Supporting Information

Visible-Light-Promoted Catalytic Epoxidation of Alkenes under Metal-Free Conditions

Dabao Tan,[a] Xiaoyan Cai,[c] Boyu Liu,[a] Lele Zhang,[b] Feiming Li,[a] Zhixiong Cai,[a] Mingqiang Huang,[a] Xiaoping Chen,[a] and Shunyou Cai*[a,b]

[a] *Fujian Provincial Key Laboratory of Modern Analytical Science and Separation Technology, School of Chemistry, Chemical Engineering and Environment, Minnan Normal University, Zhangzhou, 363000, China.*

[b] *Guangdong Provincial Key Laboratory of Chemical Genomics, Shenzhen Graduate School, Peking University, Shenzhen, 518055, China.*

E-mail: caishy05@mnnu.edu.cn

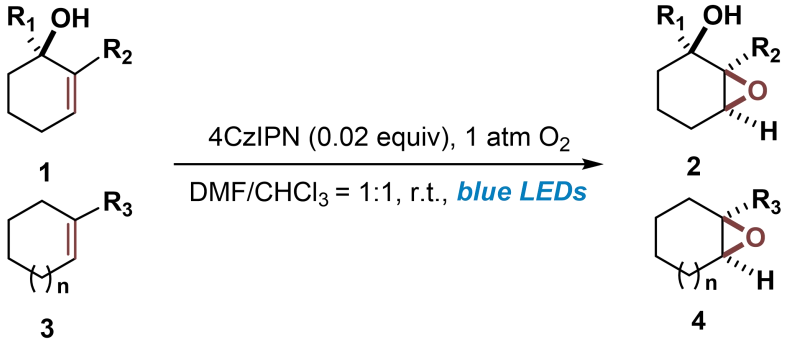
Table of Contents

(100 Pages)

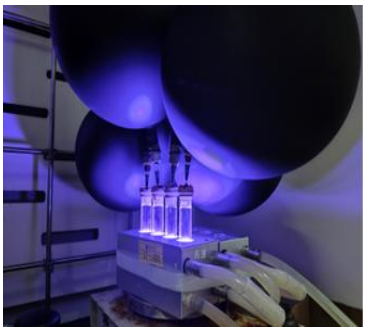
Materials and methods

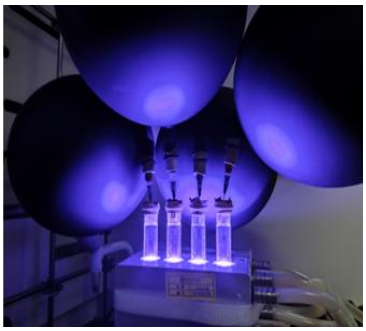
All the chemicals were purchased commercially and used without further purification. Thin-layer chromatography (TLC) was conducted with 0.25 mm Tsingdao silica gel plates (60F-254) and visualized by exposure to UV light (254 nm) or stained with potassium permanganate. Flash column chromatography was performed using Tsingdao silica gel (60, particle size 0.040–0.063 mm). Reagents were purchased at the highest commercial quality and used without further purification, unless otherwise stated. 1H NMR spectra were recorded on JEOL spectrometers (at 400 MHz) and were reported relative to deuterated solvent signals. Data for 1H NMR spectra were reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. 13C NMR spectrawere recorded on JEOL Spectrometers (at 100 MHz). Data for 13C NMR spectra were reported in terms of chemical shift. Mass spectrometric data were obtained using Bruker Apex IV RTMS. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, br = broad.

General procedure for Epoxidation synthesis

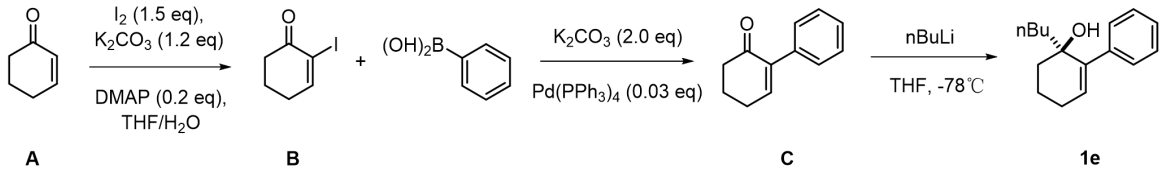


A flame-dried reaction tube was equipped with magnetic stir bar and charged with 5',6'-dihydro-[1,1':2',1"-terphenyl]-1'(4'H)-ol **1 or 3** (0.1199 mmol, 1.0 equiv), 4CzIPN (0.0024 mmol, 0.02 equiv), and DMF/$CHCl_3$ (1:1) (3.0 mL). The reaction mixture was irradiated by blue LEDs (12 W, wavelength 450 nm) under a balloon oxygen atmosphere at room temperature until the starting material disappeared from the TLC. After that, the reaction mixture was directly concentrated under reduced pressure and the crude residue was purified by silica gel column chromatography using Hexane/EtOAc (*v*/*v* = 2/1) to afford the desired pure product **2 or 4** in 41-92% yields.



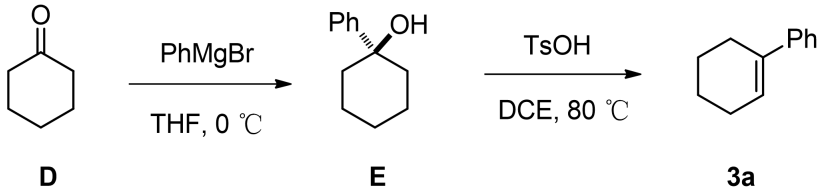


General procedure for 1e synthesis



Cyclohexenone (A) (1.0 eq, 5.20 mmol) was dissolved in THF-H2O (24 mL, v/v=1:1) solvent in a dry 50 mL round-bottomed flask with (1.5 eq, 7.80 mmol) of I2, (1.2 eq, 6.24 mmol) of K2CO3 and (0.2 eq, 1.04 mmol) of DMAP. At the end of the reaction, the reaction system was diluted with ethyl acetate (EA) and was washed sequentially by adding saturated sodium thiosulfate and 0.1 M aqueous HCI to the reaction system, followed by extraction with EA and purification by column chromatography to obtain 2-iodocyclohexa-2 -enone (B). Then, B (1.0 eq, 3.37 mmol) was further reacted with (1.5 eq, 5.06 mmol) of phenylboronic acid, (2.0 eq, 6.74 mmol) of potassium carbonate, and 0.03 eq of tetrakis(triphenylphosphine)palladium catalyst dissolved in 20 mL of toluene solvent in a dry 50 mL round-bottomed flask at 110° for 18h, and the reaction was tracked by TLC The reaction was followed by TLC. The reaction system was rinsed with EA solvent through diatomaceous earth was filtered by sand core funnel extraction, the filtrate was washed with saturated aqueous sodium bicarbonate solution, extracted, dried, and finally separated and purified by column chromatography to give 4,5-dihydro-[1,1′-biphenyl]-2(3H)-One (**C**). A dry 10 mL of the test tube reactor was taken and protected with nitrogen, and anhydrous treatment was done with an electric gun, then **C** (1.0 eq, 2.03 mmol) was dissolved with 2 mL of dewatered THF and added to the test tube reactor, and then (1.5 eq, 3.04 mmol) butyllithium reagent was slowly added dropwise to the test tube reactor for a reaction of 3 h at -78 °C, and then the reaction was bursted with a saturated ammonium chloride solution, and the EA extraction, and purification by column chromatographic separation in 90% yield to afford **1e**.

General procedure for 3a synthesis

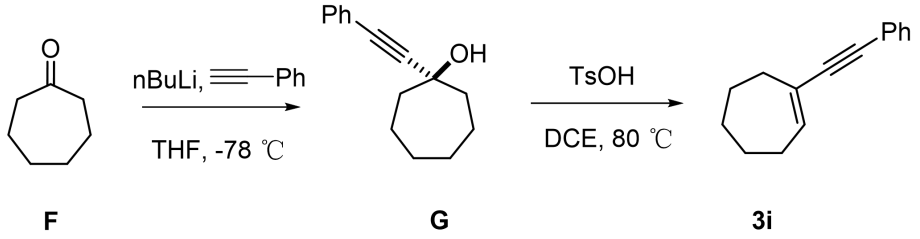


D **E** **3a**

A 10 mL test tube reactor was taken and a magnetic stir bar was placed therein. Under the protection of ordinary nitrogen, the reactor was purged with an electric gun for three times and then evacuated. Cyclohexanone (**D**) (2.0 mmol, 1.0 eq) and anhydrous THF (3 mL) were added into the reactor. Finally, phenylmagnesium bromide reagent (2.8 mol/L, 1.5 eq) of 1.0 mL was slowly dropped at 0 °C. After the dropwise addition was completed, the reaction was allowed to slowly rise to room temperature and react for 5 h until the starting materials disappeared as detected by TLC. Then 5.0 mL of saturated ammonium chloride solution was slowly added to the reaction mixture. Subsequently, the organic phase was evaporated and concentrated under reduced pressure. The resulting residue was extracted with EtOAc (3×20.0 mL) and 15 mL of water. The organic phases were combined and washed with 20 mL of saturated brine, and dried over anhydrous sodium sulfate. After the organic phase was evaporated and concentrated under reduced pressure, it was separated and purified by column chromatography using n-hexane:ethyl acetate (4:1) to obtain 1-phenylcyclohexan-1-ol (**E**) with a separation yield of 95%. Next, a 10 mL test tube reactor was taken and a magnetic stir bar was placed therein. Under the protection of ordinary nitrogen, **E** (1.0 mmol, 1.0 eq), p-toluenesulfonic acid (0.3 mmol, 0.3 eq), and 2.0 mL of 1,2-dichloroethane were added. The reaction was heated at 80 °C until the disappearance of the reaction starting materials. Then saturated sodium bicarbonate solution (2.0 mL) was slowly added to the reaction mixture. Subsequently, the organic phase was evaporated and concentrated under reduced pressure. The resulting residue was extracted with EtOAc (3 × 20.0 mL) and 15 mL of water. The organic phases were combined and washed with 20 mL of saturated brine, and dried over anhydrous sodium sulfate. After the organic phase was evaporated and concentrated under reduced

pressure, it was separated and purified by column chromatography to obtain 2,3,4,5-tetrahydro-1,1'-biphenyl (**3a**) with a separation yield of 70%.

General procedure for 3i synthesis



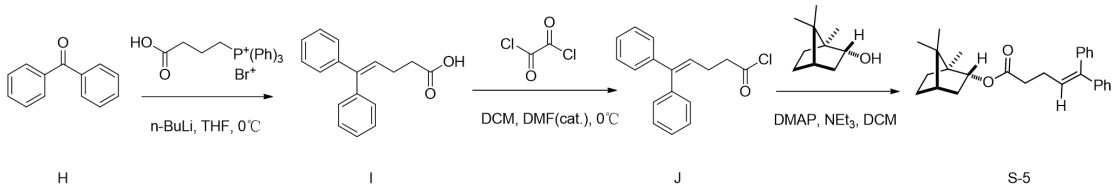
F **G** **3i**

A 10 mL test tube reactor was taken and a magnetic stir bar was placed inside. Under the protection of ordinary nitrogen, the reactor was purged with an electric gun for three times and then evacuated. Phenylacetylene (2.4 mmol, 1.2 eq) was added to the reactor followed by the addition of anhydrous THF (3 mL). Then, 2 mL of n-butyl lithium reagent (1.6 mol/L, 1.3 eq) was slowly dropped at -78 °C and stirred for half an hour. After that, cycloheptanone (F) (0.2 mL, 2.0 mmol, 1.0 eq) was slowly dropped at -78 °C. After the dropwise addition was completed, the reaction was allowed to slowly rise to room temperature until the starting materials disappeared as detected by TLC. Then, 5.0 mL of saturated ammonium chloride solution was slowly added to quench the reaction. Subsequently, the organic phase was evaporated and concentrated under reduced pressure. The resulting residue was extracted with EtOAc (3×20.0 mL) and 15 mL of water. The combined organic phase was washed with 20 mL of saturated brine, dried over anhydrous sodium sulfate, and evaporated and concentrated under reduced pressure. After separation and purification by column chromatography using n-hexane:ethyl acetate (4:1), 1-(phenylethynyl)cycloheptan-1-ol (**G**) was obtained with a separation yield of 90%.

Next, another 10 mL test tube reactor was taken and a magnetic stir bar was placed inside. Under the protection of ordinary nitrogen, **G** (1.0 mmol, 1.0 eq), *p*-toluenesulfonic acid (0.3 mmol, 0.3 eq), and 2.0 mL of 1,2-dichloroethane were added. The reaction was heated at 80 °C until the starting materials disappeared. Then, 2.0 mL of saturated sodium

bicarbonate solution was slowly added to the reaction mixture. Subsequently, the organic phase was evaporated and concentrated under reduced pressure. The resulting residue was extracted with EtOAc (3 × 20.0 mL) and 15 mL of water. The combined organic phase was washed with 20 mL of saturated brine, dried over anhydrous sodium sulfate, and evaporated and concentrated under reduced pressure. After separation and purification by column chromatography, 1-(phenylethynyl)cyclohept-1-ene (**3i**) was obtained with a separation yield of 70%.

General procedure for S-5 synthesis



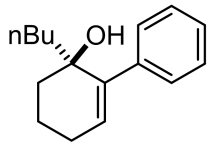
A 10 mL test tube reactor was taken into a magnetic stirrer and purged 3 times with an electric gun and evacuated under normal nitrogen protection. Weigh (3-carboxypropyl)triphenylphosphonium bromide (0.5227 mmol, 1 eq) into the test tube reactor add dewatered THF solvent and add *n*-BuLi (1.0453 mmol, 2 eq) slowly dropwise at 0 °C in an ice bath. After stirring for 45 min then THF solution of benzophenone was added dropwise to it. The reaction was stirred at room temperature for 12 h. At the end of the reaction, the organic phase was evaporated and concentrated under reduced pressure, and the resulting residue was extracted with EtOAc (3 × 20.0 mL) and 15 mL of water, the organic phases were combined and washed with 20 mL of saturated saline, dried with anhydrous sodium sulfate, and the organic phases were evaporated and concentrated under reduced pressure. The organic phase was evaporated and concentrated under reduced pressure. 5,5-diphenylpentanoic acid (**I**) was purified by column chromatography.

A 10 mL test tube reactor was taken into a magnetic stirrer and purged 3 times with an electric gun and evacuated under normal nitrogen protection. Acid (**I**) (0.8878 mmol, 1

eq.) was weighed into the tube reactor and dissolved with 2 mL of DCM, oxalyl chloride (4.4390 mmol, 5 eq.) was added dropwise at 0 °C, followed by 10 μL of DMF at room temperature with stirring. At the end of the reaction, the organic phase was evaporated and concentrated under reduced pressure, and the resulting residue was extracted with EtOAc (3 × 20.0 mL) and 15 mL of water, the organic phases were combined and washed with 20 mL of saturated saline, dried with anhydrous sodium sulfate, and the organic phases were evaporated and concentrated under reduced pressure. The organic phase was evaporated and concentrated under reduced pressure. 5,5-diphenylpentanoyl chloride (**J**) was purified by column chromatography.

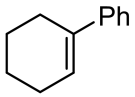
A 10 mL test tube reactor was taken into a magnetic stirrer and purged 3 times with an electric gun and evacuated under normal nitrogen protection. Borneol (0.3409 mmol, 1 eq), DMAP (0.0341 mmol, 0.1 eq), and NEt_3 (0.6819 mmol, 2 eq) were dissolved in DCM and subsequently added dropwise at 0 °C After the dropwise addition, the reaction was allowed to slowly warm up to room temperature until the material disappeared from the TLC. The organic phase was concentrated by evaporation under reduced pressure and the resulting residue was extracted with EtOAc (3 × 20.0 mL) with 15 mL of water, the organic phases were combined and washed with 20 mL of saturated NaCl (aq.), dried over anhydrous sodium sulfate, and the organic phase was concentrated by evaporation under reduced pressure. S-5 was purified by column chromatography.

^{1}H and ^{13}C spectral data of some representative substrates



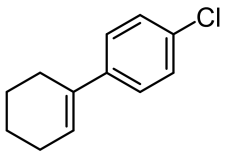
1e

2-butyl-2,3,4,5-tetrahydro-[1,1'-biphenyl]-2-ol (1e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.42 (m, 2H), 7.29-7.20 (m, 3H), 5.84-5.82 (m, 1H), 2.27-2.20 (m, 1H), 2.13-2.04 (m, 1H), 1.88 (s, 1H), 1.83-1.75 (m, 4H), 1.59-1.41 (m, 2H), 1.27-1.20 (m, 1H), 1.18-1.00 (m, 2H), 0.73-0.70 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 141.7, 130.7, 128.7, 127.8, 126.6, 72.4, 39.7, 35.8, 26.2, 26.1, 23.1, 18.7, 13.9; HRMS calculated for $C_{16}H_{22}ONa$ ($M + Na^+$): 253.1568, found: 253.1563. (Yellow oil)



3a

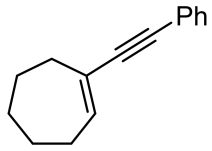
2,3,4,5-tetrahydro-1,1'-biphenyl (3a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.37 (m, 2H), 7.35-7.28 (m, 2H), 7.24-7.19 (m, 1H), 6.13-6.11 (m, 1H), 2.43-2.40 (m, 2H), 2.23-2.19 (m, 2H), 1.81-1.75 (m, 2H), 1.69-1.63 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 136.7, 128.3, 126.6, 125.0, 124.9, 27.5, 25.9, 23.2, 22.3; HRMS calculated for $C_{12}H_{15}$ ($M + H^+$): 159.1174, found: 159.1168. (Colourless oil)



3c

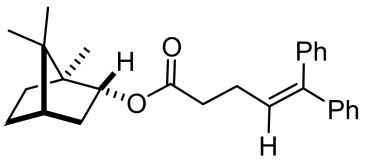
4'-chloro-2,3,4,5-tetrahydro-1,1'-biphenyl (3c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.24 (m, 4H), 6.10 (s, 1H), 2.36-2.35 (m, 2H), 2.22-2.18 (m, 2H), 1.80-1.74 (m, 2H), 1.68-1.62 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.2, 135.6, 132.2, 128.3, 126.3,

125.5, 27.4, 25.9, 23.0, 22.1; HRMS calculated for $C_{12}H_{14}Cl$ ($M + H^+$): 193.0784, found: 193.0779. (White solid)



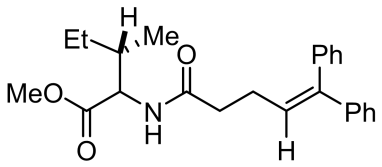
3i

1-(phenylethynyl)cyclohept-1-ene (3i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.39 (m, 2H), 7.30-7.25 (m, 3H), 6.41-6.38 (t, *J* = 6.8 Hz, 1H), 2.44-2.42 (m, 2H), 2.25-2.21 (m, 2H), 1.80-1.74 (m, 2H), 1.64-1.51 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.4, 131.9, 131.4, 128.3, 127.7, 127.0, 123.9, 93.0, 86.9, 34.4, 32.3, 29.4, 26.7, 26.6; HRMS calculated for $C_{15}H_{17}$ ($M + H^+$): 197.1330, found: 197.1325. (Yellow oil)



(from Borneol)
s-5

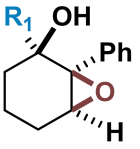
1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 5,5-diphenylpent-4-enoate (s-5): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.35 (m, 2H), 7.33-7.30 (m, 1H), 7.26-7.23 (m, 3H), 7.22-7.17 (m, 4H), 6.09-6.06 (m, 1H), 4.90-4.86 (m, 1H), 2.46-2.45 (m, 4H), 2.38-2.30 (m, 1H), 1.92-1.86 (m, 1H), 1.75-1.68 (m, 1H), 1.67-1.64 (m, 1H), 1.30-1.15 (m, 2H), 0.95-0.90 (m, 1H), 0.89 (s, 3H), 0.86 (s, 3H), 0.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ173.4, 142.9, 142.5, 139.8, 129.9, 128.3, 128.2, 127.6, 127.4, 127.2, 127.1, 79.9, 48.8, 47.9, 44.9, 36.9, 34.9, 28.1, 27.2, 25.6, 19.8, 18.9, 13.6; HRMS calculated for $C_{27}H_{32}O_2Na$ ($M + Na^+$): 411.2300, found: 411.2295. (Colourless oil)



(from L-Isoleucine)
s-6

methyl 2-(5,5-diphenylpent-4-enamido)-3-methylpentanoate (s-6): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.35 (m, 2H), 7.33-7.17 (m, 8H), 6.08-6.05 (t, *J* = 7.2 Hz 1H), 5.99-5.97 (d, *J* = 8.8 Hz 1H), 4.62-4.58 (m, 1H), 3.71 (s, 3H), 2.51-2.45 (m, 2H), 2.36-2.32 (m, 2H), 1.88-1.81 (m, 1H), 1.44-1.37 (m, 1H), 1.62-1.09 (m, 1H), 0.91-0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 172.0, 143.0, 142.5, 139.8, 129.9, 128.4, 128.2, 127.6, 127.4, 127.3, 127.2, 56.4, 52.2, 38.1, 36.7, 25.9, 25.3, 15.5, 11.6; HRMS calculated for $C_{24}H_{29}O_3NNa$ ($M + Na^+$): 402.2045, found: 402.2040. (Colourless oil)

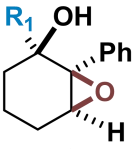
^{1}H, ^{13}C and ^{19}Fspectra data of compounds 2a-2l, 4a-4t



R_1 = Ph

2a

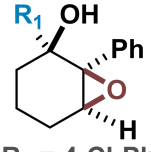
1,2-diphenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.38 (d, *J* = 7.2 Hz, 2H), 7.18-7.13 (m, 4H), 7.08-7.01 (m, 4H), 3.69 (s, 1H), 2.82-2.81 (d, *J* = 3.2 Hz, 1H), 2.23-2.12 (m, 1H), 2.06-1.92 (m, 2H), 1.62-1.42 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 137.9, 128.8, 128.7, 127.7, 127.6, 127.5, 126.8, 126.3, 76.1, 66.2, 63.9, 38.6, 23.4, 16.2; HRMS calculated for $C_{18}H_{18}O_2Na$ ($M + Na^+$): 289.1204, found: 289.1199. (Colourless solid, 21.3 mg, 67% isolated yield)



R_1 = 4-OMe-Ph

2b

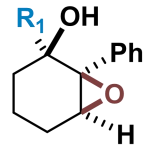
2-(4-methoxyphenyl)-1-phenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2b): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.39-7.36 (d, *J* = 8.4 Hz, 2H), 7.25-7.23 (m, 2H), 7.11-7.10 (d, *J* = 4.8 Hz, 3H), 6.78-6.76 (d, *J* = 8.4 Hz, 2H), 3.75 (s. 3H), 3.73 (s, 1H), 2.83 (s, 1H), 2.26-2.19 (m, 1H), 2.11-2.04 (m, 2H), 1.67-1.61 (m, 2H), 1.54-1.49 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 137.9, 136.3, 128.7, 127.7, 127.6, 127.4, 113.1, 75.9, 66.1, 64.0, 55.2, 38.4, 23.2, 16.4; HRMS calculated for $C_{19}H_{20}O_3Na$ ($M + Na^+$): 319.1310, found: 319.1305. (Yellow oil, 25.1 mg, 78% isolated yield)



R_1 = 4-Cl-Ph

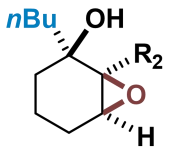
2c

2-(4-chlorophenyl)-1-phenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2c): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.38-7.35 (m, 2H), 7.23-7.19 (m, 2H), 7.18-7.16 (m, 2H), 7.12-7.10 (m, 3H), 3.78-3.77 (m, 1H), 2.98 (s, 1H), 2.32-2.25 (m, 1H), 2.13-1.99 (m, 2H), 1.69-1.63 (m, 2H), 1.54-1.45 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.8, 137.7, 132.5, 128.7, 128.6, 127.8, 127.8, 127.7, 75.7, 66.2, 63.6, 38.9, 23.5, 15.9; HRMS calculated for $C_{18}H_{17}O_2ClNa$ (M + Na^+): 323.0815, found: 323.0809. (Yellow oil, 21.1 mg, 69% isolated yield)



R_1 = 4-F-Ph
2d

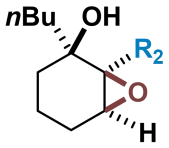
2-(4-fluorophenyl)-1-phenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2d): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.42-7.38 (m, 2H), 7.22-7.19 (m, 2H), 7.11-7.09 (m, 3H), 6.91-6.87 (m, 2H), 3.77-3.76 (t, *J* = 2.0 Hz, 1H), 3.04 (s, 1H), 2.32-2.23 (m, 1H), 2.19-1.99 (m, 2H), 1.72-1.67 (m, 2H), 1.56-1.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 162.8, 160.3, 139.9, 137.9, 128.8, 128.7, 128.0, (d, *J* = 8.6 Hz), 127.6, 114.5, (d, *J* = 21.1 Hz) 75.6, 66.4, 63.7, 38.8, 23.6, 15.9; ^{19}F NMR (376 MHz, CDCl3) δ -116.1; HRMS calculated for $C_{18}H_{17}O_2FNa$ (M + Na^+): 307.1110, found: 307.1105. (White solid, 20.9 mg, 66% isolated yield)



R_2 = Ph
2e

2-butyl-1-phenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2e): ^{1}H NMR (400 Hz, $CDCl_3$) δ

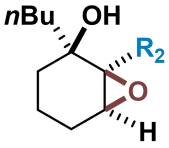
7.41-7.39 (m, 2H), 7.34-7.29 (m, 3H), 3.50-3.49 (d, J = 2.0 Hz. 1H), 2.30 (s, 1H), 2.13-2.06 (m, 1H), 1.98-1.90 (m, 1H), 1.73-1.66 (m, 1H), 1.61-1.51 (m, 3H), 1.49-1.39 (m, 2H), 1.37-1.28 (m, 1H), 1.19-1.07 (m, 3H), 0.79-0.76 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 128.9, 127.9, 127.8, 73.0, 68.0, 62.7, 37.9, 32.6, 25.3, 23.8, 23.3, 16.9, 14.1; HRMS calculated for $C_{16}H_{21}O_2$ (M - H^+): 245.1542, found: 245.1547. (Yellow oil, 24.7 mg, 77% isolated yield)



R_2 = 4-F-Ph

2f

2-butyl-1-(4-fluorophenyl)-7-oxabicyclo[4.1.0]heptan-2-ol (2f): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.39-7.36 (m, 2H), 7.03-6.99 (t, J = 8.4 Hz, 2H), 3.48 (s, 1H), 2.25 (s, 1H), 2.12-2.06 (m, 1H), 1.97-1.91 (m, 1H), 1.70-1.51 (m, 4H), 1.48-1.39 (m, 2H), 1.34-1.28 (m, 1H), 1.17-1.05 (m, 3H), 0.81-0.78 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.3, 130.6, (d, J = 8.6 Hz), 114.9, 114.7, 73.1, 67.4, 62.8, 37.8, 32.6, 25.3, 23.7, 23.3, 16.9, 14.1; ^{19}F NMR (376 MHz, CDCl3) δ -113.9; HRMS calculated for $C_{16}H_{21}O_2FNa$ (M + Na^+): 287.1423, found: 287.1418. (Yellow oil, 21.4 mg, 67% isolated yield)

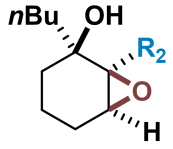


R_2 = 4-Cl-Ph

2g

2-butyl-1-(4-chlorophenyl)-7-oxabicyclo[4.1.0]heptan-2-ol (2g): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.35-7.29 (m, 4H), 3.47 (s, 1H), 2.23 (s, 1H), 2.12-2.05 (m, 1H), 1.96-1.91 (m, 1H), 1.71-1.65 (m, 1H), 1.57-1.32 (m, 5H), 1.17-1.07 (m, 4H), 0.82-0.78 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.9, 133.8, 130.3, 128.0, 72.9, 67.4, 62.7, 37.8,

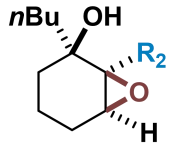
32.6, 25.3, 23.7, 23.3, 16.9, 14.1; HRMS calculated for $C_{16}H_{21}O_2ClNa$ (M + Na^+): 303.1128, found: 303.1122. (White solid, 20.0 mg, 63% isolated yield)



R_2 = 4-Me-Ph

2h

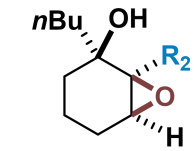
2-butyl-1-(p-tolyl)-7-oxabicyclo[4.1.0]heptan-2-ol (2h): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.29-7.27 (m, 2H), 7.13-7.12 (d, *J* = 8.0 Hz, 2H), 3.48 (s, 1H), 2.34 (s, 3H), 2.25 (s, 1H), 2.12-2.05 (m, 1H), 1.95-1.91 (m, 1H), 1.72-1.67 (m, 1H), 1.52-1.42 (m, 3H), 1.37-1.08 (m, 6H), 0.81-0.77 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 135.4, 128.7, 128.5, 73.1, 67.9, 62.7, 37.9, 32.5, 25.3, 23.8, 23.3, 21.3, 16.9, 14.1; HRMS calculated for $C_{17}H_{24}O_2Na$ (M + Na^+): 283.1674, found: 283.1669. (Colourless oil, 24.9 mg, 78% isolated yield)



R_2 = 3,4-diF-Ph

2i

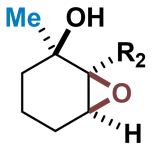
2-butyl-1-(3,4-difluorophenyl)-7-oxabicyclo[4.1.0]heptan-2-ol (2i): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.28-7.24 (m, 1H), 7.13-7.09 (m, 2H), 3.47 (s, 1H), 2.19 (s, 1H), 2.11-2.04 (m, 1H), 1.96-1.91 (m, 1H), 1.69-1.62 (m, 1H), 1.57-1.51 (m, 2H), 1.47-1.32 (m, 3H), 1.25-1.11 (m, 4H), 0.83-0.80 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, (d, *J* = 11.5 Hz), 148.4 (d, *J* = 11.5 Hz), 135.3, 125.0, 118.3, (d, *J* = 17.3 Hz), 116.6, (d, *J* = 17.2 Hz) 73.1, 67.2, 62.9, 37.6, 32.5, 25.2, 23.5, 23.2, 17.1, 14.1; ^{19}F NMR (376 MHz, CDCl3) δ -137.8, -138.5; HRMS calculated for $C_{16}H_{20}O_2F_2Na$ (M + Na^+): 305.1329, found: 305.1324. (White solid, 20.2 mg, 64% isolated yield)



R_2 = 3-Me-4-F-Ph

2j

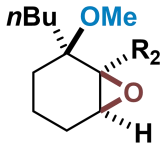
2-butyl-1-(4-fluoro-3-methylphenyl)-7-oxabicyclo[4.1.0]heptan-2-ol (2j): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.24-7.23 (d, *J* = 1.2 Hz, 1H), 7.17-7.14 (m, 1H), 6.96-6.91 (m, 1H), 3.47-3.46 (m, 1H), 2.27-2.26 (m, 4H), 2.12-2.05 (m, 1H), 1.97-1.89 (m, 1H), 1.71-1.65 (m, 1H), 1.58-1.50 (m, 2H), 1.48-1.40 (m, 2H), 1.37-1.29 (m, 1H), 1.19-1.12 (m, 4H), 0.82-0.78 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 133.9, 132.0, (d, *J* = 4.8 Hz) 127.7, (d, *J* = 8.6 Hz) 124.3, (d, *J* = 17.3 Hz) 114.3, (d, *J* = 22 Hz) 73.1, 67.5, 62.8, 37.9, 32.6, 25.3, 23.7, 23.3, 16.9, 14.7, 14.6, 14.1; ^{19}F NMR (376 MHz, CDCl3) δ -118.3; HRMS calculated for $C_{17}H_{23}O_2FNa$ ($M + Na^+$): 301.1580, found: 301.1574. (White solid, 19.1 mg, 60% isolated yield)



R_2 = Ph

2k

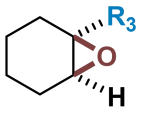
2-methyl-1-phenyl-7-oxabicyclo[4.1.0]heptan-2-ol (2k): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.40-7.38 (d, *J* = 6.8 Hz, 2H), 7.34-.7.29 (m, 3H), 3.49 (s, 1H), 2.4 (s, 1H), 2.13-1.93 (m, 2H), 1.81-1.74 (m, 1H), 1.68-1.63 (m, 1H), 1.53-1.45 (m, 2H), 1.08 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.4, 128.5, 127.9, 127.8, 71.0, 67.5, 62.9, 37.4, 26.5, 24.0, 17.4; HRMS calculated for $C_{13}H_{16}O_2Na$ ($M + Na^+$): 227.1048, found: 227.1043. (Yellow oil, 18.2 mg, 56% isolated yield)



R_2 = Ph

2l

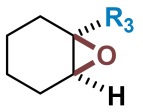
2-butyl-2-methoxy-1-phenyl-7-oxabicyclo[4.1.0]heptane (2l): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.40-7.37 (m, 2H), 7.34-7.28 (m, 3H), 3.52 (s, 3H), 3.19-3.18 (d, *J* = 1.6 Hz, 1H), 2.22-2.14 (m, 1H), 1.99-1.96 (m, 2H), 1.68-1.63 (m, 2H), 1.56-1.48 (m, 1H), 1.45-1.39 (m, 1H), 1.34-1.25 (m, 2H), 1.22-1.13 (m, 3H), 0.85-0.81 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.3, 129.1, 127.7, 127.6, 78.3, 67.2, 58.2, 51.5, 36.3, 25.3, 23.9, 23.3, 22.3, 18.7, 14.2; HRMS calculated for $C_{17}H_{24}O_2Na$ ($M + Na^+$): 283.1674, found: 283.1668. (Colourless oil, 16.8 mg, 56% isolated yield)



R_3 = Ph

4a

1-([1,1'-biphenyl]-4-yl)-7-oxabicyclo[4.1.0]heptane (4a): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.39-7.32 (m, 4H), 7.28-7.24 (m, 1H), 3.08 (s, 1H), 2.32-2.25 (m, 1H), 2.15-2.09 (m, 1H), 2.00-1.98 (m, 2H), 1.56-1.55 (m, 1H), 1.51-1.43 (m, 1H), 1.37-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 128.3, 127.3, 125.4, 62.0, 60.3, 28.9, 24.8, 20.2, 19.9; HRMS calculated for $C_{12}H_{15}O$ ($M + H^+$): 175.1123, found: 175.1117. (Yellow oil, 23.7 mg, 72% isolated yield)

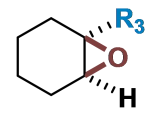


R_3 = 4-*t*Bu-Ph

4b

1-(4-(tert-butyl)phenyl)-7-oxabicyclo[4.1.0]heptane (4b): ^{1}H NMR (400 Hz, $CDCl_3$) δ

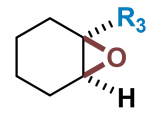
7.30-7.28 (m, 2H), 7.26-7.22 (m, 2H), 3.01 (s, 1H), 2.24-2.18 (m, 1H), 2.08-2.03 (m, 1H), 1.93-1.89 (m, 1H), 1.53-1.48 (m, 3H), 1.26-1.21 (m, 11H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.2, 139.5, 137.6, 130.3, 125.3, 125.1, 62.1, 60.1, 43.5, 34.6, 31.4, 28.8, 24.8, 20.2, 19.9; HRMS calculated for $C_{16}H_{23}O$ ($M + H^+$): 231.1749, found: 231.1743. (Colourless solid, 23.2 mg, 72% isolated yield)



R_3 = 4-Cl-Ph

4c

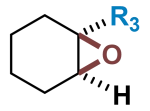
1-(4-chlorophenyl)-7-oxabicyclo[4.1.0]heptane (4c): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.29 (s, 4H), 3.03 (s, 1H), 2.27-2.20 (m, 1H), 2.12-2.05 (m, 1H), 2.01-1.97 (m, 2H), 1.61-1.54 (m, 2H), 1.51-1.44 (m, 1H), 1.36-1.24 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.1, 133.1, 128.5, 126.9, 62.1, 59.9, 28.8, 24.7, 20.1, 19.8; HRMS calculated for $C_{12}H_{14}ClO$ ($M + H^+$): 209.0733, found: 209.0728. (White solid, 25.3 mg, 78% isolated yield)



R_3 = 2-Naphthyl

4d

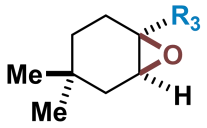
1-(naphthalen-2-yl)-7-oxabicyclo[4.1.0]heptane (4d): ^{1}H NMR (400 Hz, $CDCl_3$) δ 8.03-8.01 (d, J = 7.6 Hz, 1H), 7.88-7.86 (d, J = 8.0 Hz, 1H), 7.78-7.76 (d, J = 8.4 Hz, 1H), 7.56-7.42 (m, 4H), 3.27 (s, 1H), 2.22-2.09 (m, 4H), 1.73-1.64 (m, 2H), 1.57-1.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 133.6, 130.5, 128.9, 127.8, 126.2, 125.7, 125.5, 124.0, 123.9, 60.9, 59.8, 30.9, 25.0, 20.7, 19.2; HRMS calculated for $C_{16}H_{17}O$ ($M + H^+$): 225.1279, found: 225.1274. (White solid, 21.6 mg, 67% isolated yield)



R_3 = 4-F-Ph

4e

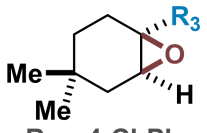
1-(4-fluorophenyl)-7-oxabicyclo[4.1.0]heptane (4e): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.36-7.31 (m, 2H), 7.04-6.98 (m, 2H), 3.05-3.04 (t, *J* = 1.2 Hz, 1H), 2.27-2.20 (m, 1H), 2.14-2.07 (m, 1H), 2.01-1.97 (m, 2H), 1.64-1.59 (m, 1H), 1.58-1.52 (m, 1H), 1.51-1.44 (m, 1H), 1.36-1.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 127.2, 127.1, 115.3, 115.0, 62.0, 59.9, 29.0, 24.7, 20.1, 19.8; ^{19}F NMR (376 MHz, CDCl3) δ -115.5; HRMS calculated for $C_{12}H_{14}FO$ ($M + H^+$): 193.1029, found: 193.1023. (White solid, 21.6 mg, 69% isolated yield)



R_3 = 4-F-Ph

4f

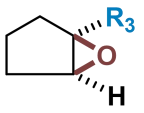
1-(4-fluorophenyl)-4,4-dimethyl-7-oxabicyclo[4.1.0]heptane (4f): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.36-7.33 (m, 2H), 7.04-6.98 (m, 2H), 3.02-3.01 (d, *J* = 5.2 Hz, 1H), 2.38-2.30 (m, 1H), 2.07-2.02 (m, 1H), 1.80-1.74 (m, 2H), 1.54-1.47 (m, 1H), 1.26-1.18 (m, 1H), 0.97 (s, 3H), 0.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 137.8, (d, *J* = 40.2 Hz) 127.2, (d, *J* = 8.6 Hz) 115.2, (d, *J* = 21.1 Hz) 60.9, 59.6, 38.5, 32.2, 31.4, 27.4, 26.5, 25.9, 25.4; ^{19}F NMR (376 MHz, CDCl3) δ -115.3; HRMS calculated for $C_{14}H_{18}FO$ ($M + H^+$): 221.1342, found: 221.1336. (Colourless oil, 23.8 mg, 74% isolated yield)



R_3 = 4-Cl-Ph

4g

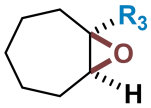
1-(4-chlorophenyl)-4,4-dimethyl-7-oxabicyclo[4.1.0]heptane (4g): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.31-7.30 (m, 4H), 3.01-3.00 (d, *J* = 4.4 Hz, 1H), 2.38-2.29 (m, 1H), 2.07-2.01 (m, 1H), 1.80-1.73 (m, 2H), 1.54-1.45 (m, 1H), 1.25-1.18 (m, 1H), 0.97 (s, 3H), 0.94 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.6, 130.3, 128.6, 126.9, 61.0, 59.5, 38.5, 32.1, 31.4, 27.4, 26.5, 25.2; HRMS calculated for $C_{14}H_{18}ClO$ ($M + H^+$): 237.1046, found: 237.1041. (White solid, 23.4 mg, 73% isolated yield)



R_3 = Ph

4h

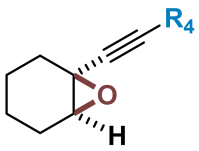
1-phenyl-6-oxabicyclo[3.1.0]hexane (4h): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.40-7.32 (m, 4H), 7.30-7.27 (m, 1H), 3.56 (s, 1H), 2.28-2.19 (m, 2H), 2.14-2.09 (m, 1H), 1.83-1.78 (m, 1H), 1.75-1.70 (m, 1H), 1.65-1.60 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.0, 128.4, 127.7, 126.0, 67.0, 66.5, 29.0, 28.1, 19.4; HRMS calculated for $C_{11}H_{13}O$ ($M + H^+$): 161.0966, found: 161.0961. (White solid, 20.0 mg, 63% isolated yield)



R_3 = Ph

4i

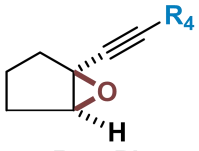
1-phenyl-8-oxabicyclo[5.1.0]octane (4j): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.37-7.30 (m,4H), 7.26-7.22 (m, 1H), 3.04-3.02 (m, 1H), 2.44-2.38 (m, 1H), 2.16-2.09 (m, 1H), 2.07-2.00 (m, 2H), 1.71-1.64 (m, 3H), 1.63-1.60 (m, 1H), 1.58-1.54 (m, 1H), 1.38-1.31 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ143.8, 128.3, 127.1, 125.2, 65.6, 63.3, 33.7, 31.5, 29.7, 25.2, 24.6; HRMS calculated for $C_{13}H_{17}O$ ($M + H^+$): 189.1279, found: 189.1274.(Yellow oil, 21.5 mg, 68% isolated yield)



R_4 = Ph

4j

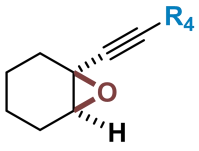
1-(phenylethynyl)-7-oxabicyclo[4.1.0]heptane (4j): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.43-7.42 (d, *J* = 6.0 Hz, 2H), 7.30-7.29 (d, *J* = 4.4 Hz, 3H), 3.45 (s, 1H), 2.28-2.21 (m, 1H), 2.14-2.07 (m, 1H), 1.96-1.95 (m, 2H), 1.47-1.45 (m, 2H), 1.39-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.9, 128.6, 128.3, 122.4, 89.7, 82.1, 60.5, 50.8, 29.9, 24.3, 19.6, 19.0; HRMS calculated for $C_{14}H_{15}O$ ($M + H^+$): 199.1123, found: 199.1117. (Colourless oil, 23.3 mg, 72% isolated yield)



R_4 = Ph

4k

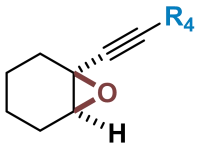
1-(phenylethynyl)-6-oxabicyclo[3.1.0]hexane (4k): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.42-7.40 (m, 2H), 7.31-7.25(m, 3H), 2.55-2.50 (m, 1H), 2.21-2.19 (m, 1H), 2.14-2.06 (m, 1H), 1.94-1.81 (m, 2H), 1.78-1.69 (m, 1H), 1.67-1.62 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.6, 128.3, 127.6, 124.1, 92.6, 84.7, 49.9, 44.6, 38.7, 32.9, 26.2; HRMS calculated for $C_{13}H_{13}O$ ($M + H^+$): 185.0966, found: 185.0961 (Colourless oil, 23.0 mg, 70% isolated yield)



R_3 = 4-F-Ph

4l

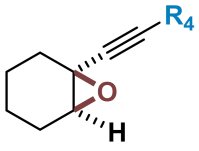
1-((4-fluorophenyl)ethynyl)-7-oxabicyclo[4.1.0]heptane (4l): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.43-7.39 (m, 2H), 7.01-6.97 (t, *J* = 8.0 Hz, 2H), 3.44 (s, 1H), 2.27-2.20 (m, 1 H), 2.13-2.06 (m, 1H), 1.98-1.94 (m, 2H), 1.48-1.43 (m, 2H), 1.39-1.28 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 133.8, (d, *J* = 7.7 Hz) 118.5, 115.6, (d, *J* = 22.1 Hz) 89.4, 81.1, 60.5, 50.7, 29.8, 24.3, 19.5, 18.9; ^{19}F NMR (376 MHz, CDCl3) δ -110.4; HRMS calculated for $C_{14}H_{14}FO$ ($M + H^+$): 217.1029, found: 217.1023. (Colourless oil, 22.6 mg, 70% isolated yield)



R_4 = 4-Cl-Ph

4m

1-((4-chlorophenyl)ethynyl)-7-oxabicyclo[4.1.0]heptane (4m): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.37-7.35 (m, 2H), 7.28-7.26 (m, 2H), 3.44-3.43 (t, *J* = 2.8 Hz, 1H), 2.27-2.19 (m, 1H), 2.13-2.01 (m, 1H), 1.98-1.94 (m, 2H), 1.50-1.25 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 134.6, 133.3 128.7, 120.9, 90.7, 80.9, 60.5, 50.7, 29.8, 24.3, 19.5, 18.9; HRMS calculated for $C_{14}H_{14}ClO$ ($M + H^+$): 233.0733, found: 233.0728. (Colourless oil, 21.9 mg, 68% isolated yield)

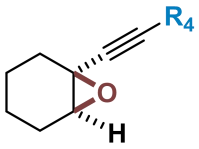


R_4 = 4-Me-Ph

4n

1-(p-tolylethynyl)-7-oxabicyclo[4.1.0]heptane (4n): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.33-7.31 (d, *J* = 8.4 Hz, 2H), 7.12-7.09 (d, *J* = 7.6 Hz, 2H), 3.44-3.43 (m, 1H), 2.34 (s, 3H), 2.27-2.20 (m, 1H), 2.14-2.08 (m, 1H), 1.97-1.93 (m, 2H), 1.51-1.42 (m, 2H), 1.37-1.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.7, 137.6, 131.8, 130.3, 129.1,

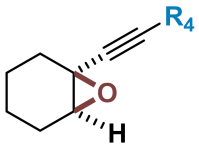
119.3, 89.0, 82.3, 60.5, 50.9, 29.9, 24.3, 21.6, 19.6, 19.0; HRMS calculated for $C_{15}H_{17}O$ ($M + H^+$): 213.1279, found: 213.1274. (Colourless oil, 23.3 mg, 72% isolated yield)



R_4 = 4-Et-Ph

4o

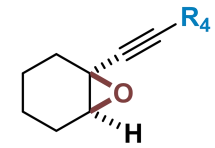
1-((4-ethylphenyl)ethynyl)-7-oxabicyclo[4.1.0]heptane (4o): ^1H NMR (400 Hz, $CDCl_3$) δ 7.35-7.33 (d, *J* = 8.0 Hz, 2H), 7.13-7.11 (d, *J* = 8.4 Hz, 2H), 3.44-3.43 (m, 1H), 2.66-2.60 (m, 2H), 2.27-2.21 (m, 1H), 2.14-2.07 (m, 1H), 1.98-1.94 (m, 2H), 1.51-1.43 (m, 2H), 1.39-1.28 (m, 2H), 1.24-1.20 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.9, 131.9, 127.9, 119.6, 89.1, 82.3, 60.5, 50.9, 29.9, 28.9, 24.3, 19.6, 19.0, 15.4; HRMS calculated for $C_{16}H_{19}O$ ($M + H^+$): 227.1436, found: 227.1430. (Colourless oil, 22.9 mg, 71% isolated yield)



R_4 = 4-*n*Pr-Ph

4p

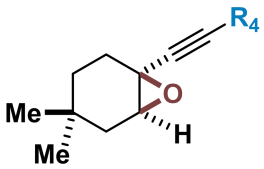
1-((4-propylphenyl)ethynyl)-7-oxabicyclo[4.1.0]heptane (4p): ^1H NMR (400 Hz, $CDCl_3$) δ 7.35-7.33 (d, *J* = 8.4 Hz, 2H), 7.11-7.09 (d, *J* = 8.0 Hz, 2H), 3.44-3.43 (m, 1H), 2.58-2.55 (t, *J* = 7.2 Hz, 2H), 2.27-2.20 (m, 1H), 2.13-2.06 (m, 1H), 1.97-1.93 (m, 2H), 1.64-1.59 (m, 2H), 1.51-1.43 (m, 2H), 1.39-1.24 (m, 2H), 0.94-0.90 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.5, 131.8, 128.5, 119.6, 89.0, 82.3, 60.5, 50.7, 38.0, 29.9, 24.4, 19.6, 19.0, 13.8; HRMS calculated for $C_{17}H_{21}O$ ($M + H^+$): 241.1592, found: 241.1587. (Yellow oil, 24.1 mg, 75% isolated yield)



R_4 = 4-*n*Pentyl-Ph

4q

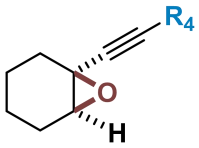
1-((4-pentylphenyl)ethynyl)-7-oxabicyclo[4.1.0]heptane (4q): ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.35-7.33 (d, *J* = 7.6 Hz, 2H), 7.11-7.09 (d, *J* = 8.4 Hz, 2H), 3.43 (s, 1H), 2.59-2.56 (t, *J* = 7.2 Hz, 2H), 2.27-2.20 (m, 1H), 2.13-2.06 (m, 1H), 1.97-1.93 (m, 2H), 1.62-1.55 (m, 2H), 1.50-1.41 (m, 2H), 1.33-1.26 (m, 6H), 0.89-0.86 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.7, 131.8, 128.5, 119.5, 89.0, 82.3, 60.5, 50.9, 35.9, 31.5, 30.9, 29.9, 24.3, 22.6, 19.6, 19.0, 14.1; HRMS calculated for $C_{19}H_{24}ONa$ ($M + Na^+$): 291.1725, found: 291.1719. (Yellow oil, 22.5 mg, 71% isolated yield)



R_4 = Ph

4r

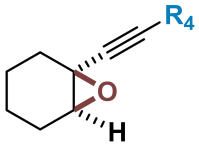
4,4-dimethyl-1-(phenylethynyl)-7-oxabicyclo[4.1.0]heptane (4r) : ^{1}H NMR (400 Hz, $CDCl_3$) δ 7.45-7.43 (m, 2H), 7.31-7.30 (m, 3H), 3.41-3.40 (d, *J* = 5.6 Hz, 1H), 2.28-2.22 (m, 1H), 2.20-2.12 (m, 1H), 1.80-1.74 (m, 1H), 1.62-1.60 (m, 1H), 1.40-1.32 (m, 1H), 1.14-1.09 (m, 1H), 0.94 (s, 3H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 131.9, 128.6, 128.3, 122.4, 89.3, 82.2, 59.5, 50.6, 37.8, 31.6, 31.2, 27.3, 26.6, 26.5; HRMS calculated for $C_{16}H_{19}O$ ($M + H^+$): 227.1436, found: 227.1430. (Yellow oil, 24.5 mg, 76% isolated yield)



R_4 = *n*Pentyl

4s

(1S,6S)-1-(hept-1-yn-1-yl)-7-oxabicyclo[4.1.0]heptane (4s): ^{1}H NMR (400 Hz, $CDCl_3$) δ 3.29 (s, 1H), 2.20-2.09 (m, 3H), 1.99-1.88 (m, 3H), 1.53-1.46 (m, 2H), 1.43-1.18 (m, 8H), 0.91-0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 83.2, 80.7, 60.2, 50.7, 31.1, 30.2, 28.3, 24.3, 22.3, 19.6, 19.1, 18.8, 14.0; HRMS calculated for $C_{13}H_{21}O$ ($M + H^+$): 193.1592, found: 193.1587. (Colourless oil, 22.9 mg, 70% isolated yield)

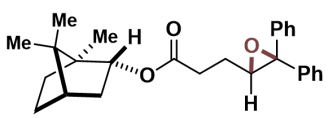


R_4 = *n*Hexyl

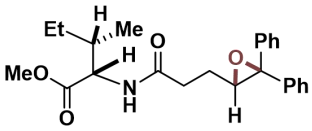
4t

1-(oct-1-yn-1-yl)-7-oxabicyclo[4.1.0]heptane (4t): ^{1}H NMR (400 Hz, $CDCl_3$) δ 3.29-3.28 (t, *J* = 2 Hz, 1H), 2.20-2.17 (m, 2H), 2.15-2.09 (m, 1H), 2.00-1.93 (m, 1H), 1.93-1.88 (m, 2H), 1.53-1.44 (m, 2H), 1.43-1.36 (m, 3H), 1.34-1.26 (m, 7H), 0.90-0.87 (t, *J* = 8.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 83.2, 80.7, 60.2, 50.7, 31.4, 30.2, 28.6, 28.5, 24.3, 22.6, 19.6, 19.1, 18.8, 14.1; HRMS calculated for $C_{14}H_{23}O$ ($M + H^+$): 207.1749, found: 207.1743. (Colourless oil, 22.4 mg, 69% isolated yield)

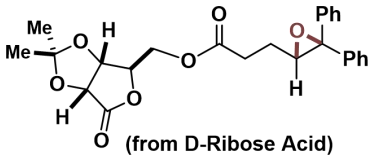
Late-stage diversification of substances derived from natural products and drugs



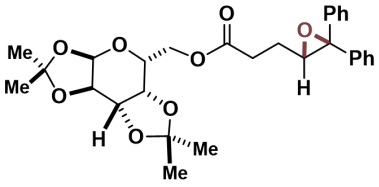
(from Borneol)
5: 91%



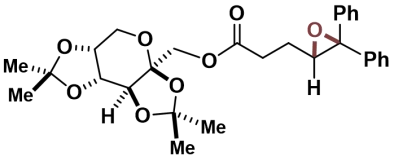
(from L-Isoleucine)
6: 70%



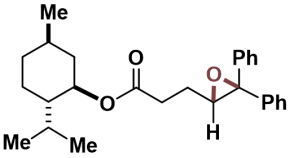
(from D-Ribose Acid)
7: 87%



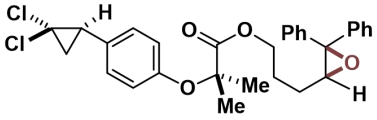
(from D-Galactopyranose)
8: 89%



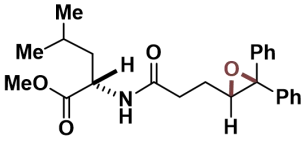
(from D-Fructopyranose)
9: 92%



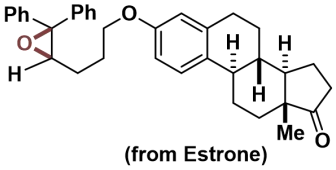
(from L-Menthol)
10: 90%



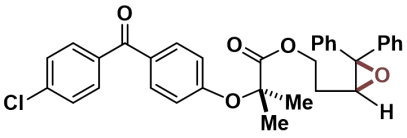
(from Ciprofibrate)
11: 76%



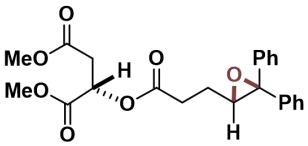
(from L-Leucine)
12: 77%



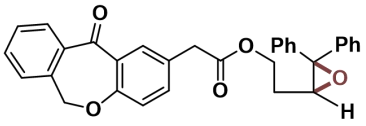
(from Estrone)
13: 56%



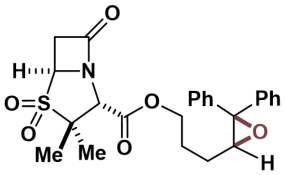
(from Fenofibric Acid)
14: 78%



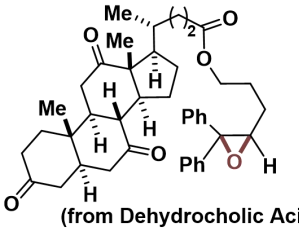
(from Malate)
15: 88%



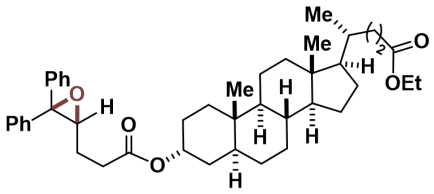
(from Isoxepac)
16: 83%



(from Sulbactam)
17: 69%

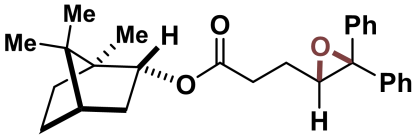


(from Dehydrocholic Acid)
18: 41%



(from Lithocholic Acid)
19: 68%

^{1}H and ^{13}C spectra data of compounds 5-19

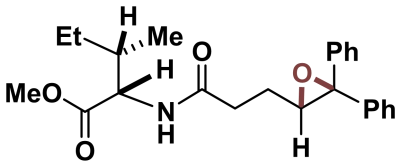


(from Borneol)

5

1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl 3-(3,3-diphenyloxiran-2-yl)propanoate (5):

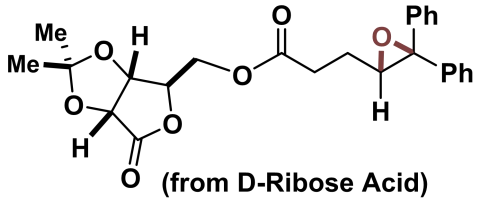
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.35 (m, 4H), 7.33-7.30 (m, 5H), 7.29-7.27 (m, 1H), 4.88-4.84 (m, 1H), 3.51-3.48 (m, 1H), 2.49-2.46 (t, *J* = 7.2 Hz, 1H), 2.34-2.30 (m, 1H), 1.90-1.81 (m, 2H), 1.76-1.70 (m, 1H), 1.67-1.64 (m, 1H), 1.57-1.52 (m, 1H), 1.30-1.18 (m, 3H), 0.96-0.90 (m, 1H), 0.89 (s, 3H), 0.86 (s, 3H), 0.80-0.78 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.2, 140.8, 137.3, 130.3, 128.4, 128.3, 128.0, 127.9, 127.8, 127.1, 80.2, 66.6, 65.4, 48.8, 47.9, 44.9, 36.8, 31.2, 28.1, 27.2, 25.3, 19.8, 18.9, 13.6; HRMS calculated for $C_{27}H_{32}O_3Na$ (M + Na^+): 427.2249, found: 427.2244. (Yellow oil, 28.4 mg, 91% isolated yield)



(from L-Isoleucine)

6

methyl 2-(3-(3,3-diphenyloxiran-2-yl)propanamido)-3-methylpentanoate (6): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.35 (m, 4H), 7.33-7.28 (m, 6H), 6.08-6.04 (t, *J* = 7.2 Hz, 1H), 4.55-4.55 (m, 1H), 3.72 (s, 3H), 3.50-3.46 (m, 1H), 2.42-2.37 (m, 2H), 2.02-1.95 (m, 1H), 1.88-1.82 (m, 1H), 1.49-1.37 (m, 2H), 1.20-1.12 (m, 1H), 0.92-0.86 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ `172.6, 171.6, 140.8, 137.3, 128.3, 128.0, 127.9, 127.8, 127.0, 66.7, 65.6, 56.5, 52.2, 37.9, 33.0, 25.8, 25.3, 15.5, 11.7; HRMS calculated for $C_{24}H_{29}O_4NNa$ (M + Na^+): 418.1994, found: 418.1989. (Colourless oil, 21.3 mg, 70% isolated yield)

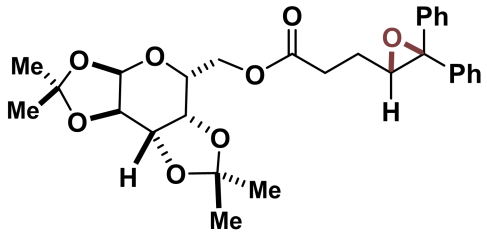


(from D-Ribose Acid)

7

(2,2-dimethyl-6-oxotetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)methyl 3-(3,3-diphenyl-

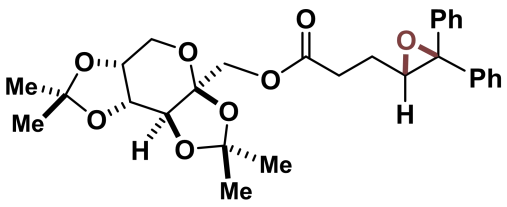
oxiran-2-yl)propanoate (7)： ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.38 (m, 4H), 7.37-7.27 (m, 6H), 4.76-4.75 (m, 1H), 4.71-4.65 (m, 2H), 4.38-4.33 (m, 1H), 4.25-4.22 (m, 1H), 3.47-3.42 (m, 1H), 2.50-2.45 (m, 2H), 1.93-1.86 (m, 1H), 1.53-1.41 (m, 4H), 1.38-1.36 (d, *J* = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.5, 171.7, 140.5, 137.0, 128.5, 128.1, 128.0, 127.9, 127.1, 127.0, 113.9, 79.6, 77.7, 75.2, 65.1, 64.7, 63.7, 30.7, 26.8, 25.6, 25.1; HRMS calculated for $C_{25}H_{26}O_7Na$ ($M + Na^+$): 461.1576, found: 461.1571. (Yellow oil, 27.1 mg, 87% isolated yield)



(from D-Galactopyranose)

8

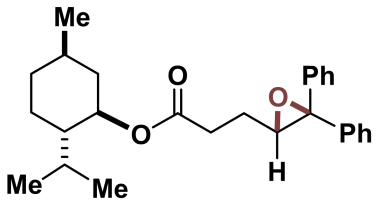
(2,2,7,7-tetramethyltetrahydro-5*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methyl 3-(3,3-diphenyloxiran-2-yl)propanoate (8)： ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.34 (m, 4H), 7.33-7.27 (m, 6H), 5.53-5.51 (m, 1H), 4.62-4.59 (m, 1H), 4.33-4.30 (m, 1H), 4.29-4.25 (m, 1H), 4.22-4.17 (m, 2H), 4.02-3.98 (m, 1H), 3.51-3.48 (m, 1H), 2.53-2.49 (m, 2H), 1.89-1.83 (m, 1H), 1.57-1.49 (m, 1H), 1.45-1.44 (d, *J* = 5.2 Hz, 6H), 1.32 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 137.3, 128.4, 128.3, 128.0, 127.9, 127.8, 127.2, 127.1, 109.7, 108.9, 96.3, 71.1, 70.7, 70.5, 66.6, 65.9, 65.2, 63.6, 30.8, 26.0, 25.2, 25.0, 24.5, 23.9; HRMS calculated for $C_{29}H_{34}O_8Na$ ($M + Na^+$): 533.2151, found: 533.2146. (Colourless oil, 26.7 mg, 89% isolated yield)



(from D-Fructopyranose)

9

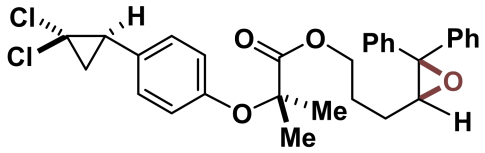
2,2,7,7-tetramethyltetrahydro-3aH-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-3a-yl)methyl 3-((S)-3,3-diphenyloxiran-2-yl)propanoate (9)： ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.35 (m, 5H), 7.33-7.28 (m, 5H), 4.60-4.58 (m, 1H), 4.23-4.40 (m, 1H), 4.28-4.27 (m, 1H), 4.25-4.23 (m, 1H), 4.04-4.00 (m, 1H), 3.92-3.88 (m, 1H), 3.77-3.74 (m, 1H), 3.50-3.47 (m, 1H), 2.55-2.51 (m, 2H), 1.94-1.87 (m, 1H), 1.60 (s, 2H), 1.53-1.52 (d, *J* = 3.6 Hz, 4H), 1.36-1.34 (m, 7H). ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 140.7, 137.2, 128.4, 128.4, 128.0, 127.9, 127.8, 127.1, 109.2, 108.8, 101.5, 7, 66.6, 65.4, 65.2, 61.3, 30.7, 26.5, 26.0, 25.3, 25.1, 24.1; HRMS calculated for $C_{29}H_{34}O_8Na$ (M + Na^+): 533.2151, found: 533.2146. (Yellow oil, 27.6 mg, 92% isolated yield)



(from L-Menthol)

10

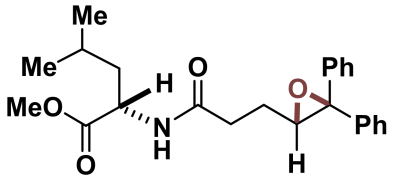
2-isopropyl-5-methylcyclohexyl 3-((S)-3,3-diphenyloxiran-2-yl)propanoate (10)： ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.35 (m, 4H), 7.33-7.27 (m, 6H), 4.70-4.63 (m, 1H), 3.49-3.45 (m, 1H), 2.45-2.42 (m, 2H), 1.97-1.93 (m, 1H), 1.86-1.79 (m, 2H), 1.68-1.64 (m, 2H), 1.56-1.50 (m, 1H), 1.49-1.43 (m, 1H), 1.38-1.31 (m, 1H), 1.05-0.97 (m, 1H), 0.96-0.92 (m, 1H), 0.90-0.86 (m, 6H), 0.84-0.83 (m, 1H), 0.73-0.69 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.4, 140.9, 137.3, 128.4, 128.3, 128.0, 127.9, 127.8, 127.1, 74.5, 66.6, 65.3, 47.0, 41.0, 34.3, 31.4, 31.2, 26.3, 25.3, 23.5, 22.1, 20.8, 16.4; HRMS calculated for $C_{27}H_{34}O_3Na$ (M + Na^+): 429.2406, found: 429.2400. (Colourless oil, 27 mg, 90% isolated yield)



(from Ciprofibrate)

11

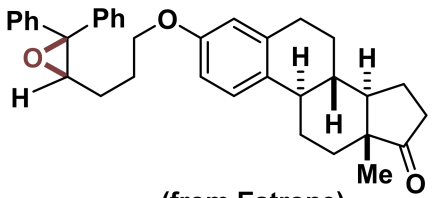
3-(3,3-diphenyloxiran-2-yl)propyl-2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methyl propanoate (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.35 (d, *J* = 4.4 Hz, 4H), 7.31-7.26 (m, 6H), 7.09-7.07 (d, *J* = 8.8 Hz, 2H), 6.77-6.75 (d, *J* = 8.0 Hz, 2H), 4.20-4.08 (m, 2H), 3.35-3.32 (m, 1H), 2.81-2.76 (m, 1H), 1.93-1.87 (m, 1H), 1.81-1.73 (m, 3H), 1.53-1.52 (d, *J* = 2.4 Hz, 6H), 1.49-1.40 (m, 1H), 1.23-1.15 (m, 1H) ; ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.2, 155.0, 140.9, 137.3, 129.7, 128.4, 128.3, 128.0, 127.9, 127.0, 118.6, 79.2, 66.3, 65.9, 64.9, 60.9, 34.9, 26.2, 25.9, 25.5, 25.4, 25.3, 25.3; HRMS calculated for $C_{30}H_{30}O_4Cl_2Na$ (M + Na^+): 547.1419, found: 547.1413. (Colourless oil, 22.8 mg, 76% isolated yield)



(from L-Leucine)

12

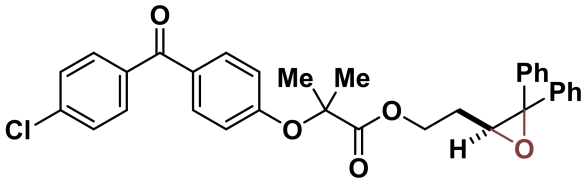
methyl (3-(3,3-diphenyloxiran-2-yl)propanoyl)leucinate (12): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.35 (m, 4H), 7.33-7.26 (m, 6H), 5.95-5.90 (t, *J* = 9.2 Hz, 1H), 4.65-4.57 (m, 1H), 3.71-3.70 (d, *J* = 1.2 Hz, 3H), 3.51-3.45 (m, 1H), 2.41-2.36 (m, 2H), 2.03-1.95 (m, 1H), 1.65-1.59 (m, 2H) , 1.48-1.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 171.6, 140.8, 137.3, 128.4, 128.4, 128.1, 127.9, 127.9, 127.0, 65.6, 52.4, 50.8, 41.7, 32.9, 25.6, 24.9, 22.9, 22.0. HRMS calculated for $C_{24}H_{29}O_4NNa$ (M + Na^+): 418.1994, found: 418.1989. (Colourless oil, 23.1 mg, 77% isolated yield)



(from Estrone)

13

3-(3-(3,3-diphenyloxiran-2-yl)propoxy)-13-methyl-6,7,8,9,11,12,13,14,15,16-decahydro-17*H*-cyclopenta[a]phenanthren-17-one (13): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.38 (m, 3H), 7.36-7.30 (m, 7H), 7.18-7.16 (d, *J* = 8.4 Hz, 1H), 6.66-6.63 (m, 1H), 6.57-6.56 (d, *J* = 2.4 Hz, 1H), 3.96-3.86 (m, 2H), 3.50-3.47 (m, 1H), 2.89-2.85 (m, 2H), 2.54-2.47 (m, 1H), 2.40-2.36 (m, 1H), 2.24 (s, 1H), 2.17-2.10 (m, 1H), 2.05-1.92 (m, 4H), 1.68-1.61 (m, 2H), 1.54-1.41 (m, 6H), 1.25 (s, 1H), 0.90 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 221.2, 156.9, 141.1, 137.8, 137.5, 132.1, 128.4, 128.2, 128.1, 127.9, 127.7, 127.1, 126.4, 114.6, 112.2, 67.3, 66.2, 50.5, 44.0, 38.4, 36.0, 31.6, 29.7, 26.6, 26.5, 26.2, 26.0, 21.7, 14.0. HRMS calculated for $C_{35}H_{38}O_3Na$ ($M + Na^+$): 529.2719, found: 529.2713. (Colourless oil, 17.3 mg, 56% isolated yield)

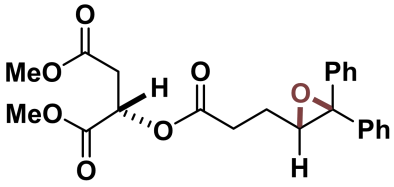


(from Fenofibric Acid)

14

2-(3,3-diphenyloxiran-2-yl)ethyl2-(4-(4-chlorobenzoyl)phenoxy)-2-methylpropanoate (14): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.65 (m, 4H), 7.44-7.42 (d, *J* = 8.4 Hz, 2H), 7.36-7.34 (m, 5H), 7.24-7.21 (m, 3H), 7.18-7.16 (m, 2H), 6.86-6.84 (m, 2H), 4.32-4.29 (m, 2H), 3.32-3.29 (m, 1H), 1.87-1.81 (m, 2H), 1.68 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.2, 173.8, 159.6, 140.4, 137.0, 136.4, 132.2, 131.3, 130.4, 128.6, 128.4, 128.3, 128.0, 127.9, 127.0, 117.1, 98.9, 79.4, 66.1, 63.0, 29.2, 25.8; HRMS calculated for $C_{33}H_{29}O_5ClNa$ ($M + Na^+$): 563.1601, found: 563.1596. (Yellow oil, 23.4 mg, 78%

