Supporting Information

Photocatalytic Dehydrogenated Etherification of 2-Aryl Benzylic Alcohols

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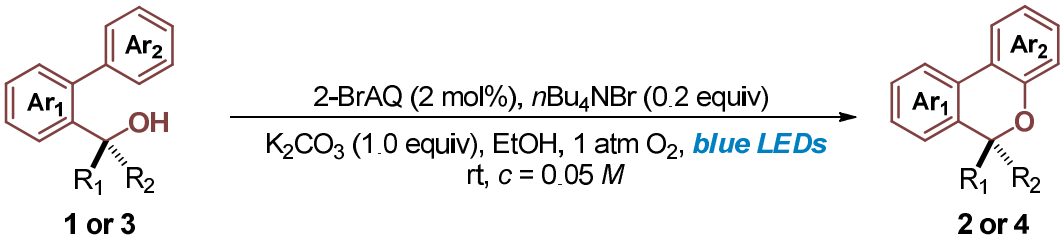
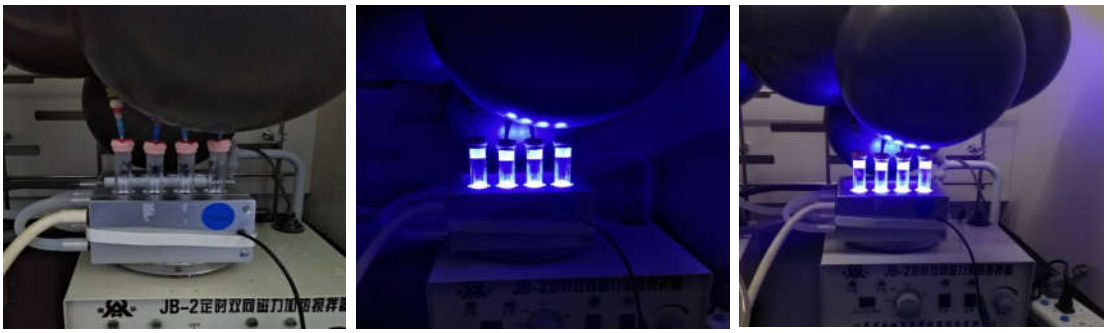
Materials and methods

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. ^{1}H NMR spectra were recorded on JEOL spectrometers (at 400 MHz) and were reported relative to deuterated solvent signals. Data for ^{1}H NMR spectra were reported as follows: chemical shift (δ ppm), multiplicity, coupling constant (Hz) and integration. ^{13}C NMR spectrawere recorded on JEOL Spectrometers (at 100 MHz). Data for ^{13}C 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.

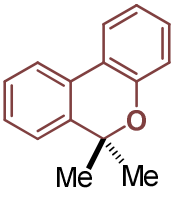
General procedure for 6*H*-benzo[*c*]chromenes synthesis



A flame-dried reaction tube was equipped with magnetic stir bar and charged with 2-aryl benzylic alcohols **1** or **3** (0.14 mmol, 1.0 equiv), 2-BrAQ (0.0028 mmol, 0.02 equiv), K_2CO_3 (0.14 mmol, 1.0 equiv), *n*Bu_4NBr (0.028 mmol, 0.2 equiv) and EtOH (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* = 20/1) to afford the desired pure product **2-4** in 34-91% yields.

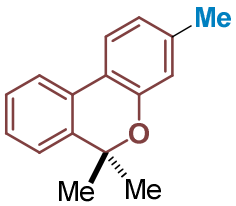


^{1}H, ^{13}C and ^{19}F spectra data of compounds 2a-2zc, 4a-4y



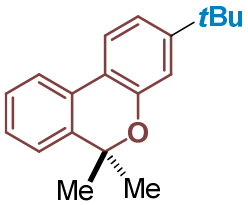
2a

6,6-dimethyl-6*H*-benzo[*c*]chromene (2a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.72 (d, *J* = 8.0 Hz, 2H), 7.35-7.28 (m, 2H), 7.25-7.20 (m, 2H), 7.04-7.00 (m, 1H), 6.96-6.94 (d, *J* = 8.4 Hz, 1H), 1.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 139.6, 129.5, 128.7, 128.0, 127.8, 123.3, 123.2, 122.9, 122.5, 122.3, 121.6, 118.1, 27.6. These data are consistent with literature values, see: L. Mahendar, J. Krishna, A. G. K. Reddy, B. V. Ramulu, G. Satyanarayana. *Org. Lett.* **2012**, *14*, 628. (Yellow oil, 25.3 mg, 84% isolated yield)



2b

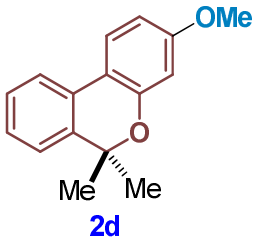
3,6,6-trimethyl-6*H*-benzo[*c*]chromene (2b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.67 (d, *J* = 7.6 Hz, 1H), 7.61-7.59 (d, *J* = 8.0 Hz, 1H), 7.34-7.21 (m, 3H), 6.84-6.82 (dd, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H), 6.77 (s, 1H), 2.32 (s, 3H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 139.9, 139.2, 128.8, 127.7, 127.6, 123.3, 122.8, 122.5, 121.9, 119.8, 118.6, 76.8, 27.7, 21.5. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Yellow oil, 30.8 mg, 91% isolated yield)



2c

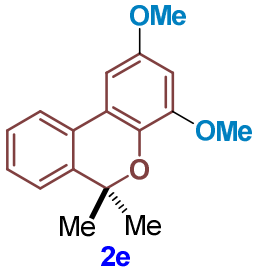
3-(tert-butyl)-6,6-dimethyl-6*H*-benzo[*c*]chromene (2c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.69 (d, *J* = 7.6 Hz, 1H), 7.66-7.64 (d, *J* = 7.4 Hz, 1H), 7.34-7.22 (m, 3H), 7.06-7.03 (m, 1H), 6.97-6.96 (d, *J* = 1.6 Hz, 1H), 1.64 (s, 6H), 1.32 (s, 9H); ^{13}C NMR

(100 MHz, $CDCl_3$) δ 153.4, 152.4, 139.2, 128.7, 127.7, 127.6, 123.2, 122.4, 122.0, 119.6, 118.7, 115.0, 77.0, 34.8, 31.3, 27.8; HRMS calculated for $C_{19}H_{23}O$ ($M + H^+$): 267.1750, found: 267.1745. (Pale yellow oil, 28.2 mg, 80% isolated yield)



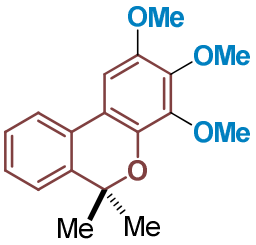
2d

3-methoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64-7.62 (m, 2H), 7.33-7.29 (m, 1H), 7.24-7.22 (dd, J_1 = 1.2 Hz, J_2 = 6.4 Hz, 2H), 6.61-6.59 (m, 1H), 6.52-6.51 (d, J = 2.4 Hz, 1H), 3.81 (s, 3H), 1.63 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.1, 154.0, 138.3, 128.8, 127.7, 127.0, 123.9, 123.2, 121.5, 115.5, 108.4, 102.8, 78.0, 55.4, 27.6. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Yellow oil, 21.6 mg, 71% isolated yield)



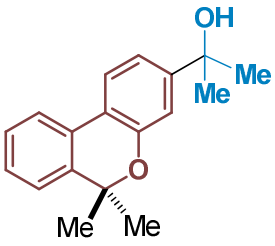
2e

2,4-dimethoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67-7.65 (m, 1H), 7.34-7.30 (m, 2H), 6.85-6.84 (d, J = 2.8 Hz, 1H), 6.50-6.49 (d, J = 2.8 Hz, 1H), 3.87 (s, 3H), 3.85 (s, 3H), 1.66 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 150.4, 140.0, 136.5, 128.8, 128.2, 127.6, 123.3, 123.2, 122.6, 100.5, 98.2, 77.5, 56.3, 55.8, 27.3; HRMS calculated for $C_{17}H_{19}O_3$ ($M + H^+$): 271.1335, found: 271.1329. (Yellow oil, 29.6 mg, 82% isolated yield)



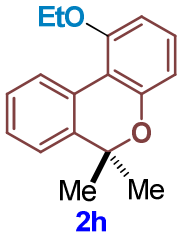
2f

2,3,4-trimethoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.61 (m, 1H), 7.36-7.23 (m, 3H), 7.01 (s, 1H), 3.95 (s, 3H), 3.94 (s, 3H), 3.92 (s, 3H), 1.67 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.3, 150.4, 140.0, 136.5, 128.8, 128.2, 127.6, 123.3, 123.2, 122.6, 100.5, 98.2, 77.5, 56.3, 55.8, 27.3; HRMS calculated for $C_{18}H_{20}O_4Na$ (M + Na^+): 323.1260, found: 323.1254. (Pale yellow solid, Mp 83-85 ℃, 31.6 mg, 87% isolated yield)



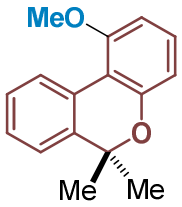
2g

2-(6,6-dimethyl-6*H*-benzo[*c*]chromen-3-yl)propan-2-ol (2g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.68 (m, 2H), 7.36-7.23 (m, 3H), 7.16-7.14 (m, 1H), 7.07-7.06 (d, J = 2.0 Hz, 1H), 1.64 (s, 6H), 159(s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 151.0, 139.3, 128.5, 127.9, 127.7, 123.3, 122.8, 122.2, 120.8, 117.8, 114.2, 77.8, 72.5, 31.7, 27.8; HRMS calculated for $C_{18}H_{20}O_2Na$ (M + Na^+): 291.1361, found: 291.1356. (Yellow oil, 20.0 mg, 65% isolated yield)



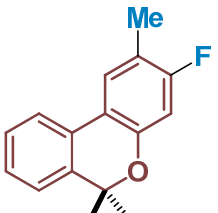
2h

1-ethoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39-7.35 (m, 1H), 7.31-7.28 (m, 1H), 7.20-7.18 (d, *J* = 8.0 Hz, 1H), 6.96-6.94 (d, *J* = 7.6 Hz, 1H), 6.55-6.53 (d, *J* = 10.0 Hz, 1H), 6.12-6.10 (m, 1H), 5.54-5.53 (d, *J* = 2.0 Hz, 1H), 3.98-3.91 (m, 1H), 3.84-3.76 (m, 1H), 1.69 (s, 3H), 1.63 (s, 3H), 1.25-1.21 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.9, 173.6, 147.7, 146.9, 137.6, 129.2, 128.2, 125.9, 121.6, 121.4, 120.6, 101.9, 88.6, 64.7, 31.4, 29.5, 13.9; HRMS calculated for $C_{17}H_{19}O_2$ (M + H^+): 255.1385, found: 255.1379. (Yellow oil, 22.1 mg, 68% isolated yield)



2i

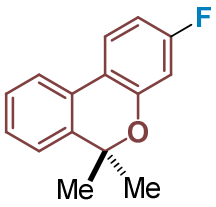
1-methoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.34 (m, 1H), 7.31-7.29 (m, 1H), 7.21-7.19 (d, *J* = 8.0 Hz, 1H), 6.96-6.94 (d, *J* = 7.6 Hz, 1H), 6.55-6.53 (d, *J* = 10.4 Hz, 1H), 6.14-6.11 (m, 1H), 5.58-5.57 (m, 1H), 3.65 (s, 3H), 1.68 (s, 3H), 1.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.7, 174.2, 147.7, 146.8, 137.5, 129.4, 128.3, 125.9, 121.4, 101.6, 88.6, 83.4, 56.1, 31.4, 29.5; HRMS calculated for $C_{16}H_{17}O_2$ (M + H^+): 241.1229, found: 241.1223. (Pale yellow solid, Mp 97-99 ℃, 23.5 mg, 79% isolated yield)



2j

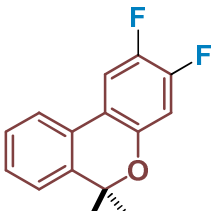
3-fluoro-2,6,6-trimethyl-6*H*-benzo[*c*]chromene (2j): ^{1}H NMR (400 MHz, $CDCl_3$) δ

7.66-7.64 (m, 1H), 7.52-7.50 (d, J = 8.8 Hz, 1H), 7.35-7.21 (m, 3H), 6.64-6.62 (d, J = 10.4 Hz, 1H), 2.27 (s, 3H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 158.3, 144.2, 138.9, 128.2, 127.8, 127.7, 125.3, 125.2, 123.3, 121.9, 105.2, 104.9, 78.1, 27.5, 14.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.3; HRMS calculated for $C_{16}H_{16}OF$ ($M + H^+$): 243.1186, found: 243.1180. (Yellow oil, 21.8 mg, 73% isolated yield)



2k

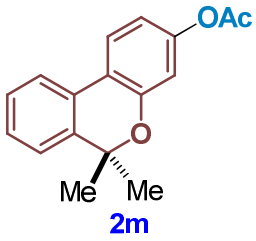
3-fluoro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.64 (m, 2H), 7.37-7.32 (m, 1H), 7.31-7.27 (m, 1H), 7.25-7.22 (m, 1H), 6.76-6.66 (m, 2H), 1.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.1, 138.7, 128.1, 127.9, 124.1, 124.0, 123.3, 122.0, 108.8, 108.6, 105.5, 105.3, 78.4, 27.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.9. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Yellow oil, 19.7 mg, 68% isolated yield)



2l

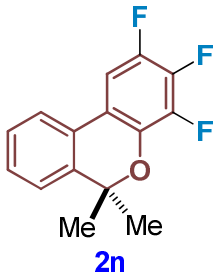
2,3-difluoro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67-7.64 (m, 1H), 7.39-7.35 (m, 1H), 7.26-7.22 (m, 1H), 7.16-7.11 (m, 2H), 7.05-7.02 (m, 1H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 138.1, 132.2, 128.1, 126.4, 126.1, 125.8, 125.7, 118.9, 118.8, 116.5, 116.4, 74.0, 32.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -138.2, -140.3; HRMS calculated for $C_{15}H_{13}OF_2$ ($M + H^+$): 247.0935, found:

247.0929. (Pale yellow oil, 25.5 mg, 84% isolated yield)



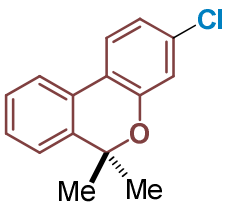
2m

6,6-dimethyl-6*H*-benzo[*c*]chromen-3-yl acetate (2m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72-7.67 (m, 2H), 7.36-7.27 (m, 2H), 7.25-7.22 (m, 1H), 6.79-6.76 (dd, J_1 = 8.4 Hz, J_2 = 2.4 Hz, 1H), 6.72-6.71 (d, J = 2.4 Hz, 1H), 2.30 (s, 3H), 1.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 153.6, 151.5, 139.1, 128.1, 128.0, 127.8, 123.6, 123.3, 122.2, 120.3, 114.8, 111.4, 78.2, 27.7, 21.3; HRMS calculated for $C_{17}H_{17}O_3$ ($M + H^+$): 269.1178, found: 269.1172. (Colorless oil, 10.8 mg, 60% isolated yield)



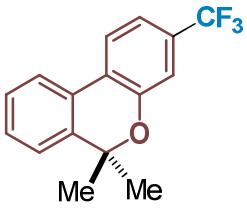
2n

2,3,4-trifluoro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.61 (m, 1H), 7.39-7.35 (m, 1H), 7.27-7.23 (m, 1H), 7.03-7.01 (dd, J_1 = 7.6 Hz, J_2 = 0.8 Hz, 1H), 6.95-6.91 (m, 1H), 1.49 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4, 149.0, 148.9, 146.0, 140.2, 137.4, 131.9, 128.3, 126.5, 126.3, 114.2, 114.1, 114.0, 113.9, 73.9, 32.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -135.2, -135.3, -163.1; HRMS calculated for $C_{15}H_{12}OF_3$ ($M + H^+$): 265.0841, found: 265.0835. (Pale yellow solid, Mp 93-95 ℃, 21.8 mg, 68% isolated yield)



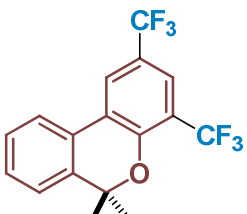
2o

3-chloro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.35-7.30 (m, 2H), 7.25-7.22 (m, 1H), 7.00-6.96 (m, 2H), 1.63 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 139.2, 134.5, 128.3, 127.9, 127.8, 123.9, 123.4, 122.2, 121.9, 121.2, 118.4, 78.4, 27.7; These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Yellow oil, 22.0 mg, 73% isolated yield)



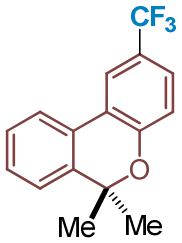
2p

6,6-dimethyl-3-(trifluoromethyl)-6*H*-benzo[*c*]chromene (2p): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.44-7.36 (m, 3H), 7.28-7.24 (m, 1H), 7.04-7.02 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 1.46 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 146.0, 138.8, 131.9, 131.6, 129.9, 128.0, 126.3, 126.1, 125.6, 124.6, 124.5, 122.9, 74.0, 32.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.2; HRMS calculated for $C_{16}H_{14}O_3$ (M + H^+): 279.0997, found: 279.0991. (White solid, Mp 68-70 ℃, 23.1 mg, 64% isolated yield)



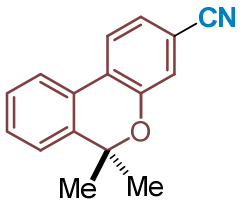
2q

6,6-dimethyl-2,4-bis(trifluoromethyl)-6*H*-benzo[*c*]chromene (2q): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (s, 1H), 7.78 (s, 1H), 7.62-7.60 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.43-7.39 (m, 1H), 7.31-7.26 (m, 1H), 7.07-7.04 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 1.48 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.6, 146.0, 137.6, 132.0, 130.6, 130.3, 129.8, 128.5, 127.2, 126.7, 126.3, 124.8, 122.1, 120.5, 73.8, 32.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.6, -62.6; HRMS calculated for $C_{17}H_{13}OF_6$ ($M + H^+$): 347.0871, found: 347.0865. (White solid, Mp 74-76 ℃, 22.8 mg, 77% isolated yield)



2r

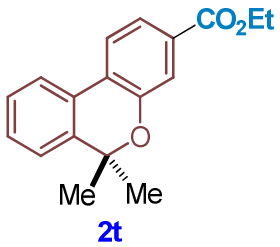
6,6-dimethyl-2-(trifluoromethyl)-6*H*-benzo[*c*]chromene (2r): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.66 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.61-7.58 (m, 2H), 7.50-7.49 (m, 1H), 7.41-7.36 (m, 1H), 7.29-7.25 (m, 1H), 7.06-7.04 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 1.45 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.2, 144.9, 138.7, 132.9, 132.1, 130.1, 129.8, 128.0, 126.4, 126.1, 125.5, 123.7, 123.7, 122.8, 79.9, 32.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.4; HRMS calculated for $C_{16}H_{14}O_3$ ($M + H^+$): 279.0997, found: 279.0991. (Orange oil, 22.0 mg, 64% isolated yield)



2s

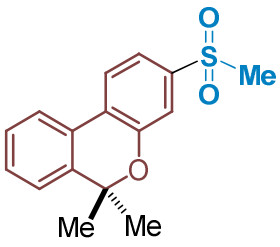
6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carbonitrile (2s): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.61 (m, 2H), 7.43-7.37 (m, 3H), 7.29-7.25 (m, 1H), 7.02-6.99 (dd, J_1 = 7.6 Hz,

J_2 = 1.2 Hz, 1H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.7, 145.9, 138.5, 131.6, 131.3, 130.4, 128.2, 126.4, 126.2, 119.0, 110.6, 73.9, 32.8. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (White solid, Mp 162-165 ℃, 11.2 mg, 36% isolated yield)



2t

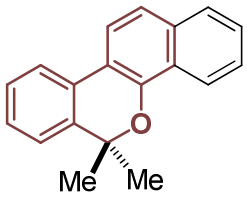
ethyl 6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (2t): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.04 (m, 2H), 7.68-7.65 (dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 7.39-7.37 (m, 2H), 7.29-7.25 (m, 1H), 7.05-7.02 (dd, J_1 = 7.6 Hz, J_2 = 1.6 Hz, 1H), 4.43-4.48 (q, J= 7.2 Hz, 2H), 1.45 (s, 6H), 1.41 (t, J= 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.5, 149.1, 146.1, 139.2, 131.6, 129.6, 129.1, 128.9, 127.8, 126.3, 126.1, 74.0, 61.1, 32.7, 14.4; HRMS calculated for $C_{18}H_{19}O_3$ (M + H^+): 283.1335, found: 283.1329. (Yellow solid, Mp 97-99 ℃, 24.8 mg, 79% isolated yield)



2u

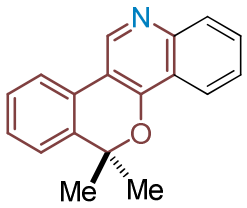
6,6-dimethyl-3-(methylsulfonyl)-6*H*-benzo[*c*]chromene (2u): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94-7.92 (m, 2H), 7.65-7.62 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 7.53-7.50 (m, 2H), 7.42-7.38 (m, 1H), 7.02-7.00 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 3.12 (s, 3H), 1.47 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 150.0, 149.2, 145.9, 138.7, 138.3, 131.7, 130.5, 128.2, 126.6, 126.4, 126.2, 73.9, 68.0, 44.6, 32.8; HRMS calculated for

$C_{16}H_{17}O_3S$ (M + H^+): 289.0899, found: 289.0893. (White solid, Mp 182-184 ℃, 23.5 mg, 78% isolated yield)



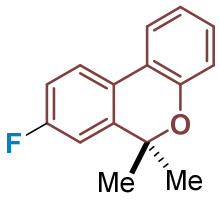
2v

6,6-dimethyl-6*H*-dibenzo[*c,h*]chromene (2v): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31-8.29 (m, 1H), 7.86-7.84 (d, *J* = 8.8 Hz, 1H), 7.80-7.77 (m, 2H), 7.52-7.46 (m, 3H), 7.40-7.36 (m, 1H), 7.34-7.23 (m, 2H), 1.73 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 139.0, 134.5, 129.1, 127.9, 127.8, 127.6, 126.5, 126.2, 125.6, 123.3, 122.5, 122.2, 120.9, 120.8, 116.4, 78.3, 27.6; HRMS calculated for $C_{19}H_{17}O$ (M + H^+): 261.1280, found: 261.1274. (White solid, Mp 93-95 ℃, 13.6 mg, 47% isolated yield)



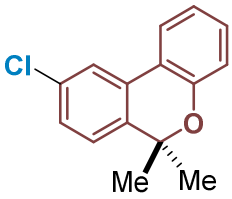
2w

6,6-dimethyl-6*H*-isochromeno[*4,3-c*]quinoline (2w): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.93-7.88 (m, 2H), 7.83-7.81 (m, 1H), 7.65-7.61 (m, 1H), 7.44-7.40 (m, 3H), 7.38-7.33 (m, 1H), 1.77 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 147.7, 140.4, 130.9, 129.9, 129.1, 128.2, 127.7, 127.6, 127.4, 126.2, 124.8, 123.8, 123.2, 117.8, 80.2, 28.8; HRMS calculated for $C_{18}H_{16}ON$ (M + H^+): 262.1233, found: 262.1226. (Yellow solid, Mp 125-127 ℃, 15.5 mg, 52% isolated yield)



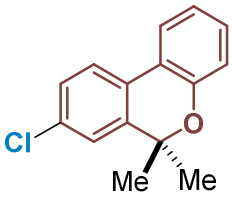
2x

8-fluoro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2x): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.65 (m, 2H), 7.24-7.20 (m, 1H), 7.07-7.00 (m, 2H), 6.96-6.93(m, 2H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.9, 152.2, 141.8, 141.7, 129.4, 129.0, 124.9, 124.2, 124.1, 122.7, 121.8, 119.5, 118.1, 114.8, 114.5, 110.6, 110.4, 27.3. ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.5; HRMS calculated for $C_{15}H_{14}OF$ ($M + H^+$): 229.1029, found: 229.1023. (Pale yellow oil, 17.6 mg, 59% isolated yield)



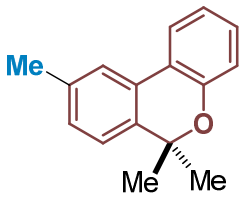
2y

9-chloro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2y): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.65 (m, 2H), 7.27-7.23 (m, 2H), 7.17-7.15 (d, J = 8.0 Hz, 1H), 7.05-7.00 (m, 1H), 6.96-6.93 (m, 1H), 1.61 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 137.8, 137.7, 130.6, 130.2, 127.7, 124.8, 123.0, 122.3, 121.7, 118.2, 27.5; HRMS calculated for $C_{15}H_{14}OCl$ ($M + H^+$): 245.0734, found: 245.0728. (Pale yellow solid, Mp 70-72 ℃ 15.6 mg, 48% isolated yield)



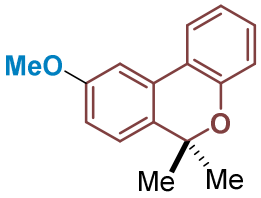
2z

8-chloro-6,6-dimethyl-6*H*-benzo[*c*]chromene (2z): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68-7.62 (m, 2H), 7.32-7.29 (dd, J_1 = 8.0 Hz, J_2= 2.4 Hz, 1H), 7.23-7.21 (m, 2H), 7.04-7.00 (m, 1H), 6.95-6.93 (m, 1H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 141.2, 133.6, 129.8, 127.9, 127.3, 123.7, 123.6, 122.8, 121.8, 121.6, 118.2, 27.4. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Yellow oil, 20.2 mg, 61% isolated yield)



2za

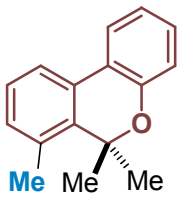
6,6,9-trimethyl-6*H*-benzo[*c*]chromene (2za): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.71 (m, 1H), 7.54 (s, 1H), 7.23-7.19 (m, 1H), 7.15-7.09 (m, 2H), 7.03-6.99 (m, 1H), 6.94-6.92 (m, 1H), 2.40 (s, 3H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 137.3, 136.8, 129.3, 128.9, 128.7, 128.4, 123.2, 122.8, 122.5, 121.5, 118.1, 77.5, 27.7, 21.4. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Pale yellow solid, Mp 59-61 ℃, 16.0 mg, 52% isolated yield)



2zb

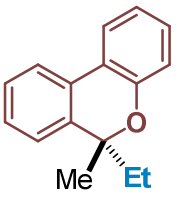
9-methoxy-6,6-dimethyl-6*H*-benzo[*c*]chromene (2zb): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67-7.63 (m, 2H), 7.19-7.15 (m, 1H), 7.02-6.98 (m, 1H), 6.94-6.87 (m, 2H), 6.79-6.78 (d, J = 2.0 Hz, 1H), 3.85 (s, 3H), 1.61 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$)

δ 169.4, 162.8, 159.6, 151.9, 141.3, 128.5, 123.7, 122.6, 122.2, 121.7, 121.6, 117.9, 112.5, 109.5, 55.4, 27.5; HRMS calculated for $C_{16}H_{17}O_2$ ($M + H^+$): 241.1229, found: 241.1223. (Yellow oil, 21.4 mg, 67% isolated yield)



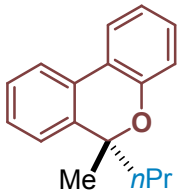
2zc

6,6,7-trimethyl-6*H*-benzo[*c*]chromene (2zc): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.25-7.20 (m, 3H), 7.16-7.13 (m, 1H) 7.09-6.99 (m, 2H), 2.66 (s, 3H), 1.59 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.0, 142.5, 134.2, 131.5, 128.7, 127.7, 127.3, 121.0, 120.9, 118.3, 78.0, 21.7, 23.6; HRMS calculated for $C_{16}H_{17}O$ ($M + H^+$): 225.1280, found: 225.1274. (Colorless oil, 16.1 mg, 63% isolated yield)



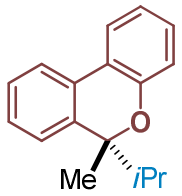
4a

(*R*)-6-ethyl-6-methyl-6*H*-benzo[*c*]chromene (4a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.71 (m, 2H), 7.36-7.27 (m, 2H), 7.24-7.17 (m, 2H), 7.03-6.99 (m, 1H), 6.96-6.93 (dd, J_1 = 8.0 Hz, J_2 = 0.8 Hz, 1H), 2.03-1.94 (m, 1H), 1.81-1.71(m, 1H), 1.64 (s, 3H), 0.93-0.90 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 138.7, 129.5, 129.0, 127.8, 127.7, 124.1, 122.9, 122.5, 122.3, 121.5, 118.0, 80.0, 32.5, 25.1, 8.5. These data are consistent with literature values, see: C. Shekhar, G. Satyanarayana. *Eur. J. Org. Chem.* **2022**, e202101444. (Colorless oil, 25.0 mg, 85% isolated yield)



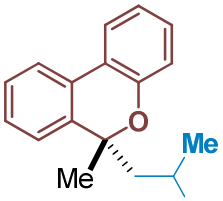
4b

6-methyl-6-propyl-6*H*-benzo[*c*]chromene (4b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.70 (m, 2H), 7.35-7.17 (m, 4H), 7.02-6.98 (m, 1H), 6.94-6.92 (d, J = 7.6 Hz, 1H), 1.95-1.87 (m, 1H), 1.78-1.70 (m, 1H), 1.65 (s, 3H), 1.45-1.34 (m, 2H), 0.86-0.82 (t, J = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 138.8, 129.5, 128.9, 127.8, 127.6, 124.1, 122.9, 122.4, 122.2, 121.4, 118.0, 79.9, 42.2, 25.8, 17.4, 14.4; HRMS calculated for $C_{17}H_{19}O$ ($M + H^+$): 239.1437, found: 239.1430. (Yellow oil, 20.1 mg, 67% isolated yield)



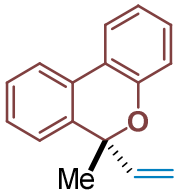
4c

6-isopropyl-6-methyl-6*H*-benzo[*c*]chromene (4c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.70 (m, 2H), 7.37-7.28 (m, 2H), 7.25-7.17 (m, 2H), 7.03-6.94 (m, 2H), 2.19-2.12 (m, 1H), 1.64 (s, 3H), 0.97-0.96 (d, J = 6.4 Hz, 3H), 0.78-0.77 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 138.4, 129.5, 128.8, 127.6, 127.3, 125.3, 122.7, 122.3, 121.4, 117.9, 82.2, 33.5, 19.8, 17.5, 16.8; HRMS calculated for $C_{17}H_{19}O$ ($M + H^+$): 239.1437, found: 239.1430. (Pale yellow oil, 19.6 mg, 64% isolated yield)



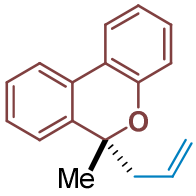
4d

6-isobutyl-6-methyl-6*H*-benzo[*c*]chromene (4d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.71 (m, 2H), 7.35-7.26 (m, 2H), 7.23-7.17 (m, 2H), 7.02-6.98 (m, 1H), 6.92-6.90 (m, 1H), 1.93-1.88 (m, 1H), 1.69 (s, 3H), 1.60-1.58 (m, 2H), 0.93-0.92 (d, J = 6.4 Hz, 3H), 0.83-0.81 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.7, 139.3, 129.4, 128.7, 127.8, 127.6, 127.3, 124.0, 122.8, 122.1, 121.3, 118.2, 80.4, 47.9, 26.2, 24.5, 24.0; HRMS calculated for $C_{18}H_{21}O$ ($M + H^+$): 253.1593, found: 253.1587. (Colorless oil, 18.9 mg, 59% isolated yield)



4e

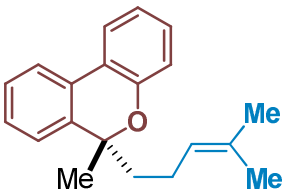
6-methyl-6-vinyl-6*H*-benzo[*c*]chromene (4e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.70 (m, 2H), 7.38-7.20 (m, 4H), 7.04-6.97 (m, 2H), 6.09-6.02 (dd, J_1 = 17.2 Hz, J_2 = 10.4 Hz, 1H), 5.14-5.12 (d, J = 11.6 Hz, 1H), 5.03-4.98 (d, J = 17.6 Hz, 1H), 1.79 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 141.5, 136.7, 129.5, 129.3, 128.2, 127.9, 124.7, 123.0, 122.6, 122.3, 121.8, 118.0, 115.9, 79.8, 25.6; HRMS calculated for $C_{16}H_{14}O$ ($M + H^+$): 223.1124, found: 223.1117. (Pale yellow solid, Mp 75-77 ℃, 10.7 mg, 36% isolated yield)



4f

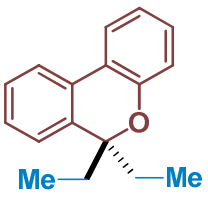
6-allyl-6-methyl-6*H*-benzo[*c*]chromene (4f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 2H), 7.37-7.27 (m, 2H), 7.25-7.18 (m, 2H), 7.05-7.00 (m, 1H), 6.96-6.94

(dd, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1H), 5.84-5.74 (m, 1H), 5.08-4.98 (m, 2H), 2.71-2.66 (m, 1H), 2.48-2.43 (m, 1H), 1.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 138.3, 133.4, 129.6, 128.9, 127.9, 127.8, 124.2, 122.9, 122.5, 122.3, 121.7, 118.3, 118.2, 79.2, 44.0, 25.0; HRMS calculated for $C_{16}H_{15}O$ ($M + H^+$): 237.1280, found: 237.1274. (Pale yellow oil, 10.1 mg, 32% isolated yield)



4g

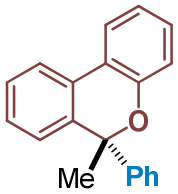
6-methyl-6-(4-methylpent-3-en-1-yl)-6*H*-benzo[*c*]chromene (4g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63-7.60 (m, 1H), 7.37-7.33 (m, 3H), 7.30-7.21 (m, 3H), 7.07-7.04 (m, 1H), 4.88 (s, 1H), 4.81-4.78 (m, 1H), 3.98-3.92 (m, 1H), 1.87-1.78 (m, 1H), 1.63 (s, 3H), 1.58-1.51 (m, 1H), 1.45-1.44 (d, J = 3.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.2, 144.8, 143.8, 139.8, 132.2, 127.8, 127.5, 127.2, 126.7, 126.6, 126.1, 111.0, 75.1, 40.0, 39.2, 31.7, 29.9, 29.4, 18.0; HRMS calculated for $C_{20}H_{23}O$ ($M + H^+$): 279.1750, found: 279.1743. (White solid, Mp 104-106 ℃, 15.9 mg, 53% isolated yield)



4h

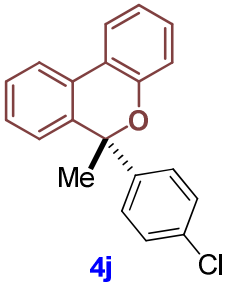
6,6-diethyl-6*H*-benzo[*c*]chromene (4h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.69 (m, 2H), 7.34-7.25 (m, 2H), 7.22-7.18 (m, 1H), 7.12-7.10 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.00-6.92 (m, 2H), 2.00-1.87 (m, 4H), 0.90-0.87 (t, J = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.2, 136.4, 129.7, 129.5, 127.5, 127.4, 125.0, 122.8, 122.1, 121.9, 121.1, 117.8, 82.9, 31.1, 8.3. These data are consistent with literature values, see:

Mahendar, L.; Krishna, J.; Reddy, A. G. K.; Ramulu, B. V.; Satyanarayana, G. *Org. Lett.* **2012**, *14*, 628. (Colorless oil, 25.4 mg, 82% isolated yield)



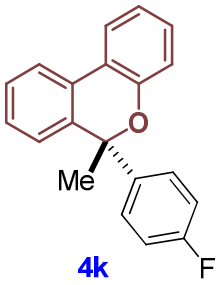
4i

6-methyl-6-phenyl-6*H*-benzo[*c*]chromene (4i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (d, J = 7.2 Hz, 1H), 7.66-7.64 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.43-7.39 (m, 1H), 7.36-7.16 (m, 8H), 7.03-7.01 (m, 1H), 7.00-6.93 (m, 1H), 2.03 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 144.9, 137.6, 129.6, 129.5, 128.3, 128.0, 127.6, 127.4, 126.6, 125.7, 123.0, 122.9, 122.6, 121.9, 118.3, 81.2, 28.6. These data are consistent with literature values, see: Mahendar, L.; Satyanarayana, G. *J. Org. Chem.* **2014**, *79*, 2059. (Colorless oil, 20.0 mg, 65% isolated yield)



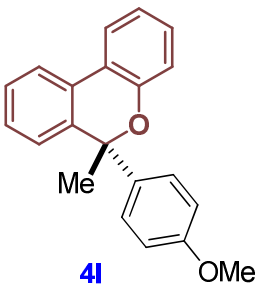
4j

6-(4-chlorophenyl)-6-methyl-6*H*-benzo[*c*]chromene (4j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (m, 1H), 7.66-7.64 (m, 1H), 7.45-7.41 (m, 1H), 7.38-7.34 (m, 1H), 7.29-7.27 (m, 1H), 7.23-7.15 (m, 5H), 7.02-6.95 (m, 2H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 143.6, 137.0, 133.2, 129.7, 129.6, 128.5, 128.2, 128.1, 127.7, 125.5, 123.1, 122.9, 122.7, 122.1, 118.3, 80.7, 28.6; HRMS calculated for $C_{20}H_{16}OCl$ ($M + H^+$): 307.0890, found: 307.0884. (Pale yellow solid, Mp 92-94 ℃, 34.8 mg, 84% isolated yield)



4k

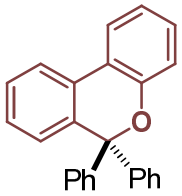
6-(4-fluorophenyl)-6-methyl-6*H*-benzo[*c*]chromene (4k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.74 (d, J = 7.6 Hz, 1H), 7.66-7.64 (dd, J_1 = 8.0 Hz, J_2 = 1.6 Hz, 1H), 7.44-7.40 (m, 1H), 7.37-7.33 (m, 1H), 7.27-7.24 (m, 3H), 7.21-7.17 (m, 1H), 7.01-6.94 (m, 2H), 6.90-6.86 (m, 2H), 2.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ162.0, 152.8, 140.8, 137.3, 129.6, 129.5, 128.4, 128.3, 127.7, 125.5, 123.1, 122.9, 122.7, 122.0, 118.3, 114.8, 80.7, 28.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -115.3; HRMS calculated for $C_{20}H_{16}OF$ ($M + H^+$): 291.1186, found: 291.1180. (White solid, Mp 87-89 ℃, 29.8 mg, 82% isolated yield)



4l

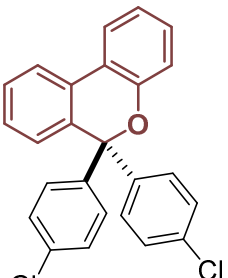
6-(4-methoxyphenyl)-6-methyl-6*H*-benzo[*c*]chromene (4l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (dd, J_1 = 8 Hz, J_2 = 1.2 Hz, 1H), 7.66-7.64 (dd, J_1 = 7.6 Hz, J_2 = 1.2 Hz, 1H), 7.43-7.38 (m, 2H), 7.35-7.30 (m, 1H), 7.24-7.16 (m, 3H), 7.00-6.93 (m, 2H), 6.75-6.72 (m, 2H), 3.71 (s, 3H), 2.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 153.0, 137.9, 137.1, 130.9, 130.4, 129.5, 129.0, 128.8, 128.2, 127.9, 127.6, 125.6, 123.0, 122.5, 121.8, 118.3, 113.3, 80.9, 55.2, 28.4. These data are consistent with literature values, see: Wang, B.; Li, M.; Xu, S.; Song, H.; Wang B. *J. Org. Chem.*

2006, *71*, 8291. (Pale yellow solid, Mp 66-68 ℃, 31.2 mg, 83% isolated yield)



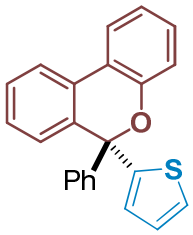
4m

6,6-diphenyl-6*H*-benzo[*c*]chromene (4m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.76 (m, 2H), 7.66-7.63 (m, 1H), 7.61-7.56 (m, 1H), 7.50-7.46 (m, 2H), 7.42-7.38 (m, 1H), 7.28-7.20 (m, 6H), 7.19-7.14 (m, 2H), 7.05-7.03 (m, 1H), 6.95-6.91 (m, 1H), 6.72-6.70 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 143.6, 137.6, 137.1, 132.5, 130.1, 129.6, 128.9, 128.3, 128.1, 127.8, 127.1, 122.9, 122.4, 122.0, 118.6, 86.6. These data are consistent with literature values, see: Wang, B.; Li, M.; Xu, S.; Song, H.; Wang B. *J. Org. Chem.* **2006**, *71*, 8291. (Brown solid, Mp 60-62 ℃, 24.3 mg, 82% isolated yield)



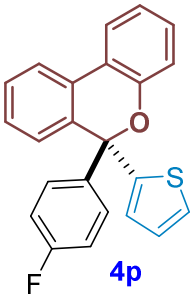
4n

6,6-bis(4-chlorophenyl)-6*H*-benzo[*c*]chromene (4n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.77 (m, 1H), 7.66-7.64 (m, 1H), 7.45-7.40 (m, 1H), 7.25-7.20 (m, 5H), 7.15-7.12 (m, 5H), 7.02-6.95 (m, 2H), 6.69-6.66 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 141.8, 136.1, 134.0, 130.2, 129.8, 128.8, 128.1, 128.0, 127.3, 123.0, 122.9, 122.6, 122.4, 118.5, 85.7; HRMS calculated for $C_{25}H_{17}OCl_2$ ($M + H^+$): 403.0657, found: 403.0651. (Pale yellow solid, Mp 173-175 ℃, 21.6 mg, 64% isolated yield)



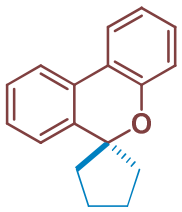
4o

6-phenyl-6-(thiophen-2-yl)-6*H*-benzo[*c*]chromene (4o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.77 (m, 1H), 7.69-7.67 (m, 1H), 7.44-7.40 (m, 1H), 7.34-7.28 (m, 6H), 7.24-7.18 (m, 2H), 7.09-7.07 (m, 1H), 7.00-6.96 (m, 1H), 6.87-6.82 (m, 2H), 6.58-6.56 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 148.4, 143.4, 137.0, 129.8, 129.7, 128.9, 128.7, 128.4, 128.2, 127.9, 127.7, 127.3, 126.9, 125.8, 123.0, 122.7, 122.3, 118.8, 84.5; HRMS calculated for $C_{23}H_{17}OS$ ($M + H^+$): 341.1001, found: 341.0995. (Yellow solid, Mp 184-186 ℃, 19.7 mg, 63% isolated yield)



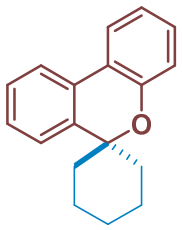
4p

6-(4-fluorophenyl)-6-(thiophen-2-yl)-6*H*-benzo[*c*]chromene (4p): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.77 (d, J = 7.6 Hz, 1H), 7.69-7.67 (m, 1H), 7.45-7.41 (m, 1H), 7.32-7.26 (m, 3H), 7.22-7.18 (m, 1H), 7.07-7.05 (m, 1H), 7.01-6.94 (m, 4H), 6.88-6.85 (m, 1H), 6.82-6.80 (d, J = 8.0 Hz, 1H), 6.57-6.56 (dd, J_1 = 3.6 Hz, J_2 = 0.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 148.1, 134.7, 134.4, 131.8, 131.7, 130.3, 130.2, 129.7, 129.0, 128.9, 128.4, 128.1, 127.5, 127.4, 127.0, 125.0, 123.0, 122.5, 115.5, 114.8, 114.6, 84.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.0; HRMS calculated for $C_{23}H_{16}OFS$ ($M + H^+$): 359.0907, found: 359.0900. (Yellow solid, Mp 53-55 ℃, 17.9 mg, 61% isolated yield)



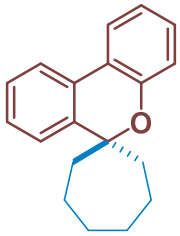
4q

spiro[benzo[*c*]chromene-6,1'-cyclopentane] (4q): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.71 (m, 2H), 7.36-7.26 (m, 3H), 7.25-7.19 (m, 1H), 7.04-7.00 (m, 1H), 6.95-6.92 (m, 1H), 2.28-2.21 (m, 2H), 2.05-1.92 (m, 4H), 1.85-1.79 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.0, 137.9, 129.6, 129.2, 127.9, 127.7, 123.2, 123.0, 122.9, 122.2, 121.7, 118.2, 88.7, 38.0, 23.9; HRMS calculated for $C_{17}H_{17}O$ ($M + H^+$): 237.1280, found: 237.1274. (Pale yellow oil, 24.8mg, 80% isolated yield)



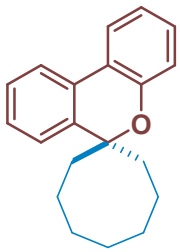
4r

spiro[benzo[*c*]chromene-6,1'-cyclohexane] (4r): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.70 (m, 2H), 7.35-7.27 (m, 2H), 7.24-7.21 (m, 2H), 7.02-7.00 (m, 2H), 2.13-2.10 (d, *J* = 12.8 Hz, 2H), 1.89-1.82 (m, 3H), 1.70-1.67 (m, 2H), 1.64-1.58 (m, 2H), 1.30-1.27 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 140.0, 129.3, 129.0, 128.0, 127.6, 123.2, 123.0, 122.9, 122.4, 121.6, 118.1, 77.7, 34.7, 25.5, 21.6. These data are consistent with literature values, see: Wang, B.; Li, M.; Xu, S.; Song, H.; Wang B. *J. Org. Chem.* **2006**, *71*, 8291. (White solid, Mp 106-108 ℃, 21.8 mg, 61% isolated yield)



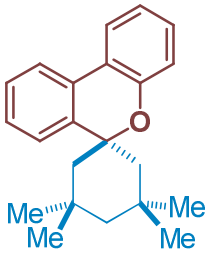
4s

spiro[benzo[*c*]chromene-6,1'-cycloheptane] (4s): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71-7.69 (m, 2H), 7.34-7.27 (m, 3H), 7.24-7.20 (m, 1H), 7.02-6.96 (m, 2H), 2.26-2.20 (m, 2H), 2.02-1.96 (m, 2H), 1.93-1.84 (m, 2H), 1.76-1.70 (m, 2H), 1.66-1.54 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 141.4, 129.4, 128.6, 127.9, 127.5, 123.3, 122.9, 122.8, 122.2, 121.5, 118.2, 81.8, 39.2, 29.8, 22.8. These data are consistent with literature values, see: Wang, B.; Li, M.; Xu, S.; Song, H.; Wang B. *J. Org. Chem.* **2006**, *71*, 8291. (Yellow solid, Mp 115-117 ℃, 19.8 mg, 60% isolated yield)



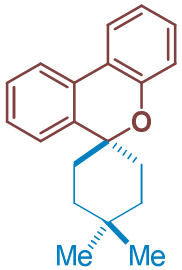
4u

spiro[benzo[*c*]chromene-6,1'-cyclooctane] (4u): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73-7.69 (m, 2H), 7.36-7.31 (m, 1H), 7.29-7.27 (m, 2H), 7.24-7.19 (m, 1H), 7.02-6.95 (m, 2H), 2.14-2.11 (m, 3H), 1.88-1.85 (m, 2H), 1.70-1.69 (m, 3H), 1.58 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 139.9, 129.4, 127.5, 123.8, 122.9, 122.8, 122.5, 121.4, 118.0, 81.4, 33.8, 28.4, 24.7, 21.9; HRMS calculated for $C_{20}H_{23}O$ ($M + H^+$): 279.1750, found: 279.1743. (Pale yellow solid, Mp 114-116 ℃, 22.6 mg, 65% isolated yield)



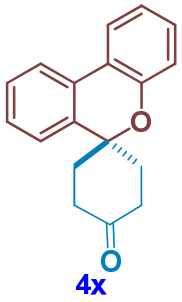
4v

3',3',5',5'-tetramethylspiro[benzo[*c*]chromene-6,1'-cyclohexane] (4v): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75-7.72 (m, 2H), 7.35-7.27 (m, 3H), 7.24-7.19 (m, 1H), 7.04-7.00 (m, 1H), 6.94-6.91 (m, 1H), 2.07-2.03 (m, 2H), 1.54-1.49 (m, 3H), 1.33 (s, 6H), 1.25-1.21 (d, J = 14.0 Hz, 1H), 0.93 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 139.7, 129.3, 129.0, 128.0, 127.6, 123.1, 122.7, 122.5, 122.4, 121.4, 118.5, 81.0, 51.8, 45.7, 36.6, 31.7, 28.4; HRMS calculated for $C_{22}H_{27}O$ (M + H^+): 307.2062, found: 307.2056. (Colorless oil, 27.4 mg, 87% isolated yield)



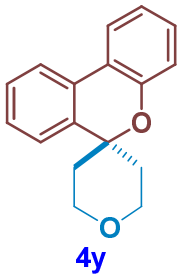
4w

4',4'-dimethylspiro[benzo[*c*]chromene-6,1'-cyclohexane] (4w): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74-7.71 (m, 2H), 7.37-7.27 (m, 3H), 7.26-7.21 (m, 1H), 7.05-7.00 (m, 2H), 1.99-1.78 (m, 5H), 1.27-1.23 (m, 3H), 1.03 (s, 3H), 1.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 139.7, 129.4, 129.2, 128.0, 127.7, 123.2, 123.0, 122.9, 122.4, 121.6, 118.1, 77.5, 34.4, 32.9, 30.8, 29.4, 24.0; HRMS calculated for $C_{20}H_{23}O$ (M + H^+): 279.1749, found: 279.1744. (Colorless oil, 23.9 mg, 78% isolated yield)



4x

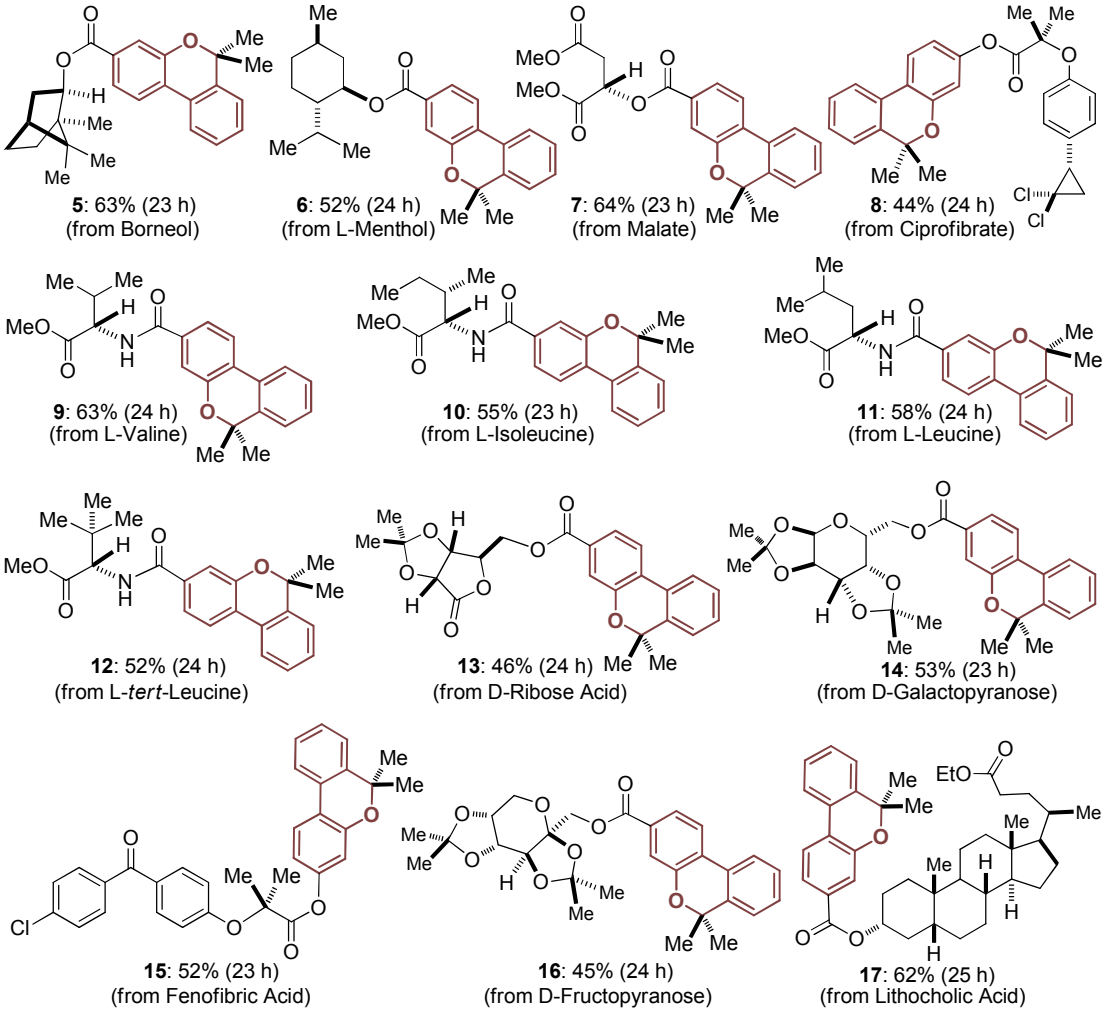
spiro[benzo[*c*]chromene-6,1'-cyclohexan]-4'-one (4x): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.76 (m, 2H), 7.42-7.28 (m, 3H), 7.25-7.22 (m, 1H), 7.12-7.04 (m, 2H), 2.98-2.88 (m, 2H), 2.53-2.46 (m, 2H), 2.39-2.34 (m, 2H), 2.25-2.17 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 211.1, 151.6, 137.4, 129.8, 129.6, 129.1, 128.4, 128.3, 123.3, 122.8, 122.7, 122.5, 117.9, 76.3, 37.1, 34.5; HRMS calculated for $C_{18}H_{17}O_2$ ($M + H^+$): 265.1229, found: 265.1224. (White solid, Mp 153-155 ℃, 16.1 mg, 54% isolated yield)



4y

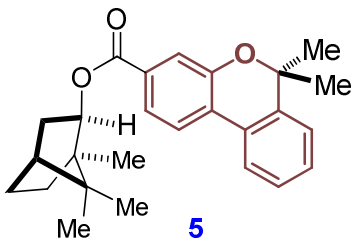
2',3',5',6'-tetrahydrospiro[benzo[*c*]chromene-6,4'-pyran] (4y): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76-7.73 (m, 2H), 7.40-7.32 (m, 2H), 7.28-7.23 (m, 2H), 7.07-7.04 (m, 2H), 4.06-3.99 (m, 2H), 3.89-3.85 (m, 2H), 2.15-2.08 (m, 2H), 2.03-1.99(d, J = 12.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 138.2, 134.2, 129.6, 129.0, 128.3, 128.1, 123.2, 123.0, 122.6, 122.1, 118.1, 75.3, 63.6, 34.6; HRMS calculated for $C_{17}H_{17}O_2$ ($M + H^+$): 253.1229, found: 253.1223. (White solid, Mp 126-128 ℃, 20.6 mg, 69% isolated yield)

Late-stage functionalization of substances derived from natural products



The reactions were conducted in a 1:1 mixed solvent of MeCN and CF_3CH_2OH.

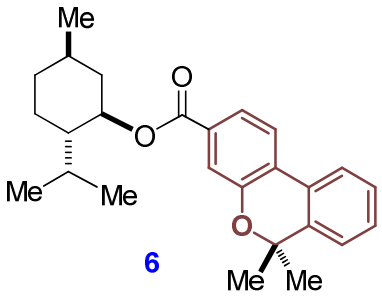
^{1}H and ^{13}C spectra data of compounds 5-17



5

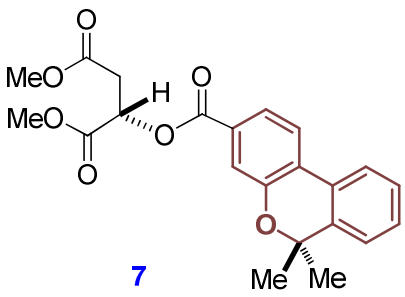
1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (5): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.72 (m, 3H), 7.63-7.62 (d, J = 2.0 Hz, 1H), 7.41-7.34 (m, 2H), 7.29-7.27 (m, 1H), 5.13-5.09 (m, 1H), 2.52-2.44 (m, 1H),

2.21-2.14 (m, 1H), 1.86-1.73 (m, 2H), 1.66 (s, 6H), 1.46-1.25 (m, 2H), 1.16-1.11 (m, 1H), 0.97 (s, 3H), 0.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 152.6, 140.1, 131.7, 129.1, 128.0, 127.8, 126.8, 123.4, 123.0, 122.9, 122.8, 119.2, 80.7, 78.1, 49.2, 48.0, 45.1, 37.0, 28.2, 27.7, 27.5, 19.8, 19.0, 13.7; HRMS calculated for $C_{26}H_{32}O_3Na$ ($M + Na^+$): 413.2093, found: 413.2087. (Colorless oil, 12.9 mg, 63% isolated yield)



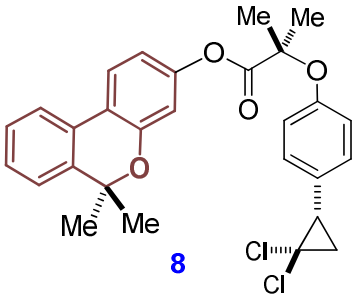
6

2-isopropyl-5-methylcyclohexyl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (6): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.75 (m, 2H), 7.72-7.69 (dd, J_1 = 8.4 Hz, J_2 = 2.0 Hz, 1H), 7.62-7.61 (d, J = 1.2 Hz, 1H), 7.40-7.34 (m, 2H), 7.28-7.27 (m, 1H), 4.96-4.90 (m, 1H), 2.16-2.11 (m, 2H), 2.03-1.96 (m, 1H), 1.76-1.71 (m, 2H), 1.68 (s, 3H), 1.64 (s, 3H), 1.58 (s, 2H), 1.57-1.52 (m, 1H), 1.14-1.06(m, 2H), 0.94-0.92 (d, J = 7.2 Hz, 6H), 0.81-0.79 (d, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.8, 152.5, 140.1, 131.7, 129.1, 128.0, 127.8, 126.7, 123.4, 123.0, 122.9, 122.8, 119.3, 78.0, 74.9, 47.3, 41.0, 34.4, 31.5, 27.8, 27.7, 26.4, 23.6, 22.2, 21.0, 16.5; HRMS calculated for $C_{26}H_{32}O_3Na$ ($M + Na^+$): 415.2249, found: 415.2244. (Colorless oil, 10.5 mg, 52% isolated yield)



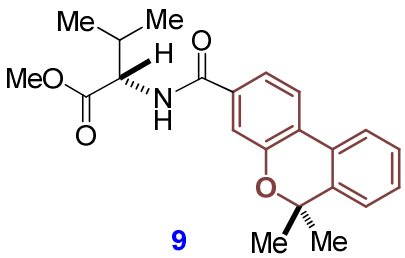
7

dimethyl-2-((6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carbonyl)oxy)succinate (7): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.11 (m, 2H), 7.61-7.59 (m, 1H), 7.47 (d, J = 8.4 Hz, 2H), 7.43-7.35 (m, 2H), 5.78-5.75 (dd, J_1 = 7.2 Hz, J_2= 4.8 Hz, 1H), 3.82 (s, 3H), 3.76 (d, J = 0.8 Hz, 3H), 3.09-3.06 (m, 1H), 2.78-2.76 (m, 1H), 1.61 (s, 3H), 1.35-1.34 (d, J = 4.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.7, 169.5, 165.4, 147.0, 139.3, 137.1, 133.4, 132.2, 130.0, 129.9, 129.3, 128.3, 127.9, 127.4, 127.4, 68.8, 57.9, 56.3, 52.9, 52.4, 36.2, 24.1, 24.0; HRMS calculated for $C_{22}H_{22}O_7Na$ (M + Na^+): 421.1264, found: 421.1258. (Yellow oil, 14.3 mg, 64% isolated yield)



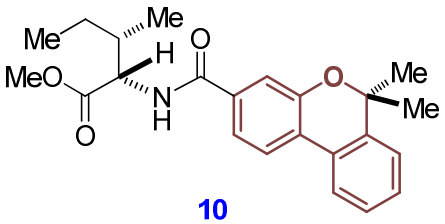
8

6,6-dimethyl-6*H*-benzo[*c*]chromen-3-yl-2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropanoate (8): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.65 (m, 2H), 7.34-7.27 (m, 2H), 7.24-7.22 (m, 1H), 7.19-7.17 (m, 2H), 7.00-6.93 (m, 2H), 6.66-6.64 (m, 1H), 6.60-6.59 (d, J = 2.0 Hz, 1H), 2.90-2.85 (m, 1H), 1.99-1.94 (m, 1H), 1.84-1.80 (m, 1H), 1.76 (s, 6H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.8, 155.1, 153.6, 151.3, 139.1, 129.9, 128.5, 128.2, 127.9, 127.3, 123.6, 123.3, 122.2, 120.6, 118.5, 114.5, 111.2, 79.4, 78.3, 60.9, 34.9, 27.7, 25.9, 25.6; HRMS calculated for $C_{28}H_{26}Cl_2O_4Na$ (M + Na^+): 519.1106, found: 519.1101. (Colorless oil, 11.2 mg, 44% isolated yield)



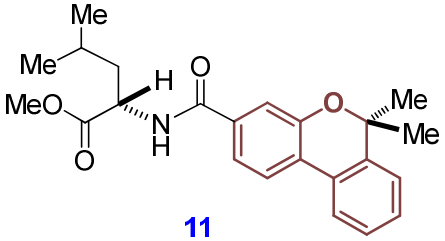
9

methyl-2-(6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxamido)-3-methylbutanoat e (9): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.74 (m, 2H), 7.51-7.48 (dd, J_1 = 8.4 Hz, J_2= 2.0 Hz, 1H), 7.40-7.33 (m, 3H), 7.28-7.26 (m, 1H), 6.65-6.62 (d, J = 8.8 Hz, 1H), 4.81-4.78 (m, 1H), 3.79 (s, 3H), 2.31-2.26 (m, 1H), 1.66-1.65 (d, J = 4.0 Hz, 6H), 1.05-0.99 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 166.9, 152.8, 139.9, 134.9, 129.0, 128.8, 128.0, 125.8, 123.5, 123.3, 122.8, 120.6, 116.7, 78.2, 57.5, 52.4, 31.8, 27.8, 27.7, 19.1, 18.1; HRMS calculated for $C_{22}H_{25}O_4NNa$ (M + Na^+): 390.1682, found: 390.1676. (Colorless oil, 12.6 mg, 63% isolated yield)



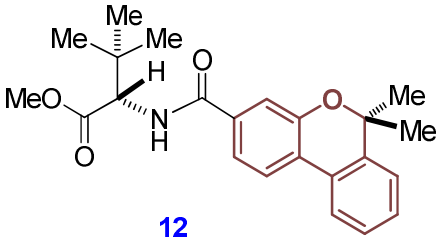
10

methyl-2-(6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxamido)-3-methylpentanoa te (10): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.74 (m, 2H), 7.50-7.48 (m, 1H), 7.38-7.35 (m, 3H), 7.28-7.27 (m, 1H), 6.66-6.64 (d, J = 8.8 Hz, 1H), 4.84-4.81 (m, 1H), 3.78 (s, 3H), 2.04-2.00 (m, 1H), 1.65 (s, 6H), 1.57-1.51 (m, 1H), 1.31-1.24 (m, 1H), 1.01-0.97 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 166.6, 152.8, 139.9, 134.9, 129.0, 128.0, 127.7, 125.8, 123.4, 122.8, 120.6, 116.7, 78.2, 56.9, 52.3, 38.4, 27.8, 25.4, 15.6, 11.7; HRMS calculated for $C_{23}H_{27}O_4NNa$ (M + Na^+): 404.1838, found: 404.1832. (Colorless oil, 11.5 mg, 55% isolated yield)



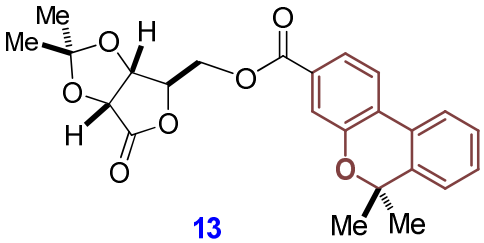
11

methyl-2-(6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxamido)-4-methylpentanoate (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80-7.74 (m, 2H), 7.50-7.47 (m, 1H), 7.38-7.35 (m, 3H), 7.28-7.27 (m, 1H), 6.52-6.50 (d, *J* = 8.4 Hz, 1H), 4.90-4.84 (m, 1H), 3.78 (s, 3H), 1.79-1.67 (m, 3H), 1.65-1.64 (d, *J* = 4.8 Hz, 6H), 1.01-0.98 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 166.7, 152.8, 139.9, 134.8, 129.0, 128.0, 127.7, 125.8, 123.4, 123.2, 122.8, 120.6, 116.7, 78.1, 52.5, 51.2, 42.0, 27.7, 25.1, 23.0, 22.2; HRMS calculated for $C_{23}H_{27}O_4NNa$ (M + Na^+): 404.1838, found: 404.1832. (Colorless oil, 12.1 mg, 58% isolated yield)



12

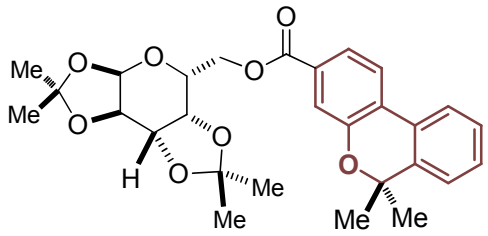
methyl-2-(6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxamido)-3,3-dimethylbutanoate (12): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.74 (m, 2H), 7.50-7.43 (m, 2H), 7.38-7.34 (m, 3H), 6.67-6.65 (d, *J* = 9.6 Hz, 1H), 4.72-4.70 (d, *J* = 9.2 Hz, 1H), 3.77 (s, 3H), 1.66-1.65 (d, *J* = 4.8 Hz, 6H), 1.06 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 166.7, 152.8, 139.9, 135.0, 129.0, 128.0, 127.3, 125.8, 123.5, 123.3, 122.8, 120.6, 116.6, 78.2, 60.3, 52.0, 35.3, 27.8, 26.8; HRMS calculated for $C_{23}H_{27}O_4NNa$ (M + Na^+): 404.1838, found: 404.1832. (Colorless oil, 10.4 mg, 52% isolated yield)



13

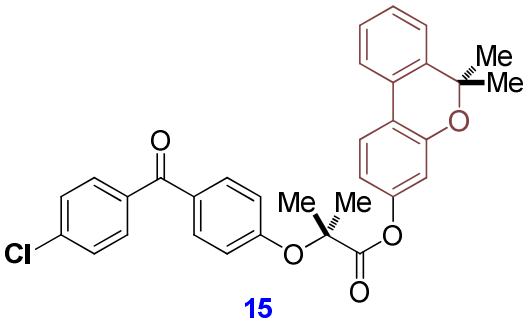
2,2-dimethyl-6-oxotetrahydrofuro[3,4-d][1,3]dioxol-4-yl)methyl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (13): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81-7.75 (m,

2H), 7.61-7.56 (m, 1H), 7.40-7.37 (m, 2H), 7.30-7.27 (m, 1H), 4.93-4.86 (m, 2H), 4.81-4.79 (m, 1H), 4.72-4.62 (m, 1H), 4.56-4.47 (m, 1H), 1.67-1.64 (m, 6H), 1.52 (s, 3H), 1.41-1.40 (d, J = 6.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.6, 165.4, 152.9, 140.3, 129.5, 129.3, 128.1, 127.3, 123.5, 123.3, 123.1, 122.8, 119.3, 114.0, 80.0, 78.3, 77.9, 75.3, 63.9, 27.8, 27.7, 26.9, 25.7; HRMS calculated for $C_{24}H_{24}O_7Na$ (M + Na^+): 447.1420, found: 447.1414. (Colorless oil, 10.2 mg, 46% isolated yield)



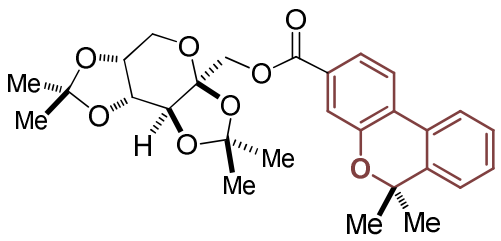
14

2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-5-yl)methyl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (14): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.70 (m, 3H), 7.63-7.62 (d, J = 1.2 Hz, 1H), 7.40-7.34 (m, 2H), 7.28-7.27 (m, 1H), 5.58-5.57 (d, J = 4.8 Hz, 1H), 4.68-4.65 (m, 1H), 4.55-4.50 (m, 1H), 4.45-4.40 (m, 1H), 4.37-4.35 (m, 2H), 4.21-4.17 (m, 1H), 1.64 (s, 6H), 1.54 (s, 3H), 1.49 (s, 3H), 1.37-1.35 (d, J = 9.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 152.6, 140.2, 130.8, 129.2, 128.0, 127.0, 123.4, 123.0, 122.9, 119.5, 109.8, 108.9, 96.4, 78.0, 71.2, 70.8, 70.6, 66.1, 63.8, 27.7, 26.2, 26.1, 25.1, 24.6; HRMS calculated for $C_{28}H_{32}O_8Na$ (M + Na^+): 519.1995, found: 519.1989. (Colorless oil, 10.5 mg, 53% isolated yield)



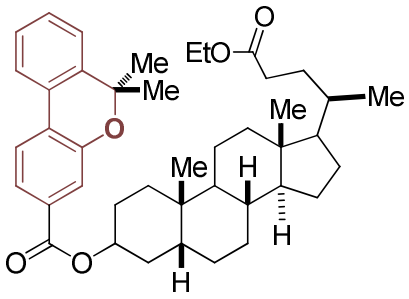
15

6,6-dimethyl-6*H*-benzo[*c*]chromen-3-yl-2-(4-(4-chlorobenzoyl)phenoxy)-2-methyl propanoate (15): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82-7.79 (m, 2H), 7.75-7.71 (m, 3H), 7.69-7.65 (m, 1H), 7.48-7.45 (m, 2H), 7.36-7.28 (m, 2H), 7.24-7.22 (m, 1H), 7.01-6.99 (m, 2H), 6.69-6.66 (dd, J_1 = 8.4 Hz, J_2= 2.4 Hz, 1H), 6.61-6.60 (d, J = 2.4 Hz, 1H), 1.83 (s, 6H), 1.62 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.4, 172.3, 159.6, 153.6, 151.1, 139.0, 138.5, 136.4, 132.3, 131.3, 130.7, 128.6, 128.2, 127.9, 127.8, 123.6, 123.3, 122.2, 120.3, 117.3, 114.3, 111.0, 79.5, 78.3, 27.7, 25.5; HRMS calculated for $C_{32}H_{27}O_5ClNa$ ($M + Na^+$): 549.1445, found: 549.1439. (Colorless oil, 15.5 mg, 52% isolated yield)



16

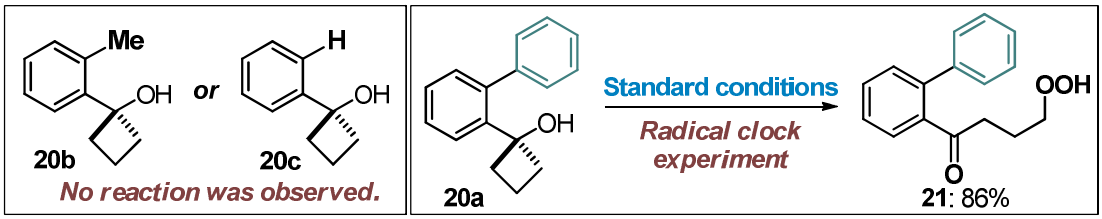
2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-b:4',5'-d]pyran-3a-yl)methyl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (16): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79-7.72 (m, 3H), 7.67-7.66 (d, J = 1.2 Hz, 1H), 7.39-7.36 (m, 2H), 7.28-7.27 (m, 1H), 4.73-4.65 (m, 2H), 4.51-4.50 (m, 1H), 4.32-4.26 (m, 1H), 3.99-3.95 (m, 1H), 3.83-3.80 (d, J = 12.8 Hz, 1H), 1.64 (s, 3H), 1.56 (s, 3H), 1.48 (s, 3H), 1.40 (s, 3H), 1.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.7, 152.6, 140.2, 130.6, 129.2, 128.8, 128.0, 127.7, 123.5, 123.1, 123.0, 122.9, 119.6, 109.3, 108.9, 101.8, 78.0, 70.9, 70.6, 70.2, 65.4, 61.5, 27.7, 26.6, 26.0, 25.6, 24.1; HRMS calculated for $C_{28}H_{32}O_8Na$ ($M + Na^+$): 519.1995, found: 519.1989. (Colorless oil, 9.1 mg, 45% isolated yield)



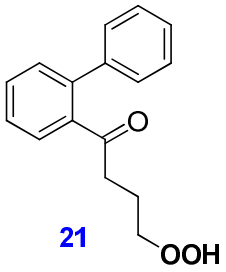
17

5-ethoxy-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl-6,6-dimethyl-6*H*-benzo[*c*]chromene-3-carboxylate (17): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13-8.11 (m, 2H), 7.61-7.59 (m, 1H), 7.46-7.44 (m, 2H), 7.42-7.35 (m, 2H), 5.04-4.98 (m, 1H), 4.15-4.10 (q, *J* = 7.6 Hz, 2H), 2.75 (s, 3H), 2.37-2.31 (m, 1H), 2.25-2.17 (m, 1H), 2.02-1.96 (m, 2H), 1.90-1.84 (m, 3H), 1.61 (s, 3H), 1.48-1.41 (m, 4H), 1.34 (s, 3H), 1.28-1.24 (m, 8H), 1.19-1.07 (m, 6H), 0.97 (s, 3H), 0.92-0.91 (d, *J* = 6.4 Hz, 3H), 0.66 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 166.0, 146.1, 139.5, 139.1, 129.9, 129.8, 129.6, 129.1, 129.1, 128.2, 127.8, 127.3, 77.3, 75.2, 60.3, 57.9, 56.6, 56.3, 56.1, 42.8, 42.0, 40.5, 40.2, 35.9, 35.4, 35.1, 34.7, 32.4, 31.4, 31.0, 28.2, 27.1, 26.8, 26.4, 24.2, 24.0, 23.4, 20.9, 18.3, 14.3, 12.1; HRMS calculated for $C_{42}H_{56}O_5Na$ ($M + Na^+$): 663.4026, found: 663.4020. (Pale yellow solid, Mp 80-82 ℃, 18.4 mg, 62% isolated yield)

Radical clock experiment



^{1}H and ^{13}C spectra data of compounds 21



1-([1,1'-biphenyl]-2-yl)-4-hydroperoxybutan-1-one (21) ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53-7.51 (m, 2H), 7.44-7.41 (m, 5H), 7.40-7.35 (m, 2H), 3.79 (t, J = 5.6 Hz, 2H), 2.41 (t, J = 6.4 Hz, 2H), 1.88-1.82 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 209.1, 140.6, 140.4, 130.9, 130.4, 129.0, 128.8, 128.0, 127.6, 76.2, 39.9, 21.6; HRMS calculated for $C_{16}H_{16}O_3Na$ ($M + Na^+$): 279.0997, found: 279.0992. (White solid, Mp 41-43 ℃, 23.9 mg, 86% isolated yield)

UV-Vis absorption experiments

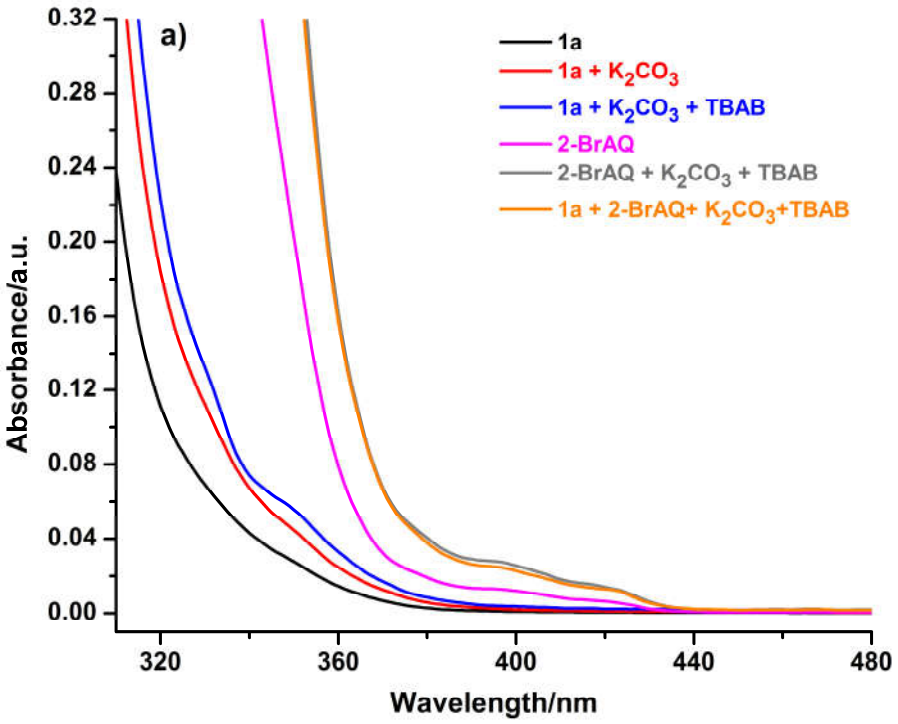


Figure 1. UV−Vis absorption spectra of the individual reaction components and the reaction mixtures

Fluorescence quenching experiments

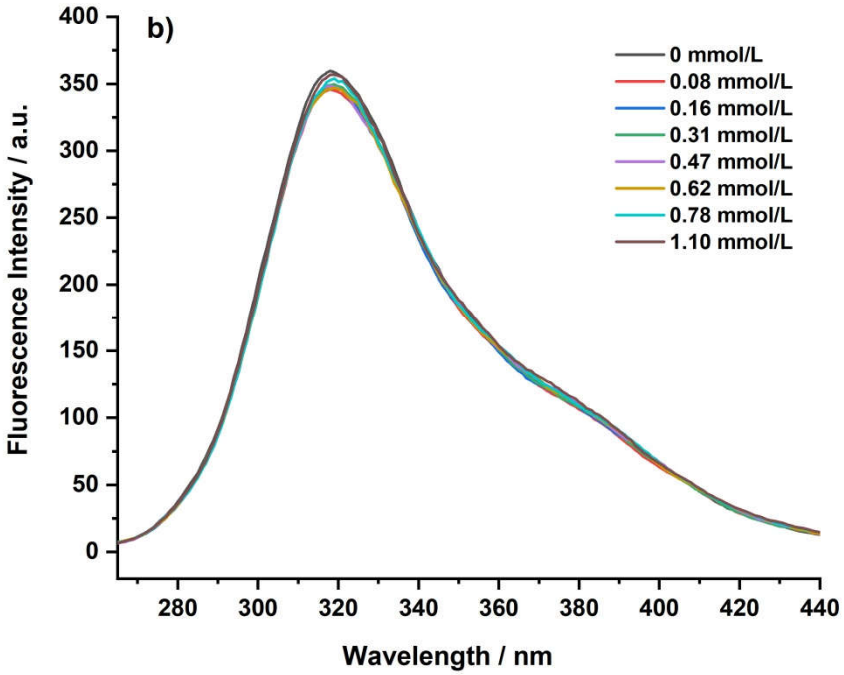


Figure 2. Fluorescence spectra of 2-BrAQ with different concentrations of nBu$_4$NBr

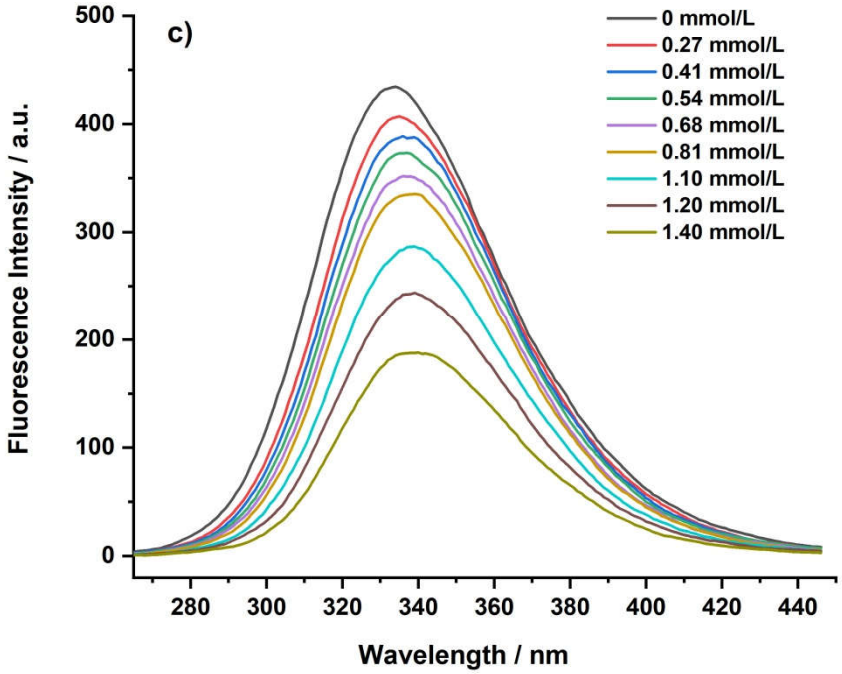


Figure 3. Fluorescence spectra of 2-BrAQ with different concentrations of substrate **1a**

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 -2.5 to +2.3 V). nBu$_4$NPF$_6$ (0.1 M MeCN) was used as the supporting electrolyte.

