Demand Diels-Alder Cycloaddition of Oxocarbenium Ions.

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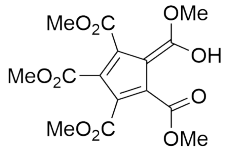
General information

All reactions were performed open to the atmosphere, unless otherwise noted. Organic solutions were concentrated using a Buchi rotary evaporator. Methylene chloride, diethyl ether, benzene and toluene were dried using a J.C. Meyer solvent purification system. All other solvents and commercial reagents were used as provided. Flash column chromatography was performed employing 40-63 μm silica gel (SiliaFlash® P60 from Silicycle). Thin-layer chromatography (TLC) was performed on 250 μm glass-backed silica plates (SiliaPlateTM G TLC from Silicycle).

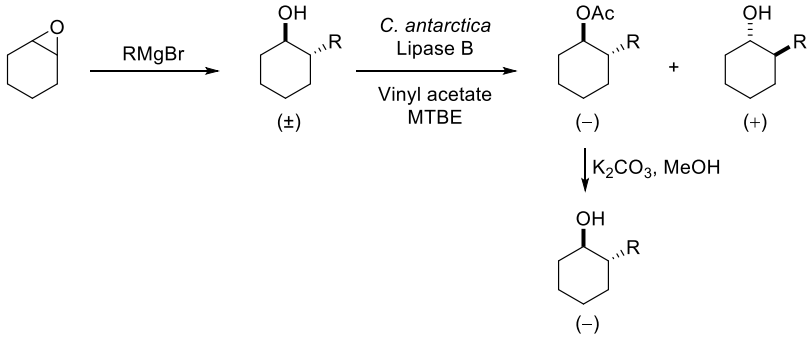
^{1}H and ^{13}C NMR spectra were recorded in $CDCl_3$ (except where noted) on Bruker DRX-300, DRX-400 or DRX-500 spectrometers as noted. Data for ^{1}H NMR are reported as follows: chemical shift (δ ppm), multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, p = pentet, dd = doublet of doublets, td = triplet of doublets, m = multiplet), coupling constant (Hz), integration, and assignment. All ^{1}H-NMR experiments were measured relative to the signals of tetramethylsilane (TMS, 0.00 ppm) or residual chloroform (7.26 ppm). Data for ^{13}C are reported in terms of chemical shift relative to deuterochloroform (77.16 ppm). Data for ^{19}F are reported in terms of chemical shift relative to hexafluorobenzene (-164.90 ppm). Optical rotations were measured using a Jasco DIP-1000 digital polarimeter. High-resolution mass spectra were obtained from the Columbia University Mass Spectrometry Facility on a Waters XEVO G2XS QToF mass spectrometer equipped with a UPC2 SFC inlet, electrospray ionization (ESI) probe, atmospheric pressure chemical ionization (APCI) probe, and atmospheric solids analysis probe (ASAP). Low-resolution mass spectrometry (LRMS) was performed on a Waters SQD2 quadrupole mass spectrometer equipped with a UPC2 SFC inlet and a dual ESI/APCI probe.

Preparation of Pentakis(methoxycarbonyl)cyclopentadiene



Cyclopentadiene acid **2** was prepared according to the procedure by Bruce and White[1] to produce 50.68 g of **2** (61% overall yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 20.08 (s, 1H, O**H**), 4.04 (s, 6H, CO_2Me x 2), 3.90 (s, 6H, CO_2Me x 2), 3.77 (s, 3H, CO_2Me). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 167.8, 163.2, 133.7, 117.7, 106.4, 55.7, 52.6, 51.9. IR (thin film, cm^{-1}) 1725, 1710, 1602, 1456, 1351, 1211, 1093, 1073, 986, 933, 793, 759, 701, 604.

General procedure for epoxide opening & kinetic resolution of cyclohexanol derivatives

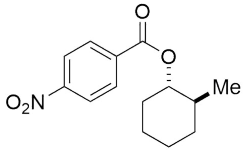


Arylhalide (1.2 equiv.) was dissolved in dry THF (1 mL/mmol) with activated magnesium turnings (1.4 equiv; these were washed first with 1 M HCl followed by deionized H_2O, acetone, and diethyl ether). A drop of 1,2-dibromo ethane was added to the solution mixture. This solution was refluxed for 1 h or until all the Mg was dissolved. The reaction was then cooled down to -30 °C and CuCN (0.05 equiv) was added at this temperature. Cyclohexene oxide (1.0 equiv) as a solution in THF (0.1 mL/mmol) was syringe pumped into the reaction flask over 1.5 h. This reaction mixture was then warmed to room temperature and stirred for 2 h. The reaction was quenched with sat. NH_4Cl and extracted into ether. The crude material was purified with column chromatography.

The pure racemic alcohol (1.0 equiv.) and vinyl acetate (10.0 equiv.) were dissolved in MTBE (8.14 mL/mmol with respect to the alcohol). ^{1}H-NMR was taken prior to adding *Candia antarctica* Lipase B (50 mg/mmol with respect to the alcohol). After 24 h, the reaction was checked by ^{1}H-NMR to monitor the conversion of alcohol. If complete or close to 50% conversion, the reaction was filtered, concentrated *in vacuo*, and purified via column chromatography. The acetylated alcohol has a higher R_f than the free alcohol.

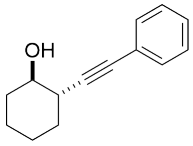
The acetylated alcohol (1.0 equiv) was deprotected by dissolving the alcohol in MeOH (4.38 mL/mmol) and adding crushed K_2CO_3 (3.0 equiv). This was stirred at room temperature for 24 h and extracted out of EtOAc-H_2O to obtain the free alcohol. This was not further purified and used as is. In the case of 2-alkylcyclohexyl alcohols, these were further derivatized with 4-nitrobenzoyl chloride to determine the ee.

(1*S*,2*S*)-2-methylcyclohexyl 4-nitrobenzoate:



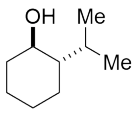
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.33-8.17 (m, 4H, Ar**H**), 4.71 (td, *J* = 10.1, 4.5 Hz, 1H, C**H**O), 2.17-1.07 (m, 9H), 0.97 (d, *J* = 6.6 Hz, 3H, C**H$_3$**). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.5, 150.6, 136.4, 130.7, 123.6, 80.5, 37.5, 33.6, 31.8, 25.3, 24.8, 18.6. HPLC analysis: Chiralpak AD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 8.0 min (major), >99% ee.

(1*R*,2*S*)-2-(phenylethynyl)cyclohexan-1-ol:



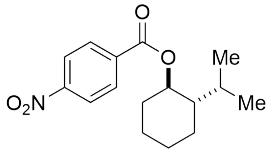
The general procedure was followed to obtain the title product as a colorless oil (from deprotected alcohol, 0.720g, 29% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48-7.21 (m, 5H, Ar**H**), 3.65-3.51 (m, 1H, C**H**OH), 2.47 (ddd, J = 11.6, 9.3, 3.8 Hz, 1H, C**H**C ≡CPh), 2.34 (d, J = 2.3 Hz, 1H, O**H**), 2.19-2.01 (m, 2H), 1.87-1.68 (m, 2H), 1.59-1.18 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 131.9, 128.4, 128.1, 123.5, 91.0, 82.9, 73.7, 39.8, 33.3, 31.2, 25.0, 24.3. $[\alpha]_D^{23}$ = –38.20 (1.0 c, MeOH). HPLC analysis: Chiralpak AD-H (Hex/IPA = 96/4, 1.0 mL/min, 254 nm, 23 °C) 11.4 min (minor), 12.6 min (major), 98% ee.

(1*R*,2*S*)-2-isopropylcyclohexan-1-ol:



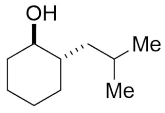
The general procedure was followed to obtain the title product as a white solid (from deprotected alcohol, 0.240 g, 16% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.39 (td, J = 10.0, 4.2 Hz, 1H, C**H**OH), 2.17 (pd, J = 7.0, 3.0 Hz, 1H), 1.98 (dd, J = 7.5, 5.5, 3.8, 1.7 Hz, 1H), 1.80-1.57 (m, 3H), 1.43 (s, 1H, O**H**), 1.33-1.06 (m, 4H), 1.02-0.88 (m, 4H), 0.82 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 72.0, 50.7, 36.4, 26.1, 25.9, 25.2, 23.8, 21.0, 16.4. $[\alpha]_D^{23}$ = –9.40 (1.0 c, MeOH). IR (thin film, cm^{-1}) 3324, 2943, 2831, 1448, 1114, 1021, 619.

(1*R*,2*S*)-2-isopropylcyclohexyl 4-nitrobenzoate:



^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32-8.18 (m, 4H, Ar**H**), 4.97 (td, *J* = 10.2, 4.4 Hz, 1H, C**H**O), 2.23-1.07 (m, 10H), 0.93 (d, *J* = 6.9 Hz, 3H, CH_3), 0.82 (d, *J* = 7.0 Hz, 3H, CH_3). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 150.6, 136.4, 130.8, 123.6, 76.5, 47.7, 32.3, 26.8, 25.4, 24.8, 24.3, 20.8, 16.9. HPLC analysis: Chiralpak AD-H (Hex/IPA = 99/1, 1.0 mL/min, 254 nm, 23 °C) 6.9 min (minor), 7.8 min (major), 99% ee.

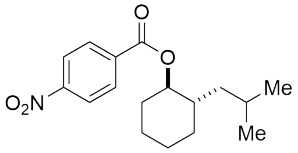
(1*R*,2*S*)-2-isobutylcyclohexan-1-ol:



The general procedure was followed to obtain the title product as a white solid (from deprotected alcohol, 0.658 g, 26% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 3.16 (td, J = 9.4, 4.5 Hz, 1H, C**H**OH), 2.14-0.57 (m, 19H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 75.5, 43.0, 42.1, 35.8, 30.4, 25.7, 25.1, 25.0,

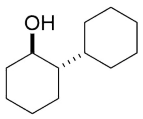
24.4, 21.8. $[\alpha]_D^{23}$ = –56.88 (1.0 c, MeOH).

(1*R*,2*S*)-2-isobutylcyclohexyl 4-nitrobenzoate:



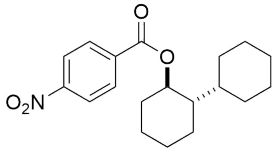
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.32-8.17 (m, 4H, Ar**H**), 4.76 (td, J = 9.7, 4.2 Hz, 1H, C**H**O), 2.16-0.96 (m, 12H), 0.92-0.80 (m, 6H, C**H$_3$** x 2). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.4, 150.6, 136.4, 130.7, 123.6, 79.4, 42.0, 39.7, 31.7, 30.5, 25.2, 25.0, 24.5, 24.0, 21.9. HPLC analysis: Chiralpak AD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 6.7 min (minor), 9.7 min (major), 93% ee.

(1*S*,2*R*)-[1,1'-bi(cyclohexan)]-2-ol:



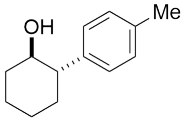
The general procedure was followed to obtain the title product as a colorless oil (from deprotected alcohol, 0.840 g, 39% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.45-3.26 (m, 1H, C**H**OH), 2.03-0.58 (m, 21H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 71.3, 50.9, 37.3, 36.5, 31.7, 27.5, 27.3, 27.09, 27.07, 26.1, 25.5, 25.1. $[\alpha]_D^{23}$ = –44.00 (1.0 c, MeOH). IR (thin film, cm^{-1}) 3334, 2921, 2851, 1448, 1352, 1287, 1196, 1053, 984, 922, 895, 851.

(1*S*,2*R*)-[1,1'-bi(cyclohexan)]-2-yl 4-nitrobenzoate:



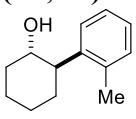
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.28-8.08 (m, 4H, Ar**H**), 4.93 (td, *J* = 10.1, 4.3 Hz, 1H, C**H**O), 2.05 (dt, *J* = 12.0, 4.0 Hz, 1H), 1.82-0.82 (m, 19H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.3, 150.6, 136.4, 130.8, 123.6, 75.9, 47.6, 38.0, 32.3, 31.3, 27.9, 27.2, 27.0, 26.8, 25.8, 25.5, 24.6. HPLC analysis: Chiralpak AD-H (Hex/IPA = 99/1, 1.0 mL/min, 254 nm, 23 °C) 10.2 min (minor), 17.8 min (major), >99% ee.

(1*R*,2*S*)-2-(*p*-tolyl)cyclohexan-1-ol:



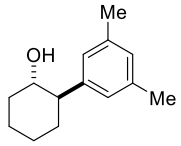
The general procedure was followed to obtain the title product as a white solid (from deprotected alcohol, 0.200 g, 40% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.14 (s, 4H, Ar**H**), 3.62 (td, J = 10.0, 4.2 Hz, 1H, C**H**OH), 2.39 (ddd, J = 12.4, 10.0, 3.6 Hz, 1H, C**H**Ar), 2.33 (s, 3H, C**H$_3$**), 2.14-2.07 (m, 1H, C**H**), 1.88-1.79 (m, 2H, C**H$_2$**), 1.79-1.69 (m, 1H, C**H**), 1.56 (s, 1H, O**H**), 1.54-1.25 (m, 4H, C**H$_2$** x 2). ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.3, 136.5, 129.6, 127.9, 74.6, 52.9, 34.6, 33.5, 26.2, 25.2, 21.2. $[\alpha]_D^{23}$ = –58.05 (1.0 c, MeOH). HPLC analysis: Chiralpak AD-H (Hex/IPA = 96/4, 1.0 mL/min, 254 nm, 23 °C) 8.6 min, 9.9 min, >99% ee.

(1*S*,2*R*)-2-(*o*-tolyl)cyclohexan-1-ol:



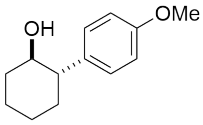
The general procedure was followed to obtain the title product as a clear oil (from recovered alcohol, 0.857 g, 43% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.40-7.03 (m, 4H), 3.88-3.66 (m, 1H), 2.78 (ddd, J = 11.7, 9.9, 3.5 Hz, 1H), 2.37 (s, 3H), 2.20-2.07 (m, 1H), 1.93-1.69 (m, 3H), 1.63-1.52 (m, 1H), 1.51-1.28 (m, 3H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 141.5, 137.3, 130.8, 126.7, 126.4, 125.6, 74.5, 48.0, 34. 7, 33.3, 26.4, 25.3, 20.0. $[\alpha]_D^{23}$ = +28.70 (1.0 c, MeOH). HPLC analysis: Chiralpak OD-H (Hex/IPA = 99.5/0.5, 1.0 mL/min, 254 nm, 23 °C) 34.3 min (minor), 35.2 min (major), 94% ee.

(1*S*,2*R*)-2-(3,5-dimethylphenyl)cyclohexan-1-ol:



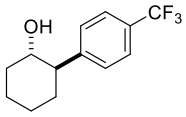
The general procedure was followed to obtain the title product as a white solid (from recovered alcohol, 0.723 g, 36% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (s, 3H, Ar**H**), 3.63 (td, *J* = 10.1, 4.2 Hz, 1H, C**H**OH), 2.41-1.09 (m, 16H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.2, 138.3, 128.6, 125.8, 74.5, 53.2, 34.5, 33.4, 26.2, 25.2, 21.5. $[\alpha]_D^{23}$ = +36.36 (1.0 c, MeOH).HPLC analysis (of ROAc): Chiralpak OJ-H (Hex/IPA = 98/2, 1.0 mL/min, 254 nm, 23 °C) 10.0 min (minor), 10.8 min (major), 97% ee.

(1*R*,2*S*)-2-(4-methoxyphenyl)cyclohexan-1-ol:



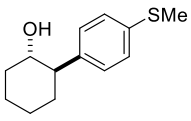
The general procedure was followed to obtain the title product as a white solid (from deprotected alcohol, 0.800 g, 47% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22-7.11 (m, 2H, Ar**H**), 6.93-6.79 (m, 2H, Ar**H**), 3.79 (s, 3H, OMe), 3.65-3.48 (m, 1H, C**H**OH), 2.48-2.24 (m, 1H, C**H**Ar), 2.10 (m, 1H, C**H**), 1.92-1.69 (m, 3H, C**H₂** + C**H**), 1.58 (d, *J* = 2.0 Hz, 1H, O**H**), 1.54-1.21 (m, 4H, C**H₂** x 2). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.6, 135.3, 128.9, 114.3, 74.7, 55.4, 52.5, 34.6, 33.6, 26.3, 25.2. IR (thin film, cm^{-1}) 3568, 3403, 3004, 2922, 2853, 1611, 1581, 1510, 1447, 1324, 1302, 1279, 1243, 1177, 1126, 1059, 1032, 962, 898, 828, 786, 752, 577. $[\alpha]_D^{23}$ = –51.83 (1.0 c, MeOH). HPLC analysis: Chiralpak OJ-H (Hex/IPA = 97:3, 1.0 mL/min, 230 nm, 23 °C) 25.6 min (major), >99% ee.

(1*S*,2*R*)-2-(4-(trifluoromethyl)phenyl)cyclohexan-1-ol:



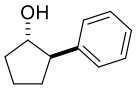
The general procedure was followed to obtain the title product as a white solid (from recovered alcohol, 0.570 g, 39% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.0 Hz, 2H, Ar**H**), 7.36 (d, *J* = 8.0 Hz, 2H, Ar**H**), 3.74-3.57 (m, 1H, C**H**OH), 2.50 (ddd, *J* = 12.8, 10.0, 3.6 Hz, 1H, C**H**Ar), 2.10 (ddt, *J* = 9.3, 3.1, 2.0 Hz, 1H), 1.94-1.71 (m, 3H), 1.61-1.21 (m, 5H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, [129.6, 129.3, 128.9, 128.6], 128.3, [125.74, 125.70, 125.67, 125.63], 123.0, 74.3, 53.1, 35.0, 33.4, 26.0, 25.1. IR (thin film, cm^{-1}) 3373, 2932, 2858, 1618, 1449, 1419, 1324, 1161, 1119, 1068, 1019, 962, 833, 822, 755, 657. $[\alpha]_D^{23}$ = +46.80 (1.0 c, MeOH). HPLC analysis: Chiralpak OJ-H (Hex/IPA = 96:4, 1.0 mL/min, 230 nm, 23 °C) 9.2 min (minor), 14.2 min (major), 98% ee.

(1*R*,2*S*)-2-(4-(methylthio)phenyl)cyclohexan-1-ol:



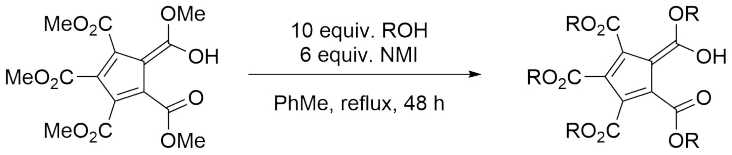
The general procedure was followed to obtain the title product as a white solid (from recovered alcohol, 0.959 g, 46% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.28-7.16 (m, 4H, ArH), 3.63 (td, J = 10.0, 4.2 Hz, 1H, C**H**OH), 2.50 (s, 3H, SMe), 2.41 (ddd, J = 12.3, 9.9, 3.5 Hz, 1H, C**H**Ar), 2.16-2.07 (m, 1H), 1.92-1.74 (m, 3H), 1.61 (s, 1H), 1.57-1.29 (m, 4H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 140.4, 136.6, 128.5, 127.3, 74.5, 52.8, 34.6, 33.4, 26.1, 25.1, 16.2. IR (thin film, cm^{-1}) 3428, 2920, 2852, 1497, 1448, 1406, 1345, 1323, 1307, 1264, 1201, 1096, 1057, 1014, 958, 809, 779. $[\alpha]_D^{23}$ = +53.00 (1.0 c, MeOH). HPLC analysis: Chiralpak AD-H (Hex/IPA = 90/10, 1.0 mL/min, 254 nm, 23 °C) 8.7 min (major), >99% ee.

(1*S*,2*R*)-2-phenylcyclopentan-1-ol:

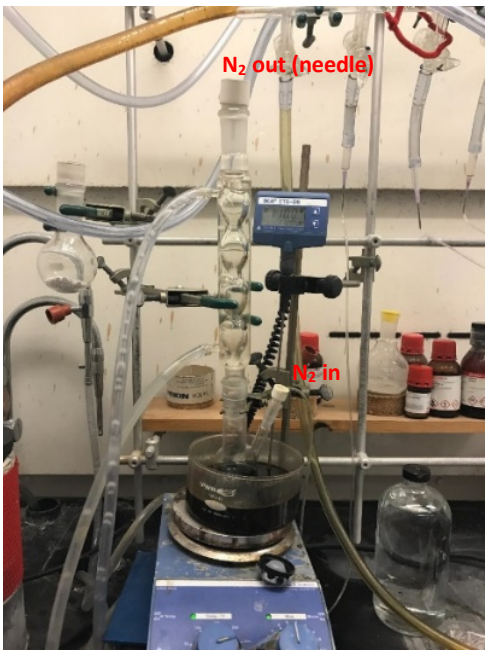


The general procedure was followed to obtain the title product as a white solid (from recovered alcohol, 0.911 g, 46% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.13 (m, 5H, Ar**H**), 4.16 (q, J = 7.1 Hz, 1H, C**H**OH), 2.94-2.72 (m, 1H, C**H**Ar), 2.25-2.00 (m, 2H, C**H₂**), 1.97-1.59 (m, 5H, C**H₂** x 2 + O**H**). ^{13}C NMR (100 MHz, $CDCl_3$) δ 143. 5, 128.7, 127.5, 126.5, 80.6, 54.6, 34.2, 32.0, 21.9. $[\alpha]_D^{23}$ = +71.88 (1.0 c, MeOH). HPLC analysis: Chiralpak OD-H (Hex/IPA = 97/3, 1.0 mL/min, 254 nm, 23 °C) 10.7 min (major), >99% ee.

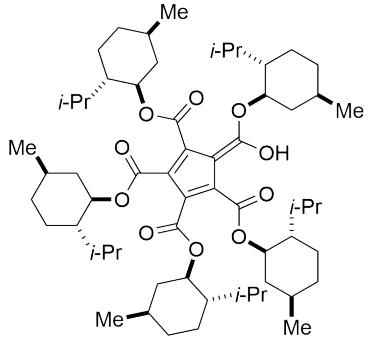
General Procedure for Transesterification



Cyclopentadiene **2** (1.0 equiv), alcohol (10 equiv), and *N*-methylimidazole (6.0 equiv) were dissolved in toluene (0.1 M) in a flame-dried two-neck round-bottom flask. A steady flow of N_2 allowed for the removal of methanol (see photo below). The reaction solution was refluxed for 48 hours while being monitored by SFC-MS. Upon completion, the reaction solution was cooled down to room temperature and concentrated *in vacuo*. The crude material was purified by silica gel column chromatography (0 → 5% MeOH/CH_2Cl_2). The purified material was subsequently washed with 1 M HCl/CH_2Cl_2 (3 x), dried with anhydrous magnesium sulfate, and concentrated *in vacuo* to yield the title product. The transesterified PCCPs were stored in a sealed vial in the freezer.

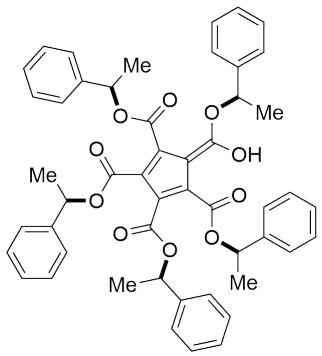


Pentakis((1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (4):



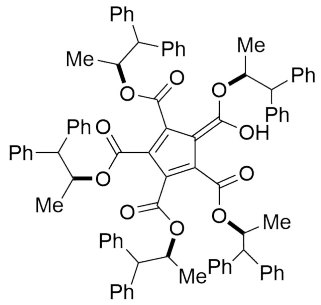
The general procedure was followed using cyclopentadiene (0.100 g, 0.281 mmol, 1.0 equiv), (1*R*,2*S*,5*R*)-(−)-Menthol (0.439 g, 2.807 mmol, 10 equiv), and *N*-methylimidazole (0.134 mL, 1.684 mmol, 6.0 equiv) dissolved in 2.81 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.262 g, 96% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 20.30 (s, 1H, O**H**), 5.39-4.41 (m, 5H, CO_2C**H** x 5), 2.85-0.28 (m, 90H, Alkyl **H**). ^{13}C NMR (100 MHz, CDCl3) δ 172.1, 167.0, 162.6, 134.3, 118.9, 106.5, 81.3, 77.5, 77.2, 76.8, 76.7, 75.7, 47.5, 46.3, 46.2, 41.6, 40.8, 40.3, 34.6, 34.5, 34.1, 32.0, 31.7, 31.6, 25.6, 25.44, 25.36, 23.34, 23.30, 23.2, 23.1, 22.6, 22.4, 22.3, 22.2, 21.9, 21.3, 21.0, 16.8, 16.1, 15.8. IR (thin film, cm^{-1}) 2952, 2868, 1734, 1704, 1590, 1454, 1410, 1387, 1370, 1319, 1213, 1178, 980, 963, 904, 640. $[\alpha]_D^{23}$ = –56.3 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{60}H_{95}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 975.6931, found *m/z* 975.6951.

Pentakis((*R*)-1-phenylethan-1-ol) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (5):



Cyclopentadiene (0.350 g, 0.982 mmol) and 50 µL of DMF are dissolved in 5.0 mL $SOCl_2$ under an inert atmosphere of N_2. After refluxing for 5 h, the $SOCl_2$ is distilled off and the remaining yellow semisolid is dried under high vacuum. 5.0 mL of dry CH_2Cl_2 is then added to the flask and (*R*)-1-phenylethanol is added. The mixture is stirred for 30 minutes and then concentrated *in vacuo*. The crude material was purified by silica gel chromatography (0 → 10% MeOH/CH_2Cl_2), washed with 1 M HCl/CH2Cl2 (3 x), and dried with anhydrous MgSO4 to yield the title product as a light yellow solid (0.126 g, 16% y).^{1}H NMR (500 MHz, $CDCl_3$) δ 19.86 (s, 1H, O**H**), 7.81-6.74 (m, 25H, Ar**H**), 6.30-5.56 (m, 5H, C**H**O x 5), 1.83-1.08 (m, 15H, C**H$_3$** x 5). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.4, 166.5, 162.3, 142.1, 141.7, 139.9, 133.9, 128.5, 128.3, 127.8, 127.4, 126.64, 126.2, 125.9, 118.5, 106.8, 78.8, 74.2, 72.9, 29.8, 23.0, 22.1, 21.9. IR (thin film, cm^{-1}) 3032, 2980, 2931, 1709, 1604, 1494, 1451, 1405, 1197, 1060, 1028, 759, 698. $[\alpha]_D^{23}$ = +4.50 (1.0 c, $CHCl_3$). LRMS (ESI-) exact mass calc'd for $C_{50}H_{45}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 805.30, found *m/z* 805.63.

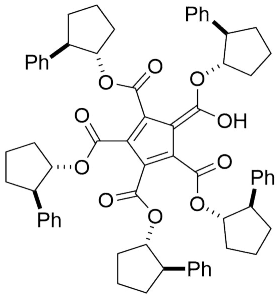
Pentakis((*S*)-1,1-diphenylpropan-2-yl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (6):



The general procedure was followed using cyclopentadiene (0.118 g, 0.331 mmol, 1.0 equiv), (*S*)-1,1-diphenylpropan-2-ol (0.702 g, 3.307 mmol, 10 equiv), and *N*-methylimidazole

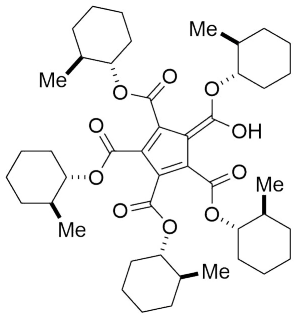
(0.158 mL, 0.1.984 mmol, 6.0 equiv) dissolved in 1.4 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 8% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.299 g, 72% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 19.66 (s, 1H, O**H**), 7.72-6.54 (m, 50H, Ar**H**), 6.02-5.10 (m, 5H, Ph_2C**H** x 5), 4.60-3.37 (m, 5H, OC**H** x 5), 1.79-0.67 (m, 15H, CH_3 x 5). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.3, 166.5, 162.5, 160.9, 160.8, 159.8, 142.2-140.3, 139.3, 134.9, 133.6, 130.4, 129.0-126.4, 118.7, 106.7, 78.6, 74.8, 74.4, 74.1, 73.9, 71.9, 59.5, 57.2, 57.1, 56.9, 56.6, 56.5, 56.4, 54.7, 29.8, 19.4, 19.2, 19.1, 19.0, 18.8, 18.5, 17.8. IR (thin film, cm^{-1}) 3027, 1731, 1598, 1494, 1452, 1406, 1321, 1238, 1046, 756, 700. $[\alpha]_D^{23}$ = +4.92 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{85}H_{75}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1255.5366, found *m/z* 1255.5364.

Pentakis((1*S*,2*R*)-2-phenyl-1-cyclopentanol) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (7):



The general procedure was followed using cyclopentadiene (0.200 g, 0.561 mmol, 1.0 equiv), (1*S*,2*R*)-2-phenyl-1-cyclopentanol (0.911 g, 5.614 mmol, 10 equiv), and *N*-methylimidazole (0.268 mL, 3.368 mmol, 6.0 equiv) dissolved in 5.6 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.300 g, 53% yield). ^{1}H NMR (400 MHz, $CDCl_3$) 19.82 (s, 1H, O**H**), 7.30-7.12 (m, 25H, Ar**H**), 5.38-5.35 (m, 5H, OC**H** x 5), 3.53-3.04 (5H, C**H**Ph x 5), 2.19-0.88 (m, 30H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 166.8, 162.6, 143.7, 141.9, 128.6, 127.5, 126.7, 126.3, 106.8, 87.9, 84.6, 82.4, 51.0, 34.8, 34.7, 32.6, 32.3, 31.9, 31.7, 27.1, 25.4, 24.0, 23.3, 22.8, 20.9, 14.3. IR (thin film, cm^{-1}) 3027, 2958, 2873, 1731, 1703, 1596, 1493, 1453, 1411, 1329, 1213, 1193, 1141, 1090, 1060, 1029, 939, 844, 755, 699. $[\alpha]_D^{23}$ = –5.2 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{65}H_{65}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1005.4583, found *m/z* 1005.4574.

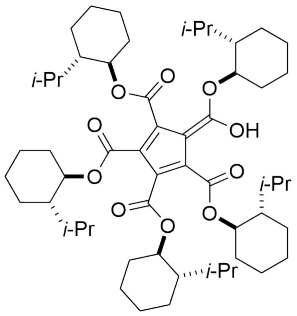
Pentakis((1*S*,2*S*)-2-methyl-1-cyclohexanol) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (8):



The general procedure was followed using cyclopentadiene (0.150 g, 0.421 mmol, 1.0 equiv), (1*S*,2*S*)-2-methyl-1-cyclohexanol (0.385 g, 3.368 mmol, 8.0 equiv), and *N*-methylimidazole (0.201 mL, 2.526 mmol, 6.0 equiv) dissolved in 4.2 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 10% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.273 g, 85% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 20.24 (s, 1H, O**H**), 4.82-4.34 (m, 5H, C**H**O x 5), 2.49-0.67 (m, 60H, alkyl **H**). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.2, 166.9, 162.9, 134.1, 118.7, 106.7, 85.4, 79.8, 79.1, 37.4, 37.3, 36.3, 33.8, 32.8, 31.9, 31.7, 30.8, 25.7, 25.4, 25.0, 24.9, 24.5, 24.2, 18.7. IR (thin

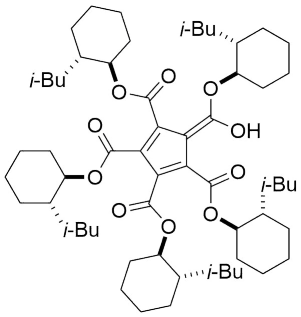
film, cm^{-1}) 2930, 2857, 1733, 1704, 1593, 1453, 1411, 1373, 1352, 1336, 1305, 1215, 1192, 1156, 1130, 1054, 1054, 999, 984, 912, 756, 640, 568. $[\alpha]_D^{23}$ = +70.12 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{45}H_{65}O_{10}^-$ $[M\text{-}H^+]^-$ requires m/z 765.4583, found *m/z* 765.4579.

Pentakis((1*R*,2*S*)-2-isopropyl-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (9):



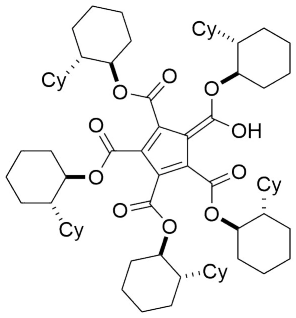
The general procedure was followed using cyclopentadiene (80.0 mg, 0.225 mmol, 1.0 equiv), (1*R*,2*S*)-2-isopropyl-1-cyclohexanol (0.240 g, 1.688 mmol, 7.5 equiv), and *N*-methylimidazole (0.108 mL, 1.350 mmol, 6.0 equiv) dissolved in 3.0 mL toluene (0.075 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a beige solid (0.169 g, 83% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 20.32 (s, 1H, O**H**), 5.04-4.81 (m, 5H, OC**H** x 5), 2.21-0.75 (m, 80H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 166.8, 162.7, 134.2, 118.9, 106.6, 81.4, 75.3, 75.0, 47.1, 46.0, 32.3, 32.1, 29.8, 25.8, 25.7, 25.6, 25.4, 25.1, 25.0, 23.8, 23.6, 23.5, 23.3, 21.5, 21.1, 21.0, 20.9, 20.7, 18.8, 16.2, 15.9. IR (thin film, cm^{-1}) 2934, 2862, 1732, 1594, 1453, 1410, 1370, 1336, 1322, 1222, 1192, 1138, 1054, 1010, 978, 907, 861, 757. $[\alpha]_D^{23}$ = –67.0 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{55}H_{85}O_{10}^-$ $[M\text{-}H^+]^-$ requires *m/z* 905.6148, found *m/z* 905.6143.

Pentakis((1*R*,2*S*)-2-isobutyl-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (10):



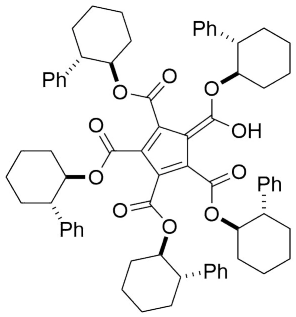
The general procedure was followed using cyclopentadiene (0.200 g, 0.561 mmol, 1.0 equiv), (1*R*,2*S*)-2-isobutyl-1-cyclohexanol (0.658 g, 4.208 mmol, 7.5 equiv), and *N*-methylimidazole (0.268 mL, 3.368 mmol, 6.0 equiv) dissolved in 5.6 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a beige solid (0.283 g, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 20.26 (s, 1H, O**H**), 4.81-4.61 (m, 5H, OC**H** x 5), 2.19-0.82 (m, 90H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 166.6, 162.9, 134.3, 118.8, 106.7, 84.4, 78.0, 60.1, 41.1, 40.9, 40.9, 40.6, 40.4, 39.3, 39.2, 39.0, 37.4, 34.8, 31.7, 31.4, 29.8, 29.7, 29.4, 28.3, 25.4, 25.0, 25.0, 24.9, 24.8, 24.6, 24.6, 24.4, 24.3, 24.3, 24.0, 23.1, 22.0, 21.5, 21.2. IR (thin film, cm^{-1}) 2932, 2865, 1734, 1594, 1454, 1411, 1367, 1333, 1309, 1218, 1190, 1134, 1084, 1057, 1024, 996, 909, 758, 639. $[\alpha]_D^{23}$ = –61.8 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{60}H_{95}O_{10}^-$ $[M\text{-}H^+]^-$ requires *m/z* 975.6931, found *m/z* 975.6939.

Pentakis((1*S*,2*R*)-[1,1'-bi(cyclohexan)]-2-yl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (11):



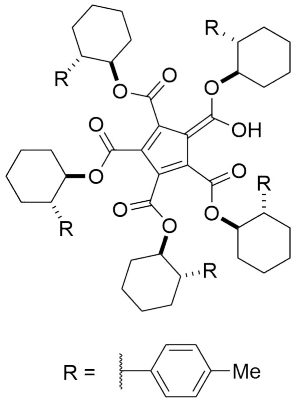
The general procedure was followed using cyclopentadiene (0.164 g, 0.461 mmol, 1.0 equiv), (1*S*,2*R*)-[1,1'-bi(cyclohexan)]-2-ol (0.840 g, 4.608 mmol, 10 equiv), and *N*-methylimidazole (0.220 mL, 2.765 mmol, 6.0 equiv) dissolved in 4.6 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a beige solid (0.312 g, 61% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 20.32 (s, 1H), 5.14-4.88 (m, 5H), 2.14-0.89 (m, 100H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 172.1, 166.7, 162.6, 134. 7, 118.4, 106.7, 80.8, 74.4, 73.6, 47.3, 44.3, 36.5, 36.3, 35.8, 32.6, 32.1, 31.8, 31.7, 31.6, 29.8, 29.8, 29.5, 29.5, 28.9, 27.1, 27.1, 27.0, 26.9, 26.82, 26.75, 26.64, 26.59, 26.0, 25.6, 25.5, 25.4, 25.0, 24.9, 23.7, 22.8, 22.7, 22.6. IR (thin film, cm^{-1}) 2923, 2852, 1730, 1593, 1449, 1410, 1373, 1335, 1307, 124, 1191, 1127, 1087, 1057, 996, 973, 907, 757. $[\alpha]_D^{23}$ = –49.8 (1.0 c, $CHCl_3$). LRMS (ESI-) exact mass calc'd for $C_{70}H_{10}5O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1105.77, found *m/z* 1106.25.

Pentakis((1*R*,2*S*)-2-phenyl-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (12):



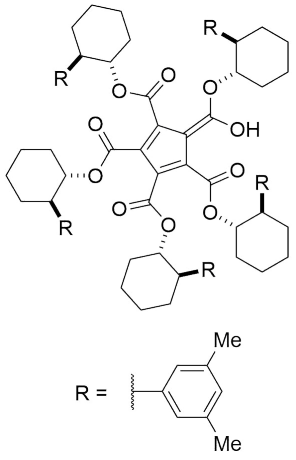
The general procedure was followed using cyclopentadiene (0.200 g, 0.561 mmol, 1.0 equiv), (1*R*,2*S*)-2-phenyl-1-cyclohexanol (0.989 g, 5.614 mmol, 10 equiv), and *N*-methylimidazole (0.268 mL, 3.368 mmol, 6.0 equiv) dissolved in 5.6 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.441 g, 73% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 18.76 (s, 1H, O**H**), 7.73-6.47 (m, 15H, Ar**H**), 5.26-4.25 (m, 5H), 3.06-0.61 (m, 45H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 166.5, 163.4, 162.6, 162.2, 160.6, 160.3, 159.7, 144.5, 143.5, 143.3, 143.1, 143.0, 142.7, 142.3, 141.4, 139.9, 138.9, 135.6, 132.3, 128.9, 128.49, 128.45, 128.37, 128.33, 128.30, 128.2, 128.1, 128.0, 127.9, 127.79, 127.75, 127.63, 127.60, 126.59, 126.4, 126.34, 126.29, 126.2, 119.1, 106.8, 82.4, 78.6, 78.2, 77.9, 77.3, 76.1, 59.4, 48.9, 48.5, 48.4, 48.2, 48.1, 46.2, 34.4, 34.3, 34.0, 33.3, 32.6, 32.03, 31.98, 31.8, 31.5, 31.3, 31.2, 30.1, 29.8, 26.0, 25.84, 25.80, 25.7, 25.6, 25.41, 25.35, 24.9, 24.7, 24.6, 24.5, 24.4, 23.6. IR (thin film, cm^{-1}) 3028, 2932, 2858, 1721, 1597, 1493, 1450, 1406, 1334, 1334, 1306, 1190, 1123, 1086, 1056, 1012, 750, 698. $[\alpha]_D^{23}$ = –159.7 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{70}H_{75}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1075.5366, found *m/z* 1075.5363.

Pentakis((1*R*,2*S*)-2-(*p*-tolyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (13):



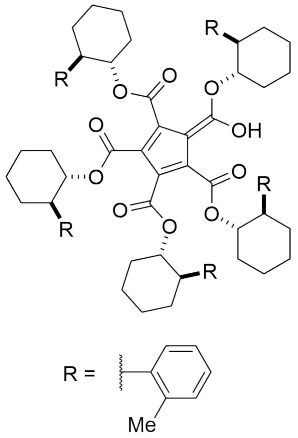
The general procedure was followed using cyclopentadiene (0.050 g, 0.140 mmol, 1.0 equiv), (1*R*,2*S*)-2-(*p*-tolyl)-1-cyclohexanol (0.200 g, 4.208 mmol, 7.5 equiv), and *N*-methylimidazole (0.067 mL, 0.841 mmol, 6.0 equiv) dissolved in 1.4 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.075 g, 47% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 18.84, (s, 1H), 7.52-6.69 (m, 20H, ArH), 5.14-4.88 (m, 5H), 2.89-0.79 (m, 60H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 129.61, 129.26, 127.88, 127.65, 34.55, 29.84, 24.72, 21.10. IR (thin film, cm^{-1}) 2924, 2852, 1727, 1593, 1514, 1448, 1409, 1374, 1335, 1306, 1224, 1190, 1126, 1057, 997, 961, 935, 908, 850, 808, 752, 666. $[\alpha]_D^{23}$ = –28.9 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{75}H_{85}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1145.6148, found *m/z* 1145.6155.

Pentakis((1*S*,2*R*)-2-(3,5-dimethylphenyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (14):



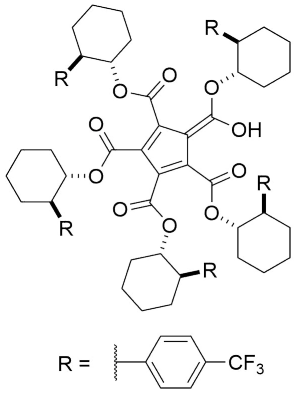
The general procedure was followed using cyclopentadiene (0.126 g, 0.354 mmol, 1.0 equiv), (1*S*,2*R*)-2-(3,5-dimethylphenyl)-1-cyclohexanol (0.723 g, 3.539 mmol, 10 equiv), and *N*-methylimidazole (0.169 mL, 2.122 mmol, 6.0 equiv) dissolved in 3.5 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.207 g, 48% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 19.11, (s, 1H, O**H**), 7.02-6.61 (m, 15H, Ar**H**), 5.19-4.89 (m, 5H, OC**H**), 2.98-1.05 (m, 75H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 171.0, 166.2, 162.4, 143.2, 141.0, 137.5, 137.2, 132.5, 128.2, 127.9, 126.0, 125.9, 125.8, 125.6, 125.4, 119.2, 106.8, 82.5, 48.5, 48.2, 45.7, 34.1, 33.4, 31.8, 31.5, 30.6, 29.8, 26.2, 25.9, 25.4, 25.2, 24.8, 24.7, 24.4, 23.2, 21.6, 21.1. IR (thin film, cm^{-1}) 2929, 2857, 1710, 1603, 1448, 1408, 1332, 1307, 1240, 1190, 1118, 1031, 839, 755. $[\alpha]_D^{23}$ = –0.1 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{80}H_{95}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1215.6931, found *m/z* 1215.6926.

Pentakis((1*S*,2*R*)-2-(*o*-tolyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (15):



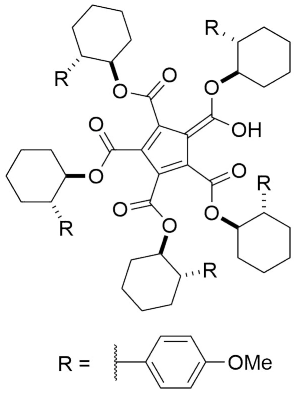
The general procedure was followed using cyclopentadiene (0.150 g, 0.420 mmol, 1.0 equiv), (1*S*,2*R*)-2-(*o*-tolyl)-1-cyclohexanol (0.800 g, 4.204 mmol, 10 equiv), and *N*-methylimidazole (0.201 mL, 2.526 mmol, 6.0 equiv) dissolved in 4.2 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.123 g, 25% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 19.29, (s, 1H), 7.28-6.81 (m, 20H, ArH), 5.26-4.92 (m, 5H), 2.94-0.89 (m, 60H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.4, 162.2, 160.41, 160.12, 159.53, 145.24, 141.21, 141.11, 141.04, 140.87, 140.34, 139.02, 138.85, 136.05, 135.92, 135.85, 134.62, 130.74, 130.61, 130.43, 130.36, 130.30, 130.26, 130.15, 126.63, 126.45, 126.36, 126.34, 126.27, 126.07, 126.04, 126.01, 125.94, 125.86, 125.65, 125.53, 125.47, 125.29, 124.83, 79.69, 77.87, 74.43, 59.45, 44.08, 43.98, 43.86, 43.34, 34.70, 34.65, 34.23, 33.94, 33.65, 33.25, 32.71, 32.40, 32.10, 31.97, 31.78, 29.80, 26.37, 26.22, 26.15, 25.96, 25.92, 25.87, 25.23, 24.91, 24.85, 24.77, 24.73, 19.92, 19.82, 19.77, 19.71, 19.62, 19.6, 19.5. LRMS (ESI-) exact mass calc'd for $C_{75}H_{85}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1145.61, found *m/z* 1146.35.

Pentakis((1*S*,2*R*)-2-(4-(trifluoromethyl)phenyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (16):



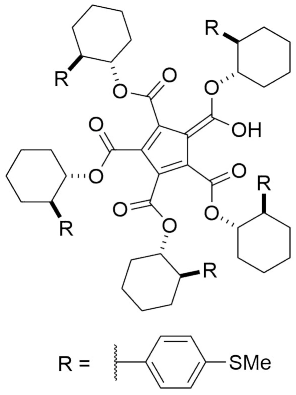
The general procedure was followed using cyclopentadiene (0.100 g, 0.281 mmol, 1.0 equiv), (1*S*,2*R*)-2-(4-(trifluoromethyl)phenyl)-1-cyclohexanol (0.514 g, 2.105 mmol, 7.5 equiv), and *N*-methylimidazole (0.134 mL, 1.684 mmol, 6.0 equiv) dissolved in 2.8 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 10% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.164 g, 41% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 18.80 (s, 1H, O**H**), 7.53-6.91 (m, 20H, Ar**H**), 5.05-4.16 (m, 5H, OC**H**), 1.93-0.88 (m, 45H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.4, 170.3, 166.8, 162.2, 148.0, 147.9, 147.0, 146.4, 145.9, 145.5, 128.9, 128.4, 128.3, 128.2, 128.1, 128.01, 127.96, 127.8, 127.7, 125.7, 125.5, 125.4, 125.3, 125.3, 125.2, 125.0, 81.8, 80.5, 74.5, 74.3, 53.1, 49.8, 49.5, 48.8, 48.5, 35.0, 34.5, 34.3, 33.5, 33.4, 32.6, 32.0, 31.9, 29.9, 26.0, 25.6, 25.5, 25.1, 24.6, 24.3. IR (thin film, cm^{-1}) 2935, 2860, 1727, 1618, 1451, 1407, 1325, 1242, 1163, 1122, 1069, 1018, 866, 756, 657. $\overline{[a]_D^{23}}$ = –16.7 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{75}H_{70}F_{15}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1415.4735, found *m/z* 1415.4727.

Pentakis((1*R*,2*S*)-2-(4-methoxyphenyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (17):



The general procedure was followed using cyclopentadiene (0.138 g, 0.387 mmol, 1.0 equiv), (1*R*,2*S*)-2-(4-methoxyphenyl)-1-cyclohexanol (0.800 g, 3.878 mmol, 10 equiv), and *N*-methylimidazole (0.152 mL, 1.910 mmol, 6.0 equiv) dissolved in 7.8 mL toluene (0.05 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 10% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.356 g, 75% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 18.90 (s, 1H, O**H**), 7.28-6.63 (m, 20H, Ar**H**), 5.14-4.90 (m, 5H, OC**H**), 3.82-3.61 (m, 15H, OC**H$_3$** x 5), 2.90-0.93 (m, 45H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.8, 166.5, 163.6, 162.8, 161.9, 160.6, 160.4, 159.7, 158.2, 158.1, 158.0, 157.93, 157.86, 144.2, 140.4, 138.9, 136.7, 135.6, 135.4, 135.2, 135.1, 135.0, 134.6, 133.4, 132.1, 128.89, 128.85, 128.81, 128.63, 128.57, 128.53, 128.49, 119.4, 114.3, 113.9, 113.80, 113.78, 113.73, 113.68, 113.5, 106.9, 82.56, 78.9, 78.6, 78.2, 78.0, 77.0, 76.5, 74.7, 59.6, 55.3, 55.21, 55.18, 55.09, 55.05, 54.99, 52.4, 47.9, 47.6, 47.4, 47.12, 47.08, 46.8, 45.7, 34.5, 34.3, 34.2, 34.1, 33.5, 33.4, 32.7, 32.0, 31.9, 31.7, 31.5, 31.1, 30.8, 30.0, 29.8, 26.2, 26.0, 25.83, 25.79, 25.65, 25.60, 25.4, 25.3, 25.2, 24.9, 24.8, 24.7, 24.6, 24.3, 23.6. IR (thin film, cm^{-1}) 2932, 2857, 1726, 1609, 1514, 153, 1406, 1371, 1333, 1306, 1283, 1247, 1213, 1192, 1180, 1126, 1087, 1035, 911, 824, 754. $[\alpha]_D^{23}$ = –92.7 (1.0 c, $CHCl_3$). HRMS (ESI-) exact mass calc'd for $C_{75}H_{85}O_{15}^-$ [M-H$^+$]$^-$ requires *m/z* 1225.5894, found *m/z* 1125.5894.

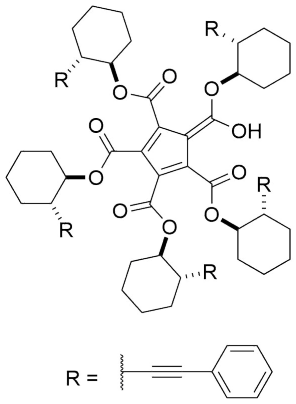
Pentakis((1*S*,2*R*)-2-(4-(methylthio)phenyl)-1-cyclohexanol) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (18):



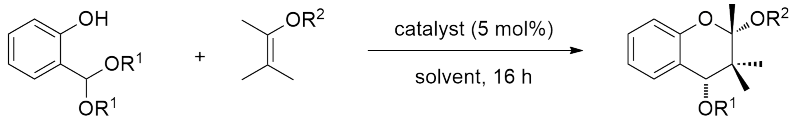
The general procedure was followed using cyclopentadiene (0.150 g, 0.421 mmol, 1.0 equiv), (1*S*,2*R*)-2-(4-(methylthio)phenyl)-1-cyclohexanol (0.936 g, 4.210 mmol, 10 equiv), and *N*-methylimidazole (0.201 mL, 2.526 mmol, 6.0 equiv) dissolved in 4.2 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 10% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.399 g, 72% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 18.70 (s, 1H, O**H**), 7.18-6.60 (m, 20H, Ar**H**), 5.03-4.74 (m, 5H, OC**H**), 2.79-0.79 (m, 60H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.73, 166.49, 161.76, 144.01, 140.51, 140.31, 140.20, 139.45, 138.37, 137.05, 136.18, 135.83, 135.69, 132.07, 128.62, 128.37, 128.31, 128.24, 128.16, 127.39, 126.98, 126.89, 126.84, 126.76, 126.70, 119.23, 106.90, 82.43, 59.51, 48.36, 48.09, 47.56, 47.41, 46.31, 34.33, 32.51, 32.04, 31.58, 30.21, 26.03, 25.42, 24.81, 24.60, 23.69, 16.19, 16.14, 16.05, 15.94, 15.86, 15.66. IR (thin film, cm^{-1}) 2931, 2857, 1726, 1597, 1495, 1448, 1407, 1332, 1306, 1189, 1126, 1093, 1056, 1016, 956, 911, 811, 753. $[\alpha]_D^{23}$ = –17.08 (1.0 c, $CHCl_3$). LRMS (ESI-) exact mass calc'd for $C_{75}H_{70}F_{15}O_{10}^-$ [M-H$^+$]$^-$ requires *m/z* 1305.48, found *m/z* 1306.54.

Pentakis((1*R*,2*S*)-2-(phenylethynyl)-1-cyclohexyl) Cyclopenta-1,3-diene-1,2,3,4,5-pentacarboxylate (19):

The general procedure was followed using cyclopentadiene (156 mg, 0.438 mmol, 1.0 equiv), (1*R*,2*S*)-2-(phenylethynyl)-1-cyclohexanol (0.700 g, 3.503 mmol, 8 equiv), and *N*-methylimidazole (0.209 mL, 2.627 mmol, 6.0 equiv) dissolved in 4.4 mL toluene (0.1 M). Upon completion of the reaction, the crude material was purified by silica gel chromatography (0 → 5% MeOH/CH_2Cl_2), washed with 1 M HCl/CH_2Cl_2 (3 x), and dried with anhydrous $MgSO_4$ to yield the title product as a brown solid (0.181 g, 35% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 20.32 (s, 1H, O**H**), 7.96-6.81 (m, 25H, Ar**H**), 5.18 (dd, J = 32.6, 22.2 Hz, 5H, OC**H** x 5), 3.55-0.62 (m, 45H, Cy**H**). ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.7, 166.3, 162.3, 134.1, 132.1, 131.8, 128.2, 127.9, 127.5, 123.7, 123.3, 118.5, 107.0, 90.5, 89.3, 83.1, 80.5, 74.7, 74.0, 37.2, 34.9, 34.8, 34.6, 32.6, 32.0, 31.7, 30.3, 30.1, 29.8, 29.5, 29.1, 27.4, 27.0, 25.4, 23.7, 23.2, 22.79, 22.75, 22.1, 21.5, 20.8, 14.2, 11.5. IR (thin film, cm^{-1}) 2935, 2860, 1734, 1597, 1454, 1409, 1378, 1322, 1215, 1154, 1050, 756, 691. $[\alpha]_D^{23}$ = –52.5 (1.0 c, $CHCl_3$). LRMS (ESI-) exact mass calc'd for $C_{80}H_{75}O_{10}^-$ $[M\text{-}H^+]^-$ requires *m/z* 1195.54, found *m/z* 1196.48.

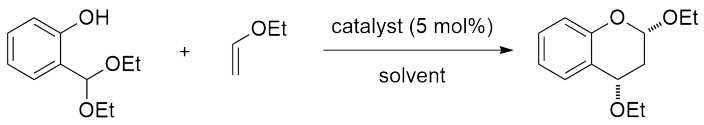


General Procedure for [4+2]-Cycloaddition



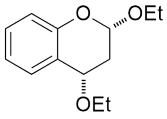
Salicylaldehyde acetal (1.0 equiv) and vinyl ether (3.0 equiv) were mixed in benzene (0.2 M) at room temperature. The optimal PCCP catalyst (0.05 equiv) was then added and the reaction vial was stirred for 16 hours at this temperature. Upon completion of the reaction, as monitored by ^{1}H-NMR, $NaBH_4$ (15.0 mg) was added, followed by MeOH (0.1 mL). After stirring for 30 minutes, the crude material was washed with H_2O and extracted with Et_2O, dried with $MgSO_4$ and concentrated *in vacuo*. The crude was subjected to silica gel column chromatography (Et_2O/Hex eluent as noted). Potassium permanganate stain was used to visualize the products. The products are characterized below.

Solvent & Concentration Screen



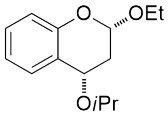
Catalyst	Solvent	Concentration (M)	Yield (%)	Enantiomeric Ratio
4	THF	0.2	29	59.5:40.5
4	EtOAc	0.2	53	61:39
4	Hexanes	0.2	77	62:38
4	Et_2O	0.2	61	63:37
4	$CHCl_3$	0.2	50	75:25
4	PhH	0.2	69	84.5:15.5
17	PhH	0.1	61	94:6
17	PhH	0.2	78	94:6
17	PhH	0.3	62	94:6
17	PhH	0.4	67	94:6

(2*S*,4*S*)-2,4-diethoxychromane (3):



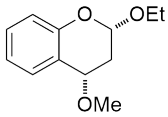
The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and ethyl vinyl ether (58.6 μL, 0.611 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (35.3 mg, 78% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36-7.25 (m, 1H, Ar**H**), 7.10 (td, J = 7.7, 1.7 Hz, 1H, Ar**H**), 6.87 (td, J = 7.5, 1.2 Hz, 1H, Ar**H**), 6.77 (d, J = 8.1 Hz, 1H, Ar**H**), 5.12 (dd, J = 7.7, 2.7 Hz, 1H, OC**H**OEt), 4.57 (dd, J = 8.4, 5.9 Hz, 1H, C**H**OEt), 3.95 (dq, J = 9.7, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.72-3.40 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.33 (ddd, J = 13.2, 6.0, 2.7 Hz, 1H, ring C**H$_a$**H$_b$), 2.05 (dt, J = 13.2, 8.0 Hz, 1H, ring CH$_a$**H$_b$**), 1.31-1.09 (m, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 129.2, 128.0, 123.9, 121.2, 117.0, 98.4, 70.8, 64.7, 63.8, 33.8, 15.7, 15.2. IR (thin film, cm^{-1}) 2974, 2929, 1610, 1585, 1487, 1463, 1409, 1347, 1285, 1120, 1200, 1118, 1096, 1049, 1014, 945, 865, 834, 756. $[\alpha]_D^{23}$ = +295.0 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{13}O_2^+$ [M-OEt]$^+$ requires m/z 177.09, found m/z 177.04. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 5.6 min (minor), 7.0 min (major), 94:6 er.

(2*S*,4*S*)-2-ethoxy-4-isopropoxychromane (20):



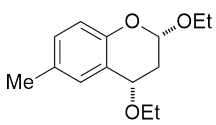
The general procedure was followed using cyclopentadiene (10.9 mg, 0.009 mmol, 0.05 equiv), salicylaldehyde diisopropyl acetal (40.0 mg, 0.178 mmol, 1.0 equiv), and ethyl vinyl ether (51.2 μL, 0.535 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (36.7 mg, 87% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.36 (dt, J = 7.5, 1.3 Hz, 1H, Ar**H**), 7.16 (tdd, J = 8.1, 1.8, 0.7 Hz, 1H, Ar**H**), 6.94 (td, J = 7.5, 1.3 Hz, 1H, Ar**H**), 6.83 (dd, J = 8.2, 1.2 Hz, 1H, Ar**H**), 5.20 (dd, J = 8.1, 2.6 Hz, 1H, OC**H**OEt), 4.66 (dd, J = 8.8, 5.8 Hz, 1H, ArC**H**O^{i}Pr), 4.03 (dq, J = 9.5, 7.1 Hz, 1H, OC$\mathbf{H_a}H_bCH_3$), 3.87 (hept, J = 6.1 Hz, 1H, OC**H**$(CH_3)_2$), 3.64 (dq, J = 9.5, 7.1 Hz, 1H, $OCH_a\mathbf{H_b}CH_3$), 2.39 (ddd, J = 13.1, 5.9, 2.6 Hz, 1H, ring C$\mathbf{H_a}H_b$), 2.08 (ddd, J = 13.0, 8.7, 8.0 Hz, 1H, ring $CH_a\mathbf{H_b}$), 1.34-1.18 (m, 9H, C$\mathbf{H_3}$ x 3). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.4, 129.1, 127.9, 124.7, 121.2, 116.9, 98.6, 70.3, 69.0, 64.7, 35.0, 23.6, 22.3, 15.3. IR (thin film, cm^{-1}) 2973, 2931, 1658, 1610, 1585, 1486, 1459, 1378, 1324, 1297, 1271, 1221, 1142, 1115, 1078, 1053, 1018, 942, 891, 756. $[a]_D^{23}$ = +133.8 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{13}O_2^+$ [M-O^{i}Pr]$^+$ requires m/z 177.09, found m/z 176.98. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.5 min (major), 5.5 min (minor), 94.5:5.5 er.

(2*S*,4*S*)-2-ethoxy-4-methoxychromane (21):



The general procedure was followed using cyclopentadiene (14.6 mg, 0.012 mmol, 0.05 equiv), salicylaldehyde dimethyl acetal (40.0 mg, 0.238 mmol, 1.0 equiv), and ethyl vinyl ether (68.3 μL, 0.713 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-10% Et_2O/Hex) to yield the title product as a colorless oil (37.7 mg, 76% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.37 (d, J = 7.7 Hz, 1H, Ar**H**), 7.24-7.15 (m, 1H, Ar**H**), 6.95 (td, J = 7.5, 1.2 Hz, 1H, Ar**H**), 6.86 (dd, J = 8.2, 1.2 Hz, 1H, Ar**H**), 5.22 (dd, J = 6.9, 2.8 Hz, 1H, OC**H**OEt), 4.61-4.41 (m, 1H, C**H**OMe), 4.00 (dq, J = 9.8, 7.1 Hz, 1H, OC$\mathbf{H_a}H_bCH_3$), 3.66 (dq, J = 9.8, 7.1 Hz, 1H, $OCH_a\mathbf{H_b}CH_3$), 3.46 (s, 3H, OC$\mathbf{H_3}$), 2.38 (ddd, J = 13.4, 5.9, 2.8 Hz, 1H, ring C$\mathbf{H_a}H_b$), 2.17 (dt, J = 13.4, 7.2 Hz, 1H, ring $CH_a\mathbf{H_b}$), 1.27 (t, J = 7.1 Hz, 3H, $OCH_2C\mathbf{H_3}$). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.3, 129.4, 128.4, 123.3, 121.1, 117.1, 98.0, 72.0, 64.7, 56.0, 32.9, 15.2. IR (thin film, cm^{-1}) 2976, 2932, 1640, 1610, 1585, 1486, 1464, 1408, 1347, 1222, 1194, 1091, 1046, 1018, 889, 865, 757. $[a]_D^{23}$ = +185.3 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{13}O_2^+$ [M-OMe]$^+$ requires m/z 177.09, found m/z 177.01. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 6.5 min (major), 8.5 min (minor), 90:10 er.

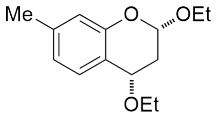
(2*S*,4*S*)-2,4-diethoxy-6-methylchromane (22):



The general procedure was followed using cyclopentadiene (8.8 mg, 0.007 mmol, 0.05 equiv), 5-methylsalicylaldehyde diethyl acetal (30.0 mg, 0.143 mmol, 1.0 equiv), and ethyl vinyl ether (41.0 μL, 0.428 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (31.6 mg, 94% yield). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.22-7.14 (m, 1H,

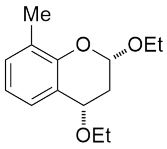
Ar**H**), 7.03-6.90 (m, 1H, Ar**H**), 6.74 (d, J = 8.3 Hz, 1H, Ar**H**), 5.16 (dd, J = 7.6, 2.6 Hz, 1H, OC**H**OEt), 4.61 (dd, J = 8.2, 6.0 Hz, 1H, ArC**H**OEt), 4.00 (dq, J = 9.6, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.79-3.51 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.38 (ddd, J = 13.2, 6.0, 2.6 Hz, 1H, ring C**H$_a$**H$_b$), 2.28 (s, 3H, ArC**H$_3$**), 2.11 (ddd, J = 13.2, 8.3, 7.6 Hz, 1H, ring CH$_a$**H$_b$**), 1.38-1.13 (m, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (125 MHz, $CDCl_3$) δ 150.1, 130.5, 129.9, 128.3, 123.5, 116.8, 98.3, 70.8, 64.6, 63.8, 33.8, 20.8, 15.7, 15.2. IR (thin film, cm^{-1}) 2974, 2929, 2869, 1618, 1589, 1495, 1444, 1378, 1349, 1271, 1246, 1218, 1151, 1095, 1056, 1023, 951, 890, 815. $[a]_D^{23}$ = +299.6 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{12}H_{15}O_2^+$ [M-OEt]$^+$ requires m/z 191.11, found m/z 190.96. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 5.3 min (minor), 6.9 min (major), 94:6 er.

