Supporting Information

Syntheses of Functionalized Benzocoumarins by Photoredox Catalysis

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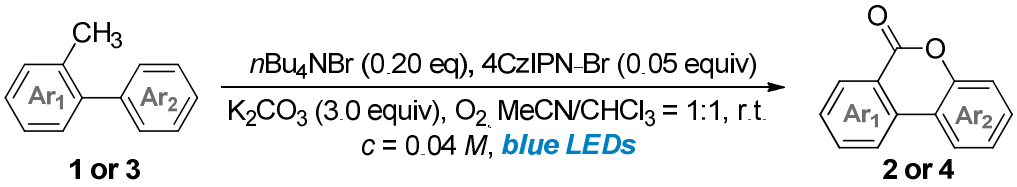
Materials and methods

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 phosphomolybdic acid. 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 synthesis of 6*H*-benzo[*c*]chromen-6-ones

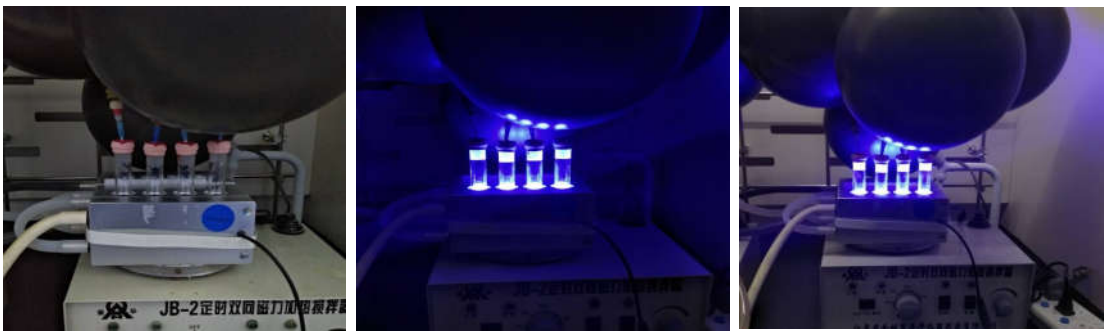


1 or 3 **2 or 4**

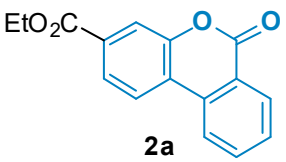
Condition A: A flame-dried reaction tube was equipped with magnetic stir bar and charged with 2-methyl-1,1'-biphenyl **1** or **3** (0.0416 mmol, 1.0 equiv), nBu$_4$NBr (0.0083 mmol, 0.2 equiv), 4CzIPN-Br (0.0021 mmol, 0.05 equiv), K_2CO_3 (0.1248mmol, 3.0 equiv) and MeCN/$CHCl_3$ (1:1).

Condition B: A flame-dried reaction tube was equipped with magnetic stir bar and charged with 2-methyl-1,1'-biphenyl **1** (0.0416 mmol, 1.0 equiv), nBu$_4$NBr (0.0166 mmol, 0.4 equiv), 2-BrAQ (0.0017 mmol, 0.04 equiv), KF (0.1248 mmol, 3.0 equiv) and MeCN/CF_3CH_2OH (1:1).

Then, 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 = 6/1) to afford the desired pure product **2-4** in 29-89% yields. (The substrates **1d**, **1e** and **1o** were carried out under the condition B.)

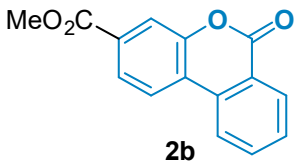


^{1}H, ^{13}C and ^{19}F spectra data of compounds 2a-2q, 4a-4t



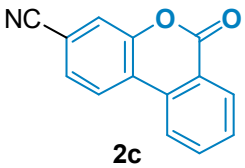
2a

ethyl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (2a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (d, J = 7.2 Hz, 1H), 8.20-8.18 (d, J = 8.4 Hz, 1H), 8.15-8.13 (d, J = 8.4 Hz, 1H), 8.03-8.00 (m, 2H), 7.91-7.87 (m, 1H), 7.69-7.86 (t, J = 7.2 Hz, 1H), 4.46-4.41 (q, J = 7.2Hz, 2H), 1.46-1.42 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.4, 160.7, 151.0, 135.1, 133.8, 132.3, 130.8, 130.1, 125.3, 122.9, 122.5, 121.9, 121.8, 119.1, 61.7, 14.4. These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (White solid, 17.6 mg, 77% isolated yield)



2b

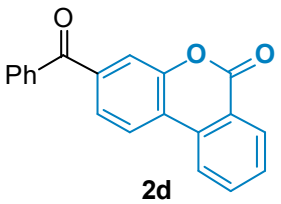
methyl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (2b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.43 (dd, J_1 = 0.8 Hz, J_2 = 7.6 Hz, 1H), 8.19-8.13 (m, 2H), 8.02-7.99 (m, 2H), 7.90-7.89 (m, 1H), 7.69-7.67 (m, 1H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 160.8, 151.0, 135.2, 133.8, 131.9, 130.9, 130.1, 125.4, 123.0, 122.5, 122.0, 121.8, 119.2, 52.7. These data are consistent with literature values, see: C. Pan, L. Wang and J. Han, *Org. Lett.*, 2020, **22**, 4776. (White solid, 14.4 mg, 62% isolated yield)



2c

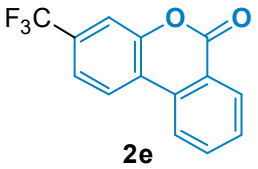
6-oxo-6*H*-benzo[*c*]chromene-3-carbonitrile (2c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (m, 1H), 8.20-8.16 (m, 2H), 7.95-7.91 (m, 1H), 7.75-7.71 (m, 1H), 7.68-7.67 (d, J = 1.6Hz, 1H), 7.64-7.62 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H); ^{13}C NMR

(100 MHz, $CDCl_3$) δ 159.9, 151.0, 135.5, 133.0, 131.1, 130.8, 127.8, 124.0, 122.5, 122.4, 121.9, 121.8, 117.7, 113.6. These data are consistent with literature values, see: Y. Wang, A. V. Gulevich, V. Gevorgyan, *Chem. Eur. J.*, 2013, **19**, 15836. (White solid, 14.5 mg, 63% isolated yield)



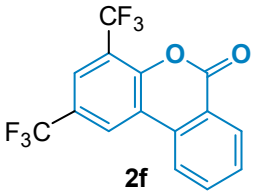
2d

3-benzoyl-6*H*-benzo[*c*]chromen-6-one (2d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 8.22-8.20 (m, 2H), 7.93-7.88 (m, 1H), 7.86-7.78 (m, 4H), 7.71-7.63 (m, 2H), 7.55-7.51 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.0, 160.8, 150.9, 139.1, 137.0, 135.2, 133.9, 133.1, 130.9, 130.1, 128.6, 127.2, 125.8, 123.1, 122.5, 121.8, 121.5, 119.8; HRMS calculated for $C_{20}H_{13}O_3$ ($M + H^+$): 301.0865, found: 301.0860. (White solid, 10.8 mg, 49% isolated yield)



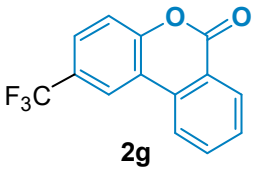
2e

3-**(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (2e):** ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 8.22-8.18 (t, J = 8.0 Hz, 2H), 7.93-7.89 (m, 1H), 7.72-7.59 (m, 3H), 7.46-7.43 (t, J = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 151.1, 135.3, 133.5, 132.5, 132.2, 131.0, 130.2, 124.7, 123.7, 122.3, 122.0, 121.8, 121.2, 121.1, 115.4, 115.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.68. These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (White solid, 11.3 mg, 50% isolated yield)



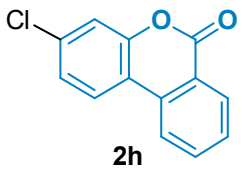
2f

2,4-bis(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (2f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53-8.46 (m, 2H), 8.22-8.20 (d, J = 8.0 Hz, 1H), 8.03 (s, 1H), 7.98-7.94 (m, 1H), 7.78-7.72 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 150.7, 135.8, 133.8, 132.6, 131.6, 131.5, 131.2, 130.9, 128.9, 128.8, 126.7, 126.4, 124.7, 124.5, 124.2, 123.4, 122.2, 121.8, 121.1, 120.6, 120.5, 120.2, 120.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.04, -62.74. These data are consistent with literature values, see: Y. Wang, A. V. Gulevich, V. Gevorgyan, *Chem. Eur. J.*, 2013, **19**, 15836. (White solid, 11.3 mg, 53% isolated yield)



2g

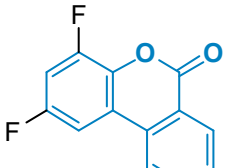
2-(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (2g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 8.30-8.28 (d, J = 8.4 Hz, 1H), 8.17-8.15 (d, J = 8.0 Hz, 1H), 7.91-7.87 (m, 1H), 7.80-7.79 (d, J = 7.6 Hz, 1H), 7.69-7.65 (m, 1H), 7.46-7.42 (t, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.4, 153.2, 135.4, 133.6, 130.9, 130.0, 127.2, 127.1, 126.9, 125.2, 122.5, 122.0, 121.3, 120.6, 120.5, 118.6, 118.5, 116.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.63. These data are consistent with literature values, see: Z. Luo, Z.-H. Gao, Z.-Y. Song, Y.-F. Han and S. Ye, *Org. Biomol. Chem.,* 2019, **17**, 4212. (White solid, 10.0 mg, 44% isolated yield)



2h

3-chloro-6*H*-benzo[*c*]chromen-6-one (2h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38-8.36 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 8.06-8.04 (d, J = 7.6 Hz, 1H), 7.97-7.95 (d, J = 8.4 Hz, 1H), 7.85-7.81 (m, 1H), 7.62-7.57 (m, 1H), 7.35-7.34 (d, J = 2.0 Hz, 1H), 7.32-7.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 151.6, 136.0, 135.2, 134.1, 130.8, 129.3, 125.1, 123.9, 121.8, 121.0, 118.1, 116.8. These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (White solid, 22.5 mg, 62% isolated yield)

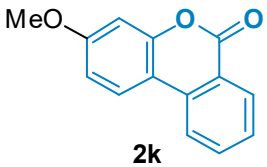
3-fluoro-6*H*-benzo[*c*]chromen-6-one (2i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.41-8.39 (d, J = 7.6 Hz, 1H), 8.07-8.03 (m, 2H), 7.86-7.82 (m, 1H), 7.61-7.57 (m, 1H), 7.11-7.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 162.3, 161.0, 152.2, 135.2, 134.4, 130.8, 128.9, 124.5, 124.4, 121.6, 120.5, 114.7, 112.7, 112.4, 105.4, 105.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -108.26; These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (Yellow solid, 11.2 mg, 48% isolated yield)



2j

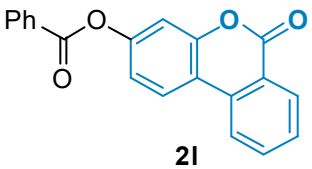
2,4-difluoro-6*H*-benzo[*c*]chromen-6-one (2j): ^{1}H NMR (400 MHz, $CDCl_3$) δ

8.47-8.44 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 8.05-8.03 (d, J = 8.0 Hz, 1H), 7.91-7.87 (m, 1H), 7.71-7.67 (m, 1H), 7.56-7.53 (m, 1H), 7.10-7.04 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.5, 157.2, 157.1, 151.7, 149.3, 149.2, 135.3, 133.4, 131.1, 130.3, 122.3, 121.5, 120.5, 106.0, 105.8, 105.7, 105.5, 104.3, 104.2, 104.1, 104.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.18, -127.46. These data are consistent with literature values, see: X.-Z. Tao, J.-J. Dai, J. Z., J. X. and H.-J. Xu, *Chem. Eur. J.*, 2018, **24**, 6932. (White solid, 9.7 mg, 43% isolated yield)



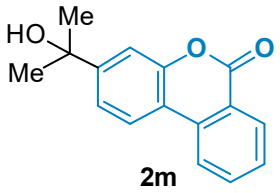
2k

3-methoxy-6*H*-benzo[*c*]chromen-6-one (2k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38-8.36 (m, 1H), 8.03-7.95 (m, 2H), 7.82-7.77 (m, 1H), 7.53-7.50 (m, 1H), 6.94-6.91 (m, 1H), 6.89-6.88 (d, J = 2.8 Hz, 1H), 3.89 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.6, 152.7, 137.6, 130.3, 129.7, 128.4, 127.8, 127.6, 123.9, 120.8, 115.4, 112.6, 101.7, 55.8. These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (Orange solid, 14.3 mg, 63% isolated yield)



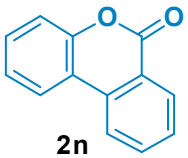
2l

6-oxo-6*H*-benzo[*c*]chromen-3-yl benzoate (2l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43-8.41 (m, 1H), 8.24-8.22 (d, J = 7.6 Hz, 2H), 8.13-8.11 (m, 3H), 7.87-7.83 (m, 1H), 7.70-7.46 (m, 4H), 7.28-7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 164.8, 152.3, 151.9, 135.2, 134.4, 134.1, 133.9, 130.8, 130.4, 130.3, 129.4, 129.0, 128.8, 128.6, 123.8, 121.8, 120.9, 118.7, 116.1, 111.4; HRMS calculated for $C_{20}H_{13}O_4$ ($M + H^+$): 317.0814, found: 317.0808. (Yellow solid, 12.7 mg, 58% isolated yield)



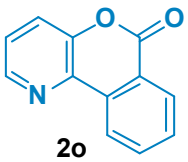
2m

3-(2-hydroxypropan-2-yl)-6*H*-benzo[*c*]chromen-6-one (2m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.39 (dd, J_1 = 0.8 Hz, J_2 = 8.4 Hz, 1H), 8.12-8.10 (d, J = 8.0 Hz, 1H), 8.04-8.02 (d, J = 8.0 Hz, 1H), 7.85-7.81 (m, 1H), 7.60-7.56 (m, 1H), 7.50-7.47 (m, 2H), 1.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.5, 152.5, 151.3, 135.0, 134.8, 130.7, 128.8, 122.8, 121.7, 121.1, 119.2, 116.5, 113.9, 72.5, 31.8; HRMS calculated for $C_{16}H_{15}O_3$ ($M + H^+$): 255.1021, found: 255.1016. (Pale yellow solid, 6.5 mg, 29% isolated yield)



2n

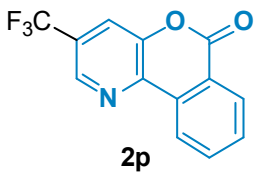
6*H*-benzo[*c*]chromen-6-one (2n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.39 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 8.14-8.12 (d, J = 8.0 Hz, 1H), 8.08-8.05 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 7.85-7.81 (m, 1H), 7.61-7.57 (m, 1H), 7.51-7.46 (m, 1H), 7.38-7.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 151.3, 136.1, 135.0, 130.7, 130.5, 129.0, 125.8, 124.7, 122.9, 121.8, 121.3, 117.9. These data are consistent with literature values, see: Y. Li, Y. Ding, J. Wang, Y. Su, X. Wang, *Org. Lett.*, 2013, **15**, 2574. (Yellow oil, 13.9 mg, 60% isolated yield)



2o

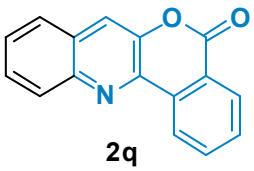
6*H*-isochromeno[4,3-*b*]pyridin-6-one (2o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71-8.69

(d, J = 7.2 Hz, 1H), 8.64-8.62 (m, 1H), 8.41-8.39 (m, 1H), 7.96-7.91 (m, 1H), 7.74-7.67 (m, 2H), 7.47-7.44 (, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 152.6, 147.8, 146.2, 136.9, 135.7, 135.4, 130.7, 130.2, 124.9, 123.5, 122.5. These data are consistent with literature values, see: X.-Z. Tao, J.-J. Dai, J. Z., J. X. and H.-J. Xu, *Chem. Eur. J.*, 2018, **24**, 6932. (White solid, 12.3 mg, 52% isolated yield)



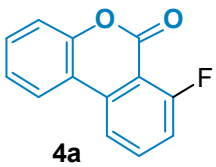
2p

3-(trifluoromethyl)-6*H*-isochromeno[4,3-*b*]pyridin-6-one (2p): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86-8.85 (d, J = 1.2 Hz, 1H), 8.74-8.72 (d, J = 8.0 Hz, 1H), 8.43-8.41 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 8.00-7.96 (m, 1H), 7.89-7.88 (d, J = 1.2 Hz, 1H), 7.82-7.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 147.0, 142.6, 142.5, 140.0, 135.7, 134.5, 131.9, 130.5, 127.7, 127.4, 124.2, 122.9, 122.3, 122.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.91; HRMS calculated for $C_{13}H_7F_3NO_2$ ($M + H^+$): 266.0429, found: 266.0423. (White solid, 16.5mg, 71% isolated yield)



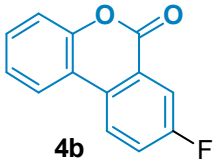
2q

5*H*-isochromeno[4,3-*b*]quinolin-5-one (2q): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96-8.94 (d, J = 8.0 Hz, 1H), 8.44-8.42 (m, 1H), 8.23-8.21 (d, J = 8.8 Hz, 1H), 8.05 (s, 1H), 8.00-7.95 (m, 1H), 7.91-7.89 (d, J = 8.0 Hz, 1H), 7.79-7.73 (m, 2H), 7.64-7.59 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.3, 145.7, 145.2, 138.7, 135.6, 135.3, 131.3, 130.4, 129.7, 129.3, 128.9, 127.9, 127.5, 124.4, 123.4, 121.1; HRMS calculated for $C_{16}H_{10}NO_2$ ($M + H^+$): 248.0712, found: 248.0706. (White solid, 14.5 mg, 62% isolated yield)



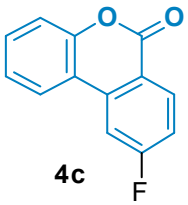
4a

7-fluoro-6*H*-benzo[*c*]chromen-6-one (4a): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.03 (m, 1H), 7.96-7.93 (d, *J* = 8.4 Hz, 1H), 7.83-7.78 (m, 1H), 7.54-7.49 (m, 1H), 7.37-7.33 (m, 2H), 7.30-7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 162.4, 156.8, 151.6, 137.4, 136.3, 136.2, 131.3, 124.8, 123.3, 117.8, 117.7, 117.6, 117.1, 116.6, 116.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -105.75. These data are consistent with literature values, see: S. Xia, K. Hu, C. Lei and J. Jin. *Org. Lett.*, 2020, **22**, 1385. (Yellow solid, 17.5 mg, 72% isolated yield)



4b

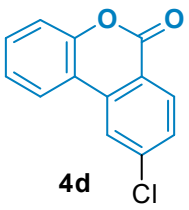
8-fluoro-6*H*-benzo[*c*]chromen-6-one (4b): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.13 (m, 1H), 8.08-8.02 (m, 2H), 7.59-7.54 (m, 1H), 7.52-7.48 (m, 1H), 7.40-7.35 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 161.3, 160.4, 150.9, 131.4, 130.5, 128.3, 124.9, 124.4, 124.3, 123.3, 123.1, 122.7, 118.0, 117.5, 116.4, 116.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -110.04. These data are consistent with literature values, see: Y. Wang, J.-Y. Gu and Z.-J. Shi, *Org. Lett.*, 2017, **19**, 1326. (White solid, 10.0 mg, 43% isolated yield)



4c

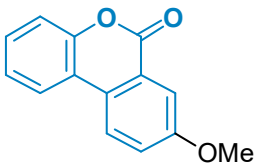
9-fluoro-6*H*-benzo[*c*]chromen-6-one (4c): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.42 (m, 1H), 7.98-7.96 (m, 1H), 7.76-7.73 (m, 1H), 7.55-7.51 (m, 1H), 7.40-7.34 (m, 2H),

7.31-7.26 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 165.8, 160.4, 151.7, 137.8, 134.1, 134.0, 131.4, 124.8, 123.1, 118.0, 117.8, 117.5, 117.3, 117.0, 108.4, 108.2; ^{19}F NMR (376 MHz, $CDCl_3$) δ -100.94. These data are consistent with literature values, see: S. Xia, K. Hu, C. Lei and J. Jin. *Org. Lett.*, 2020, **22**, 1385. (White solid, 12.0 mg, 51% isolated yield)



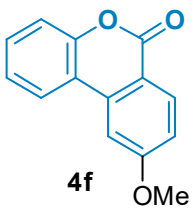
4d

9-chloro-6*H*-benzo[*c*]chromen-6-one (4d): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34-8.32 (d, *J* = 8.0 Hz, 1H), 8.07-8.06 (d, *J* = 2.0 Hz, 1H), 8.00-7.98 (d, *J* = 7.6 Hz, 1H), 7.55-7.50 (m, 2H), 7.38-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 151.7, 141.9, 136.4, 132.3, 131.3, 129.4, 124.9, 123.0, 121.9, 119.6, 118.0, 117.1. These data are consistent with literature values, see: M. Chao, F. Wang, L. Xu, Y. Ju, Z. Chen, B. Wang, P.Gong, J. You, M. Jin and D. Shen. *J. Org. Chem.*, 2021, **86**, 13371. (White solid, 16.5 mg, 71% isolated yield)

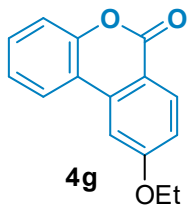


4e

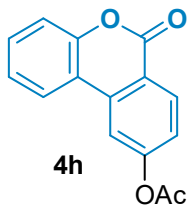
8-methoxy-6*H*-benzo[*c*]chromen-6-one (4e): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06-8.04 (d, *J* = 9.2 Hz, 1H), 8.01-7.98 (m, 1H), 7.83-7.82 (d, *J* = 3.2 Hz, 1H), 7.46-7.31 (m, 4H), 3.95 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.1, 150.5, 129.4, 128.2, 127.2, 124.7, 124.4, 123.5, 122.5, 122.3, 118.3, 117.7, 111.2, 55.9. These data are consistent with literature values, see: S. Xia, K. Hu, C. Lei and J. Jin. *Org. Lett.*, 2020, **22**, 1385. (Yellow solid, 10.9 mg, 48% isolated yield)



9-methoxy-6*H*-benzo[*c*]chromen-6-one (4f): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.34 (d, J = 9.2 Hz, 1H), 8.02-8.00 (m, 1H), 7.51-7.47 (m, 2H), 7.38-7.31 (m, 2H), 7.14-7.11 (m, 1H), 4.00 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 151.7, 137.0, 133.0, 130.7, 129.7, 124.5, 122.8, 117.9, 115.4, 114.4, 105.2, 55.8. These data are consistent with literature values, see: S. Xia, K. Hu, C. Lei and J. Jin. *Org. Lett.*, 2020, **22**, 1385. (Yellow solid, 13.6 mg, 80% isolated yield)

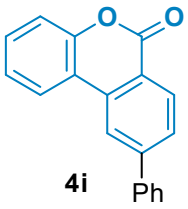


9-ethoxy-6*H*-benzo[*c*]chromen-6-one (4g): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33-8.31 (d, J = 8.8 Hz, 1H), 8.00-7.98 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 7.50-7.46 (m, 2H), 7.37-7.30 (m, 2H), 7.11-7.08 (m, 1H), 4.25-4.20 (q, J = 7.2 Hz, 2H), 1.53-1.50 (t, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 161.2, 151.7, 137.0, 133.0, 130.6, 124.4, 122.8, 118.2, 117.9, 116.5, 114.2, 105.8, 64.2, 14.8; HRMS calculated for $C_{15}H_{13}O_3$ ($M + H^+$): 241.0865, found: 241.0859. (White solid, 16.9 mg, 72% isolated yield)



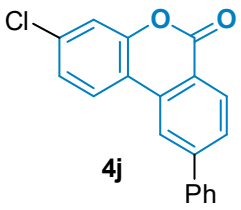
6-oxo-6*H*-benzo[*c*]chromen-9-yl acetate (4h): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.43 (d, J = 8.4 Hz, 1H), 7.99-7.97 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 7.87-7.86 (d, J = 2.4 Hz, 1H), 7.53-7.49 (m, 1H), 7.39-7.31 (m, 3H), 2.40 (s, 3H), 2.01 (s, 2H);

^{13}C NMR (100 MHz, $CDCl_3$) δ 168.8, 160.6, 156.0, 151.6, 136.8, 132.7, 131.1, 124.7, 123.1, 122.8, 118.8, 118.0, 117.6, 114.7, 21.3; HRMS calculated for $C_{15}H_{11}O_4$ (M + H^+): 255.0657, found: 255.0652. (White solid, 10.9 mg, 47% isolated yield)



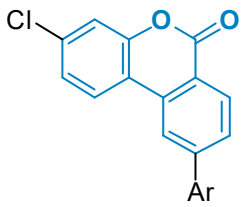
4i

9-phenyl-6*H*-benzo[*c*]chromen-6-one (4i): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (d, J = 8.4 Hz, 1H), 8.29-8.28 (d, J = 2.0 Hz, 1H), 8.16-8.14 (dd, J_1 = 0.8 Hz, J_2 = 8.0 Hz, 1H), 7.81-7.78 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 7.73-7.71 (m, 2H), 7.56-7.46 (m, 4H), 7.40-7.34 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 151.6, 147.9, 139.7, 135.2, 131.3, 130.7, 129.3, 128.9, 128.0, 127.6, 124.7, 122.9, 120.2, 120.0, 118.2, 118.0. These data are consistent with literature values, see: C. Pan, L. Wang and J. Han, *Org. Lett.*, 2020, **22**, 4776. (Yellow solid, 9.7 mg, 43% isolated yield)



4j

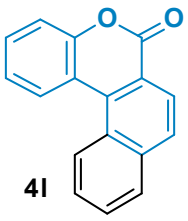
3-chloro-9-phenyl-6*H*-benzo[*c*]chromen-6-one (4j): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (d, J = 8.0 Hz, 1H), 8.23-8.22 (d, J = 2.0 Hz, 1H), 8.09-8.06 (d, J = 8.4 Hz, 1H), 7.83-7.80 (dd, J_1 = 2.0 Hz, J_2 = 8.4 Hz, 1H), 7.72-7.70 (m, 2H), 7.57-7.53 (m, 2H), 7.51-7.48 (m, 1H), 7.40-7.39 (m, 1H), 7.35-7.33 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 151.8, 148.2, 139.5, 136.1, 134.5, 131.4, 129.3, 129.1, 128.3, 127.6, 125.1, 123.9, 120.2, 119.6, 118.1, 116.9; HRMS calculated for $C_{19}H_{11}ClNaO_2$ (M + Na^+): 329.0345, found: 329.0340. (White solid, 12.8 mg, 58% isolated yield)



Ar = 4-Cl-Ph

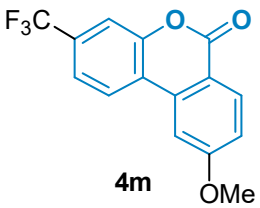
4k

3-chloro-9-(4-chlorophenyl)-6*H*-benzo[*c*]chromen-6-one (4k): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (d, *J* = 8.4 Hz, 1H), 8.19 (s, 1H), 8.08-8.06 (d, *J* = 8.4 Hz, 1H), 7.78-7.76 (d, *J* = 8.0 Hz, 1H), 7.65-7.63 (d, *J* = 8.0 Hz, 2H), 7.52-7.50 (d, *J* = 8.4 Hz, 2H), 7.41 (s, 1H), 7.36-7.34 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 151.9, 146.9, 137.9, 136.3, 135.4, 134.6, 131.6, 129.5, 128.9, 128.1, 125.2, 123.9, 120.0, 119.9, 118.2, 116.7; HRMS calculated for $C_{19}H_{11}Cl_2O_2$ ($M + H^+$): 341.0136, found: 341.0131. (White solid, 10.0 mg, 46% isolated yield)



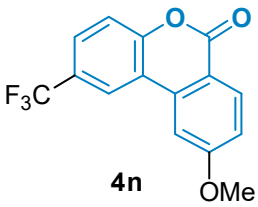
4l

6*H*-naphtho[2,1-*c*]chromen-6-one (4l): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91-8.88 (m, 1H), 8.55-8.53 (m, 1H), 8.35-8.33 (d, *J* = 8.8 Hz, 1H), 8.03-8.00 (m, 1H), 7.98-7.96 (d, *J* = 8.8 Hz, 1H), 7.76-7.70 (m, 2H), 7.56-7.50 (m, 2H), 7.44-7.40 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.8, 151.7, 137.2, 134.5, 130.2, 129.7, 129.3, 129.1, 128.4, 128.0, 127.6, 127.3, 124.6, 124.3, 120.2, 118.9, 118.1. These data are consistent with literature values, see: S. Xia, K. Hu, C. Lei and J. Jin. *Org. Lett.*, 2020, **22**, 1385. (Yellow oil, 17.7 mg, 76% isolated yield)



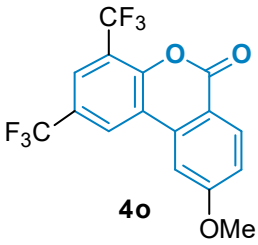
4m

9-methoxy-3-(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (4m): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36-8.34 (d, J = 8.8 Hz, 1H), 8.12-8.10 (d, J = 8.4 Hz, 1H), 7.60-7.55 (m, 2H), 7.51-7.50 (d, J = 2.4 Hz, 1H), 7.19-7.16 (dd, J_1 = 2.4 Hz, J_2 = 9.2 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 160.2, 151.4, 135.6, 133.3, 132.6, 132.2, 123.7, 121.1, 120.9, 117.2, 115.4, 114.7, 110.3, 106.0, 56.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.31; HRMS calculated for $C_{15}H_{10}F_3O_3$ ($M + H^+$): 295.0582, found: 295.0577. (Yellow solid, 19.8mg, 85% isolated yield)



4n

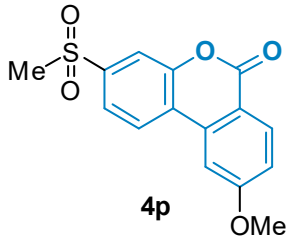
9-methoxy-2-(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (4n): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37-8.35 (d, J = 8.8 Hz, 1H), 8.25-8.24 (d, J = 1.2 Hz, 1H), 7.75-7.72 (dd, J_1 = 1.6 Hz, J_2 = 8.8 Hz, 1H), 7.51-7.46 (m, 2H), 7.20-7.17 (dd, J_1 = 2.4 Hz, J_2 = 9.2 Hz, 1H), 4.01 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.3, 160.3, 153.6, 135.8, 133.3, 127.3, 127.2, 127.0, 120.6, 120.5, 118.7, 118.5, 117.2, 114.3, 105.4, 56.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -61.81. These data are consistent with literature values, see: L. Pan, J. Dong, D. Xie, Y. Li and Q. Liu, *Adv. Synth. Catal.*, 2018, **360**, 958. (Yellow solid, 10.9 mg, 56% isolated yield)



4o

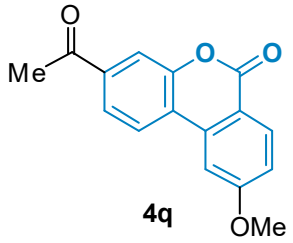
9-methoxy-2,4-bis(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-one (4o): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43-8.37 (m, 2H), 8.02 (s, 1H), 7.52-7.51 (d, J = 2.0 Hz, 1H), 7.25-7.22 (m, 1H), 4.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.5, 158.2, 134.7, 133.6, 126.1, 124.8, 124.1, 120.0, 117.8, 113.9, 106.0, 56.2; ^{19}F NMR (376 MHz,

$CDCl_3$) δ -62.04, -62.07; HRMS calculated for $C_{16}H_9F_6O_3$ ($M + H^+$): 363.0456, found: 363.0450. (Yellow solid, 15.7 mg, 72% isolated yield)



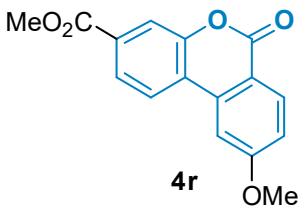
4p

9-methoxy-3-(methylsulfonyl)-6*H*-benzo[*c*]chromen-6-one (4p): ^1H NMR (400 MHz, $CDCl_3$) δ 8.40-8.38 (d, J = 8.8 Hz, 1H), 8.22-8.20 (d, J = 8.0 Hz, 1H), 7.93-7.87 (m, 2H), 7.55 (s, 1H), 7.27-7.23 (m, 1H), 4.03 (s, 3H), 3.14 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 159.9, 151.6, 142.0, 135.1, 133.5, 127.2, 124.3, 122.7, 117.7, 117.5, 114.8, 106.4, 56.1, 44.5; HRMS calculated for $C_{15}H_{12}NaO_5S$ ($M + Na^+$): 327.0303, found: 327.0298. (Pale yellow solid, 15.6 mg, 70% isolated yield)



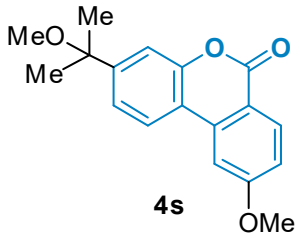
4q

3-acetyl-9-methoxy-6*H*-benzo[*c*]chromen-6-one (4q): ^1H NMR (400 MHz, $CDCl_3$) δ 8.34-8.32 (d, J = 8.8 Hz, 1H), 8.07-8.04 (m, 1H), 7.90-7.86 (m, 2H), 7.50-7.49 (d, J = 2.4 Hz, 1H), 7.18-7.16 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 4.02 (s, 3H), 2.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 165.1, 160.0, 151.5, 138.5, 135.8, 133.2, 123.7, 123.2, 122.0, 118.0, 117.3, 114.7, 106.0, 56.0, 26.8; HRMS calculated for $C_{16}H_{13}O_4$ ($M + H^+$): 269.0814, found: 269.0808. (Yellow solid, 18.6 mg, 81% isolated yield)



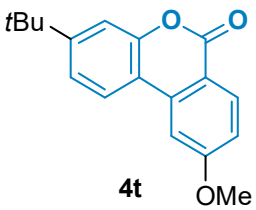
4r

methyl 9-methoxy-6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (4r): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.38-8.36 (d, J = 8.8 Hz, 1H), 8.09-8.07 (d, J = 8.0 Hz, 1H), 8.01-7.97 (m, 2H), 7.54-7.53 (d, J = 2.8 Hz, 1H), 7.20-7.17 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 4.02 (s, 3H), 3.98 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.9, 165.0, 160.6, 151.4, 135.9, 133.2, 132.0, 125.2, 123.0, 122.0, 119.2, 117.2, 114.8, 106.0, 55.9, 52.7; HRMS calculated for $C_{16}H_{13}O_5$ ($M + H^+$): 285.0763, found: 285.0760. (White solid, 13.8 mg, 62% isolated yield)



4s

9-methoxy-3-(2-methoxypropan-2-yl)-6*H*-benzo[*c*]chromen-6-one (4s): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34-8.32 (d, J = 8.8 Hz, 1H), 8.09-8.05 (m, 1H), 7.96-7.94 (d, J = 9.2Hz, 1H), 7.61-7.58 (d, J = 8.8 Hz, 1H), 7.48-7.45 (m, 3H), 7.12-7.09 (dd, J_1 = 2.8 Hz, J_2 = 9.2 Hz, 1H), 4.00 (s, 3H), 1.64 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 152.6, 151.6, 136.9, 133.0, 130.3, 124.7, 122.8, 120.9, 116.5, 116.1, 114.0, 105.1, 56.9, 31.7; HRMS calculated for $C_{18}H_{19}O_4$ ($M + H^+$): 299.1283, found: 299.1278. (Pale yellow solid, 10.7 mg, 48% isolated yield)

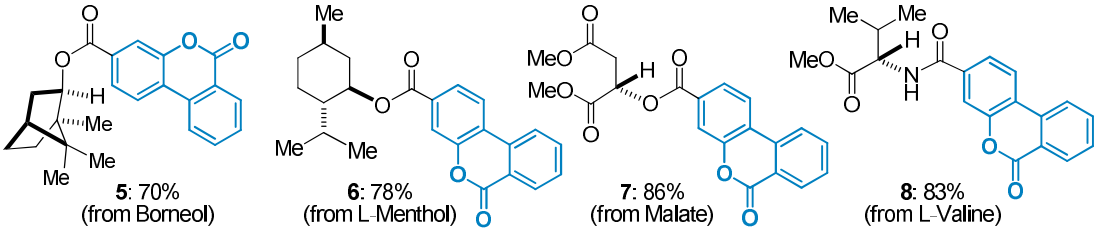


4t

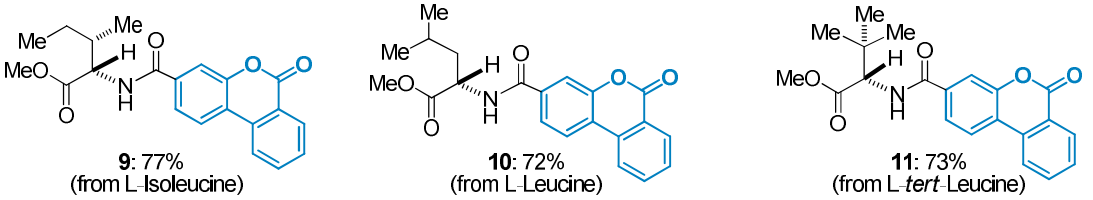
3-(*tert*-butyl)-9-methoxy-6*H*-benzo[*c*]chromen-6-one (4t): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34-8.32 (d, J = 8.8 Hz, 1H), 7.93-7.91 (d, J = 9.2 Hz, 1H), 7.47-7.46 (d, J = 2.4 Hz, 1H), 7.38-7.35 (m, 2H), 7.10-7.08 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 4.00 (s, 3H), 1.37 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 161.5, 154.9, 151.7, 137.2, 133.0, 130.2, 127.2, 125.6, 122.5, 121.9, 115.8, 105.0, 55.8, 35.1, 31.2; HRMS

calculated for $C_{18}H_{19}O_3$ ($M + H^+$): 283.1334, found: 283.1329. (Orange solid, 13.1 mg, 59% isolated yield)

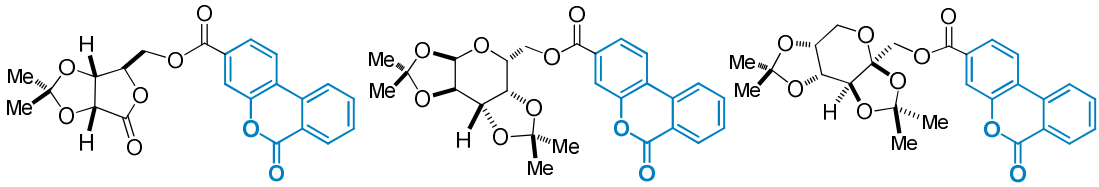
Late-stage functionalization of substances derived from natural products



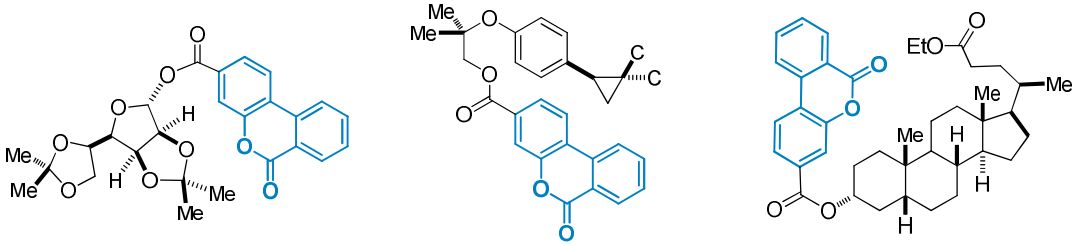
5: 70% (from Borneol) **6**: 78% (from L-Menthol) **7**: 86% (from Malate) **8**: 83% (from L-Valine)



9: 77% (from L-Isoleucine) **10**: 72% (from L-Leucine) **11**: 73% (from L-*tert*-Leucine)



12: 52% (from D-Ribose Acid) **13**: 89% (from D-Galactopyranose) **14**: 80% (from D-Fructopyranose)



15: 85% (from D-Mannofuranose) **16**: 51% (from Ciprofibrate) **17**: 58% (from Lithocholic Acid)

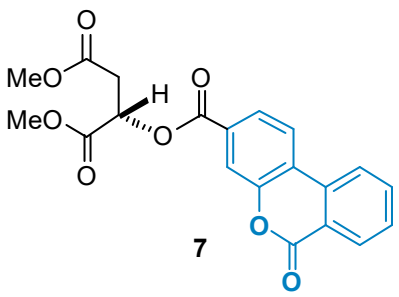
These reactions were conducted in the solvent of MeCN/DCE (1:1) under otherwise identical reaction conditions

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

4,7,7-trimethylbicyclo[2.2.1]heptan-2-yl-6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (5): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (m, 1H), 8.20-8.15 (m, 2H), 8.06-8.01 (m, 2H), 7.92-7.87 (m, 1H), 7.70-7.66 (t, *J* = 7.2 Hz, 1H), 5.17-5.14 (m,

1H), 2.55-2.47 (m, 1H), 2.17-2.11 (m, 1H), 1.88-1.76 (m, 2H), 1.49-1.42 (m, 1H), 1.35-1.31 (m, 1H), 1.18-1.14 (m, 1H), 0.99 (s, 3H), 0.94 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 165.6, 160.8, 151.0, 135.2, 133.9, 132.7, 130.9, 130.1, 125.4, 123.0, 122.5, 121.8, 119.1, 81.4, 49.3, 48.0, 45.1, 37.0, 28.2, 27.5, 19.8, 19.0, 13.7; HRMS calculated for $C_{24}H_{24}NaO_4$ ($M + Na^+$): 399.1572, found: 399.1567. (Yellow solid, 15.2 mg, 70% isolated yield)

2-isopropyl-5-methylcyclohexyl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (6): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (d, J = 7.6 Hz, 1H), 8.20-8.18 (d, J = 8.4 Hz, 1H), 8.15-8.13 (d, J = 8.0 Hz, 1H), 8.03-8.00 (m, 2H), 7.91-7.87 (m, 1H), 7.69-7.65 (t, J = 8.0 Hz, 1H), 4.99-4.93 (m, 1H), 2.18-2.15 (d, J = 12.0 Hz, 1H), 1.99-1.97 (m, 1H), 1.78-1.74 (m, 2H), 1.63-1.60 (m, 3H), 1.25 (s, 1H), 1.18-1.13 (m, 1H), 0.96-0,94 (dd, J_1 = 1.6 Hz, J_2 = 7.2 Hz, 6H), 0.82-0.80 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 160.8, 151.0, 135.2, 133.9, 132.7, 130.9, 130.0, 125.4, 122.9, 122.4, 121.8, 119.1, 75.8, 47.3, 41.0, 34.3, 31.6, 26.7, 23.7, 22.1, 20.9, 16.6; HRMS calculated for $C_{24}H_{26}NaO_4$ ($M + Na^+$): 401.1729, found: 401.1723. (Yellow solid, 17.3 mg, 78% isolated yield)



7

dimethyl 2-((6-oxo-6*H*-benzo[*c*]chromene-3-carbonyl)oxy)succinate (7): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.43 (d, *J* = 8.0 Hz, 1H), 8.20-8.14 (m, 2H), 8.03-8.00 (m, 2H), 7.92-7.88 (t, *J* = 8.0 Hz, 1H), 7.71-7.67 (t, *J* = 7.6 Hz, 1H), 5.77-5.74 (m, 1H), 3.82 (s, 3H), 3.77 (s, 3H), 3.10-3.07 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 169.2, 164.3, 160.6, 151.0, 135.2, 133.7, 130.9, 130.8, 130.3, 125.7, 123.1, 122.6, 121.9, 119.6, 69.2, 53.0, 52.5, 36.1; HRMS calculated for $C_{20}H_{16}NaO_8$ ($M + Na^+$): 407.0743, found: 407.0737. (Yellow solid, 20.1mg, 86% isolated yield)

methyl (6-oxo-6*H*-benzo[*c*]chromene-3-carbonyl)valinate (8): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.43 (d, *J* = 8.0 Hz, 1H), 8.18-8.13 (d, *J* = 8.8 Hz, 2H), 7.90-7.86 (d, *J* = 7.6 Hz, 1H), 7.80-7.78 (m, 2H), 7.70-7.64 (m, 1H), 6.80-6.78 (d, *J* = 8.4 Hz, 1H), 4.82-4.79 (m, 1H), 3.81 (s, 3H), 1.06-1.02 (t, *J* = 7.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 165.9, 160.7, 151.1, 135.9, 135.2, 133.8, 130.9, 130.0, 123.4, 123.3, 122.3, 121.7, 121.0, 116.7, 57.8, 52.5, 31.7, 19.1, 18.0; HRMS calculated for $C_{20}H_{19}NNaO_5$ ($M + Na^+$): 376.1161, found: 376.1155. (White solid, 19.1 mg, 83% isolated yield)

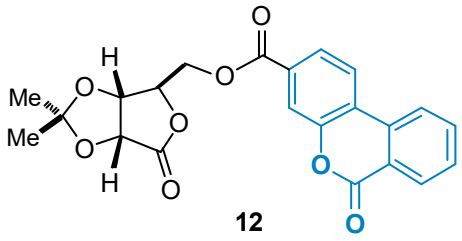
methyl (6-oxo-6*H*-benzo[*c*]chromene-3-carbonyl)-*L*-isoleucinate (9): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.45-8.42 (d, *J* = 8.4 Hz, 1H), 8.17-8.12 (m, 2H), 7.90-7.86 (m, 1H), 7.79-7.78 (m, 2H), 7.68-7.64 (m, 1H), 6.83-6.81 (d, *J* = 8.4 Hz, 1H), 4.86-4.82

(m, 1H), 3.81 (s, 3H), 2.10-2.01 (m, 1H), 1.60-1.53 (m, 1H), 1.32-1.23 (m, 1H), 1.02-1.00 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.6, 165.7, 160.8, 151.1, 136.0, 135.2, 133.8, 130.9, 130.0, 123.3, 123.2, 122.3, 121.6, 121.0, 116.6, 57.1, 52.5, 38.3, 25.5, 15.6, 11.7; HRMS calculated for $C_{21}H_{21}NNaO_5$ (M + Na^+): 390.1317, found: 390.1312. (Yellow solid, 17.4 mg, 77% isolated yield)

methyl (6-oxo-6*H*-benzo[*c*]chromene-3-carbonyl)-*L*-leucinate (10): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.43-8.41 (m, 1H), 8.16-8.10 (m, 2H), 7.90-7.86 (m, 1H), 7.78-7.76 (m, 2H), 7.68-7.64 (t, *J* = 7.6 Hz, 1H), 6.78-6.76 (d, *J* = 8.4 Hz, 1H), 4.91-4.86 (m, 1H), 3.81 (s, 3H), 1.82-1.71 (m, 2H), 1.03-1.00 (t, *J* = 5.6 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.7, 165.7, 160.7, 151.1, 135.8, 135.2, 133.8, 130.9, 129.9, 124.8, 123.3, 122.3, 121.6, 121.0, 116.7, 52.7, 51.5, 41.8, 25.1, 22.9, 22.1; HRMS calculated for $C_{21}H_{21}NNaO_5$ (M + Na^+): 390.1317, found: 390.1312. (Yellow oil, 16.0 mg, 72% isolated yield)

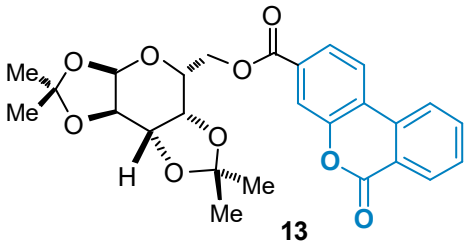
Methyl-3,3-dimethyl-2-(6-oxo-6*H*-benzo[*c*]chromene-3-carboxamido) butan-oate (11): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.42-8.40 (m, 1H), 8.15-8.11 (t, *J* = 9.2 Hz, 2H), 7.88-7.84 (m, 1H), 7.76-7.74 (m, 2H), 7.66-7.63 (m, 1H), 4.71-4.69 (d, *J* = 9.6 Hz, 1H), 3.77 (s, 3H), 3.71 (s, 1H), 1.07 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.1, 165.7, 160.7, 151.1, 136.1, 135.2, 133.8, 130.9, 130.0, 123.4, 123.2, 122.3, 121.6, 121.0, 116.6, 60.6, 52.2, 43.5, 35.3, 26.8; HRMS calculated for $C_{21}H_{21}NNaO_5$ (M +

Na^+): 390.1317, found: 390.1312. (Yellow solid, 16.6 mg, 73% isolated yield)



12

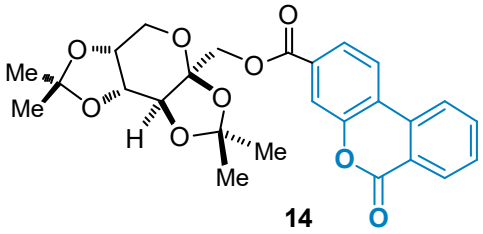
2,2-dimethyl-6-oxotetrahydrofuro[3,4-*d*][1,3]dioxol-4-yl)methyl-6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (12): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.44-8.41 (dd, J_1 = 1.2Hz, J_2 = 8.0 Hz, 1H), 8.18-8.14 (m, 2H), 7.92-7.88 (m, 2H), 7.86-7.84 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 7.71-7.67 (m, 1H), 4.95-4.93 (t, J = 2.8 Hz, 1H), 4.90-4.89 (d, J = 5.2 Hz, 1H), 4.87-4.85 (d, J = 5.6 Hz, 1H), 4.65-4.64 (d, J = 2.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 164.5, 160.4, 151.1, 135.3, 133.4, 130.9, 130.5, 125.1, 123.5, 122.8, 122.6, 121.9, 119.2, 114.2, 79.9, 77.8, 75.3, 64.4, 26.8, 25.7; HRMS calculated for $C_{22}H_{18}NaO_8$ (M + Na^+): 433.0899, found: 433.0894. (White solid, 17.6 mg, 82% isolated yield)



13

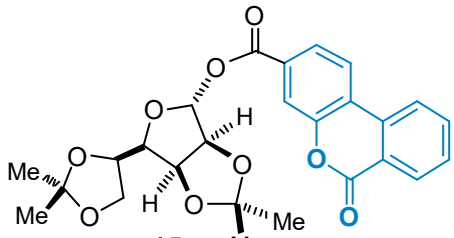
2,2,7,7-tetramethyltetrahydro-5*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-5-yl)methyl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (13): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (d, J = 7.6 Hz, 1H), 8.20-8.13 (q, J = 8.0 Hz, 2H), 8.03-8.01 (m, 2H), 7.91-7.87 (m, 1H), 7.69-7.66 (t, J = 7.2 Hz, 1H), 5.59-5.58 (d, J = 4.4 Hz, 1H), 4.69-4.67 (m, 1H), 4.56-4.52 (m, 2H), 4.38-4.34 (m, 2H), 4,23-4.20 (m, 1H), 1.55-1.50 (d, J = 22.0 Hz, 6H), 1.38-1.35 (d, J = 10.0 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.2, 160.8, 151.0, 135.2, 133.8, 131.9, 130.9, 130.1, 125.5, 123.0, 122.5, 122.1, 121.9, 119.3, 109.9, 109.0, 96.4, 71.2, 70.8, 70.6, 66.1, 64.5, 26.2, 26.1, 25.1,

24.6; HRMS calculated for $C_{26}H_{26}NaO_9$ ($M + Na^+$): 505.1475, found: 505.1469. (Yellow solid, 18.9 mg, 89% isolated yield)



14

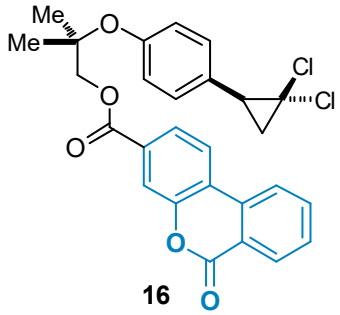
2,2,7,7-tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-3a-yl)methyl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (14): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (m, 1H), 8.20-8.15 (m, 2H), 8.08-8.04 (m, 2H), 7.92-7.87 (m, 1H), 7.70-7.66 (m, 1H), 4.75-4.72 (d, *J* = 12.0 Hz, 1H), 4.69-4.66 (m, 1H), 4.49-4.48 (d, *J* = 2.8 Hz, 1H), 4.39-4.36 (d, *J* = 11.6 Hz, 1H), 4.30-4.27 (m, 1H), 4.00-3.96 (m, 1H), 3.84-3.81 (d, *J* = 13.4 Hz, 1H), 1.57 (s, 3H), 1.49 (s, 3H), 1.40 (s, 3H), 1.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.8, 160.7, 151.0, 137.5, 135.2, 130.9, 130.3, 130.2, 125.6, 123.1, 122.5, 122.2, 121.9, 119.3, 109.3, 109.0, 101.6, 70.8, 70.7, 70.2, 65.9, 61.5, 26.6, 26.0, 25.7, 24.1; HRMS calculated for $C_{26}H_{26}NaO_9$ ($M + Na^+$): 505.1475, found: 505.1469. (Yellow oil, 19.0 mg, 80% isolated yield)



15

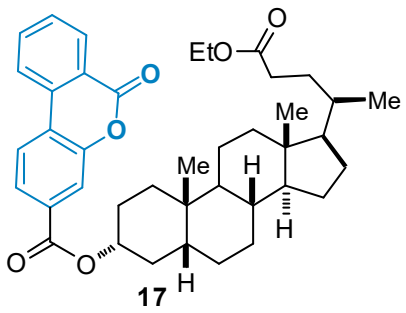
2,2-dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydro-furo[3,4-*d*][1,3]dioxol-4-yl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (15): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (d, *J* = 7.6 Hz, 1H), 8.21-8.15 (m, 2H), 8.00-7.98 (m, 2H), 7.92-7.89 (t, *J* = 7.6 Hz, 1H), 7.71-7.68 (t, *J* = 7.2 Hz, 1H), 6.41 (s, 1H), 5.00-4.98 (m, 1H), 4.92-4.91 (m, 1H), 4.47-4.46 (m, 1H), 4.18-4.06 (m, 3H), 1.55-1.48 (d, *J* = 24.8 Hz, 6H), 1.40 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.8, 160.6, 151.0, 137.6, 135.2, 133.6, 131.2,

130.9, 130.3, 125.6, 123.2, 122.6, 121.9, 119.4, 113.6, 109.5, 102.0, 85.3, 82.8, 79.4, 72.9, 66.9, 27.1, 26.1, 25.2, 24.8; HRMS calculated for $C_{26}H_{26}NaO_9$ ($M + Na^+$): 505.1475, found: 505.1469. (Yellow solid, 18.1 mg, 85% isolated yield)



16

2-(4-(2,2-dichlorocyclopropyl)phenoxy)-2-methylpropyl-6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (16): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47-8.45 (dd, J_1 = 1.6 Hz, J_2 = 8.0 Hz, 1H), 8.21-8.16 (m, 2H), 8.04-8.02 (m, 2H), 7.92-7.88 (m, 1H), 7.71-7.67 (m, 1H), 7.18-7.16 (m, 2H), 7.05-7.02 (m, 2H), 4.40 (s, 2H), 2.90-2.86 (m, 1H), 2.00-1.94 (m, 1H), 1.83-1.79 (m, 1H), 1.45 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 160.7, 154.1, 151.0, 135.2, 133.8, 131.8, 130.9, 130.4, 130.2, 129.7, 125.5, 124.1, 123.1, 122.5, 122.2, 121.9, 119.2, 78.9, 70.7, 60.9, 35.0, 26.0, 24.3; HRMS calculated for $C_{27}H_{22}C_{l2}NaO_5$ ($M + Na^+$): 519.0742, found: 519.0737. (Pale yellow solid, 11.0 mg, 51% isolated yield)

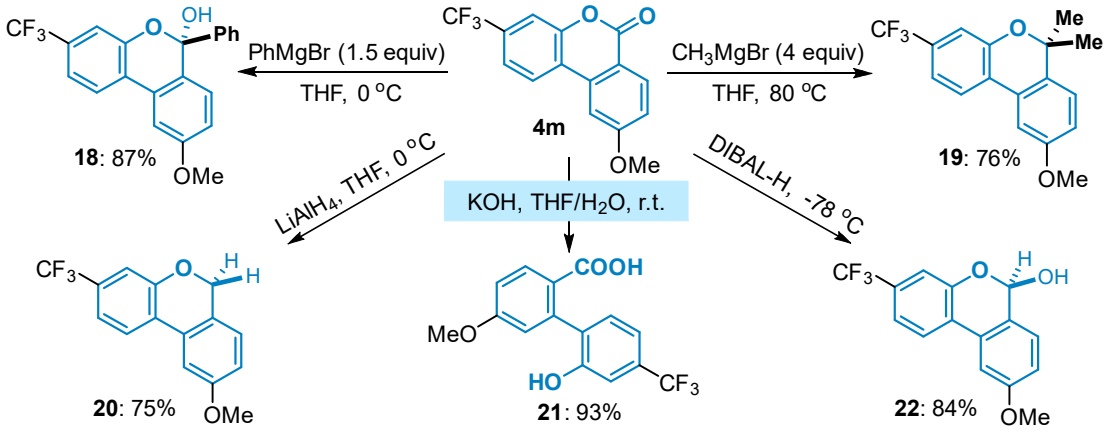


17

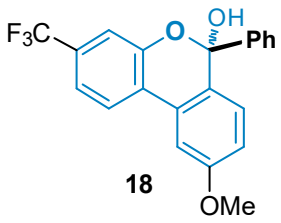
17-(5-ethoxy-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl 6-oxo-6*H*-benzo[*c*]chromene-3-carboxylate (17): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.46-8.44 (dd, J_1 = 1.2 Hz, J_2 = 8.0 Hz, 1H), 8.20-8.18 (d, J = 8.4 Hz, 1H), 8.14-8.12 (d, J = 8.4 Hz, 1H), 8.04-8.00 (m, 2H), 7.91-7.86 (m, 1H), 7.69-7.65

(m, 1H), 5.04-4.98 (m, 1H), 4.15-4.10 (q, *J* = 7.2 Hz, 2H), 2.37-2.31 (m, 1H), 2.25-2.17 (m, 1H), 2.06-1.97 (m, 2H), 1.92-1.78 (m, 3H), 1.61 (s, 3H), 1.49-1.38 (m, 4H), 1.28-1.22 (m, 11H), 1.18-1.07 (m, 6H), 0.98 (s, 3H), 0.94-0.92 (d, *J* = 6.4 Hz, 1H), 0.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.5, 174.5, 164.9, 160.8, 151.0, 135.1, 133.9, 132.8, 130.9, 130.0, 125.4, 122.9, 122.5, 121.9, 121.8, 119.2, 75.9, 60.3, 56.6, 56.1, 42.8, 42.1, 40.6, 40.2, 35.9, 35.4, 35.1, 34.7, 32.4, 31.4, 31.1, 28.3, 27.1, 26.8, 26.4, 24.3, 23.5, 21.0, 18.4, 14.4, 12.1; HRMS calculated for $C_{40}H_{50}NaO_6$ ($M + Na^+$): 649.3505, found: 649.3500. (Pale yellow solid, 12.4 mg, 58% isolated yield)

Synthetic applications



^{1}H, ^{13}C and ^{19}F spectra data of compounds 18-22



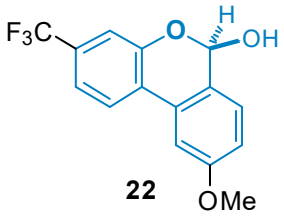
9-methoxy-6-phenyl-3-(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-ol (18): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.29 (m, 2H), 7.27-7.25 (m, 1H), 7.19-7.14 (m, 1H), 7.07 (s, 1H), 6.98-6.96 (m, 1H), 6.84-6.82 (d, *J* = 8.4 Hz, 1H), 6.79-6.72 (m, 2H), 6.61-6.60 (d, *J* = 2.4 Hz, 1H), 6.32-6.30 (d, *J* = 8.0 Hz, 1H), 3.76 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 153.2, 146.3, 145.6, 138.4, 137.2, 134.3, 131.4, 131.3, 130.7, 130.4, 128.3, 128.2, 127.9, 127.8, 127.2, 125.3, 122.6, 118.3, 116.4, 116.3, 113.5, 113.4, 112.7, 82.9, 55.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.53; HRMS calculated for $C_{21}H_{16}F_3O_3$ ($M + H^+$): 373.1052, found: 373.1046. (Pale yellow solid, 33.0 mg, 87% isolated yield)

9-methoxy-6,6-dimethyl-3-(trifluoromethyl)-6*H*-benzo[*c*]chromene (19): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51-7.49 (d, J = 8.4 Hz, 1H), 7.26-7.20 (m, 3H), 6.92-6.89 (dd, J_1 = 2.8 Hz, J_2 = 8.4 Hz, 1H), 6.58-6.57 (d, J = 2.4 Hz, 1H), 3.78 (s, 3H), 1.62 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.5, 153.4, 137.9, 135.8, 131.4, 131.1, 127.5, 125.3, 122.6, 118.0, 117.1, 117.0, 114.2, 113.9, 73.7, 55.4, 32.0, 31.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.45; HRMS calculated for $C_{17}H_{16}F_3O_2$ ($M + H^+$): 309.1102, found: 309.1097. (White solid, 41.0 mg, 76% isolated yield)

9-methoxy-3-(trifluoromethyl)-6*H*-benzo[*c*]chromene (20): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40-7.38 (d, J = 8.8 Hz, 1H), 7.25-7.17 (m, 3H), 6.95-6.92 (dd, J_1 = 2.4 Hz, J_2 = 8.4 Hz, 1H), 6.74-6.73 (d, J = 2.4 Hz, 1H), 4.36 (s, 2H), 3.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 153.6, 137.6, 131.9, 131.5, 131.4, 130.4, 129.1, 128.3, 125.4, 117.5, 116.0, 114.5, 113.8, 63.3, 55.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.57; HRMS calculated for $C_{15}H_{12}F_3O_2$ ($M + H^+$): 281.0789, found: 281.0784. (Brown solid, 38.0 mg, 75% isolated yield)

2'-hydroxy-5-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid (21):

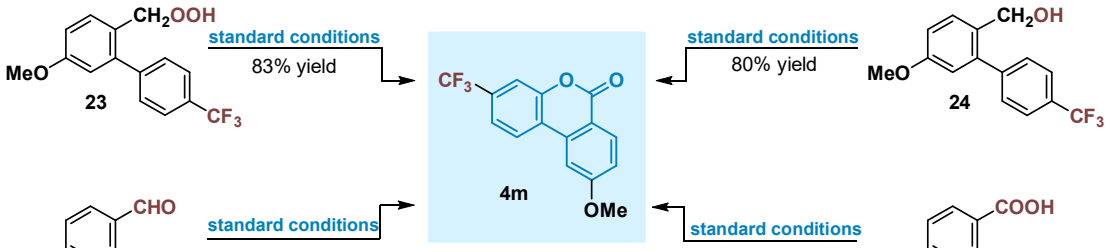
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.37-8.35 (d, J = 8.8 Hz, 1H), 8.12-8.10 (d, J = 8.4 Hz, 1H), 7.60-7.55 (m, 2H), 7.51 (s, 1H), 7.19-7.17 (d, J = 9.2 Hz, 1H), 4.02 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 160.2, 151.4, 135.6, 133.3, 123.7, 121.1, 120.9, 117.2, 115.4, 114.7, 106.0, 56.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.69; HRMS calculated for $C_{15}H_{12}F_3O_4$ ($M + H^+$): 313.0688, found: 313.0682. (White solid, 22.2 mg, 75% isolated yield)



22

(*R*)-9-methoxy-3-(trifluoromethyl)-6*H*-benzo[*c*]chromen-6-ol (22): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.42 (d, J = 8.8 Hz, 1H), 7.24 (s, 3H), 6.99-6.96 (dd, J_1 = 2.8 Hz, J_2 = 8.8 Hz, 1H), 6.75-6.74 (d, J = 2.8 Hz, 1H), 4.42-4.41 (d, J = 6.4 Hz, 1H), 3.82 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.9, 153.6, 137.3, 131.9, 131.5, 131.4, 130.4, 117.5, 116.0, 114.7, 114.2, 63.4, 55.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.57; HRMS calculated for $C_{15}H_{12}F_3O_3$ ($M + H^+$): 297.0739, found: 297.0734. (Yellow oil, 43.0 mg, 84% isolated yield)

Synthesis of benzocoumarins from peroxide, alcohol aldehyde, and carbonyl acid.



^{1}H, ^{13}C and ^{19}F spectra data of compounds 23-26

2-(hydroperoxymethyl)-5-methoxy-4'-(trifluoromethyl)-1,1'-biphenyl (23): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.70-7.68 (d, J = 8.0 Hz, 2H), 7.54-7.52 (d, J = 7.6 Hz, 2H), 7.49-7.46 (d, J = 8.8 Hz, 1H), 6.98-6.95 (dd, J_1 = 2.8 Hz, J_2 = 8.4 Hz, 1H), 6.84-6.83 (d, J = 2.8 Hz, 1H), 4.83 (s, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.8, 144.1, 143.5, 133.1, 129.9, 129.8, 129.6, 125.2, 125.1, 124.6, 122.9, 115.6, 113.7, 76.4, 55.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.99; HRMS calculated for $C_{15}H_{13}F_3O_3$ ($M + H^+$): 299.0895, found: 299.0890. (Yellow oil)

(5-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-yl)methanol (24): ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, J = 8.0 Hz, 2H), 7.55-7.53 (d, J = 8.0 Hz, 2H), 7.47-7.45 (d, J = 8.0 Hz, 1H), 6.98-6.95 (dd, J_1 = 2.8 Hz, J_2 = 8.8 Hz, 1H), 6.82-6.81 (d, J = 2.8 Hz, 1H), 4.50 (s, 2H), 3.84 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2,

144.4, 141.8, 130.9, 130.3, 129.6, 129.5, 125.3, 125.2, 115.5, 113.8, 62.7, 55.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.63; HRMS calculated for $C_{15}H_{14}F_3O_2$ ($M + H^+$): 283.0946, found: 283.0941. (Yellow oil)

5-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carbaldehyde (25): ^1H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.06-8.04 (d, *J* = 9.2 Hz, 1H), 7.75-7.73 (d, *J* = 8.4 Hz, 2H), 7.53-7.51 (d, *J* = 7.6 Hz, 2H), 7.07-7.04 (m, 1H), 6.86-6.85 (d, *J* = 2.0 Hz, 1H), 3.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 163.7, 146.8, 141.7, 130.7, 130.3, 127.3, 125.5, 125.4, 115.5, 114.4, 55.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.06; HRMS calculated for $C_{15}H_{12}F_3O_2$ ($M + H^+$): 281.0789, found: 281.0784. (Yellow solid)

5-methoxy-4'-(trifluoromethyl)-[1,1'-biphenyl]-2-carboxylic acid (26): ^1H NMR (400 MHz, $CDCl_3$) δ 8.07-8.05 (d, *J* = 8.8 Hz, 1H), 7.64-7.62 (d, *J* = 7.6 Hz, 2H), 7.42-7.40 (d, *J* = 8.4 Hz, 2H), 6.97-6.95 (dd, J_1 = 2.4 Hz, J_2 = 8.8 Hz, 1H), 6.78-6.77 (d, *J* = 2.8 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 162.7, 145.3, 134.0, 128.8, 128.7, 124.9, 120.5, 117.0, 113.2, 55.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.85; HRMS calculated for $C_{15}H_{12}F_3O_3$ ($M + H^+$): 297.0739, found: 297.0733. (Yellow solid)

UV-Vis absorption experiments

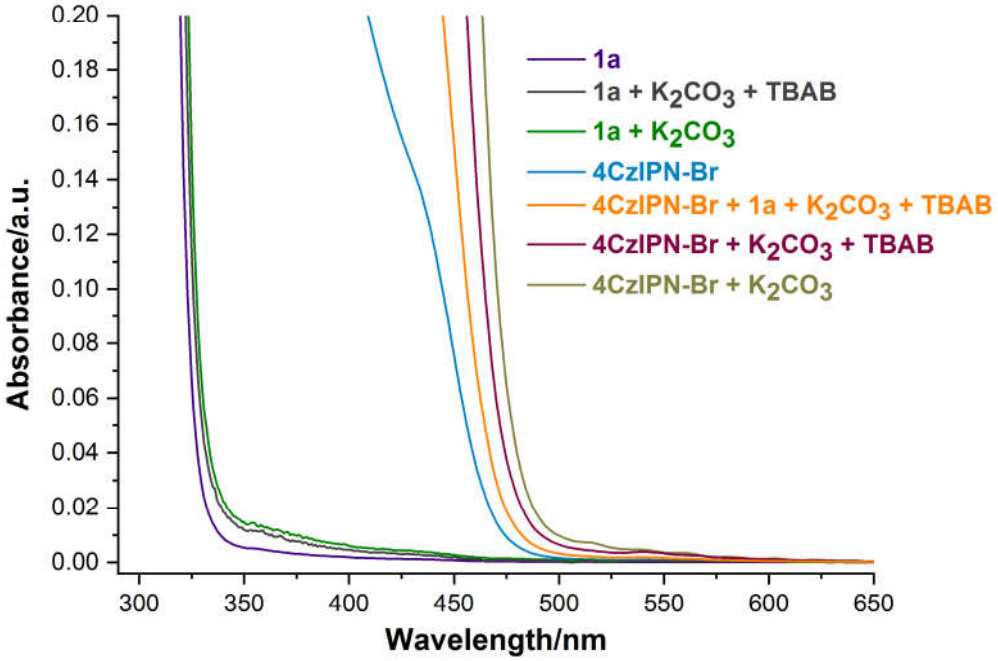


Figure 1. UV−Vis absorption spectra of the individual reaction components and the reaction mixtures

Fluorescence quenching experiments

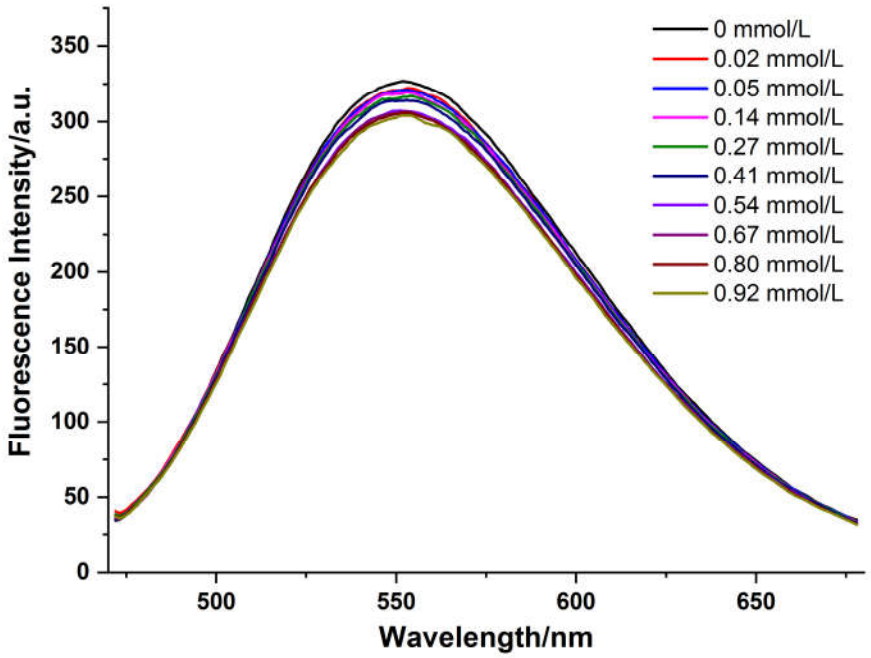


Figure 2. Fluorescence spectra of 4-BrCZIPN with different concentrations of substrate **1a**

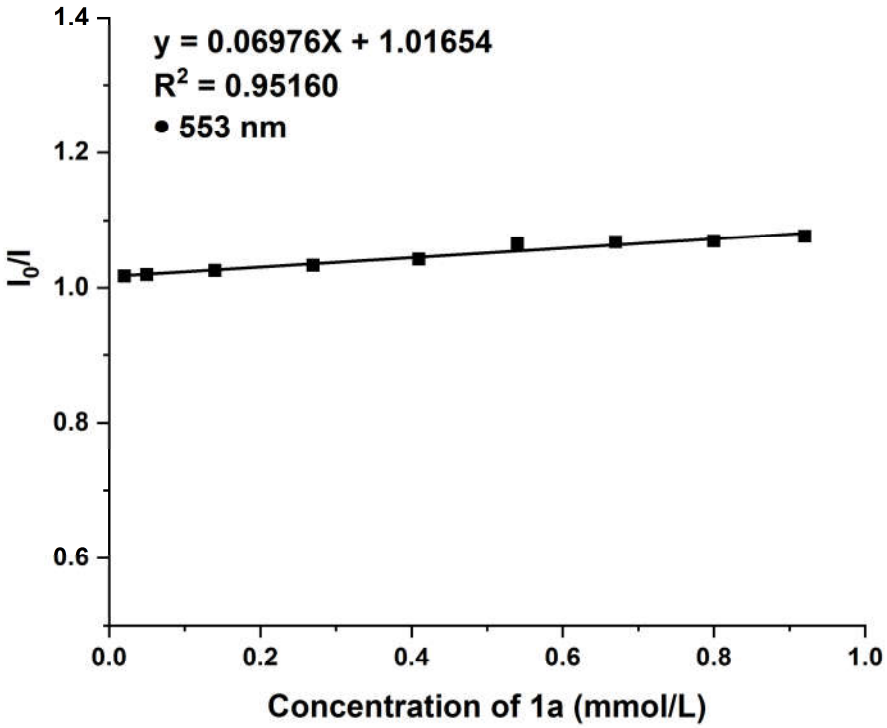


Figure 3. Stern Volmer plots of the substrate **1a**

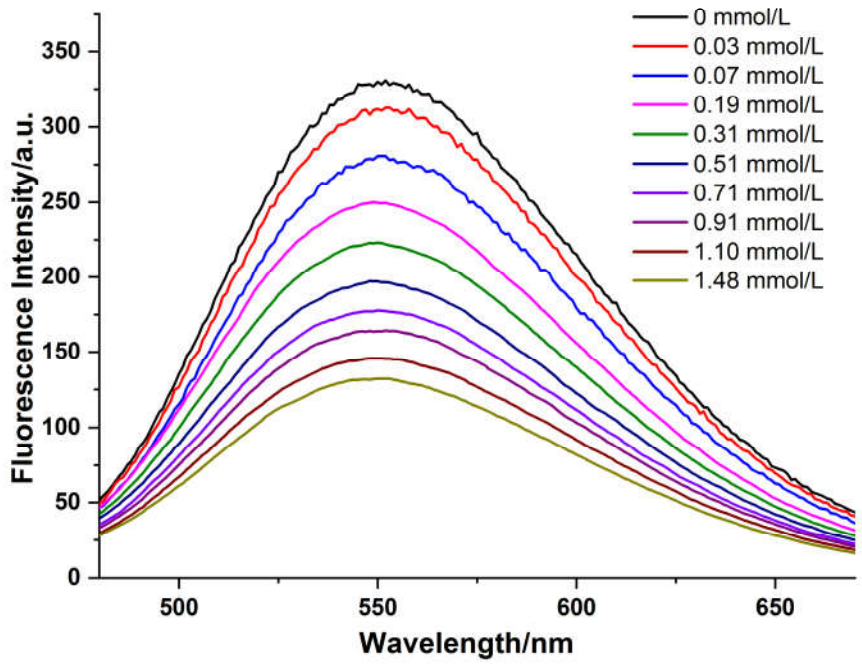


Figure 4. Fluorescence spectra of 4-BrCZIPN with different concentrations of substrate **TBAB**

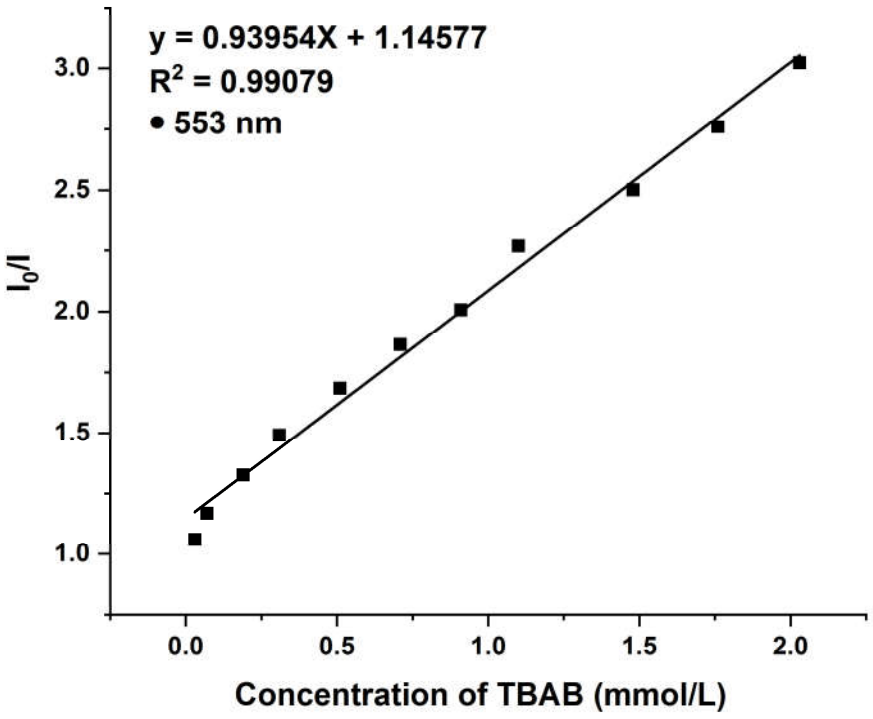


Figure 5. Stern Volmer plots of the TBAB

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 -1.7 to +2.4 V). nBu$_4$NPF$_6$ (0.1 M MeCN) was used as the supporting electrolyte.

