An Umpolung Strategy for Chemically Selective Intermolecular Cross-Enolate-Type Coupling of N-Alkenoxypyridiniums with Aldehydes

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Supporting Information

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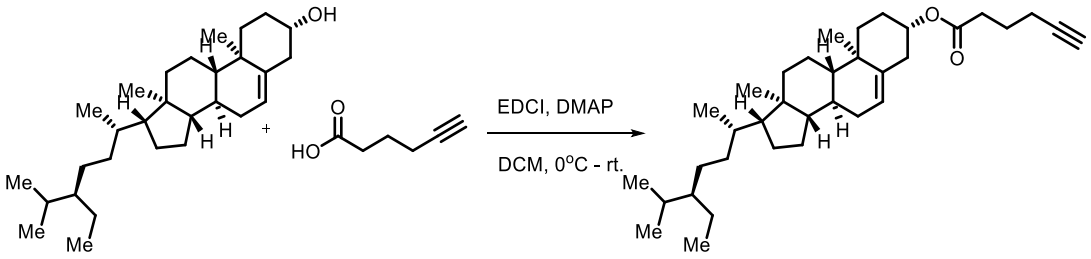
1. General procedures

All reagents and solvents were purchased from commercial sources and used without further purification unless otherwise stated. All reactions were monitored by thin-layer chromatography (TLC). All reactions were carried out in air unless otherwise stated. Column chromatography was performed on silica gel (200 - 300 mesh) and visualized with ultraviolet light. Ethyl acetate and petroleum ether were used as eluents. ^{1}H, ^{13}C and ^{19}F spectra were recorded at room temperature on a JEOL ECZ400 with MDB as an internal standard and $CDCl_3$ as solvent. Multiplicity abbreviated as: s, singlet; d, doublet; t, triplet; q, quartet; se-Pt, Septet; m, multiplet; Fourier transform infrared spectra (FT-IR) were recorded on Agilent Technologies Cary 630 instrument. HRMS analyses were made by means of ESI-TOF. Melting points were measured on micro melting point apparatus and uncorrected.

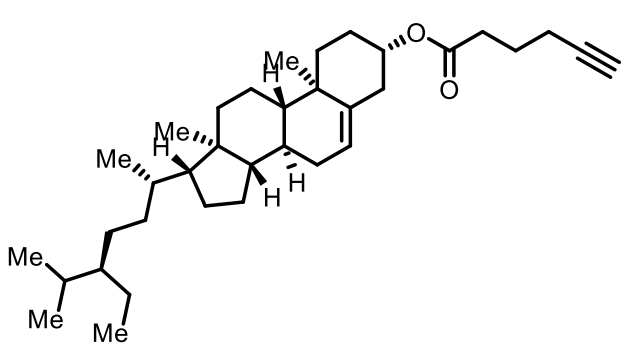
2. Synthesis of substrates

2.1. Synthesis of S1ah-S1al [1]



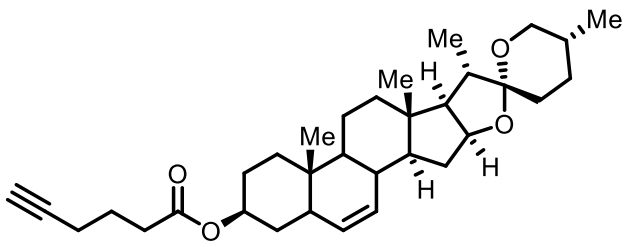
To a solution of Beta-Sitosterol (5.0 mmol, 2.07 g) and 5-Hexynoic Acid (5.0 mmol, 1 equiv) in DCM (20.0 mL) was added EDCI (6.0 mmol, 1.2 equiv, 1.15 g) and DMAP (0.5 mmol, 0.1 equiv, 0.061 g) at 0 °C. After addition, the mixture was stirred at room temperature until TLC indicating completion. The reaction was quenched with H_2O and extracted with CH_2Cl_2 (2 × 20 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated in vacuo. The crude product was purified by flash chromatography (silica gel, 50:1 petroleum ether/EtOAc) to afford 4-acetylbenzoate **S1ah - S1al**.

(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*S*,5*R*)-5-Ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl-hex-5-ynoate (S1ah)



White solid after purification by column chromatography (petroleum ether/ethyl acetate = 50/1); mp: 155.0 - 155.6 °C, 2.5 g, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.37 (d, *J* = 4.1 Hz, 1H), 4.68 − 4.54 (m, 1H), 2.42 (t, *J* = 7.3 Hz, 2H), 2.35 − 2.22 (m, 4H), 2.03 − 1.91 (m, 2H), 1.91 − 1.79 (m, 4H), 1.63 − 1.44 (m, 7H), 1.42 (s, 3H), 1.33 − 1.21 (m, 4H), 1.19 − 1.07 (m, 4H), 1.01 (s, 3H), 0.94 − 0.89 (m, 4H), 0.86 (t, *J* = 5.5 Hz, 4H), 0.85 − 0.79 (m, 10H), 0.67 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.5, 139.6, 122.7, 83.4, 76.7, 73.9, 69.0, 56.6, 55.9, 49.9, 45.8, 42.3, 39.7, 38.1, 36.9, 36.6, 36.1, 33.9, 33.3, 31.9, 31.8, 29.1, 28.2, 27.8, 25.9, 24.3, 23.7, 23.0, 20.9, 19.8, 19.3, 18.9, 18.7, 17.8, 11.9, 11.8. IR (KBr, cm^{-1}): 3263, 2954, 2870, 1720, 1465, 1381, 1323, 1265, 1195, 1153, 1010, 921, 879, 802, 736, 682, 536. HRMS (ESI^{+}) m/z: $[M+H]^{+}$ calcd for $C_{35}H_{57}O_2^{+}$: 509.4353; found: 509.4344.

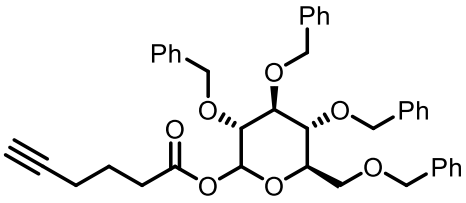
(4*S*,5'*R*,6a*S*,8a*S*,8b*R*,9*S*,10*R*,11a*S*,12a*S*,12b*R*)-5',6a,8a,9-Tetramethyl-2a,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4-yl-hex-5-ynoate (S1ai)



White solid after purification by column chromatography (petroleum ether/ethyl acetate = 50/1); mp: 167.5 − 168.2 °C, 2.5 g, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.37 (d, *J* = 4.6 Hz, 1H), 4.68 − 4.54 (m, 1H), 4.41 (q, *J* = 7.5 Hz, 1H), 3.47 (dd, *J* = 11.0, 4.1 Hz, 1H), 3.37 (t, *J* = 10.7 Hz, 1H), 2.42 (t, *J* = 7.5 Hz, 2H), 2.35 − 2.21 (m, 4H), 2.05 − 1.93 (m, 3H), 1.91 − 1.81 (m, 5H), 1.81 − 1.69 (m, 2H), 1.66 − 1.55 (m, 7H), 1.55 − 1.36 (m, 4H), 1.28 (td, *J* = 12.7, 6.3 Hz, 1H), 1.23 − 1.05 (m, 3H), 1.03 (s, 3H), 0.97 (d, *J* = 6.9 Hz, 3H), 0.79 (d, *J* = 4.6 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.3, 139.6, 122.3, 109.2, 83.3, 80.7, 73.8, 69.1, 66.7, 61.9, 56.3, 49.8, 41.5, 40.2, 39.6, 38.0, 36.9, 36.6, 33.2, 31.9, 31.8, 31.3, 30.2, 28.7, 27.7, 23.6, 20.7, 19.3, 17.8, 17.1, 16.2, 14.5. IR (KBr, cm^{-1}): 2931, 2885, 1724, 1450, 1377, 1246, 1165, 1049, 1006, 983, 960, 918, 898, 864, 840, 798, 702, 597, 536. HRMS (ESI^{+}) m/z: $[M+H]^{+}$ calcd for $C_{33}H_{49}O_4^{+}$: 509.3625; found: 509.3647.

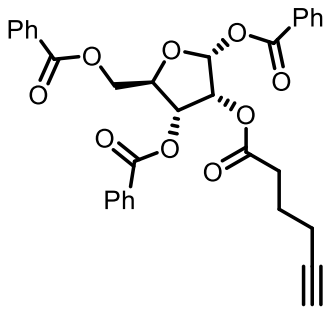
(3*R*,4*S*,5*R*,6*R*)-3,4,5-5Tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl-hex-5-ynoate (S1aj)

White solid after purification by column chromatography (petroleum ether/ethyl acetate



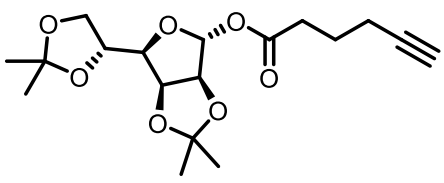
= 20/1); mp: 65.3 − 67.5 °C, 3054.10 g, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 (q, *J* = 2.4 Hz, 20H), 7.16 (q, *J* = 2.7 Hz, 2H), 6.46 − 5.60 (m, 1H), 4.95 (dd, *J* = 24.5, 10.7 Hz, 1H), 4.89 − 4.81 (m, 2H), 4.79 (d, *J* = 4.1 Hz, 1H), 4.75 − 4.60 (m, 2H), 4.58 − 4.47 (m, 2H), 4.00 − 3.86 (m, 1H), 3.82 − 3.69 (m, 4H), 3.69−3.56 (m, 1H), 2.62 − 2.44 (m, 1H), 2.27 (tt, *J* = 7.0, 2.2 Hz, 2H), 1.99 (q, *J* = 2.6 Hz, 1H), 1.92 − 1.81 (m, 2H), 0.94 − 0.84 (2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.6, 202.8, 171.7, 166.2, 165.8, 165.3, 138.0, 133.8, 133.7, 133.5, 130.0, 129.9, 129.8, 129.6, 129.5, 129.2, 129.0, 128.8, 128.7, 128.7, 128.6, 128.5, 126.9, 94.8, 82.9, 82.8, 77.2, 70.8, 70.7, 64.1, 60.5, 48.4, 41.3, 40.8, 34.6, 32.6, 21.2, 18.3, 14.3. IR (KBr, cm^{-1}): 3290, 3030, 2912, 2858, 1743, 1608, 1585, 1496, 1444, 1359, 1205, 1076, 732, 700, 636, 459. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{40}H_{42}O_7Na^{+}$: 657.2823; found: 657.2810.

(2*R*,3*R*,4*R*,5*R*)-5-((Benzoyloxy)methyl)-3-(hex-5-ynoyloxy)tetrahydrofuran-2,4-diyl-dibenzoate (S1ak)



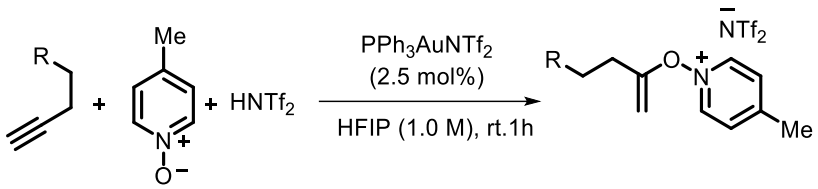
Transparent viscous liquid after purification by column chromatography (petroleum ether/ethyl acetate = 20/1); 2.7 g, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.12 − 8.07 (m, 6H), 7.67 − 7.57 (m, 3H), 7.52 − 7.37 (m, 6H), 6.81 (d, *J* = 4.6 Hz, 1H), 5.79 (dd, *J* = 6.4, 2.3 Hz, 1H), 5.57 (dd, *J* = 6.4, 4.6 Hz, 1H), 4.86 (q, *J* = 2.9 Hz, 1H), 4.72 (dd, *J* = 12.3, 3.2 Hz, 1H), 4.65 − 4.57 (1H), 2.42 (t, *J* = 7.5 Hz, 2H), 2.13 (td, *J* = 7.0, 2.6 Hz, 2H), 1.80 (t, *J* = 2.5 Hz, 1H), 1.78 − 1.68 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.7, 166.2, 165.8, 165.3, 133.8, 133.6, 133.5, 130.1, 130.0, 129.9, 129.8, 129.7, 129.5, 129.3, 128.7, 128.7, 128.5, 94.8, 83.0, 82.9, 77.1, 70.9, 70.7, 69.3, 64.1, 32.3, 23.3, 17.7. IR (KBr, cm^{-1}): 3277, 3047, 2927, 2360, 1724, 1598, 1450, 1315, 1265, 1114, 1022, 707. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{32}H_{28}O_9Na^{+}$: 579.1626; found: 579.1617.

(3a*S*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl-hex-5-ynoate (S1al)



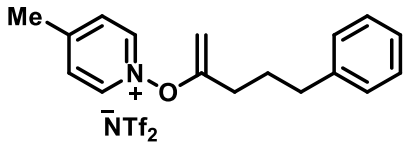
Transparent viscous liquid after purification by column chromatography (petroleum ether/ethyl acetate = 20/1); 1.7 g, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 6.14 (s, 1H), 4.85 (q, *J* = 3.2 Hz, 1H), 4.69 (d, *J* = 5.9 Hz, 1H), 4.43 − 4.36 (m, 1H), 4.13 − 4.06 (1H), 4.02 (td, *J* = 7.9, 3.7 Hz, 2H), 2.46 (t, *J* = 7.5 Hz, 2H), 2.27 (td, *J* = 6.9, 2.7 Hz, 2H), 1.99 (t, *J* = 2.7 Hz, 1H), 1.90 − 1.77 (m, 2H), 1.47 (d, *J* = 10.5 Hz, 6H), 1.35 (d, *J* = 13.7 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.5, 113.2, 109.3, 100.6, 85.0, 83.0, 82.2, 79.2, 77.0, 72.8, 69.3, 66.8, 32.7, 26.9, 25.9, 25.1, 24.6, 23.1, 17.6. IR (KBr, cm^{-1}): 3251, 3010, 2987, 2902, 1743, 1490, 1463, 1280, 1165, 1151, 1120, 1071, 1039, 974, 846, 707, 680, 563, 516, 468, 418. HRMS (ESI+) m/z: [M+Na]$^{+}$ calcd for $C_{18}H_{26}O_7Na^{+}$: 377.1751; found: 377.1569.

2.2. General procedure for B [2]



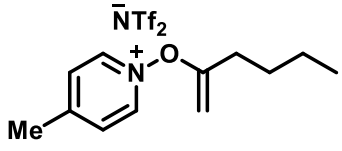
p-Methylpyridine oxide and Tf_2NH were premixed in a molar ratio of 1.2/1.1 which was then stored in a vial and used forreaction directly. PPh_3AuNTf_2 (5.5 mg, 0.025 equiv.) was added into a mixture of pent-4-yn-1-ylbenzene (43.8 mg, 0.3 mmol), the above premixed salt (126.9 mg, 1.2 equiv, in the p-methylpyridine oxide) and HFIP (0.3 mL) in a vial at room temperature. The reaction mixture was then stirred at room temperature, and the progress of the reaction was monitored by TLC (CH_2Cl_2/MeOH = 10/1). After the reaction was completed, the N-alkenoxypyridinium salt was purified by column chromatography on silica with greater than 90 % isolated yield (CH_2Cl_2/ MeOH = 100/1).

4-Methyl-1-((5-phenylpent-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2a)



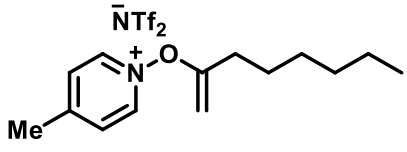
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1040.1 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.55 − 8.48 (m, 2H), 7.96 (d, *J* = 6.7 Hz, 2H), 7.28 (t, *J* = 7.4 Hz, 2H), 7.19 (dt, *J* = 9.8, 3.0 Hz, 3H), 4.46 (d, *J* = 5.4 Hz, 1H), 3.68 (d, *J* = 5.5 Hz, 1H), 2.69 (d, *J* = 5.5 Hz, 5H), 2.38 (t, *J* = 7.7 Hz, 2H), 1.96 (p, *J* = 7.6 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.2, 161.4, 141.1, 140.5, 130.4, 128.4, 128.4, 126.0, 121.3, 118.1, 88.9, 34.7, 30.3, 27.7, 22.2. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3113, 2939, 1716, 1666, 1639, 1624, 1496, 1454, 1350, 1192, 1138, 1056, 786, 740, 651, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{17}H_{20}NO^+$:254.1539 ; found:254.1540.

1-(Hex-1-en-2-yloxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2b)



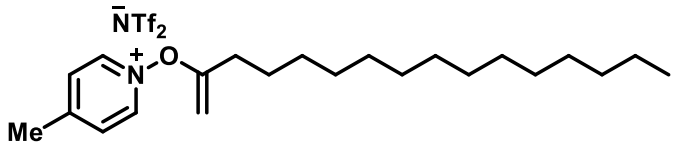
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 910.8 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 6.9 Hz, 2H), 7.98 (d, *J* = 6.4 Hz, 2H), 4.42 (d, *J* = 5.5 Hz, 1H), 3.64 (d, *J* = 5.5 Hz, 1H), 2.69 (s, 3H), 2.33 (t, *J* = 7.8 Hz, 2H), 1.65 − 1.48 (m, 2H), 1.36 (q, *J* = 7.5 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.7, 161.3, 140.6, 130.3, 121.2, 118.0, 88.2, 30.4, 28.3, 22.1, 21.7, 13.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.89. IR (KBr, cm^{-1}): 3116, 2962, 2935, 2873, 1666, 1624, 1496, 1462, 1350, 1138, 1056, 871, 852, 786, 740, 655, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{12}H_{18}NO^+$: 192.1383; found: 192.1391.

4-Methyl-1-(oct-1-en-2-yloxy)pyridine-1-ium bis((trifluoromethyl)sulfonyl)amide (2c)



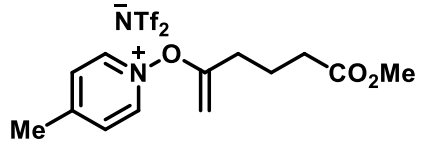
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 960.0 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 − 8.59 (m, 2H), 8.03 (d, *J* = 6.7 Hz, 2H), 4.47 (d, *J* = 5.4 Hz, 1H), 3.69 (d, *J* = 5.3 Hz, 1H), 2.74 (s, 3H), 2.36 (t, *J* = 7.7 Hz, 2H), 1.61 (p, *J* = 7.9, 7.4 Hz, 2H), 1.44 − 1.20 (m, 6H), 0.93 − 0.82 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.8, 161.3, 140.6, 130.4, 121.2, 118.0, 88.3, 31.1, 30.7, 28.3, 26.2, 22.2, 22.1, 13.8. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 2927, 2854, 1666, 1624, 1496, 1458, 1354, 1192, 1138, 1056, 848, 786, 740, 690, 651, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{14}H_{22}NO^+$: 220.1696; found: 220.1670.

1-(Hexadec-1-en-2-yloxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2d)



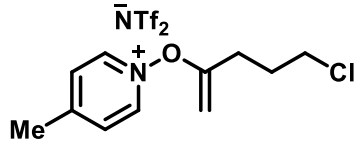
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1164.1 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.62 (d, *J* = 7.1 Hz, 2H), 8.03 (d, *J* = 6.4 Hz, 2H), 4.50 − 4.39 (d, *J* = 5.5 Hz,1H), 3.67 (d, *J* = 5.5 Hz, 1H), 2.80 − 2.67 (s, 3H), 2.35 (t, *J* = 7.8 Hz, 2H), 1.67 − 1.52 (m, 2H), 1.34 − 1.14 (m, 18H), 0.84 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 166.0, 161.5, 140.7, 134.0, 130.6, 88.5, 31.9, 30.9, 29.7, 29.6, 29.6, 29.4, 29.3, 29.2, 28.9, 26.5, 22.7, 22.4, 14.1. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.89. IR (KBr, cm^{-1}): 3116, 2927, 2854, 1666, 1624, 1496, 1462, 1350, 1192, 1138, 1060, 848, 786, 740, 655, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{22}H_{38}NO^+$: 332.2948; found: 332.2954.

1-((6-Methoxy-6-oxohex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2e)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 996.7 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.77 − 8.64 (m, 2H), 8.01 (d, *J* = 6.6 Hz, 2H), 4.51 − 4.45 (m, 1H), 3.74 − 3.66 (m, 1H), 3.64 (d, *J* = 0.9 Hz, 3H), 2.73 (s, 3H), 2.52 − 2.30 (m, 4H), 1.96 (h, *J* = 7.5 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 173.5, 164.5, 161.6, 140.7, 130.5, 121.3, 118.1, 89.1, 51.6, 32.6, 30.4, 22.3, 21.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.92. IR (KBr, cm^{-1}): 3116, 2958, 1732, 1666, 1624, 1496, 1458, 1438, 1350, 1192, 1138, 1056, 848, 786, 740, 651, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{13}H_{18}NO_3^+$: 236.1281; found: 236.1284.

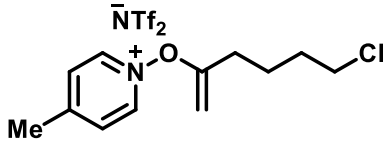
1-((5-Chloropent-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2f)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 956.0 mg, 97% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.67 (d, *J* = 5.8 Hz, 2H), 7.99 (d, *J* = 5.5 Hz, 2H), 4.53 (d, *J* = 5.4 Hz,

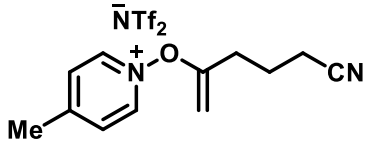
1H), 3.73 (d, *J* = 5.5 Hz, 1H), 3.62 (t, *J* = 6.1 Hz, 2H), 2.73 (s, 3H), 2.57 (t, *J* = 7.4 Hz, 2H), 2.09 (h, *J* = 7.1, 6.6 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 164.2, 161.7, 140.8, 130.6, 90.0, 43.6, 29.1, 28.4, 22.6. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.92. IR (KBr, cm^{-1}): 3116, 1666, 1624, 1496, 1350, 1192, 1138, 1056, 786, 740, 617, 570, 513. HRMS (ESI$^+$) m/z: [M]$^+$ calcd for $C_{11}H_{15}ClNO^+$: 212.0837; found: 212.0847.

1-((6-Chlorohex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2g)



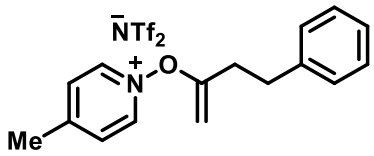
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 993.3 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.66 (d, *J* = 5.8 Hz, 2H), 8.01 (d, *J* = 5.8 Hz, 2H), 4.50 (dd, *J* = 5.5, 0.9 Hz, 1H), 3.71 (d, *J* = 5.5 Hz, 1H), 3.57 (t, *J* = 6.1 Hz, 2H), 2.73 (s, 3H), 2.42 (t, *J* = 7.3 Hz, 2H), 1.87 − 1.71 (m, 4H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 165.0, 161.5, 140.7, 130.4, 121.2, 118.1, 88.9, 44.4, 31.3, 30.1, 23.5, 22.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.89. IR (KBr, cm^{-1}): 3116, 2877, 1666, 1624, 1496, 1458, 1350, 1192, 1138, 1056, 852, 786, 740, 617, 570, 513. HRMS (ESI$^+$) m/z: [M]$^+$ calcd for $C_{12}H_{17}ClNO^+$: 226.0993; found: 226.1003.

1-((6-Cyanohex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2h)



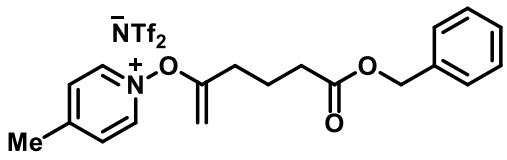
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 918.5 mg, 95% yield. ^{1}H NMR (400 MHz, Methanol-*d*$_4$) δ 9.08 (d, *J* = 7.3 Hz, 2H), 8.08 (d, *J* = 4.6 Hz, 2H), 4.82 (s, 2H), 4.63 (d, *J* = 5.5 Hz, 1H), 3.86 (d, *J* = 5.5 Hz, 1H), 3.37 − 3.20 (1H), 2.67 − 2.49 (4H), 2.13 − 1.96 (m, 2H). ^{13}C NMR (100 MHz, Methanol-*d*$_4$) δ 165.2, 163.3, 142.5, 131.3, 122.8, 120.7, 119.6, 89.9, 31.2, 23.7, 22.3, 16.6. ^{19}F NMR (376 MHz, Methanol-*d*$_4$) δ -78.98. IR (KBr, cm^{-1}): 3116, 2947, 1666, 1624, 1496, 1458, 1350, 1192, 1138, 1056, 867, 786, 740, 651, 617, 570, 513. HRMS (ESI$^+$) m/z: [M]$^+$ calcd for $C_{12}H_{15}N_2O^+$: 203.1179; found: 203.1180.

4-Methyl-1-((4-phenylbut-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2i)



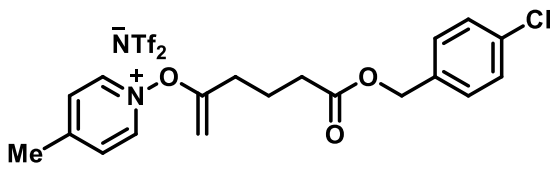
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1019.4 mg, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.54 − 8.39 (m, 2H), 8.05 − 7.91 (m, 2H), 7.40 − 7.28 (m, 2H), 7.26 (td, *J* = 5.2, 2.8 Hz, 3H), 4.50 (d, *J* = 5.5 Hz, 1H), 3.69 (d, *J* = 5.5 Hz, 1H), 2.97 (p, *J* = 7.5 Hz, 2H), 2.78 − 2.63 (m, 1H), 2.72 (s, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 164.6, 161.5, 140.6, 139.5, 130.4, 128.6, 128.5, 126.6, 121.3, 118.1, 89.3, 32.8, 32.4, 22.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.79. IR (KBr, cm^{-1}): 3113, 1666, 1624, 1496, 1454, 1350, 1192, 1056, 786, 740, 702, 651, 617, 570, 513. HRMS (ESI$^+$) m/z: [M]+ calcd for $C_{16}H_{18}NO^+$: 240.1383; found: 240.1387.

1-((6-(Benzyloxy)-6-oxohex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2j)



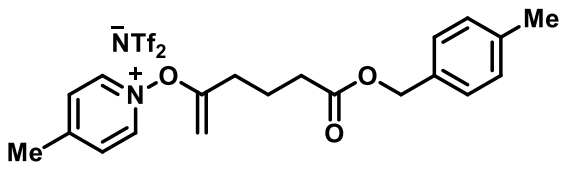
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1125.2 mg, 95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.70 − 8.64 (m, 2H), 8.00 (d, *J* = 6.6 Hz, 2H), 7.36 − 7.24 (m, 3H), 5.07 (s, 2H), 4.48 (d, *J* = 5.5 Hz, 1H), 3.70 (d, *J* = 5.5 Hz, 1H), 2.75 (s, 3H), 2.46 (dt, *J* = 17.5, 7.2 Hz,5H), 1.99 (p, *J* = 7.3 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.8, 164.4, 161.6, 140.7, 134.3, 134.1, 130.5, 129.6, 128.7, 121.3, 118.1, 89.3, 65.6, 32.8, 30.6, 22.5, 21.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3113, 2951, 1732, 1666, 1624, 1496, 1458, 1350, 1192, 1138, 1056, 887, 848, 786, 740, 698, 651, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{19}H_{22}NO_3^+$: 312.1594; found: 312.1592.

1-((6-((4-Chlorobenzyl)oxy)-6-oxohex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2k)



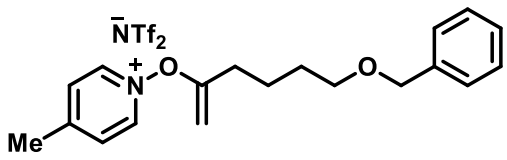
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1191.1 mg ,95% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.67 − 8.53 (m, 2H), 7.99 − 7.88 (m, 2H), 7.28 (s, 2H), 7.35 − 7.19 (m, 2H), 5.06 (s, 2H), 4.40 (d, *J* = 5.5 Hz, 1H), 3.60 (d, *J* = 5.5 Hz, 1H), 2.66 (s, 3H), 2.52 − 2.26 (m, 5H), 1.94 (h, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.8, 164.4, 161.6, 140.7, 134.3, 134.1, 130.5, 129.6, 128.7, 89.3, 65.6, 32.8, 30.6, 22.5, 21.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3113, 2947, 1723, 1666, 1624, 1492, 1458, 1350, 1188, 1056, 740, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{19}H_{21}ClNO_3^+$: 346.1204; found: 346.1199.

4-Methyl-1-((6-((4-methylbenzyl)oxy)-6-oxohex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2l)



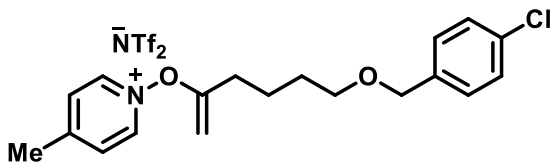
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1164.7 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.73 − 8.60 (m, 2H), 8.06 − 7.92 (m, 2H), 7.31 − 7.17 (m, 2H), 7.17 − 7.10 (m, 2H), 7.06 (dd, *J* = 8.3, 5.9 Hz, 0H), 5.07 (s, 3H), 4.46 (d, *J* = 5.5 Hz, 1H), 3.67 (d, *J* = 5.5 Hz, 1H), 2.74 (s, 3H), 2.45 (dt, *J* = 13.3, 7.2 Hz, 4H), 2.32 (s, 3H), 1.98 (p, *J* = 7.2 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.9, 164.4, 161.5, 140.7, 138.2, 132.7, 130.5, 129.2, 128.3, 121.3, 118.1, 89.2, 66.4, 32.9, 30.5, 22.4, 21.3, 21.1. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3113, 2951, 1732, 1666, 1624, 1496, 1458, 1354, 1192, 1138, 1056, 844, 810, 740, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{20}H_{24}NO_3^+$: 326.1751; found: 326.1747.

1-((6-(Benzyloxy)hex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2m)



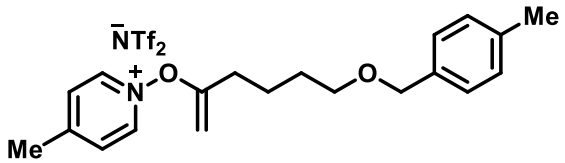
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1110.7 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 7.3 Hz, 2H), 7.93 (d, *J* = 7.3 Hz, 2H), 7.33 − 7.19 (m, 4H), 4.46 (d, *J* = 5.5 Hz, 1H), 4.43 (s, 2H), 3.67 (d, *J* = 5.5 Hz, 1H), 3.50 (t, *J* = 5.7 Hz, 2H), 2.69 (s, 3H), 2.38 (t, *J* = 7.1 Hz, 2H), 1.81 − 1.56 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.4, 161.4, 140.6, 137.0, 133.2, 130.4, 129.1, 128.4, 121.3, 118.1, 88.9, 72.1, 69.8, 53.4, 30.7, 28.6, 23.1, 22.3. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3116, 2939, 2866, 1666, 1624, 1492, 1458, 1350, 1195, 1138, 1056, 848, 813, 740, 651, 617, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{19}H_{24}NO_2^+$: 298.1802; found: 298.1804.

1-((6-((4-Chlorobenzyl)oxy)hex-1-en-2-yl)oxy)-4-methylpyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2n)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1176.9 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.61 − 8.51 (m, 2H), 7.87 (d, *J* = 6.7 Hz, 2H), 7.31 (s, 2H), 7.31 − 7.30 (s, 2H), 4.45 (d, *J* = 10.0 Hz, 3H), 3.67 (d, *J* = 5.4 Hz, 1H), 3.52 (t, *J* = 5.7 Hz, 2H), 2.66 (s, 3H), 2.37 (t, *J* = 7.1 Hz, 2H), 1.79 − 1.66 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.4, 161.4, 140.7, 136.9, 133.2, 130.4, 129.1, 128.5, 121.3, 118.1, 89.0, 72.2, 69.8, 30.7, 28.6, 23.1, 22.4. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.79. IR (KBr, cm^{-1}): 3113, 2939, 2866, 1666, 1624, 1496, 1458, 1354, 1195, 1138, 1056, 852, 786, 740, 651, 617, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{19}H_{23}ClNO_2^+$: 332.1412; found: 332.1416.

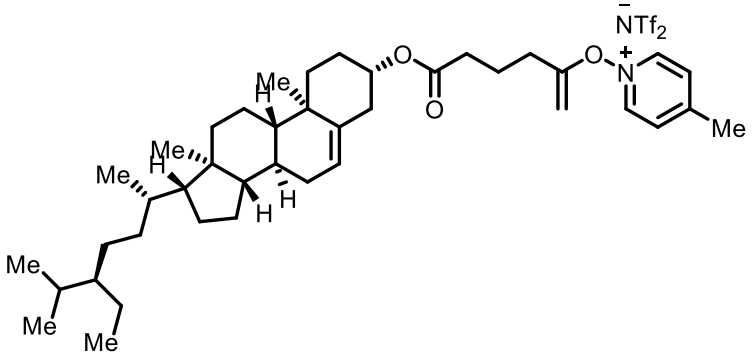
4-Methyl-1-((6-((4-methylbenzyl)oxy)hex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2o)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1137.8 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, *J* = 6.9 Hz, 2H), 7.89 (d, *J* = 6.9 Hz, 2H), 7.23 (d, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 4.50 (d, *J* = 5.0 Hz, 1H), 4.45 (s, 2H), 3.77 − 3.71 (1H), 3.53 (t, *J* = 5.7 Hz, 2H), 2.71 (s, 3H), 2.40 (t, *J* = 7.1 Hz, 2H), 2.33 (s, 3H), 1.86 − 1.60 (m, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.3, 161.3, 140.6, 137.3, 135.2, 130.3, 129.0, 127.9, 121.3, 118.1, 89.0, 72.8, 69.5, 30.7, 28.5, 23.0, 22.2, 21.0. ^{19}F NMR (376 MHz, Chloroform-*d*) δ -78.83. IR (KBr, cm^{-1}): 3113, 2935, 2866, 1666, 1624, 1496, 1458, 1354, 1195, 1138, 1056, 848, 806, 786, 740, 651, 617, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{20}H_{26}NO_2^+$: 312.1958; found: 312.1956.

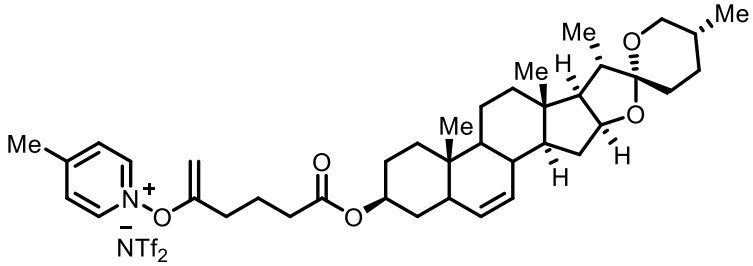
1-((6-(((3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*S*,5*R*)-5-Ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-6-oxohex-1-en-2-yl)oxy)-4-methylpyridin-1-

ium bis((trifluoromethyl)sulfonyl)amide (2ah)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 1.7 g, 92% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 6.9 Hz, 2H), 8.03 (d, *J* = 6.9 Hz, 2H), 5.29 (s, 1H), 4.59 (t, *J* = 5.0 Hz, 1H), 4.50 (d, *J* = 5.5 Hz, 1H), 3.73 (d, *J* = 5.5 Hz, 1H), 2.75 (s, 3H), 2.42 (dt, *J* = 18.0, 7.3 Hz, 4H), 2.29 (d, *J* = 6.4 Hz, 2H), 2.04 − 1.90 (m, 4H), 1.89 − 1.76 (m, 3H), 1.72−1.39 (m, 7H), 1.37−1.03 (m, 12H), 1.00 (s, 4H), 0.91 (d, *J* = 6.9 Hz, 4H), 0.86−0.73 (m, 10H), 0.65 (d, *J* = 12.8 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ172.4, 164.6, 161.6, 140.8, 139.5, 130.5, 122.7, 121.3, 118.1, 89.2, 74.2, 56.6, 55.9, 53.4, 49.9, 45.7, 42.2, 39.6, 38.0, 36.9, 36.5, 36.1, 35.4, 33.8, 33.2, 31.8, 31.7, 30.5, 29.0, 28.2, 27.7, 25.9, 24.2, 22.9, 22.4, 21.5, 20.9, 19.8, 19.2, 18.9, 18.7, 11.9, 11.8. IR (KBr, cm^{-1}): 3116, 2939, 1728, 1666, 1624, 1456, 1350, 1138, 1056, 844, 790, 740, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{41}H_{64}NO_3^+$: 618.4881; found: 618.4884.

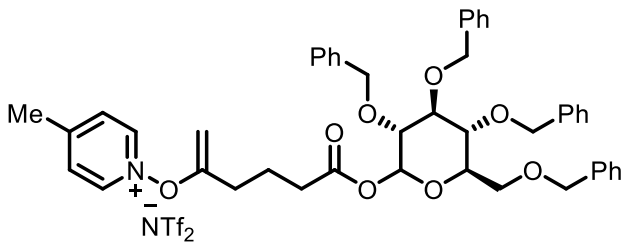
4-Methyl-1-((6-oxo-6-(((4*S*,5'*R*,6a*S*,8a*S*,8b*R*,9*S*,10*R*,11a*S*,12a*S*,12b*R*)-5',6a,8a,9-tetramethyl-2a,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4-yl)oxy)hex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2ai)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 1.6 g, 90% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.71 (d, *J* = 6.9 Hz, 2H), 8.03 (d, *J* = 6.4 Hz, 2H), 5.40 − 5.31 (m, 1H), 4.65 − 4.53 (m, 1H), 4.53 − 4.48 (m, 1H), 4.45 − 4.33 (m, 1H), 3.73 (d, *J* = 5.5 Hz, 1H), 3.46 (dd, *J* = 10.5, 3.2 Hz, 1H), 3.35 (t, *J* = 10.7 Hz, 1H), 2.75 (s, 3H), 2.42 (dt, *J* = 18.6, 7.2 Hz, 4H), 2.29 (d, *J* = 7.8 Hz, 2H), 1.96 (td, *J* = 14.4, 6.7 Hz, 4H), 1.90 − 1.68 (m, 6H), 1.68 − 1.51 (m, 7H), 1.51 − 1.35 (m, 3H), 1.33 − 1.22 (m, 1H), 1.21 − 1.04 (m, 3H), 1.02 (s, 3H), 0.95 (d, *J* = 6.9 Hz, 3H), 0.77 (d, *J* = 5.5 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 172.4, 164.6, 161.6, 140.8, 139.6, 130.5, 122.4, 121.3, 118.1, 109.2, 89.3, 80.7, 74.2, 66.8, 61.9, 56.4, 53.4, 49.8, 41.5, 40.2, 39.6, 37.9, 36.8, 36.7, 33.2, 31.9, 31.8, 31.3, 30.5, 30.2, 28.7, 27.6, 22.4, 21.5, 20.7, 19.2, 17.1, 16.2, 14.5. IR (KBr, cm^{-1}): 2943, 2900, 1732, 1666, 1624, 1496, 1454, 1350, 1192, 1380, 1056, 790, 736, 617, 570, 513. HRMS (ESI^+) m/z: $[M]^+$ calcd for $C_{39}H_{56}NO_5^+$: 618.4153; found: 618.4159.

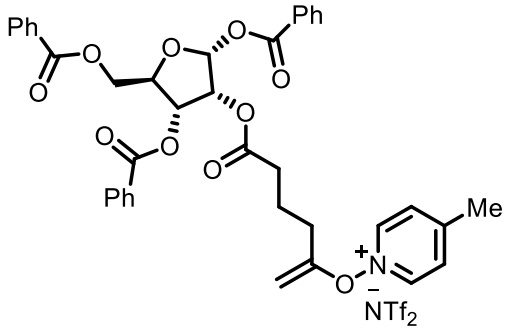
1-((6-Oxo-6-(((3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-

((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl)oxy)hex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2aj)



Transparent viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1.4 g, 70% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.57 (dd, *J* = 18.1, 5.3 Hz, 2H), 7.90 (dd, *J* = 29.7, 6.9 Hz, 2H), 7.35 − 7.26 (m, 20H), 7.20 − 7.08 (m, 4H), 6.42 − 5.56 (m, 1H), 4.97 − 4.86 (m, 1H), 4.82 (dq, *J* = 11.0, 3.0 Hz, 2H), 4.67 (d, *J* = 4.6 Hz, 1H), 4.56 (dd, *J* = 12.1, 3.4 Hz, 2H), 4.51 − 4.42 (m, 2H), 3.78 − 3.68 (m, 4H), 2.71 (d, *J* = 5.5 Hz, 3H), 2.58 − 2.30 (4H), 2.08 − 1.87 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.6, 164.3, 161.5, 140.6, 138.4, 138.1, 138.0, 137.8, 137.7, 137.6, 137.5, 130.4, 130.4, 128.4, 128.0, 127.9, 127.86, 127.89, 127.7, 127.6, 121.3, 118.1, 94.1, 90.2, 89.5, 89.4, 84.7, 81.5, 80.9, 78.8, 75.6, 75.5, 75.4, 75.2, 74.9, 73.5, 73.4, 73.3, 73.0, 68.2, 53.4, 32.7, 30.2, 22.4, 21.3, 21.0. IR (KBr, cm^{-1}): 3477, 2360, 1643, 1625, 1496, 1452, 1350, 1118, 1134, 1055, 738, 698, 611, 569, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{46}H_{50}NO_8^+$: 744.3531; found: 744.3533.

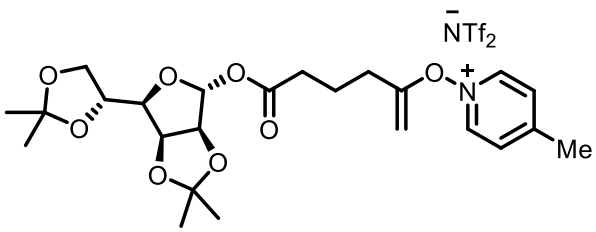
1-((6-(((2*R*,3*R*,4*R*,5*R*)-2,4-Bis(benzoyloxy)-5-((benzoyloxy)methyl)tetrahydrofuran-3-yl)oxy)-6-oxohex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2ak)



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1.9 g, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.17 (d, J = 6.9 Hz, 2H), 7.77-7.62 (m, 5H), 7.57 (d, J = 6.9 Hz, 2H), 7.27-7.12 (m, 3H), 7.11-6.91 (m, 6H), 6.39 (d, J = 4.1 Hz, 1H), 5.39 (dd, J = 6.4, 2.3 Hz, 1H), 5.16 (dd, J = 6.4, 4.6 Hz, 1H), 4.89 (s, 2H), 4.47 (q, J = 3.0 Hz, 1H), 4.25 (ddd, J = 36.5, 12.2, 3.5 Hz, 2H), 3.89 (d, J = 5.5 Hz, 1H), 3.22 (d, J = 5.5 Hz, 1H), 2.32 (s, 3H), 1.97 (t, J = 6.9 Hz, 2H), 1.90 (t, J = 7.3 Hz, 2H), 1.54-1.33 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.5, 166.1, 165.7, 165.2, 164.2, 161.6, 140.6, 133.9, 133.8, 133.5, 130.4, 129.8, 129.7, 129.7, 128.7, 128.6, 128.5, 121.3, 118.1, 94.7, 89.4, 82.7, 70.9, 70.5, 63.9, 32.2, 30.1, 22.4, 20.9. IR (KBr, cm^{-1}): 3103, 2362, 2337, 1718, 1450, 1350, 1267, 1195, 1138, 1056, 711, 615, 570, 518. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{38}H_{36}NO_{10}^+$: 666.2334; found: 666.2330.

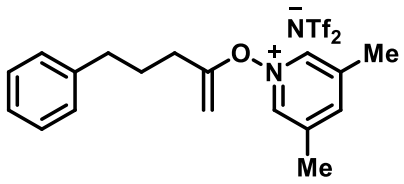
1-((6-(((3a*S*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl)oxy)-6-oxohex-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide (2al)

Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH =



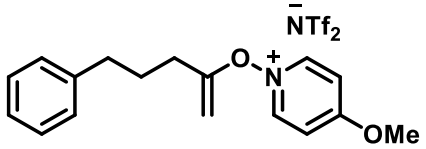
100/1); 1.5 g, 98% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.74 (d, *J* = 6.9 Hz, 2H), 8.01 (d, *J* = 6.9 Hz, 2H), 6.14-6.07 (m, 1H), 4.85 (dd, *J* = 9.1, 5.5 Hz, 1H), 4.69 (d, *J* = 5.9 Hz, 1H), 4.52 (d, *J* = 5.5 Hz, 1H), 4.45 − 4.30 (m, 2H), 4.07−3.93 (m, 4H), 3.74 (d, *J* = 5.5 Hz, 1H), 2.75 (s, 3H), 2.52−2.30 (m, 4H), 1.97 (t, *J* = 7.3 Hz, 2H), 1.52 − 1.39 (d, *J* = 9.6 Hz,6H), 1.33 (d, *J* = 9.6 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.7, 204.9, 171.6, 145.2, 140.7, 130.4, 126.9, 125.7, 121.2, 117.9, 113.1, 109.2, 100.6, 89.8, 82.1, 79.1, 72.7, 66.6, 44.0, 41.8, 41.1, 32.8, 26.8, 25.8, 24.9, 24.4, 18.3. IR (KBr, cm^{-1}): 2993, 2947, 2360, 2337, 1739, 1350, 1190, 1058, 962, 837, 615, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{24}H_{30}NO_8^+$: 464.2279; found: 464.2282.

3,5-Dimethyl-1-((5-phenylpent-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide



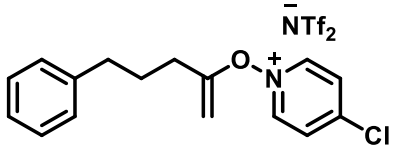
Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 818.8 mg, 75% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.31 − 8.26 (s, 2H), 8.22 − 8.17 (s, 1H), 7.30 (t, *J* = 7.5 Hz, 2H), 7.24 − 7.18 (m, 3H), 4.49 (d, *J* = 5.5 Hz, 1H), 3.74 (d, *J* = 5.5 Hz, 1H), 2.72 (t, *J* = 7.3 Hz, 2H), 2.58 (s, 6H), 2.41 (t, *J* = 7.8 Hz, 2H), 2.04 − 1.91 (m, 2H) ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.2, 148.2, 141.3, 141.1, 138.1, 128.6, 128.5, 126.1, 121.3, 118.1, 89.0, 34.9, 30.5, 27.8, 18.4. IR (KBr, cm^{-1}): 3116, 2939, 1728, 1666, 1624, 1462, 1350, 1192, 1138, 1056, 910, 844, 790, 736, 617, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{18}H_{22}NO^+$: 268.1696; found: 268.1694.

4-Methoxy-1-((5-phenylpent-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide



Transparent viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 1.1 g, 99% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.46 (d, *J* = 7.8 Hz, 2H), 7.54 (d, *J* = 7.8 Hz, 2H), 7.36 − 7.27 (m, 2H), 7.21 (t, *J* = 7.8 Hz, 3H), 4.45 (d, *J* = 5.5 Hz, 1H), 4.17 (s, 3H), 3.71 (d, *J* = 5.5 Hz, 1H), 2.72 (t, *J* = 7.3 Hz, 2H), 2.38 (t, *J* = 7.5 Hz, 2H), 2.07 − 1.84 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 171.5, 165.1, 142.9, 141.0, 128.5, 126.1, 121.3, 118.1, 114.7, 88.3, 58.9, 34.8, 30.4, 27.9. IR (KBr, cm^{-1}): 3128, 3026，2939, 1627, 1512, 1354, 1195, 1138, 1056, 852, 740, 702, 617, 570, 513. HRMS (ESI$^+$) m/z: $[M]^+$ calcd for $C_{17}H_{20}NO_2^+$: 270.1489; found: 270.1488.

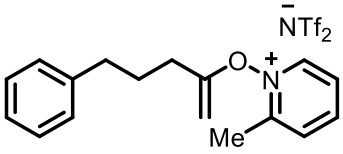
4-Chloro-1-((5-phenylpent-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide



Transparent viscous liquid after purification by column chromatography (CH_2Cl_2/MeOH = 100/1); 9211.3 mg, 83% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.70 (d, *J* = 7.3 Hz, 2H), 8.14 (d, *J* = 6.9 Hz, 2H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.21 (dd, *J* = 10.5, 7.8 Hz, 3H), 4.57 (d, *J* = 5.5

Hz, 1H), 3.81 (d, *J* = 5.9 Hz, 1H), 2.73 (t, *J* = 7.3 Hz, 2H), 2.42 (t, *J* = 7.5 Hz, 2H), 2.03 − 1.92 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 165.6, 155.6, 142.8, 141.0, 130.5, 128.6, 128.6, 126.2, 121.3, 118.1, 89.9, 34.8, 30.4, 27.7. IR (KBr, cm^{-1}): 3109, 3028, 2931, 1612, 1473, 1350, 1195, 1138, 1056, 852, 740, 702, 617, 570, 513. HRMS (ESI$^+$) m/z: [M]$^+$ calcd for $C_{16}H_{17}NO^+$: 274.0993; found: 274.1001.

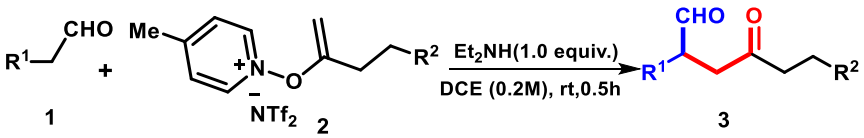
2-Methyl-1-((5-phenylpent-1-en-2-yl)oxy)pyridin-1-ium bis((trifluoromethyl)sulfonyl)amide



Yellow viscous liquid after purification by column chromatography (CH_2Cl_2/ MeOH = 100/1); 930.0 mg, 87 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.60 (d, J = 6.4 Hz, 1H), 8.48 (t, *J* = 7.8 Hz, 1H), 8.17 − 8.07 (1H), 8.03 (t, *J* = 7.1 Hz, 1H), 7.31 (t, *J* = 7.5 Hz, 2H), 7.21 (t, *J* = 8.0 Hz, 3H), 4.49 (d, *J* = 5.5 Hz, 1H), 3.61 − 3.50 (d, *J* = 5.5 Hz, 1H), 2.79 − 2.71 (m, 5H), 2.46 (t, *J* = 7.8 Hz, 2H), 2.07 − 1.94 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 163.5, 153.6, 146.3, 141.9, 140.8, 131.4, 128.5, 128.4, 127.7, 126.2, 121.3, 118.1, 87.9, 53.4, 34.9, 30.4, 28.0, 17.1. IR (KBr, cm^{-1}): 3066, 2920, 1666, 1616, 1496, 1458, 1350, 1195, 1138, 1056, 786, 740, 702, 613, 570, 513. HRMS (ESI$^+$) m/z: [M]$^+$ calcd for $C_{17}H_{20}NO_2^+$: 254.1539; found: 254.1540.

3. Experimental procedures and characterization of products

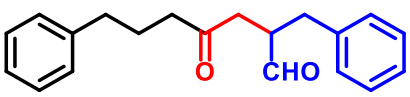
3.1 General procedure for the preparation of 1, 4-dicarbonyl compounds(0.2mmol scale)



In a 10 mL reaction bottle, **1a** and compound **2a** were dissolved in 1, 2-dichloroethane, stirred evenly, then added into Et_2NH (1equiv) and reacted at room temperature for 30 min. During the reaction, petroleum ether : EtOAc = 5:1 was used to monitor and a product point with R_f = 0.43 was obtained. After the band reaction, the solvent was dried in vacuum and purified with petroleum ether: EtOAc =20:1 in silica gel column to obtain the pure products.

3.2 Characterization of products

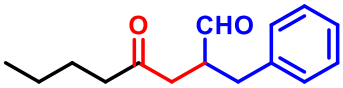
2-Benzyl-4-oxo-7-phenylheptanal (3a)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 44.1 mg, 75% yield. ^{1}H NMR (400 MHz, Chloroform-d) δ 9.77 (s, 1H), 7.33 − 7.17 (m, 6H), 7.14 (d, *J* = 7.7 Hz, 5H), 3.21 (tt, *J* = 8.1, 4.7 Hz, 1H), 3.07 (dd, *J* = 13.8, 6.4 Hz, 1H), 2.76 (dd, *J* = 18.0, 8.0 Hz, 1H), 2.68 (dd, *J* = 13.9, 8.5 Hz, 1H), 2.58 (t, *J* = 7.5 Hz, 2H), 2.50 − 2.27 (m, 3H), 1.87 (pd, *J* = 7.2, 3.1 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.4, 202.8, 141.4, 138.0,

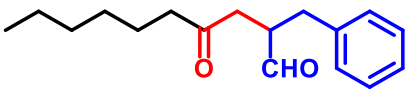
128.9, 128.7, 128.4, 128.4, 126.7, 125.9, 48.3, 41.9, 40.9, 34.9, 34.5, 25.0. IR (KBr, cm^{-1}) :3056, 3021, 2930, 2856, 1713, 1598, 1493, 1444, 1410, 1375, 1186, 1092, 1026, 750, 697. HRMS (ESI^+) m/z: $[M+H]^+$ calcd for $C_{20}H_{23}O_2^+$: 295.1693; found: 295.1712.

2-Benzyl-4-oxooctanal (3b)



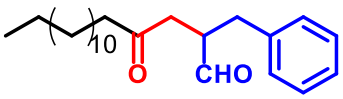
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 32.1 mg, 69% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 9.79 (s, 1H), 7.36 − 7.20 (m, 3H), 7.19 − 7.11 (m, 2H), 3.22 (tdd, *J* = 8.1, 6.4, 4.6 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.87 − 2.63 (m, 2H), 2.52 − 2.28 (m, 3H), 1.59 − 1.40 (m, 2H), 1.38 − 1.19 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.9, 202.9, 138.0, 129.0, 128.7, 128.5, 126.7, 48.2, 42.6, 40.8, 34.5, 25.8, 22.2, 13.8. IR (KBr, cm^{-1}) : 2956, 2924, 2861, 1713, 1454, 1366, 744, 702. HRMS (ESI^+) m/z: $[M+Na]^+$ calcd for $C_{15}H_{20}O_2Na^+$: 255.1356 ; found: 255.1359.

2-Benzyl-4-oxodecanal (3c)



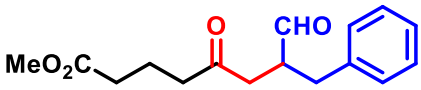
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 35.4 mg, 68% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.33 − 7.23 (m, 2H), 7.26 − 7.18 (m, 1H), 7.18 − 7.11 (m, 2H), 3.26 − 3.14 (m, 1H), 3.07 (dd, *J* = 13.8, 6.4 Hz, 1H), 2.78 (dd, *J* = 18.0, 7.9 Hz, 1H), 2.68 (dd, *J* = 13.9, 8.5 Hz, 1H), 2.45 − 2.26 (m, 3H), 1.57 − 1.45 (m, 2H), 1.24 (dtd, *J* = 10.0, 7.2, 4.6 Hz, 6H), 0.85 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 203.0, 138.0, 129.0, 128.7, 126.7, 48.2, 42.9, 40.8, 34.5, 31.5, 28.7, 23.6, 22.4, 14.0. IR (KBr, cm^{-1}) : 2930, 2856, 1713, 1497, 1455, 1410, 1368, 746, 694. HRMS (ESI^+) m/z: $[M+Na]^+$ calcd for $C_{17}H_{24}O_2Na^+$: 283.1699 ; found: 283.1695.

2-Benzyl-4-oxoheptadecanal (3d)



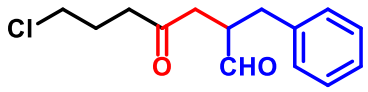
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 41.0 mg, 55% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.36 − 7.22 (m, 2H), 7.25 − 7.10 (m, 3H), 2.99 − 2.76 (m, 1H), 2.62 (p, *J* = 7.0 Hz, 2H), 2.54 − 2.33 (m, 2H), 2.12 (s, 2H), 1.99 − 1.83 (m, 2H), 1.56 (s, 2H), 1.44 − 1.17 (m, 10H), 0.92 − 0.84 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.0, 203.0, 138.0, 129.2 - 128.2 (m), 126.7, 77.2, 48.2, 42.9, 40.8, 34.5, 31.9, 29.7 - 28.7 (m), 28.1, 23.2 (d, *J* = 103.6 Hz), 14.1.IR (KBr, cm^{-1}) : 2923, 2856, 1713, 1451, 1266, 914, 750, 690. HRMS (ESI^+) m/z: $[M+H]^+$ calcd for $C_{25}H_{41}O_2^+$: 373.3101 ; found: 373.3126.

Methyl-7-benzyl-5,8-dioxooctanoate (3e)



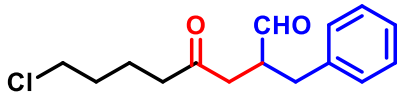
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 38.1 mg, 69% yield. ^1H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.37 − 7.20 (m, 3H), 7.18 − 7.09 (m, 2H), 3.65 (s, 2H), 3.28 − 3.17 (m, 1H), 3.09 (dd, *J* = 13.9, 6.3 Hz, 1H), 2.83 − 2.62 (m, 2H), 2.58 − 2.35 (m, 3H), 2.30 (t, *J* = 7.3 Hz, 2H), 1.94 − 1.75 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.9, 202.8, 173.6, 137.9, 129.0, 128.7, 126.8, 51.5, 48.4, 41.6, 40.8, 34.5, 32.8, 18.7. IR (KBr, cm^{-1}) : 2954, 2924, 1732, 1422, 1172, 748, 702. HRMS (ESI^+) m/z: $[M+Na]^+$ calcd for $C_{16}H_{20}O_4Na^+$: 299.1254 ; found: 299.1250.

2-Benzyl-7-chloro-4-oxoheptanal (3f)



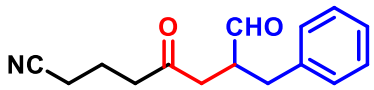
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 38.9 mg, 74% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.30 (td, *J* = 7.1, 6.1, 1.4 Hz, 2H), 7.26 − 7.17 (m, 1H), 7.15 (dd, *J* = 7.2, 1.6 Hz, 2H), 3.52 (t, *J* = 6.3 Hz, 2H), 3.22 (tdd, *J* = 8.3, 6.2, 4.6 Hz, 1H), 3.09 (dd, *J* = 13.9, 6.3 Hz, 1H), 2.79 (dd, *J* = 17.9, 8.1 Hz, 1H), 2.69 (dd, *J* = 13.9, 8.7 Hz, 1H), 2.57 (qt, *J* = 17.8, 6.9 Hz, 2H), 2.40 (dd, *J* = 17.9, 4.6 Hz, 1H), 2.07 − 1.91 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.1, 202.8, 137.9, 128.9, 128.7, 126.8, 48.4, 44.6, 41.8, 40.7, 34.5, 31.7, 20.8. IR (KBr, cm^{-1}) : 2921, 2854, 1713, 1496, 1447, 1415, 1373, 1093, 1023, 744, 705. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{14}H_{17}ClO_2Na^{+}$: 275.0809 ; found: 275.0825.

2-Benzyl-8-chloro-4-oxooctanal (3g)



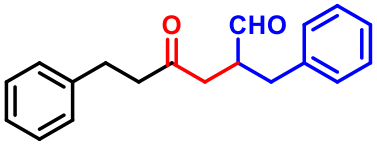
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 38.4 mg, 72% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.79 (s, 1H), 7.39 − 7.27 (m, 2H), 7.31 − 7.19 (m, 1H), 7.16 (dd, *J* = 6.9, 1.8 Hz, 2H), 3.51 (t, *J* = 6.2 Hz, 2H), 3.24 (tdd, *J* = 8.4, 6.3, 4.5 Hz, 1H), 3.10 (dd, *J* = 13.9, 6.3 Hz, 1H), 2.89 − 2.60 (m, 2H), 2.48 (dd, *J* = 17.5, 7.4 Hz, 1H), 2.45 − 2.30 (m, 2H), 1.79 − 1.62 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.1, 202.8, 137.9, 128.9, 128.7, 126.8, 48.4, 44.6, 41.8, 40.7, 34.5, 31.7, 20.8. IR (KBr, cm^{-1}) : 2930, 2867, 1720, 1455, 1410, 1375, 743, 701. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{15}H_{19}ClO_2Na^{+}$: 289.0966; found: 289.0956.

8-Benzyl-6,9-dioxononanenitrile (3h)



Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 41.4 mg, 85% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.31 (tt, *J* = 6.8, 1.2 Hz, 2H), 7.27 − 7.21 (m, 1H), 7.17 − 7.13 (m, 2H), 4.16 − 4.06 (m, 1H), 3.31 − 3.19 (m, 1H), 3.11 (dd, *J* = 13.9, 6.1 Hz, 1H), 2.83 − 2.72 (m, 1H), 2.75 − 2.58 (m, 1H), 2.52 (dt, *J* = 18.2, 6.9 Hz, 1H), 2.48 − 2.28 (m, 1H), 1.88 (h, *J* = 7.2 Hz, 2H), 1.25 (td, *J* = 7.2, 0.9 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.0, 202.5, 137.7, 128.9, 128.8, 126.9, 119.2, 77.3, 77.2, 77.0, 76.7, 48.7, 40.7, 40.5, 34.4, 19.2, 16.4. IR (KBr, cm^{-1}) : 2933, 2849, 2241, 1713, 1490, 1451, 1413, 1371, 1095, 753, 701. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{15}H_{17}NO_2Na^{+}$: 266.1151 ; found: 266.1138.

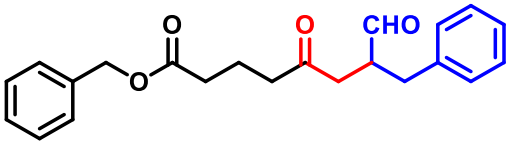
2-Benzyl-4-oxo-6-phenylhexanal (3i)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 43.2 mg, 77% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.79 (s, 1H), 7.45 − 6.96 (m, 5H), 3.22 (tdd, *J* = 8.1, 6.4, 4.6 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.87 − 2.63 (m, 2H), 2.52 − 2.28 (m, 3H), 1.59 − 1.40 (m, 2H), 1.38 − 1.19 (m, 2H), 0.88 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.8, 202.8, 140.8, 137.9, 129.0, 128.7, 128.5, 128.3, 126.7, 126.1, 48.3, 44.3, 41.0, 34.4, 29.6. IR (KBr, cm^{-1}) : 3024, 1717, 1490, 1437, 1399, 1357, 1095,

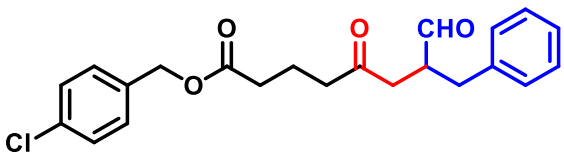
1078, 734, 697. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{19}H_{21}O_2^+$: 281.1536; found:281.1546.

Benzyl-7-benzyl-5,8-dioxooctanoate (3j)



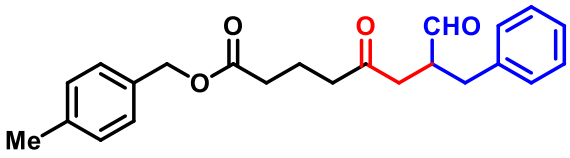
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 45.8 mg, 65% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.40 − 7.31 (m, 5H), 7.31 − 7.18 (m, 3H), 7.18 − 7.11 (m, 2H), 5.10 (s, 2H), 3.22 (tdd, *J* = 8.3, 6.3, 4.6 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.82 − 2.61 (m, 2H), 2.56 − 2.26 (m, 5H), 1.97 − 1.79 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.8, 202.7, 172.9, 137.9, 135.9, 128.9, 128.7, 128.5, 128.4, 128.2, 128.2, 126.7, 66.2, 48.3, 41.5, 40.8, 34.5, 33.1, 18.7. IR (KBr, cm^{-1}) : 3031, 2944, 2716, 1727, 1493, 1455, 1413, 1382, 1162, 746, 694. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{22}H_{24}O_4Na^+$: 375.1567 ; found: 375.1559.

4-Chlorobenzyl-7-benzyl-5,8-dioxooctanoate (3k)



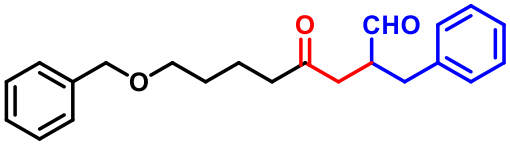
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 51.8 mg, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.37 − 7.21 (m, 7H), 7.19 − 7.11 (m, 2H), 5.06 (d, *J* = 5.5 Hz, 2H), 3.22 (tdd, *J* = 8.3, 6.2, 4.5 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.3 Hz, 1H), 2.86 − 2.62 (m, 2H), 2.56 − 2.29 (m, 5H), 1.98 − 1.76 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.8, 202.7, 172.8, 137.8, 134.4, 134.1, 129.6, 128.9, 128.7, 126.8, 65.3, 48.4, 41.5, 40.8, 34.4, 33.0, 18.6. IR (KBr, cm^{-1}) : 2936, 1734, 1493, 1455, 1417, 1371, 1162, 1085, 1015 806, 743, 697. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{22}H_{23}ClO_4Na^+$: 409.1177; found: 409.1167.

4-Methylbenzyl-7-benzyl-5,8-dioxooctanoate (3l)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 48.4 mg, 66% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.38 − 7.26 (m, 2H), 7.30 − 7.19 (m, 3H), 7.23 − 7.08 (m, 4H), 5.06 (s, 2H), 3.21 (tdd, *J* = 8.3, 6.4, 4.5 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.83 − 2.70 (m, 1H), 2.68 (dd, *J* = 13.9, 8.6 Hz, 1H), 2.53 − 2.37 (m, 3H), 2.34 (d, *J* = 6.7 Hz, 5H), 1.94 − 1.81 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.8, 202.7, 172.9, 138.1, 137.9, 132.9, 129.2, 128.9, 128.7, 128.4, 126.7, 66.2, 48.3, 41.5, 40.8, 34.5, 33.1, 21.2, 18.7. IR (KBr, cm^{-1}) : 2937, 1713, 1514, 1468, 1462, 1410, 1368, 1169, 806, 739, 694. HRMS (ESI$^+$) m/z: $[M+Na]^+$ calcd for $C_{23}H_{26}O_4Na^+$: 389.1723 ; found: 389.1715.

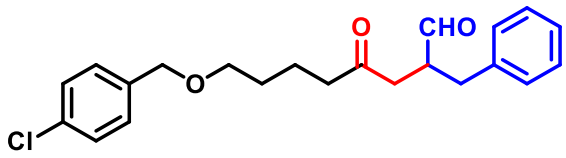
2-Benzyl-8-(benzyloxy)-4-oxooctanal (3m)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 44.7 mg, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.33 (d,

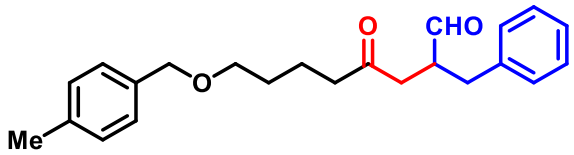
J = 6.0 Hz, 4H), 7.31 − 7.22 (m, 4H), 7.22 − 7.08 (m, 2H), 4.48 (s, 2H), 3.45 (t, *J* = 6.0 Hz, 2H), 3.27 − 3.14 (m, 1H), 3.07 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.87 − 2.56 (m, 2H), 2.52 − 2.31 (m, 3H), 1.62 (dtt, *J* = 15.6, 9.3, 3.4 Hz, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 202.9, 138.5, 138.0, 129.0, 128.7, 128.3, 127.6, 127.5, 126.7, 72.9, 69.9, 48.3, 42.5, 40.8, 34.5, 29.0, 20.4.IR (KBr, cm^{-1}) : 2930, 2860, 1717, 1497, 1455, 1357, 1102, 739, 679. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{22}H_{26}O_3Na^+$: 361.1774 ; found: 361.1764.

2-Benzyl-8-((4-chlorobenzyl)oxy)-4-oxooctanal (3n)



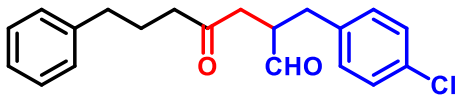
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 50.0 mg, 67% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.30 (ddd, *J* = 8.2, 4.0, 2.8 Hz, 4H), 7.30 − 7.17 (m, 2H), 7.21 − 7.08 (m, 2H), 4.43 (s, 2H), 3.51 − 3.36 (m, 2H), 3.22 (ddd, *J* = 13.8, 10.2, 6.7 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.88 − 2.61 (m, 2H), 2.51 − 2.31 (m, 3H), 1.71 − 1.49 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 202.9, 137.9, 137.0, 133.2, 128.9, 128.9, 128.7, 128.5, 126.7, 72.0, 70.0, 48.3, 42.4, 40.8, 34.4, 29.0, 20.4. IR (KBr, cm^{-1}) : 2944, 2863, 1713, 1497, 1451, 1406, 1357, 1095, 1019, 809, 750, 701. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{22}H_{25}ClO_3Na^+$: 395.1384 ; found: 395.1370.

2-Benzyl-8-((4-methylbenzyl)oxy)-4-oxooctanal (3o)



Light yellow liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 47.9 mg, 68% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.38 − 7.25 (m, 2H), 7.28 − 7.17 (m, 3H), 7.21 − 7.08 (m, 4H), 4.44 (s, 2H), 3.43 (q, *J* = 5.5 Hz, 2H), 3.21 (tdd, *J* = 8.2, 6.4, 4.6 Hz, 1H), 3.08 (dd, *J* = 13.9, 6.4 Hz, 1H), 2.86 − 2.62 (m, 2H), 2.50 − 2.34 (m, 3H), 2.34 (s, 3H), 1.61 (tddt, *J* = 15.1, 9.1, 6.1, 2.6 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 202.9, 138.0, 137.2, 135.4, 129.0, 128.9, 128.7, 127.7, 126.7, 72.7, 69.7, 48.2, 42.5, 40.8, 34.4, 29.0, 21.1, 20.4. IR (KBr, cm^{-1}) : 2926, 2860, 1710, 1455, 1413, 1364, 1099, 802, 750, 694. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{23}H_{28}O_3Na^+$: 375.1931 ; found: 375.1922.

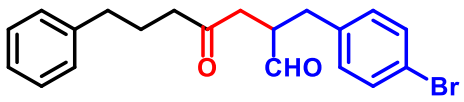
2-(4-Chlorobenzyl)-4-oxo-7-phenylheptanal (3p)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 46.6 mg, 71 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.31 − 7.22 (m, 4H), 7.26 − 7.14 (m, 1H), 7.18 − 7.11 (m, 2H), 7.11 − 7.04 (m, 2H), 3.16 (qd, *J* = 7.7, 4.9 Hz, 1H), 3.03 (dd, *J* = 14.0, 6.5 Hz, 1H), 2.74 (dd, *J* = 18.0, 7.8 Hz, 1H), 2.65 (dd, *J* = 13.9, 8.3 Hz, 1H), 2.58 (t, *J* = 7.5 Hz, 2H), 2.48 − 2.28 (m, 3H), 1.87 (pd, *J* = 7.3, 2.5 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.3, 202.4, 141.4, 136.5, 132.6, 130.3, 128.8, 128.4, 128.4, 126.0, 48.1, 41.9, 40.8, 34.9, 33.8, 25.0. IR (KBr, cm^{-1}) : 3026, 2921, 2854, 1713, 1492, 1450, 1408, 1359, 1090, 1009, 740, 698. HRMS (ESI$^+$) m/z: [M-H]$^-$ calcd for $C_{20}H_{20}ClO_2^-$:

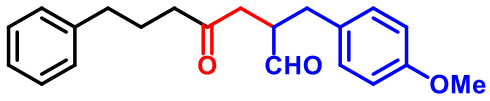
327.1157 ; found: 327.1154.

2-(4-Bromobenzyl)-4-oxo-7-phenylheptanal (3q)



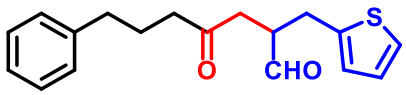
Light green liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 53.8 mg, 72% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.45 − 7.30 (m, 2H), 7.30 − 7.25 (m, 1H), 7.25 − 7.15 (m, 1H), 7.18 − 7.08 (m, 2H), 7.02 (s, 1H), 7.03 − 6.90 (m, 1H), 3.16 (tdd, *J* = 7.9, 6.4, 4.8 Hz, 1H), 3.01 (dd, *J* = 14.0, 6.5 Hz, 1H), 2.80 − 2.67 (m, 1H), 2.67 − 2.61 (m, 1H), 2.61 − 2.55 (m, 2H), 2.47 − 2.25 (m, 3H), 1.95 − 1.78 (m, 2H).^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.2, 202.4, 141.4, 137.0, 131.8, 130.7, 128.4, 128.4, 126.0, 120.6, 53.4, 48.0, 41.9, 40.8, 34.9, 33.8, 25.0. IR (KBr, cm^{-1}) : 2930, 2849, 1713, 1493, 1444, 1410, 1368, 1071, 1012, 750, 697. HRMS (ESI^{+}) m/z: [M-H]$^{-}$ calcd for $C_{20}H_{20}BrO_2^-$: 371.0652 ; found: 371.0641.

2-(4-Methoxybenzyl)-4-oxo-7-phenylheptanal (3r)



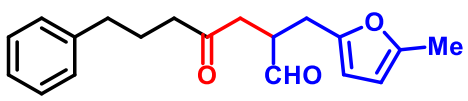
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 44.8 mg, 69% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.30 − 7.22 (m, 3H), 7.21 − 7.11 (m, 3H), 7.04 (d, *J* = 8.7 Hz, 2H), 6.82 (d, *J* = 8.7 Hz, 2H), 3.77 (s, 3H), 3.21 − 3.12 (m, 1H), 3.00 (q, *J* = 6.9 Hz, 1H), 2.74 (dd, *J* = 18.1, 8.0 Hz, 1H), 2.68 − 2.61 (m, 1H), 2.57 (t, *J* = 7.5 Hz, 2H), 2.47 − 2.28 (m, 3H), 1.93 − 1.78 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.6, 203.1, 158.4, 141.5, 129.9, 128.4, 128.3, 125.9, 114.1, 55.2, 48.5, 41.9, 40.8, 34.9, 33.6, 25.1. IR (KBr, cm^{-1}) : 2935, 2854, 1713, 1486, 1425, 1388, 1051, 1023, 745, 693. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{21}H_{24}O_3Na^+$: 347.1618 ; found: 347.1615.

4-Oxo-7-phenyl-2-(thiophen-2-ylmethyl)heptanal (3s)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 41.5 mg, 69% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.35 - 7.21 (m, 2H), 7.24 - 7.15 (m, 1H), 7.19 - 7.07 (m, 3H), 6.91 (dd, *J* = 5.2, 3.4 Hz, 1H), 6.77 (dt, *J* = 3.5, 1.0 Hz, 1H), 3.48 (s, 1H), 3.46 - 3.09 (m, 3H), 3.00 (ddd, *J* = 14.6, 7.5, 0.8 Hz, 1H), 2.88 - 2.71 (m, 1H), 2.60 (q, *J* = 7.8 Hz, 2H), 2.53 - 2.45 (m, 1H), 2.44 - 2.35 (m, 2H), 1.98 - 1.80 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.3, 202.4, 141.4, 140.2, 128.4, 128.4, 127.1, 126.1, 126.0, 124.3, 48.3, 41.9, 40.9, 34.9, 28.4, 25.0. IR (KBr, cm^{-1}) : 2919, 2856, 1713, 1451, 1406, 1364, 1092, 1022, 746, 694. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{18}H_{20}O_2SNa^+$: 323.1076 ; found: 323.1085.

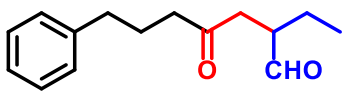
2-((4-Methylcyclopetroleum-etherna-1,3-dien-1-yl)methyl)-4-oxo-7-phenylheptanal (3t)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 35.8 mg, 63% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.76 (s, 1H), 7.27 (td, *J* = 6.2, 2.9 Hz, 2H), 7.22 − 7.12 (m, 3H), 5.88 (d, *J* = 3.1 Hz, 1H), 5.84 − 5.79 (m, 1H), 3.22 − 3.11 (m, 1H), 2.99 (dd, *J* = 15.3, 6.2 Hz, 1H), 2.85 − 2.74 (m, 2H), 2.60 (t, *J* = 7.5 Hz, 2H), 2.51 − 2.41 (m, 2H), 2.43 − 2.31

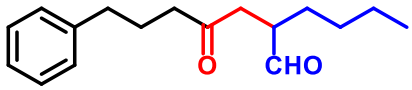
(m, 1H), 2.21 (s, 3H), 1.89 (pd, *J* = 7.4, 1.8 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.5, 202.7, 151.5, 149.9, 141.6, 128.6, 128.5, 126.1, 107.9, 106.1, 46.1, 42.1, 40.9, 35.1, 27.0, 25.2, 13.6. IR (KBr, cm^{-1}) : 3028, 2926, 2853, 1713, 1605, 1574, 1574, 1497, 1406, 1364, 1211, 1029, 785, 753, 704. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{19}H_{23}O_3^+$: 299.1642 ; found: 299.1648.

2-Ethyl-4-oxo-7-phenylheptanal (3u)



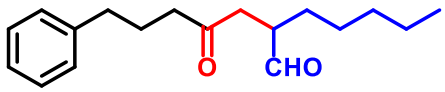
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 29.3 mg, 63% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.69 (s, 1H), 7.31 − 7.23 (m, 3H), 7.22 − 7.13 (m, 3H), 2.92 − 2.76 (m, 2H), 2.61 (t, *J* = 7.5 Hz, 2H), 2.50 (dt, *J* = 13.9, 5.7 Hz, 1H), 2.48 − 2.38 (m, 1H), 2.42 − 2.31 (m, 1H), 1.99 − 1.83 (m, 2H), 1.81 − 1.66 (m, 1H), 1.56 − 1.35 (m, 1H), 0.93 (t, *J* = 7.5 Hz, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 203.5, 141.5, 128.5, 128.4, 126.0, 48.0, 42.1, 40.8, 35.0, 25.2, 21.6, 11.4. IR (KBr, cm^{-1}) : 3061, 2954, 1713, 1454, 1408, 1380, 1181, 751, 702. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{15}H_{20}O_2Na^+$:255.1356 ; found:255.1371.

2-Butyl-4-oxo-7-phenylheptanal (3v)



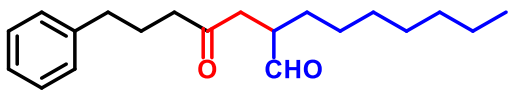
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 32.3 mg, 62% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.33 − 7.24 (m, 2H), 7.23 − 7.14 (m, 3H), 2.91 (dtd, *J* = 12.6, 6.4, 3.9 Hz, 1H), 2.83 (dd, *J* = 17.3, 8.4 Hz, 1H), 2.62 (t, *J* = 7.6 Hz, 2H), 2.56 − 2.34 (m, 3H), 2.00 − 1.84 (m, 2H), 1.76 − 1.63 (m, 1H), 1.39 − 1.22 (m, 4H), 0.90 (t, *J* = 6.9 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 203.5, 141.5, 128.5, 128.4, 125.9, 46.7, 42.0, 41.3, 35.0, 29.1, 28.3, 25.1, 22.7, 13.8. IR (KBr, cm^{-1}) : 2935, 2865, 1713, 1461, 1408, 1373, 740, 702. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{17}H_{24}O_2Na^+$:283.1669 ; found:283.1700.

4-Oxo-2-petroleum etherntyl-7-phenylheptanal (3w)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 33.5 mg, 61% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.28 (t, *J* = 7.8 Hz, 2H), 7.19 (dd, *J* = 10.6, 7.4 Hz, 3H), 2.91 (qd, *J* = 6.4, 3.8 Hz, 1H), 2.83 (dd, *J* = 17.4, 8.3 Hz, 1H), 2.62 (t, *J* = 7.5 Hz, 2H), 2.56 − 2.34 (m, 3H), 2.00 − 1.84 (m, 2H), 1.75 − 1.62 (m, 1H), 1.43 − 1.24 (m, 7H), 0.88 (t, *J* = 6.5 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 203.5, 141.5, 128.5, 128.4, 125.9, 46.7, 42.0, 41.3, 35.0, 31.7, 28.5, 26.7, 25.1, 22.4, 13.9. IR (KBr, cm^{-1}) : 2973, 2863, 1713, 1455, 1410, 1368, 750, 697. HRMS (ESI$^+$) m/z: [M+H]$^+$ calcd for $C_{18}H_{27}O_2^+$: 275.2006 ; found: 275.1994.

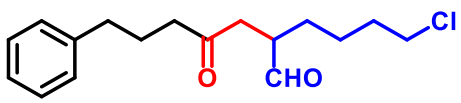
2-(2-Oxo-5-phenylpetroleum etherntyl)nonanal (3x)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 36.9 mg, 61% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.36 − 7.22 (m, 2H), 7.25 − 7.10 (m, 3H), 2.96 − 2.75 (m, 2H), 2.62 (p, *J* = 7.0 Hz, 2H), 2.54 − 2.33 (m, 2H), 2.12 (s, 2H), 1.99 − 1.83

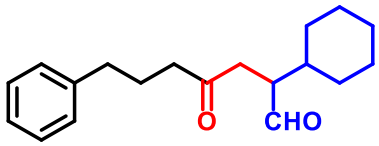
(m, 2H), 1.56 (s, 2H), 1.44 − 1.17 (m, 10H), 0.92 − 0.84 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.7, 203.6, 141.5, 128.5, 128.5, 128.4, 125.9, 53.4, 46.7, 42.8, 42.0, 41.3, 35.0, 31.7, 30.0, 29.6, 29.0, 28.6, 27.0, 25.2, 22.6, 14.1. IR (KBr, cm^{-1}) : 2924, 2858, 1713, 1454, 1408, 1356, 747, 689. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{20}H_{30}NaO_2^+$: 325.2138 ; found: 325.2146.

2-(4-Chlorobutyl)-4-oxo-7-phenylheptanal (3y)



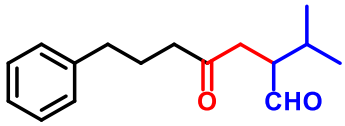
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 44.2 mg, 75% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.70 (s, 1H), 7.35 − 7.27 (m, 2H), 7.23 − 7.07 (m, 3H), 3.53 (t, *J* = 6.5 Hz, 2H), 2.97 − 2.86 (m, 1H), 2.84 (dd, *J* = 17.3, 8.1 Hz, 1H), 2.62 (t, *J* = 7.5 Hz, 2H), 2.61 − 2.37 (m, 3H), 2.02 − 1.86 (m, 2H), 1.89 − 1.65 (m, 3H), 1.56 − 1.38 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 208.4, 203.0, 141.4, 128.5, 128.4, 126.0, 46.4, 44.5, 42.0, 41.2, 35.0, 32.3, 27.7, 25.1, 24.2. IR (KBr, cm^{-1}) : 2933, 2863, 1713, 1451, 1399, 1361, 750, 694. HRMS (ESI$^+$) m/z: $[M+K]^+$ calcd for $C_{17}H_{23}ClKO_2^+$: 333.1018 ; found: 333.1014.

2-Cyclohexyl-4-oxo-7-phenylheptanal (3z)



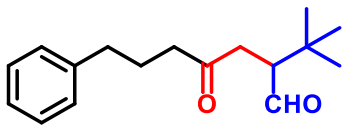
Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 18.3 mg, 32% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.36 − 7.15 (m, 2H), 7.19 − 7.10 (m, 3H), 2.99 − 2.77 (m, 3H), 2.70 − 2.57 (m, 2H), 2.54 − 2.36 (m, 2H), 2.36 − 2.24 (m, 2H), 2.12 (s, 1H), 1.91 (pd, *J* = 7.4, 2.7 Hz, 2H), 1.83 − 1.64 (m, 2H), 1.55 (d, *J* = 15.8 Hz, 2H), 1.36 − 1.18 (m, 2H), 1.14 − 0.98 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.1, 204.0, 128.5, 128.5, 128.4, 125.9, 52.2, 42.8, 42.1, 38.4, 37.8, 35.0, 31.0, 29.9, 26.4, 26.4, 26.1, 25.2, 25.2. IR (KBr, cm^{-1}) : 2926, 2856, 1713, 1451, 1413, 1357, 743, 701. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{19}H_{27}O_2^+$: 287.2006 ; found: 287.2014.

2-Isopropyl-4-oxo-7-phenylheptanal (3aa)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 28.6 mg, 58% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.74 (s, 1H), 7.31 − 7.27 (m, 2H), 7.21 − 7.17 (m, 3H), 2.96 − 2.92 (m, 1H), 2.86 (dd, *J* = 17.2, 9.7 Hz, 1H), 2.64 − 2.60 (m, 2H), 2.54 − 2.41 (m, 2H), 2.26 (dd, *J* = 17.2, 2.9 Hz, 1H), 2.20 − 2.13 (m, 1H), 1.96 − 1.88 (m, 2H), 0.99 (d, *J* = 6.9 Hz, 3H), 0.90 (d, *J* = 6.9 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.9, 203.8, 141.6, 128.5, 128.4, 125.9, 52.5, 42.1, 37.7, 35.0, 27.5, 25.2, 20.4, 19.3. IR (KBr, cm^{-1}): 3026, 2962, 2935, 1712, 1496, 1454, 1373, 1242, 1180, 748, 702. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{17}H_{25}O_2^+$: 261.1849 ; found: 261.1842.

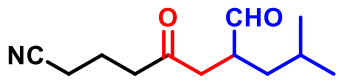
2-(Tert-butyl)-4-oxo-7-phenylheptanal (3ab)



Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 22.4 mg, 43% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.91 (s, 1H), 7.28 (d, *J* = 6.9 Hz, 2H), 7.20 − 7.14 (m, 3H), 2.91 (s, 1H), 2.64 − 2.58 (m, 1H), 2.51 − 2.38 (m, 2H), 2.11 (s, 1H), 1.95 − 1.86 (m, 2H),

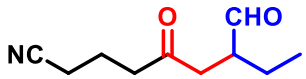
1.57 (s, 2H), 1.00 (s, 9H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 209.3, 204.7, 141.6, 128.5, 128.5, 128.4, 125.9, 56.0, 42.8, 42.0, 38.2, 35.0, 33.3, 29.9, 28.2, 25.2, 25.2. IR (KBr, cm^{-1}) : 2961, 2870, 1717, 1456, 1361, 750, 701. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{17}H_{24}O_2Na^+$: 283.1669 ; found: 283.1669.

7-Formyl-9-methyl-5-oxodecanenitrile (3ac)



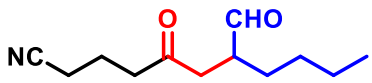
Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 29.3 mg, 70% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.69 − 9.65 (1H), 3.05 − 2.92 (m, 1H), 2.81 (q, J = 8.8 Hz, 1H), 2.75 − 2.58 (m, 2H), 2.48 − 2.31 (m, 4H), 2.20 − 2.14 (s, 1H), 1.97 − 1.88 (m, 3H), 1.70 − 1.51 (m, 3H), 1.35 − 1.14 (m, 2H), 0.94 (q, J = 6.6 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.3, 203.5, 119.4, 45.4, 41.8, 41.2, 40.7, 37.7, 25.9, 23.0, 22.3, 19.4, 16.5. IR (KBr, cm^{-1}) : 2956, 2914, 2322, 1713, 1524, 1454, 1373. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{12}H_{19}NO_2Na^+$: 232.1308 ; found: 232.1305.

7-Formyl-5-oxononanenitrile (3ad)



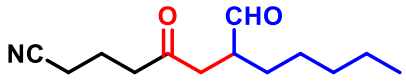
Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 27.9 mg, 77% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.68 (d, *J* = 1.4 Hz, 1H), 2.97 − 2.88 (m, 1H), 2.91 − 2.79 (m, 1H), 2.69 (qtd, *J* = 18.2, 6.9, 1.5 Hz, 2H), 2.41 (qdd, *J* = 9.9, 5.5, 3.0 Hz, 4H), 1.93 (pd, *J* = 7.0, 1.6 Hz, 2H), 1.85 − 1.72 (m, 1H), 1.69 − 1.47 (m, 2H), 0.96 (td, *J* = 7.5, 1.6 Hz, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.20, 203.36, 119.25, 45.32, 41.71, 40.57, 37.56, 25.77, 22.86, 22.15, 19.26, 16.39. IR (KBr, cm^{-1}) : 2965, 2973, 2248, 1717, 1458, 1410, 1371. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{10}H_{15}NO_2Na^+$: 204.0995 ; found: 204.0995.