(2*S*,4*S*)-2,4-diethoxy-7-methylchromane (23):



The general procedure was followed using cyclopentadiene (11.7 mg, 0.010 mmol, 0.05 equiv), 4-methylsalicylaldehyde diethyl acetal (40.0 mg, 0.190 mmol, 1.0 equiv), and ethyl vinyl ether (55.0 μL, 0.571 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a white solid (37.6 mg, 84% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (d, J = 7.8 Hz, 1H, Ar**H**), 6.82-6.73 (m, 1H, Ar**H**), 6.67 (t, J = 1.1 Hz, 1H, Ar**H**), 5.17 (dd, J = 7.7, 2.6 Hz, 1H, OC**H**OEt), 4.63 (dd, J = 8.2, 6.0 Hz, 1H, ArC**H**OEt), 4.01 (dq, J = 9.7, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.75-3.49 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.37 (ddd, J = 13.2, 6.0, 2.6 Hz, 1H, ring C**H$_a$**H$_b$), 2.28 (s, 3H, ArC**H$_3$**), 2.11 (ddd, J = 13.2, 8.3, 7.6 Hz, 1H, ring CH$_a$**H$_b$**), 1.34-1.19 (m, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 139.3, 127.9, 122.2, 120.8, 117.3, 98.4, 70.7, 64.6, 63.5, 33.8, 21.3, 15.7, 15.2. IR (thin film, cm^{-1}) 2978, 2960, 2926, 1624, 1578, 1502, 1444, 1421, 1379, 1343, 1297, 1266, 1246, 1207, 1166, 1142, 1127, 1100, 1056, 1023, 951, 898, 875, 857, 808, 745. $[a]_D^{23}$ = +293.1 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{12}H_{15}O_2^+$ [M-OEt]$^+$ requires m/z 191.11, found m/z 191.04. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 5.2 min (minor), 8.7 min (major), 95.5:4.5 er.

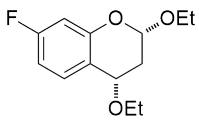
(2*S*,4*S*)-2,4-diethoxy-8-methylchromane (24):



The general procedure was followed using cyclopentadiene (14.6 mg, 0.012 mmol, 0.05 equiv), 3-methylsalicylaldehyde diethyl acetal (50.0 mg, 0.238 mmol, 1.0 equiv), and ethyl vinyl ether (68.3 μL, 0.713 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a white solid (54.1 mg, 96% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28-7.20 (m, 1H, Ar**H**), 7.08-7.00 (m, 1H, Ar**H**), 6.86 (t, J = 7.5 Hz, 1H, Ar**H**), 5.22 (dd, J = 7.8, 2.7 Hz, 1H, OC**H**OEt), 4.66 (dd, J = 8.7, 6.0 Hz, 1H, ArC**H**OEt), 4.05 (dq, J = 9.7, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.76-3.51 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.42 (ddd, J = 13.1, 6.0, 2.7 Hz, 1H, ring C**H$_a$**H$_b$), 2.22 (s, 3H, ArC**H$_3$**), 2.11 (ddd, J = 13.1, 8.6, 7.8 Hz, 1H, , ring CH$_a$**H$_b$**), 1.37-1.22 (m, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.5, 130.3, 126.1, 125.4, 123.5, 120.6, 98.5, 71.1, 64.6, 63.6, 33.9, 16.0, 15.7, 15.3. IR (thin film, cm^{-1}) 2974, 2930, 2873, 1597, 1468, 1440, 1379, 1338, 1301, 1263, 1212, 1172, 1105, 1076, 1033, 1012, 929, 863, 777, 746, 609. $[a]_D^{23}$ = +190.2 (1.0 c, $CHCl_3$). LRMS (ESI+) exact

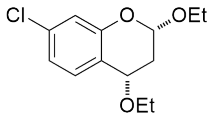
mass calc'd for $C_{12}H_{15}O_2^+$ [M-OEt]$^+$ requires m/z 191.11, found m/z 191.06. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 5.3 min (minor), 6.3 min (major), 80:20 er.

(2*S*,4*S*)-2,4-diethoxy-7-fluorochromane (25):



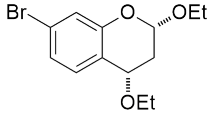
The general procedure was followed using cyclopentadiene (10.0 mg, 0.008 mmol, 0.05 equiv), 4-fluorosalicylaldehyde diethyl acetal (35.0 mg, 0.163 mmol, 1.0 equiv), and ethyl vinyl ether (47.0 µL, 0.490 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a white solid (28.0 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 (ddd, J = 8.6, 6.6, 0.9 Hz, 1H, Ar**H**), 6.66 (td, J = 8.5, 2.6 Hz, 1H, Ar**H**), 6.55 (dd, J = 10.1, 2.6 Hz, 1H, Ar**H**), 5.20 (dd, J = 7.4, 2.6 Hz, 1H, OC**H**OEt), 4.58 (ddt, J = 8.0, 5.8, 1.1 Hz, 1H, ArC**H**OEt), 4.00 (dq, J = 9.6, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.77-3.49 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.37 (ddd, J = 13.3, 5.9, 2.7 Hz, 1H, ring C**H$_a$**H$_b$), 2.20-2.03 (m, 1H, ring CH$_a$**H$_b$**), 1.27 (td, J = 7.0, 5.7 Hz, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 153.6, 129.4, 119.8, 108.4, 104.08, 98.7, 70.3, 64.9, 63.8, 33.5, 15.6, 15.2. ^{19}F NMR (375 MHz, $CDCl_3$) δ -116.08. IR (thin film, cm^{-1}) 2976, 2878, 1619, 1599, 1499, 1434, 1380, 1342, 1300, 1261, 1129, 1097, 1052, 1020, 968, 877, 847, 805. $\boxed{[a]_D^{23}}$ = +257.1 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{12}FO_2^+$ [M-OEt]$^+$ requires m/z 195.08, found m/z 194.79. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.5 min (minor), 6.2 min (major), 94:6 er.

(2*S*,4*S*)-7-chloro-2,4-diethoxychromane (26):



The general procedure was followed using cyclopentadiene (13.3 mg, 0.011 mmol, 0.05 equiv), 4-chlorosalicylaldehyde diethyl acetal (50.0 mg, 0.217 mmol, 1.0 equiv), and ethyl vinyl ether (62.3 µL, 0.650 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (33.3 mg, 78% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dd, J = 8.3, 0.9 Hz, 1H, Ar**H**), 6.95-6.78 (m, 2H, Ar**H**), 5.19 (dd, J = 7.5, 2.7 Hz, 1H, OC**H**OEt), 4.57 (ddd, J = 8.3, 5.9, 0.9 Hz, 1H, ArC**H**OEt), 3.99 (dq, J = 9.7, 7.1 Hz, 1H, OC**H$_a$**H$_b$), 3.77-3.49 (m, 3H, OCH$_a$**H$_b$** + OC**H$_a$H$_b$**), 2.38 (ddd, J = 13.3, 5.9, 2.7 Hz, 1H, ring C**H$_a$**H$_b$), 2.10 (ddd, J = 13.3, 8.3, 7.5 Hz, 1H, ring CH$_a$**H$_b$**), 1.27 (td, J = 7.0, 5.8 Hz, 6H, OCH$_2$C**H$_3$** x 2). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 134.3, 129.1, 122.6, 121.4, 117.2, 98.7, 70.3, 64.9, 63.9, 33.5, 15.6, 15.2. IR (thin film, cm^{-1}) 2975, 2930, 2873, 1604, 1576, 1483, 1443, 1414, 1379, 1341, 1293, 1226, 1195, 1156, 1121, 1098, 1051, 1017, 951, 921, 894, 856, 807, 766, 721. $\boxed{[a]_D^{23}}$ = +221.5 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{12}ClO_2^+$ [M-OEt]$^+$ requires m/z 211.05, found m/z 211.54. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.9 min (minor), 7.5 min (major), 88:12 er.

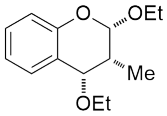
(2*S*,4*S*)-7-bromo-2,4-diethoxychromane (27):



The general procedure was followed using cyclopentadiene (12.3 mg, 0.010 mmol, 0.05 equiv), 4-bromosalicylaldehyde diethyl acetal (55.0mg, 0.200 mmol, 1.0 equiv), and ethyl vinyl ether (57.0 µL, 0.600

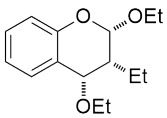
mmol, 3.0 equiv). The reaction was complete after 16 h and purified by silica gel chromatography (5% Et_2O/Hex) to yield the title product as a colorless oil (40.8 mg, 68% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.32-7.18 (m, 1H, Ar**H**), 7.11-6.98 (m, 2H, Ar**H**), 5.19 (dd, J = 7.5, 2.7 Hz, 1H, OC**H**OEt), 4.56 (dd, J = 8.2, 5.9 Hz, 1H, ArC**H**OEt), 3.99 (dq, J = 9.6, 7.1 Hz, 1H, OC$\mathbf{H_a}H_b$), 3.77-3.46 (m, 3H, $OCH_a\mathbf{H_b}$ + OC$\mathbf{H_aH_b}$), 2.38 (ddd, J = 13.4, 5.9, 2.7 Hz, 1H, ring C$\mathbf{H_a}H_b$), 2.10 (dt, J = 13.3, 7.9 Hz, 1H, ring $CH_a\mathbf{H_b}$), 1.33-1.17 (m, 6H. $OCH_2C\mathbf{H_3}$ x 2). ^{13}C NMR (125 MHz, $CDCl_3$) δ 153.2, 129.4, 124.3, 123.1, 122.1, 120.2, 98.7, 70.3, 64.9, 63.9, 33.4, 15.6, 15.2. IR (thin film, cm^{-1}) 2975, 2931, 1644, 1573, 1480, 1419, 1339, 1291, 1205, 1181, 1097, 1069, 1010, 904, 860, 811, 776. $[a]_D^{23}$ = +210.3 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{12}BrO_2^+$ [M-OEt]$^+$ requires m/z 255.00, found m/z 254.71. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 5.0 min (major), 7.8 min (minor), 62:38 er.

(2*S*,3*R*,4*S*)-2,4-diethoxy-3-methylchromane (28):



The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and ethyl-1-propenyl ether [mixture of cis + trans] (68.0 µL, 0.612 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (37.1 mg, 77% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.42 (dt, J = 7.6, 1.3 Hz, 1H, Ar**H**), 7.15 (dddd, J = 8.1, 7.2, 1.7, 0.8 Hz, 1H, Ar**H**), 6.93 (td, J = 7.5, 1.2 Hz, 1H, Ar**H**), 6.80 (dd, J = 8.2, 1.2 Hz, 1H, Ar**H**), 5.07 (d, J = 2.0 Hz, 1H, OC**H**OEt), 4.65 (d, J = 5.6 Hz, 1H, EtOC**H**), 4.06 (dq, J = 9.7, 7.1 Hz, 1H, OC$\mathbf{H_a}H_b$), 3.80-3.52 (m, 3H, $OCH_a\mathbf{H_b}$ + OC$\mathbf{H_aH_b}$), 2.58-2.39 (m, 1H, C**H**CH_3), 1.30 (dt, J = 11.5, 7.0 Hz, 6H, $OCH_2C\mathbf{H_3}$ x 2), 0.97 (d, J = 6.8 Hz, 3H, CHC$\mathbf{H_3}$). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 128.9, 128.2, 122.63, 121.2, 116.3, 101.1, 75.0, 65.2, 64.7, 34.6, 15.6, 15.3, 5.9. IR (thin film, cm^{-1}) 2976, 2928, 2873, 1610, 1585, 1484, 1457, 1375, 1352, 1294, 1272, 1235, 1198, 1163, 1144, 1106, 1086, 1036, 965, 931, 895, 851, 799, 755, 722. $[a]_D^{23}$ = +201.5 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{12}H_{15}O_2^+$ [M-OEt]$^+$ requires m/z 191.11, found m/z 191.05. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.2 min (minor), 4.6 min (major), 89:11 er. NOESY experiment suggests all syn configuration; single X-ray crystal structure of lactone (shown below) confirms syn configuration.

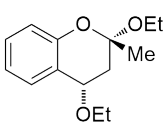
(2*S*,3*R*,4*S*)-2,4-diethoxy-3-ethylchromane (29):



The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and 1-butenyl ethyl ether [mixture of cis + trans] (79.0 µL, 0.612 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (39.8 mg, 78% yield). ^1H NMR (500 MHz, $CDCl_3$) δ 7.37-7.29 (m, 1H, Ar**H**), 7.22-7.11 (m, 1H, Ar**H**), 6.92 (td, J = 7.4, 1.2 Hz, 1H, Ar**H**), 6.82 (dd, J = 8.2, 1.2 Hz, 1H, Ar**H**), 5.12 (d, J = 2.5 Hz, 1H, OC**H**OEt), 4.53 (d, J = 5.2 Hz, 1H, EtOC**H**), 3.97 (dq, J = 9.9, 7.1 Hz, 1H, OC$\mathbf{H_a}H_b$), 3.74-3.57 (m, 3H, $OCH_a\mathbf{H_b}$ + OC$\mathbf{H_aH_b}$), 2.12 (tdd, J = 6.6, 5.1, 2.5 Hz, 1H, C**H**Et), 1.69-1.56 (m, 2H, CHC$\mathbf{H_2}CH_3$),

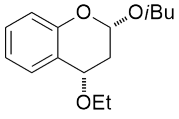
1.31-1.18 (m, 6H, OCH_2CH_3 x 2), 1.06 (t, J = 7.5 Hz, 3H, $CHCH_2CH_3$). ^{13}C NMR (125 MHz, $CDCl_3$) δ 152.1, 129.2, 129.1, 123.0, 120.8, 116.8, 100.4, 73.6, 65.3, 65.1, 42.5, 17.3, 15.6, 15.2, 13.1. IR (thin film, cm^{-1}) 2973, 2874, 1610, 1585, 1484, 1456, 1375, 1354, 1295, 1258, 1221, 1195, 1167, 1094, 1045, 1015, 982, 937, 891, 869, 852, 800, 754, 717. $[\alpha]_D^{23}$ = +149.0 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{13}H_{17}O_2^+$ $[M\text{-}OEt]^+$ requires m/z 205.12, found m/z 204.81. HPLC Analysis: Chiralpak OJ-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.4 min (minor), 4.7 min (major), 93:7 er.

(2*S*,4*S*)-2,4-diethoxy-2-methylchromane (30):



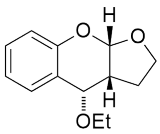
The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and 2-ethoxy-1-propene (68.3 µL, 0.612 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (5-8% Et_2O/Hex) to yield the title product as a colorless oil (24.1 mg, 50% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.40 (d, J = 6.8 Hz, 1H, Ar**H**), 7.17 (dddd, J = 8.1, 7.3, 1.7, 0.7 Hz, 1H, Ar**H**), 6.94 (td, J = 7.5, 1.2 Hz, 1H, Ar**H**), 6.83 (dd, J = 8.2, 1.2 Hz, 1H, Ar**H**), 4.54 (t, J = 6.7 Hz, 1H, ArC**H**OEt), 3.81-3.52 (m, 4H, OCH_2CH_3 x 2), 2.34-2.12 (m, 2H, ring CH_2), 1.51 (s, 3H, $CHCH_3$), 1.29 (t, J = 7.0 Hz, 3H, OCH_2CH_3), 1.14 (t, J = 7.1 Hz, 3H, OCH_2CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 129.2, 128.2, 123.5, 121.0, 117.2, 100.4, 71.0, 64.1, 57.3, 37.2, 24.3, 15.7, 15.7. IR (thin film, cm^{-1}) 2975, 2933, 2879, 1611, 1585, 1484, 1456, 1377, 1340, 1303, 1272, 1243, 1218, 1189, 1164, 1121, 1095, 1064, 1028, 942, 922, 876, 754. $[\alpha]_D^{23}$ = +98.1 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{12}H_{15}O_2^+$ $[M\text{-}OEt]^+$ requires m/z 191.11, found m/z 191.01. HPLC Analysis: Chiralpak OJ-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 4.5 min (major), 7.3 min (minor), 83:17 er.

(2*S*,4*S*)-4-ethoxy-2-isobutoxychromane (31):



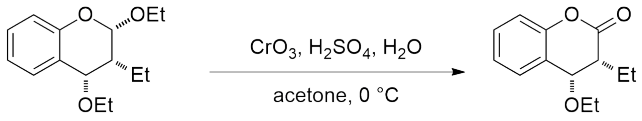
The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and isobutyl vinyl ether (79.7 µL, 0.612 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (3% Et_2O/Hex) to yield the title product as a colorless oil (22.9 mg, 45% yield). ^1H NMR (400 MHz, $CDCl_3$) δ 7.42 (dt, *J* = 7.7, 1.3 Hz, 1H, ArH), 7.18 (td, *J* = 7.8, 1.7 Hz, 1H, ArH), 6.96 (td, *J* = 7.4, 1.2 Hz, 1H, ArH), 6.83 (dd, *J* = 8.2, 1.2 Hz, 1H, ArH), 5.41 (dd, *J* = 8.9, 2.4 Hz, 1H, OCHO), 4.77 (dd, *J* = 9.7, 6.1 Hz, 1H, EtOCH), 3.71 (dq, *J* = 9.0, 7.0 Hz, 1H, ring CH_aH_b), 3.60 (dq, *J* = 9.1, 7.0 Hz, 1H, ring CH_aH_b), 2.35 (ddd, *J* = 12.9, 6.1, 2.4 Hz, 1H, $OCH_aH_bCH_3$), 2.12 (dt, *J* = 12.9, 9.3 Hz, 1H, $OCH_aH_bCH_3$), 1.37 (s, 9H, *t*-Bu), 1.31 (t, *J* = 7.0 Hz, 3H, OCH_2CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 129.1, 127.6, 123.8, 121.0, 117.2, 93.8, 76.0, 71.6, 63.4, 35.2, 28.8, 15.7. $[\alpha]_D^{23}$ = +287.4 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{13}H_{17}O_2^+$ $[M\text{-}OEt]^+$ requires m/z 205.12, found m/z 205.07. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 254 nm, 23 °C) 4.6 min (minor), 5.0 min (major), 91:9 er.

(3aR,4S,9aS)-4-ethoxy-2,3,3a,9a-tetrahydro-4H-furo[2,3-b]chromene (32):



The general procedure was followed using cyclopentadiene (12.5 mg, 0.010 mmol, 0.05 equiv), salicylaldehyde diethyl acetal (40.0 mg, 0.204 mmol, 1.0 equiv), and 2,3-dihydrofuran (46.2 μL, 0.612 mmol, 3.0 equiv). After completion of the reaction, the crude mixture was purified by silica gel chromatography (10% Et_2O/Hex) to yield the title product as a colorless oil (31.9 mg, 71% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44 (dt, *J* = 7.6, 1.5 Hz, 1H, Ar**H**), 7.22-7.12 (m, 1H, Ar**H**), 7.00 (td, *J* = 7.5, 1.2 Hz, 1H, Ar**H**), 6.96-6.83 (m, 1H, Ar**H**), 5.84 (d, *J* = 5.9 Hz, 1H, OC**H**O), 4.73 (d, *J* = 5.5 Hz, 1H, ArC**H**O), 3.90-3.76 (m, 3H), 3.68 (dq, *J* = 9.2, 7.0 Hz, 1H), 3.13 (tt, *J* = 9.1, 5.6 Hz, 1H), 2.00-1.84 (m, 1H), 1.79-1.66 (m, 1H), 1.34 (t, *J* = 7.0 Hz, 3H, C**H$_3$**). ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 128.7, 125.9, 125.3, 121.9, 117.0, 102.6, 72.3, 68.6, 65.1, 43.3, 24.5, 15.6. LRMS (ESI+) exact mass calc'd for $C_{11}H_{11}O_2^+$ $[M\text{-}OEt]^+$ requires m/z 175.08, found m/z 175.03. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 98/2, 1.0 mL/min, 280 nm, 23 °C) 8.0 min (major), 10.7 min (minor), 59:41 er.

(3*R*,4*S*)-4-ethoxy-3-ethylchroman-2-one:



91.5:8.5 er

45.5 mg
52% yield
91.5:8.5 er

Jones reagent was prepared utilizing 2.5 g Cr(VI)O_3 dissolved in 2.5 mL H_2SO_4 (conc.). The solution was added very slowly to 7.5 mL H_2O that had been cooled to 0 °C and was stirring. (2*S*,3*R*,4*S*)-2,4-diethoxy-3-ethylchromane (100 mg, 0.400 mmol) was dissolved in acetone at 0 °C. 1.0 mL of the prepared Jones reagent was added to the acetone solution and the reaction was stirred for 2 hours. The reaction was extracted with H_2O-ethyl acetate, dried with $MgSO_4$, and concentrated in vacuo. The crude mixture was purified by silica gel chromatography (20% Et_2O/Hex) to yield the title product as a colorless solid (45.5 mg, 52% yield).^{1}H NMR (300 MHz, $CDCl_3$) δ 7.44-6.98 (m, 4H, Ar**H**), 4.40 (d, *J* = 3.2 Hz, 1H, ArC**H**), 3.54-3.26 (m, 2H, OC**H$_2$**CH_3), 2.62 (ddd, *J* = 8.3, 6.0, 3.2 Hz, 1H, ArO_2CC**H**Et), 2.23-1.97 (m, 1H, C**H$_a$**$CH_b$$CH_3$), 1.84 (ddt, *J* = 14.1, 8.3, 7.5 Hz, 1H, CH_aC**H$_b$**CH_3), 1.09 (dt, *J* = 12.4, 7.2 Hz, 6H, C**H$_3$** x 2). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.5, 151.8, 130.3, 128.7, 123.7, 123.4, 117.3, 73.3, 63.9, 47.1, 19.0, 15.0, 11.8. IR (thin film, cm^{-1}) 2972, 2878, 1771, 1613, 1592, 1486, 1459, 1365, 1339, 1235, 1223, 1199, 1144, 1118, 1092, 1079, 978, 943, 918, 802, 760, 643, 605. $[a]_D^{23}$ = –92.2 (1.0 c, $CHCl_3$). LRMS (ESI+) exact mass calc'd for $C_{11}H_{11}O_2^+$ $[M\text{-}OEt]^+$ requires m/z 175.08, found m/z 175.06. HPLC Analysis: Chiralpak OD-H (Hex/IPA = 99/1, 1.0 mL/min, 280 nm, 23 °C) 7.4 min (major), 9.2 min (minor), 91.5:8.5 er.

Single crystal X-ray diffraction. Data for all compounds was collected on an Agilent SuperNova diffractometer using mirror-monochromated Cu Kα radiation. Data collection, integration, scaling (ABSPACK) and absorption correction (face-indexed Gaussian integration[2] or numeric analytical methods[3]) were performed in CrysAlisPro.[4]

Structure solution was performed using ShelXT.[5] Subsequent refinement was performed by full-matrix least-squares on F^2 in ShelXL. Olex2[6] was used for viewing and to prepare CIF files. PLATON[7] was used for Bijvoet difference analysis of absolute structure (further details within). ORTEP graphics were prepared in CrystalMaker.[8] Thermal ellipsoids are rendered at the 50% probability level.

A single crystal of **Chirag6** was grown as colorless rods from a sample of **83%** enantiomeric purity (as determined by **HPLC**) by cooling a saturated hexanes solution. Part of a crystal (0.14 x 0.11 x 0.08 mm) was separated carefully, mounted with Paratone oil, and cooled to 100 K on the diffractometer. A highly redundant set of data (8x redundant in 222) was collected to 0.800 Å resolution. 19062 reflections were collected (2330 unique, 2307 observed) with R(int) 3.6% and R(sigma) 1.8% after Gaussian absorption and beam profile correction (Tmin .814).

The space group was assigned as $P2_12_12$ based on the systematic absences. The structure solved routinely in ShelXT with 1 molecule in the asymmetric unit. All non-H atoms were located in the initial solution and refined anisotropically with no restraints. C-H hydrogens were placed in calculated positions and refined with riding coordinates and ADPs.

The final refinement (2330 data, 0 restraints, 147 parameters) converged with R_1 ($F_o > 4\sigma(F_o)$) = 2.8%, wR_2 = 7.0%, S = 1.08. The largest Fourier features were 0.15 and -0.15 $e^- A^{-3}$.

A crystal with molecular formula $C_{13}H_{16}O_3$ is a reasonable target for absolute structure determination using Cu Kα radiation.[9] The Flack x parameter was -0.05(5) by the Parsons selected quotients method implemented in ShelXL. For confirmation of the absolute structure, the data set was analyzed by the probabilistic approach of Hooft, Straver, and Spek[10] as implemented in PLATON. Errors were assumed to be Gaussian; a normal probabilities plot was linear with correlation coefficient 0.999 and slope 0.899. Using an outlier criterion of 16.32 and sigma criterion of 0.25, 379 Bijvoet pairs were selected for analysis. The Hooft y parameter was -0.05(4) using these parameters. The probability of a racemic twin, P3(rac-twin), was calculated as 9×10^{-33} and the probability of an incorrect absolute structure, P3(false), was 6×10^{-119}. Therefore, we state with high confidence that the absolute structure is correctly assigned.

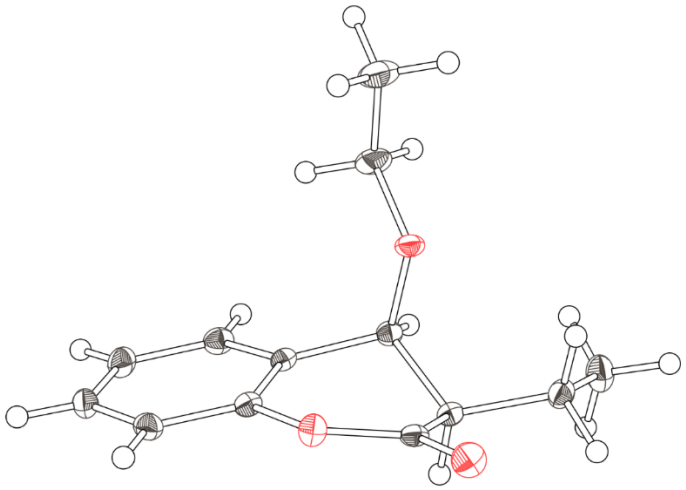


Figure S1. Molecular structure of **Chirag6**.

Compound	**Chirag6**
Formula	$C_{13}H_{16}O_3$
MW	220.26
Space group	$P2_12_12$
***a* (Å)**	28.7833(4)
***b* (Å)**	7.66350(10)
***c* (Å)**	5.26380(10)
***α* (°)**	90
***β* (°)**	90
***γ* (°)**	90
V (Å^3)	1161.09(3)
Z	4
ρ_{calc} (g cm^{-3})	1.260
T (K)	100
λ (Å)	1.54184
$2\theta_{min}$, $2\theta_{max}$	12, 146
Nref	19062
R(int), R(σ)	.0363, .0184
μ(mm^{-1})	0.720
Size (mm)	.14 x .11 x

	.08
T_{max}, T_{min}	1, .814
Data	2330
Restraints	0
Parameters	147
R_1(obs)	0.0276
wR_2(all)	0.0699
S	1.081
Peak, hole (e^- Å^{-3})	0.15, -0.15
Flack	-0.05(5)

Single crystal X-ray diffraction. Data for all compounds was collected on an Agilent SuperNova diffractometer using mirror-monochromated Cu Kα radiation. Data collection, integration, scaling (ABSPACK) and absorption correction (face-indexed Gaussian integration[11]) were performed in CrysAlisPro.[12] Structure solution was performed using SuperFlip.[13] Subsequent refinement was performed by full-matrix least-squares on F^2 in ShelXL.[14] Olex2[15] was used for viewing and to prepare CIF files. Many disordered solvent molecules were modeled as rigid fragments from the Idealized Molecular Geometry Library.[16] ORTEP graphics were prepared in CrystalMaker.[17] Thermal ellipsoids are rendered at the 50% probability level.

A chloroform solution of Chirag5c was diluted with diethyl ether by vapor diffusion to afford bunches of large, colorless needles. A crystal (.37 x .08 x .05 mm) was separated carefully, mounted with STP oil treatment, and cooled to 100 K on the diffractometer. A full sphere of data were collected to 0.8 Å resolution. 307530 reflections were collected (58110 unique, 46998 observed) with R(int) 7.6% and R(sigma) 5.8% after absorption and beam profile correction (Tmin .459).

The space group was assigned as $P2_1$ based on the systematic absences. The cell volume indicated Z=8, or nearly 400 non-H atoms in the asymmetric unit. Since no heavy atom was necessarily present, this suggested a difficult case for structure solution. Previous experience indicated that charge-flipping in Superflip, with a reasonable number of cycles per trial and a large number of trials, could be an effective strategy for a large equal-atom structure. Superflip runs are most importantly configured by the parameters k_{ed}, which modifies the fraction of charges that are flipped per cycle, and w, the fraction of reflections treated as weak. We tested k_{ed} set to automatic or 1.3, and w set to 0.1 or 0.2. The resulting four parameter sets were configured with 100 trials each; the 400 trials took about 8 hours on a personal computer. The algorithm converged in 1 trial out of 400. The successful solution was obtained with the default parameters chosen by flipsmall[18] (k_{ed} automatic, w=0.2).

When a successful solution had been obtained, the refinement proceeded routinely using ShelXL. Constrained-gradient least-squares refinement was employed until the final stages because the large number of reflections and parameters resulted in very slow full-matrix least-squares refinement.

The asymmetric unit contains two partially occupied chloroform molecules, which were important for determination of the absolute structure. The chloroform molecules appear to be part of a mixed-occupancy disorder with an Et_2O molecule disordered over several additional positions, but it was not possible to explicitly model the partially occupied diethyl ether. Instead, the $CHCl_3$ occupancies were freely refined (one at 24% occupancy and the other at 60% occupancy) and additional solvent was not modeled.

All four tetramethylammonium cations are disordered over two positions, which were modeled with standard distance and ADP restraints. Several of the flexible side chains on the **PCCP** anions may have some slight unresolved disorder, which was addressed by restraining ADPs to be chemically reasonable with SIMU or RIGU restraints as needed.

C-H hydrogens were placed in calculated positions and refined with riding coordinates and ADPs. The final refinement (58110 data, 917 restraints, 3669 parameters) converged with R_1 ($F_o > 4\sigma(F_o)$) = 7.2%, wR_2 = 19.9%, S = 1.01. The largest Fourier features were 1.00 and -0.59 $e^- A^{-3}$ and occurred near the partially occupied chloroform molecules. The Flack parameter was 0.024(13), indicating the absolute structure is determined with extremely high confidence.

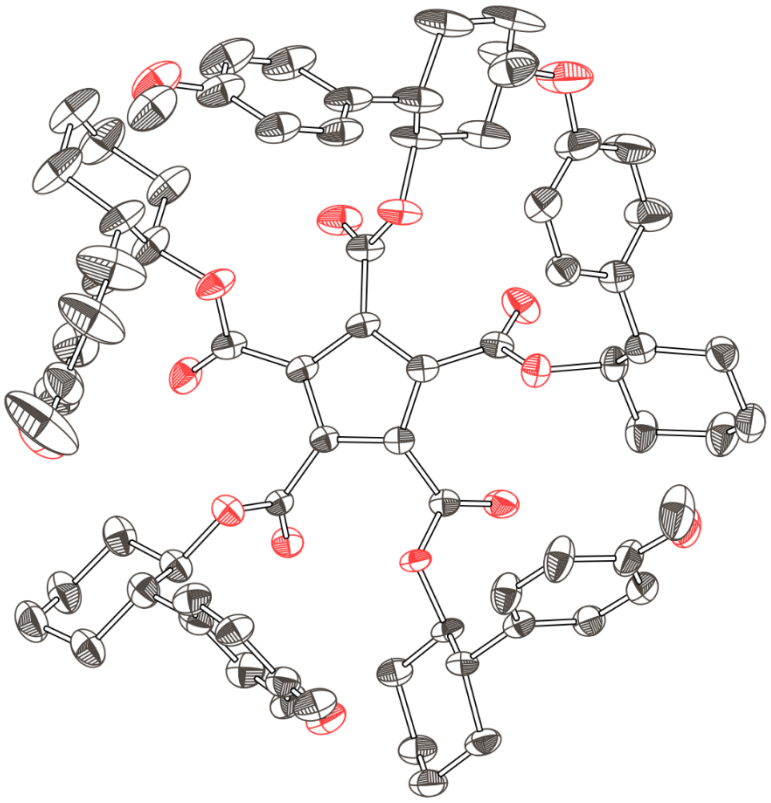


Figure S2. Molecular structure of **Chirag5**$^{-}$. One of four independent molecules is shown.

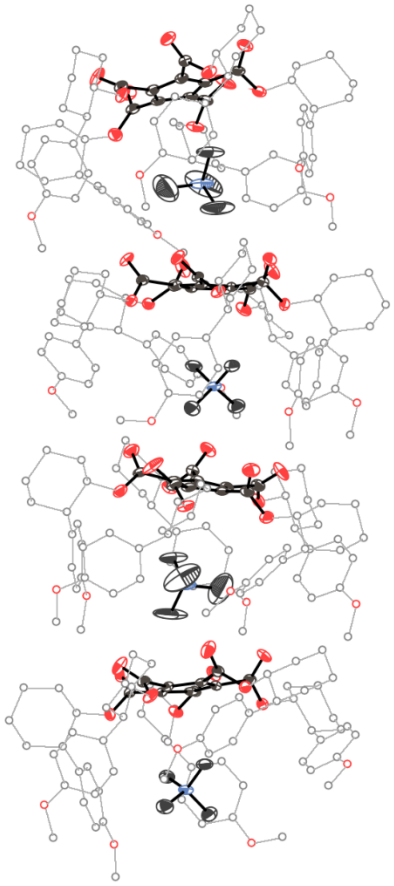


Figure S3. Helical stack of **Chirag5NMe$_4$** aligned along *b* axis. One of the two independent stacks is shown; every second molecule is related by a 2_1 screw axis.

Compound	**Chirag5c**
Formula	$C_{79.2}Cl_{0.63}NO_{15}H_{97.2}$
MW	1325.69
Space group	$P2_1$
***a* (Å)**	15.7236(3)
***b* (Å)**	33.2669(4)
***c* (Å)**	27.9753(5)
***α* (°)**	90
***β* (°)**	90.4715(15)
***γ* (°)**	90
V (Å^3)	14632.7(4)
Z	8
ρ_{calc} (g cm^{-3})	1.204
T (K)	100
λ (Å)	1.54184
$2\theta_{min}$, $2\theta_{max}$	7, 147
Nref	307530
R(int), R(σ)	.0761, .0580
μ(mm^{-1})	0.867
Size (mm)	.37 x .08 x .05
T_{max}, T_{min}	1.00, .459
Data	58110
Restraints	917
Parameters	3669
R_1(obs)	0.0717
wR_2(all)	0.1989
S	1.014
Peak, hole (e$^-$ Å^{-3})	1.00, -.59
Flack	0.024(13)

Theoretical methods (*all structure numbers in discussion and SI figures are from the manuscript)***:** The 4+2 cycloaddition transition state (TS) was explored using the oxocarbenium ion-PCCP anion complex (**35**) and ethyl vinyl ether **2** using B3LYP/6-31G* calculations as implemented in Gaussian 09.[19] For initial TS explorations we used the PCCP anion derived from catalyst **8** since it had 55 atoms less than the optimal catalyst **17**. We explored TSs leading to both (*S,S*) and (*R,R*) cycloaddition product with PCCP anion conformation # 1 (Figure S4), which has all carboxyl groups geared in the same direction and with all carbonyl oxygen atoms on the same face of the cyclopentadienyl ring and the 2-substituted cyclohexyl moiety on the opposite face of the cyclopentadienyl ring. Different orientations of the substrates with respect to the PCCP anion were explored; however, majority of the orientations explored converged to one of two TSs for both (*S,S*) and (*R,R*) cycloaddition product. The coordinates of these four TSs are included in the SI as SS1Me.log SS2Me.log RR1Me.log and RR2Me.log.

As a next step in our TS explorations, we took the lowest energy TS (SS1Me.log) and explored different conformations of the PCCP anion (conformations #2 and #3, Figure S4) by rotating one or two of the carbonyl oxygen atoms to the face opposite the remaining carbonyl oxygen atoms. The (*S,S*) TS located using PCCP anion conformation # 2 (coordinates labeled as SS3Me.log) was found to be ~ 3.0 kcal/mol higher in Free energy than SS1Me.log, while the (*S,S*) TS located using PCCP anion conformation # 3 (coordinates labeled as SS4Me.log) was found to be ~ 4.2 kcal/mol higher in Free energy than SS1Me.log. Based on this trend, we surmised that rotating additional carbonyl oxygen atoms would only further increase the energy of the resulting TSs and so additional modifications to the PCCP anion structure along these lines were not explored.

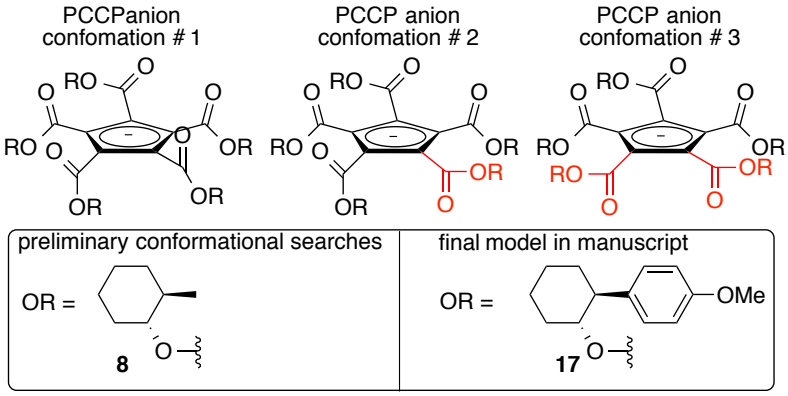


Figure S4. Conformations of the PCCP anion explored during TS searches.

The helical chirality of the PCCP anion is determined by the relative stereochemistry of the two adjacent chiral centers on the cyclohexyl ester. One enantiomer of the PCCP anion strongly favors one helical chiral arrangement of the carboxyl group while the opposite enantiomer of the PCCP anion favors the other helically chiral arrangement. The origin of this preference stems from the orientation of the 2-substituent on the cyclohexanol ring (Me in **8** or *p*-OMePh in **17**) toward the opposite face of the cyclopentadienyl anion relative to the orientation of the carbonyl oxygen atoms (which are oriented towards the active site of the catalyst).

However, for each enantiomer of the PCCP anion, the two helically chiral forms can exist in a dynamic equilibrium with each other depending on the size of this 2-substituent. The consequence of this dynamic equilibrium is that rather than the paradigm presented in the manuscript where the same gearing of the carboxyl groups stabilizes opposite enantiomers of the cycloaddition product via different non-covalent interactions, one can imagine conformations with opposite gearing of the carboxyl groups (for the *same* enantiomer of the PCCP anion) stabilizing both enantiomers of the cycloaddition product with identical stabilizing non-covalent interactions. Under this scenario, the only differentiating factor between the TSs leading to the opposite enantiomers of product would be the steric interaction of the TS with the 2-substituent on the cyclohexanol ring. Upon exploration, we found that for catalyst **8**, this paradigm might contribute to the origin of enantioselectivity since both helically chiral forms are close in energy and the interaction of the Me-group with the active site is minimal – The transition structures leading to the minor enantiomer of product stabilized by the opposite-geared PCCP anion (RR1Me-opp.log) is only 1.2 kcal/mol higher in energy than the RR TS having the same gearing as the lowest energy SS TS (RR1Me.log). However, for the bulkier PCCP anion derived from catalyst **17**, it was found that the opposite enantiomers of product resulted exclusively from the same gearing of the

carboxyl groups since the structure corresponding to the opposite gearing of the carboxyl groups (analogous to RR1Me-opp.log) was found to be ~10 kcal/mol higher in energy (not fully converged structure, therefore not included in SI).

Based on these explorations, it was determined that the lowest energy transition structure leading to the major and minor enantiomer of the cycloaddition product using catalyst **8** were SS1Me.log and RR1Me.log. We then proceeded to replace the 2-methyl group (catalyst **8**) by the 2-*p*-OMePh group (catalyst **17**) for these two transition structures to arrive at the two structures presented in the manuscript. The coordinates for these two structures for catalyst **17** are labeled SS1p-OMe and RR1p-OMe (highlighted in blue). We are currently working on a comprehensive exploration of a number of PCCP anion stabilized TSs to understand which of the two above-described paradigms dictate enantioselectivity for the different 2-substituents shown in Table 1 in the manuscript. This is the subject of a more detailed study exploring structure-activity relationships in PCCP catalysis.

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19 Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A. Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2013.

SS1Me.log
Free Energy = -3237.534830
Zero-point Energy = -3237.415913
Potential Energy = -3238.76985135
Nimag = 1 (-80.7085 cm-1)

Charge = 0 Multiplicity = 1
C 0.63214 -1.42578 -0.18342
C -0.67444 -0.98451 -0.46258
C -0.63729 0.43081 -0.61897
C 0.70106 0.85145 -0.43143
C 1.48976 -0.28583 -0.15398
C -1.87452 -1.84035 -0.41076
C -1.75488 1.34547 -0.81285
O -1.77371 2.51751 -0.43702
C 1.14303 2.27043 -0.46194
O 1.52946 2.90839 0.50745
C 2.86971 -0.29820 0.34783
O 3.26898 -1.03954 1.23556
C 0.98677 -2.82644 0.09823
O 0.28749 -3.59762 0.74417
O -2.81533 -1.67773 0.38034
C -2.50807 1.83267 3.68981
C -3.13748 2.23429 4.88950
C -4.04826 1.40265 5.51415
C -4.34898 0.14963 4.94582
C -3.74176 -0.27691 3.77344
C -2.80451 0.55463 3.13481
H -2.90298 3.21102 5.30014
H -4.53571 1.71403 6.43252
H -5.07025 -0.50022 5.43449
H -3.97346 -1.24418 3.33738
O -2.15629 0.22910 2.02224
H -2.50710 -0.56531 1.50602
O 1.05823 2.77237 -1.70959
O -1.85806 -2.83633 -1.29358
O -2.79862 0.76425 -1.45412
O 3.65641 0.63725 -0.24375
O 2.16220 -3.17947 -0.46322
C -1.62224 2.68285 2.95226
H -1.34620 2.42204 1.93419
C 0.54656 1.92565 3.65906
H 1.02959 2.64711 3.01158
H 0.33236 2.18967 4.68907
C 0.58485 0.62160 3.26925
H 0.90369 0.34447 2.26699
O -1.49877 3.93653 3.32037
C -0.85659 4.85260 2.37658
H -0.11429 4.29850 1.79491
H -0.35090 5.58076 3.01451
C -1.90882 5.49807 1.49183
H -1.43227 6.25611 0.86036
H -2.37157 4.75283 0.83774
H -2.68081 5.98769 2.09431
O 0.20266 -0.36406 4.07103
C 0.27652 -1.70533 3.50391
H 1.28048 -1.84720 3.09226
H -0.44294 -1.77374 2.68444
C -0.03249 -2.69449 4.60766
H -1.03050 -2.51754 5.02226
H -0.00166 -3.70860 4.19637
H 0.69863 -2.62292 5.41945
C -4.01926 1.52946 -1.61166
C -4.67382 1.08193 -2.92661
C -4.92048 1.29825 -0.39477
H -3.74431 2.58813 -1.67472
C -6.04290 1.77395 -3.08079
H -4.84609 -0.00272 -2.84881
C -6.28257 1.98522 -0.56953
H -5.05411 0.21596 -0.26593
H -4.41190 1.66836 0.50227
C -6.96281 1.54376 -1.87318
H -6.52385 1.41887 -4.00138
H -5.88305 2.85513 -3.21428
H -6.92414 1.76804 0.29361
H -6.14222 3.07620 -0.58666
H -7.90982 2.08093 -2.01146
H -7.21520 0.47534 -1.80683
C 1.36655 4.17287 -1.93737
C 2.22948 4.25810 -3.20550
C 0.05040 4.94169 -2.07934
H 1.93037 4.53927 -1.07272
C 2.46308 5.73741 -3.57357
H 1.65051 3.78994 -4.01618
C 0.30309 6.41288 -2.44069
H -0.54543 4.46141 -2.86707
H -0.52761 4.84680 -1.15532
C 1.15571 6.52960 -3.71244
H 3.04260 5.78977 -4.50444
H 3.08821 6.20266 -2.79565
H -0.65287 6.93635 -2.56865
H 0.82410 6.91220 -1.60975
H 1.37277 7.58256 -3.93321
H 0.58369 6.14103 -4.56754
C 4.98000 0.83866 0.32290
C 5.92771 1.22471 -0.82021
C 4.89587 1.90836 1.41610
H 5.29950 -0.11255 0.76122
C 7.31440 1.56902 -0.23892
H 5.52170 2.13241 -1.28973
C 6.28693 2.24588 1.97285
H 4.42656 2.80530 0.99193
H 4.23404 1.55162 2.21323
C 7.24946 2.65178 0.84792
H 7.97846 1.88503 -1.05412
H 7.76020 0.65623 0.18548
H 6.20669 3.04558 2.71992
H 6.69391 1.36910 2.49771
H 8.25218 2.84245 1.25171
H 6.90666 3.59631 0.40037
C 2.67976 -4.50594 -0.18672
C 3.55829 -4.89788 -1.38325
C 3.45224 -4.49036 1.13612
H 1.82629 -5.18978 -0.10964
C 4.24801 -6.24726 -1.09870
H 4.33942 -4.12758 -1.47242
C 4.13849 -5.83965 1.39588
H 4.19419 -3.68349 1.09505
H 2.76134 -4.24344 1.94897
C 5.03720 -6.24127 0.21814
H 4.90767 -6.49886 -1.93953
H 3.48317 -7.03853 -1.06010
H 4.72020 -5.78857 2.32485
H 3.37501 -6.61691 1.54932
H 5.48457 -7.22784 0.39559
H 5.87058 -5.52805 0.13820
C -2.93469 -3.82255 -1.26325
C -3.05963 -4.37889 -2.68768
C -2.60909 -4.90075 -0.22780
H -3.85482 -3.29765 -0.98386
C -4.09569 -5.52182 -2.70168
H -2.07919 -4.80213 -2.95338
C -3.65318 -6.02700 -0.26230
H -1.61043 -5.30004 -0.44218
H -2.55357 -4.44482 0.76514
C -3.78530 -6.61798 -1.67283
H -4.14577 -5.94721 -3.71236
H -5.09250 -5.10204 -2.49517
H -3.38008 -6.80685 0.45919
H -4.62952 -5.63390 0.05836

H -4.56726 -7.38769 -1.69487
H -2.84468 -7.11796 -1.94592
C -3.76907 1.34197 -4.13682
C 3.55326 3.50136 -3.05671
C 6.02036 0.12652 -1.88627
C 2.76382 -4.93516 -2.69420
C -3.40891 -3.28726 -3.70631
H 4.11688 3.51470 -3.99707
H 4.18151 3.96645 -2.28564
H 3.38527 2.45930 -2.77074
H -4.38992 -2.84524 -3.48613
H -2.66667 -2.48400 -3.69663
H -3.45218 -3.70220 -4.72011
H 2.29208 -3.96964 -2.89757
H 3.41817 -5.18229 -3.53868
H 1.97362 -5.69651 -2.65177
H 5.03700 -0.10138 -2.30768
H 6.68128 0.43394 -2.70546
H 6.42701 -0.79970 -1.45935
H -3.56615 2.41501 -4.25110
H -2.80993 0.82695 -4.03181
H -4.24602 0.99333 -5.06043

SS2Me.log
Free Energy = -3237.532918
Zero-point Energy = -3237.411791
Potential Energy = -3238.76545539
Nimag = 1 (-197.0527 cm-1)

Charge = 0 Multiplicity = 1
C 0.10907 -1.12451 -0.43662
C -1.01701 -0.27167 -0.54904
C -0.56996 1.06662 -0.47918
C 0.84414 1.04163 -0.31577
C 1.25907 -0.30504 -0.28071
C -2.42436 -0.71675 -0.55980
C -1.40628 2.27086 -0.44315
O -1.13863 3.30147 0.15241
C 1.75330 2.19280 -0.17237
O 2.65288 2.26649 0.65825
C 2.63353 -0.78512 -0.02217
O 2.94485 -1.56576 0.86863
C 0.04935 -2.58434 -0.43481
O -0.87901 -3.24472 0.03018
O -3.24585 -0.44906 0.32837
C -0.63676 0.68285 4.34128
C -0.74005 1.15484 5.66420
C -1.97749 1.47341 6.20098
C -3.13503 1.32347 5.41843
C -3.06529 0.84381 4.11595
C -1.81553 0.51084 3.56940
H 0.16761 1.28822 6.24337
H -2.05216 1.85014 7.21624
H -4.10374 1.58601 5.83542
H -3.95973 0.72686 3.51052
O -1.63354 0.00600 2.34897
H -2.41658 -0.00752 1.72414
O 1.51374 3.15255 -1.08513
O -2.73688 -1.45336 -1.62456
O -2.55803 2.10551 -1.15601
O 3.52139 -0.25395 -0.88656
O 1.13991 -3.14742 -1.00261
C 0.63326 0.43222 3.69408
H 0.67434 0.45779 2.60788
C 0.86130 -1.76153 3.64638
H 1.69704 -1.75310 2.95238
H 1.06160 -1.80707 4.71202
C -0.31646 -2.27990 3.16780
H -0.49301 -2.44387 2.10724
O 1.72146 0.77642 4.35694
C 2.98093 0.82476 3.61476
H 2.79602 1.28384 2.63881
H 3.31476 -0.20727 3.46642
C 3.96476 1.62232 4.44604
H 4.92607 1.66166 3.92322
H 3.61236 2.64825 4.59031
H 4.12321 1.16256 5.42716
O -1.31534 -2.56813 3.98562
C -2.53289 -3.06584 3.36194
H -2.30299 -4.02501 2.88612
H -2.83287 -2.35776 2.58397
C -3.58018 -3.20622 4.44761
H -3.78287 -2.23836 4.91614
H -4.51137 -3.58488 4.01294
H -3.25018 -3.90648 5.22142
C -3.52680 3.18078 -1.11292
C -4.30947 3.14294 -2.43311
C -4.42927 3.01066 0.11410
H -2.97457 4.12400 -1.03367
C -5.44053 4.19030 -2.39406
H -4.77102 2.14596 -2.50652
C -5.55378 4.05686 0.13049
H -4.85372 1.99795 0.09301
H -3.81542 3.08746 1.01849
C -6.35968 4.02432 -1.17560
H -6.02163 4.12795 -3.32346
H -4.99423 5.19659 -2.37699
H -6.21064 3.88739 0.99318
H -5.11869 5.05824 0.26299
H -7.12768 4.80845 -1.17153
H -6.89152 3.06428 -1.24968
C 2.27285 4.38625 -0.99513
C 2.31876 4.98294 -2.40872
C 1.61351 5.32232 0.02210
H 3.28682 4.13168 -0.66480
C 3.00711 6.36183 -2.36313
H 1.27585 5.13201 -2.72739
C 2.30801 6.69184 0.04707
H 0.55529 5.43214 -0.24374
H 1.64213 4.85206 1.01032
C 2.35371 7.31710 -1.35423
H 2.99813 6.80215 -3.36890
H 4.06684 6.22294 -2.09793
H 1.79153 7.35820 0.74936
H 3.33494 6.57726 0.42535
H 2.89630 8.27114 -1.33164
H 1.32930 7.54653 -1.68217
C 4.92381 -0.59787 -0.73805
C 5.54973 -0.49678 -2.13686
C 5.58288 0.34196 0.27600
H 4.97731 -1.63124 -0.37583
C 7.07284 -0.71621 -2.04222
H 5.37359 0.53043 -2.49090
C 7.10001 0.11086 0.34743
H 5.36760 1.37706 -0.01746
H 5.12000 0.18793 1.25634
C 7.74564 0.23165 -1.03965
H 7.51651 -0.59715 -3.03927
H 7.26563 -1.75793 -1.74190
H 7.55294 0.82460 1.04716
H 7.29995 -0.89219 0.75272
H 8.82095 0.01955 -0.98120
H 7.64875 1.26747 -1.39627
C 1.27457 -4.59063 -0.94952
C 2.05125 -5.01689 -2.20344
C 1.98483 -4.98469 0.34956
H 0.26727 -5.02163 -0.96996
C 2.34345 -6.52948 -2.13864
H 3.01284 -4.48136 -2.18388
C 2.27563 -6.49238 0.39054

H 2.91802 -4.41212 0.42151
H 1.36426 -4.68612 1.20206
C 3.06664 -6.93784 -0.84744
H 2.93405 -6.82042 -3.01708
H 1.39244 -7.07969 -2.21065
H 2.82223 -6.74215 1.30853
H 1.32686 -7.04775 0.43163
H 3.22496 -8.02380 -0.83001
H 4.06407 -6.47505 -0.82666
C -4.08258 -2.00091 -1.74017
C -4.34206 -2.19557 -3.24055
C -4.18294 -3.30760 -0.94833
H -4.77787 -1.25936 -1.33059
C -5.70676 -2.88326 -3.44211
H -3.55897 -2.87281 -3.61383
C -5.54737 -3.97906 -1.16699
H -3.37200 -3.97262 -1.27012
H -4.01609 -3.09998 0.11314
C -5.82808 -4.19881 -2.65997
H -5.86528 -3.05828 -4.51400
H -6.50394 -2.19460 -3.12189
H -5.58261 -4.93196 -0.62427
H -6.33998 -3.34749 -0.73867
H -6.82604 -4.63284 -2.80186
H -5.10876 -4.92778 -3.06055
C -3.39772 3.34356 -3.64934
C 3.00080 4.04318 -3.41020
C 4.90002 -1.46818 -3.12951
C 1.31379 -4.63880 -3.49350
C -4.25572 -0.87759 -4.01921
H 1.89933 -4.92726 -4.37445
H 0.34467 -5.15117 -3.55514
H 1.13026 -3.56175 -3.54271
H 5.05763 -2.50950 -2.81776
H 3.82248 -1.29700 -3.20278
H 5.33545 -1.35151 -4.12903
H 4.04694 3.86285 -3.12874
H 2.49200 3.07606 -3.45385
H 2.99795 4.47889 -4.41653
H -2.60983 2.58578 -3.68200
H -3.97272 3.28195 -4.58104
H -2.91647 4.32990 -3.61923
H -3.28664 -0.39227 -3.87403
H -4.39539 -1.05193 -5.09255
H -5.03659 -0.17835 -3.69191

SS3Me.log
Free Energy = -3237.529621
Zero-point Energy = -3237.411048
Potential Energy = -3239.20334622
Nimag = 1 (-202.0653 cm-1)

Charge = 0 Multiplicity = 1
C -1.34617 0.31214 -0.37209
C -0.11189 1.00009 -0.38952
C 0.91811 0.05650 -0.65905
C 0.30982 -1.21117 -0.80675
C -1.08021 -1.06824 -0.63506
C 0.07532 2.43399 -0.08538
C 2.35761 0.27380 -0.73567
O 3.20715 -0.58647 -0.50816
C 1.04955 -2.49179 -0.97954
O 1.19280 -3.32242 -0.09245
C -1.97717 -2.23320 -0.66173
O -1.82103 -3.19252 -1.39887
C -2.61452 1.01318 -0.12634
O -2.72033 1.97682 0.62454
O 0.76231 2.87123 0.84958
C 3.00739 -0.30930 3.75218
C 3.65408 -0.37260 5.00411
C 3.68096 0.73486 5.83444
C 3.05927 1.92801 5.42312
C 2.40815 2.01830 4.19976
C 2.36799 0.89724 3.35365
H 4.14181 -1.29755 5.29443
H 4.18562 0.68769 6.79426
H 3.08726 2.79854 6.07327
H 1.92897 2.93983 3.88219
O 1.75807 0.86824 2.17180
H 1.41236 1.74183 1.80367
O 1.55594 -2.60889 -2.21670
O -0.56719 3.24444 -0.92281
O 2.67451 1.54155 -1.09589
O -2.95798 -2.17340 0.28216
O -3.64820 0.54017 -0.86020
C 2.99947 -1.40083 2.81436
H 2.74202 -1.20768 1.77666
C 0.92359 -2.34120 3.13448
H 1.10448 -3.07149 2.35478
H 1.14631 -2.59533 4.16528
C 0.01337 -1.36106 2.85199
H -0.33183 -1.18759 1.83436
O 3.75165 -2.44979 3.07234
C 4.01151 -3.36935 1.96232
H 3.12327 -3.41570 1.32601
H 4.16298 -4.33481 2.44971
C 5.23732 -2.91940 1.18629
H 5.46639 -3.66471 0.41617
H 5.04854 -1.96501 0.68573
H 6.10767 -2.82442 1.84380
O -0.46239 -0.56242 3.79546
C -1.40729 0.45738 3.35742
H -2.24775 -0.04422 2.86766
H -0.91520 1.09563 2.62016
C -1.84830 1.23591 4.57881
H -0.99263 1.71518 5.06525
H -2.55523 2.01343 4.27192
H -2.34089 0.58350 5.30705
C 4.07469 1.91393 -1.14561
C 4.23166 2.95045 -2.26728
C 4.50329 2.45445 0.22178
H 4.65100 1.01402 -1.38671
C 5.68168 3.47564 -2.28192
H 3.56615 3.79314 -2.02339
C 5.94541 2.98205 0.18685
H 3.81188 3.25925 0.50588
H 4.39828 1.66068 0.96938
C 6.12533 4.02960 -0.92059
H 5.77763 4.24597 -3.05802
H 6.35467 2.65592 -2.57750
H 6.21301 3.40293 1.16413
H 6.63614 2.14460 0.00897
H 7.17111 4.35901 -0.96888
H 5.52714 4.92005 -0.67760
C 2.43800 -3.72286 -2.52421
C 1.79004 -4.59883 -3.60797
C 3.77070 -3.11973 -2.97471
H 2.56870 -4.30956 -1.60933
C 2.79587 -5.68209 -4.05106
H 1.59041 -3.94421 -4.47054
C 4.75622 -4.21289 -3.41139
H 3.57401 -2.44192 -3.81696
H 4.18034 -2.50511 -2.16590
C 4.14325 -5.10141 -4.50339
H 2.34777 -6.27933 -4.85570
H 2.96343 -6.37500 -3.21175
H 5.68995 -3.75649 -3.76356
H 5.02240 -4.83698 -2.54451
H 4.83435 -5.91103 -4.77153
H 3.99408 -4.50233 -5.41365

C -3.87188 -3.30070 0.36733
C -3.53907 -4.15147 1.60673
C -5.28950 -2.73089 0.41587
H -3.73674 -3.90624 -0.53387
C -4.61166 -5.24788 1.78015
H -3.59263 -3.48159 2.48001
C -6.33797 -3.83914 0.58556
H -5.35616 -2.02675 1.25669
H -5.47269 -2.15460 -0.49808
C -6.04043 -4.68981 1.82765
H -4.39473 -5.82003 2.69167
H -4.52848 -5.95945 0.94439
H -7.34083 -3.39835 0.64919
H -6.33643 -4.48408 -0.30530
H -6.76441 -5.51032 1.91296
H -6.16102 -4.07035 2.72876
C -4.84877 1.35699 -0.91903
C -5.55666 0.99972 -2.23456
C -5.73976 1.14426 0.30845
H -4.52660 2.40563 -0.94681
C -6.87837 1.78712 -2.33964
H -5.80176 -0.07276 -2.18898
C -7.04861 1.94018 0.18034
H -5.96510 0.07482 0.39862
H -5.18824 1.44246 1.20477
C -7.78713 1.58903 -1.11825
H -7.40150 1.49126 -3.25819
H -6.64665 2.85795 -2.44905
H -7.68723 1.74846 1.05173
H -6.82384 3.01694 0.19064
H -8.69468 2.19790 -1.21957
H -8.11648 0.54048 -1.07578
C -0.52694 4.68353 -0.68111
C -0.79103 5.35851 -2.03399
C -1.55896 5.06236 0.38381
H 0.48150 4.93043 -0.33013
C -0.87733 6.88572 -1.83698
H -1.77267 5.00299 -2.38244
C -1.62704 6.58652 0.56101
H -2.53598 4.66923 0.07820
H -1.30448 4.56881 1.32619
C -1.90929 7.28896 -0.77441
H -1.11251 7.35774 -2.79961
H 0.11397 7.26434 -1.54297
H -2.39719 6.83925 1.30023
H -0.67275 6.95277 0.96821
H -1.90950 8.37850 -0.64260
H -2.91580 7.01452 -1.12211
C 3.82017 2.38918 -3.63331
C 0.46464 -5.21677 -3.14772
C -2.13519 -4.76663 1.54794
C -4.66205 1.23795 -3.45712
C 0.26099 4.98371 -3.08461
H 0.02331 -5.81602 -3.95371
H 0.62164 -5.87971 -2.28703
H -0.26013 -4.45409 -2.85150
H 1.25904 5.32494 -2.77875
H 0.30513 3.90125 -3.23409
H 0.03064 5.45372 -4.04795
H -3.73785 0.65804 -3.39083
H -5.18232 0.95225 -4.37897
H -4.39092 2.29863 -3.54309
H -1.35353 -4.00603 1.47474
H -1.94295 -5.36125 2.44964
H -2.03036 -5.42479 0.67800
H 4.45896 1.54312 -3.91881
H 2.78383 2.03980 -3.62217
H 3.91468 3.15512 -4.41206

SS4Me.log
Free Energy = -3237.527116
Zero-point Energy = -3237.408085
Potential Energy = -3239.20108359
Nimag = 1 (-159.0584 cm-1)

Charge = 0 Multiplicity = 1
C -0.69274 1.28830 -0.63844
C 0.69128 0.99283 -0.60975
C 0.84461 -0.41285 -0.67892
C -0.45881 -0.98624 -0.72722
C -1.40075 0.04667 -0.73254
C 1.77732 1.97712 -0.39200
C 2.06876 -1.19809 -0.71913
O 2.13696 -2.40083 -0.46884
C -0.75870 -2.44247 -0.82169
O -0.84680 -3.20816 0.12752
C -2.87124 -0.15744 -0.84416
O -3.56133 0.12963 -1.80079
C -1.23352 2.62030 -0.38017
O -0.56816 3.58715 -0.02414
O 2.50660 2.00004 0.61065
C 2.27282 -1.63422 3.80325
C 2.78138 -1.98244 5.07145
C 3.50897 -1.06533 5.81143
C 3.74107 0.22029 5.29063
C 3.24531 0.59495 4.04853
C 2.49799 -0.32597 3.29470
H 2.60630 -2.98554 5.44658
H 3.90654 -1.33853 6.78380
H 4.31886 0.93706 5.86831
H 3.42572 1.58694 3.64449
O 1.96392 -0.06119 2.10412
H 2.24922 0.79671 1.65294
O -0.96095 -2.81518 -2.09701
O 1.91919 2.84173 -1.38845
O 3.15345 -0.46052 -1.07376
O -3.36306 -0.76355 0.27401
O -2.58083 2.68545 -0.54843
C 1.57109 -2.56825 2.95657
H 1.46569 -2.35117 1.89725
C -0.60555 -2.04737 3.28744
H -0.92935 -2.81332 2.59369
H -0.56475 -2.27472 4.34735
C -0.75368 -0.75074 2.87267
H -0.94862 -0.51065 1.82871
O 1.55610 -3.83511 3.32239
C 1.19614 -4.81985 2.30002
H 0.43775 -4.38661 1.64303
H 0.76392 -5.64454 2.87106
C 2.42852 -5.24652 1.52074
H 2.15288 -6.05576 0.83482
H 2.81293 -4.41614 0.92110
H 3.21223 -5.61497 2.19085
O -0.62989 0.25816 3.72023
C -0.72359 1.59841 3.15926
H -1.69945 1.69784 2.67223
H 0.05655 1.71161 2.40233
C -0.55747 2.58586 4.29561
H 0.41404 2.45521 4.78267
H -0.61332 3.60529 3.90012
H -1.34337 2.45934 5.04710
C 4.45512 -1.09734 -1.05125
C 5.26989 -0.52807 -2.22178
C 5.10912 -0.83604 0.30894
H 4.30350 -2.17280 -1.19255
C 6.71459 -1.06394 -2.15453
H 5.30522 0.56432 -2.08997
C 6.54983 -1.36572 0.35238
H 5.09898 0.24680 0.49274

