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Towards engineering of self-assembled nanostructures using non-ionic dendritic amphiphiles

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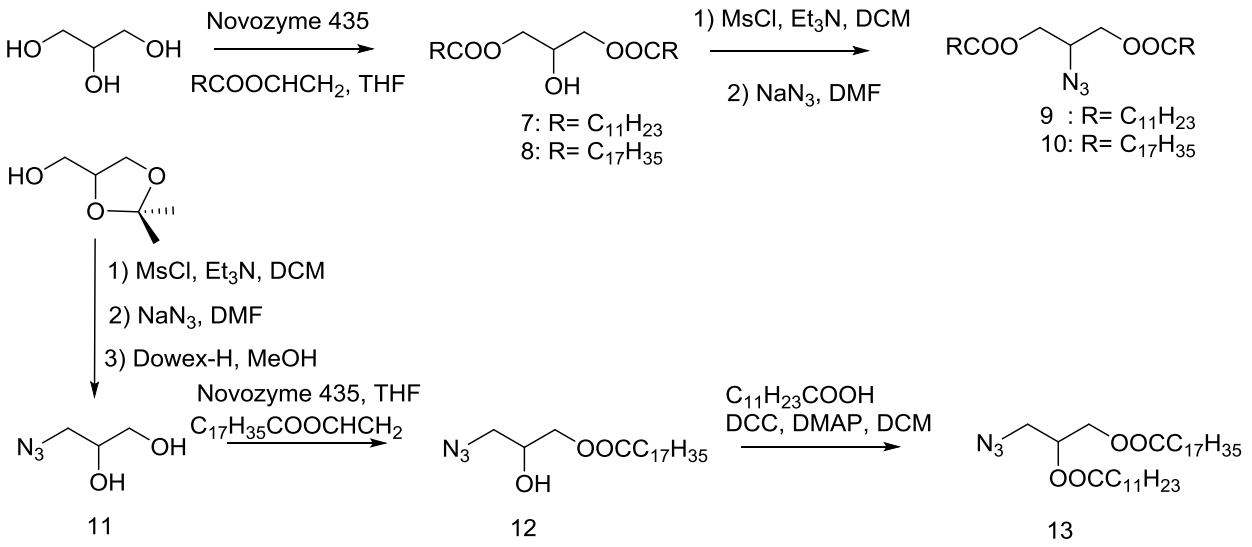
Content:

1) General synthetic and Analytic methods

All commercially available compounds were used as received without further purification. Millipore water was obtained from a *Merck* Millipore Milli-Q Integral System. UV/Vis measurements were performed on a *PerkinElmer* LAMBDA 950 UV/Vis/NIR spectrophotometer. Standard disposable PMMA UV/Vis cuvettes with a path length of 1 cm from *PLASTIBRAND* were used. DLS measurements were performed on *Malvern* Zetasizer ZS. Disposable *BRAND* UV-Cuvettes micro were used. NMR spectra were recorded on JOEL ECX400, JOEL ECP500 and *BRUKER* AV500 spectrometers. IR spectra were recorded on a *JASCO* FT/IR 4100 spectrometer. Mass analyses were performed on an Agilent 6210 ESI-TOF, Agilent Technologies, Santa Clara, CA, USA. Surface tension measurements were performed on a *Dataphysics* OCA 20.

2) Synthetic procedures and Characterization data



Scheme S1. Synthesis of lipophilic azides

Synthesis of glycerol symmetric esters:

To a solution of Glycerol (1 equiv.) in THF, vinyl ester of the corresponding alkyl chain (2.5 equiv.) was added followed by addition of the enzyme (20% wt. of the glycerol), Novozyme 435. The reaction mixture was left stirring at room temperature, without breaking the beads of the enzyme. The progress of the reaction was followed by TLC. After complete conversion of the starting materials, stopped stirring, filtered the reaction mixture and washed the beads with excess THF. The filtrate was concentrated, dried and purified by column chromatography to obtain the pure product as a white solid.

Compound 7: 4.3 g of the product was obtained from 1 g of glycerol. Yield 86%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.19 (dd, *J*= 4, 11Hz, 2H, -COO**CH$_2$-**), 4.14 (dd, *J*= 6, 11Hz, 2H, COO**CH$_2$-**), 4.08 (m, 1H, HO**CH**(CH_2O-)$_2$), 2.35 (t, *J*=7.5 Hz, 4H, -**CH$_2$**COO-), 1.63 (m, 4H, -**CH$_2$**CH2COO-), 1.33-1.22 (m, 32H, Alkyl chain), 0.88 (t, *J*= 7Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.08, 77.38, 68.58, 65.20, 34.26, 32.06, 29.75, 29.60, 29.48, 29.40, 29.28, 25.05, 22.83, 14.26. MS (ESI) m/z = 479.3709 $[M+Na]^+$ (calcd. 479.3712). IR: 2911, 2845, 1722,1182.