7-Formyl-5-oxoundecanenitrile (3ae)



Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 32.2 mg, 77 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.67 (d, *J* = 2.8 Hz, 1H), 2.95 (ddp, *J* = 9.8, 6.9, 3.2 Hz, 1H), 2.84 (ddd, *J* = 17.2, 9.0, 2.9 Hz, 1H), 2.69 (dddd, *J* = 25.0, 16.0, 10.6, 6.9 Hz, 2H), 2.41 (ddp, *J* = 9.7, 6.9, 3.3 Hz, 3H), 1.93 (pd, *J* = 7.0, 2.8 Hz, 2H), 1.74 (dt, *J* = 14.4, 7.2 Hz, 1H), 1.52 - 1.39 (m, 1H), 1.32 (tt, *J* = 7.3, 3.6 Hz, 4H), 0.90 (td, *J* = 6.9, 2.9 Hz, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.2, 203.3, 119.3, 47.0, 41.1, 40.6, 29.1, 28.1, 22.6, 19.2, 16.4, 13.8. IR (KBr, cm^{-1}) : 2926, 2860, 2248, 1720, 1458, 1413, 1378, 1095. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{12}H_{19}NO_2Na^+$: 232.1308 ; found: 232.1307.

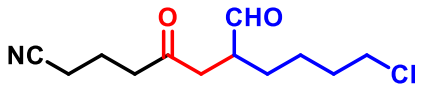
7-Formyl-5-oxotetradecanenitrile (3af)



Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 33.5 mg, 75% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.68 (s, 1H), 3.01 − 2.90 (m, 1H), 2.84 (ddd, *J* = 17.2, 9.0, 1.2 Hz, 1H), 2.77 − 2.56 (m, 2H), 2.50 − 2.33 (m, 3H), 2.03 − 1.84 (m, 2H), 1.79 − 1.66 (m, 1H), 1.43 (dt, *J* = 13.9, 7.2 Hz, 1H), 1.37 − 1.23 (m, 6H), 0.96 − 0.81 (m, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.2, 203.3, 119.3, 47.1, 41.1, 40.6, 31.7, 28.4, 26.7, 22.4, 19.2, 16.4, 13.9. IR (KBr, cm^{-1}): 2930, 2853, 2244, 1713, 1462, 1417, 1371, 1095.

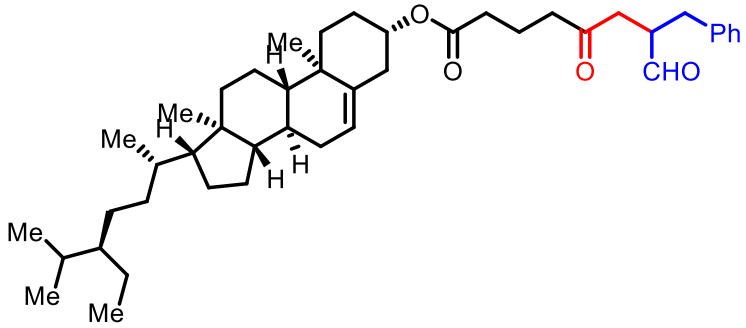
HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{13}H_{21}NO_2Na^+$: 246.1465 ; found: 246.1456.

11-Chloro-7-formyl-5-oxoundecanenitrile (3ag)



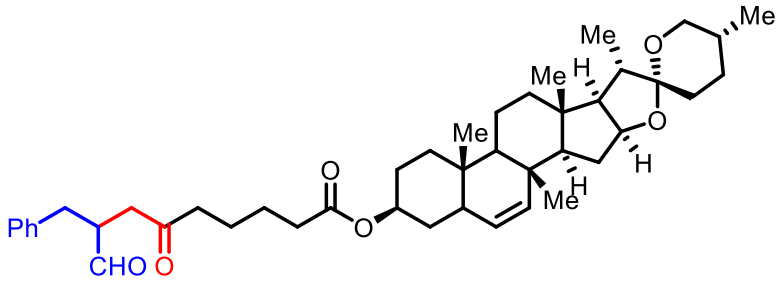
Colorless liquid after purification by column chromatography (dichloromethane/ethyl acetate = 50/1); 36.8 mg, 80.4% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 4.10 (q, *J* = 7.2 Hz, 1H), 3.53 (td, *J* = 6.4, 2.3 Hz, 3H), 3.00 − 2.79 (m, 2H), 2.79 − 2.48 (m, 4H), 2.48 − 2.40 (m, 1H), 2.44 − 2.28 (m, 3H), 2.04 − 1.90 (m, 3H), 1.93 − 1.85 (m, 1H), 1.89 − 1.69 (m, 4H), 1.60 − 1.40 (m, 4H), 1.24 (td, *J* = 7.1, 0.7 Hz, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 206.9, 202.7, 119.2, 60.3, 46.8, 44.5, 41.1, 40.6, 32.2, 27.6, 24.2, 19.2, 16.3. IR (KBr, cm^{-1}): 2939, 2862, 2245, 1712, 1411, 1373, 1195, 1099, 736, 648. HRMS (ESI$^+$) m/z: [M+K]$^+$ calcd for $C_{12}H_{21}NO_2K^+$: 285.0892 ; found: 285.0884.

(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-17-((2*S*,5*R*)-5-Ethyl-6-methylheptan-2-yl)-10,13-dimethyl-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1*H*-cyclopetroleum ethernta[*a*]phenanthren-3-yl 7-benzyl-5,8-dioxooctanoate (3ah)



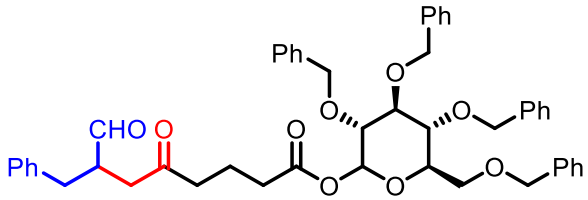
Transparent viscous liquid after purification by column chromatography (petroleum ether : EtOAc = 20/1); 94.9 mg, 72% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.29 (t, *J* = 7.1 Hz, 2H), 7.22 (t, *J* = 7.3 Hz, 1H), 7.14 (d, *J* = 6.9 Hz, 2H), 5.35 (d, *J* = 4.6 Hz, 1H), 4.58 (tt, *J* = 11.8, 4.3 Hz, 1H), 3.26-3.17 (m, 1H), 3.07 (q, *J* = 6.9 Hz, 1H), 2.81 − 2.63 (m, 2H), 2.54 − 2.34 (m, 3H), 2.32 − 2.18 (m, 4H), 2.04 − 1.91 (m, 2H), 1.88 − 1.76 (m, 5H), 1.65 (q, *J* = 6.9 Hz, 3H), 1.59 − 1.43 (m, 6H), 1.41 (s, 2H), 1.34 − 1.19 (m, 4H), 1.19 − 1.05 (m, 4H), 1.00 (s, 4H), 0.93 − 0.87 (m, 4H), 0.87 − 0.77 (m, 10H), 0.66 (s, 3H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.9, 202.8, 172.5, 139.6, 137.9, 128.9, 128.7, 126.8, 122.7, 73.9, 56.6, 55.9, 49.9, 48.4, 45.8, 42.3, 41.6, 40.8, 39.7, 38.1, 36.9, 36.5, 36.1, 34.5, 33.9, 33.5, 31.9, 31.8, 29.0, 28.2, 27.7, 26.8, 25.9, 24.3, 22.9, 20.9, 19.8, 19.3, 18.9, 18.8, 18.7, 11.9, 11.8. IR (KBr, cm^{-1}): 2954, 2870, 1728, 1454, 1377, 1253, 1176, 736, 702. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{44}H_{66}O_4Na^+$: 681.4853; found: 681.4845.

(4*S*,5'*R*,6a*S*,8a*S*,8b*R*,9*S*,10*R*,11a*S*,12a*S*,12b*R*)-5',6a,8a,9-Tetramethyl-2a,3,3',4,4',5,5',6,6a,6b,6',7,8,8a,8b,9,11a,12,12a,12b-icosahydrospiro[naphtho[2',1':4,5]indeno[2,1-b]furan-10,2'-pyran]-4-yl 8-benzyl-6,9-dioxononanoate (3ai)



Transparent viscous liquid after purification by column chromatography (petroleum ether : EtOAc = 15/1); 100.9 mg, 75% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.78 (s, 1H), 7.30 (t, *J* = 7.3 Hz, 2H), 7.26 − 7.20 (m, 1H), 7.15 (d, *J* = 6.9 Hz, 2H), 5.42 − 5.29 (1H), 4.65 − 4.52 (m, 1H), 4.41 (q, *J* = 7.5 Hz, 1H), 3.47 (dd, *J* = 10.7, 2.5 Hz, 1H), 3.37 (t, *J* = 11.0 Hz, 1H), 3.27 − 3.17 (m, 1H), 3.09 (dd, *J* = 14.0, 6.2 Hz, 1H), 2.86 − 2.64 (m, 2H), 2.56 − 2.33 (m, 3H), 2.33 − 2.21 (m, 4H), 2.06 − 1.92 (m, 2H), 1.91 − 1.74 (m, 6H), 1.66 − 1.57 (m, 7H), 1.56 − 1.45 (m, 4H), 1.42 (s, 2H), 1.35 − 1.23 (m, 2H), 1.23 − 1.06 (m, 3H), 1.03 (s, 3H), 0.97 (d, *J* = 6.9 Hz, 3H), 0.79 (d, *J* = 5.9 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.9, 202.8, 172.5, 139.6, 137.9, 128.9, 128.7, 126.8, 122.4, 109.3, 80.8, 73.8, 66.8, 61.9, 56.4, 49.8, 48.4, 41.6, 41.5, 40.8, 40.2, 39.7, 38.0, 36.9, 36.7, 34.5, 33.4, 31.9, 31.8, 31.3, 30.3, 28.7, 27.7, 26.9, 20.8, 19.3, 18.8, 17.1, 16.3, 14.5. IR (KBr, cm^{-1}): 2947, 2900, 1728, 1454, 1377, 1176, 1053, 983, 898, 736, 702. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{44}H_{62}O_6Na^{+}$: 709.4439; found: 709.4438.

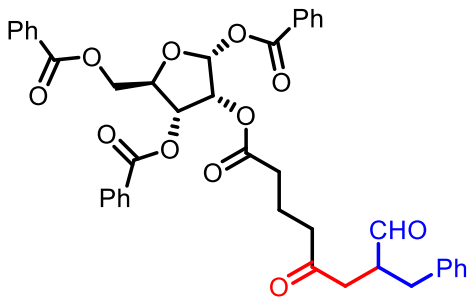
(3*R*,4*S*,5*R*,6*R*)-3,4,5-Tris(benzyloxy)-6-((benzyloxy)methyl)tetrahydro-2*H*-pyran-2-yl-7-benzyl-5,8-dioxooctanoate (3aj)



Transparent viscous liquid after purification by column chromatography (petroleum ether : EtOAc = 5/1); 112.2 mg, 72 % yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.79 − 9.72 (m, 1H), 7.43 − 7.27 (m, 24H), 7.19 − 7.11 (m, 5H), 6.47 − 5.58 (m, 1H), 5.01 − 4.91 (m, 1H), 4.91 − 4.71 (m, 4H), 4.70 − 4.58 (m, 2H), 4.52 (dd, *J* = 21.3, 11.2 Hz, 2H), 3.98 − 3.83 (m, 1H), 3.82 − 3.51 (m, 6H), 3.29 − 3.12 (m, 1H), 3.11 − 2.98 (m, 1H), 2.80 − 2.59 (m, 2H), 2.55 − 2.18 (m, 6H), 2.14 − 2.00 (m, 1H), 1.96 − 1.76 (m, 2H), 1.32 − 1.23 (m, 1H), 0.95 − 0.78 (m, 2H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.7, 202.7, 171.5, 138.5, 138.2, 138.0, 137.9, 137.8, 137.7, 137.5, 128.8, 128.7, 128.4, 128.1, 127.9, 127.8, 127.7, 127.65, 127.61, 126.7, 93.9, 89.9, 84.7, 81.6, 80.9, 78.9, 75.6, 75.4, 75.2, 74.9, 73.5, 73.4, 73.1, 72.6, 67.9, 48.2, 42.3, 40.7, 34.4, 33.1, 32.9, 18.5, 18.2. IR (KBr, cm^{-1}): 2981, 2858, 1743, 1708, 1494, 1452, 1355, 1070, 1024, 906, 734, 696. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{49}H_{52}O_9Na^{+}$: 807.2504; found: 807.3484.

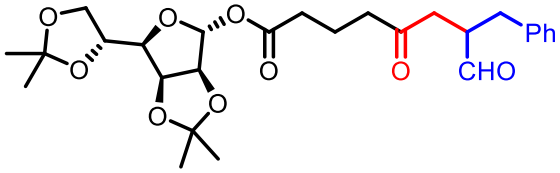
(2*R*,3*R*,4*R*,5*R*)-5-((Benzoyloxy)methyl)-3-((7-benzyl-5,8-dioxooctanoyl)oxy)tetrahydrofuran-2,4-diyl-dibenzoate (3ak)

Transparent viscous liquid after purification by column chromatography (petroleum ether : EtOAc = 3/1); 106.7 mg, 76% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.67 (s, 1H), 8.14 − 8.01 (m, 7H), 7.63 − 7.52 (m, 4H), 7.50 − 7.32 (m, 8H), 7.29 − 7.16 (m, 4H), 7.09 (d, *J* = 6.9 Hz, 2H), 6.77 (d, *J* = 5.5 Hz, 1H), 5.76 (d, *J* = 7.8 Hz, 1H), 5.54 (dd, *J* = 6.6, 4.3 Hz, 1H), 4.84 (q, *J* = 2.9 Hz, 1H), 4.64 (ddd, *J* = 42.2, 12.2, 3.1



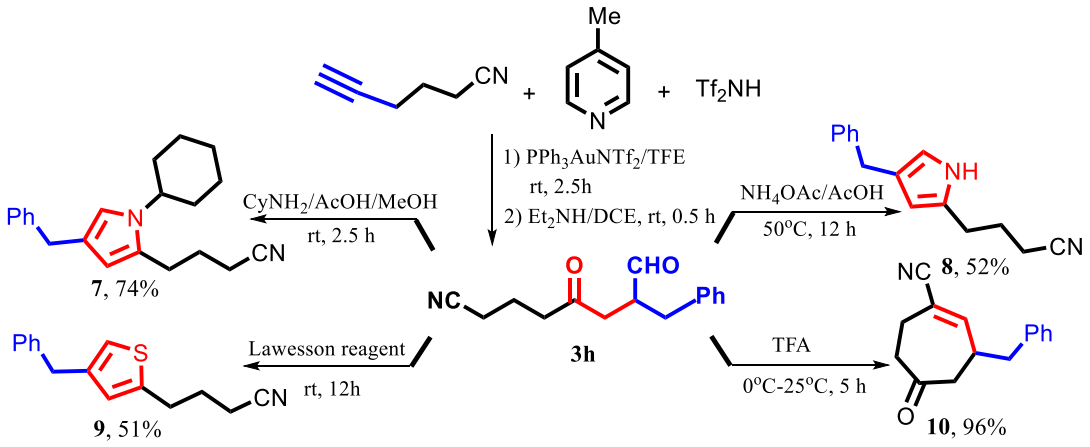
Hz, 2H), 4.10 (q, *J* = 7.2 Hz, 2H), 3.16 − 3.06 (m, 1H), 3.00 (q, *J* = 6.7 Hz, 1H), 2.65 − 2.52 (2H), 2.43 − 2.14 (m, 6H), 2.06 − 1.96 (3H), 1.77 − 1.65 (m, 2H), 1.24 (t, J = 7.3 Hz, 4H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.5, 202.6, 171.6, 166.0, 165.6, 165.1, 137.8, 133.7, 133.5, 133.4, 129.9, 129.8, 129.7, 129.5, 129.3, 129.1, 128.9, 128.7, 128.6, 128.5, 128.4, 128.4, 126.7, 94.7, 82.7, 82.7, 70.7, 70.6, 63.9, 60.3, 48.3, 41.2, 40.6, 34.4, 32.4, 21.0, 18.1, 14.1. IR (KBr, cm^{-1}): 2924, 2370, 2337, 1714, 1558, 1508, 1458, 1267, 1112, 1069, 1024, 709, 491, 420. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{41}H_{38}O_{11}Na^+$: 729.2306; found: 729.2291.

(3a*S*,4*R*,6*R*,6a*S*)-6-((*R*)-2,2-Dimethyl-1,3-dioxolan-4-yl)-2,2-dimethyltetrahydrofuro[3,4-d][1,3]dioxol-4-yl 7-benzyl-5,8-dioxooctanoate (3al)

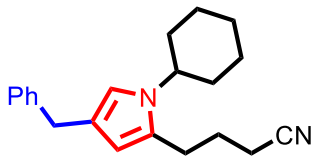


Transparent viscous liquid after purification by column chromatography (petroleum ether : EtOAc = 3/1); 73.6 mg, 73% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 9.77 (s, 1H), 7.30 (t, J = 7.1 Hz, 2H), 7.23 (t, J = 7.3 Hz, 1H), 7.15 (d, J = 7.3 Hz, 2H), 6.14 − 6.08 (m, 1H), 4.90 − 4.79 (1H), 4.67 (q, J = 2.9 Hz, 1H), 4.45 − 4.34 (m, 1H), 4.11 − 4.05 (1H), 4.05 − 3.97 (1H), 3.29 − 3.17 (m, 1H), 3.09 (dd, J = 14.0, 6.2 Hz, 1H), 2.84 − 2.61 (m, 2H), 2.58 − 2.34 (m, 4H), 2.30 (t, J = 7.1 Hz, 2H), 1.94 − 1.78 (m, 2H), 1.46 (d, J = 12.3 Hz, 6H), 1.35 (d, J = 13.7 Hz, 6H). ^{13}C NMR (100 MHz, Chloroform-*d*) δ 207.8, 202.7, 171.5, 137.8, 128.9, 128.7, 126.8, 113.2, 109.3, 100.6, 85.0, 82.2, 79.2, 72.8, 66.8, 48.5, 41.3, 40.8, 34.5, 33.1, 32.9, 27.0, 25.9, 25.1, 24.6, 18.3. IR (KBr, cm^{-1}): 3433, 2987, 2941, 1714, 1726, 1708, 1635, 1454, 1369, 1209, 1161, 1066, 960, 848, 702. HRMS (ESI$^+$) m/z: [M+Na]$^+$ calcd for $C_{27}H_{36}O_9Na^+$: 527.2252; found: 527.2257.

3.3 Synthesis of diverse heterocycles starting from compound 3h [3 − 4]

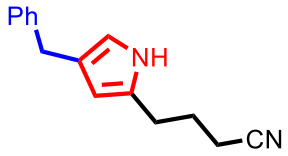


4-(4-Benzyl-1-cyclohexyl-1H-pyrrol-2-yl)butanenitrile (7)



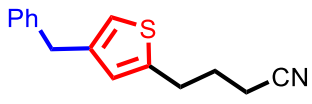
Compound 3h (0.20 mmol, 1.0 equiv) and cyclohexylamine (0.40 mmol, 2.0 equiv) were dissolved in methanol (2 mL). At 0°C, the glacial acetic acid (0.40 mmol, 2.0 equiv) was slowly added dropwise. The reaction mixture was kept at this temperature for 15 min. Then the mixture was warmed to room temperature and stirred for 2.5 h. The reaction was then diluted with brine and dichloromethane, separated and extracted twice with dichloromethane. The combined solution was dried with anhydrous $MgSO_4$. Then the solvents were evaporated and the chromatography on silica gel of the residue gave the target product 7. Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 5/1); 45.4 mg, 74% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 − 7.15 (m, 5H) , 6.43 (s, 1H), 5.71 (s, 1H), 3.78 (s, 2H), 3.74 − 3.64 (m, 1H), 2.69 (t, *J* = 7.4 Hz, 2H), 2.42 (t, *J* = 7.0 Hz, 2H), 2.02 − 1.83 (m, 6H), 1.78 − 1.69 (m, 1H), 1.57 (qd, *J* = 12.4, 3.1 Hz, 2H), 1.47 − 1.32 (m, 2H), 1.29 − 1.16 (m, 1H).^{13}C NMR (100 MHz, Chloroform-*d*) δ129.4, 128.6, 128.2, 125.6, 121.8, 119.6, 114.7, 106.1, 54.8, 34.6, 33.6, 25.9, 25.0, 24.7, 16.7. IR (KBr, cm^{-1}): 2936, 2851, 2319, 2243, 1699, 1495, 1452, 1413, 1136, 702. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{21}H_{28}N_2^+$: 307.2169 ; found: 307.2163.

4-(4-Benzyl-1*H*-pyrrol-2-yl)butanenitrile (8)



A 15mL reaction tube was charged with compound 3h (0.2 mmol, 1.0 equiv) and ammonium acetate (1mmol, 5.0 equiv) in ethanol (2 mL), under an argon atmosphere. Glacial acetic acid (17.8 μL, 0.312 mmol, 4.0 equiv) was added dropwise to the mixture, and then the reaction tube was put into the 50°C oil bath and was kept for 12 h until the completion of starting material. For the work-up, solid sodium carbonate (4 equiv) was added into the mixture and stirred for 15 min. The reaction was then diluted with brine and dichloromethane, separated and extracted twice with dichloromethane. The combined solution was dried with anhydrous $MgSO_4$. Then the solvents were evaporated and the chromatography on silica gel of the residue gave the target product 8. Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 10/1); 20.2 mg, 45% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.28 (d, *J* = 7.3 Hz, 2H), 7.24 − 7.14 (m, 3H), 6.40 (s, 1H), 5.79 (s, 1H), 3.78 (s, 2H), 2.71 (t, *J* = 7.3 Hz, 2H), 2.34 (t, *J* = 7.1 Hz, 2H), 1.99 − 1.84 (m, 2H). ^{3}C NMR (100 MHz, Chloroform-*d*) δ 142.1, 129.8, 128.9, 128.6, 128.3, 125.7, 123.7, 119.5, 114.7, 106.7, 33.5, 26.5, 25.4, 16.4. IR (KBr, cm^{-1}): 2924, 2850, 2345, 2310, 1720, 1512, 1454, 1060, 702. HRMS (ESI$^+$) m/z: $[M+H]^+$ calcd for $C_{15}H_{17}N_2^+$: 255.1386 ; found: 255.1379.

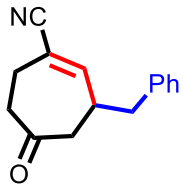
4-(4-Benzylthiophen-2-yl)butanenitrile (9)



Compound 3h (0.20 mmol, 1.0 equiv) was dissolved in anhydrous THF (2 mL). The reaction mixture was cooled to 0°C, and at this temperature Lawesson's reagent (0.40 mmol, 2.0 equiv) was added in portions over 10 min. The reaction was stirred for another 30 min, and then warmed to room temperature and stirred until completion of 3 g. After 12 h, the solvents were evaporated carefully under vacuum and the chromatography on silica gel of the residue gave the target product 9. Colorless liquid after purification by

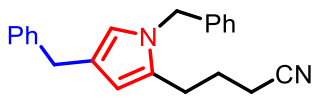
column chromatography (petroleum ether : EtOAc = 10/1); 24.1 mg, 50% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 − 7.26 (t, *J* = 7.4 Hz, 2H), 7.26 − 7.17 (m, 2H), 6.76 − 6.71 (s, 1H), 6.66 − 6.62 (s, 1H), 3.92 − 3.87 (s, 2H), 2.98 − 2.84 (t, *J* = 7.3 Hz, 2H), 2.44 − 2.28 (t, *J* = 7.1 Hz, 2H), 2.07 − 1.91 (p, *J* = 7.3 Hz, 2H), 0.09 − 0.05 (s, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.4, 141.5, 140.4, 132.3, 132.2, 128.7, 128.5, 126.8, 126.2, 119.6, 119.2, 36.8, 28.7, 27.1, 16.3, 1.0. IR (KBr, cm^{-1}): 2379, 2324, 1869, 1723, 1657, 1557, 1505, 710, 674. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{15}H_{15}NSNa^{+}$: 264.0817; found: 264.0807.

3-Benzyl-5-oxocyclohept-1-ene-1-carbonitrile (10)



Compound 3h (0.20 mmol, 1.0 equiv) was dissolved in cold trifluoroacetic acid (2 mL). The reaction mixture was stirred at 0°C for 30 min. Then the mixture was warmed to room temperature and stirred until completion of 3h After 5h, the solvents were evaporated carefully under vacuum and the chromatography on silica gel of the residue gave the target product 10. Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 5/1); 43.3 mg, 96% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (t, *J* = 1.4 Hz, 1H), 7.37 − 7.29 (m, 2H), 7.28 − 7.24 (m, 1H), 7.19 (d, *J* = 6.9 Hz, 2H), 3.32 − 3.10 (m, 1H), 2.80 (dd, *J* = 7.5, 1.6 Hz, 2H), 2.66 − 2.48 (m, 5H), 2.17 (dd, *J* = 19.2, 2.3 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.0, 163.1, 141.9, 138.7, 128.8, 128.6, 126.6, 118.9, 41.0, 41.0, 40.6, 21.2, 15.9. IR (KBr, cm^{-1}): 3028, 2920, 2850, 2254, 1701, 1635, 1600, 1496, 1454, 1357, 1199, 1064, 748, 705, 493. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{15}H_{15}NONa^{+}$: 248.1046; found: 248.1038.

4-(1,4-Dibenzyl-1*H*-pyrrol-2-yl)butanenitrile (11)



Compound 3h (0.20 mmol, 1.0 equiv) and benzylamine (0.40 mmol, 2.0 equiv) were dissolved in methanol (2 mL). At 0°C, the glacial acetic acid (0.40 mmol, 2.0 equiv) was slowly added dropwise. The reaction mixture was kept at this temperature for 15 min. Then the mixture was warmed to room temperature and stirred for 2.5 h. The reaction was then diluted with brine and dichloromethane, separated and extracted twice with dichloromethane. The combined solution was dried with anhydrous $MgSO_4$. Then the solvents were evaporated and the chromatography on silica gel of the residue gave the target product 11. Colorless liquid after purification by column chromatography (petroleum ether : EtOAc = 10/1); 53.4 mg, 85% yield. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 − 7.15 (m, 8H), 7.04 − 6.94 (m, 2H), 6.41 (s, 1H), 5.81 (s, 1H), 4.96 (s, 2H), 3.80 (s, 2H), 2.56 (t, *J* = 7.5 Hz, 2H), 2.29 (t, *J* = 7.1 Hz, 2H), 1.88 − 1.73 (m, 2H).^{13}C NMR (100 MHz, Chloroform-*d*) δ 142.2, 138.3, 130.2, 128.8, 128.6, 128.2, 127.4, 126.2, 125.7, 122.3, 119.7, 119.4, 107.6, 50.2, 33.4, 24.9, 24.5, 16.5. IR (KBr, cm^{-1}): 3029, 2928, 2318, 1700, 1496, 1447, 1352, 730, 698. HRMS (ESI^{+}) m/z: [M+Na]$^{+}$ calcd for $C_{22}H_{22}N_2Na^{+}$: 315.1856 ; found: 315.1848.

4. Evaluation of proliferation inhibitory activity of the compounds on tumor cells[5]

In order to investigate the relationship between protein-tyrosine kinase inhibitory activity and antitumor activity of the compounds, we further investigated whether the

compounds had inhibitory effects on tumor cell proliferation. The tumor cells we selected were human ovarian cancer cells (SKOV3), human breast cancer cells (MCF-7) and human liver cancer cells (HepG2). It was used to test whether compound 10 could inhibit the proliferation activity of cancer cells after administration.

Typically, Take cells at logarithmic growth stage and configure them into 5×10^4 μmol/L cell suspension, planking on 96 well plate, adding PBS solution in a circle of holes around, 100μL for each hole. To eliminate the edge effect. Select 5 adjacent wells, and add DMEM high sugar medium (containing 10% fetal bovine serum) into the wells, 100 μL for each hole. As a contrast, eliminate the influence of background values. Add prepared cell suspension into the remaining holes, 100 μL for each hole. To ensure that the cell concentration in the hole is uniform, after adding a row of holes, blow the cell suspension with a straw and add all the cells, write a mark, and put the 96 hole plate into a 37 ºC, 5% CO_2 cell incubator for 24 hours.

Next, compound 10 was weighed and added biological DMSO solution to prepare compound mother solution of 100 μM/mL, mix evenly, use gradient dilution method, dilute with DMEM high sugar medium, and prepare 80, 40, 20, 10, 5 μM/mL successively for standby. The prepared drug solution was administered to the cells, and after the treatment, the 96-well plates were placed in a 37 ºC, 5% CO_2 cell incubator for 48 h.

Finally, the 96-well plate was removed from the incubator, 10 μL CCK-8 solution was added to each well, and then incubated again in a 37 ºC cell incubator with 5% CO_2 for 1−3 h. The operating environment was required to be shielded from light during the entire operation. A 96-well plates was removed from the cell incubator and the absorbance (OD) value was measured at 450 nm using a microplate reader (Fig.S1).

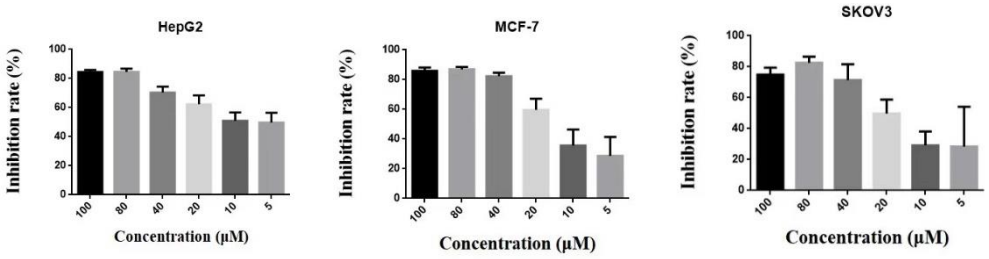


Fig.S1 MTS assay showed the inhibitory effect of HepG2 cell lines, McF-7 cell lines and SKOV3 cell lines at different concentrations after compound 10 treatment.

Calculation formula:

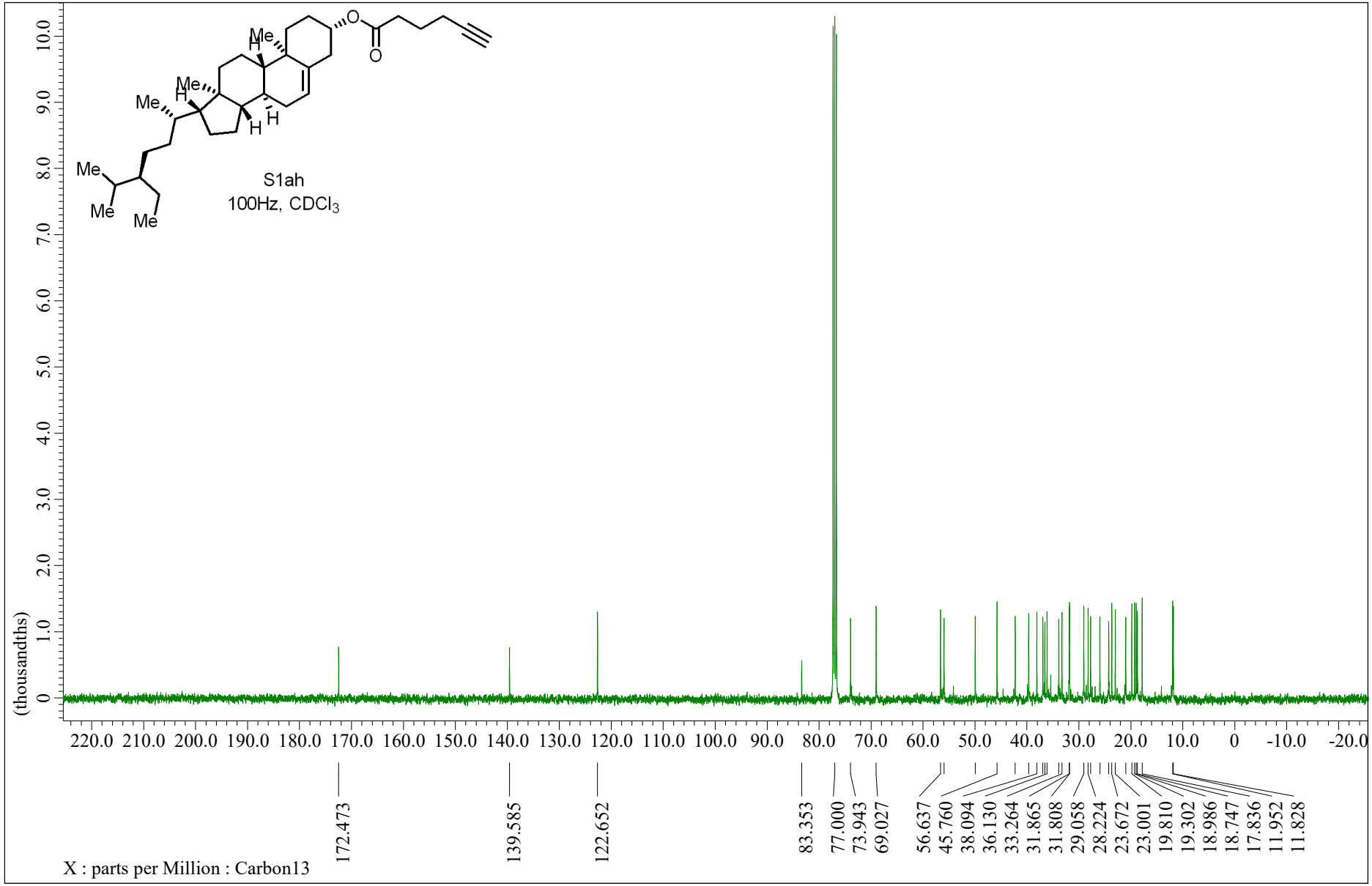
$$\text{Inhibition rate} = \frac{1-(\text{absorbance value after administration} - \text{background value})}{(\text{blank control value} - \text{background value})} \times 100\%$$

Compound	HepG2	MCF-7	SKOV3
	IC_{50} (μM)	IC_{50} (μM)	IC_{50} (μM)
10	36.86	18.94	21.85

5. Reference

[1] Huang M, Zhang L, Pan T, Luo S. *Science*. **2022**: 375, 869 − 874.
[2] Xu Z, Chen H, Wang Z, Ying A, Zhang L. *J Am Chem Soc*, **2016**, 138: 5515 − 5518.
[3] García-Santos WH, Mateus-Ruiz JB, Cordero-Vargas A. *Org Lett*, **2019**, 21: 4092 – 4096.
[4] Zhou W, Voituriez A. *Org Lett*, **2021**, 23: 247 – 252.
[5] Ganapathy-Kanniappan S, Geschwind JFH, Kunjithapatham R, Buijs M, Syed LH, Rao PP, Ota S, Vali M. *ASSAY and Drug Development Technologies*, 2010, 8: 258–262.

6. NMR spectra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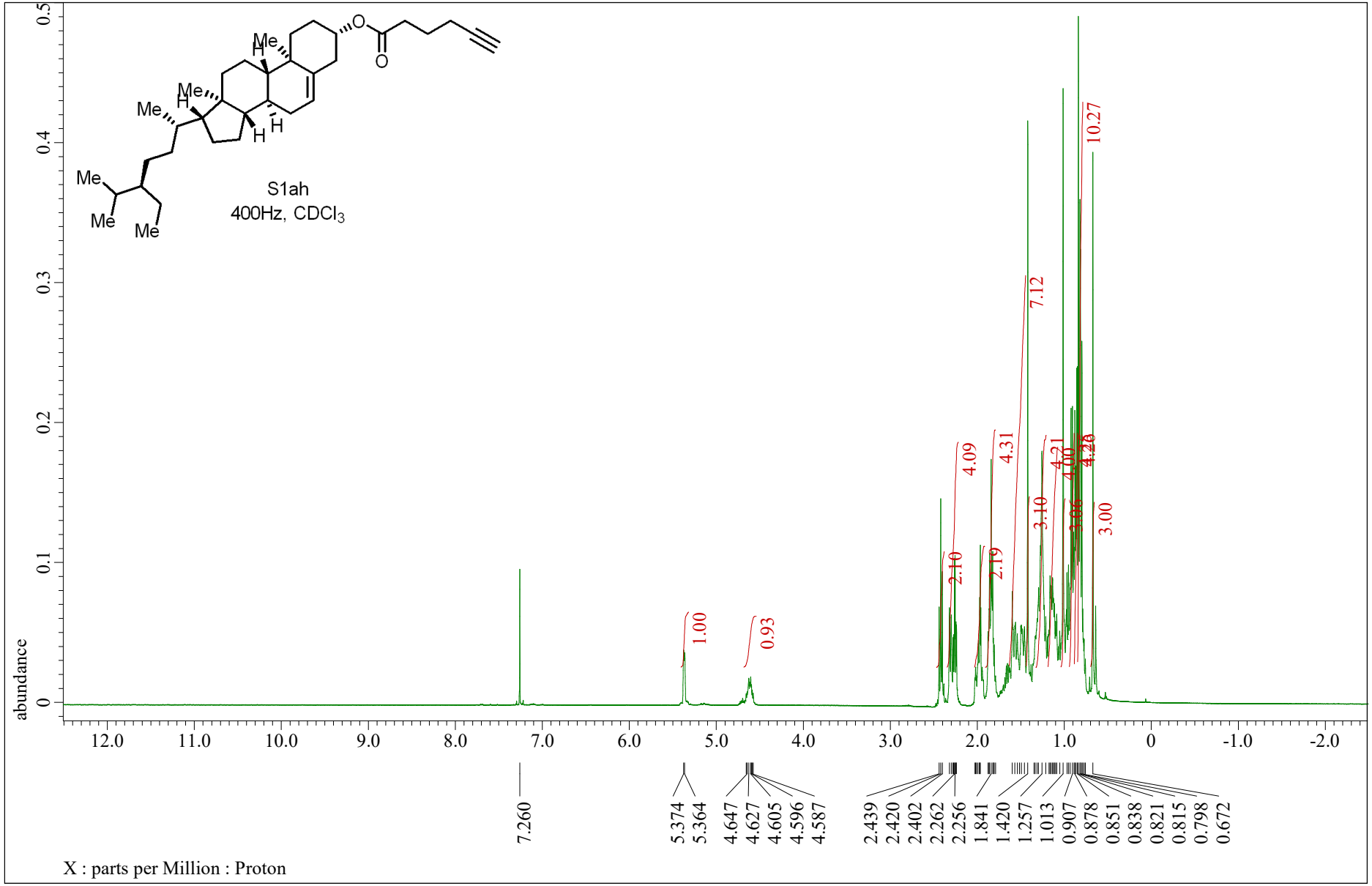
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
172.473
139.585
122.652
83.353
77.000
73.943
69.027
56.637
45.760
38.094
36.130
33.264
31.865
31.808
29.058
28.224
23.672
23.001
19.810
19.302
18.986
18.747
17.836
11.952
11.828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400Hz, CDCl3
abundance
X : parts per Million : Proton
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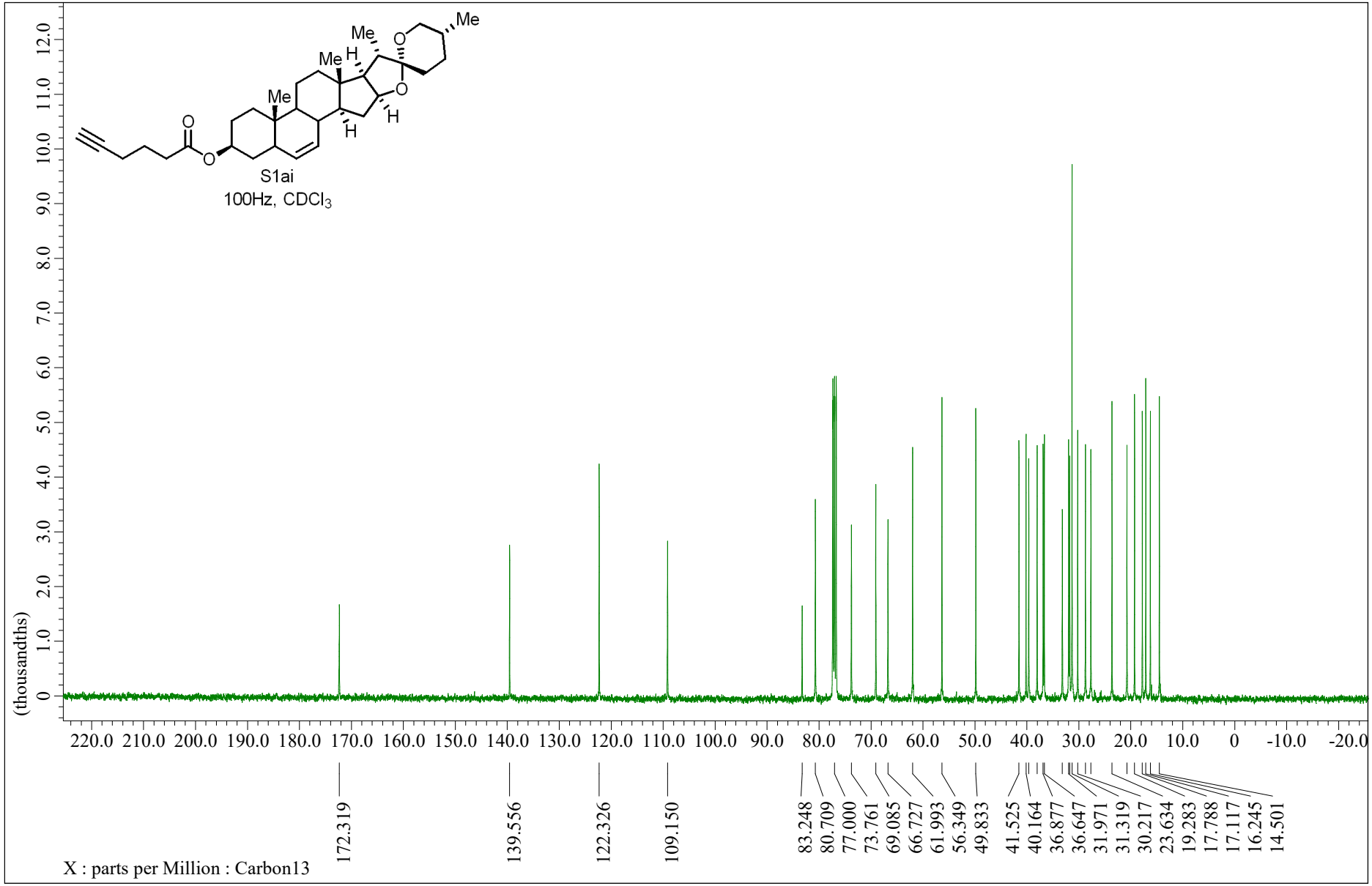
2.10
2.19
4.09
4.31
7.12
3.10
10.27
3.00
7.260
5.374
5.364
4.647
4.627
4.605
4.596
4.587
2.439
2.420
2.402
2.262
2.256
1.841
1.420
1.257
1.013
0.907
0.878
0.851
0.838
0.821
0.815
0.798
0.672


S1ai
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
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122.326
109.150
83.248
80.709
77.000
73.761
69.085
66.727
61.993
56.349
49.833
41.525
40.164
36.877
36.647
31.971
31.319
30.217
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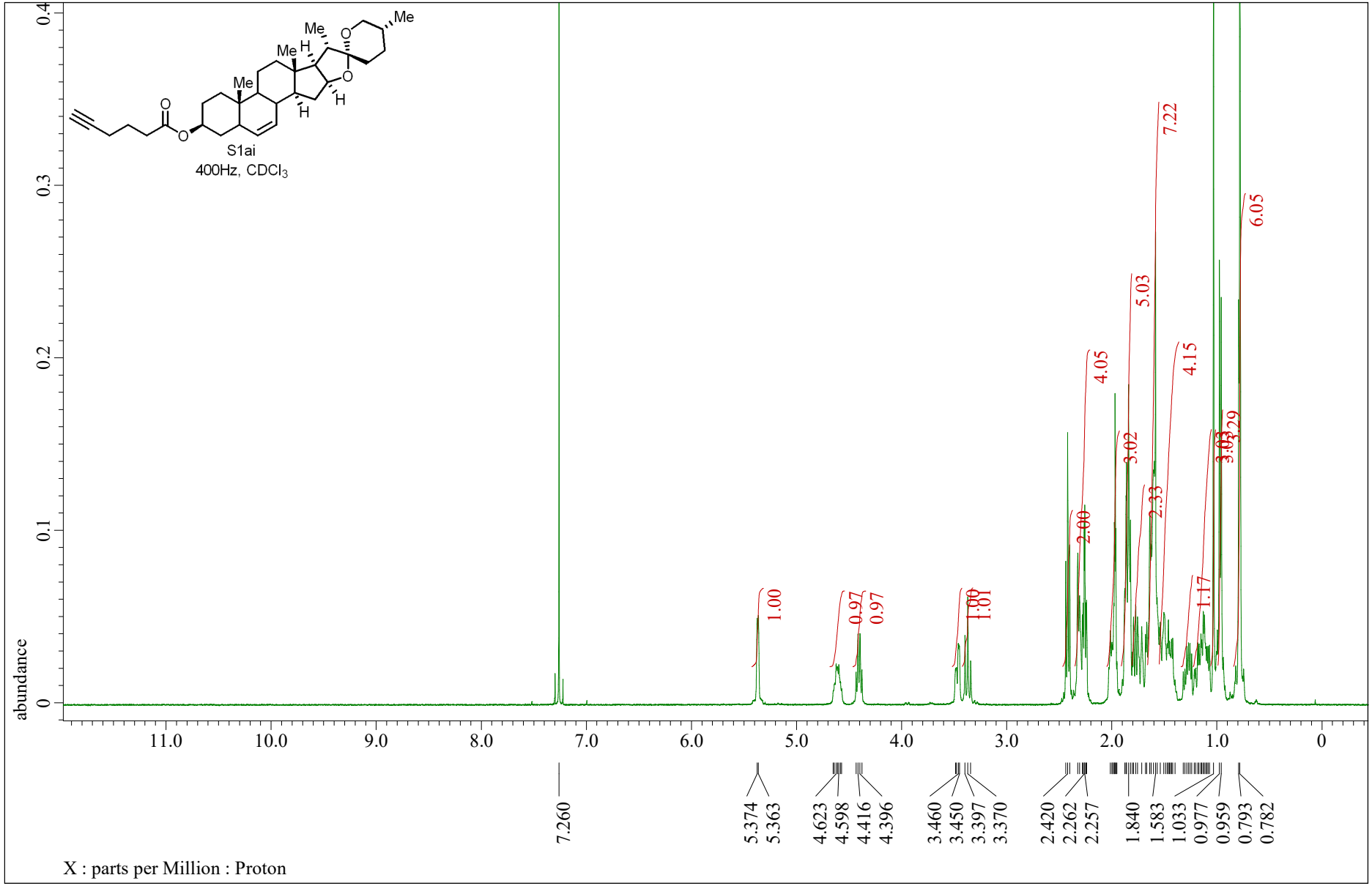
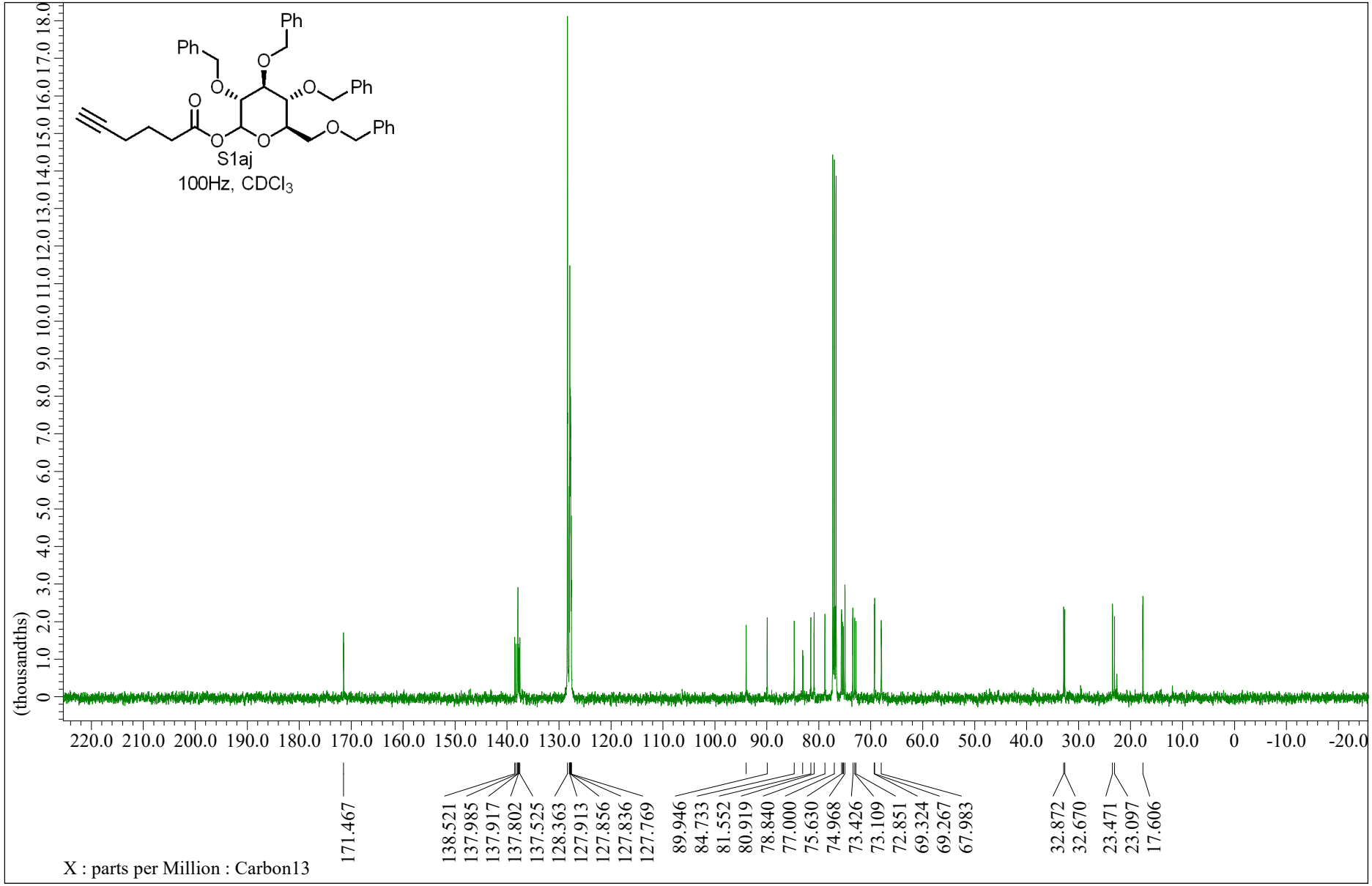
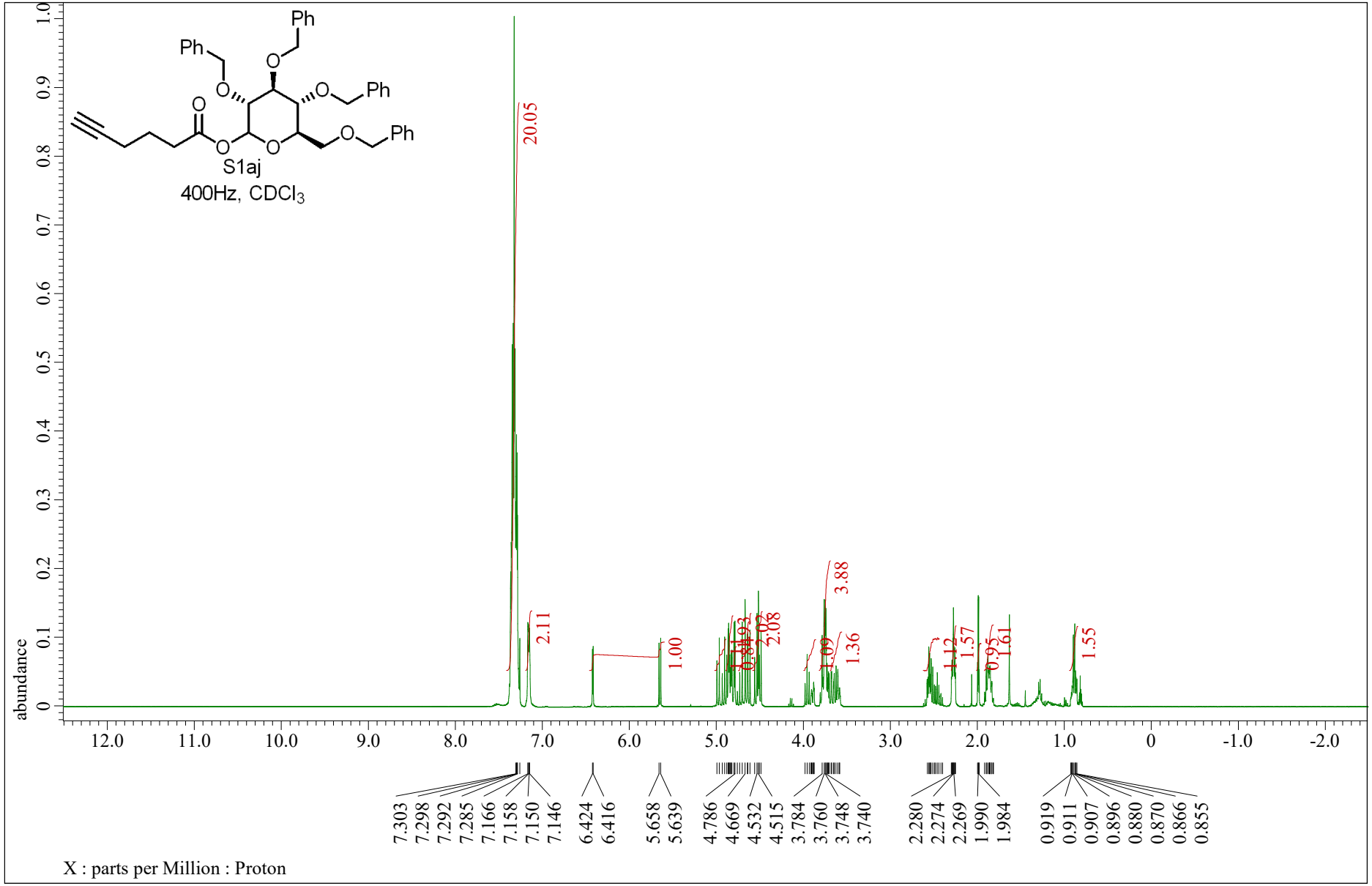
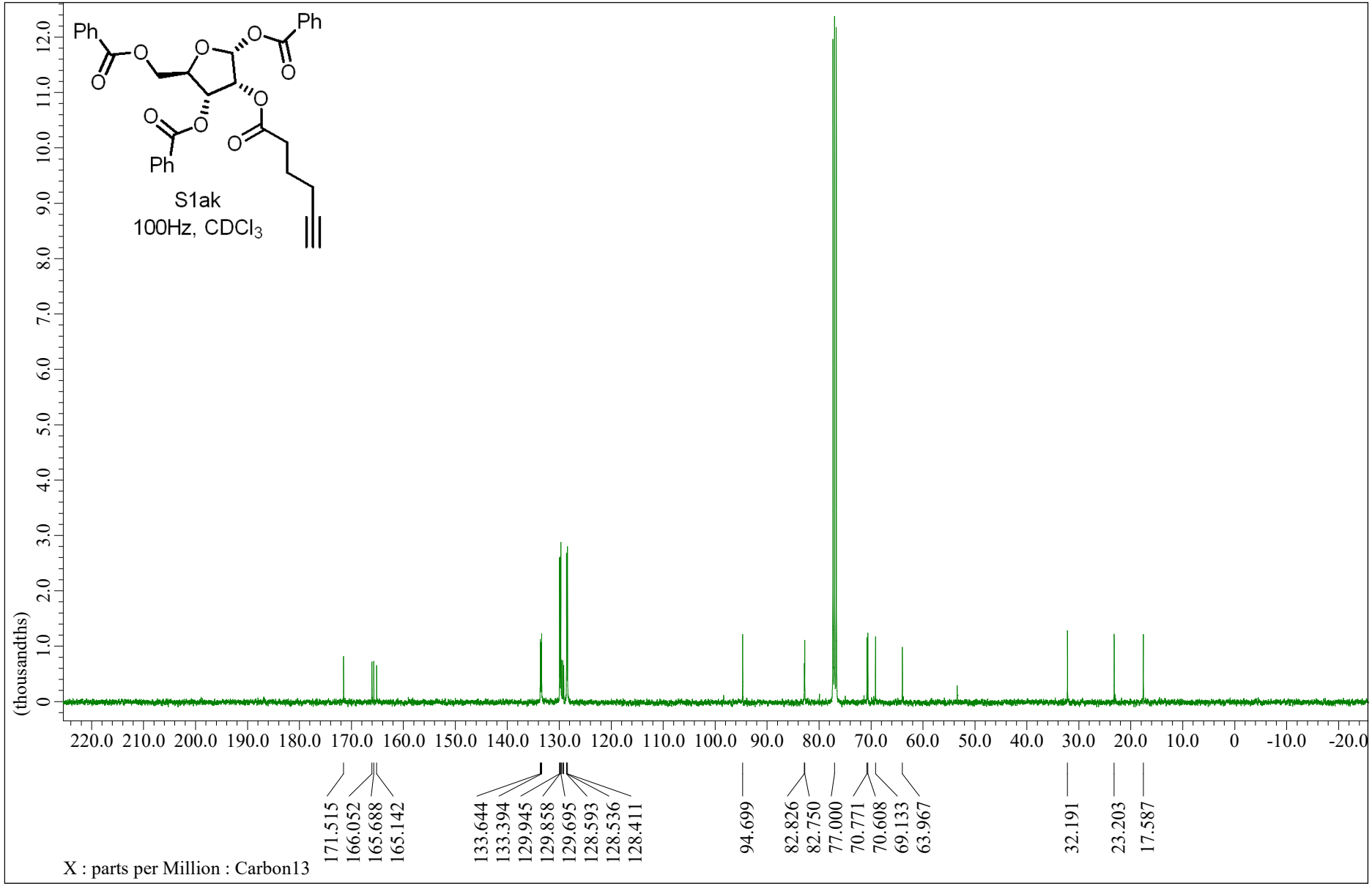
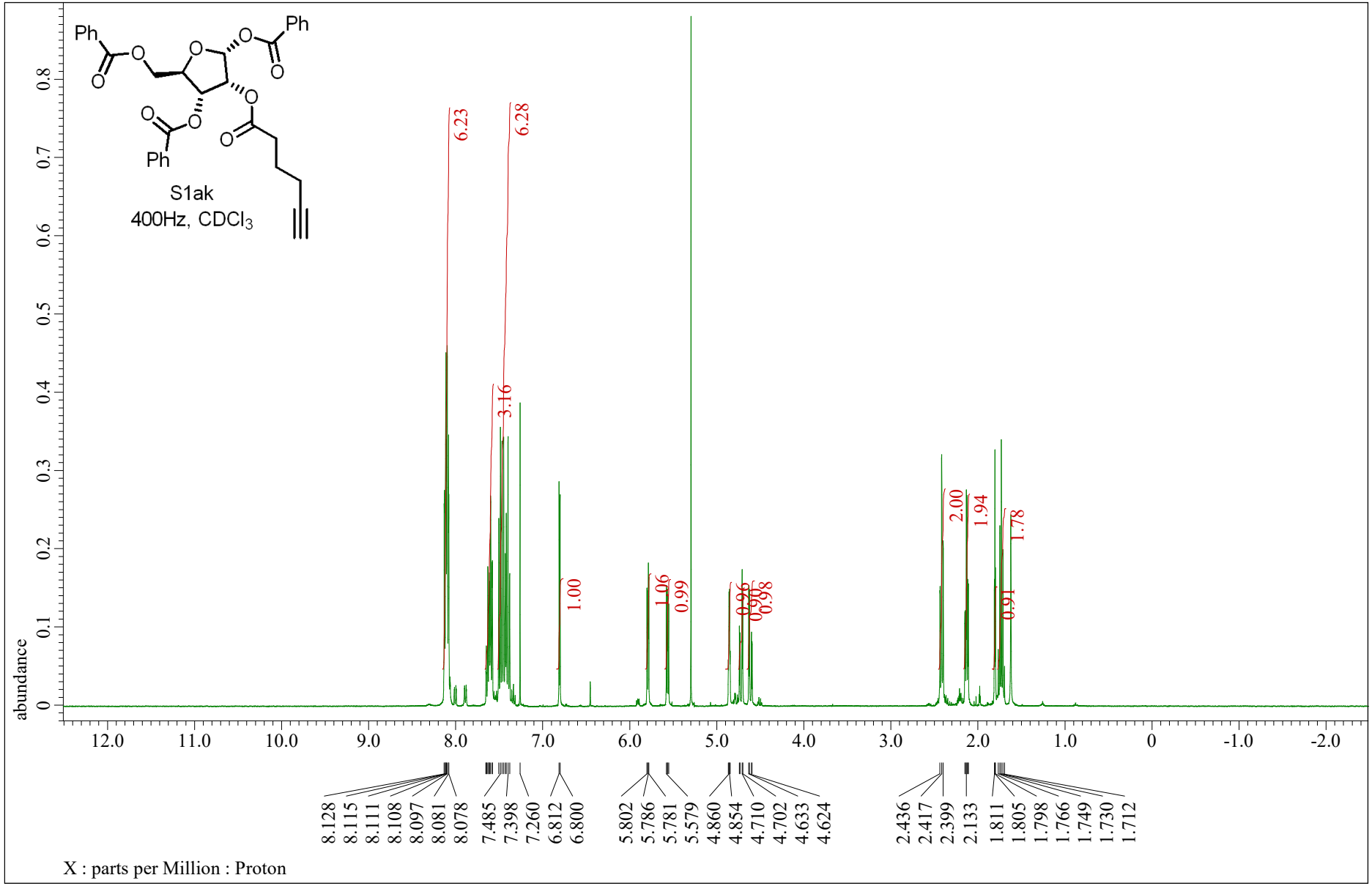
19.283
17.788
17.117
16.245
14.501

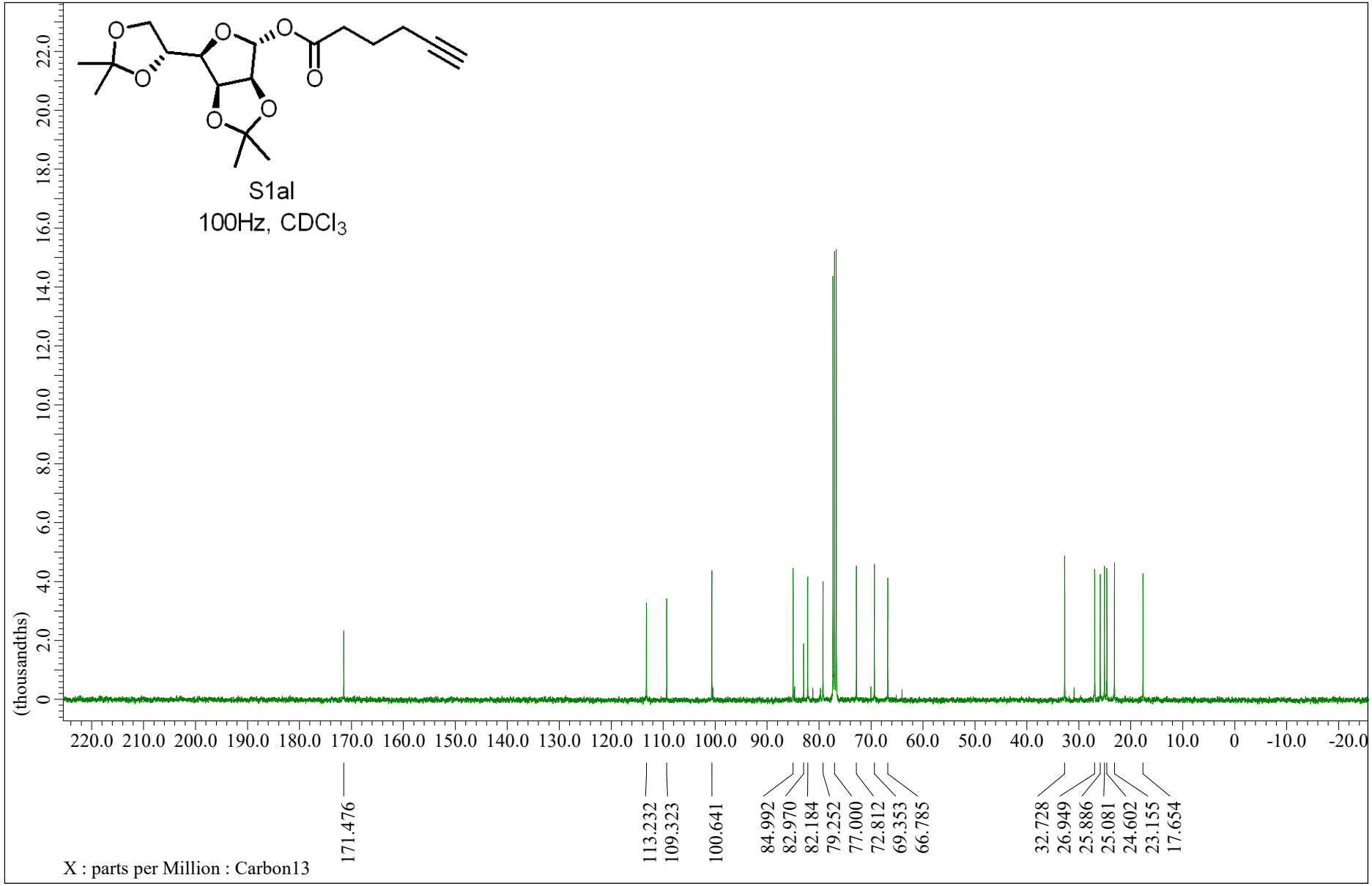

S1ai
400Hz, CDCl3
abundance
X : parts per Million : Proton
7.260
5.374
5.363
4.623
4.598
4.416
4.396
3.460
3.450
3.397
3.370
2.420
2.262
2.257
1.840
1.583
1.033
0.977
0.959
0.793
0.782
1.00
0.97
0.97
1.00
1.01
2.00
4.05
3.02
5.03
2.33
7.22
4.15
1.17
3.03
3.29
6.05


Ph
Ph
O
O
O
Ph
O
O
O
Ph
O
O
S1aj
100Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
171.467
138.521
137.985
137.917
137.802
137.525
128.363
127.913
127.856
127.836
127.769
89.946
84.733
81.552
80.919
78.840
77.000
75.630
74.968
73.426
73.109
72.851
69.324
69.267
67.983
32.872
32.670
23.471
23.097
17.606
X : parts per Million : Carbon13


S1aj
400Hz, CDCl3
abundance
X : parts per Million : Proton
20.05
2.11
1.00
3.88
1.36
1.09
2.08
2.02
1.57
1.55
1.61
1.12
0.95
7.303
7.298
7.292
7.285
7.166
7.158
7.150
7.146
6.424
6.416
5.658
5.639
4.786
4.669
4.532
4.515
3.784
3.760
3.748
3.740
2.280
2.274
2.269
1.990
1.984
0.919
0.911
0.907
0.896
0.880
0.870
0.866
0.855


S1ak
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
171.515
166.052
165.688
165.142
133.644
133.394
129.945
129.858
129.695
128.593
128.536
128.411
94.699
82.826
82.750
77.000
70.771
70.608
69.133
63.967
32.191
23.203
17.587


Ph
O
O
O
O
Ph
O
O
Ph
O
O
S1ak
400Hz, CDCl3
abundance
6.23
6.28
3.16
1.00
1.06
0.99
0.96
0.96
0.98
2.00
1.94
1.78
0.91
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.128
8.115
8.111
8.108
8.097
8.081
8.078
7.485
7.398
7.260
6.812
6.800
5.802
5.786
5.781
5.579
4.860
4.854
4.710
4.702
4.633
4.624
2.436
2.417
2.399
2.133
1.811
1.805
1.798
1.766
1.749
1.730
1.712
X : parts per Million : Proton


S1al
100Hz, CDCl3
(thousandths)
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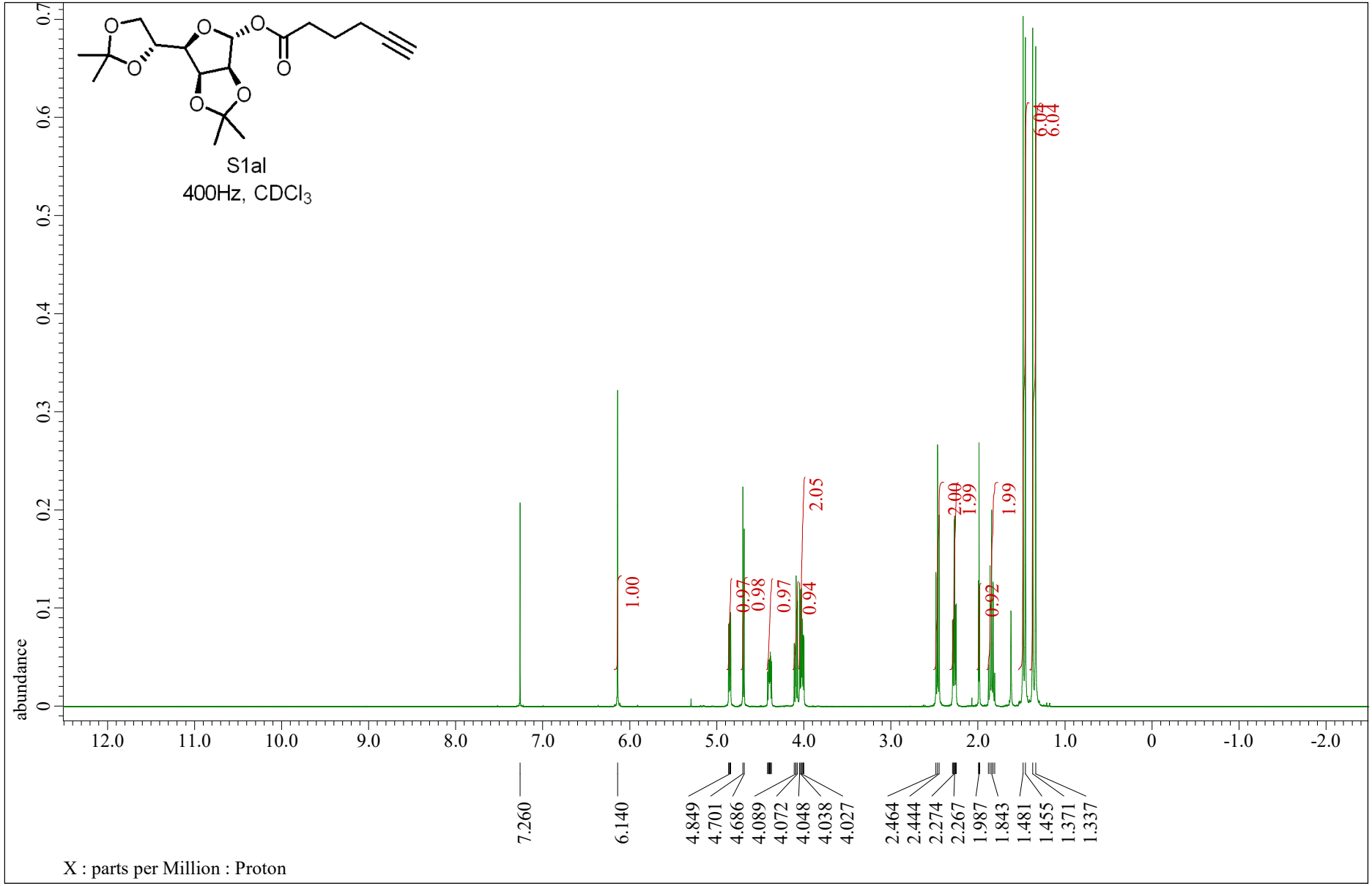
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
22.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
171.476
113.232
109.323
100.641
84.992
82.970
82.184
79.252
77.000
72.812
69.353
66.785
32.728
26.949
25.886
25.081
24.602
23.155
17.654
X : parts per Million : Carbon13


S1al
400Hz, CDCl3
abundance
X : parts per Million : Proton
7.260
6.140
4.849
4.701
4.686
4.089
4.072
4.048
4.038
4.027
2.464
2.444
2.274
2.267
1.987
1.843
1.481
1.455
1.371
1.337
1.00
0.97
0.98
0.97
0.94
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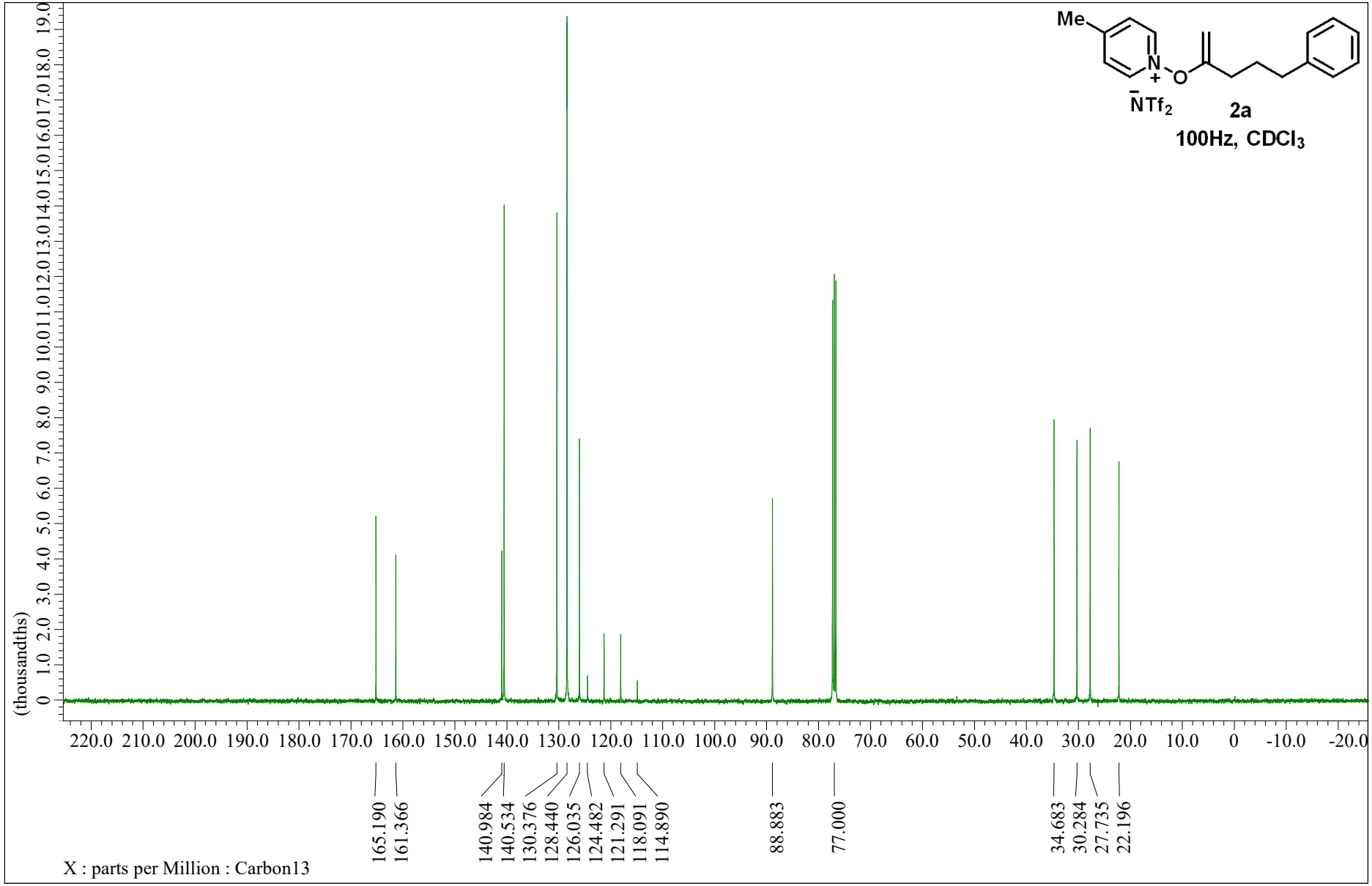
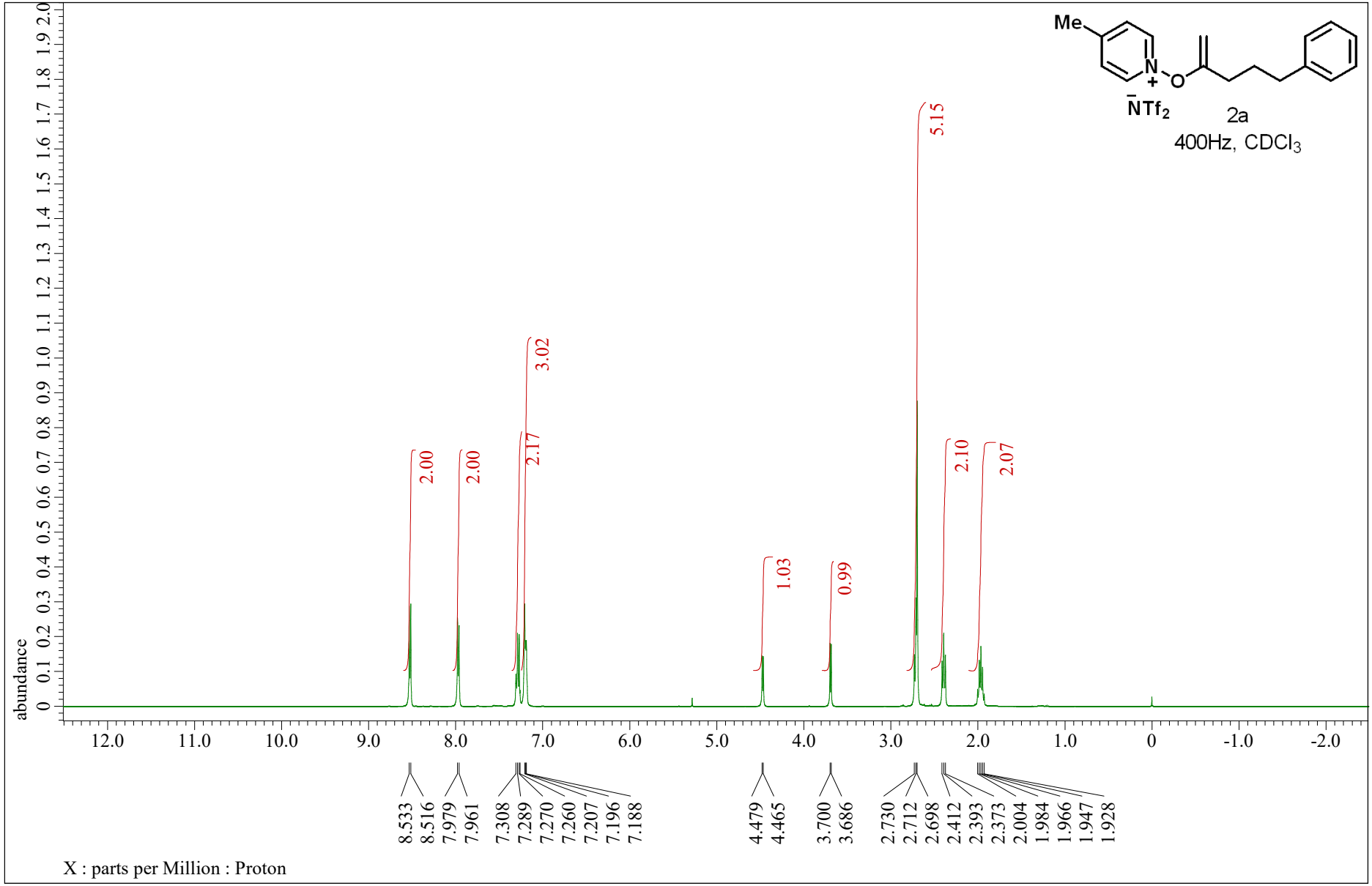
2.00
1.99
0.92
1.99
6.04


Me
N
+
O
NTf2
2a
100Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.190
161.366
140.984
140.534
130.376
128.440
126.035
124.482
121.291
118.091
114.890
88.883
77.000
34.683
30.284
27.735
22.196
X : parts per Million : Carbon13


Me
N
+
O
NTf2
2a
400Hz, CDCl3
abundance
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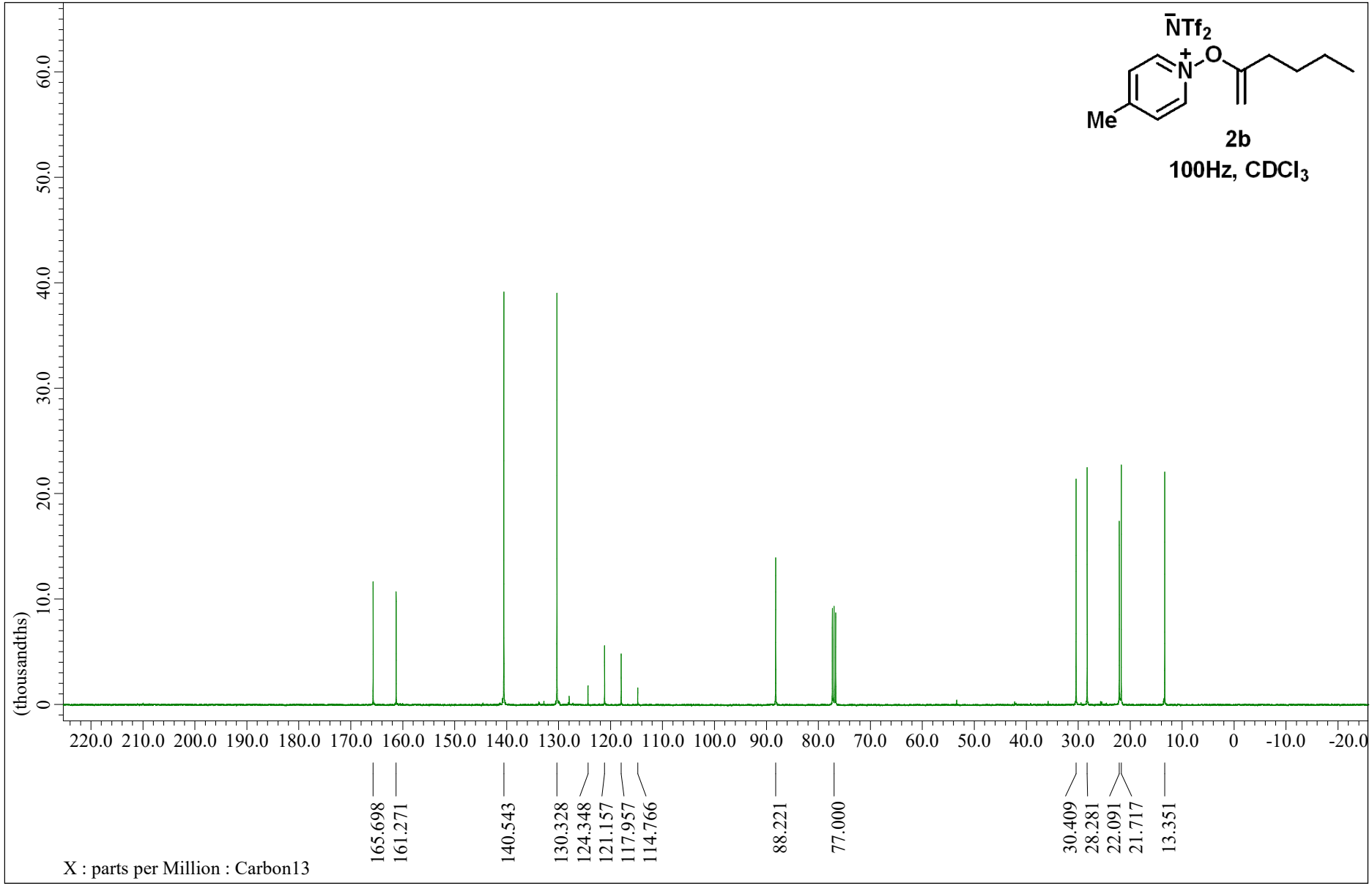
3.02
2.17
2.00
2.00
2.10
2.07
1.03
0.99
8.533
8.516
7.979
7.961
7.308
7.289
7.270
7.260
7.207
7.196
7.188
4.479
4.465
3.700
3.686
2.730
2.712
2.698
2.412
2.393
2.373
2.004
1.984
1.966
1.947
1.928
X : parts per Million : Proton


