Supporting Information for:

Oleic Amide Derivatives as Small Molecule Stimulators of the Human Proteasome's Core Particle

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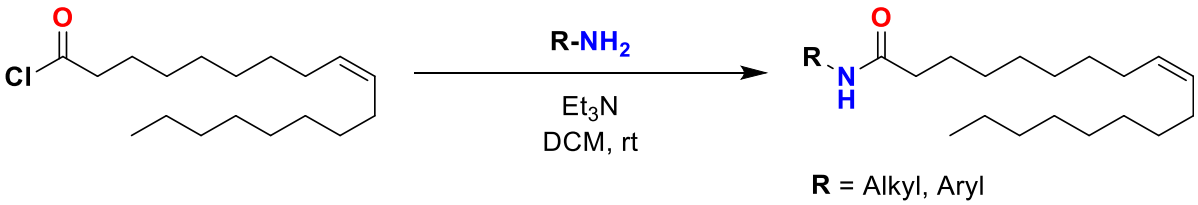
General Methods and Materials.

All chemicals, reagents and solvents were procured from commercial providers and were used as such. The reactions were monitored by thin layer chromatography (TLC) and/or LCMS on Agilent 1260 Infinity II system with Single Quadrupole LC/MS System. ^{1}H and ^{13}C NMR spectra were obtained on Bruker DRX500-2 spectrometer (500 and 125 MHz for ^{1}H and ^{13}C NMR respectively). Chemical shifts (δ) are reported in ppm relative to tetramethyl silane (TMS) as internal standard or calibrated using residual $CHCl_3$ peak as δ 7.26 for 1H and δ 77.16 for ^{13}C NMR. Spin multiplicities for ^{1}H NMR are reported as s (singlet), brs (broad singlet), d (doublet), dd (double doublet), t (triplet), q (quartet) and m (multiplet). Coupling constant (J) values are reported in hertz (Hz). Mass of the synthesized molecules were recorded using ESI or APCI probe on Advion Expression CMS single quadrupole mass spectrometer. Column chromatography was performed using silica gel 60-120 or 100- 200 mesh.

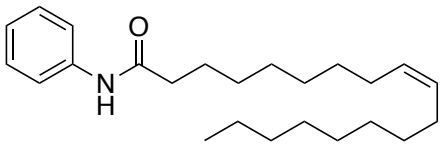
General Synthesis of the amide derivatives



Supporting Information Figure S1. General amide coupling reaction.

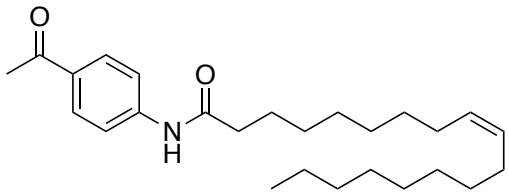
In a typical reaction, the corresponding amine (1 eq, 0.1 M) and triethylamine (2 eq) was dissolved in dichloromethane, and oleoyl chloride (1.2 eq) was subsequently added to the solution. The reaction was stirred at room temperature and monitored using TLC and/or LCMS. Upon completion, the reaction mixture washed 1X with *sat.* citric acid, then 3X with 1 M NaOH, and 1X with water. All the aqueous layers were quickly washed with DCM. The combined DCM layer was washed with brine, and dried using *anh.* sodium sulfate. Solvent was removed using rotavap, and the crude product purity was analyzed using NMR and LCMS. The crude was purified using silica gel flash chromatography, if needed, to afford the pure product. The NMR of all the synthesized products matched with the reported spectra.

NMR and APCI-MS characterization of synthesized compounds

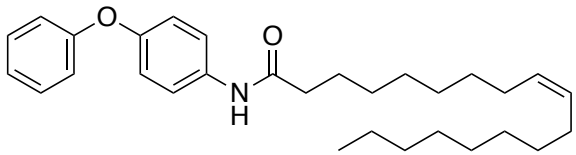


N-phenyloleamide (1). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (2H, d, *J* = 8.0 Hz), 7.32 (2H, t, *J* = 7.9 Hz), 7.17 (1H, s), 7.10 (1H, t, *J* = 7.4 Hz), 5.34 (2H, m), 2.35 (2H, t, *J* = 8.7, 6.5 Hz), 2.01 (4H, m), 1.74 (2H, p, *J* = 7.5 Hz), 1.30 (20H, m), 0.88 (3H, t, *J* = 6.9 Hz) ppm; ^{13}C NMR (126

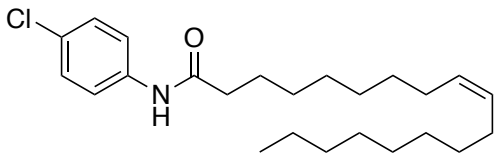
MHz, $CDCl_3$) δ 171.24, 137.83, 129.92, 129.63, 128.89, 124.06, 119.62, 76.91, 37.75, 31.80, 29.66, 29.60, 29.42, 29.22, 29.18, 29.14, 29.02, 27.12, 27.06, 25.51, 22.58, 14.02 ppm; APCI-MS (m/z). For $C_{24}H_{40}NO^+$ 358.31 $[M+H]^+$; found 358.3.



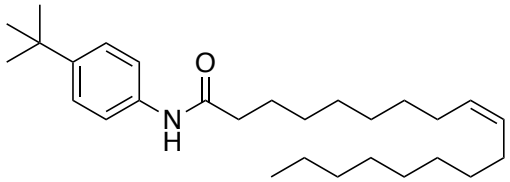
N-(4-acetylphenyl)oleamide (2). ^1H NMR (800 MHz, $CDCl_3$) δ 7.95 (2H, d, *J* = 8.3 Hz), 7.66 (2H, d, *J* = 8.3 Hz), 7.62 (1H, s), 5.36 (2H, m), 2.59 (3H, s), 2.41 (2H, t, *J* = 7.6 Hz), 2.03 (4H, m), 1.75 (2H, p, *J* = 7.6 Hz), 1.31 (20H, m), 0.90 (4H, m) ppm; ^{13}C NMR (201 MHz, $CDCl_3$) δ 197.08, 171.80, 142.44, 132.73, 130.06, 129.77, 129.69, 118.82, 77.04, 37.88, 31.91, 29.77, 29.70, 29.53, 29.33, 29.28, 29.23, 29.11, 27.23, 27.16, 26.44, 25.45, 22.69, 14.13 ppm; APCI-MS (m/z). For $C_{26}H_{42}NO_2^+$ 400.32 $[M+H]^+$; found 400.3.



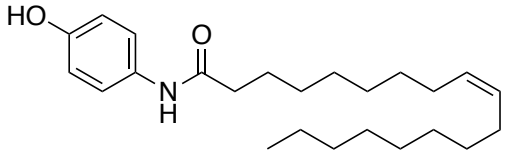
N-(4-phenoxyphenyl)oleamide (3). ^1H NMR (500 MHz, $CDCl_3$) δ 7.48 (2H, d, *J* = 8.9 Hz), 7.31 (2H, t, *J* = 7.8 Hz), 7.08 (1H, t, *J* = 7.4 Hz), 6.97 (4H, m), 5.35 (2H, m), 2.35 (2H, t, *J* = 7.6 Hz), 2.01 (4H, m), 1.73 (2H, p, *J* = 7.4 Hz), 1.31 (20H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.49, 157.46, 153.22, 133.41, 129.93, 129.62, 122.94, 121.56, 119.50, 118.27, 76.96, 37.56, 31.82, 29.68, 29.63, 29.45, 29.24, 29.19, 29.06, 27.14, 27.09, 25.61, 22.61, 14.06 ppm; APCI-MS (m/z). For $C_{30}H_{44}NO_2^+$ 450.34 $[M+H]^+$; found 450.2.



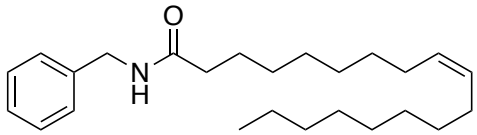
N-(4-chlorophenyl)oleamide (4). ^1H NMR (500 MHz, $CDCl_3$) δ 7.47 (2H, d, *J* = 8.5 Hz), 7.31 (1H, s), 7.26 (2H, d, *J* = 8.5 Hz), 5.34 (2H, m), 2.34 (2H, t, *J* = 7.6 Hz), 2.00 (4H, m), 1.72 (2H, p, *J* = 7.5 Hz), 1.31 (18H, m), 0.88 (4H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.33, 136.45, 129.93, 129.58, 128.97, 128.85, 120.87, 76.91, 60.30, 37.62, 31.79, 29.65, 29.58, 29.41, 29.21, 29.16, 29.12, 29.00, 27.11, 27.05, 25.42, 22.57, 20.93, 14.07, 13.99 ppm; APCI-MS (m/z). For $C_{24}H_{39}ClNO^+$ 392.27 $[M+H]^+$; found 392.2.



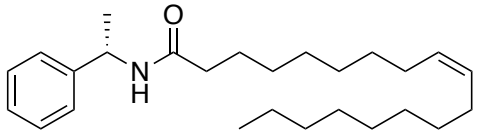
N-(4-(tert-butyl)phenyl)oleamide (5). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 (3H, d, *J* = 8.6, 6.4 Hz), 7.32 (2H, d, *J* = 8.6 Hz), 5.34 (2H, m), 2.34 (2H, t, *J* = 7.6 Hz), 2.01 (4H, q, *J* = 6.6 Hz), 1.71 (2H, p, *J* = 7.2 Hz), 1.29 (29H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.41, 147.00, 135.27, 129.90, 129.63, 125.62, 119.60, 76.94, 37.63, 34.22, 31.80, 31.25, 29.67, 29.61, 29.42, 29.22, 29.15, 29.05, 27.12, 27.07, 25.63, 22.58, 14.01 ppm; APCI-MS (m/z). For $C_{28}H_{48}NO^+$ 414.37 $[M+H]^+$; found 414.4.



N-(4-hydroxyphenyl)oleamide (6). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (1H, s), 7.23 (1H, d, *J* = 8.5 Hz), 6.73 (1H, d, *J* = 8.5 Hz), 5.35 (2H, m), 2.32 (2H, t, *J* = 7.9 Hz), 2.00 (4H, m), 1.70 (2H, p, *J* = 7.4 Hz), 1.29 (20H, m), 0.87 (4H, t, *J* = 6.7 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.57, 154.67, 129.91, 129.75, 129.64, 122.73, 116.51, 115.07, 76.93, 36.55, 32.49, 29.67, 29.62, 29.43, 29.23, 29.18, 29.16, 29.05, 27.60, 27.08, 25.65, 22.59, 14.93 ppm; APCI-MS (m/z). For $C_{24}H_{40}NO_2^+$ 374.31 $[M+H]^+$; found 374.3.

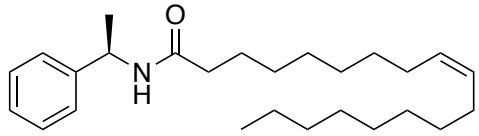


N-benzyloleamide (7). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (2H, m), 7.29 (2H, m), 7.27 (1H, m), 5.70 (1H, s), 5.35 (2H, m), 4.45 (2H, d, *J* = 5.7 Hz), 2.21 (2H, d, *J* = 8.5 Hz), 2.01 (4H, m), 1.66 (2H, p, *J* = 7.5 Hz), 1.29 (20H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.85, 138.28, 129.90, 129.64, 128.61, 127.74, 127.41, 76.91, 43.50, 36.71, 31.80, 29.66, 29.59, 29.42, 29.22, 29.18, 29.15, 29.03, 27.12, 27.07, 25.65, 22.58, 14.02 ppm; APCI-MS (m/z). For $C_{25}H_{42}NO^+$ 372.33 $[M+H]^+$; 372.4 found.

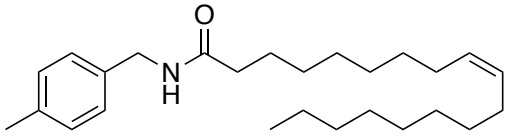


(S)-N-(1-phenylethyl)oleamide (8). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.32 (4H, m), 7.26 (1H, m), 5.82 (1H, d, *J* = 8.1 Hz), 5.35 (2H, m), 5.14 (1H, p, *J* = 7.1 Hz), 2.16 (2H, t, *J* = 7.2 Hz), 2.01

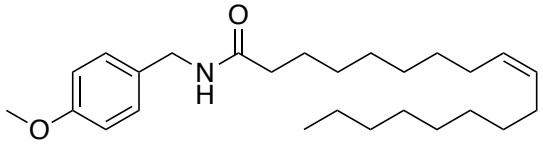
(4H, m), 1.61 (2H, p, *J* = 7.2 Hz), 1.48 (3H, d, *J* = 6.9 Hz), 1.29 (20H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.20, 143.14, 129.89, 129.65, 128.55, 127.23, 126.09, 76.95, 48.48, 36.75, 31.81, 29.67, 29.60, 29.44, 29.23, 29.15, 29.05, 27.12, 27.08, 25.67, 22.60, 21.60, 14.04 ppm; APCI-MS $C_{26}H_{44}NO^+$ 386.34 (m/z). For $[M+H]^+$; 386.4 found.



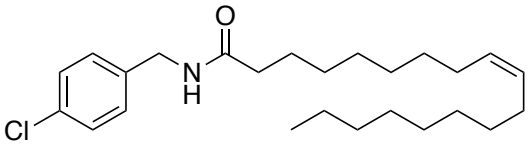
(R)-N-(1-phenylethyl)oleamide (9). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.31 (4H, m), 7.26 (1H, m), 5.85 (1H, d, *J* = 7.9 Hz), 5.35 (2H, m), 5.13 (1H, p, *J* = 7.1 Hz), 2.17 (2H, d, *J* = 8.1 Hz), 2.00 (4H, m), 1.62 (2H, p, *J* = 7.2 Hz), 1.48 (3H, d, *J* = 6.9 Hz), 1.28 (20H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.22, 143.14, 129.89, 129.65, 128.55, 127.23, 126.09, 76.96, 48.48, 36.74, 31.81, 29.67, 29.60, 29.44, 29.23, 29.15, 29.05, 27.12, 27.08, 25.67, 22.60, 21.60, 14.05 ppm; APCI-MS $C_{26}H_{44}NO^+$ 386.34 (m/z). For $[M+H]^+$; 386.4 found.



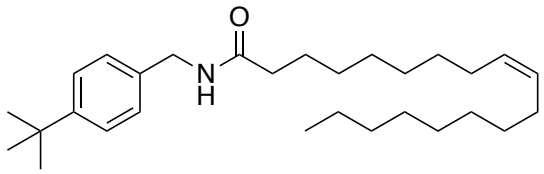
N-(4-methylbenzyl)oleamide (10). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.15 (4H, d, *J* = 6.1 Hz), 5.78 (1H, t, *J* = 5.7 Hz), 5.35 (2H, m), 4.38 (2H, d, *J* = 5.6 Hz), 2.33 (3H, s), 2.19 (2H, d, *J* = 7.8 Hz), 2.00 (4H, m), 1.64 (2H, p, *J* = 7.2 Hz), 1.28 (20H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.93, 137.11, 135.22, 129.90, 129.65, 129.27, 127.75, 76.95, 43.25, 36.71, 31.81, 29.67, 29.60, 29.43, 29.23, 29.18, 29.16, 29.05, 27.12, 27.08, 25.67, 22.60, 21.00, 14.04 ppm; APCI-MS (m/z). For $C_{26}H_{44}NO^+$ 386.34 $[M+H]^+$; 386.4 found.



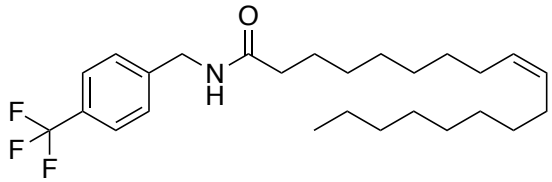
N-(4-methoxybenzyl)oleamide (11). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (2H, d, *J* = 8.2 Hz), 6.85 (2H, d, *J* = 8.5 Hz), 5.78 (1H, t, *J* = 5.8 Hz), 5.34 (2H, m), 4.35 (2H, d, *J* = 5.5 Hz), 3.78 (3H, s), 2.18 (2H, t, *J* = 7.6 Hz), 2.00 (4H, m), 1.63 (2H, p, *J* = 7.3 Hz), 1.28 (20H, m), 0.88 (3H, t, *J* = 6.7 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.86, 158.91, 130.39, 129.88, 129.63, 129.06, 113.96, 76.94, 55.17, 42.95, 36.67, 31.79, 29.65, 29.59, 29.41, 29.21, 29.17, 29.14, 29.02, 27.11, 27.06, 25.66, 22.57, 14.00 ppm; APCI-MS (m/z). For $C_{26}H_{44}NO_2^+$ 402.34 $[M+H]^+$; 402.3 found.



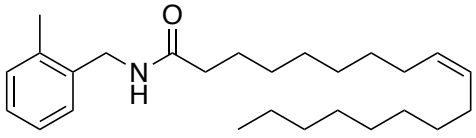
N-(4-chlorobenzyl)oleamide (12). ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.30 (2H, d, *J* = 7.9 Hz), 7.21 (2H, d, *J* = 8.7 Hz), 5.97 (1H, t, *J* = 6.2 Hz), 5.36 (2H, m), 4.40 (2H, d, *J* = 5.9 Hz), 2.22 (2H, t, *J* = 7.9 Hz), 2.02 (4H, q, *J* = 6.8 Hz), 1.65 (2H, m), 1.29 (20H, m), 0.89 (3H, t, *J* = 7.1 Hz) ppm; ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.20, 137.04, 133.25, 130.03, 129.72, 129.10, 128.79, 77.06, 60.42, 42.82, 36.71, 31.91, 29.77, 29.71, 29.53, 29.33, 29.28, 29.26, 29.15, 27.23, 27.18, 25.75, 22.69, 14.13 ppm; APCI-MS (m/z). For $C_{25}H_{41}ClNO^+$ 406.29 $[M+H]^+$; 406.2 found.



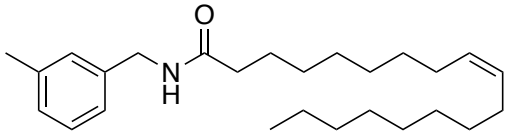
N-(4-(tert-butyl)benzyl)oleamide (13). ^{1}H NMR (800 MHz, $CDCl_3$) δ 7.38 (2H, d, *J* = 7.7 Hz), 7.23 (2H, d, *J* = 8.4 Hz), 5.80 (1H, t, *J* = 5.6 Hz), 5.37 (2H, m), 4.43 (2H, d, *J* = 5.6 Hz), 2.22 (2H, m), 2.03 (4H, m), 1.67 (2H, p, *J* = 8.8 Hz), 1.32 (29H, m), 0.90 (3H, t, *J* = 7.2 Hz) ppm; ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.06, 150.55, 135.31, 130.01, 129.76, 127.68, 125.64, 77.06, 43.32, 36.81, 34.52, 31.92, 31.34, 31.08, 29.78, 29.72, 29.54, 29.34, 29.31, 29.27, 29.16, 27.24, 27.19, 25.79, 22.70, 14.14 ppm; APCI-MS (m/z). For $C_{29}H_{50}NO^+$ 428.39 $[M+H]^+$; 428.3 found.



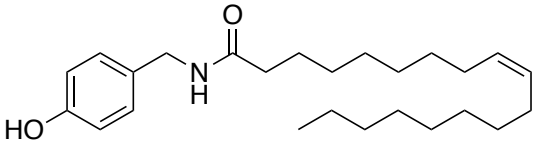
N-(4-(trifluoromethyl)benzyl)oleamide (14). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.58 (2H, d, *J* = 8.0 Hz), 7.38 (2H, d, *J* = 7.9 Hz), 5.90 (1H, t, *J* = 6.1 Hz), 5.35 (2H, m), 4.49 (2H, d, *J* = 5.9 Hz), 2.23 (2H, t, *J* = 7.6 Hz), 2.00 (4H, m), 1.65 (2H, p, *J* = 7.5 Hz), 1.28 (21H, m), 0.87 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.12, 142.46, 129.93, 129.74, 129.59, 129.48, 127.78, 125.52, 122.87, 76.92, 42.88, 36.60, 31.80, 29.66, 29.59, 29.42, 29.22, 29.17, 29.14, 29.02, 27.11, 27.05, 25.61, 22.58, 14.02; APCI-MS (m/z). For $C_{26}H_{41}F_3NO^+$ 440.31 $[M+H]^+$; 440.4 found.



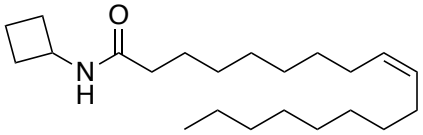
N-(2-methylbenzyl)oleamide (15). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.19 (4H, m), 5.71 (1H, t, *J* = 5.4 Hz), 5.34 (2H, m), 4.42 (2H, d, *J* = 5.3 Hz), 2.31 (3H, s), 2.18 (2H, t, *J* = 7.5 Hz), 2.01 (4H, m), 1.64 (2H, p, *J* = 7.3 Hz), 1.28 (19H, m), 0.88 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.82, 136.36, 135.82, 130.42, 129.88, 129.62, 128.48, 127.65, 126.08, 76.95, 60.28, 41.64, 36.59, 31.80, 29.66, 29.59, 29.41, 29.21, 29.14, 29.03, 27.11, 27.06, 25.70, 22.57, 18.86, 14.00 ppm; For $C_{26}H_{44}NO^+$ 386.34 $[M+H]^+$; 386.4 found.



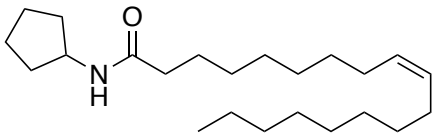
N-(3-methylbenzyl)oleamide (16). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.21 (1H, t, *J* = 7.8 Hz), 7.08 (2H, t, *J* = 4.8 Hz), 5.82 (1H, s), 5.34 (2H, m), 4.39 (2H, d, *J* = 5.6 Hz), 2.33 (3H, s), 2.20 (2H, m), 2.00 (3H, m), 1.64 (2H, p, *J* = 7.4 Hz), 1.27 (22H, m), 0.88 (3H, t, *J* = 6.9 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.94, 138.30, 138.18, 129.89, 129.64, 128.50, 128.13, 124.75, 76.95, 60.32, 43.46, 36.69, 31.81, 29.67, 29.60, 29.43, 29.23, 29.20, 29.18, 29.06, 27.12, 27.07, 25.68, 22.59, 21.26, 14.04 ppm; For $C_{26}H_{44}NO^+$ 386.34 $[M+H]^+$; 386.3 found.



N-(4-hydroxybenzyl)oleamide (17). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.07 (2H, d, *J* = 8.2 Hz), 6.79 (2H, d, *J* = 8.3 Hz), 5.99 (1H, t, *J* = 4.9 Hz), 5.33 (2H, m), 4.32 (2H, d, *J* = 5.5 Hz), 2.20 (2H, t, *J* = 7.4 Hz), 2.00 (4H, m), 1.63 (2H, m), 1.27 (28H, m), 0.87 (4H, t, *J* = 6.7 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.71, 156.01, 129.91, 129.64, 129.08, 115.63, 76.95, 43.23, 36.70, 31.81, 29.67, 29.61, 29.43, 29.23, 29.15, 29.12, 29.04, 27.12, 27.07, 25.69, 22.59, 14.04 ppm; APCI-MS (m/z). For $C_{25}H_{42}NO_2^+$ 388.32 $[M+H]^+$; 388.3 found.

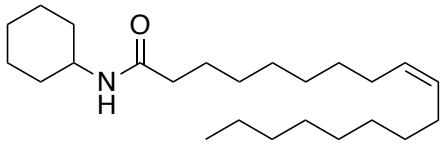


N-cyclobutyloleamide (18). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.72 (1H, s), 5.32 (2H, m), 4.38 (1H, h, *J* = 8.2 Hz), 2.33 (2H, m), 2.11 (2H, t, *J* = 7.4 Hz), 1.99 (4H, m), 1.82 (2H, m), 1.69 (2H, m), 1.61 (2H, p, *J* = 6.8 Hz), 1.26 (22H, m), 0.87 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.19, 171.05, 129.86, 129.62, 76.92, 60.27, 44.49, 36.62, 31.78, 31.19, 29.64, 29.58, 29.40, 29.20, 29.15, 29.01, 27.09, 27.05, 25.62, 22.56, 20.91, 14.92, 14.06, 13.98, -0.14 ppm; APCI-MS (m/z). For $C_{22}H_{42}NO^+$ 336.33 $[M+H]^+$; 336.5 found.

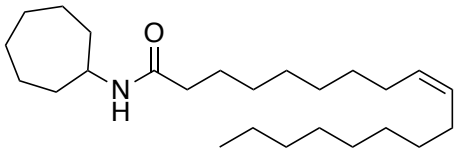


N-cyclopentyloleamide (19). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.49 (1H, s), 5.34 (2H, m), 4.20 (1H, h, *J* = 7.0 Hz), 2.13 (2H, t, *J* = 7.5 Hz), 1.99 (4H, m), 1.96 (2H, m), 1.66 (2H, m), 1.60 (4H, m), 1.28 (24H, m), 0.87 (3H, t, *J* = 6.7 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.73, 129.87,

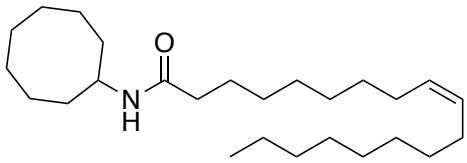
129.63, 76.91, 60.28, 50.99, 36.80, 33.04, 31.78, 29.65, 29.59, 29.40, 29.20, 29.14, 29.02, 27.10, 27.05, 25.74, 23.59, 22.56, 20.92, 14.07, 13.99 ppm; APCI-MS (m/z). For $C_{23}H_{44}NO^+$ 350.34 $[M+H]^+$; 350.5 found.



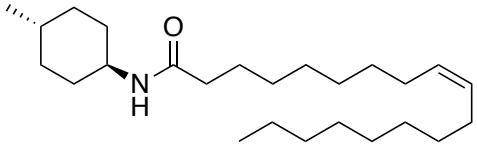
N-cyclohexyloleamide (20). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.34 (2H, m), 5.28 (1H, d, *J* = 7.8 Hz), 3.77 (1H, m), 2.12 (2H, t, *J* = 7.4 Hz), 2.00 (4H, m), 1.91 (2H, m), 1.69 (2H, m), 1.61 (2H, m), 1.29 (21H, m), 1.11 (4H, m), 0.88 (3H, m) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.06, 129.88, 129.65, 76.91, 47.89, 37.01, 33.18, 31.80, 29.66, 29.60, 29.42, 29.22, 29.16, 29.13, 29.04, 27.11, 27.06, 25.78, 25.44, 24.77, 22.58, 14.01 ppm; APCI-MS (m/z). For $C_{24}H_{46}NO^+$ 364.36 $[M+H]^+$; 364.4 found.



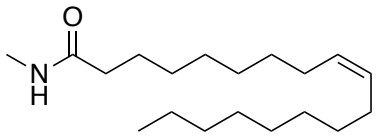
N-cycloheptyloleamide (21). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.58 (1H, d, *J* = 8.2 Hz), 5.33 (2H, m), 3.92 (1H, m), 2.12 (2H, t, *J* = 7.6 Hz), 1.99 (4H, m), 1.89 (2H, m), 1.59 (6H, m), 1.49 (4H, m), 1.39 (2H, m), 1.27 (20H, m), 0.86 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.95, 129.86, 129.63, 76.95, 50.22, 36.88, 35.06, 31.80, 29.66, 29.60, 29.42, 29.22, 29.17, 29.14, 29.04, 27.91, 27.10, 27.06, 25.81, 23.96, 22.58, 14.02 ppm; APCI-MS (m/z). For $C_{25}H_{48}NO^+$ 378.37 $[M+H]^+$; 378.3 found.



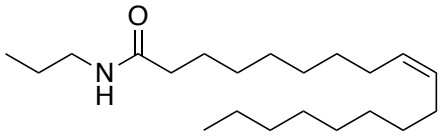
N-cyclooctyloleamide (22). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.47 (1H, d, *J* = 8.2 Hz), 5.33 (2H, m), 3.98 (1H, m), 2.12 (2H, t, *J* = 7.6 Hz), 2.00 (4H, m), 1.80 (2H, m), 1.58 (14H, m), 1.28 (20H, m), 0.87 (4H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.85, 129.87, 129.65, 76.94, 49.11, 36.94, 32.15, 31.80, 29.66, 29.61, 29.42, 29.22, 29.18, 29.14, 29.05, 27.11, 27.08, 25.79, 25.27, 23.53, 22.59, 14.03 ppm; APCI-MS (m/z). For $C_{26}H_{50}NO^+$ 392.39 $[M+H]^+$; 392.3 found.



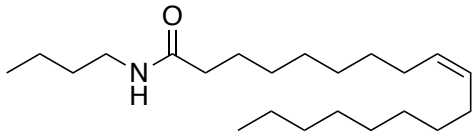
N-((1r,4r)-4-methylcyclohexyl)oleamide (23). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.36 (1H, s), 5.32 (2H, m), 3.68 (1H, m), 2.11 (2H, t, *J* = 7.5 Hz), 1.99 (4H, m), 1.92 (2H, m), 1.68 (2H, m), 1.59 (2H, t, *J* = 7.4 Hz), 1.27 (21H, m), 1.06 (4H, m), 0.86 (6H, t, *J* = 6.5 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.31, 129.87, 129.64, 76.94, 48.18, 36.97, 33.70, 33.13, 31.86, 31.80, 29.66, 29.59, 29.42, 29.21, 29.16, 29.13, 29.04, 27.10, 27.05, 25.78, 22.58, 22.06, 14.02 ppm; APCI-MS (m/z). For $C_{25}H_{48}NO^+$ 378.37 $[M+H]^+$; 378.4 found.



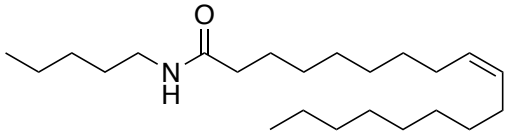
N-methyloleamide (24). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.50 (1H, s), 5.33 (2H, m), 2.80 (3H, d, *J* = 4.8 Hz), 2.16 (2H, t, *J* = 7.6 Hz), 2.00 (4H, m), 1.62 (2H, p, *J* = 7.4 Hz), 1.27 (20H, m), 0.87 (3H, t, *J* = 6.9 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 129.90, 129.65, 76.92, 36.62, 31.81, 29.66, 29.60, 29.42, 29.22, 29.03, 27.11, 26.21, 25.69, 22.59, 14.03 ppm; APCI-MS (m/z). For $C_{19}H_{38}NO^+$ 296.29 $[M+H]^+$; 296.3 found.



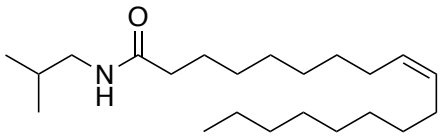
N-propyloleamide (25). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.59 (1H, s), 5.33 (2H, m), 3.19 (2H, q, *J* = 6.8 Hz), 2.15 (2H, t, *J* = 7.5 Hz), 1.99 (4H, m), 1.61 (2H, p, *J* = 7.4 Hz), 1.50 (2H, h, *J* = 7.3 Hz), 1.27 (20H, m), 0.91 (3H, t, *J* = 7.4 Hz), 0.87 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.14, 129.86, 129.62, 76.92, 41.07, 36.76, 31.78, 29.64, 29.58, 29.40, 29.19, 29.15, 29.02, 27.09, 27.05, 25.73, 22.77, 22.55, 13.98, 11.22 ppm; APCI-MS (m/z). For $C_{21}H_{42}NO^+$ 324.33 $[M+H]^+$; 324.4 found.



N-butyloleamide (26). ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.47 (1H, s), 5.34 (2H, m), 3.24 (2H, q, *J* = 6.8 Hz), 2.15 (2H, t, *J* = 7.5 Hz), 2.00 (4H, m), 1.63 (2H, m), 1.47 (2H, p, *J* = 7.5 Hz), 1.30 (23H, m), 0.91 (3H, t, *J* = 7.3 Hz), 0.86 (3H, t, *J* = 6.8 Hz) ppm; ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.19, 129.89, 129.65, 76.92, 39.12, 36.80, 31.80, 31.62, 29.66, 29.60, 29.43, 29.22, 29.17, 29.04, 27.11, 27.06, 25.74, 22.59, 19.96, 14.03, 13.66 ppm; APCI-MS (m/z). For $C_{22}H_{44}NO^+$ 338.34 $[M+H]^+$; 338.4 found.



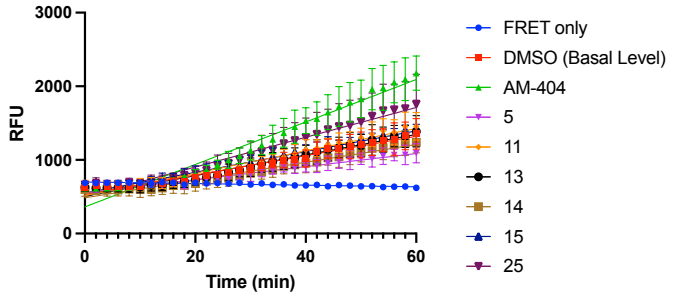
N-pentyloleamide (27). ^{1}H NMR (800 MHz, $CDCl_3$) δ 5.59 (1H, s), 5.35 (2H, m), 3.25 (2H, q, *J* = 7.1 Hz), 2.17 (2H, t, *J* = 7.7 Hz), 2.01 (4H, m), 1.63 (2H, p, *J* = 7.5 Hz), 1.50 (2H, p, *J* = 7.3 Hz), 1.31 (24H, m), 0.91 (3H, t, *J* = 6.2 Hz), 0.89 (4H, t, *J* = 7.0 Hz) ppm; ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.22, 129.99, 129.74, 77.04, 39.51, 36.88, 31.91, 29.77, 29.71, 29.53, 29.35, 29.32, 29.28, 29.15, 29.07, 27.22, 27.18, 25.85, 22.69, 22.36, 14.11, 13.98 ppm; APCI-MS (m/z). For $C_{23}H_{46}NO^+$ 352.36 $[M+H]^+$; 352.4 found.