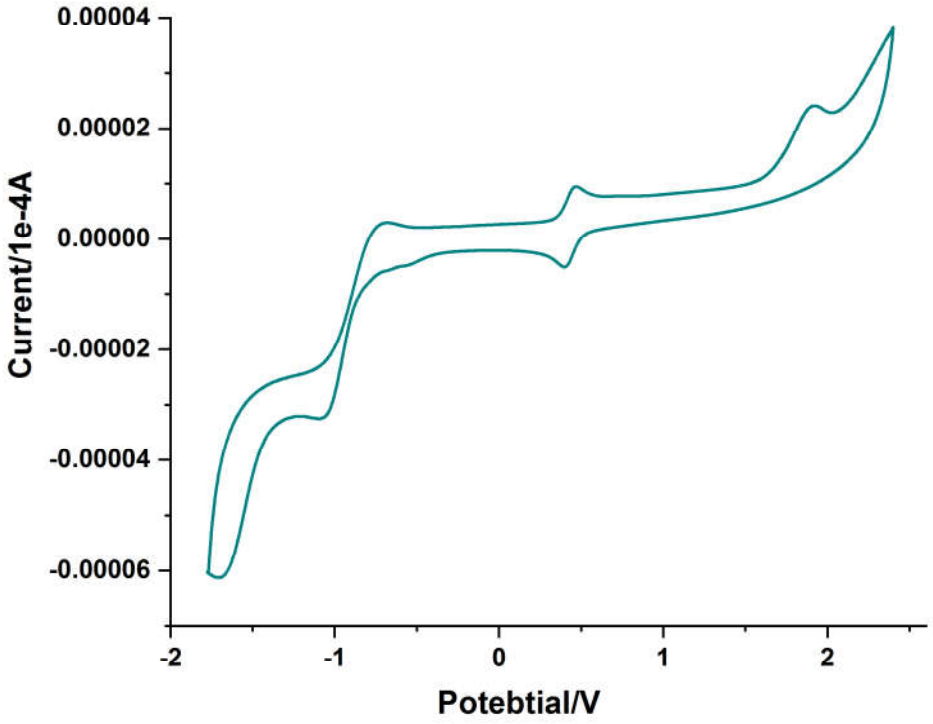


Figure 6. Cyclic voltammetry of the substrate **1a**

In-situ NMR spectroscopic experiments

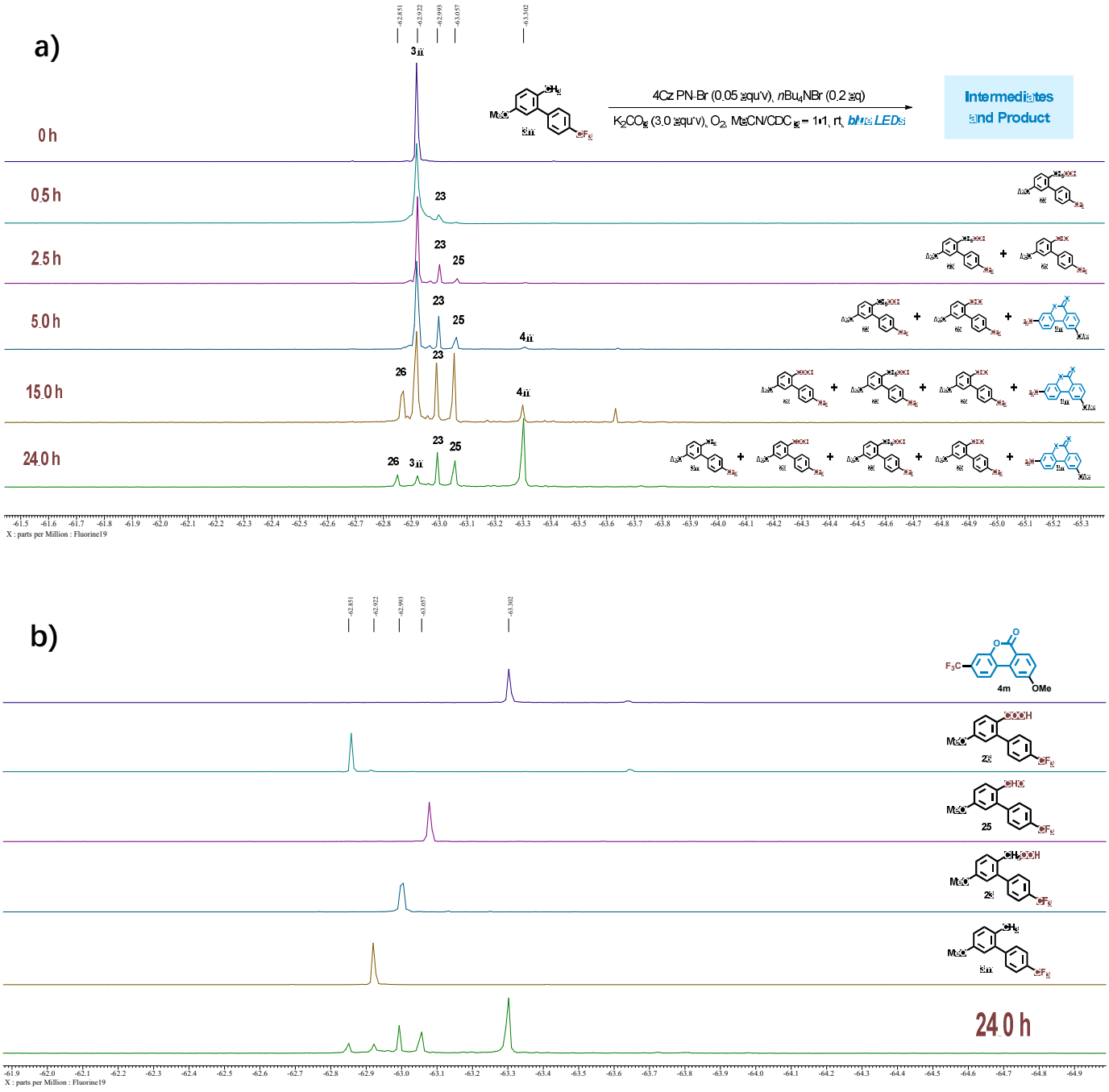
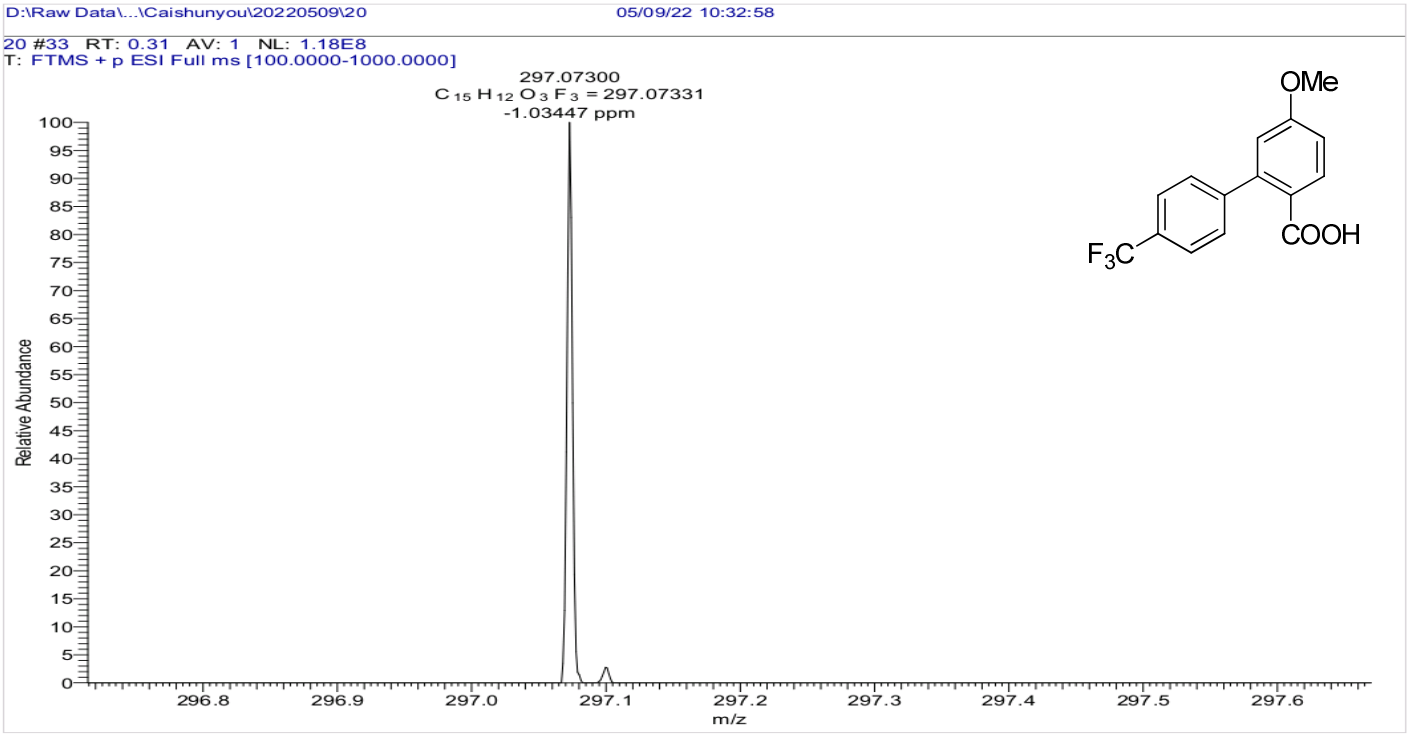
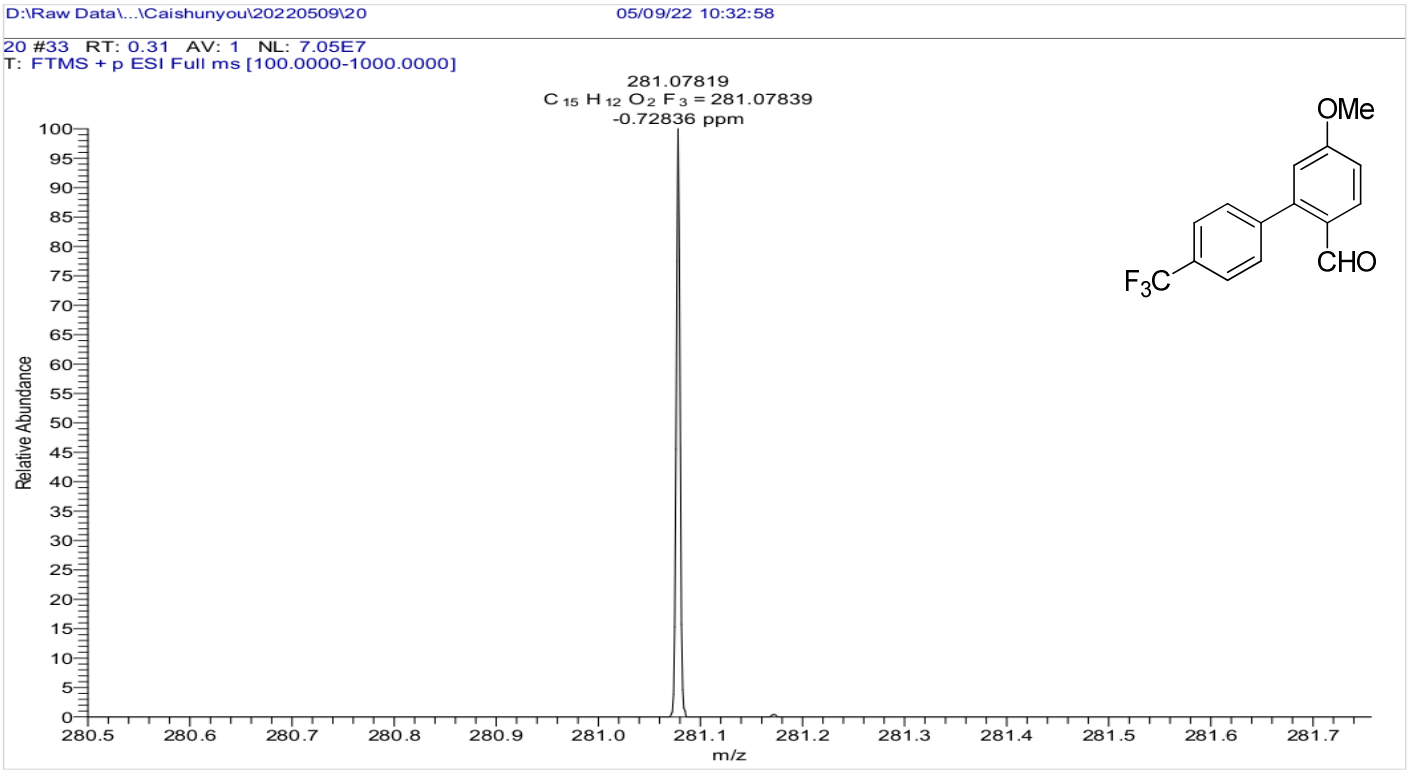
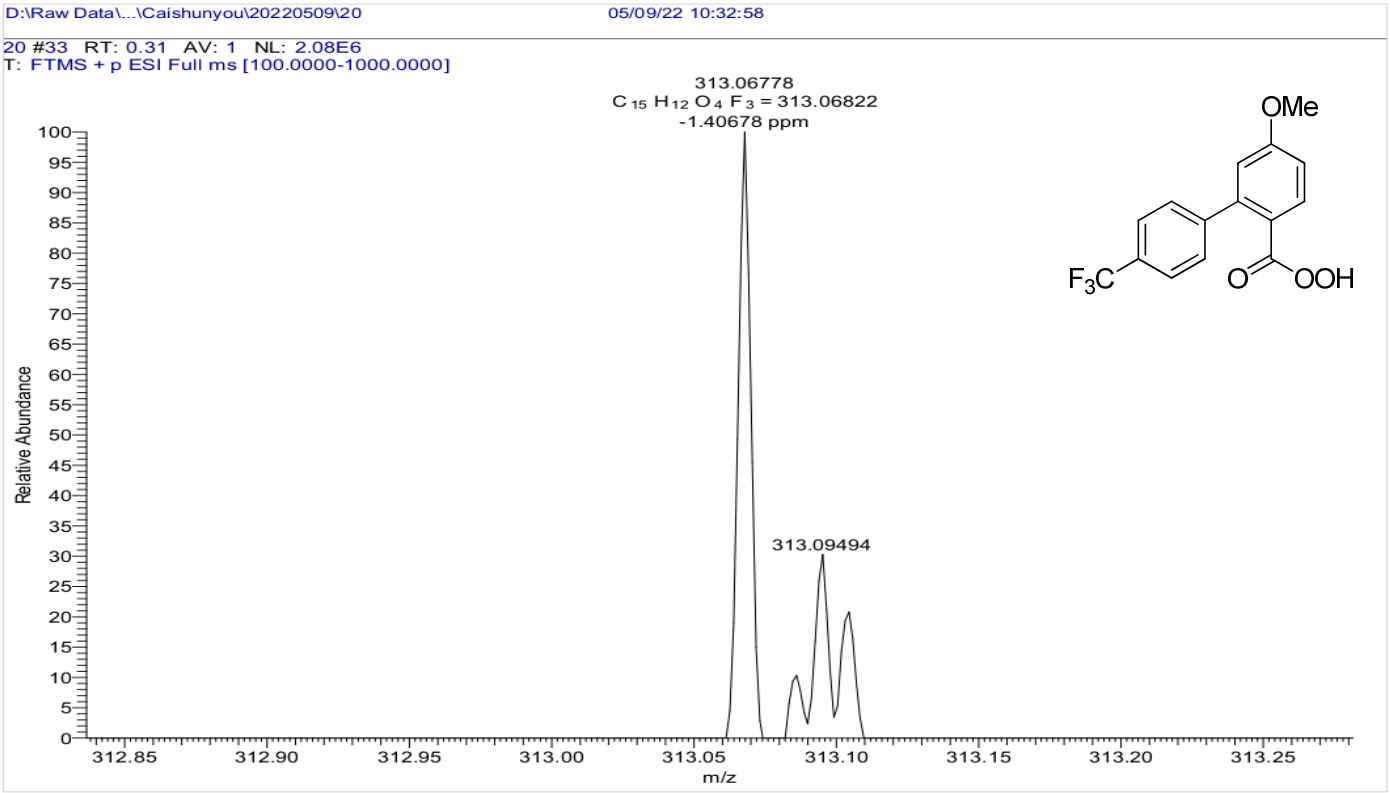


Figure 6. Reaction progress of **3m** monitored by in-situ ^{19}F-NMR

High-resolution mass spectrum analysis of the reaction mixture (3m)



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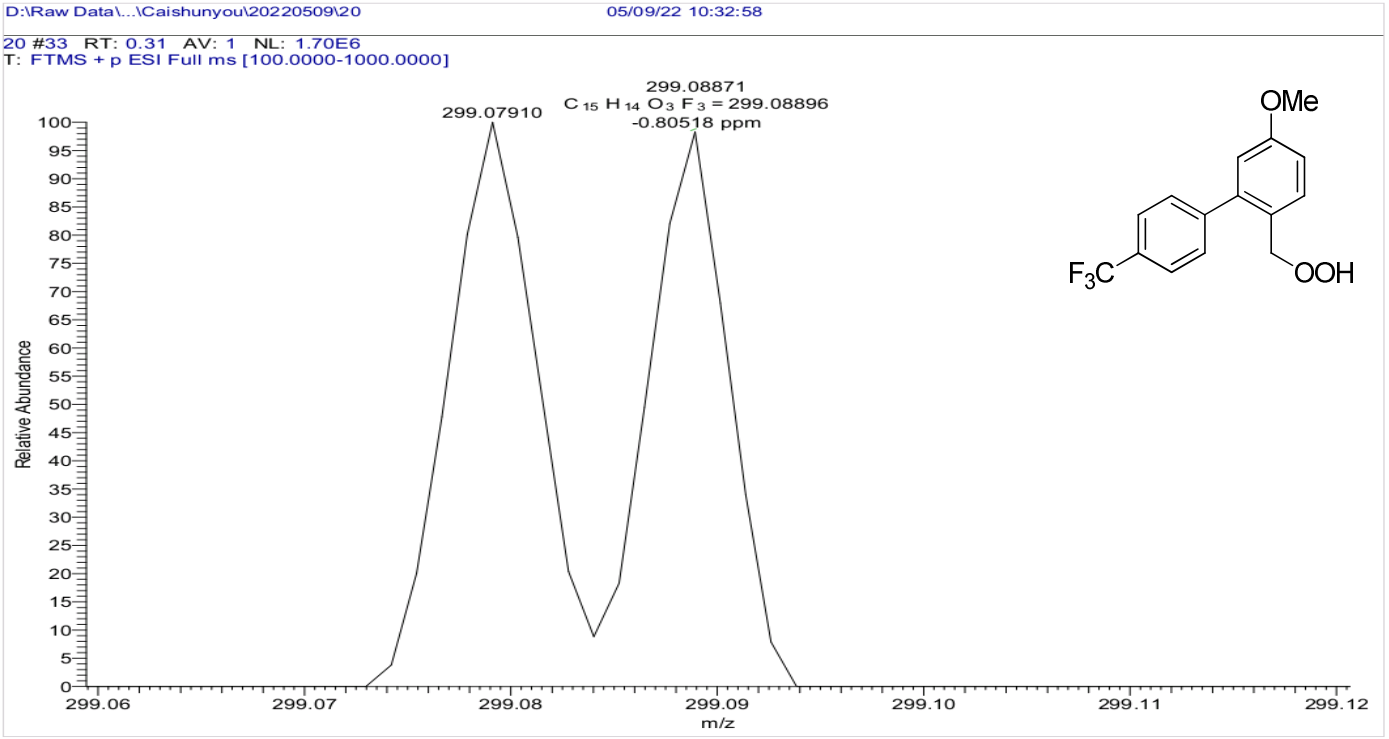
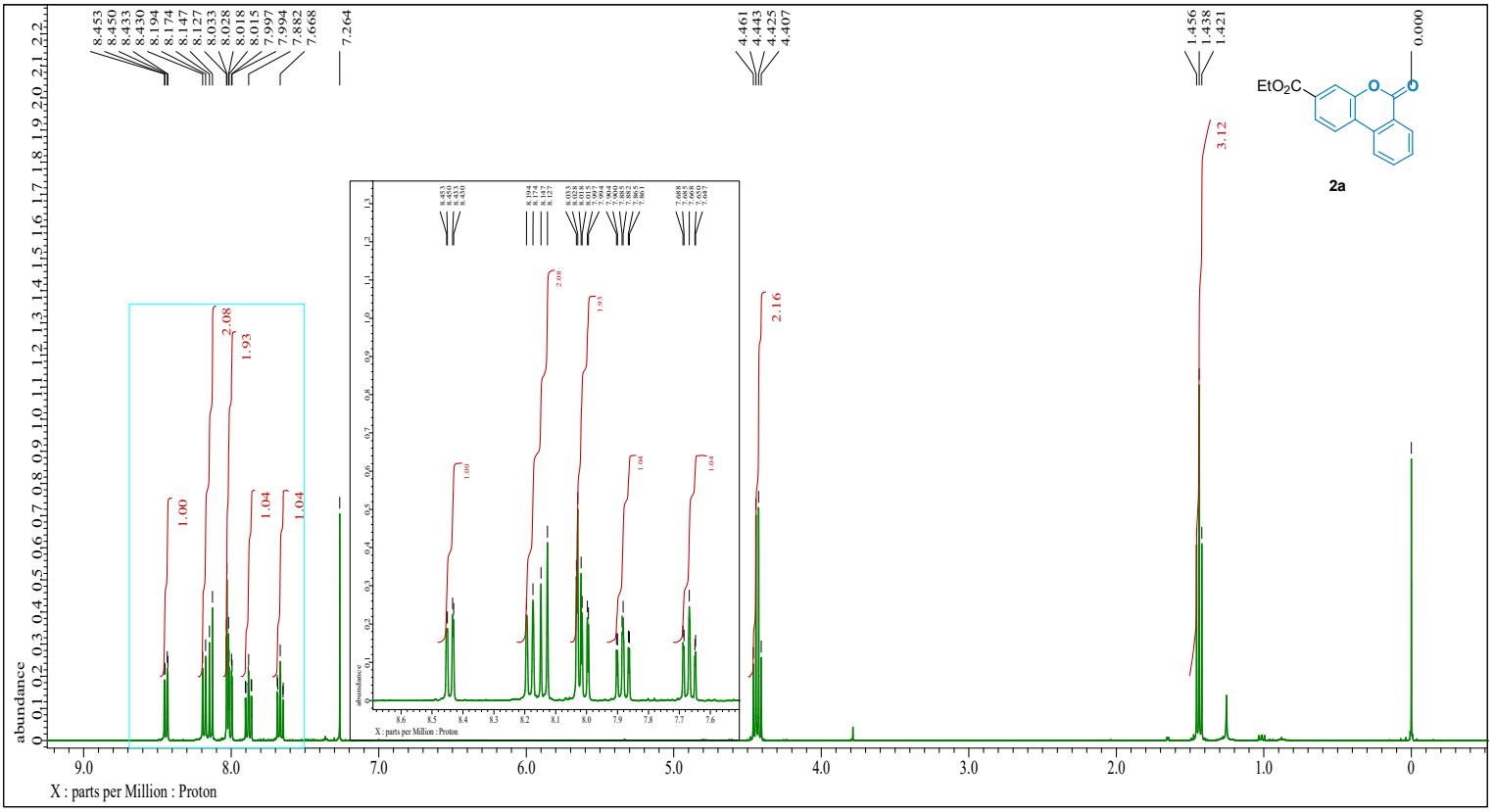
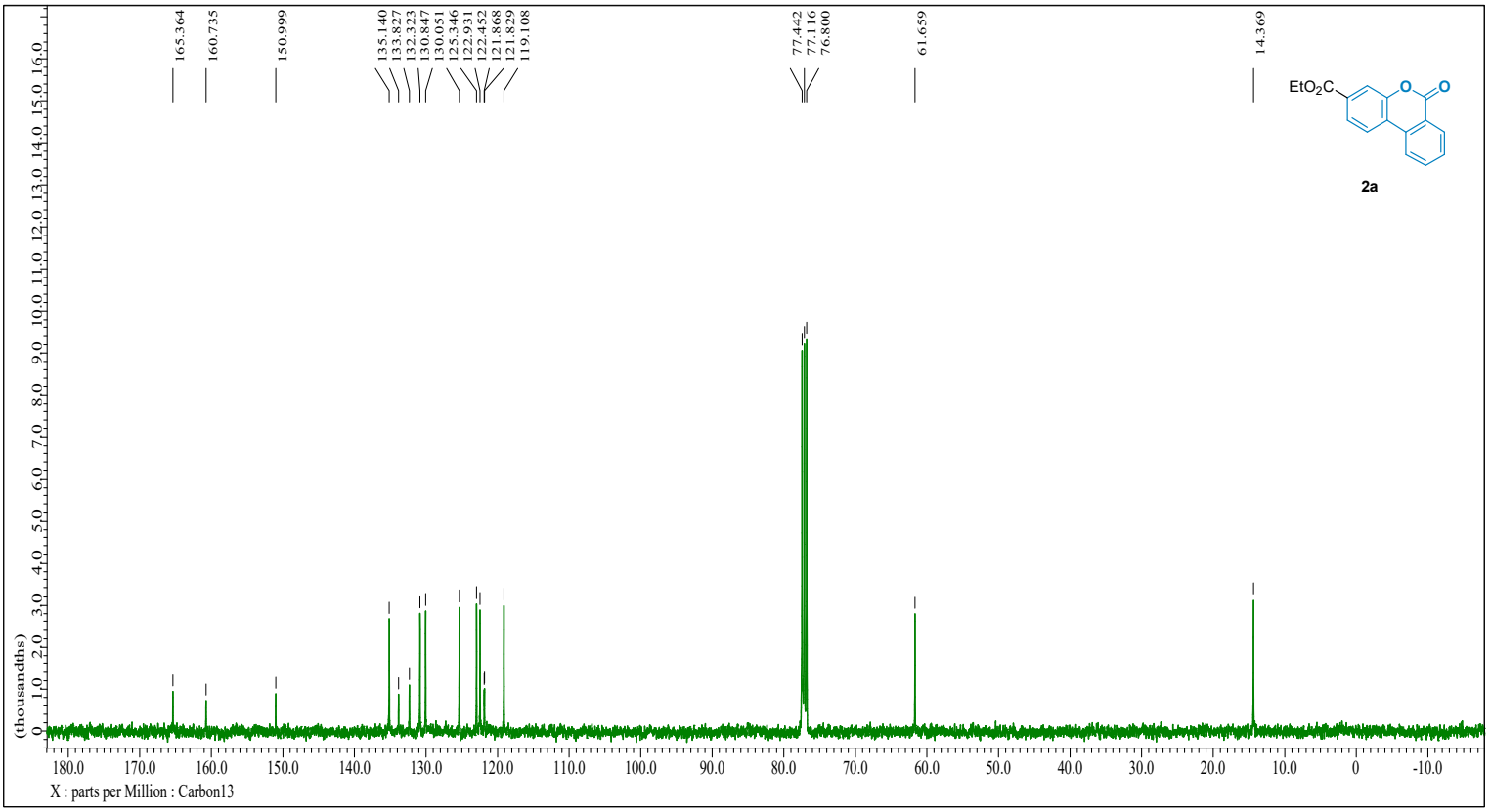
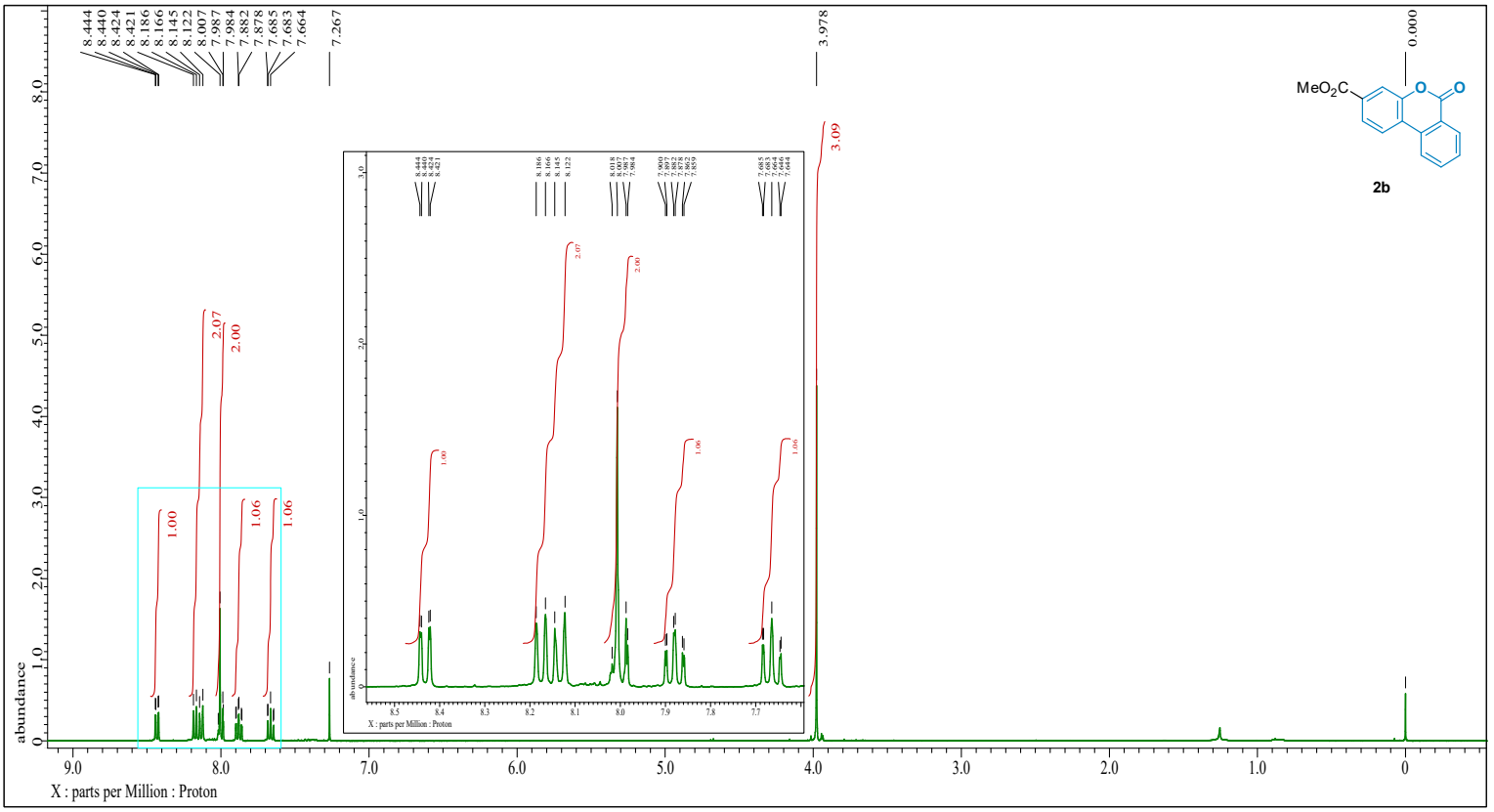
05/09/22 10:32:58
20 #33 RT: 0.31 AV: 1 NL: 2.08E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]
313.06778
C 15 H 12 O 4 F 3 = 313.06822
-1.40678 ppm
313.09494
Relative Abundance
m/z
OMe
F3C
O
OOH


D:\Raw Data\...\Caishunyou\20220509\20
05/09/22 10:32:58
20 #33 RT: 0.31 AV: 1 NL: 1.70E6
T: FTMS + p ESI Full ms [100.0000-1000.0000]
299.07910
299.08871
C 15 H 14 O 3 F 3 = 299.08896
-0.80518 ppm
Relative Abundance
m/z
OMe
F3C
OOH