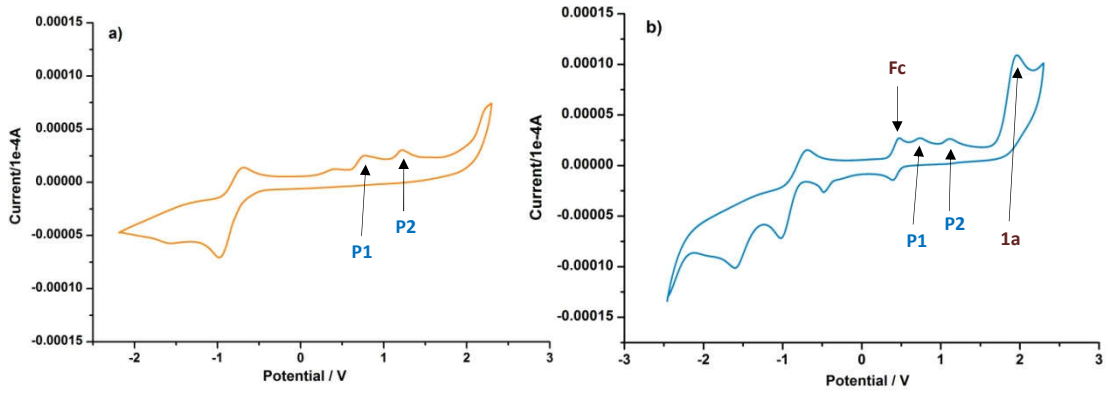
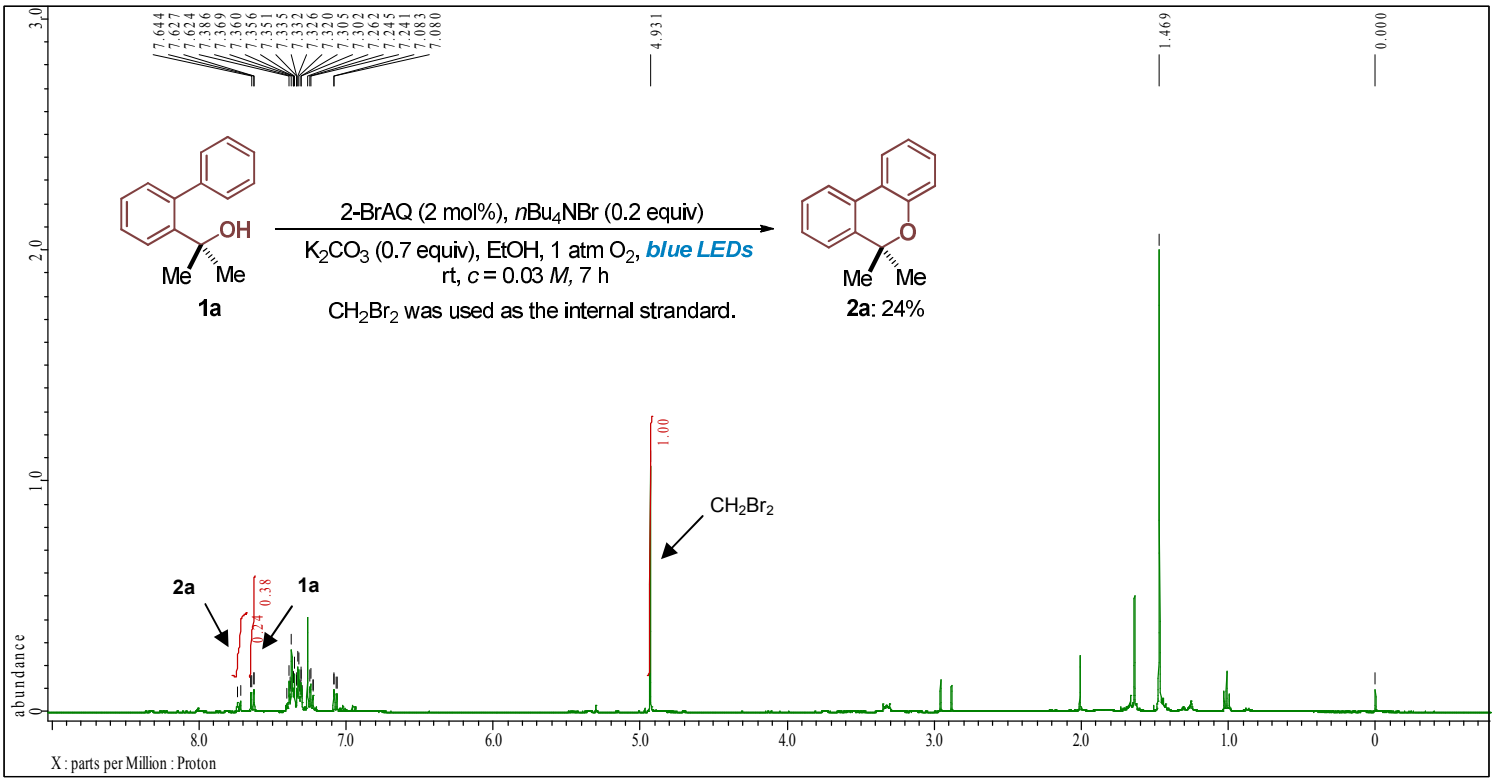
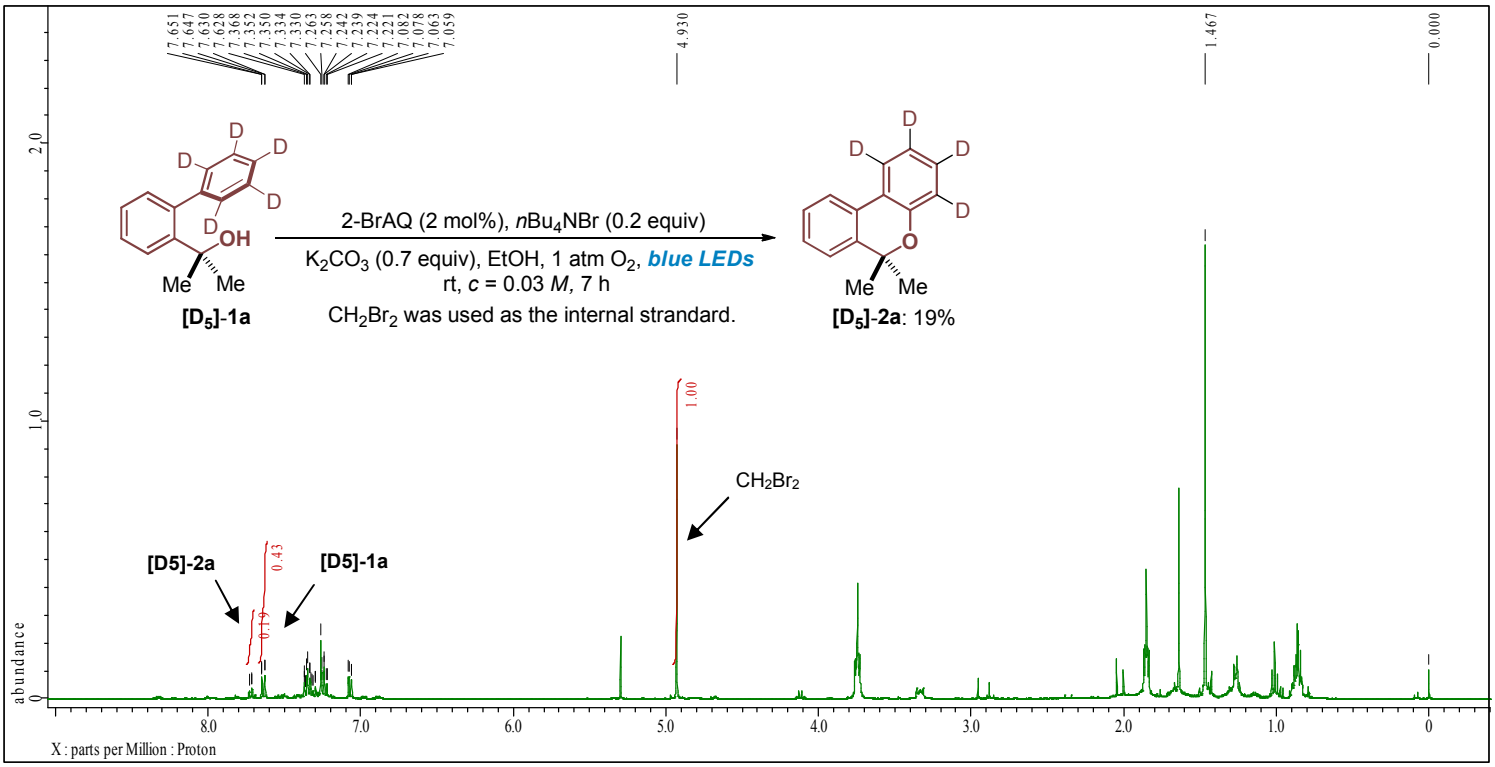


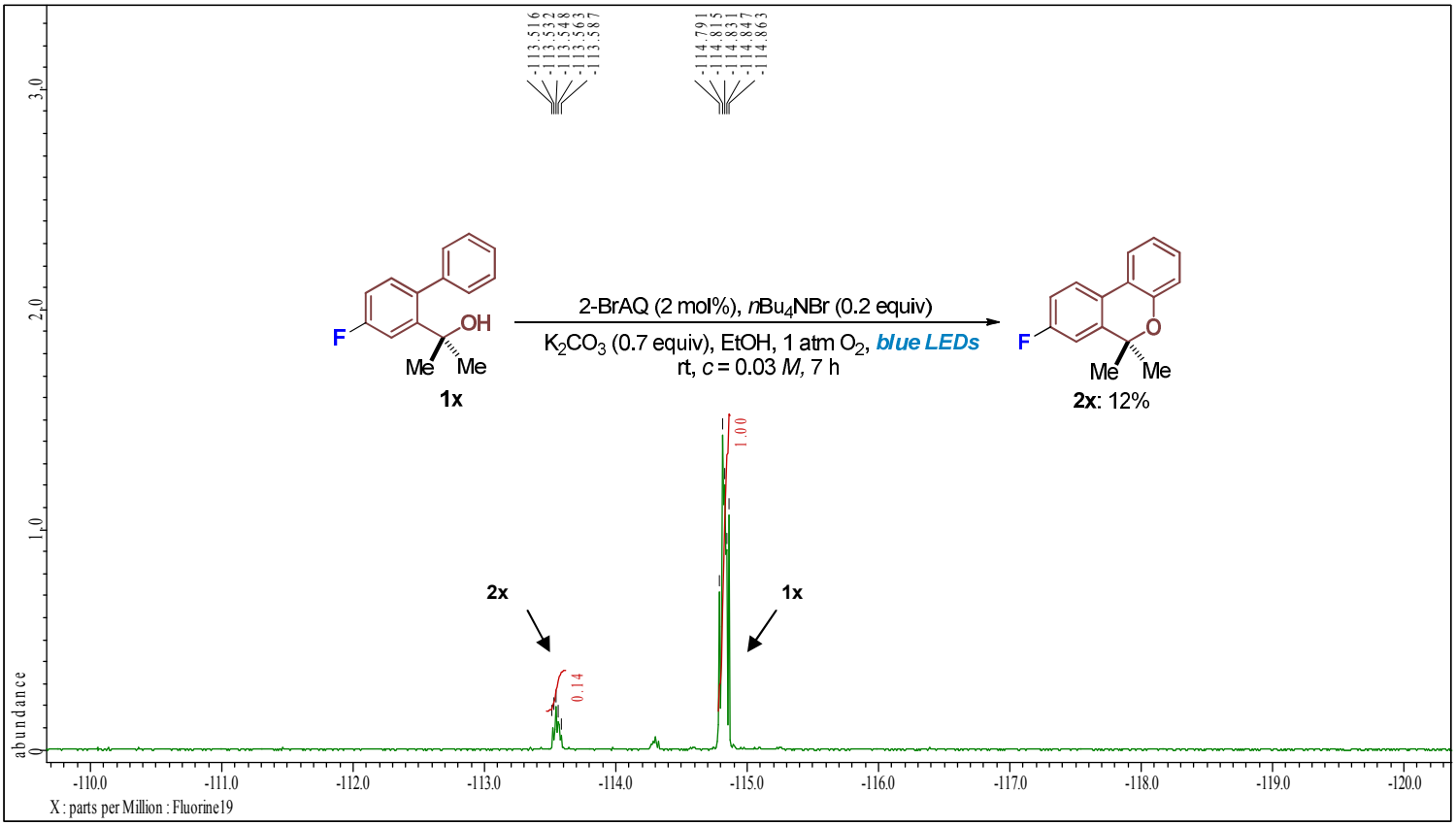
Figure 4. a) Cyclic voltammetry of background; b) Cyclic voltammetry of the substrate **1a**

Compared with CV curve of the background (Figure 4a), signal peak 1 (P1) and peak 2 (P2) in CV curve of the substrate **1a** (Figure 4b) are the original signal peaks of the background. In addition, the signal peak (Fc) at +0.49 V is the oxidation potential of the internal standard ferrocene.

Kinetic isotope experiments on reaction mechanism



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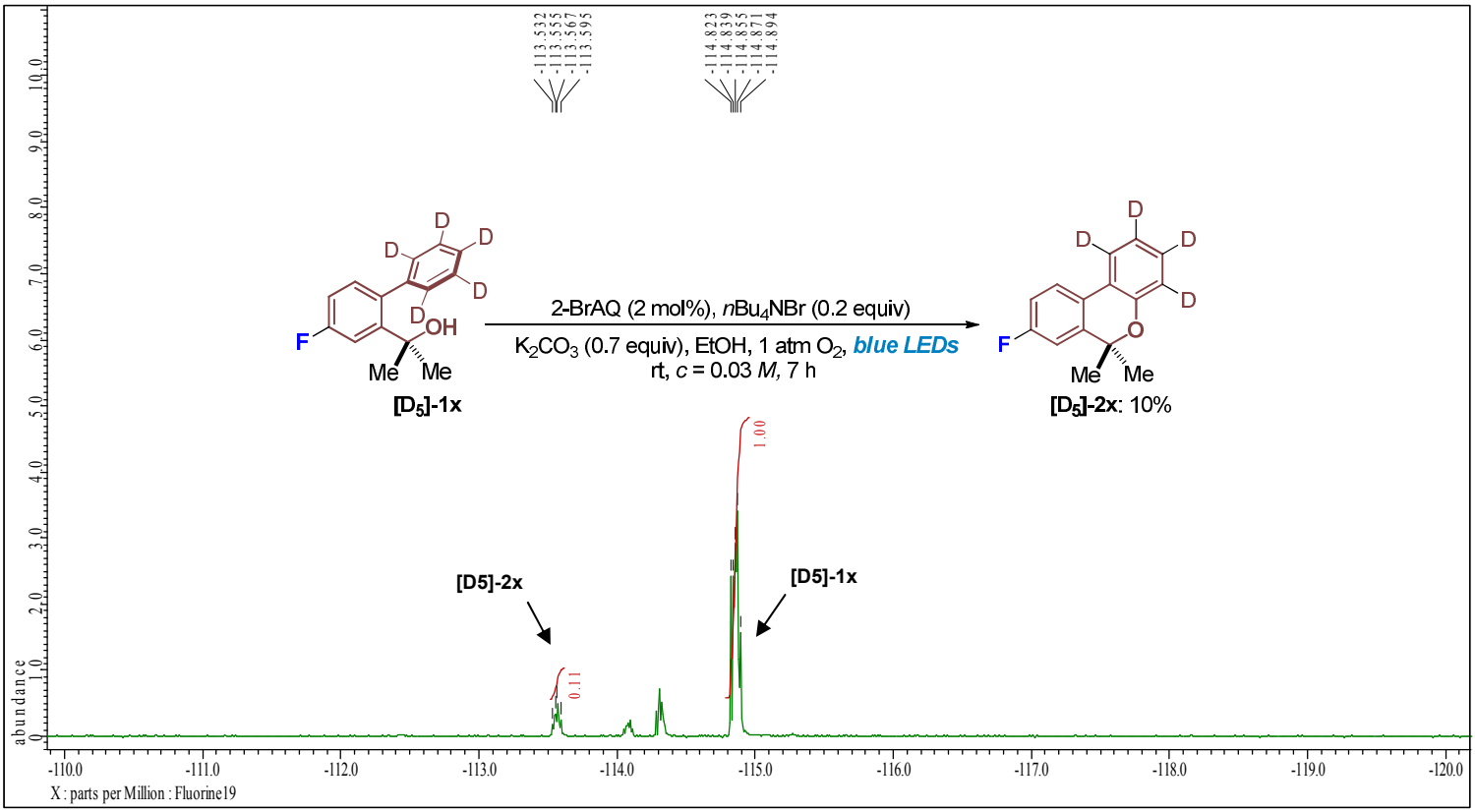
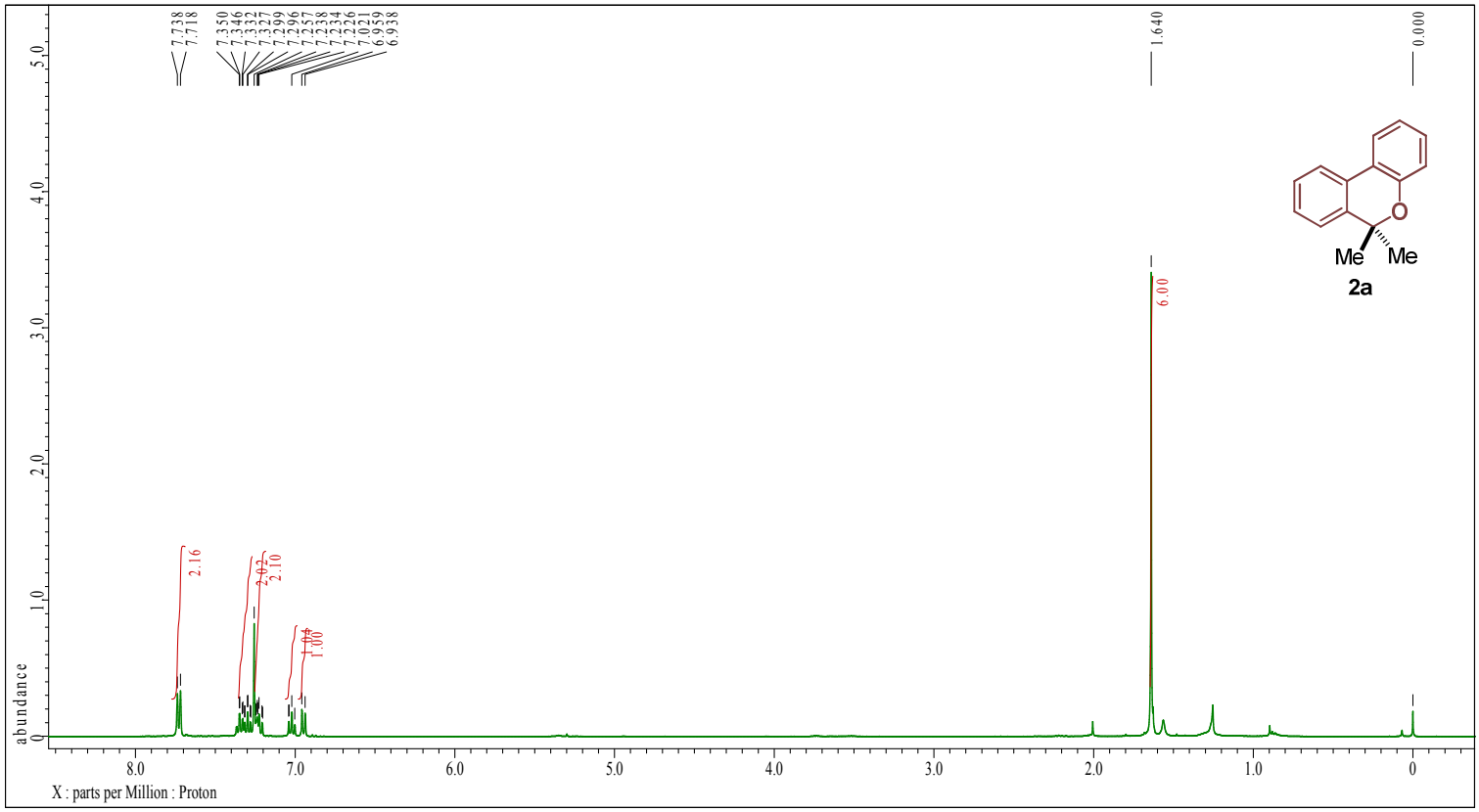
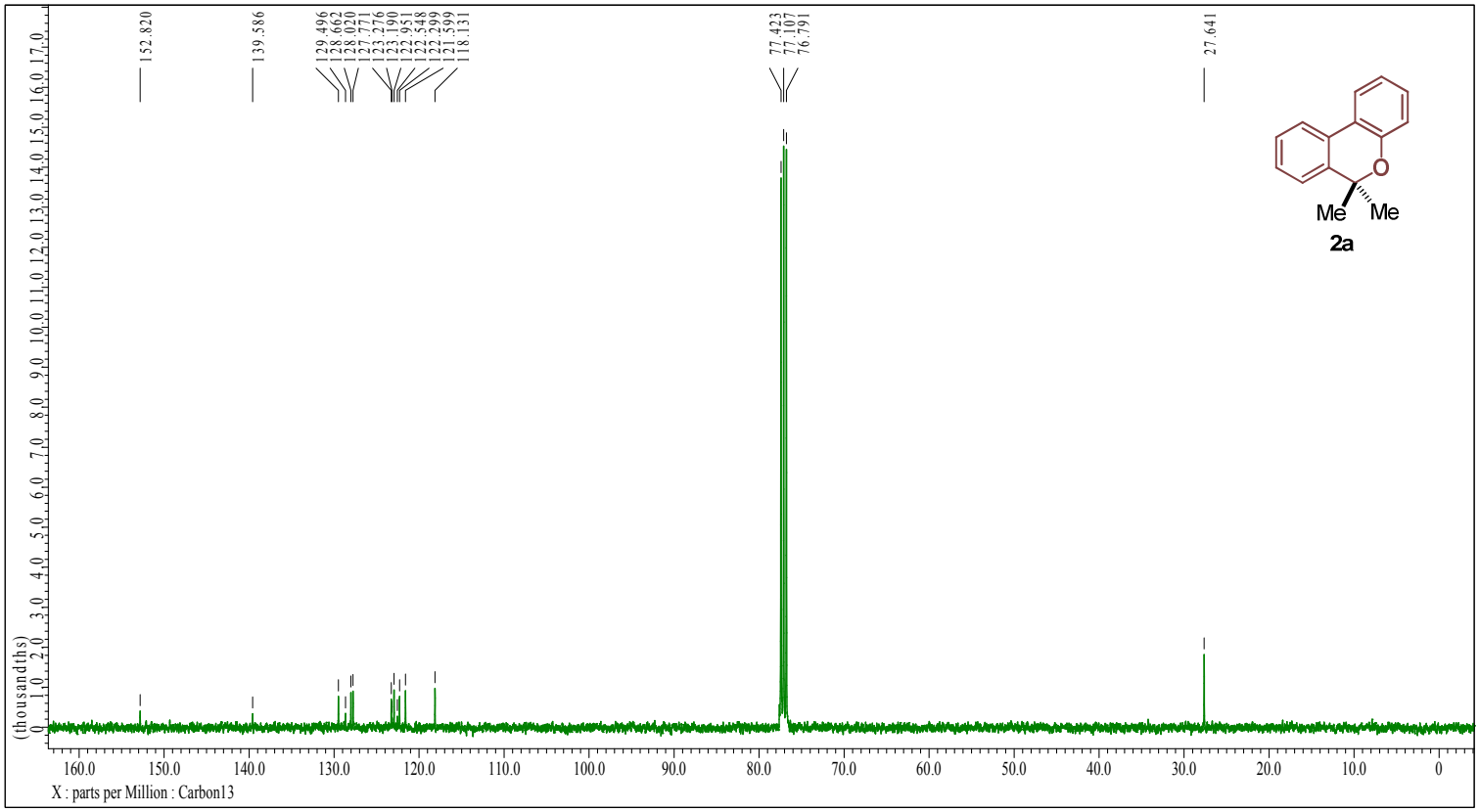
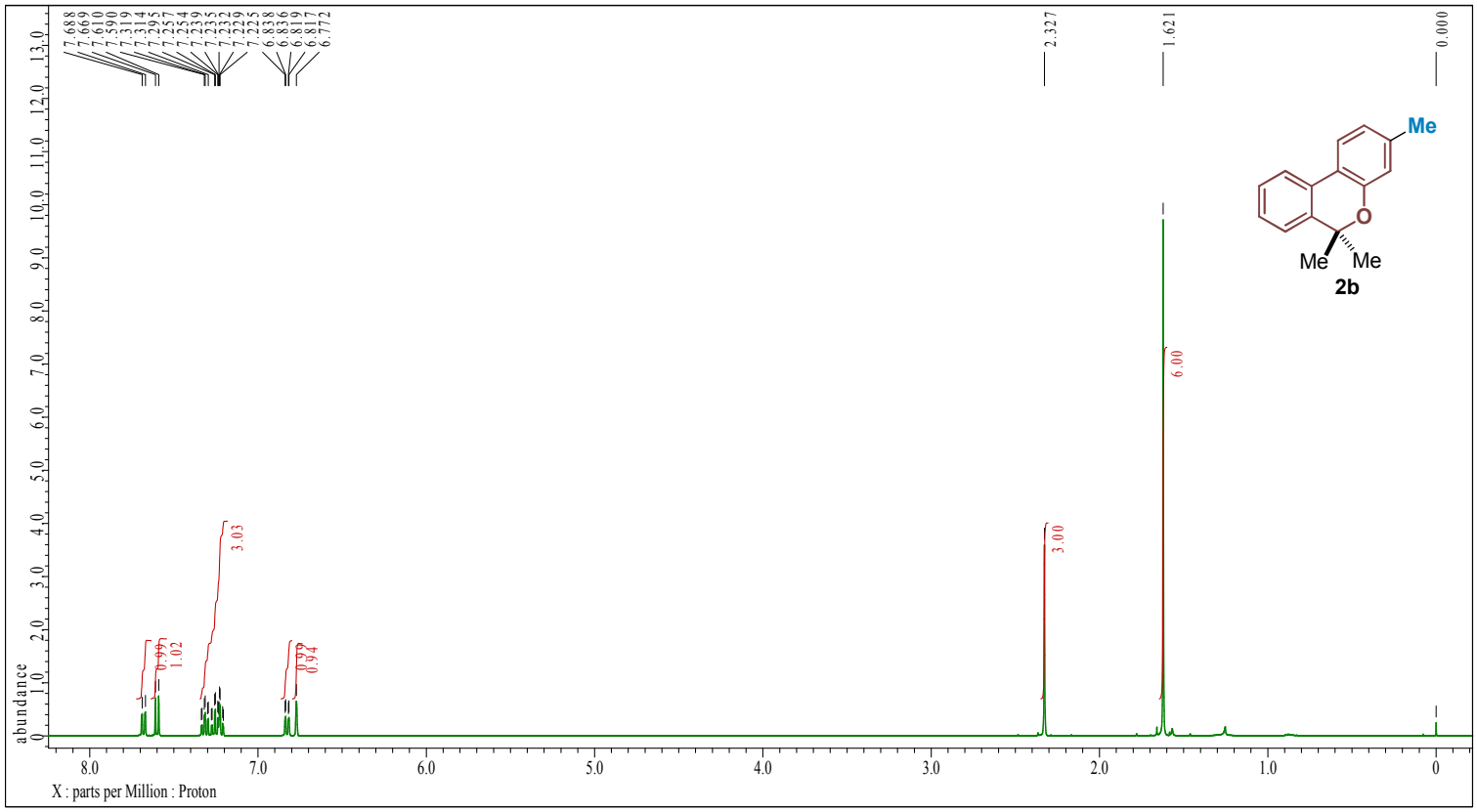
-113.532
-113.548
-113.563
-113.587
-114.791
-114.815
-114.831
-114.847
-114.863
F
OH
Me Me
1x
2-BrAQ (2 mol%), nBu4NBr (0.2 equiv)
K2CO3 (0.7 equiv), EtOH, 1 atm O2, blue LEDs
rt, c = 0.03 M, 7 h
F
O
Me Me
2x: 12%
1.00
2x
1x
0.14
abundance
X : parts per Million : Fluorine19


-113.532
-113.555
-113.567
-113.595
-114.823
-114.839
-114.855
-114.871
-114.894
D
F
OH
Me Me
[D5]-1x
2-BrAQ (2 mol%), nBu4NBr (0.2 equiv)
K2CO3 (0.7 equiv), EtOH, 1 atm O2, blue LEDs
rt, c = 0.03 M, 7 h
F
O
Me Me
[D5]-2x: 10%
1.00
[D5]-2x
[D5]-1x
0.11
abundance
X : parts per Million : Fluorine19