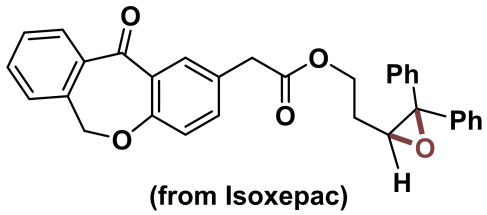
isolated yield)



(from Malate)

15

dimethyl 2-((3-(3,3-diphenyloxiran-2-yl)propanoyl)oxy)succinate (15): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.35 (m, 5H), 7.33-7.27 (m, 5H), 5.50-5.44 (m, 1H), 3.74-3.73 (d, *J* = 2.4 Hz, 3H), 3.68-3.67 (d, *J* = 5.2 Hz, 3H), 3.52-3.48 (m, 1H), 2.89-2.87 (m, 2H), 2.59-2.53 (m, 2H), 1.93-1.84 (m, 1H), 1.56-1.50 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 169.7, 169.4, 140.8, 137.2, 128.5, 128.4, 128.0, 127.8, 127.1, 125.9, 82.5, 68.3, 65.0, 52.8, 52.3, 35.9, 30.5, 25.1; HRMS calculated for $C_{23}H_{24}O_7Na$ ($M + Na^+$): 435.1420, found: 435.1414. (Yellow oil, 27.5 mg, 88% isolated yield)

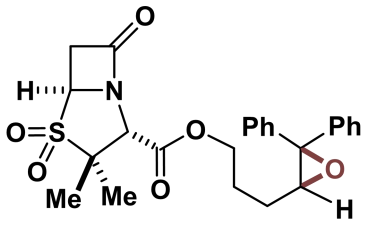


(from Isoxepac)

16

2-(3,3-diphenyloxiran-2-yl)ethyl2-(11-oxo-6,11-dihydrodibenzo[*b*,*e*]oxepin-3-yl) acetate (16): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.11 (d, *J* = 2.4 Hz, 1H), 7.88-7.86 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 7.72-7.69 (m, 2H), 7.57-7.54 (m, 1H), 7.49-7.47 (m, 1H), 7.43-7.41 (dd, J_1 = 2.0 Hz, J_2 = 8.0 Hz, 1H), 7.38-7.36 (m, 4H), 7.33-7.31 (m, 2H), 7.29-7.28 (m, 2H), 7.13-7.09 (m, 2H), 7.03-7.00 (d, *J* = 8.8 Hz, 1H), 5.16 (s, 2H), 4.26-4.22 (m, 2H), 3.65 (s, 2H), 3.49-3.46 (m, 1H), 1.86-1.85 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.9, 171.4, 160.6, 140.6, 137.6, 137.2, 136.4, 135.6, 132.9, 132.6, 130.3, 129.6, 129.4, 128.4, 128.3, 128.0, 127.9, 127.8, 127.7, 127.6, 127.1, 121.2, 73.7,

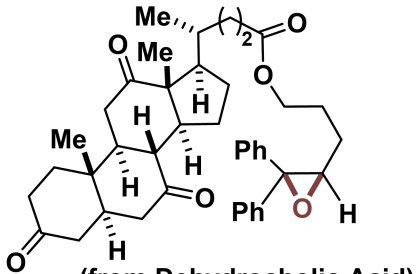
66.2, 63.3, 62.2, 40.3, 29.1, 1.125; HRMS calculated for $C_{32}H_{26}O_5Na$ ($M + Na^+$): 513.1678, found: 513.1673. (Colourless oil, 25.7 mg, 83% isolated yield)



(from Sulbactam)

17

2-(3,3-diphenyloxiran-2-yl)propyl 3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0] heptane-2-carboxylate 4,4-dioxide (17): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.38 (t, 4H), 7.32-7.30 (m, 6H), 4.54-4.52 (m, 1H), 4.31-4.28 (d, *J* = 12.0 Hz, 1H), 4.24-4.18 (m, 2H), 3.45-3.42 (m, 2H), 3.40-3.38 (m, 1H), 1.91-1.85 (m, 2H), 1.67-1.62 (m, 1H), 1.48-1.45 (d, *J* = 13.2 Hz, 3H), 1.35-1.31 (d, *J* = 16.0 Hz, 3H), 1.28-1.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.8, 167.0, 140.7, 137.2, 128.5, 128.4, 128.0, 127.9, 127.0, 126.9, 66.1, 38.4, 26.6, 25.6, 20.4, 18.6. HRMS calculated for $C_{25}H_{27}O_6NNaS$ ($M + Na^+$): 492.1457, found: 492.1451. (Yellow oil, 21.4 mg, 69% isolated yield)

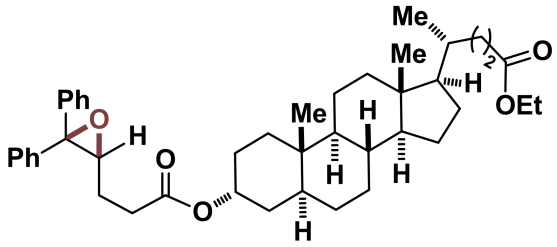


(from Dehydrocholic Acid)

18

3-(3,3-diphenyloxiran-2-yl)propyl4-(10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate : ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41-7.37 (m, 4H), 7.34-7.28 (m, 6H), 4.10-4.00 (m, 2H), 3.44-3.41 (m, 1H), 2.96-2.82 (m, 4H), 2.38-2.24 (m, 6H), 2.21-2.12 (m, 4H), 2.06-1.95 (m, 4H), 1.87-1.76 (m, 4H),

1.40 (s, 3H), 1.37-1.24 (m, 6H), 1.06 (s, 3H), 0.83-0.82 (d, J = 4.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 212.1, 209.2, 208.9, 174.1, 140.9, 137.4, 128.4, 128.3, 128.0, 127.9, 127.8, 127.1, 66.4, 66.0, 63.8, 57.0, 51.8, 49.1, 46.9, 45.7, 45.6, 45.1, 42.9, 38.7, 36.6, 36.1, 35.6, 35.4, 31.5, 30.4, 27.7, 26.3, 25.5, 25.2, 22.0, 18.7, 11.9; HRMS calculated for $C_{41}H_{50}O_6Na$ ($M + Na^+$): 661.3505, found: 661.3500. (Yellow oil, 12.6 mg, 41% isolated yield)



(from Lithocholic Acid)

19

Ethyl 4-(-2-((3-(3,3-diphenyloxiran-2-yl)propanoyl)oxy)-10,13-dimethylhexadeca hydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate (19): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42-7.36 (m, 4H), 7.35-7.28 (m, 6H), 4.74-4.68 (m, 1H), 4.15-4.09 (m, 2H), 3.50-3.47 (m, 1H), 2.45-2.41 (t, J = 7.2 Hz, 2H), 2.38-2.30 (m, 1H), 2.24-2.17 (m, 1H), 1.98-1.95 (d, J = 12.0 Hz, 1H), 1.87-1.75 (m, 6H), 1.68-1.62 (m, 1H), 1.56-1.51 (m, 2H), 1.47-1.33 (m, 8H), 1.29-1.24 (m, 6H), 1.21-0.97 (m, 7H), 0.94-0.88 (m, 6H), 0.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 172.4, 140.9, 137.3, 128.4, 128.3, 128.0, 127.9, 127.8, 127.1, 74.7, 66.6, 65.4, 60.3, 56.6, 56.1, 42.8, 42.0, 40.5, 40.2, 35.9, 35.5, 35.1, 34.7, 31.4, 31.1, 28.3, 27.1, 26.7, 26.4, 25.2, 24.3, 23.4, 20.9, 18.4, 14.4, 12.1. HRMS calculated for $C_{43}H_{58}O_5Na$ ($M + Na^+$): 677.4182, found: 677.4177. (Colourless oil, 20.9 mg, 68% isolated)

UV-Vis absorption experiments

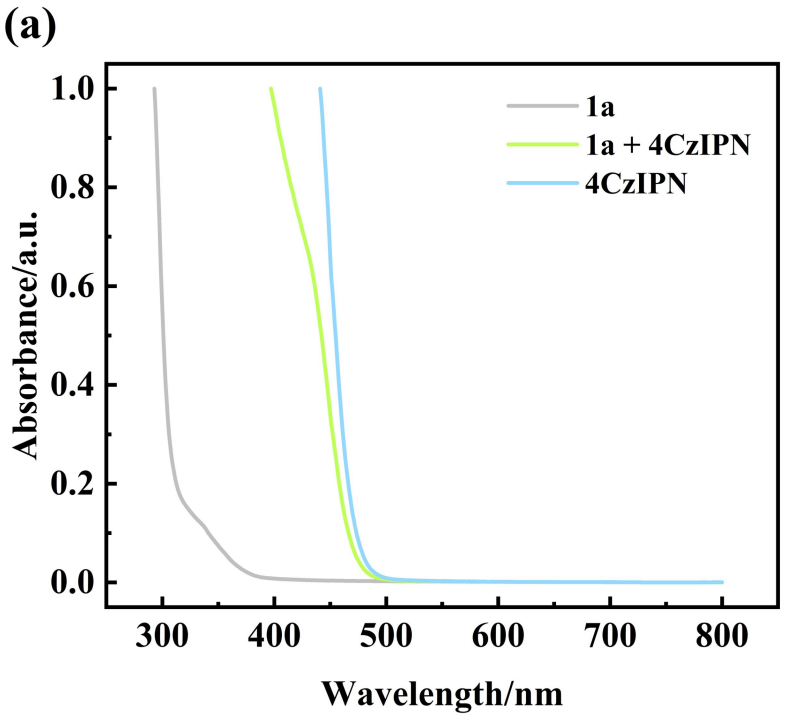


Figure 1. UV−Vis absorption spectra of the individual reaction components and the reaction mixtures

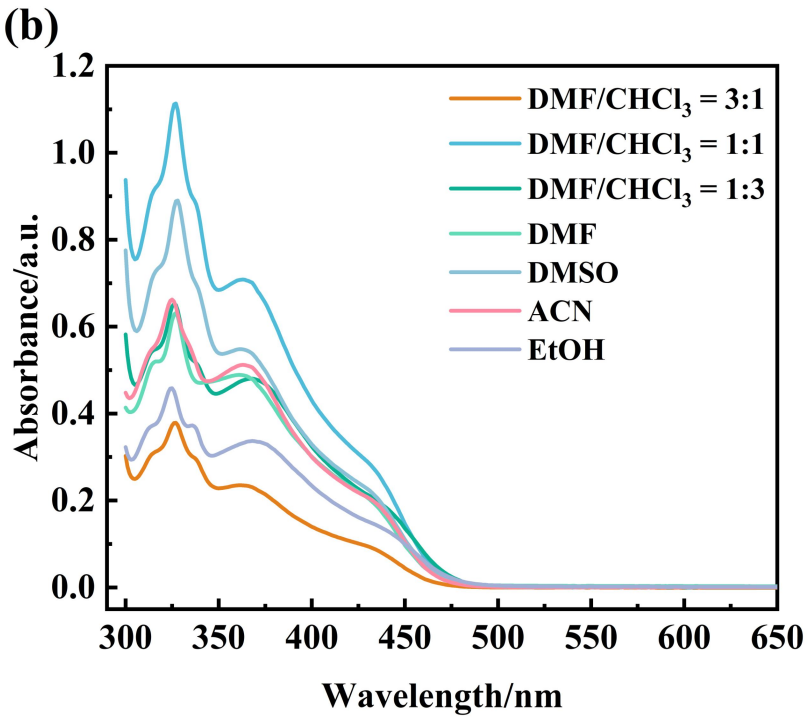


Figure 2. UV-Vis absorption spectra of 4CzIPN in different solvents.

Transient fluorescence spectroscopy

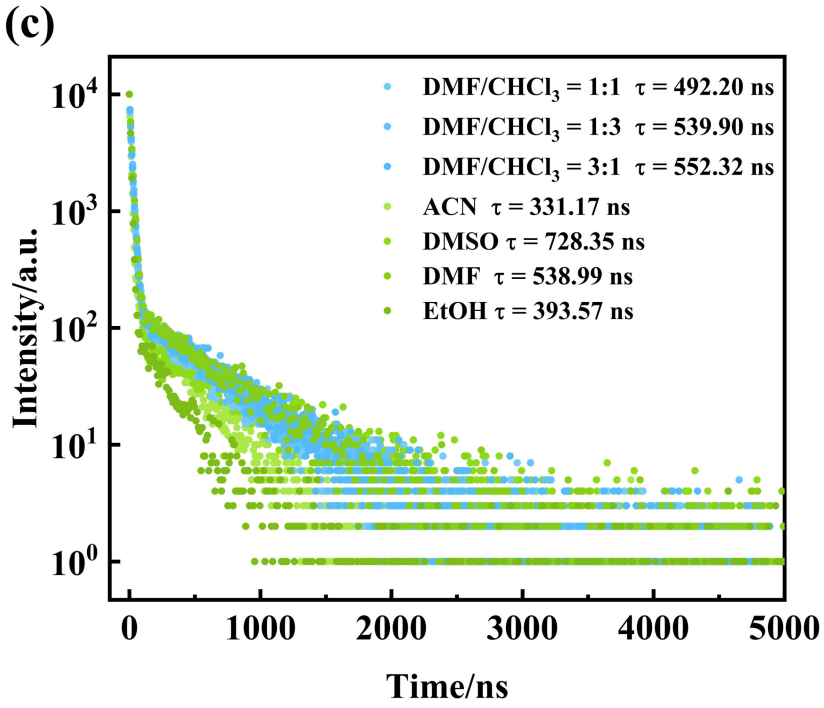


Figure 3. Transient fluorescence spectra of 4CzIPN in different solvents

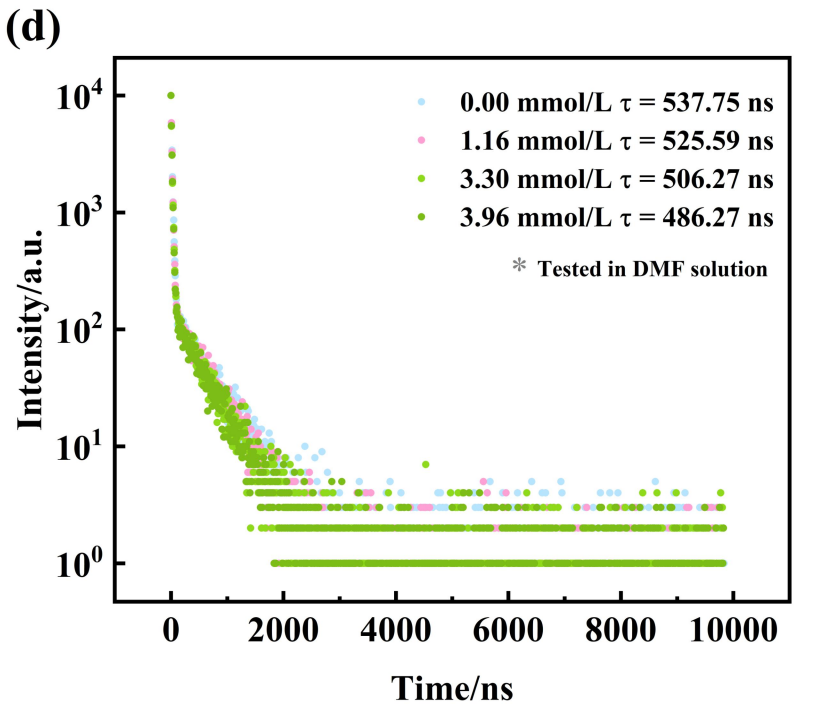


Figure 4. Transient fluorescence spectra of 4CzIPN at different concentrations of 1a

Fluorescence quenching experiments

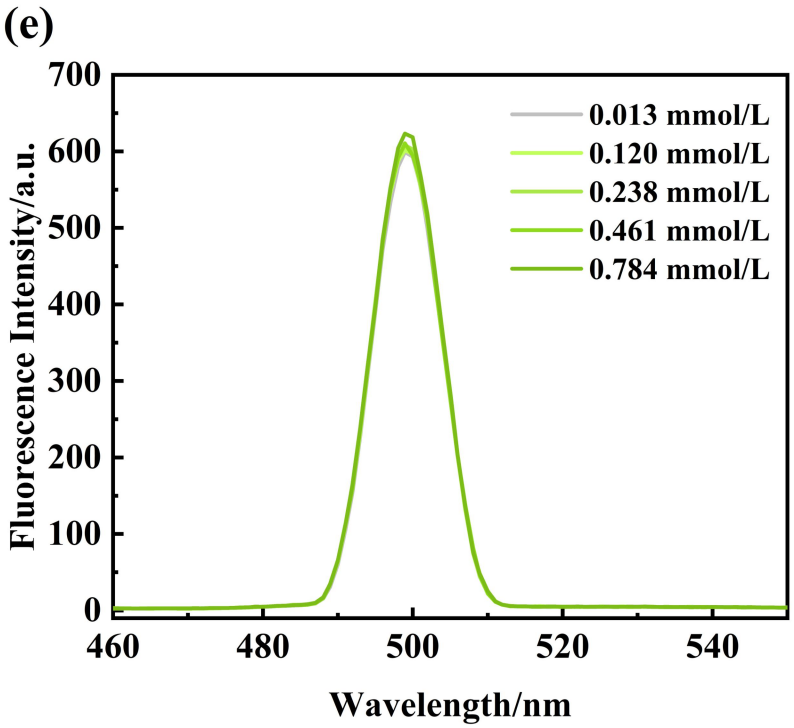


Figure 5. Fluorescence spectra of 4CzIPN with different concentrations of 1a

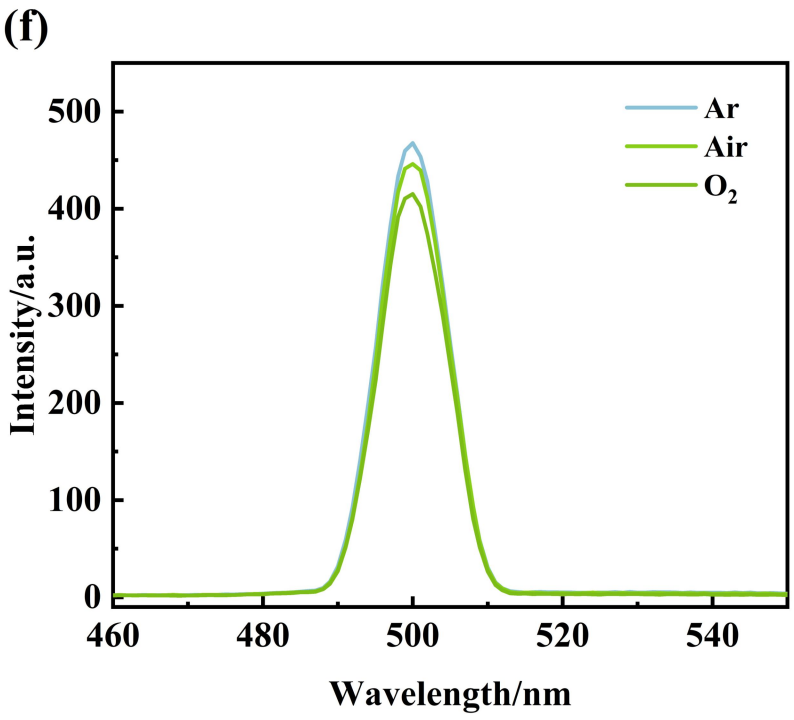


Figure 6. Fluorescence spectra of 4CzIPN with different concentrations of O_2

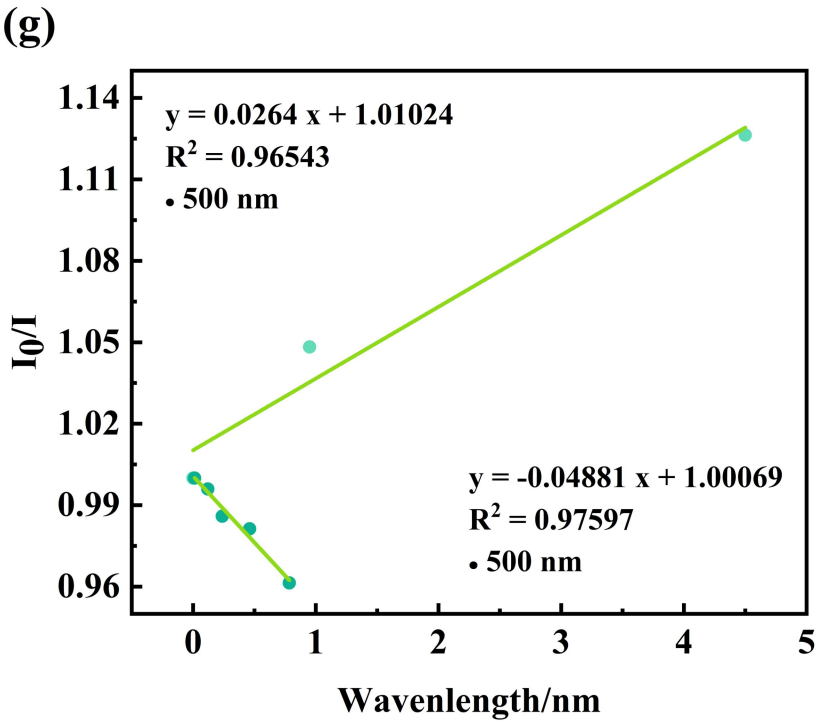


Figure 7. Stern Volmer plots of the substrate 1a and O_2

EPR experiments

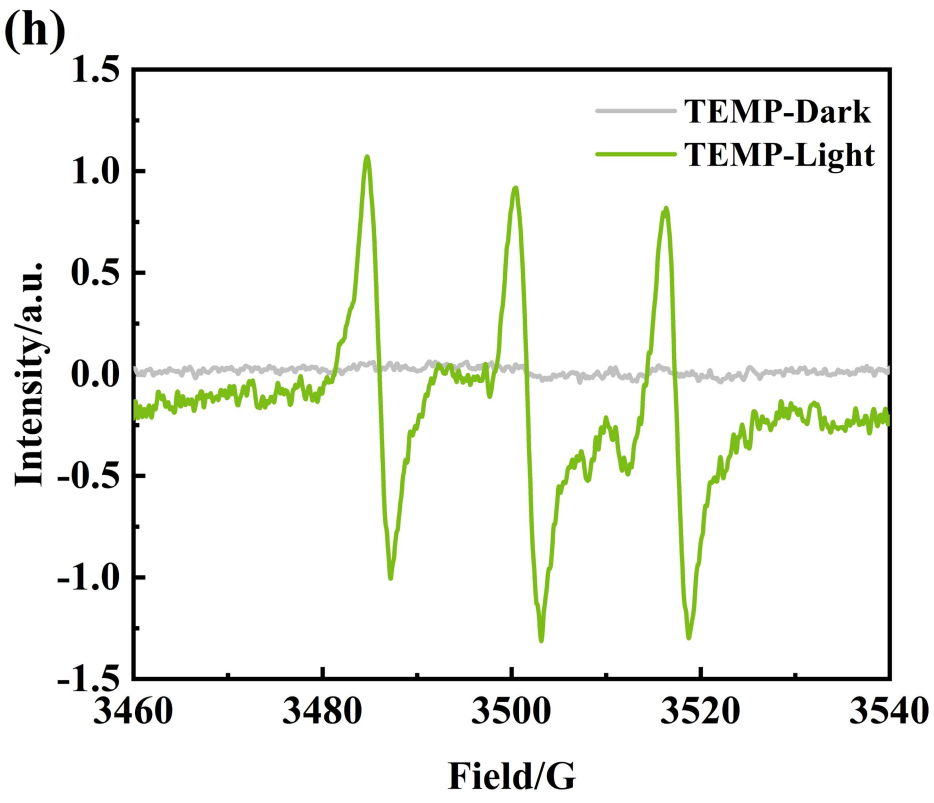


Figure 8. EPR experiments on reaction of 1a by adding TEMP

CV curve of the substrate 1a

Cyclic voltammetry (CV) was performed using an Epsilon electrochemical workstation (a BASi three-electrode cell system): glassy carbon electrode as the working electrode, Pt wire as the counter electrode, Ag/AgCl (KCl, 3 *M*) electrode as the reference electrode, and ferrocenium/ferrocene (Fc^{+}/Fc) as the internal standard. Scan rate: 100 mV s^{-1} (in the range -0.78 to +2.39 V). *n*Bu_4NPF_6 (0.1 M MeCN) was used as the supporting electrolyte.

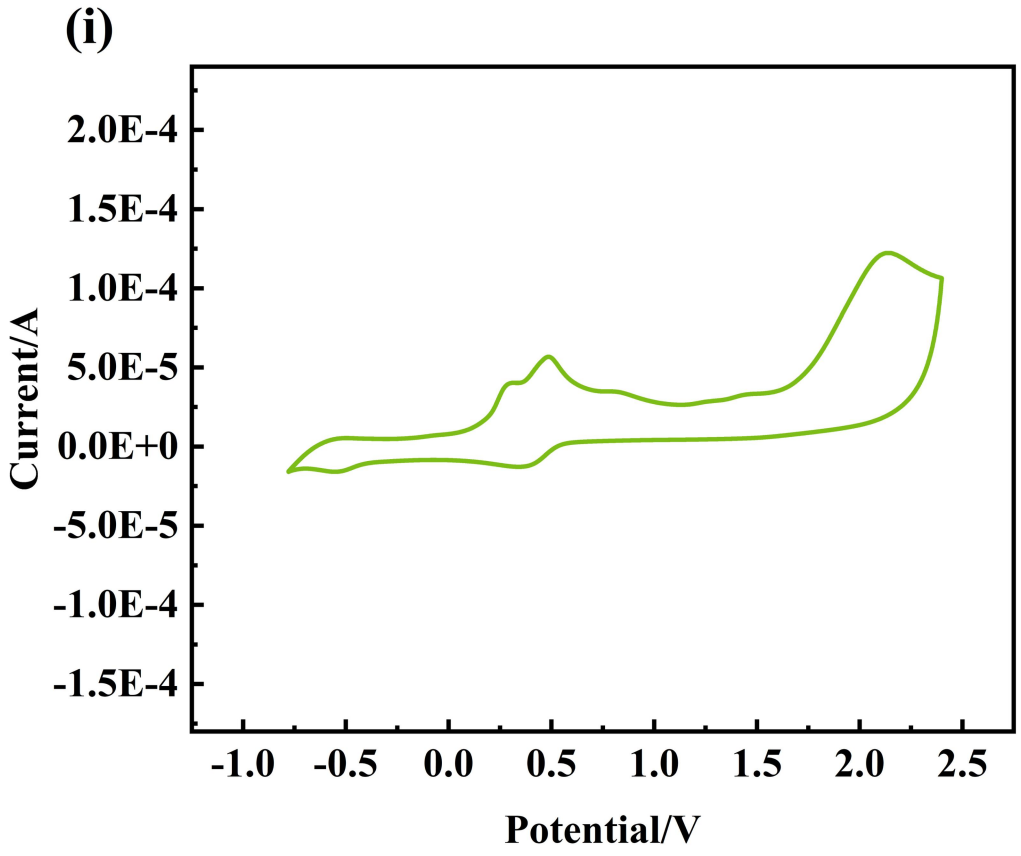
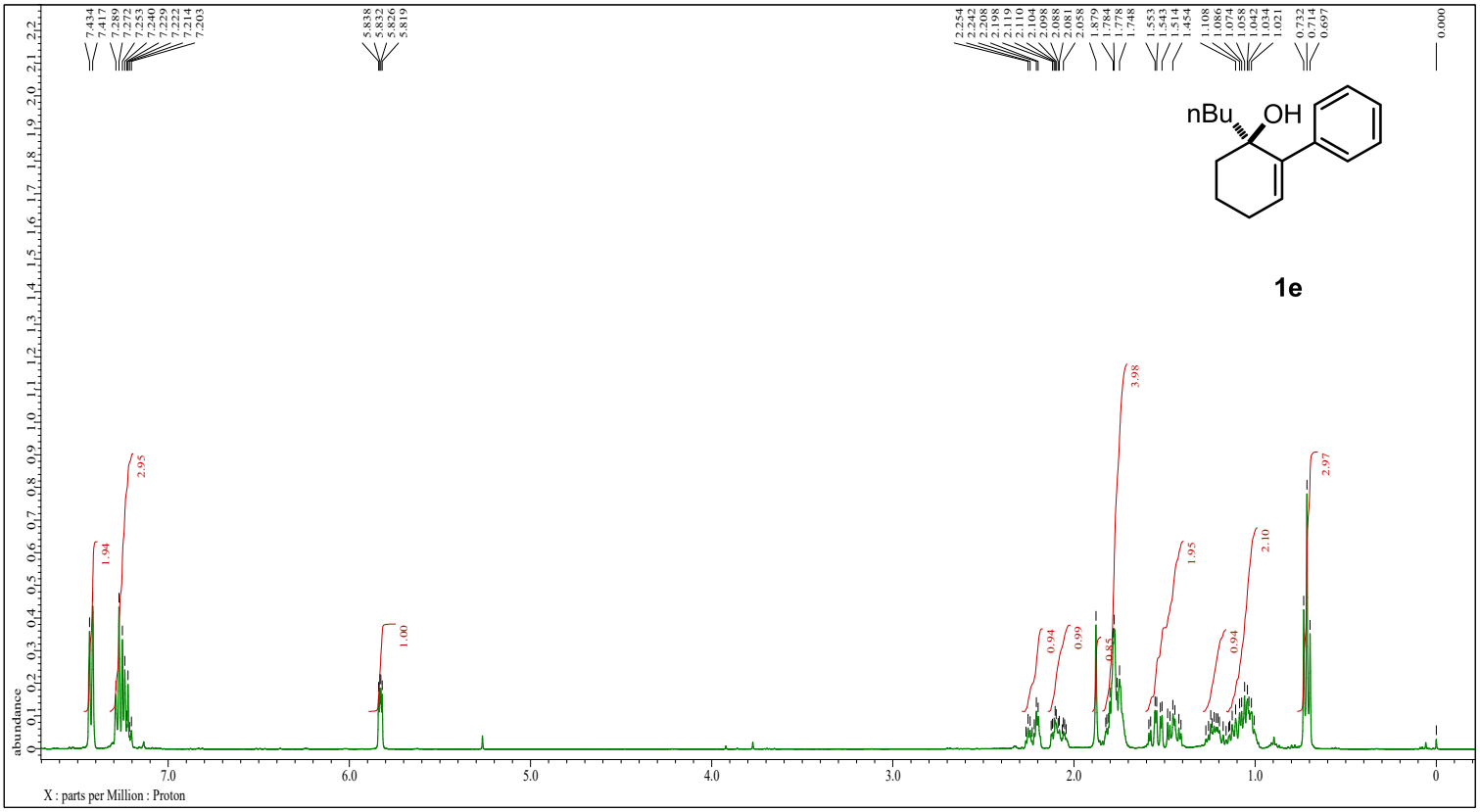
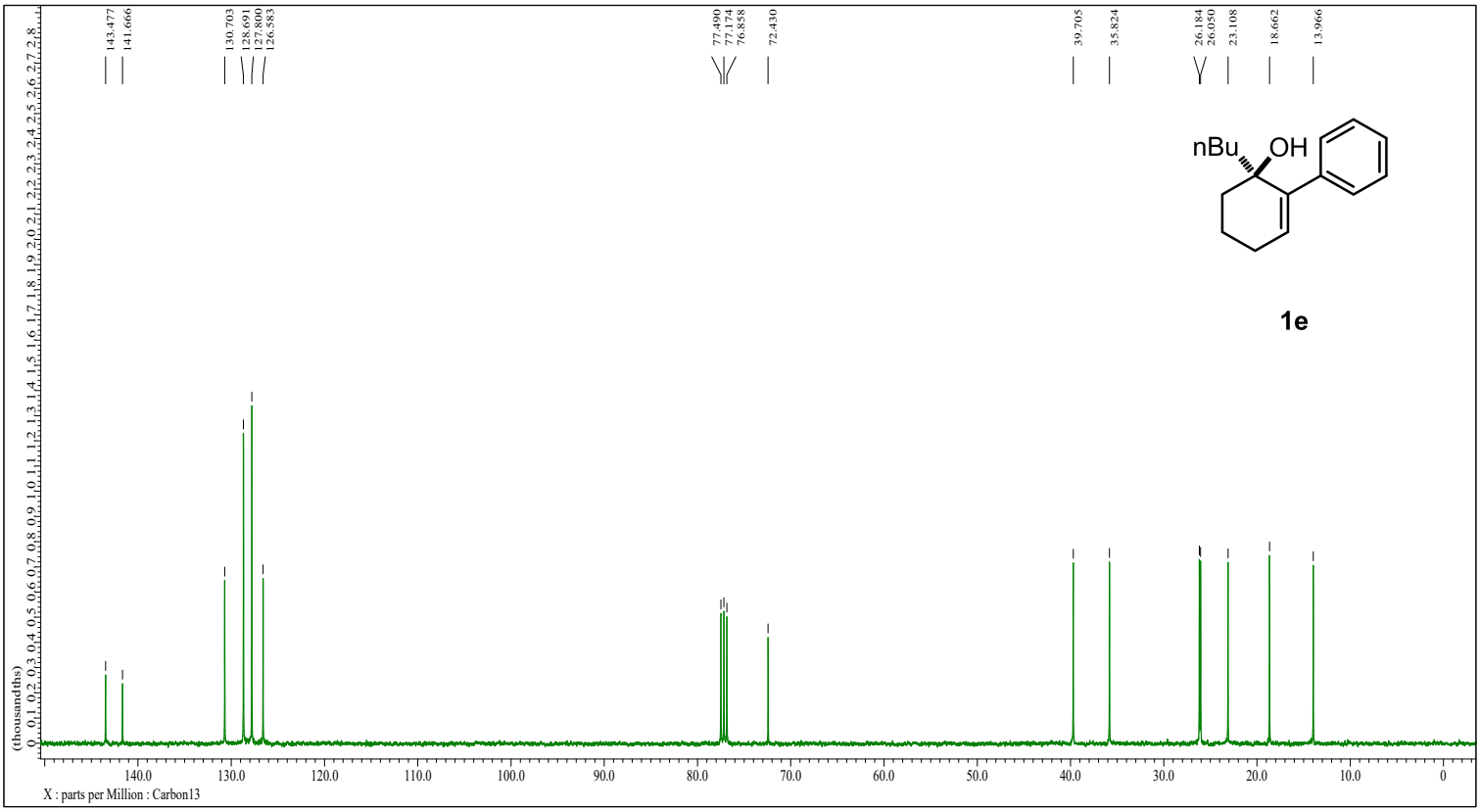
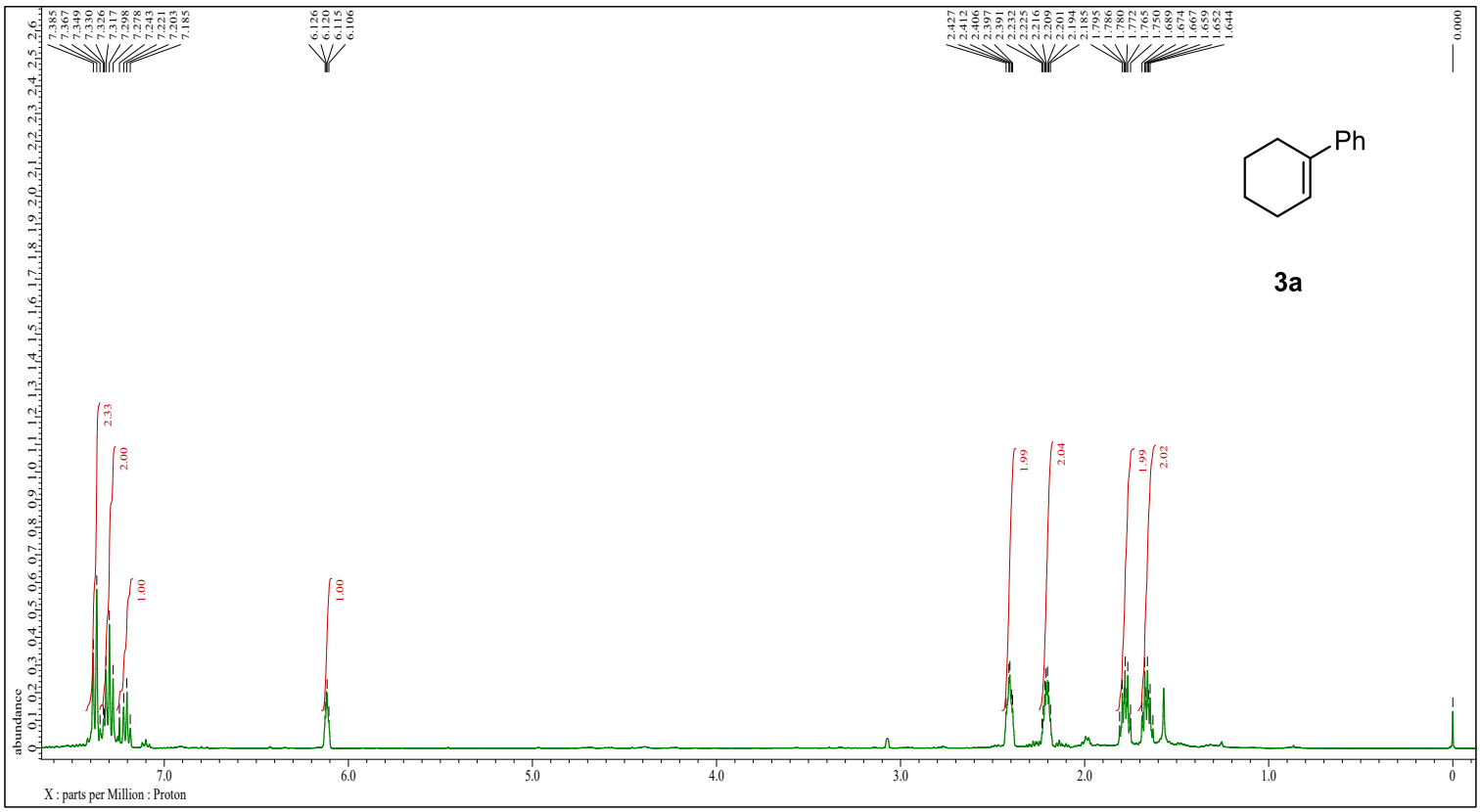


Figure 9. Cyclic voltammetry of the substrate 1a

Copies of ^{1}H NMR, ^{13}C NMR and ^{19}F NMR spectra



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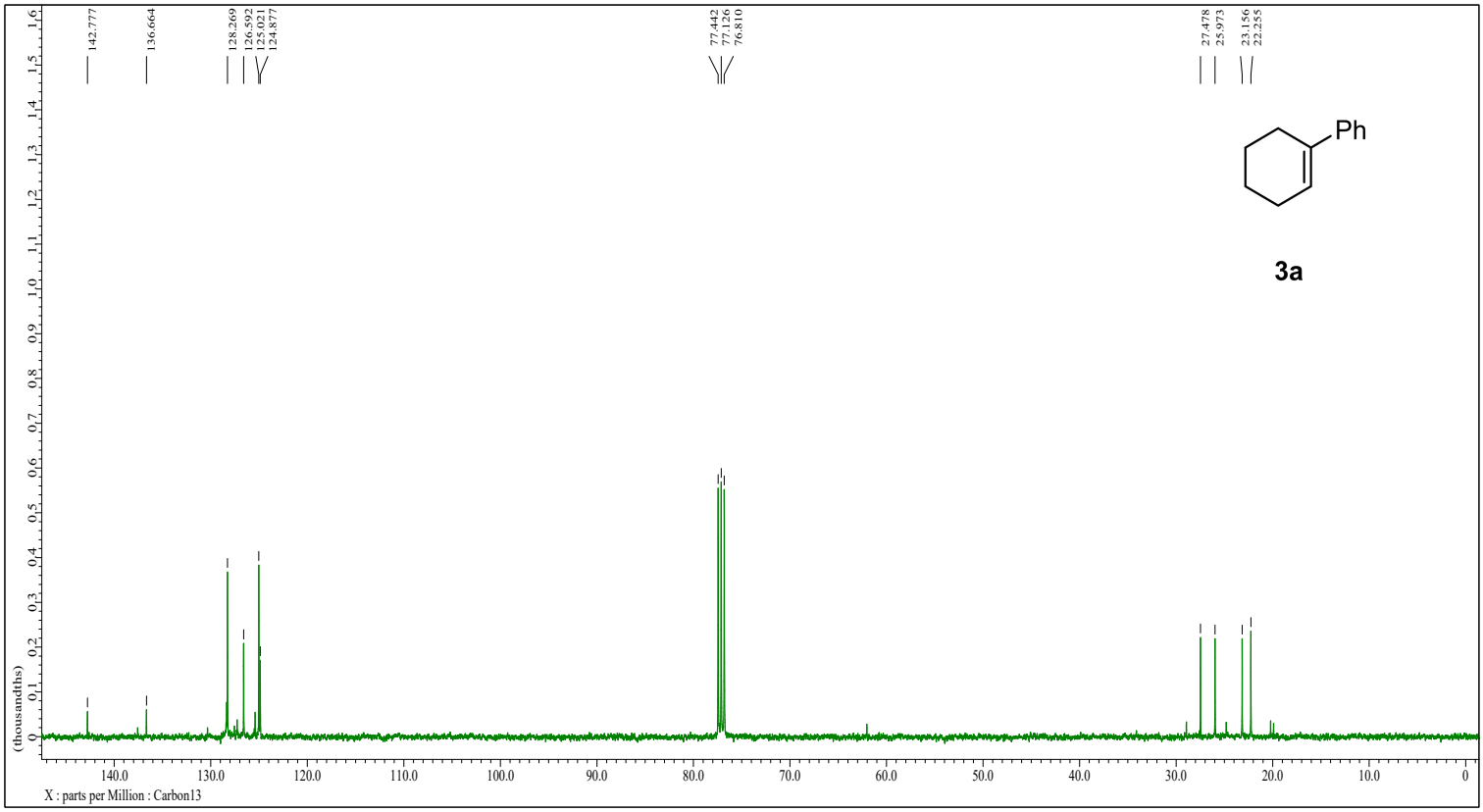
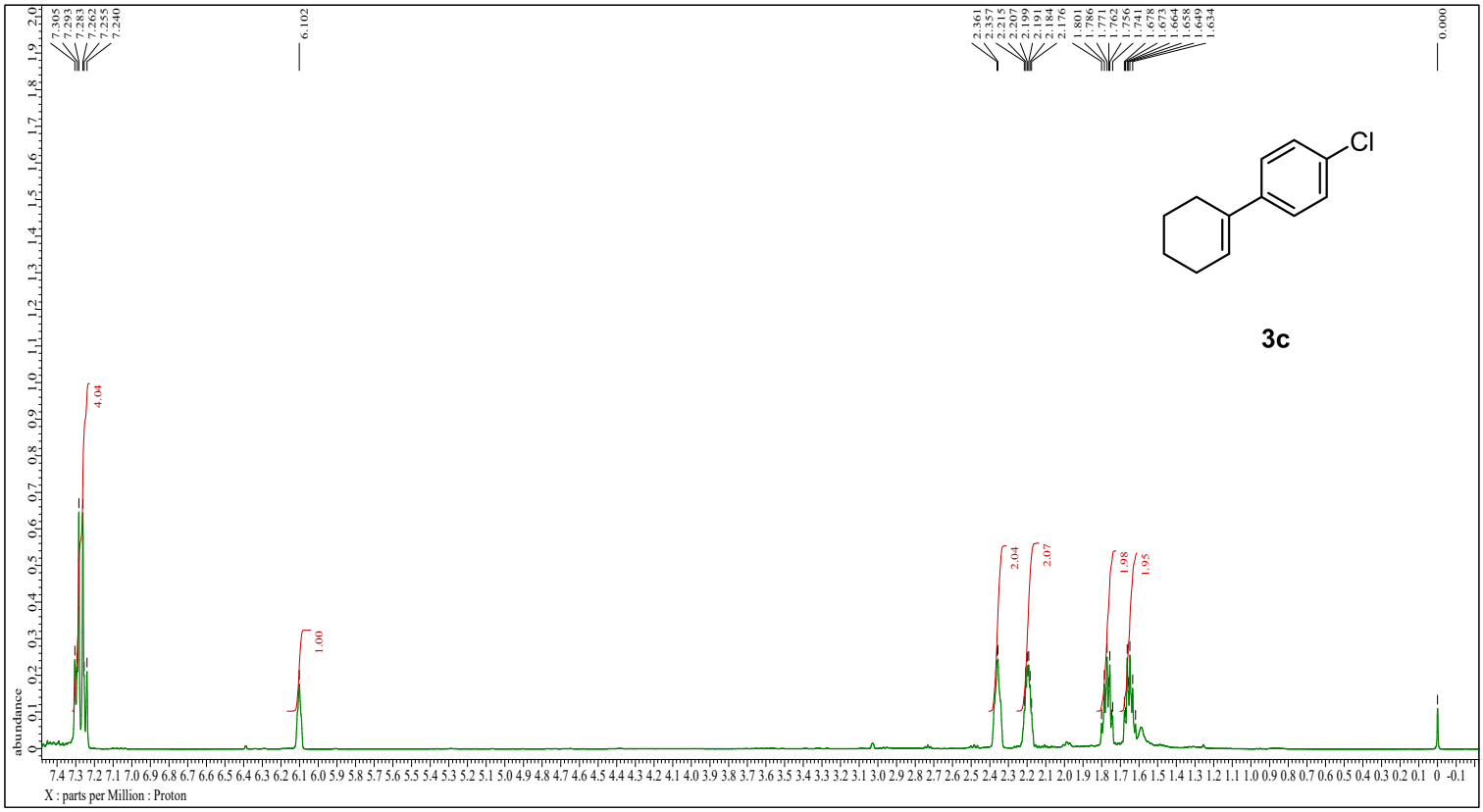
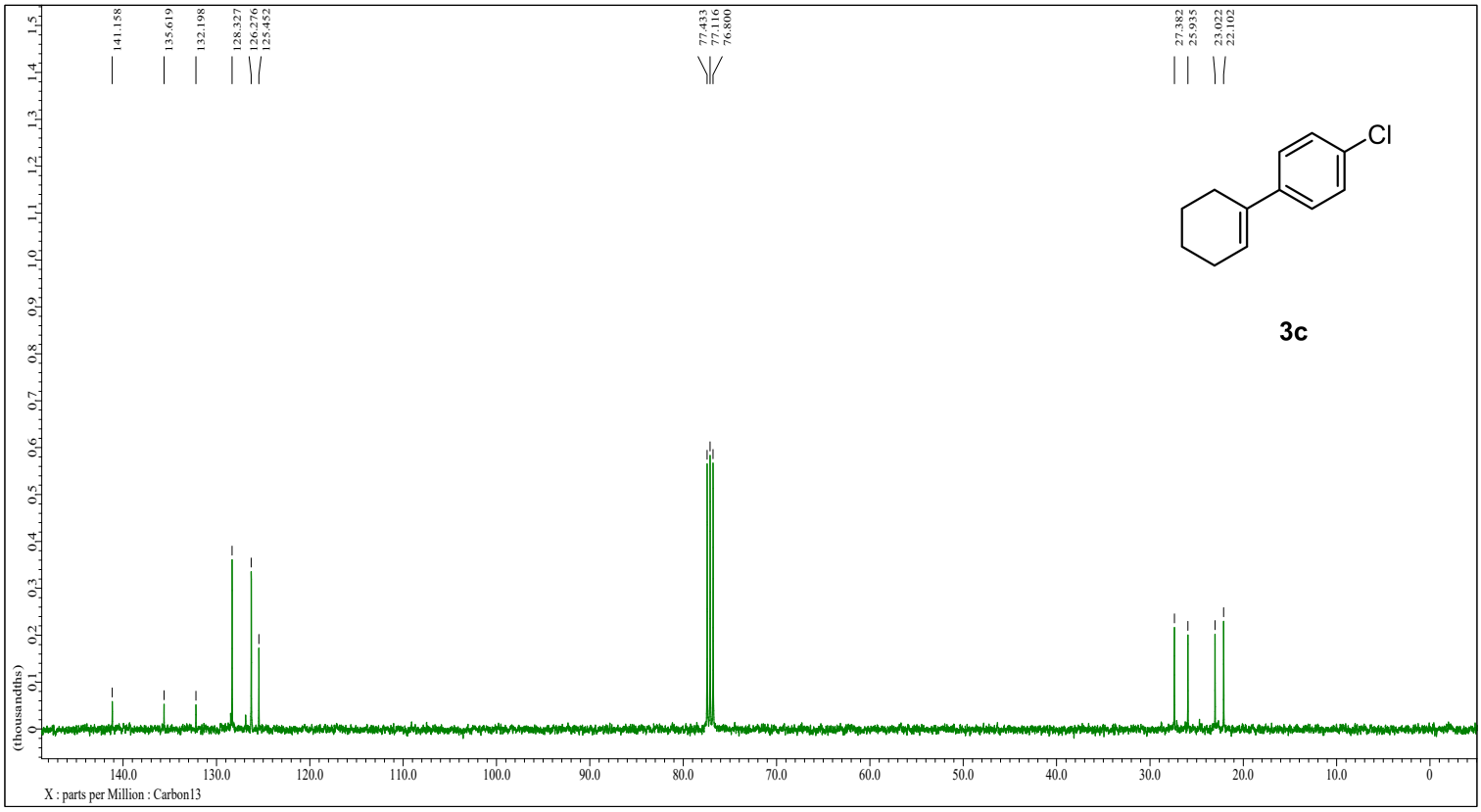
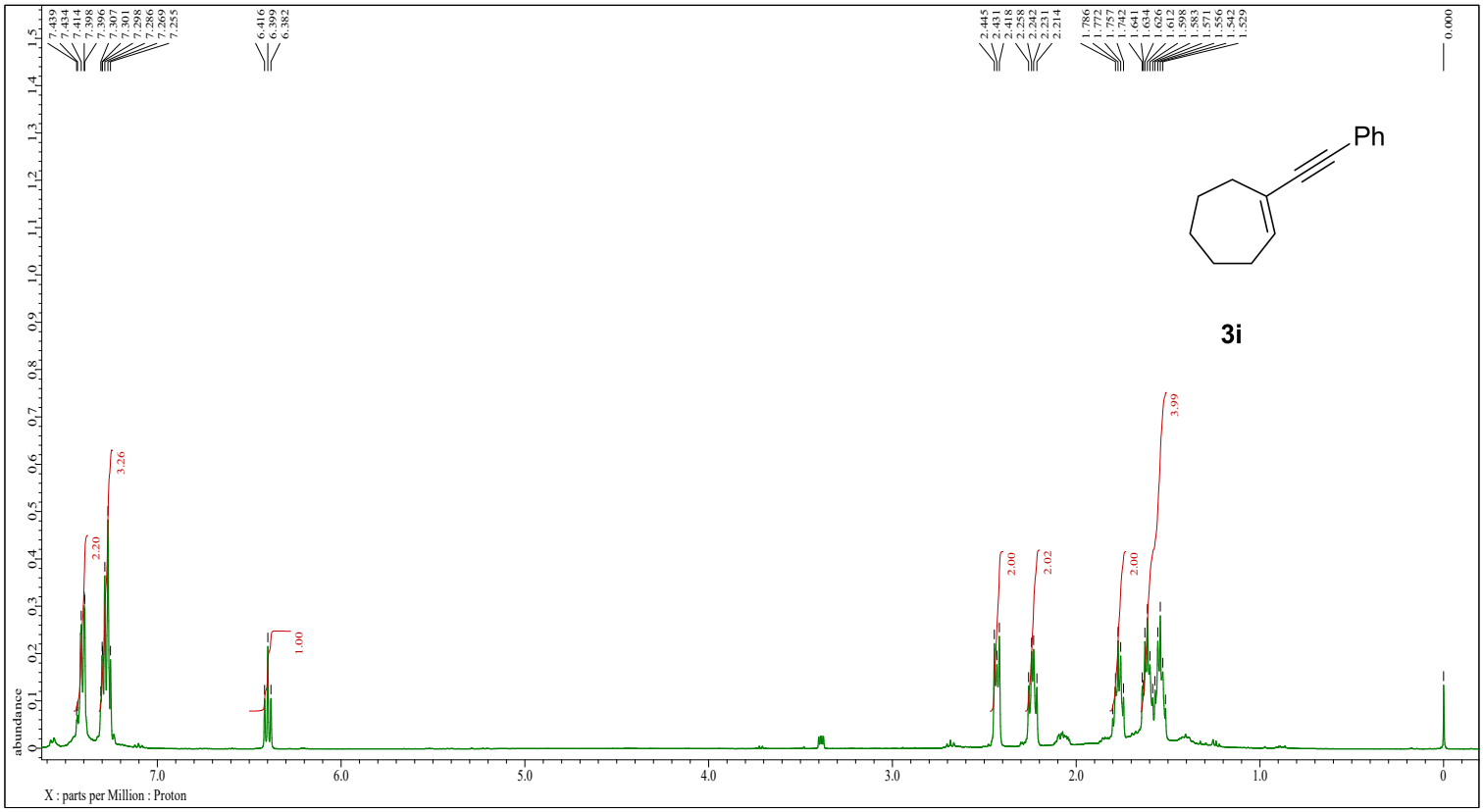
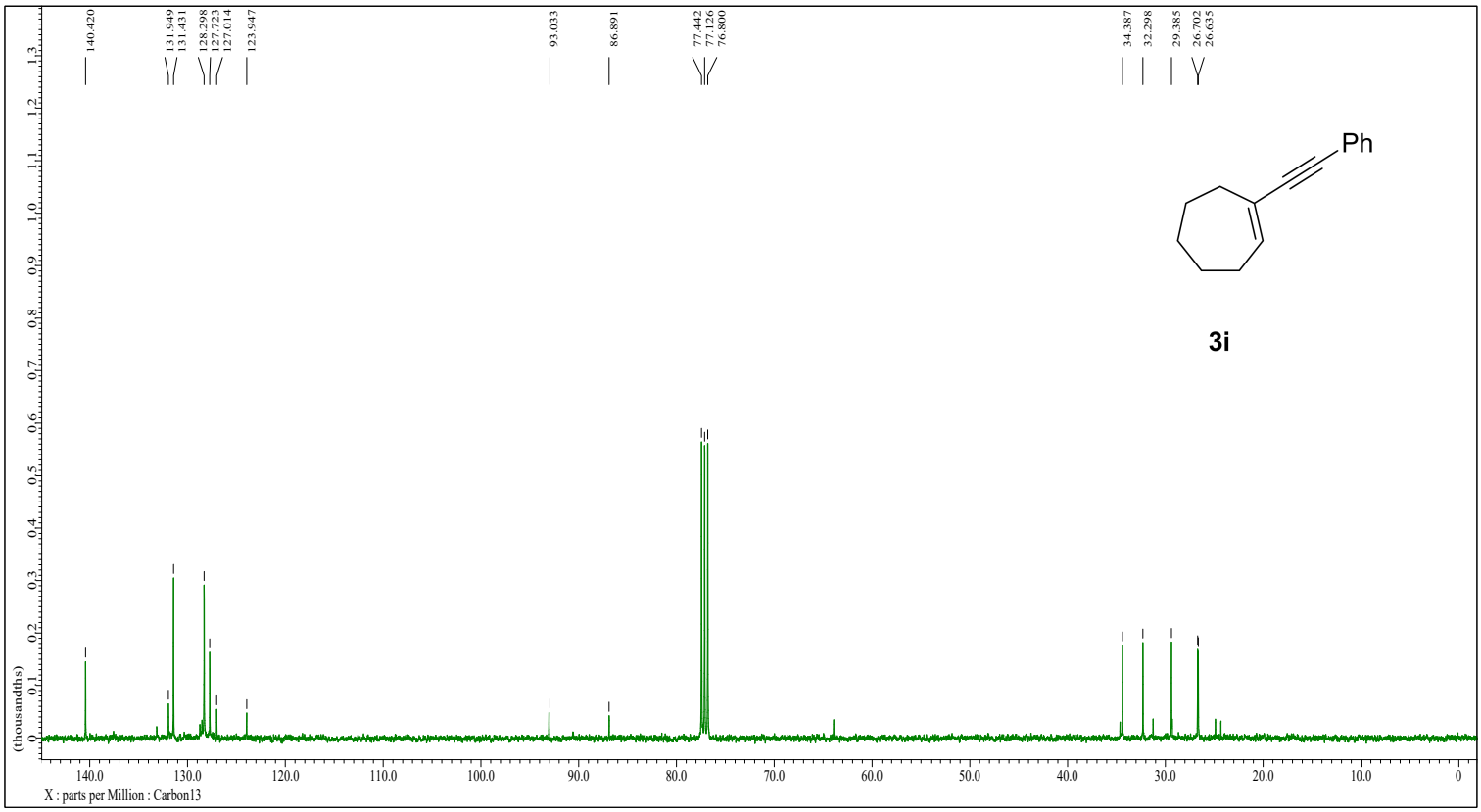
7.367
7.349
7.330
7.326
7.317
7.298
7.278
7.243
7.221
7.203
7.185
6.126
6.120
6.115
6.106
2.427
2.412
2.406
2.397
2.391
2.232
2.225
2.216
2.209
2.201
2.194
2.185
1.795
1.786
1.780
1.772
1.765
1.750
1.689
1.674
1.667
1.659
1.652
1.644
0.000
Ph
3a
2.33
2.00
1.00
1.00
1.99
2.04
1.99
2.02
abundance
X : parts per Million : Proton


142.777
136.664
128.269
126.592
125.021
124.877
77.442
77.126
76.810
27.478
25.973
23.156
22.255
Ph
3a
(thousandths)
X : parts per Million : Carbon13


7.305
7.293
7.283
7.262
7.255
7.240
6.102
2.361
2.357
2.215
2.207
2.199
2.191
2.184
2.176
1.801
1.786
1.771
1.762
1.756
1.741
1.678
1.673
1.664
1.658
1.649
1.634
0.000
Cl
3c
4.04
1.00
2.04
2.07
1.98
1.95
abundance
X : parts per Million : Proton


141.158
135.619
132.198
128.327
126.276
125.452
77.433
77.116
76.800
27.382
25.935
23.022
22.102
Cl
3c
(thousandths)
X : parts per Million : Carbon13


7.439
7.434
7.414
7.398
7.396
7.307
7.301
7.298
7.286
7.269
7.255
6.416
6.399
6.382
2.445
2.431
2.418
2.258
2.242
2.231
2.214
1.786
1.772
1.757
1.742
1.641
1.634
1.626
1.613
1.598
1.583
1.571
1.556
1.542
1.529
0.000
Ph
3i
3.26
2.20
1.00
2.00
2.02
2.00
3.99
abundance
X : parts per Million : Proton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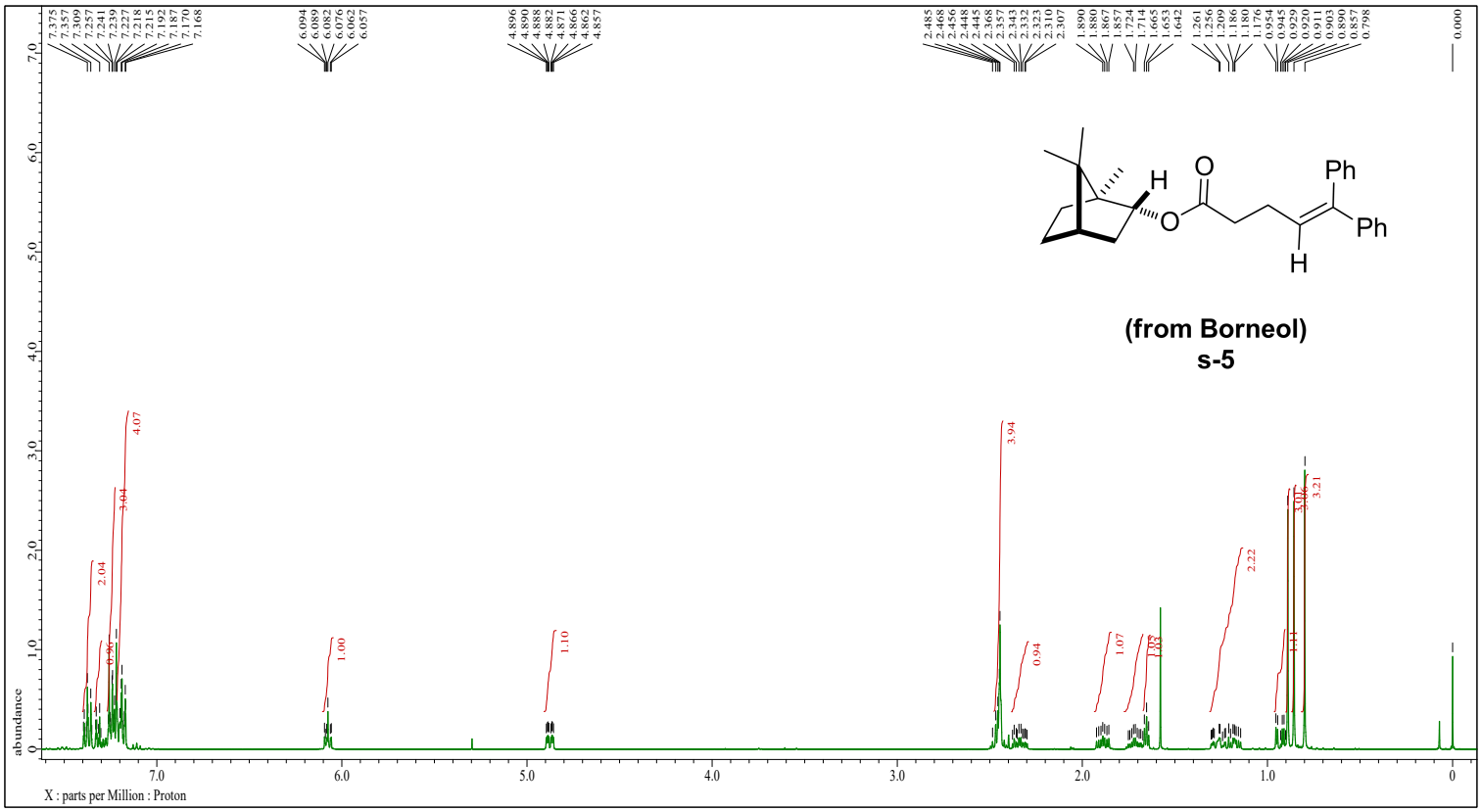
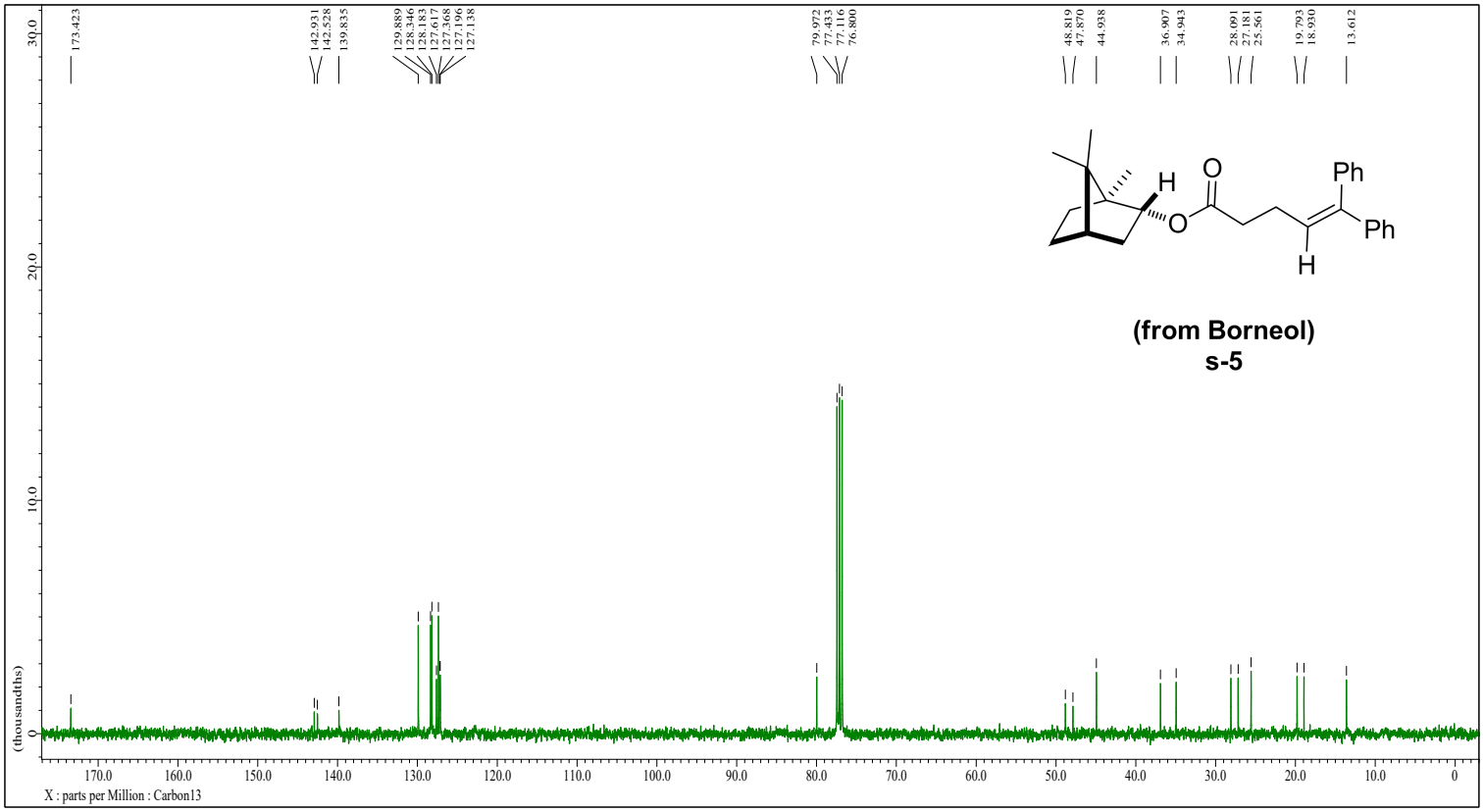
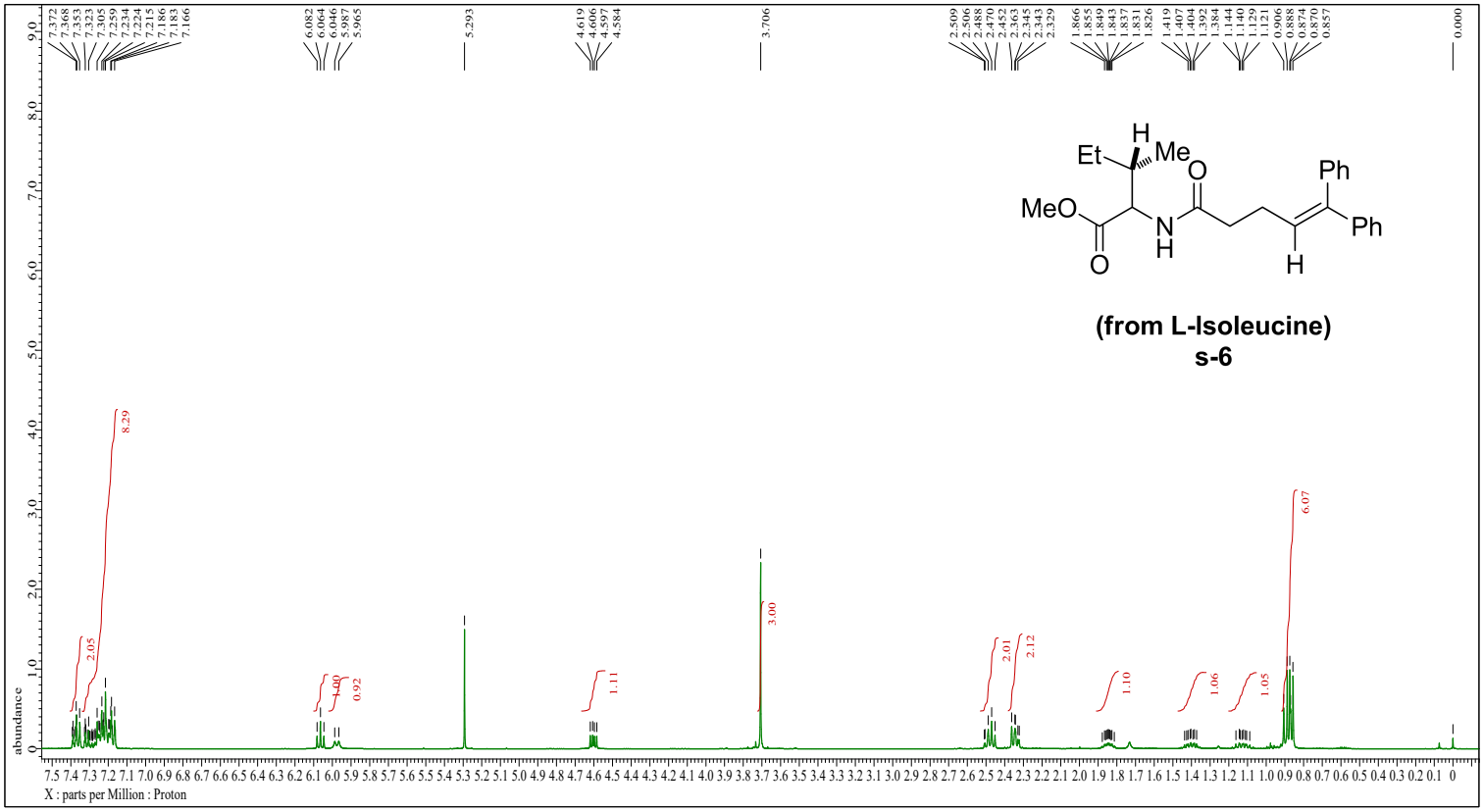
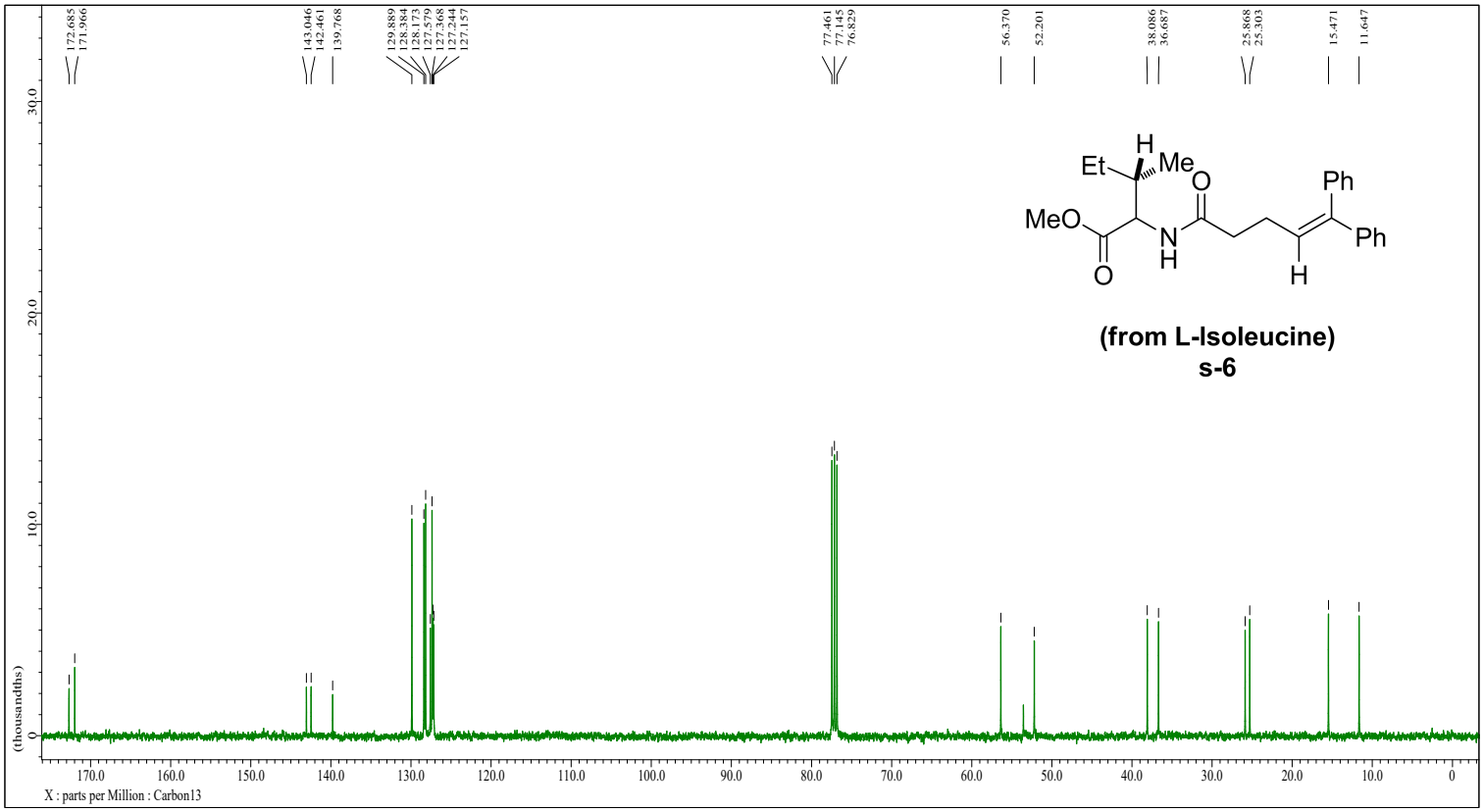
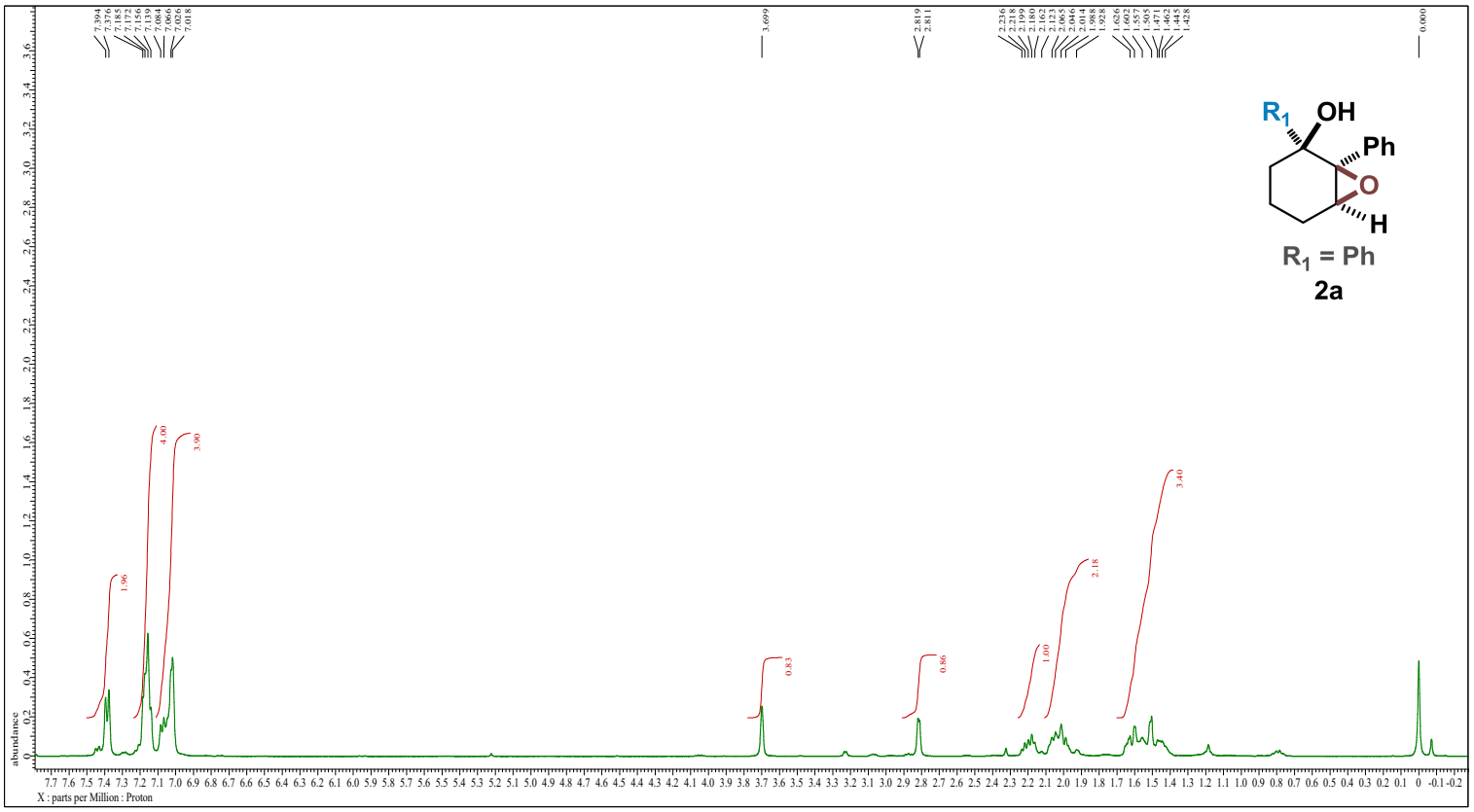
131.949
131.431
128.298
127.723
127.014
123.947
93.033
86.891
77.442
77.126
76.800
34.387
32.298
29.385
26.702
26.635
Ph
3i
(thousandths)
X : parts per Million : Carbon13