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



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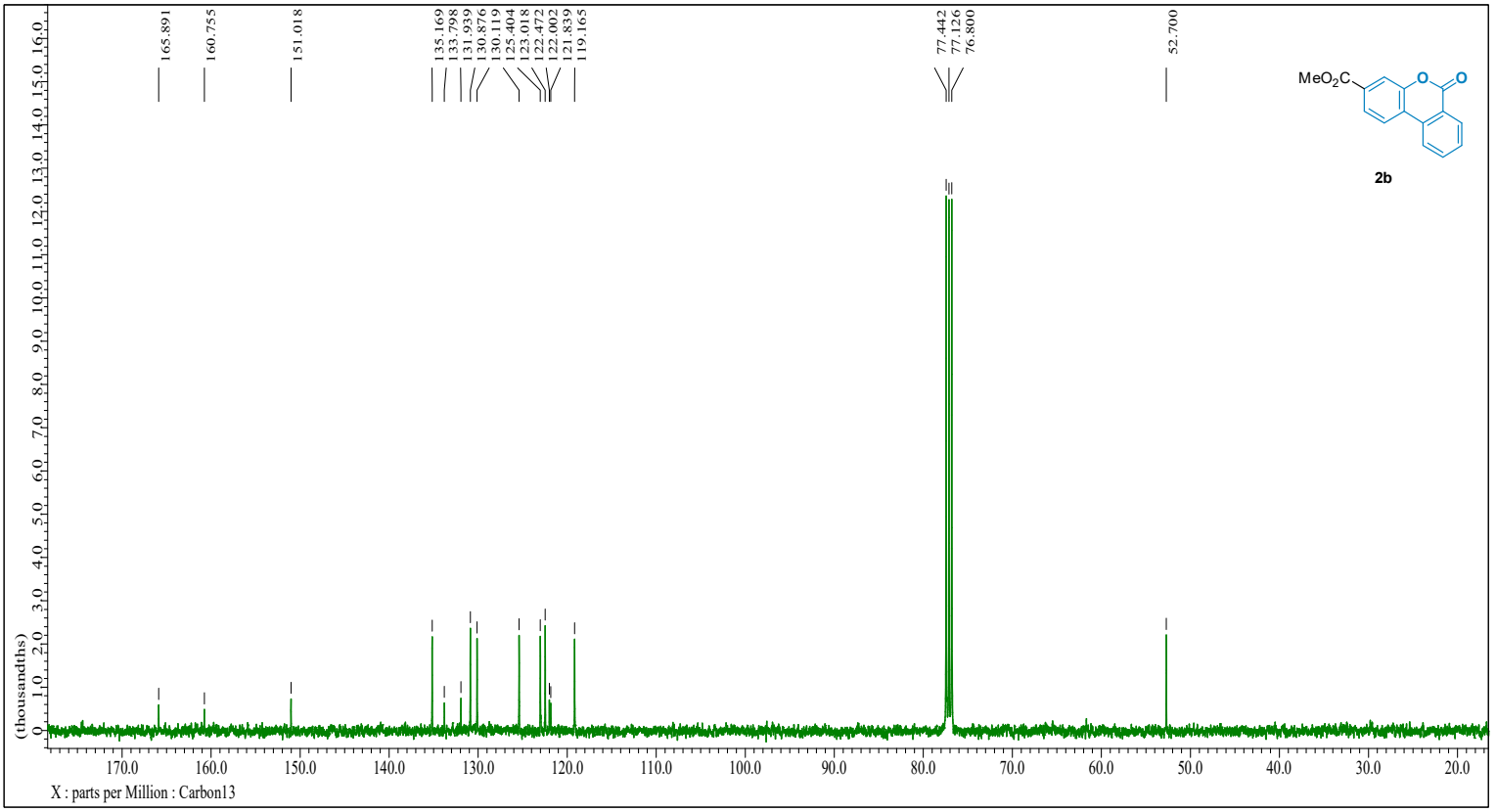
8.424
8.421
8.186
8.166
8.145
8.122
8.007
7.987
7.984
7.882
7.878
7.685
7.683
7.664
7.267
3.978
0.000
3.09
2.07
2.00
1.00
1.06
1.06
MeO2C
O
O
2b
abundance
X : parts per Million : Proton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160.755
151.018
135.169
133.798
131.939
130.876
130.119
125.404
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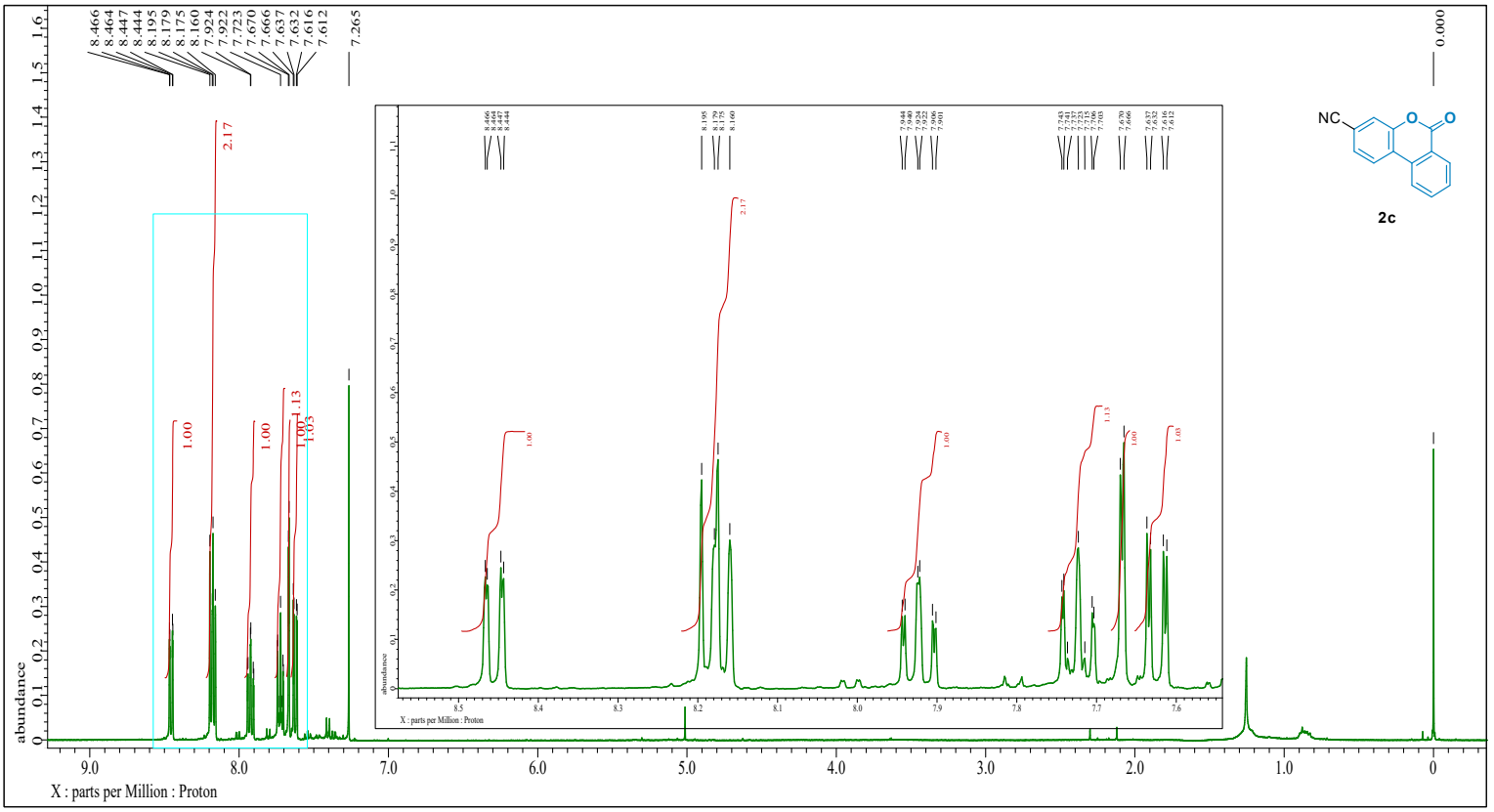
122.472
122.002
121.839
119.165
77.442
77.126
76.800
52.700
MeO2C
O
O
2b
(thousandths)
X : parts per Million : Carbon13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8.160
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7.922
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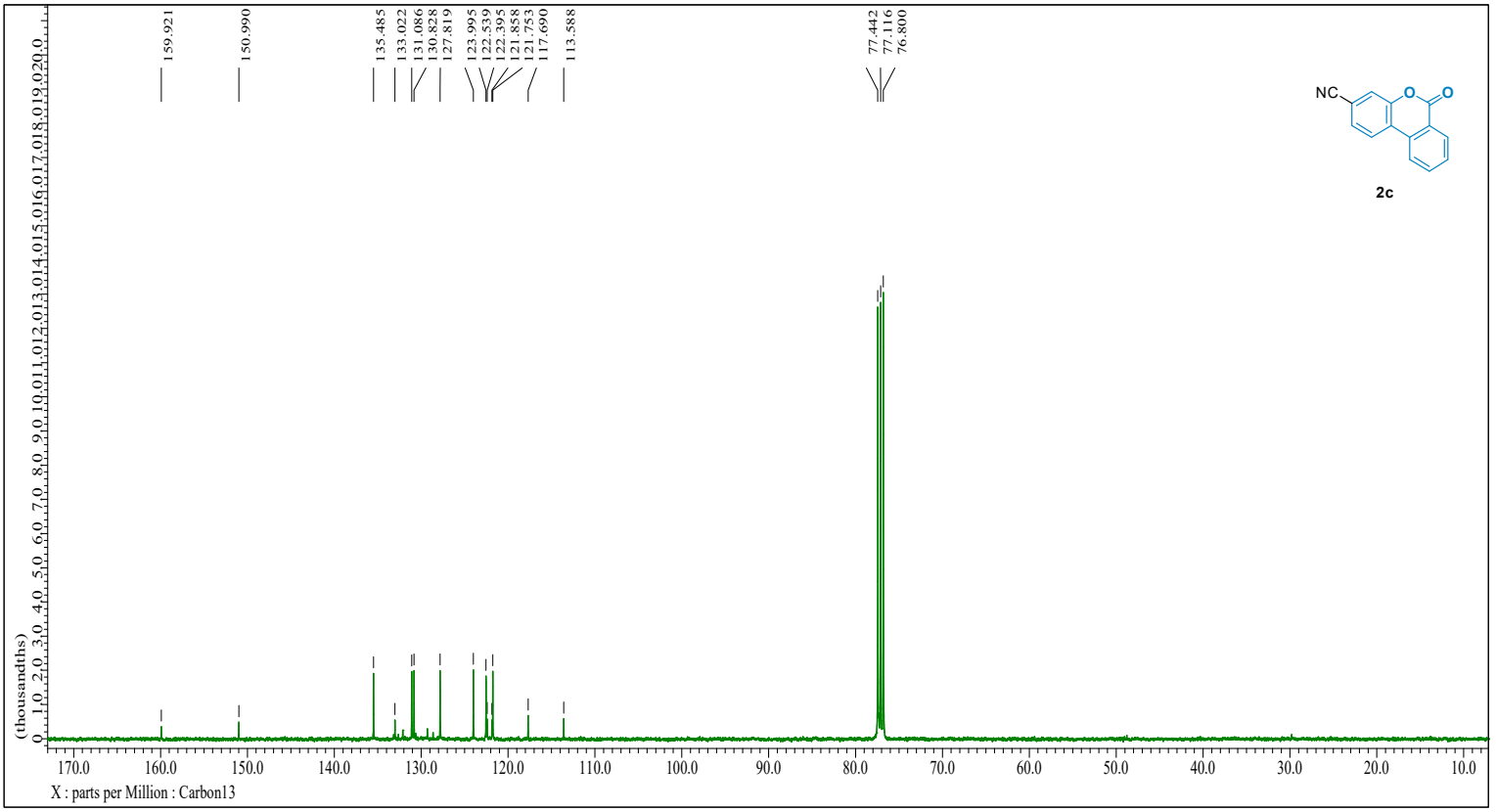
7.670
7.666
7.637
7.632
7.616
7.612
7.265
0.000
2.17
1.00
1.00
1.13
1.03
NC
O
O
2c
abundance
X : parts per Million : Proton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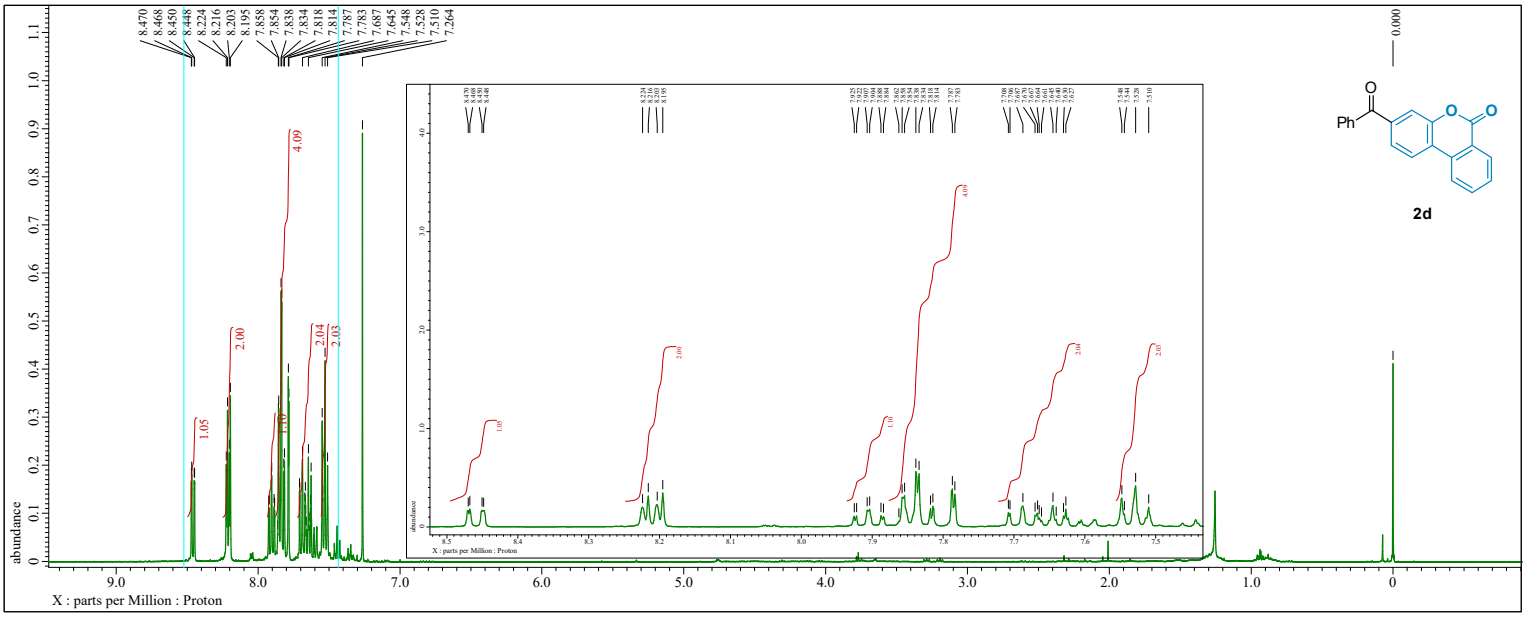
135.485
133.022
131.086
130.828
127.819
123.995
122.539
122.395
121.858
121.753
117.690
113.588
77.442
77.116
76.800
NC
O
O
2c
(thousandths)
X : parts per Million : Carbon13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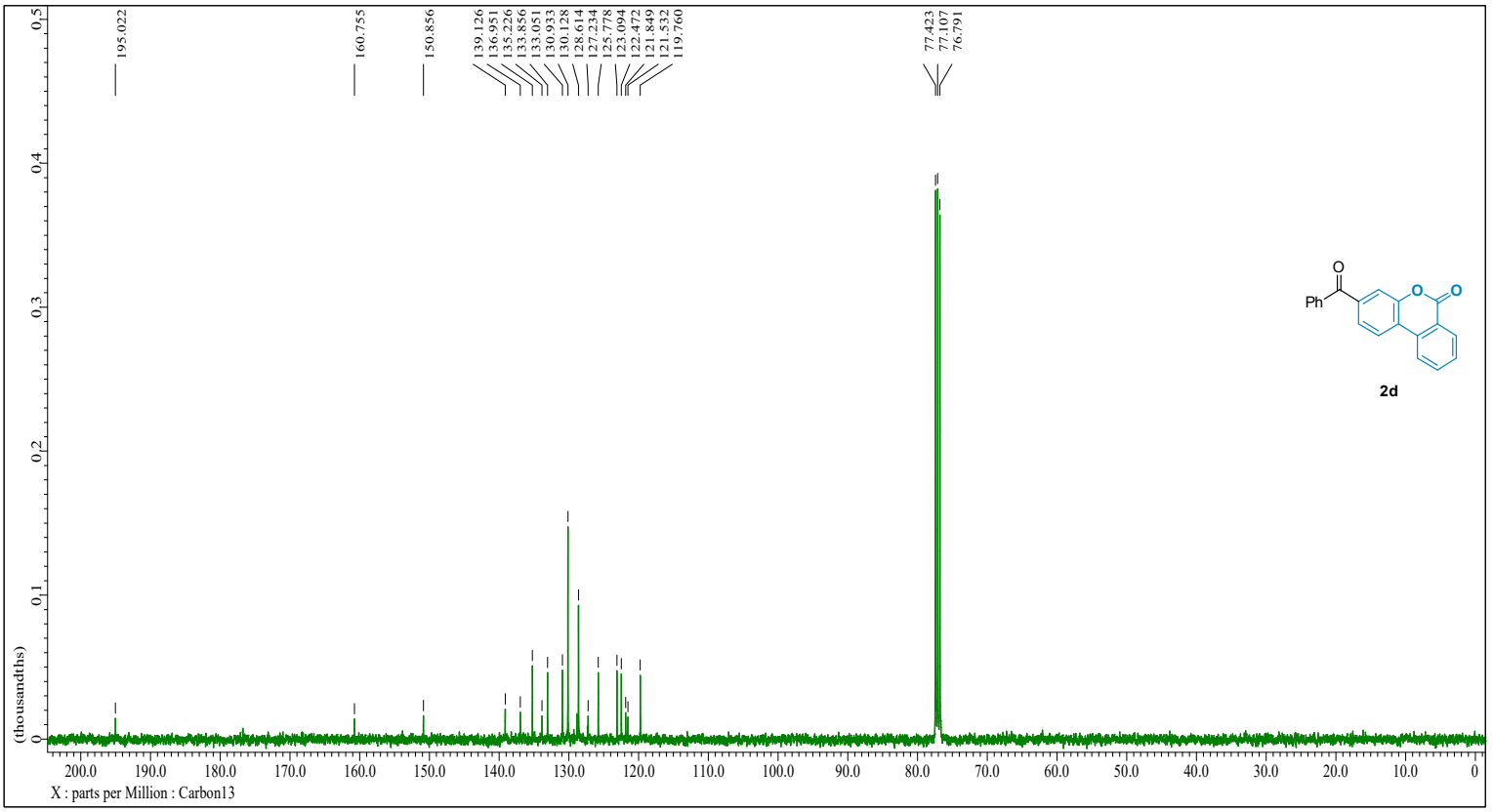
7.818
7.814
7.787
7.783
7.687
7.645
7.548
7.528
7.510
7.264
0.000
1.05
2.00
1.10
4.09
2.04
2.03
abundance
X : parts per Million : Proton
Ph
O
O
O
2d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130.128
128.614
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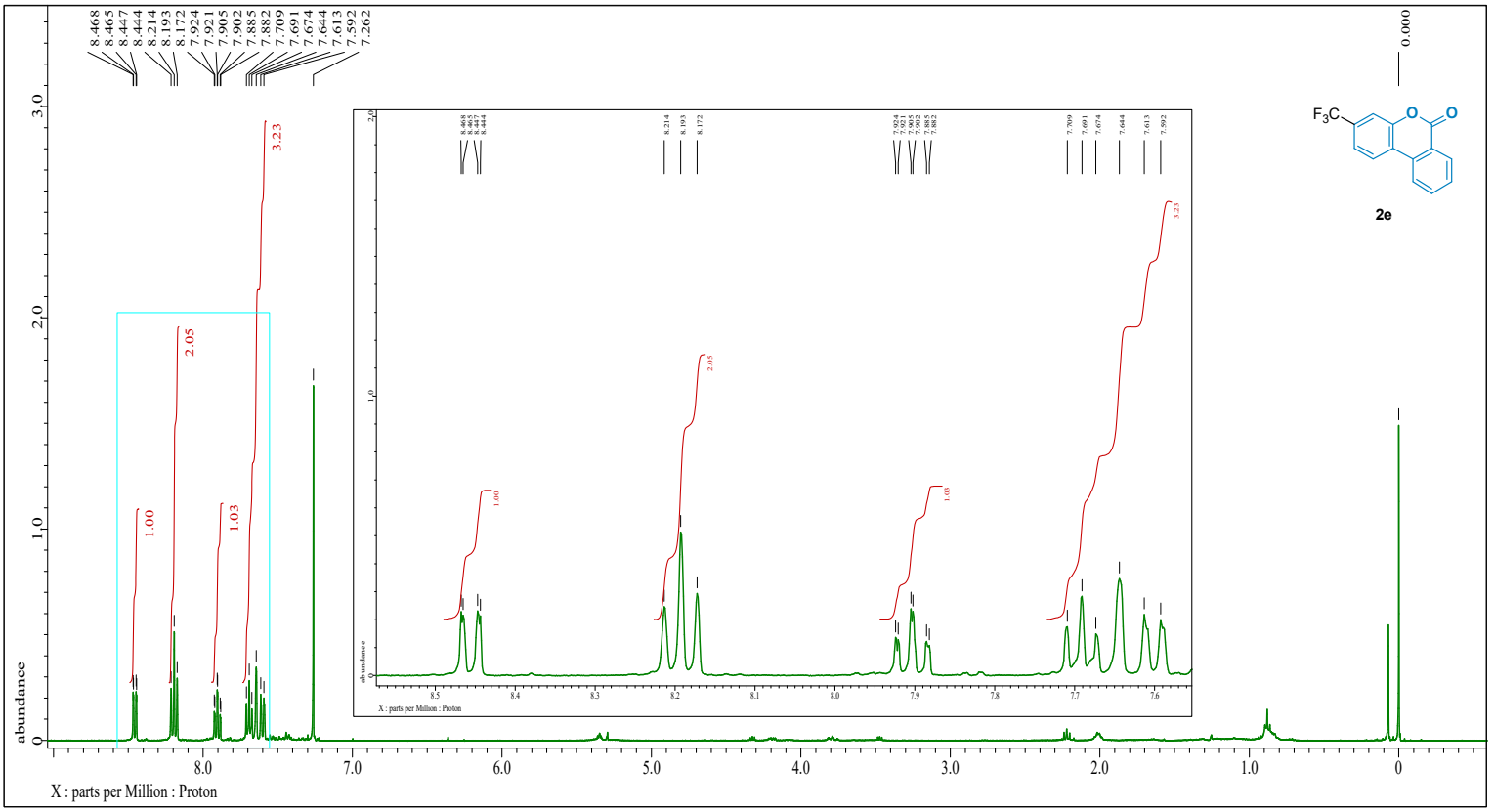
123.094
122.472
121.849
121.532
119.760
77.423
77.107
76.791
(thousandths)
X : parts per Million : Carbon13
Ph
O
O
O
2d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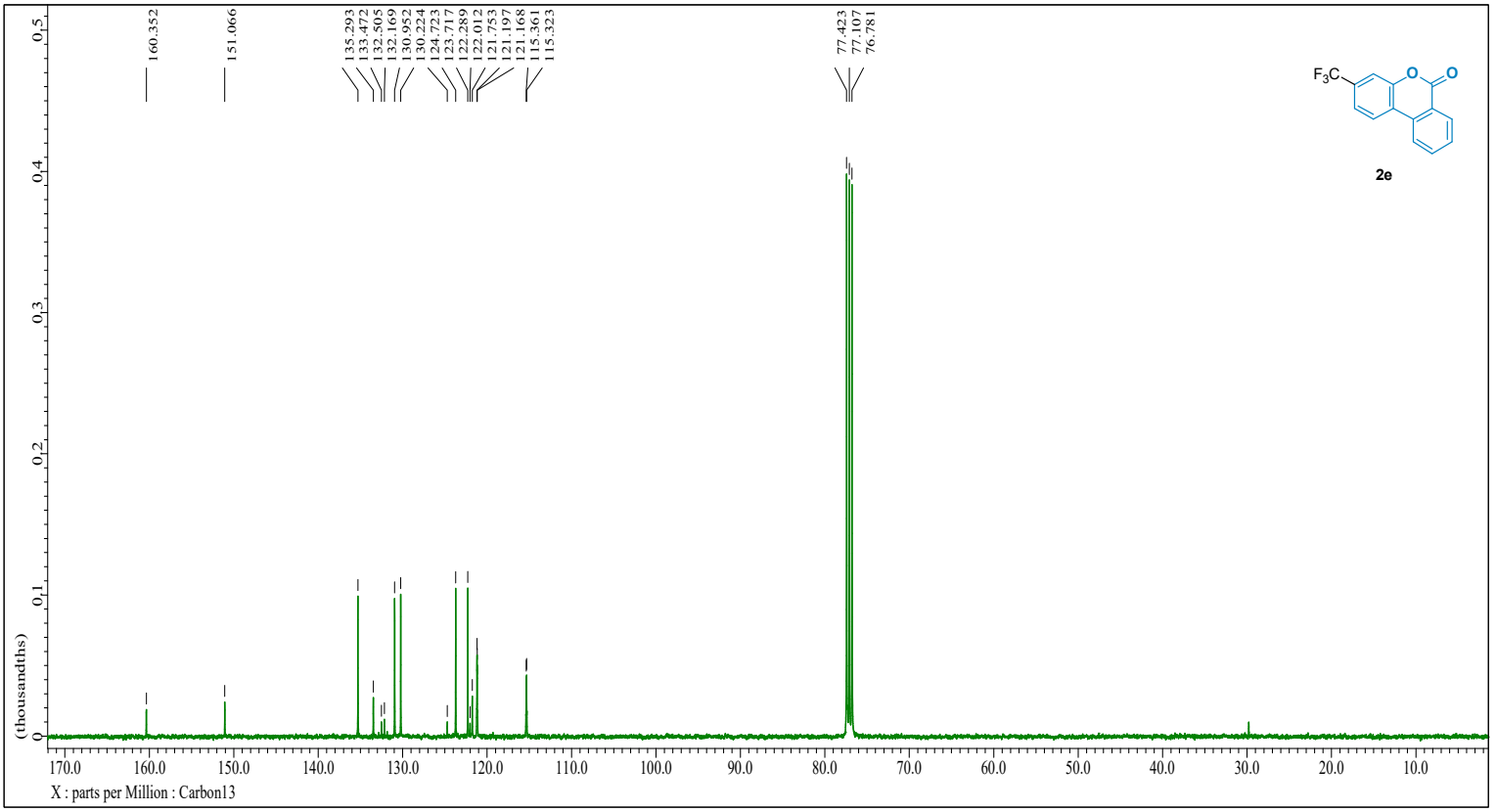
7.882
7.709
7.691
7.674
7.644
7.613
7.592
7.262
0.000
1.00
2.05
1.03
3.23
abundance
X : parts per Million : Proton
2e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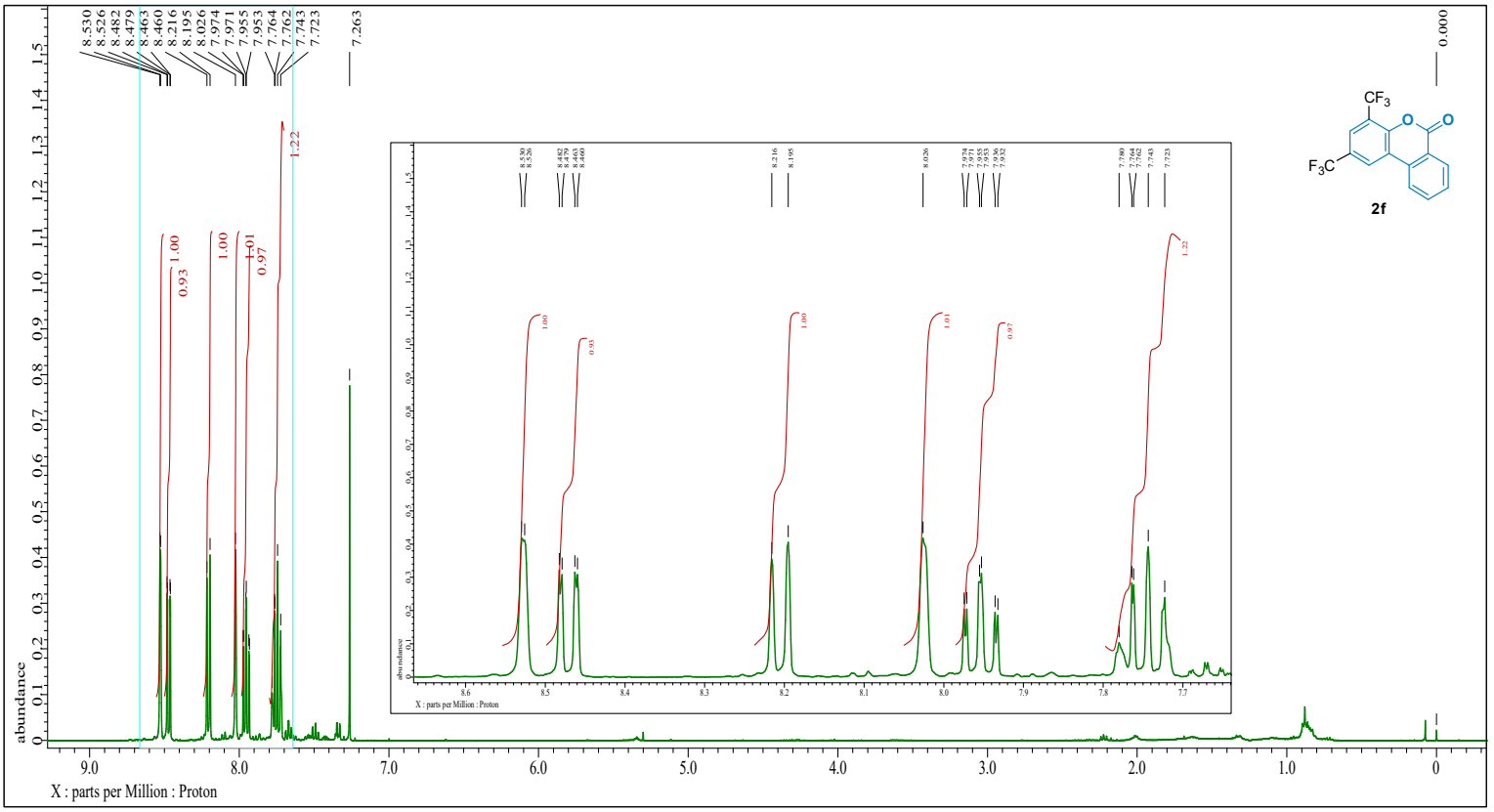
135.293
133.472
132.505
132.169
130.952
130.224
124.723
123.717
122.289
122.012
121.753
121.197
121.168
115.361
115.323
77.423
77.107
76.781
(thousandths)
X : parts per Million : Carbon13
2e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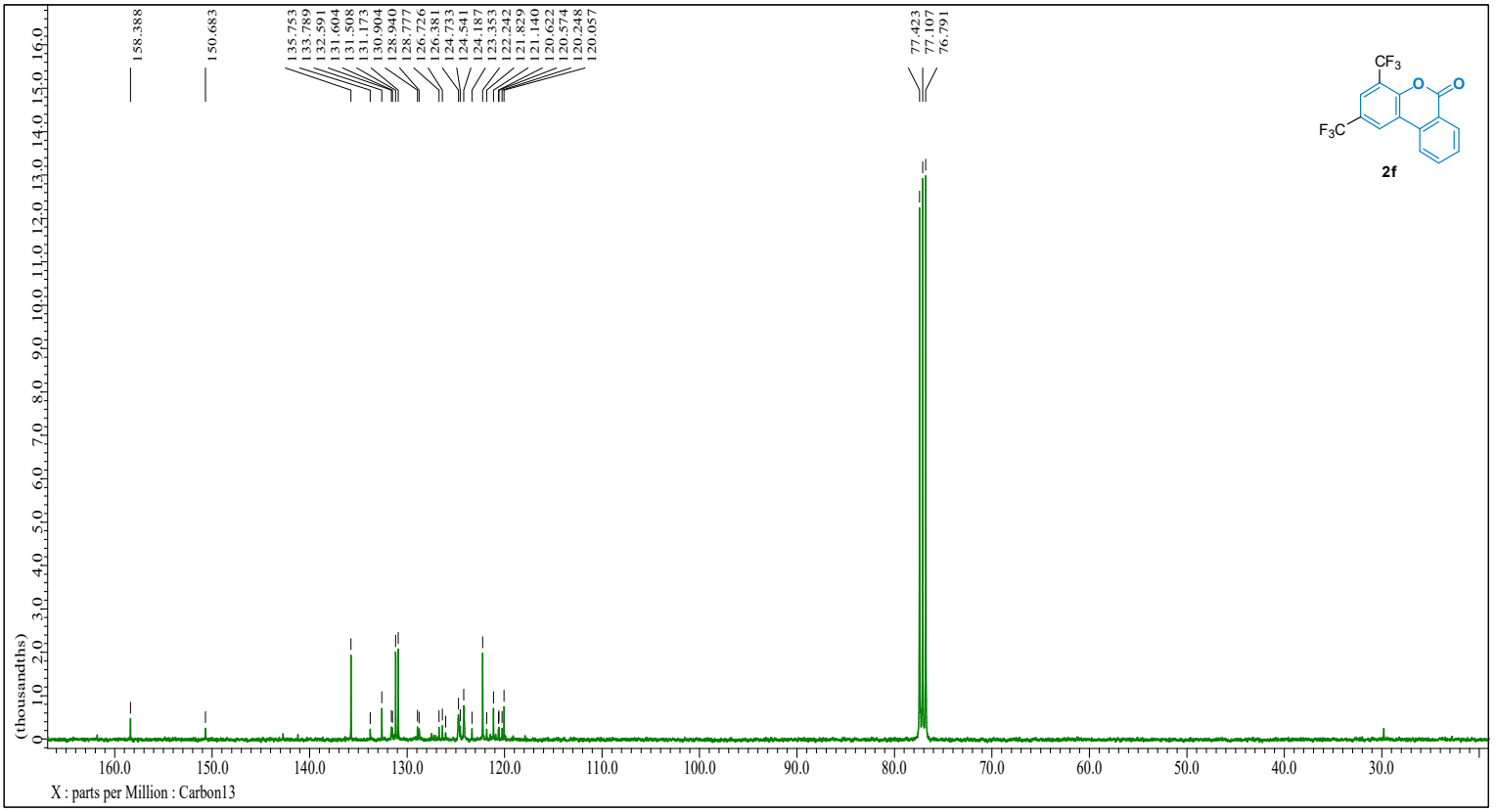
8.460
8.216
8.195
8.026
7.974
7.971
7.955
7.953
7.764
7.762
7.743
7.723
7.263
0.000
1.00
0.93
1.00
1.01
0.97
1.22
abundance
X : parts per Million : Proton
CF3
F3C
O
O
2f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150.683
135.753
133.789
132.591
131.604
131.508
131.173
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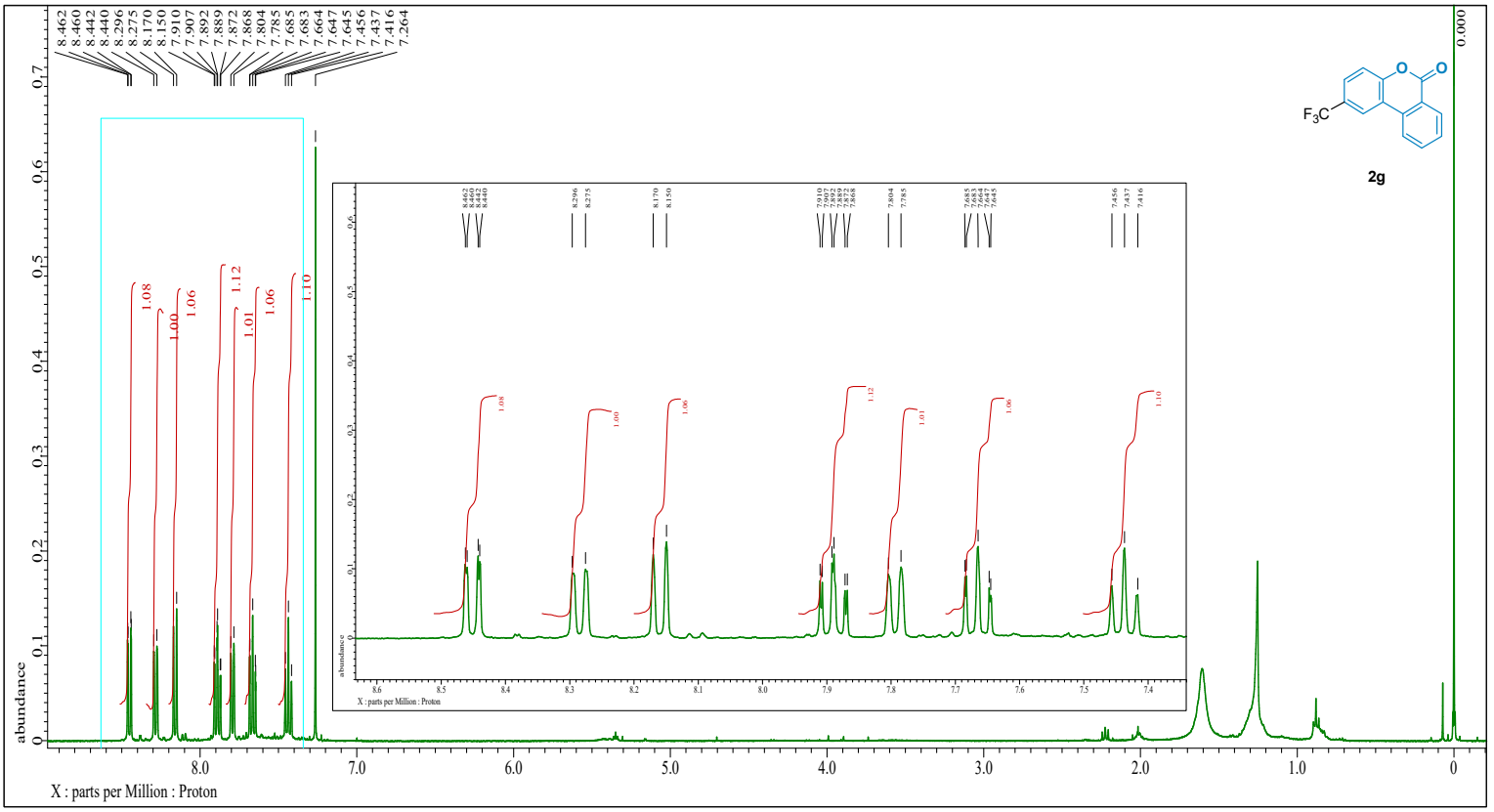
128.940
128.777
126.726
126.381
124.733
124.541
124.187
123.353
122.242
121.829
121.140
120.622
120.574
120.248
120.057
77.423
77.107
76.791
(thousandths)
X : parts per Million : Carbon13
CF3
F3C
O
O
2f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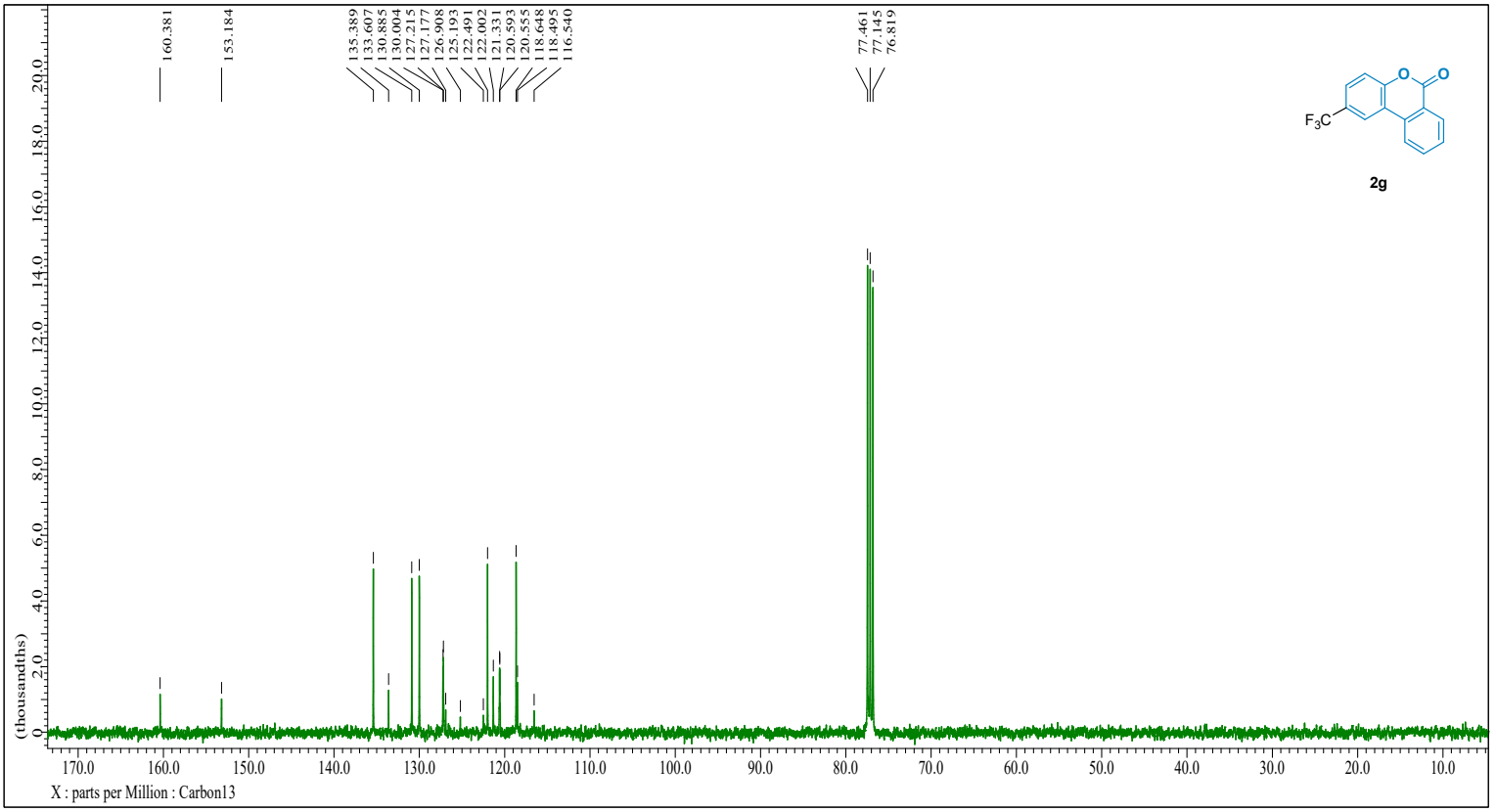
8.460
8.442
8.440
8.296
8.275
8.170
8.150
7.910
7.907
7.892
7.889
7.872
7.868
7.804
7.785
7.685
7.683
7.664
7.647
7.645
7.456
7.437
7.416
7.264
1.08
1.00
1.06
1.12
1.01
1.06
1.10
0.000
abundance
X : parts per Million : Proton
F3C
O
O
2g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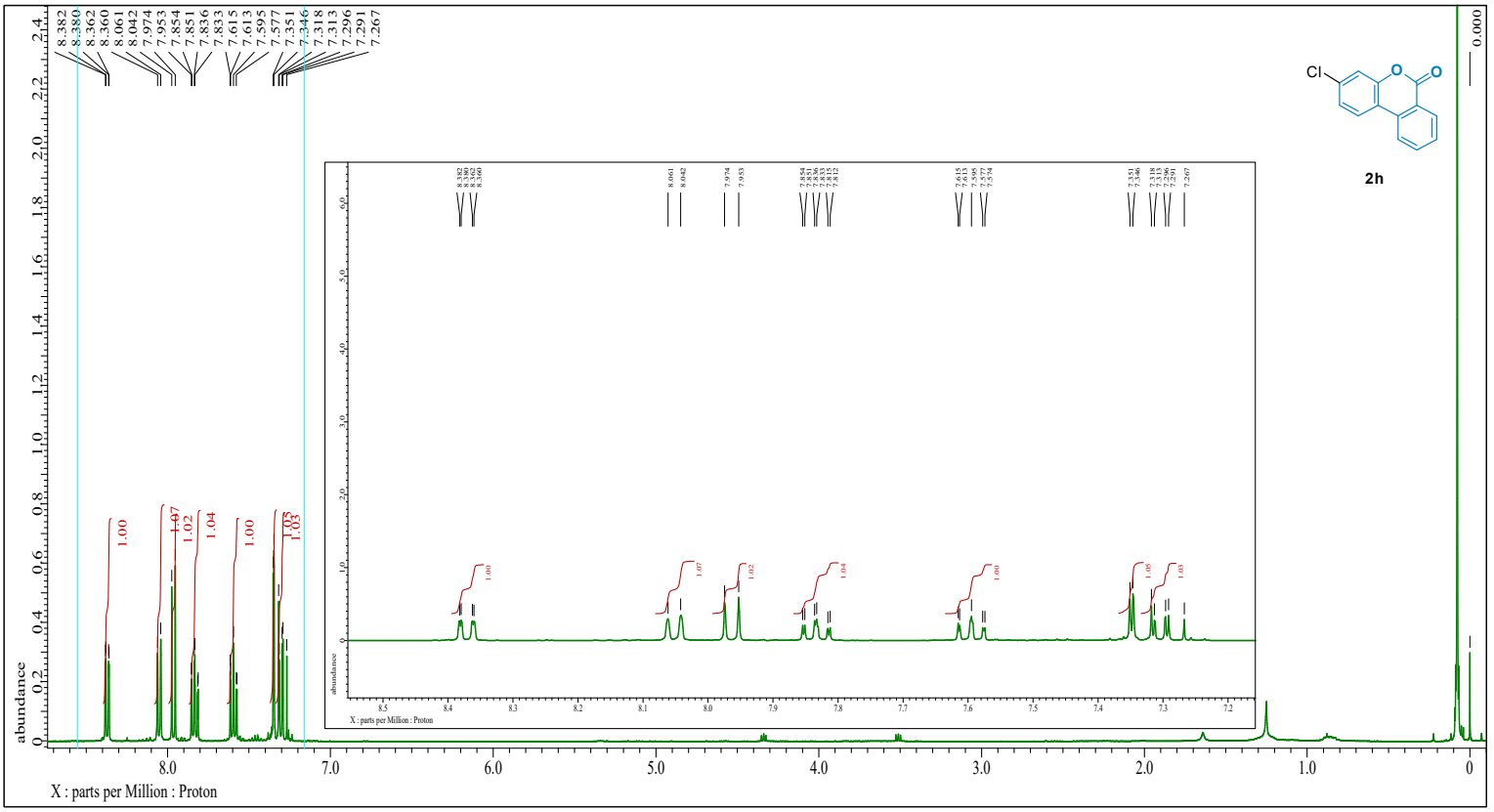
130.004
127.215
127.177
126.908
125.193
122.491
122.002
121.331
120.593
120.555
118.648
118.495
116.540
77.461
77.145
76.819
(thousandths)
X : parts per Million : Carbon13
F3C
O
O
2g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8.380
8.362
8.360
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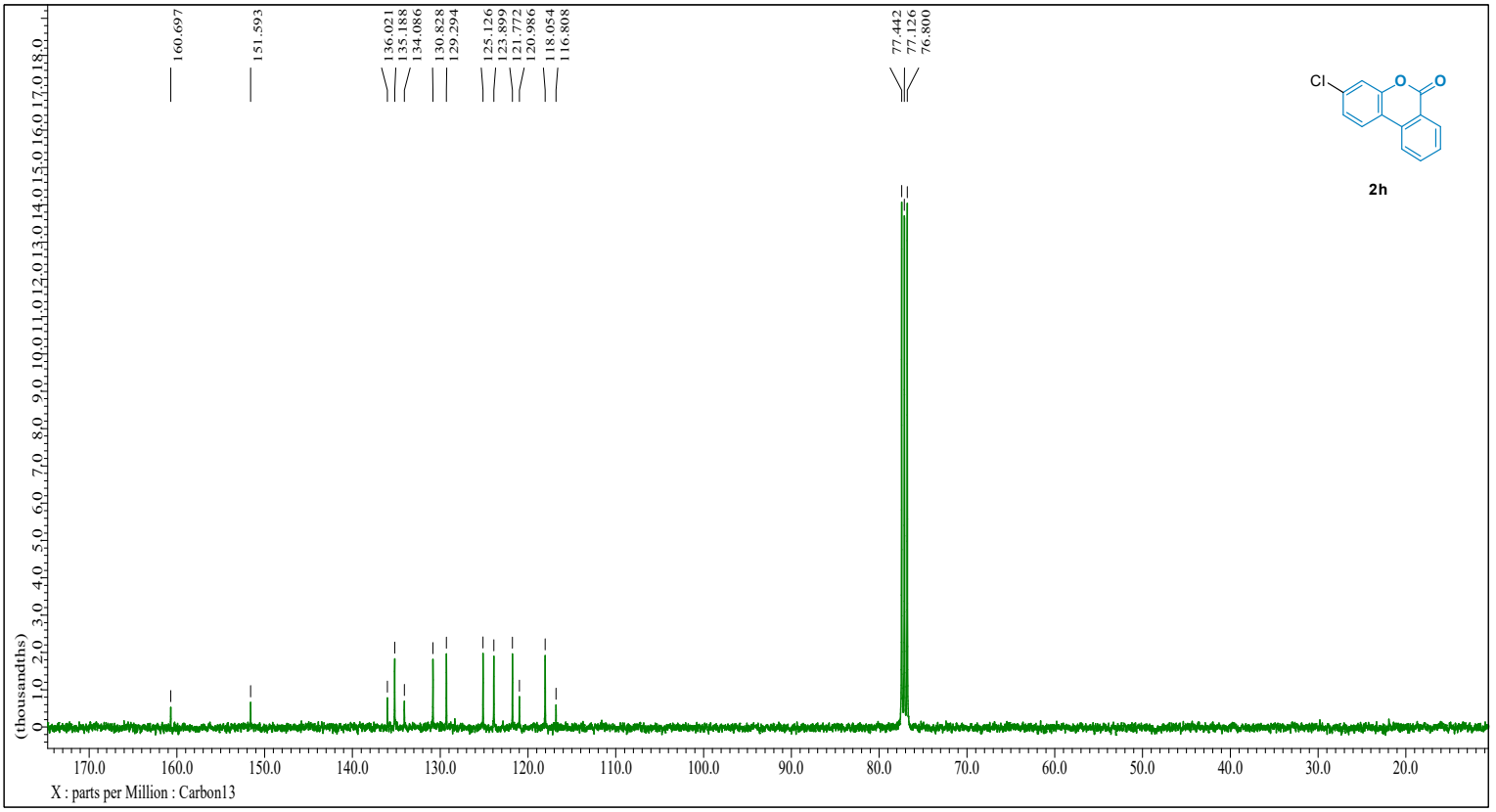
8.042
7.974
7.953
7.854
7.851
7.836
7.833
7.615
7.613
7.595
7.577
7.351
7.346
7.318
7.313
7.296
7.291
7.267
1.00
1.07
1.02
1.04
1.00
1.05
1.03
abundance
X : parts per Million : Proton
Cl
O
O
2h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134.086
130.828
129.294
125.126
123.899
121.772
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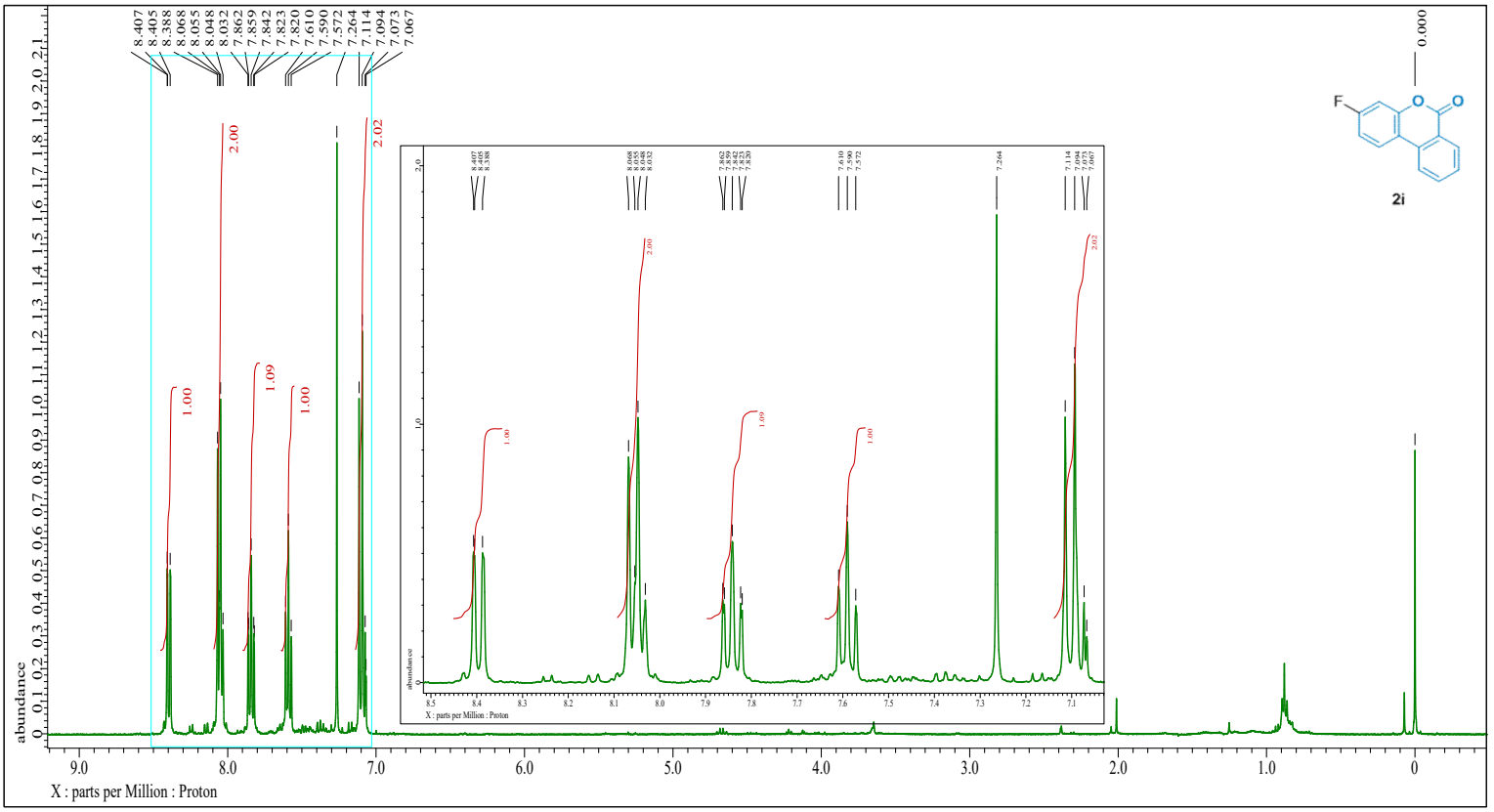
118.054
116.808
77.442
77.126
76.800
(thousandths)
X : parts per Million : Carbon13
Cl
O
O
2h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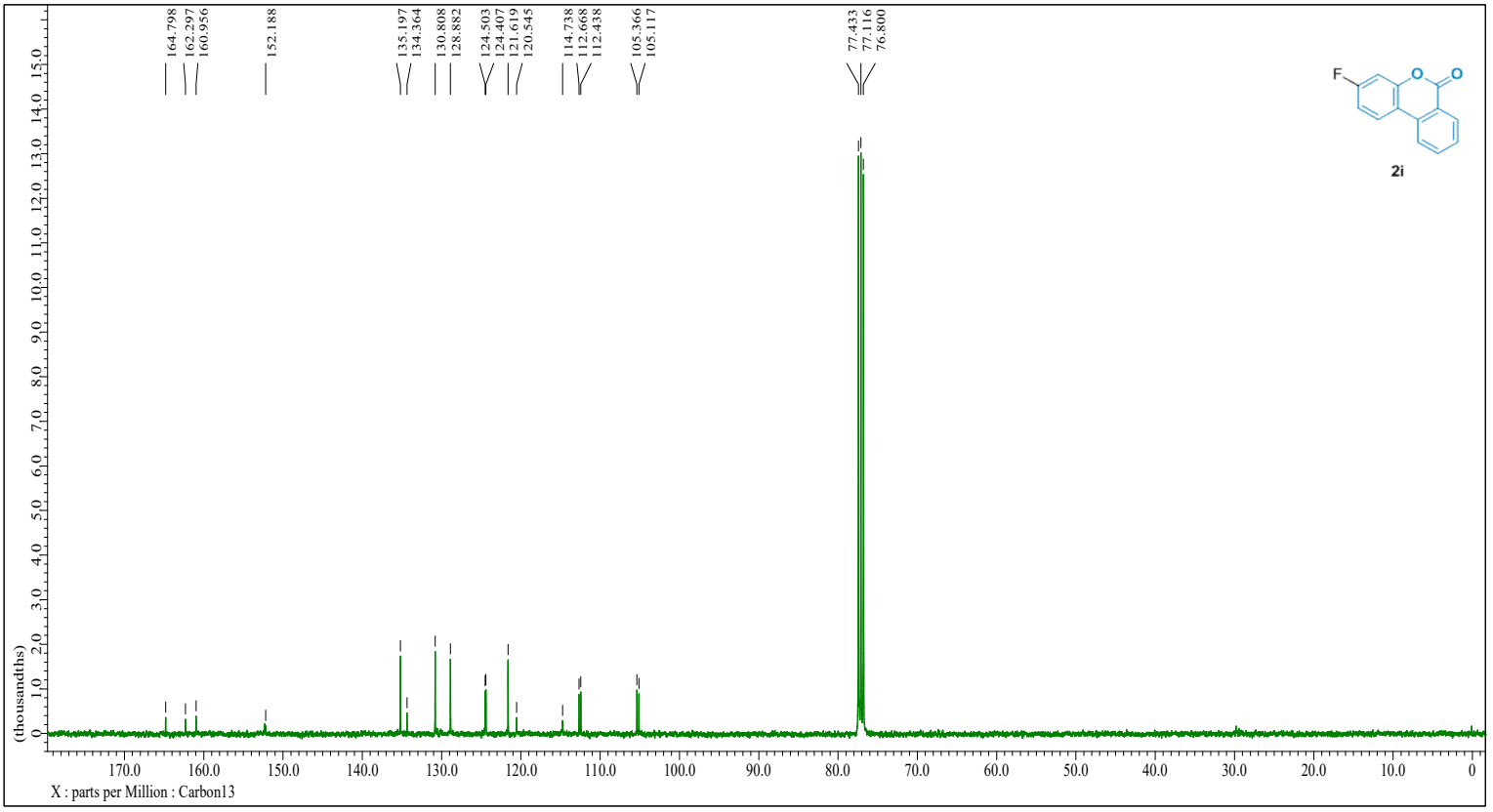
8.388
8.068
8.055
8.048
8.032
7.862
7.859
7.842
7.823
7.820
7.610
7.590
7.572
7.264
7.114
7.094
7.073
7.067
0.000
1.00
2.00
1.09
1.00
2.02
abundance
X : parts per Million : Proton
2i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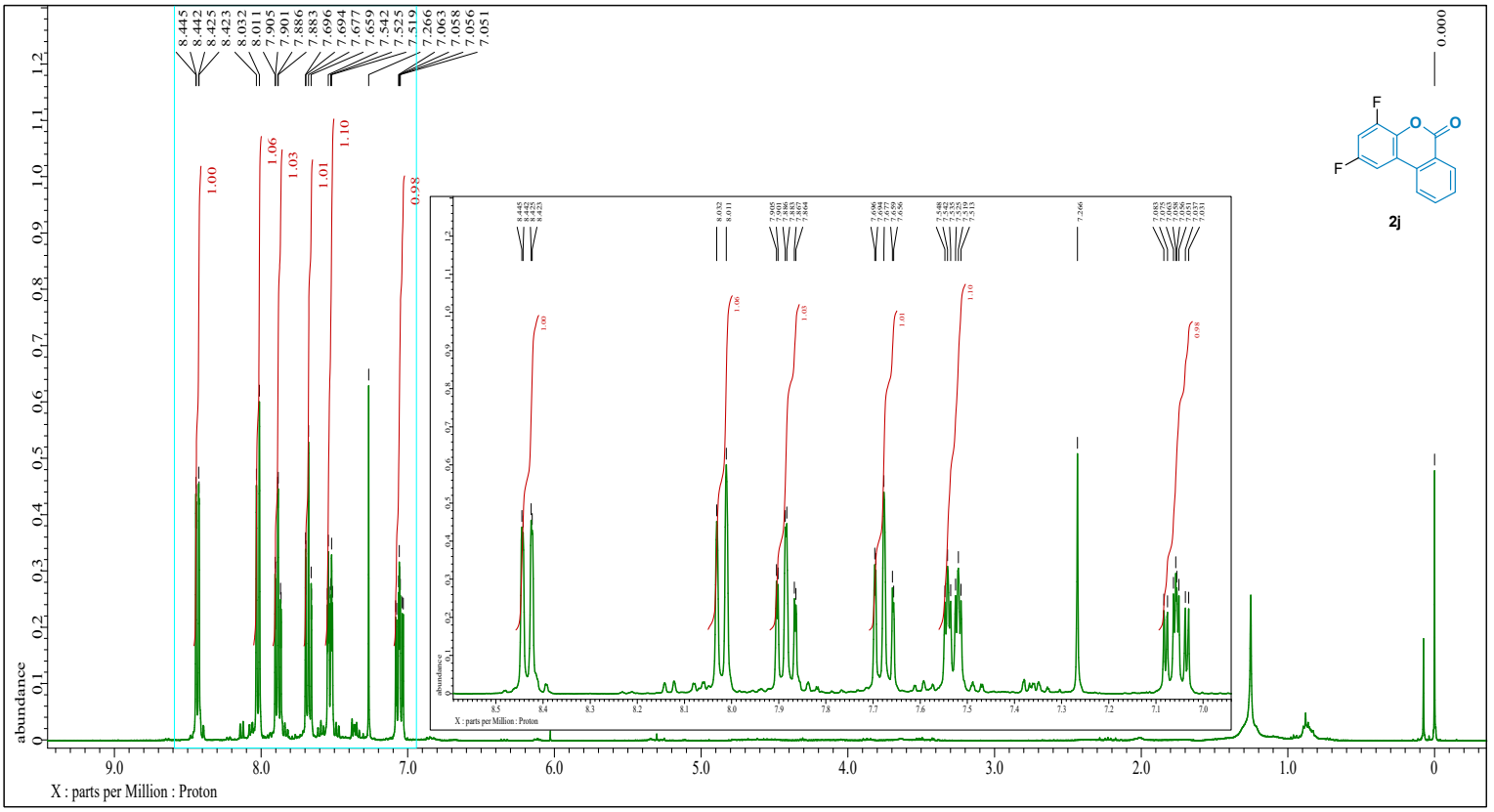
162.297
160.956
152.188
135.197
134.364
130.808
128.882
124.503
124.407
121.619
120.545
114.738
112.668
112.438
105.366
105.117
77.433
77.116
76.800
(thousandths)
X : parts per Million : Carbon13
2i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8.442
8.425
8.423
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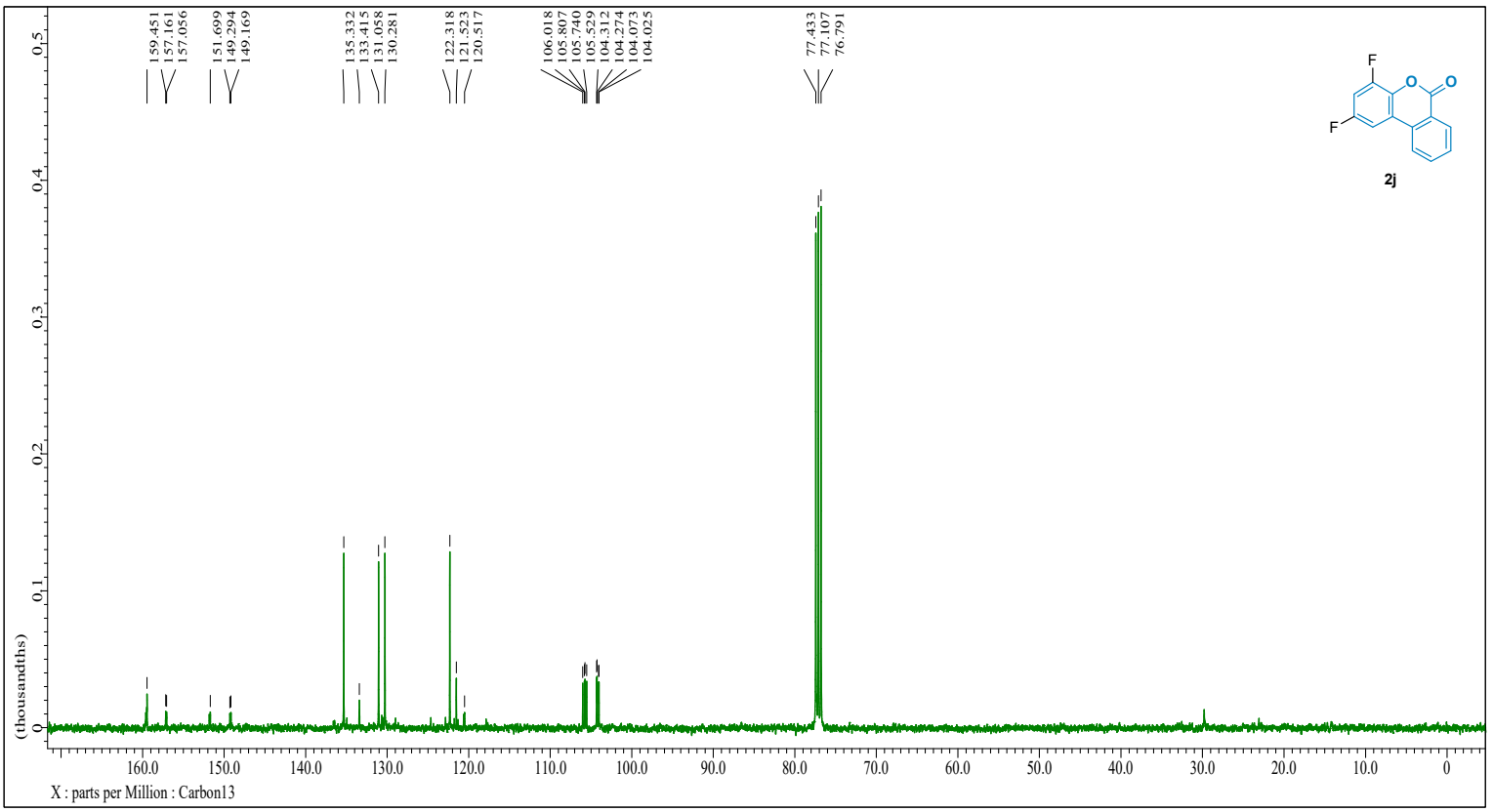
8.011
7.905
7.901
7.886
7.883
7.696
7.694
7.677
7.659
7.542
7.525
7.519
7.266
7.063
7.058
7.056
7.051
1.00
1.06
1.03
1.01
1.10
0.98
0.000
F
O
O
F
2j
abundance
X : parts per Million : Proton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157.056
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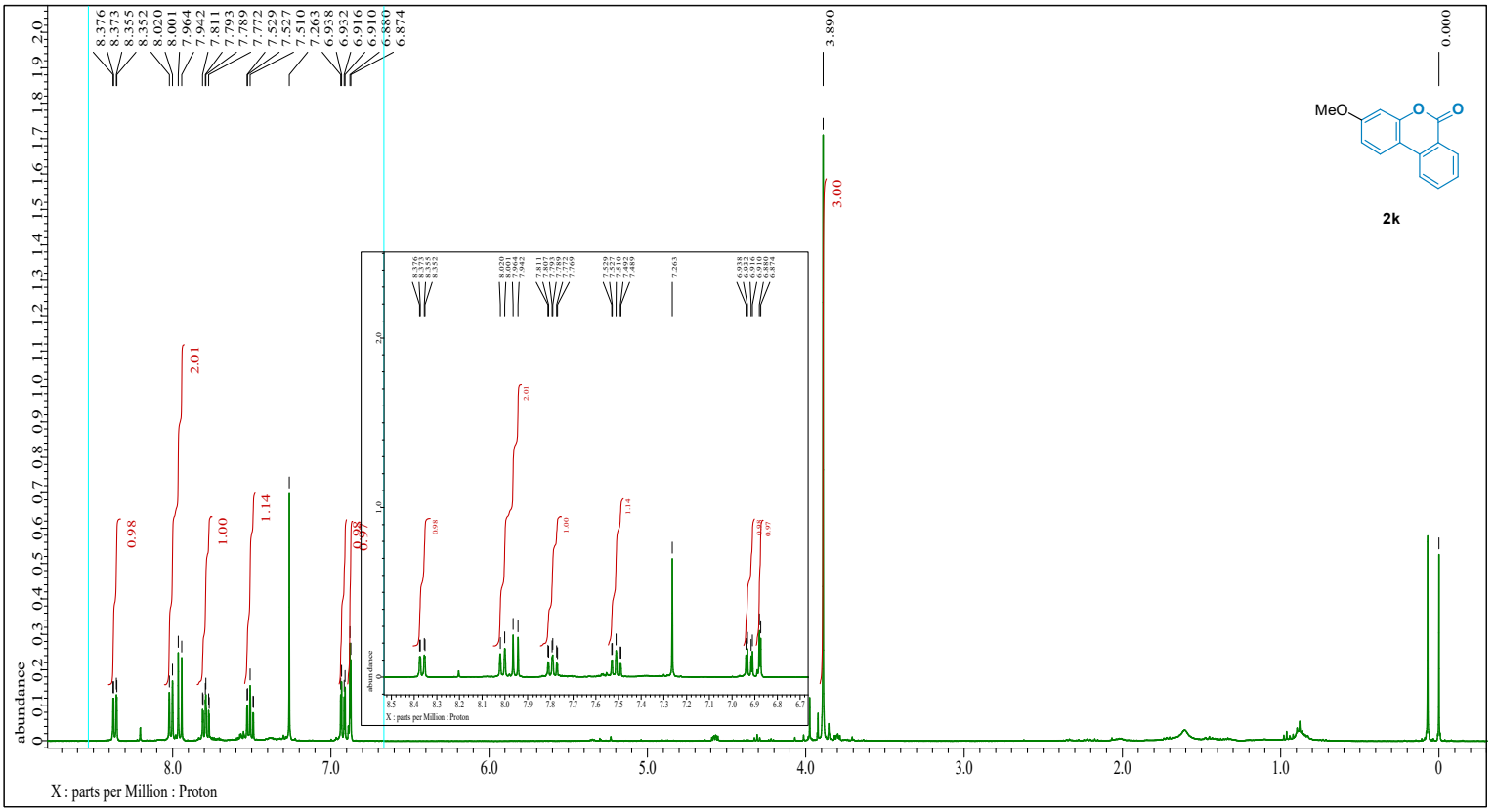
149.169
135.332
133.415
131.058
130.281
122.318
121.523
120.517
106.018
105.807
105.740
105.529
104.312
104.274
104.073
104.025
77.433
77.107
76.791
F
O
O
F
2j
(thousandths)
X : parts per Million : Carbon13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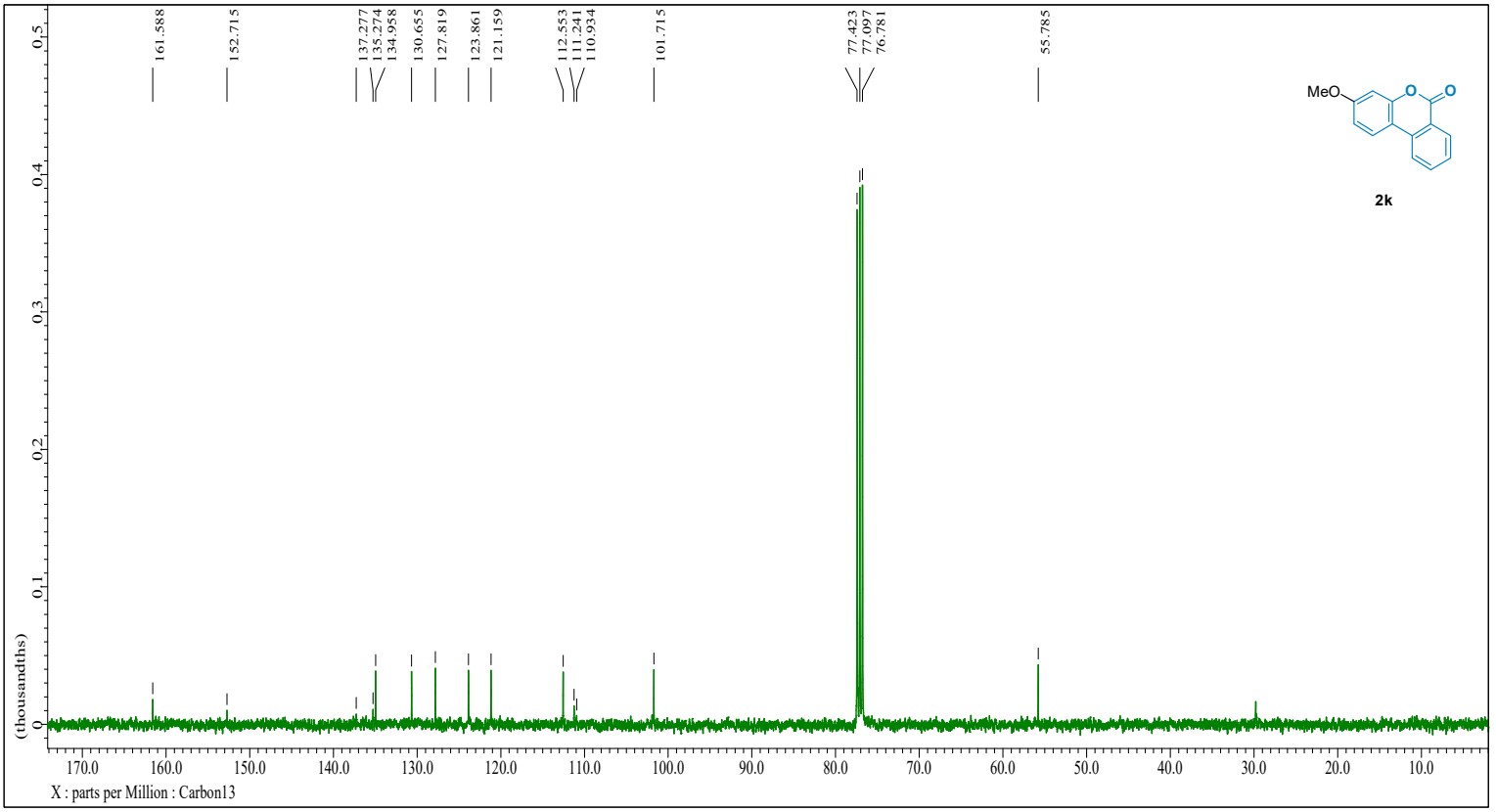
8.373
8.355
8.352
8.020
8.001
7.964
7.942
7.811
7.793
7.789
7.772
7.529
7.527
7.510
7.263
6.938
6.932
6.916
6.910
6.880
6.874
3.890
0.000
2.01
0.98
1.00
1.14
3.00
MeO
O
O
2k
abundance
X : parts per Million : Proton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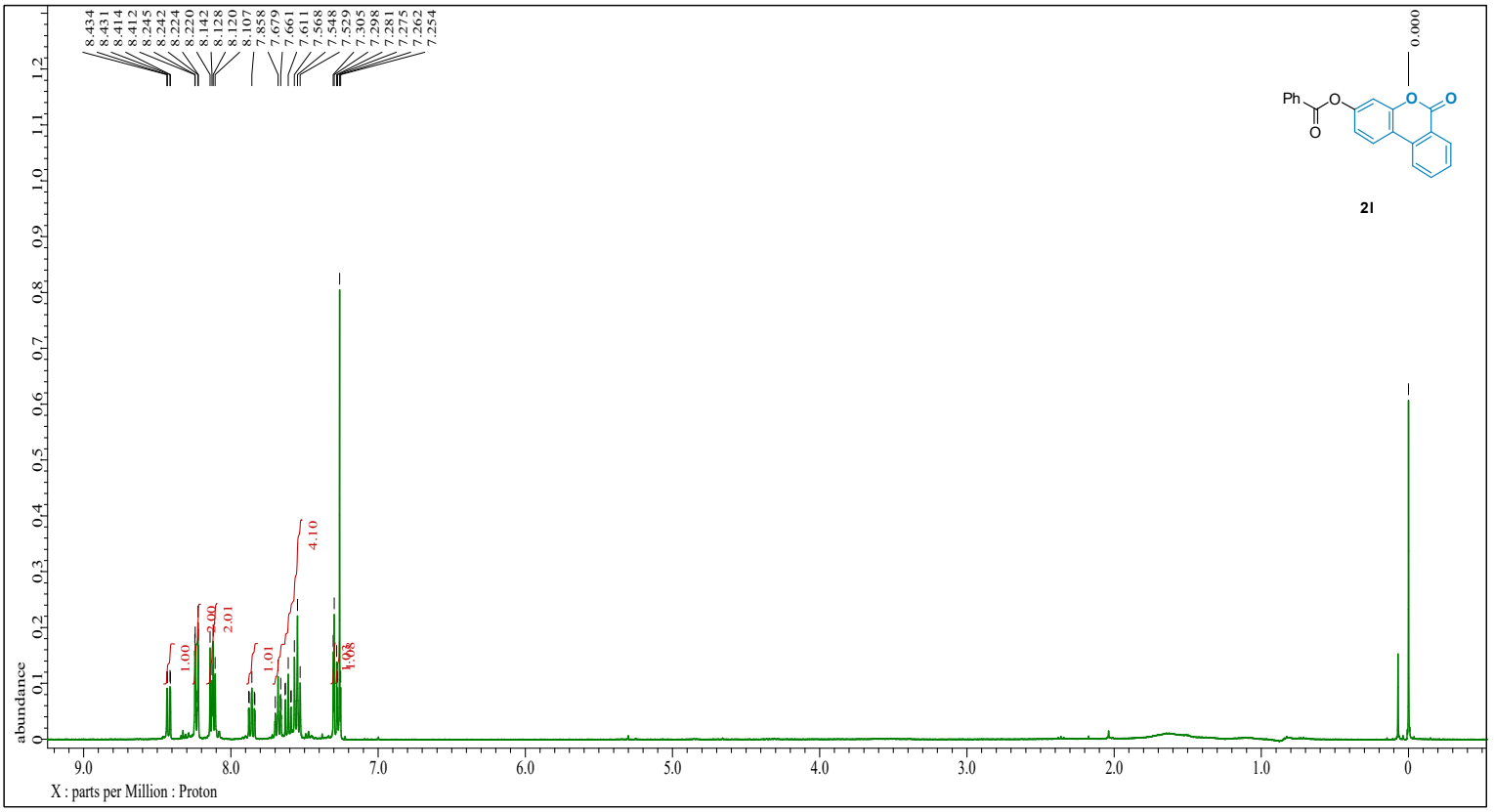
135.274
134.958
130.655
127.819
123.861
121.159
112.553
111.241
110.934
101.715
77.423
77.097
76.781
55.785
MeO
O
O
2k
(thousandths)
X : parts per Million : Carbon13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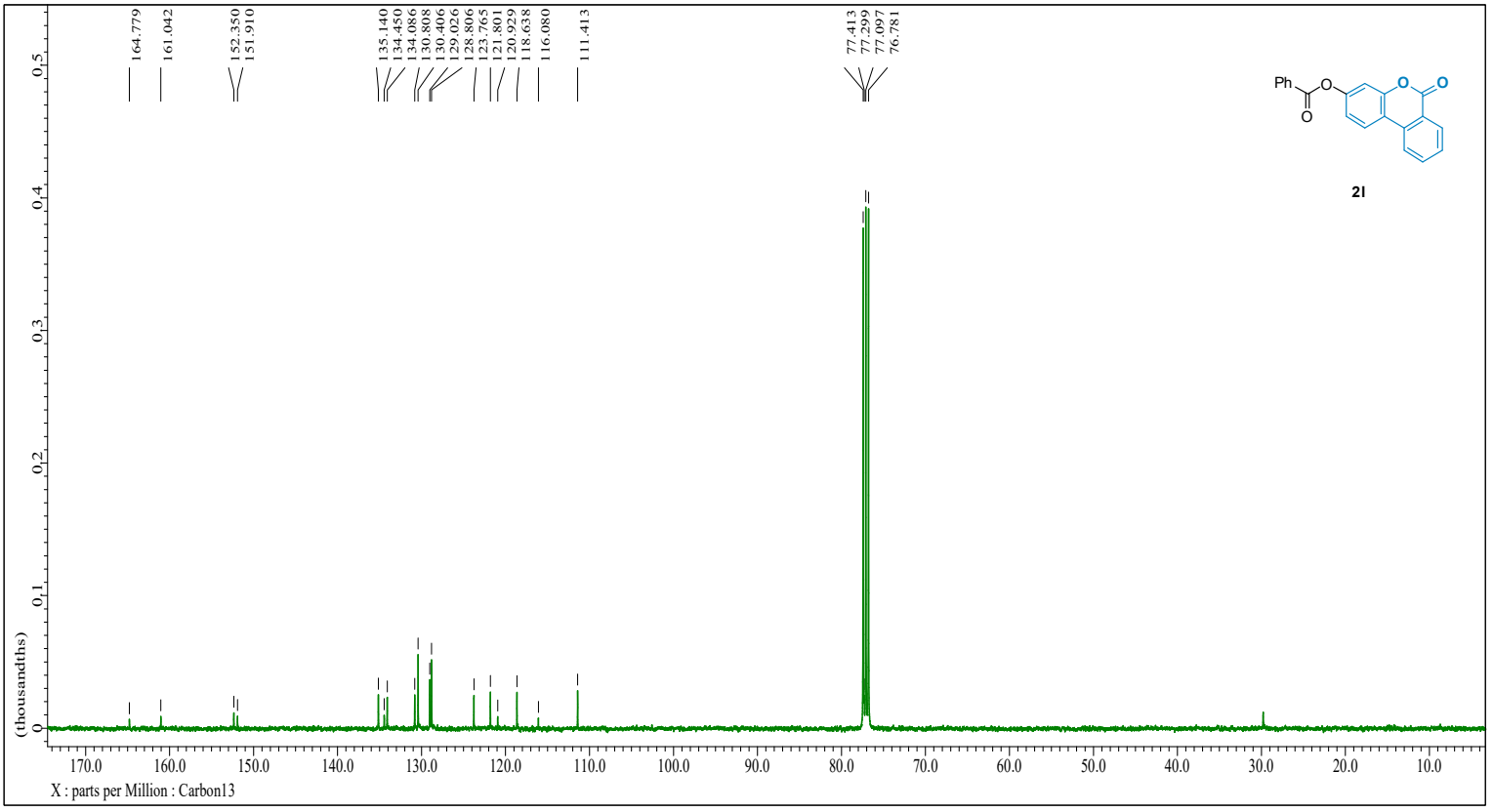
8.431
8.414
8.412
8.245
8.242
8.224
8.220
8.142
8.128
8.120
8.107
7.858
7.679
7.661
7.611
7.568
7.548
7.529
7.305
7.298
7.281
7.275
7.262
7.254
0.000
Ph
O
O
O
O
2l
1.00
2.00
2.01
4.10
1.01
1.08
abundance
X : parts per Million : Proton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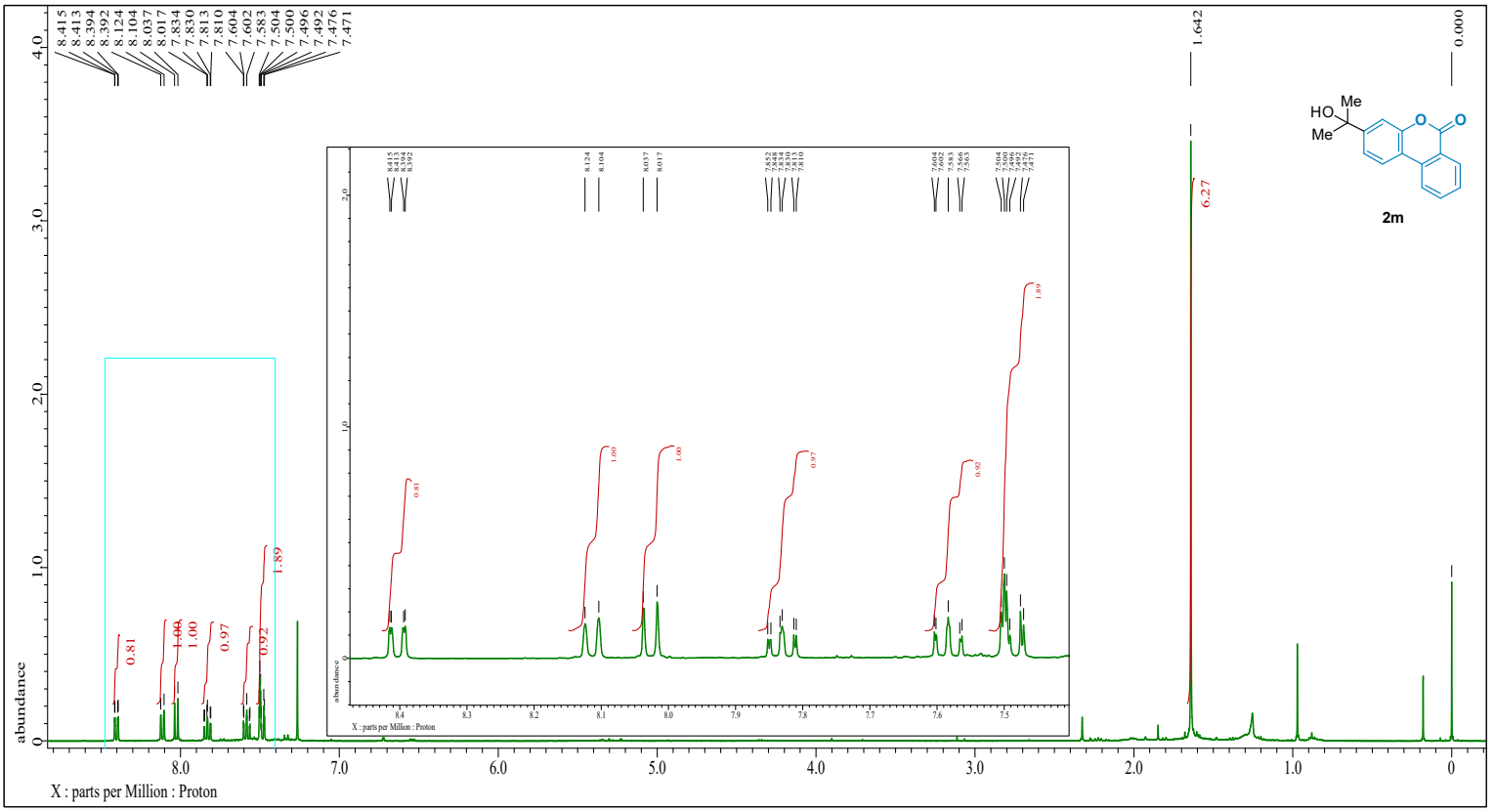
151.910
135.140
134.450
134.086
130.808
130.406
129.026
128.806
123.765
121.801
120.929
118.638
116.080
111.413
77.413
77.299
77.097
76.781
Ph
O
O
O
O
2l
(thousandths)
X : parts per Million : Carbon13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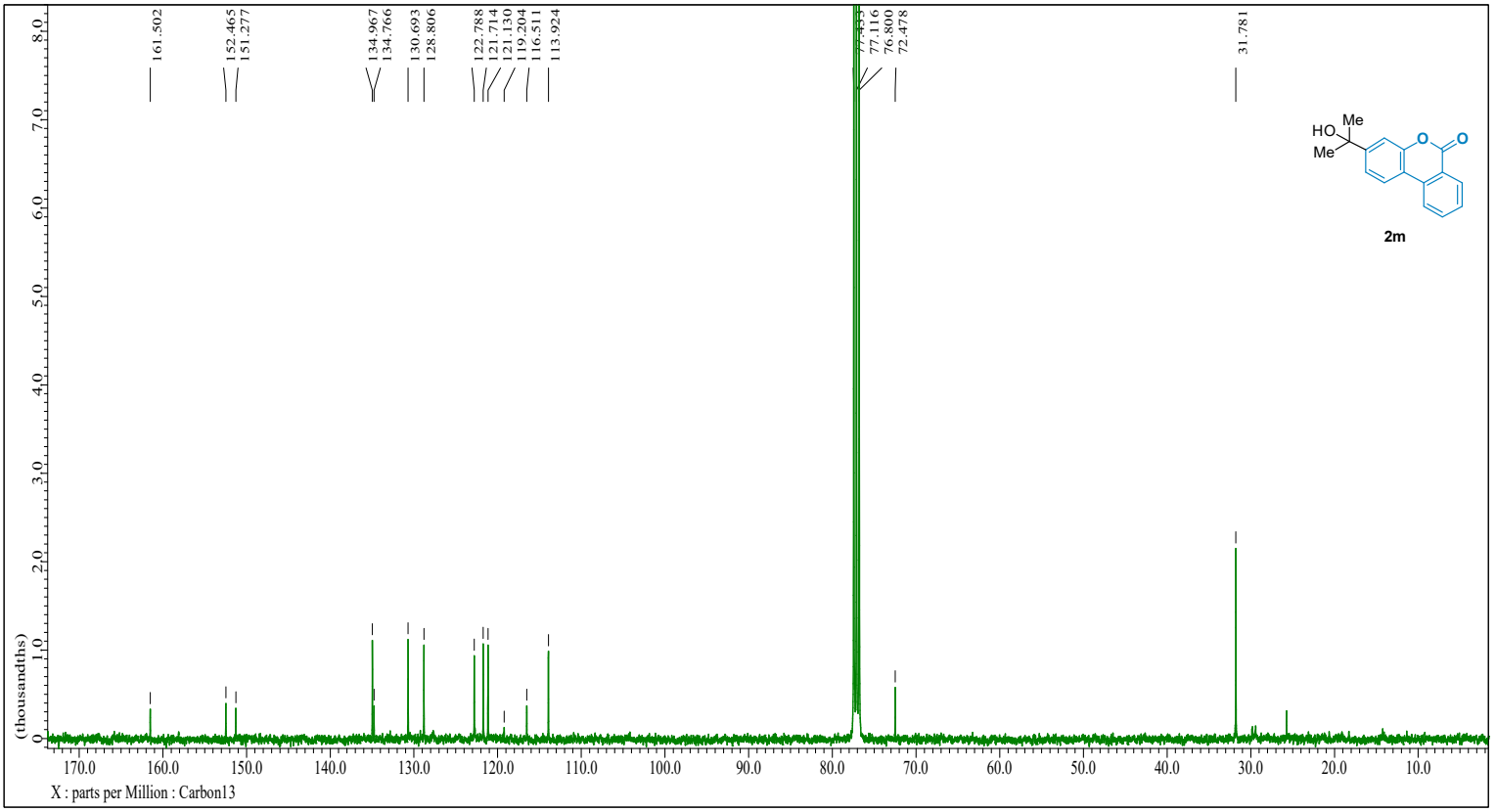
8.413
8.394
8.392
8.124
8.104
8.037
8.017
7.834
7.830
7.813
7.810
7.604
7.602
7.583
7.504
7.500
7.496
7.492
7.476
7.471
1.642
0.000
6.27
0.81
1.00
1.00
0.97
0.92
1.89
HO
Me
Me
O
O
2m
abundance
X : parts per Million : Proton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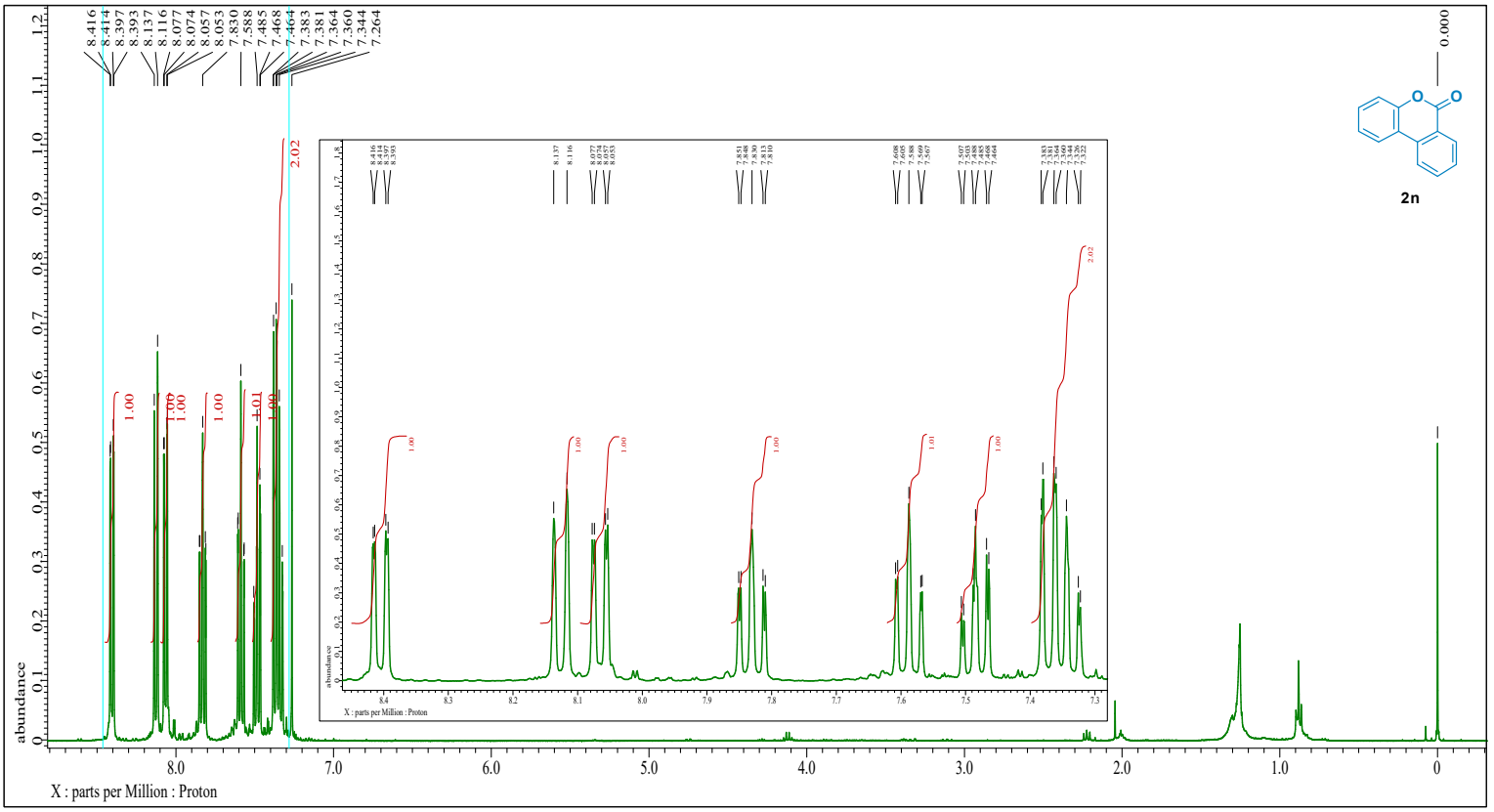
151.277
134.967
134.766
130.693
128.806
122.788
121.714
121.130
119.204
116.511
113.924
77.433
77.116
76.800
72.478
31.781
HO
Me
Me
O
O
2m
(thousandths)
X : parts per Million : Carbon13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8.393
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8.116
8.077
8.074
8.057
8.053
7.830
7.588
7.485
7.468
7.464
7.383
7.381
7.364
7.360
7.344
7.264
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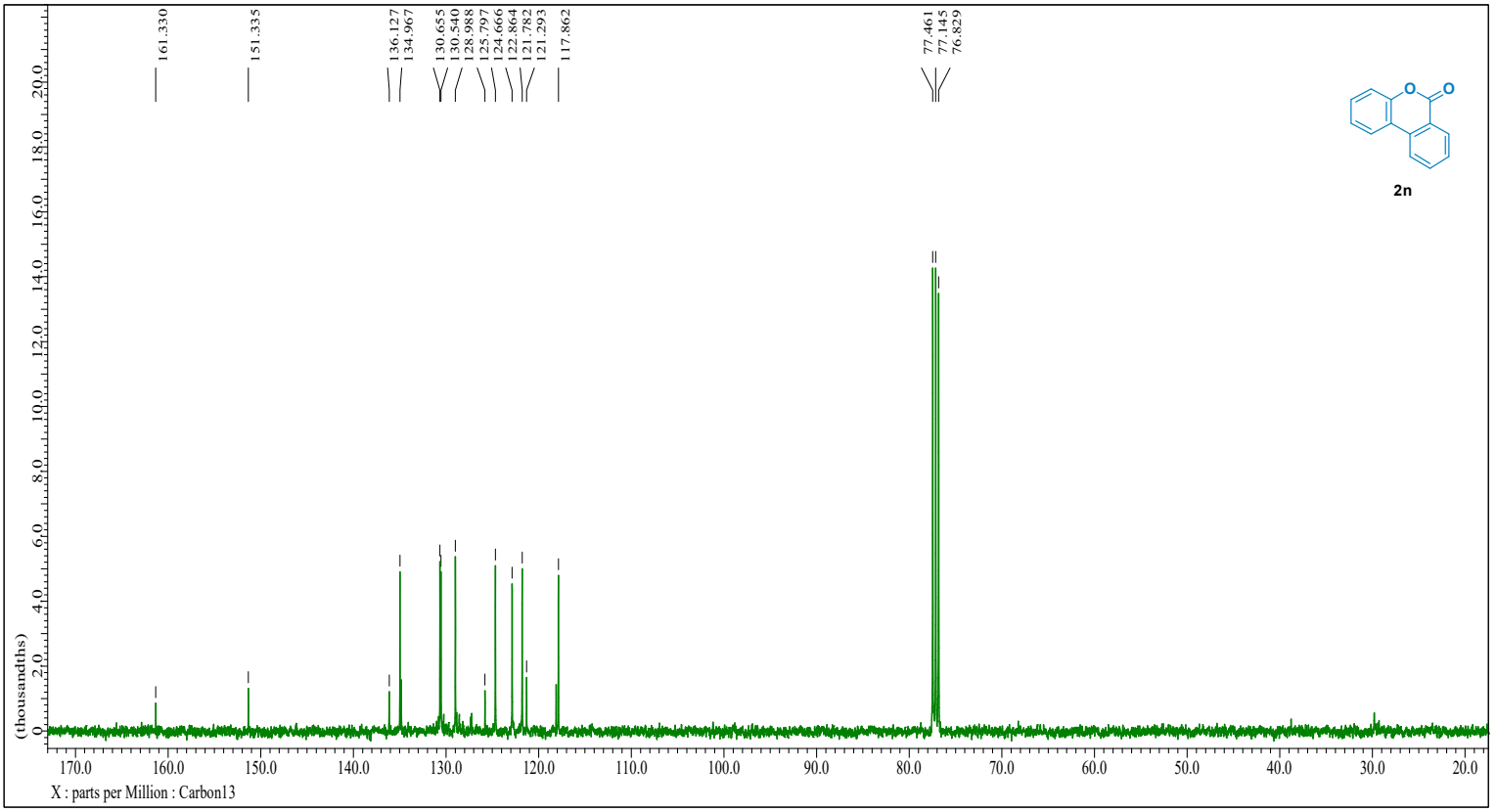
1.00
1.00
1.01
1.02
2.02
0.000
2n
abundance
X : parts per Million : Proton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151.335
136.127
134.967
130.655
130.540
128.988
125.797
124.666
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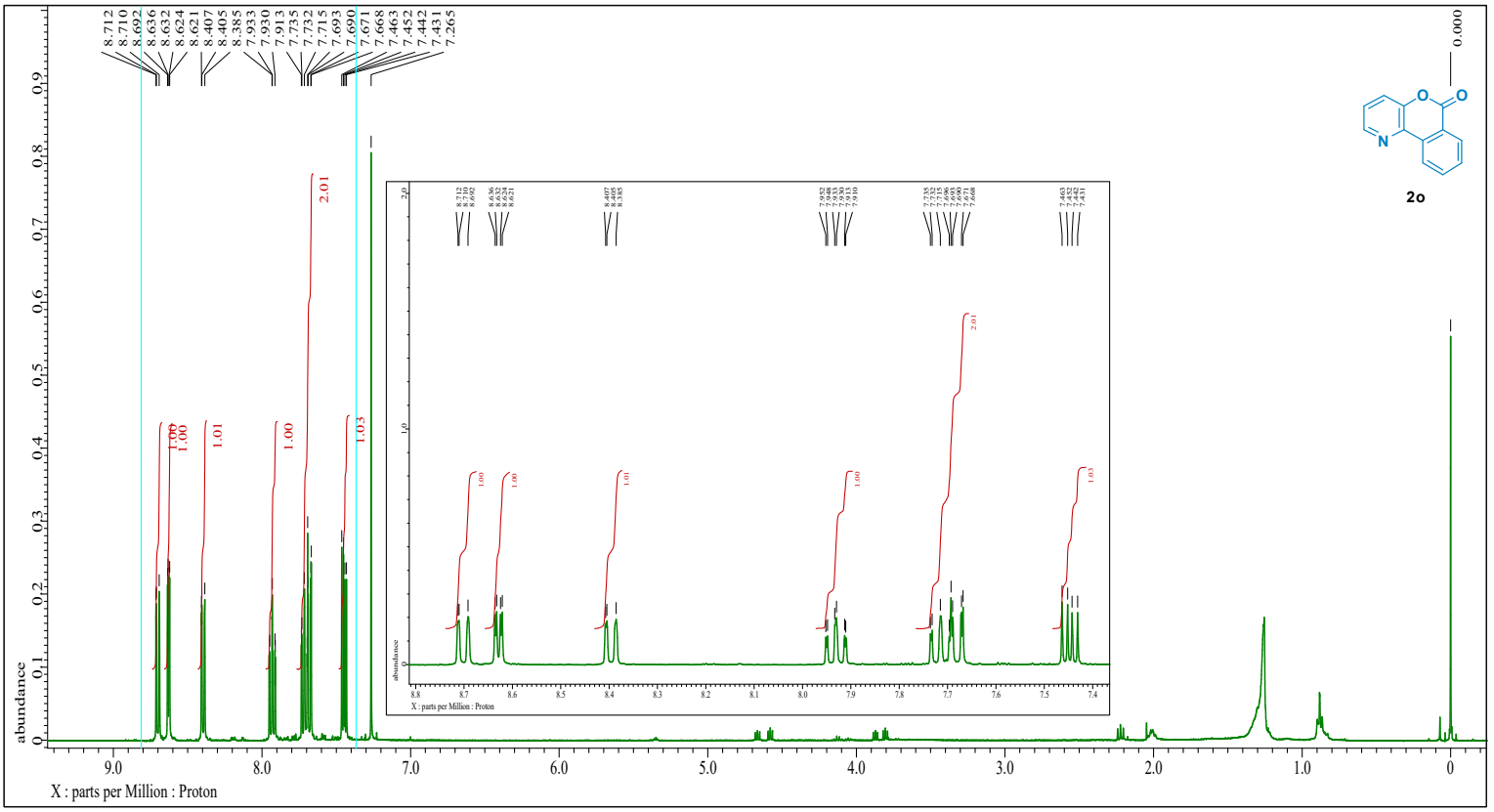
121.782
121.293
117.862
77.461
77.145
76.829
2n
(thousandths)
X : parts per Million : Carbon13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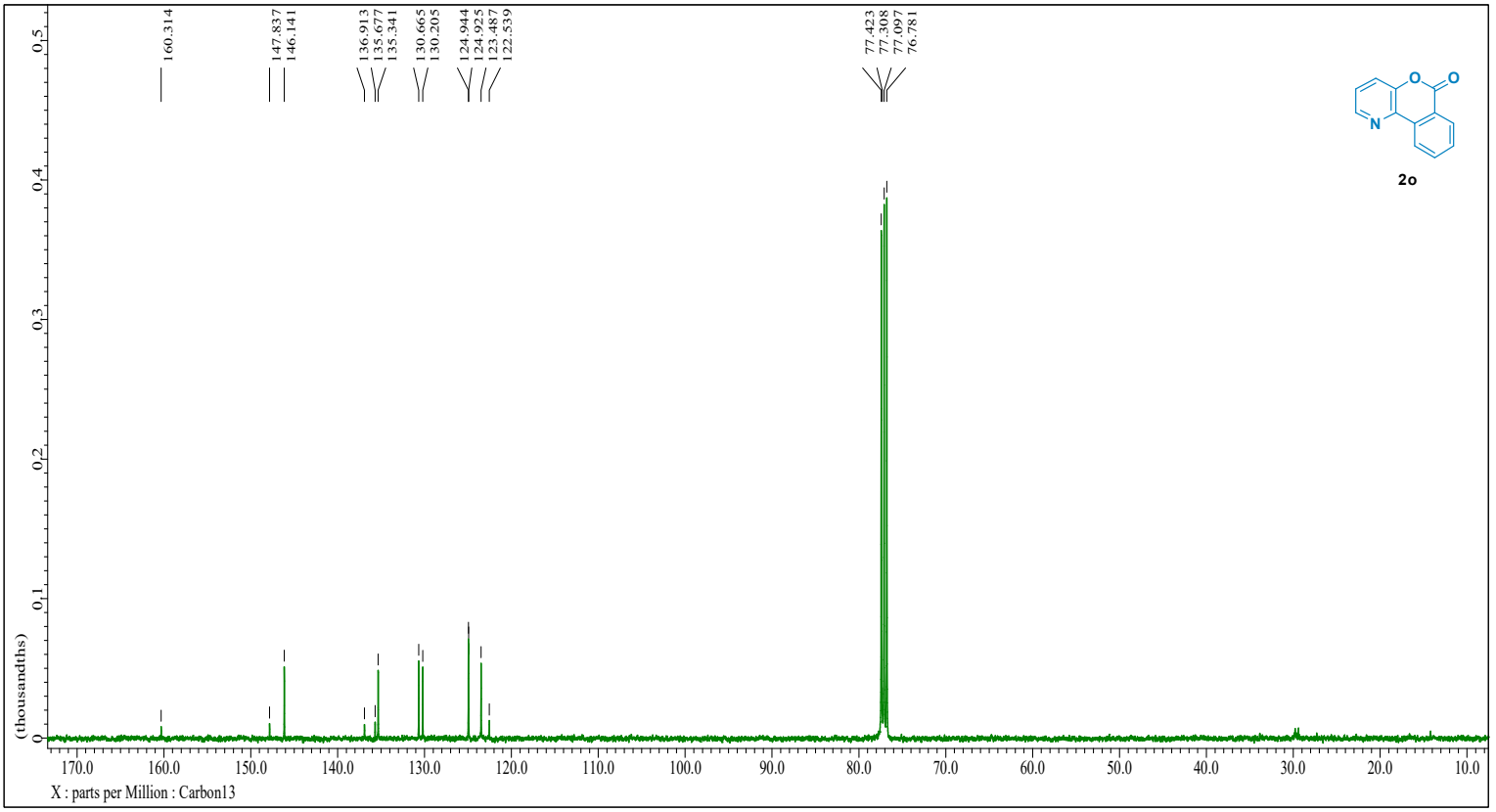
8.624
8.621
8.407
8.405
8.385
7.933
7.930
7.913
7.735
7.732
7.715
7.693
7.690
7.671
7.668
7.463
7.452
7.442
7.431
7.265
0.000
2.01
1.03
1.01
1.00
1.00
1.00
abundance
X : parts per Million : Proton
2o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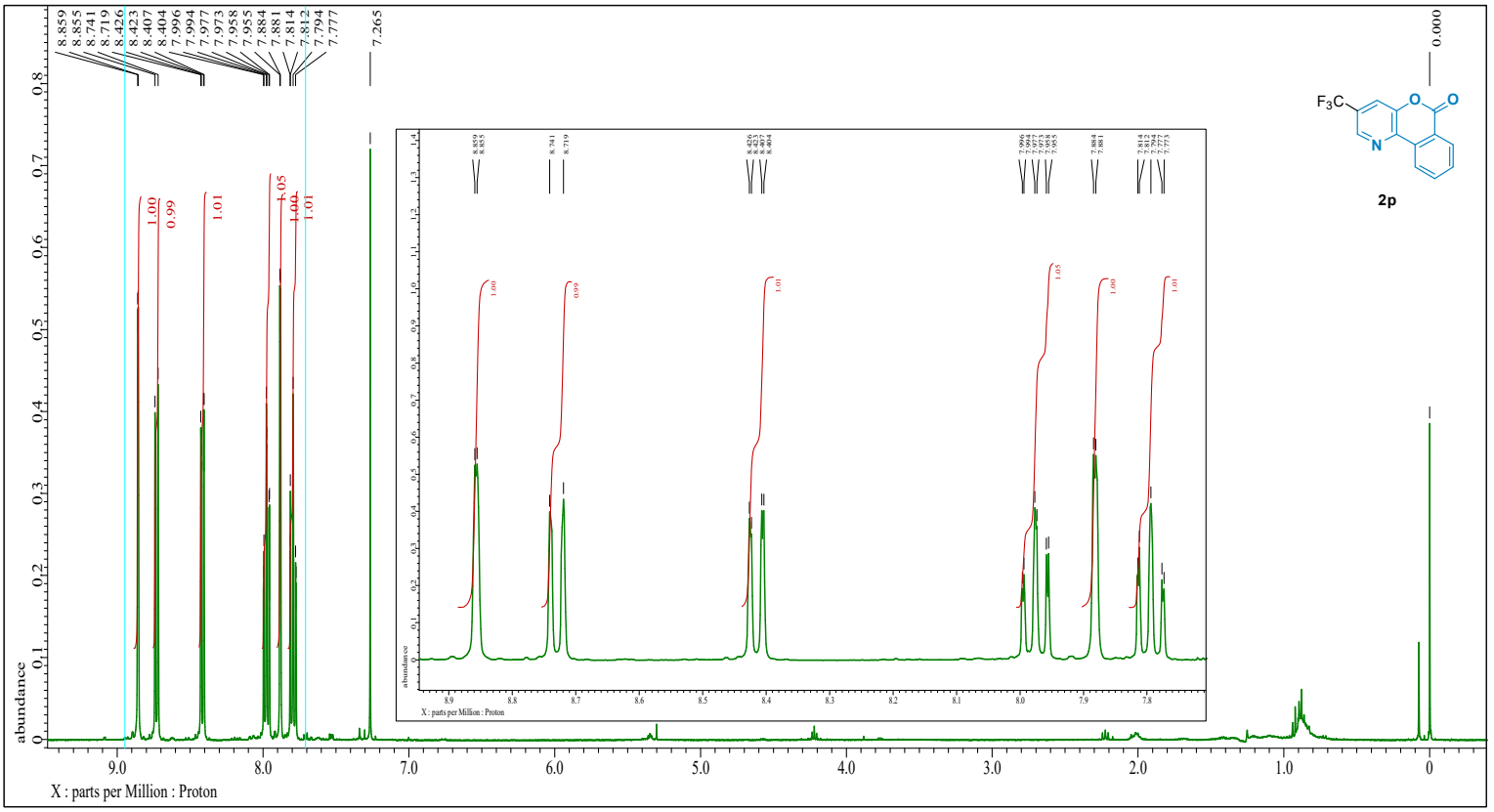
147.837
146.141
136.913
135.677
135.341
130.665
130.205
124.944
124.925
123.487
122.539
77.423
77.308
77.097
76.781
(thousandths)
X : parts per Million : Carbon13
2o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8.719
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8.423
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8.404
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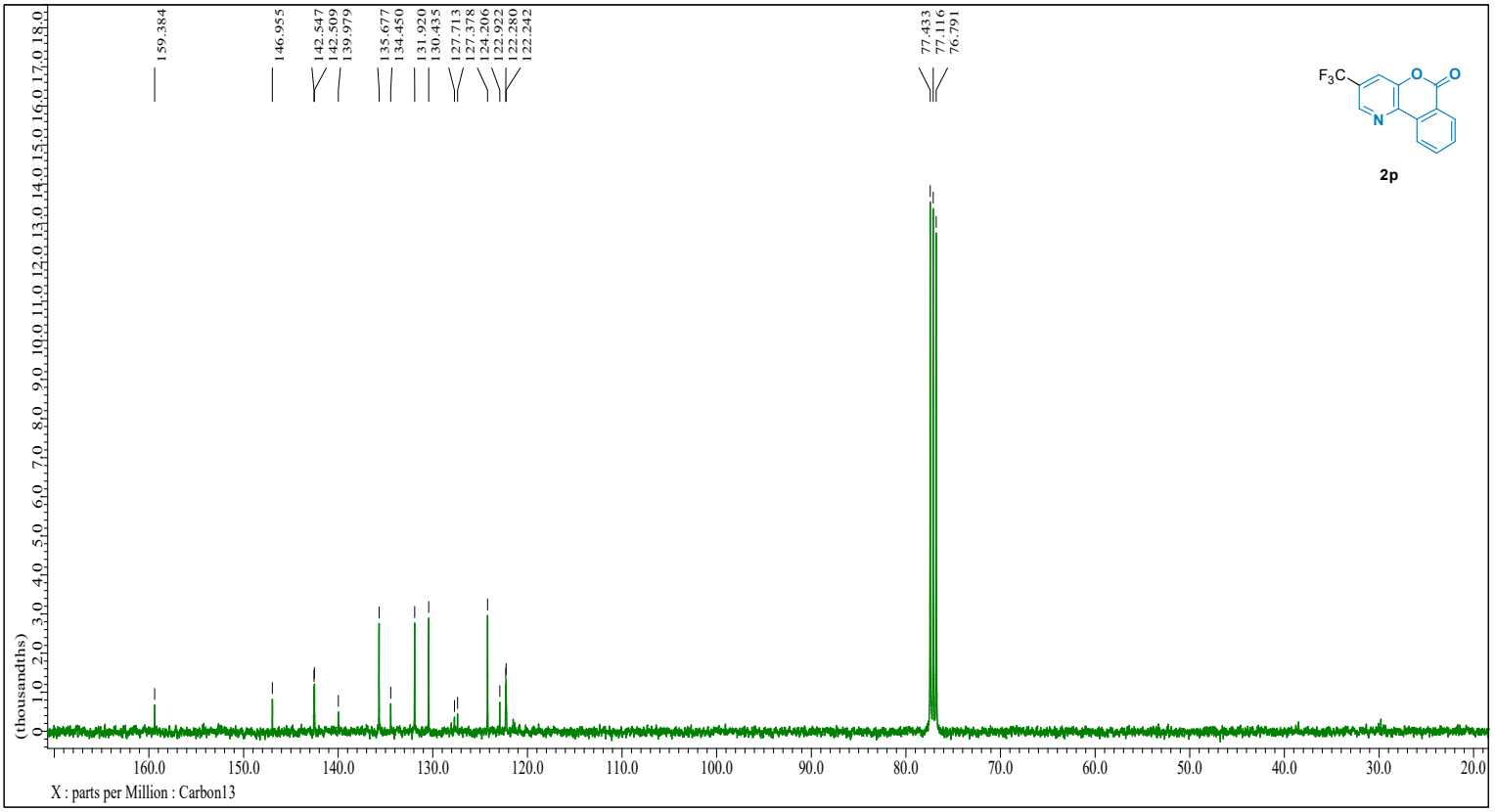
7.994
7.977
7.973
7.958
7.955
7.884
7.881
7.814
7.812
7.794
7.777
7.265
0.000
1.00
0.99
1.01
1.05
1.00
1.01
F3C
O
O
N
2p
abundance
X : parts per Million : Proton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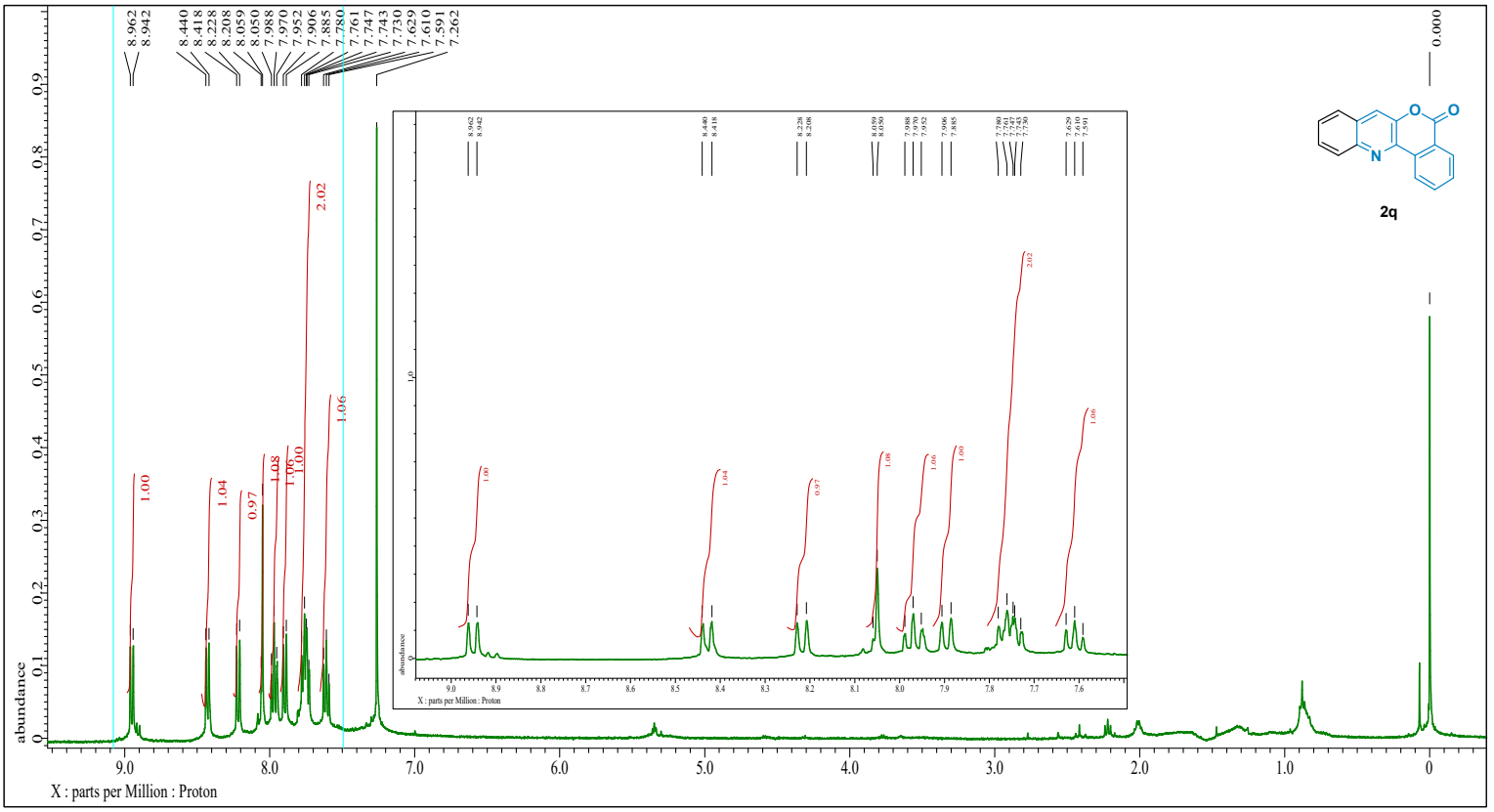
135.677
134.450
131.920
130.435
127.713
127.378
124.206
122.922
122.280
122.242
77.433
77.116
76.791
F3C
O
O
N
2p
(thousandths)
X : parts per Million : Carbon13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8.228
8.208
8.059
8.050
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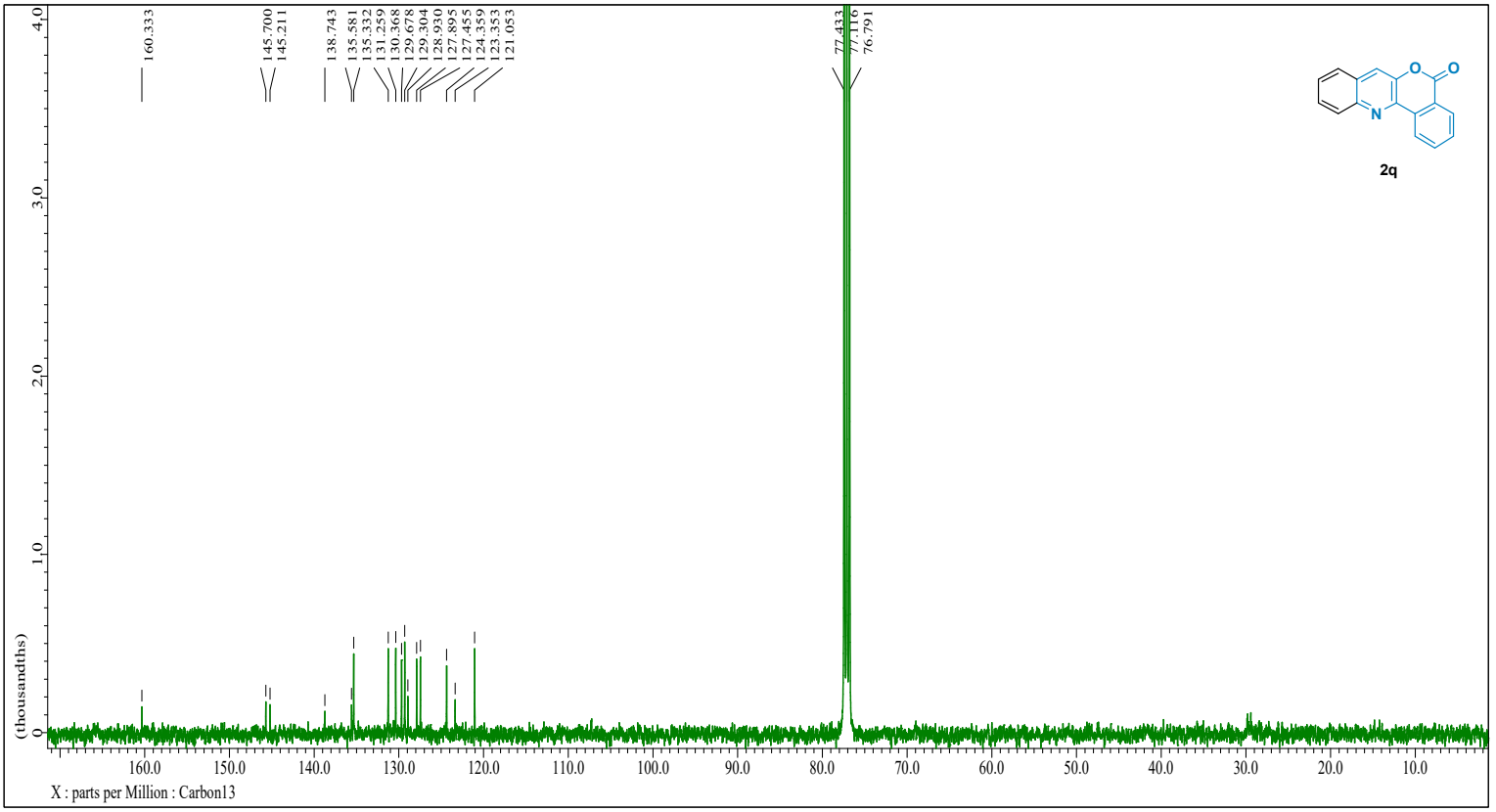
7.970
7.952
7.906
7.885
7.780
7.761
7.747
7.743
7.730
7.629
7.610
7.591
7.262
0.000
1.00
1.04
0.97
1.08
1.06
1.00
2.02
1.06
abundance
X : parts per Million : Proton
2q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135.332
131.259
130.368
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129.304
128.930
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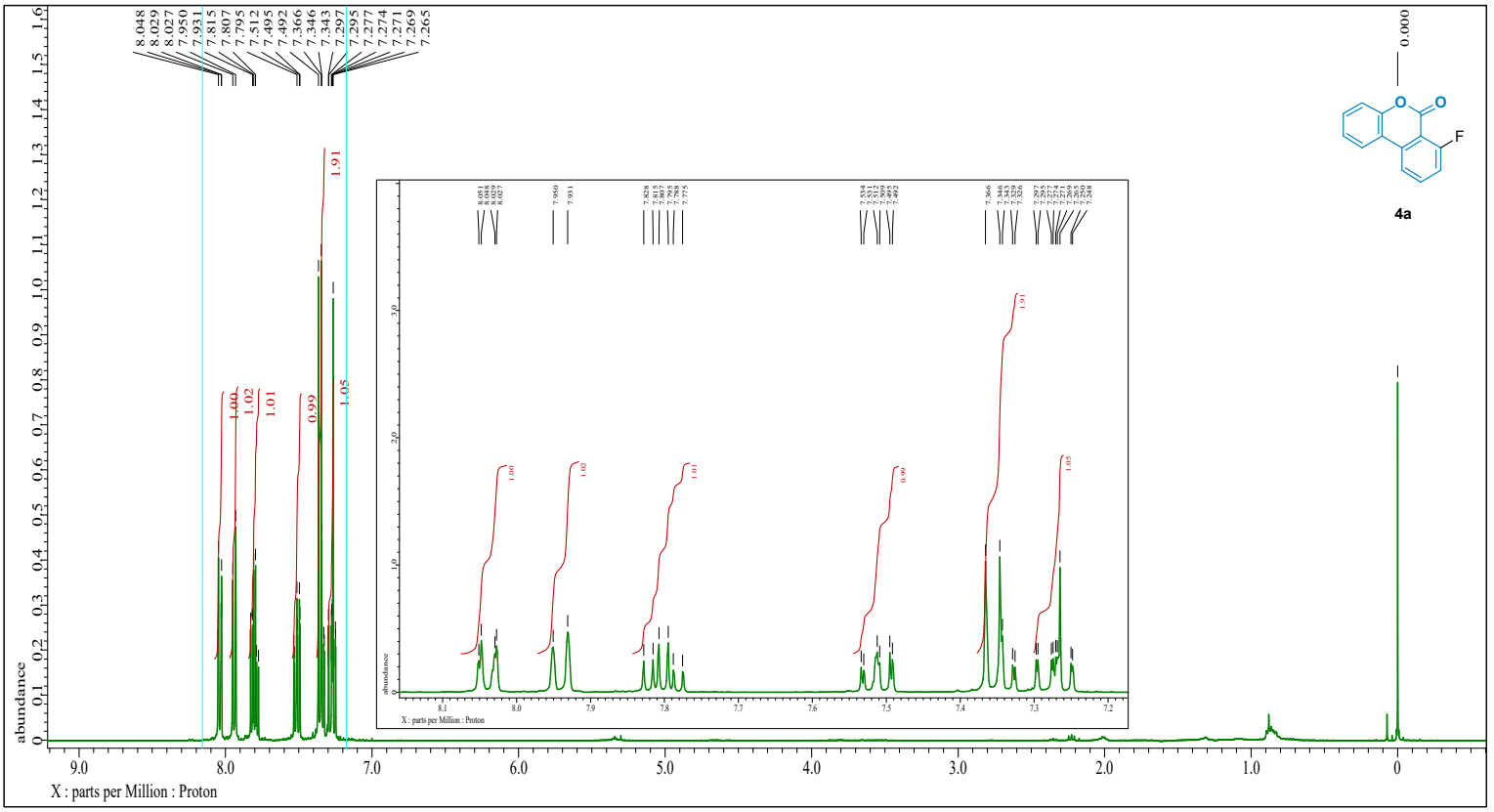
127.455
124.359
123.353
121.053
77.433
77.116
76.791
(thousandths)
X : parts per Million : Carbon13
2q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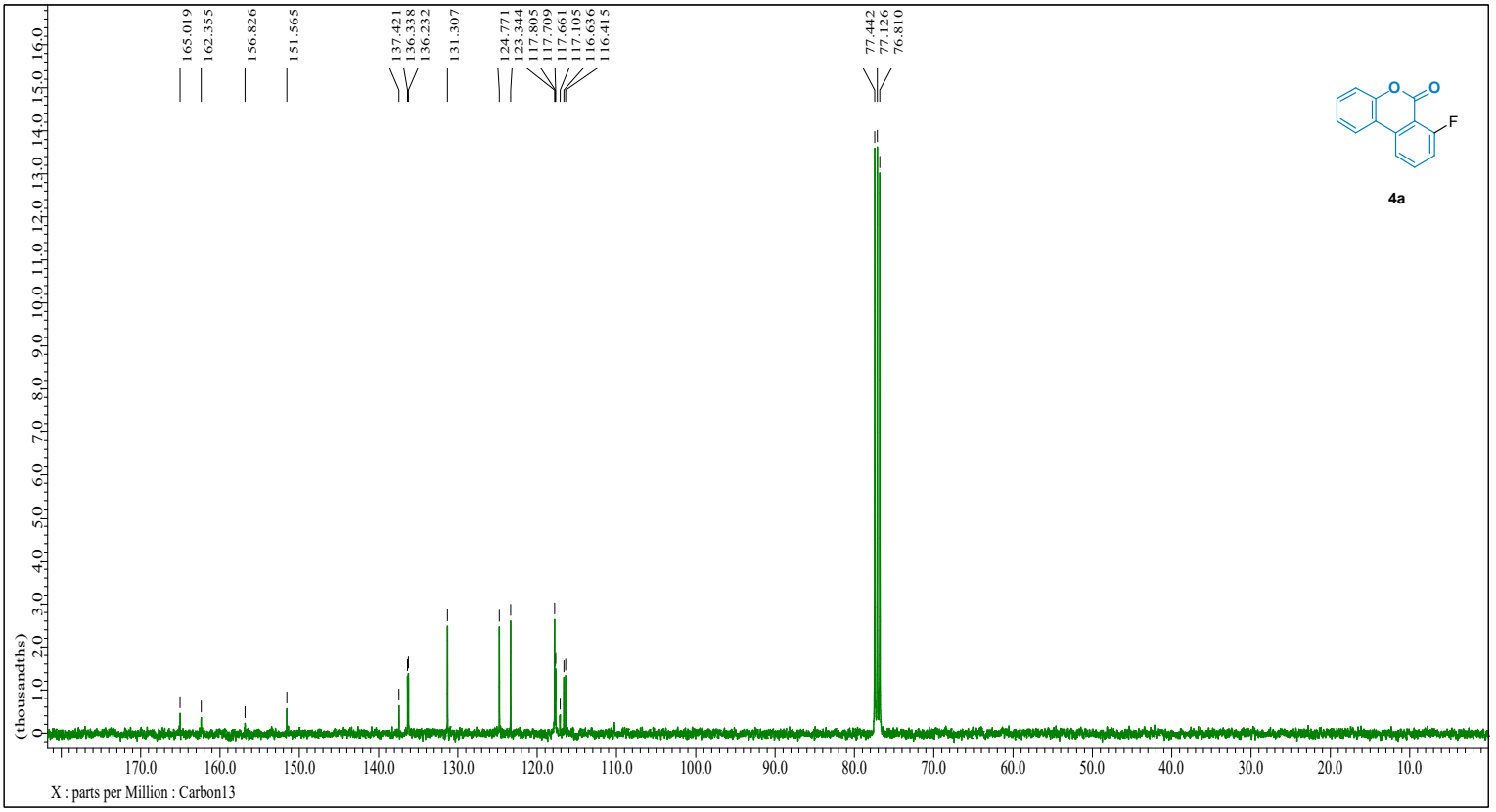
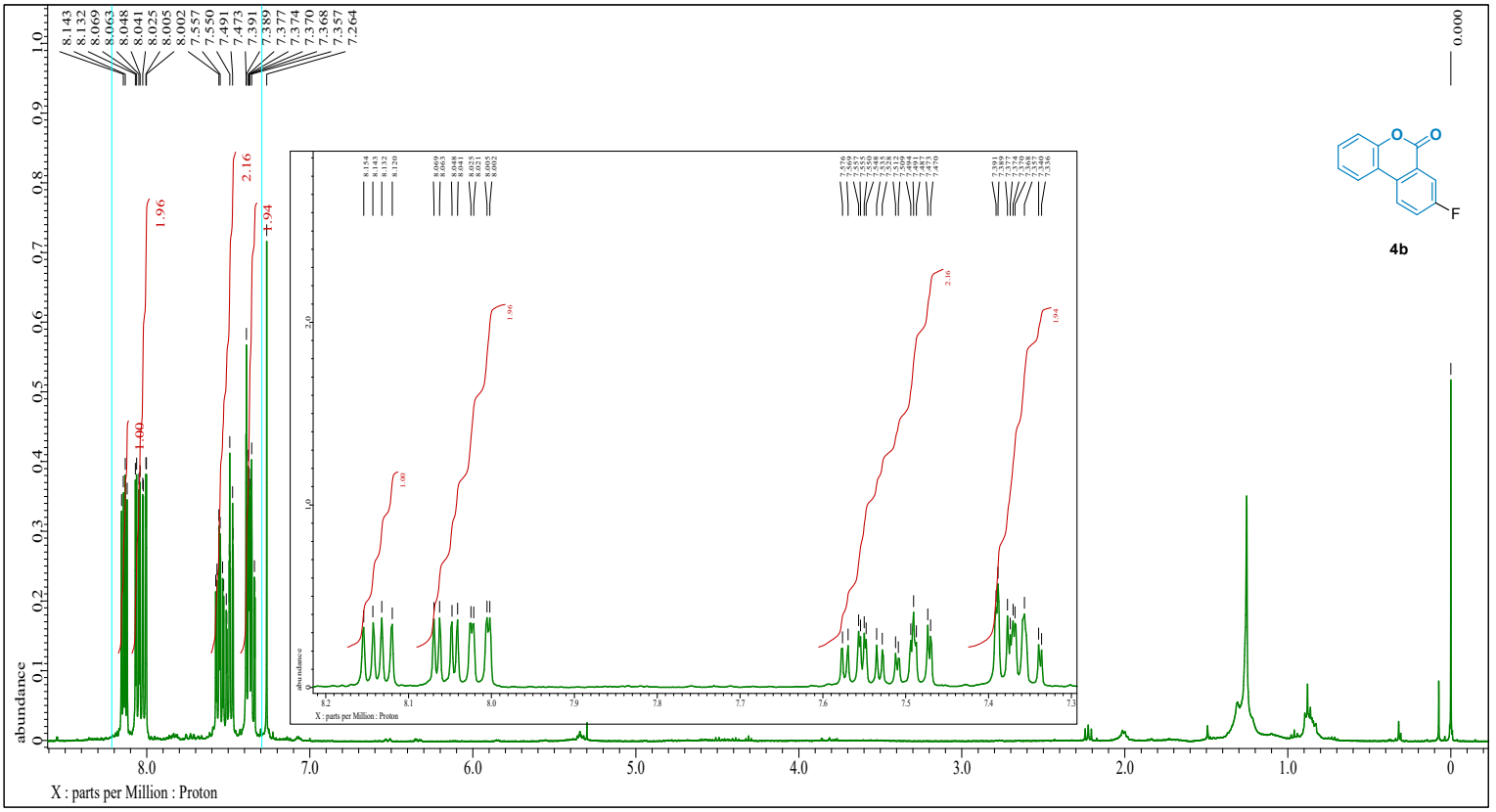
8.027
7.950
7.931
7.815
7.807
7.795
7.512
7.495
7.492
7.366
7.346
7.343
7.297
7.295
7.277
7.274
7.271
7.269
7.265
1.00
1.02
1.01
0.99
1.91
1.05
0.000
F
4a
abundance
X : parts per Million : Proton