Compound 8: 5.0 g of product was obtained from 1g of glycerol. Yield 76%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.19 (dd, *J*= 4.5, 11 Hz, 2H, -COO**CH$_2$-**), 4.14 (dd, *J*= 6, 11 Hz, 2H, COO**CH$_2$-**), 4.08 (m, 1H, HO**CH**(CH_2O-)$_2$), 2.34 (t, *J*= 7.5 Hz, 4H, -**CH$_2$**COO-), 1.62 (m, 4H,

CH_2CH2COO-), 1.32-1.22 (m, 56H, Alkyl chain), 0.88 (t, *J*= 7 Hz, 6H, -**CH_3**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.09, 77.36, 68.56, 65.19, 34.26, 32.08, 29.85, 29.83, 29.81, 29.80, 29.75, 29.61, 29.51, 29.40, 29.28, 25.04, 22.84, 14.27. MS (ESI) m/z = 647.5607 $[M+Na]^+$ (calcd. 647.5590). IR: 2915, 2849, 1756,1149.

Synthesis of azido derivatives: To a solution of alcohol (**7**/**8**) in dichloromethane, triethyl amine (1.2 equiv.) and methanesulfonyl chloride (1.2 equiv.) were added at 0 °C. Reaction mixture was allowed to warm-up to room temperature during the progress of the reaction. After complete conversion of the alcohol, the reaction mixture was quenched by adding water and both the phases were separated. Compound was extracted from aqueous phase using DCM. The combined organic phase was washed further with dil. HCl, satd. $NaHCO_3$ and water, then dried over anhyd. Na_2SO_4. The reaction mixture was concentrated and subjected for the next step.

The mesylate was dissolved in DMF followed by addition of sodium azide (5 equiv.). The reaction mixture was left stirring at 90 °C. Progress of the reaction was monitoring by TLC. After completion of the reaction, the reaction mixture was filtered and DMF was removed under reduced pressure. Reaction mixture was dissolved in DCM and washed with water, and dried over anhyd. Na_2SO_4. The crude mixture was purified by column chromatography using DCM/Hexane.

Compound 9: 3.2 g of product was obtained from 3.1 g of compound **7**. Yield 95%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.23 (dd, *J*= 4.5, 11.5 Hz, 2H, -COO**CH_2**-), 4.14 (dd, *J*= 6.5, 11.5 Hz, 2H, COO**CH_2**-), 3.87 (m, 1H, N_3**CH**$(CH_2O)_2$), 2.35(t, *J*= 7.5 Hz, 4H, -**CH_2**COO-), 1.63 (m, 4H, **CH_2**CH2COO-), 1.33-1.25 (m, 32H, Alkyl chain), 0.88 (t, J= 7Hz, 6H, -**CH_3**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.41, 77.36, 63.15, 58.84, 34.16, 32.05, 29.73, 29.58, 29.47, 29.37, 29.24, 24.96, 22.82, 14.25. MS (ESI) m/z = 504.3781 $[M+Na]^+$ (calcd. for $C_{27}H_{51}N_3NaO_4$: 504.3777). IR: 2923, 2853, 2116, 1743.

Compound 10: 5 g of product was obtained from 5.2 g of compound **7**. Yield 92%.

^{1}H NMR (500 MHz, $CDCl_3$) δ 4.23 (dd, *J*= 4.5 Hz, 11.5 Hz, -COO**CH_2**-), 4.14 (dd, *J*= 7, 11.5 Hz, 2H, COO**CH_2**-), 3.87 (m, 1H, N_3**CH**$(CH_2O)_2$-), 2.35 (t, *J*= 7.5 Hz, 4H, -**CH_2**COO-), 1.61 (m, 4H, **CH_2**CH2COO-), 1.33-1.20 (m, 56H, Alkyl chain), 0.88 (t, *J*= 7 Hz, 6H, -**CH_3**).^{13}C NMR (126 MHz, $CDCl_3$) δ 173.42, 63.16, 58.82, 34.16, 32.07, 29.85, 29.82, 29.80, 29.80, 29.74, 29.60, 29.51, 29.38, 29.25, 24.96, 22.84, 14.27. MS (ESI) m/z = 672.5667 $[M+Na]^+$ (calcd. for $C_{39}H_{75}N_3NaO_4$: 672.5655). IR: 2917, 2850, 2126, 1741.

Synthesis of dissymmetric azide (11): To a solution of protected glycerol (4.05g, 36.9 mmol) in DCM, triethylamine (1.2 equiv.) and methanesulfonyl chloride (1.2 equiv.) were added at 0 °C and left stirring in the ice bath. Reaction mixture was allowed to warm-up to room temperature during the progress of the reaction and monitored the conversion using TLC. After completion of the reaction, it was quenched by adding water and both the phases were separated and organic compound was extracted from aqueous phase using DCM. Combined organic phase was washed with dil. HCl, satd. $NaHCO_3$ solution and water. Finally the reaction mixture was dried over anhyd. Na_2SO_4. The reaction mixture was concentrated and dried, and the crude product was subjected for the next step by dissolving in DMF and adding sodium azide (5 equiv.). The reaction mixture was left stirring at 90 °C overnight and the reaction mixture was filtered to remove excess sodium azide. DMF was removed under reduced pressure and the reaction mixture was dissolved in DCM. This organic phase was washed with water and dried over anhyd. Na_2SO_4. The organic phase was concentrated under reduced pressure. To a methanolic solution of this crude mixture, Dowex-H was added and left stirring at reflux for 5 h. Finally the reaction mixture was cooled to room temperature and filter to remove Dowex. The filtrate was concentrated and purified by column chromatography using EtOH/DCM, yield-81%.