H 4.50132 -1.30025 1.09359
C 7.38465 -0.79145 -0.80058
H 7.30152 -0.61919 -2.96858
H 6.70204 -2.14888 -2.34131
H 7.00776 -1.12355 1.31957
H 6.53841 -2.46332 0.27932
H 8.39709 -1.21485 -0.78751
H 7.49664 0.29387 -0.66174
C -1.24588 -4.21328 -2.37993
C -2.11928 -4.24921 -3.64128
C 0.07672 -4.96402 -2.55680
H -1.79725 -4.62422 -1.52664
C -2.34585 -5.71592 -4.06236
H -1.55004 -3.74835 -4.43900
C -0.16983 -6.42147 -2.97377
H 0.66383 -4.44960 -3.32952
H 0.65391 -4.90525 -1.62818
C -1.03350 -6.49304 -4.24128
H -2.93133 -5.73660 -4.99058
H -2.96226 -6.21490 -3.29859
H 0.78838 -6.93232 -3.13105
H -0.67832 -6.95605 -2.15759
H -1.24560 -7.53798 -4.50144
H -0.47180 -6.06734 -5.08547
C -4.79553 -1.01614 0.31910
C -5.03534 -2.16071 1.31450
C -5.52179 0.27132 0.72201
H -5.11326 -1.31748 -0.68590
C -6.55263 -2.37191 1.50316
H -4.61194 -1.84126 2.27971
C -7.02826 0.03626 0.90113
H -5.08744 0.63030 1.66623
H -5.33253 1.03709 -0.03602
C -7.29366 -1.09061 1.90797
H -6.71285 -3.15939 2.25113
H -6.97686 -2.75268 0.56126
H -7.51504 0.96558 1.22261
H -7.47423 -0.22911 -0.06852
H -8.37036 -1.28703 1.99014
H -6.95601 -0.77305 2.90563
C -3.20474 3.98987 -0.46372
C -4.42314 3.97506 -1.39783
C -3.58003 4.30641 0.98714
H -2.47535 4.72875 -0.81551
C -5.16144 5.32447 -1.28690
H -5.10224 3.18830 -1.03520
C -4.32968 5.64474 1.08489
H -4.21504 3.49436 1.36898
H -2.66823 4.32681 1.59410
C -5.55359 5.66505 0.15841
H -6.05218 5.30232 -1.92808
H -4.51426 6.12073 -1.68617
H -4.62854 5.83211 2.12406
H -3.64928 6.46206 0.80455
H -6.04445 6.64604 0.19757
H -6.29119 4.93172 0.51642
C 2.91427 3.90225 -1.27107
C 3.21934 4.36700 -2.70190
C 2.37988 5.03228 -0.38698
H 3.81110 3.46248 -0.81854
C 4.19020 5.56433 -2.65831
H 2.26776 4.71341 -3.13254
C 3.36149 6.21374 -0.35870
H 1.40758 5.35105 -0.78063
H 2.19920 4.65000 0.62144
C 3.67825 6.71101 -1.77575
H 4.36855 5.91810 -3.68199
H 5.16464 5.22016 -2.27798
H 2.94436 7.02552 0.25011
H 4.29566 5.90463 0.13402
H 4.41790 7.52121 -1.74202
H 2.76750 7.13543 -2.22252
C 4.61785 -0.83068 -3.57587
C -3.44645 -3.50376 -3.45379
C -4.34639 -3.46322 0.89154
C -4.03906 3.64304 -2.84440
C 3.76290 3.23415 -3.58018
H -4.03734 -3.53204 -4.37690
H -4.04752 -3.97086 -2.66191
H -3.28766 -2.45512 -3.18629
H 4.72278 2.86510 -3.19474
H 3.06682 2.39167 -3.61708
H 3.93055 3.58557 -4.60510
H -3.58902 2.64903 -2.90909
H -4.92474 3.66083 -3.49090
H -3.32399 4.37697 -3.23969
H -3.26646 -3.33487 0.78463
H -4.52747 -4.25136 1.63288
H -4.74303 -3.81833 -0.06932
H 4.56412 -1.91296 -3.75204
H 3.60108 -0.43040 -3.62341
H 5.19792 -0.38821 -4.39423

RR1Me.log
Free Energy = -3237.532664
Zero-point Energy = -3237.412405
Potential Energy = -3238.76638255
Nimag = 1 (-186.0436 cm-1)

Charge = 0 Multiplicity = 1
C -0.54270 -0.93333 -0.29384
C -1.35059 0.21649 -0.15214
C -0.50884 1.35898 -0.22471
C 0.81785 0.90631 -0.41074
C 0.80325 -0.50950 -0.46481
C -2.81820 0.21641 0.02645
C -0.89106 2.77210 -0.09208
O -0.18823 3.64036 0.40337
C 2.03302 1.73680 -0.32878
O 2.92521 1.56051 0.51497
C 1.96760 -1.37976 -0.61647
O 2.11853 -2.47965 -0.08881
C -1.04563 -2.31498 -0.20404
O -1.80488 -2.71659 0.67328
O -3.43291 0.83516 0.88106
C 1.79148 0.52691 3.67605
C 2.80101 1.30022 4.27081
C 2.69705 1.65261 5.61053
C 1.59881 1.24392 6.38614
C 0.58659 0.50033 5.80145
C 0.65746 0.14515 4.43949
H 3.65085 1.61187 3.67056
H 3.48255 2.25137 6.06415
H 1.53589 1.52580 7.43254
H -0.28800 0.20700 6.37263
O 2.10015 2.69626 -1.24680
O -3.42117 -0.57584 -0.89308
O -2.12021 3.01220 -0.60781
O 2.89967 -0.82942 -1.43554
O -0.59032 -3.09952 -1.20088
C 1.33628 -2.66197 3.01806
H 1.48487 -2.62839 1.93799
C 0.08768 -2.63732 3.58513
H -0.74904 -2.86308 2.93273
C -2.67909 4.33826 -0.44082
C -3.70360 4.53026 -1.56820
C -3.30268 4.46187 0.95346
H -1.86279 5.06267 -0.54845
C -4.44101 5.87067 -1.37715
H -4.44058 3.71827 -1.47050

C -4.03881 5.79976 1.11933
H -3.99573 3.62274 1.09414
H -2.51333 4.35781 1.70540
C -5.08240 5.99968 0.01159
H -5.20103 5.97917 -2.16215
H -3.72659 6.69549 -1.52470
H -4.51237 5.84494 2.10820
H -3.31222 6.62510 1.08445
H -5.56850 6.97859 0.11420
H -5.87365 5.24318 0.11829
C 3.19386 3.66012 -1.18072
C 3.39177 4.19300 -2.60599
C 2.84568 4.76103 -0.17628
H 4.09082 3.12184 -0.85400
C 4.44794 5.31720 -2.59289
H 2.43145 4.62900 -2.91969
C 3.91139 5.86730 -0.18311
H 1.86393 5.17236 -0.43783
H 2.74171 4.32176 0.82038
C 4.11353 6.43462 -1.59496
H 4.54911 5.72544 -3.60688
H 5.42726 4.88360 -2.33692
H 3.62271 6.66274 0.51492
H 4.86644 5.46214 0.18379
H 4.90918 7.19061 -1.59519
H 3.19415 6.94574 -1.91541
C 4.14113 -1.54296 -1.65726
C 4.53813 -1.32215 -3.12473
C 5.20057 -1.02937 -0.67740
H 3.95200 -2.60701 -1.47872
C 5.92168 -1.95145 -3.38422
H 4.62319 -0.23497 -3.27533
C 6.57327 -1.65976 -0.95595
H 5.25899 0.06302 -0.76696
H 4.87642 -1.24293 0.34778
C 6.99658 -1.43952 -2.41498
H 6.21836 -1.75404 -4.42243
H 5.83924 -3.04536 -3.29026
H 7.32196 -1.24421 -0.26978
H 6.52837 -2.74013 -0.75236
H 7.95425 -1.93718 -2.61416
H 7.15985 -0.36555 -2.58666
C -0.95468 -4.50425 -1.19006
C -1.05521 -4.95442 -2.65432
C 0.09080 -5.29487 -0.39794
H -1.93272 -4.59269 -0.70419
C -1.31473 -6.47325 -2.70919
H -0.07737 -4.75680 -3.11974
C -0.17940 -6.80498 -0.47224
H 1.08277 -5.06277 -0.80564
H 0.08645 -4.95132 0.64245
C -0.26915 -7.28221 -1.92857
H -1.34383 -6.79629 -3.75795
H -2.31438 -6.67891 -2.29589
H 0.60607 -7.35145 0.06495
H -1.12454 -7.03376 0.04216
H -0.51318 -8.35163 -1.96645
H 0.71320 -7.16747 -2.40993
C -4.86391 -0.71303 -0.83677
C -5.35427 -0.89343 -2.28087
C -5.23099 -1.89521 0.06508
H -5.27072 0.21373 -0.41674
C -6.86997 -1.17676 -2.28092
H -4.84091 -1.77884 -2.68673
C -6.74298 -2.16603 0.04398
H -4.68161 -2.78077 -0.27941
H -4.88658 -1.68802 1.08413
C -7.24999 -2.36804 -1.39059
H -7.20468 -1.34748 -3.31244
H -7.40094 -0.27835 -1.92982
H -6.97371 -3.04310 0.66180
H -7.27382 -1.31632 0.49842
H -8.33809 -2.51205 -1.39512
H -6.81031 -3.28712 -1.80513
C 3.76477 3.08024 -3.59304
C 3.48054 -1.86315 -4.09406
C -5.00586 0.31288 -3.16089
H -0.01710 -2.81769 4.65003
C -0.43877 -0.49616 3.74606
O -1.58220 -0.60730 4.39528
H -0.47963 -0.41022 2.66284
O 1.83779 0.09051 2.41201
H 2.37460 0.66170 1.77941
O 2.41709 -2.65653 3.78154
C 3.70106 -2.58952 3.10278
H 3.63903 -1.81448 2.33474
H 4.39354 -2.26713 3.88328
C 4.09731 -3.93532 2.51876
H 5.11299 -3.86992 2.11211
H 4.08333 -4.71461 3.28762
H 3.42740 -4.21897 1.70154
C -2.78539 -0.82753 3.58865
H -2.99898 0.10293 3.05638
H -2.56978 -1.60103 2.84522
C -3.90037 -1.22551 4.53227
H -4.82278 -1.36610 3.95919
H -3.66938 -2.16262 5.04929
H -4.07862 -0.44715 5.28125
C -3.05844 4.43283 -2.95572
H -2.31633 5.22923 -3.09988
H -2.55245 3.47234 -3.08822
H -3.81335 4.53508 -3.74449
C -2.12448 -4.16995 -3.42426
H -3.12169 -4.34819 -3.00000
H -1.92951 -3.09447 -3.38618
H -2.15108 -4.47807 -4.47619
H 3.85525 3.47795 -4.61068
H 4.72982 2.62858 -3.32620
H 3.01065 2.28805 -3.60025
H 3.77205 -1.67008 -5.13318
H 3.36048 -2.94830 -3.97775
H 2.50732 -1.39557 -3.91981
H -5.50377 1.22089 -2.79557
H -3.92831 0.49956 -3.16714
H -5.33206 0.14757 -4.19459

RR2Me.log
Free Energy = -3237.532953
Zero-point Energy = -3237.412304
Potential Energy = -3238.76621798
Nimag = 1 (-190.8083 cm-1)

Charge = 0 Multiplicity = 1
C -0.60702 -0.93681 -0.30588
C -1.36769 0.24114 -0.13278
C -0.48703 1.35230 -0.22396
C 0.81618 0.85259 -0.45275
C 0.74751 -0.56167 -0.51488
C -2.82811 0.29556 0.08828
C -0.81219 2.77765 -0.06863
O -0.06615 3.61188 0.42210
C 2.06228 1.63802 -0.40672
O 2.97890 1.42012 0.40102
C 1.87305 -1.47396 -0.71331
O 2.00280 -2.58264 -0.20044
C -1.15555 -2.30068 -0.20648
O -1.89658 -2.68225 0.69519
O -3.39515 0.94151 0.95562
C 1.93044 0.40132 3.58543
C 2.98664 1.13011 4.15532

C	2.93163	1.48394	5.49782
C	1.83677	1.12003	6.29991
C	0.77997	0.42031	5.74007
C	0.80179	0.06471	4.37668
H	3.83257	1.40813	3.53336
H	3.75238	2.04885	5.93206
H	1.81149	1.40254	7.34774
H	-0.09143	0.16274	6.33294
O	2.13003	2.60752	-1.31413
O	-3.48617	-0.47905	-0.80852
O	-2.04079	3.07194	-0.55651
O	2.79500	-0.95041	-1.56124
O	-0.76252	-3.09328	-1.22245
C	1.33076	-2.76276	2.92446
H	1.43875	-2.75567	1.83855
C	0.10776	-2.68217	3.54189
H	-0.76217	-2.88967	2.92795
C	-2.54113	4.41776	-0.36404
C	-3.57858	4.66673	-1.46823
C	-3.13153	4.55121	1.04371
H	-1.69748	5.10878	-0.47983
C	-4.25202	6.03601	-1.24788
H	-4.34835	3.88659	-1.36426
C	-3.80408	5.91804	1.23953
H	-3.85787	3.74158	1.18894
H	-2.33310	4.40351	1.77852
C	-4.85898	6.17822	0.15511
H	-5.02247	6.18644	-2.01562
H	-3.50506	6.83019	-1.40214
H	-4.25627	5.97162	2.23795
H	-3.04247	6.71101	1.20029
H	-5.29738	7.17716	0.27774
H	-5.68211	5.45781	0.26988
C	3.25445	3.53743	-1.26984
C	3.42020	4.08848	-2.69231
C	2.97184	4.62966	-0.23614
H	4.14507	2.96706	-0.98272
C	4.50619	5.18433	-2.69605
H	2.46222	4.55497	-2.96709
C	4.06577	5.70770	-0.26116
H	1.99309	5.07128	-0.45598
H	2.89004	4.17592	0.75609
C	4.23519	6.29300	-1.66991
H	4.58502	5.60678	-3.70622
H	5.48143	4.72071	-2.47999
H	3.82152	6.49862	0.45866
H	5.02166	5.27225	0.06693
H	5.05022	7.02790	-1.68535
H	3.31949	6.83342	-1.95050
C	4.00123	-1.70682	-1.82979
C	4.37317	-1.46035	-3.29958
C	5.10131	-1.26408	-0.86012
H	3.77309	-2.76710	-1.67505
C	5.72659	-2.13091	-3.60939
H	4.49477	-0.37311	-3.42248
C	6.44300	-1.93498	-1.19023
H	5.19814	-0.17218	-0.91707
H	4.79065	-1.49951	0.16445
C	6.84070	-1.68555	-2.65164
H	6.00639	-1.91414	-4.64841
H	5.60725	-3.22357	-3.54441
H	7.22215	-1.56814	-0.51014
H	6.36296	-3.01866	-1.01809
H	7.77537	-2.21000	-2.88790
H	7.03781	-0.61322	-2.79595
C	-1.17117	-4.48598	-1.20599
C	-1.30440	-4.92883	-2.66993
C	-0.14081	-5.31013	-0.42813
H	-2.14540	-4.54336	-0.70774
C	-1.60573	-6.43974	-2.72758
H	-0.32770	-4.75617	-3.14743
C	-0.45430	-6.81163	-0.50593
H	0.85323	-5.10328	-0.84397
H	-0.12520	-4.97226	0.61391
C	-0.57256	-7.27941	-1.96311
H	-1.65595	-6.75712	-3.77729
H	-2.60552	-6.62097	-2.30320
H	0.32115	-7.38212	0.02073
H	-1.40017	-7.01634	0.01725
H	-0.84427	-8.34205	-2.00343
H	0.40699	-7.18691	-2.45479
C	-4.93143	-0.55510	-0.71530
C	-5.46288	-0.73913	-2.14426
C	-5.32725	-1.70472	0.21600
H	-5.28911	0.39497	-0.30256
C	-6.98892	-0.95708	-2.10518
H	-4.99709	-1.65248	-2.54557
C	-6.84967	-1.91047	0.23396
H	-4.82441	-2.61912	-0.12419
H	-4.95148	-1.49392	1.22316
C	-7.39864	-2.11508	-1.18467
H	-7.35433	-1.13151	-3.12561
H	-7.47284	-0.03056	-1.75922
H	-7.10293	-2.76609	0.87268
H	-7.33293	-1.03110	0.68506
H	-8.49172	-2.21176	-1.16152
H	-7.00892	-3.05948	-1.59222
C	-2.96588	4.55736	-2.86953
C	3.73000	2.98282	-3.70851
C	3.27407	-1.93455	-4.25759
C	-2.36173	-4.11206	-3.42261
C	-5.08447	0.43595	-3.05373
H	0.04130	-2.84804	4.61217
C	-0.33647	-0.53417	3.71146
O	-1.46530	-0.60152	4.39213
H	-0.40414	-0.44129	2.63012
O	1.92877	-0.03554	2.32027
H	2.45284	0.52827	1.66867
O	2.44075	-2.78839	3.64306
C	3.69527	-2.75272	2.90901
H	3.71463	-3.60098	2.21688
H	3.71338	-1.82775	2.32683
C	4.81997	-2.81540	3.92211
H	5.78419	-2.78821	3.40338
H	4.77055	-1.96302	4.60676
H	4.76933	-3.73785	4.50915
C	-2.69888	-0.77057	3.61946
H	-2.90885	0.18194	3.12620
H	-2.52513	-1.52262	2.84372
C	-3.79107	-1.17633	4.58621
H	-4.73493	-1.27675	4.04025
H	-3.56487	-2.13584	5.06272
H	-3.92655	-0.42096	5.36705
H	-3.73023	4.70533	-3.64176
H	-2.19000	5.31999	-3.01857
H	-2.50824	3.57613	-3.02387
H	-5.53681	1.37005	-2.69497
H	-4.00058	0.57765	-3.08609
H	-5.43976	0.26594	-4.07701
H	-3.35784	-4.26496	-2.98608
H	-2.13694	-3.04247	-3.38277
H	-2.41048	-4.41460	-4.47537
H	3.54836	-1.72298	-5.29782
H	3.11595	-3.01737	-4.16818
H	2.32356	-1.43635	-4.04673
H	3.79412	3.39408	-4.72276
H	4.69214	2.50307	-3.48351
H	2.95610	2.20994	-3.70017

RR1-Me-opp.log
Free Energy = -3237.530334
Zero-point Energy = -3237.411865
Potential Energy = -3239.20324100
Nimag = 1 (-82.6868 cm-1)

Charge = 0 Multiplicity = 1
C 0.96061 -1.14211 -0.02119
C 1.02641 0.22377 0.33011
C -0.29406 0.70413 0.49856
C -1.18685 -0.37929 0.25277
C -0.41558 -1.51616 -0.06036
C 2.27557 1.02260 0.44744
C -0.59147 2.09492 0.82093
O 0.15141 3.03581 0.54300
C -2.66052 -0.28870 0.21306
O -3.28487 0.49647 -0.51488
C -1.00890 -2.82886 -0.37279
O -2.01720 -2.96971 -1.05421
C 2.06474 -2.00824 -0.45427
O 1.96934 -2.84076 -1.34534
O 3.02791 1.26665 -0.48667
C -1.85560 2.53067 -3.08844
C -3.09419 2.57822 -3.75134
C -3.24526 3.40111 -4.85842
C -2.18216 4.19150 -5.33670
C -0.96146 4.15929 -4.68813
C -0.77880 3.34016 -3.55180
H -3.91429 1.96626 -3.38751
H -4.20546 3.43221 -5.36668
H -2.32553 4.82669 -6.20502
H -0.13305 4.77203 -5.02862
O -3.27770 -1.12548 1.04592
O 2.50444 1.42341 1.71294
O -1.76495 2.26313 1.47983
O -0.36493 -3.85857 0.21592
O 3.21554 -1.78019 0.23037
C 0.60353 0.32155 -3.35190
H 0.56233 -0.21166 -2.40424
C 1.50968 1.31550 -3.56657
H 2.30274 1.42798 -2.83687
C -2.06431 3.59370 1.98208
C -3.58738 3.78266 1.97718
C -1.45860 3.72233 3.38415
H -1.59743 4.31981 1.30815
C -3.93892 5.12447 2.65510
H -4.01828 2.97052 2.58342
C -1.82416 5.06190 4.03874
H -1.83542 2.89280 3.99818
H -0.37153 3.60489 3.31691
C -3.34529 5.26189 4.06364
H -5.03085 5.23224 2.68804
H -3.56805 5.94760 2.02482
H -1.41063 5.10615 5.05392
H -1.35839 5.88429 3.47604
H -3.59705 6.24348 4.48500
H -3.79938 4.51038 4.72600
C -4.72792 -1.03954 1.22149
C -5.43206 -2.22241 0.53779
C -4.95044 -1.00852 2.73612
H -5.06172 -0.10282 0.76587
C -6.92805 -2.20868 0.92019
H -4.98352 -3.14276 0.94234
C -6.44517 -0.99802 3.08505
H -4.47127 -1.89342 3.17632
H -4.44212 -0.13175 3.15476
C -7.16716 -2.18577 2.43565
H -7.41562 -3.08240 0.46929
H -7.40157 -1.32484 0.46513
H -6.57178 -1.01439 4.17456
H -6.89835 -0.05989 2.73210
H -8.24287 -2.14280 2.64865
H -6.79674 -3.12186 2.87853
C -0.96632 -5.17854 0.10239
C 0.16232 -6.21938 0.11854
C -1.95124 -5.35143 1.26447
H -1.50462 -5.22354 -0.85032
C -0.44300 -7.63732 0.19330
H 0.74547 -6.04710 1.03648
C -2.53656 -6.76984 1.30865
H -1.41632 -5.14175 2.20096
H -2.74469 -4.60131 1.17179
C -1.41843 -7.81970 1.36316
H 0.37289 -8.36908 0.25682
H -0.96928 -7.84691 -0.75081
H -3.20659 -6.87064 2.17184
H -3.15221 -6.94149 0.41344
H -1.84157 -8.83245 1.34878
H -0.87375 -7.72055 2.31360
C 4.36896 -2.61347 -0.06853
C 5.49446 -1.76045 -0.67580
C 4.78052 -3.28945 1.24209
H 4.05241 -3.36571 -0.79707
C 6.75669 -2.63291 -0.84132
H 5.72563 -0.96045 0.04471
C 6.04354 -4.14368 1.05945
H 4.96384 -2.51257 1.99736
H 3.94583 -3.89789 1.60997
C 7.18907 -3.31245 0.46555
H 7.57190 -2.01338 -1.23751
H 6.55854 -3.40365 -1.60209
H 6.34071 -4.58145 2.02063
H 5.82131 -4.98620 0.38823
H 8.06921 -3.94443 0.29055
H 7.49441 -2.54440 1.19162
C 3.79496 2.01299 2.04007
C 3.57077 3.27284 2.88915
C 4.59508 0.93643 2.78142
H 4.29257 2.27750 1.10185
C 4.92675 3.78590 3.41975
H 2.95595 2.97356 3.75189
C 5.93829 1.47414 3.29261
H 3.98984 0.58353 3.62756
H 4.73690 0.07809 2.11544
C 5.72827 2.71458 4.17106
H 4.75040 4.65610 4.06543
H 5.52373 4.15130 2.56956
H 6.46665 0.69004 3.84912
H 6.58006 1.73713 2.43863
H 6.69343 3.12380 4.49602
H 5.18647 2.42558 5.08350
C -5.25750 -2.22402 -0.98608
C 1.09633 -6.08455 -1.08971
C 2.83102 4.37358 2.11990
H 1.62325 1.75063 -4.55361
C 0.43001 3.32005 -2.78578
O 1.38170 4.17558 -3.07759
H 0.43027 2.88013 -1.79258
O -1.59556 1.76368 -2.03662
H -2.37289 1.30688 -1.58835
O -0.29598 -0.01242 -4.27039
C -1.18217 -1.11844 -3.93630
H -1.53579 -0.99569 -2.90871
H -2.02587 -0.99524 -4.61927
C -0.49532 -2.46080 -4.12485
H -1.21323 -3.25955 -3.91148
H -0.13218 -2.57348 -5.15196
H 0.34390 -2.57900 -3.43114
C 2.45208 4.33709 -2.09014
H 2.04750 4.95671 -1.28414

H 2.70420 3.35482 -1.68172
C 3.62434 4.99489 -2.78702
H 4.42959 5.15799 -2.06307
H 4.00941 4.35981 -3.59081
H 3.34021 5.96355 -3.21051
C -4.18020 3.70380 0.56527
H -3.75823 4.48709 -0.07856
H -3.97986 2.73402 0.10363
H -5.26665 3.85178 0.59545
C 5.08243 -1.11082 -2.00186
H 4.79177 -1.87071 -2.73796
H 4.24194 -0.42745 -1.85921
H 5.91761 -0.53708 -2.42248
H -5.81048 -3.06311 -1.42612
H -5.65006 -1.29782 -1.42445
H -4.20820 -2.32743 -1.26843
H 1.90808 -6.82025 -1.02948
H 0.54930 -6.27416 -2.02320
H 1.53331 -5.08550 -1.15297
H 3.43774 4.72373 1.27276
H 1.87361 4.02066 1.72868
H 2.64681 5.23875 2.76884

SS1p-OMe ($TS_{(S,S)}$ in manuscript)
Free Energy = -4768.421226
Zero-point Energy = -4768.268276
Potential Energy = -4770.05101772
Nimag = 1 (-190.9914 cm-1)

Charge = 0 Multiplicity = 1
C -0.18193 -0.87110 -1.60545
C 0.90164 -1.17352 -0.74548
C 1.52816 0.05352 -0.37940
C 0.81895 1.10401 -1.01184
C -0.22709 0.53580 -1.77867
C 1.37203 -2.53377 -0.45698
C 2.76632 0.24042 0.38146
O 3.60753 1.10722 0.14620
C 1.17111 2.54067 -0.97190
O 1.33367 3.24196 -1.96079
C -1.07645 1.23740 -2.75896
O -1.29921 0.82613 -3.89018
C -0.99014 -1.87404 -2.32259
O -0.53294 -2.89918 -2.81501
O 2.54354 -2.92346 -0.61180
C 5.67537 -0.44264 -3.26239
C 6.77809 -0.70289 -4.10896
C 7.06690 -1.99477 -4.50407
C 6.25683 -3.05716 -4.05463
C 5.16435 -2.83467 -3.23024
C 4.85008 -1.52170 -2.83171
H 7.39892 0.12795 -4.42831
H 7.91570 -2.19448 -5.15030
H 6.49024 -4.07368 -4.36056
H 4.54109 -3.65355 -2.88363
O 3.81994 -1.20769 -2.05906
H 3.37579 -1.97292 -1.56109
O 1.29486 2.99850 0.29301
O 0.41522 -3.35639 -0.03160
O 2.90944 -0.66395 1.37755
O -1.56263 2.40626 -2.28861
O -2.29536 -1.54126 -2.38895
C 5.38221 0.85619 -2.74327
H 4.64883 0.96856 -1.94723
C 3.69485 1.68651 -4.26640
H 3.54044 2.62097 -3.73996
H 4.42875 1.64502 -5.06361
C 2.70109 0.75737 -4.18652
H 1.88494 0.86615 -3.47431
O 6.26890 1.81375 -2.91682
C 6.10211 3.02521 -2.12269
H 5.04170 3.29107 -2.11635
H 6.65924 3.78254 -2.67767
C 6.64152 2.83110 -0.71568
H 6.58852 3.78389 -0.17738
H 6.04088 2.10044 -0.16540
H 7.68660 2.50597 -0.74027
O 2.70568 -0.33028 -4.94267
C 1.60951 -1.27051 -4.72417
H 0.66684 -0.71719 -4.77551
H 1.71127 -1.68603 -3.71946
C 1.70178 -2.34571 -5.78565
H 2.66767 -2.85960 -5.73725
H 0.90887 -3.08016 -5.61216
H 1.58069 -1.92561 -6.78951
C 4.15879 -0.67756 2.10965
C 3.84231 -1.17682 3.53180
C 5.15691 -1.58383 1.38031
H 4.54007 0.34786 2.14653
C 5.15811 -1.37972 4.32145
H 3.36786 -2.16152 3.41630
C 6.45114 -1.76835 2.18413
H 4.67523 -2.55544 1.21087
H 5.36641 -1.15714 0.39363
C 6.15001 -2.29642 3.59277
H 4.91616 -1.78076 5.31309
H 5.63407 -0.40388 4.49351
H 7.12729 -2.44904 1.65172
H 6.97767 -0.80536 2.26358
H 7.07548 -2.38634 4.17607
H 5.72630 -3.30867 3.51813
C 1.72946 4.36696 0.49072
C 1.42293 4.69964 1.96593
C 3.22445 4.49503 0.17148
H 1.14587 5.00983 -0.17893
C 2.01839 6.07815 2.34146
H 1.95220 3.93978 2.55804
C 3.78490 5.87094 0.55781
H 3.75220 3.70200 0.71506
H 3.36304 4.30473 -0.89668
C 3.51719 6.17721 2.03573
H 1.82561 6.26620 3.40469
H 1.49346 6.87094 1.79056
H 4.86159 5.90932 0.34395
H 3.31898 6.64985 -0.06390
H 3.88931 7.17636 2.29688
H 4.06860 5.46120 2.66269
C -2.27041 3.26029 -3.22363
C -3.20828 4.14773 -2.38331
C -1.25666 4.07786 -4.03226
H -2.85299 2.61794 -3.89242
C -3.87934 5.20908 -3.28791
H -2.56591 4.68125 -1.66846
C -1.94847 5.12634 -4.91516
H -0.57028 4.56532 -3.32914
H -0.65469 3.39283 -4.63782
C -2.85726 6.03607 -4.07865
H -4.50713 5.85862 -2.66570
H -4.55797 4.71254 -3.99579
H -1.19446 5.71814 -5.44930
H -2.55156 4.62277 -5.68543
H -3.37685 6.75850 -4.72156
H -2.24246 6.62231 -3.37986
C -3.16119 -2.37203 -3.20343
C -4.59437 -2.15340 -2.68104
C -3.00915 -1.97887 -4.67733
H -2.86181 -3.41591 -3.05896
C -5.60606 -2.87569 -3.60219
H -4.78824 -1.07441 -2.75877
C -4.02928 -2.70129 -5.56811

H -3.13338 -0.89247 -4.75669
H -1.98700 -2.20311 -4.99819
C -5.46089 -2.46086 -5.07212
H -6.62131 -2.67327 -3.23945
H -5.46405 -3.96291 -3.52563
H -3.91842 -2.36479 -6.60660
H -3.82273 -3.78211 -5.56785
H -6.18125 -3.01255 -5.69010
H -5.70774 -1.39425 -5.17738
C 0.71610 -4.77708 0.11242
C -0.42572 -5.36323 0.96568
C 0.80789 -5.43886 -1.26733
H 1.67204 -4.86217 0.64084
C -0.28528 -6.90251 1.04881
H -1.35360 -5.14484 0.41903
C 0.95025 -6.96308 -1.15107
H -0.09512 -5.18203 -1.83240
H 1.65242 -5.01127 -1.81464
C -0.20036 -7.56183 -0.33328
H -1.13284 -7.30122 1.61920
H 0.61722 -7.15882 1.62142
H 0.98390 -7.40686 -2.15388
H 1.90696 -7.21277 -0.66773
H -0.07340 -8.64665 -0.22398
H -1.14690 -7.40792 -0.87144
C 2.86284 -0.28115 4.27465
C 1.57660 -0.74514 4.58902
C 3.20004 1.01182 4.68684
C 0.67110 0.03520 5.29790
H 1.27354 -1.73586 4.26216
C 2.30251 1.81814 5.39501
H 4.18368 1.41664 4.45922
C 1.02948 1.32666 5.70836
H -0.31830 -0.34023 5.53975
H 2.60605 2.81445 5.69653
C -0.05251 4.60344 2.32504
C -0.52589 3.51837 3.07999
C -0.97671 5.58828 1.96269
C -1.85364 3.43209 3.47979
H 0.15999 2.72206 3.35396
C -2.31906 5.51933 2.35090
H -0.65920 6.44131 1.36786
C -2.76108 4.43802 3.12170
H -2.20447 2.59425 4.07389
H -3.00095 6.30646 2.04925
C -4.22186 3.35112 -1.57591
C -4.08130 3.23561 -0.18441
C -5.32188 2.72128 -2.16593
C -5.00510 2.54291 0.58895
H -3.22380 3.69050 0.30267
C -6.26259 2.01496 -1.40805
H -5.46610 2.77333 -3.24243
C -6.10819 1.92872 -0.01967
H -4.88614 2.46660 1.66528
H -7.10223 1.54480 -1.90778
C -4.76134 -2.53987 -1.21909
C -4.89390 -1.54505 -0.23779
C -4.79966 -3.87159 -0.79473
C -5.07639 -1.86056 1.10306
H -4.84074 -0.50070 -0.53039
C -4.97617 -4.21249 0.55101
H -4.69317 -4.67735 -1.51715
C -5.11982 -3.20129 1.50819
H -5.18986 -1.08005 1.84868
H -5.00170 -5.25865 0.83529
C -0.54810 -4.72531 2.34120
C -1.62389 -3.87090 2.62955
C 0.36824 -4.97668 3.36677
C -1.79242 -3.30836 3.88874
H -2.34038 -3.63516 1.84808
C 0.21995 -4.41853 4.64128
H 1.22277 -5.62570 3.18847
C -0.87044 -3.58227 4.90780
H -2.63573 -2.65821 4.09900
H 0.95264 -4.64361 5.40838
O -6.96365 1.27051 0.82230
O -5.29878 -3.41522 2.84891
O -1.11818 -2.98503 6.11473
O -4.04539 4.26933 3.56465
O 0.07376 2.01920 6.39913
C 0.36215 3.35121 6.79202
H 0.54713 3.99461 5.92251
H -0.52665 3.70675 7.31674
H 1.22495 3.39524 7.47081
C -0.21047 -3.22327 7.17889
H 0.79458 -2.85197 6.94120
H -0.60265 -2.67164 8.03538
H -0.15497 -4.29120 7.43004
C -5.34941 -4.75479 3.31185
H -4.40675 -5.28329 3.12040
H -5.51137 -4.69270 4.38972
H -6.17866 -5.30962 2.85199
C -8.06271 0.57842 0.25295
H -7.72854 -0.21191 -0.43122
H -8.59655 0.12463 1.09017
H -8.73867 1.26114 -0.28004
C -5.00750 5.25500 3.22249
H -5.94295 4.93096 3.68252
H -4.73169 6.24187 3.61835
H -5.14510 5.32233 2.13598

RR1p-OMe ($TS_{(R,R)}$ in manuscript)
Free Energy = -4768.418086
Zero-point Energy = -4768.265059
Potential Energy = -4770.04847893
Nimag = 1 (-174.1375 cm-1)

Charge = 0 Multiplicity = 1
C -0.82140 1.26466 0.82247
C -0.03633 0.53451 1.75322
C -0.33139 -0.84306 1.59171
C -1.29252 -0.96391 0.55758
C -1.59447 0.33871 0.07632
C 0.89262 1.11266 2.74421
C 0.12791 -1.96602 2.43152
O -0.59730 -2.87333 2.81231
C -2.00772 -2.19256 0.19494
O -3.24689 -2.27785 0.11858
C -2.58754 0.67439 -0.95097
O -3.35886 1.63069 -0.90787
C -0.91422 2.73533 0.77879
O -1.00792 3.44434 1.77815
O 0.97262 0.77725 3.91834
C -4.81450 -0.83295 2.87769
C -5.74772 -1.88022 2.93513
C -6.42993 -2.12827 4.11970
C -6.20767 -1.34325 5.26398
C -5.27088 -0.32362 5.22429
C -4.54773 -0.06580 4.04199
H -5.92604 -2.47782 2.04585
H -7.15176 -2.94000 4.15684
H -6.75406 -1.54829 6.17931
H -5.05610 0.26805 6.10793
O -1.21721 -3.23648 -0.04490
O 1.65921 2.08891 2.20547
O 1.44031 -1.88521 2.74256
O -2.57765 -0.20719 -1.97578
O -0.91099 3.23415 -0.47269
C -4.83660 2.26329 1.86365
H -4.33477 2.04853 0.92240

C	-4.17901	2.71709	2.97613
H	-3.18230	3.12139	2.83422
C	1.95223	-2.83666	3.70822
C	3.46821	-2.94676	3.45635
C	1.62227	-2.34844	5.12372
H	1.46874	-3.80176	3.52210
C	4.12774	-3.80360	4.56344
H	3.86909	-1.92709	3.54160
C	2.28977	-3.22036	6.19565
H	1.95943	-1.30880	5.21336
H	0.53433	-2.34219	5.24770
C	3.80602	-3.29289	5.97427
H	5.21149	-3.82538	4.39533
H	3.78335	-4.84384	4.47680
H	2.06333	-2.82306	7.19322
H	1.86956	-4.23674	6.16287
H	4.27576	-3.94317	6.72376
H	4.24063	-2.29154	6.10918
C	-1.82410	-4.54847	-0.23110
C	-0.73476	-5.43317	-0.86657
C	-2.30643	-5.10384	1.11358
H	-2.66846	-4.43126	-0.91939
C	-1.25211	-6.88653	-0.98872
H	0.10361	-5.44024	-0.15609
C	-2.80717	-6.54882	0.97321
H	-1.47434	-5.05258	1.82464
H	-3.09550	-4.45760	1.50824
C	-1.73068	-7.45001	0.35568
H	-0.45484	-7.51016	-1.41071
H	-2.08312	-6.92208	-1.70750
H	-3.11283	-6.92933	1.95577
H	-3.70575	-6.57062	0.33807
H	-2.11191	-8.47053	0.22103
H	-0.87749	-7.52069	1.04582
C	-3.61998	-0.10408	-2.97545
C	-3.04582	-0.71184	-4.27124
C	-4.86104	-0.85733	-2.48457
H	-3.84816	0.95668	-3.12126
C	-4.15511	-0.83047	-5.34371
H	-2.72312	-1.73037	-4.01337
C	-5.94344	-0.95481	-3.56894
H	-4.54838	-1.86182	-2.17452
H	-5.26237	-0.37120	-1.58797
C	-5.38343	-1.59917	-4.84169
H	-3.73331	-1.31071	-6.23497
H	-4.47199	0.17360	-5.65856
H	-6.79735	-1.53049	-3.18958
H	-6.32470	0.04978	-3.80647
H	-6.15003	-1.63516	-5.62640
H	-5.10315	-2.64061	-4.62677
C	-1.17434	4.65302	-0.63518
C	-0.65227	5.03883	-2.03281
C	-2.67806	4.91859	-0.48725
H	-0.61975	5.18950	0.14240
C	-1.04853	6.49880	-2.36426
H	-1.17373	4.38348	-2.74445
C	-3.04015	6.37171	-0.82194
H	-3.20920	4.22978	-1.15540
H	-2.98288	4.67510	0.53497
C	-2.55538	6.74853	-2.22678
H	-0.70644	6.73262	-3.37971
H	-0.51030	7.18413	-1.69417
H	-4.12509	6.51288	-0.73559
H	-2.58020	7.04713	-0.08518
H	-2.78414	7.79939	-2.44679
H	-3.09573	6.14558	-2.97124
C	2.51641	2.84843	3.09527
C	3.61420	3.47248	2.20972
C	1.67952	3.90583	3.82607
H	2.95818	2.15340	3.81772
C	4.45976	4.47482	3.03158
H	3.08943	4.04400	1.43126
C	2.54946	4.88479	4.62560
H	1.08647	4.44750	3.07940
H	0.97117	3.39371	4.48454
C	3.60235	5.54079	3.72442
H	5.19732	4.94066	2.36652
H	5.03530	3.93458	3.79640
H	1.91428	5.64611	5.09634
H	3.05518	4.35194	5.44489
H	4.24179	6.21732	4.30617
H	3.09830	6.15727	2.96568
C	3.79599	-3.45292	2.05937
C	4.32086	-2.58037	1.09358
C	3.59471	-4.78426	1.68254
C	4.64640	-3.01615	-0.18548
H	4.46810	-1.53404	1.34606
C	3.91204	-5.24483	0.39984
H	3.18061	-5.49464	2.39419
C	4.44510	-4.35662	-0.54117
H	5.05868	-2.33105	-0.91950
H	3.74080	-6.28643	0.15156
C	-0.20322	-4.89447	-2.18578
C	1.09277	-4.35939	-2.25417
C	-0.94813	-4.93274	-3.36843
C	1.63196	-3.90127	-3.44999
H	1.68970	-4.29386	-1.34897
C	-0.42856	-4.46886	-4.58216
H	-1.95861	-5.33518	-3.36317
C	0.87247	-3.95382	-4.62692
H	2.64094	-3.50287	-3.48877
H	-1.04006	-4.51902	-5.47620
C	-1.82309	0.03250	-4.78937
C	-0.54334	-0.52645	-4.64427
C	-1.91677	1.26955	-5.43407
C	0.58934	0.10537	-5.14216
H	-0.43183	-1.47313	-4.12417
C	-0.78887	1.92548	-5.93964
H	-2.88553	1.74719	-5.55935
C	0.47350	1.33750	-5.79967
H	1.57153	-0.34349	-5.03382
H	-0.90849	2.88124	-6.43758
C	0.84000	4.80872	-2.21319
C	1.30087	3.82495	-3.10103
C	1.80065	5.57817	-1.54949
C	2.65668	3.62673	-3.33359
H	0.58147	3.19378	-3.61562
C	3.17085	5.39247	-1.76316
H	1.48983	6.34864	-0.84716
C	3.60469	4.41389	-2.66586
H	2.99527	2.86560	-4.02958
H	3.88124	6.01185	-1.22680
C	4.47792	2.43543	1.50611
C	4.31358	2.19186	0.13313
C	5.46835	1.70914	2.17459
C	5.11951	1.28871	-0.54892
H	3.53322	2.71569	-0.41023
C	6.28764	0.79105	1.50859
H	5.62275	1.85279	3.24125
C	6.11891	0.58399	0.13489
H	4.99037	1.11772	-1.61299
H	7.04487	0.25151	2.06656
O	1.64271	1.88135	-6.26074
O	4.91333	4.14868	-2.95980
O	6.86493	-0.27988	-0.62188
O	1.48582	-3.48045	-5.75414
O	4.79140	-4.69250	-1.82341
C	4.61386	-6.03858	-2.23371
H	3.55670	-6.33230	-2.20647
H	4.97104	-6.08665	-3.26426

H	5.20062	-6.73028	-1.61388
C	7.88423	-1.02664	0.02328
H	7.47105	-1.69150	0.79240
H	8.35203	-1.62977	-0.75718
H	8.63970	-0.36993	0.47586
C	5.91596	4.84348	-2.23640
H	5.84200	4.64530	-1.15959
H	6.86985	4.46317	-2.60690
H	5.86581	5.92669	-2.41337
C	1.58138	3.12565	-6.94002
H	1.19762	3.92187	-6.28969
H	2.60838	3.36130	-7.22509
H	0.95962	3.06055	-7.84331
C	0.73719	-3.44166	-6.95815
H	1.40403	-3.01743	-7.71124
H	0.42770	-4.44711	-7.27508
H	-0.14873	-2.80134	-6.85933
H	-4.75592	3.03968	3.83694
C	-3.44264	0.86488	3.99614
O	-3.04914	1.39195	5.13800
H	-2.70051	0.74266	3.21117
O	-4.17085	-0.47396	1.76083
H	-3.95880	-1.22825	1.12300
O	-6.12981	1.98657	1.92149
C	-6.72594	1.43461	0.71878
H	-6.11400	0.58888	0.38410
H	-7.69246	1.05653	1.05859
C	-6.88716	2.48355	-0.37034
H	-7.45062	2.05471	-1.20687
H	-7.43589	3.35346	0.00493
H	-5.91433	2.80676	-0.75304
C	-1.70908	1.98199	5.17534
H	-0.98431	1.17266	5.05193
H	-1.60642	2.66138	4.32364
C	-1.56516	2.69249	6.50463
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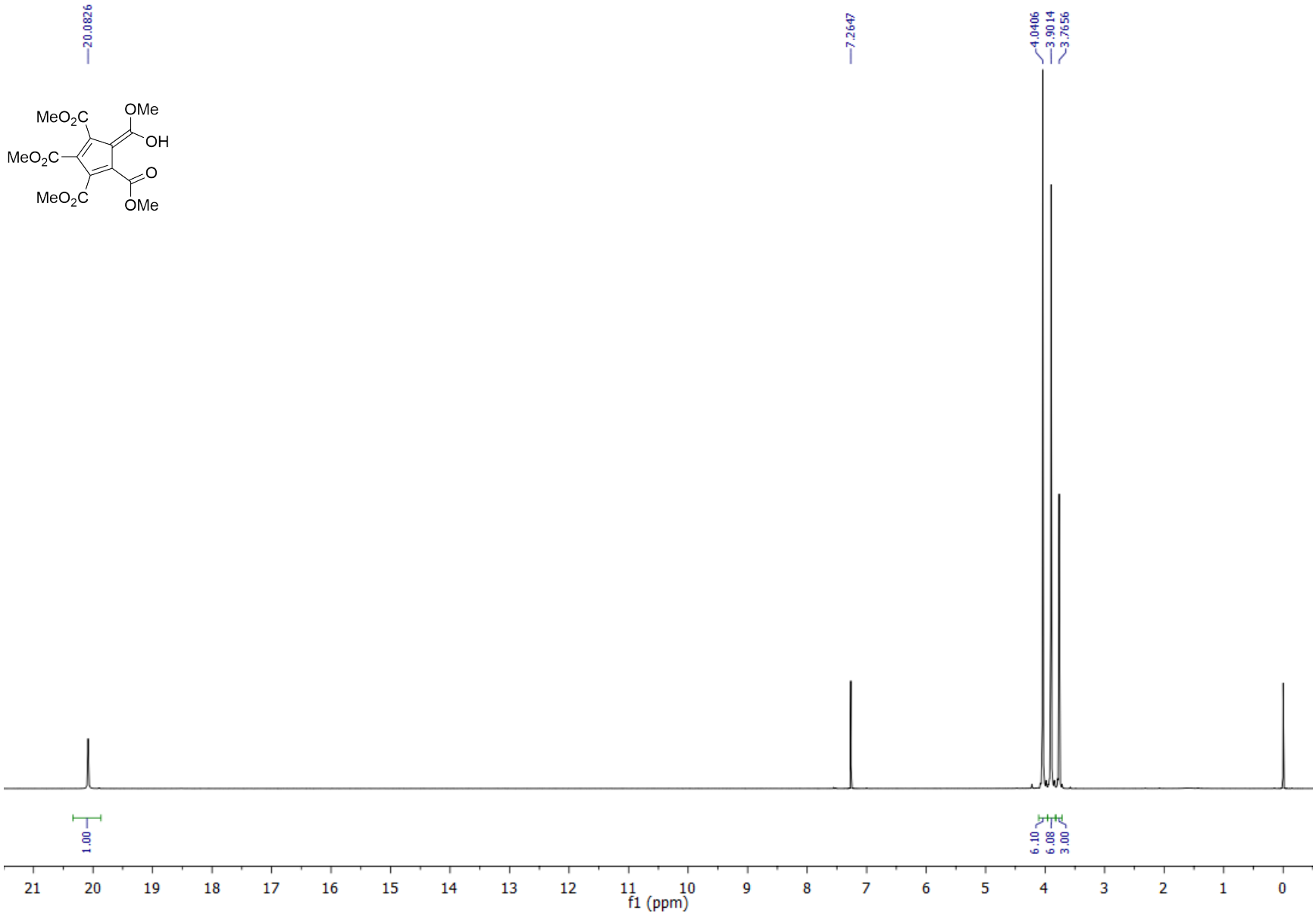
H	-2.29278	3.50475	6.60323
H	-1.70264	1.99622	7.33819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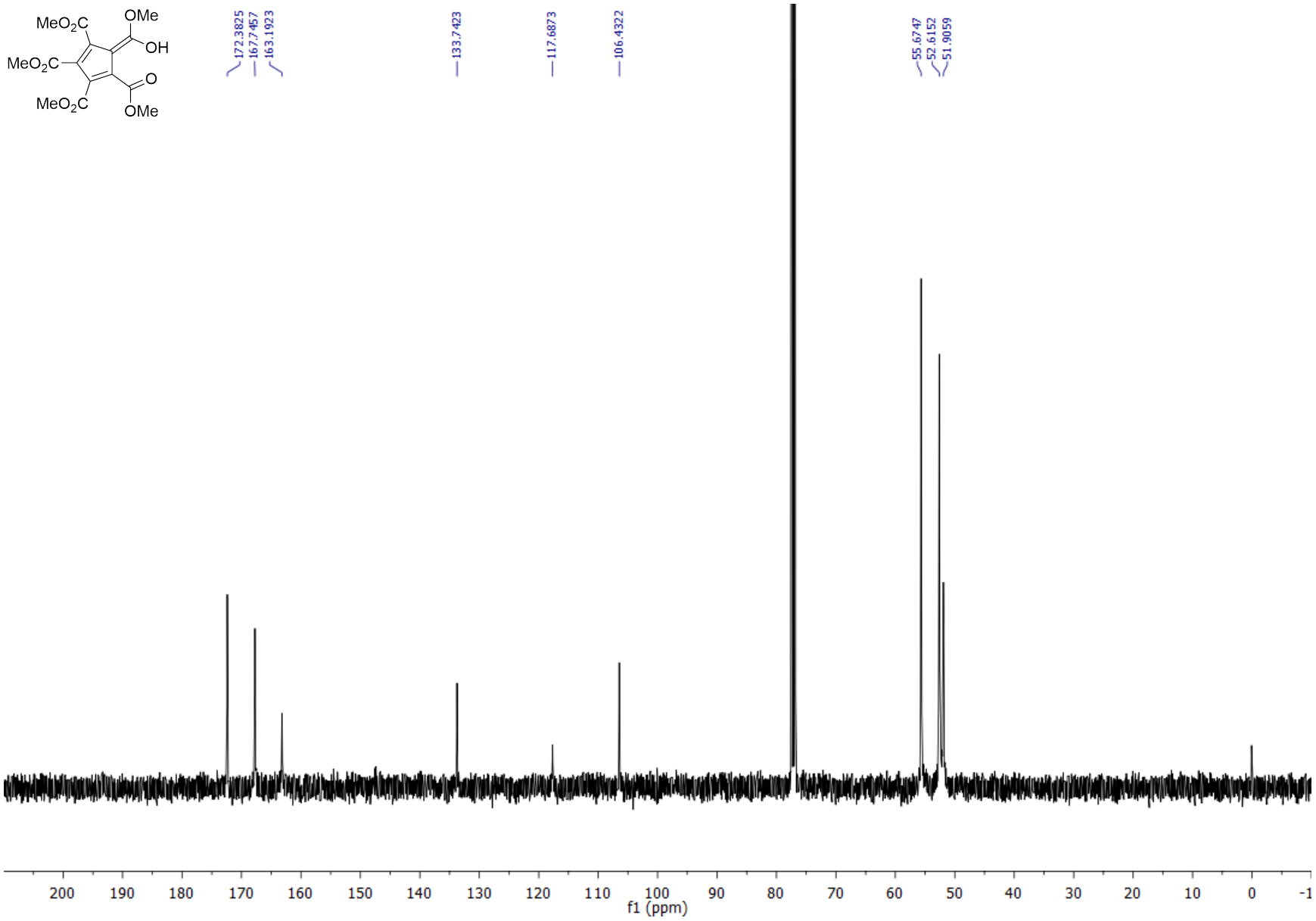
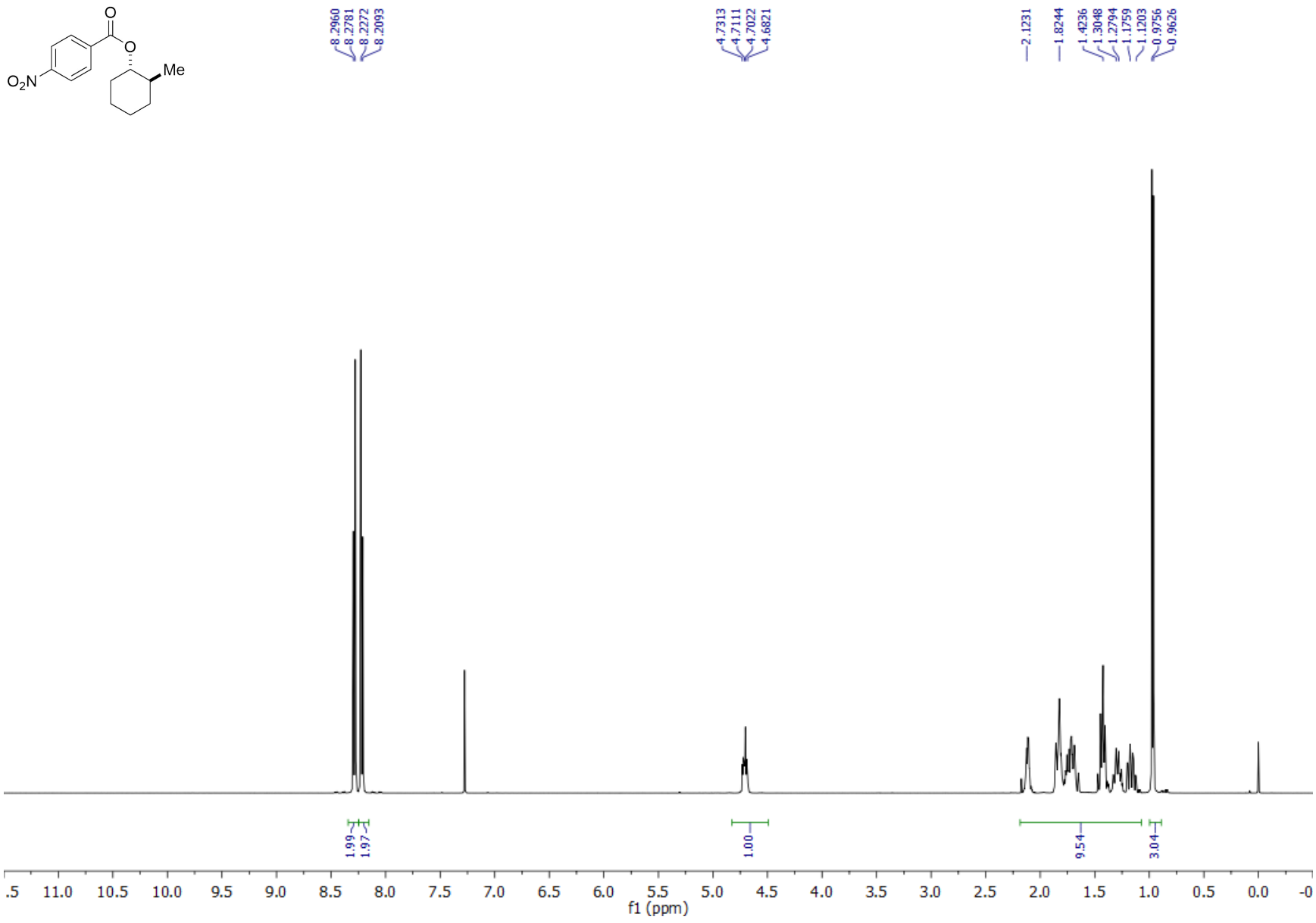
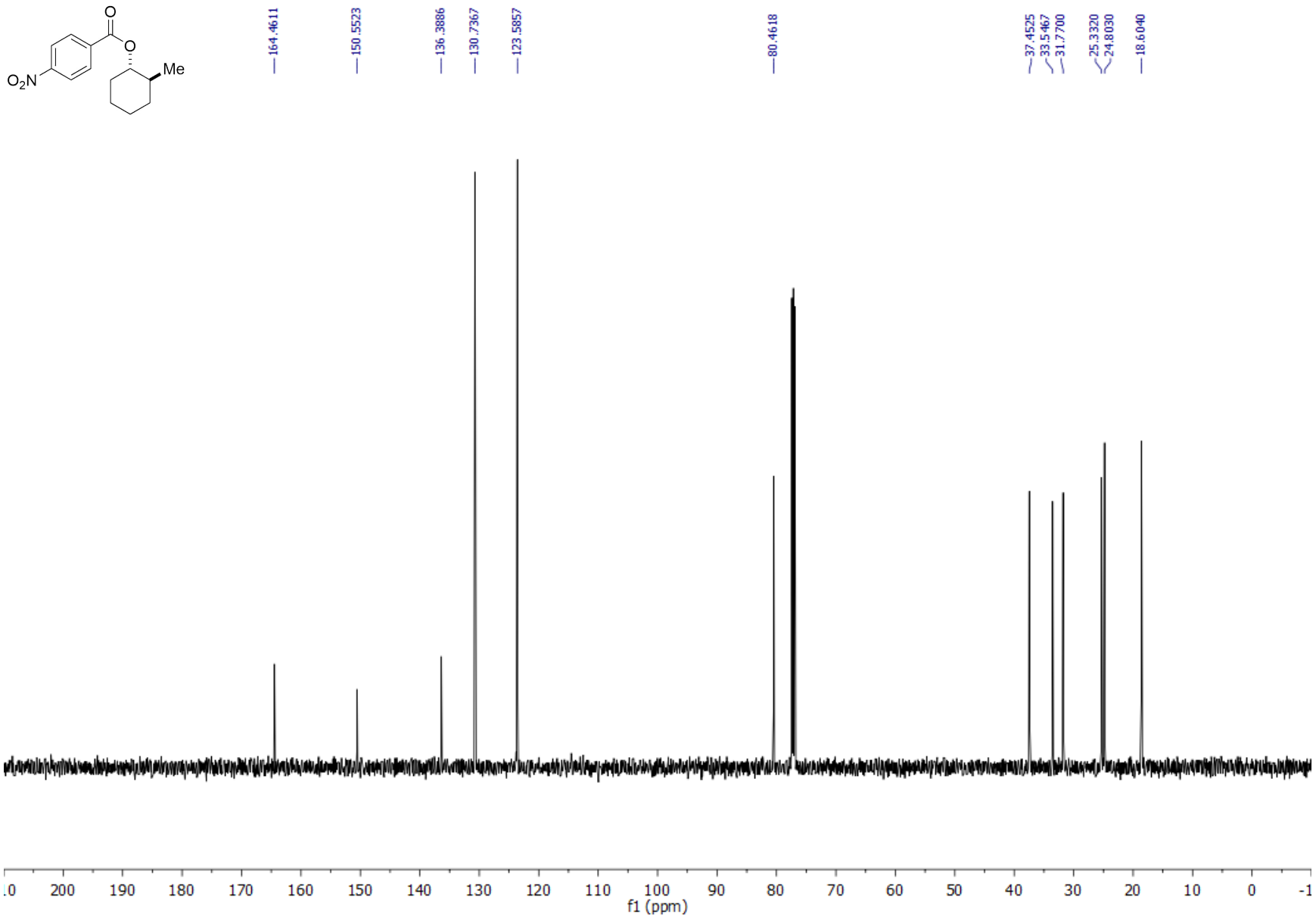
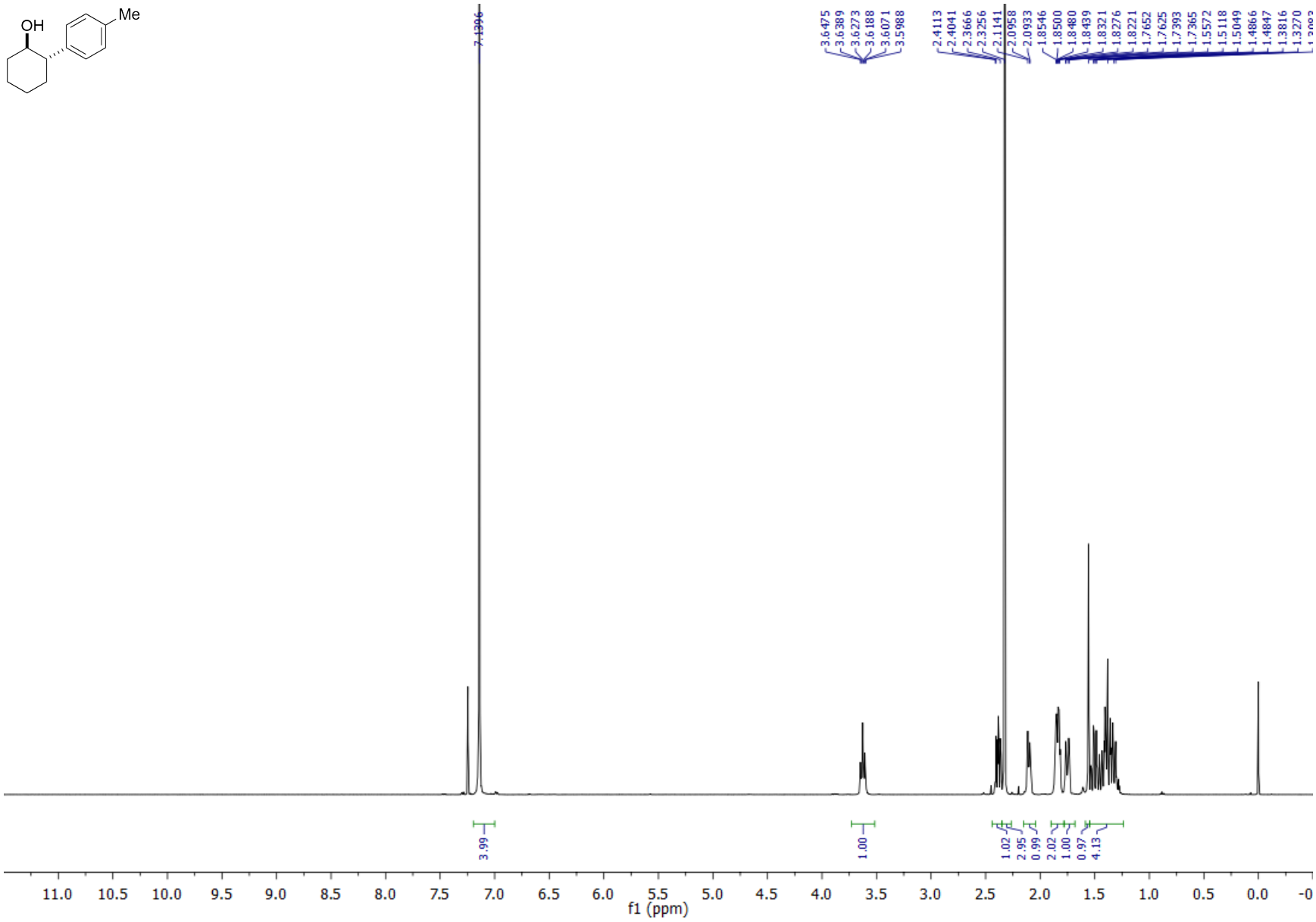
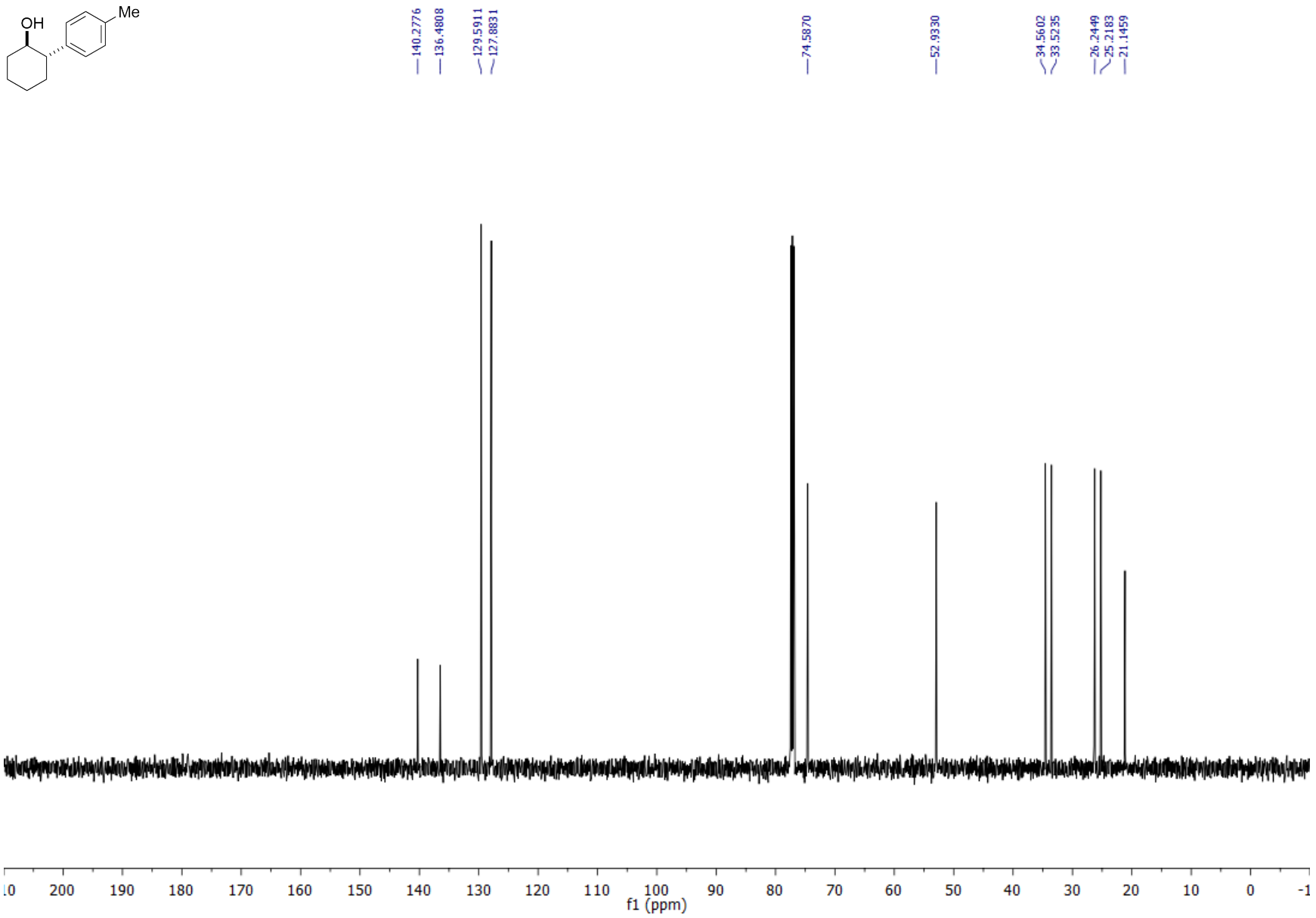
7.2647
4.0406
3.9014
3.7656
MeO2C
OMe
OH
MeO2C
O
MeO2C
OMe
1.00
6.10
6.08
3.00
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