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



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7.610
7.590
7.319
7.314
7.295
7.257
7.254
7.239
7.235
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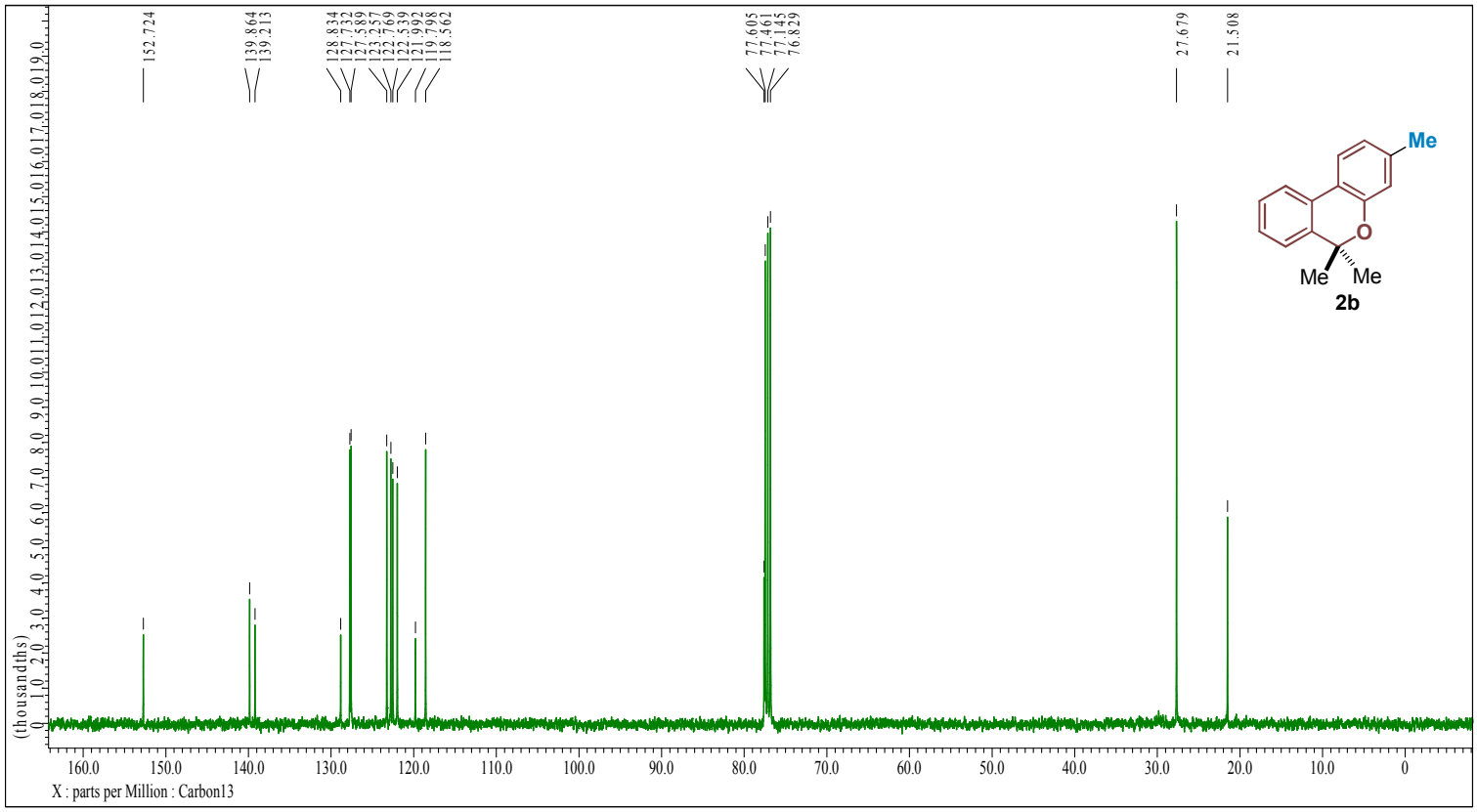
7.229
7.225
6.838
6.836
6.819
6.817
6.772
2.327
1.621
0.000
Me
O
Me
Me
2b
3.03
3.00
6.00
0.99
1.02
0.99
0.94
abundance
X : parts per Million : Proton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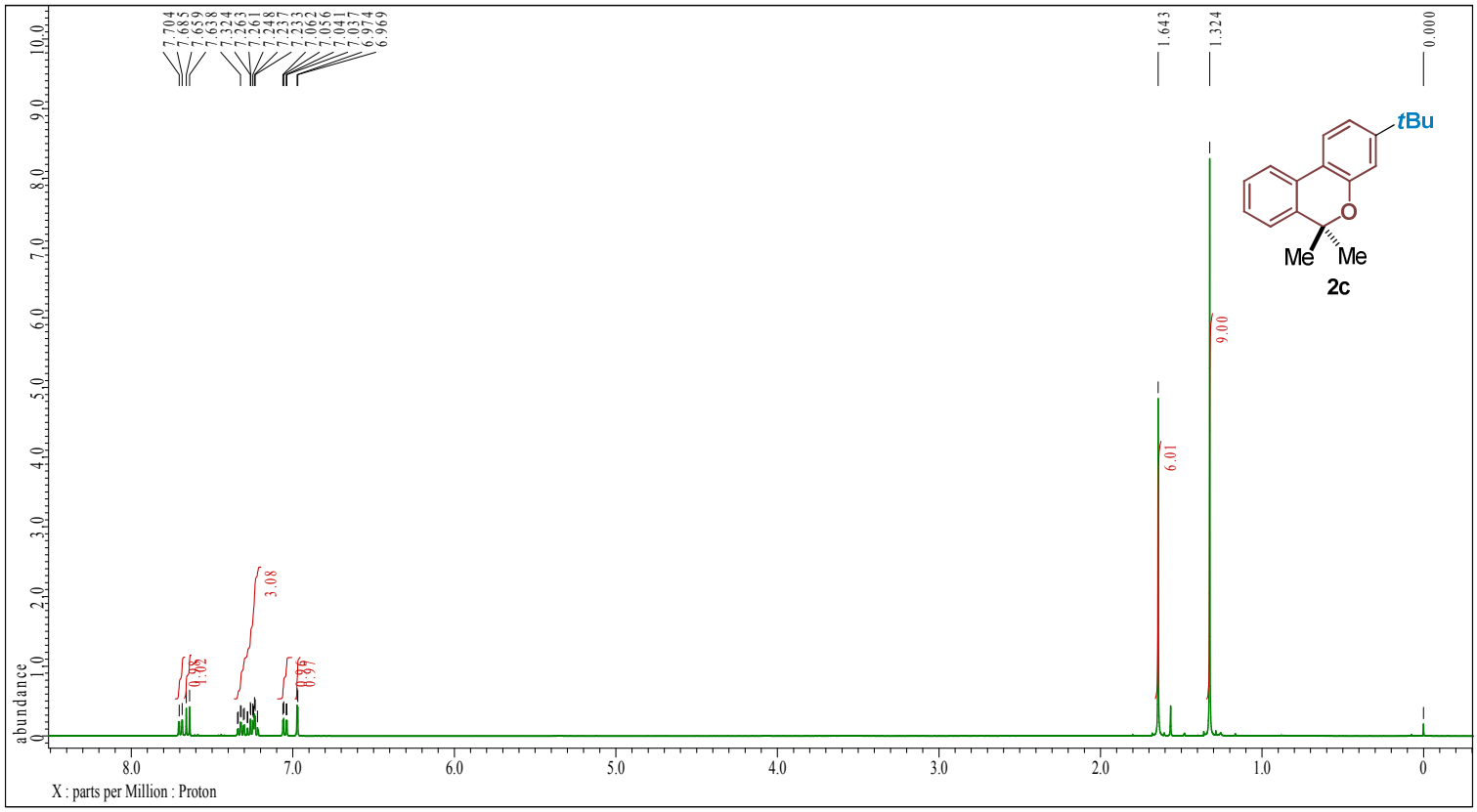
139.864
139.213
128.834
127.732
127.589
123.257
122.769
122.539
121.992
119.798
118.562
77.605
77.461
77.145
76.829
27.679
21.508
Me
O
Me
Me
2b
(thousandths)
X : parts per Million : Carbon13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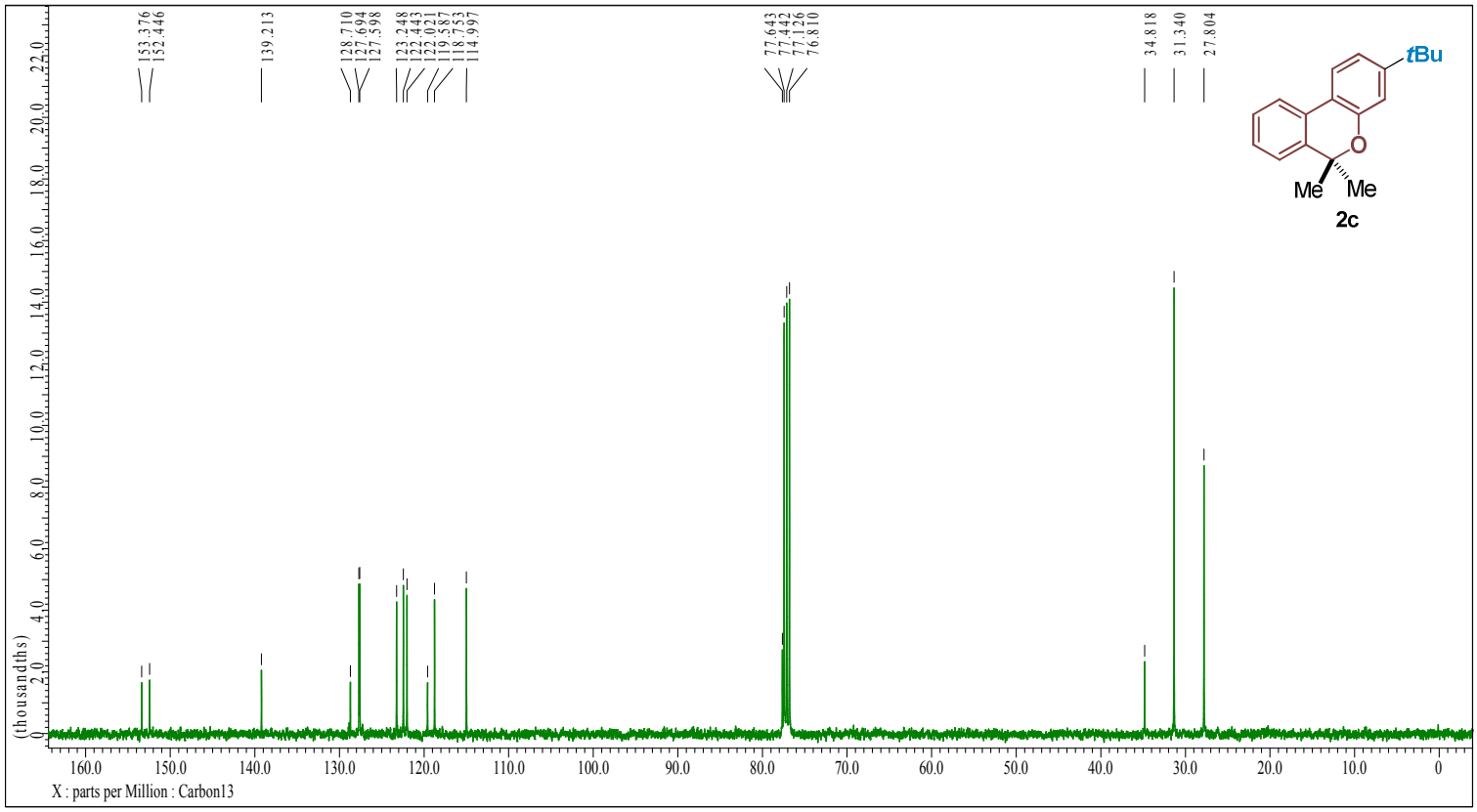
7.685
7.659
7.638
7.324
7.263
7.261
7.248
7.237
7.233
7.062
7.056
7.041
7.037
6.974
6.969
1.643
1.324
0.000
3.08
6.01
9.00
tBu
Me
Me
2c
abundance
X : parts per Million : Proton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128.710
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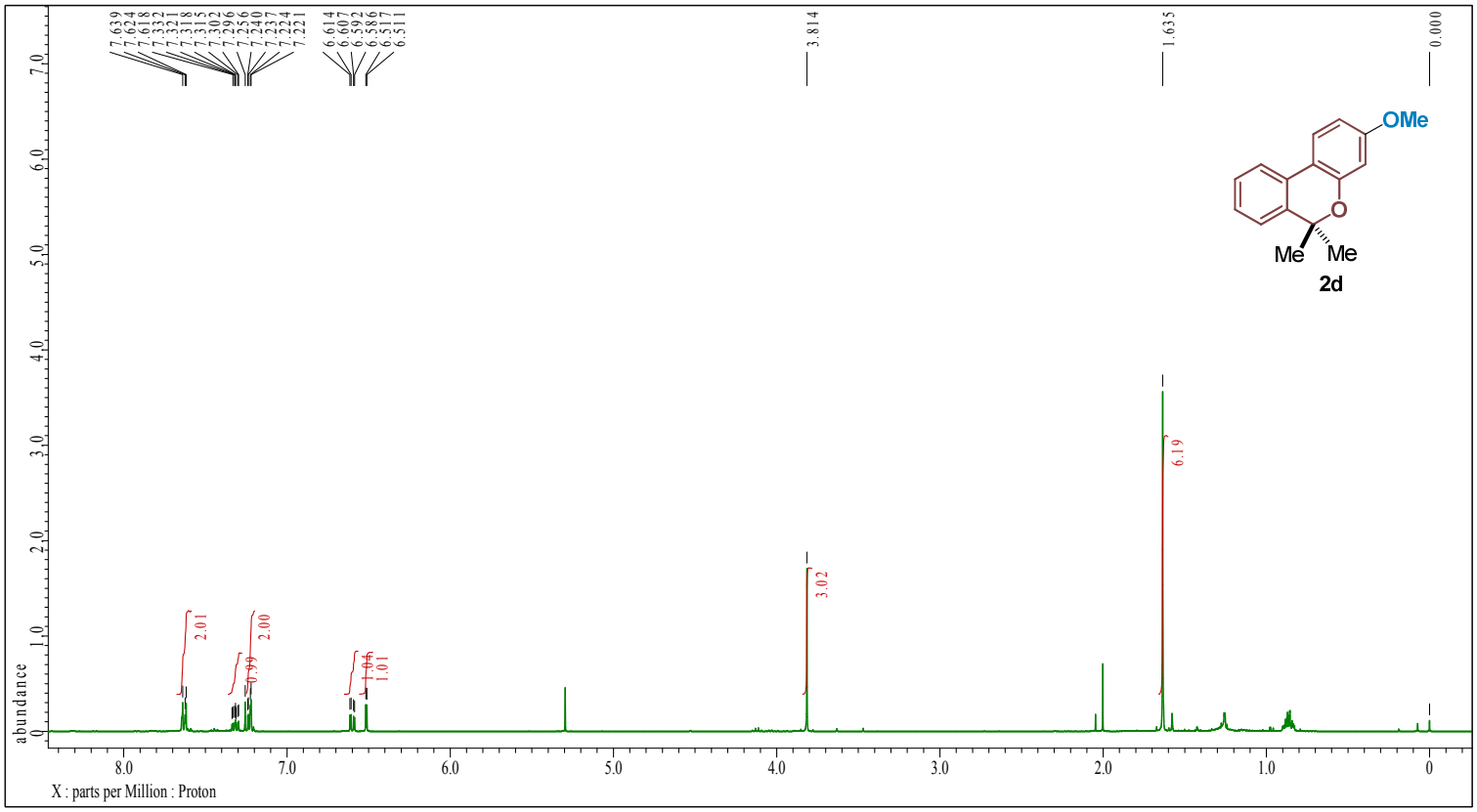
127.598
123.248
122.443
122.021
119.587
118.753
114.997
77.643
77.442
77.126
76.810
34.818
31.340
27.804
tBu
Me
Me
2c
(thousandths)
X : parts per Million : Carbon13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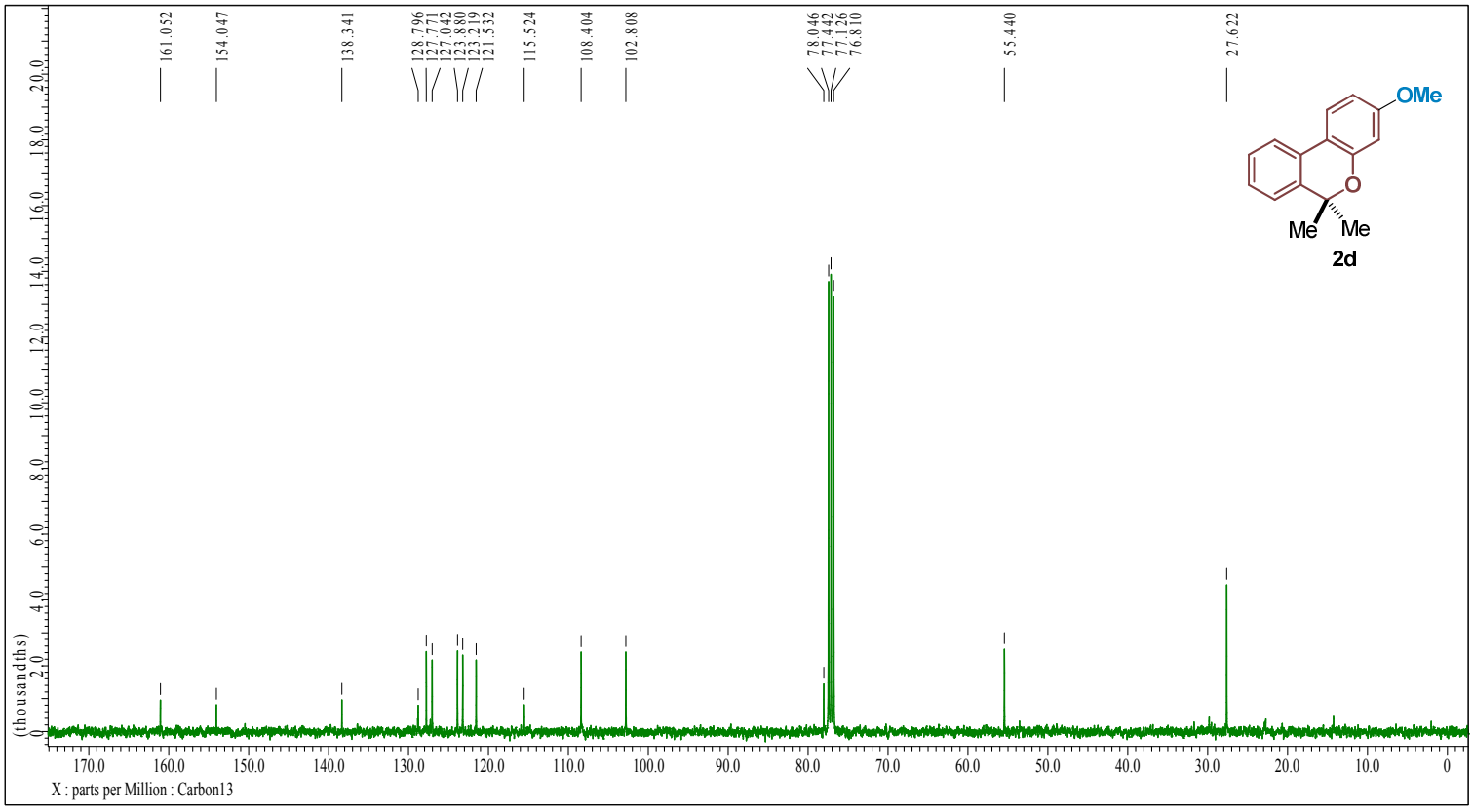
7.624
7.618
7.332
7.321
7.318
7.315
7.302
7.296
7.256
7.240
7.237
7.224
7.221
6.614
6.607
6.592
6.386
6.317
6.511
3.814
1.635
0.000
OMe
O
Me
Me
2d
2.01
2.00
0.99
1.04
1.01
3.02
6.19
abundance
X : parts per Million : Proton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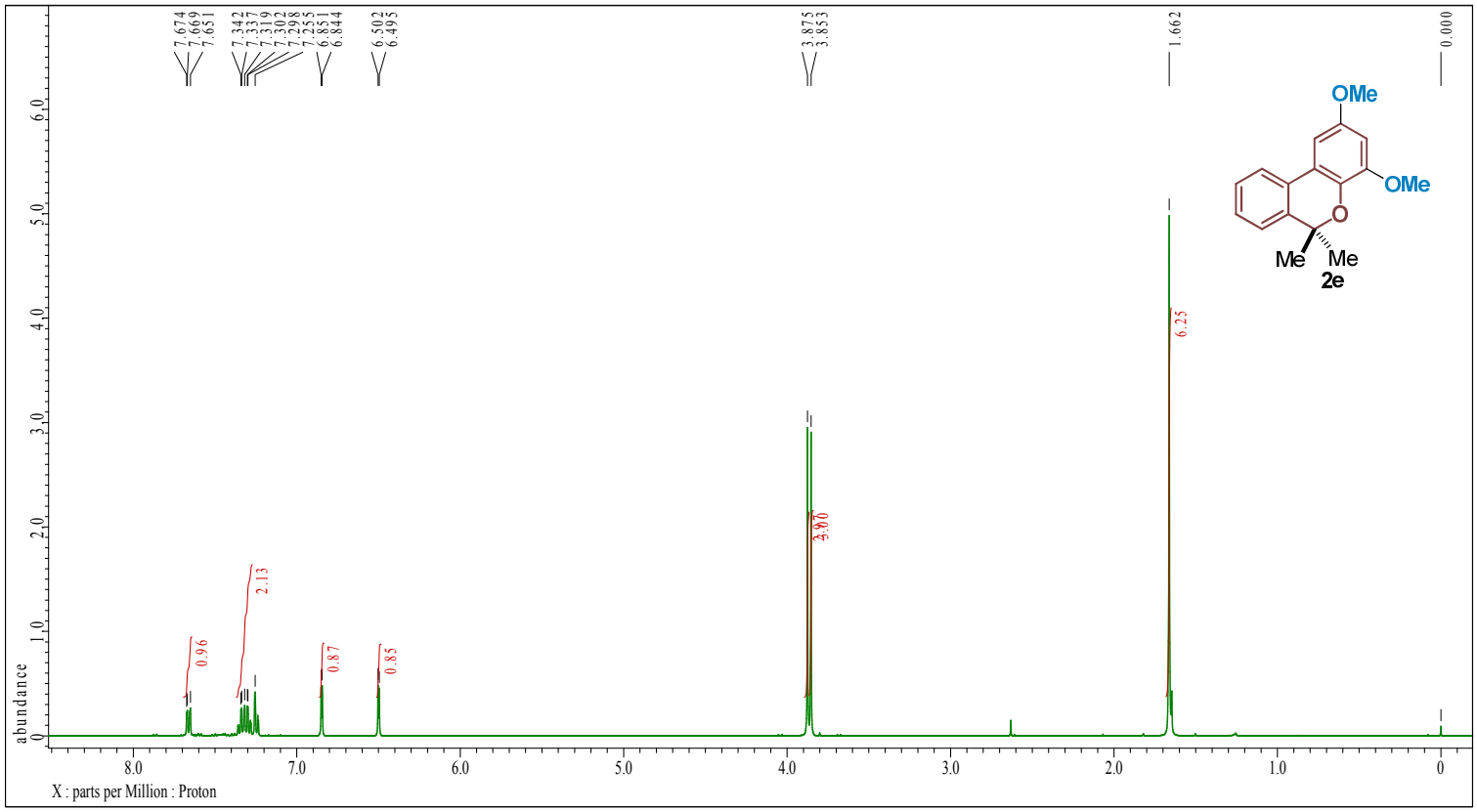
128.796
127.771
127.042
123.880
123.219
121.532
115.524
108.404
102.808
78.046
77.442
77.126
76.810
55.440
27.622
OMe
O
Me
Me
2d
(thousandths)
X : parts per Million : Carbon13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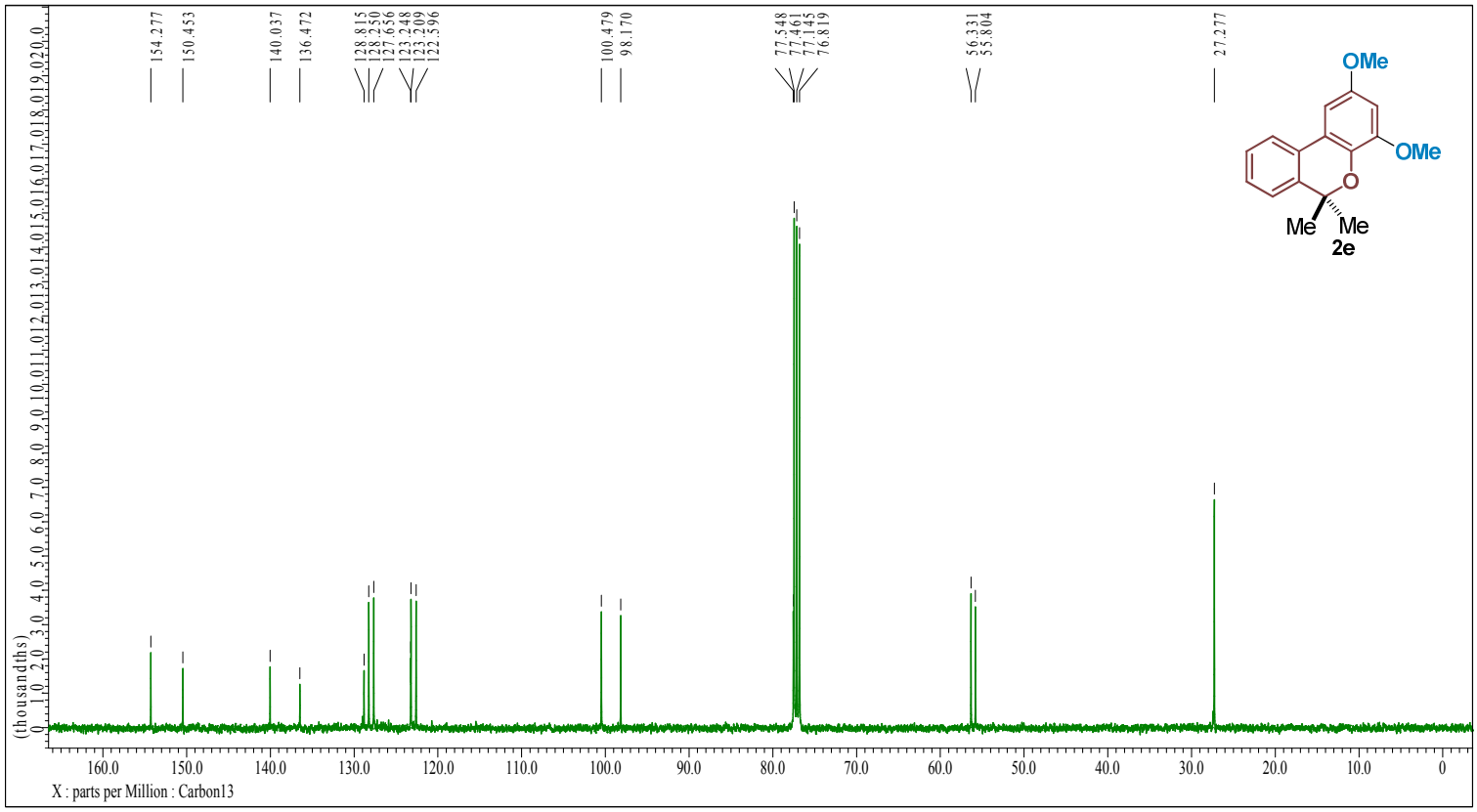
7.669
7.651
7.342
7.337
7.319
7.302
7.298
7.255
6.851
6.844
6.502
6.495
3.875
3.853
1.662
0.000
OMe
OMe
Me
Me
2e
6.25
3.00
2.13
0.96
0.87
0.85
abundance
X : parts per Million : Proton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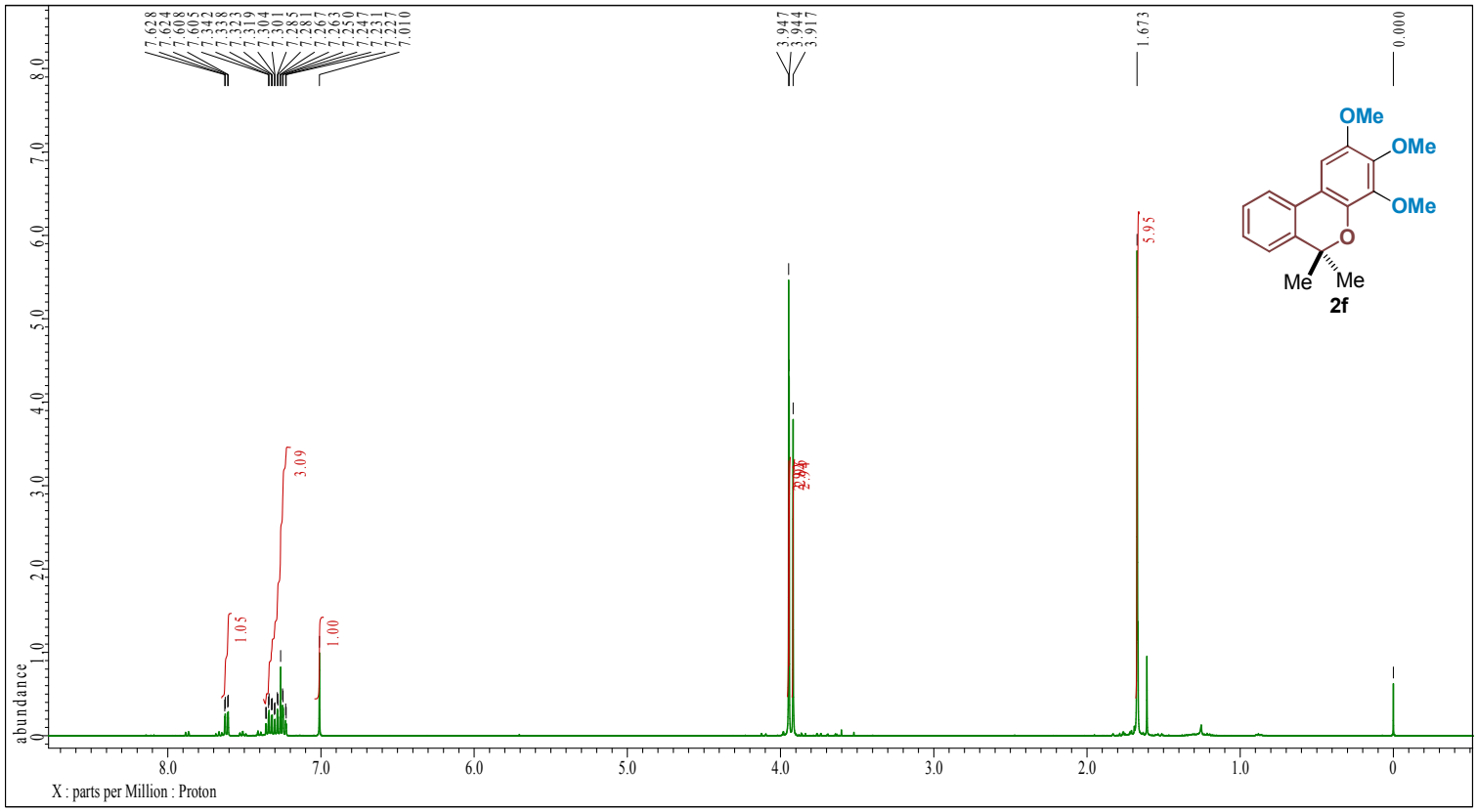
128.250
127.656
123.248
123.209
122.596
100.479
98.170
77.548
77.461
77.145
76.819
56.331
55.804
27.277
OMe
OMe
Me
Me
2e
(thousandths)
X : parts per Million : Carbon13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7.605
7.342
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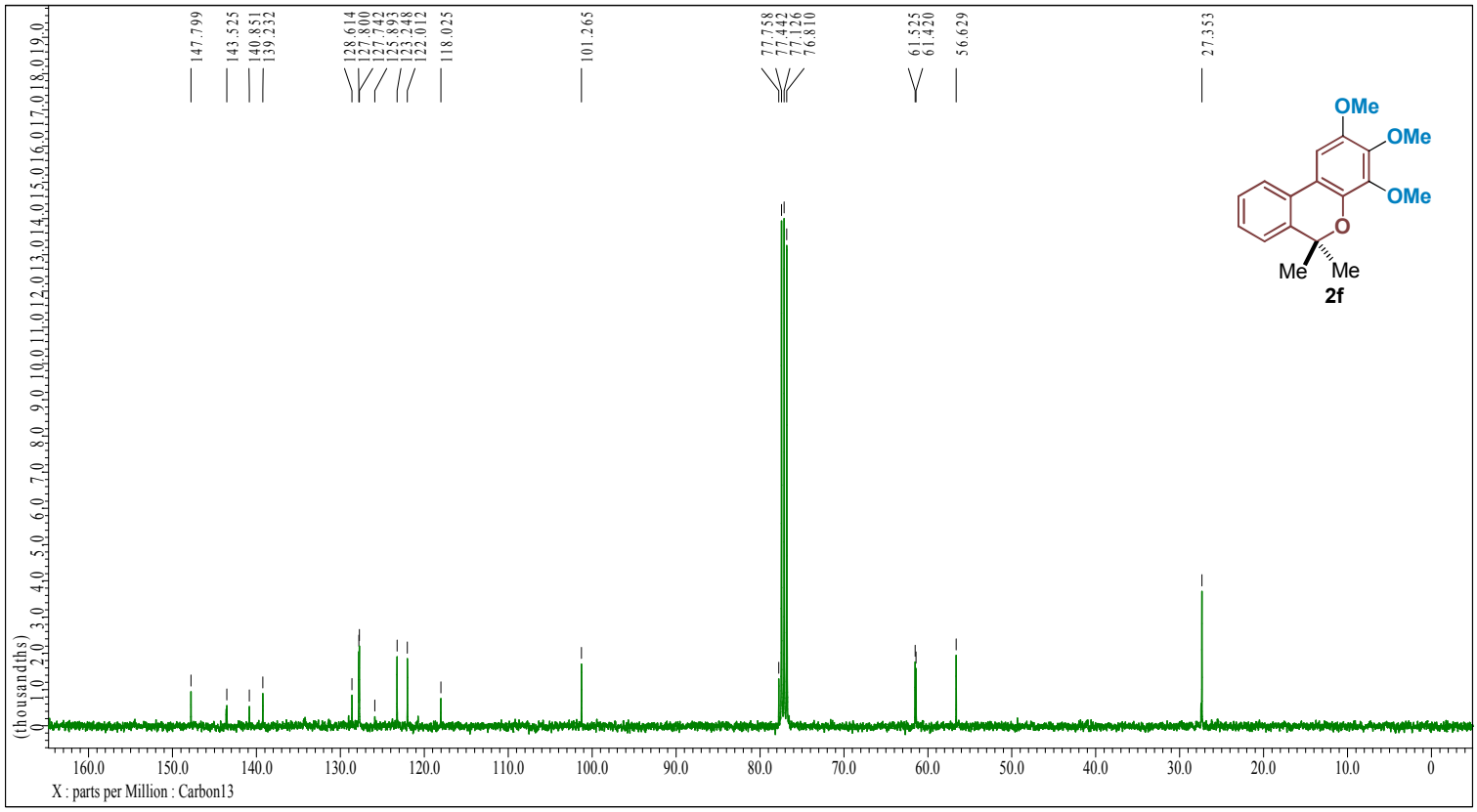
7.323
7.319
7.304
7.301
7.285
7.281
7.267
7.263
7.250
7.247
7.231
7.227
7.010
3.947
3.944
3.917
1.673
0.000
5.95
3.09
1.05
1.00
abundance
X : parts per Million : Proton
OMe
OMe
OMe
Me
Me
2f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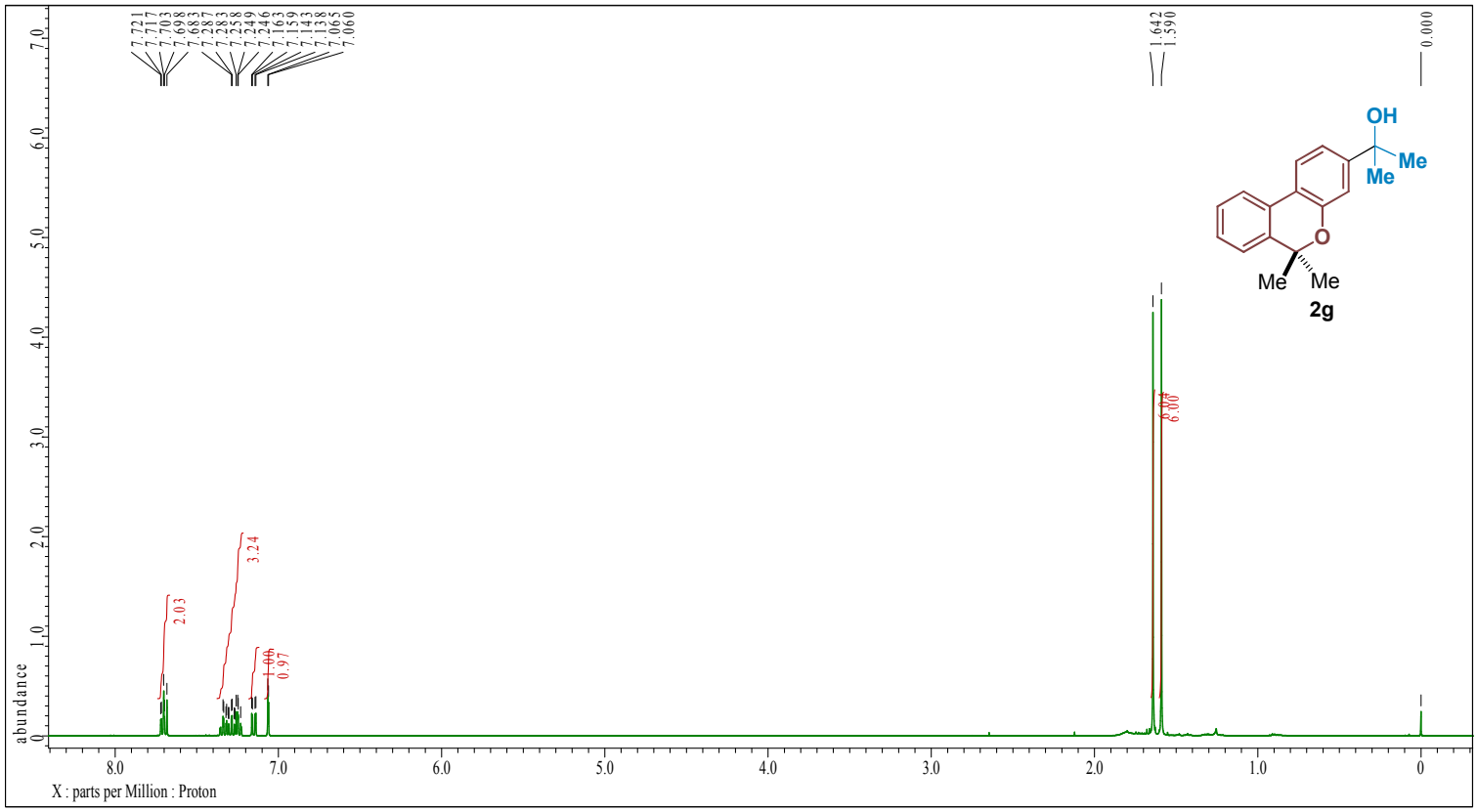
127.800
127.742
125.893
123.248
122.012
118.025
101.265
77.758
77.442
77.126
76.810
61.525
61.420
56.629
27.353
(thousandths)
X : parts per Million : Carbon13
OMe
OMe
OMe
Me
Me
2f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7.683
7.287
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7.246
7.163
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7.138
7.065
7.060
1.642
1.590
0.000
OH
Me
Me
O
Me
Me
2g
3.24
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1.00
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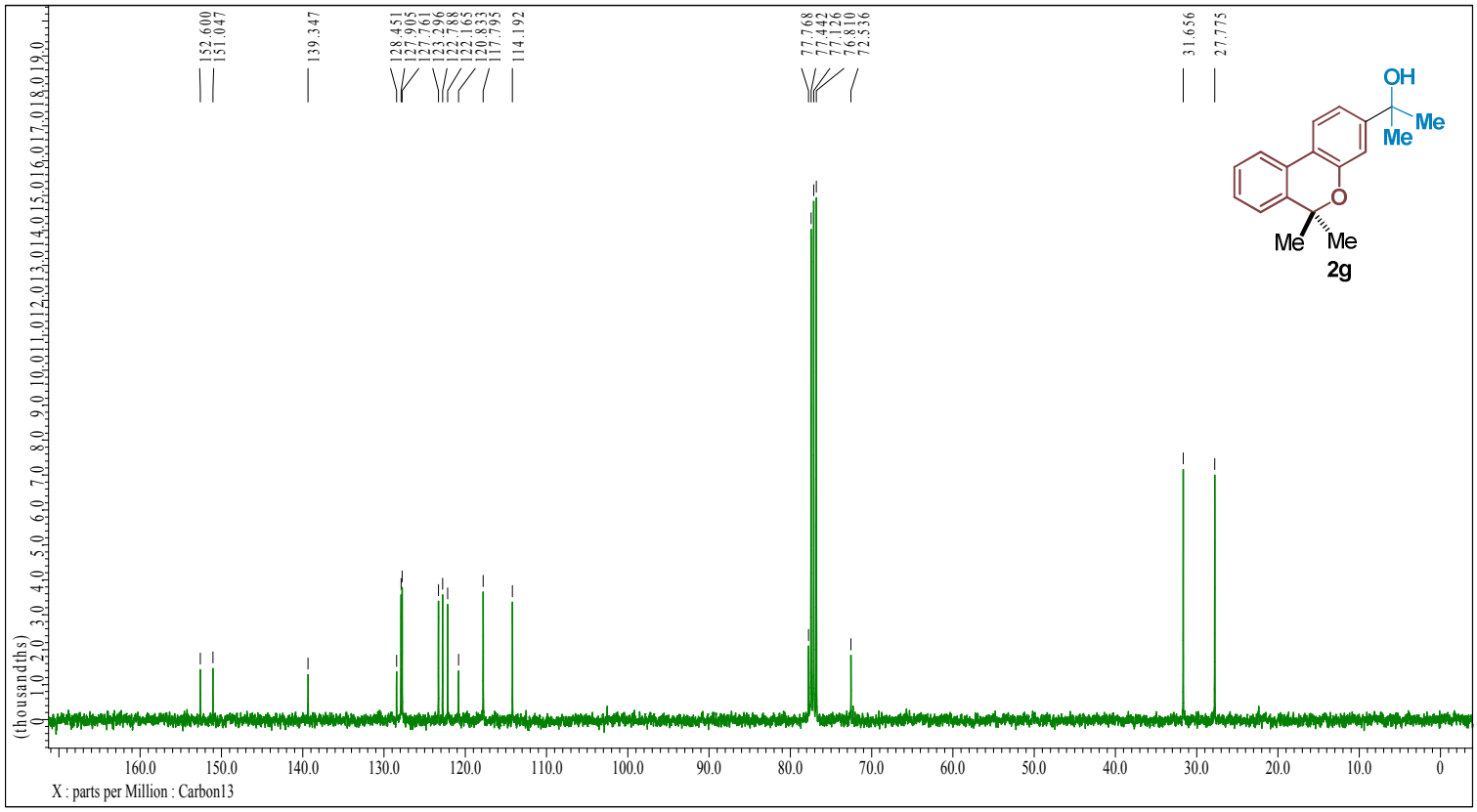
abundance
X : parts per Million : Proton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77.768
77.442
77.126
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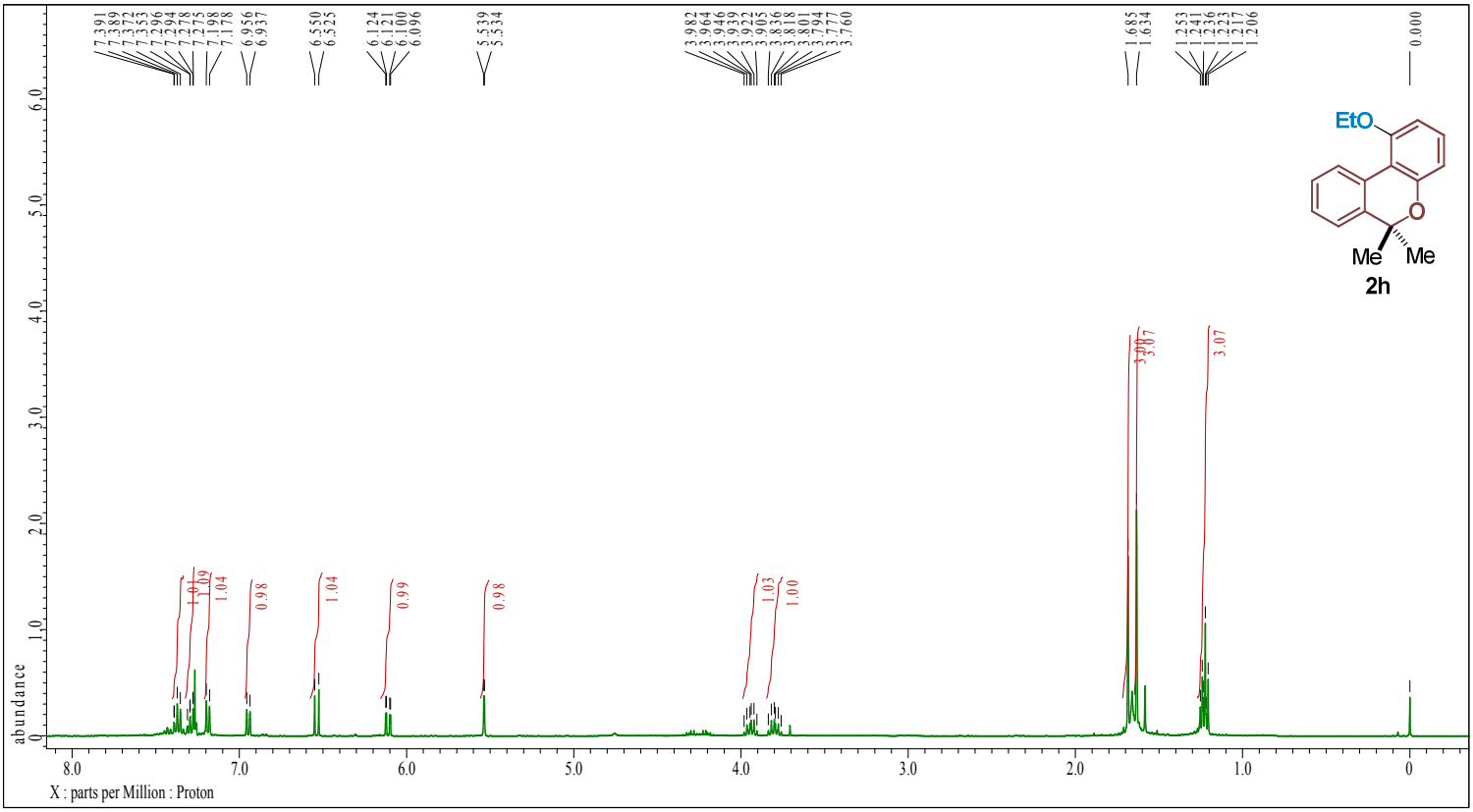
O
Me
Me
2g
(thousandths)
X : parts per Million : Carbon13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6.550
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6.121
6.100
6.096
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5.534
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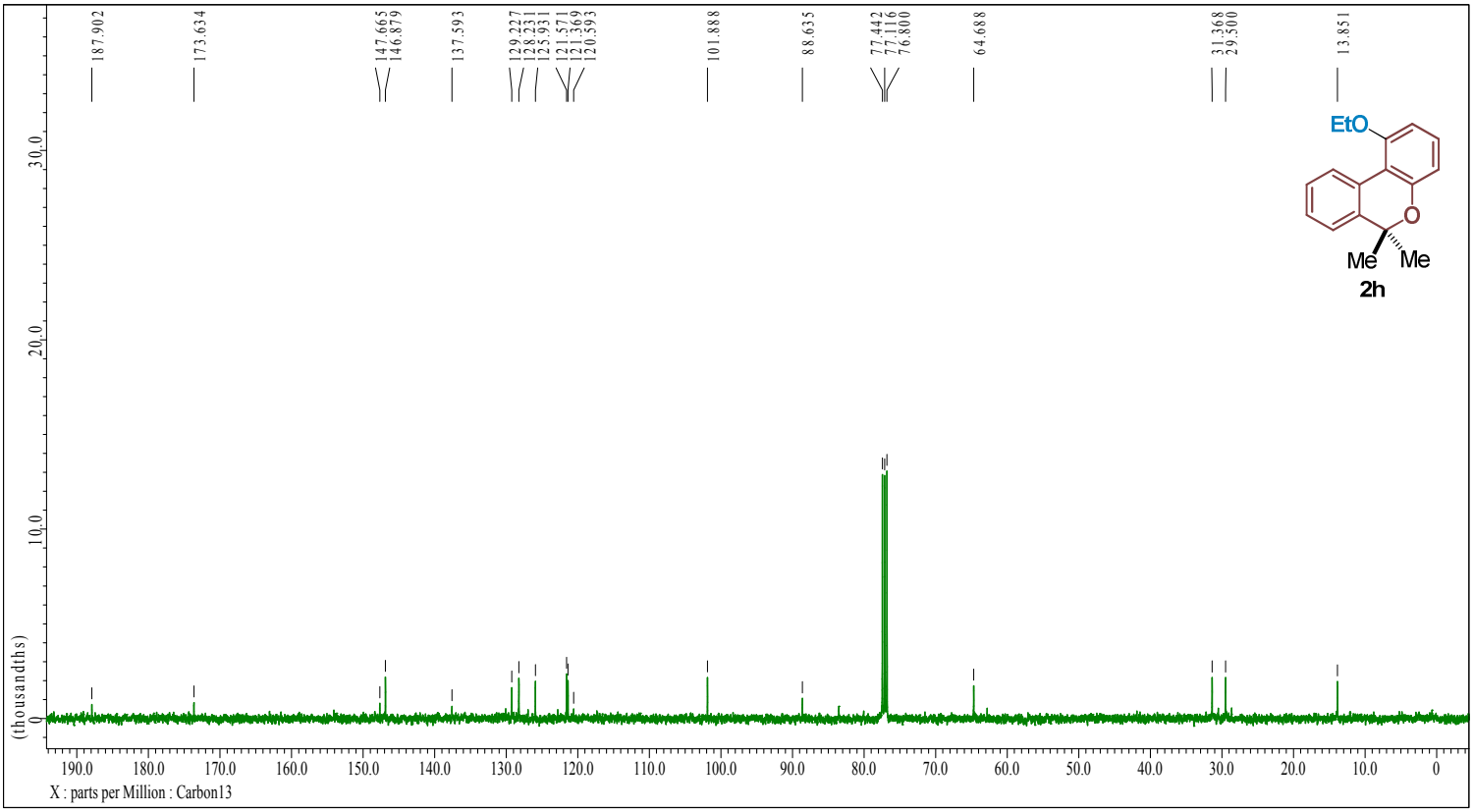
3.964
3.946
3.939
3.922
3.905
3.836
3.818
3.801
3.794
3.777
3.760
1.685
1.634
1.253
1.241
1.236
1.223
1.217
1.206
0.000
EtO
O
Me
Me
2h
1.01
1.09
1.04
0.98
1.04
0.99
0.98
1.03
1.00
3.00
3.07
3.07
abundance
X : parts per Million : Proton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88.635
77.442
77.116
76.800
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31.368
29.500
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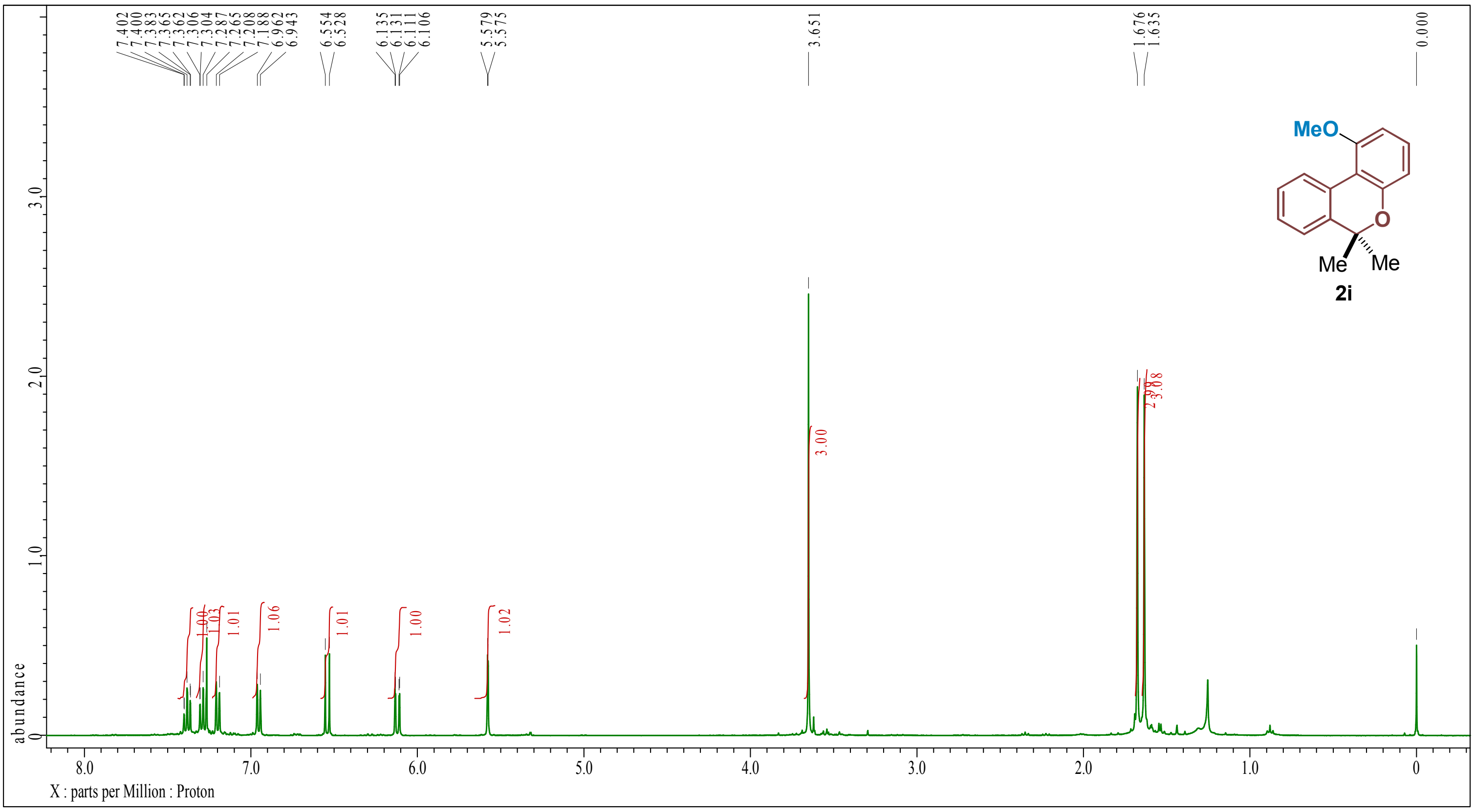
EtO
O
Me
Me
2h
(thousandths)
X : parts per Million : Carbon13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6.943
6.554
6.528
6.135
6.131
6.111
6.106
5.579
5.575
3.651
1.676
1.635
0.000
MeO
O
Me
Me
2i
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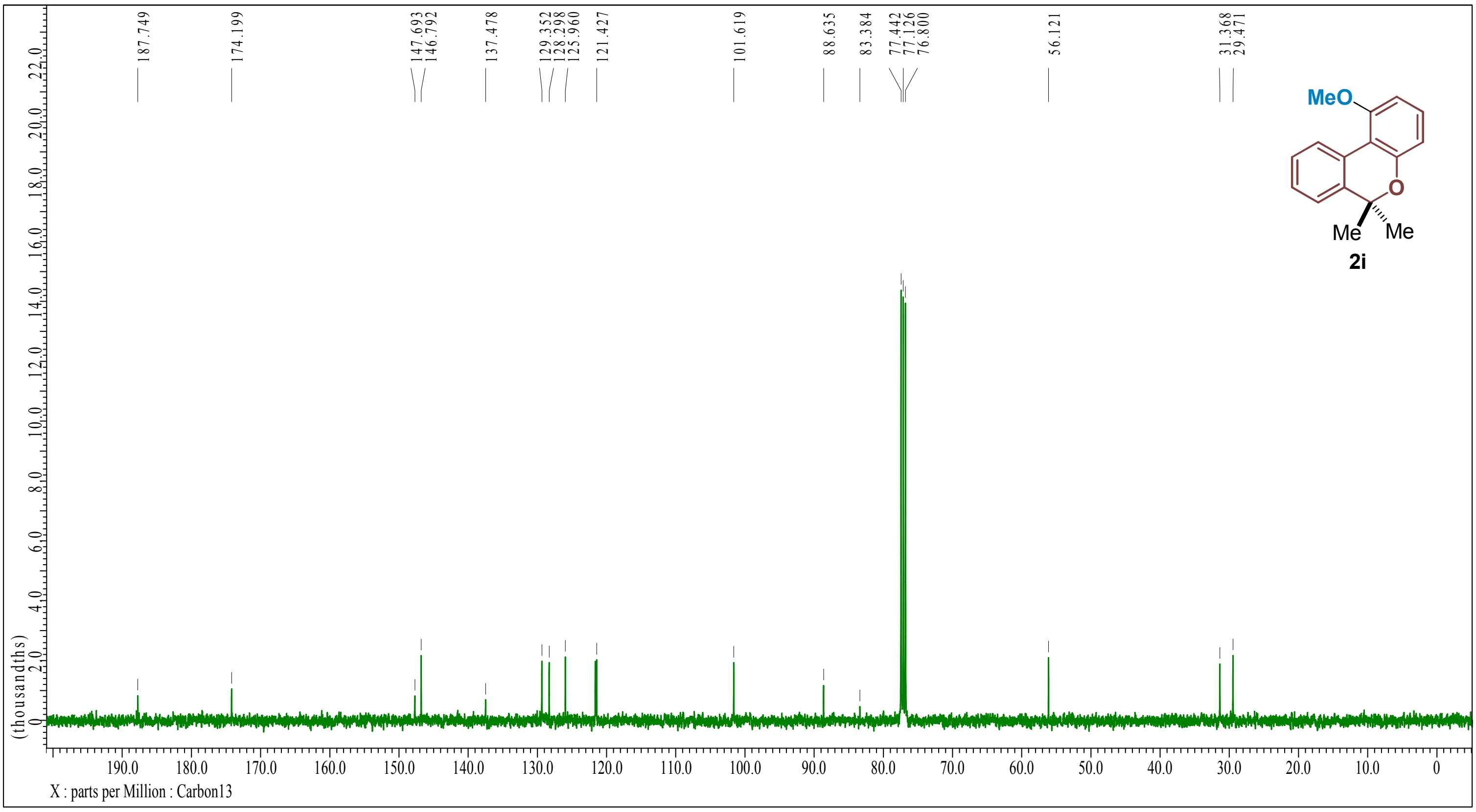
1.01
1.06
1.01
1.00
1.02
3.00
3.08
abundance
X : parts per Million : Proton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77.442
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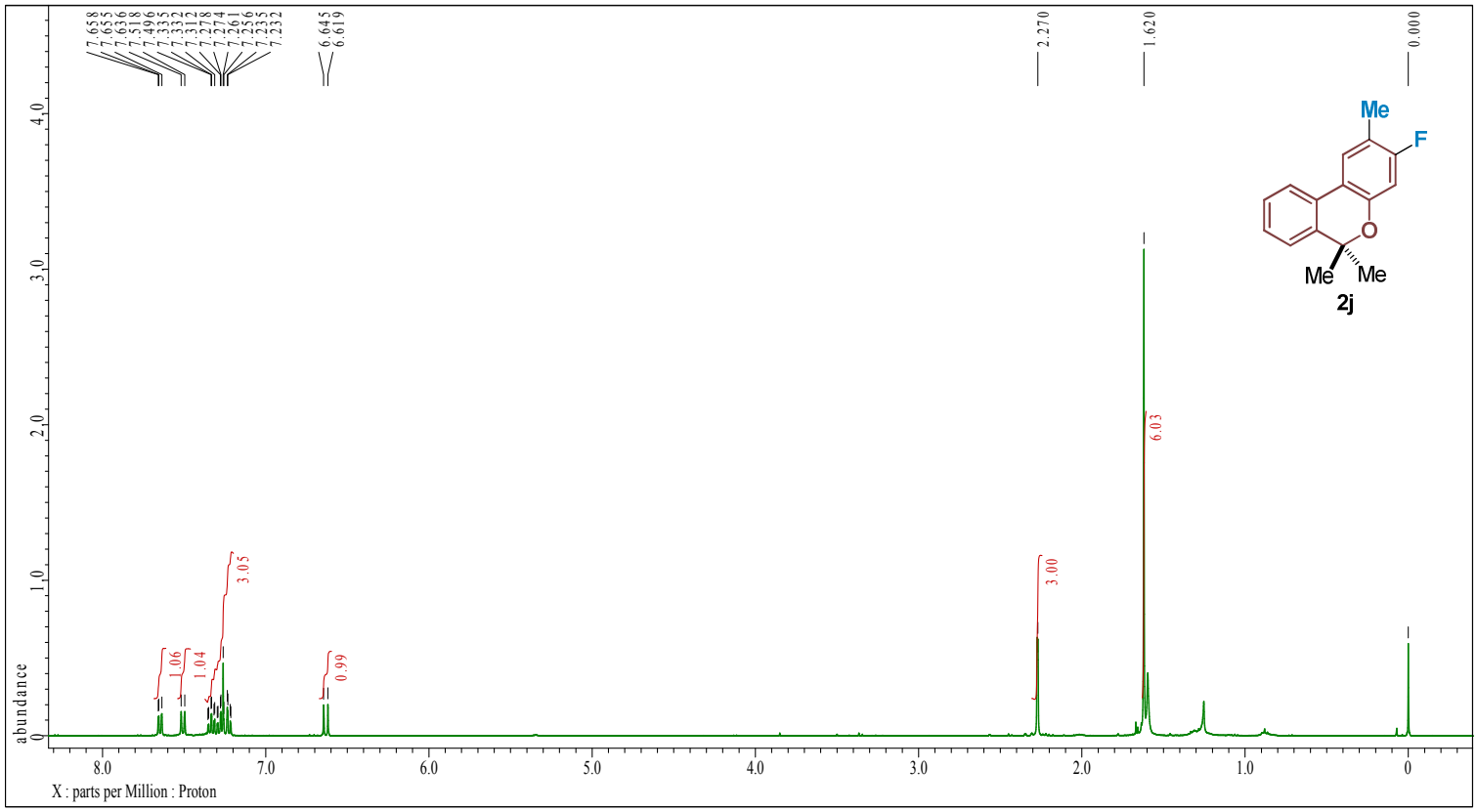
31.368
29.471
MeO
O
Me
Me
2i
(thousandths)
X : parts per Million : Carbon13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2.270
1.620
0.000
Me
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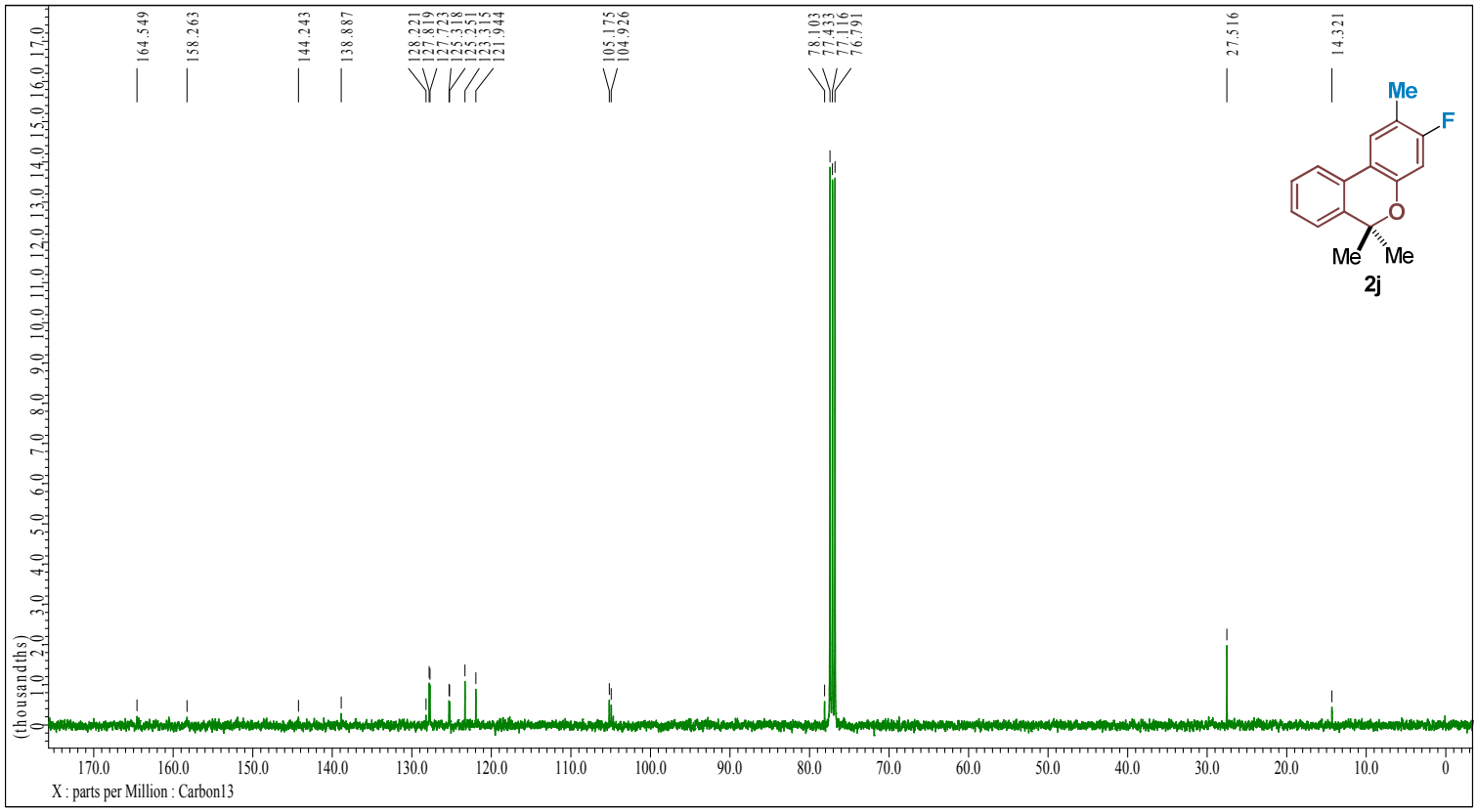
3.00
1.06
1.04
0.99
abundance
X : parts per Million : Proton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104.926
78.103
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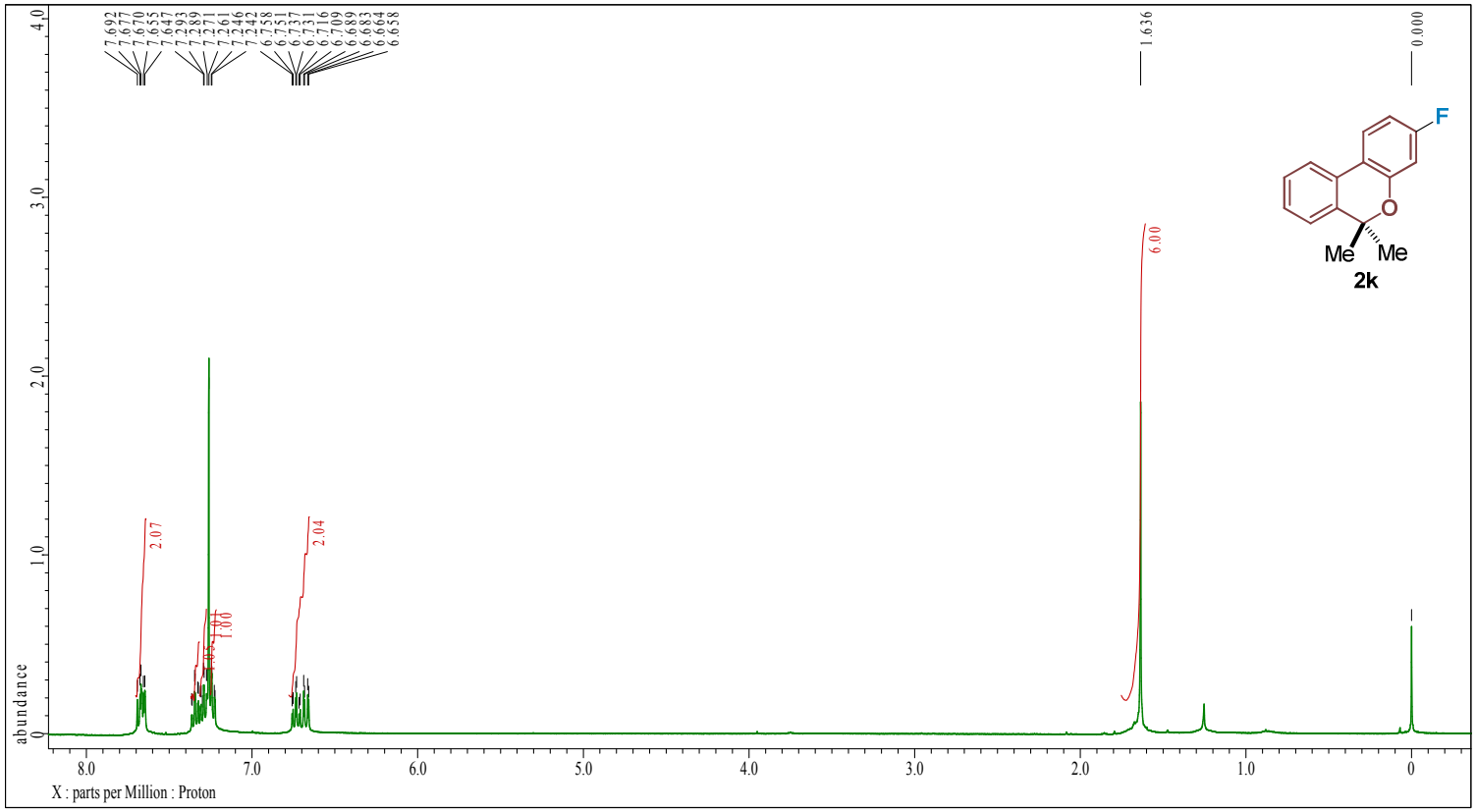
14.321
Me
F
O
Me
Me
2j
(thousandths)
X : parts per Million : Carbon13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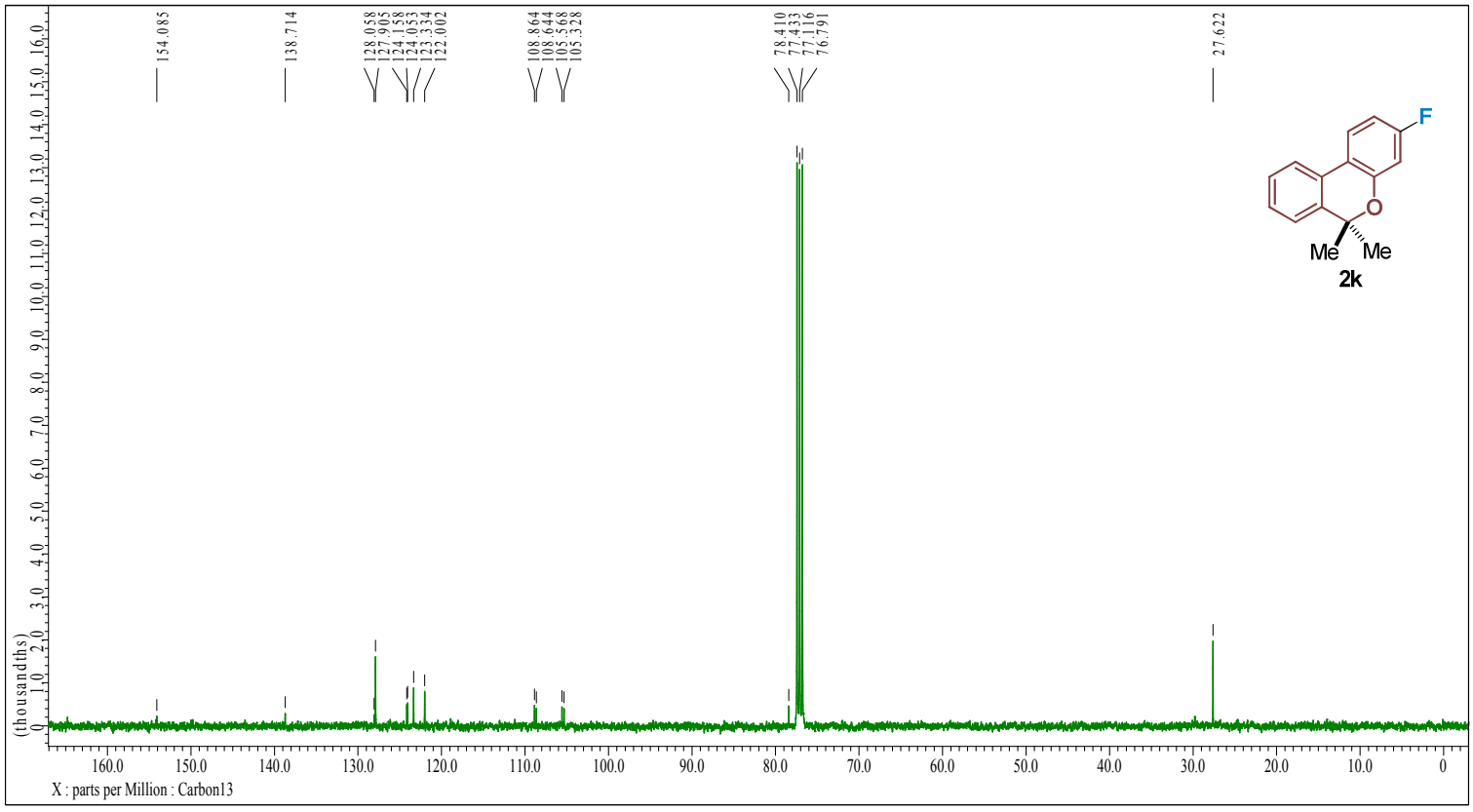
6.709
6.689
6.683
6.664
6.658
1.636
0.000
6.00
2.07
2.04
1.01
1.00
abundance
X : parts per Million : Proton
F
O
Me
Me
2k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122.002
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108.644
105.568
105.328
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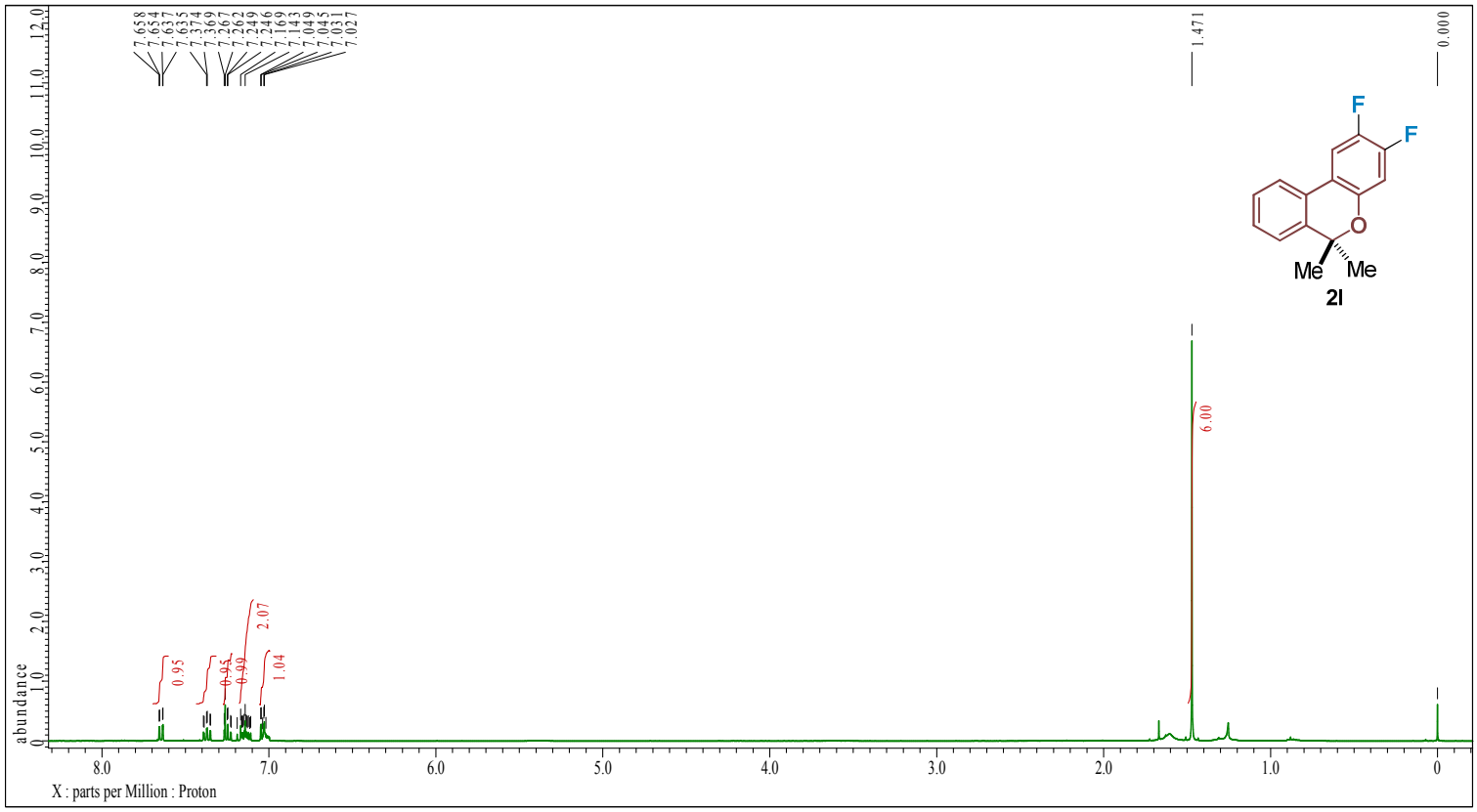
77.116
76.791
27.622
(thousandths)
X : parts per Million : Carbon13
F
O
Me
Me
2k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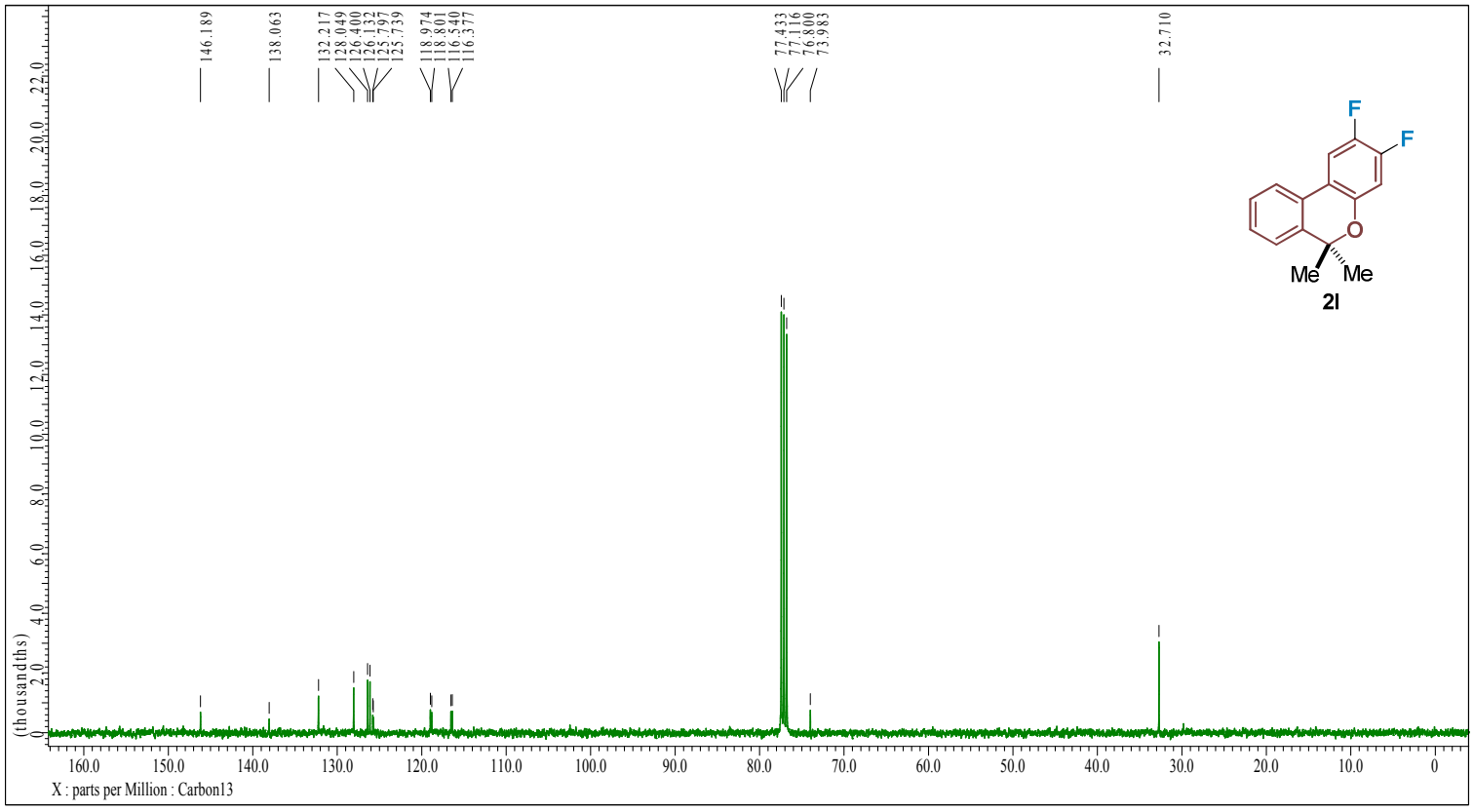
7.369
7.267
7.262
7.249
7.246
7.169
7.143
7.049
7.045
7.031
7.027
1.471
0.000
F
F
O
Me
Me
2l
6.00
2.07
1.04
0.95
0.95
0.99
abundance
X : parts per Million : Proton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125.739
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118.801
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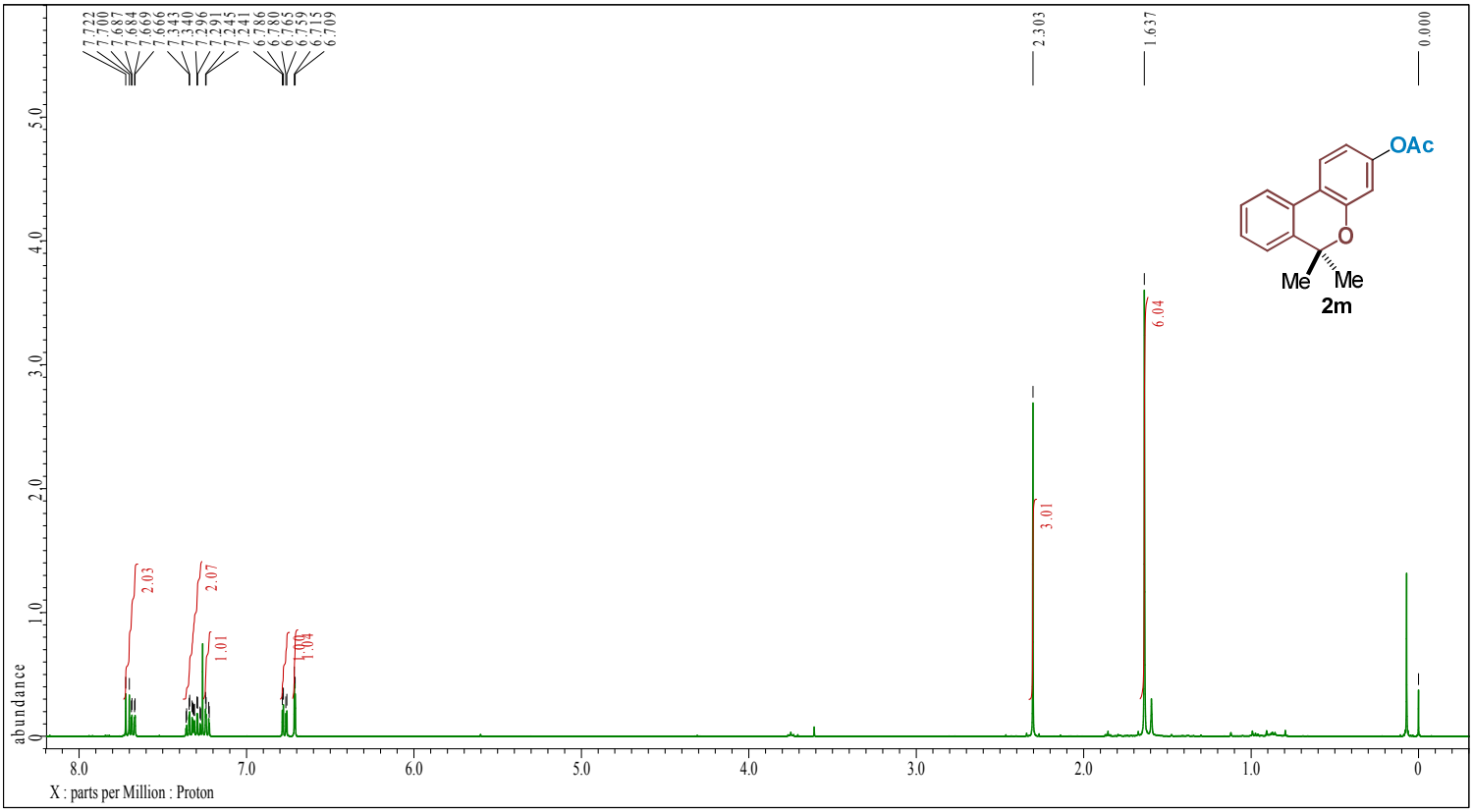
116.377
77.433
77.116
76.800
73.983
32.710
F
F
O
Me
Me
2l
(thousandths)
X : parts per Million : Carbon13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7.340
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7.291
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7.241
6.786
6.780
6.765
6.759
6.715
6.709
2.303
1.637
0.000
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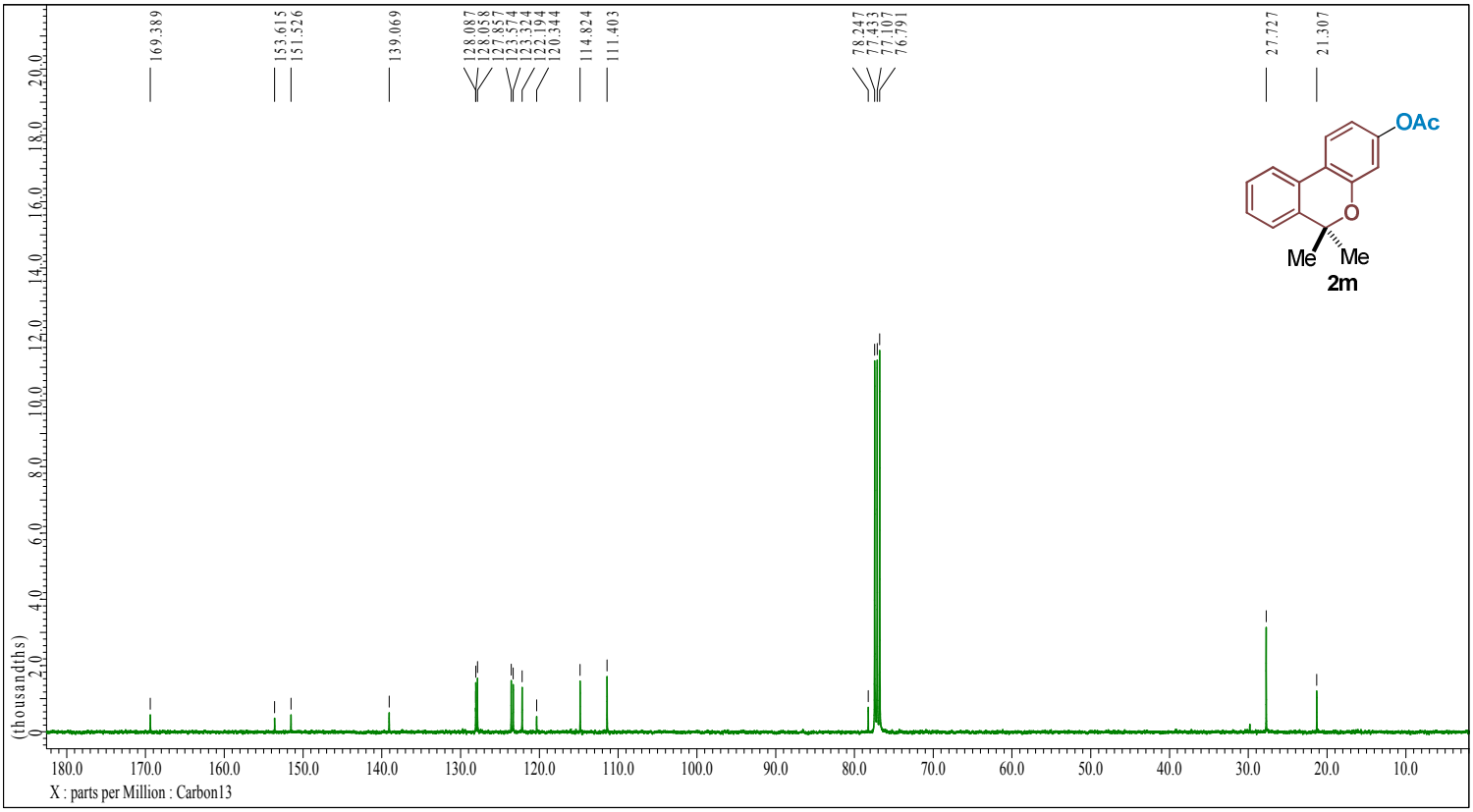
O
Me
Me
2m
6.04
3.01
2.03
2.07
1.01
1.04
abundance
X : parts per Million : Proton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139.069
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128.058
127.857
123.574
123.324
122.194
120.344
114.824
111.403
78.247
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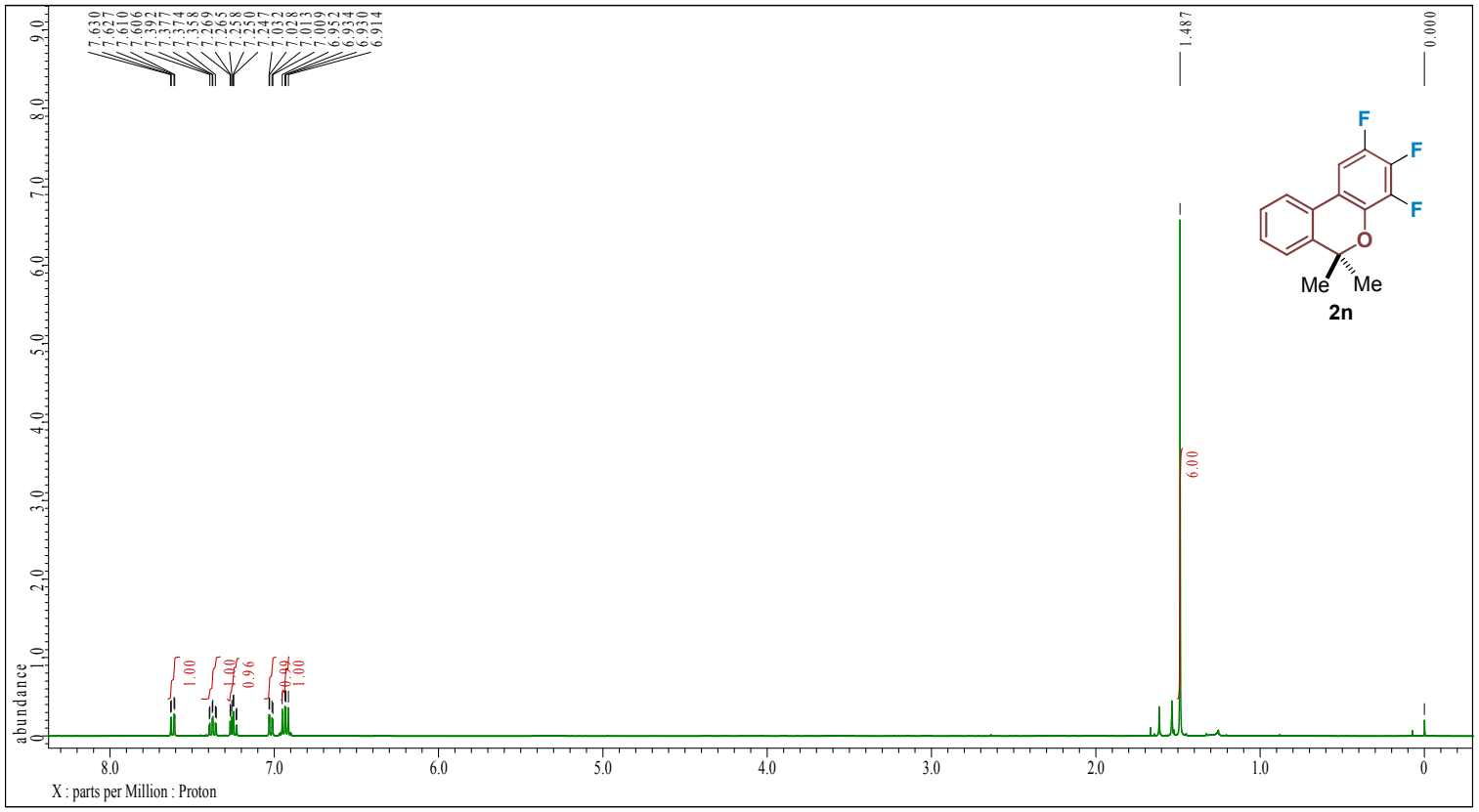
77.107
76.791
27.727
21.307
OAc
O
Me
Me
2m
(thousandths)
X : parts per Million : Carbon13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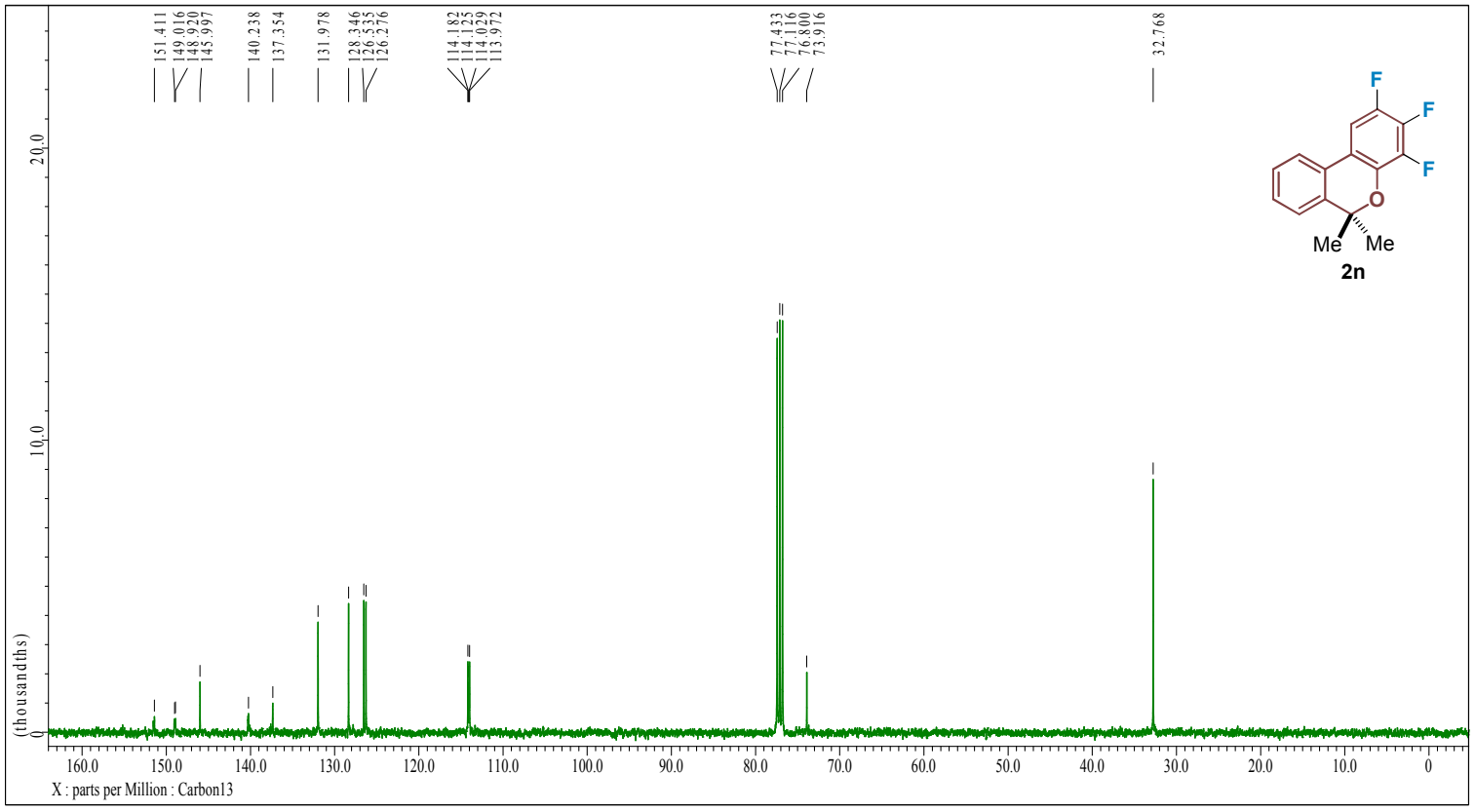
7.606
7.392
7.377
7.374
7.358
7.269
7.265
7.258
7.250
7.247
7.032
7.028
7.013
7.009
6.952
6.934
6.930
6.914
1.487
0.000
6.00
1.00
1.00
0.96
1.00
abundance
X : parts per Million : Proton
F
F
F
O
Me
Me
2n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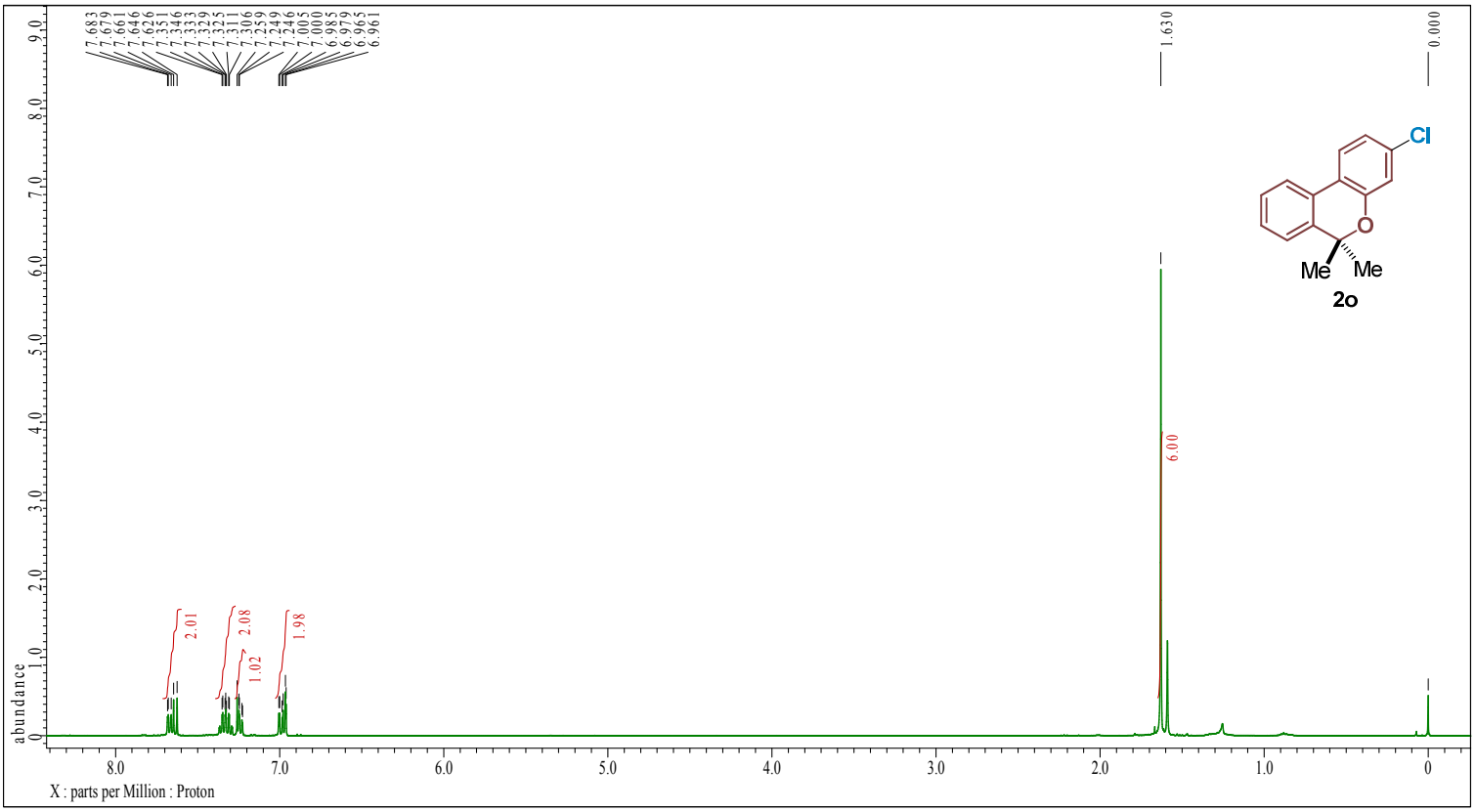
137.354
131.978
128.346
126.335
126.276
114.182
114.125
114.029
113.972
77.433
77.116
76.800
73.916
32.768
(thousandths)
X : parts per Million : Carbon13
F
F
F
O
Me
Me
2n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7.646
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7.333
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7.311
7.306
7.259
7.249
7.246
7.005
7.000
6.985
6.979
6.965
6.961
1.630
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6.00
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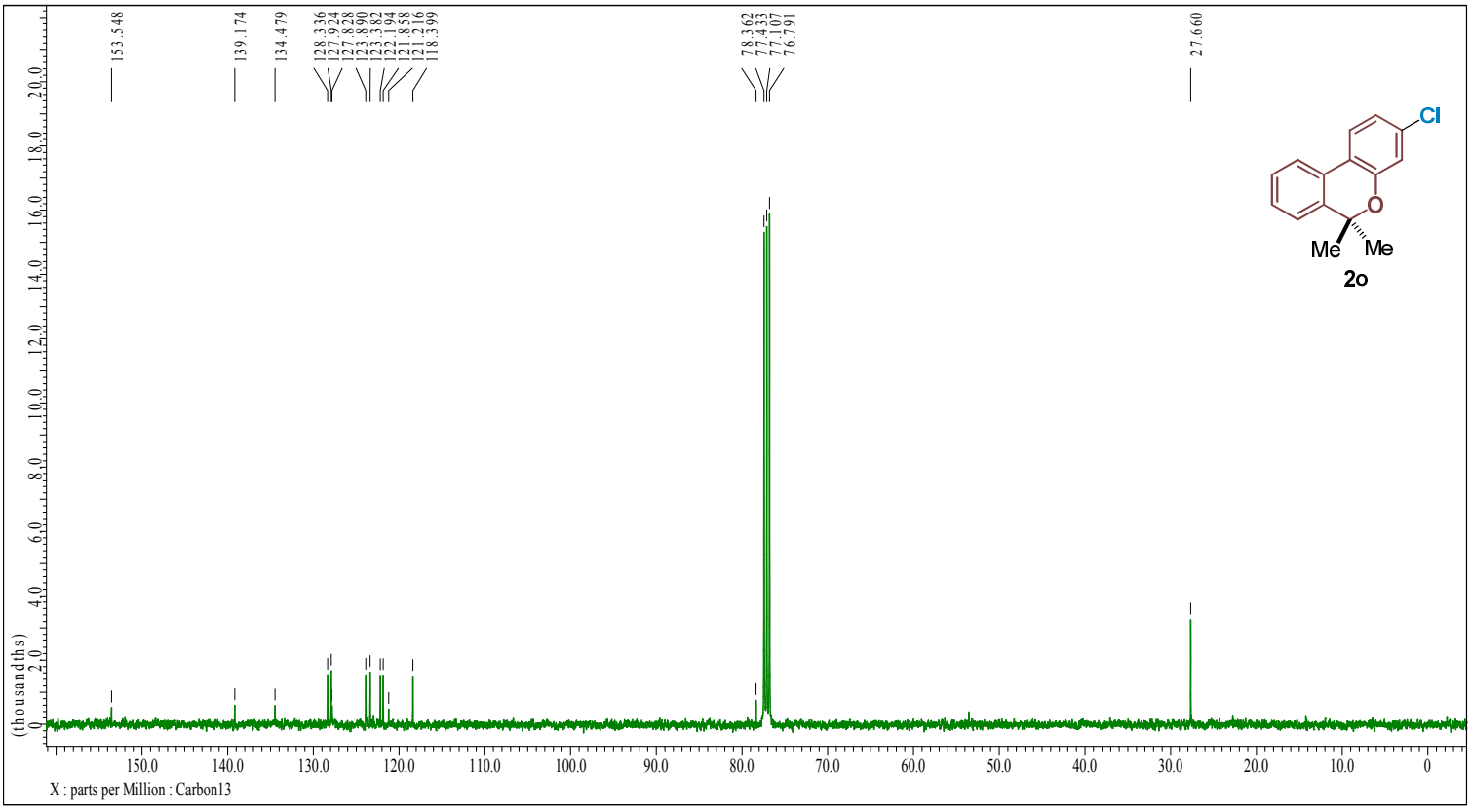