N-isobutyloleamide (28). ^{1}H NMR (800 MHz, $CDCl_3$) δ 5.62 (1H, s), 5.35 (2H, t, *J* = 5.3 Hz), 3.09 (2H, t, *J* = 6.4 Hz), 2.19 (2H, t, *J* = 7.6 Hz), 2.02 (4H, m), 1.64 (2H, p, *J* = 7.4 Hz), 1.31 (26H, m), 0.92 (7H, d, *J* = 6.8 Hz), 0.89 (4H, t, *J* = 7.1 Hz) ppm; ^{13}C NMR (201 MHz, $CDCl_3$) δ 173.30, 129.99, 129.74, 77.04, 46.83, 36.93, 31.91, 29.77, 29.71, 29.53, 29.32, 29.30, 29.27, 29.15, 28.50, 27.22, 27.17, 25.91, 22.68, 20.09, 14.11 ppm; APCI-MS (m/z). For $C_{22}H_{44}NO^+$ 338.34 $[M+H]^+$; 338.4 found.

FRET Assay Protocol

Each compound's stimulation of the 20S CP was tested at 25 μM using the FRET assay. For each instance, the following controls were performed in triplicate: FRET Only, Basal Level, and 25 μM AM-404 (positive control). Each well contained 24.5 μL 20 μM FRET reporter in Tris-HCl (50 mM, pH 7.63). Every well except for the Fret Only control contained 5 nM 20S CP in addition to 20 μM FRET reporter in Tris-HCl. For each well of the FRET Only and Basal Level controls, 0.5 μL DMSO was added to obtain a final DMSO concentration of 2% in a total volume of 25 μL. For each well of the 25 μM AM-404 and test compounds, 0.5 μL of a 1250 μM stock solution in DMSO was added to obtain a final DMSO concentration of 2% in a total volume of 25 μL. Each compound was tested in triplicate. The plate was placed in the plate reader heated to 37 °C. The excitation and emission wavelengths were set to 335 nm and 493 nm, respectively. The fluorescence was recorded every 2 min over a 60 min period, and the resulting data was plotted against time. The slope of the linear portion of the curve was determined to be the rate of hydrolysis of the FRET reporter by the 20S CP.



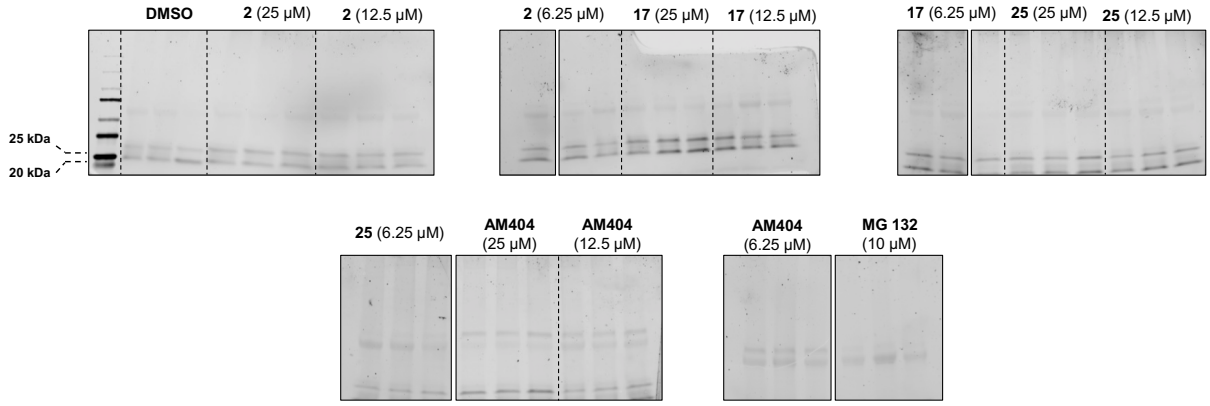
	Slope	Error in Slope		% Stimulation
FRET only	-1.1	0.1		0
DMSO (Basal)	13.2	0.6		100.0
AM-404	28.8	1.0		219.1
5	8.9	0.4		67.6
11	15.2	0.6		115.8
13	14.0	0.6		106.5
14	12.1	0.6		91.7
15	14.1	0.5		106.8
25	20.2	1.1		153.6

Supporting Information Figure S2. Example of raw data obtained for determining the ability of molecules to stimulated the cleavage of our FRET peptide probe to monitor proteasome activity. All molecules were run in triplicate and AM-404 was included in all run as a positive control.

In cell activity assay with Me4BodipyFL-Ahx3Leu3VS proteasome probe

HEK-293T cells were plated in a 24-well plate at a density of 200.000 cells/well (500 μL total volume). The plate was placed in the cell culture incubator overnight to allow full attachment to the wells. Once cells reached >95% confluency the media was vacuum aspirated and subsequently dosed with the corresponding molecule dissolved in fresh warm media (500 μL total volume) and returned to the incubator for 2 hour. DMSO was used a control (final concentration, 0.5%). After the 2 hour incubation period, cells were dosed with 1 μM Me4BodipyFL-Ahx3Leu3VS by adding 1 μL 500x solution in DMSO, and the plate was returned to the incubator for 1 hour. After incubation cells were physically detached, and the resulting suspension was collected. Samples were subsequently pelleted (5 min at 1000xg) followed by replacement of PBS supernatant with M-PER lysis buffer + 100x HALT protease inhibitor cocktail. Cells were subsequently sonicated in an ice bath for 10 min, and pelleted at 14,000xg, 4°C for 15 min. The supernatant was transferred to new tubes and the total protein

concentration was measured on a NanoDrop One instrument. Concentrations were normalized for SDS-PAGE analysis (50 µg total protein). Samples were mixed with 4x loading buffer (9:1 Laemmli sample buffer:βME) and run in 4–15% Mini-PROTEAN® TGX™ Precast Protein Gels (Bio-Rad) for 50 min at 160 V. Gels were subsequently scanned for fluorescence in a Sapphire™ RGBNIR Biomolecular Imager at 488 nm.



Supporting Information Figure S3. SDS PAGE gels of the *in cell* proteasome activity with the Me4BodipyFL-Ahx3Leu3VS proteasome probe

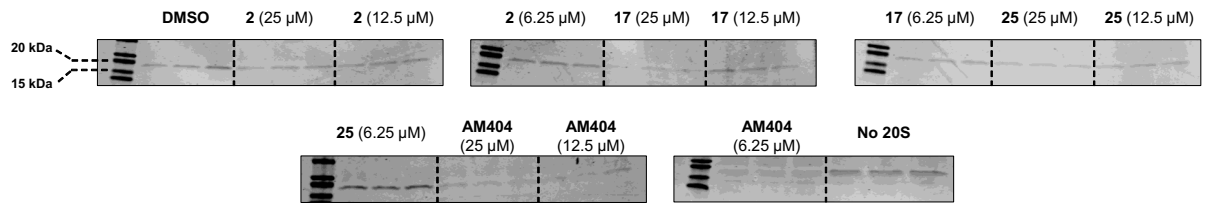
	RFU		RFU
DMSO	165000	D3 (25 µM)	294000
	160000		243000
	160000		244000
A4 (25 µM)	219000	D3 (12.5 µM)	142000
	203000		176000
	245000		260000
A4 (12.5 µM)	228000	D3 (6.25 µM)	176000
	220000		158000
	203000		145000
A4 (6.25 µM)	186000	AM404 (25 µM)	288000
	190000		277000
	137000		351000
B12 (25 µM)	253000	AM404 (12.5 µM)	204000
	311000		211000
	339000		253000
B12 (12.5 µM)	285000	AM404 (6.25 µM)	179000
	236000		205000
	258000		182000
B12 (6.25 µM)	262000	MG132 (10 µM)	21100
	262000		40600
	205000		27400

Table S1. Raw fluorescent values from the gel band density analysis to determine the % increase in proteasome activity in cells.

Degradation of purified alpha-synuclein with sCP and stimulators

Each of the samples contained a total volume of 18 µL, a final DMSO concentration of 2%, final 20S CP concentration of 5 nM, and 400 ng of α-Syn. The 20S CP was omitted for the positive control. Alpha-synuclein (α-Syn) monomer was diluted in Tris-HCl (50 mM, pH 7.6, henceforth called reaction buffer) to a final concentration of 66.66 ng/µL. The small molecule 20S CP stimulators were dissolved in DMSO, and a 3X stock in reaction buffer, containing 6% DMSO was prepared. A solution of 15 nM 20S CP was made by diluting the 3.7 µM purchased stock solution of human 20S CP (South Bay Bio, Cat. # SBB-PP0005) in Tris-HCl.
For the assay, 6 µL of 15 nM 20S CP was added to 6 µL of stimulator solution in a 600 µL microcentrifuge tube kept on ice. Subsequently, 6 µL of the 66.66 ng/µL a-Syn was added to the reaction vial and pipetted up and down thrice to mix the components thoroughly. Samples were prepared for each compound in triplicate.

Following preparation, the samples were incubated for 2 hr at 37°C. After this period, 10 µL of 4x SDS gel loading buffer was added to each sample, which were then heated for 5 min at 95°C. The samples were then loaded onto a 50 µL 10-well 4–15% Mini-PROTEAN® TGX™ Precast Protein Gels (Bio-Rad) and ran for 30 min at 160 V. The gels were stained with Coomassie, imaged with a LICOR Odyssey, and quantitated using ImageJ. For each protein, the calculated band intensities were normalized to the total α-Syn loaded (no 20S CP).

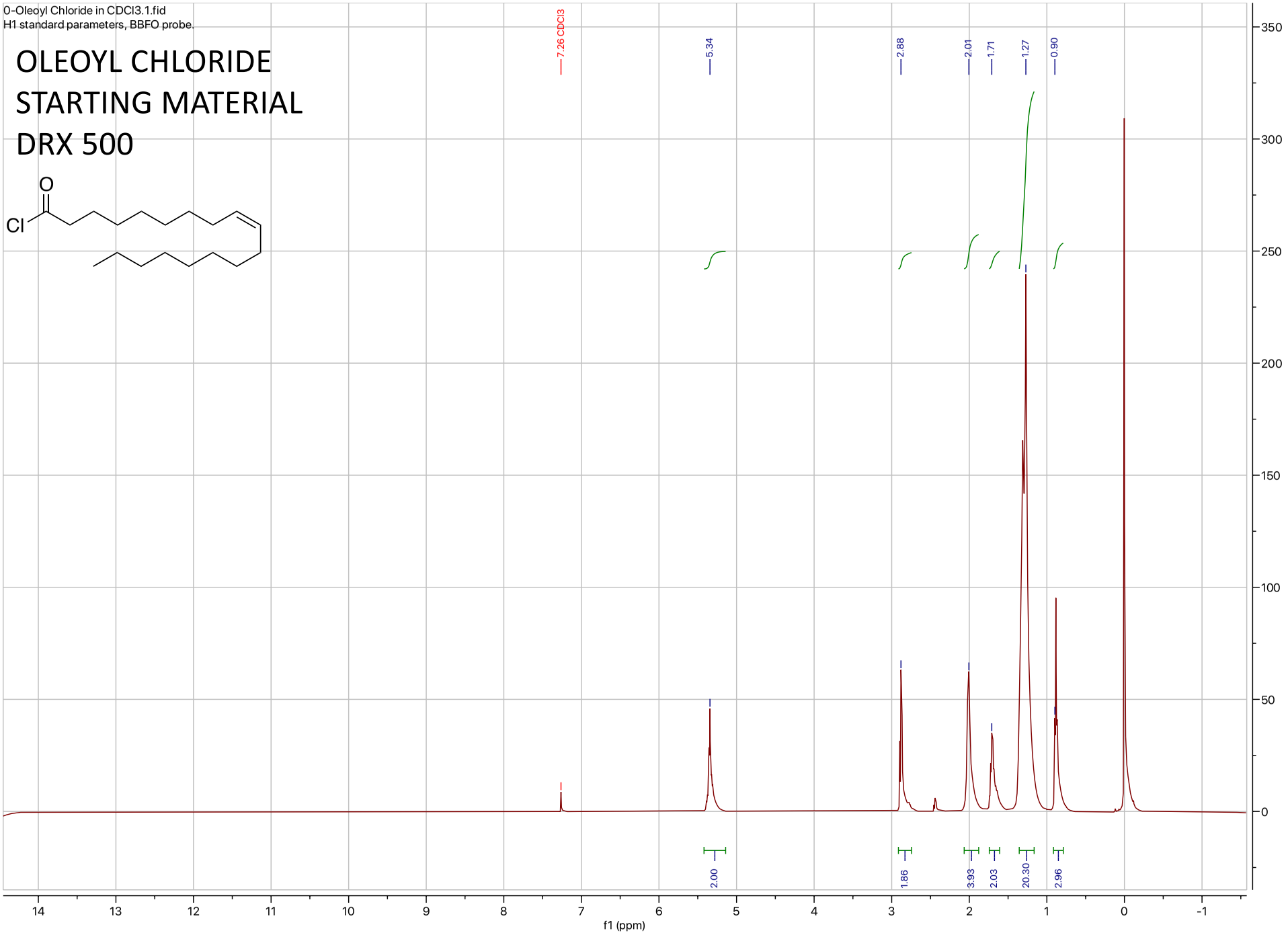


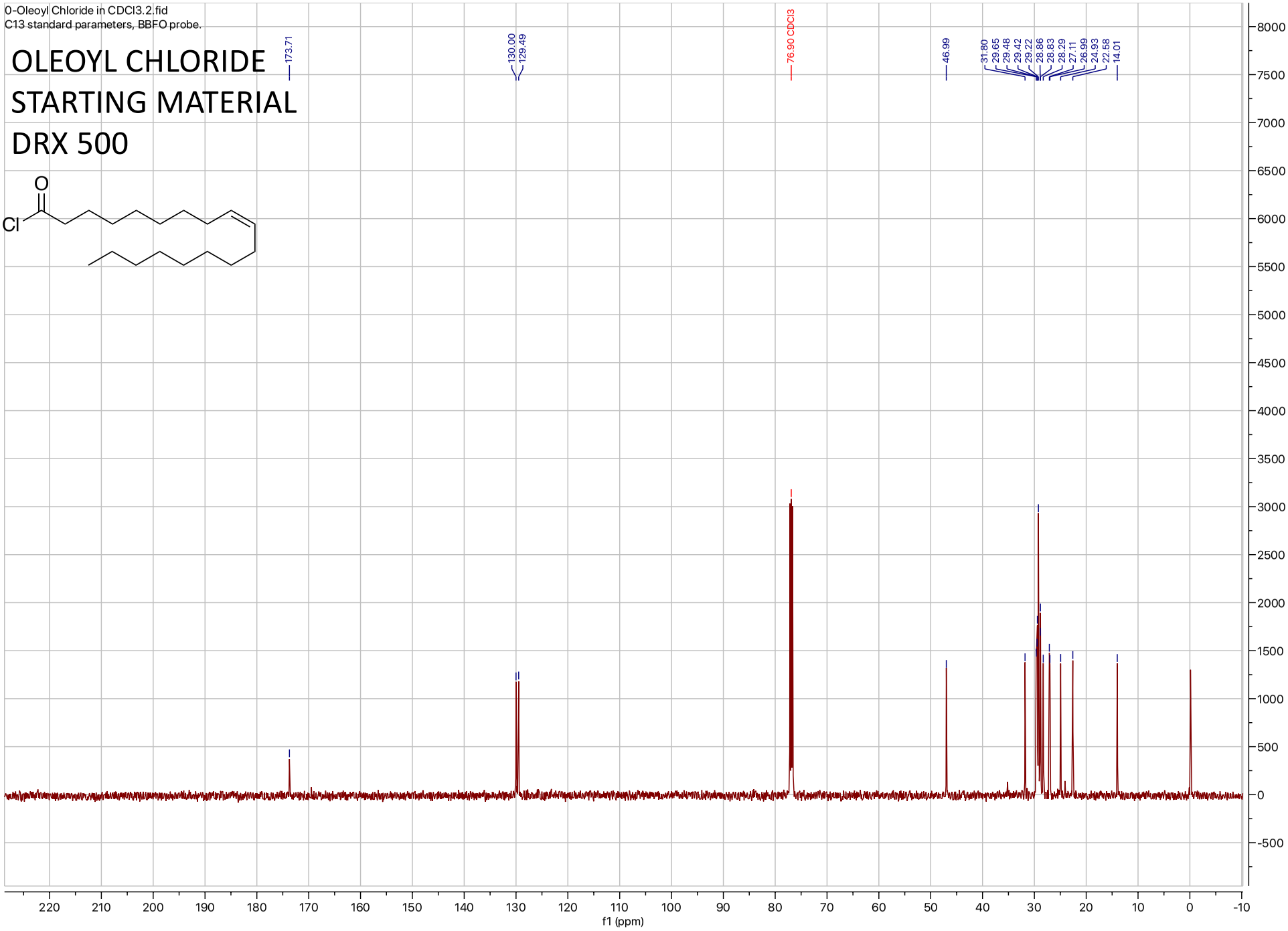
Supporting Information Figure S4. SDS-PAGE gel images showing the amount of alpha synuclein remaining after incubating with purified 20S CP and a stimulator.

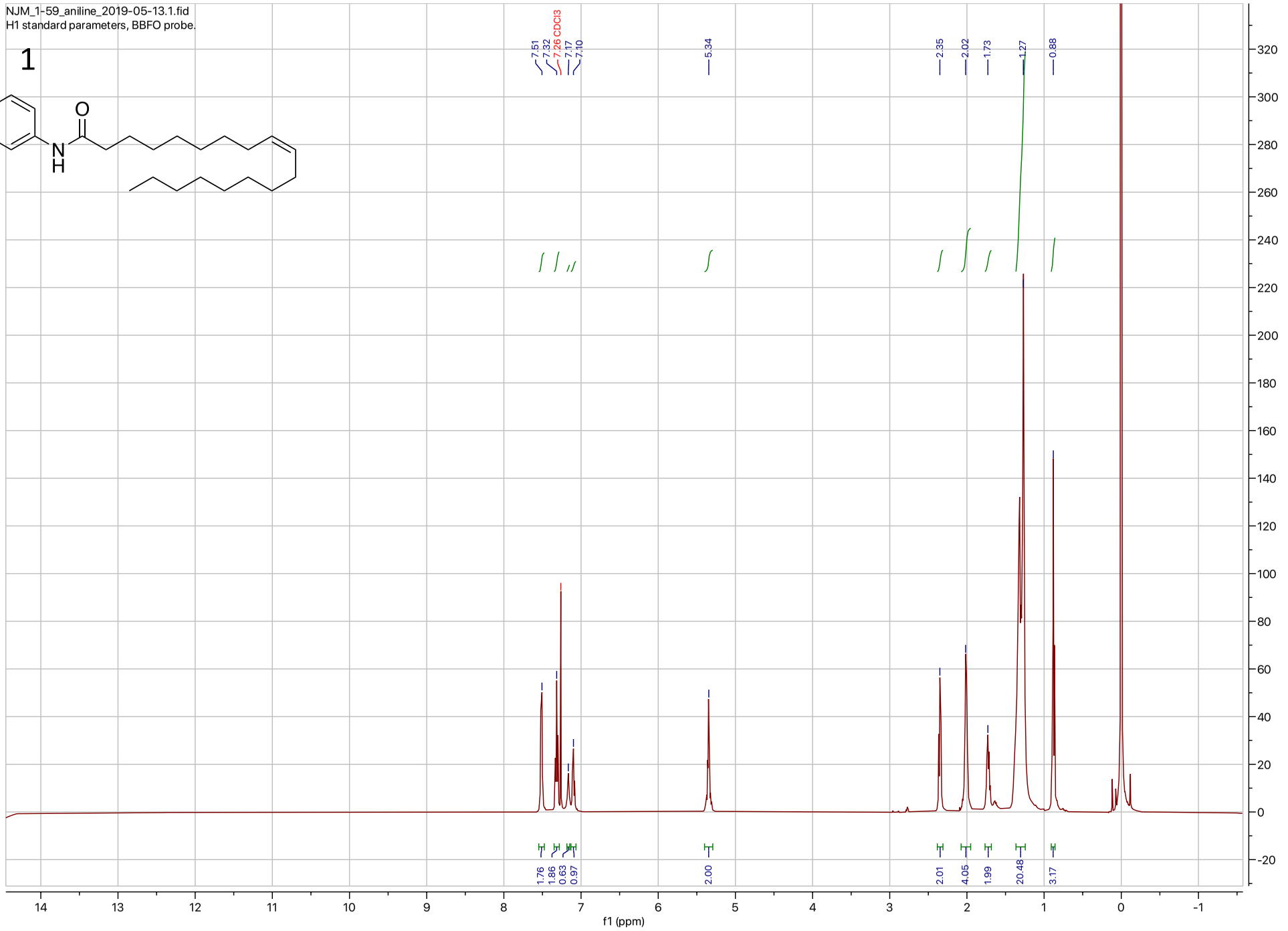
Luminescent cell viability assay

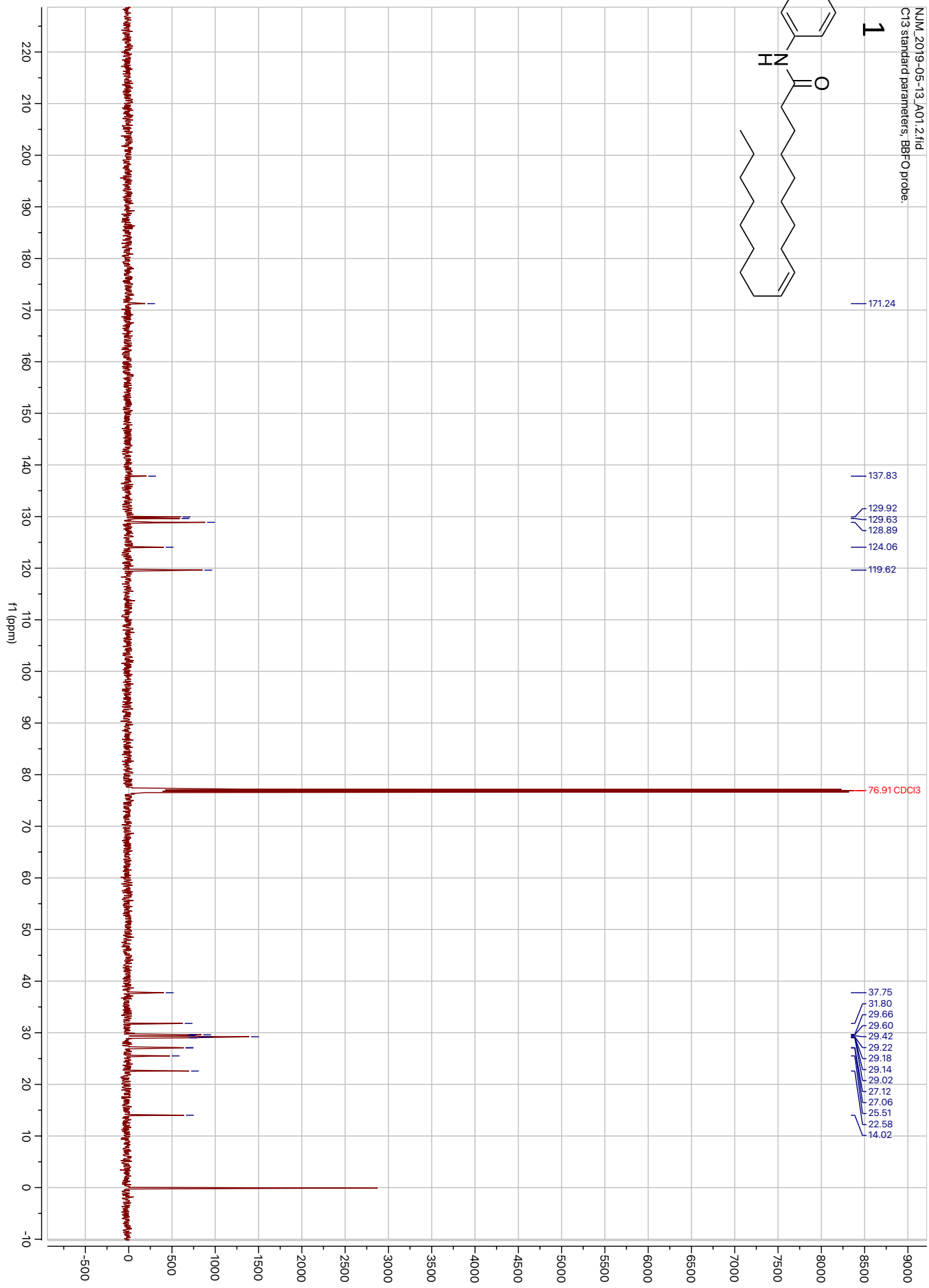
The CellTiter Glo® viability assay was performed by plating HEK-293T cells at a density of 5000 cells/well in a white 96-well plate (100 µL total volume). The plate was placed in the cell culture incubator overnight to allow full attachment to the wells. The next day media from all wells was vacuum aspirated and 50 µL of fresh warm media was added. Stock solutions of 50 µL of either (1) or (2) in DMSO were prepared and subsequently added in triplicate to the wells. (Final concentration of DMSO of 1%). After returning the plate to the incubator for 24 hours, the plate was taken out and allowed to reach room temperature for 30 min. The CellTiter-Glo® Reagent (prepared per manufacturer's protocol) was thawed and equilibrated to room temperature and subsequently added (50 µL) to each well. The plate was covered with aluminum foil and orbital shaken gently for 10 min. The plate was subsequently removed from orbital shaker and allowed to stabilize luminescent signal for 10 min. at room temperature. Luminescence was recorded

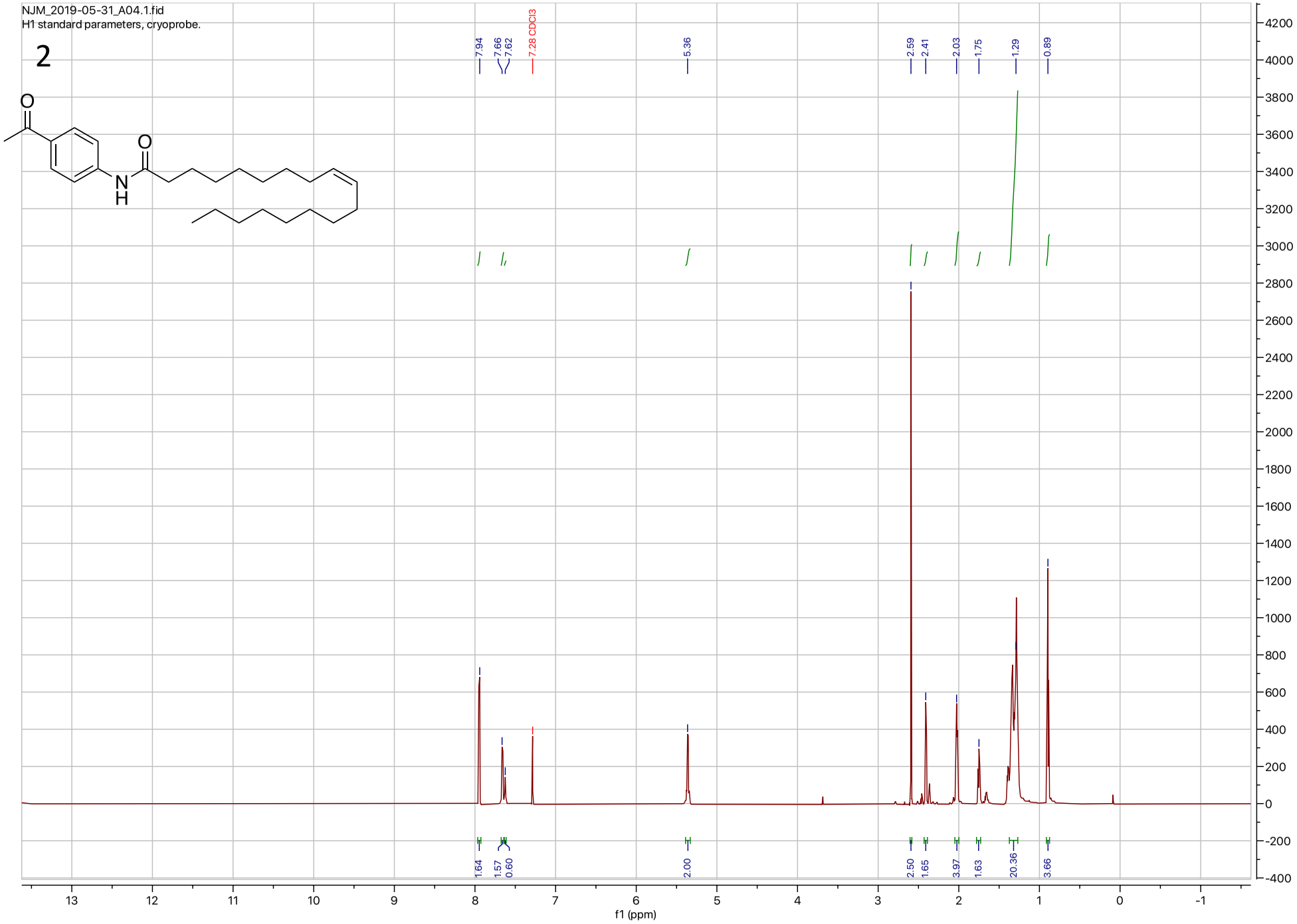
using a BioTek Synergy™ Neo2 Multimode Microplate Reader. The gain was adjusted to 120. Data was plotted as seen in Figure 3 in the article.