165.019
162.355
156.826
151.565
137.421
136.338
136.232
131.307
124.771
123.344
117.805
117.709
117.661
117.105
116.636
116.415
77.442
77.126
76.810
F
4a
(thousandths)
X : parts per Million : Carbon13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8.063
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8.041
8.025
8.005
8.002
7.557
7.550
7.491
7.473
7.391
7.389
7.377
7.374
7.370
7.368
7.357
7.264
0.000
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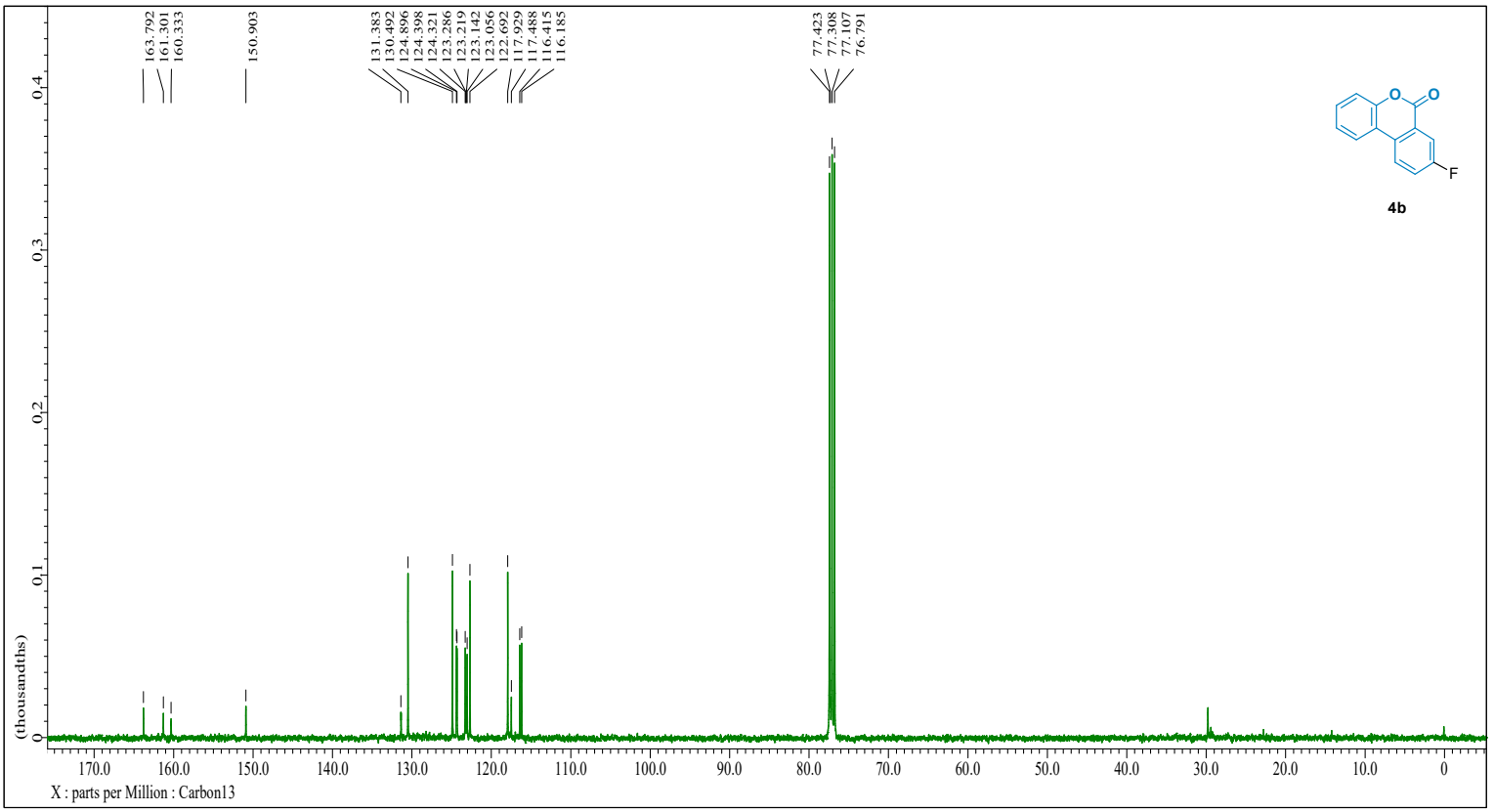
1.94
1.00
4b
abundance
X : parts per Million : Proton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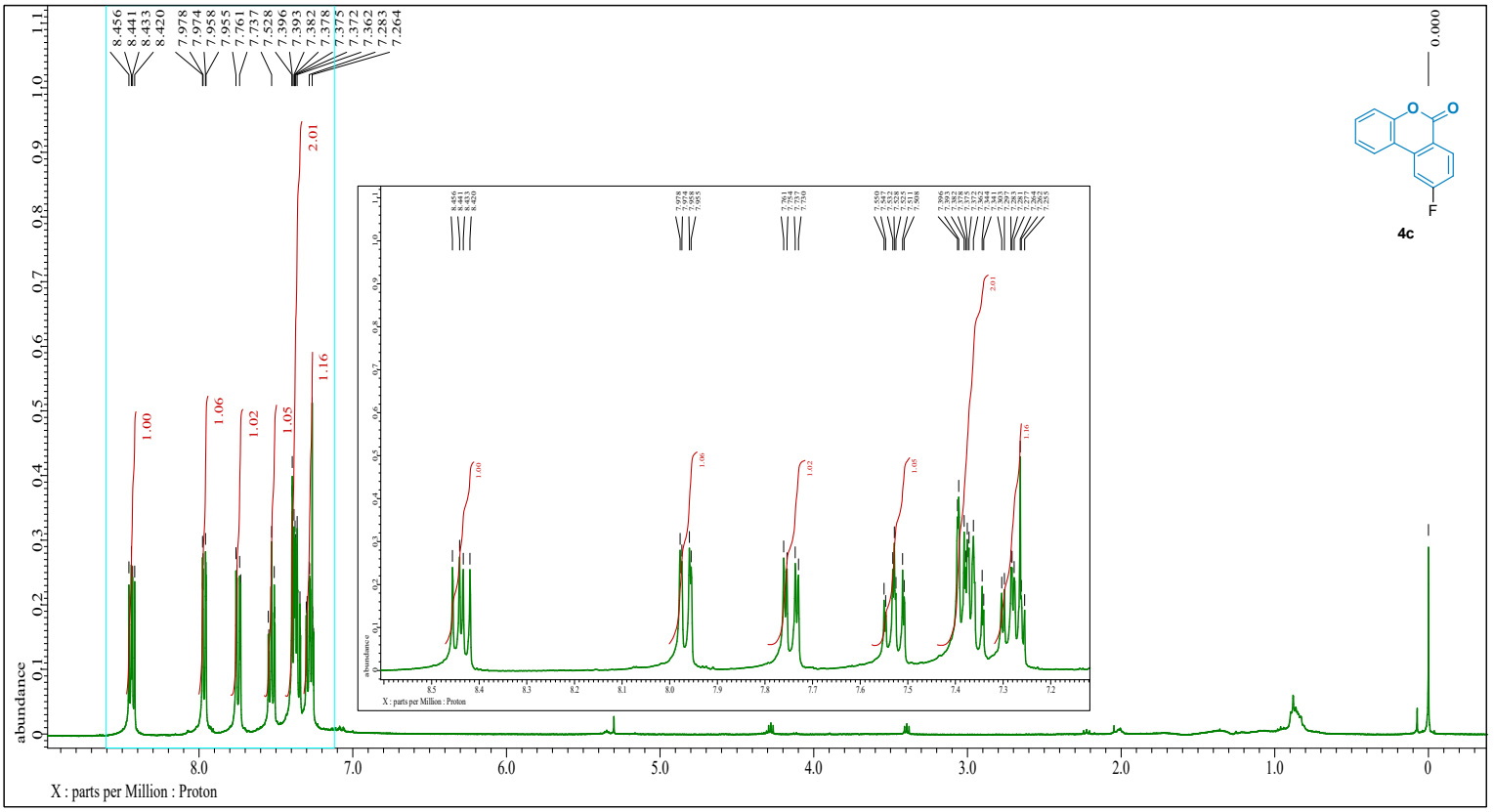
123.142
123.056
122.692
117.929
117.488
116.415
116.185
77.423
77.308
77.107
76.791
4b
(thousandths)
X : parts per Million : Carbon13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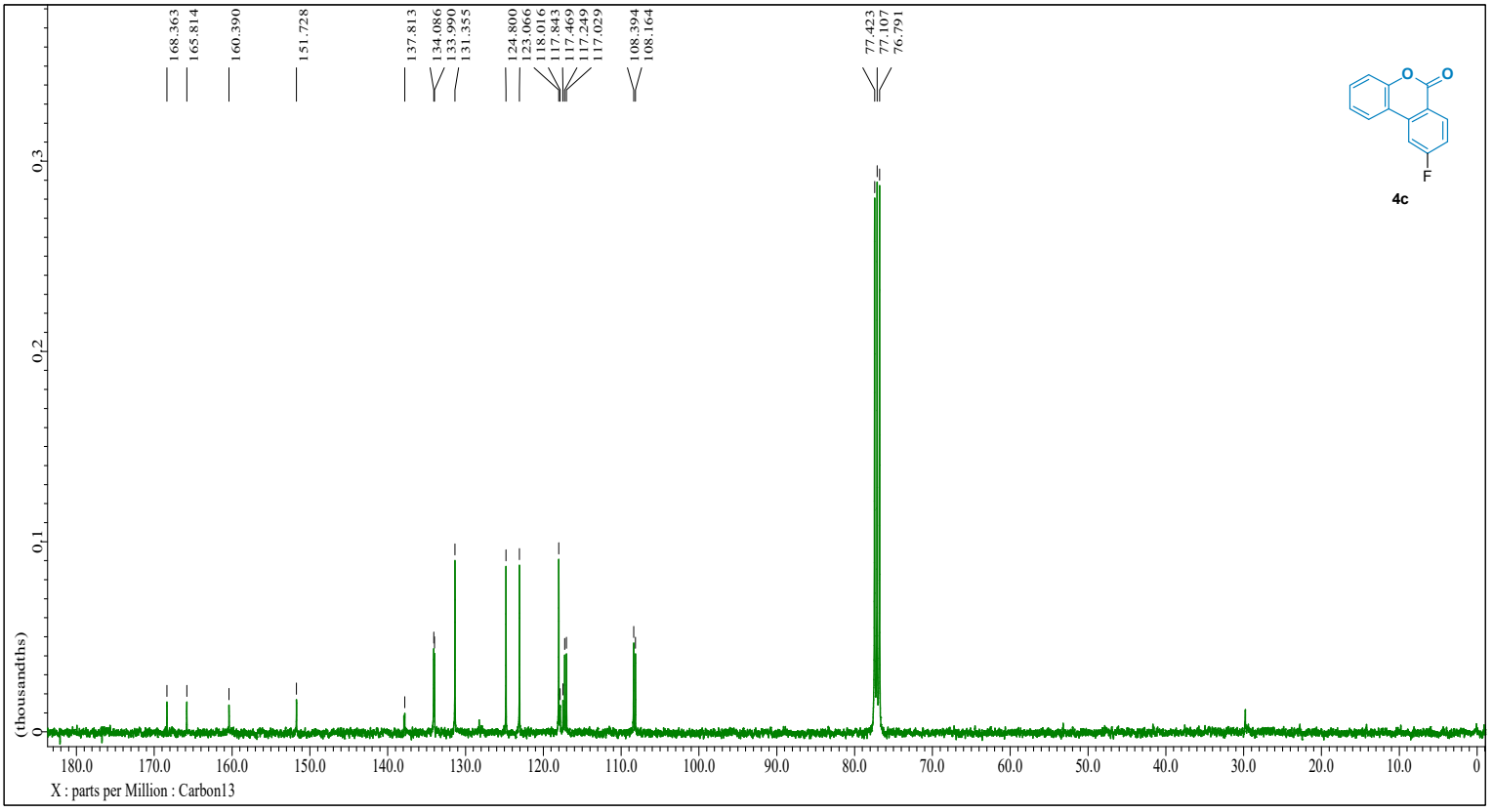
8.441
8.433
8.420
7.978
7.974
7.958
7.955
7.761
7.737
7.528
7.396
7.393
7.382
7.378
7.375
7.372
7.362
7.283
7.264
0.000
2.01
1.16
1.00
1.06
1.02
1.05
4c
abundance
X : parts per Million : Proton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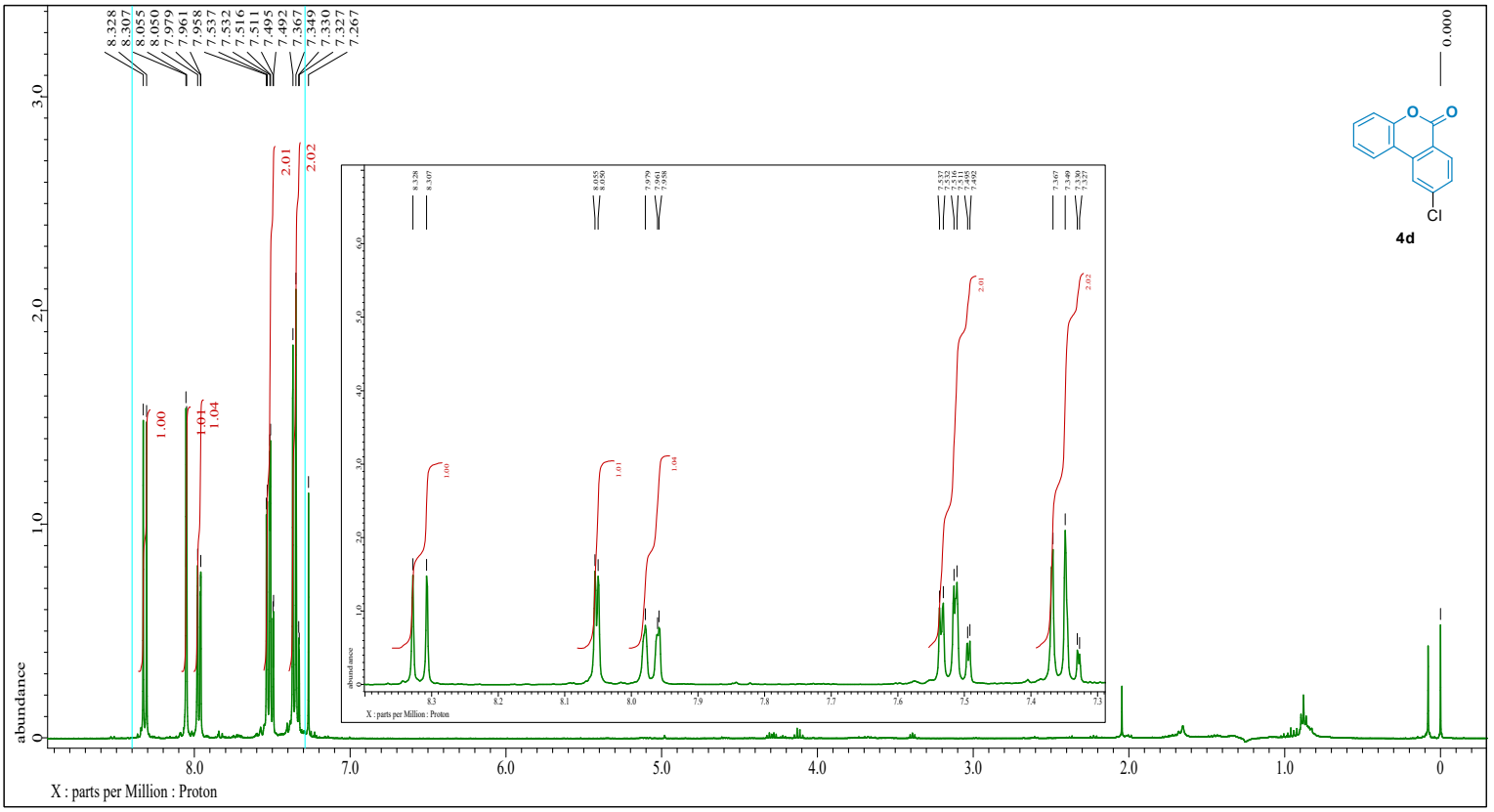
165.814
160.390
151.728
137.813
134.086
133.990
131.355
124.800
123.066
118.016
117.843
117.469
117.249
117.029
108.394
108.164
77.423
77.107
76.791
4c
(thousandths)
X : parts per Million : Carbon13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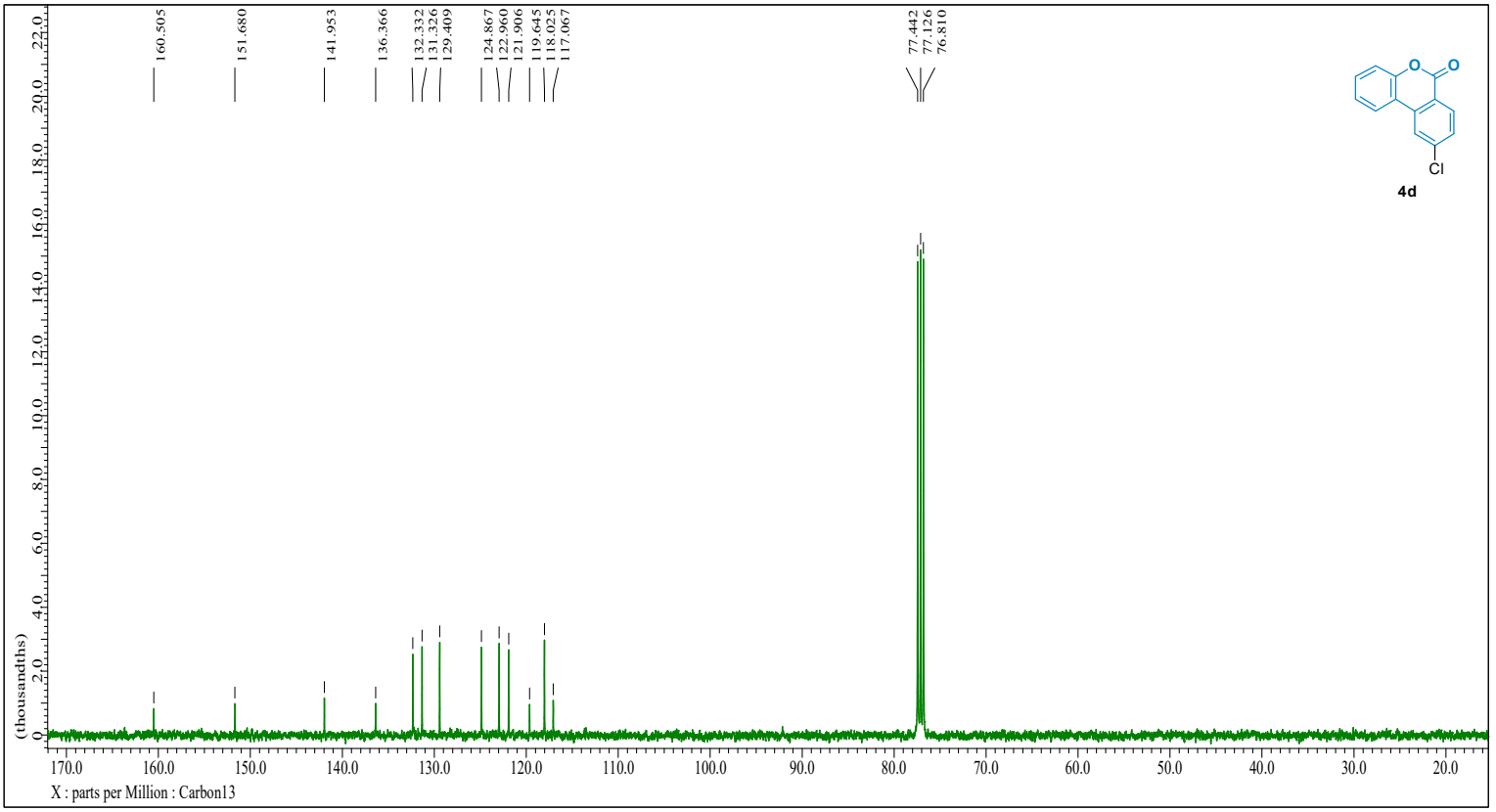
8.307
8.055
8.050
7.979
7.961
7.958
7.537
7.532
7.516
7.511
7.495
7.492
7.367
7.349
7.330
7.327
7.267
0.000
1.00
1.01
1.04
2.01
2.02
abundance
X : parts per Million : Proton
Cl
4d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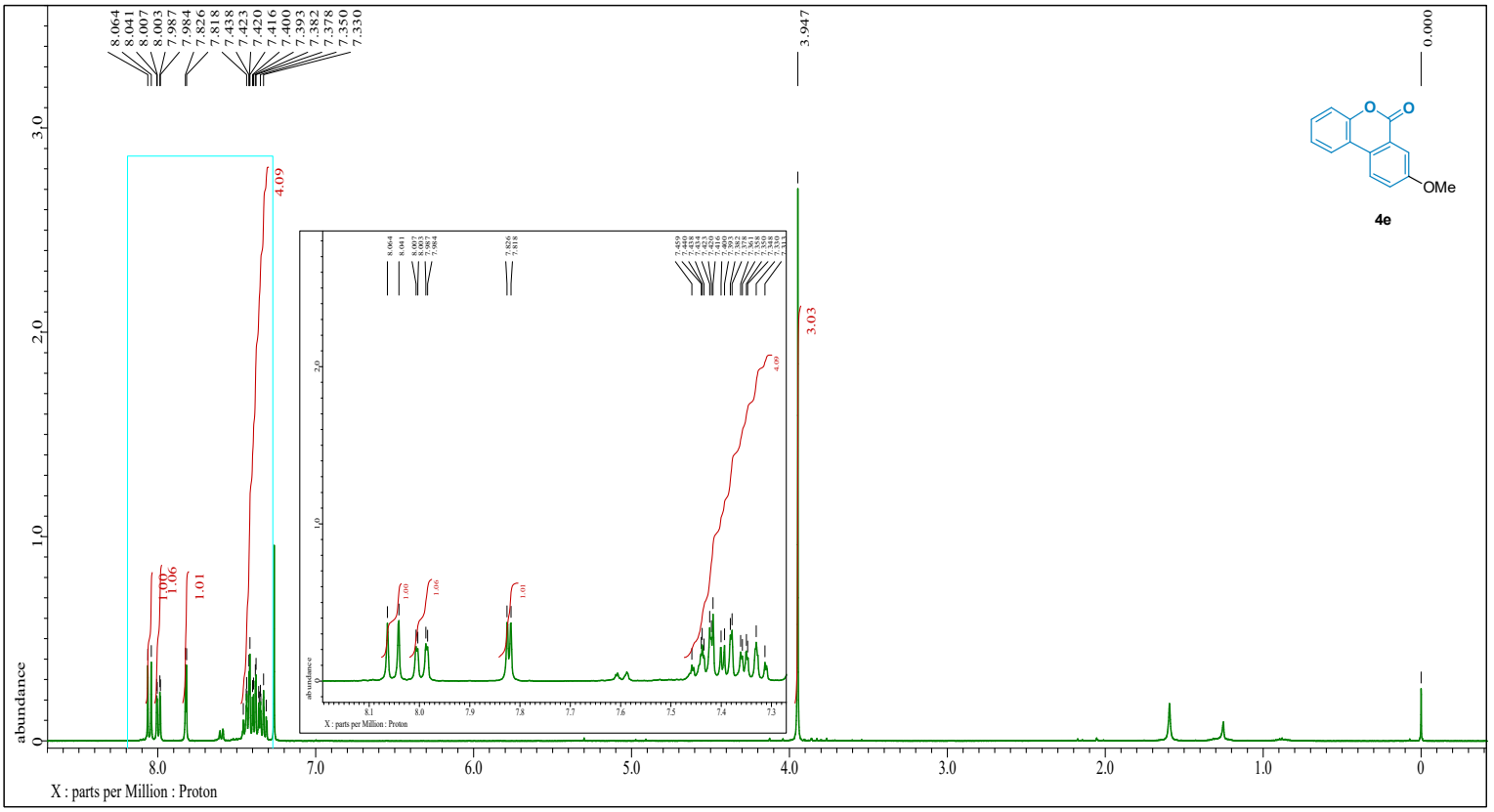
151.680
141.953
136.366
132.332
131.326
129.409
124.867
122.960
121.906
119.645
118.025
117.067
77.442
77.126
76.810
(thousandths)
X : parts per Million : Carbon13
Cl
4d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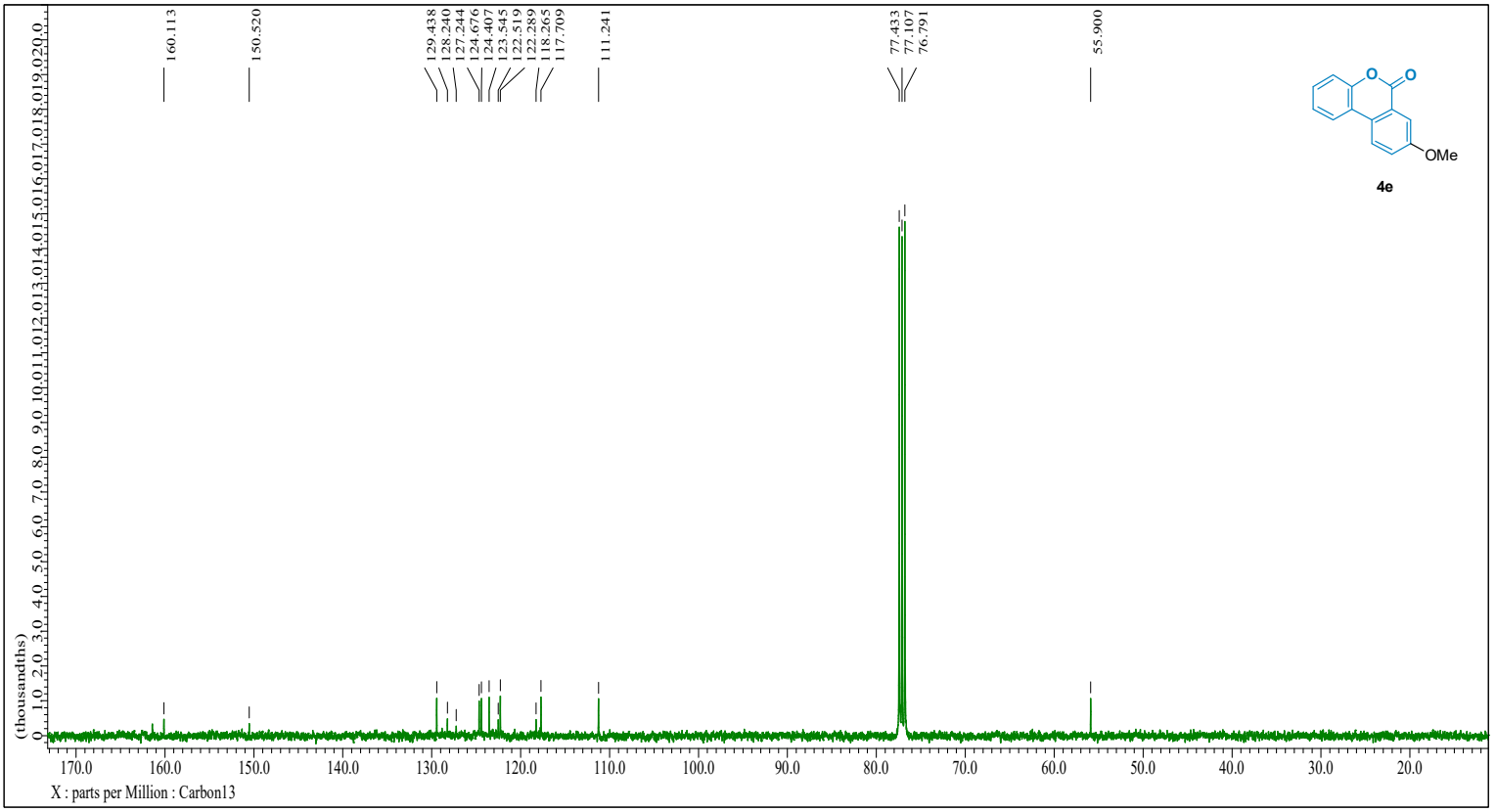
8.041
8.007
8.003
7.987
7.984
7.826
7.818
7.438
7.423
7.420
7.416
7.400
7.393
7.382
7.378
7.350
7.330
3.947
0.000
4.09
3.03
1.00
1.06
1.01
OMe
4e
abundance
X : parts per Million : Proton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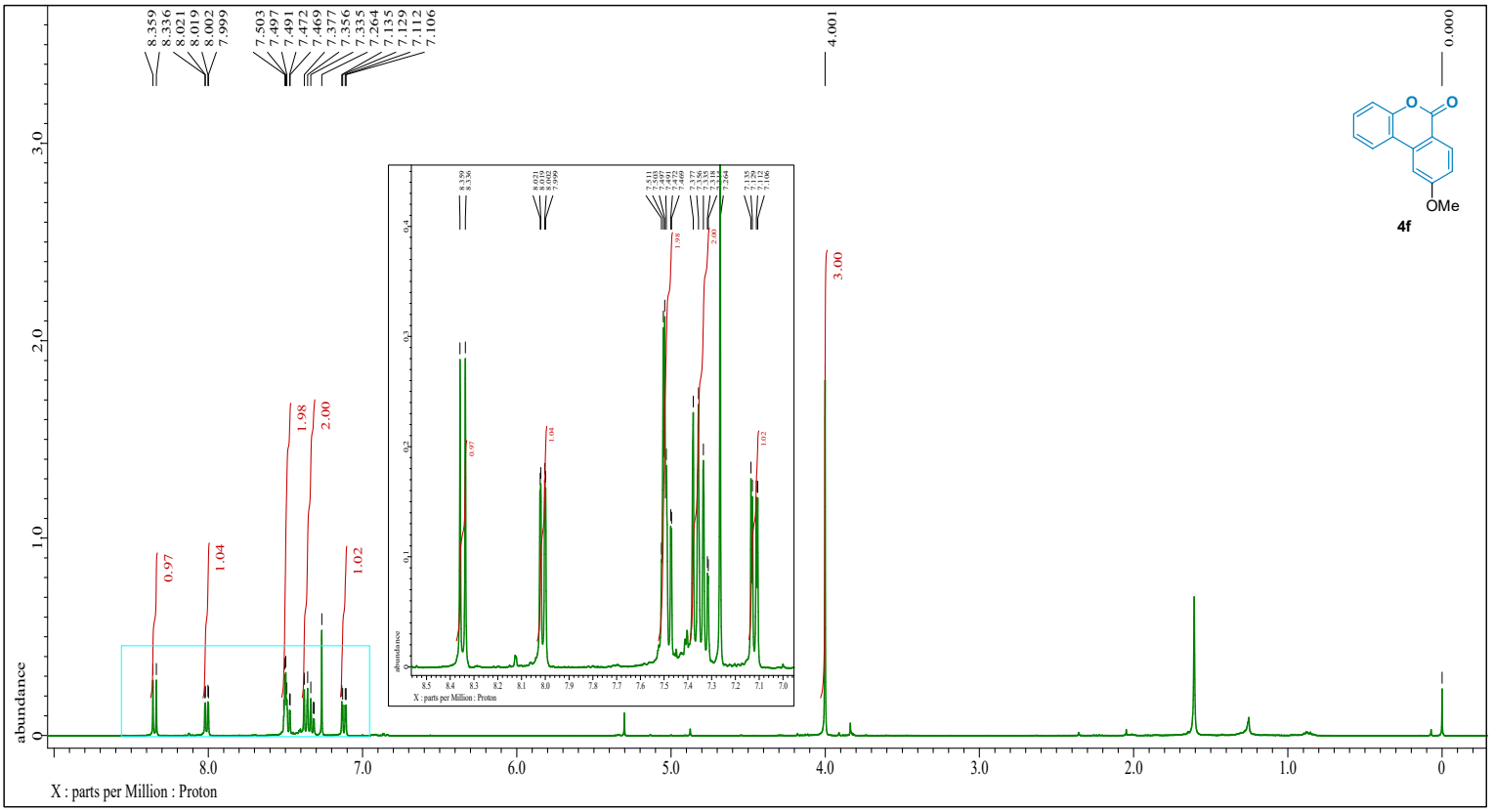
150.520
129.438
128.240
127.244
124.676
124.407
123.545
122.519
122.289
118.265
117.709
111.241
77.433
77.107
76.791
55.900
OMe
4e
(thousandths)
X : parts per Million : Carbon13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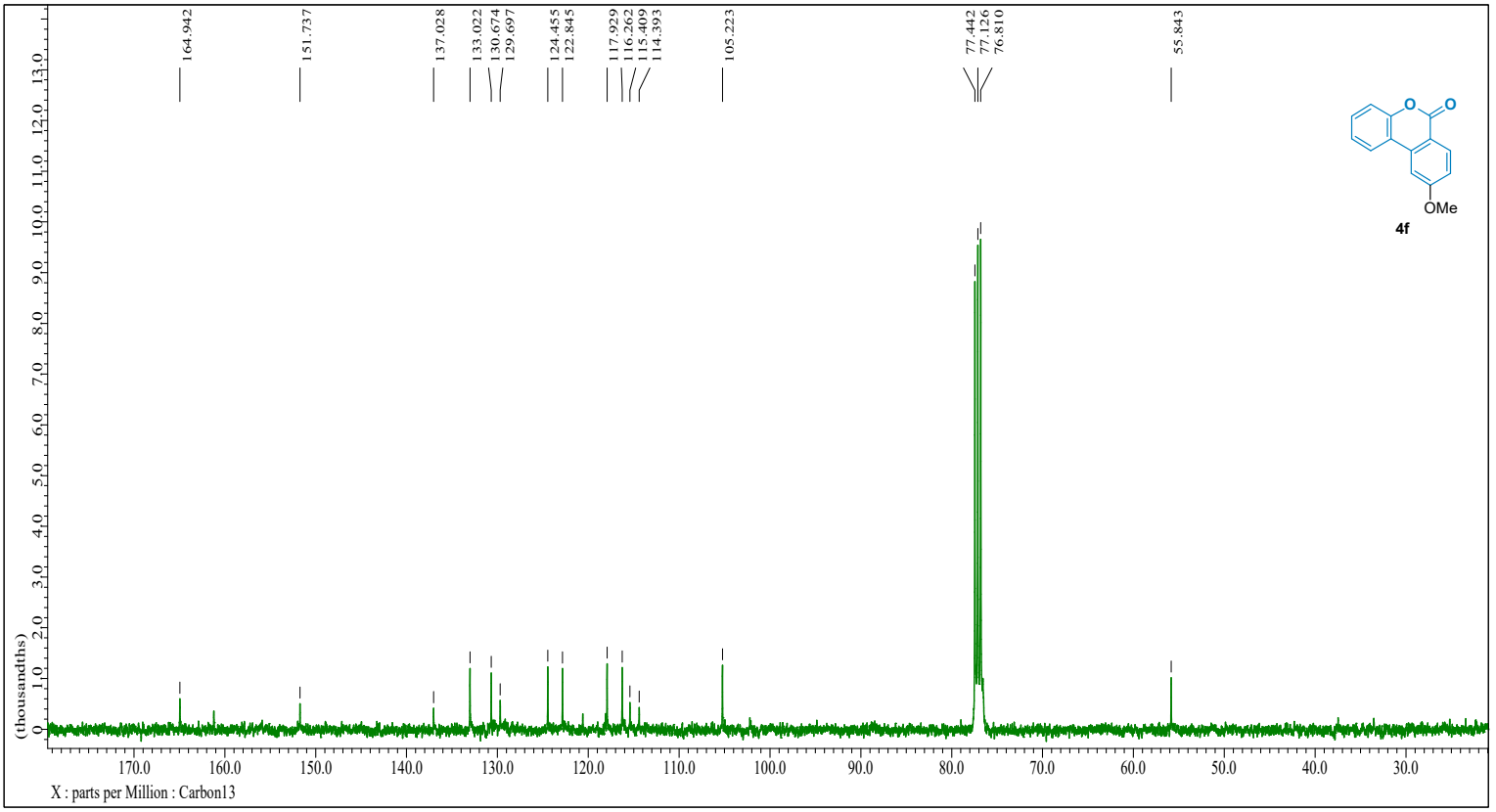
8.336
8.021
8.019
8.002
7.999
7.503
7.497
7.491
7.472
7.469
7.377
7.356
7.335
7.264
7.135
7.129
7.112
7.106
4.001
0.000
3.00
1.98
2.00
0.97
1.04
1.02
OMe
4f
abundance
X : parts per Million : Proton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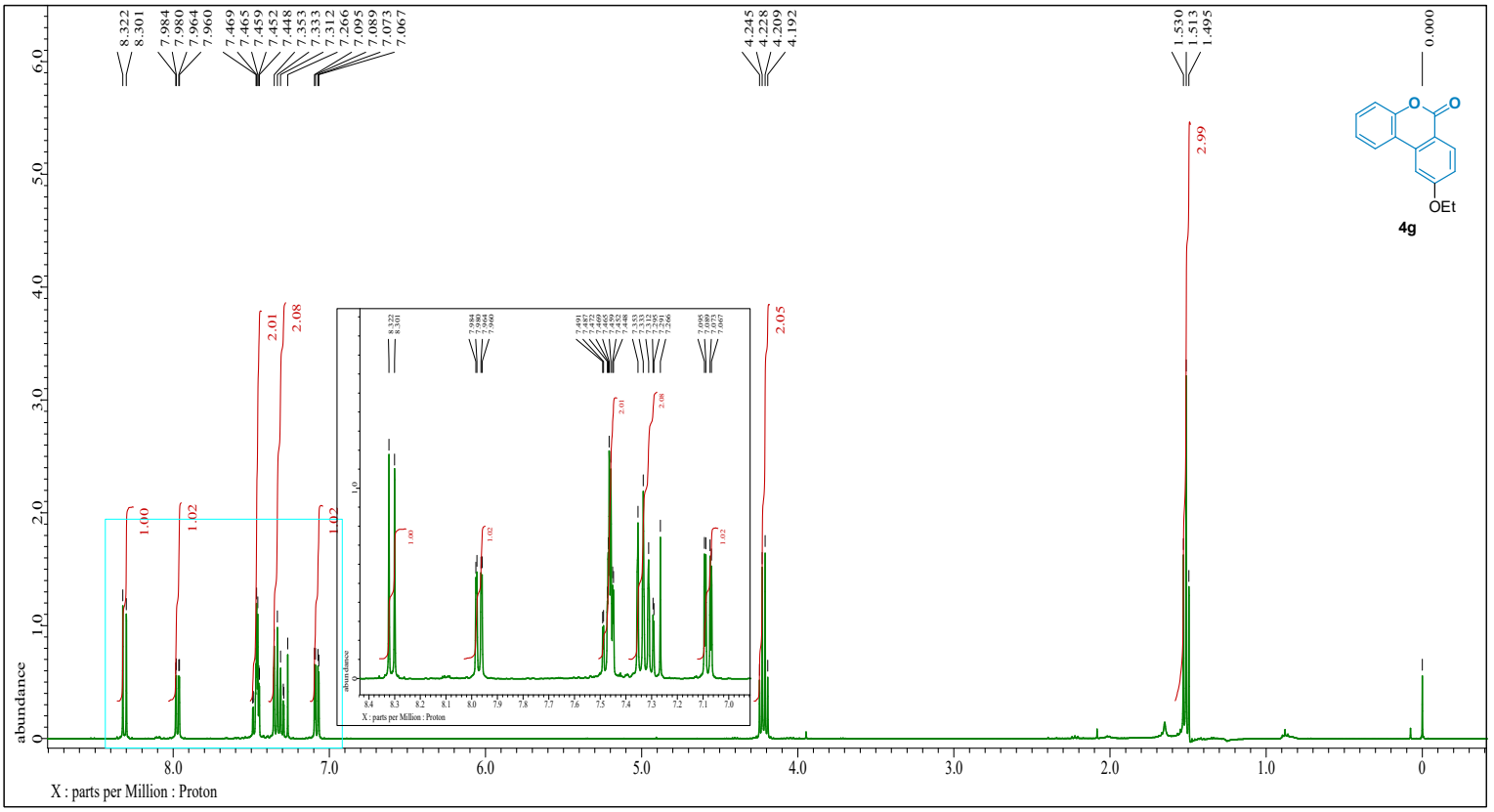
151.737
137.028
133.022
130.674
129.697
124.455
122.845
117.929
116.262
115.409
114.393
105.223
77.442
77.126
76.810
55.843
OMe
4f
(thousandths)
X : parts per Million : Carbon13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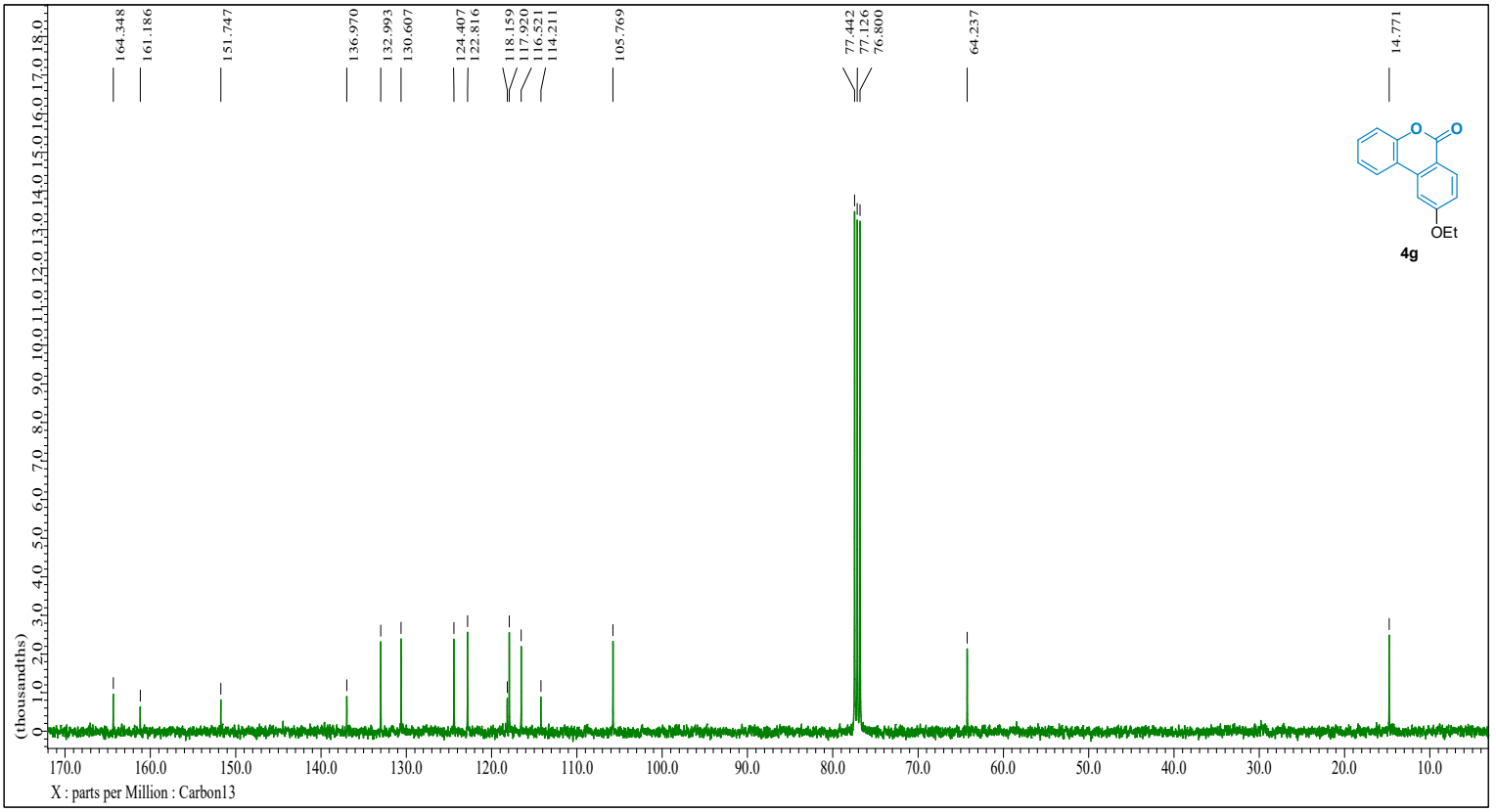
8.301
7.984
7.980
7.964
7.960
7.469
7.465
7.459
7.452
7.448
7.353
7.333
7.312
7.266
7.095
7.089
7.073
7.067
4.245
4.228
4.209
4.192
1.530
1.513
1.495
0.000
2.99
2.01
2.08
2.05
1.00
1.02
1.02
OEt
4g
abundance
X : parts per Million : Proton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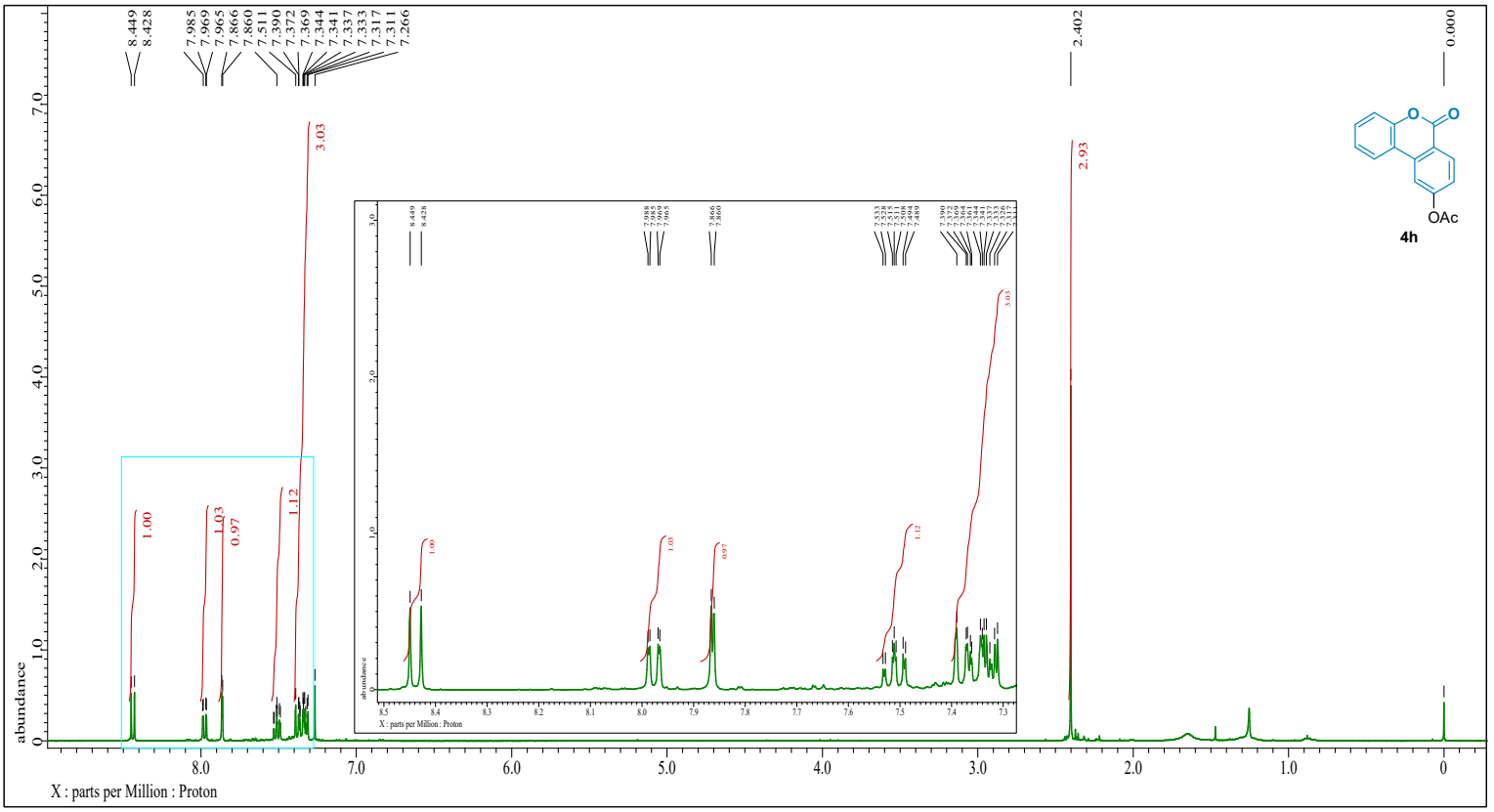
151.747
136.970
132.993
130.607
124.407
122.816
118.159
117.920
116.521
114.211
105.769
77.442
77.126
76.800
64.237
14.771
OEt
4g
(thousandths)
X : parts per Million : Carbon13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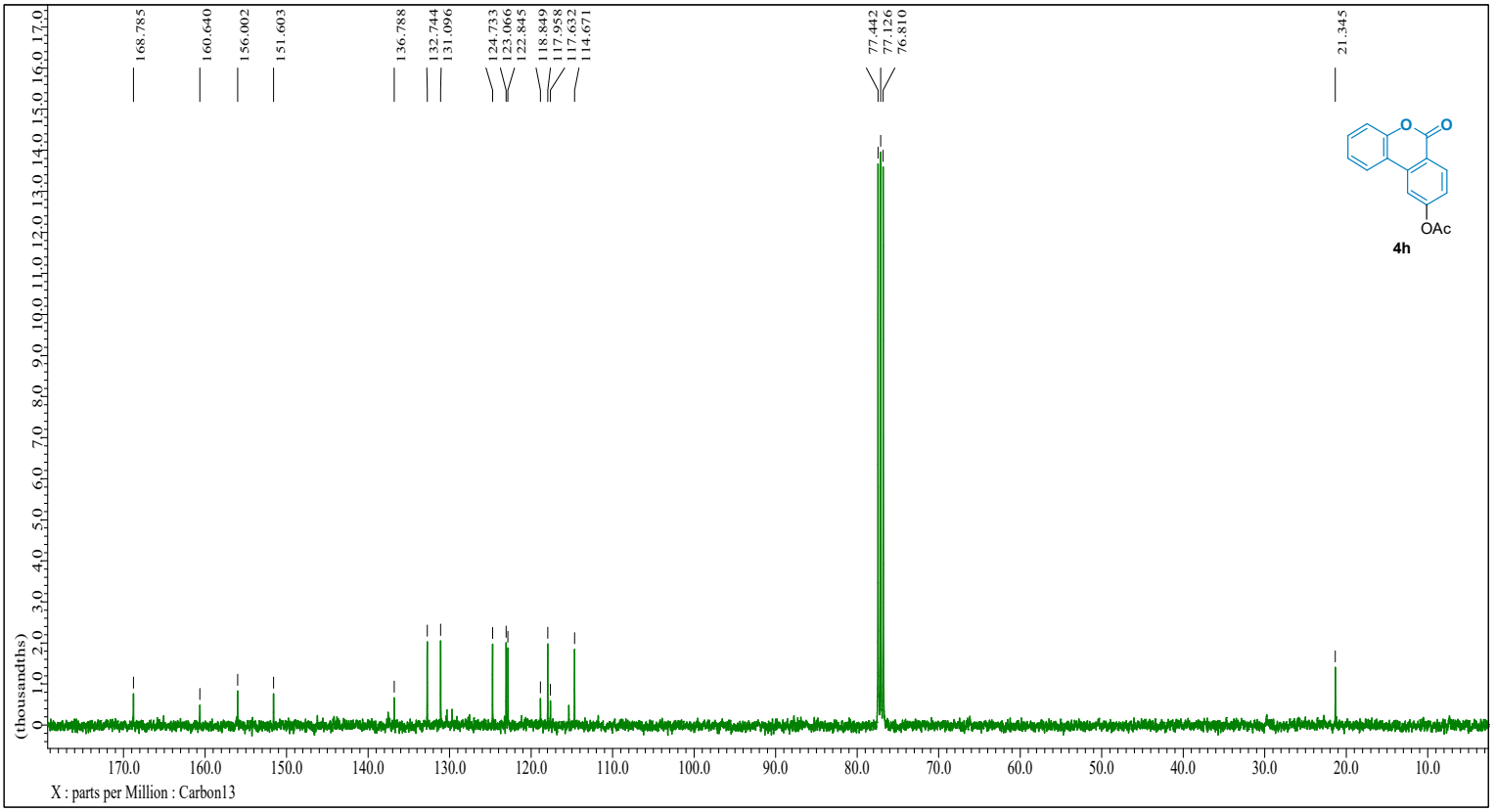
8.428
7.985
7.969
7.965
7.866
7.860
7.511
7.390
7.372
7.369
7.344
7.341
7.337
7.333
7.317
7.311
7.266
2.402
0.000
3.03
2.93
1.00
1.03
0.97
1.12
4h
OAc
abundance
X : parts per Million : Proton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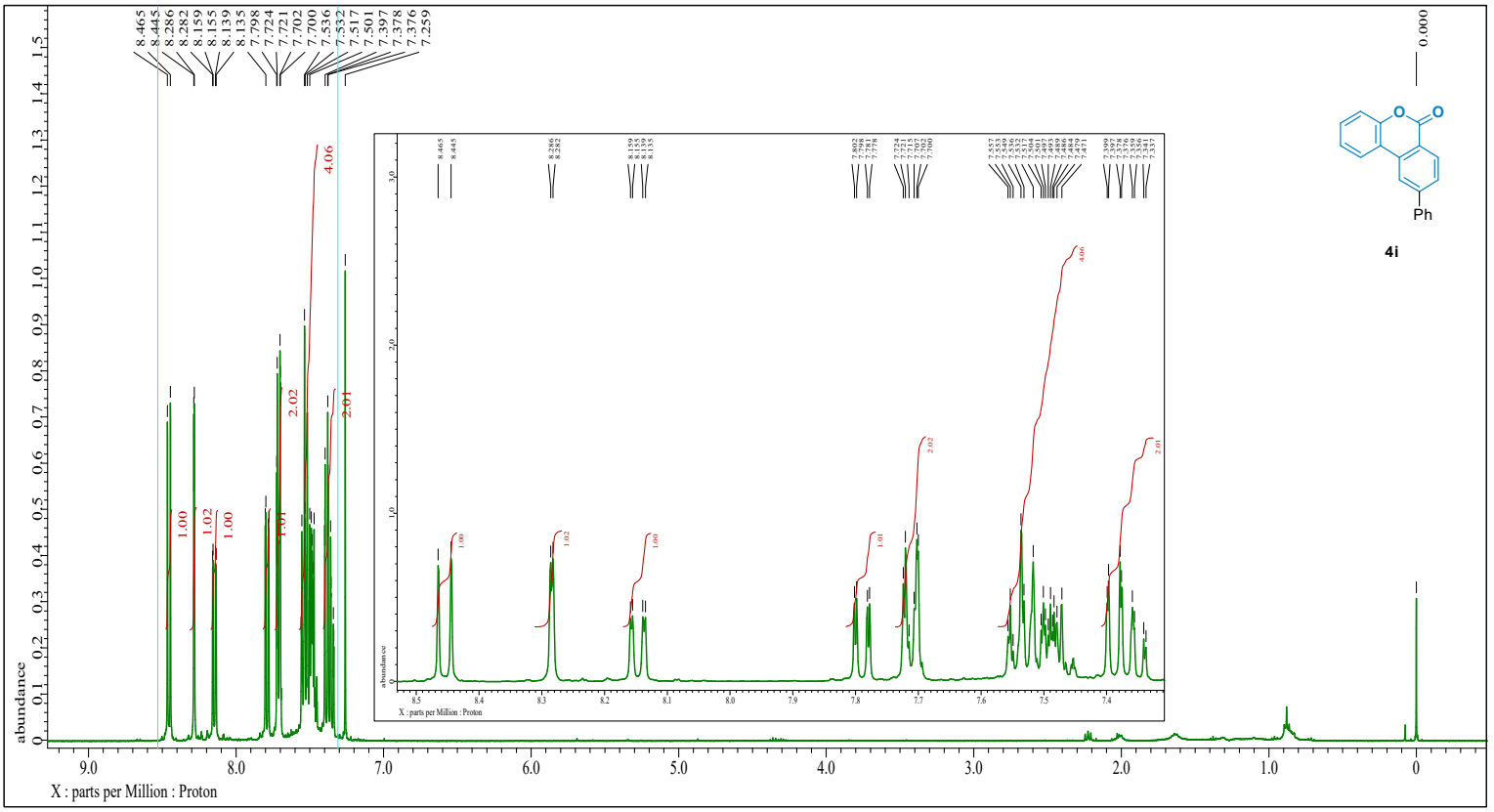
151.603
136.788
132.744
131.096
124.733
123.066
122.845
118.849
117.958
117.632
114.671
77.442
77.126
76.810
21.345
4h
OAc
(thousandths)
X : parts per Million : Carbon13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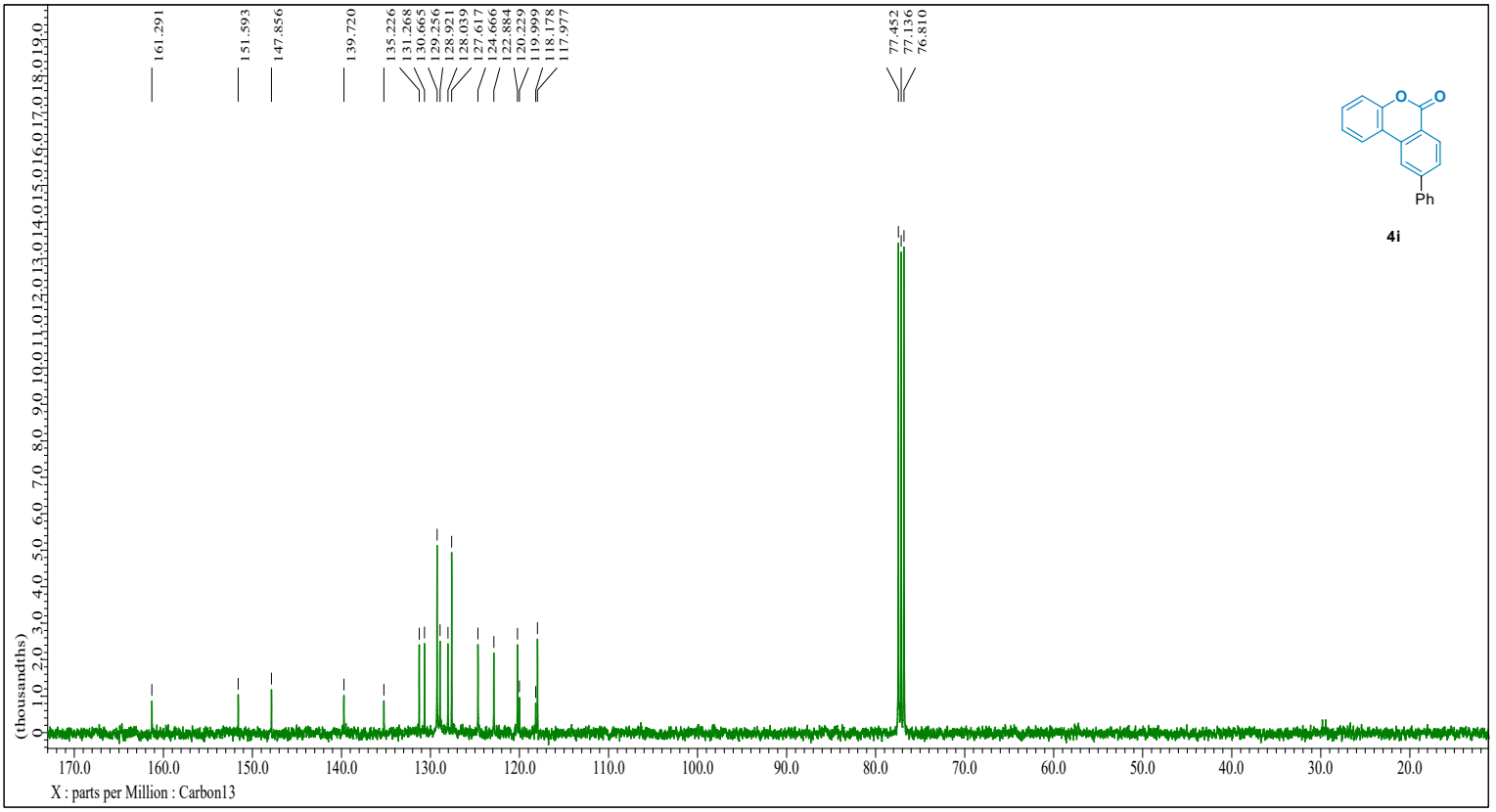
8.445
8.286
8.282
8.159
8.155
8.139
8.135
7.798
7.724
7.721
7.702
7.700
7.536
7.532
7.517
7.501
7.397
7.378
7.376
7.259
0.000
4.06
2.02
2.01
1.00
1.02
1.00
1.01
abundance
X : parts per Million : Proton
Ph
4i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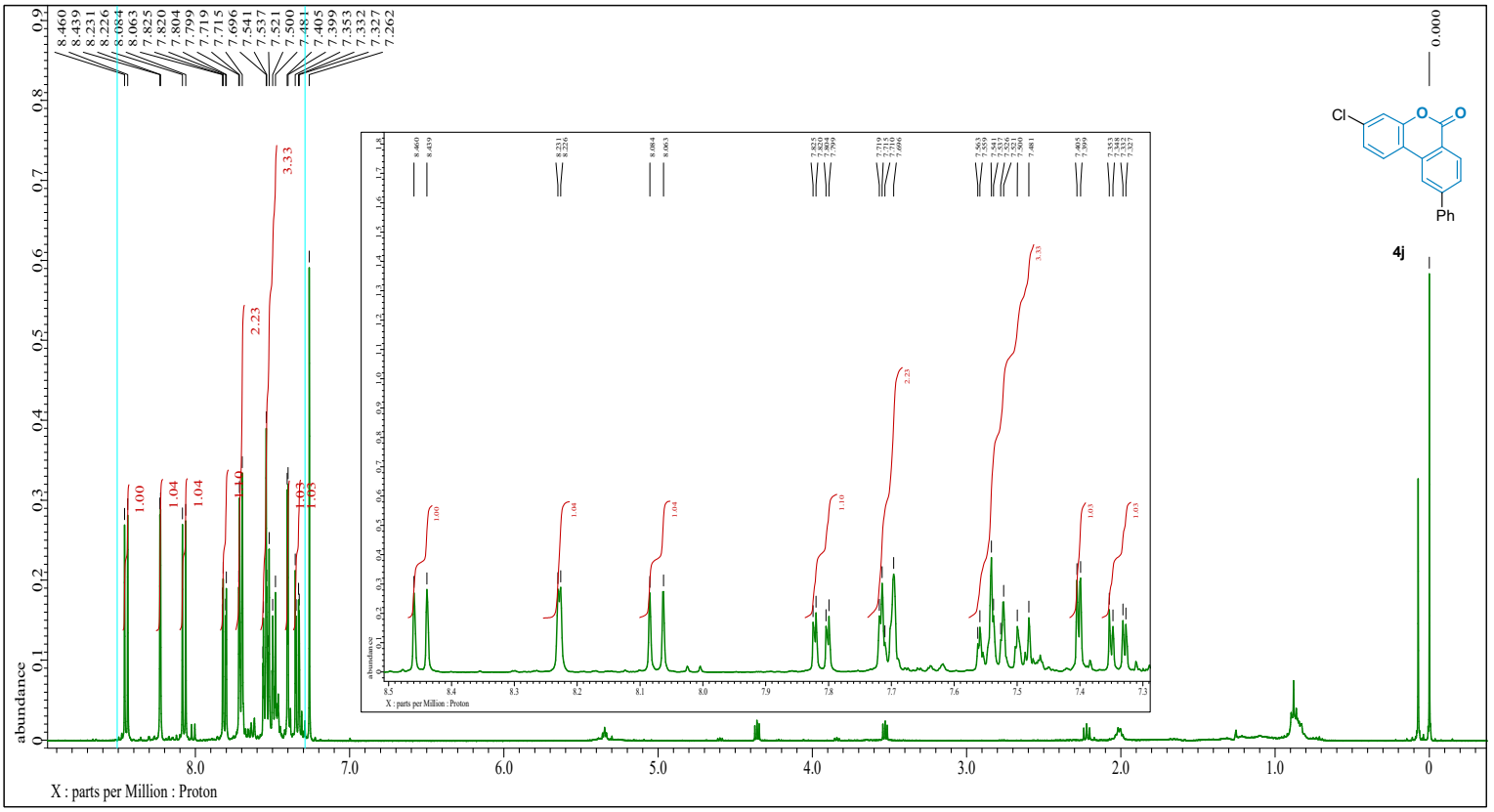
151.593
147.856
139.720
135.226
131.268
130.665
129.256
128.921
128.039
127.617
124.666
122.884
120.229
119.999
118.178
117.977
77.452
77.136
76.810
(thousandths)
X : parts per Million : Carbon13
Ph
4i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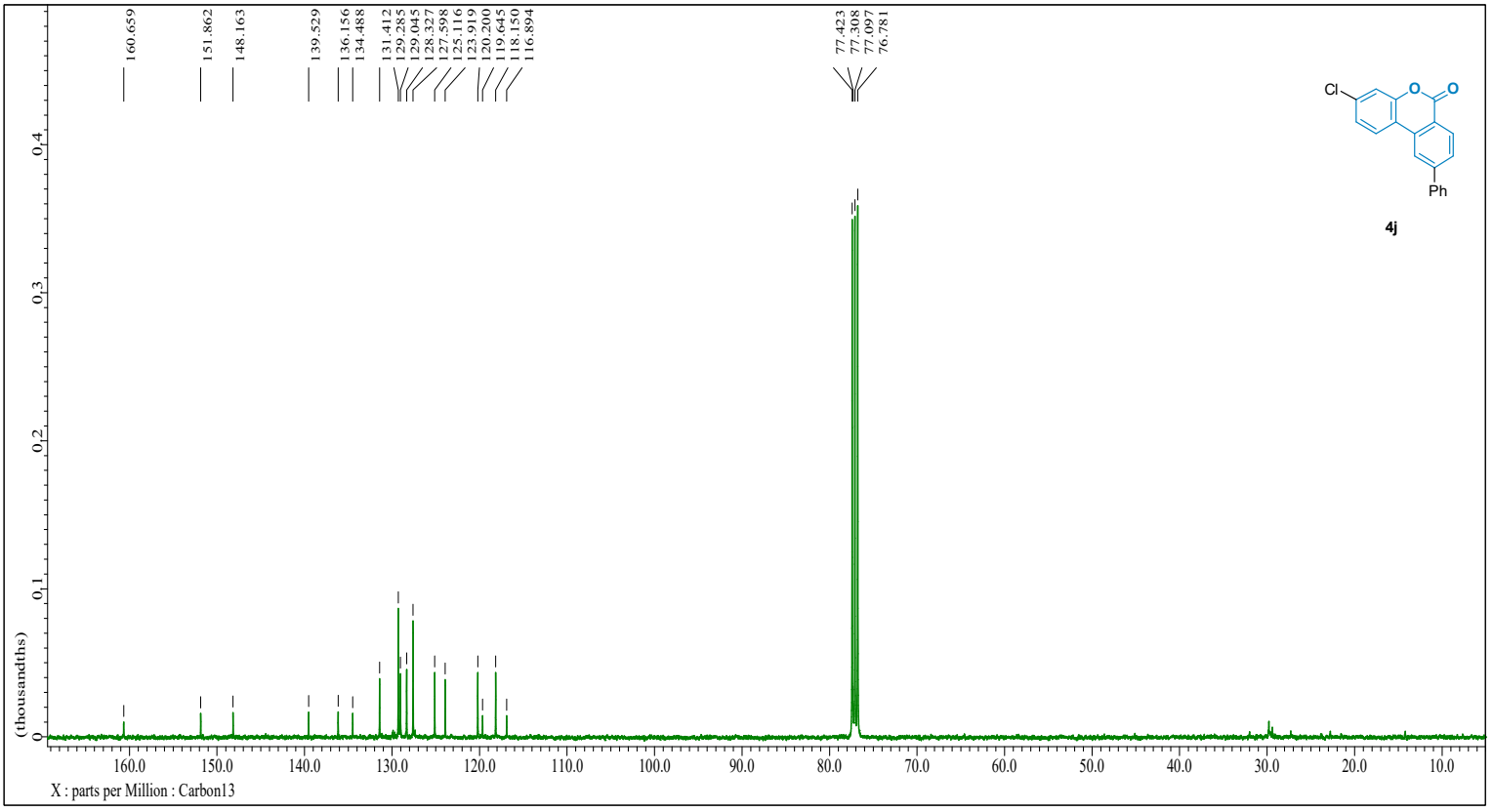
8.439
8.231
8.226
8.084
8.063
7.825
7.820
7.804
7.799
7.719
7.715
7.696
7.541
7.537
7.521
7.500
7.481
7.405
7.399
7.353
7.332
7.327
7.262
0.000
1.00
1.04
1.04
1.10
2.23
3.33
1.03
1.03
Cl
O
O
Ph
4j
abundance
X : parts per Million : Proton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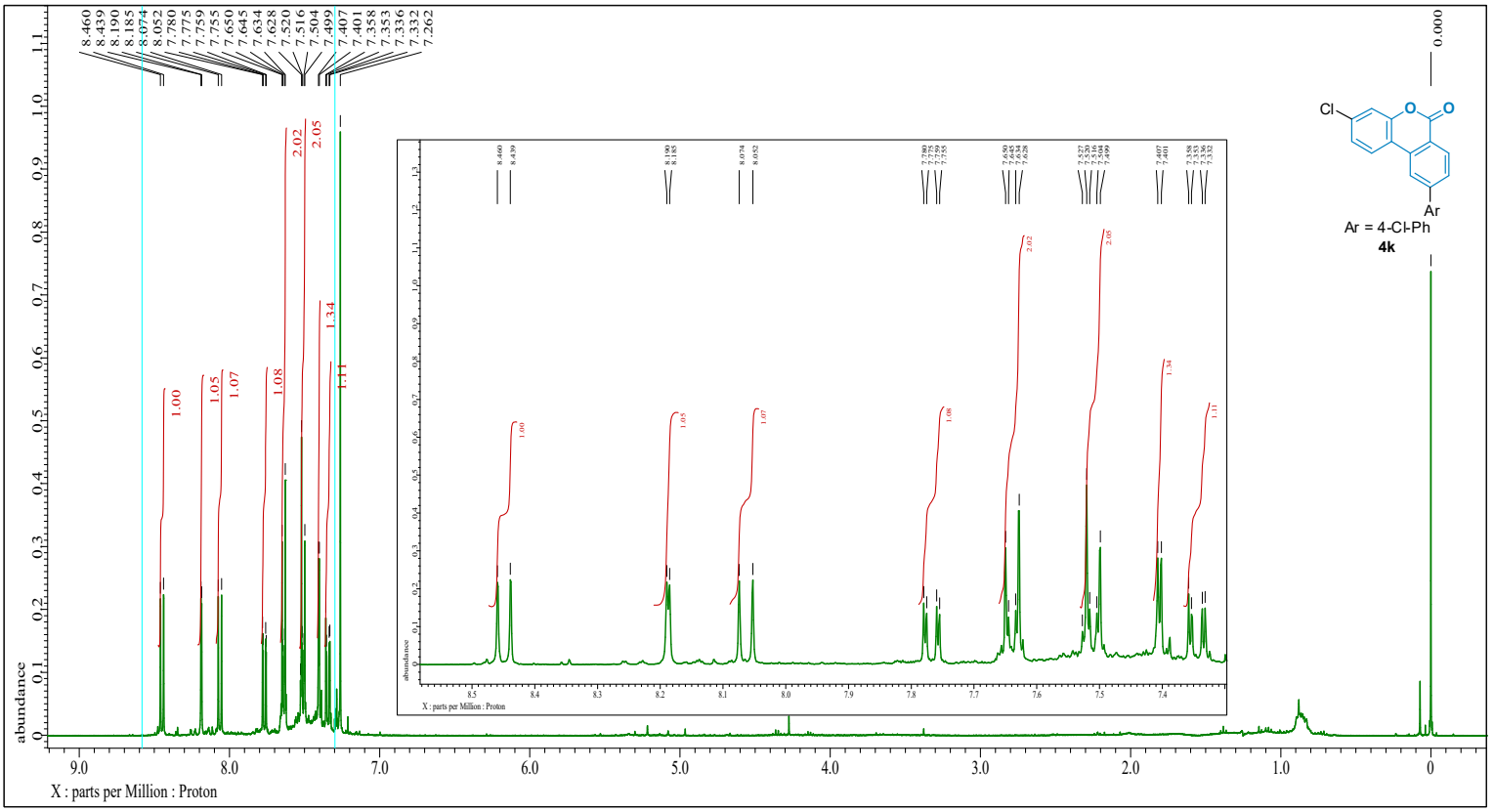
151.862
148.163
139.529
136.156
134.488
131.412
129.285
129.045
128.327
127.598
125.116
123.919
120.200
119.645
118.150
116.894
77.423
77.308
77.097
76.781
Cl
O
O
Ph
4j
(thousandths)
X : parts per Million : Carbon13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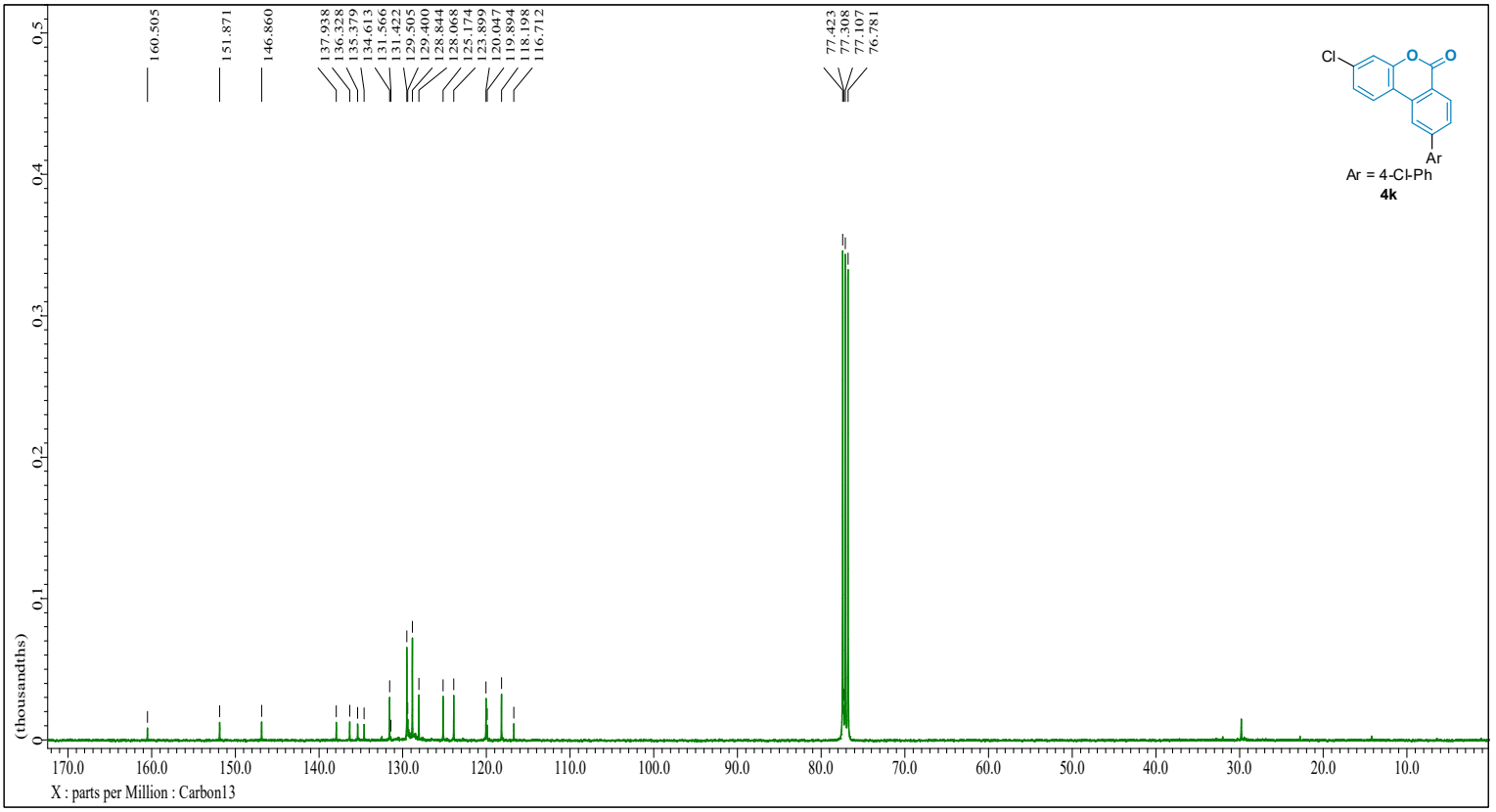
8.439
8.190
8.185
8.074
8.052
7.780
7.775
7.759
7.755
7.650
7.645
7.634
7.628
7.520
7.516
7.504
7.499
7.407
7.401
7.358
7.353
7.336
7.332
7.262
0.000
1.00
1.05
1.07
1.08
2.02
2.05
1.34
1.11
abundance
X : parts per Million : Proton
Cl
O
O
Ar
Ar = 4-Cl-Ph
4k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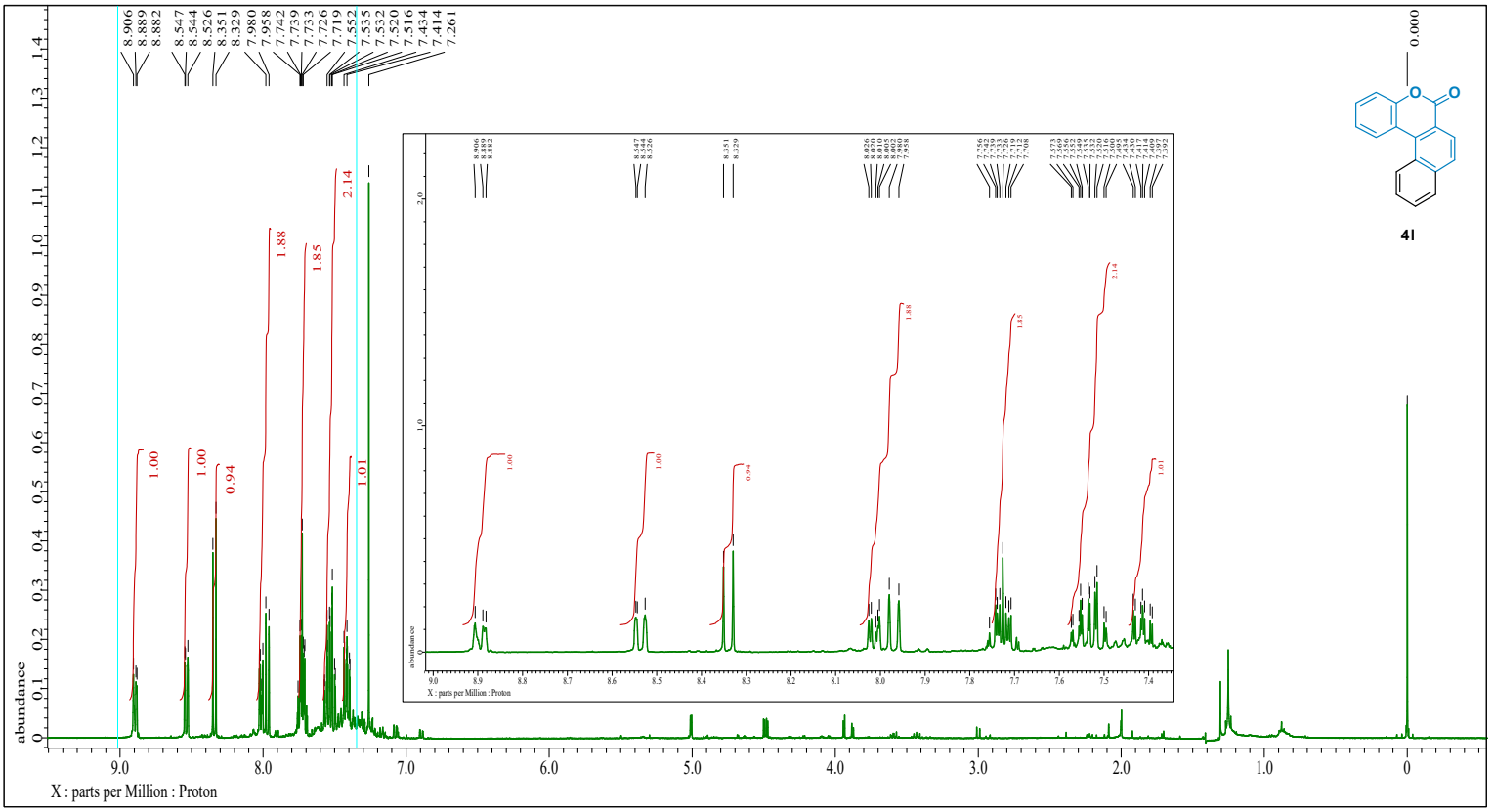
146.860
137.938
136.328
135.379
134.613
131.566
131.422
129.505
129.400
128.844
128.068
125.174
123.899
120.047
119.894
118.198
116.712
77.423
77.308
77.107
76.781
(thousandths)
X : parts per Million : Carbon13
Cl
O
O
Ar
Ar = 4-Cl-Ph
4k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8.882
8.547
8.544
8.526
8.351
8.329
7.980
7.958
7.742
7.739
7.733
7.726
7.719
7.552
7.535
7.532
7.520
7.516
7.434
7.414
7.261
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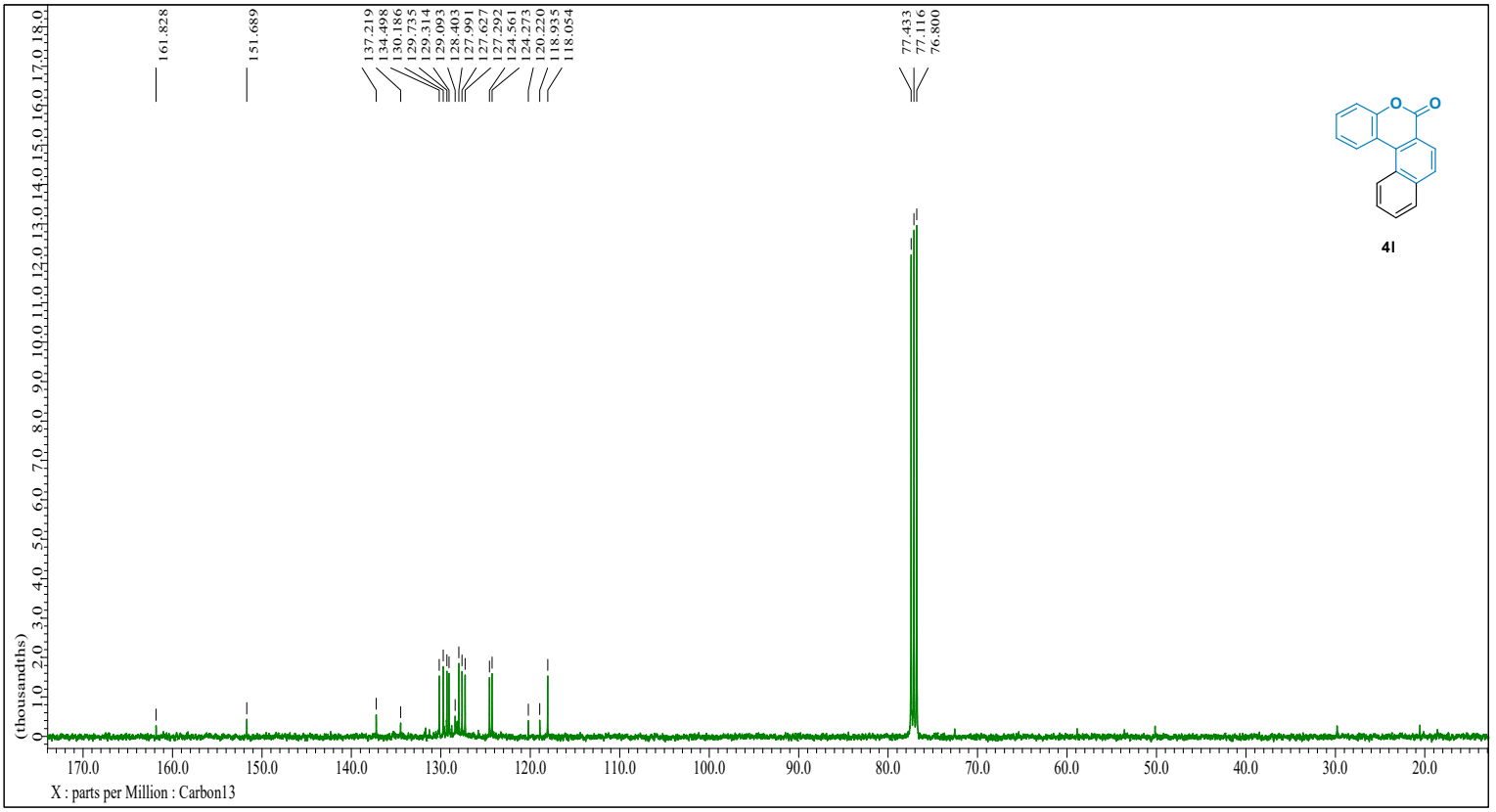
1.00
0.94
1.88
1.85
2.14
1.01
abundance
X : parts per Million : Proton
4l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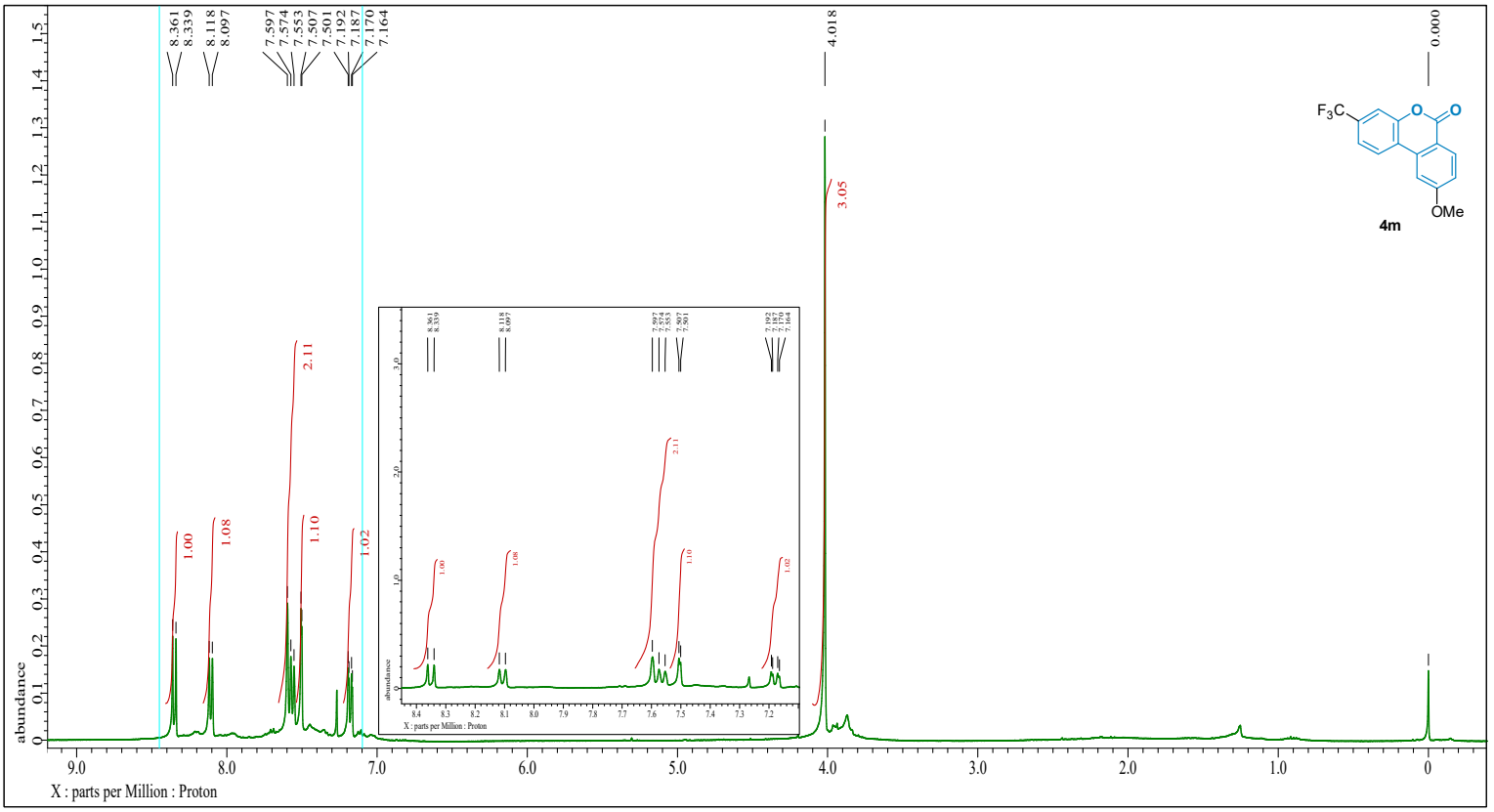
129.735
129.314
129.093
128.403
127.991
127.627
127.292
124.561
124.273
120.220
118.935
118.054
77.433
77.116
76.800
(thousandths)
X : parts per Million : Carbon13
4l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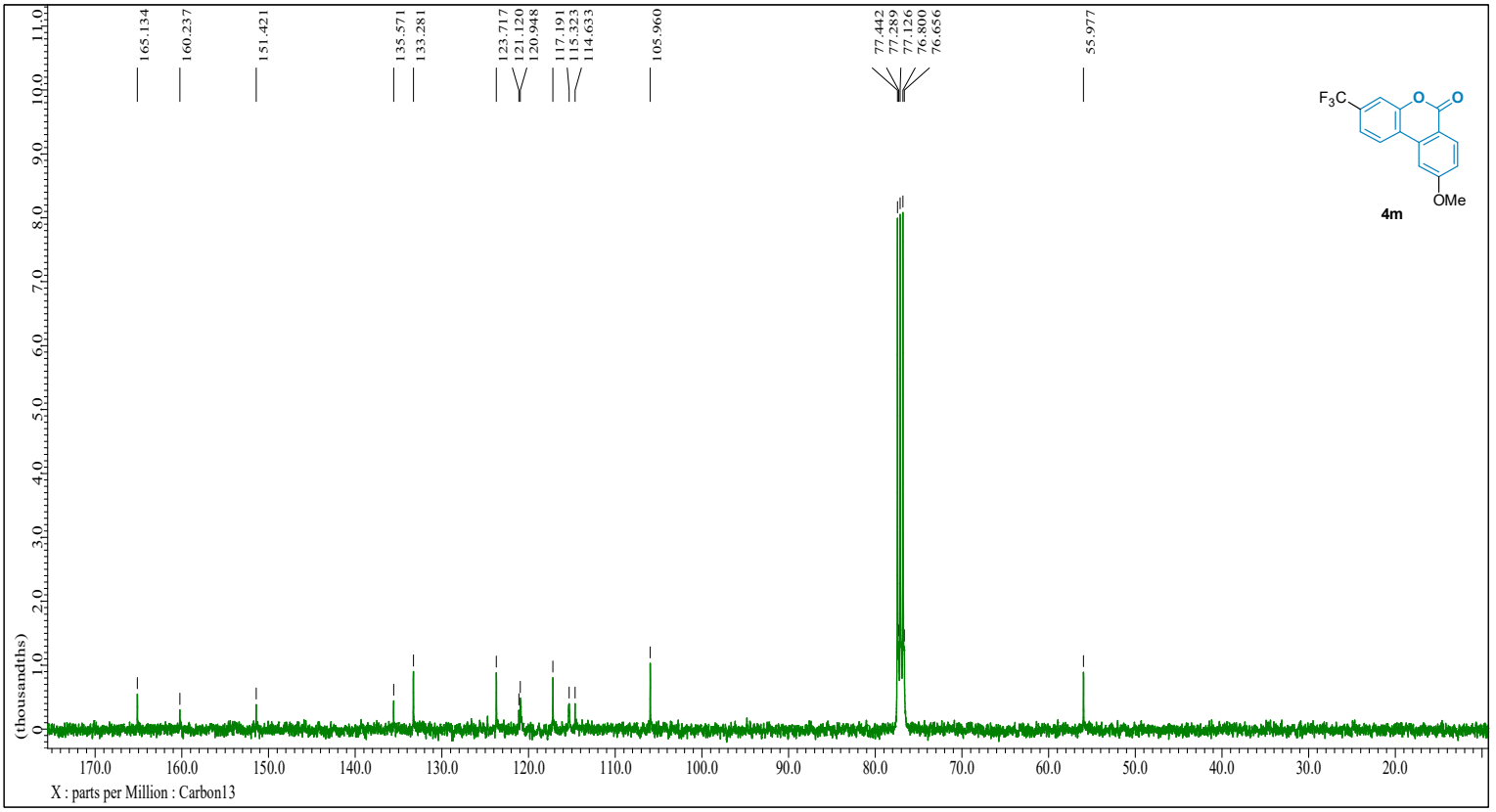
8.339
8.118
8.097
7.597
7.574
7.553
7.507
7.501
7.192
7.187
7.170
7.164
4.018
0.000
3.05
2.11
1.00
1.08
1.10
1.02
abundance
X : parts per Million : Proton
F3C
O
O
OMe
4m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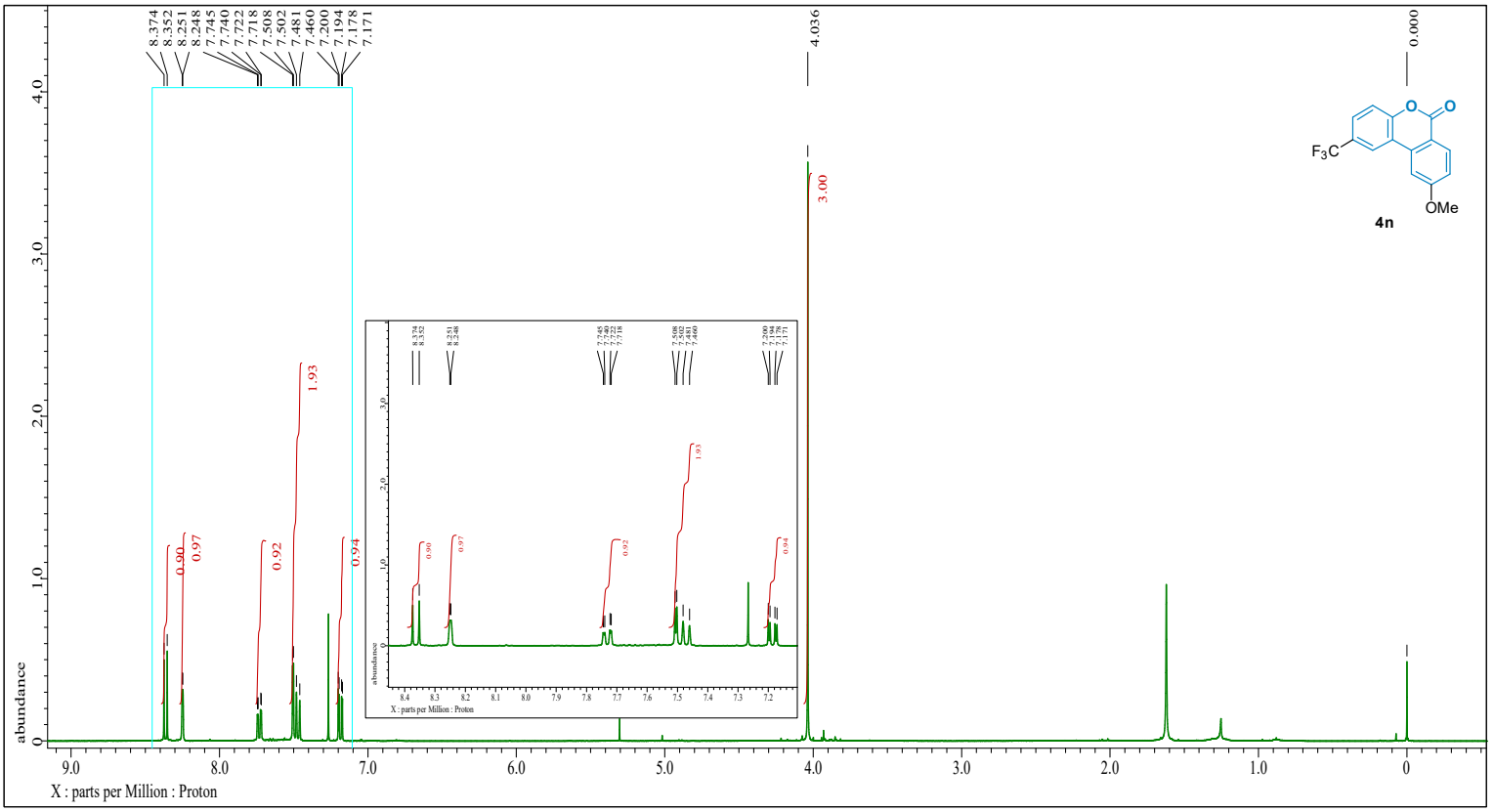
160.237
151.421
135.571
133.281
123.717
121.120
120.948
117.191
115.323
114.633
105.960
77.442
77.289
77.126
76.800
76.656
55.977
(thousandths)
X : parts per Million : Carbon13
F3C
O
O
OMe
4m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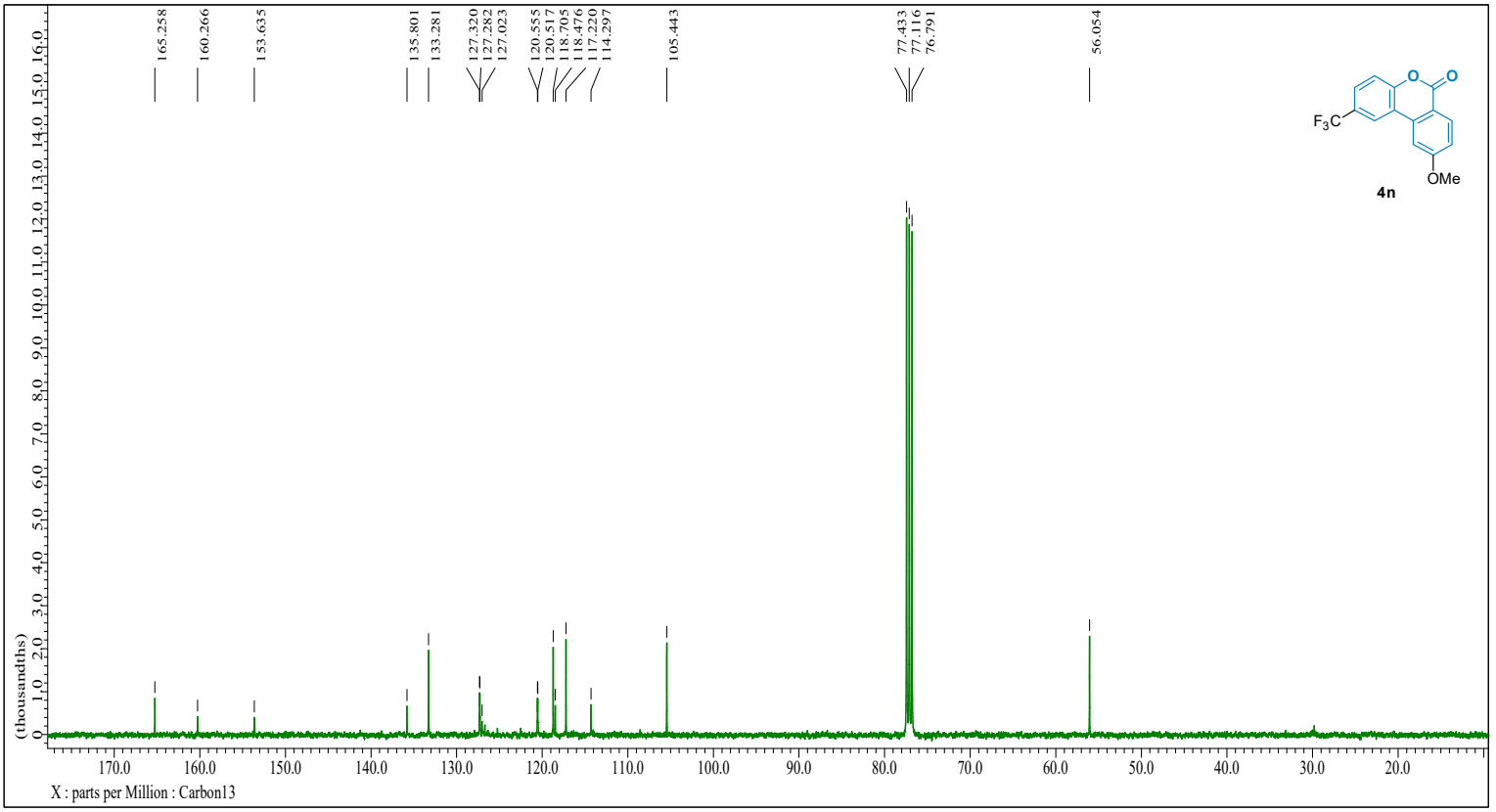
8.251
8.248
7.745
7.740
7.722
7.718
7.508
7.502
7.481
7.460
7.200
7.194
7.178
7.171
4.036
0.000
3.00
1.93
0.90
0.97
0.92
0.94
abundance
X : parts per Million : Proton
F3C
OMe
4n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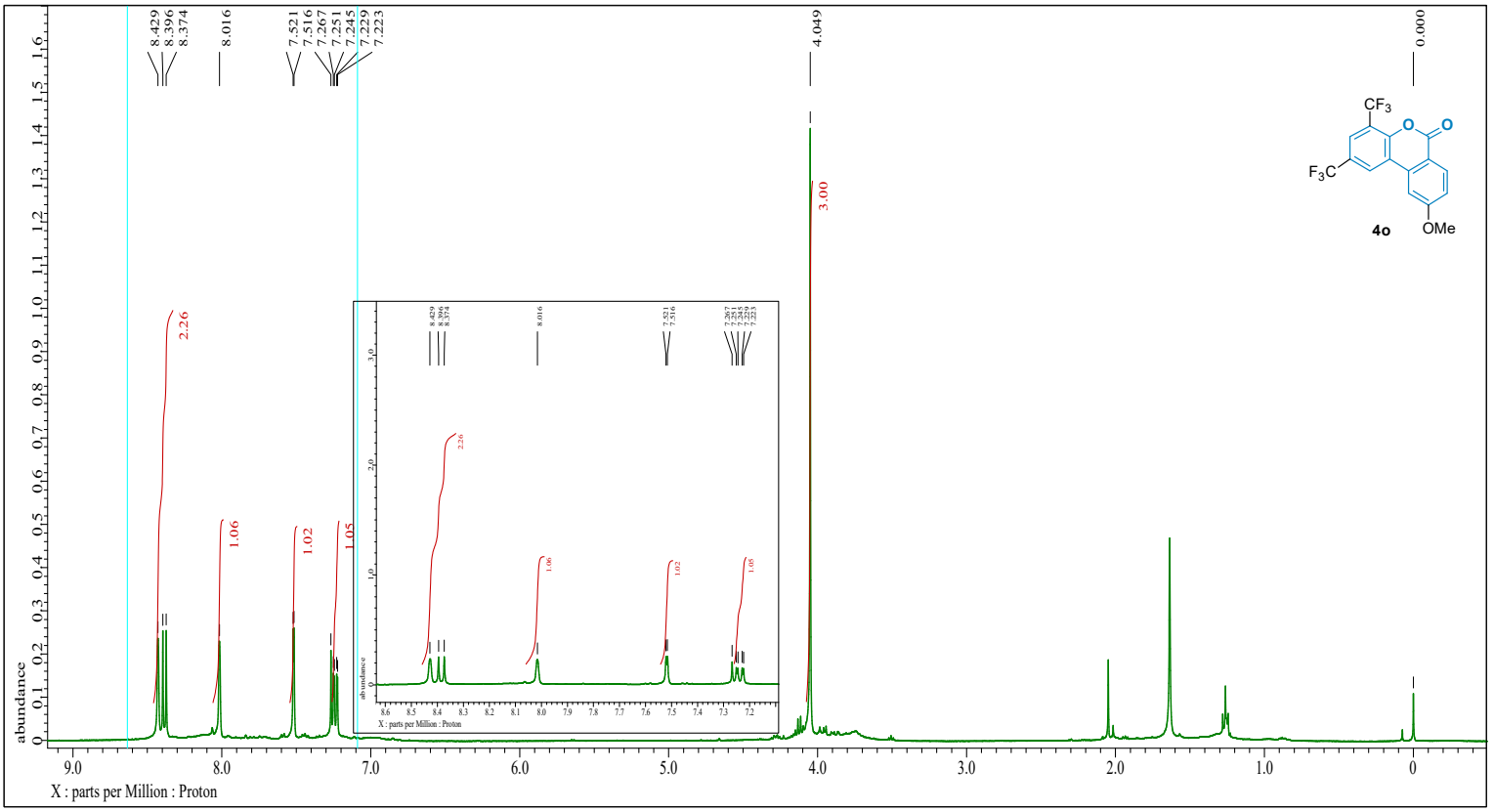
160.266
153.635
135.801
133.281
127.320
127.282
127.023
120.555
120.517
118.705
118.476
117.220
114.297
105.443
77.433
77.116
76.791
56.054
(thousandths)
X : parts per Million : Carbon13
F3C
OMe
4n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8.016
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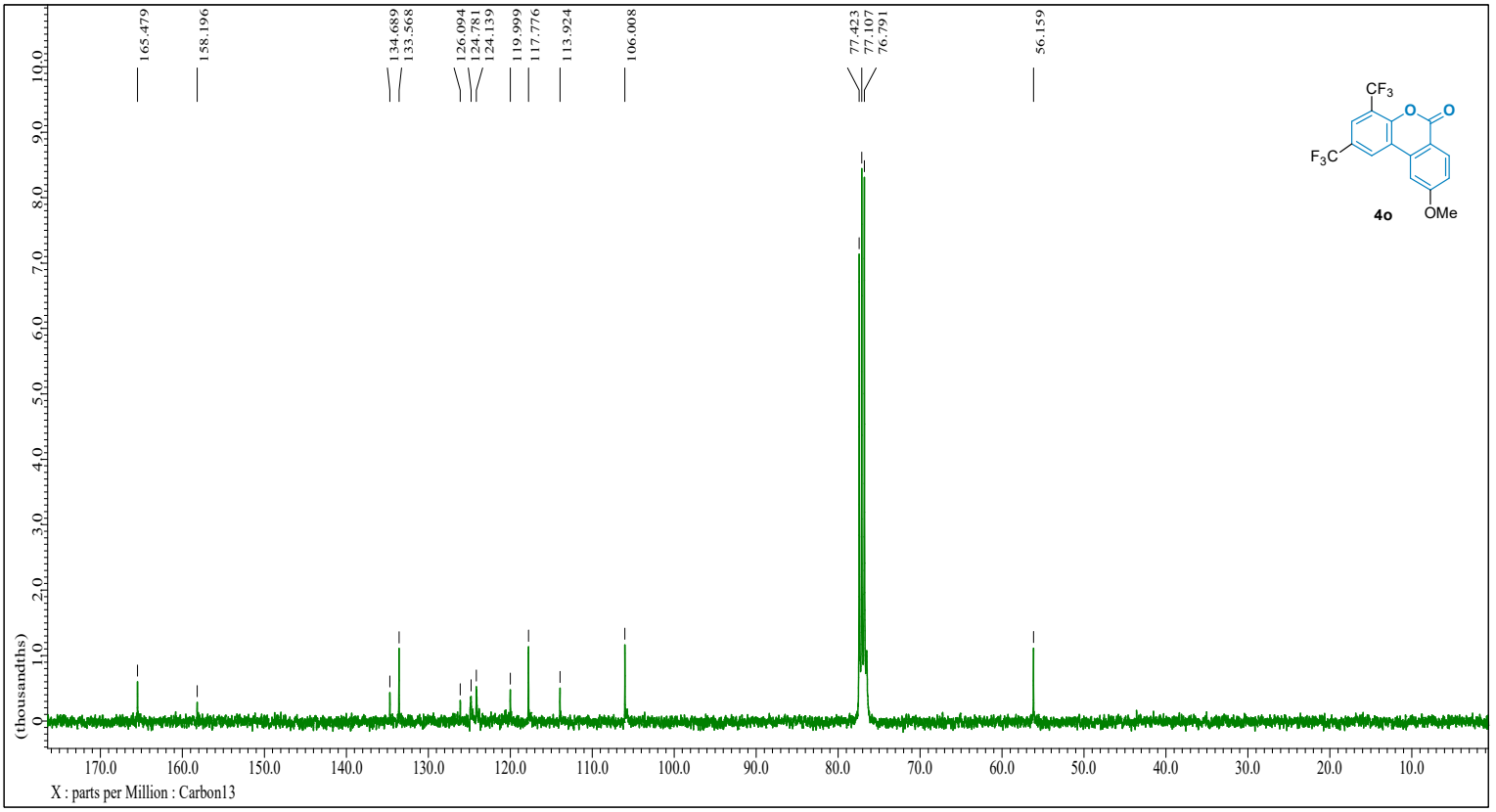
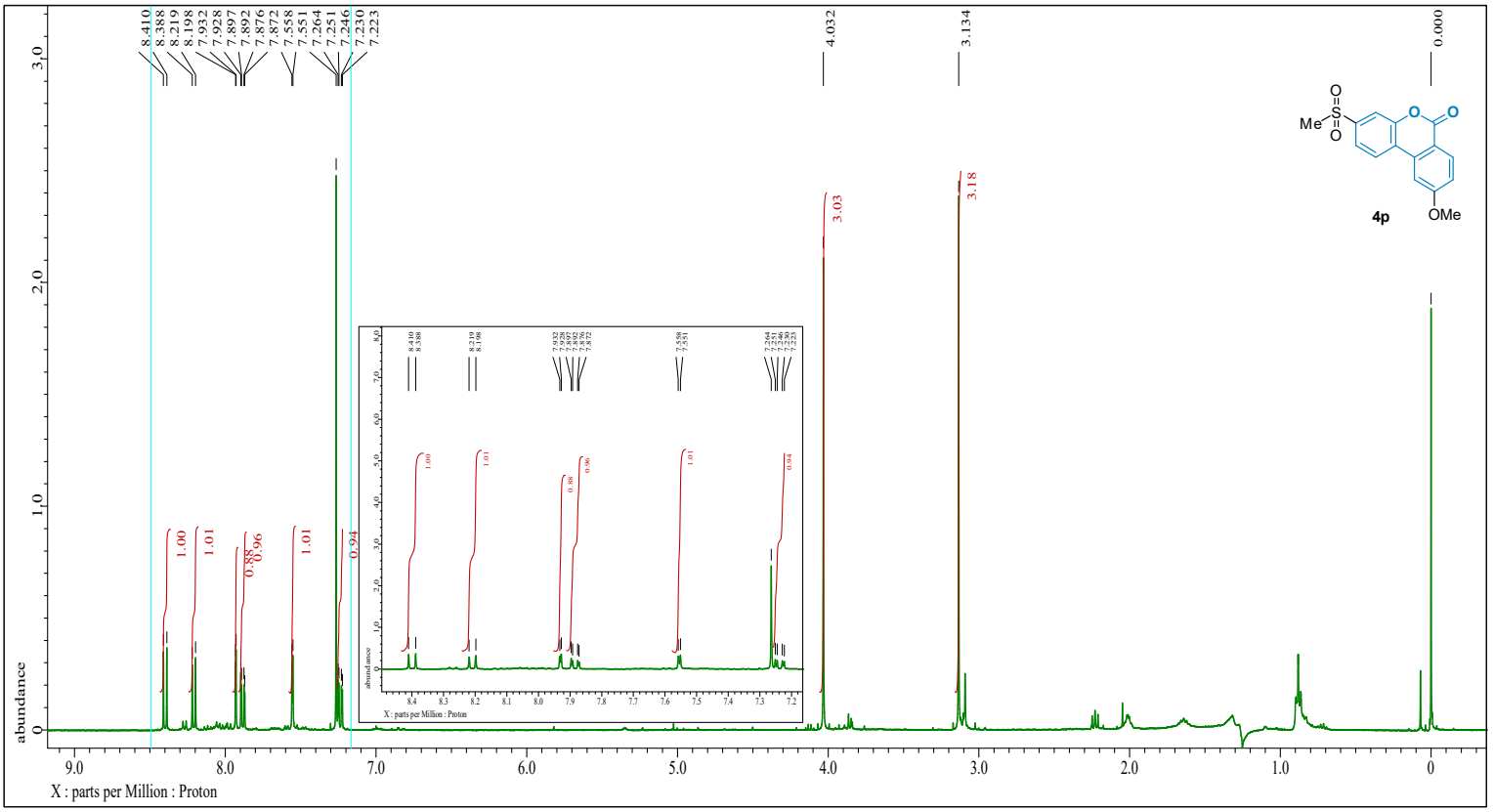
7.516
7.267
7.251
7.245
7.229
7.223
4.049
0.000
3.00
2.26
1.06
1.02
1.05
abundance
X : parts per Million : Proton
CF3
F3C
O
O
4o
OMe