$\bar{N}Tf_2$
Me
2b
100Hz, $CDCl_3$
(thousandths)
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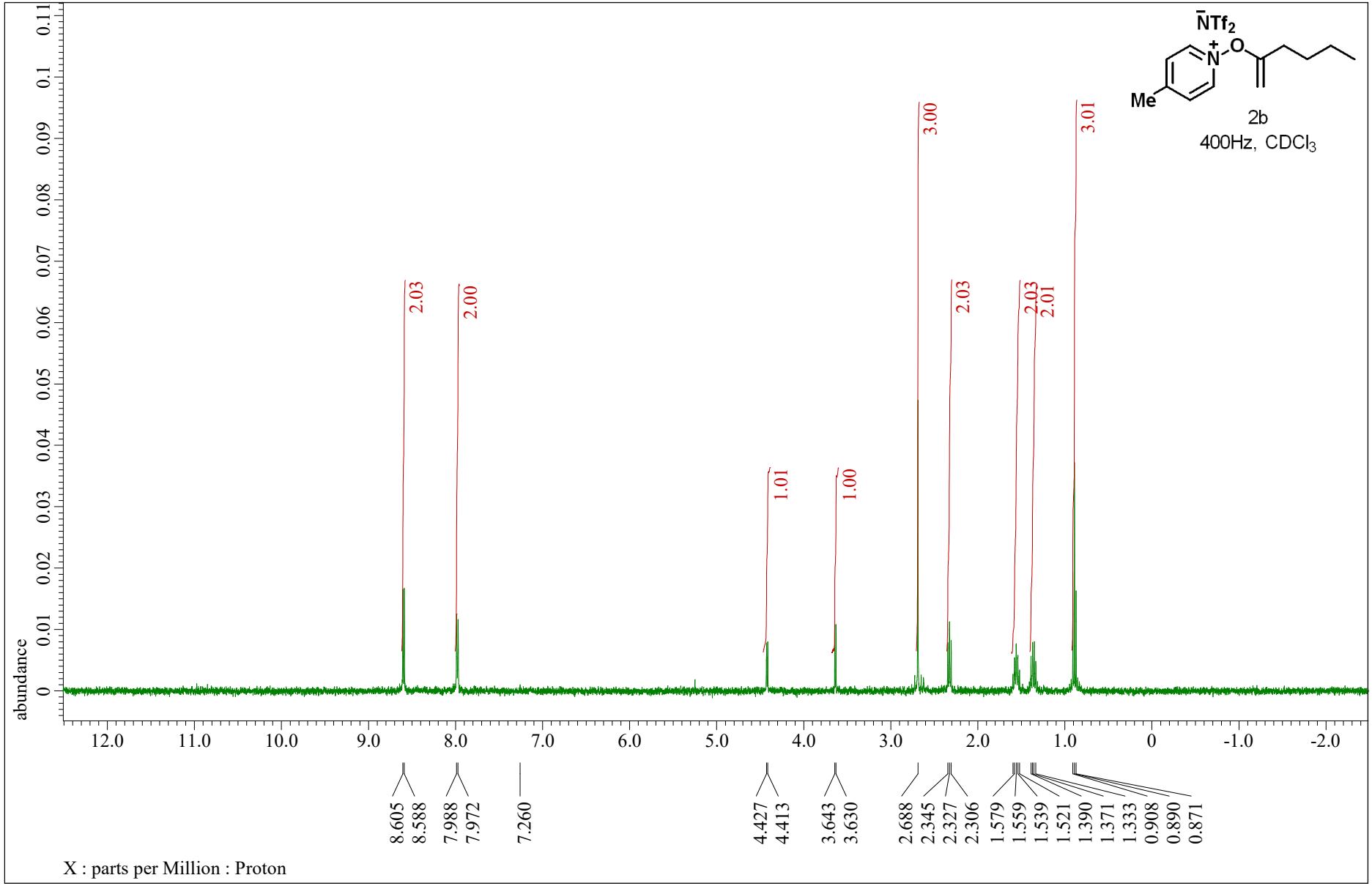
50.0
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.698
161.271
140.543
130.328
124.348
121.157
117.957
114.766
88.221
77.000
30.409
28.281
22.091
21.717
13.351
X : parts per Million : Carbon13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N
O
Me
2b
400Hz, CDCl3
abundance
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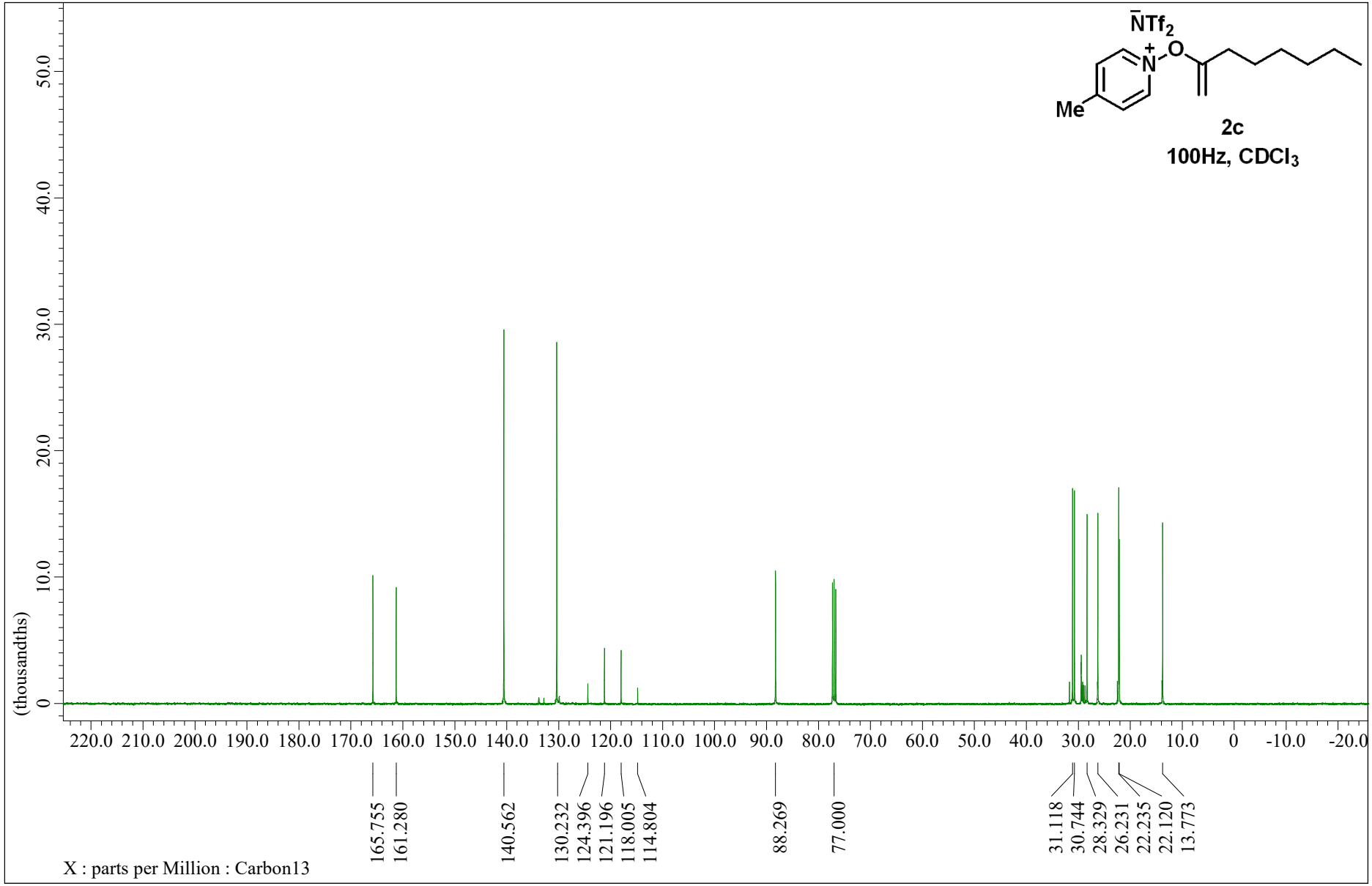
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
0.11
2.03
2.00
1.01
1.00
3.00
2.03
2.03
2.01
3.01
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.605
8.588
7.988
7.972
7.260
4.427
4.413
3.643
3.630
2.688
2.345
2.327
2.306
1.579
1.559
1.539
1.521
1.390
1.371
1.333
0.908
0.890
0.871
X : parts per Million : Proton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Me
2c
100Hz, CDCl3
(thousandths)
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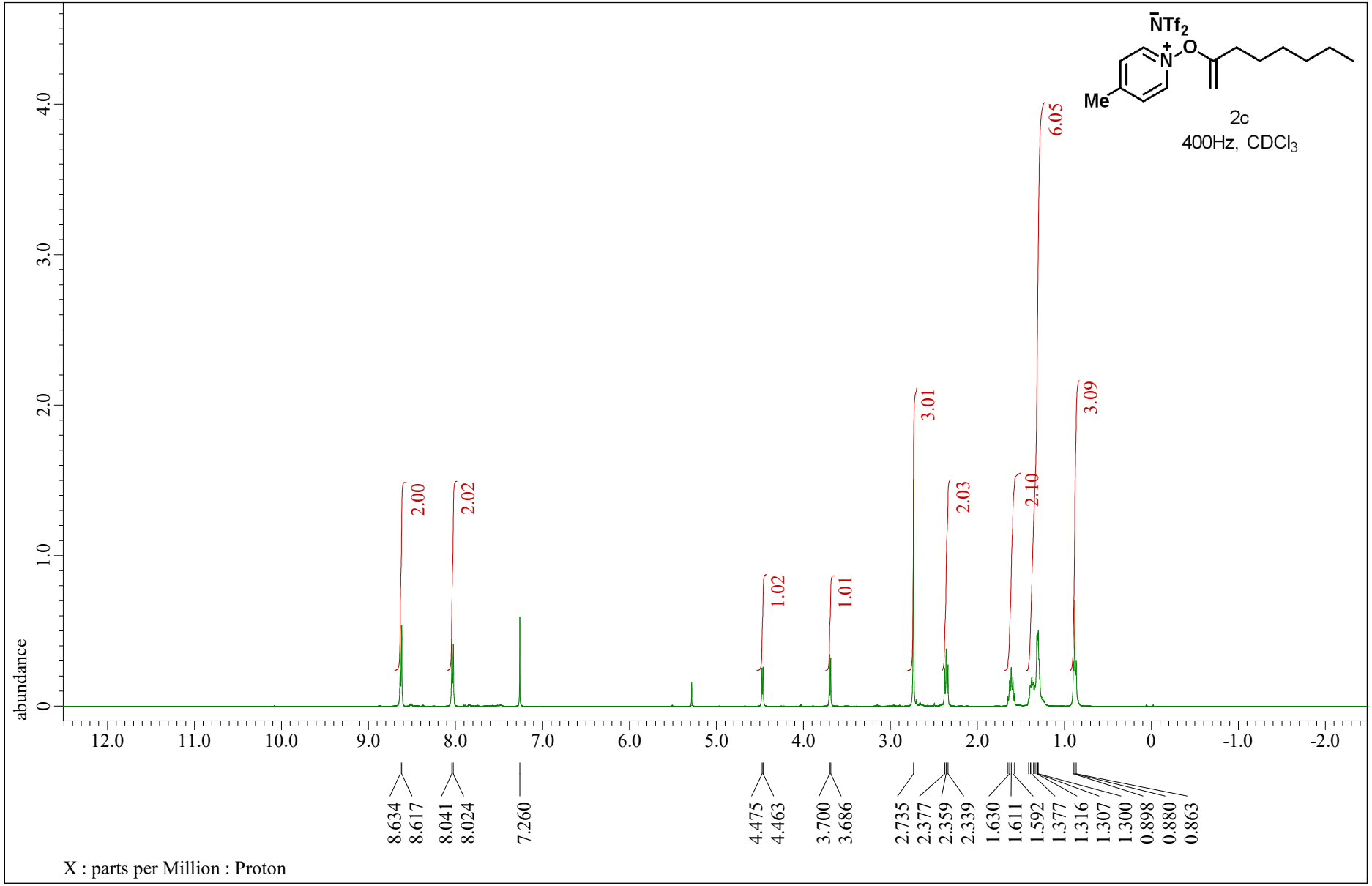
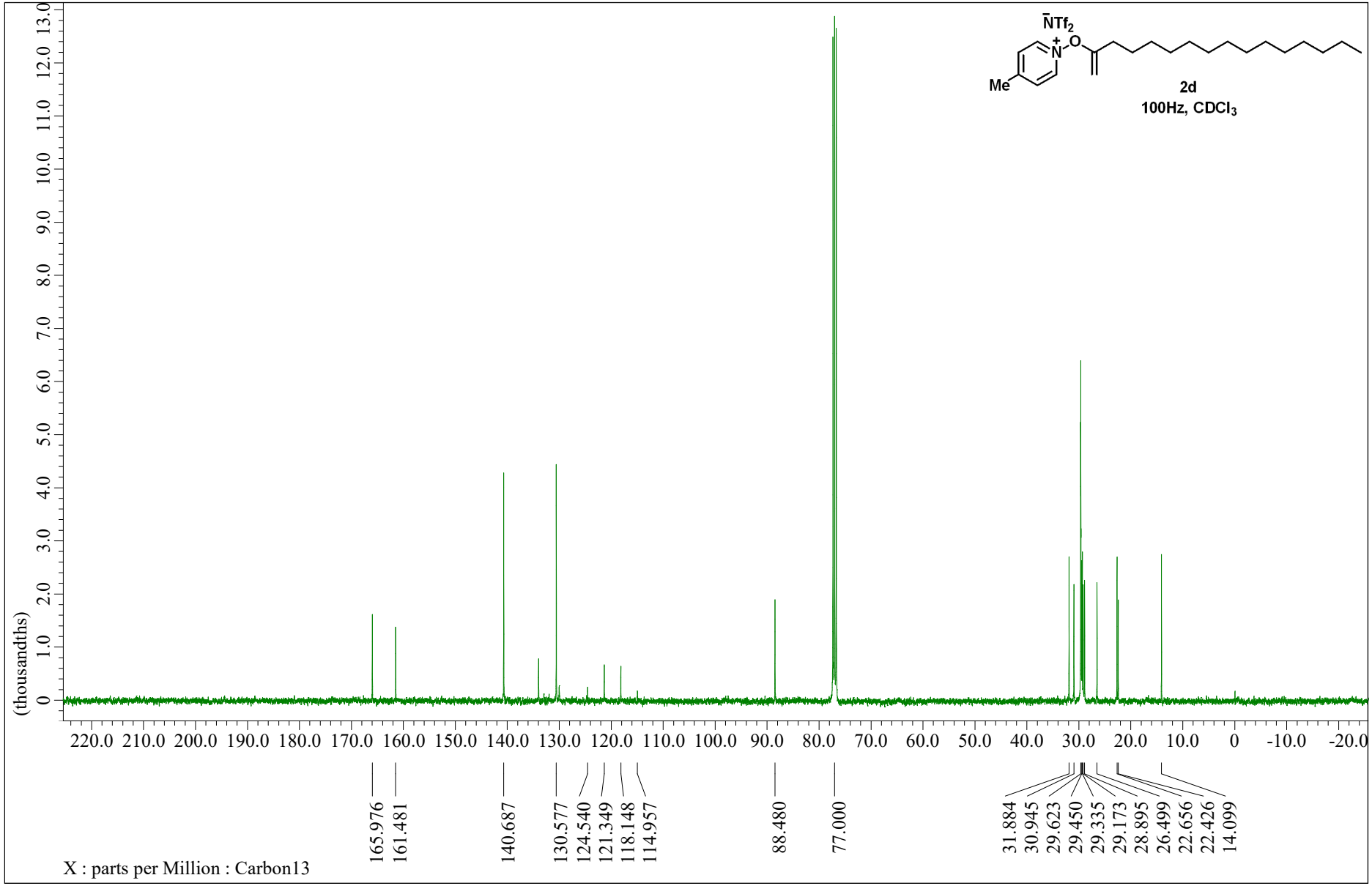
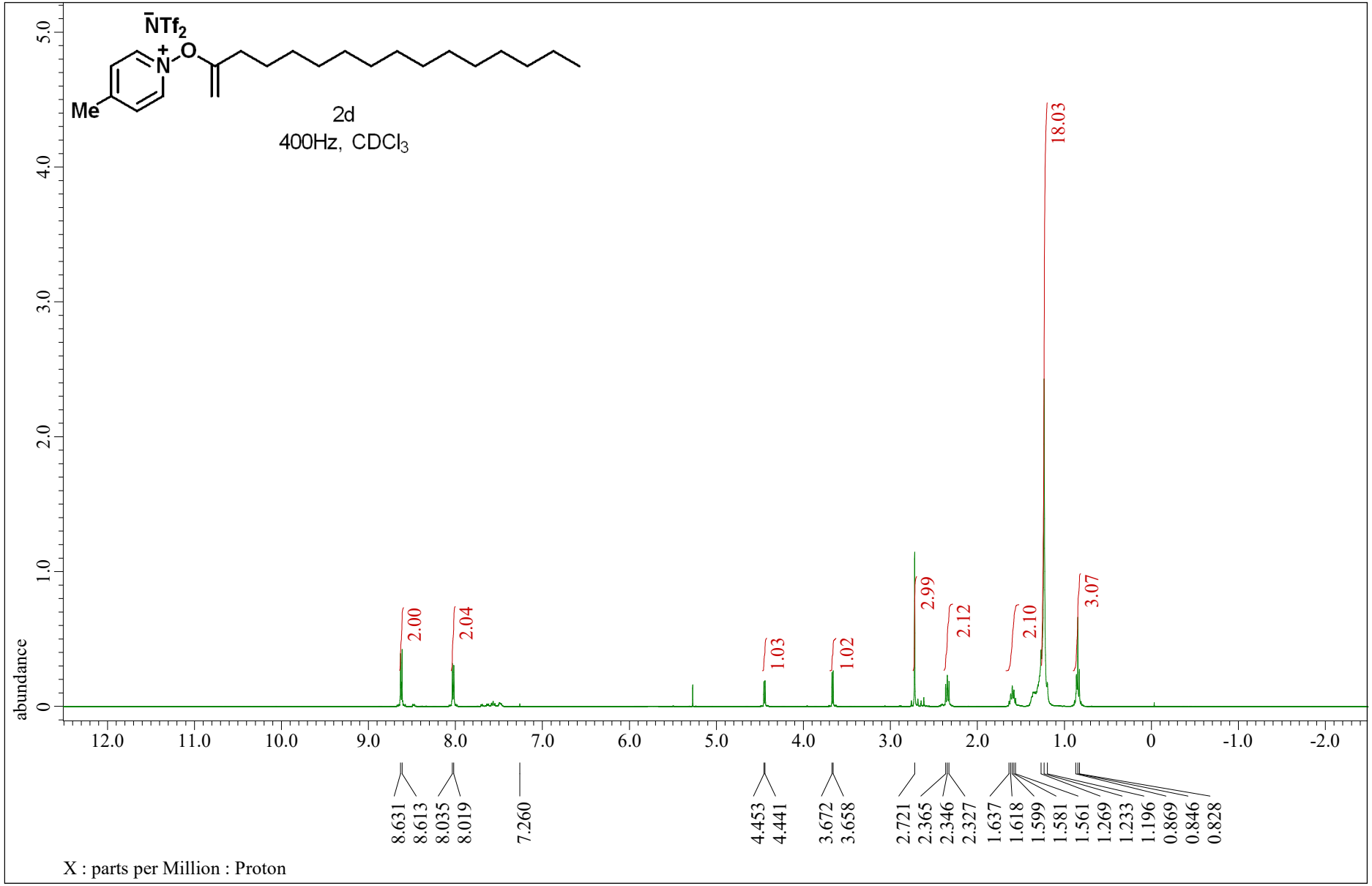
40.0
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.755
161.280
140.562
130.232
124.396
121.196
118.005
114.804
88.269
77.000
31.118
30.744
28.329
26.231
22.235
22.120
13.773
X : parts per Million : Carbon13


NTf2
N
O
Me
2c
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.02
1.02
1.01
3.01
2.03
2.10
6.05
3.09
8.634
8.617
8.041
8.024
7.260
4.475
4.463
3.700
3.686
2.735
2.377
2.359
2.339
1.630
1.611
1.592
1.377
1.316
1.307
1.300
0.898
0.880
0.863


NTf2
N
O
Me
2d
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.976
161.481
140.687
130.577
124.540
121.349
118.148
114.957
88.480
77.000
31.884
30.945
29.623
29.450
29.335
29.173
28.895
26.499
22.656
22.426
14.099
X : parts per Million : Carbon13


NTf2
Me
2d
400Hz, CDCl3
abundance
18.03
2.00
2.04
1.03
1.02
2.99
2.12
2.10
3.07
8.631
8.613
8.035
8.019
7.260
4.453
4.441
3.672
3.658
2.721
2.365
2.346
2.327
1.637
1.618
1.599
1.581
1.561
1.269
1.233
1.196
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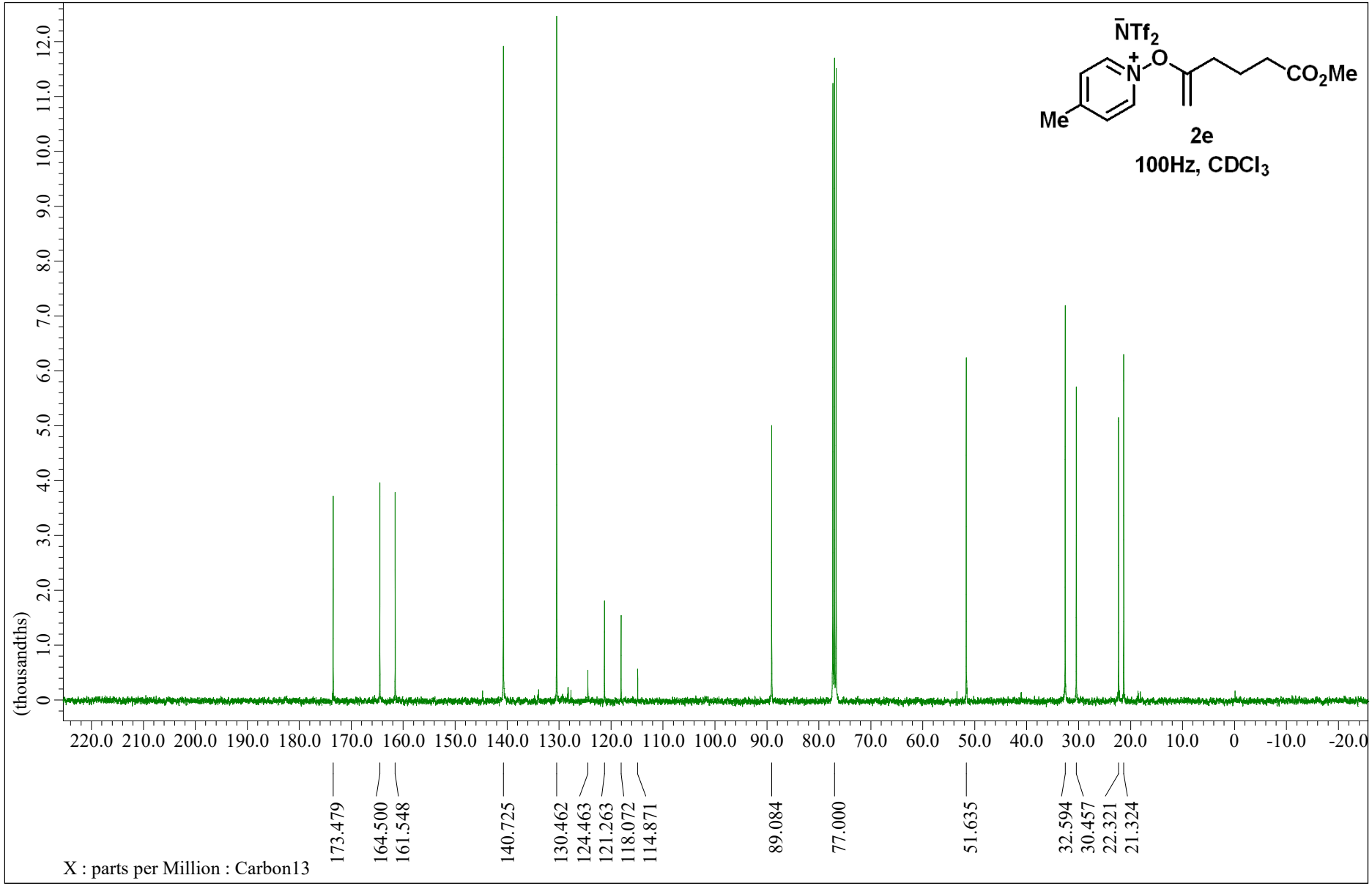
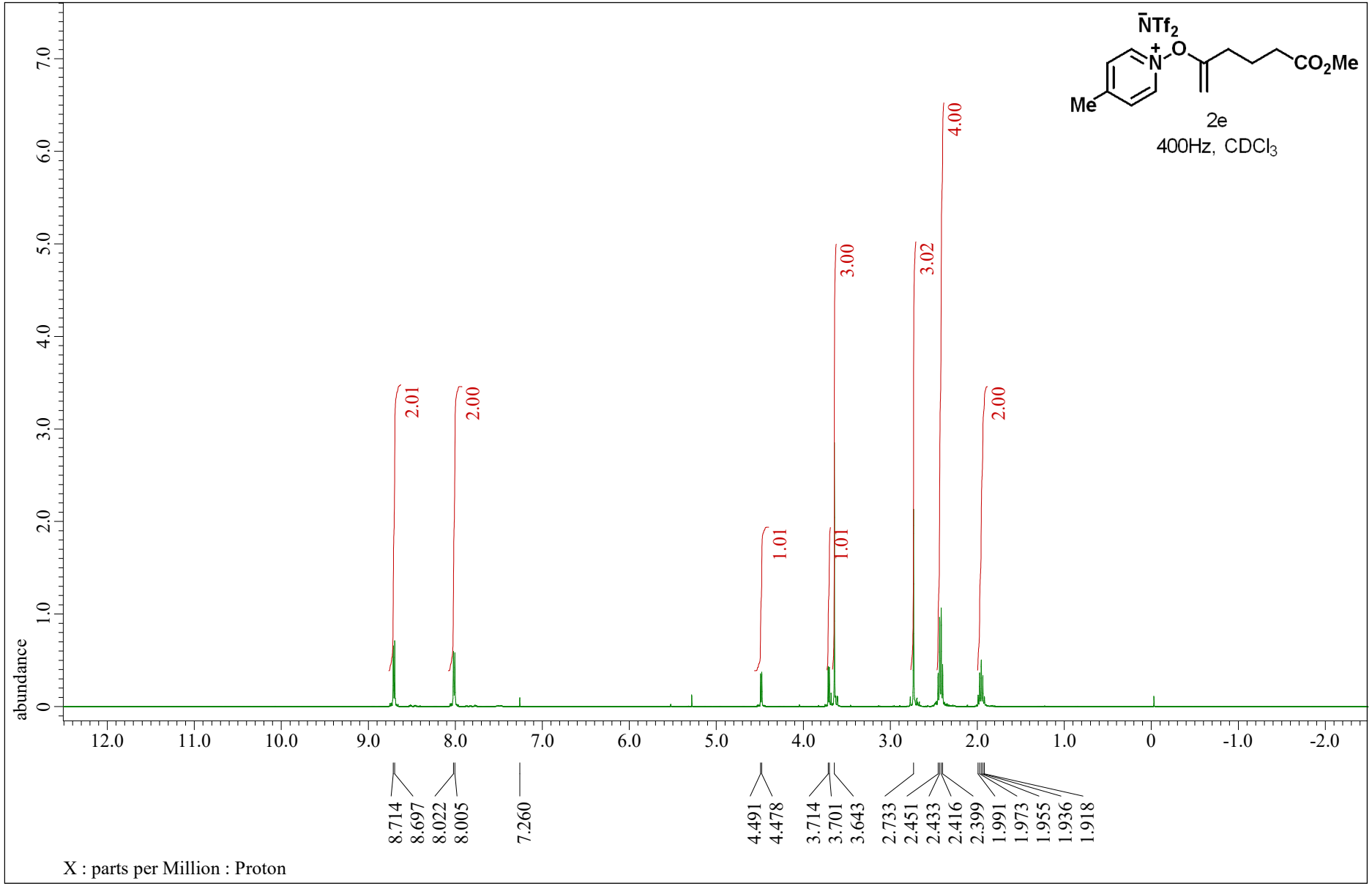
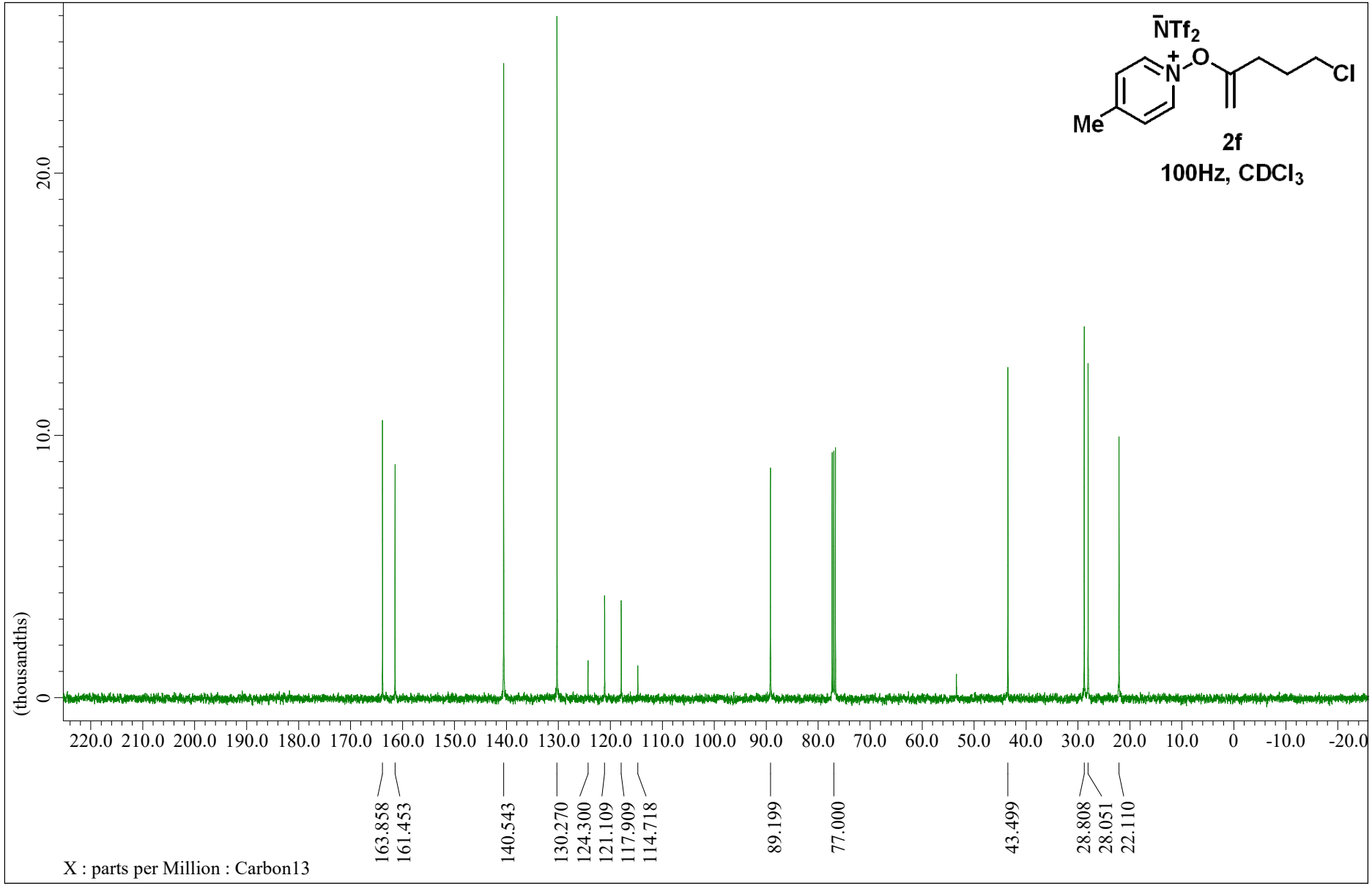
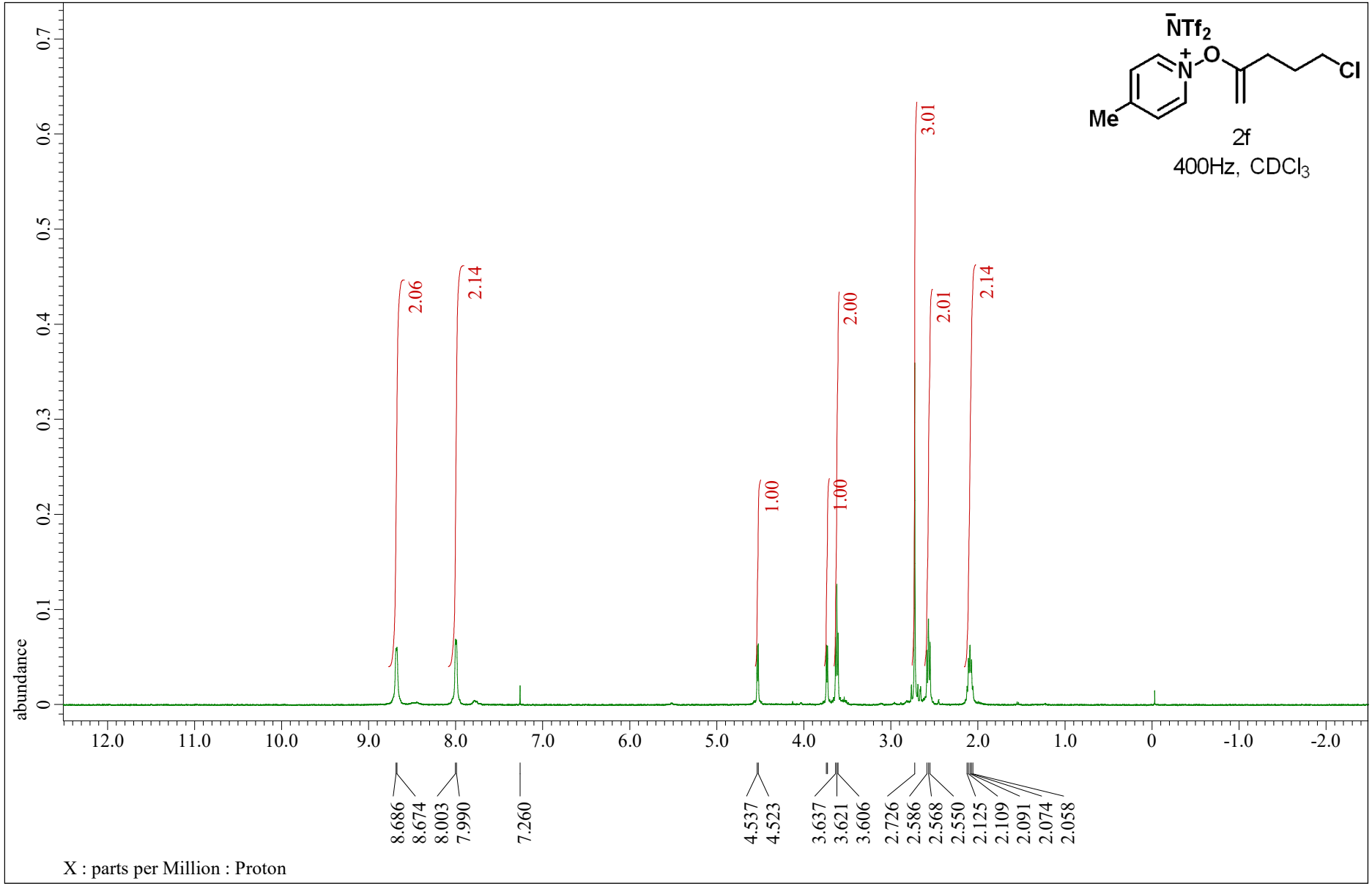
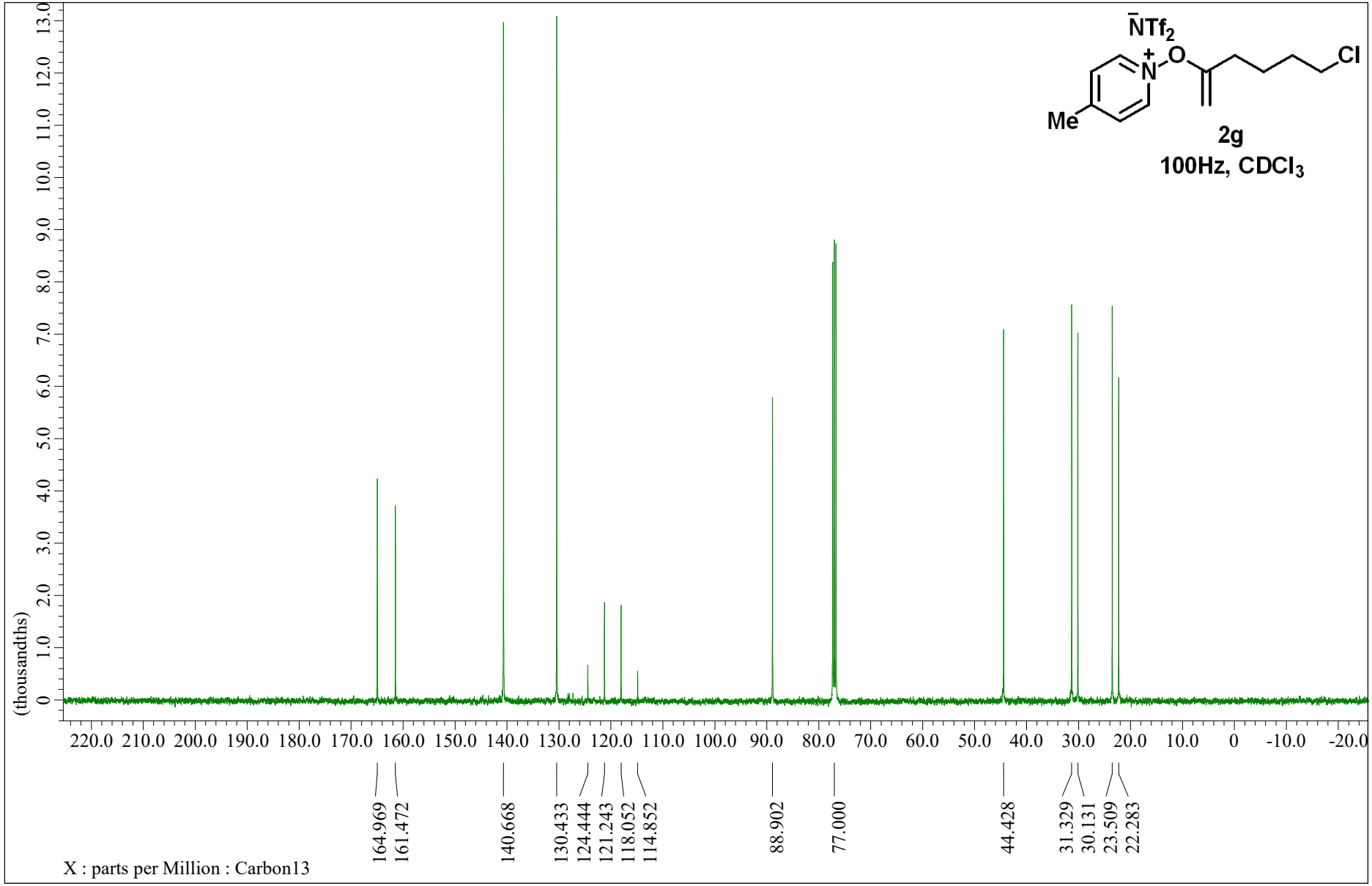
0.846
0.828
X : parts per Million : Proton

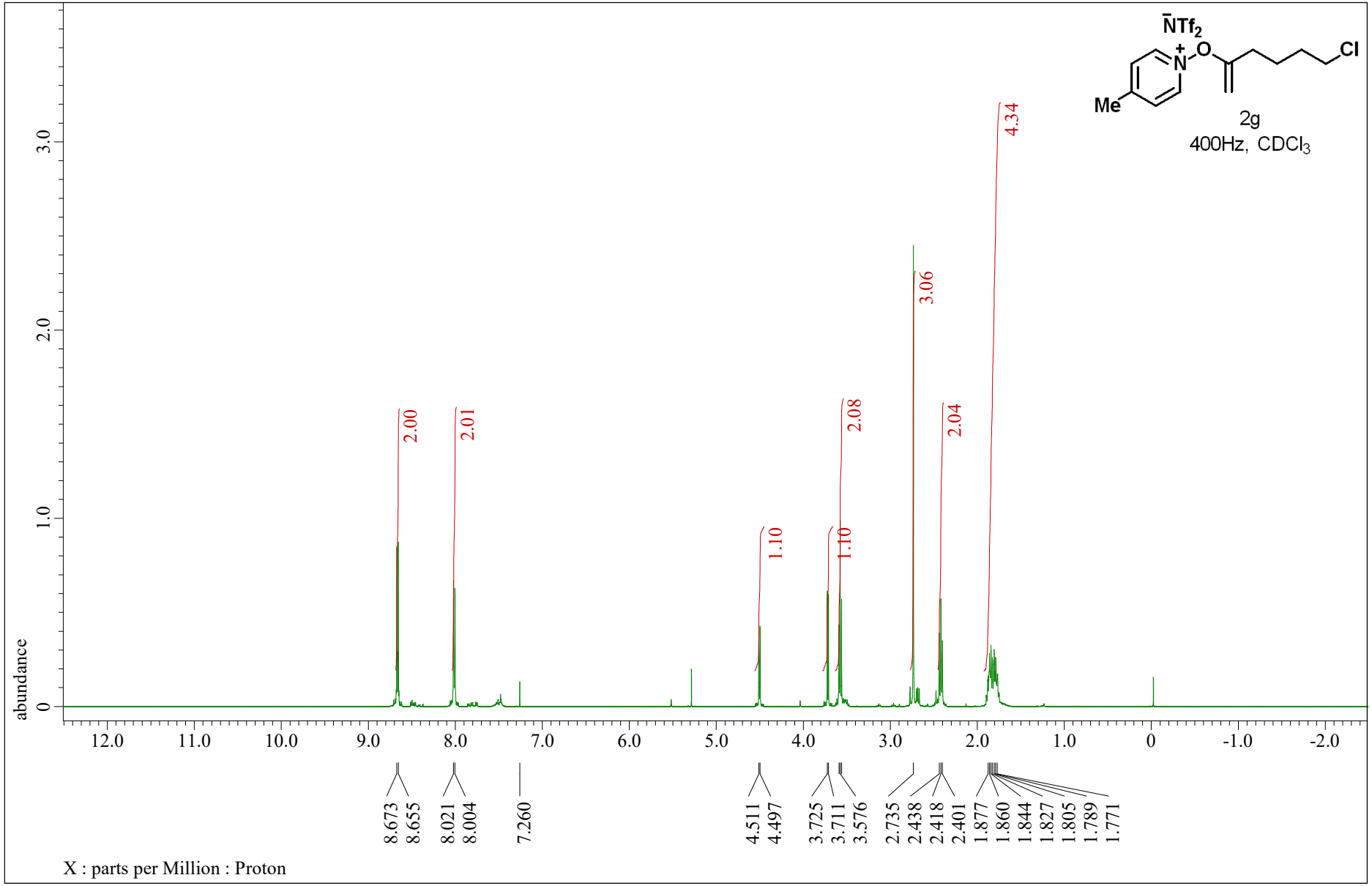

NTf2
O
N
CO2Me
Me
2e
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
173.479
164.500
161.548
140.725
130.462
124.463
121.263
118.072
114.871
89.084
77.000
51.635
32.594
30.457
22.321
21.324
X : parts per Million : Carbon13

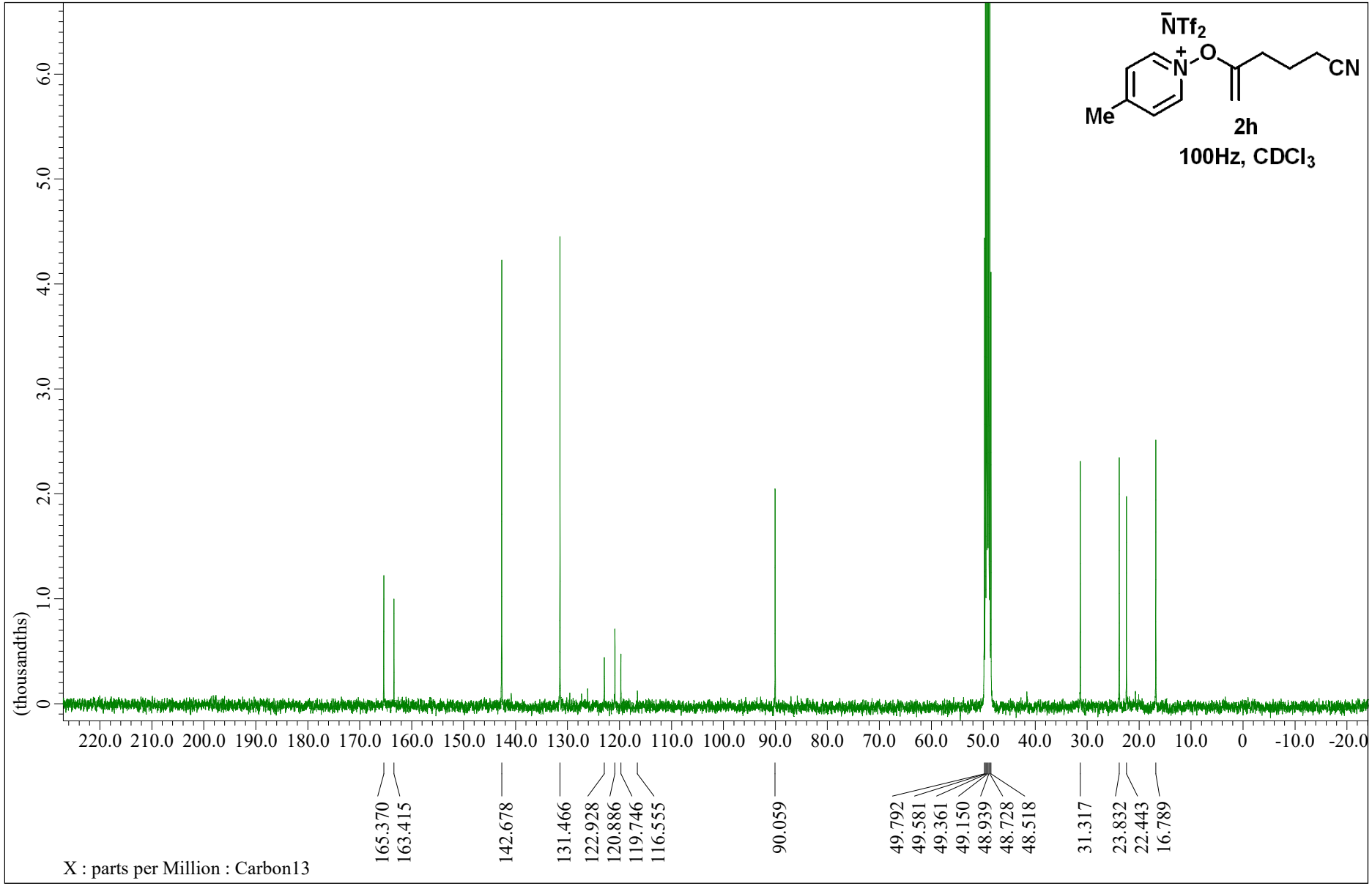

NTf2
N
O
CO2Me
Me
2e
400Hz, CDCl3
abundance
2.01
2.00
1.01
1.01
3.00
3.02
4.00
2.00
8.714
8.697
8.022
8.005
7.260
4.491
4.478
3.714
3.701
3.643
2.733
2.451
2.433
2.416
2.399
1.991
1.973
1.955
1.936
1.918
X : parts per Million : Proton

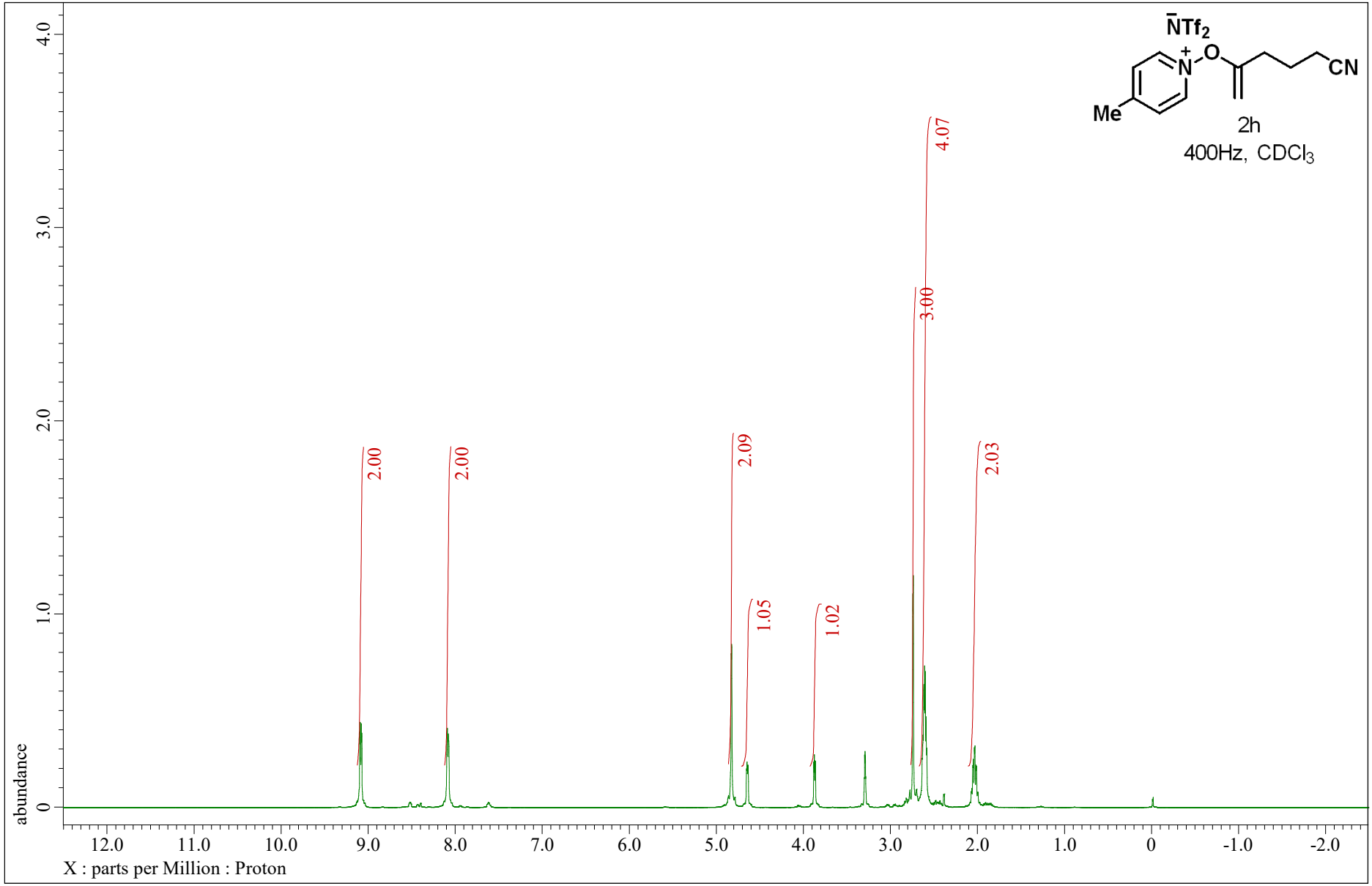

NTf2
N
O
Cl
Me
2f
100Hz, CDCl3
(thousandths)
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.858
161.453
140.543
130.270
124.300
121.109
117.909
114.718
89.199
77.000
43.499
28.808
28.051
22.110
X : parts per Million : Carbon13

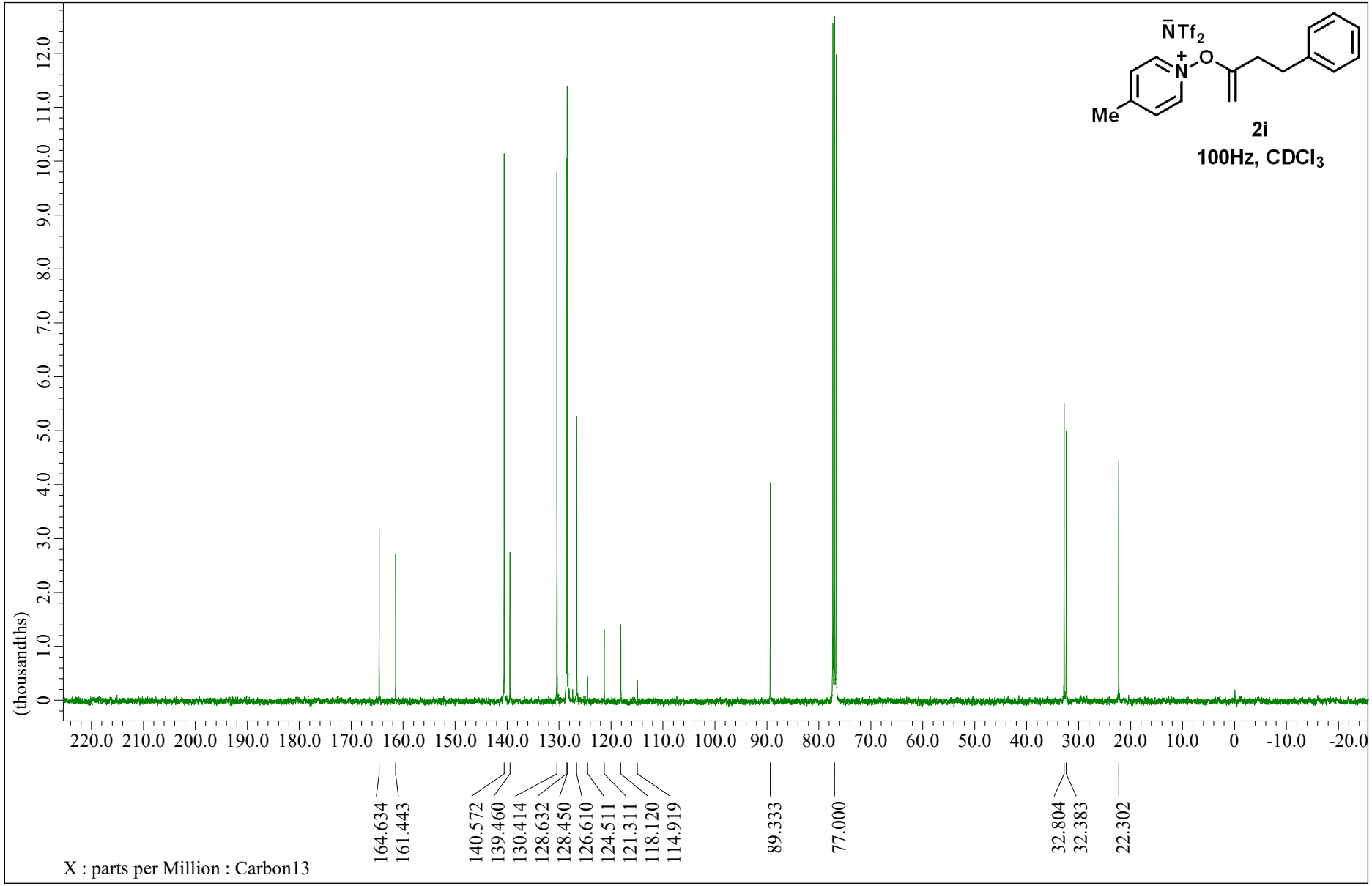

NTf2
N
O
Cl
Me
2f
400Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
2.06
2.14
1.00
1.00
2.00
3.01
2.01
2.14
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.686
8.674
8.003
7.990
7.260
4.537
4.523
3.637
3.621
3.606
2.726
2.586
2.568
2.550
2.125
2.109
2.091
2.074
2.058
X : parts per Million : Proton

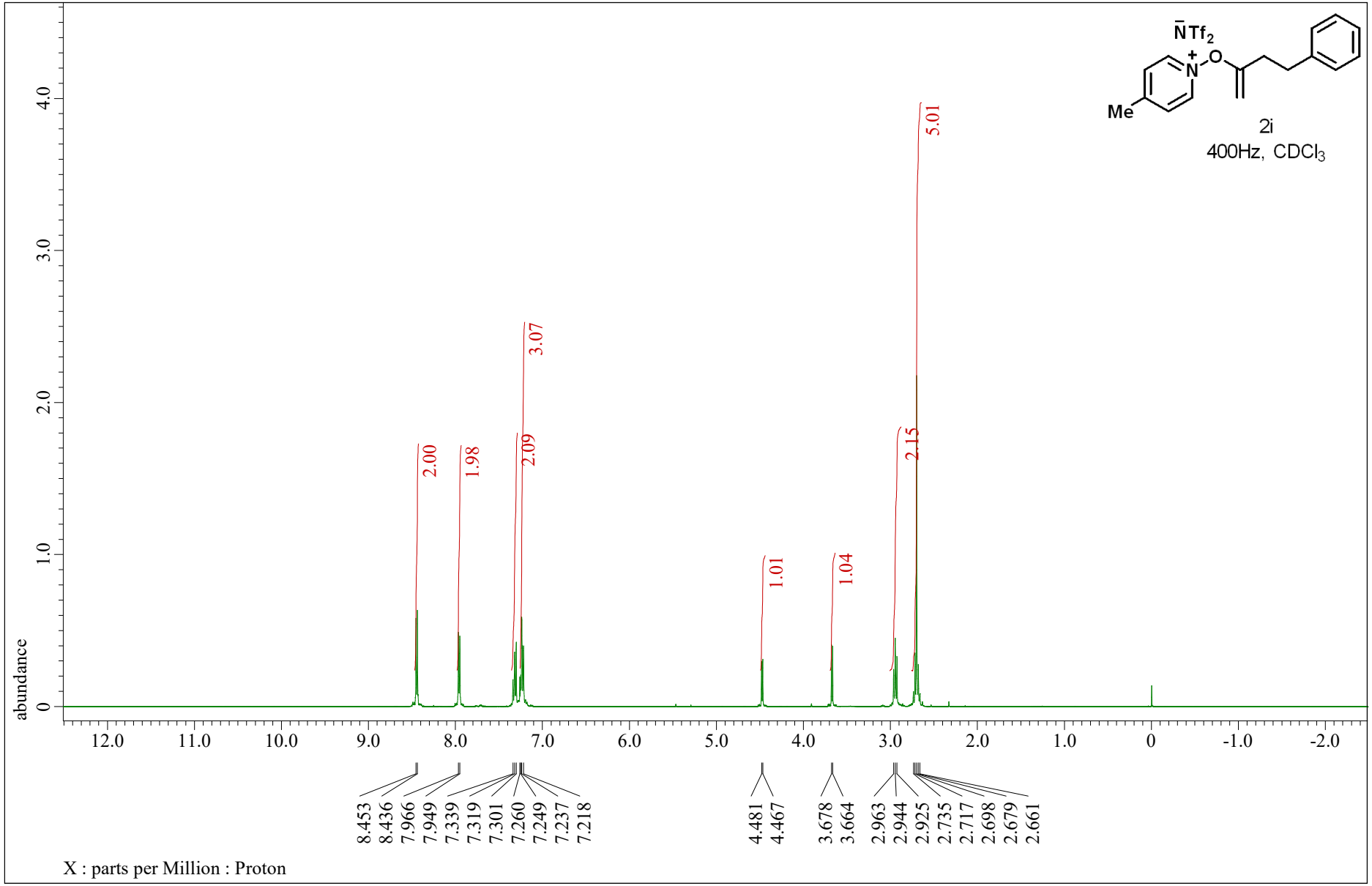

NTf2
N
O
Cl
Me
2g
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
164.969
161.472
140.668
130.433
124.444
121.243
118.052
114.852
88.902
77.000
44.428
31.329
30.131
23.509
22.283
X : parts per Million : Carbon13

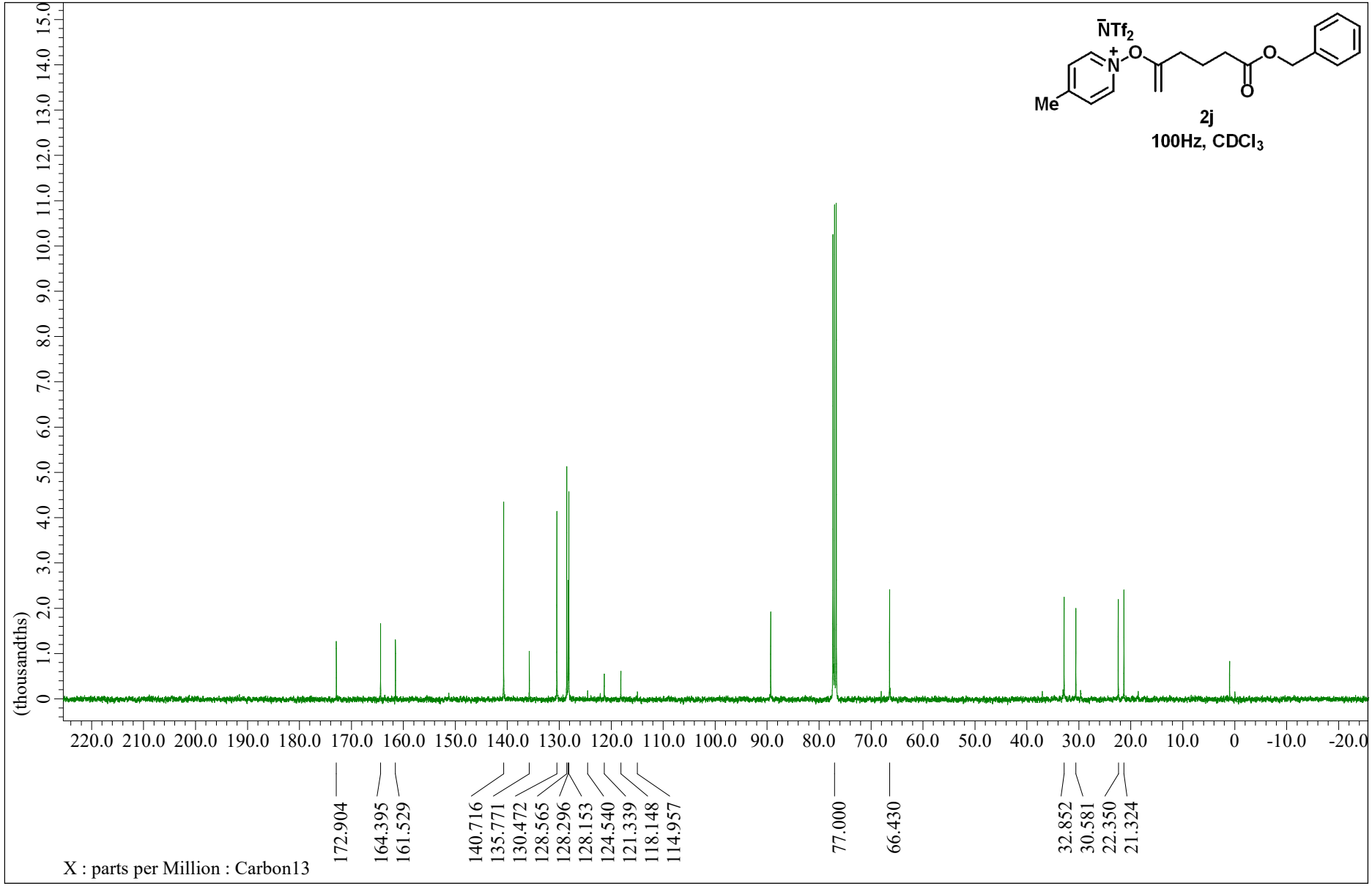

NTf2
O
N
Cl
Me
2g
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.01
1.10
2.08
1.10
3.06
2.04
4.34
8.673
8.655
8.021
8.004
7.260
4.511
4.497
3.725
3.711
3.576
2.735
2.438
2.418
2.401
1.877
1.860
1.844
1.827
1.805
1.789
1.771

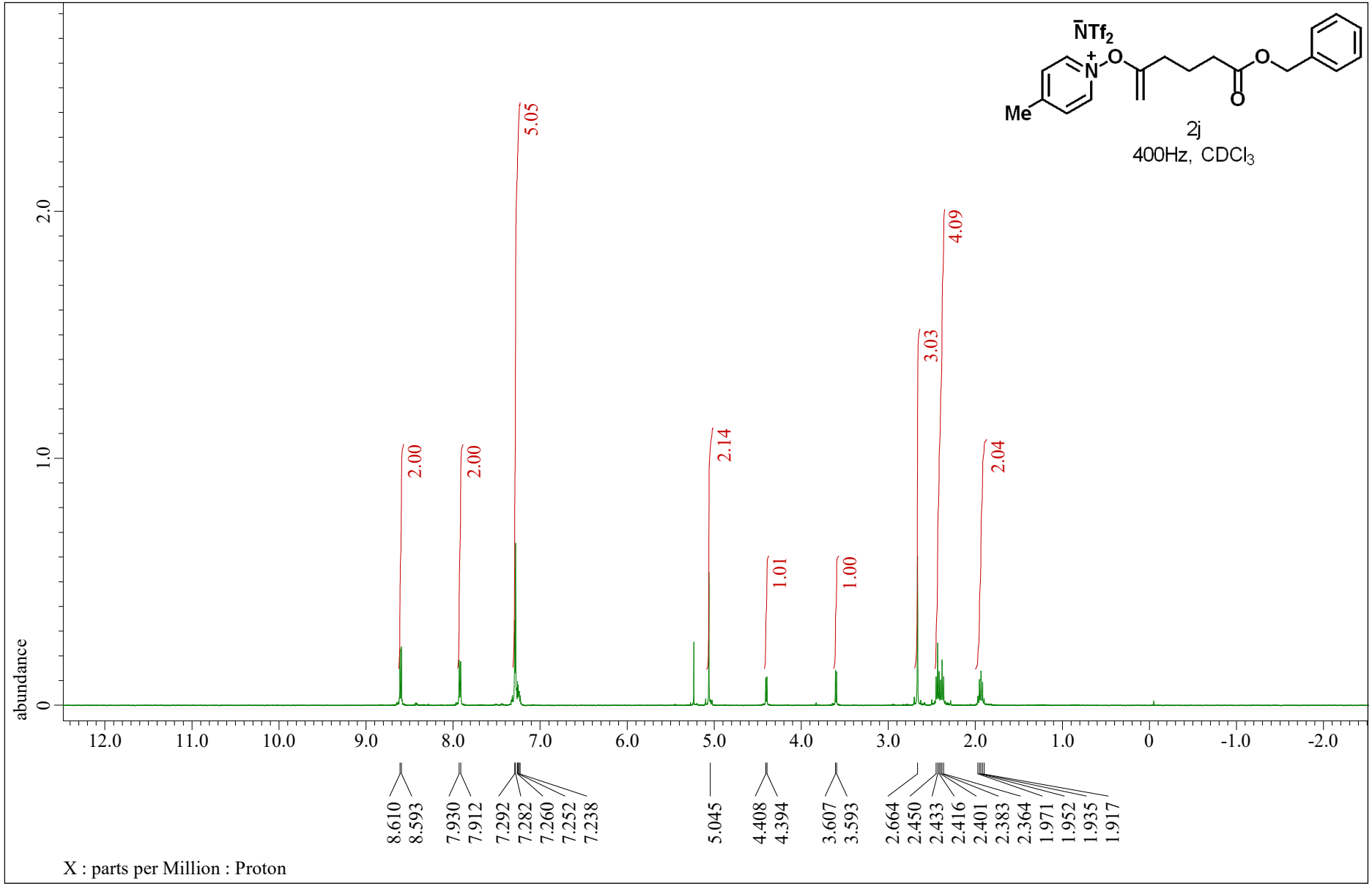

$\bar{N}Tf_2$
Me
CN
2h
100Hz, $CDCl_3$
(thousandths)
6.0
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.370
163.415
142.678
131.466
122.928
120.886
119.746
116.555
90.059
49.792
49.581
49.361
49.150
48.939
48.728
48.518
31.317
23.832
22.443
16.789
X : parts per Million : Carbon13

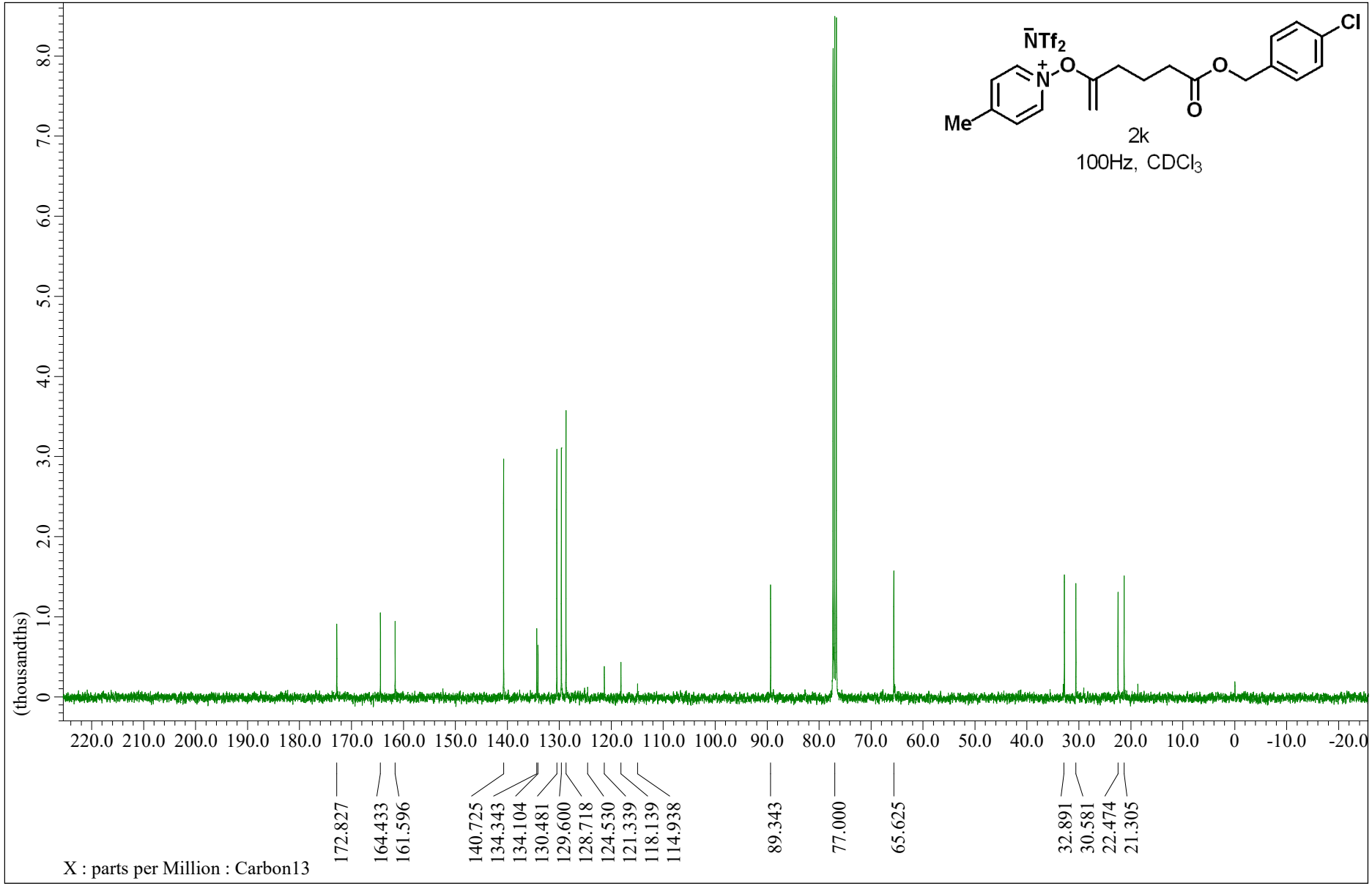

NTf2
N
O
CN
Me
2h
400Hz, CDCl3
4.07
3.00
2.09
2.00
2.00
2.03
1.05
1.02
abundance
X : parts per Million : Proton

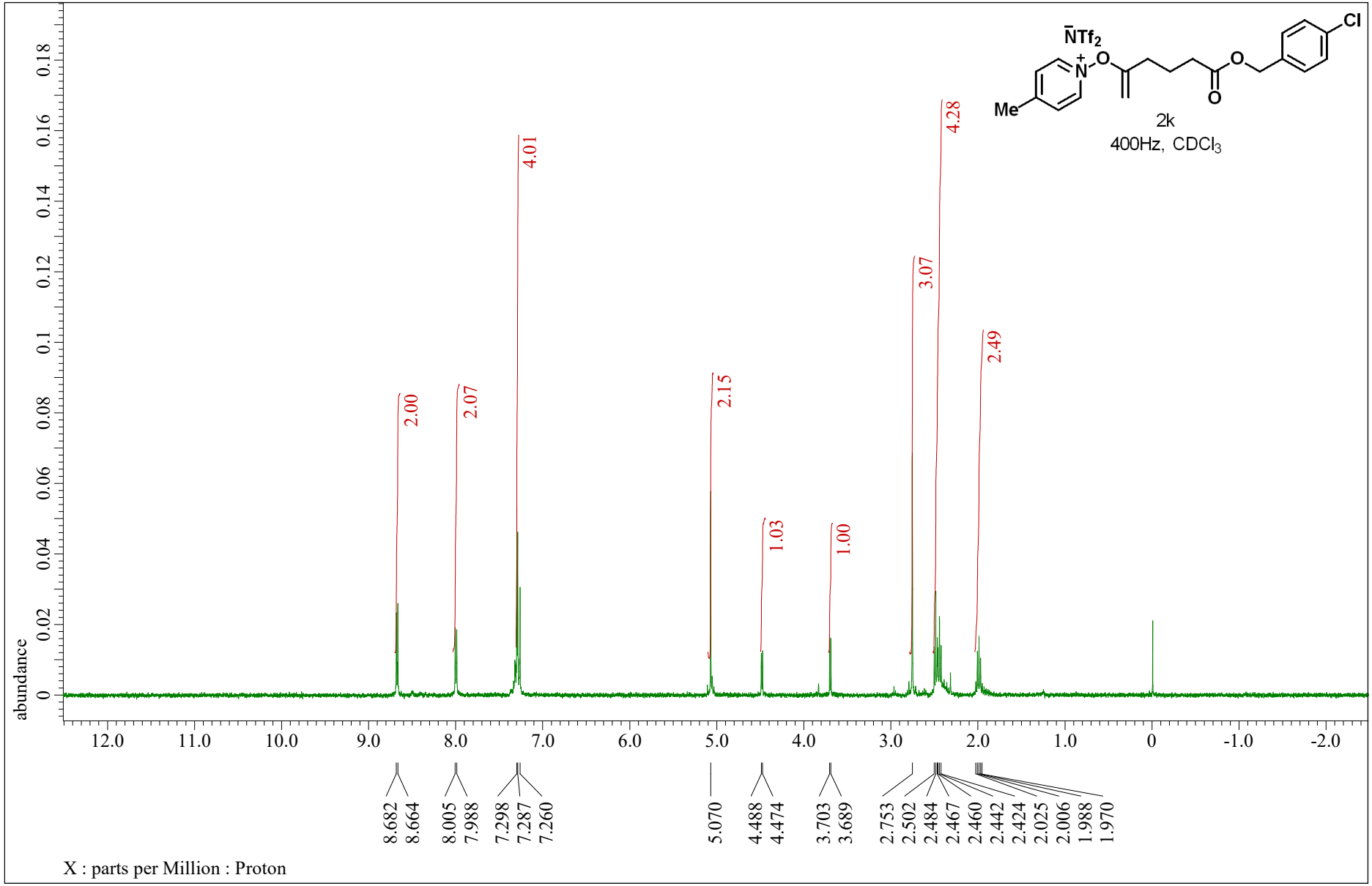

(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
164.634
161.443
140.572
139.460
130.414
128.632
128.450
126.610
124.511
121.311
118.120
114.919
89.333
77.000
32.804
32.383
22.302
X : parts per Million : Carbon13
NTf2
O
N
Me
2i
100Hz, CDCl3

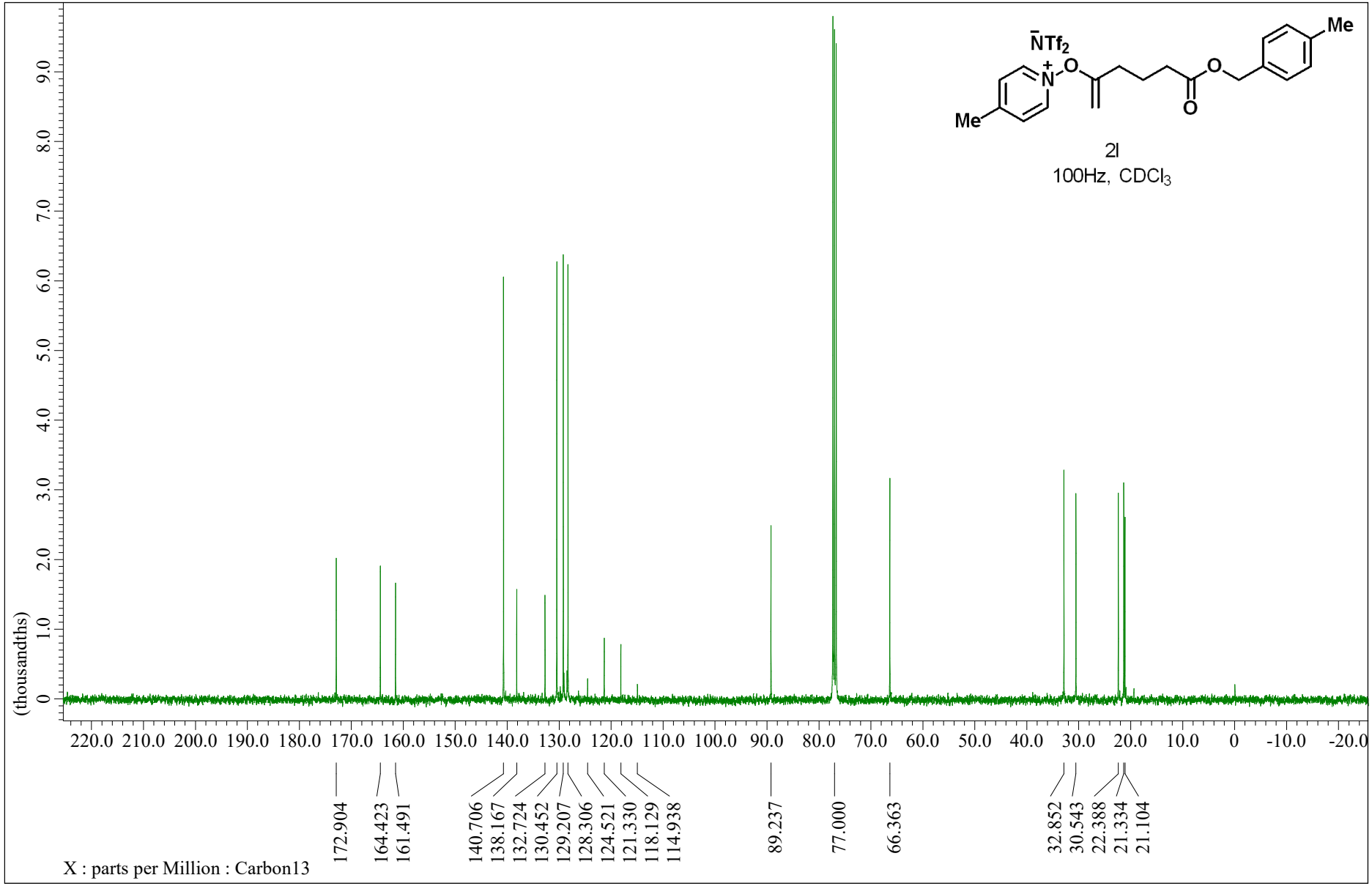

NTf2
Me
2i
400Hz, CDCl3
abundance
X : parts per Million : Proton
5.01
3.07
2.15
2.09
2.00
1.98
1.01
1.04
8.453
8.436
7.966
7.949
7.339
7.319
7.301
7.260
7.249
7.237
7.218
4.481
4.467
3.678
3.664
2.963
2.944
2.925
2.735
2.717
2.698
2.679
2.661

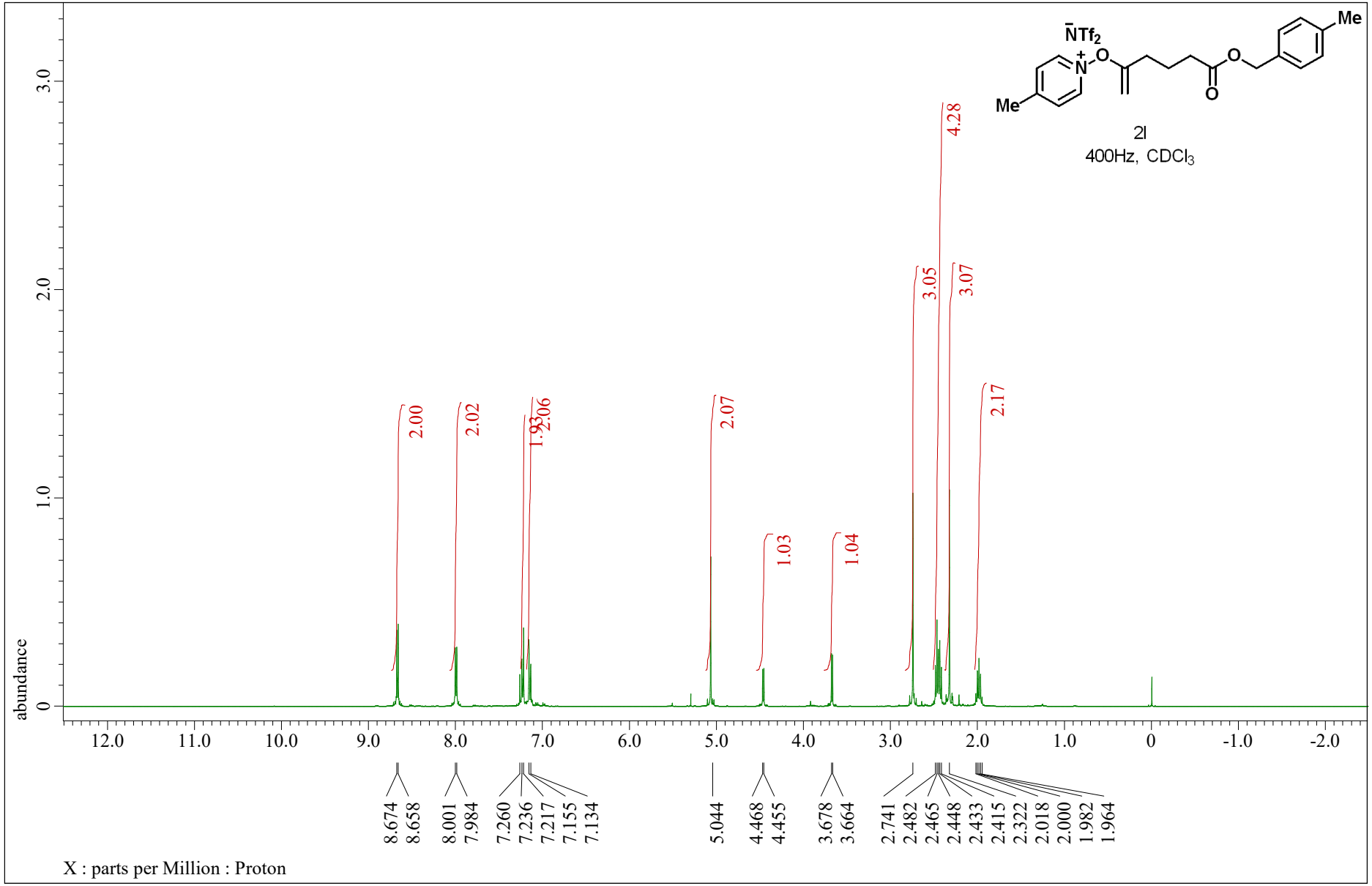

NTf2
N+
O
O
O
Me
2j
100Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
172.904
164.395
161.529
140.716
135.771
130.472
128.565
128.296
128.153
124.540
121.339
118.148
114.957
77.000
66.430
32.852
30.581
22.350
21.324
X : parts per Million : Carbon13

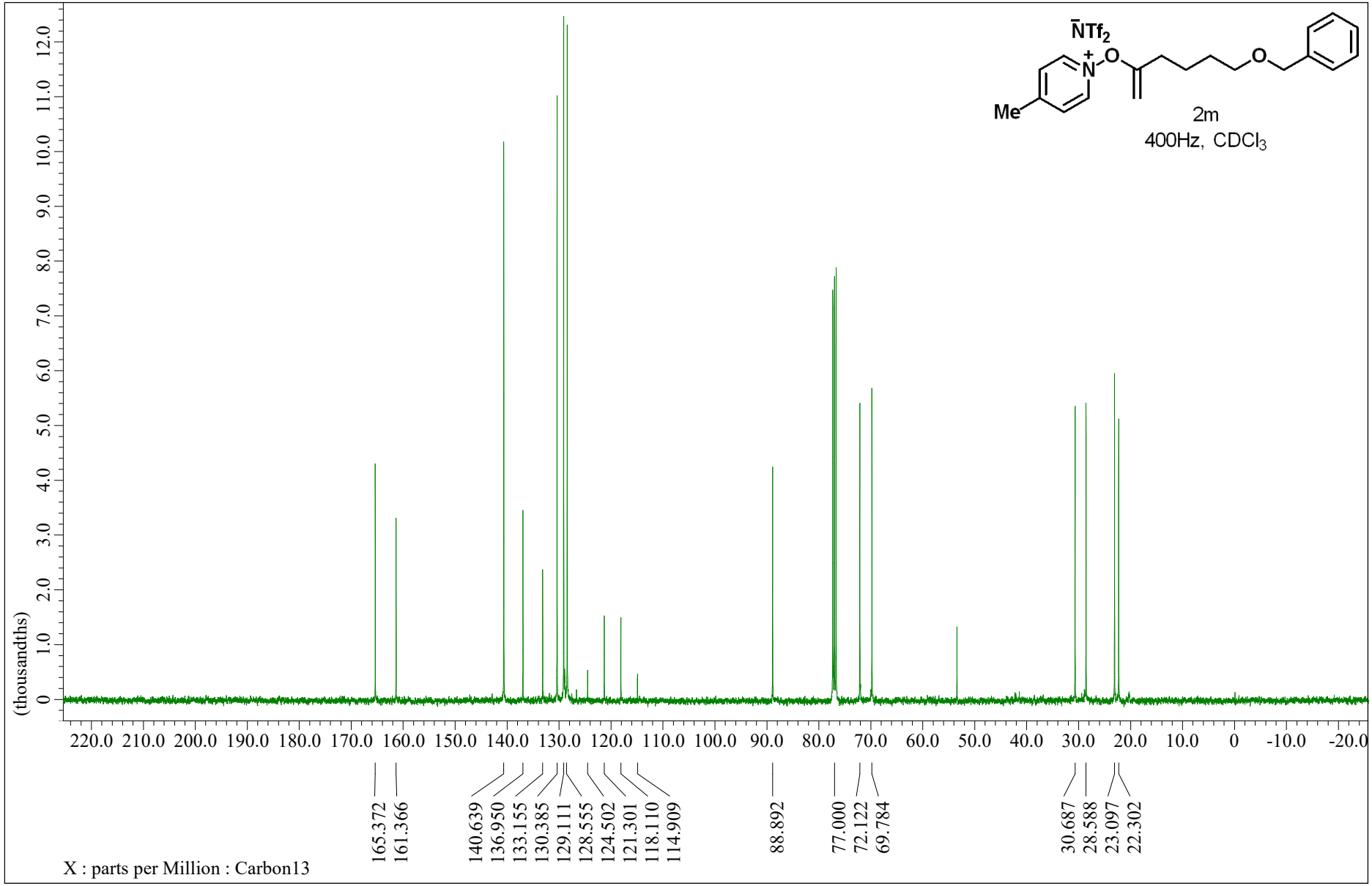

$\bar{N}Tf_2$
Me
2j
400Hz, $CDCl_3$
abundance
2.00
2.00
5.05
2.14
1.01
1.00
3.03
4.09
2.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.610
8.593
7.930
7.912
7.292
7.282
7.260
7.252
7.238
5.045
4.408
4.394
3.607
3.593
2.664
2.450
2.433
2.416
2.401
2.383
2.364
1.971
1.952
1.935
1.917
X : parts per Million : Proton

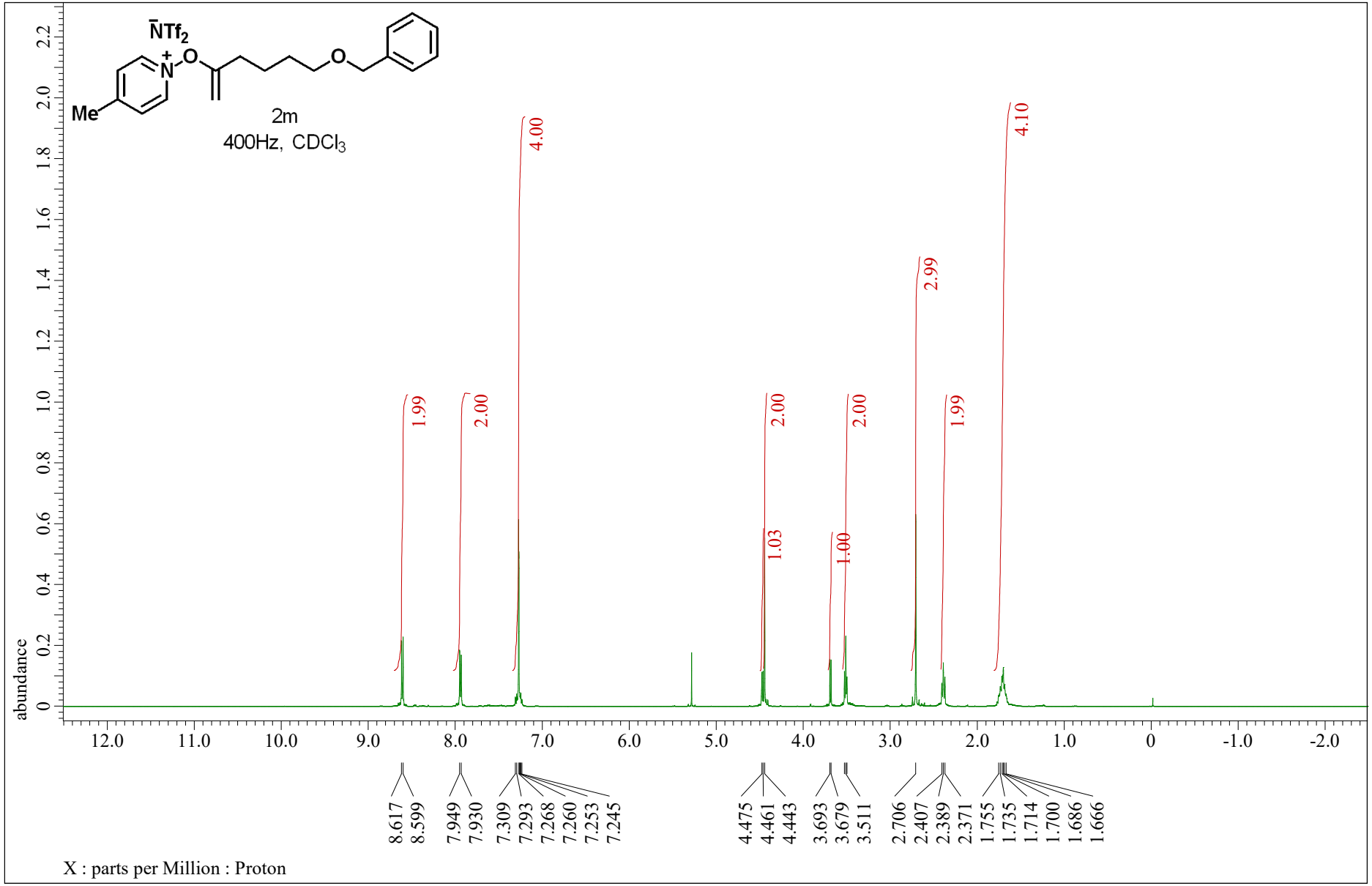

NTf2
Me
Cl
2k
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
172.827
164.433
161.596
140.725
134.343
134.104
130.481
129.600
128.718
124.530
121.339
118.139
114.938
89.343
77.000
65.625
32.891
30.581
22.474
21.305