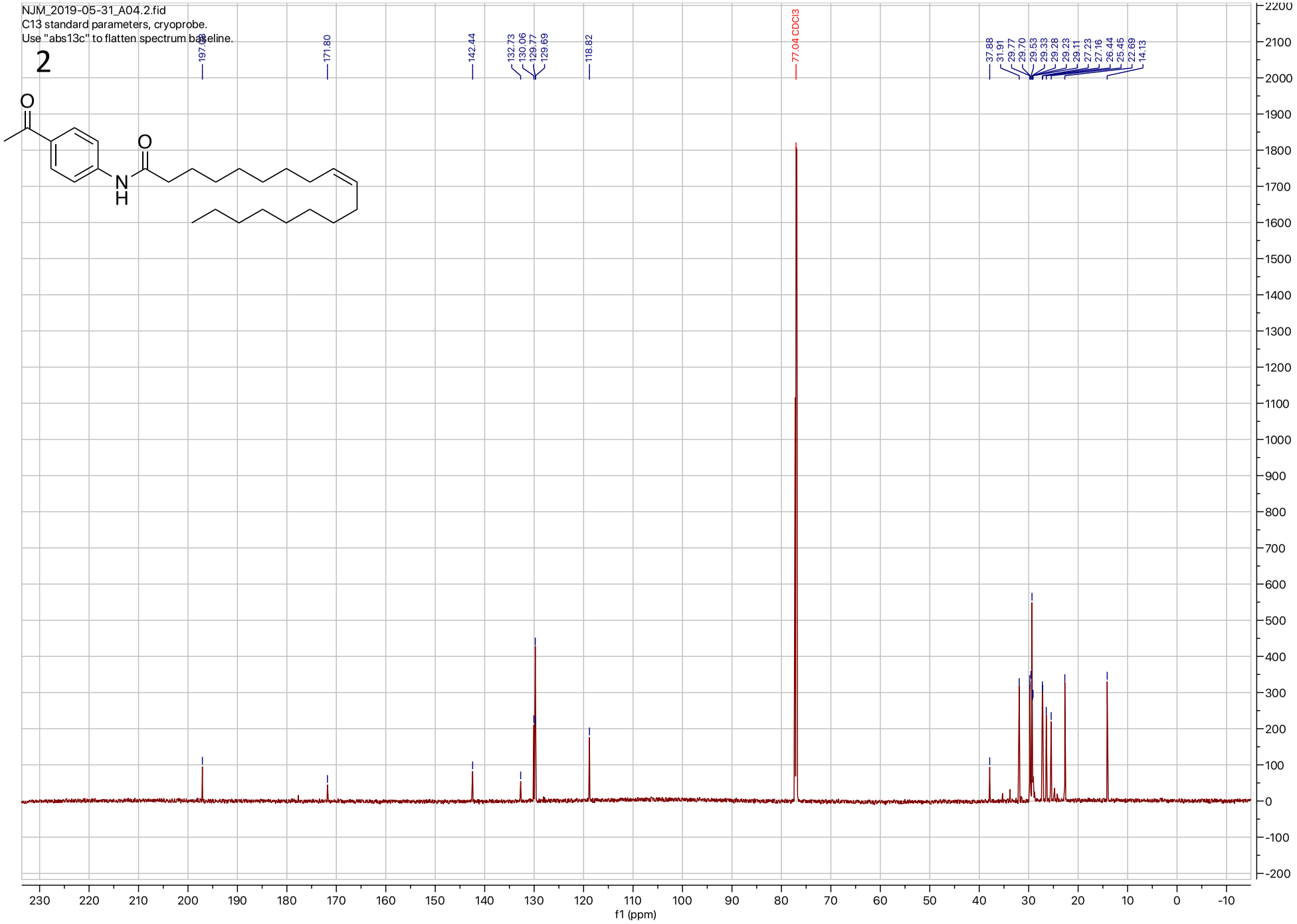

0-Oleoyl Chloride in CDCl3.1.fid
H1 standard parameters, BBFO probe.
OLEOYL CHLORIDE
STARTING MATERIAL
DRX 500
O
Cl
7.26 CDCl3
5.34
2.88
2.01
1.71
1.27
0.90
2.00
1.86
3.93
2.03
20.30
2.96
f1 (ppm)

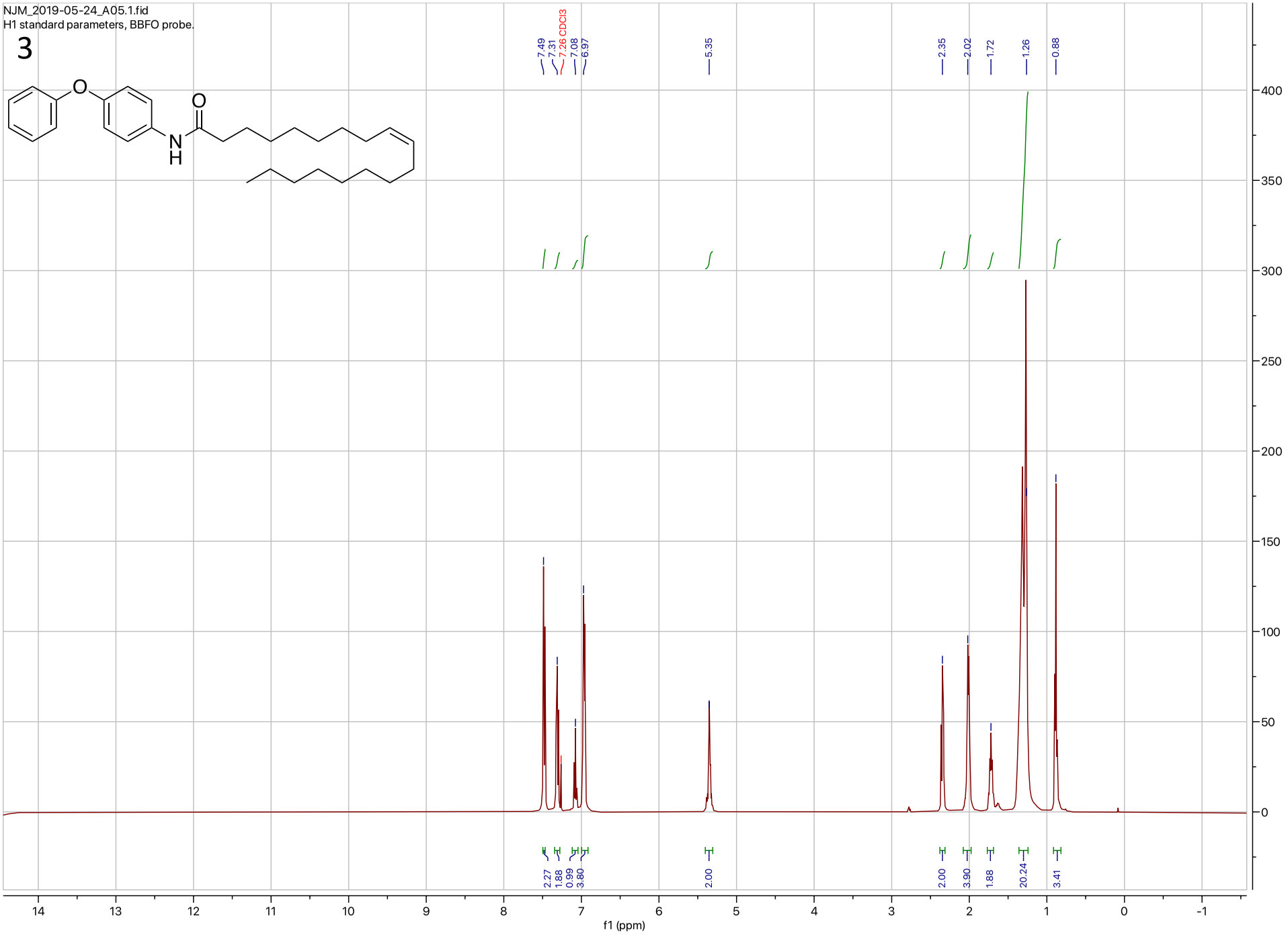

0-Oleoyl Chloride in CDCl3.2.fid
C13 standard parameters, BBFO probe.
OLEOYL CHLORIDE
STARTING MATERIAL
DRX 500
O
Cl
173.71
130.00
129.49
76.90 CDCl3
46.99
31.80
29.65
29.48
29.42
29.22
28.86
28.83
28.29
27.11
26.99
24.93
22.58
14.01
f1 (ppm)

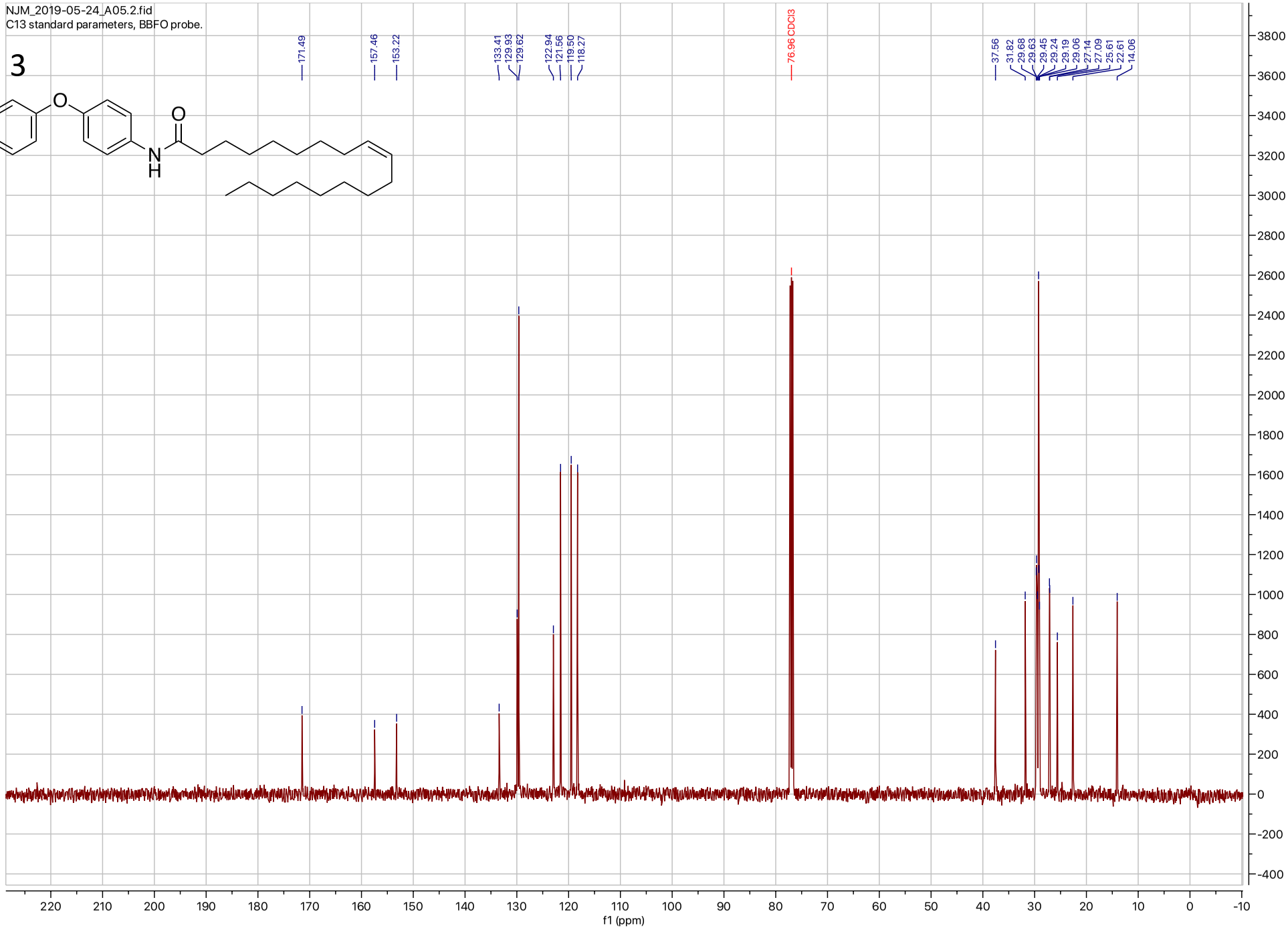

NJM_1-59_aniline_2019-05-13.1.fid
H1 standard parameters, BBFO probe.
1
O
N
H
7.51
7.32
7.26 CDCl3
7.17
7.10
5.34
2.35
2.02
1.73
1.27
0.88
1.76
1.86
0.63
0.97
2.00
2.01
4.05
1.99
20.48
3.17
f1 (ppm)

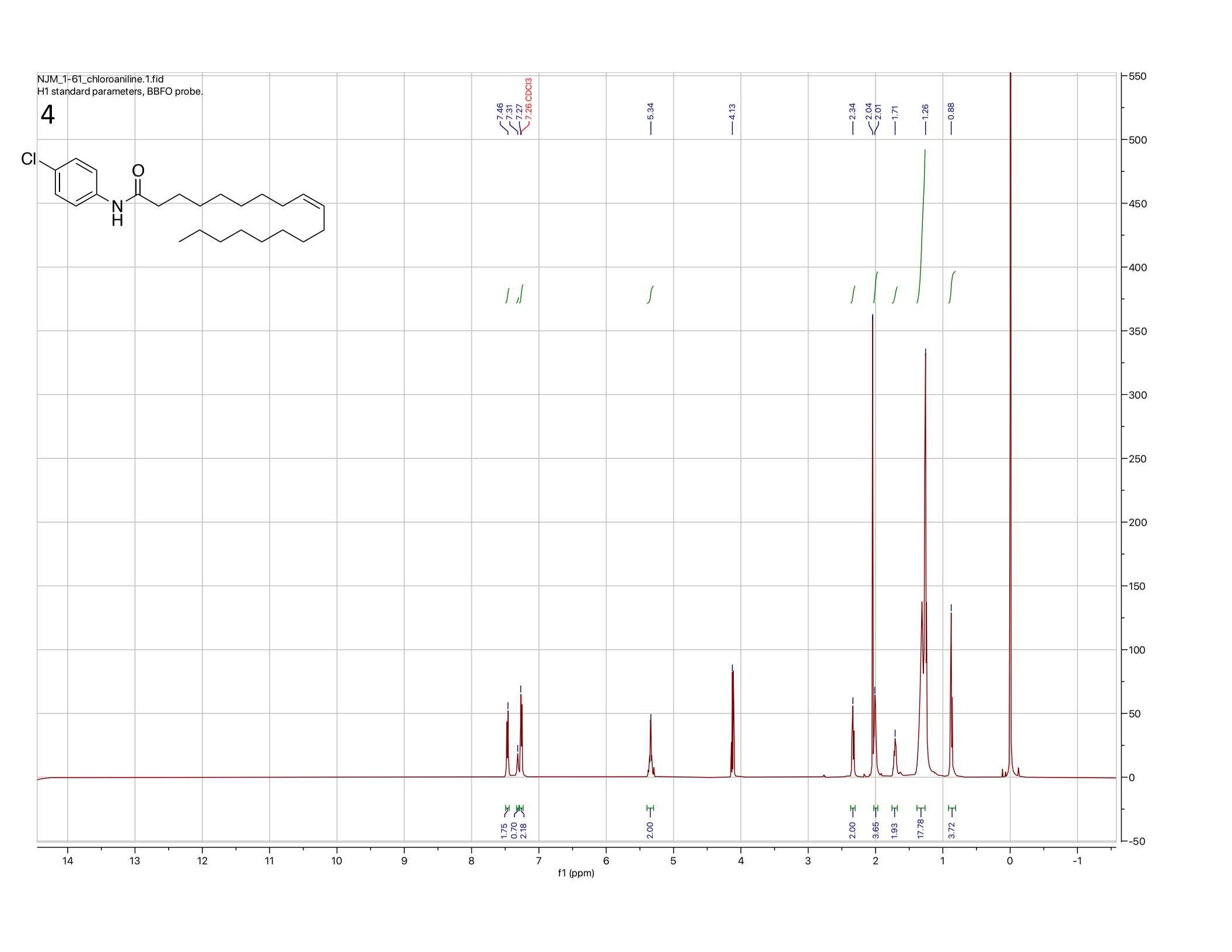

NJM_2019-05-13_A01.2.fid
C13 standard parameters, BBFO probe.
1
171.24
137.83
129.92
129.63
128.89
124.06
119.62
76.91 CDCl3
37.75
31.80
29.66
29.60
29.42
29.22
29.18
29.14
29.02
27.12
27.06
25.51
22.58
14.02
f1 (ppm)

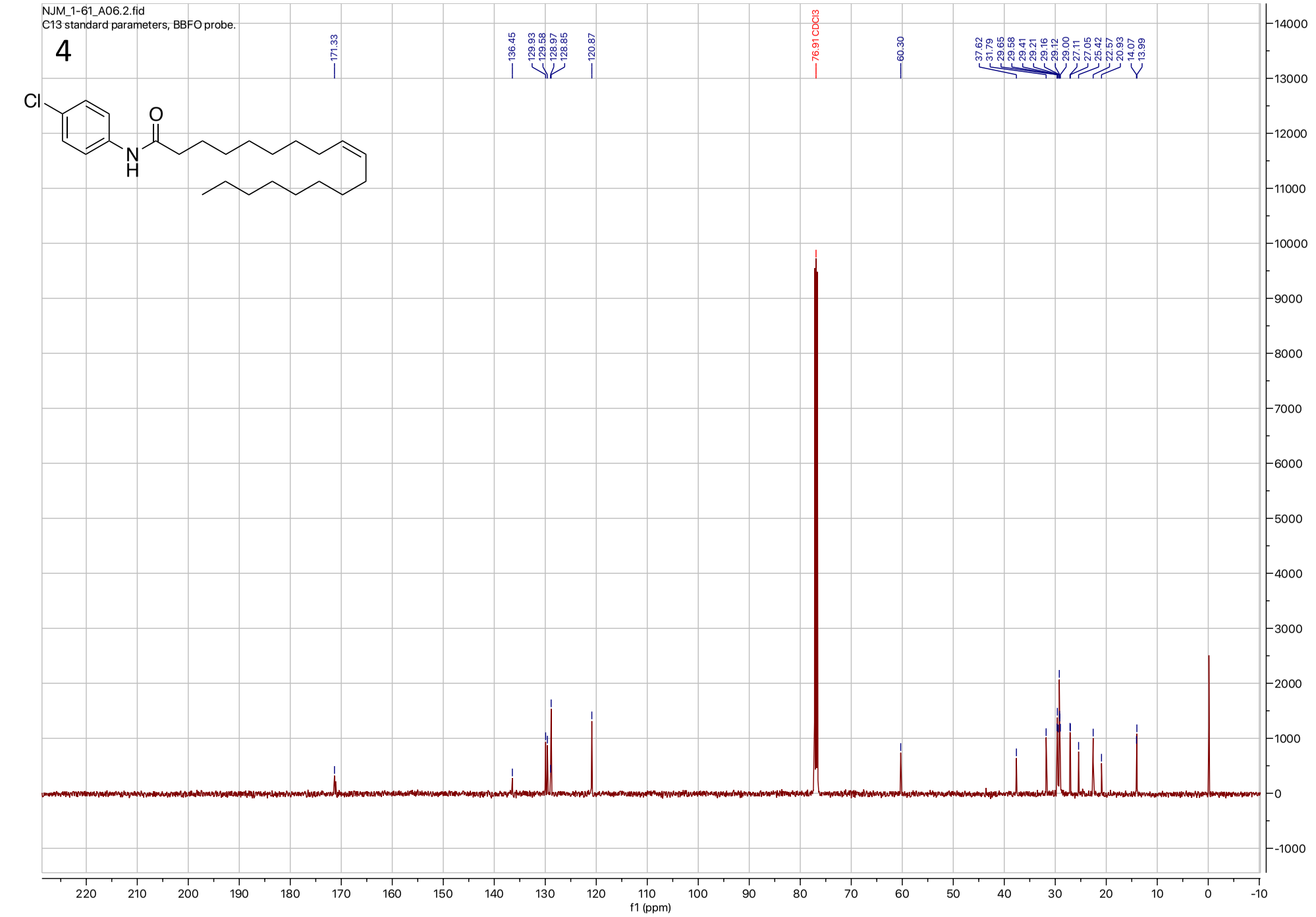

NJM_2019-05-31_A04.1.fid
H1 standard parameters, cryoprobe.
2
O
O
N
H
7.94
7.66
7.62
7.28 CDCl3
5.36
2.59
2.41
2.03
1.75
1.29
0.89
1.64
1.57
0.60
2.00
2.50
1.65
3.97
1.63
20.36
3.66
f1 (ppm)

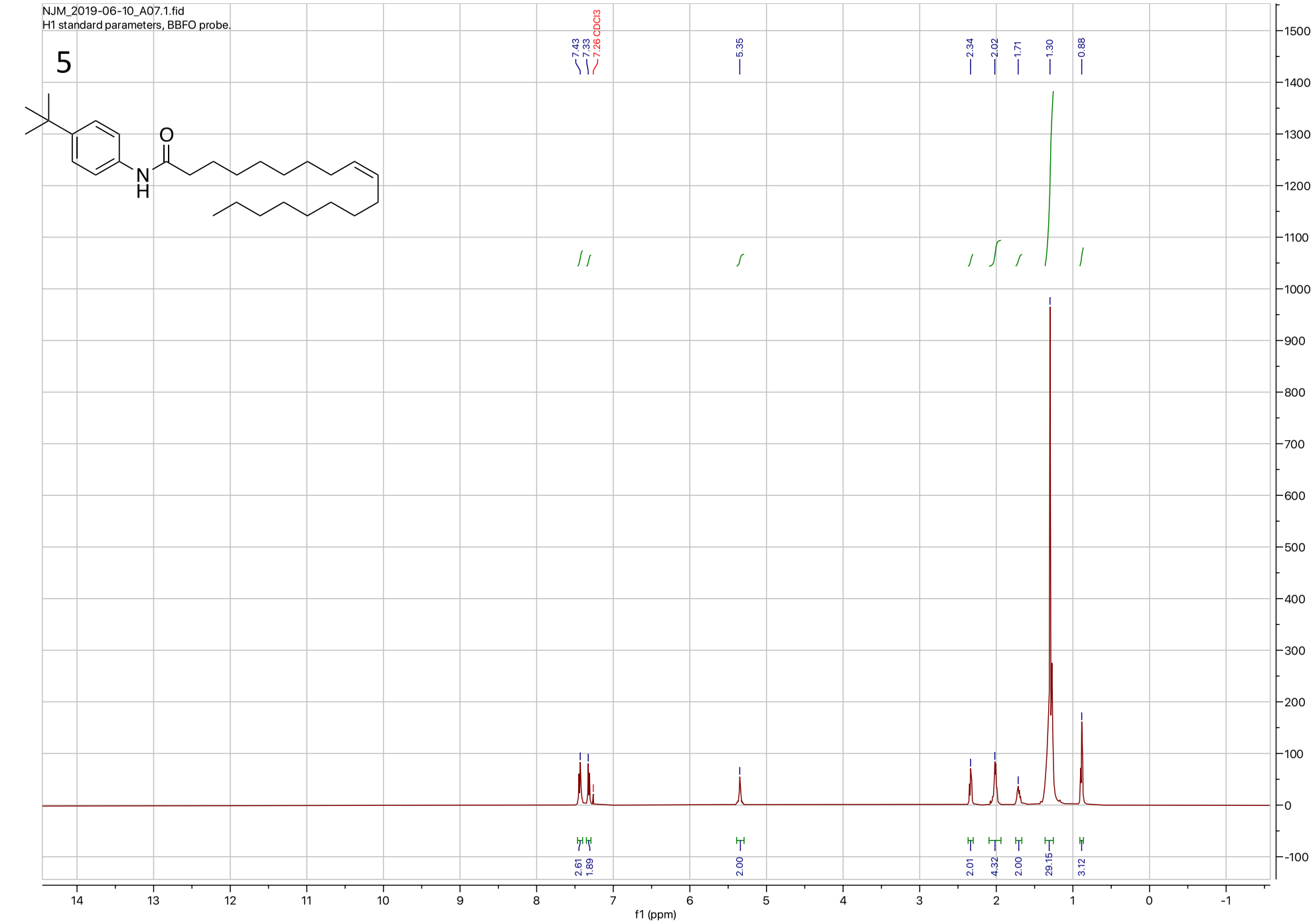

NJM_2019-05-31_A04.2.fid
C13 standard parameters, cryoprobe.
Use "abs13c" to flatten spectrum baseline.
2
O
O
N
H
197.83
171.80
142.44
132.73
130.06
129.77
129.69
118.82
77.04 CDCl3
37.88
31.91
29.77
29.70
29.53
29.33
29.28
29.23
29.11
27.23
27.16
26.44
25.45
22.69
14.13
f1 (ppm)

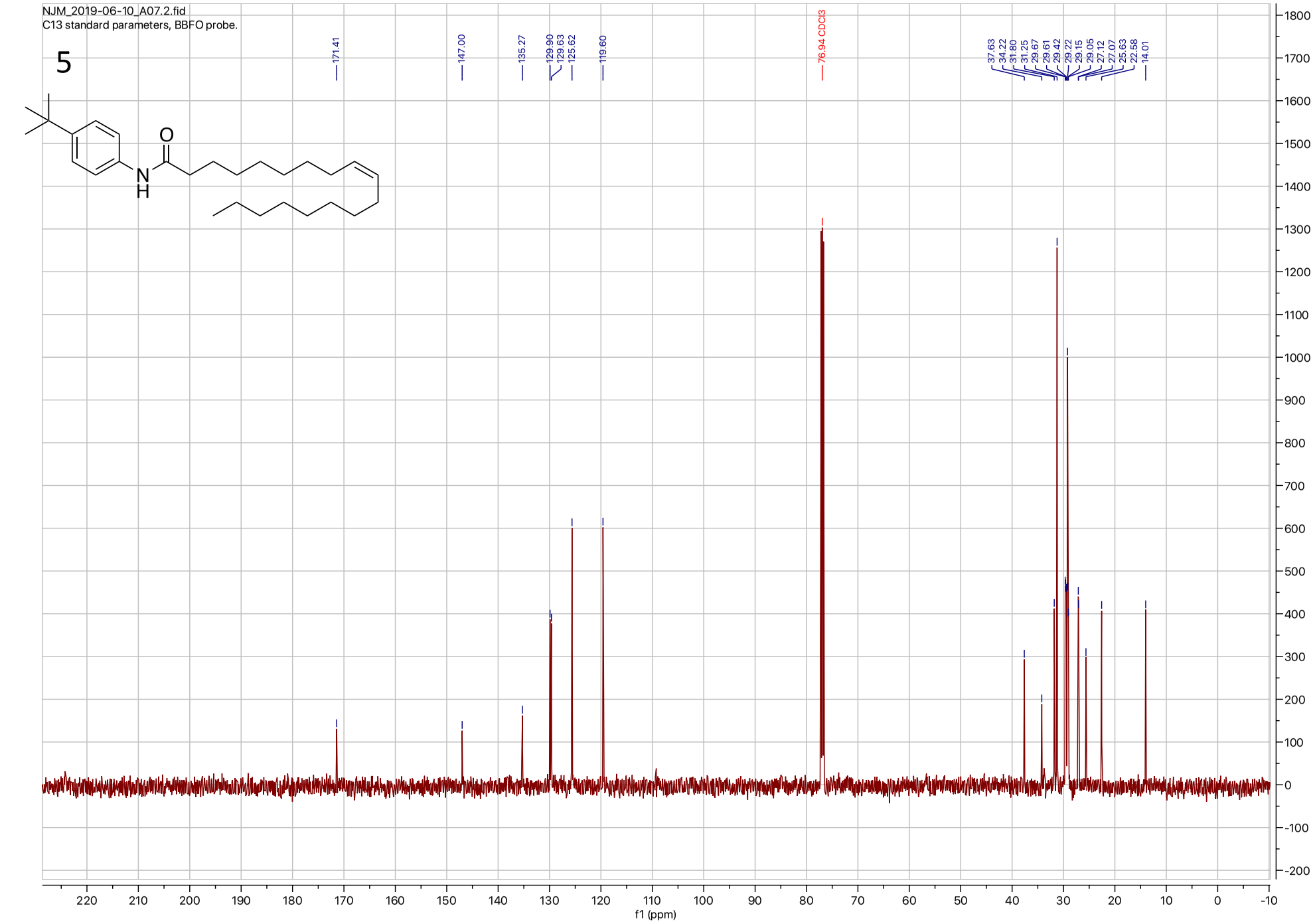

NJM_2019-05-24_A05.1.fid
H1 standard parameters, BBFO probe.
3
O
O
N
H
7.49
7.31
7.26 CDCl3
7.08
6.97
5.35
2.35
2.02
1.72
1.26
0.88
2.27
1.88
0.99
3.80
2.00
2.00
3.90
1.88
20.24
3.41
f1 (ppm)

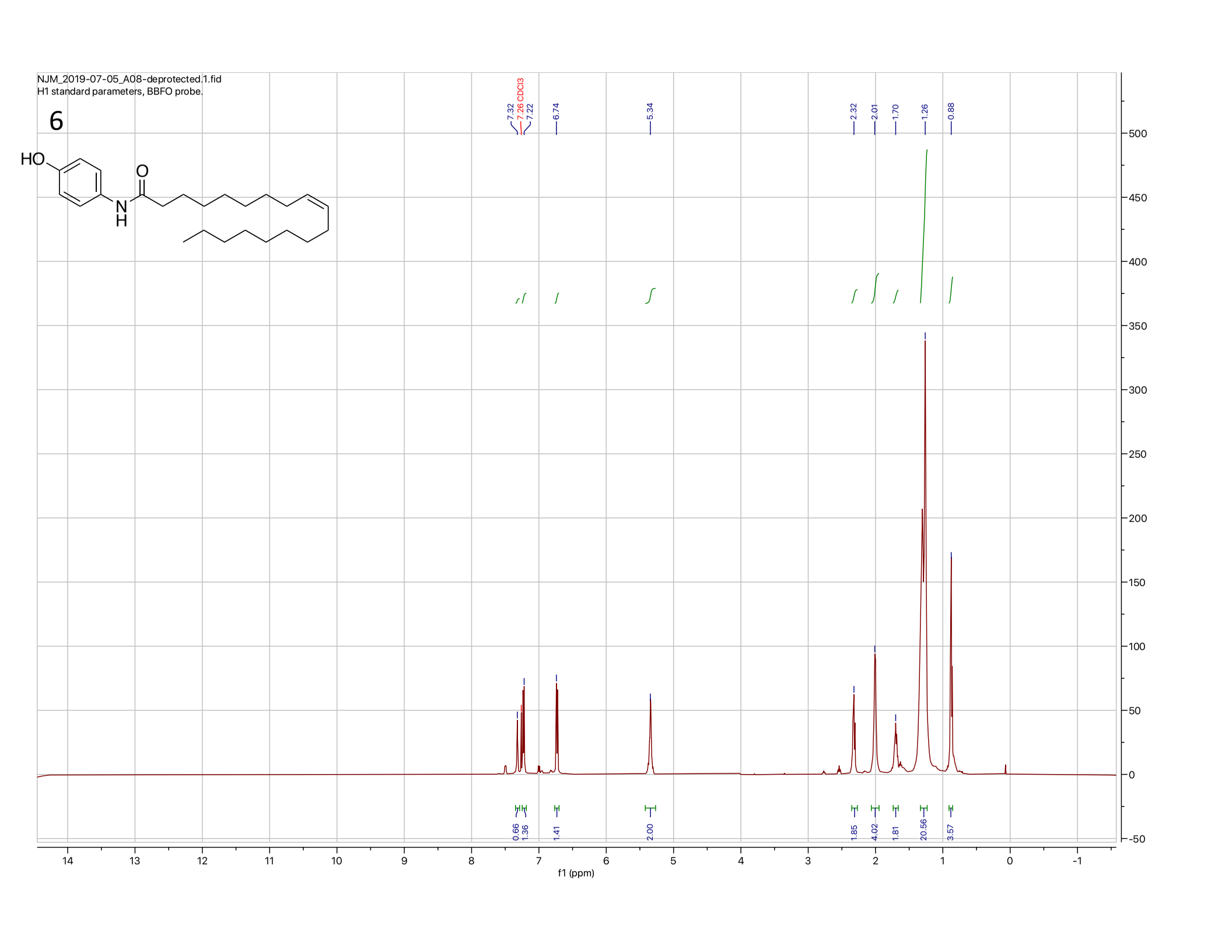

NJM_2019-05-24_A05.2.fid
C13 standard parameters, BBFO probe.
3
171.49
157.46
153.22
133.41
129.93
129.62
122.94
121.56
119.50
118.27
76.96 CDCl3
37.56
31.82
29.68
29.63
29.45
29.24
29.19
29.06
27.14
27.09
25.61
22.61
14.06
f1 (ppm)

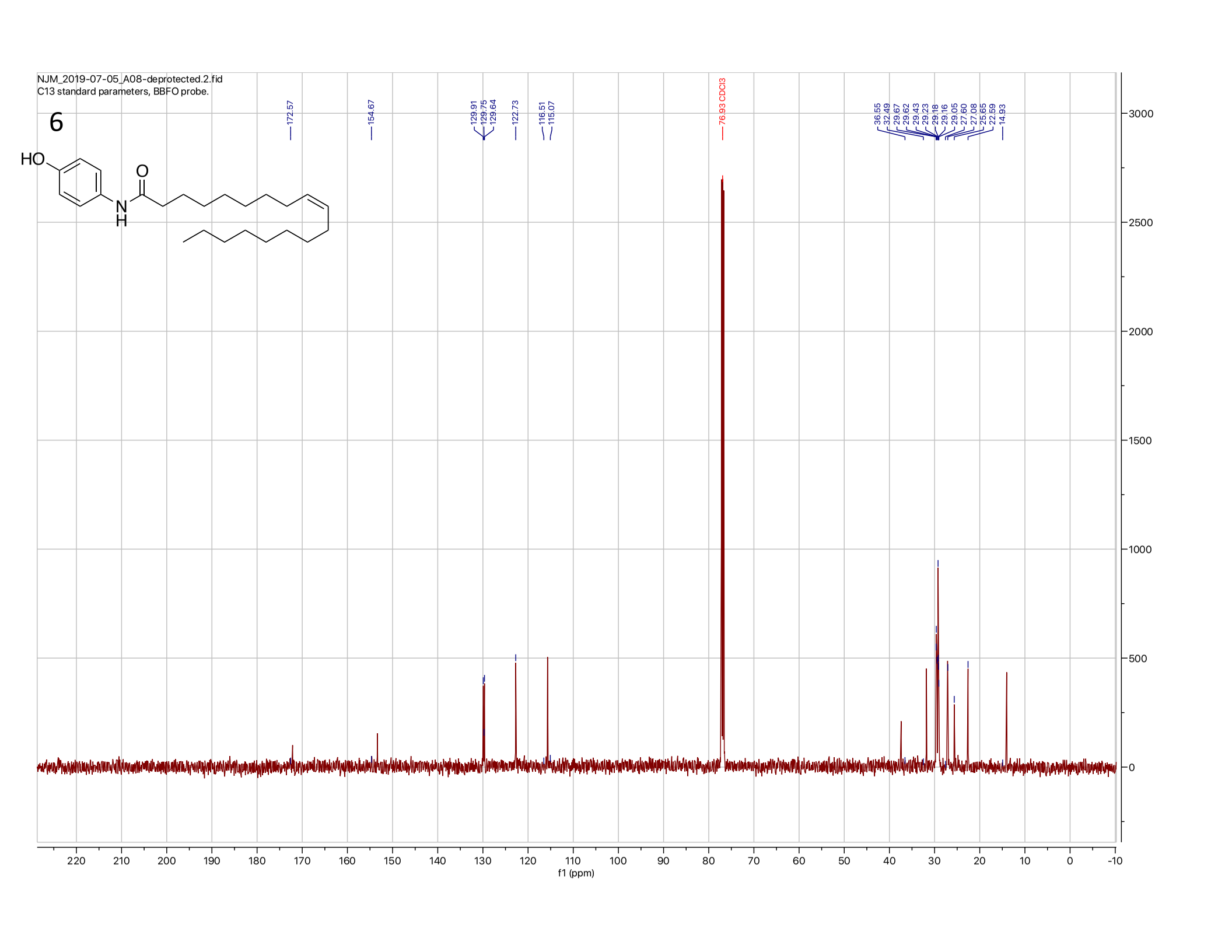

NJM_1-61_chloroaniline.1.fid
H1 standard parameters, BBFO probe.
4
Cl
O
N
H
7.46
7.31
7.27
7.26 CDCl3
5.34
4.13
2.34
2.04
2.01
1.71
1.26
0.88
1.75
0.70
2.18
2.00
2.00
3.65
1.93
17.78
3.72
f1 (ppm)