165.479
158.196
134.689
133.568
126.094
124.781
124.139
119.999
117.776
113.924
106.008
77.423
77.107
76.791
56.159
(thousandths)
X : parts per Million : Carbon13
CF3
F3C
O
O
4o
OMe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8.198
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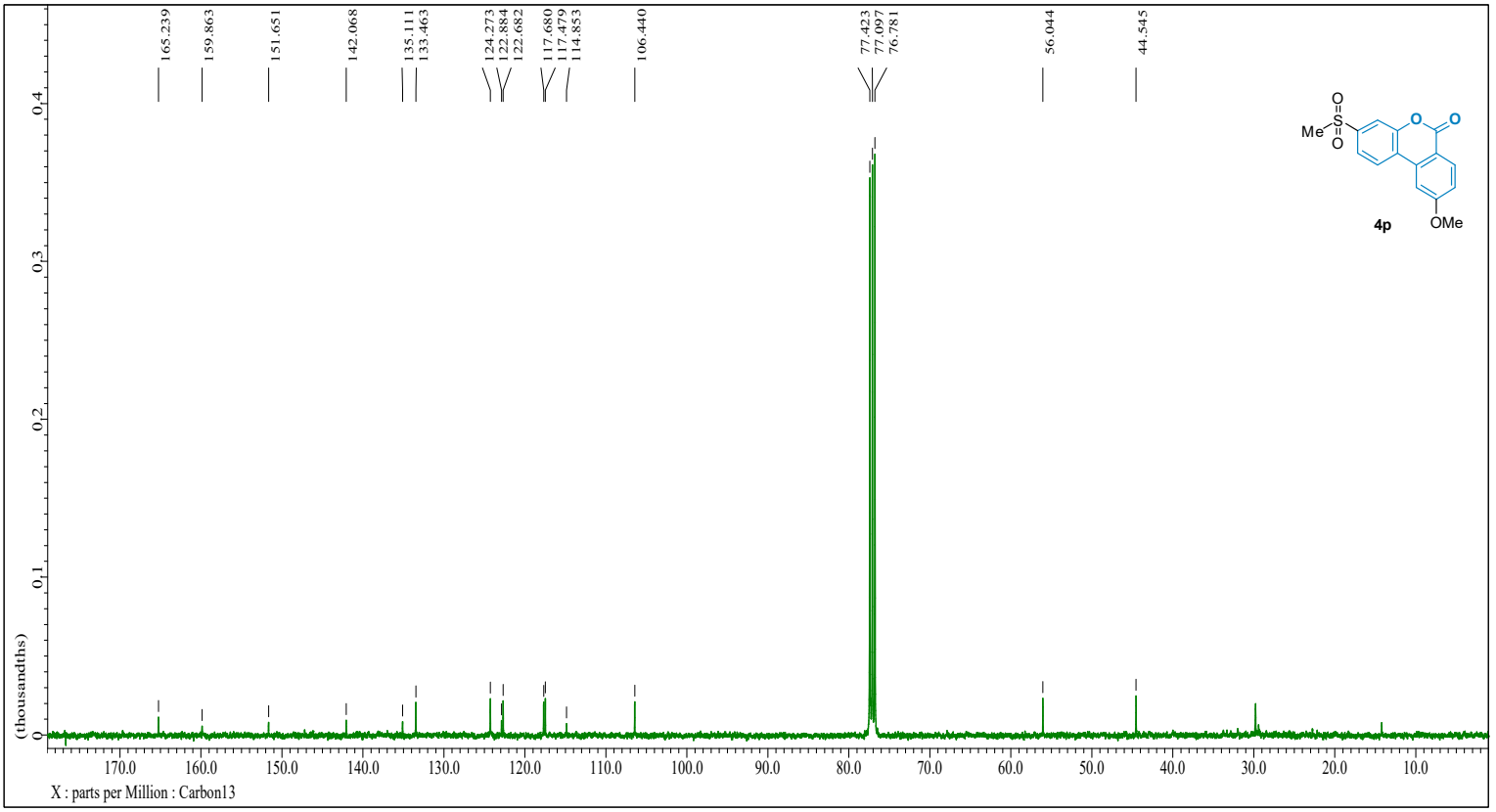
7.928
7.897
7.892
7.876
7.872
7.558
7.551
7.264
7.251
7.246
7.230
7.223
4.032
3.134
0.000
3.03
3.18
1.00
1.01
0.88
0.96
1.01
0.94
abundance
X : parts per Million : Proton
Me
O
S
O
O
O
O
OMe
4p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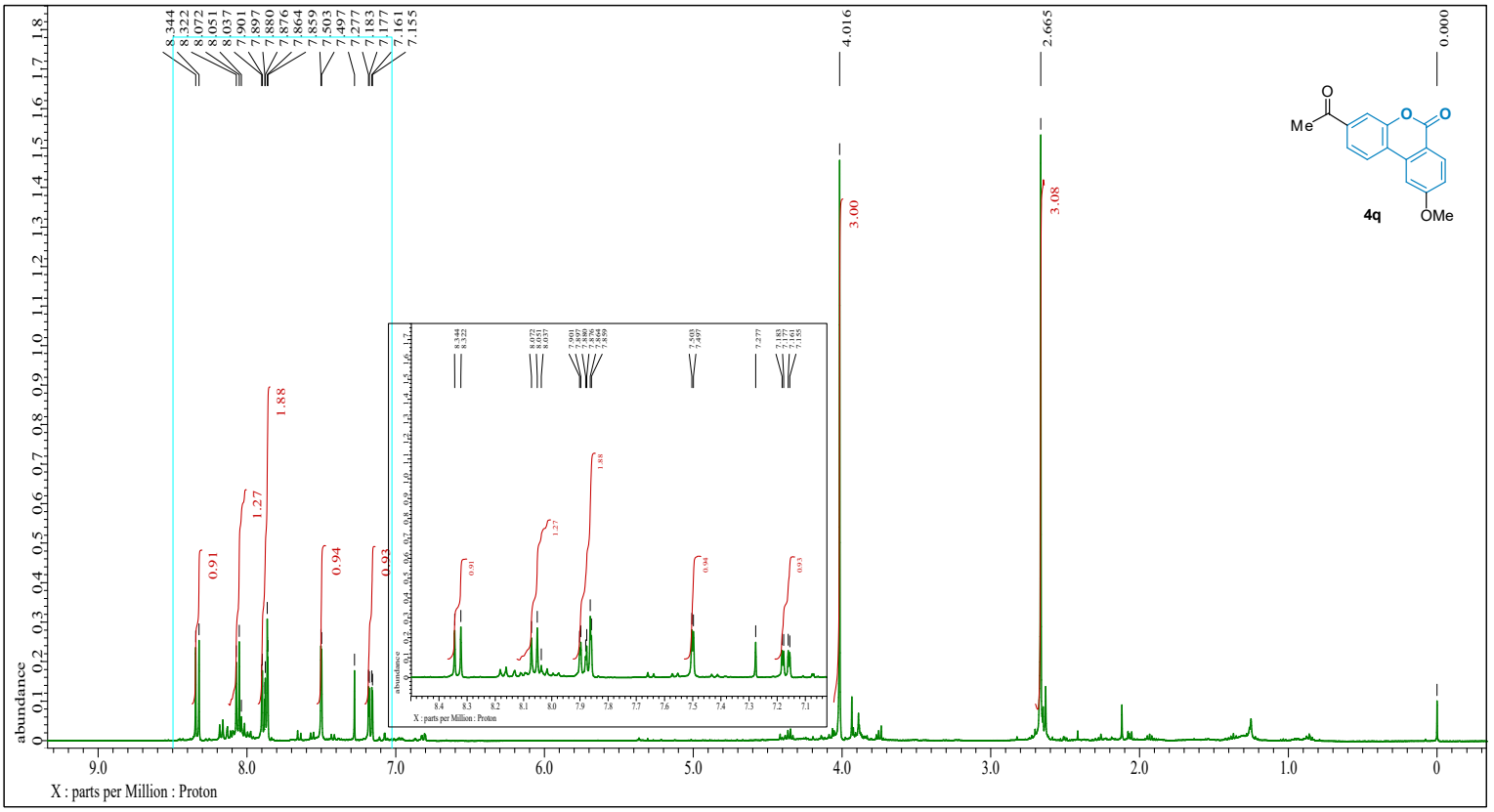
142.068
135.111
133.463
124.273
122.884
122.682
117.680
117.479
114.853
106.440
77.423
77.097
76.781
56.044
44.545
(thousandths)
X : parts per Million : Carbon13
Me
O
S
O
O
O
O
OMe
4p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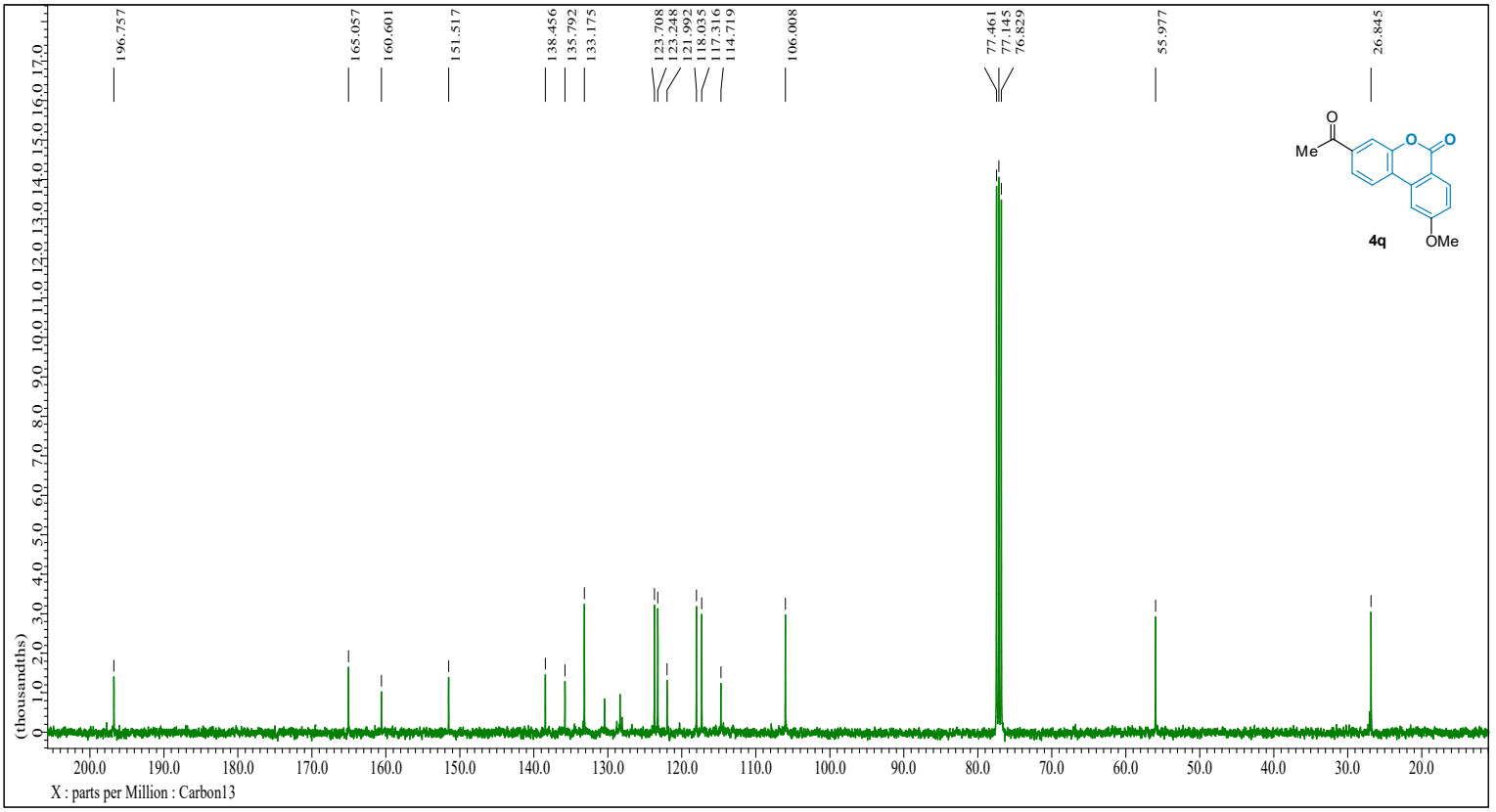
8.051
8.037
7.901
7.897
7.880
7.876
7.864
7.859
7.503
7.497
7.277
7.183
7.177
7.161
7.155
4.016
2.665
0.000
3.00
3.08
1.88
1.27
0.91
0.94
0.93
abundance
X : parts per Million : Proton
Me
O
O
O
OMe
4q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160.601
151.517
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135.792
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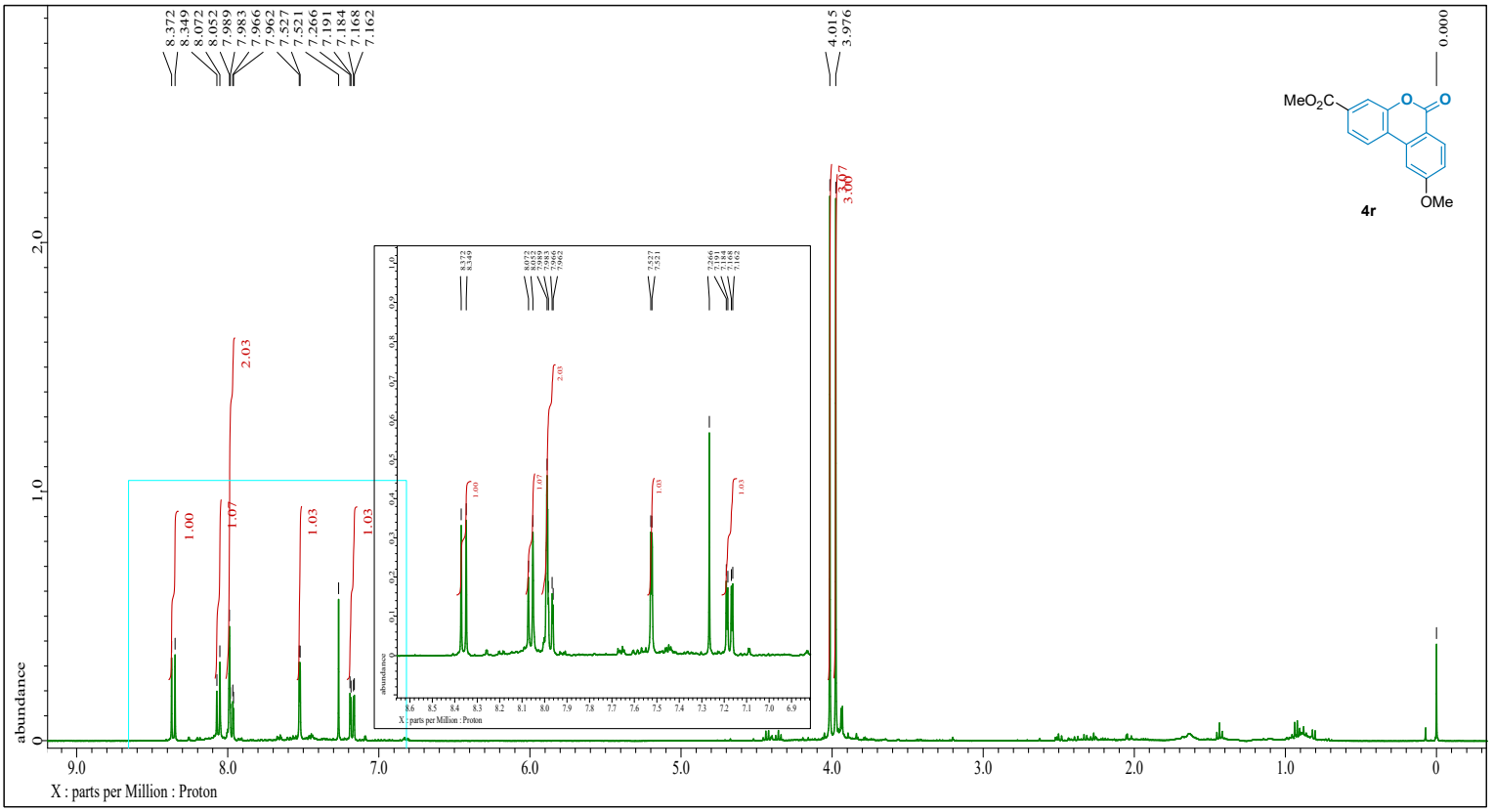
123.708
123.248
121.992
118.035
117.316
114.719
106.008
77.461
77.145
76.829
55.977
26.845
(thousandths)
X : parts per Million : Carbon13
Me
O
O
O
OMe
4q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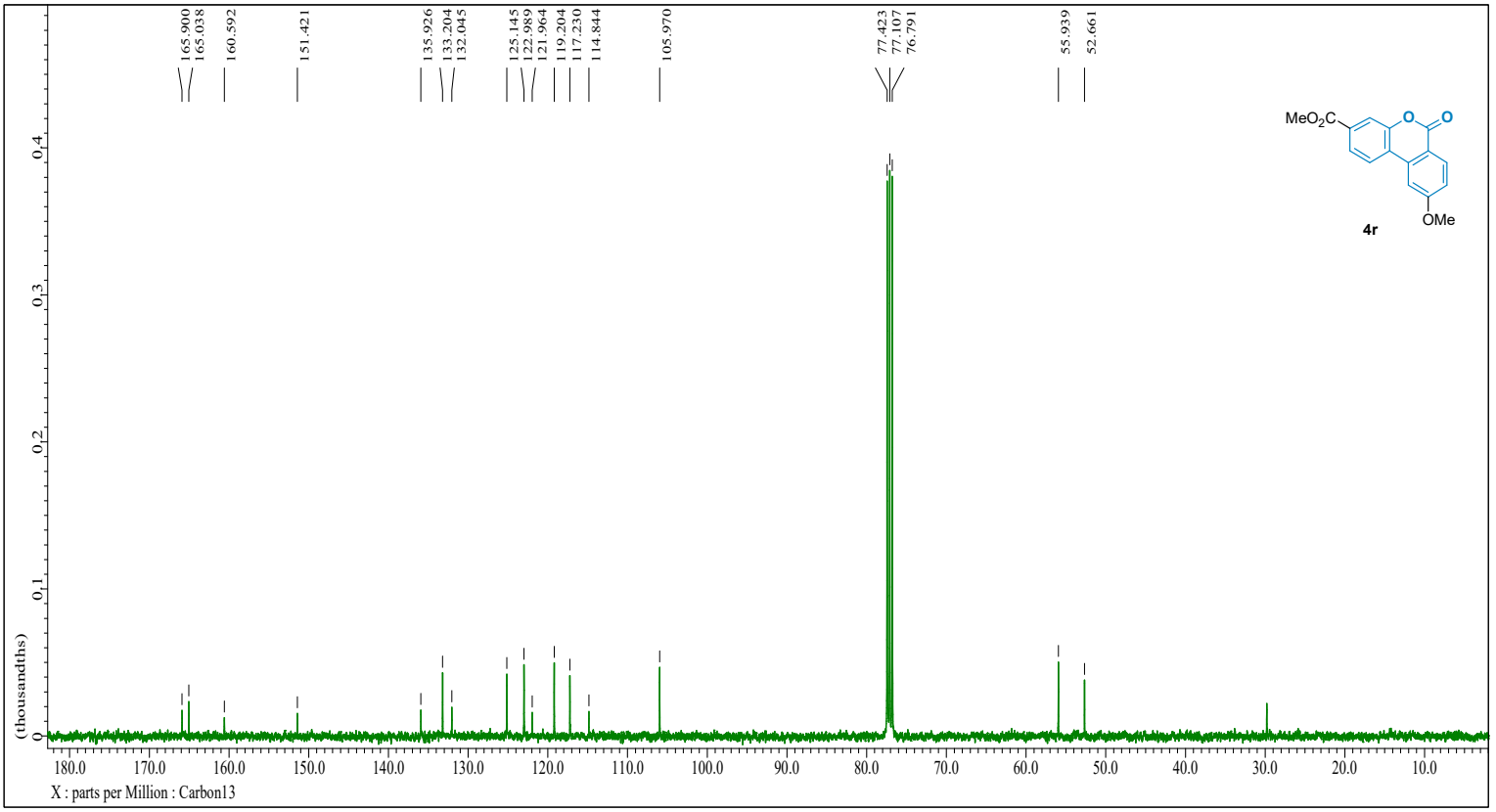
8.349
8.072
8.052
7.989
7.983
7.966
7.962
7.527
7.521
7.266
7.191
7.184
7.168
7.162
4.015
3.976
0.000
MeO2C
OMe
4r
2.03
1.00
1.07
1.03
1.03
3.00
abundance
X : parts per Million : Proton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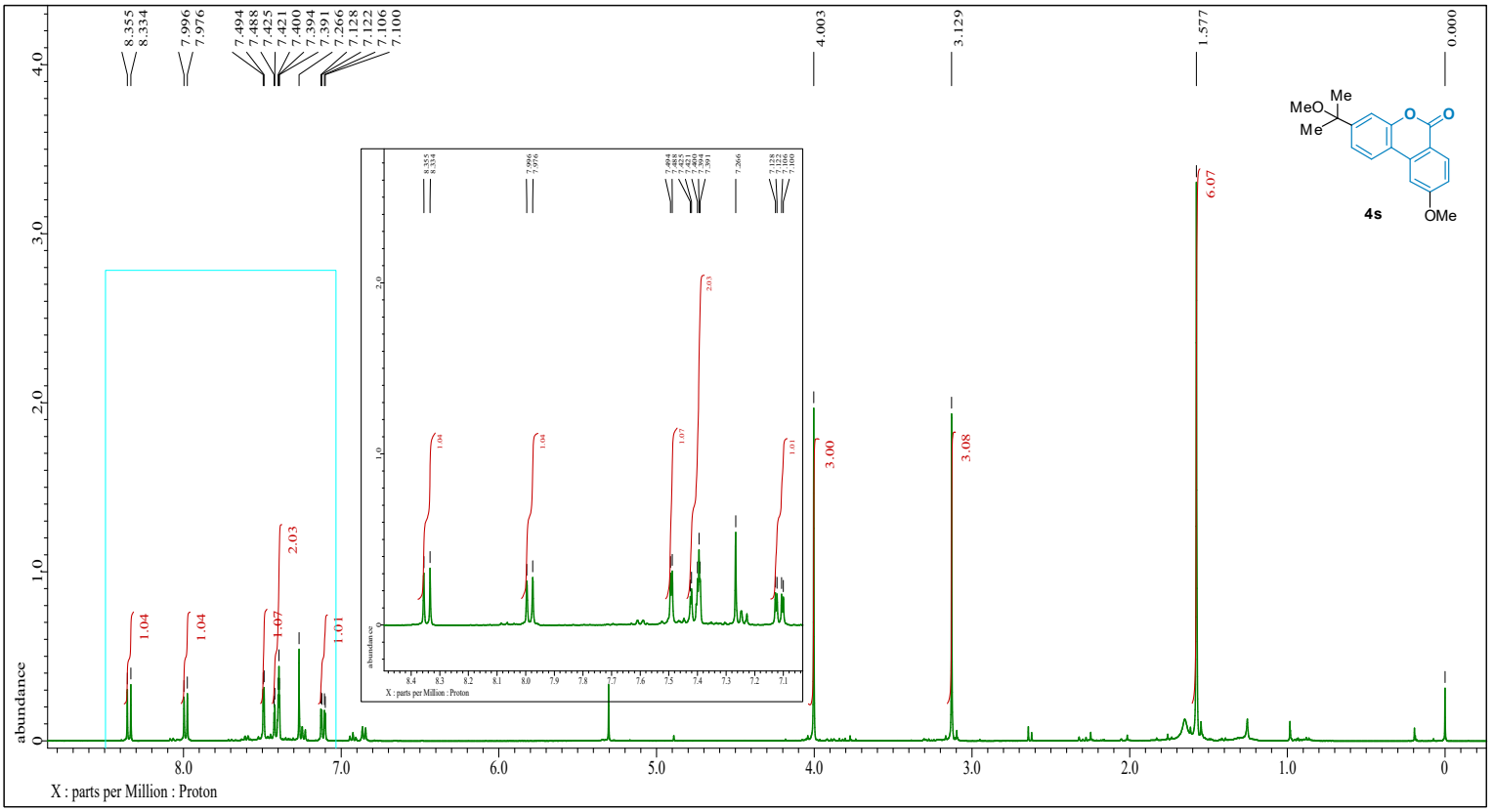
165.038
160.592
151.421
135.926
133.204
132.045
125.145
122.989
121.964
119.204
117.230
114.844
105.970
77.423
77.107
76.791
55.939
52.661
MeO2C
OMe
4r
(thousandths)
X : parts per Million : Carbon13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8.334
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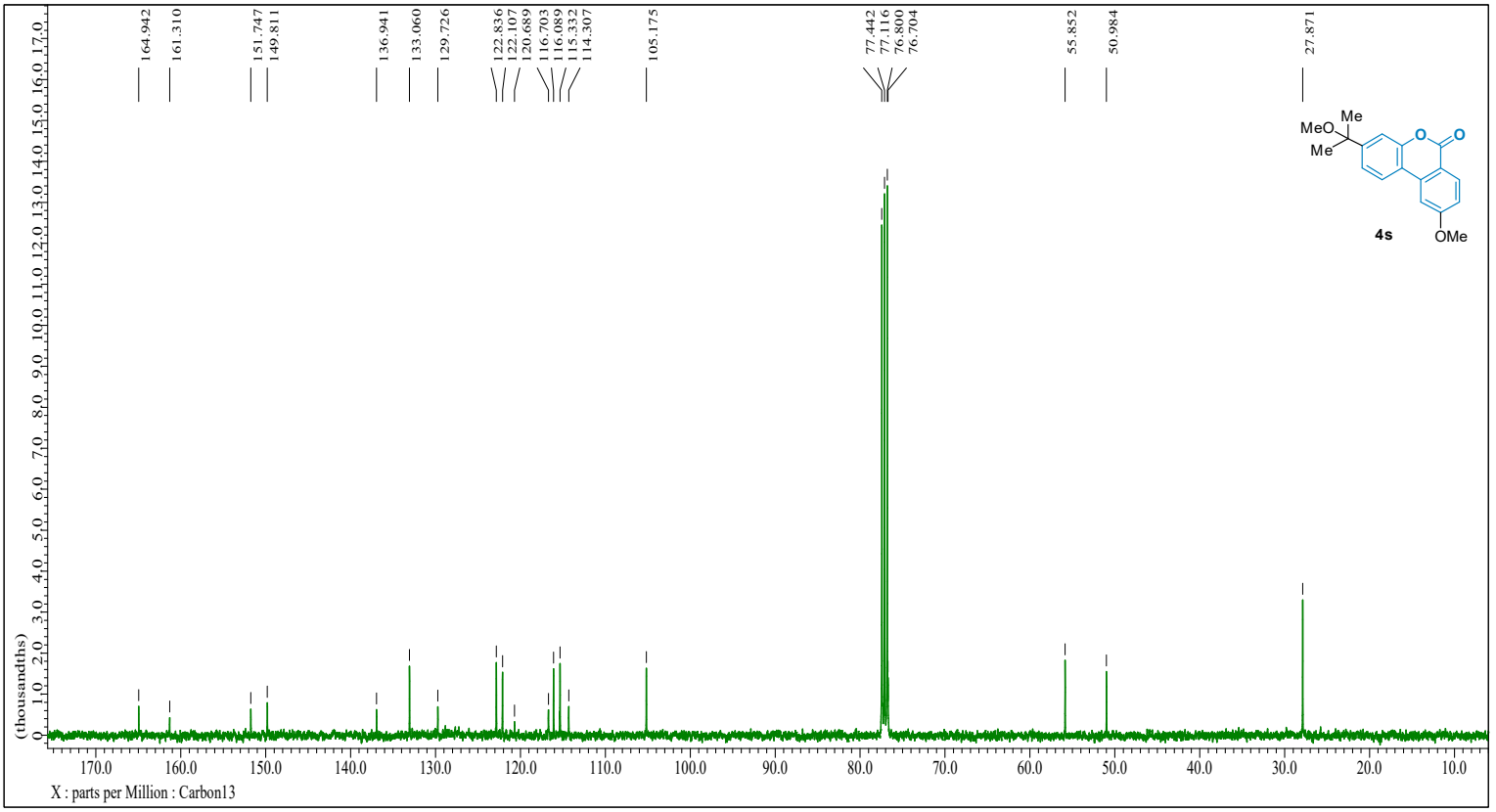
7.976
7.494
7.488
7.425
7.421
7.400
7.394
7.391
7.266
7.128
7.122
7.106
7.100
4.003
3.129
1.577
0.000
1.04
1.04
2.03
1.07
1.01
3.00
3.08
6.07
Me
MeO
Me
O
O
4s
OMe
abundance
X : parts per Million : Proton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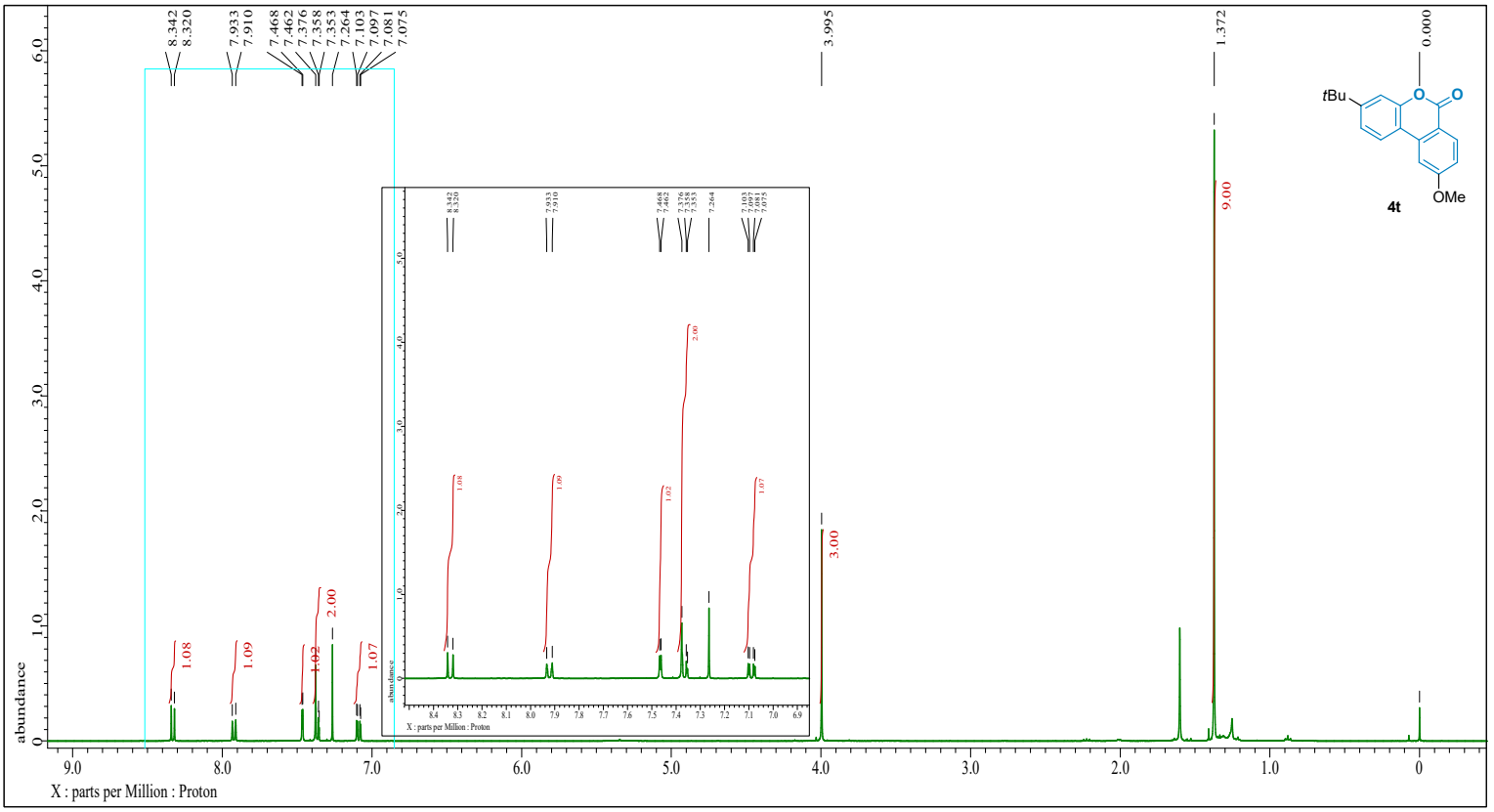
151.747
149.811
136.941
133.060
129.726
122.836
122.107
120.689
116.703
116.089
115.332
114.307
105.175
77.442
77.116
76.800
76.704
55.852
50.984
27.871
Me
MeO
Me
O
O
4s
OMe
(thousandths)
X : parts per Million : Carbon13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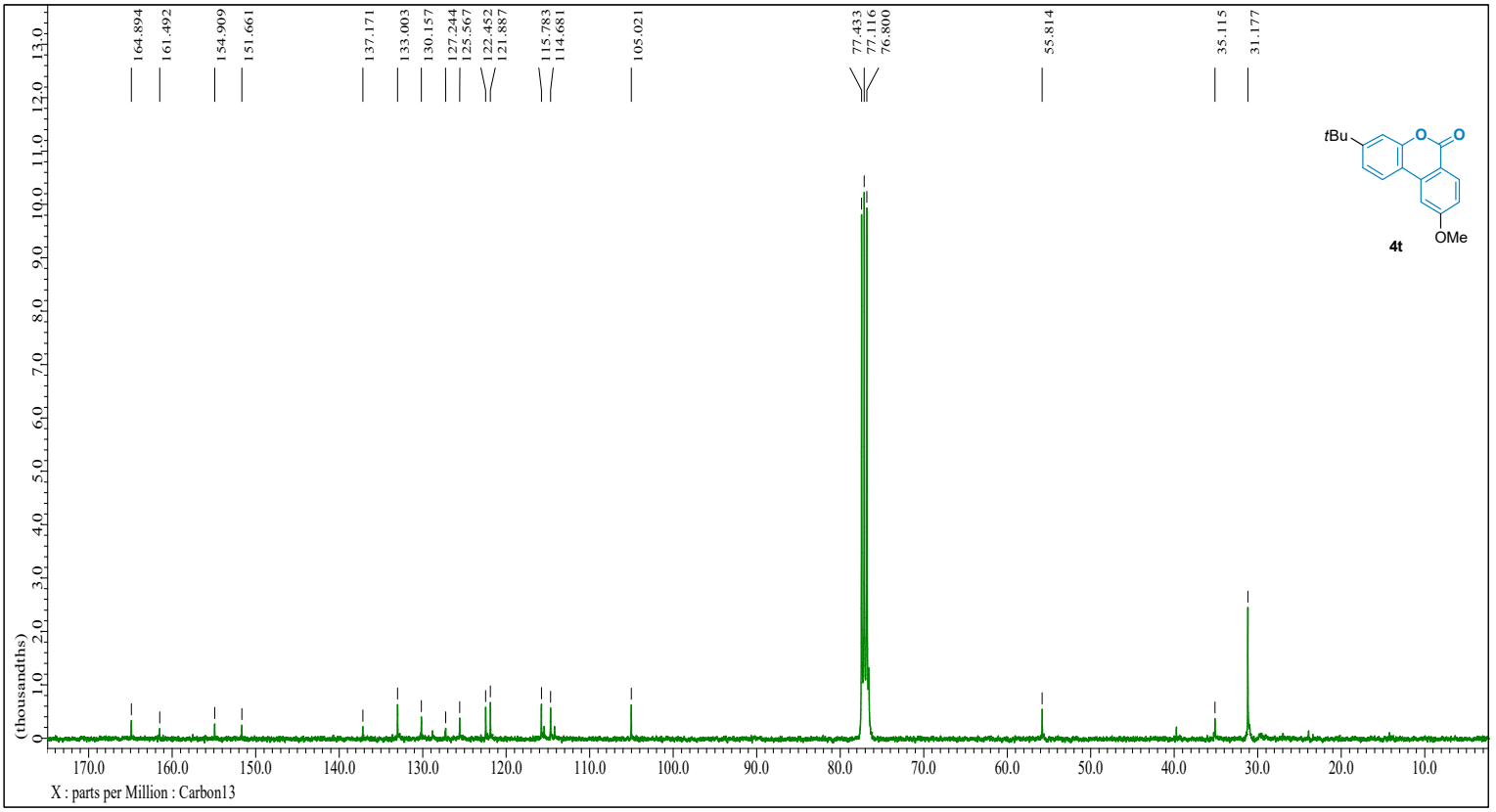
8.320
7.933
7.910
7.468
7.462
7.376
7.358
7.353
7.264
7.103
7.097
7.081
7.075
3.995
1.372
0.000
1.08
1.09
2.00
1.02
1.07
3.00
9.00
tBu
O
O
OMe
4t
abundance
X : parts per Million : Proton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161.492
154.909
151.661
137.171
133.003
130.157
127.244
125.567
122.452
121.887
115.783
114.681
105.021
77.433
77.116
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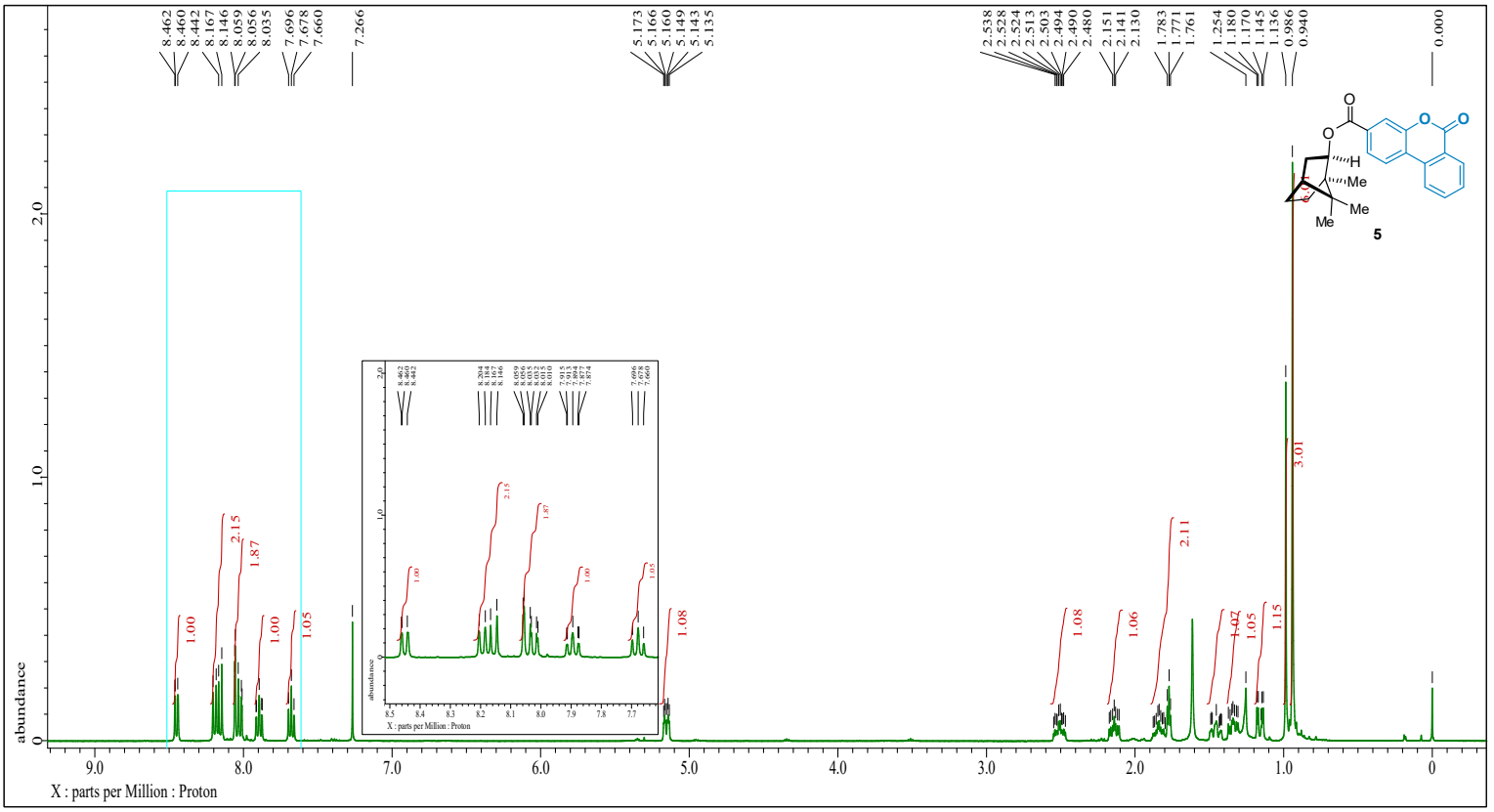
55.814
35.115
31.177
tBu
O
O
OMe
4t
(thousandths)
X : parts per Million : Carbon13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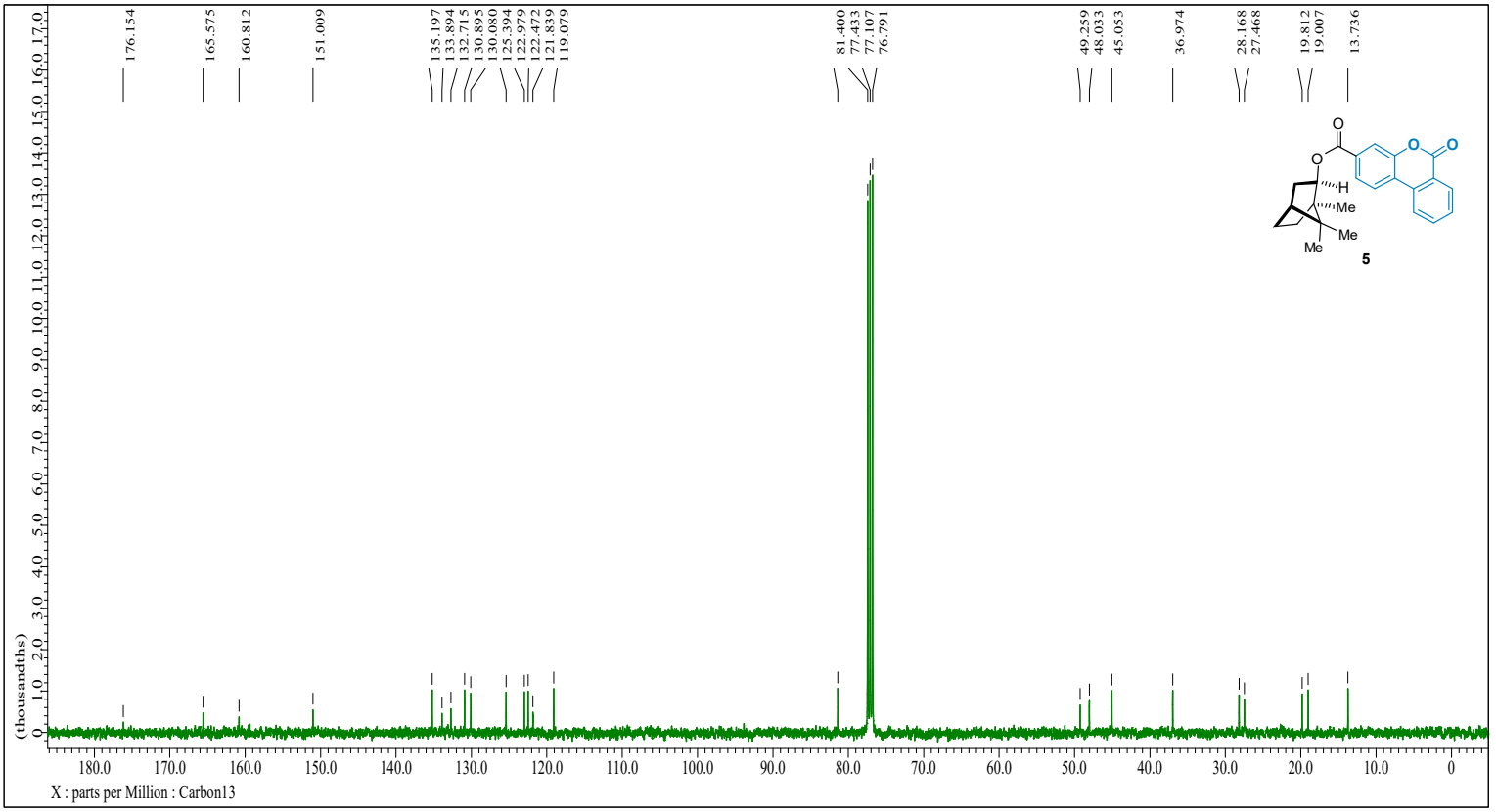
8.460
8.442
8.167
8.146
8.059
8.056
8.035
7.696
7.678
7.660
7.266
5.173
5.166
5.160
5.149
5.143
5.135
2.538
2.528
2.524
2.513
2.503
2.494
2.490
2.480
2.151
2.141
2.130
1.783
1.771
1.761
1.254
1.180
1.170
1.145
1.136
0.986
0.940
0.000
1.00
2.15
1.87
1.00
1.05
1.08
1.08
1.06
2.11
1.07
1.05
1.15
3.01
abundance
X : parts per Million : Proton
5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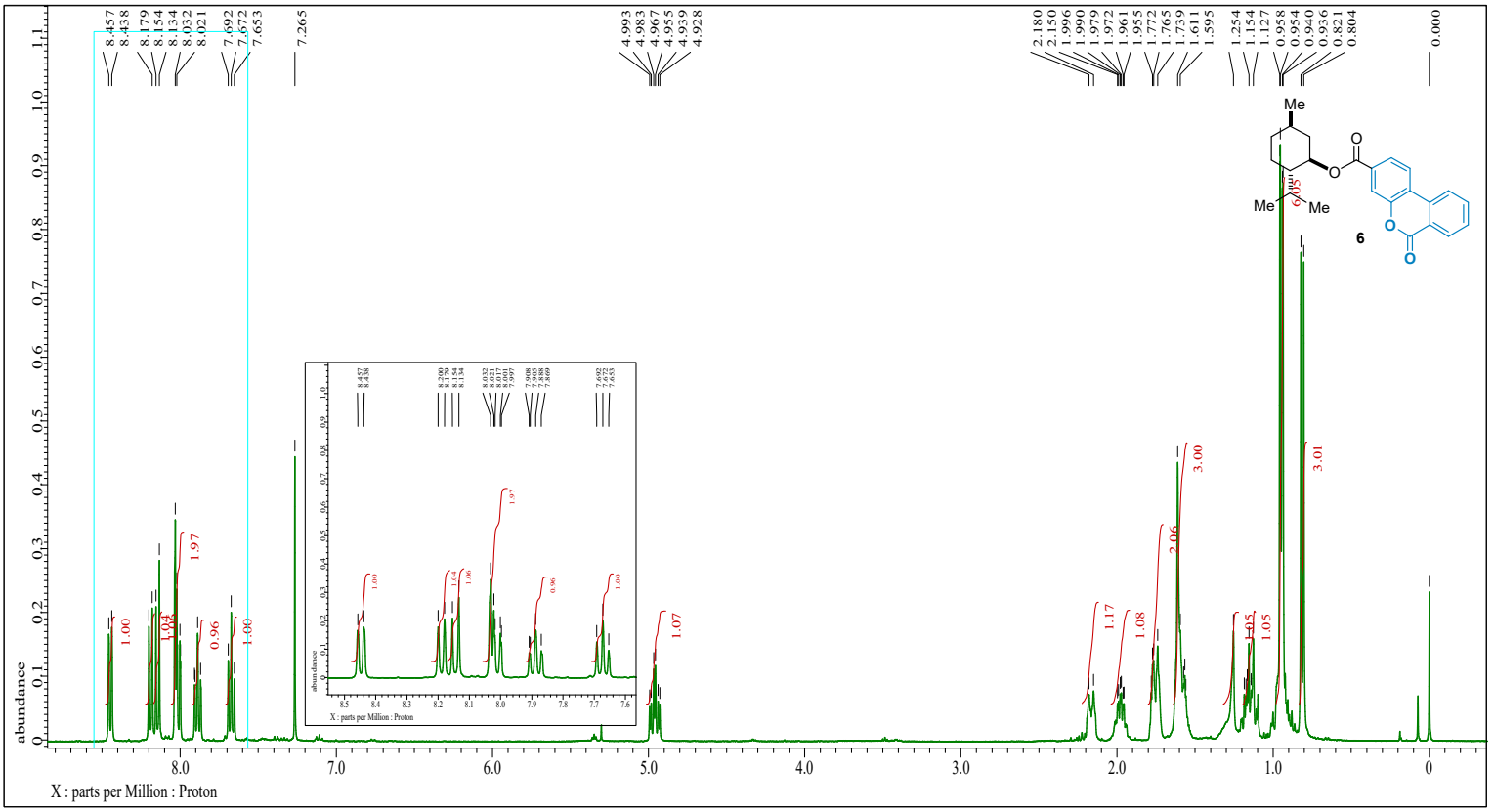
165.575
160.812
151.009
135.197
133.894
132.715
130.895
130.080
125.394
122.979
122.472
121.839
119.079
81.400
77.433
77.107
76.791
49.259
48.033
45.053
36.974
28.168
27.468
19.812
19.007
13.736
(thousandths)
X : parts per Million : Carbon13
5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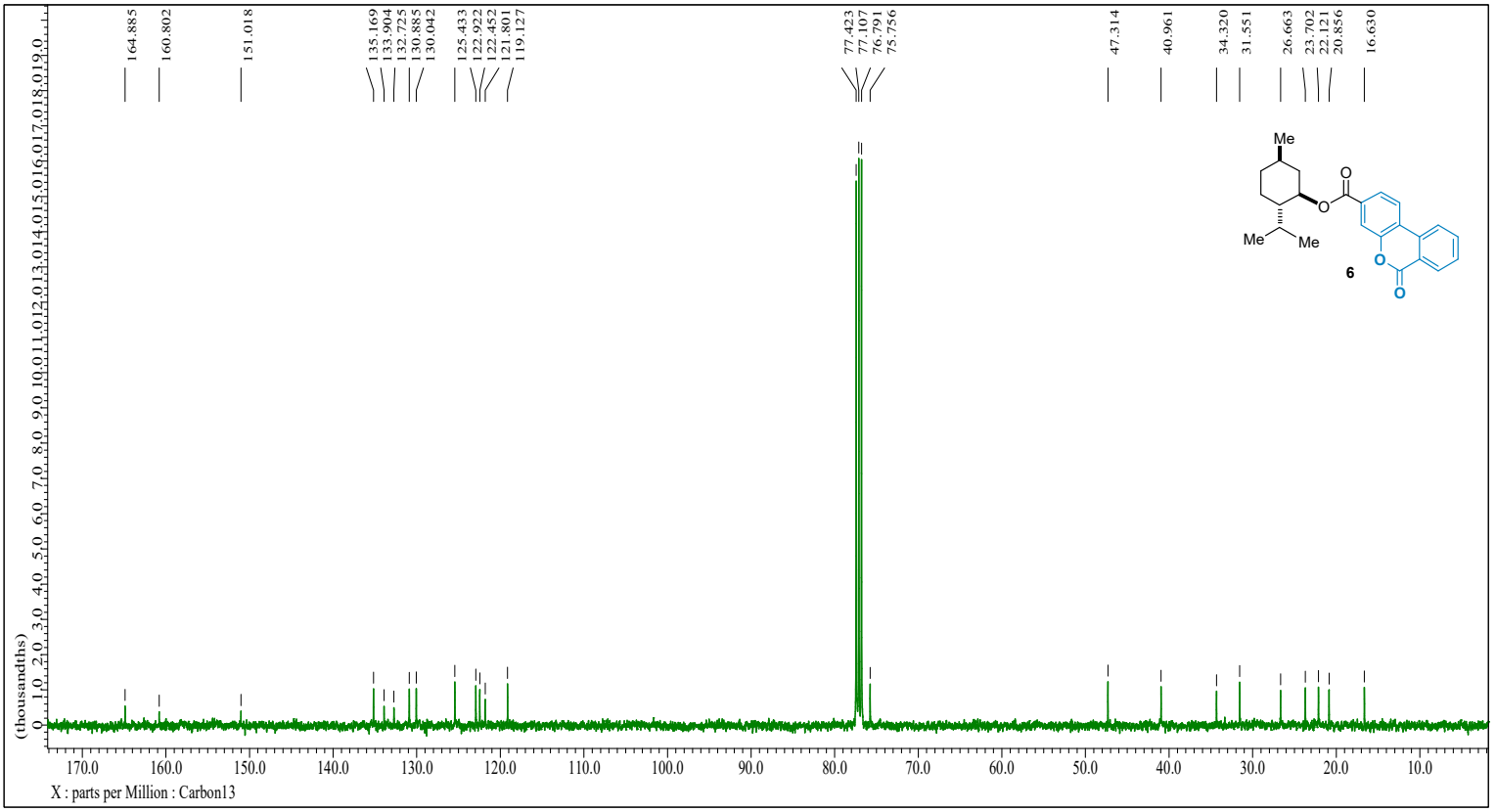
8.438
8.179
8.154
8.134
8.032
8.021
7.692
7.672
7.653
7.265
4.993
4.983
4.967
4.955
4.939
4.928
2.180
2.150
1.996
1.990
1.979
1.972
1.961
1.955
1.772
1.765
1.739
1.611
1.595
1.254
1.154
1.127
0.958
0.954
0.940
0.936
0.821
0.804
0.000
Me
Me
Me
O
O
O
O
6
1.00
1.03
1.97
0.96
1.00
1.07
1.17
1.08
2.06
3.00
1.05
1.05
3.01
abundance
X : parts per Million : Proton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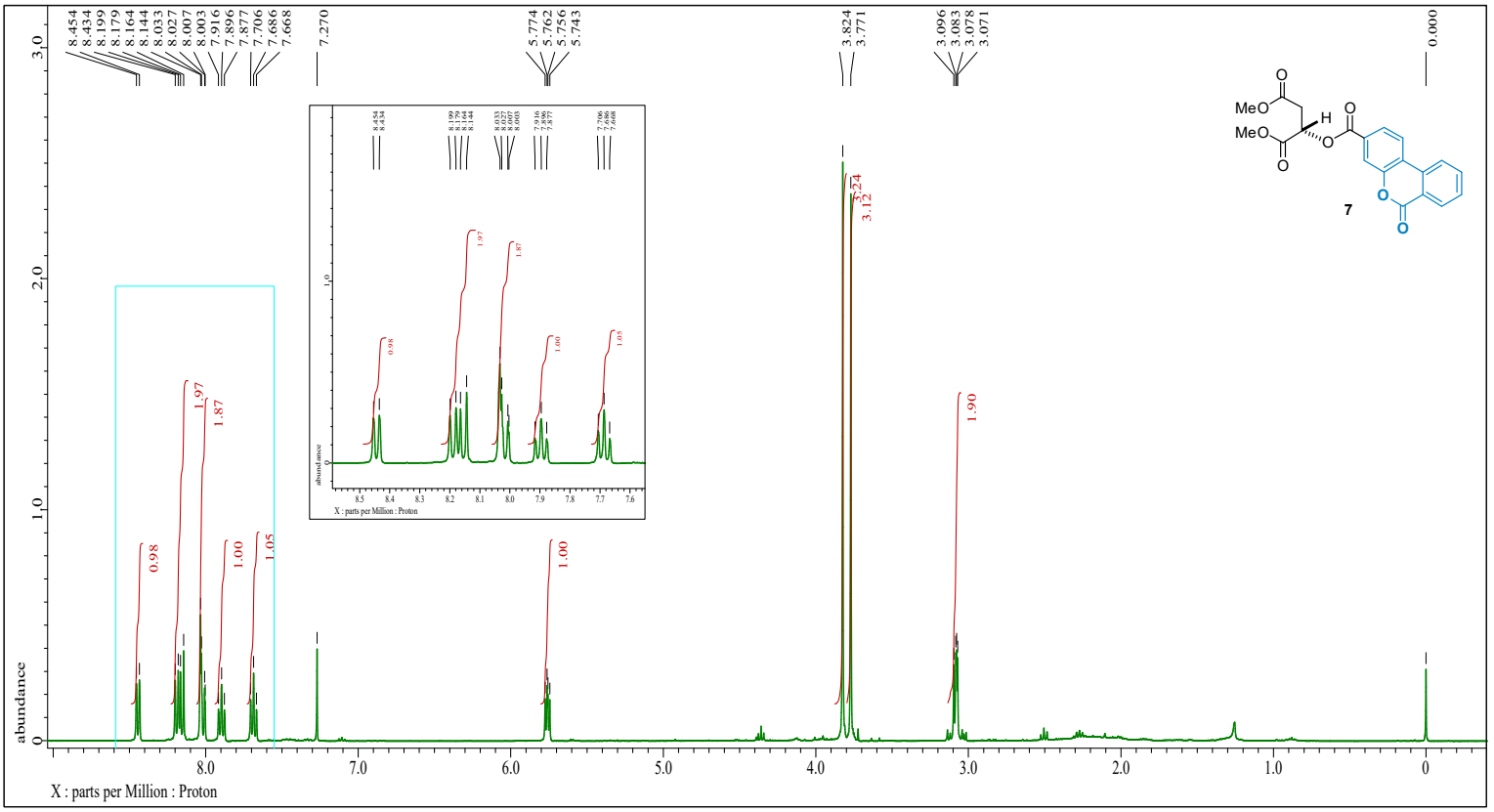
151.018
135.169
133.904
132.725
130.885
130.042
125.433
122.922
122.452
121.801
119.127
77.423
77.107
76.791
75.756
47.314
40.961
34.320
31.551
26.663
23.702
22.121
20.856
16.630
Me
Me
Me
O
O
O
O
6
(thousandths)
X : parts per Million : Carbon13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8.434
8.199
8.179
8.164
8.144
8.033
8.027
8.007
8.003
7.916
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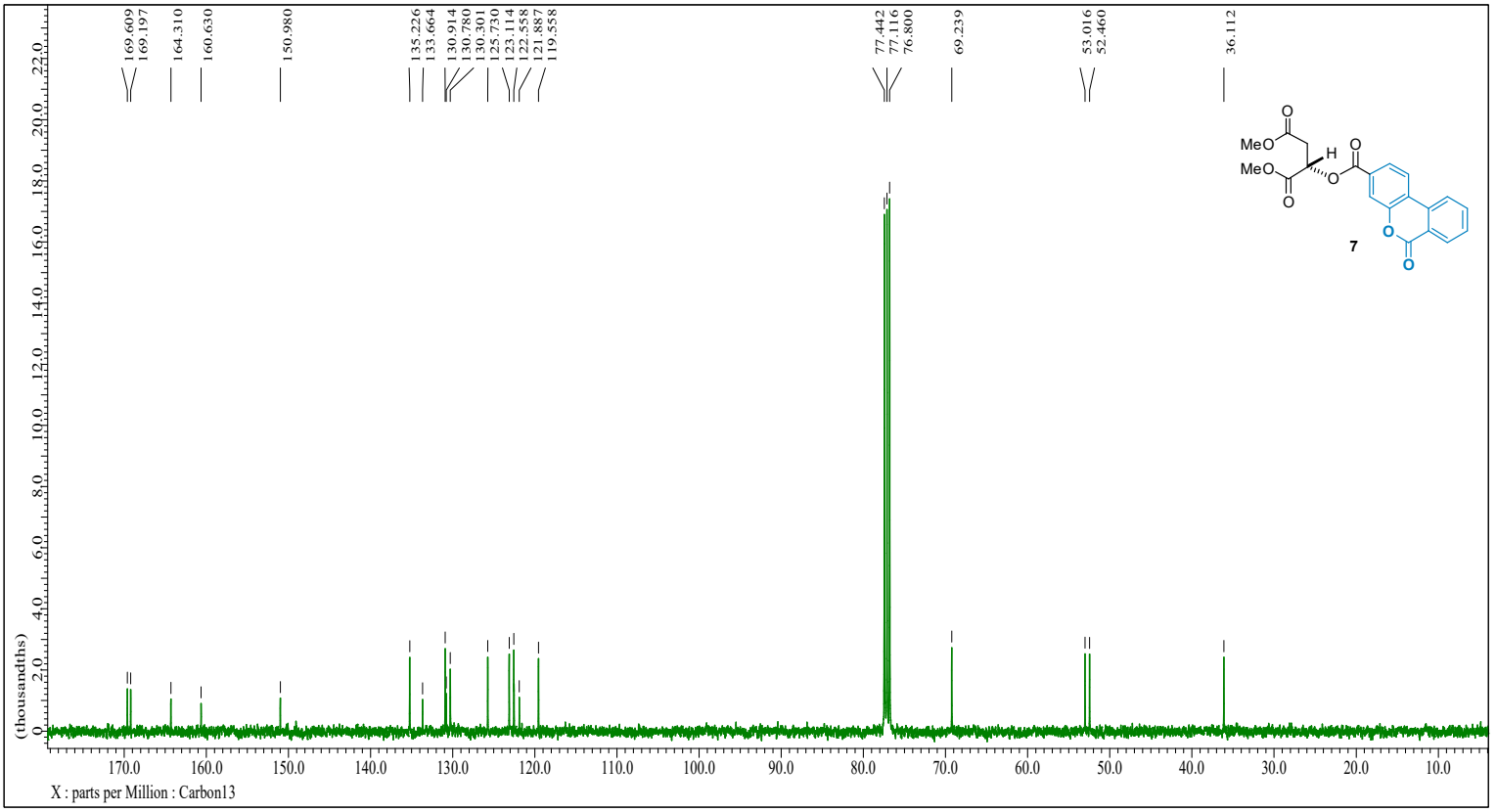
7.877
7.706
7.686
7.668
7.270
5.774
5.762
5.756
5.743
3.824
3.771
3.096
3.083
3.078
3.071
0.000
0.98
1.97
1.87
1.00
1.05
1.00
1.90
3.24
3.12
MeO
MeO
H
O
7
abundance
X : parts per Million : Proton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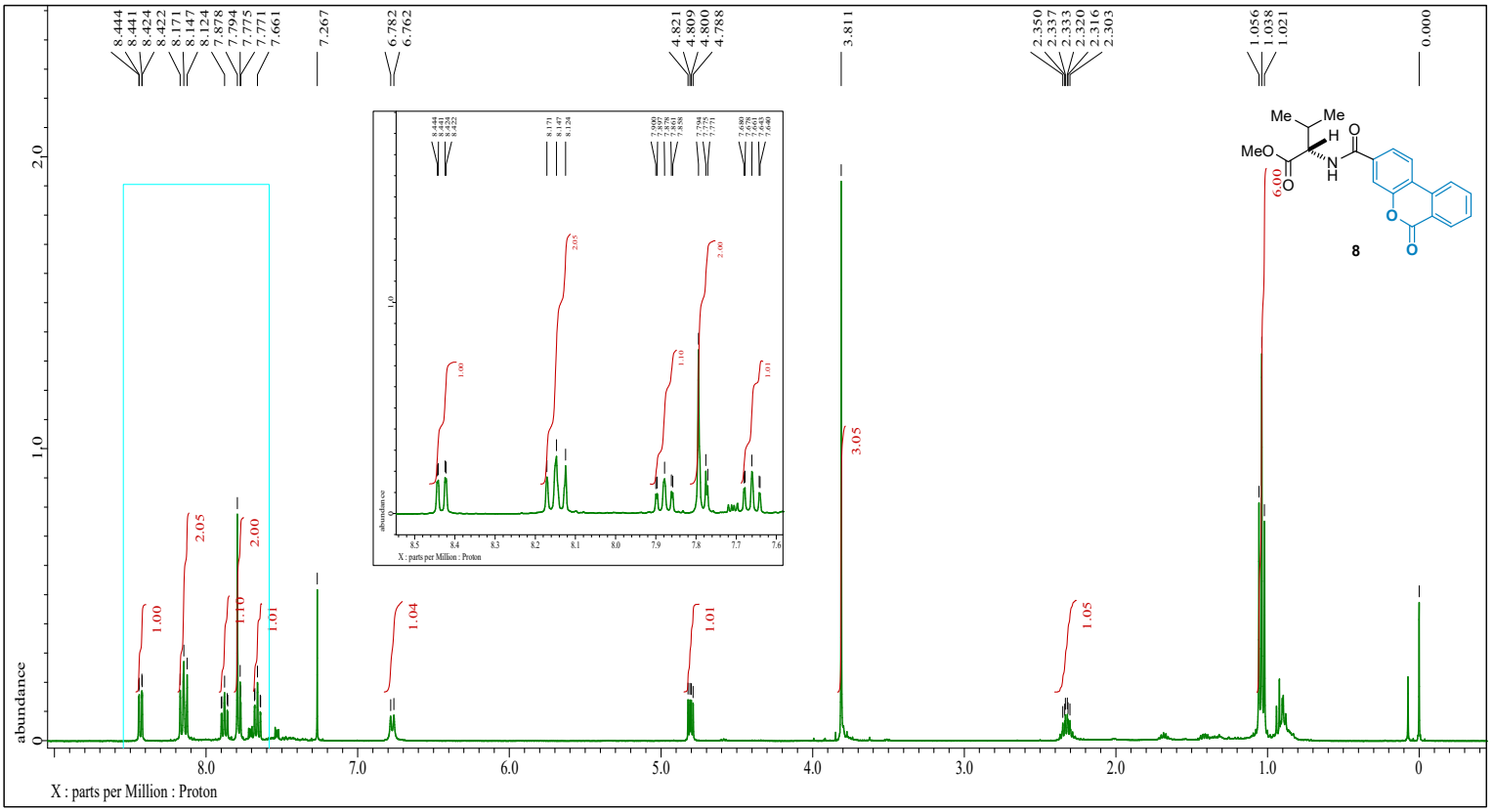
160.630
150.980
135.226
133.664
130.914
130.780
130.301
125.730
123.114
122.558
121.887
119.558
77.442
77.116
76.800
69.239
53.016
52.460
36.112
MeO
MeO
H
O
7
(thousandths)
X : parts per Million : Carbon13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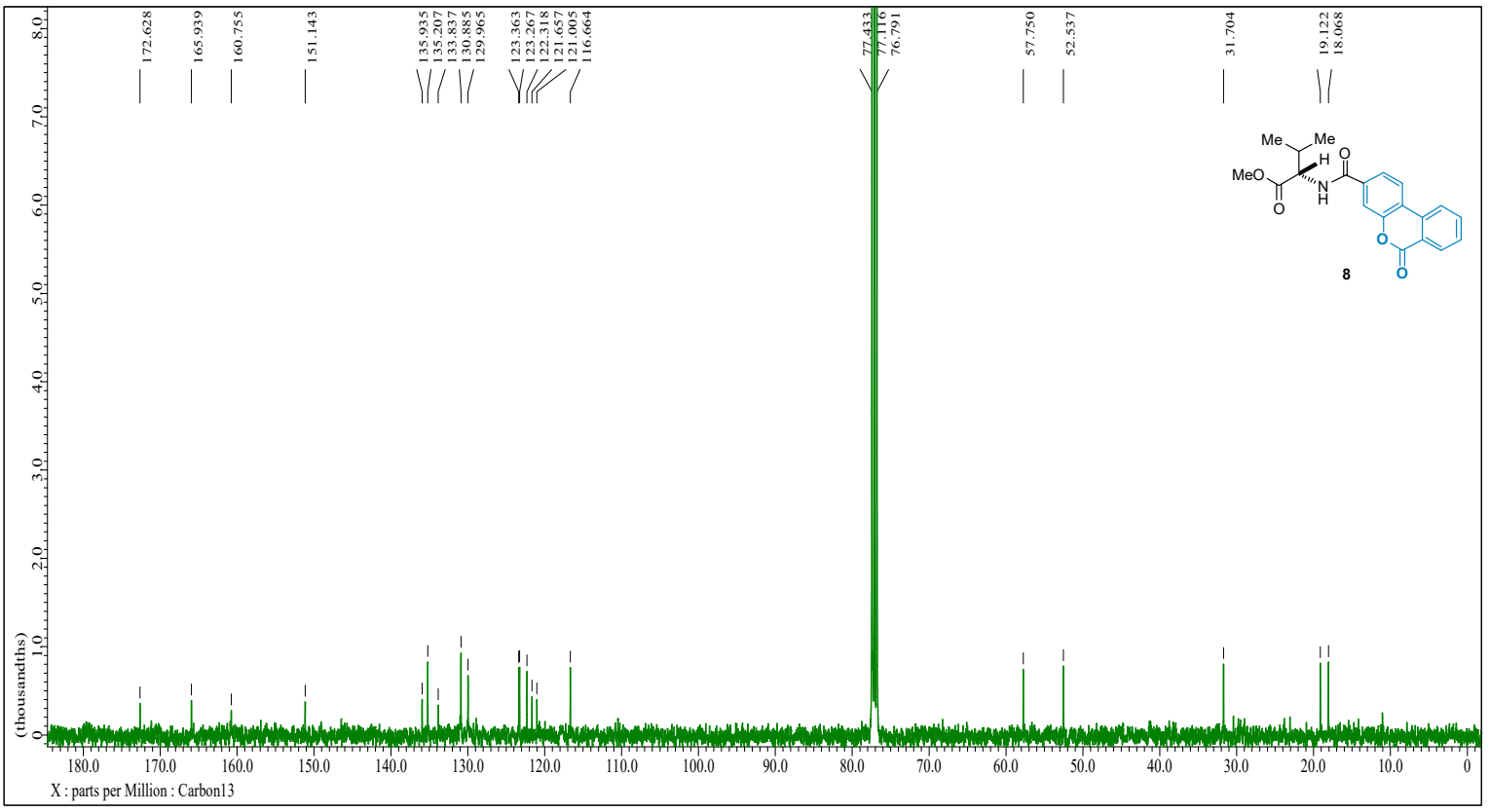
8.441
8.424
8.422
8.171
8.147
8.124
7.878
7.794
7.775
7.771
7.661
7.267
6.782
6.762
4.821
4.809
4.800
4.788
3.811
2.350
2.337
2.333
2.320
2.316
2.303
1.056
1.038
1.021
0.000
1.00
2.05
2.00
1.10
1.01
1.04
1.01
3.05
1.05
6.00
Me
Me
H
MeO
O
N
H
O
O
O
O
8
abundance
X : parts per Million : Proton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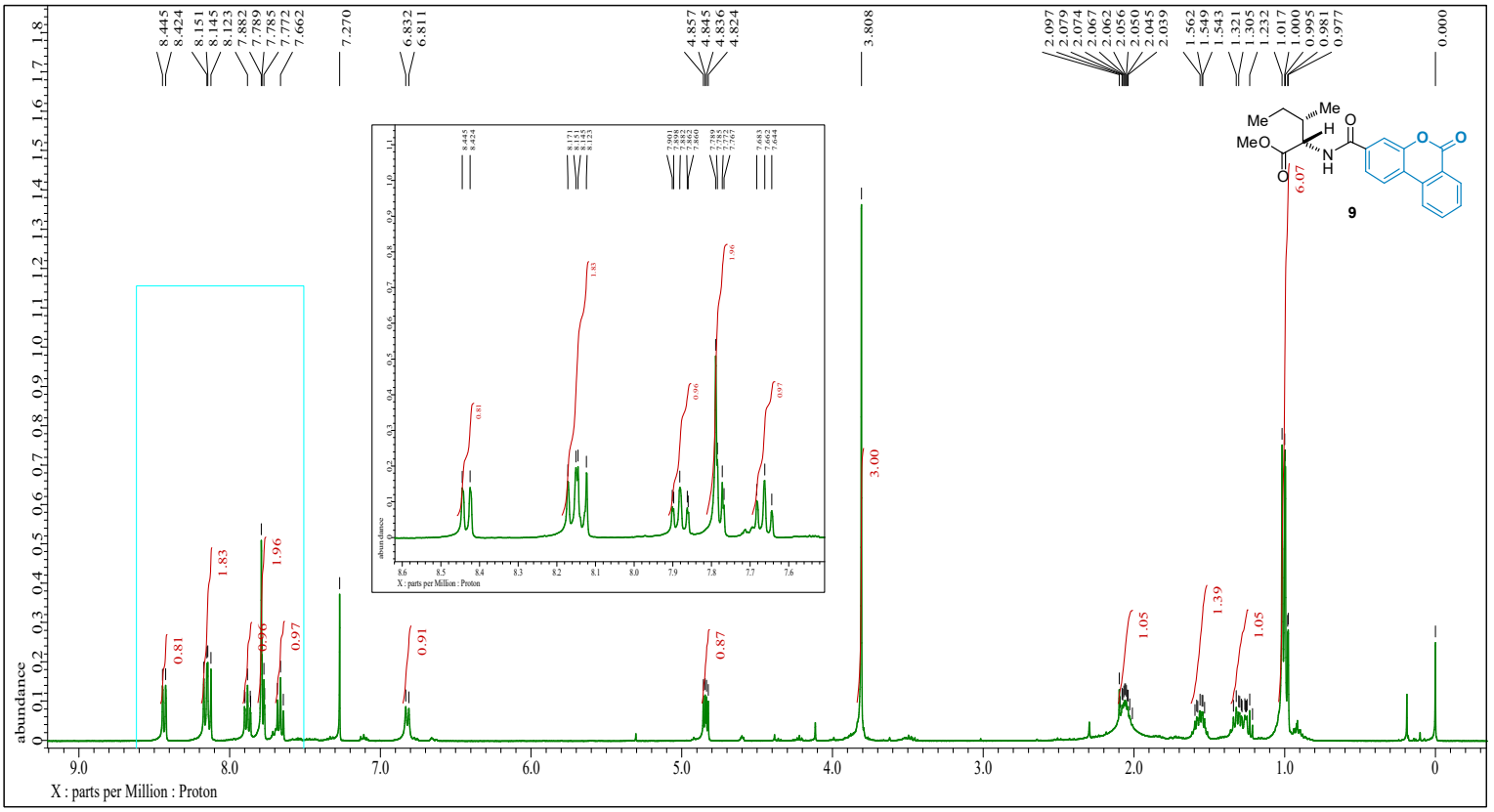
165.939
160.755
151.143
135.935
135.207
133.837
130.885
129.965
123.363
123.267
122.318
121.657
121.005
116.664
77.433
77.116
76.791
57.750
52.537
31.704
19.122
18.068
Me
Me
H
MeO
O
N
H
O
O
O
O
8
(thousandths)
X : parts per Million : Carbon13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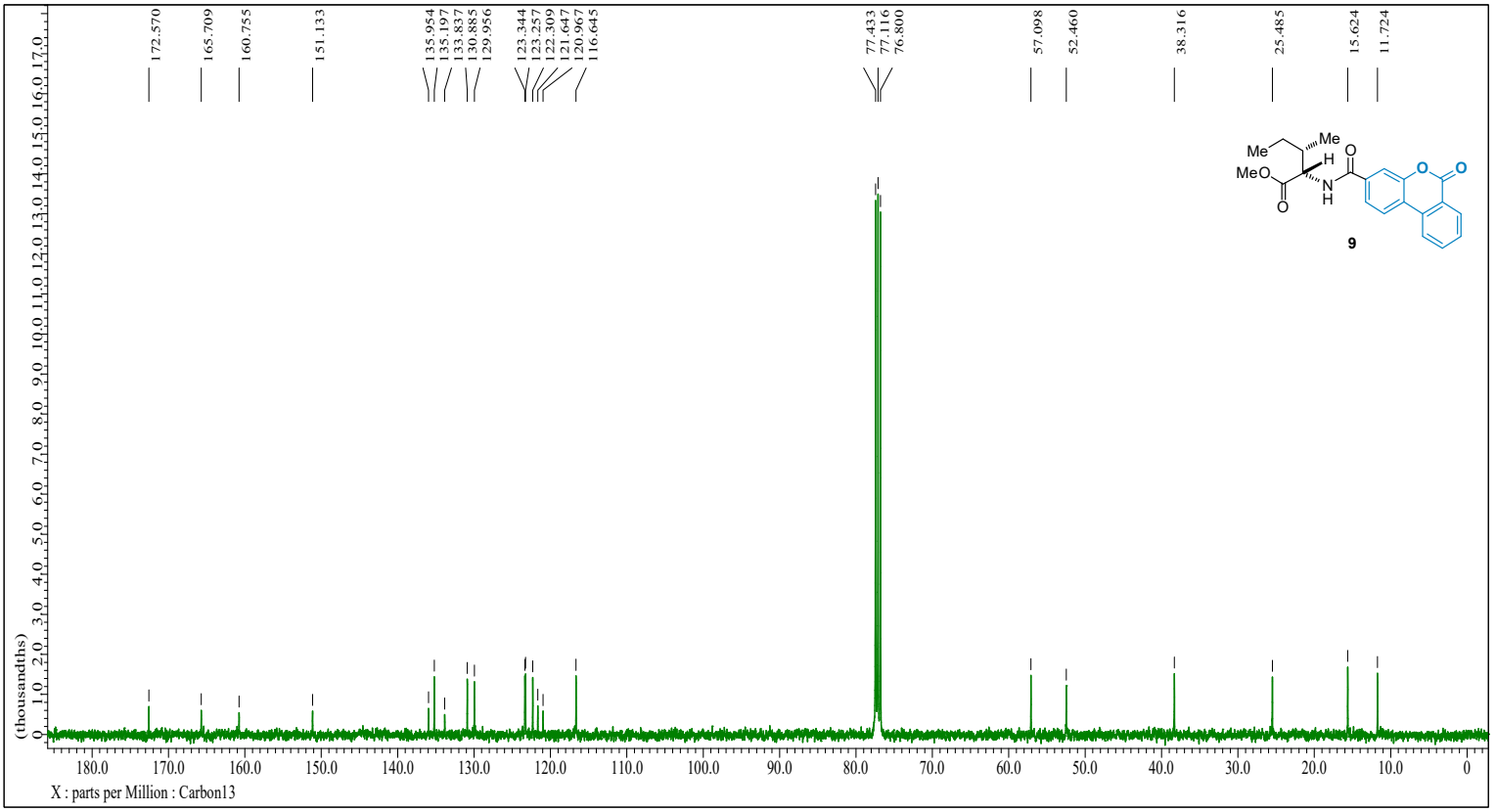
8.424
8.151
8.145
8.123
7.882
7.789
7.785
7.772
7.662
7.270
6.832
6.811
4.857
4.845
4.836
4.824
3.808
2.097
2.079
2.074
2.067
2.062
2.056
2.050
2.045
2.039
1.562
1.549
1.543
1.321
1.305
1.232
1.017
1.000
0.995
0.981
0.977
0.000
0.81
1.83
1.96
0.96
0.97
0.91
0.87
3.00
1.05
1.39
1.05
6.07
Me
MeO
H
N
H
O
O
O
O
9
abundance
X : parts per Million : Proton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135.197
133.837
130.885
129.956
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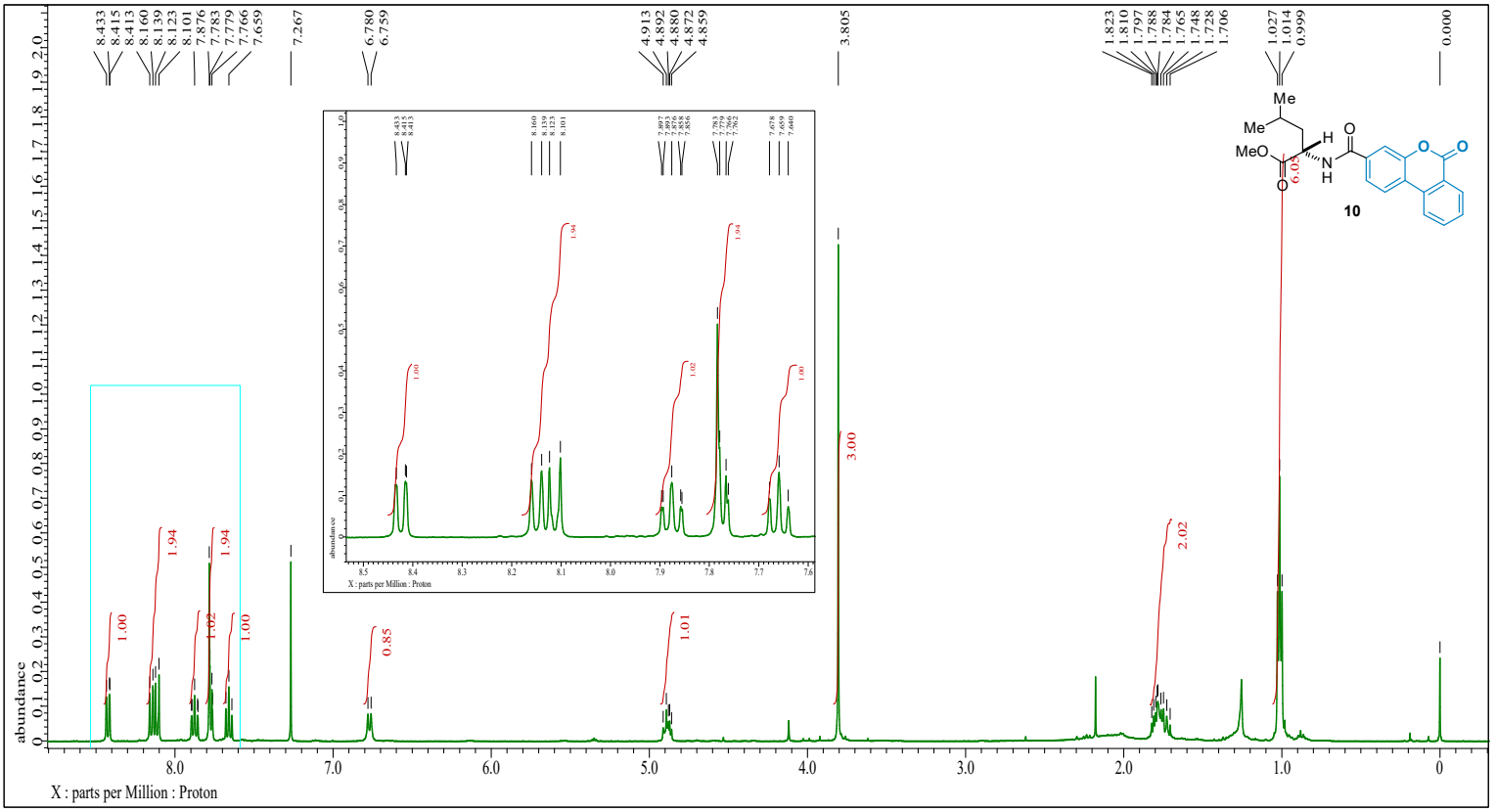
123.257
122.309
121.647
120.967
116.645
77.433
77.116
76.800
57.098
52.460
38.316
25.485
15.624
11.724
Me
MeO
H
N
H
O
O
O
O
9
(thousandths)
X : parts per Million : Carbon13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8.413
8.160
8.139
8.123
8.101
7.876
7.783
7.779
7.766
7.659
7.267
6.780
6.759
4.913
4.892
4.880
4.872
4.859
3.805
1.823
1.810
1.797
1.788
1.784
1.765
1.748
1.728
1.706
1.027
1.014
0.999
0.000
1.00
1.94
1.94
1.02
1.00
0.85
1.01
3.00
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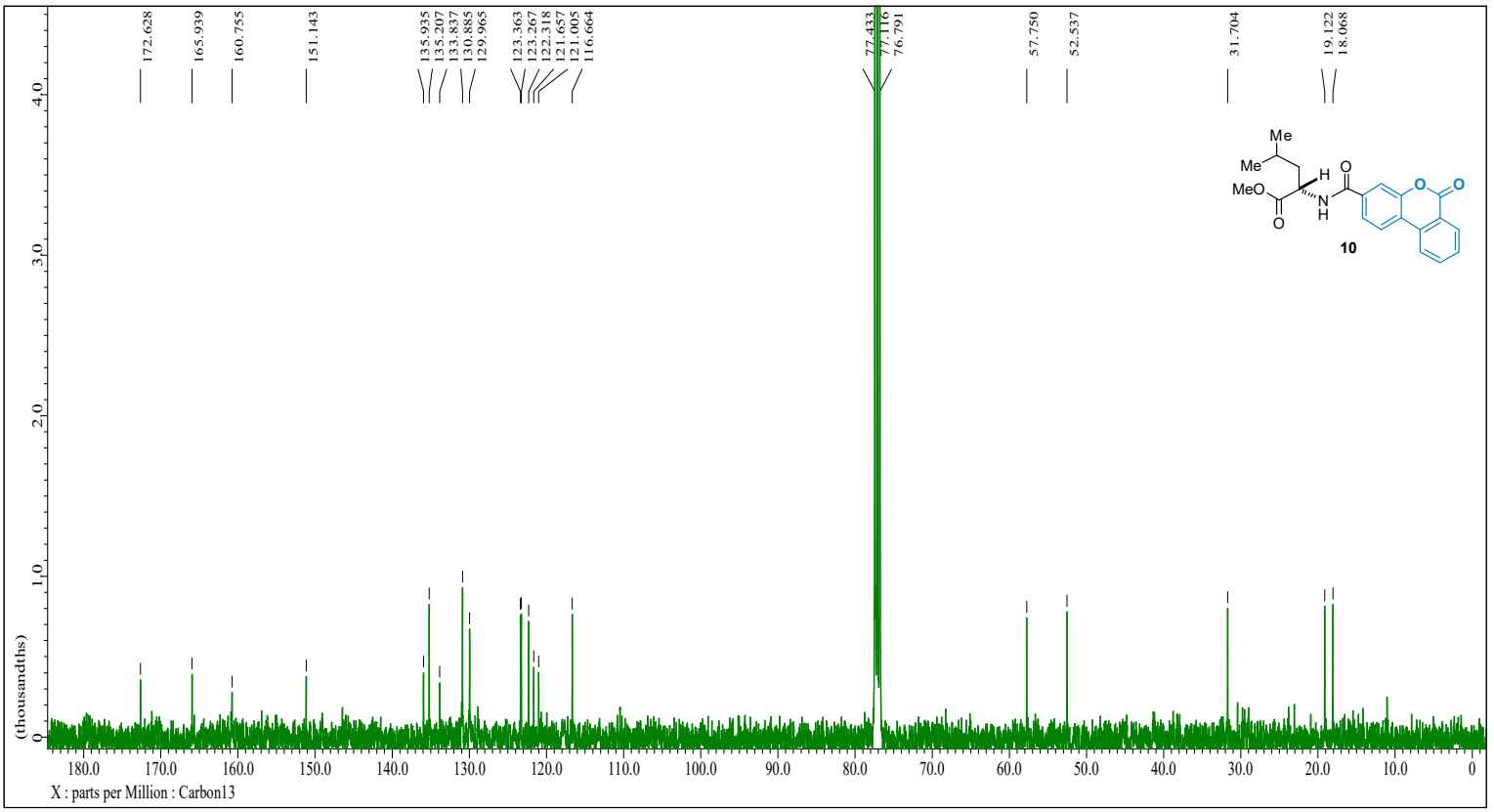
Me
Me
MeO
H
N
H
O
O
O
O
10
abundance
X : parts per Million : Proton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151.143
135.935
135.207
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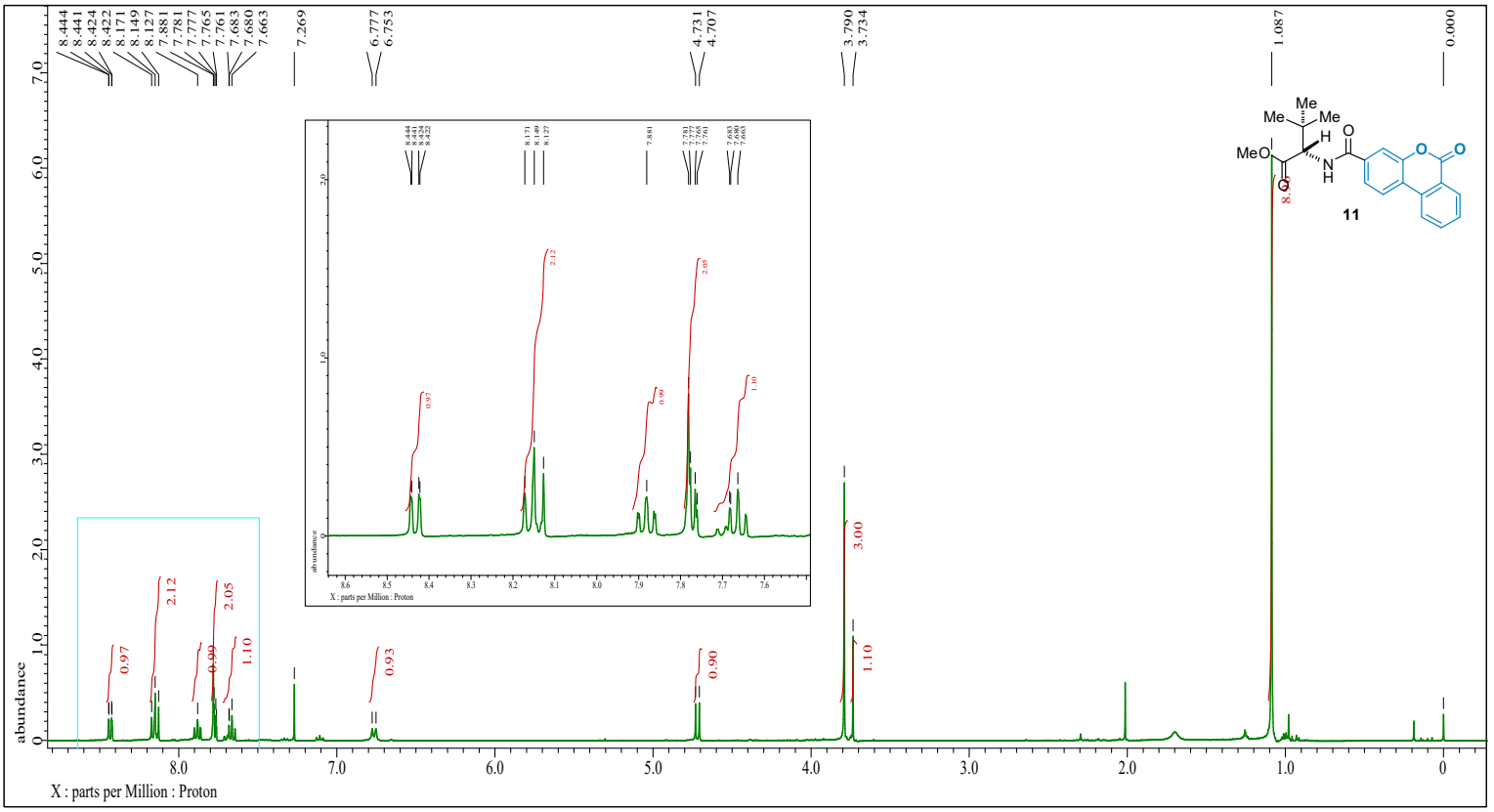
130.885
129.965
123.363
123.267
122.318
121.657
121.005
116.664
77.433
77.116
76.791
57.750
52.537
31.704
19.122
18.068
Me
Me
MeO
H
N
H
O
O
O
O
10
(thousandths)
X : parts per Million : Carbon13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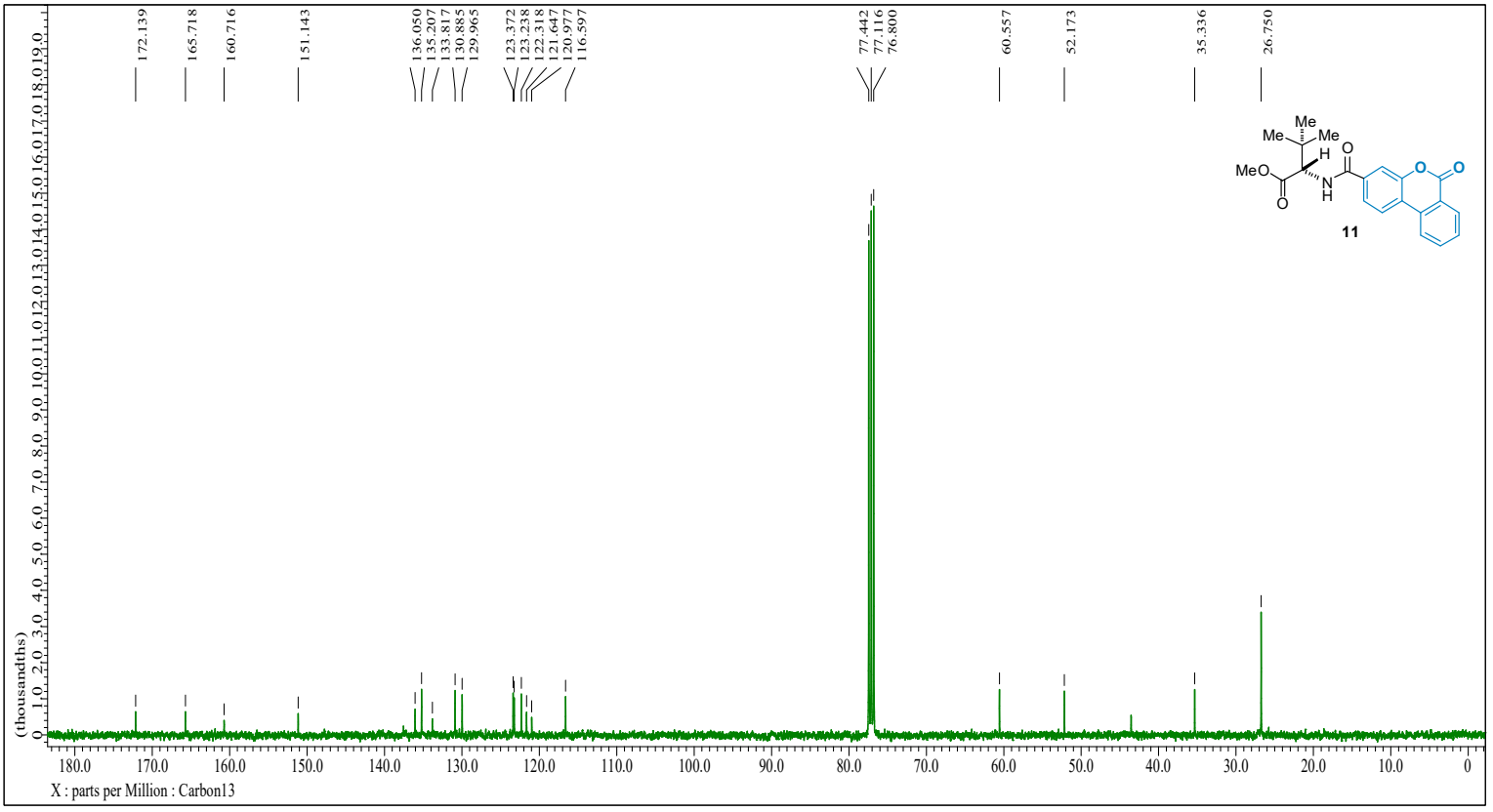
8.424
8.422
8.171
8.149
8.127
7.881
7.781
7.777
7.765
7.761
7.683
7.680
7.663
7.269
6.777
6.753
4.731
4.707
3.790
3.734
1.087
0.000
0.97
2.12
2.05
0.99
1.10
0.93
0.90
3.00
1.10
abundance
X : parts per Million : Proton
Me
Me
Me
H
N
H
O
MeO
O
O
O
11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135.207
133.817
130.885
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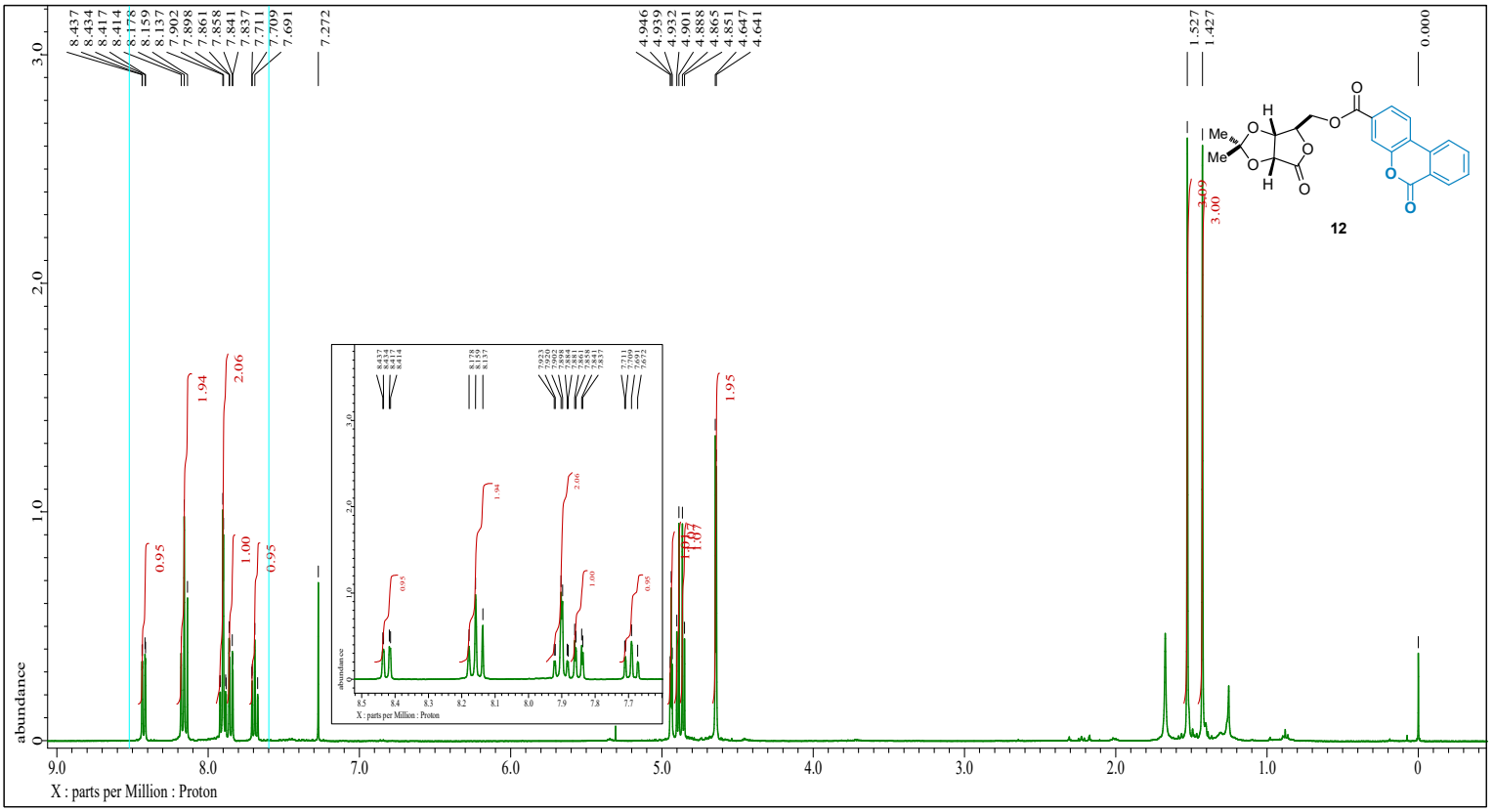
123.372
123.238
122.318
121.647
120.977
116.597
77.442
77.116
76.800
60.557
52.173
35.336
26.750
(thousandths)
X : parts per Million : Carbon13
Me
Me
Me
H
N
H
O
MeO
O
O
O
11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8.414
8.178
8.159
8.137
7.902
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7.861
7.858
7.841
7.837
7.711
7.709
7.691
7.272
4.946
4.939
4.932
4.901
4.888
4.865
4.851
4.647
4.641
1.527
1.427
0.000
0.95
1.94
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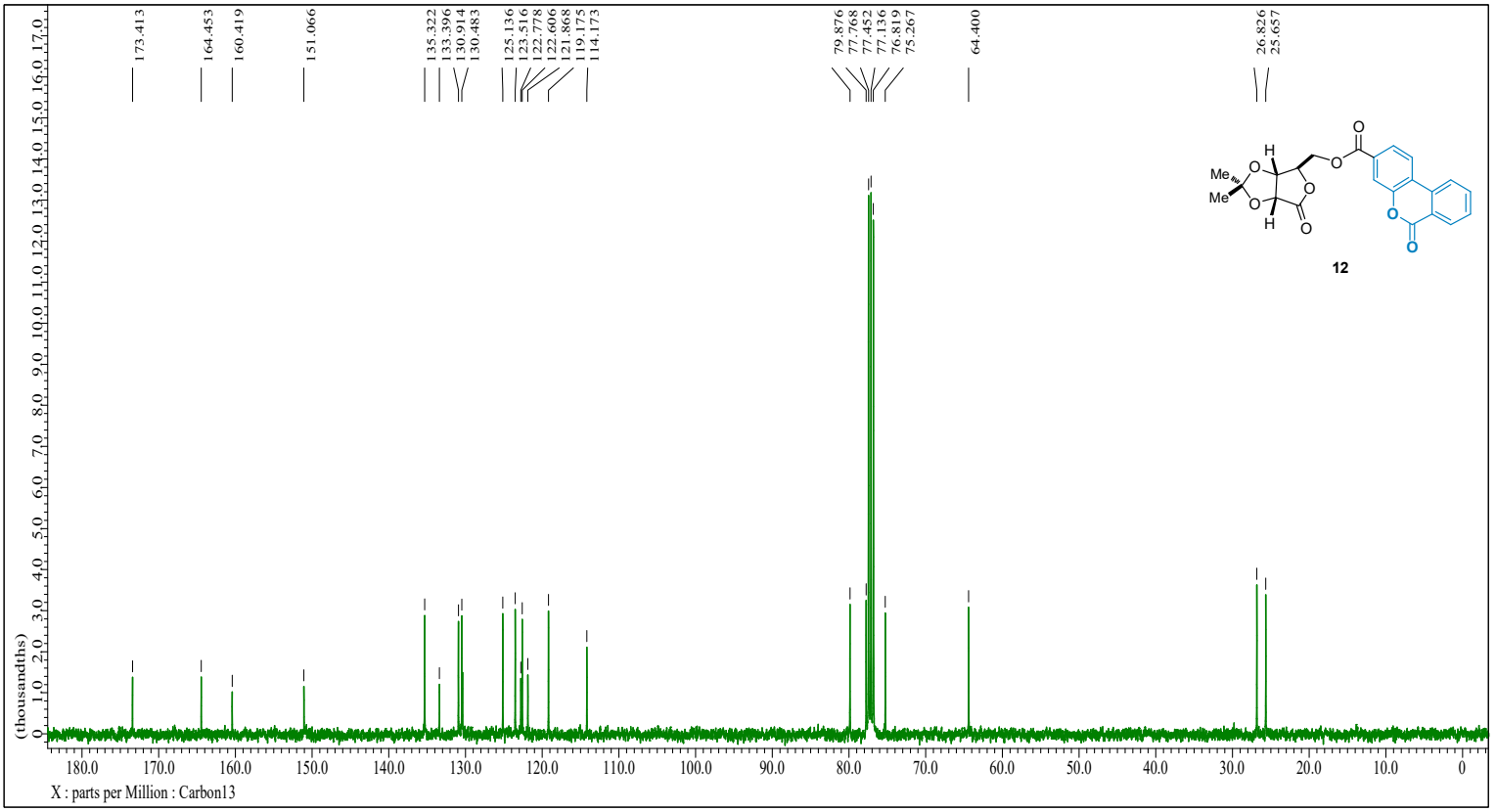
0.95
1.95
1.07
3.09
3.00
Me
Me
12
abundance
X : parts per Million : Proton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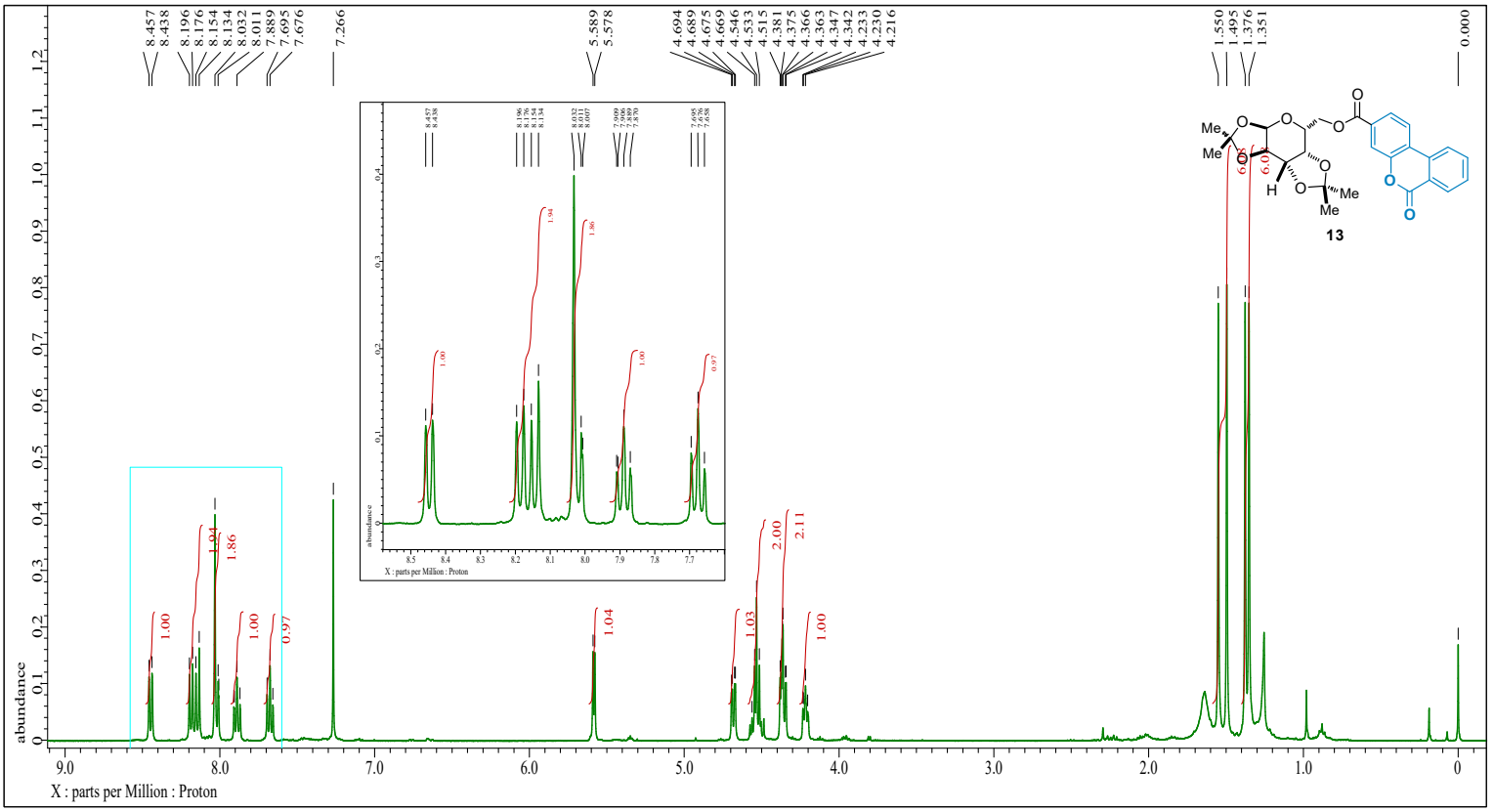
151.066
135.322
133.396
130.914
130.483
125.136
123.516
122.778
122.606
121.868
119.175
114.173
79.876
77.768
77.452
77.136
76.819
75.267
64.400
26.826
25.657
Me
Me
12
(thousandths)
X : parts per Million : Carbon13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8.176
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8.134
8.032
8.011
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7.676
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5.589
5.578
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4.689
4.675
4.669
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4.533
4.515
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4.375
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4.216
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1.495
1.376
1.351
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1.00
1.04
1.86
1.00
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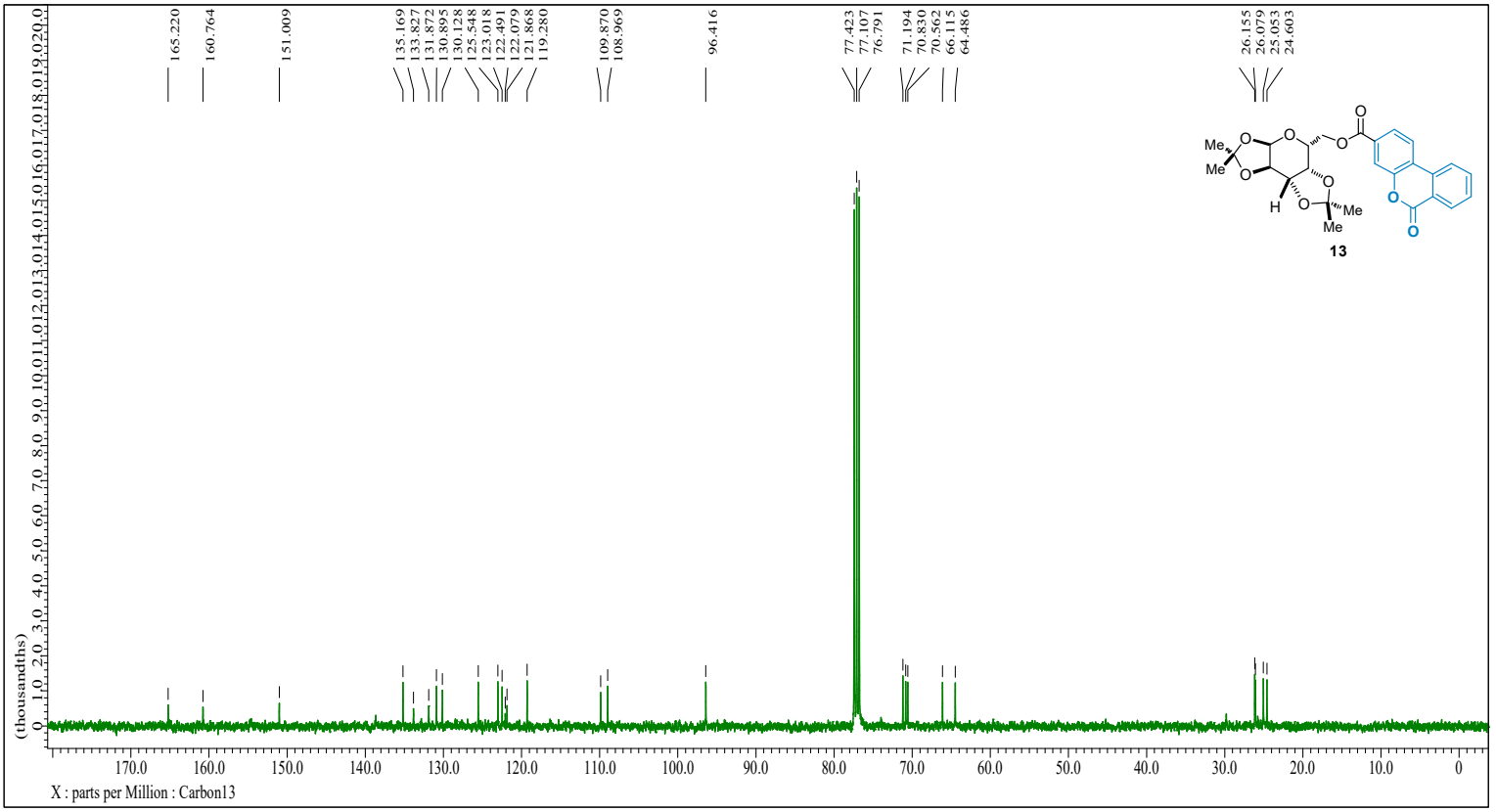
1.03
2.00
2.11
1.00
6.0
6.0
13
abundance
X : parts per Million : Proton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122.079
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109.870
108.969
96.416
77.423
77.107
76.791
71.194
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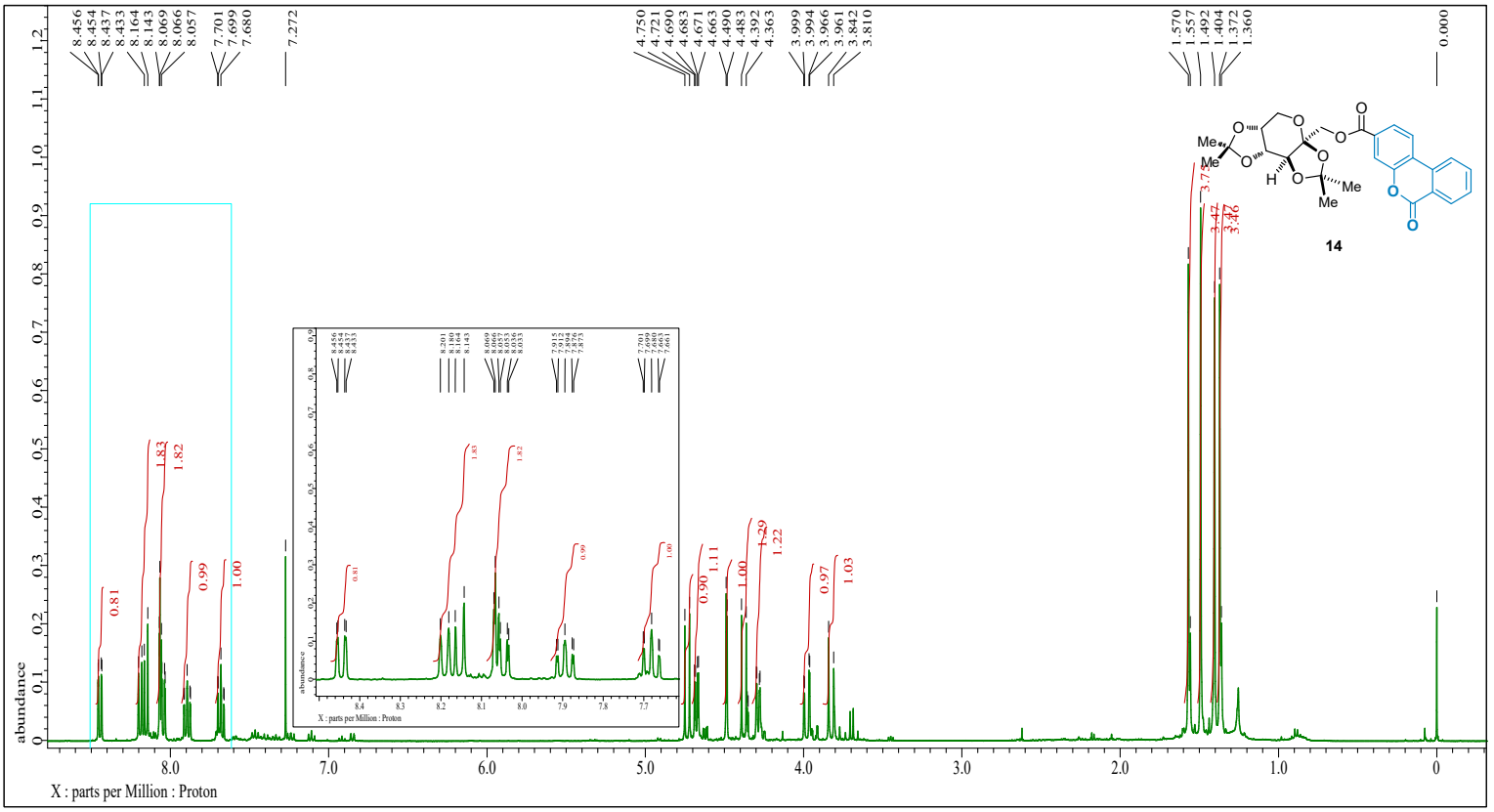
66.115
64.486
26.155
26.079
25.053
24.603
13
(thousandths)
X : parts per Million : Carbon13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8.066
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7.699
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7.272
4.750
4.721
4.690
4.683
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4.663
4.490
4.483
4.392
4.363
3.999
3.994
3.966
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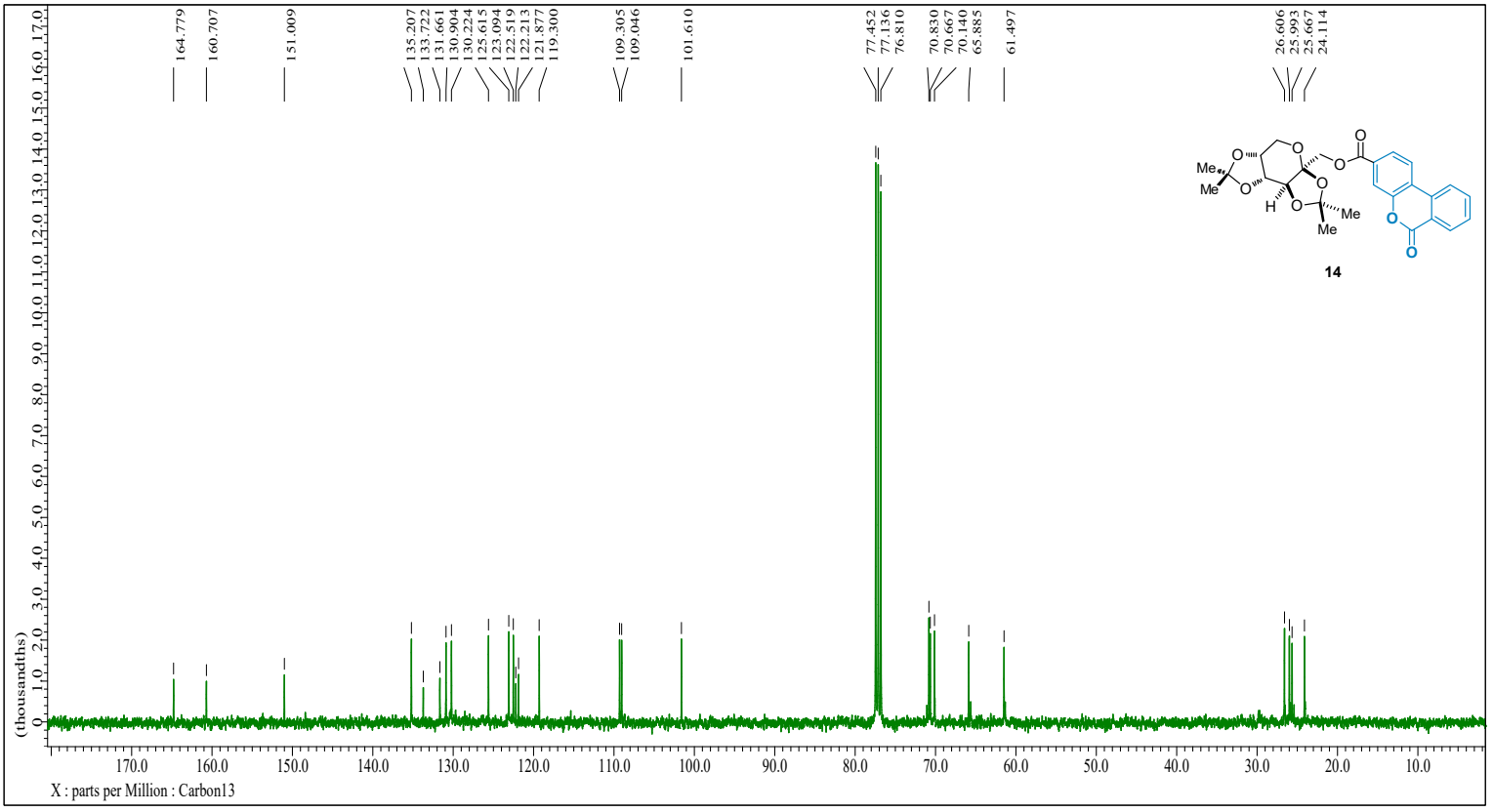
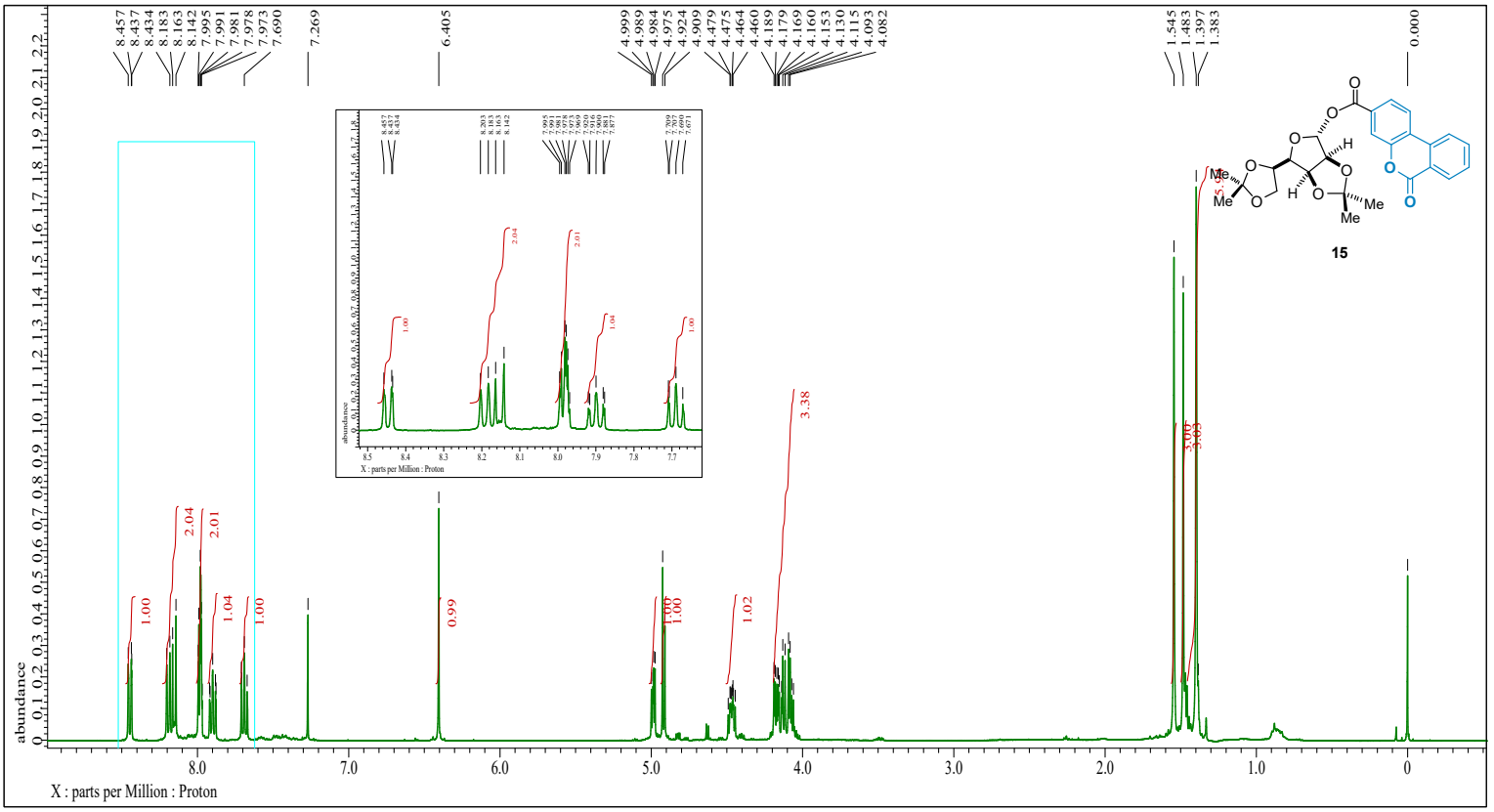
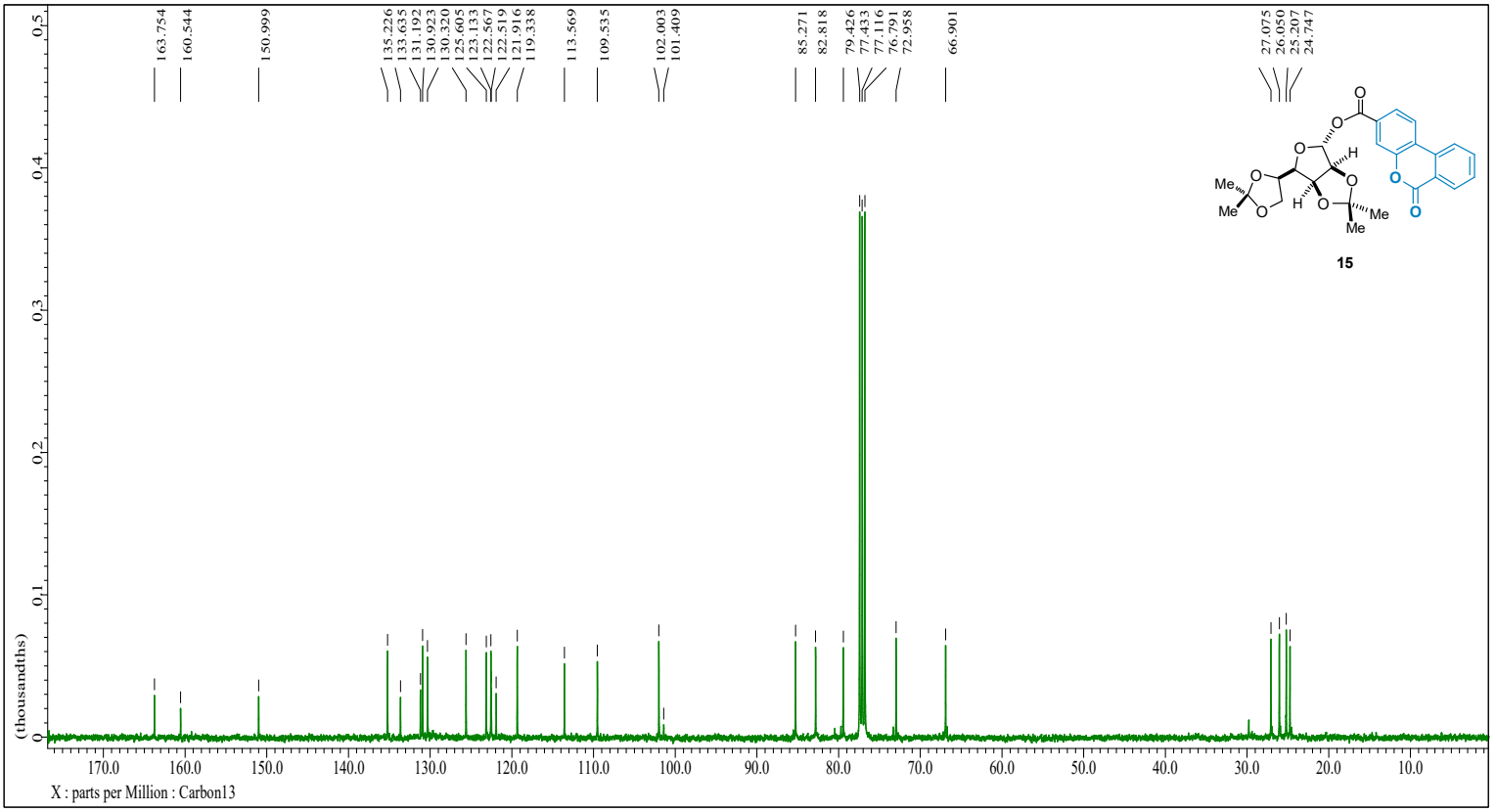
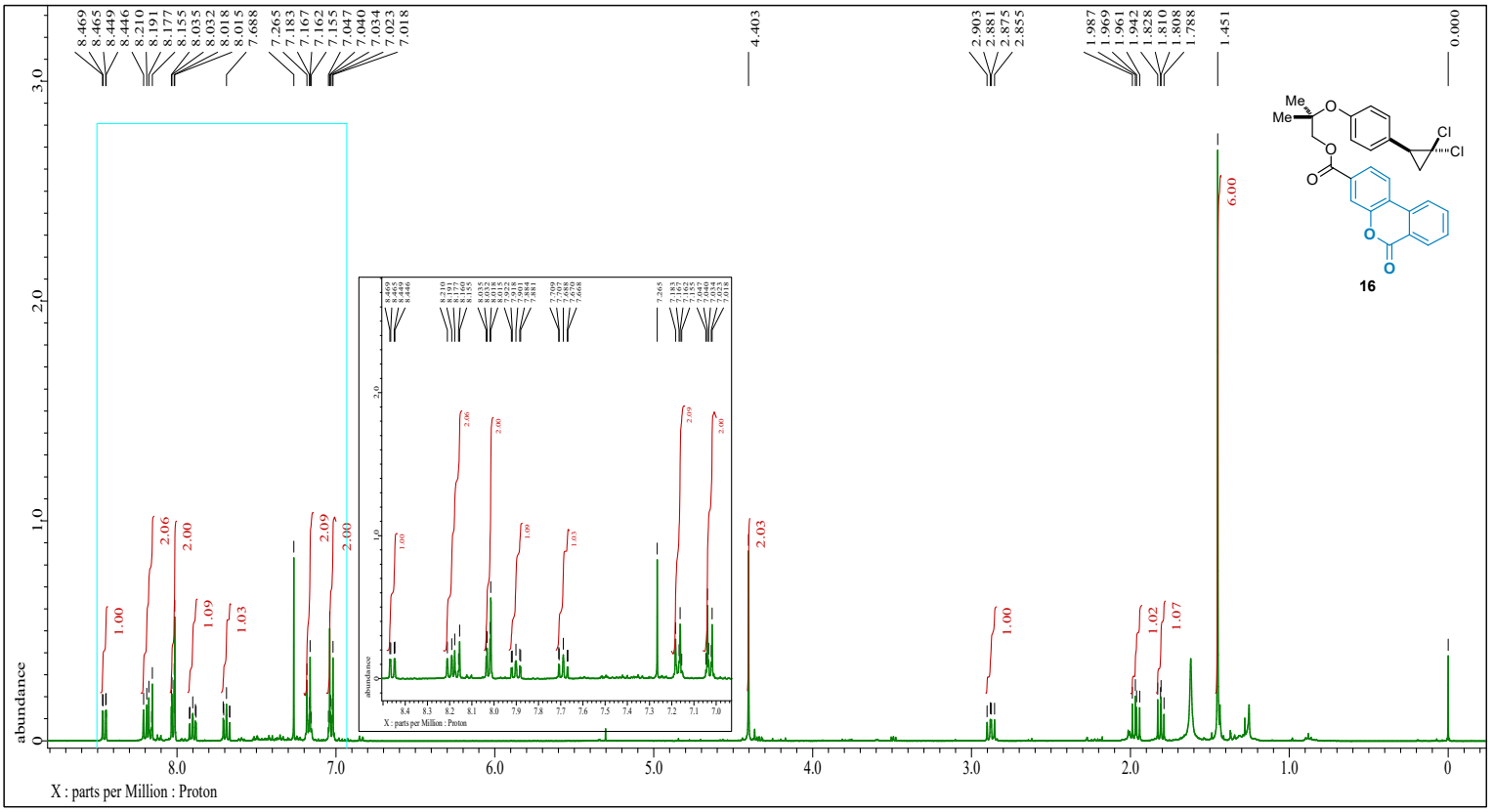
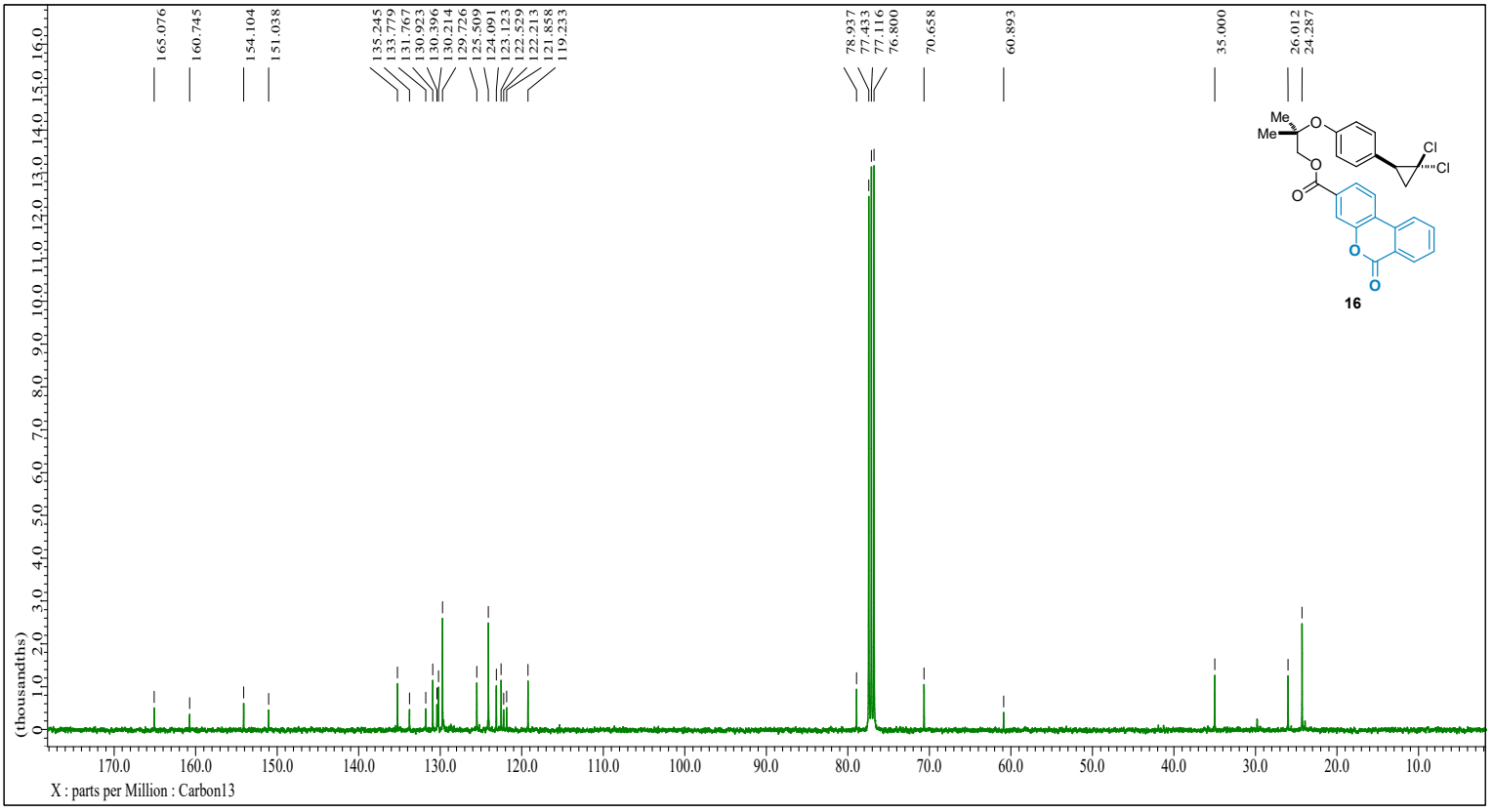
3.810
1.570
1.557
1.492
1.404
1.372
1.360
0.000
0.81
1.83
1.82
0.99
1.00
0.90
1.11
1.00
1.29
1.22
0.97
1.03
3.47
3.46
14
abundance
X : parts per Million : Proton