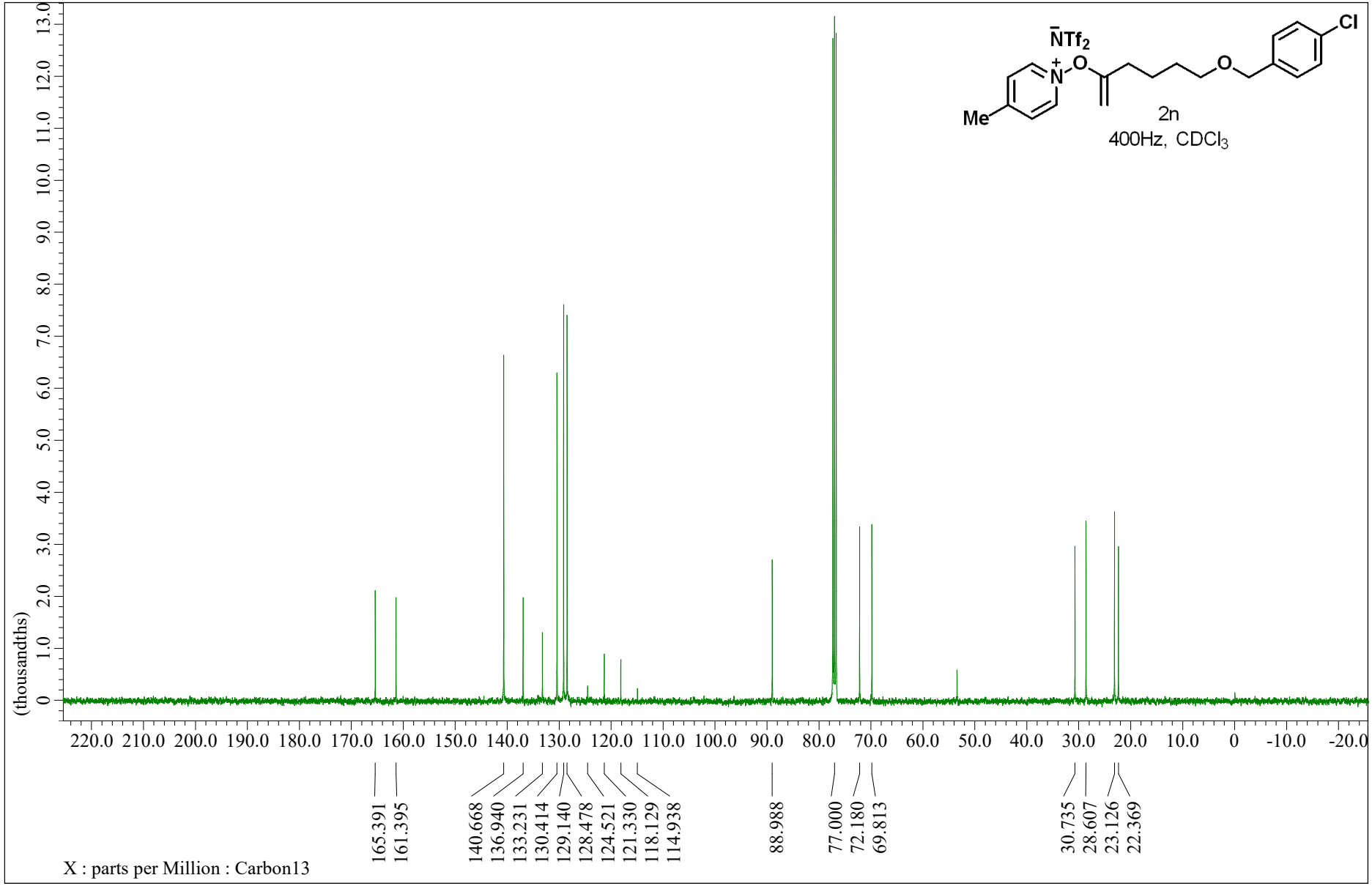

abundance
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
2.00
2.07
4.01
2.15
1.03
1.00
3.07
4.28
2.49
8.682
8.664
8.005
7.988
7.298
7.287
7.260
5.070
4.488
4.474
3.703
3.689
2.753
2.502
2.484
2.467
2.460
2.442
2.424
2.025
2.006
1.988
1.970
X : parts per Million : Proton
NTf2
O
N
O
O
O
Me
Cl
2k
400Hz, CDCl3

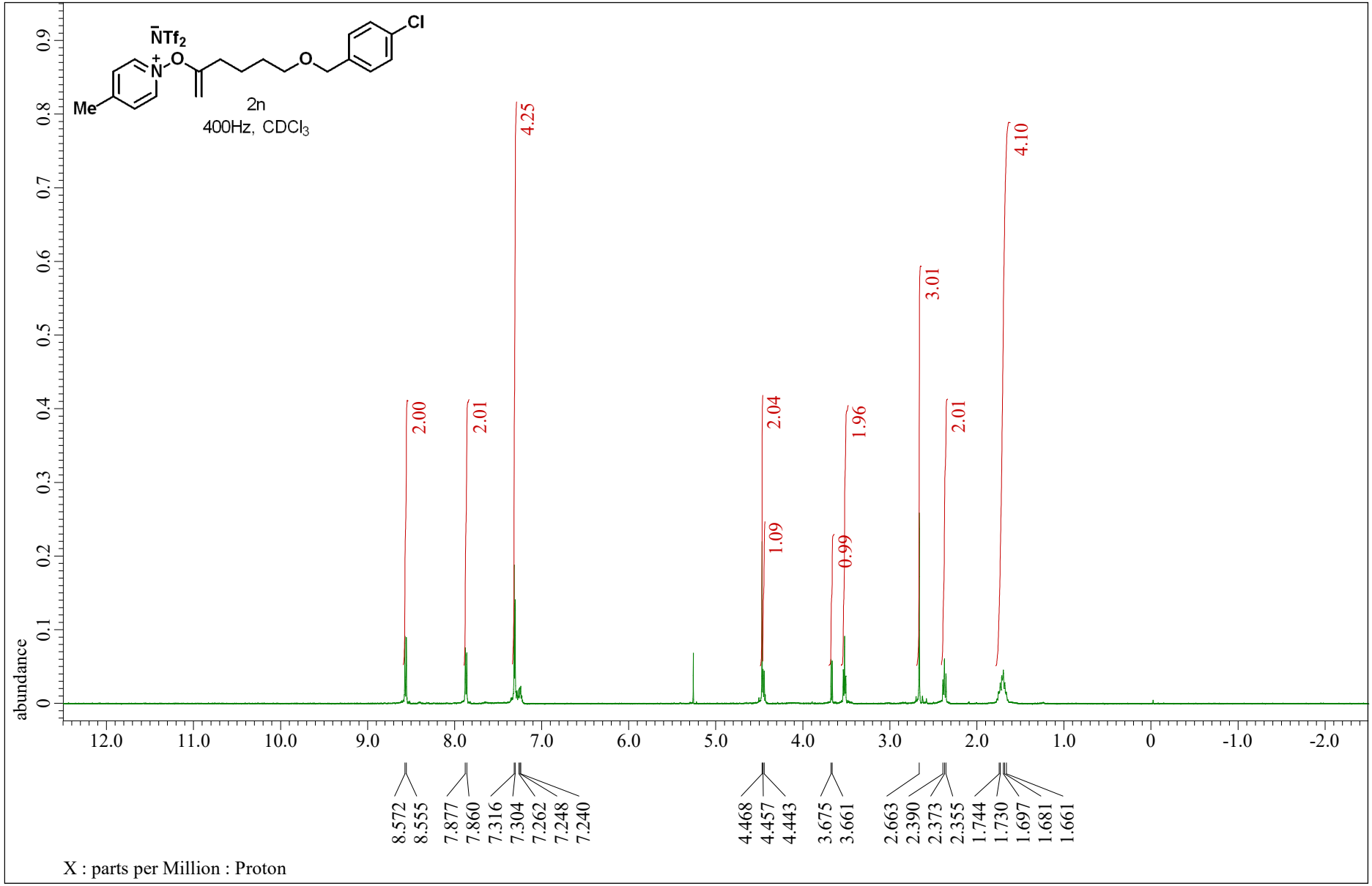

NTf2
Me
Me
2l
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
172.904
164.423
161.491
140.706
138.167
132.724
130.452
129.207
128.306
124.521
121.330
118.129
114.938
89.237
77.000
66.363
32.852
30.543
22.388
21.334
21.104
X : parts per Million : Carbon13

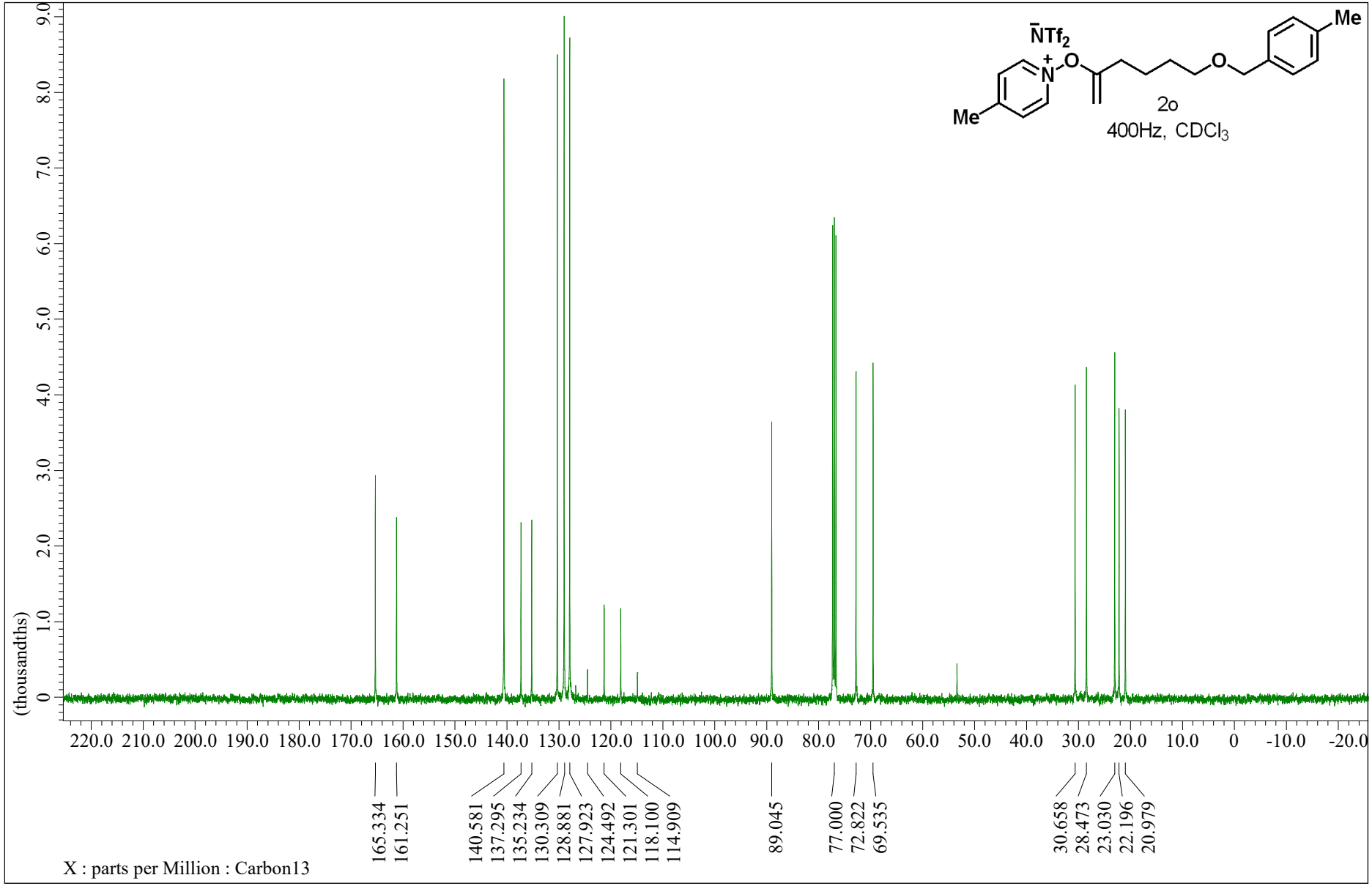

NTf2
Me
Me
2l
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.02
1.93
2.06
2.07
1.03
1.04
3.05
4.28
3.07
2.17
8.674
8.658
8.001
7.984
7.260
7.236
7.217
7.155
7.134
5.044
4.468
4.455
3.678
3.664
2.741
2.482
2.465
2.448
2.433
2.415
2.322
2.018
2.000
1.982
1.964

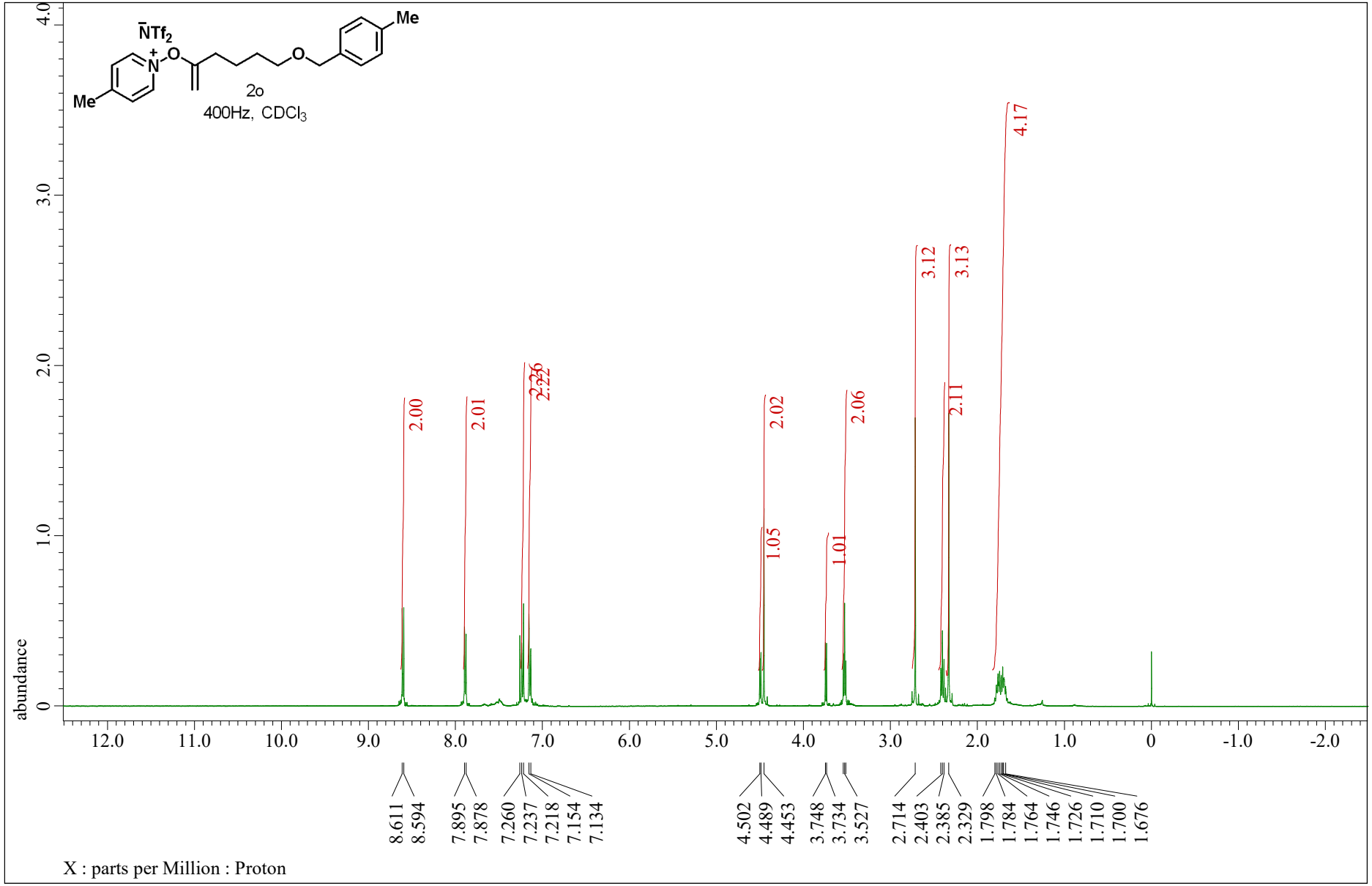

NTf2
Me
2m
400Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.372
161.366
140.639
136.950
133.155
130.385
129.111
128.555
124.502
121.301
118.110
114.909
88.892
77.000
72.122
69.784
30.687
28.588
23.097
22.302
X : parts per Million : Carbon13

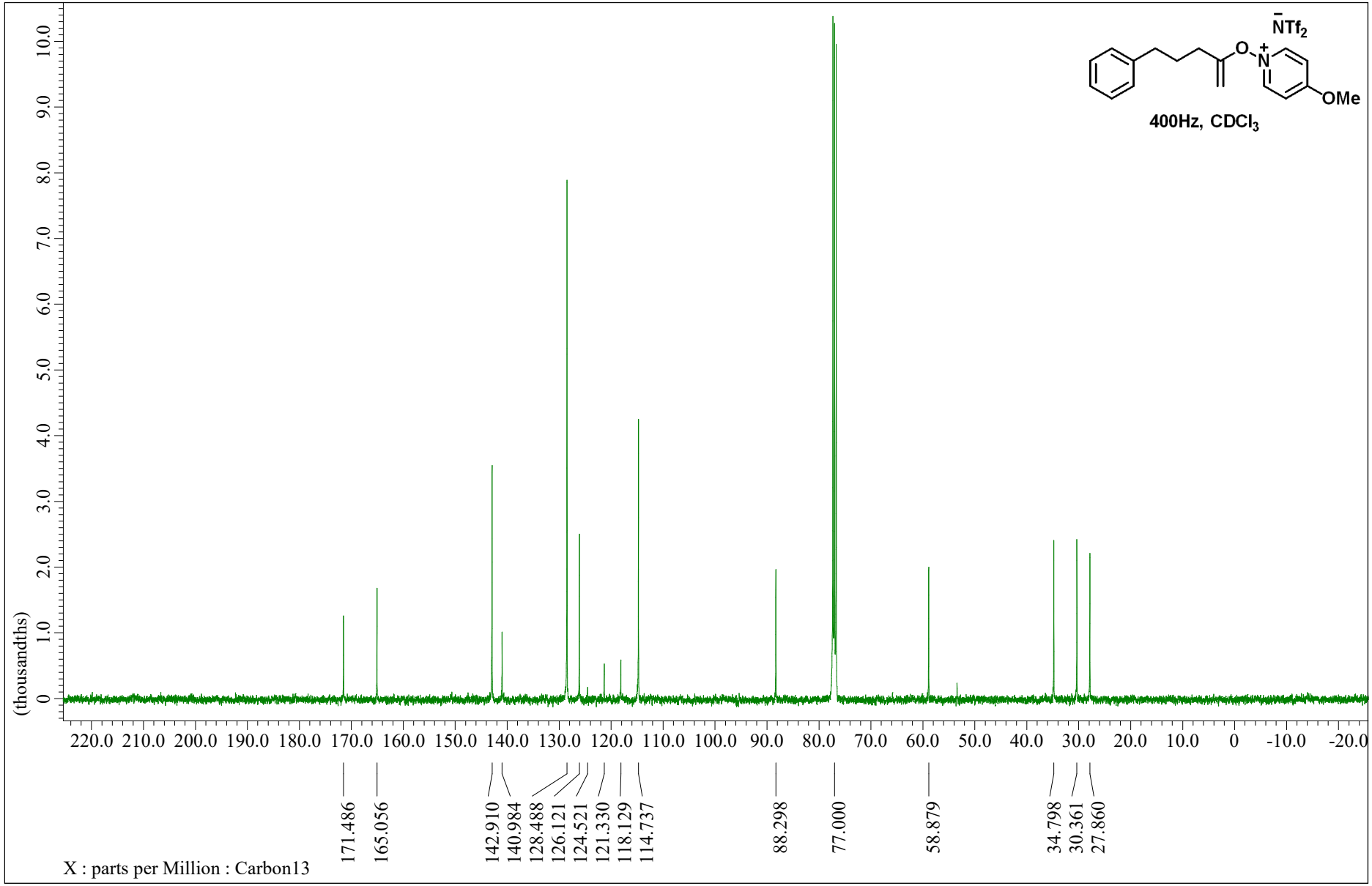

NTf2
Me
2m
400Hz, CDCl3
abundance
X : parts per Million : Proton
1.99
2.00
4.00
1.03
2.00
1.00
2.00
2.99
1.99
4.10
8.617
8.599
7.949
7.930
7.309
7.293
7.268
7.260
7.253
7.245
4.475
4.461
4.443
3.693
3.679
3.511
2.706
2.407
2.389
2.371
1.755
1.735
1.714
1.700
1.686
1.666

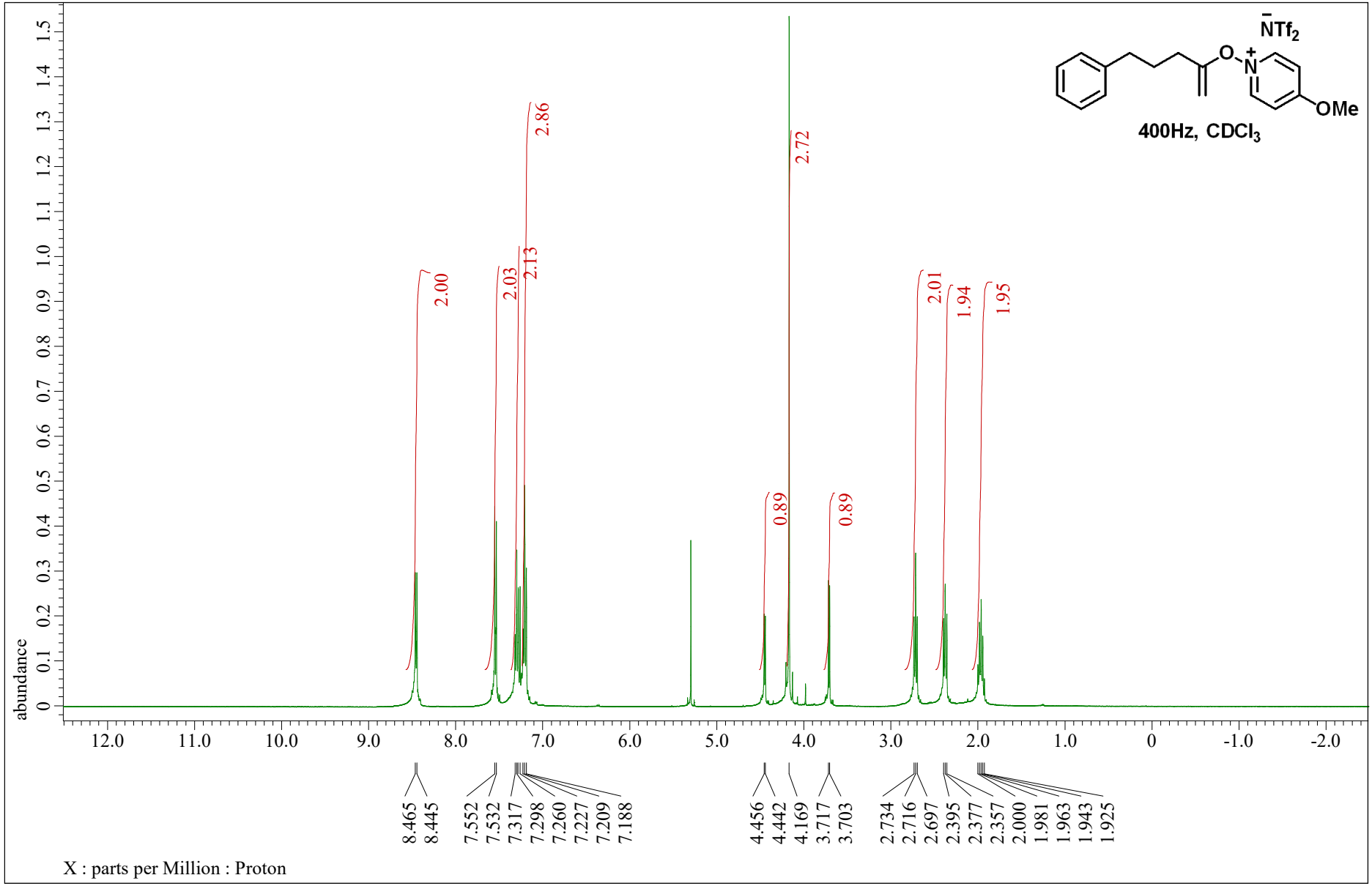

NTf2
Cl
Me
2n
400Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
165.391
161.395
140.668
136.940
133.231
130.414
129.140
128.478
124.521
121.330
118.129
114.938
88.988
77.000
72.180
69.813
30.735
28.607
23.126
22.369

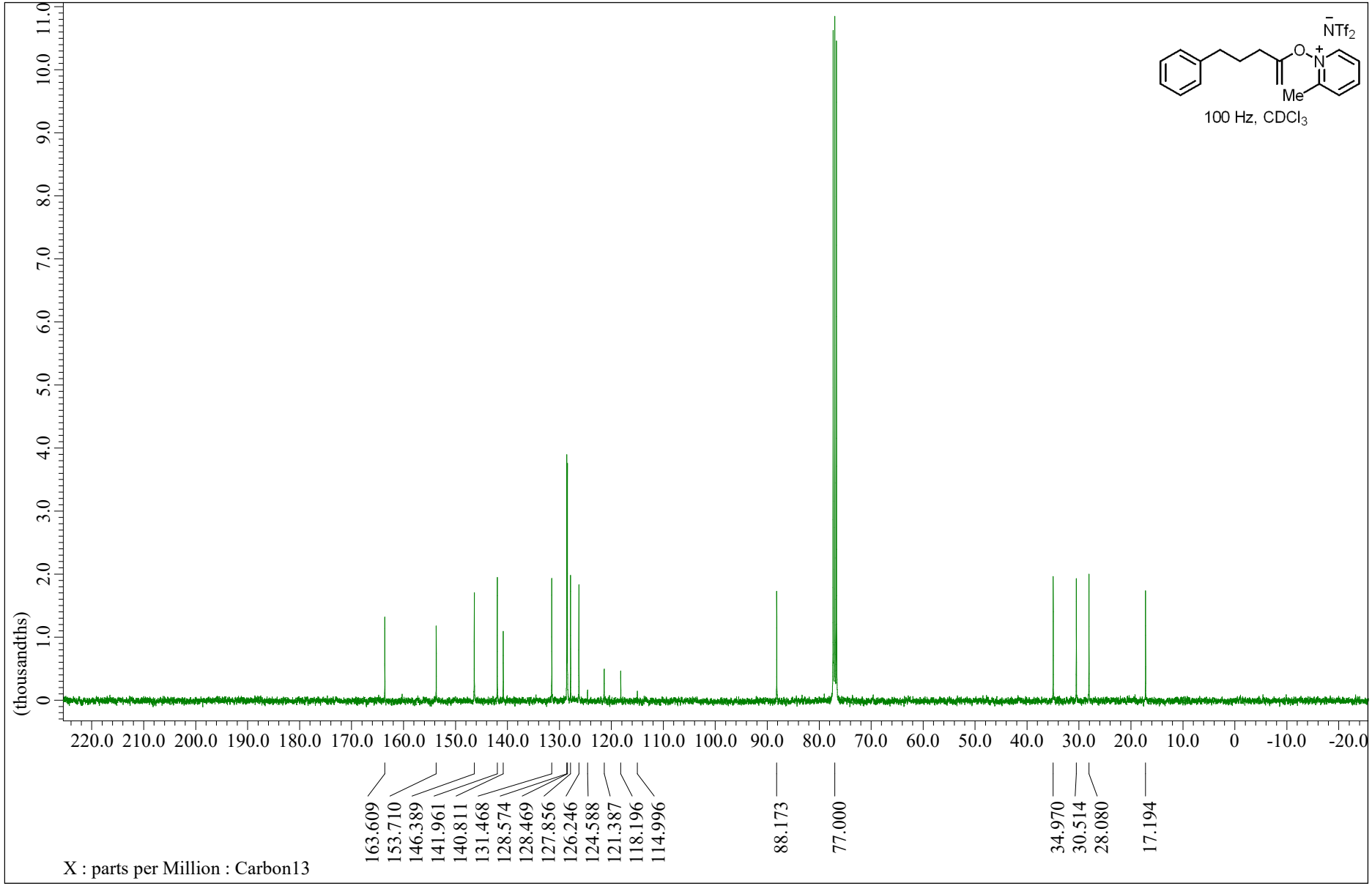

NTf2
Cl
Me
2n
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.01
4.25
2.04
1.09
0.99
1.96
3.01
2.01
4.10
8.572
8.555
7.877
7.860
7.316
7.304
7.262
7.248
7.240
4.468
4.457
4.443
3.675
3.661
2.663
2.390
2.373
2.355
1.744
1.730
1.697
1.681
1.661

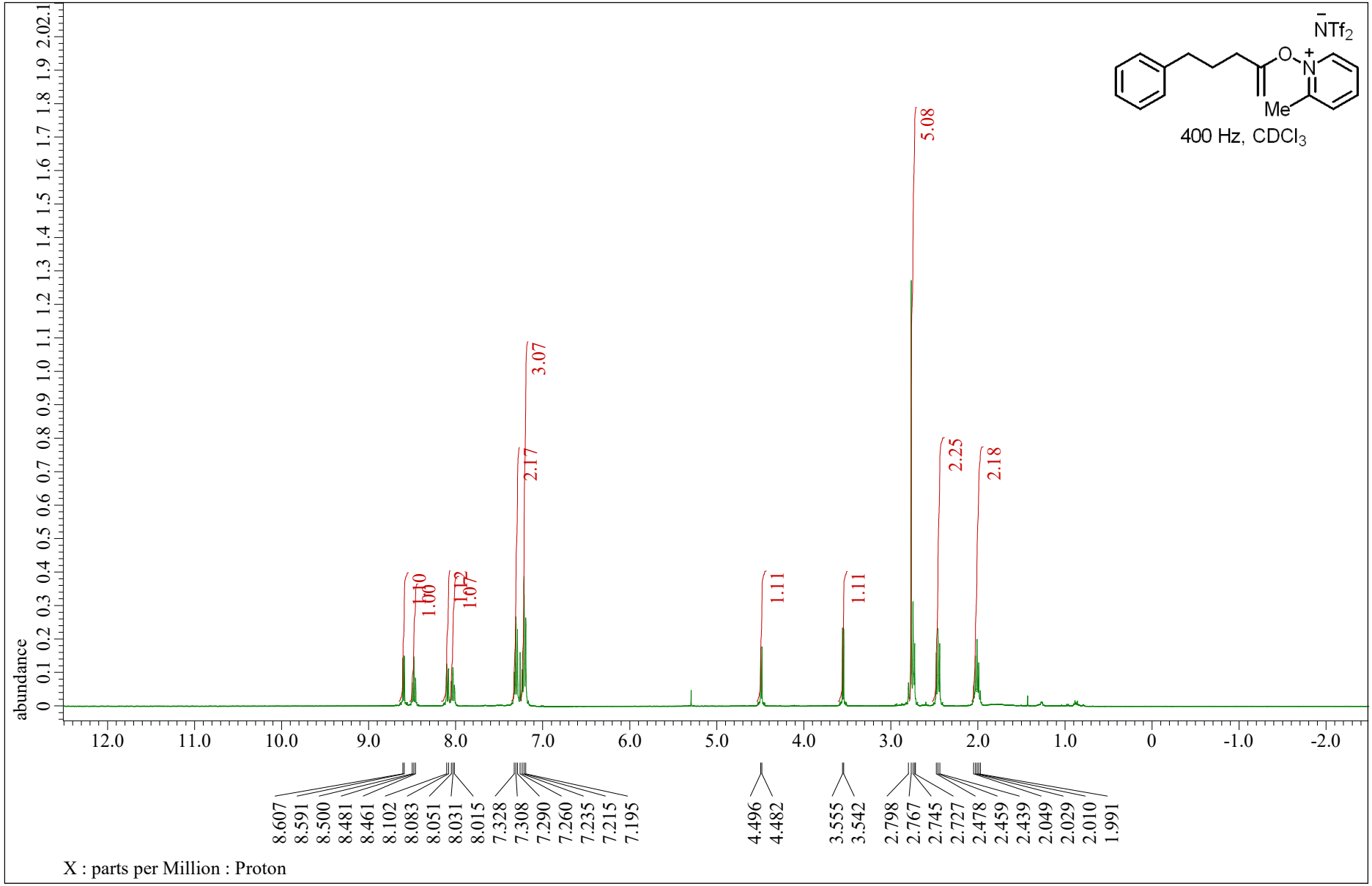

NTf2
Me
Me
2o
400Hz, CDCl3
(thousandths)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.334
161.251
140.581
137.295
135.234
130.309
128.881
127.923
124.492
121.301
118.100
114.909
89.045
77.000
72.822
69.535
30.658
28.473
23.030
22.196
20.979
X : parts per Million : Carbon13

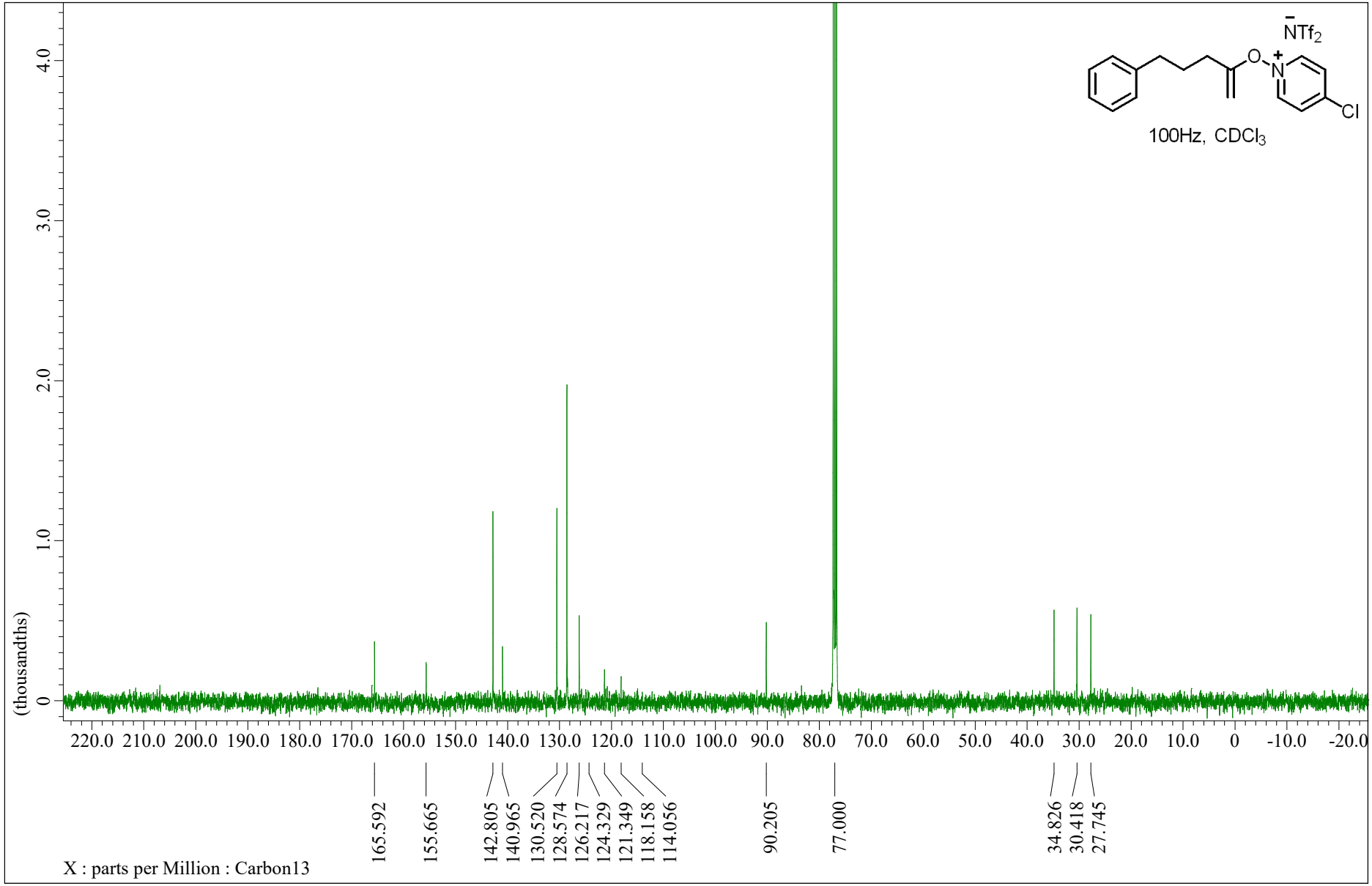

NTf2
Me
Me
2o
400Hz, CDCl3
abundance
4.0
3.0
2.0
1.0
0
2.00
2.01
2.26
2.22
2.02
1.05
2.06
1.01
3.12
3.13
2.11
4.17
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.611
8.594
7.895
7.878
7.260
7.237
7.218
7.154
7.134
4.502
4.489
4.453
3.748
3.734
3.527
2.714
2.403
2.385
2.329
1.798
1.784
1.764
1.746
1.726
1.710
1.700
1.676
X : parts per Million : Proton

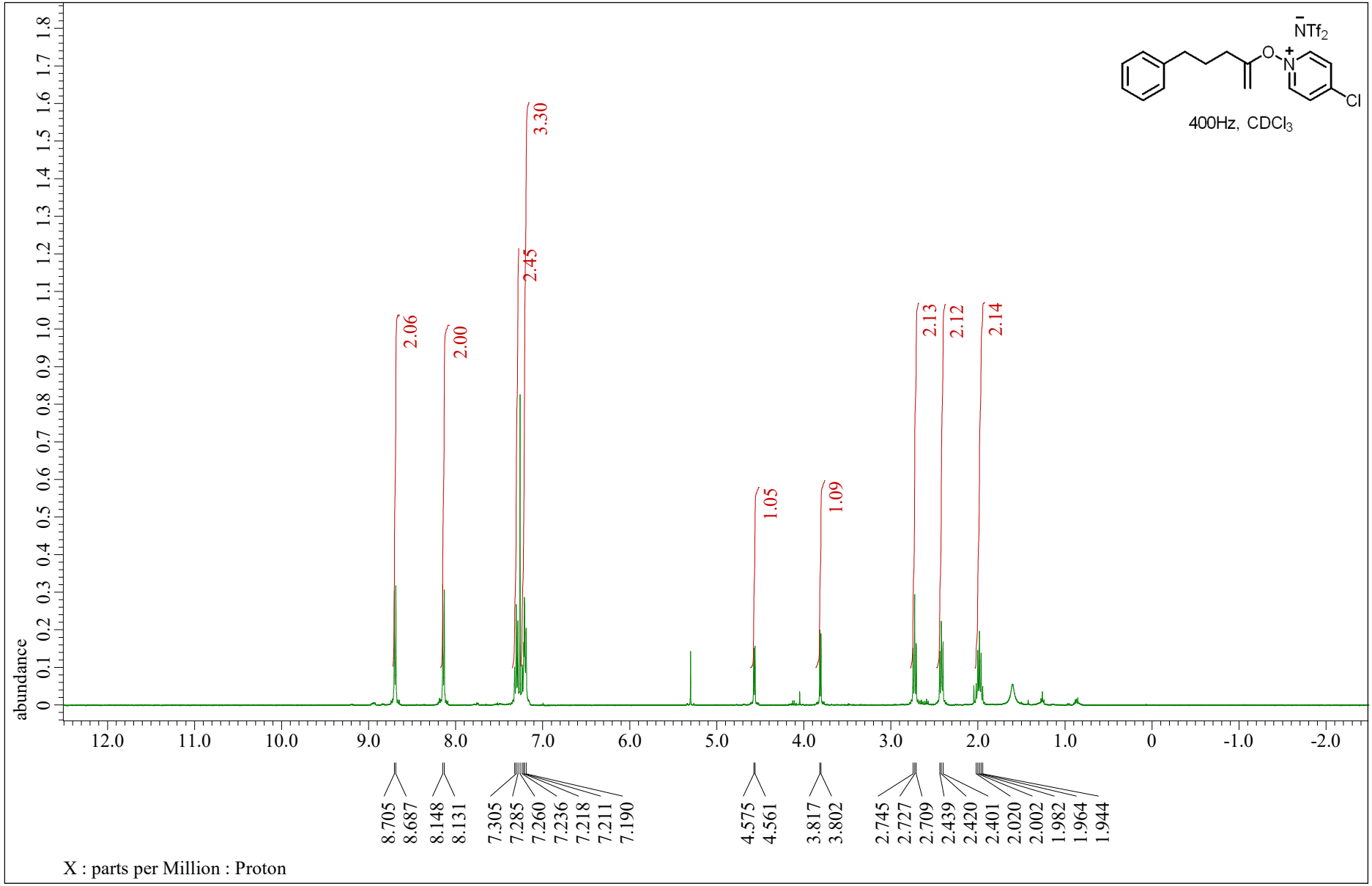

$\bar{N}Tf_2$
O
N
OMe
400Hz, $CDCl_3$
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
171.486
165.056
142.910
140.984
128.488
126.121
124.521
121.330
118.129
114.737
88.298
77.000
58.879
34.798
30.361
27.860
X : parts per Million : Carbon13

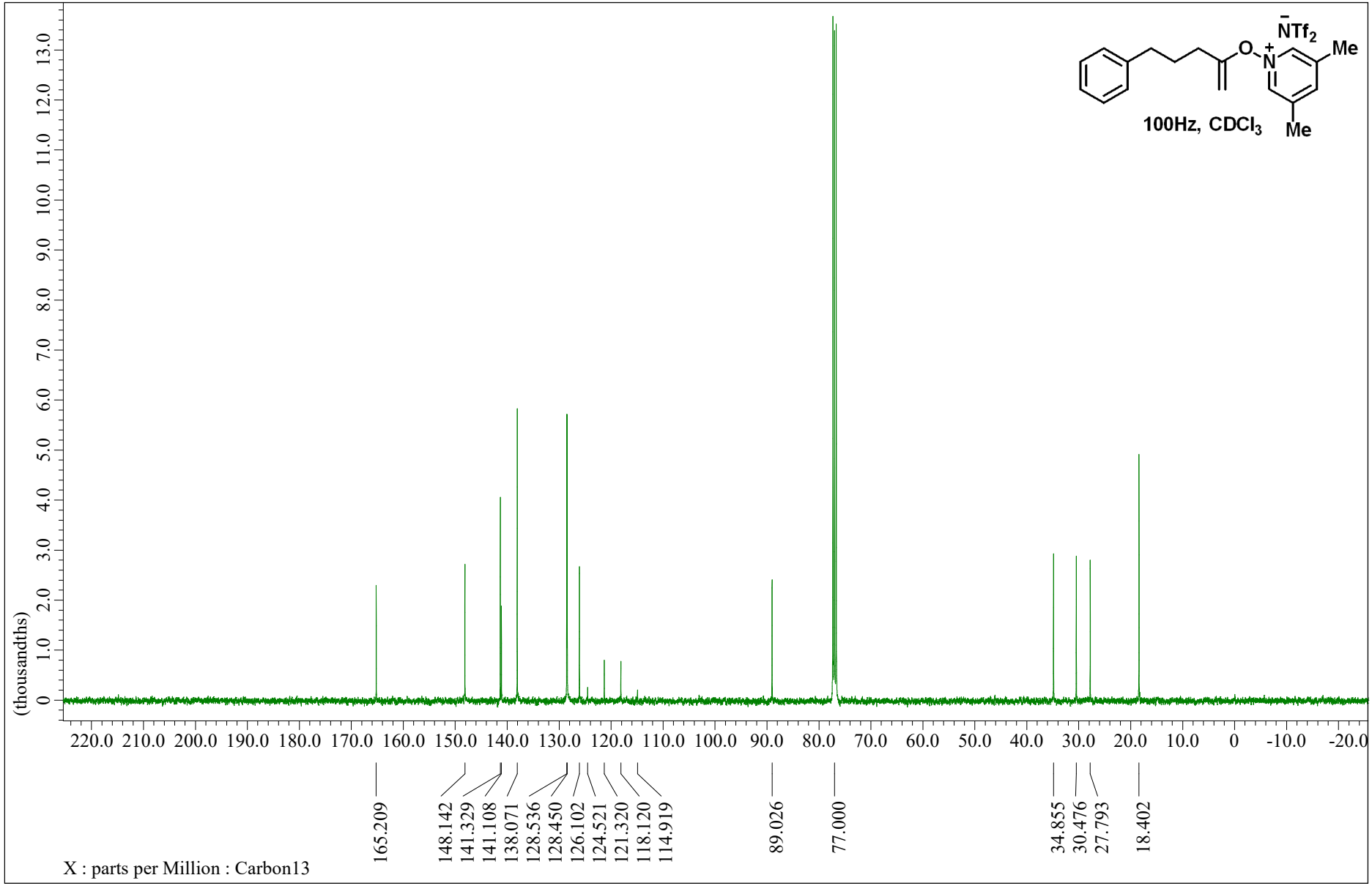

NTf2
OMe
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.03
2.13
2.86
2.72
0.89
0.89
2.01
1.94
1.95
8.465
8.445
7.552
7.532
7.317
7.298
7.260
7.227
7.209
7.188
4.456
4.442
4.169
3.717
3.703
2.734
2.716
2.697
2.395
2.377
2.357
2.000
1.981
1.963
1.943
1.925

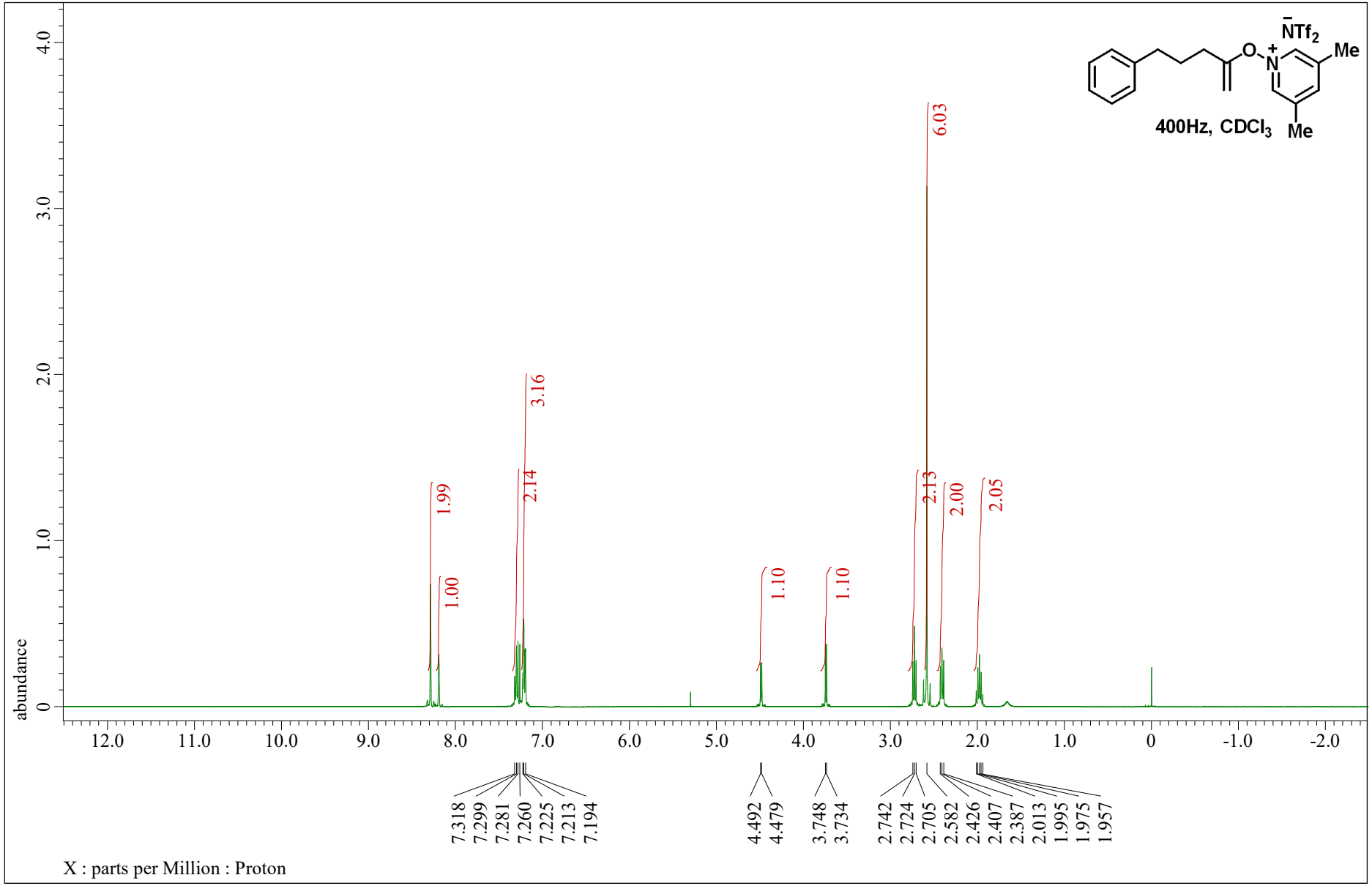

NTf2
O
N
Me
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
163.609
153.710
146.389
141.961
140.811
131.468
128.574
128.469
127.856
126.246
124.588
121.387
118.196
114.996
88.173
77.000
34.970
30.514
28.080
17.194
X : parts per Million : Carbon13

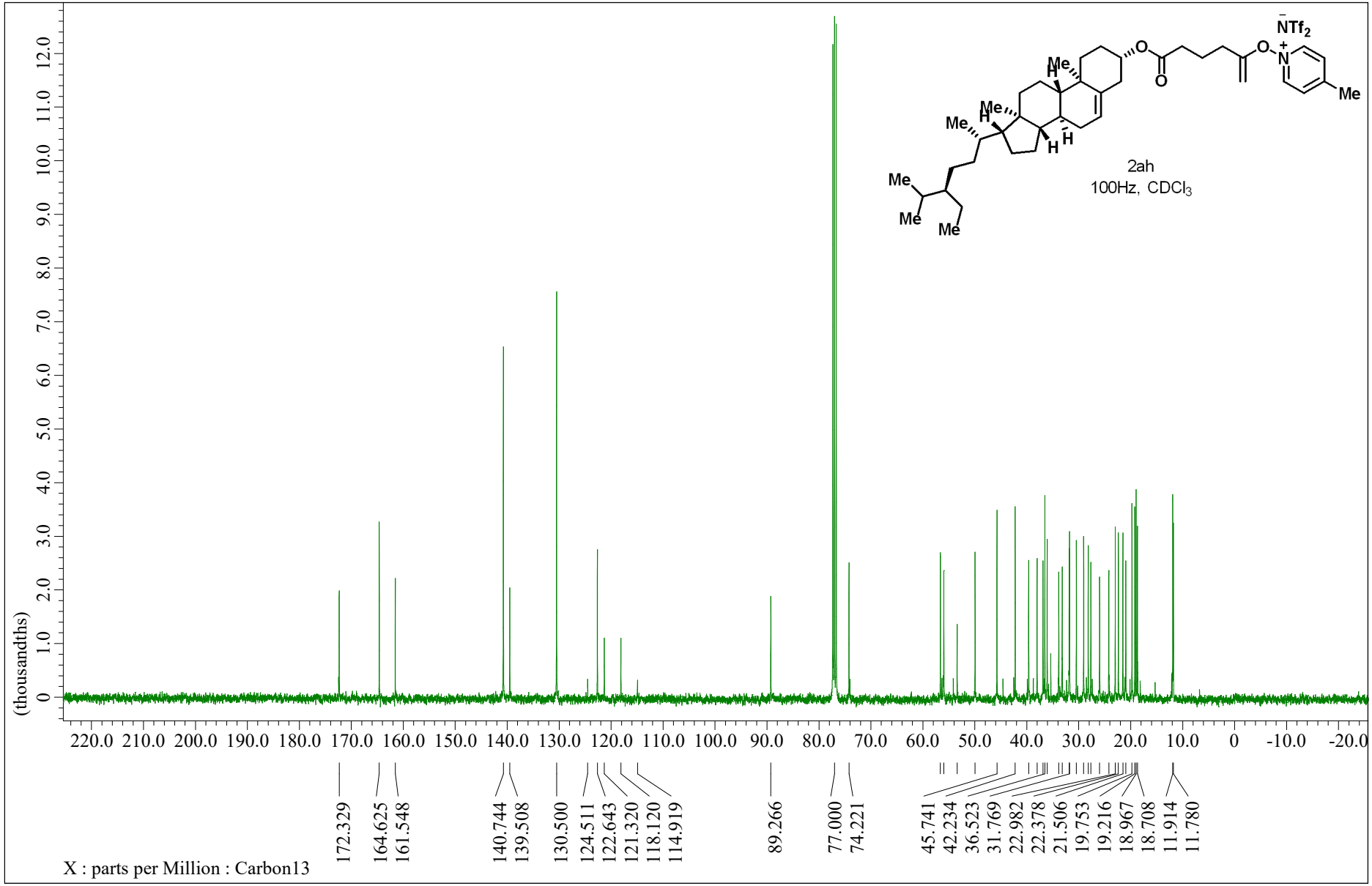

NTf2
Me
400 Hz, CDCl3
abundance
X : parts per Million : Proton
5.08
3.07
2.25
2.18
2.17
1.11
1.11
1.10
1.00
1.12
1.07
8.607
8.591
8.500
8.481
8.461
8.102
8.083
8.051
8.031
8.015
7.328
7.308
7.290
7.260
7.235
7.215
7.195
4.496
4.482
3.555
3.542
2.798
2.767
2.745
2.727
2.478
2.459
2.439
2.049
2.029
2.010
1.991

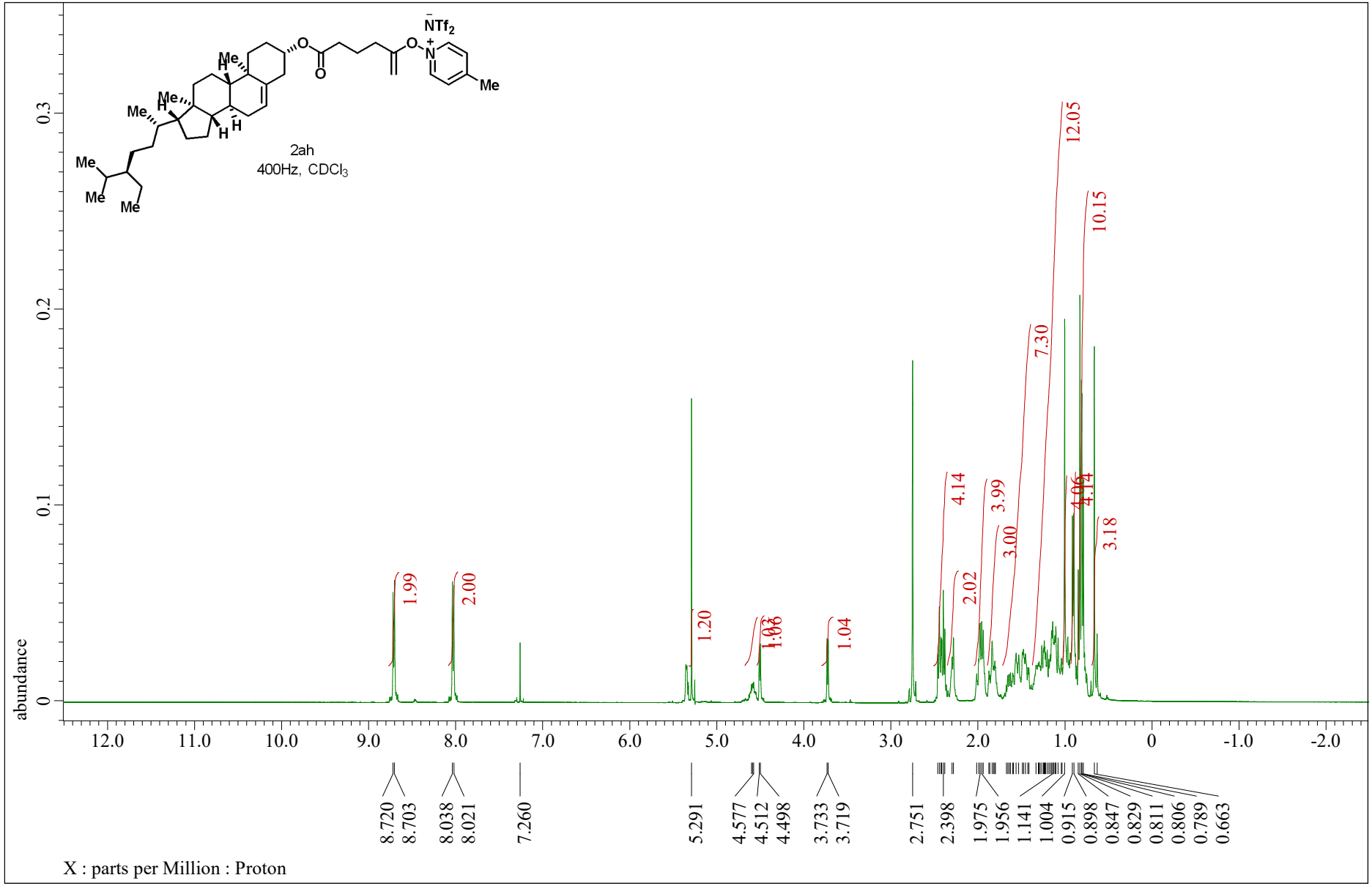

NTf2
O
N
Cl
100Hz, CDCl3
(thousandths)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.592
155.665
142.805
140.965
130.520
128.574
126.217
124.329
121.349
118.158
114.056
90.205
77.000
34.826
30.418
27.745
X : parts per Million : Carbon13

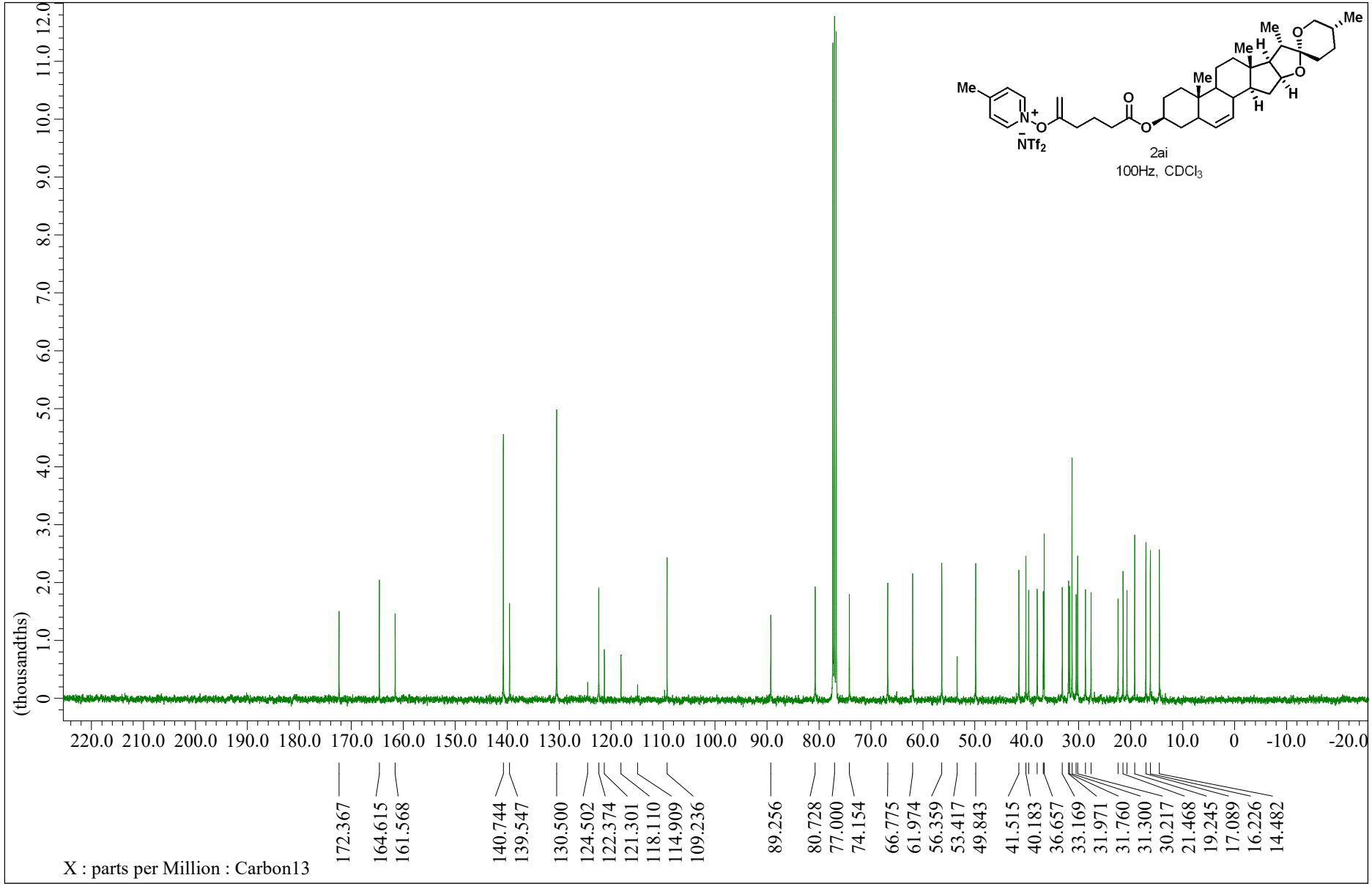

NTf2
Cl
400Hz, CDCl3
abundance
2.06
2.00
3.30
2.45
1.05
1.09
2.13
2.12
2.14
8.705
8.687
8.148
8.131
7.305
7.285
7.260
7.236
7.218
7.211
7.190
4.575
4.561
3.817
3.802
2.745
2.727
2.709
2.439
2.420
2.401
2.020
2.002
1.982
1.964
1.944
X : parts per Million : Proton

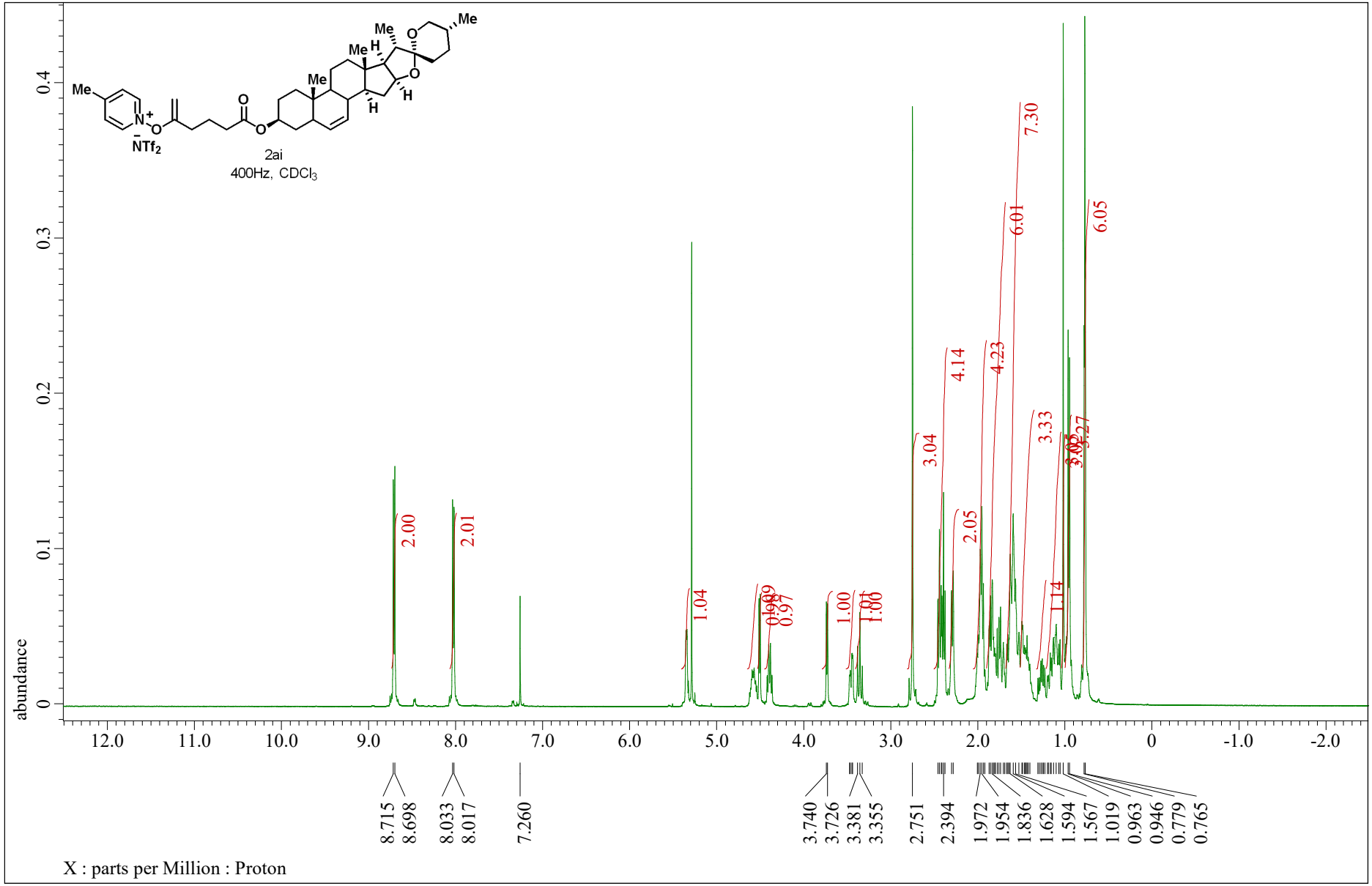

100Hz, CDCl3
NTf2
Me
Me
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
165.209
148.142
141.329
141.108
138.071
128.536
128.450
126.102
124.521
121.320
118.120
114.919
89.026
77.000
34.855
30.476
27.793
18.402
X : parts per Million : Carbon13

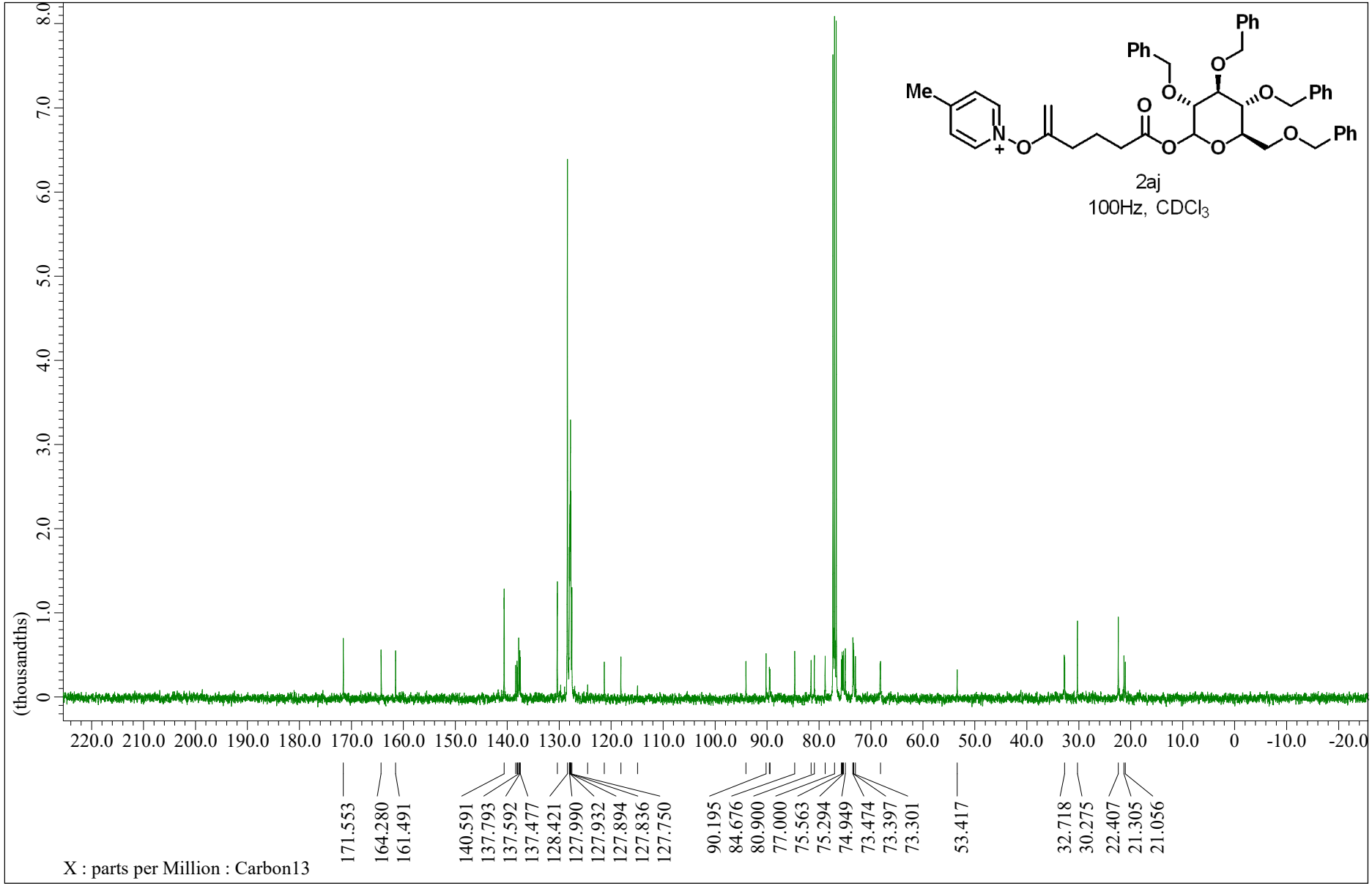

400Hz, CDCl3
NTf2
Me
Me
abundance
X : parts per Million : Proton
6.03
3.16
2.14
1.99
1.00
1.10
1.10
2.13
2.00
2.05
7.318
7.299
7.281
7.260
7.225
7.213
7.194
4.492
4.479
3.748
3.734
2.742
2.724
2.705
2.582
2.426
2.407
2.387
2.013
1.995
1.975
1.957

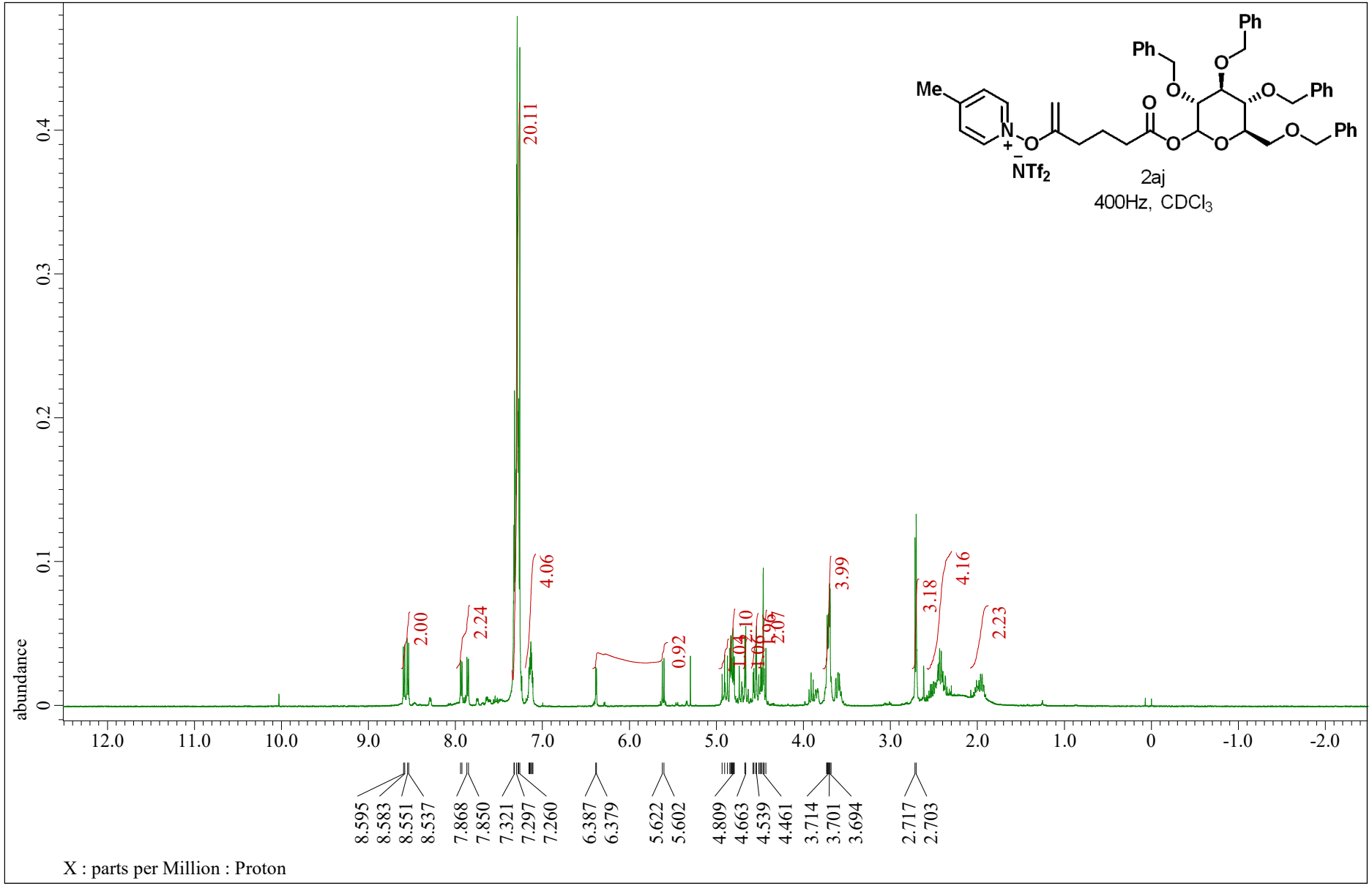

2ah
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
172.329
164.625
161.548
140.744
139.508
130.500
124.511
122.643
121.320
118.120
114.919
89.266
77.000
74.221
45.741
42.234
36.523
31.769
22.982
22.378
21.506
19.753
19.216
18.967
18.708
11.914
11.780

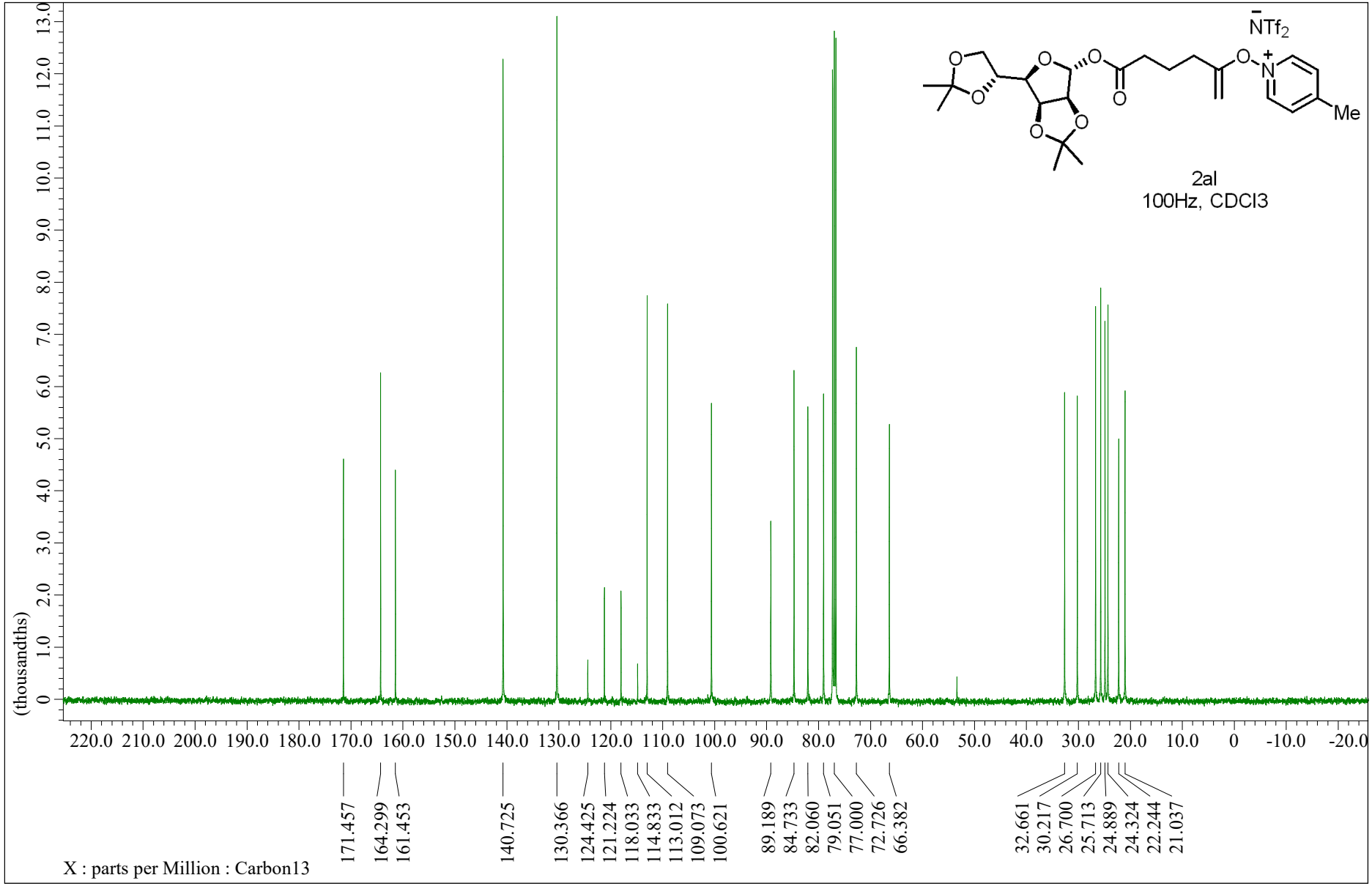

2ah
400Hz, CDCl3
abundance
X : parts per Million : Proton
1.99
2.00
1.20
1.04
4.14
2.02
3.99
3.00
7.30
12.05
10.15
4.06
4.14
3.18
8.720
8.703
8.038
8.021
7.260
5.291
4.577
4.512
4.498
3.733
3.719
2.751
2.398
1.975
1.956
1.141
1.004
0.915
0.898
0.847
0.829
0.811
0.806
0.789
0.663

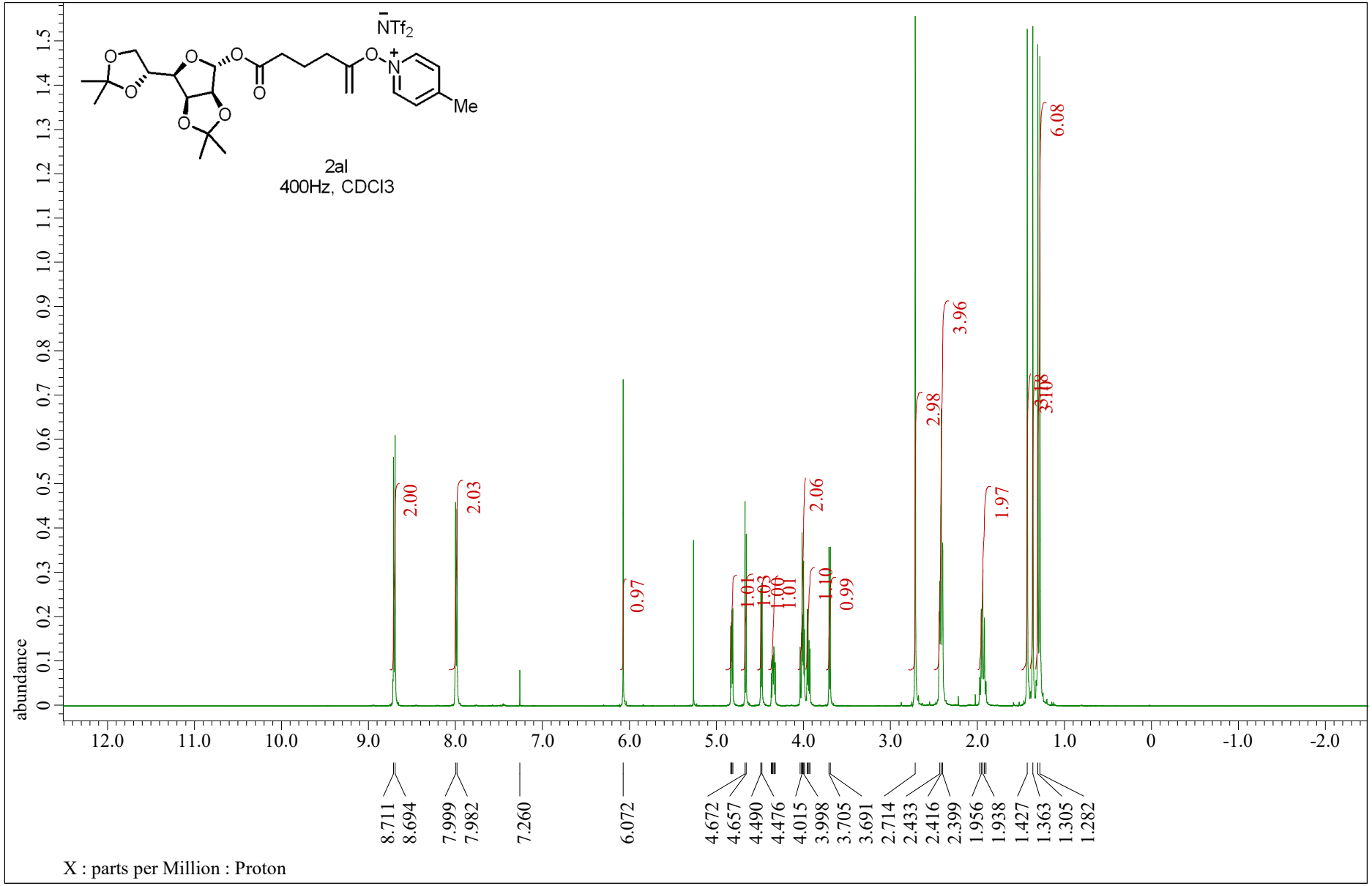

2ai
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
172.367
164.615
161.568
140.744
139.547
130.500
124.502
122.374
121.301
118.110
114.909
109.236
89.256
80.728
77.000
74.154
66.775
61.974
56.359
53.417
49.843
41.515
40.183
36.657
33.169
31.971
31.760
31.300
30.217
21.468
19.245
17.089
16.226
14.482

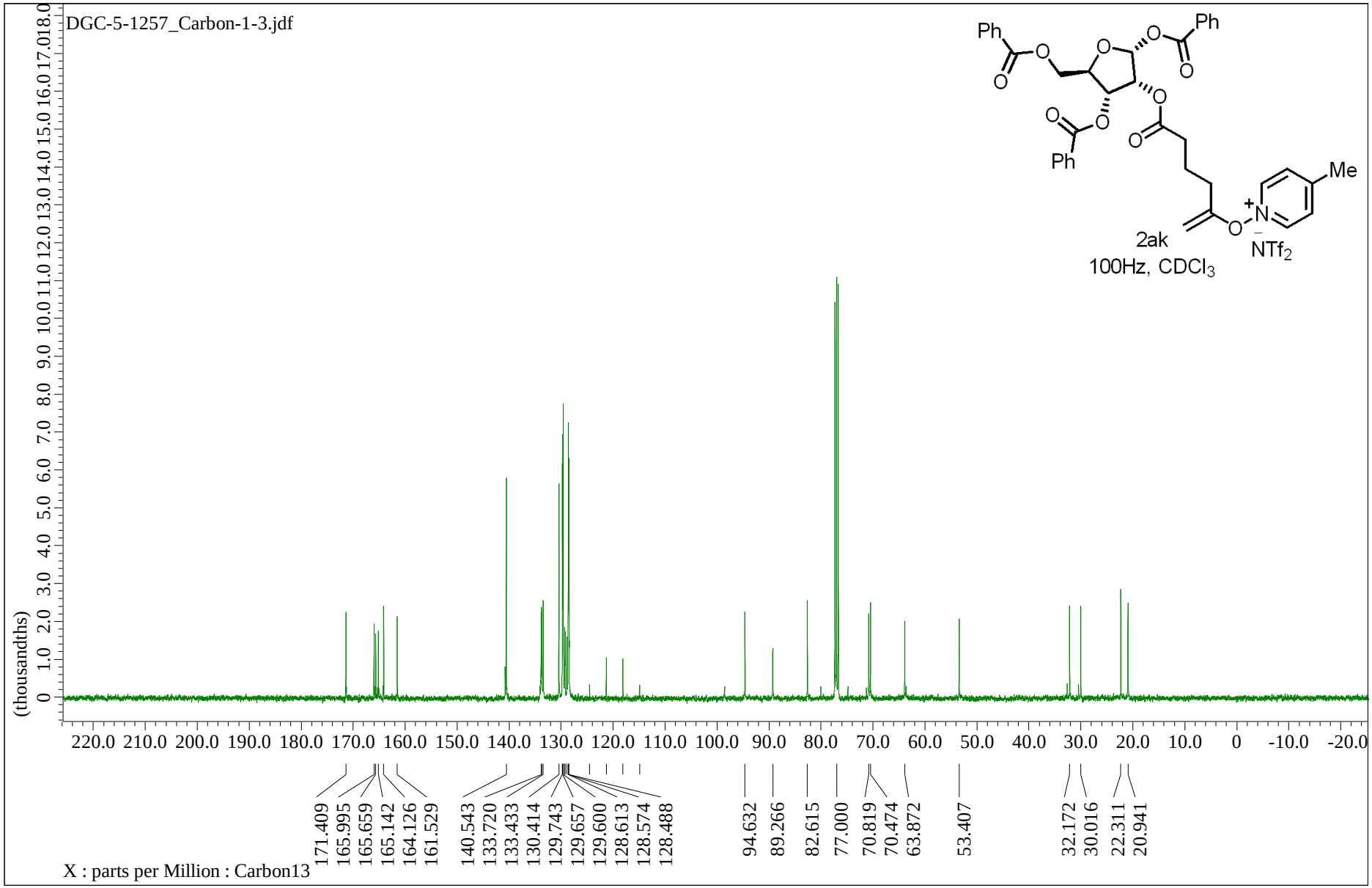

2ai
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.01
1.04
0.97
1.00
3.04
4.14
4.23
2.05
6.01
7.30
3.33
1.14
6.05
8.715
8.698
8.033
8.017
7.260
3.740
3.726
3.381
3.355
2.751
2.394
1.972
1.954
1.836
1.628
1.594
1.567
1.019
0.963
0.946
0.779
0.765

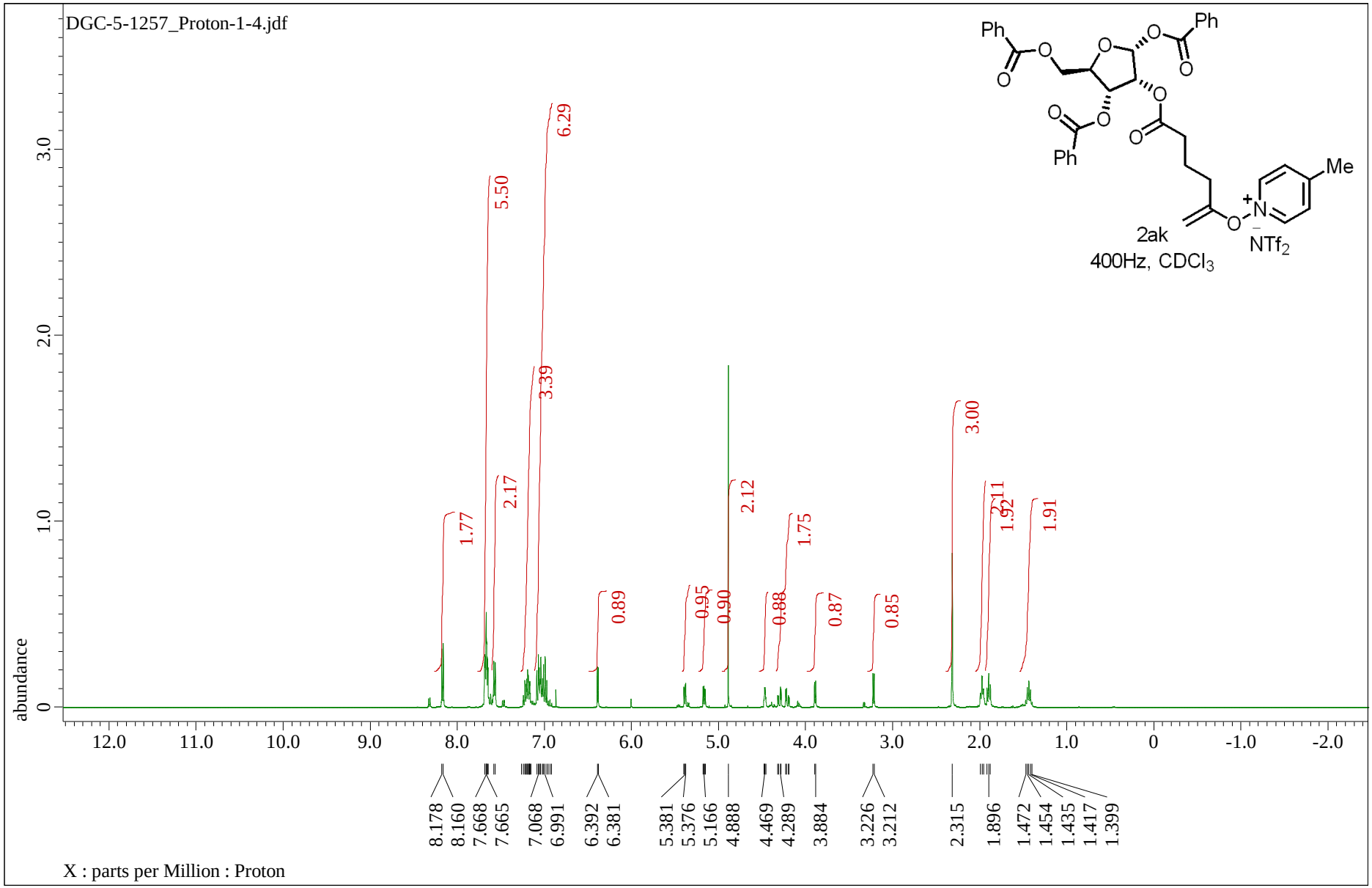

2aj
100Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
171.553
164.280
161.491
140.591
137.793
137.592
137.477
128.421
127.990
127.932
127.894
127.836
127.750
90.195
84.676
80.900
77.000
75.563
75.294
74.949
73.474
73.397
73.301
53.417
32.718
30.275
22.407
21.305
21.056