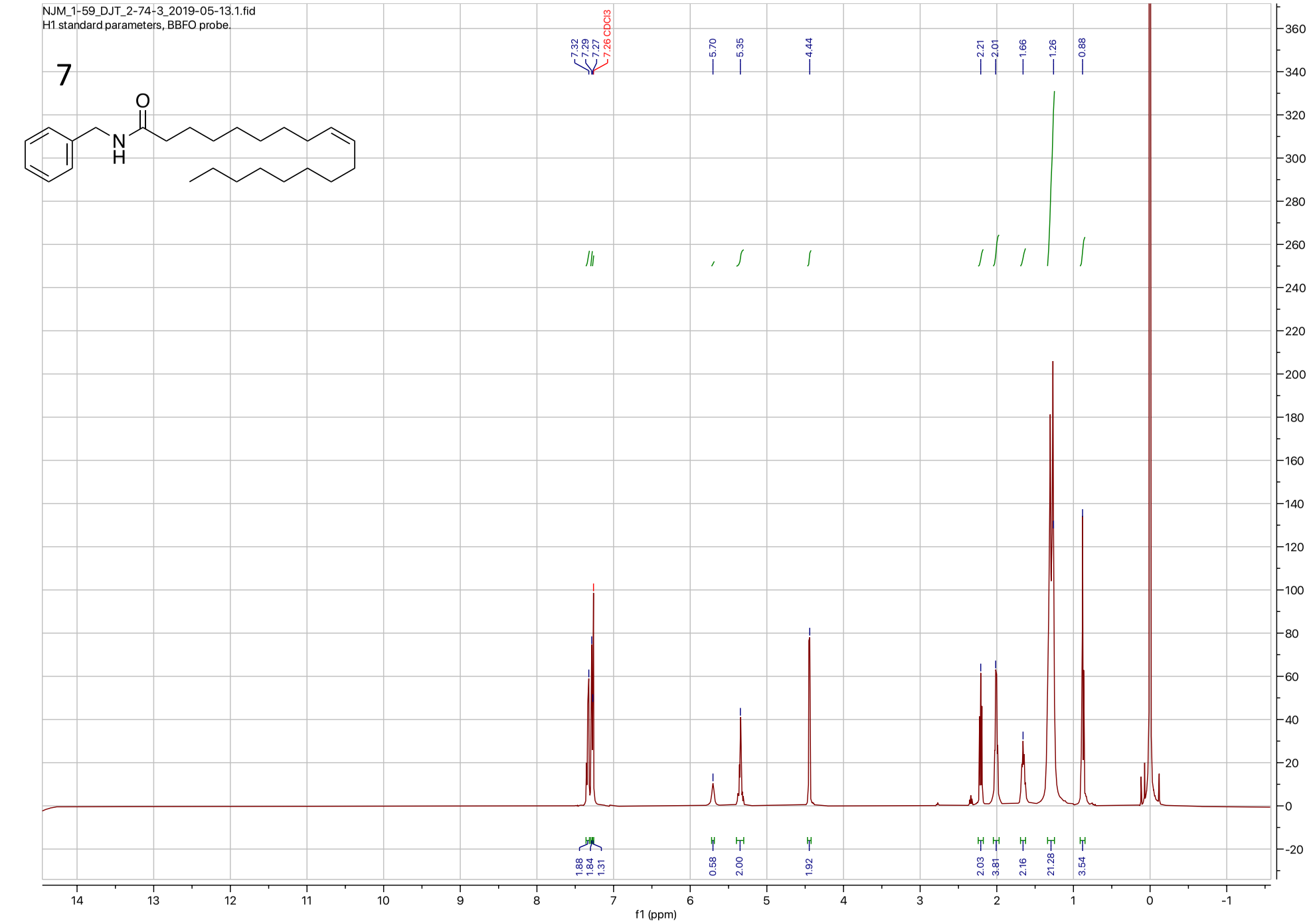

NJM_1-61_A06.2.fid
C13 standard parameters, BBFO probe.
4
Cl
O
N
H
171.33
136.45
129.93
129.58
128.97
128.85
120.87
76.91 CDCl3
60.30
37.62
31.79
29.65
29.58
29.41
29.21
29.16
29.12
29.00
27.11
27.05
25.42
22.57
20.93
14.07
13.99
f1 (ppm)

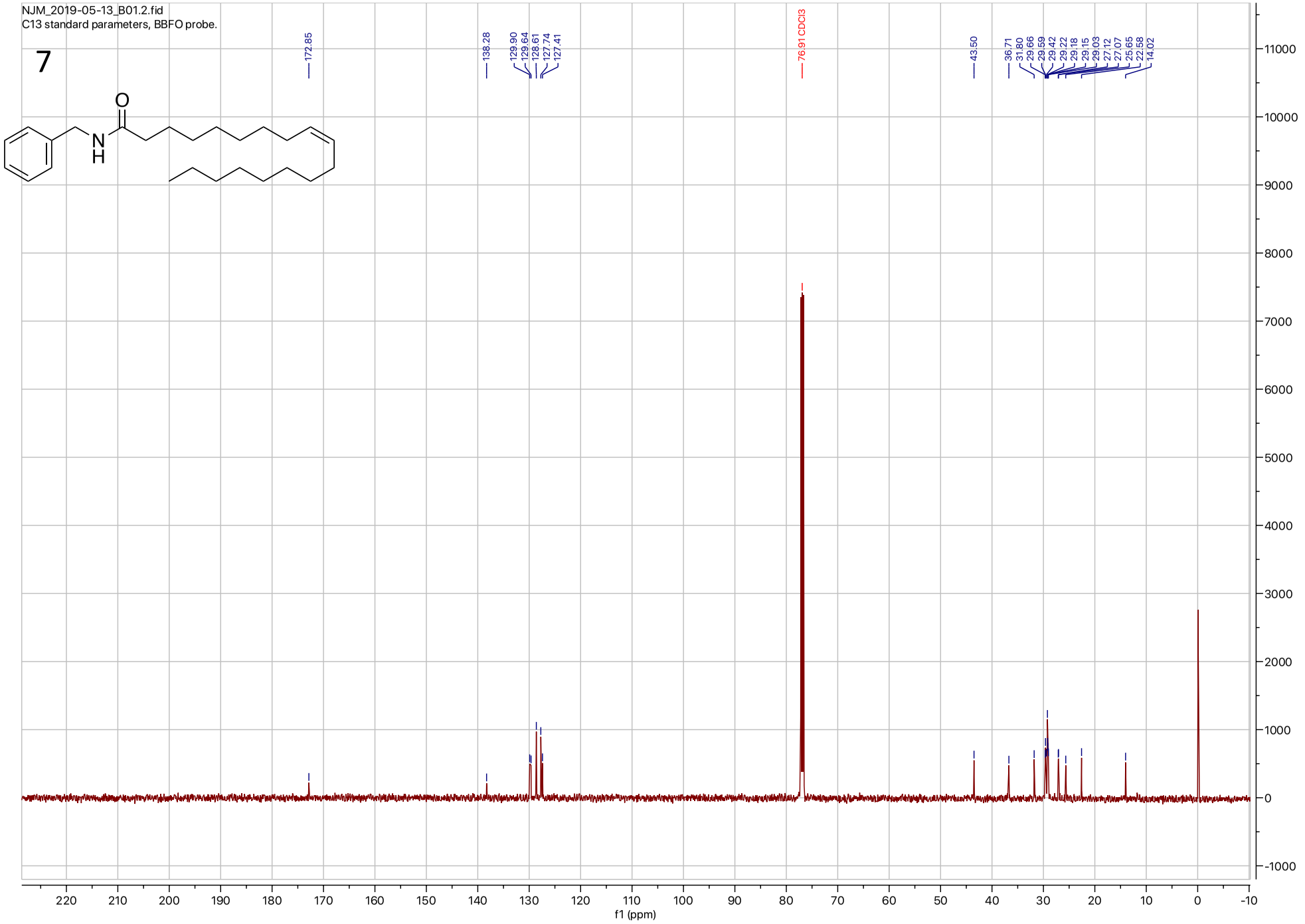

NJM_2019-06-10_A07.1.fid
H1 standard parameters, BBFO probe.
5
O
N
H
7.43
7.33
7.26 CDCl3
5.35
2.34
2.02
1.71
1.30
0.88
2.61
1.89
2.00
2.01
4.32
2.00
29.15
3.12
f1 (ppm)

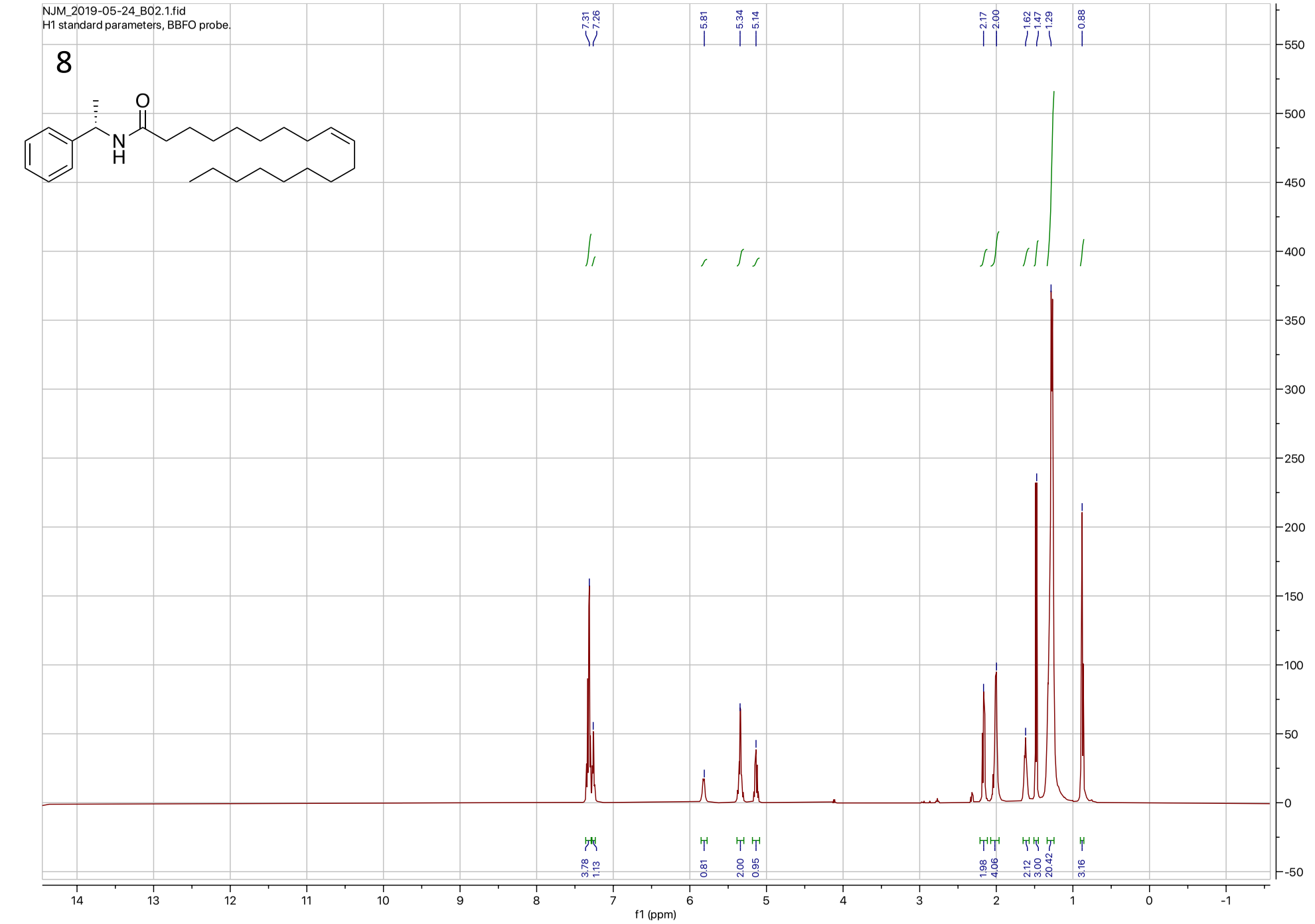

NJM_2019-06-10_A07.2.fid
C13 standard parameters, BBFO probe.
5
171.41
147.00
135.27
129.90
129.63
125.62
119.60
76.94 CDCl3
37.63
34.22
31.80
31.25
29.67
29.61
29.42
29.22
29.15
29.05
27.12
27.07
25.63
22.58
14.01
O
N
H
f1 (ppm)

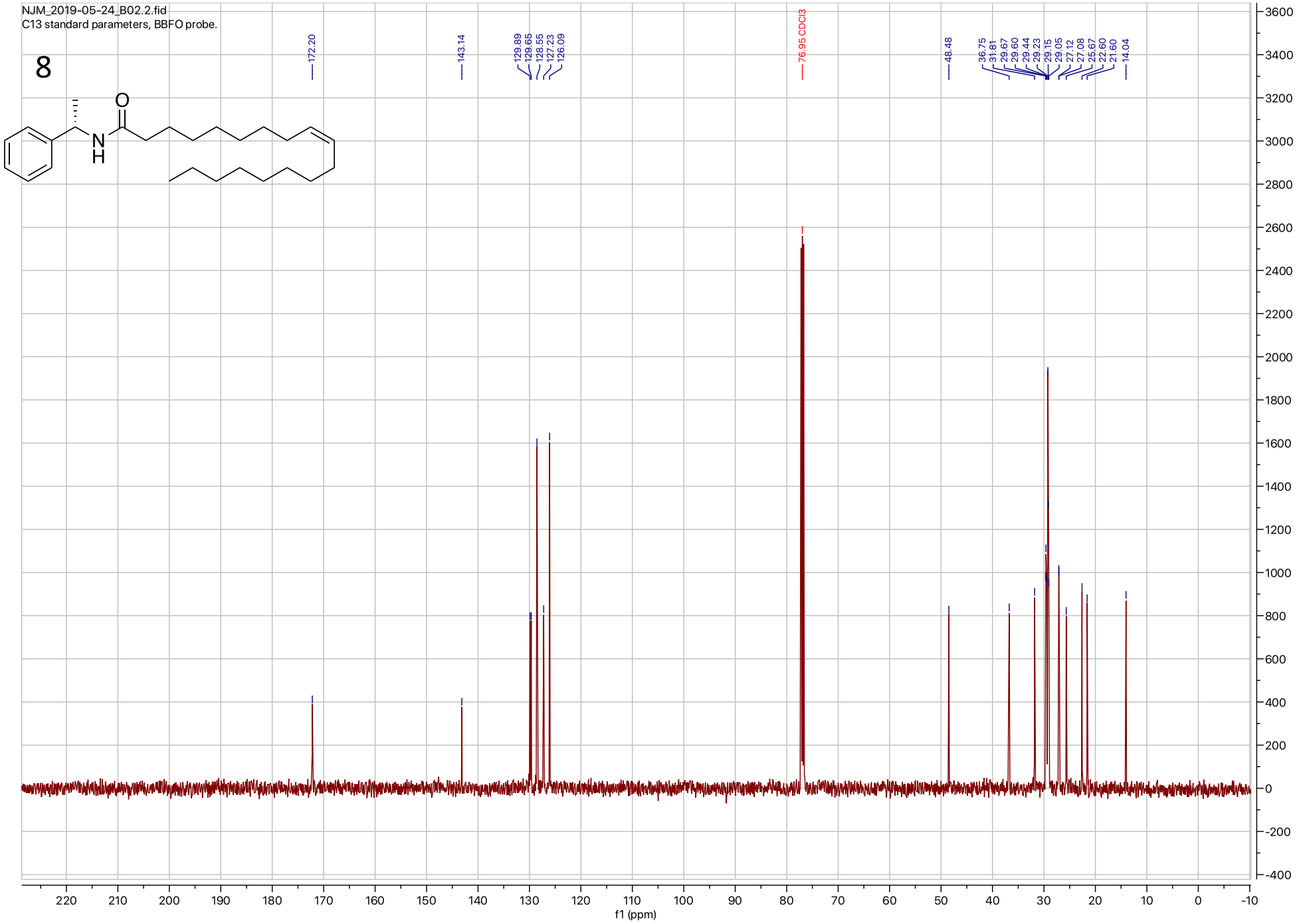

NJM_2019-07-05_A08-deprotected.1.fid
H1 standard parameters, BBFO probe.
6
HO
O
N
H
7.32
7.26 CDCl3
7.22
6.74
5.34
2.32
2.01
1.70
1.26
0.88
0.66
1.36
1.41
2.00
1.85
4.02
1.81
20.56
3.57
f1 (ppm)

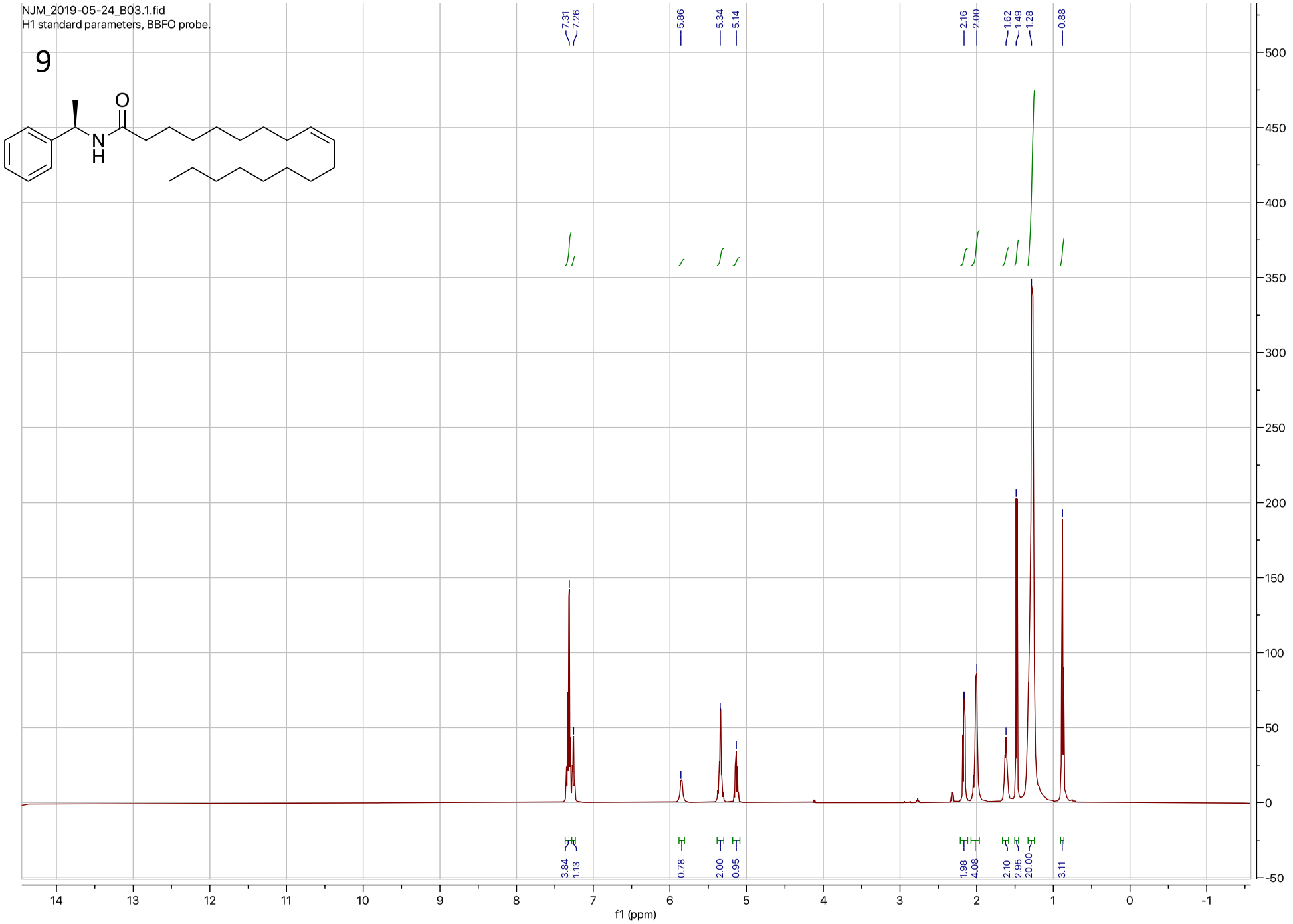

NJM_2019-07-05_A08-deprotected.2.fid
C13 standard parameters, BBFO probe.
6
HO
O
N
H
172.57
154.67
129.91
129.75
129.64
122.73
116.51
115.07
76.93 CDCl3
36.55
32.49
29.67
29.62
29.43
29.23
29.18
29.16
29.05
27.60
27.08
25.65
22.59
14.93
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

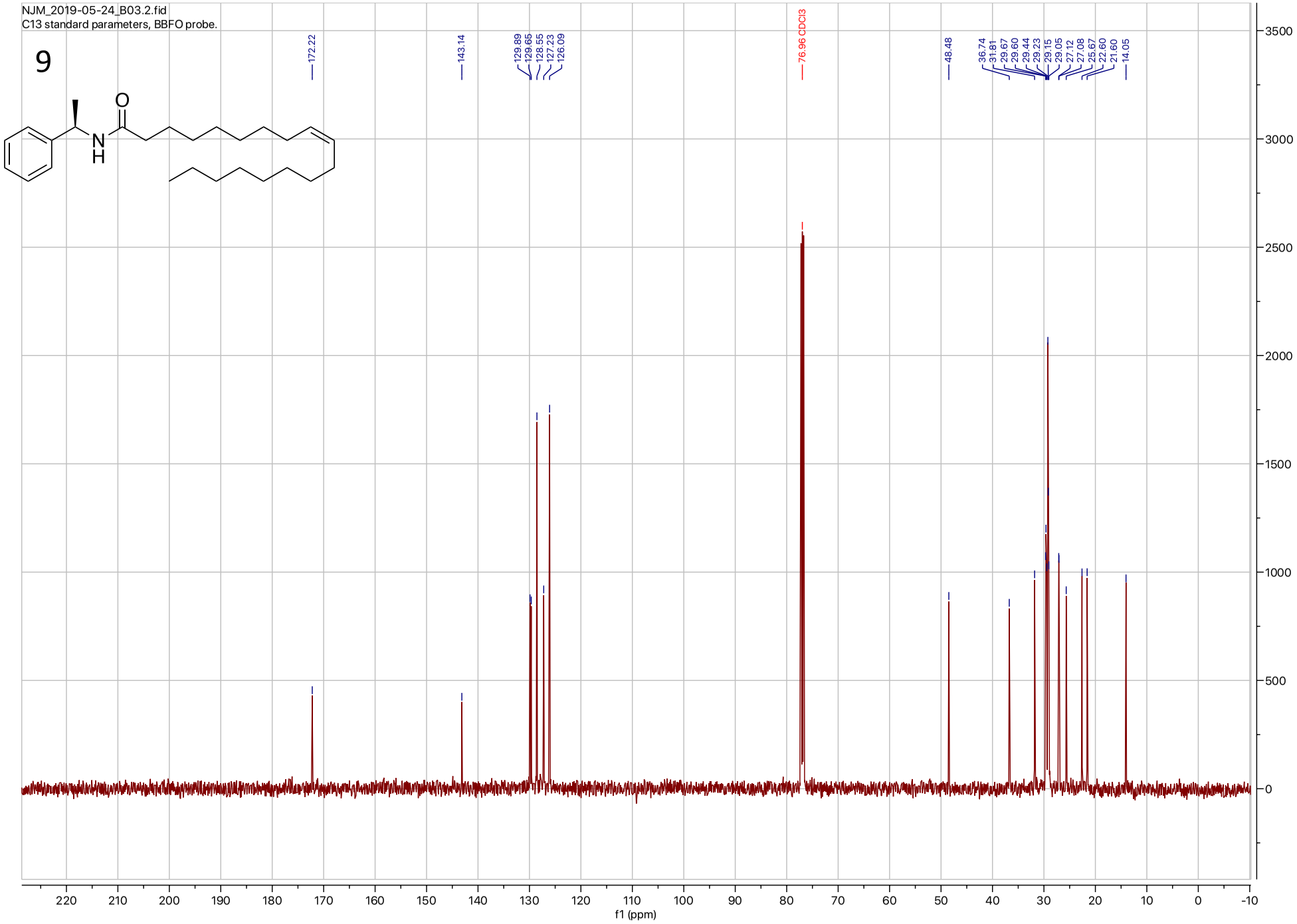

NJM_1-59_DJT_2-74-3_2019-05-13.1.fid
H1 standard parameters, BBFO probe.
7
O
N
H
7.32
7.29
7.27
7.26 CDCl3
5.70
5.35
4.44
2.21
2.01
1.66
1.26
0.88
1.88
1.84
1.31
0.58
2.00
1.92
2.03
3.81
2.16
21.28
3.54
f1 (ppm)


NJM_2019-05-13_B01.2.fid
C13 standard parameters, BBFO probe.
7
O
N
H
172.85
138.28
129.90
129.64
128.61
127.74
127.41
76.91 CDCl3
43.50
36.71
31.80
29.66
29.59
29.42
29.22
29.18
29.15
29.03
27.12
27.07
25.65
22.58
14.02
f1 (ppm)


NJM_2019-05-24_B02.1.fid
H1 standard parameters, BBFO probe.
8
O
N
H
7.31
7.26
5.81
5.34
5.14
2.17
2.00
1.62
1.47
1.29
0.88
3.78
1.13
0.81
2.00
0.95
1.98
4.06
2.12
3.00
20.42
3.16
f1 (ppm)


NJM_2019-05-24_B02.2.fid
C13 standard parameters, BBFO probe.
8
O
N
H
172.20
143.14
129.89
129.65
128.55
127.23
126.09
76.95 CDCl3
48.48
36.75
31.81
29.67
29.60
29.44
29.23
29.15
29.05
27.12
27.08
25.67
22.60
21.60
14.04
f1 (ppm)


NJM_2019-05-24_B03.1.fid
H1 standard parameters, BBFO probe.
9
O
N
H
7.31
7.26
5.86
5.34
5.14
2.16
2.00
1.62
1.49
1.28
0.88
3.84
1.13
0.78
2.00
0.95
1.98
4.08
2.10
2.95
20.00
3.11
f1 (ppm)


NJM_2019-05-24_B03.2.fid
C13 standard parameters, BBFO probe.
9
O
N
H
172.22
143.14
129.89
128.65
128.55
127.23
126.09
76.96 CDCl3
48.48
36.74
31.81
29.67
29.60
29.44
29.23
29.15
29.05
27.12
27.08
25.67
22.60
21.60
14.05
3500
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

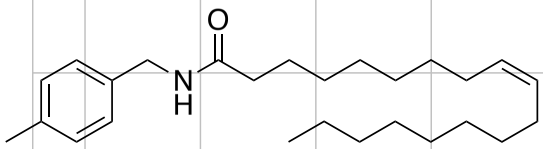
10

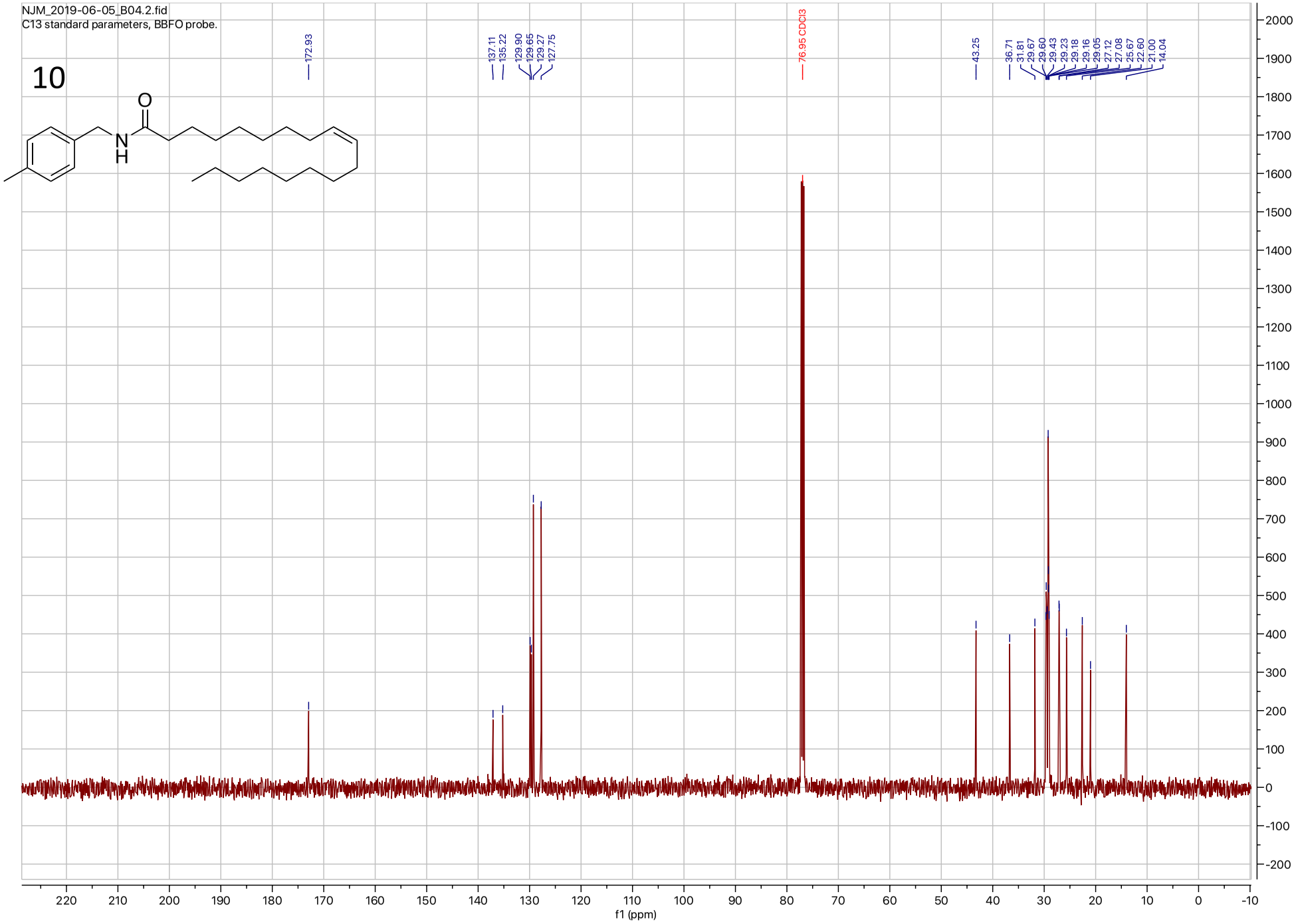
NJM 2019-06-05_B04.1.fid

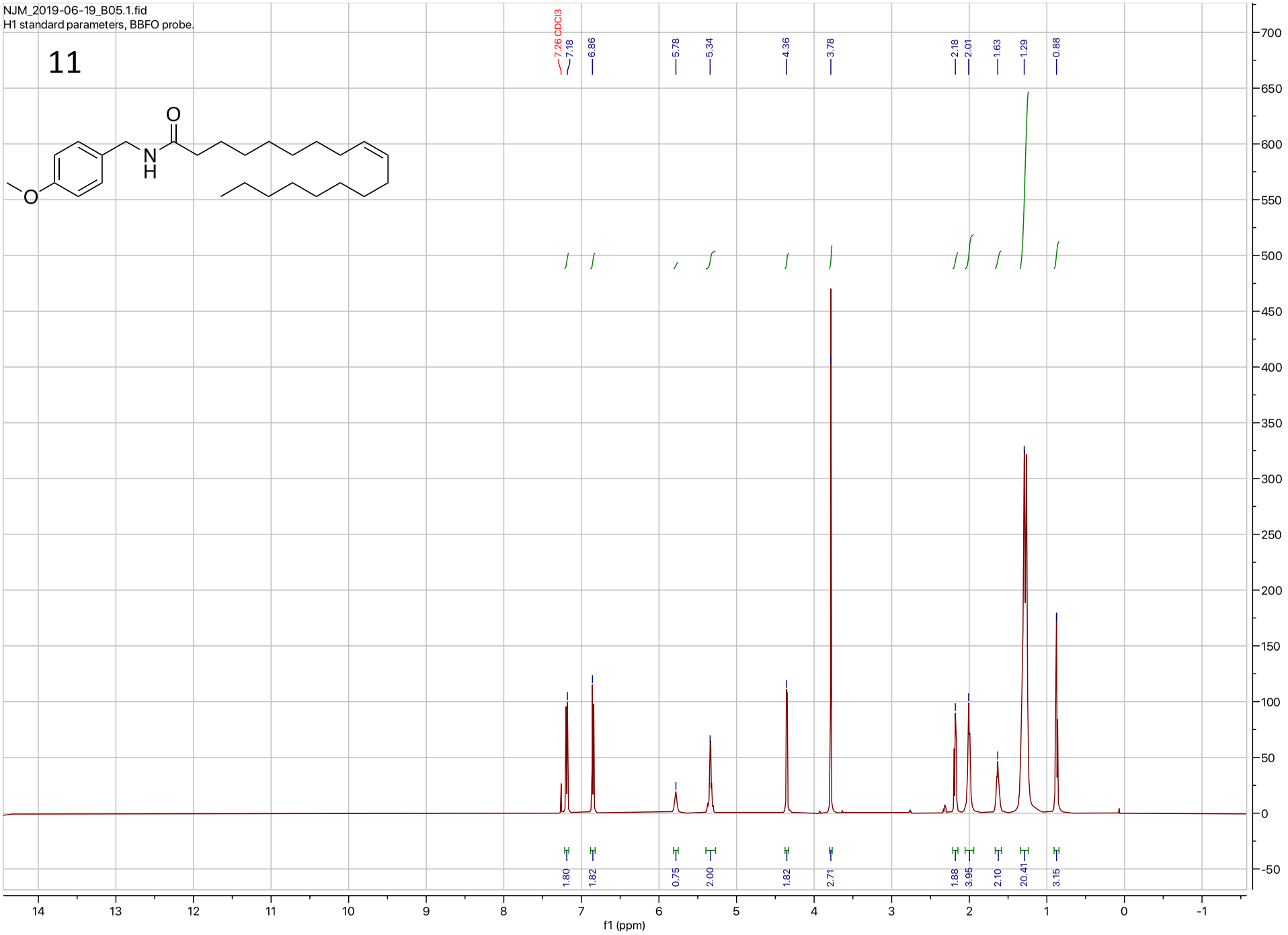
NJM standard parameters, BBFO probe.