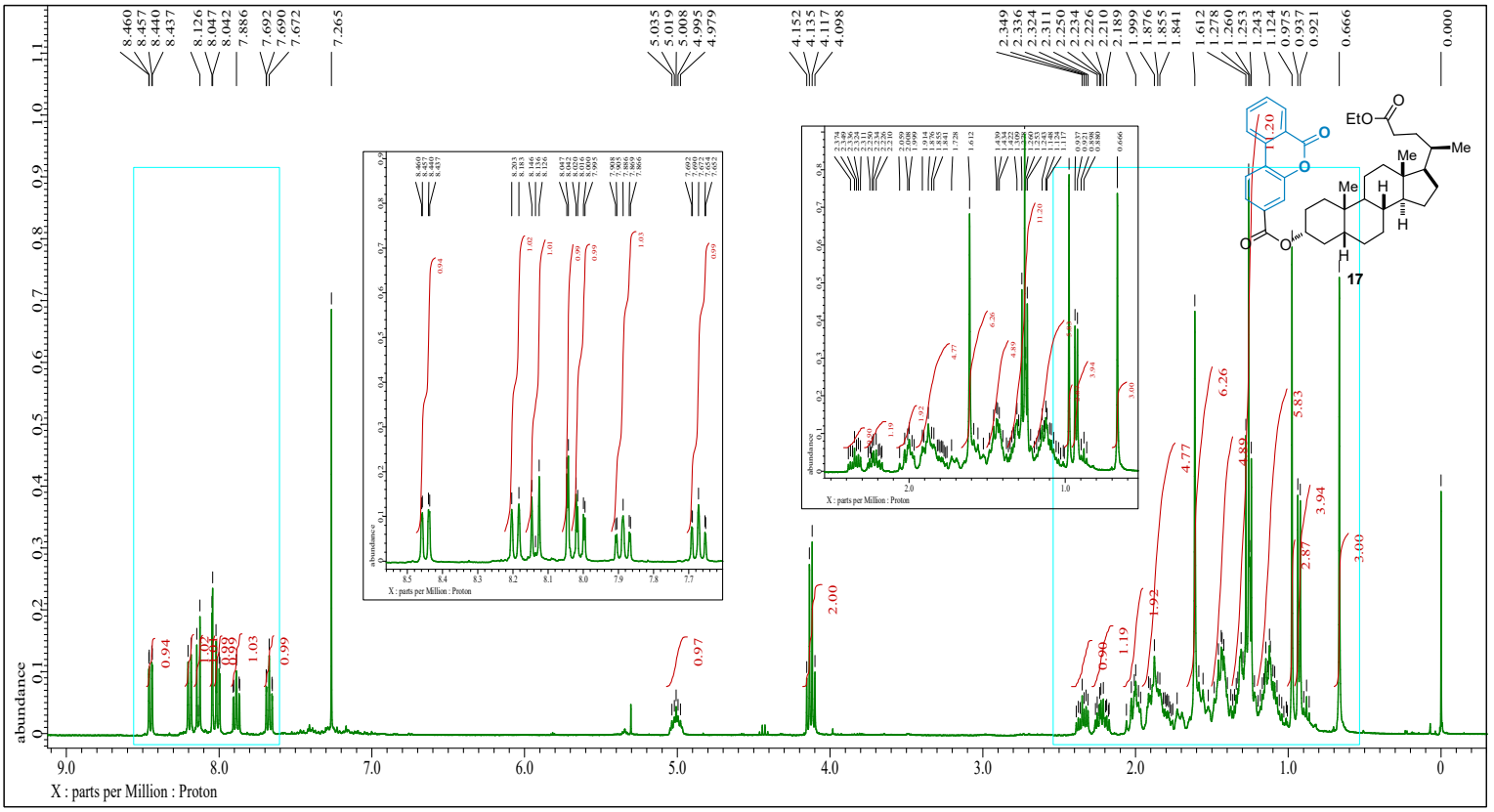

164.779
160.707
151.009
135.207
133.722
131.661
130.904
130.224
125.615
123.094
122.519
122.213
121.877
119.300
109.305
109.046
101.610
77.452
77.136
76.810
70.830
70.667
70.140
65.885
61.497
26.606
25.993
25.667
24.114
14
(thousandths)
X : parts per Million : Carbon13