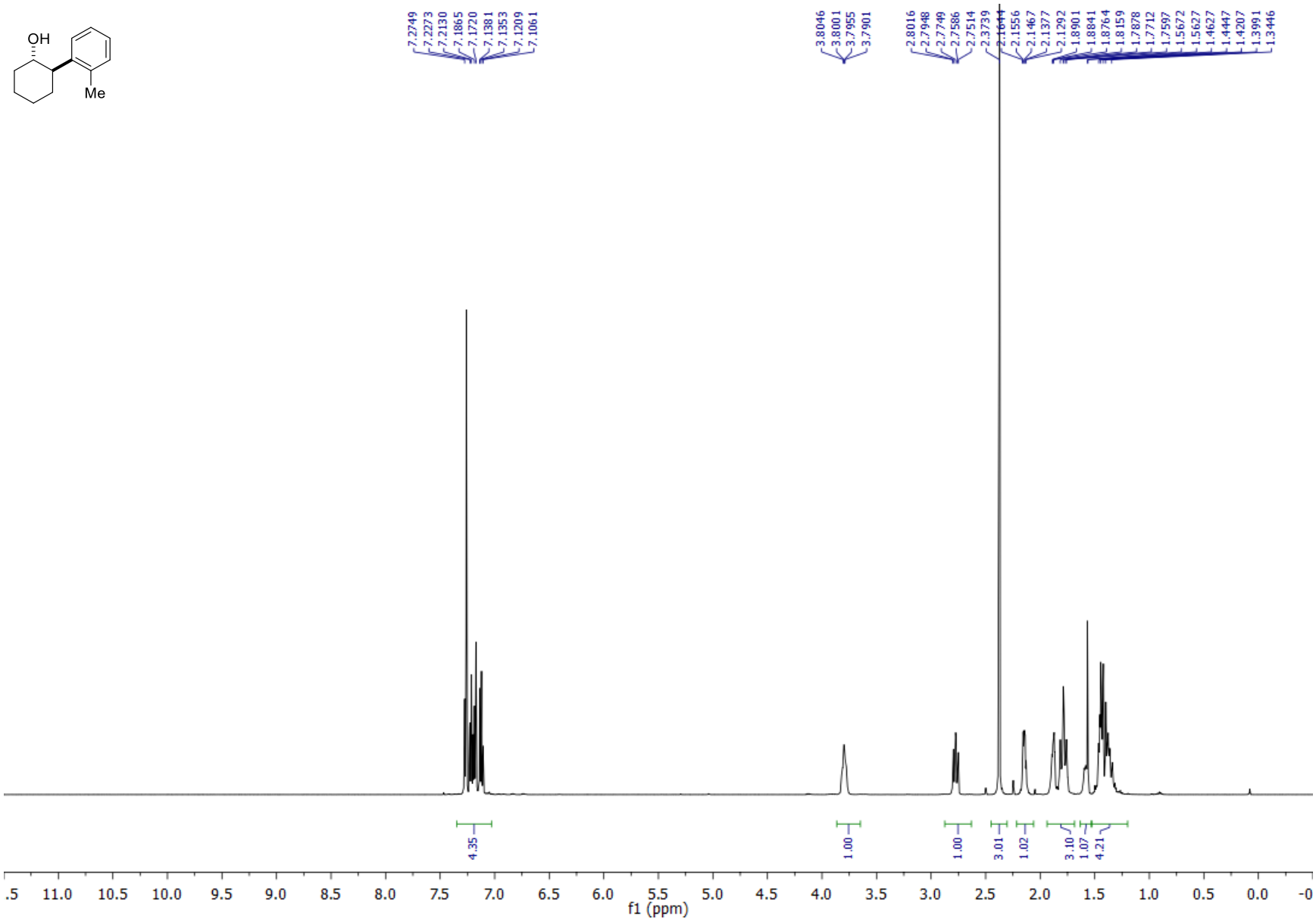

MeO2C
OMe
OH
MeO2C
O
MeO2C
OMe
172.3825
167.7457
163.1923
133.7423
117.6873
106.4322
55.6747
52.6152
51.9059
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

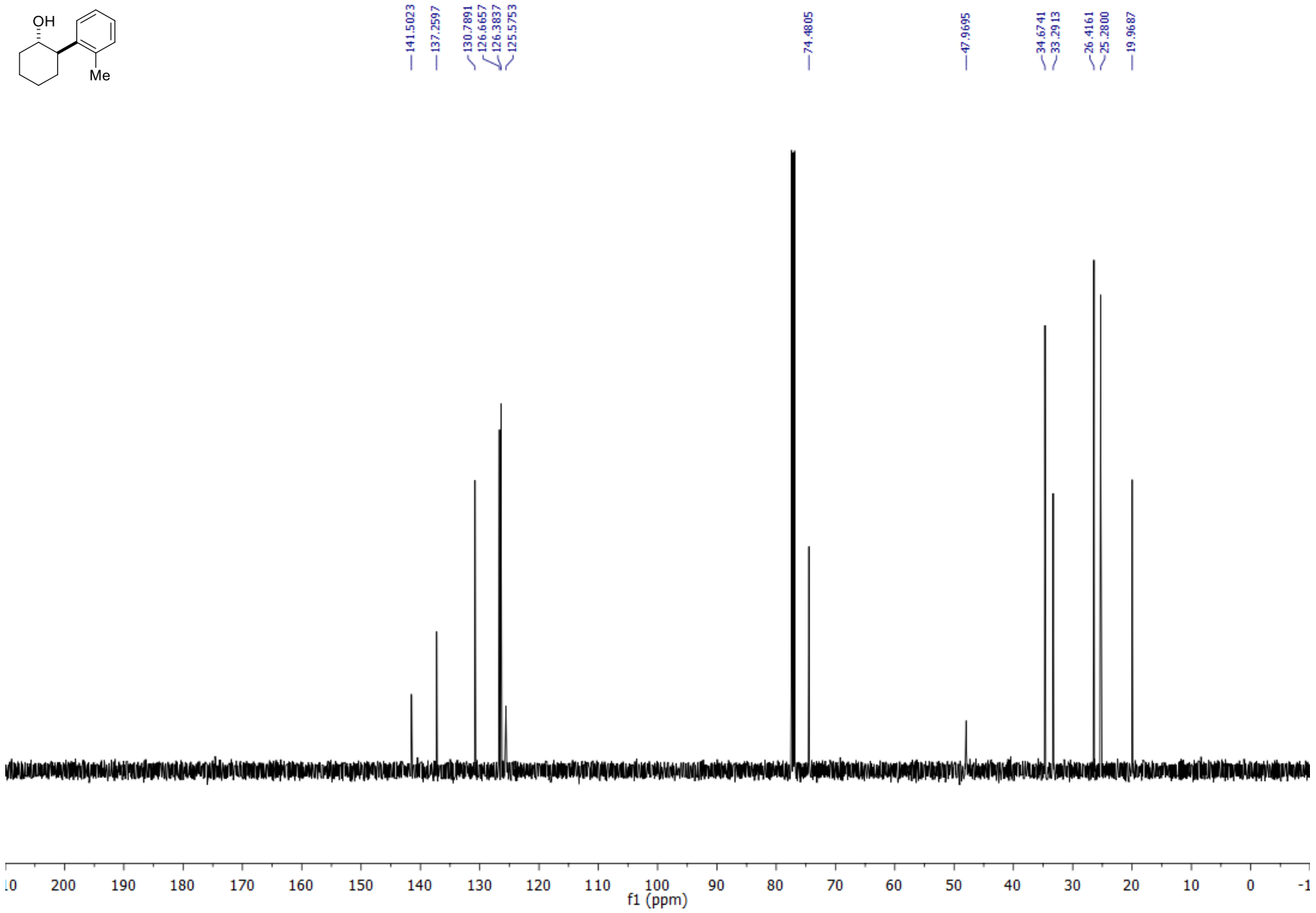

O
O
O2N
Me
8.2960
8.2781
8.2272
8.2093
4.7313
4.7111
4.7022
4.6821
2.1231
1.8244
1.4236
1.3048
1.2794
1.1759
1.1203
0.9756
0.9626
1.99
1.97
1.00
9.54
3.04
f1 (ppm)

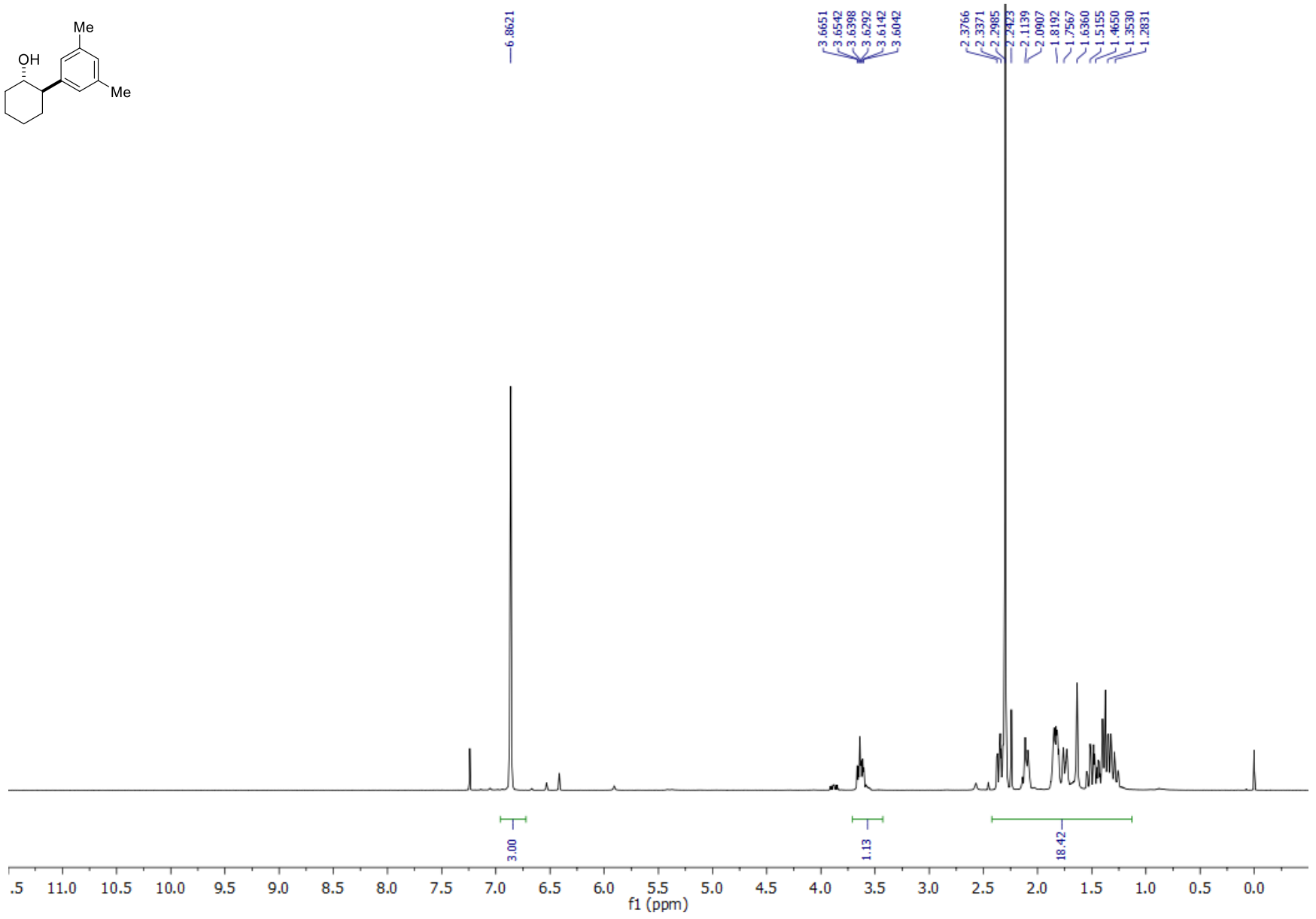

O
O
O2N
Me
164.4611
150.5523
136.3886
130.7367
123.5857
80.4618
37.4525
33.5467
31.7700
25.3320
24.8030
18.6040
f1 (ppm)

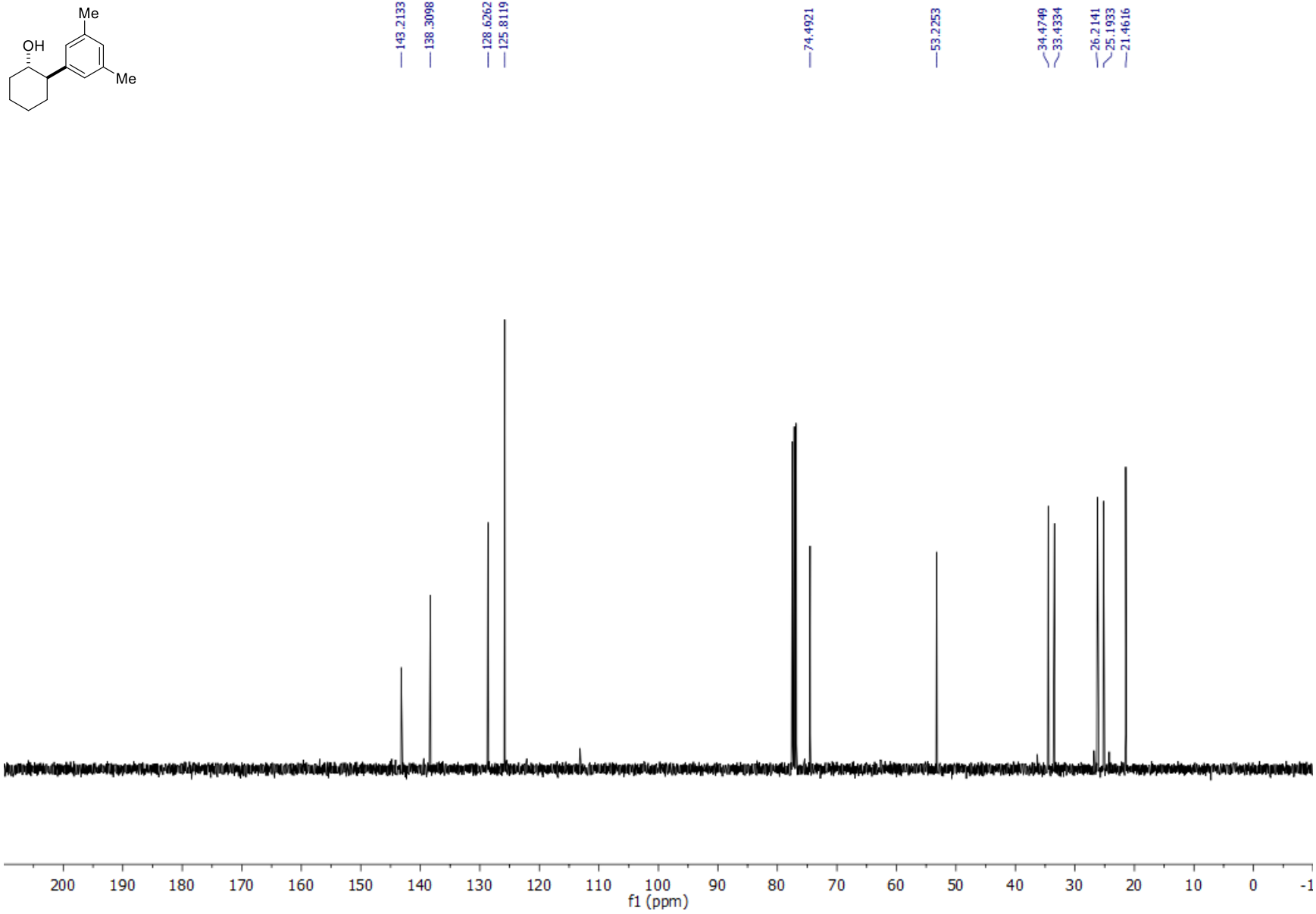

OH
Me
7.1396
3.6475
3.6389
3.6273
3.6188
3.6071
3.5988
2.4113
2.4041
2.3666
2.3256
2.1141
2.0958
2.0933
1.8546
1.8500
1.8480
1.8439
1.8321
1.8276
1.8221
1.7652
1.7625
1.7393
1.7365
1.5572
1.5118
1.5049
1.4866
1.4847
1.3816
1.3270
3.99
1.00
1.02
2.95
0.99
2.02
1.00
0.97
4.13
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

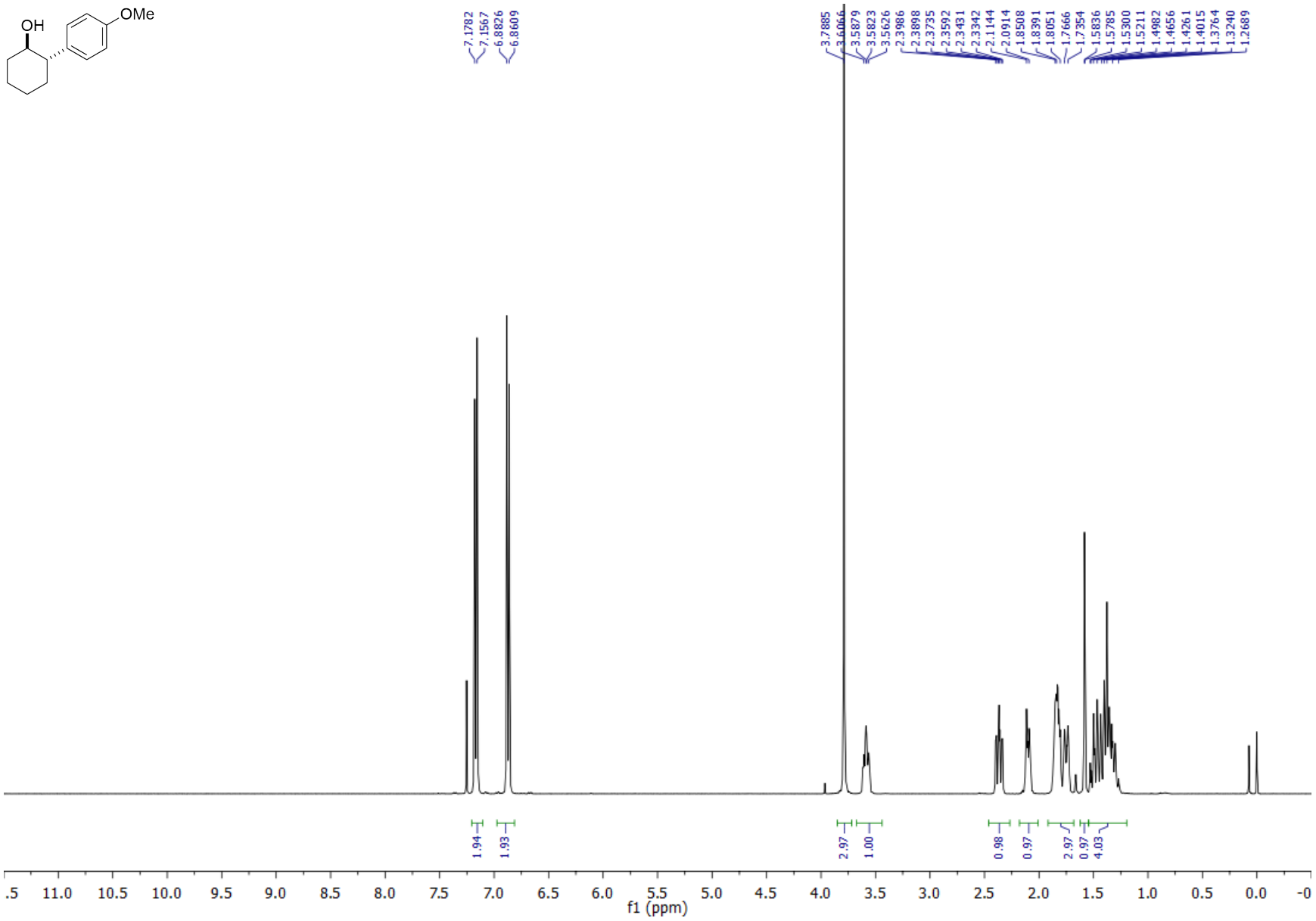

OH
Me
140.2776
136.4808
129.5911
127.8831
74.5870
52.9330
34.5602
33.5235
26.2449
25.2183
21.1459
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

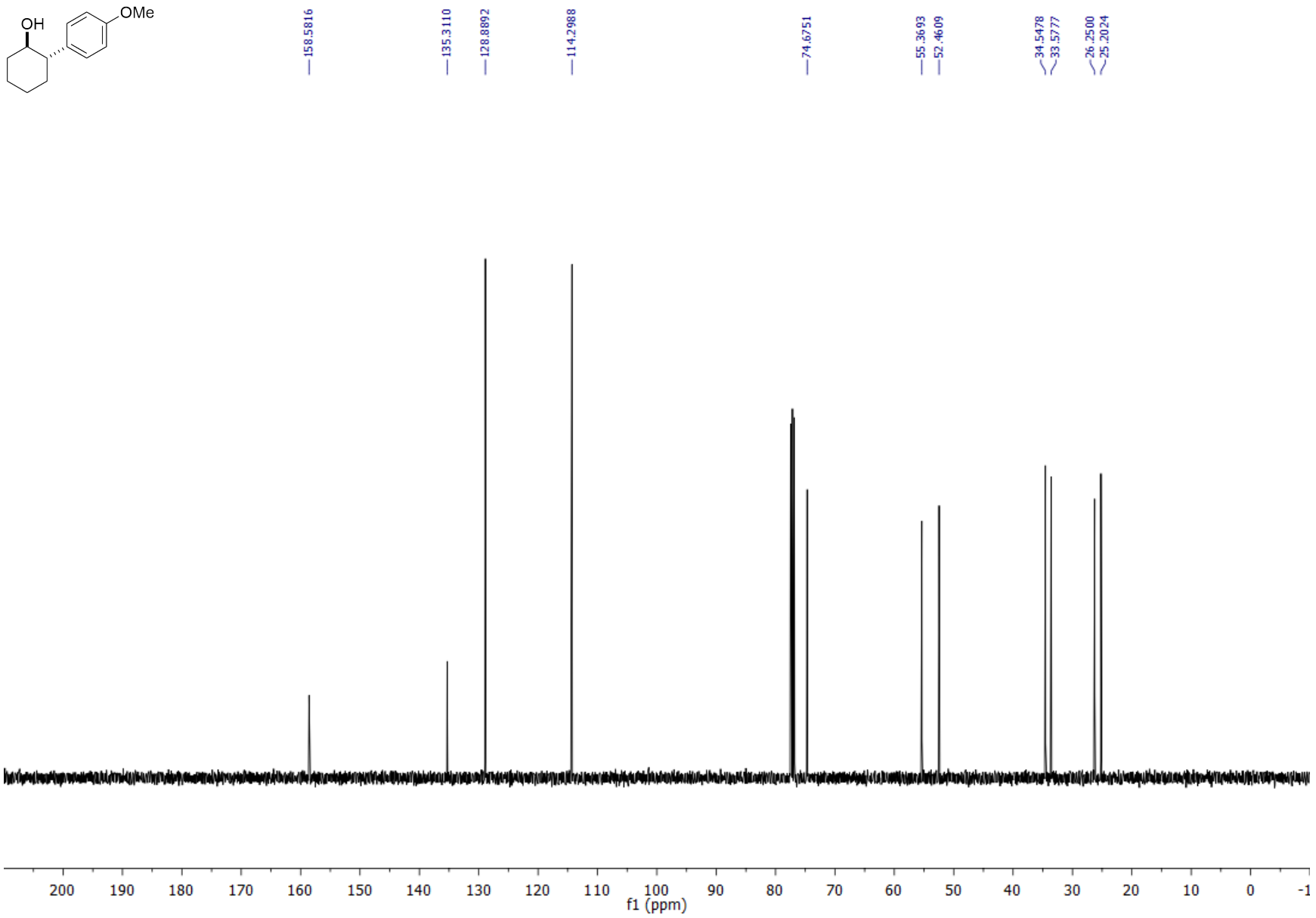

OH
Me
7.2749
7.2273
7.2130
7.1865
7.1720
7.1381
7.1353
7.1209
7.1061
3.8046
3.8001
3.7955
3.7901
2.8016
2.7948
2.7749
2.7586
2.7514
2.3739
2.1644
2.1556
2.1467
2.1377
2.1292
1.8901
1.8841
1.8764
1.8159
1.7878
1.7712
1.7597
1.5672
1.5627
1.4627
1.4447
1.4207
1.3991
1.3446
4.35
1.00
1.00
3.01
1.02
3.10
1.07
4.21
f1 (ppm)

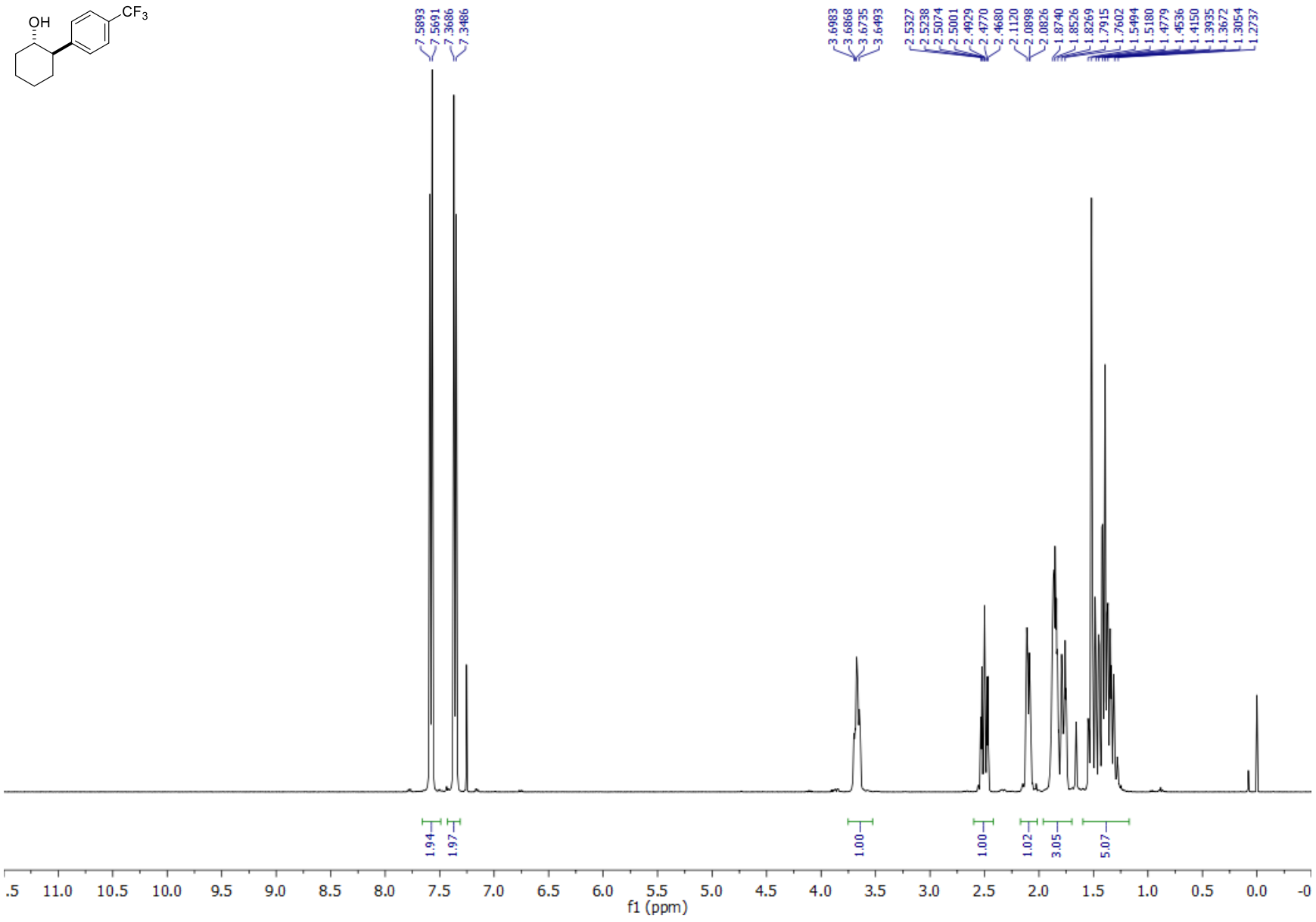

OH
Me
141.5023
137.2597
130.7891
126.6657
126.3837
125.5753
74.4805
47.9695
34.6741
33.2913
26.4161
25.2800
19.9687
f1 (ppm)

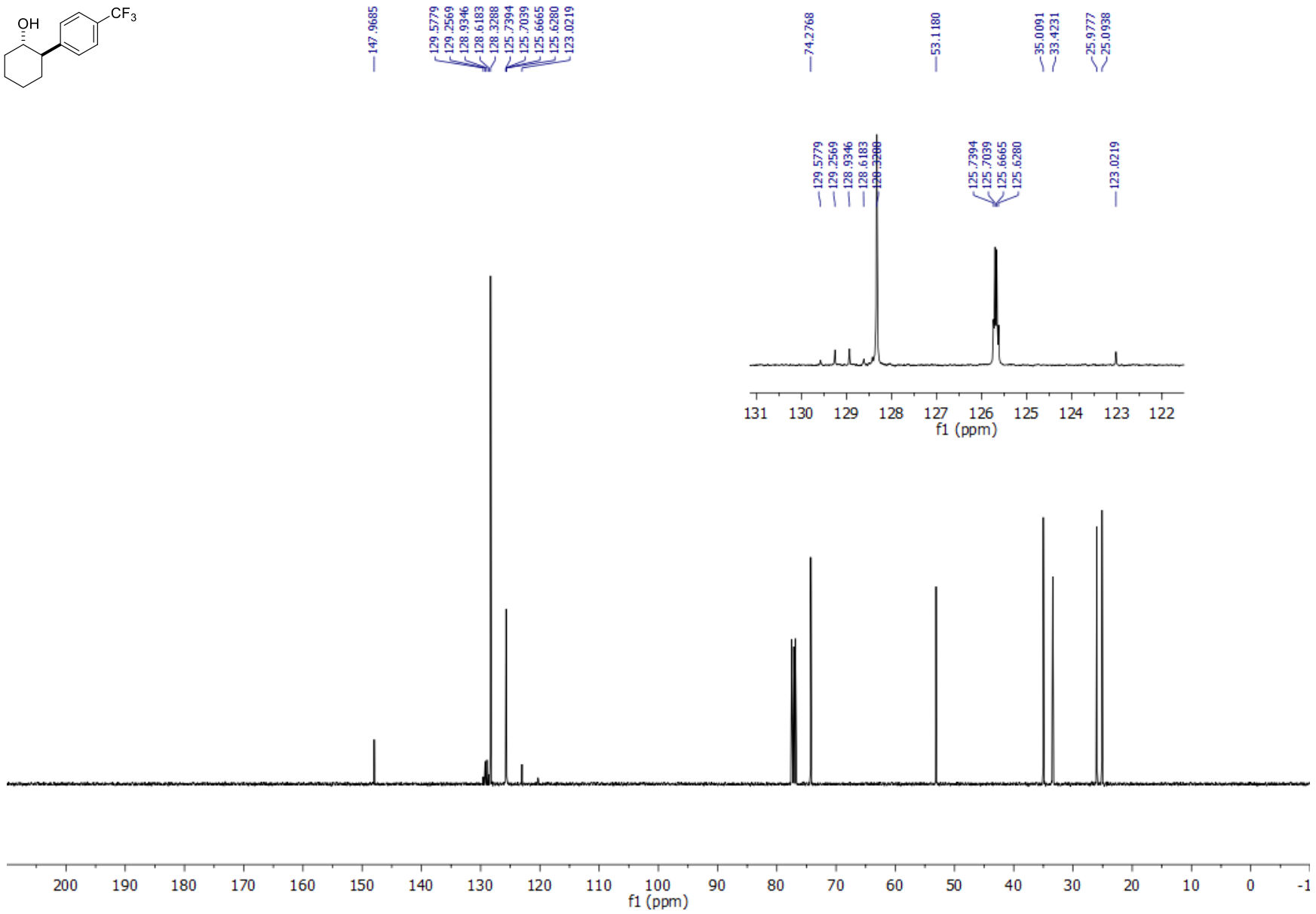

Me
OH
Me
6.8621
3.6651
3.6542
3.6398
3.6292
3.6142
3.6042
2.3766
2.3371
2.2985
2.2423
2.1139
2.0907
1.8192
1.7567
1.6360
1.5155
1.4650
1.3530
1.2831
3.00
1.13
18.42
f1 (ppm)

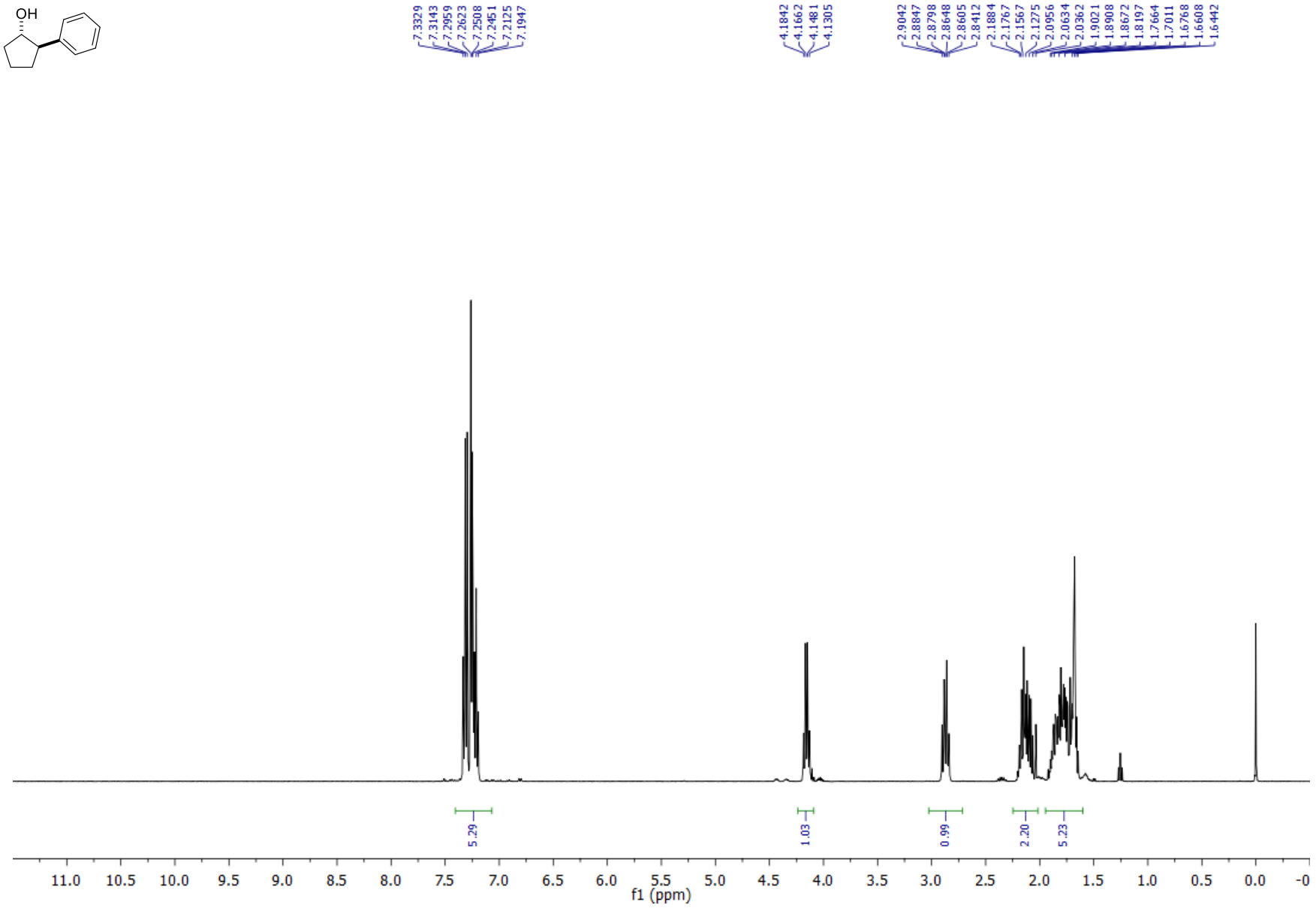

Me
OH
Me
143.2133
138.3098
128.6262
125.8119
74.4921
53.2253
34.4749
33.4334
26.2141
25.1933
21.4616
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

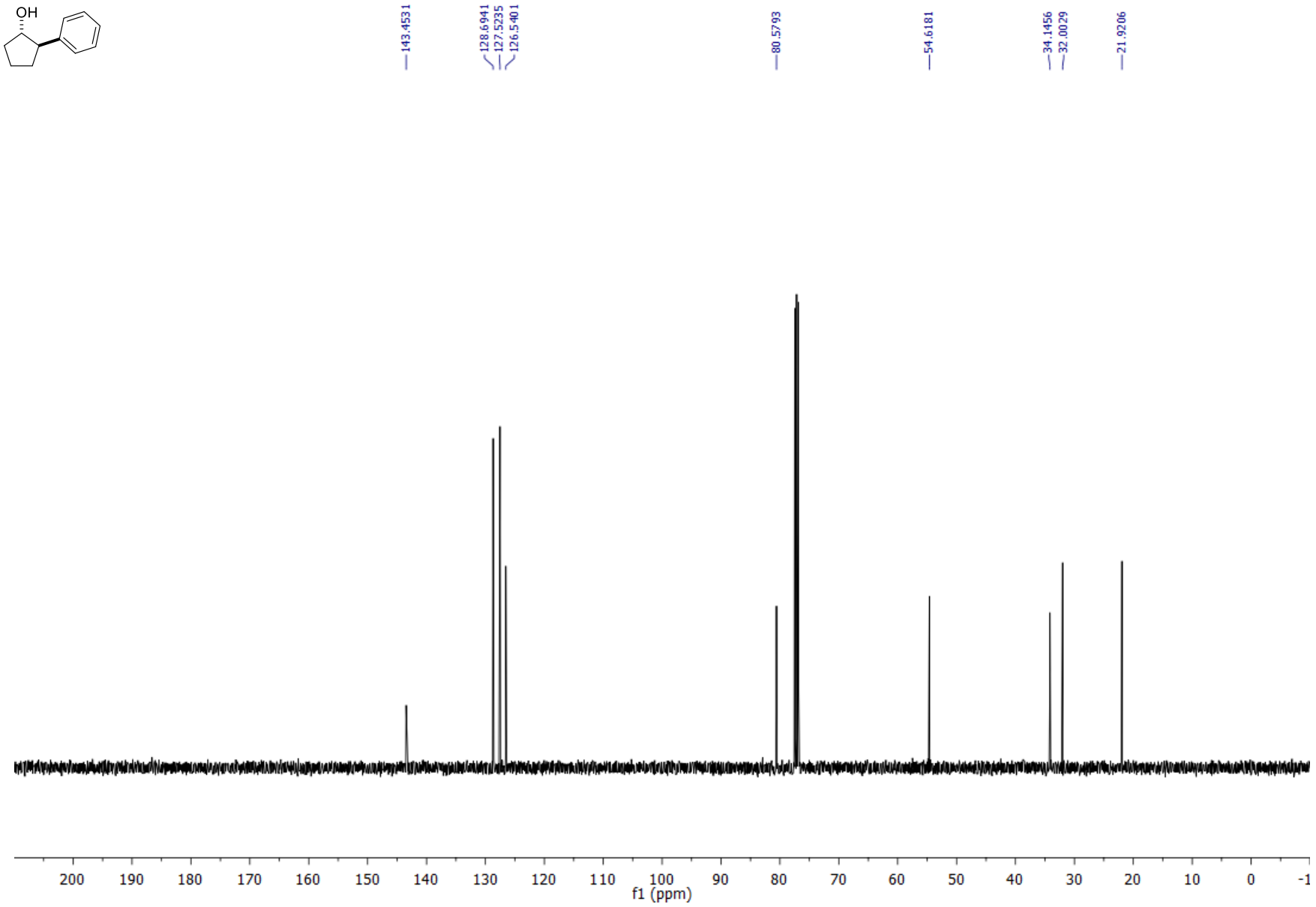

OH
OMe
7.1782
7.1567
6.8826
6.8609
3.7885
3.6066
3.5879
3.5823
3.5626
2.3986
2.3898
2.3735
2.3592
2.3431
2.3342
2.1144
2.0914
1.8508
1.8391
1.8051
1.7666
1.7354
1.5836
1.5785
1.5300
1.5211
1.4982
1.4656
1.4261
1.4015
1.3764
1.3240
1.2689
1.94
1.93
2.97
1.00
0.98
0.97
2.97
0.97
4.03
f1 (ppm)

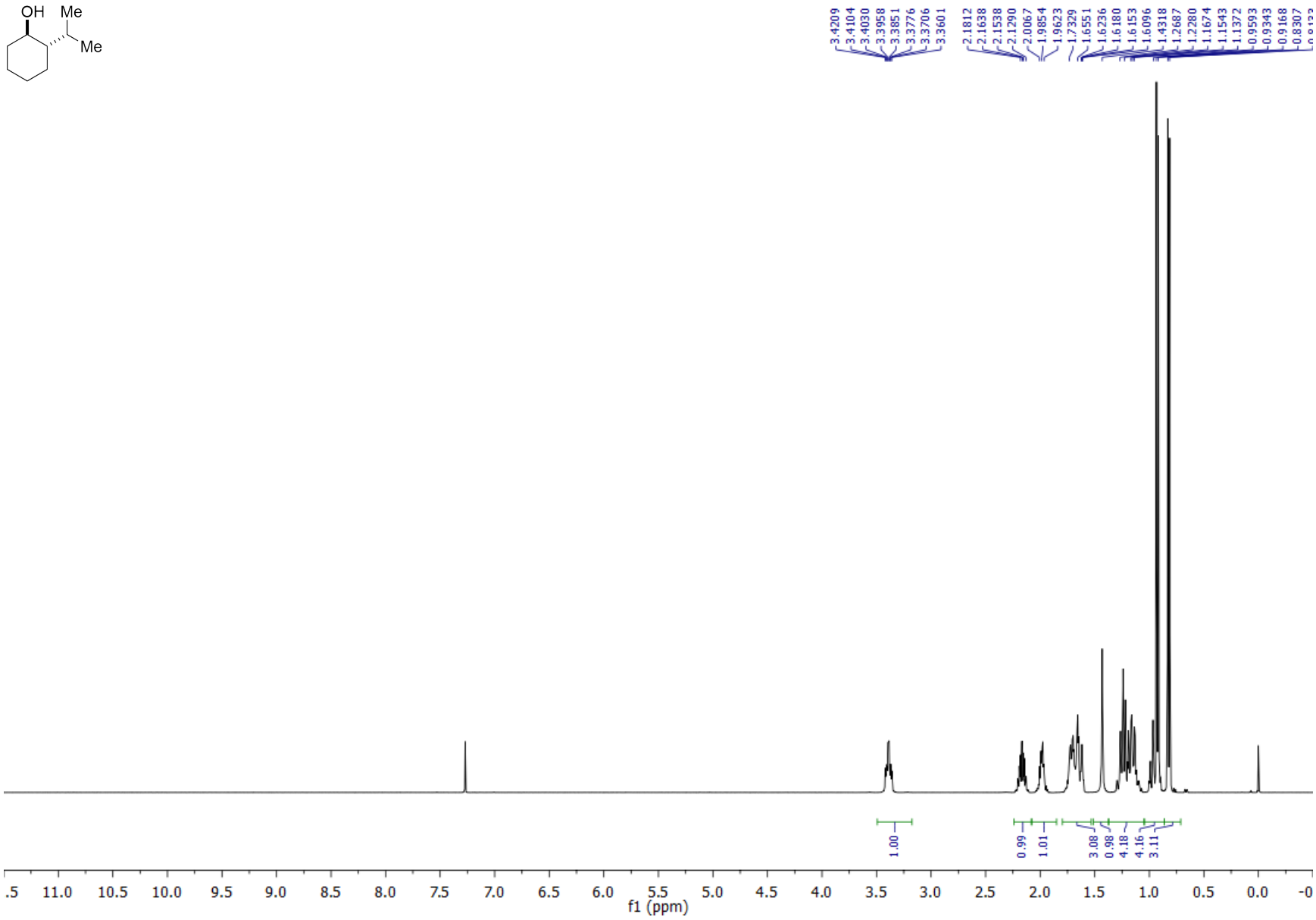

OH
OMe
158.5816
135.3110
128.8892
114.2988
74.6751
55.3693
52.4609
34.5478
33.5777
26.2500
25.2024
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

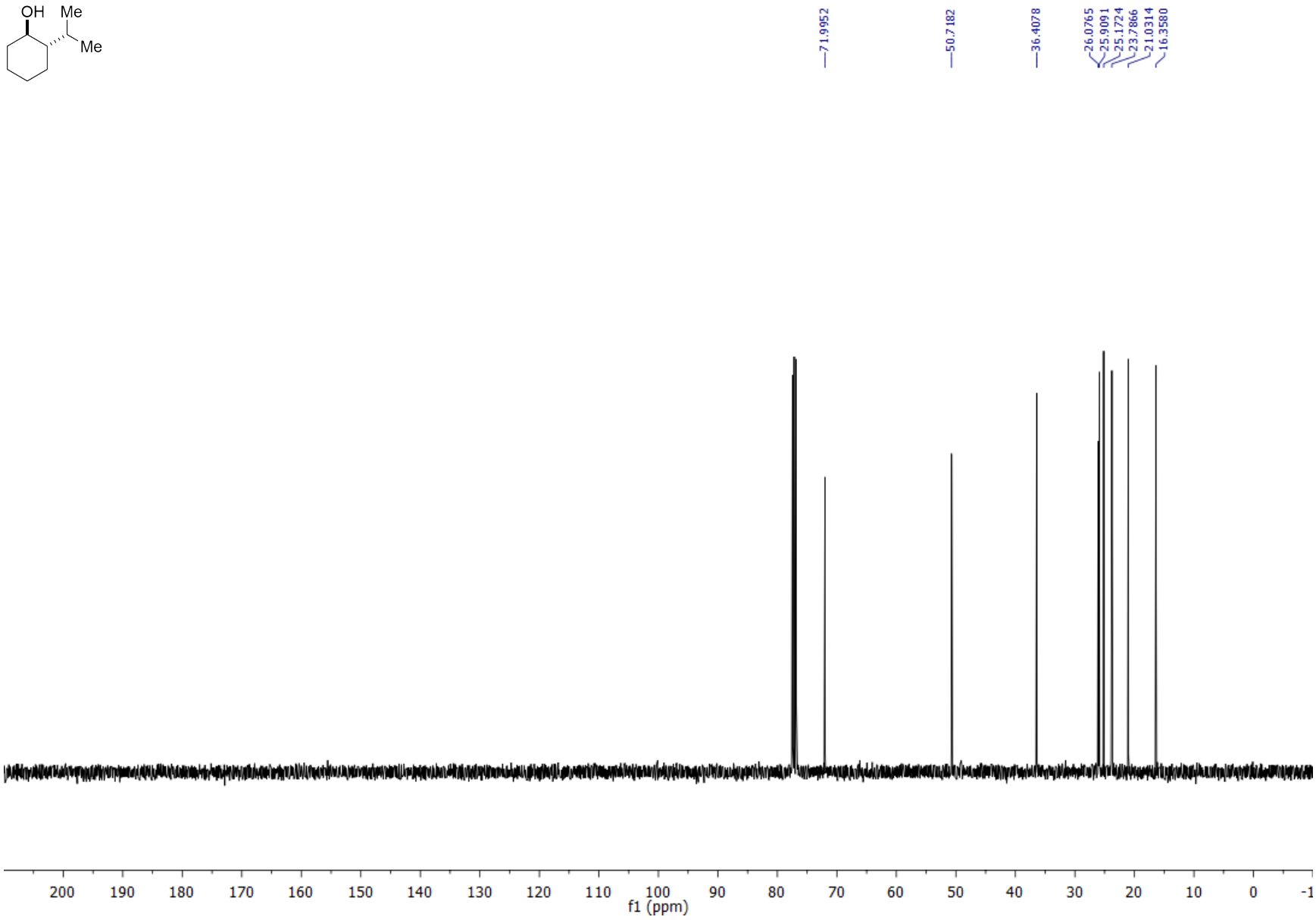

OH
CF3
7.5893
7.5691
7.3686
7.3486
3.6983
3.6868
3.6735
3.6493
2.5327
2.5238
2.5074
2.5001
2.4929
2.4770
2.4680
2.1120
2.0898
2.0826
1.8740
1.8526
1.8269
1.7915
1.7602
1.5494
1.5180
1.4779
1.4536
1.4150
1.3935
1.3672
1.3054
1.2737
1.94
1.97
1.00
1.00
1.02
3.05
5.07
f1 (ppm)

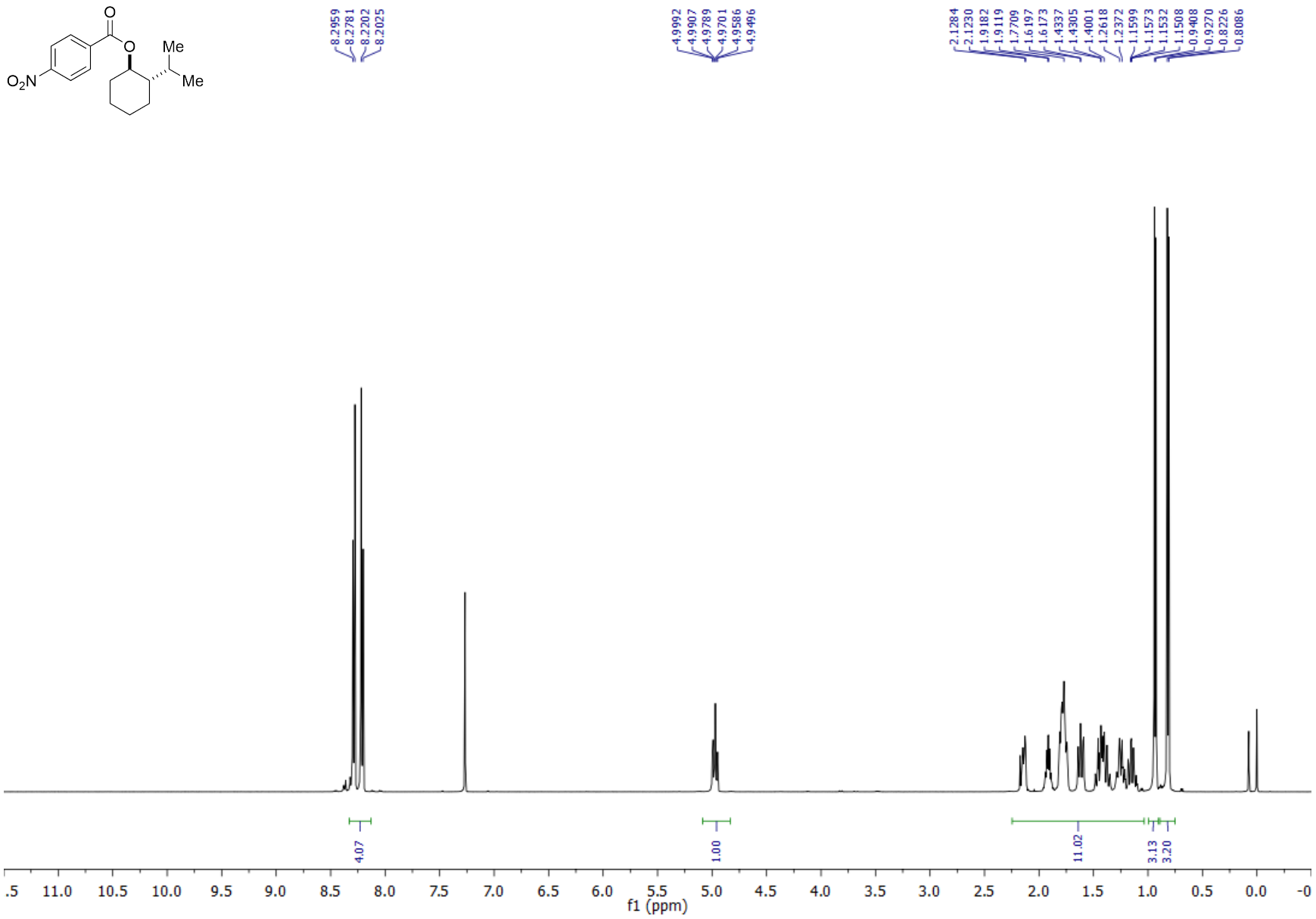

OH
CF3
147.9685
129.5779
129.2569
128.9346
128.6183
128.3288
125.7394
125.7039
125.6665
125.6280
123.0219
74.2768
53.1180
35.0091
33.4231
25.9777
25.0938
f1 (ppm)
f1 (ppm)

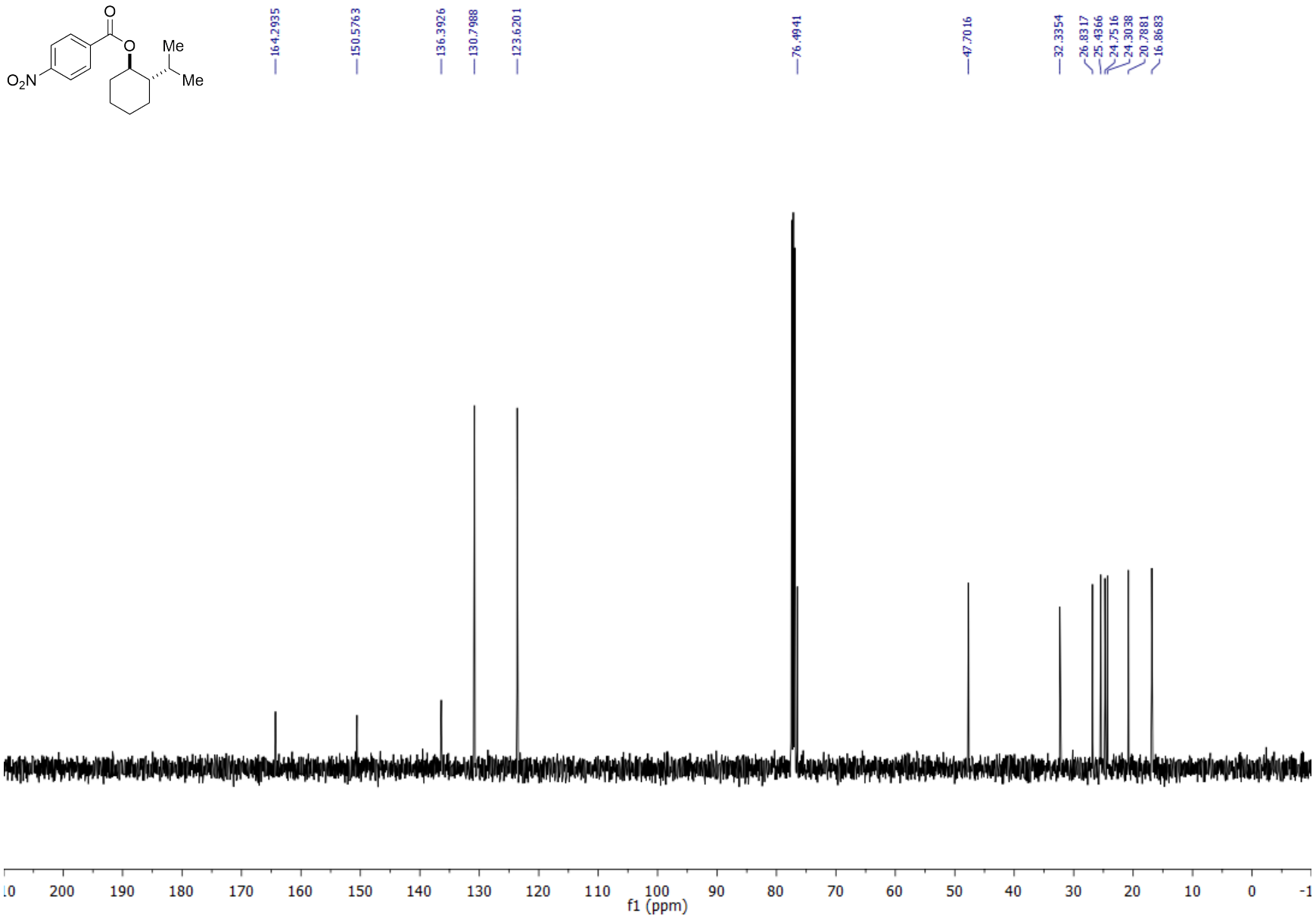

OH
7.3329
7.3143
7.2959
7.2623
7.2508
7.2451
7.2125
7.1947
4.1842
4.1662
4.1481
4.1305
2.9042
2.8847
2.8798
2.8648
2.8605
2.8412
2.1884
2.1767
2.1567
2.1275
2.0956
2.0634
2.0362
1.9021
1.8908
1.8672
1.8197
1.7664
1.7011
1.6768
1.6608
1.6442
5.29
1.03
0.99
2.20
5.23
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

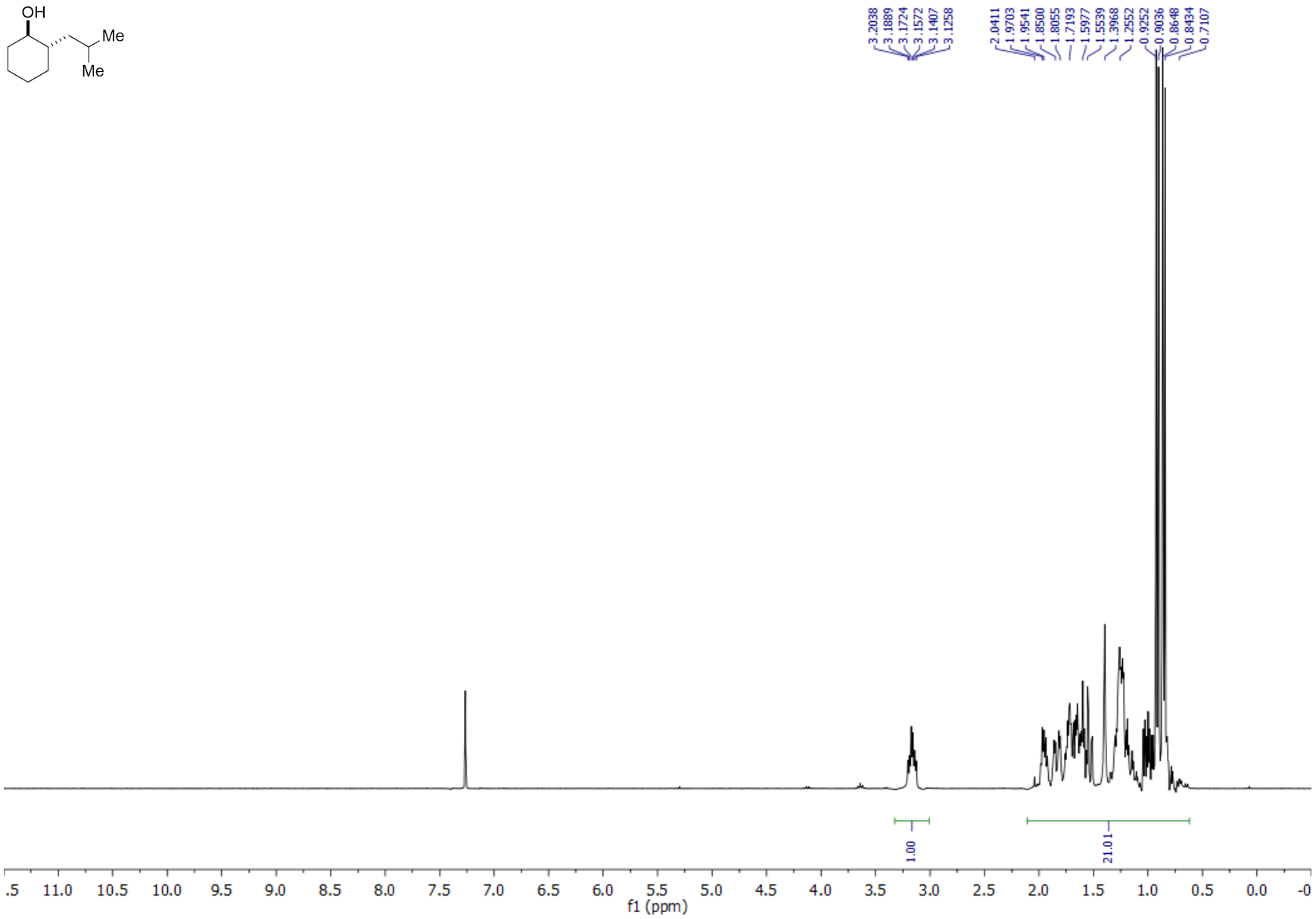

OH
143.4531
128.6941
127.5235
126.5401
80.5793
54.6181
34.1456
32.0029
21.9206
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