2.08
1.02
1.98
abundance
X : parts per Million : Proton
Cl
O
Me
Me
2o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127.828
123.890
123.382
122.194
121.858
121.216
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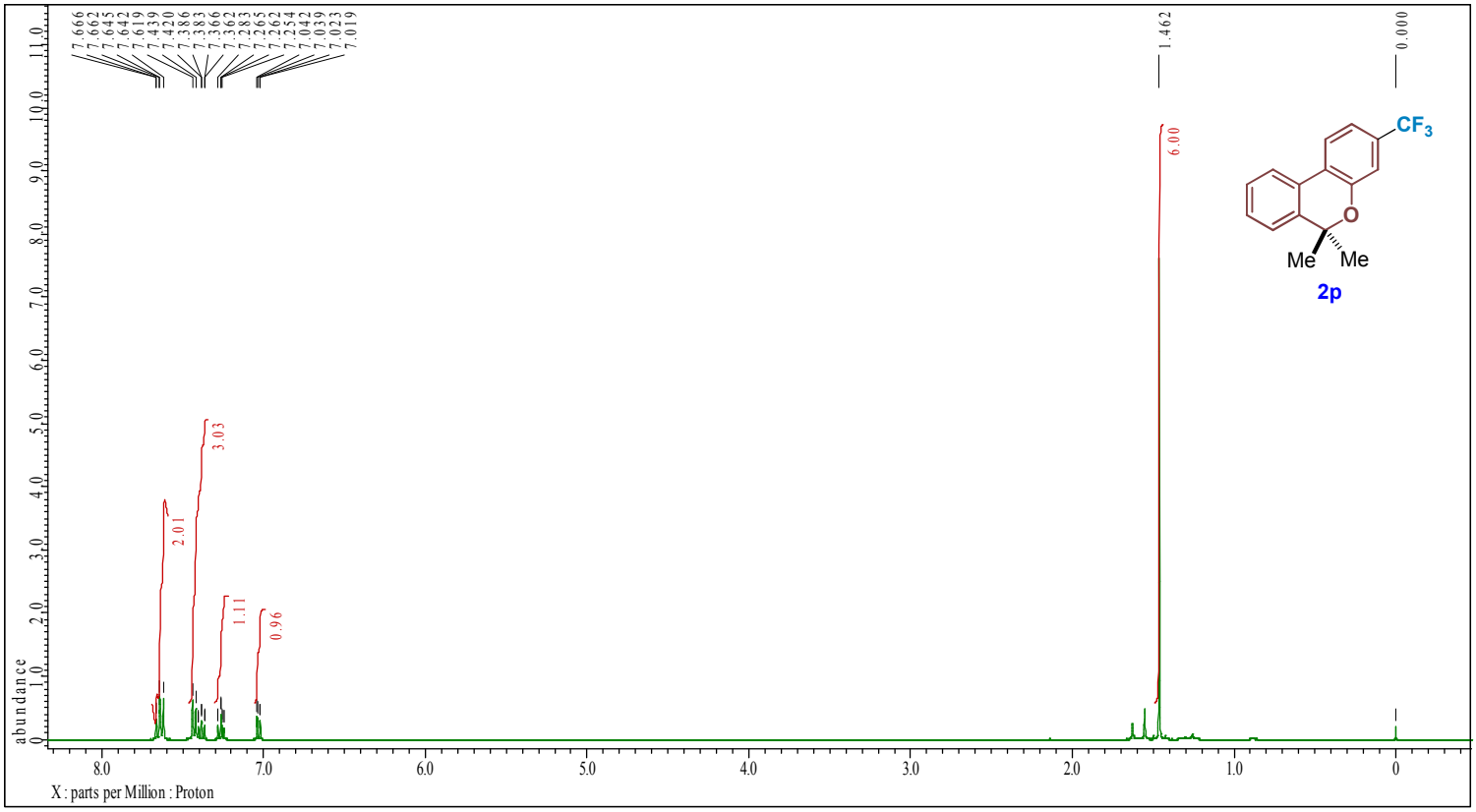
77.433
77.107
76.791
27.660
(thousandths)
X : parts per Million : Carbon13
Cl
O
Me
Me
2o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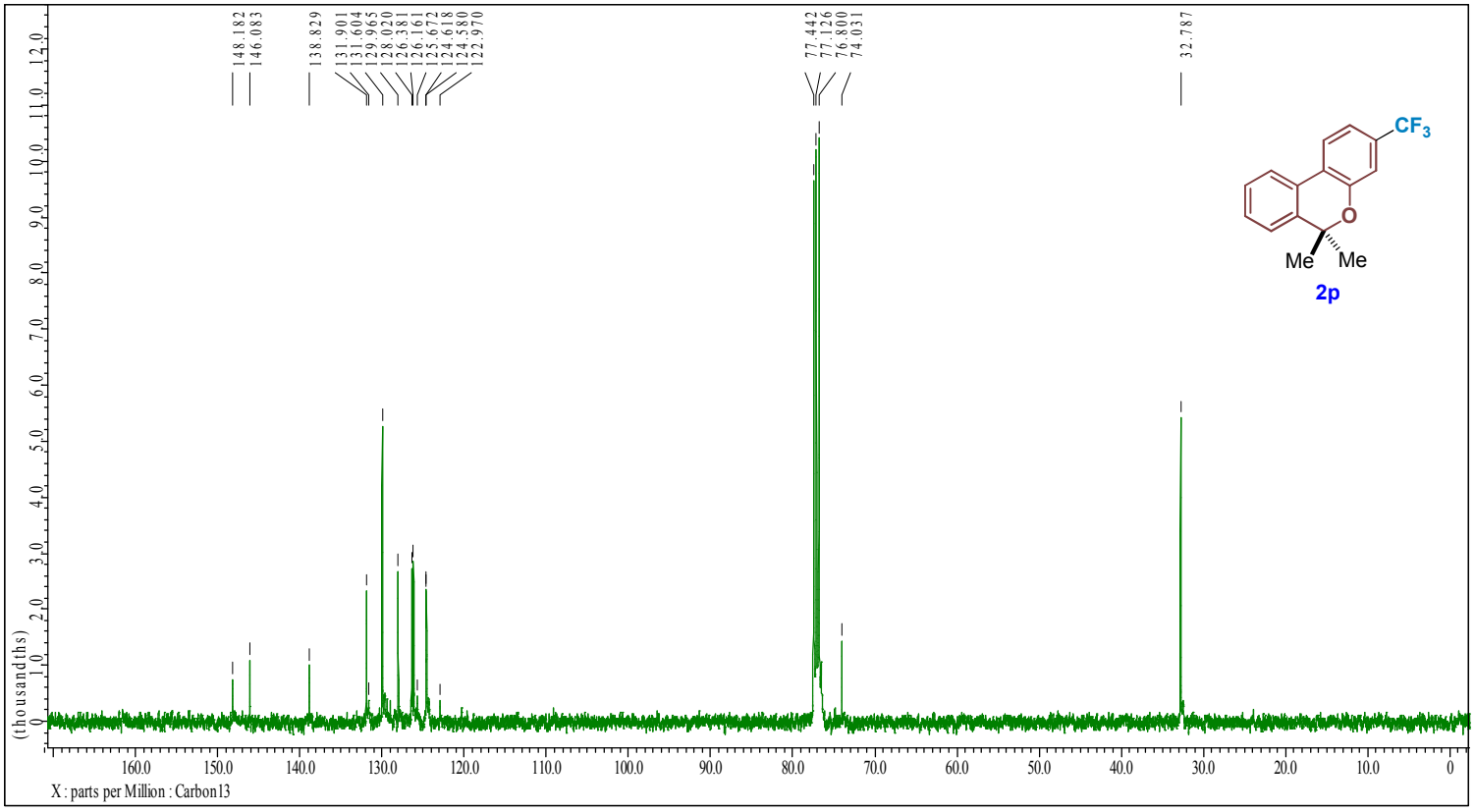
7.642
7.619
7.439
7.420
7.386
7.383
7.366
7.362
7.283
7.265
7.262
7.254
7.042
7.039
7.023
7.019
1.462
0.000
6.00
3.03
2.01
1.11
0.96
abundance
X : parts per Million : Proton
CF3
O
Me
Me
2p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146.083
138.829
131.901
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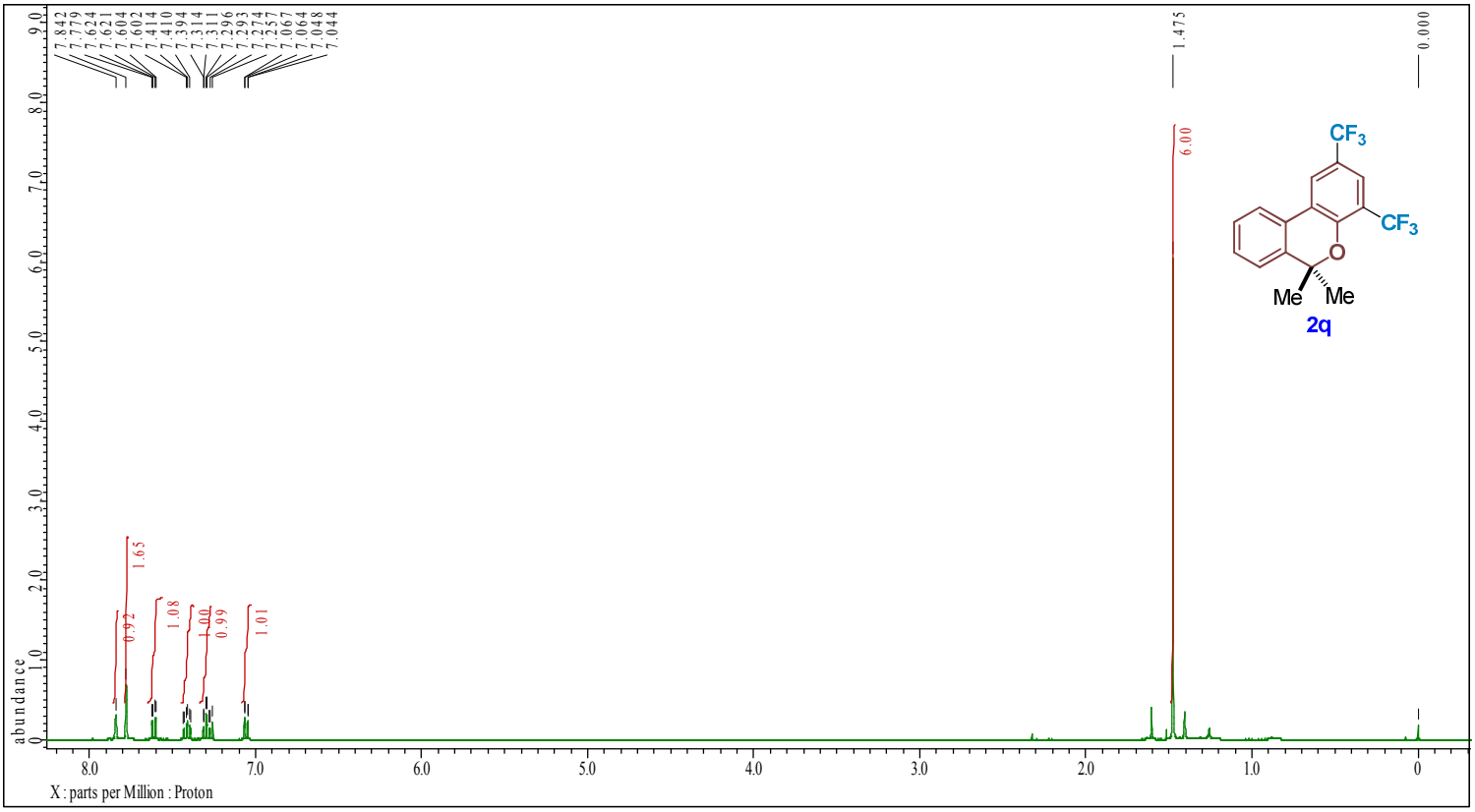
129.965
128.020
126.381
126.161
125.672
124.618
124.580
122.970
77.442
77.126
76.800
74.031
32.787
(thousandths)
X : parts per Million : Carbon13
CF3
O
Me
Me
2p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7.779
7.624
7.621
7.604
7.602
7.414
7.410
7.394
7.314
7.311
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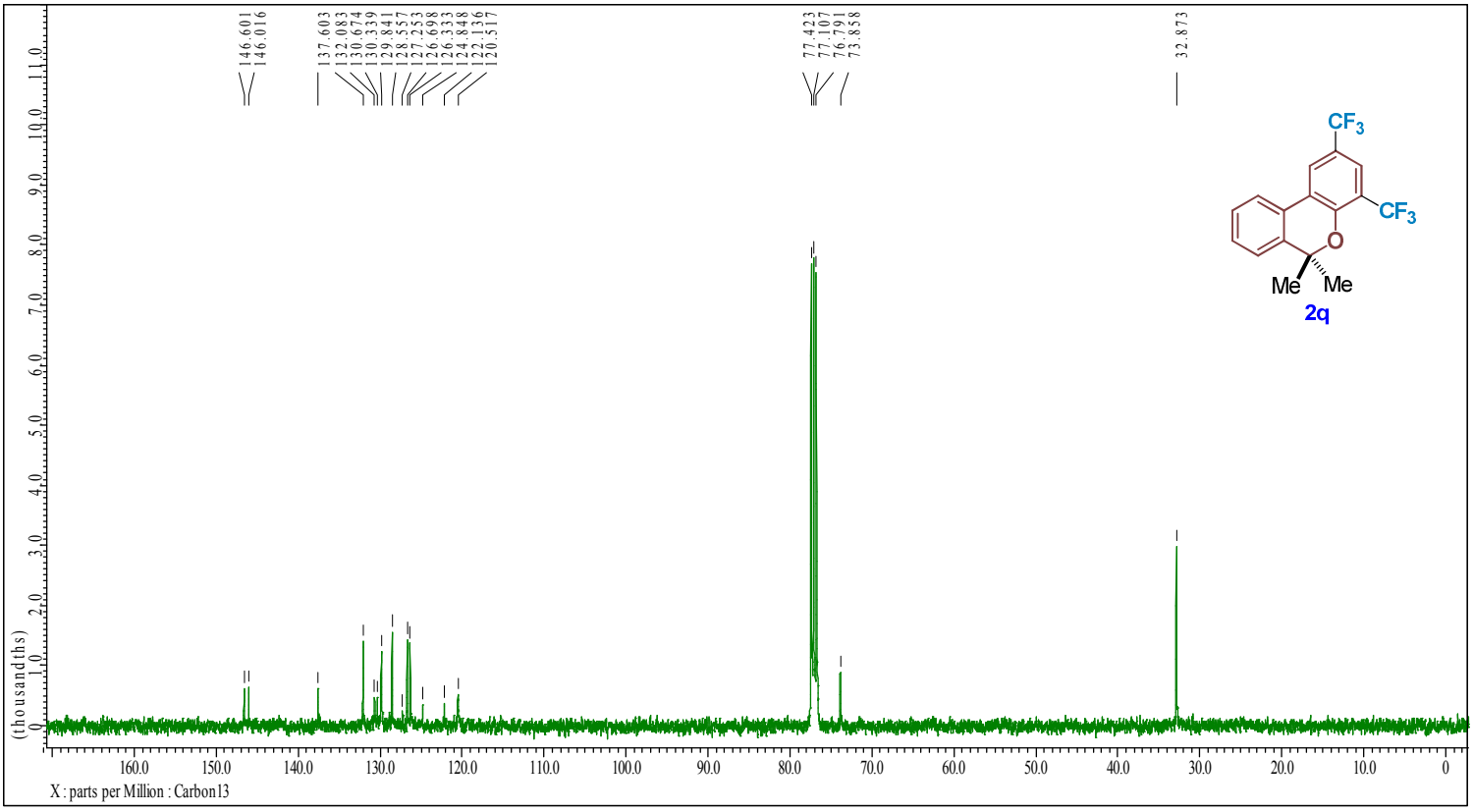
7.293
7.274
7.257
7.067
7.064
7.048
7.044
1.475
0.000
6.00
1.65
0.92
1.08
1.00
0.99
1.01
abundance
X : parts per Million : Proton
CF3
CF3
O
Me
Me
2q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146.016
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129.841
128.557
127.253
126.698
126.333
124.848
122.136
120.517
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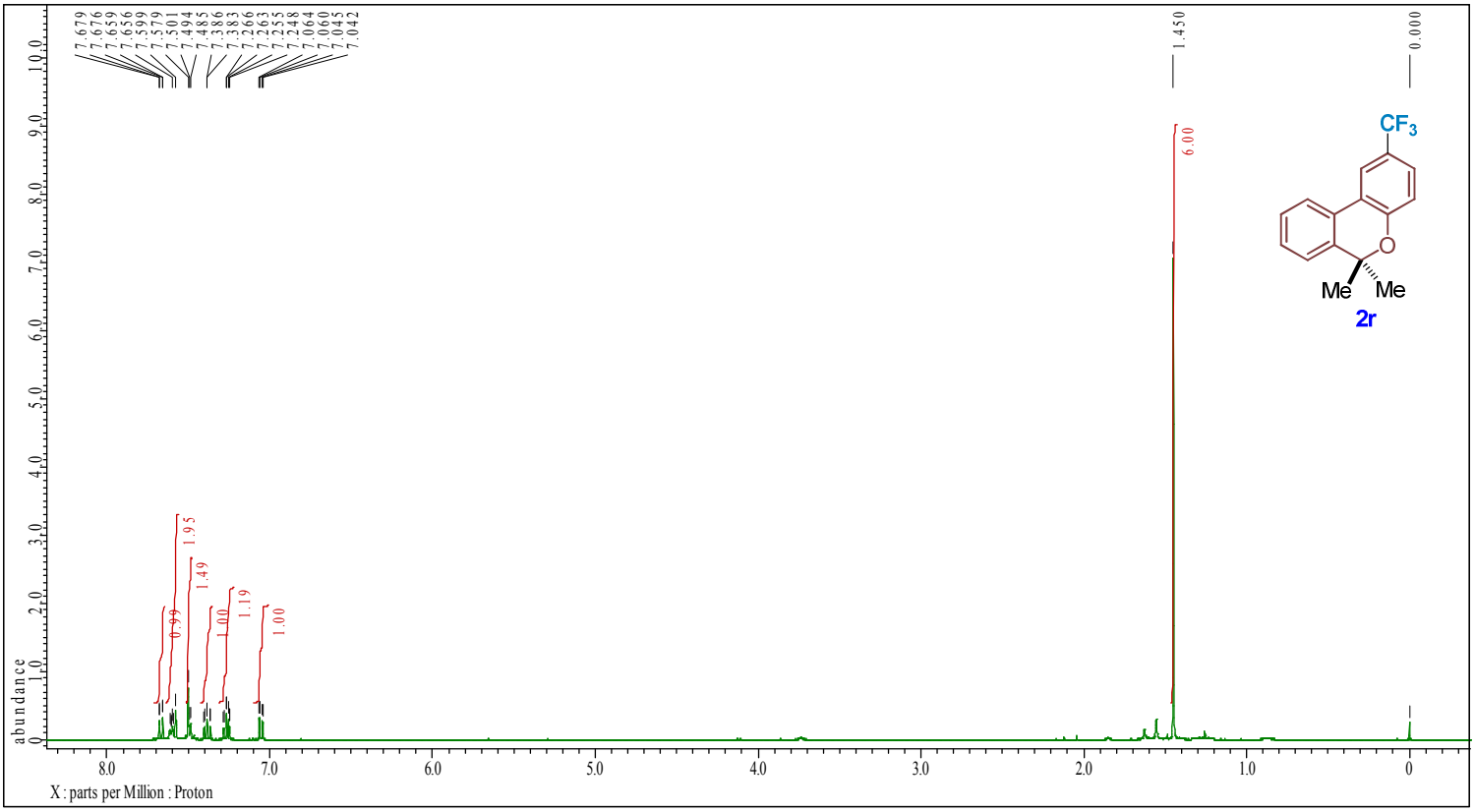
77.107
76.791
73.858
32.873
(thousandths)
X : parts per Million : Carbon13
CF3
CF3
O
Me
Me
2q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7.494
7.485
7.386
7.383
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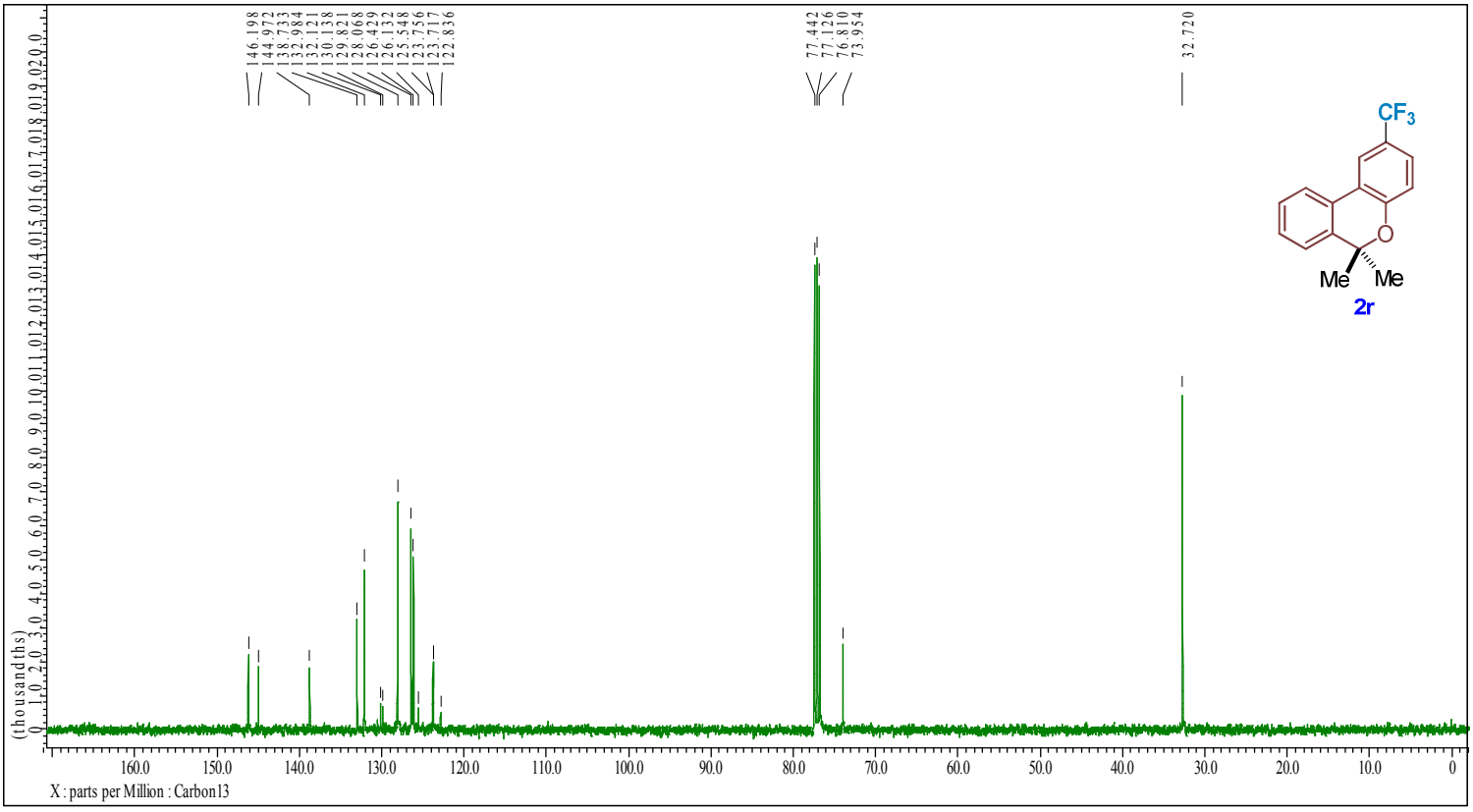
7.263
7.255
7.248
7.064
7.060
7.045
7.042
1.450
0.000
6.00
1.95
1.49
1.00
1.19
1.00
0.99
CF3
O
Me
Me
2r
abundance
X : parts per Million : Proton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126.132
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123.756
123.717
122.836
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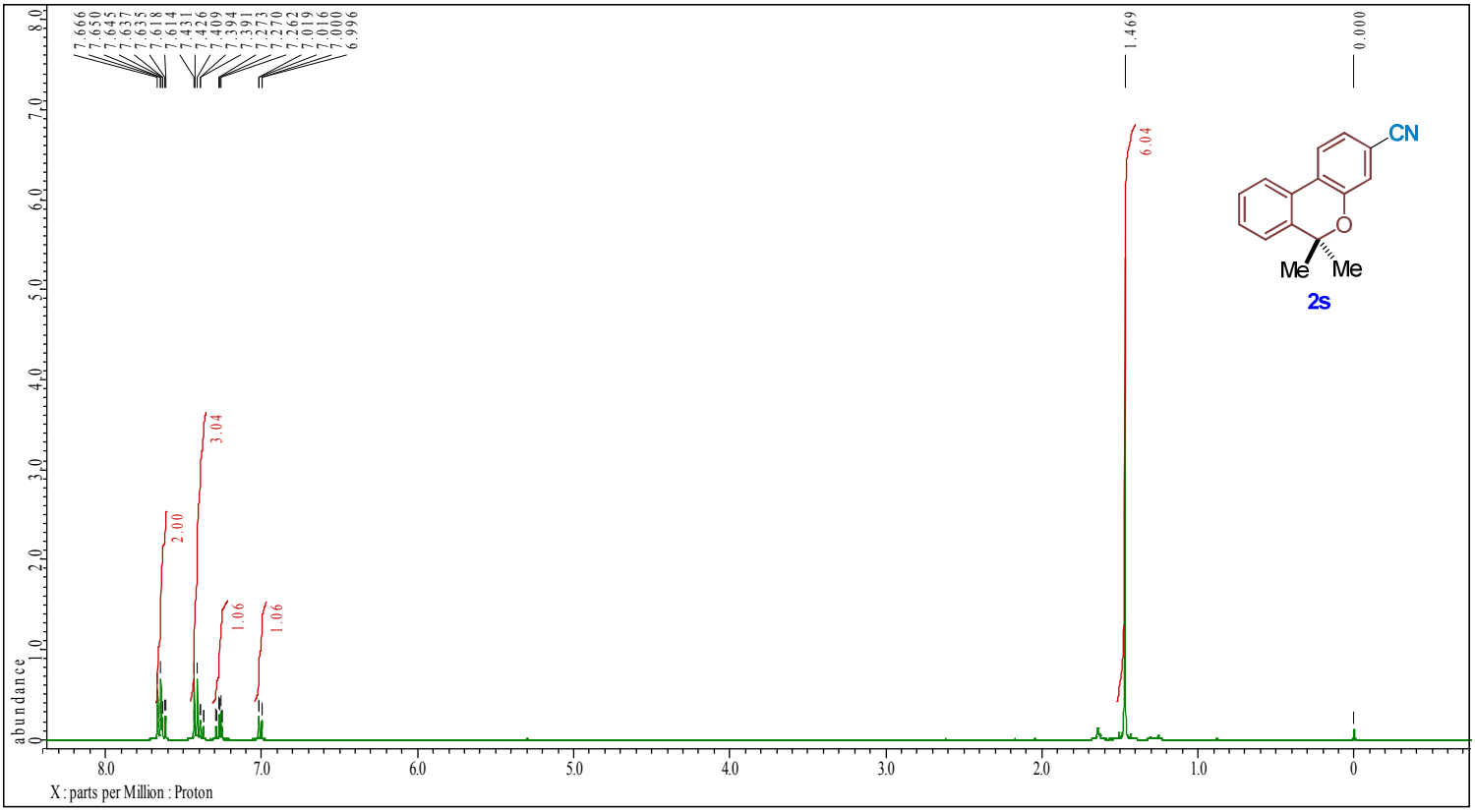
73.954
32.720
CF3
O
Me
Me
2r
(thousandths)
X : parts per Million : Carbon13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7.645
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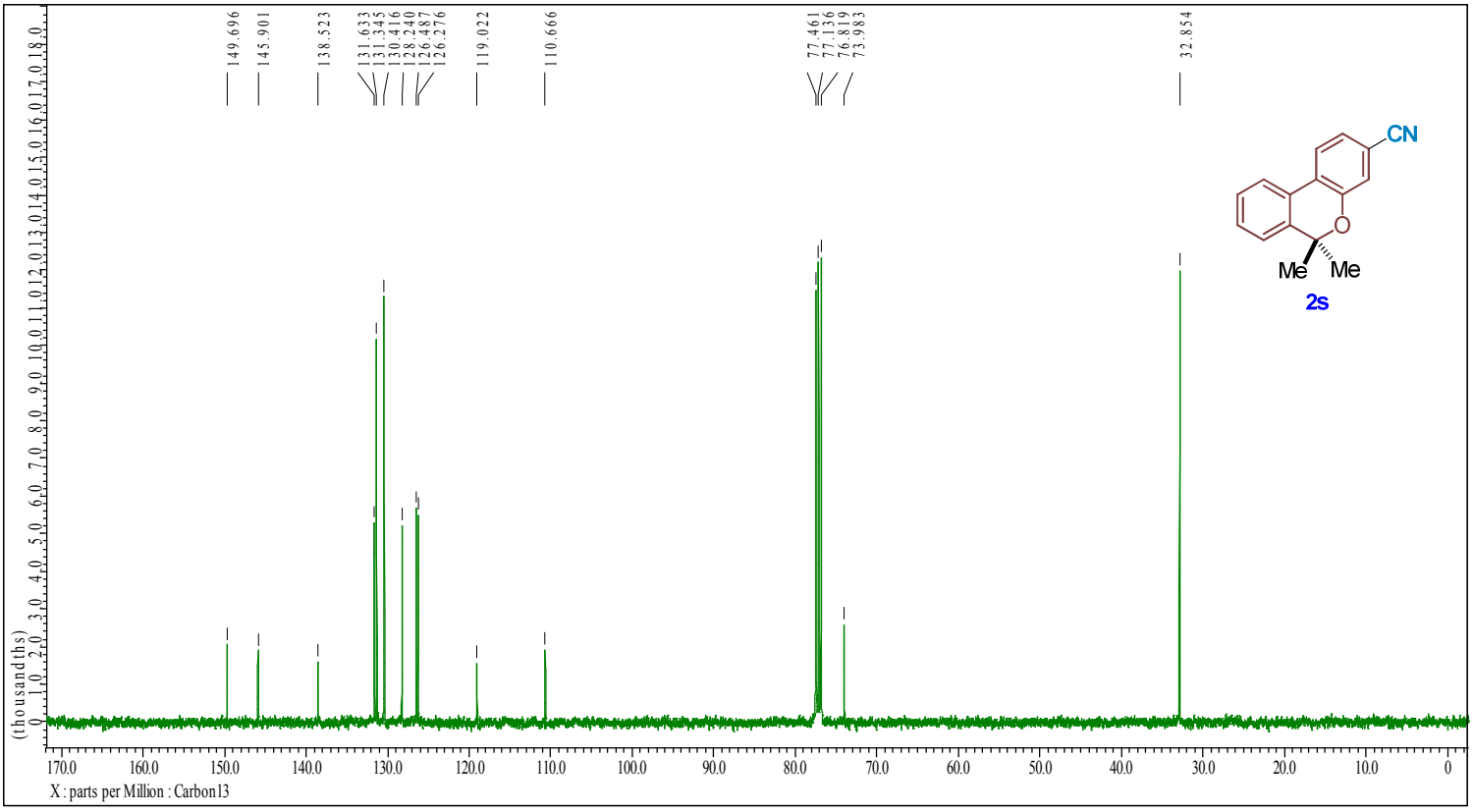
7.614
7.431
7.426
7.409
7.394
7.391
7.273
7.270
7.262
7.019
7.016
7.000
6.996
1.469
0.000
6.04
3.04
2.00
1.06
1.06
abundance
X : parts per Million : Proton
CN
Me
Me
2s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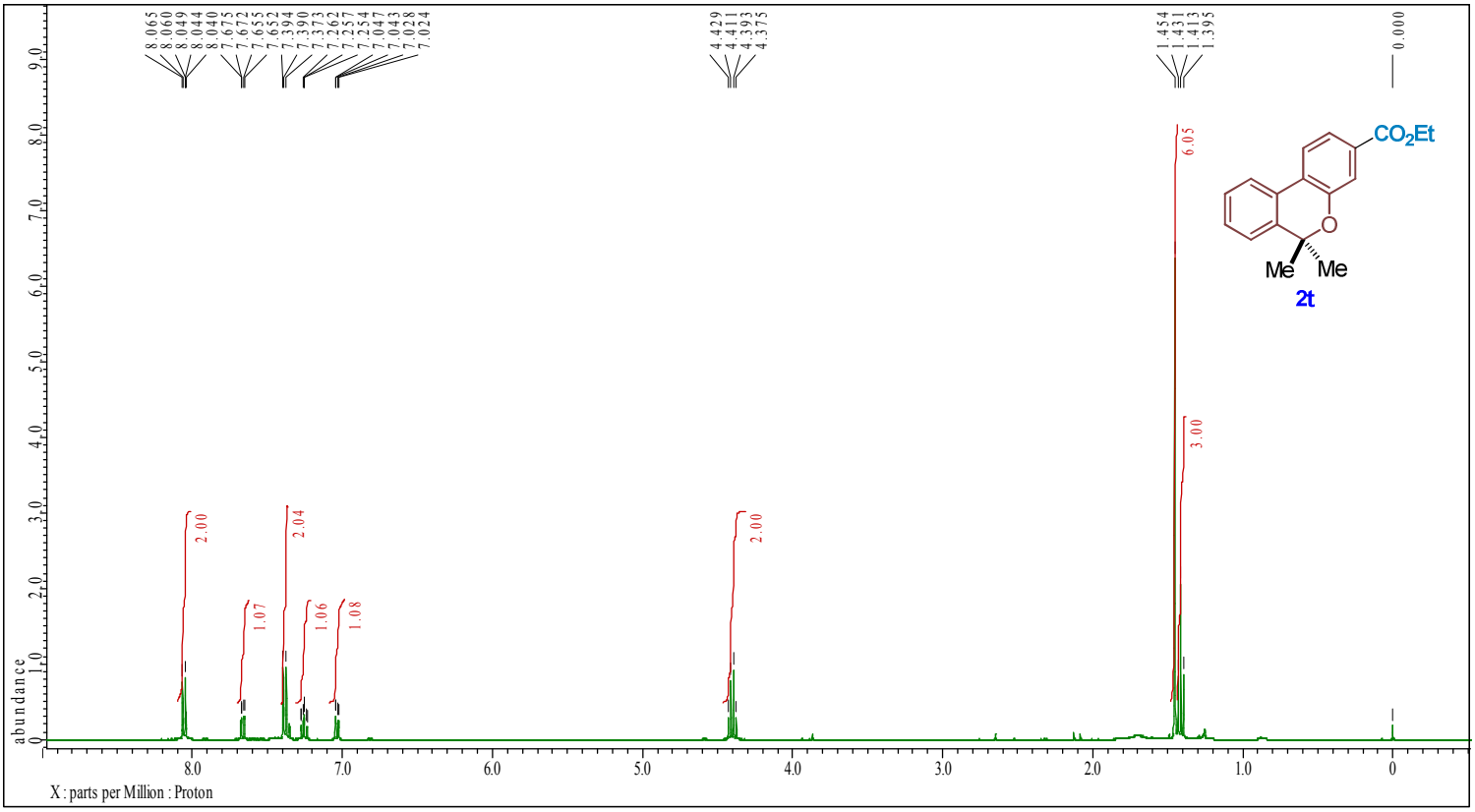
130.416
128.240
126.487
126.276
119.022
110.666
77.461
77.136
76.819
73.983
32.854
(thousandths)
X : parts per Million : Carbon13
CN
Me
Me
2s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8.044
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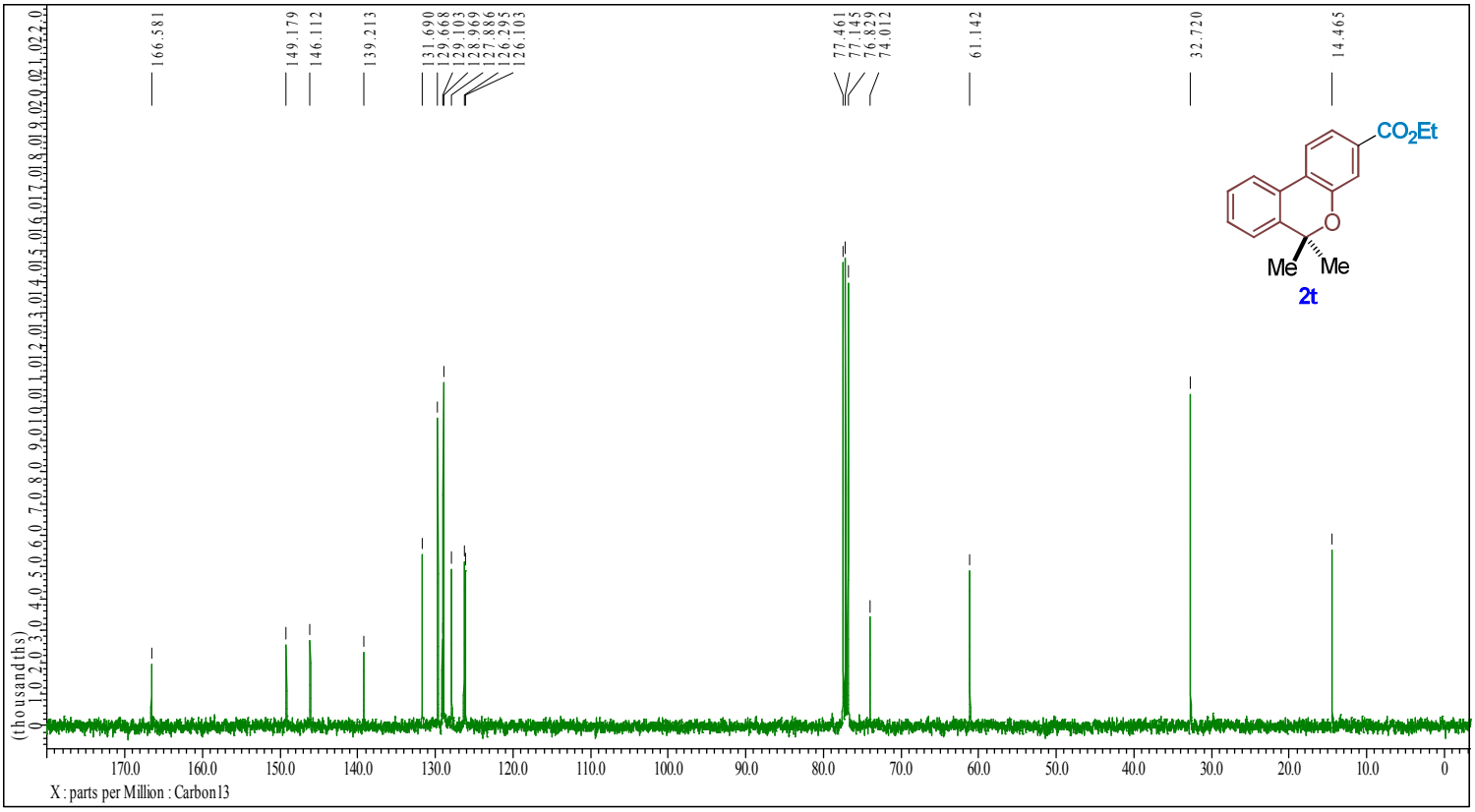
7.652
7.394
7.390
7.373
7.262
7.257
7.254
7.047
7.043
7.028
7.024
4.429
4.411
4.393
4.375
1.454
1.431
1.413
1.395
0.000
6.05
3.00
2.00
2.04
2.00
1.07
1.06
1.08
CO2Et
Me
Me
2t
abundance
X : parts per Million : Proton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128.969
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126.295
126.103
77.461
77.145
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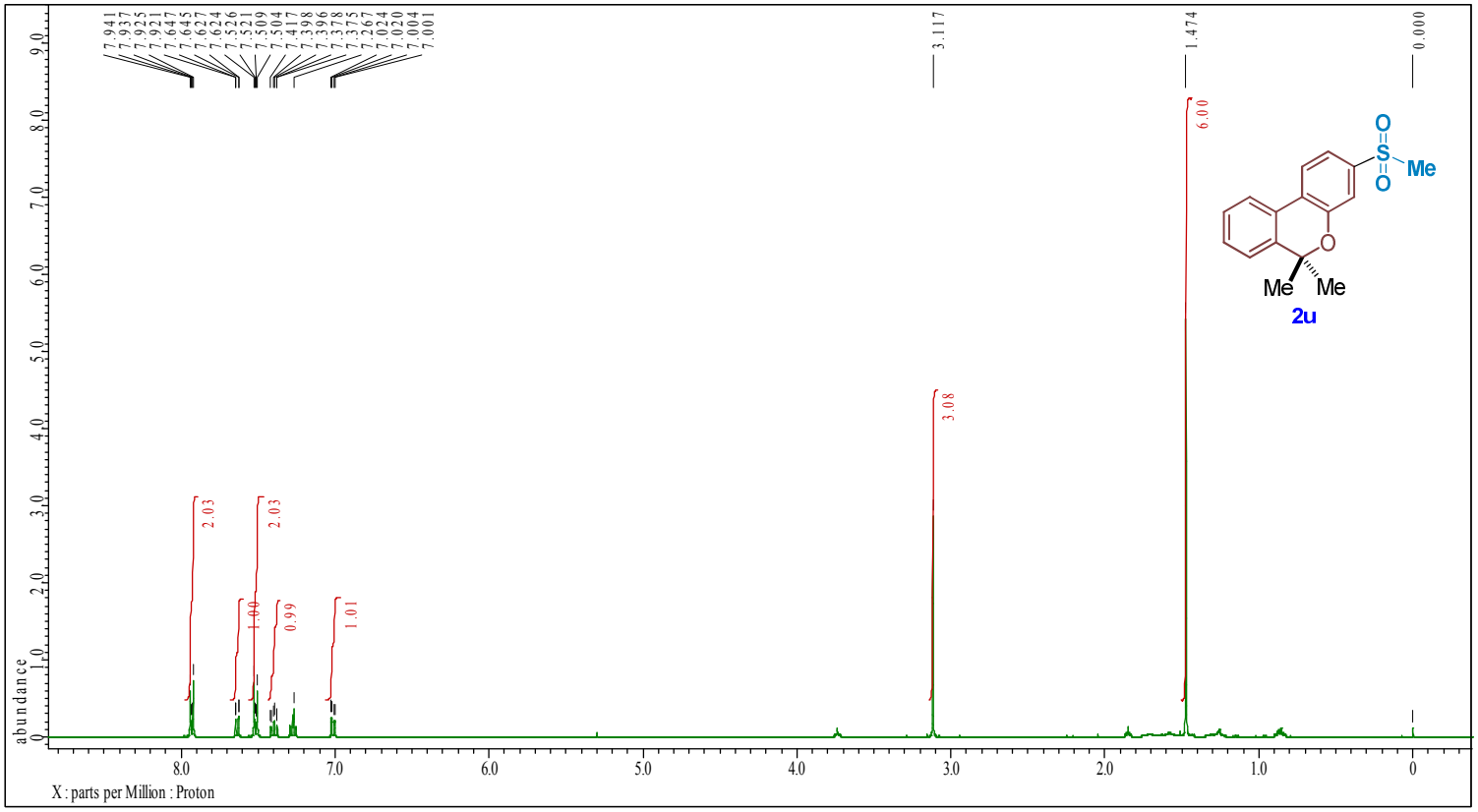
74.012
61.142
32.720
14.465
CO2Et
Me
Me
2t
(thousandths)
X : parts per Million : Carbon13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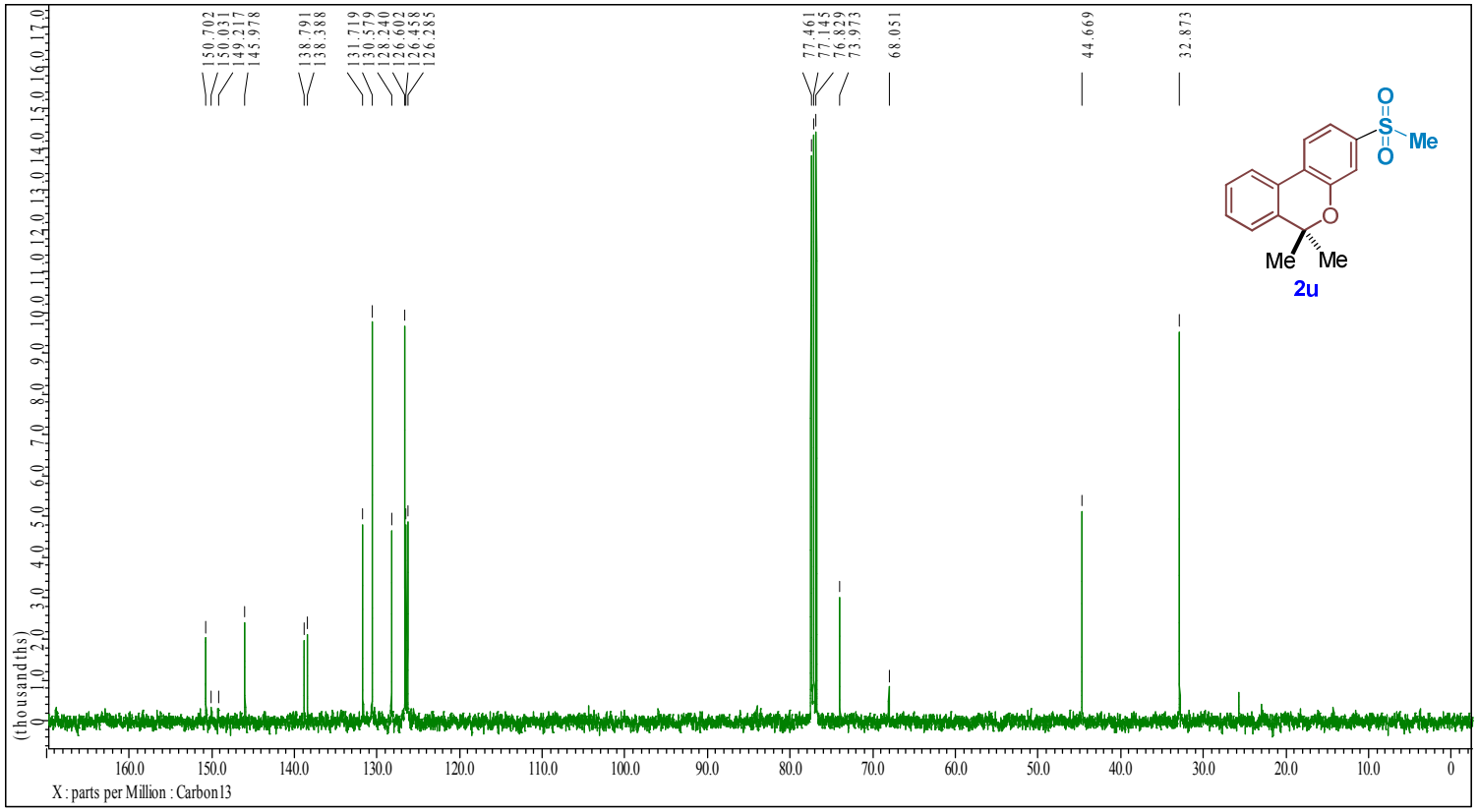
7.627
7.624
7.526
7.521
7.509
7.504
7.417
7.398
7.396
7.378
7.375
7.267
7.024
7.020
7.004
7.001
3.117
1.474
0.000
6.00
3.08
2.03
2.03
1.00
0.99
1.01
abundance
X : parts per Million : Proton
O
S
Me
O
Me
Me
2u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145.978
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131.719
130.579
128.240
126.602
126.458
126.285
77.461
77.145
76.829
73.973
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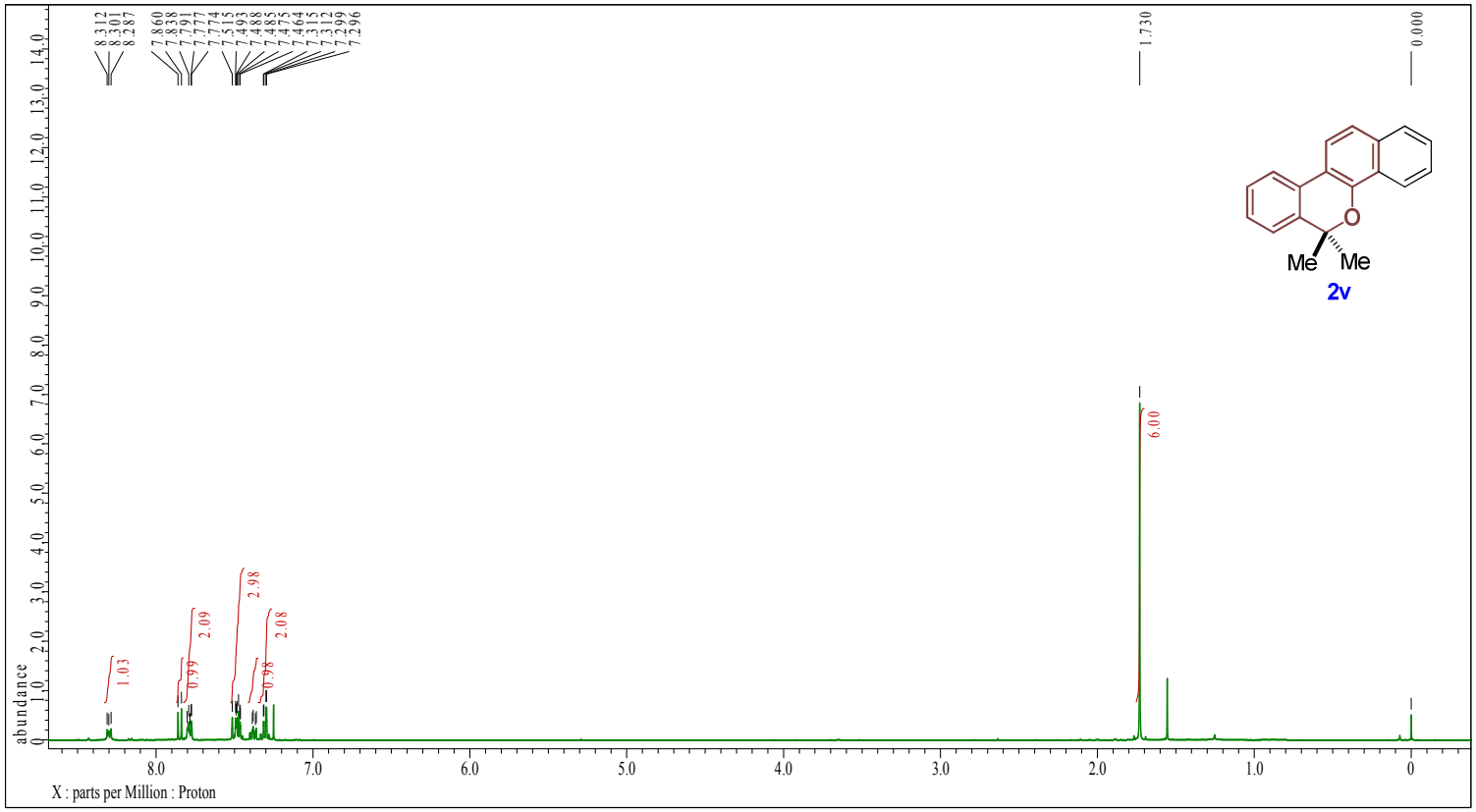
44.669
32.873
(thousandths)
X : parts per Million : Carbon13
O
S
Me
O
Me
Me
2u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7.791
7.777
7.774
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7.488
7.485
7.475
7.464
7.315
7.312
7.299
7.296
1.730
0.000
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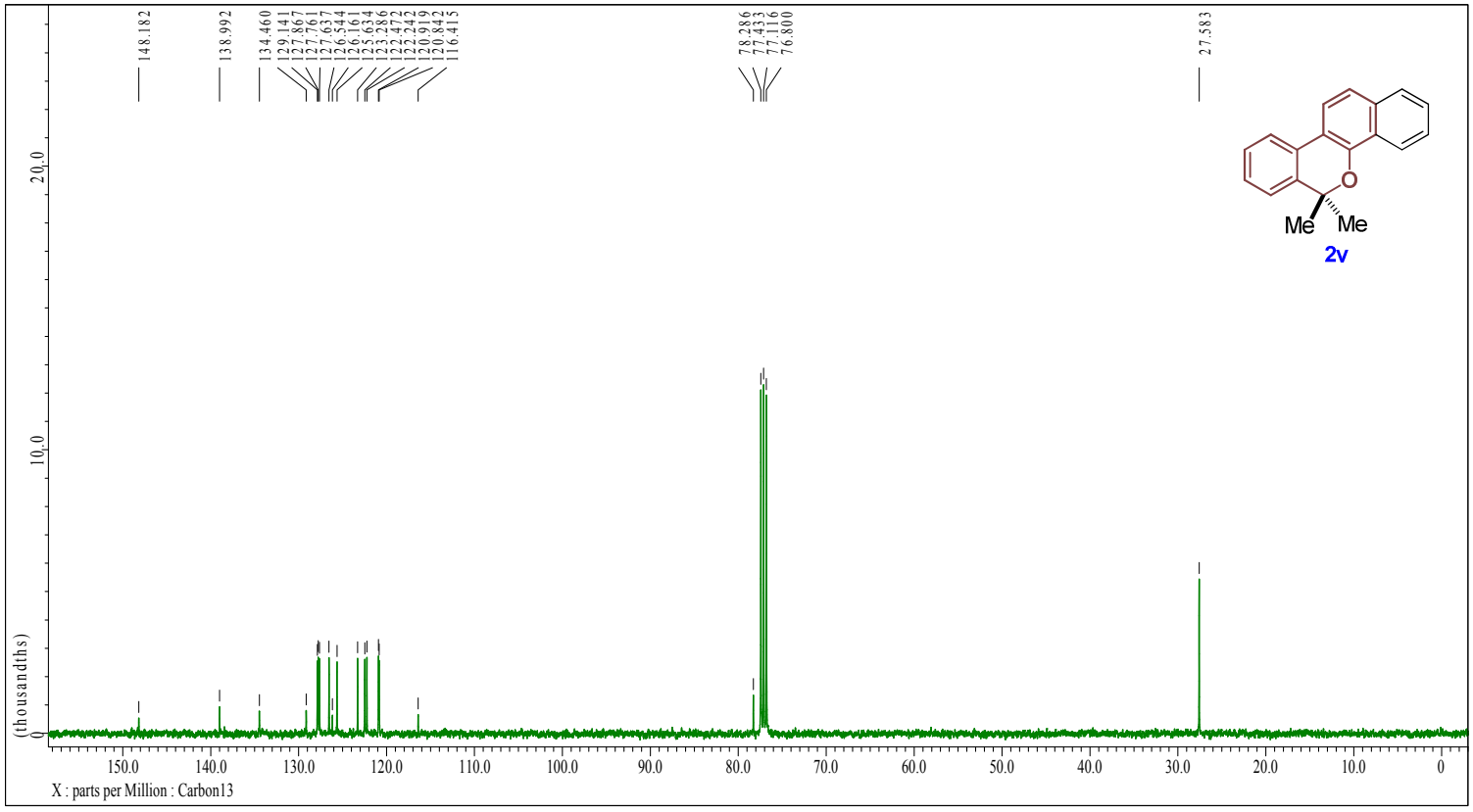
2.08
1.03
0.99
0.98
abundance
X : parts per Million : Proton
Me
Me
O
2v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127.637
126.544
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125.634
123.286
122.472
122.242
120.916
120.842
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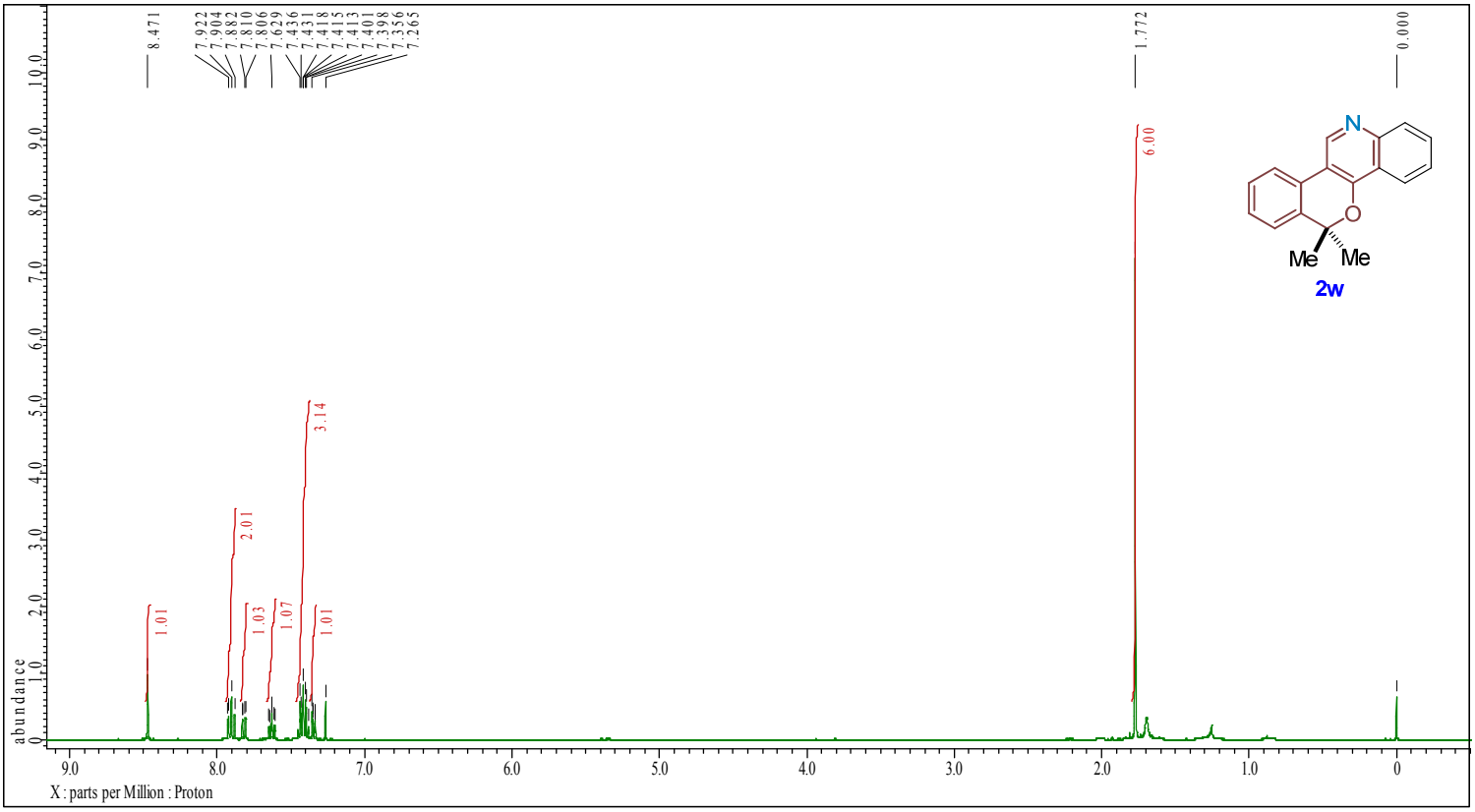
77.116
76.800
27.583
(thousandths)
X : parts per Million : Carbon13
Me
Me
O
2v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7.418
7.415
7.413
7.401
7.398
7.356
7.265
1.772
0.000
6.00
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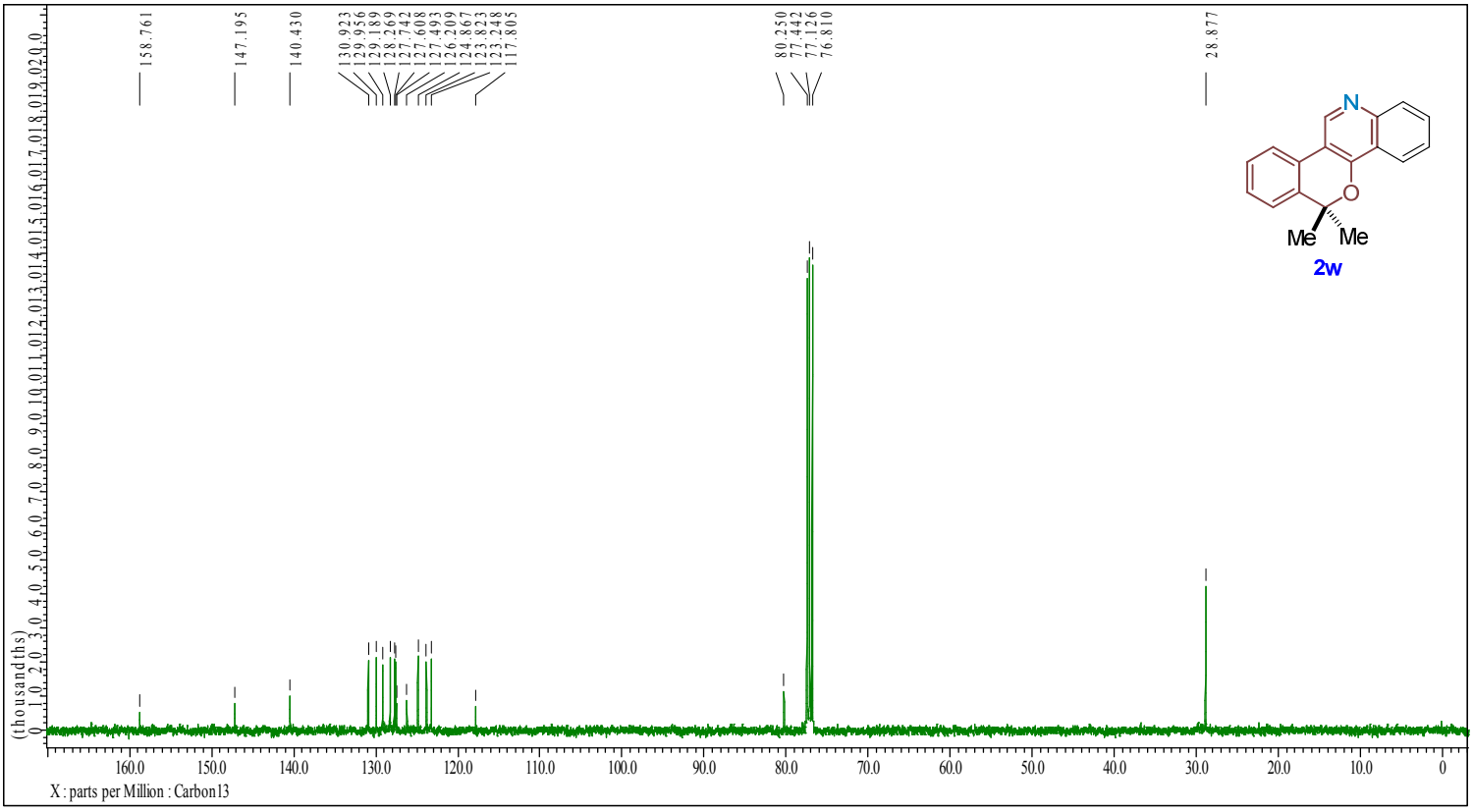
1.07
1.01
1.01
abundance
X : parts per Million : Proton
N
O
Me
Me
2w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129.956
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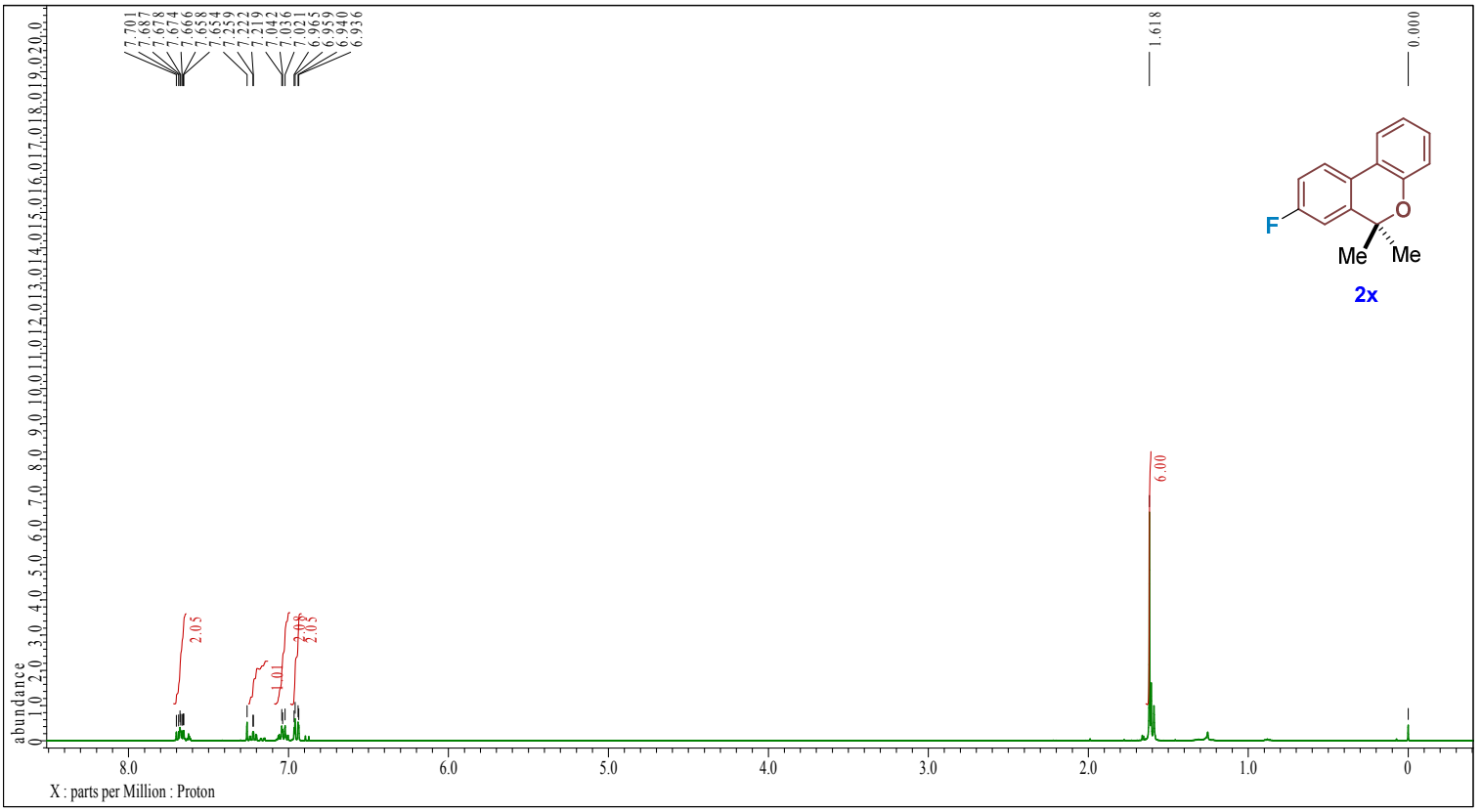
128.269
127.742
127.608
127.493
126.209
124.867
123.823
123.248
117.805
80.250
77.442
77.126
76.810
28.877
(thousandths)
X : parts per Million : Carbon13
N
O
Me
Me
2w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7.658
7.654
7.259
7.222
7.219
7.042
7.036
7.021
6.965
6.959
6.940
6.936
1.618
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O
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Me
2x
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2.05
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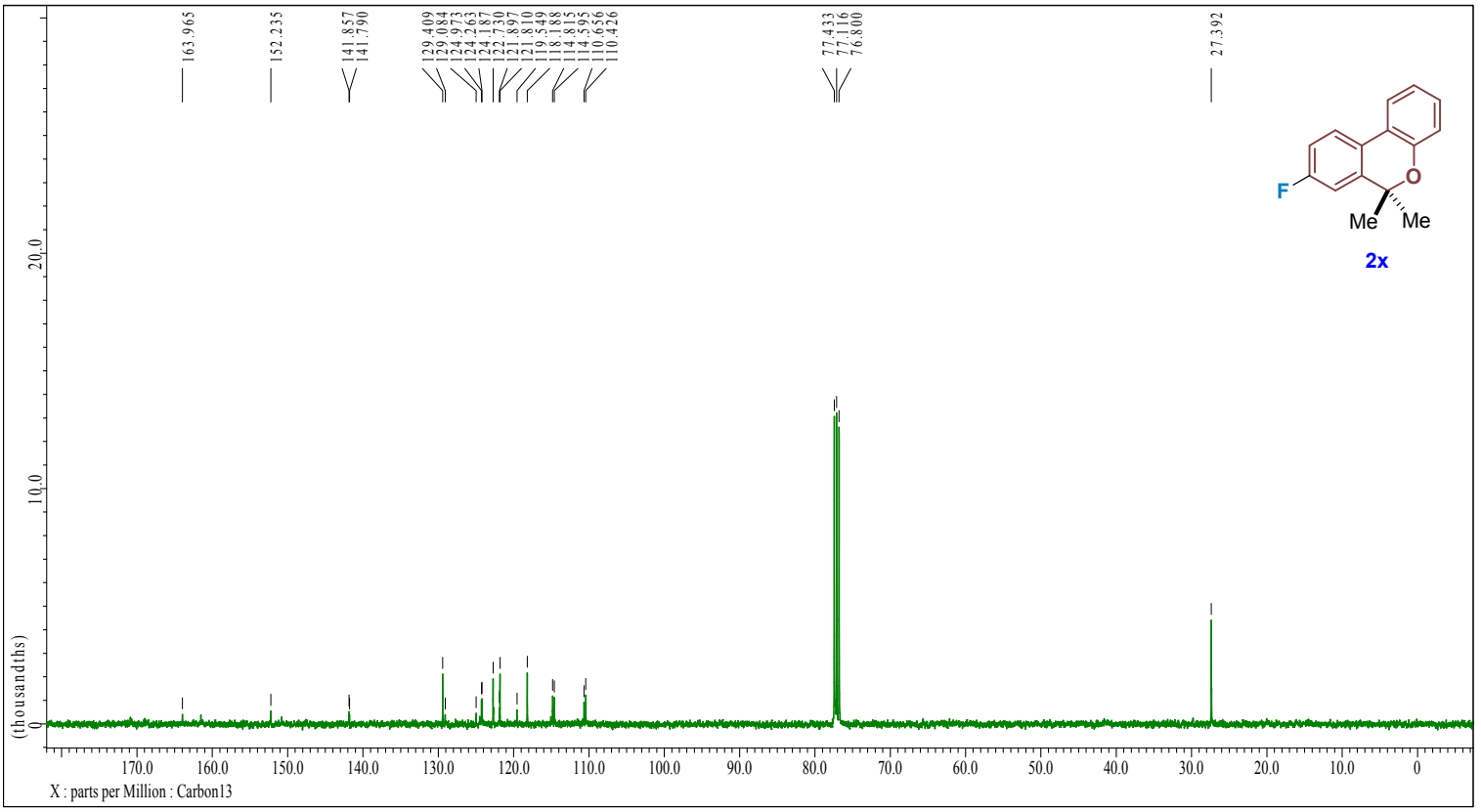
2.08
2.05
abundance
X : parts per Million : Proton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141.790
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129.084
124.973
124.263
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122.730
121.897
121.810
119.549
118.188
114.815
114.595
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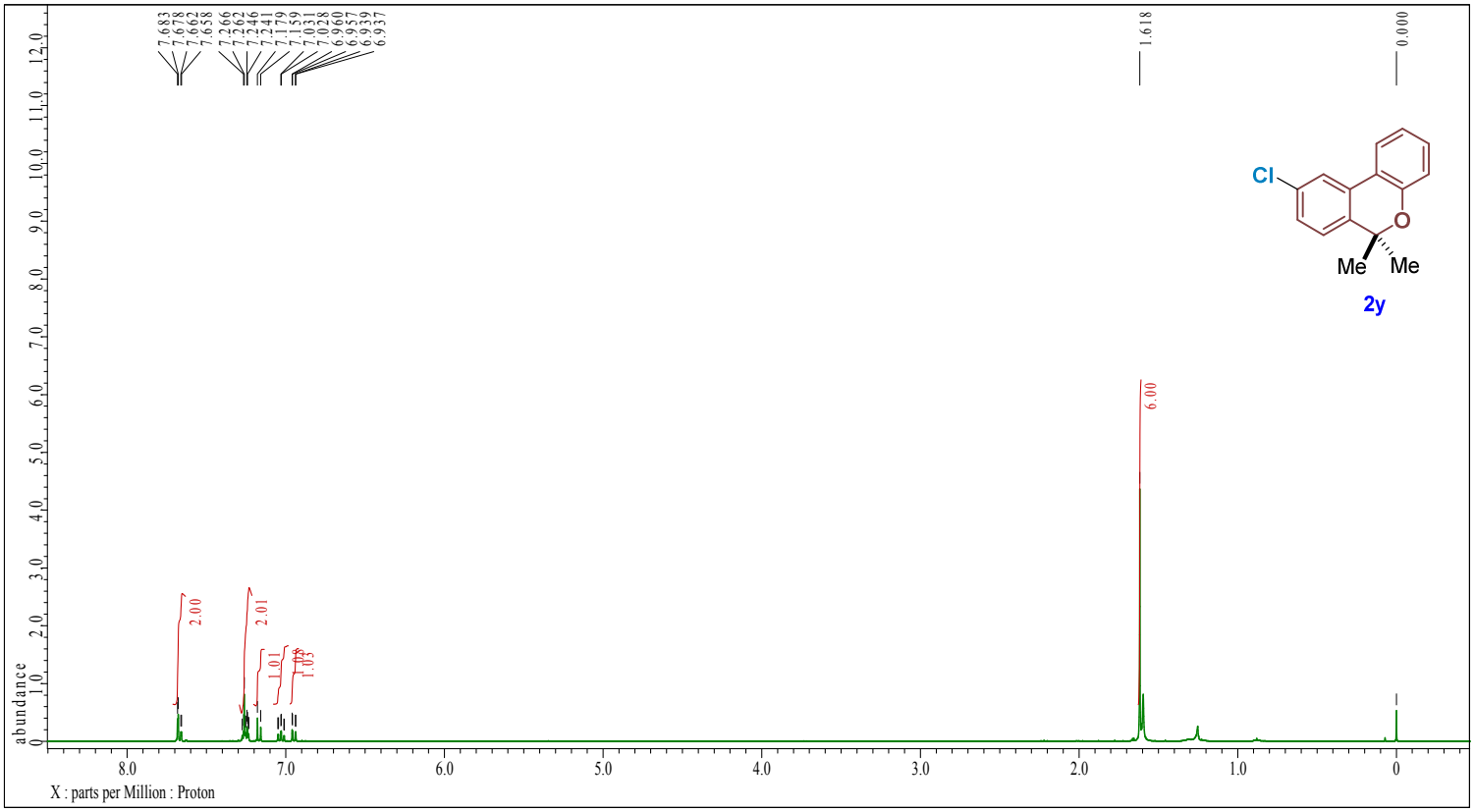
77.116
76.800
27.392
F
O
Me
Me
2x
(thousandths)
X : parts per Million : Carbon13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7.266
7.262
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7.241
7.179
7.159
7.031
7.028
6.960
6.957
6.939
6.937
1.618
0.000
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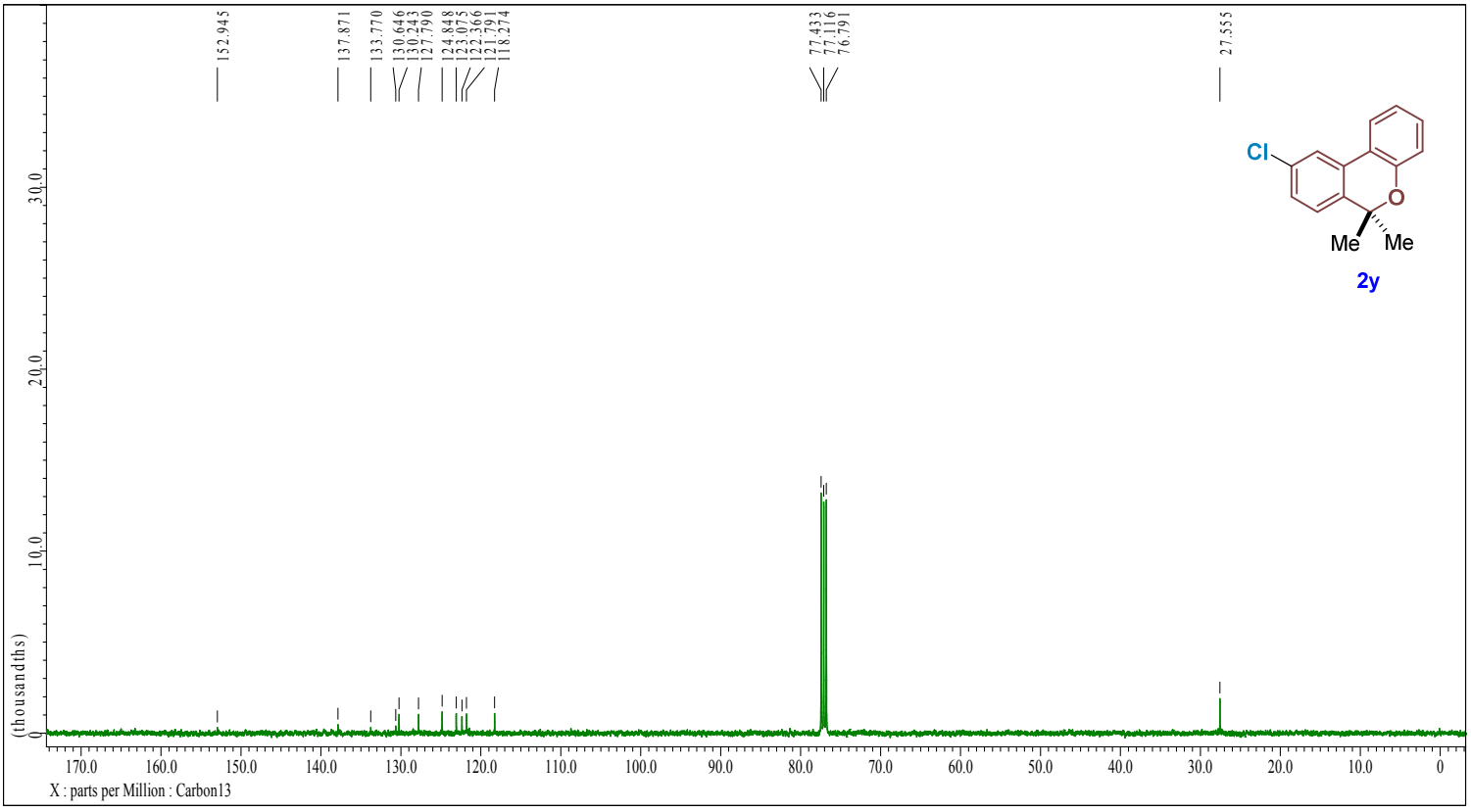
O
Me
Me
2y
6.00
2.00
2.01
1.01
1.03
abundance
X : parts per Million : Proton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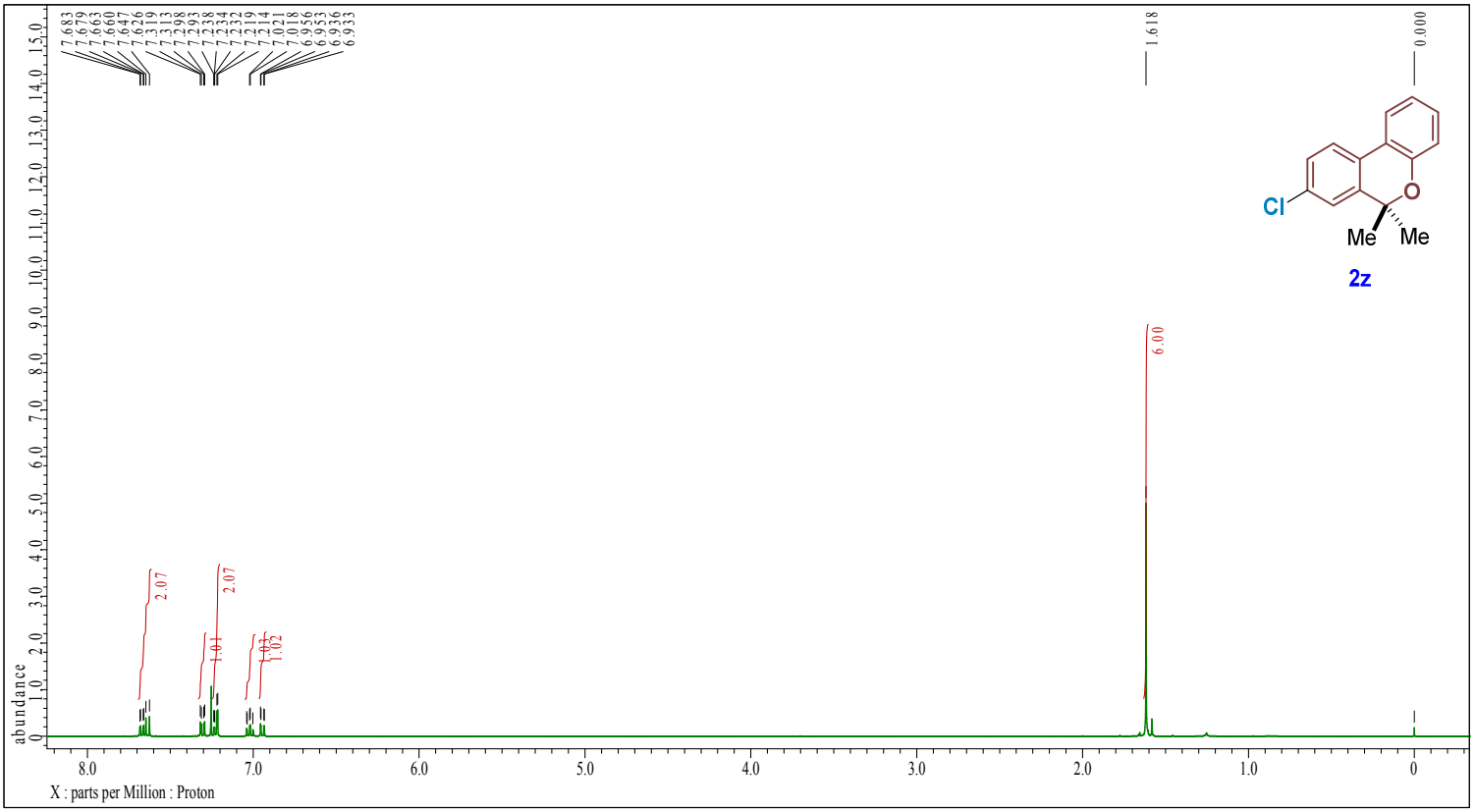
76.791
27.555
Cl
O
Me
Me
2y
(thousandths)
X : parts per Million : Carbon13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7.232
7.219
7.214
7.021
7.018
6.956
6.953
6.936
6.933
1.618
0.000
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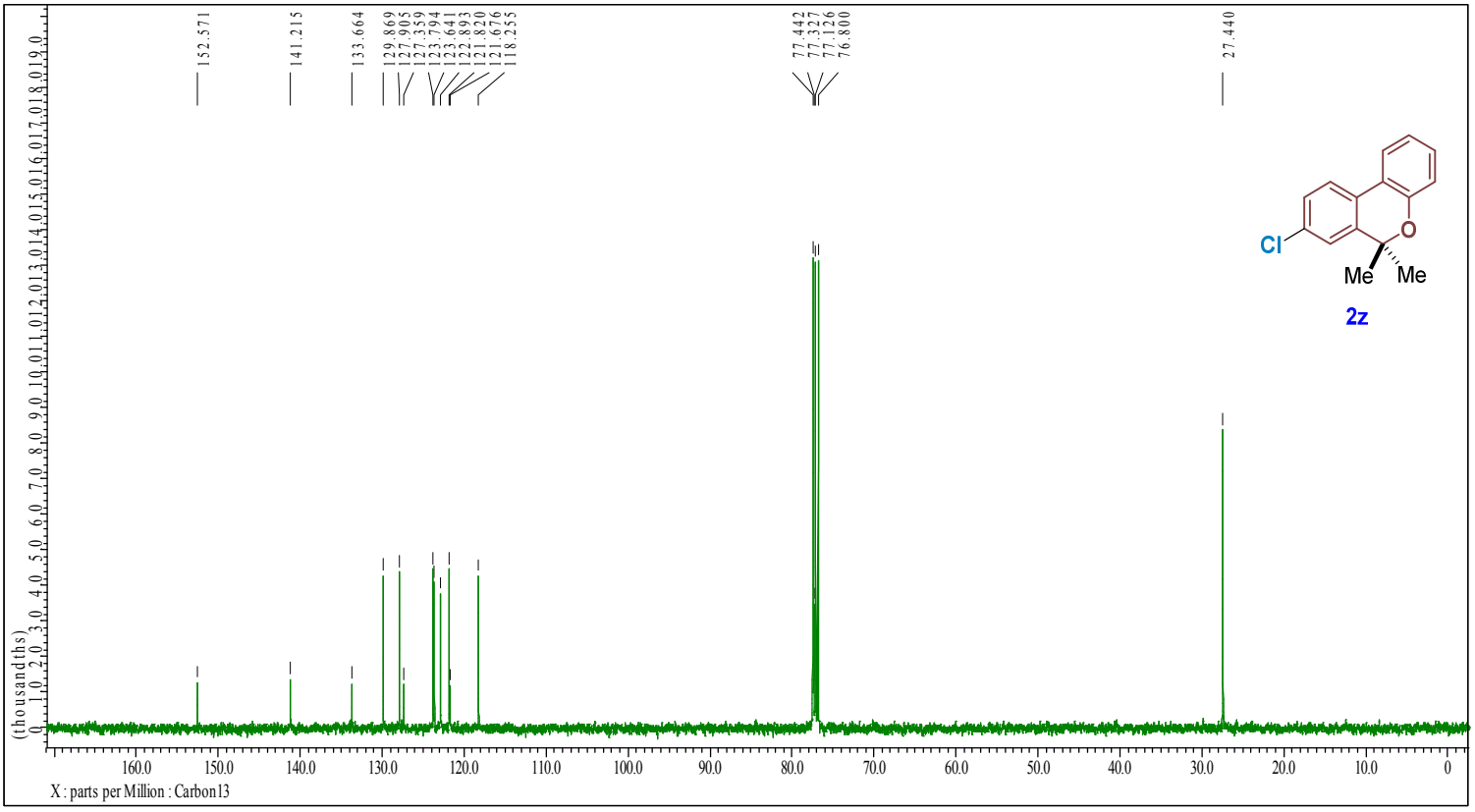
2.07
2.07
1.01
1.02
1.02
abundance
X : parts per Million : Proton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129.869
127.905
127.399
123.794
123.641
122.893
121.820
121.676
118.255
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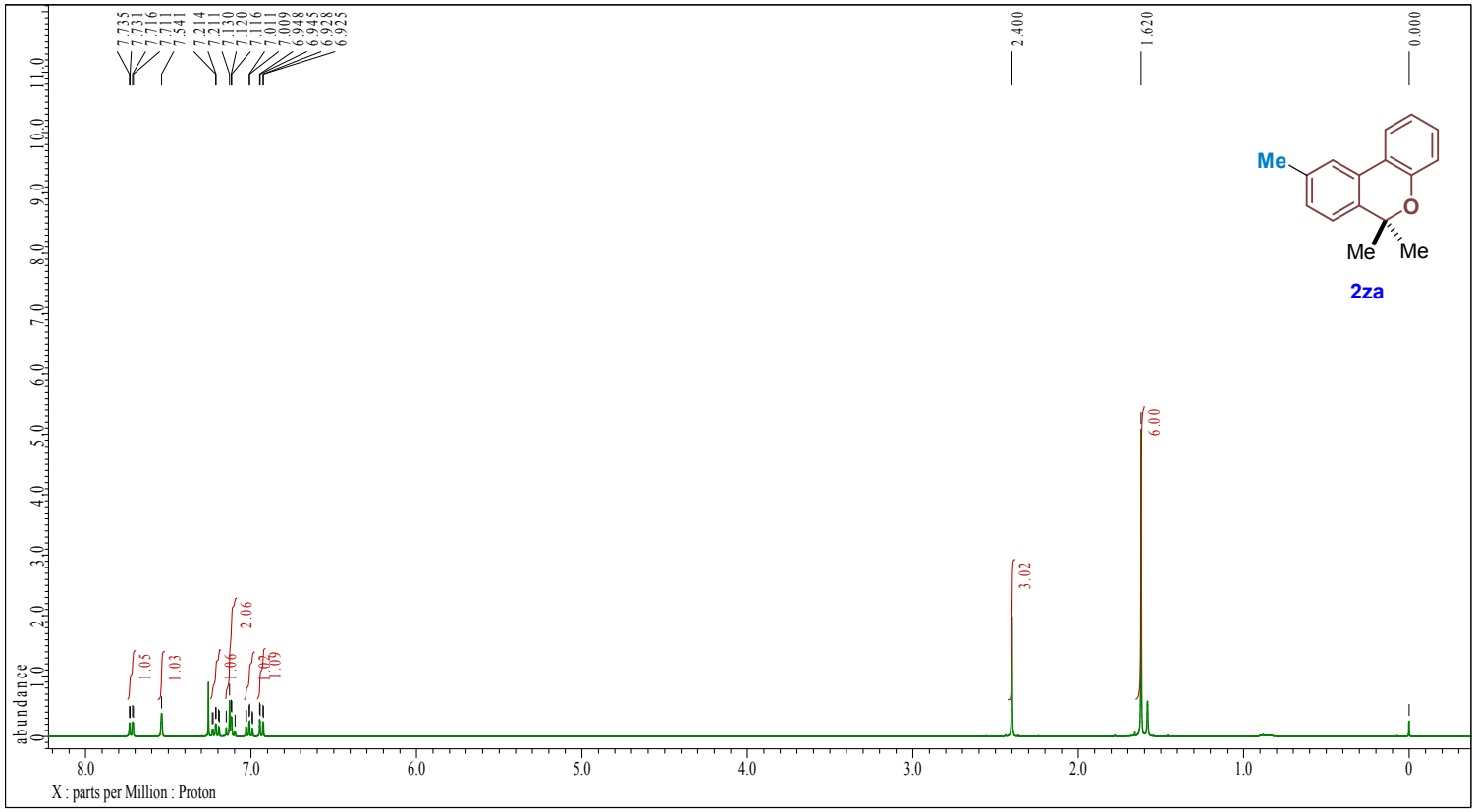
77.327
77.126
76.800
27.440
Cl
O
Me
Me
2z
(thousandths)
X : parts per Million : Carbon13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7.130
7.120
7.116
7.011
7.009
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6.945
6.928
6.925
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1.620
0.000
Me
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Me
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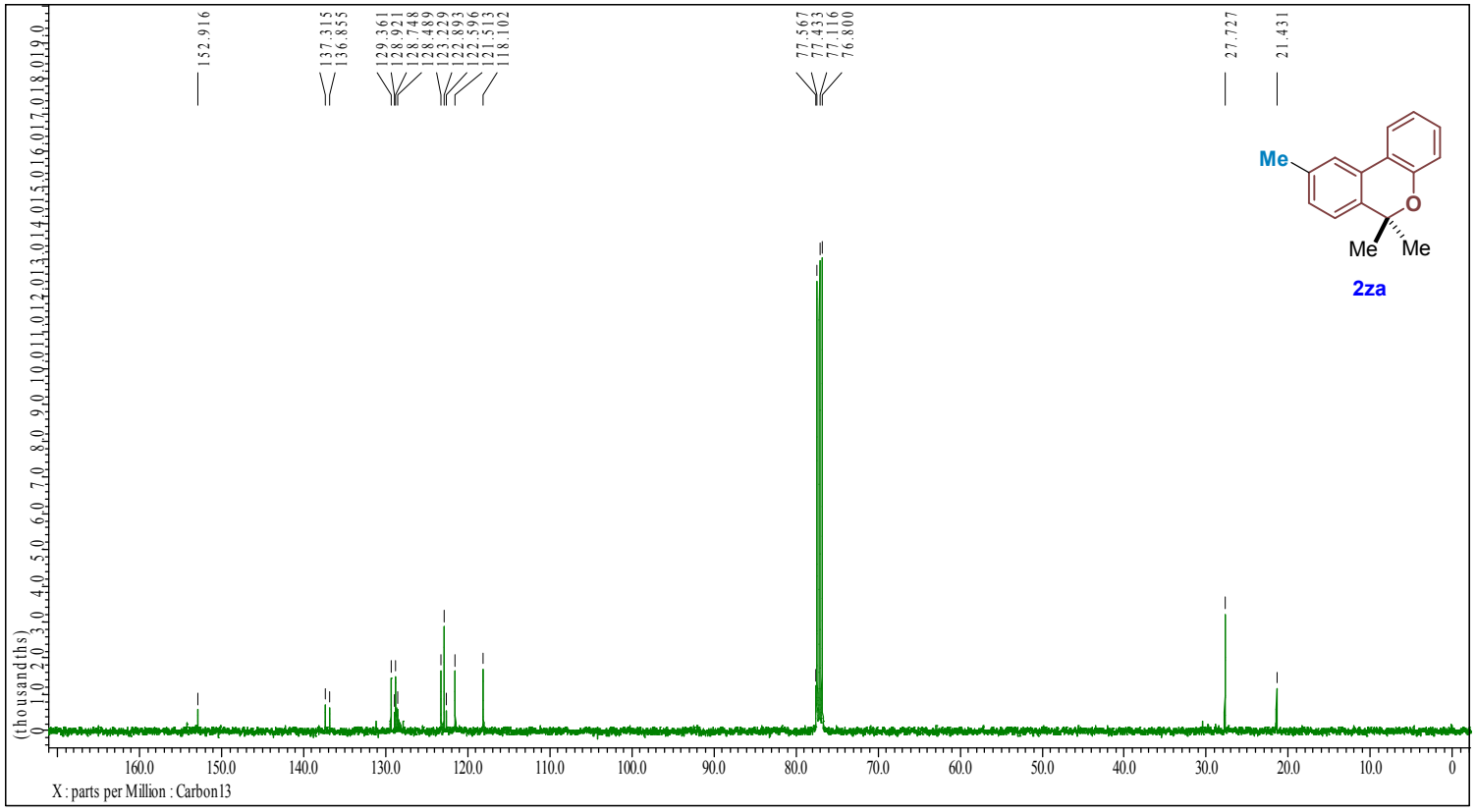
3.02
2.06
1.05
1.03
1.06
1.09
abundance
X : parts per Million : Proton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Me
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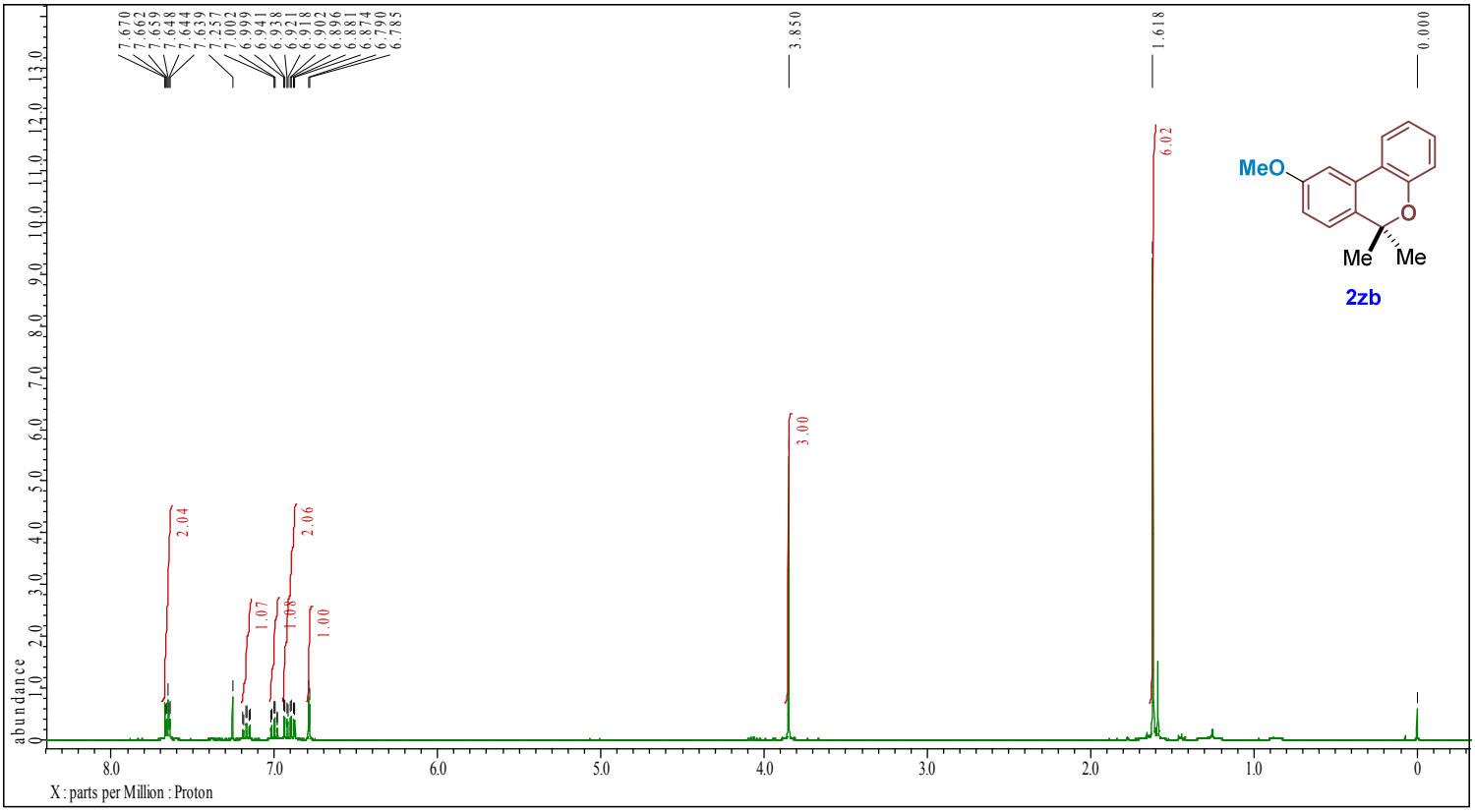
Me
Me
2za
(thousandths)
X : parts per Million : Carbon13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6.918
6.902
6.896
6.881
6.874
6.790
6.785
3.850
1.618
0.000
6.02