^{1}H NMR (400 MHz, $CDCl_3$) δ 3.85 (m, 1H, HO**CH**-), 3.65 (dd, *J*= 3.6, 12 Hz, 1H, HO**CH$_2$**-), 3.55 (dd, *J*= 6.4, 11.6 Hz, 1H, HO**CH$_2$**-), 3.37-3.32 (m, 2H, N_3**CH$_2$**-). ^{13}C NMR (101 MHz, $CDCl_3$) δ 71.13, 64.05, 53.47.

Compound 12: To compound **11** (2.3 g, 19.64 mmol) in THF (50 mL), vinyl stearate (1.2 equiv.) was added, followed by addition of the enzyme (20% wt.), Novozyme 435. The reaction mixture was left stirring at room temperature. After complete consumption of the starting material, the reaction mixture was filtered to remove the enzyme. The filtrate was concentrated under reduced pressure and the crude mixture was purified by column chromatography (10-25% EtOAc/Hexane) to obtain the compound **12** (5.9 g, yield 79%) as white solid.

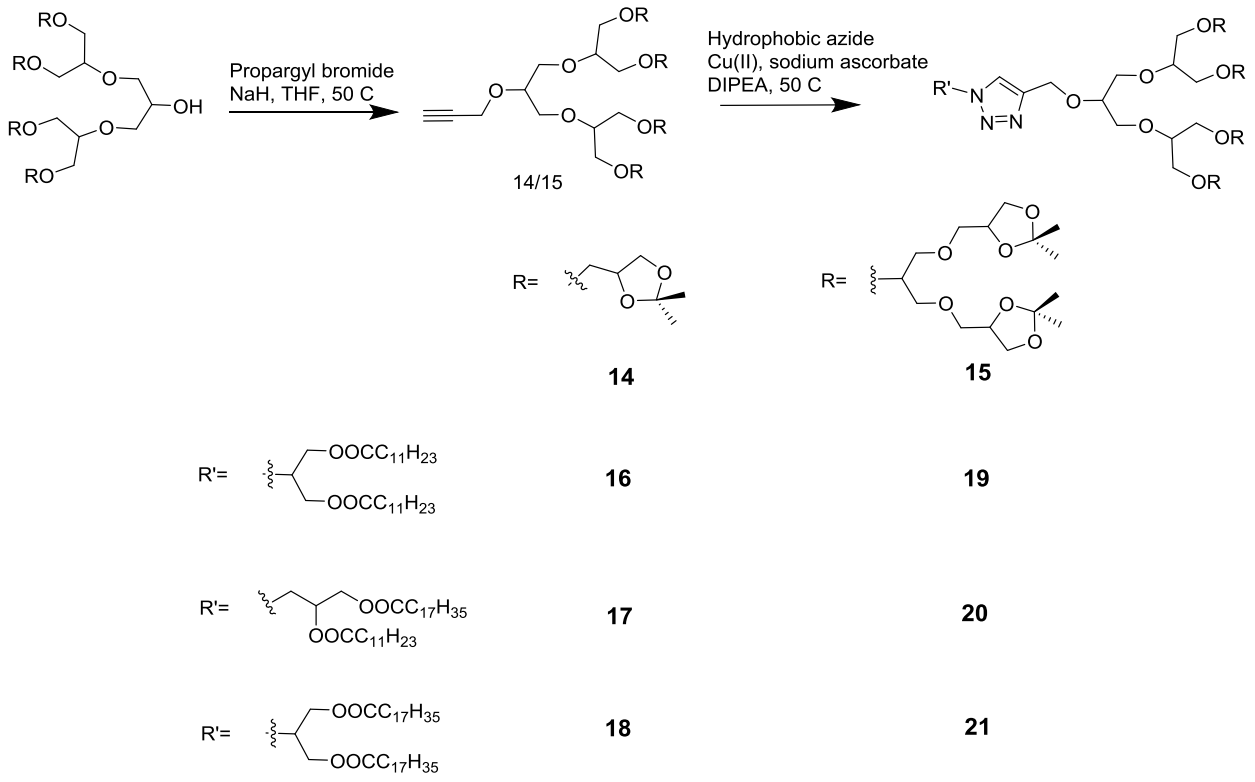
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.17 (dd, *J*= 4.4, 11.6 Hz, 1H, -COO**CH$_2$**-), 4.12 (dd, *J*= 6, 11.6 Hz, 1H, -COO**CH$_2$**-), 4.01 (m, 1H, HO**CH**-), 3.4 (m, 2H, N_3**CH$_2$**-), 2.35 (t, *J*= 7.6 Hz, 2H, -OOC**CH$_2$**-), 1.62 (m, 2H, -OOCCH$_2$**CH$_2$**-), 1.29-1.20 (m, 28H, Alkyl chain), 0.87 (t, *J*= 7.2 Hz, 3H, -**CH$_3$**)