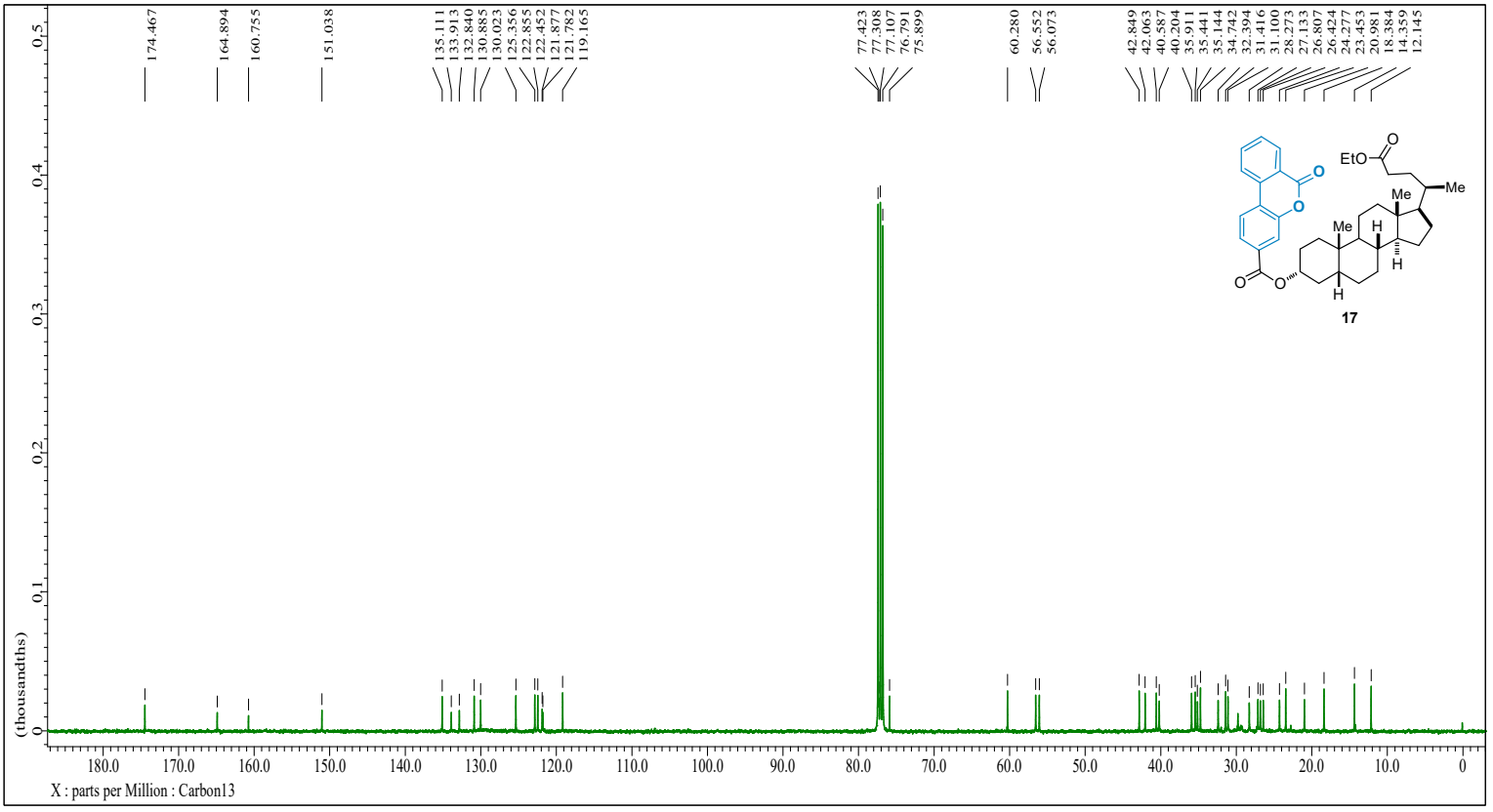

8.457
8.437
8.434
8.183
8.163
8.142
7.995
7.991
7.981
7.978
7.973
7.690
7.269
6.405
4.999
4.989
4.984
4.975
4.924
4.909
4.479
4.475
4.464
4.460
4.189
4.179
4.169
4.160
4.153
4.130
4.115
4.093
4.082
1.545
1.483
1.397
1.383
0.000
1.00
2.04
2.01
1.04
1.00
0.99
1.00
1.00
1.02
3.38
3.06
3.03
15
abundance
X : parts per Million : Proton

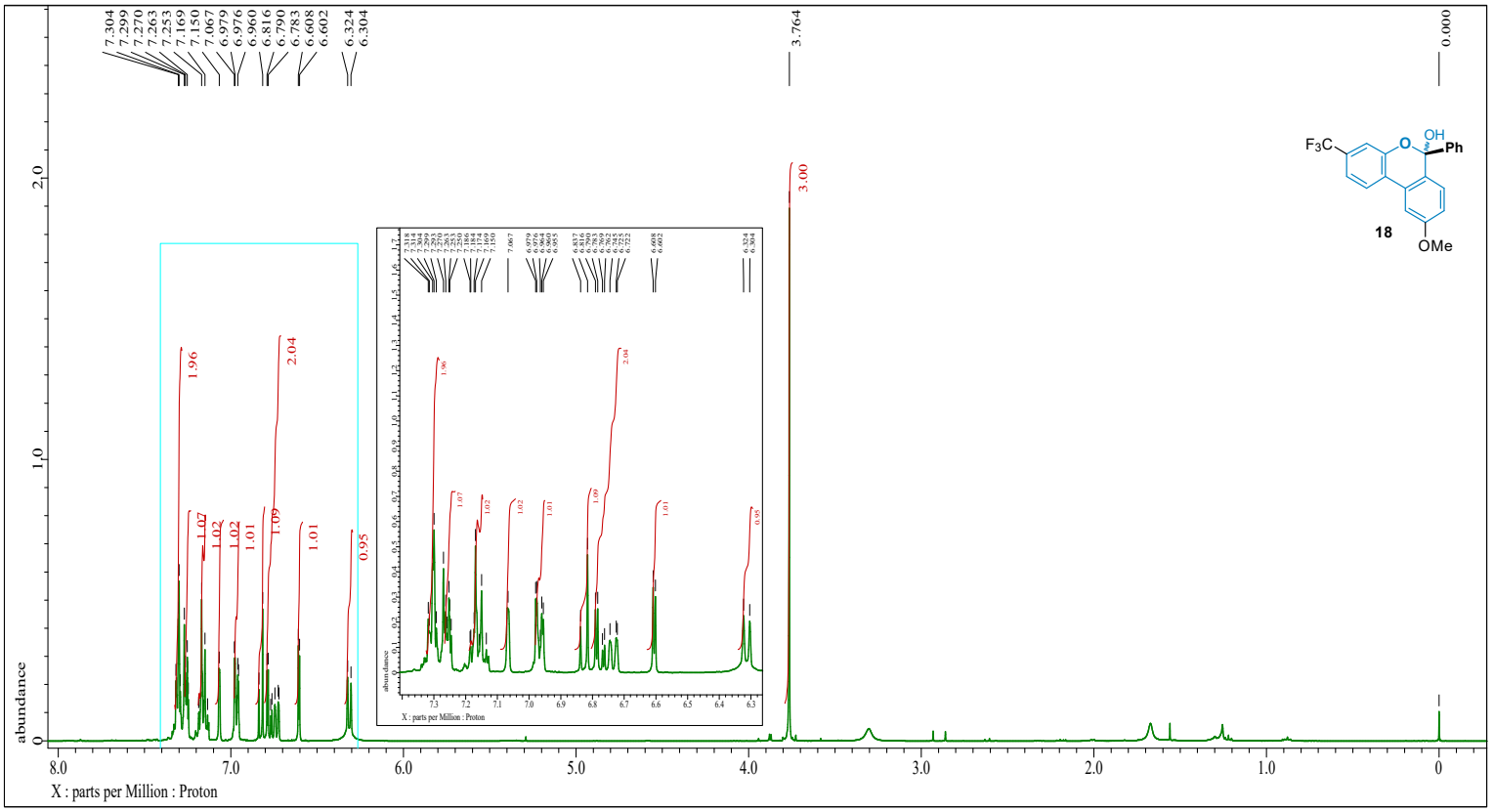

163.754
160.544
150.999
135.226
133.635
131.192
130.923
130.320
125.605
123.133
122.567
122.519
121.916
119.338
113.569
109.535
102.003
101.409
85.271
82.818
79.426
77.433
77.116
76.791
72.958
66.901
27.075
26.050
25.207
24.747
15
(thousandths)
X : parts per Million : Carbon13


8.469
8.465
8.449
8.446
8.210
8.191
8.177
8.155
8.035
8.032
8.018
8.015
7.688
7.265
7.183
7.167
7.162
7.155
7.047
7.040
7.034
7.023
7.018
4.403
2.903
2.881
2.875
2.855
1.987
1.969
1.961
1.942
1.828
1.810
1.808
1.788
1.451
0.000
1.00
2.06
2.00
1.09
1.03
2.09
2.00
2.03
1.00
1.02
1.07
6.00
abundance
X : parts per Million : Proton
Me
Me
O
O
O
Cl
Cl
O
O
16


165.076
160.745
154.104
151.038
135.245
133.779
131.767
130.923
130.396
130.214
129.726
125.509
124.091
123.123
122.529
122.213
121.858
119.233
78.937
77.433
77.116
76.800
70.658
60.893
35.000
26.012
24.287
(thousandths)
X : parts per Million : Carbon13
Me
Me
O
O
O
Cl
Cl
O
O
16


abundance
X : parts per Million : Proton
17


(thousandths)
X : parts per Million : Carbon13
17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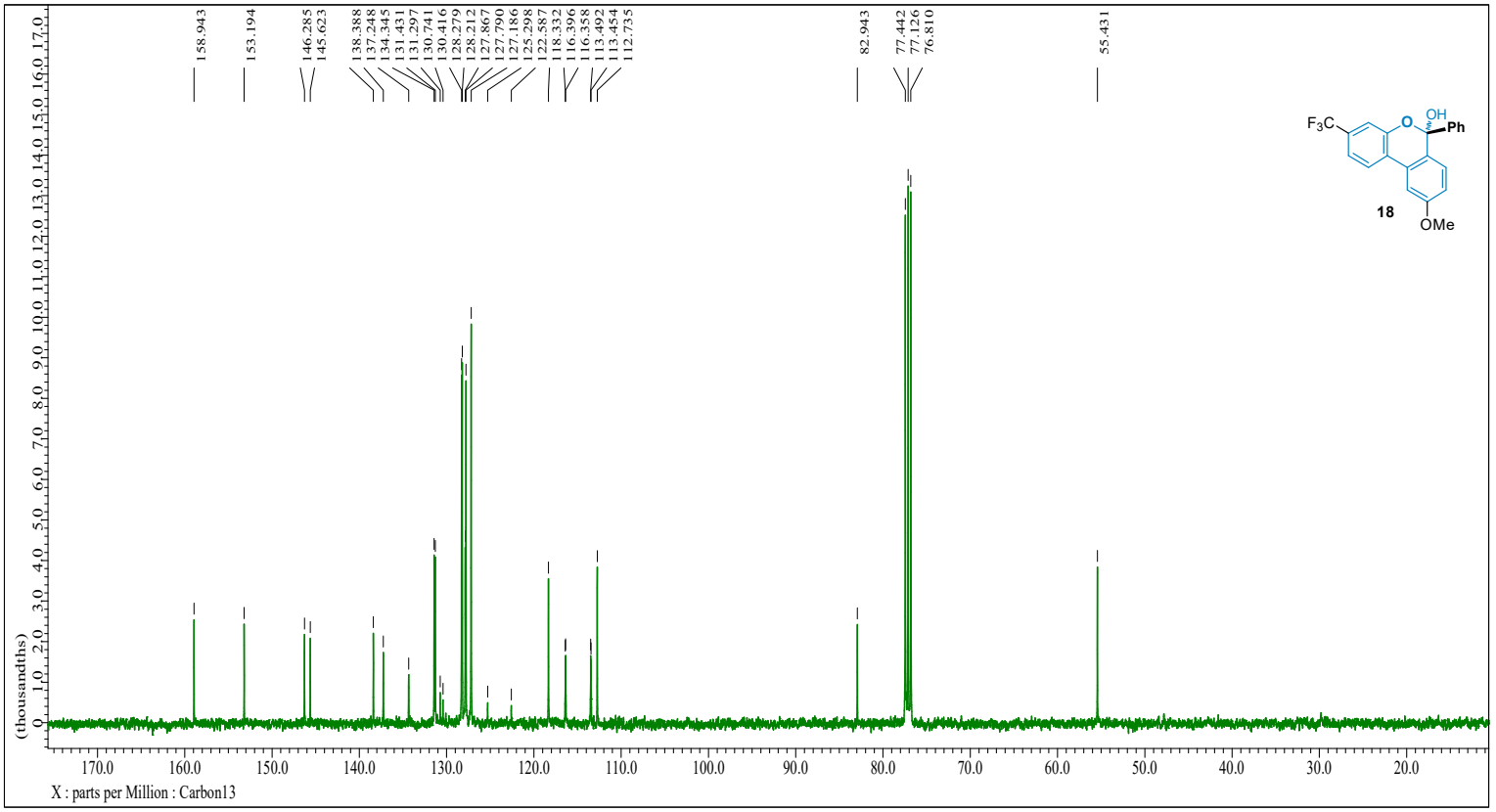
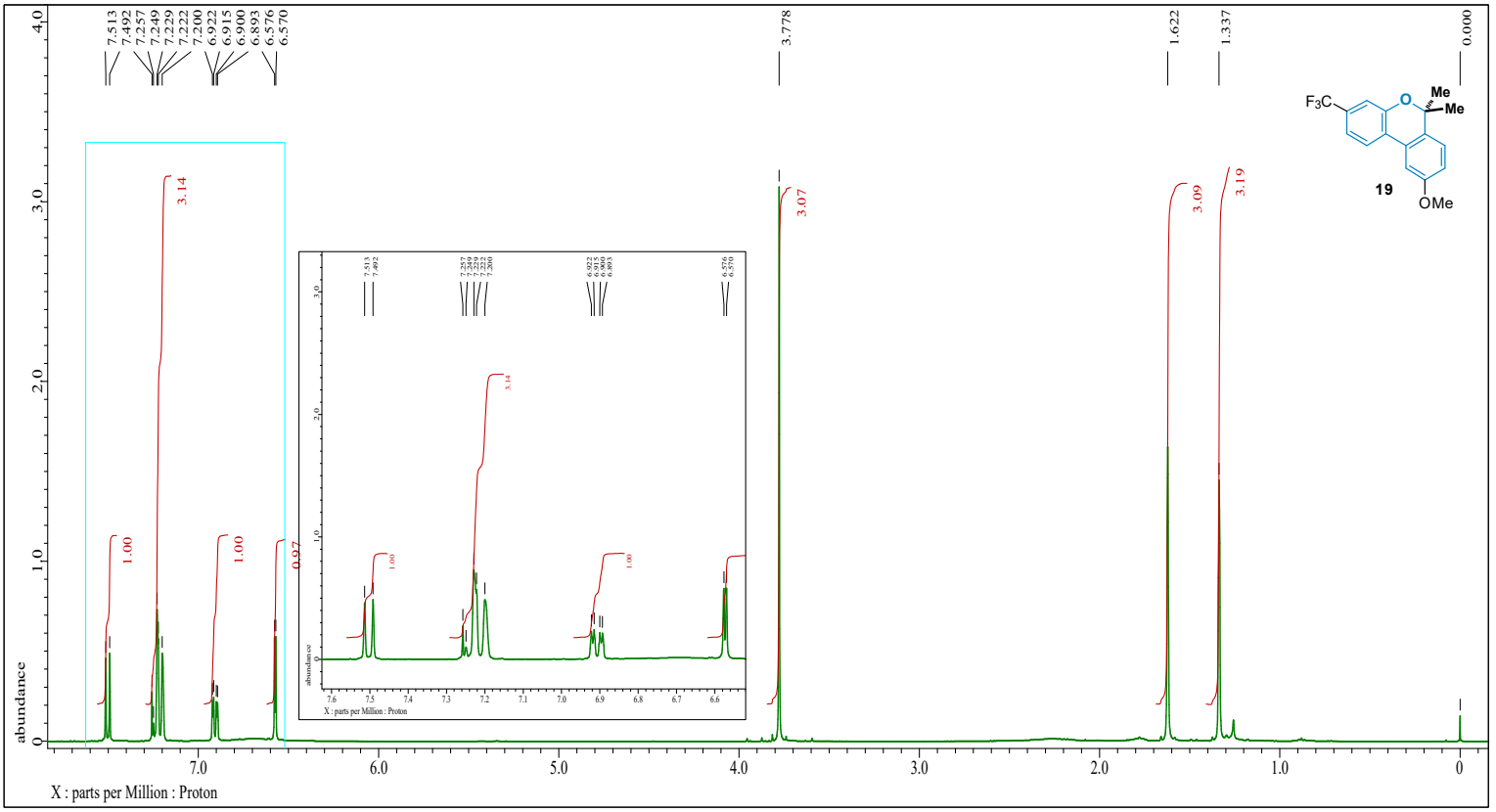
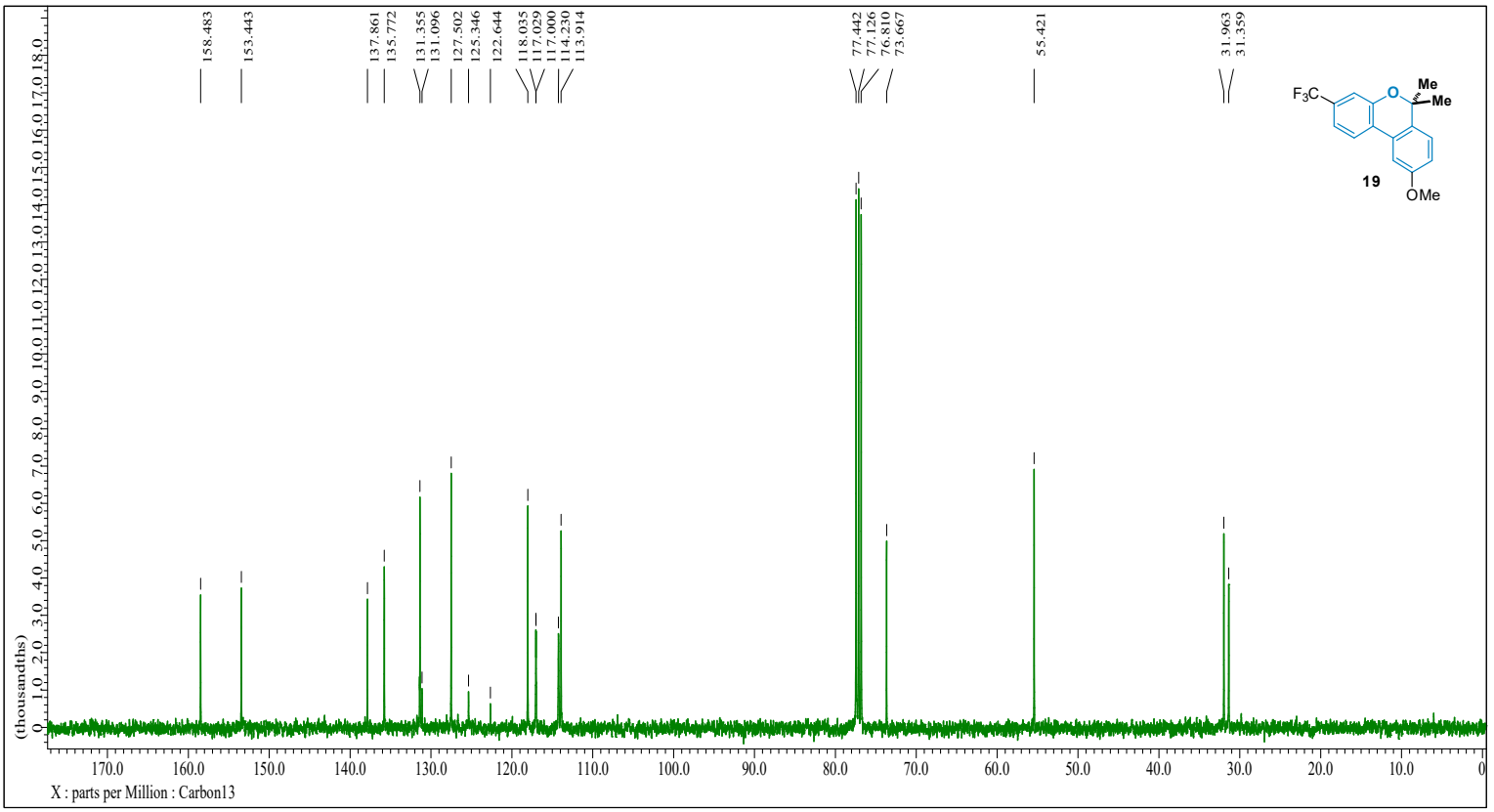
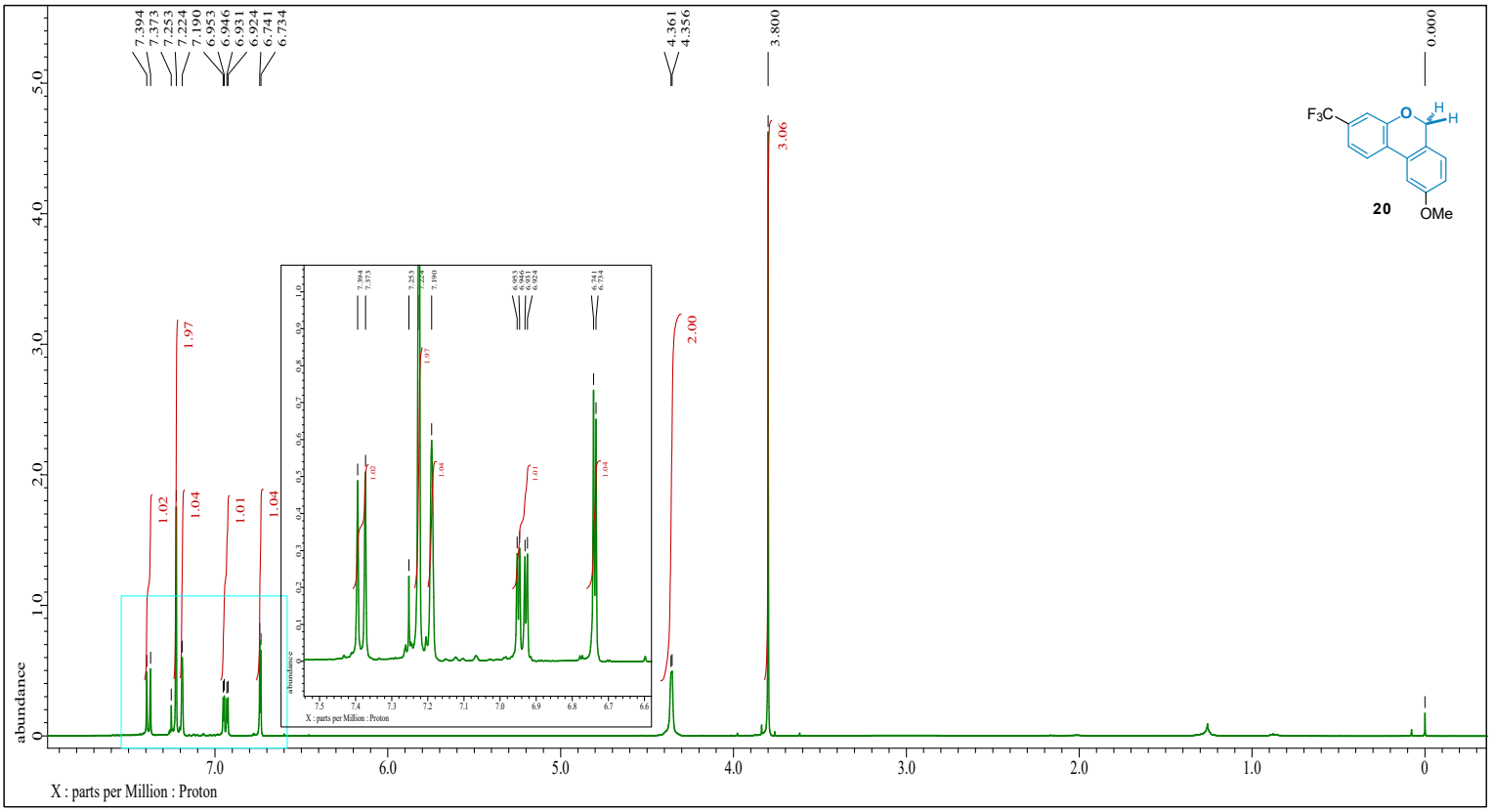
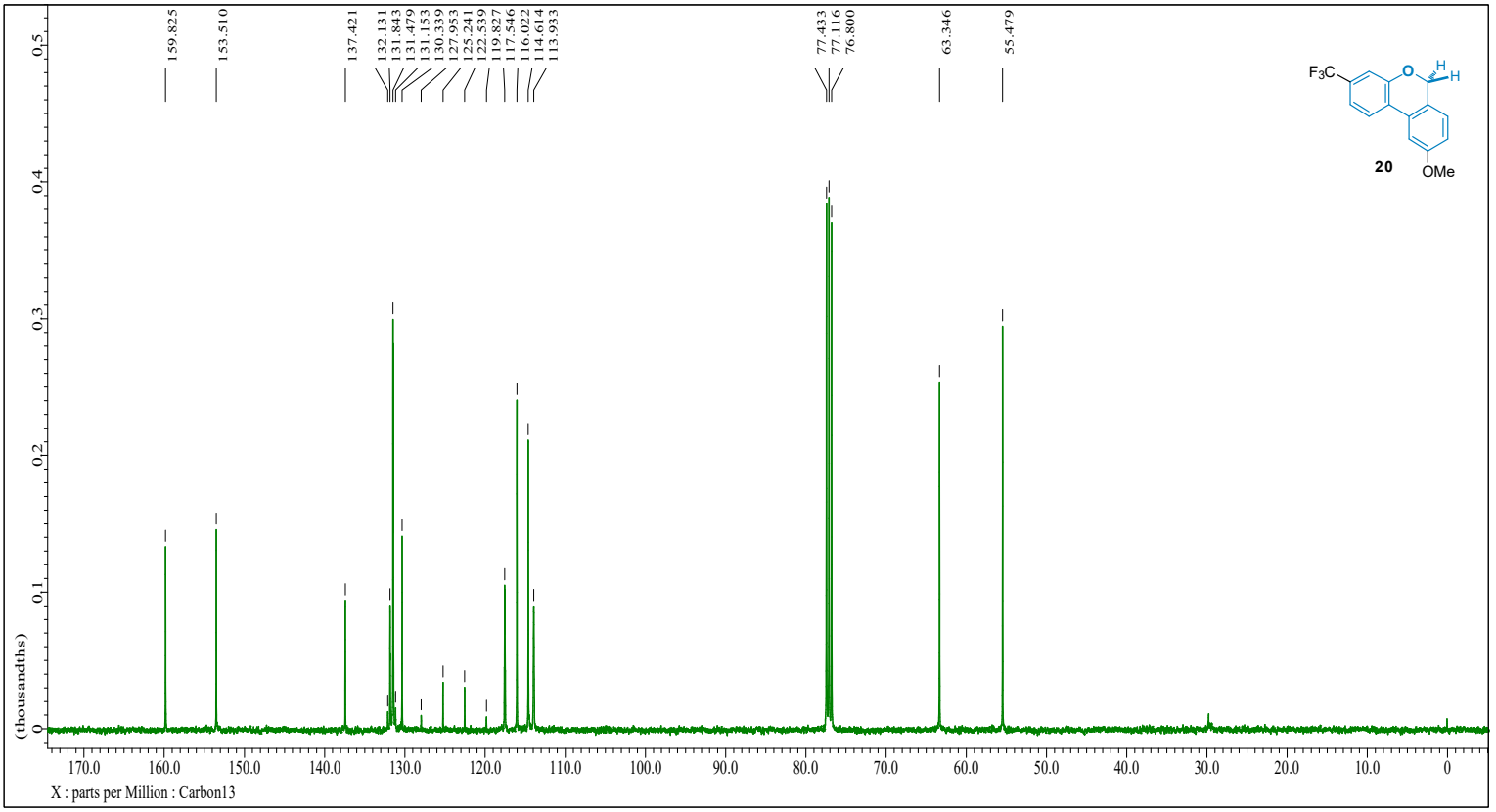
7.299
7.270
7.263
7.253
7.169
7.150
7.067
6.979
6.976
6.960
6.816
6.790
6.783
6.608
6.602
6.324
6.304
3.764
0.000
3.00
1.96
2.04
1.07
1.02
1.02
1.01
1.09
1.01
0.95
abundance
X : parts per Million : Proton
F3C
OH
Ph
O
18
OMe


158.943
153.194
146.285
145.623
138.388
137.248
134.345
131.431
131.297
130.741
130.416
128.279
128.212
127.867
127.790
127.186
125.298
122.587
118.332
116.396
116.358
113.492
113.454
112.735
82.943
77.442
77.126
76.810
55.431
(thousandths)
X : parts per Million : Carbon13
F3C
OH
Ph
O
18
OMe


7.513
7.492
7.257
7.249
7.229
7.222
7.200
6.922
6.915
6.900
6.893
6.576
6.570
3.778
1.622
1.337
0.000
3.14
3.07
3.09
3.19
1.00
1.00
0.97
abundance
X : parts per Million : Proton
F3C
Me
Me
O
19
OMe


158.483
153.443
137.861
135.772
131.355
131.096
127.502
125.346
122.644
118.035
117.029
117.000
114.230
113.914
77.442
77.126
76.810
73.667
55.421
31.963
31.359
(thousandths)
X : parts per Million : Carbon13
F3C
Me
Me
O
19
OMe


7.394
7.373
7.253
7.224
7.190
6.953
6.946
6.931
6.924
6.741
6.734
4.361
4.356
3.800
0.000
3.06
2.00
1.97
1.02
1.04
1.01
1.04
abundance
X : parts per Million : Proton
F3C
O
H
H
20
OMe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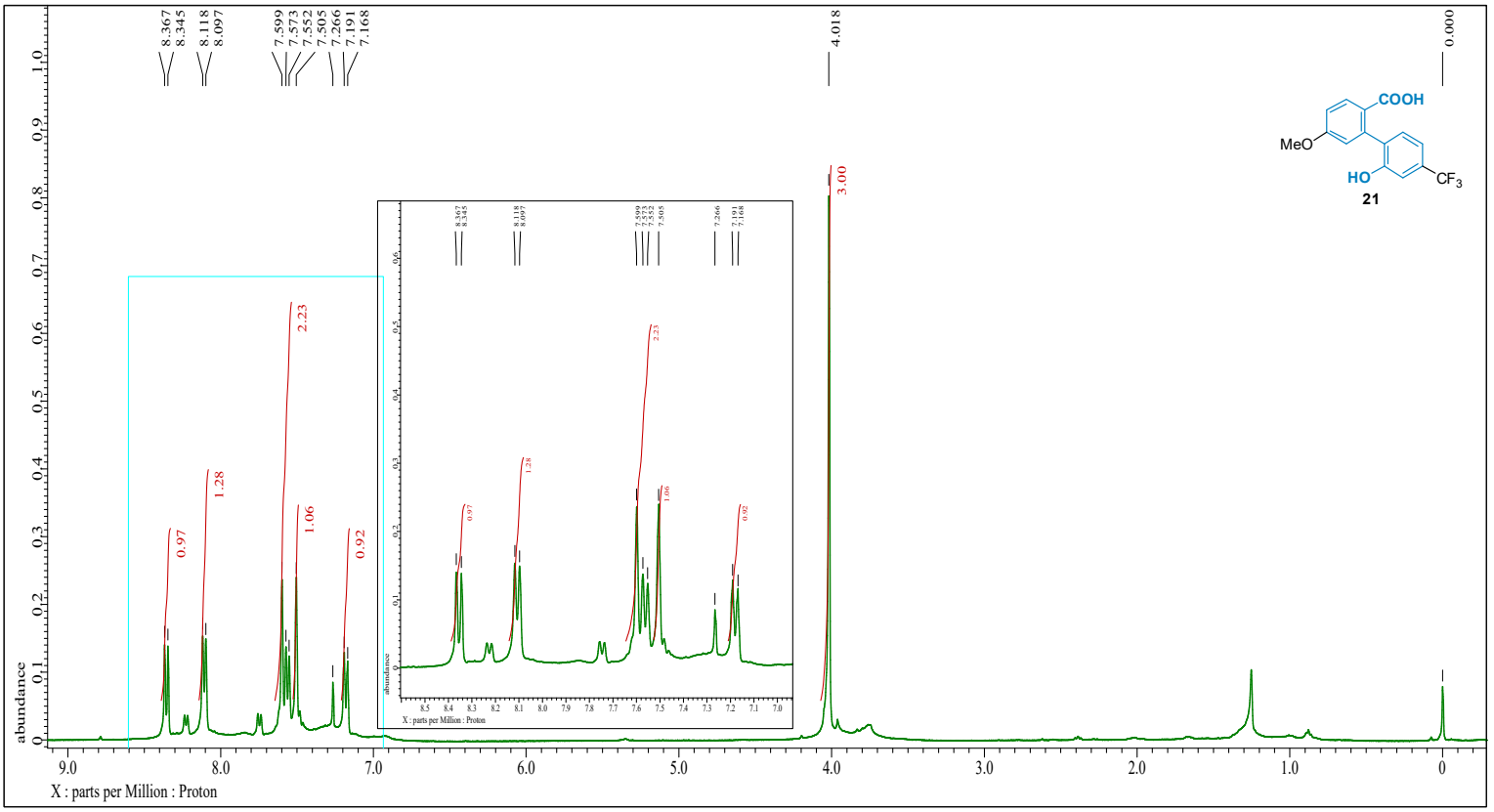
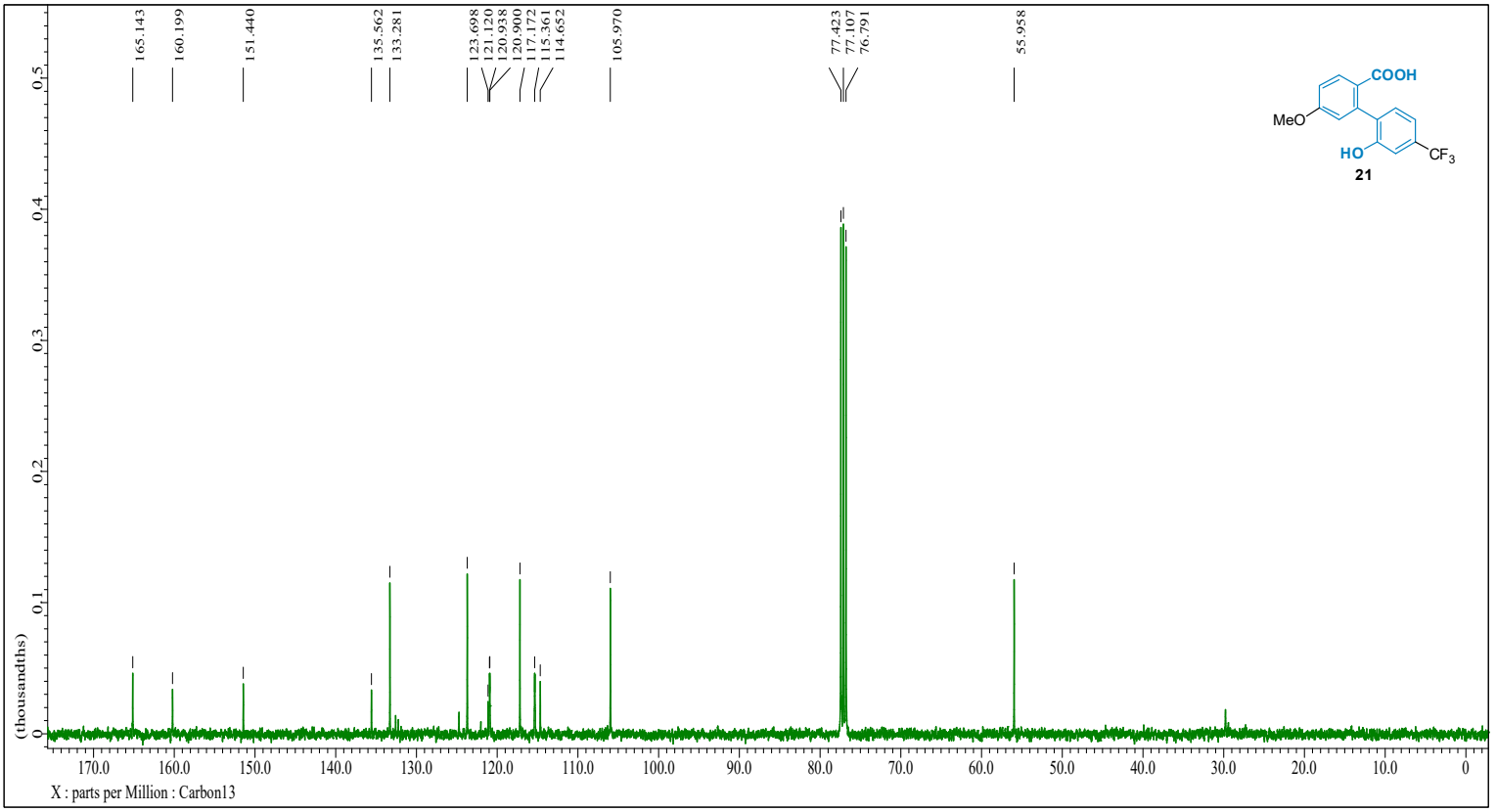
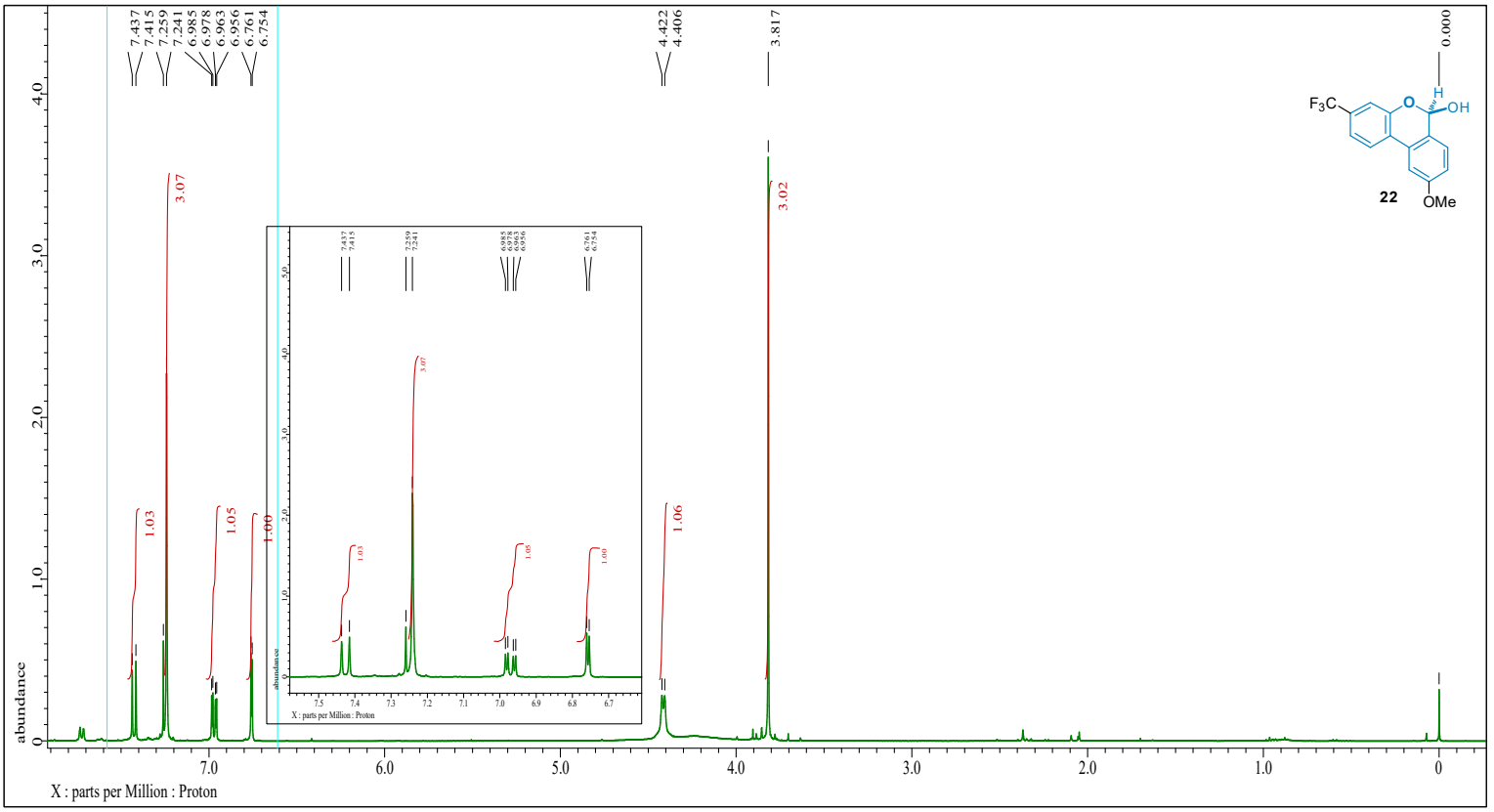
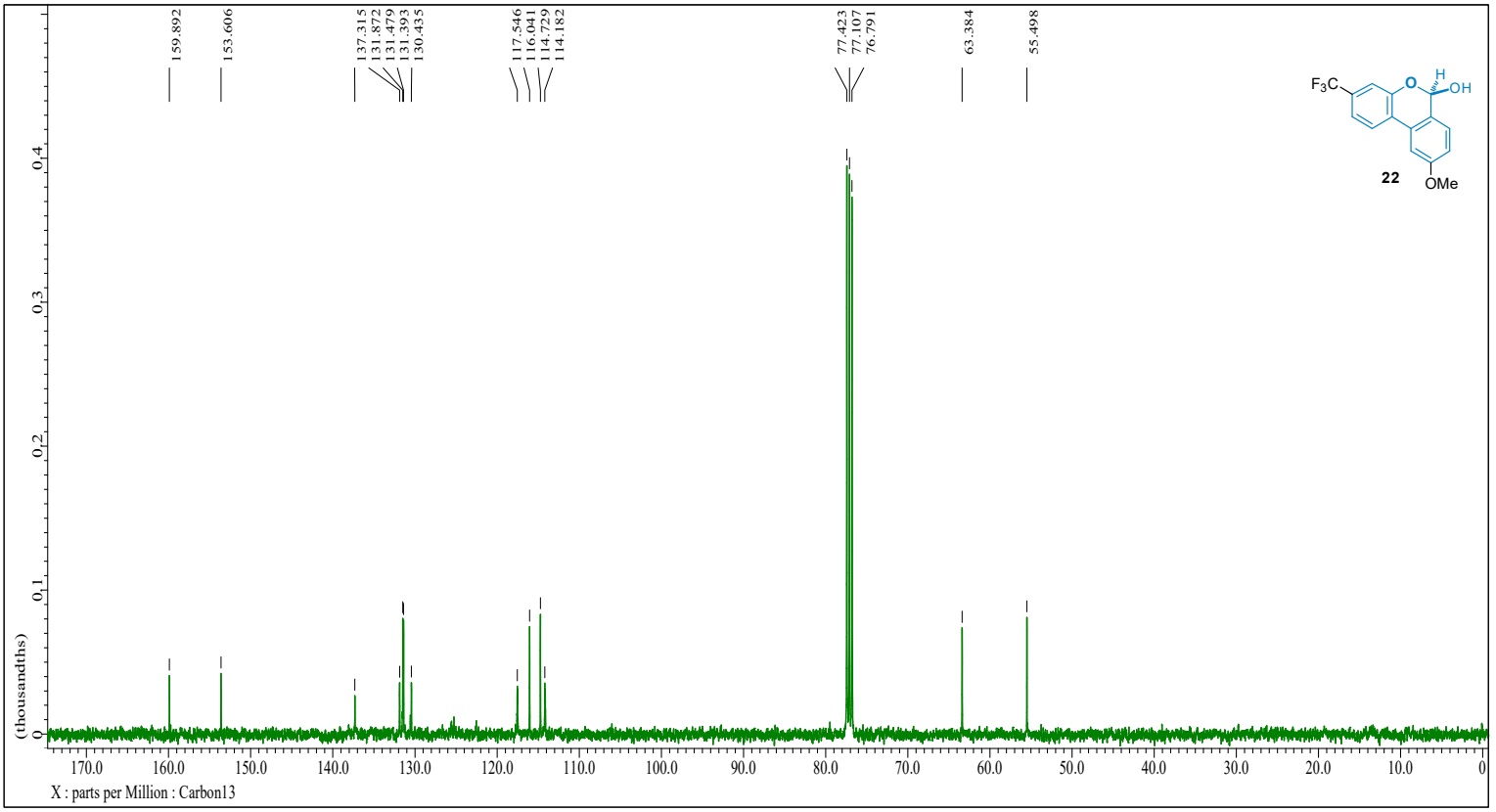
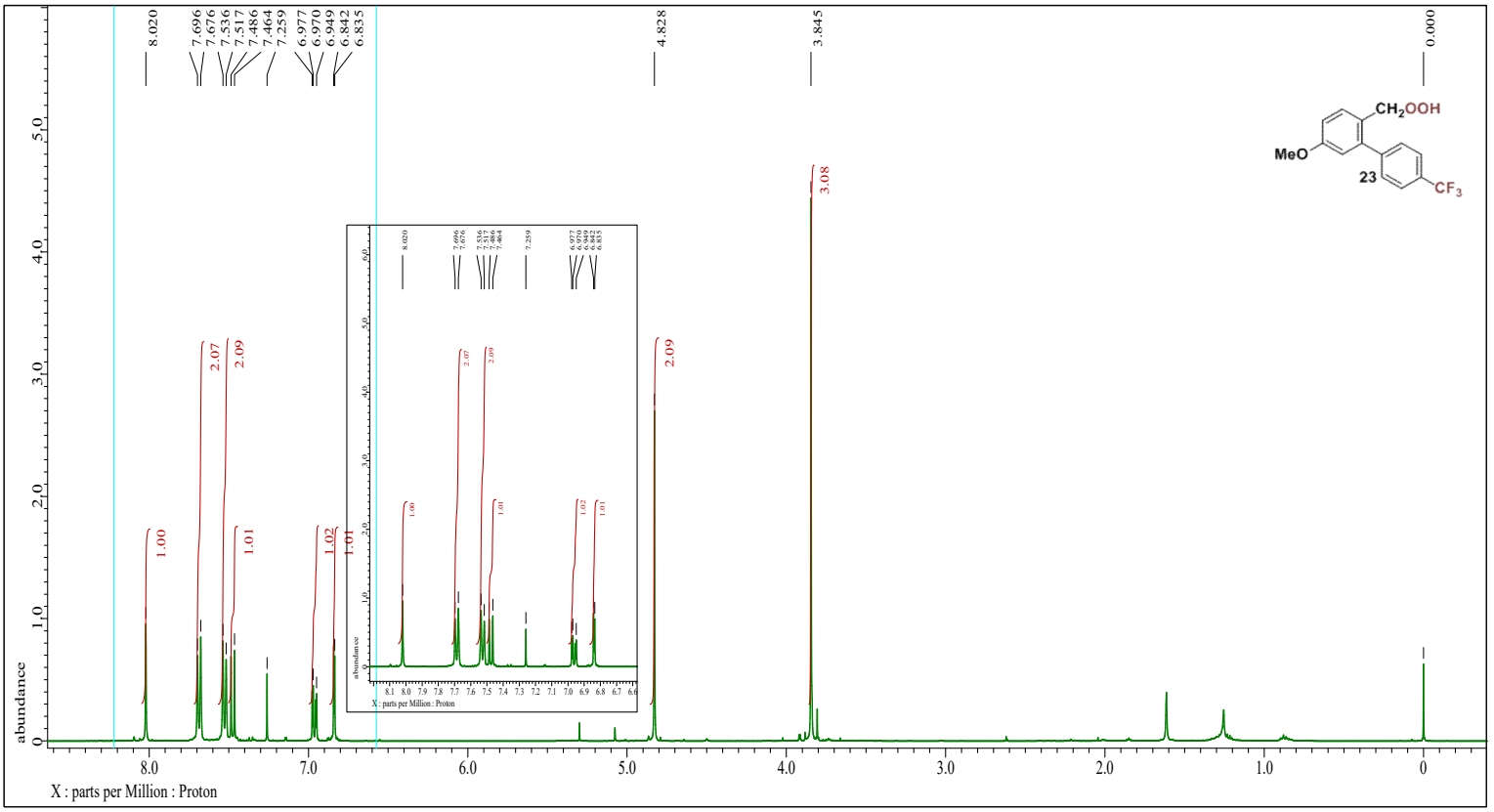
153.510
137.421
132.131
131.843
131.479
131.153
130.339
127.953
125.241
122.539
119.827
117.546
116.022
114.614
113.933
77.433
77.116
76.800
63.346
55.479
(thousandths)
X : parts per Million : Carbon13
F3C
O
H
H
20
OMe

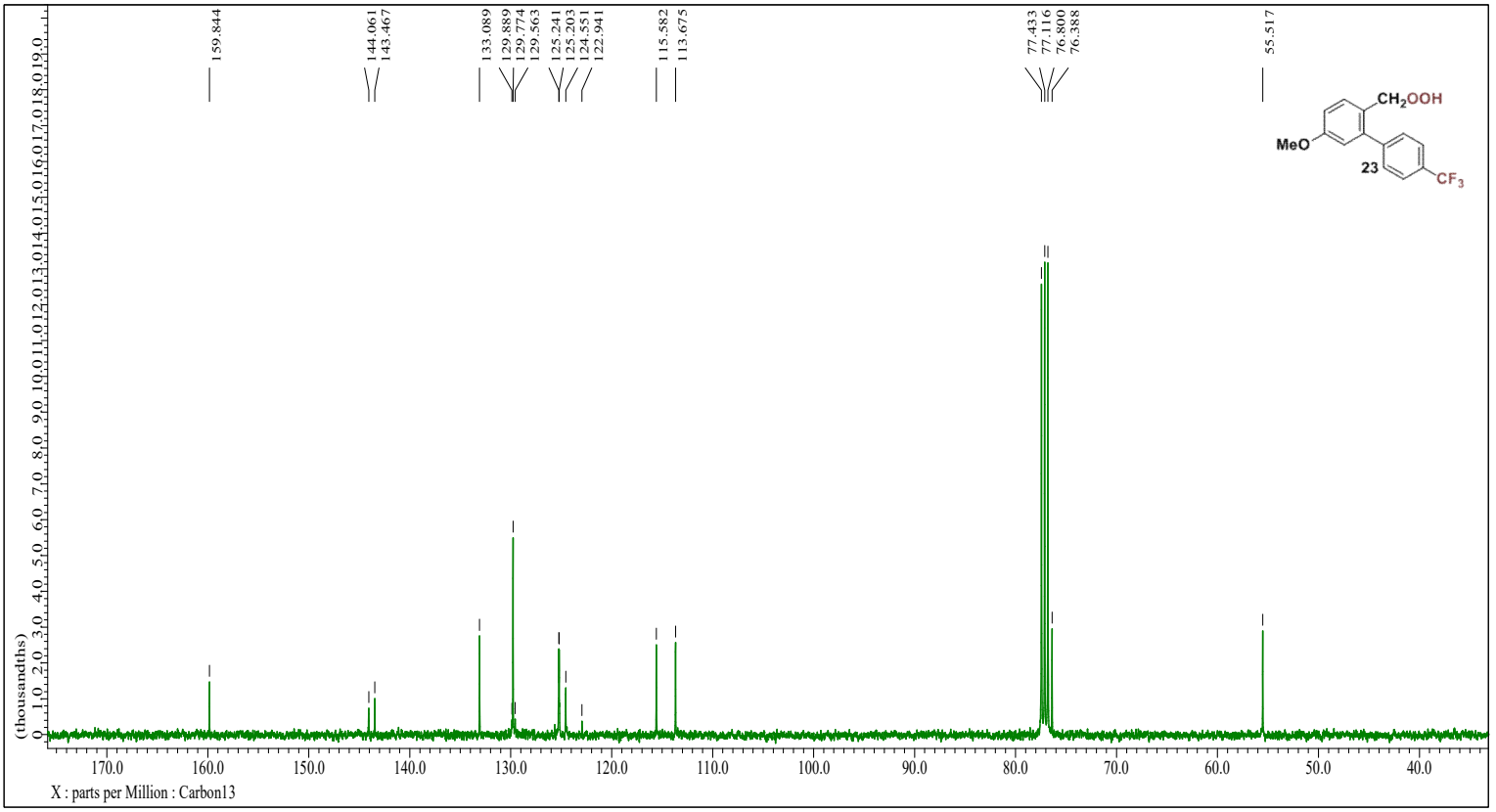

8.367
8.345
8.118
8.097
7.599
7.573
7.552
7.505
7.266
7.191
7.168
4.018
0.000
COOH
MeO
HO
CF3
21
3.00
2.23
1.28
1.06
0.97
0.92
abundance
X : parts per Million : Proton


165.143
160.199
151.440
135.562
133.281
123.698
121.120
120.938
120.900
117.172
115.361
114.652
105.970
77.423
77.107
76.791
55.958
COOH
MeO
HO
CF3
21
(thousandths)
X : parts per Million : Carbon13


7.437
7.415
7.259
7.241
6.985
6.978
6.963
6.956
6.761
6.754
4.422
4.406
3.817
0.000
3.07
3.02
1.03
1.05
1.00
1.06
abundance
X : parts per Million : Proton
F3C
OH
OMe
22


159.892
153.606
137.315
131.872
131.479
131.393
130.435
117.546
116.041
114.729
114.182
77.423
77.107
76.791
63.384
55.498
(thousandths)
X : parts per Million : Carbon13
F3C
OH
OMe
22


8.020
7.696
7.676
7.536
7.517
7.486
7.464
7.259
6.977
6.970
6.949
6.842
6.835
4.828
3.845
0.000
CH2OOH
MeO
23
CF3
3.08
2.09
2.07
1.00
1.01
1.02
abundance
X : parts per Million : Proton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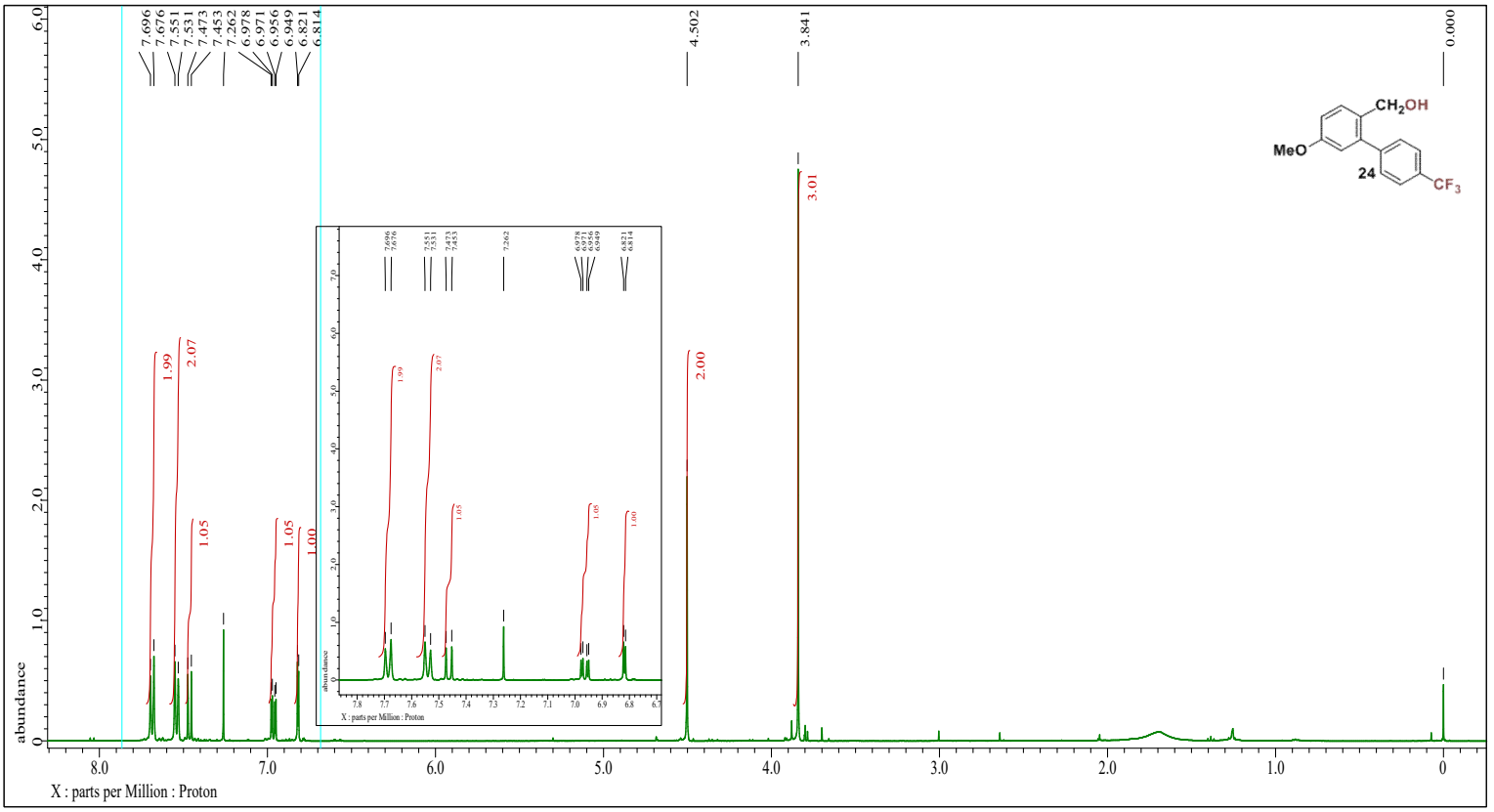
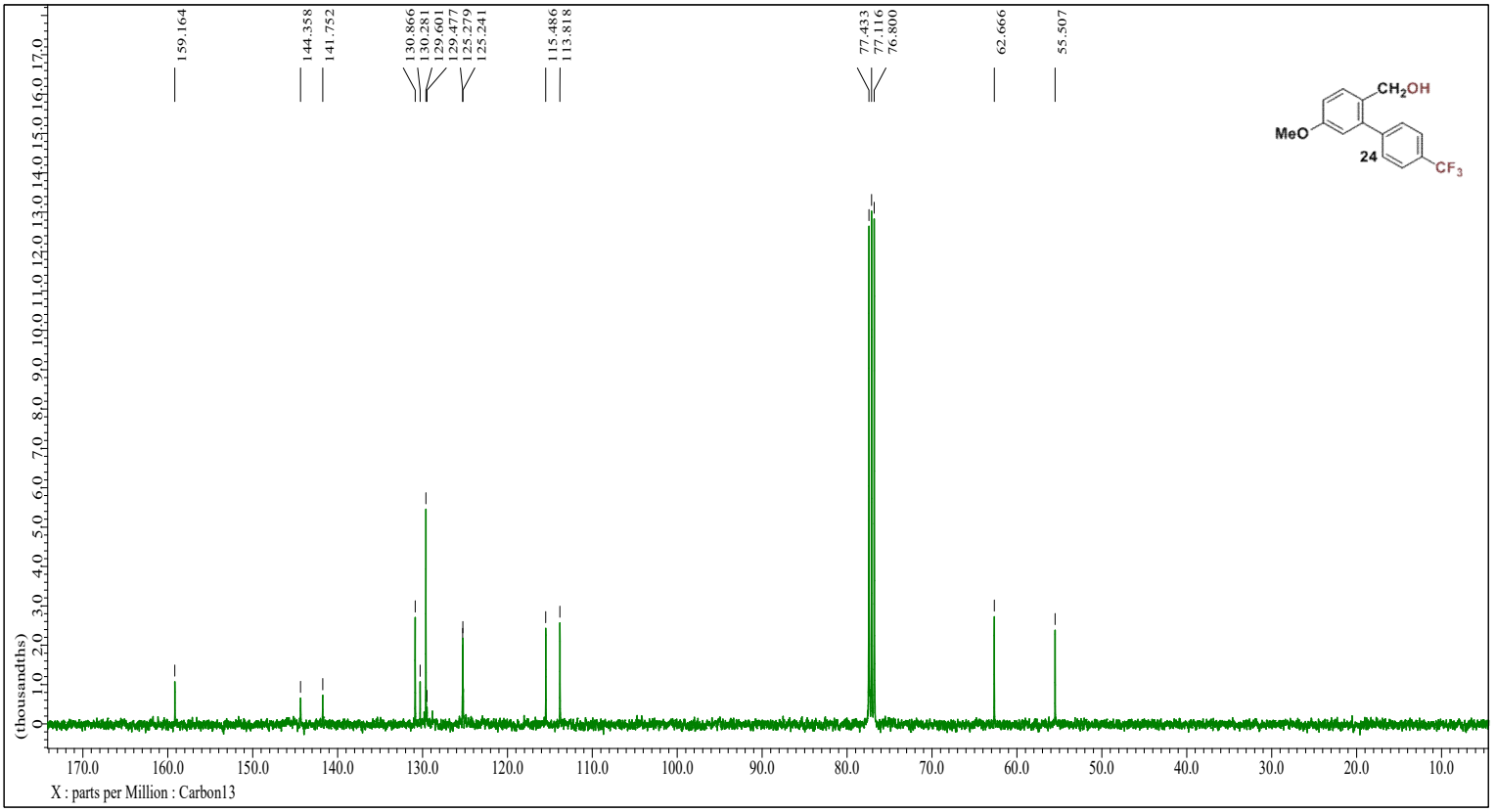
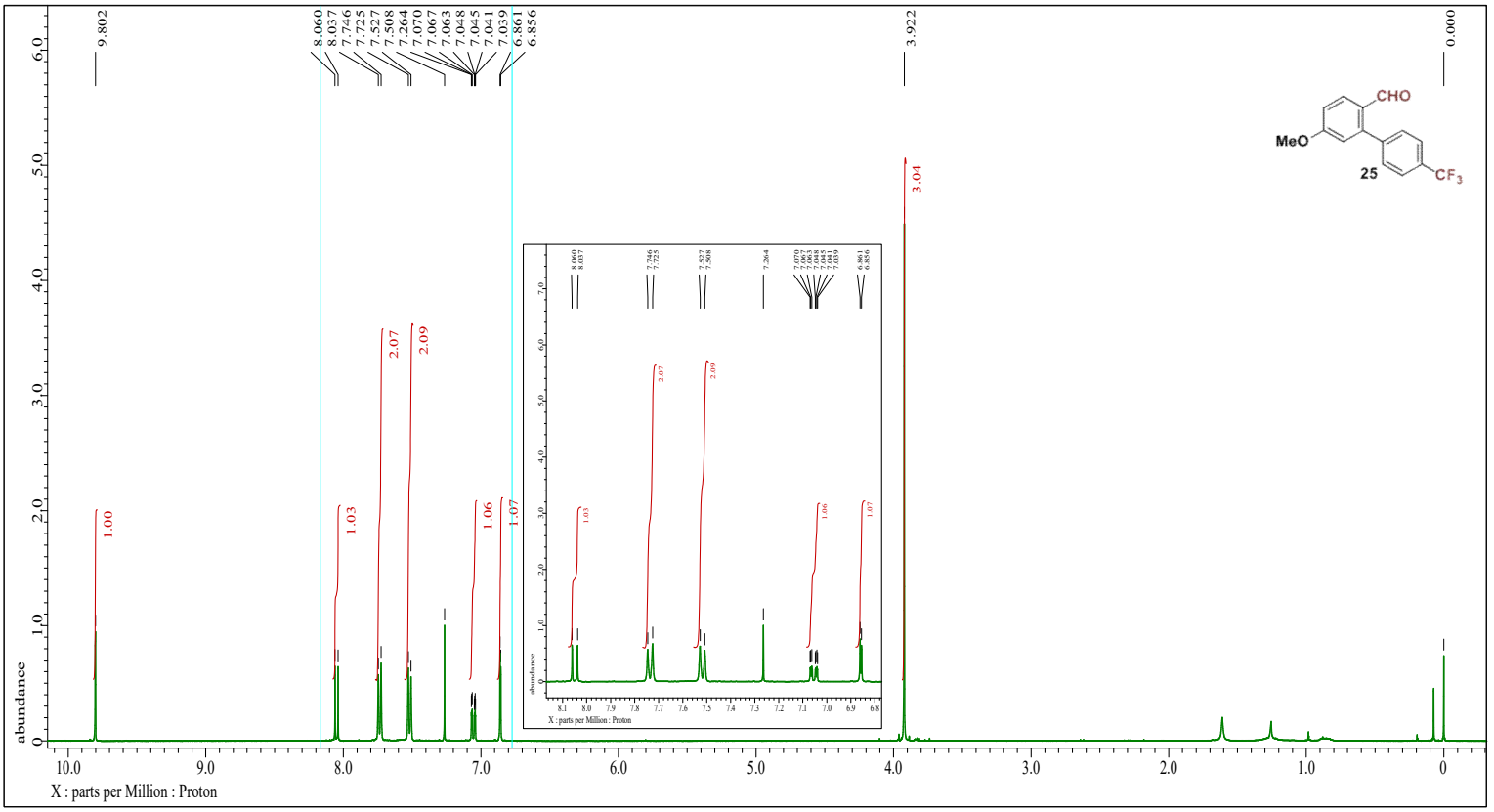
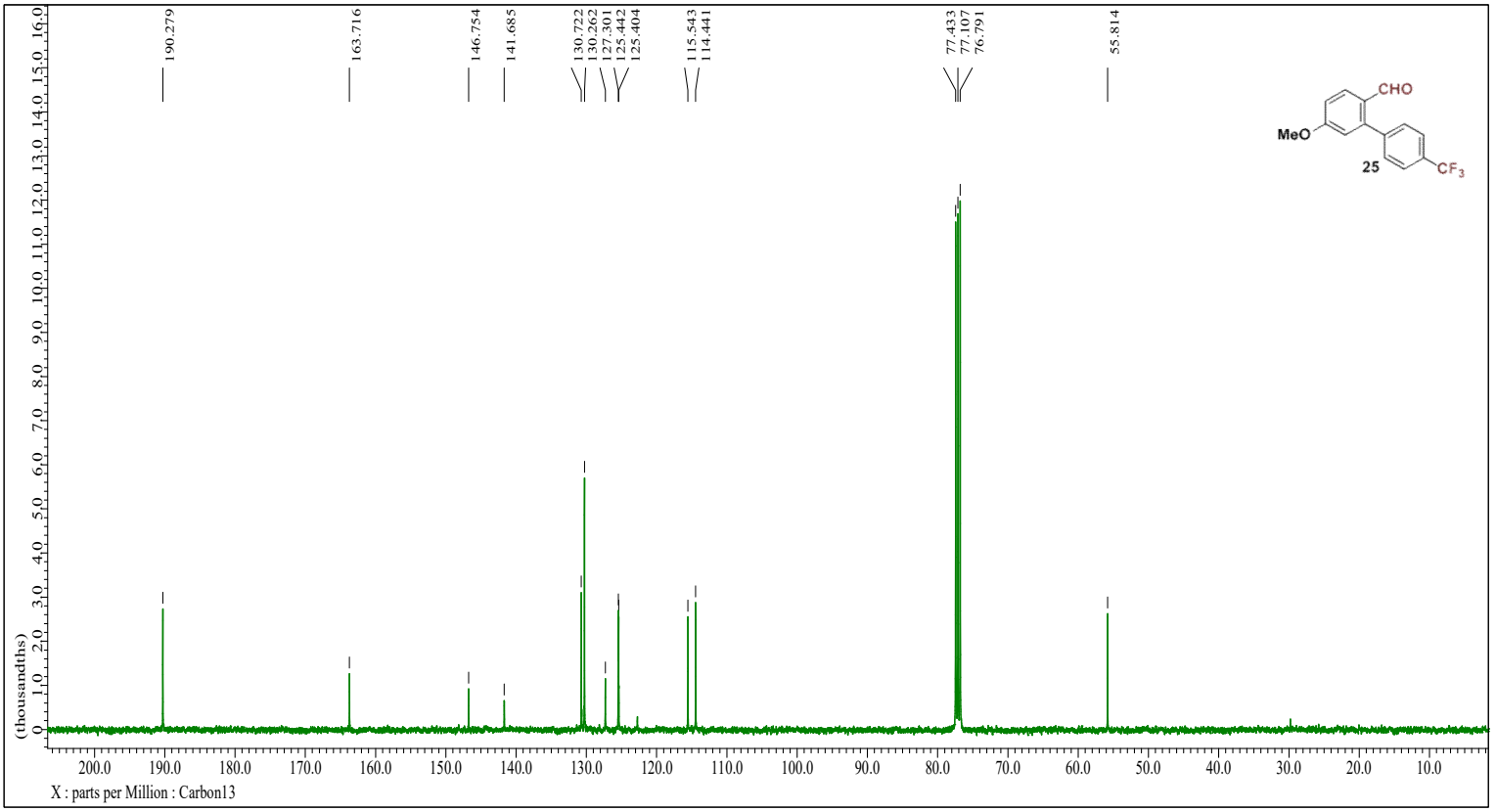
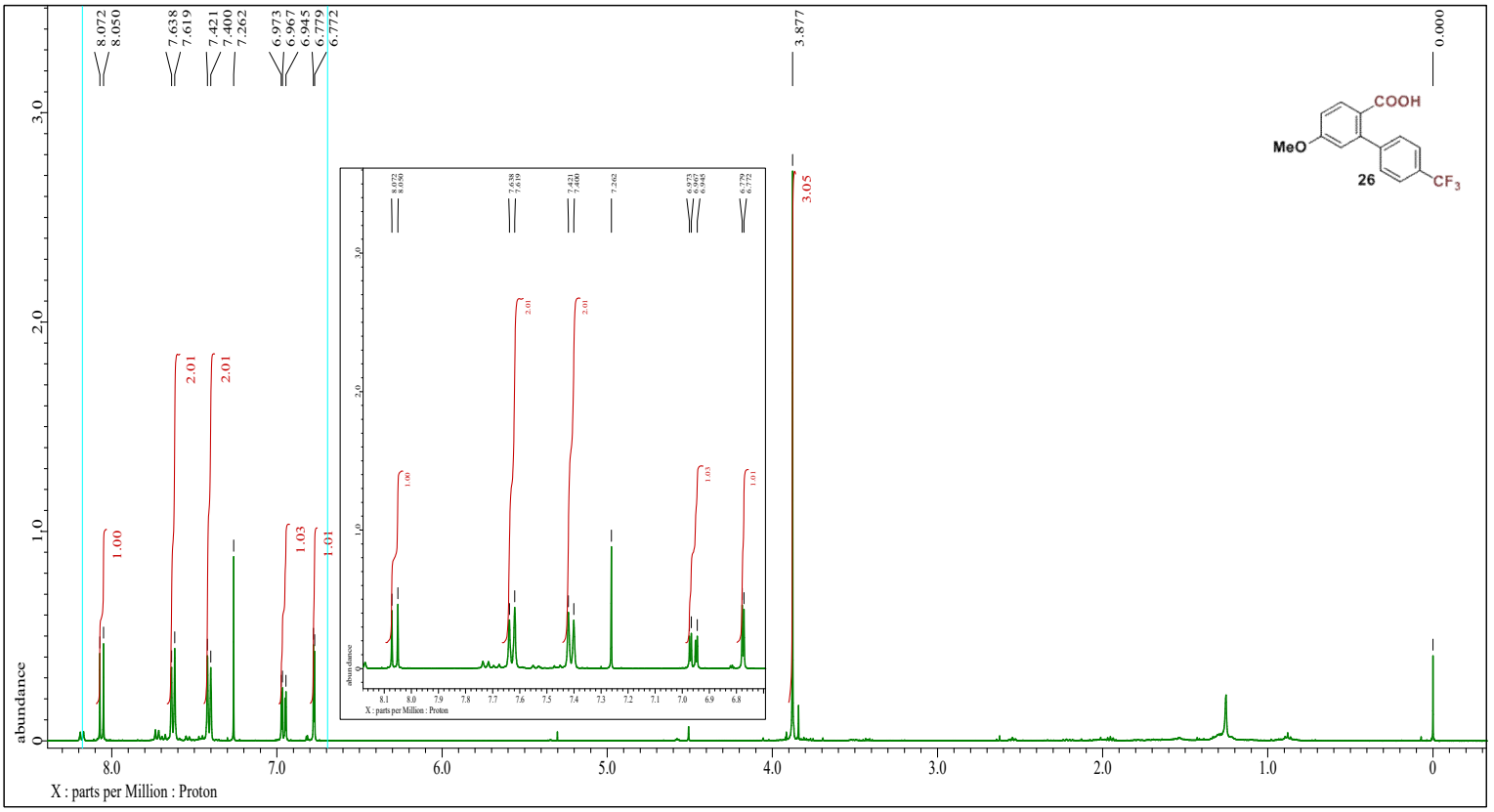
143.467
133.089
129.889
129.774
129.563
125.241
125.203
124.551
122.941
115.582
113.675
77.433
77.116
76.800
76.388
55.517
CH2OOH
MeO
23
CF3
(thousandths)
X : parts per Million : Carbon13

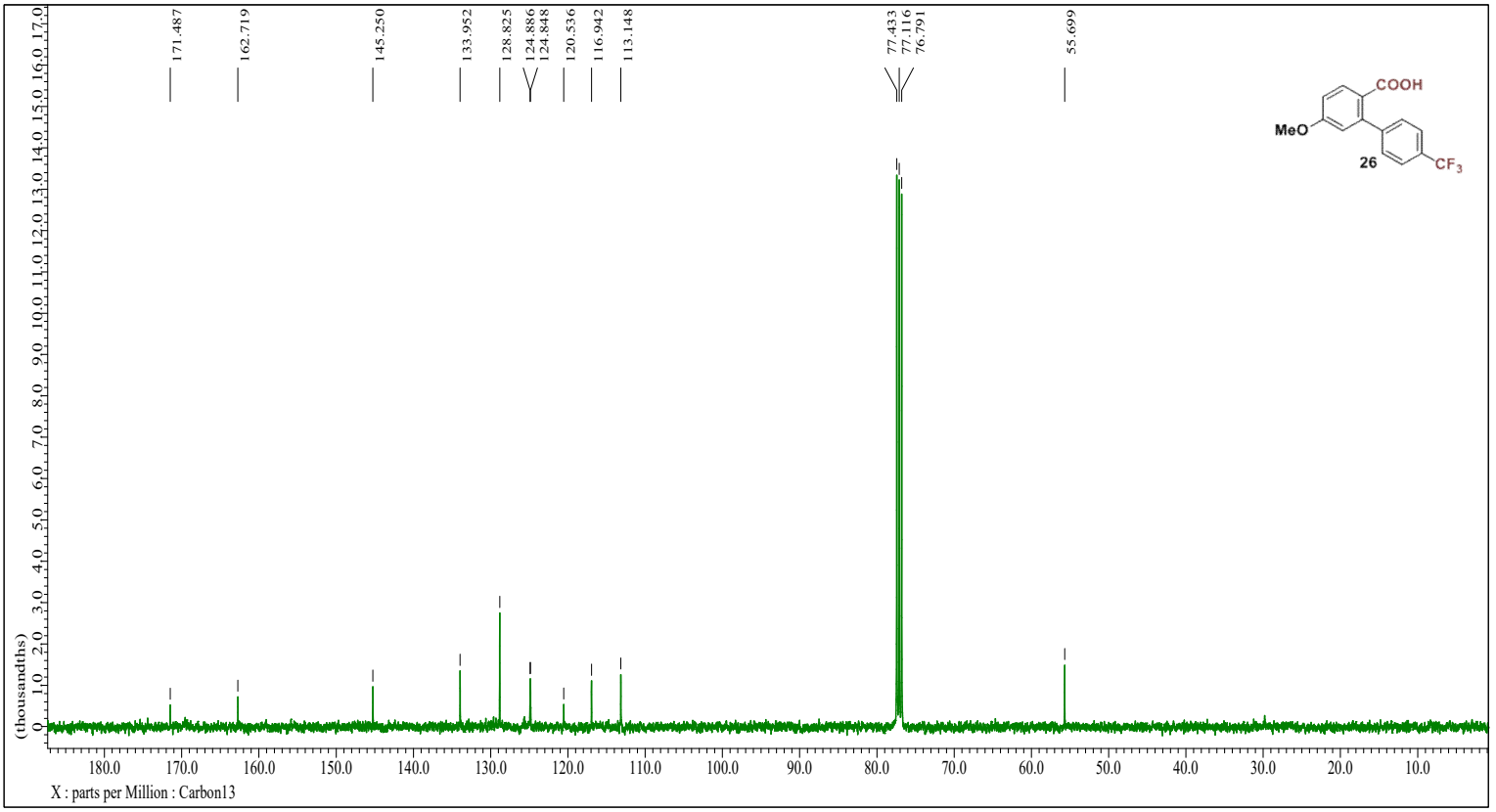

7.696
7.676
7.551
7.531
7.473
7.453
7.262
6.978
6.971
6.956
6.949
6.821
6.814
4.502
3.841
0.000
1.99
2.07
1.05
1.05
1.00
2.00
3.01
CH2OH
MeO
24
CF3
abundance
X : parts per Million : Proton