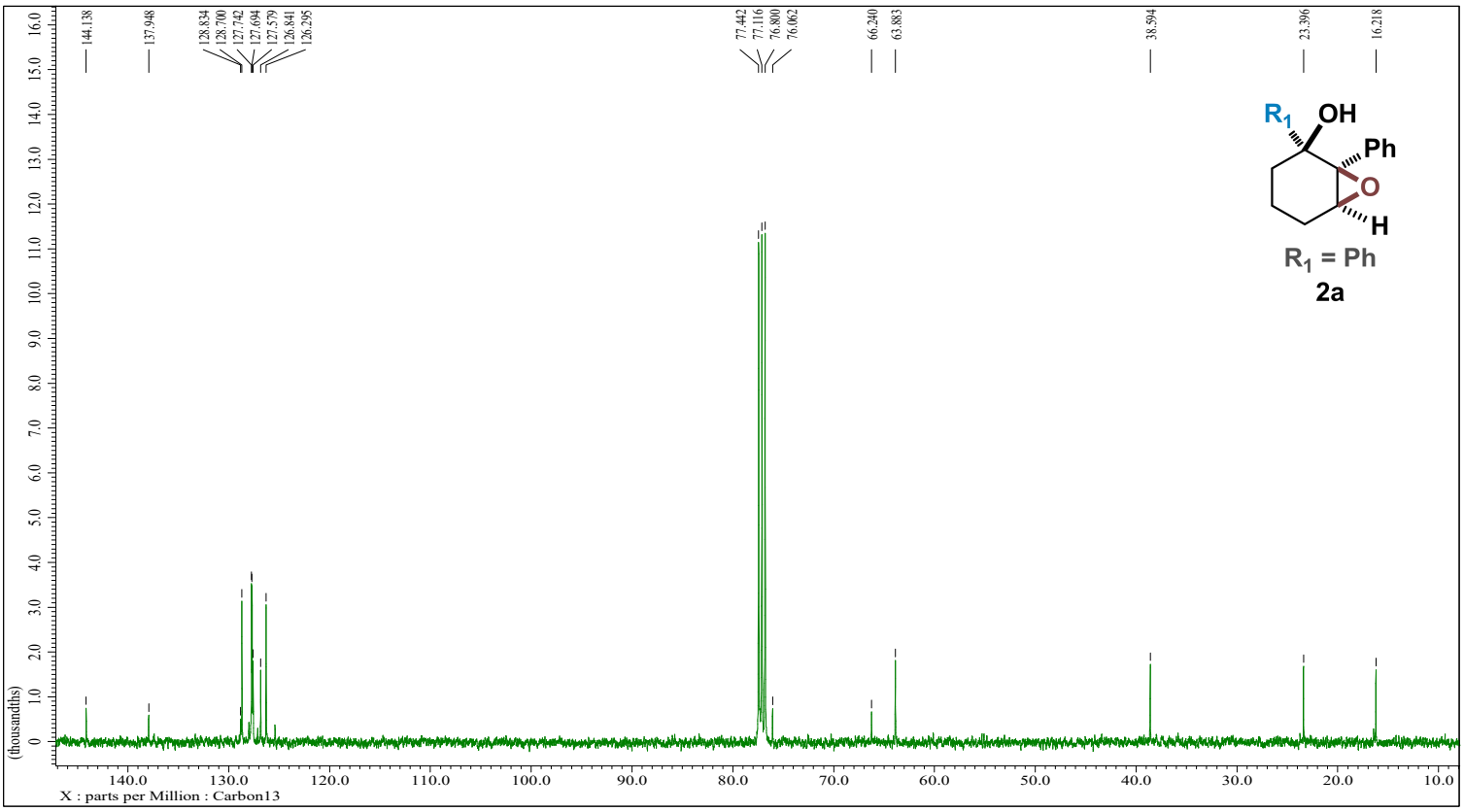

(from Borneol)
s-5
abundance
X : parts per Million : Proton

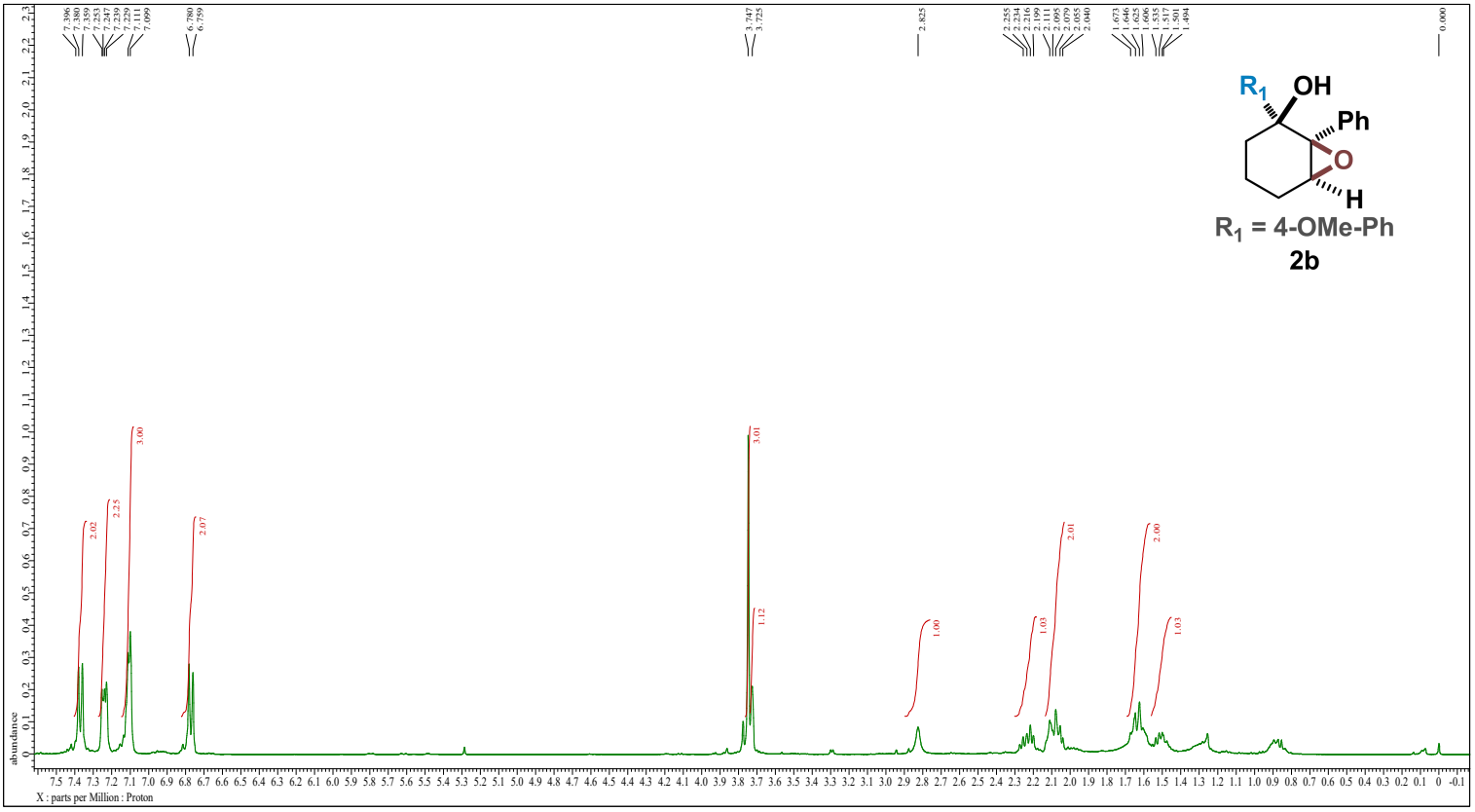

(from Borneol)
s-5
(thousandths)
X : parts per Million : Carbon13

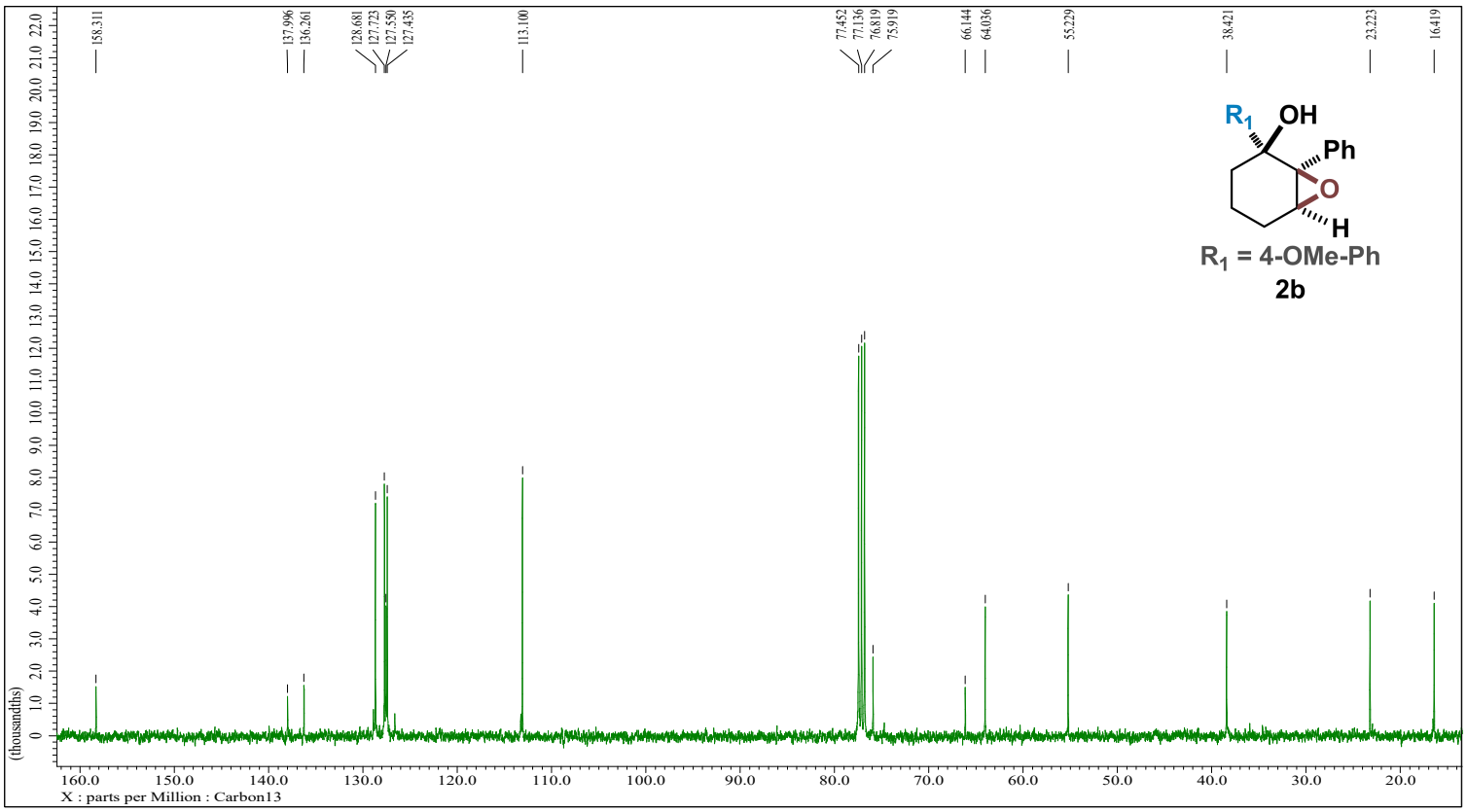

abundance
X : parts per Million : Proton
(from L-Isoleucine)
s-6

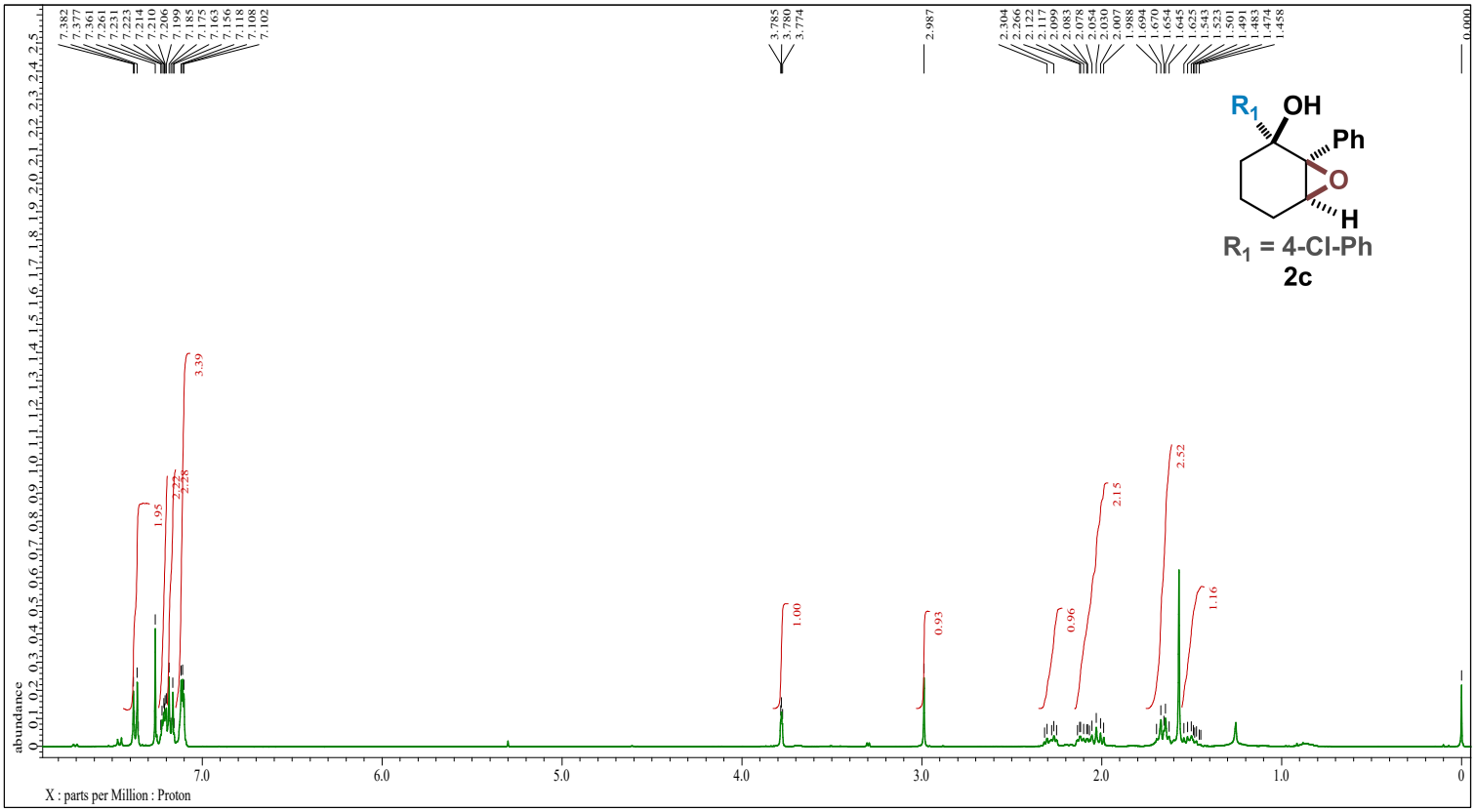

(thousandths)
X : parts per Million : Carbon13
(from L-Isoleucine)
s-6


R1 OH
Ph
O
H
R1 = Ph
2a
abundance
X : parts per Million : Proton


R1 OH
Ph
O
H
R1 = Ph
2a
(thousandths)
X : parts per Million : Carbon13


R1 OH
Ph
O
H
R1 = 4-OMe-Ph
2b
X : parts per Million : Proton


R1 OH
Ph
O
H
R1 = 4-OMe-Ph
2b
X : parts per Million : Carbon13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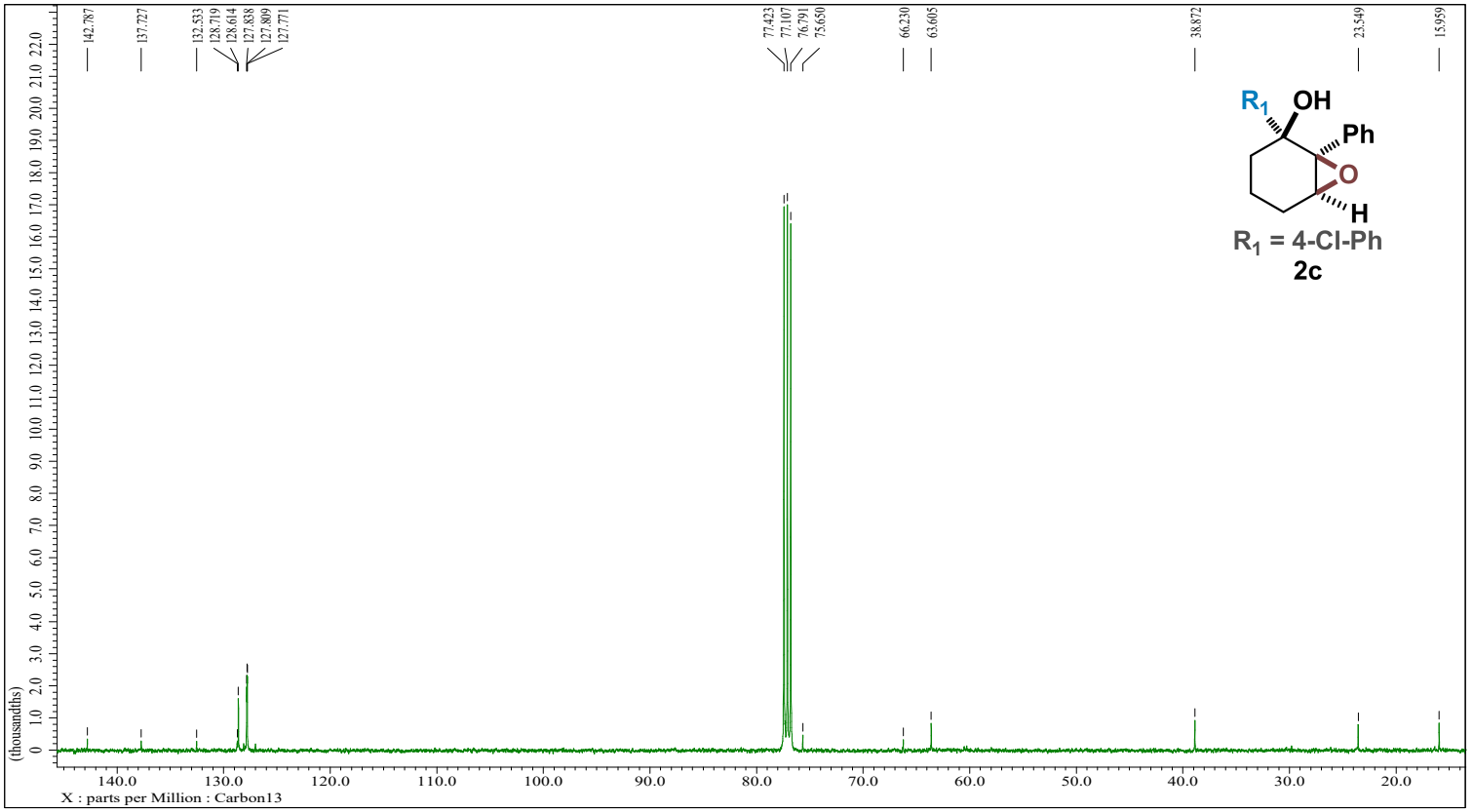
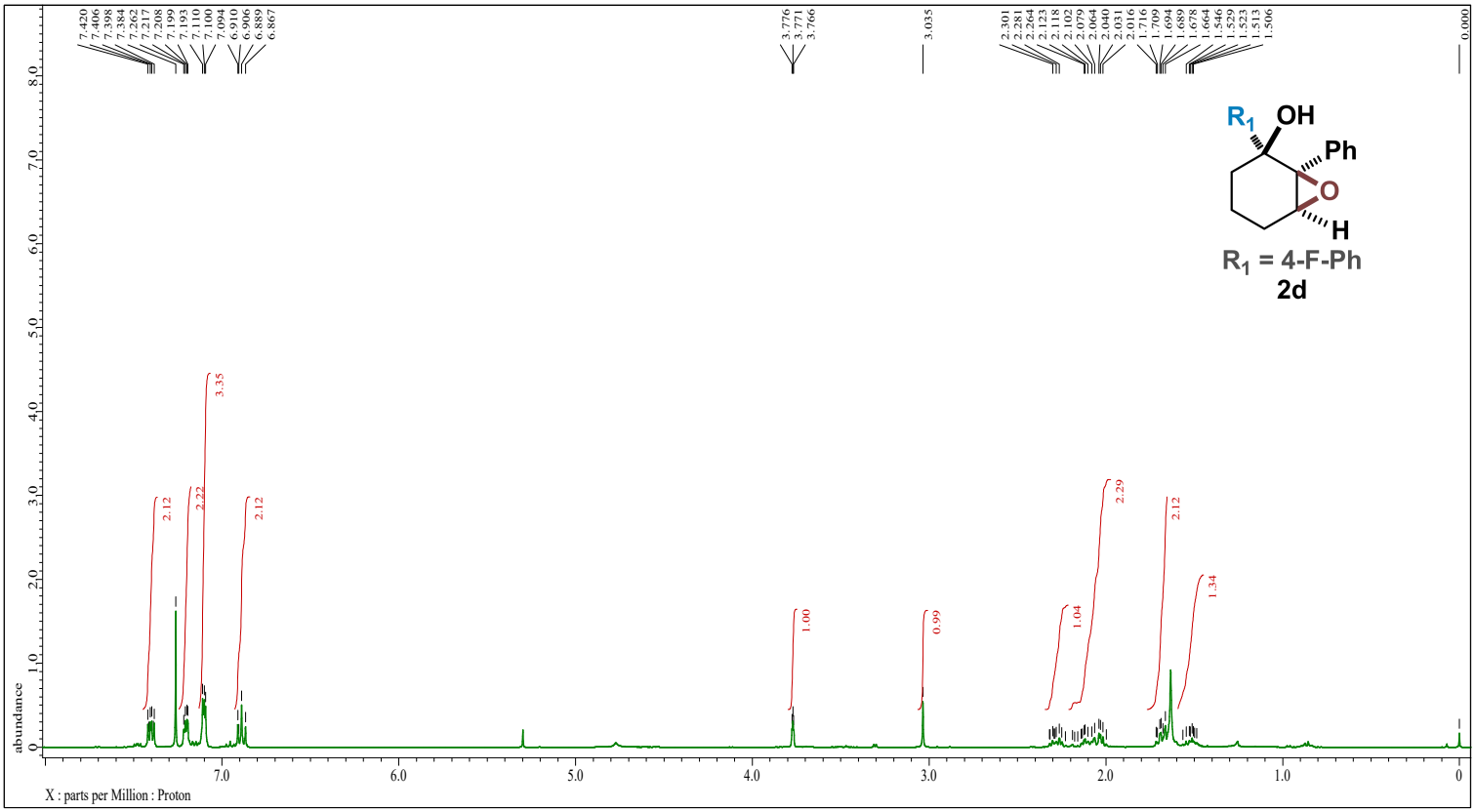
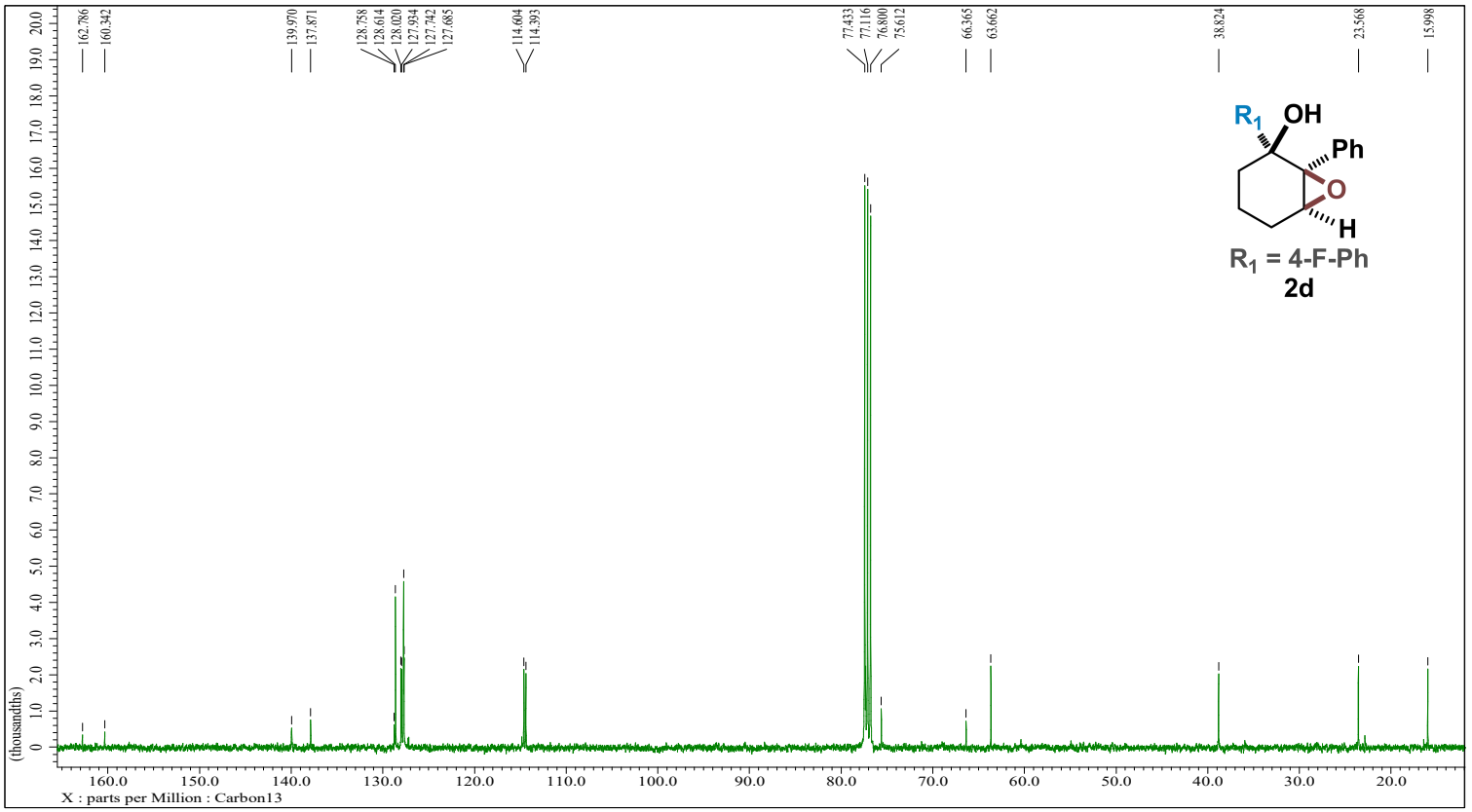
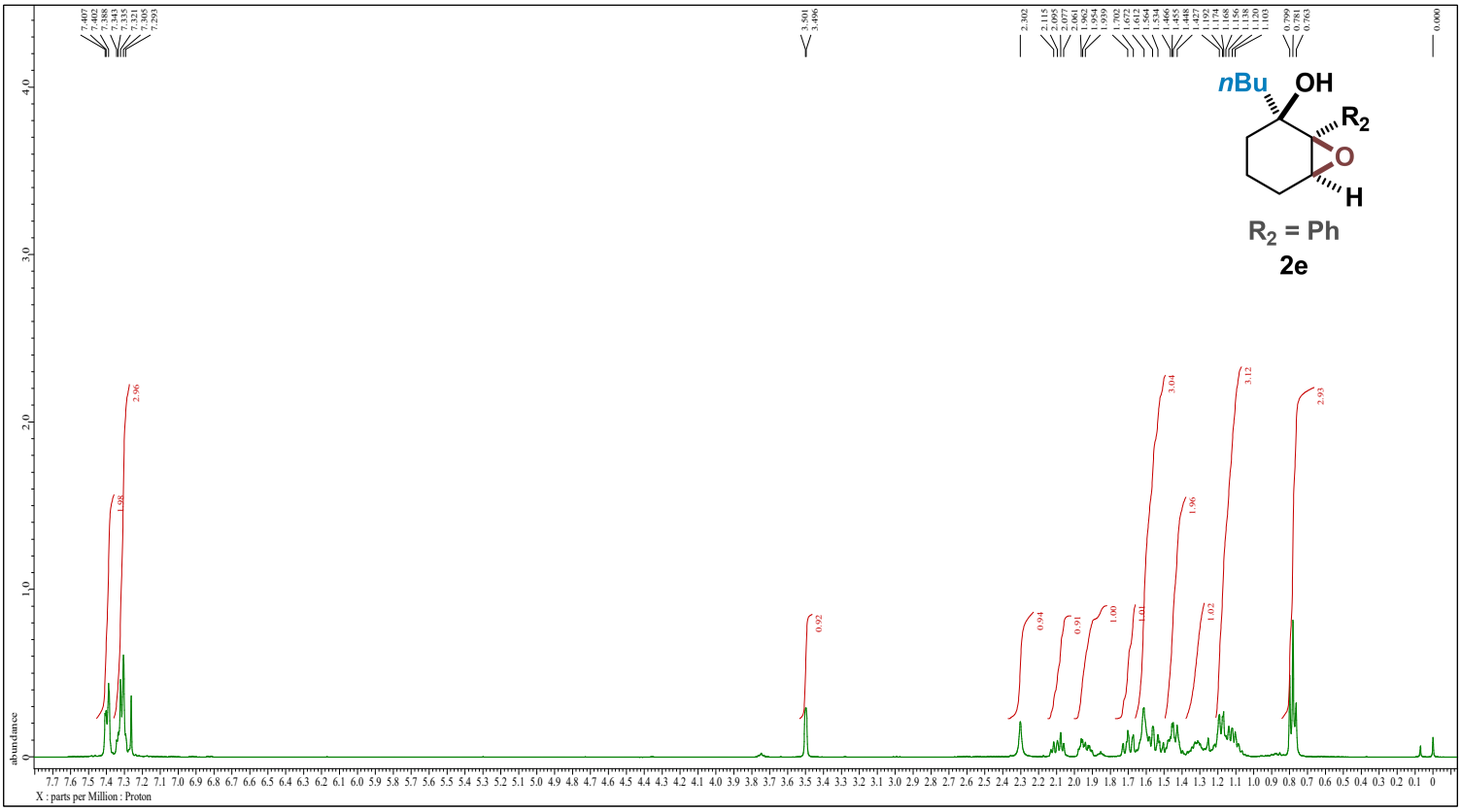
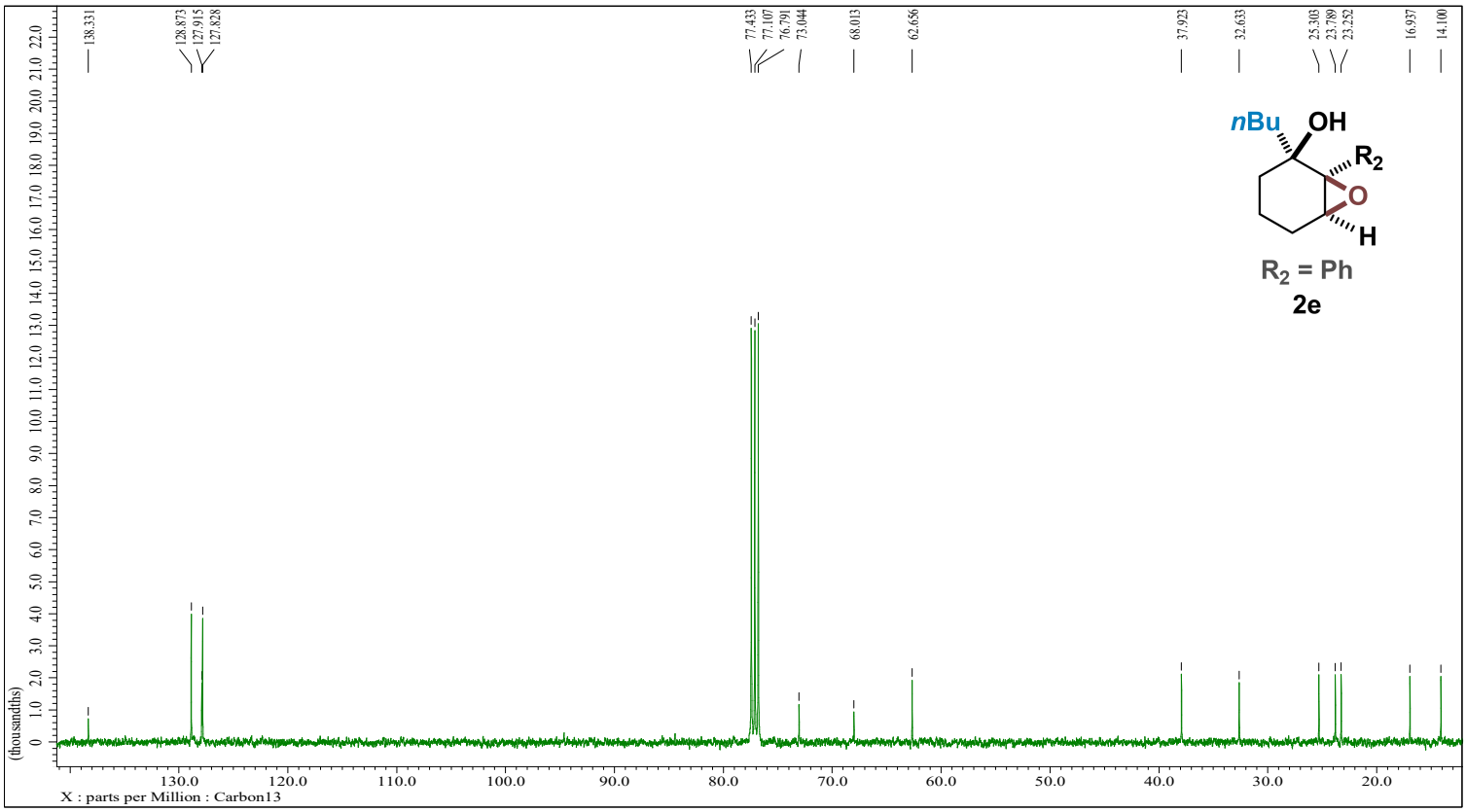
7.377
7.361
7.261
7.231
7.223
7.214
7.210
7.206
7.199
7.185
7.175
7.163
7.156
7.118
7.108
7.102
3.785
3.780
3.774
2.987
2.304
2.266
2.122
2.117
2.099
2.088
2.078
2.054
2.030
2.007
1.988
1.694
1.670
1.654
1.645
1.625
1.543
1.523
1.501
1.491
1.483
1.474
1.458
0.000
R1
OH
Ph
O
H
R1 = 4-Cl-Ph
2c
3.39
2.77
2.28
1.95
1.00
0.93
0.96
2.15
2.52
1.16
abundance
X : parts per Million : Proton

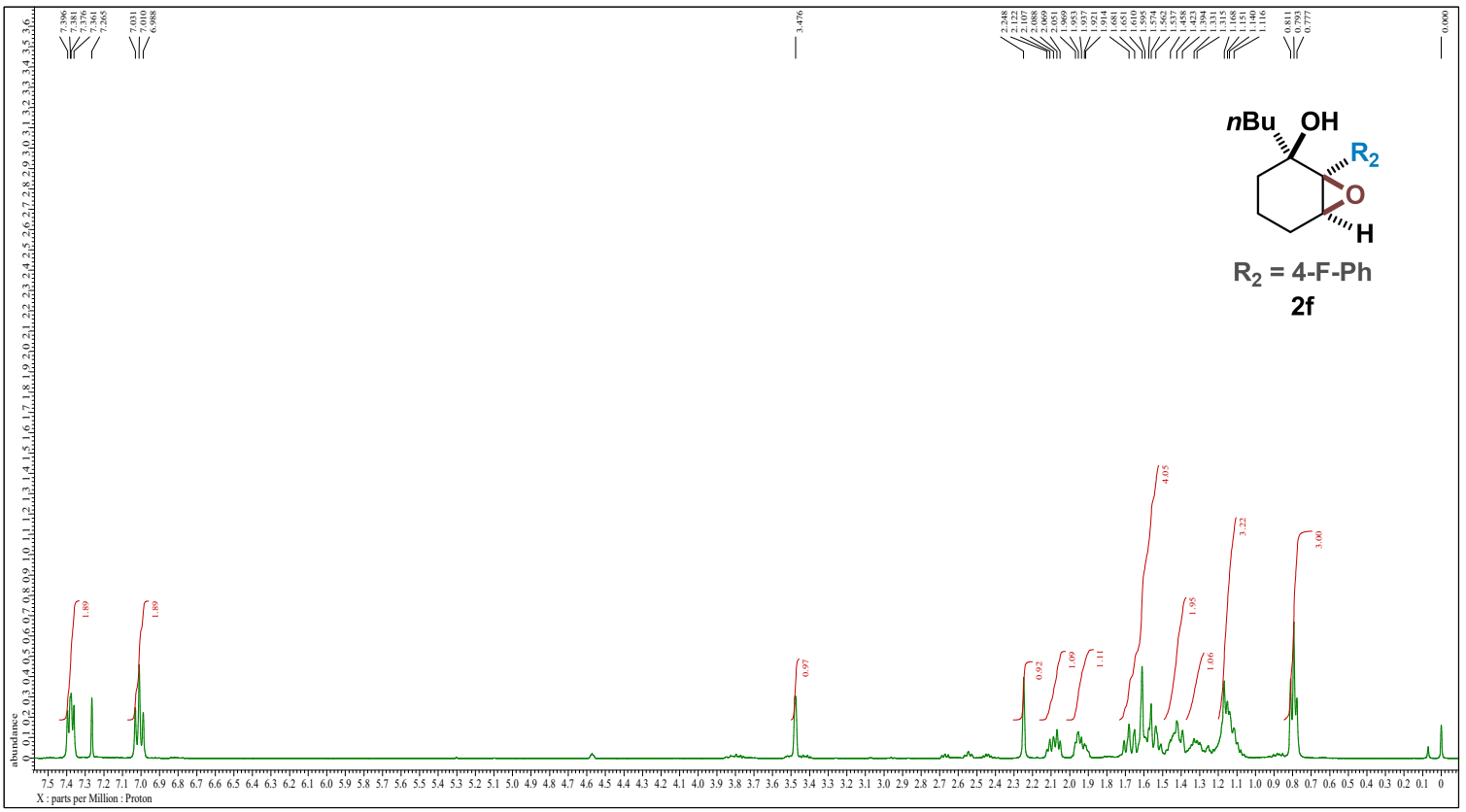

142.787
137.727
132.533
128.719
128.614
127.838
127.809
127.771
77.423
77.107
76.791
75.650
66.230
63.605
38.872
23.549
15.959
R1
OH
Ph
O
H
R1 = 4-Cl-Ph
2c
(thousandths)
X : parts per Million : Carbon13

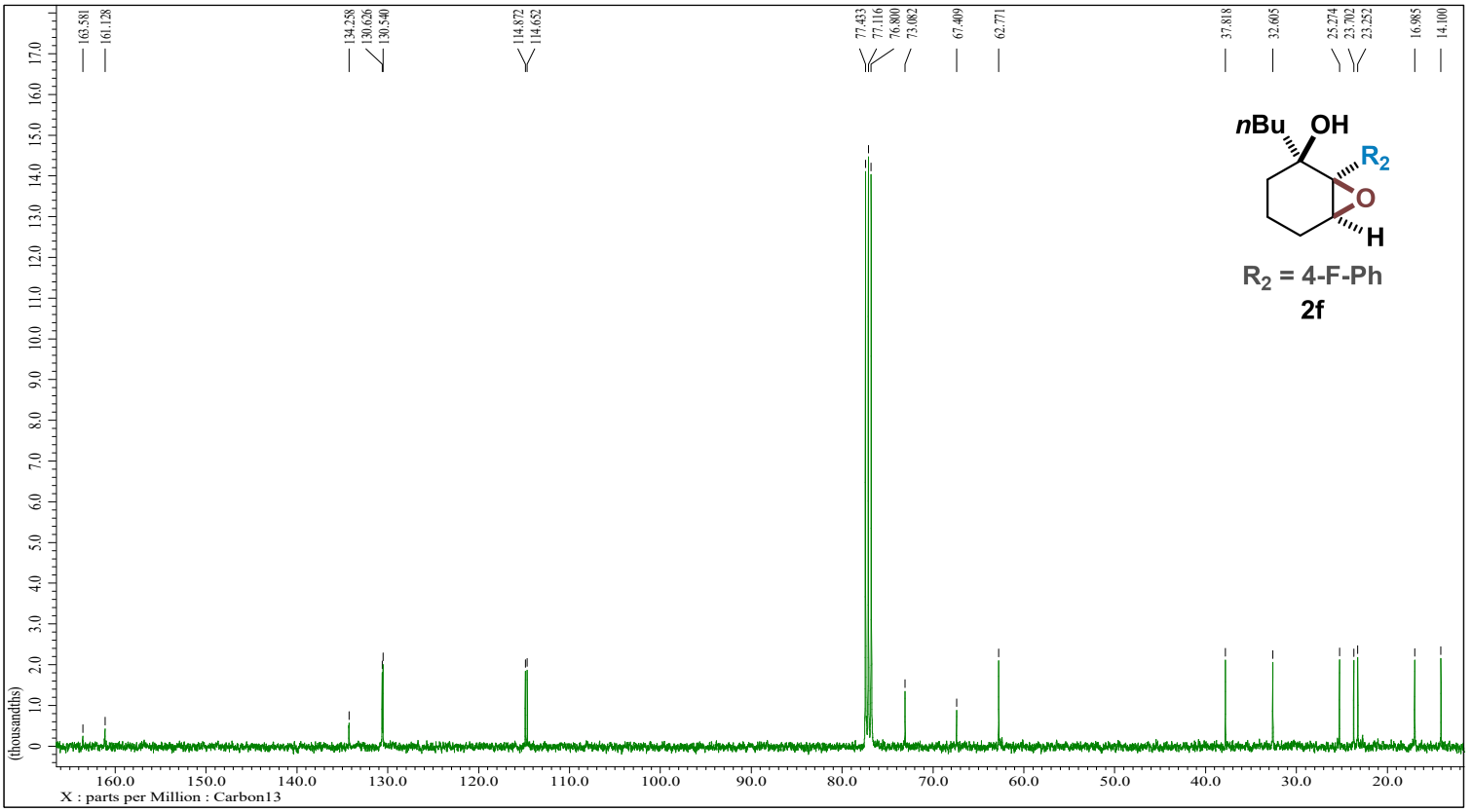

7.420
7.406
7.398
7.384
7.262
7.217
7.208
7.199
7.193
7.110
7.100
7.094
6.910
6.906
6.889
6.867
3.776
3.771
3.766
3.035
2.301
2.281
2.264
2.123
2.118
2.102
2.079
2.064
2.040
2.031
2.016
1.716
1.709
1.694
1.680
1.678
1.664
1.546
1.529
1.523
1.513
1.506
0.000
R1 OH
Ph
O
H
R1 = 4-F-Ph
2d
2.12
2.22
3.35
2.12
1.00
0.99
1.04
2.29
2.12
1.34
abundance
X : parts per Million : Proton

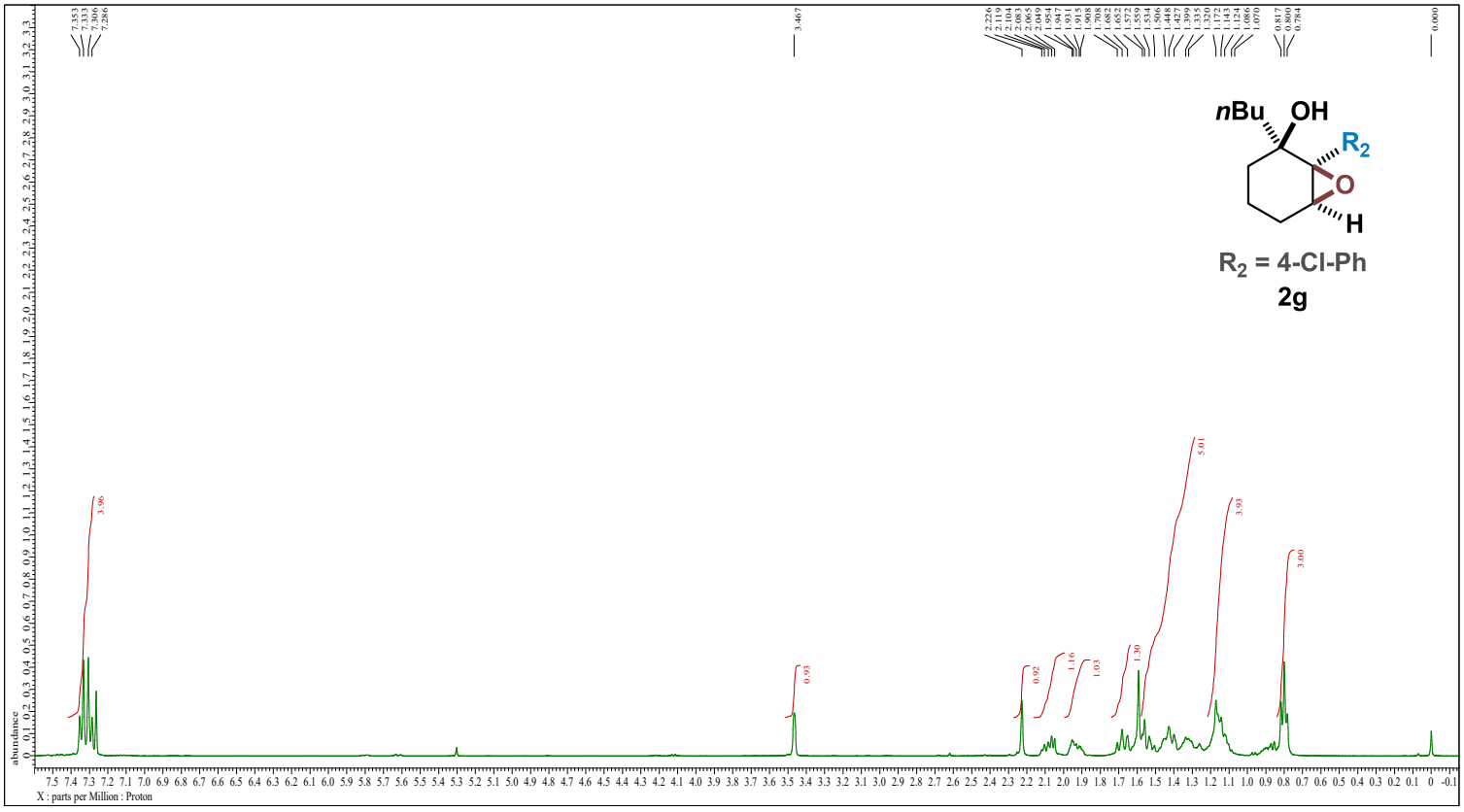

162.786
160.342
139.970
137.871
128.758
128.614
128.020
127.934
127.742
127.685
114.604
114.393
77.433
77.116
76.800
75.612
66.365
63.662
38.824
23.568
15.998
R1 OH
Ph
O
H
R1 = 4-F-Ph
2d
(thousandths)
X : parts per Million : Carbon13