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1.00
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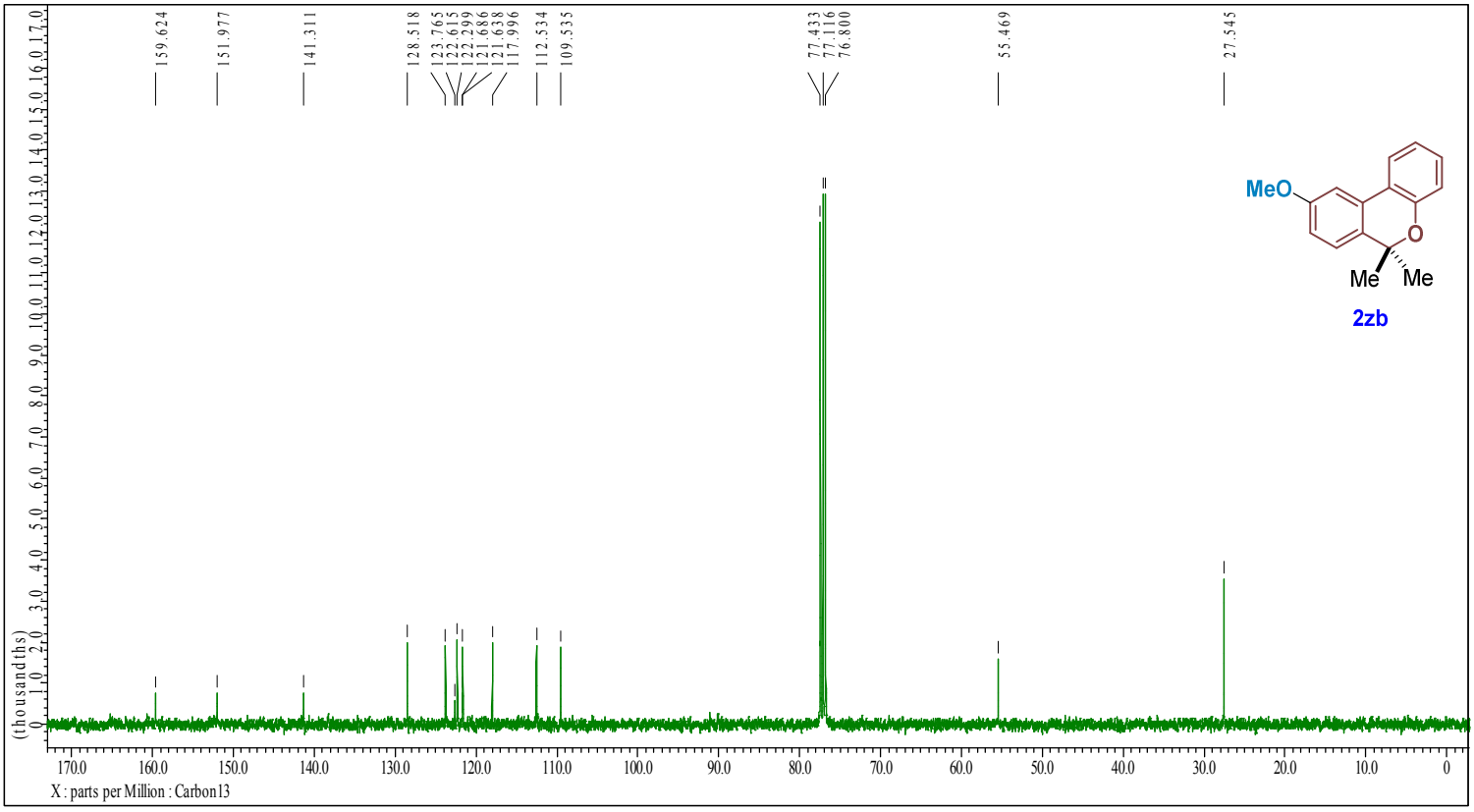
Me
Me
2zb
abundance
X : parts per Million : Proton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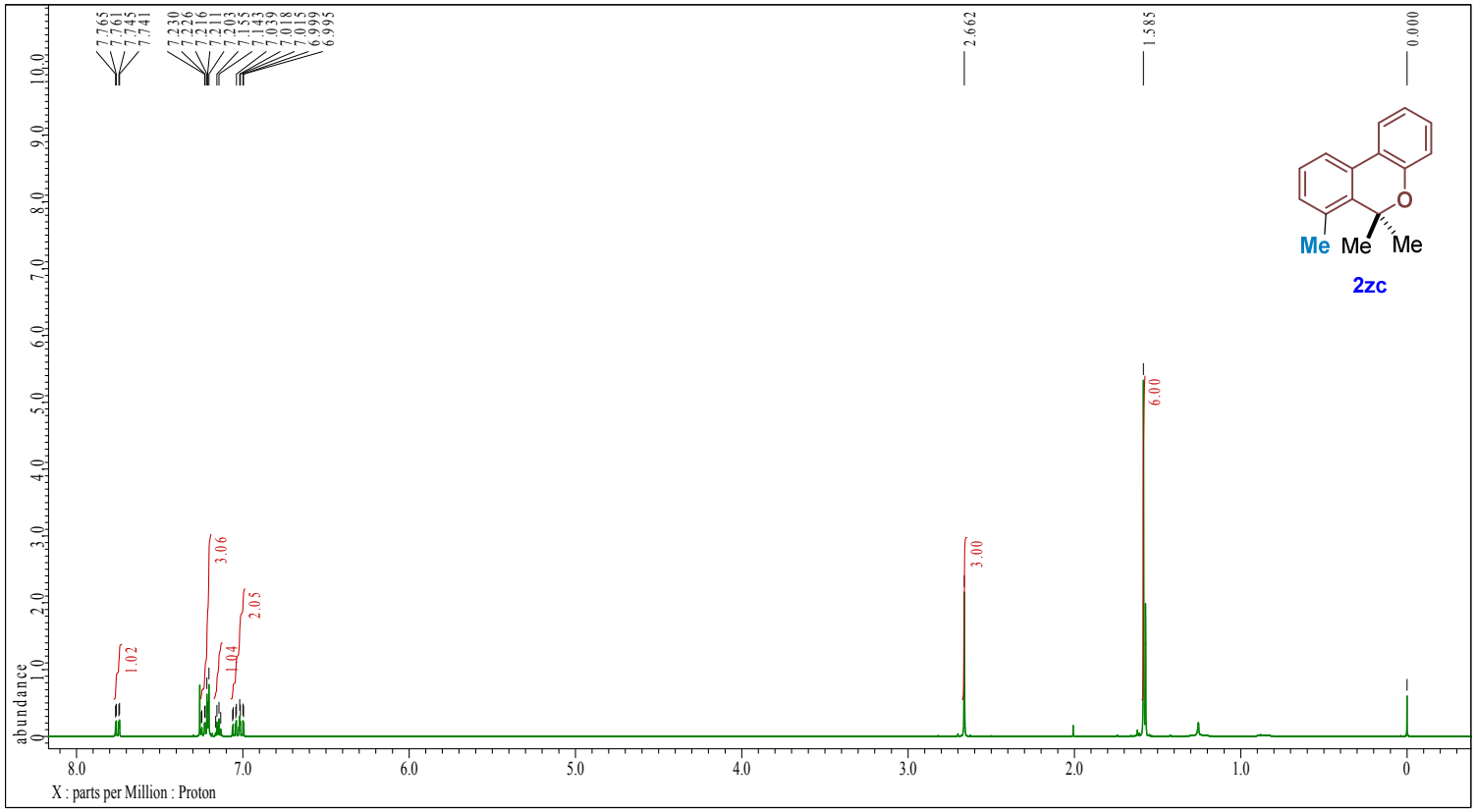
Me
Me
2zb
(thousandths)
X : parts per Million : Carbon13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7.211
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7.155
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7.039
7.018
7.015
6.999
6.995
2.662
1.585
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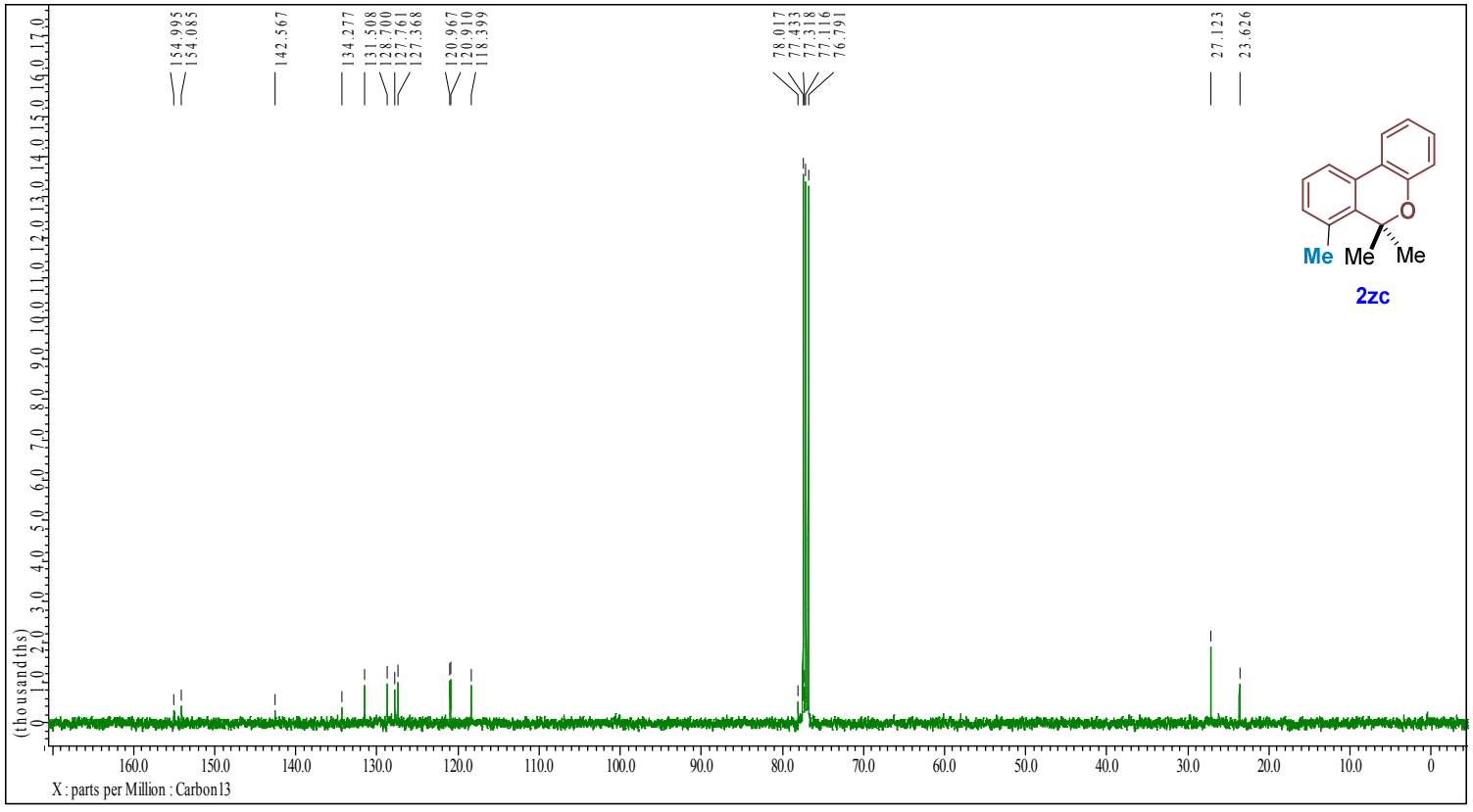
6.00
abundance
X : parts per Million : Proton
Me Me Me
2zc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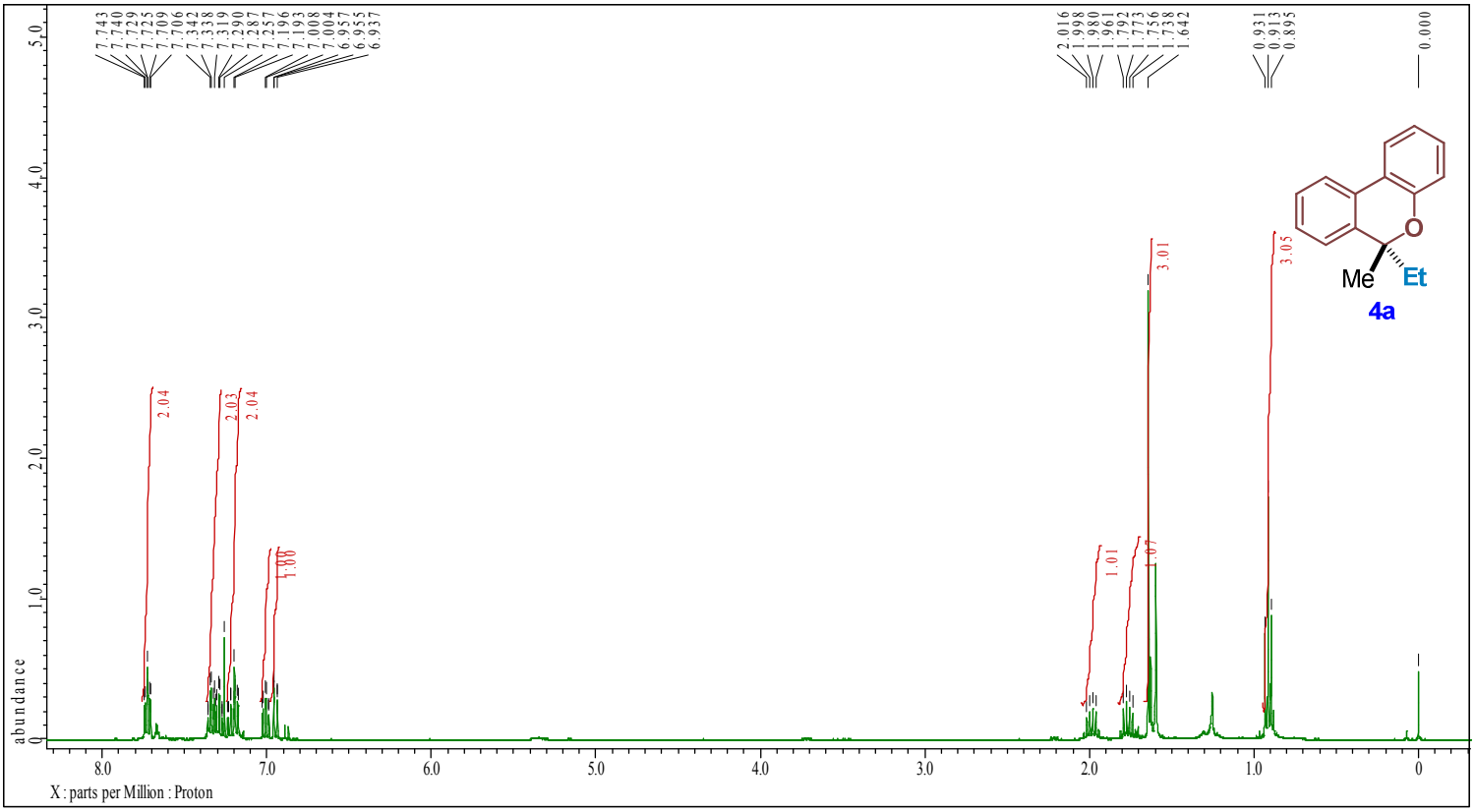
23.626
(thousandths)
X : parts per Million : Carbon13
Me Me Me
2zc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7.196
7.193
7.008
7.004
6.957
6.955
6.937
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1.998
1.980
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1.773
1.756
1.738
1.642
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0.895
0.000
2.04
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1.01
1.07
3.01
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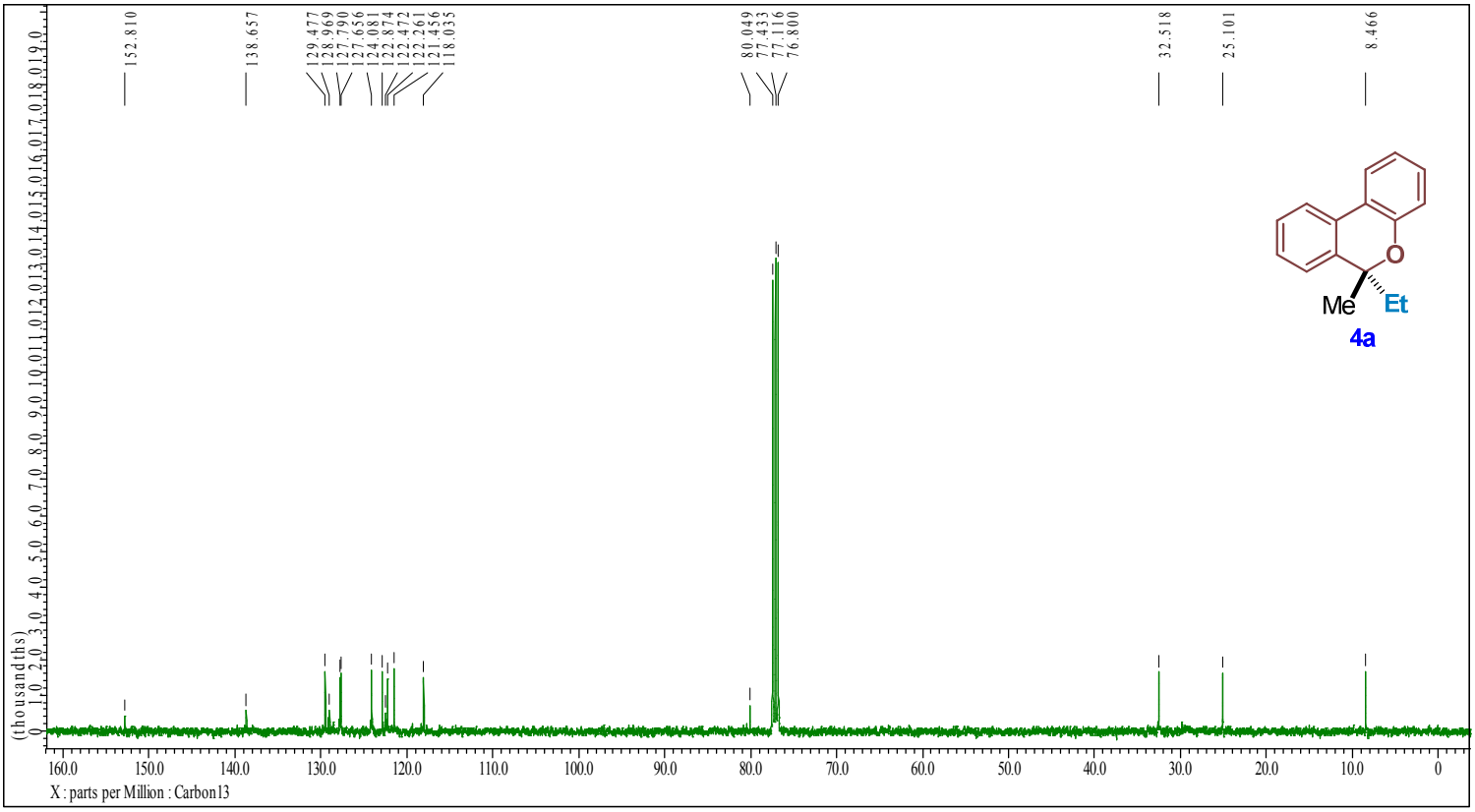
Me
Et
4a
abundance
X : parts per Million : Proton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122.874
122.472
122.261
121.456
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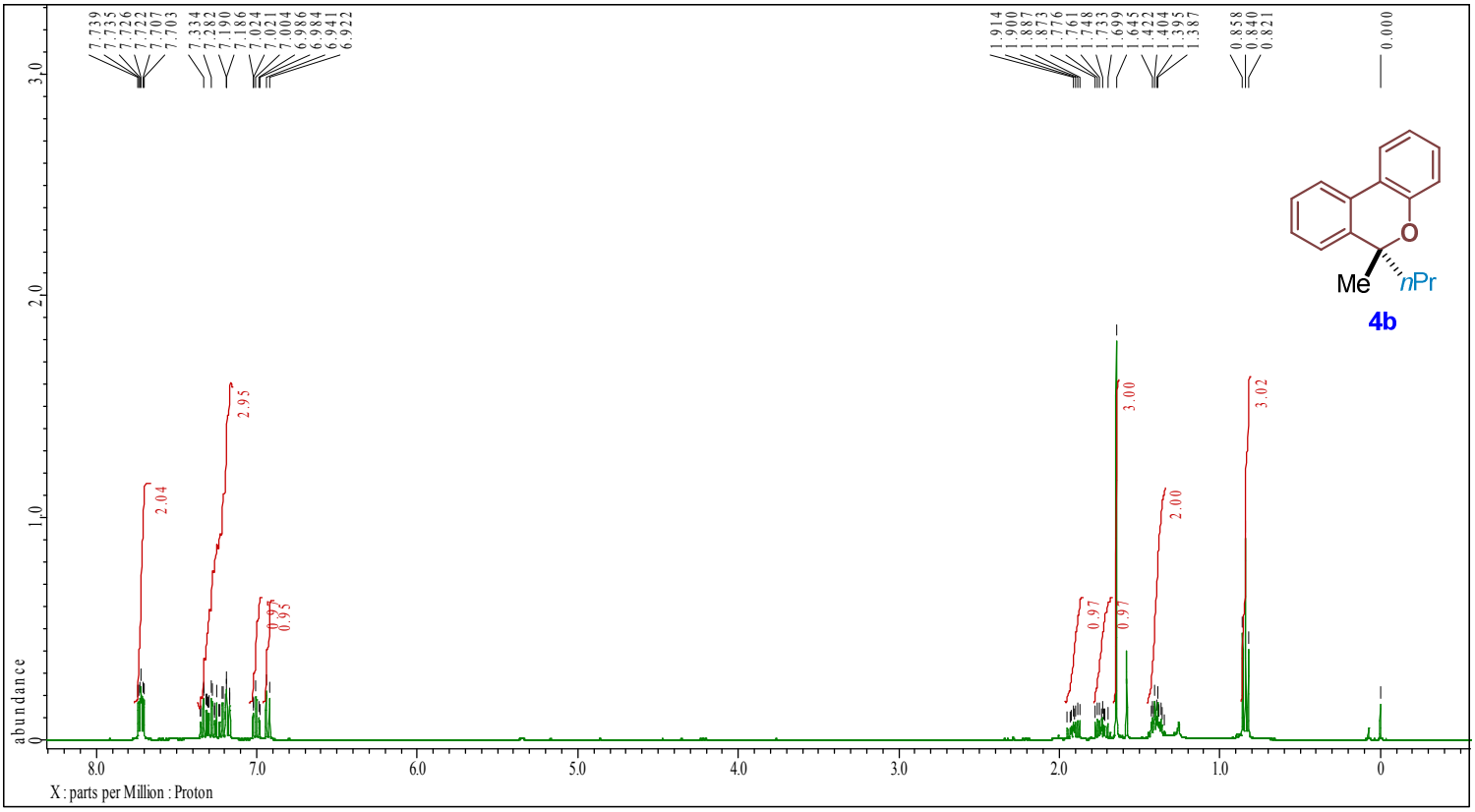
76.800
32.518
25.101
8.466
Me
Et
4a
(thousandths)
X : parts per Million : Carbon13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7.186
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7.021
7.004
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6.984
6.941
6.922
1.914
1.900
1.887
1.873
1.776
1.761
1.748
1.733
1.699
1.645
1.422
1.404
1.395
1.387
0.858
0.840
0.821
0.000
2.04
2.95
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0.97
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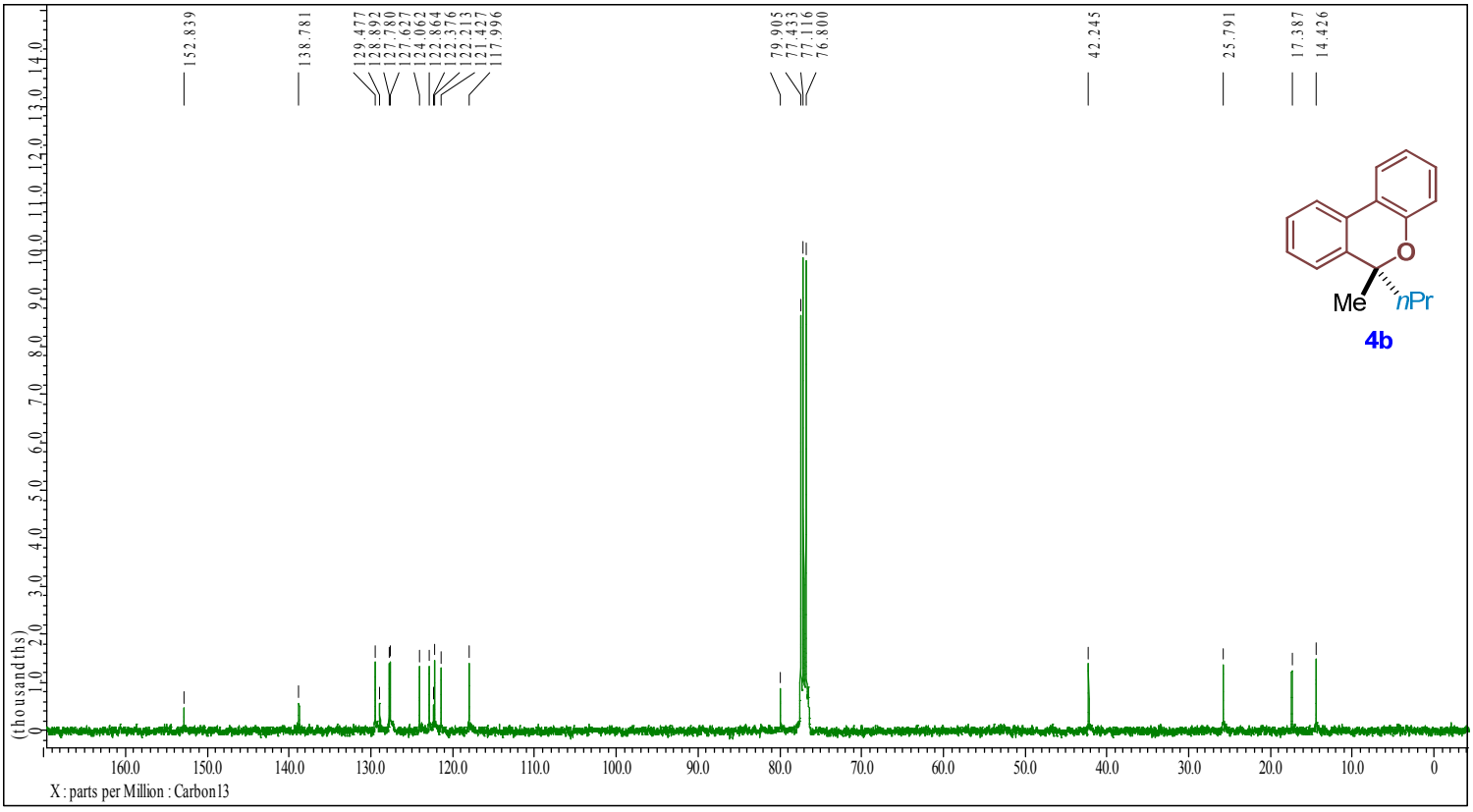
3.02
Me
nPr
4b
abundance
X : parts per Million : Proton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nPr
4b
(thousandths)
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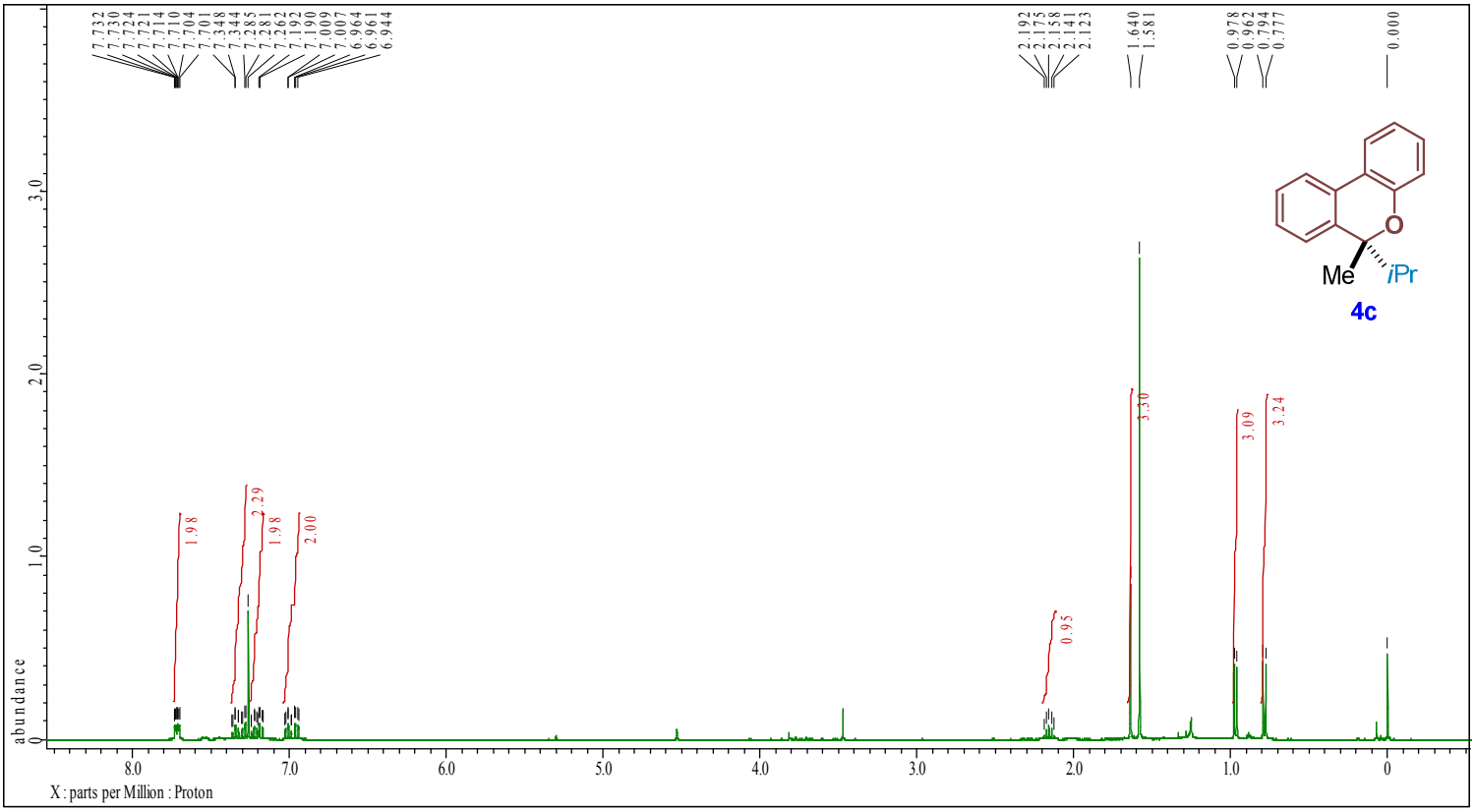
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7.344
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7.281
7.262
7.192
7.190
7.009
7.007
6.964
6.961
6.944
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2.141
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0.777
0.000
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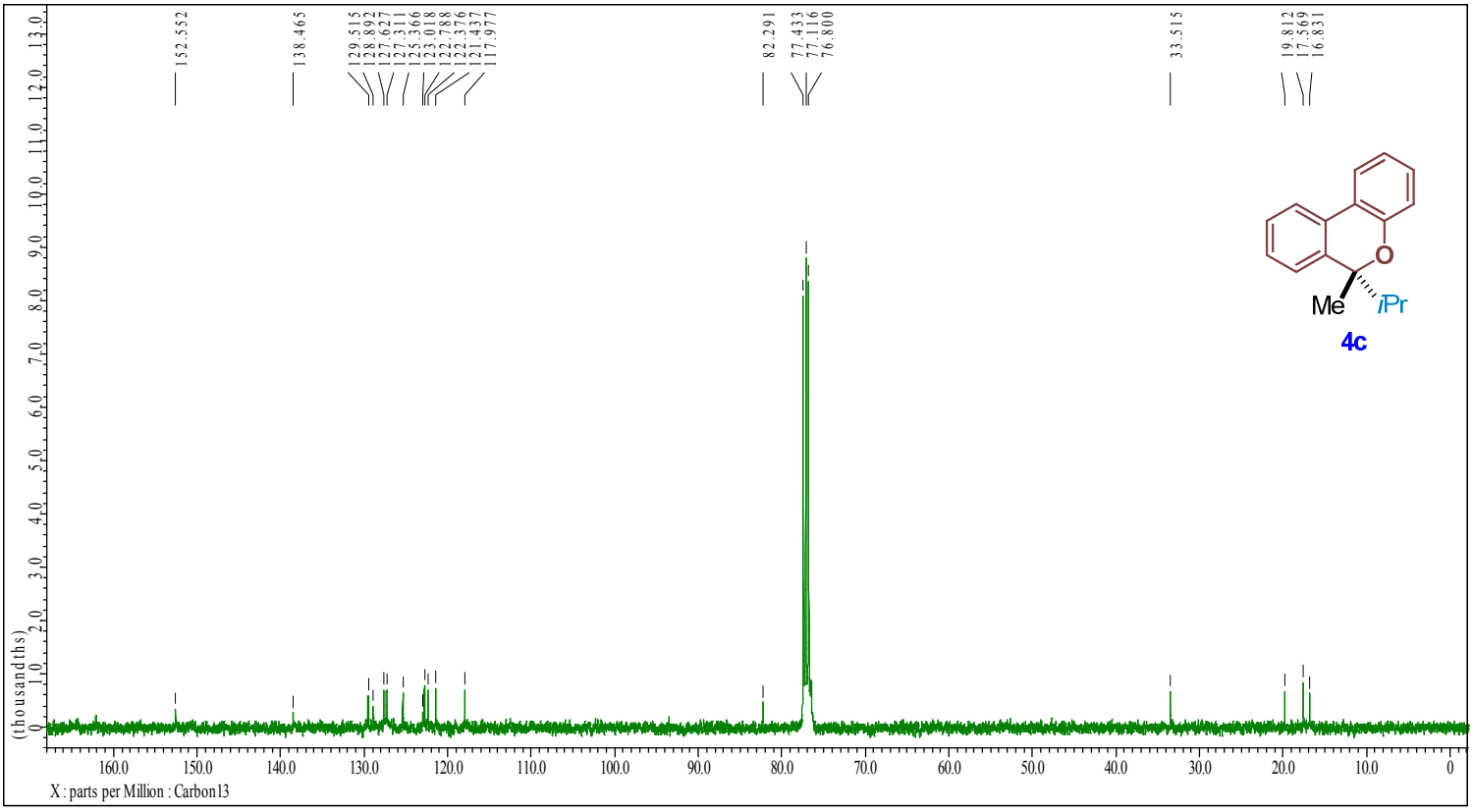
3.09
3.24
abundance
X : parts per Million : Proton
Me
iPr
4c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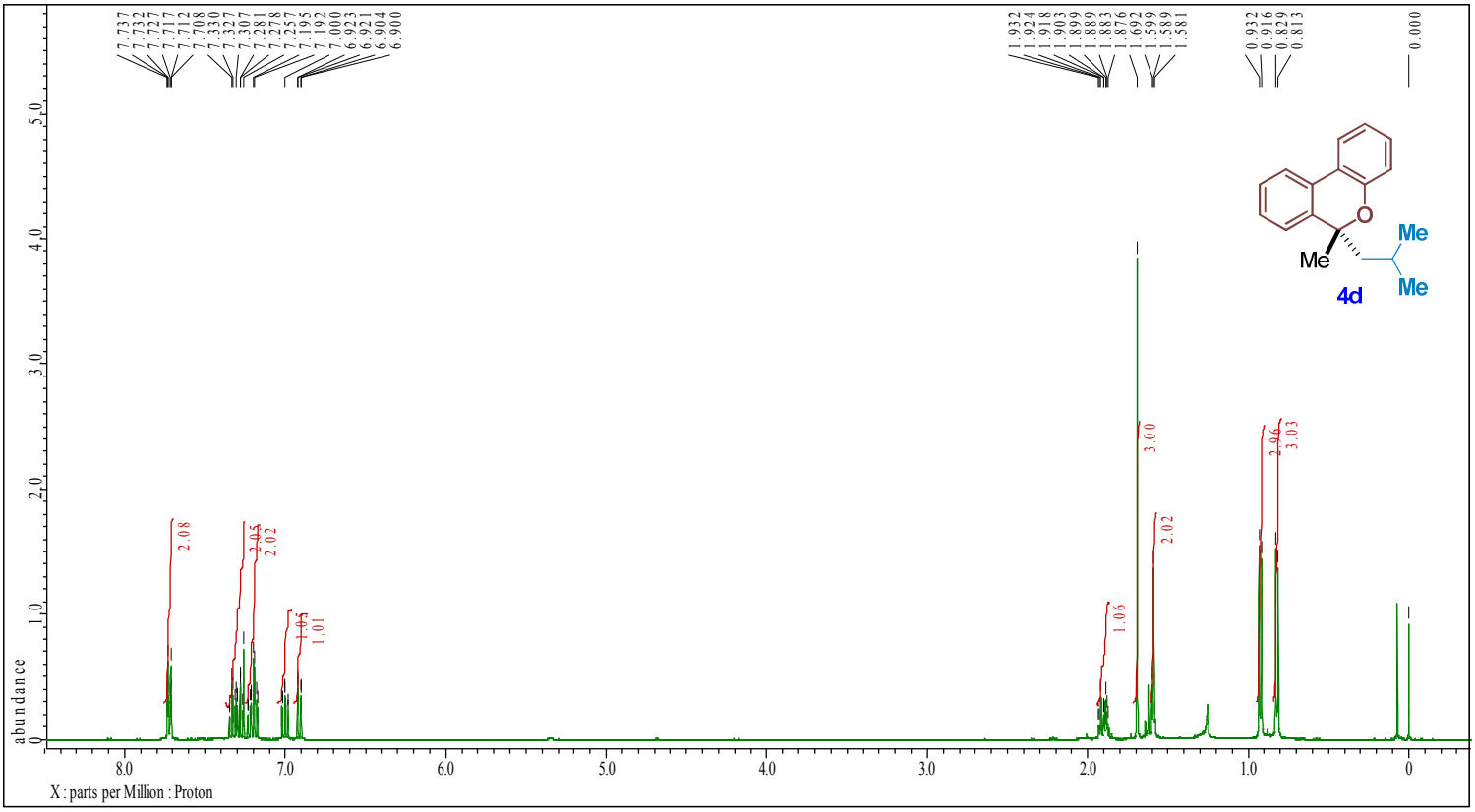
16.831
(thousandths)
X : parts per Million : Carbon13
Me
iPr
4c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7.278
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7.192
7.000
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6.921
6.904
6.900
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1.599
1.589
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2.05
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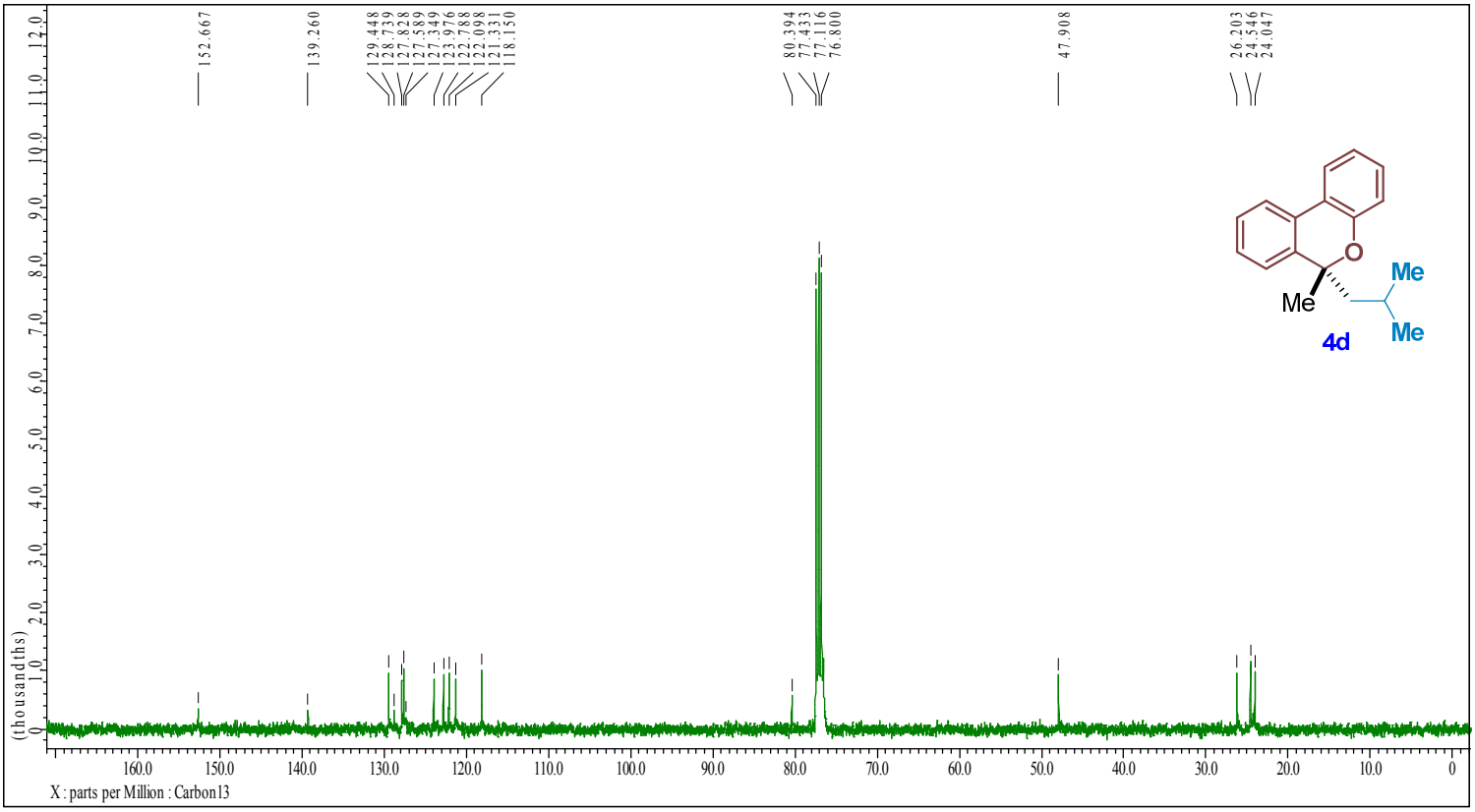
Me
Me
4d
abundance
X : parts per Million : Proton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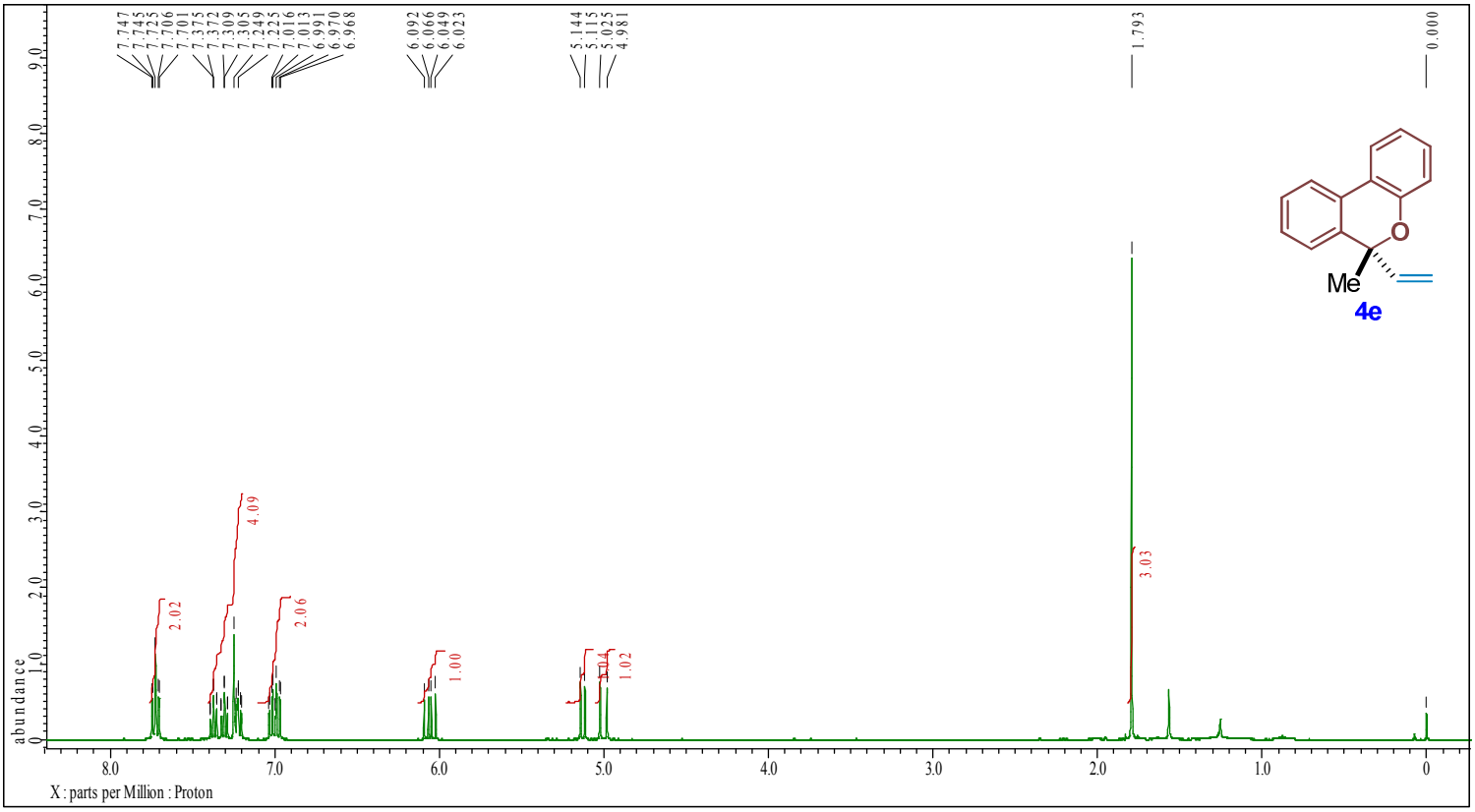
Me
4d
(thousandths)
X : parts per Million : Carbon13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6.049
6.023
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5.025
4.981
1.793
0.000
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1.00
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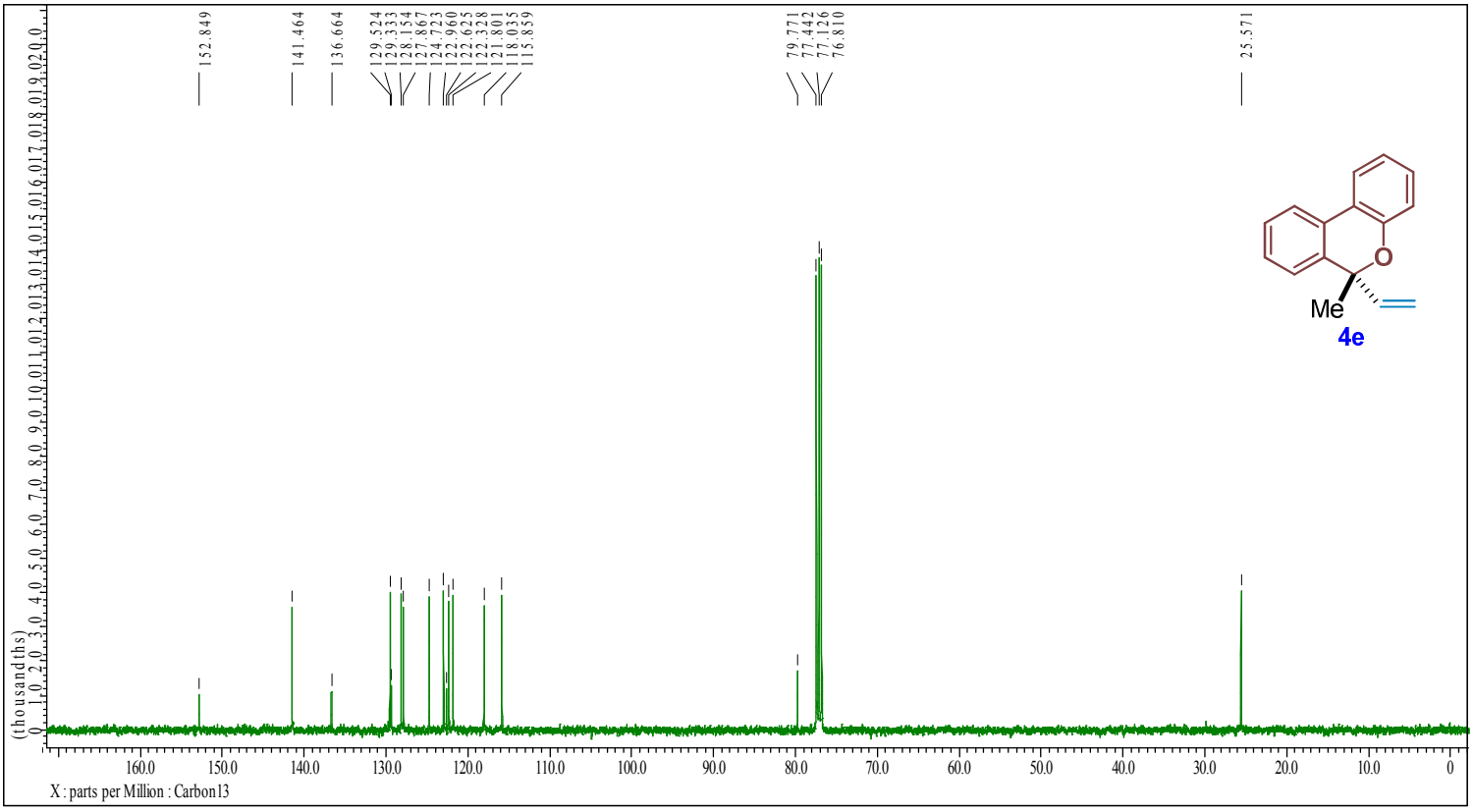
1.02
3.03
abundance
X : parts per Million : Proton
O
Me
4e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121.801
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25.571
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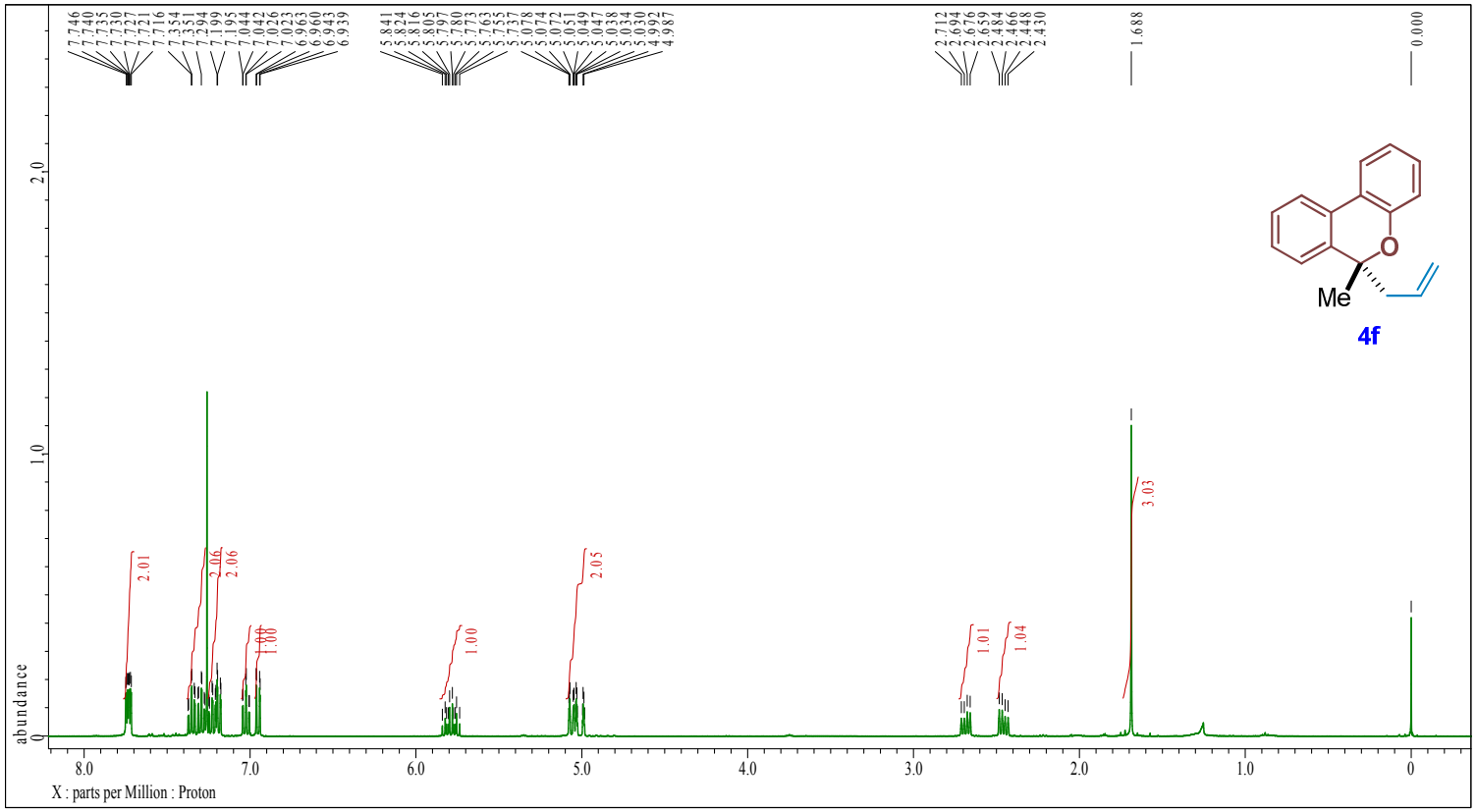
Me
4e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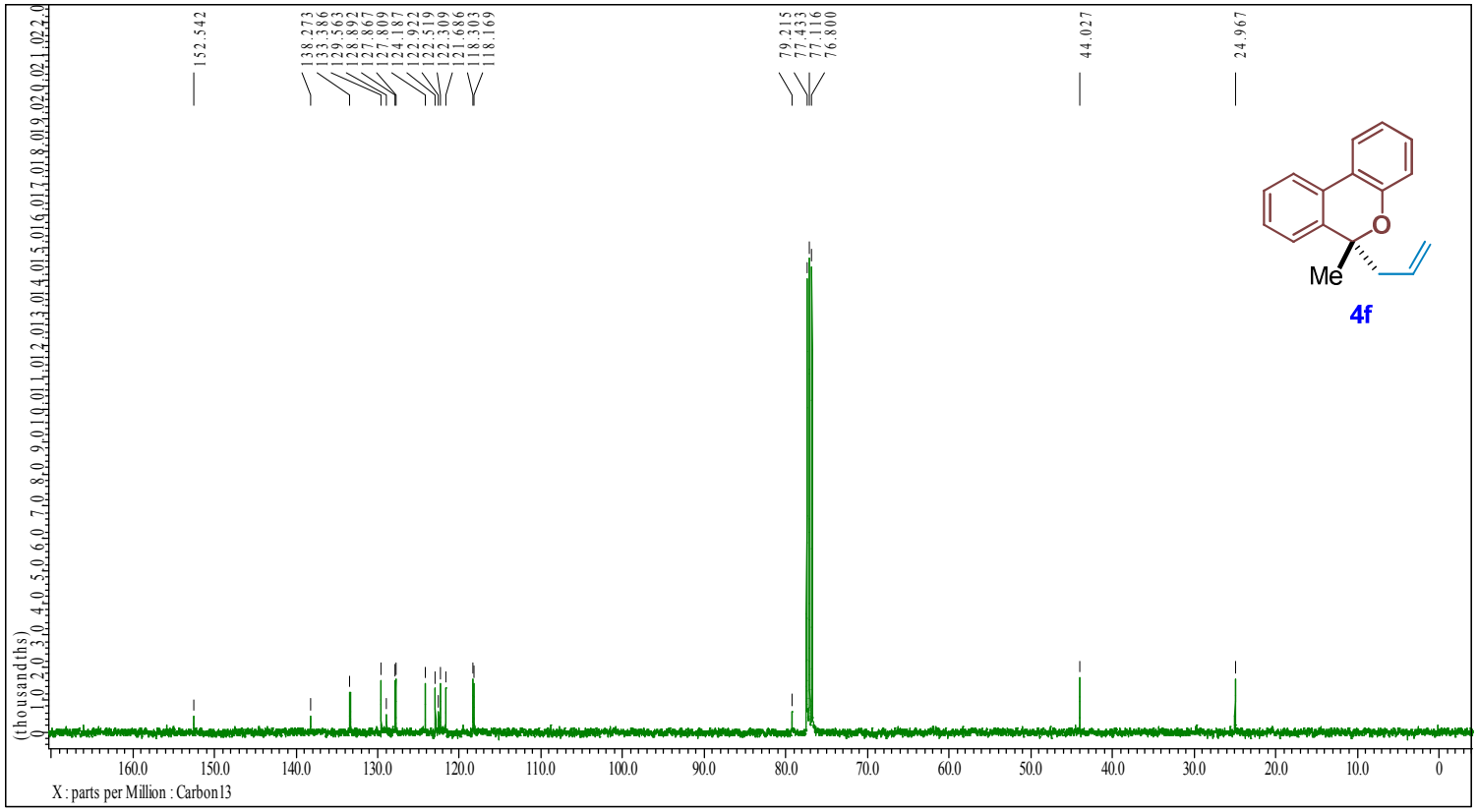
abundance
X : parts per Million : Proton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Me
4f
(thousandths)
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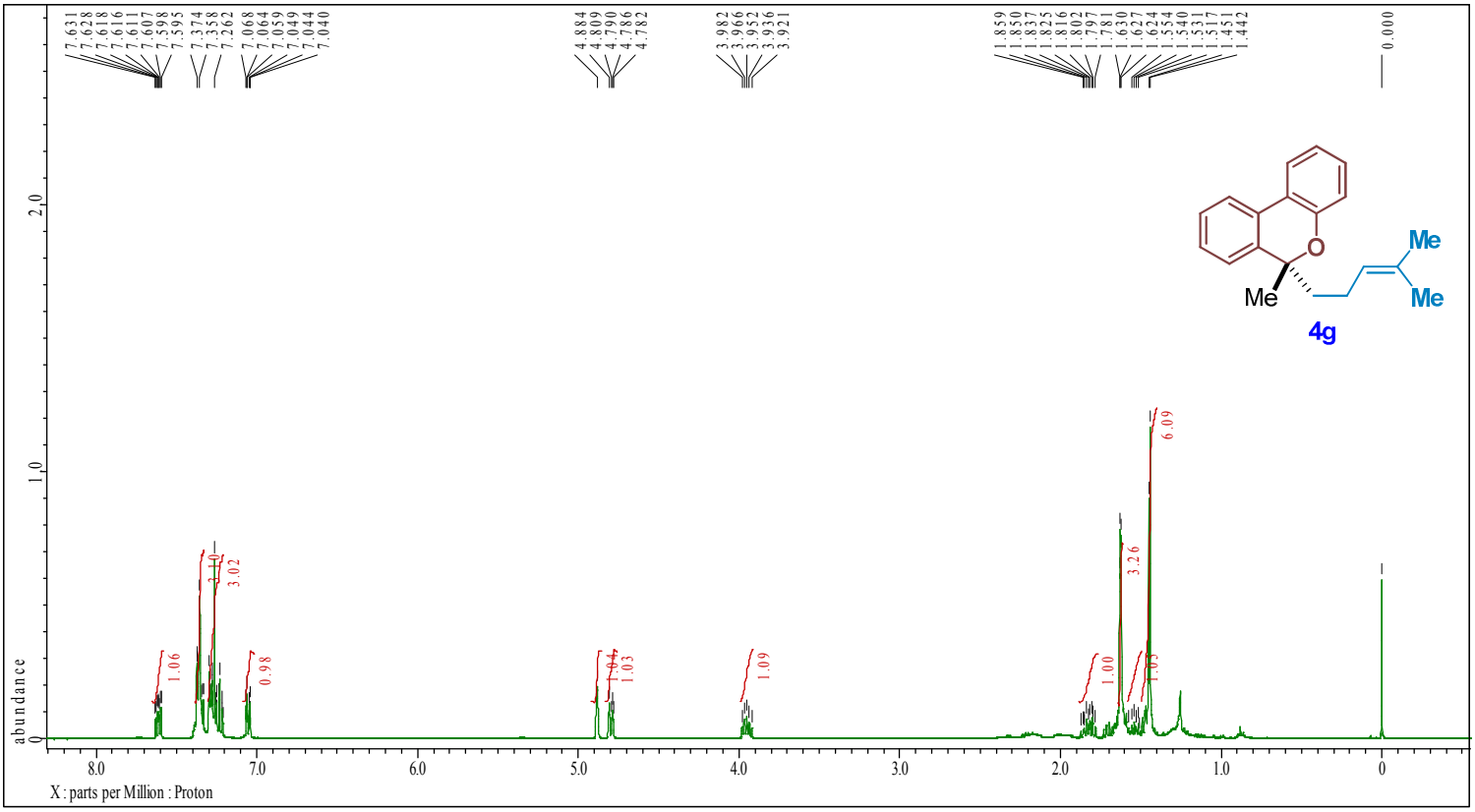
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abundance
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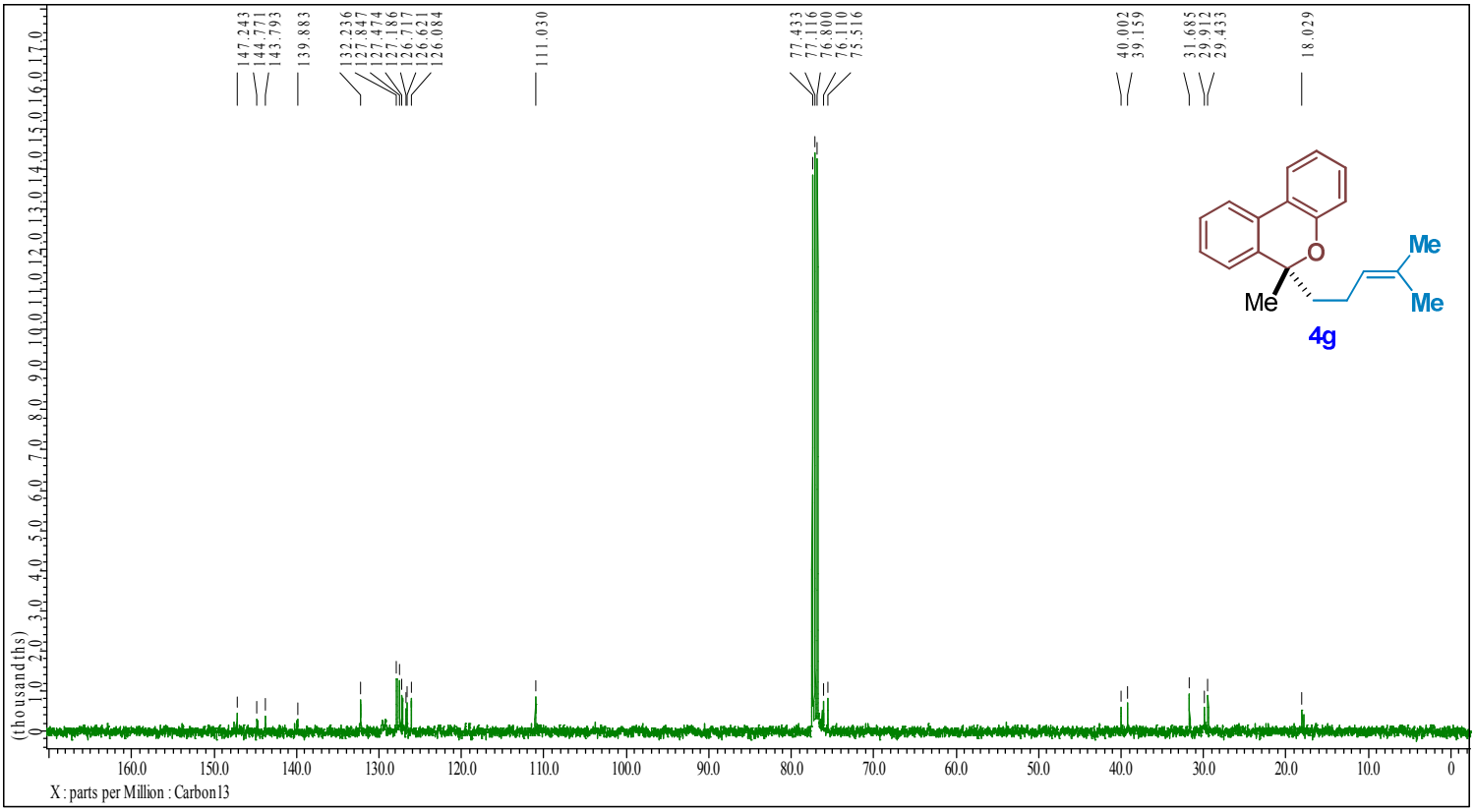
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76.800
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75.516
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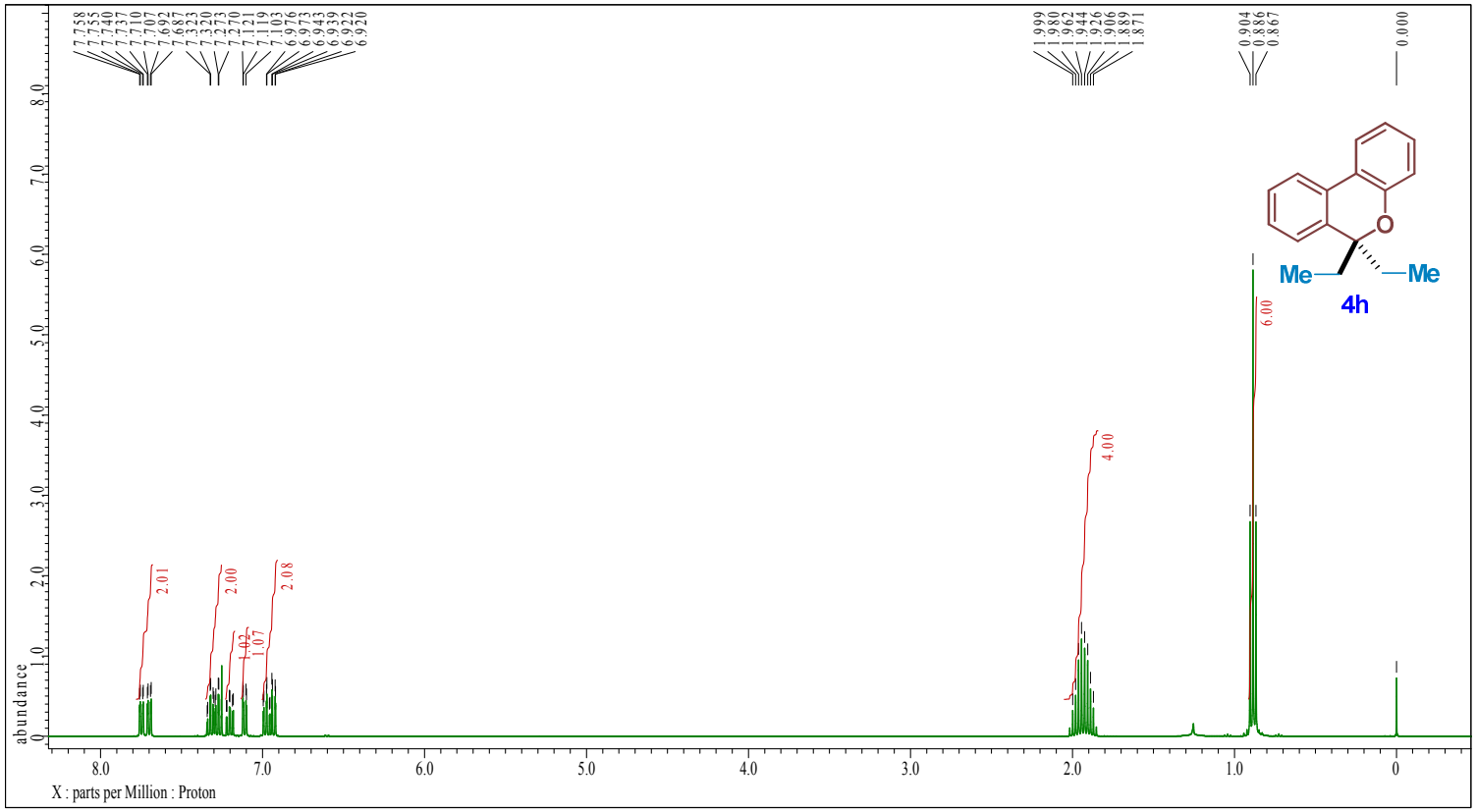
Me
Me
4g
(thousandths)
X : parts per Million : Carbon13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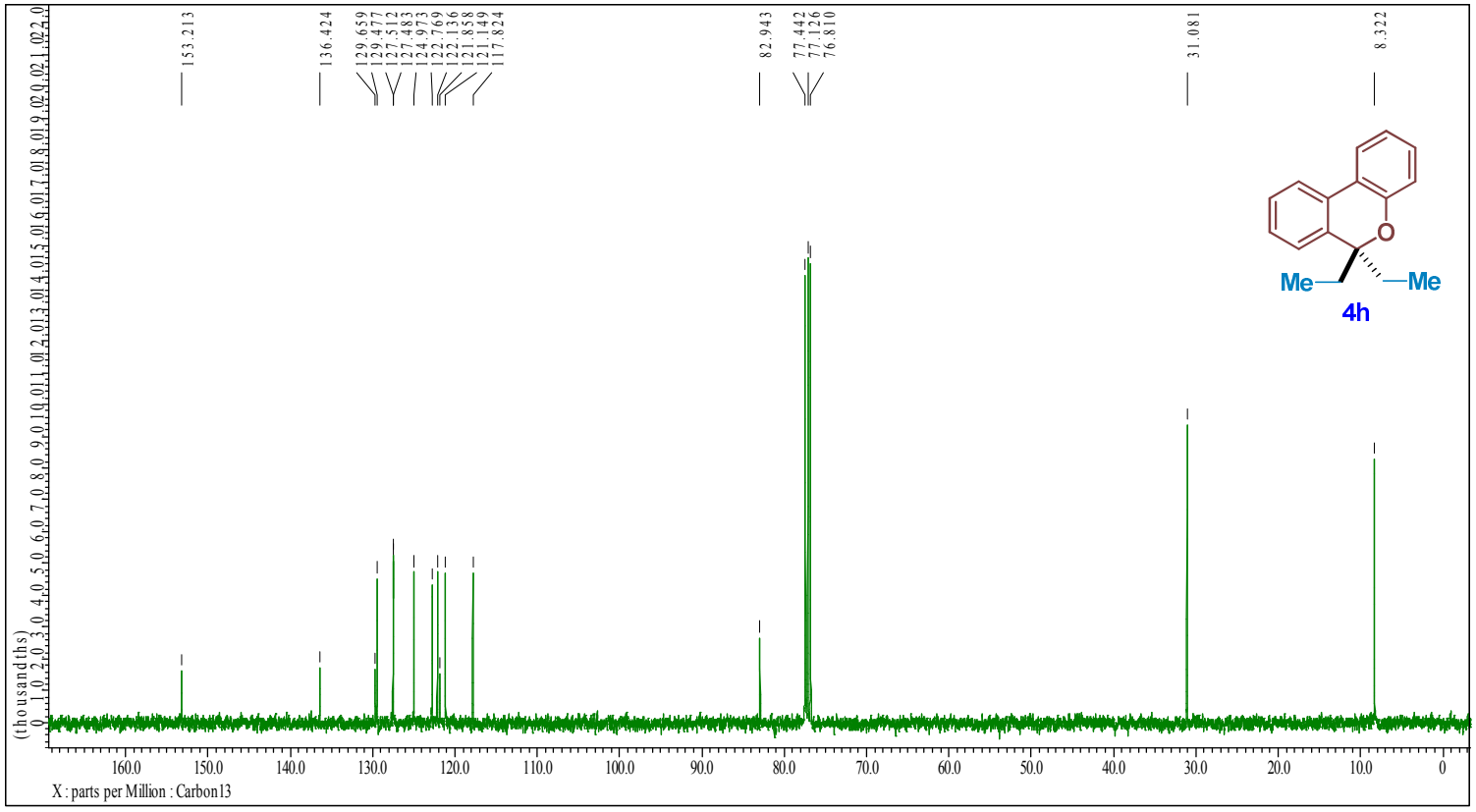
Me
4h
abundance
X : parts per Million : Proton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77.126
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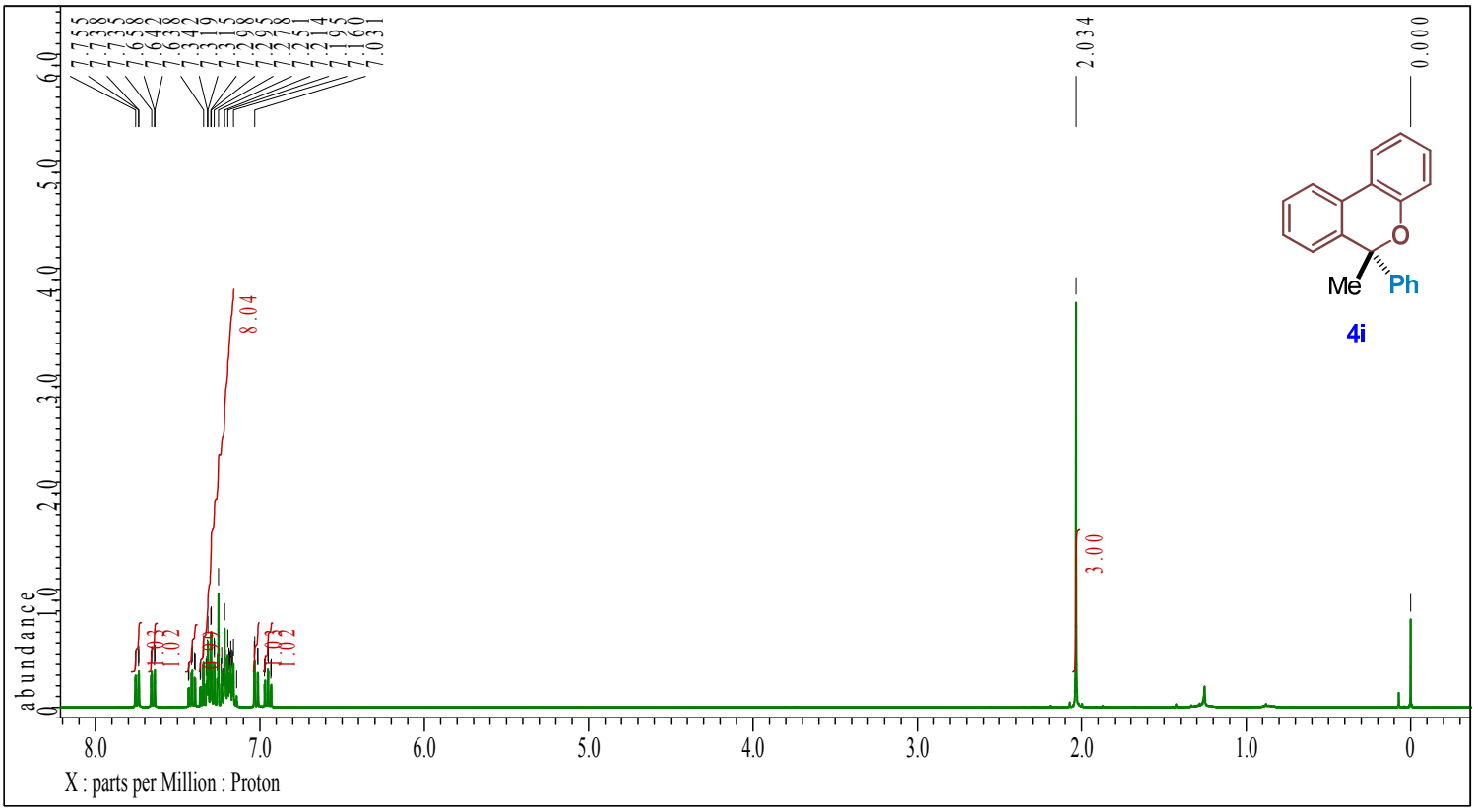
31.081
8.322
Me
Me
4h
(thousandths)
X : parts per Million : Carbon13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7.214
7.195
7.160
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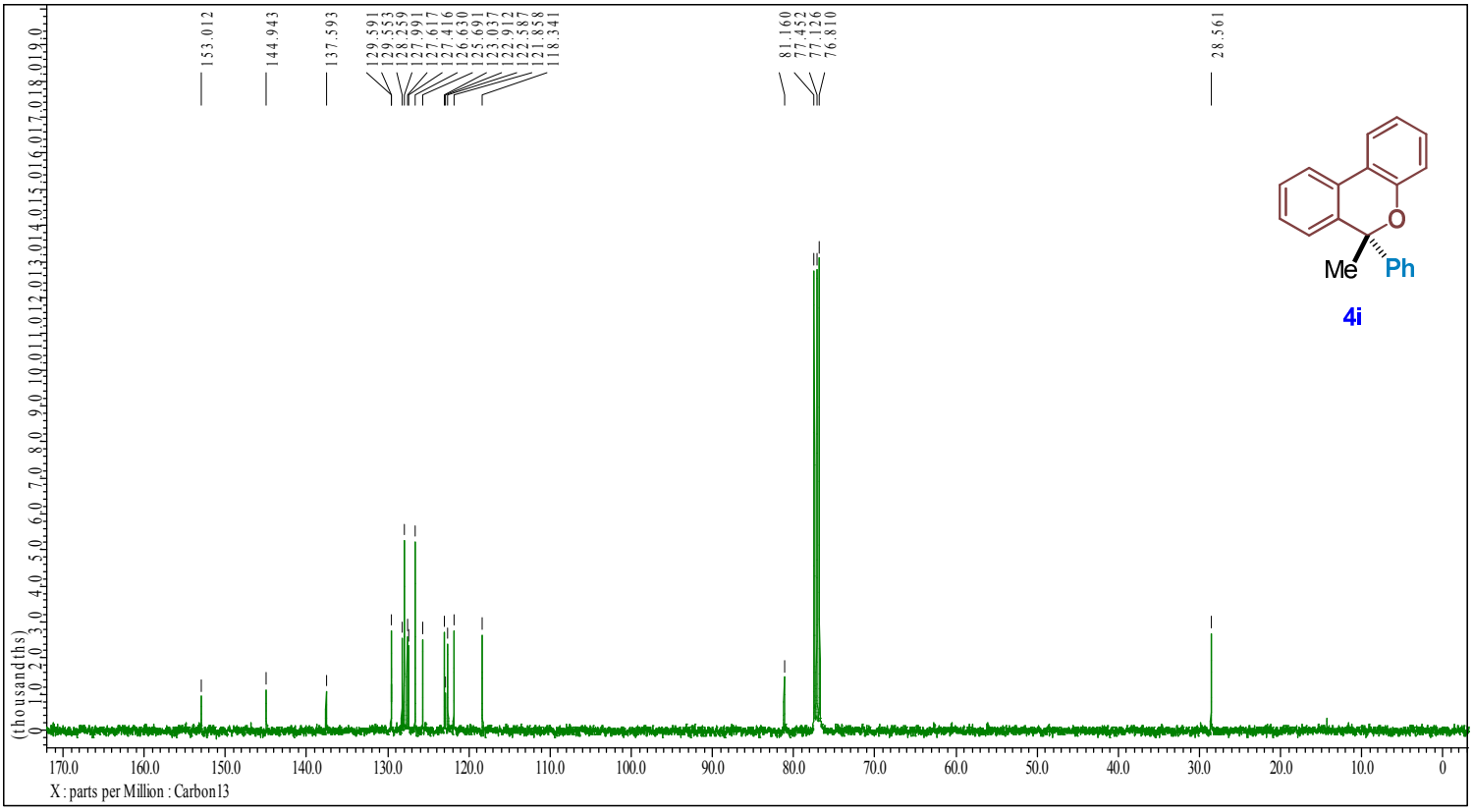
3.00
1.02
1.02
1.02
abundance
X : parts per Million : Proton
Me
Ph
4i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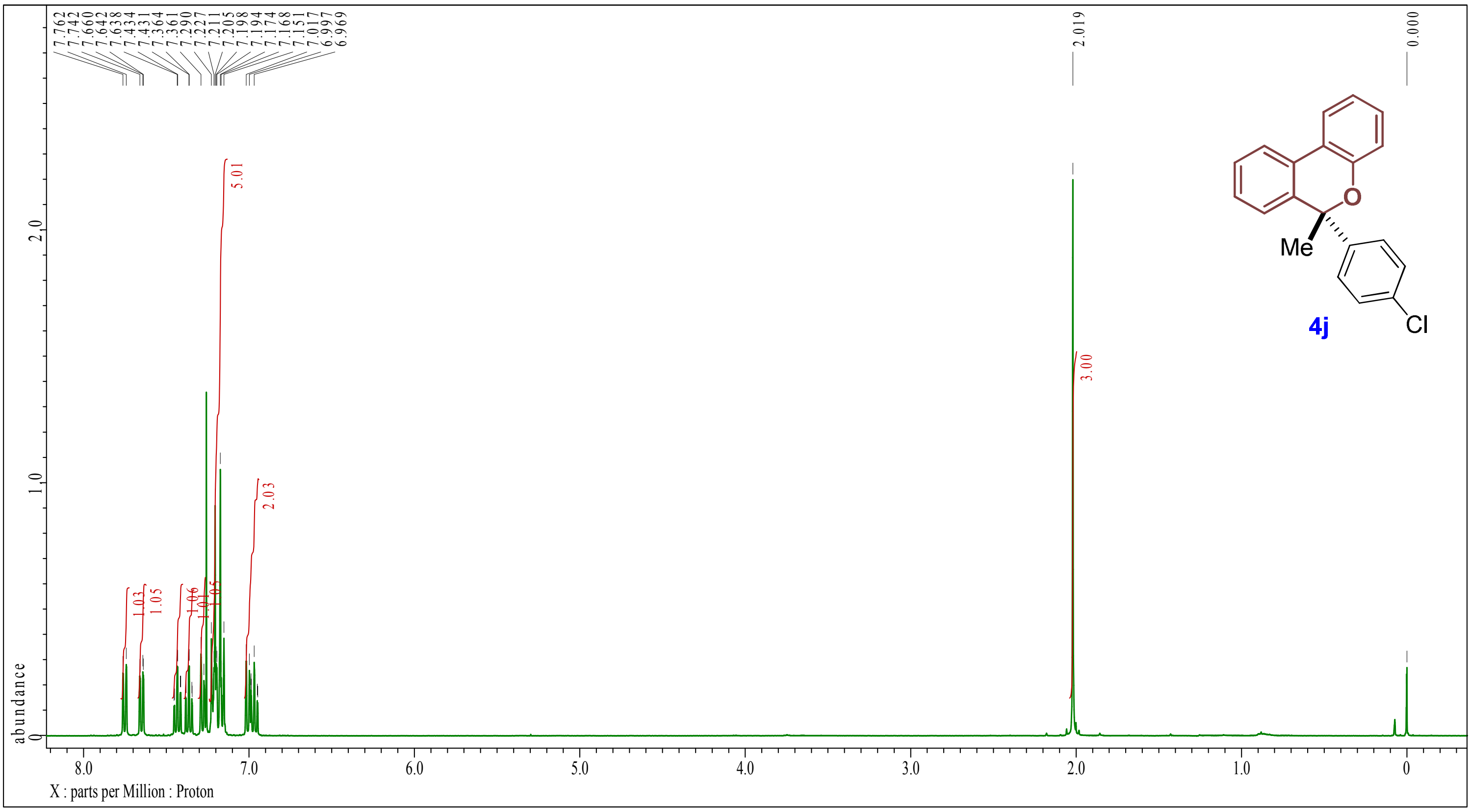
28.561
(thousandths)
X : parts per Million : Carbon13
Me
Ph
4i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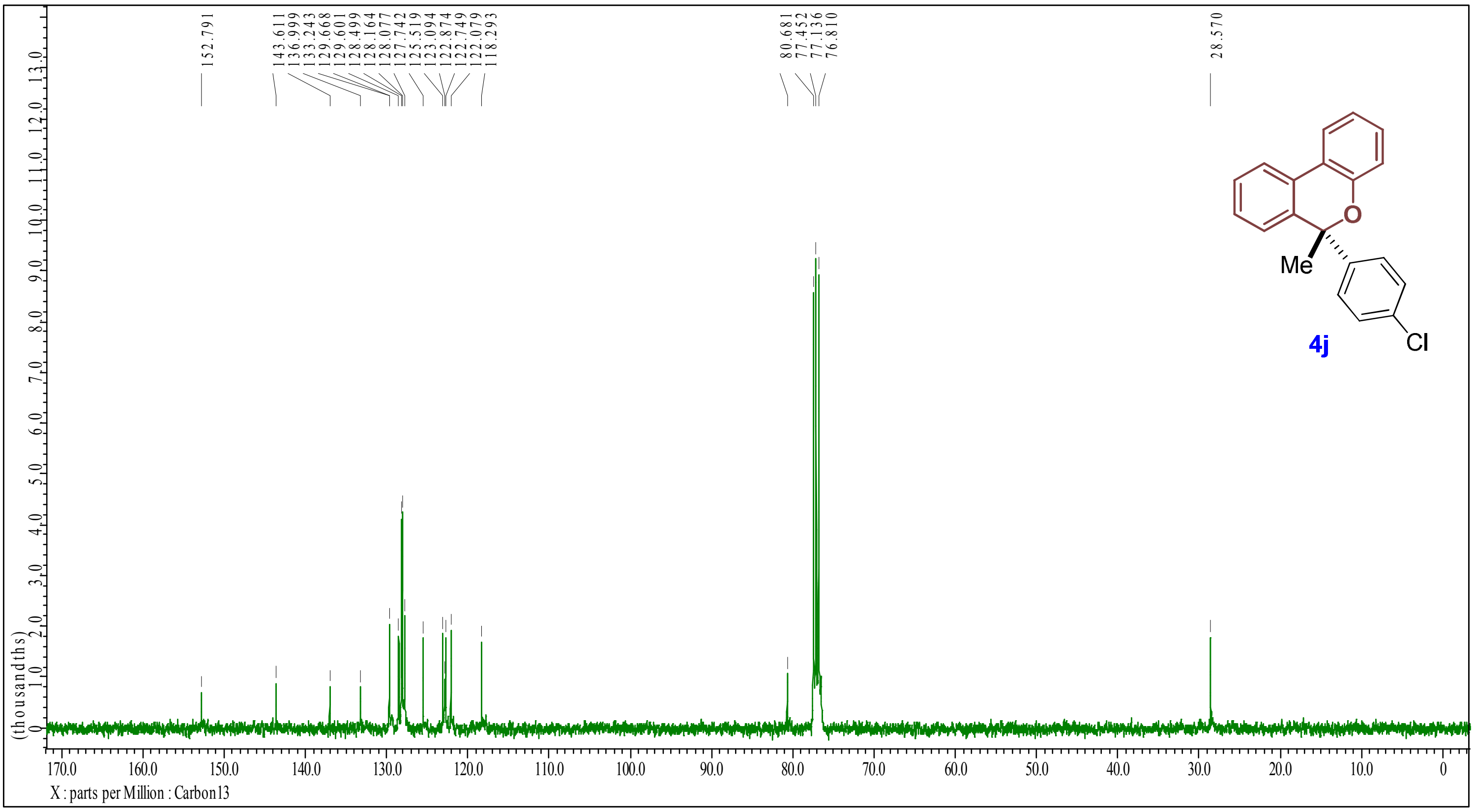
1.06
1.01
1.05
Me
O
Cl
4j
abundance
X : parts per Million : Proton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28.570
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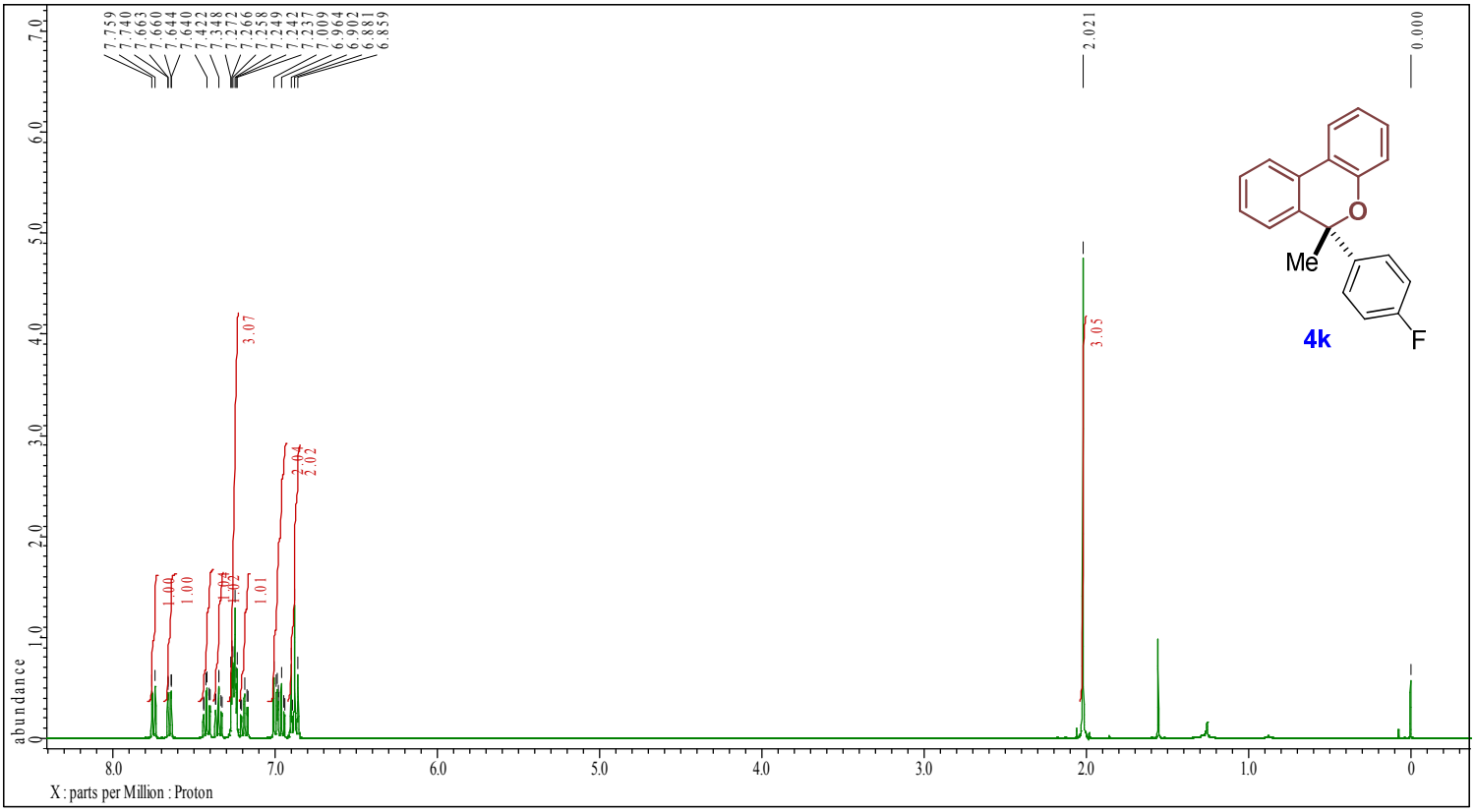
(thousandths)
X : parts per Million : Carbon13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7.348
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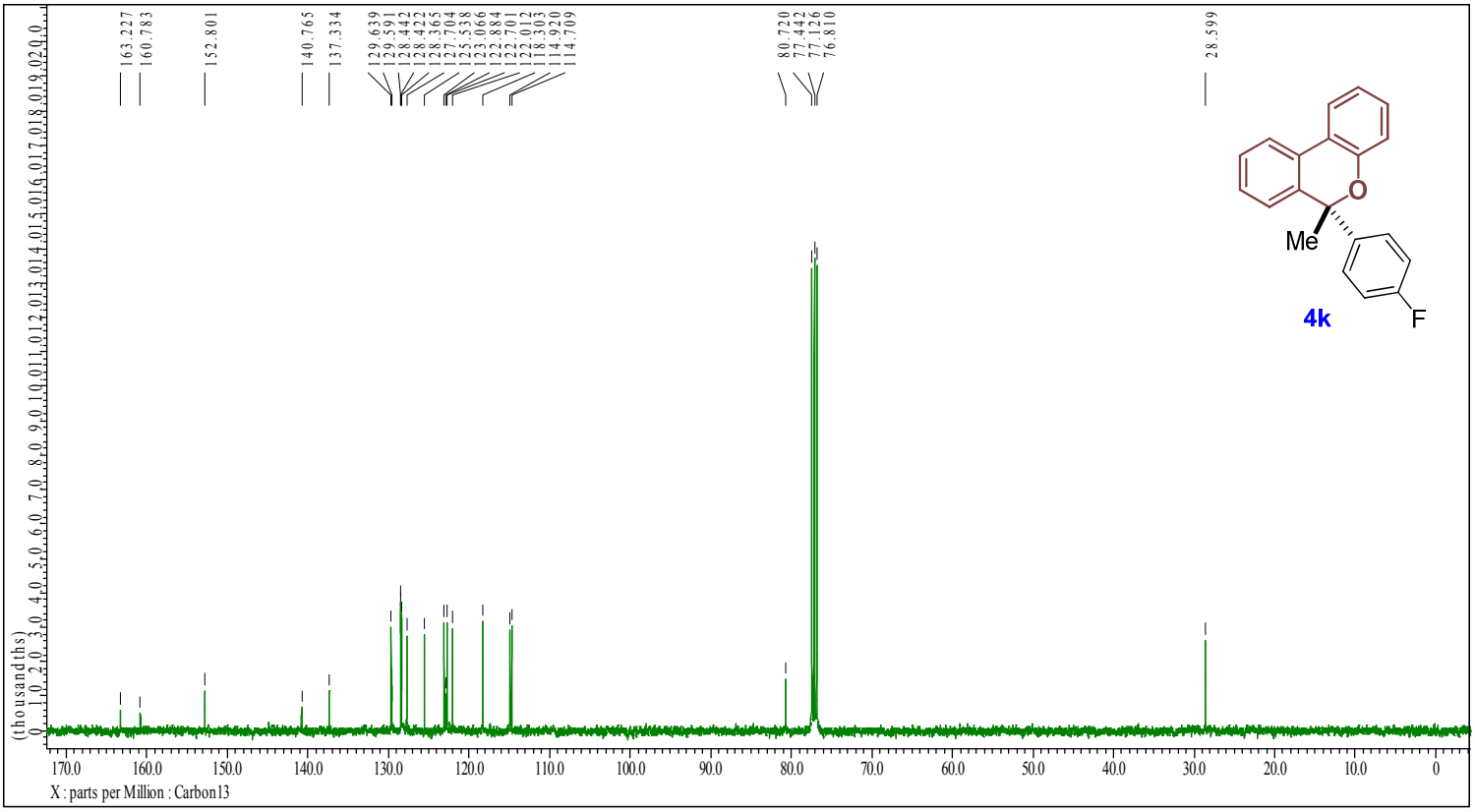
7.266
7.258
7.249
7.242
7.237
7.009
6.964
6.902
6.881
6.859
2.021
0.000
3.07
3.05
3.04
2.02
1.04
1.00
1.01
Me
O
F
4k
abundance
X : parts per Million : Proton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140.765
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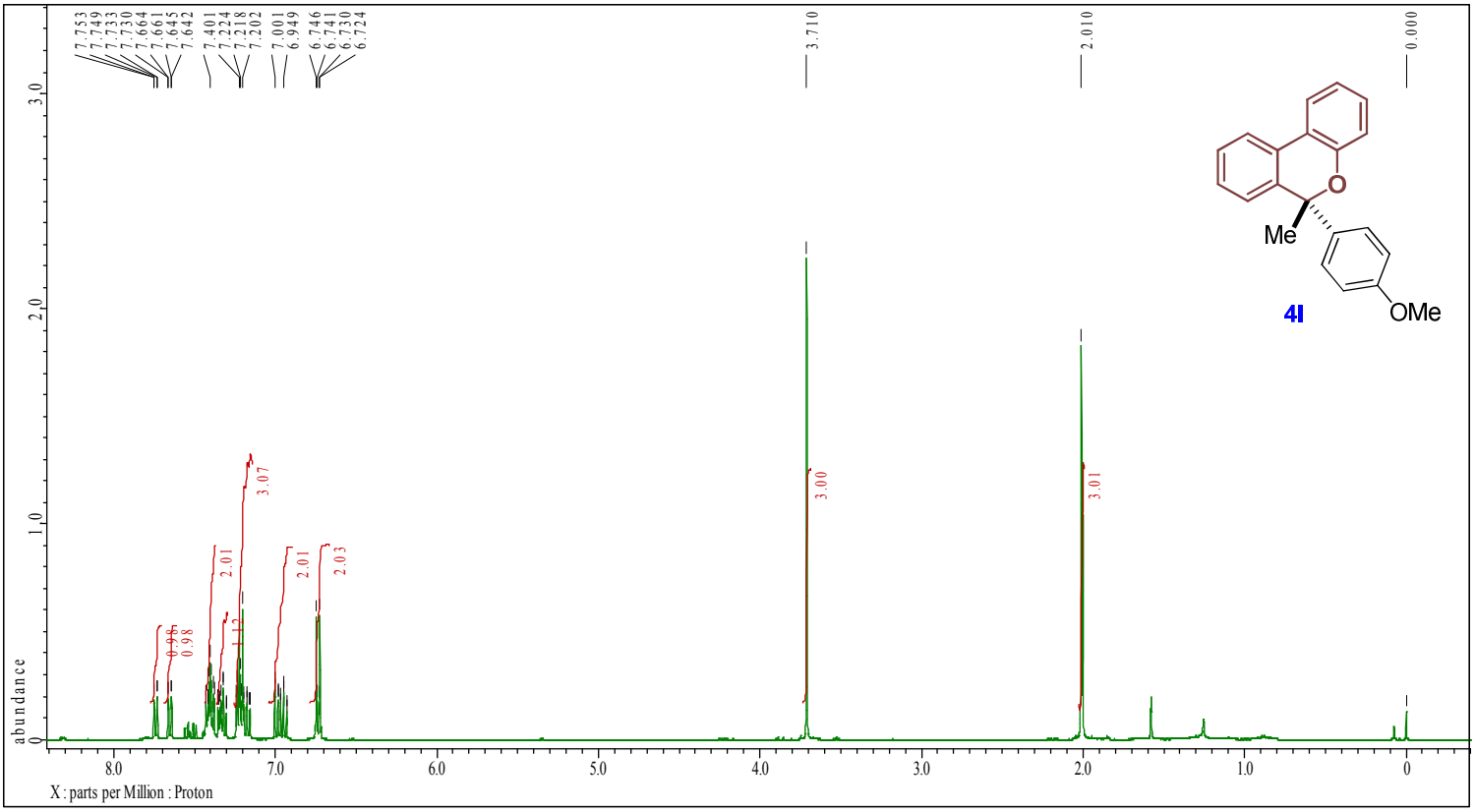
129.591
128.442
128.422
128.365
127.704
125.538
123.066
122.884
122.701
122.012
118.303
114.920
114.709
80.720
77.442
77.126
76.810
28.599
Me
O
F
4k
(thousandths)
X : parts per Million : Carbon13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7.730
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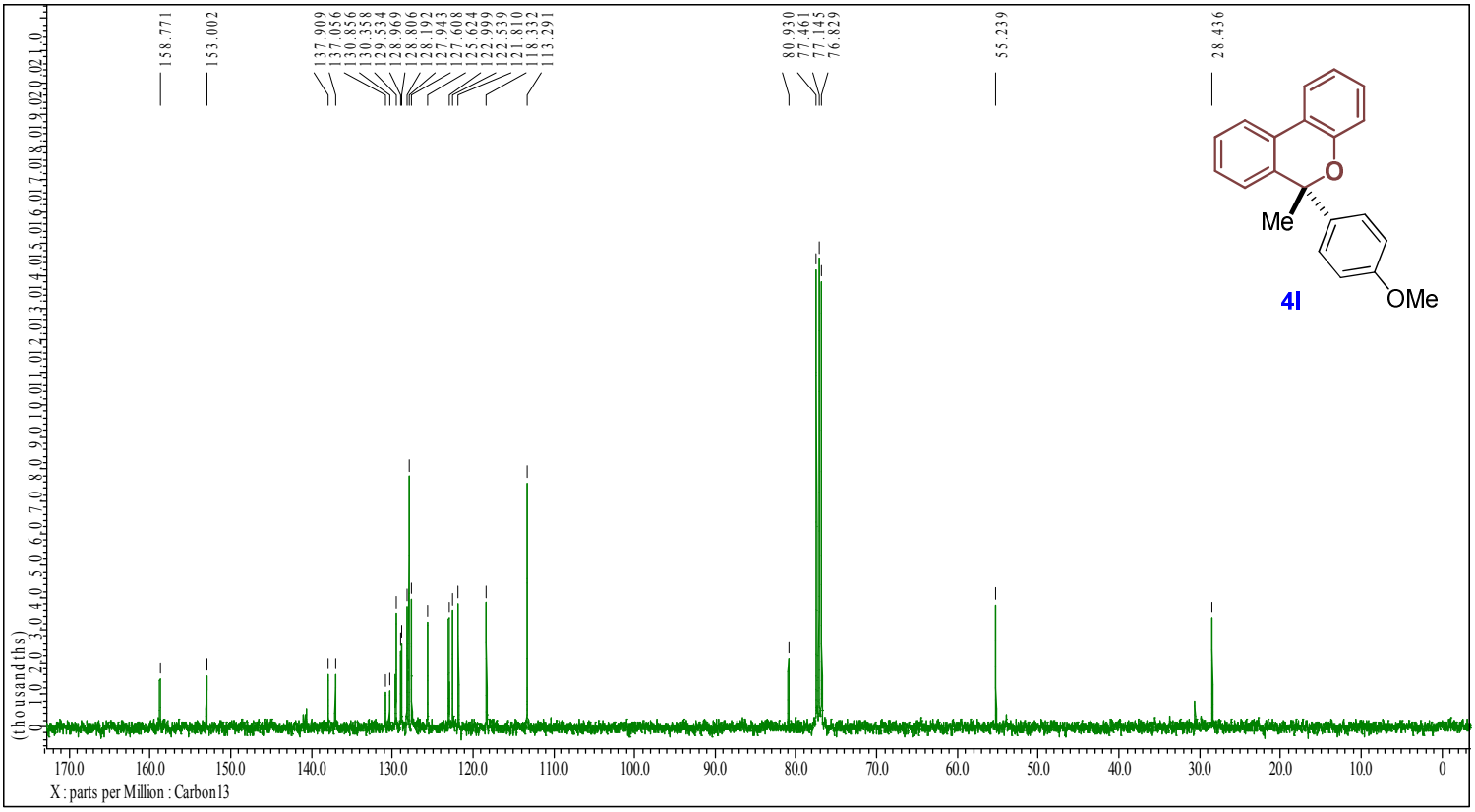
7.661
7.645
7.642
7.401
7.224
7.218
7.202
7.001
6.949
6.746
6.741
6.730
6.724
3.710
2.010
0.000
3.07
2.01
2.01
2.03
0.98
0.98
3.00
3.01
abundance
X : parts per Million : Proton
Me
OMe
4l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137.909
137.056
130.856
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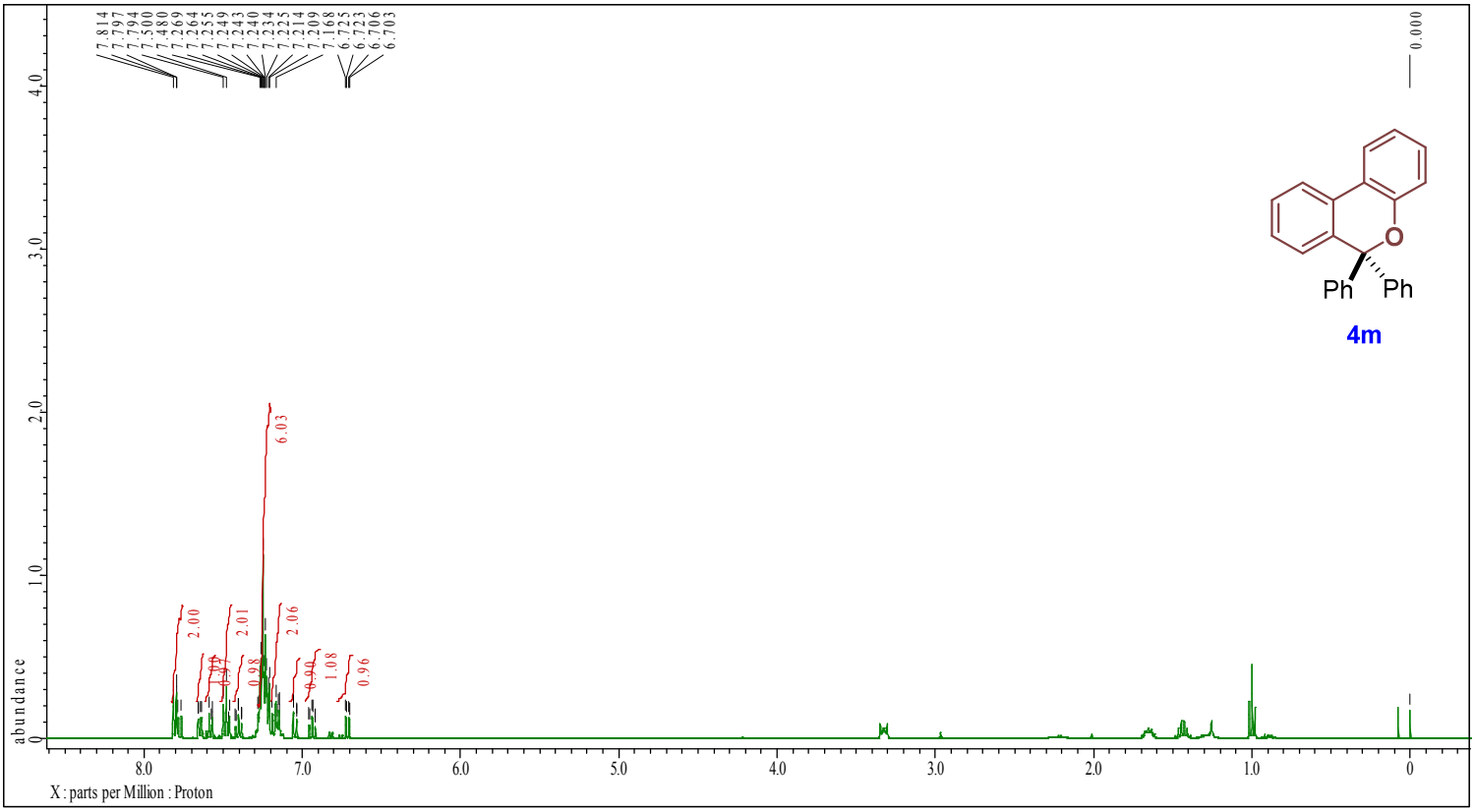
129.534
128.969
128.806
128.192
127.943
127.608
125.624
122.999
122.539
121.810
118.332
113.291
80.930
77.461
77.145
76.829
55.239
28.436
(thousandths)
X : parts per Million : Carbon13
Me
OMe
4l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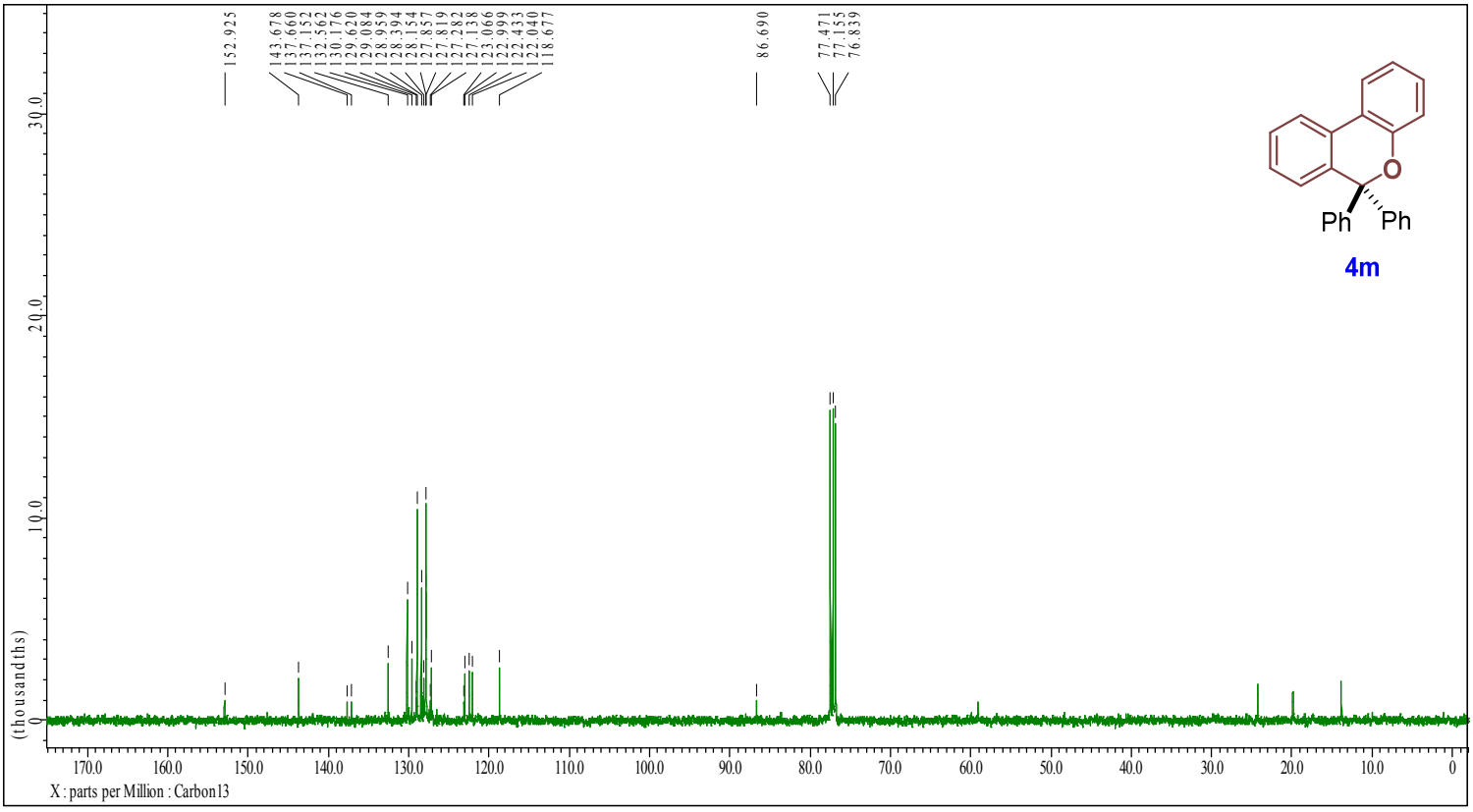
7.797
7.794
7.500
7.480
7.269
7.264
7.255
7.249
7.243
7.240
7.234
7.225
7.214
7.209
7.168
6.725
6.723
6.706
6.703
0.000
6.03
2.00
2.01
2.06
0.98
0.90
1.08
0.96
abundance
X : parts per Million : Proton
Ph
Ph
O
4m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143.678
137.660
137.152
132.562
130.176
129.620
129.084
128.959
128.394
128.154
127.857
127.819
127.282
127.138
123.066
122.999
122.433
122.040
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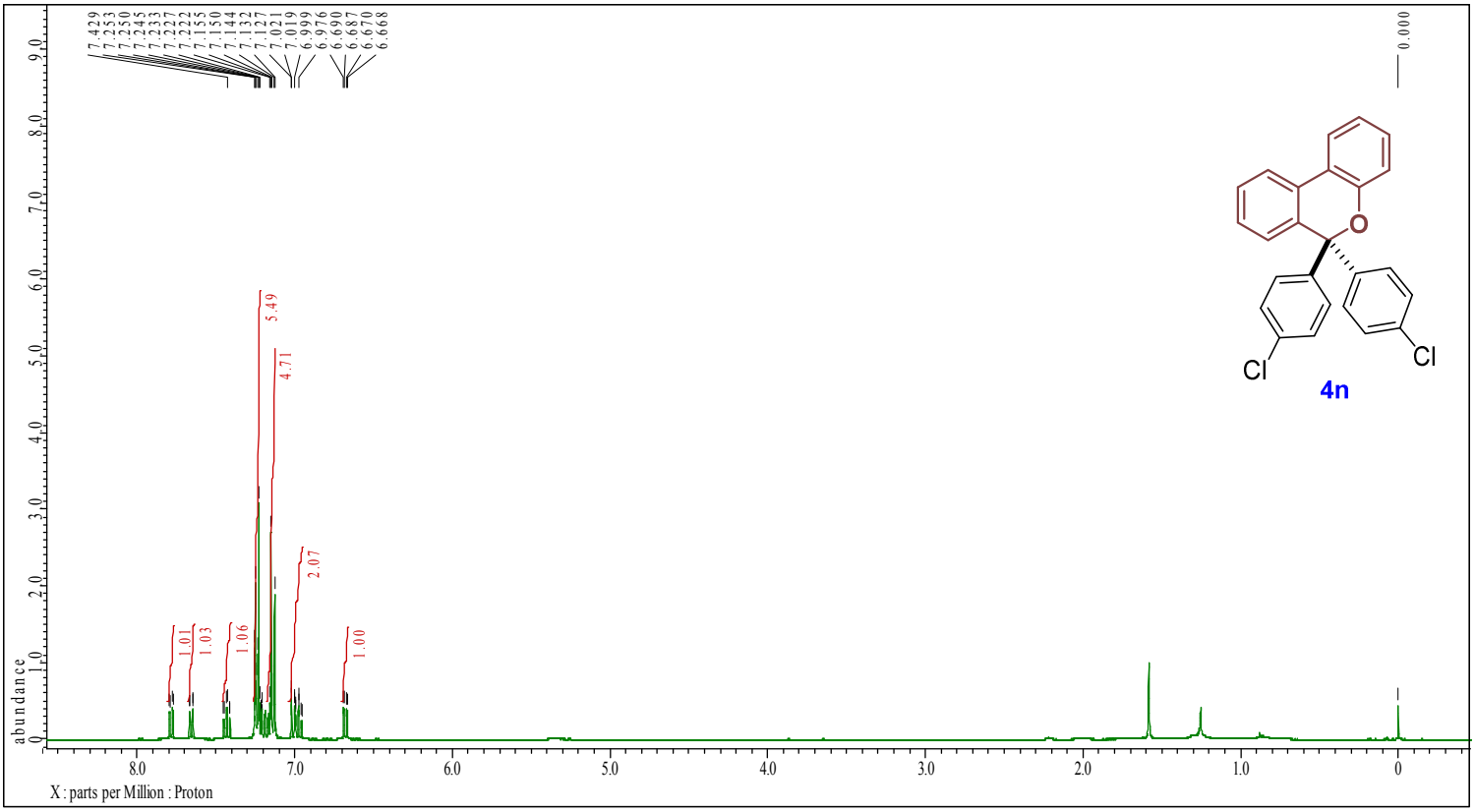
77.471
77.155
76.839
(thousandths)
X : parts per Million : Carbon13
Ph
Ph
O
4m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7.245
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7.227
7.222
7.155
7.150
7.144
7.132
7.127
7.021
7.019
6.999
6.976
6.690
6.687
6.670
6.668
0.000
5.49
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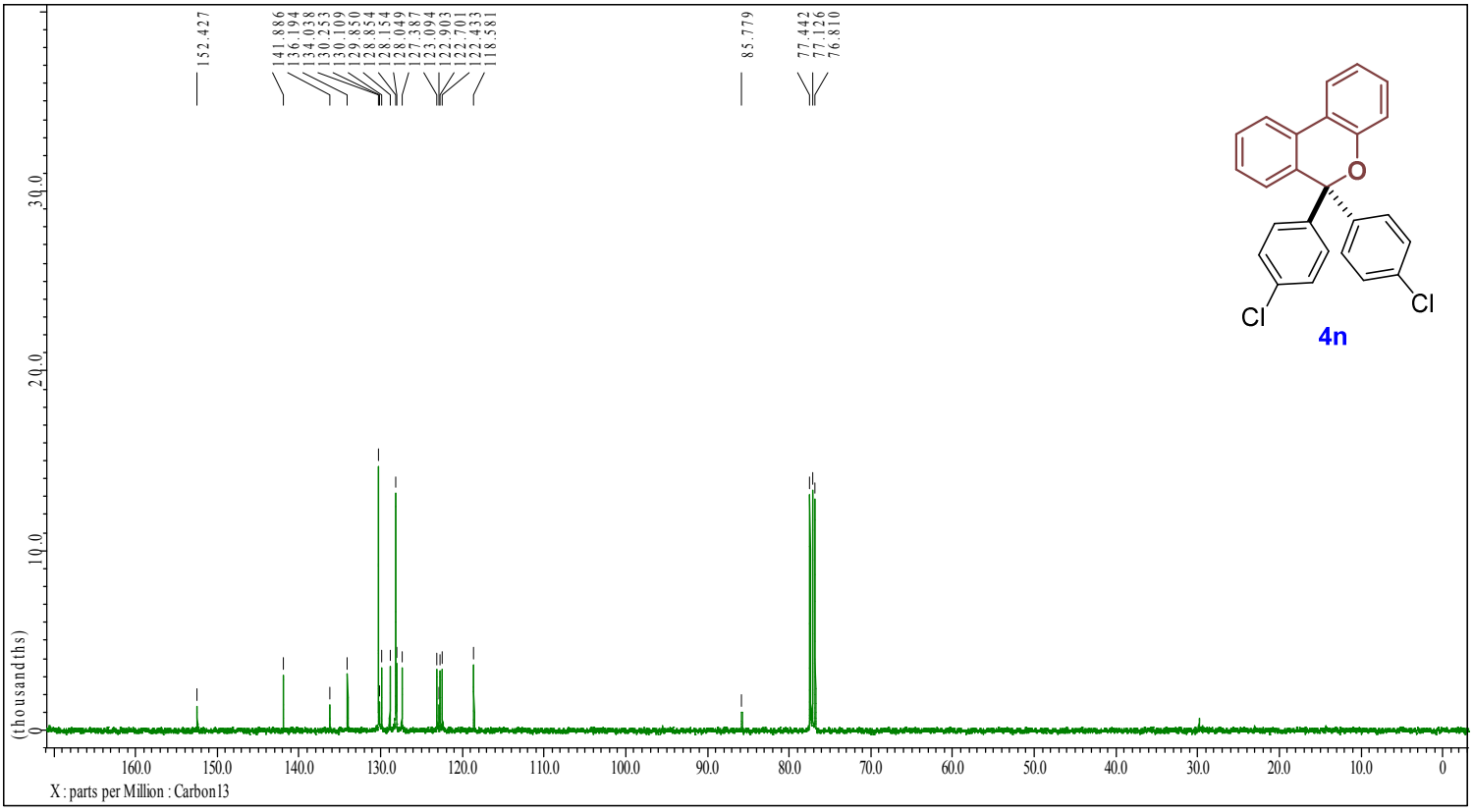
2.07
1.01
1.03
1.06
1.00