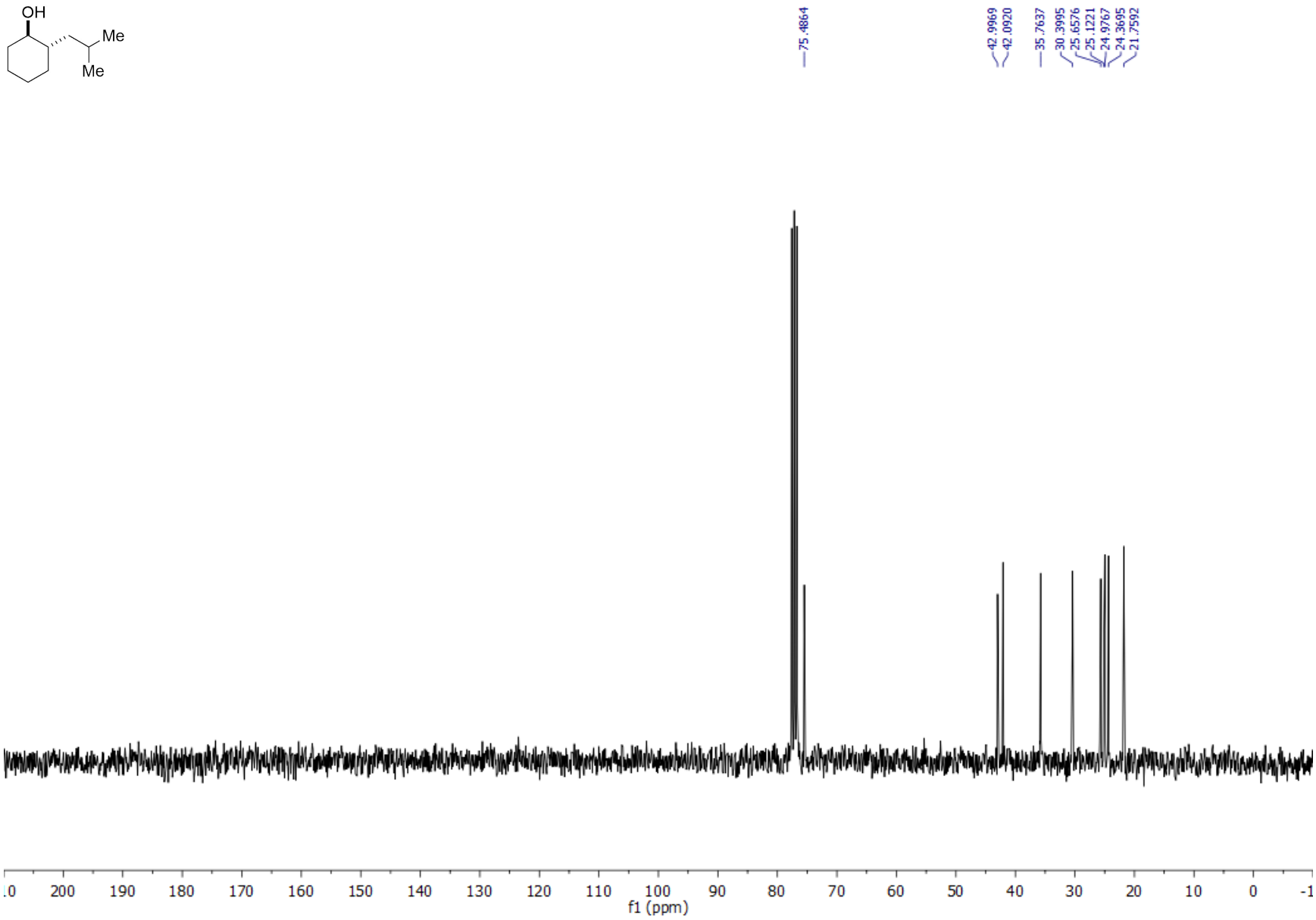

OH
Me
Me
3.4209
3.4104
3.4030
3.3958
3.3851
3.3776
3.3706
3.3601
2.1812
2.1638
2.1538
2.1290
2.0067
1.9854
1.9623
1.7329
1.6551
1.6236
1.6180
1.6153
1.6096
1.4318
1.2687
1.2280
1.1674
1.1543
1.1372
0.9593
0.9343
0.9168
0.8307
1.00
0.99
1.01
3.08
0.98
4.18
4.16
3.11
f1 (ppm)

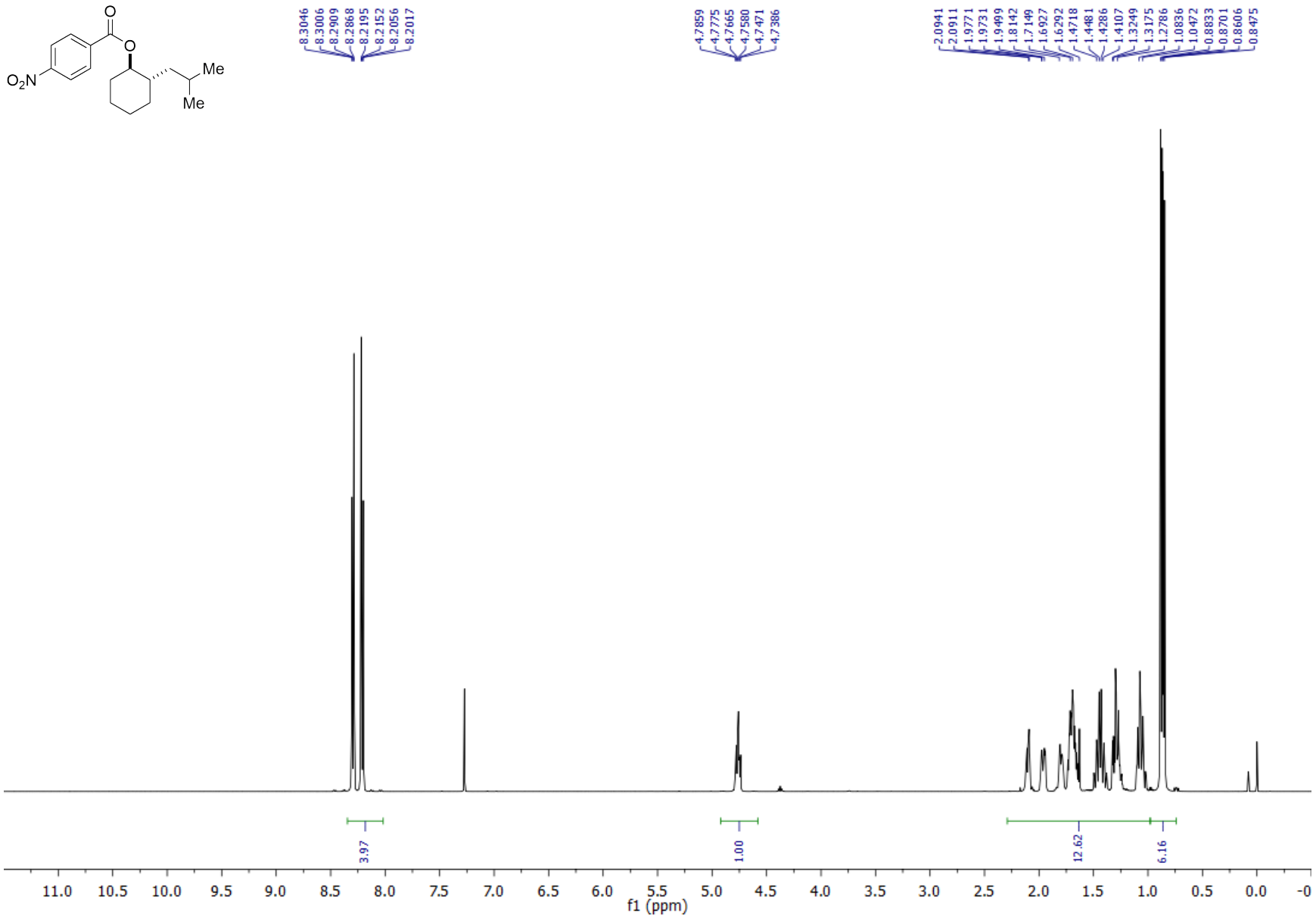

OH
Me
Me
71.9952
50.7182
36.4078
26.0765
25.9091
25.1724
23.7866
21.0314
16.3580
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

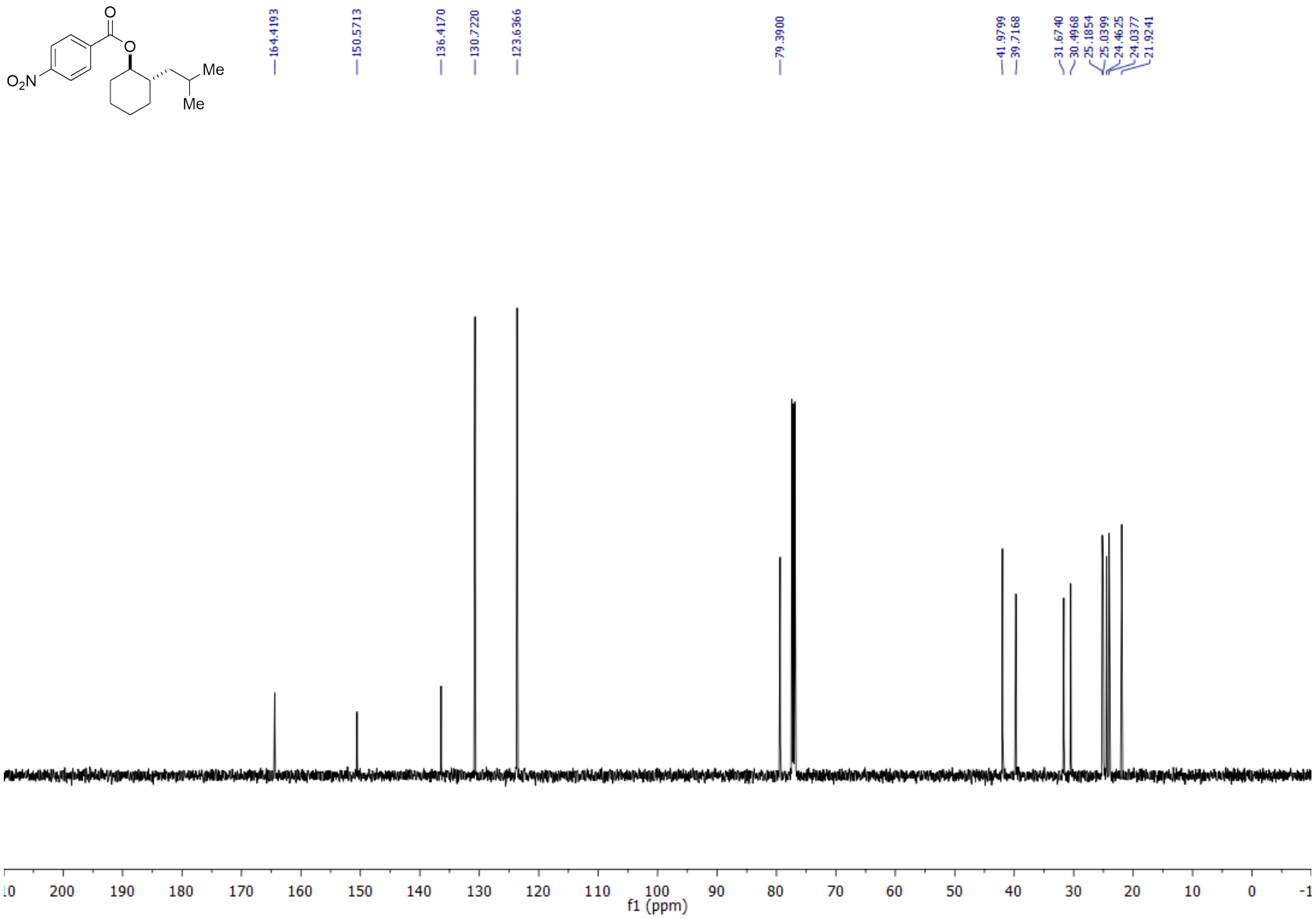

O
O
Me
Me
O_2N
8.2959
8.2781
8.2202
8.2025
4.9992
4.9907
4.9789
4.9701
4.9586
4.9496
2.1284
2.1230
1.9182
1.9119
1.7709
1.6197
1.6173
1.4337
1.4305
1.4001
1.2618
1.2372
1.1599
1.1573
1.1532
1.1508
0.9408
0.9270
0.8226
0.8086
4.07
1.00
11.02
3.13
3.20
f1 (ppm)

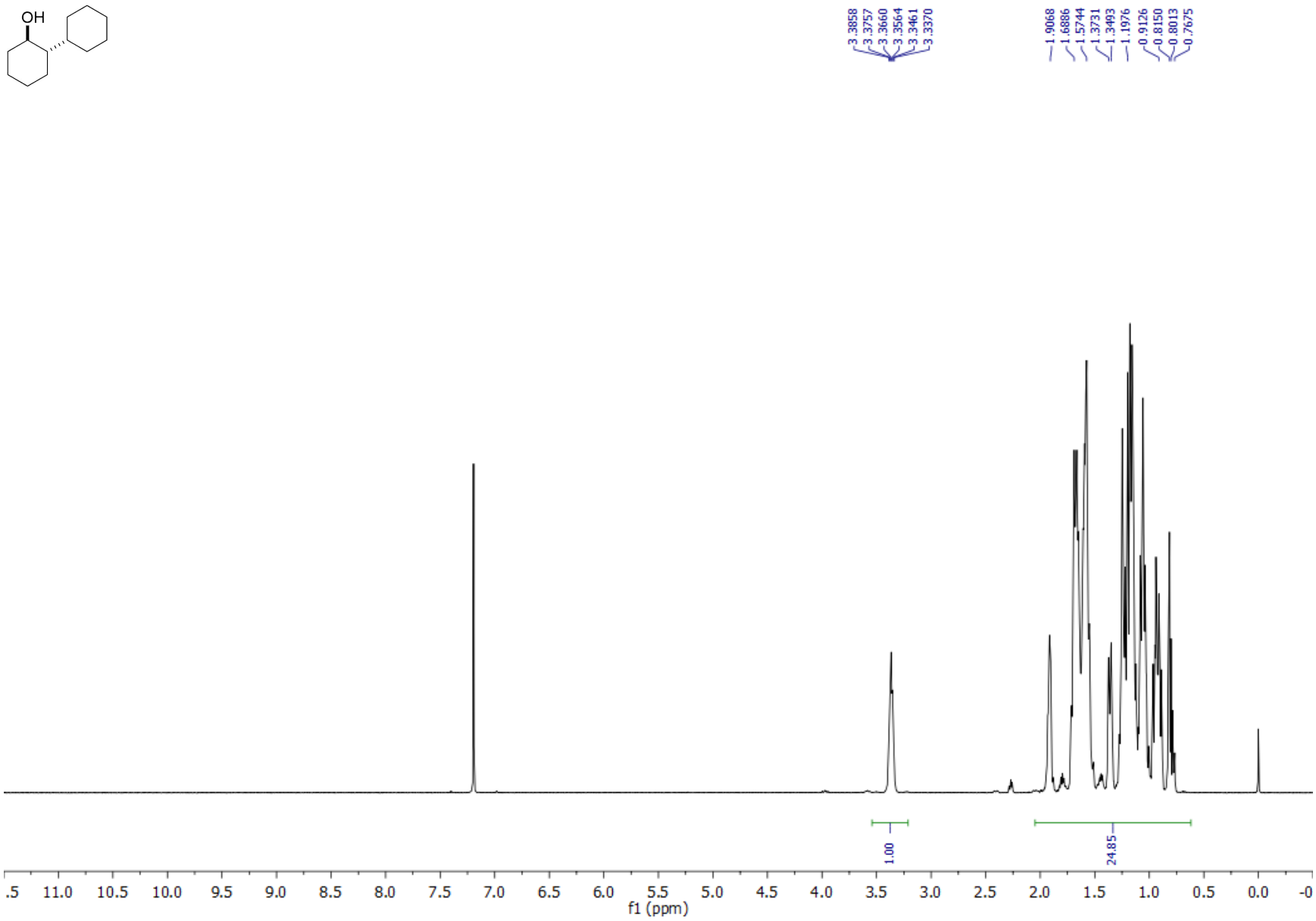

O
O
Me
Me
O_2N
164.2935
150.5763
136.3926
130.7988
123.6201
76.4941
47.7016
32.3354
26.8317
25.4366
24.7516
24.3038
20.7881
16.8683
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

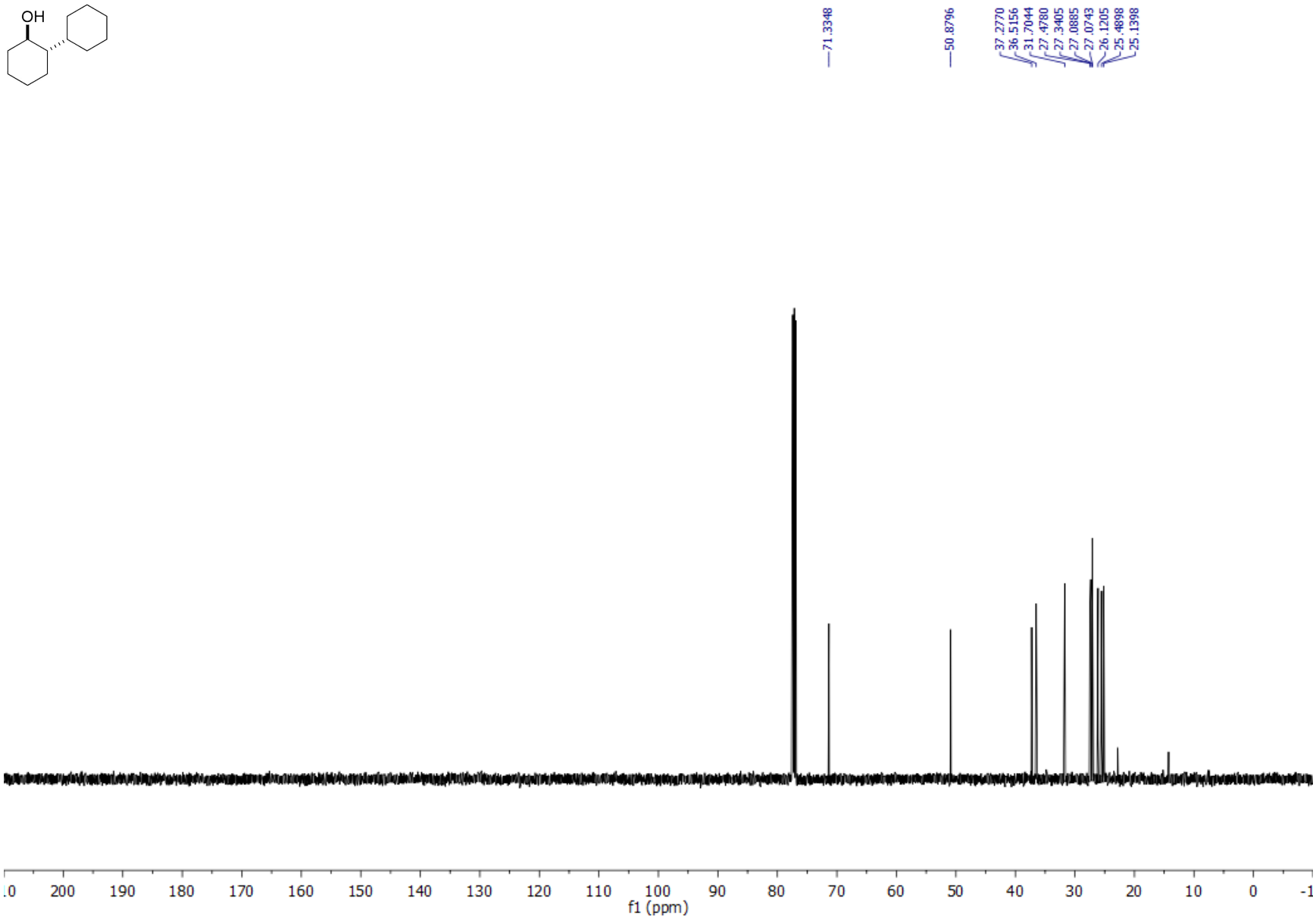

OH
Me
Me
3.2038
3.1889
3.1724
3.1572
3.1407
3.1258
2.0411
1.9703
1.9541
1.8500
1.8055
1.7193
1.5977
1.5539
1.3968
1.2552
0.9252
0.9036
0.8648
0.8434
0.7107
1.00
21.01
f1 (ppm)

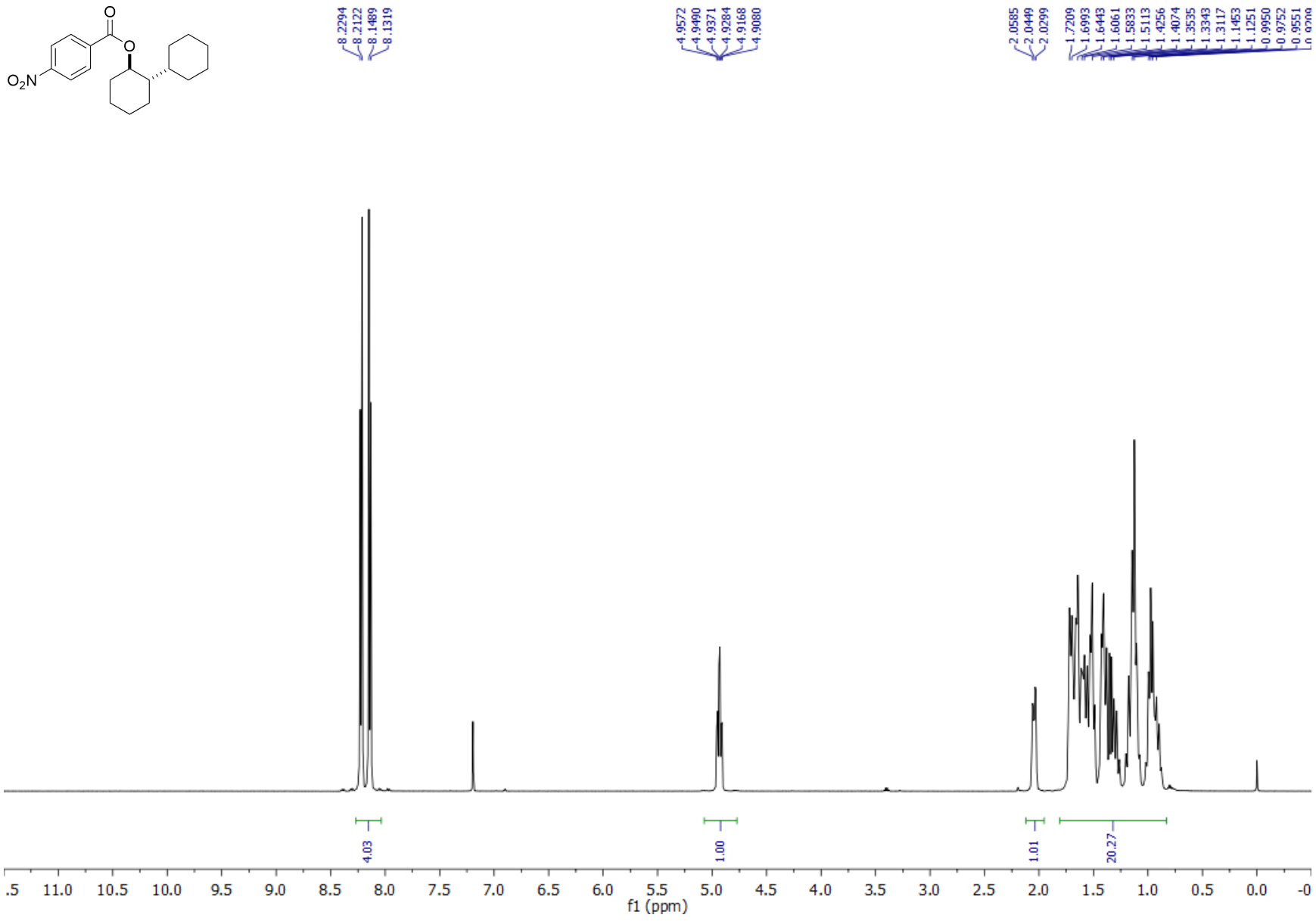

OH
Me
Me
75.4864
42.9969
42.0920
35.7637
30.3995
25.6576
25.1221
24.9767
24.3695
21.7592
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

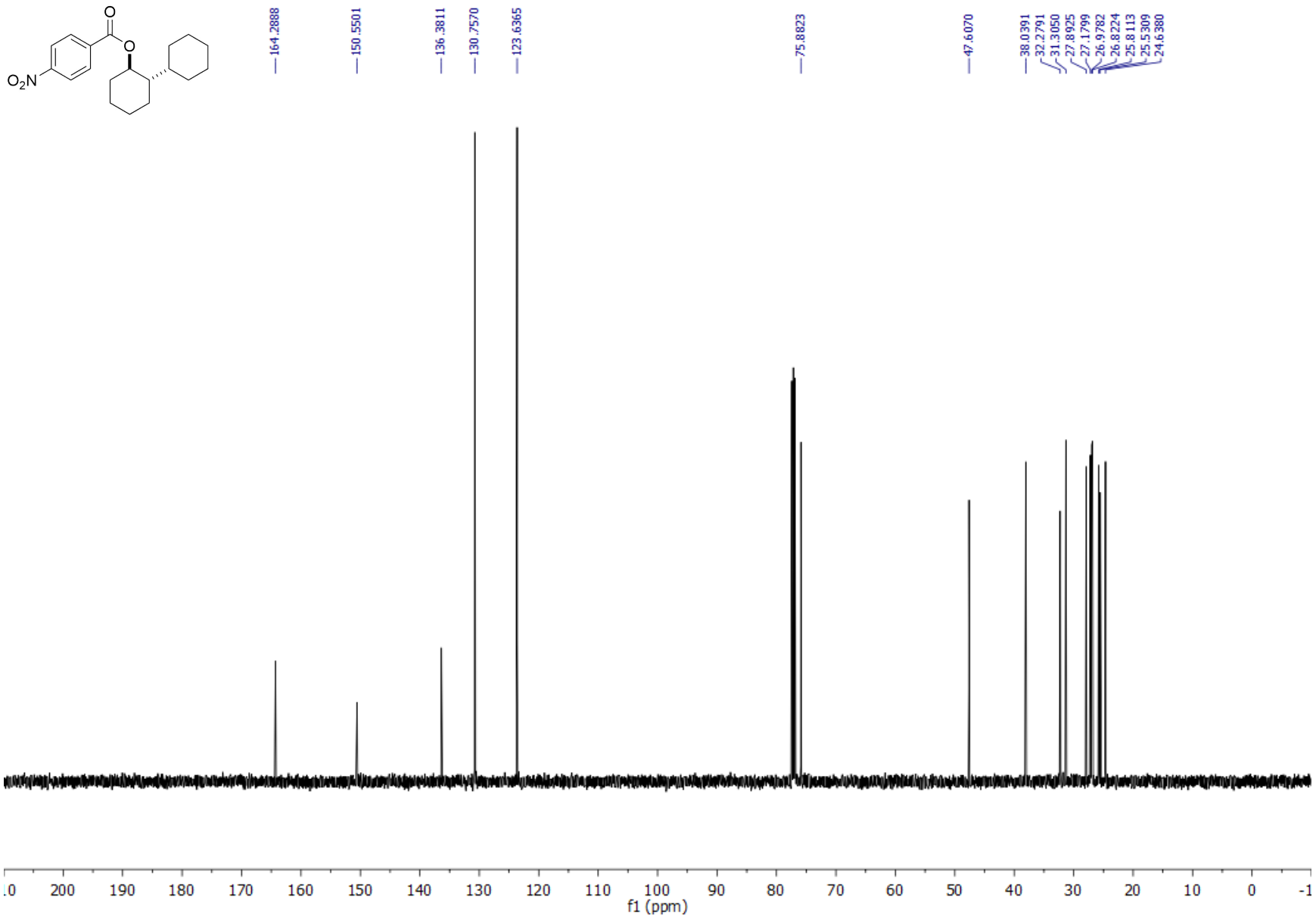

O
O
O2N
Me
Me
8.3046
8.3006
8.2909
8.2868
8.2195
8.2152
8.2056
8.2017
4.7859
4.7775
4.7665
4.7580
4.7471
4.7386
2.0941
2.0911
1.9771
1.9731
1.9499
1.8142
1.7149
1.6927
1.6292
1.4718
1.4481
1.4286
1.4107
1.3249
1.3175
1.2786
1.0836
1.0472
0.8833
0.8701
0.8606
0.8475
3.97
1.00
12.62
6.16
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

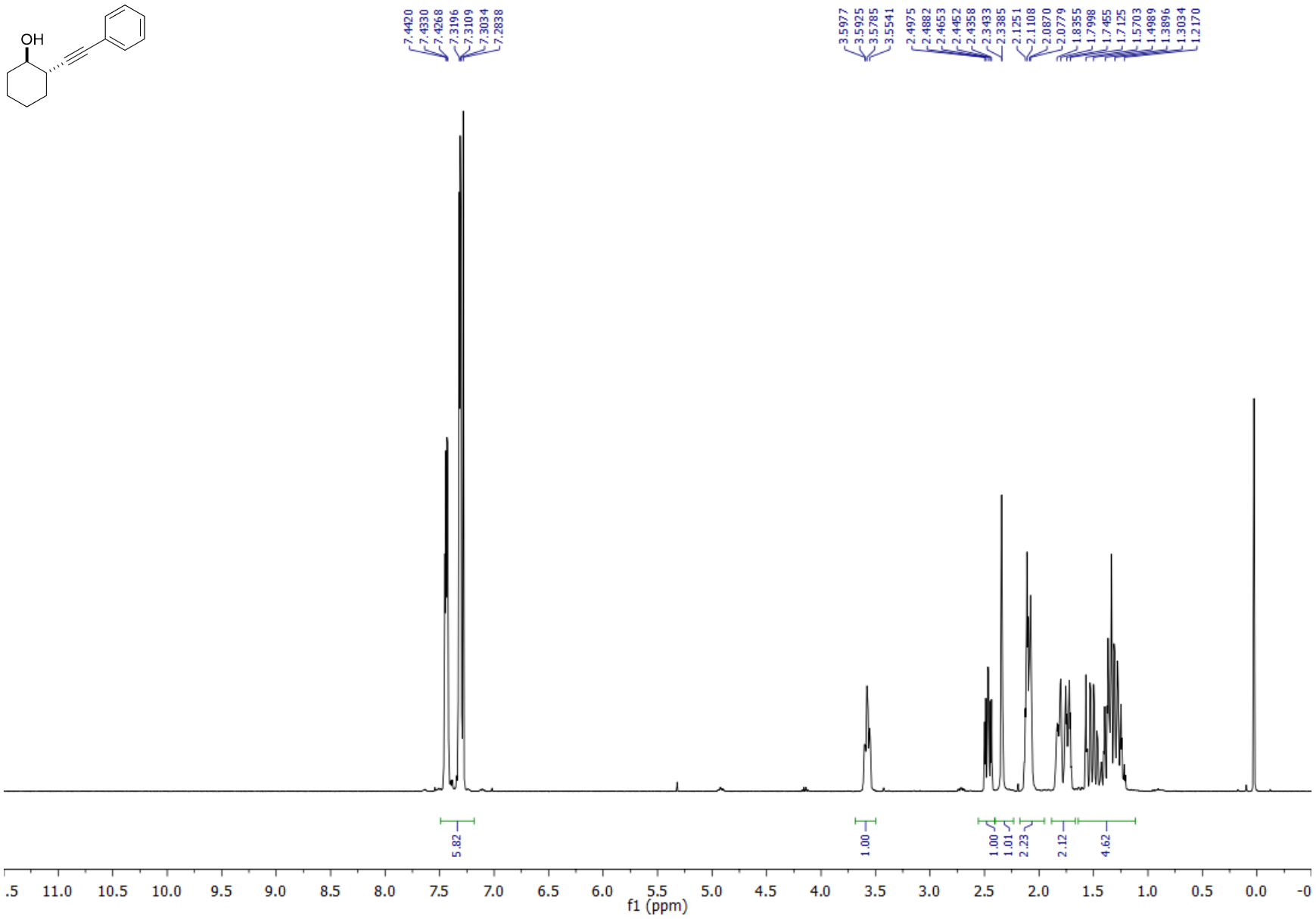

O
O
O2N
Me
Me
164.4193
150.5713
136.4170
130.7220
123.6366
79.3900
41.9799
39.7168
31.6740
30.4968
25.1854
25.0399
24.4625
24.0377
21.9241
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

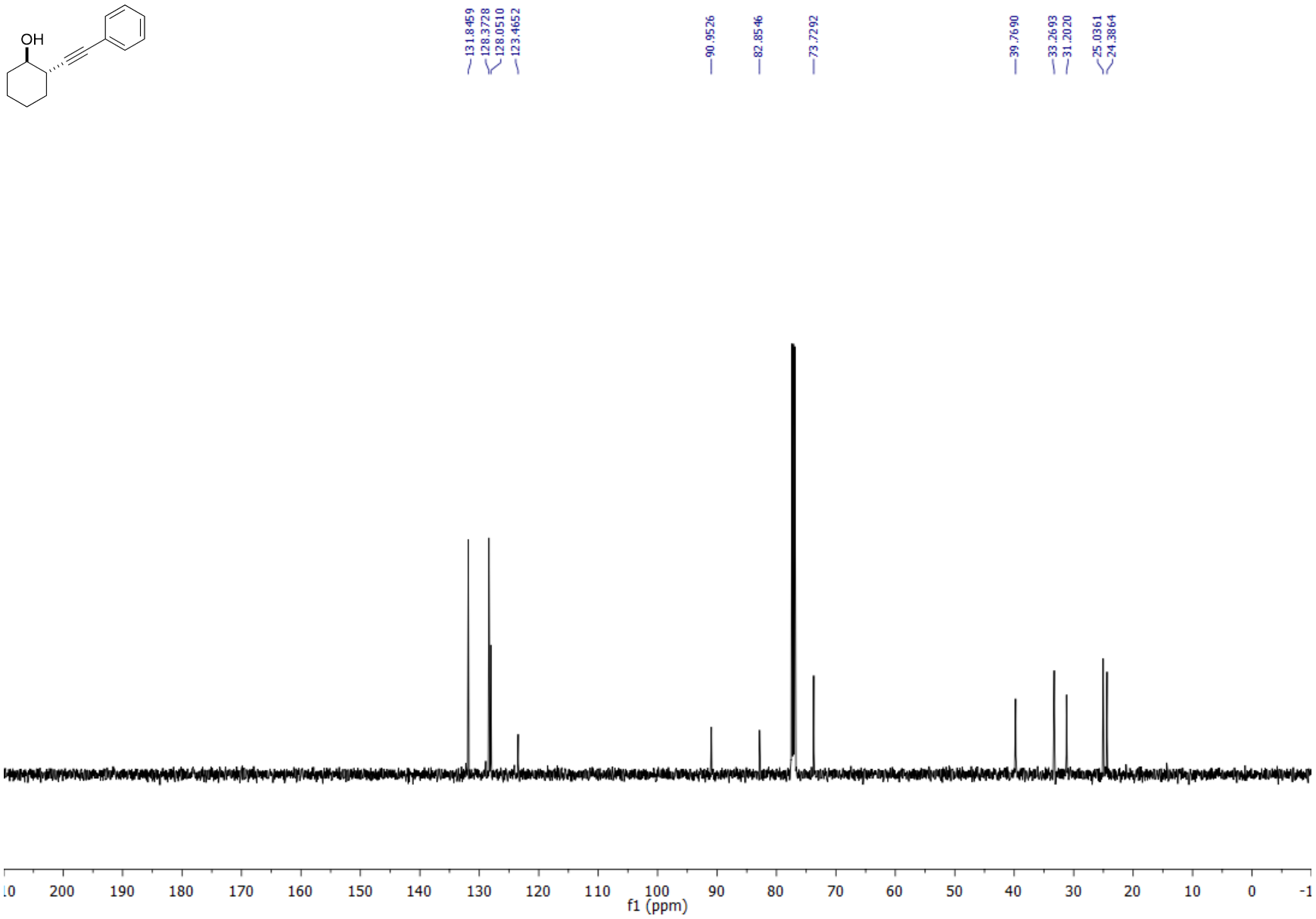

OH
3.3858
3.3757
3.3660
3.3564
3.3461
3.3370
1.9068
1.6886
1.5744
1.3731
1.3493
1.1976
0.9126
0.8150
0.8013
0.7675
1.00
24.85
f1 (ppm)

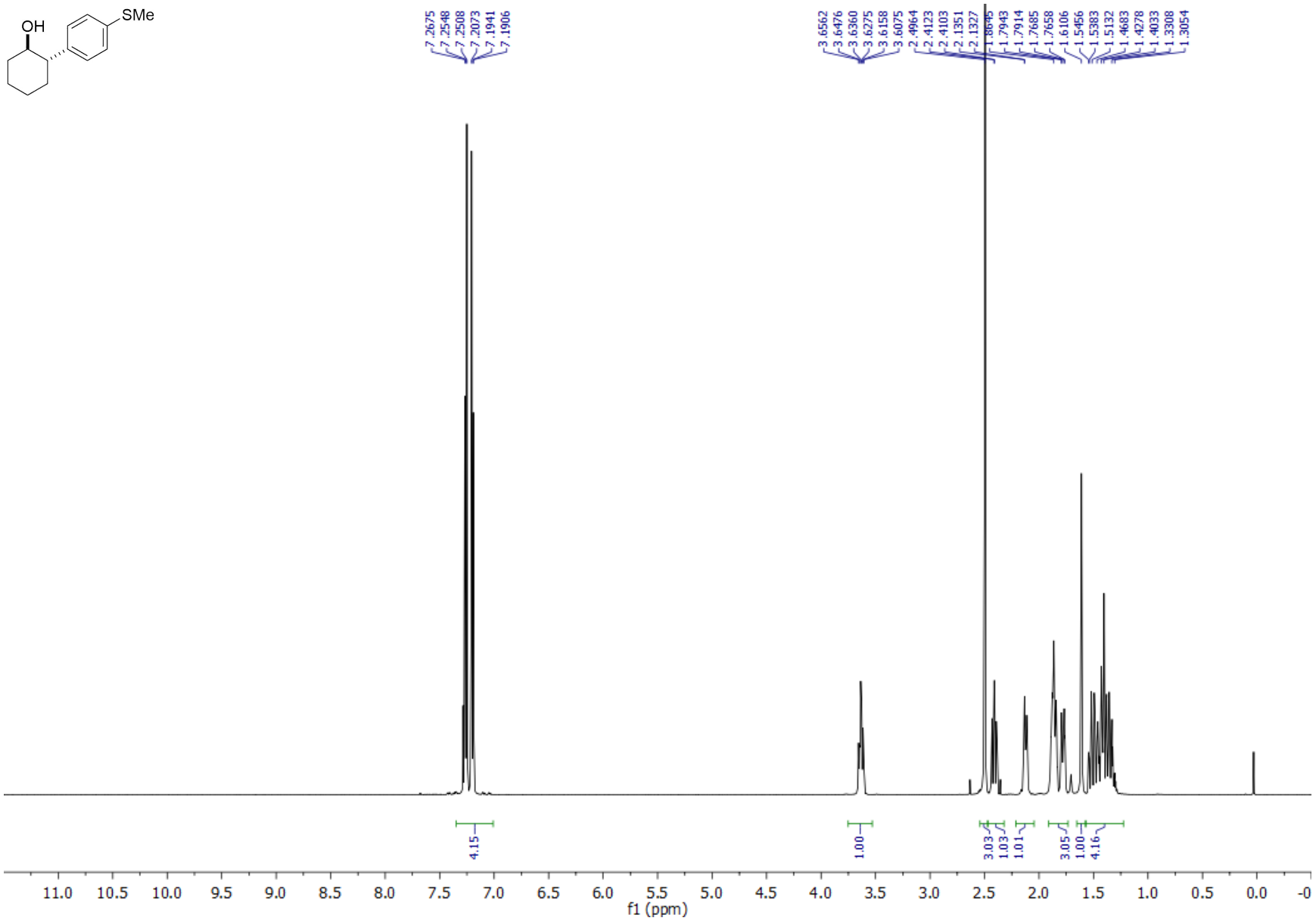

OH
71.3348
50.8796
37.2770
36.5156
31.7044
27.4780
27.3405
27.0885
27.0743
26.1205
25.4898
25.1398
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

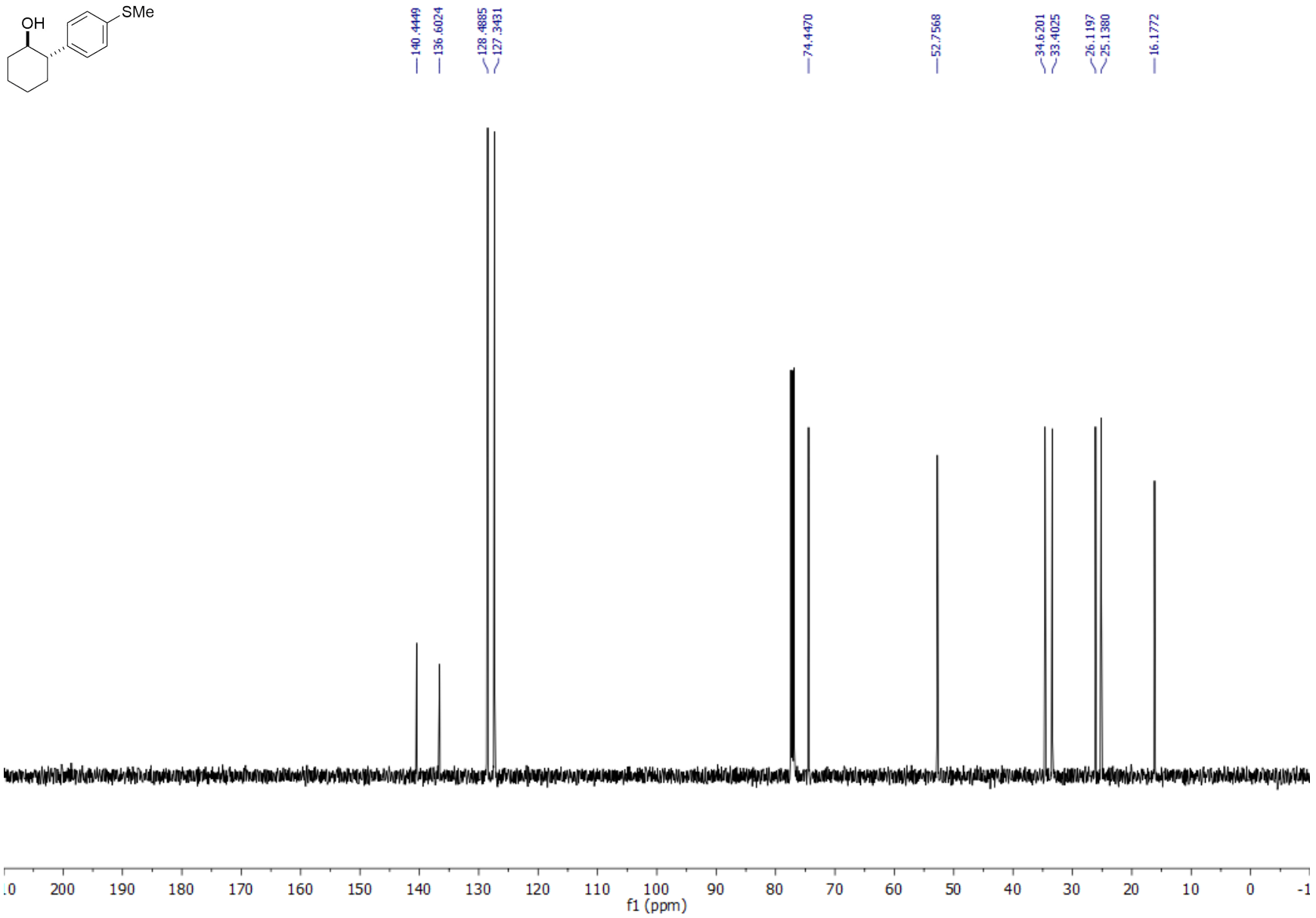

O2N
8.2294
8.2122
8.1489
8.1319
4.9572
4.9490
4.9371
4.9284
4.9168
4.9080
2.0585
2.0449
2.0299
1.7209
1.6993
1.6443
1.6061
1.5833
1.5113
1.4256
1.4074
1.3535
1.3343
1.3117
1.1453
1.1251
0.9950
0.9752
0.9551
4.03
1.00
1.01
20.27
f1 (ppm)

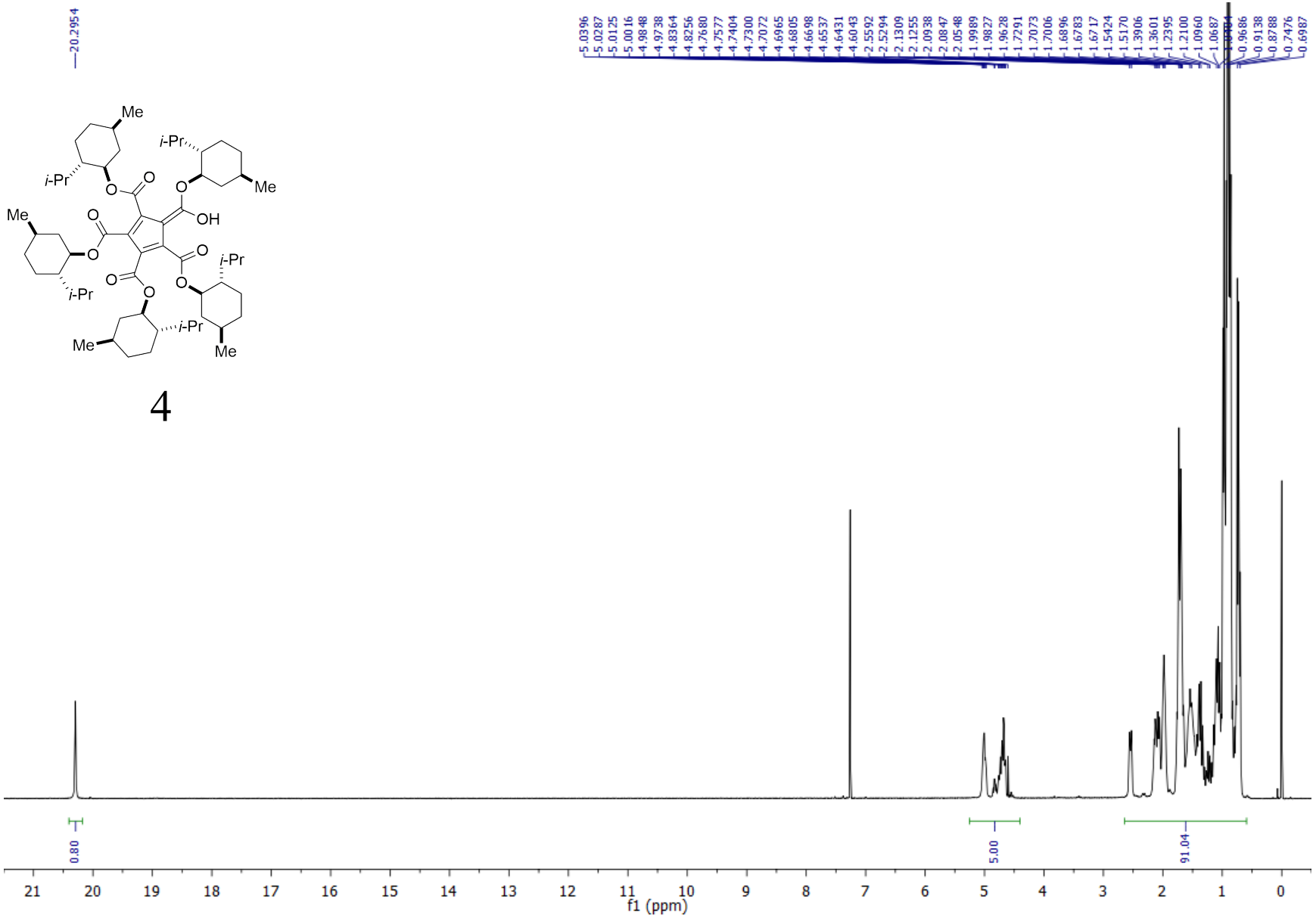

O2N
O
O
164.2888
150.5501
136.3811
130.7570
123.6365
75.8823
47.6070
38.0391
32.2791
31.3050
27.8925
27.1799
26.9782
26.8224
25.8113
25.5309
24.6380
f1 (ppm)


OH
7.4420
7.4330
7.4268
7.3196
7.3109
7.3034
7.2838
3.5977
3.5925
3.5785
3.5541
2.4975
2.4882
2.4653
2.4452
2.4358
2.3433
2.3385
2.1251
2.1108
2.0870
2.0779
1.8355
1.7998
1.7455
1.7125
1.5703
1.4989
1.3896
1.3034
1.2170
5.82
1.00
1.00
1.01
2.23
2.12
4.62
f1 (ppm)


OH
131.8459
128.3728
128.0510
123.4652
90.9526
82.8546
73.7292
39.7690
33.2693
31.2020
25.0361
24.3864
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

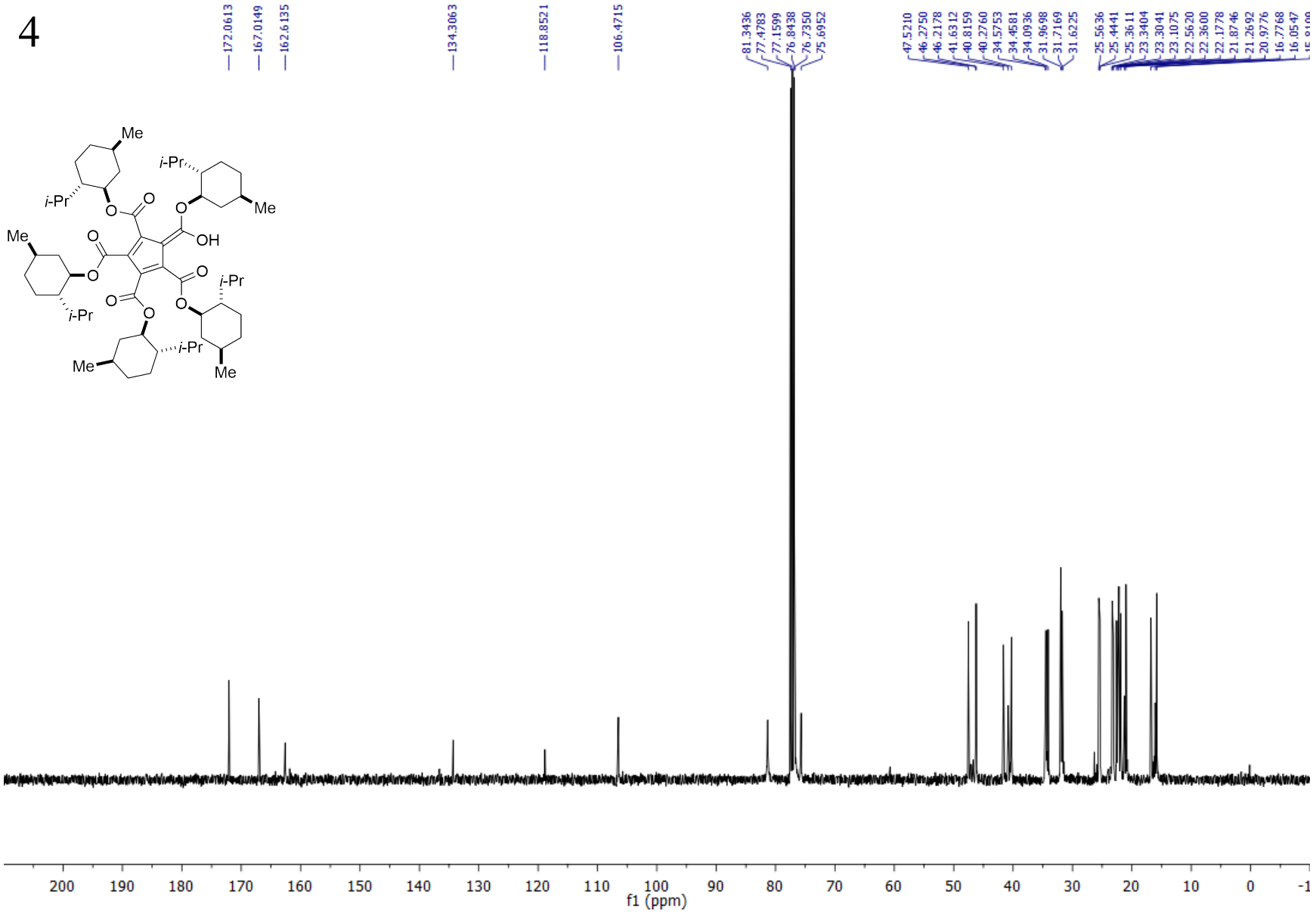

OH
SMe
7.2675
7.2548
7.2508
7.2073
7.1941
7.1906
3.6562
3.6476
3.6360
3.6275
3.6158
3.6075
2.4964
2.4123
2.4103
2.1351
2.1327
1.8645
1.7943
1.7914
1.7685
1.7658
1.6106
1.5456
1.5383
1.5132
1.4683
1.4278
1.4033
1.3308
1.3054
4.15
1.00
3.03
1.03
1.01
3.05
1.00
4.16
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

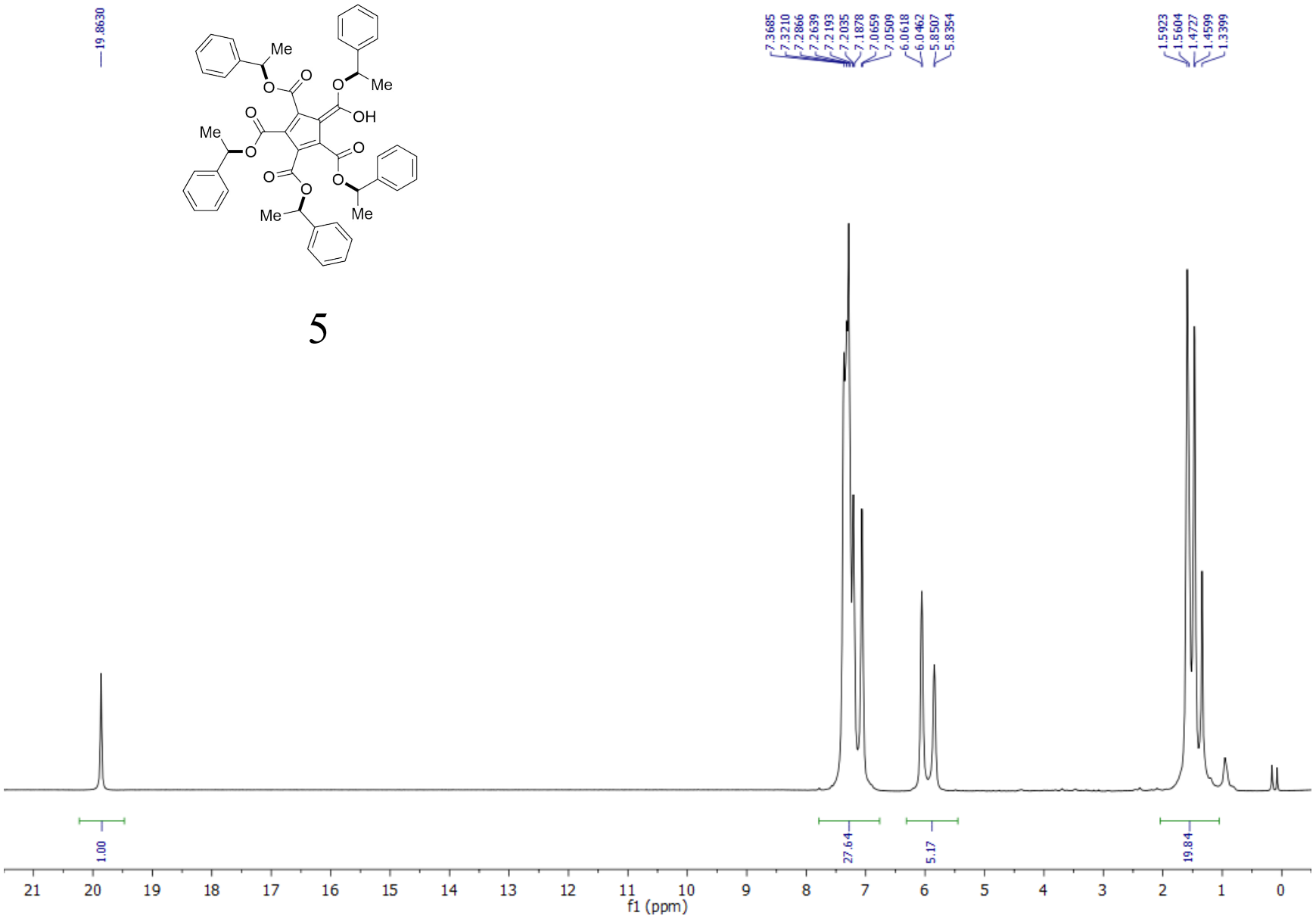

OH
SMe
140.4449
136.6024
128.4885
127.3431
74.4470
52.7568
34.6201
33.4025
26.1197
25.1380
16.1772
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


20.2954
5.0396
5.0287
5.0125
5.0016
4.9848
4.9738
4.8364
4.8256
4.7680
4.7577
4.7404
4.7300
4.7072
4.6965
4.6805
4.6698
4.6537
4.6431
4.6043
2.5592
2.5294
2.1309
2.1255
2.0938
2.0847
2.0548
1.9989
1.9827
1.9628
1.7291
1.7073
1.7006
1.6896
1.6783
1.6717
1.5424
1.5170
1.3906
1.3601
1.2395
1.2100
1.0960
1.0687
0.9686
0.9138
0.8788
0.7476
0.6987
0.80
5.00
91.04
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

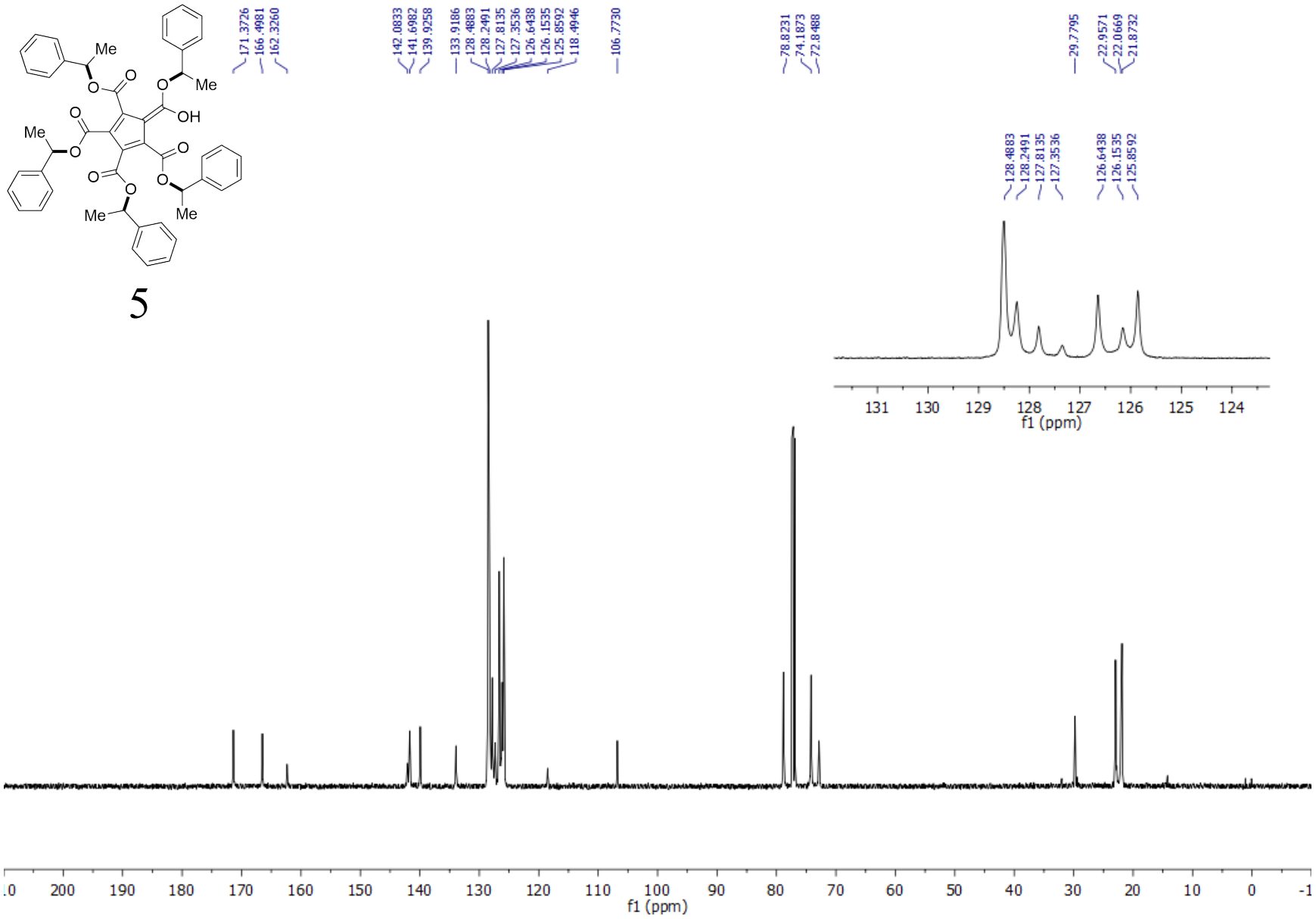
4

4

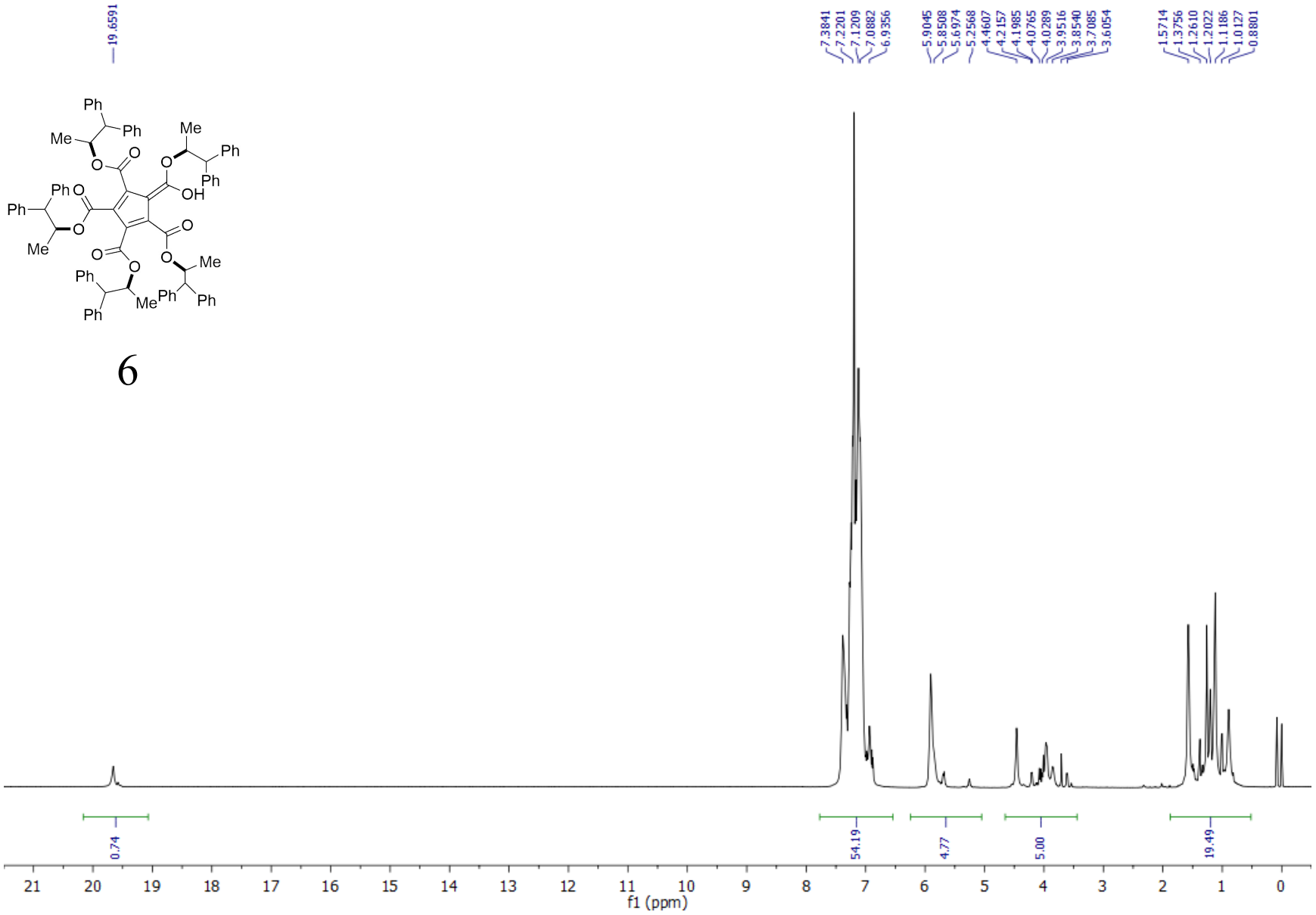

172.0613
167.0149
162.6135
134.3063
118.8521
106.4715
81.3436
77.4783
77.1599
76.8438
76.7350
75.6952
47.5210
46.2750
46.2178
41.6312
40.8159
40.2760
34.5753
34.4581
34.0936
31.9698
31.7169
31.6225
25.5636
25.4441
25.3611
23.3404
23.3041
23.1075
22.5620
22.3600
22.1778
21.8746
21.2692
20.9776
16.7768
16.0547
Me
i-Pr
i-Pr
Me
O
O
O
OH
Me
O
i-Pr
O
O
O
i-Pr
Me
i-Pr
Me
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