^{13}C NMR (101 MHz, $CDCl_3$) δ 174.18, 69.27, 65.64, 53.59, 34.22, 32.05, 29.83, 29.80, 29.77, 29.76, 29.73, 29.58, 29.50, 29.48, 29.37, 29.35, 29.24, 25.01, 22.82, 14.26, 14.24. MS (ESI) m/z = 406.3055 $[M+Na]^+$ (calcd. for $C_{21}H_{41}N_3NaO_3$: 406.3046).

Compound 13: To a solution of the compound **12** (2.1 g, 5.3 mmol) in DCM, lauric acid (1.2 equiv.) was added followed by addition of DMAP (0.2 equiv.). The reaction mixture was cooled to 0 °C and added

DCC (1.2 equiv.), left stirring in the ice bath for 8 h. The reaction mixture was allowed to warm up to room temperature during the progress of the reaction. The progress of the reaction was monitored by TLC. Reaction mixture was filtered to remove the by-products and the precipitate was washed with DCM/Hexane. The combined organic layer was washed with dil. HCl, satd. $NaHCO_3$ solution, water and dried over anhyd. Na_2SO_4. The reaction mixture was concentrated and purified by column chromategraphy to obtain the compound **13** (2.2 g, yield 74%) as a white solid.

^{1}H NMR (500 MHz, $CDCl_3$) δ 5.17 (m, 1H. –COO**CH**-), 4.29 (dd, *J*= 4.5, 12 Hz, 1H, -COO**CH$_2$**-), 4.15 (dd, *J*= 6, 12 Hz, 1H, -COO**CH$_2$**-), 3.46 (m, 2H, -**CH$_2$**N$_3$), 2.35 (t, *J*=7.5 Hz, 2H, -**CH$_2$**COO-), 2.31 (t, *J*= 7.5 Hz, 2H, -**CH$_2$**COO-), 1.62 (m, 4H, -**CH$_2$**CH$_2$COO-), 1.32-1.22 (m, 44H, Alkyl chain), 0.88 (t, *J*= 7 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, $CDCl_3$) δ 173.38, 173.01, 70.01, 62.43, 51.03, 34.33, 34.19, 32.07, 32.05, 29.85, 29.83, 29.81, 29.77, 29.75, 29.62, 29.61, 29.51, 29.48, 29.47, 29.41, 29.40, 29.26, 29.21, 25.01, 24.96, 22.83, 14.26. MS (ESI) m/z = 588.4730 $[M+Na]^+$ (calcd. for $C_{33}H_{63}N_3NaO_4$: 588.4716). IR: 2922, 2852, 2101, 1743, 1152.



Scheme S2. Synthesis of protected dendritic amphiphiles

Synthesis of Propargyl ethers of dendrons (14/15): All the dendrons were synthesized by a literature reported procedure.[1] To a solution of protected dendron in THF, sodium hydride (5 equiv.) was added and left stirring at 50 °C for 1h. To this reaction mixture, propargyl bromide was added slowly and left stirring at the same temperature for 8 h. The progress of the reaction was checked by TLC and excess of NaH was quenched by drop wise addition of water, keeping the reaction flask in ice bath. The reaction mixture was concentrated under reduced pressure and diluted with water. The compound was extracted into DCM. The combined organic layer was washed with water, dried over anhyd. Na_2SO_4. The reaction mixture was concentrated and purified by column chromatography to obtain a pale yellow liquid (yield 80-85%).

Compound 14: ^{1}H NMR (400 MHz, Methanol-d4) δ 4.33 (m, 2H, CHC**CH$_2$**O-), 4.28-4.23 (m, 4H, **CH** acetonide), 4.08-4.03 (m, 4H, **CH$_2$** acetonide), 3.85-3.49 (m, 27H, dendron), 2.86 (m, 1H, **CH**CCH$_2$-), 1.39 (m, 12H, -**CH$_3$**), 1.33 (m, 12H, -**CH$_3$**). ^{13}C NMR (101 MHz, Methanol-d4) δ 110.45, 81.29, 79.90, 79.86, 79.83, 78.47, 78.17, 77.87, 76.22, 76.10, 75.84, 75.78, 75.73, 73.40, 72.52, 72.45, 72.41, 72.38, 72.36, 71.15, 67.76, 67.74, 67.59, 67.56, 58.32, 49.64, 49.49, 49.43, 49.27, 49.21, 49.06, 49.00, 48.82, 48.79, 48.62, 48.57, 48.36, 27.18, 27.13, 27.12, 27.05, 26.13, 25.72, 25.71. MS (ESI) m/z = 757.3997 $[M+Na]^+$ (calcd. for $C_{36}H_{62}NaO_{15}$: 757.3986).