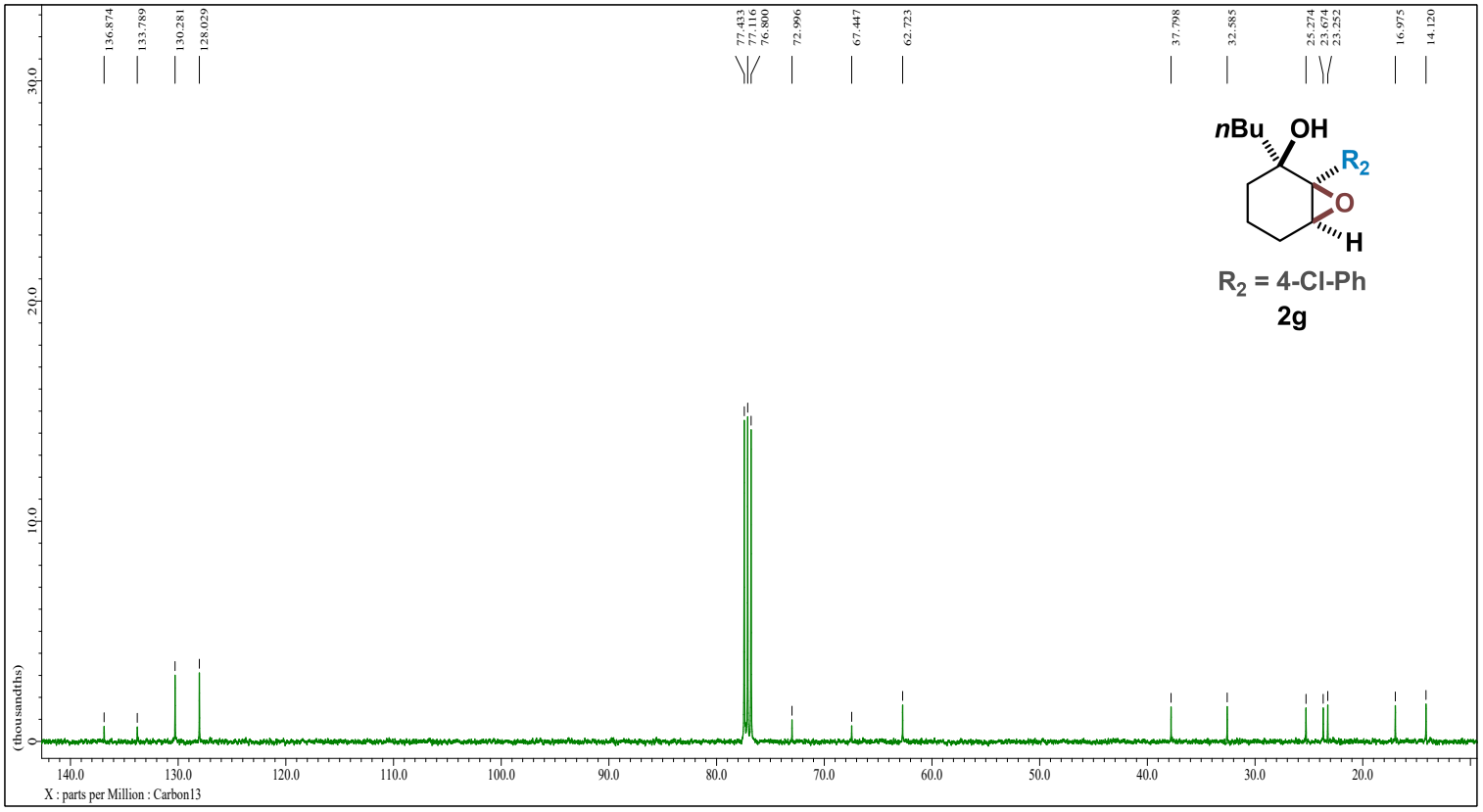

nBu
OH
R2
O
H
R2 = Ph
2e
X : parts per Million : Proton

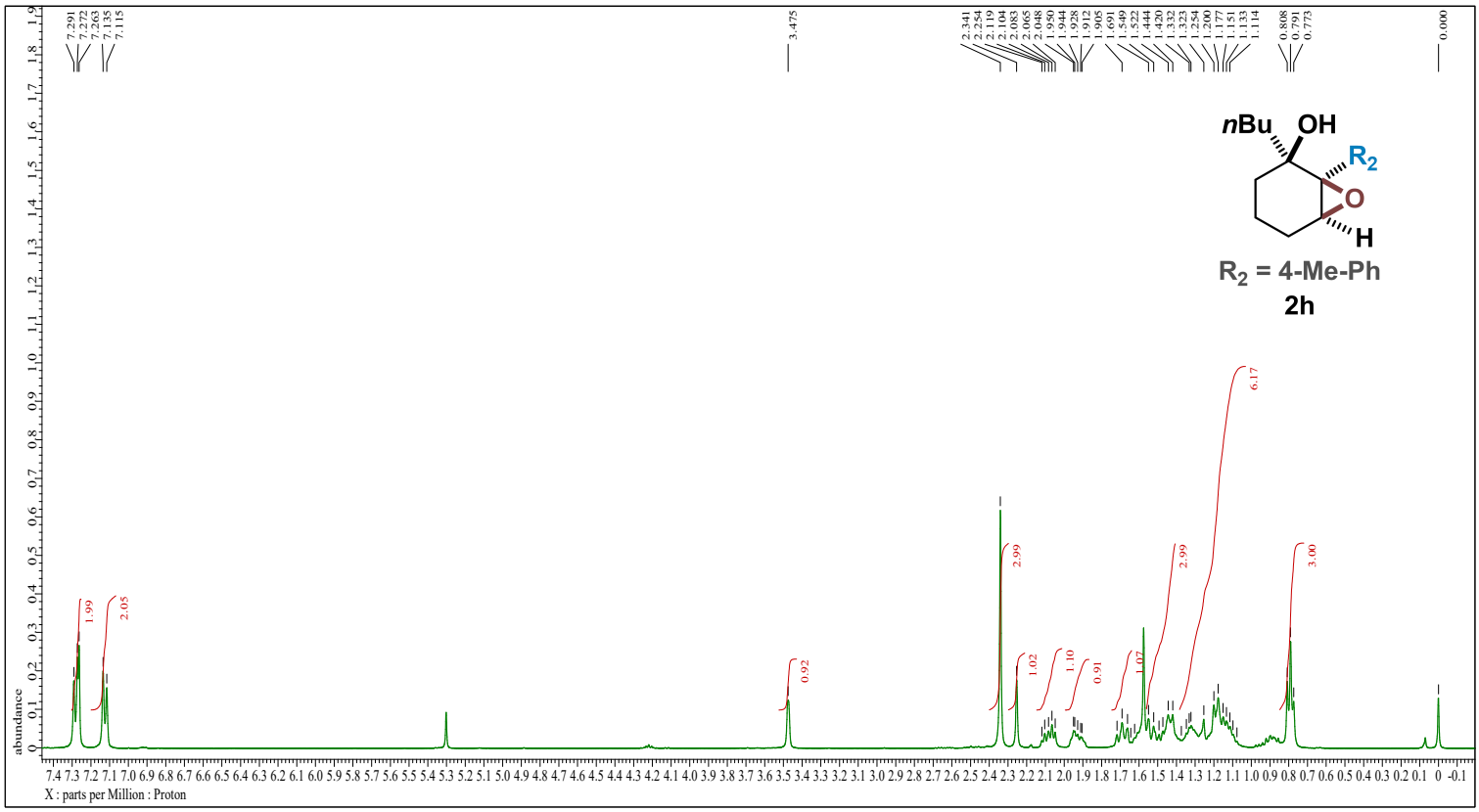

nBu
OH
R2
O
H
R2 = Ph
2e
X : parts per Million : Carbon13

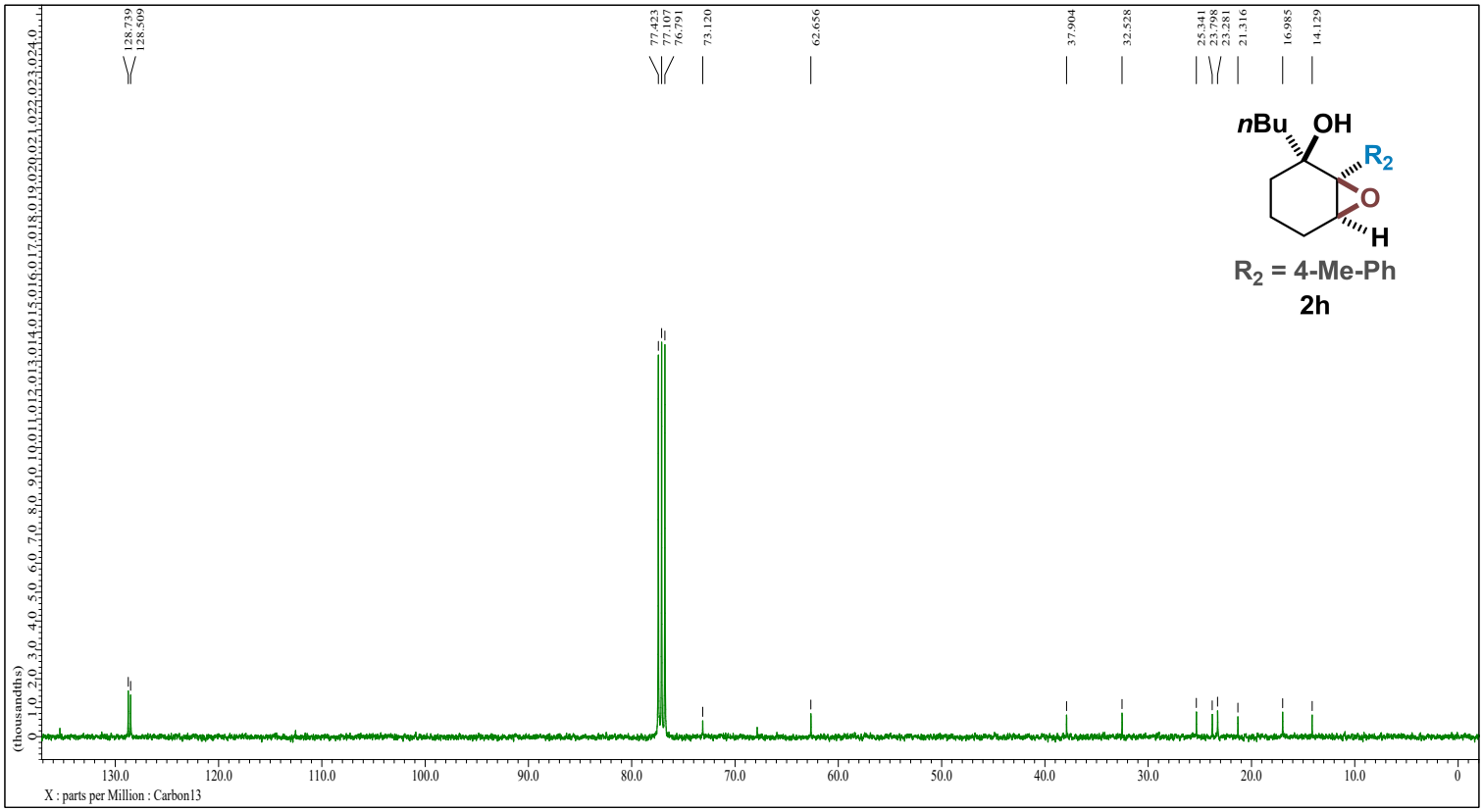

nBu
OH
R2
O
H
R2 = 4-F-Ph
2f
X : parts per Million : Proton

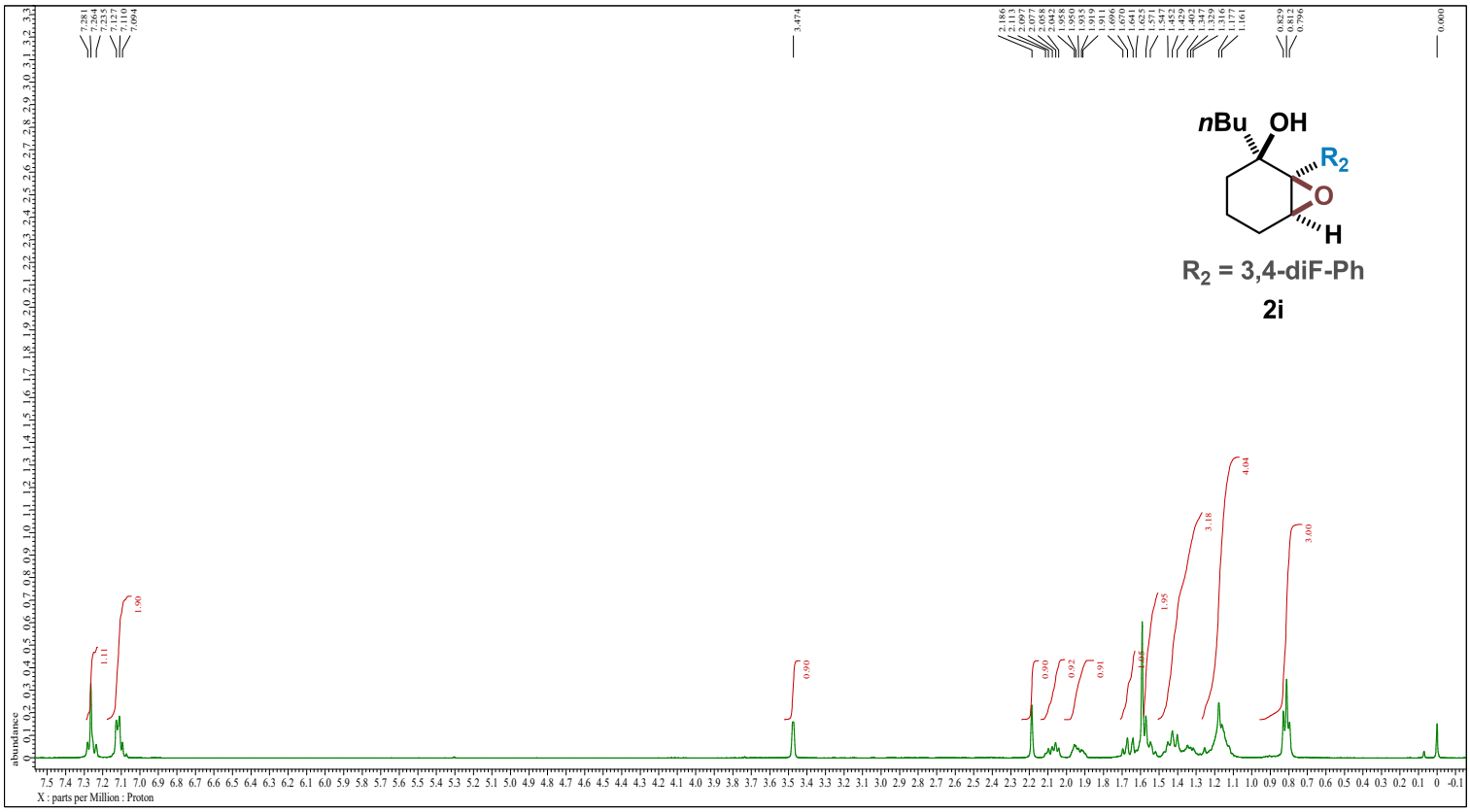

nBu
OH
R2
O
H
R2 = 4-F-Ph
2f
X : parts per Million : Carbon13

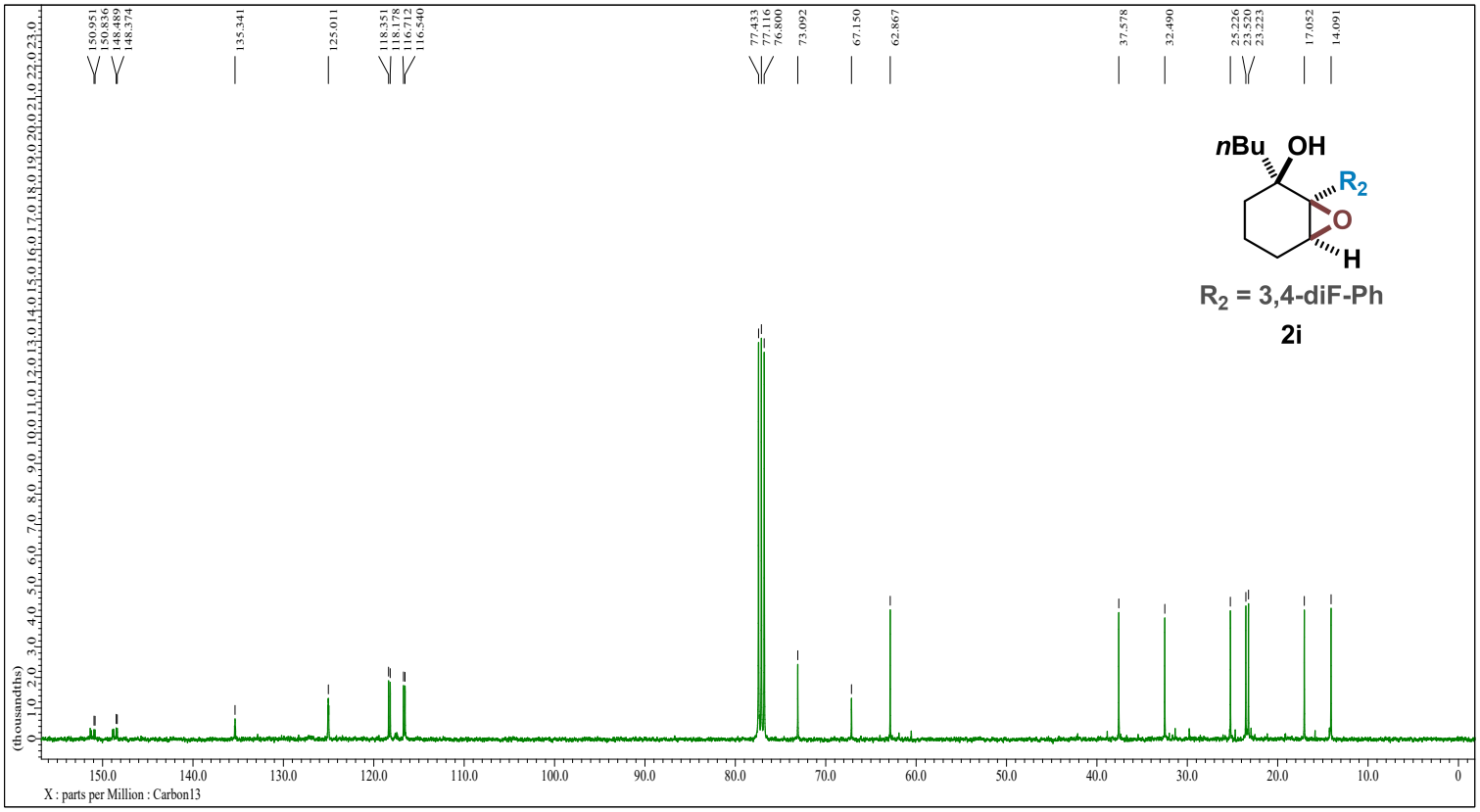

nBu
OH
R2
O
H
R2 = 4-Cl-Ph
2g
X : parts per Million : Proton

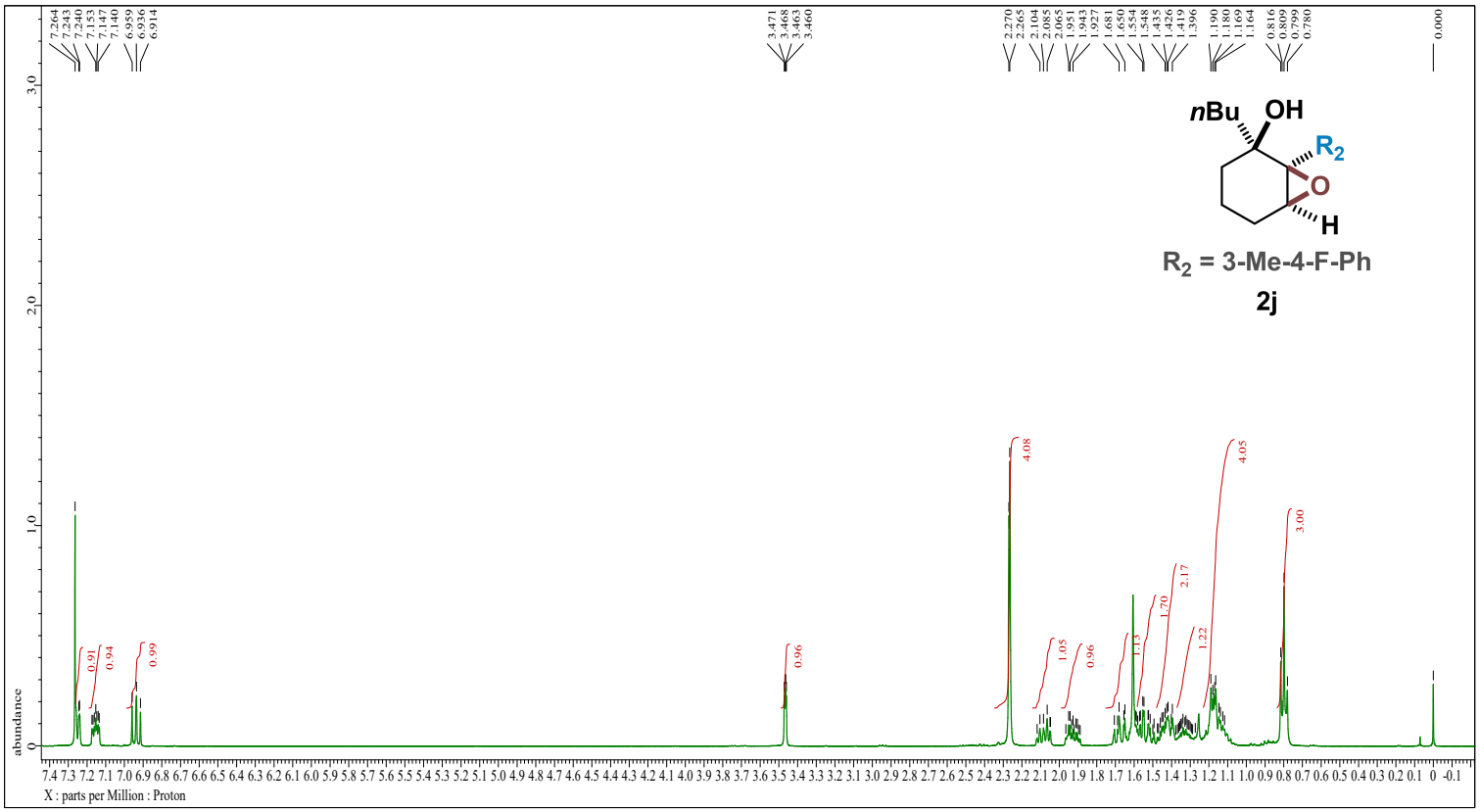

nBu
OH
R2
O
H
R2 = 4-Cl-Ph
2g
X : parts per Million : Carbon13

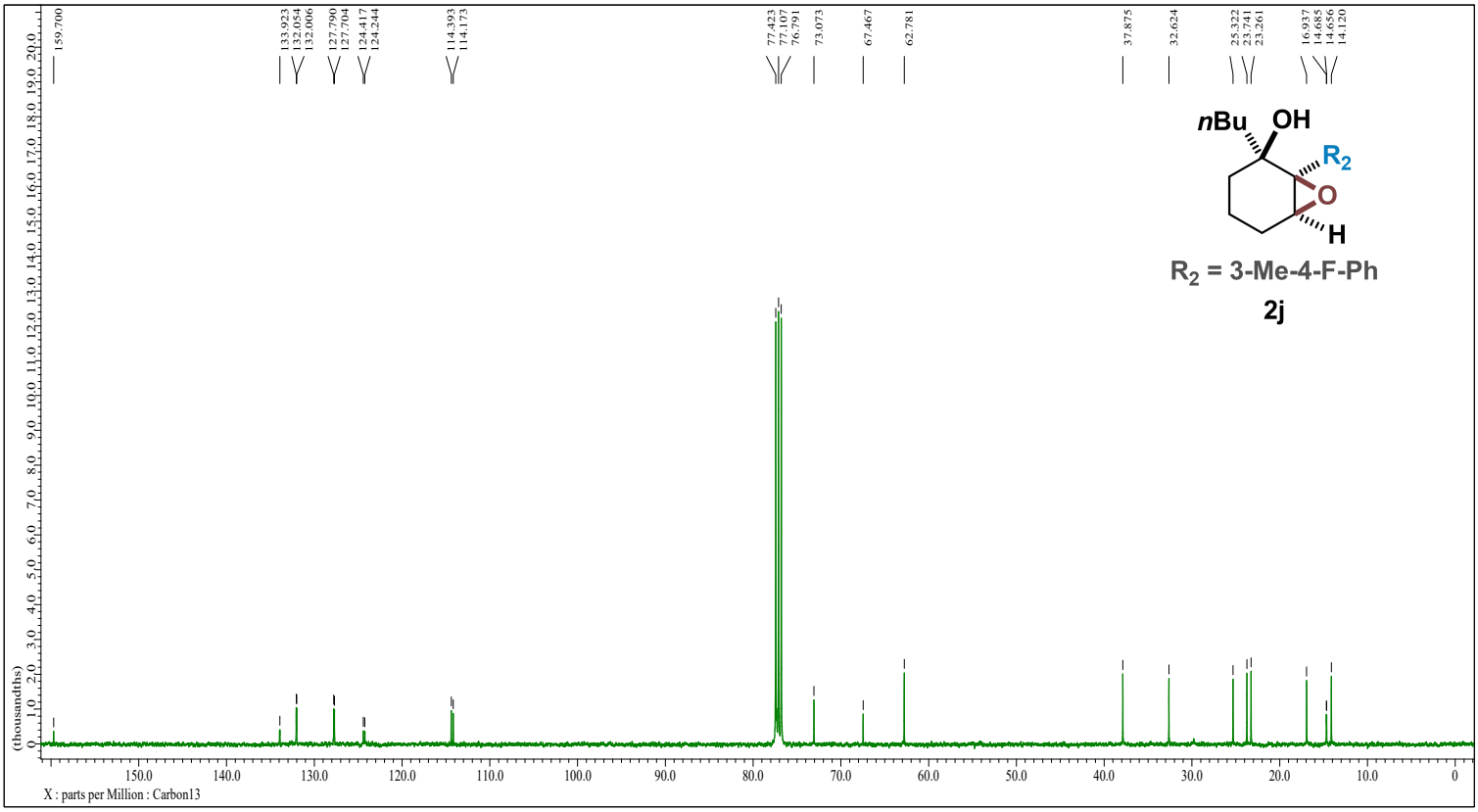

nBu
OH
R2
O
H
R2 = 4-Me-Ph
2h
abundance
X : parts per Million : Proton

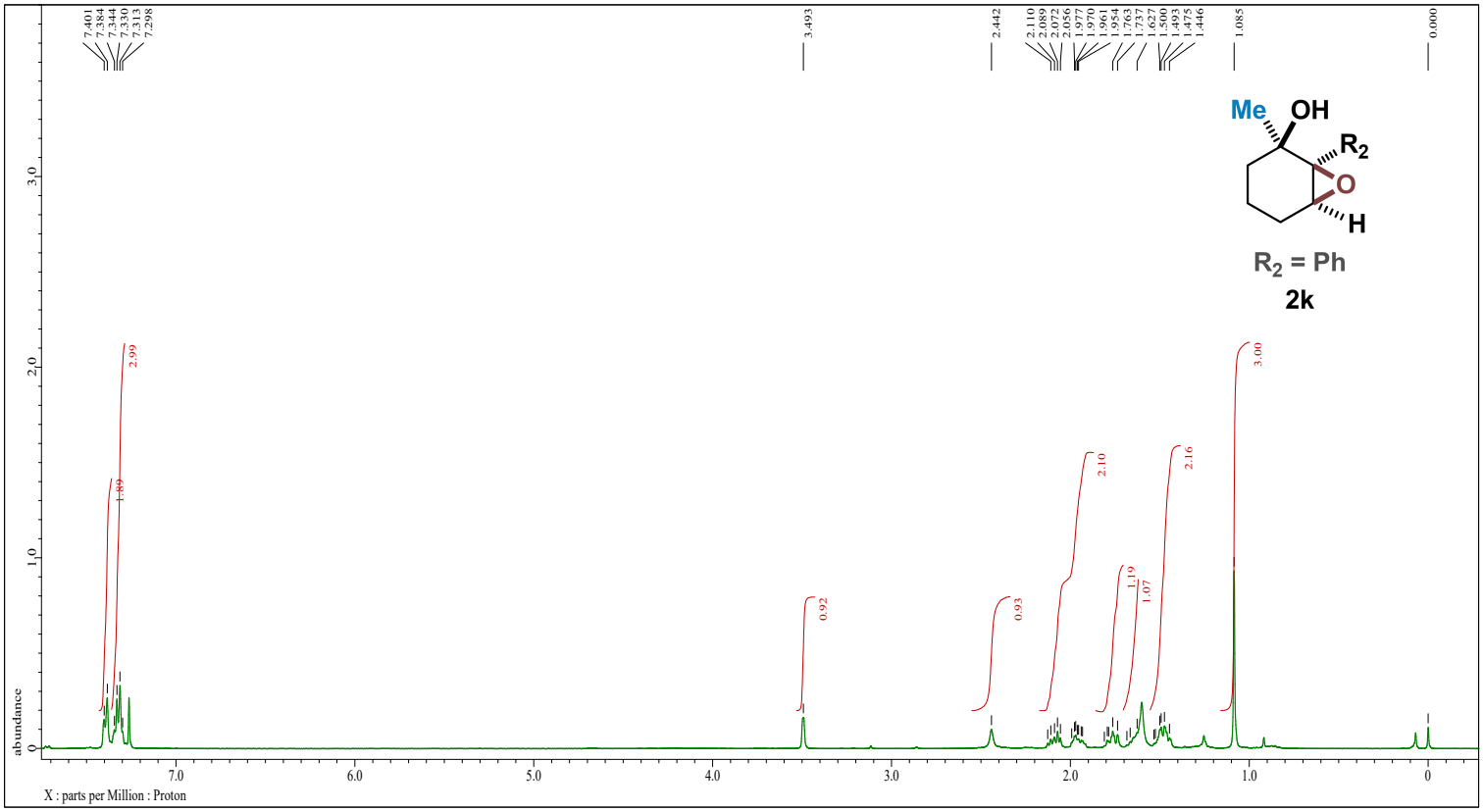

nBu
OH
R2
O
H
R2 = 4-Me-Ph
2h
(thousandths)
X : parts per Million : Carbon13

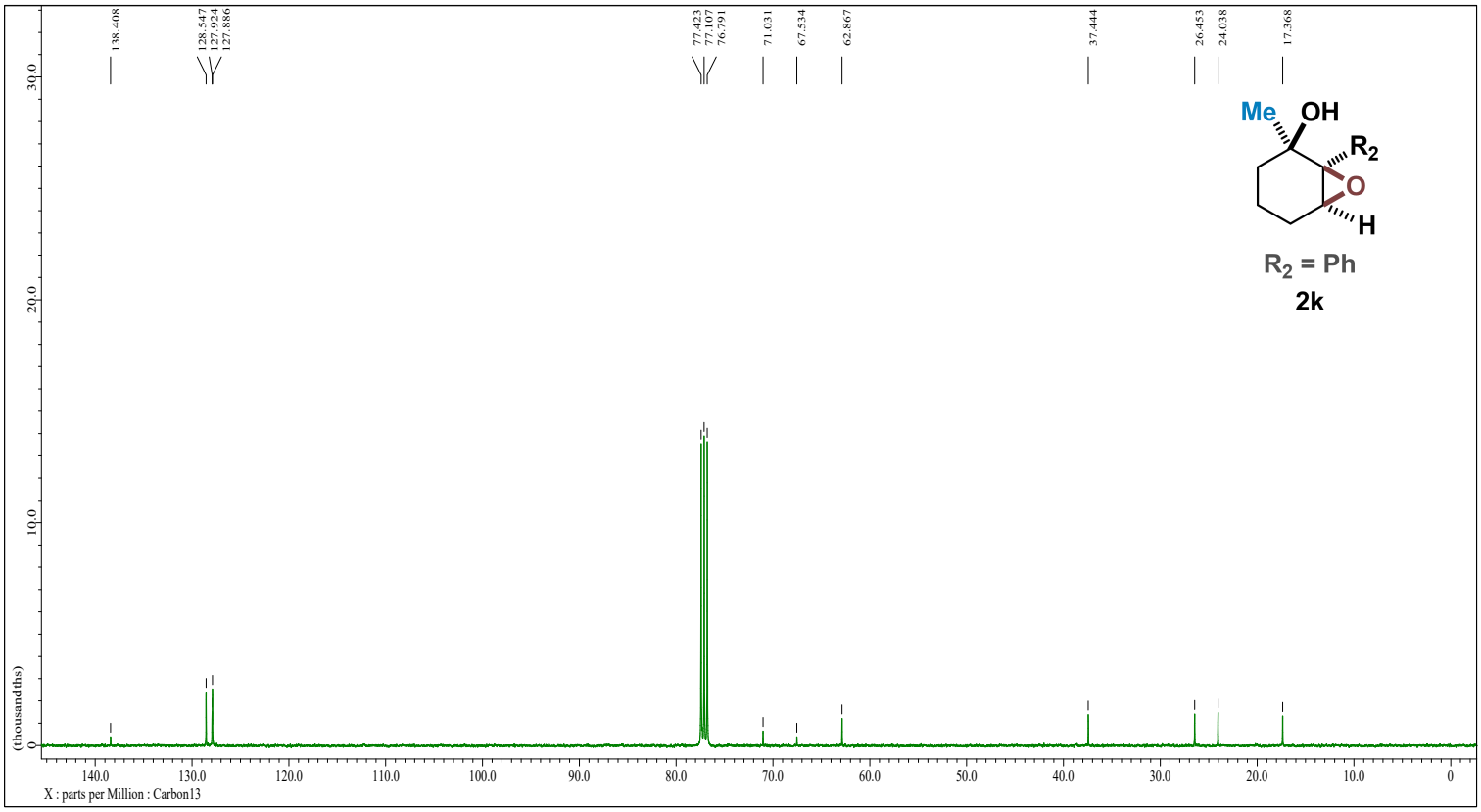

nBu
OH
R2
O
H
R2 = 3,4-diF-Ph
2i
X : parts per Million : Proton

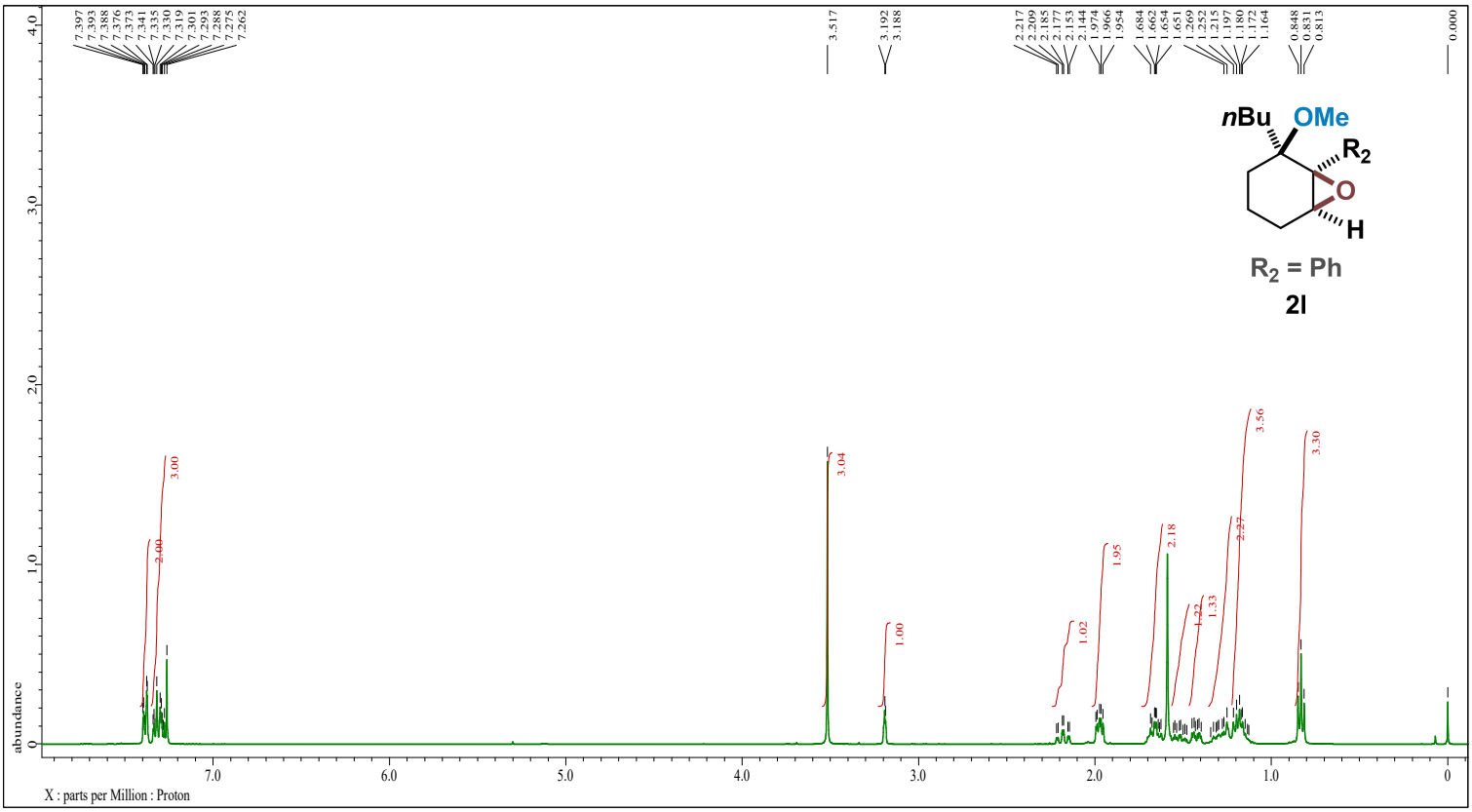

nBu
OH
R2
O
H
R2 = 3,4-diF-Ph
2i
X : parts per Million : Carbon13

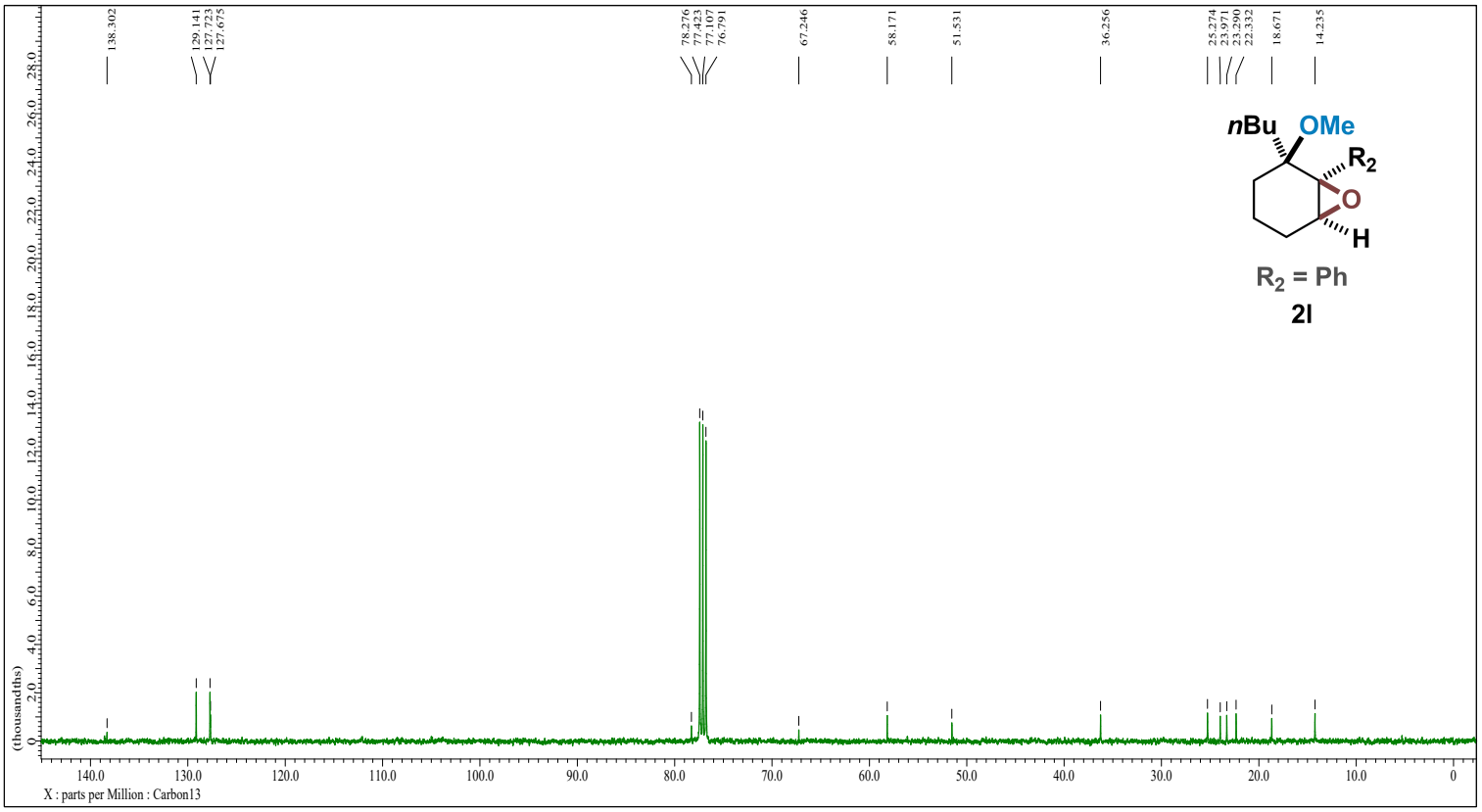

nBu
OH
R2
O
H
R2 = 3-Me-4-F-Ph
2j
abundance
X : parts per Million : Proton

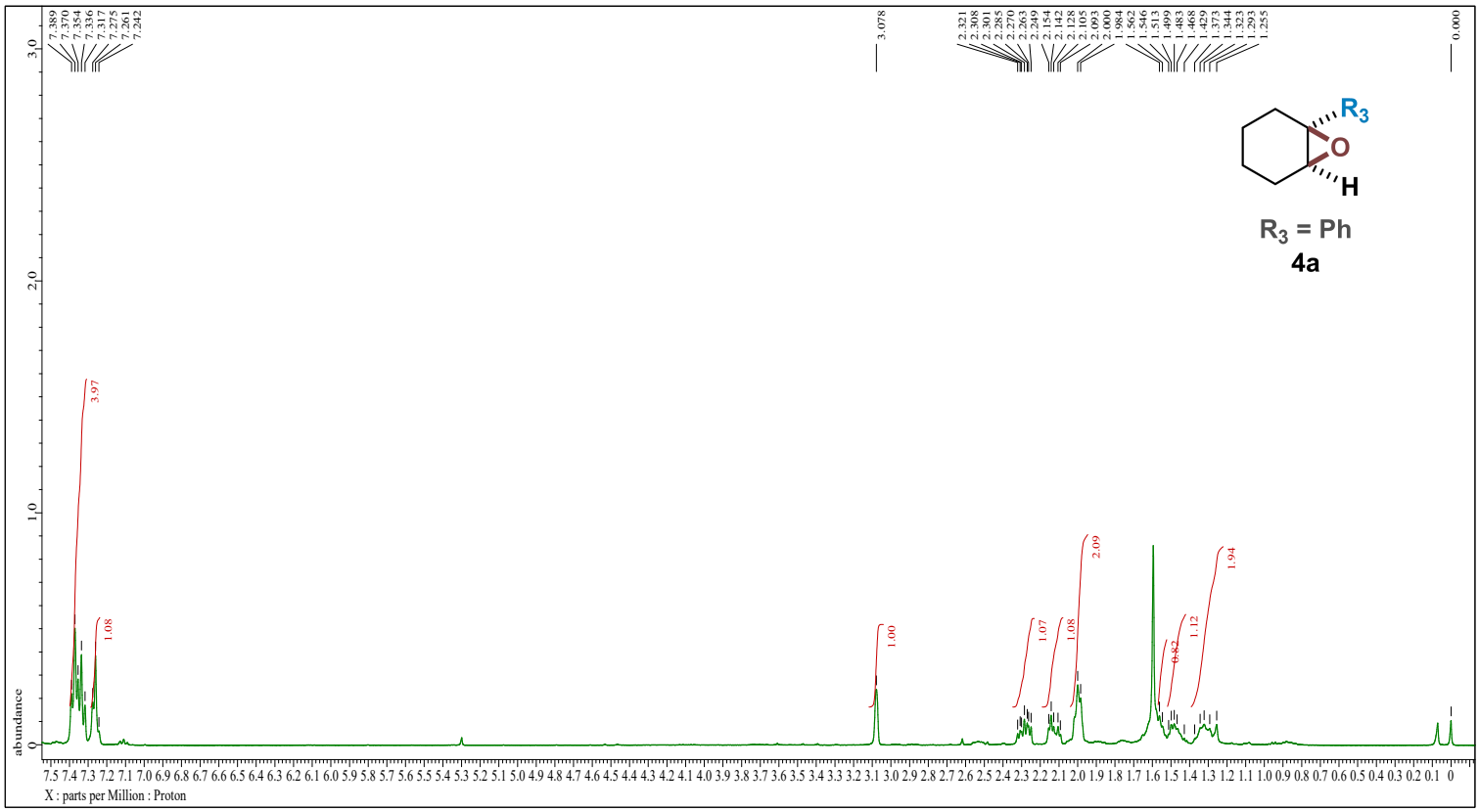

nBu
OH
R2
O
H
R2 = 3-Me-4-F-Ph
2j
(thousandths)
X : parts per Million : Carbon13

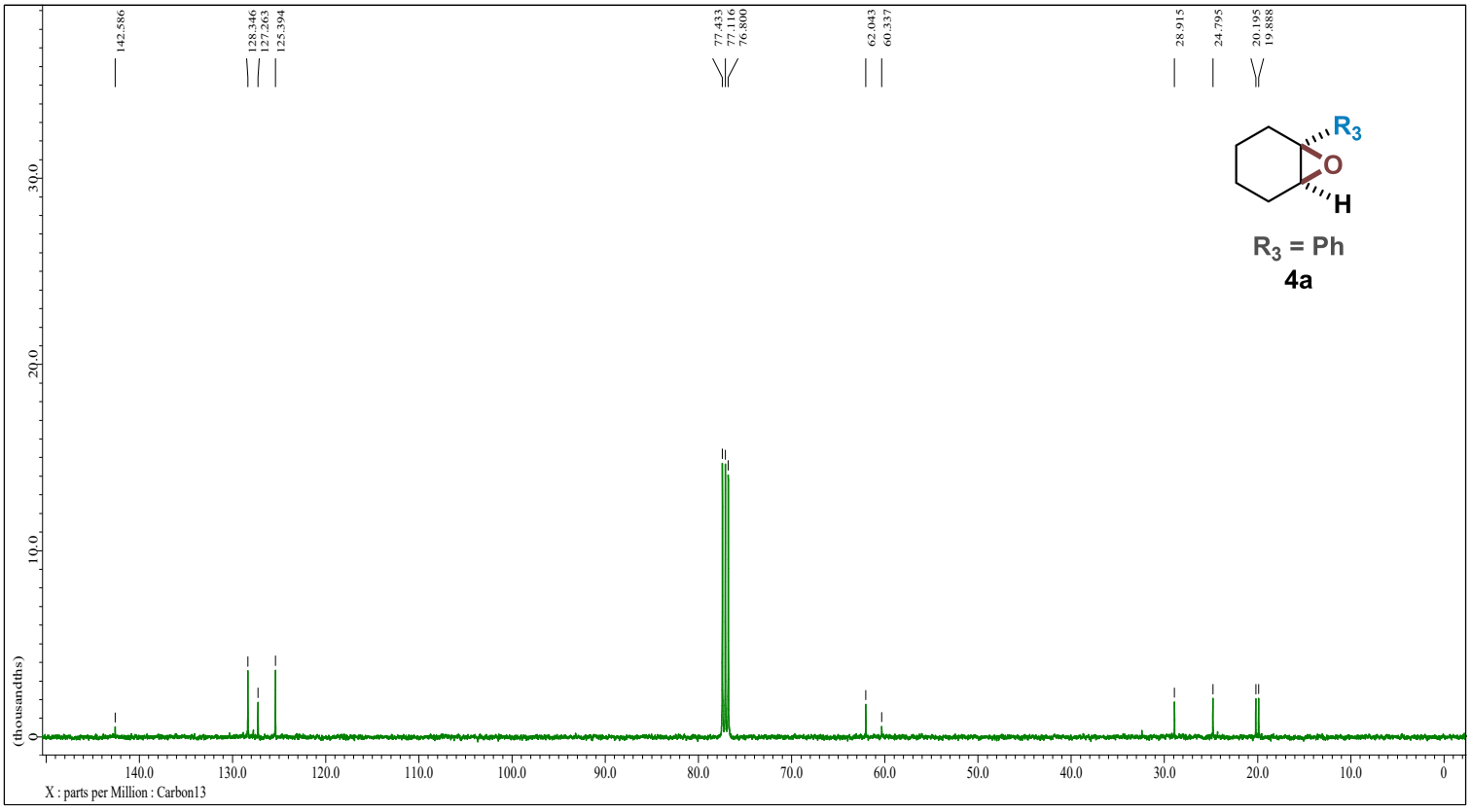

7.401
7.384
7.344
7.330
7.313
7.298
3.493
2.442
2.110
2.089
2.072
2.056
1.977
1.970
1.961
1.954
1.765
1.737
1.627
1.500
1.493
1.475
1.446
1.085
0.000
Me
OH
R2
O
H
R2 = Ph
2k
2.99
1.89
0.92
0.93
2.10
1.19
1.07
2.16
3.00
abundance
X : parts per Million : Proton

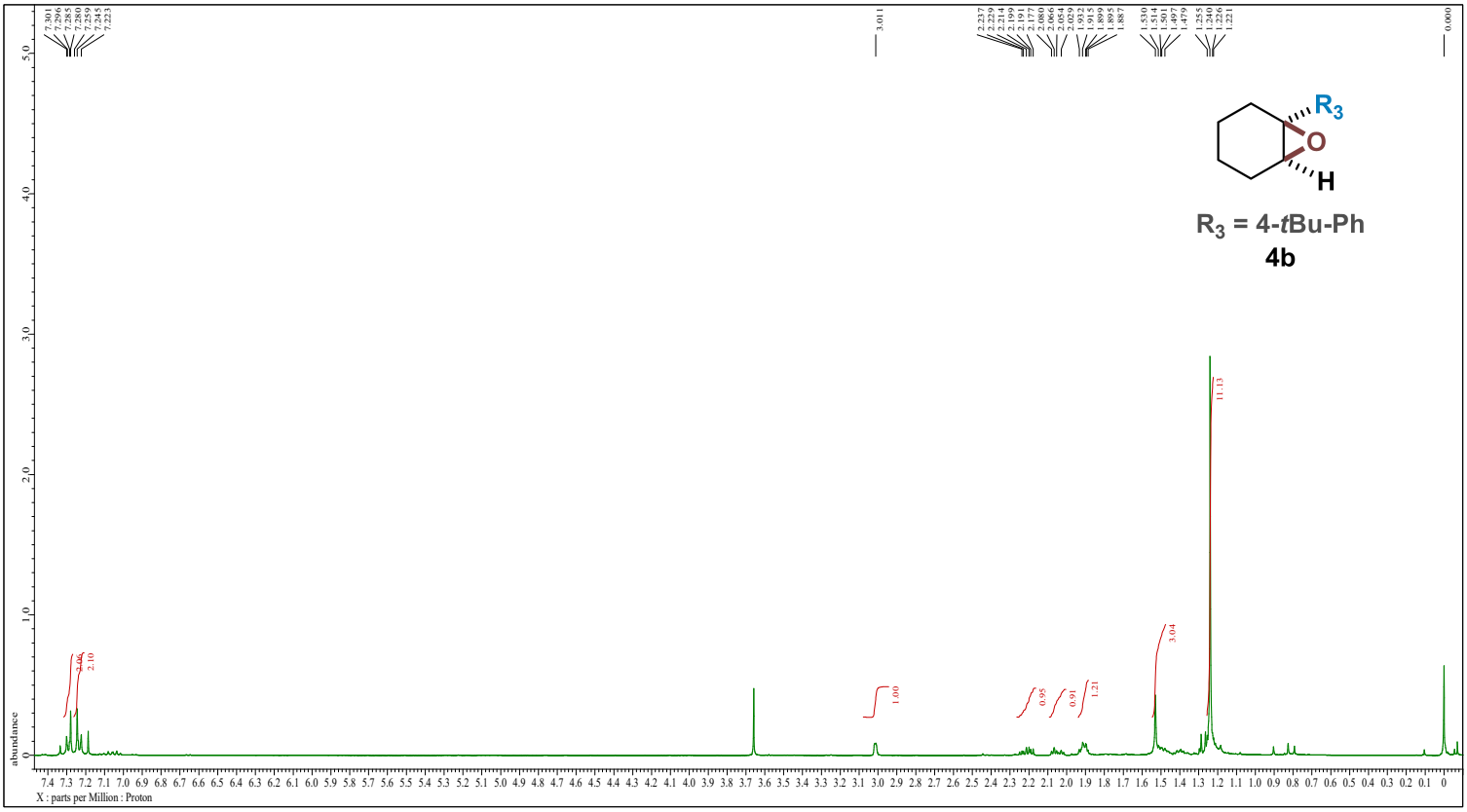

138.408
128.547
127.924
127.886
77.423
77.107
76.791
71.031
67.534
62.867
37.444
26.453
24.038
17.368
Me
OH
R2
O
H
R2 = Ph
2k
(thousandths)
X : parts per Million : Carbon13

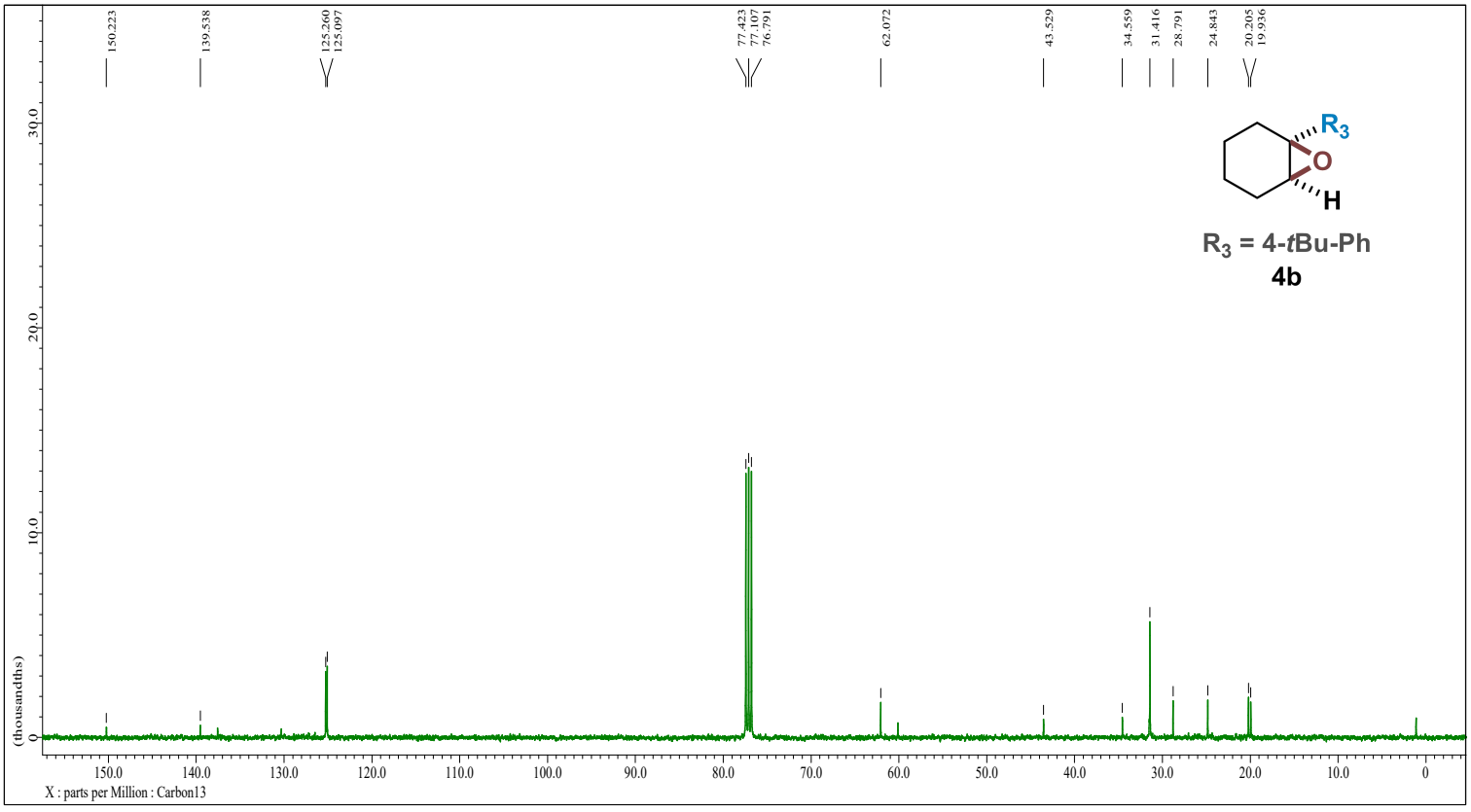

7.397
7.393
7.388
7.376
7.373
7.341
7.335
7.330
7.319
7.301
7.293
7.288
7.275
7.262
3.517
3.192
3.188
2.217
2.209
2.185
2.177
2.153
2.144
1.974
1.966
1.954
1.684
1.662
1.654
1.651
1.269
1.252
1.215
1.197
1.190
1.172
1.164
0.848
0.831
0.813
0.000
nBu
OMe
R2
O
H
R2 = Ph
2l
3.00
2.00
3.04
1.00
1.02
1.95
2.18
1.23
1.33
2.27
3.56
3.30
abundance
X : parts per Million : Proton

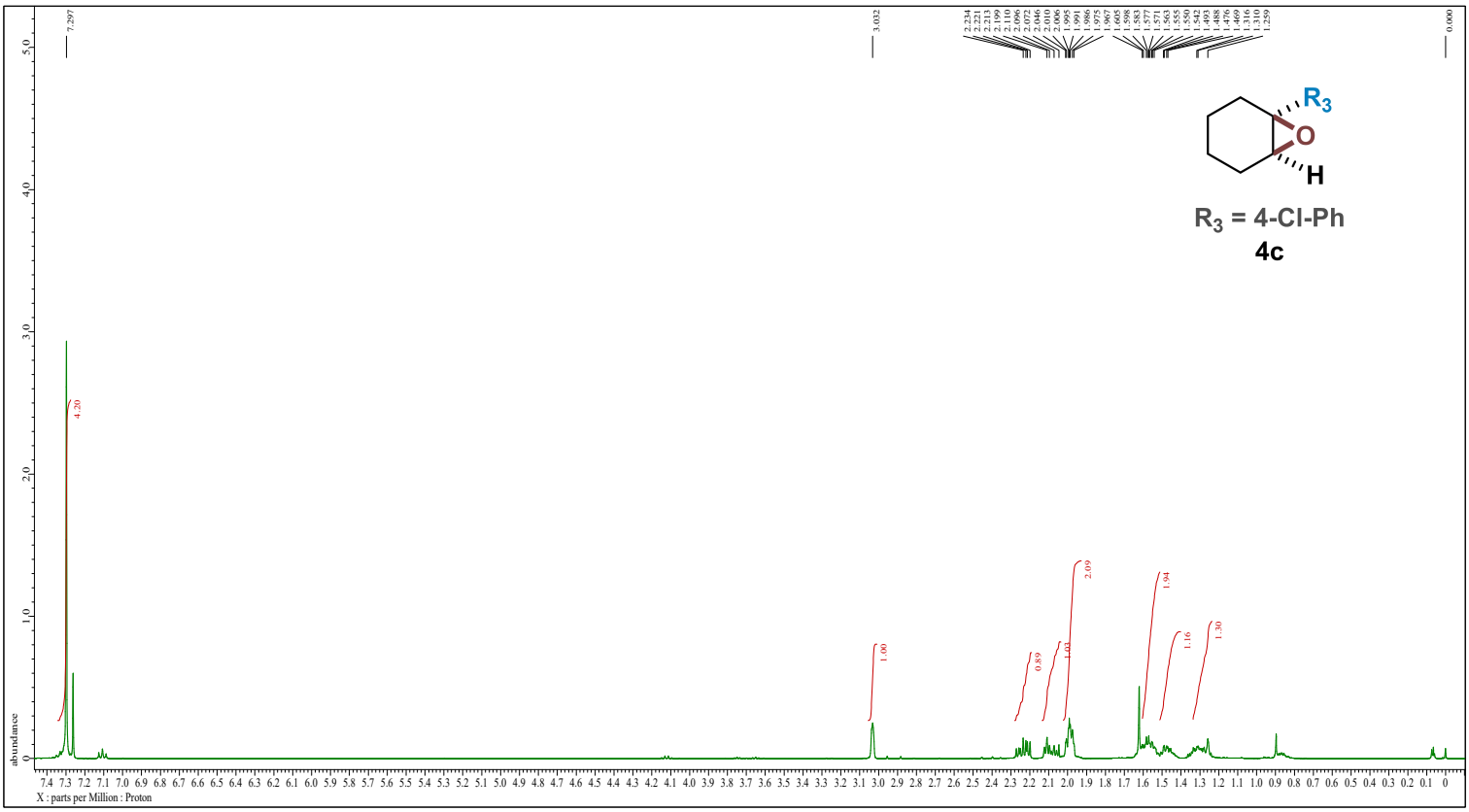

138.302
129.141
127.723
127.675
78.276
77.423
77.107
76.791
67.246
58.171
51.531
36.256
25.274
23.971
23.290
22.352
18.671
14.235
nBu
OMe
R2
O
H
R2 = Ph
2l
(thousandths)
X : parts per Million : Carbon13

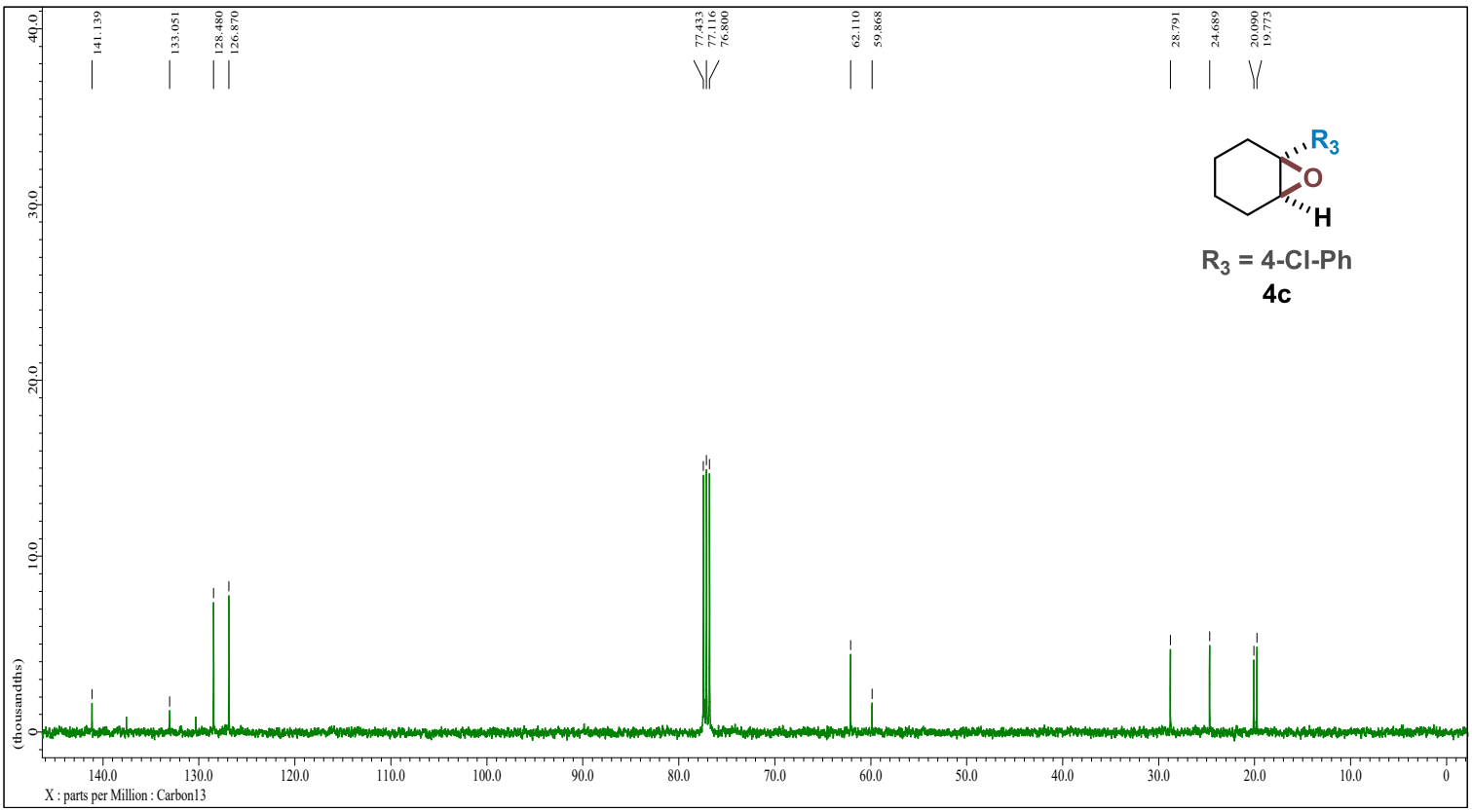

7.389
7.370
7.354
7.336
7.317
7.275
7.261
7.242
3.078
2.321
2.308
2.301
2.285
2.270
2.263
2.249
2.154
2.142
2.128
2.105
2.093
2.000
1.984
1.562
1.546
1.513
1.499
1.483
1.468
1.429
1.373
1.344
1.323
1.293
1.255
0.000
R3
O
H
R3 = Ph
4a
3.97
1.08
1.00
1.07
1.08
2.09
0.82
1.12
1.94
abundance
X : parts per Million : Proton

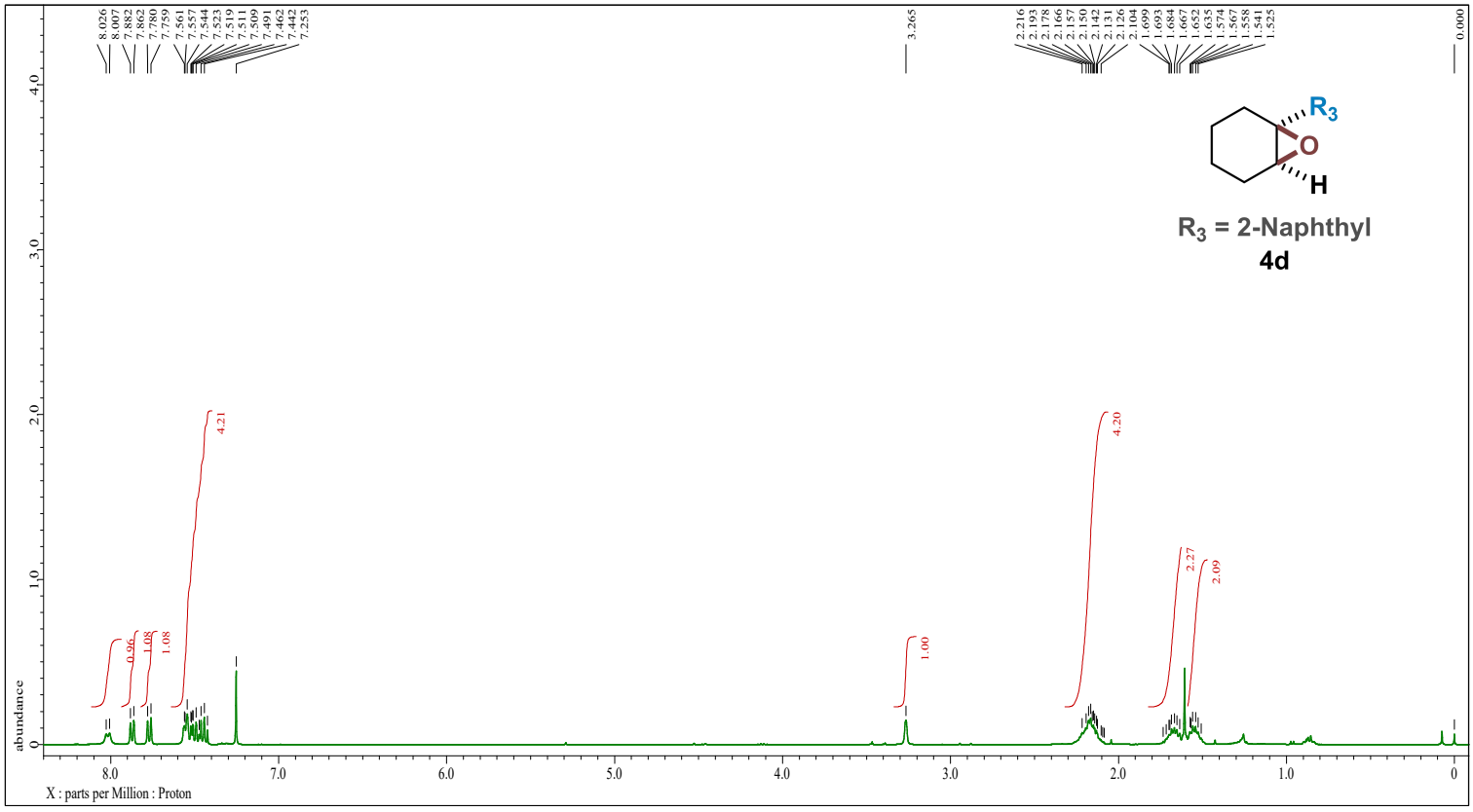

142.586
128.346
127.263
125.394
77.433
77.116
76.800
62.043
60.337
28.915
24.795
20.195
19.888
R3
O
H
R3 = Ph
4a
(thousandths)
X : parts per Million : Carbon13

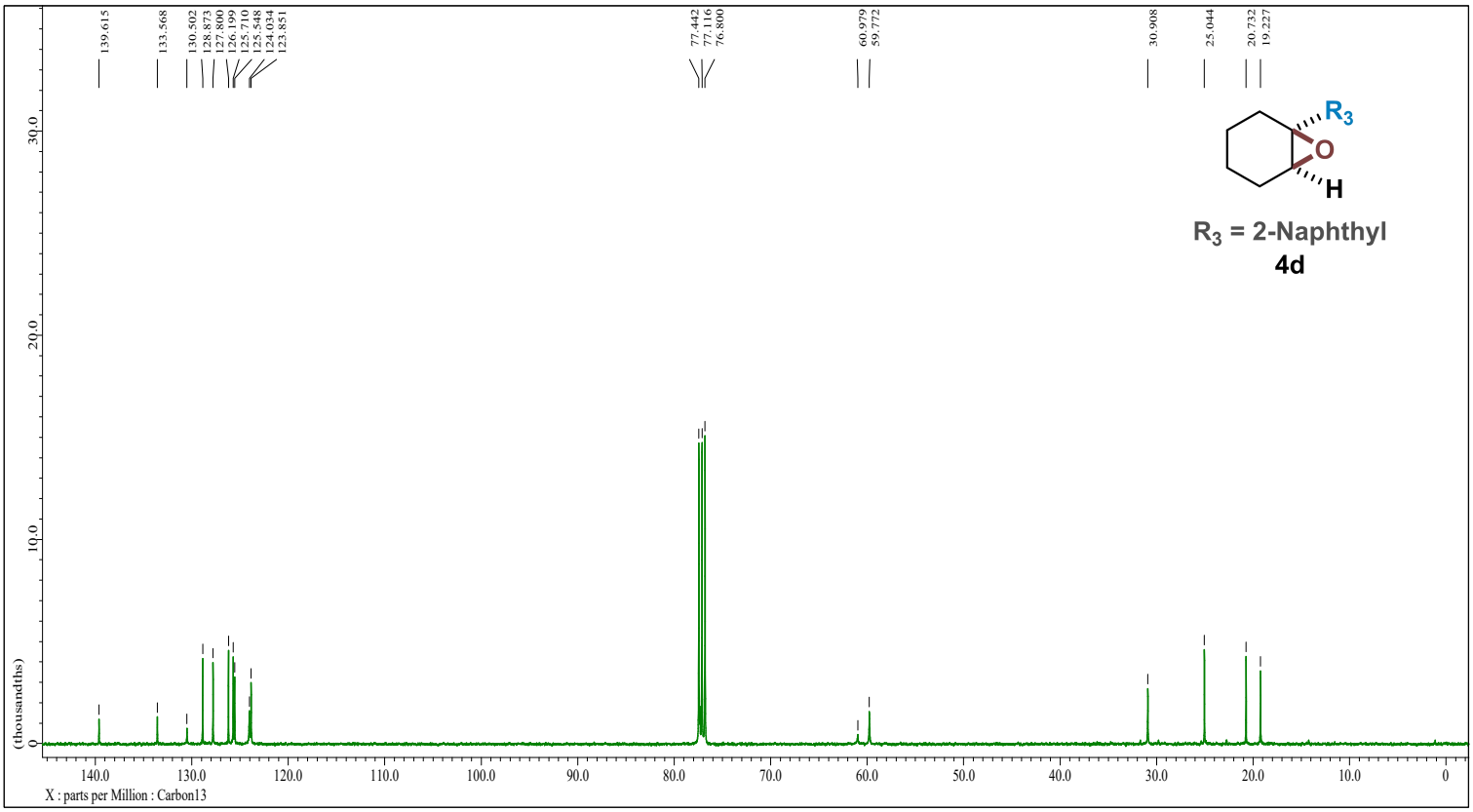

R3
O
H
R3 = 4-tBu-Ph
4b
X : parts per Million : Proton

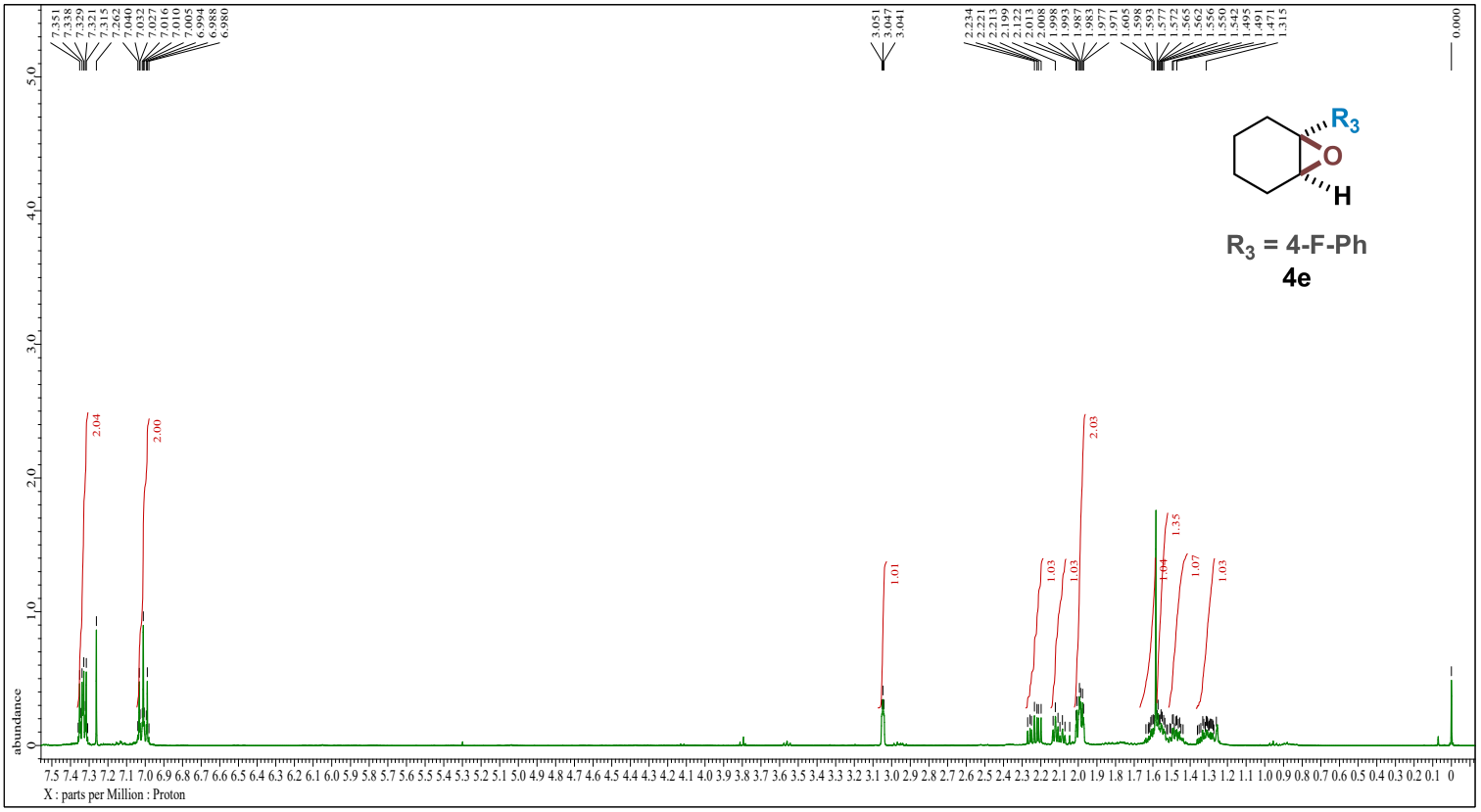

R3
O
H
R3 = 4-tBu-Ph
4b
X : parts per Million : Carbon13

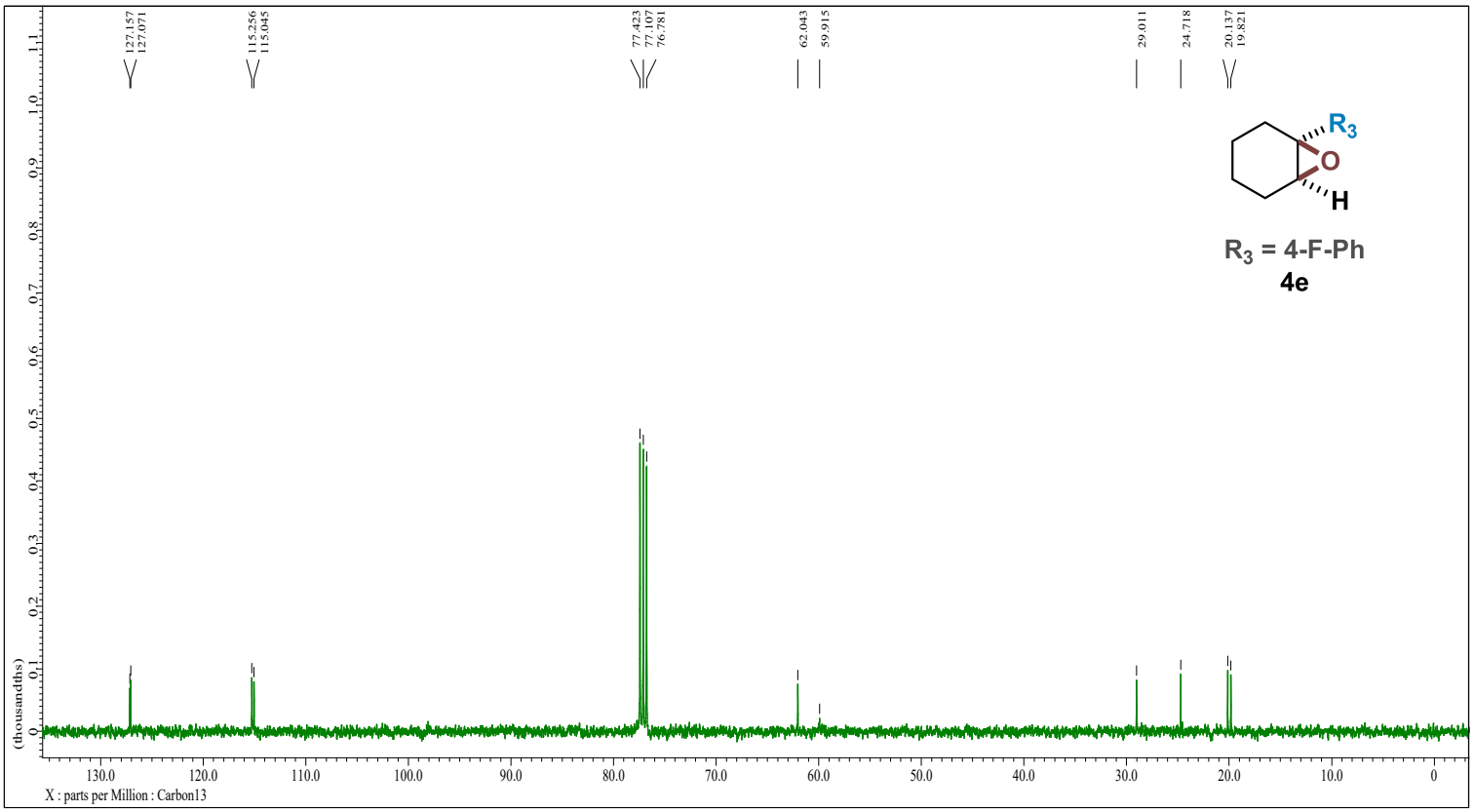

7.297
3.032
0.000
4.20
1.00
0.89
1.03
2.09
1.94
1.16
1.30
abundance
X : parts per Million : Proton
R3
O
H
R3 = 4-Cl-Ph
4c

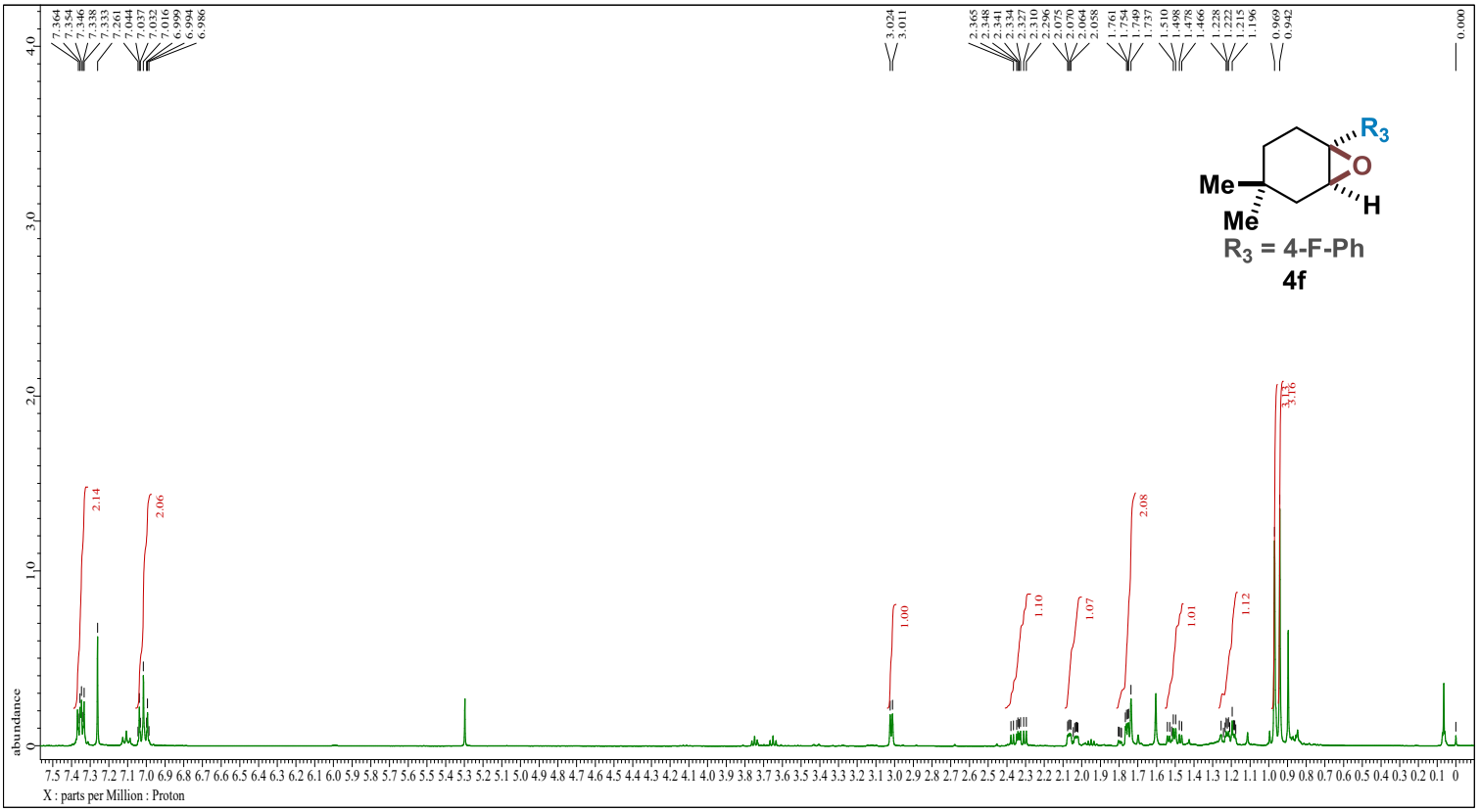

141.139
133.051
128.480
126.870
77.433
77.116
76.800
62.110
59.868
28.791
24.689
20.090
19.773
(thousandths)
X : parts per Million : Carbon13
R3
O
H
R3 = 4-Cl-Ph
4c