19.8630
7.3685
7.3210
7.2866
7.2639
7.2193
7.2035
7.1878
7.0659
7.0509
6.0618
6.0462
5.8507
5.8354
1.5923
1.5604
1.4727
1.4599
1.3399
Me
O
O
O
Me
OH
Me
O
O
O
O
O
Me
Me
1.00
27.64
5.17
19.84
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

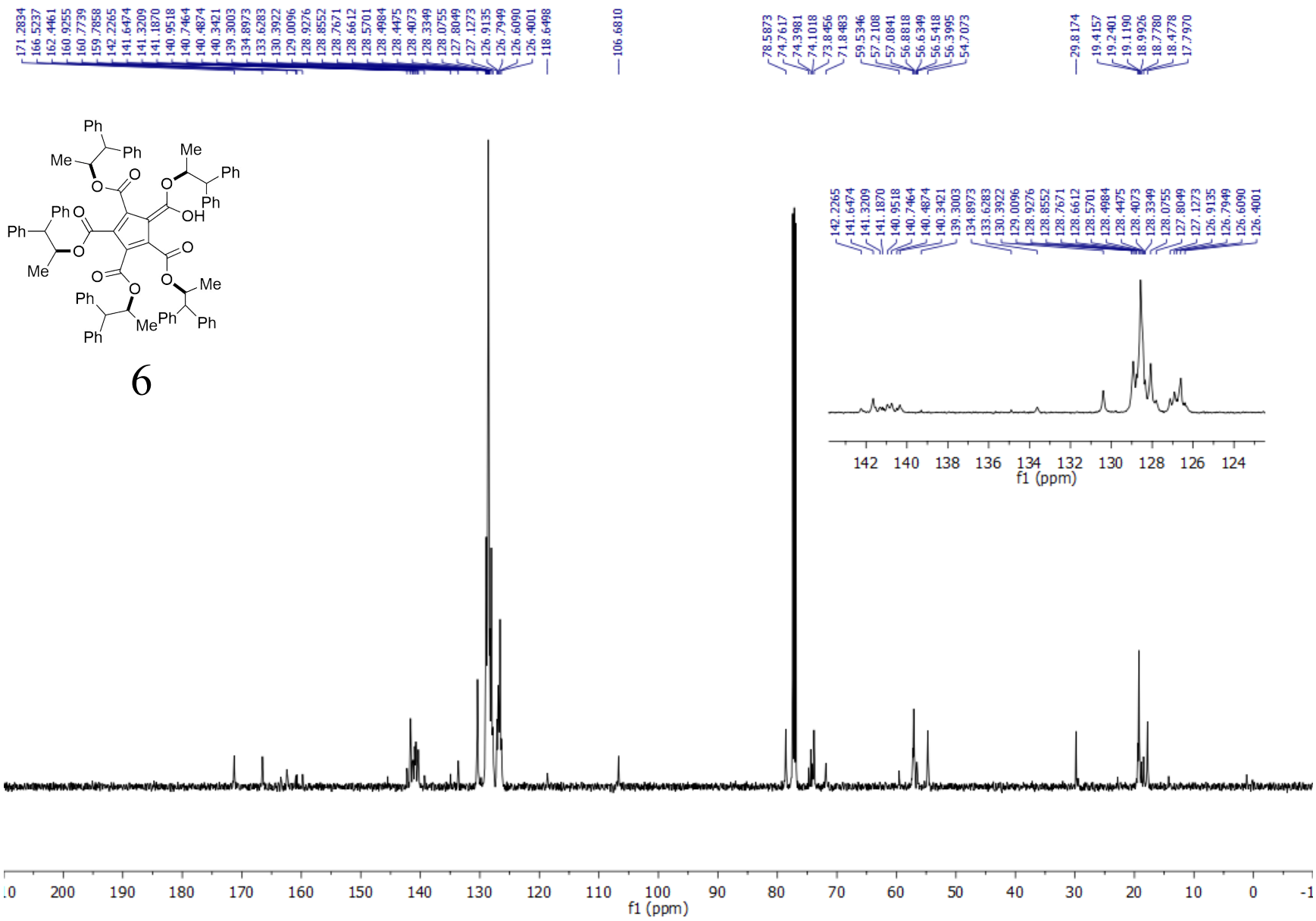
5


Me
O
O
O
OH
Me
Me
O
O
O
O
O
Me
Me
171.3726
166.4981
162.3260
142.0833
141.6982
139.9258
133.9186
128.4883
128.2491
127.8135
127.3536
126.6438
126.1535
125.8592
118.4946
106.7730
78.8231
74.1873
72.8488
29.7795
22.9571
22.0669
21.8732
f1 (ppm)

5


19.6591
7.3841
7.2201
7.1209
7.0882
6.9356
5.9045
5.8508
5.6974
5.2568
4.4607
4.2157
4.1985
4.0765
4.0289
3.9516
3.8540
3.7085
3.6054
1.5714
1.3756
1.2610
1.2022
1.1186
1.0127
0.8801
0.74
54.19
4.77
5.00
19.49
f1 (ppm)

6


171.2834
166.5237
162.4461
160.9255
160.7739
159.7858
142.2265
141.6474
141.3209
141.1870
140.9518
140.7464
140.4874
140.3421
139.3003
134.8973
133.6283
130.3922
129.0096
128.9276
128.8552
128.7671
128.6612
128.5701
128.4984
128.4475
128.4073
128.3349
128.0755
127.8049
127.1273
126.9135
126.7949
126.6090
126.4001
118.6498
106.6810
78.5873
74.7617
74.3981
74.1018
73.8456
71.8483
59.5346
57.2108
57.0841
56.8818
56.6349
56.5418
56.3995
54.7073
29.8174
19.4157
19.2401
19.1190
18.9926
18.7780
18.4778
17.7970
Ph
Me
Ph
O
O
Me
Ph
O
OH
Ph
Ph
O
O
Me
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O
Ph
Me
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Me
Ph
Ph
Ph
6
142.2265
141.6474
141.3209
141.1870
140.9518
140.7464
140.4874
140.3421
139.3003
134.8973
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130.3922
129.0096
128.9276
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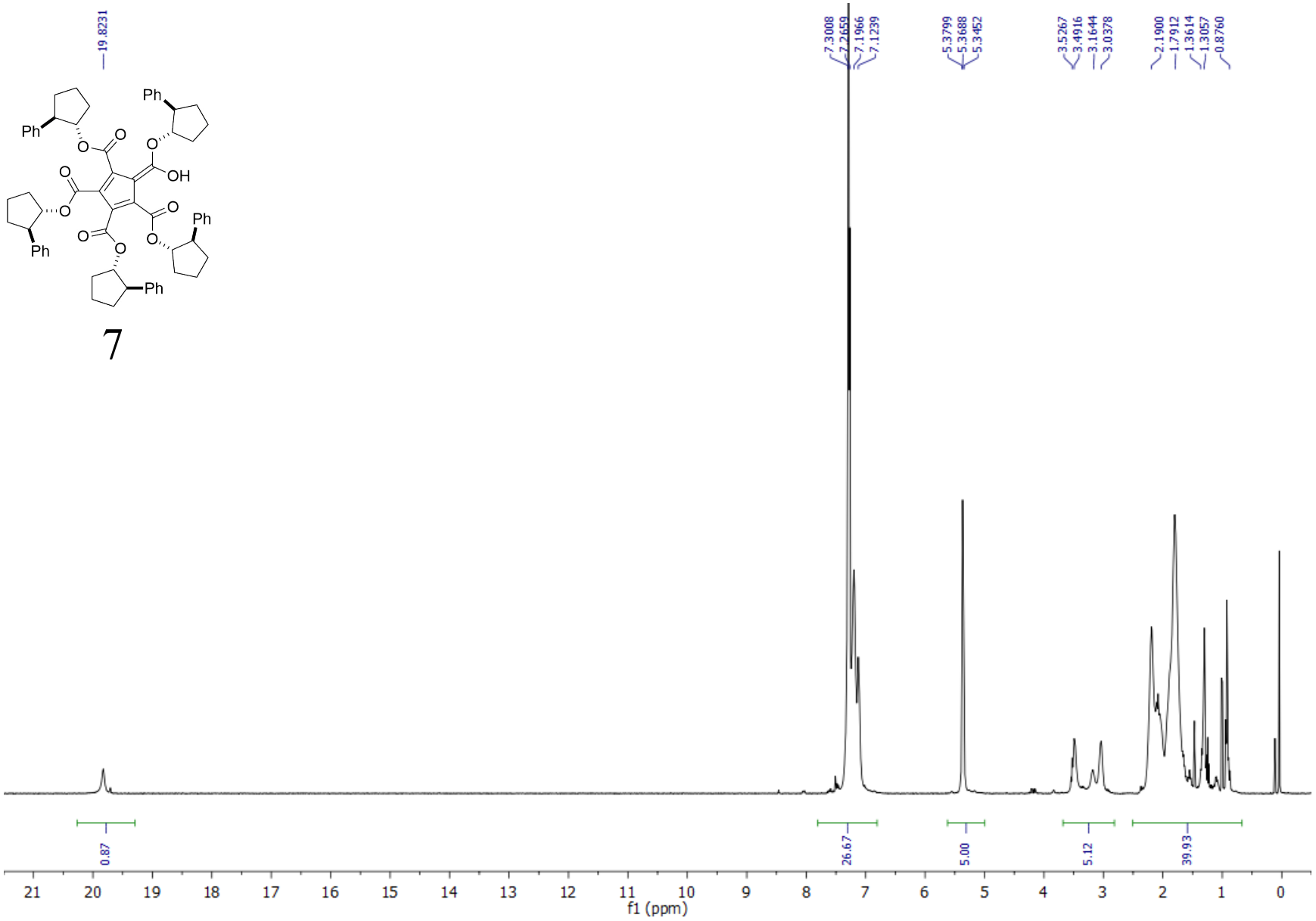
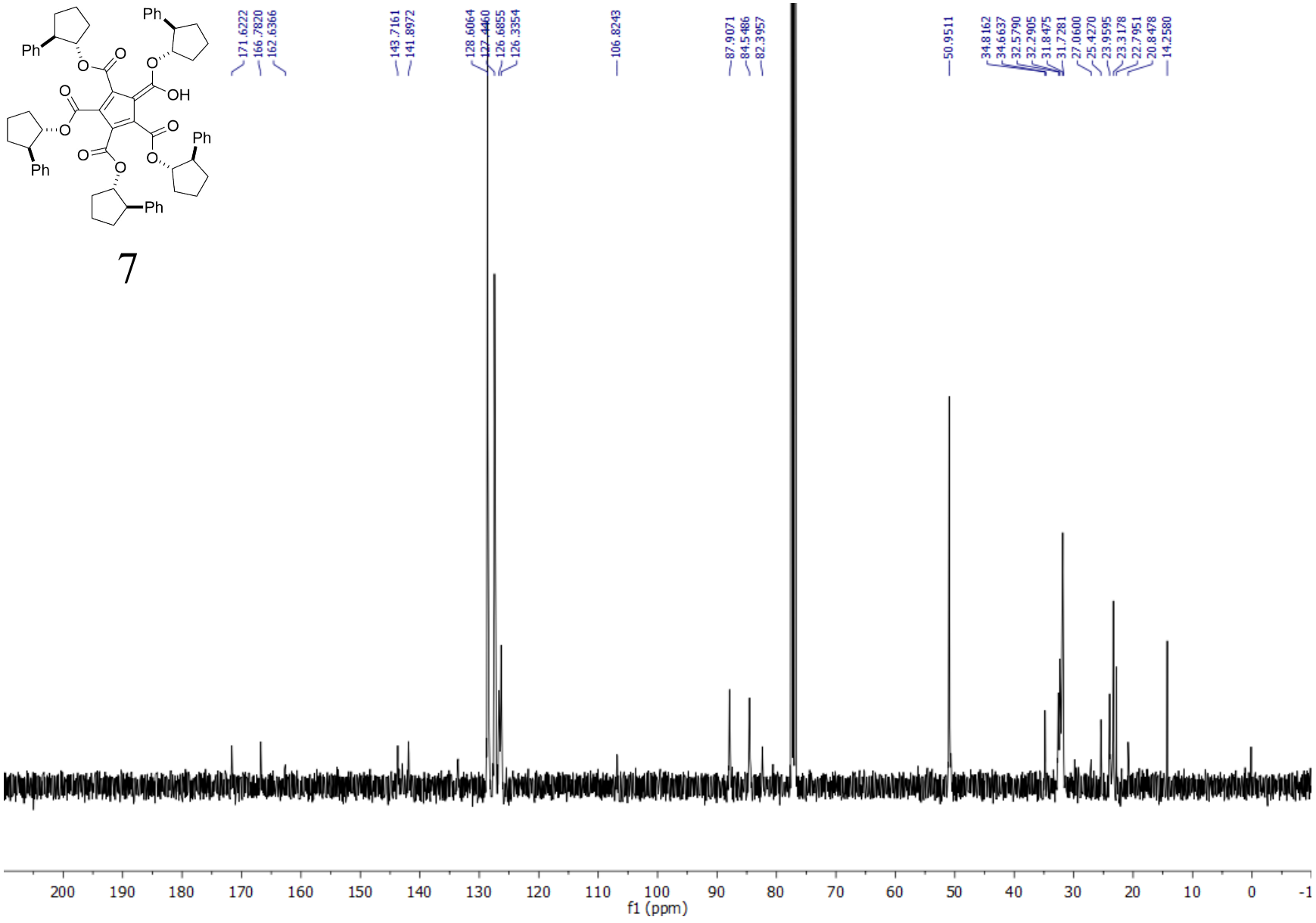
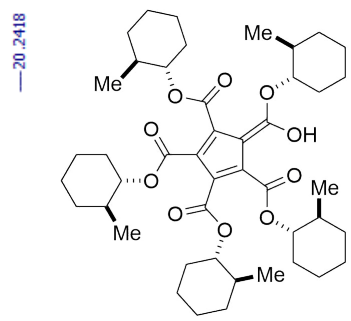
128.7671
128.6612
128.5701
128.4984
128.4475
128.4073
128.3349
128.0755
127.8049
127.1273
126.9135
126.7949
126.6090
126.4001
142 140 138 136 134 132 130 128 126 124
f1 (ppm)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)


19.8231
7.3008
7.2659
7.1966
7.1239
5.3799
5.3688
5.3452
3.5267
3.4916
3.1644
3.0378
2.1900
1.7912
1.3614
1.3057
0.8760
0.87
26.67
5.00
5.12
39.93
f1 (ppm)

7

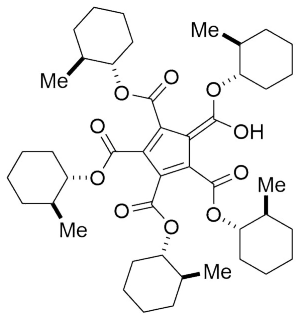

Ph
Ph
O
O
O
OH
O
O
O
O
O
O
Ph
Ph
Ph
171.6222
166.7820
162.6366
143.7161
141.8972
128.6064
127.4460
126.6855
126.3354
106.8243
87.9071
84.5486
82.3957
50.9511
34.8162
34.6637
32.5790
32.2905
31.8475
31.7281
27.0600
25.4270
23.9595
23.3178
22.7951
20.8478
14.2580
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

7


Me
Me
O
O
O
OH
O
O
O
O
O
Me
Me
O
Me

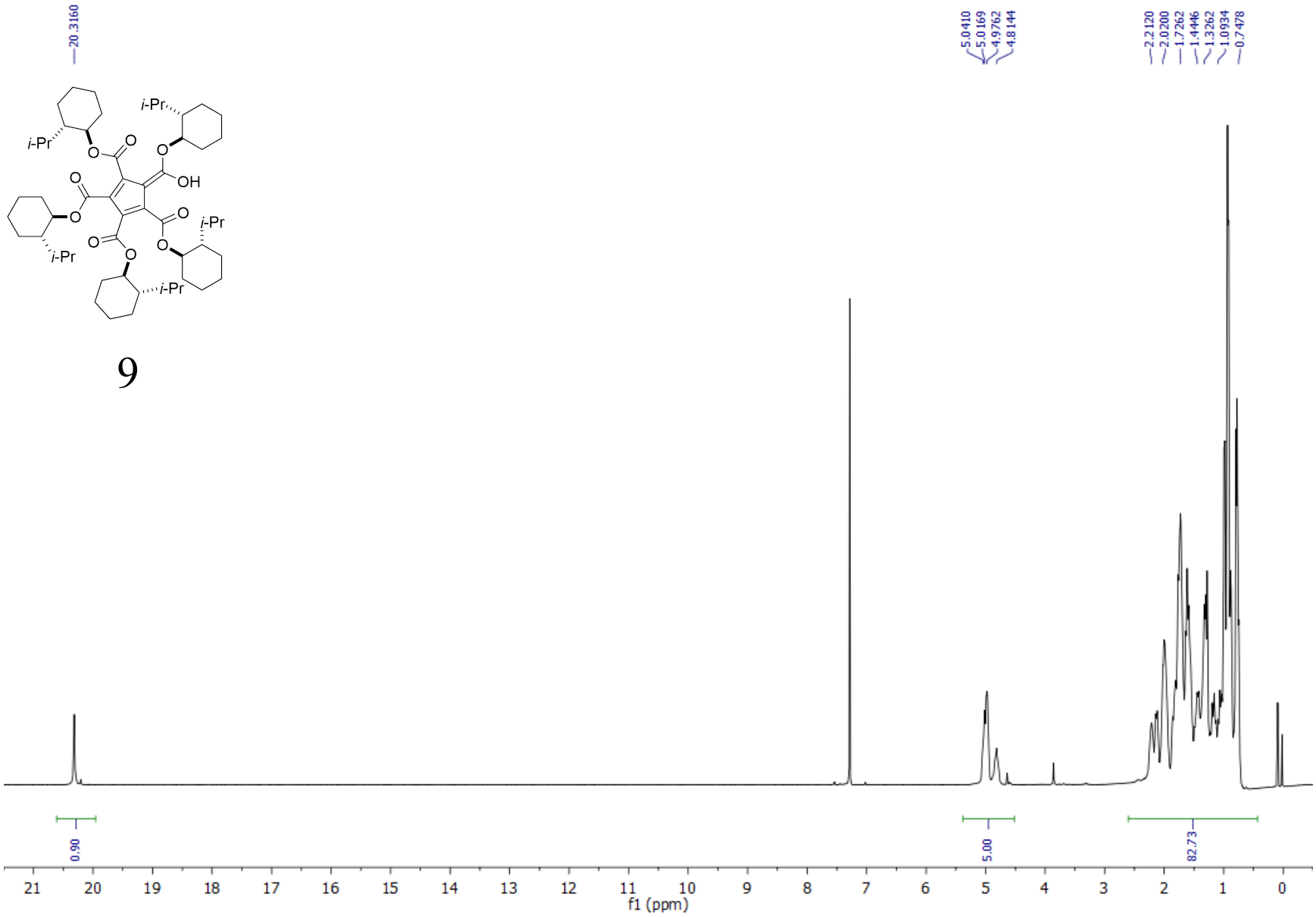
8

20.2418
4.7555
4.7473
4.7263
4.7133
4.5942
4.5103
4.4949
2.3739
2.0821
2.0634
1.9521
1.8215
1.6819
1.5545
1.4441
1.2557
1.1686
1.0909
1.0047
0.9917
0.9514
0.9389
0.8975
0.8850
0.98
5.00
64.98
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

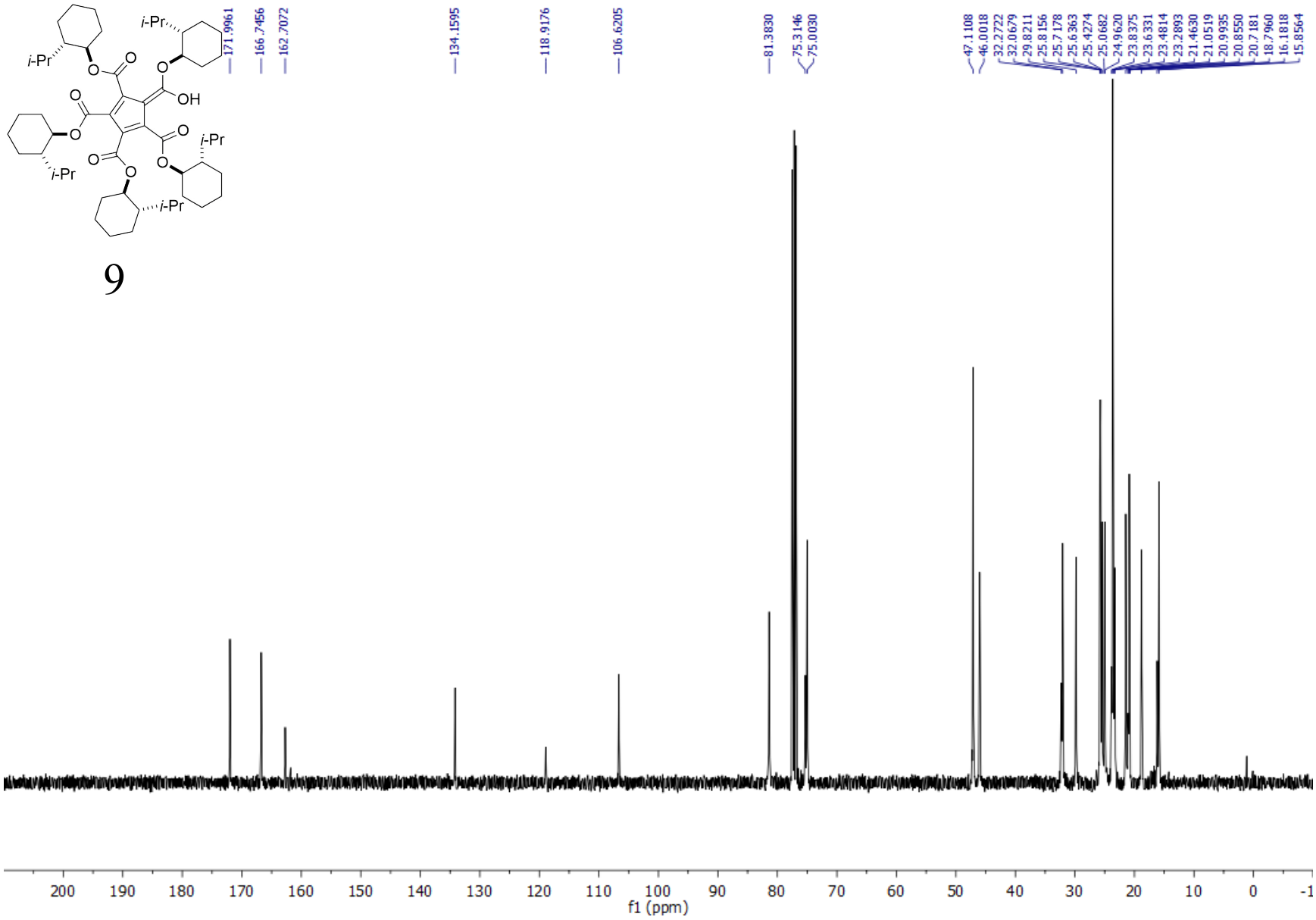

Me
Me
O
O
OH
O
O
O
O
Me
Me
O
O
Me

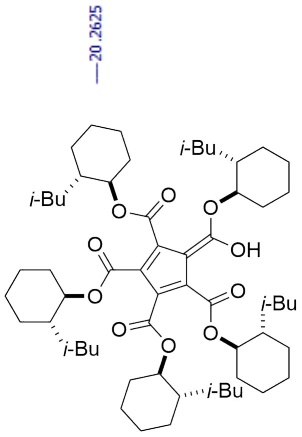
8

172.1532
166.9029
162.9201
134.1357
118.6989
106.6488
85.4034
79.8439
79.0486
37.3941
37.2490
36.3332
33.8035
32.7625
31.8627
31.6621
30.7589
25.7383
25.4192
25.0262
24.9425
24.5348
24.2057
18.7304
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


20.3160
5.0410
5.0169
4.9762
4.8144
2.2120
2.0200
1.7262
1.4446
1.3262
1.0934
0.7478
i-Pr
i-Pr
i-Pr
i-Pr
i-Pr
OH
O
0.90
5.00
82.73
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

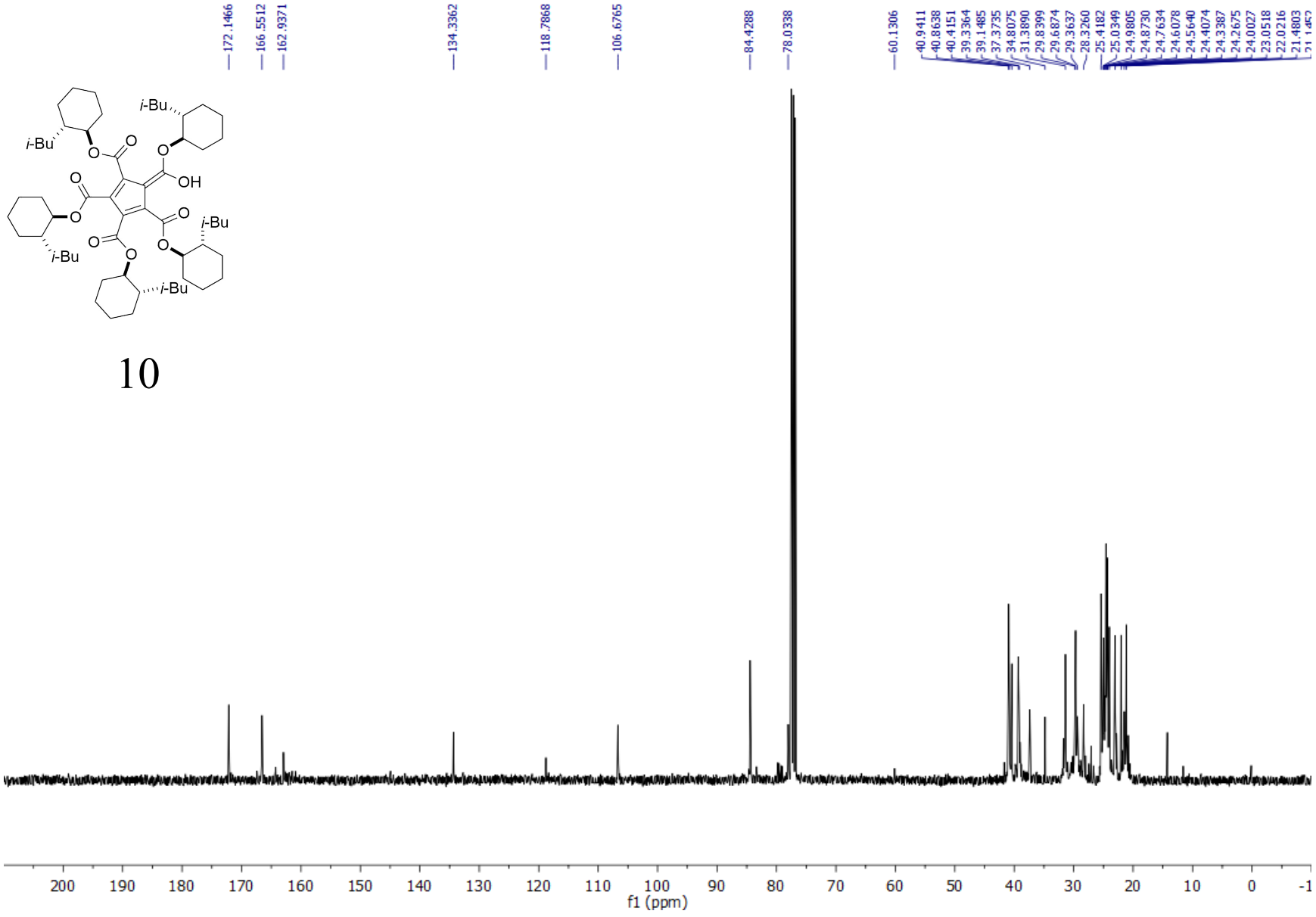
9


i-Pr
i-Pr
i-Pr
i-Pr
i-Pr
OH
O
9
171.9961
166.7456
162.7072
134.1595
118.9176
106.6205
81.3830
75.3146
75.0030
47.1108
46.0018
32.2722
32.0679
29.8211
25.8156
25.7178
25.6363
25.4274
25.0682
24.9620
23.8375
23.6331
23.4814
23.2893
21.4630
21.0519
20.9935
20.8550
20.7181
18.7960
16.1818
15.8564
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

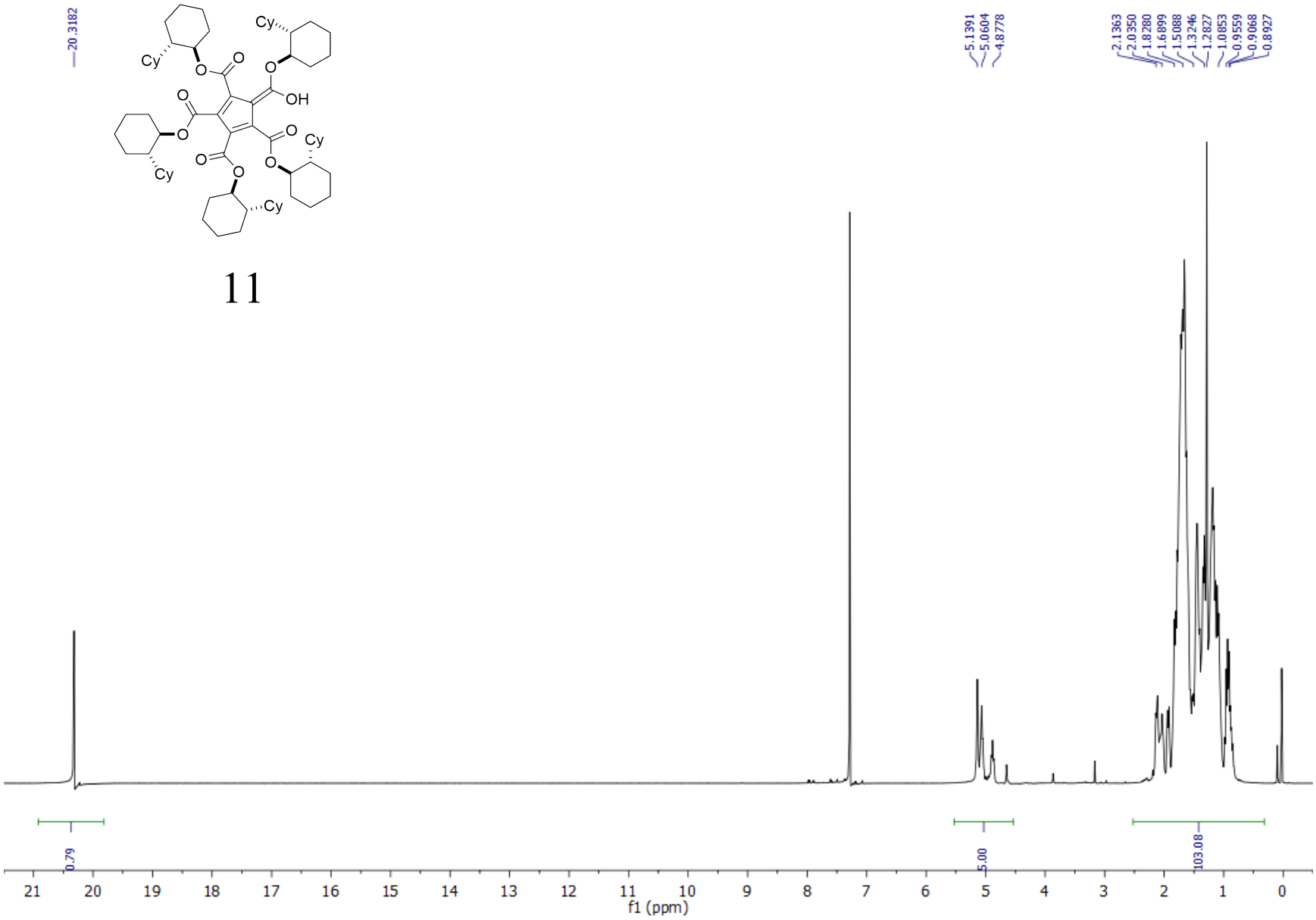

20.2625
i-Bu
i-Bu
OH
i-Bu
i-Bu
i-Bu

10

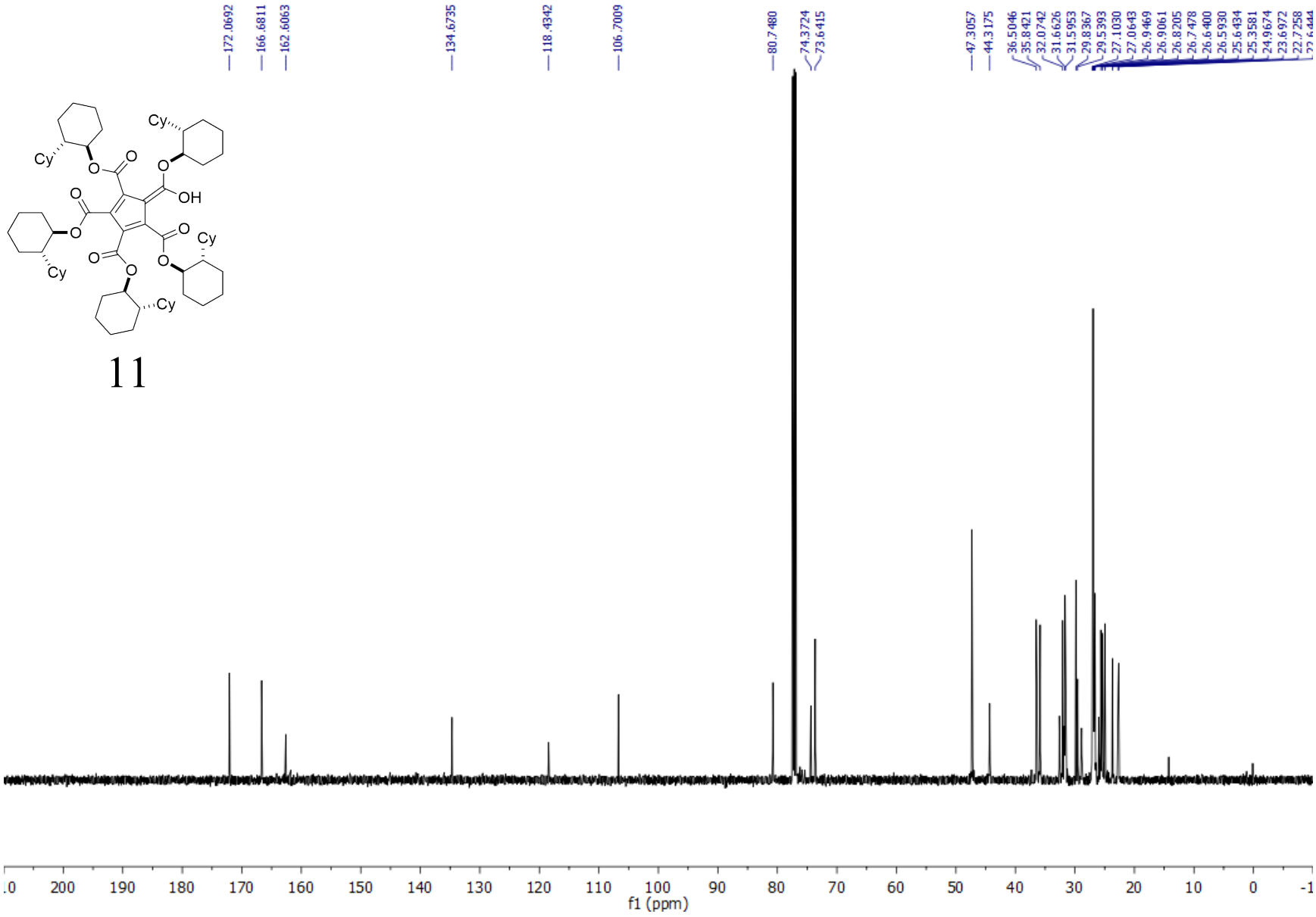
4.8054
4.7377
4.6654
4.6121
2.1889
1.9210
1.8684
1.7095
1.6016
1.5396
1.4498
1.3718
1.3273
1.2293
1.0797
0.9807
0.9033
0.8192
0.91
5.00
101.99
21 20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)


172.1466
166.5512
162.9371
134.3362
118.7868
106.6765
84.4288
78.0338
60.1306
40.9411
40.8638
40.4151
39.3364
39.1485
37.3735
34.8075
31.3890
29.8399
29.6874
29.3637
28.3260
25.4182
25.0349
24.9805
24.8730
24.7634
24.6078
24.5640
24.4074
24.3387
24.2675
24.0027
23.0518
22.0216
21.4803
i-Bu
OH
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

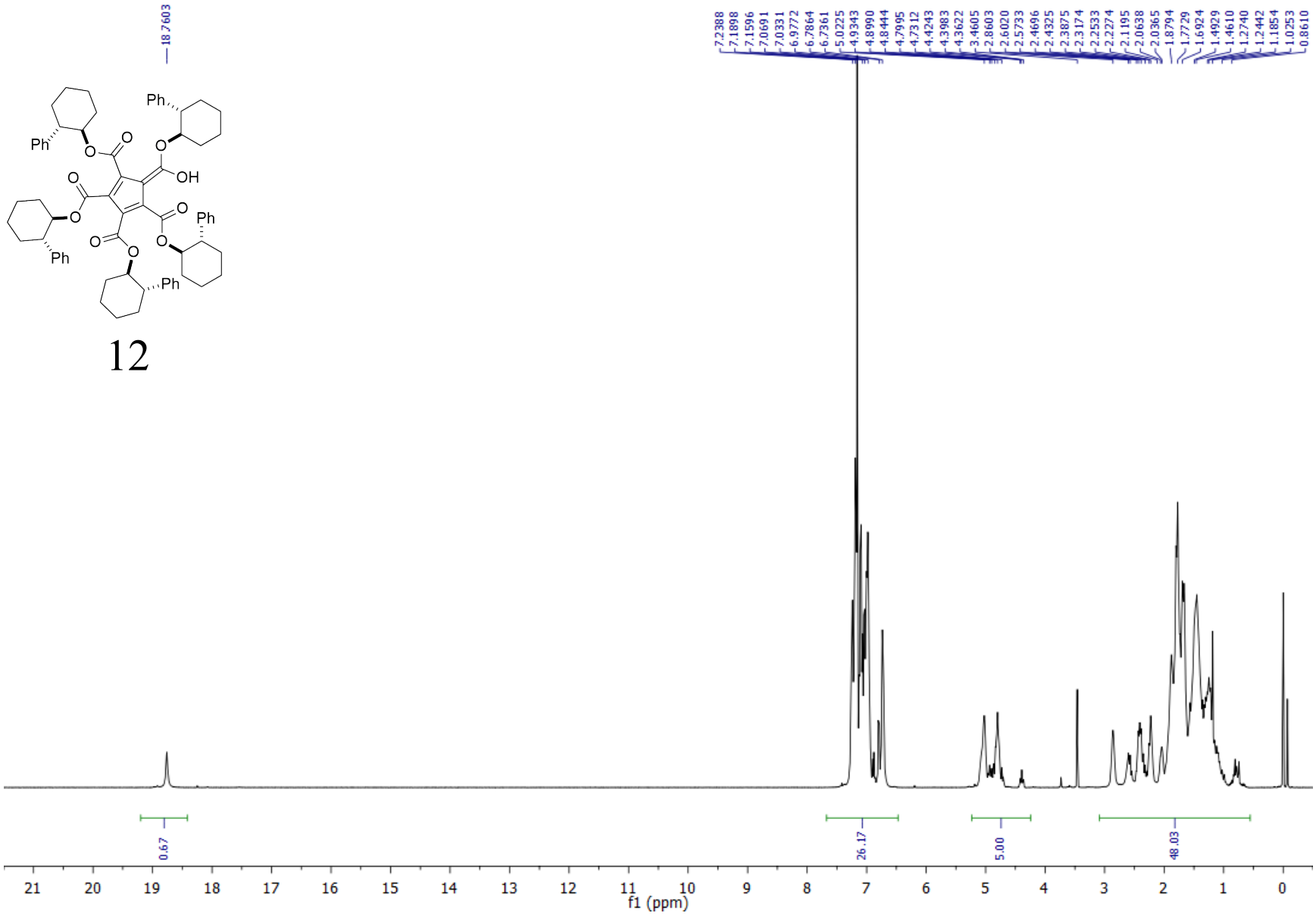
10


20.3182
5.1391
5.0604
4.8778
2.1363
2.0350
1.8280
1.6899
1.5088
1.3246
1.2827
1.0853
0.9559
0.9068
0.8927
0.79
5.00
103.08
f1 (ppm)

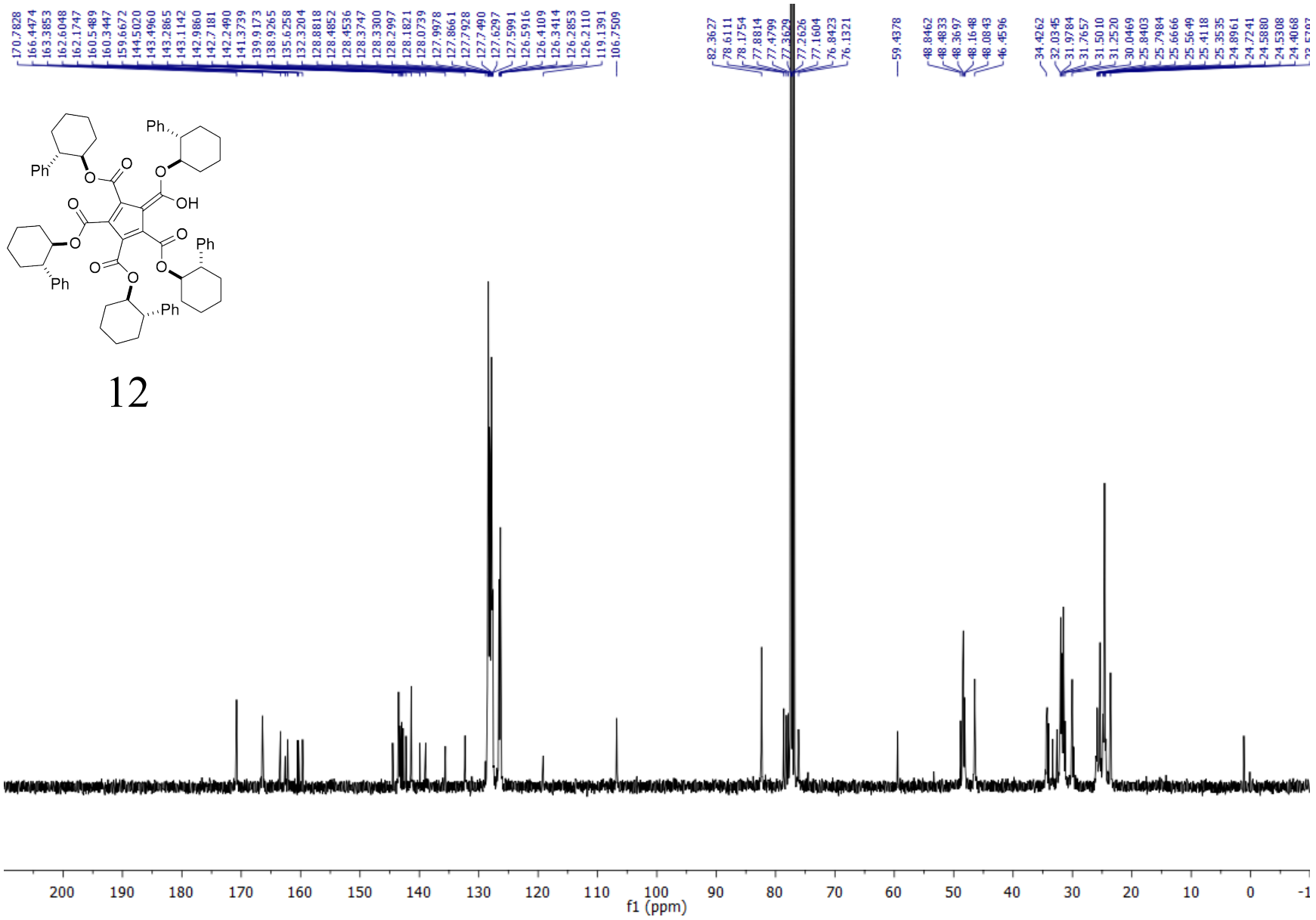
11


172.0692
166.6811
162.6063
134.6735
118.4342
106.7009
80.7480
74.3724
73.6415
47.3057
44.3175
36.5046
35.8421
32.0742
31.6626
31.5953
29.8367
29.5393
27.1030
27.0643
26.9469
26.9061
26.8205
26.7478
26.6400
26.5930
25.6434
25.3581
24.9674
23.6972
22.7258
Cy
OH
f1 (ppm)

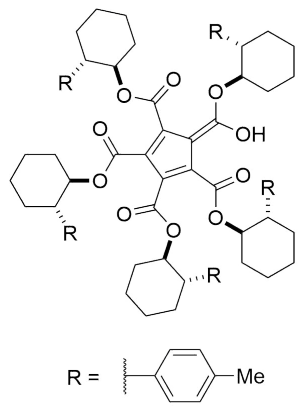
11


18.7603
Ph
Ph
O
O
O
OH
O
O
Ph
O
O
O
Ph
Ph
Ph
7.2388
7.1898
7.1596
7.0691
7.0331
6.9772
6.7864
6.7361
5.0225
4.9343
4.8990
4.8444
4.7995
4.7312
4.4243
4.3983
4.3622
3.4605
2.8603
2.6020
2.5733
2.4696
2.4325
2.3875
2.3174
2.2533
2.2274
2.1195
2.0638
2.0365
1.8794
1.7729
1.6924
1.4929
1.4610
1.2740
1.2442
1.1854
1.0253
0.8610
0.67
26.17
5.00
48.03
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

12

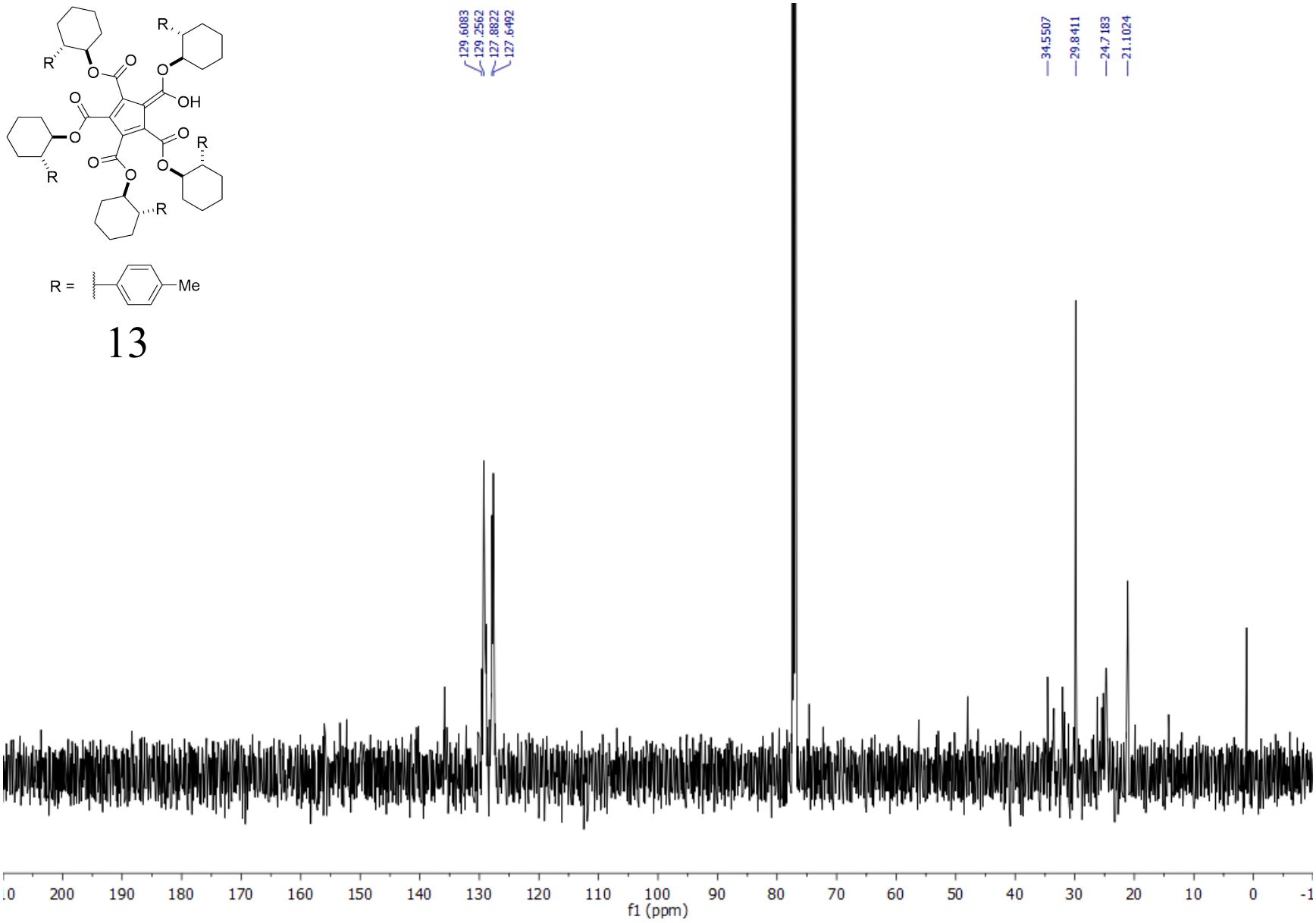

170.7828
166.4474
163.3853
162.6048
162.1747
160.5489
160.3447
159.6672
144.5020
143.4960
143.2865
143.1142
142.9860
142.7181
142.2490
141.3739
139.9173
138.9265
135.6258
132.3204
128.8818
128.4852
128.4536
128.3747
128.3300
128.2997
128.1821
128.0739
127.9978
127.8661
127.7928
127.7490
127.6297
127.5991
126.5916
126.4109
126.3414
126.2853
126.2110
119.1391
106.7509
82.3627
78.6111
78.1754
77.8814
77.4799
77.3629
77.2626
77.1604
76.8423
76.1321
59.4378
48.8462
48.4833
48.3697
48.1648
48.0843
46.4596
34.4262
32.0345
31.9784
31.7657
31.5010
31.2520
30.0469
25.8403
25.7984
25.6666
25.5649
25.4118
25.3535
24.8961
24.7241
24.5880
24.5308
24.4068
Ph
Ph
O
O
O
OH
O
O
O
O
O
Ph
Ph
Ph
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

12

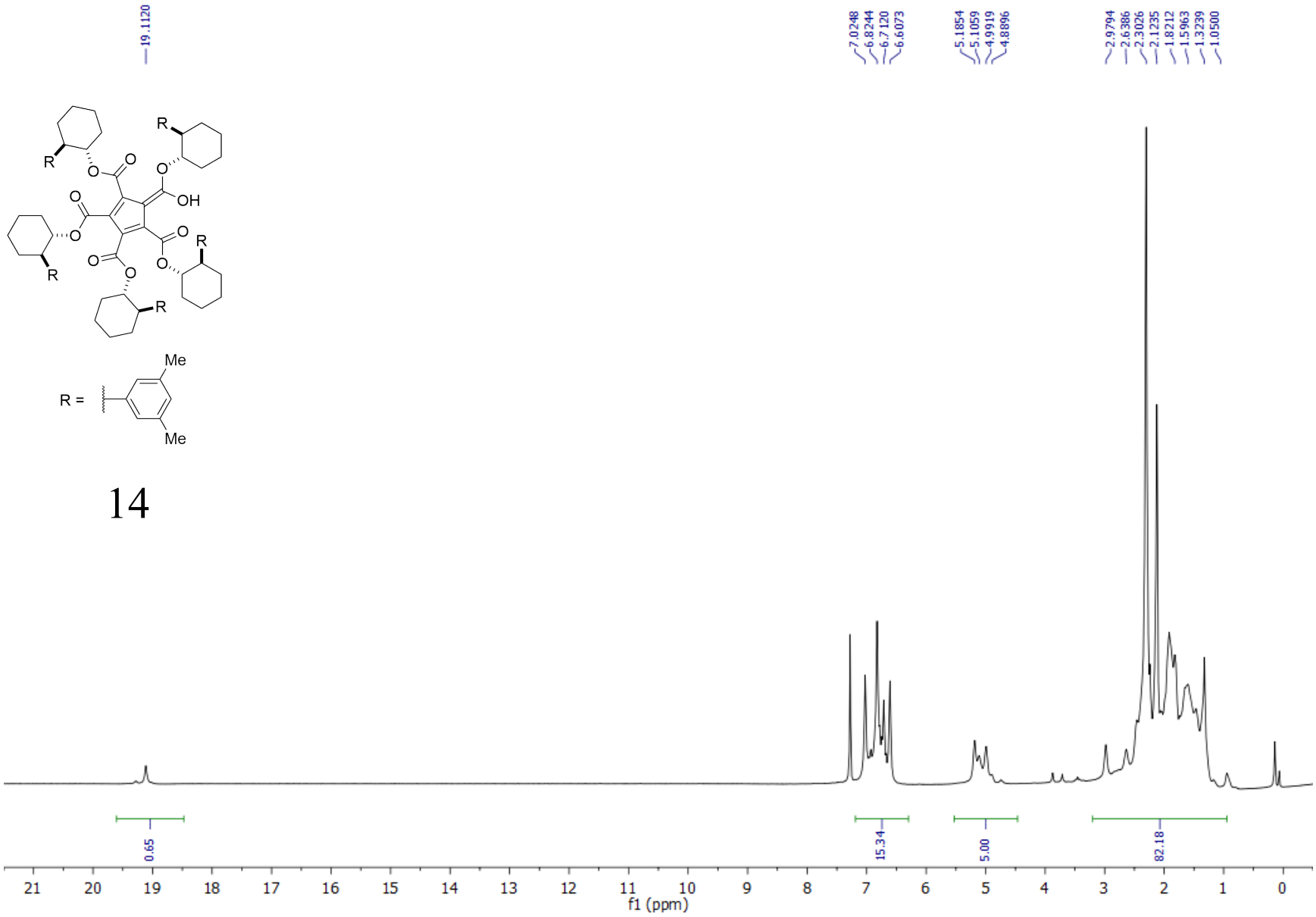

R
R
O
O
O
OH
O
O
O
R
R
O
O
O
R
R = Me

13

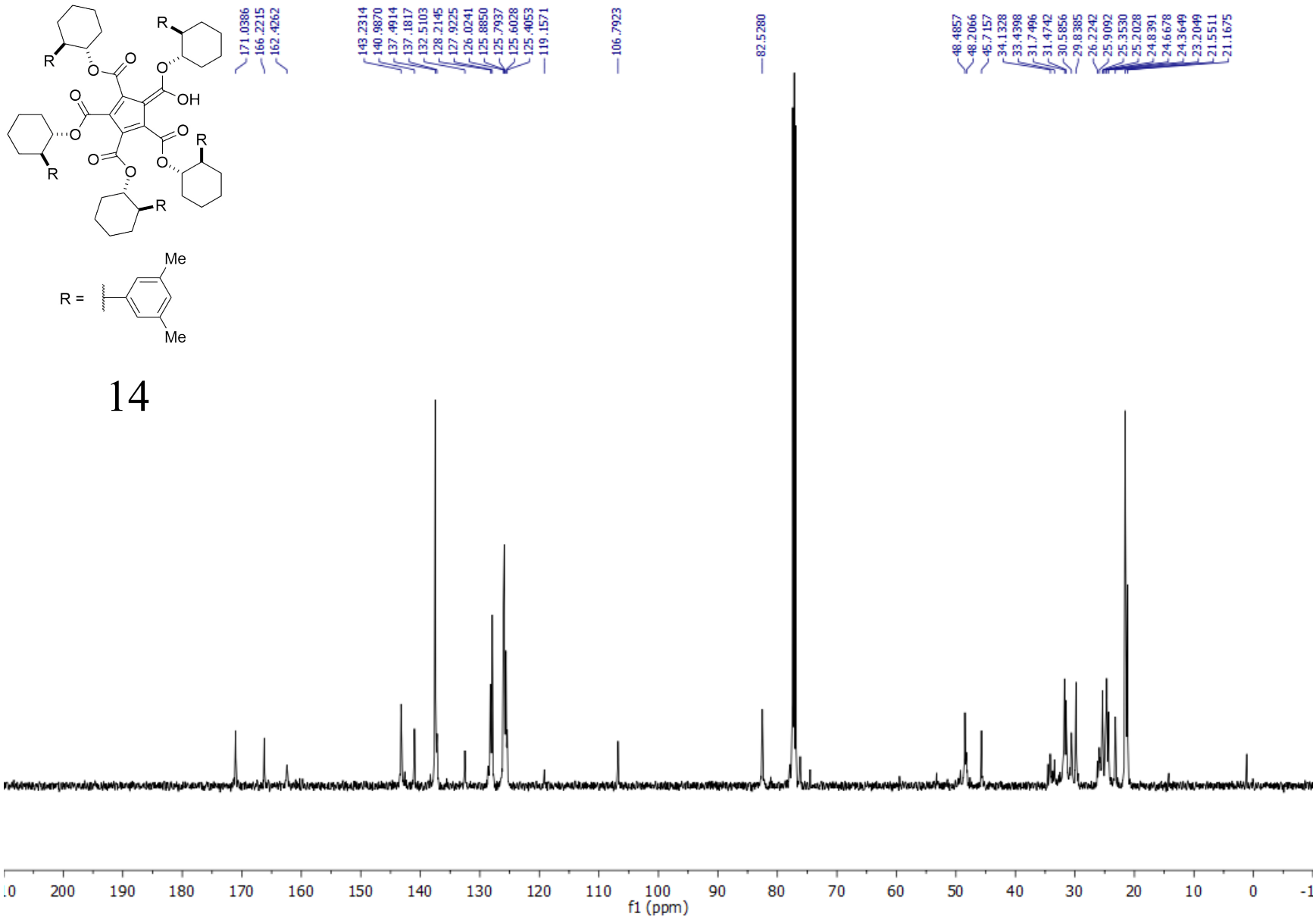
18.8448
7.5217
7.1866
7.0474
6.9513
6.6903
5.1408
4.9303
4.8794
2.8885
2.2275
2.1801
1.8069
1.8057
1.5345
1.2983
0.9228
0.7855
0.19
23.44
5.00
91.75
f1 (ppm)


R
R
O
O
O
OH
O
O
O
R
O
O
R
O
O
R
R = Me
129.6083
129.2562
127.8822
127.6492
34.5507
29.8411
24.7183
21.1024
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

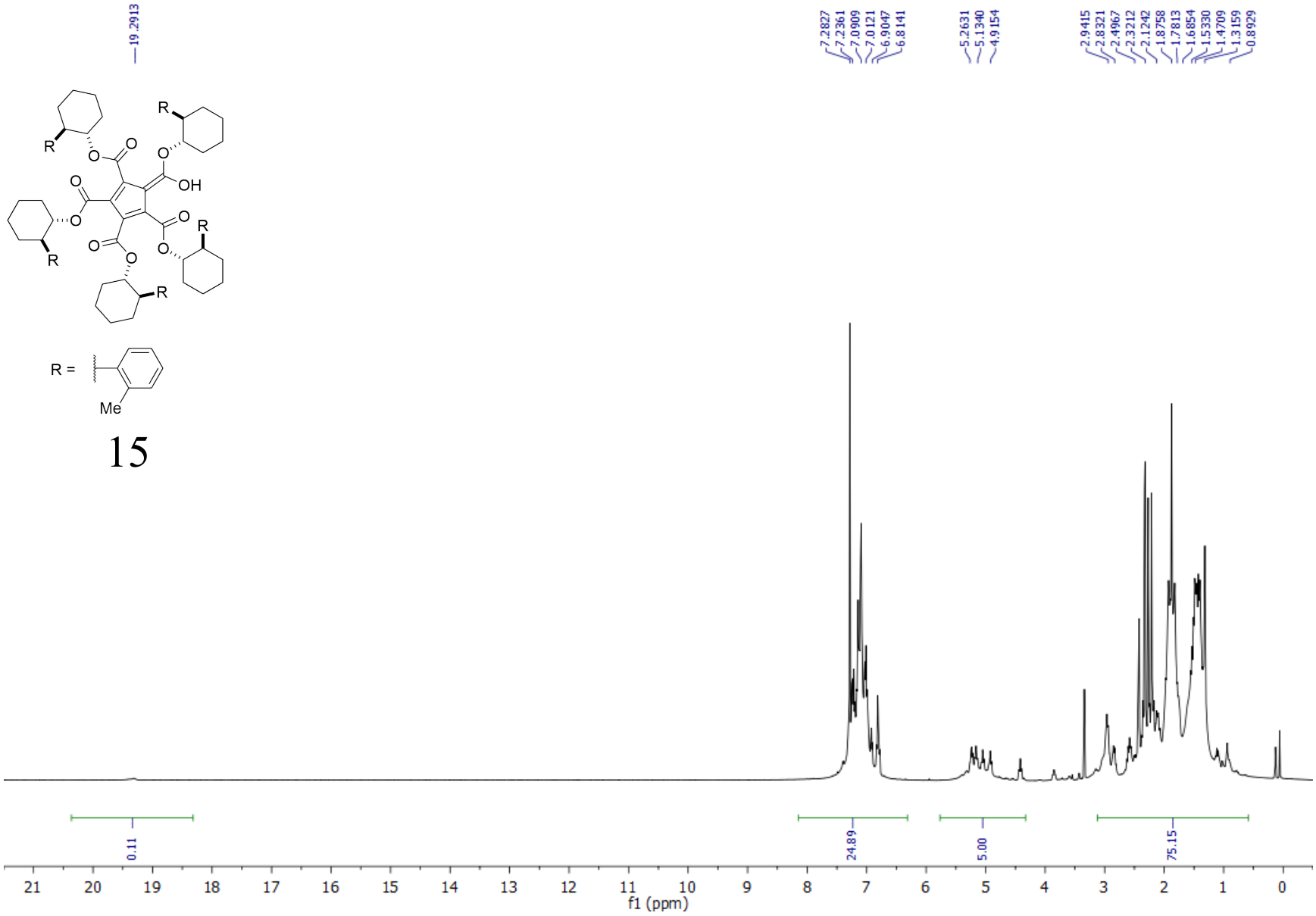
13


19.1120
7.0248
6.8244
6.7120
6.6073
5.1854
5.1059
4.9919
4.8896
2.9794
2.6386
2.3026
2.1235
1.8212
1.5963
1.3239
1.0500
R
O
OH
Me
R =
0.65
15.34
5.00
82.18
f1 (ppm)