Compound 15: ^{1}H NMR (500 MHz, Acetone-d6) δ 4.35 (m, 2H, CHC**CH$_2$**O-), 4.24-4.17 (m, 8H, **CH** acetonide), 4.05-4.01 (m, 8H, **CH** acetonide), 3.75-3.45 (m, 59H, dendron), 2.86 (m, 1H, **CH**CCH$_2$-), 1.35 (m, 24H, -**CH$_3$**), 1.29 (m, 24H, -**CH$_3$**). ^{13}C NMR (126 MHz, Acetone-d6) δ 109.49, 109.42, 79.56, 79.31, 75.59, 75.55, 75.46, 73.07, 73.05, 72.05, 70.74, 67.51, 67.35, 67.33, 67.31, 67.30, 57.90, 27.20, 27.18, 27.15, 27.13, 27.11, 27.10, 25.76, 25.74, 25.73. MS (ESI) m/z = 1509.8199 $[M+Na]^+$ (calcd. for $C_{72}H_{126}NaO_{31}$: 1509.8181).

General protocol for click reaction: To a mixture of the alkyne (1 equiv.) and azide (1.5 equiv.) in THF, diisopropylethylamine, copper sulphate solution (15% mol, aq. 0.1M) and aq. sodium ascorbate (50% mol, 0.2M) were added. The reaction mixture was left stirring at 45 °C. After complete consumption of starting material on TLC, stirring was stopped and both phases were separated from reaction mixture and organic compound were extracted from aqueous phase using DCM. The combined organic phase was washed with satd. EDTA solution, water and dried over anhyd. Na_2SO_4. The reaction mixture was concentrated and purified by column chromatography to obtain pure product as colourless, viscous liquid.

Compound 16: 2.4 g of compound **16** was obtained starting from 1.9 g of Compound **14** (yield 75%).

^{1}H NMR (500 MHz, Acetone-d_6): 8.06 (m, 1H, Triazole **CH**), 5.2 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.79-4.77 (m, 2H, -O**CH$_2$**-Triazole-), 4.60-4.57 (m, 4H, -**CH$_2$**OOC-), 4.23-4.18 (m, 4H, **CH** acetonide), 4.04 - 4.00 (m, 4H, **CH$_2$** acetonide), 3.75-3.46 (m, 27H, dendron), 2.31-2.29 (m, 4H, -**CH$_2$**COO-), 1.56-1.53 (m, 4H, -**CH$_2$**CH_2COO-), 1.34-1.28 (m, 56H, Alkyl chain and acetonide-CH_3), 0.88 (m, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Acetone-d_6) δ 206.12, 173.22, 123.59, 109.58, 79.40, 75.71, 75.57, 73.16, 72.15, 67.59, 67.41, 64.32, 63.21, 59.41, 34.30, 32.65, 30.38, 30.32, 30.30, 30.23, 30.19, 30.15, 30.10, 30.05, 30.04, 30.01, 29.99, 29.88, 29.86, 29.84, 29.73, 29.71, 29.69, 29.57, 29.53, 29.41, 29.38, 27.19, 25.78, 25.51, 23.34, 14.42, 14.39. MS (ESI) m/z = 1238.7930 $[M+Na]^+$ (calcd. for $C_{63}H_{113}N_3NaO_{19}$: 1238.7866). IR: 2984, 2923, 2855, 1744, 1456, 1370, 1253, 1213.

Compound 17: 2.9 g of compound **17** was obtained from 1.8 g of compound **14** (yield 90%)
^{1}H NMR (500 MHz, Acetone-d_6) 7.96 (m, 1H, **CH**(Triazole)), 5.48 (m, 1H, -**CH**OOC-), 4.77-4.68 (m, 4H, -**CH$_2$**-Triazole-**CH$_2$**-), 4.40 (dd, *J*=12, 4 Hz, 1H,-**CH$_2$**OOC-), 4.24-4.18 (m, 4H, **CH** acetonide), 4.15-4.11(m, 1H, -**CH$_2$**OOC-), 4.04-4.01 (m, 4H, **CH$_2$** acetonide), 3.75-3.46 (m, 27H, dendron), 2.34 (t, *J*=7.5 Hz, 2H, -OOC**CH$_2$**-), 2.29 (t, *J*=7.5 Hz, 2H, -OOC**CH$_2$**-), 1.63-1.58 (m, 2H, -OOCCH_2**CH$_2$**-), 1.57-1.53 (m, 2H, -OOCCH_2**CH$_2$**-), 1.41-1.23(m, 68H, Alkyl chain and acetonide-**CH$_3$**), 0.90-0.86 (m, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Acetone-d_6) δ 173.33, 172.84, 124.88, 109.58, 79.40, 79.35, 75.58, 75.57, 73.16, 72.08, 70.44, 67.59, 67.43, 67.41, 64.24, 63.10, 50.55, 34.51, 34.40, 32.68, 32.64, 30.42, 30.39, 30.37, 30.32, 30.30, 30.28, 30.17, 30.15, 30.09, 30.01, 29.99, 29.86, 29.84, 29.81, 29.74, 29.71, 29.69, 29.55, 29.53, 29.39, 29.38, 27.23, 27.18, 25.78, 25.60, 25.53, 23.36, 23.33, 14.40, 14.37. MS (ESI) m/z = 1322.8842 $[M+Na]^+$ (calcd. for $C_{69}H_{125}N_3NaO_{19}$: 1322.8805). IR: 2972, 2853, 1743, 1457.