abundance
X : parts per Million : Proton
Cl
Cl
O
4n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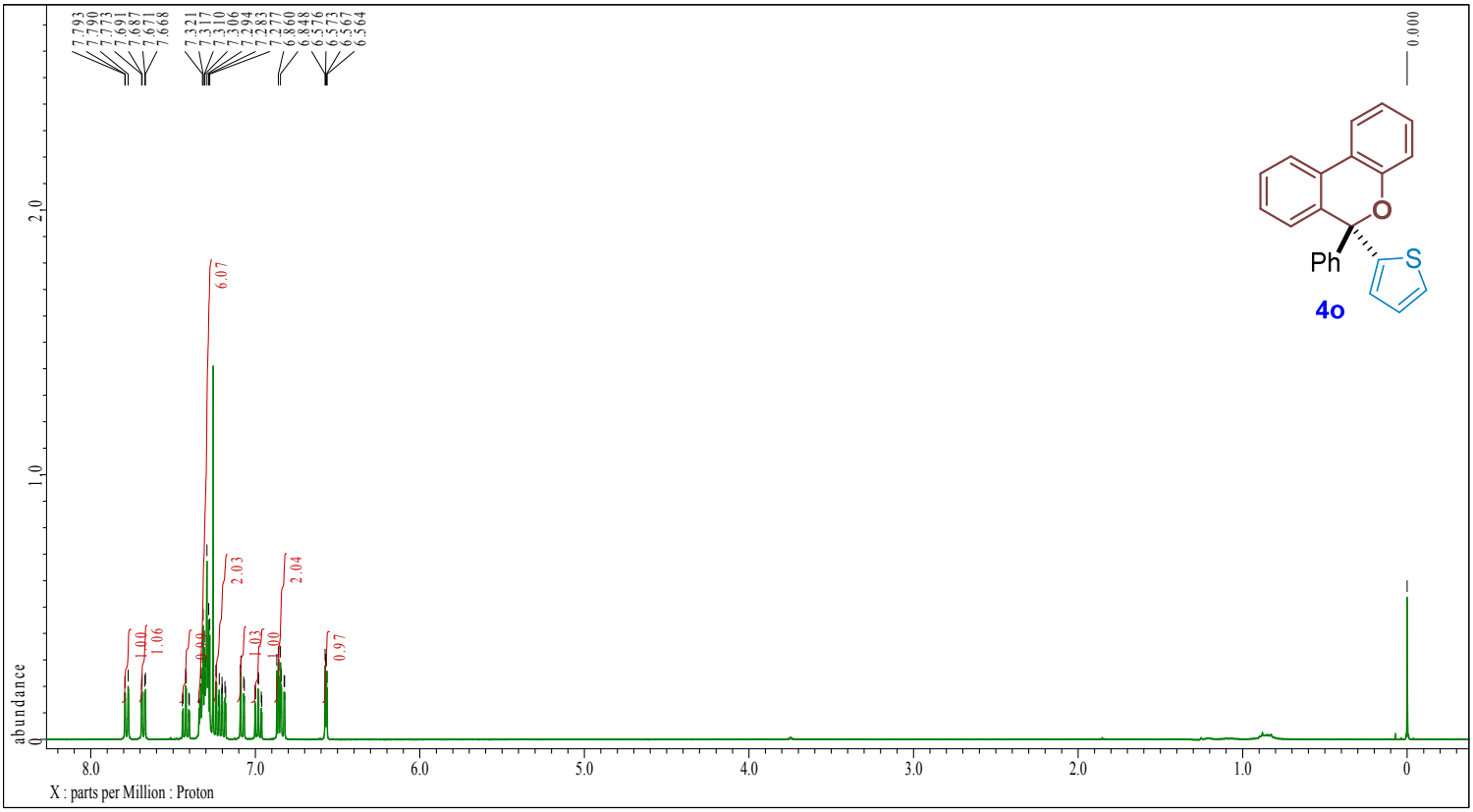
136.194
134.038
130.253
130.109
129.850
128.854
128.154
128.049
127.387
123.094
122.903
122.701
122.433
118.581
85.779
77.442
77.126
76.810
(thousandths)
X : parts per Million : Carbon13
Cl
Cl
O
4n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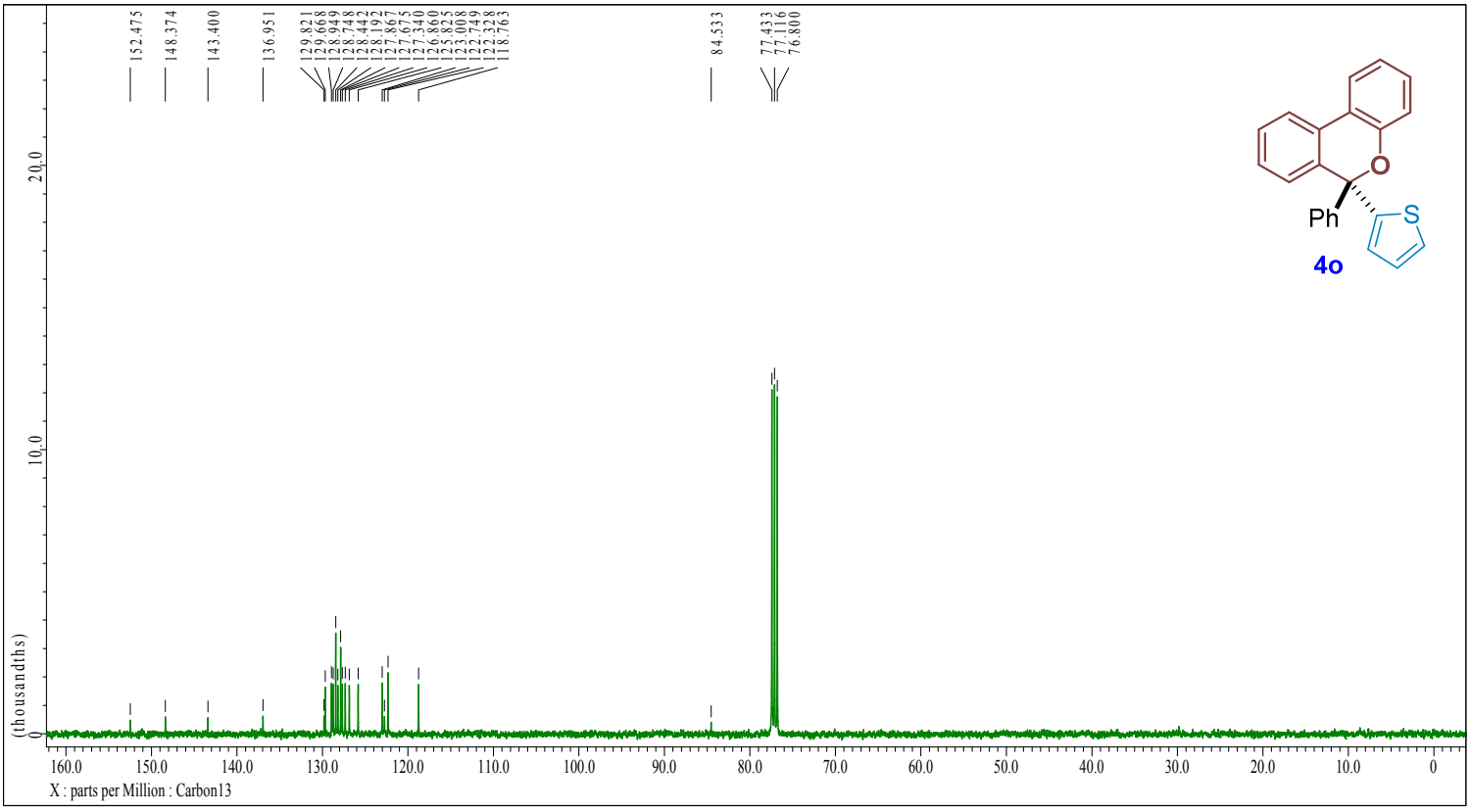
7.687
7.671
7.668
7.321
7.317
7.310
7.306
7.294
7.283
7.277
6.860
6.848
6.576
6.573
6.567
6.564
0.000
6.07
2.03
2.04
1.00
1.06
0.99
1.03
1.00
0.97
abundance
X : parts per Million : Proton
O
Ph
S
4o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128.748
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128.192
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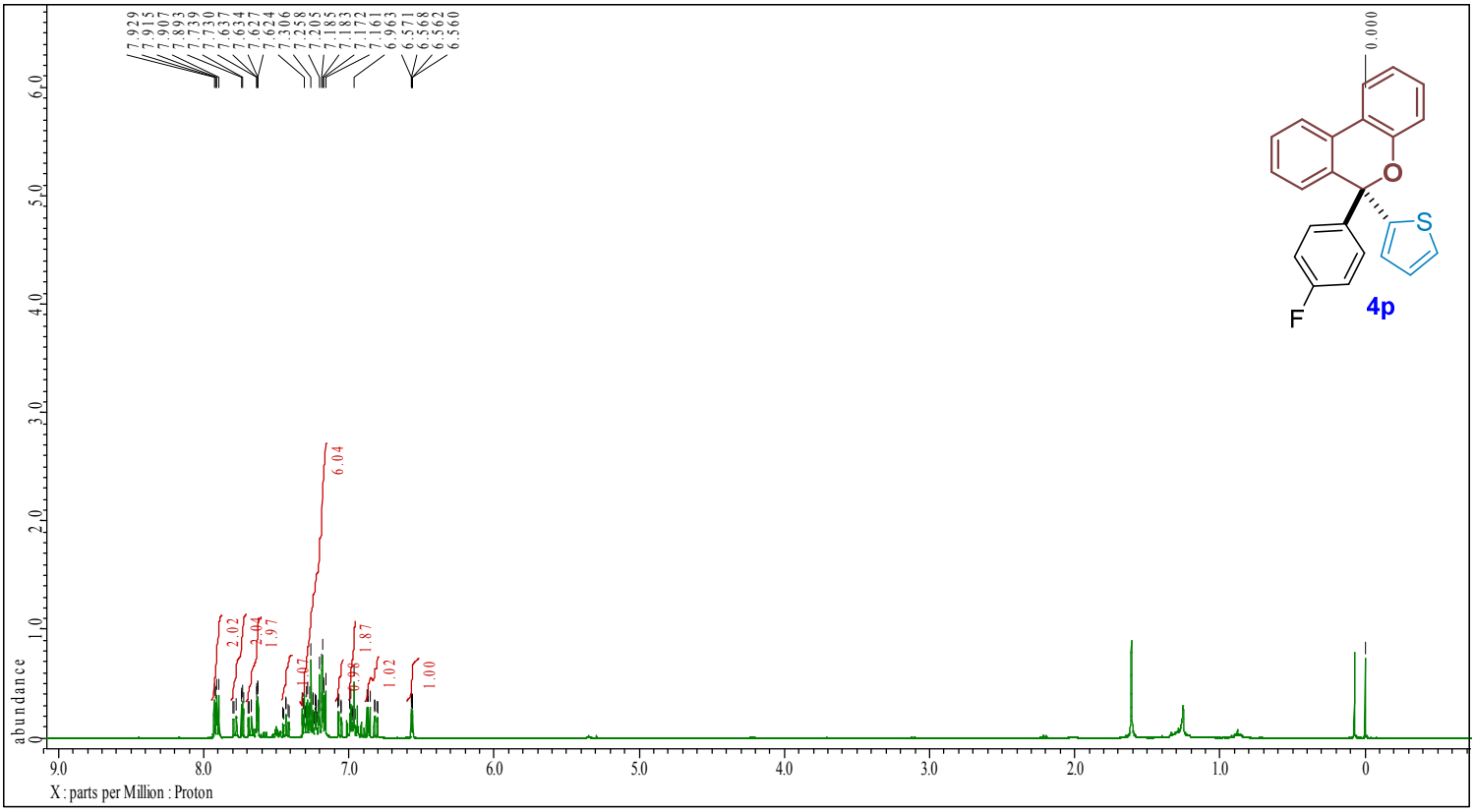
127.675
127.340
126.860
125.825
123.008
122.749
122.328
118.763
84.533
77.433
77.116
76.800
(thousandths)
X : parts per Million : Carbon13
O
Ph
S
4o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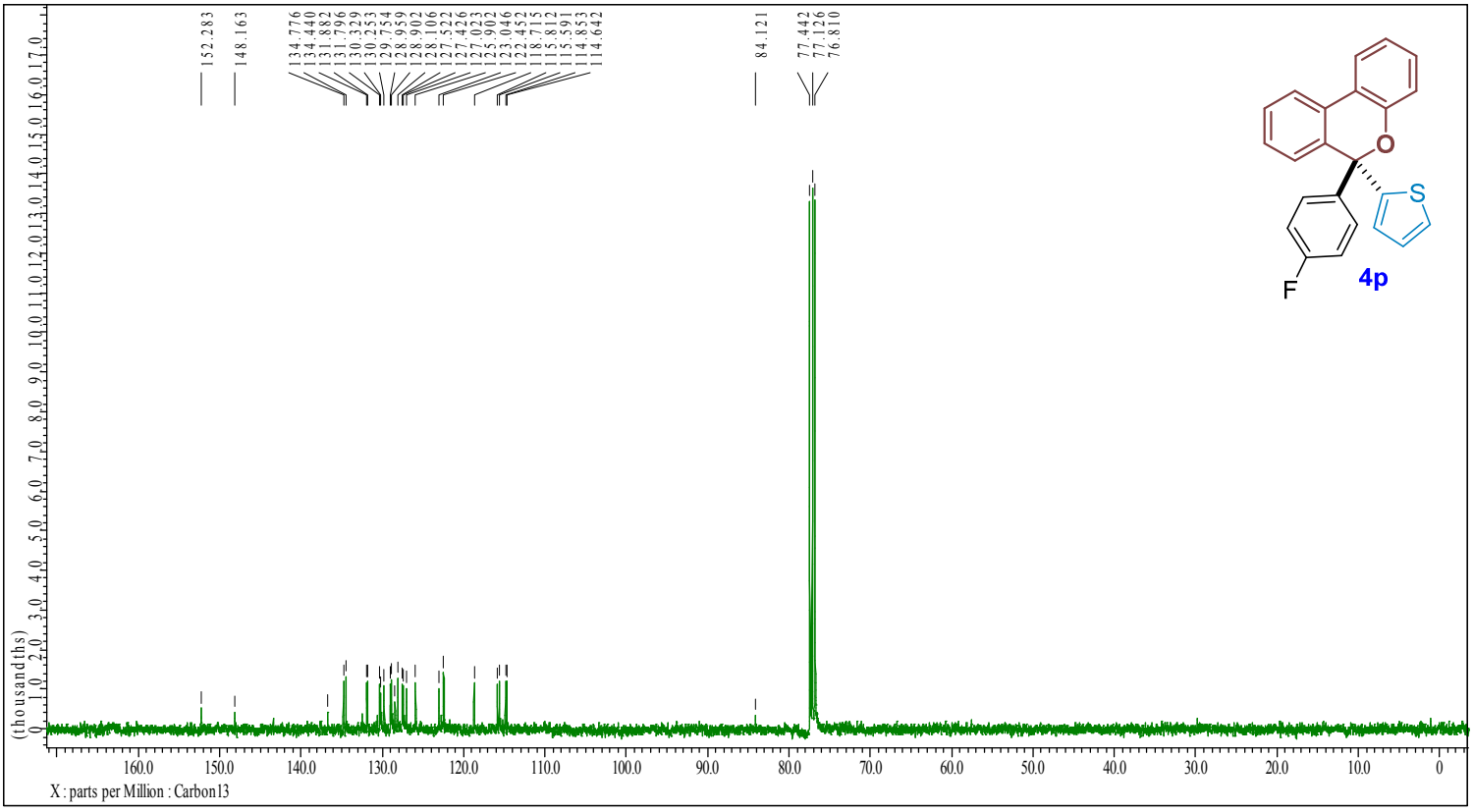
7.907
7.893
7.739
7.730
7.637
7.634
7.627
7.624
7.306
7.258
7.205
7.185
7.183
7.172
7.161
6.963
6.571
6.568
6.562
6.560
0.000
6.04
2.02
2.04
1.97
1.87
1.02
1.00
abundance
X : parts per Million : Proton
O
S
F
4p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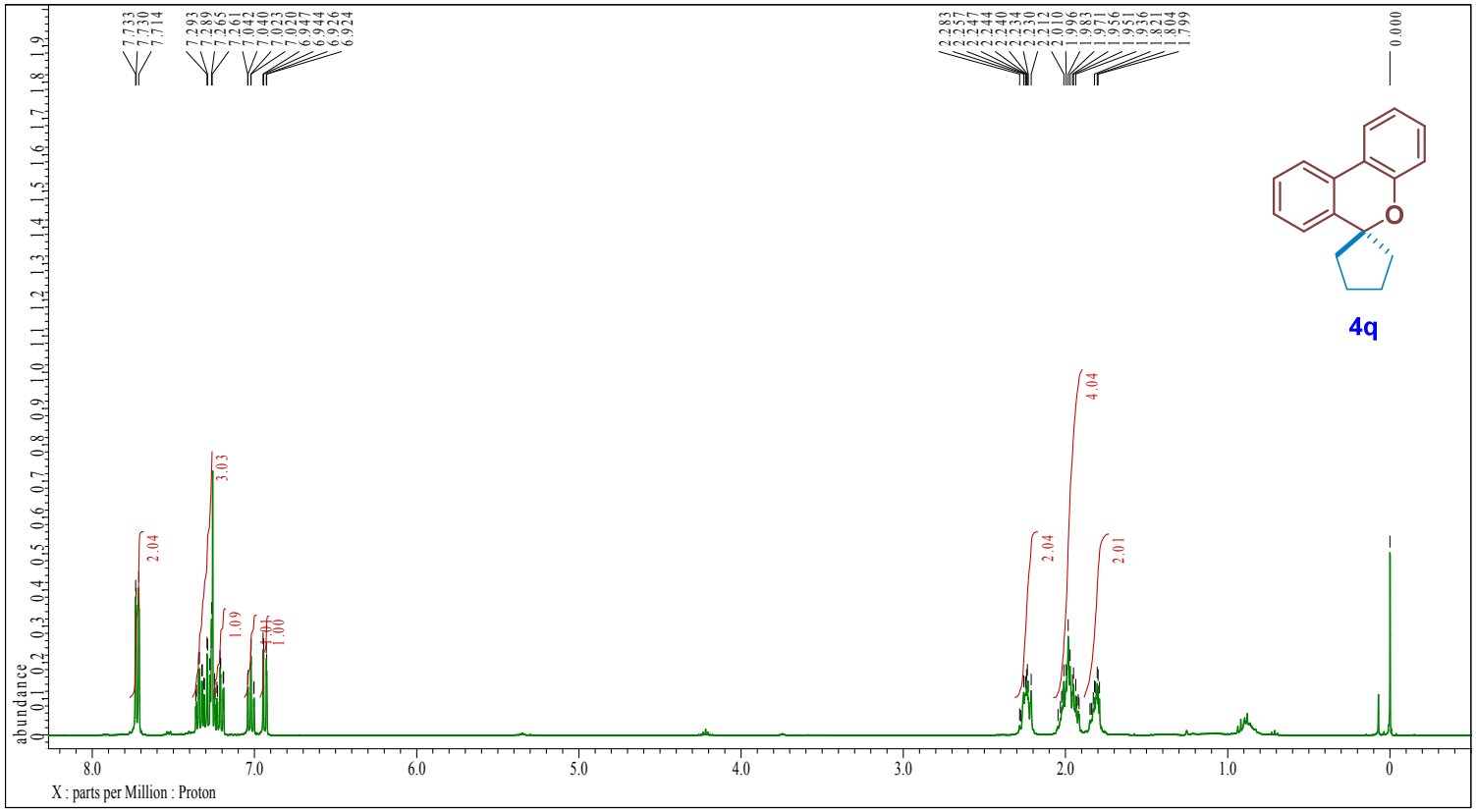
131.882
131.796
130.329
130.253
129.754
128.959
128.902
128.106
127.522
127.426
127.023
125.902
123.046
122.452
118.715
115.812
115.591
114.853
114.642
84.121
77.442
77.126
76.810
(thousandths)
X : parts per Million : Carbon13
O
S
F
4p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7.714
7.393
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7.265
7.261
7.042
7.040
7.023
7.020
6.947
6.944
6.926
6.924
2.283
2.257
2.247
2.244
2.240
2.234
2.230
2.212
2.010
1.996
1.983
1.971
1.956
1.951
1.936
1.821
1.804
1.799
0.000
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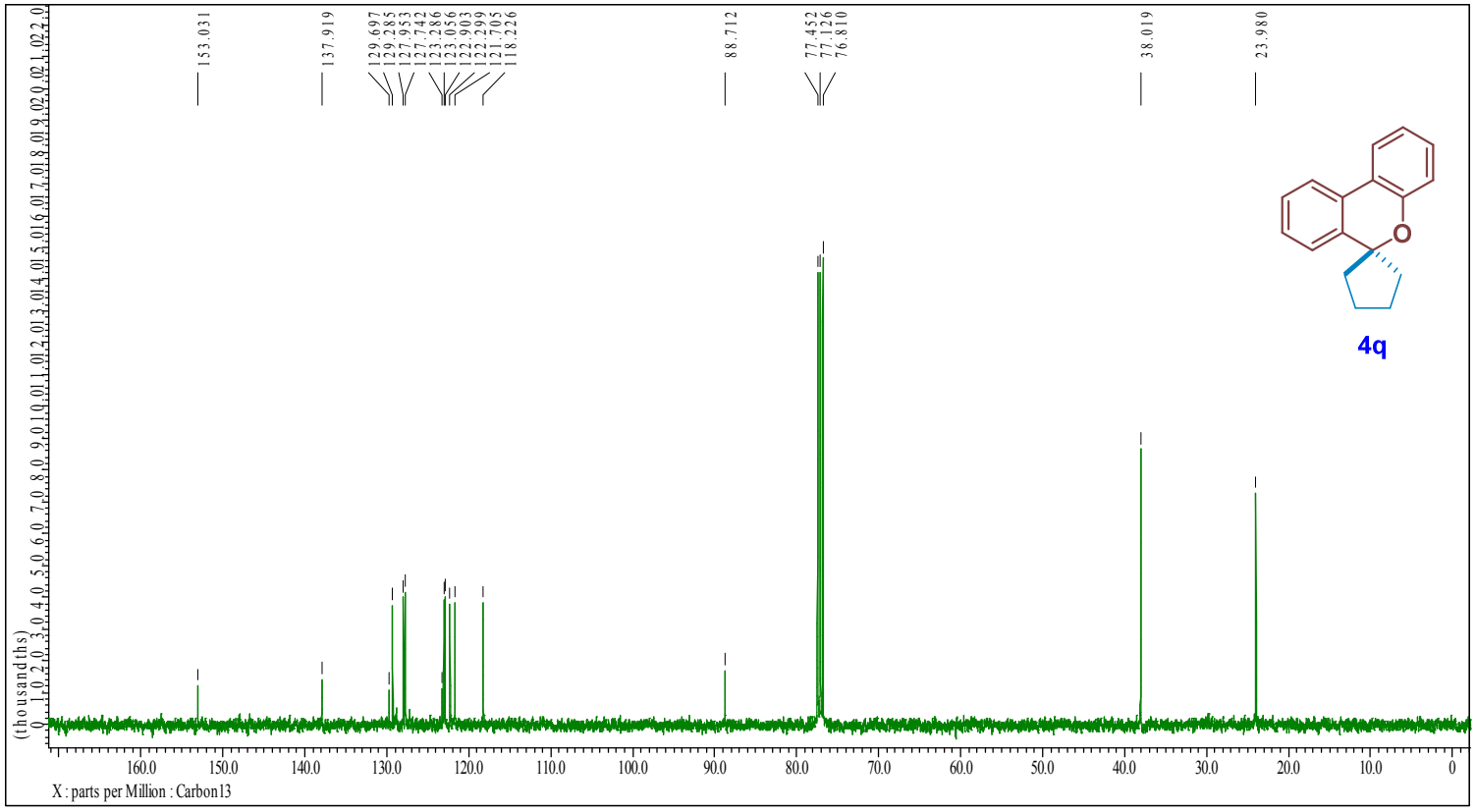
3.03
1.09
1.07
1.00
2.04
4.04
2.01
abundance
X : parts per Million : Proton
4q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123.056
122.903
122.299
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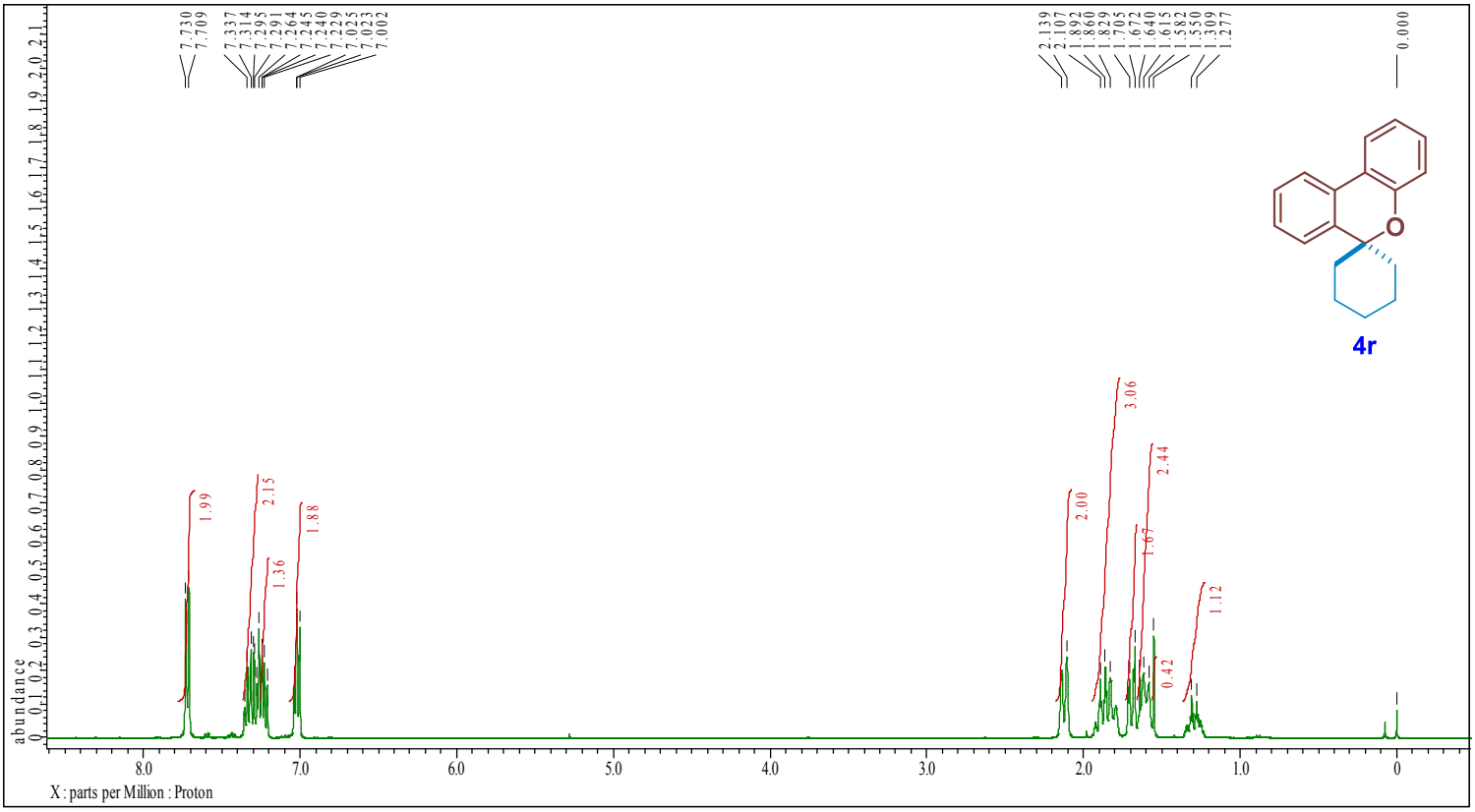
77.452
77.126
76.810
38.019
23.980
(thousandths)
X : parts per Million : Carbon13
4q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7.709
7.337
7.314
7.295
7.291
7.264
7.245
7.240
7.229
7.025
7.023
7.002
2.139
2.107
1.892
1.860
1.829
1.705
1.672
1.640
1.615
1.582
1.550
1.309
1.277
0.000
1.99
2.15
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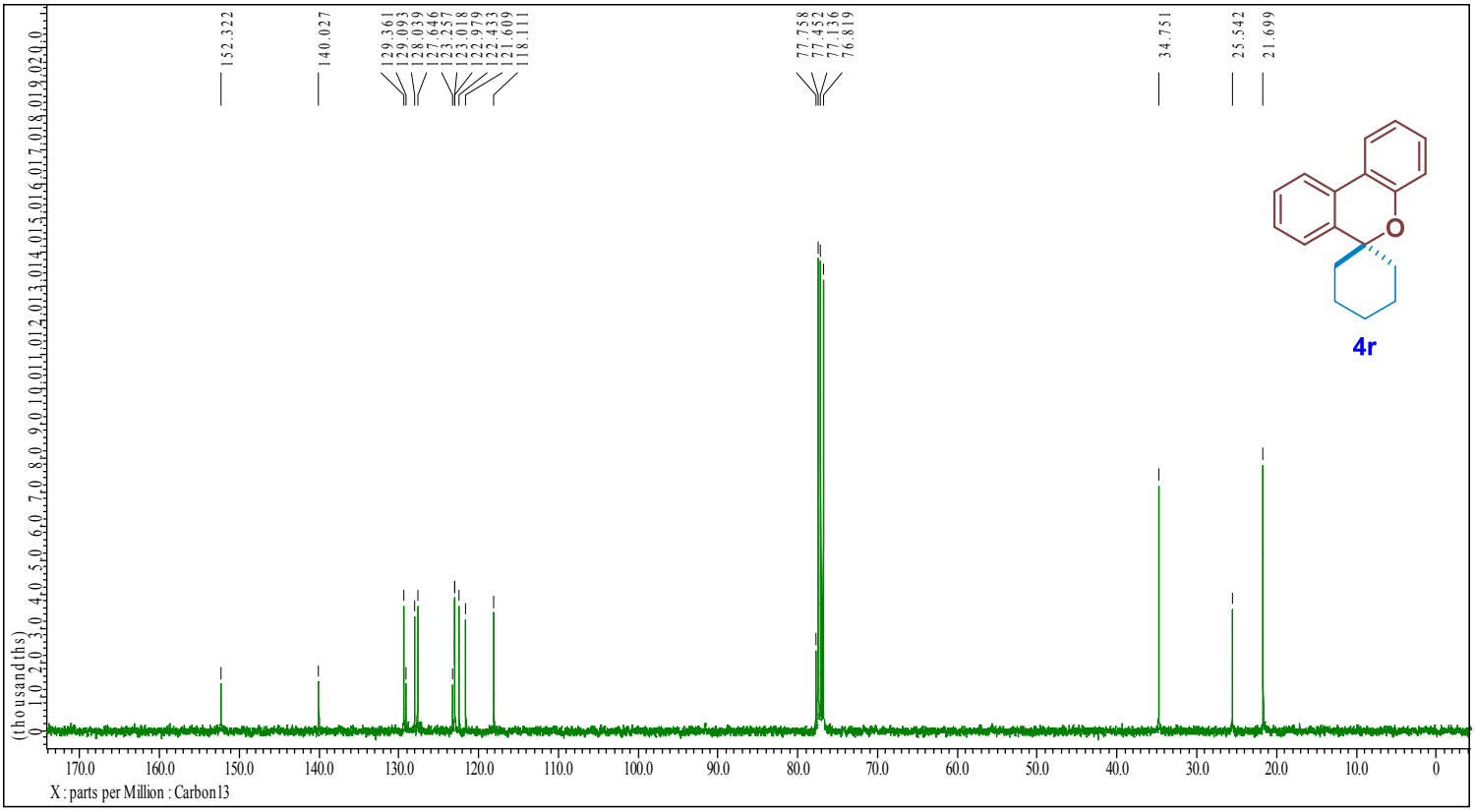
1.88
2.00
3.06
2.44
1.67
1.12
0.42
4r
abundance
X : parts per Million : Proton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122.433
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77.136
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34.751
25.542
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4r
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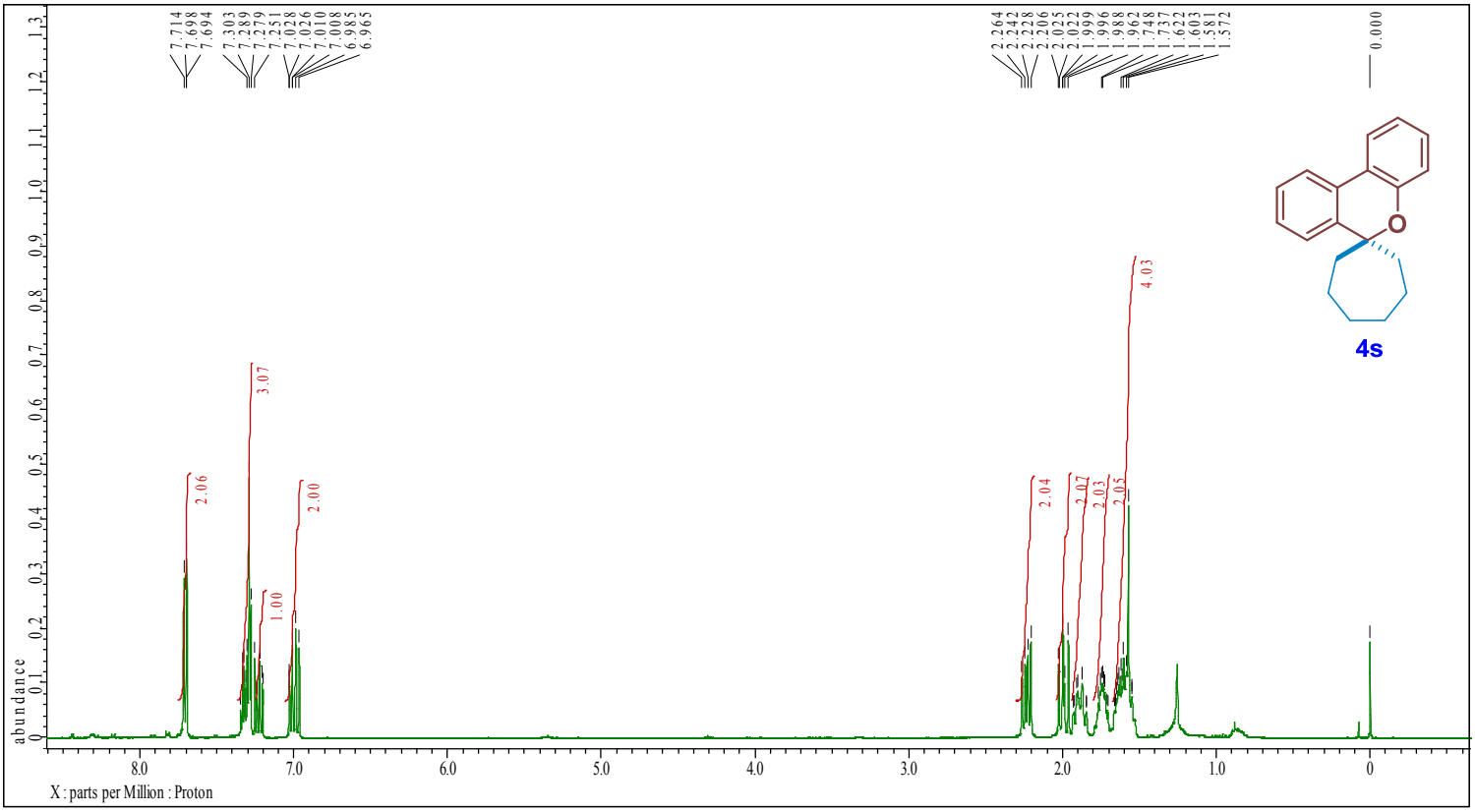
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7.028
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7.010
7.008
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6.965
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2.242
2.228
2.206
2.025
2.022
1.999
1.996
1.988
1.962
1.748
1.737
1.622
1.603
1.581
1.572
0.000
4.03
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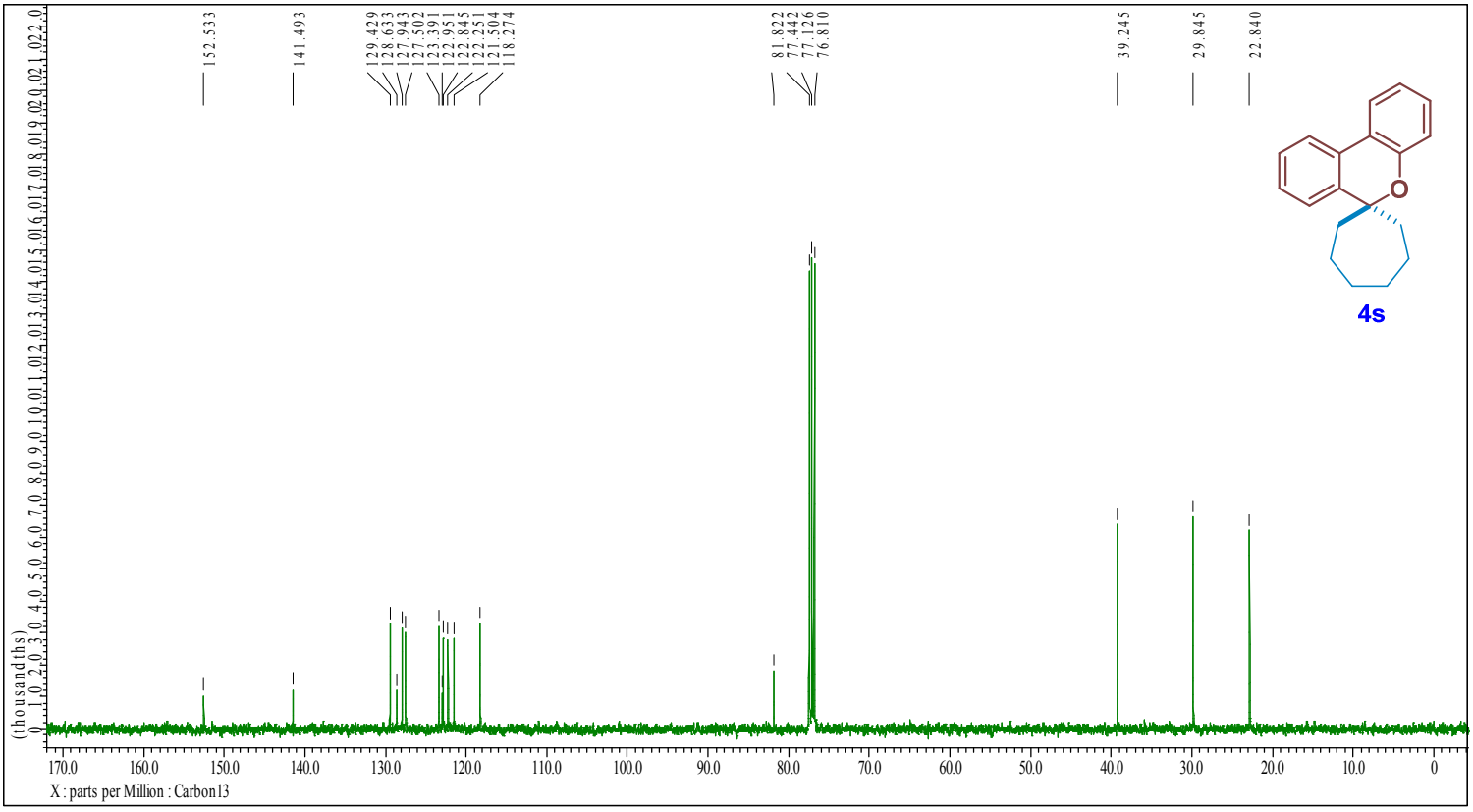
2.00
1.00
2.04
2.07
2.03
2.05
4s
abundance
X : parts per Million : Proton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122.251
121.504
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77.126
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39.245
29.845
22.840
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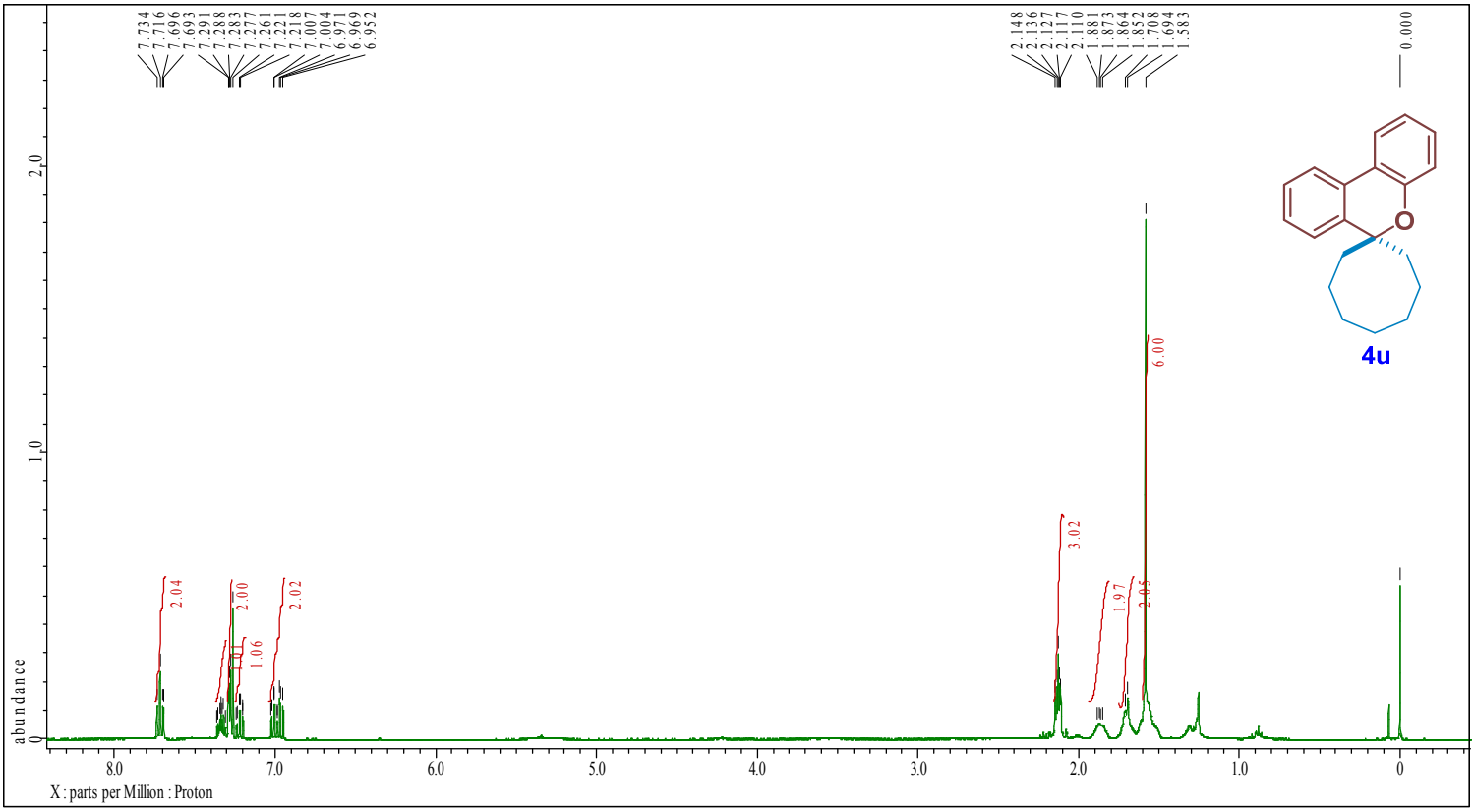
(thousandths)
X : parts per Million : Carbon13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7.283
7.277
7.261
7.221
7.218
7.007
7.004
6.971
6.969
6.952
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2.136
2.127
2.117
2.110
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1.873
1.864
1.852
1.708
1.694
1.583
0.000
2.04
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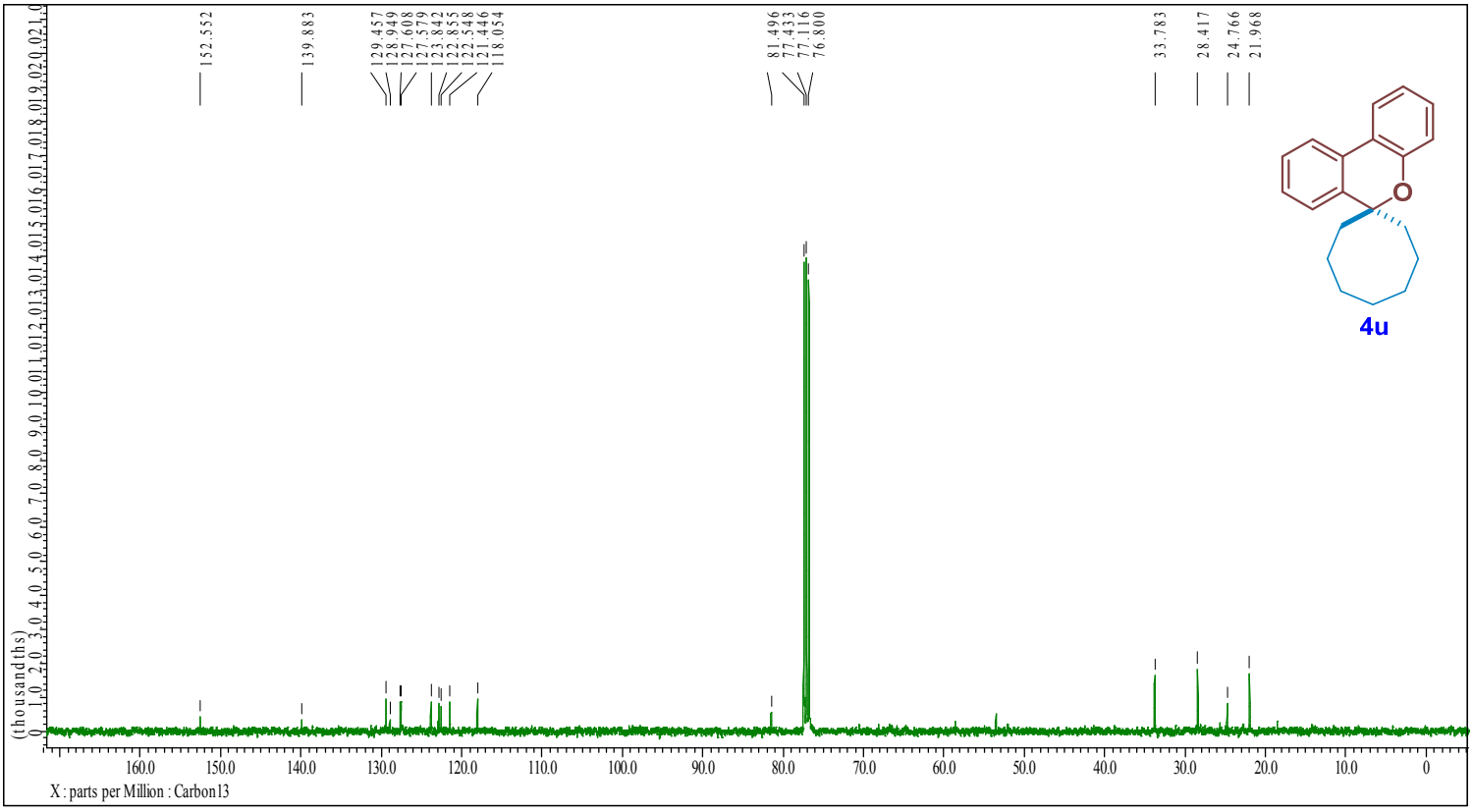
1.06
2.02
3.02
1.97
2.05
6.00
abundance
X : parts per Million : Proton
4u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121.446
118.054
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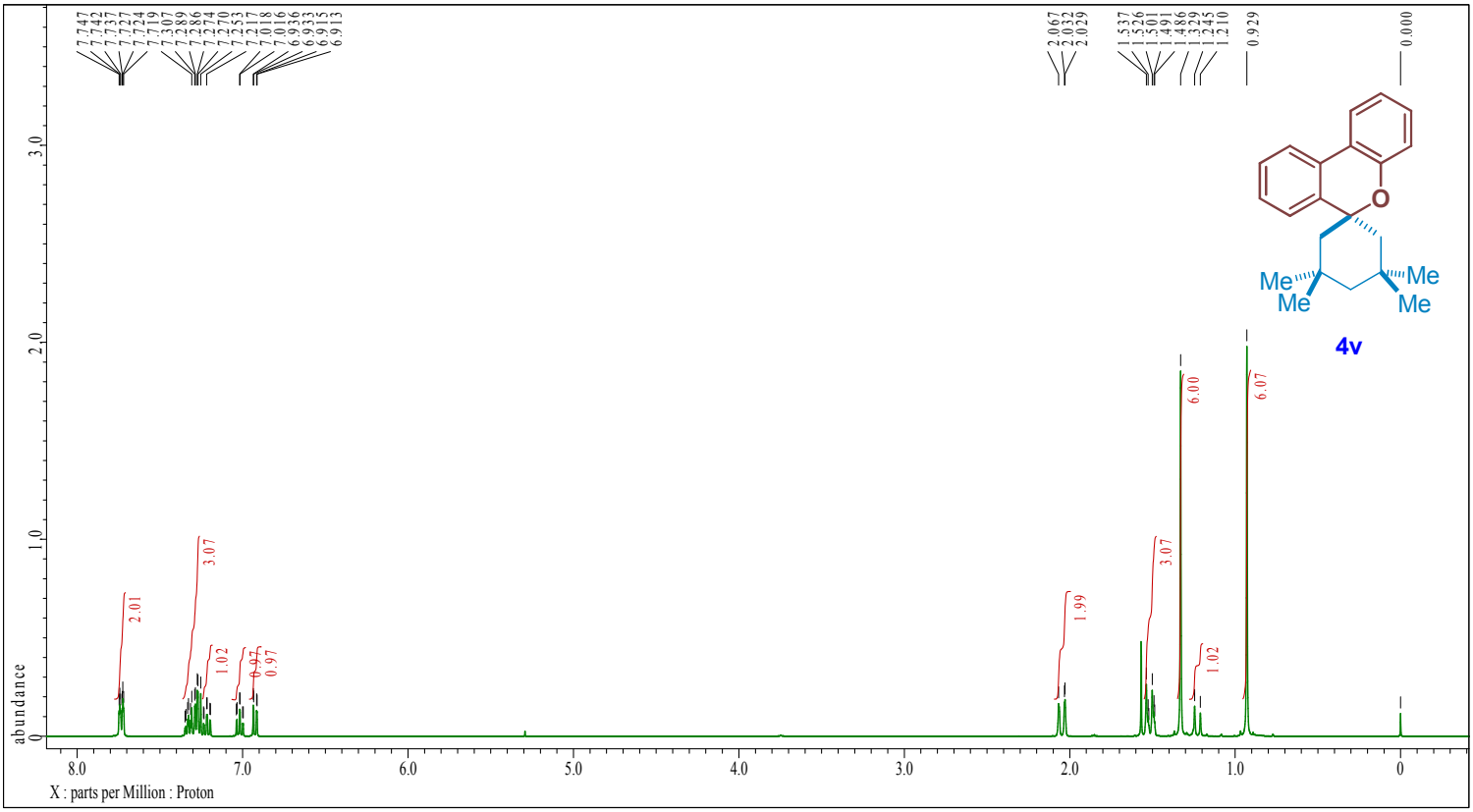
76.800
33.783
28.417
24.766
21.968
(thousandths)
X : parts per Million : Carbon13
4u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7.286
7.274
7.270
7.253
7.217
7.018
7.016
6.936
6.933
6.915
6.913
2.067
2.032
2.029
1.537
1.526
1.501
1.491
1.486
1.329
1.245
1.210
0.929
0.000
O
Me
Me
Me
Me
4v
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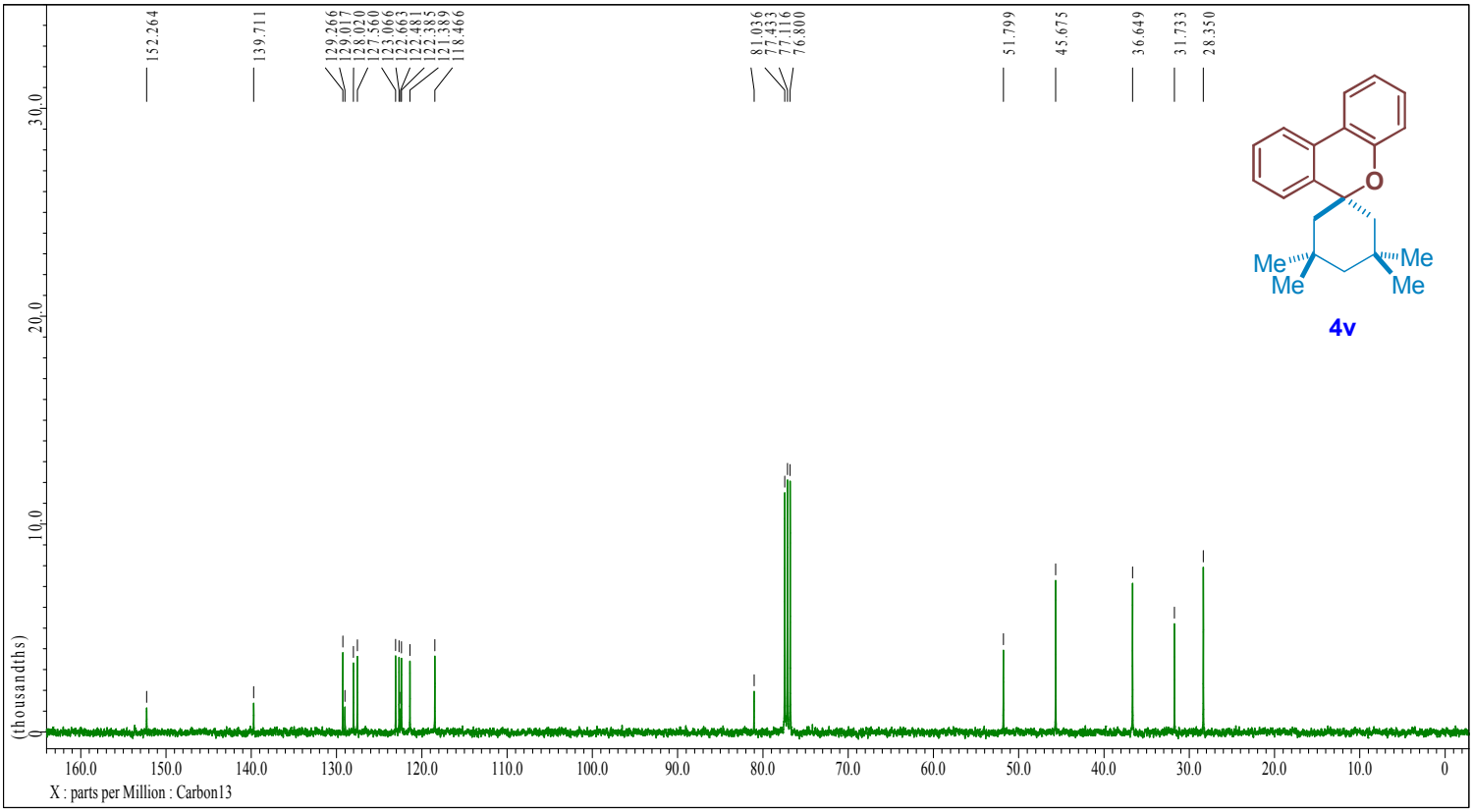
3.07
6.00
1.02
6.07
abundance
X : parts per Million : Proton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122.385
121.389
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77.433
77.116
76.800
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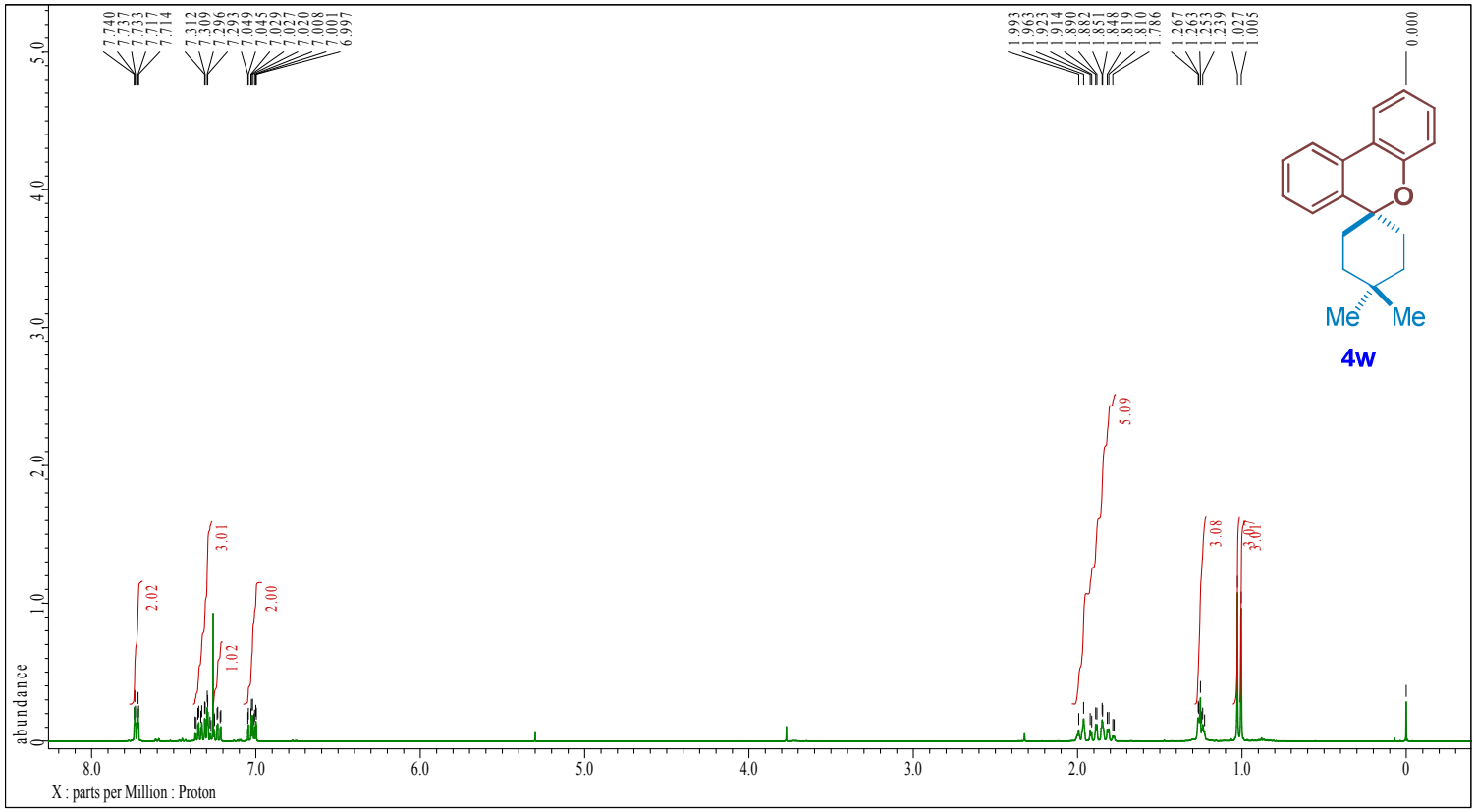
31.733
28.350
O
Me
Me
Me
Me
4v
(thousandths)
X : parts per Million : Carbon13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7.717
7.714
7.312
7.309
7.296
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7.049
7.045
7.029
7.027
7.020
7.008
7.001
6.997
1.993
1.963
1.923
1.914
1.890
1.882
1.851
1.848
1.819
1.810
1.786
1.267
1.263
1.253
1.239
1.027
1.005
0.000
2.02
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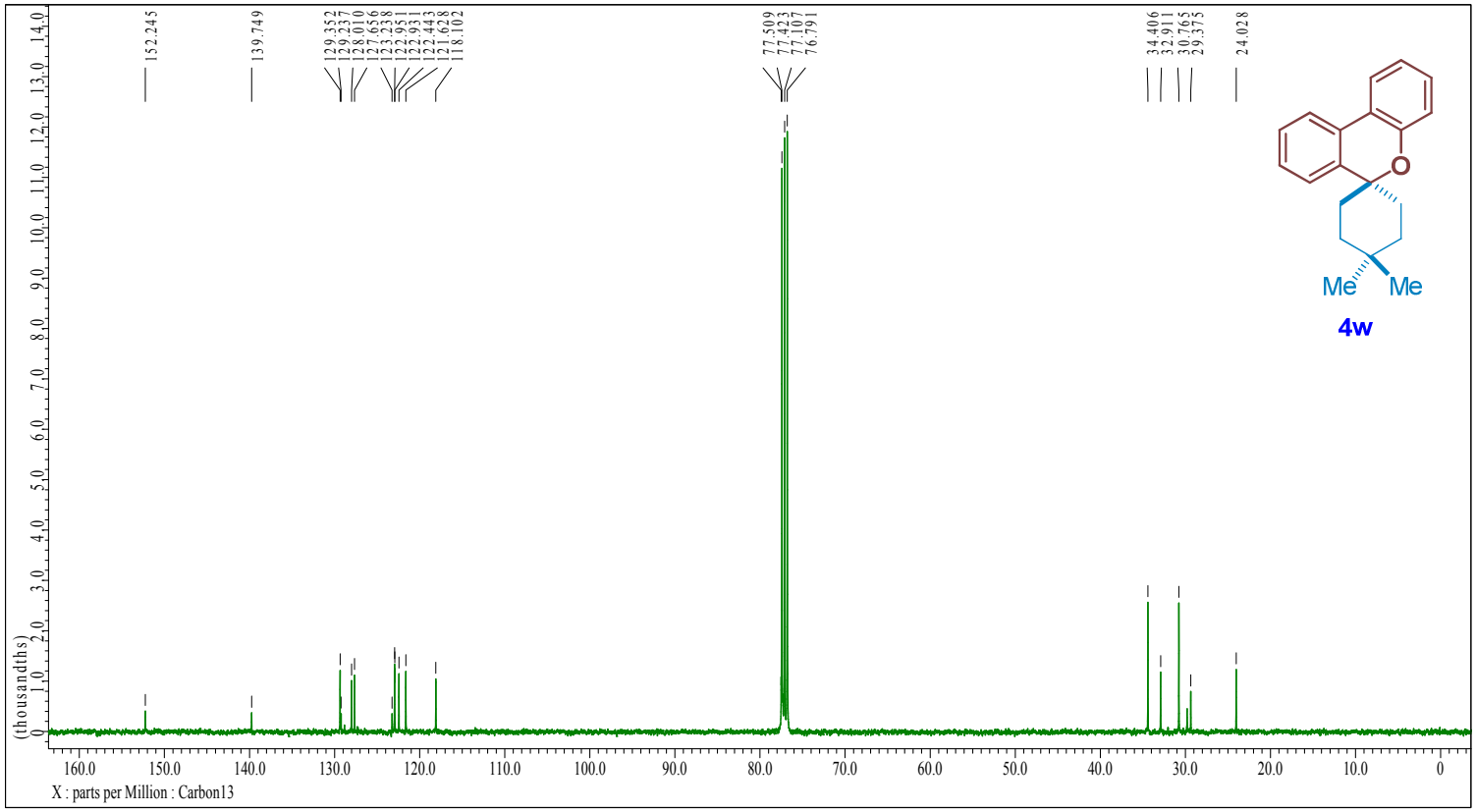
2.00
5.09
3.08
3.07
3.01
abundance
X : parts per Million : Proton
Me
Me
4w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121.628
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77.509
77.403
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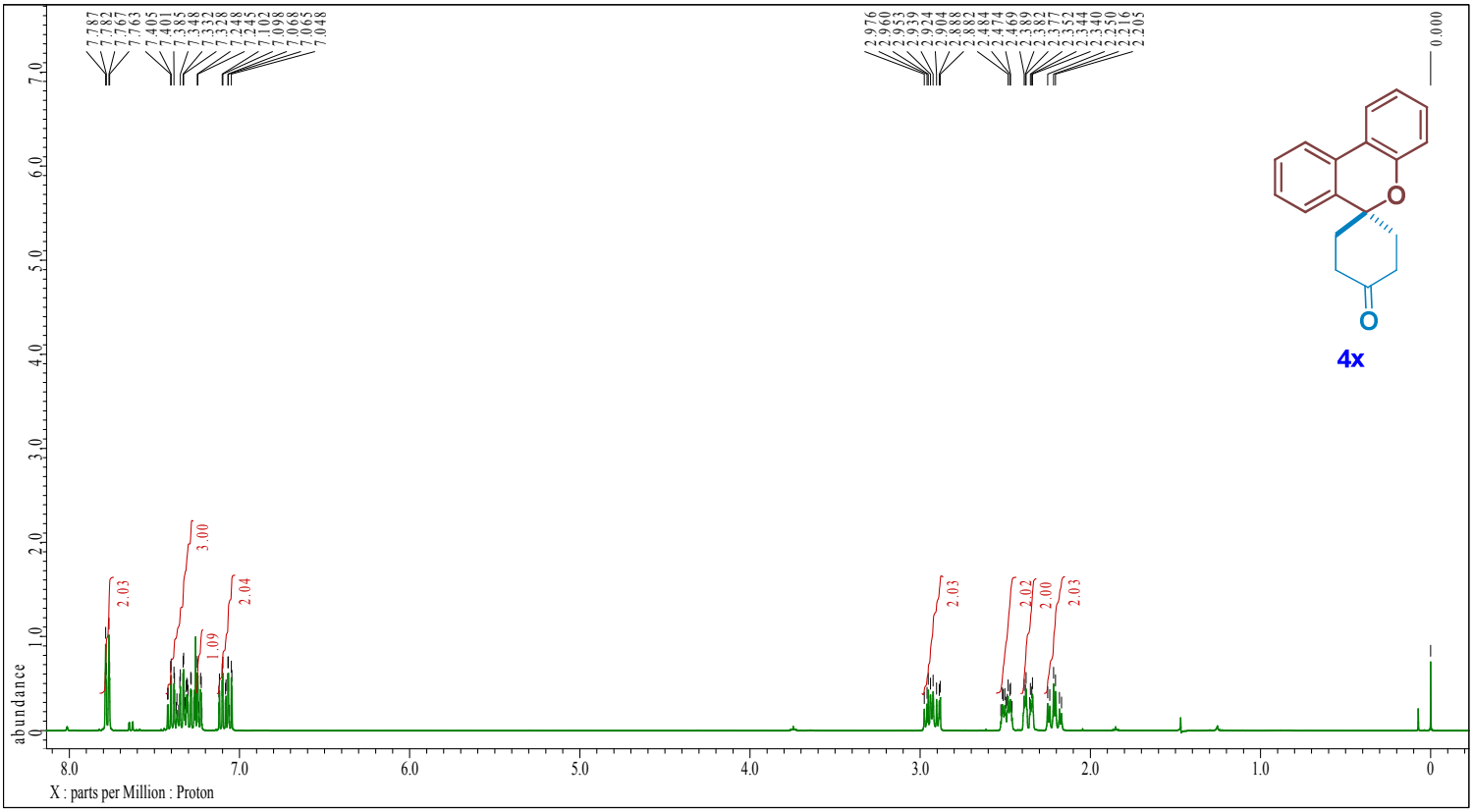
32.911
30.765
29.375
24.028
(thousandths)
X : parts per Million : Carbon13
Me
Me
4w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7.068
7.065
7.048
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2.960
2.953
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2.924
2.904
2.888
2.882
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0.000
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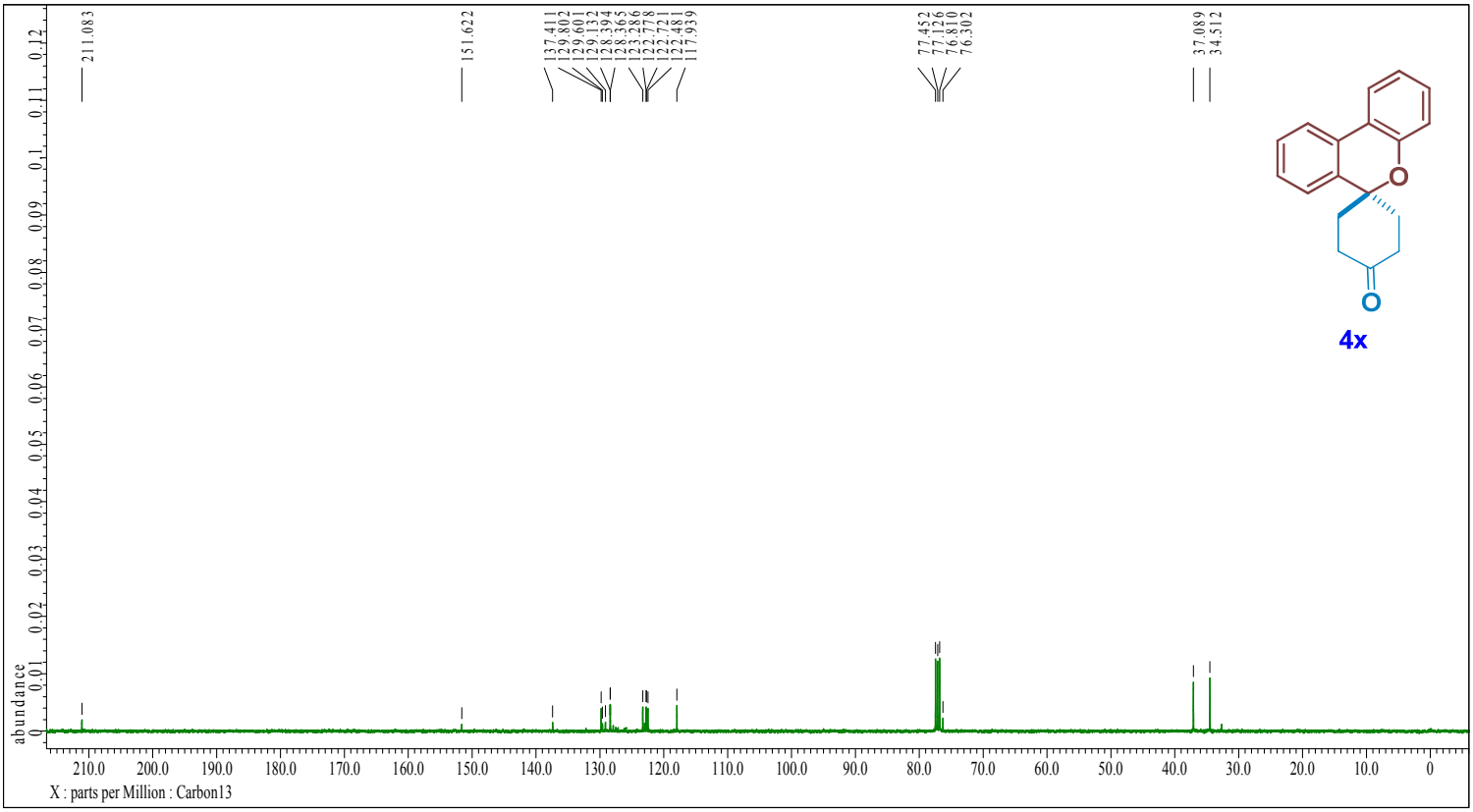
3.00
1.09
2.04
2.03
2.02
2.00
2.03
abundance
X : parts per Million : Proton
4x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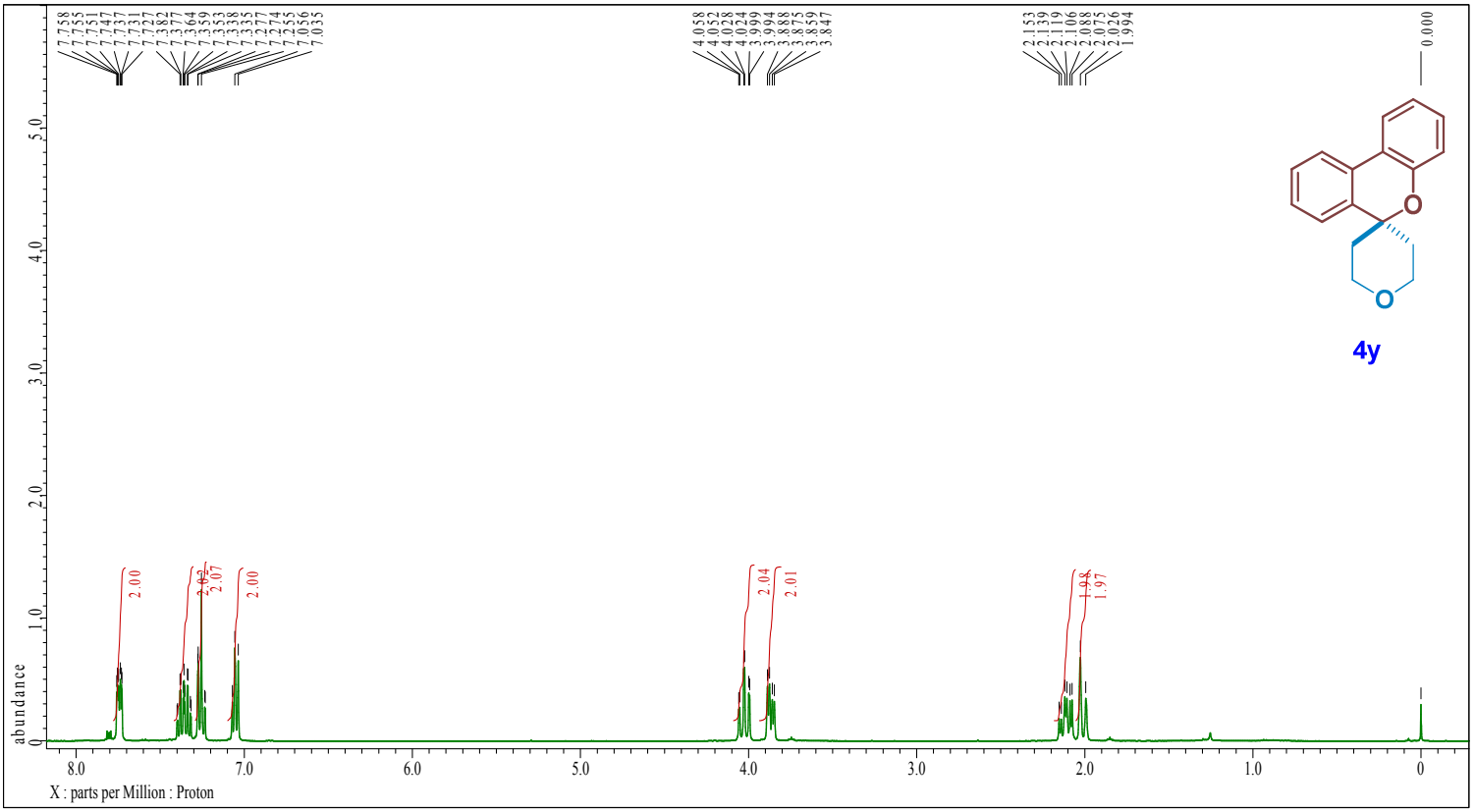
129.802
129.601
129.132
128.394
128.365
123.286
122.778
122.721
122.481
117.939
77.452
77.126
76.810
76.302
37.089
34.512
abundance
X : parts per Million : Carbon13
4x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2.106
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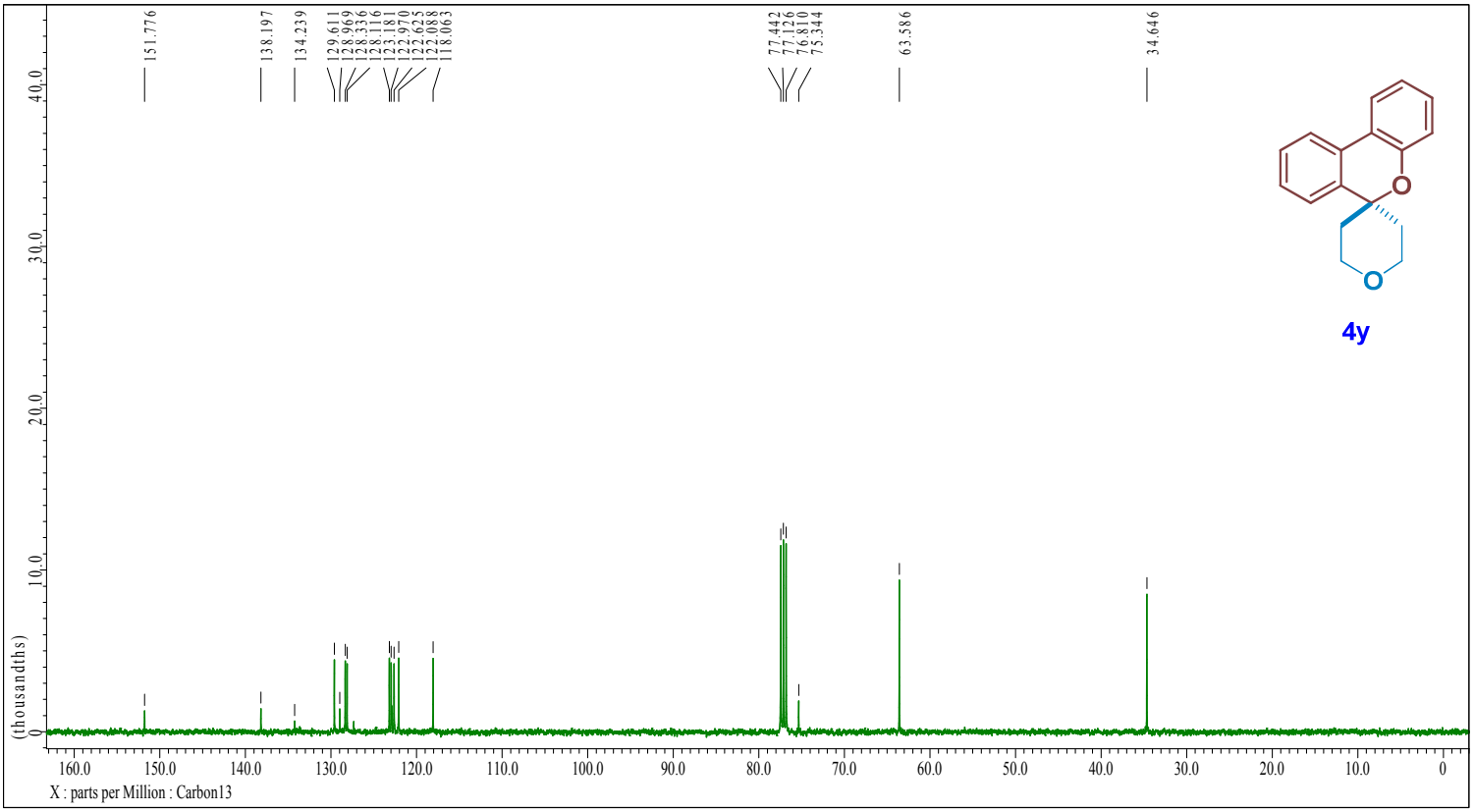
2.075
2.026
1.994
0.000
2.00
2.07
2.07
2.00
2.04
2.01
1.98
1.97
abundance
X : parts per Million : Proton
4y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134.239
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128.336
128.116
123.181
122.970
122.625
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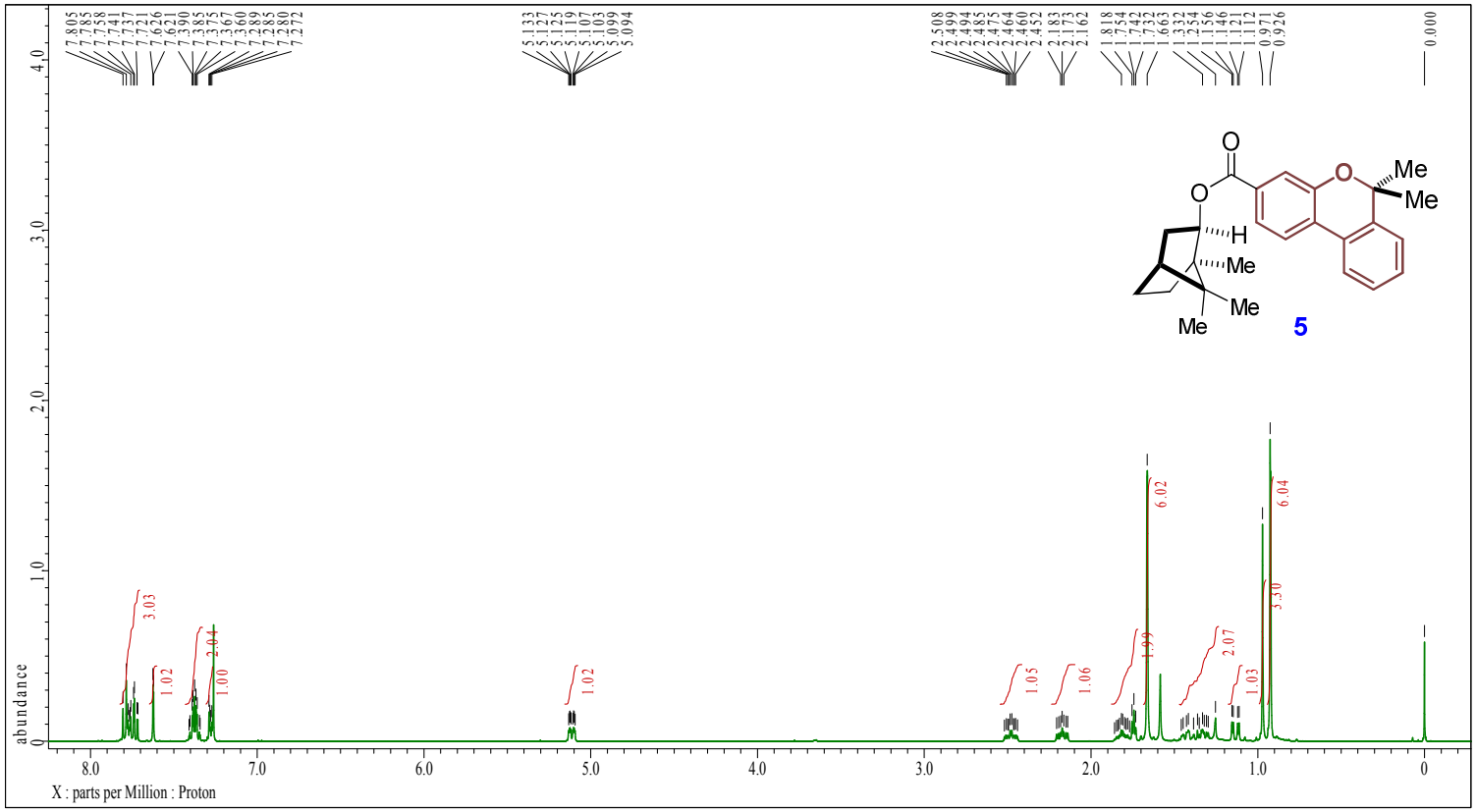
77.126
76.810
75.344
63.586
34.646
(thousandths)
X : parts per Million : Carbon13
4y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7.390
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7.375
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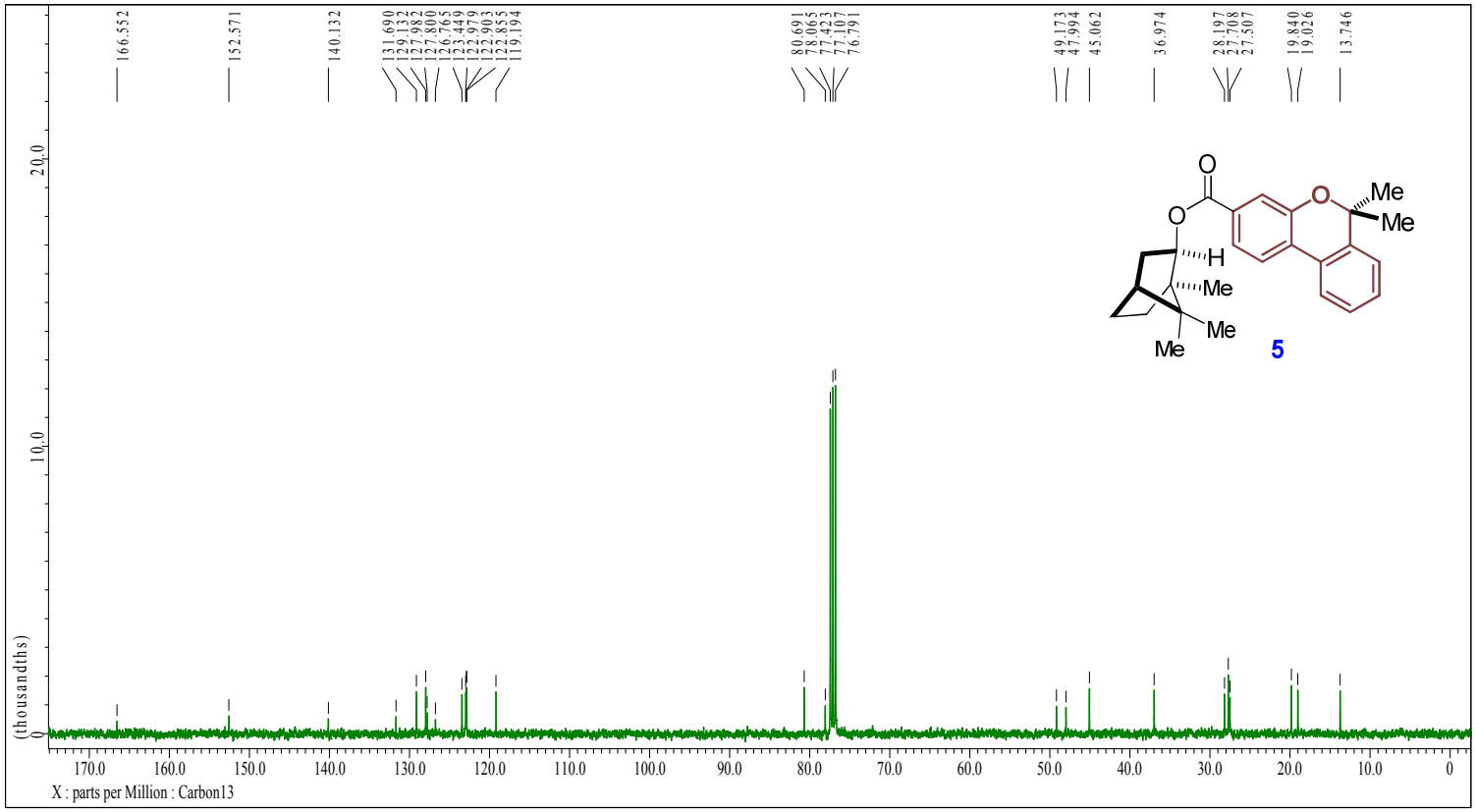
7.360
7.289
7.285
7.280
7.272
5.133
5.127
5.125
5.119
5.107
5.103
5.099
5.094
2.508
2.499
2.494
2.485
2.475
2.464
2.460
2.452
2.183
2.173
2.162
1.818
1.754
1.742
1.732
1.663
1.332
1.254
1.156
1.146
1.121
1.112
0.971
0.926
0.000
O
O
Me
Me
H
Me
Me
Me
5
3.03
1.02
2.04
1.00
1.02
1.05
1.06
1.99
6.02
2.07
1.03
3.30
6.04
abundance
X : parts per Million : Proton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140.132
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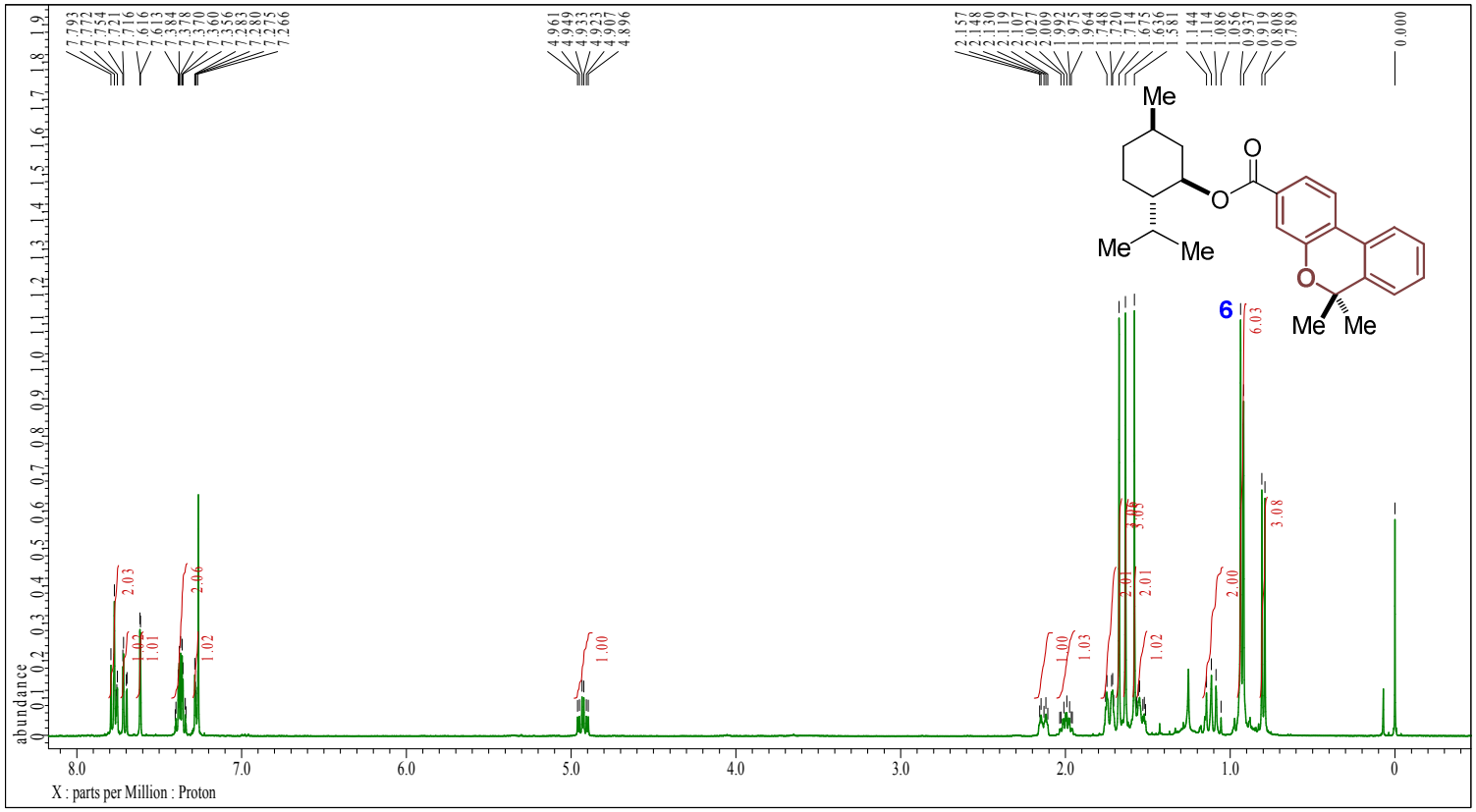
129.132
127.982
127.800
126.765
123.449
122.979
122.903
122.855
119.194
80.691
78.065
77.423
77.107
76.791
49.173
47.994
45.062
36.974
28.197
27.708
27.507
19.840
19.026
13.746
O
O
Me
Me
H
Me
Me
Me
5
(thousandths)