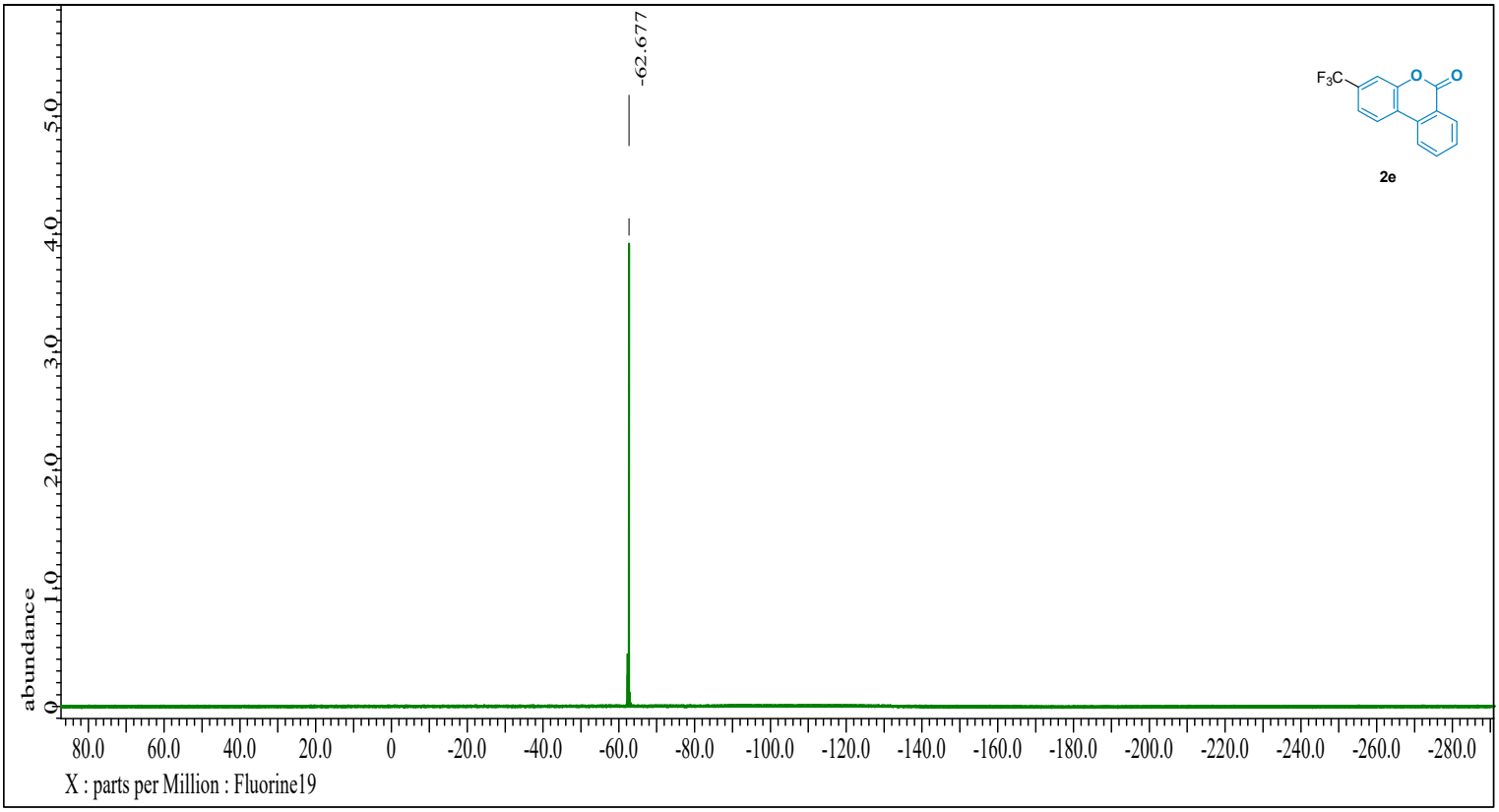

159.164
144.358
141.752
130.866
130.281
129.601
129.477
125.279
125.241
115.486
113.818
77.433
77.116
76.800
62.666
55.507
CH2OH
MeO
24
CF3
(thousandths)
X : parts per Million : Carbon13

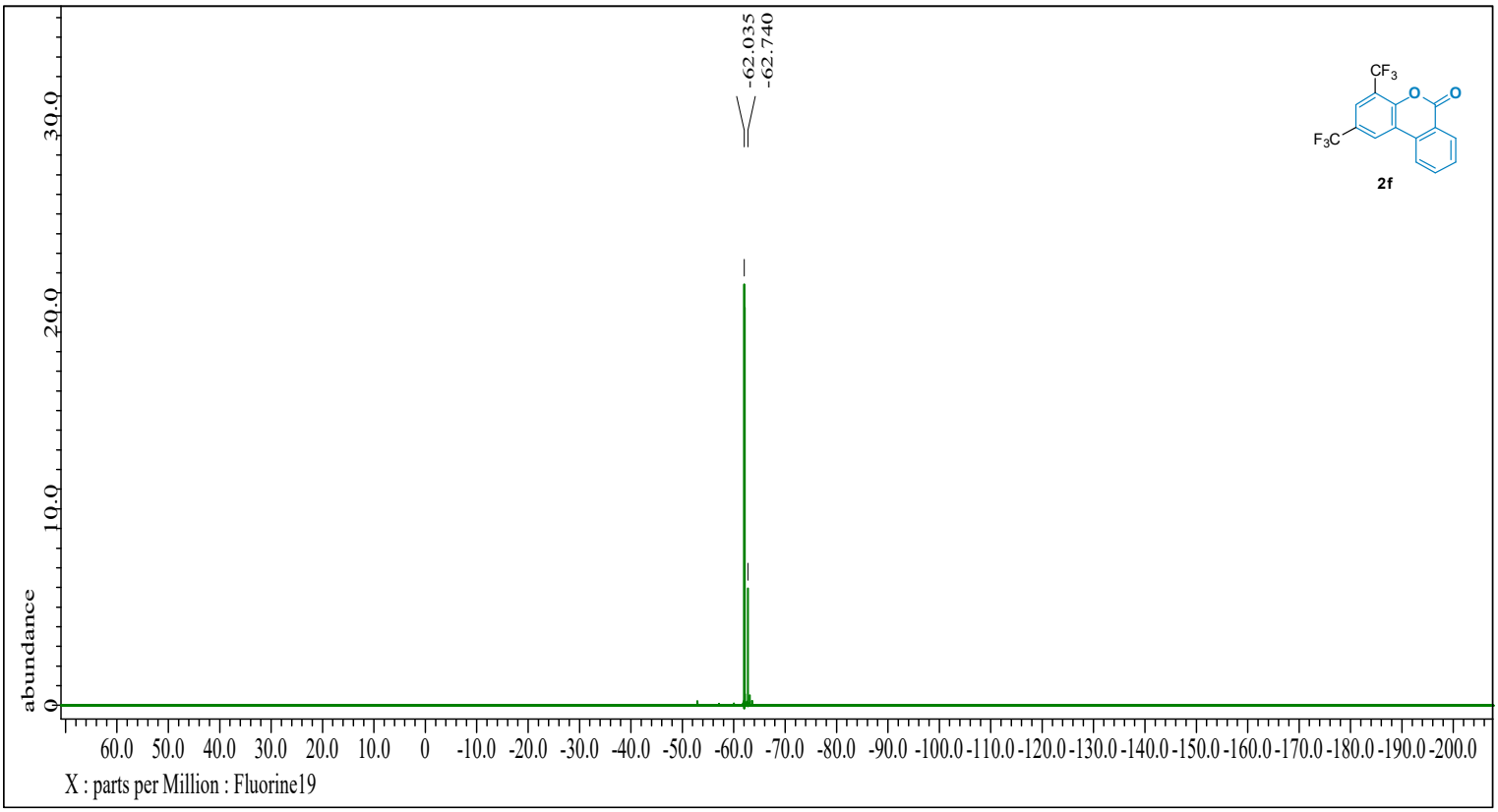

9.802
8.060
8.037
7.746
7.725
7.527
7.508
7.264
7.070
7.067
7.063
7.048
7.045
7.041
7.039
6.861
6.856
3.922
0.000
1.00
1.03
2.07
2.09
1.06
1.07
3.04
CHO
MeO
25
CF3
abundance
X : parts per Million : Proton

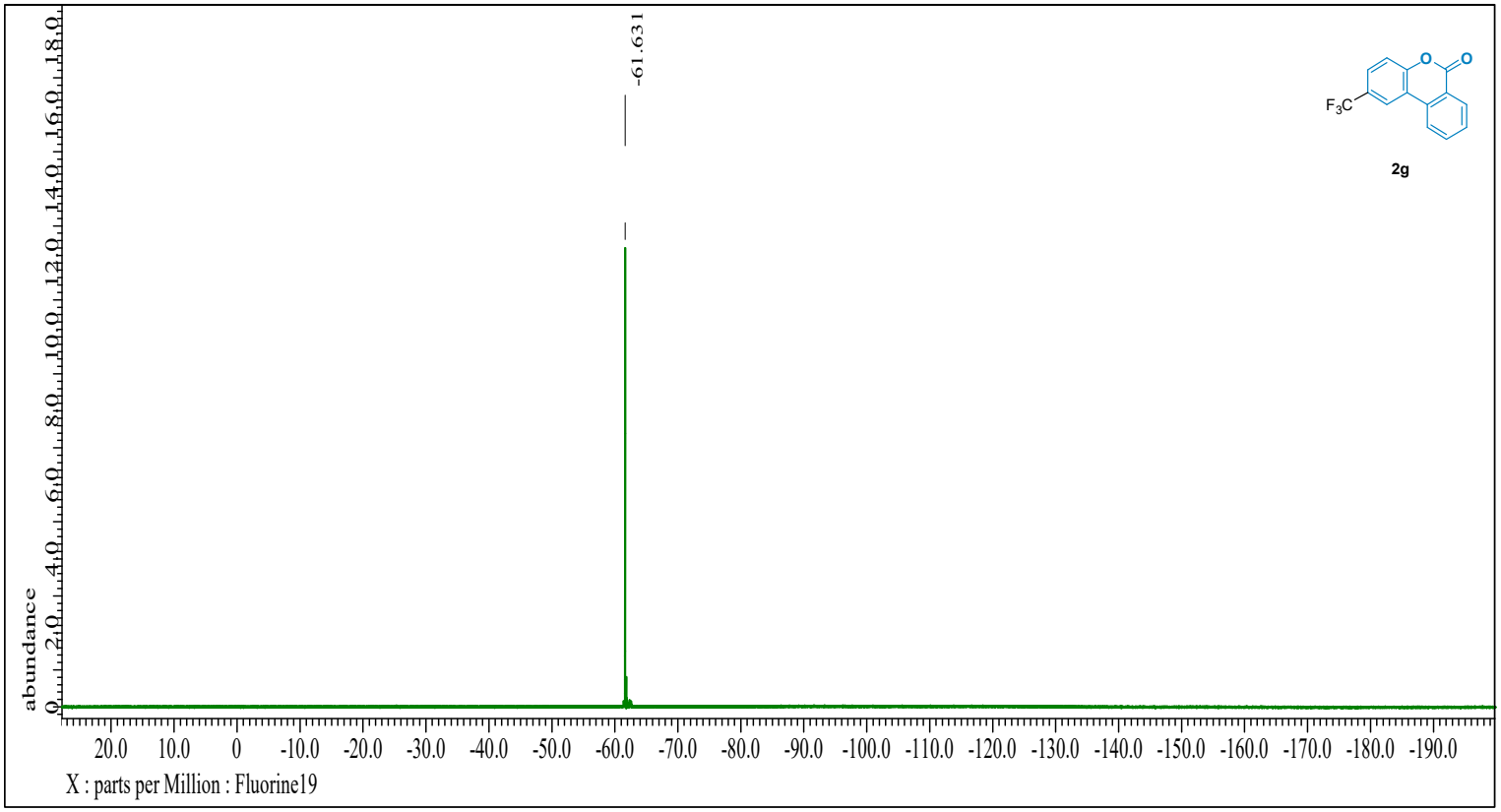

190.279
163.716
146.754
141.685
130.722
130.262
127.301
125.442
125.404
115.543
114.441
77.433
77.107
76.791
55.814
CHO
MeO
25
CF3
(thousandths)
X : parts per Million : Carbon13

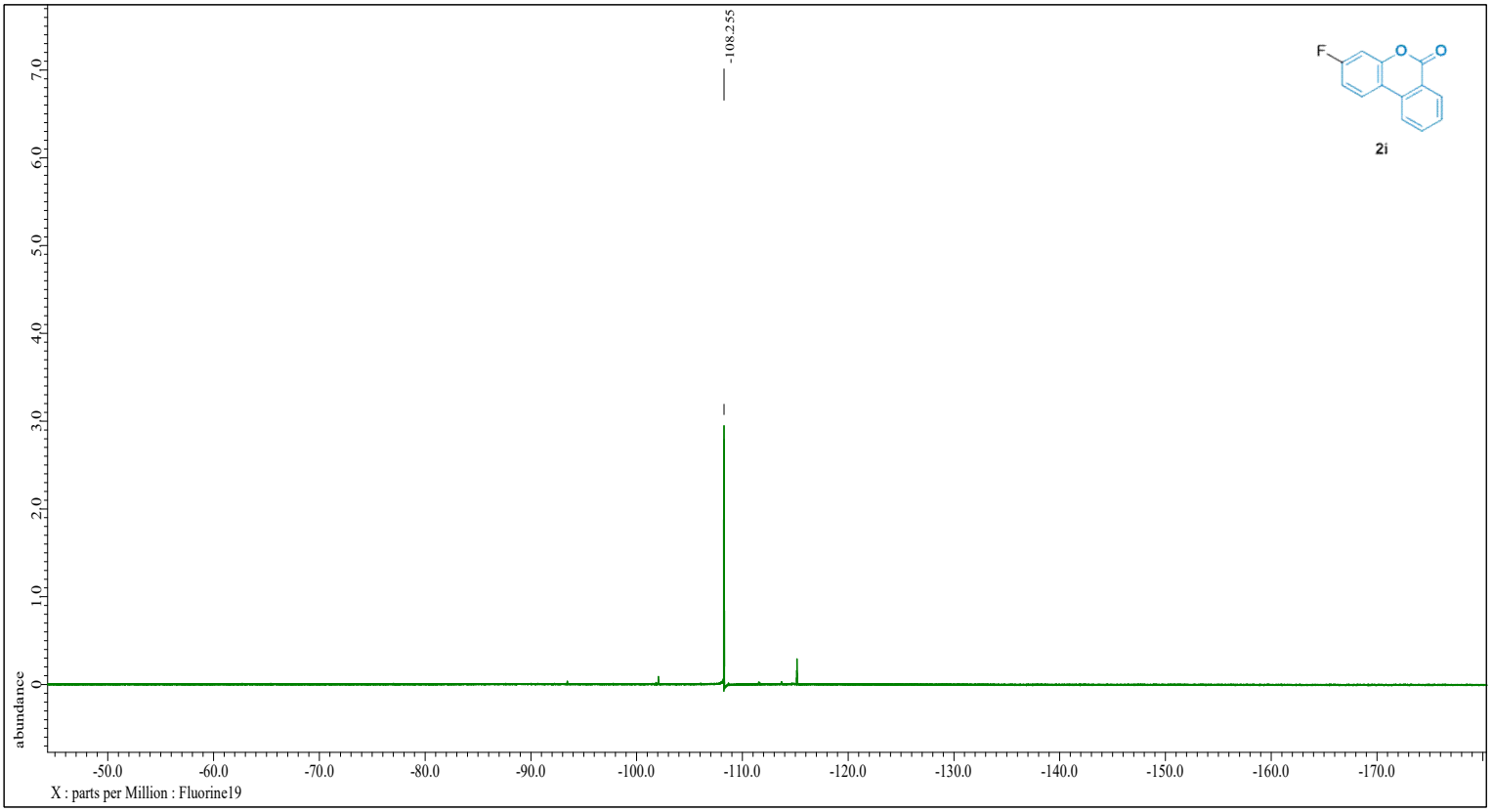

8.072
8.050
7.638
7.619
7.421
7.400
7.262
6.973
6.967
6.945
6.779
6.772
3.877
0.000
1.00
2.01
2.01
1.03
1.01
3.05
COOH
MeO
26
CF3
abundance
X : parts per Million : Proton

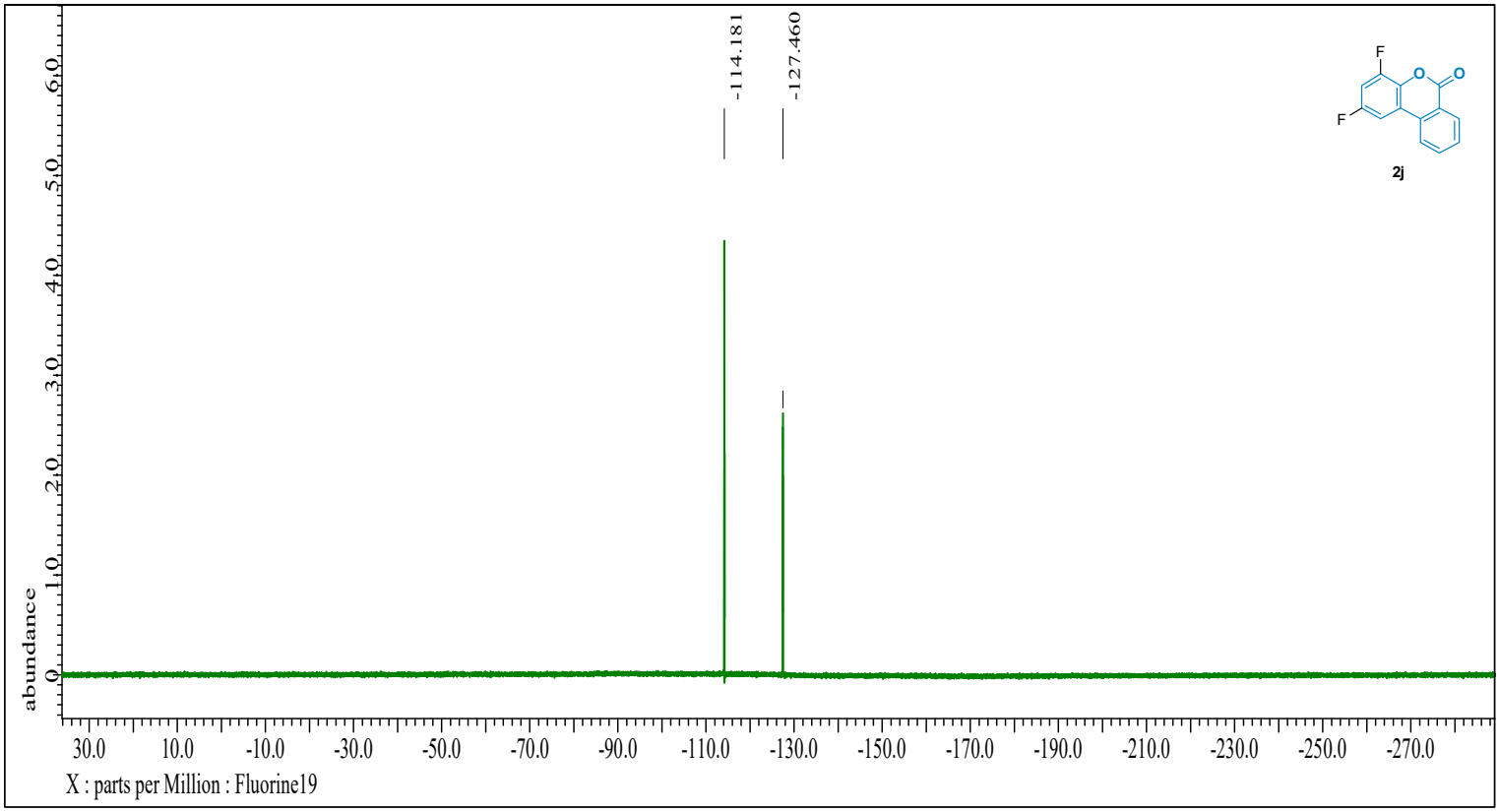

171.487
162.719
145.250
133.952
128.825
124.886
124.848
120.536
116.942
113.148
77.433
77.116
76.791
55.699
COOH
MeO
26
CF3
(thousandths)
X : parts per Million : Carbon13

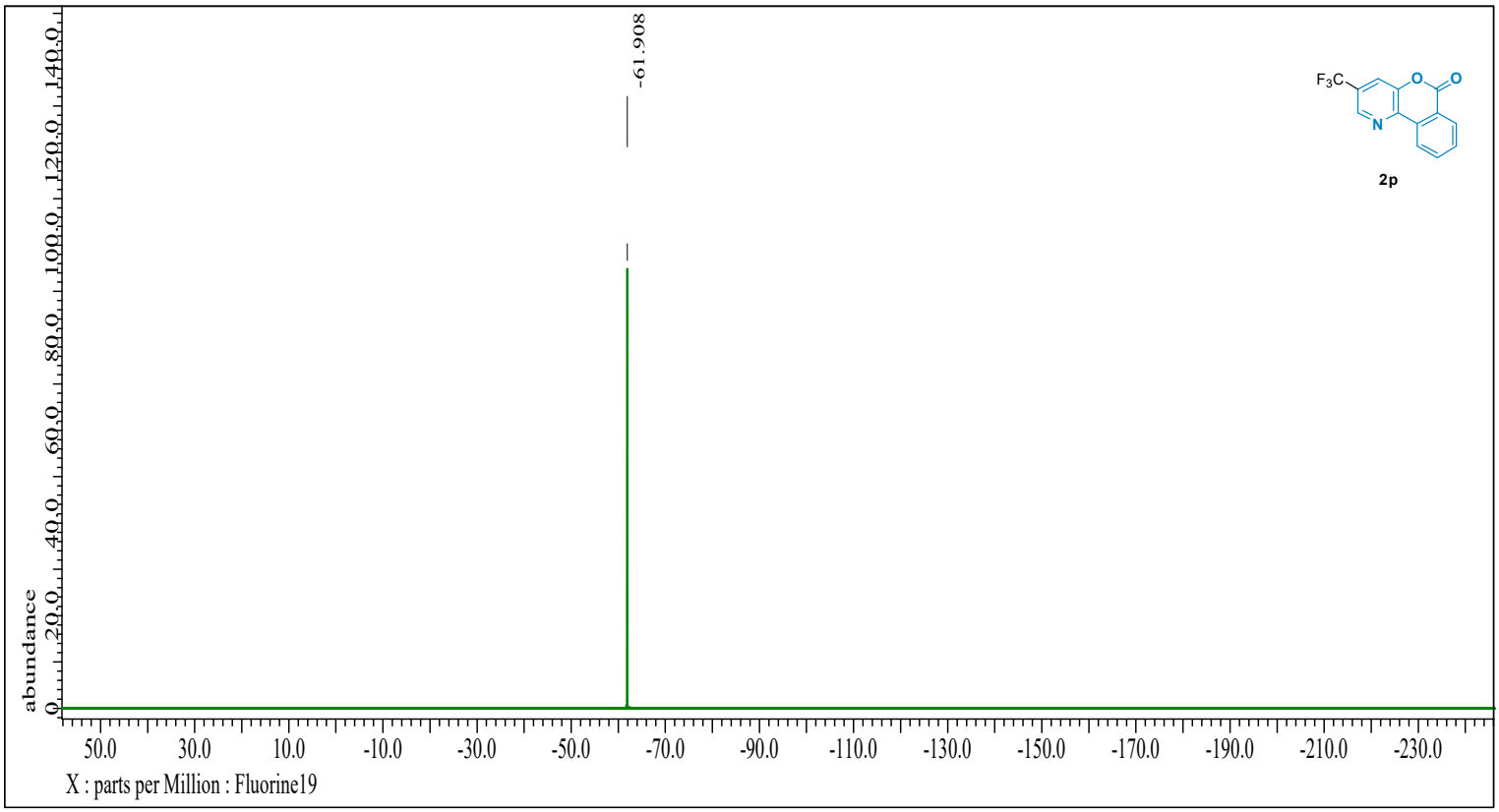

-62.677
F3C
O
O
2e
abundance
0
1.0
2.0
3.0
4.0
5.0
80.0 60.0 40.0 20.0 0 -20.0 -40.0 -60.0 -80.0 -100.0 -120.0 -140.0 -160.0 -180.0 -200.0 -220.0 -240.0 -260.0 -280.0
X : parts per Million : Fluorine19

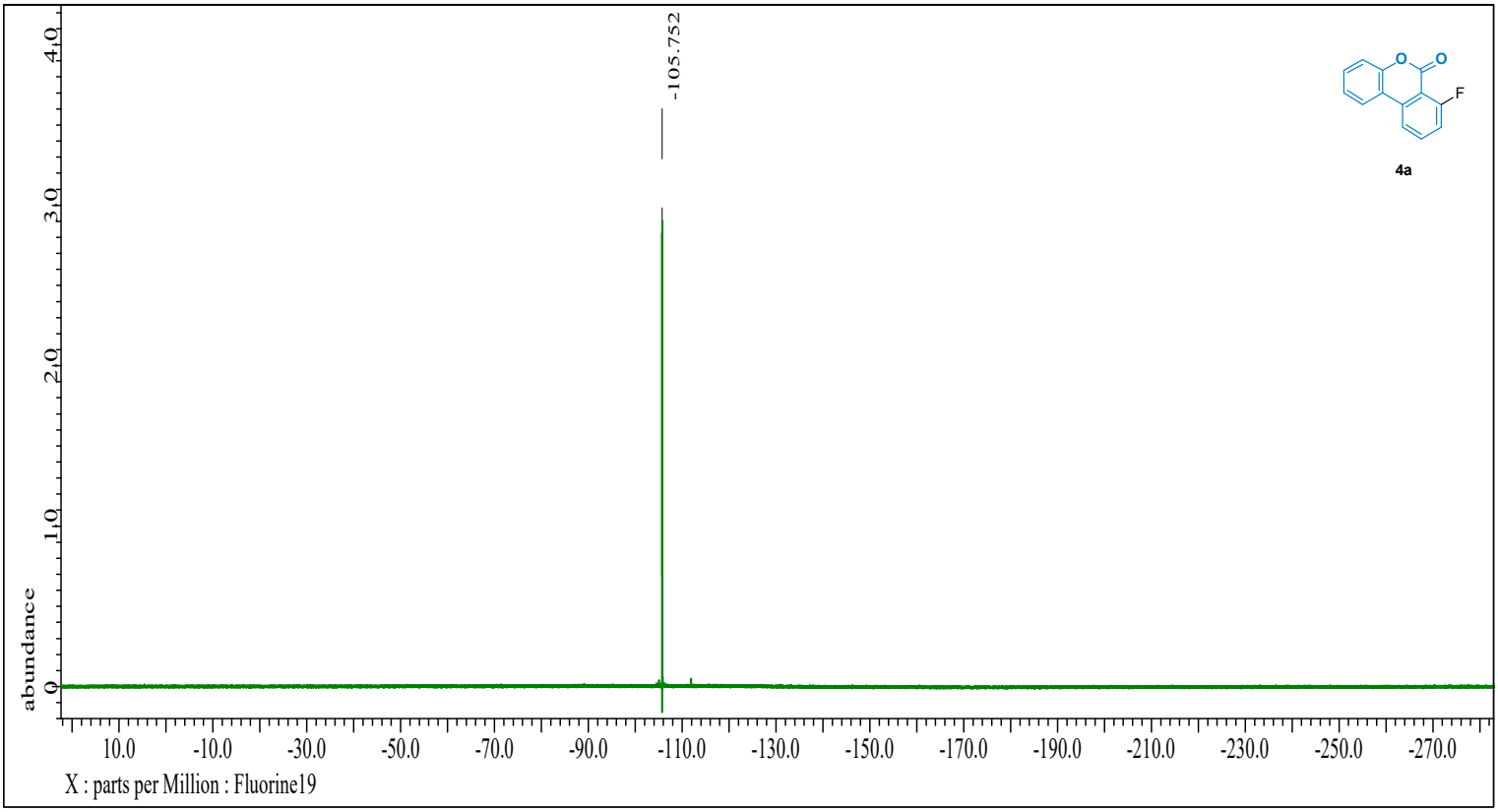

-62.035
-62.740
CF3
F3C
O
O
2f
abundance
0
10.0
20.0
30.0
60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19

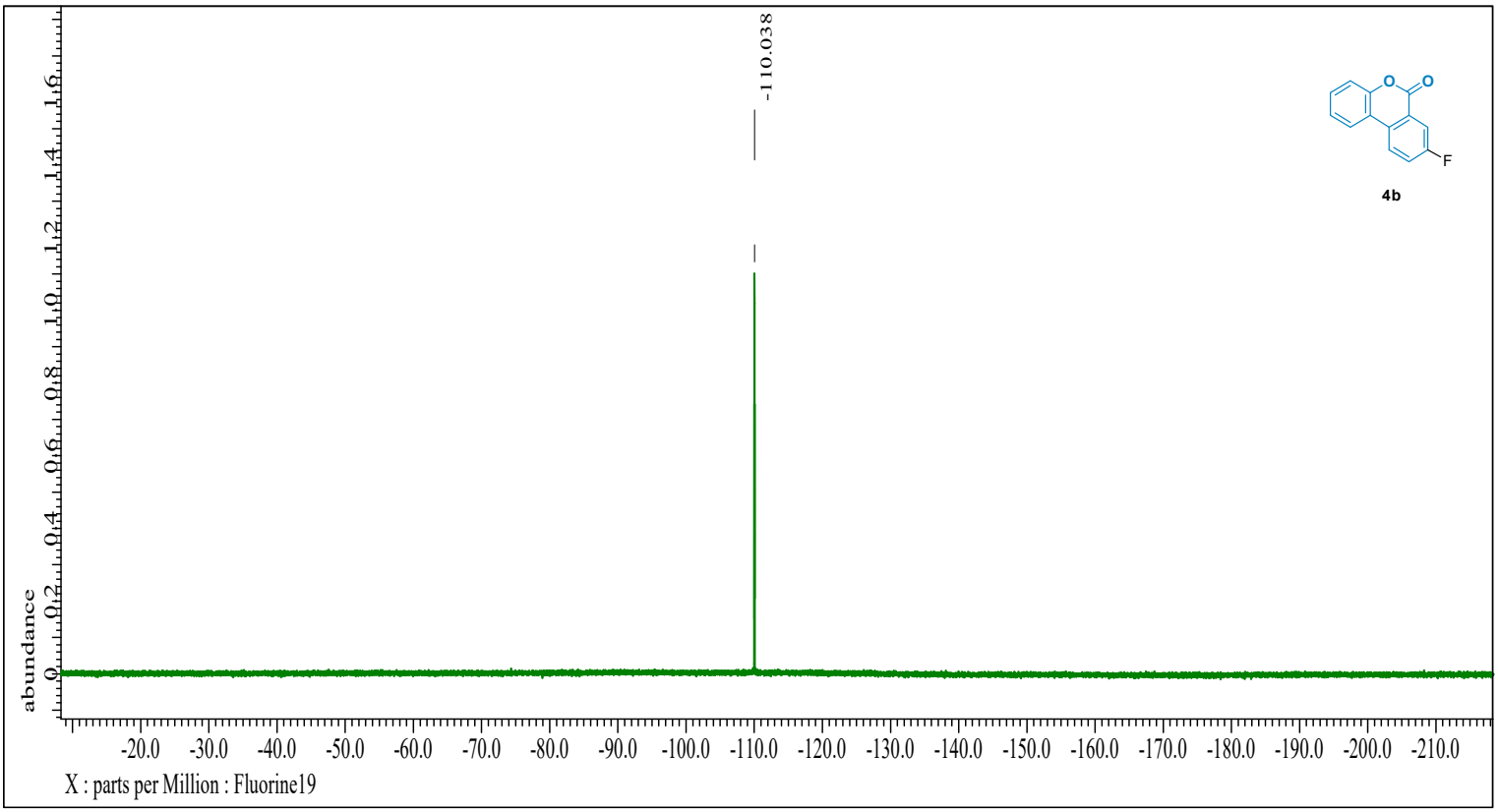

-61.631
abundance
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0
X : parts per Million : Fluorine19
F3C
O
O
2g

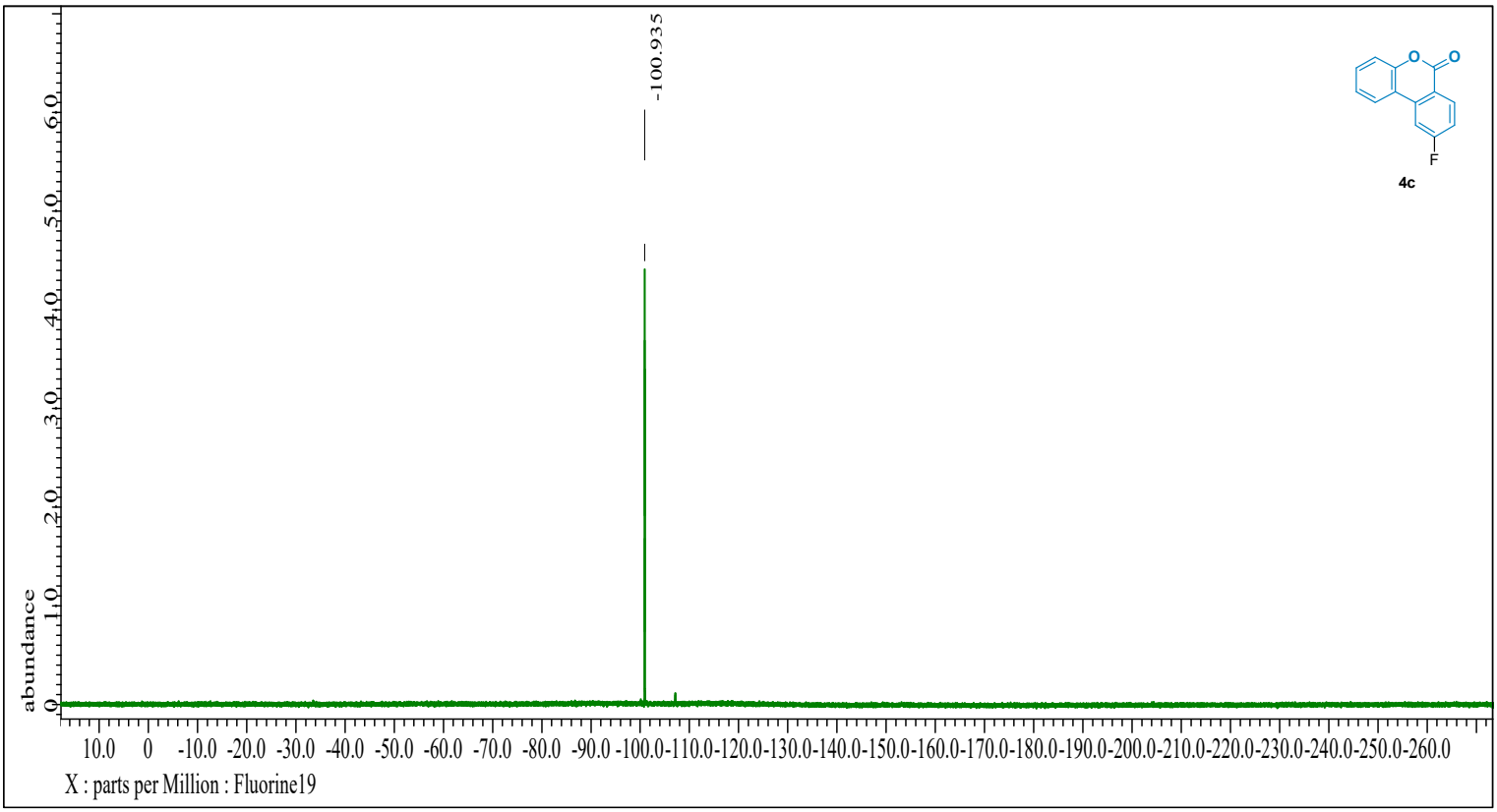

-108.255
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
-50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0
X : parts per Million : Fluorine19
F
O
O
2i

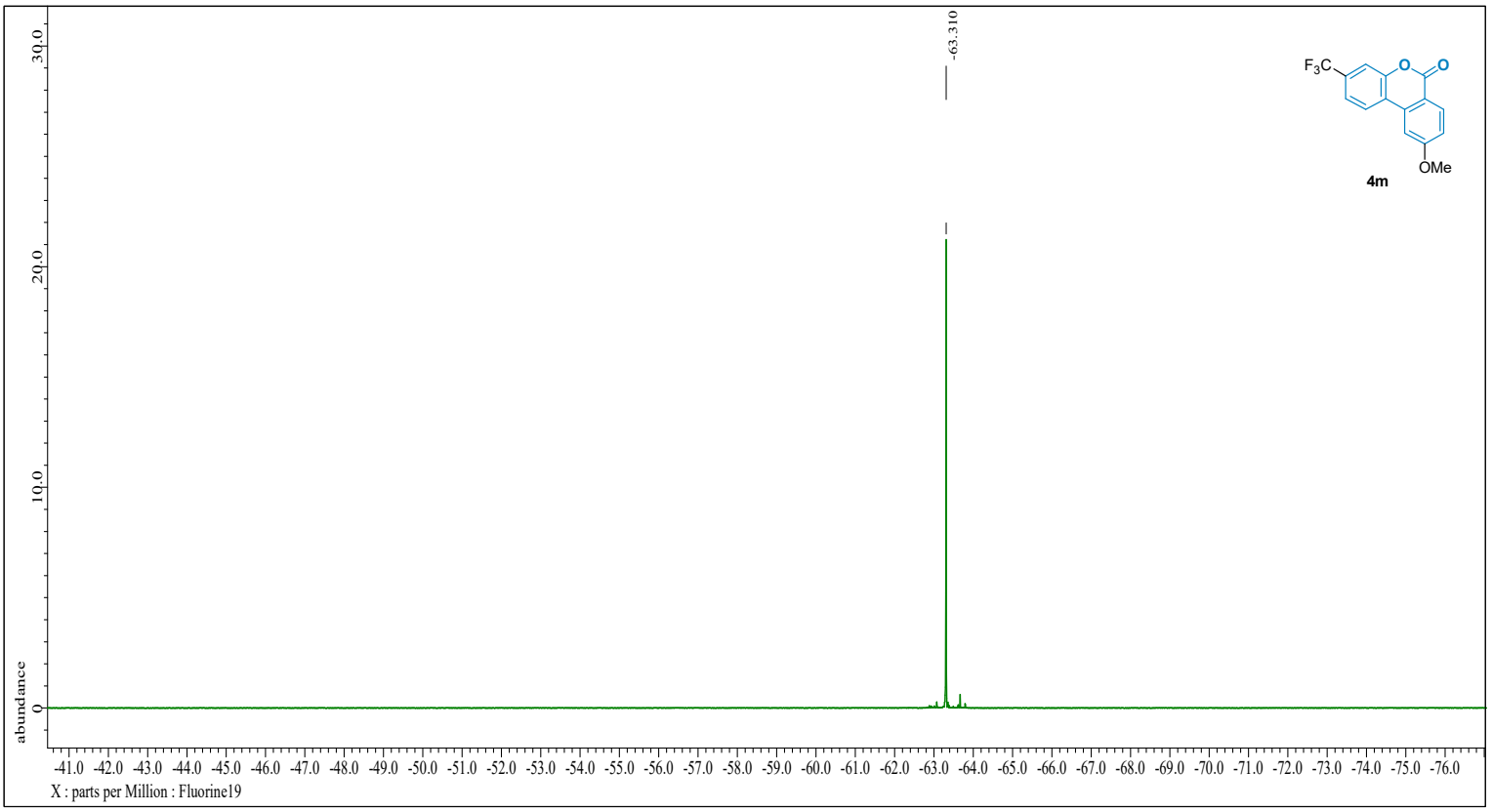

-114.181
-127.460
F
F
O
O
2j
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
X : parts per Million : Fluorine19

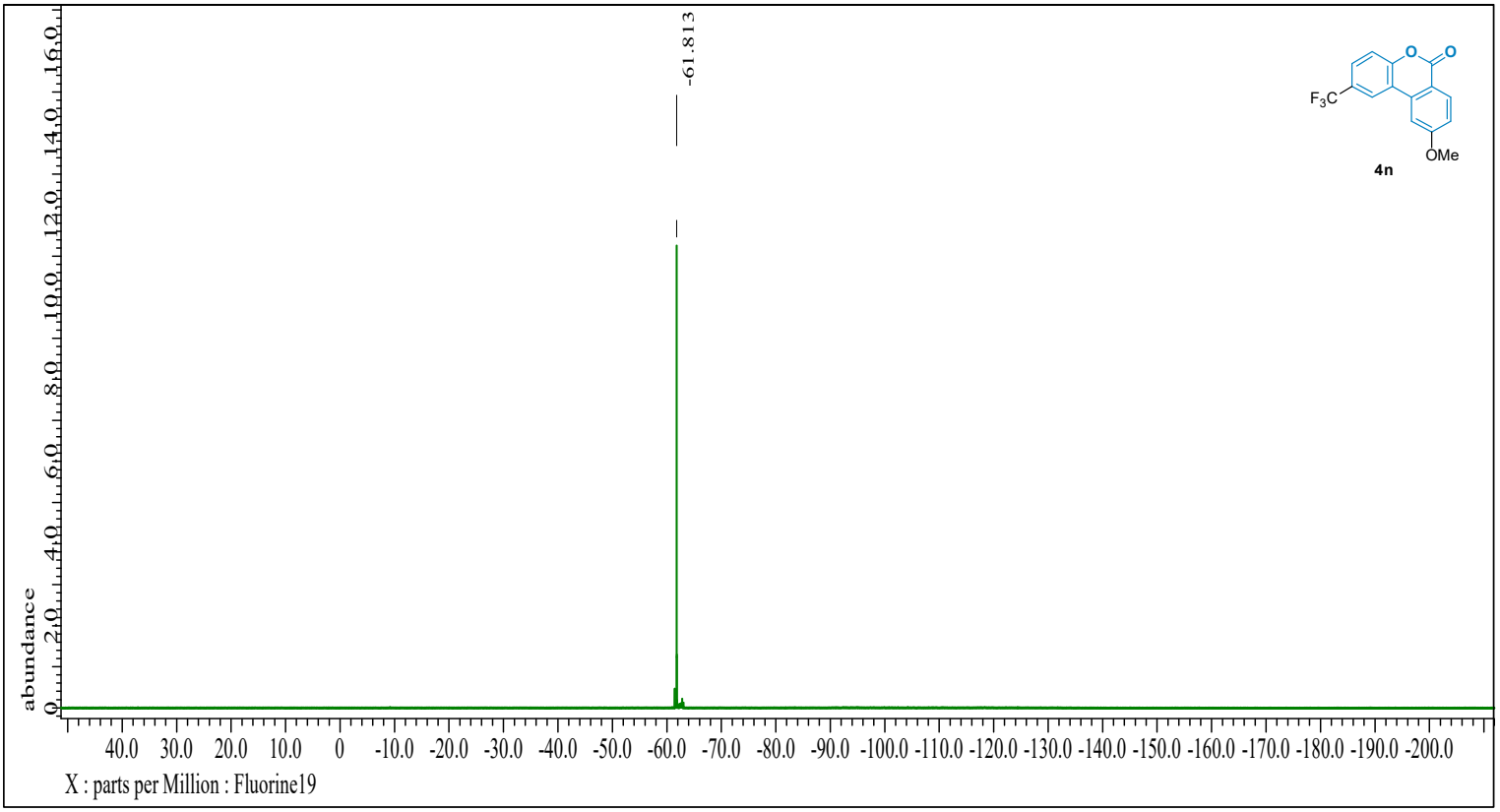

-61.908
F3C
O
O
N
2p
abundance
0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
50.0
30.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
X : parts per Million : Fluorine19

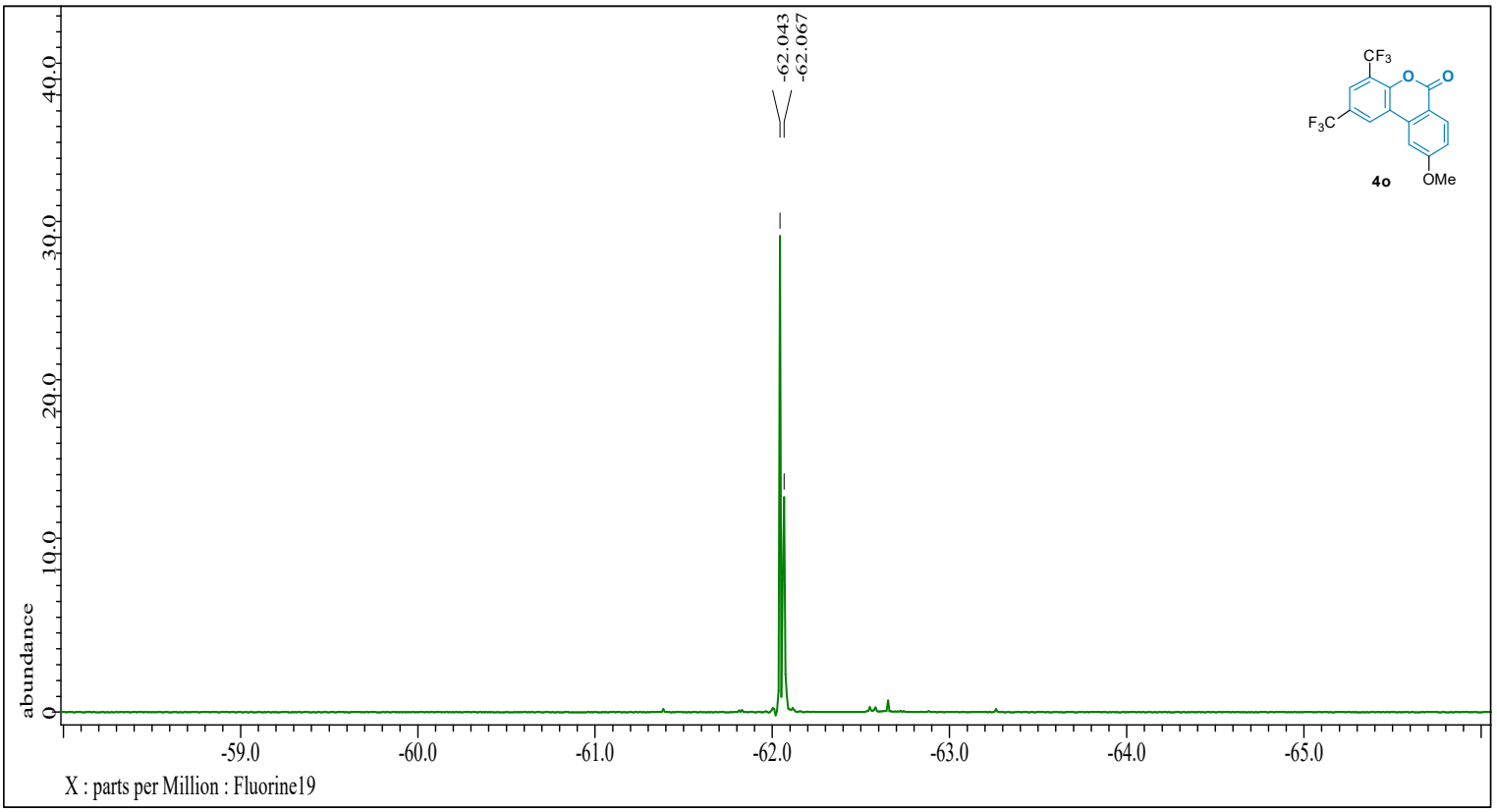

-105.752
4a
abundance
0
1.0
2.0
3.0
4.0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-190.0
-210.0
-230.0
-250.0
-270.0
X : parts per Million : Fluorine19

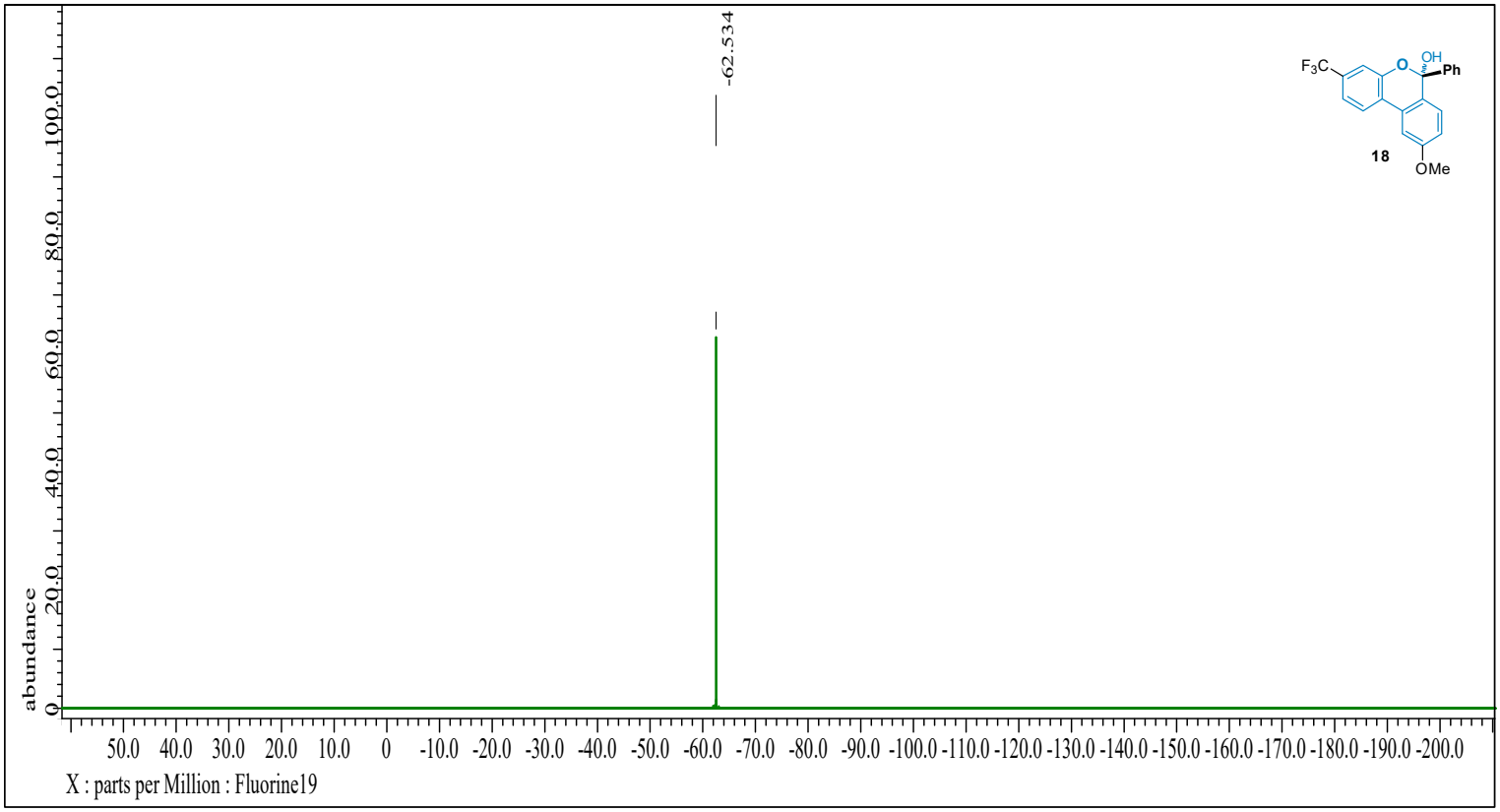

-110.038
4b
abundance
0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
-20.0
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-120.0
-130.0
-140.0
-150.0
-160.0
-170.0
-180.0
-190.0
-200.0
-210.0
X : parts per Million : Fluorine19

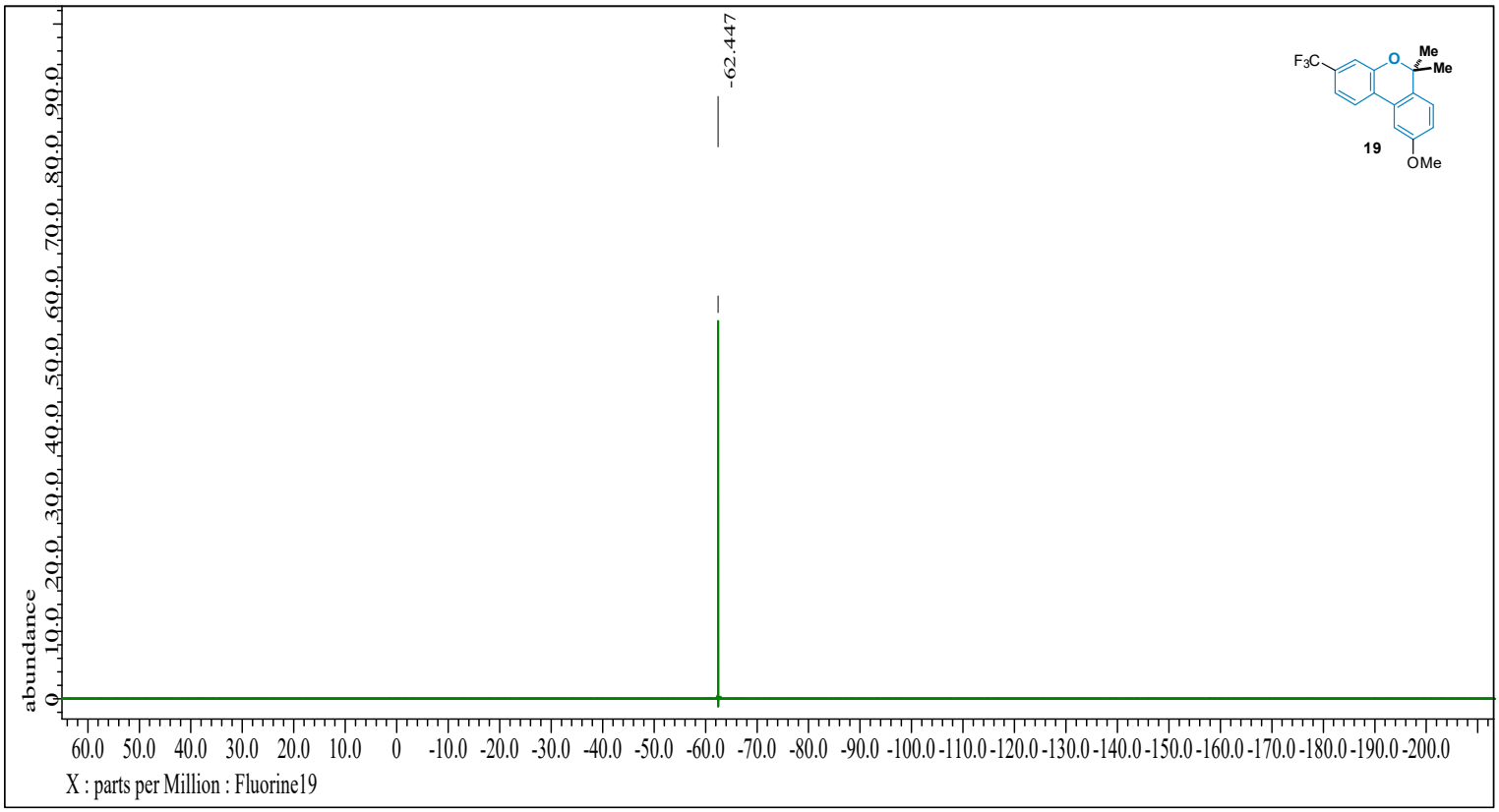

-100.935
4c
F
abundance
0
1.0
2.0
3.0
4.0
5.0
6.0
10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0 -210.0 -220.0 -230.0 -240.0 -250.0 -260.0
X : parts per Million : Fluorine19

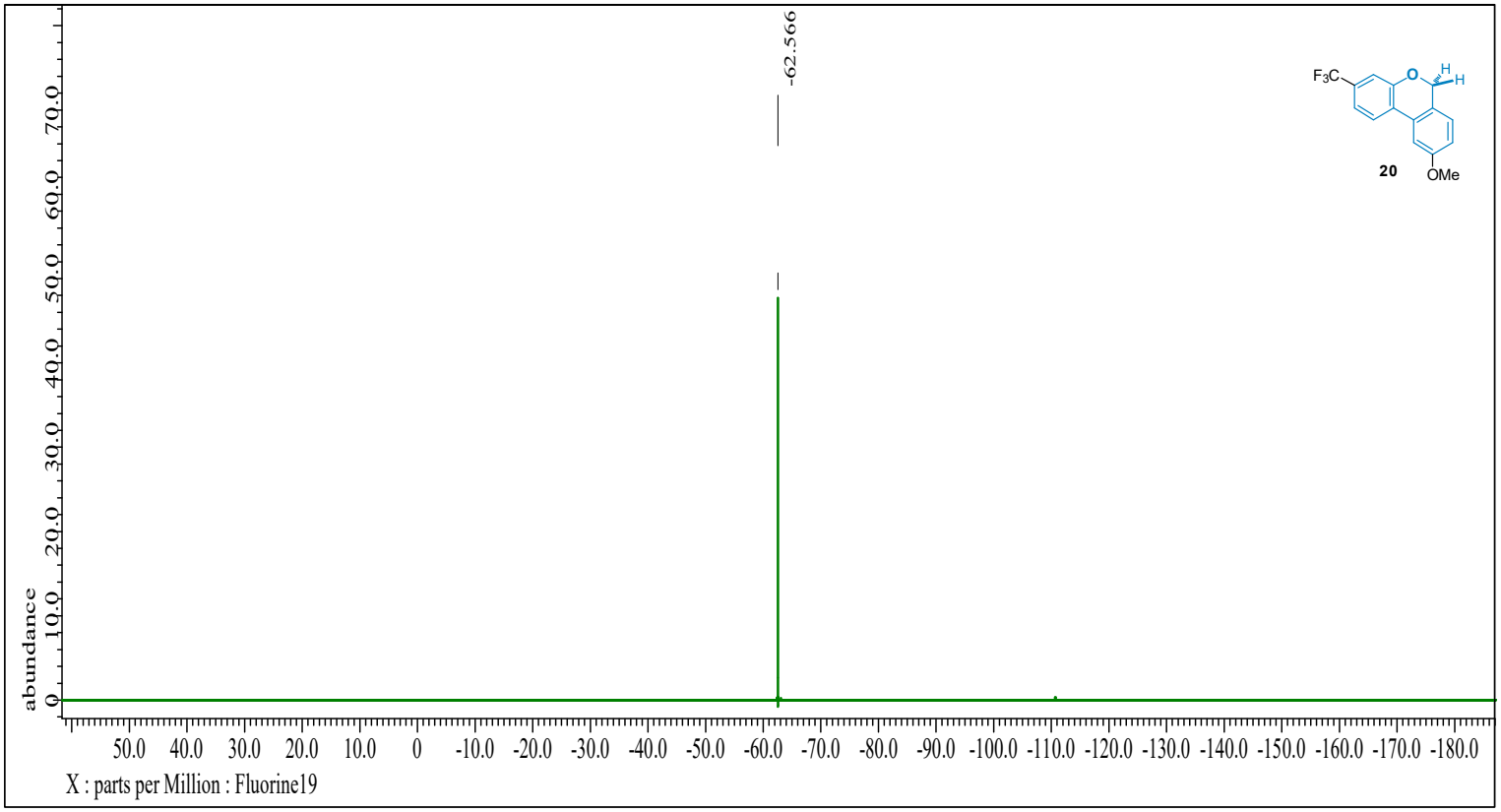

-63.310
F3C
OMe
4m
abundance
0
10.0
20.0
30.0
-41.0 -42.0 -43.0 -44.0 -45.0 -46.0 -47.0 -48.0 -49.0 -50.0 -51.0 -52.0 -53.0 -54.0 -55.0 -56.0 -57.0 -58.0 -59.0 -60.0 -61.0 -62.0 -63.0 -64.0 -65.0 -66.0 -67.0 -68.0 -69.0 -70.0 -71.0 -72.0 -73.0 -74.0 -75.0 -76.0
X : parts per Million : Fluorine19

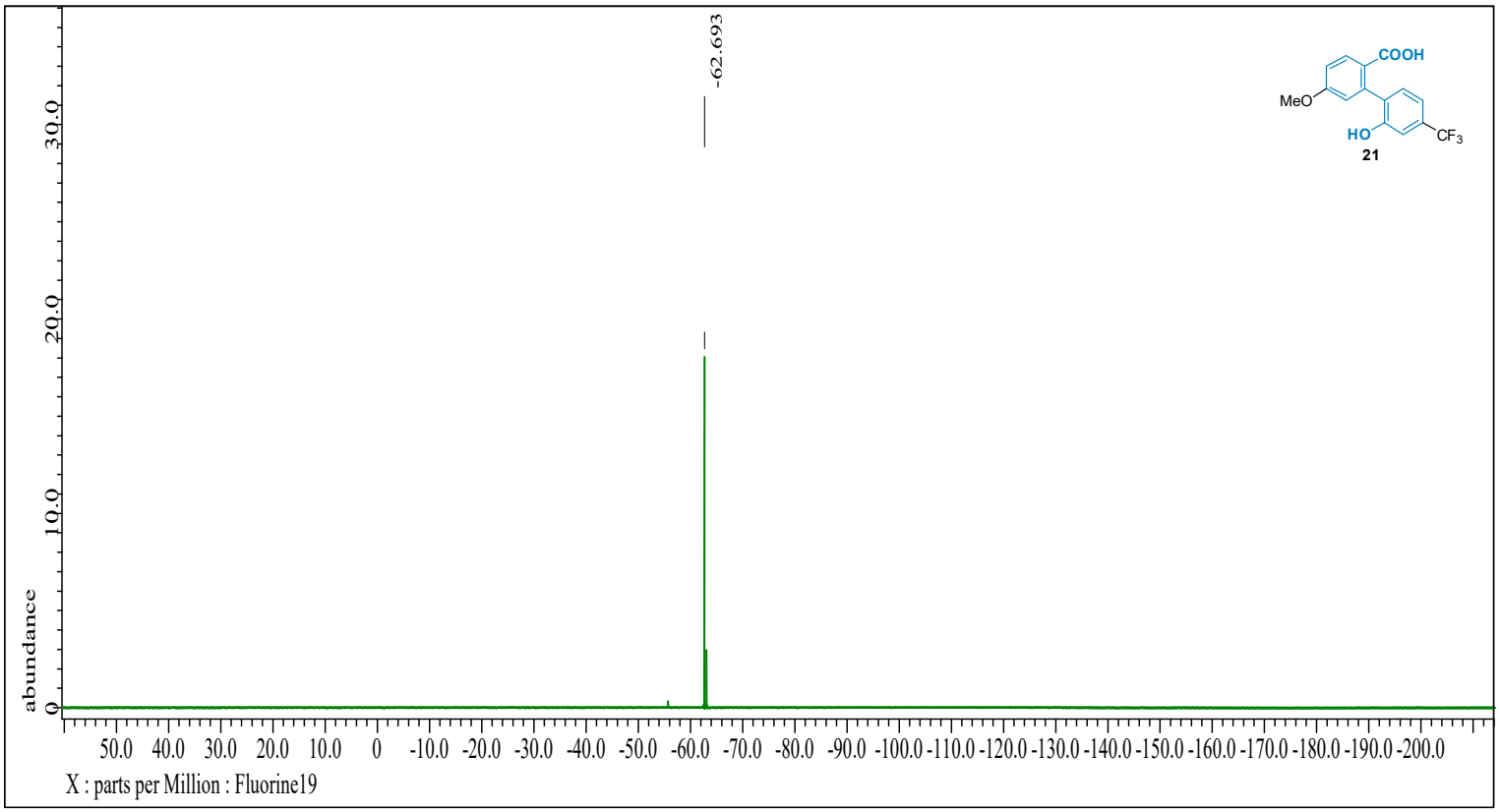

-61.813
abundance
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19
F3C
O
O
OMe
4n

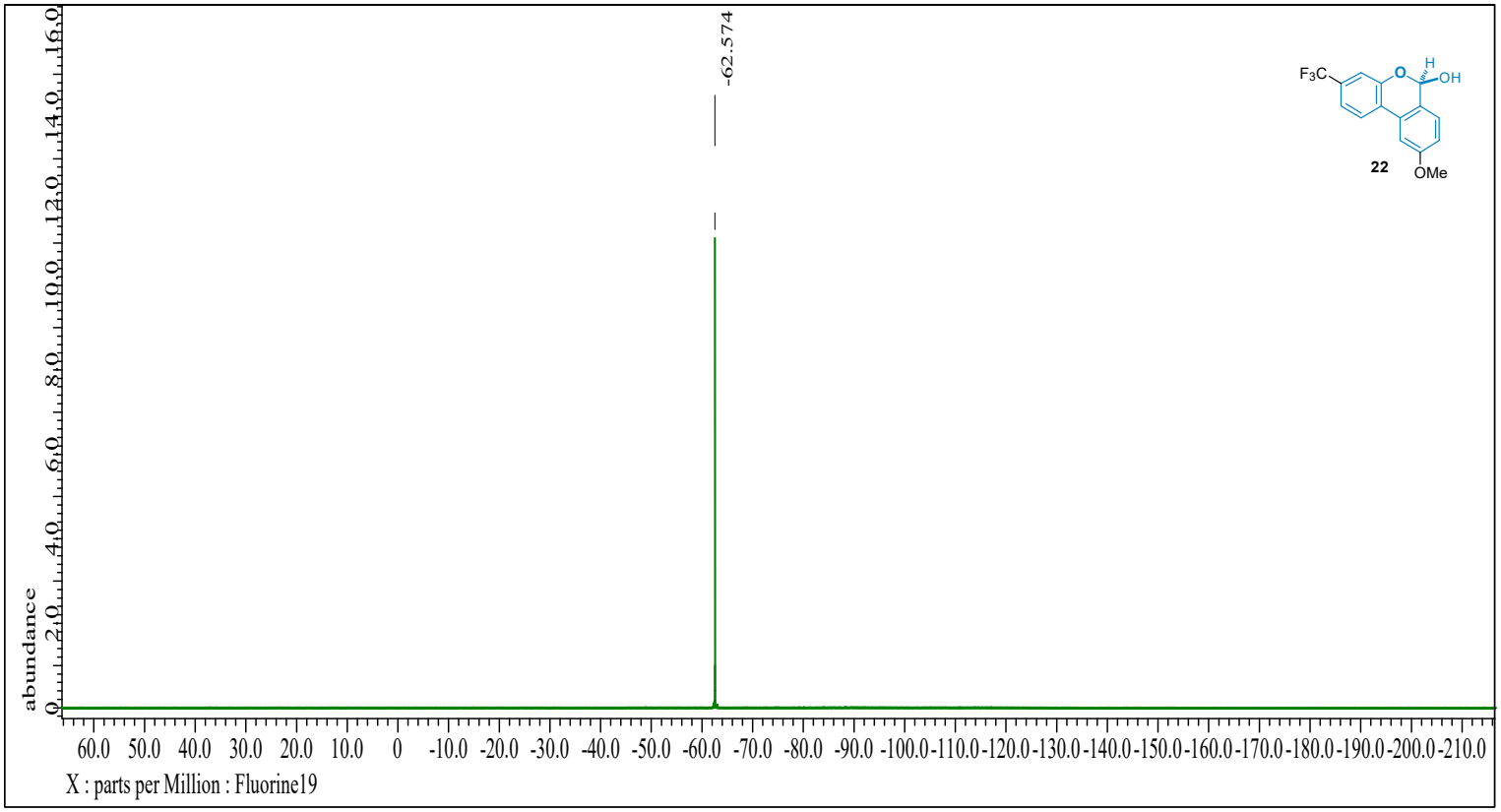

-62.043
-62.067
abundance
0
10.0
20.0
30.0
40.0
-59.0 -60.0 -61.0 -62.0 -63.0 -64.0 -65.0
X : parts per Million : Fluorine19
CF3
F3C
O
O
OMe
4o

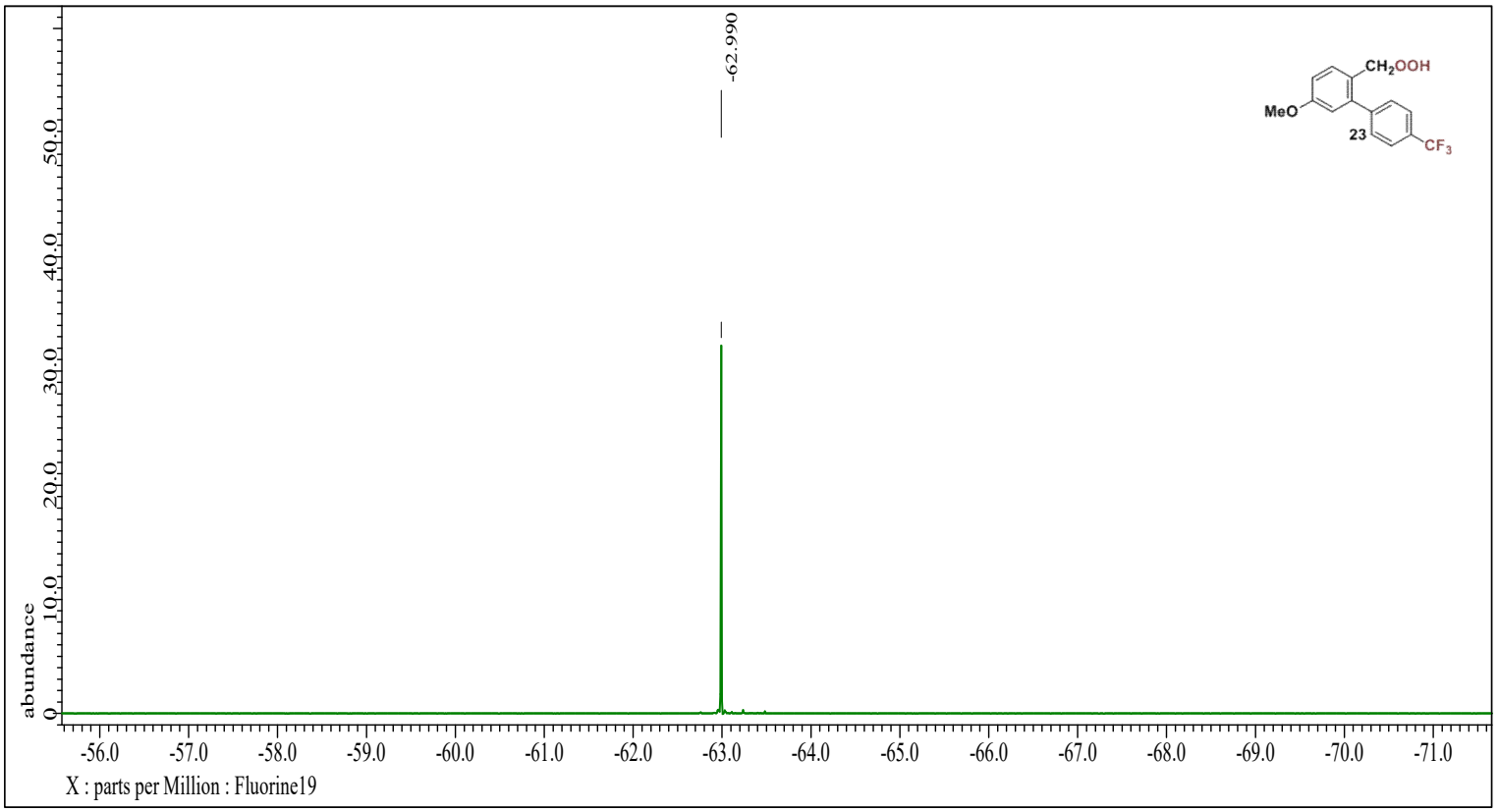

-62.534
F3C
OH
Ph
O
18
OMe
abundance
100.0
80.0
60.0
40.0
20.0
0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19

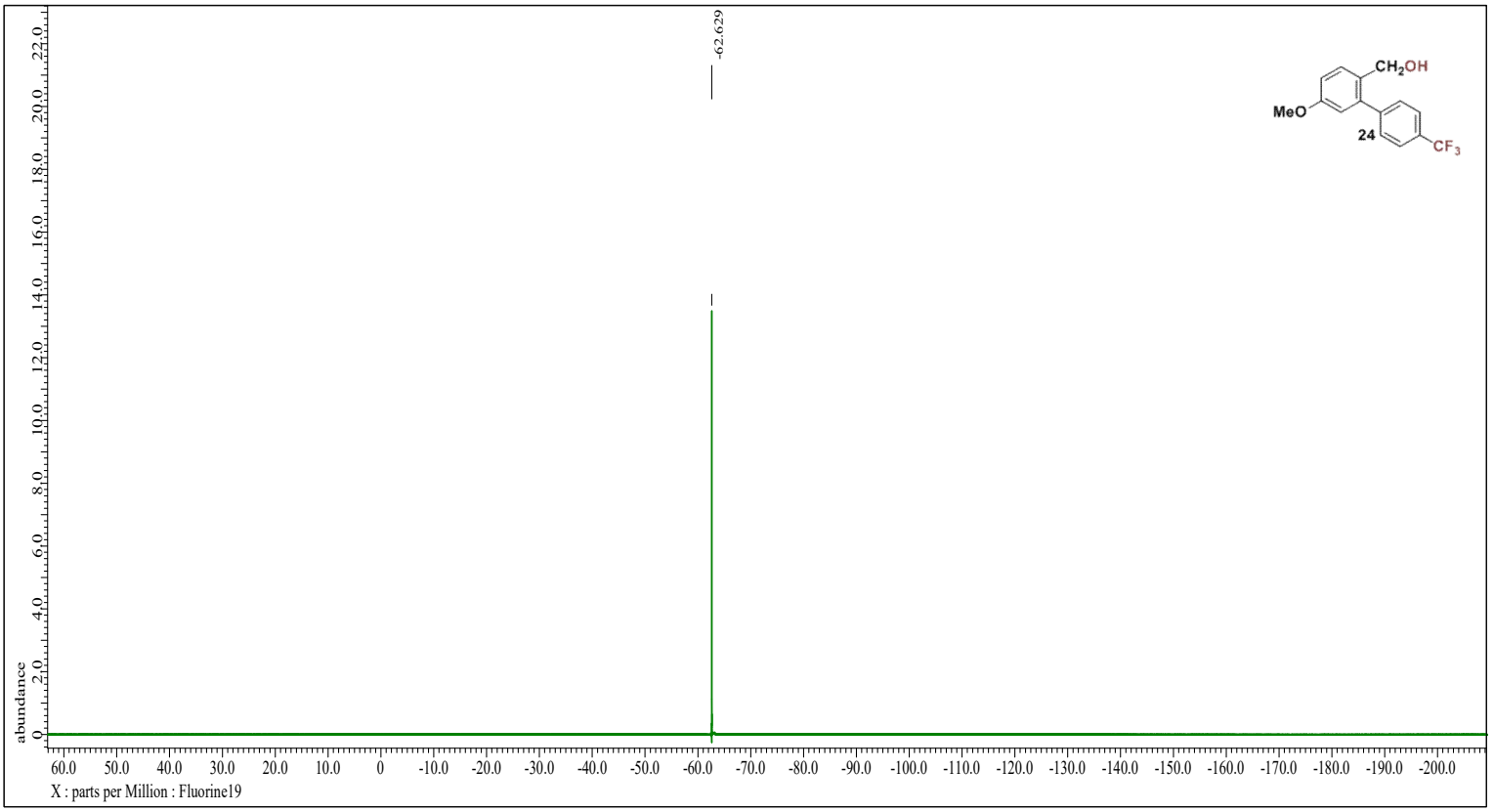

-62.447
F3C
Me
Me
O
19
OMe
abundance
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19

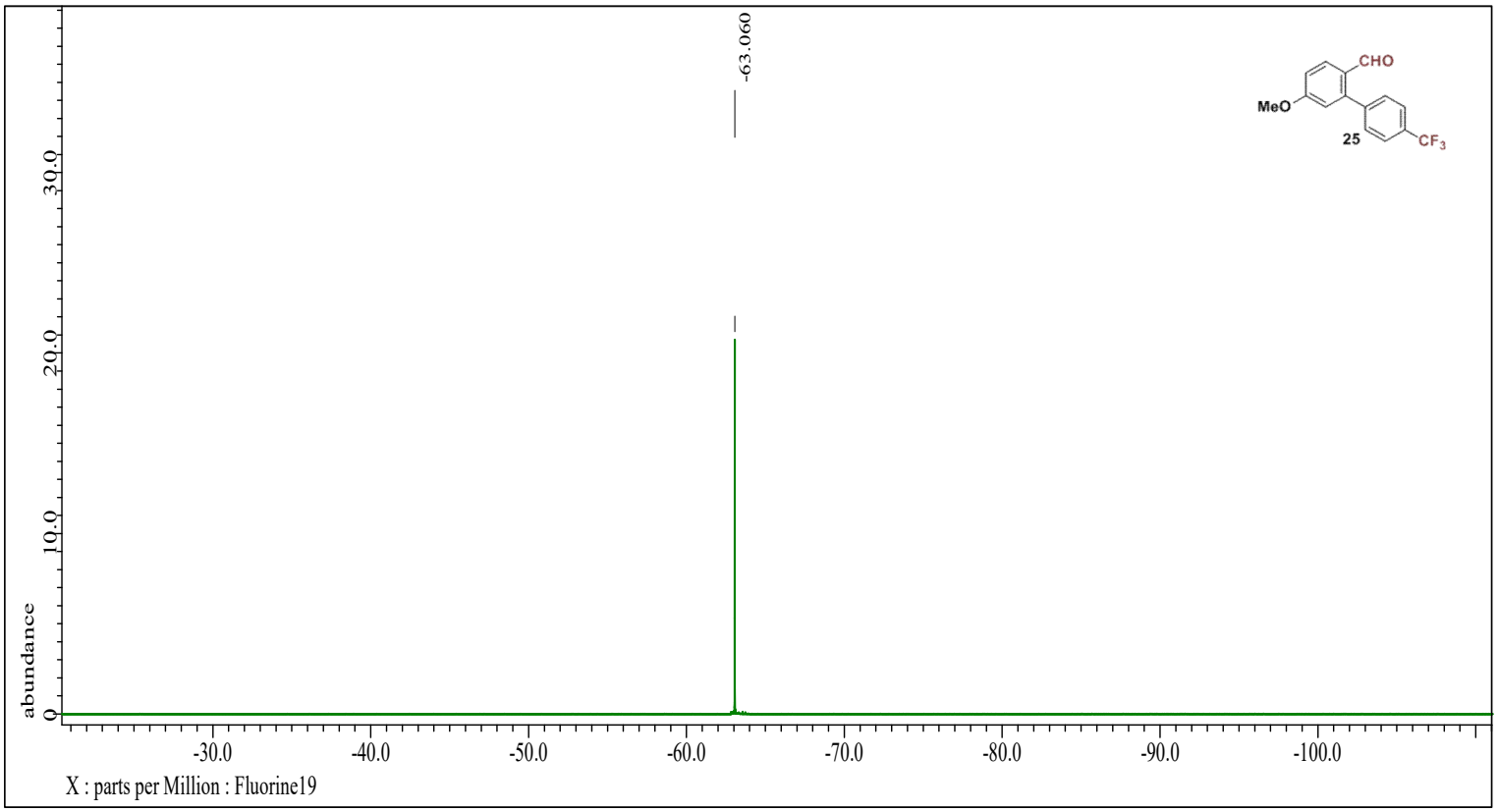

-62.566
F3C
O
H
H
20
OMe
abundance
0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0
X : parts per Million : Fluorine19

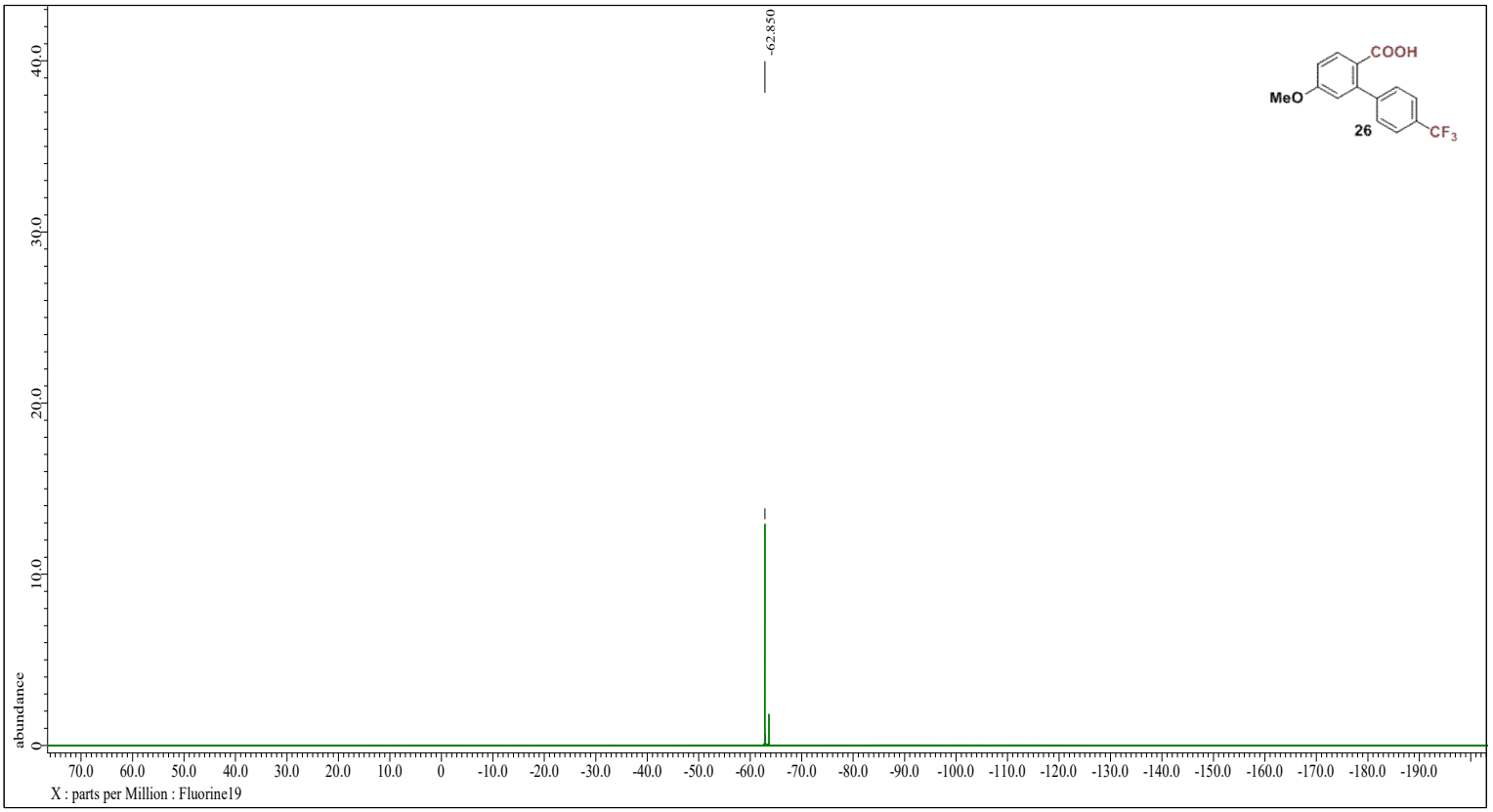

-62.693
COOH
MeO
HO
CF3
21
abundance
0
10.0
20.0
30.0
50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0 -30.0 -40.0 -50.0 -60.0 -70.0 -80.0 -90.0 -100.0 -110.0 -120.0 -130.0 -140.0 -150.0 -160.0 -170.0 -180.0 -190.0 -200.0
X : parts per Million : Fluorine19


-62.574
F3C
O
H
OH
22
OMe
abundance
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
60.0 50.0 40.0 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
X : parts per Million : Fluorine19


-62.990
CH2OOH
MeO
23
CF3
abundance
0
10.0
20.0
30.0
40.0
50.0
-56.0 -57.0 -58.0 -59.0 -60.0 -61.0 -62.0 -63.0 -64.0 -65.0 -66.0 -67.0 -68.0 -69.0 -70.0 -71.0
X : parts per Million : Fluorine19


-62.629
CH2OH
MeO
24
CF3
abundance
X : parts per Million : Fluorine19


-63.060
CHO
MeO
25
CF3
abundance
X : parts per Million : Fluorine19


-62.850
COOH
MeO
26
CF3
abundance
40.0
30.0
20.0
10.0
0
70.0 60.0 50.0 40.0 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
X : parts per Million : Fluorine19