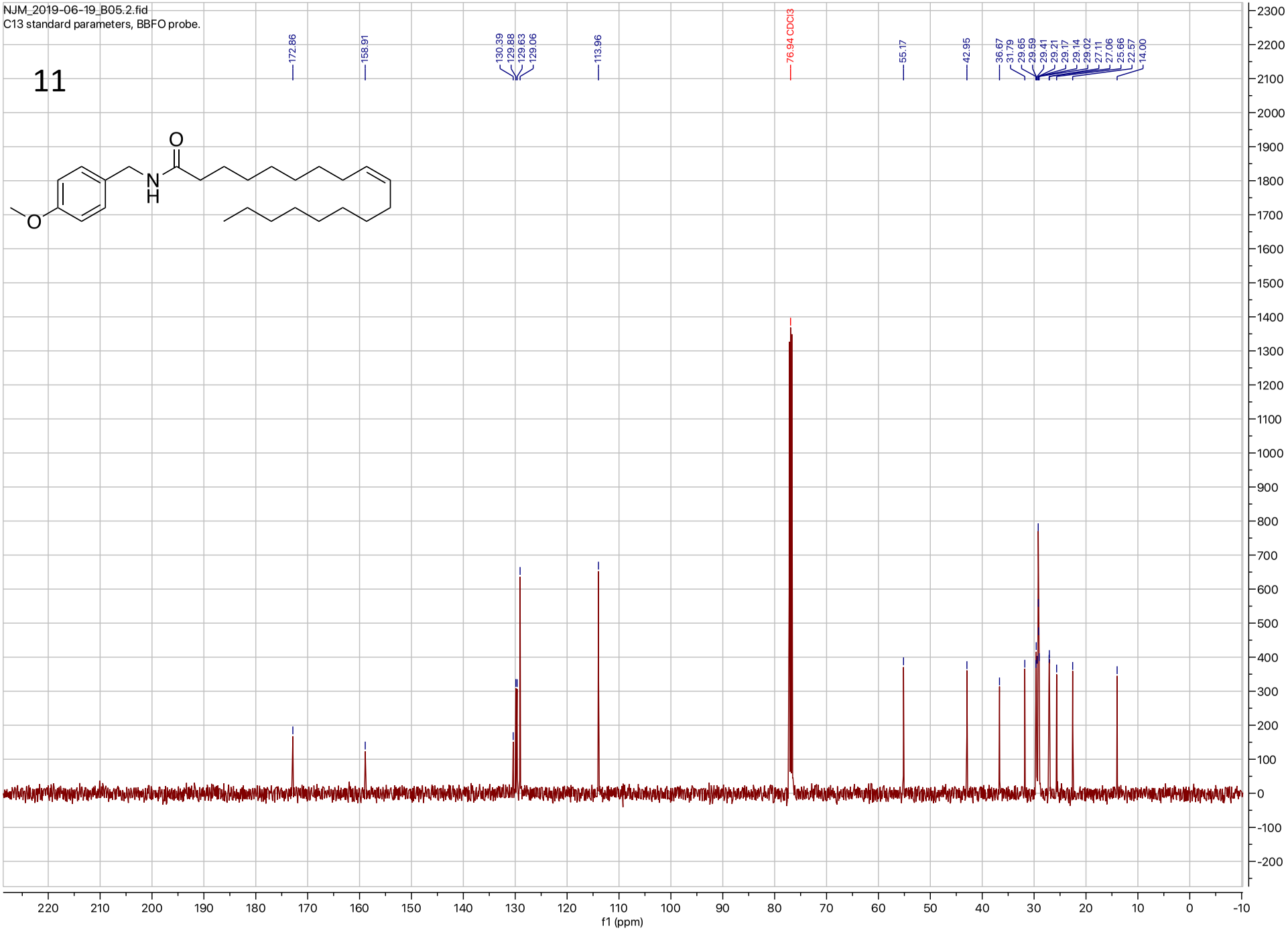
NJM 1-72

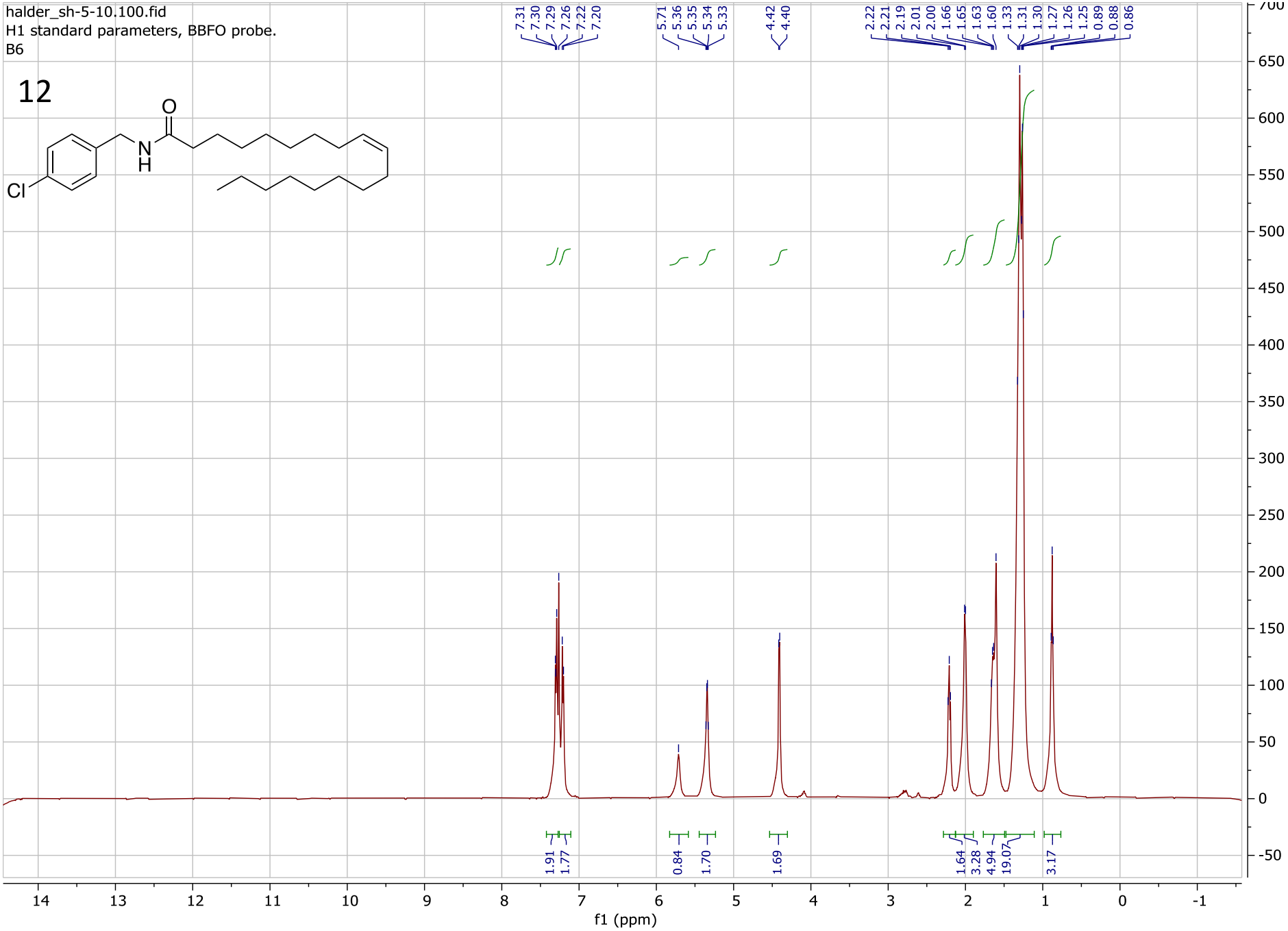
DRX 500

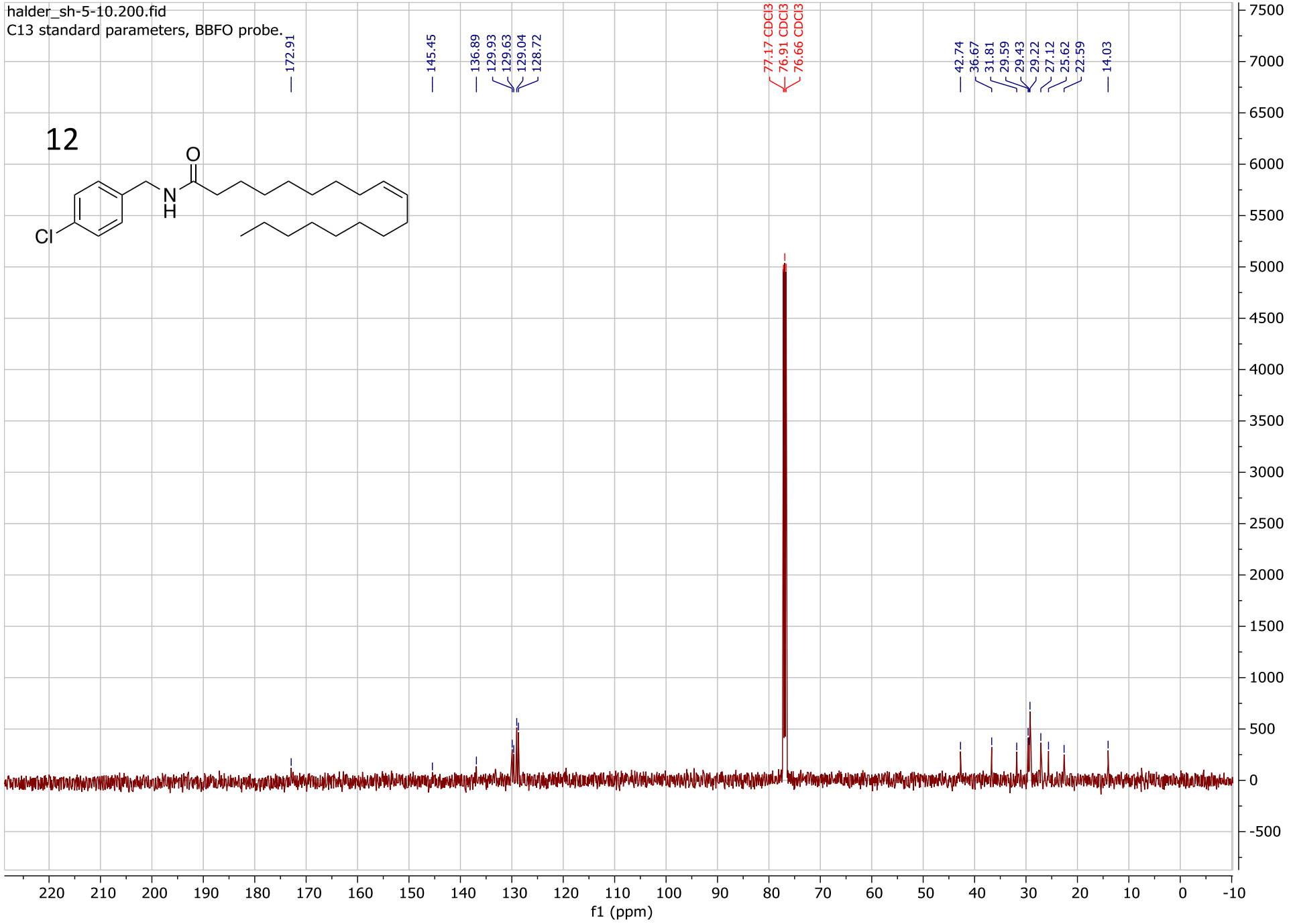


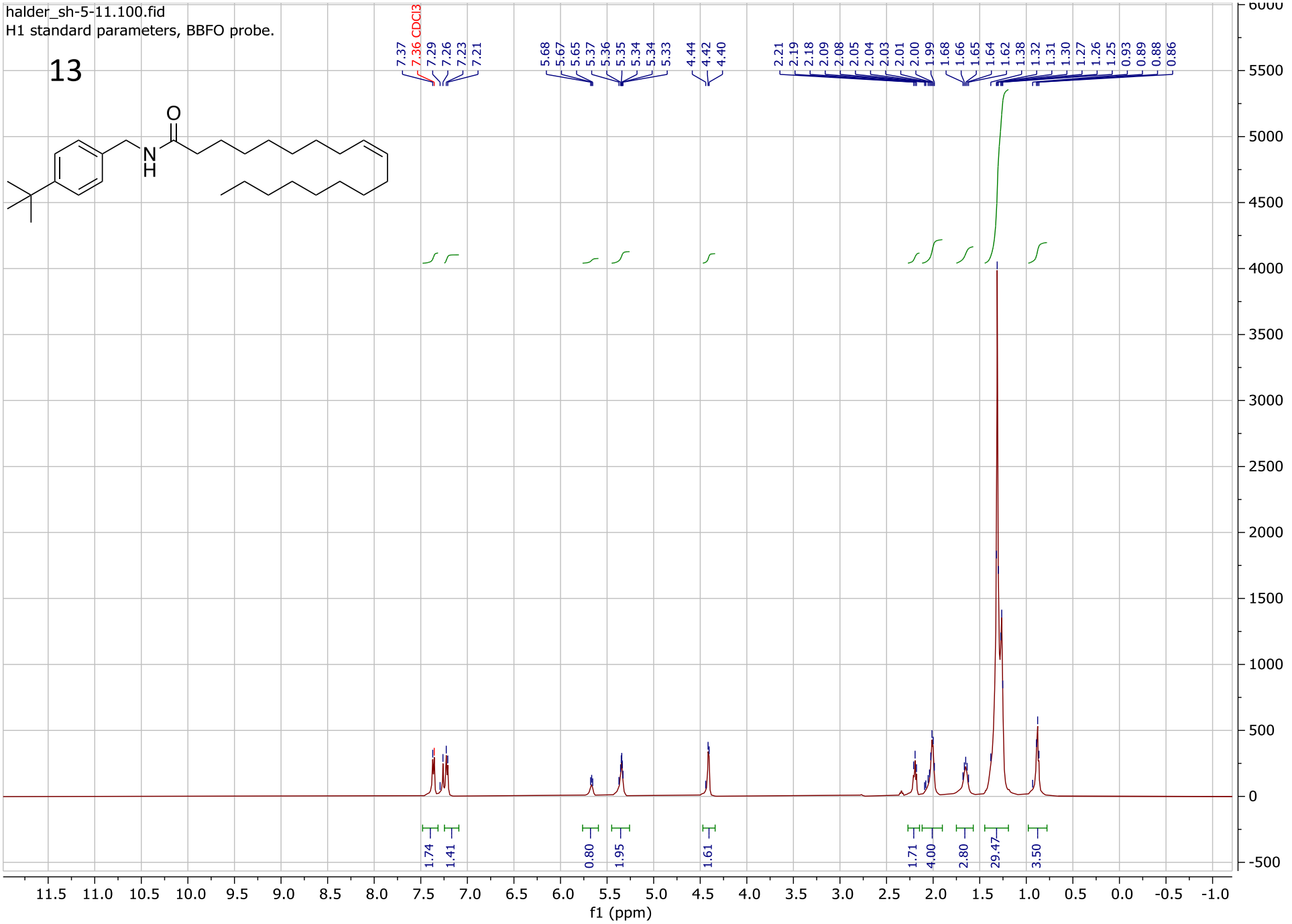

NJM_2019-06-05_B04.2.fid
C13 standard parameters, BBFO probe.
10
O
N
H
172.93
137.11
135.22
129.90
129.65
129.27
127.75
76.95 CDCl3
43.25
36.71
31.81
29.67
29.60
29.43
29.23
29.18
29.16
29.05
27.12
27.08
25.67
22.60
21.00
14.04
f1 (ppm)

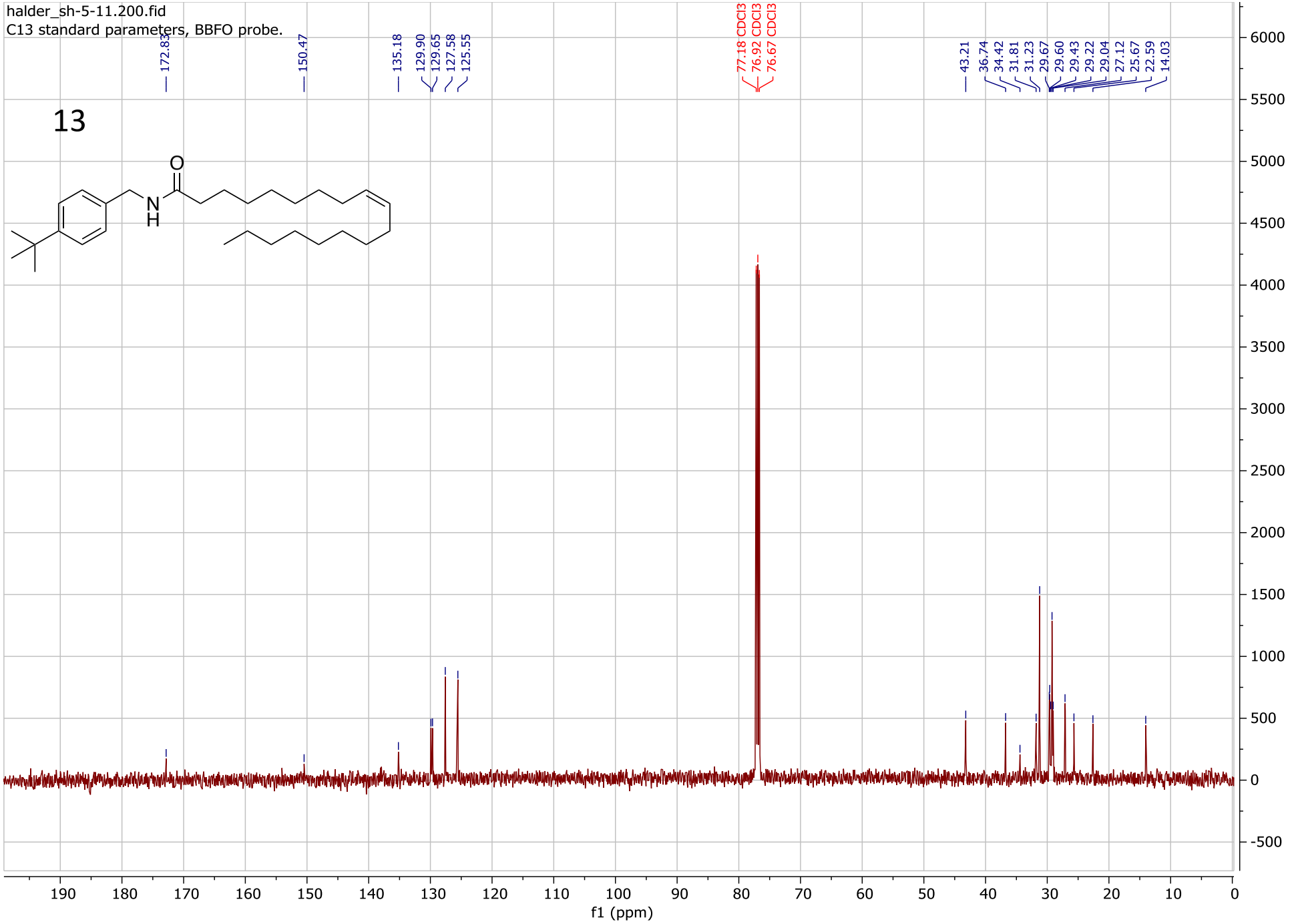

NJM_2019-06-19_B05.1.fid
H1 standard parameters, BBFO probe.
11
O
N
H
O
7.26 CDCl3
7.18
6.86
5.78
5.34
4.36
3.78
2.18
2.01
1.63
1.29
0.88
1.80
1.82
0.75
2.00
1.82
2.71
1.88
3.96
2.10
20.41
3.15
f1 (ppm)

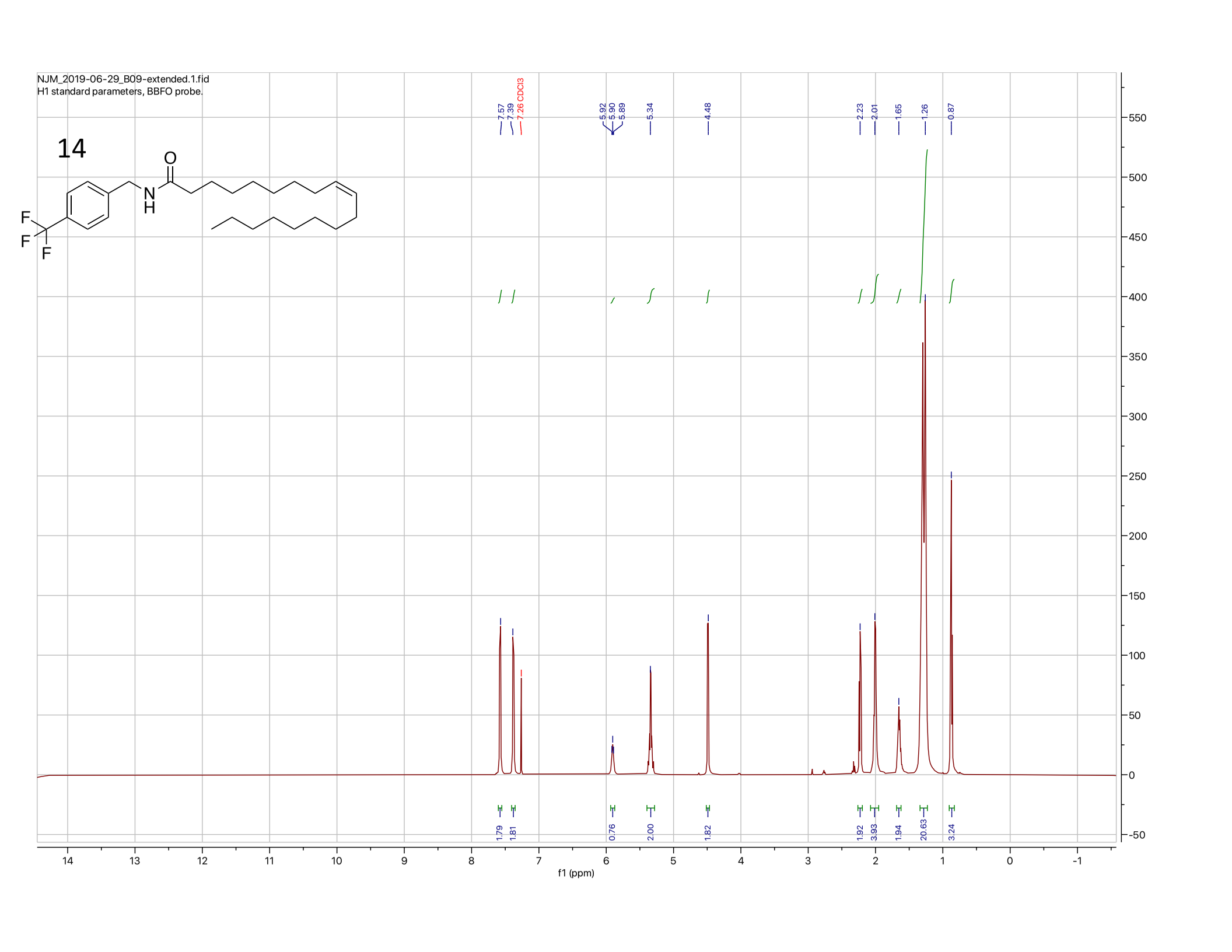

NJM_2019-06-19_B05.2.fid
C13 standard parameters, BBFO probe.
11
O
N
H
O
172.86
158.91
130.39
129.88
129.63
129.06
113.96
76.94 CDCl3
55.17
42.95
36.67
31.79
29.65
29.59
29.41
29.21
29.17
29.14
29.02
27.11
27.06
25.66
22.57
14.00
f1 (ppm)

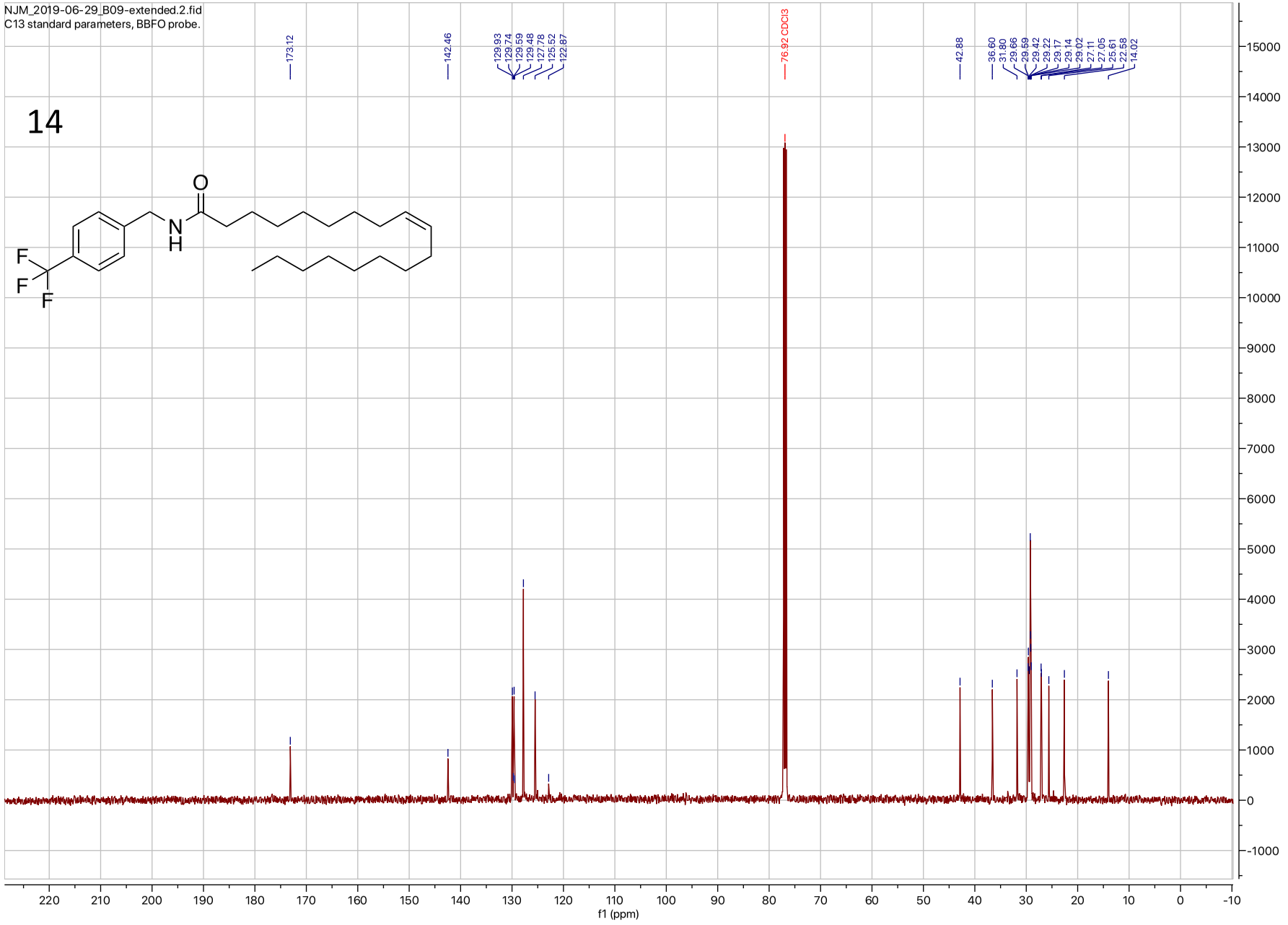

halder_sh-5-10.100.fid
H1 standard parameters, BBFO probe.
B6
12
O
N
H
Cl
7.31
7.30
7.29
7.26
7.22
7.20
5.71
5.36
5.35
5.34
5.33
4.42
4.40
2.22
2.21
2.19
2.01
2.00
1.66
1.65
1.63
1.60
1.33
1.31
1.30
1.27
1.26
1.25
0.89
0.88
0.86
1.91
1.77
0.84
1.70
1.69
1.64
3.28
4.94
19.07
3.17
f1 (ppm)

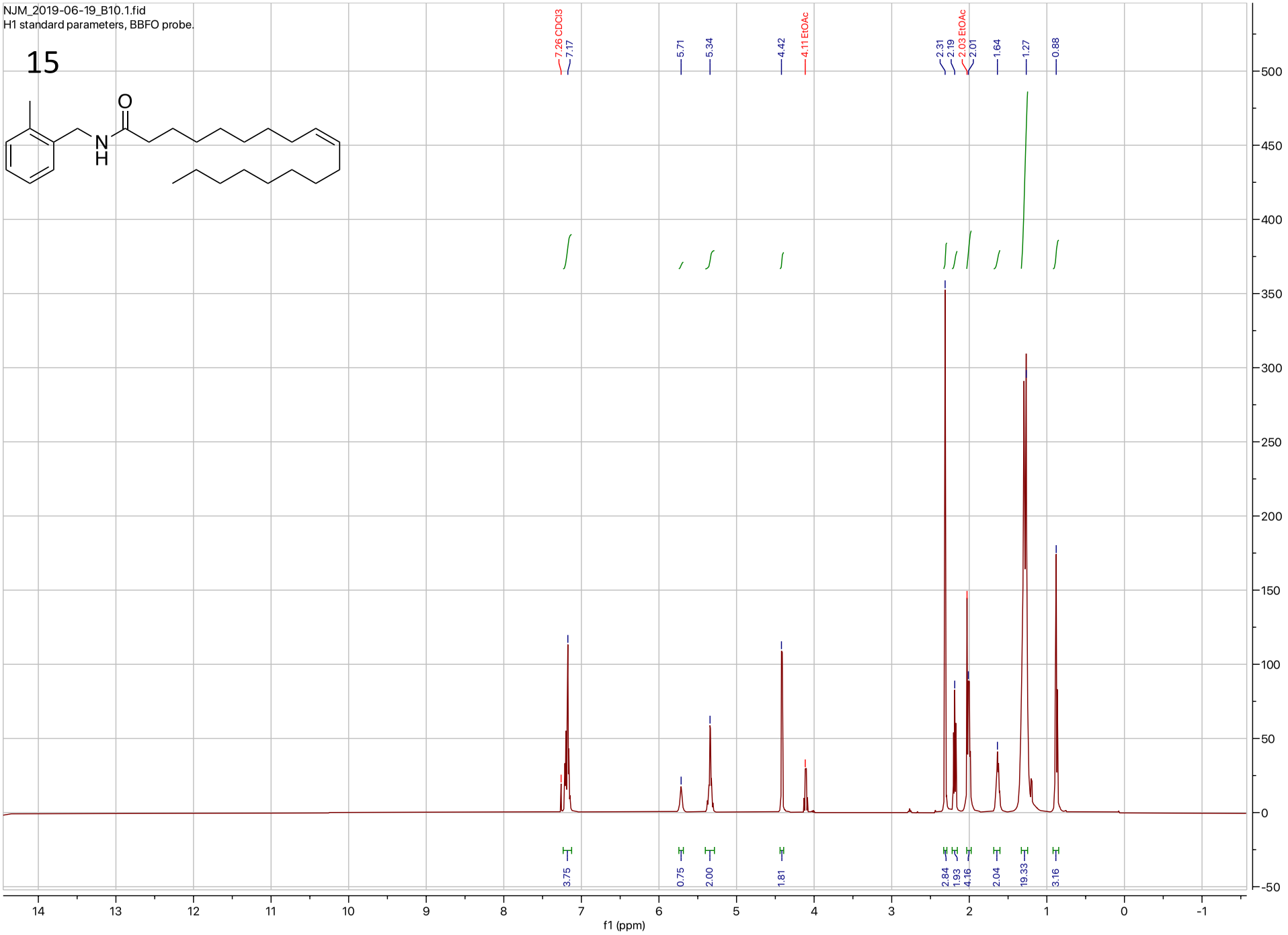

halder_sh-5-10.200.fid
C13 standard parameters, BBFO probe.
12
172.91
145.45
136.89
129.93
129.63
129.04
128.72
77.17 CDCl3
76.91 CDCl3
76.66 CDCl3
42.74
36.67
31.81
29.59
29.43
29.22
27.12
25.62
22.59
14.03
f1 (ppm)


halder_sh-5-11.100.fid
H1 standard parameters, BBFO probe.
13
O
N
H
7.37
7.36 CDCl3
7.29
7.26
7.23
7.21
5.68
5.67
5.65
5.37
5.36
5.35
5.34
5.34
5.33
4.44
4.42
4.40
2.21
2.19
2.18
2.09
2.08
2.05
2.04
2.03
2.01
2.00
1.99
1.68
1.66
1.65
1.64
1.62
1.38
1.32
1.31
1.30
1.27
1.26
1.25
0.93
0.89
0.88
0.86
1.74
1.41
0.80
1.95
1.61
1.71
4.00
2.80
29.47
3.50
f1 (ppm)


halder_sh-5-11.200.fid
C13 standard parameters, BBFO probe.
13
O
N
H
172.83
150.47
135.18
129.90
129.65
127.58
125.55
77.18 CDCl3
76.92 CDCl3
76.67 CDCl3
43.21
36.74
34.42
31.81
31.23
29.67
29.60
29.43
29.22
29.04
27.12
25.67
22.59
14.03
6000
5500
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
-500
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


NJM_2019-06-29_B09-extended.1.fid
H1 standard parameters, BBFO probe.
14
O
N
H
F
F
F
7.57
7.39
7.26 CDCl3
5.92
5.90
5.89
5.34
4.48
2.23
2.01
1.65
1.26
0.87
1.79
1.81
0.76
2.00
1.82
1.92
3.93
1.94
20.63
3.24
f1 (ppm)


NJM_2019-06-29_B09-extended.2.fid
C13 standard parameters, BBFO probe.
14
173.12
142.46
129.93
129.74
129.59
129.48
127.78
125.52
122.87
76.92 CDCl3
42.88
36.60
31.80
29.66
29.59
29.42
29.22
29.17
29.14
29.02
27.11
27.05
25.61
22.58
14.02
O
N
H
F
F
F
f1 (ppm)


NJM_2019-06-19_B10.1.fid
H1 standard parameters, BBFO probe.
15
O
N
H
7.26 CDCl3
7.17
5.71
5.34
4.42
4.11 EtOAc
2.31
2.19
2.03 EtOAc
2.01
1.64
1.27
0.88
3.75
0.75
2.00
1.81
2.84
1.93
4.16
2.04
19.33
3.16
f1 (ppm)