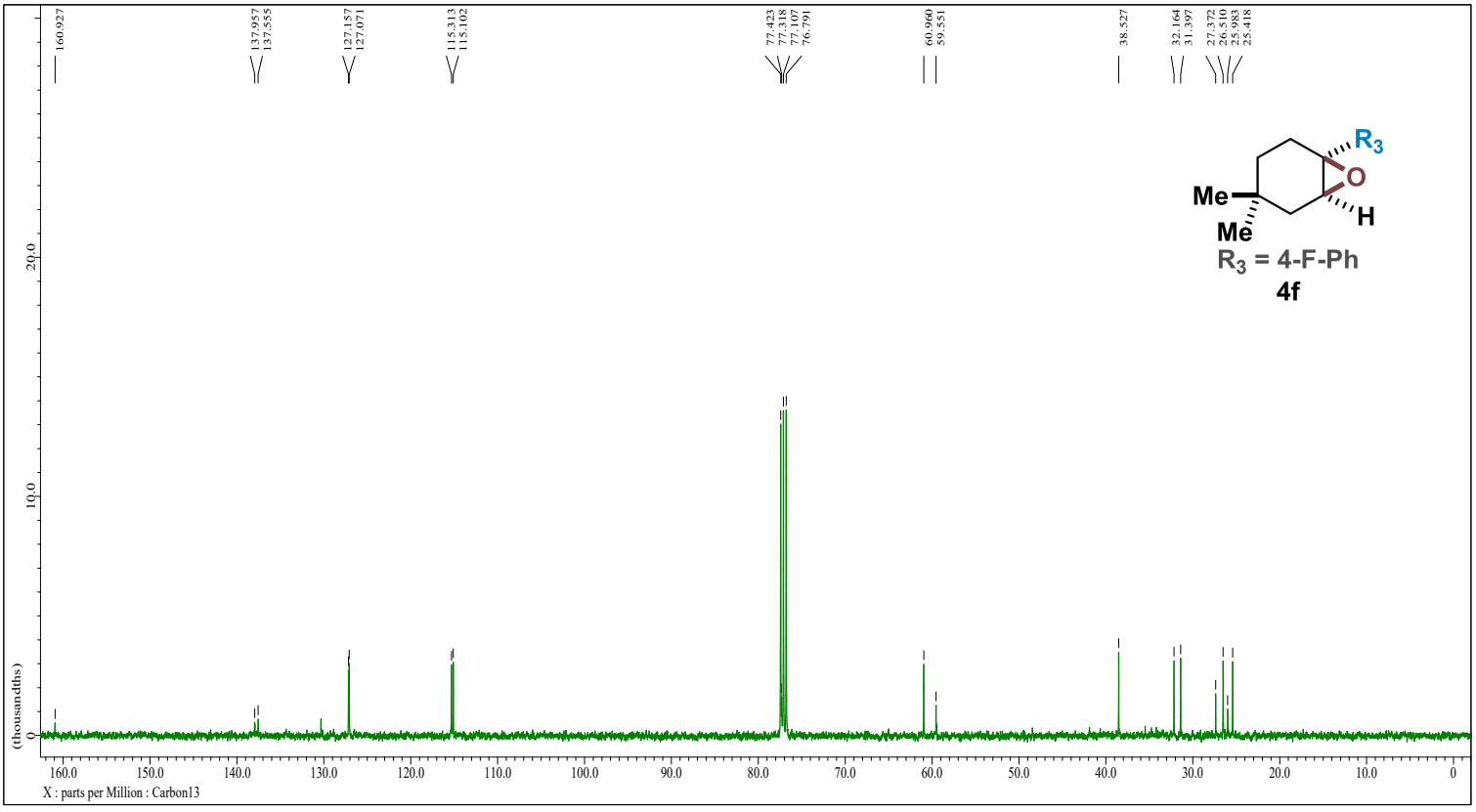

8.026
8.007
7.882
7.862
7.780
7.759
7.561
7.557
7.544
7.523
7.519
7.511
7.509
7.491
7.462
7.442
7.253
3.265
2.216
2.193
2.178
2.166
2.157
2.150
2.142
2.131
2.126
2.104
1.699
1.693
1.684
1.667
1.652
1.635
1.574
1.567
1.558
1.541
1.525
0.000
R3
O
H
R3 = 2-Naphthyl
4d
4.21
4.20
2.27
2.09
1.00
0.96
1.08
1.08
abundance
X : parts per Million : Proton

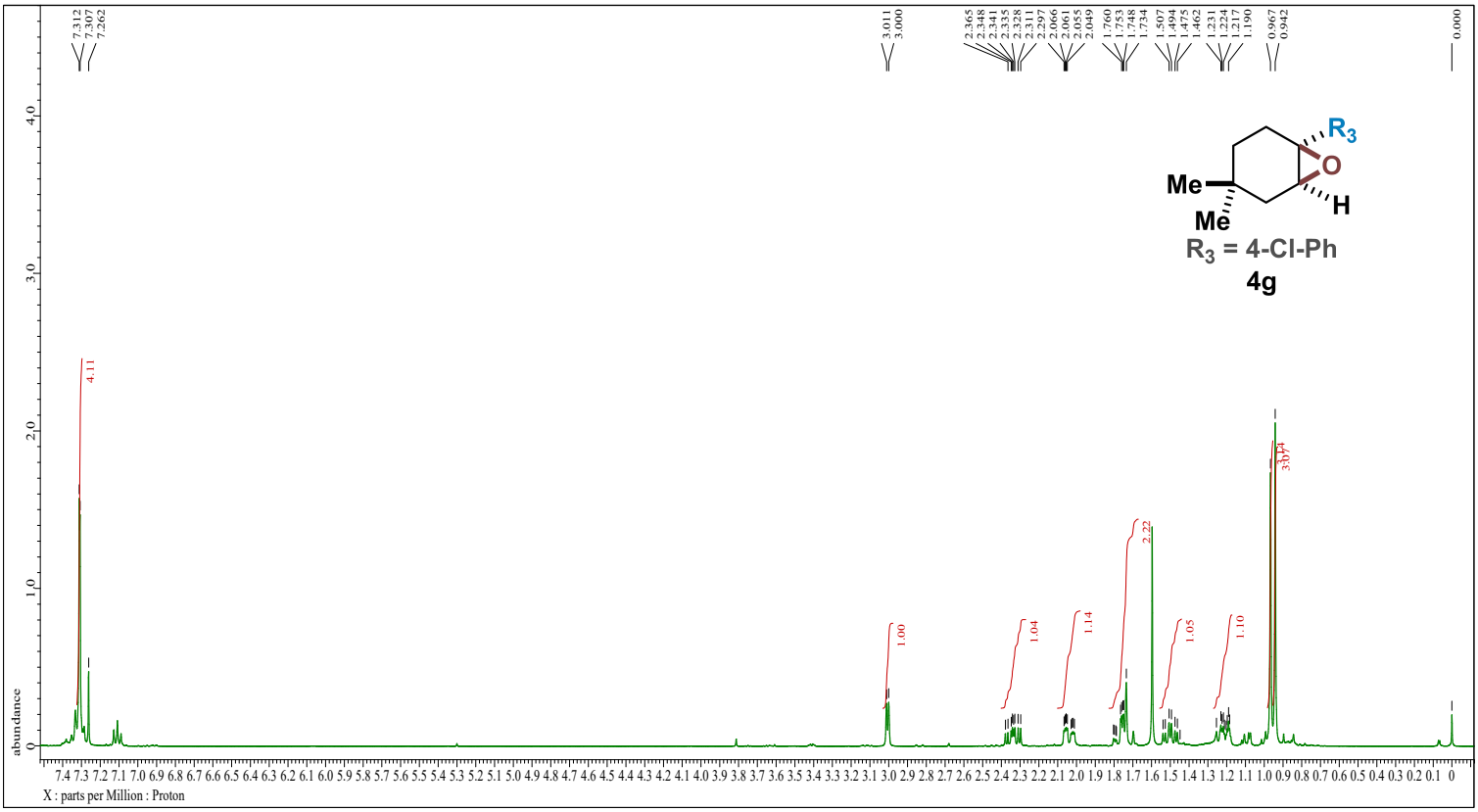

139.615
133.568
130.502
128.873
127.800
126.199
125.710
125.548
124.044
123.851
77.442
77.116
76.800
60.979
59.772
30.908
25.044
20.732
19.227
R3
O
H
R3 = 2-Naphthyl
4d
(thousandths)
X : parts per Million : Carbon13

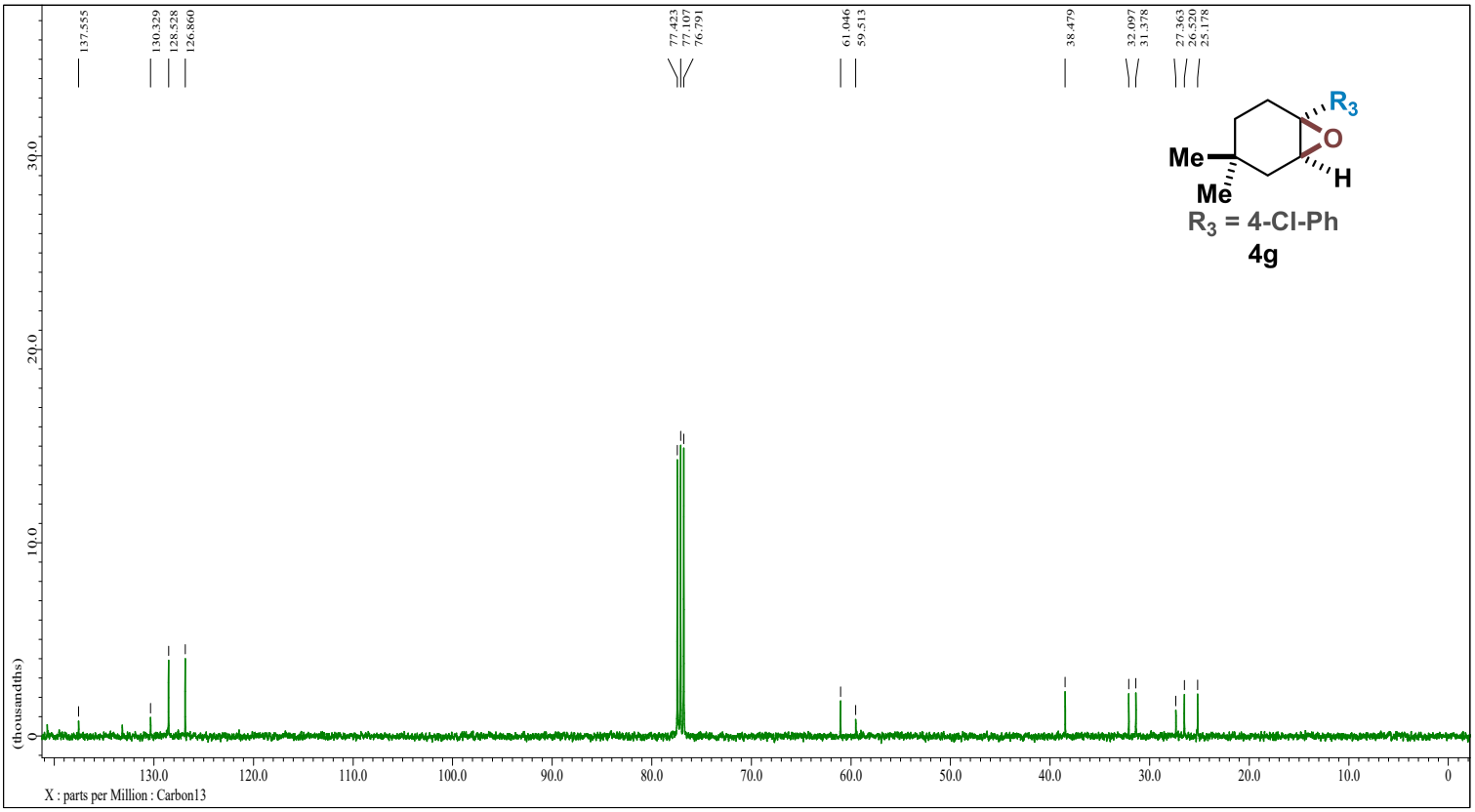

7.351
7.338
7.329
7.321
7.315
7.262
7.040
7.032
7.027
7.016
7.010
7.005
6.994
6.988
6.980
3.051
3.047
3.041
2.234
2.221
2.213
2.199
2.123
2.013
2.008
1.998
1.993
1.987
1.983
1.977
1.971
1.605
1.598
1.593
1.577
1.572
1.565
1.562
1.556
1.550
1.542
1.495
1.491
1.471
1.315
0.000
2.04
2.00
1.01
1.03
1.03
2.03
1.35
1.04
1.07
1.03
abundance
X : parts per Million : Proton
R3
O
H
R3 = 4-F-Ph
4e

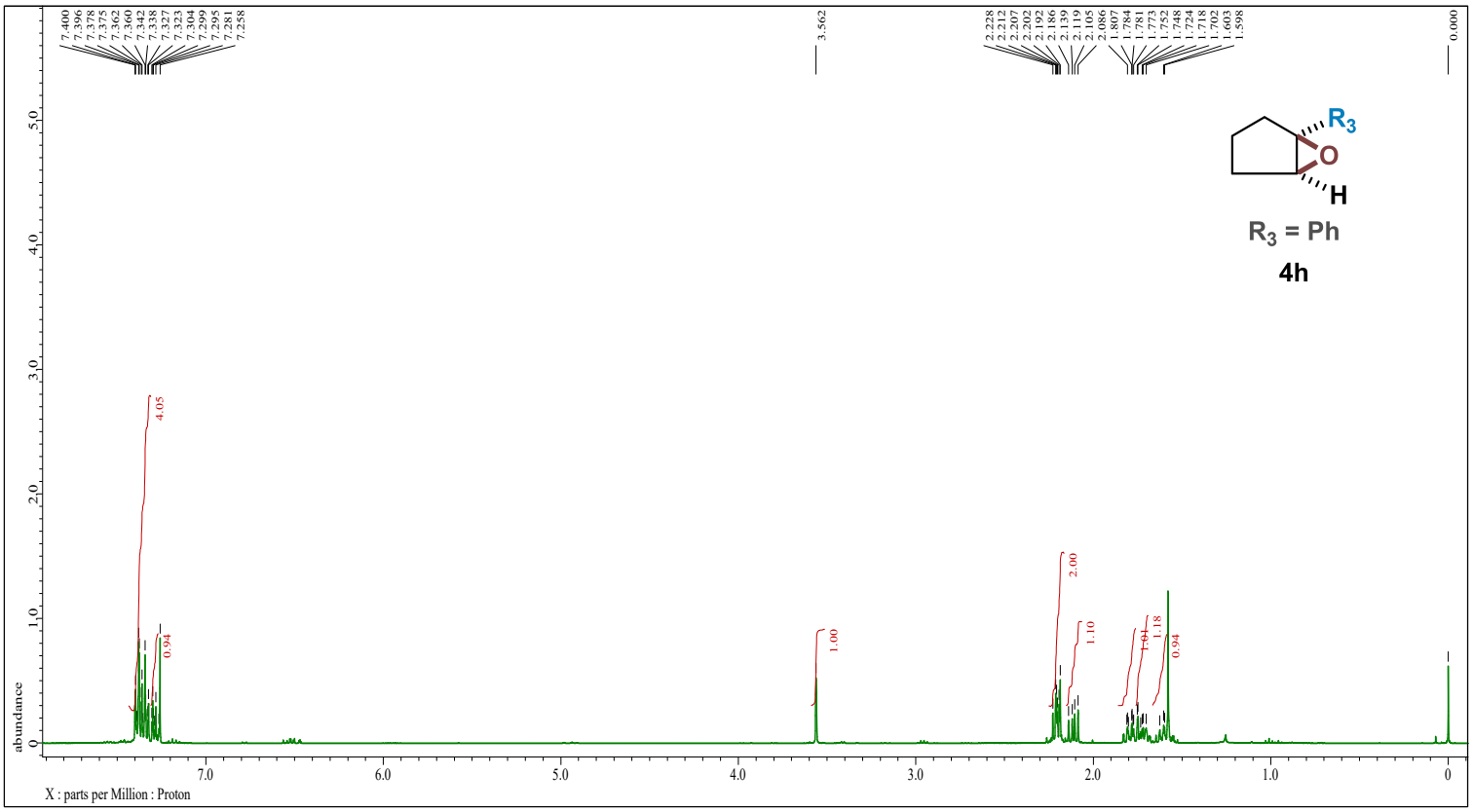

127.157
127.071
115.256
115.045
77.423
77.107
76.781
62.043
59.915
29.011
24.718
20.137
19.821
(thousandths)
X : parts per Million : Carbon13
R3
O
H
R3 = 4-F-Ph
4e

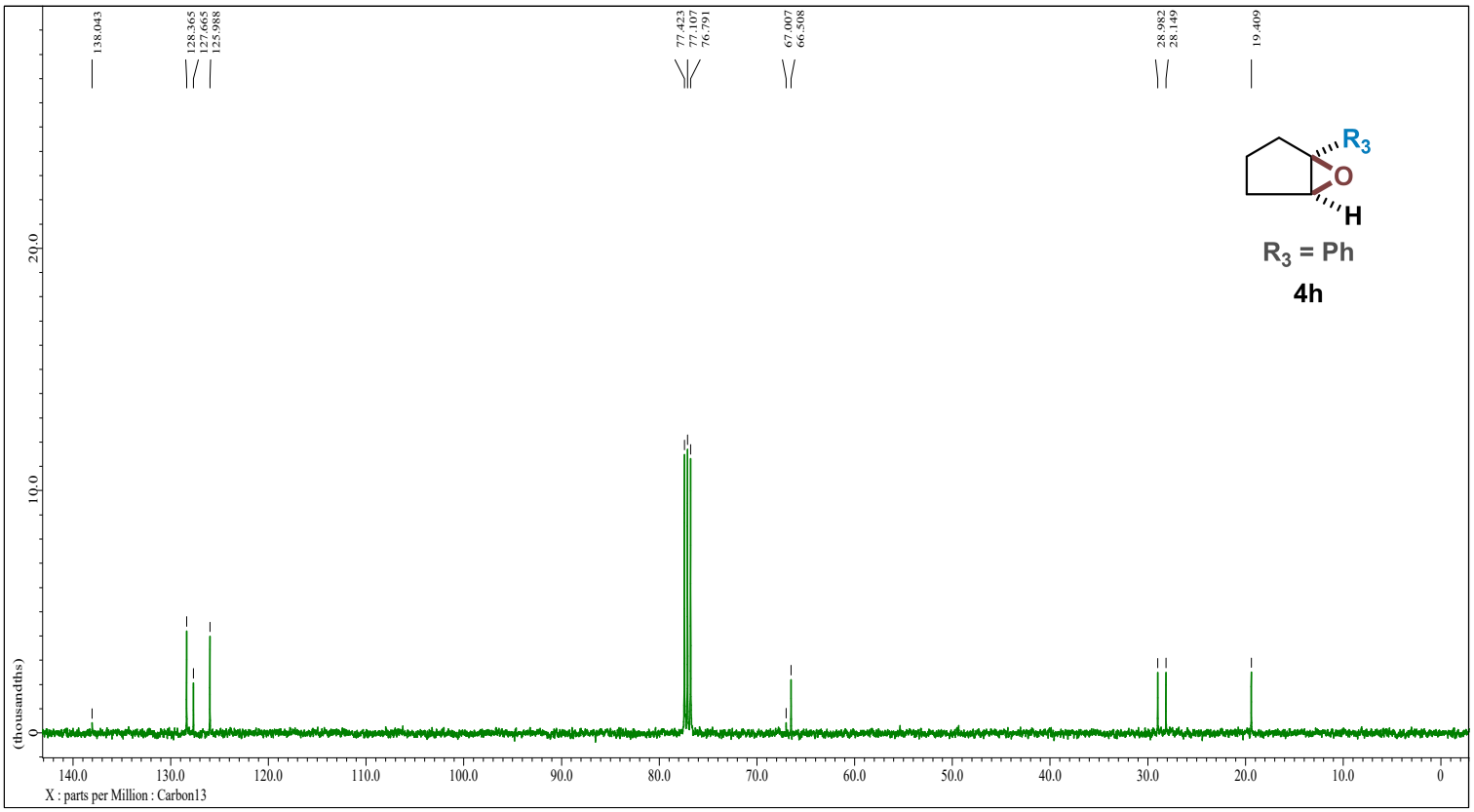

7.364
7.354
7.346
7.338
7.333
7.261
7.244
7.037
7.032
7.016
6.999
6.994
6.986
3.024
3.011
2.365
2.348
2.341
2.334
2.327
2.310
2.296
2.075
2.070
2.064
2.058
1.761
1.754
1.749
1.737
1.510
1.498
1.478
1.466
1.228
1.222
1.215
1.196
0.969
0.942
0.000
R3
O
Me
Me
H
R3 = 4-F-Ph
4f
abundance
2.14
2.06
1.00
1.10
1.07
2.08
1.01
1.12
3.16
X : parts per Million : Proton

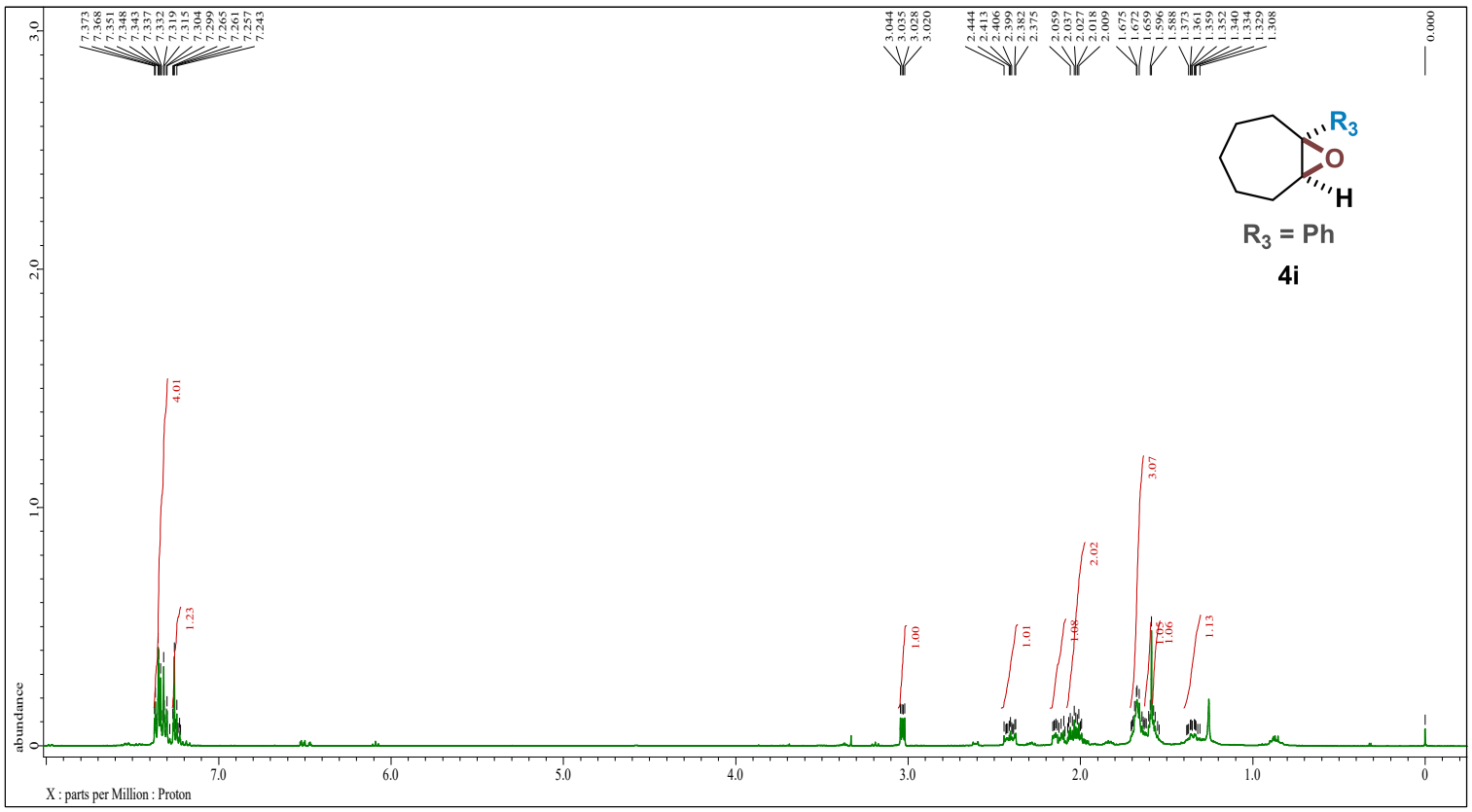

160.927
137.957
137.555
127.157
127.071
115.313
115.102
77.423
77.318
77.107
76.791
60.960
59.551
38.527
32.164
31.397
27.372
26.510
25.988
25.418
R3
O
Me
Me
H
R3 = 4-F-Ph
4f
(thousandths)
X : parts per Million : Carbon13

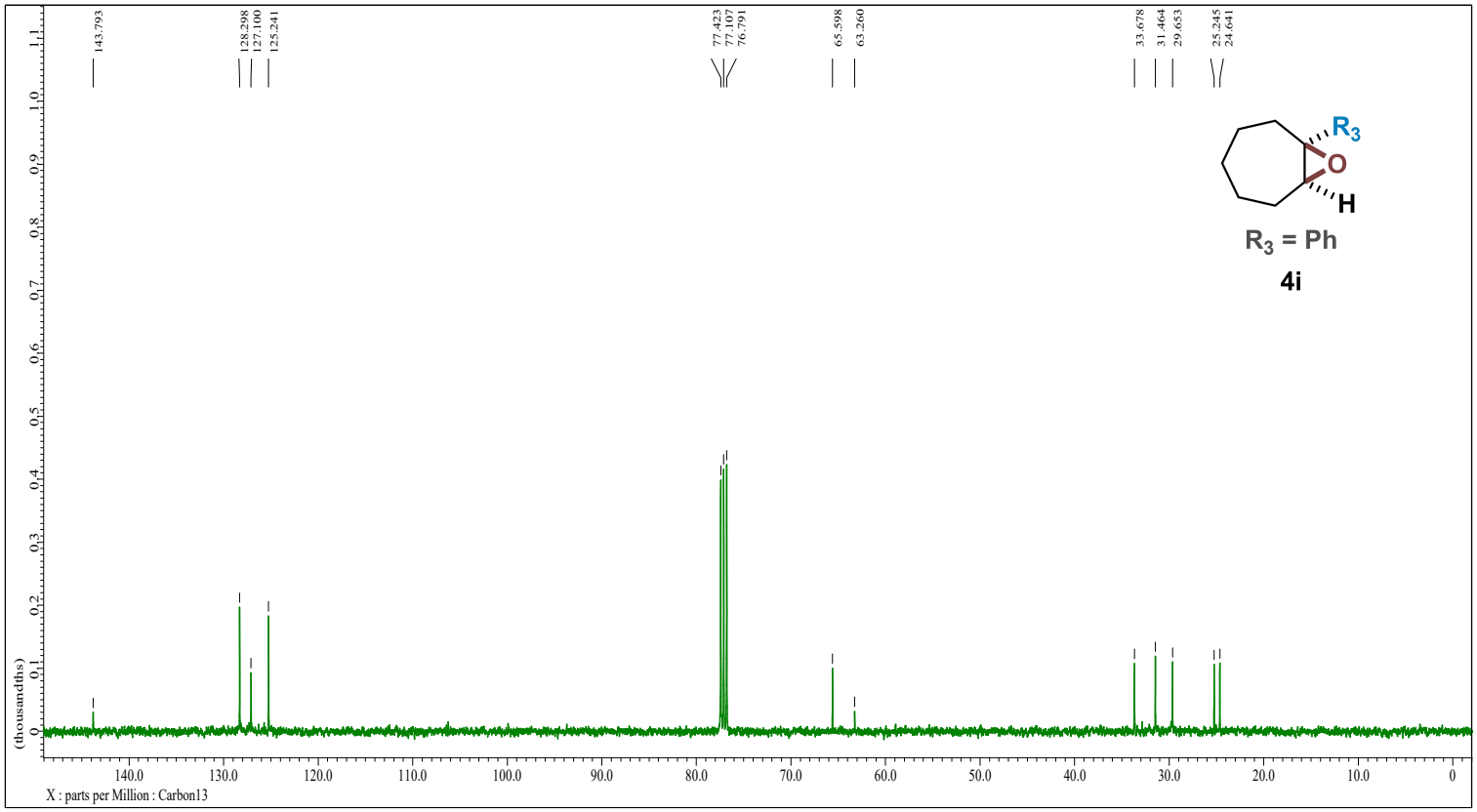

7.312
7.307
7.262
3.011
3.000
2.365
2.348
2.341
2.335
2.328
2.311
2.297
2.066
2.061
2.055
2.049
1.760
1.753
1.748
1.734
1.507
1.494
1.475
1.462
1.231
1.224
1.217
1.190
0.967
0.942
0.000
R3
O
Me
Me
H
R3 = 4-Cl-Ph
4g
4.11
1.00
1.04
1.14
2.22
1.05
1.10
3.07
abundance
X : parts per Million : Proton

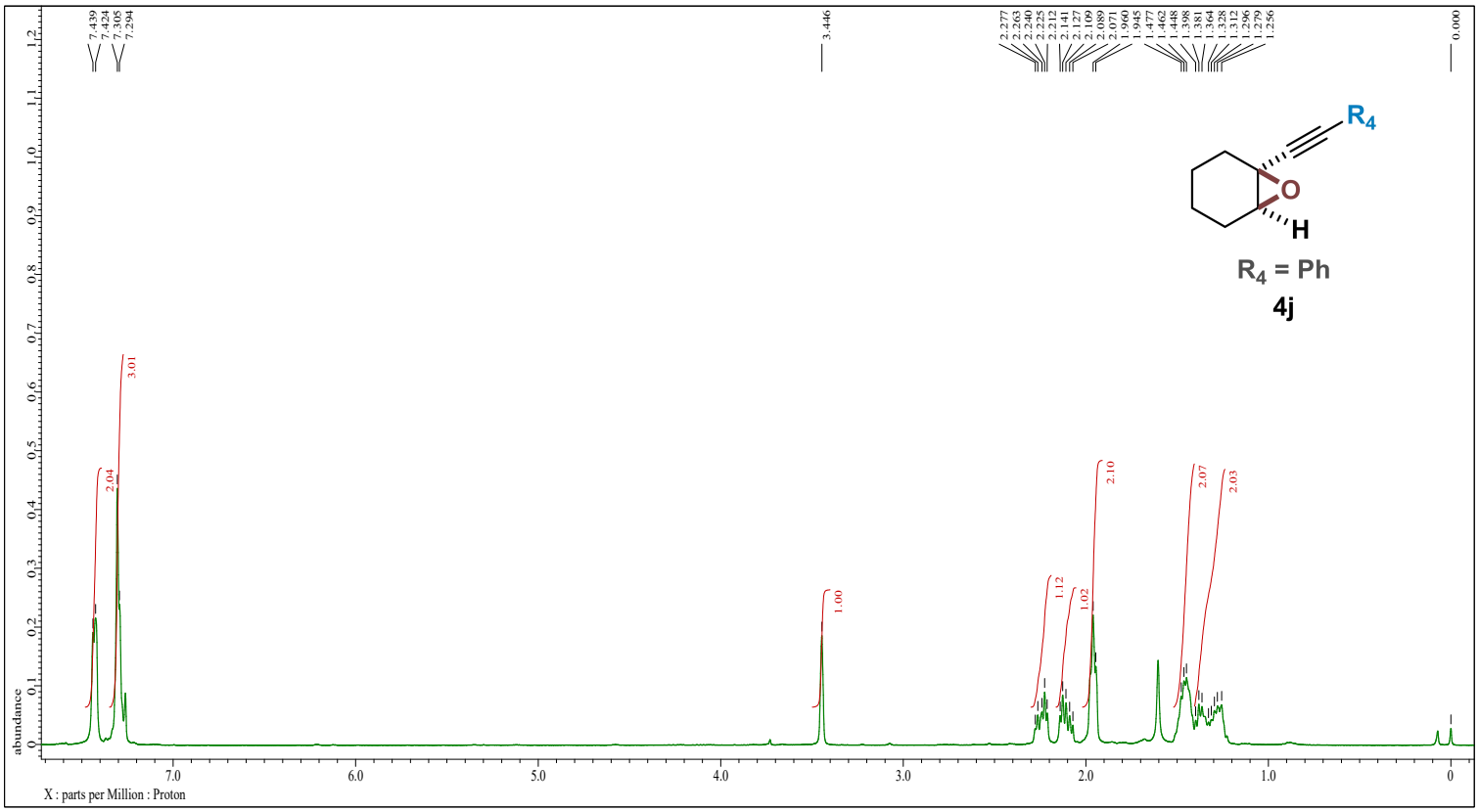

137.555
130.329
128.528
126.860
77.423
77.107
76.791
61.046
59.513
38.479
32.097
31.378
27.363
26.520
25.178
R3
O
Me
Me
H
R3 = 4-Cl-Ph
4g
(thousandths)
X : parts per Million : Carbon13

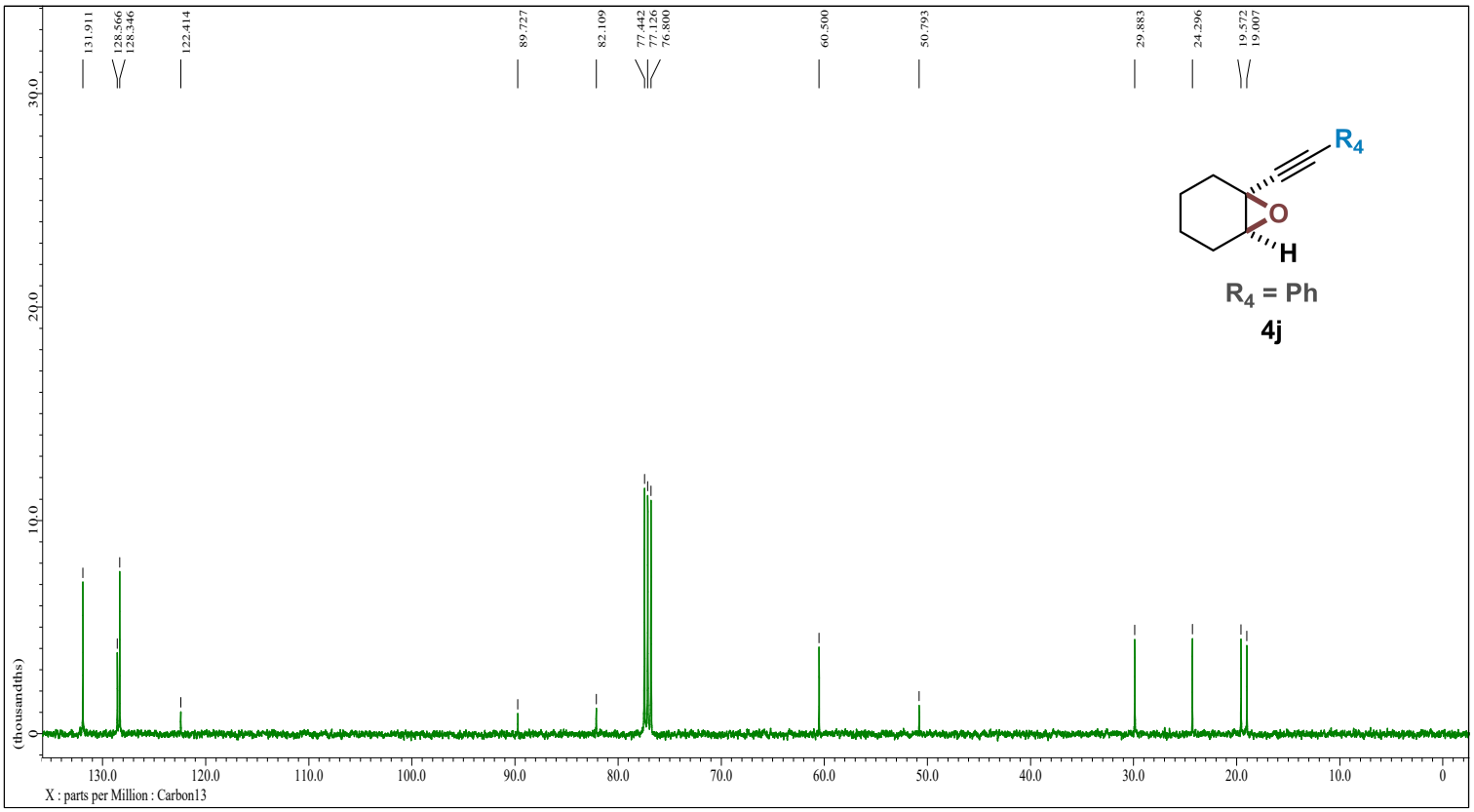

7.400
7.396
7.378
7.375
7.362
7.360
7.342
7.338
7.327
7.323
7.304
7.299
7.295
7.281
7.258
3.562
2.228
2.212
2.207
2.202
2.192
2.186
2.139
2.119
2.105
2.086
1.807
1.784
1.781
1.773
1.752
1.748
1.734
1.718
1.702
1.603
1.598
0.000
R3
O
H
R3 = Ph
4h
4.05
0.94
1.00
2.00
1.10
1.01
1.18
0.94
abundance
X : parts per Million : Proton

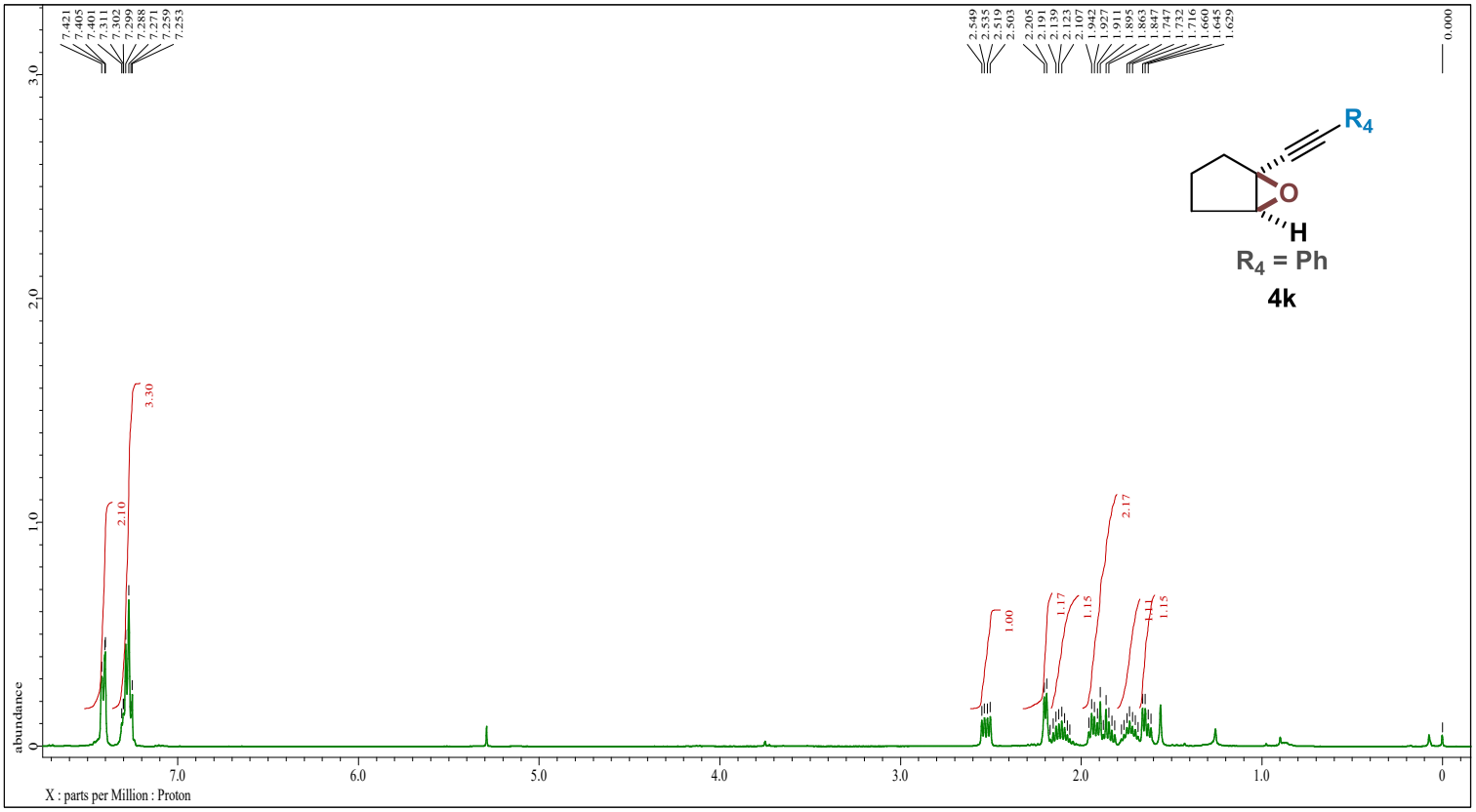

138.043
128.365
127.665
125.988
77.423
77.107
76.791
67.007
66.508
28.982
28.149
19.409
R3
O
H
R3 = Ph
4h
(thousandths)
X : parts per Million : Carbon13

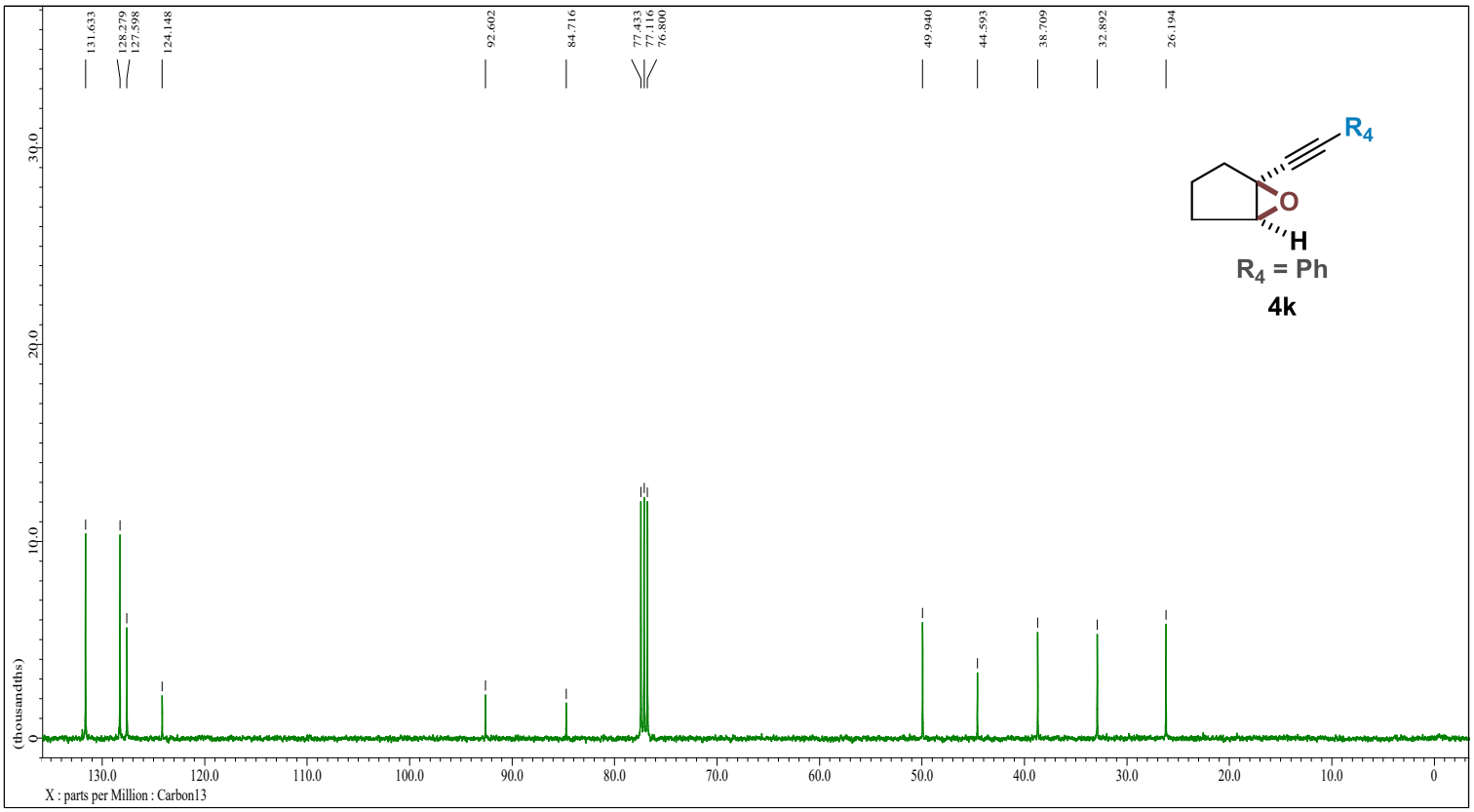

7.373
7.368
7.351
7.348
7.343
7.337
7.332
7.319
7.315
7.304
7.299
7.265
7.261
7.257
7.243
3.044
3.035
3.028
3.020
2.444
2.413
2.406
2.399
2.382
2.375
2.059
2.037
2.027
2.018
2.009
1.675
1.672
1.659
1.596
1.588
1.373
1.361
1.359
1.352
1.340
1.334
1.329
1.308
0.000
R3
O
H
R3 = Ph
4i
4.01
1.23
1.00
1.01
1.08
2.02
3.07
1.05
1.06
1.13
abundance
X : parts per Million : Proton

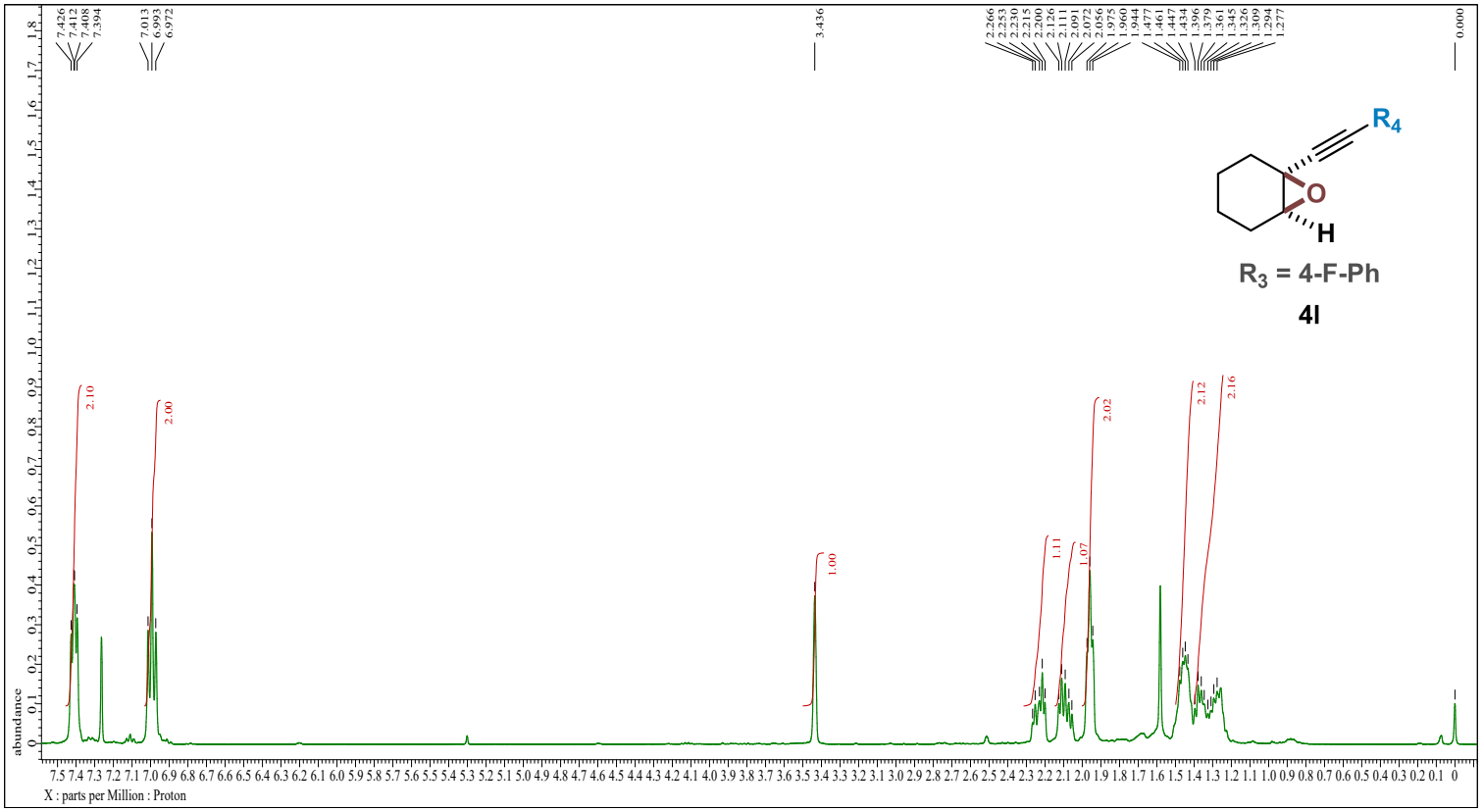

143.793
128.298
127.100
125.241
77.423
77.107
76.791
65.598
63.260
33.678
31.464
29.653
25.245
24.641
R3
O
H
R3 = Ph
4i
(thousandths)
X : parts per Million : Carbon13

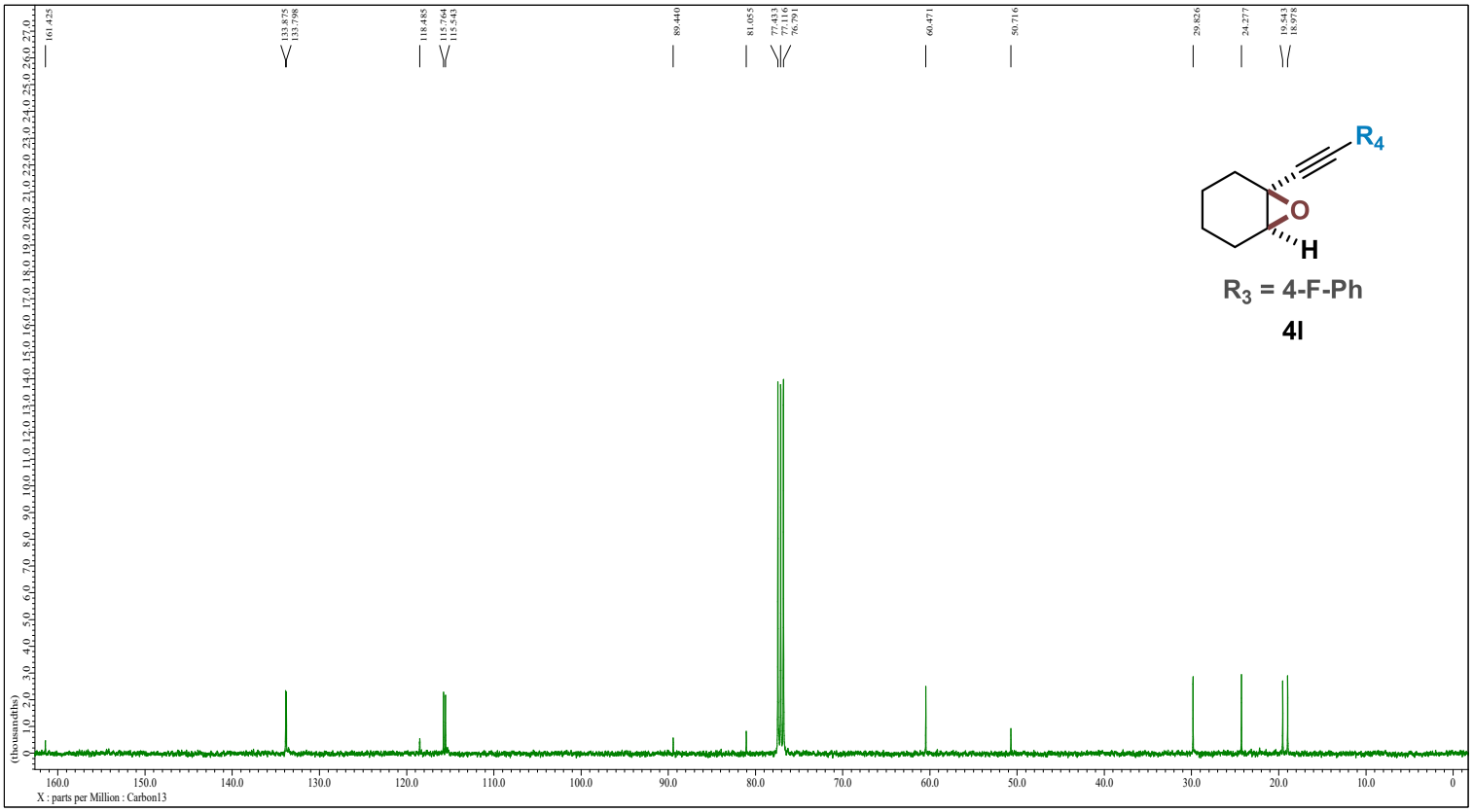

7.439
7.424
7.305
7.294
3.446
2.277
2.263
2.240
2.225
2.212
2.141
2.127
2.109
2.089
2.071
1.964
1.945
1.477
1.462
1.448
1.398
1.381
1.364
1.338
1.321
1.296
1.279
1.256
0.000
R4
O
H
R4 = Ph
4j
3.01
2.04
1.00
1.12
1.02
2.10
2.07
2.03
abundance
X : parts per Million : Proton

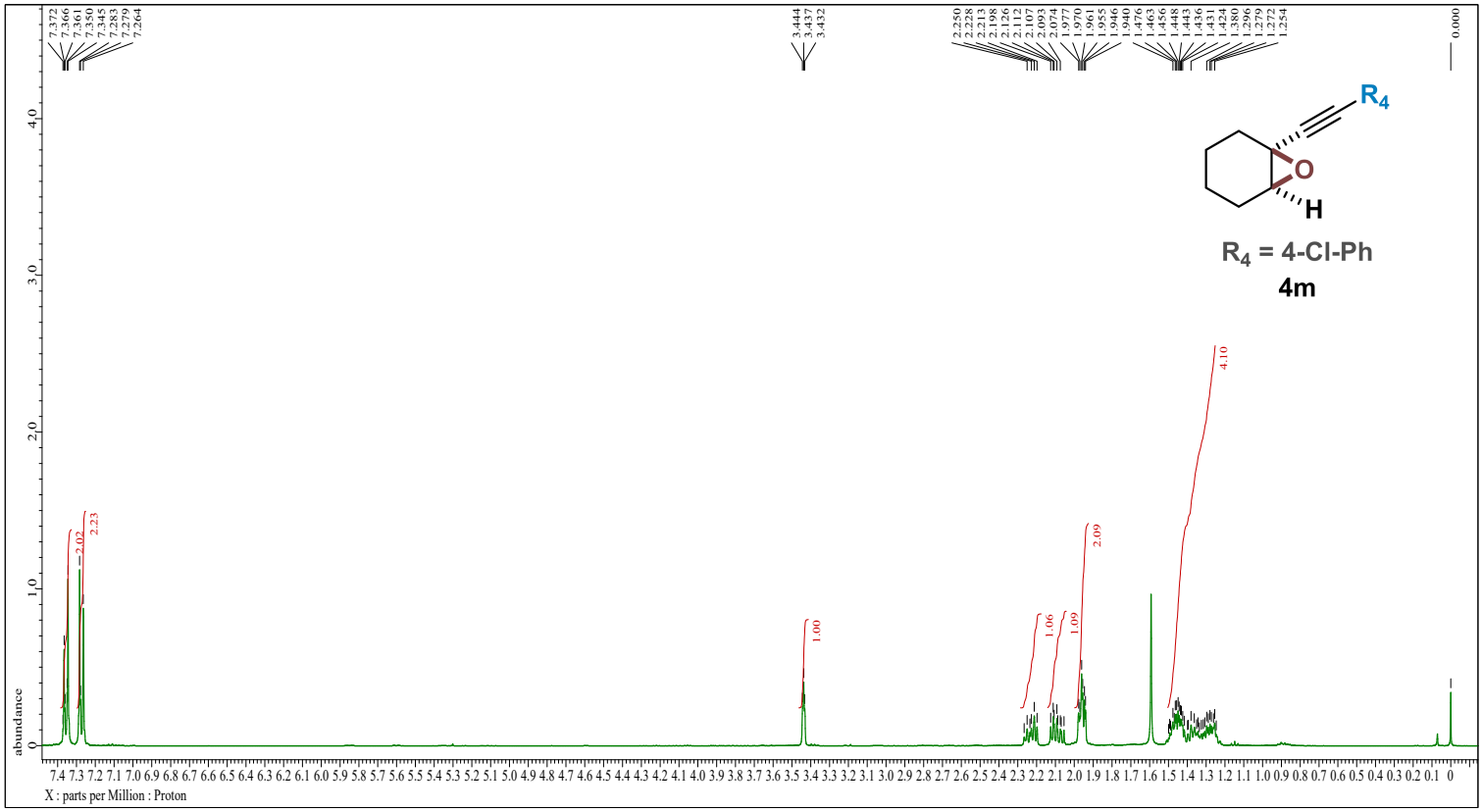

131.911
128.566
128.346
122.414
89.727
82.109
77.442
77.126
76.800
60.500
50.793
29.883
24.296
19.572
19.007
R4
O
H
R4 = Ph
4j
(thousandths)
X : parts per Million : Carbon13

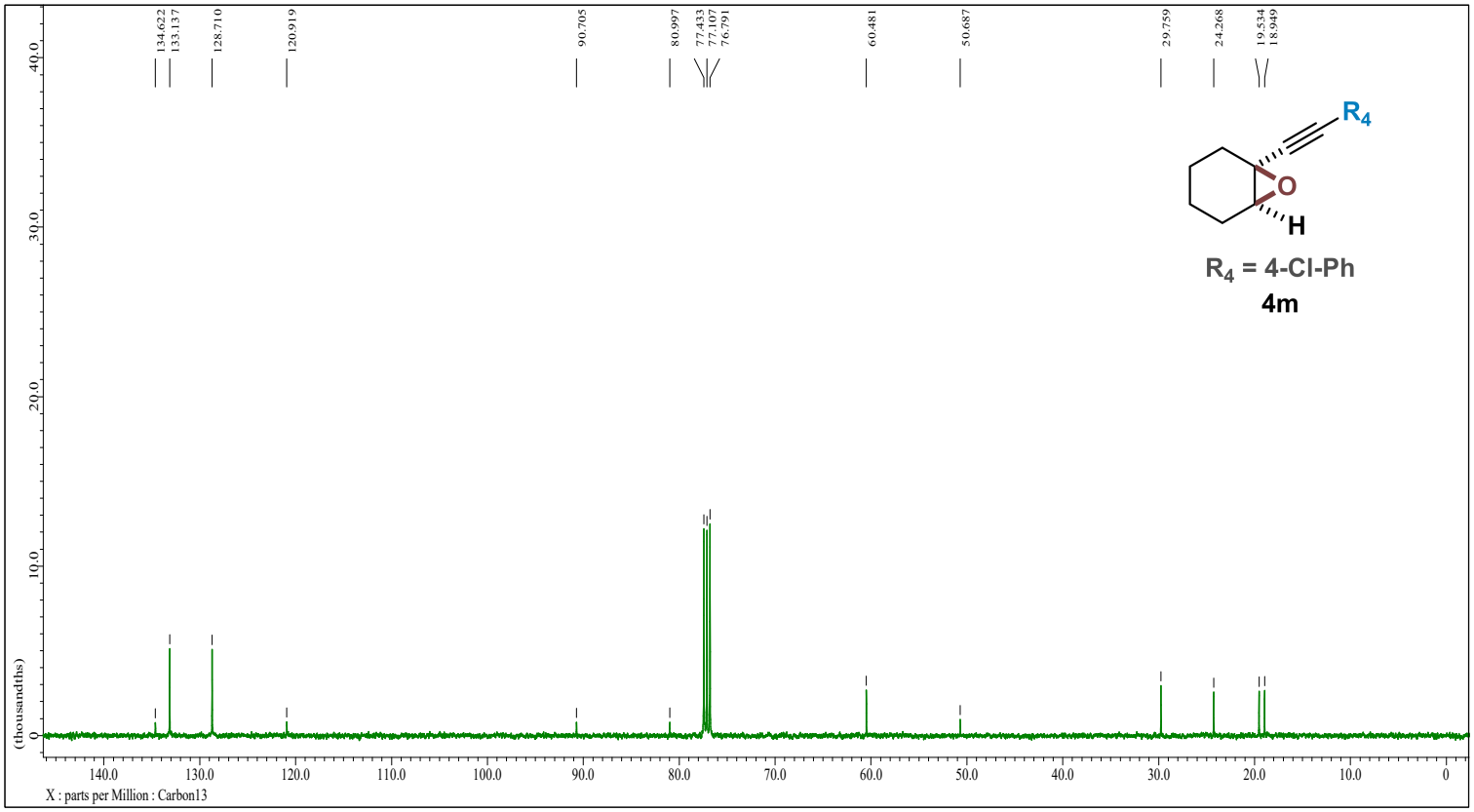

7.421
7.405
7.401
7.311
7.302
7.299
7.288
7.271
7.259
7.253
2.549
2.535
2.519
2.503
2.205
2.191
2.139
2.123
2.107
1.942
1.927
1.911
1.895
1.863
1.847
1.747
1.732
1.716
1.646
1.645
1.629
0.000
R4
O
H
R4 = Ph
4k
3.30
2.10
2.17
1.00
1.17
1.15
1.11
1.15
abundance
X : parts per Million : Proton

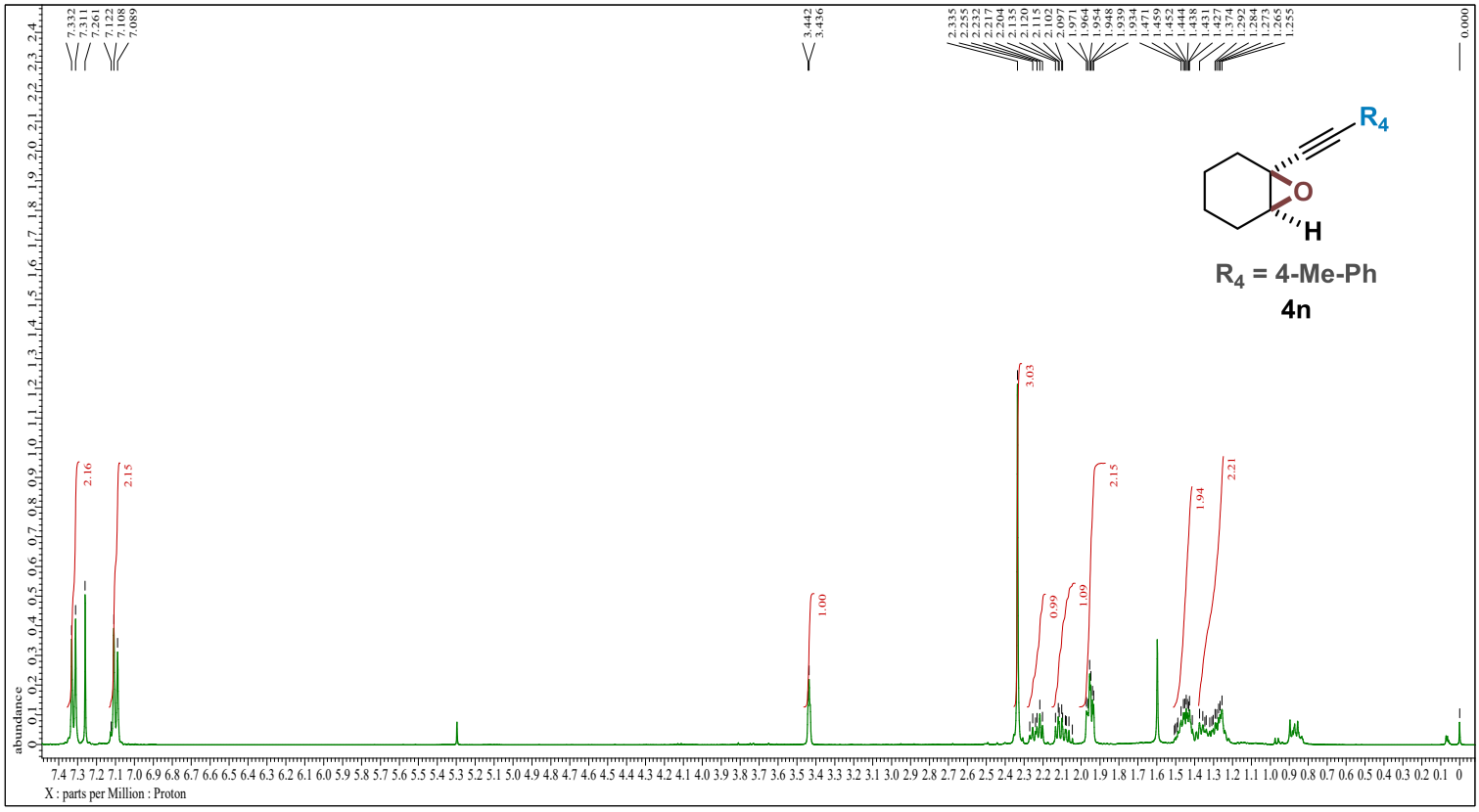

131.633
128.279
127.598
124.148
92.602
84.716
77.433
77.116
76.800
49.940
44.593
38.709
32.892
26.194
R4
O
H
R4 = Ph
4k
(thousandths)
X : parts per Million : Carbon13

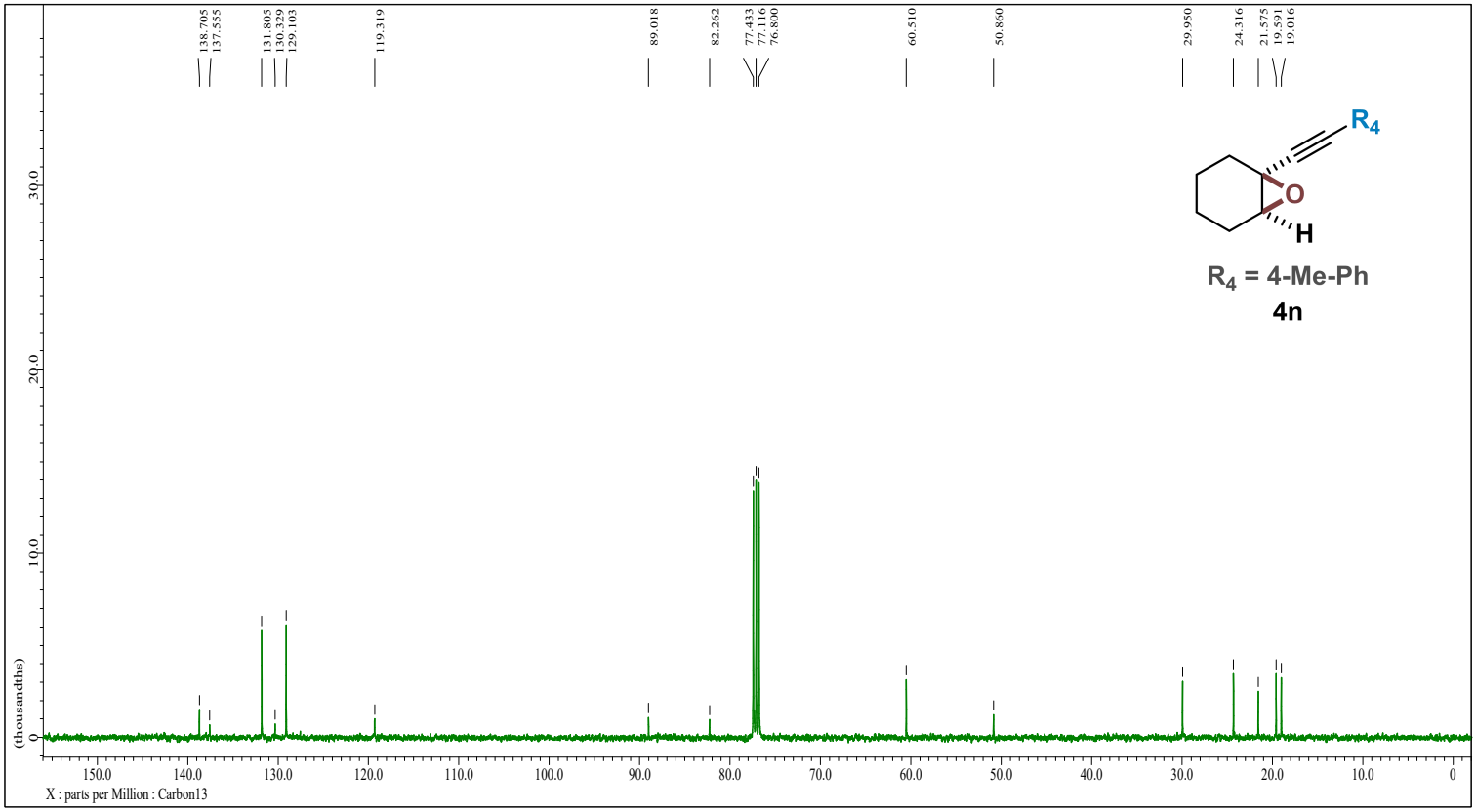

7.426
7.412
7.408
7.394
7.013
6.993
6.972
3.436
0.000
2.10
2.00
1.00
1.11
1.07
2.02
2.12
2.16
abundance
X : parts per Million : Proton
R4
O
H
R3 = 4-F-Ph
4l

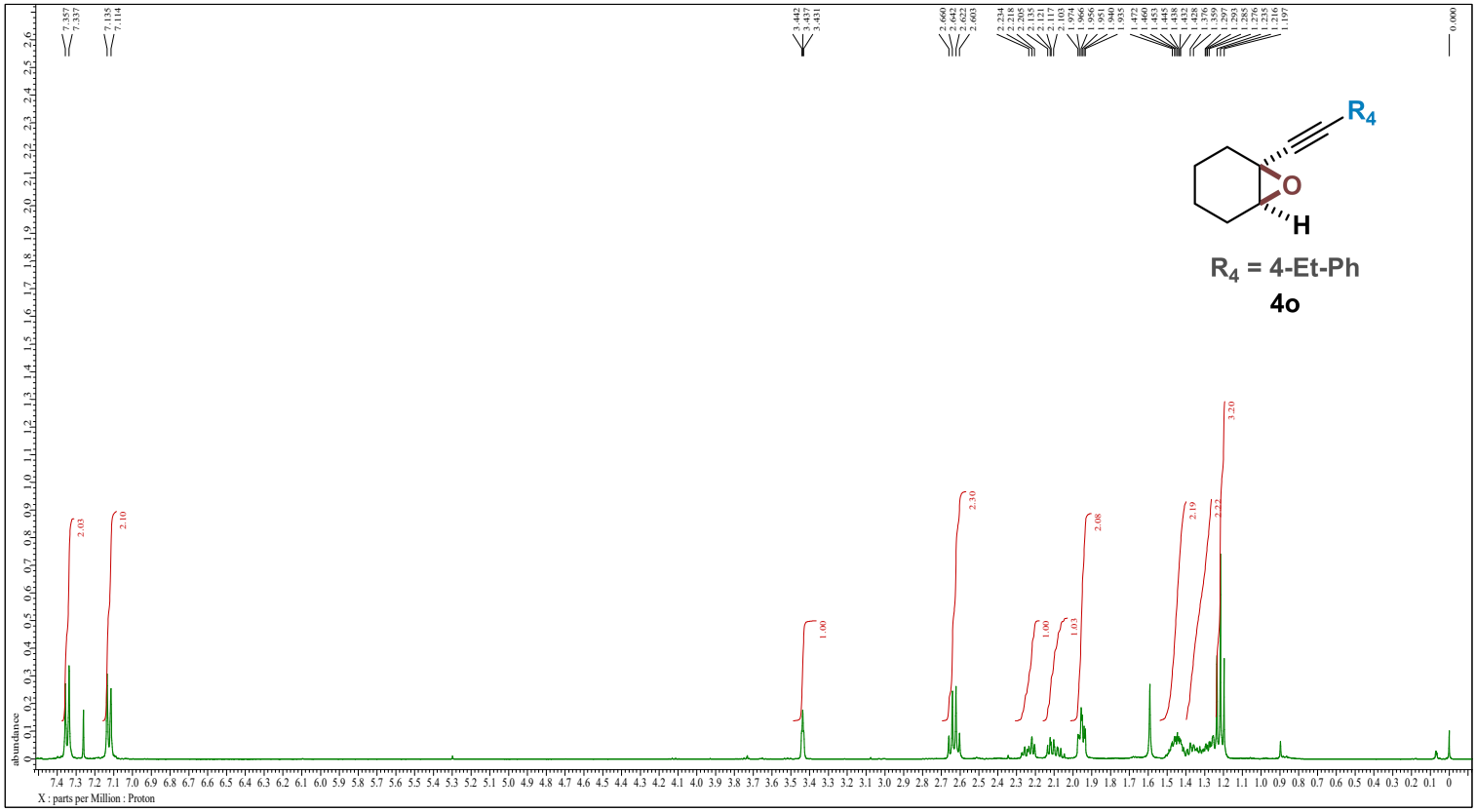

161.425
133.875
133.798
118.485
115.764
115.543
89.440
81.055
77.433
77.116
76.791
60.471
50.716
29.826
24.277
19.543
18.978
(thousandths)
X : parts per Million : Carbon13
R4
O
H
R3 = 4-F-Ph
4l