Compound 18: 3.6 g of compound **18** was obtained from 2.1 g of compound **14** (yield 91%)
^{1}H NMR (500 MHz, Acetone-d_6) 8.06 (m, 1H, **CH**(Triazole)), 5.21 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.78 (t, *J*= 2.5 Hz, 2H, -O**CH$_2$**-Triazole-), 4.59 (d, *J*= 10Hz, 4H, -**CH$_2$**OOC-), 4.23-4.18 (m, 4H, **CH** acetonide), 4.03-4.00 (m, 4H, **CH$_2$** acetonide), 3.9-3.46 (m, 27H, dendron), 2.30 (t, *J*=7.5 Hz, 4H, -OOC**CH$_2$**-), 1.55 (m, 4H, -OOCCH_2**CH$_2$**-), 1.34-1.25 (m, 80H, Alkyl chain and acetonide-CH_3), 0.88 (t, *J*=7.5 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Acetone-d_6) δ 173.20, 123.57, 109.57, 109.51, 79.41, 75.57, 75.56, 73.16, 72.14, 67.60, 67.43, 67.41, 63.19, 34.30, 30.43, 30.42, 30.38, 30.30, 30.24, 30.15, 30.08, 30.05, 29.99, 29.84, 29.73, 29.69, 29.53, 29.38, 27.22, 27.19, 27.17, 25.79, 25.77, 25.76, 25.74, 23.33. MS (ESI) m/z = 1406.9755 $[M+Na]^+$ (calcd. for $C_{75}H_{137}N_3NaO_{19}$: 1406.9744). IR: 2984, 2922, 2853, 1744, 1456, 1370, 1253, 1213.

Compound 19: 1.7 g of compound **19** was obtained starting from 1.5 g of compound **15** (yield 86%)

^{1}H NMR (500 MHz, Acetone-d_6): δ 8.06 (m, 1H, **CH**(Triazole)), 5.20 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.81 (m, 2H, -O**CH$_2$**-Triazole-), 4.60-4.58 (m, 4H, -**CH$_2$**OOC-), 4.25-4.17 (m, 8H, **CH** acetonide), 4.05-4.01 (m, 8H, **CH$_2$** acetonide), 3.91-3.87 (m, 1H), 3.74-3.35 (m, 59H, dendron), 2.31 (t, *J*= 7.5 Hz, 4H, -OOC**CH$_2$**-), 1.56 (m, 4H, -OOCCH_2**CH$_2$**-), 1.35-1.28 (m, 80H, Alkyl chain and acetonide-CH_3), 0.86 (t, *J*= 6 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Acetone-d_6) δ 173.25, 123.58, 109.59, 79.67, 79.36, 75.72, 75.68, 75.59, 75.57, 73.20, 73.19, 72.22, 72.20, 72.12, 72.11, 70.92, 67.64, 67.49, 67.46, 67.45, 67.45, 67.43, 63.70, 63.25, 59.36, 34.32, 32.65, 30.38, 30.30, 30.25, 30.15, 30.10, 30.06, 29.99, 29.84, 29.76, 29.69, 29.54, 29.53, 29.38, 27.29, 27.27, 27.23, 27.21, 25.84, 25.83, 25.83, 25.81, 25.75, 25.53, 23.34, 14.39. MS (ESI) m/z = 1991.2026 $[M+Na]^+$ (calcd. for $C_{99}H_{177}N_3NaO_{35}$: 1991.2060). IR: 2985, 2923, 2854, 1745, 1457, 1370, 1253, 1213.