15

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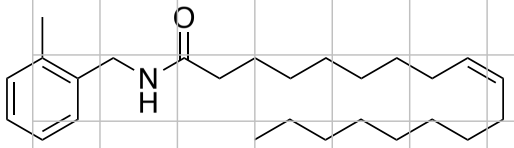
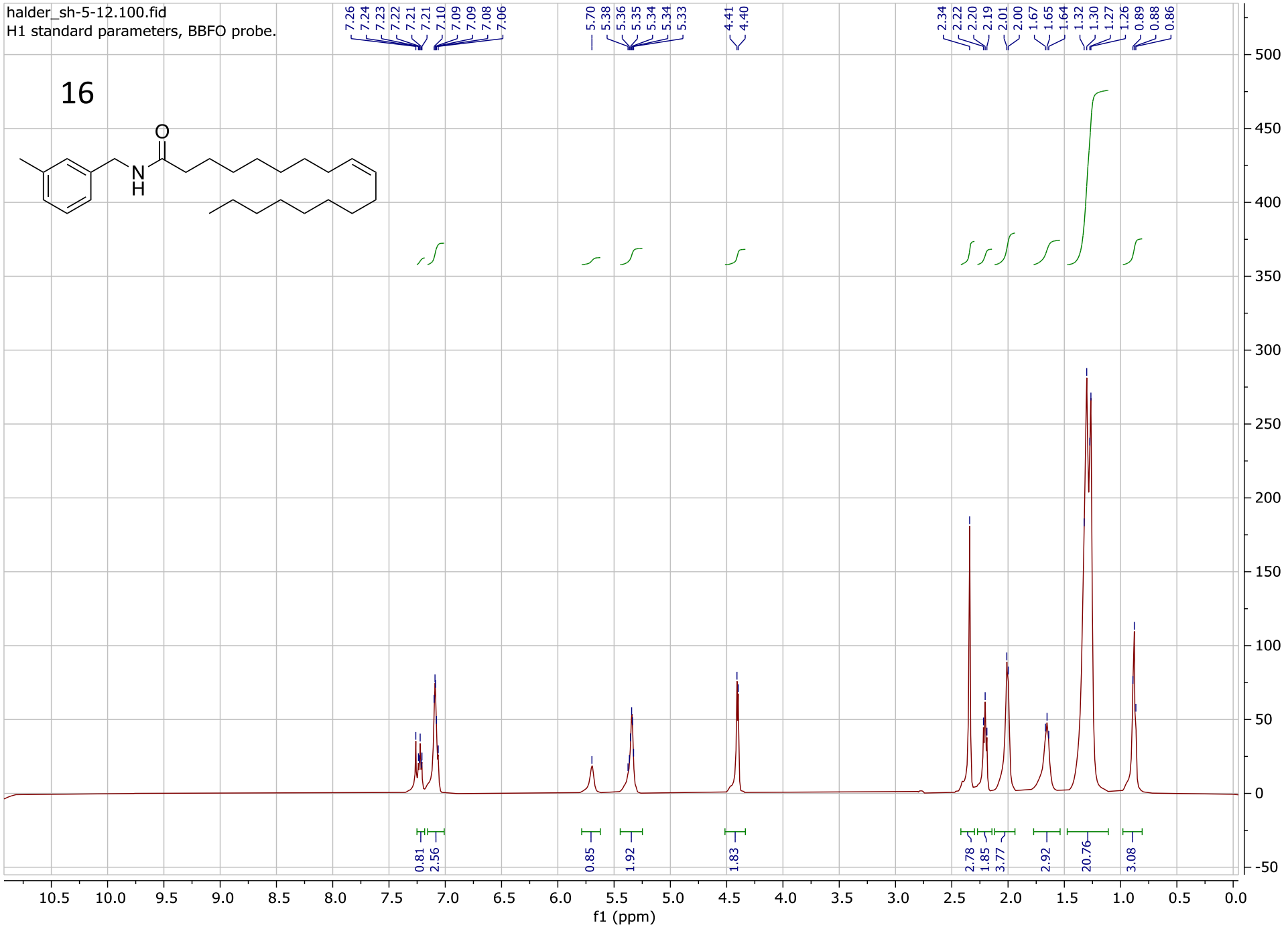
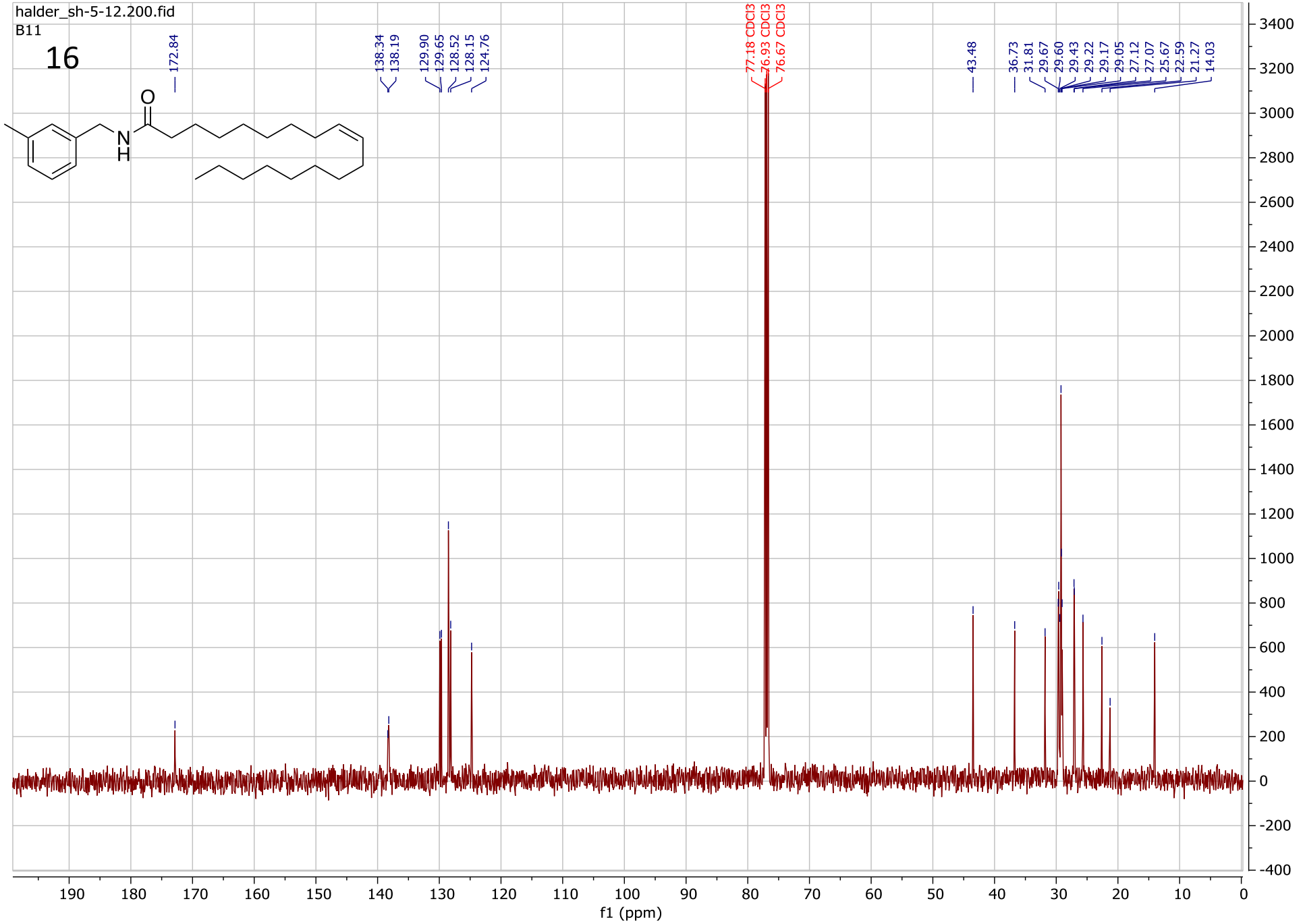
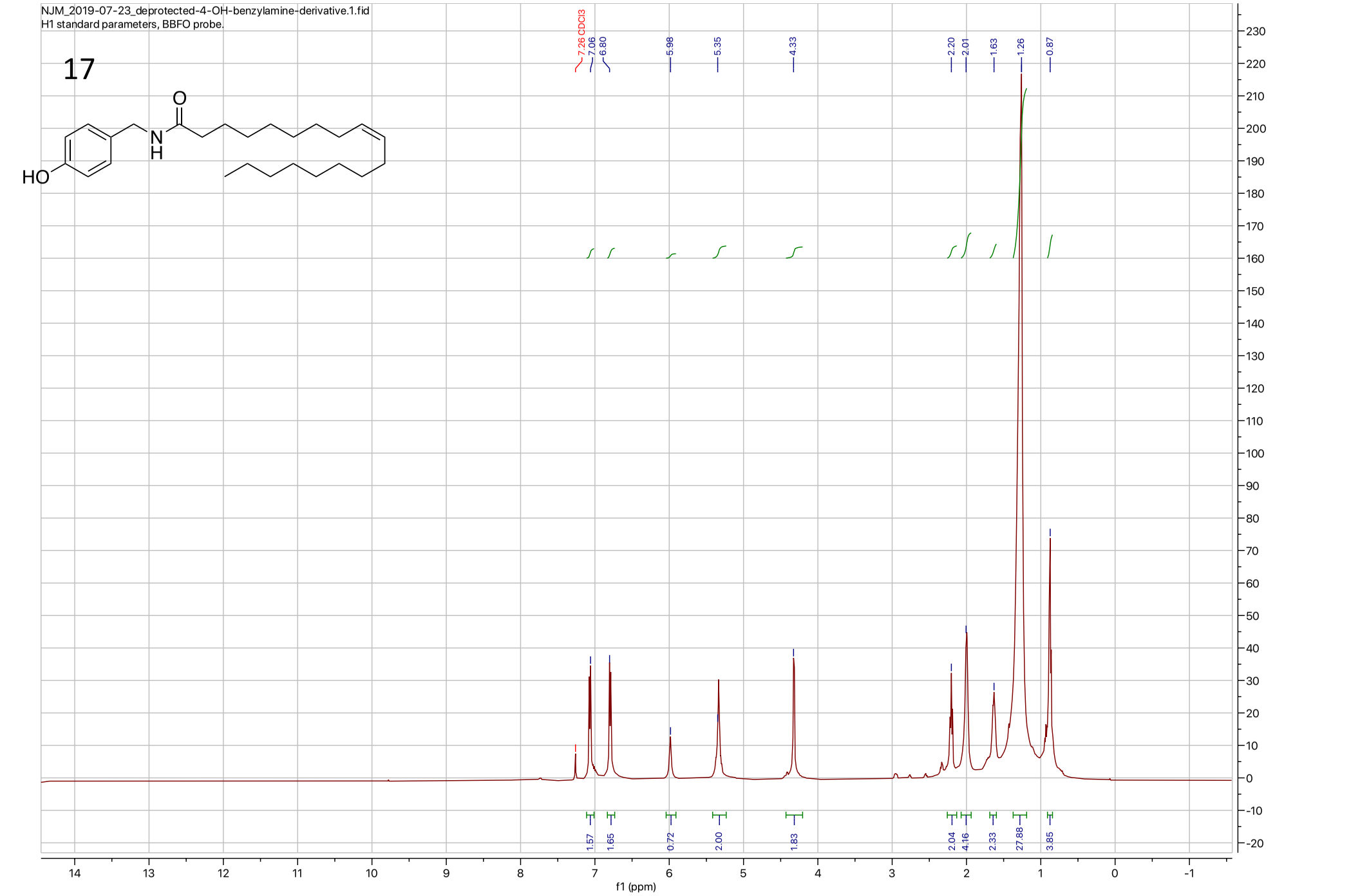
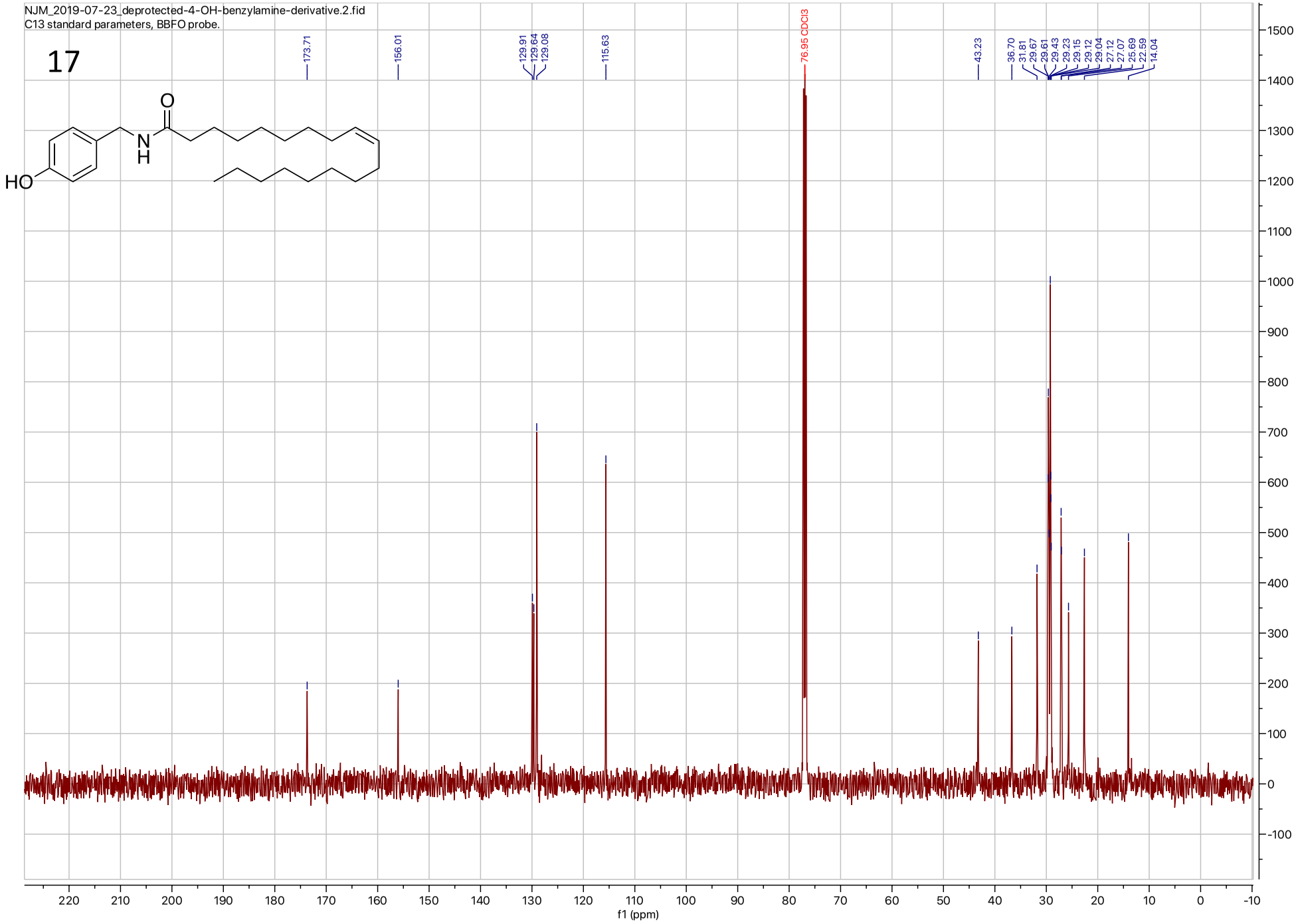
DRX 500

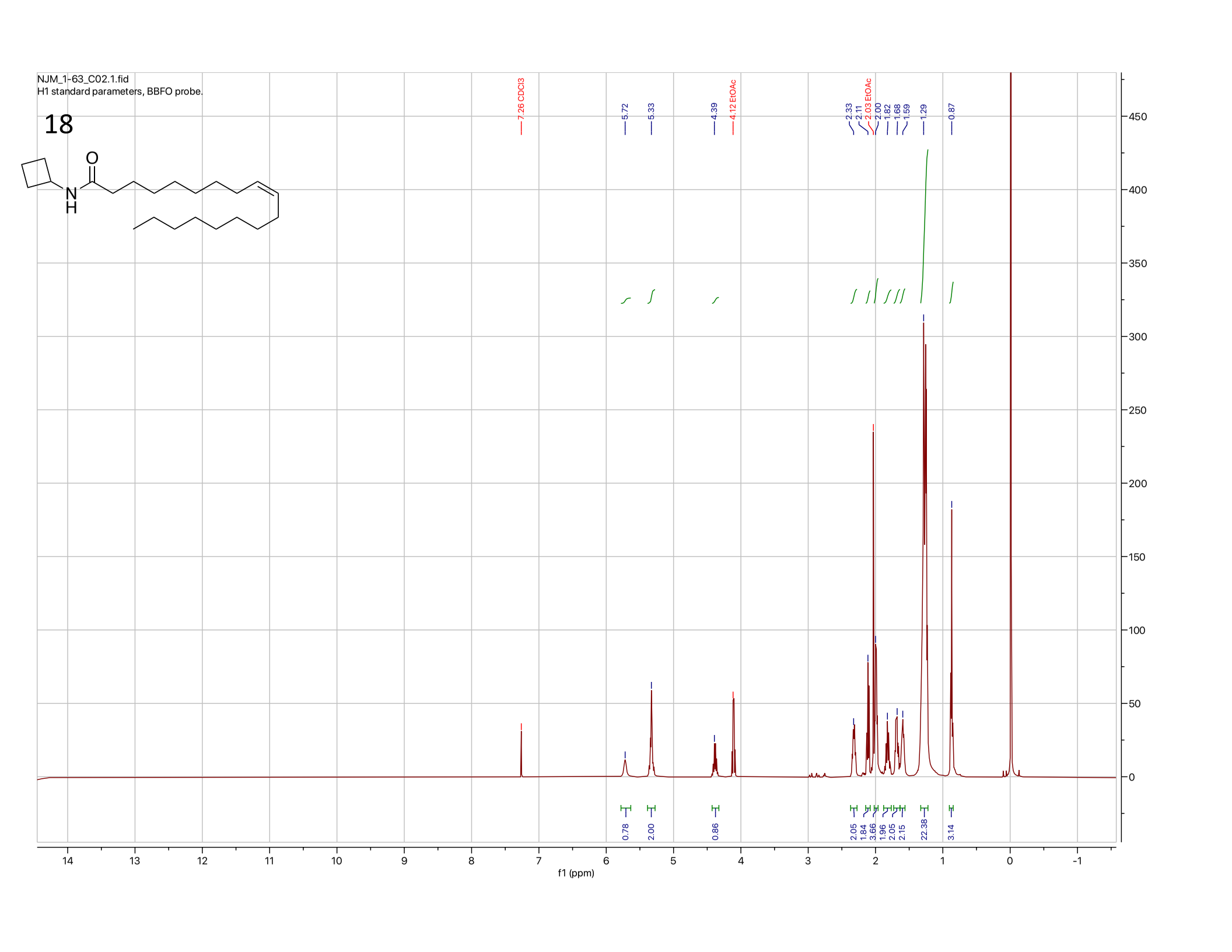


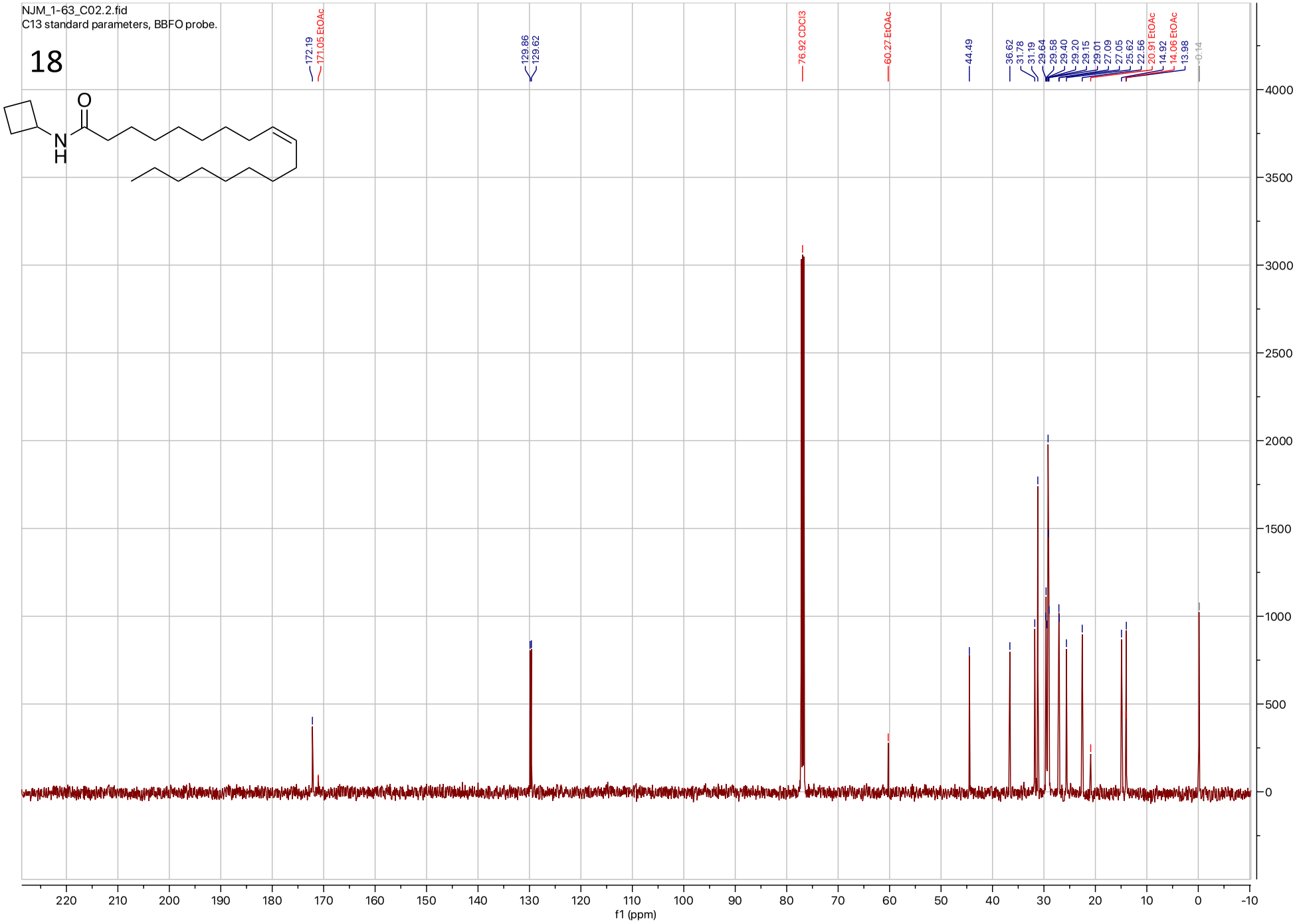

halder_sh-5-12.100.fid
H1 standard parameters, BBFO probe.
16
O
N
H
7.26 7.24 7.23 7.22 7.21 7.21 7.10 7.09 7.09 7.08 7.06
5.70 5.38 5.36 5.35 5.34 5.34 5.33
4.41 4.40
2.34 2.22 2.20 2.19 2.01 2.00 1.67 1.65 1.64 1.32 1.30 1.27 1.26 0.89 0.88 0.86
0.81 2.56 0.85 1.92 1.83 2.78 1.85 3.77 2.92 20.76 3.08
f1 (ppm)

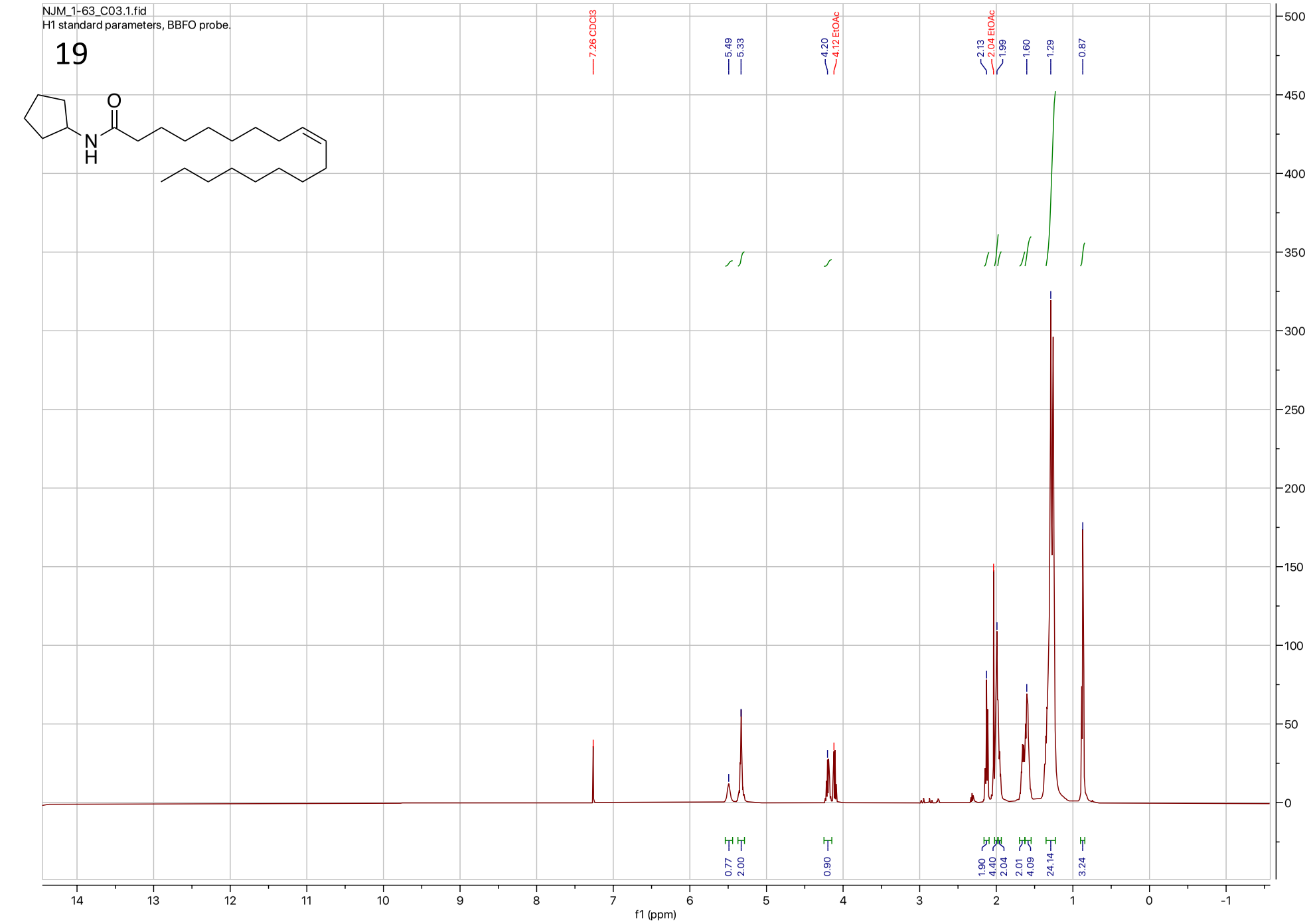

halder_sh-5-12.200.fid
B11
16
O
N
H
172.84
138.34
138.19
129.90
129.65
128.52
128.15
124.76
77.18 CDCl3
76.93 CDCl3
76.67 CDCl3
43.48
36.73
31.81
29.67
29.60
29.43
29.22
29.17
29.05
27.12
27.07
25.67
22.59
21.27
14.03
f1 (ppm)

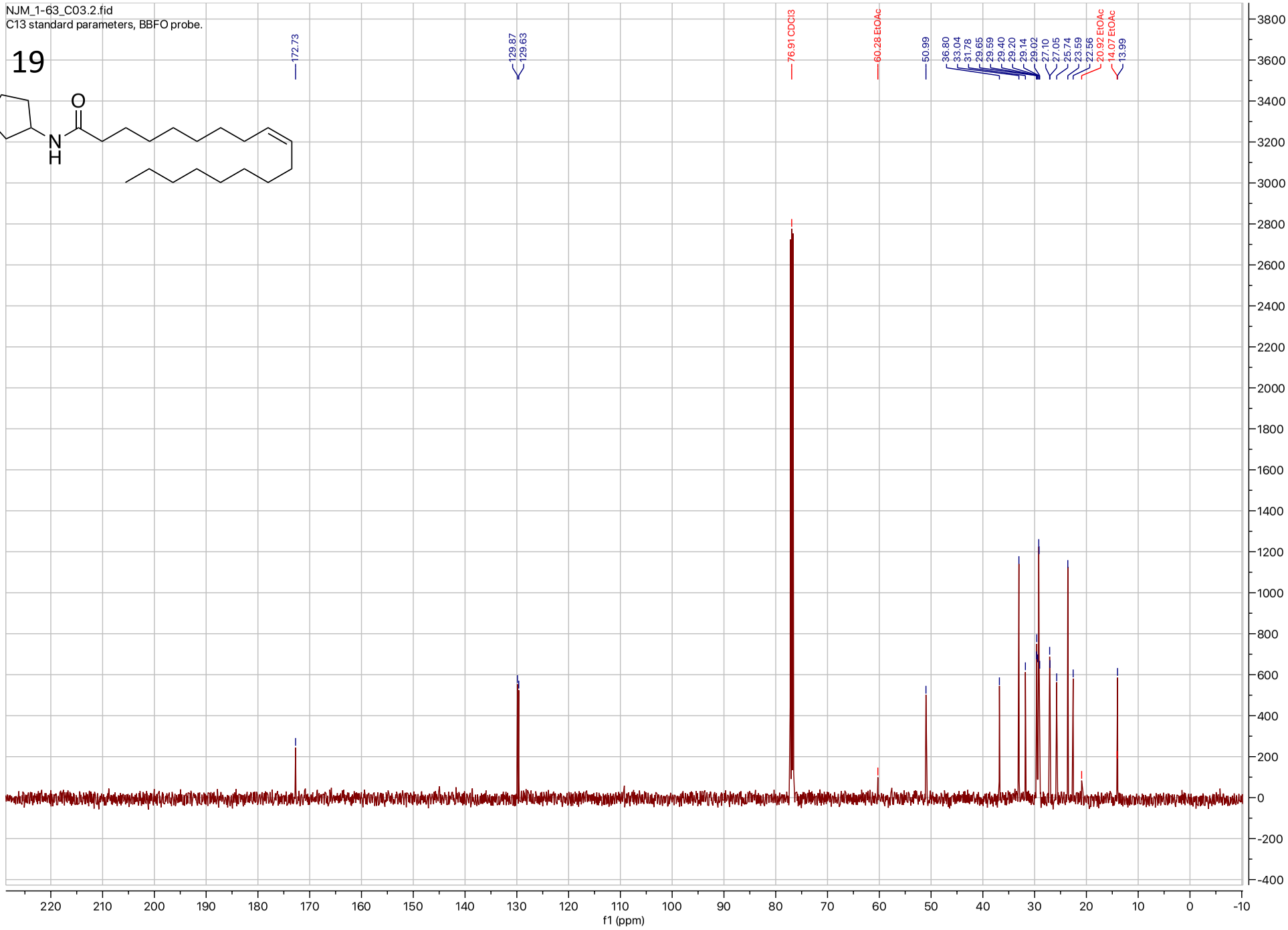

NJM_2019-07-23_deprotected-4-OH-benzylamine-derivative.1.fid
H1 standard parameters, BBFO probe.
17
HO
N
H
O
7.26 CDCl3
7.06
6.80
5.98
5.35
4.33
2.20
2.01
1.63
1.26
0.87
1.57
1.65
0.72
2.00
1.83
2.04
4.16
2.33
27.88
3.85
f1 (ppm)


NJM_2019-07-23_deprotected-4-OH-benzylamine-derivative.2.fid
C13 standard parameters, BBFO probe.
17
HO
N
H
O
173.71
156.01
129.91
129.64
129.08
115.63
76.95 CDCl3
43.23
36.70
31.81
29.67
29.61
29.43
29.23
29.15
29.12
29.04
27.12
27.07
25.69
22.59
14.04
f1 (ppm)


NJM_1-63_C02.1.fid
H1 standard parameters, BBFO probe.
18
O
N
H
7.26 CDCl3
5.72
5.33
4.39
4.12 EtOAc
2.33
2.11
2.03 EtOAc
2.00
1.82
1.68
1.59
1.29
0.87
0.78
2.00
0.86
2.05
1.84
3.66
1.96
2.05
2.15
22.38
3.14
f1 (ppm)

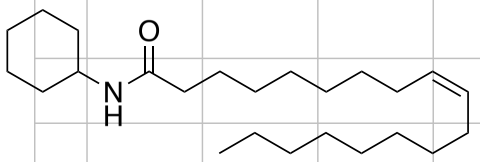

NJM_1-63_C02.2.fid
C13 standard parameters, BBFO probe.
18
O
N
H
172.19
171.05 EtOAc
129.86
129.62
76.92 CDCl3
60.27 EtOAc
44.49
36.62
31.78
31.19
29.64
29.58
29.40
29.20
29.15
29.01
27.09
27.05
25.62
22.56
20.91 EtOAc
14.92
14.06 EtOAc
13.98
-0.14
4000
3500
3000
2500
2000
1500
1000
500
0
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

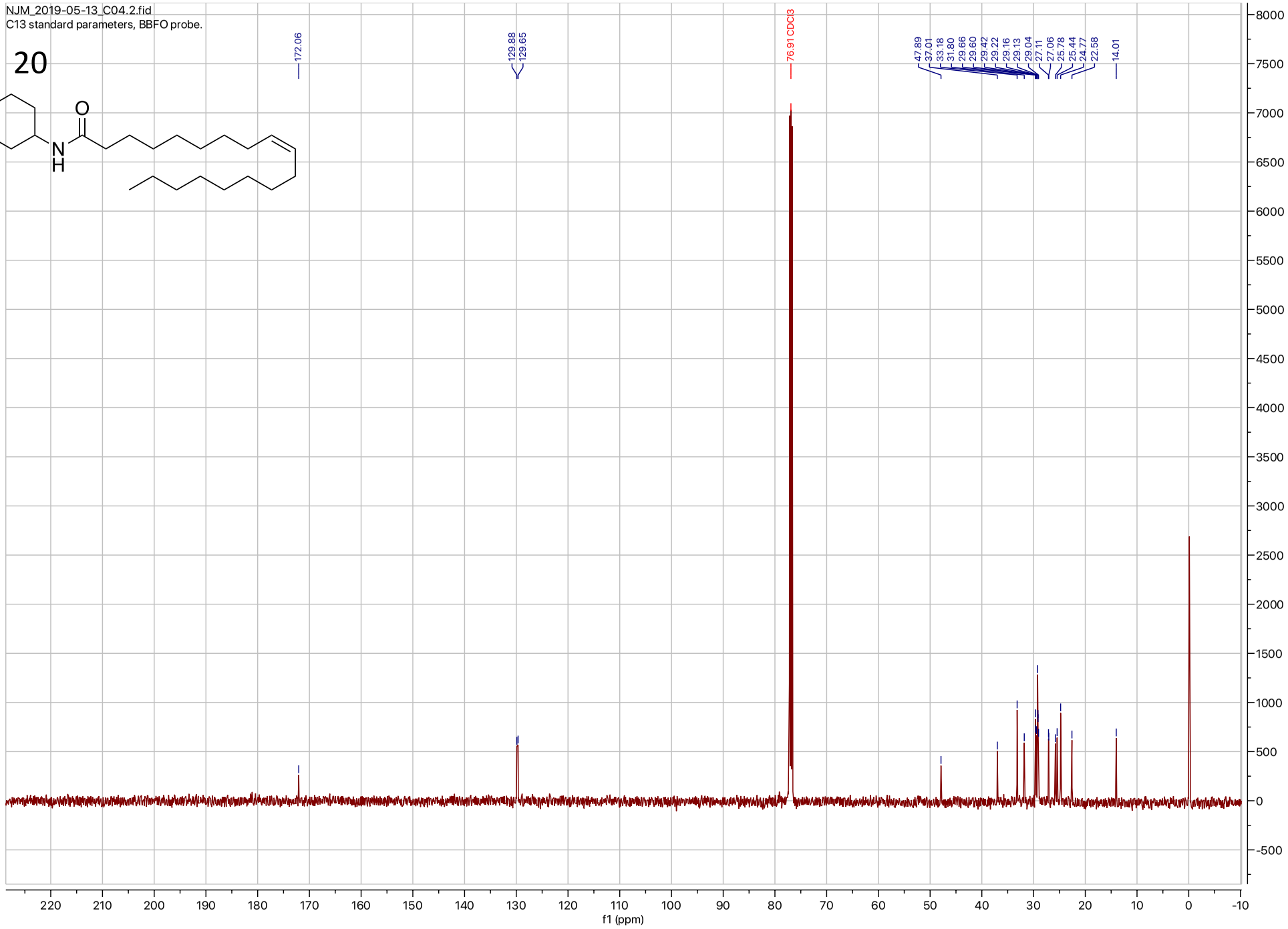

NJM_1-63_C03.1.fid
H1 standard parameters, BBFO probe.
19
O
N
H
7.26 CDCl3
5.49
5.33
4.20
4.12 EtOAc
2.13
2.04 EtOAc
1.99
1.60
1.29
0.87
0.77
2.00
0.90
1.90
4.40
2.04
2.01
4.09
24.14
3.24
f1 (ppm)