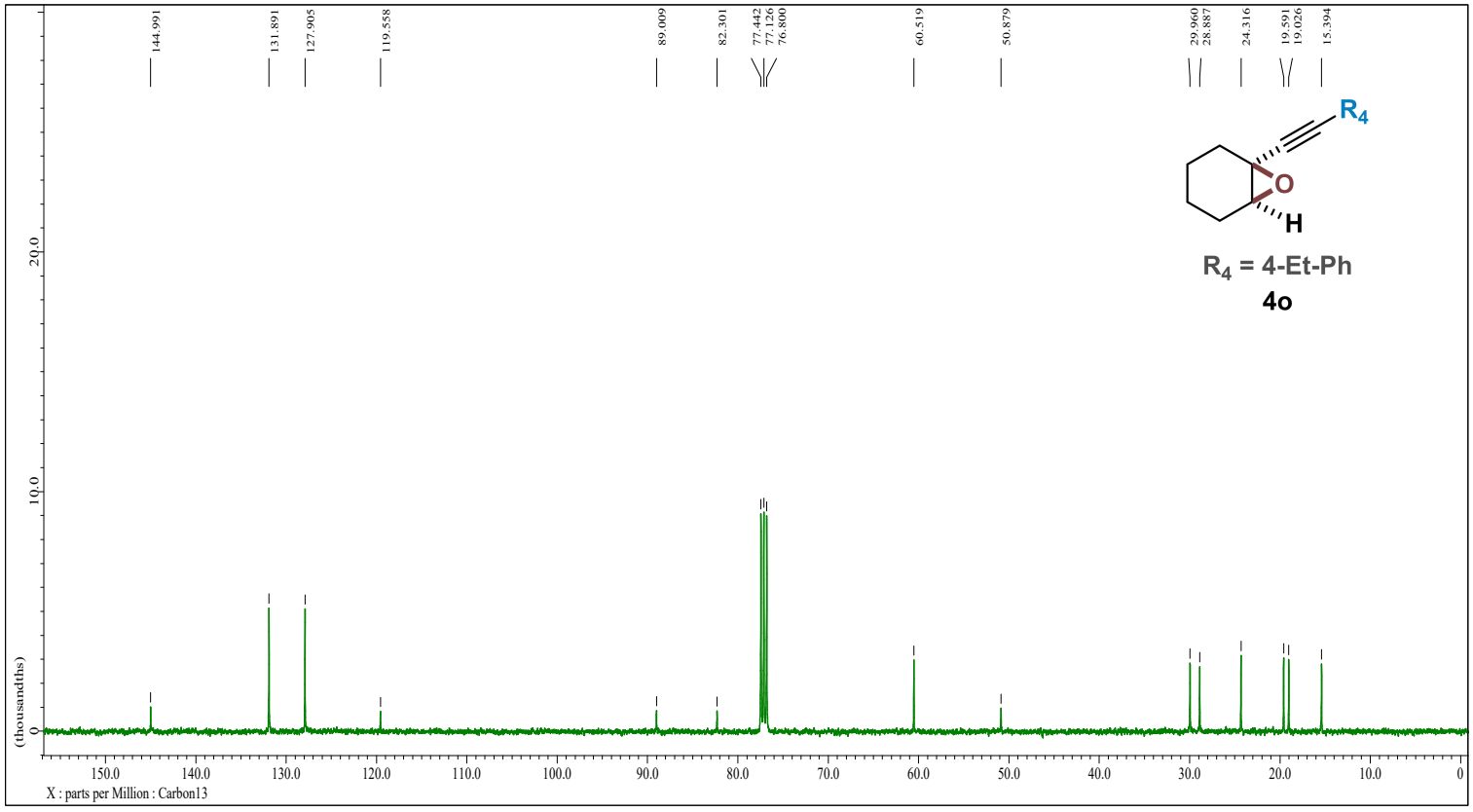

R4
O
H
R4 = 4-Cl-Ph
4m
abundance
X : parts per Million : Proton

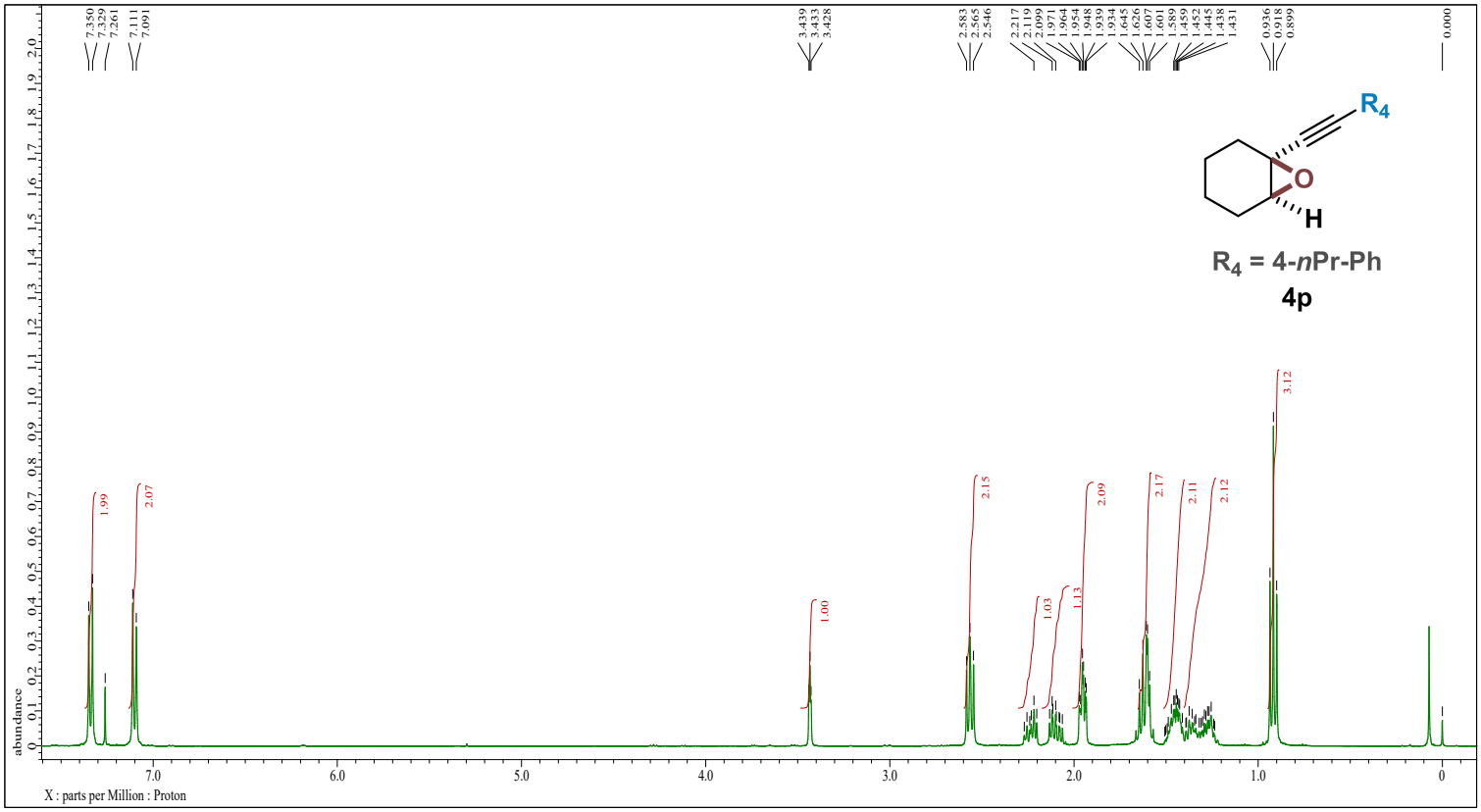

R4
O
H
R4 = 4-Cl-Ph
4m
(thousandths)
X : parts per Million : Carbon13

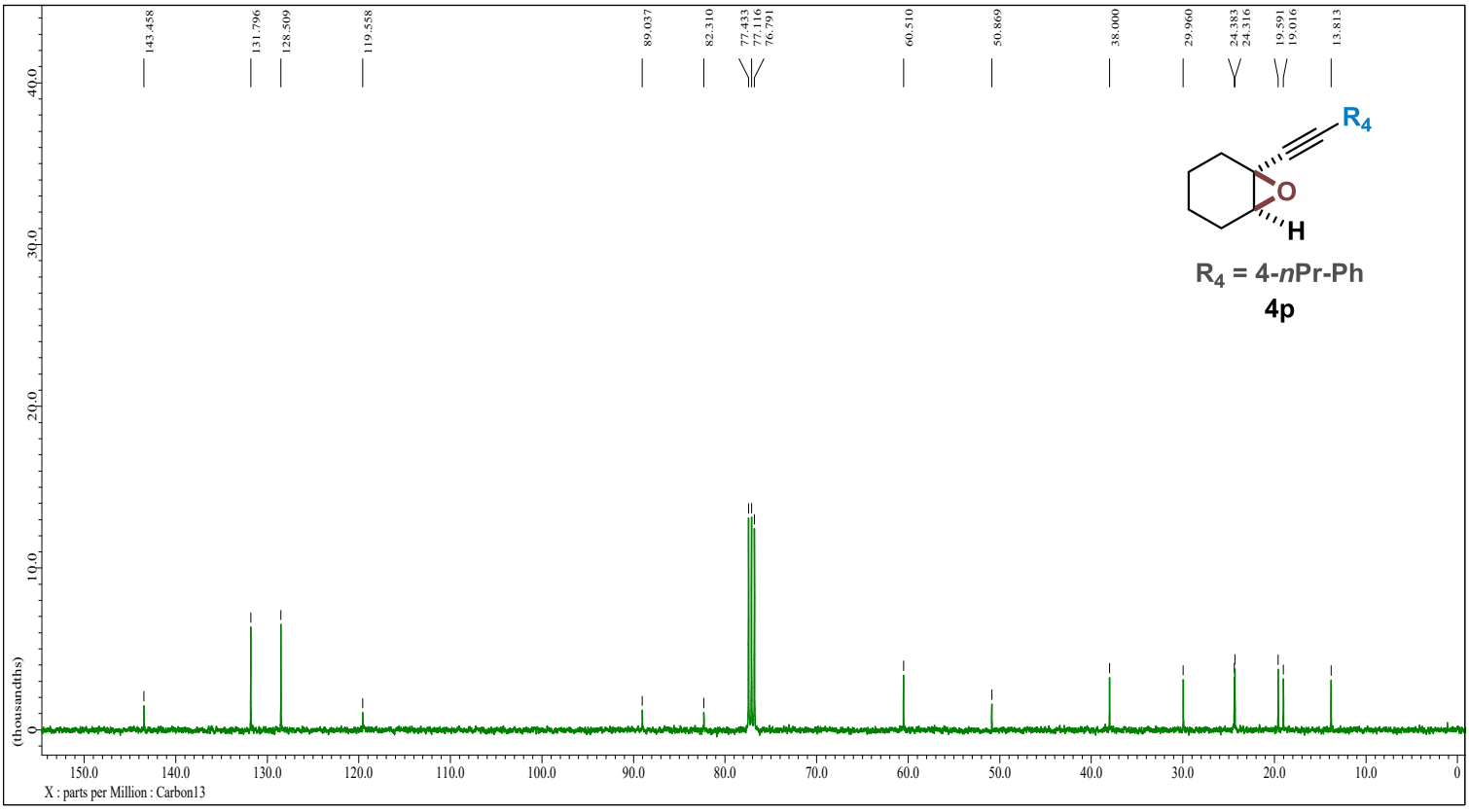

R4
O
H
R4 = 4-Me-Ph
4n
abundance
X : parts per Million : Proton

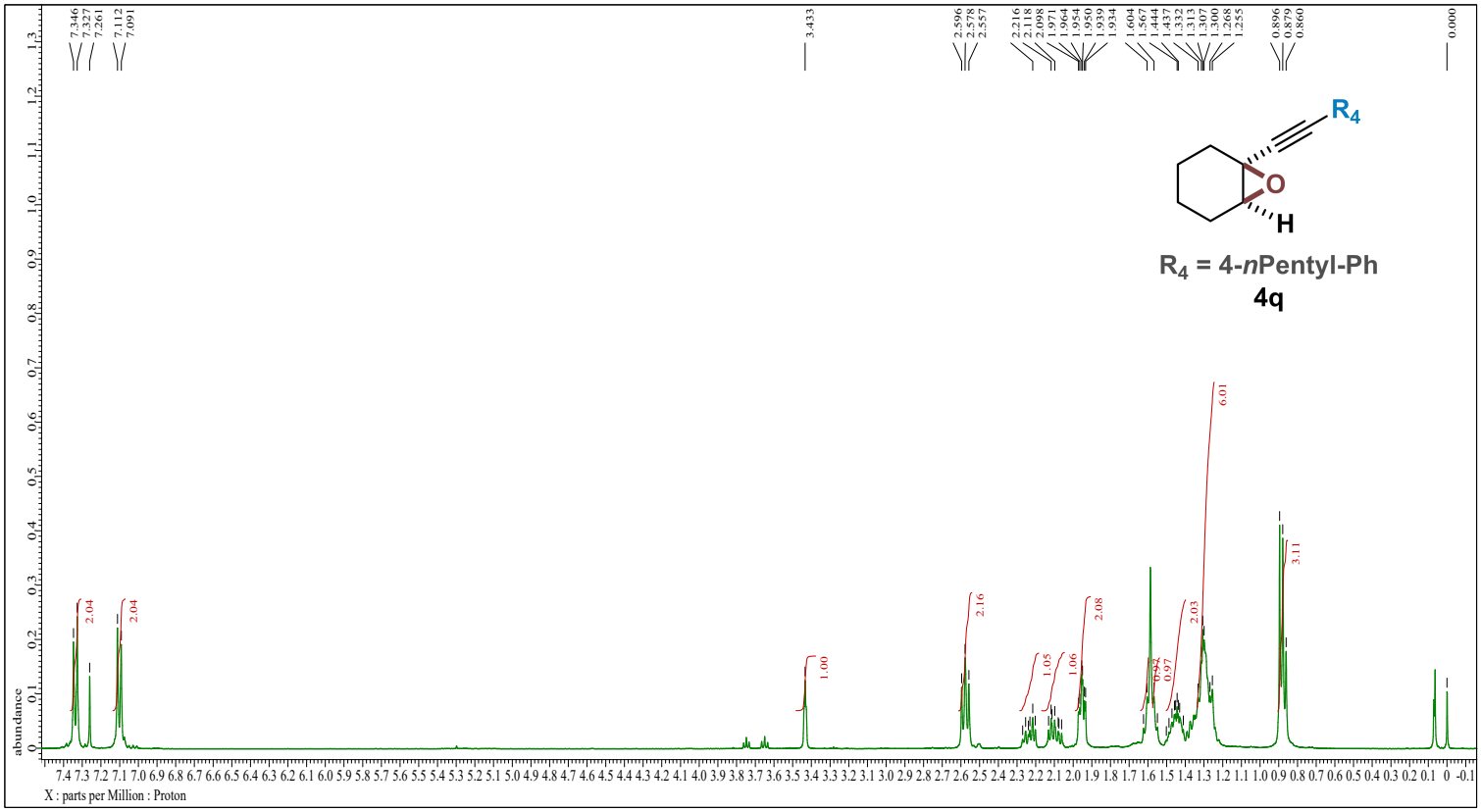

R4
O
H
R4 = 4-Me-Ph
4n
(thousandths)
X : parts per Million : Carbon13

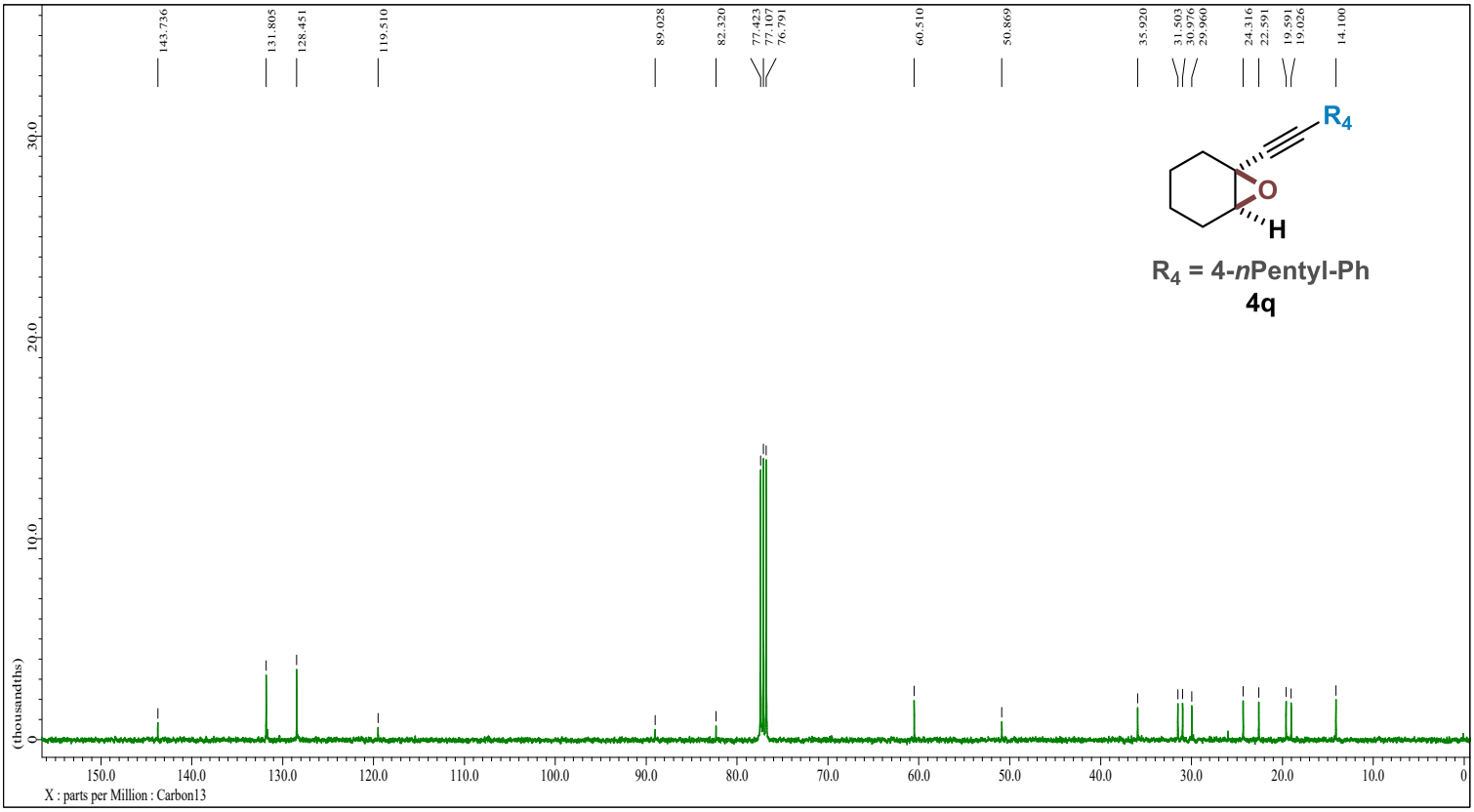

R4
O
H
R4 = 4-Et-Ph
4o
X : parts per Million : Proton

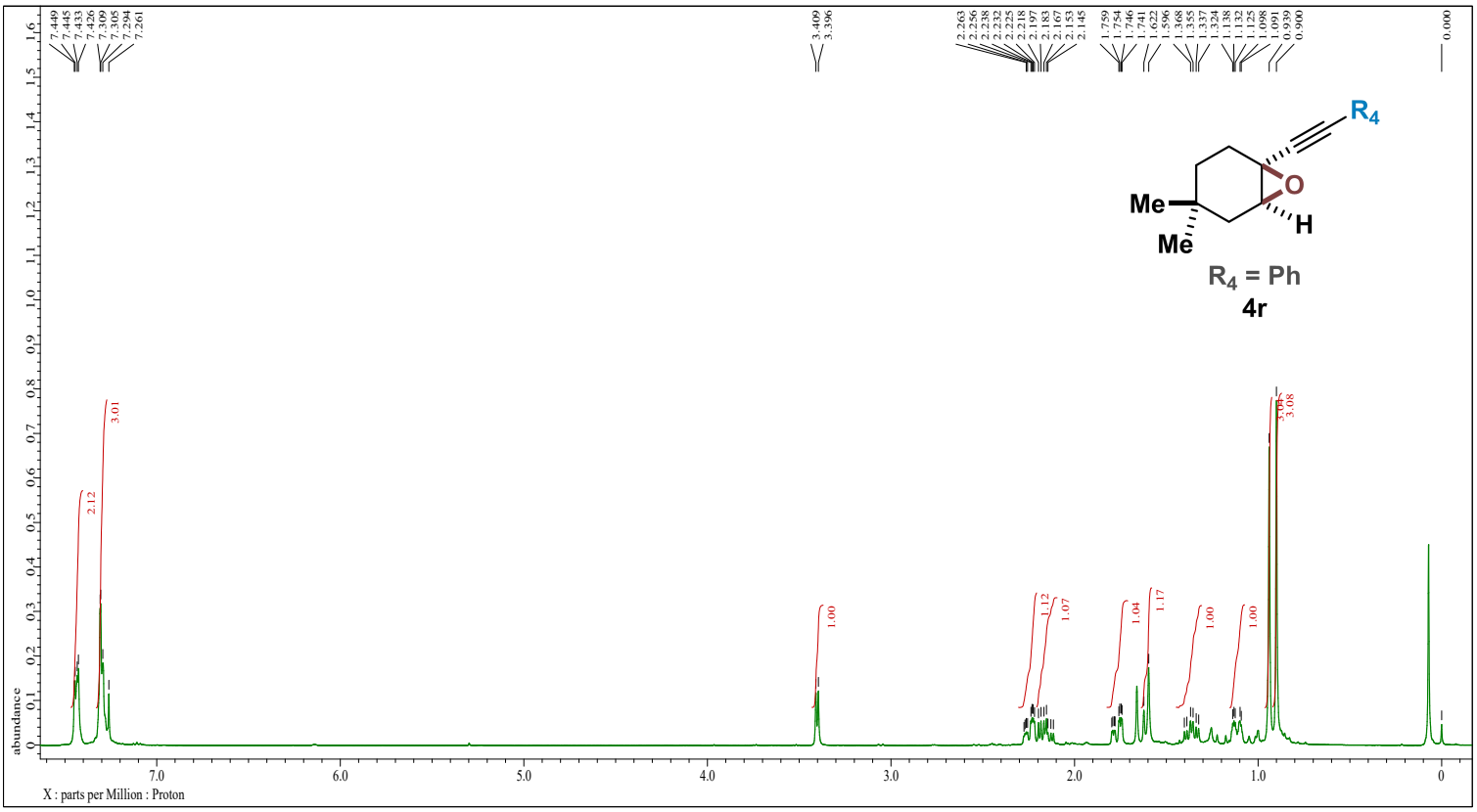

R4
O
H
R4 = 4-Et-Ph
4o
X : parts per Million : Carbon13

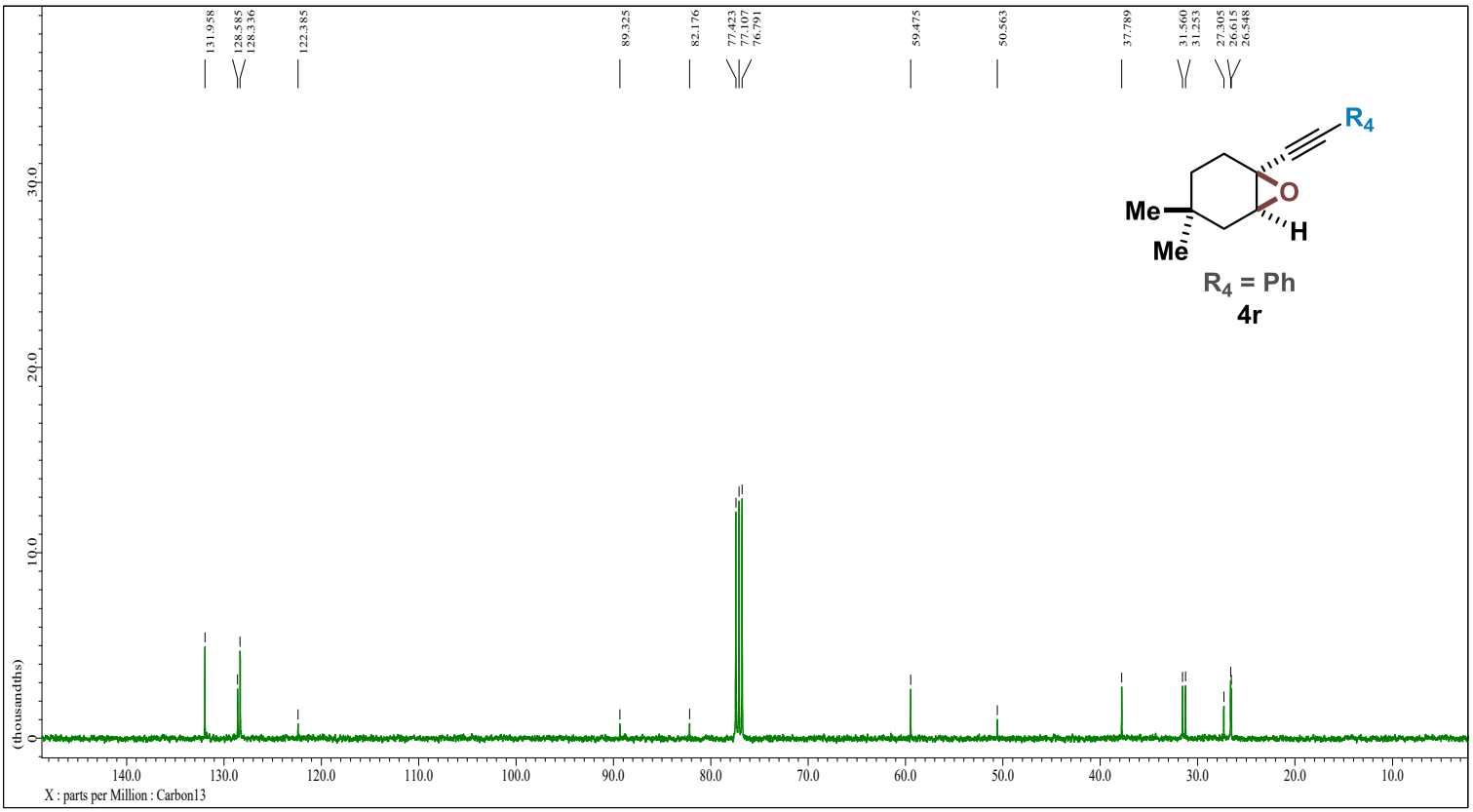

7.350
7.339
7.261
7.111
7.091
3.439
3.433
3.428
2.583
2.565
2.546
2.217
2.119
2.099
1.971
1.964
1.954
1.948
1.939
1.934
1.645
1.626
1.607
1.601
1.590
1.459
1.452
1.445
1.438
1.431
0.936
0.918
0.899
0.000
R4
O
H
R4 = 4-nPr-Ph
4p
1.99
2.07
1.00
2.15
1.03
1.13
2.09
2.17
2.11
2.12
3.12
abundance
X : parts per Million : Proton

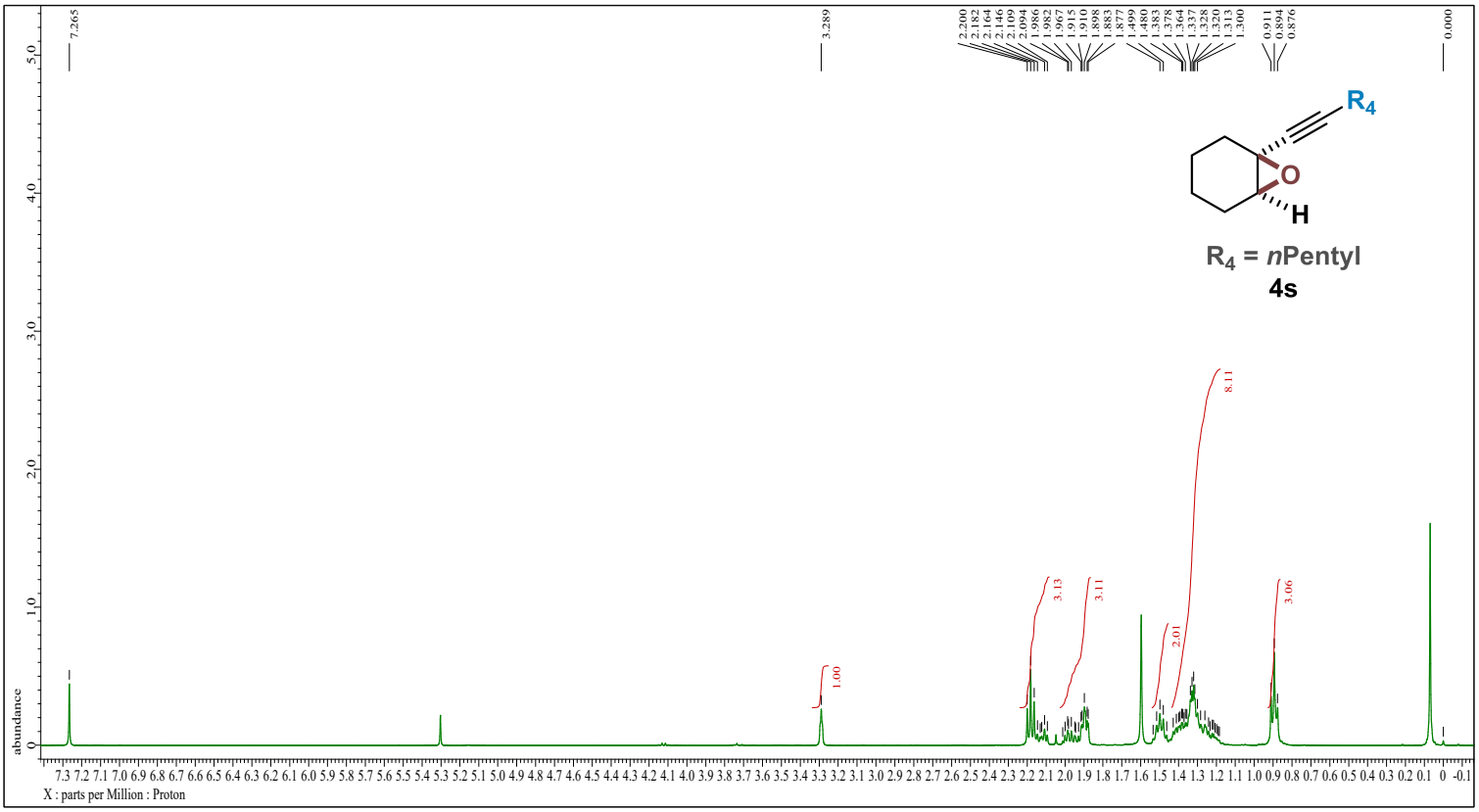

143.458
131.796
128.509
119.558
89.037
82.310
77.433
77.116
76.791
60.510
50.869
38.000
29.960
24.383
24.316
19.591
19.016
13.813
R4
O
H
R4 = 4-nPr-Ph
4p
(thousandths)
X : parts per Million : Carbon13

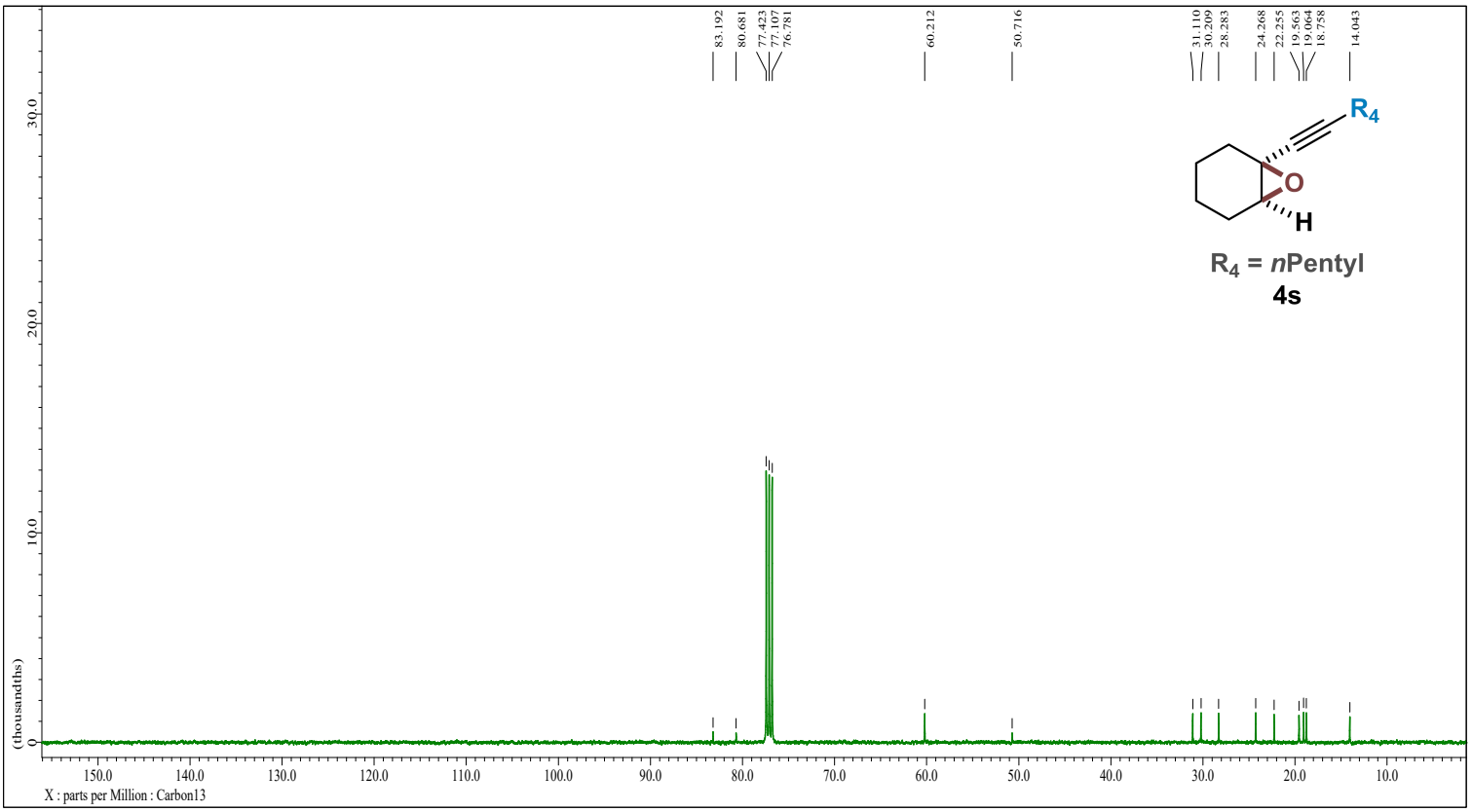

7.346
7.327
7.261
7.112
7.091
3.433
2.596
2.578
2.557
2.216
2.118
2.098
1.971
1.964
1.954
1.950
1.939
1.934
1.604
1.567
1.444
1.437
1.332
1.313
1.307
1.300
1.266
1.255
0.896
0.879
0.860
0.000
R4
O
H
R4 = 4-nPentyl-Ph
4q
abundance
X : parts per Million : Proton

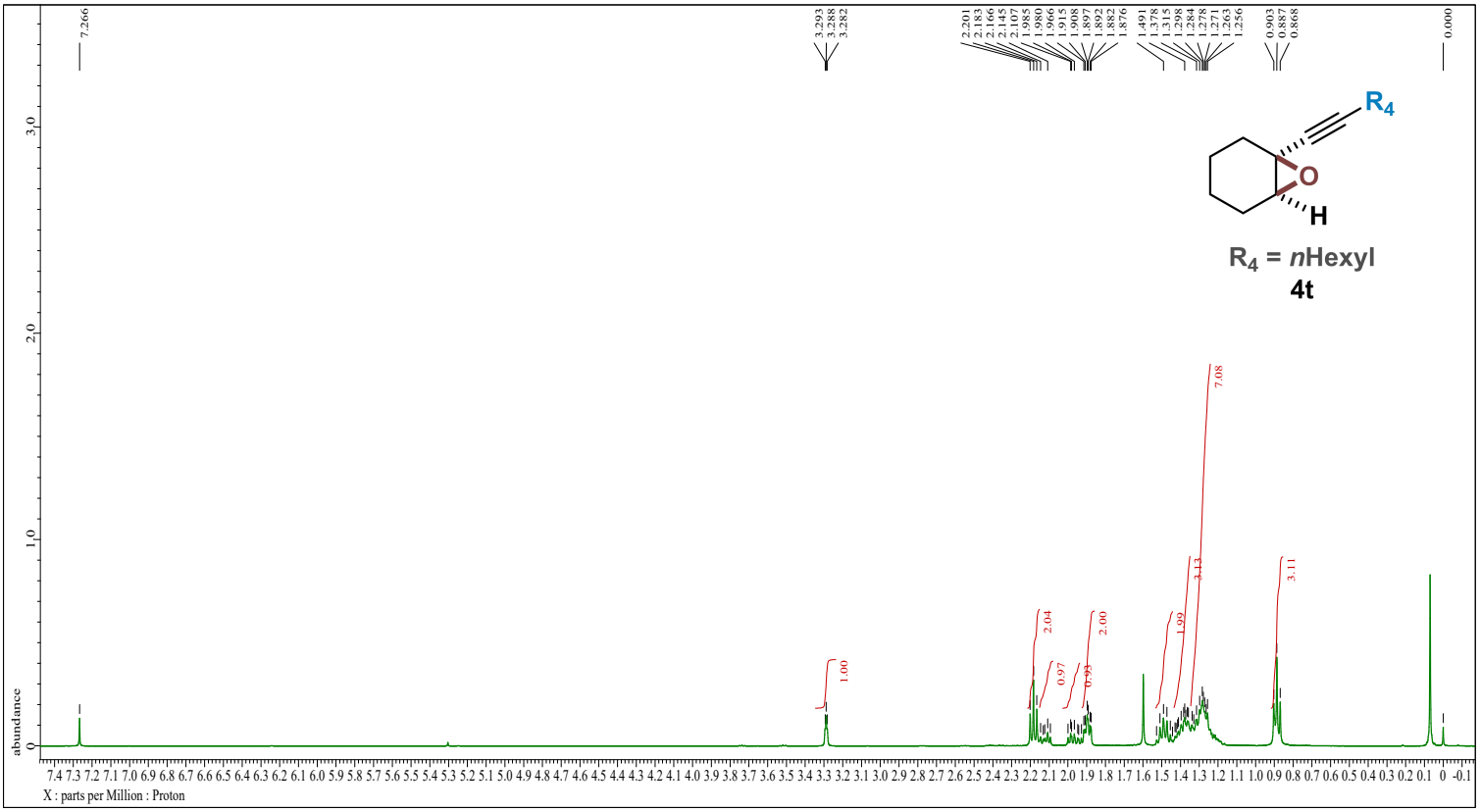

143.736
131.805
128.451
119.510
89.028
82.320
77.423
77.107
76.791
60.510
50.869
35.920
31.503
30.976
29.960
24.316
22.591
19.591
19.026
14.100
R4
O
H
R4 = 4-nPentyl-Ph
4q
(thousandths)
X : parts per Million : Carbon13

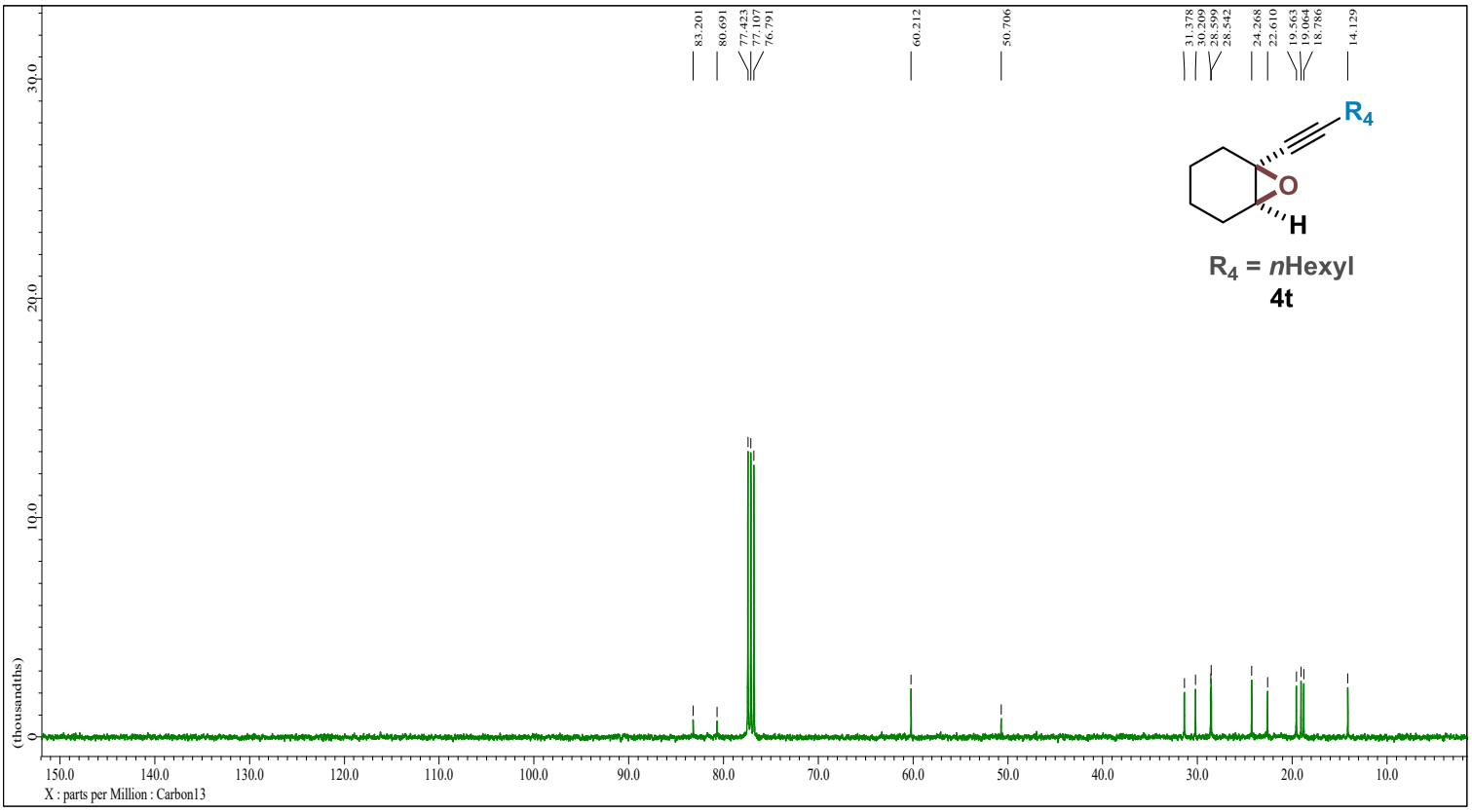

7.449
7.445
7.433
7.426
7.309
7.305
7.294
7.261
3.409
3.396
2.263
2.256
2.238
2.232
2.225
2.218
2.197
2.185
2.167
2.153
2.145
1.759
1.754
1.746
1.741
1.622
1.596
1.368
1.355
1.337
1.324
1.138
1.132
1.125
1.098
1.091
0.939
0.900
0.000
R4
O
Me
Me
H
R4 = Ph
4r
abundance
3.01
2.12
1.00
1.12
1.07
1.04
1.17
1.00
1.00
3.08
X : parts per Million : Proton

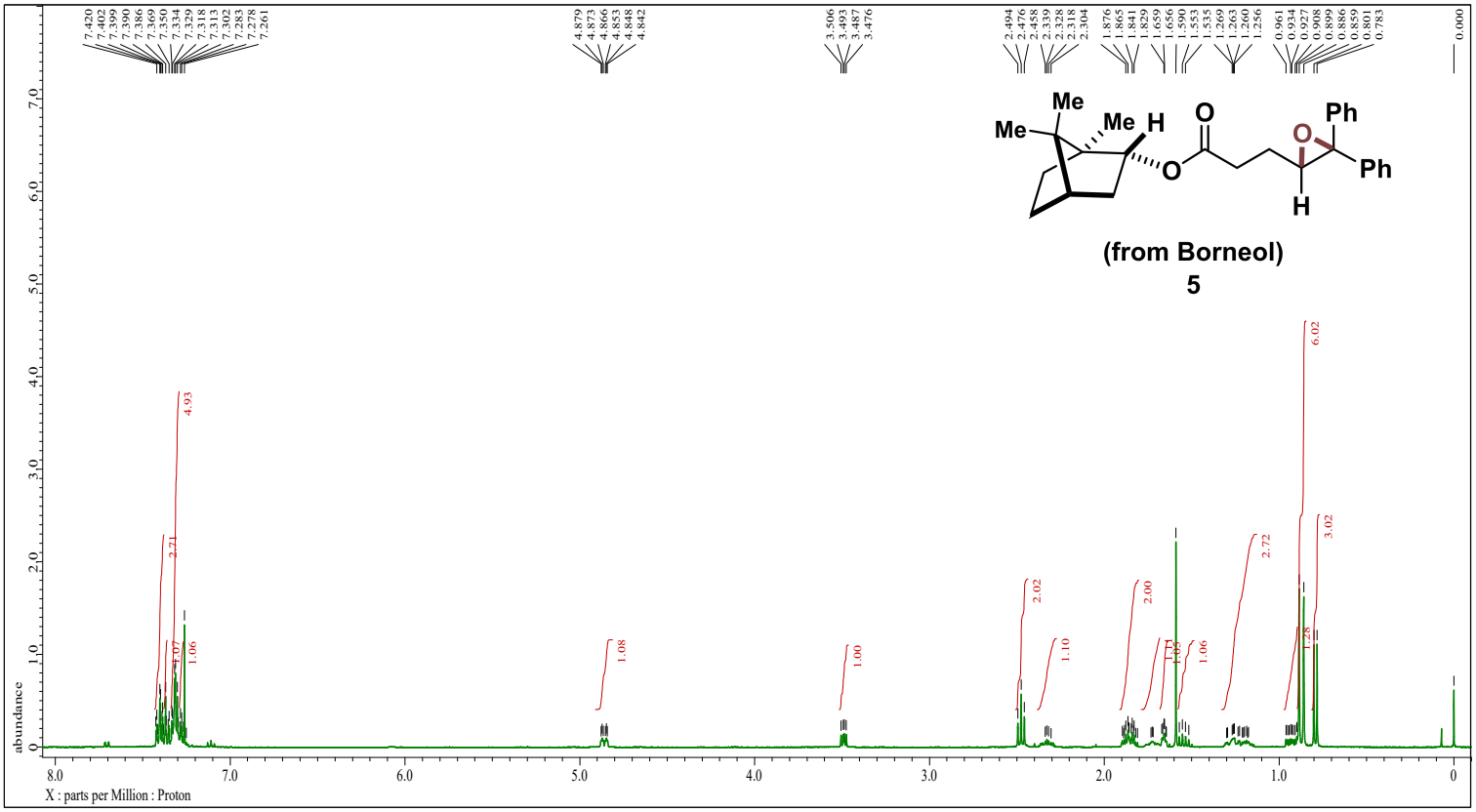

131.958
128.585
128.356
122.385
89.325
82.176
77.423
77.107
76.791
59.475
50.563
37.789
31.560
31.253
27.305
26.615
26.548
R4
O
Me
Me
H
R4 = Ph
4r
(thousandths)
X : parts per Million : Carbon13

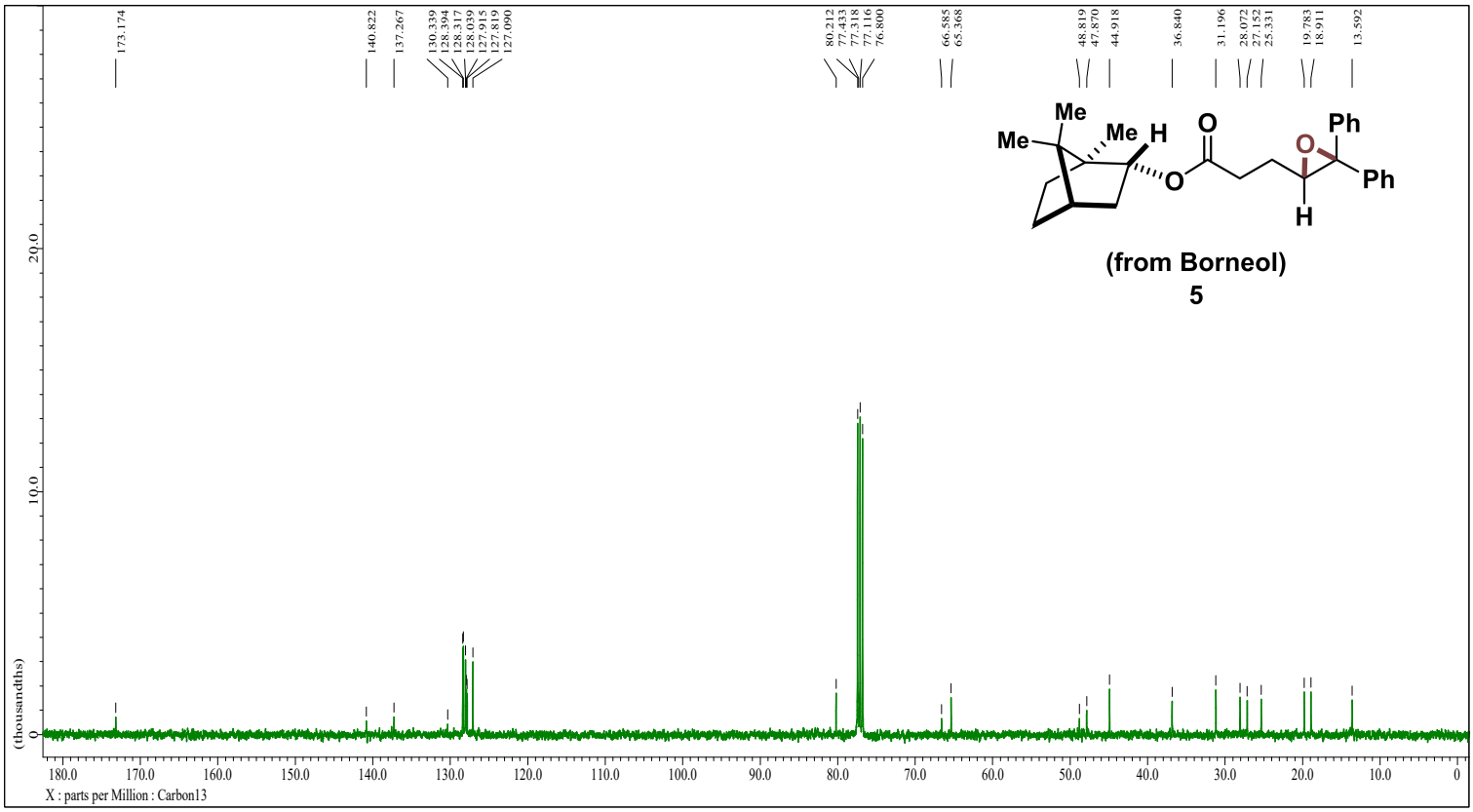

7.265
3.289
2.200
2.182
2.164
2.146
2.109
2.094
1.986
1.962
1.915
1.910
1.898
1.883
1.877
1.499
1.480
1.343
1.328
1.364
1.337
1.328
1.320
1.313
1.300
0.911
0.894
0.876
0.000
R4
O
H
R4 = nPentyl
4s
8.11
3.13
3.11
2.01
3.06
1.00
abundance
X : parts per Million : Proton

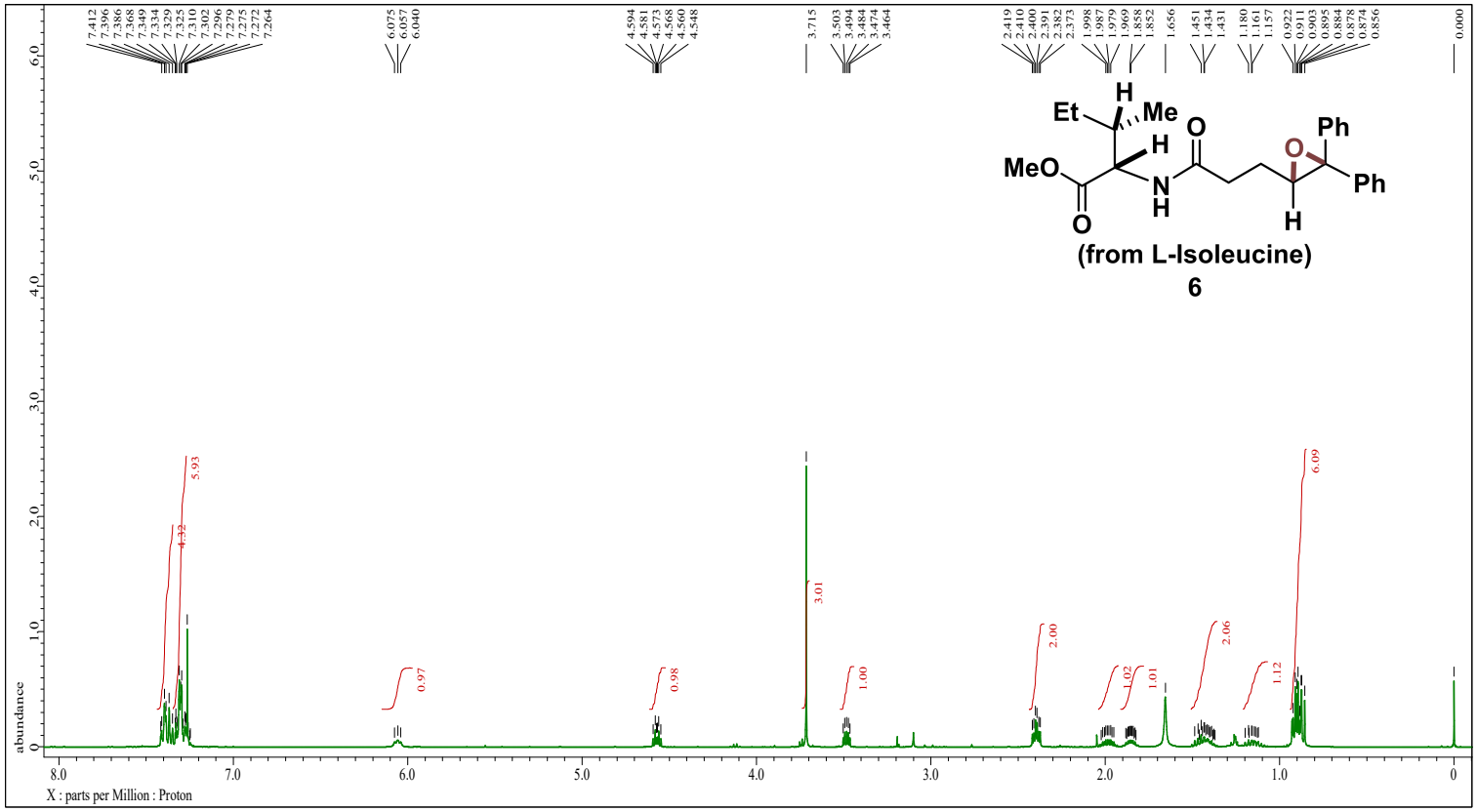

83.192
80.681
77.423
77.107
76.781
60.212
50.716
31.110
30.209
28.283
24.268
22.255
19.563
19.064
18.758
14.043
R4
O
H
R4 = nPentyl
4s
(thousandths)
X : parts per Million : Carbon13

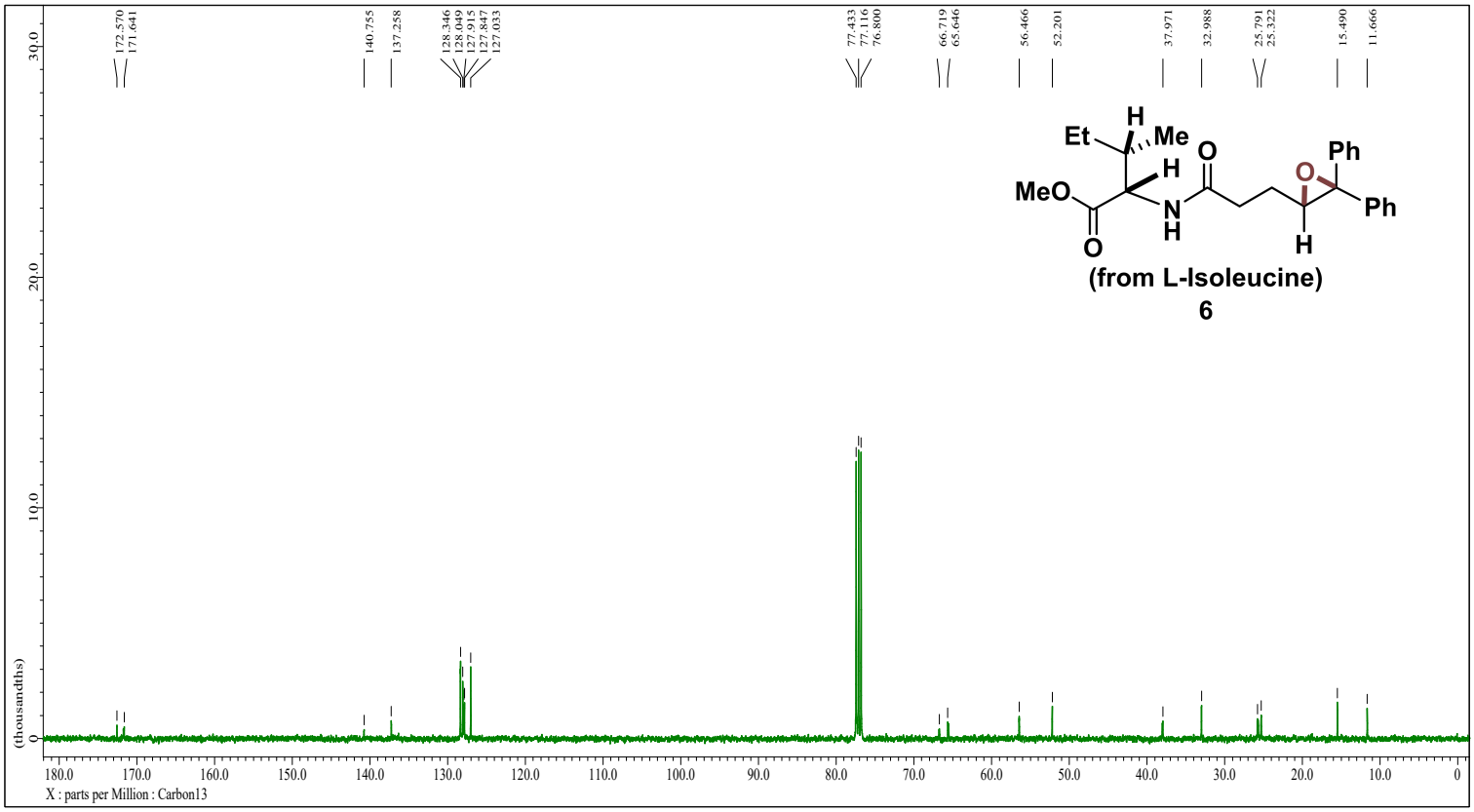

7.266
3.293
3.288
3.282
2.201
2.183
2.166
2.145
2.107
1.985
1.980
1.966
1.915
1.908
1.897
1.892
1.882
1.876
1.491
1.378
1.315
1.298
1.284
1.278
1.271
1.268
1.256
0.903
0.897
0.868
0.000
R4
O
H
R4 = nHexyl
4t
7.08
3.13
3.11
2.04
2.00
1.99
1.00
0.97
0.93
abundance
X : parts per Million : Proton

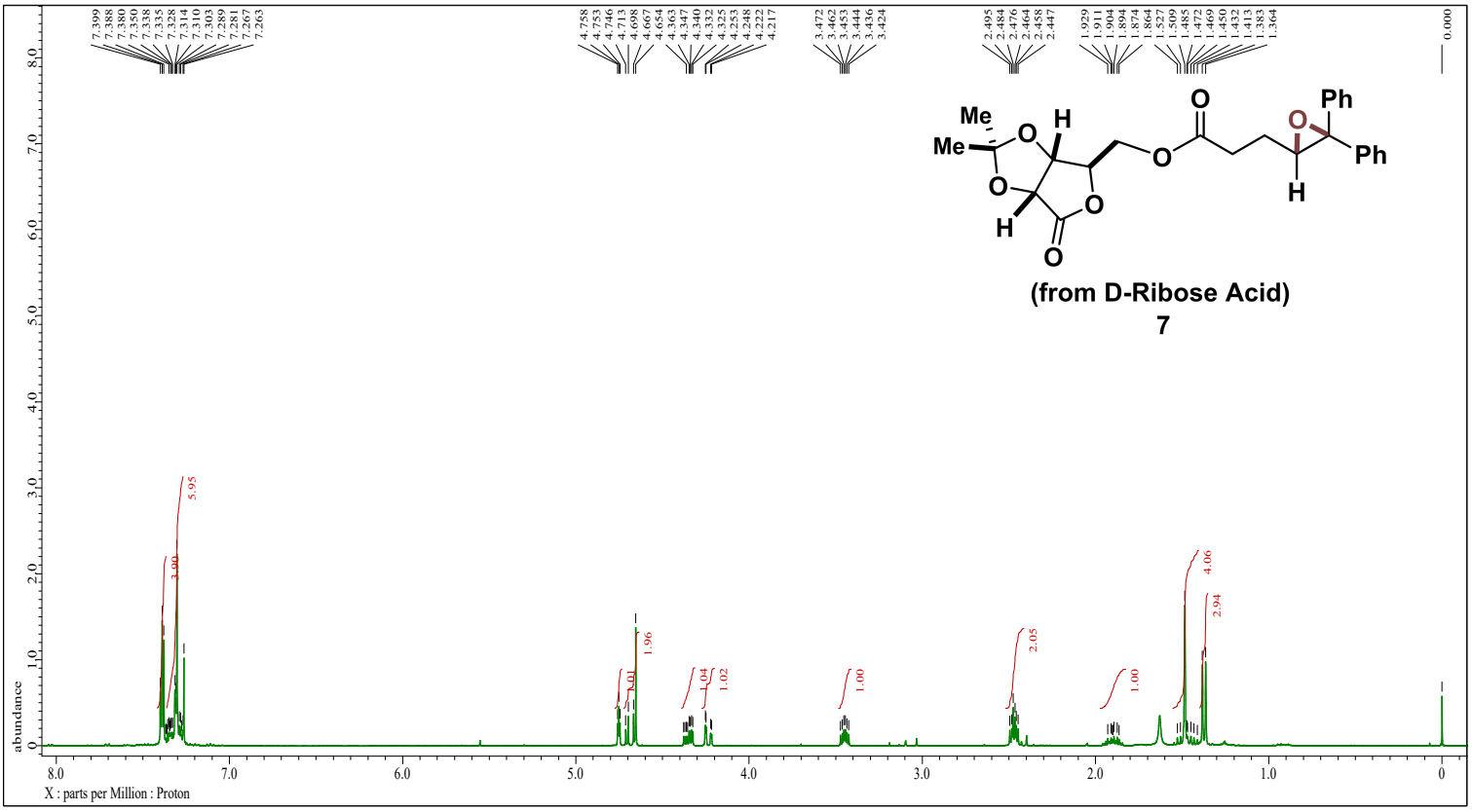

83.201
80.691
77.423
77.107
76.791
60.212
50.706
31.378
30.209
28.599
28.542
24.268
22.610
19.563
19.064
18.786
14.129
R4
O
H
R4 = nHexyl
4t
(thousandths)
X : parts per Million : Carbon13

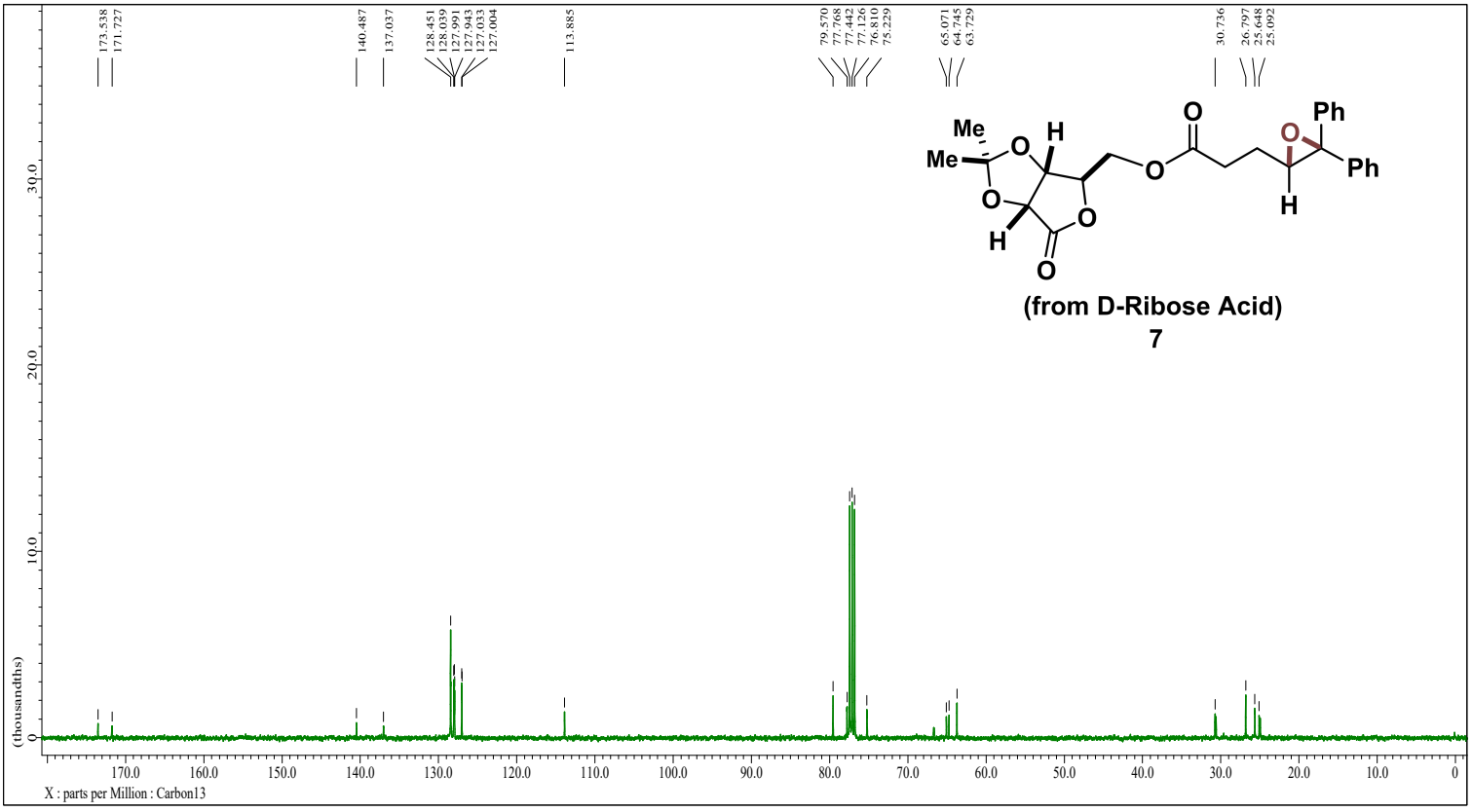

(from Borneol)
5
abundance
X : parts per Million : Proton

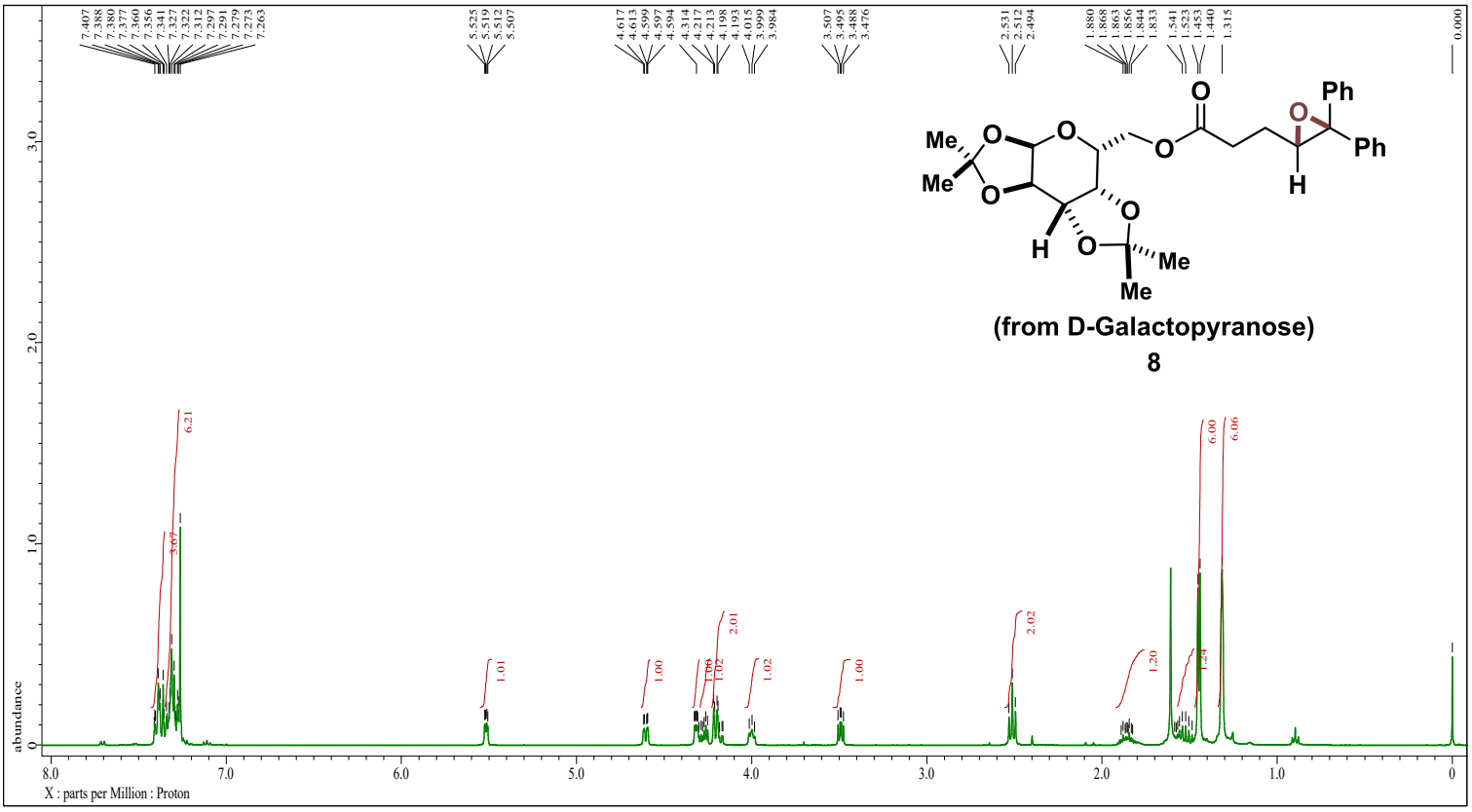

(from Borneol)
5
(thousandths)
X : parts per Million : Carbon13


7.412
7.396
7.386
7.366
7.349
7.334
7.329
7.325
7.310
7.302
7.296
7.279
7.275
7.272
7.264
6.075
6.057
6.040
4.594
4.581
4.573
4.568
4.560
4.548
3.715
3.503
3.494
3.484
3.474
3.464
2.419
2.410
2.400
2.391
2.382
2.373
1.998
1.987
1.979
1.969
1.858
1.852
1.656
1.451
1.434
1.431
1.180
1.161
1.157
0.922
0.911
0.903
0.895
0.884
0.878
0.874
0.856
0.000
5.93
4.32
0.97
0.98
3.01
1.00
2.00
1.02
1.01
2.06
1.12
6.09
abundance
X : parts per Million : Proton
Et
Me
H
MeO
O
N
H
Ph
(from L-Isoleucine)
6