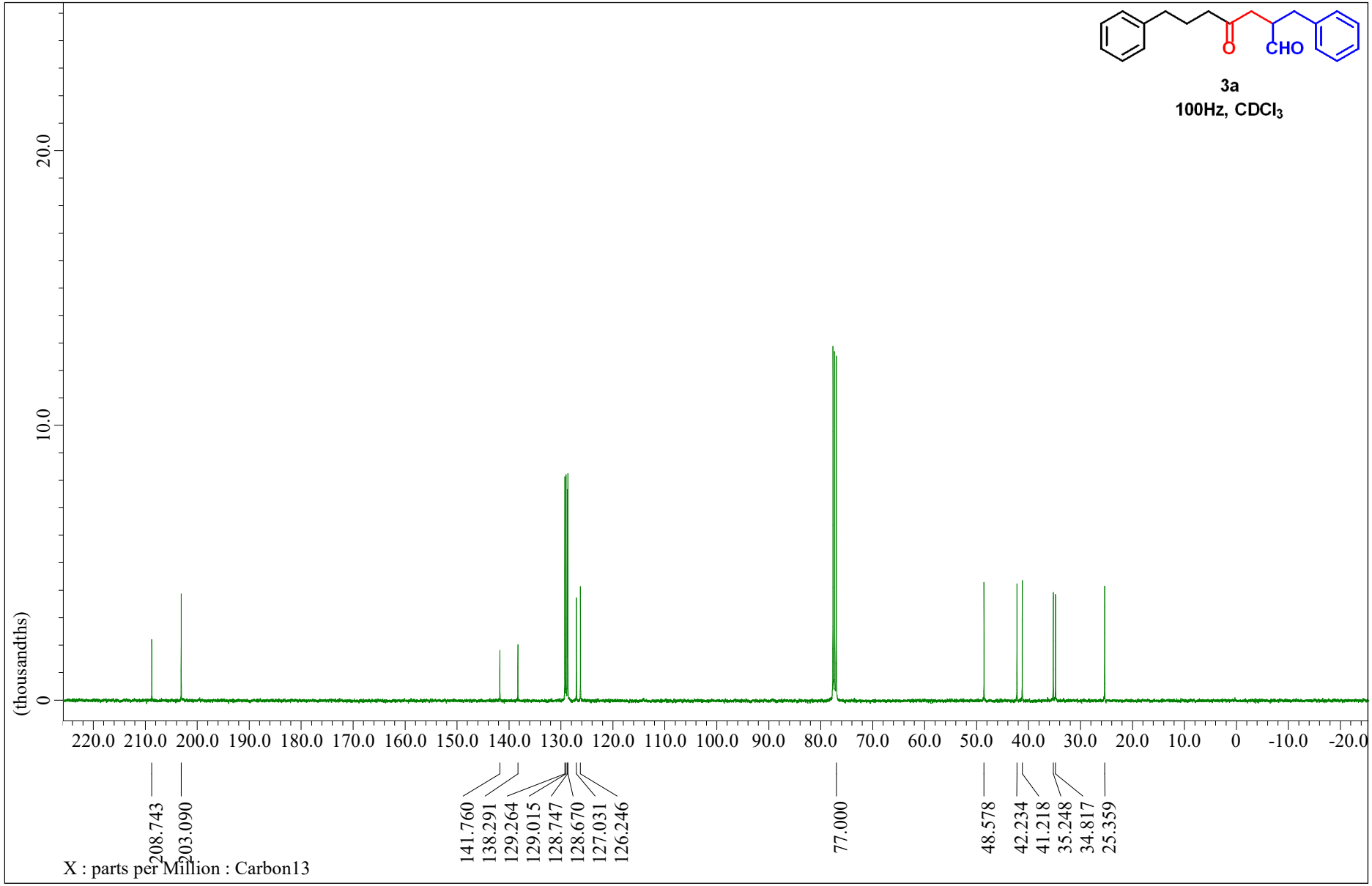

Ph
Ph
O
O
Ph
Me
O
O
O
Ph
N
+
O
−
NTf2
2aj
400Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
20.11
4.06
2.24
2.00
0.92
1.04
2.10
1.06
2.07
3.99
3.18
4.16
2.23
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.595
8.583
8.551
8.537
7.868
7.850
7.321
7.297
7.260
6.387
6.379
5.622
5.602
4.809
4.663
4.539
4.461
3.714
3.701
3.694
2.717
2.703
X : parts per Million : Proton

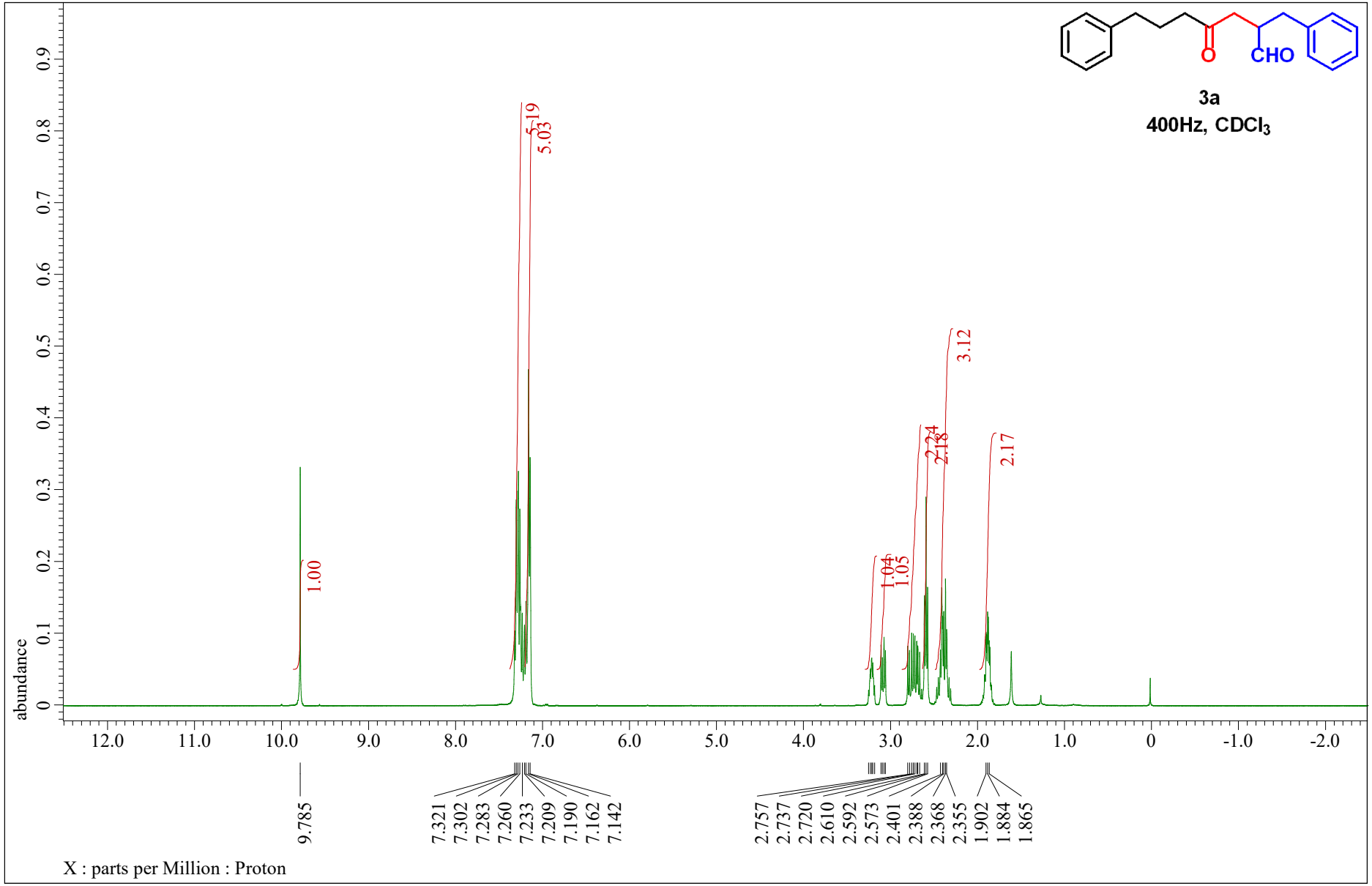

2al
100Hz, CDCl3
NTf2
Me
(thousandths)
X : parts per Million : Carbon13
171.457
164.299
161.453
140.725
130.366
124.425
121.224
118.033
114.833
113.012
109.073
100.621
89.189
84.733
82.060
79.051
77.000
72.726
66.382
32.661
30.217
26.700
25.713
24.889
24.324
22.244
21.037

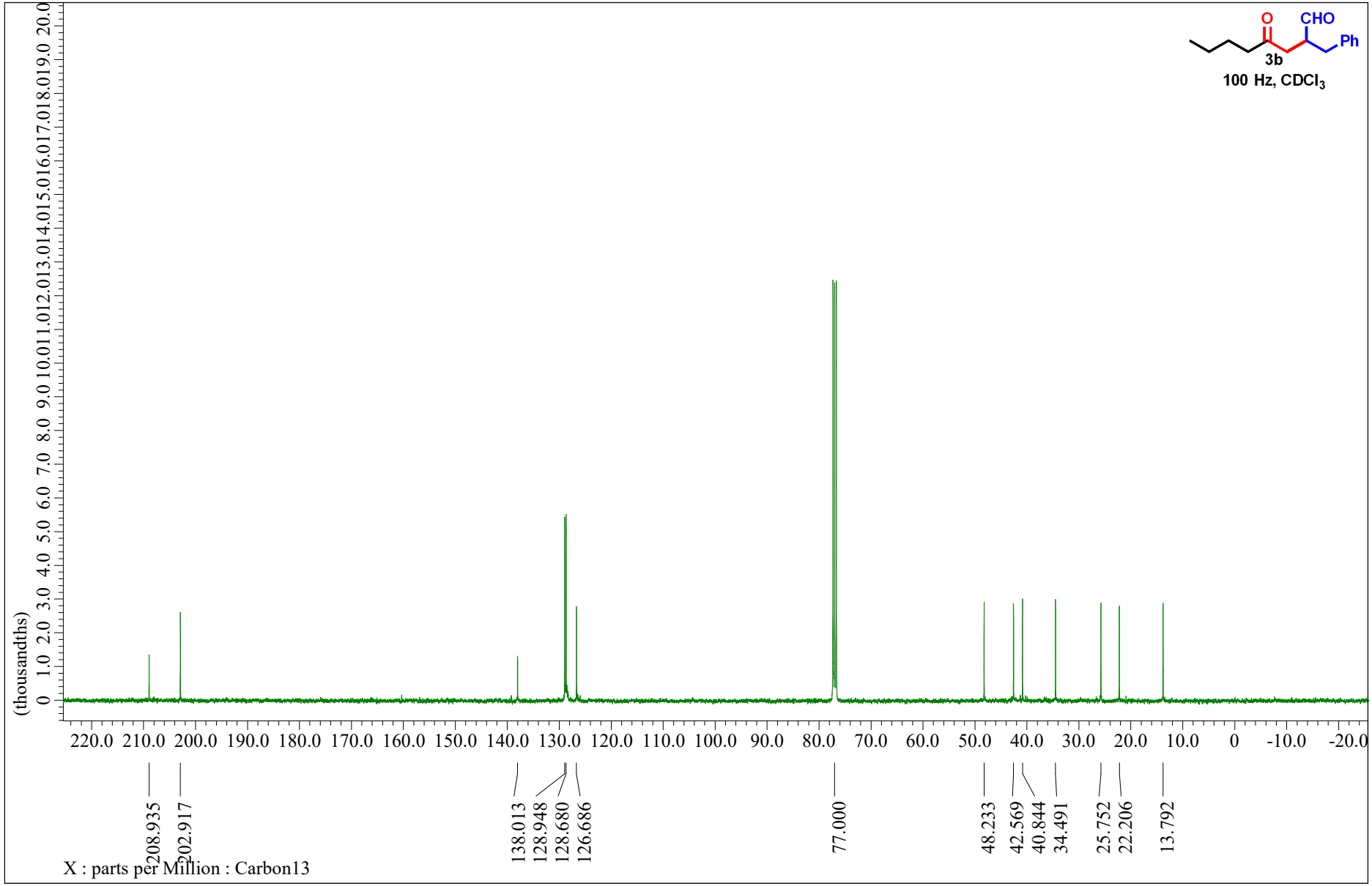

NTf2
Me
2al
400Hz, CDCl3
abundance
X : parts per Million : Proton
2.00
2.03
0.97
1.01
1.03
1.06
1.01
2.06
1.10
0.99
2.98
3.96
1.97
3.08
6.08
8.711
8.694
7.999
7.982
7.260
6.072
4.672
4.657
4.490
4.476
4.015
3.998
3.705
3.691
2.714
2.433
2.416
2.399
1.956
1.938
1.427
1.363
1.305
1.282

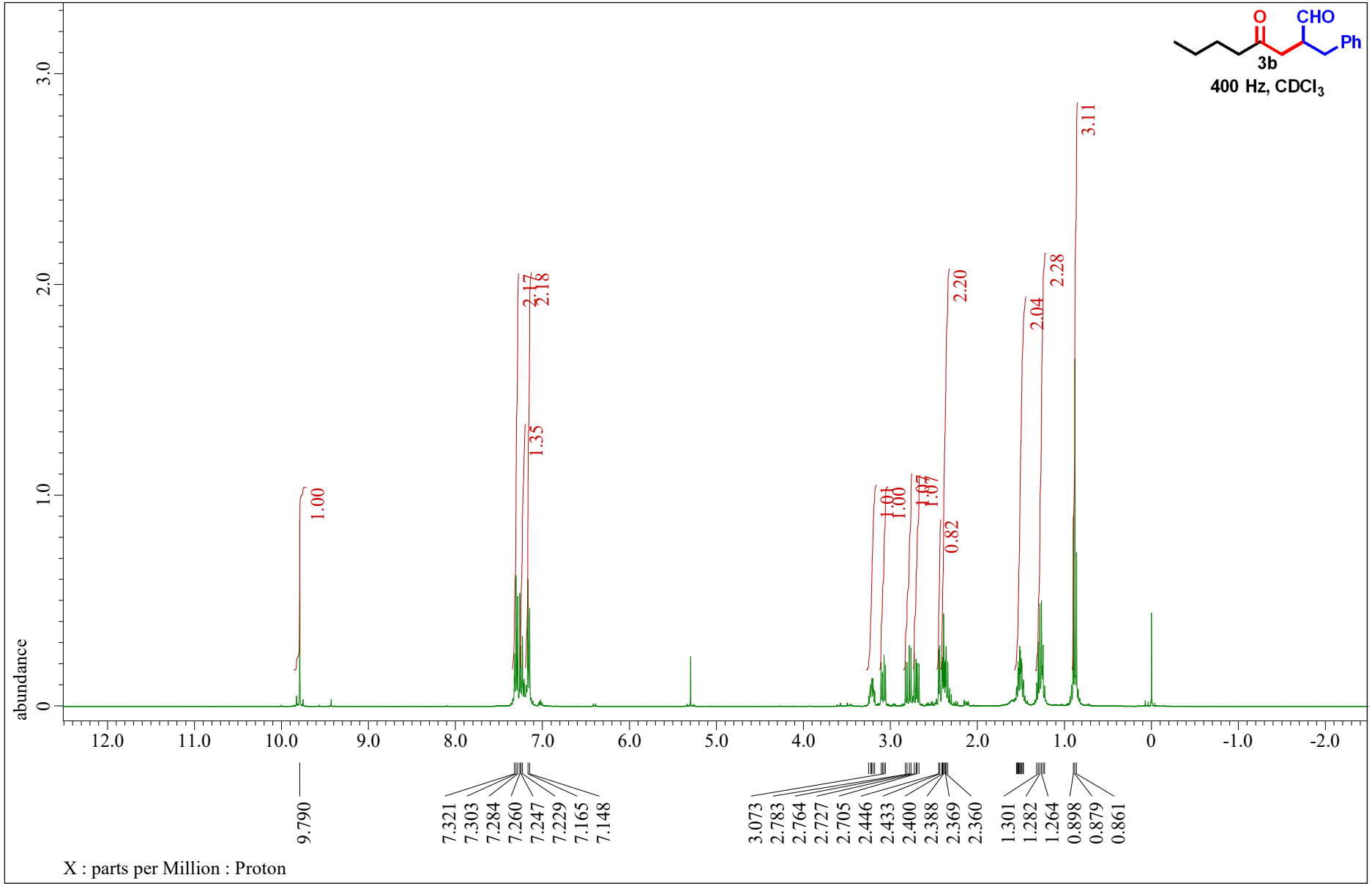

DGC-5-1257_Carbon-1-3.jdf
2ak
100Hz, CDCl3
NTf2
(thousandths)
X : parts per Million : Carbon13
171.409
165.995
165.659
165.142
164.126
161.529
140.543
133.720
133.433
130.414
129.743
129.657
129.600
128.613
128.574
128.488
94.632
89.266
82.615
77.000
70.819
70.474
63.872
53.407
32.172
30.016
22.311
20.941

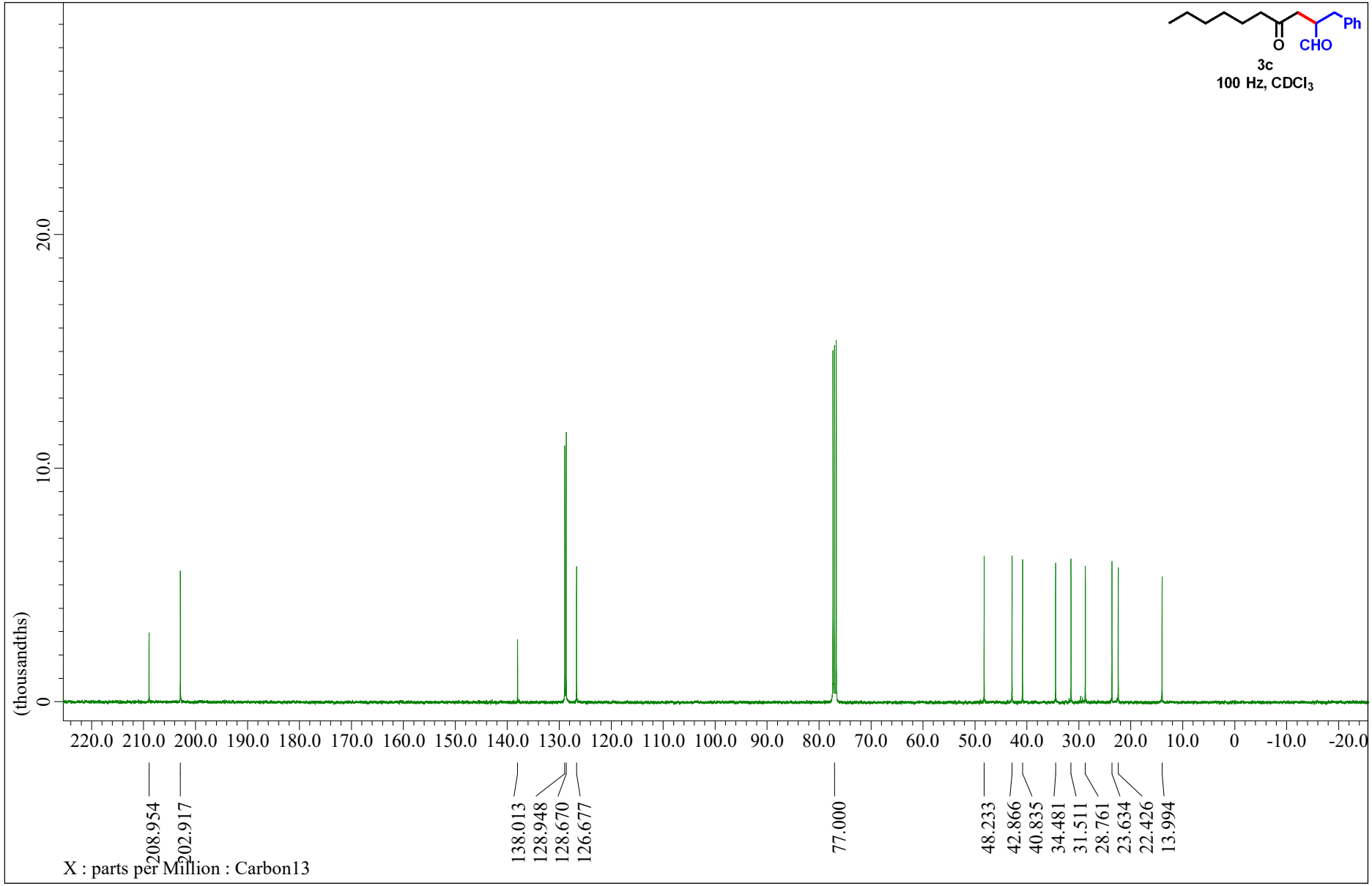

DGC-5-1257_Proton-1-4.jdf
Ph
O
O
Ph
O
O
O
Ph
O
O
O
Me
+
N
O
NTf2
2ak
400Hz, CDCl3
abundance
3.0
2.0
1.0
0
6.29
5.50
3.39
2.17
1.77
2.12
1.75
3.00
2.11
1.92
1.91
0.89
0.95
0.90
0.88
0.87
0.85
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
8.178
8.160
7.668
7.665
7.068
6.991
6.392
6.381
5.381
5.376
5.166
4.888
4.469
4.289
3.884
3.226
3.212
2.315
1.896
1.472
1.454
1.435
1.417
1.399
X : parts per Million : Proton

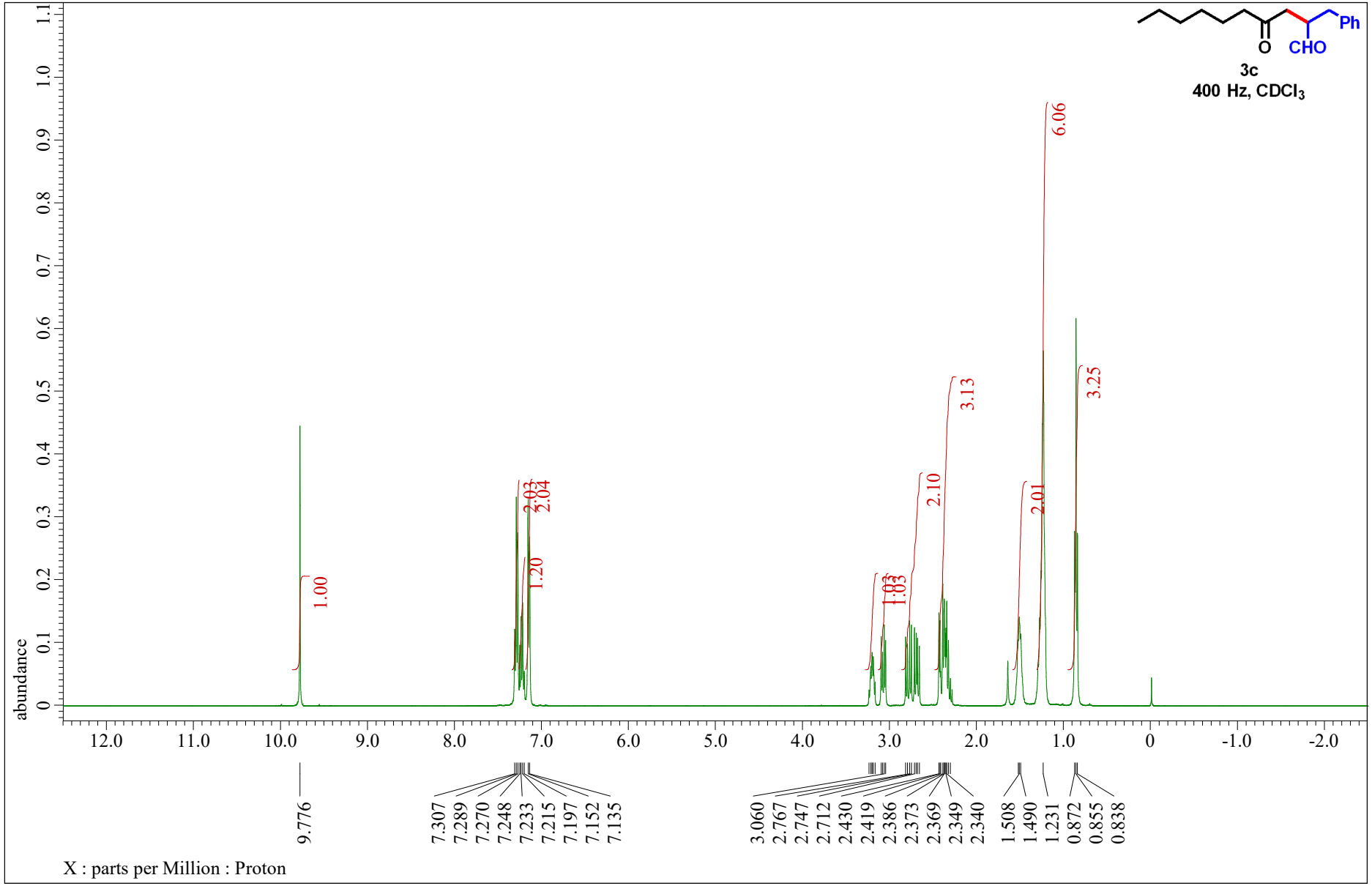

3a
100Hz, CDCl3
CHO
O
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.743
203.090
141.760
138.291
129.264
129.015
128.747
128.670
127.031
126.246
77.000
48.578
42.234
41.218
35.248
34.817
25.359
X : parts per Million : Carbon13

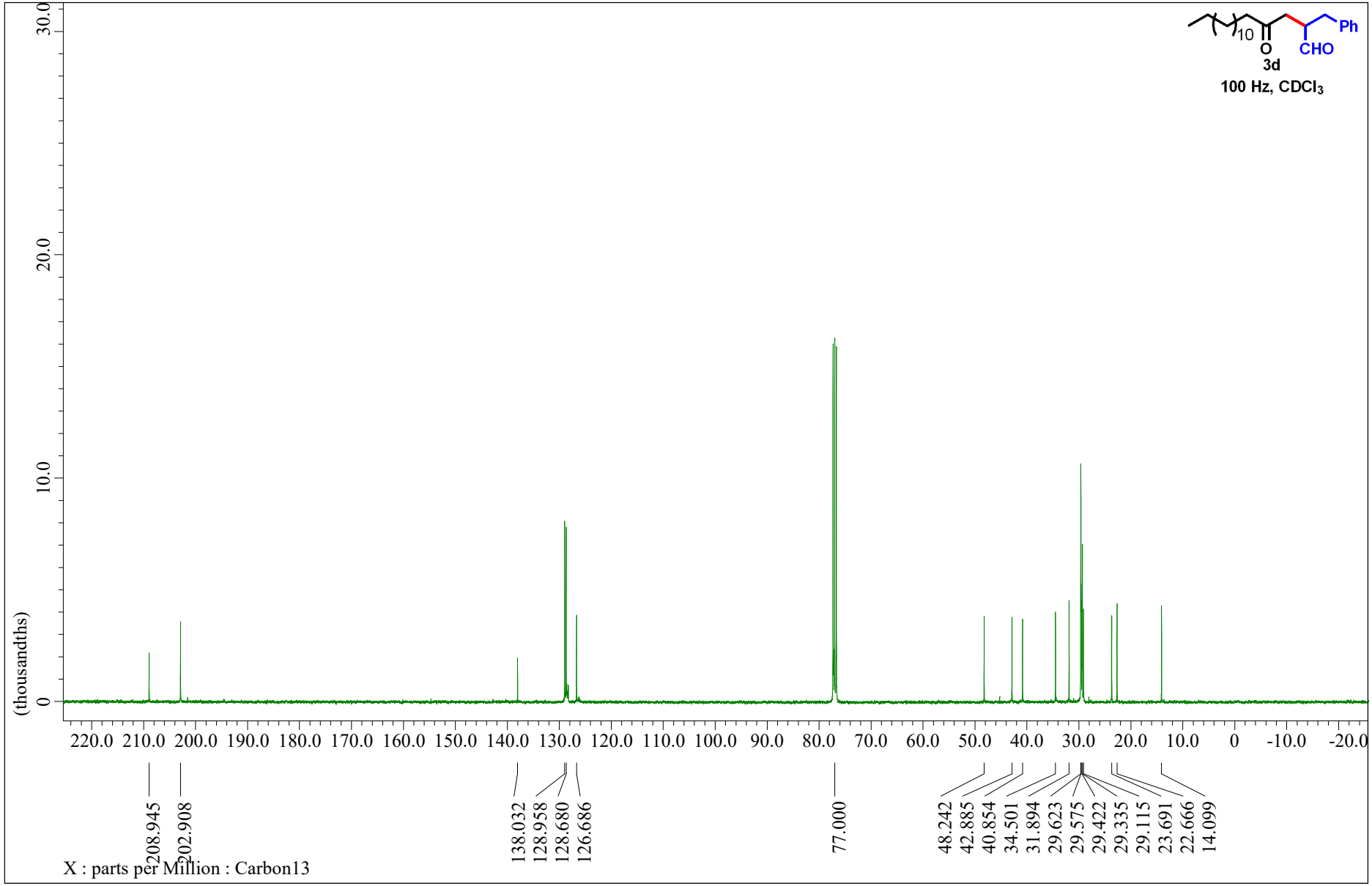

3a
400Hz, CDCl3
CHO
O
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
1.00
5.19
5.03
1.04
1.05
2.24
2.18
3.12
2.17
9.785
7.321
7.302
7.283
7.260
7.233
7.209
7.190
7.162
7.142
2.757
2.737
2.720
2.610
2.592
2.573
2.401
2.388
2.368
2.355
1.902
1.884
1.865
X : parts per Million : Proton

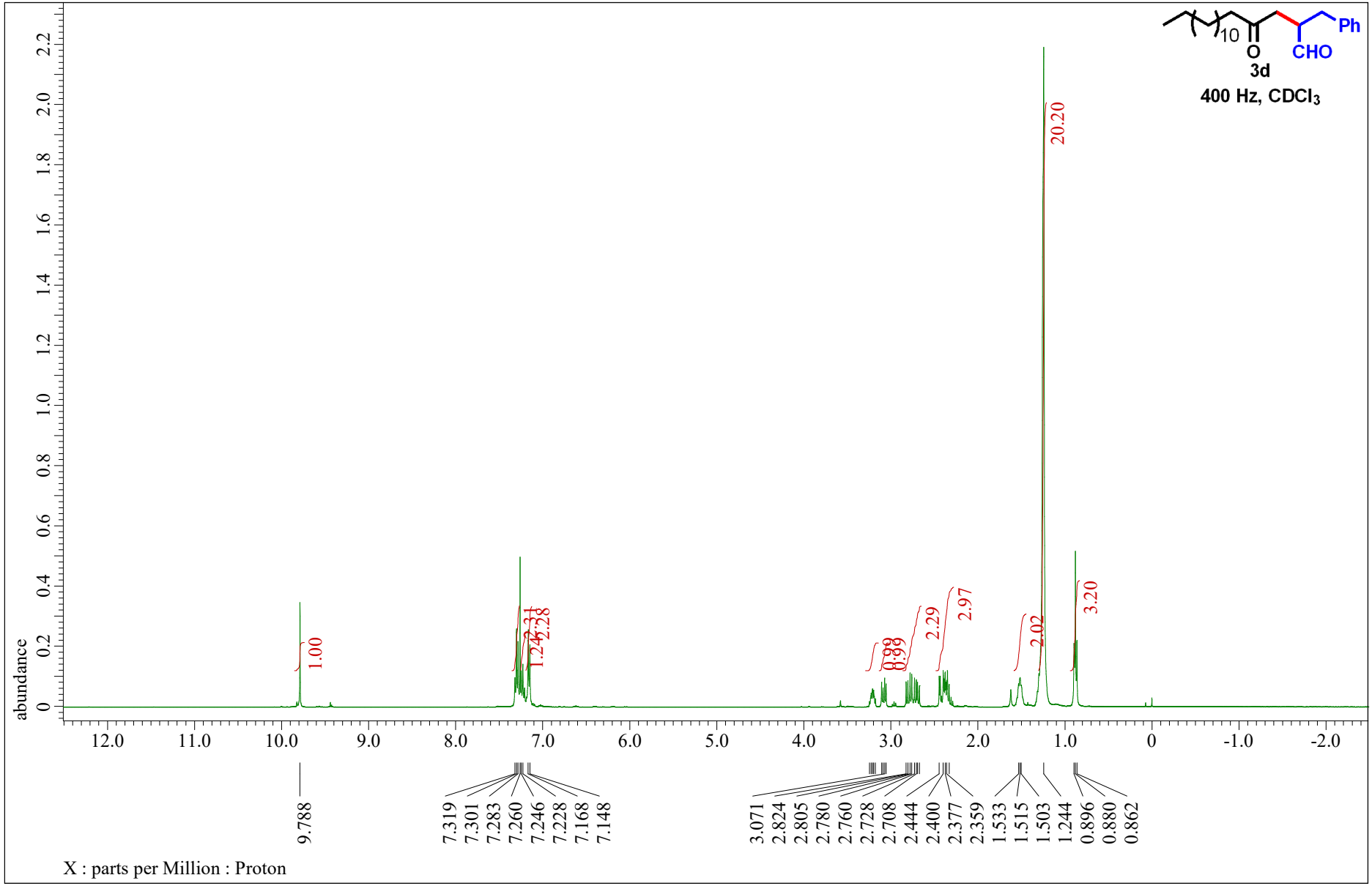

O
CHO
Ph
3b
100 Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.935
202.917
138.013
128.948
128.680
126.686
77.000
48.233
42.569
40.844
34.491
25.752
22.206
13.792
X : parts per Million : Carbon13

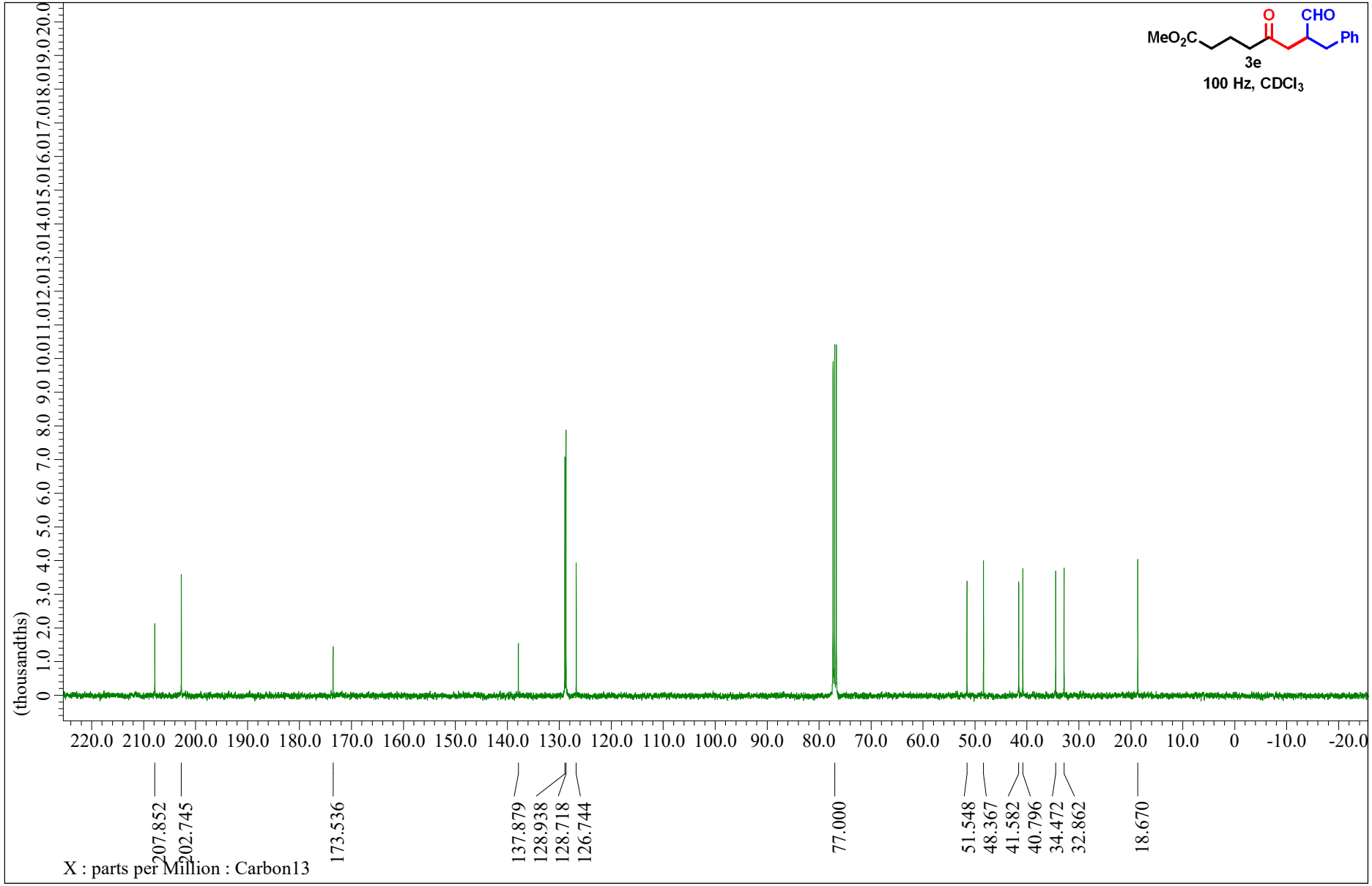

O
CHO
Ph
3b
400 Hz, CDCl3
abundance
3.0
2.0
1.0
0
1.00
2.17
2.18
1.35
1.01
1.00
1.07
0.82
2.20
2.04
2.28
3.11
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.790
7.321
7.303
7.284
7.260
7.247
7.229
7.165
7.148
3.073
2.783
2.764
2.727
2.705
2.446
2.433
2.400
2.388
2.369
2.360
1.301
1.282
1.264
0.898
0.879
0.861
X : parts per Million : Proton

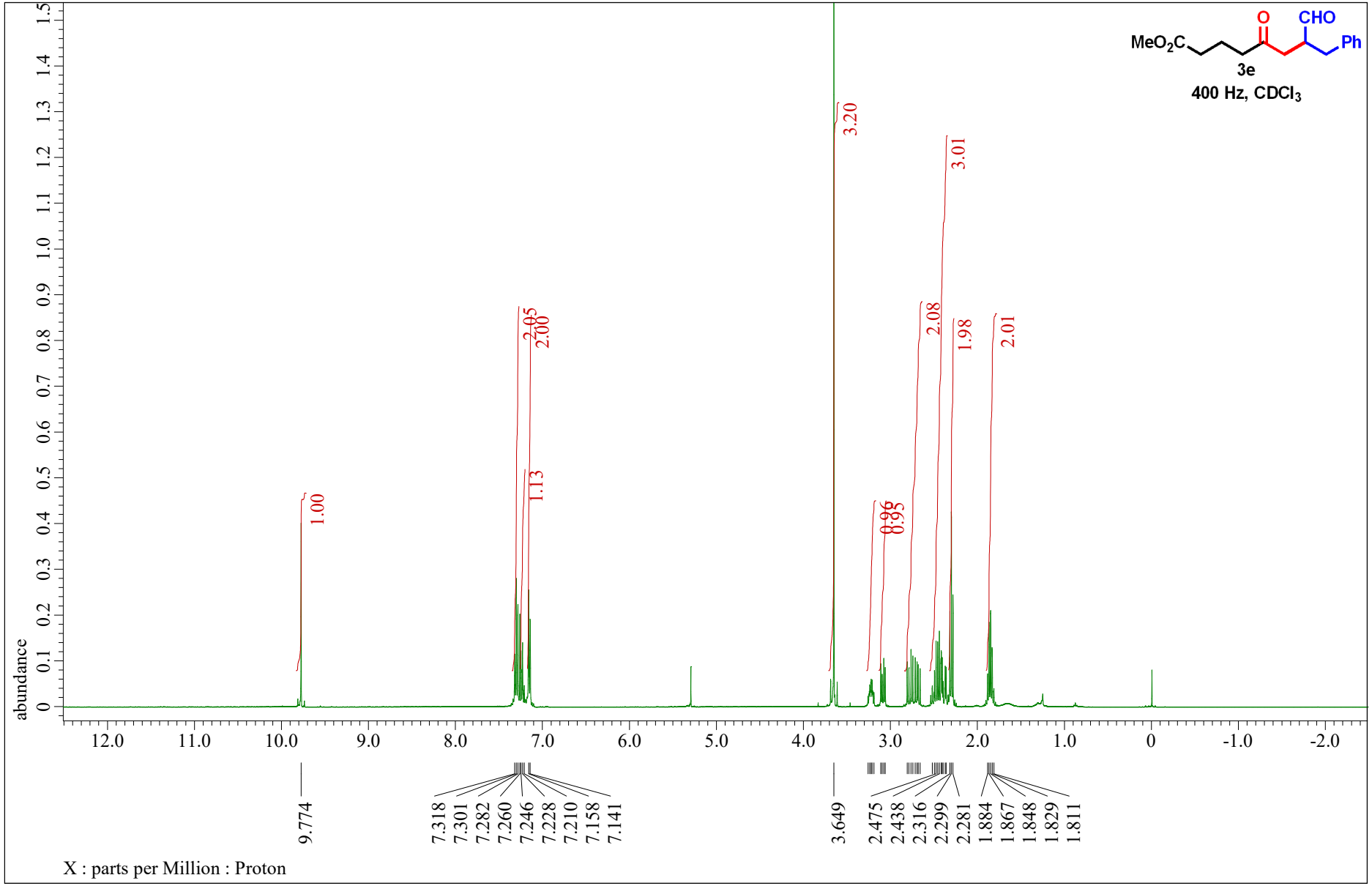

Ph
O
CHO
3c
100 Hz, CDCl3
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.954
202.917
138.013
128.948
128.670
126.677
77.000
48.233
42.866
40.835
34.481
31.511
28.761
23.634
22.426
13.994
X : parts per Million : Carbon13

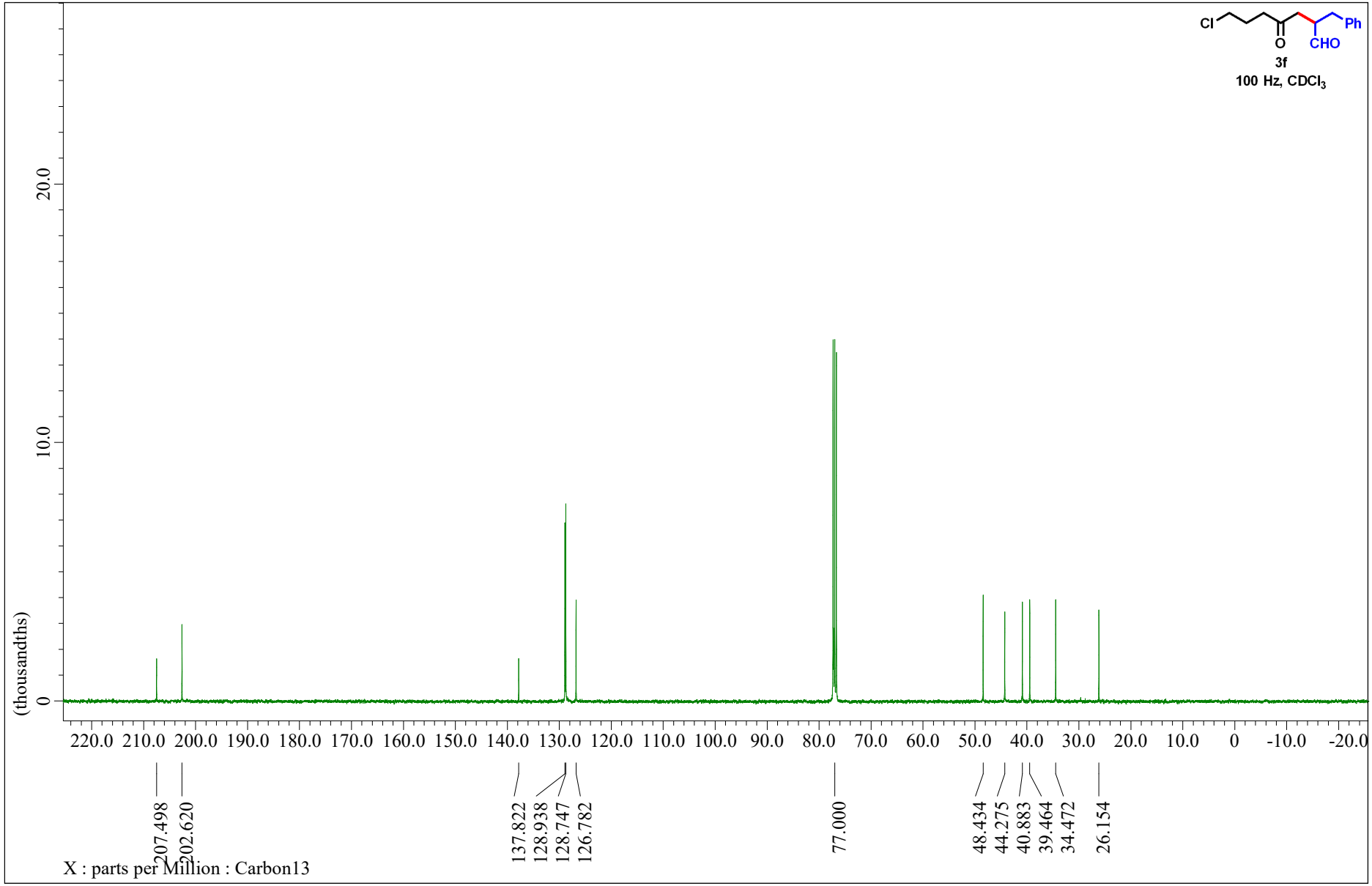

Ph
O
CHO
3c
400 Hz, CDCl3
abundance
6.06
3.25
3.13
2.10
2.01
2.04
2.03
1.20
1.03
1.03
1.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.776
7.307
7.289
7.270
7.248
7.233
7.215
7.197
7.152
7.135
3.060
2.767
2.747
2.712
2.430
2.419
2.386
2.373
2.369
2.349
2.340
1.508
1.490
1.231
0.872
0.855
0.838
X : parts per Million : Proton

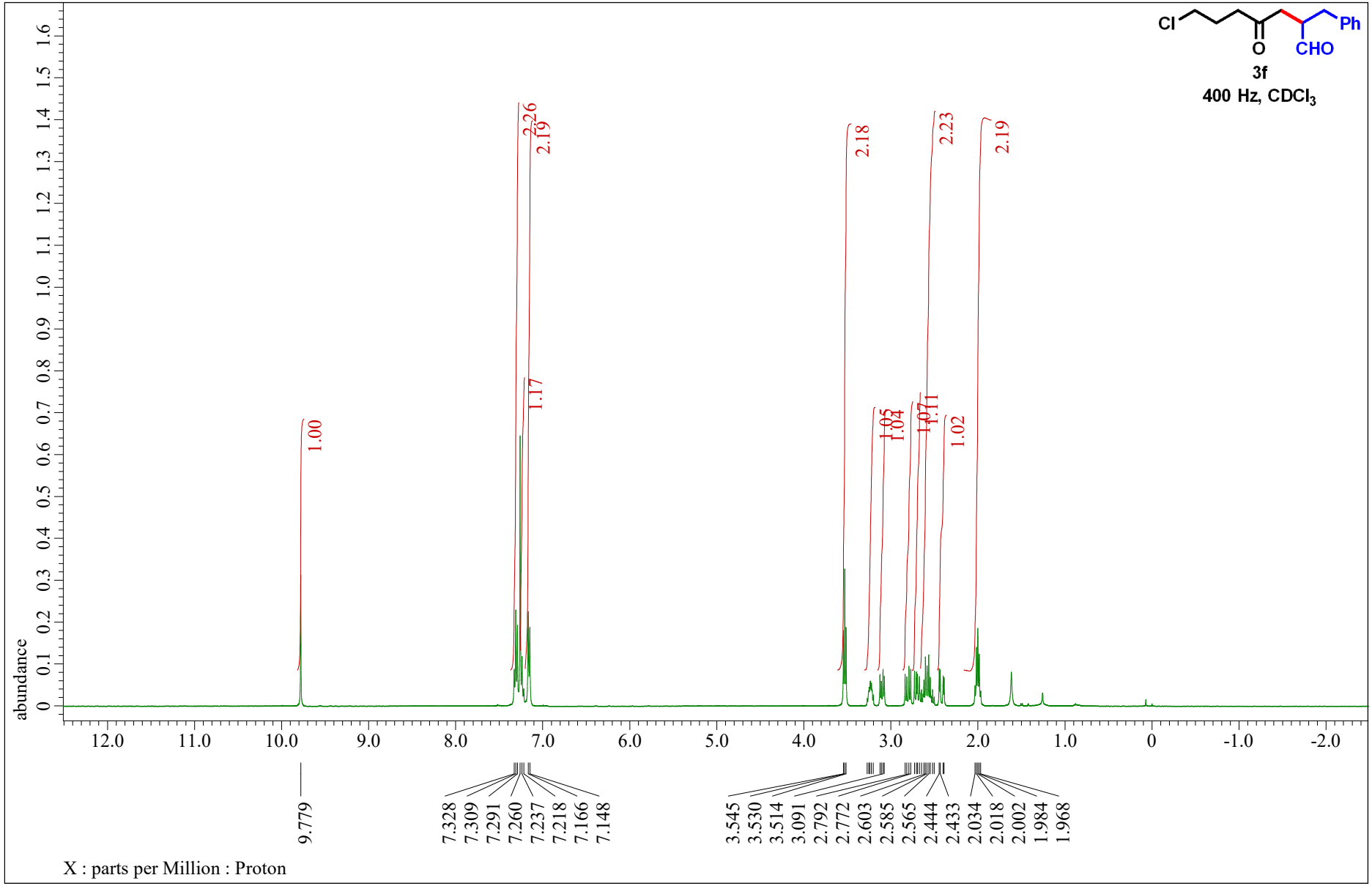

Ph
10
O
CHO
3d
100 Hz, CDCl3
(thousandths)
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.945
202.908
138.032
128.958
128.680
126.686
77.000
48.242
42.885
40.854
34.501
31.894
29.623
29.575
29.422
29.335
29.115
23.691
22.666
14.099
X : parts per Million : Carbon13

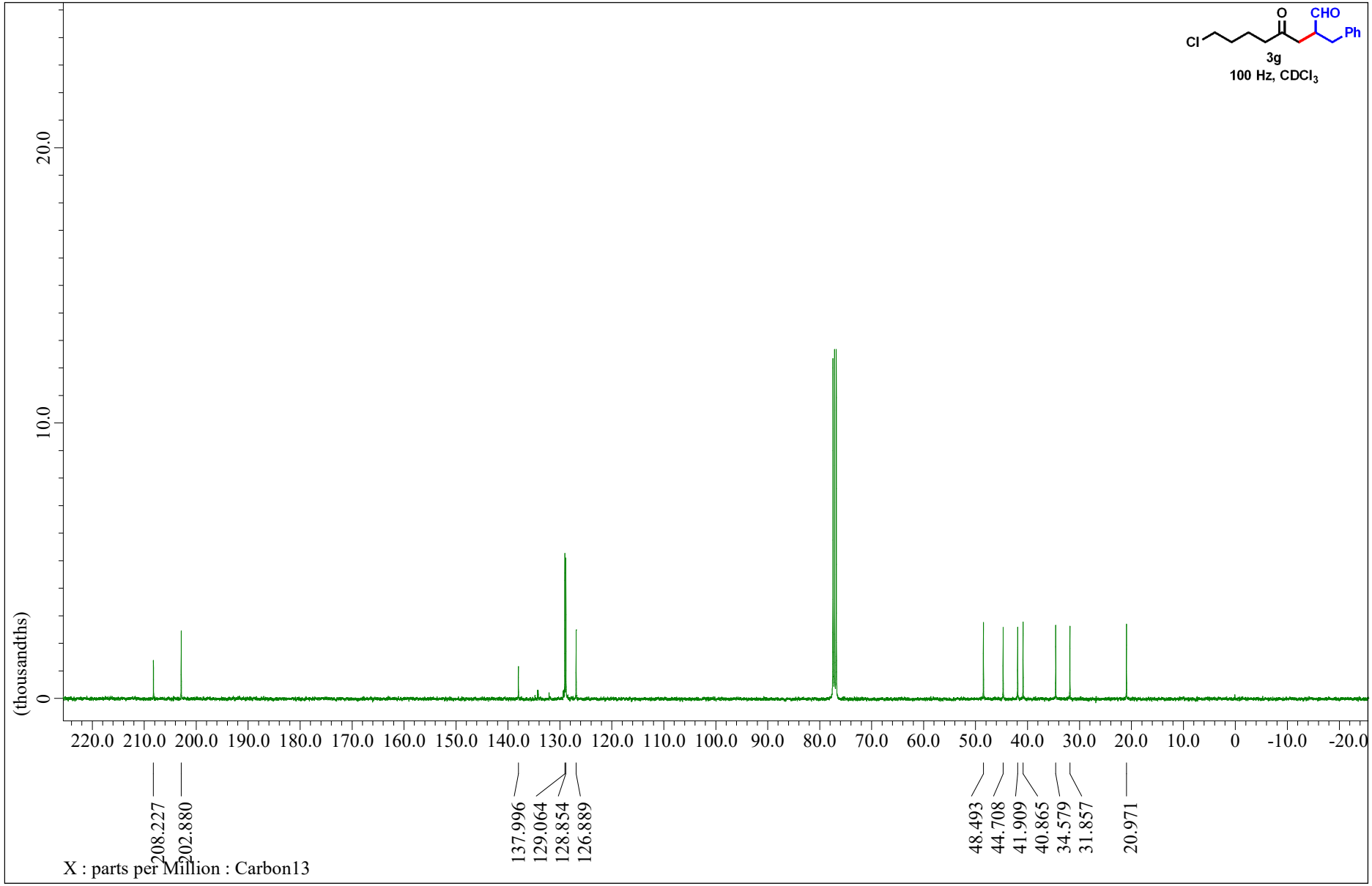

Ph
10
O
CHO
3d
400 Hz, CDCl3
abundance
20.20
3.20
2.97
2.29
2.02
1.00
2.31
2.28
1.24
X : parts per Million : Proton
9.788
7.319
7.301
7.283
7.260
7.246
7.228
7.168
7.148
3.071
2.824
2.805
2.780
2.760
2.728
2.708
2.444
2.400
2.377
2.359
1.533
1.515
1.503
1.244
0.896
0.880
0.862

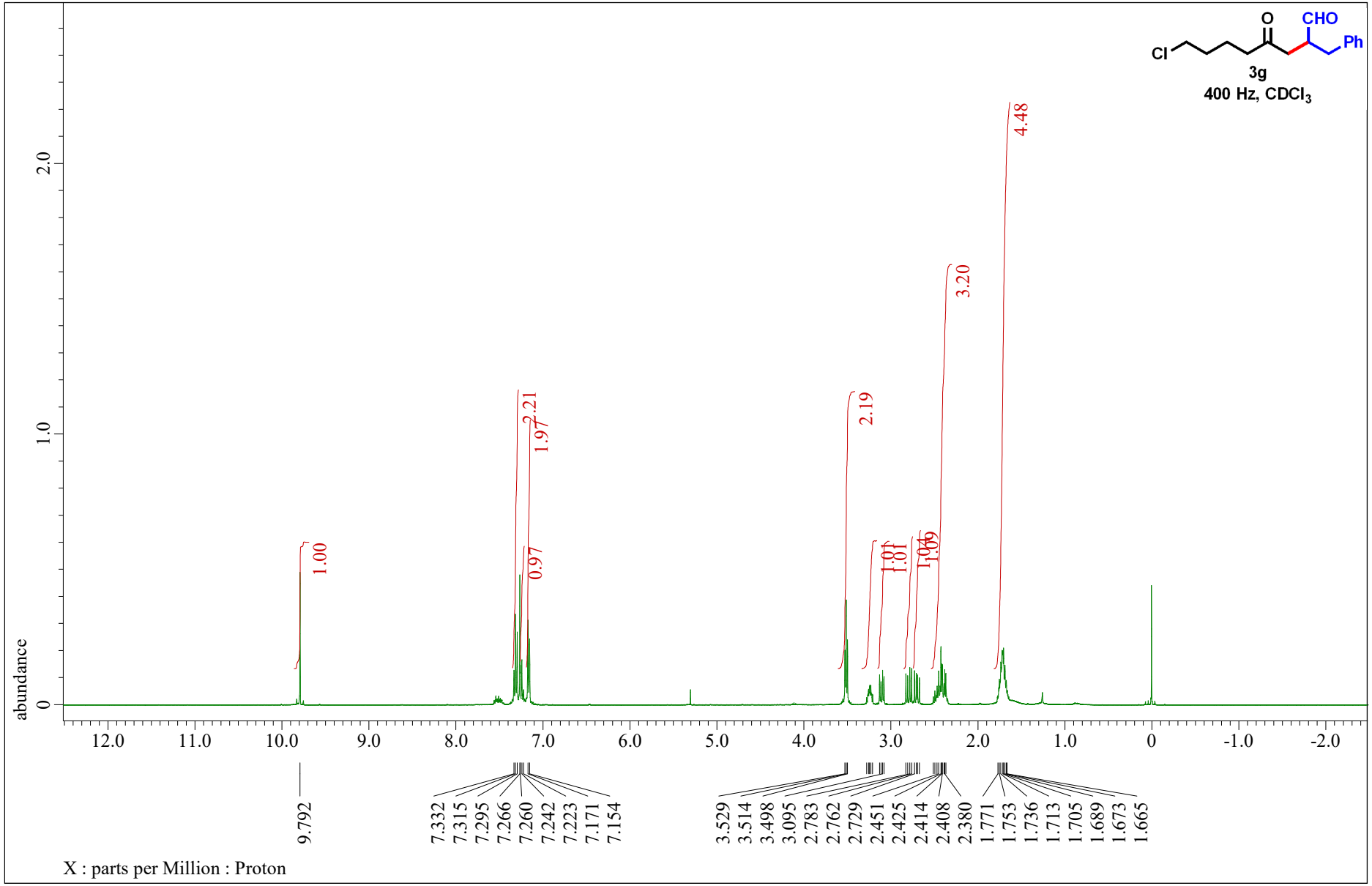

MeO2C
O
CHO
Ph
3e
100 Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0 20.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.852
202.745
173.536
137.879
128.938
128.718
126.744
77.000
51.548
48.367
41.582
40.796
34.472
32.862
18.670
X : parts per Million : Carbon13

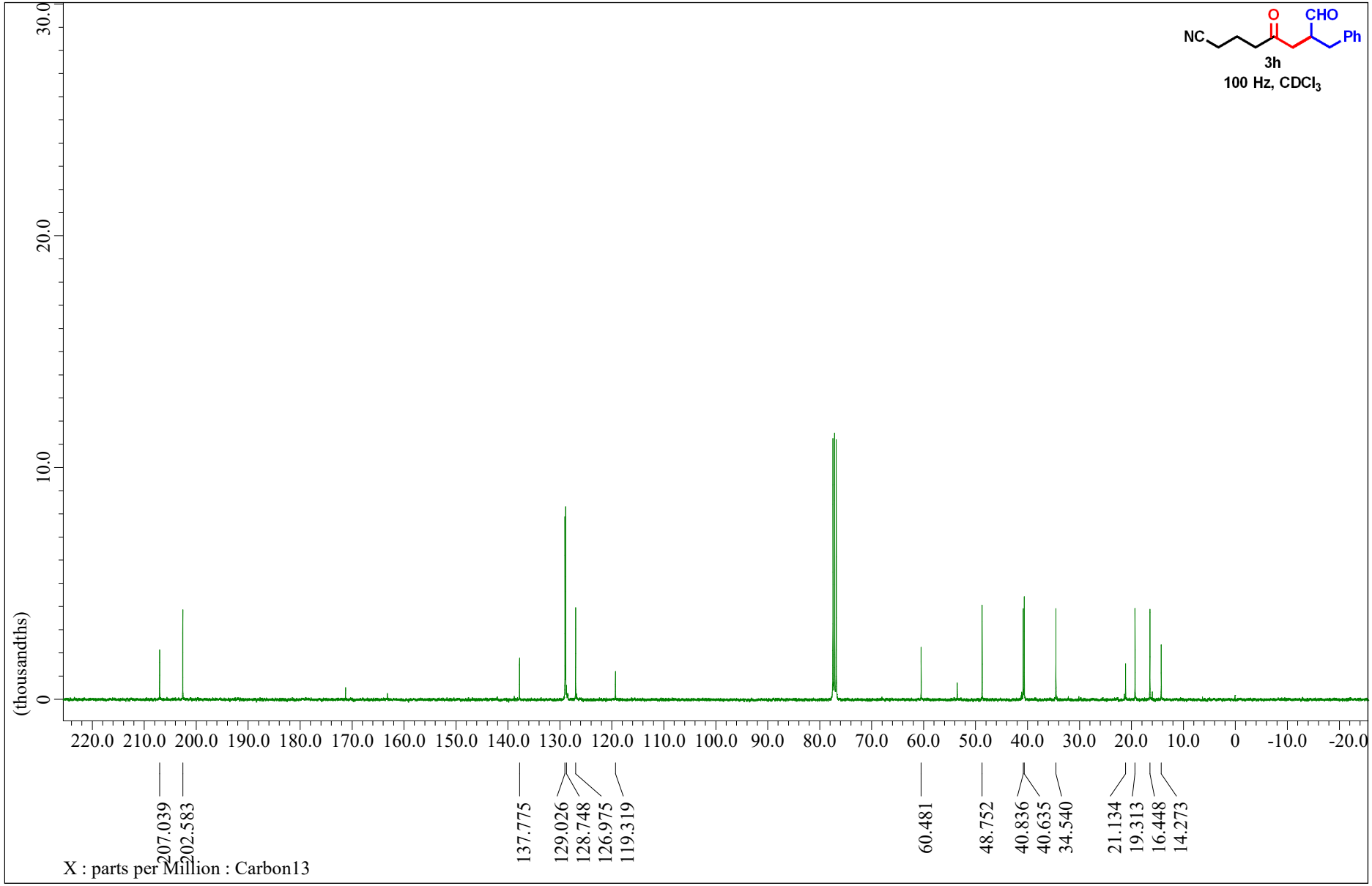

MeO2C
O
CHO
Ph
3e
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
2.05
2.00
1.13
0.96
0.95
3.20
3.01
2.08
1.98
2.01
9.774
7.318
7.301
7.282
7.260
7.246
7.228
7.210
7.158
7.141
3.649
2.475
2.438
2.316
2.299
2.281
1.884
1.867
1.848
1.829
1.811

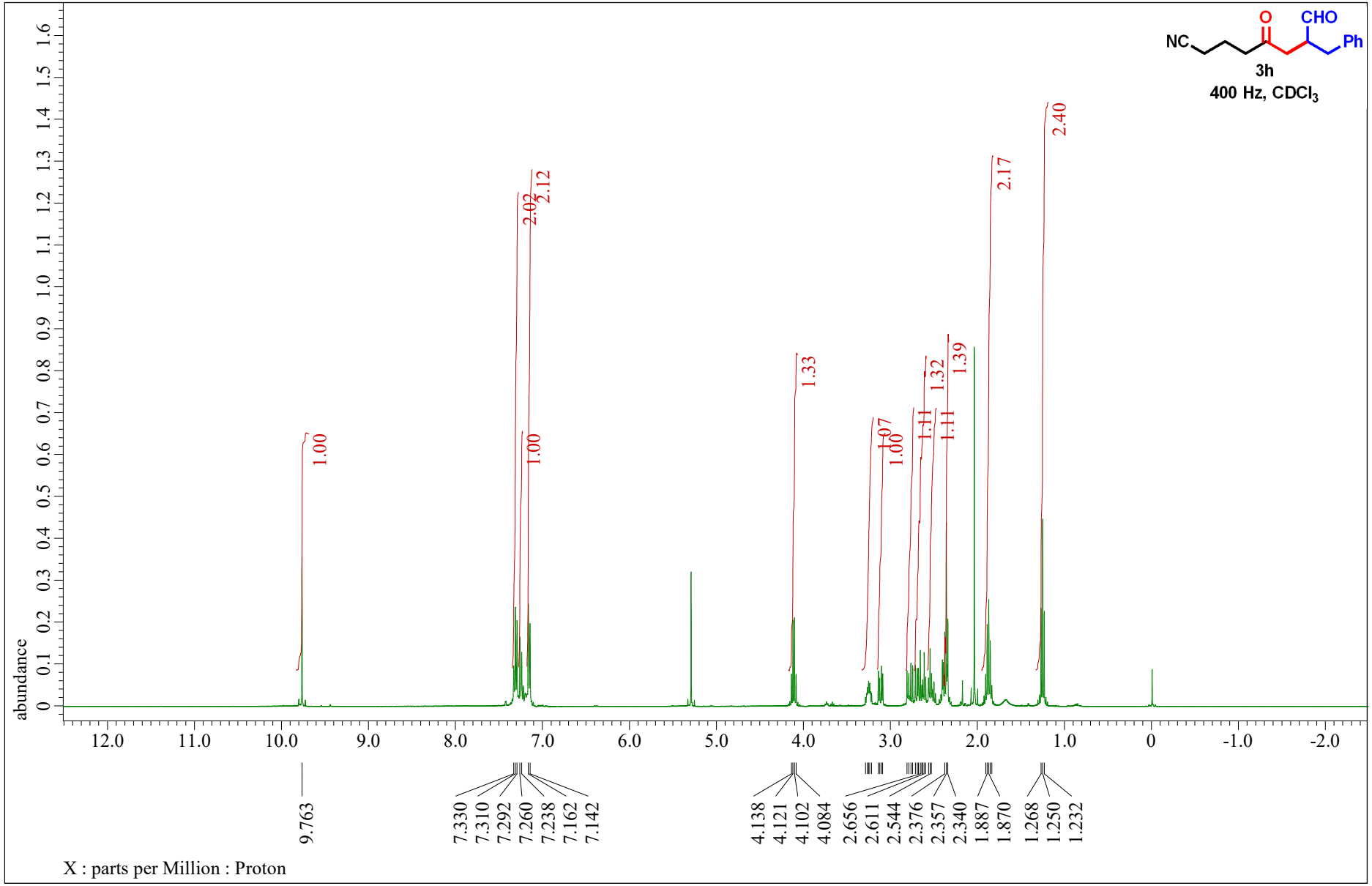

Cl
O
CHO
Ph
3f
100 Hz, CDCl3
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.498
202.620
137.822
128.938
128.747
126.782
77.000
48.434
44.275
40.883
39.464
34.472
26.154
X : parts per Million : Carbon13

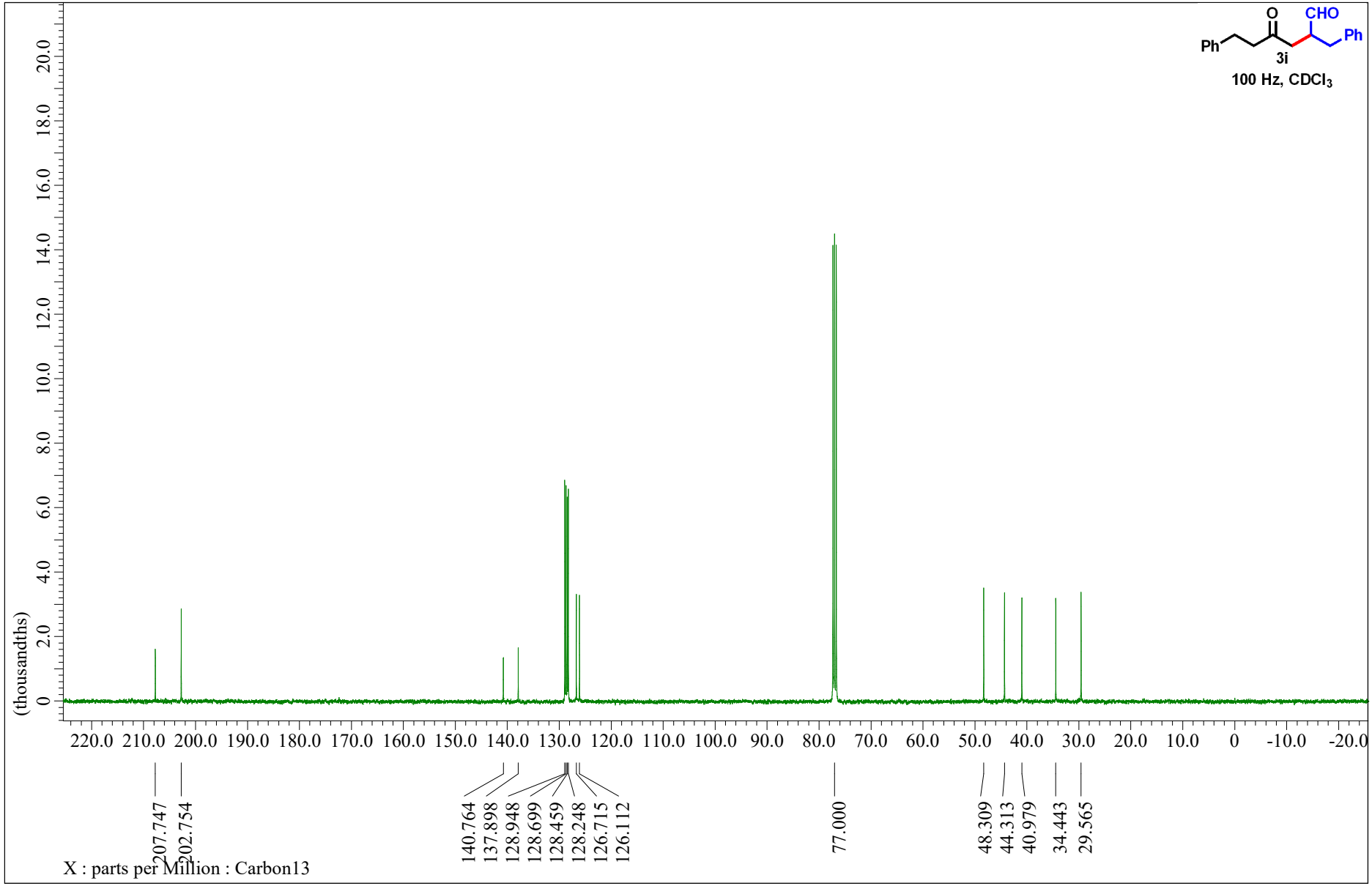

Cl
Ph
O
CHO
3f
400 Hz, CDCl3
abundance
1.00
2.26
2.19
1.17
2.18
1.05
1.04
1.07
1.11
1.02
2.23
2.19
9.779
7.328
7.309
7.291
7.260
7.237
7.218
7.166
7.148
3.545
3.530
3.514
3.091
2.792
2.772
2.603
2.585
2.565
2.444
2.433
2.034
2.018
2.002
1.984
1.968
X : parts per Million : Proton

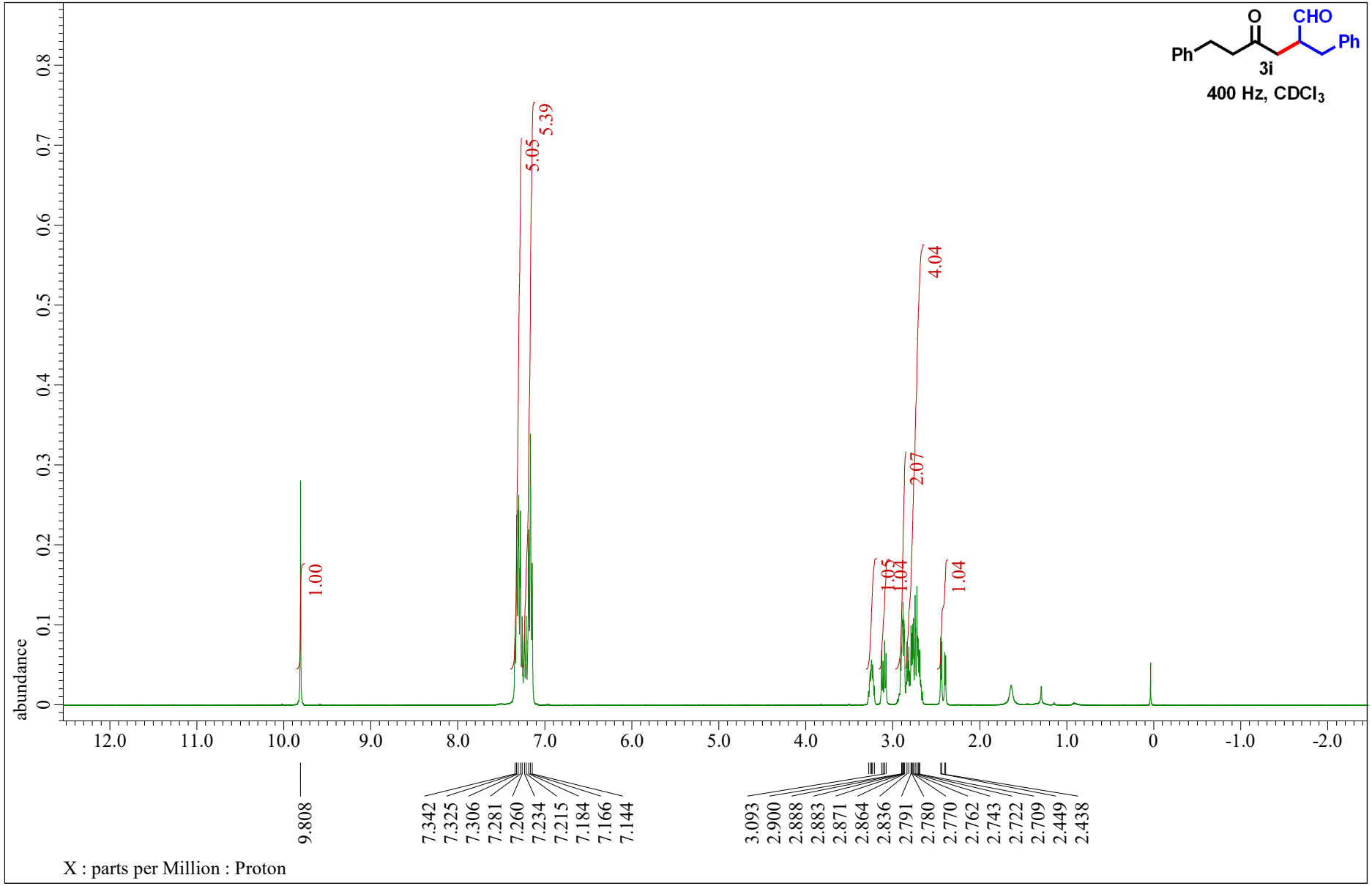

O
CHO
Cl
Ph
3g
100 Hz, CDCl3
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.227
202.880
137.996
129.064
128.854
126.889
48.493
44.708
41.909
40.865
34.579
31.857
20.971
X : parts per Million : Carbon13

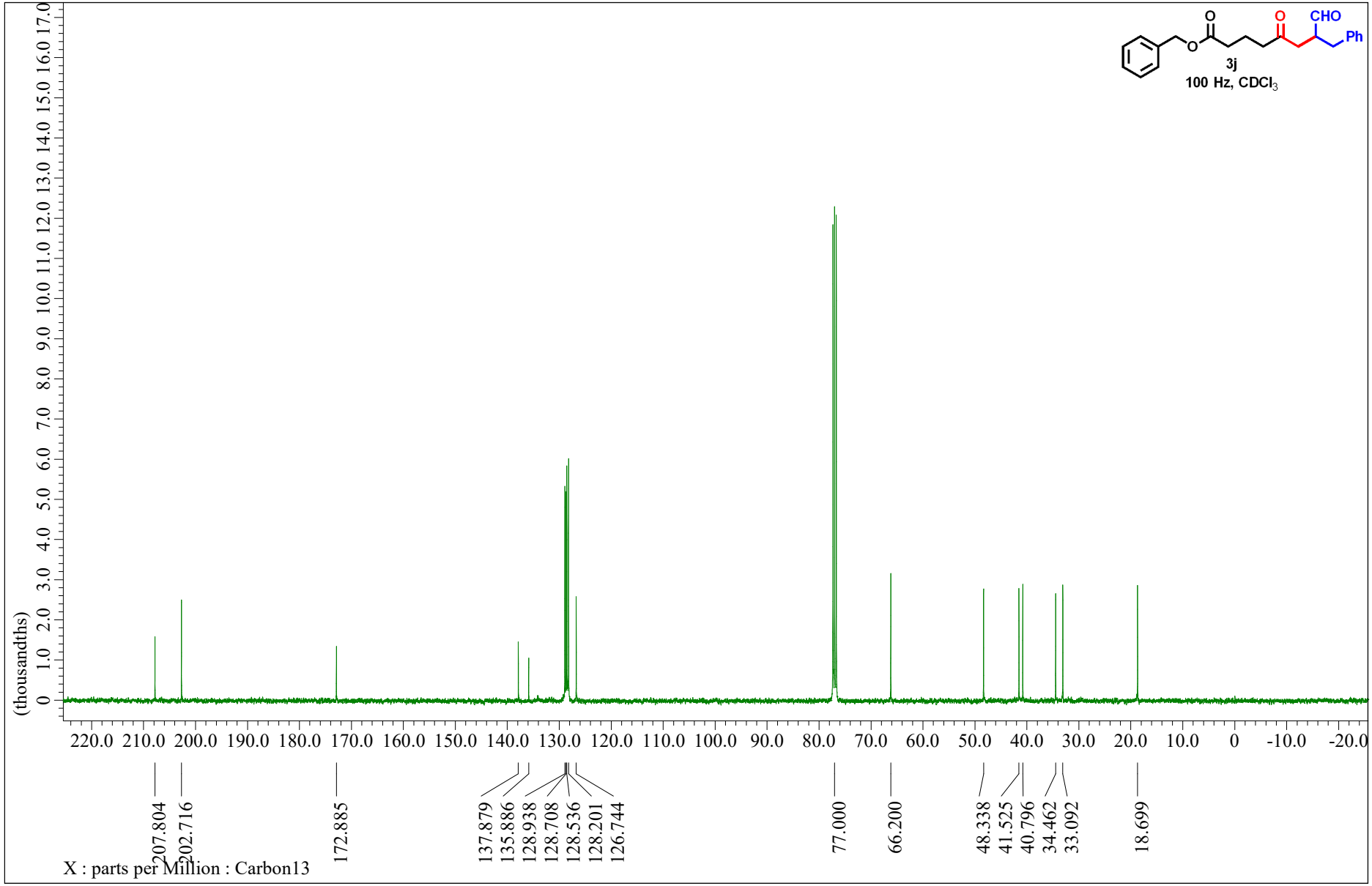

O
CHO
Cl
Ph
3g
400 Hz, CDCl3
abundance
2.0
1.0
0
4.48
3.20
2.19
2.21
1.97
1.00
0.97
1.01
1.01
1.06
1.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.792
7.332
7.315
7.295
7.266
7.260
7.242
7.223
7.171
7.154
3.529
3.514
3.498
3.095
2.783
2.762
2.729
2.451
2.425
2.414
2.408
2.380
1.771
1.753
1.736
1.713
1.705
1.689
1.673
1.665
X : parts per Million : Proton

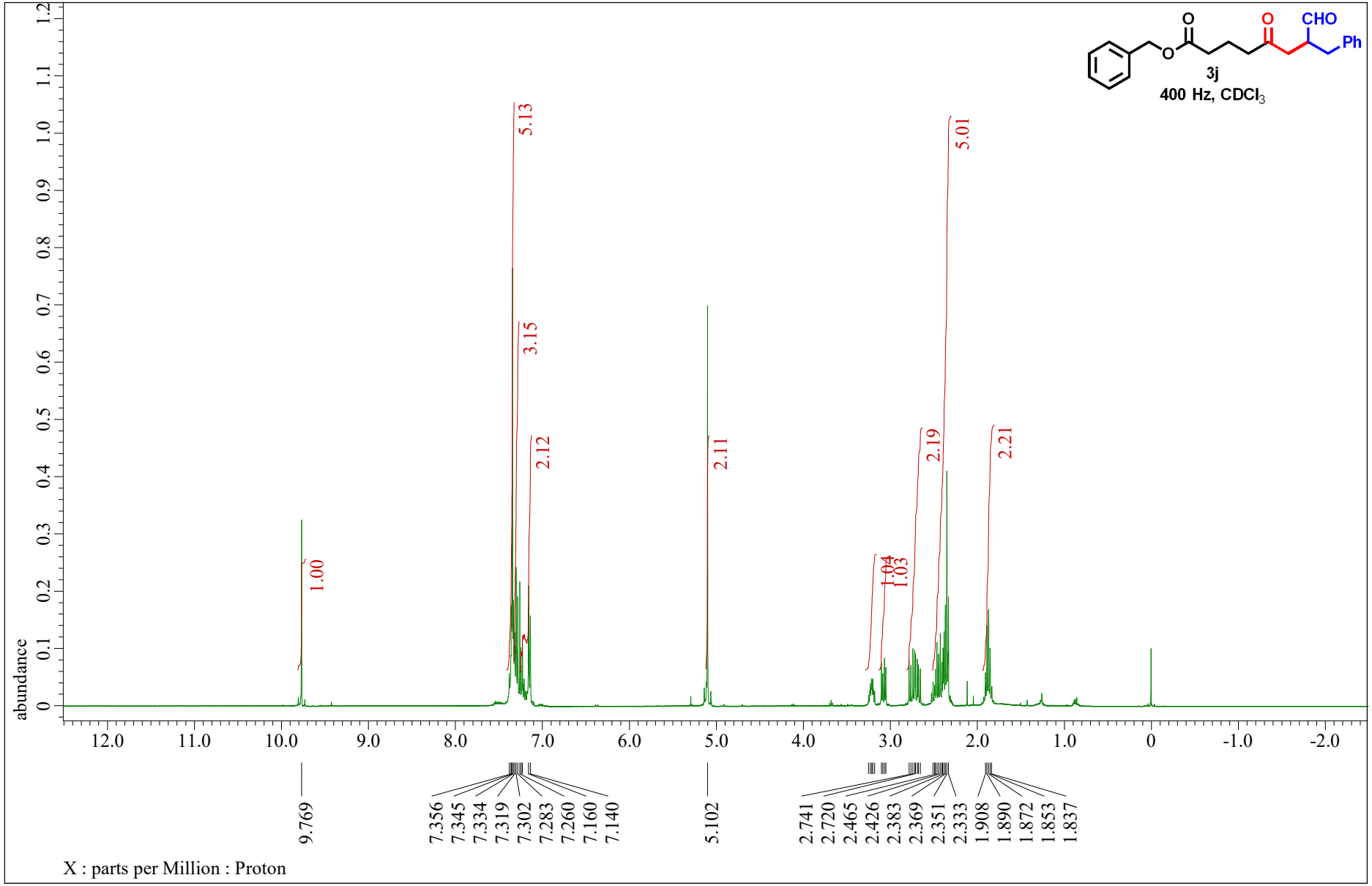

NC
O
CHO
Ph
3h
100 Hz, CDCl3
(thousandths)
30.0
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.039
202.583
137.775
129.026
128.748
126.975
119.319
60.481
48.752
40.836
40.635
34.540
21.134
19.313
16.448
14.273
X : parts per Million : Carbon13

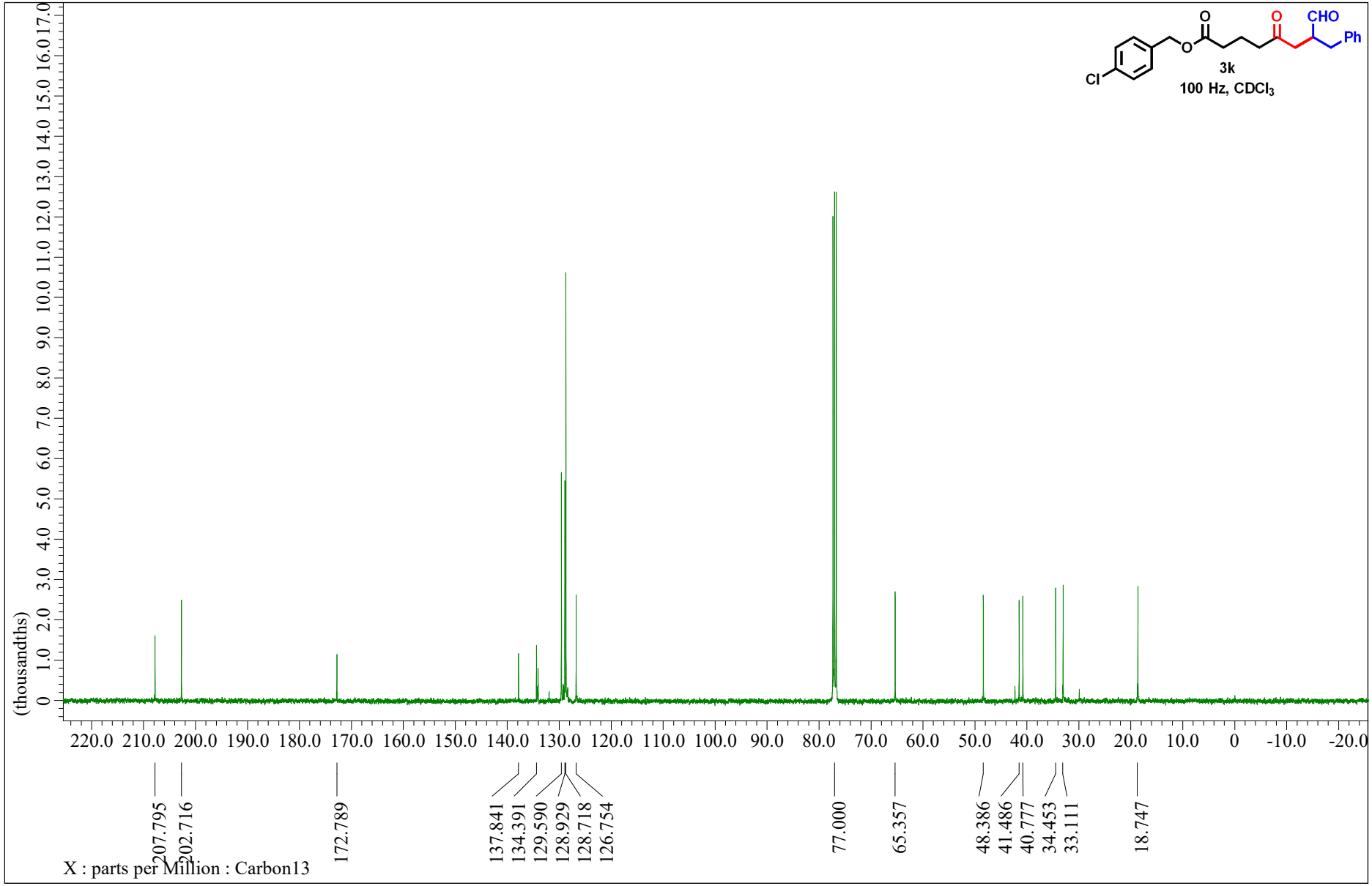

NC
O
CHO
Ph
3h
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
2.02
2.12
1.00
1.33
1.07
1.00
1.11
1.32
1.11
1.39
2.17
2.40
9.763
7.330
7.310
7.292
7.260
7.238
7.162
7.142
4.138
4.121
4.102
4.084
2.656
2.611
2.544
2.376
2.357
2.340
1.887
1.870
1.268
1.250
1.232

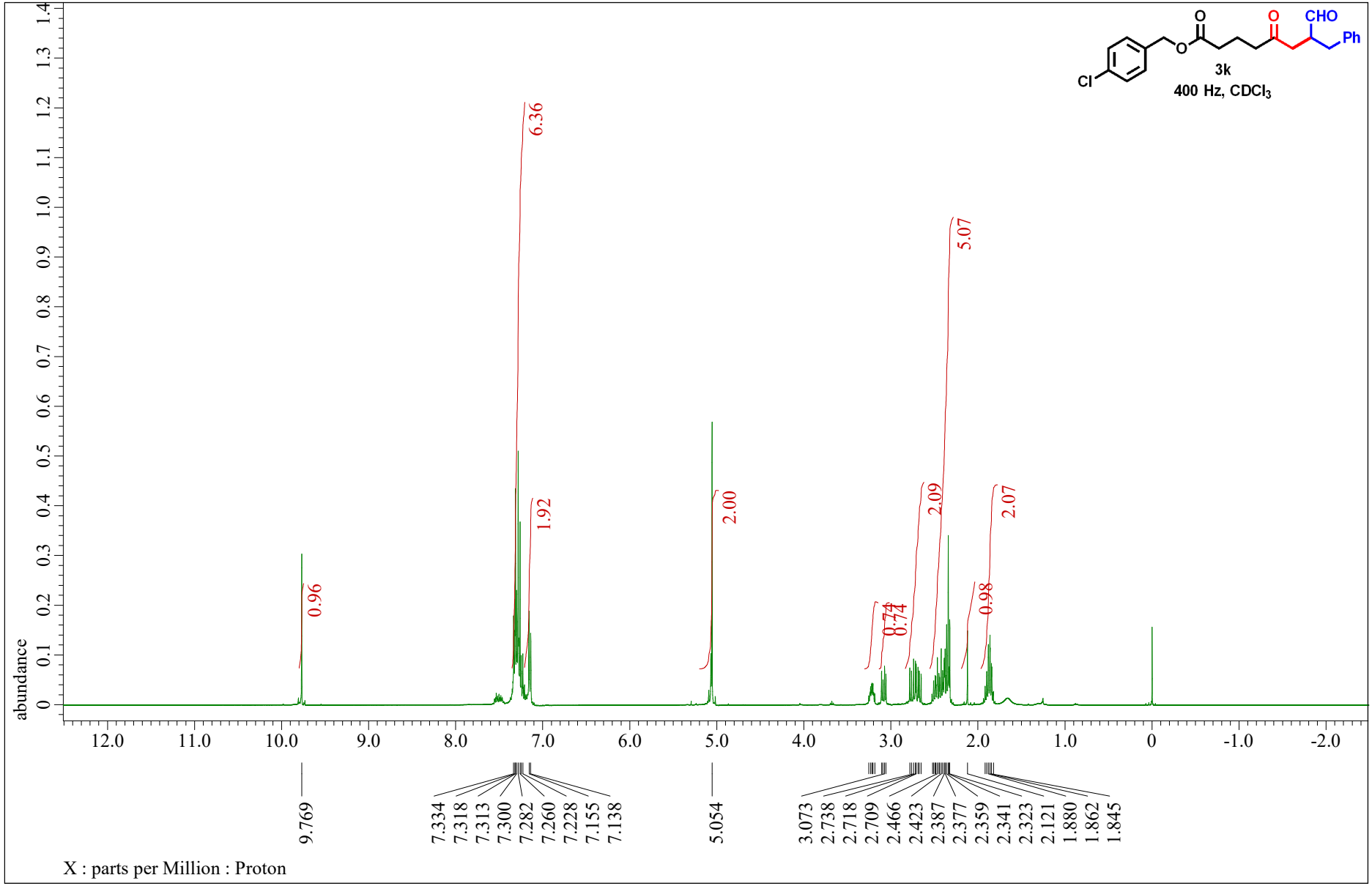

O
CHO
Ph
Ph
3i
100 Hz, CDCl3
(thousandths)
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.747
202.754
140.764
137.898
128.948
128.699
128.459
128.248
126.715
126.112
77.000
48.309
44.313
40.979
34.443
29.565
X : parts per Million : Carbon13