Compound 20: 1.8 g of compound **20** was obtained from 1.7 g of compound **15** (yield 76%)
1H NMR (500 MHz, Acetone–d6): δ 7.98 (m, 1H, **CH**(Triazole)),5.49 (m, 1H, -**CH**OOC-), 4.79 (m, 2H, -O**CH$_2$**-Triazole-), 4.75 (dd, *J*= 14.5, 4.5, 1H, Triazole-**CH$_2$**CH-), 4.70 (dd, *J*= 14.5, 7 Hz, 1H, Triazole-**CH$_2$**CH-), 4.41 (dd, *J*= 12, 4 Hz, 1H, -**CH$_2$**OOC-), 4.24-4.18 (m, 8H, **CH** acetonide), 4.13 (dd, *J*=12, 6 Hz, 1H, -**CH$_2$**OOC-), 4.05-4.01 (m, 8H, **CH$_2$** acetonide), 3.77- 3.46(m, 59H, dendron), 2.35 (t, *J*= 7.5 Hz, 2H, -OOC**CH$_2$**-), 2.30 (t, *J*=7.5 Hz, 2H, -OOC**CH$_2$**-), 1.63-1.54 (m, 4H, -OOCCH_2**CH$_2$**-), 1.35-1.25 (m, 92H, Alkyl chain and acetonide-CH_3), 0.90-0.86 (m, 6H, -**CH$_3$**). ^{13}C NMR (101 MHz, Acetone –d6) δ 173.32, 172.85, 146.53, 124.89, 109.58, 109.50, 79.91, 79.65, 79.44, 79.36, 78.76, 75.70, 75.67, 75.56, 73.17, 72.78, 72.39, 72.18, 72.10, 71.18, 70.86, 70.46, 67.62, 67.44, 64.33, 63.13, 50.53, 34.52, 34.41, 32.66, 32.63, 31.33, 30.42, 30.41, 30.28, 30.23, 30.10, 30.04, 29.84, 29.65, 29.46, 29.26, 27.63, 27.27, 27.22, 26.80, 26.22, 25.82, 25.59, 25.54, 25.41, 23.33, 14.39. MS (ESI) m/z = 2075.3006 $[M+Na]^+$ (calcd. for $C_{105}H_{189}N_3NaO_{35}$: 2075.2999). IR: 2985, 2923, 2855, 1744, 1457, 1370, 1254, 1213.

Compound 21: 1.9 g of compound **21**was obtained from 1.85 g of compound **15** (yield 71%)
^{1}H NMR (500 MHz, Acetone–d6): 8.06 (s, 1H, **CH**(Triazole)), 5.22-5.19 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.81 (t, *J*=2Hz, 2H, -O**CH$_2$**-Triazole-), 4.60-4.58 (m, 4H, -**CH$_2$**OOC-), 4.23-4.18 (m, 8H, **CH** acetonide), 4.08-3.98 (m, 8H, **CH$_2$** acetonide), 3.73-3.46 (m, 59H, dendron), 2.32 (t, *J*= 7.5 Hz, 4H, -OOC**CH$_2$**-), 1.56 (m, 4H, -OOCCH_2**CH$_2$**-), 1.35-1.25 (m, 104H, Alkyl chain and acetonide-CH_3), 0.88 (t, *J*= 7 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, ACETONE-D6) δ 173.25, 109.60, 75.73, 75.68, 75.59, 75.58, 73.21, 72.19, 72.11, 67.65, 67.49, 67.47, 63.25, 59.34, 34.33, 32.65, 30.44, 30.44, 30.40, 30.38, 30.30, 30.27, 30.15, 30.09, 30.08, 29.99, 29.84, 29.77, 29.69, 29.67, 29.53, 29.51, 29.38, 27.29, 27.27, 27.24, 27.22, 25.84, 25.83, 25.81, 25.54, 23.34, 14.38. MS (ESI) m/z = 2159.3911 $[M+Na]^+$ (calcd. for $C_{111}H_{201}N_3NaO_{35}$: 2159.3938). IR: 2985, 2923, 2854, 1745, 1456, 1370, 1253, 1213.

Deprotection of the dendrons: The protected amphiphiles (**16**-**21**) were dissolved in MeOH and added Dowex-H (2 equiv. by weight) and left stirring at room temperature (the reaction was done in EtOH and heated to 45 °C in the case of compound **3**). Deprotection reaction was monitored using NMR. After complete deprotection of the amphiphiles, the reaction mixture was filtered using filter paper and Dowex was washed with excess methanol. The filtrate was concentrated and crude mixture was purified by reverse phase HPLC using methanol/water (90-95%), yield (70-80%).

Compound 1:

1H NMR (500 MHz, Methanol-d_4) δ 8.16 (m, 1H, **CH**(Triazole)), 5.23-5.18 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.83-4.79 (2H, m, -O**CH$_2$**-Triazole-), 4.62-4.55 (m, 4H, -**CH$_2$**OOC-), 3.80-3.46 (m, 35H, dendron), 2.30 (t, *J*= 7.5Hz, 4H, -OOC**CH$_2$**-), 1.55 (m, 4H, -OOCCH$_2$**CH$_2$**-), 1.34-1.25 (m, 32H, alkylchains), 0.90 (t, *J*= 7 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Methanol-d_4) δ 174.52, 124.90, 79.81, 73.95, 72.93, 72.42, 72.28, 72.18, 64.43, 63.44, 34.67, 33.07, 30.75, 30.59, 30.48, 30.40, 30.11, 25.87, 23.74, 14.49. MS (ESI) m/z = 1078.6623 $[M+Na]^+$ (calcd. for $C_{51}H_{97}N_3NaO_{19}$: 1078.6614). IR: 3396, 2922, 2854, 1743, 1464.