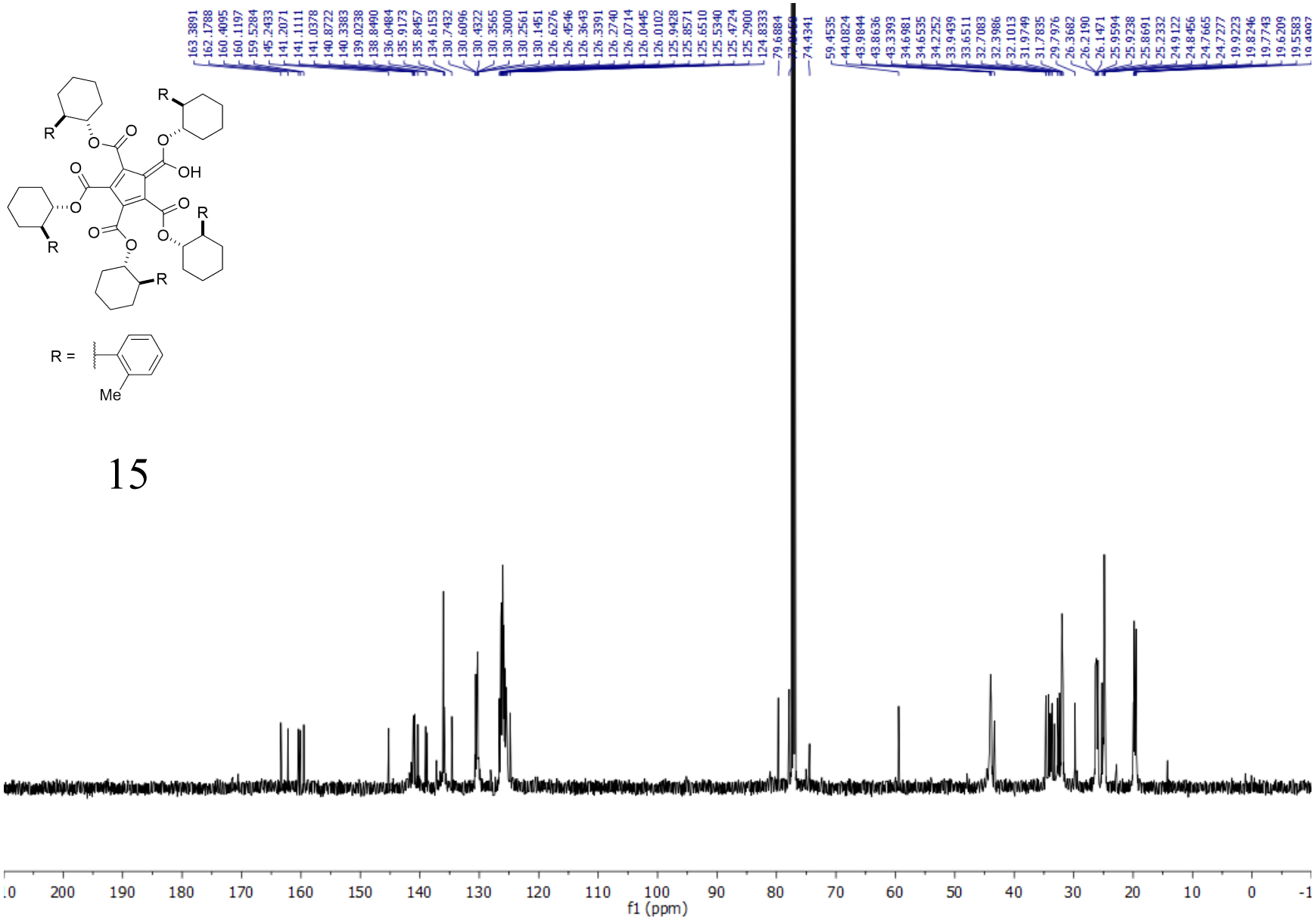
14


171.0386
166.2215
162.4262
143.2314
140.9870
137.4914
137.1817
132.5103
128.2145
127.9225
126.0241
125.8850
125.7937
125.6028
125.4053
119.1571
106.7923
82.5280
48.4857
48.2066
45.7157
34.1328
33.4398
31.7496
31.4742
30.5856
29.8385
26.2242
25.9092
25.3530
25.2028
24.8391
24.6678
24.3649
23.2049
21.5511
21.1675
R
O
OH
R =
Me
Me
f1 (ppm)

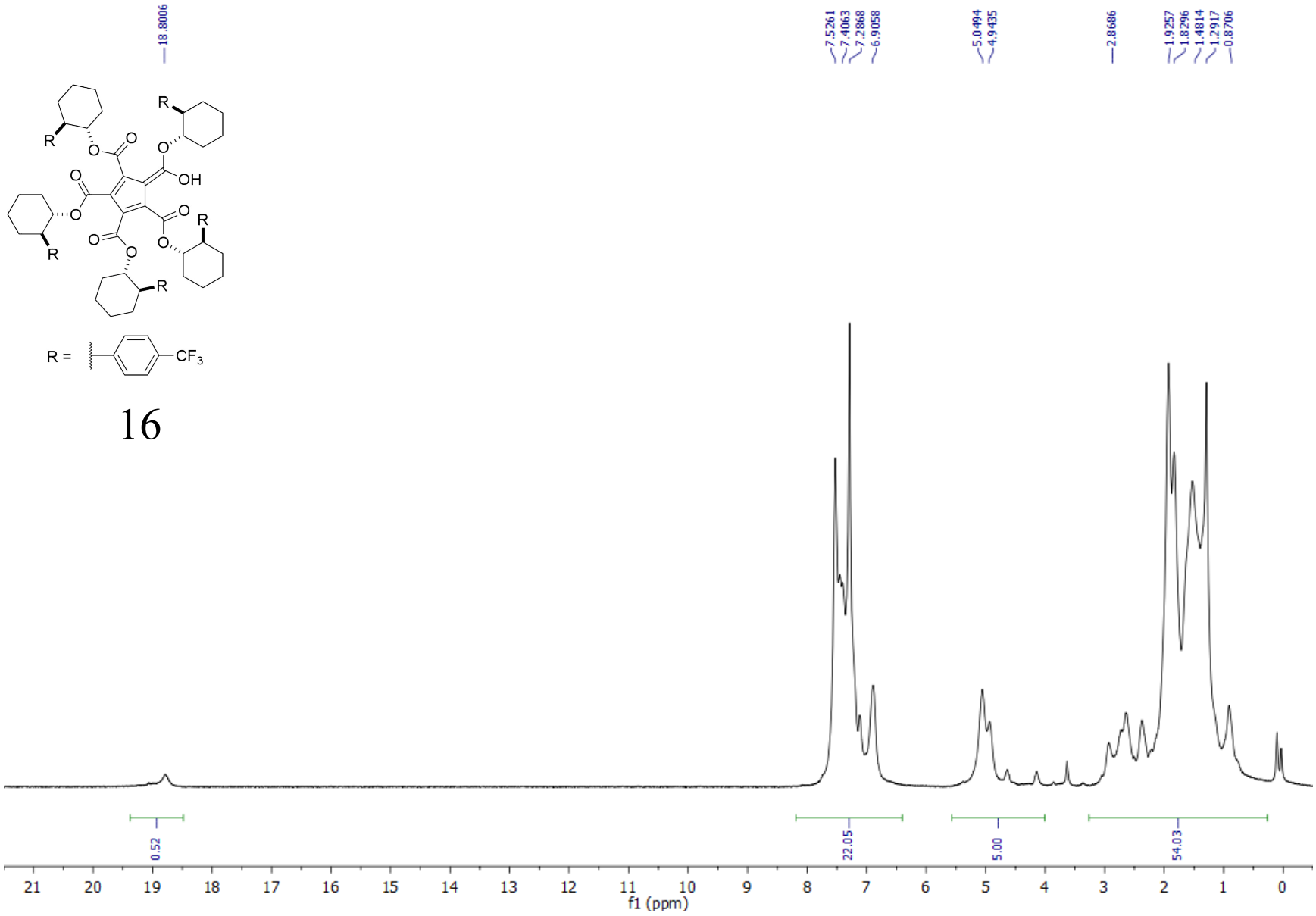
14


19.2913
7.2827
7.2361
7.0909
7.0121
6.9047
6.8141
5.2631
5.1340
4.9154
2.9415
2.8321
2.4967
2.3212
2.1242
1.8758
1.7813
1.6854
1.5330
1.4709
1.3159
0.8929
R
OH
R =
Me
0.11
24.89
5.00
75.15
f1 (ppm)

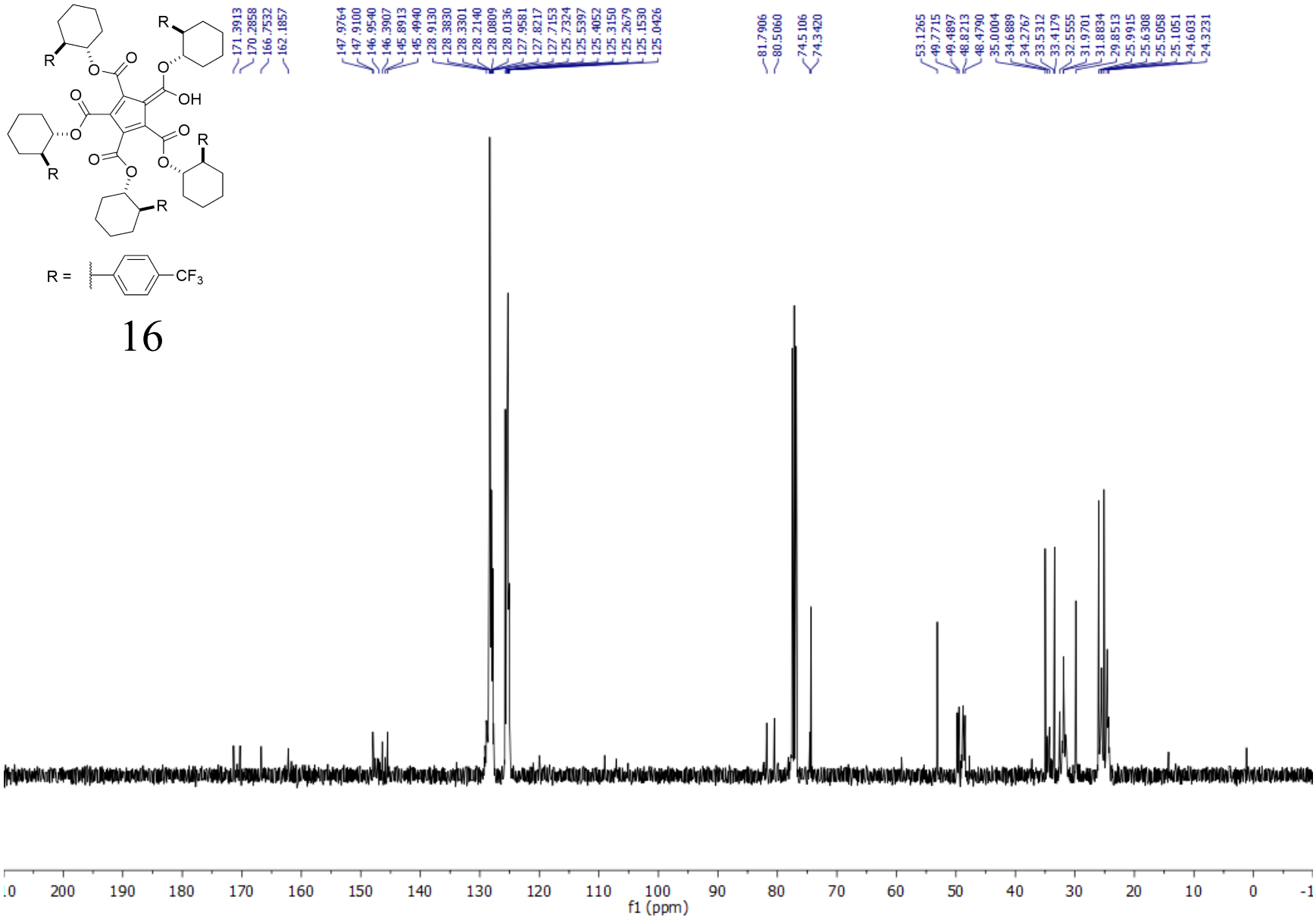
15

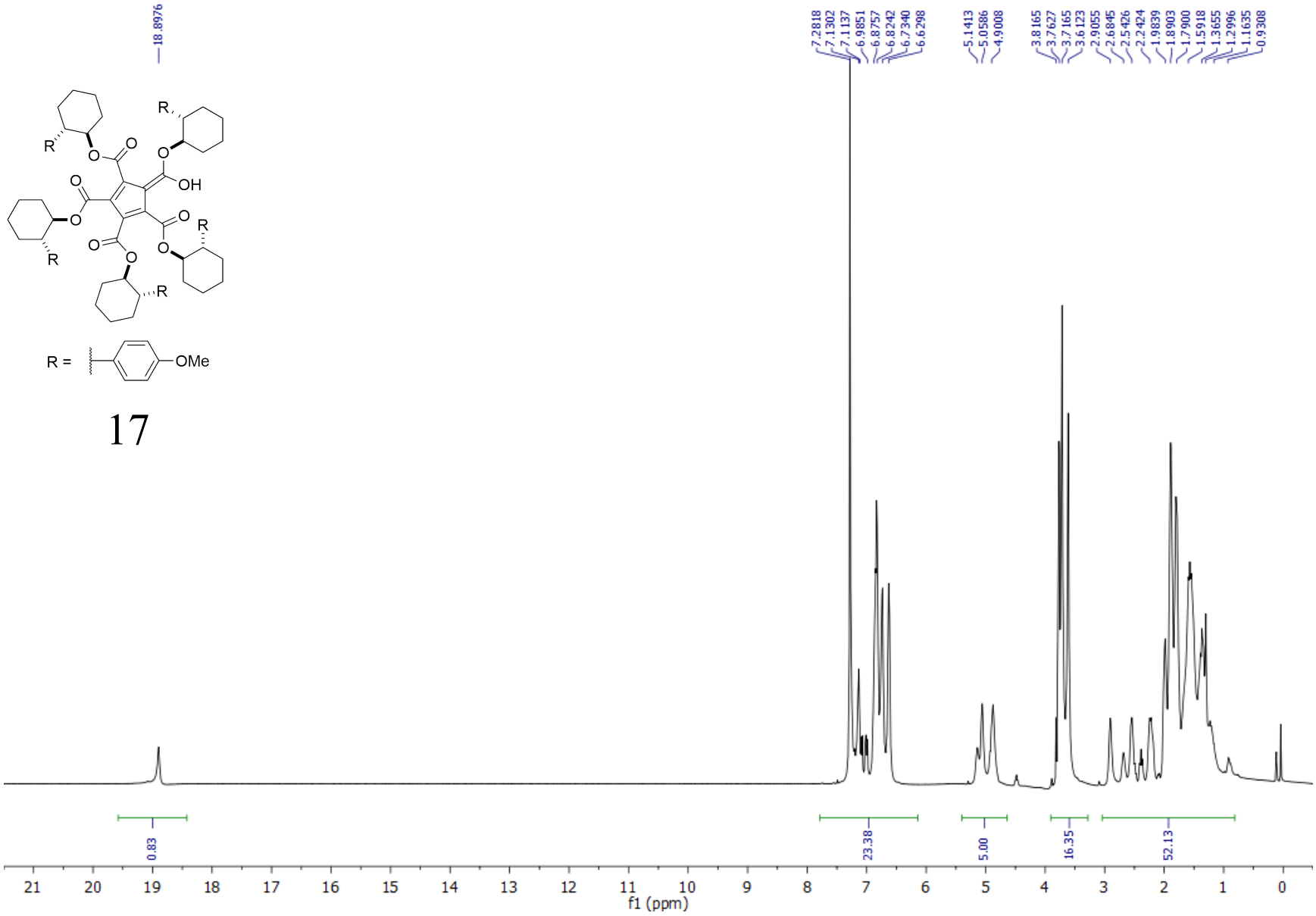

R
O
O
O
OH
O
O
O
O
O
R
R
R
R
R =
Me
163.3891
162.1788
160.4095
160.1197
159.5284
145.2433
141.2071
141.1111
141.0378
140.8722
140.3383
139.0238
138.8490
136.0484
135.9173
135.8457
134.6153
130.7432
130.6096
130.4322
130.3565
130.3000
130.2561
130.1451
126.6276
126.4546
126.3643
126.3391
126.2740
126.0714
126.0445
126.0102
125.9428
125.8571
125.6510
125.5340
125.4724
125.2900
124.8333
79.6884
74.4341
59.4535
44.0824
43.9844
43.8636
43.3393
34.6981
34.6535
34.2252
33.9439
33.6511
32.7083
32.3986
32.1013
31.9749
31.7835
29.7976
26.3682
26.2190
26.1471
25.9594
25.9238
25.8691
25.2332
24.9122
24.8456
24.7665
24.7277
19.9223
19.8246
19.7743
19.6209
19.5583
19.4987
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

15

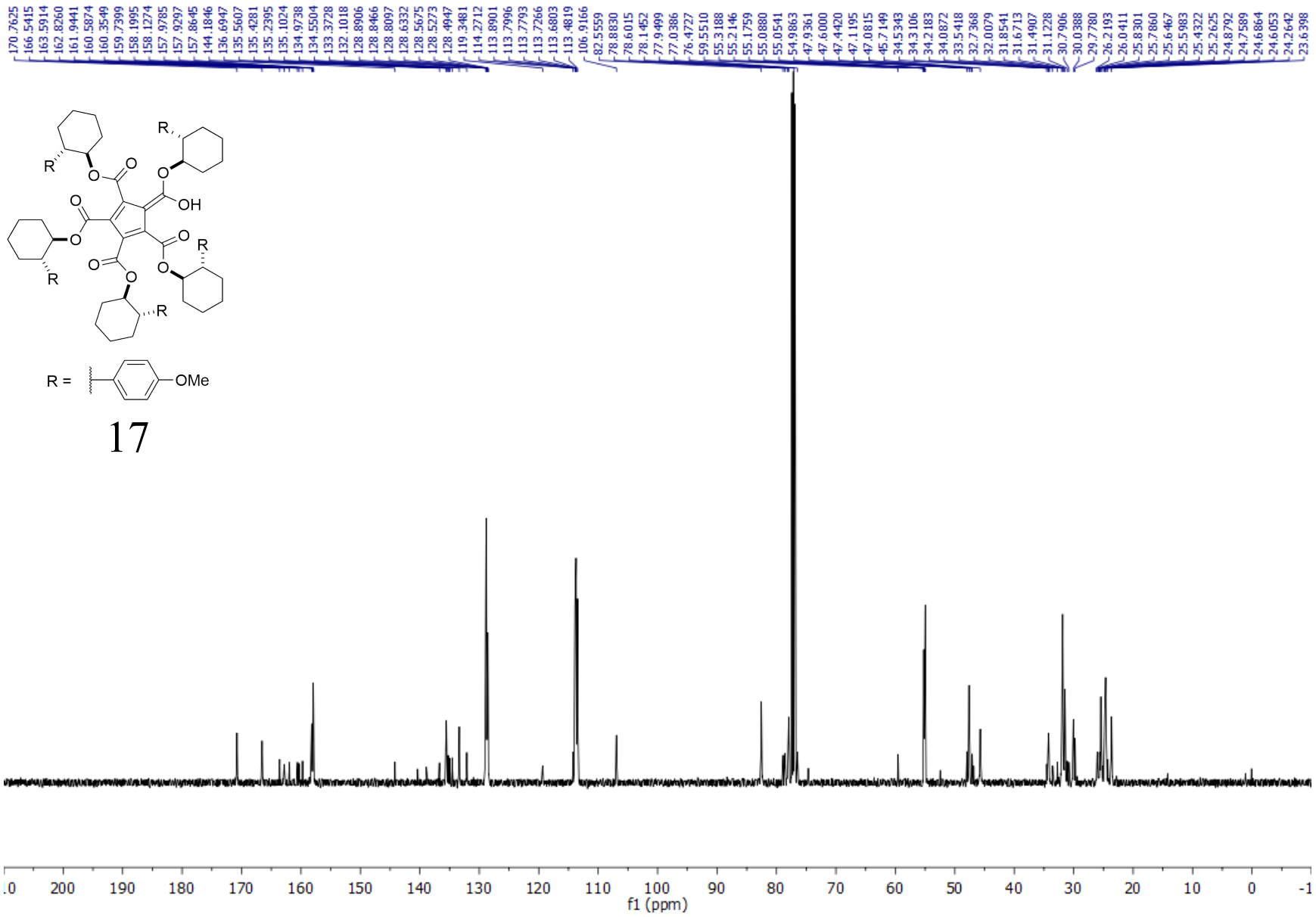

18.8006
7.5261
7.4063
7.2868
6.9058
5.0494
4.9435
2.8686
1.9257
1.8296
1.4814
1.2917
0.8706
R
O
OH
R =
CF3
0.52
22.05
5.00
54.03
21
20
19
18
17
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

16

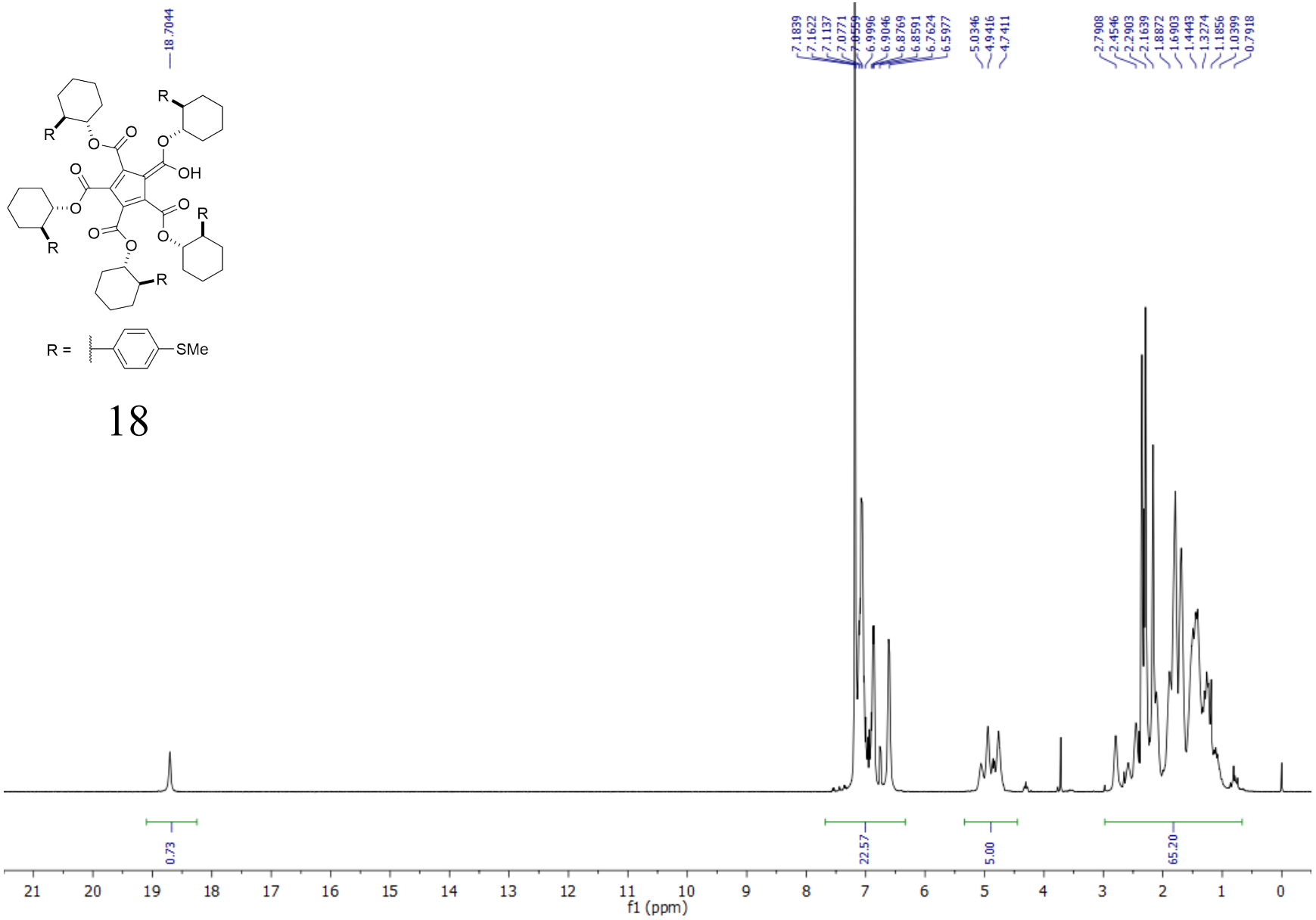

171.3913
170.2858
166.7532
162.1857
147.9764
147.9100
146.9540
146.3907
145.8913
145.4940
128.9130
128.3830
128.3301
128.2140
128.0809
128.0136
127.9581
127.8217
127.7153
125.7324
125.5397
125.4052
125.3150
125.2679
125.1530
125.0426
81.7906
80.5060
74.5106
74.3420
53.1265
49.7715
49.4897
48.8213
48.4790
35.0004
34.6889
34.2767
33.5312
33.4179
32.5555
31.9701
31.8834
29.8513
25.9915
25.6308
25.5058
25.1051
24.6031
24.3231
R =
CF3
16
f1 (ppm)


18.8976
7.2818
7.1302
7.1137
6.9851
6.8757
6.8242
6.7340
6.6298
5.1413
5.0586
4.9008
3.8165
3.7627
3.7165
3.6123
2.9055
2.6845
2.5426
2.2424
1.9839
1.8903
1.7900
1.5918
1.3655
1.2996
1.1635
0.9308
OH
R
R =
OMe
0.83
23.38
5.00
16.35
52.13
f1 (ppm)

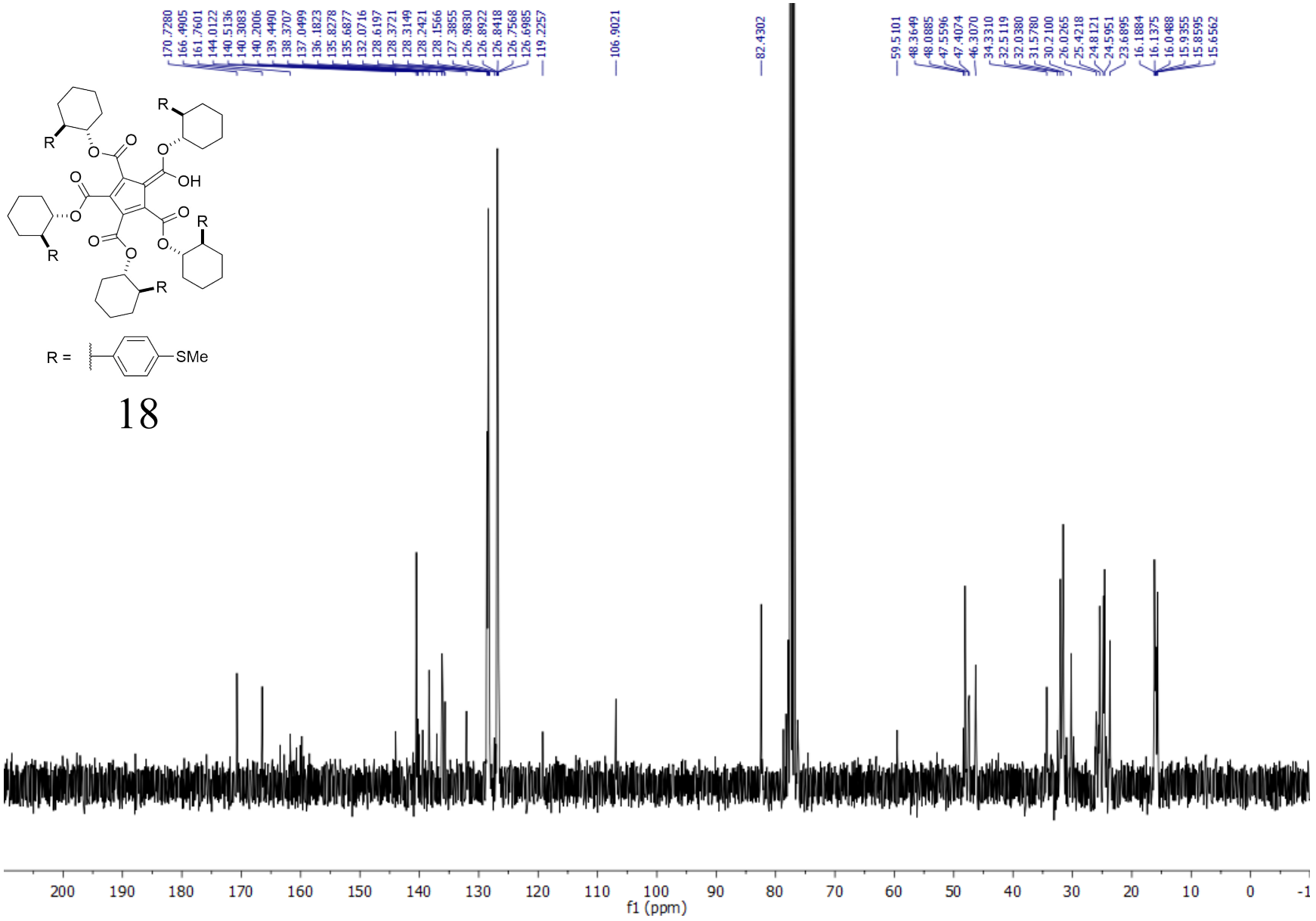
17

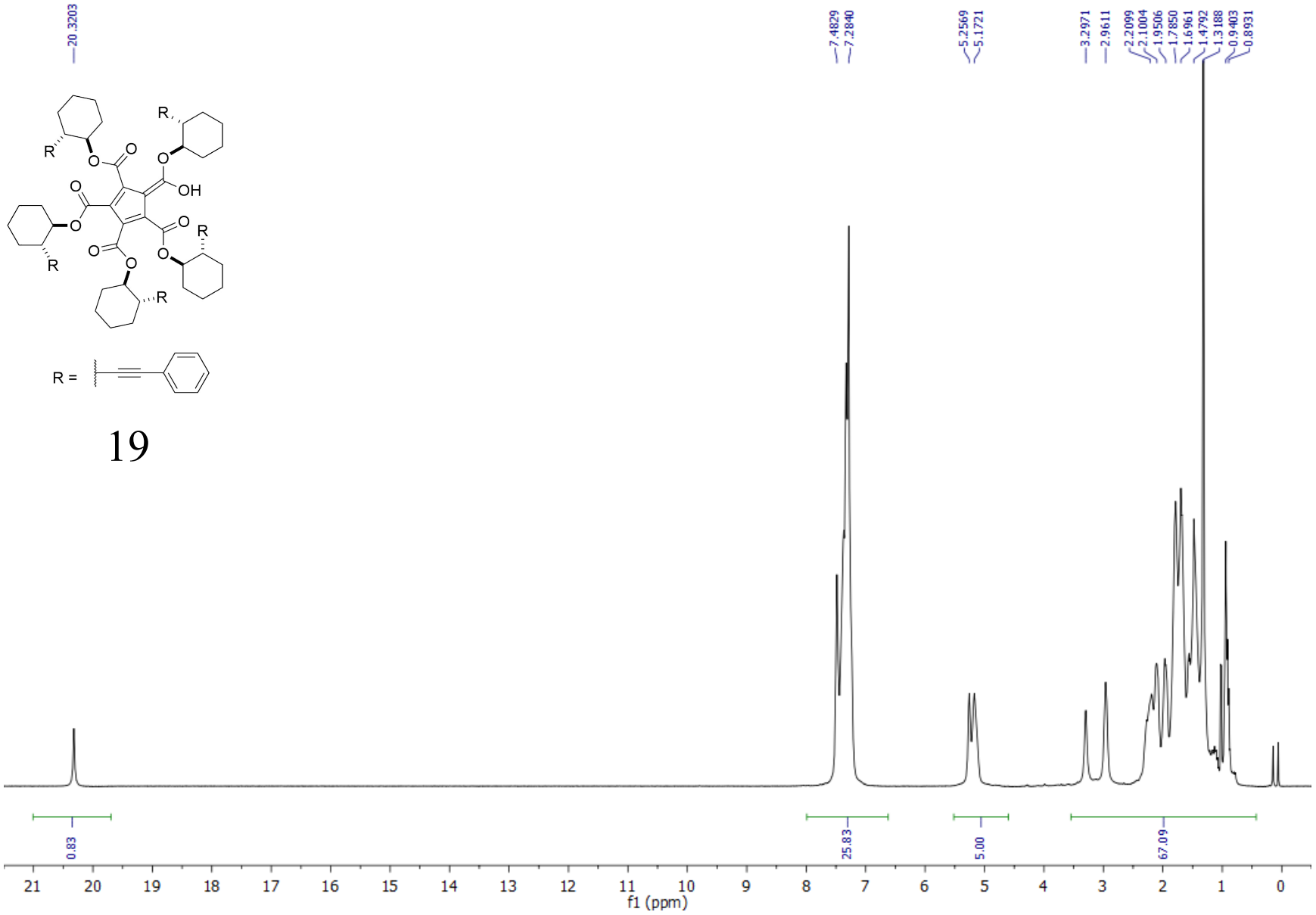

170.7625
166.5415
163.5914
162.8260
161.9441
160.5874
160.3549
159.7399
158.1995
158.1274
157.9785
157.9297
157.8645
144.1846
136.6947
135.5607
135.4281
135.2395
135.1024
134.9738
134.5504
133.3728
132.1018
128.8906
128.8466
128.8097
128.6332
128.5675
128.5273
128.4947
119.3481
114.2712
113.8901
113.7996
113.7793
113.7266
113.6803
113.4819
106.9166
82.5559
78.8830
78.6015
78.1452
77.9499
77.0386
76.4727
59.5510
55.3188
55.2146
55.1759
55.0880
55.0541
54.9863
47.9361
47.6000
47.4420
47.1195
47.0815
45.7149
34.5343
34.3106
34.2183
34.0872
33.5418
32.7368
32.0079
31.8541
31.6713
31.4907
31.1228
30.7906
30.0388
29.7780
26.2193
26.0411
25.8301
25.7860
25.6467
25.5983
25.4322
25.2625
24.8792
24.7589
24.6864
24.6053
24.2642
23.6398
OH
R
R =
OMe
f1 (ppm)

17

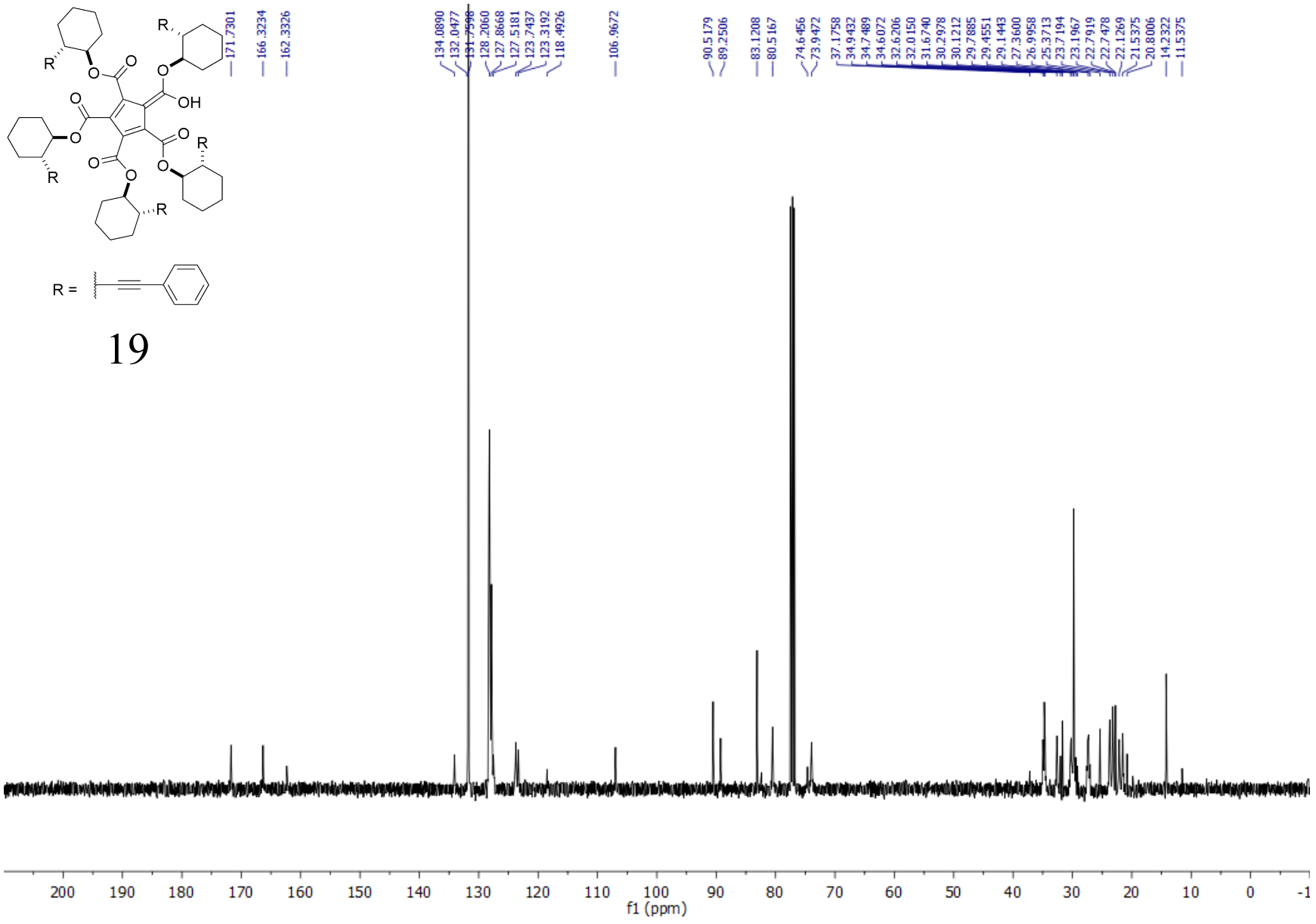

18.7044
R
O
OH
R =
SMe
7.1839
7.1622
7.1137
7.0771
7.0559
6.9996
6.9046
6.8769
6.8591
6.7624
6.5977
5.0346
4.9416
4.7411
2.7908
2.4546
2.2903
2.1639
1.8872
1.6903
1.4443
1.3274
1.1856
1.0399
0.7918
0.73
22.57
5.00
65.20
f1 (ppm)

18

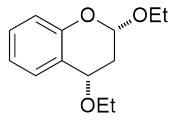

170.7280
166.4905
161.7601
144.0122
140.5136
140.3083
140.2006
139.4490
138.3707
137.0499
136.1823
135.8278
135.6877
132.0716
128.6197
128.3721
128.3149
128.2421
128.1566
127.3855
126.9830
126.8922
126.8418
126.7568
126.6985
119.2257
106.9021
82.4302
59.5101
48.3649
48.0885
47.5596
47.4074
46.3070
34.3310
32.5119
32.0380
31.5780
30.2100
26.0265
25.4218
24.8121
24.5951
23.6895
16.1884
16.1375
16.0488
15.9355
15.8595
15.6562
R
O
OH
R =
SMe
18
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


20.3203
7.4829
7.2840
5.2569
5.1721
3.2971
2.9611
2.2099
2.1004
1.9506
1.7850
1.6961
1.4792
1.3188
0.9403
0.8931
R
O
OH
R =
0.83
25.83
5.00
67.09
f1 (ppm)

19

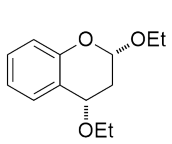

R
R
O
O
O
OH
O
O
O
O
O
R
R
R
R =
171.7301
166.3234
162.3326
134.0890
132.0477
131.7598
128.2060
127.8668
127.5181
123.7437
123.3192
118.4926
106.9672
90.5179
89.2506
83.1208
80.5167
74.6456
73.9472
37.1758
34.9432
34.7489
34.6072
32.6206
32.0150
31.6740
30.2978
30.1212
29.7885
29.4551
29.1443
27.3600
26.9958
25.3713
23.7194
23.1967
22.7919
22.7478
22.1269
21.5375
20.8006
14.2322
11.5375
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

19


O
OEt
OEt

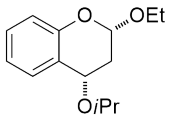
3

7.3192
7.3040
7.1177
7.1014
7.0869
6.8872
6.8727
6.7744
6.7582
5.1309
5.1256
5.1155
5.1101
4.5885
4.5766
4.5718
4.5599
3.9617
3.9475
3.9424
3.9283
3.6203
3.5761
3.5569
3.5239
2.3489
2.3319
2.3056
2.0796
2.0475
2.0211
1.2243
1.2104
1.2073
1.1965
1.1932
1.1790
1.18
1.02
1.02
1.00
1.00
1.01
1.02
3.14
1.04
1.05
6.34
f1 (ppm)


O
OEt
OEt

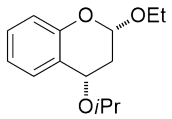
3

152.4074
129.2207
128.0236
123.9020
121.2212
117.0370
98.4275
70.8025
64.6888
63.7738
33.7716
15.6834
15.2410
f1 (ppm)


O
OEt
OiPr

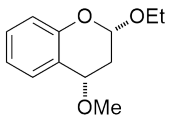
20

7.3723
7.3571
7.1806
7.1646
7.1630
7.1464
6.9570
6.9442
6.9293
6.9271
6.8396
6.8233
5.2049
5.1940
5.1888
4.6729
4.6555
4.6437
4.0621
4.0146
4.0004
3.8951
3.8585
3.8462
3.6722
3.6580
3.6106
2.4147
2.4095
2.3977
2.3768
2.3716
2.1140
2.0977
2.0715
2.0542
1.3039
1.2729
1.2602
1.2480
0.99
1.00
1.02
0.97
0.97
1.00
0.99
1.02
1.01
0.99
1.02
9.47
f1 (ppm)


O
OEt
OiPr

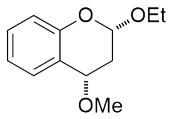
20

152.3918
129.0573
127.8760
124.6752
121.2122
116.9249
98.5781
70.3190
68.9528
64.6718
34.9912
23.6332
22.2801
15.2574
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


O
OEt
OMe

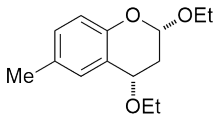
21

7.3759
7.3606
7.2115
7.1946
7.1807
6.9690
6.9539
6.9369
6.8652
6.8488
5.2220
5.2138
5.2082
4.5508
4.5373
4.5240
4.0206
4.0064
4.0011
3.9869
3.6950
3.6809
3.6472
3.6331
3.4645
2.3997
2.3729
2.3611
2.1981
2.1837
2.1569
1.2796
1.2654
1.2513
0.99
1.00
1.00
0.98
1.00
1.00
1.01
1.14
3.02
1.04
1.06
3.13
f1 (ppm)


O
OEt
OMe

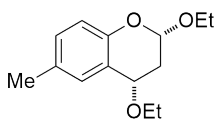
21

152.2614
129.3643
128.3475
123.2563
121.1350
117.1073
98.0022
71.9568
64.6592
56.0146
32.8452
15.1989
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


Me
OEt
OEt

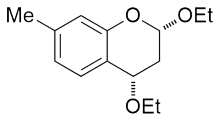
22

7.1815
6.9877
6.9668
6.7491
6.7326
5.1710
5.1658
5.1506
4.6078
4.5917
4.0318
4.0035
3.9700
3.7487
3.7067
3.6195
3.5681
3.5499
2.4045
2.3925
2.3609
2.2807
2.1361
2.1045
1.3075
1.2796
1.2440
1.00
1.04
1.01
1.02
1.03
1.04
3.19
1.09
3.20
1.09
6.62
f1 (ppm)


O
OEt
Me
OEt

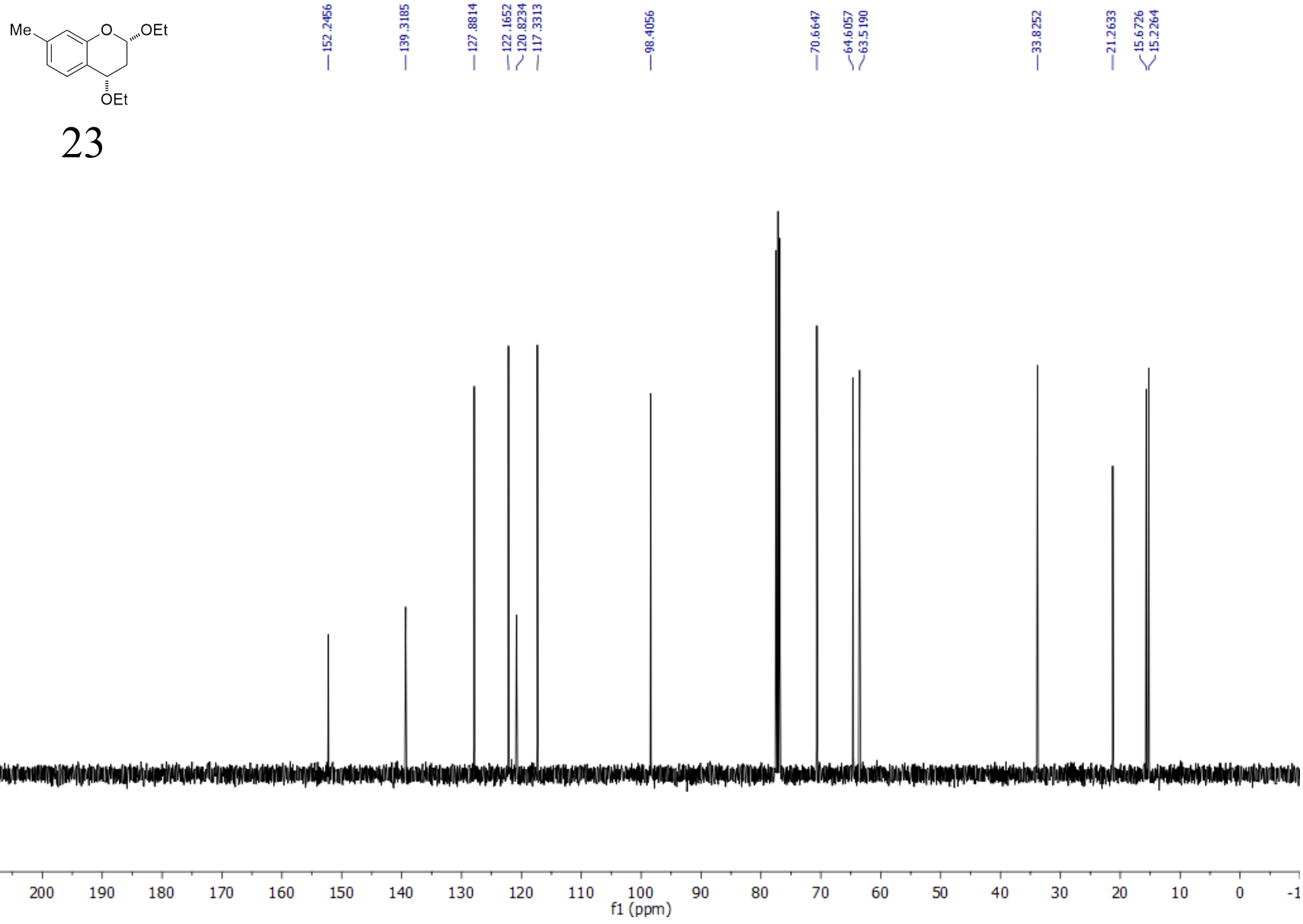
22

150.1101
130.4701
129.9073
128.2580
123.4976
116.8321
98.3064
70.8228
64.5884
63.8269
33.8380
20.7785
15.6953
15.2334
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

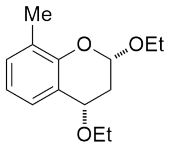

Me
O
OEt
OEt

23

7.2702
7.2507
6.7786
6.7614
6.6735
5.1780
4.6437
4.6280
4.6081
4.0505
4.0328
3.9910
3.9733
3.7242
3.6618
3.5851
3.5275
2.3956
2.3691
2.3477
2.2877
2.1462
2.0735
1.2917
1.2742
1.2512
1.08
1.01
0.99
1.00
1.00
1.03
3.13
1.03
3.09
1.08
6.43
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

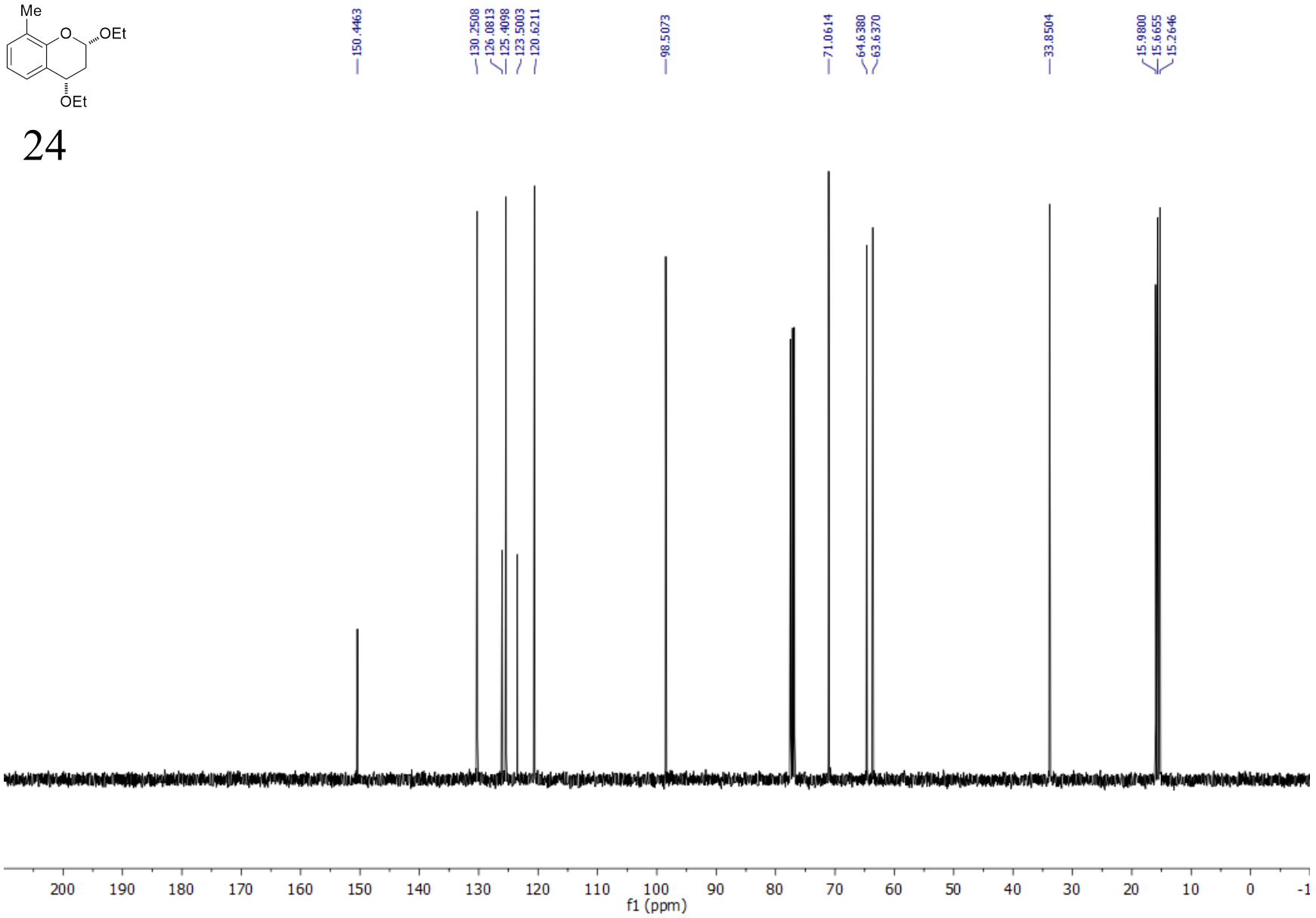

Me
O
OEt
OEt
152.2456
139.3185
127.8814
122.1652
120.8234
117.3313
98.4056
70.6647
64.6057
63.5190
33.8252
21.2633
15.6726
15.2264
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)

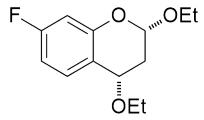
23


Me
O
OEt
OEt

23

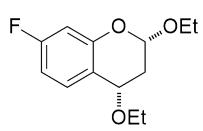
7.2339
7.2317
7.2295
7.2147
7.2125
7.2104
7.0452
7.0430
7.0408
7.0268
7.0247
7.0225
6.8628
6.8440
6.8252
5.2117
5.2050
5.1922
5.1854
4.6598
4.6449
4.6382
4.6232
4.0496
4.0319
4.0254
4.0078
3.7024
3.6849
3.6817
3.6796
3.6640
3.6622
3.6575
3.6399
3.5815
3.5641
3.5587
3.5412
2.4186
2.4036
2.3926
2.3859
2.3776
2.3708
2.2035
2.1313
2.1117
2.1096
2.0901
2.0790
2.0769
1.2944
1.2849
1.2766
1.2674
1.2589
1.08
1.02
1.02
1.00
1.03
1.02
3.21
1.06
3.13
1.08
6.46
.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Me
O
OEt
OEt
24
150.4463
130.2508
126.0813
125.4098
123.5003
120.6211
98.5073
71.0614
64.6380
63.6370
33.8504
15.9800
15.6655
15.2646
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


F
O
OEt
OEt

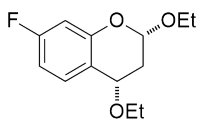
25

7.3478
7.3297
7.3267
7.3098
7.2599
6.6737
6.6526
6.6379
6.5644
6.5392
6.5328
5.2085
5.2020
5.1900
5.1834
4.5963
4.5788
4.5615
4.0342
4.0165
3.9746
3.9569
3.7402
3.6826
3.5796
3.5220
2.3944
2.3544
2.3398
2.1656
2.1304
2.1109
2.0776
1.2921
1.2781
1.2747
1.2603
1.2570
1.2426
0.98
1.00
0.96
1.00
1.01
1.02
3.11
1.03
1.20
6.36
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)


F
O
OEt
OEt

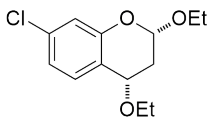
25

163.2130
153.5566
129.4294
119.7868
108.4198
104.0765
98.6796
70.2850
64.8995
63.7986
33.4538
15.6300
15.1900
f1 (ppm)


F
O
OEt
OEt

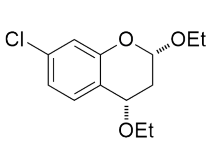
25

-116.0849
-164.8996
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
f1 (ppm)


Cl
O
OEt
OEt

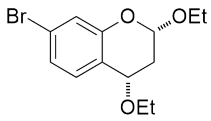
26

7.3357
7.3339
7.3151
7.3133
6.9538
6.9486
6.9332
6.9280
6.8811
5.2317
5.2249
5.2130
5.2062
4.6159
4.5964
4.5806
4.0517
4.0340
3.9921
3.9744
3.7615
3.7091
3.5893
3.5491
2.4283
2.4068
2.3735
2.1415
2.1401
2.0878
1.3158
1.3013
1.2836
1.2659
0.98
1.92
0.98
1.00
1.01
3.13
1.00
1.01
6.61
f1 (ppm)


Cl
O
OEt
OEt

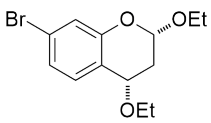
26

153.1112
134.2897
129.1195
122.6023
121.4374
117.2014
98.6645
70.2502
64.8501
63.8641
33.4842
15.6262
15.1989
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
O
OEt
OEt

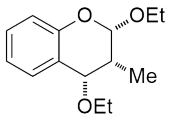
27

7.2598
7.2489
7.2324
7.0742
7.0542
7.0131
5.2020
5.1871
5.1818
4.5705
4.5547
4.5423
4.0184
4.0043
3.9709
3.9567
3.7272
3.6285
3.5282
2.3934
2.3870
2.3721
2.3551
2.1275
2.0960
2.0694
1.2852
1.2712
1.2571
1.2429
1.23
1.93
1.00
1.02
1.02
3.18
1.02
1.04
6.34
f1 (ppm)


Br
O
OEt
OEt

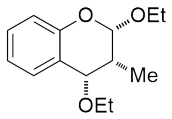
27

153.1921
129.4114
124.3310
123.0591
122.1218
120.1465
98.6471
70.2703
64.8875
63.8787
33.4104
15.6408
15.2104
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


O
OEt
Me
OEt

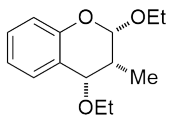
28

7.4299
7.4050
7.1720
7.1478
6.9299
6.9272
6.8163
6.7932
4.6555
4.6415
4.0809
4.0390
4.0213
3.7840
3.6914
3.6121
3.5771
3.5543
2.5224
2.4693
2.4521
1.3317
1.2968
1.2680
0.9776
0.9604
0.94
1.02
1.02
0.99
1.00
0.97
0.97
3.10
0.98
6.22
3.09
f1 (ppm)


O
OEt
Me
OEt

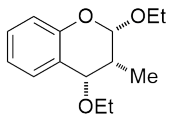
28

152.0010
128.9144
128.1481
122.6303
121.2128
116.2718
101.0935
75.0237
65.2202
64.6784
34.5618
15.5830
15.2504
5.8462
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

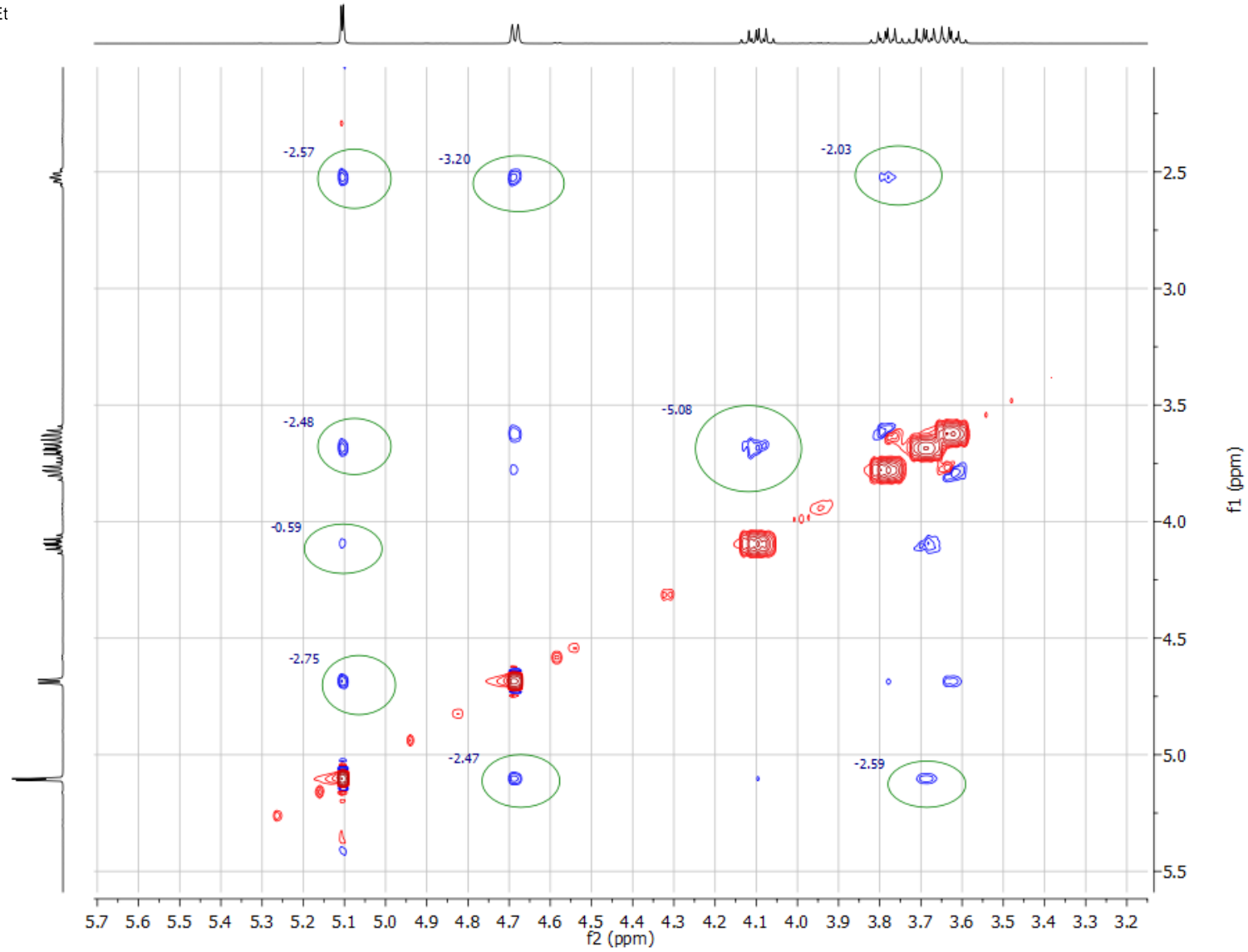

O
OEt
Me
OEt

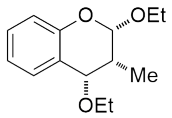
28

-2.57
-3.20
-2.03
-2.48
-5.08
-0.59
-1.00
-2.75
-2.47
-2.59
-1.26
-1.43
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f2 (ppm)
f1 (ppm)