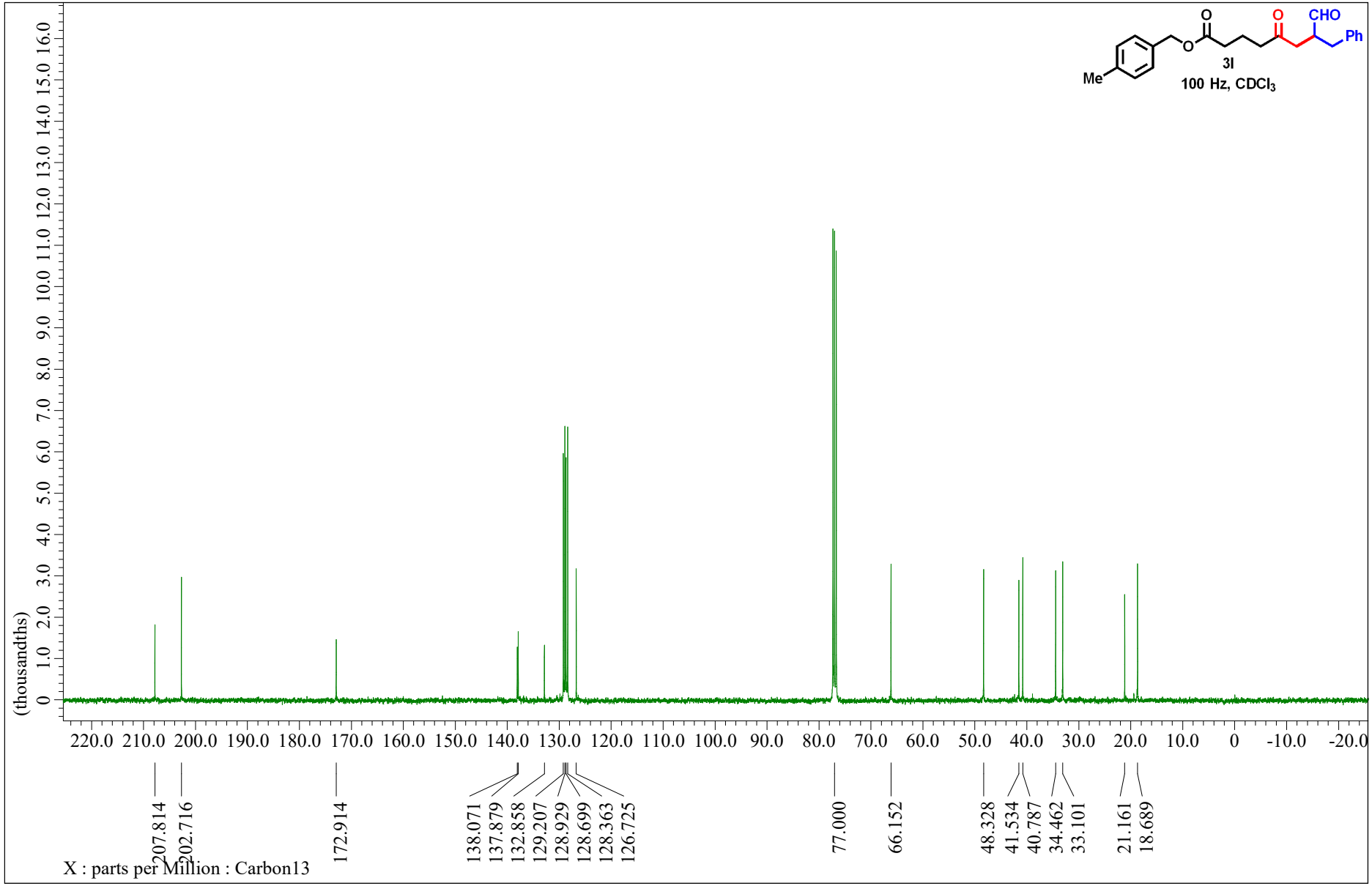

O
CHO
Ph
Ph
3i
400 Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
1.00
5.05
5.39
1.05
1.04
2.07
4.04
1.04
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.808
7.342
7.325
7.306
7.281
7.260
7.234
7.215
7.184
7.166
7.144
3.093
2.900
2.888
2.883
2.871
2.864
2.836
2.791
2.780
2.770
2.762
2.743
2.722
2.709
2.449
2.438
X : parts per Million : Proton

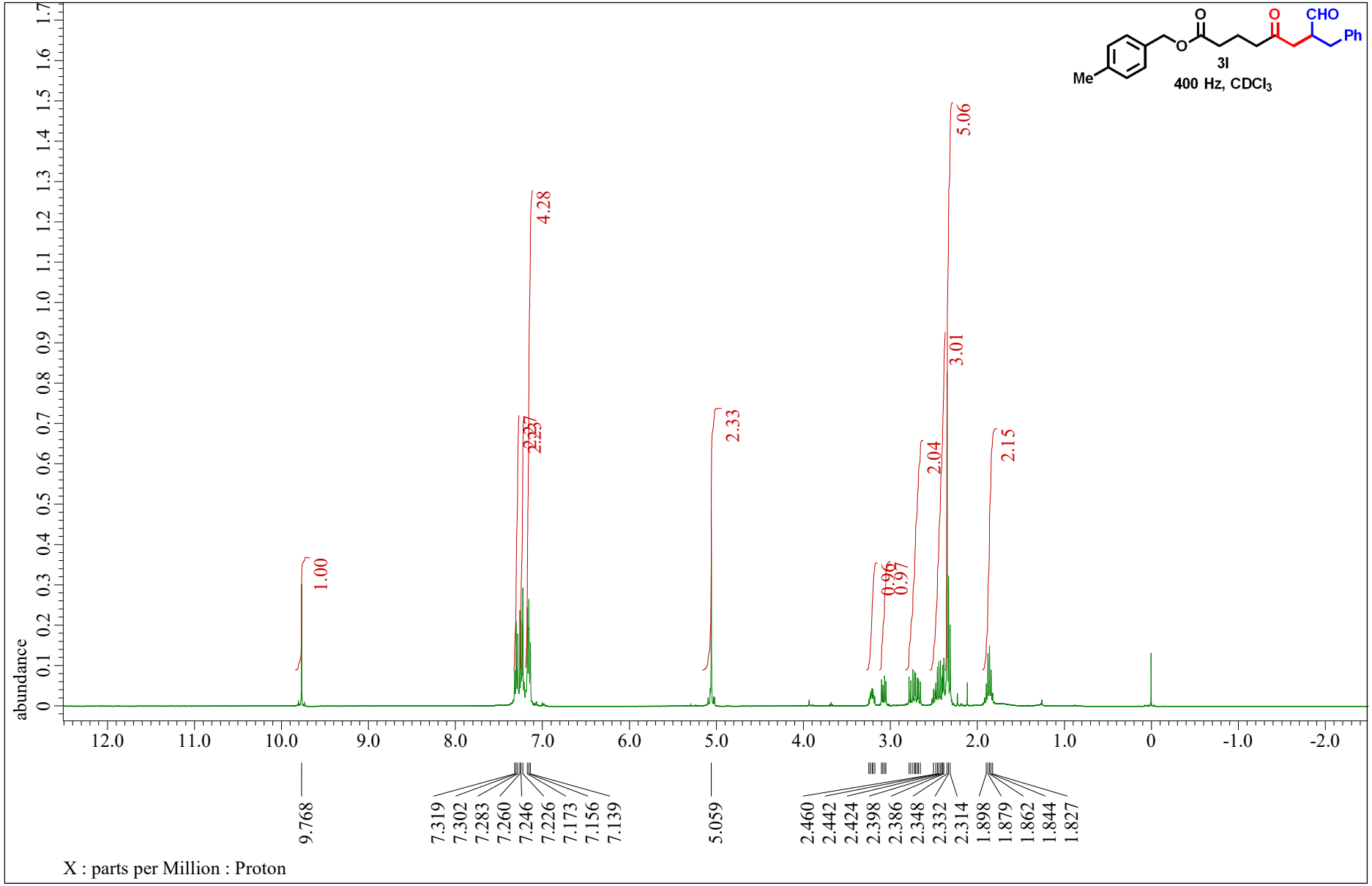

3j
100 Hz, CDCl3
CHO
Ph
(thousandths)
X : parts per Million : Carbon13
207.804
202.716
172.885
137.879
135.886
128.938
128.708
128.536
128.201
126.744
77.000
66.200
48.338
41.525
40.796
34.462
33.092
18.699

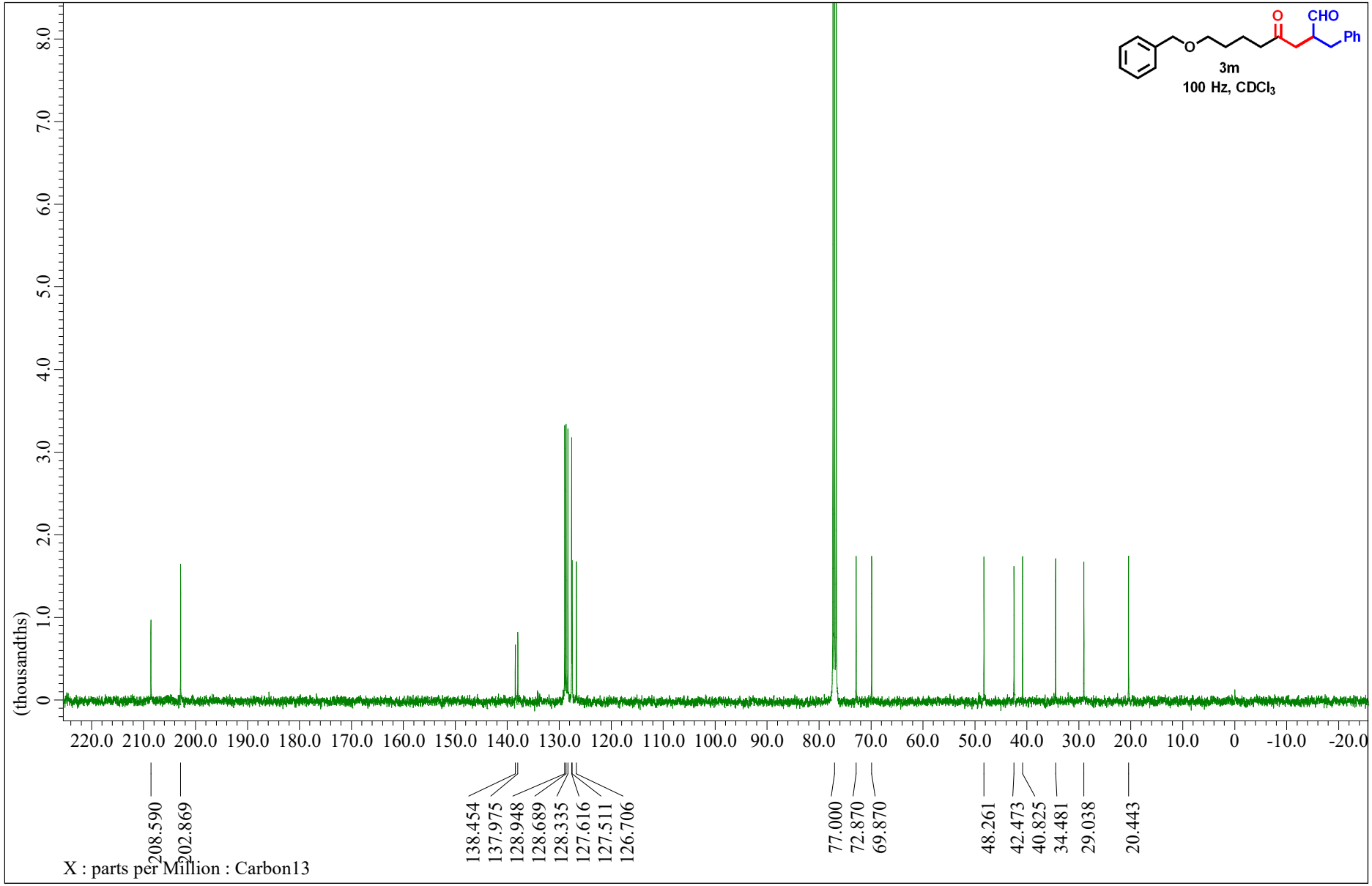

3j
400 Hz, CDCl3
abundance
X : parts per Million : Proton
5.13
3.15
2.12
1.00
2.11
5.01
2.19
2.21
1.04
1.03
9.769
7.356
7.345
7.334
7.319
7.302
7.283
7.260
7.160
7.140
5.102
2.741
2.720
2.465
2.426
2.383
2.369
2.351
2.333
1.908
1.890
1.872
1.853
1.837

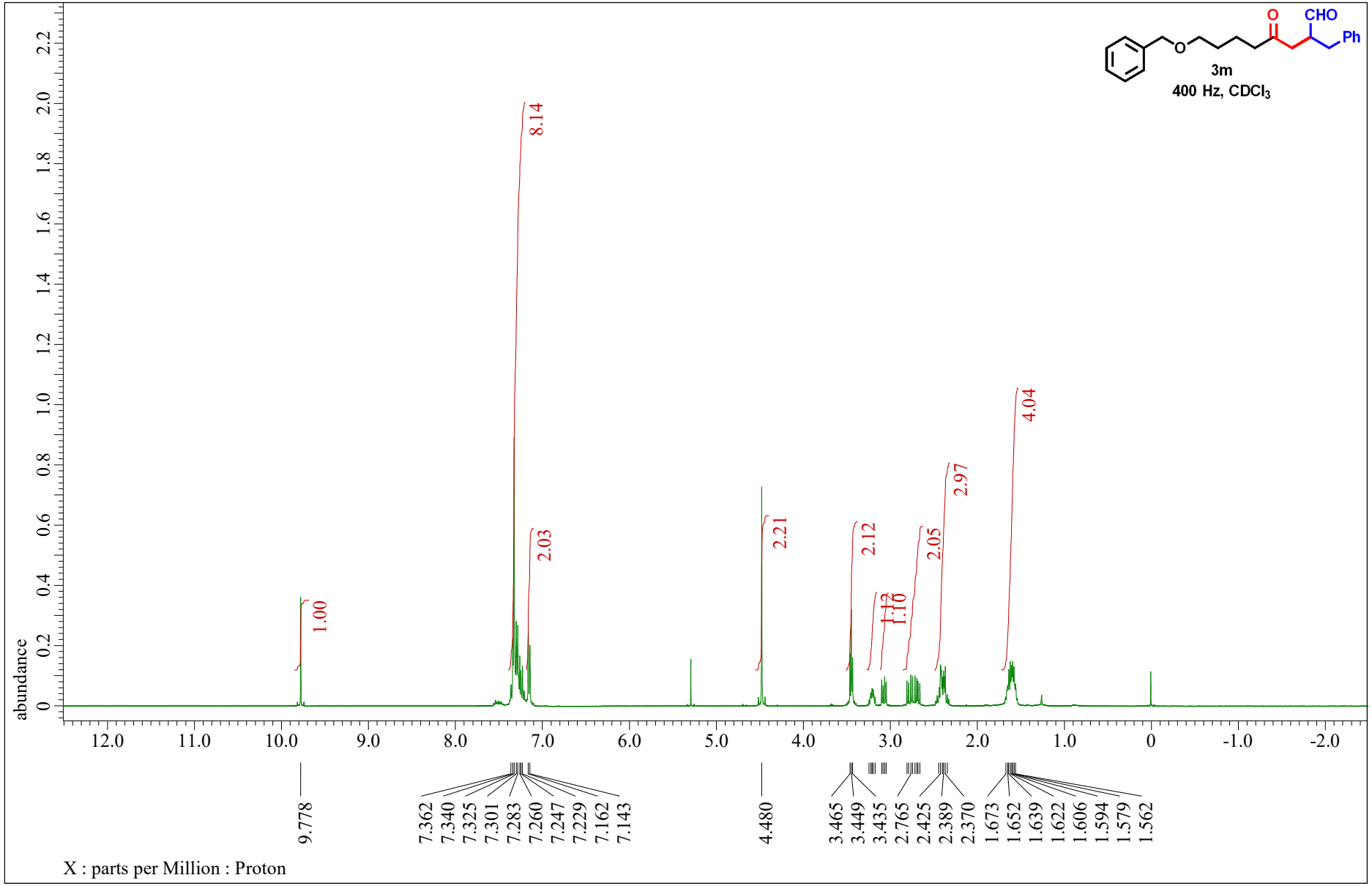

3k
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
207.795
202.716
172.789
137.841
134.391
129.590
128.929
128.718
126.754
77.000
65.357
48.386
41.486
40.777
34.453
33.111
18.747

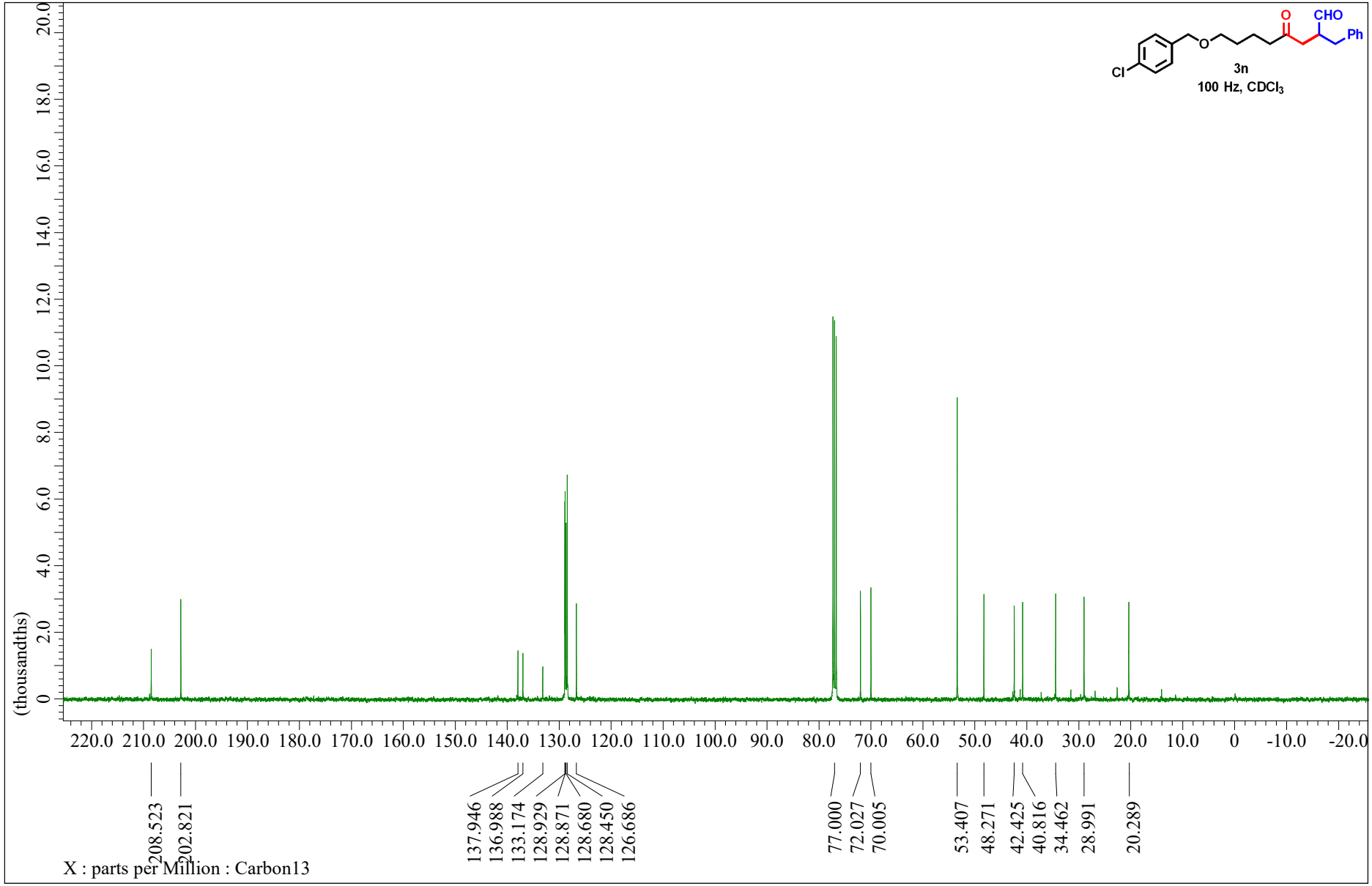

3k
400 Hz, CDCl3
abundance
X : parts per Million : Proton
6.36
5.07
2.00
1.92
2.09
2.07
0.96
0.98
9.769
7.334
7.318
7.313
7.300
7.282
7.260
7.228
7.155
7.138
5.054
3.073
2.738
2.718
2.709
2.466
2.423
2.387
2.377
2.359
2.341
2.323
2.121
1.880
1.862
1.845

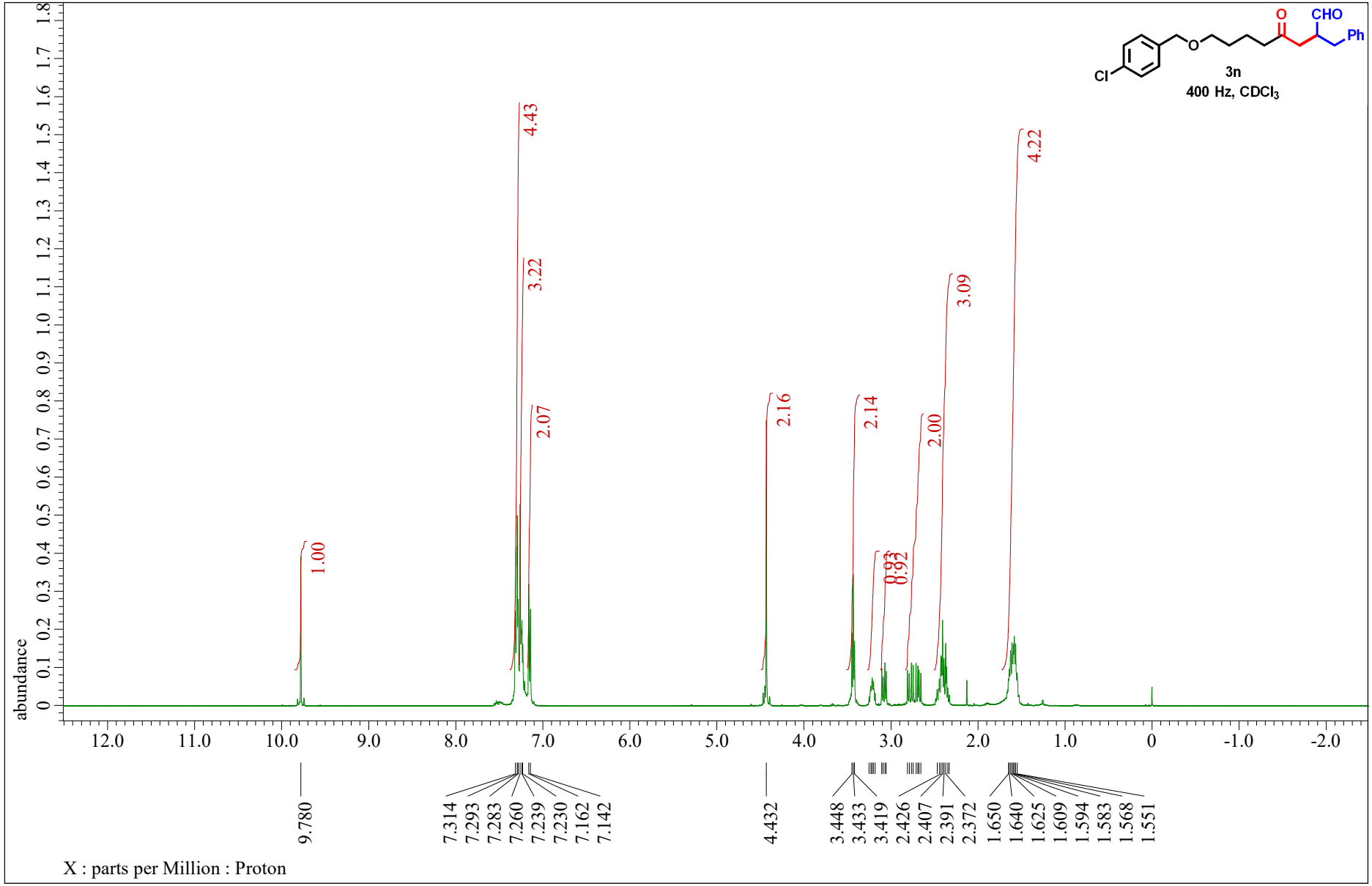

3l
100 Hz, CDCl3
Me
O
O
CHO
Ph
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.814
202.716
172.914
138.071
137.879
132.858
129.207
128.929
128.699
128.363
126.725
77.000
66.152
48.328
41.534
40.787
34.462
33.101
21.161
18.689
X : parts per Million : Carbon13

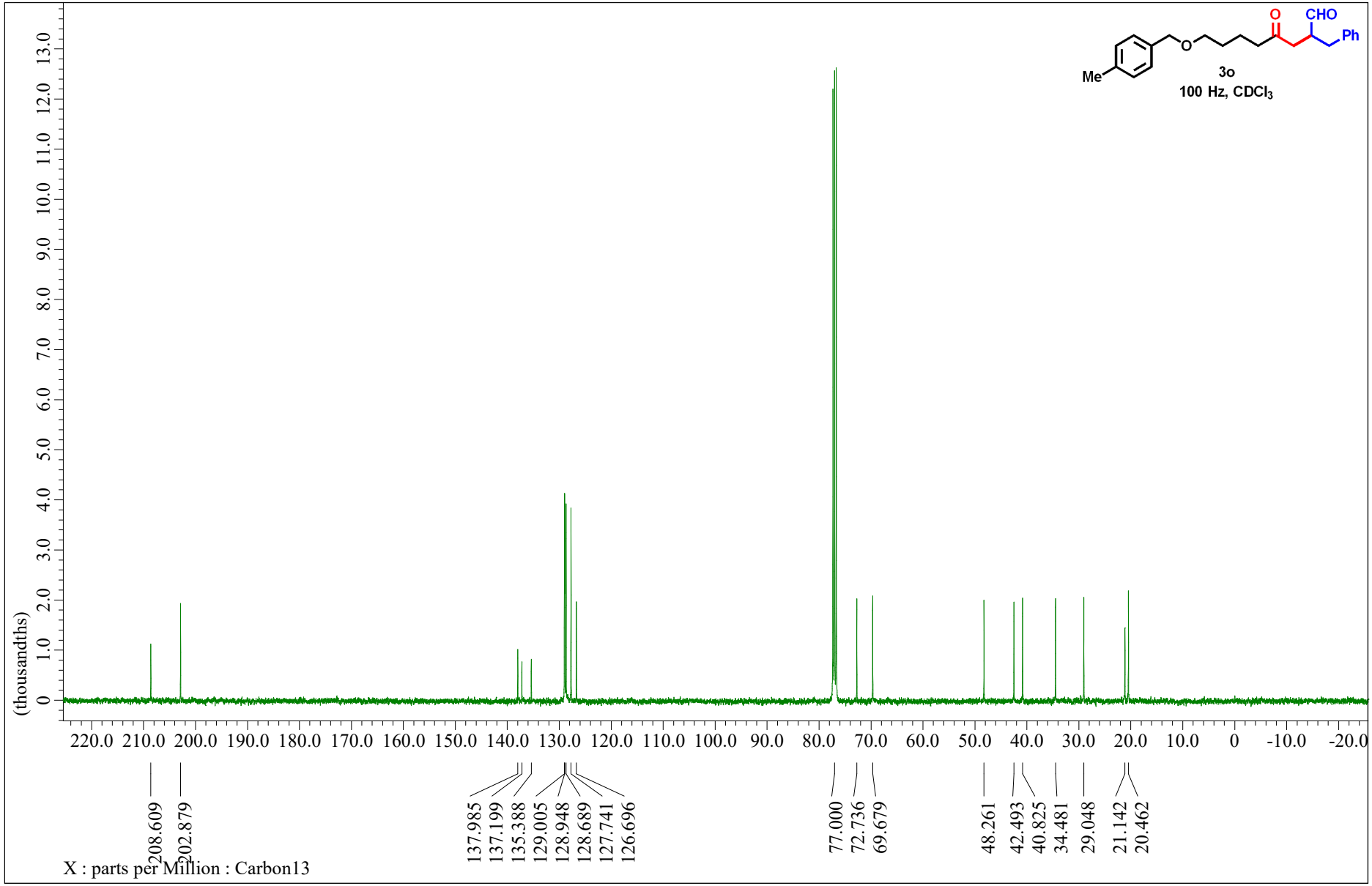

3l
400 Hz, CDCl3
Me
Ph
CHO
abundance
X : parts per Million : Proton
1.00
4.28
2.33
5.06
3.01
2.04
2.15
9.768
7.319
7.302
7.283
7.260
7.246
7.226
7.173
7.156
7.139
5.059
2.460
2.442
2.424
2.398
2.386
2.348
2.332
2.314
1.898
1.879
1.862
1.844
1.827

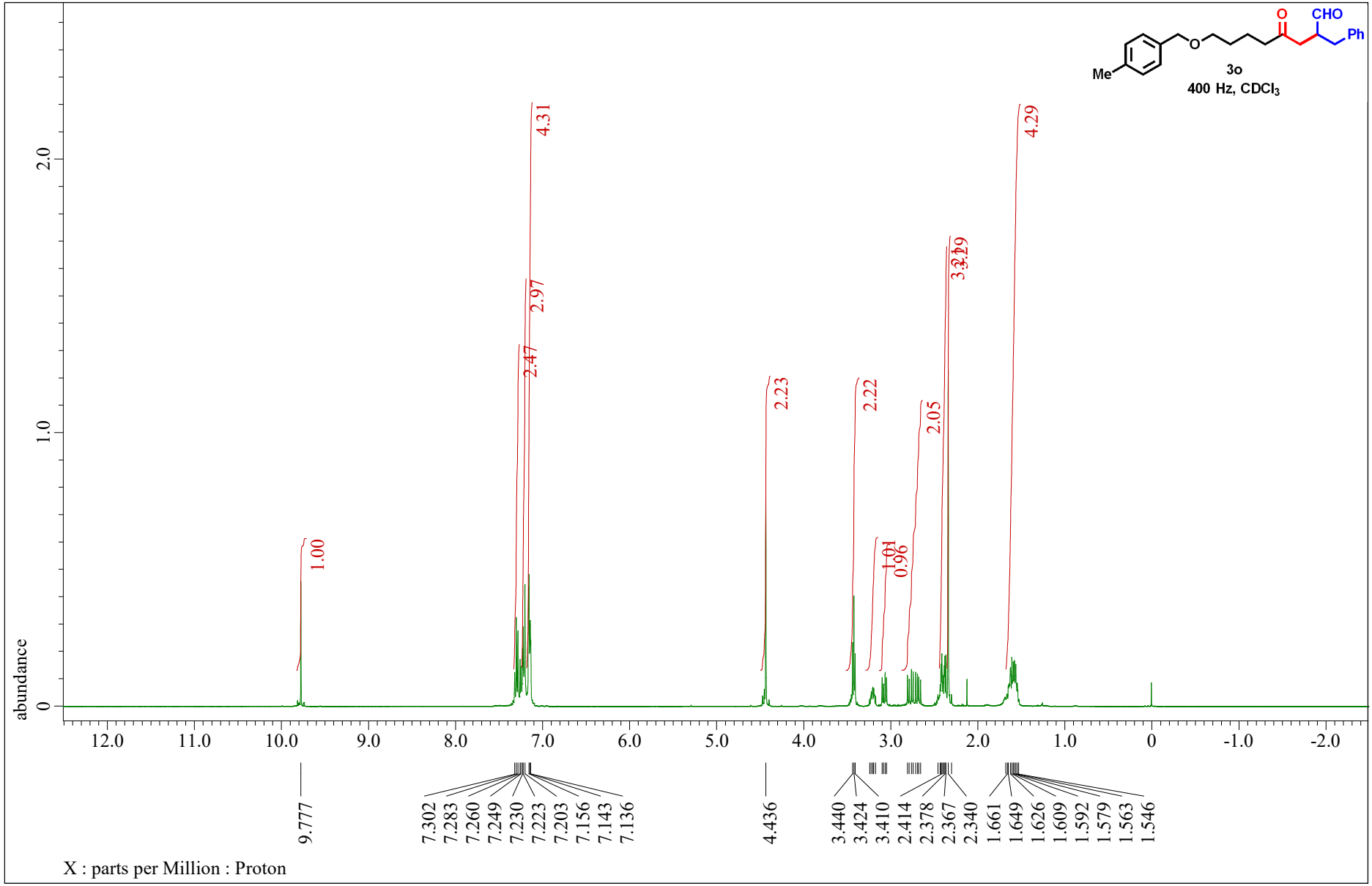

3m
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
208.590
202.869
138.454
137.975
128.948
128.689
128.335
127.616
127.511
126.706
77.000
72.870
69.870
48.261
42.473
40.825
34.481
29.038
20.443

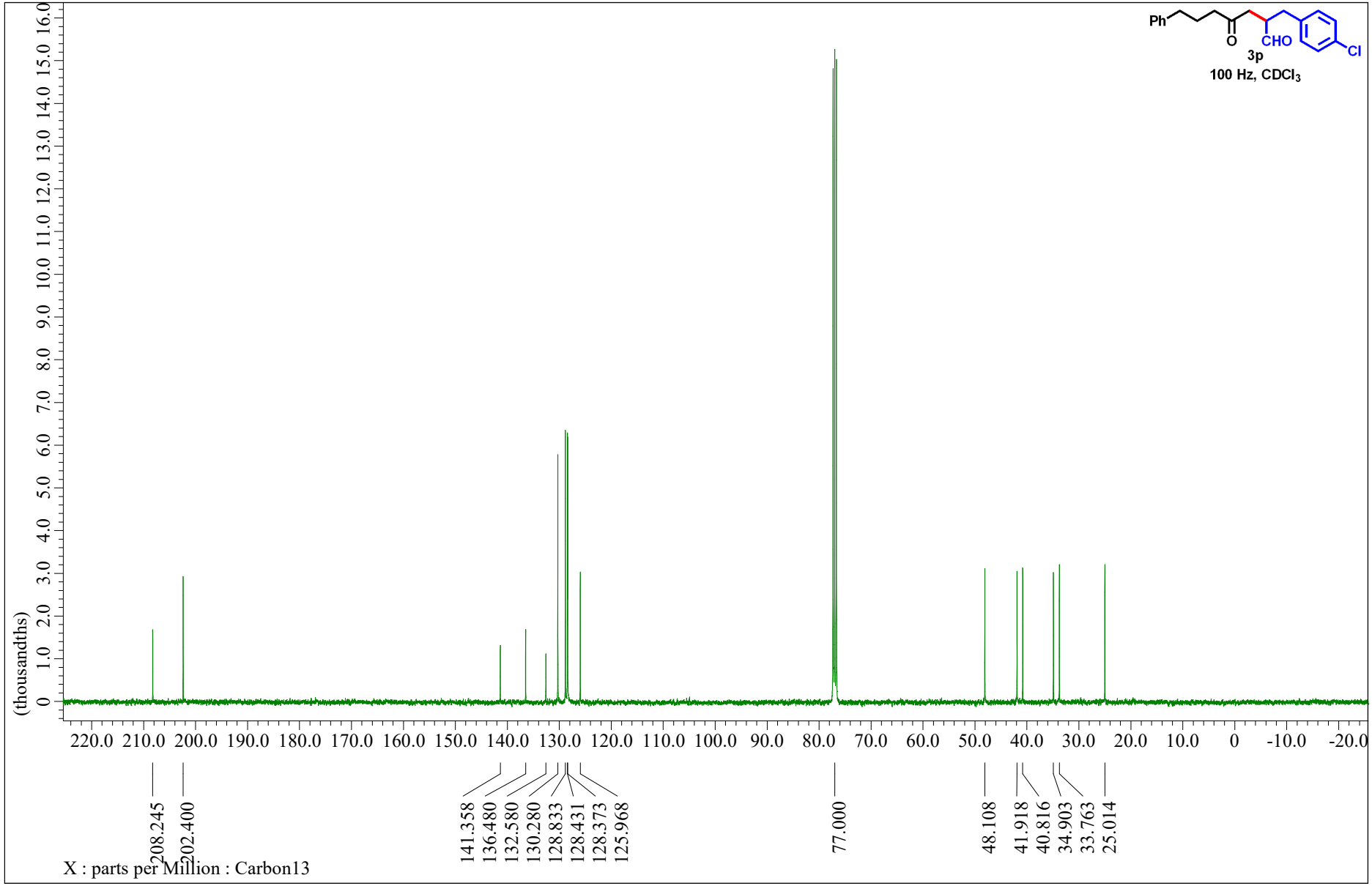

O
CHO
Ph
O
3m
400 Hz, CDCl3
abundance
8.14
4.04
2.97
2.21
2.12
2.05
2.03
1.00
1.12
1.10
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.778
7.362
7.340
7.325
7.301
7.283
7.260
7.247
7.229
7.162
7.143
4.480
3.465
3.449
3.435
2.765
2.425
2.389
2.370
1.673
1.652
1.639
1.622
1.606
1.594
1.579
1.562
X : parts per Million : Proton

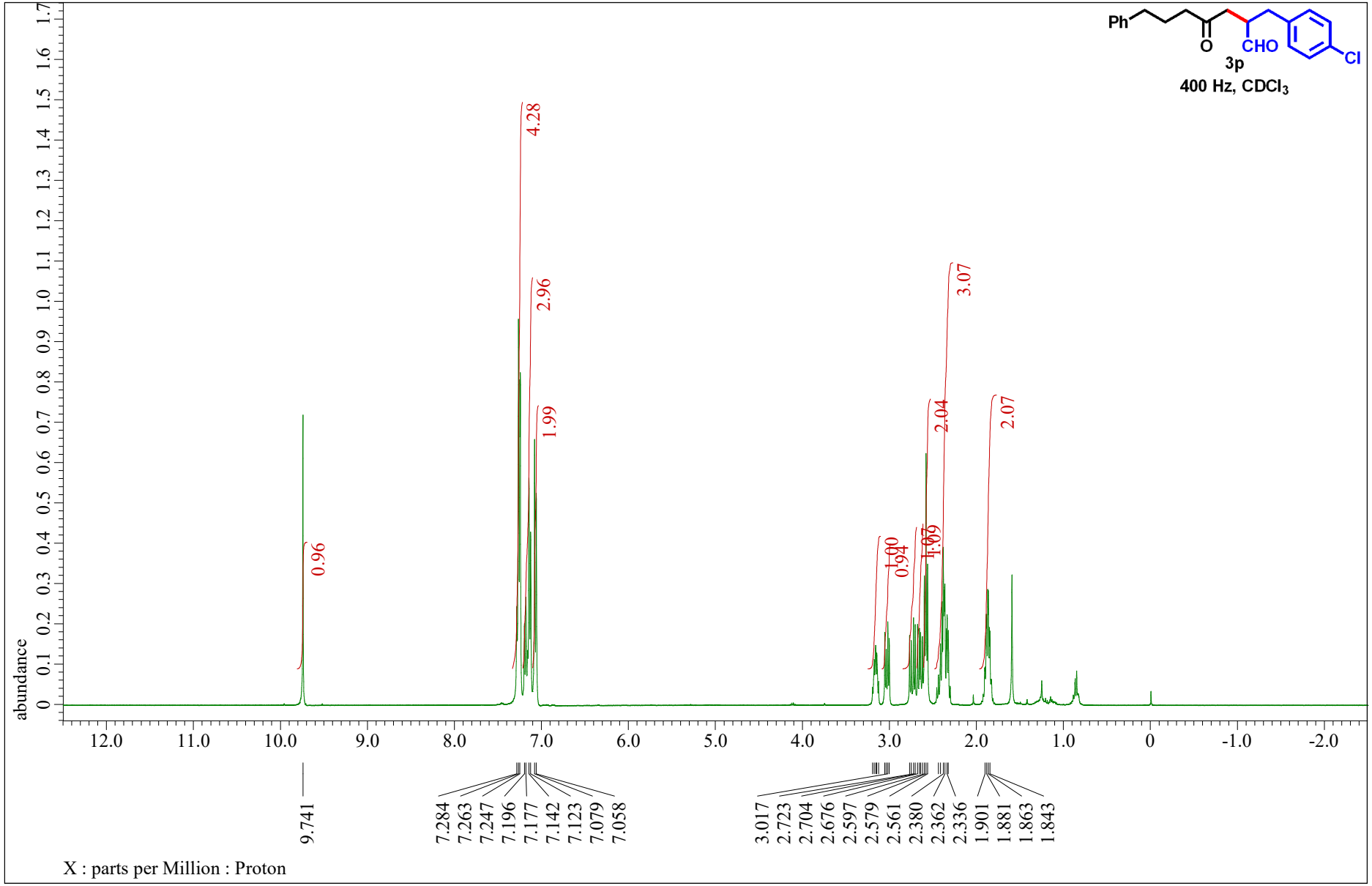

3n
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
208.523
202.821
137.946
136.988
133.174
128.929
128.871
128.680
128.450
126.686
77.000
72.027
70.005
53.407
48.271
42.425
40.816
34.462
28.991
20.289

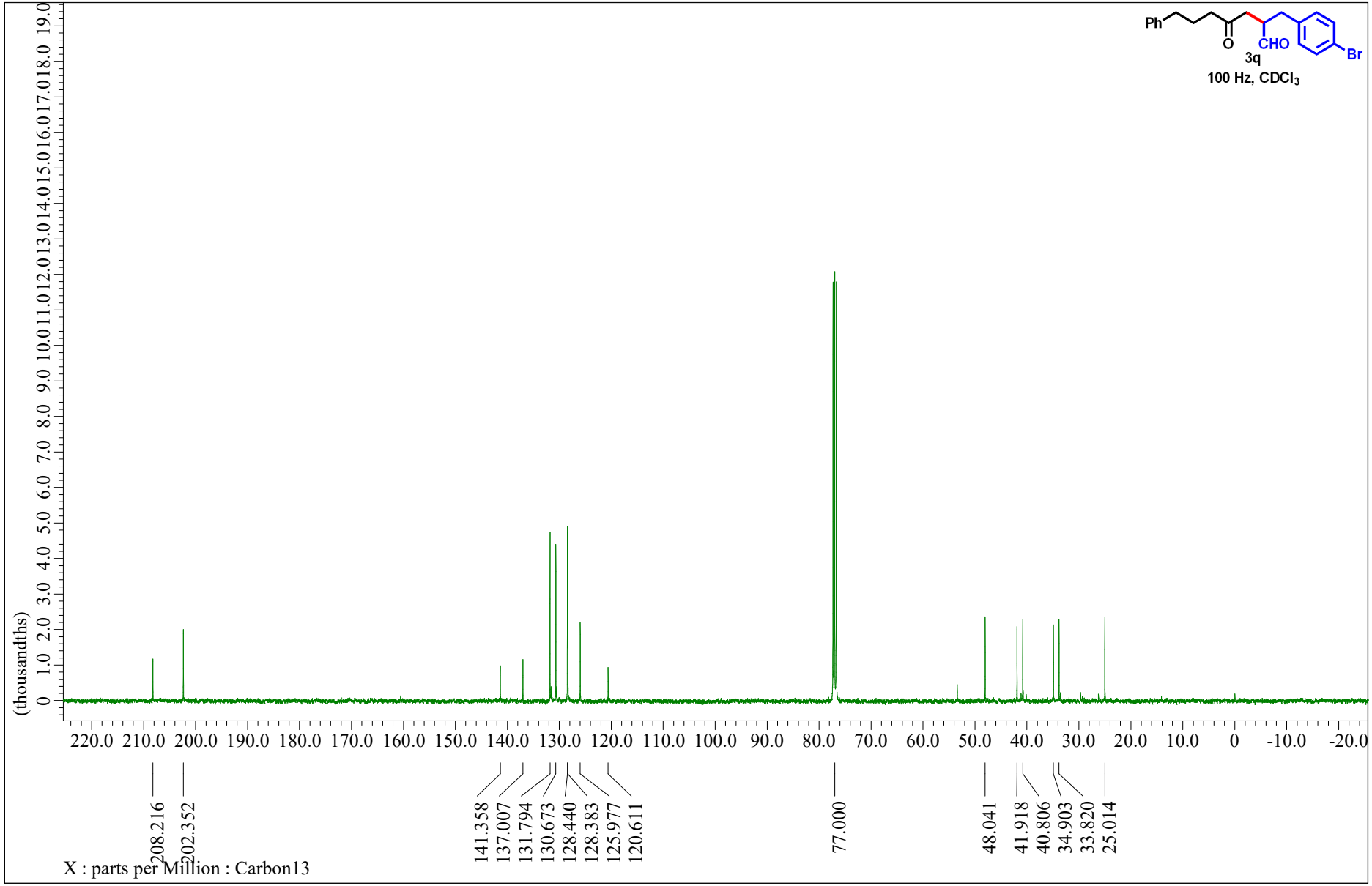

3n
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
4.43
3.22
2.07
2.16
2.14
0.93
0.92
2.00
3.09
4.22
9.780
7.314
7.293
7.283
7.260
7.239
7.230
7.162
7.142
4.432
3.448
3.433
3.419
2.426
2.407
2.391
2.372
1.650
1.640
1.625
1.609
1.594
1.583
1.568
1.551

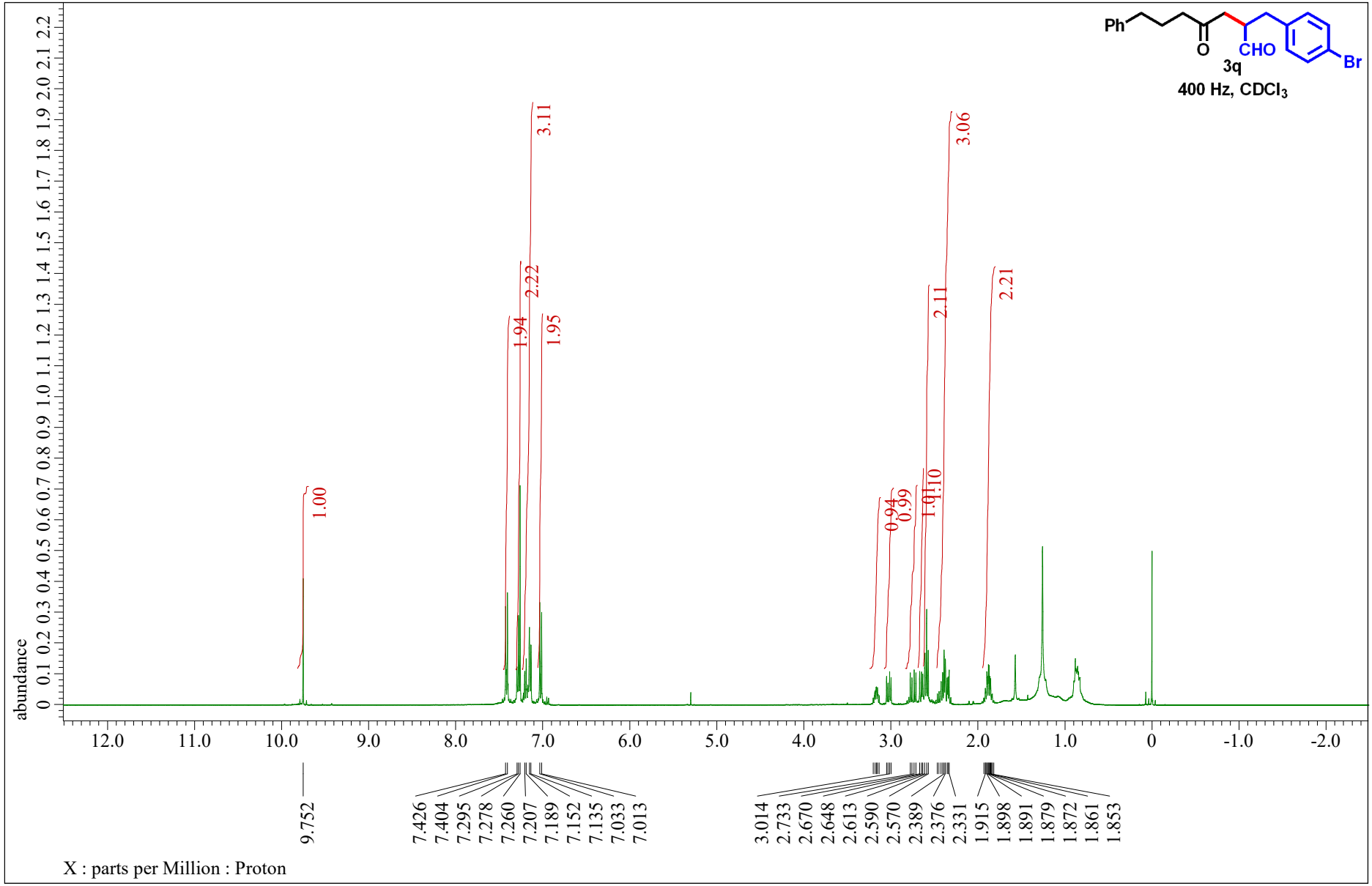

O
CHO
Ph
O
Me
3o
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.609
202.879
137.985
137.199
135.388
129.005
128.948
128.689
127.741
126.696
77.000
72.736
69.679
48.261
42.493
40.825
34.481
29.048
21.142
20.462
X : parts per Million : Carbon13

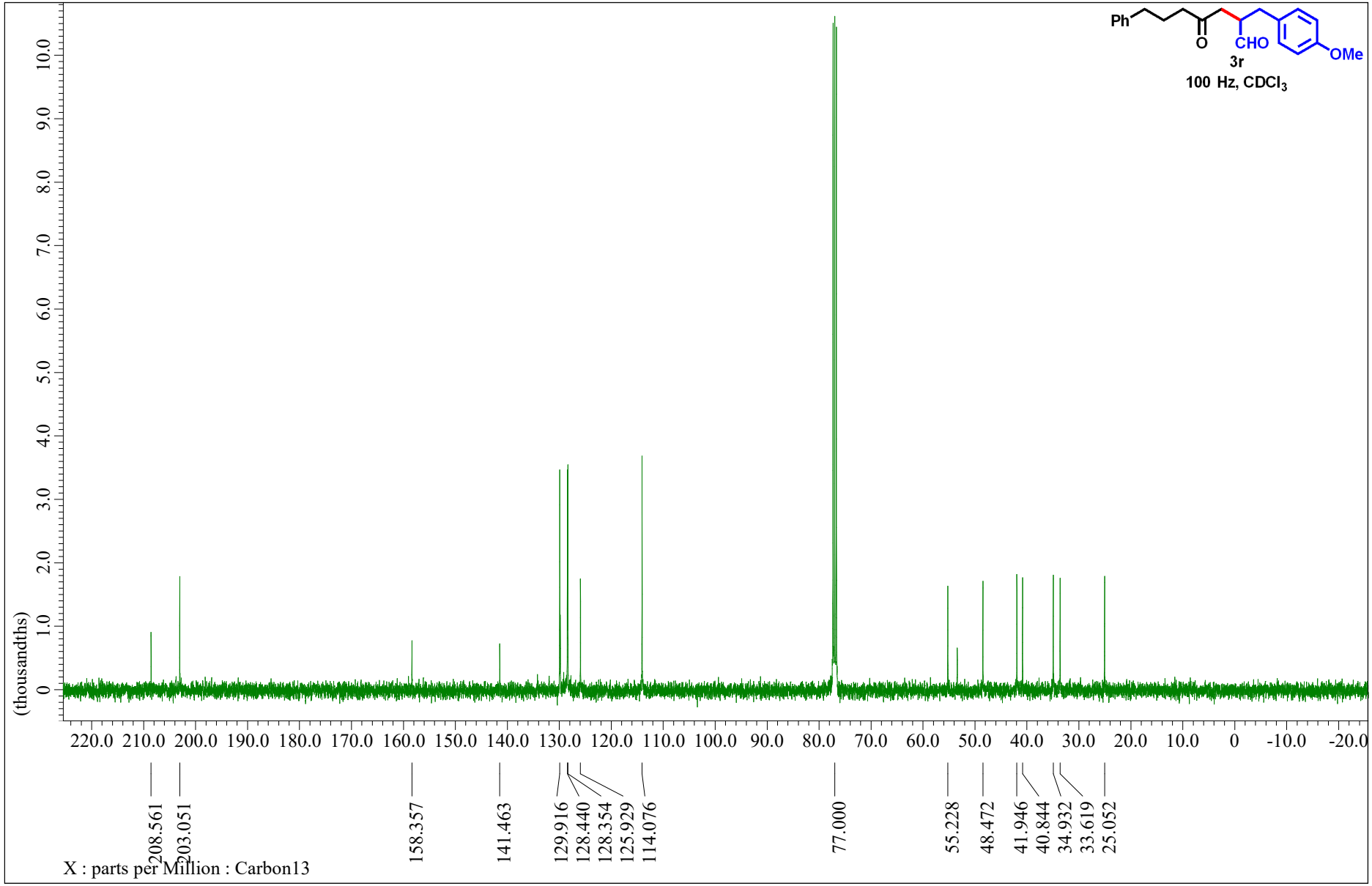

O
CHO
Ph
Me
3o
400 Hz, CDCl3
abundance
2.0
1.0
0
4.31
4.29
2.97
2.47
2.23
2.22
2.05
1.00
1.01
0.96
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.777
7.302
7.283
7.260
7.249
7.230
7.223
7.203
7.156
7.143
7.136
4.436
3.440
3.424
3.410
2.414
2.378
2.367
2.340
1.661
1.649
1.626
1.609
1.592
1.579
1.563
1.546
X : parts per Million : Proton

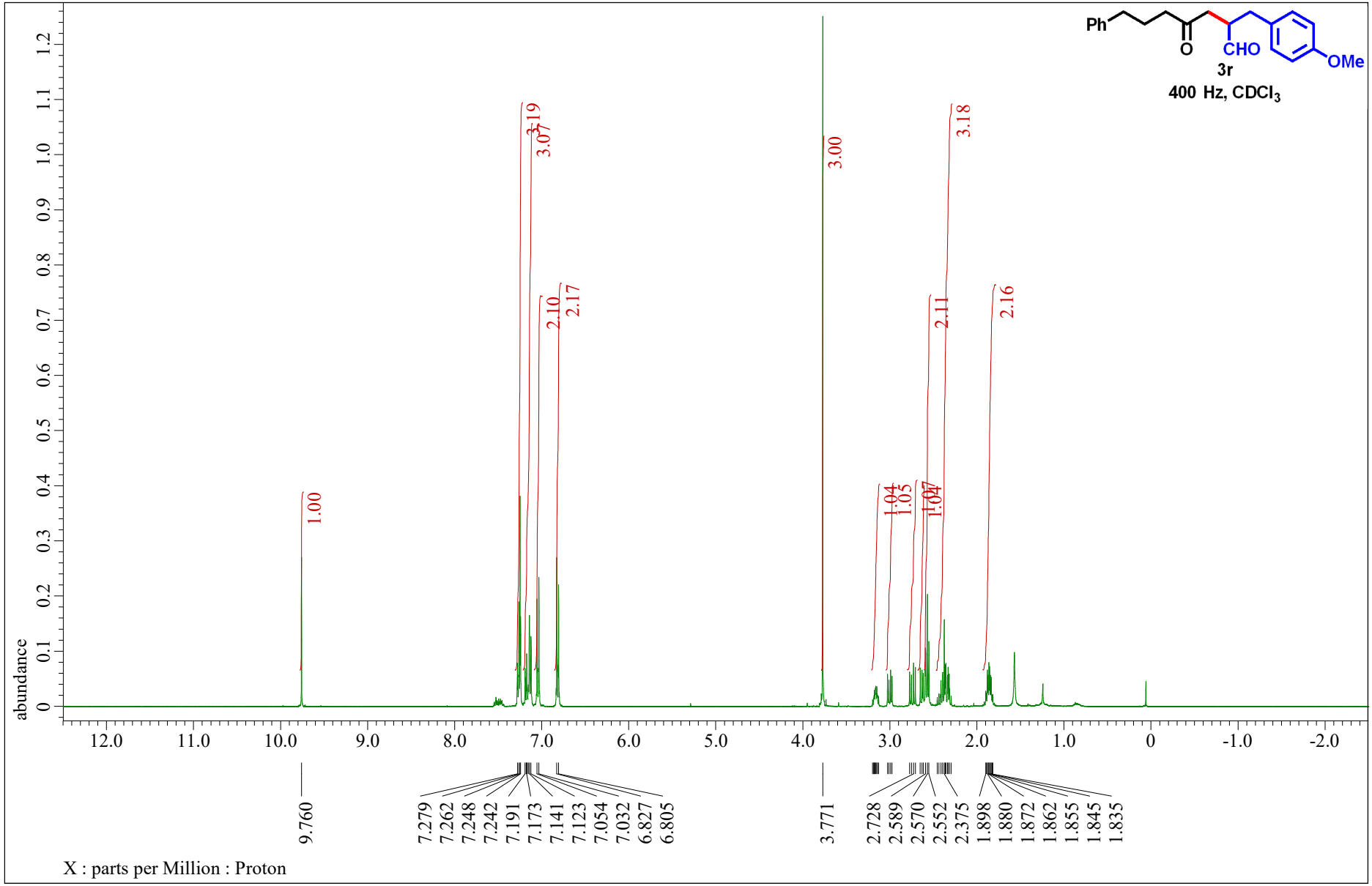

Ph
O
CHO
Cl
3p
100 Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.245
202.400
141.358
136.480
132.580
130.280
128.833
128.431
128.373
125.968
77.000
48.108
41.918
40.816
34.903
33.763
25.014
X : parts per Million : Carbon13

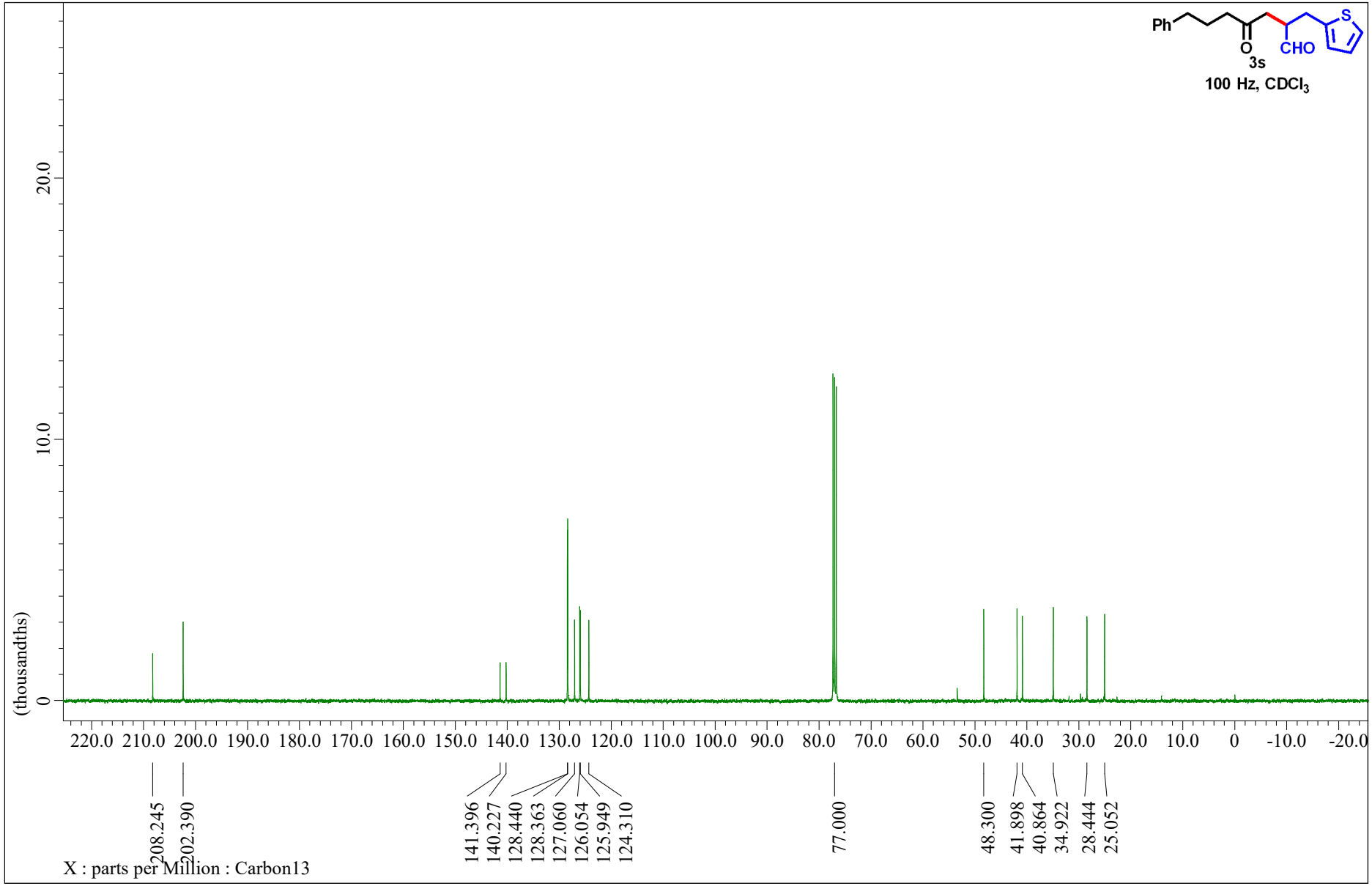

Ph
O
CHO
Cl
3p
400 Hz, CDCl3
abundance
4.28
2.96
1.99
0.96
3.07
2.04
2.07
1.00
0.94
1.05
1.09
9.741
7.284
7.263
7.247
7.196
7.177
7.142
7.123
7.079
7.058
3.017
2.723
2.704
2.676
2.597
2.579
2.561
2.380
2.362
2.336
1.901
1.881
1.863
1.843
X : parts per Million : Proton

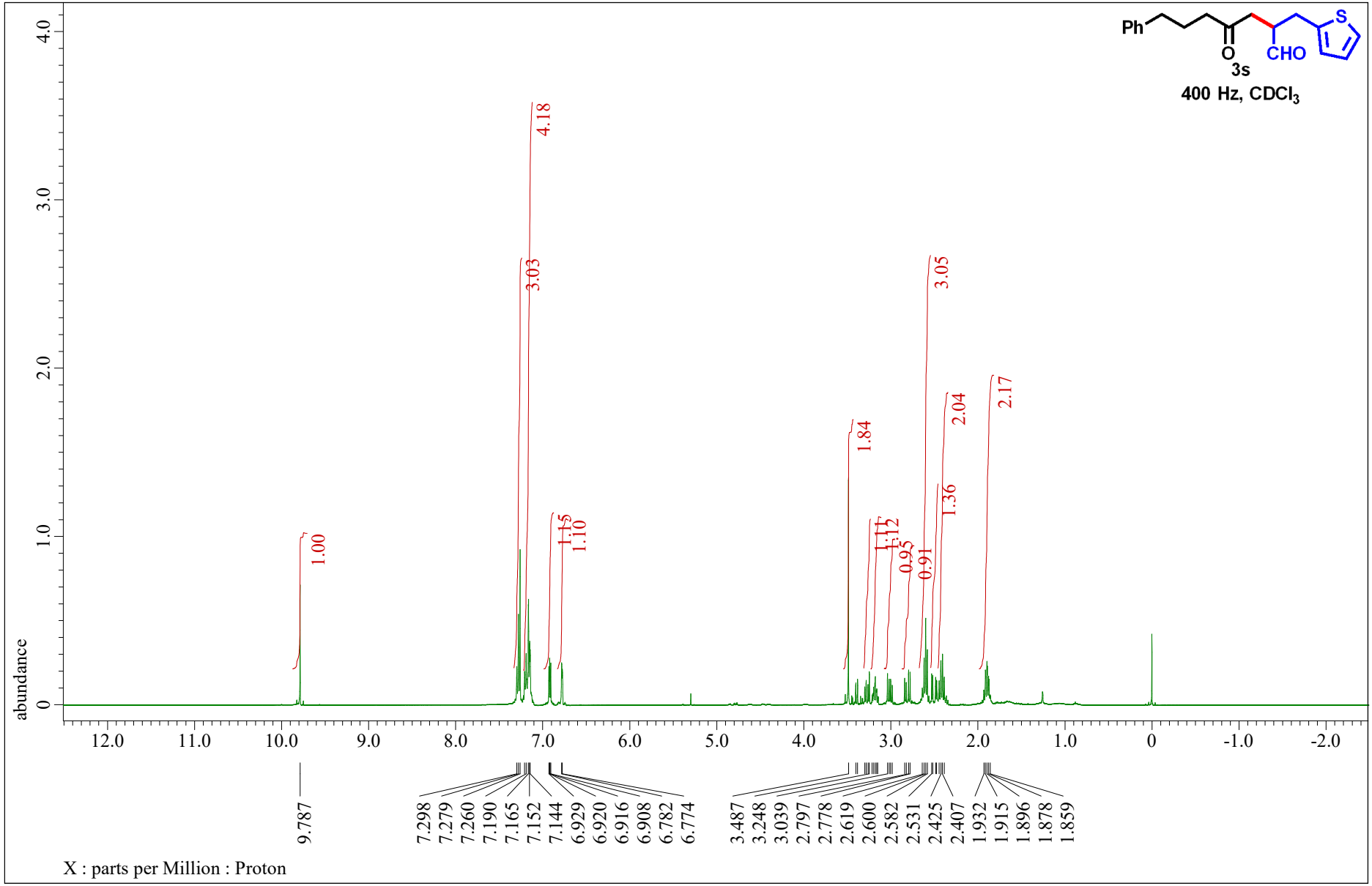

Ph
O
CHO
Br
3q
100 Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0 19.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.216
202.352
141.358
137.007
131.794
130.673
128.440
128.383
125.977
120.611
77.000
48.041
41.918
40.806
34.903
33.820
25.014
X : parts per Million : Carbon13

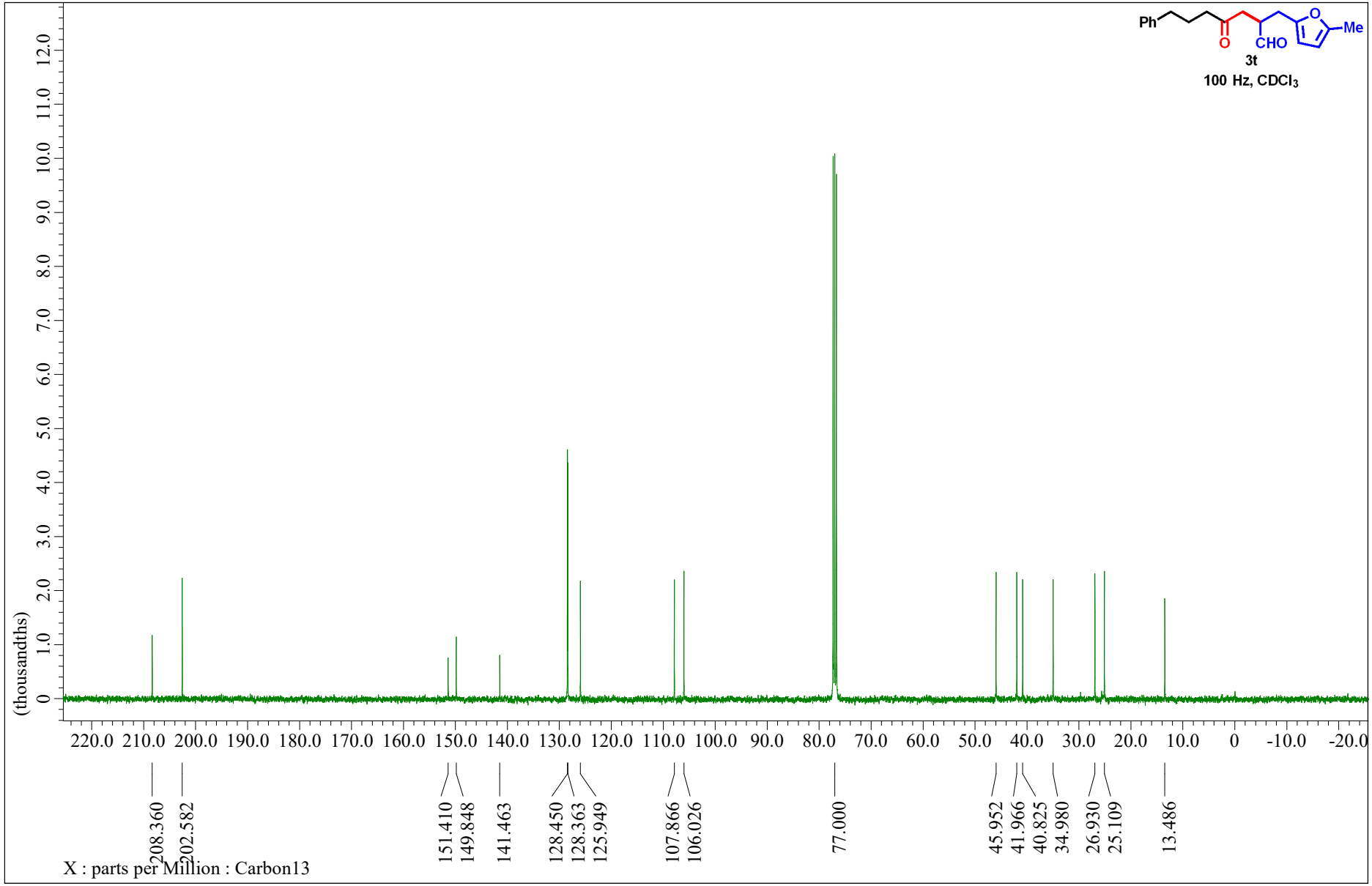

Ph
O
CHO
Br
3q
400 Hz, CDCl3
abundance
1.00
3.11
1.94
2.22
1.95
3.06
2.11
2.21
0.94
0.99
1.01
1.10
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.752
7.426
7.404
7.295
7.278
7.260
7.207
7.189
7.152
7.135
7.033
7.013
3.014
2.733
2.670
2.648
2.613
2.590
2.570
2.389
2.376
2.331
1.915
1.898
1.891
1.879
1.872
1.861
1.853
X : parts per Million : Proton

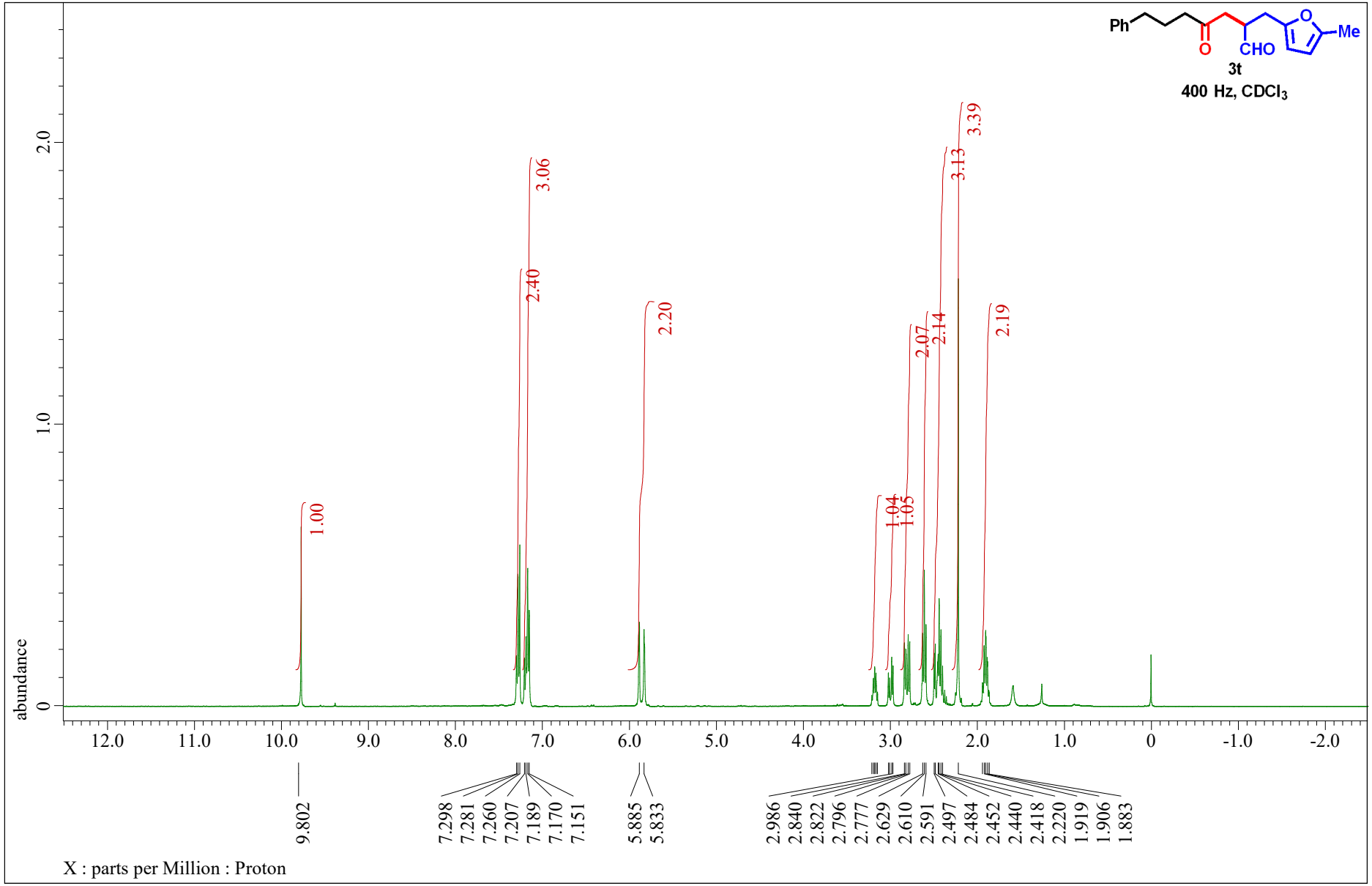

Ph
O
CHO
OMe
3r
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.561
203.051
158.357
141.463
129.916
128.440
128.354
125.929
114.076
77.000
55.228
48.472
41.946
40.844
34.932
33.619
25.052
X : parts per Million : Carbon13

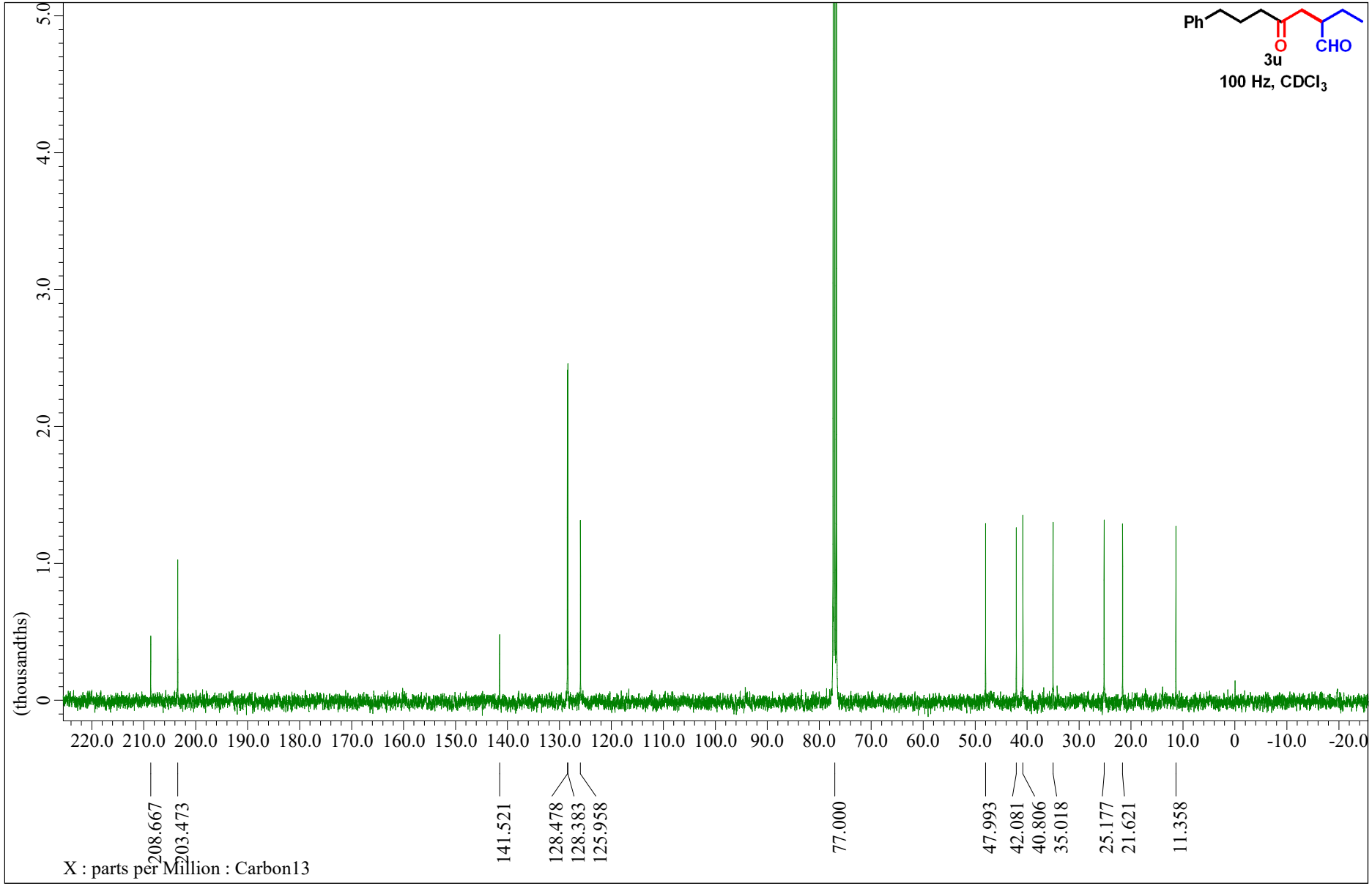

Ph
O
CHO
OMe
3r
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
3.19
3.07
2.10
2.17
3.00
1.04
1.05
1.07
1.04
2.11
3.18
2.16
9.760
7.279
7.262
7.248
7.242
7.191
7.173
7.141
7.123
7.054
7.032
6.827
6.805
3.771
2.728
2.589
2.570
2.552
2.375
1.898
1.880
1.872
1.862
1.855
1.845
1.835

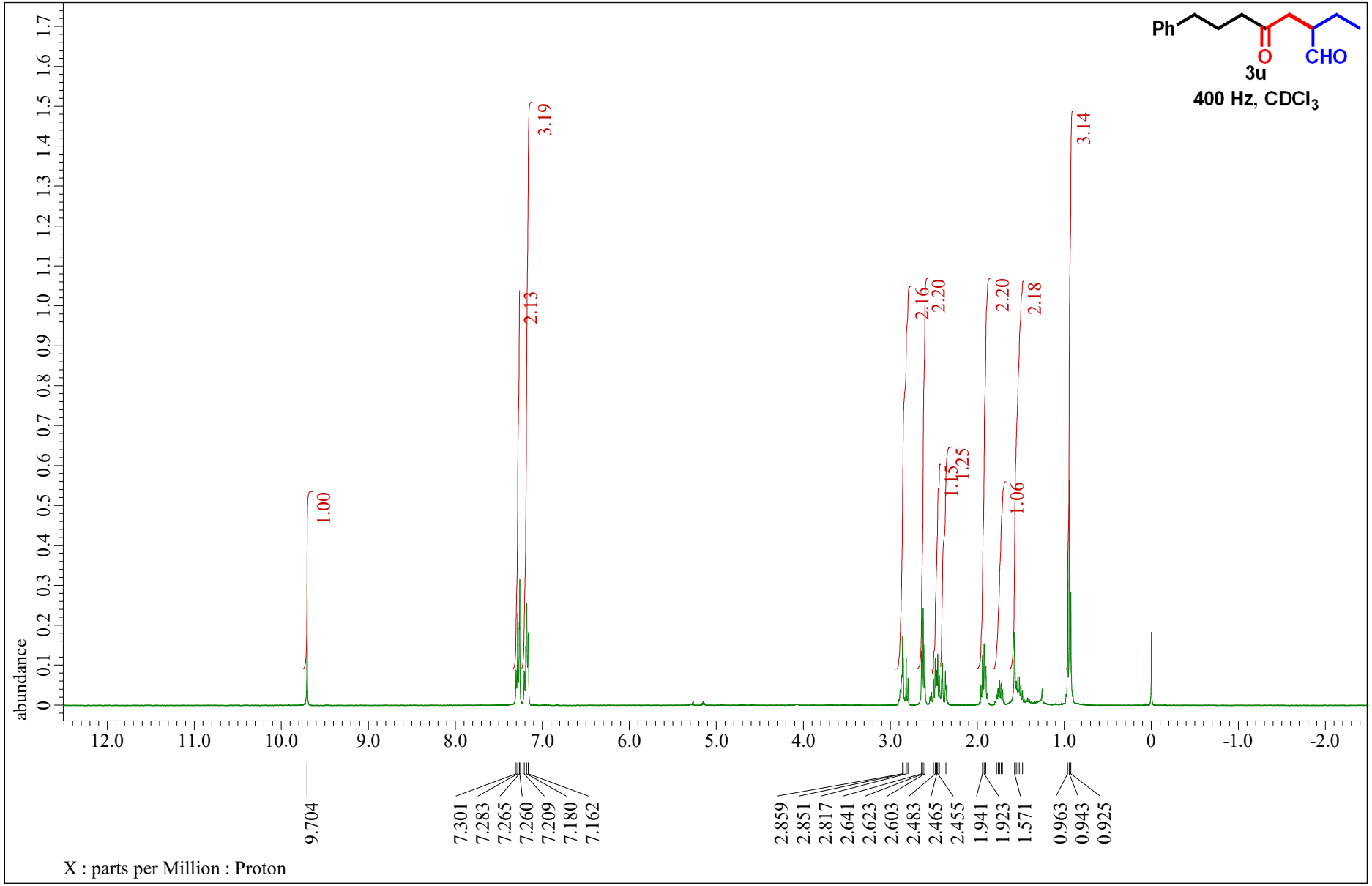

Ph
O
3s
CHO
S
100 Hz, CDCl3
20.0
10.0
0
(thousandths)
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.245
202.390
141.396
140.227
128.440
128.363
127.060
126.054
125.949
124.310
77.000
48.300
41.898
40.864
34.922
28.444
25.052
X : parts per Million : Carbon13

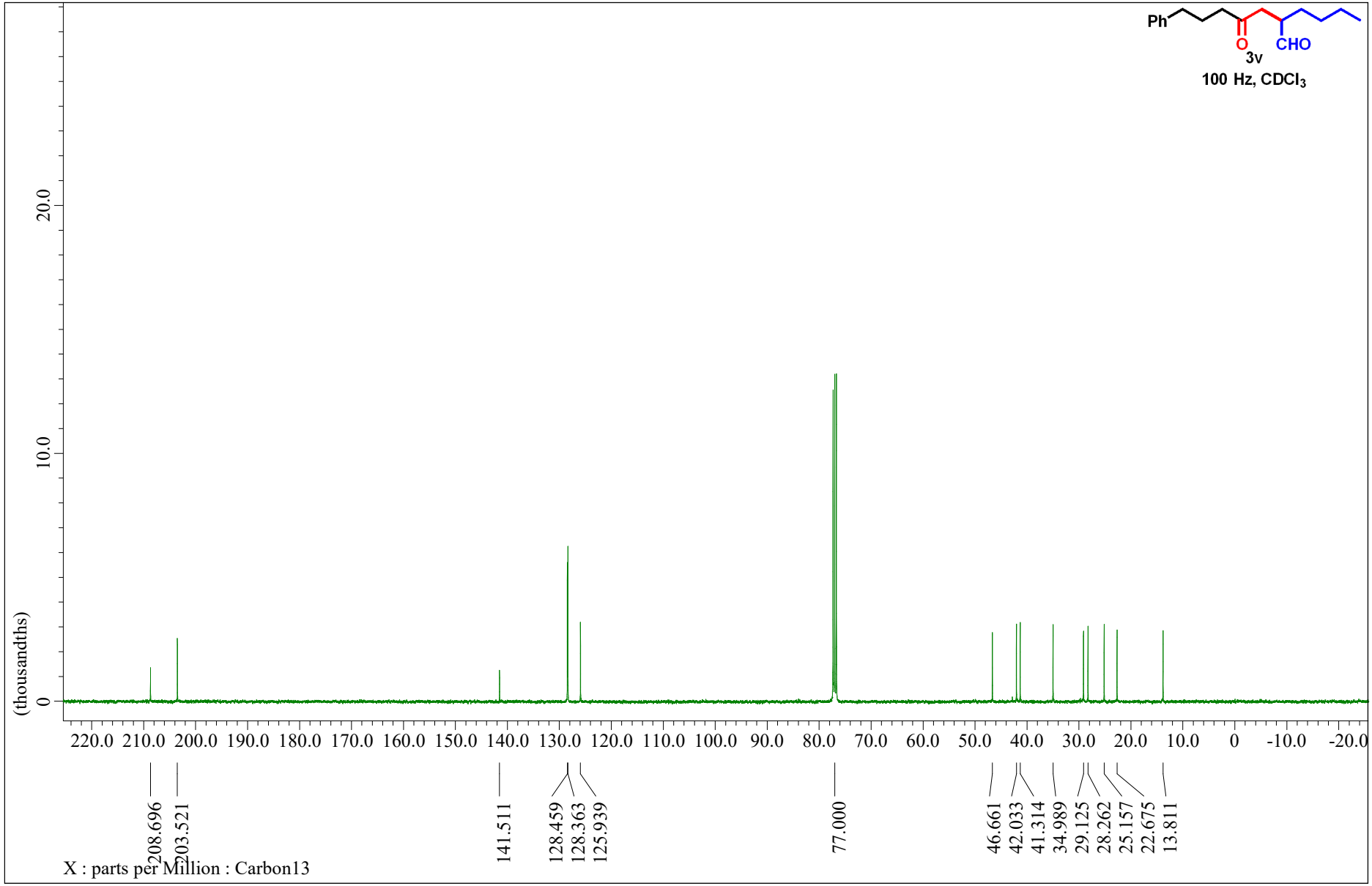

Ph
O
CHO
S
3s
400 Hz, CDCl3
abundance
4.18
3.03
3.05
1.84
2.04
2.17
1.36
1.00
1.15
1.10
1.12
0.95
0.91
9.787
7.298
7.279
7.260
7.190
7.165
7.152
7.144
6.929
6.920
6.916
6.908
6.782
6.774
3.487
3.248
3.039
2.797
2.778
2.619
2.600
2.582
2.531
2.425
2.407
1.932
1.915
1.896
1.878
1.859
X : parts per Million : Proton