X : parts per Million : Carbon13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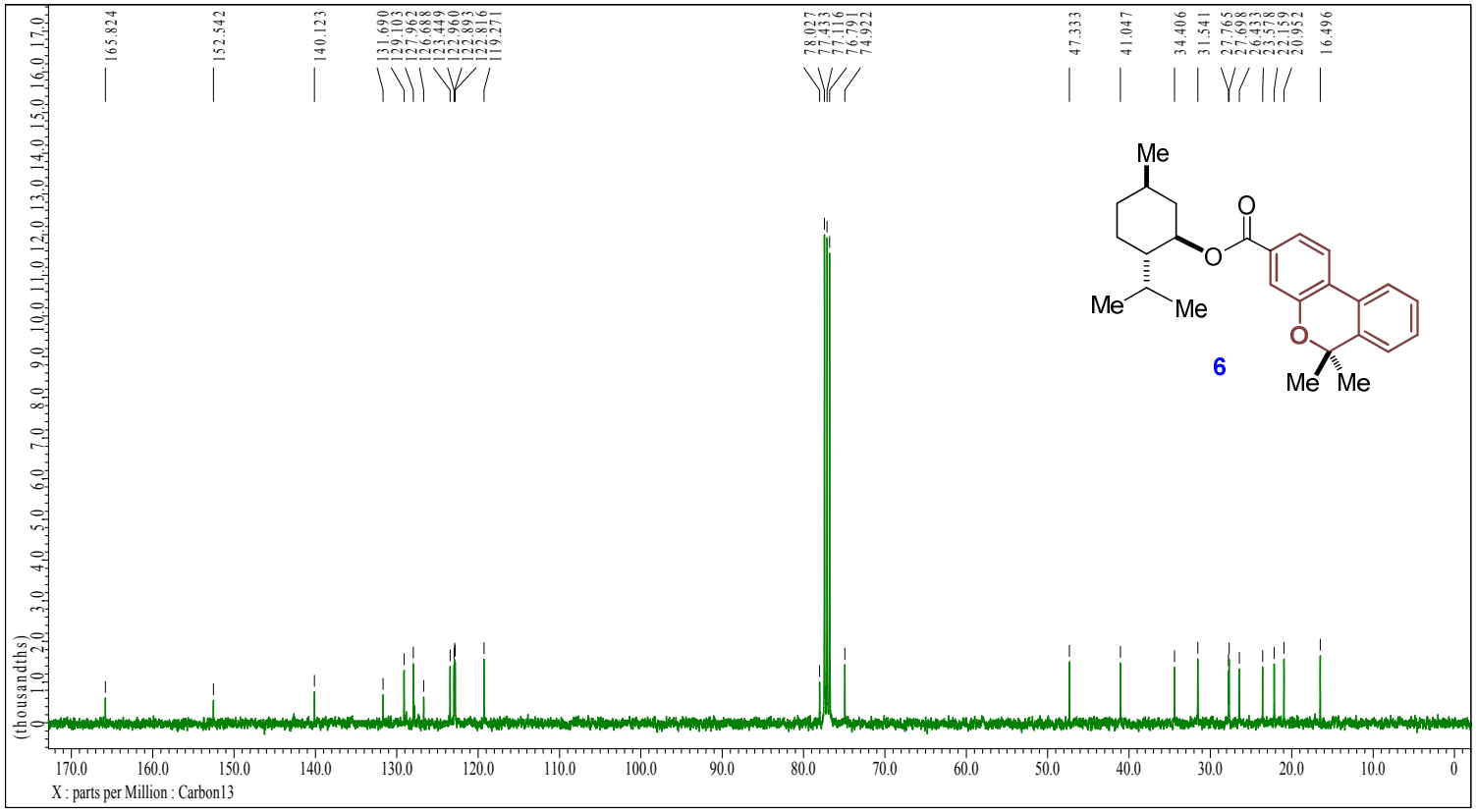
7.384
7.378
7.370
7.360
7.356
7.283
7.280
7.275
7.266
4.961
4.949
4.933
4.923
4.907
4.896
2.157
2.148
2.130
2.119
2.107
2.027
2.009
1.992
1.975
1.964
1.748
1.720
1.714
1.675
1.636
1.581
1.144
1.114
1.086
1.056
0.937
0.919
0.808
0.789
0.000
Me
O
O
Me
Me
O
Me
Me
6
6.03
3.08
3.08
2.03
2.06
2.01
2.00
1.03
1.02
1.00
1.00
1.03
1.02
1.01
1.02
abundance
X : parts per Million : Proton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140.123
131.690
129.103
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126.688
124.449
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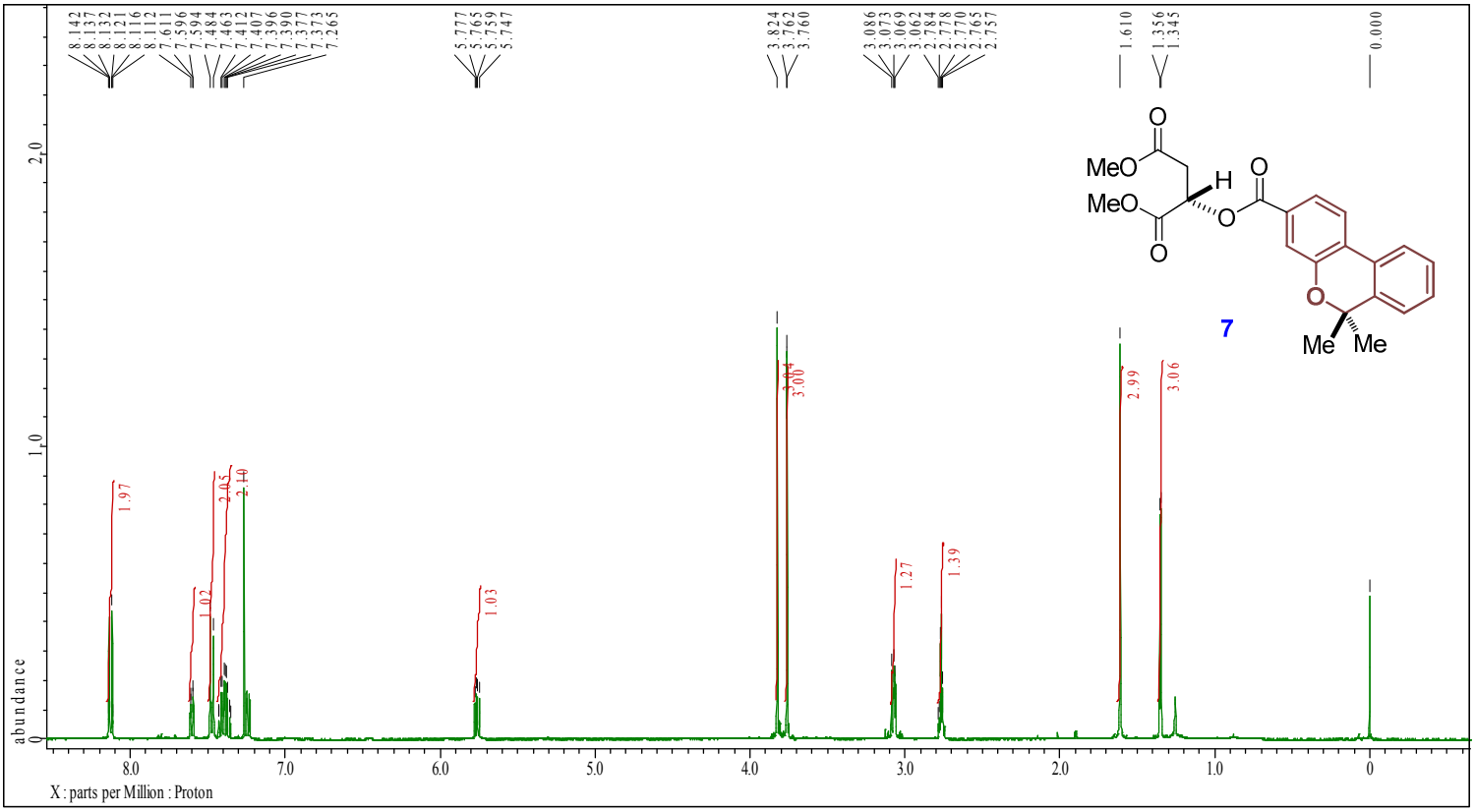
122.813
122.816
119.271
78.027
77.453
77.116
76.701
74.922
47.333
41.047
34.406
31.541
27.765
27.698
26.433
23.578
22.159
20.952
16.496
Me
O
O
Me
Me
O
Me
Me
6
(thousandths)
X : parts per Million : Carbon13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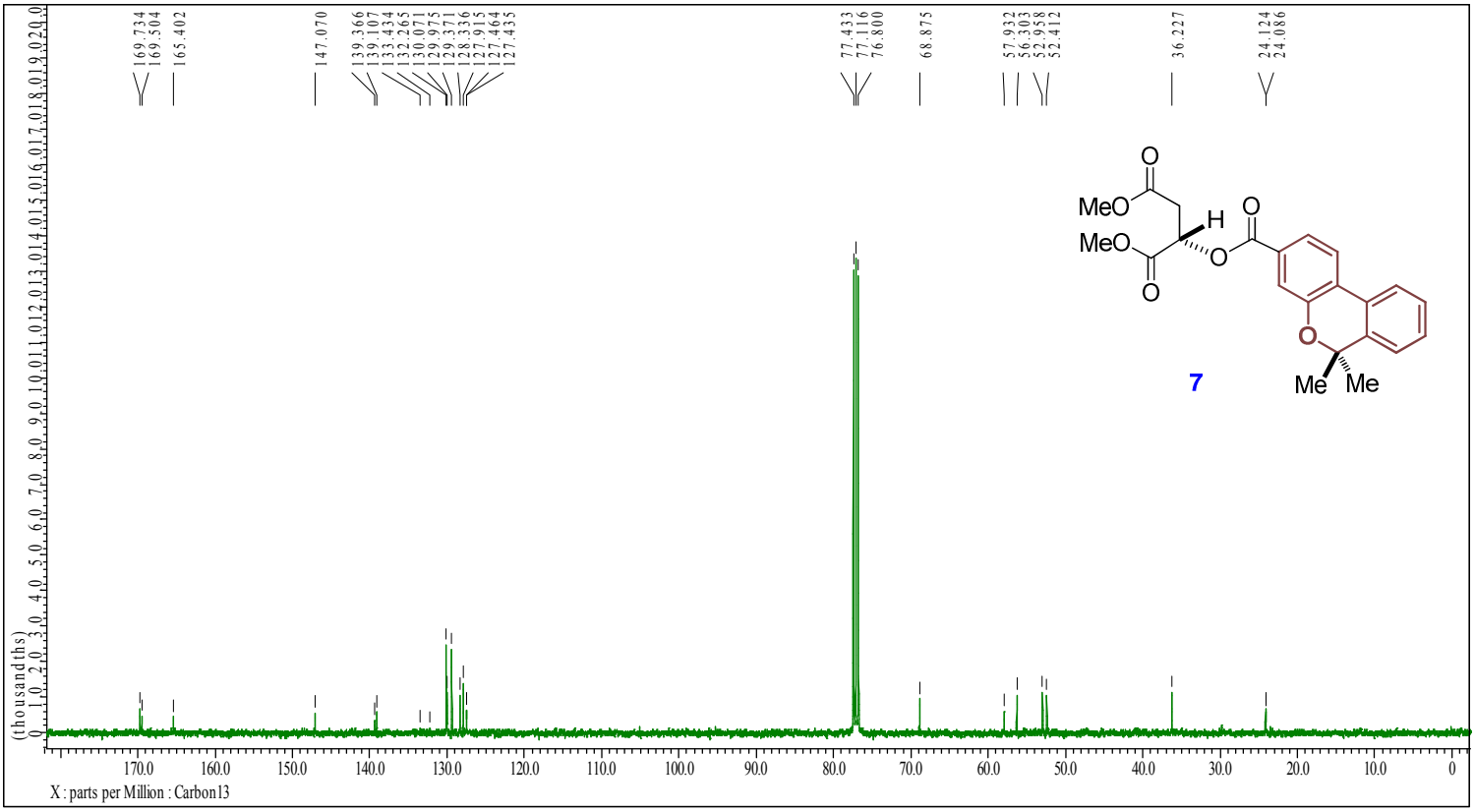
8.132
8.121
8.116
8.112
7.611
7.596
7.594
7.484
7.463
7.412
7.407
7.396
7.390
7.377
7.373
7.265
5.777
5.765
5.759
5.747
3.824
3.762
3.760
3.086
3.073
3.069
3.062
2.784
2.778
2.770
2.765
2.757
1.610
1.356
1.345
0.000
1.97
1.02
2.05
2.10
1.03
3.00
1.27
1.39
2.99
3.06
abundance
X : parts per Million : Proton
MeO
MeO
H
O
Me
Me
7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169.504
165.402
147.070
139.366
139.107
133.434
132.265
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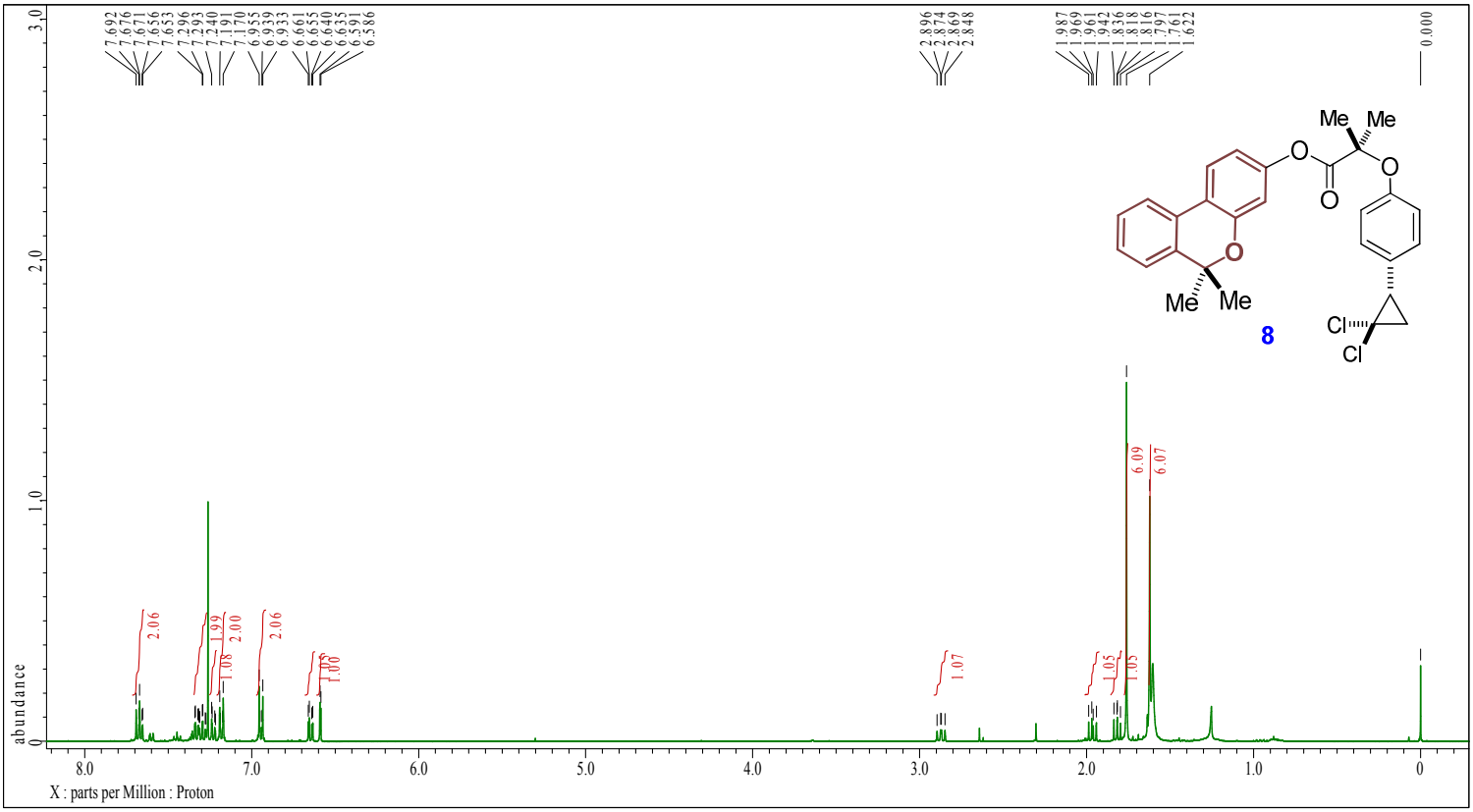
129.975
129.371
128.336
127.915
127.464
127.435
77.433
77.116
76.800
68.875
57.932
56.303
52.958
52.412
36.227
24.124
24.086
(thousandths)
X : parts per Million : Carbon13
MeO
MeO
H
O
Me
Me
7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7.656
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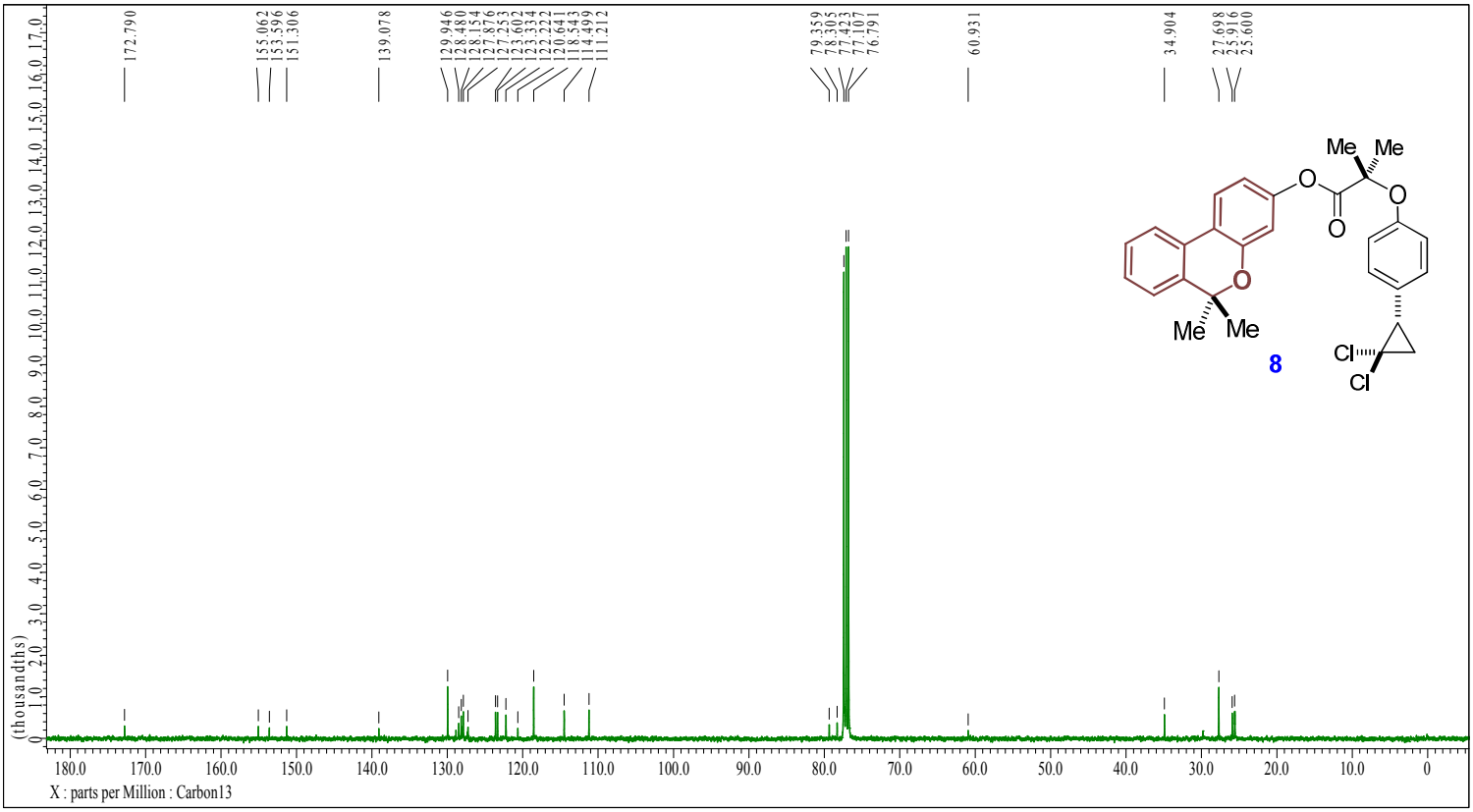
7.293
7.240
7.191
7.170
6.955
6.939
6.933
6.661
6.655
6.640
6.635
6.591
6.586
2.896
2.874
2.869
2.848
1.987
1.969
1.961
1.942
1.836
1.818
1.816
1.797
1.761
1.622
0.000
2.06
1.99
1.08
2.00
2.06
1.08
1.06
1.07
1.05
1.05
6.09
6.07
abundance
X : parts per Million : Proton
Me Me
O
O
O
O
Me Me
Cl
Cl
8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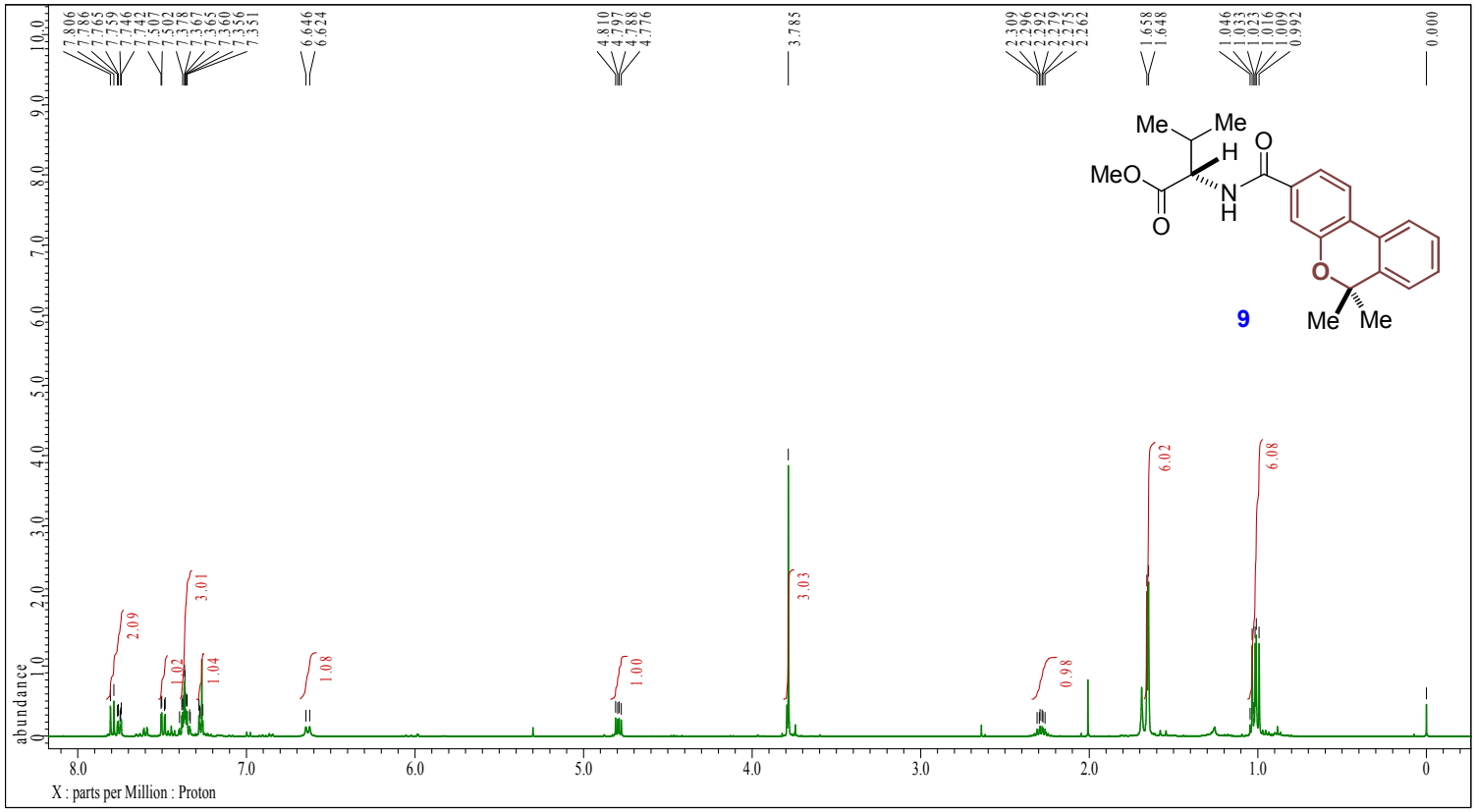
153.596
151.306
139.078
129.946
128.480
128.154
127.876
127.253
123.602
123.334
122.222
120.641
118.543
114.499
111.212
79.359
78.305
77.423
77.107
76.791
60.931
34.904
27.698
25.916
25.600
(thousandths)
X : parts per Million : Carbon13
Me Me
O
O
O
O
Me Me
Cl
Cl
8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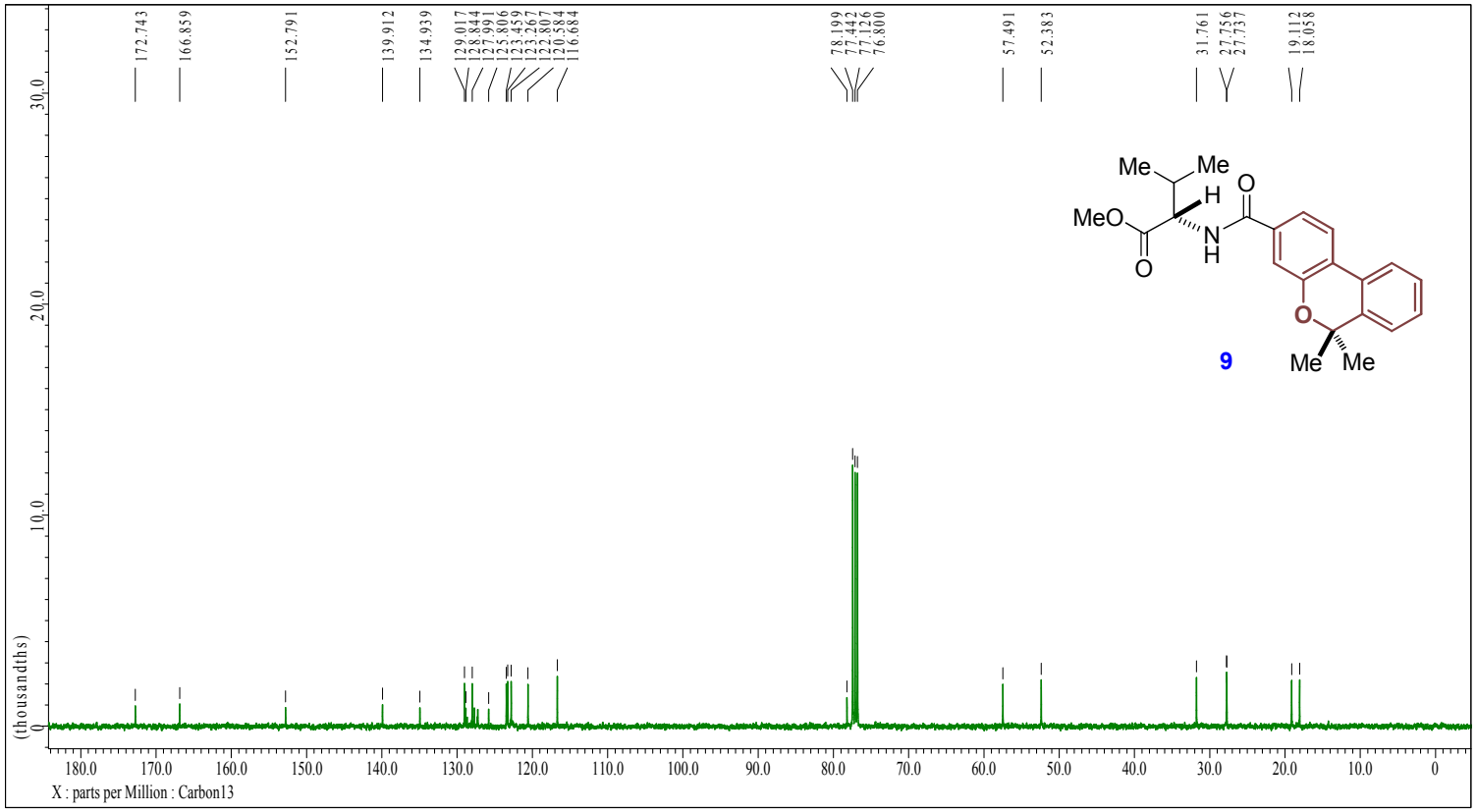
7.765
7.759
7.746
7.742
7.507
7.502
7.378
7.367
7.365
7.360
7.356
7.351
6.646
6.624
4.810
4.797
4.788
4.776
3.785
2.309
2.296
2.292
2.279
2.275
2.262
1.658
1.648
1.046
1.033
1.023
1.016
1.009
0.992
0.000
Me
Me
H
O
MeO
N
H
O
O
Me
Me
9
2.09
3.01
1.02
1.04
1.08
1.00
3.03
0.98
6.02
6.08
abundance
X : parts per Million : Proton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125.806
123.459
123.267
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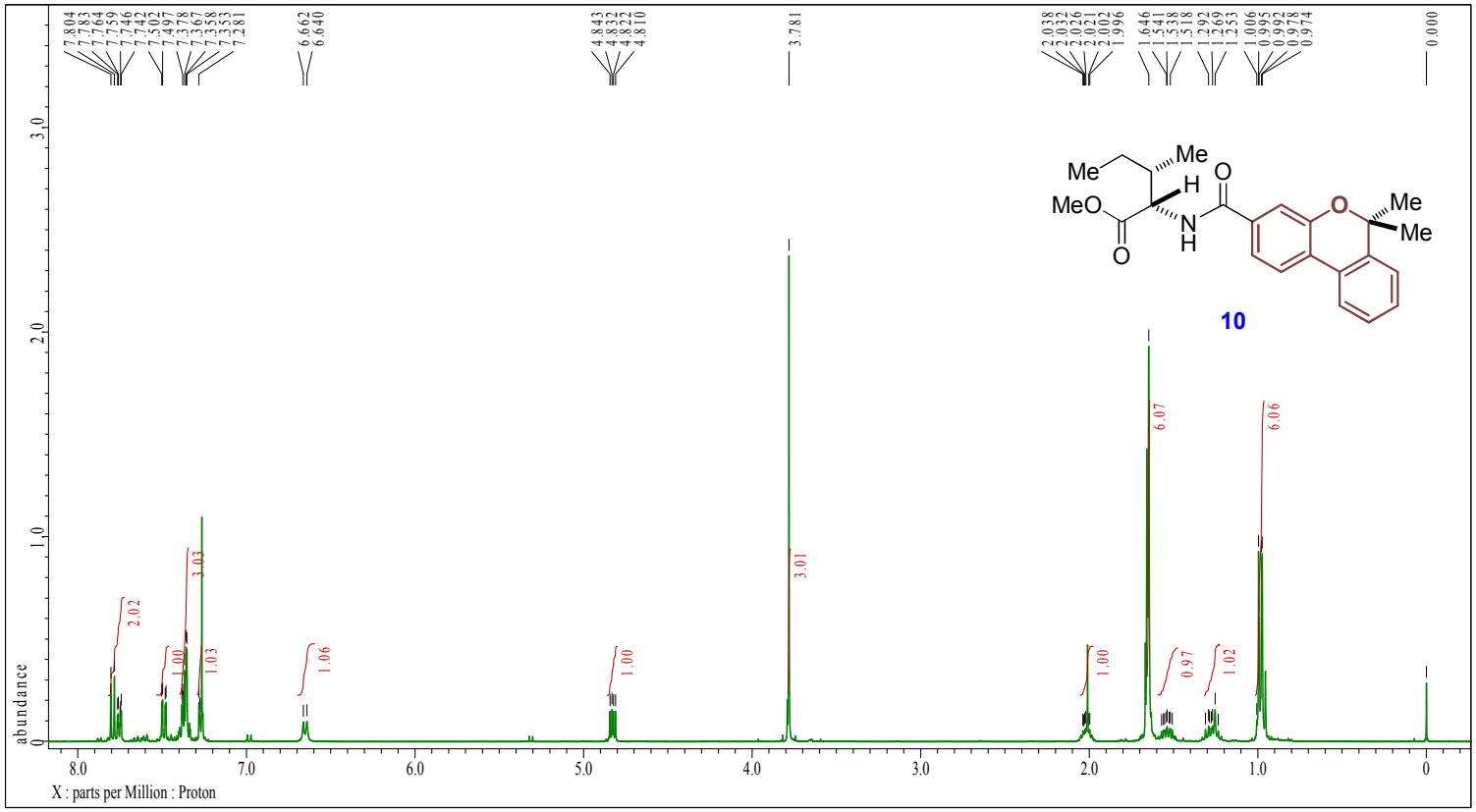
120.584
116.684
78.199
77.442
77.126
76.800
57.491
52.383
31.761
27.756
27.737
19.112
18.058
Me
Me
H
O
MeO
N
H
O
O
Me
Me
9
(thousandths)
X : parts per Million : Carbon13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7.759
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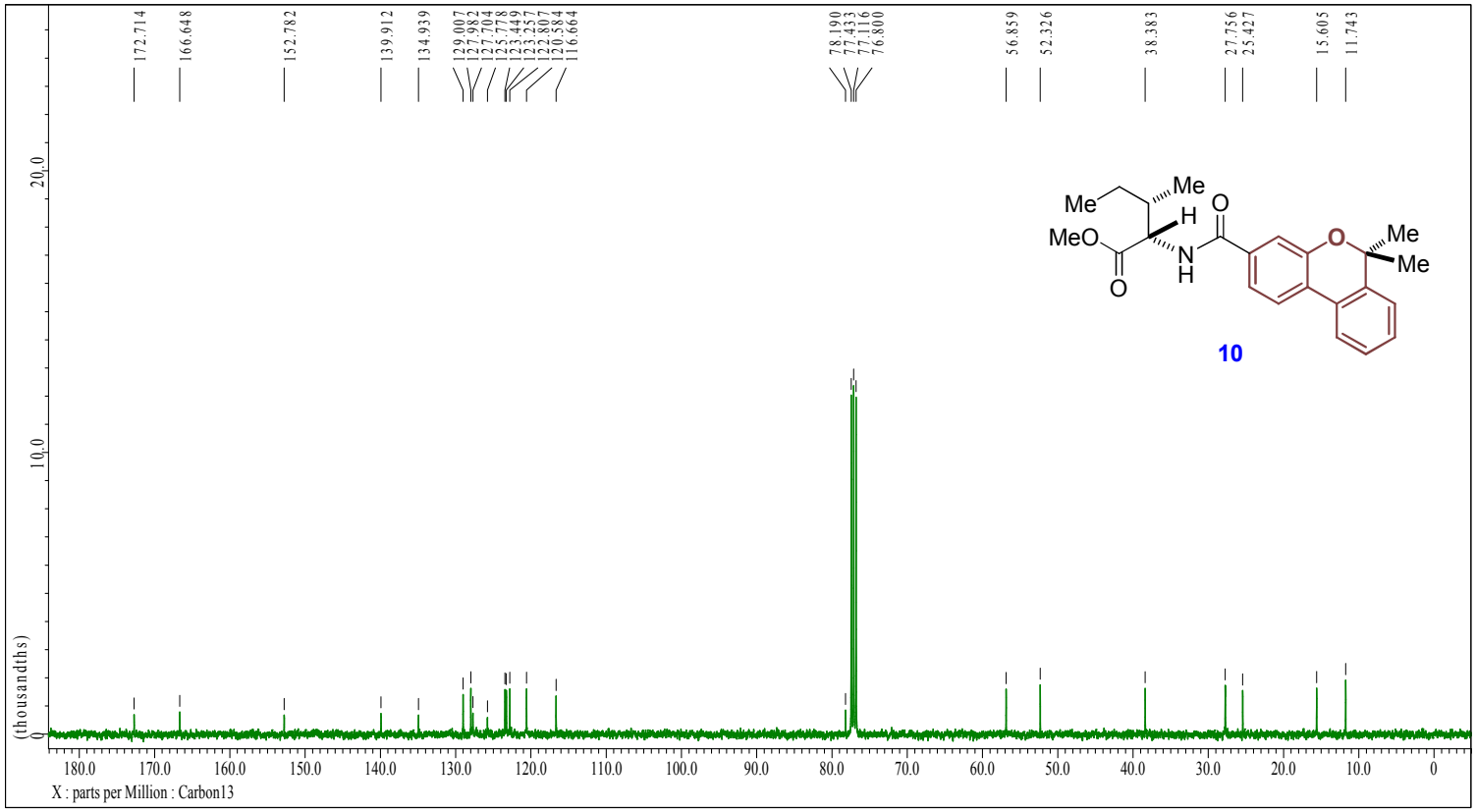
7.358
7.353
7.281
6.662
6.640
4.843
4.832
4.822
4.810
3.781
2.038
2.032
2.026
2.021
2.002
1.996
1.646
1.541
1.538
1.518
1.292
1.269
1.253
1.006
0.995
0.992
0.978
0.974
0.000
Me
Me
H
O
MeO
N
H
O
O
Me
Me
10
2.02
3.03
1.00
1.03
1.06
1.00
3.01
1.00
6.07
0.97
1.02
6.06
abundance
X : parts per Million : Proton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139.912
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127.704
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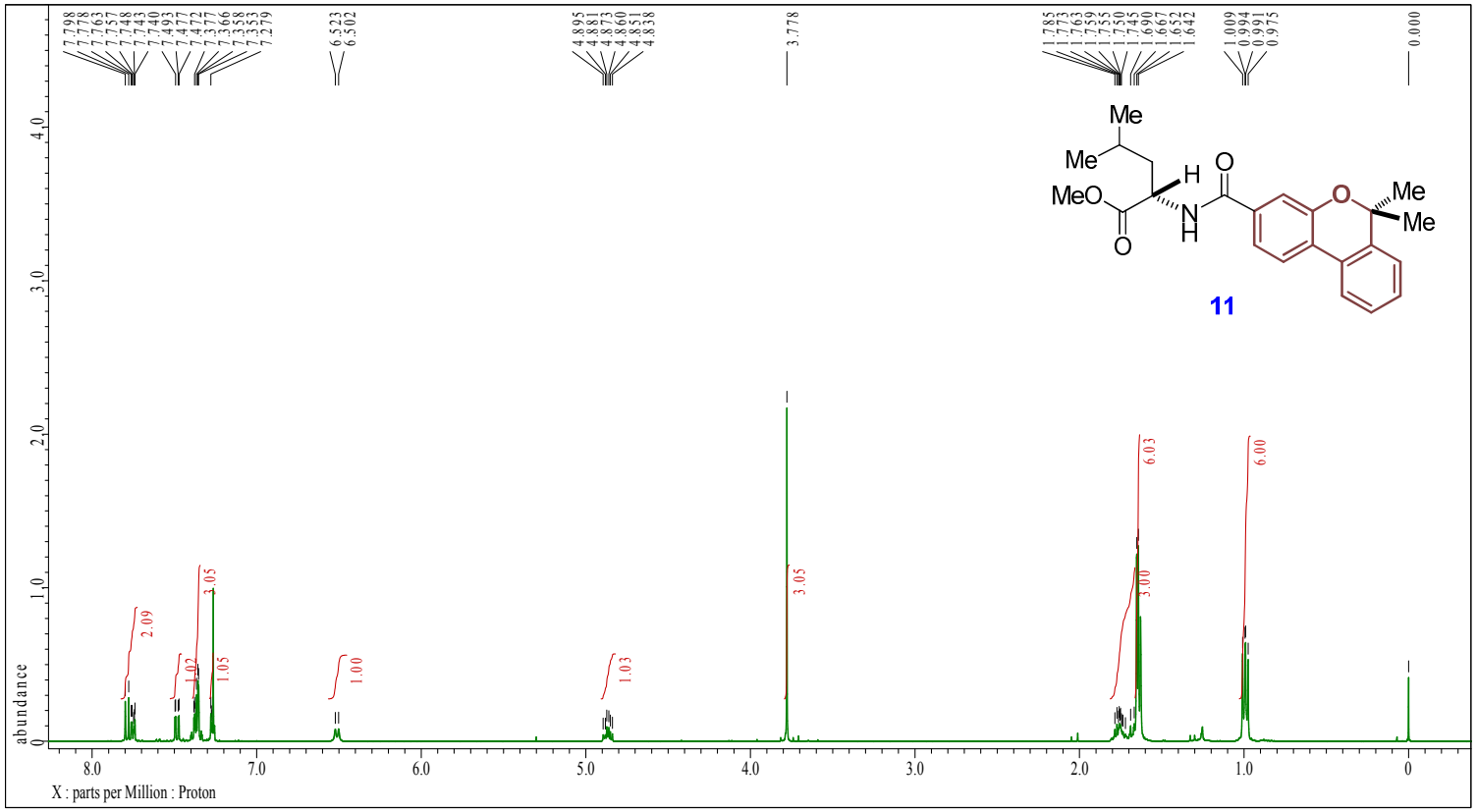
123.257
122.807
120.584
116.664
78.190
77.433
77.116
76.800
56.859
52.326
38.383
27.756
25.427
15.605
11.743
Me
Me
H
O
MeO
N
H
O
O
Me
Me
10
(thousandths)
X : parts per Million : Carbon13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7.358
7.353
7.279
6.523
6.502
4.895
4.881
4.873
4.860
4.851
4.838
3.778
1.785
1.773
1.763
1.759
1.755
1.750
1.745
1.690
1.667
1.652
1.642
1.009
0.994
0.991
0.975
0.000
Me
Me
MeO
H
N
H
O
O
O
Me
Me
11
2.09
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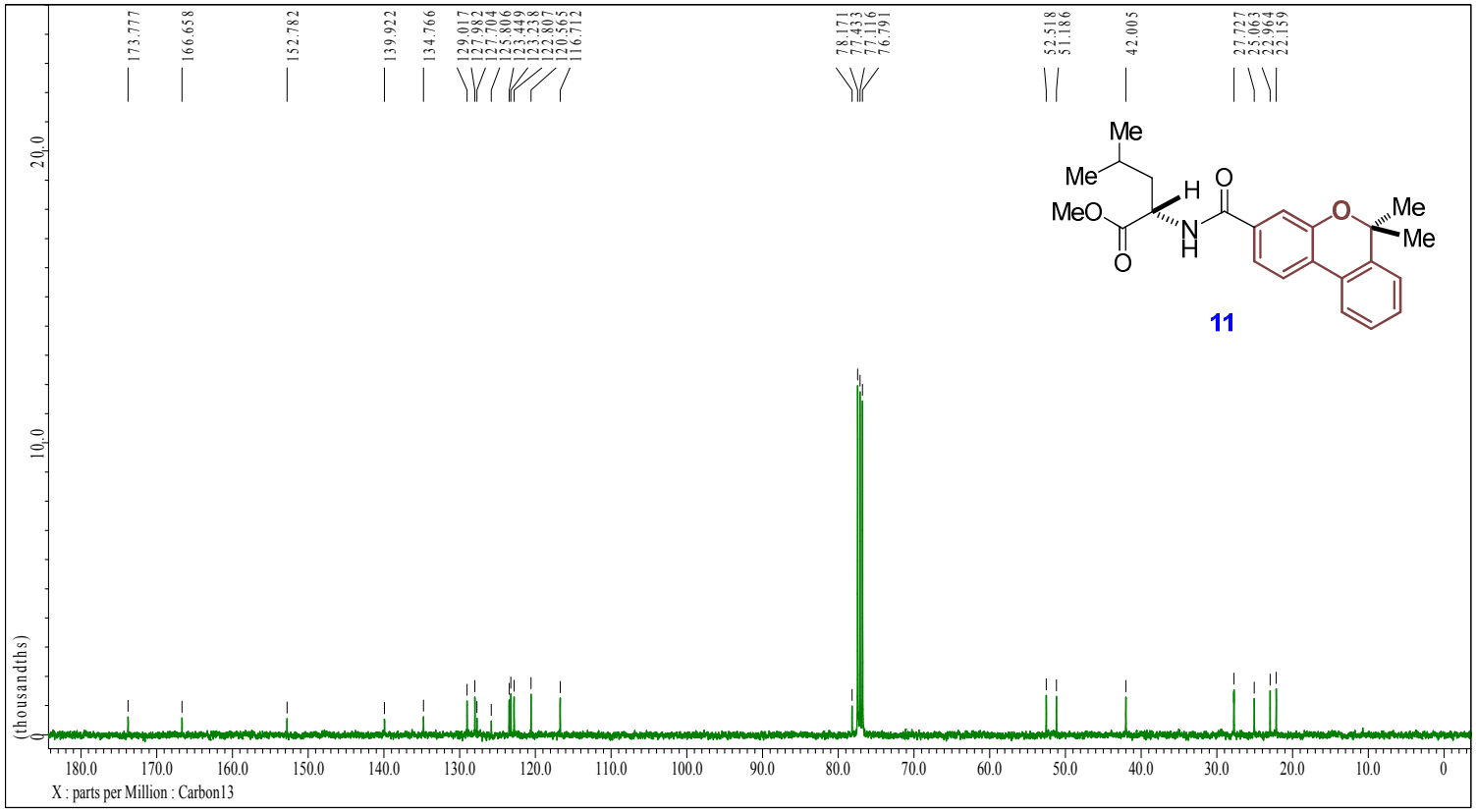
1.00
1.03
3.05
6.03
3.00
6.00
abundance
X : parts per Million : Proton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120.565
116.712
78.171
77.433
77.116
76.791
52.518
51.186
42.005
27.727
25.063
22.964
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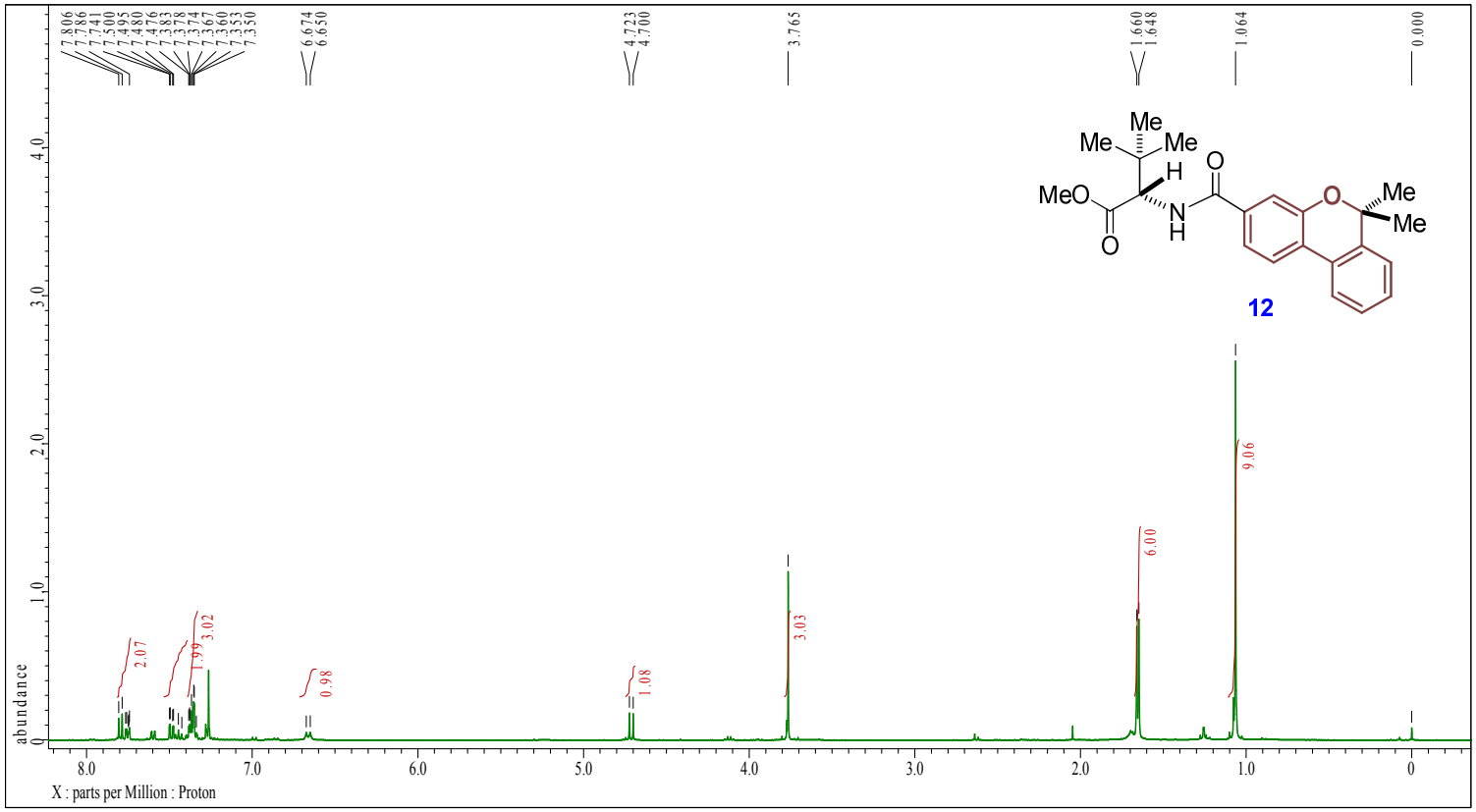
MeO
H
N
H
O
O
O
Me
Me
11
(thousandths)
X : parts per Million : Carbon13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7.374
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7.360
7.353
7.350
6.674
6.650
4.723
4.700
3.765
1.660
1.648
1.064
0.000
Me
Me
H
MeO
N
H
O
O
O
Me
Me
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3.03
3.02
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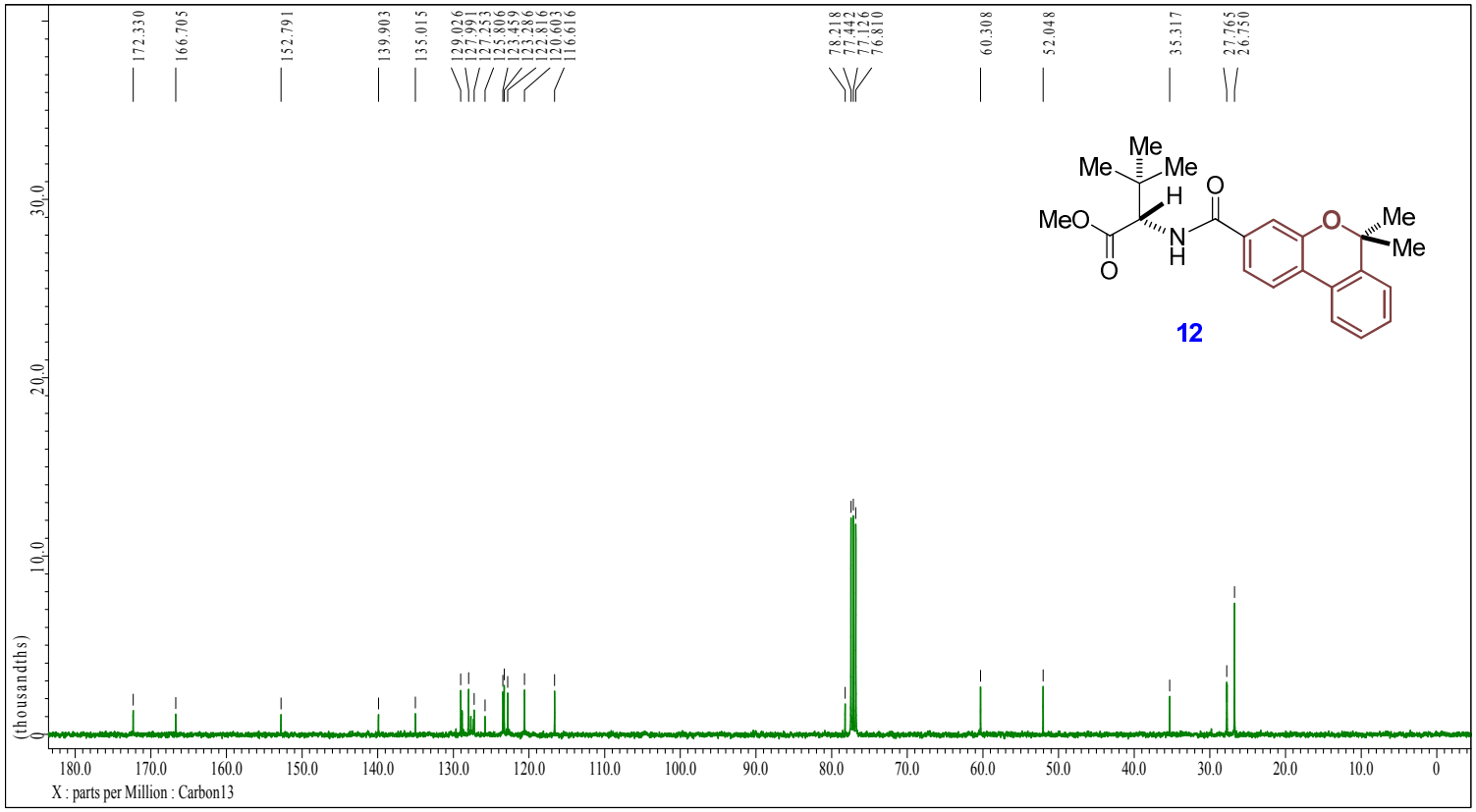
1.99
0.98
1.08
abundance
X : parts per Million : Proton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116.616
78.218
77.442
77.126
76.810
60.308
52.048
35.317
27.765
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N
H
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Me
Me
12
(thousandths)
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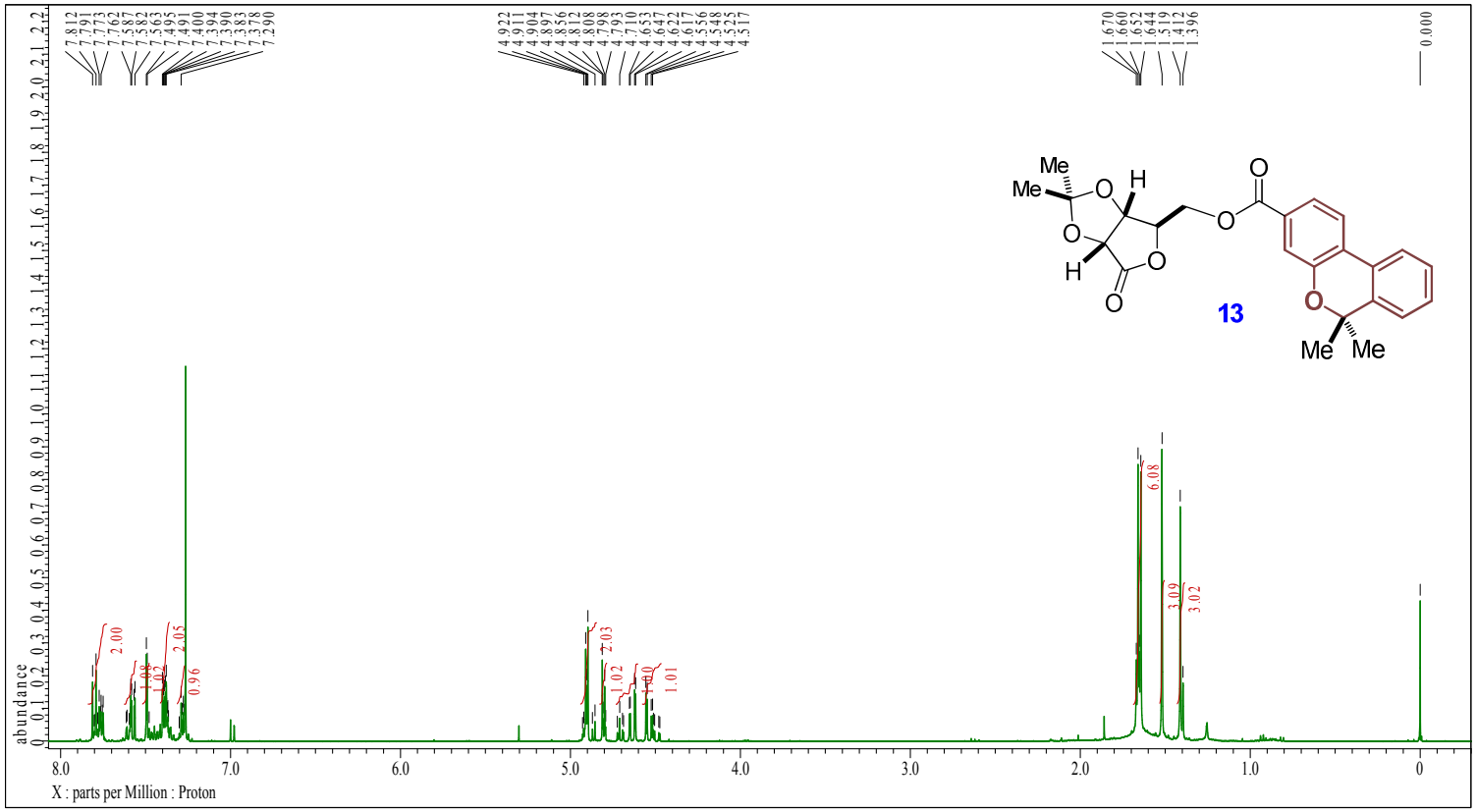
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7.383
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4.798
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4.622
4.617
4.556
4.548
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1.660
1.652
1.644
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1.412
1.396
0.000
Me
Me
O
H
O
O
H
O
O
O
O
13
Me
Me
abundance
2.00
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1.02
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6.08
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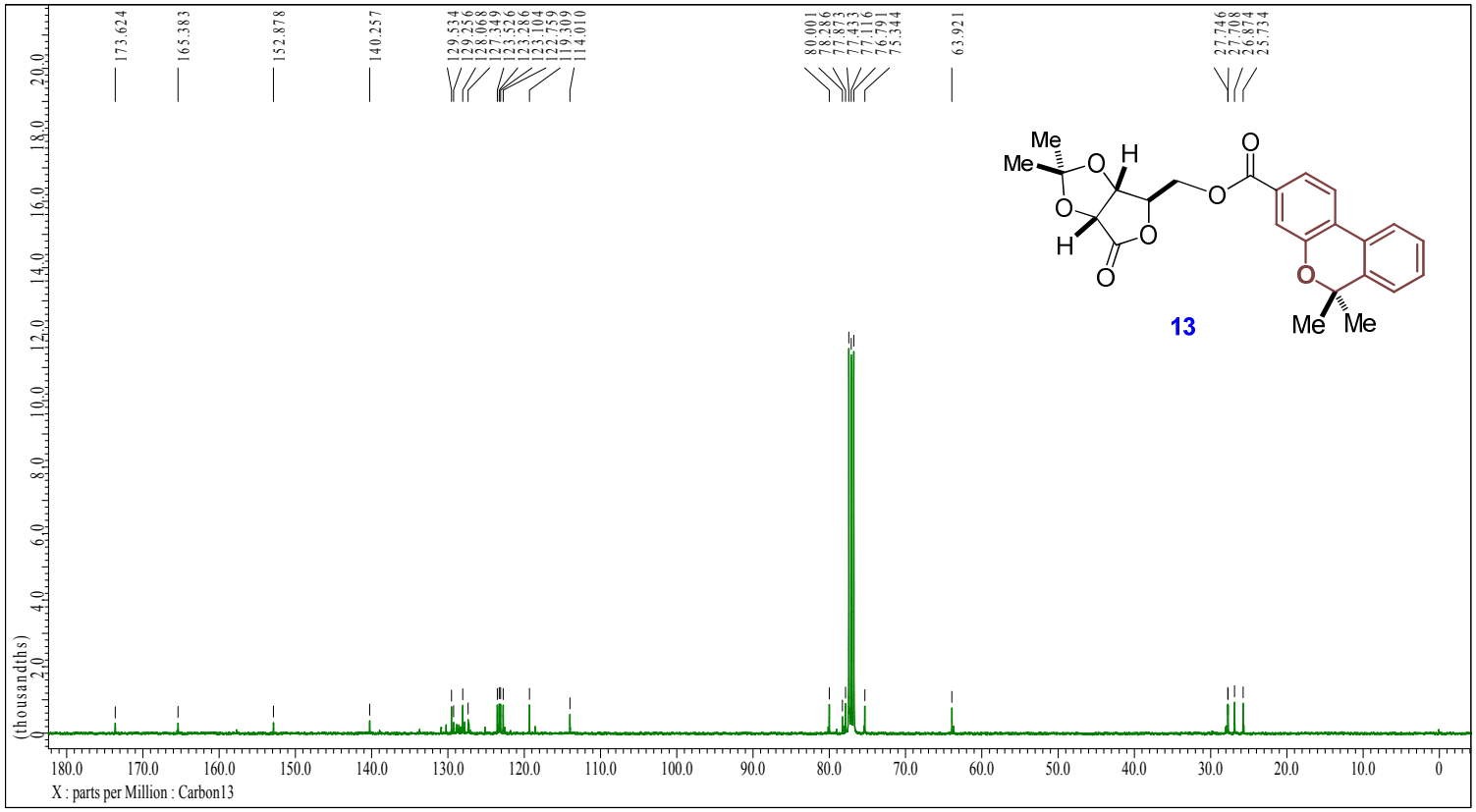
3.02
X : parts per Million : Proton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114.010
80.001
78.286
77.873
77.433
77.116
76.791
75.344
63.921
27.746
27.708
26.874
25.734
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Me
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H
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O
H
O
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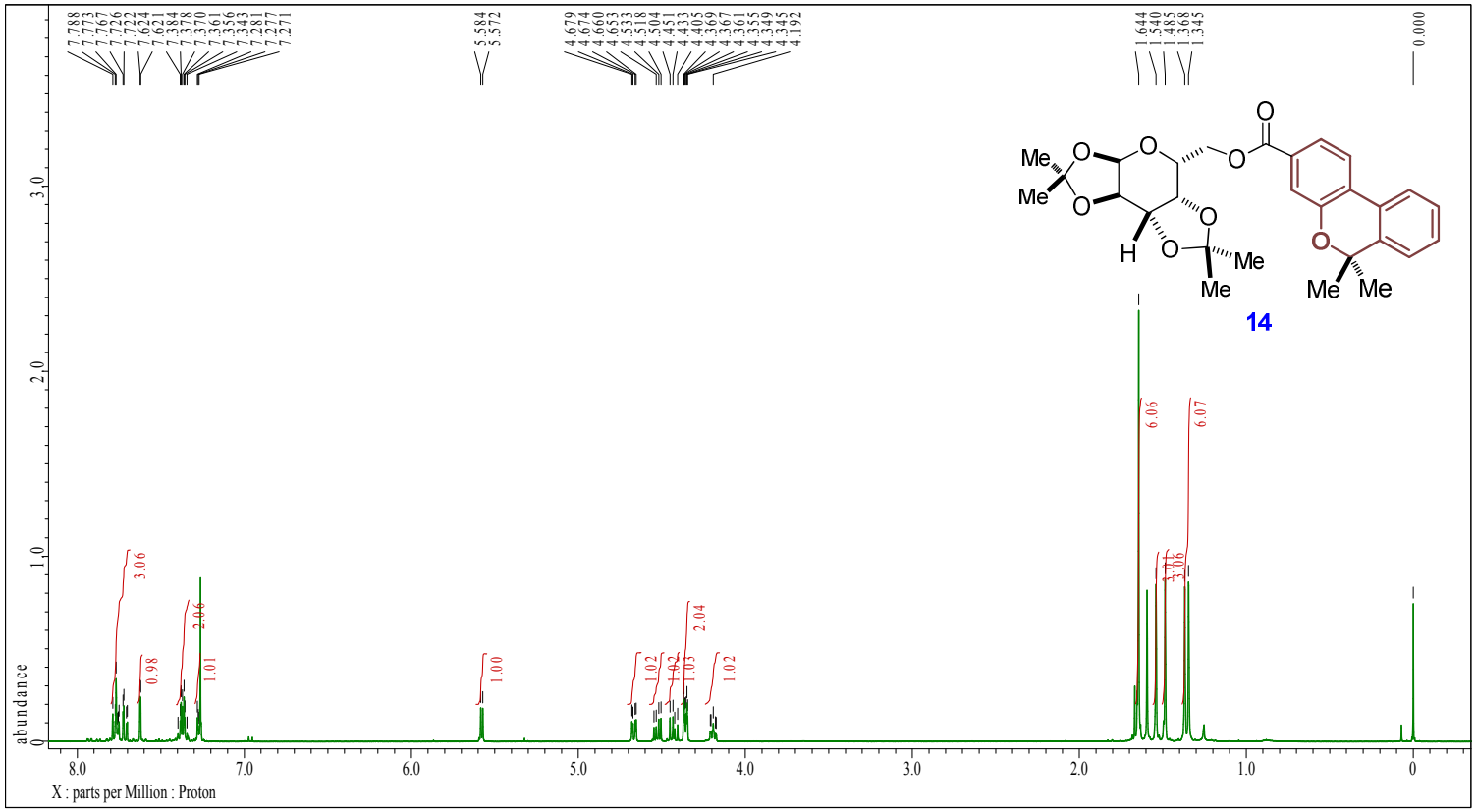
O
O
13
Me
Me
(thousandths)
X : parts per Million : Carbon13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4.433
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4.367
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1.485
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Me
O
H
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Me
Me
Me
14
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2.06
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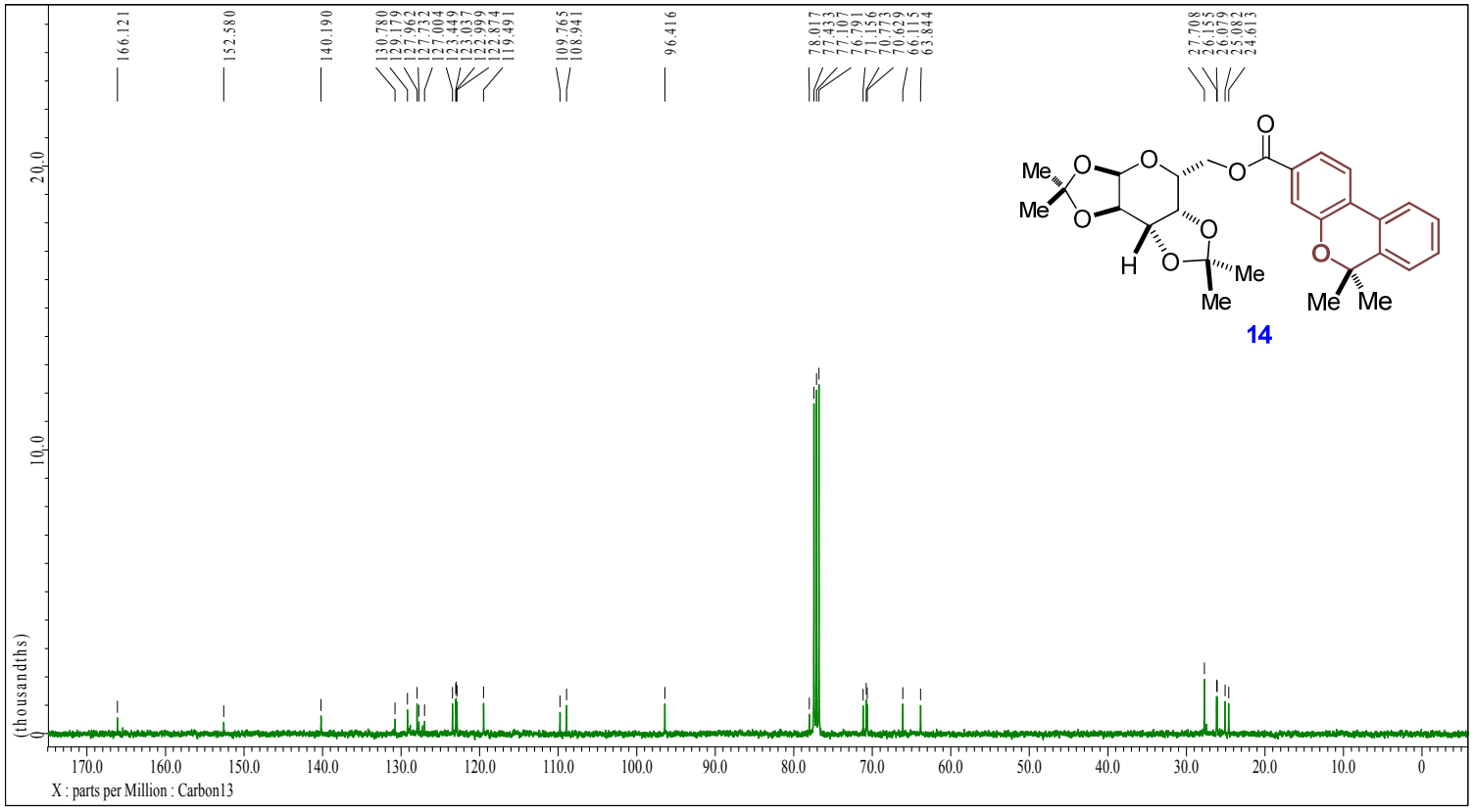
1.02
6.06
6.07
abundance
X : parts per Million : Proton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127.004
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108.941
96.416
78.017
77.433
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76.791
71.156
70.773
70.629
66.115
63.844
27.708
26.155
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O
H
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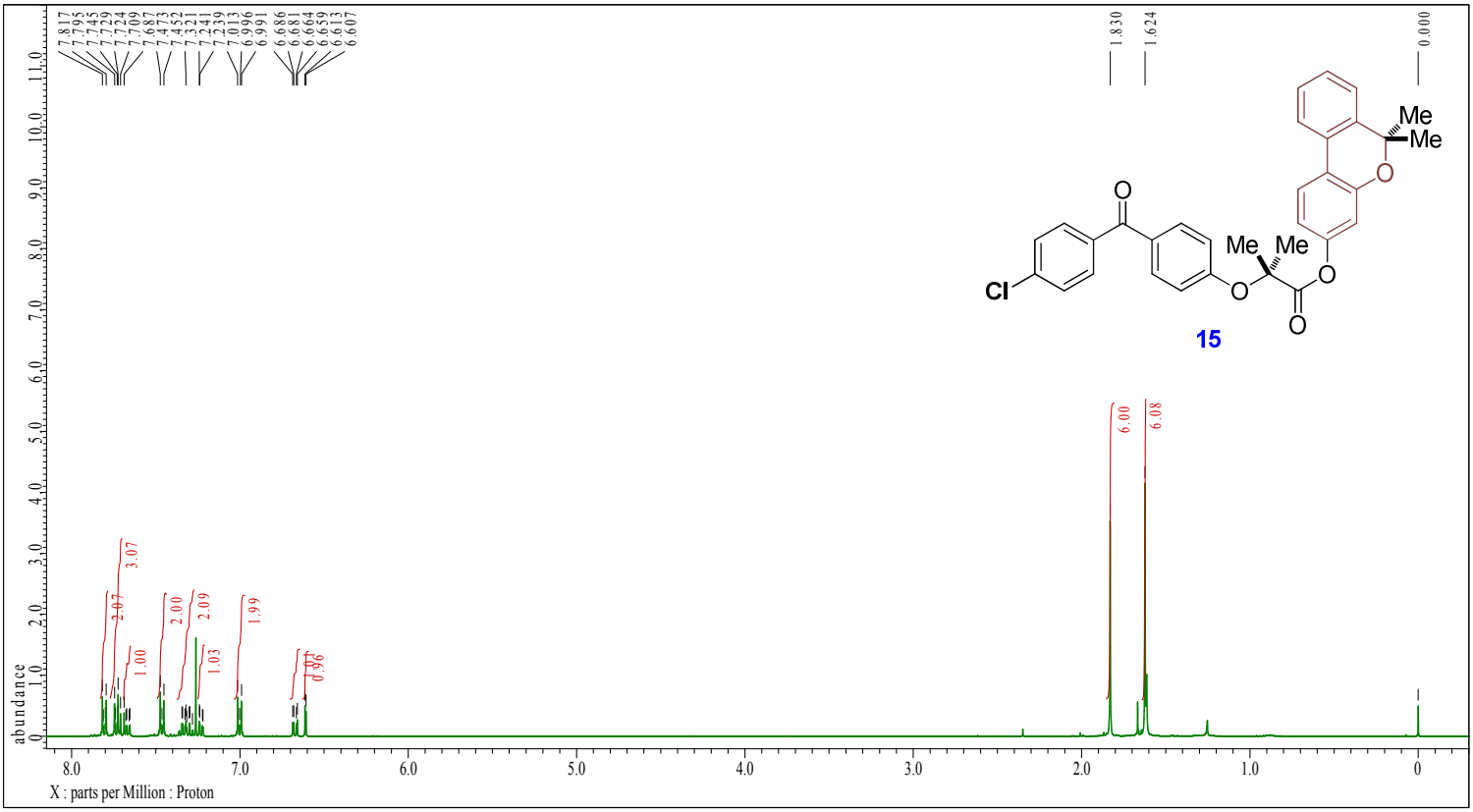
Me
Me
14
(thousandths)
X : parts per Million : Carbon13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7.239
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6.996
6.991
6.686
6.681
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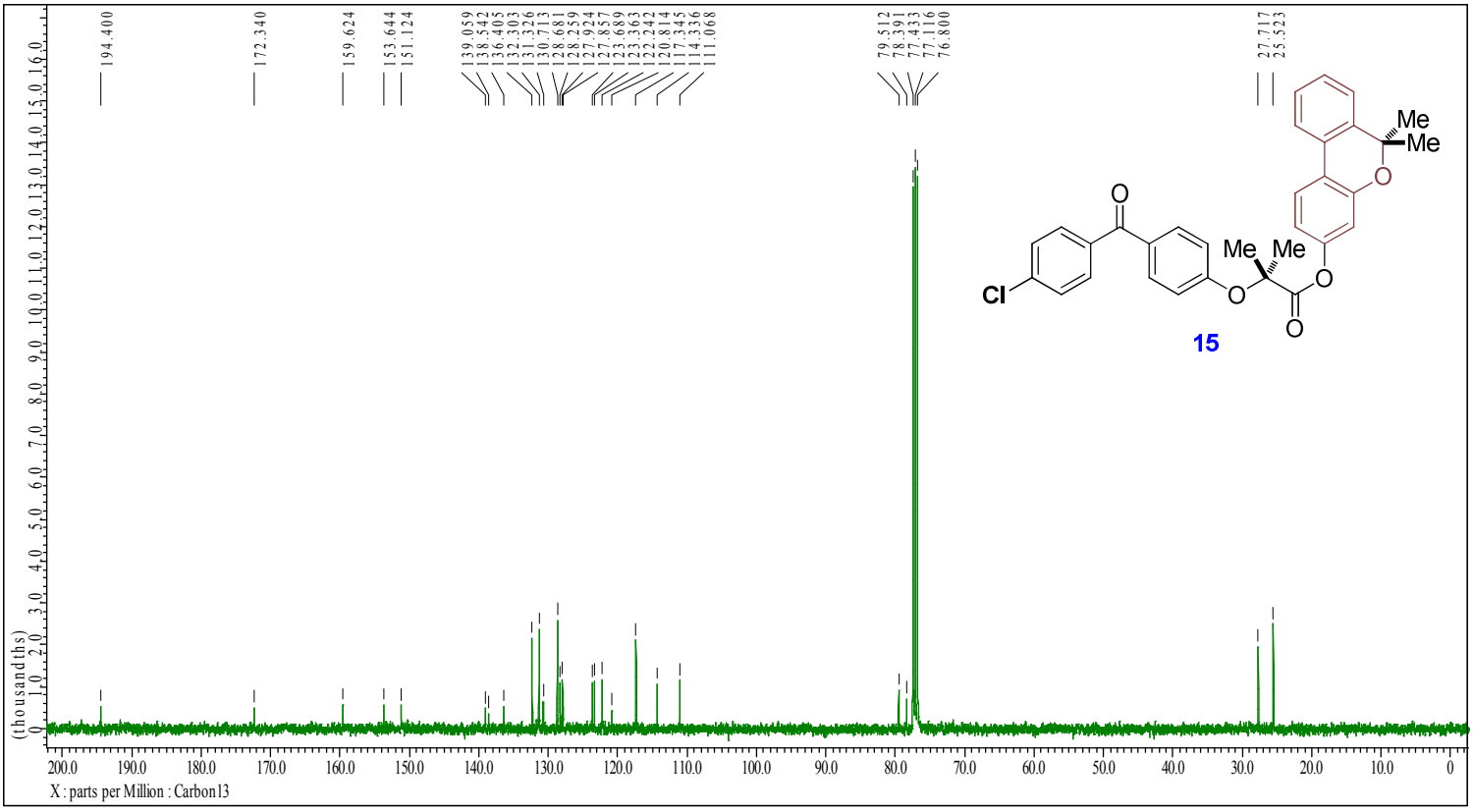
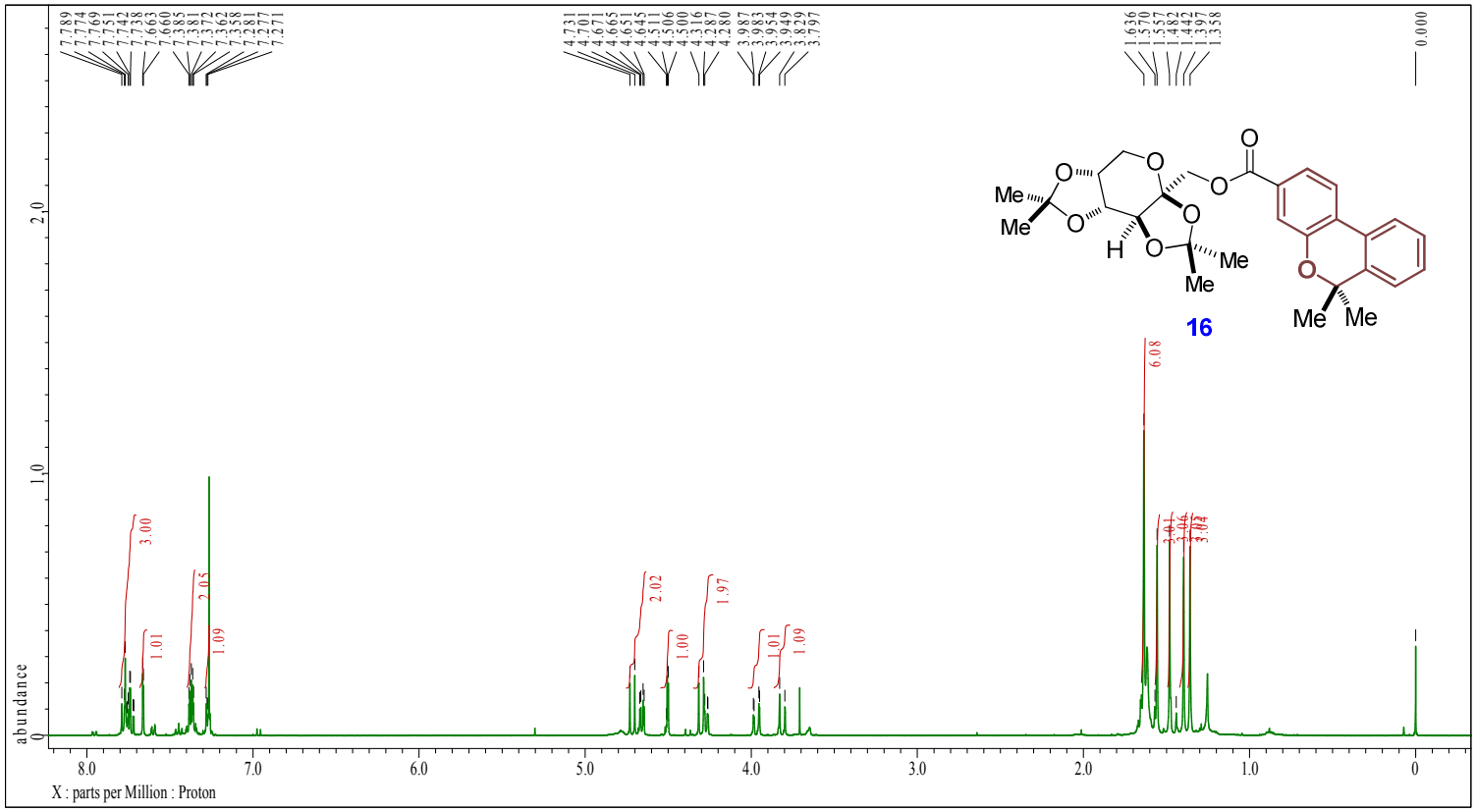
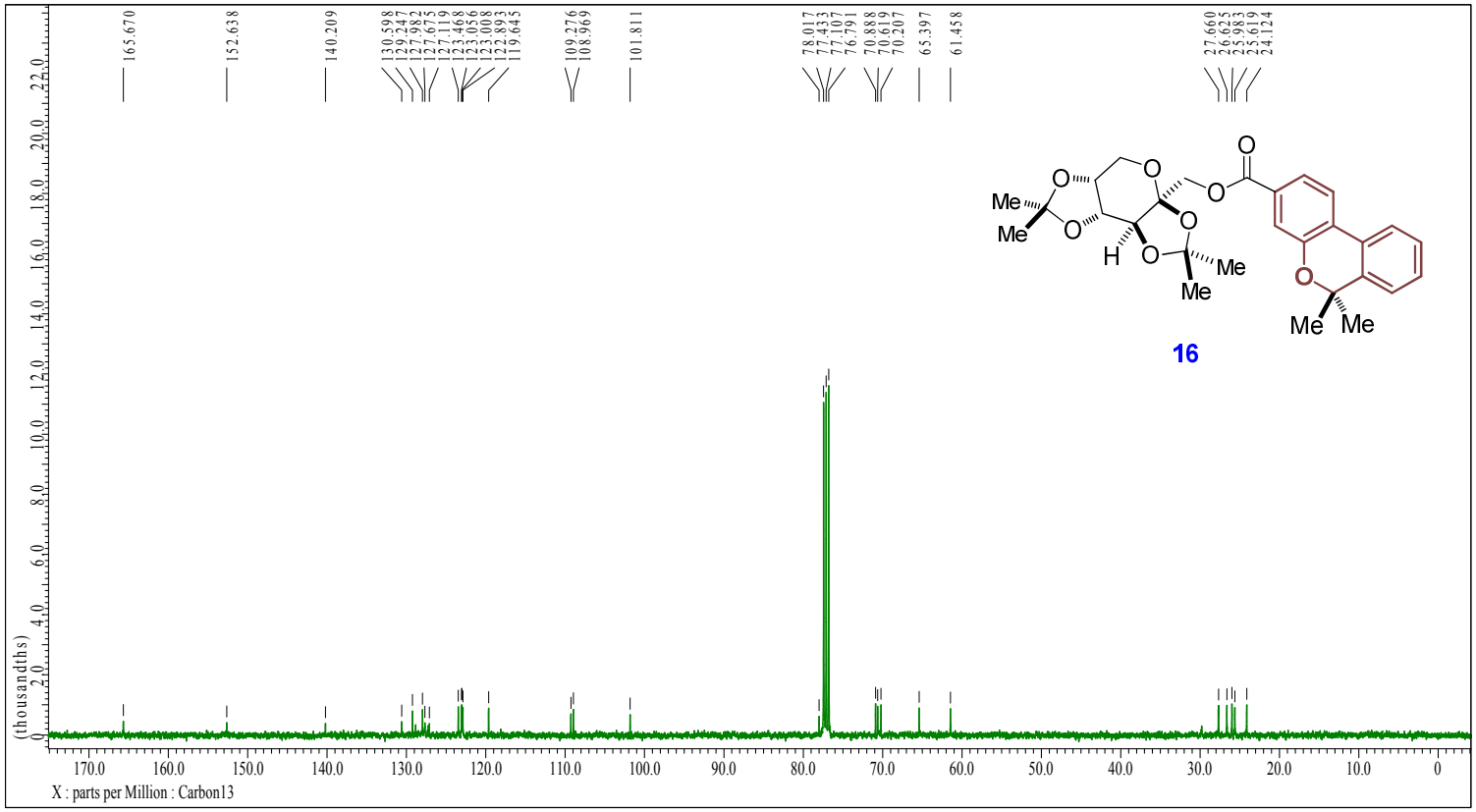
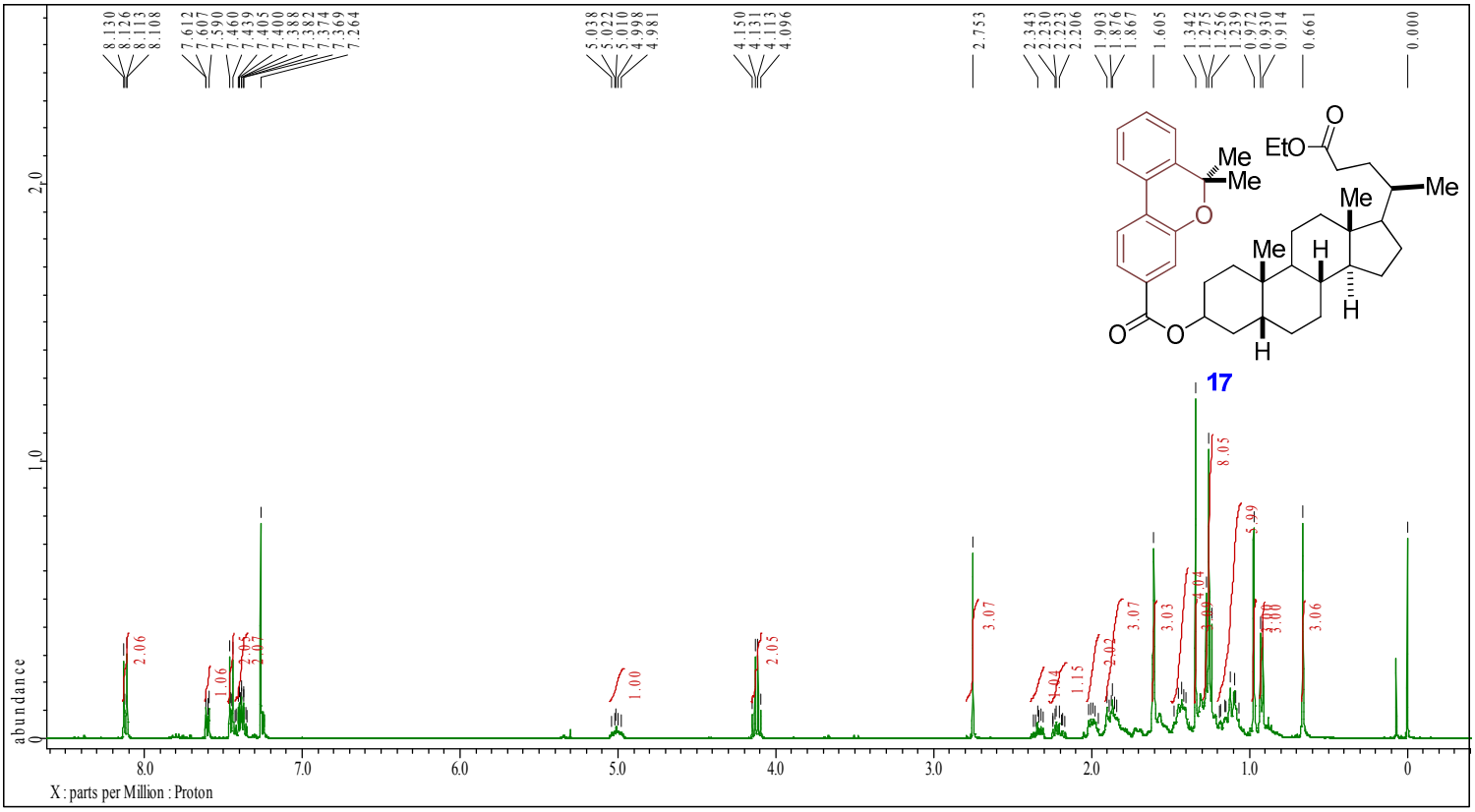
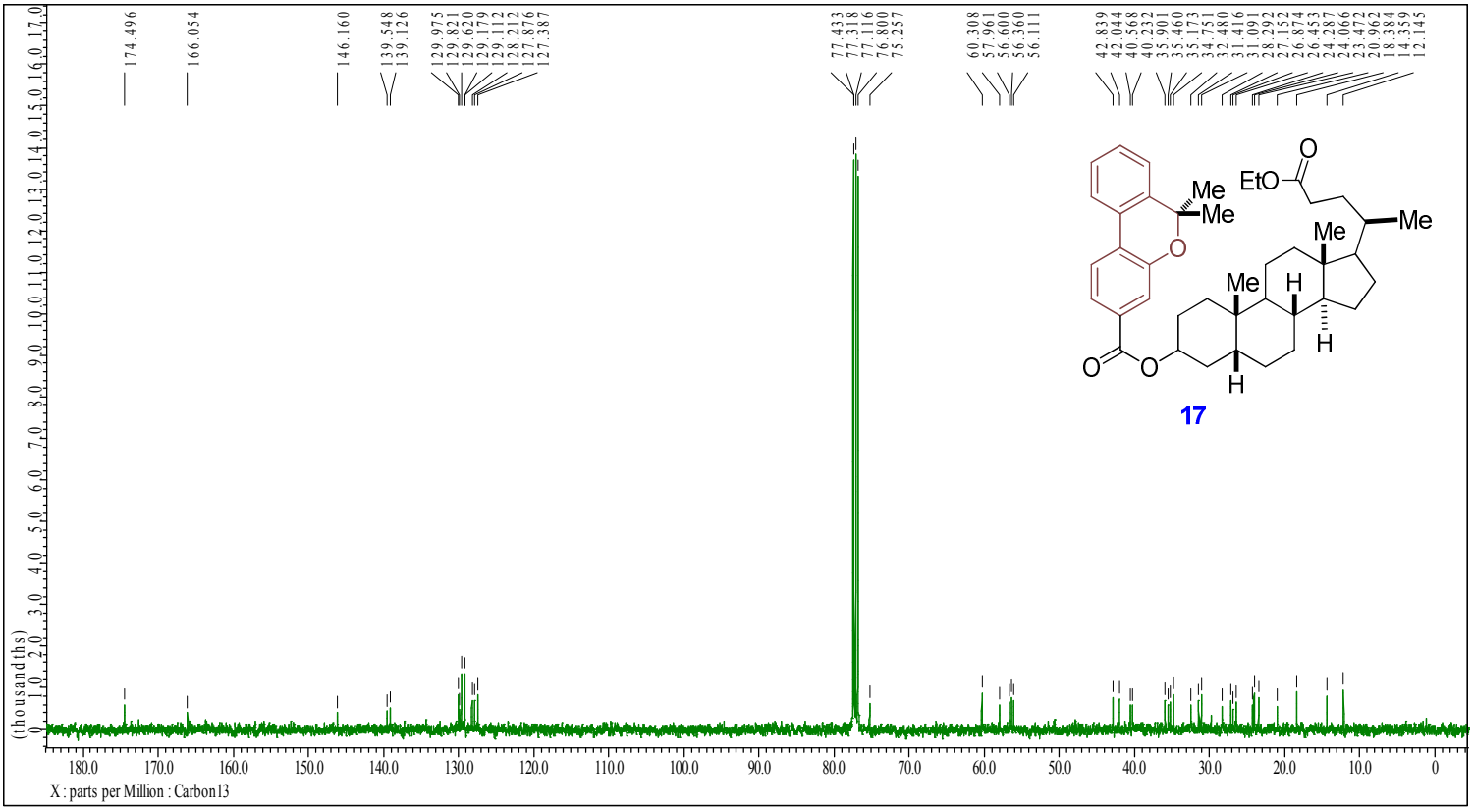
6.659
6.613
6.607
1.830
1.624
0.000
Me
Me
O
Me
Me
O
Cl
O
O
O
15
6.00
6.08
3.07
2.07
2.00
2.09
1.99
1.00
1.03
0.96
0.97
abundance
X : parts per Million : Proton