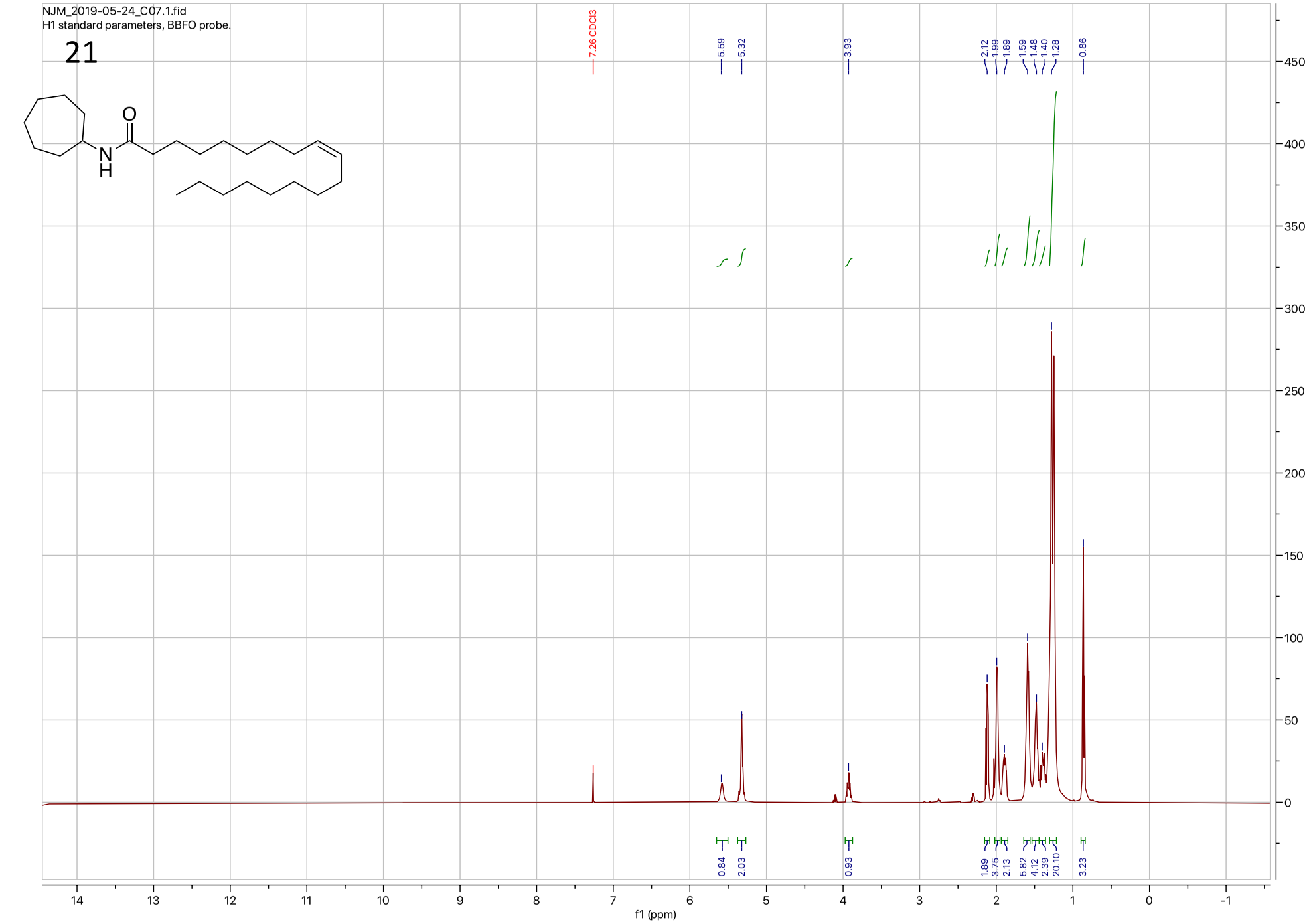

NJM_1-63_C03.2.fid
C13 standard parameters, BBFO probe.
19
O
N
H
172.73
129.87
129.63
76.91 CDCl3
60.28 EtOAc
50.99
36.80
33.04
31.78
29.65
29.59
29.40
29.20
29.14
29.02
27.10
27.05
25.74
23.59
22.56
20.92 EtOAc
14.07 EtOAc
13.99
f1 (ppm)

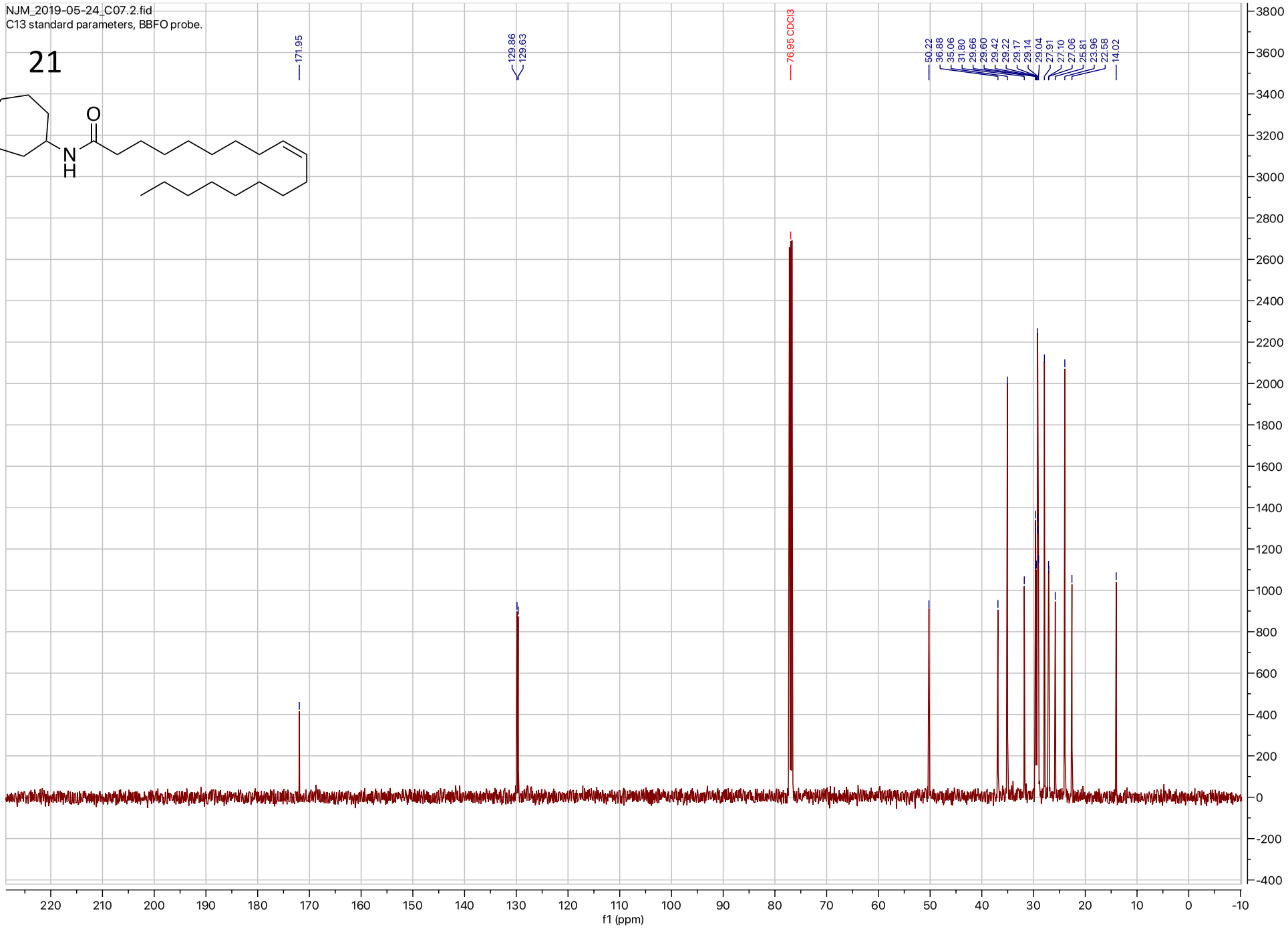
NJM_1-59_DJT_2-74-2_2019-05-13.1.fid
H1 standard parameters, BBFO probe.

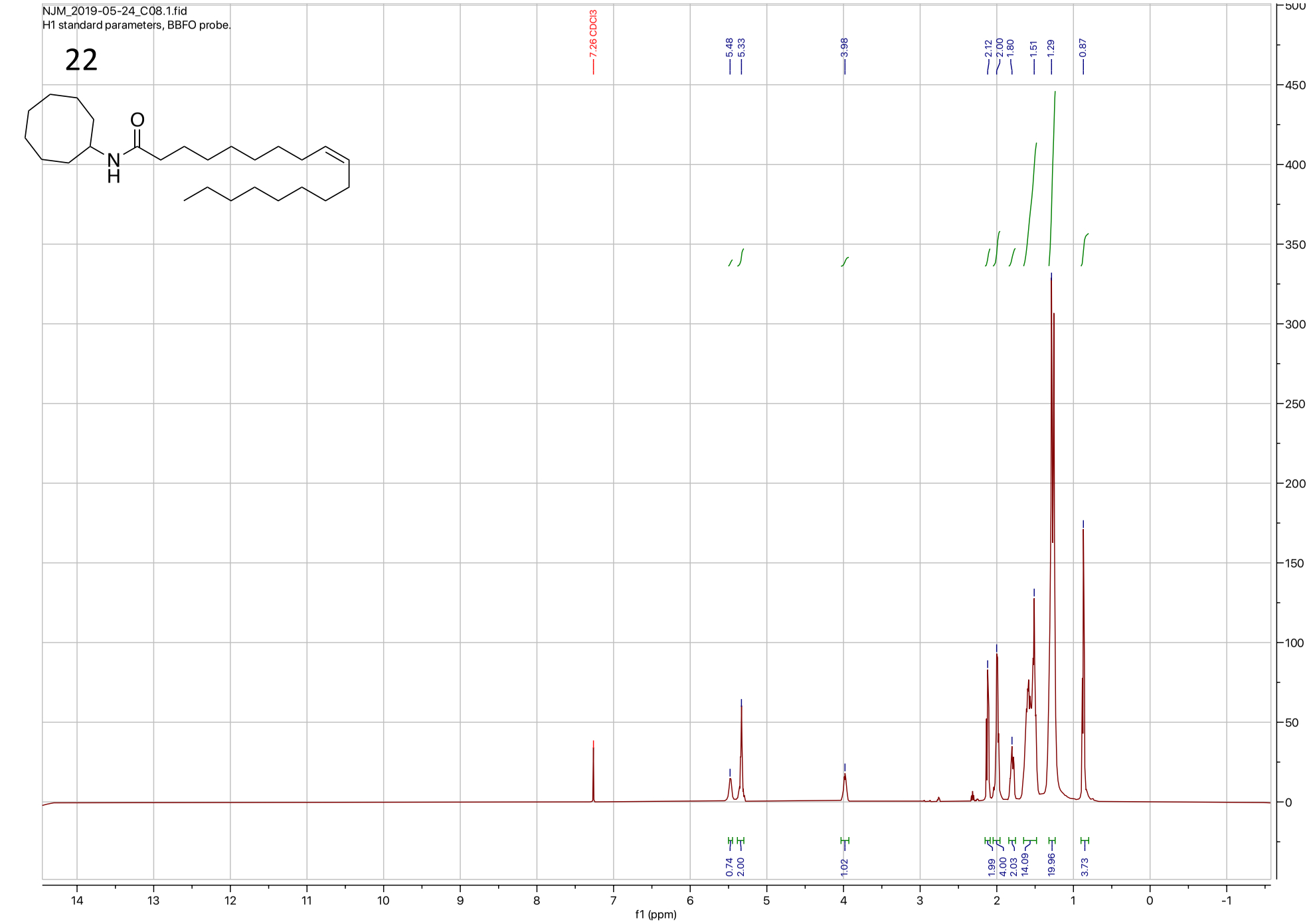
20

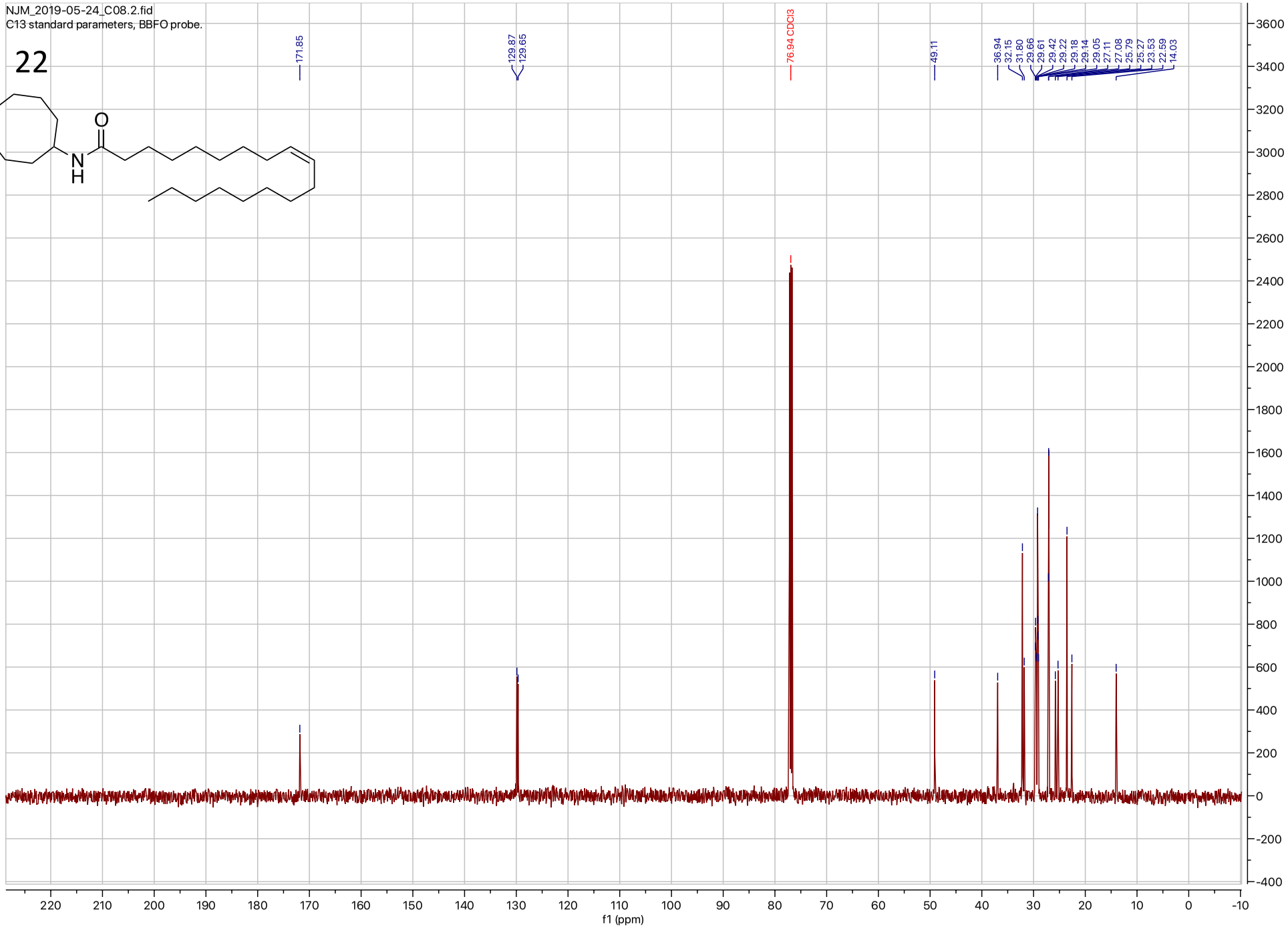


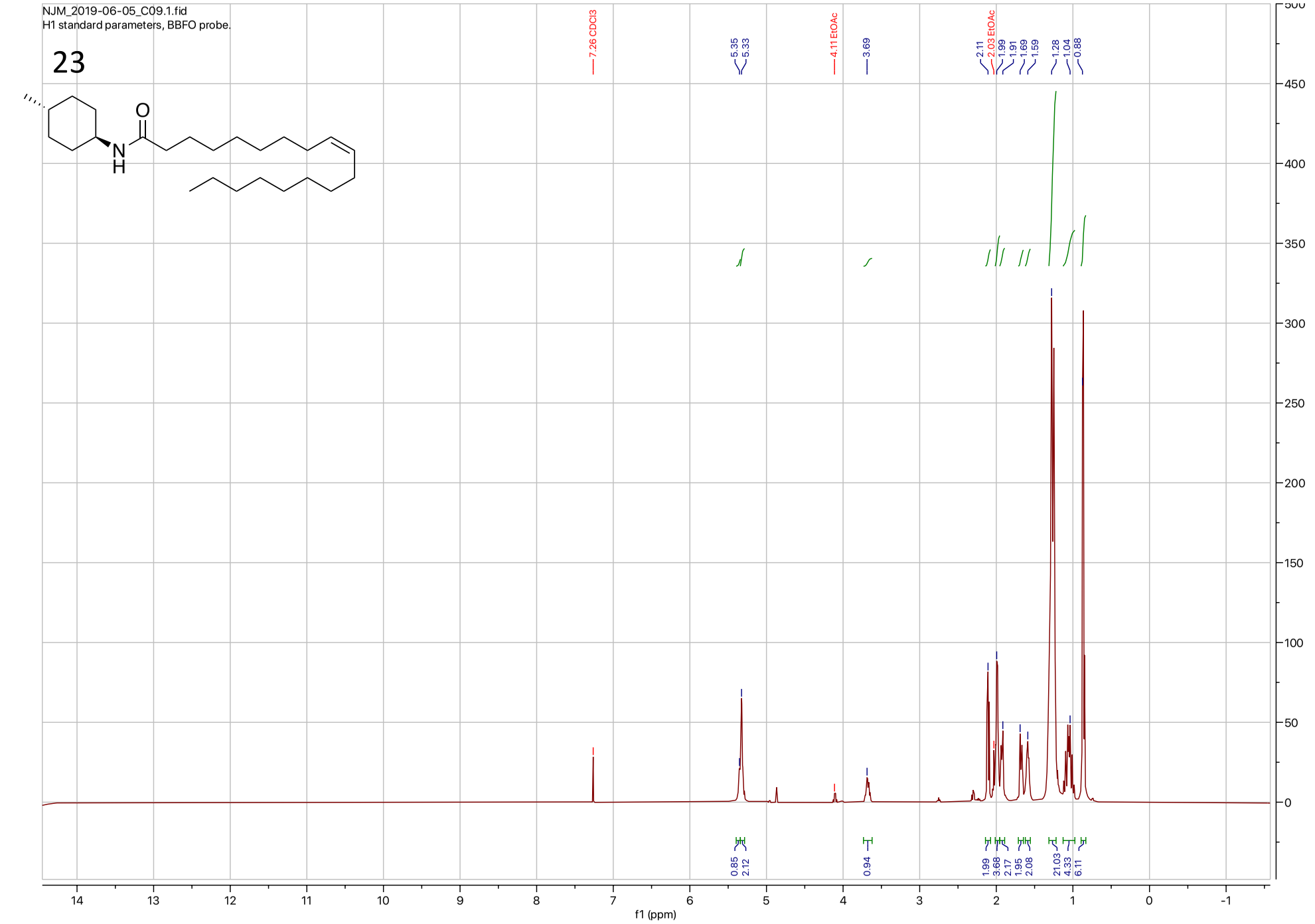

NJM_2019-05-13_C04.2.fid
C13 standard parameters, BBFO probe.
20
O
N
H
172.06
129.88
129.65
76.91 CDCl3
47.89
37.01
33.18
31.80
29.66
29.60
29.42
29.22
29.16
29.13
29.04
27.11
27.06
25.78
25.44
24.77
22.58
14.01
f1 (ppm)

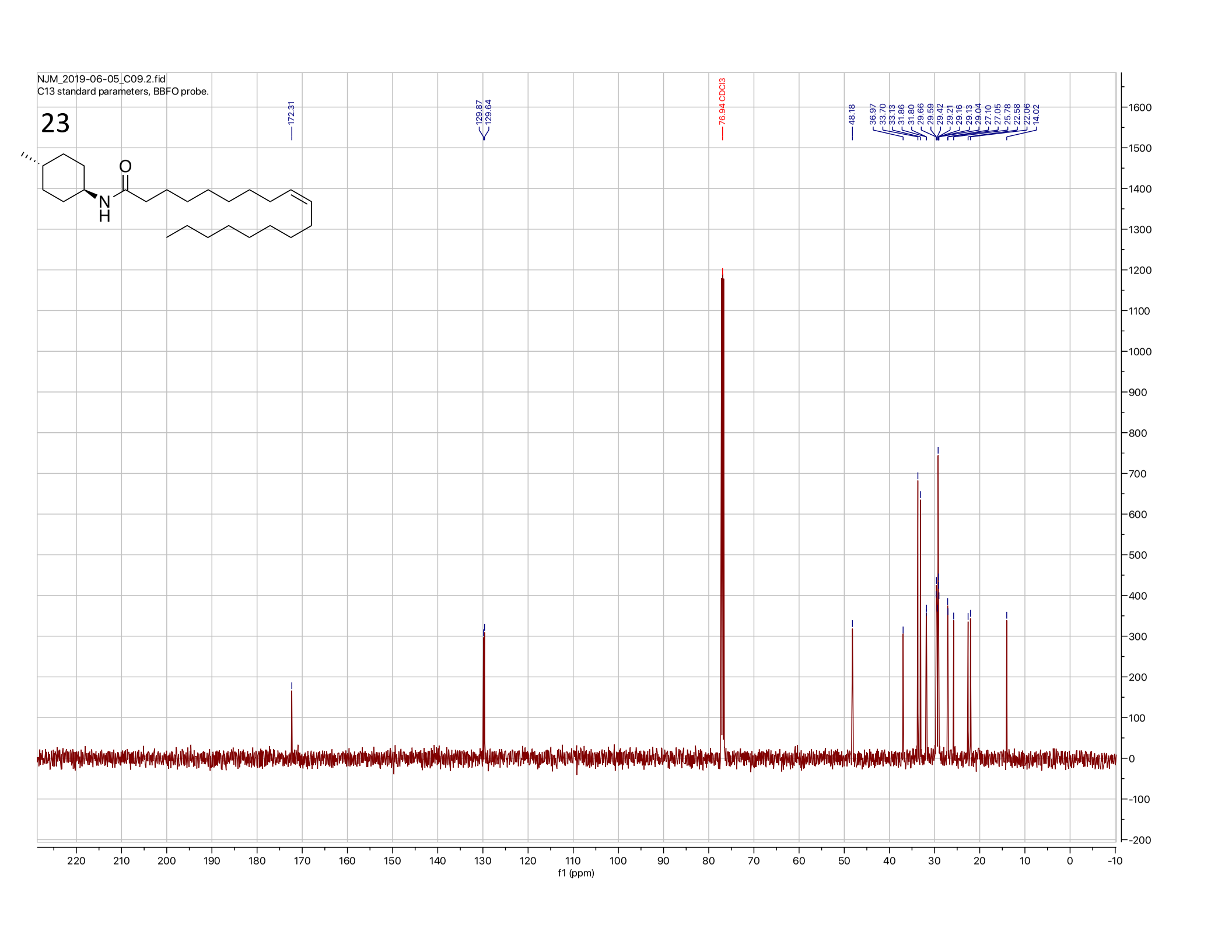

NJM_2019-05-24_C07.1.fid
H1 standard parameters, BBFO probe.
21
O
N
H
7.26 CDCl3
5.59
5.32
3.93
2.12
1.99
1.89
1.59
1.48
1.40
1.28
0.86
0.84
2.03
0.93
1.89
3.75
2.13
5.82
4.12
2.39
20.10
3.23
f1 (ppm)

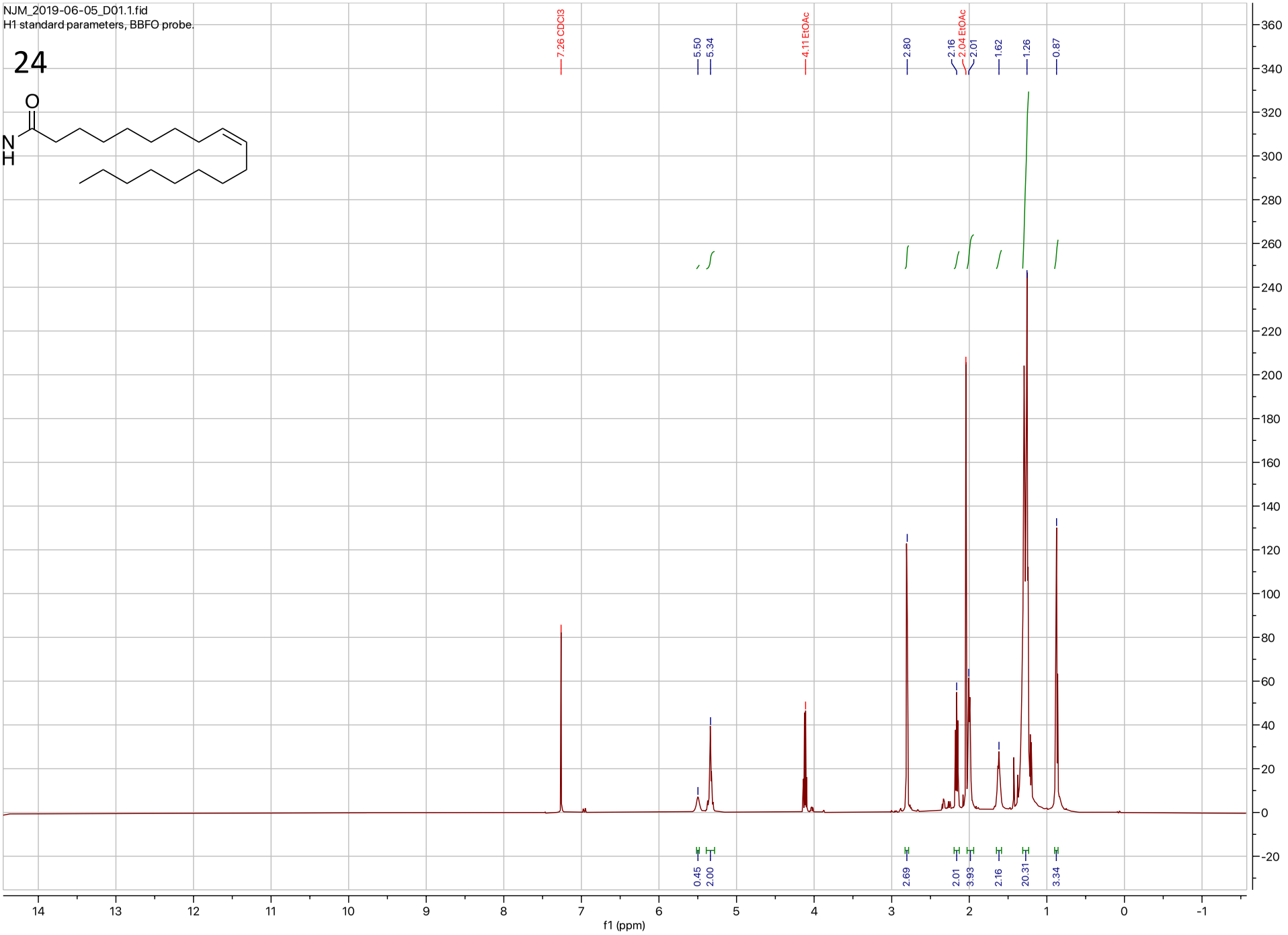

NJM_2019-05-24_C07.2.fid
C13 standard parameters, BBFO probe.
21
O
N
H
171.95
129.86
129.63
76.95 CDCl3
50.22
36.88
35.06
31.80
29.66
29.60
29.42
29.22
29.17
29.14
29.04
27.91
27.10
27.06
25.81
23.96
22.58
14.02
f1 (ppm)

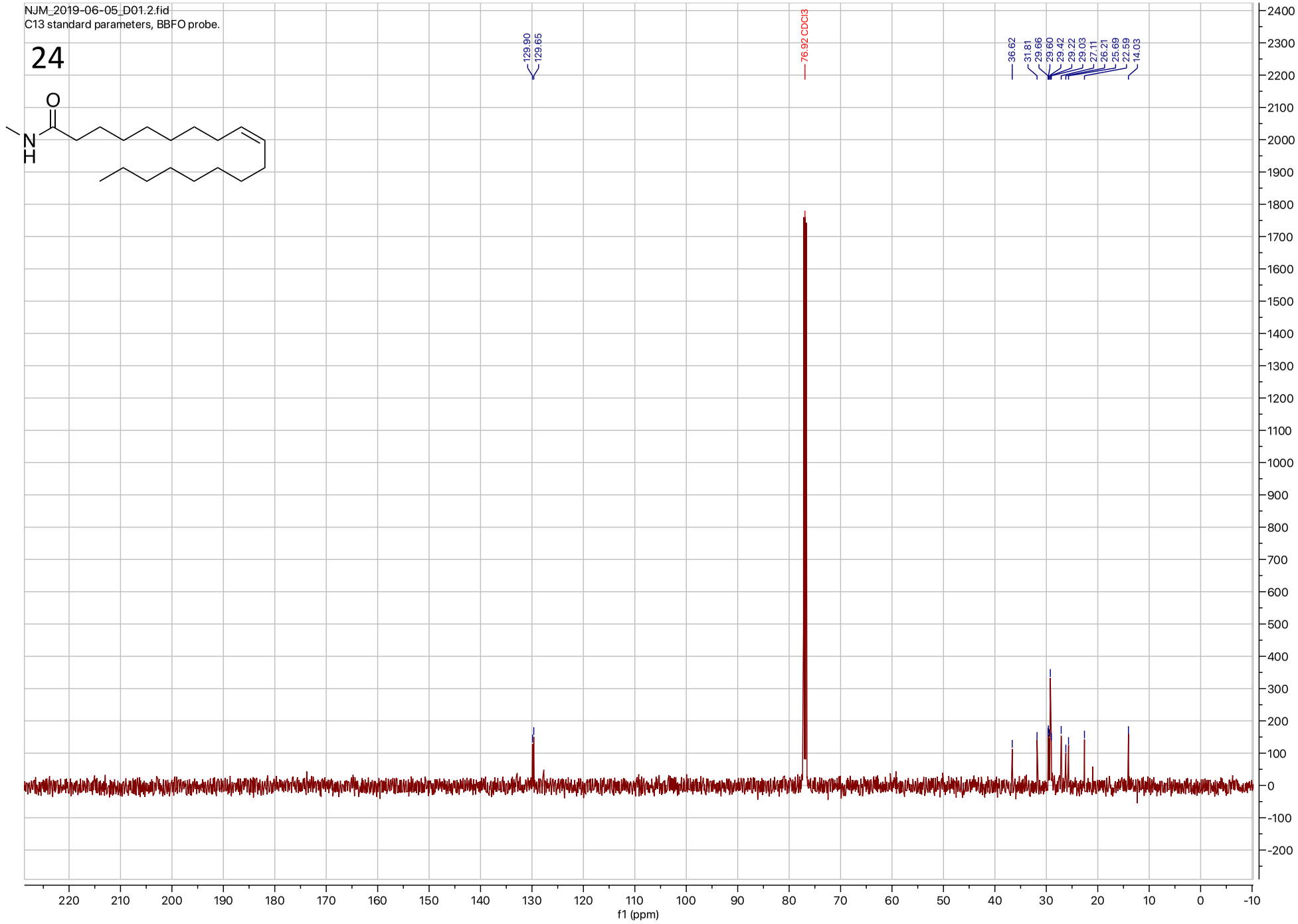

NJM_2019-05-24_C08.1.fid
H1 standard parameters, BBFO probe.
22
O
N
H
7.26 CDCl3
5.48
5.33
3.98
2.12
2.00
1.80
1.51
1.29
0.87
0.74
2.00
1.02
1.99
4.00
2.03
14.09
19.96
3.73
f1 (ppm)