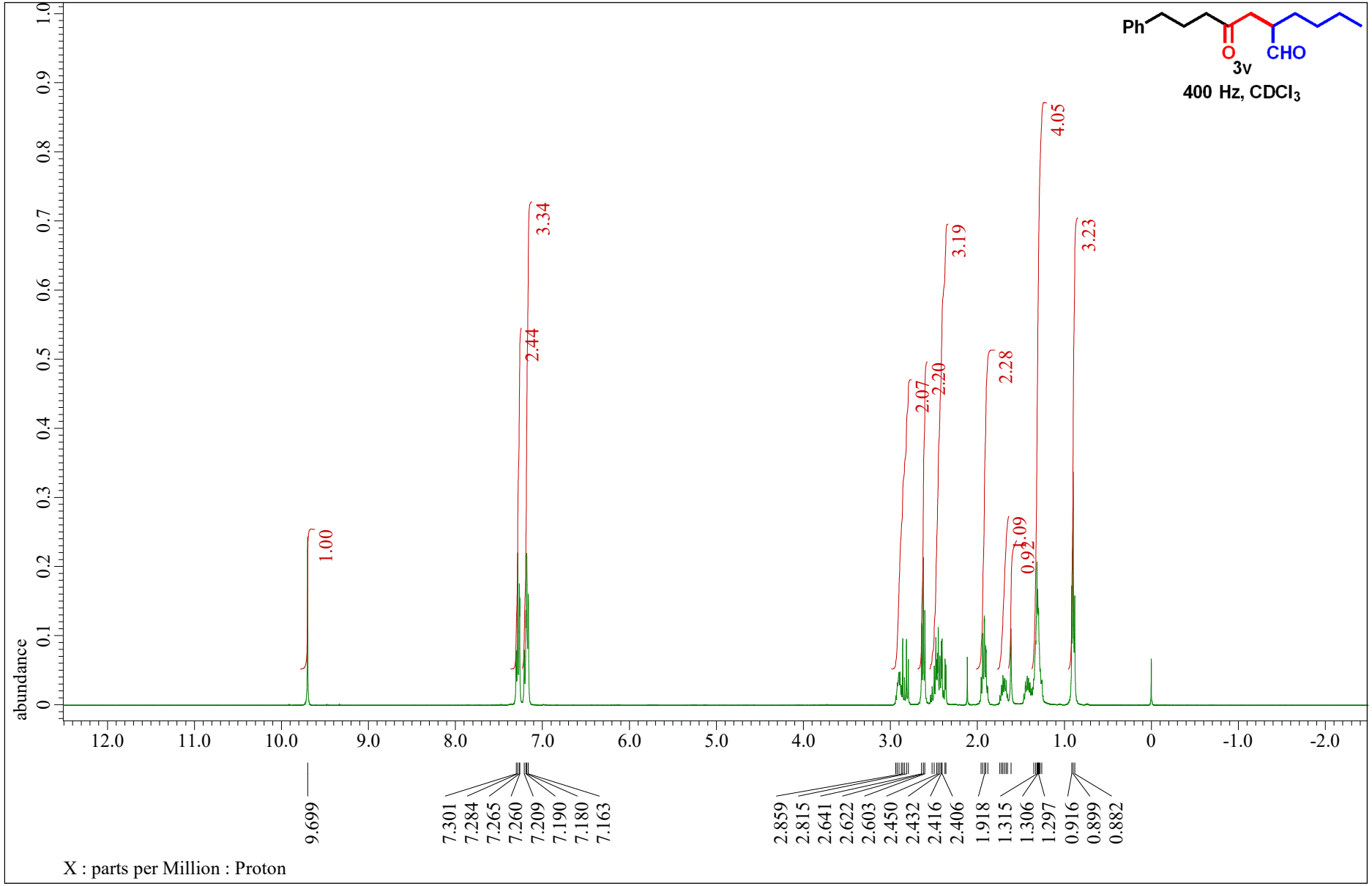

Ph
O
CHO
O
Me
3t
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.360
202.582
151.410
149.848
141.463
128.450
128.363
125.949
107.866
106.026
77.000
45.952
41.966
40.825
34.980
26.930
25.109
13.486
X : parts per Million : Carbon13

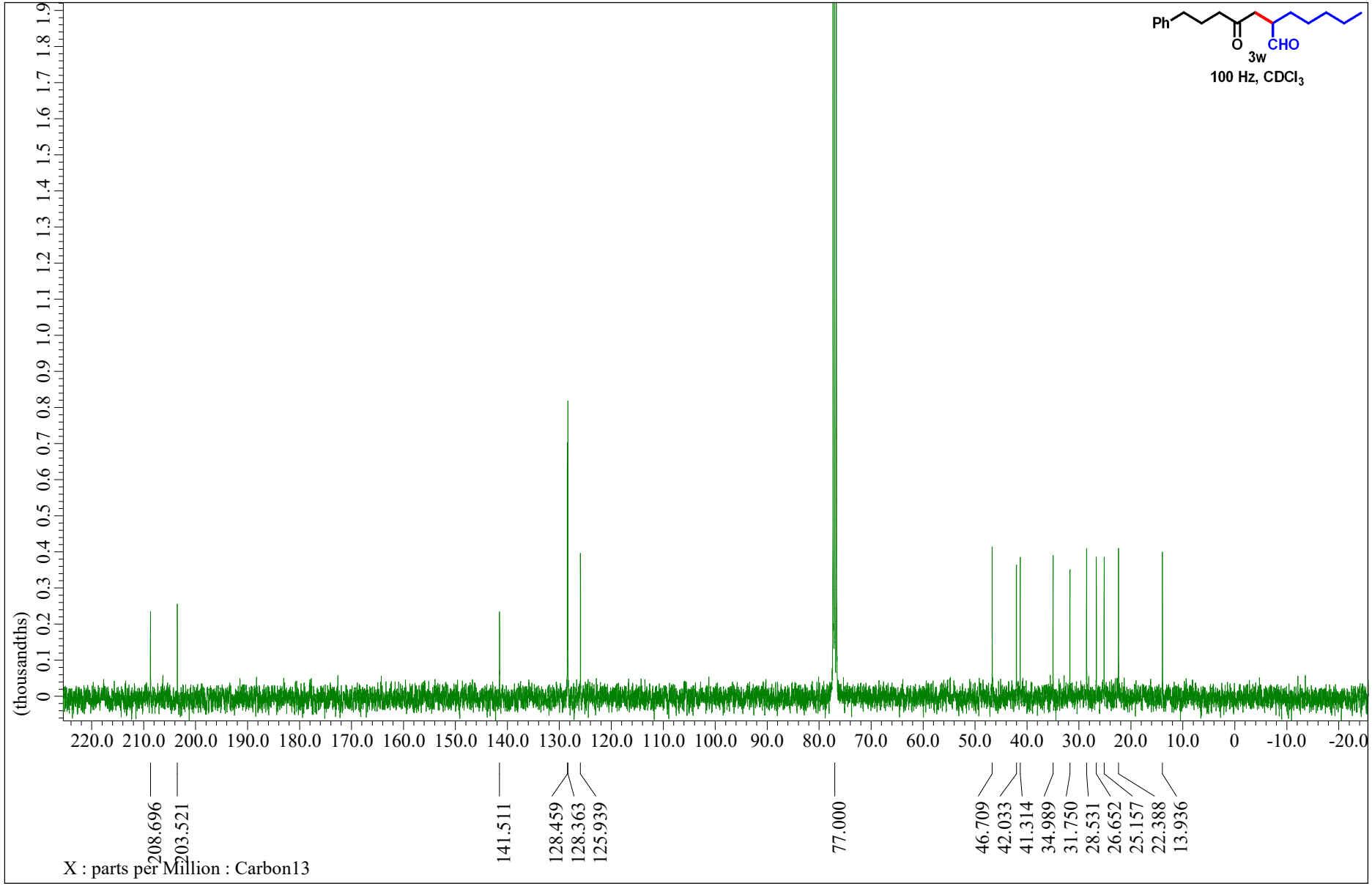

Ph
O
CHO
O
Me
3t
400 Hz, CDCl3
abundance
2.0
1.0
0
3.06
2.40
2.20
3.39
3.13
2.07
2.14
2.19
1.00
1.04
1.05
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.802
7.298
7.281
7.260
7.207
7.189
7.170
7.151
5.885
5.833
2.986
2.840
2.822
2.796
2.777
2.629
2.610
2.591
2.497
2.484
2.452
2.440
2.418
2.220
1.919
1.906
1.883
X : parts per Million : Proton

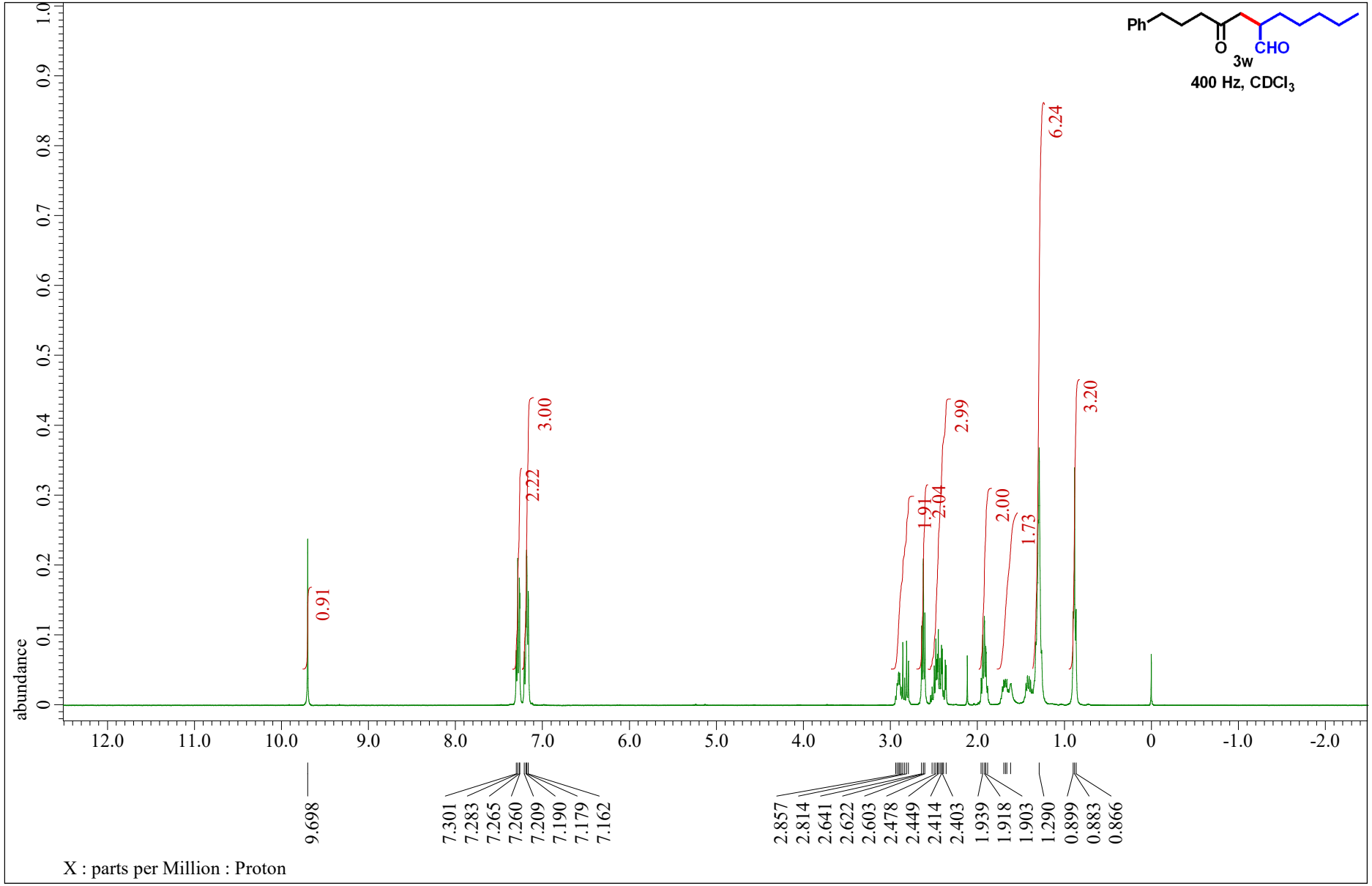

Ph
O
CHO
3u
100 Hz, CDCl3
(thousandths)
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.667
203.473
141.521
128.478
128.383
125.958
77.000
47.993
42.081
40.806
35.018
25.177
21.621
11.358
X : parts per Million : Carbon13

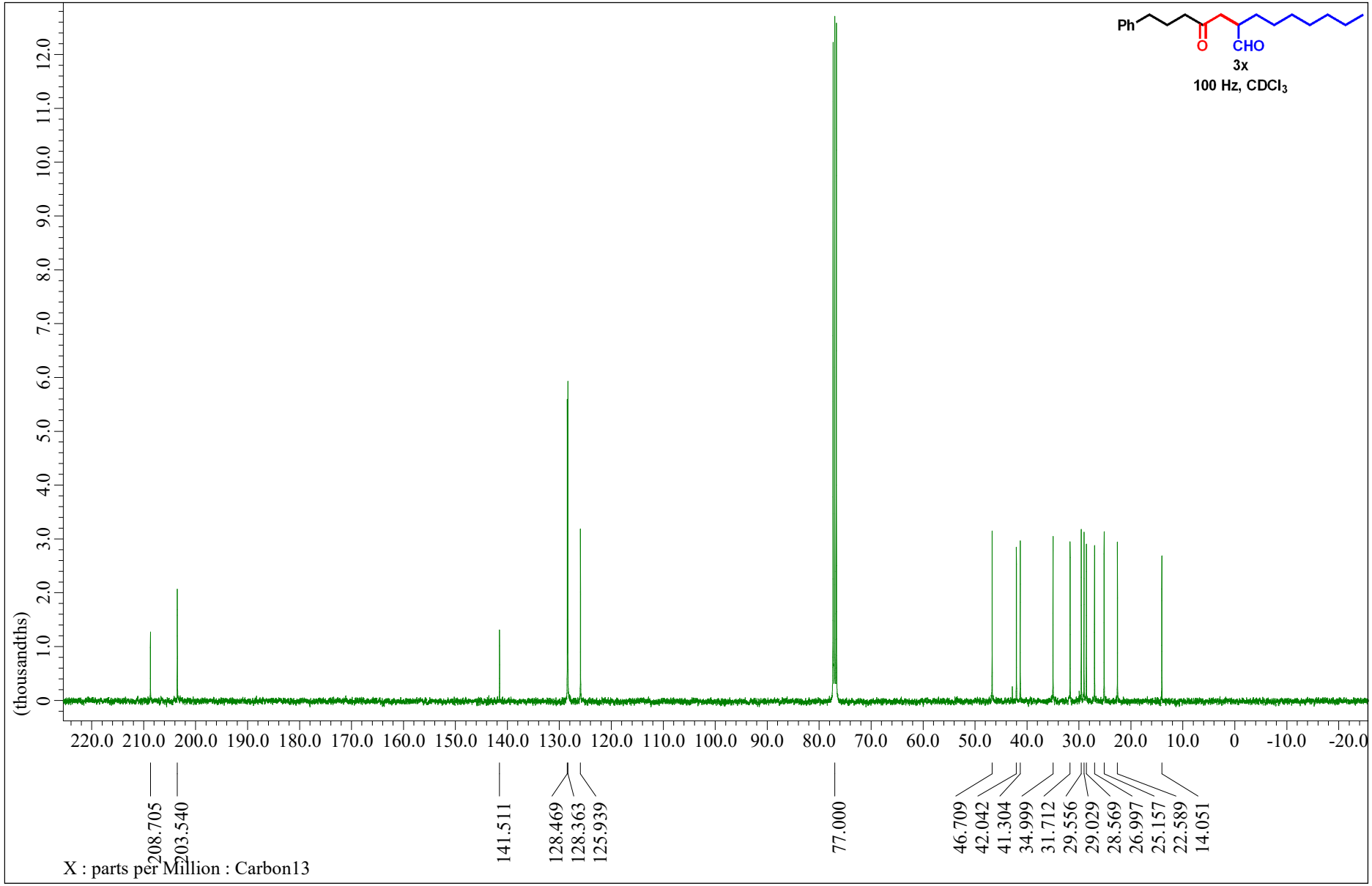

Ph
O
CHO
3u
400 Hz, CDCl3
abundance
1.00
3.19
2.13
2.16
2.20
1.15
1.25
2.20
2.18
1.06
3.14
9.704
7.301
7.283
7.265
7.260
7.209
7.180
7.162
2.859
2.851
2.817
2.641
2.623
2.603
2.483
2.465
2.455
1.941
1.923
1.571
0.963
0.943
0.925
X : parts per Million : Proton

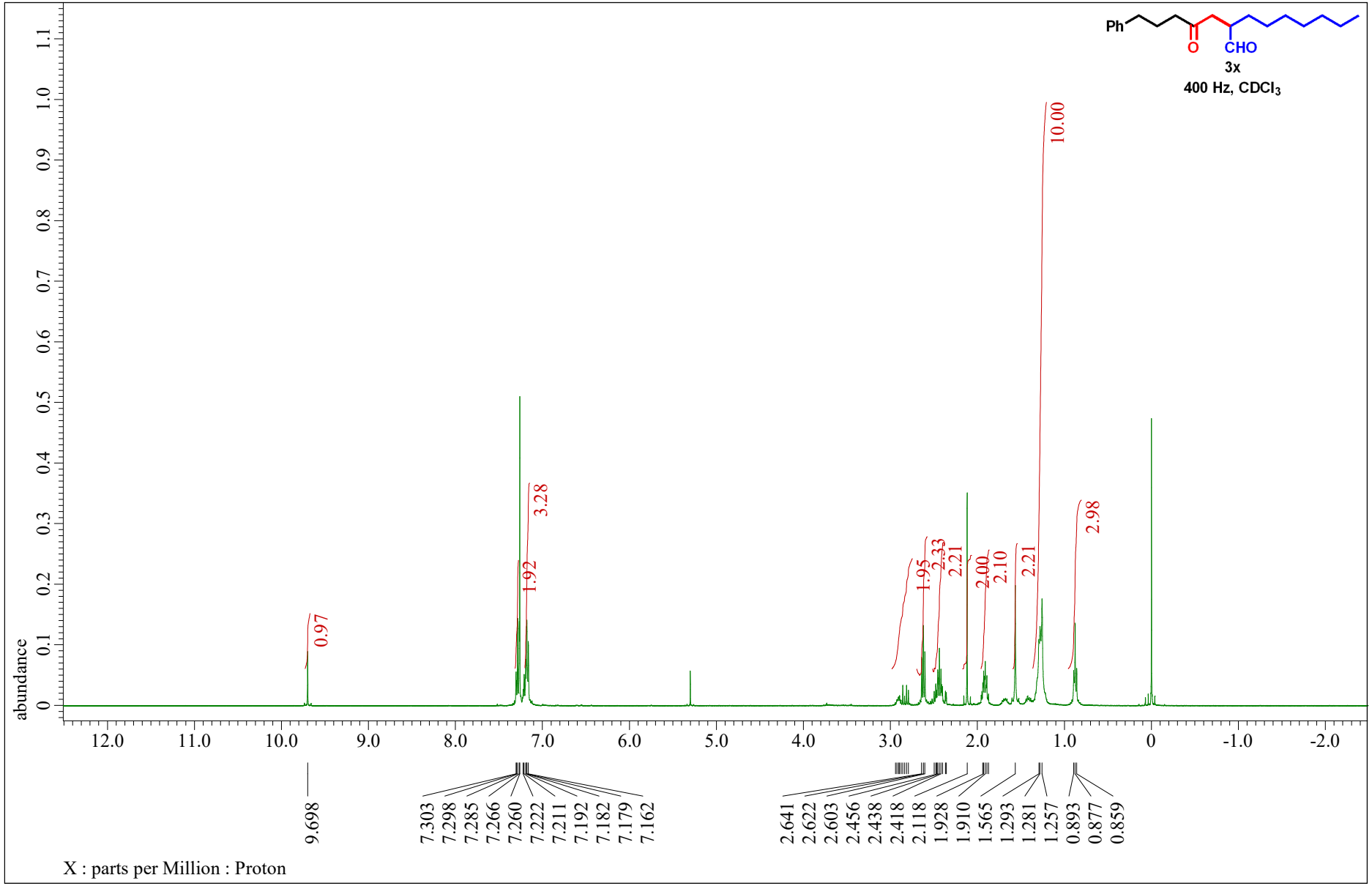

Ph
O
CHO
3v
100 Hz, CDCl3
(thousandths)
20.0
10.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.696
203.521
141.511
128.459
128.363
125.939
77.000
46.661
42.033
41.314
34.989
29.125
28.262
25.157
22.675
13.811
X : parts per Million : Carbon13

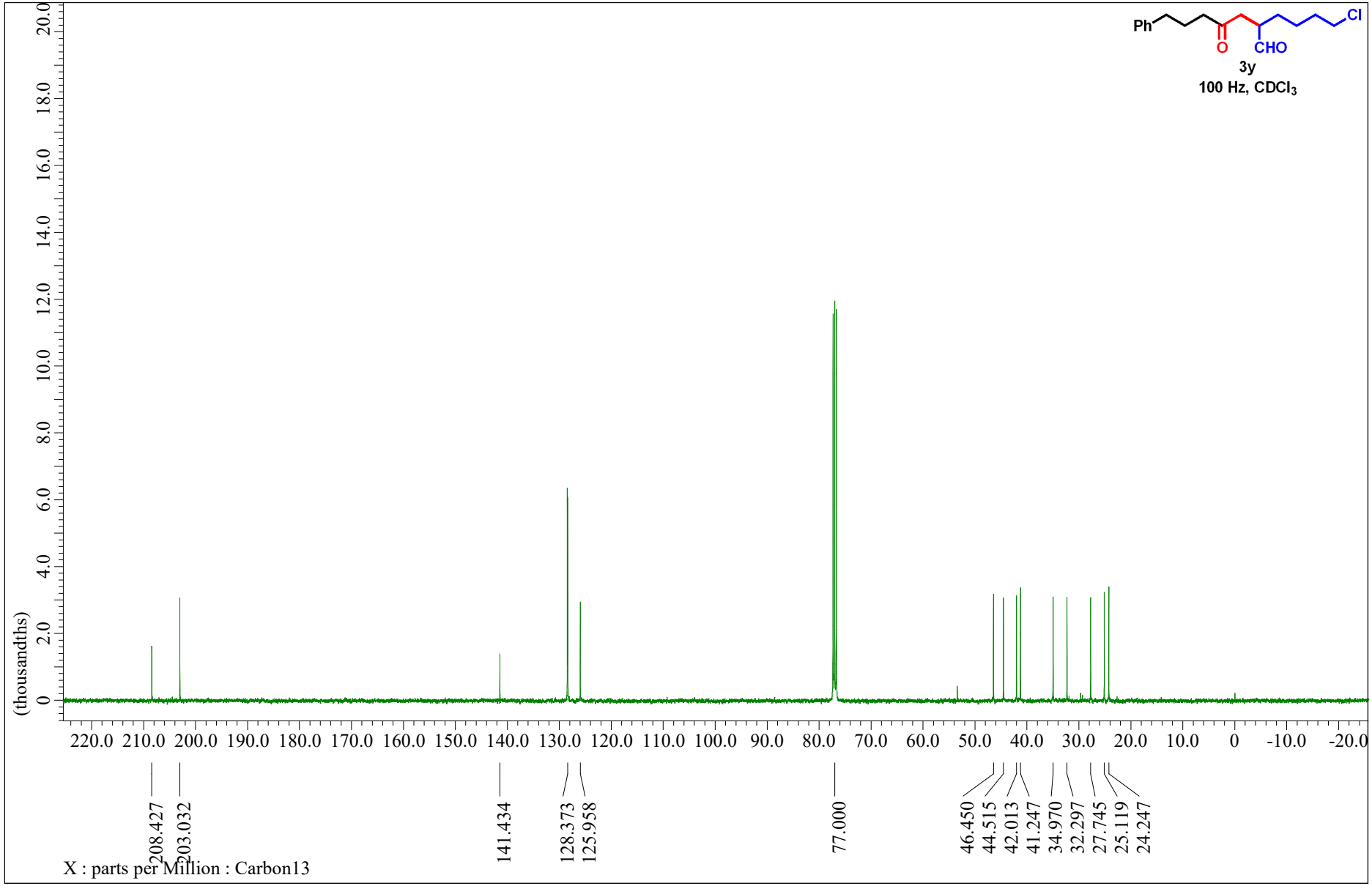

Ph
O
3v
CHO
400 Hz, CDCl3
abundance
1.00
3.34
2.44
2.07
2.20
3.19
2.28
0.92
1.09
4.05
3.23
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.699
7.301
7.284
7.265
7.260
7.209
7.190
7.180
7.163
2.859
2.815
2.641
2.622
2.603
2.450
2.432
2.416
2.406
1.918
1.315
1.306
1.297
0.916
0.899
0.882
X : parts per Million : Proton

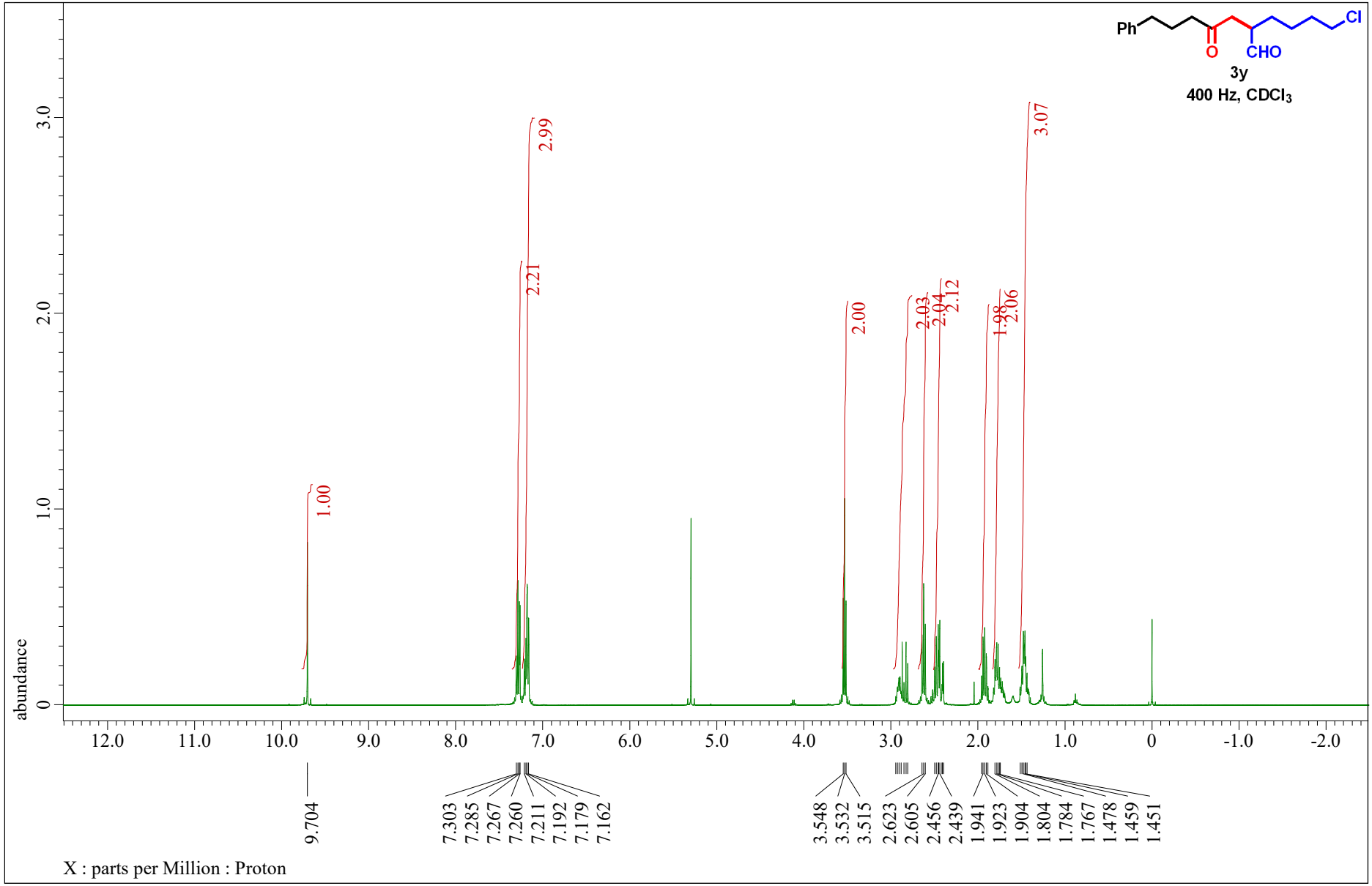

Ph
O
CHO
3w
100 Hz, CDCl3
(thousandths)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 1.1 1.2 1.3 1.4 1.5 1.6 1.7 1.8 1.9
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.696
203.521
141.511
128.459
128.363
125.939
77.000
46.709
42.033
41.314
34.989
31.750
28.531
26.652
25.157
22.388
13.936
X : parts per Million : Carbon13

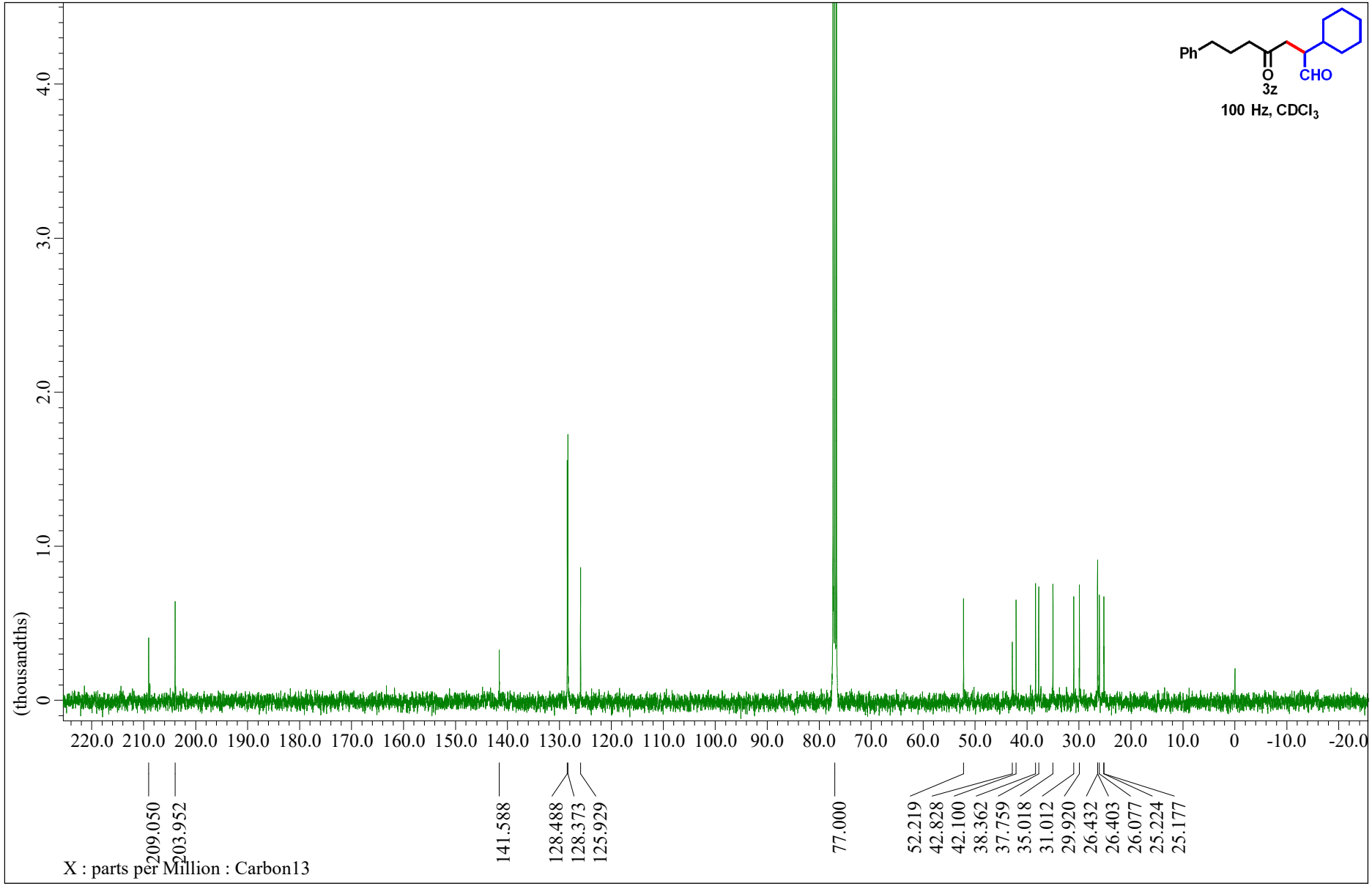

Ph
O
CHO
3w
400 Hz, CDCl3
abundance
6.24
3.20
3.00
2.99
2.22
2.04
1.91
2.00
1.73
0.91
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.698
7.301
7.283
7.265
7.260
7.209
7.190
7.179
7.162
2.857
2.814
2.641
2.622
2.603
2.478
2.449
2.414
2.403
1.939
1.918
1.903
1.290
0.899
0.883
0.866
X : parts per Million : Proton

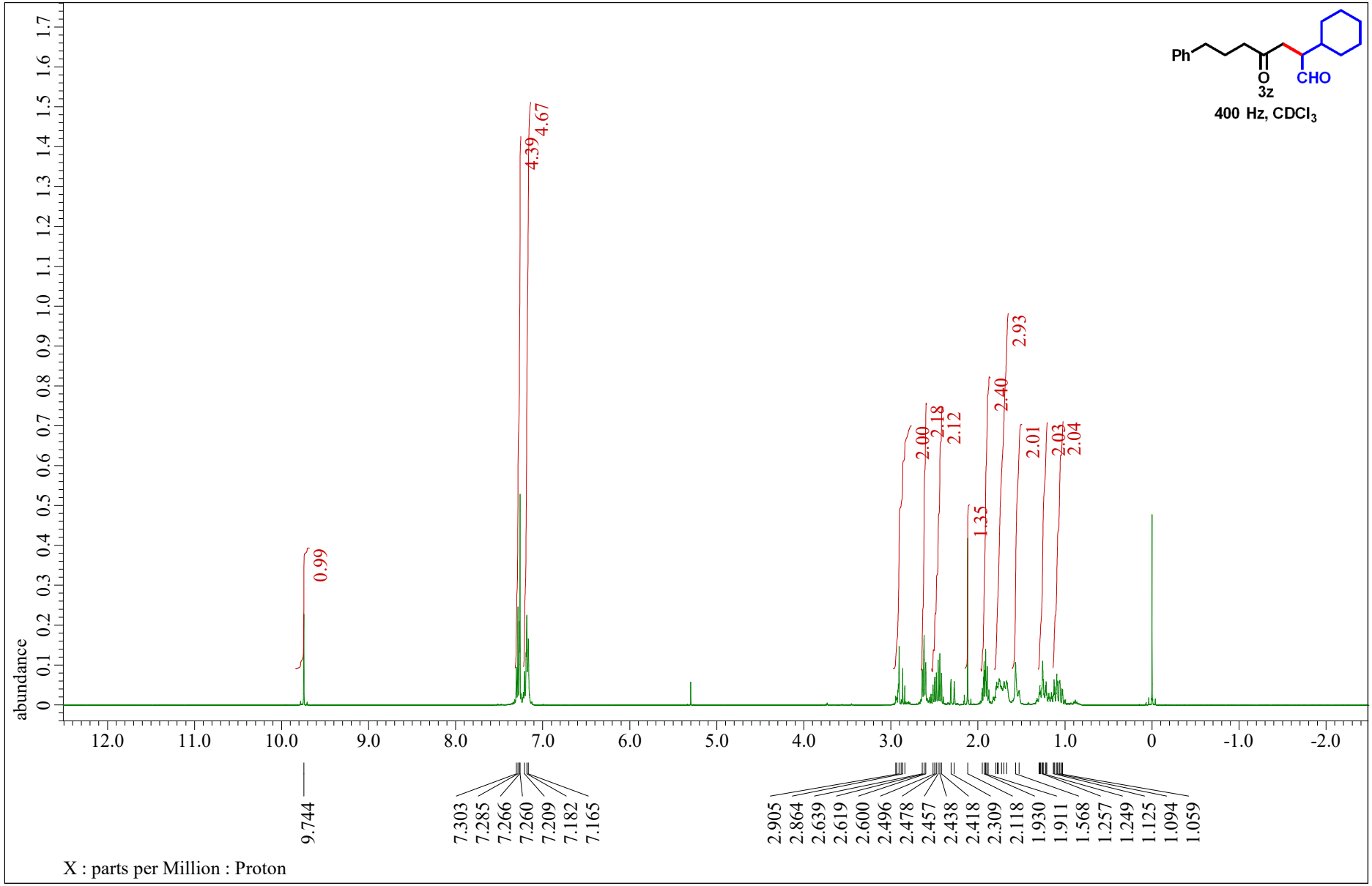

Ph
O
CHO
3x
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.705
203.540
141.511
128.469
128.363
125.939
77.000
46.709
42.042
41.304
34.999
31.712
29.556
29.029
28.569
26.997
25.157
22.589
14.051
X : parts per Million : Carbon13

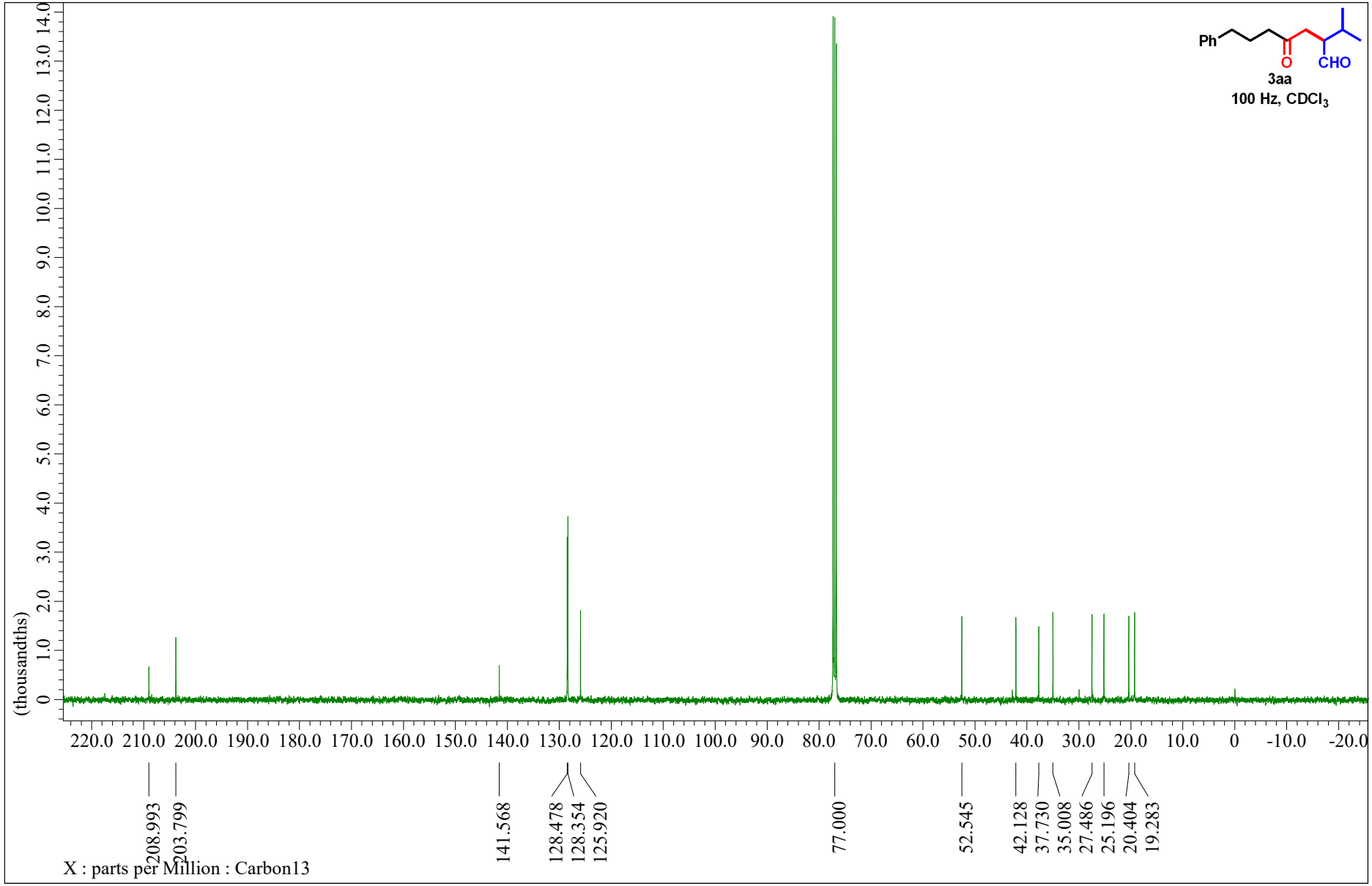

Ph
O
CHO
3x
400 Hz, CDCl3
abundance
10.00
3.28
2.98
2.33
2.21
2.21
2.10
2.00
1.95
1.92
0.97
9.698
7.303
7.298
7.285
7.266
7.260
7.222
7.211
7.192
7.182
7.179
7.162
2.641
2.622
2.603
2.456
2.438
2.418
2.118
1.928
1.910
1.565
1.293
1.281
1.257
0.893
0.877
0.859
X : parts per Million : Proton

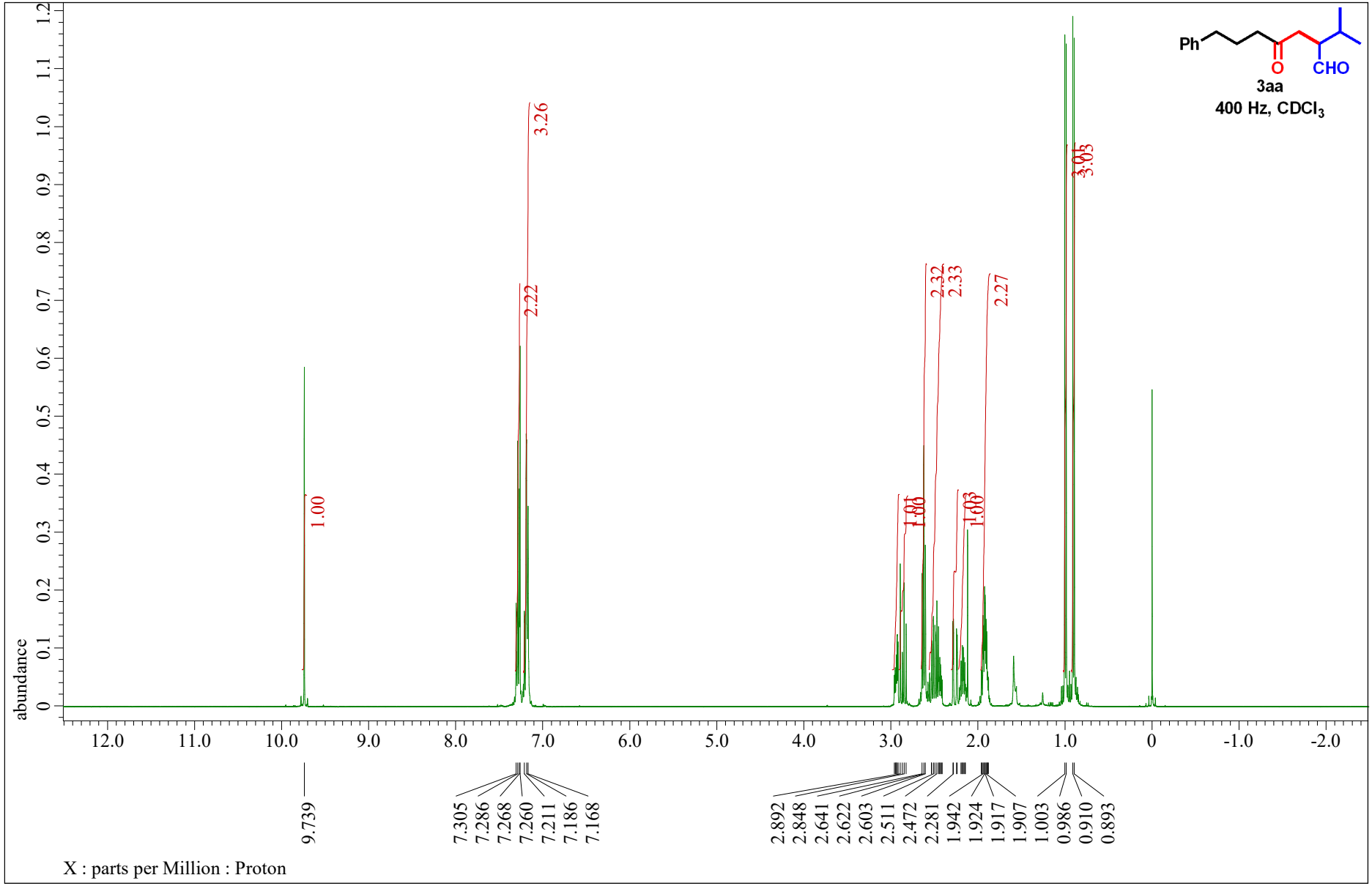

Ph
O
CHO
Cl
3y
100 Hz, CDCl3
(thousandths)
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.427
203.032
141.434
128.373
125.958
77.000
46.450
44.515
42.013
41.247
34.970
32.297
27.745
25.119
24.247
X : parts per Million : Carbon13

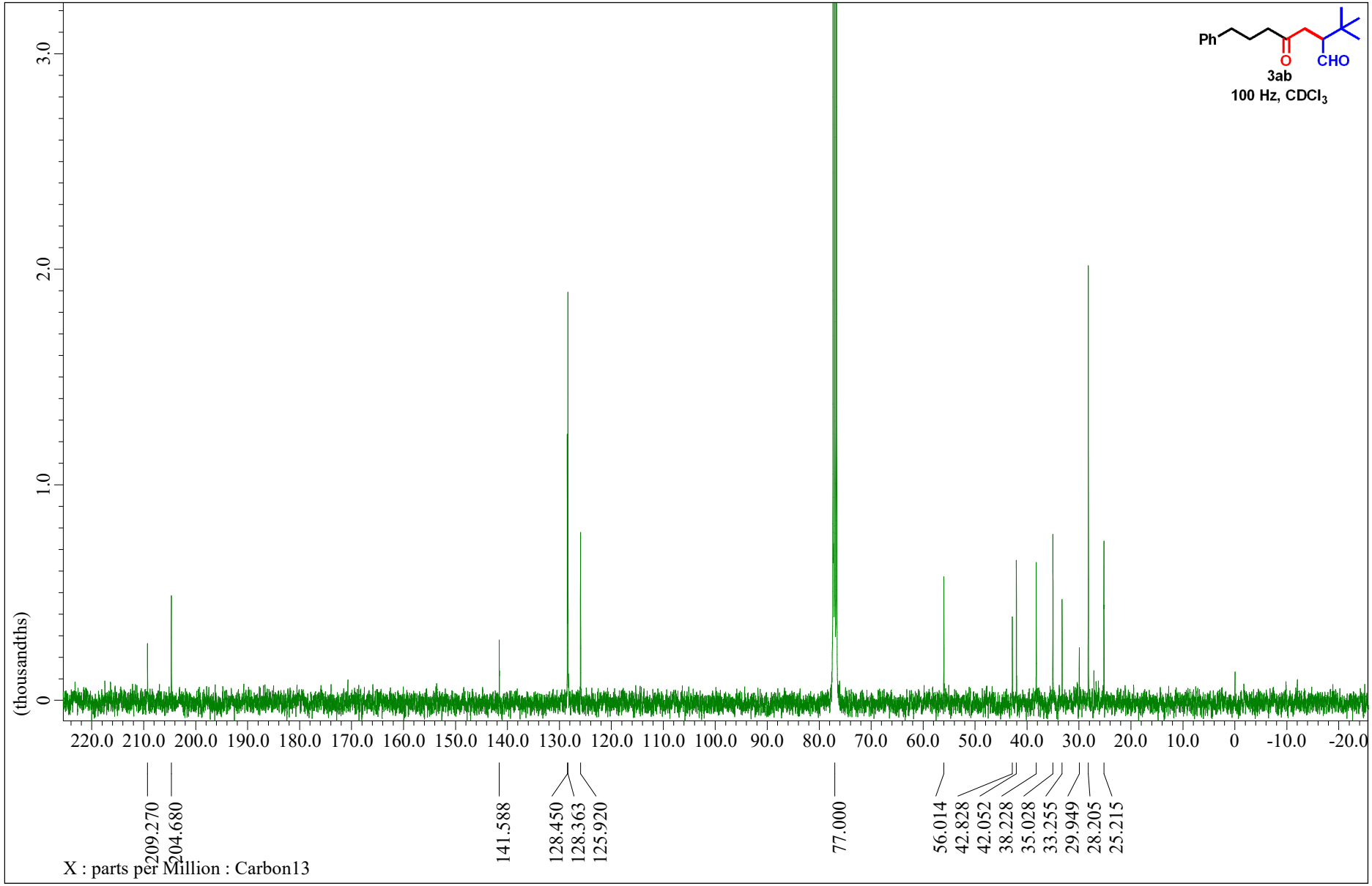

Ph
O
CHO
Cl
3y
400 Hz, CDCl3
abundance
3.0
2.0
1.0
0
1.00
2.99
2.21
2.00
2.03
2.04
2.12
1.98
2.06
3.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.704
7.303
7.285
7.267
7.260
7.211
7.192
7.179
7.162
3.548
3.532
3.515
2.623
2.605
2.456
2.439
1.941
1.923
1.904
1.804
1.784
1.767
1.478
1.459
1.451
X : parts per Million : Proton

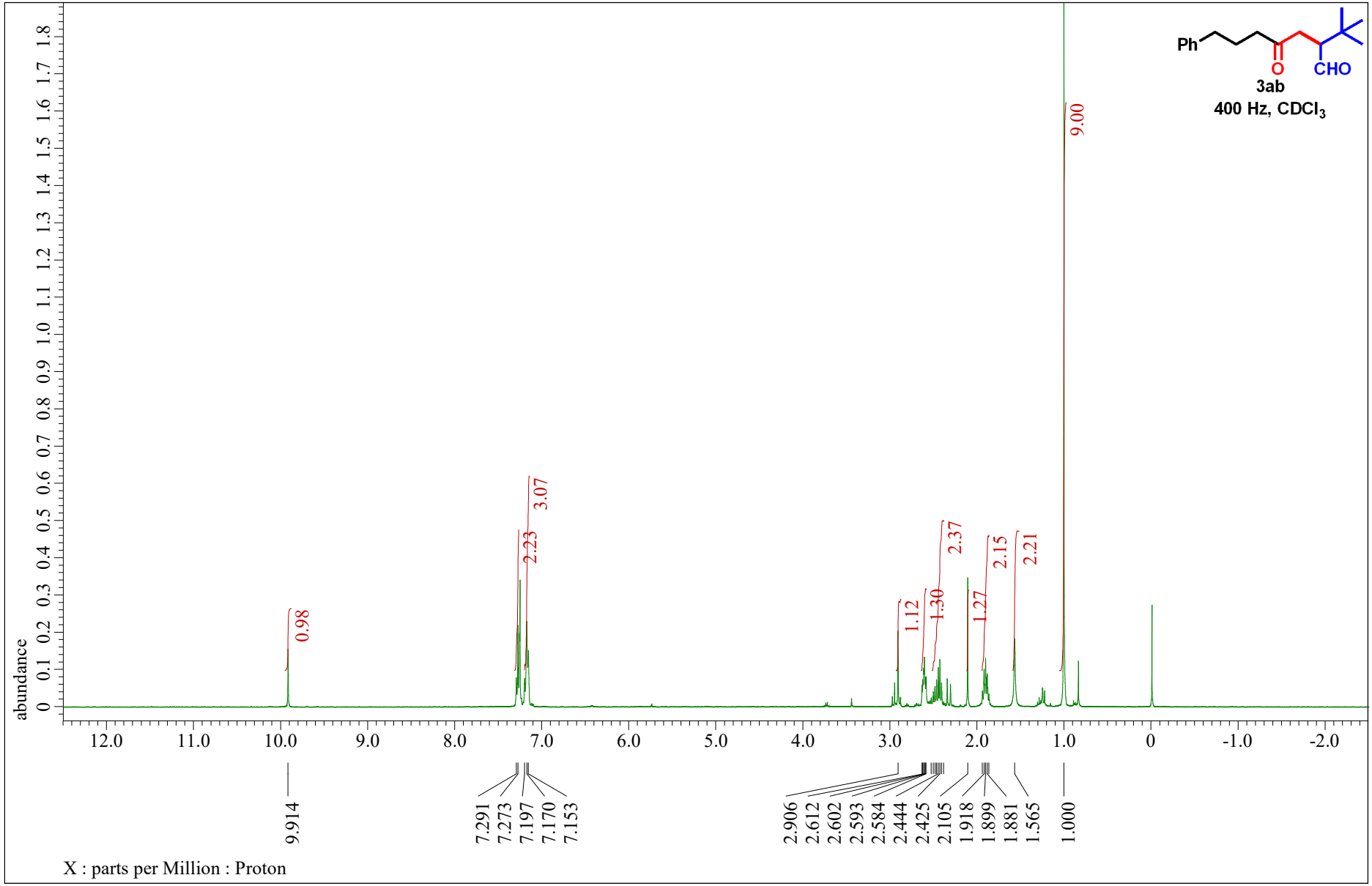

Ph
O
CHO
3z
100 Hz, CDCl3
(thousandths)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
209.050
203.952
141.588
128.488
128.373
125.929
77.000
52.219
42.828
42.100
38.362
37.759
35.018
31.012
29.920
26.432
26.403
26.077
25.224
25.177
X : parts per Million : Carbon13

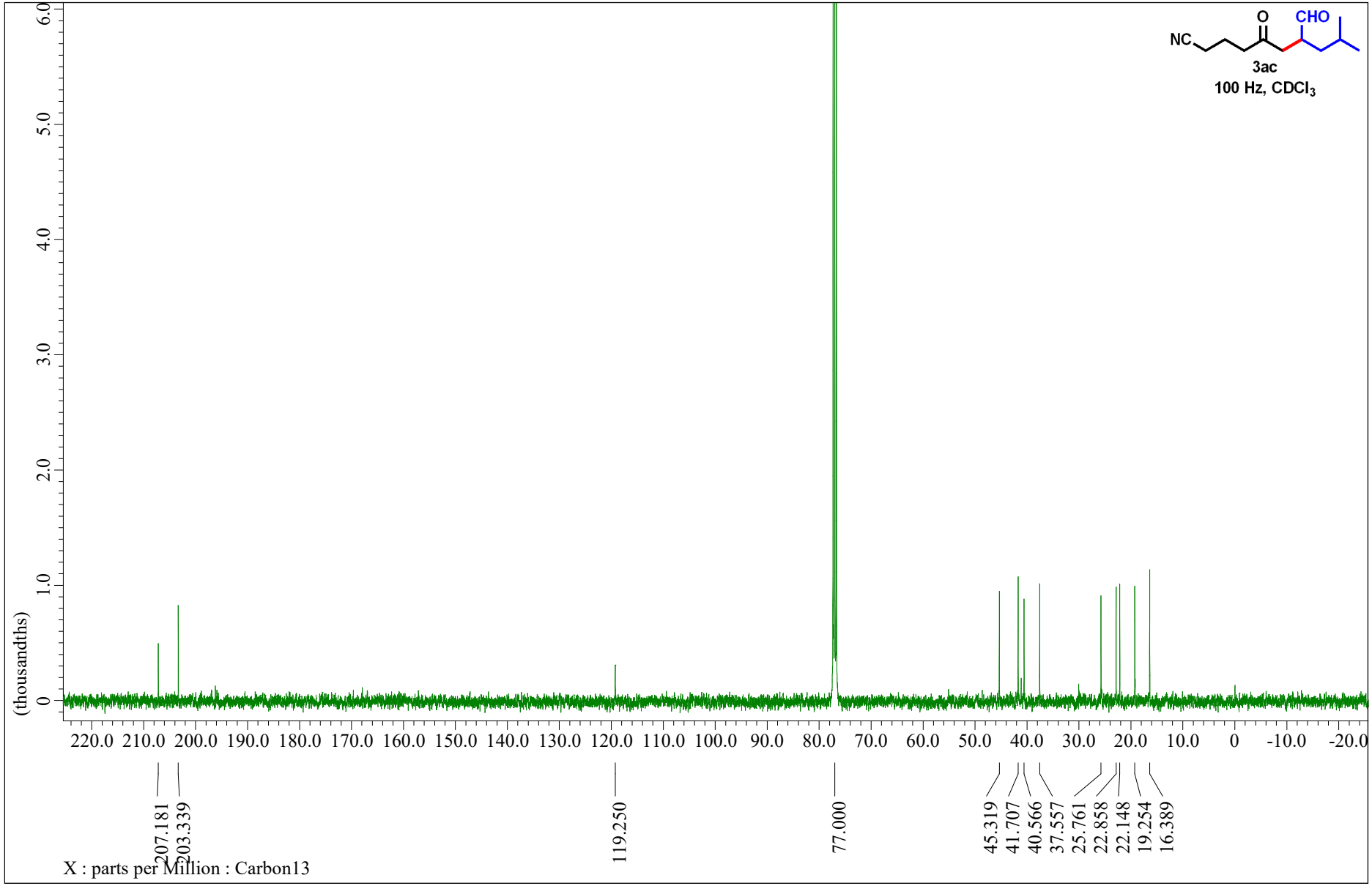

Ph
O
CHO
3z
400 Hz, CDCl3
abundance
0.99
4.39
4.67
2.00
2.18
2.12
1.35
2.40
2.93
2.01
2.03
2.04
9.744
7.303
7.285
7.266
7.260
7.209
7.182
7.165
2.905
2.864
2.639
2.619
2.600
2.496
2.478
2.457
2.438
2.418
2.309
2.118
1.930
1.911
1.568
1.257
1.249
1.125
1.094
1.059
X : parts per Million : Proton

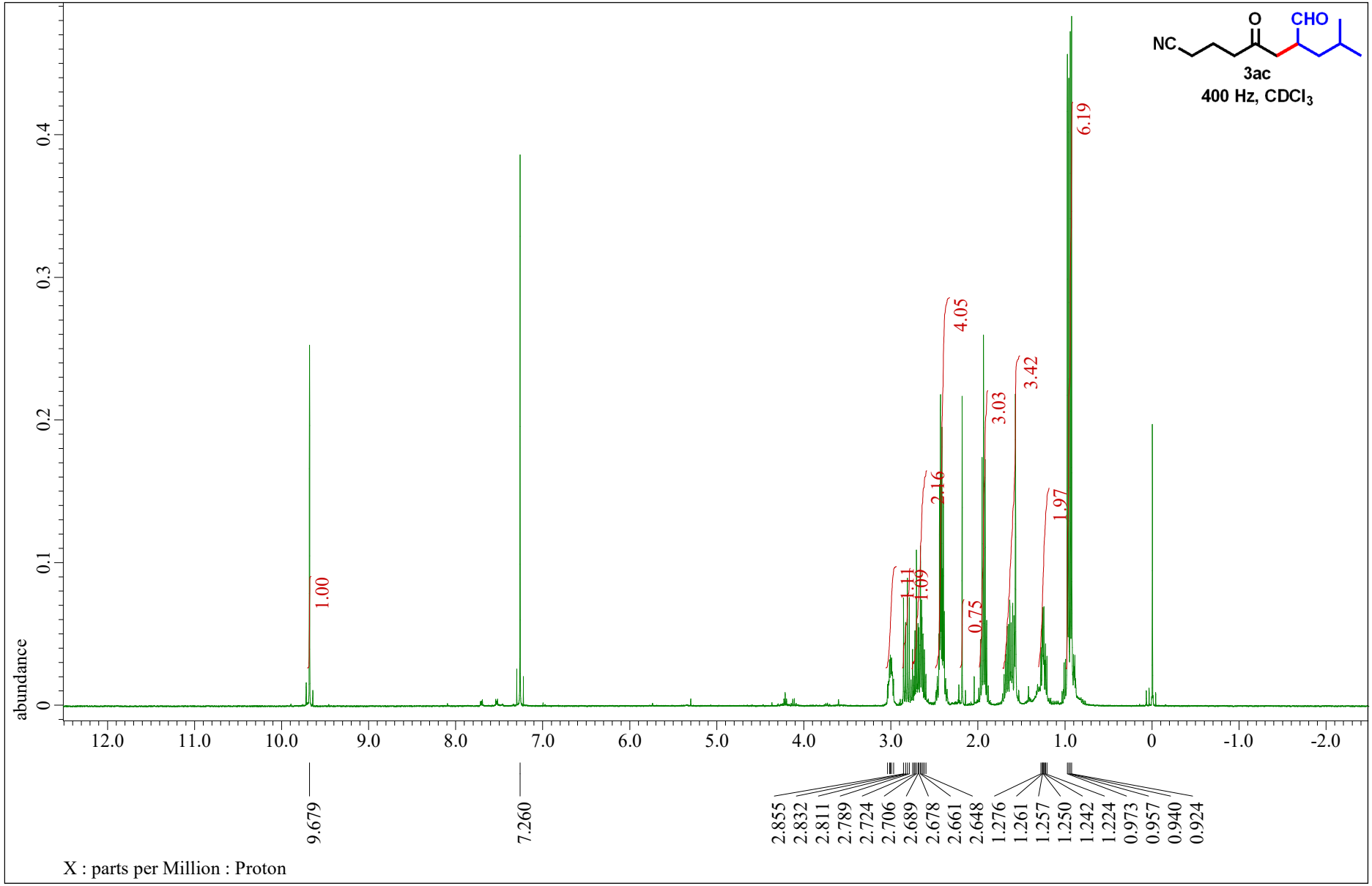

Ph
O
CHO
3aa
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
208.993
203.799
141.568
128.478
128.354
125.920
77.000
52.545
42.128
37.730
35.008
27.486
25.196
20.404
19.283
X : parts per Million : Carbon13

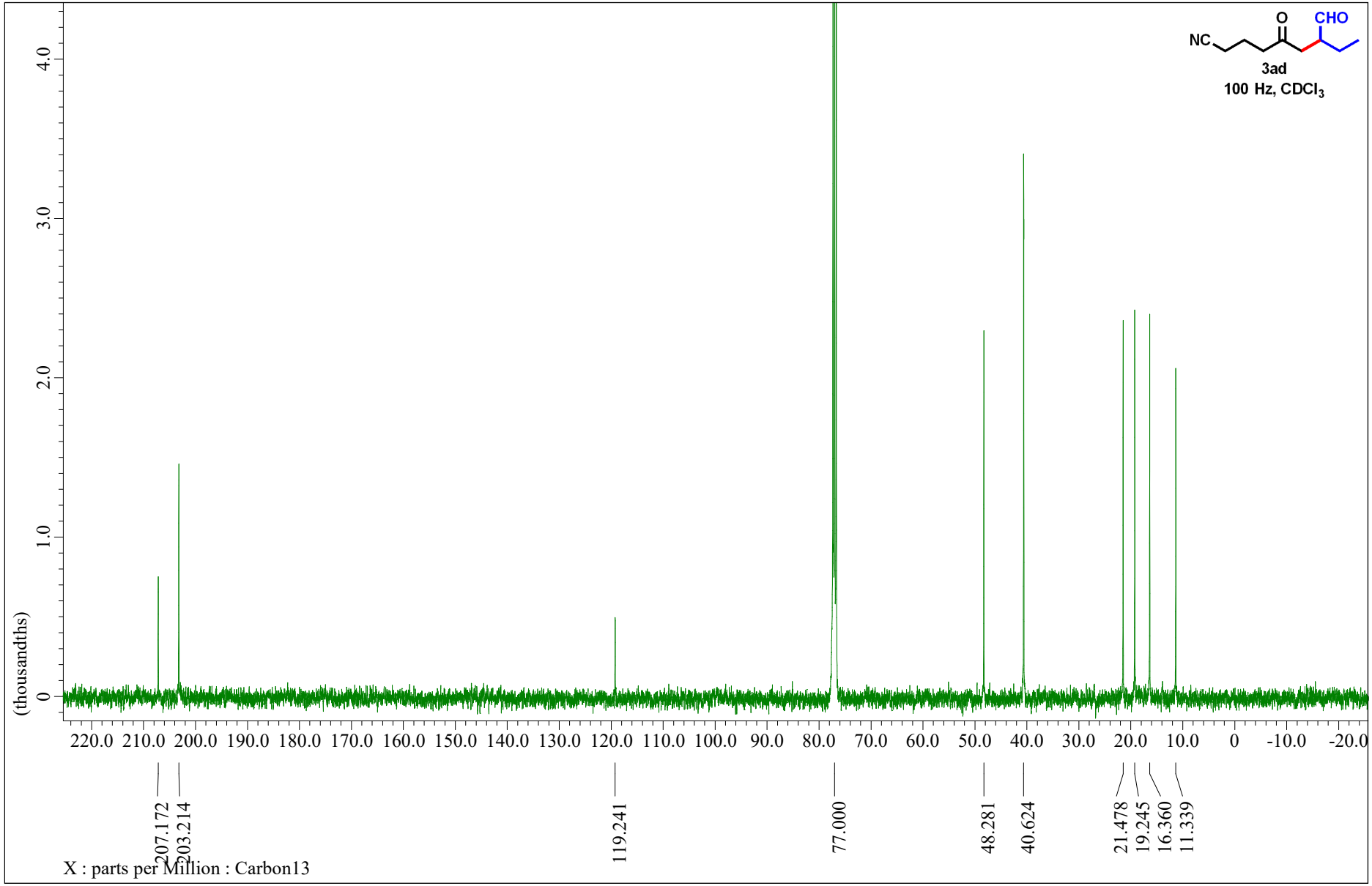

Ph
O
CHO
3aa
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
3.26
2.22
2.32
2.33
2.27
9.739
7.305
7.286
7.268
7.260
7.211
7.186
7.168
2.892
2.848
2.641
2.622
2.603
2.511
2.472
2.281
1.942
1.924
1.917
1.907
1.003
0.986
0.910
0.893

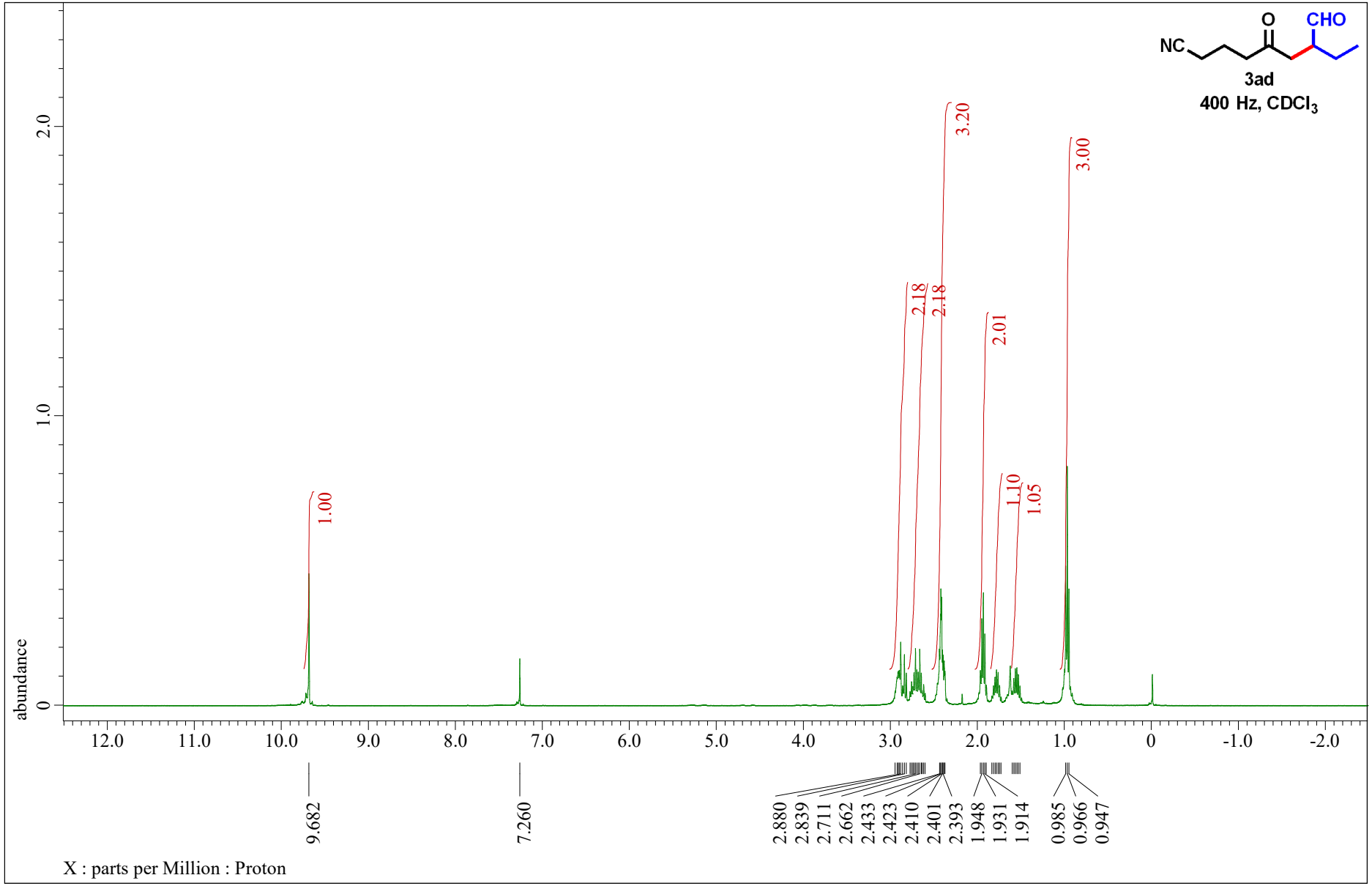

Ph
O
CHO
3ab
100 Hz, CDCl3
(thousandths)
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
209.270
204.680
141.588
128.450
128.363
125.920
77.000
56.014
42.828
42.052
38.228
35.028
33.255
29.949
28.205
25.215
X : parts per Million : Carbon13

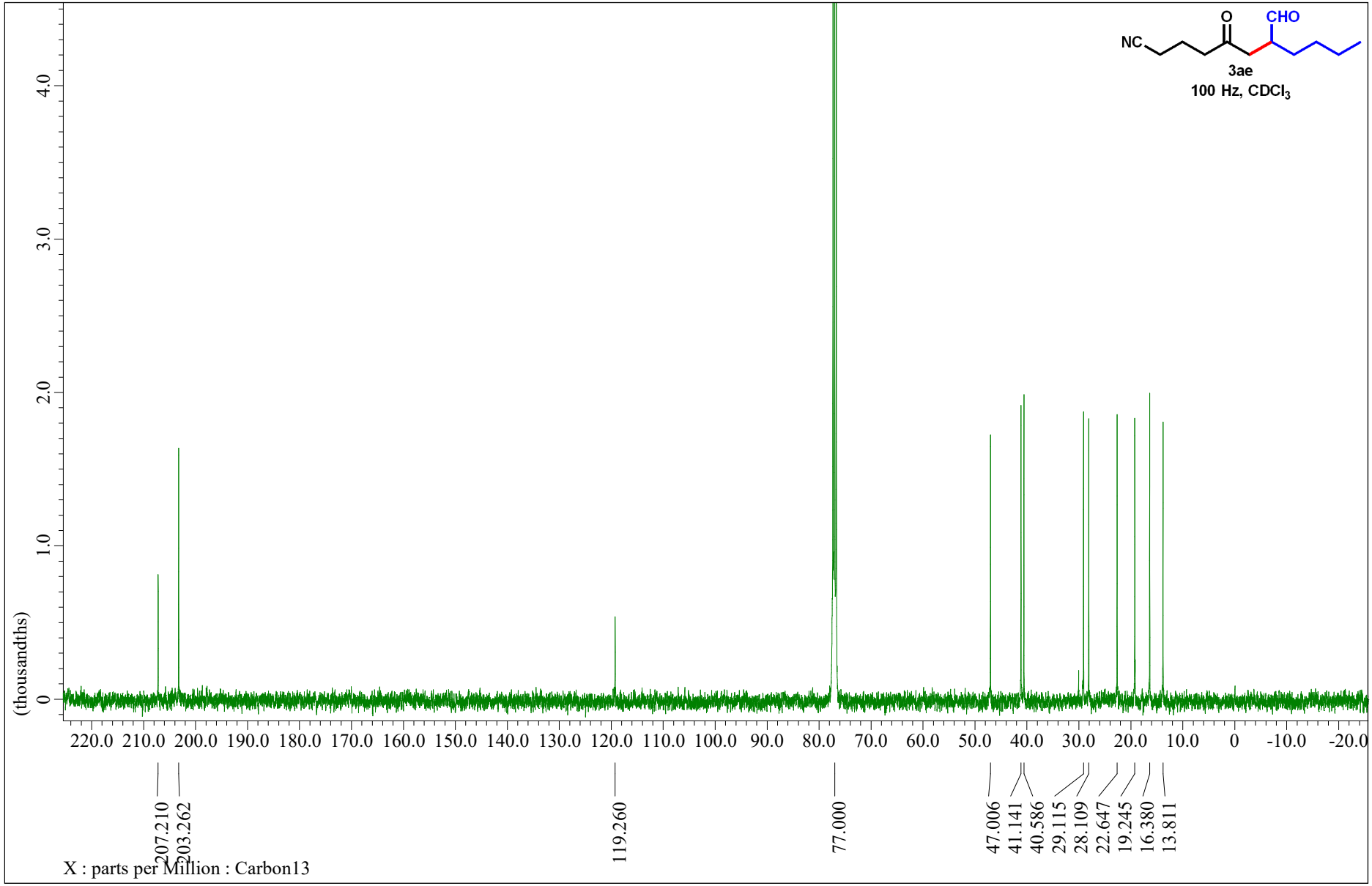

Ph
O
CHO
3ab
400 Hz, CDCl3
abundance
0.98
3.07
2.23
2.37
2.15
2.21
1.12
1.30
1.27
9.00
9.914
7.291
7.273
7.197
7.170
7.153
2.906
2.612
2.602
2.593
2.584
2.444
2.425
2.105
1.918
1.899
1.881
1.565
1.000
X : parts per Million : Proton

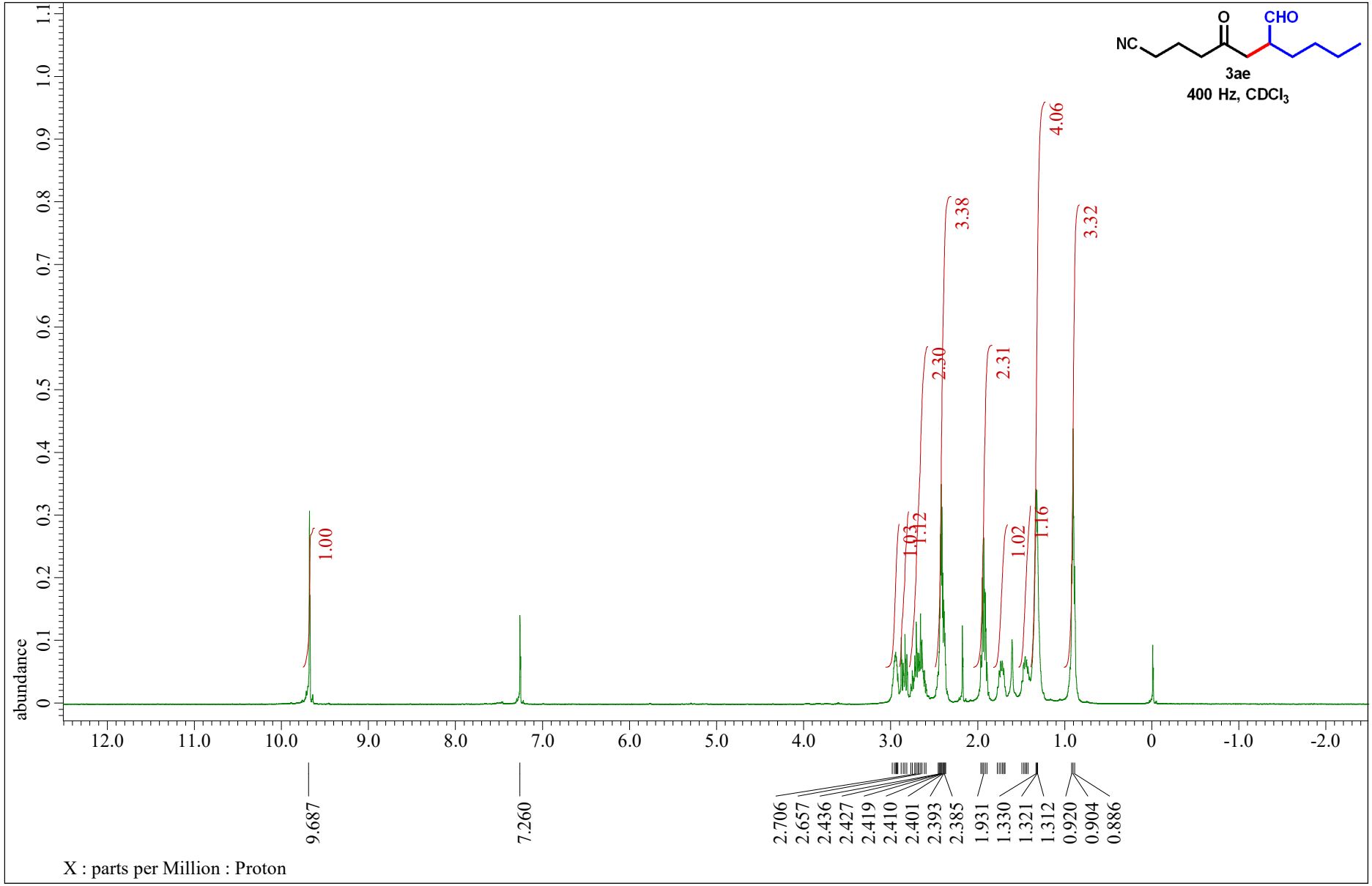

NC
O
CHO
3ac
100 Hz, CDCl3
(thousandths)
6.0
5.0
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.181
203.339
119.250
77.000
45.319
41.707
40.566
37.557
25.761
22.858
22.148
19.254
16.389
X : parts per Million : Carbon13

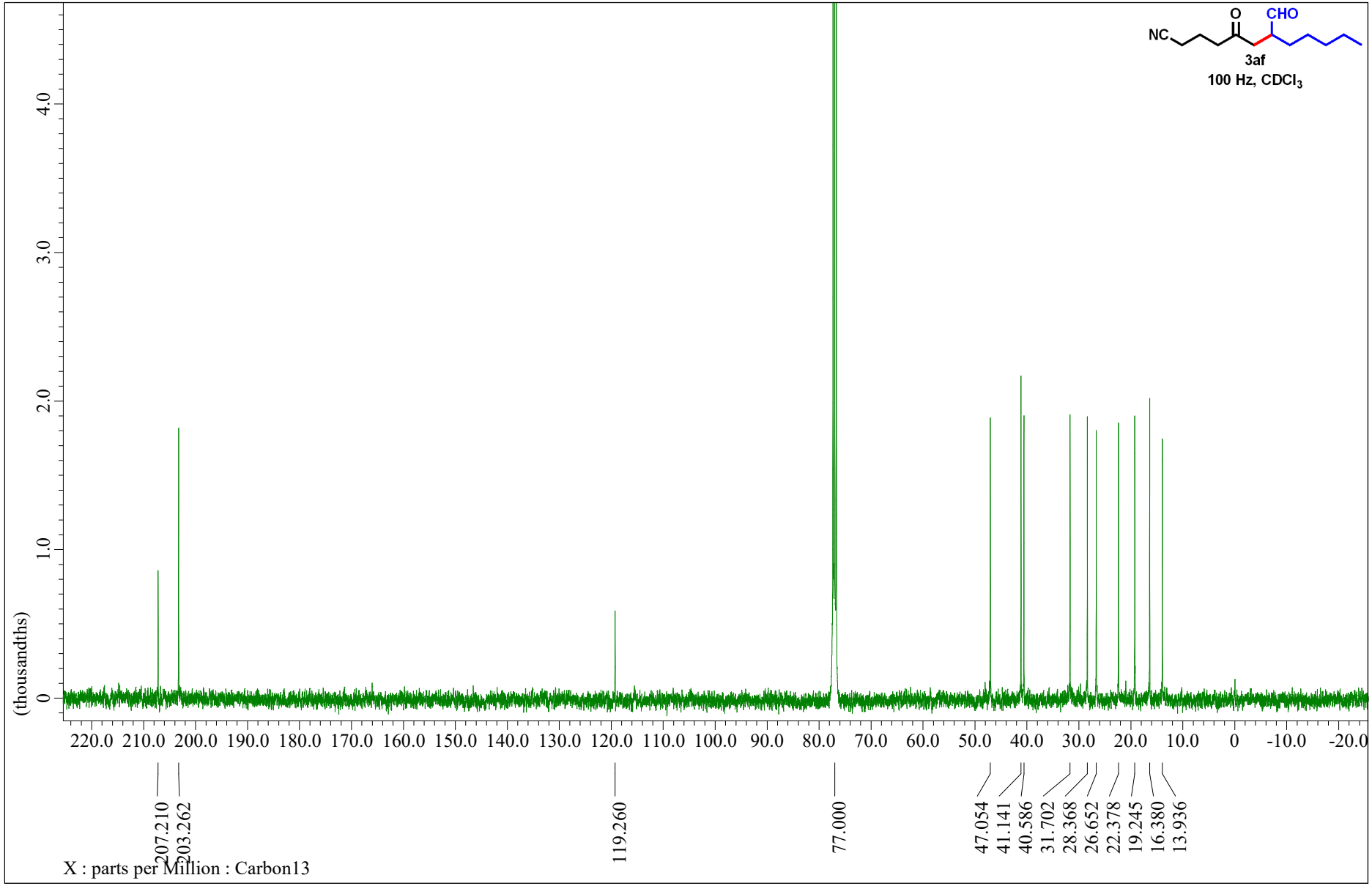

O
CHO
NC
3ac
400 Hz, CDCl3
6.19
4.05
3.42
3.03
2.16
1.97
1.11
1.09
1.00
0.75
abundance
0
0.1
0.2
0.3
0.4
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.679
7.260
2.855
2.832
2.811
2.789
2.724
2.706
2.689
2.678
2.661
2.648
1.276
1.261
1.257
1.250
1.242
1.224
0.973
0.957
0.940
0.924
X : parts per Million : Proton

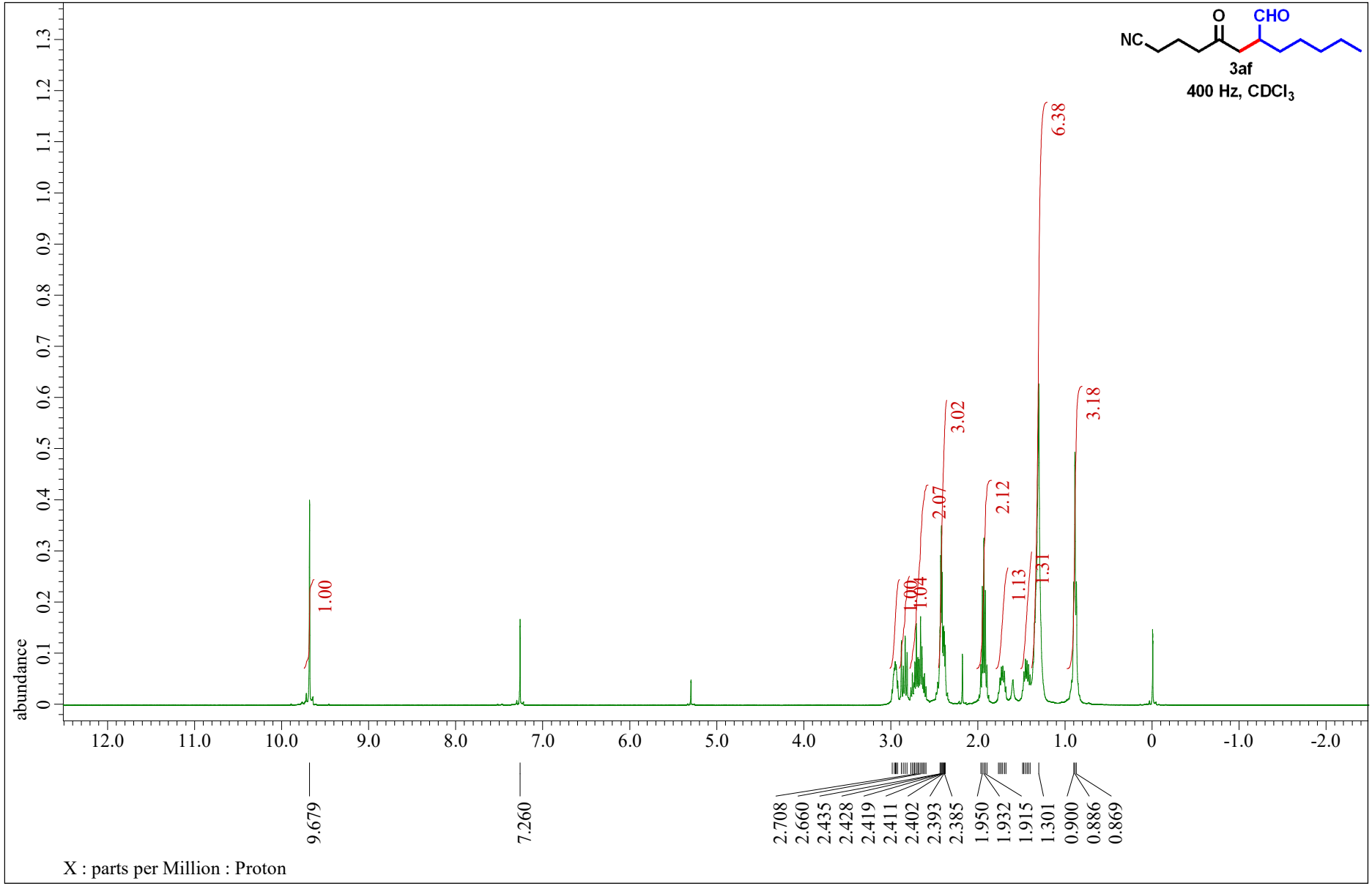

O
CHO
NC
3ad
100 Hz, CDCl3
(thousandths)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.172
203.214
119.241
77.000
48.281
40.624
21.478
19.245
16.360
11.339
X : parts per Million : Carbon13

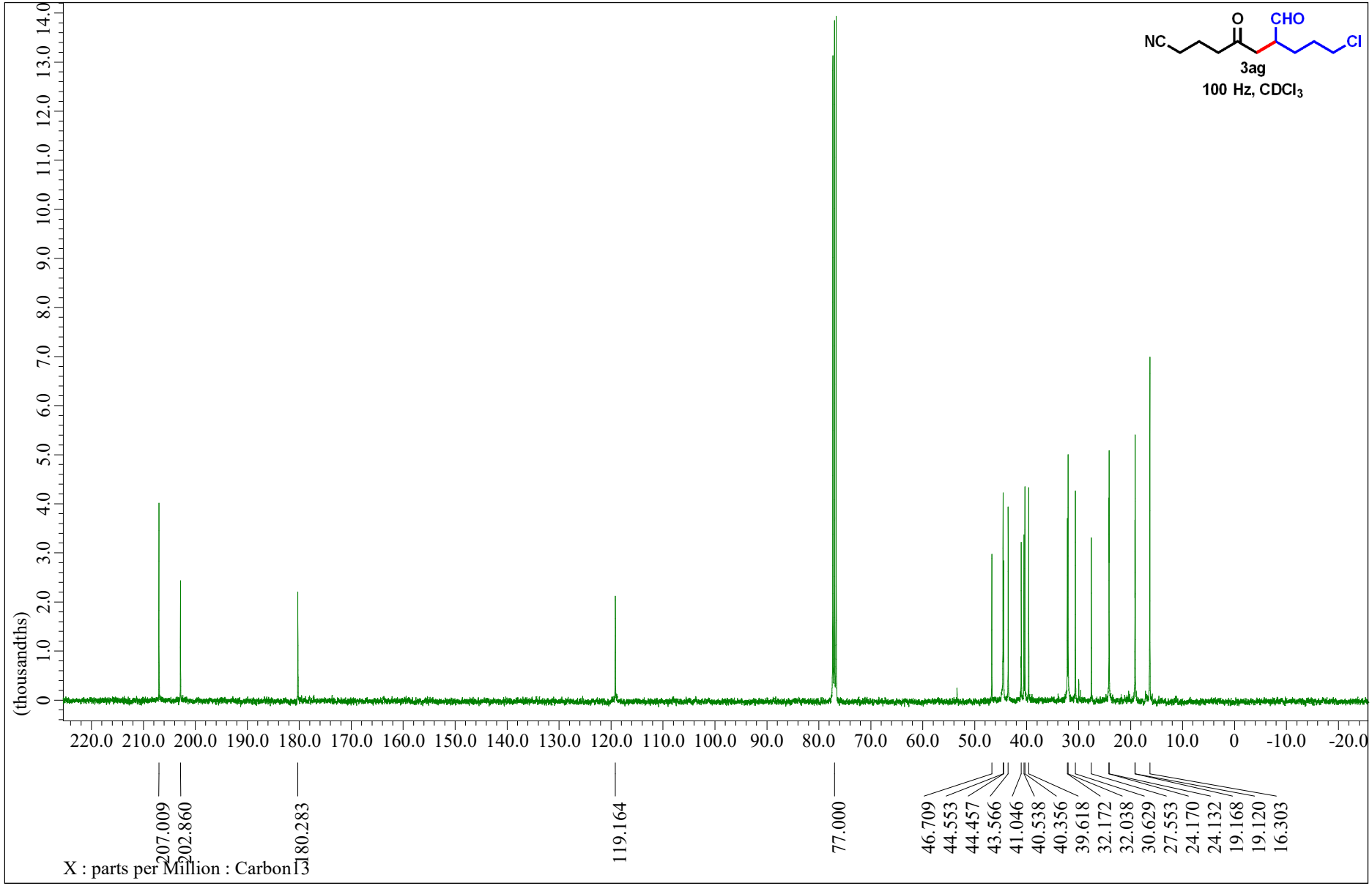

O
CHO
NC
3ad
400 Hz, CDCl3
3.20
3.00
2.18
2.18
2.01
1.10
1.05
1.00
2.0
1.0
0
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.682
7.260
2.880
2.839
2.711
2.662
2.433
2.423
2.410
2.401
2.393
1.948
1.931
1.914
0.985
0.966
0.947
X : parts per Million : Proton