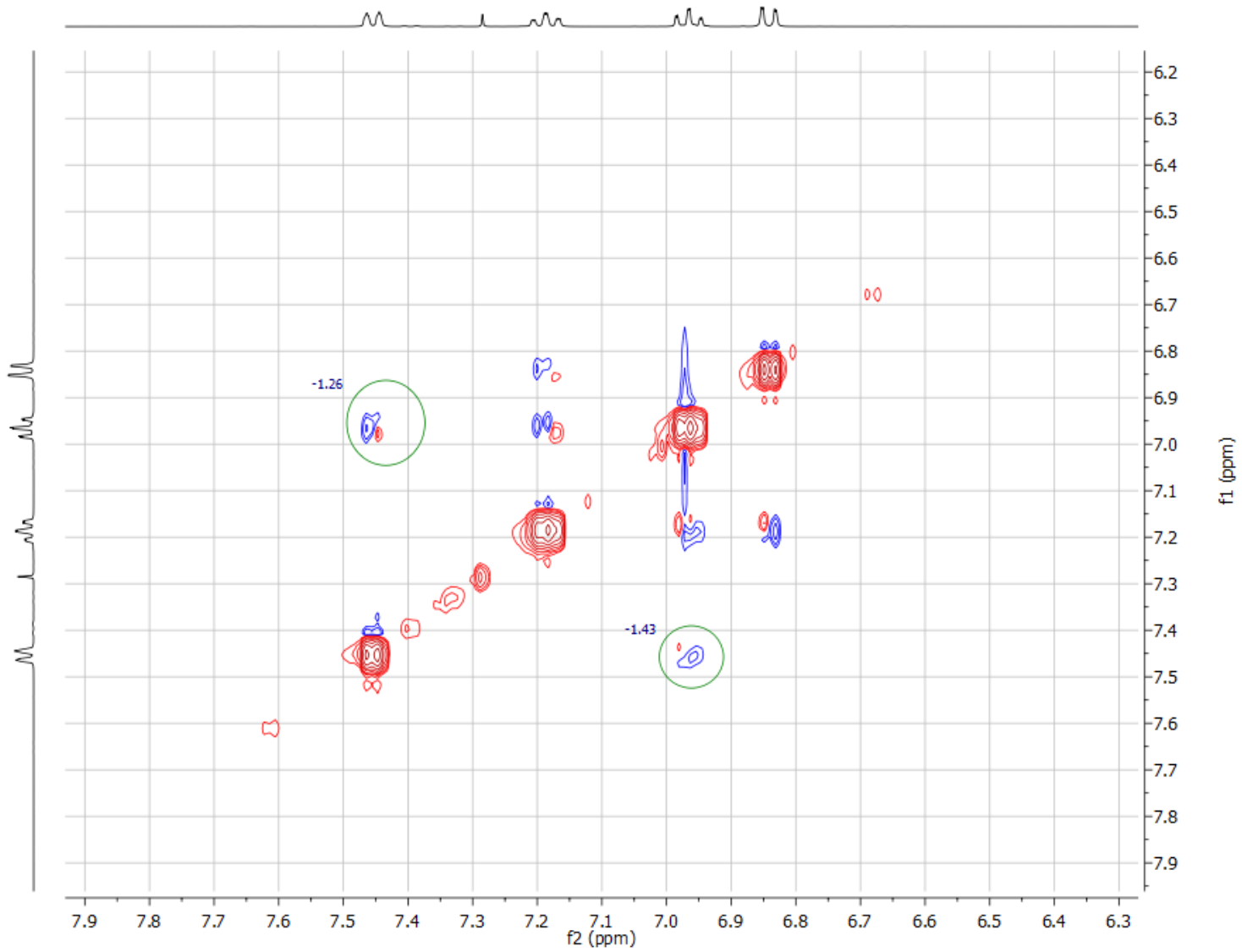

O
OEt
Me
OEt

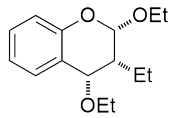
28


-2.57
-3.20
-2.03
-2.48
-5.08
-0.59
-2.75
-2.47
-2.59
2.5
3.0
3.5
4.0
4.5
5.0
5.5
f1 (ppm)
5.7 5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2
f2 (ppm)



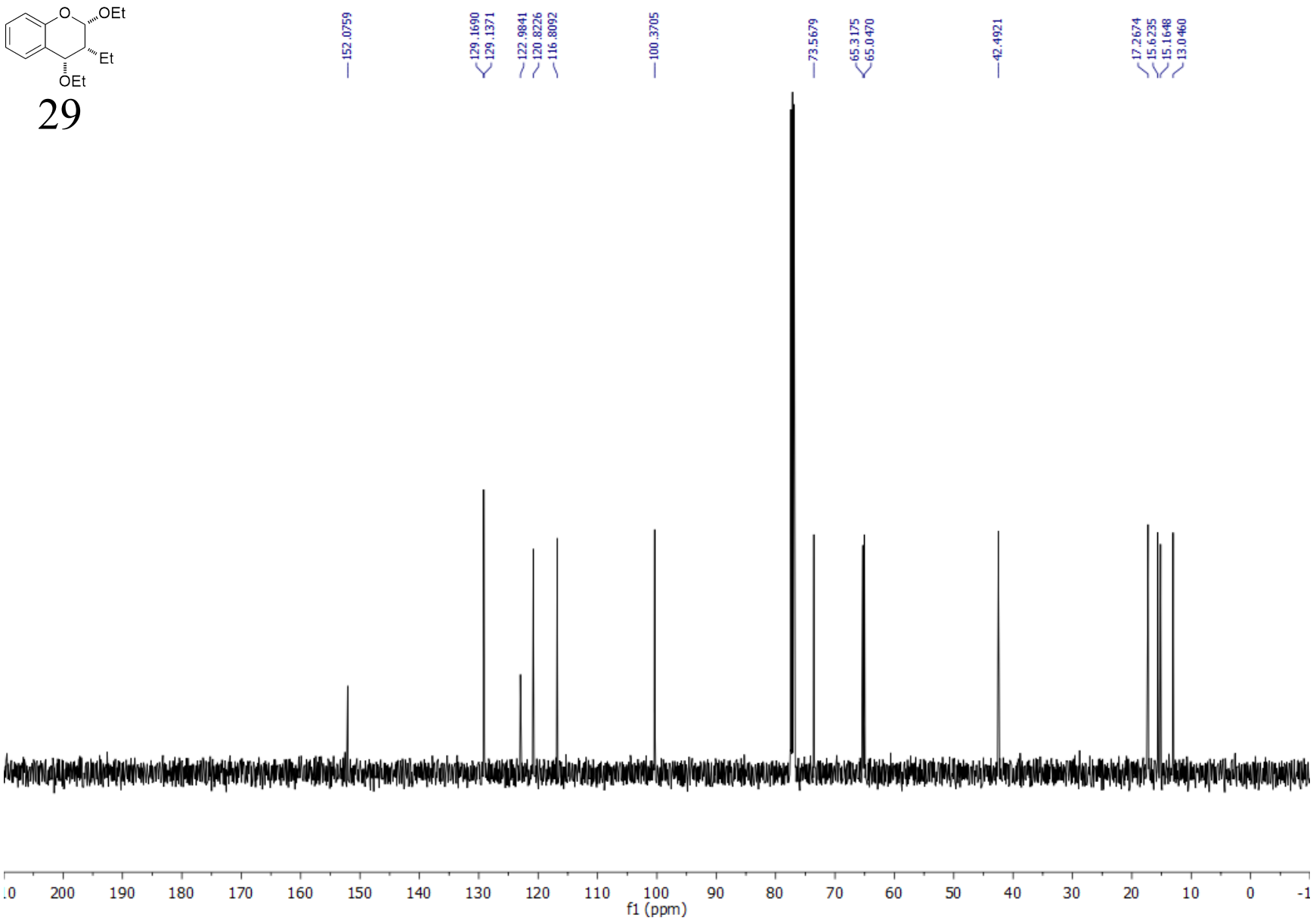
28

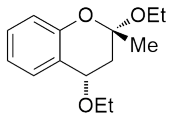



O
OEt
Et
OEt

29

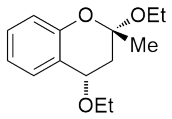
7.3560
7.3407
7.1875
7.1720
6.9332
6.9182
6.9011
6.8319
6.8155
5.1221
5.1171
4.5310
4.5206
4.0013
3.9872
3.9532
3.9390
3.7329
3.6749
3.6471
3.6125
3.5926
2.1384
2.1204
2.1100
2.0969
1.6600
1.6449
1.6167
1.5816
1.2734
1.2594
1.2380
1.2238
1.0711
1.0561
1.0409
0.99
1.00
1.01
0.98
0.99
1.00
1.00
3.08
0.99
2.36
6.42
3.06
f1 (ppm)


OEt
Et
OEt
29
152.0759
129.1690
129.1371
122.9841
120.8226
116.8092
100.3705
73.5679
65.3175
65.0470
42.4921
17.2674
15.6235
15.1648
13.0460
f1 (ppm)


O
OEt
Me
OEt

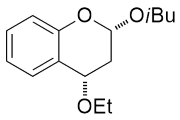
30

7.4086
7.3895
7.1948
7.1761
7.1574
6.9609
6.9423
6.8405
6.8201
4.5558
4.5394
4.5226
3.7539
3.7364
3.6252
3.5729
2.3102
2.2921
2.2767
2.2585
2.2047
2.1896
2.1712
2.1560
1.5121
1.3066
1.2891
1.2717
1.1620
1.1444
1.1268
1.01
1.05
1.04
0.99
1.00
4.26
2.07
3.05
3.31
3.28
f1 (ppm)


O
OEt
Me
OEt

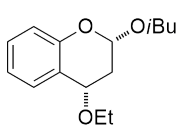
30

152.7757
129.1455
128.1968
123.4869
120.9960
117.1467
100.3996
70.9885
64.0509
57.2460
37.2036
24.3078
15.7335
15.7119
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


O
O/Bu
OEt

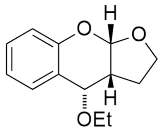
31

7.3855
7.3670
7.1913
7.1695
7.1487
6.9577
6.9389
6.9176
6.8449
6.8245
5.1707
5.1640
5.1519
5.1452
4.6601
4.6451
4.6396
4.6245
3.7651
3.7489
3.7419
3.7255
3.6968
3.6793
3.5940
3.5766
3.5366
3.3197
3.3025
3.2964
3.2790
2.4143
2.4076
2.3995
2.3599
2.1714
2.1527
2.1506
2.1317
2.1197
2.1176
2.0987
1.9362
1.9195
1.8692
1.2916
1.2740
1.2565
0.9326
0.9190
0.9157
0.9021
1.00
1.02
1.01
0.98
1.00
1.02
2.06
1.03
1.03
1.02
1.05
1.00
3.25
6.29
f1 (ppm)


O
O/Bu
OEt

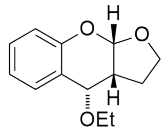
31

152.4908
129.1892
128.0462
123.9592
121.1562
117.0588
98.8681
75.9709
70.7851
63.6190
33.5986
28.6178
19.4888
19.4011
15.7132
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


H
O
O
H
OEt

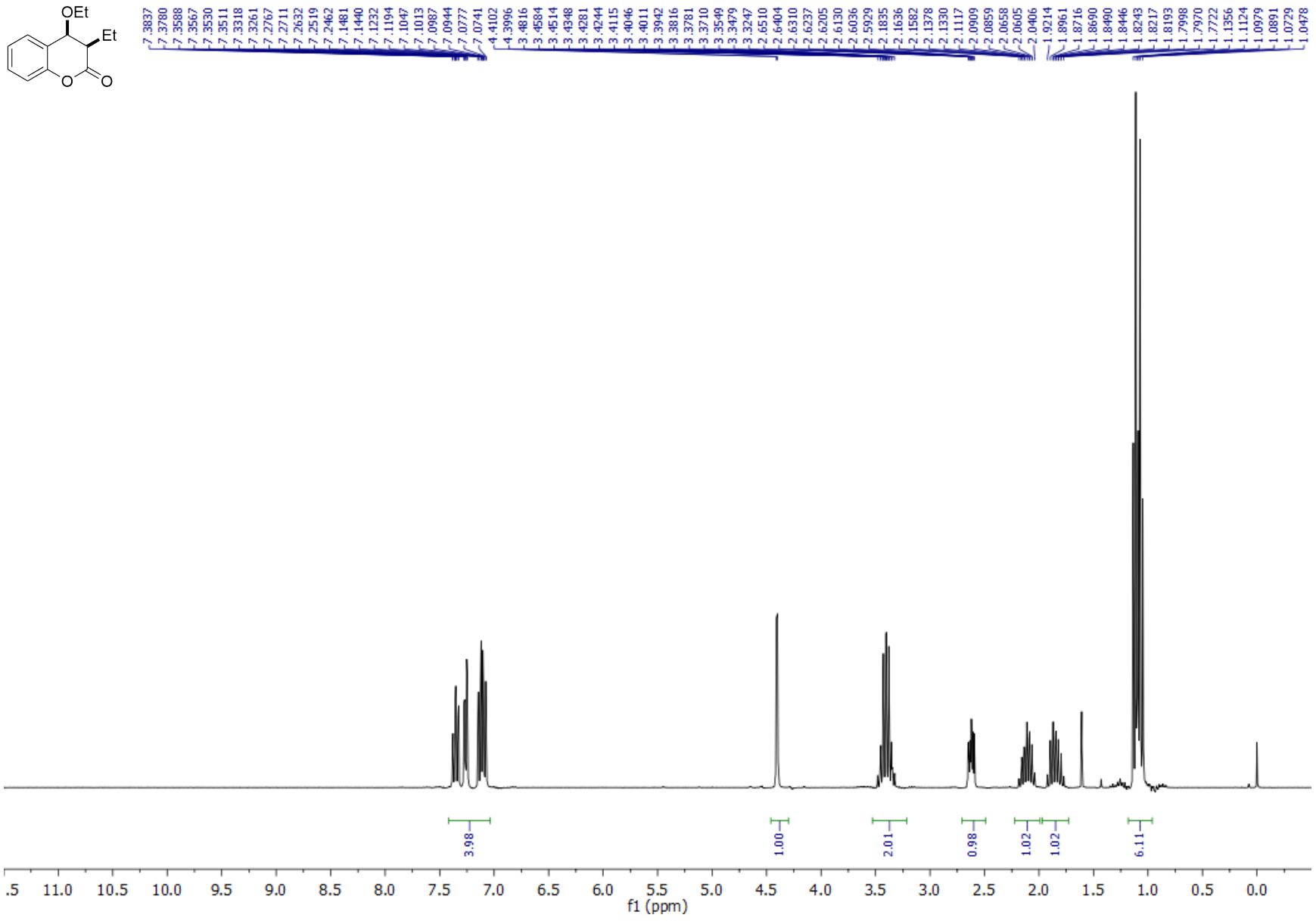
31

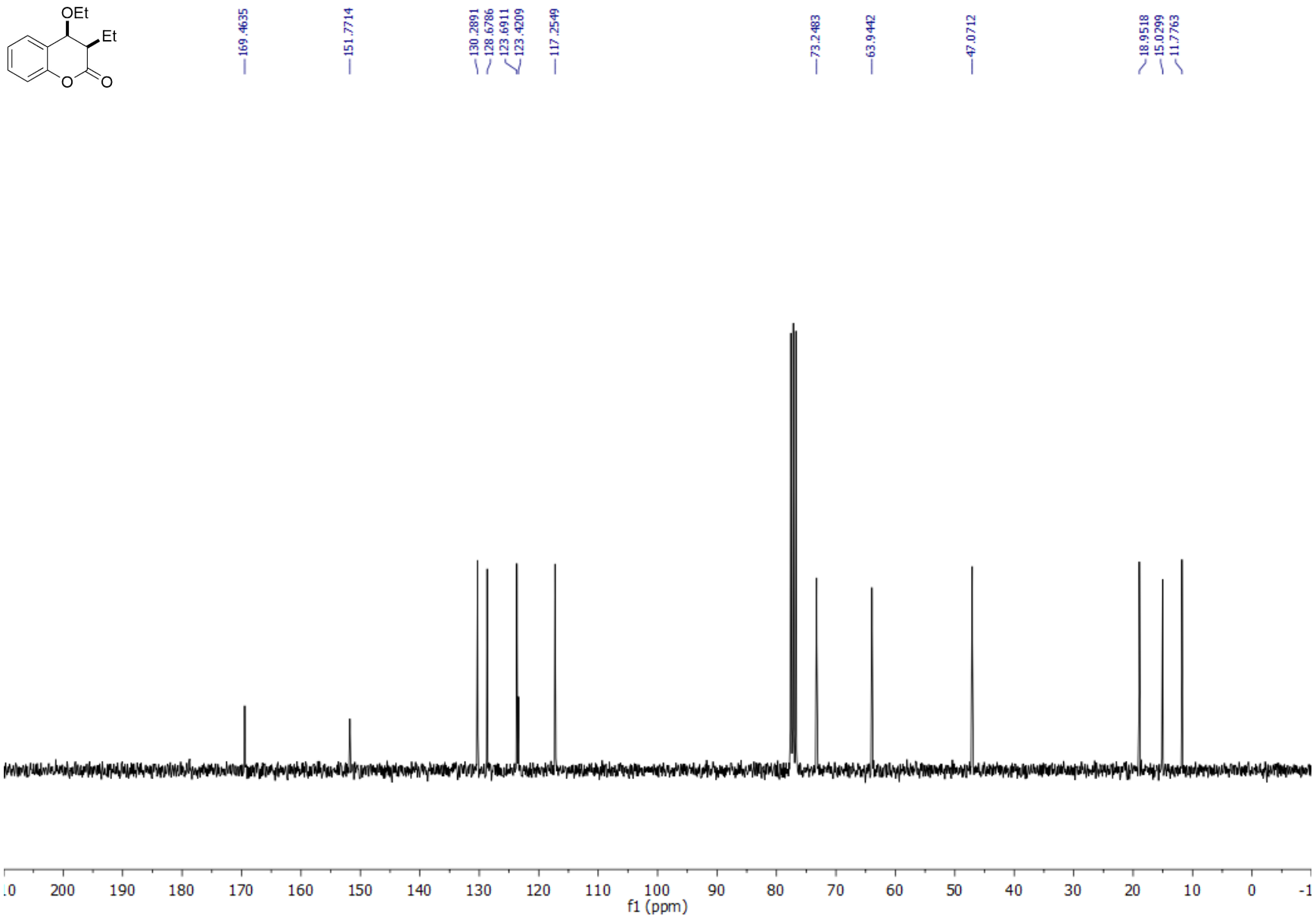
7.4560
7.4523
7.4487
7.4370
7.4333
7.4297
7.2570
7.1827
7.1803
7.1781
7.1623
7.0161
7.0131
6.9975
6.9944
6.8924
6.8894
6.8723
6.8692
5.8471
5.8325
4.7392
4.7254
4.3344
4.3278
3.8631
3.8459
3.8429
3.8316
3.8285
3.8232
3.8187
3.8101
3.8054
3.7974
3.7883
3.6959
3.6782
3.6728
3.6553
3.1517
3.1429
3.1288
3.1145
3.1059
1.9429
1.9302
1.9236
1.9197
1.7533
1.7502
1.7314
1.7284
1.7182
1.3587
1.3412
1.3238
1.2561
0.98
1.13
1.02
1.19
1.08
1.00
0.11
0.25
3.06
1.04
0.23
1.02
0.11
0.11
1.03
1.01
3.13
0.48
f1 (ppm)

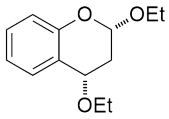

H
O
O
H
OEt

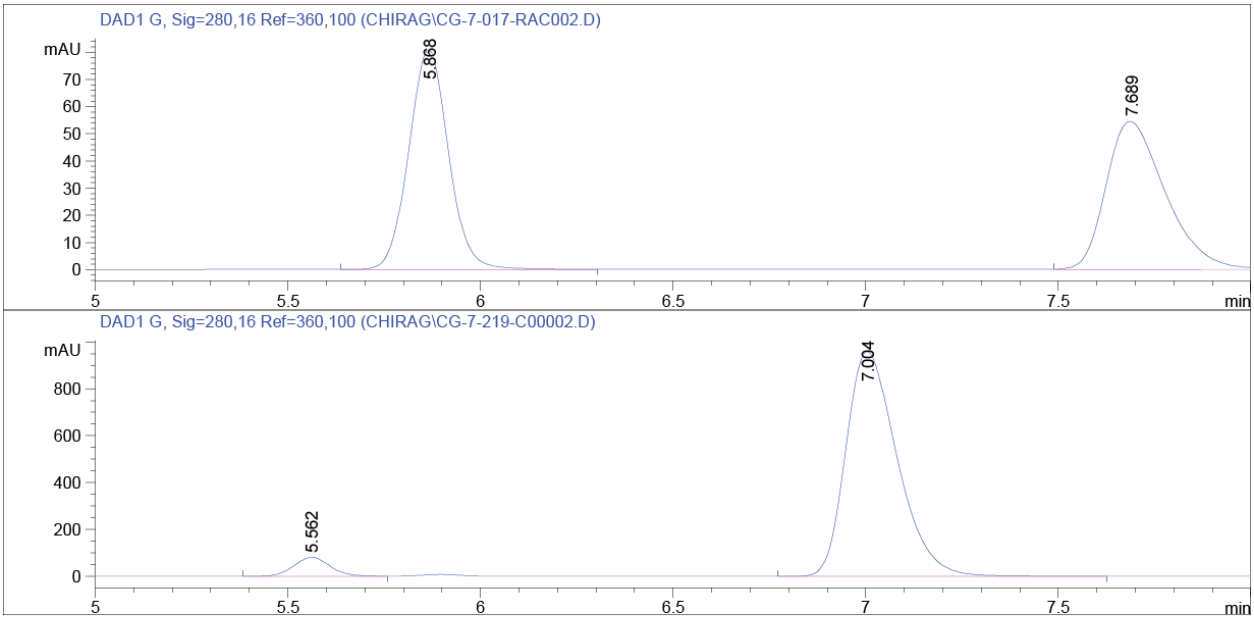
31

152.4800
128.6771
125.8907
125.2790
121.8756
116.9462
102.5635
72.3021
68.5721
65.0877
43.2970
24.4576
15.6389
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)


OEt
Et
O
O
7.3837
7.3780
7.3588
7.3567
7.3530
7.3511
7.3318
7.3261
7.2767
7.2711
7.2632
7.2519
7.2462
7.1481
7.1440
7.1232
7.1194
7.1047
7.1013
7.0987
7.0944
7.0777
7.0741
4.4102
4.3996
3.4816
3.4584
3.4514
3.4348
3.4281
3.4244
3.4115
3.4046
3.4011
3.3942
3.3816
3.3781
3.3710
3.3549
3.3479
3.3247
2.6510
2.6404
2.6310
2.6237
2.6205
2.6130
2.6036
2.5929
2.1835
2.1636
2.1582
2.1378
2.1330
2.1117
2.0909
2.0859
2.0658
2.0605
2.0406
1.9214
1.8961
1.8716
1.8690
1.8490
1.8446
1.8243
1.8217
1.8193
1.7998
1.7970
1.7722
1.1356
1.1124
1.0979
1.0891
1.0729
1.0478
3.98
1.00
2.01
0.98
1.02
1.02
6.11
.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


OEt
Et
O
O
169.4635
151.7714
130.2891
128.6786
123.6911
123.4209
117.2549
73.2483
63.9442
47.0712
18.9518
15.0299
11.7763
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)



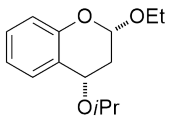


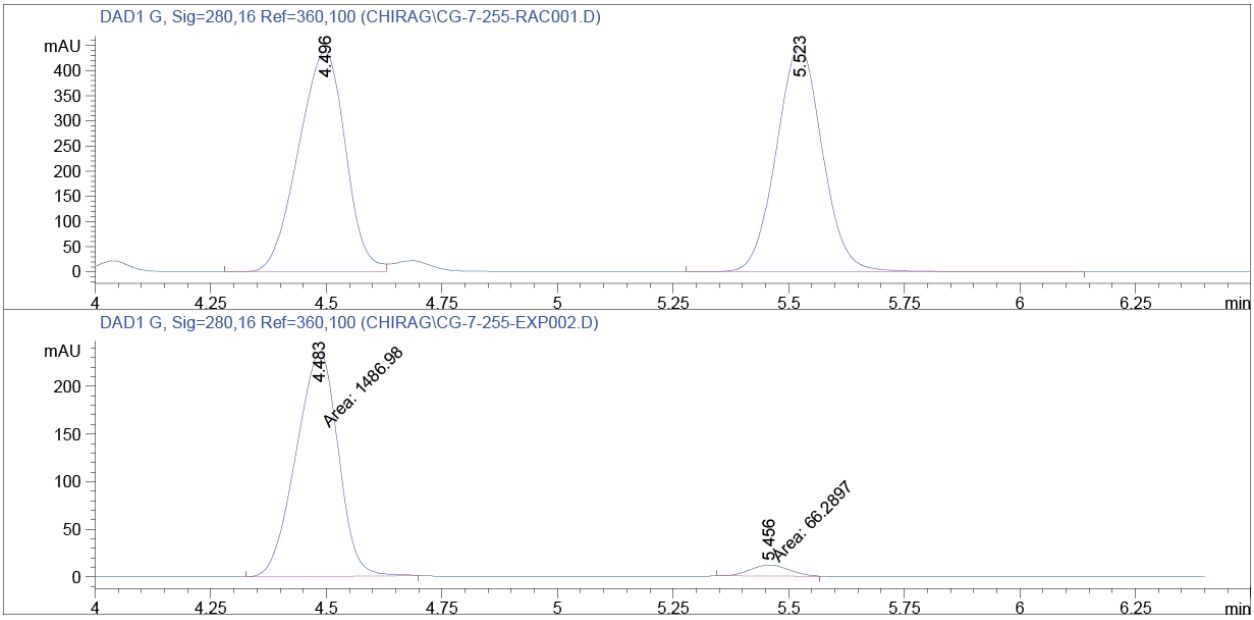
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.868	BB	0.1125	587.90741	81.13998	50.1218
2	7.689	BB	0.1653	585.05096	54.45893	49.8782
Totals :				1172.95837	135.59891	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.562	VV	0.1048	548.31958	81.22428	5.7991
2	7.004	VV	0.1422	8906.91797	960.29565	94.2009
Totals :				9455.23755	1041.51994	



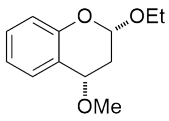


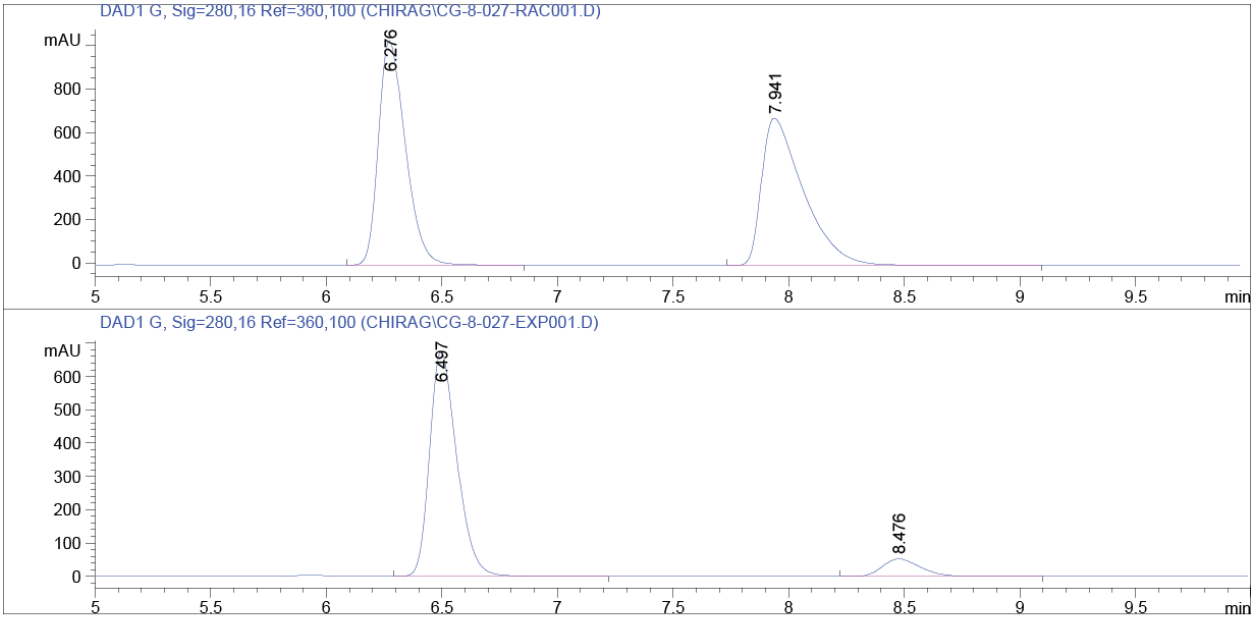
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.496	VV	0.1122	3089.45483	438.45584	49.8385
2	5.523	VB	0.1091	3109.47437	447.47980	50.1615
Totals :				6198.92920	885.93564	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.483	MM T	0.1054	1486.97681	235.10107	95.7322
2	5.456	MM T	0.0973	66.28975	11.35727	4.2678
Totals :				1553.26656	246.45834	



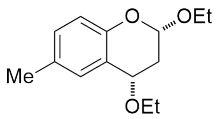


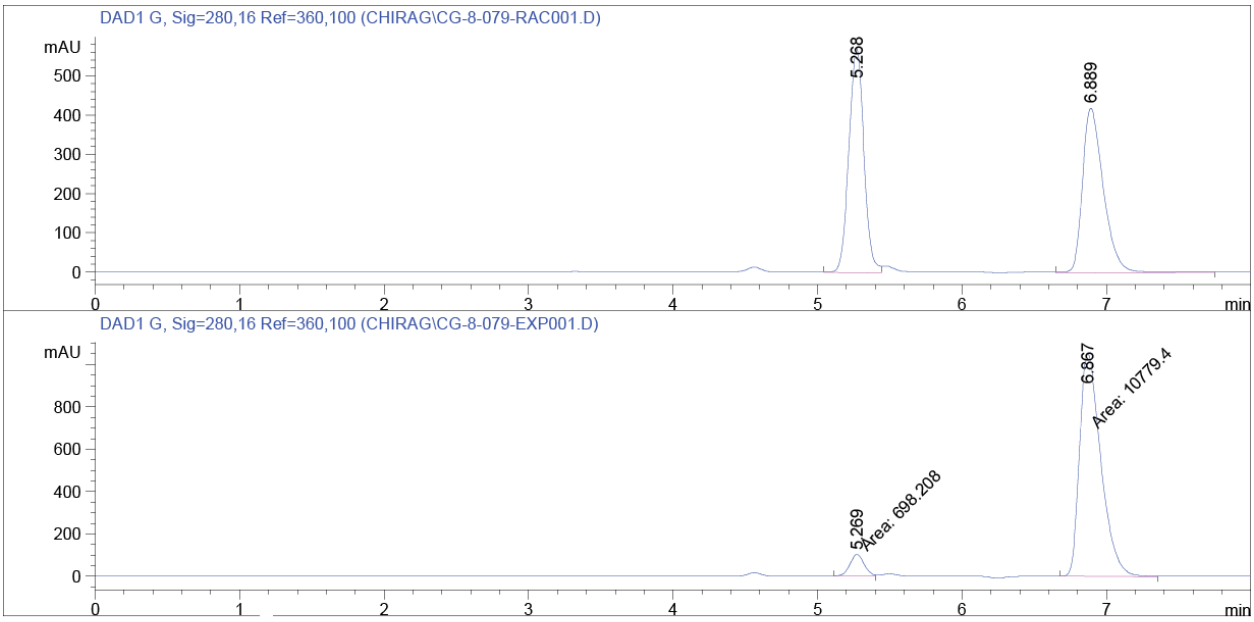
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.276	VV	0.1242	8337.82324	1032.44263	49.6907
2	7.941	VB	0.1856	8441.60449	676.24756	50.3093
Totals :				1.67794e4	1708.69019	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.497	VB	0.1260	5558.03711	675.34143	90.2153
2	8.476	BB	0.1753	602.81952	52.74452	9.7847
Totals :				6160.85663	728.08595	



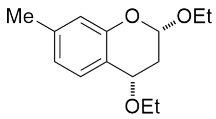


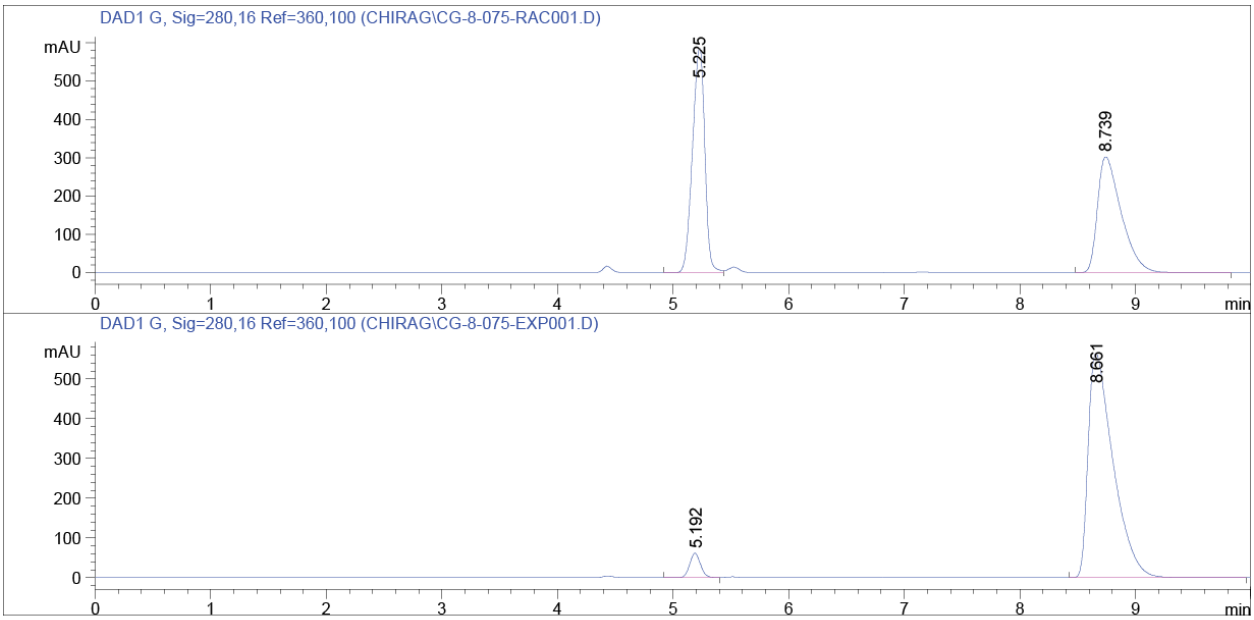
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.268	VV	0.1144	4145.64063	573.38031	49.4843
2	6.889	VB	0.1557	4232.04639	419.62384	50.5157
Totals :				8377.68701	993.00415	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.269	MM T	0.1150	698.20770	101.20574	6.0832
2	6.867	MM T	0.1704	1.07794e4	1054.28333	93.9168
Totals :				1.14776e4	1155.48907	



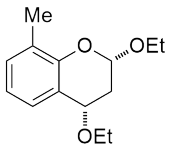


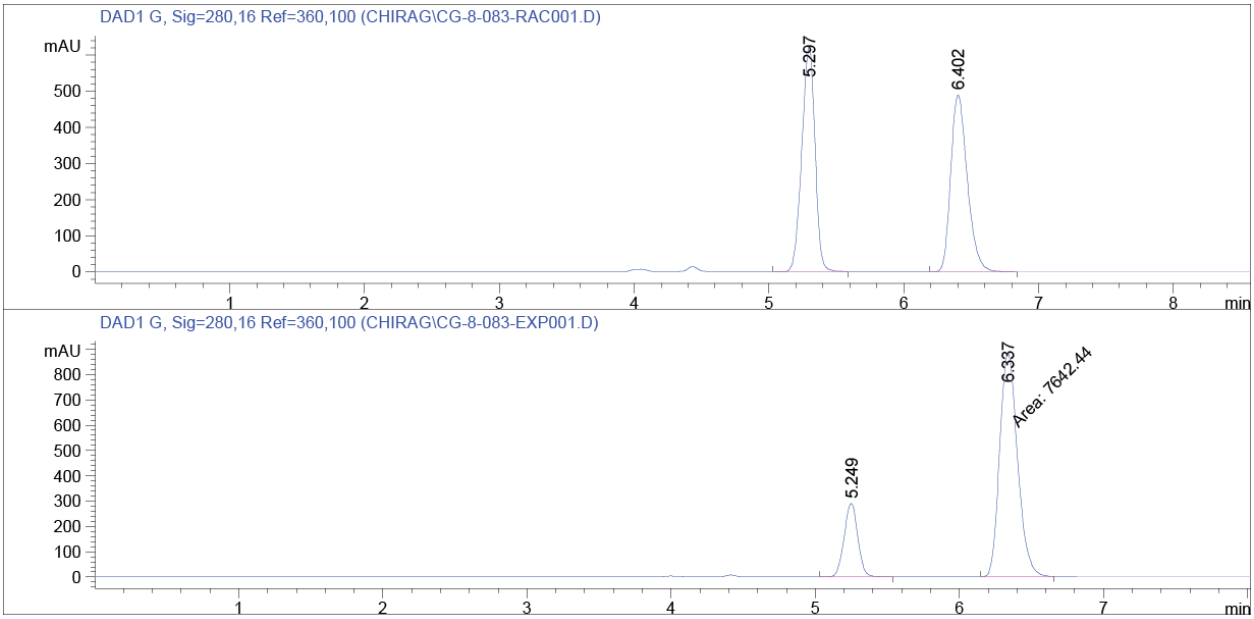
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.225	VV	0.1158	4316.51025	586.80176	49.9056
2	8.739	BB	0.2149	4332.84424	302.96524	50.0944
Totals :				8649.35449	889.76700	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.192	VV	0.1007	406.29041	61.79531	4.5816
2	8.661	BB	0.2227	8461.54102	565.11053	95.4184
Totals :				8867.83142	626.90585	



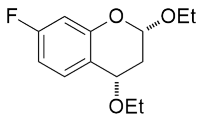


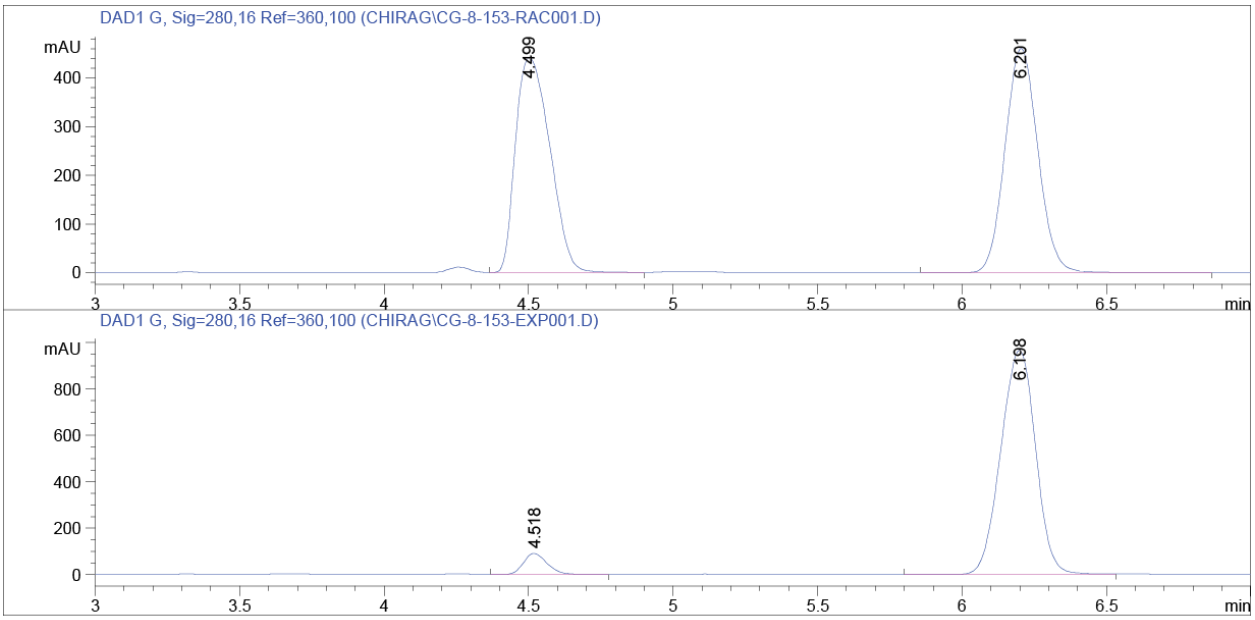
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.297	VV	0.1078	4259.59570	622.90521	50.3841
2	6.402	VV	0.1338	4194.64648	490.30670	49.6159
Totals :				8454.24219	1113.21191	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.249	BV	0.1032	1926.94690	291.04822	20.1366
2	6.337	MM T	0.1435	7642.43555	887.83368	79.8634
Totals :				9569.38245	1178.88190	



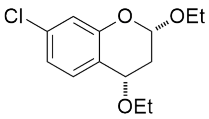


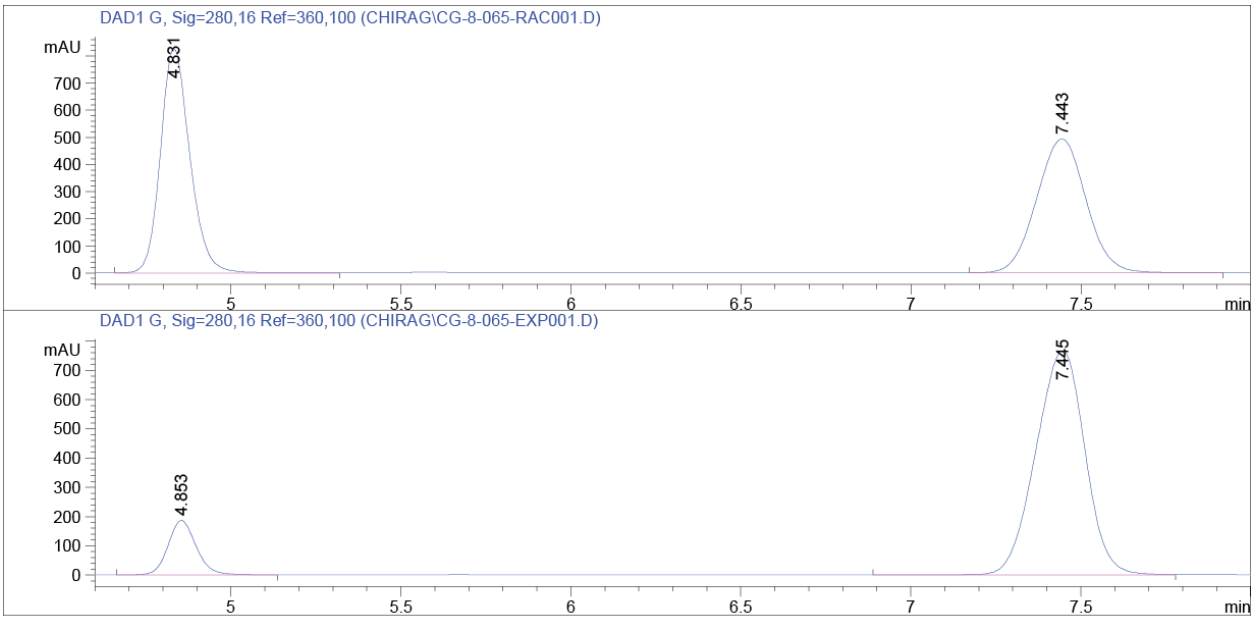
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.499	VV	0.1366	3665.06104	442.62430	50.0355
2	6.201	BB	0.1244	3659.85913	462.07532	49.9645
Totals :				7324.92017	904.69962	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.518	VV	0.0893	530.32684	91.94430	6.1292
2	6.198	BV	0.1318	8122.15771	968.48169	93.8708
Totals :				8652.48456	1060.42599	



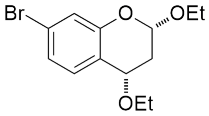


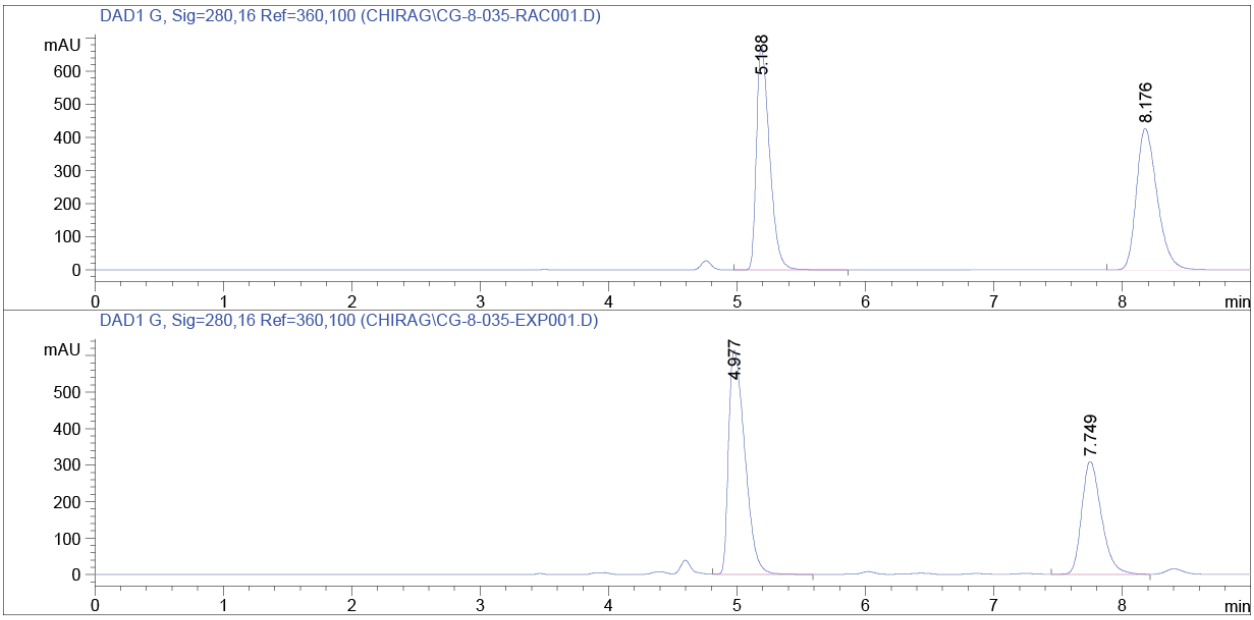
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.831	VV	0.0920	4974.62988	829.45190	49.9270
2	7.443	VV	0.1599	4989.18457	493.84140	50.0730
Totals :				9963.81445	1323.29330	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.853	VV	0.0900	1090.66516	187.09711	12.3663
2	7.445	VV	0.1593	7728.96191	768.62164	87.6337
Totals :				8819.62708	955.71875	



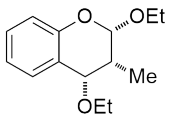


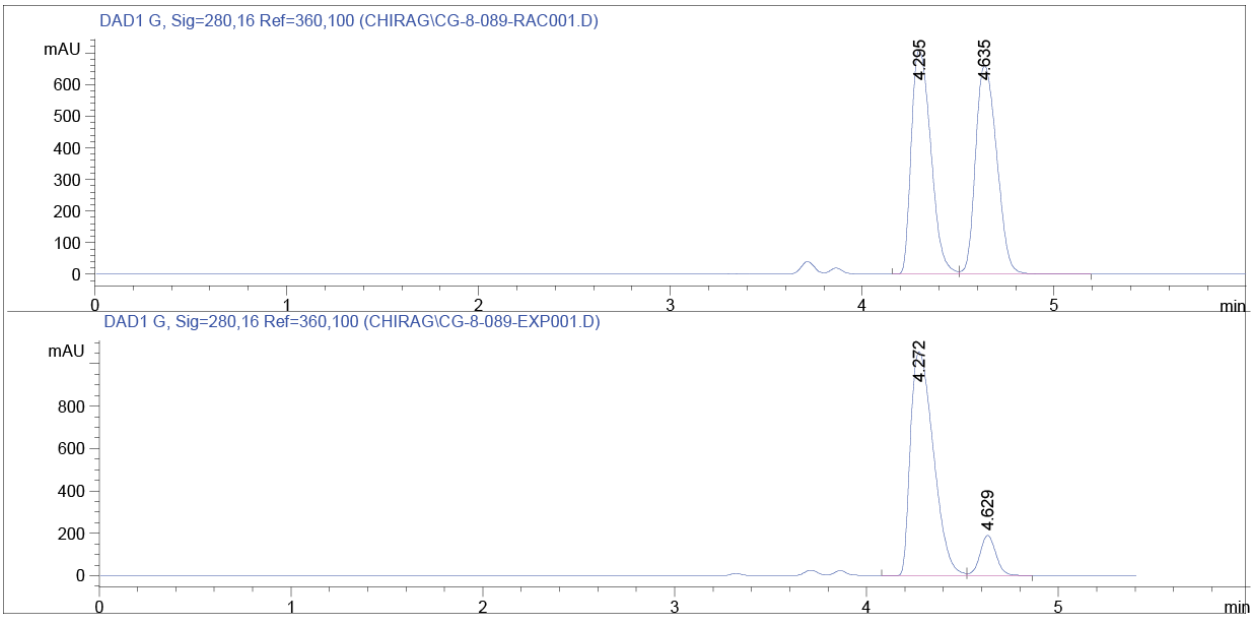
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.188	VB	0.1083	4790.23779	679.01550	49.8109
2	8.176	VB	0.1735	4826.60937	428.07718	50.1891
Totals :				9616.84717	1107.09268	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.977	VV	0.1392	5445.24902	615.36395	61.9906
2	7.749	VV	0.1653	3338.74829	310.95828	38.0094
Totals :				8783.99731	926.32224	



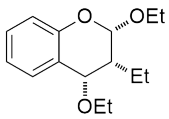


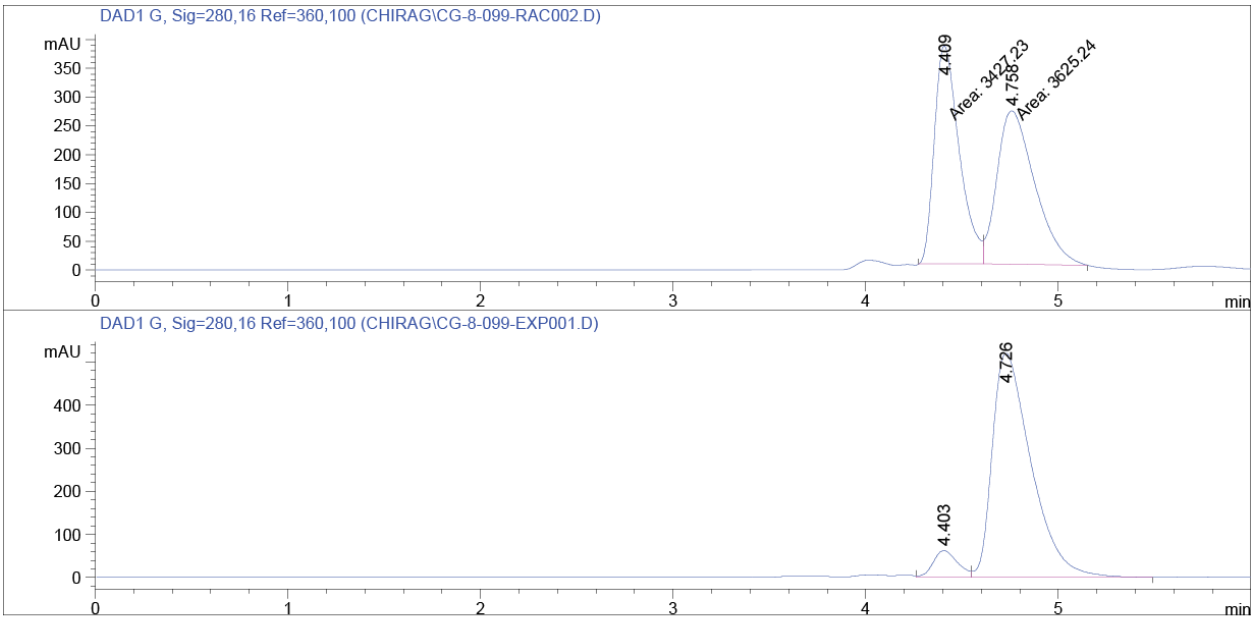
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.295	VV	0.1150	5046.10840	709.50940	49.8703
2	4.635	VV	0.1237	5072.35449	659.44153	50.1297
Totals :				1.01185e4	1368.95093	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.272	VV	0.1328	8770.82715	1057.49121	88.7892
2	4.629	VV	0.0900	1107.43213	190.12999	11.2108
Totals :				9878.25928	1247.62120	



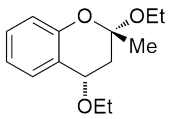


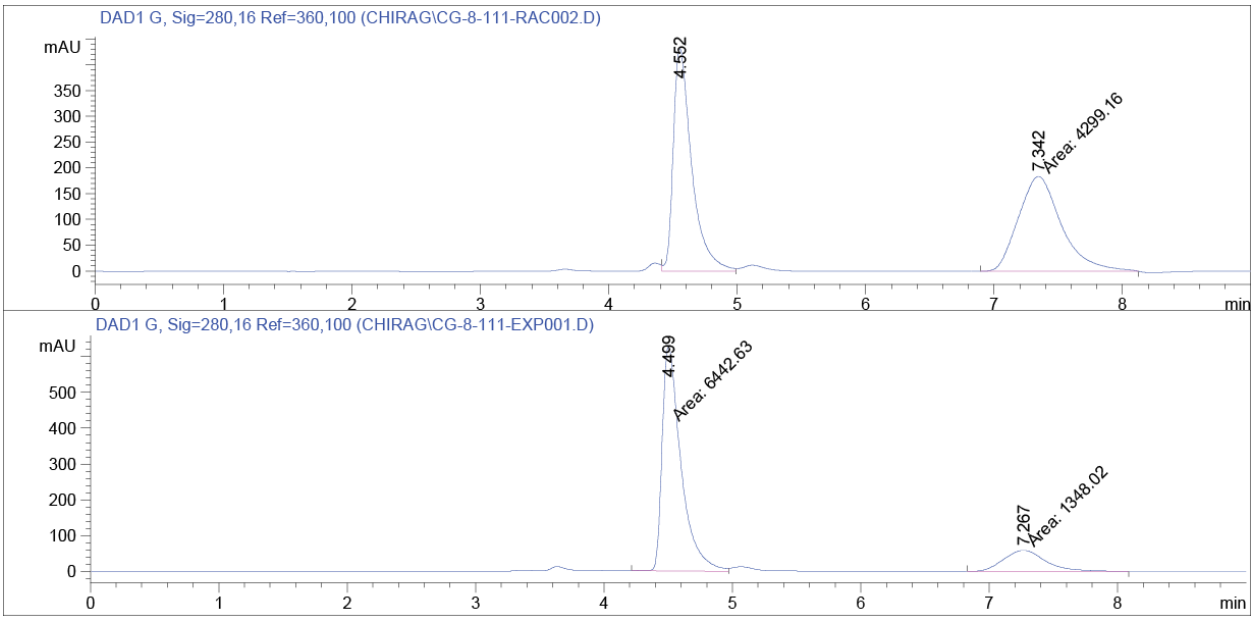
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.409	MM T	0.1506	3427.23389	379.30325	48.5962
2	4.758	MM T	0.2266	3625.23535	266.64404	51.4038
Totals :				7052.46924	645.94730	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.403	VV	0.1358	557.23846	62.61014	7.0774
2	4.726	VV	0.2138	7316.26709	521.16962	92.9226
Totals :				7873.50555	583.77975	





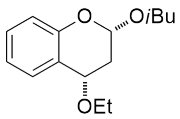
Signal 5: DAD1 G, Sig=280,16 Ref=360,100

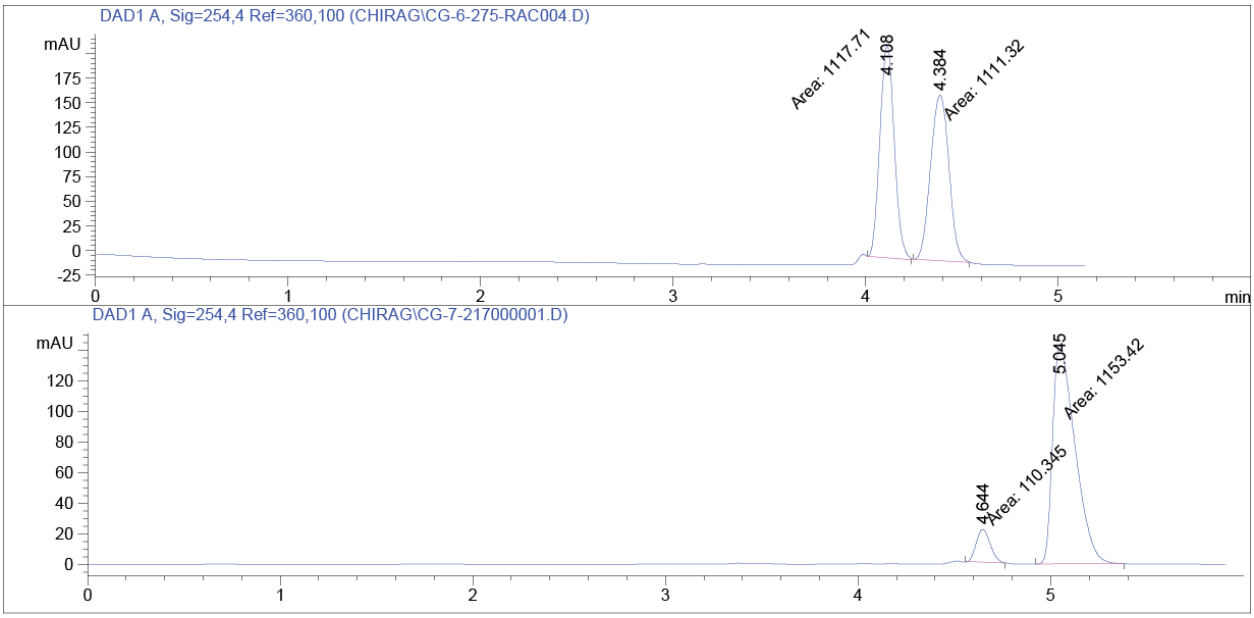
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.552	VV	0.1508	4339.83594	433.35419	50.2354
2	7.342	MM T	0.3887	4299.16016	184.34383	49.7646
Totals :				8638.99609	617.69801	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.499	MM T	0.1714	6442.63086	626.55200	82.6969
2	7.267	MM T	0.3797	1348.02368	59.17653	17.3031
Totals :				7790.65454	685.72853	

Table 2, Entry 13



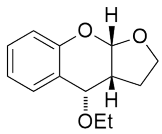


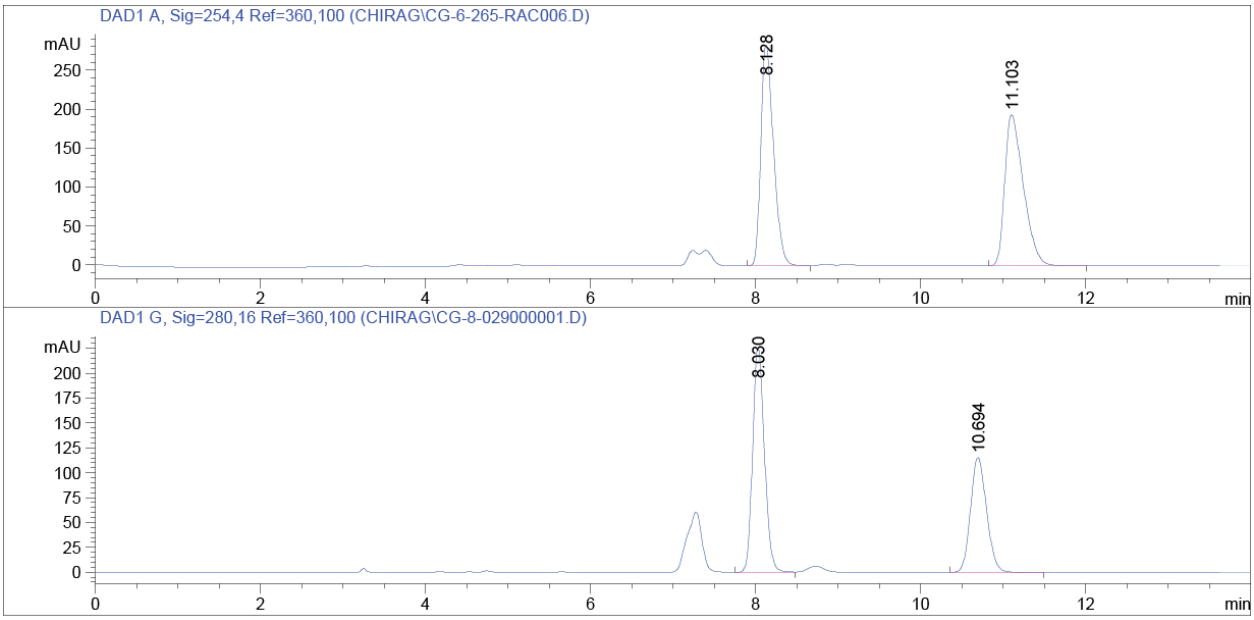
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.108	MM T	0.0858	1117.70911	217.18286	50.1433
2	4.384	MM T	0.1100	1111.32153	168.40526	49.8567
Totals :				2229.03064	385.58812	

Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.644	MM T	0.0852	110.34484	21.59715	8.7314
2	5.045	MM T	0.1337	1153.41992	143.79810	91.2686
Totals :				1263.76476	165.39525	



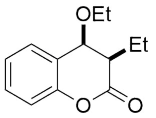


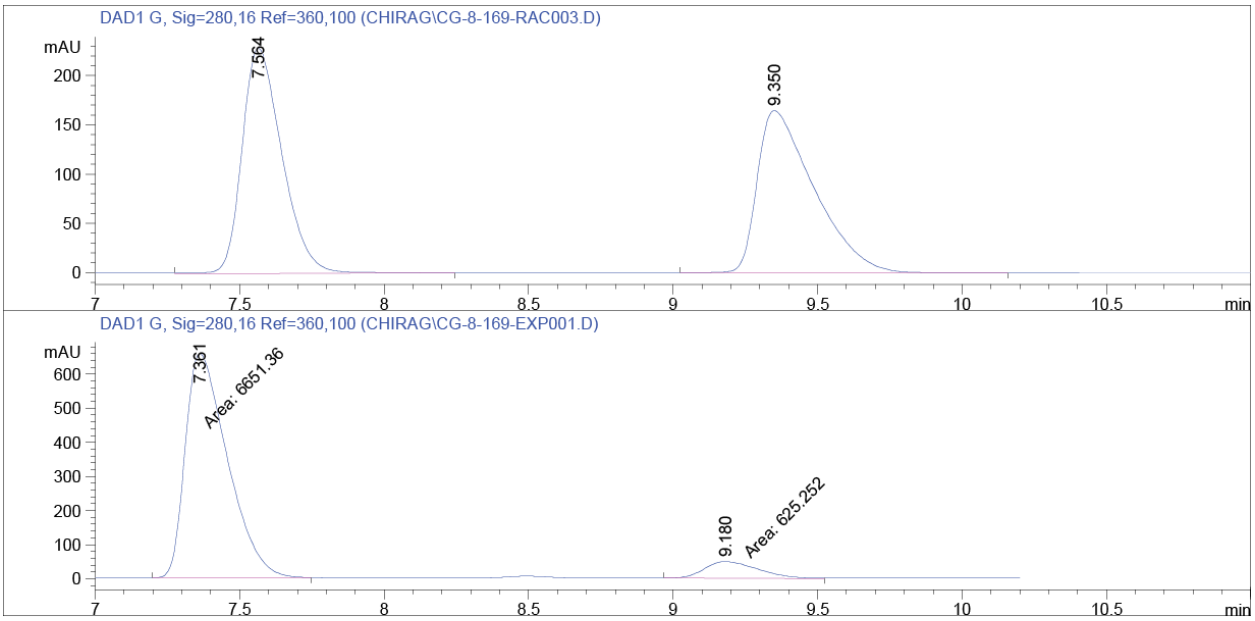
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.128	BV	0.1648	3032.90894	283.55945	49.9212
2	11.103	BB	0.2392	3042.47974	193.71185	50.0788
Totals :				6075.38867	477.27130	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.030	VV	0.1561	2247.60620	225.89848	59.0312
2	10.694	BB	0.2100	1559.88281	115.15390	40.9688
Totals :				3807.48901	341.05238	





Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.564	VB	0.1484	2206.75928	229.14566	49.4841
2	9.350	BB	0.2035	2252.76978	164.80531	50.5159
Totals :				4459.52905	393.95097	

Signal 5: DAD1 G, Sig=280,16 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.361	MM T	0.1684	6651.36475	658.48535	91.4074
2	9.180	MM T	0.2136	625.25183	48.79292	8.5926
Totals :				7276.61658	707.27827	