172.570
171.641
140.755
137.258
128.346
128.049
127.915
127.847
127.033
77.433
77.116
76.800
66.719
65.646
56.466
52.201
37.971
32.988
25.791
25.322
15.490
11.666
(thousandths)
X : parts per Million : Carbon13
Et
Me
H
MeO
O
N
H
Ph
(from L-Isoleucine)
6

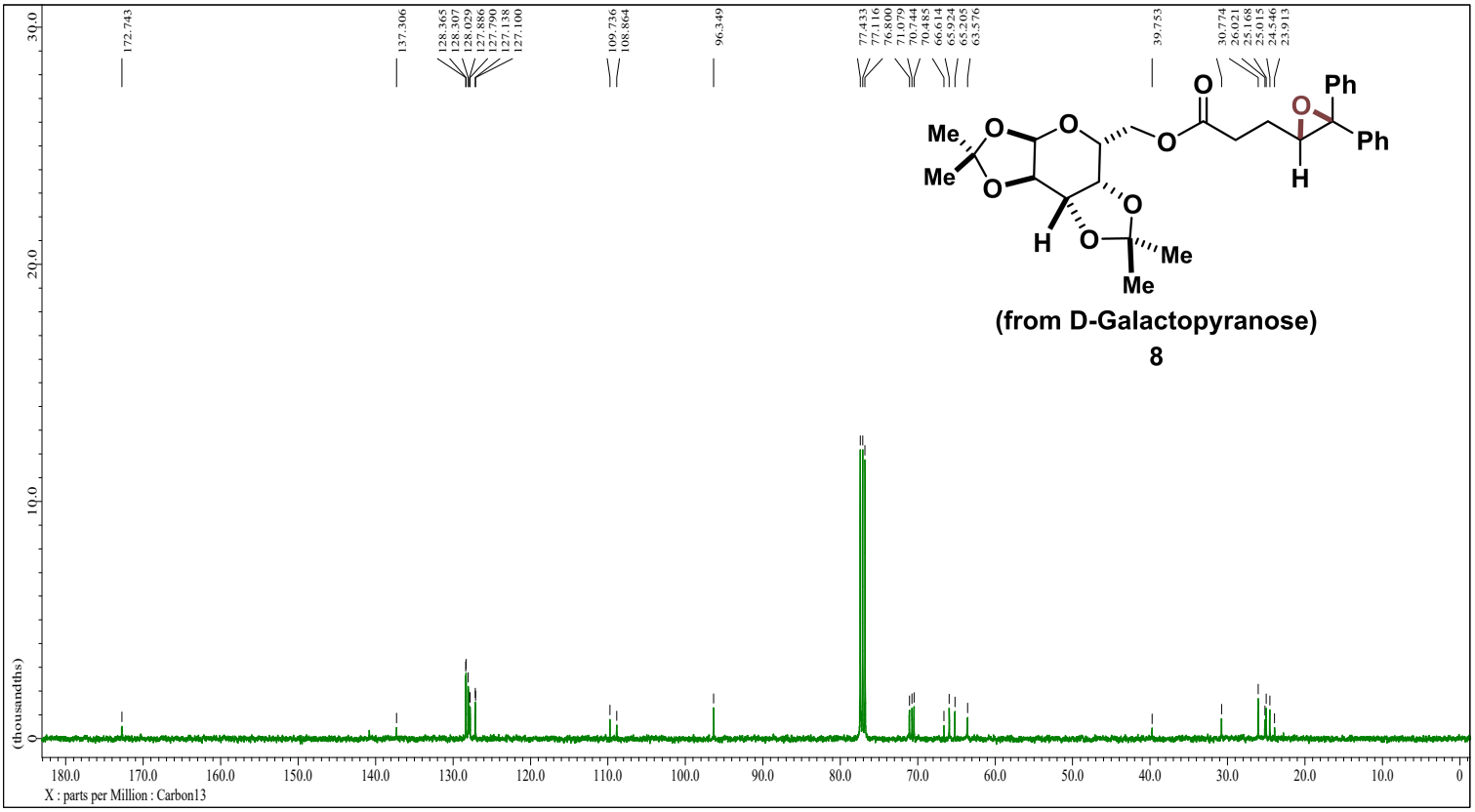

7.399 7.388 7.380 7.350 7.338 7.335 7.328 7.314 7.310 7.303 7.289 7.281 7.267 7.263
4.758 4.753 4.746 4.713 4.698 4.667 4.654 4.363 4.347 4.340 4.332 4.325 4.253 4.248 4.222 4.217
3.472 3.462 3.453 3.444 3.436 3.424
2.495 2.484 2.476 2.464 2.458 2.447
1.929 1.911 1.904 1.894 1.874 1.864 1.527 1.509 1.485 1.472 1.469 1.450 1.432 1.413 1.383 1.364
0.000
Me
Me
O
H
O
O
H
O
O
O
O
Ph
O
Ph
H
(from D-Ribose Acid)
7
5.95
3.90
1.96
1.01
1.04
1.02
1.00
2.05
1.00
4.06
2.94
abundance
X : parts per Million : Proton


173.538
171.727
140.487
137.037
128.451
128.039
127.991
127.943
127.033
127.004
113.885
79.570
77.768
77.442
77.126
76.810
75.229
65.071
64.745
63.729
30.736
26.797
25.648
25.092
Me
Me
O
H
O
O
H
O
O
O
O
Ph
O
Ph
H
(from D-Ribose Acid)
7
(thousandths)
X : parts per Million : Carbon13



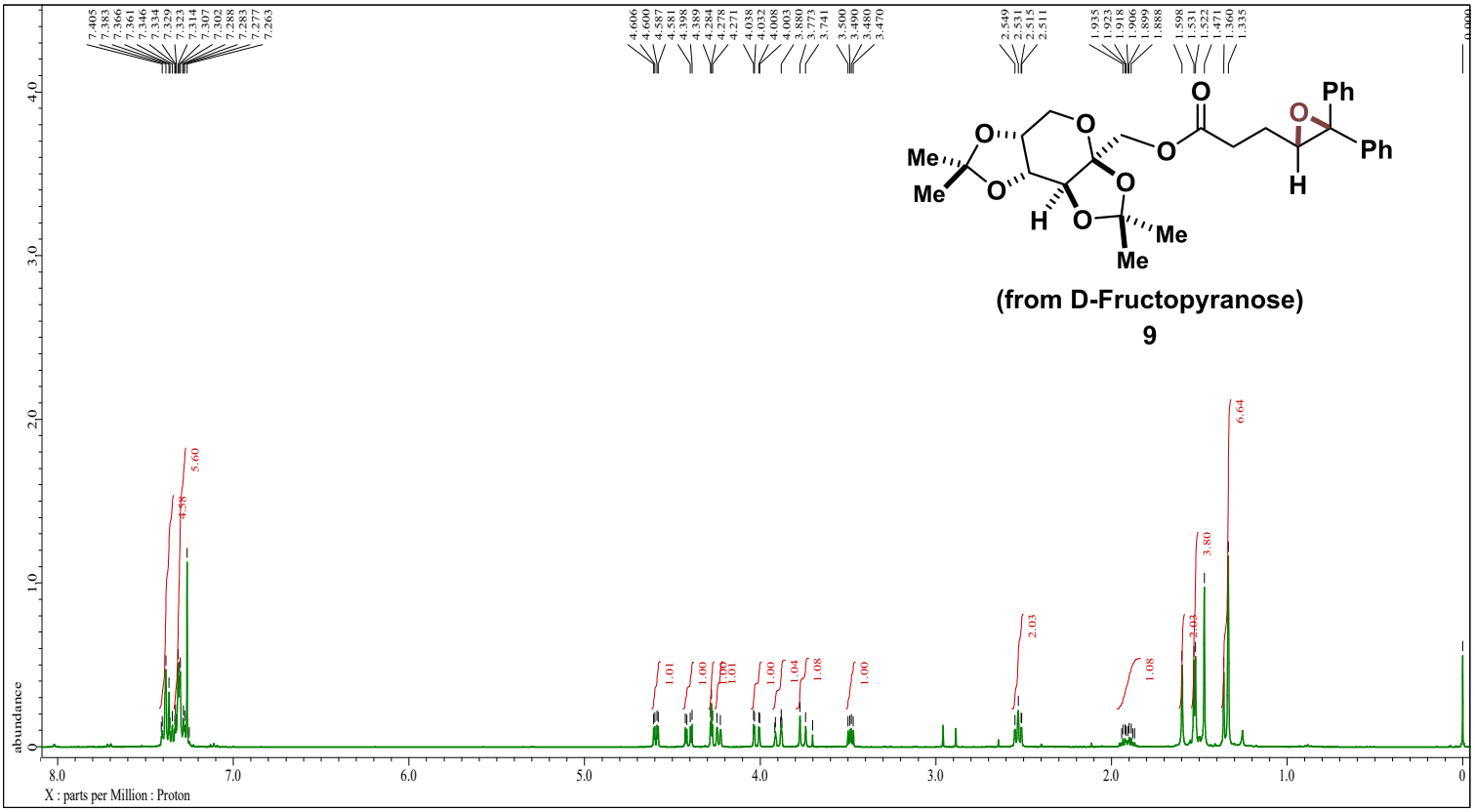
(from D-Galactopyranose)

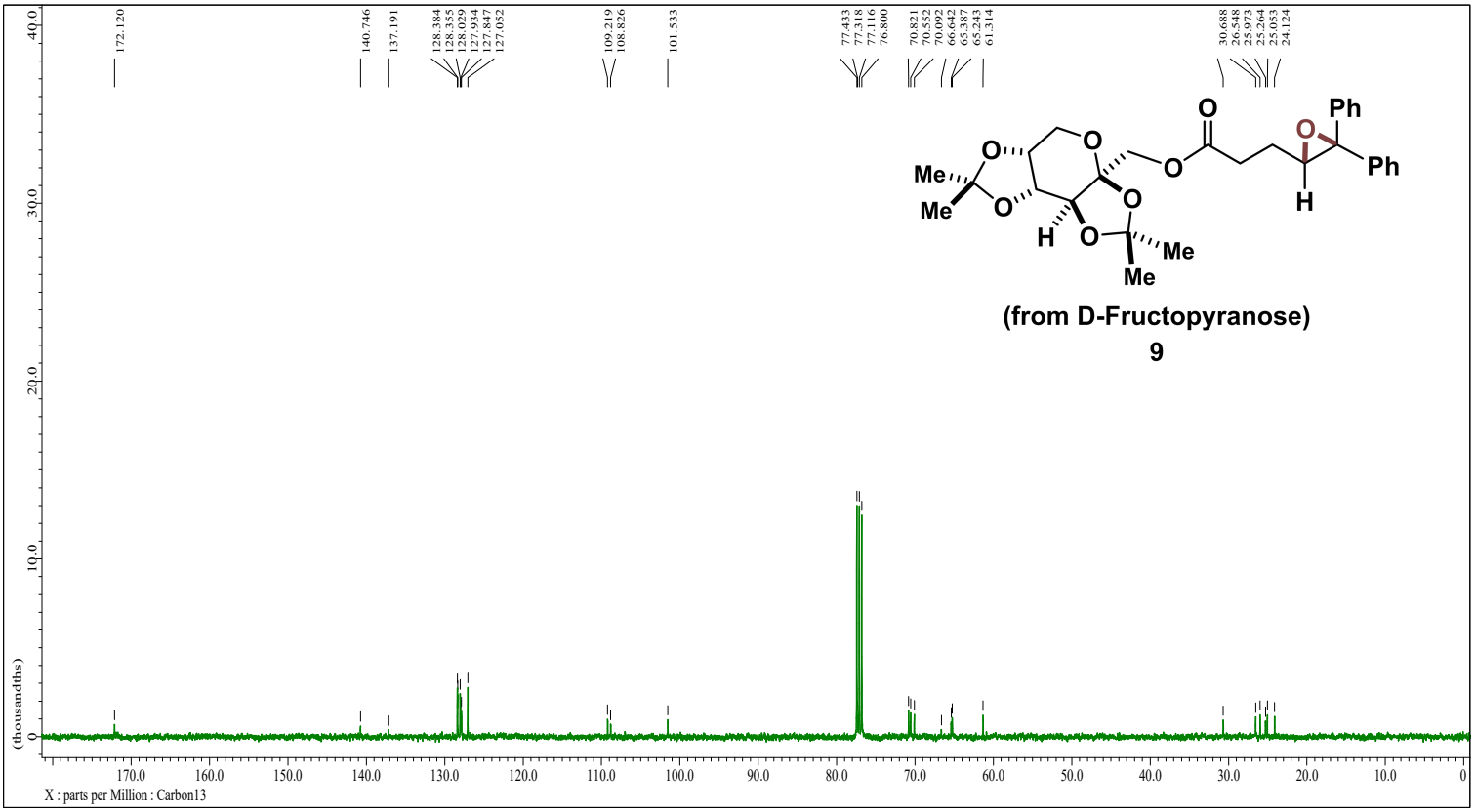
8

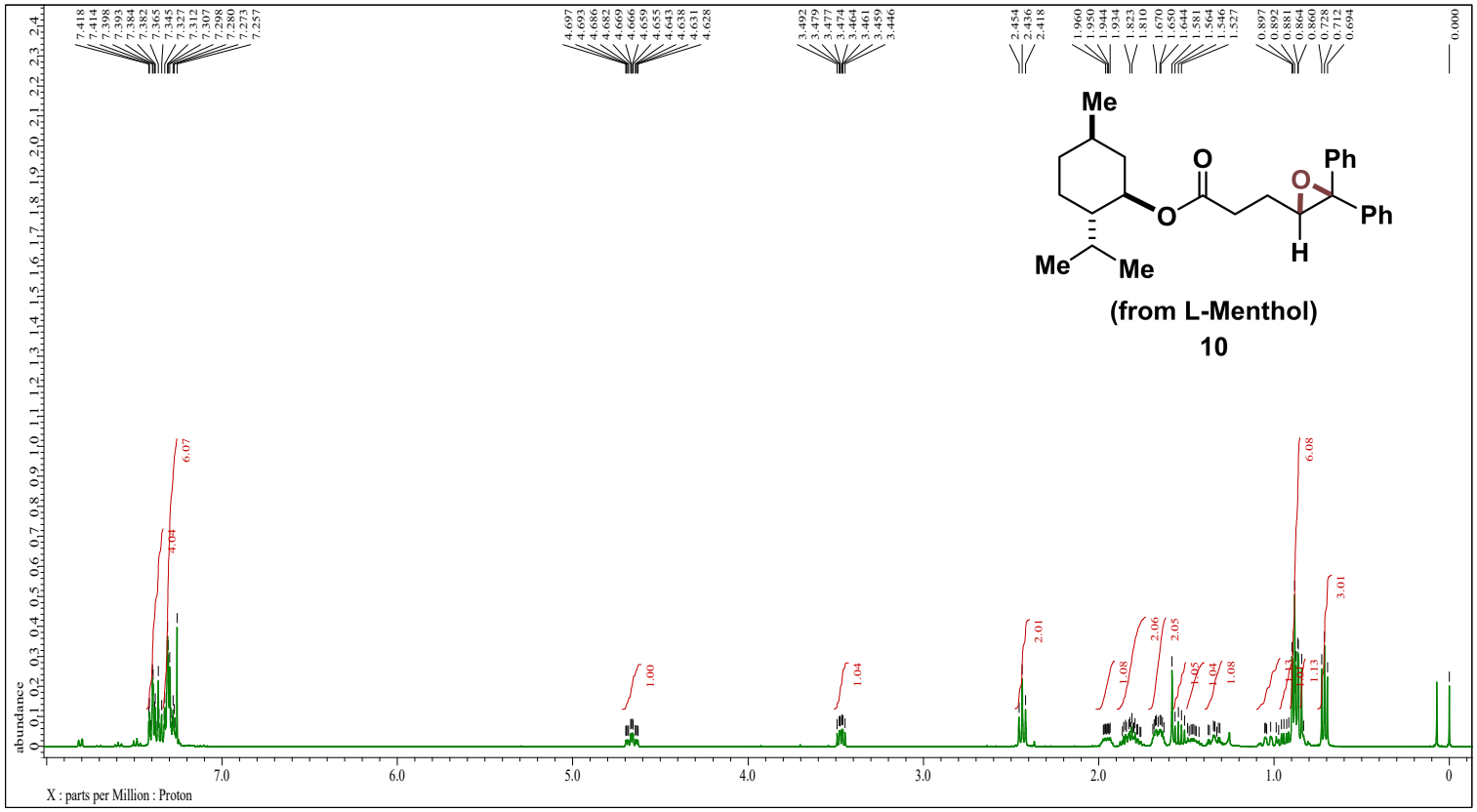


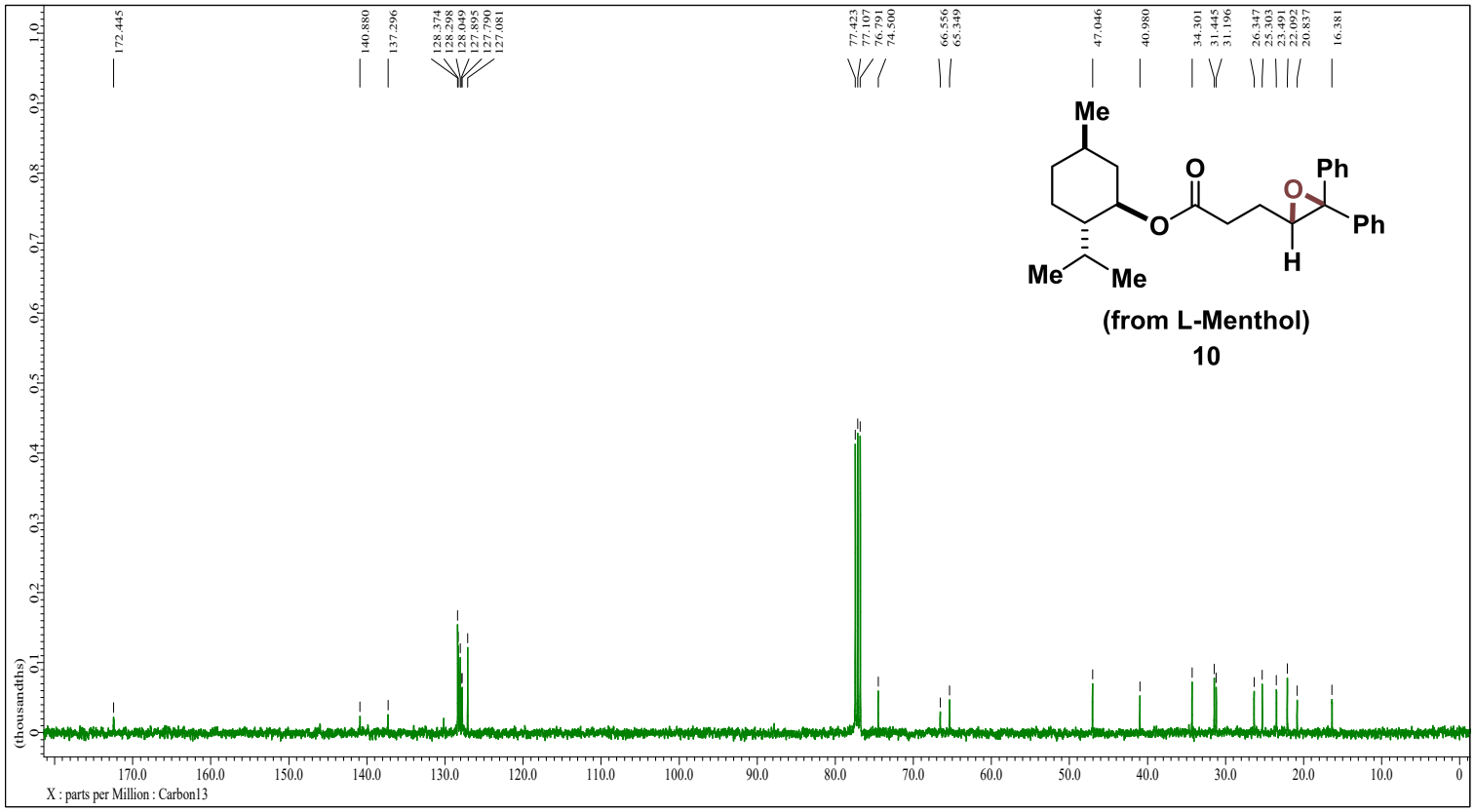
(from D-Galactopyranose)

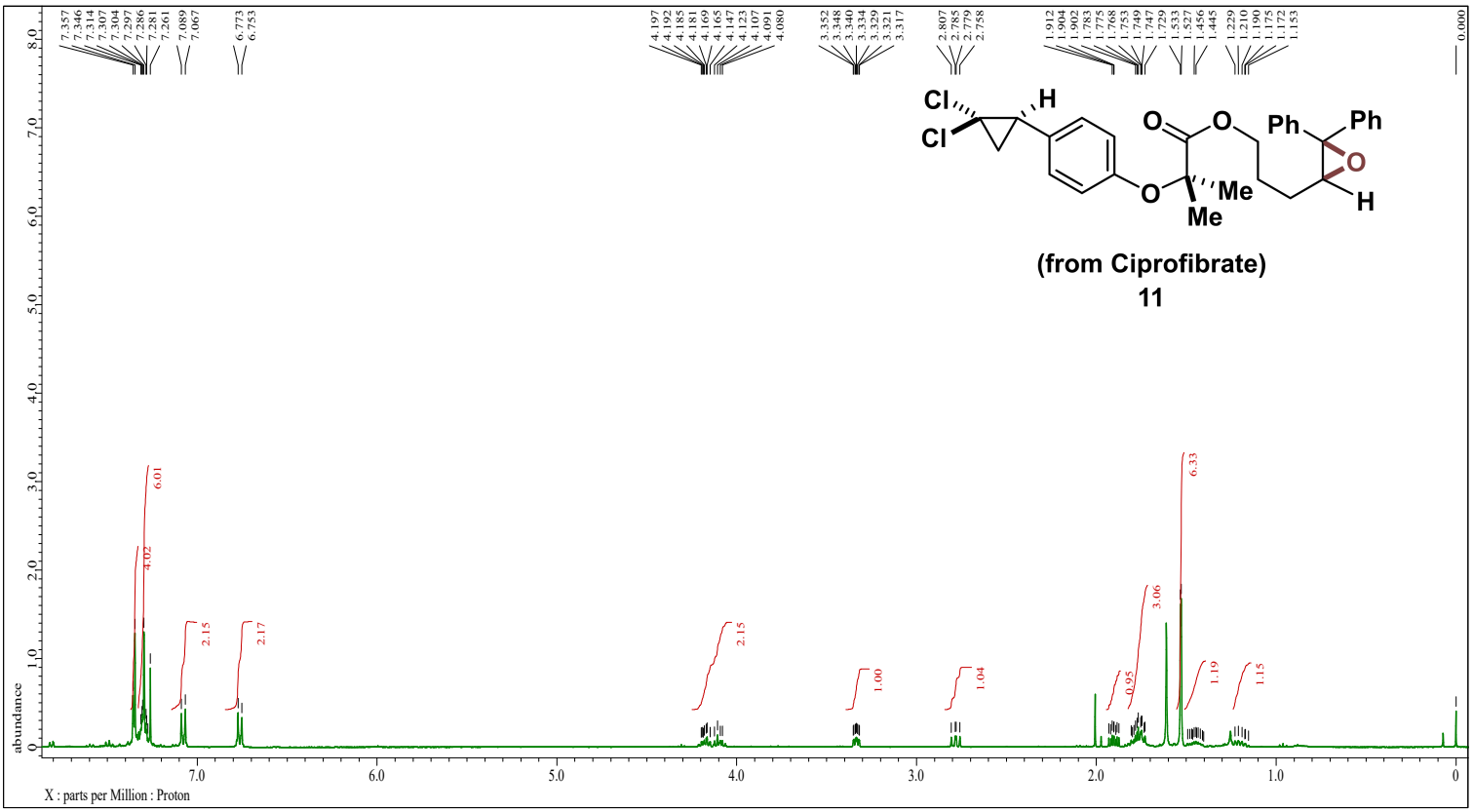
8

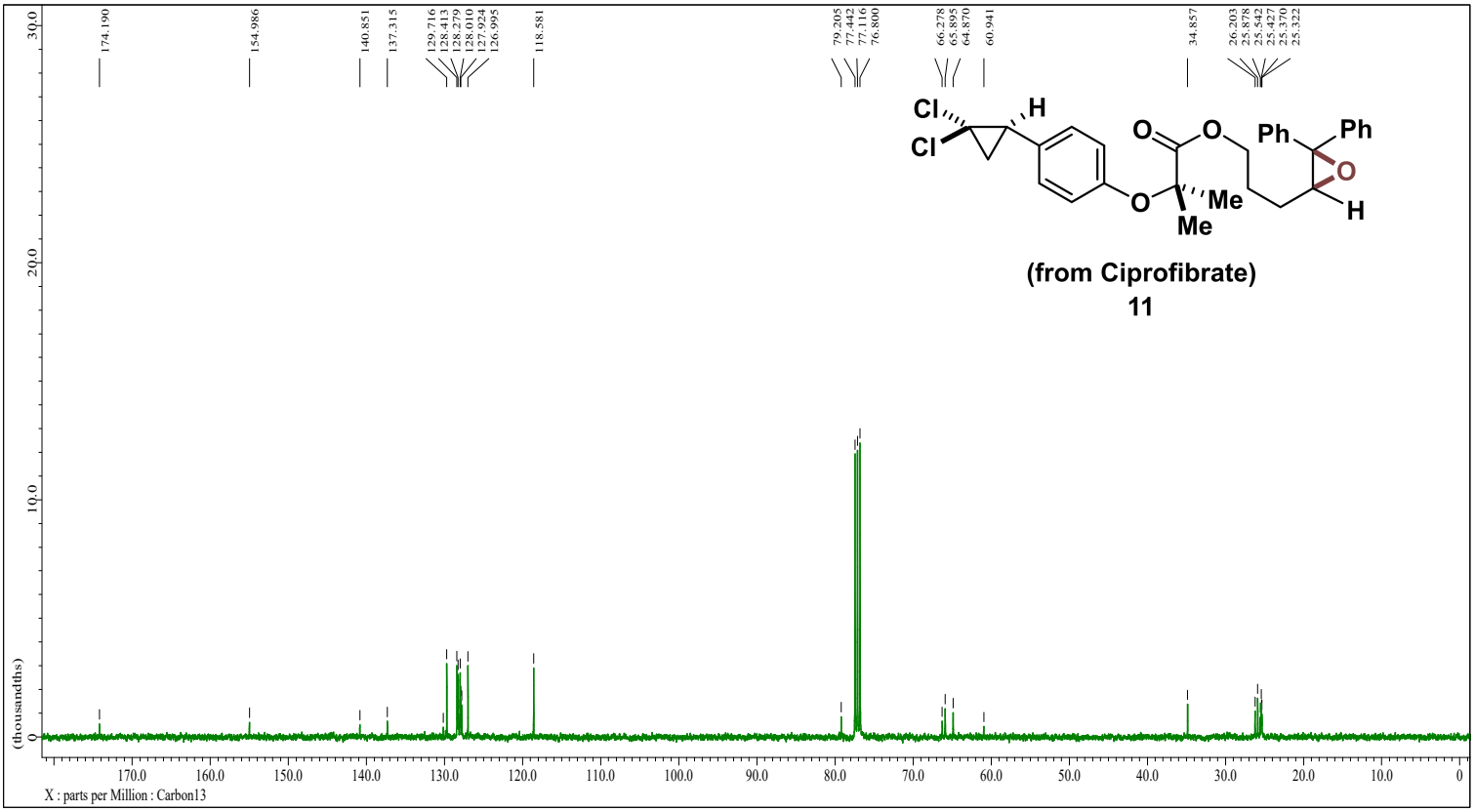

abundance
X : parts per Million : Proton
(from D-Fructopyranose)
9

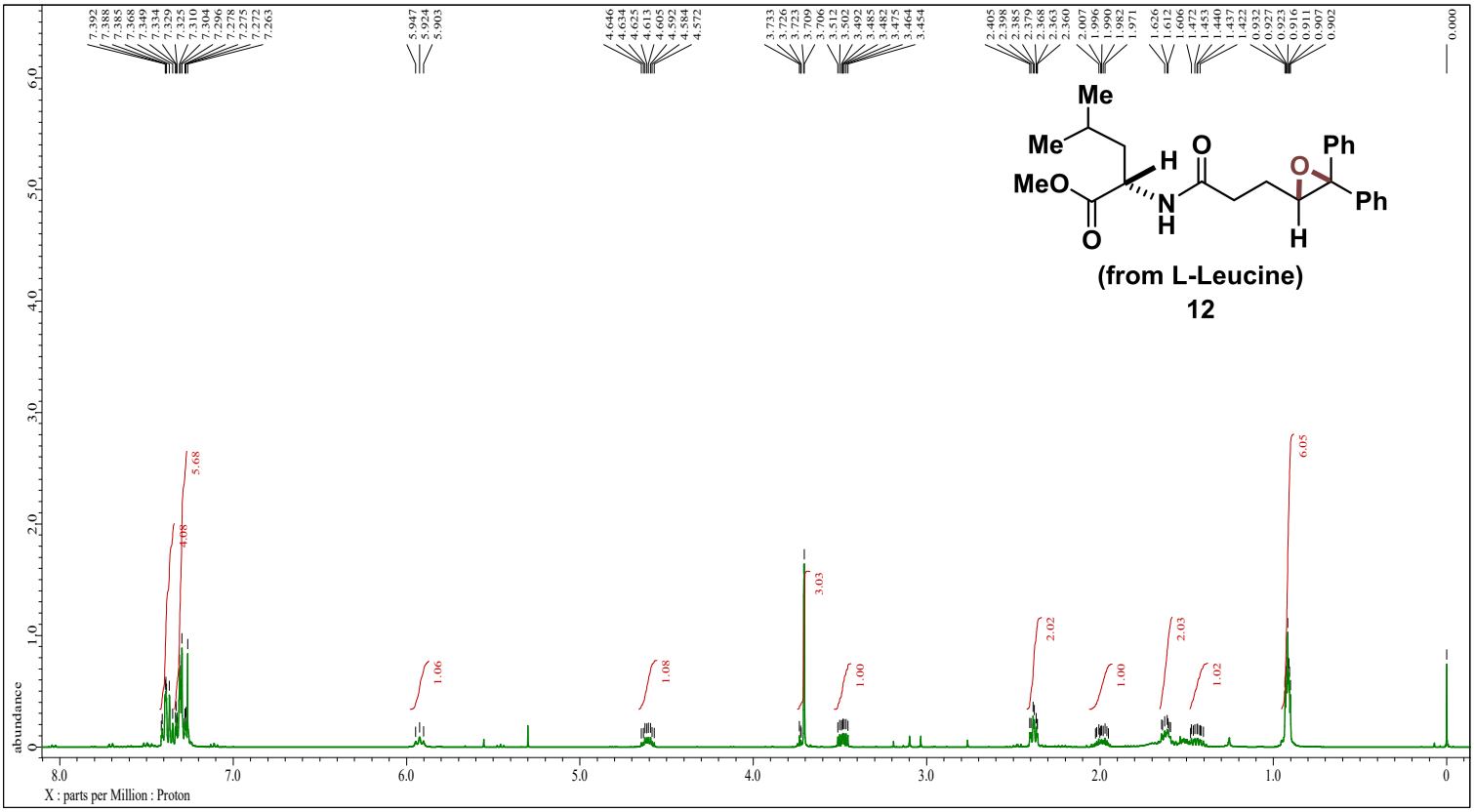

(thousandths)
X : parts per Million : Carbon13
(from D-Fructopyranose)
9

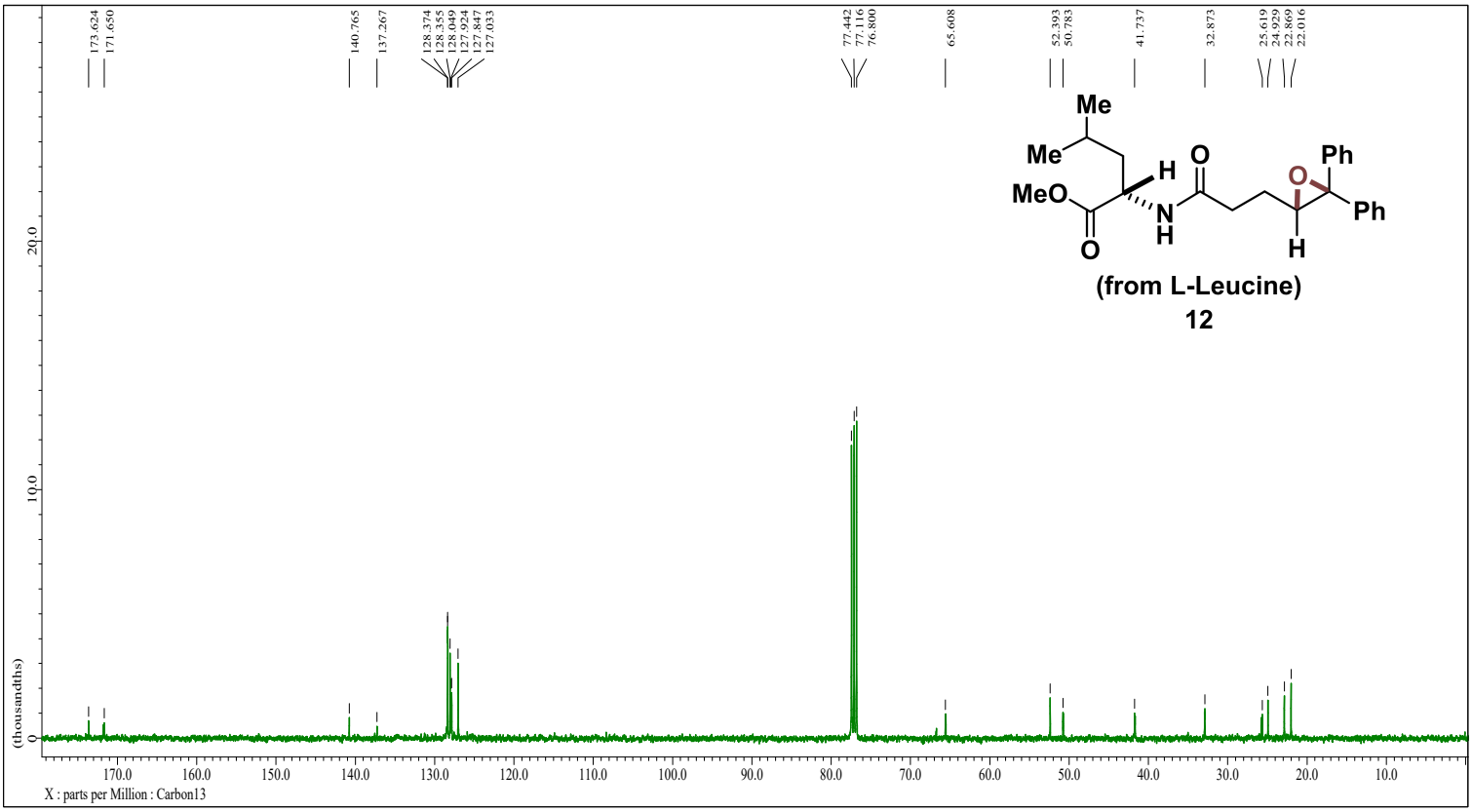

Me
O
Ph
O
O
Ph
H
Me
Me
(from L-Menthol)
10
abundance
X : parts per Million : Proton

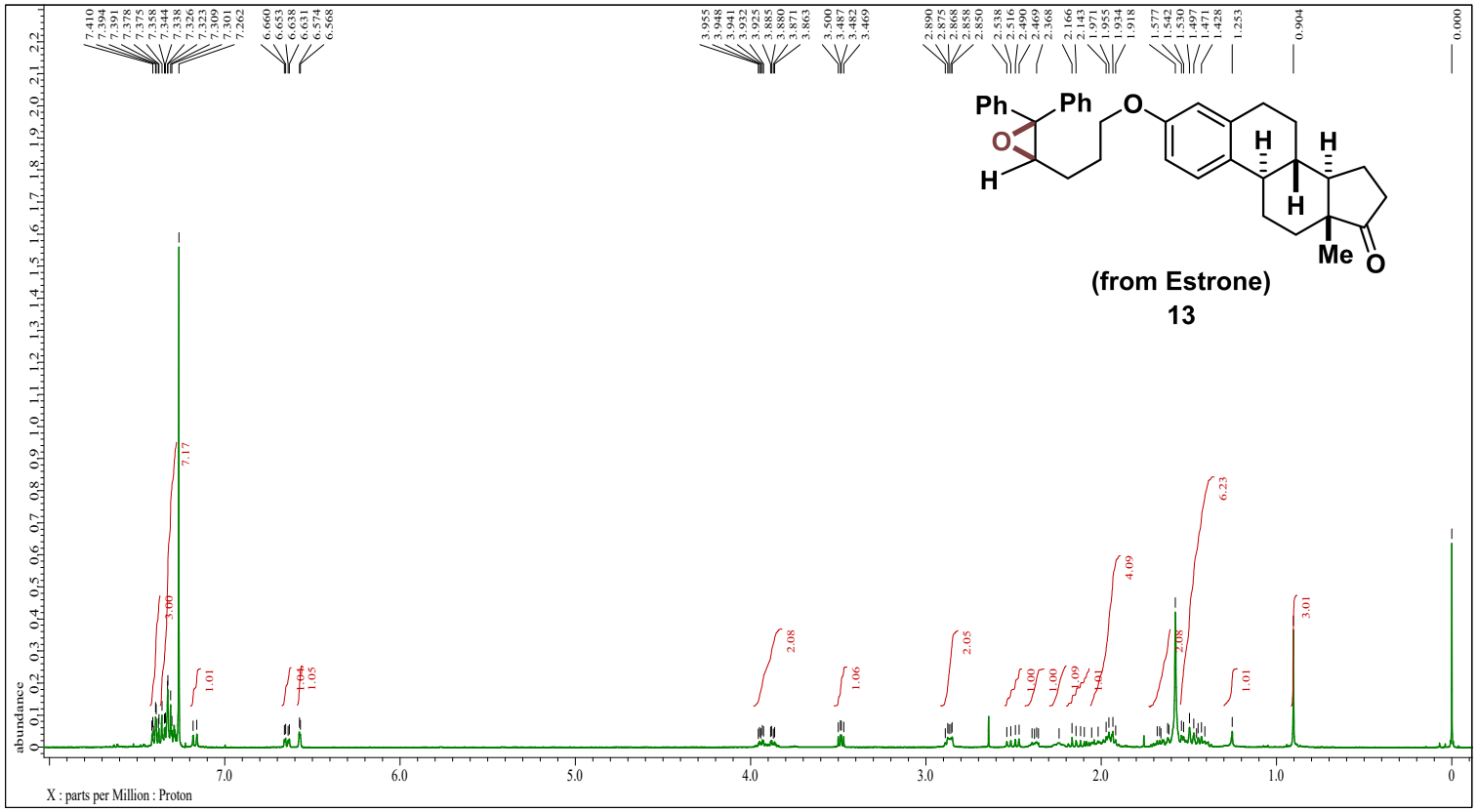

Me
O
Ph
O
O
Ph
H
Me
Me
(from L-Menthol)
10
(thousandths)
X : parts per Million : Carbon13

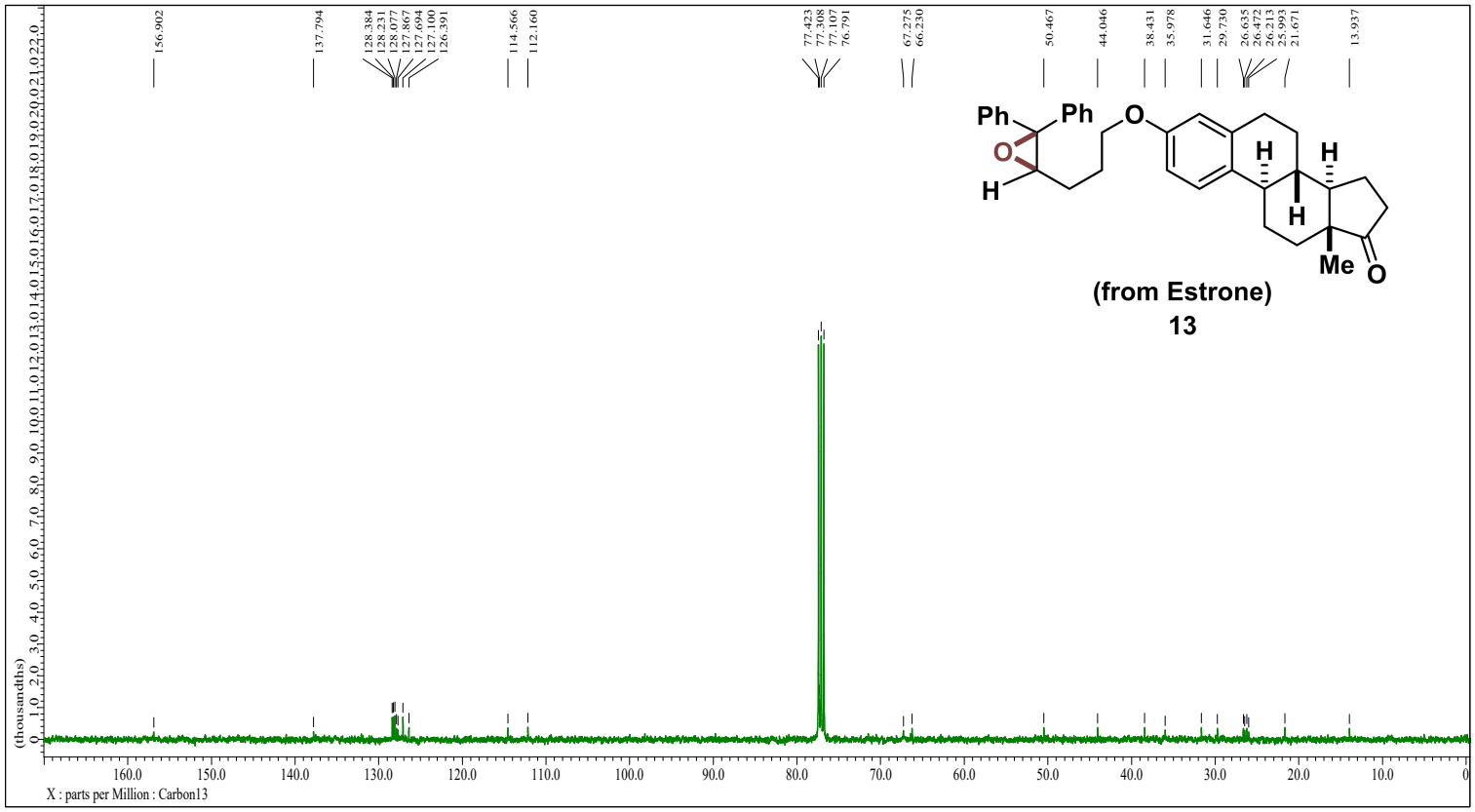

7.357 7.346 7.314 7.307 7.304 7.297 7.286 7.281 7.261 7.089 7.067 6.773 6.753
4.197 4.192 4.185 4.181 4.169 4.165 4.147 4.123 4.107 4.091 4.080
3.352 3.348 3.340 3.334 3.329 3.321 3.317
2.807 2.785 2.779 2.758
1.912 1.904 1.902 1.783 1.775 1.768 1.753 1.749 1.747 1.729 1.533 1.527 1.456 1.445 1.229 1.210 1.190 1.175 1.172 1.153
0.000
Cl H Cl O O Ph Ph O O Me Me H
(from Ciprofibrate)
11
6.01 4.02 2.15 2.17 2.15 1.00 1.04 0.95 3.06 6.33 1.19 1.15
abundance
X : parts per Million : Proton

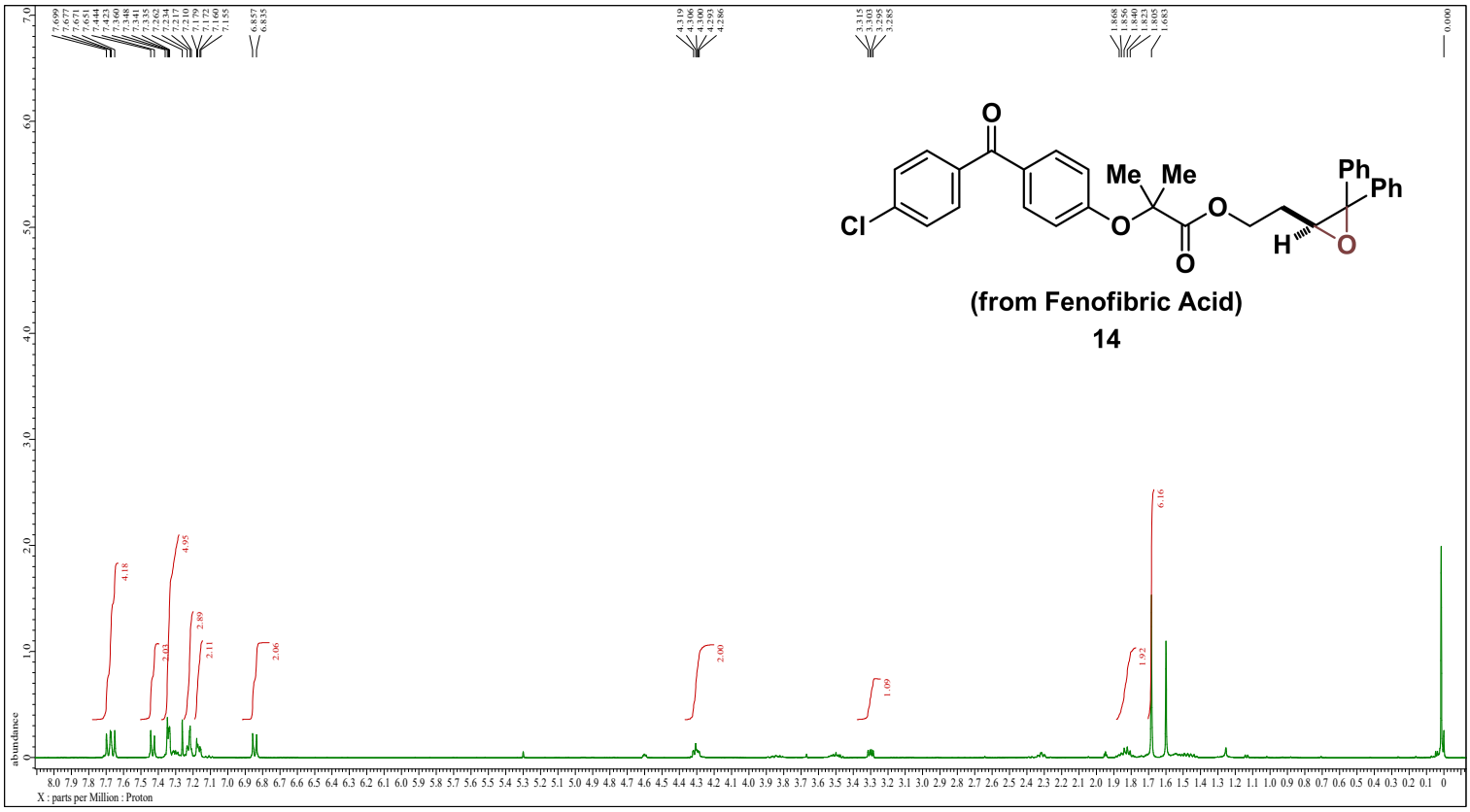

174.190 154.986 140.851 137.315 129.716 128.413 128.279 128.010 127.924 126.995 118.581
79.205 77.442 77.116 76.800 66.278 65.895 64.870 60.941
34.857 26.203 25.878 25.542 25.427 25.370 25.322
Cl H Cl O O Ph Ph O O Me Me H
(from Ciprofibrate)
11
(thousandths)
X : parts per Million : Carbon13

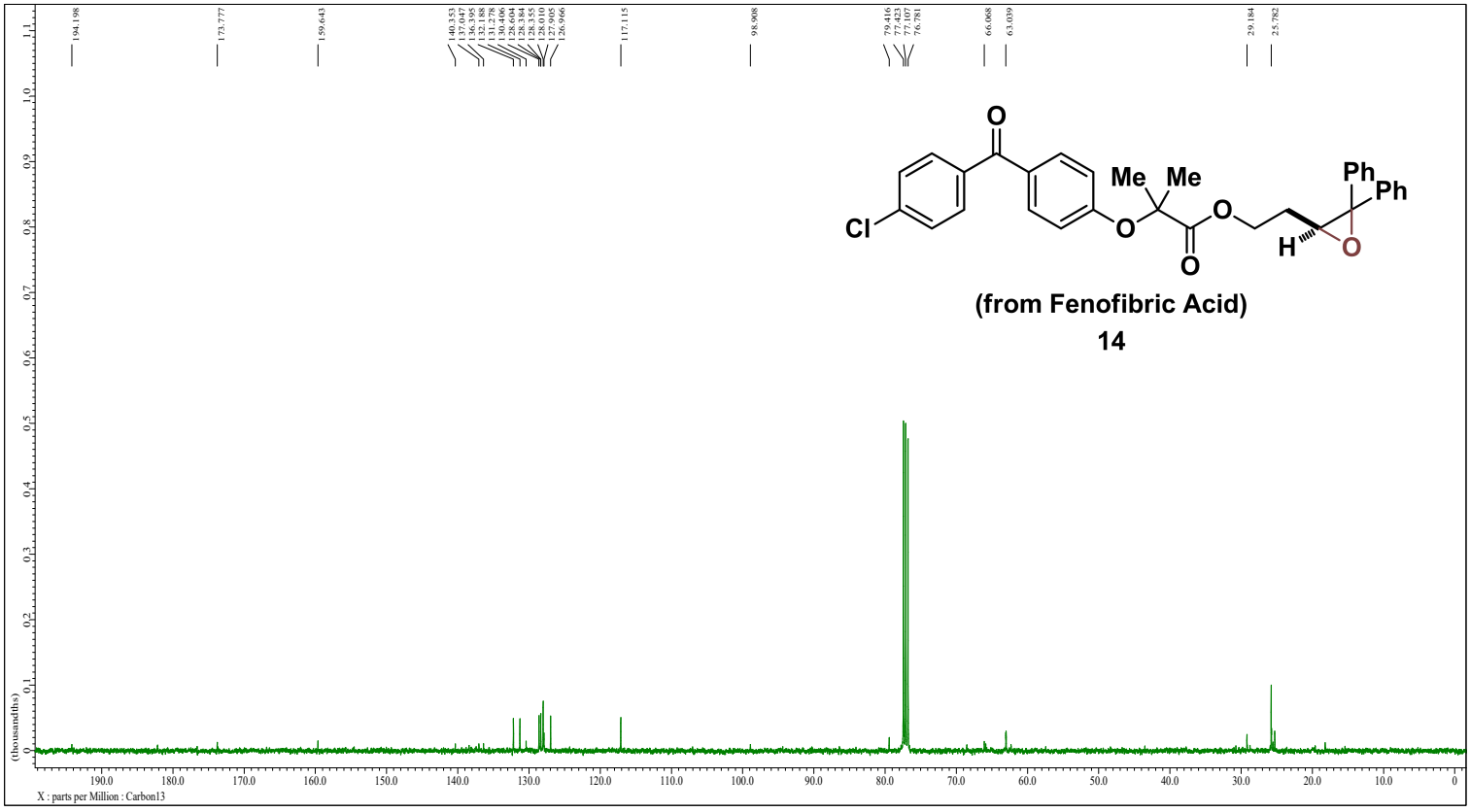

7.392 7.388 7.385 7.368 7.349 7.334 7.329 7.325 7.310 7.304 7.296 7.278 7.275 7.272 7.263
5.947 5.924 5.903
4.646 4.634 4.625 4.613 4.605 4.592 4.584 4.572
3.733 3.726 3.723 3.709 3.706 3.512 3.502 3.492 3.485 3.482 3.475 3.464 3.454
2.405 2.398 2.385 2.379 2.368 2.363 2.360 2.007 1.996 1.990 1.982 1.971 1.626 1.612 1.606 1.472 1.453 1.440 1.437 1.422 0.932 0.927 0.923 0.916 0.911 0.907 0.902
0.000
Me
Me
MeO
H
N
H
O
O
O
Ph
Ph
H
(from L-Leucine)
12
5.68
4.08
1.06
1.08
3.03
1.00
2.02
1.00
2.03
1.02
6.05
abundance
X : parts per Million : Proton

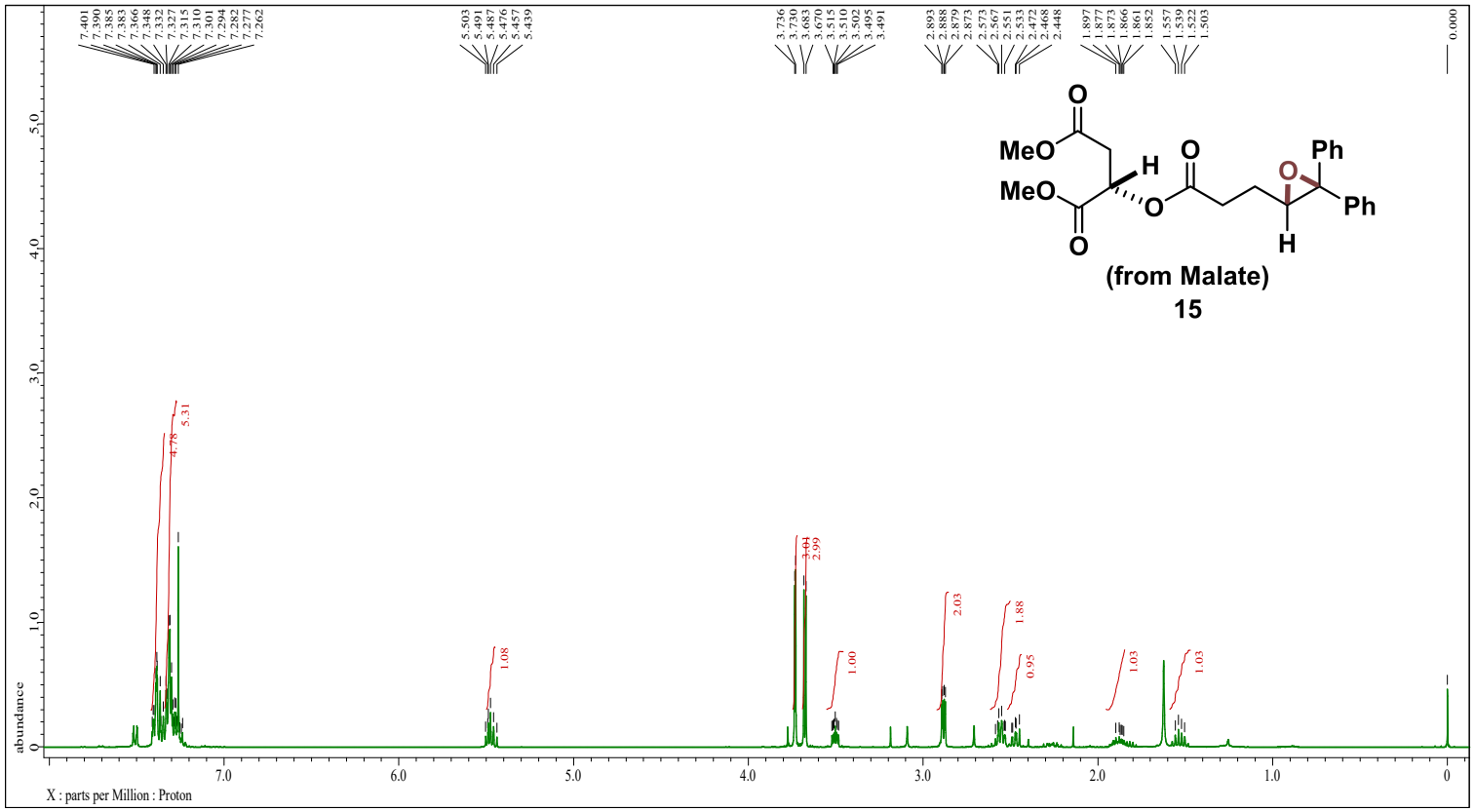

173.624 171.650
140.765 137.267
128.374 128.355 128.049 127.924 127.847 127.033
77.442 77.116 76.800
65.608
52.393 50.783
41.737
32.873
25.619 24.929 22.669 22.016
Me
Me
MeO
H
N
H
O
O
O
Ph
Ph
H
(from L-Leucine)
12
(thousandths)
X : parts per Million : Carbon13

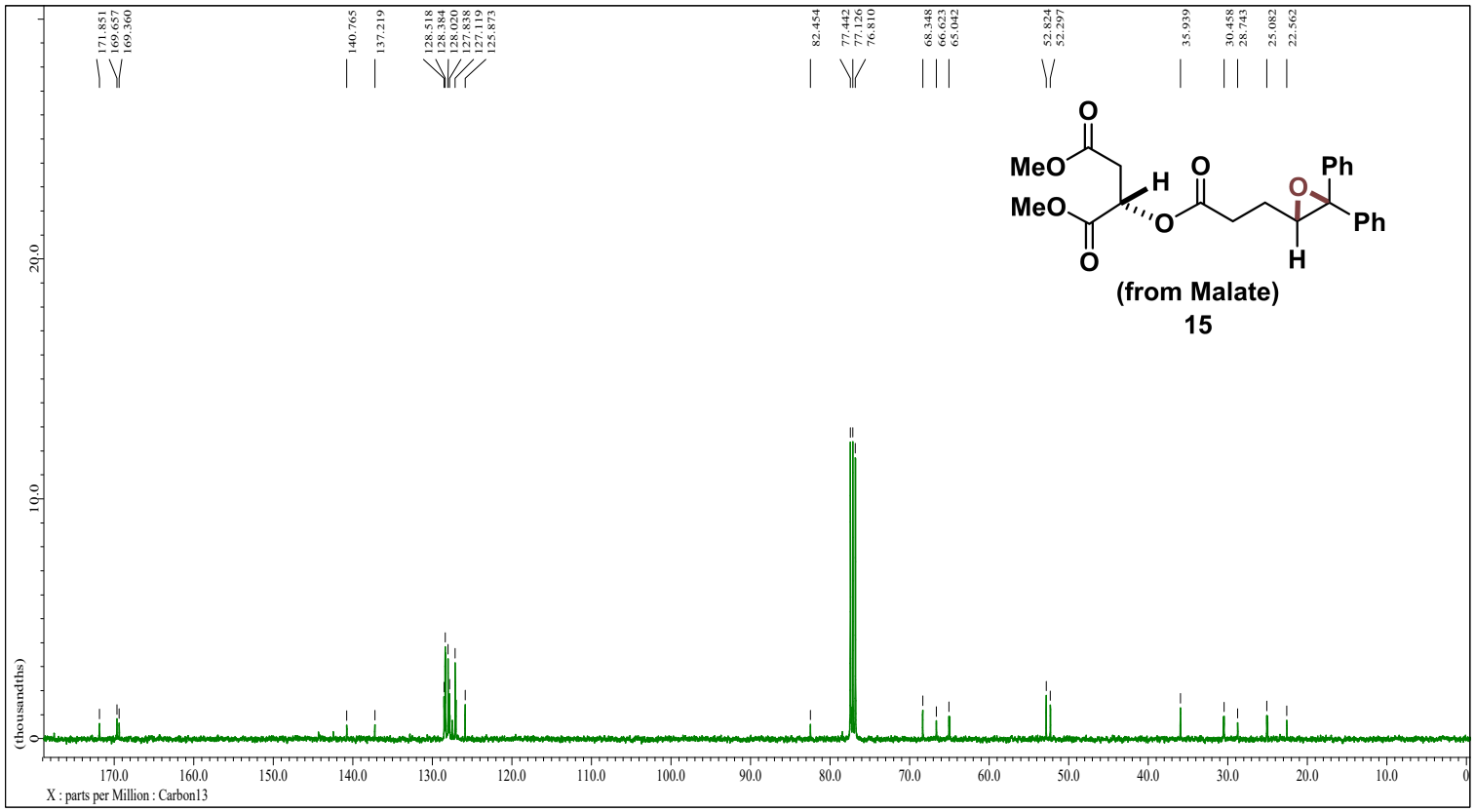

7.410
7.394
7.391
7.378
7.375
7.358
7.344
7.338
7.326
7.323
7.309
7.301
7.262
6.660
6.653
6.638
6.631
6.574
6.568
3.955
3.948
3.941
3.932
3.925
3.885
3.880
3.871
3.863
3.500
3.487
3.482
3.469
2.890
2.875
2.868
2.858
2.850
2.538
2.516
2.490
2.469
2.368
2.166
2.143
1.971
1.955
1.934
1.918
1.577
1.542
1.530
1.497
1.471
1.428
1.253
0.904
0.000
Ph
Ph
O
O
H
H
H
H
Me
O
(from Estrone)
13
7.17
3.00
1.01
1.04
1.05
2.08
1.06
2.05
1.00
1.00
1.09
1.01
4.09
2.08
6.23
1.01
3.01
abundance
X : parts per Million : Proton

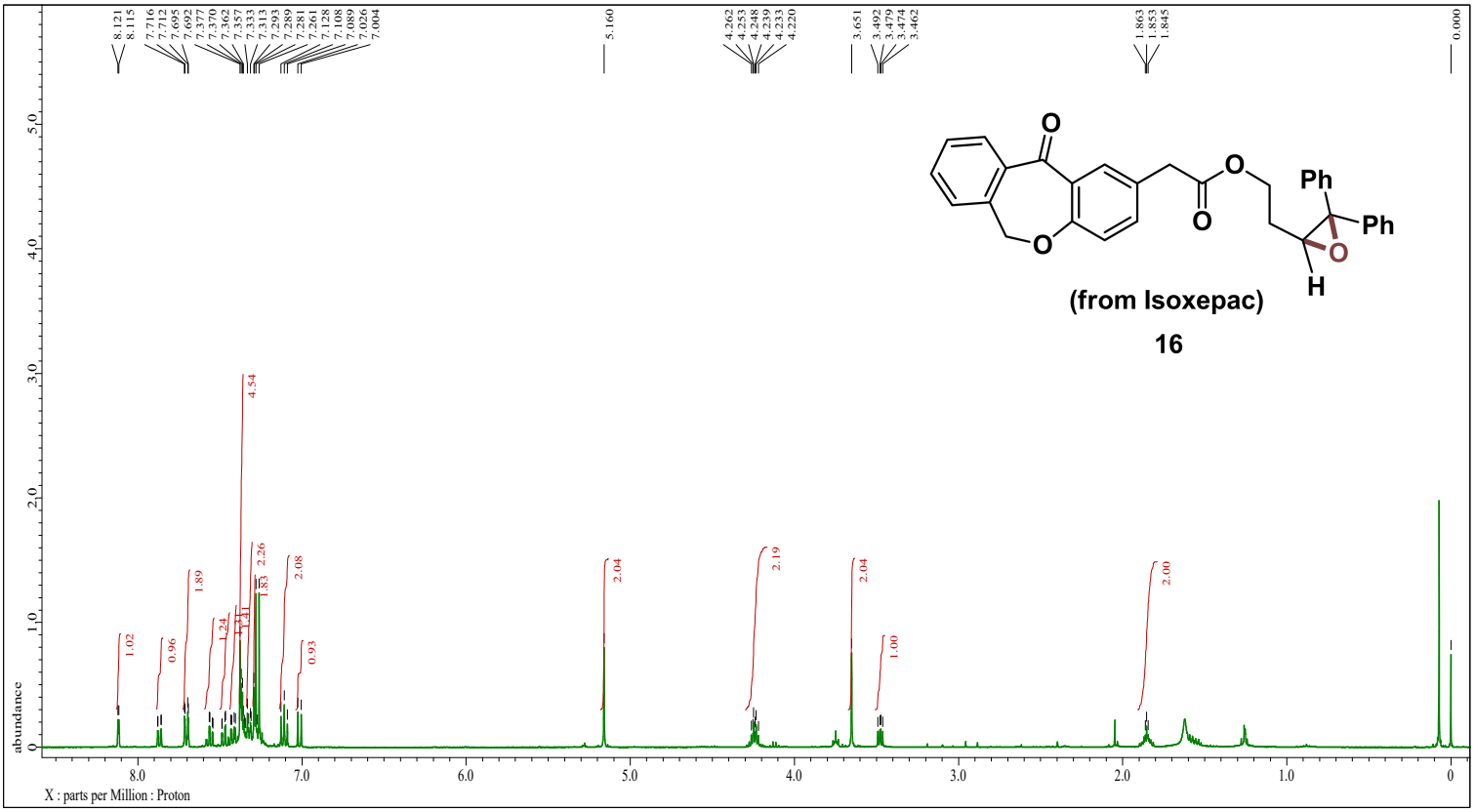

156.902
137.794
128.384
128.231
128.077
127.867
127.694
127.100
126.391
114.566
112.160
77.423
77.308
77.107
76.791
67.275
66.230
50.467
44.046
38.431
35.978
31.646
29.730
26.635
26.472
26.213
25.993
21.671
13.937
Ph
Ph
O
O
H
H
H
H
Me
O
(from Estrone)
13
(thousandths)
X : parts per Million : Carbon13