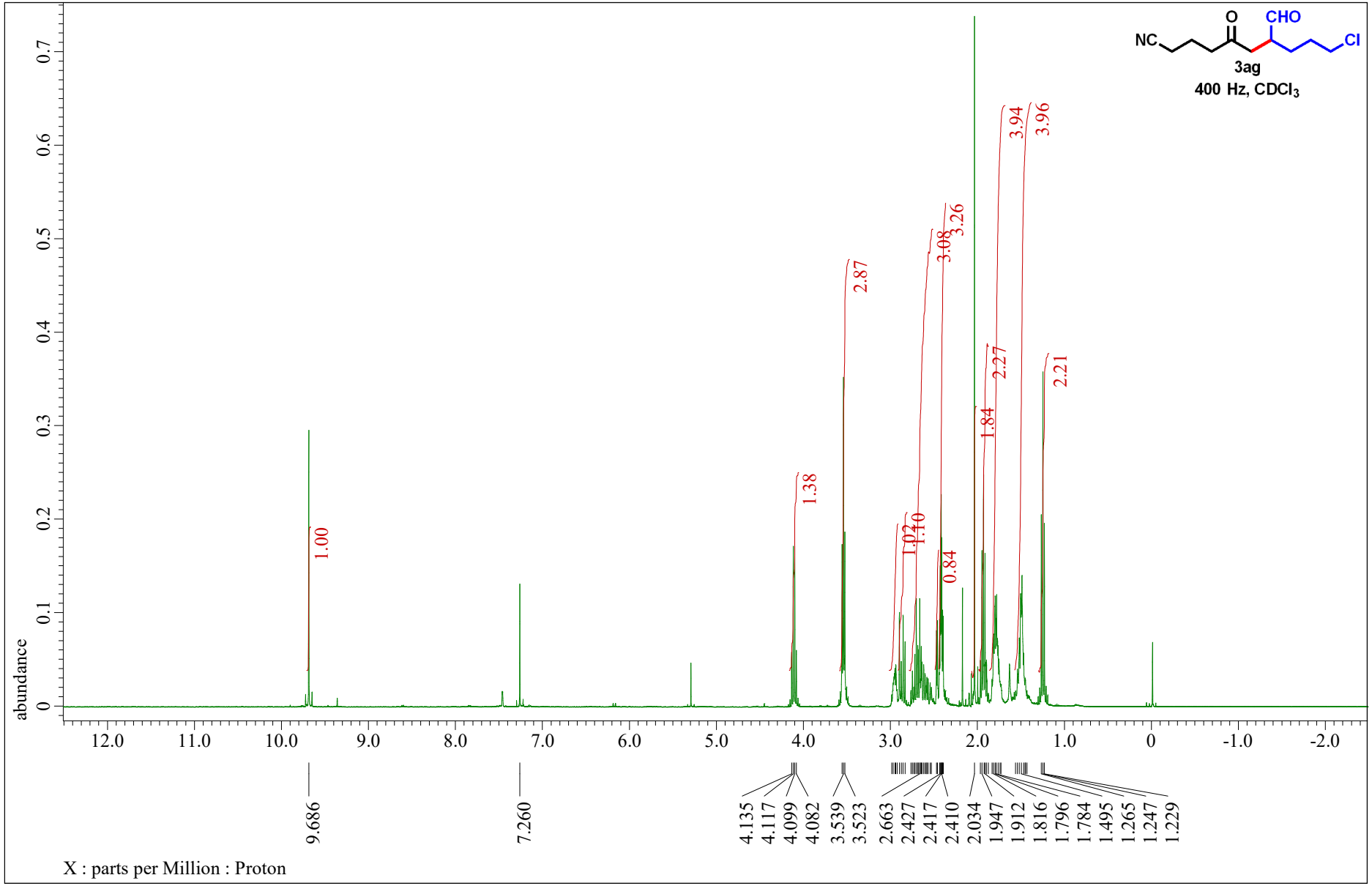

O
CHO
NC
3ae
100 Hz, CDCl3
(thousandths)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.210
203.262
119.260
77.000
47.006
41.141
40.586
29.115
28.109
22.647
19.245
16.380
13.811
X : parts per Million : Carbon13

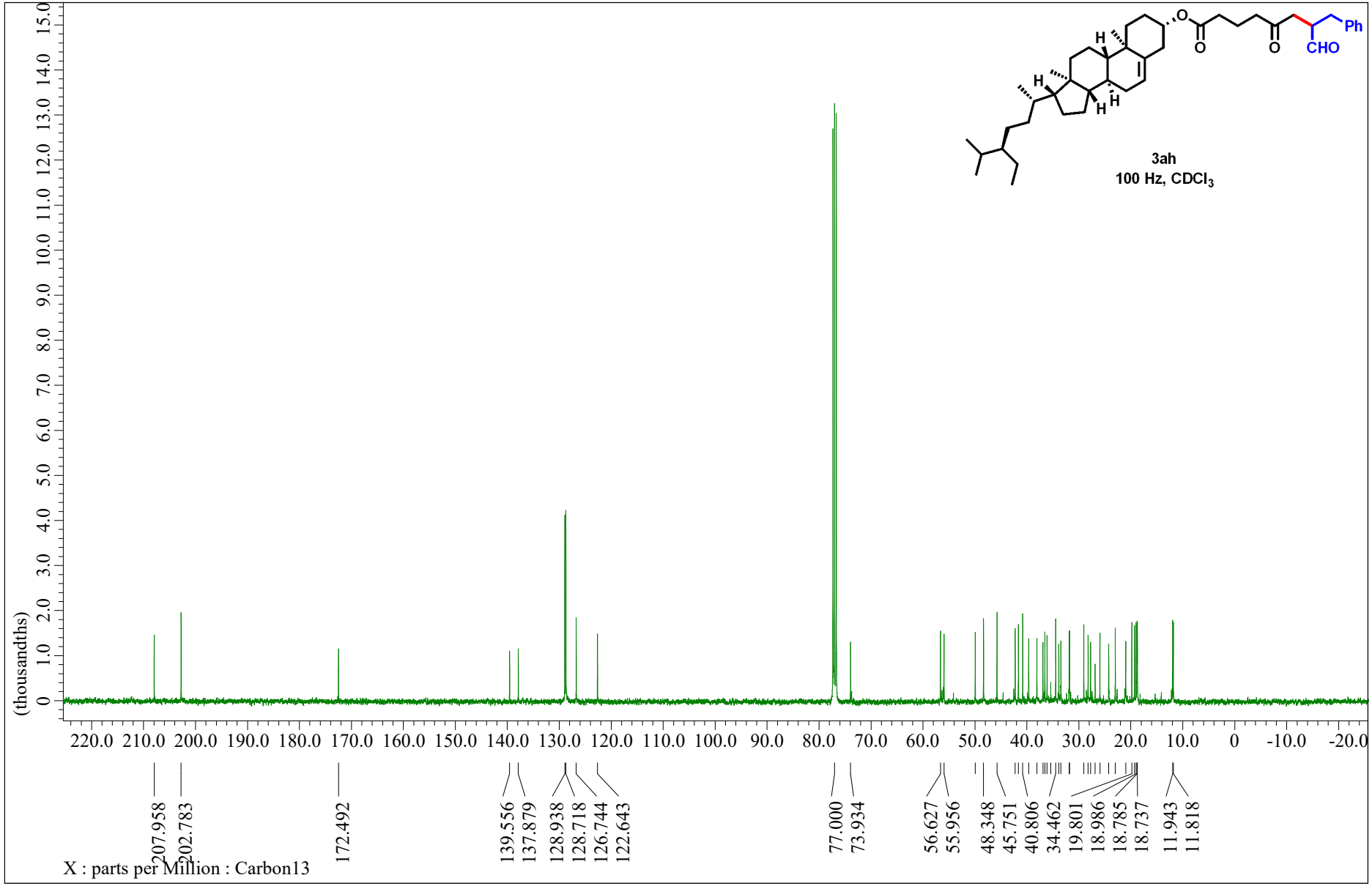

NC
O
CHO
3ae
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
1.03
1.12
2.30
3.38
2.31
1.02
1.16
4.06
3.32
9.687
7.260
2.706
2.657
2.436
2.427
2.419
2.410
2.401
2.393
2.385
1.931
1.330
1.321
1.312
0.920
0.904
0.886

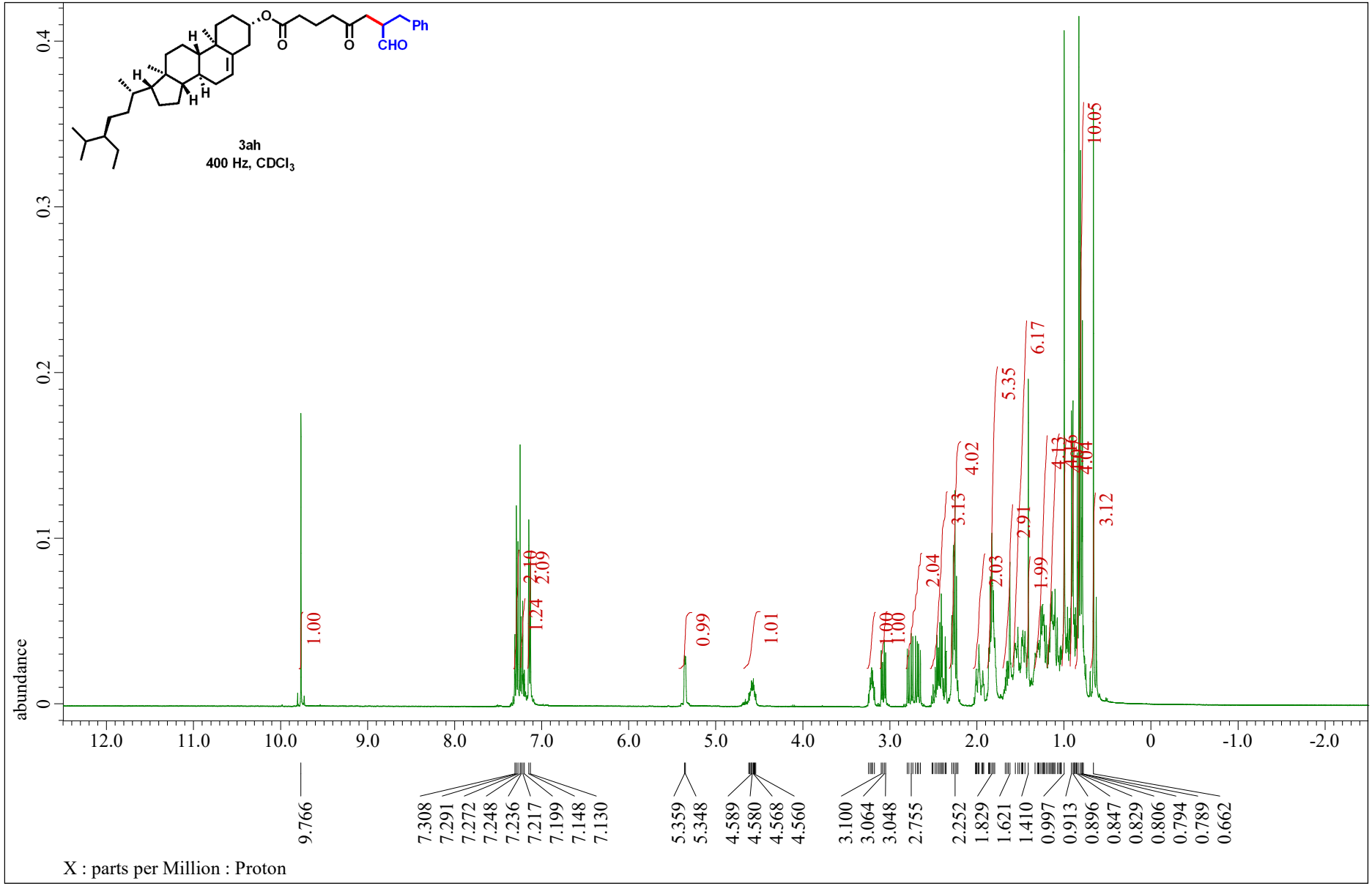

O
CHO
NC
3af
100 Hz, CDCl3
(thousandths)
4.0
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.210
203.262
119.260
77.000
47.054
41.141
40.586
31.702
28.368
26.652
22.378
19.245
16.380
13.936
X : parts per Million : Carbon13

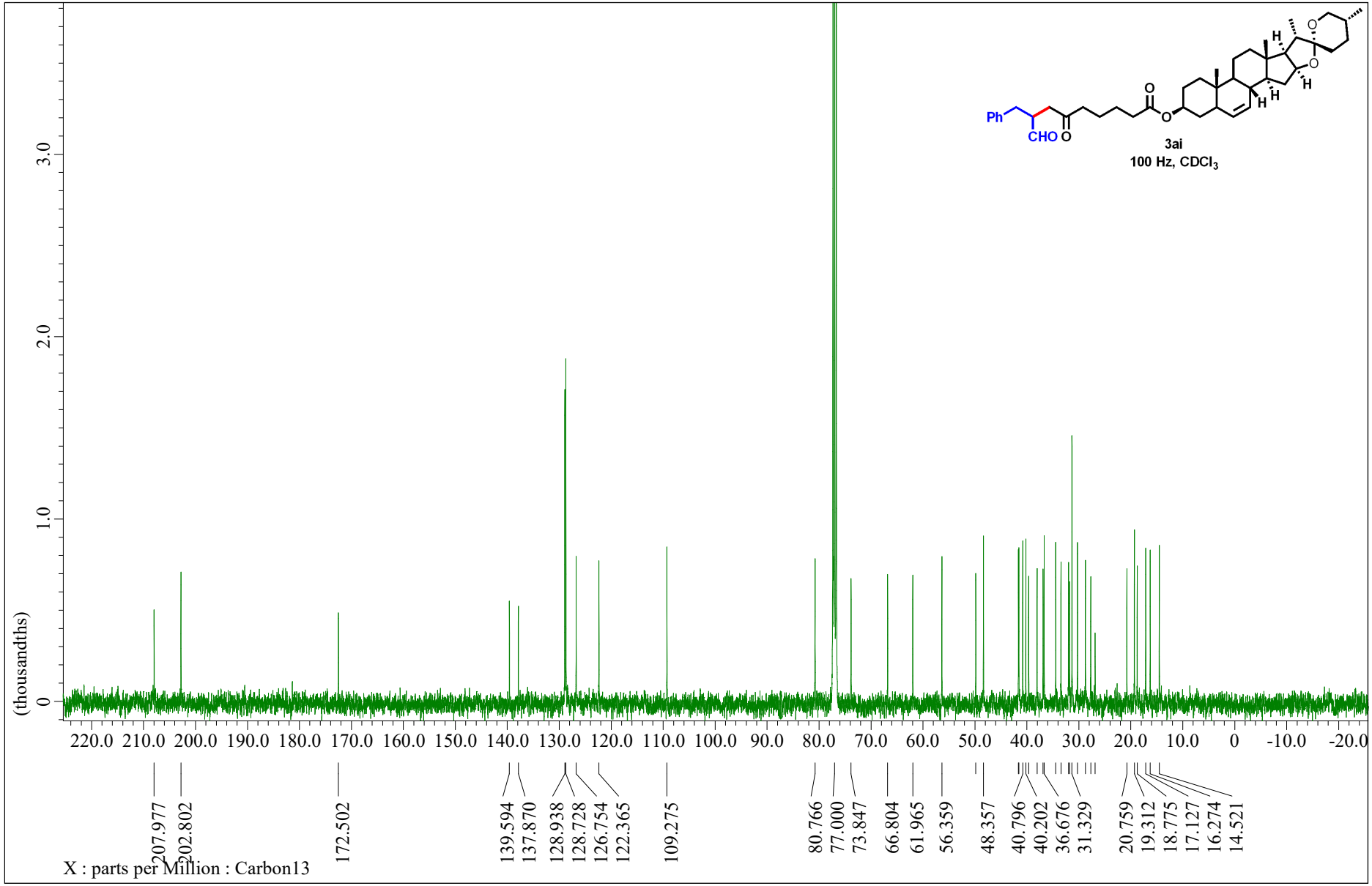

NC
O
CHO
3af
400 Hz, CDCl3
abundance
6.38
3.18
3.02
2.07
2.12
1.31
1.13
1.00
1.00
1.04
9.679
7.260
2.708
2.660
2.435
2.428
2.419
2.411
2.402
2.393
2.385
1.950
1.932
1.915
1.301
0.900
0.886
0.869
X : parts per Million : Proton

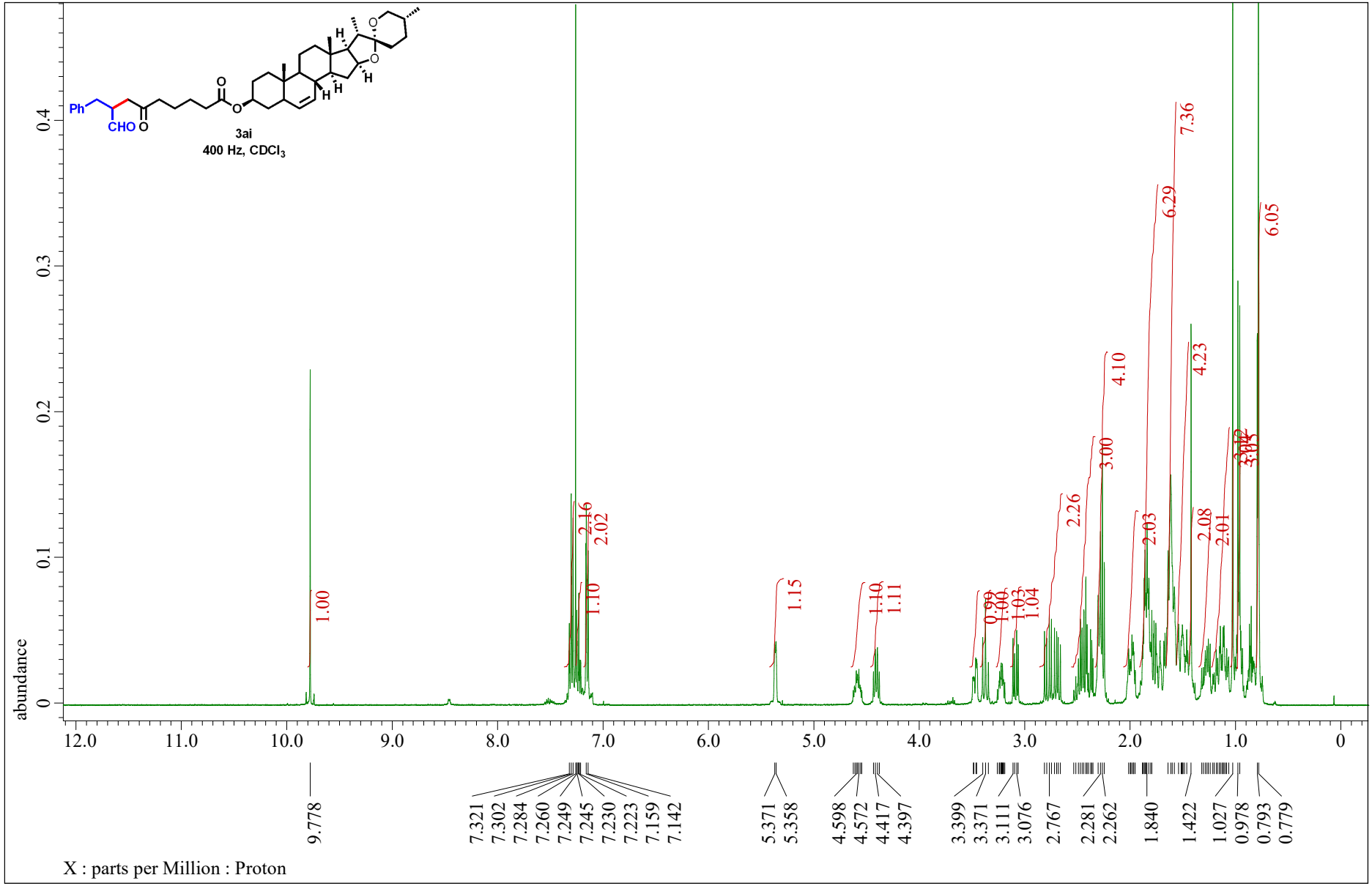

O
CHO
NC
Cl
3ag
100 Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
13.0
14.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.009
202.860
180.283
119.164
77.000
46.709
44.553
44.457
43.566
41.046
40.538
40.356
39.618
32.172
32.038
30.629
27.553
24.170
24.132
19.168
19.120
16.303
X : parts per Million : Carbon13

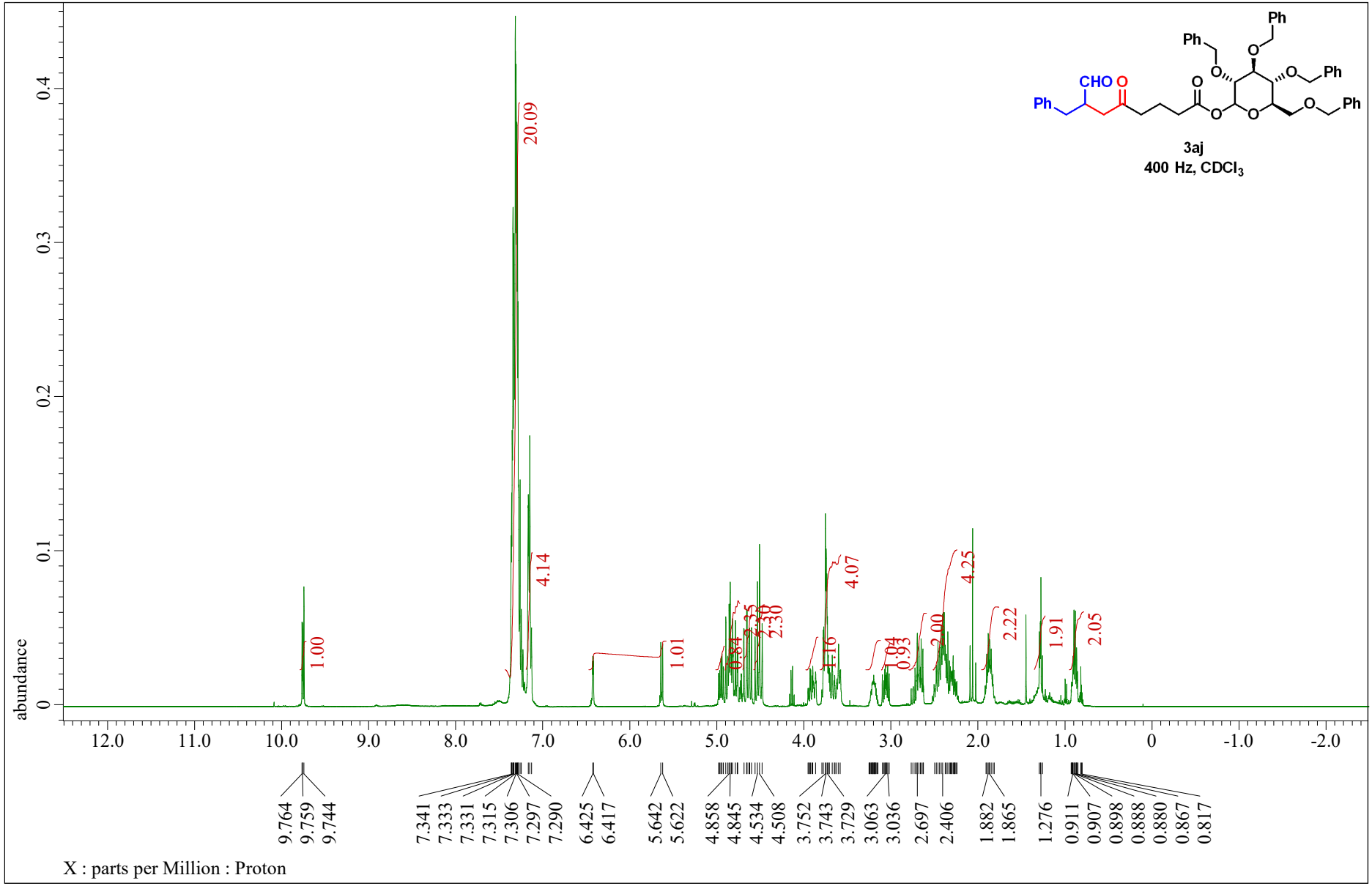

NC
O
CHO
Cl
3ag
400 Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
1.00
1.38
2.87
3.08
3.26
3.94
3.96
1.84
2.27
2.21
1.02
1.10
0.84
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
9.686
7.260
4.135
4.117
4.099
4.082
3.539
3.523
2.663
2.427
2.417
2.410
2.034
1.947
1.912
1.816
1.796
1.784
1.495
1.265
1.247
1.229
X : parts per Million : Proton

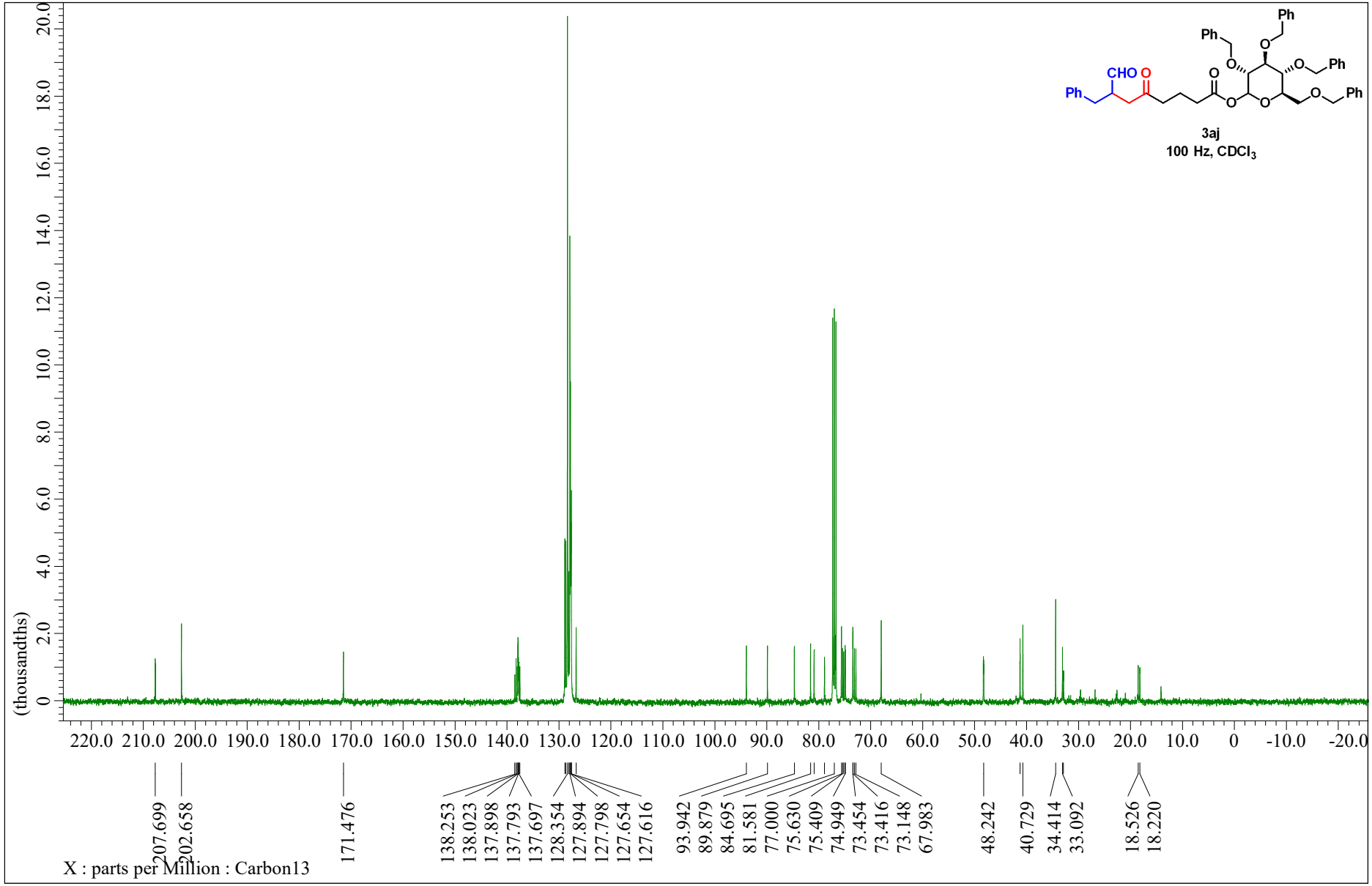

3ah
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
207.958
202.783
172.492
139.556
137.879
128.938
128.718
126.744
122.643
77.000
73.934
56.627
55.956
48.348
45.751
40.806
34.462
19.801
18.986
18.785
18.737
11.943
11.818

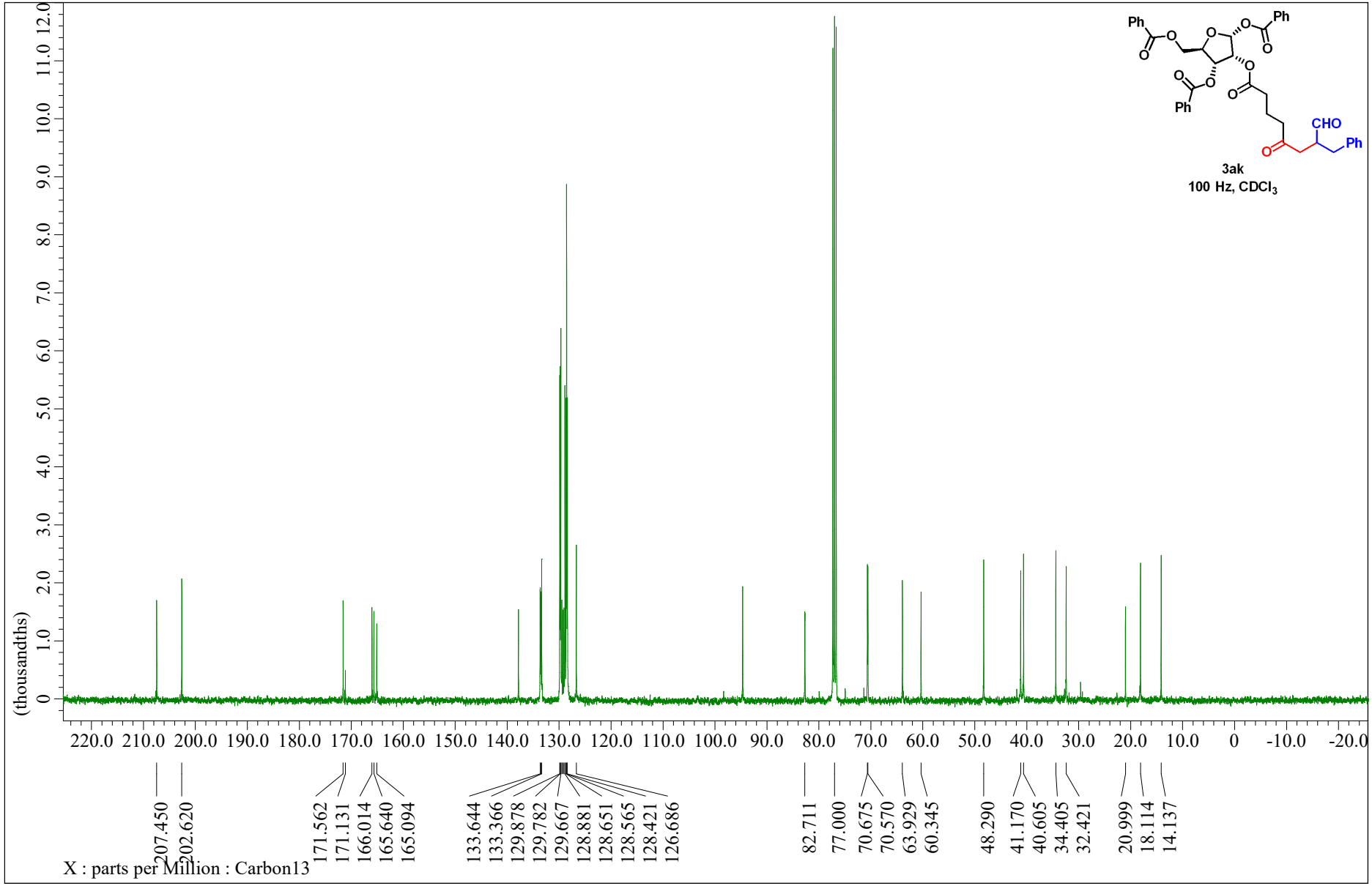

3ah
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
0.99
1.01
1.24
2.10
2.09
1.00
1.00
2.04
3.13
4.02
2.03
5.35
2.91
6.17
1.99
4.13
4.06
4.04
10.05
3.12
9.766
7.308
7.291
7.272
7.248
7.236
7.217
7.199
7.148
7.130
5.359
5.348
4.589
4.580
4.568
4.560
3.100
3.064
3.048
2.755
2.252
1.829
1.621
1.410
0.997
0.913
0.896
0.847
0.829
0.806
0.794
0.789
0.662

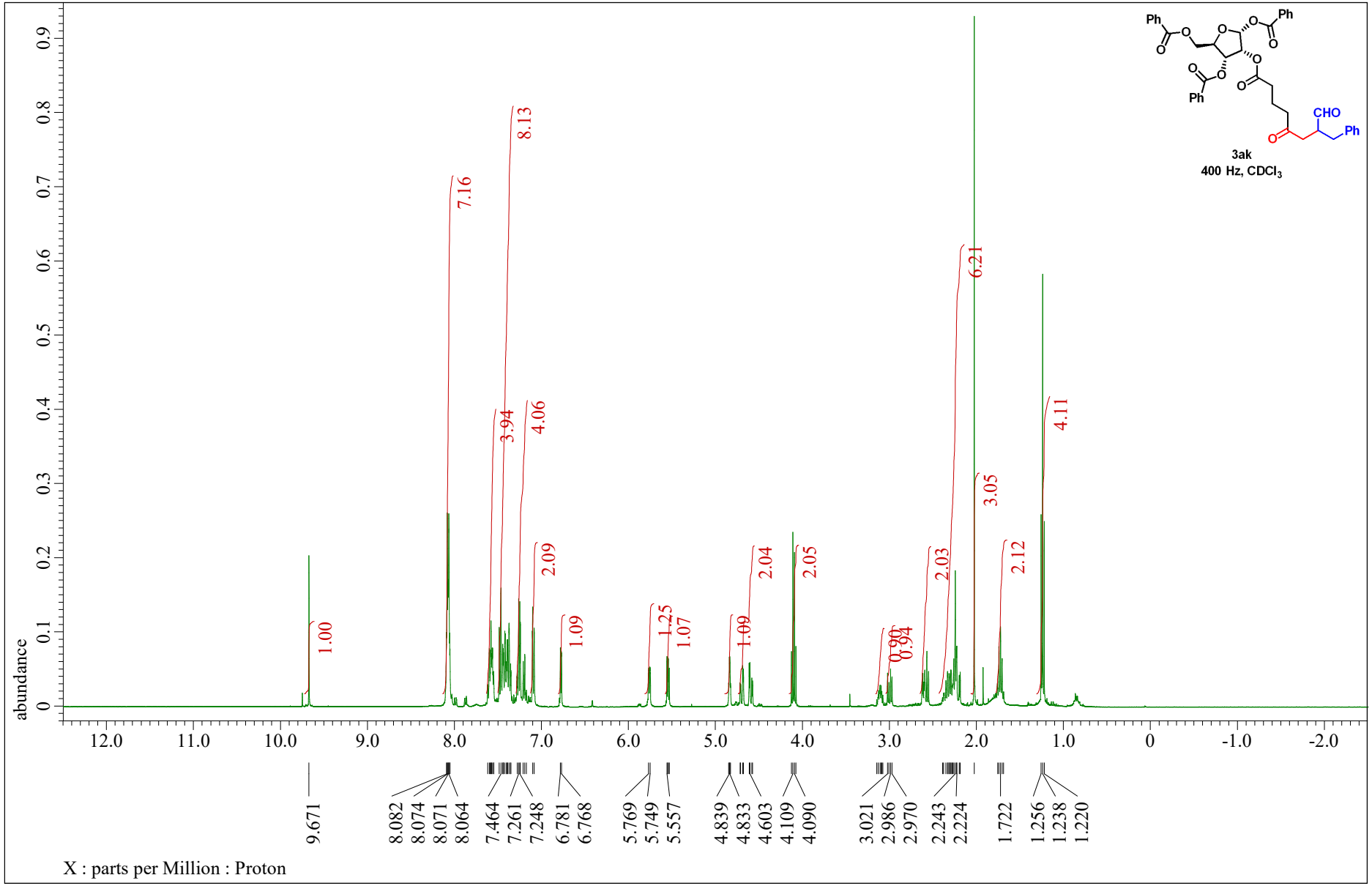

3ai
100 Hz, CDCl3
(thousandths)
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.977
202.802
172.502
139.594
137.870
128.938
128.728
126.754
122.365
109.275
80.766
77.000
73.847
66.804
61.965
56.359
48.357
40.796
40.202
36.676
31.329
20.759
19.312
18.775
17.127
16.274
14.521
X : parts per Million : Carbon13

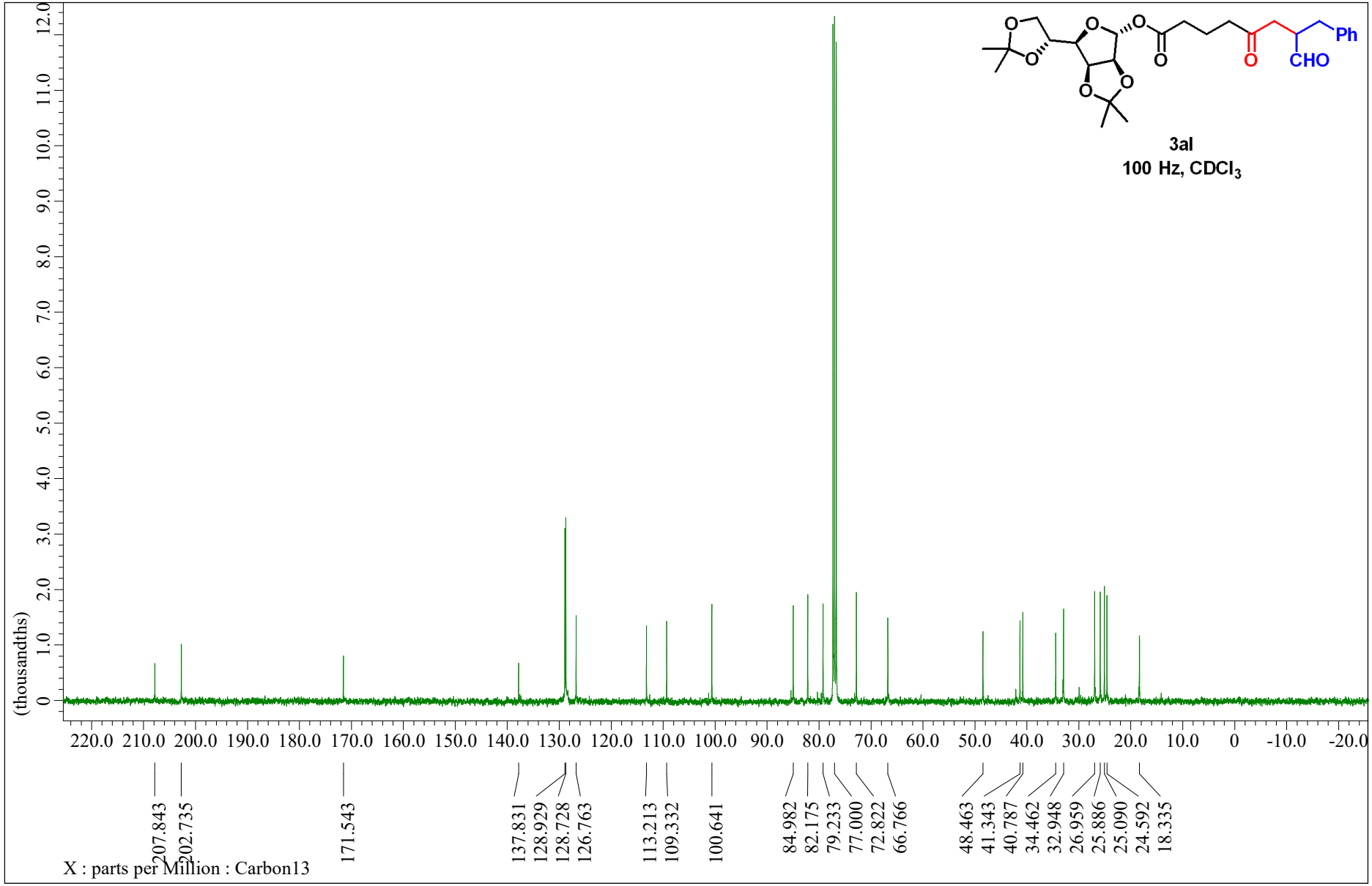

3ai
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
2.16
2.02
1.10
1.15
1.10
1.11
0.99
1.00
1.03
1.04
2.26
3.00
4.10
2.03
6.29
7.36
4.23
2.08
2.01
6.05
9.778
7.321
7.302
7.284
7.260
7.249
7.245
7.230
7.223
7.159
7.142
5.371
5.358
4.598
4.572
4.417
4.397
3.399
3.371
3.111
3.076
2.767
2.281
2.262
1.840
1.422
1.027
0.978
0.793
0.779

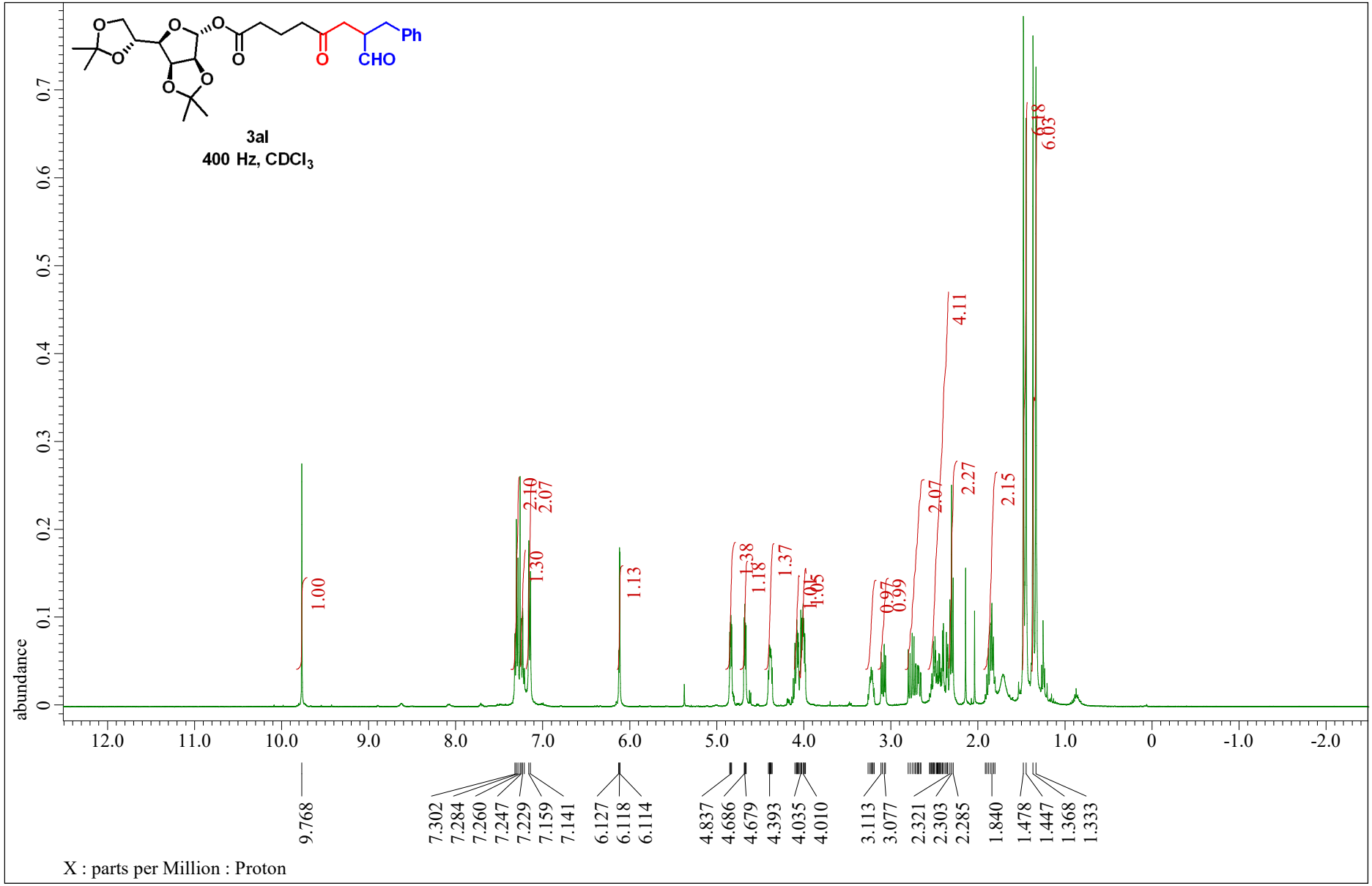

3aj
400 Hz, CDCl3
abundance
X : parts per Million : Proton
20.09
4.14
1.00
1.01
4.07
4.25
2.22
1.91
2.05
2.00
1.16
0.84
0.93
9.764
9.759
9.744
7.341
7.333
7.331
7.315
7.306
7.297
7.290
6.425
6.417
5.642
5.622
4.858
4.845
4.534
4.508
3.752
3.743
3.729
3.063
3.036
2.697
2.406
1.882
1.865
1.276
0.911
0.907
0.898
0.888
0.880
0.867
0.817

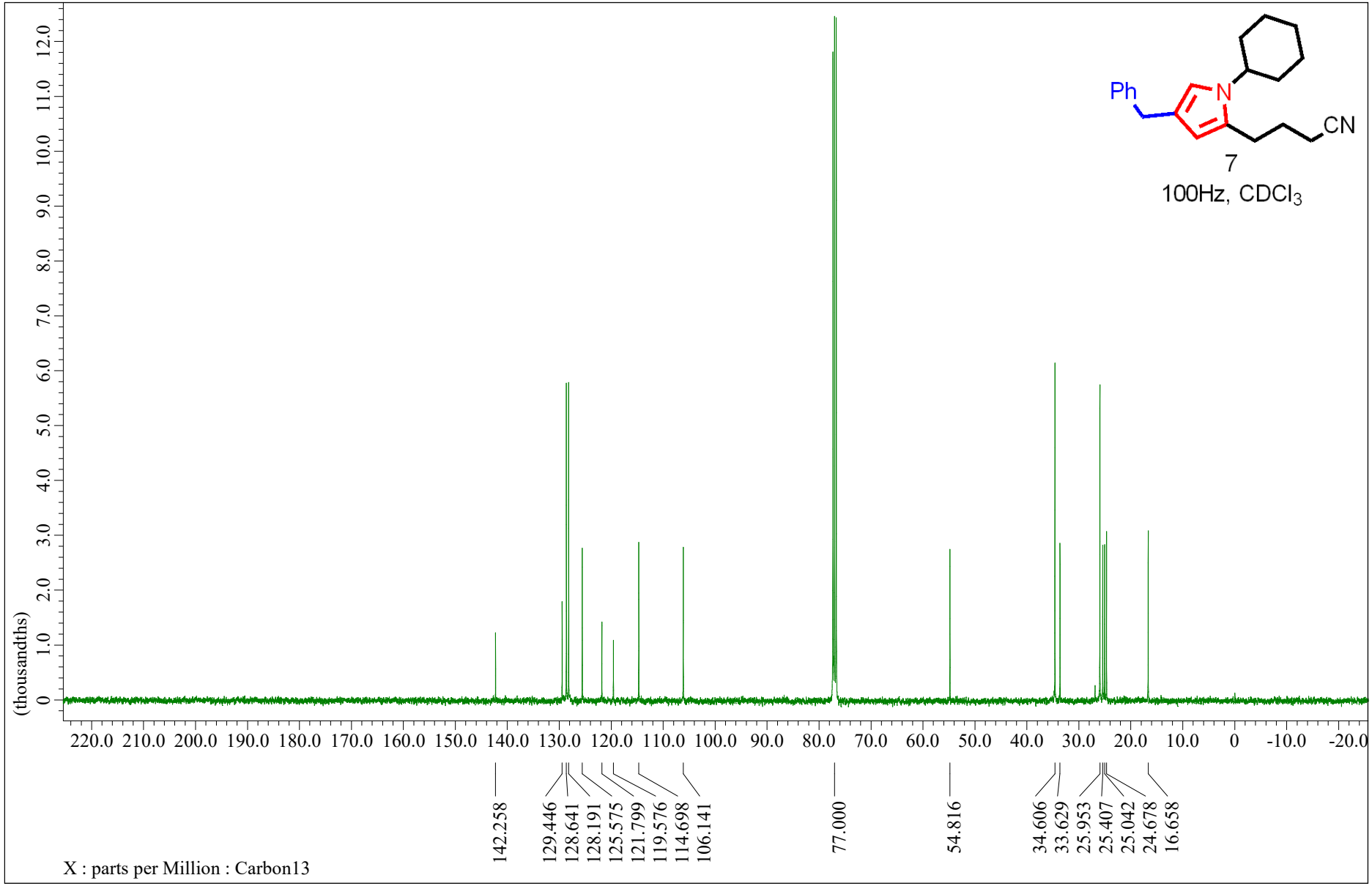

3aj
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
207.699
202.658
171.476
138.253
138.023
137.898
137.793
137.697
128.354
127.894
127.798
127.654
127.616
93.942
89.879
84.695
81.581
77.000
75.630
75.409
74.949
73.454
73.416
73.148
67.983
48.242
40.729
34.414
33.092
18.526
18.220

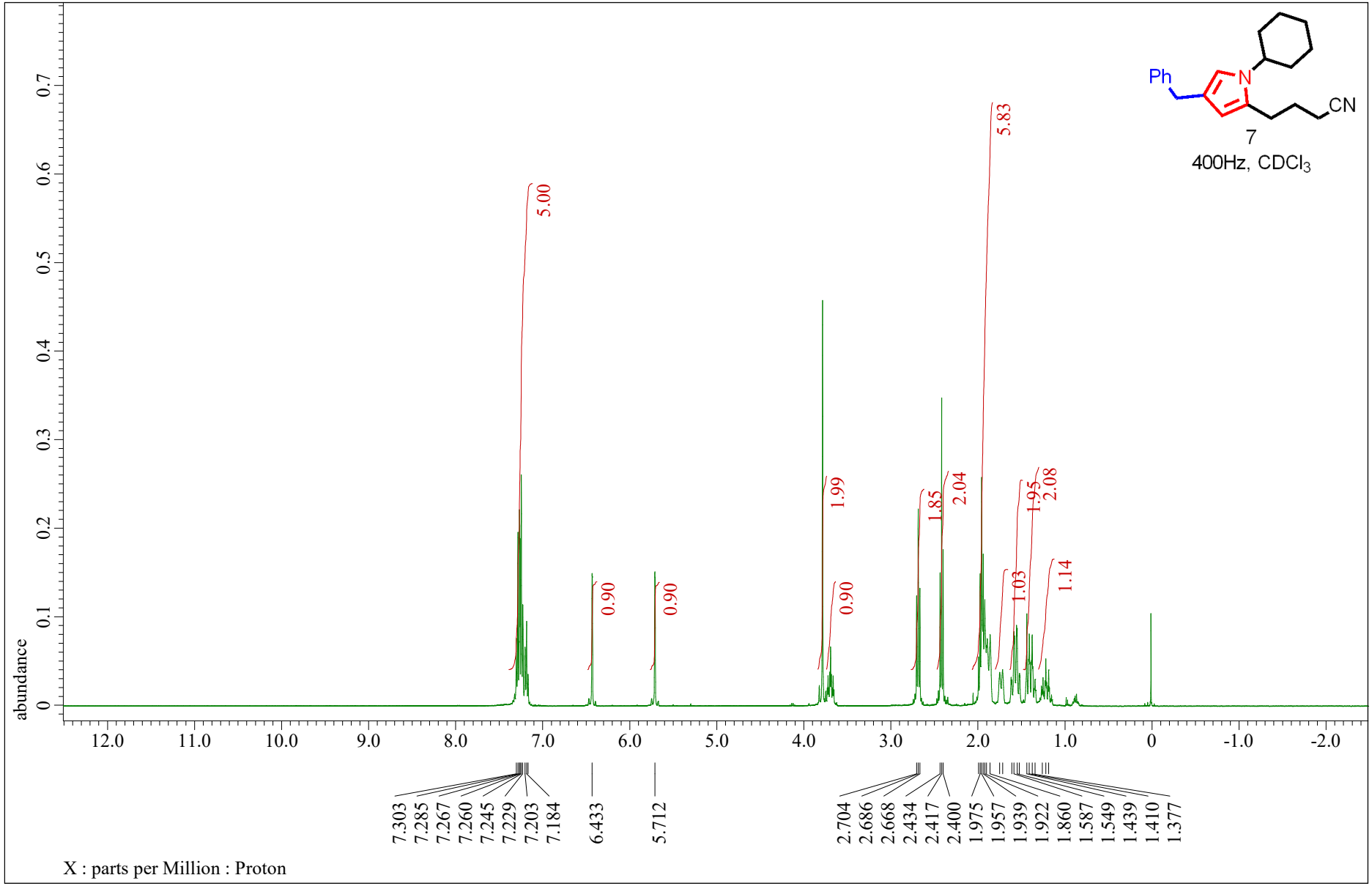

3ak
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
207.450
202.620
171.562
171.131
166.014
165.640
165.094
133.644
133.366
129.878
129.782
129.667
128.881
128.651
128.565
128.421
126.686
82.711
77.000
70.675
70.570
63.929
60.345
48.290
41.170
40.605
34.405
32.421
20.999
18.114
14.137

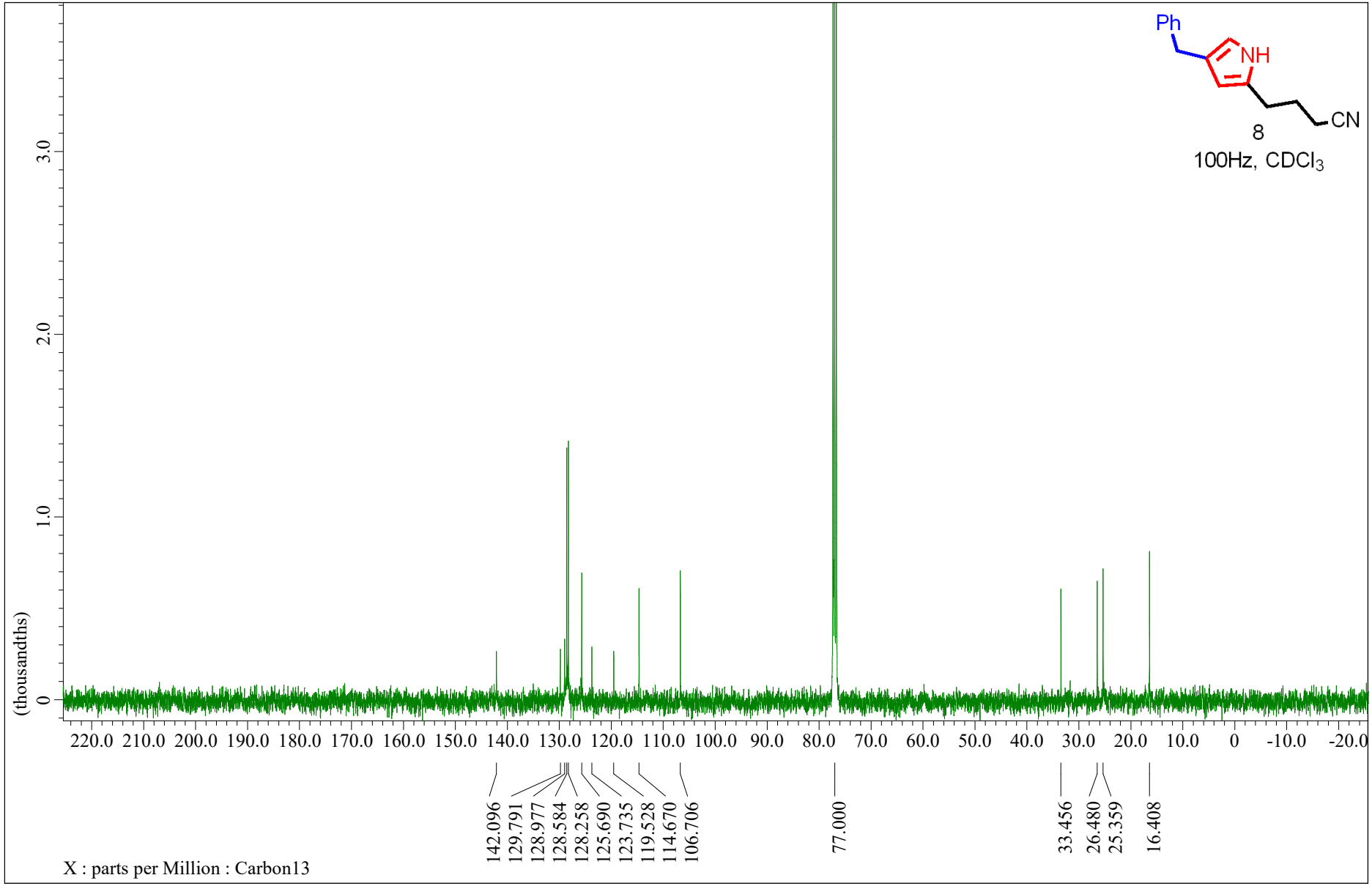

3ak
400 Hz, CDCl3
abundance
X : parts per Million : Proton
9.671
8.082
8.074
8.071
8.064
7.464
7.261
7.248
6.781
6.768
5.769
5.749
5.557
4.839
4.833
4.603
4.109
4.090
3.021
2.986
2.970
2.243
2.224
1.722
1.256
1.238
1.220

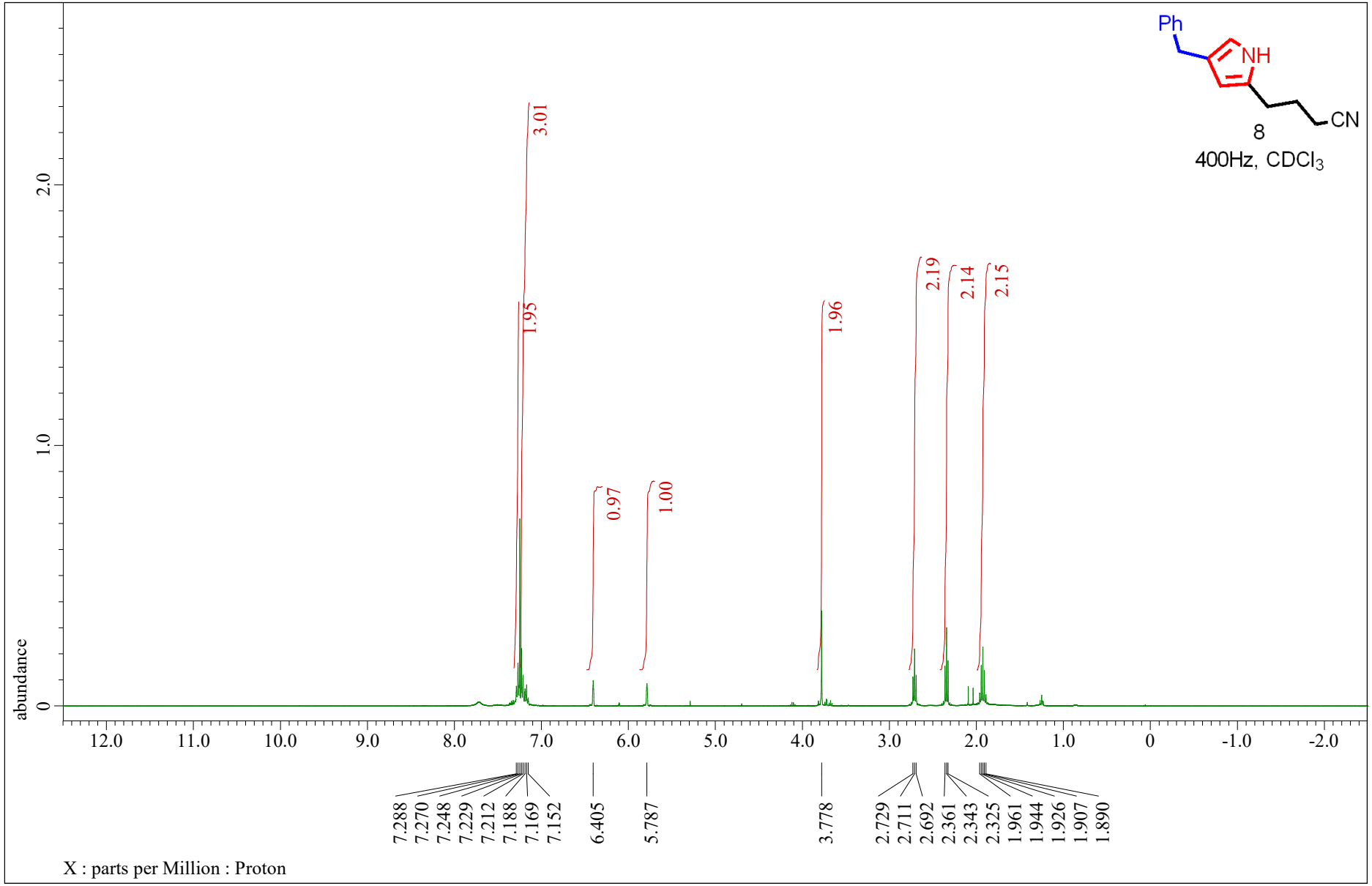

3al
100 Hz, CDCl3
(thousandths)
X : parts per Million : Carbon13
207.843
202.735
171.543
137.831
128.929
128.728
126.763
113.213
109.332
100.641
84.982
82.175
79.233
77.000
72.822
66.766
48.463
41.343
40.787
34.462
32.948
26.959
25.886
25.090
24.592
18.335

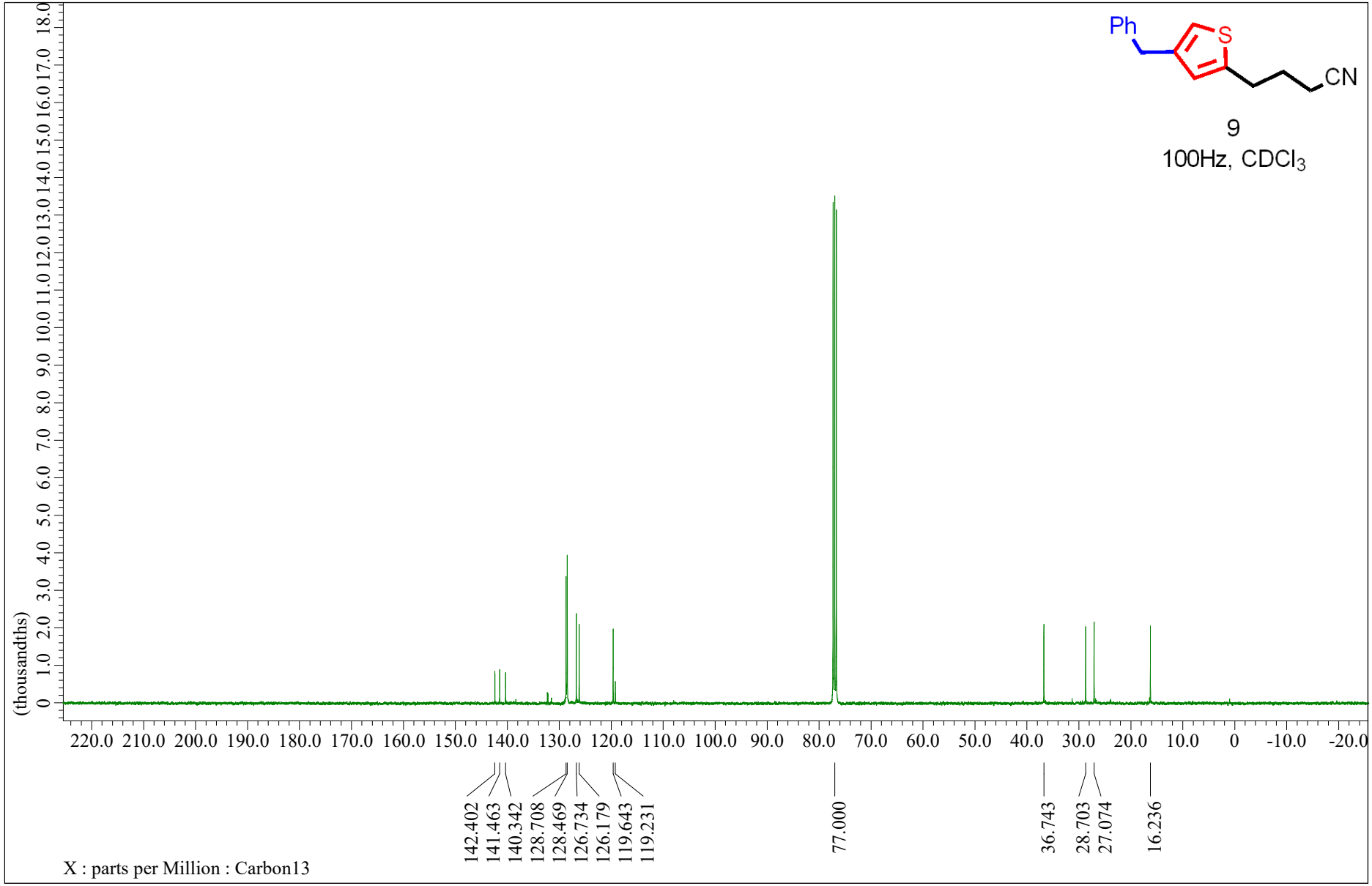

Ph
CHO
O
3al
400 Hz, CDCl3
abundance
X : parts per Million : Proton
1.00
2.10
2.07
1.30
1.13
1.38
1.18
1.37
1.05
0.97
0.99
2.07
4.11
2.27
2.15
6.18
6.03
9.768
7.302
7.284
7.260
7.247
7.229
7.159
7.141
6.127
6.118
6.114
4.837
4.686
4.679
4.393
4.035
4.010
3.113
3.077
2.321
2.303
2.285
1.840
1.478
1.447
1.368
1.333

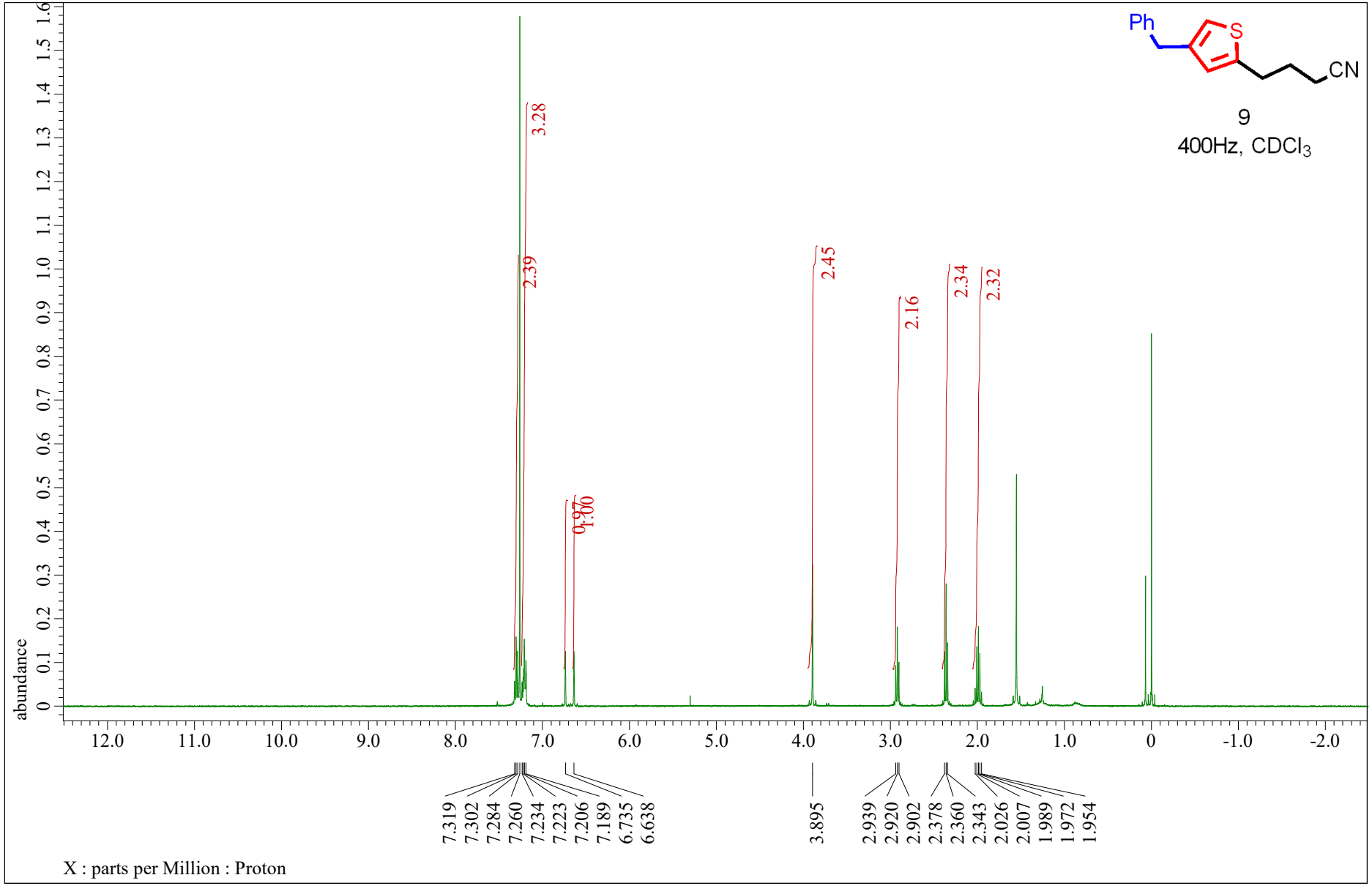

Ph
N
CN
7
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
11.0
12.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
142.258
129.446
128.641
128.191
125.575
121.799
119.576
114.698
106.141
77.000
54.816
34.606
33.629
25.953
25.407
25.042
24.678
16.658
X : parts per Million : Carbon13

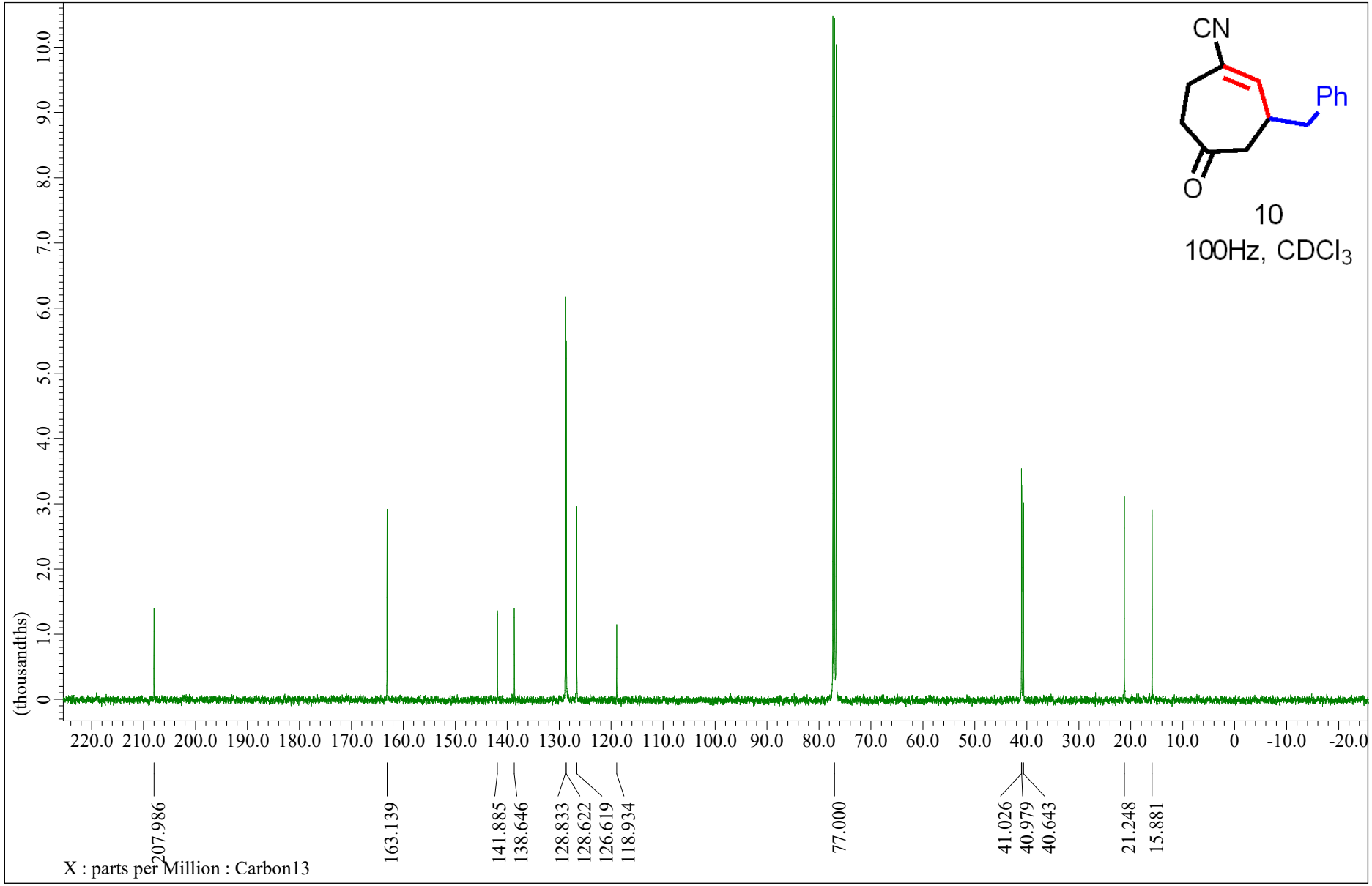

Ph
N
CN
7
400Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
5.00
0.90
0.90
1.99
0.90
1.85
2.04
5.83
1.95
2.08
1.03
1.14
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.303
7.285
7.267
7.260
7.245
7.229
7.203
7.184
6.433
5.712
2.704
2.686
2.668
2.434
2.417
2.400
1.975
1.957
1.939
1.922
1.860
1.587
1.549
1.439
1.410
1.377
X : parts per Million : Proton

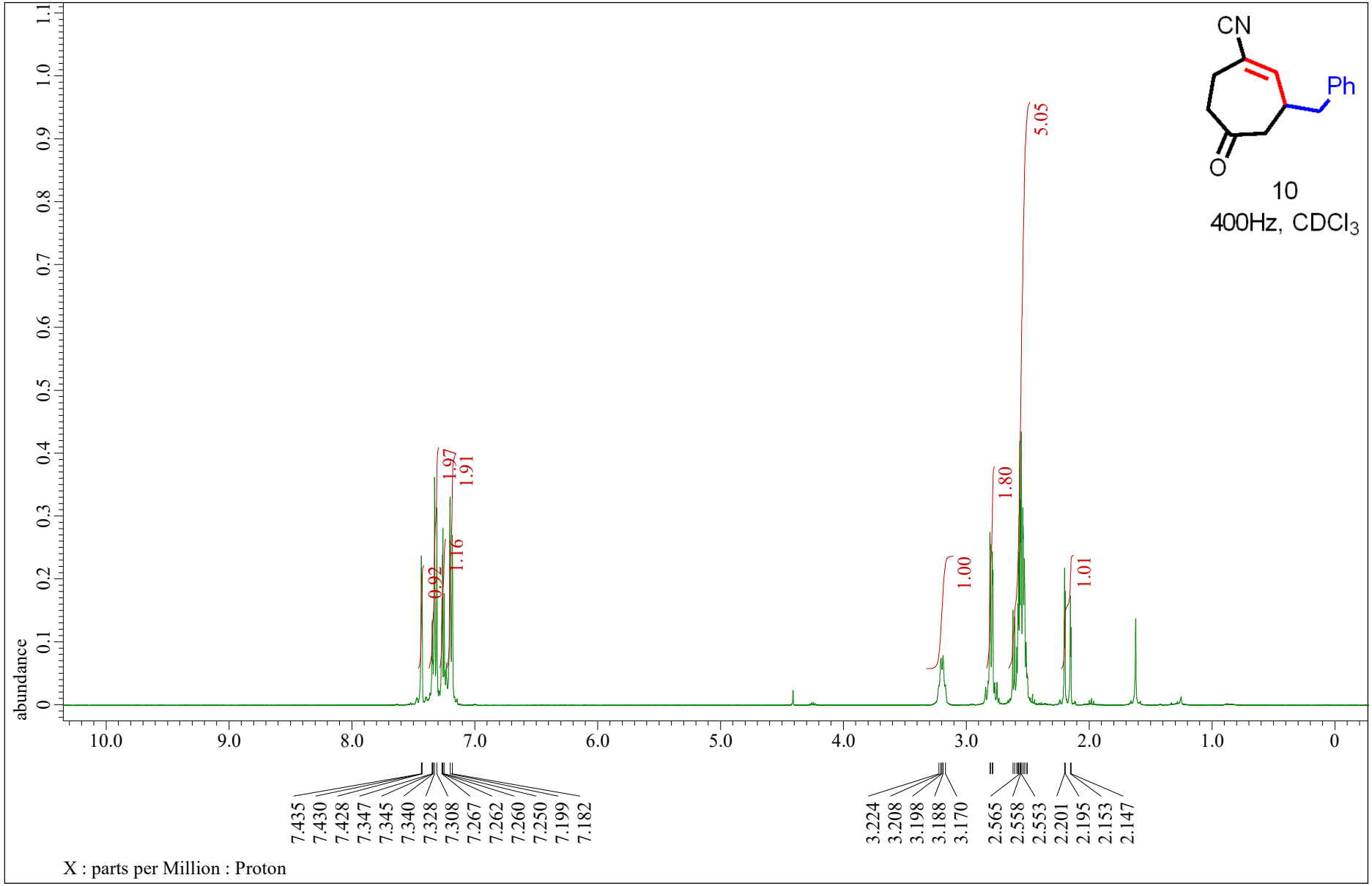

Ph
NH
CN
8
100Hz, CDCl3
(thousandths)
3.0
2.0
1.0
0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
142.096
129.791
128.977
128.584
128.258
125.690
123.735
119.528
114.670
106.706
77.000
33.456
26.480
25.359
16.408
X : parts per Million : Carbon13

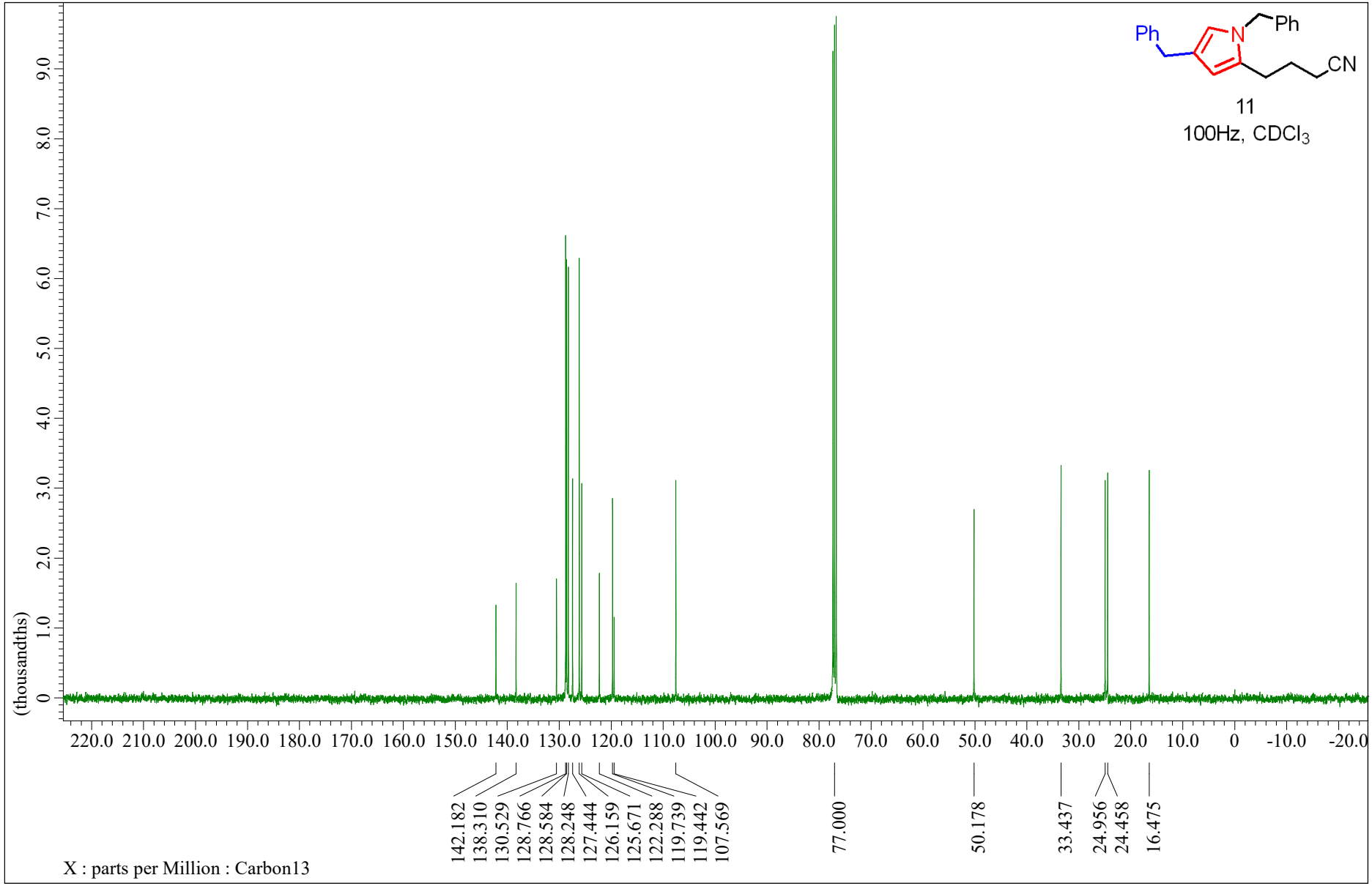

Ph
NH
CN
8
400Hz, CDCl3
abundance
2.0
1.0
0
3.01
1.95
0.97
1.00
1.96
2.19
2.14
2.15
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.288
7.270
7.248
7.229
7.212
7.188
7.169
7.152
6.405
5.787
3.778
2.729
2.711
2.692
2.361
2.343
2.325
1.961
1.944
1.926
1.907
1.890
X : parts per Million : Proton

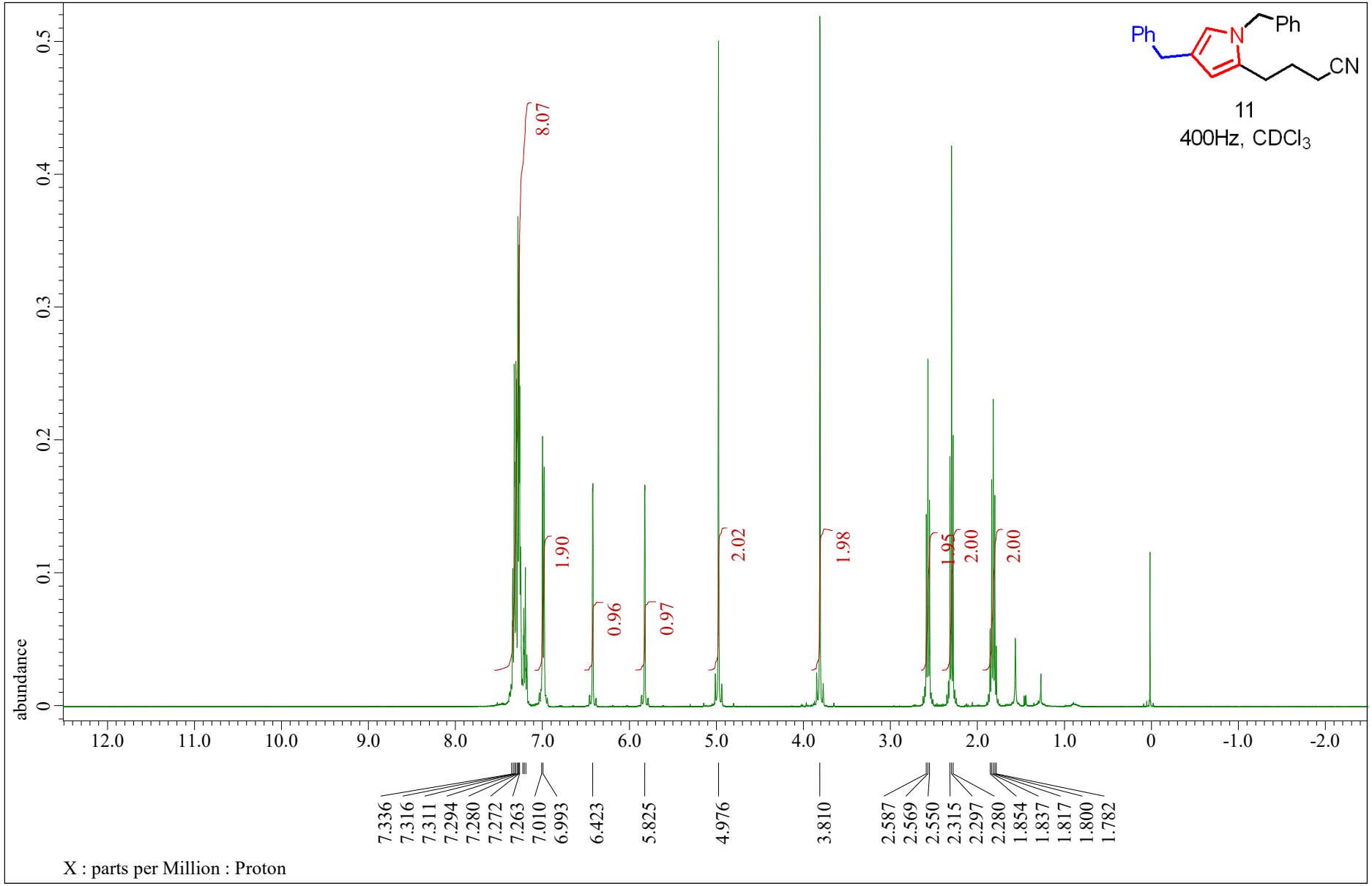

Ph
S
CN
9
100Hz, CDCl3
(thousandths)
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0 15.0 16.0 17.0 18.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
142.402
141.463
140.342
128.708
128.469
126.734
126.179
119.643
119.231
77.000
36.743
28.703
27.074
16.236
X : parts per Million : Carbon13


Ph
S
CN
9
400Hz, CDCl3
abundance
3.28
2.39
2.45
2.16
2.34
2.32
0.97
1.00
7.319
7.302
7.284
7.260
7.234
7.223
7.206
7.189
6.735
6.638
3.895
2.939
2.920
2.902
2.378
2.360
2.343
2.026
2.007
1.989
1.972
1.954
X : parts per Million : Proton


CN
Ph
O
10
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
10.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
207.986
163.139
141.885
138.646
128.833
128.622
126.619
118.934
77.000
41.026
40.979
40.643
21.248
15.881
X : parts per Million : Carbon13


CN
Ph
O
10
400Hz, CDCl3
abundance
5.05
1.97
1.91
1.80
1.16
1.00
1.01
0.92
7.435
7.430
7.428
7.347
7.345
7.340
7.328
7.308
7.267
7.262
7.260
7.250
7.199
7.182
3.224
3.208
3.198
3.188
3.170
2.565
2.558
2.553
2.201
2.195
2.153
2.147
X : parts per Million : Proton


Ph
N
Ph
CN
11
100Hz, CDCl3
(thousandths)
0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
8.0
9.0
220.0 210.0 200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0 -10.0 -20.0
142.182
138.310
130.529
128.766
128.584
128.248
127.444
126.159
125.671
122.288
119.739
119.442
107.569
77.000
50.178
33.437
24.956
24.458
16.475
X : parts per Million : Carbon13


Ph
N
Ph
CN
11
400Hz, CDCl3
abundance
0
0.1
0.2
0.3
0.4
0.5
8.07
1.90
0.96
0.97
2.02
1.98
1.95
2.00
2.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.336
7.316
7.311
7.294
7.280
7.272
7.263
7.010
6.993
6.423
5.825
4.976
3.810
2.587
2.569
2.550
2.315
2.297
2.280
1.854
1.837
1.817
1.800
1.782
X : parts per Million : Proton