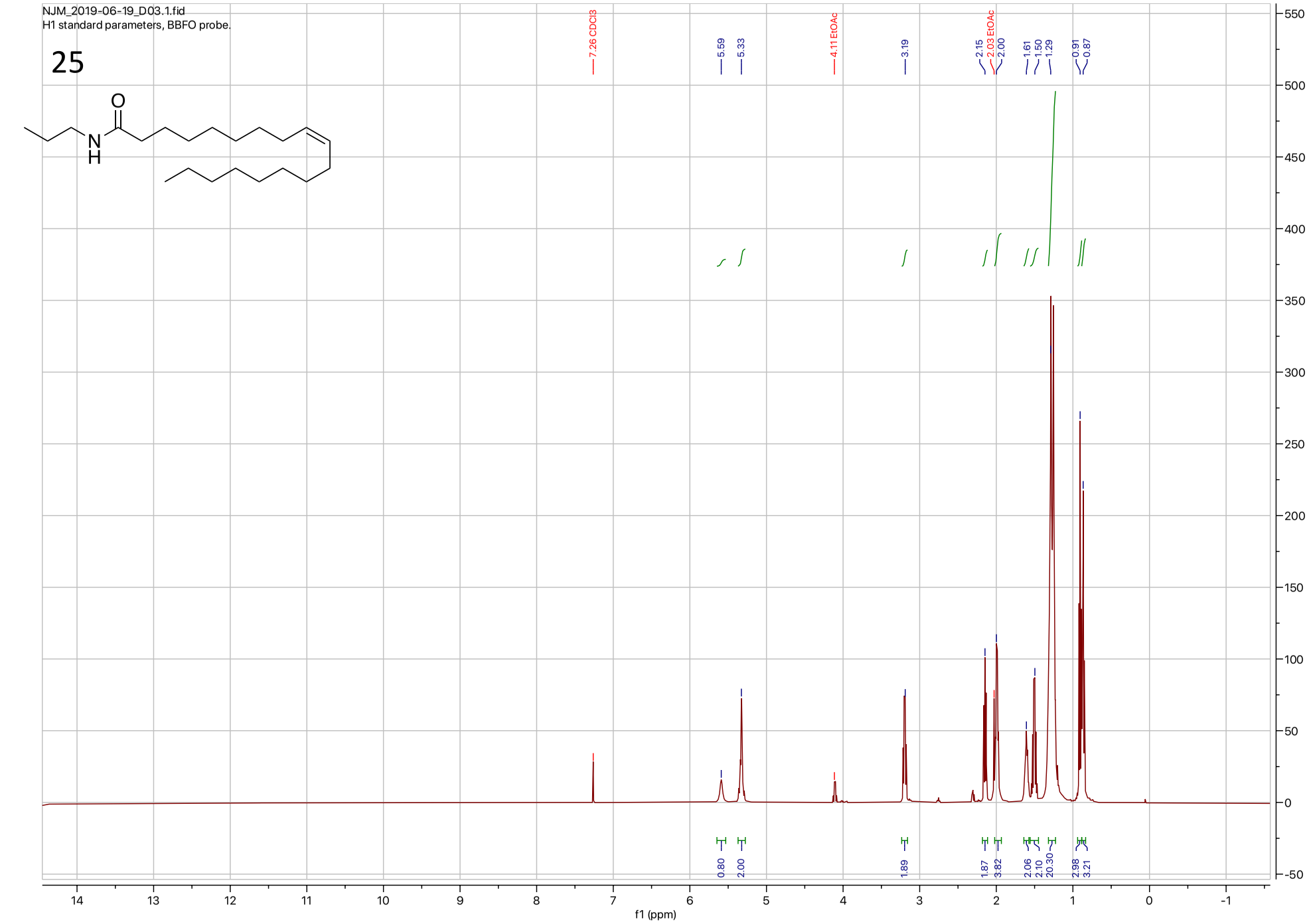

NJM_2019-05-24_C08.2.fid
C13 standard parameters, BBFO probe.
22
O
N
H
171.85
129.87
129.65
76.94 CDCl3
49.11
36.94
32.15
31.80
29.66
29.61
29.42
29.22
29.18
29.14
29.05
27.11
27.08
25.79
25.27
23.53
22.59
14.03
f1 (ppm)

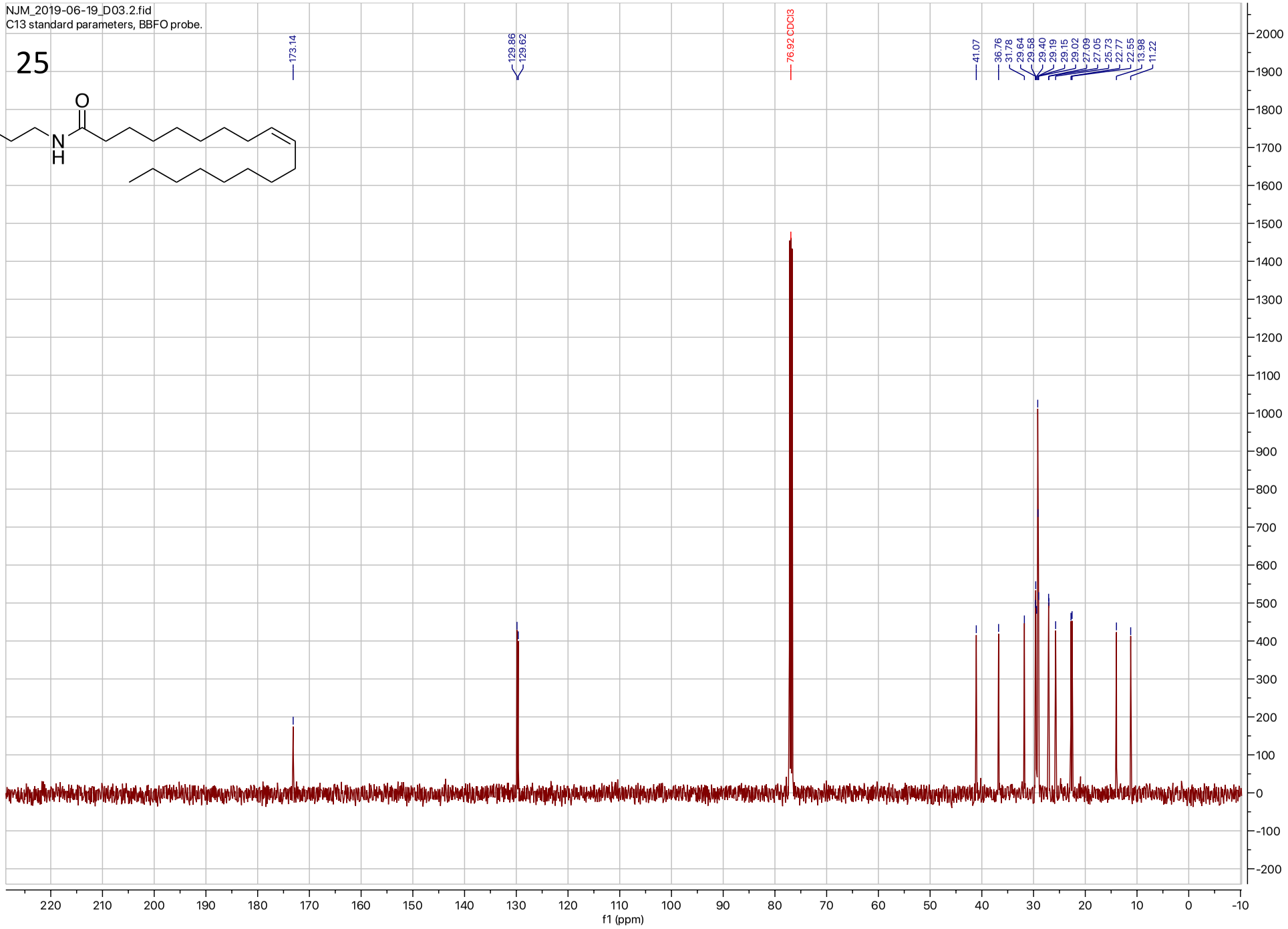

NJM_2019-06-05_C09.1.fid
H1 standard parameters, BBFO probe.
23
7.26 CDCl3
5.35
5.33
4.11 EtOAc
3.69
2.11
2.03 EtOAc
1.99
1.91
1.69
1.59
1.28
1.04
0.88
0.85
2.12
0.94
1.99
3.68
2.17
1.95
2.08
21.03
4.33
6.11
f1 (ppm)

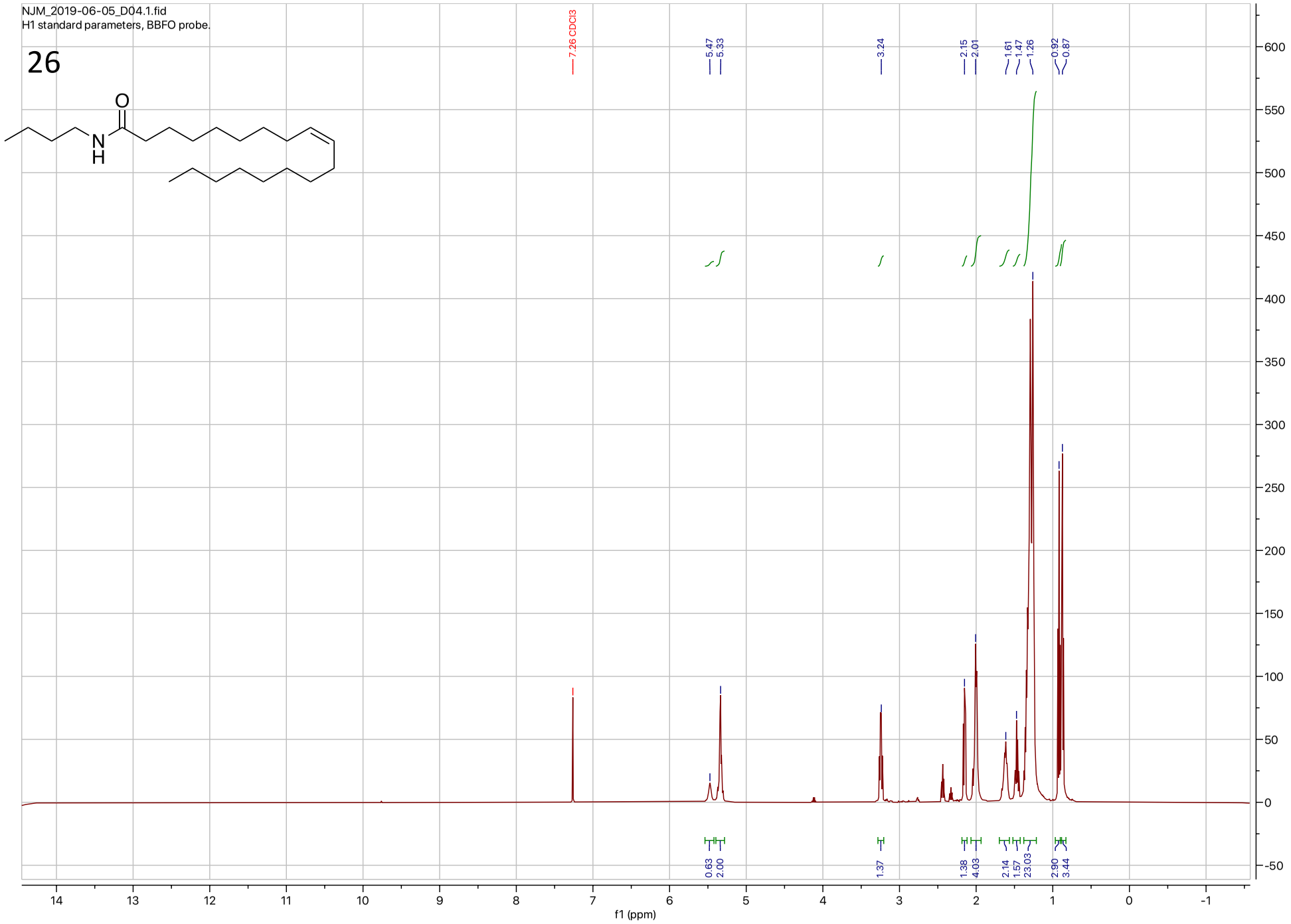

NJM_2019-06-05_C09.2.fid
C13 standard parameters, BBFO probe.
23
O
N
H
172.31
129.87
129.64
76.94 CDCl3
48.18
36.97
33.70
33.13
31.86
31.80
29.66
29.59
29.42
29.21
29.16
29.13
29.04
27.10
27.05
25.78
22.58
22.06
14.02
f1 (ppm)

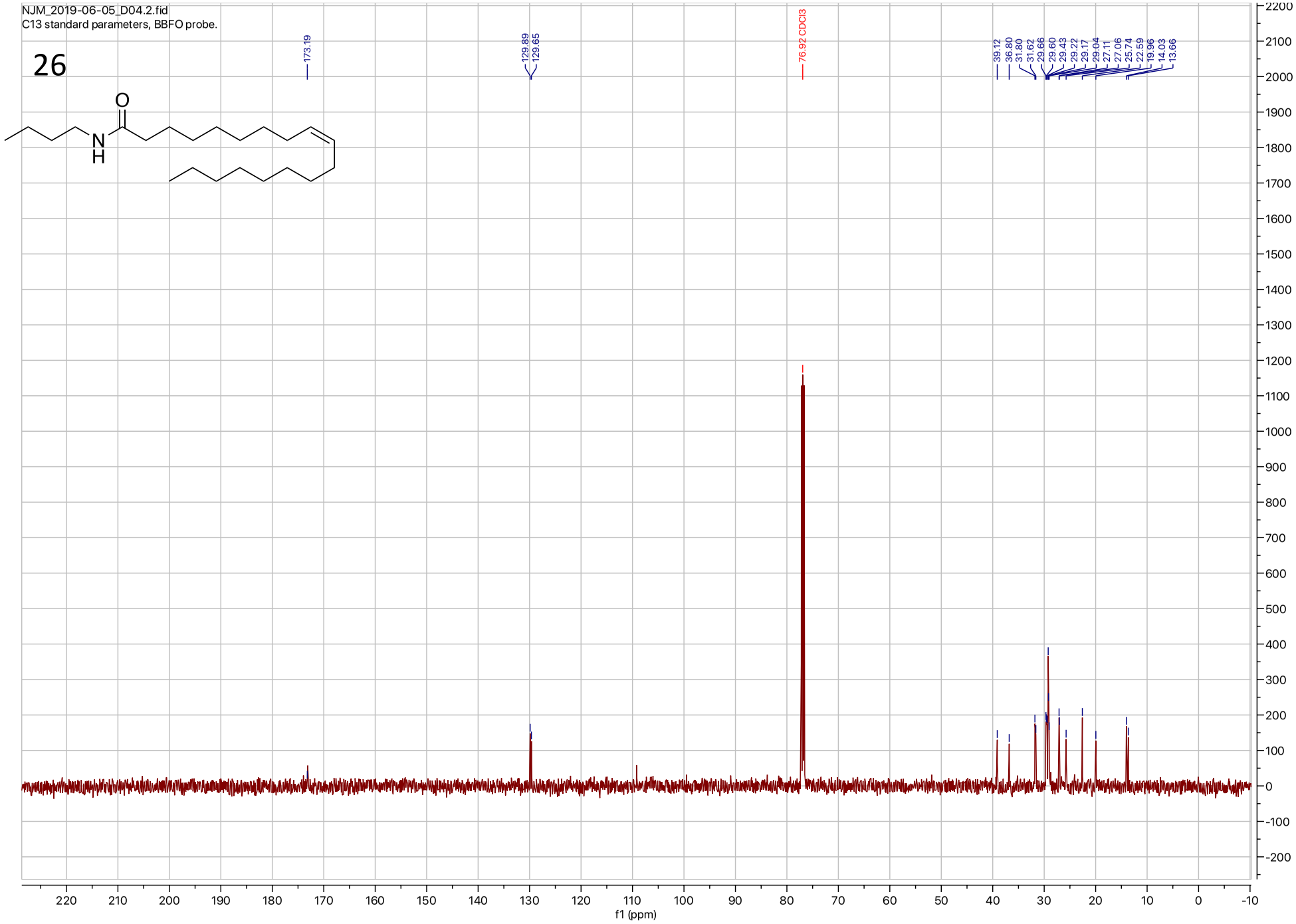

NJM_2019-06-05_D01.1.fid
H1 standard parameters, BBFO probe.
24
O
N
H
7.26 CDCl3
5.50
5.34
4.11 EtOAc
2.80
2.16
2.04 EtOAc
2.01
1.62
1.26
0.87
0.45
2.00
2.69
2.01
3.93
2.16
20.31
3.34
f1 (ppm)

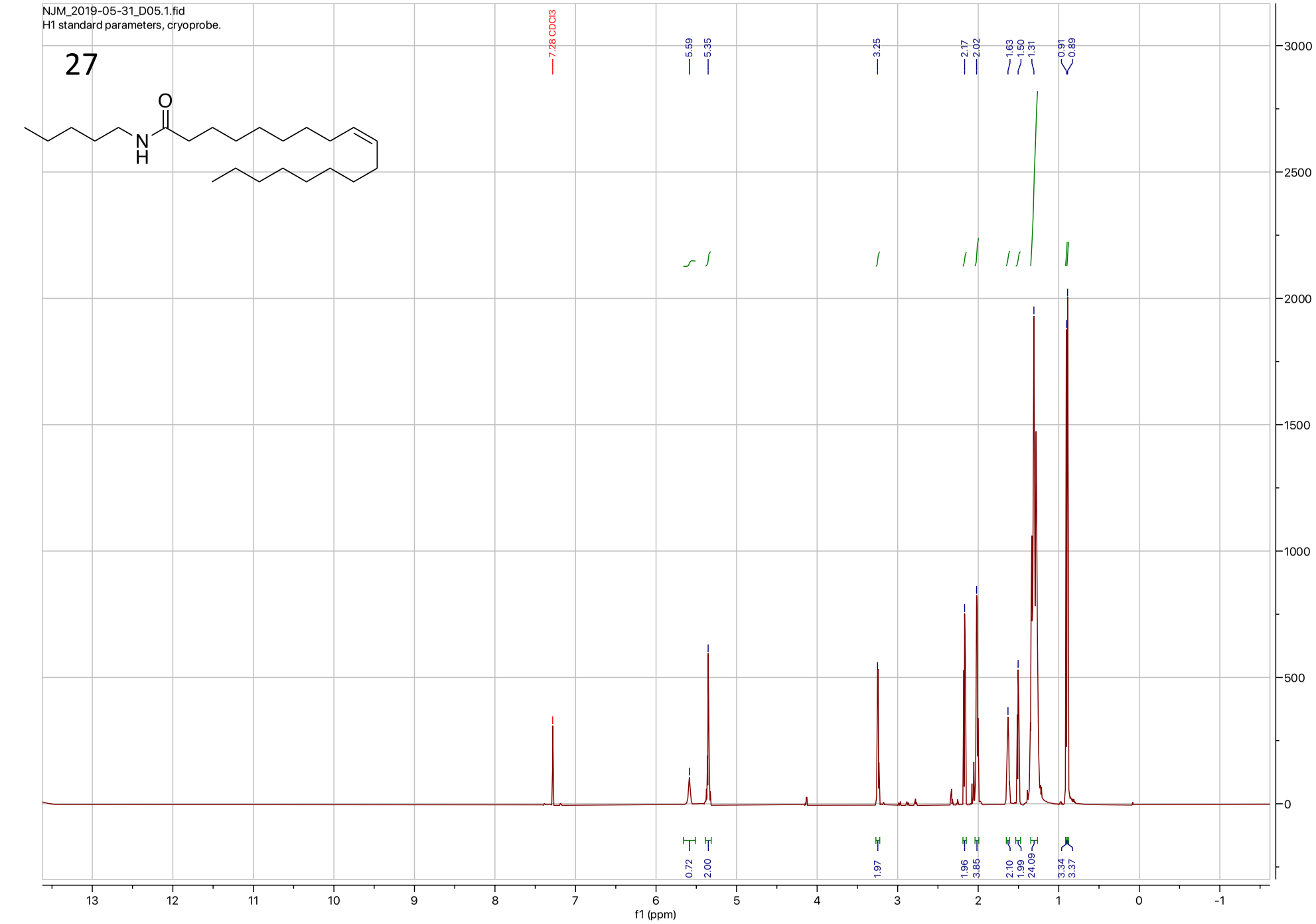

NJM_2019-06-05_D01.2.fid
C13 standard parameters, BBFO probe.
24
O
N
H
129.90
129.65
76.92 CDCl3
36.62
31.81
29.66
29.60
29.42
29.22
29.03
27.11
26.21
25.69
22.59
14.03
f1 (ppm)

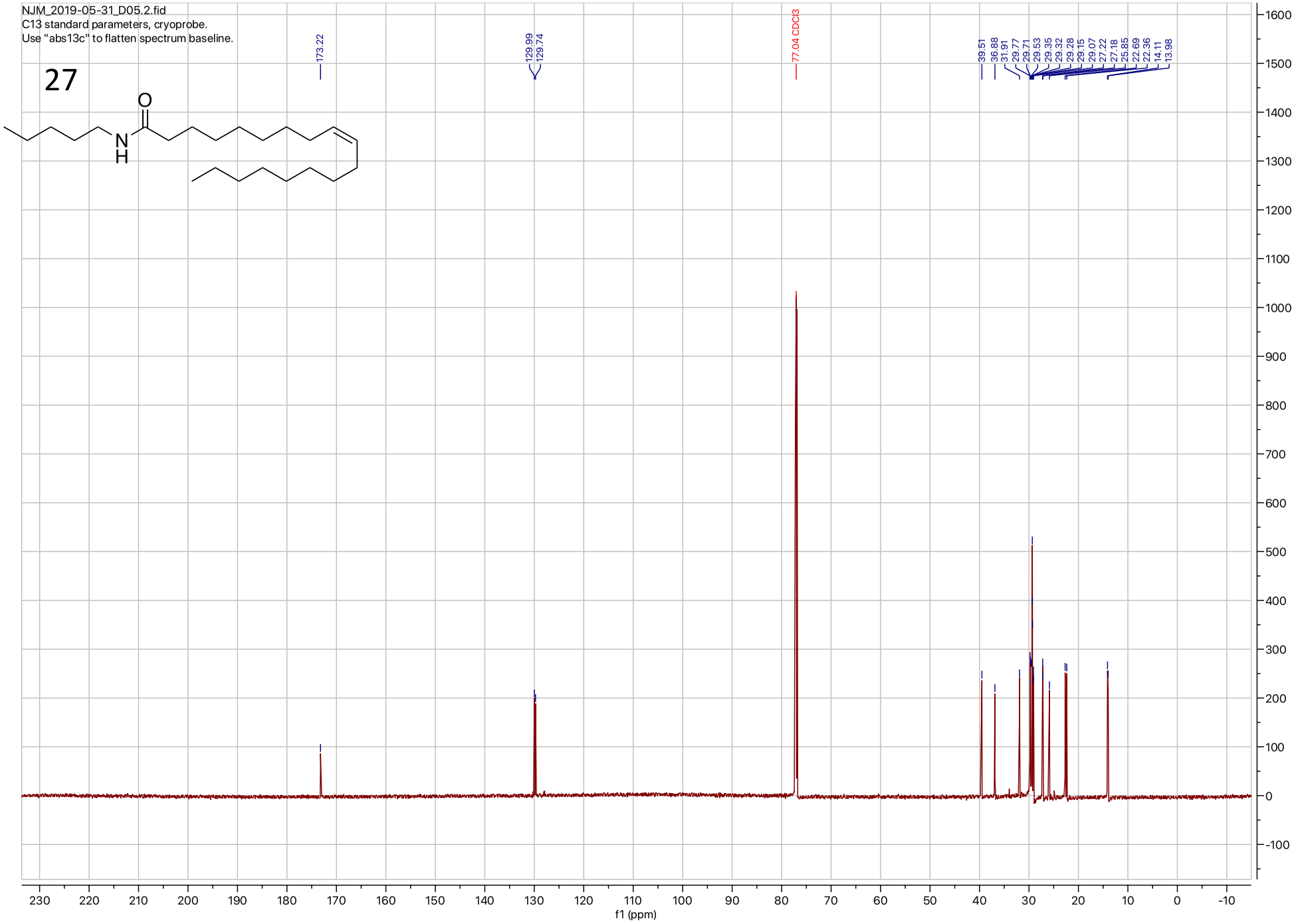

NJM_2019-06-19_D03.1.fid
H1 standard parameters, BBFO probe.
25
O
N
H
7.26 CDCl3
5.59
5.33
4.11 EtOAc
3.19
2.15
2.03 EtOAc
2.00
1.61
1.50
1.29
0.91
0.87
0.80
2.00
1.89
1.87
3.82
2.06
2.10
20.30
2.98
3.21
f1 (ppm)

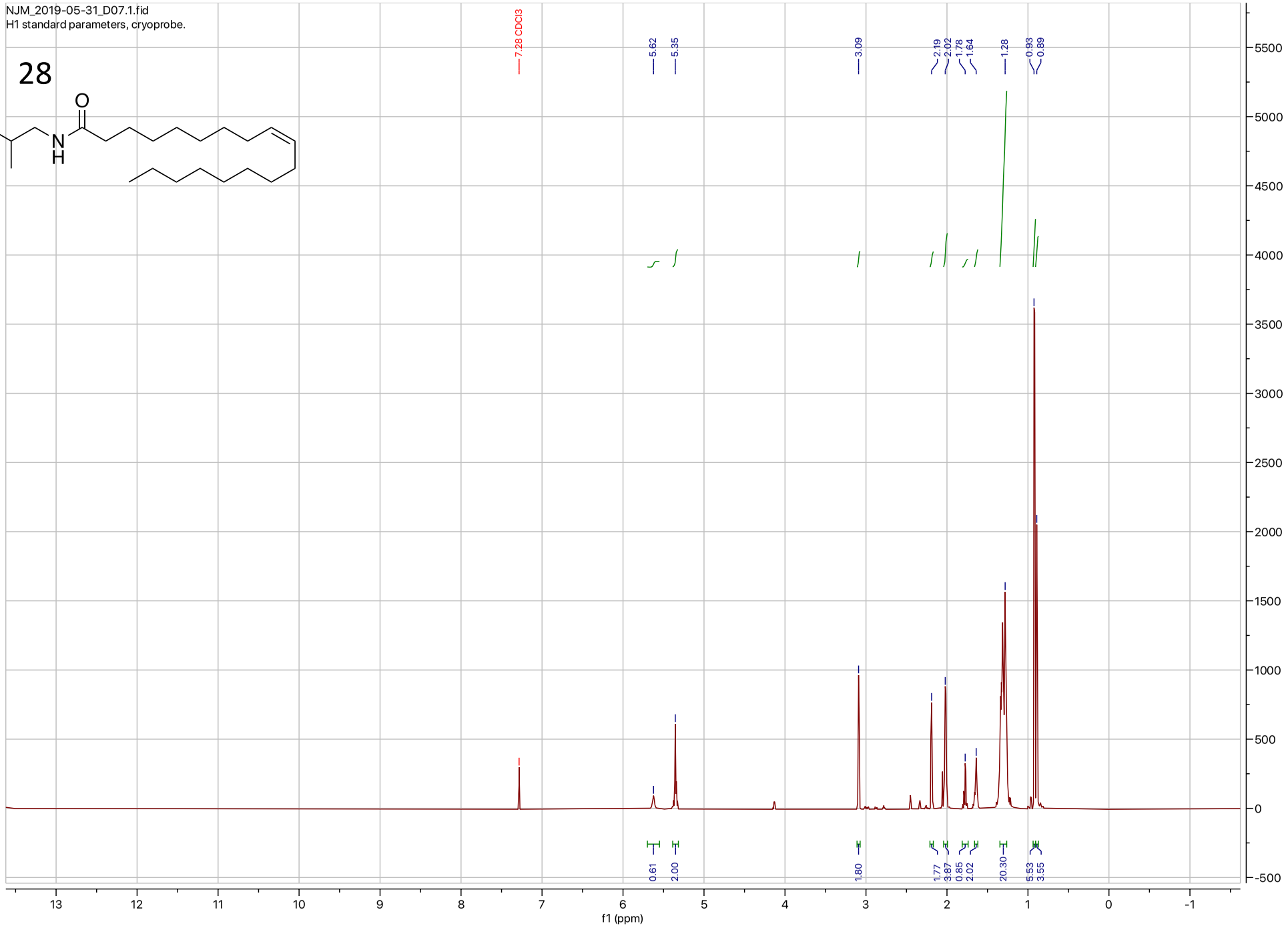

NJM_2019-06-19_D03.2.fid
C13 standard parameters, BBFO probe.
25
O
N
H
173.14
129.86
129.62
76.92 CDCl3
41.07
36.76
31.78
29.64
29.58
29.40
29.19
29.15
29.02
27.09
27.05
25.73
22.77
22.55
13.98
11.22
f1 (ppm)

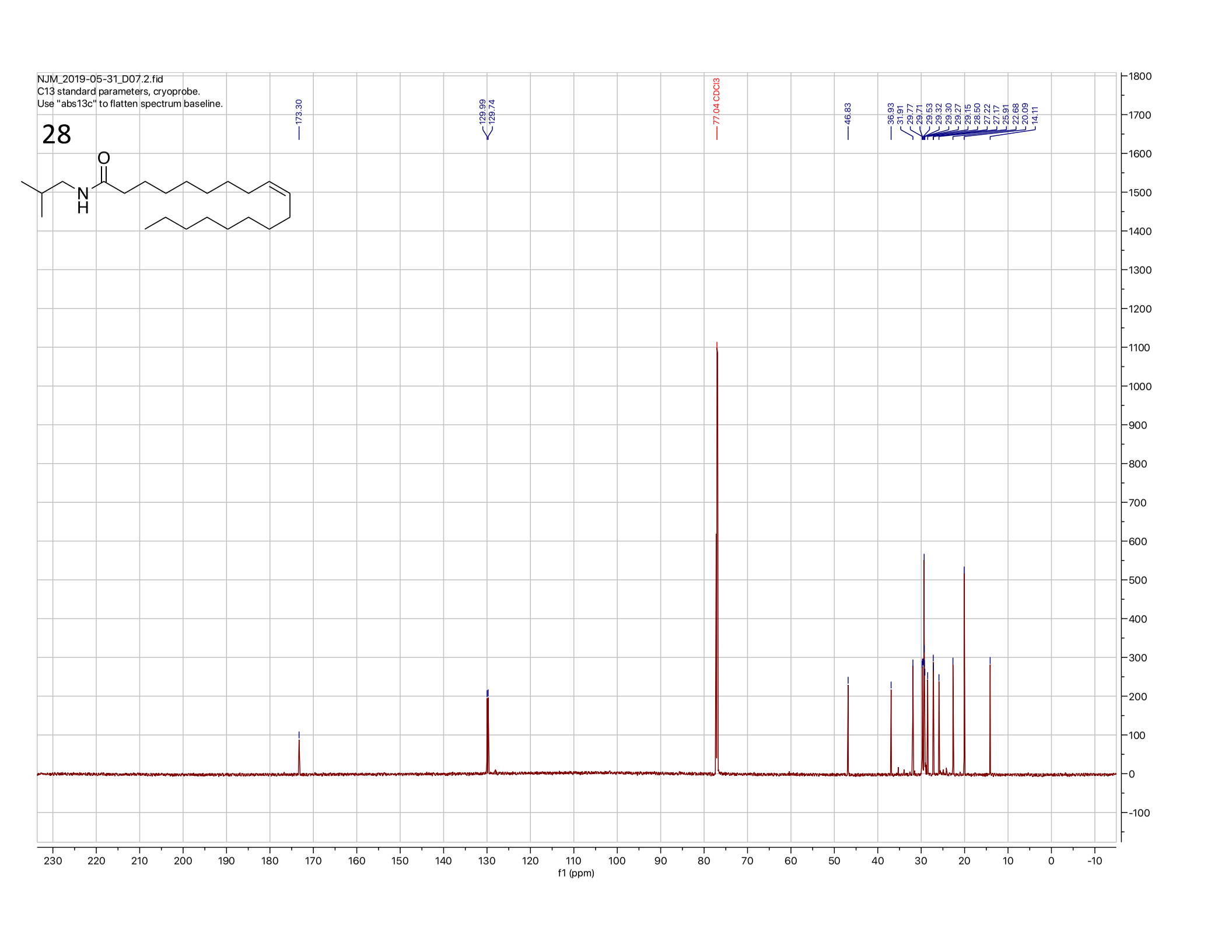

NJM_2019-06-05_D04.1.fid
H1 standard parameters, BBFO probe.
26
O
N
H
7.26 CDCl3
5.47
5.33
3.24
2.15
2.01
1.61
1.47
1.26
0.92
0.87
0.63
2.00
1.37
1.38
4.03
2.14
1.57
23.03
2.90
3.44
f1 (ppm)


NJM_2019-06-05_D04.2.fid
C13 standard parameters, BBFO probe.
26
O
N
H
173.19
129.89
129.65
76.92 CDCl3
39.12
36.80
31.80
31.62
29.66
29.60
29.43
29.22
29.17
29.04
27.11
27.06
25.74
22.59
19.96
14.03
13.66
f1 (ppm)


NJM_2019-05-31_D05.1.fid
H1 standard parameters, cryoprobe.
27
O
N
H
7.28 CDCl3
5.59
5.35
3.25
2.17
2.02
1.63
1.50
1.31
0.91
0.89
0.72
2.00
1.97
1.96
3.85
2.10
1.99
24.09
3.34
3.37
f1 (ppm)


NJM_2019-05-31_D05.2.fid
C13 standard parameters, cryoprobe.
Use "abs13c" to flatten spectrum baseline.
27
O
N
H
173.22
129.99
129.74
77.04 CDCl3
39.51
36.88
31.91
29.77
29.71
29.53
29.35
29.32
29.28
29.15
29.07
27.22
27.18
25.85
22.69
22.36
14.11
13.98
f1 (ppm)


NJM_2019-05-31_D07.1.fid
H1 standard parameters, cryoprobe.
28
O
N
H
7.28 CDCl3
5.62
5.35
3.09
2.19
2.02
1.78
1.64
1.28
0.93
0.89
0.61
2.00
1.80
1.77
3.87
0.85
2.02
20.30
5.53
3.55
f1 (ppm)


NJM_2019-05-31_D07.2.fid
C13 standard parameters, cryoprobe.
Use "abs13c" to flatten spectrum baseline.
28
O
N
H
173.30
129.99
129.74
77.04 CDCl3
46.83
36.93
31.91
29.77
29.71
29.53
29.32
29.30
29.27
29.15
28.50
27.22
27.17
25.91
22.68
20.09
14.11
f1 (ppm)