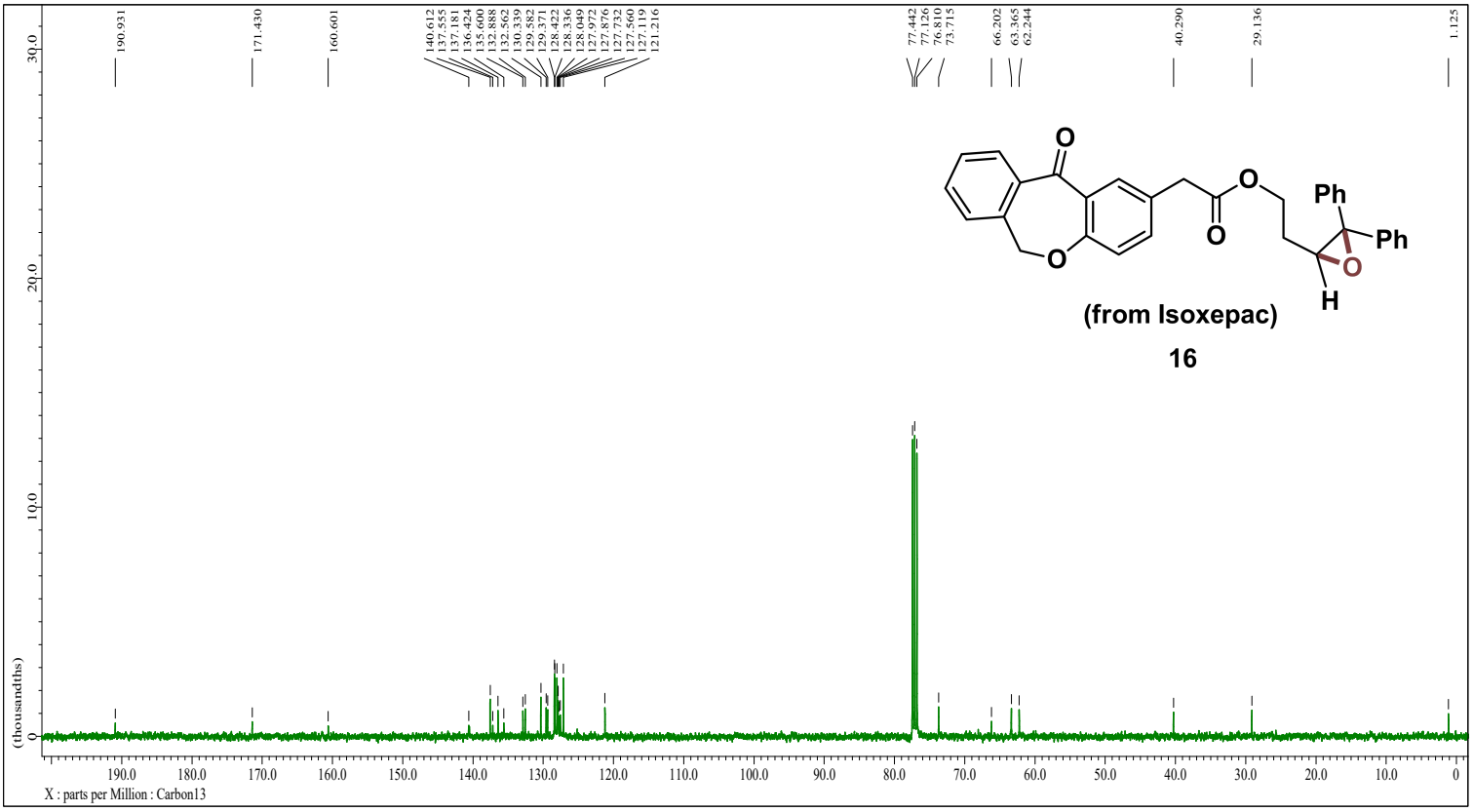

(from Fenofibric Acid)
14
X : parts per Million : Proton

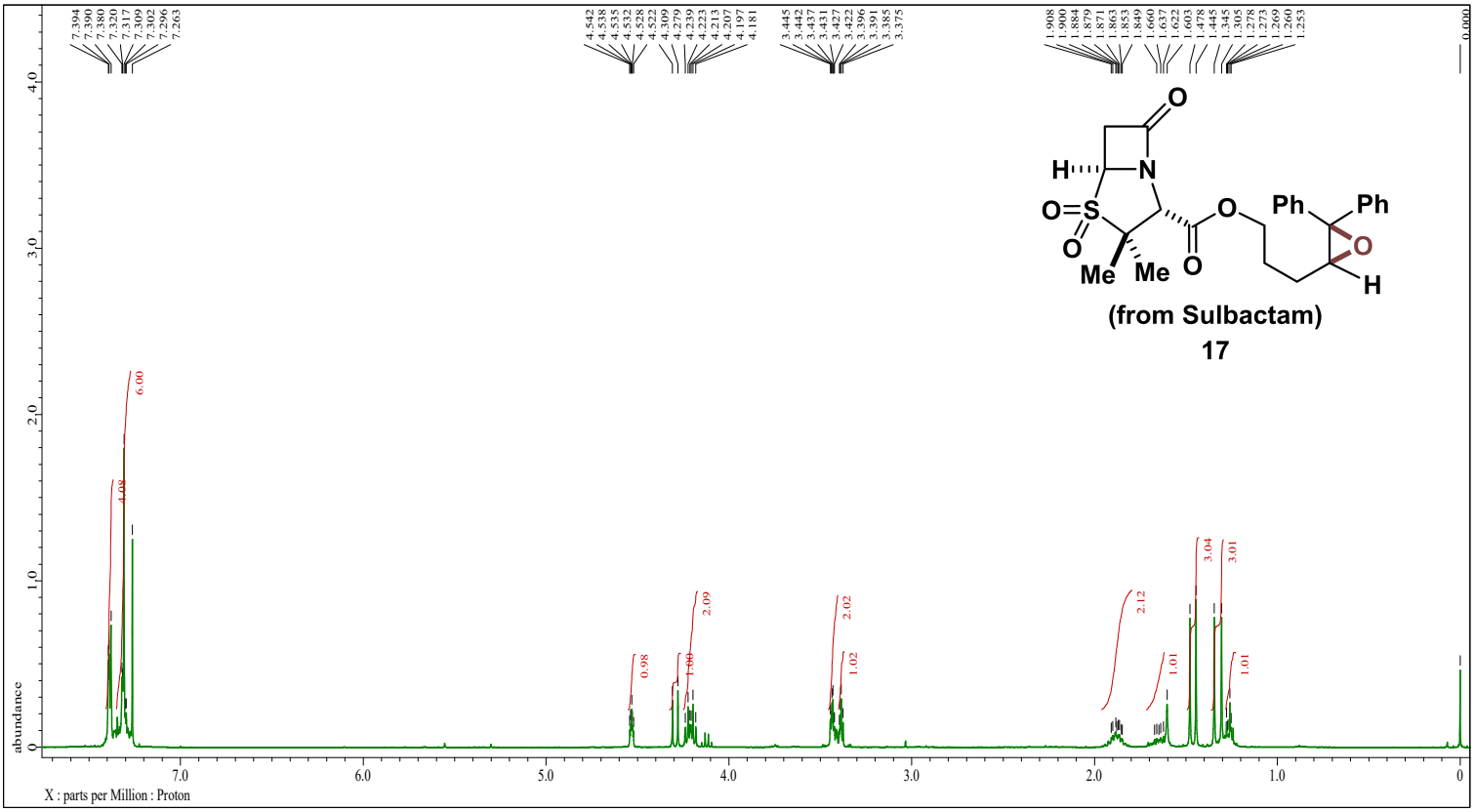

(from Fenofibric Acid)
14
X : parts per Million : Carbon13

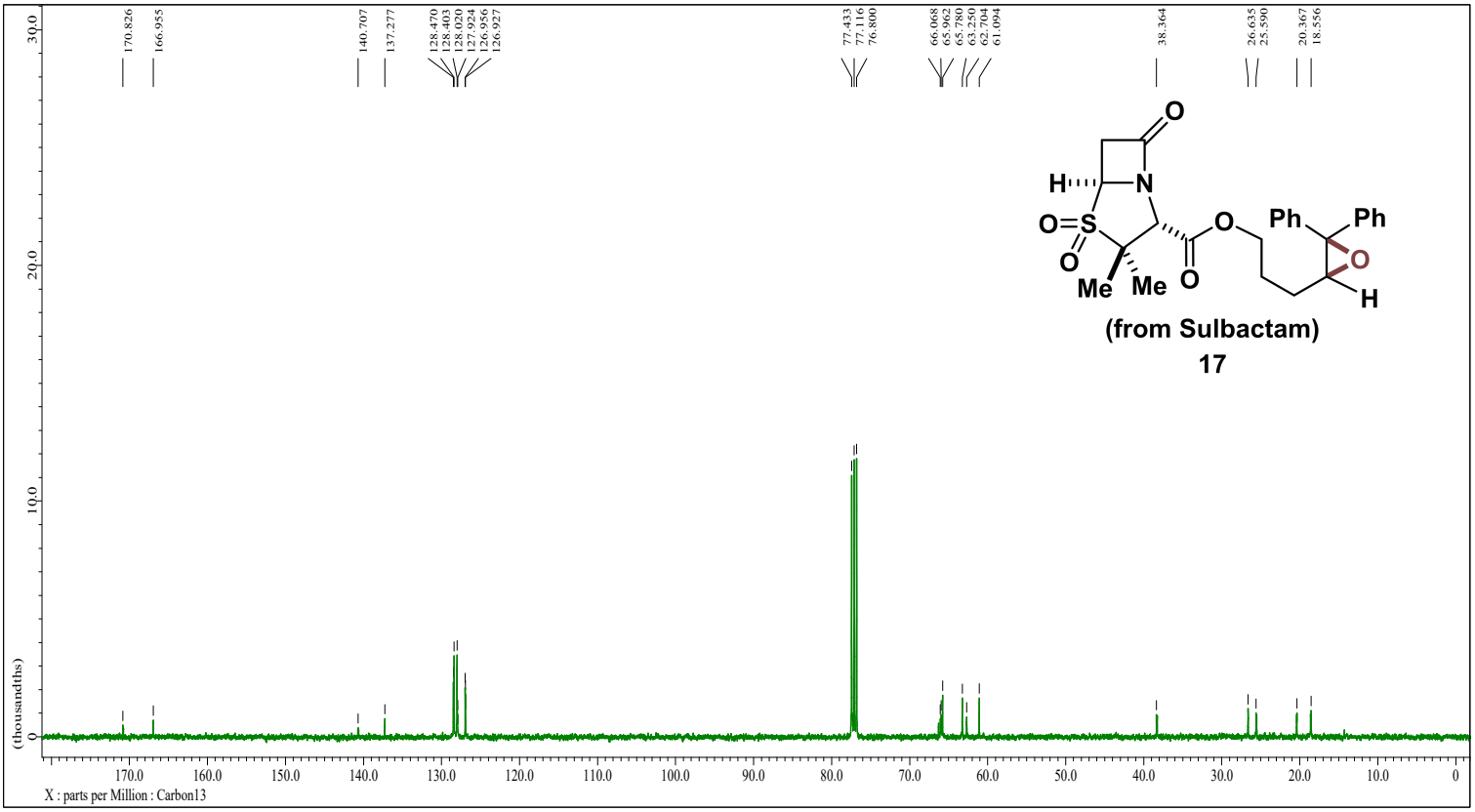

7.401
7.390
7.385
7.383
7.366
7.348
7.332
7.327
7.315
7.310
7.301
7.294
7.282
7.277
7.262
5.503
5.491
5.487
5.476
5.457
5.439
3.736
3.730
3.683
3.670
3.515
3.510
3.502
3.495
3.491
2.893
2.888
2.879
2.873
2.573
2.567
2.551
2.533
2.472
2.468
2.448
1.897
1.877
1.873
1.866
1.861
1.852
1.557
1.539
1.522
1.503
0.000
MeO
MeO
H
O
O
O
O
O
Ph
Ph
H
(from Malate)
15
abundance
X : parts per Million : Proton
5.31
4.78
3.01
2.99
2.03
1.88
1.08
1.00
0.95
1.03
1.03

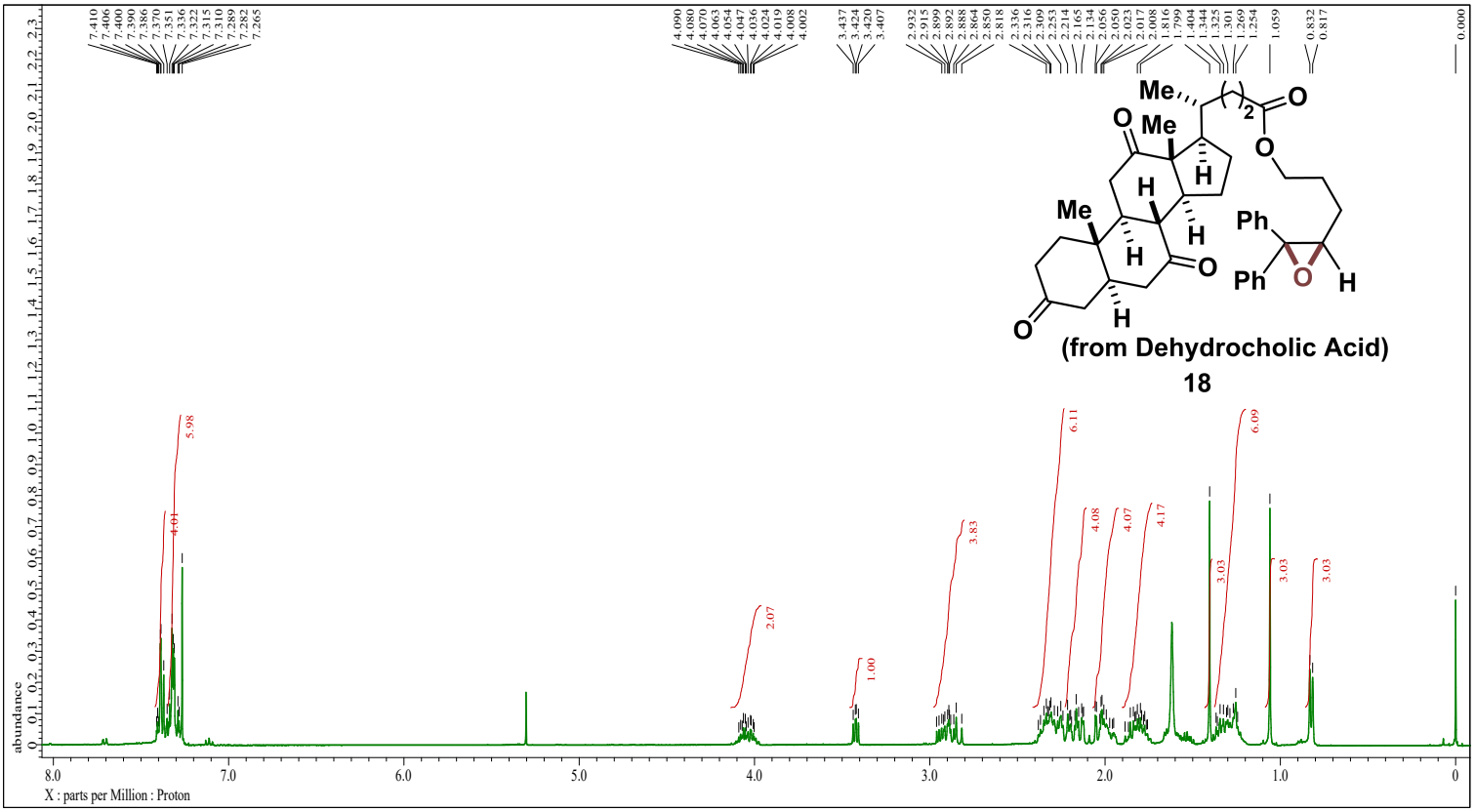

171.851
169.657
169.360
140.765
137.219
128.518
128.384
128.020
127.838
127.119
125.873
82.454
77.442
77.126
76.810
68.348
66.623
65.042
52.824
52.297
35.939
30.458
28.743
25.082
22.562
MeO
MeO
H
O
O
O
O
O
Ph
Ph
H
(from Malate)
15
(thousandths)
X : parts per Million : Carbon13

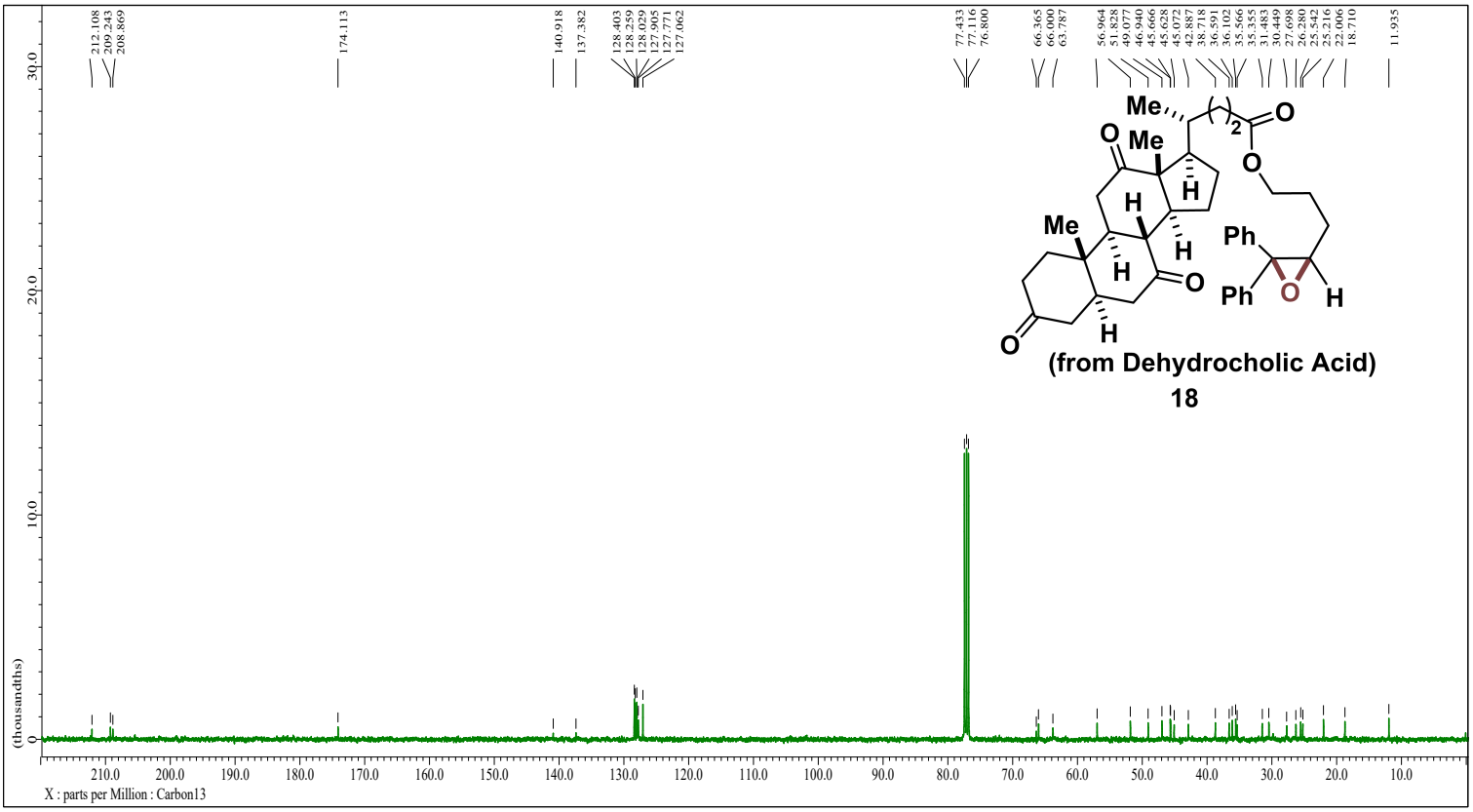

8.121
8.115
7.716
7.712
7.695
7.692
7.377
7.370
7.362
7.357
7.333
7.313
7.293
7.289
7.281
7.261
7.128
7.108
7.089
7.026
7.004
5.160
4.262
4.253
4.248
4.239
4.233
4.220
3.651
3.492
3.479
3.474
3.462
1.863
1.853
1.845
0.000
O
O
O
O
Ph
Ph
O
H
(from Isoxepac)
16
4.54
2.26
2.08
1.89
1.83
1.24
1.21
1.02
0.96
0.93
2.04
2.19
2.04
1.00
2.00
abundance
X : parts per Million : Proton

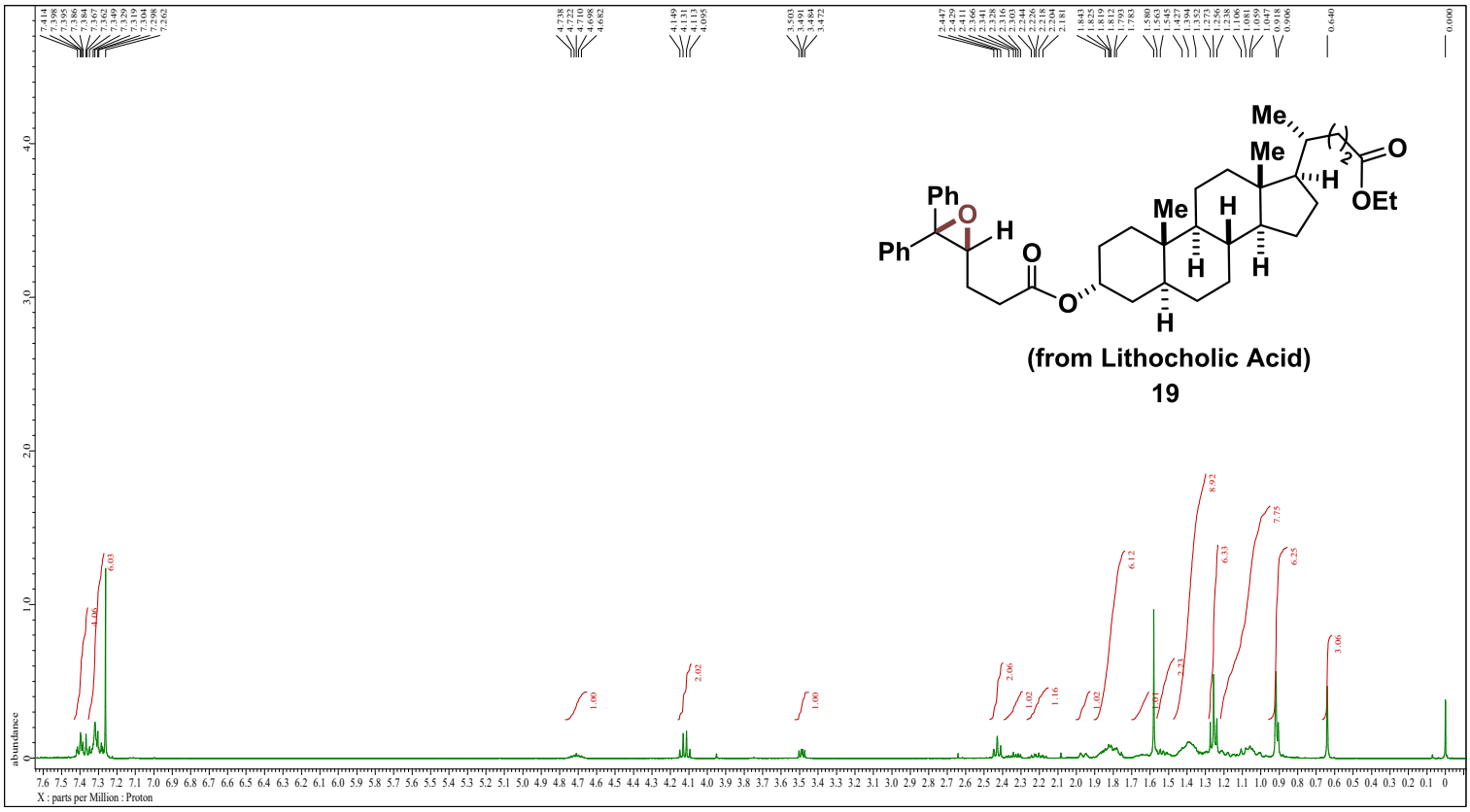

190.931
171.430
160.601
140.612
137.655
137.181
136.424
135.600
132.888
132.562
130.339
129.582
129.371
128.422
128.336
128.049
127.872
127.732
127.560
127.119
121.216
77.442
77.126
76.810
73.715
66.202
63.365
62.244
40.290
29.136
1.125
O
O
O
O
Ph
Ph
O
H
(from Isoxepac)
16
(thousandths)
X : parts per Million : Carbon13

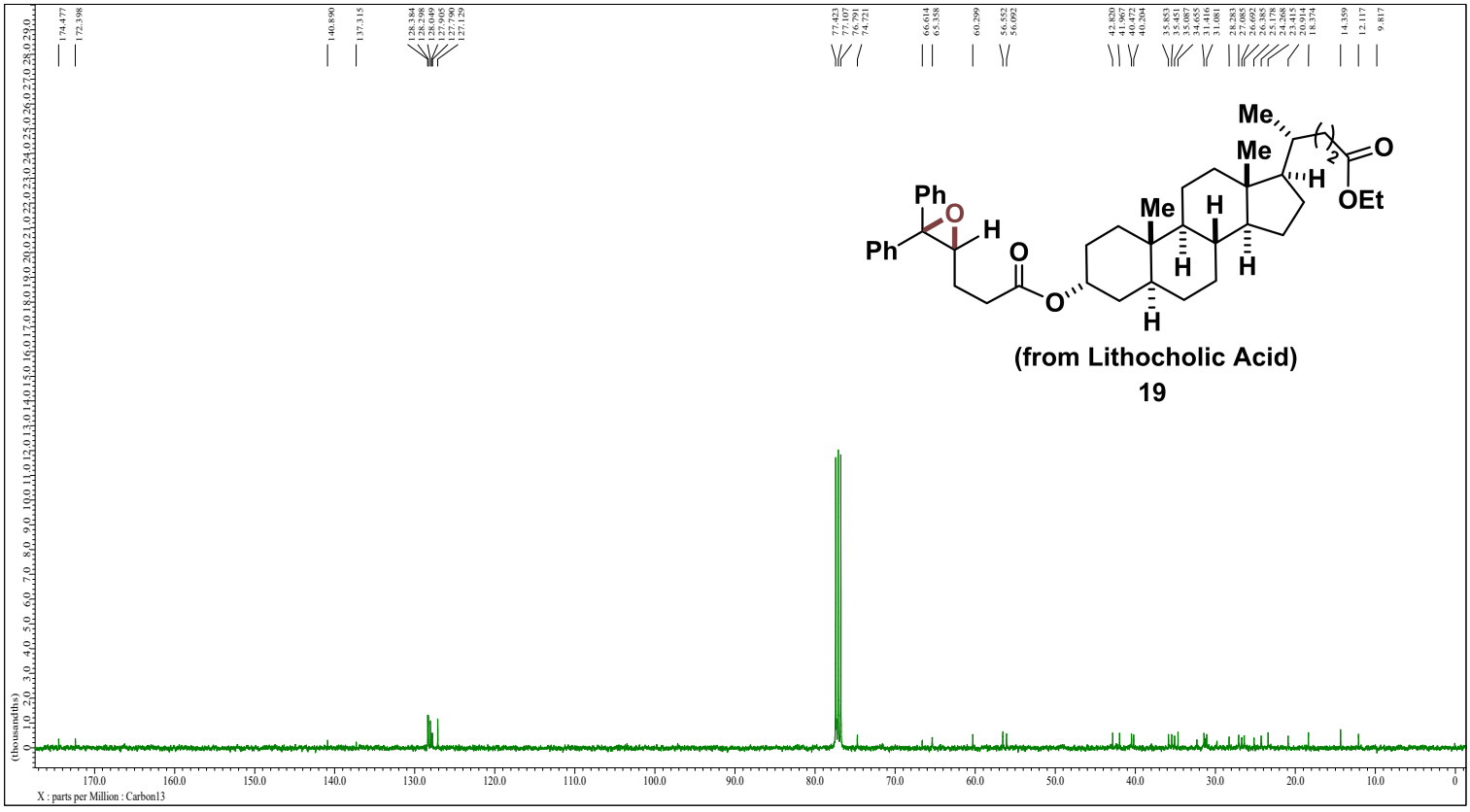

abundance
X : parts per Million : Proton
(from Sulbactam)
17

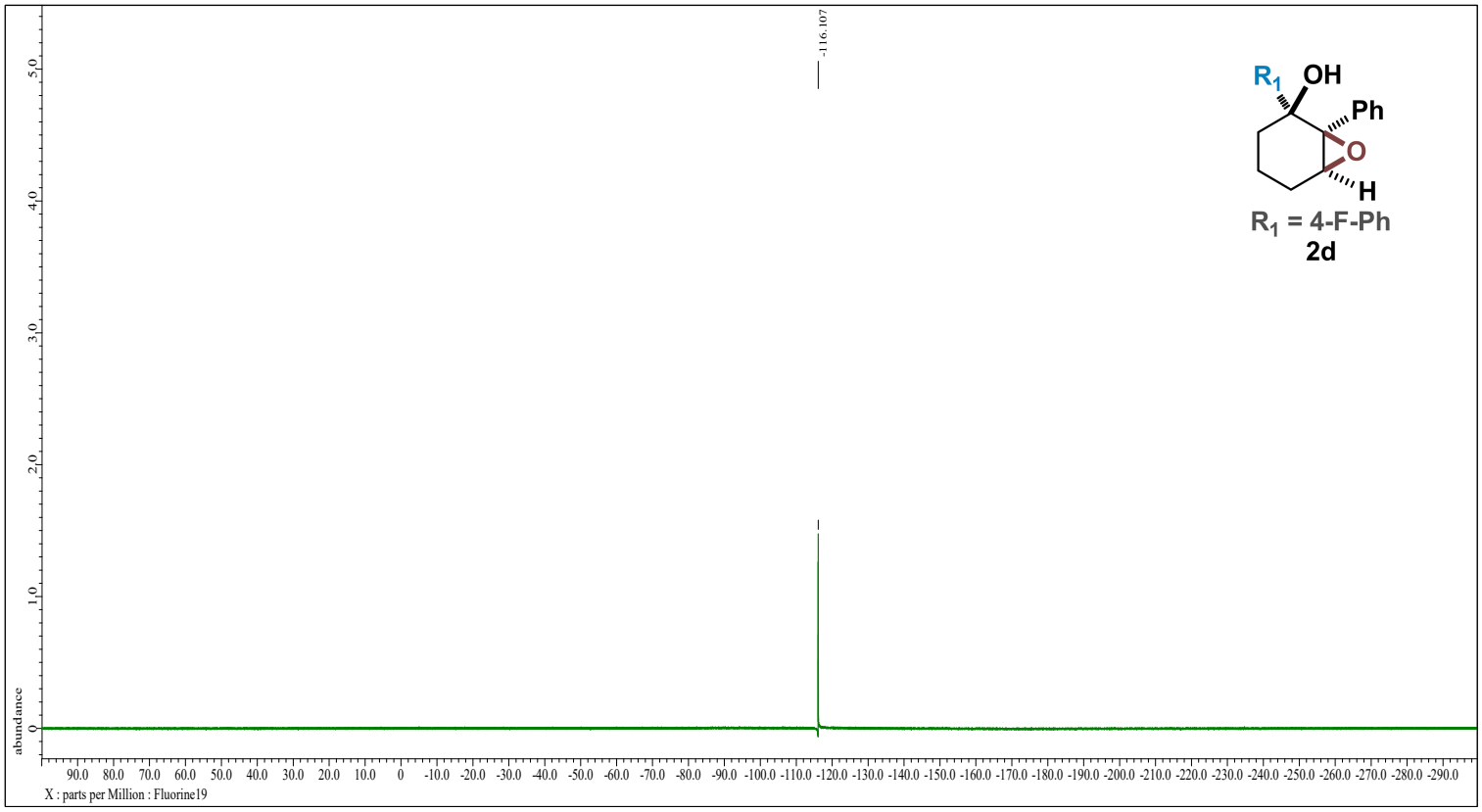

(thousandths)
X : parts per Million : Carbon13
(from Sulbactam)
17

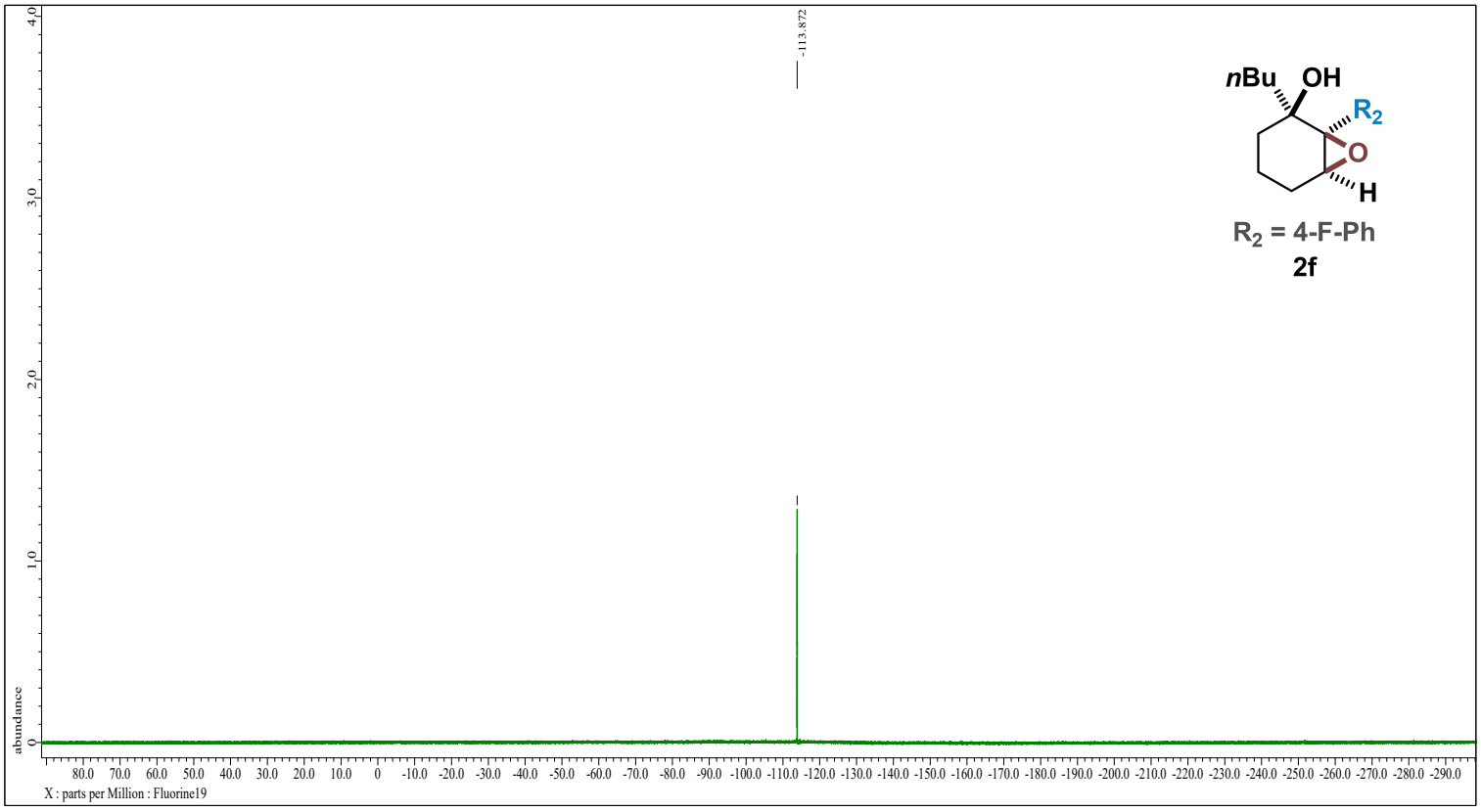

(from Dehydrocholic Acid)
18
X : parts per Million : Proton
abundance

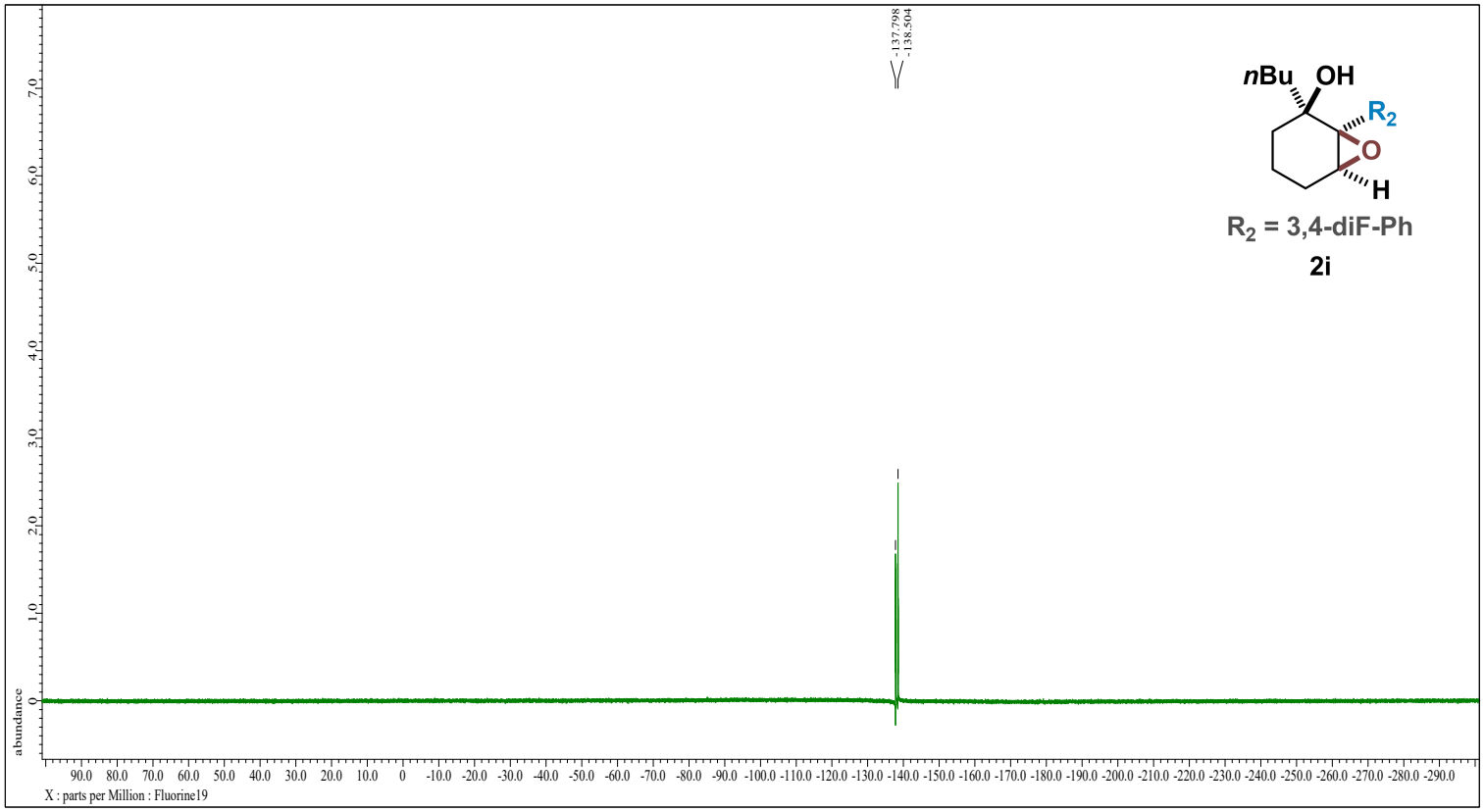

(from Dehydrocholic Acid)
18
X : parts per Million : Carbon13
(thousandths)

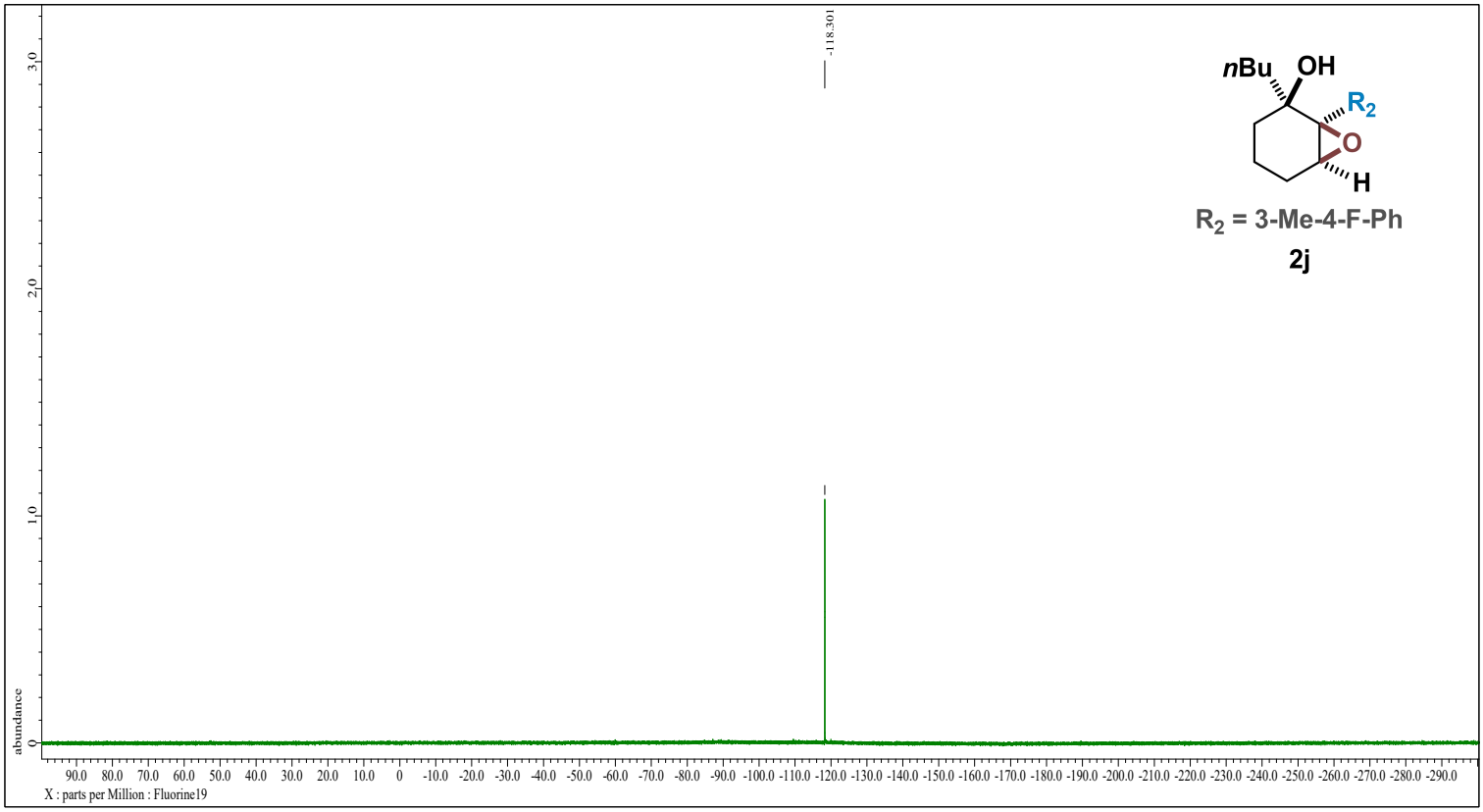

Me
Me
O
2
H
OEt
Ph
O
H
Ph
O
Me
H
H
H
O
H
(from Lithocholic Acid)
19
abundance
X : parts per Million : Proton

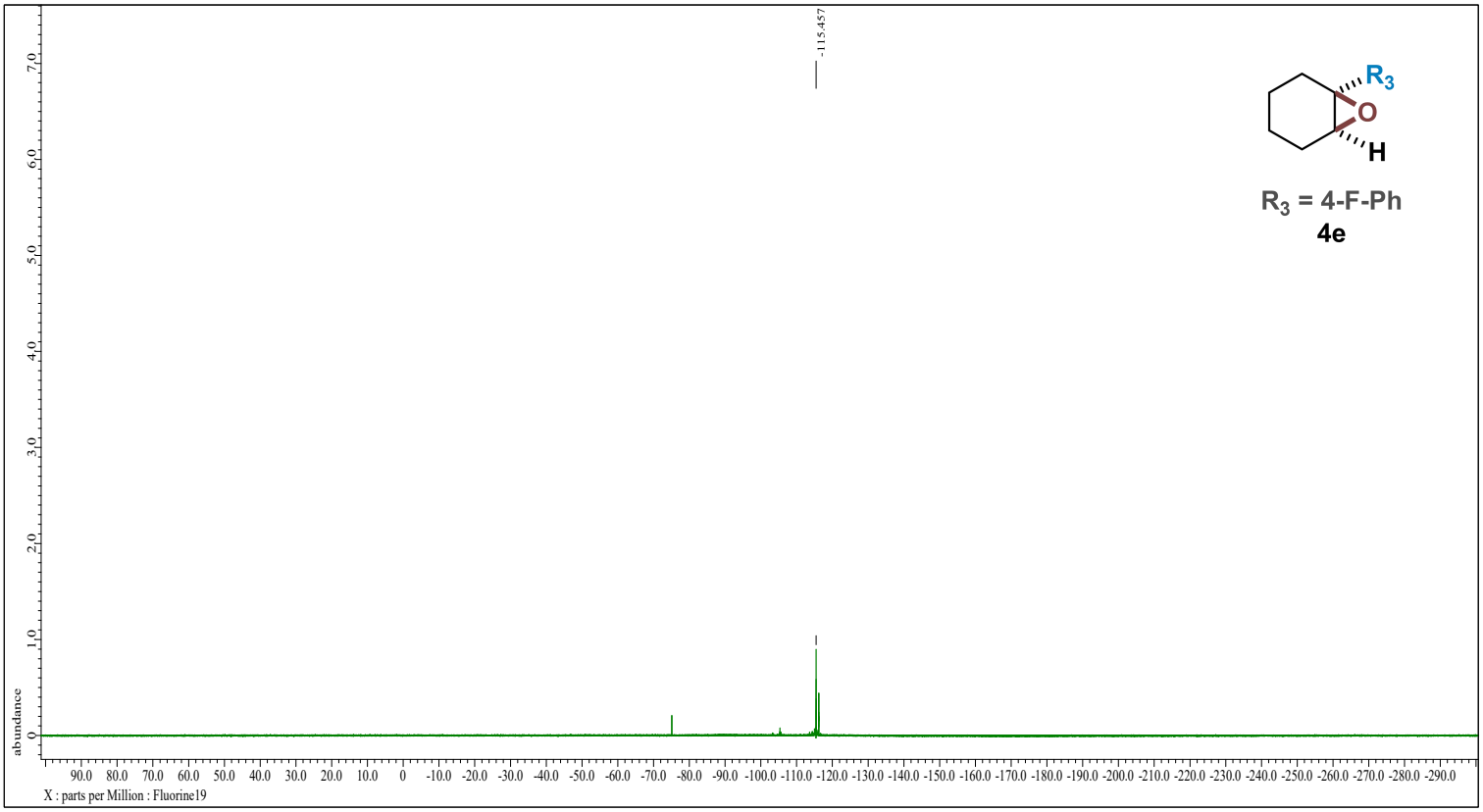

Me
Me
O
2
H
OEt
Ph
O
H
Ph
O
Me
H
H
H
O
H
(from Lithocholic Acid)
19
(thousandths)
X : parts per Million : Carbon13

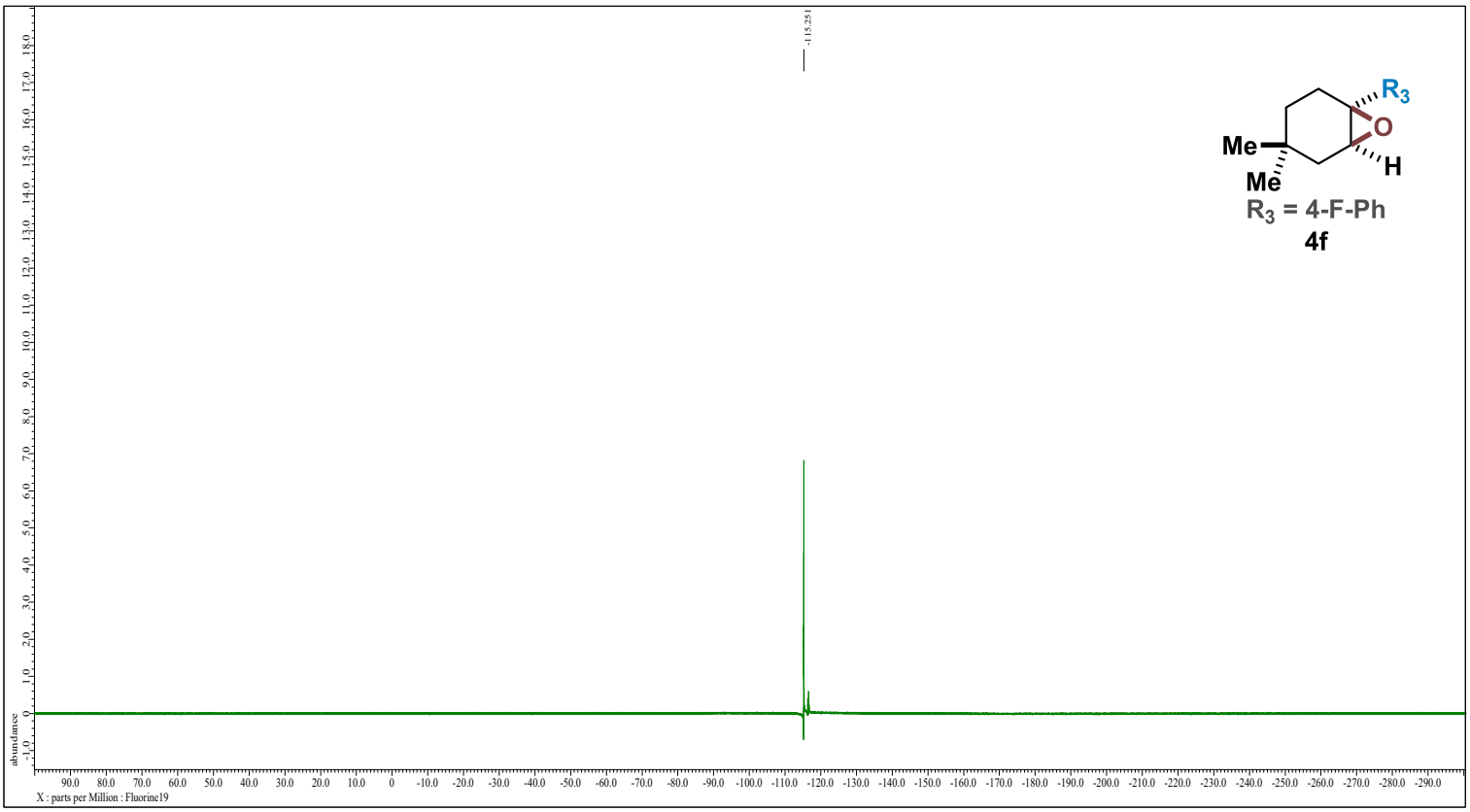

-116.107
R1 OH
Ph
O
H
R1 = 4-F-Ph
2d
abundance
X : parts per Million : Fluorine19

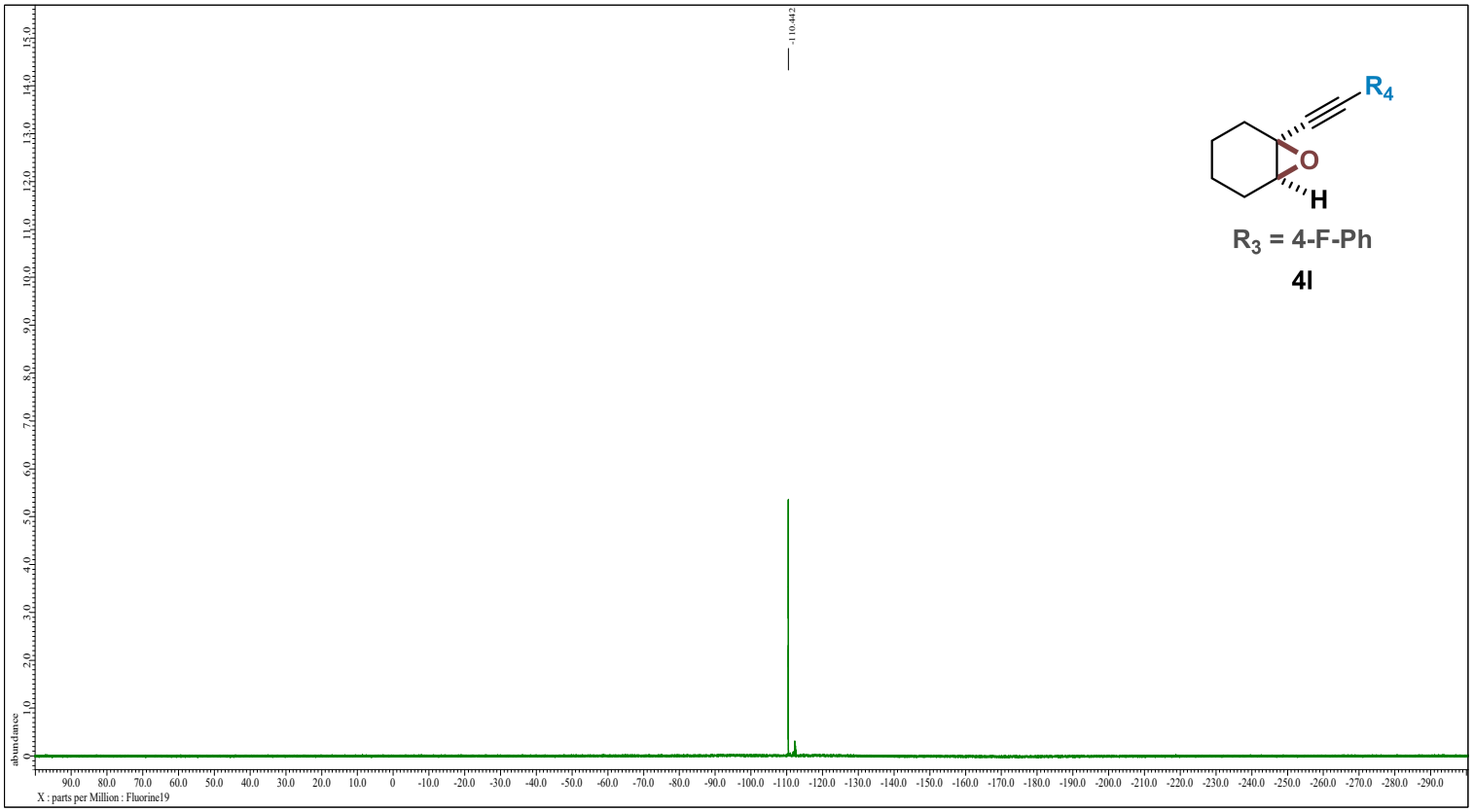

-113.872
nBu OH
R2
O
H
R2 = 4-F-Ph
2f
abundance
X : parts per Million : Fluorine19


-137.798
-138.504
nBu
OH
R2
O
H
R2 = 3,4-diF-Ph
2i
abundance
X : parts per Million : Fluorine19

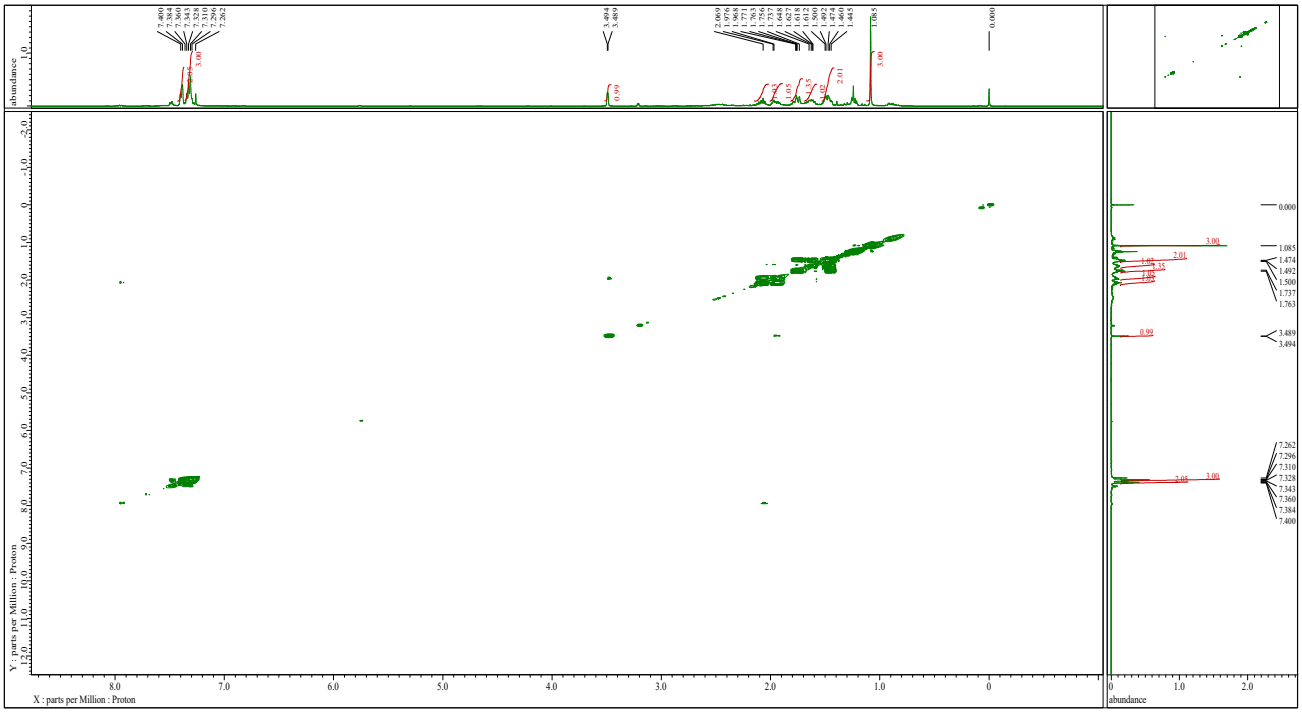

-118.301
nBu
OH
R2
O
H
R2 = 3-Me-4-F-Ph
2j
abundance
X : parts per Million : Fluorine19


-115.457
abundance
X : parts per Million : Fluorine19
R3
O
H
R3 = 4-F-Ph
4e

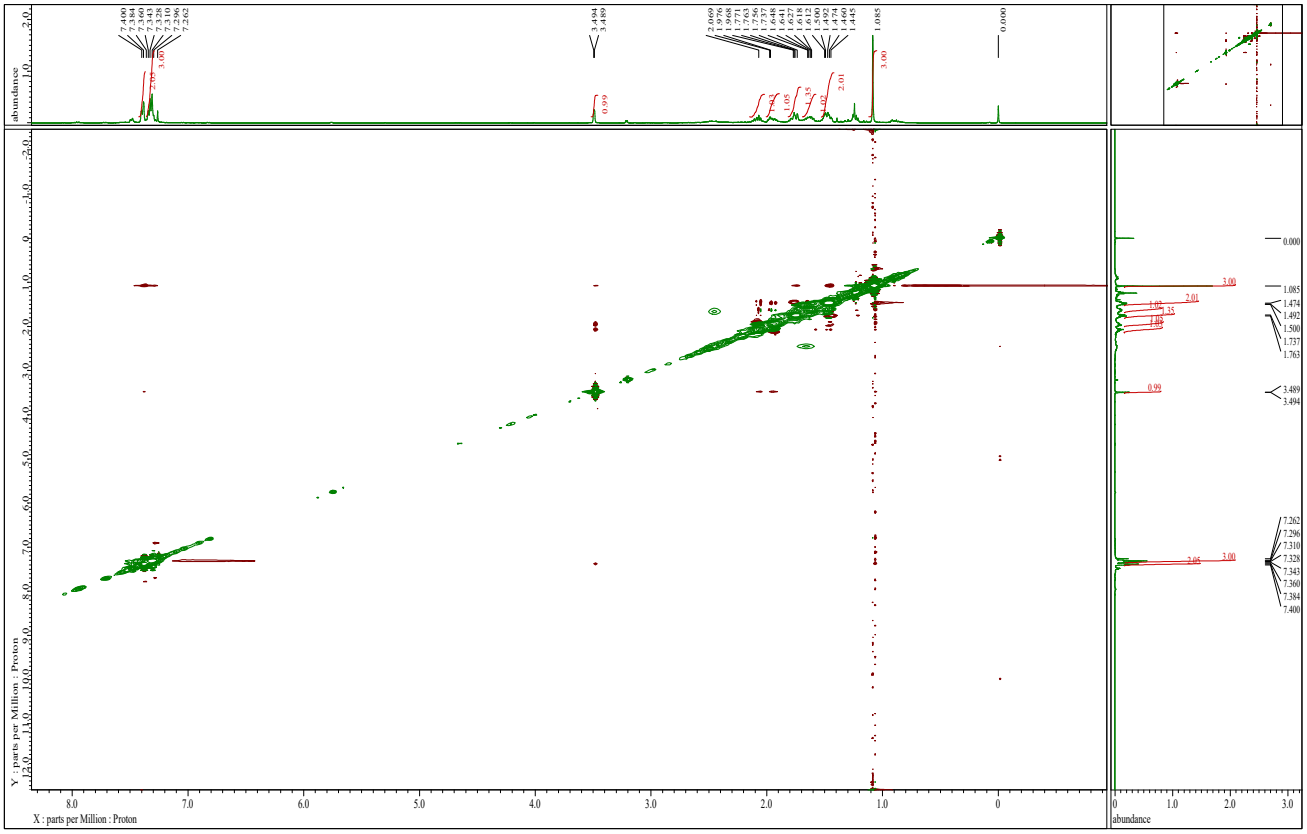

-115.251
abundance
X : parts per Million : Fluorine19
R3
O
Me
Me
H
R3 = 4-F-Ph
4f


-110.442
abundance
X : parts per Million : Fluorine19
R4
O
H
R3 = 4-F-Ph
4l

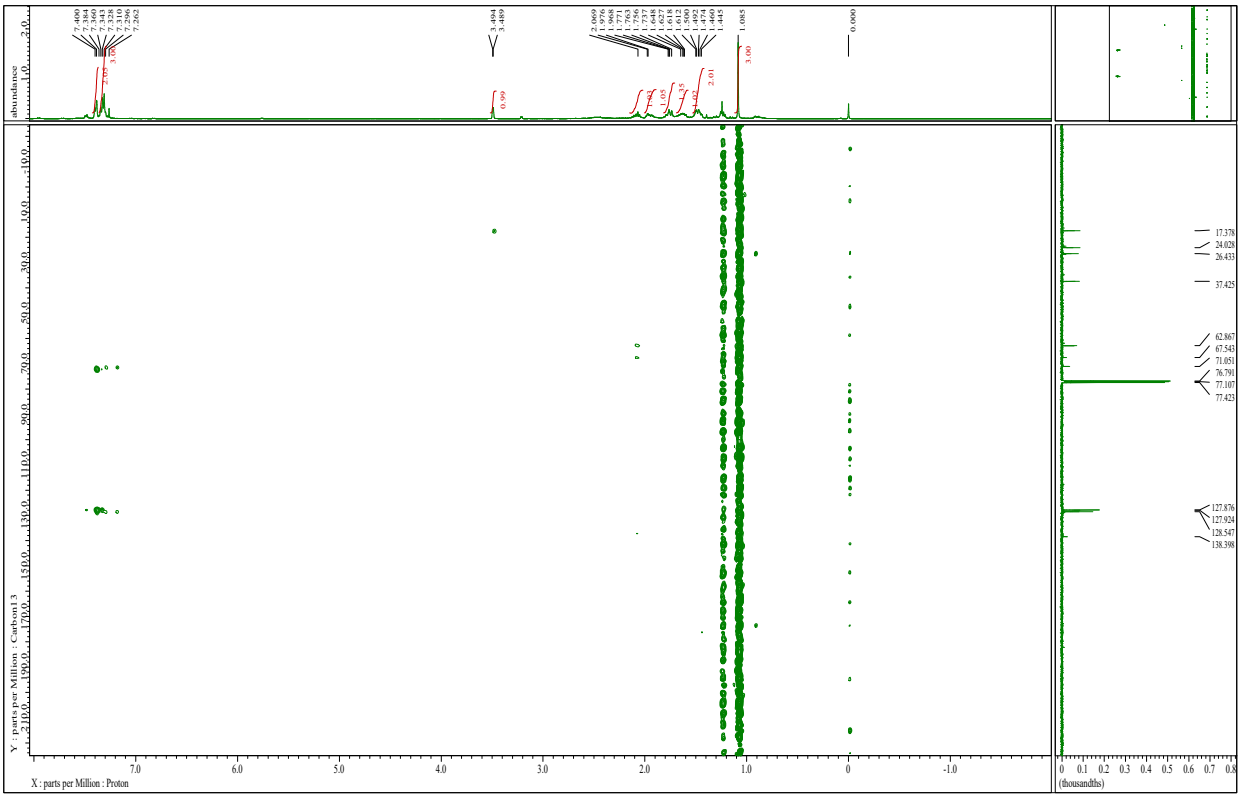
COSY, NOESY, HMBC, HMQC and 1D NOE spectra data of compounds 2k



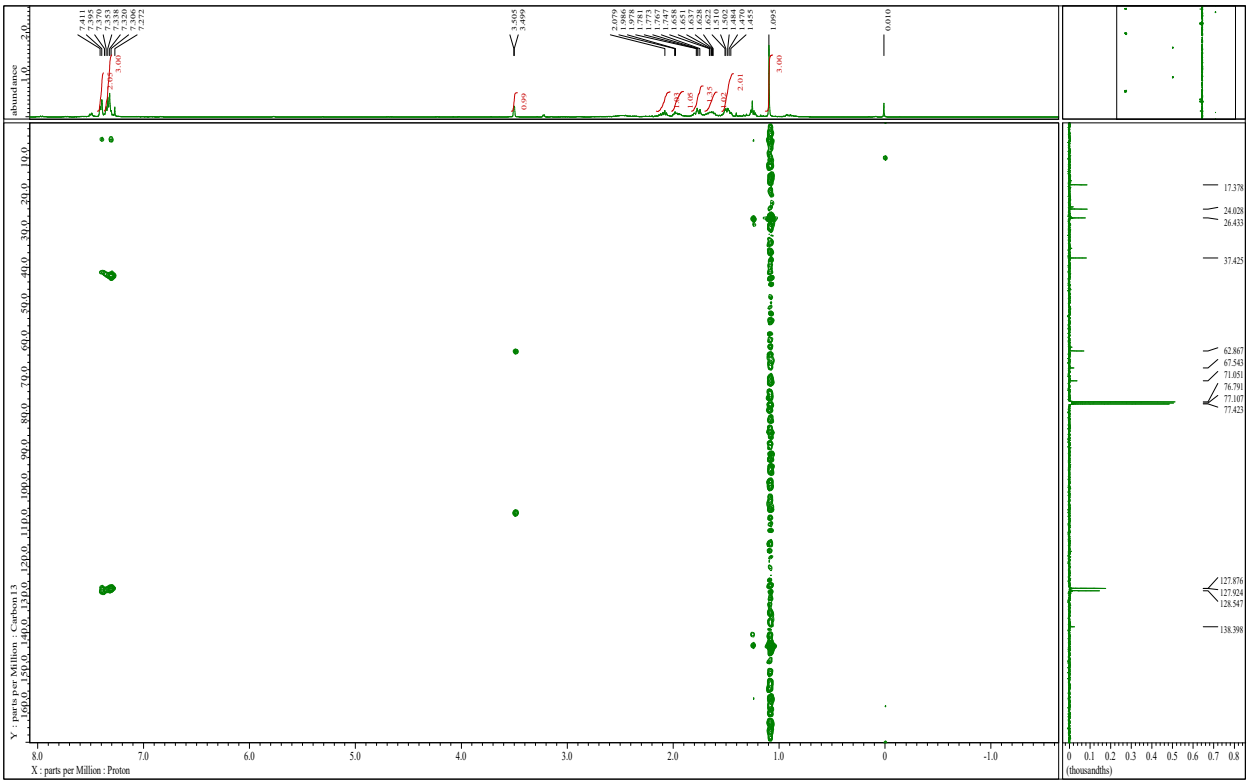
COSY



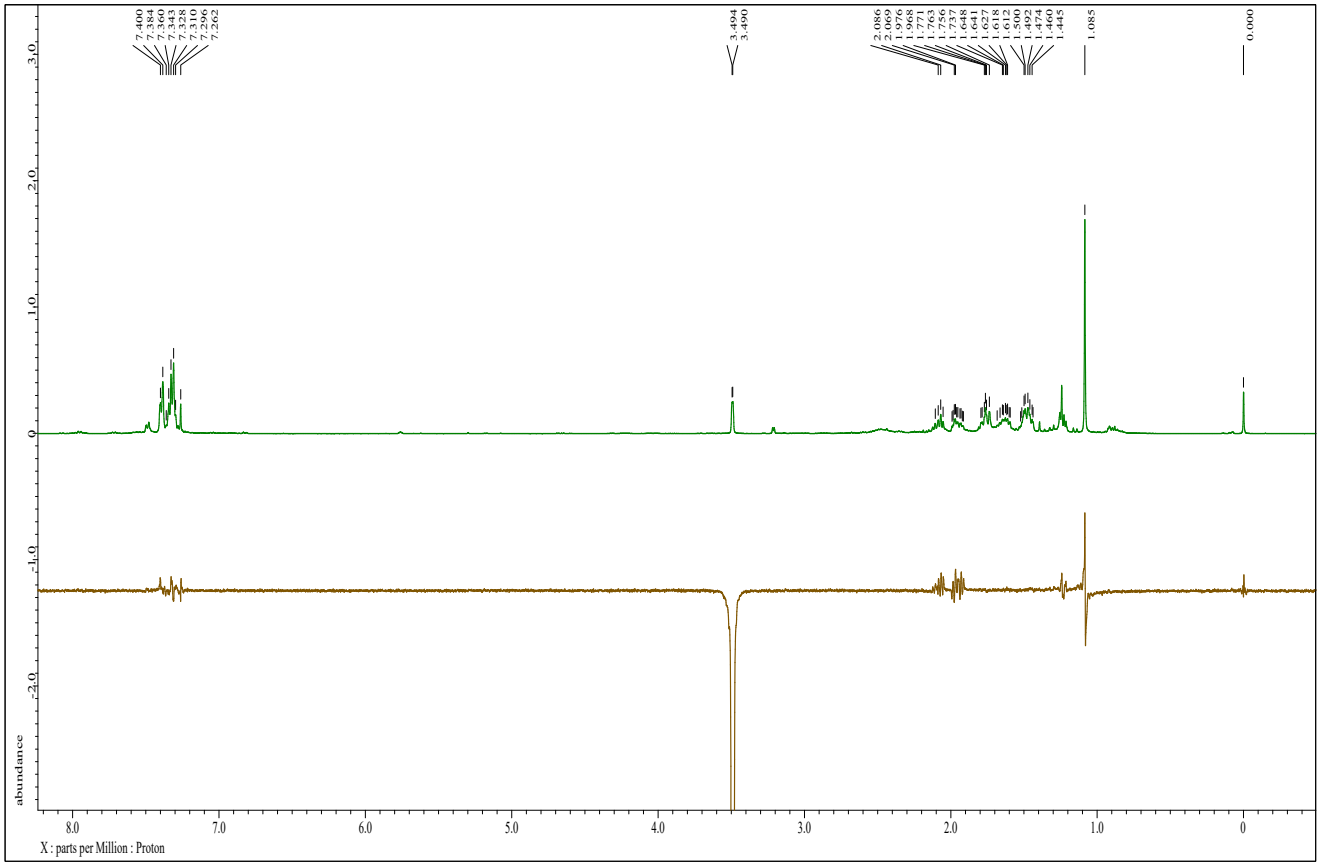
NOESY



HMBC

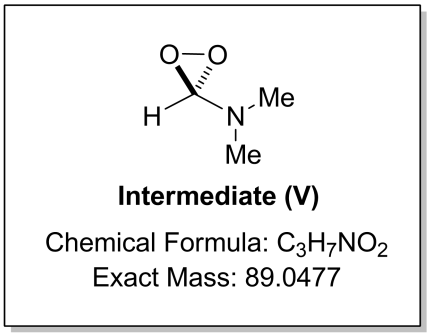


HMQC


7.400
7.384
7.360
7.343
7.328
7.310
7.296
7.262
3.494
3.490
2.086
2.069
1.976
1.968
1.771
1.763
1.756
1.737
1.648
1.641
1.627
1.618
1.612
1.500
1.492
1.484
1.460
1.445
1.085
0.000
3.0
2.0
1.0
0
-1.0
-2.0
abundance
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
X : parts per Million : Proton

1D NOE

High resolution mass spectrometry data of intermediate V



Intermediate (V)

Chemical Formula: $C_3H_7NO_2$

Exact Mass: 89.0477

HRMS calculated for $C_3H_8O_2N$ ($M + H^+$): 90.0555, found: 90.0550.