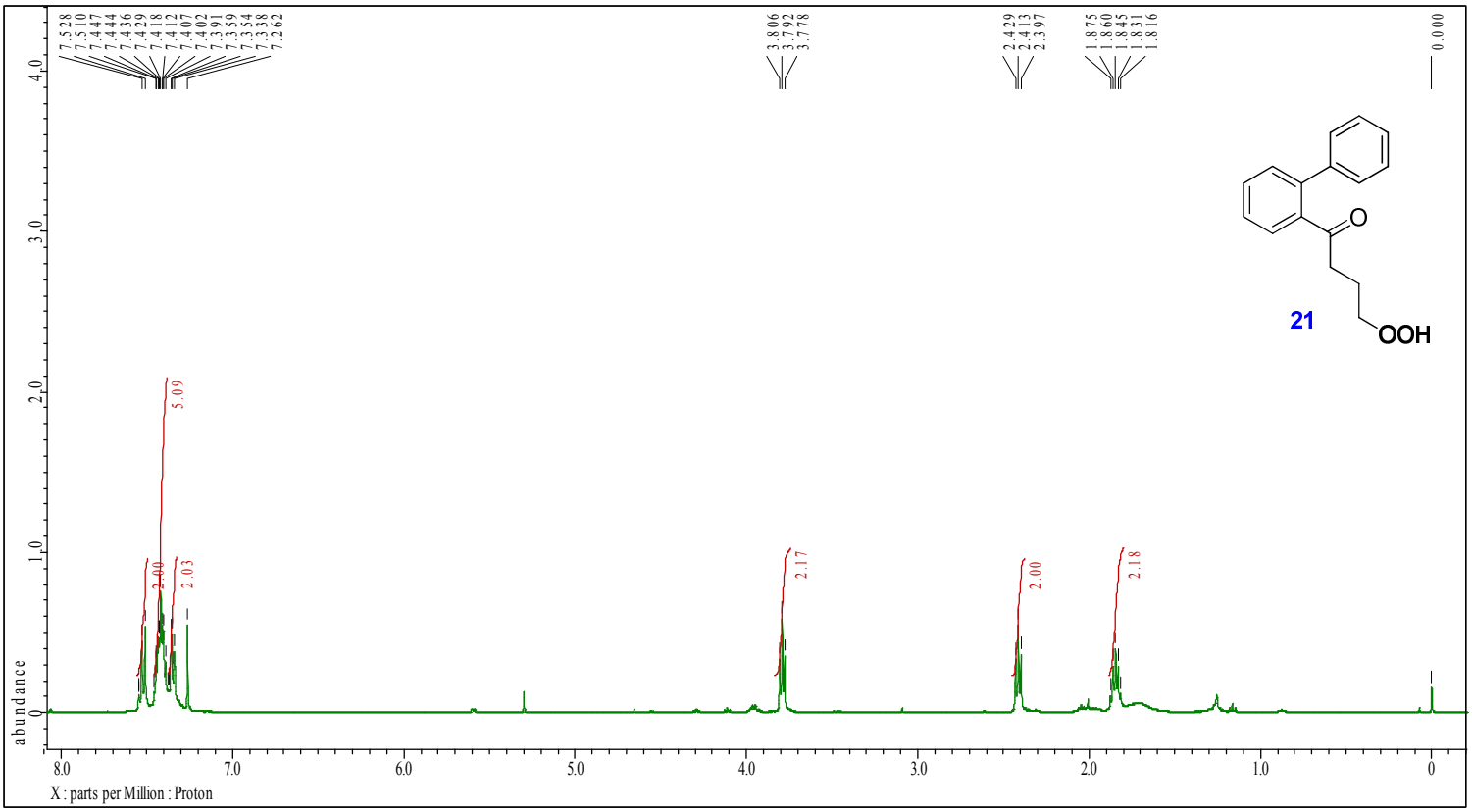

194.400
172.340
159.624
153.644
151.124
139.059
138.542
136.405
132.303
131.326
130.713
128.681
128.259
127.924
127.837
123.689
123.363
122.242
120.814
117.345
114.336
111.068
79.512
78.391
77.433
77.116
76.800
27.717
25.523
Me
Me
O
Me
Me
O
Cl
O
O
O
15
(thousandths)
X : parts per Million : Carbon13

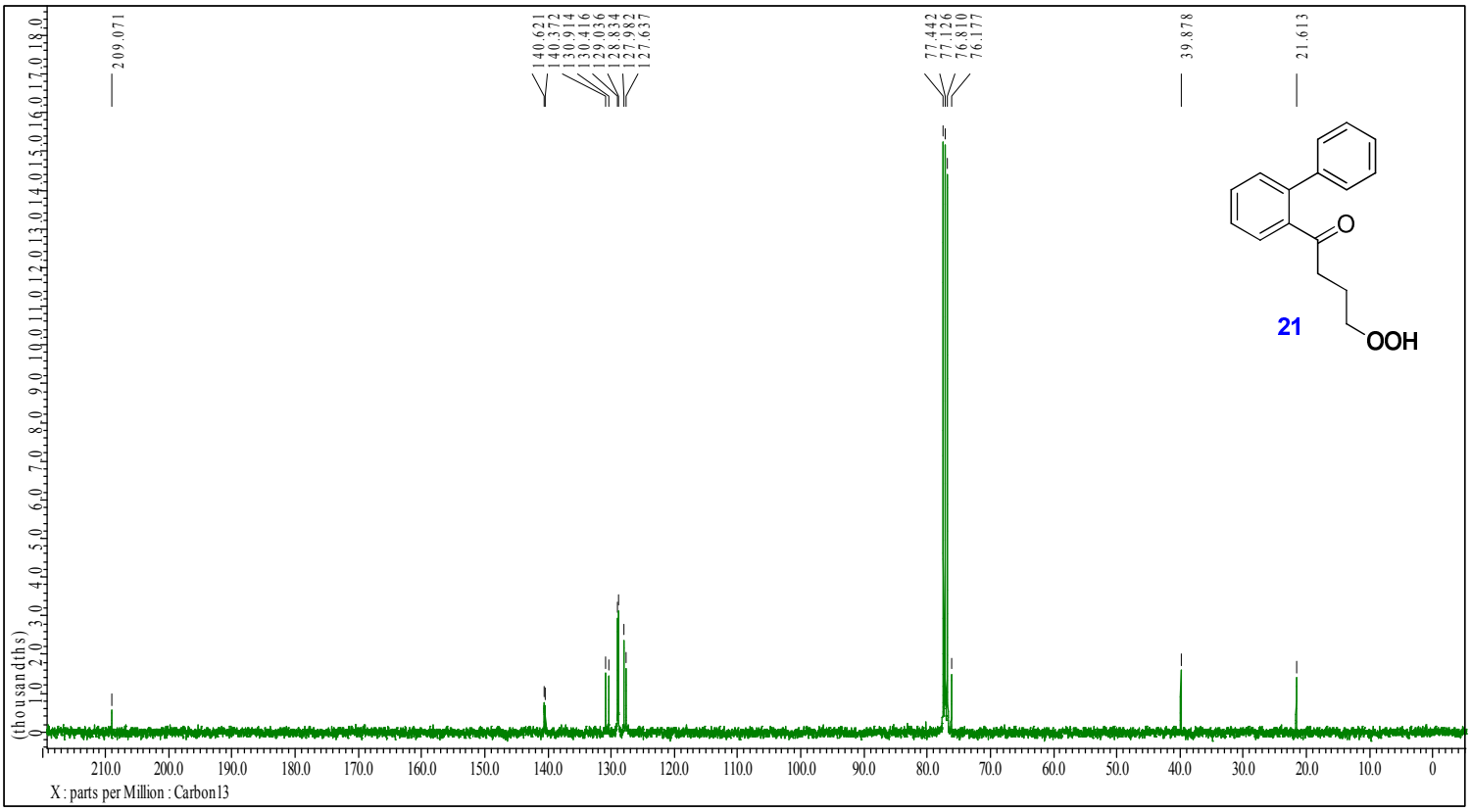

7.789
7.774
7.769
7.751
7.741
7.738
7.663
7.660
7.385
7.381
7.372
7.362
7.358
7.281
7.277
7.271
4.731
4.701
4.671
4.665
4.651
4.645
4.511
4.506
4.500
4.316
4.287
4.280
3.987
3.983
3.954
3.949
3.829
3.797
1.636
1.570
1.557
1.482
1.442
1.397
1.358
0.000
Me
Me
O
H
Me
Me
Me
Me
16
6.08
3.00
1.01
2.05
1.09
2.02
1.00
1.97
1.01
1.09
abundance
X : parts per Million : Proton

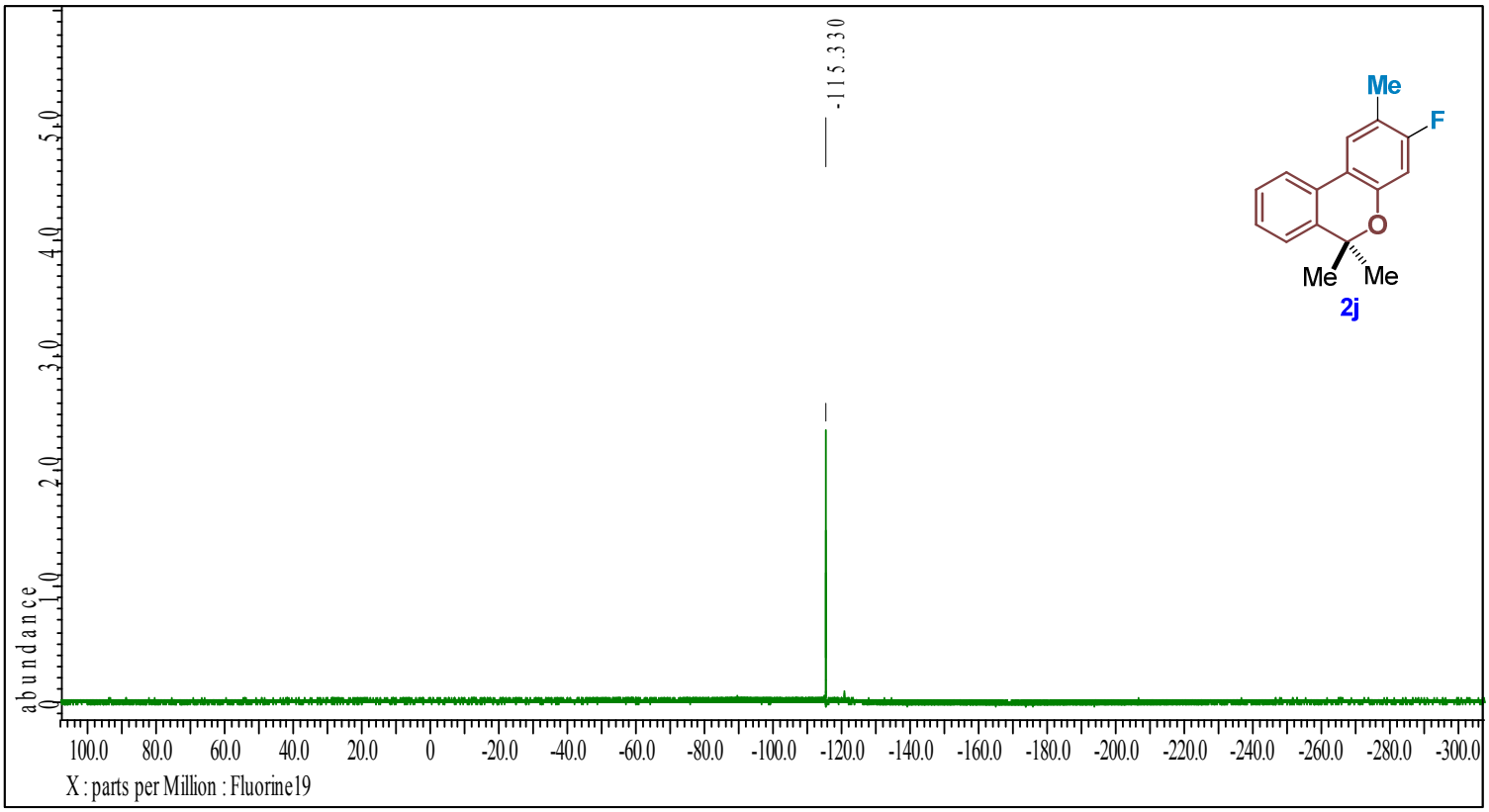

165.670
152.638
140.209
130.598
129.247
127.982
127.675
127.119
123.468
123.056
123.008
122.893
119.645
109.276
108.969
101.811
78.017
77.433
77.107
76.791
70.888
70.619
70.207
65.397
61.458
27.660
26.635
25.983
25.619
24.124
Me
Me
O
H
Me
Me
Me
Me
16
(thousandths)
X : parts per Million : Carbon13

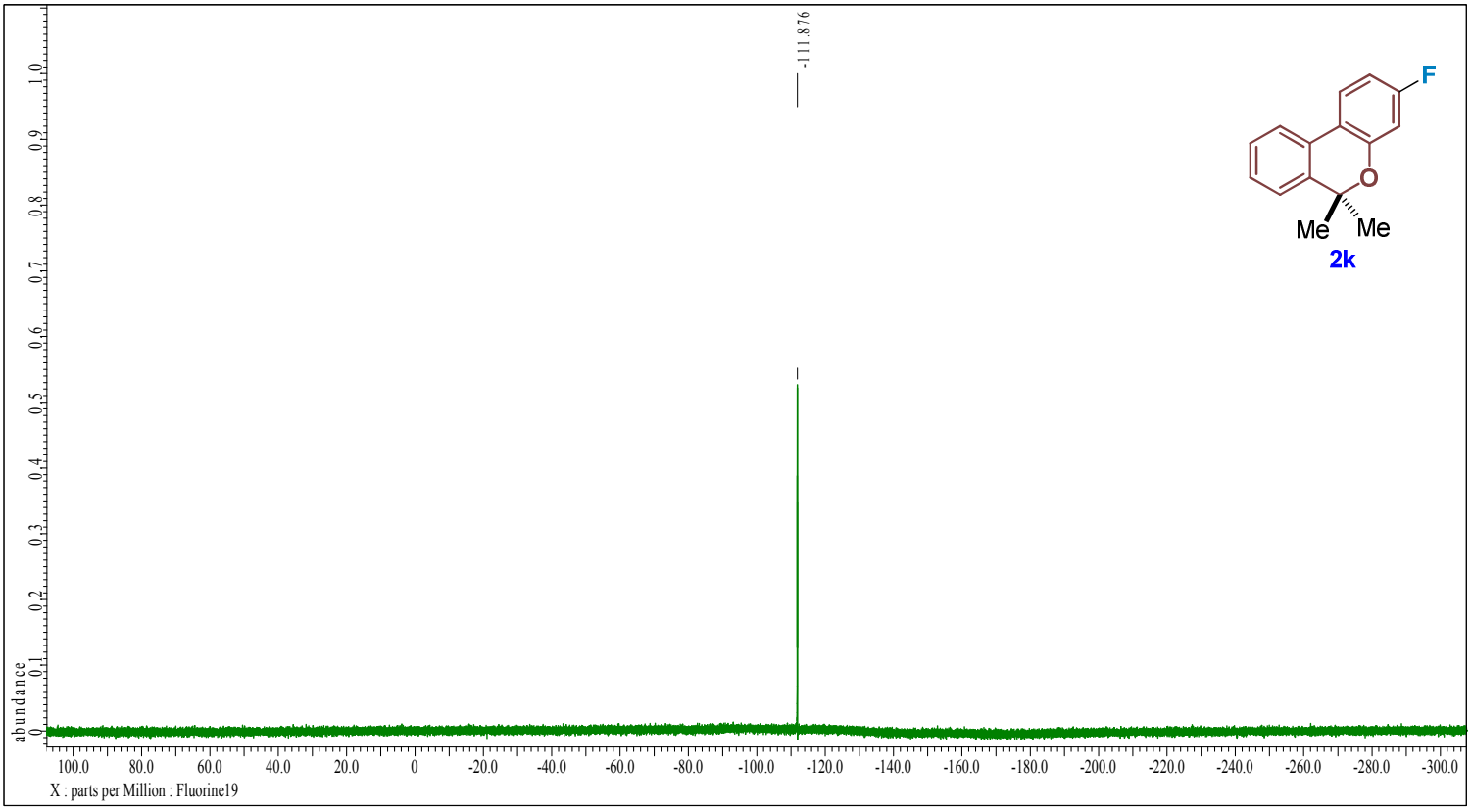

8.130
8.126
8.113
8.108
7.612
7.607
7.590
7.460
7.439
7.405
7.400
7.388
7.382
7.374
7.369
7.264
5.038
5.022
5.010
4.998
4.981
4.150
4.131
4.113
4.096
2.753
2.343
2.330
2.223
2.206
1.903
1.876
1.867
1.605
1.342
1.275
1.256
1.239
0.972
0.930
0.914
0.661
0.000
Me
Me
EtO
O
Me
Me
H
H
O
O
H
17
abundance
X : parts per Million : Proton

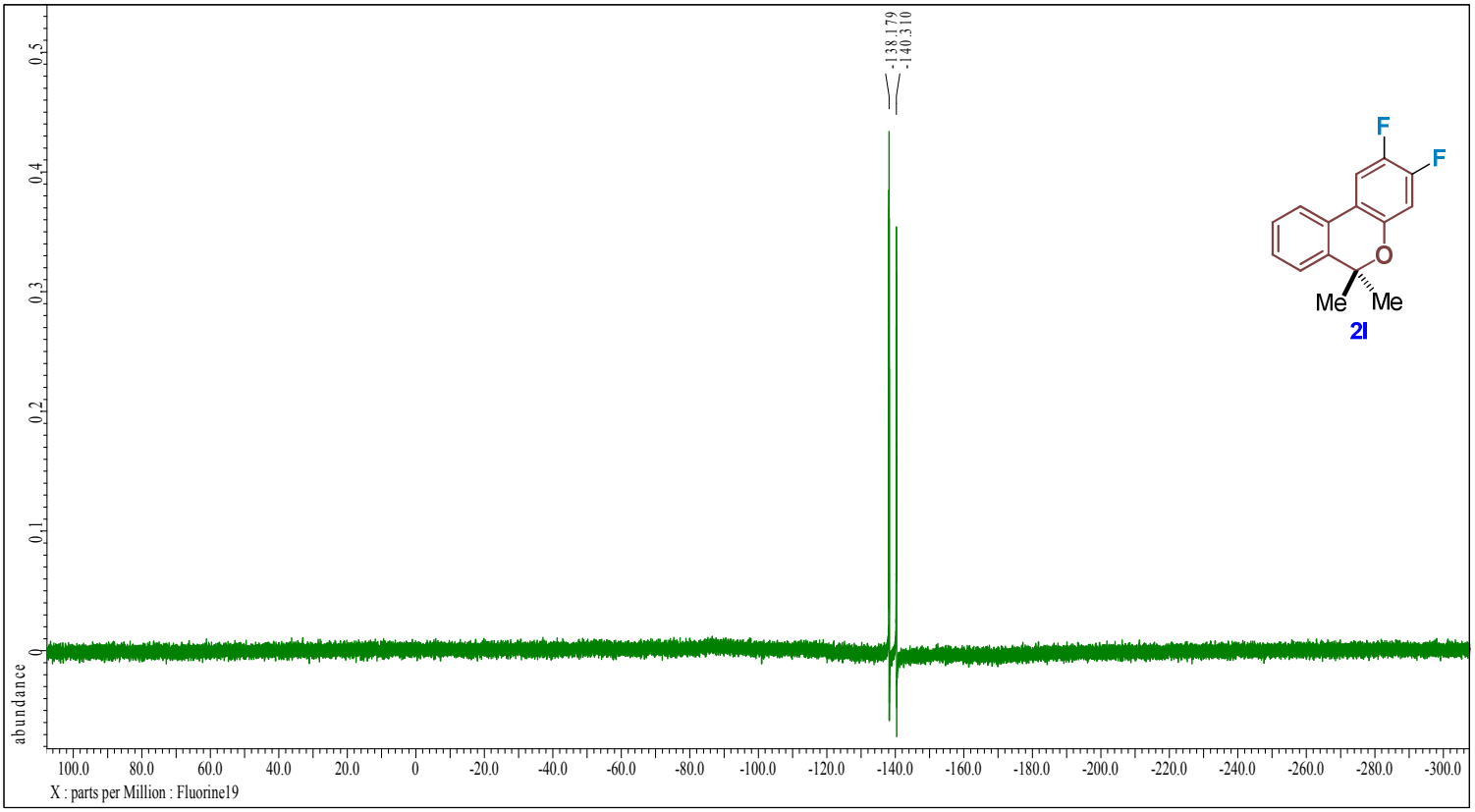

174.496
166.054
146.160
139.548
139.126
129.975
129.821
129.620
129.179
129.112
128.212
127.876
127.387
77.433
77.318
77.116
76.800
75.257
60.308
57.961
56.600
56.360
56.111
42.839
42.044
40.568
40.232
35.901
35.460
35.173
34.731
32.480
31.416
31.091
28.292
27.152
26.874
26.453
24.287
24.066
23.472
20.962
18.384
14.359
12.145
Me
Me
EtO
O
Me
Me
H
H
O
O
H
17
(thousandths)
X : parts per Million : Carbon13

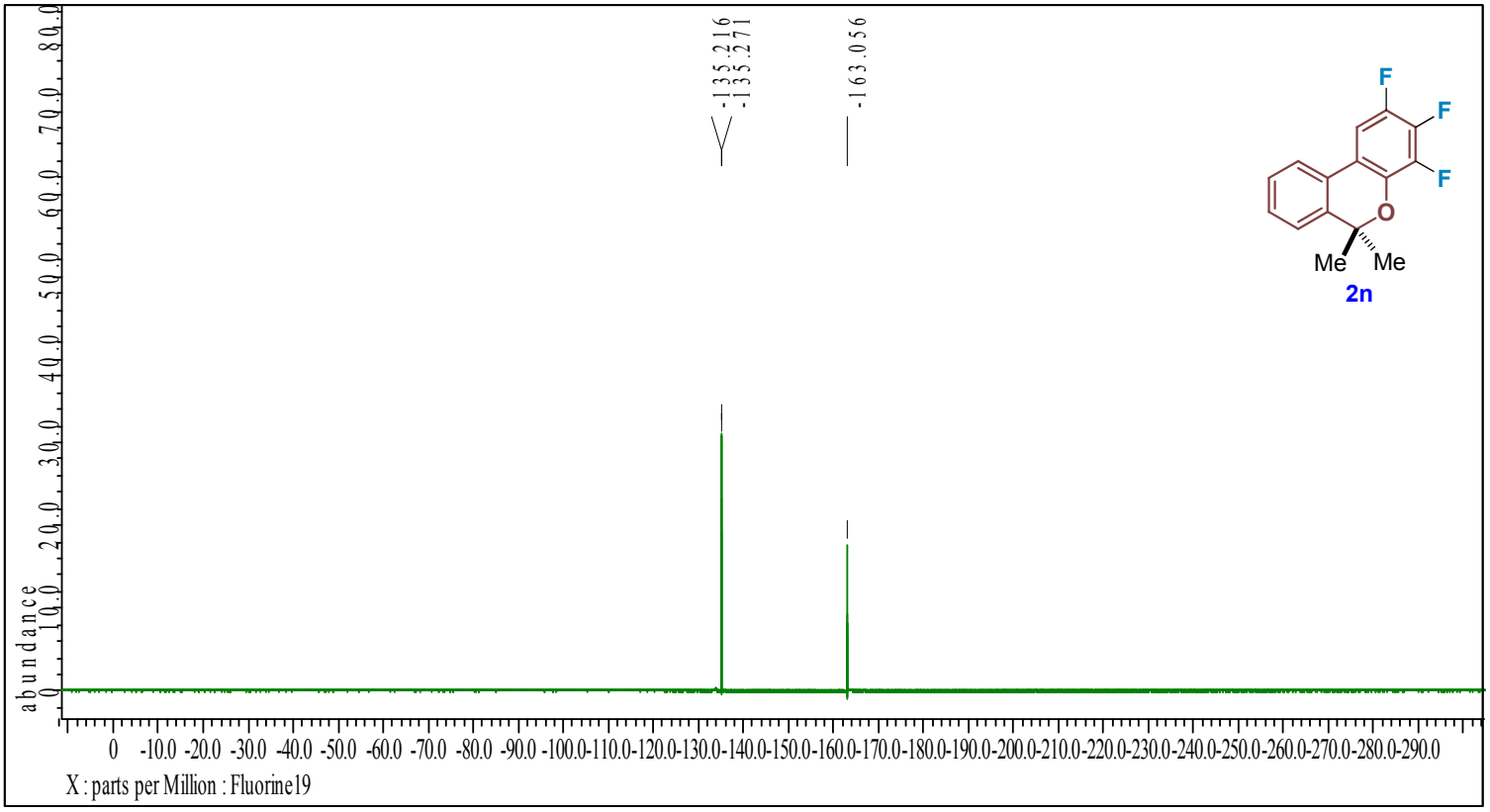

7.528
7.510
7.447
7.444
7.436
7.429
7.418
7.412
7.407
7.402
7.391
7.359
7.354
7.338
7.262
3.806
3.792
3.778
2.429
2.413
2.397
1.875
1.860
1.845
1.831
1.816
0.000
5.09
2.00
2.03
2.17
2.00
2.18
O
21
OOH
abundance
X : parts per Million : Proton

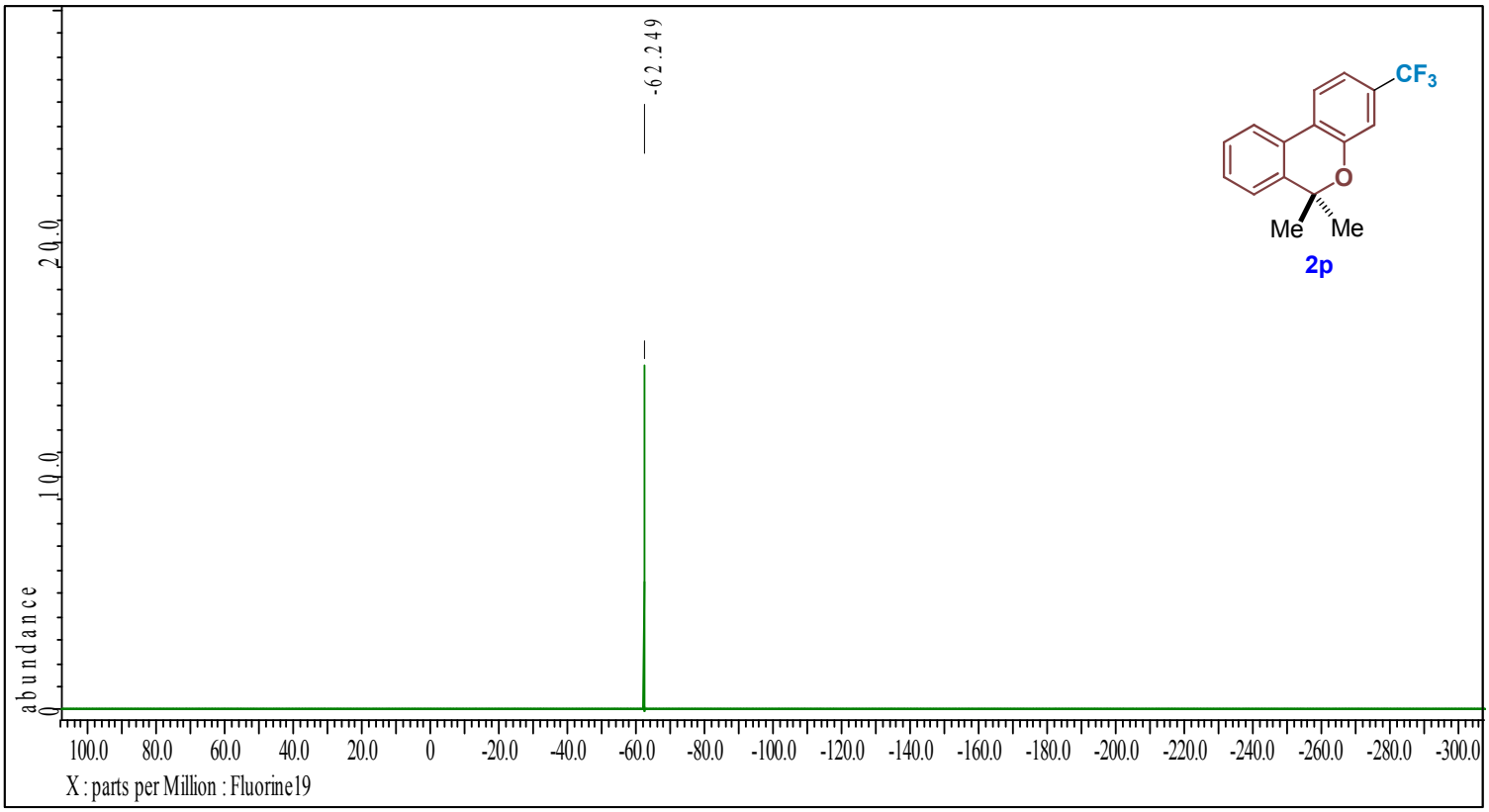

209.071
140.621
140.372
130.914
130.416
129.036
128.834
127.982
127.637
77.442
77.126
76.810
76.177
39.878
21.613
O
21
OOH
(thousandths)
X : parts per Million : Carbon13

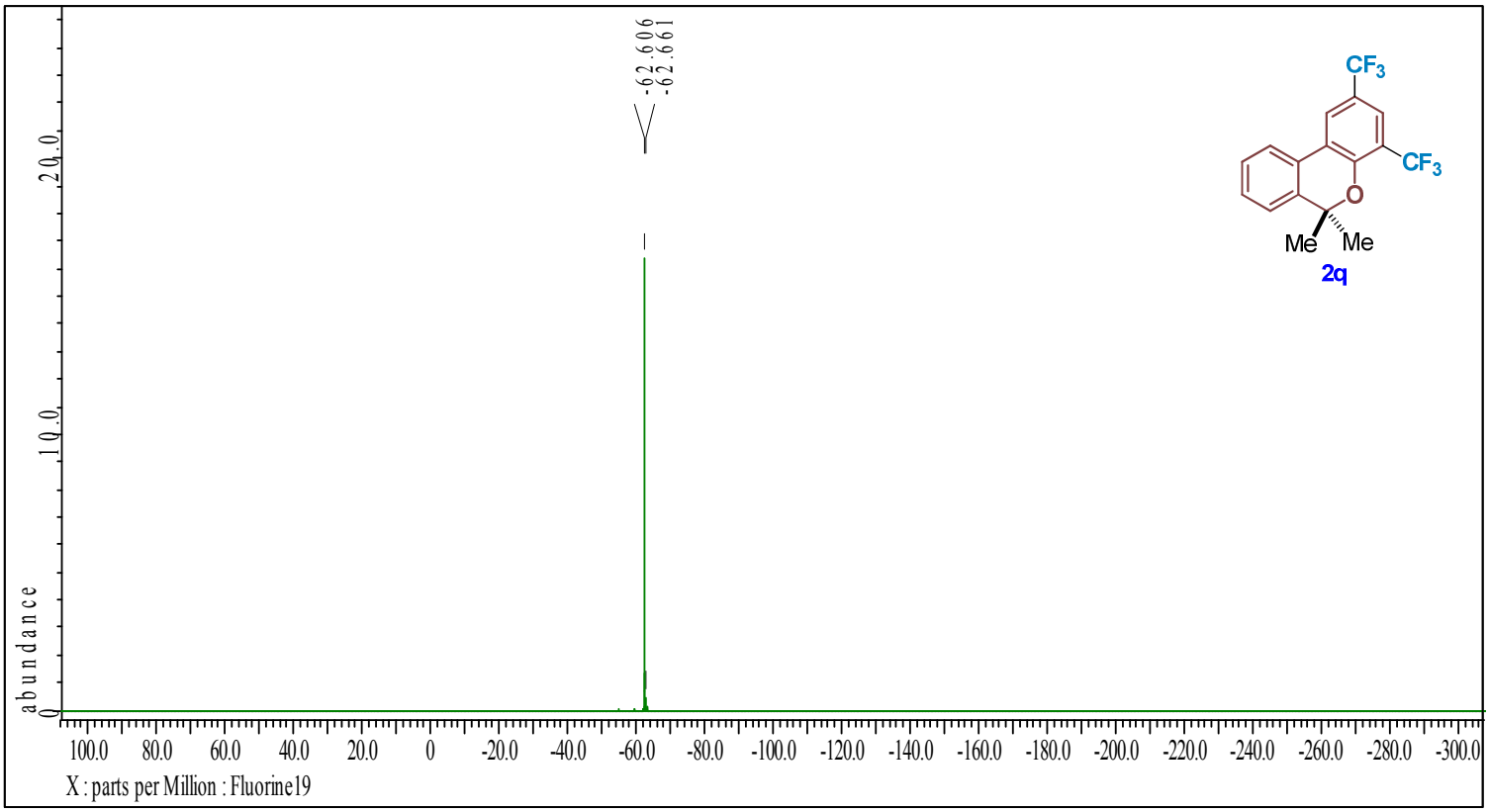

-115.330
Me
F
O
Me
Me
2j
abundance
X : parts per Million : Fluorine19

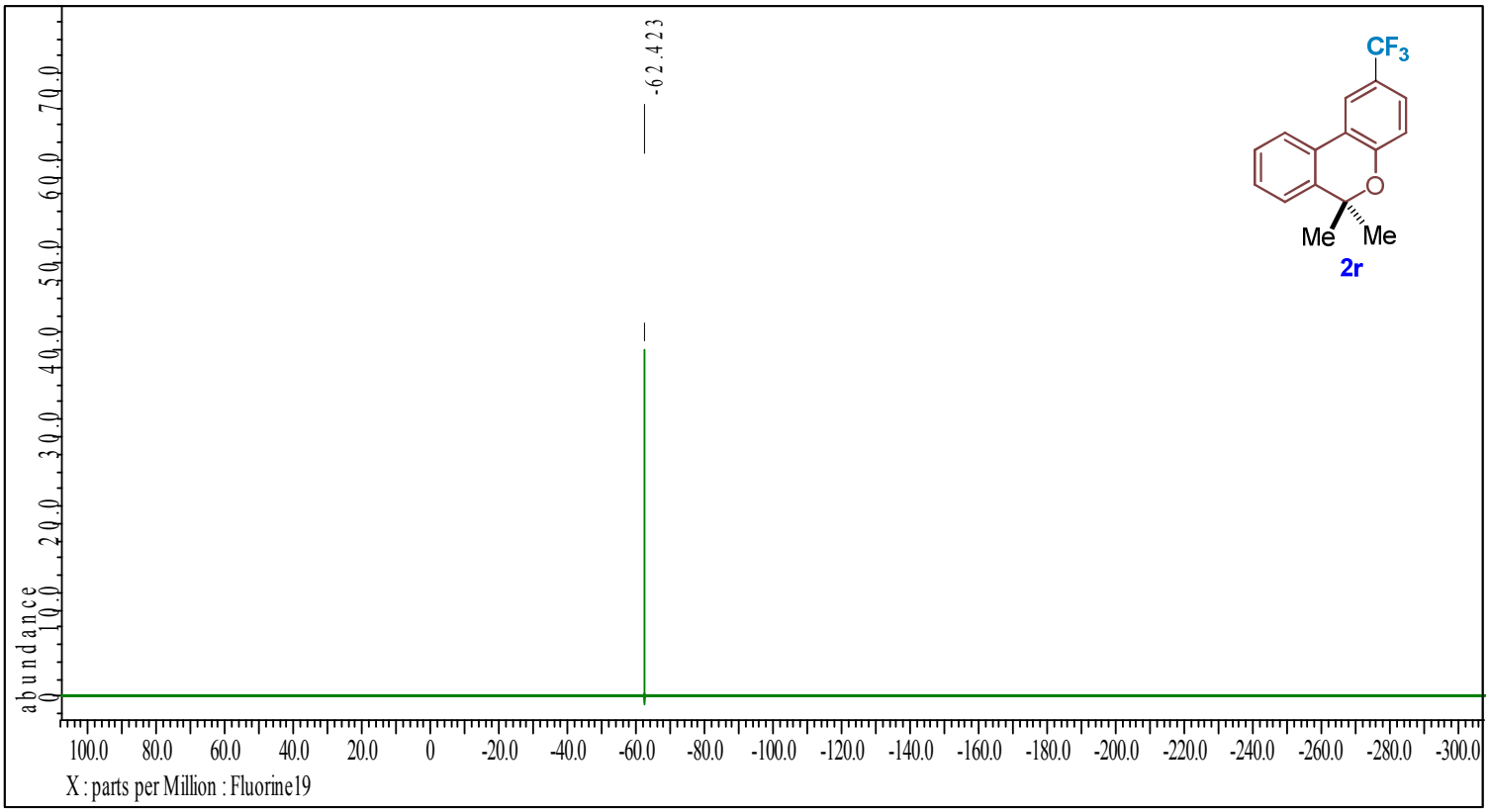

-111.876
F
O
Me
Me
2k
abundance
X : parts per Million : Fluorine19

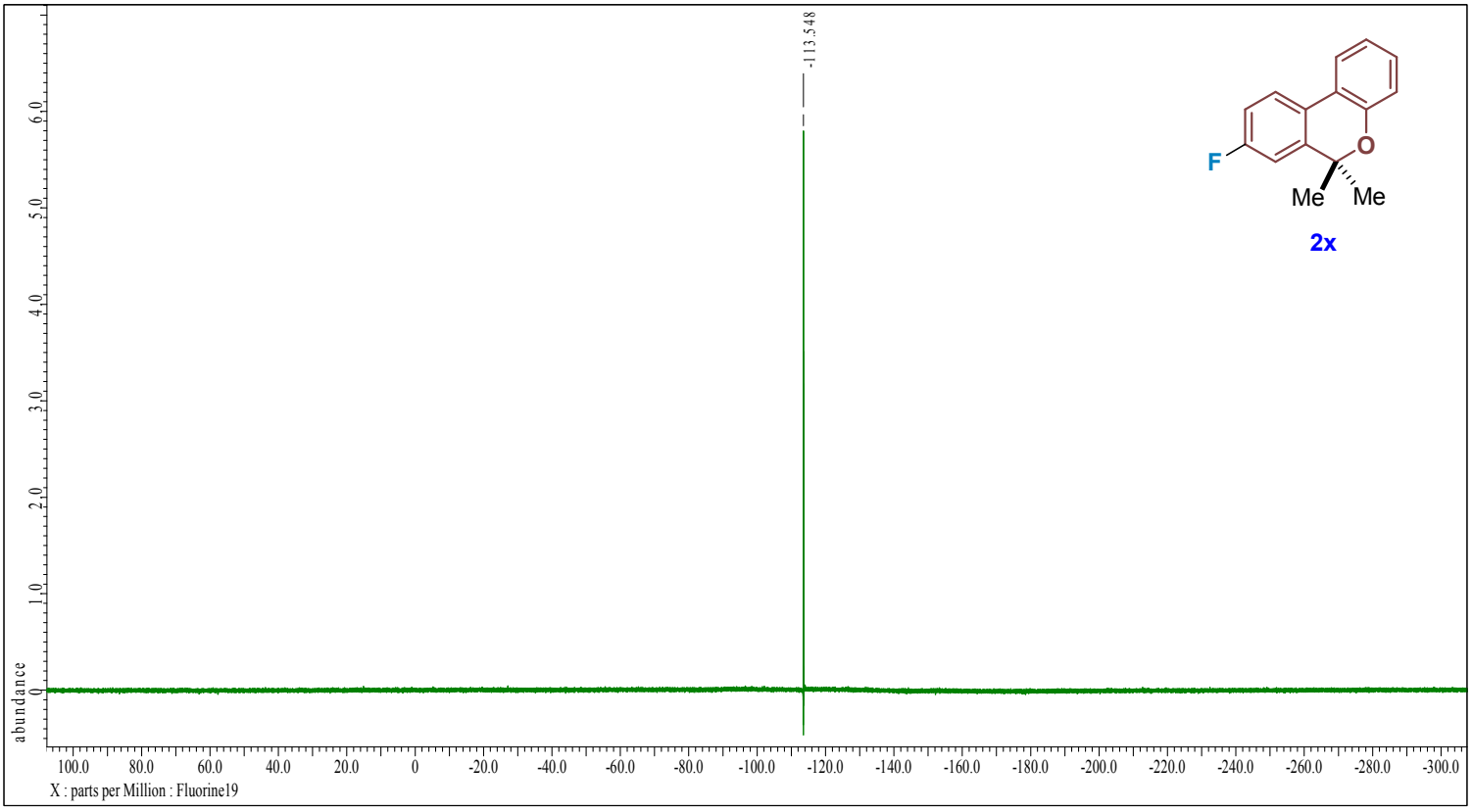

-138.179
-140.310
F
F
O
Me
Me
2l
abundance
X : parts per Million : Fluorine19

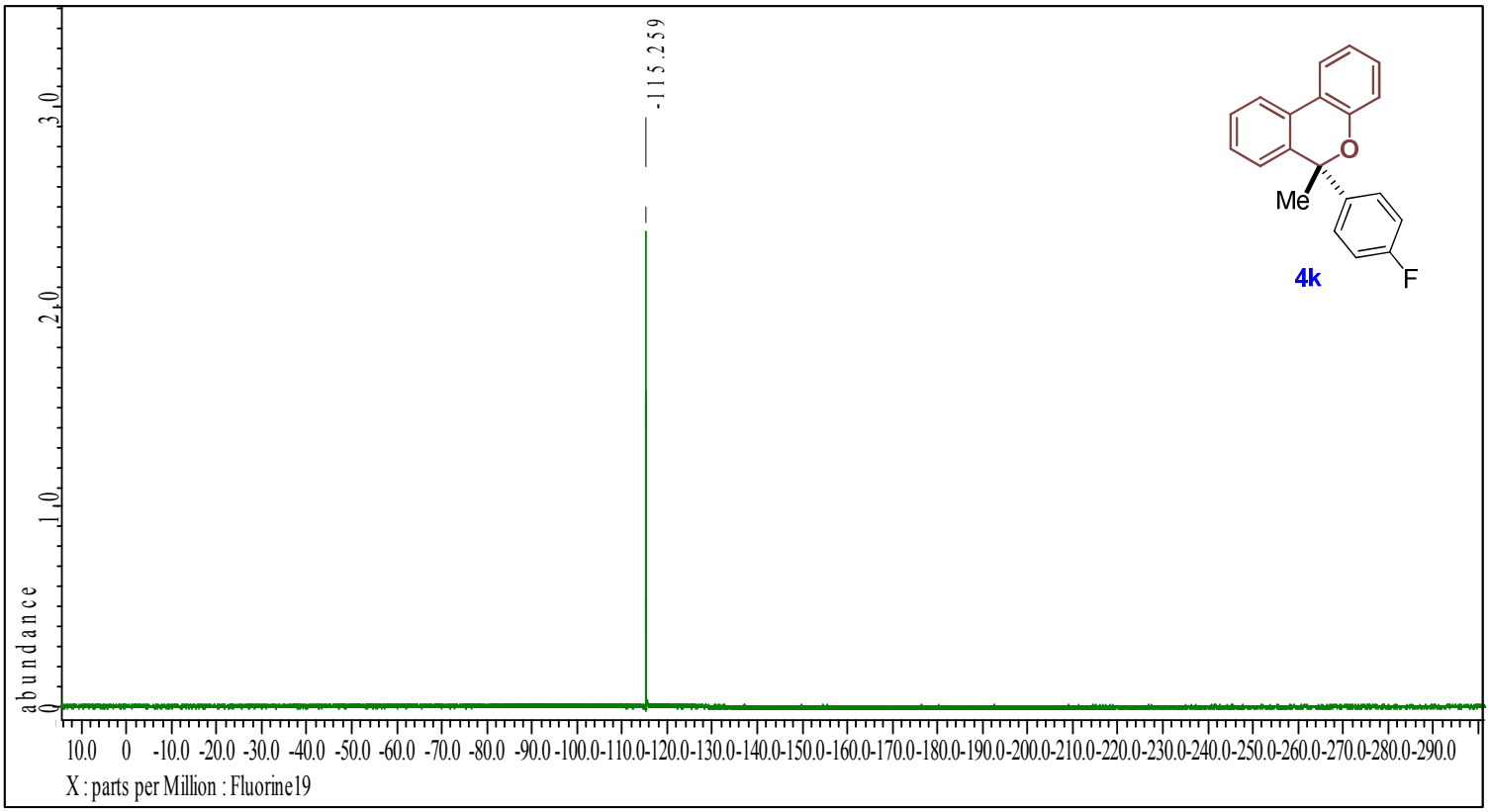

-135.216
-135.271
-163.056
F
F
F
O
Me
Me
2n
abundance
X : parts per Million : Fluorine19

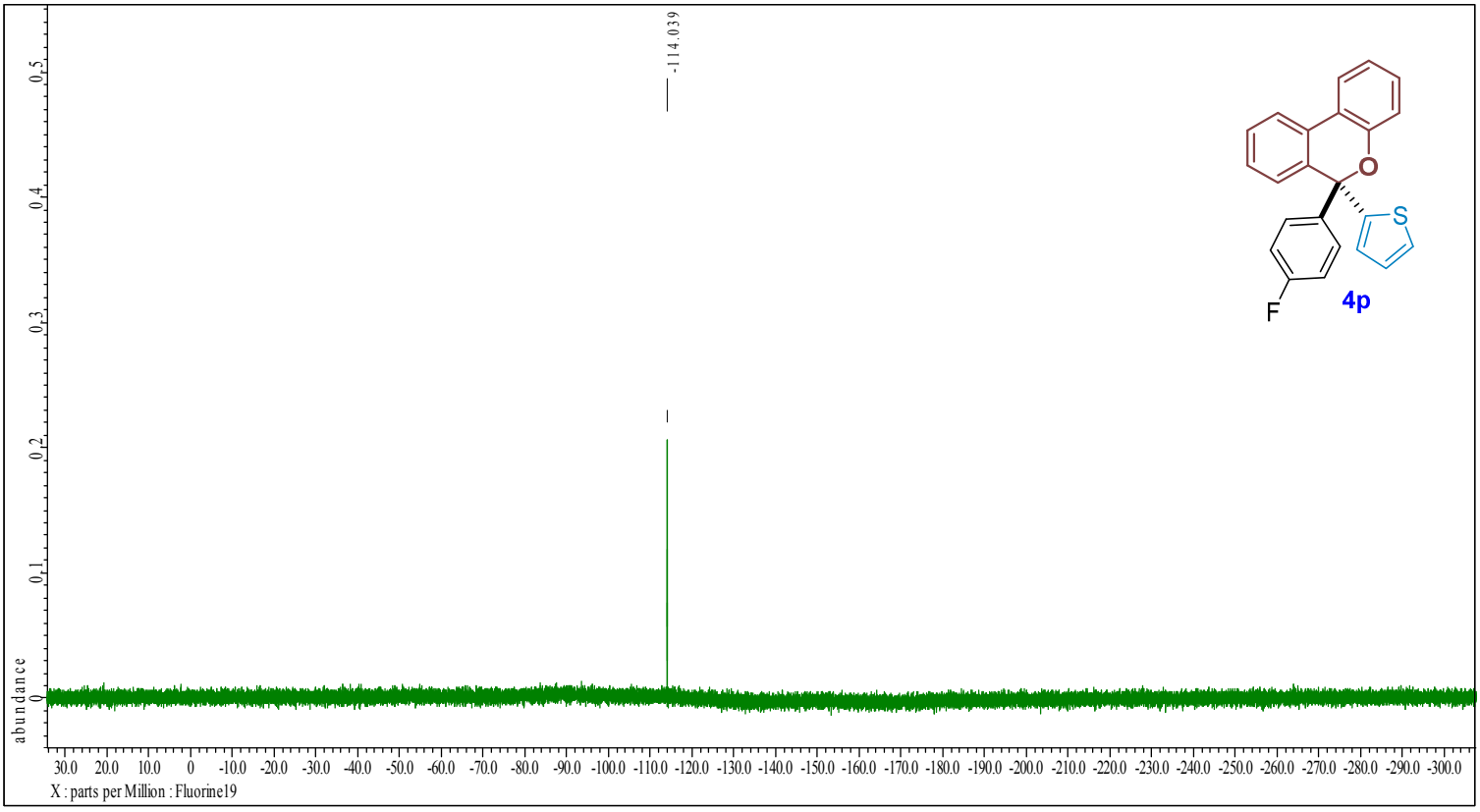

-62.249
CF3
O
Me
Me
2p
abundance
20.0
10.0
0
100.0 80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0 -280.0 -300.0
X : parts per Million : Fluorine19


-62.606
-62.661
CF3
CF3
O
Me
Me
2q
abundance
20.0
10.0
0
100.0 80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0 -280.0 -300.0
X : parts per Million : Fluorine19


-62.423
CF3
Me
Me
O
2r
abundance
X : parts per Million : Fluorine19


-113.548
F
Me
Me
O
2x
abundance
X : parts per Million : Fluorine19


-115.259
abundance
3.0
2.0
1.0
0
Me
O
F
4k
10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0 -260.0 -270.0 -280.0 -290.0
X : parts per Million : Fluorine19


-114.039
abundance
0.5
0.4
0.3
0.2
0.1
0
O
S
F
4p
30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0 -260.0 -270.0 -280.0 -290.0 -300.0
X : parts per Million : Fluorine19