Compound 2:

^{1}H NMR (500 MHz, Methanol-d_4) : δ 8.07-8.06 (m, 1H, **CH**(Triazole)), 5.48 (m, 1H, -**CH**OOC-), 4.79-4.66 (m, 4H, -**CH$_2$**-Triazole-**CH$_2$**-), 4.44 (dd, *J*=12, 3.5 Hz, 1H, -**CH$_2$**OOC-), 4.13-4.09 (m, 1H, -**CH$_2$**OOC-), 3.79-3.48 (m, 35 H, dendron), 2.35 (t, *J*= 7 Hz, 2H, -OOC**CH$_2$**-), 2.28 (t, *J*=7.5 Hz, 2H, -OOC**CH$_2$**-), 1.62 (m, 2H, -OOCCH$_2$**CH$_2$**-), 1.54 (m, 2H, -OOCCH$_2$**CH$_2$**-), 1.36-1.24 (m, 44H), 0.91 (t, *J*= 6.5 Hz, 3H), 0.90 (t, *J*= 6.5 Hz, 3H). ^{13}C NMR (126 MHz, Methanol-d_4) δ 174.70, 174.03, 146.70, 126.16, 79.91, 79.87, 79.19, 73.98, 73.95, 72.95, 72.44, 72.29, 72.21, 71.23, 70.99, 64.48, 64.46, 64.43, 64.14, 63.61, 51.22, 49.51, 49.46, 49.34, 49.29, 49.17, 49.12, 49.00, 48.83, 48.66, 48.49, 34.89, 34.82, 33.11, 33.08, 30.83, 30.80, 30.77, 30.68, 30.66, 30.53, 30.48, 30.47, 30.22, 30.14, 25.99, 25.90, 23.77, 23.74, 14.51, 14.47. MS (ESI) m/z = 1162.7564 $[M+Na]^+$ (calcd. for $C_{57}H_{109}N_3NaO_{19}$: 1162.7553). IR: 3390, 2922, 2853, 1742, 1464.

Compound 3:

^{1}H NMR (500 MHz, Methanol-d_4) δ 8.16-8.15 (m, 1H, **CH**(Triazole)), 5.24-5.18 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.81-4.79 (m, 2H, -O**CH$_2$**-Triazole-), 4.59-4.56 (m, 4H, -**CH$_2$**OOC-), 3.80-3.48 (m, 35 H, dendron), 2.31 (t, *J*= 7.5 Hz, 4H, -OOC**CH$_2$**-), 1.58-1.53 (m, 4H, -OOCCH$_2$**CH$_2$**-), 1.34-1.25 (m, 56H, alkyl chains), 0.90 (t, *J*=7.5 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Methanol-d_4) δ 174.49, 146.63, 124.89,

79.94, 79.90, 79.83, 79.30, 74.01, 73.97, 72.98, 72.48, 72.46, 72.32, 72.23, 72.22, 72.20, 71.25, 64.49, 64.45, 64.25, 63.44, 60.32, 60.30, 49.85, 49.63, 49.51, 49.47, 49.42, 49.34, 49.30, 49.29, 49.25, 49.17, 49.13, 49.08, 49.00, 48.89, 48.83, 48.66, 48.50, 48.49, 34.69, 33.09, 30.82, 30.78, 30.77, 30.62, 30.49, 30.42, 30.14, 25.89, 23.75, 14.47. MS (ESI) m/z = 1246.8552 $[M+Na]^+$ (calcd. for $C_{63}H_{121}N_3NaO_{19}$: 1246.8492). IR: 3397, 2916, 2850, 1743, 1467.

Compound 4:

^{1}H NMR (500 MHz, Methanol-d_4): 8.16-8.15 (m, 1H, **CH**(Triazole)), 5.22-5.19 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.82 (s, 2H, -O**CH$_2$**-Triazole-), 4.6-4.56 (m, 4H, -**CH$_2$**OOC-), 3.79-3.46 (m, 75H, dendron), 2.32 (t, *J*= 7.5 Hz, 4H, -OOC**CH$_2$**-), 1.56 (m, 4H, -OOCCH_2**CH$_2$**-), 1.33-1.26 (m, 32H, alkylchains), 0.90 (t, *J*= 6.5 Hz, 6H, -**CH$_3$**). ^{13}C NMR (126 MHz, Methanol-d_4) δ 174.53, 124.83, 80.03, 79.82, 79.77, 79.43, 73.99, 73.95, 72.95, 72.40, 72.29, 72.18, 72.16, 71.35, 71.02, 64.49, 64.48, 64.43, 63.46, 60.22, 49.51, 49.34, 49.17, 49.00, 48.83, 48.66, 48.49, 34.68, 33.06, 30.74, 30.59, 30.46, 30.40, 30.12, 25.87, 23.73, 14.49. MS (ESI) m/z = 1670.9556 $[M+Na]^+$ (calcd. for $C_{75}H_{145}N_3NaO_{35}$: 1670.9556). IR: 3380, 2922, 2855, 1743, 1463.

Compound 5:

1H NMR (500 MHz, Methanol-d_4): δ 8.06 (m, 1H, **CH**(Triazole)),5.48 (m, 1H, -**CH**OOC-), 4.80 (m, 2H, -O**CH$_2$**-Triazole-), 4.74 (dd, *J*= 14.5, 4.5 Hz, 1H, Triazole-**CH$_2$**CH-), 4.68 (dd, *J*= 14.5, 7.5 Hz, 1H, Triazole-**CH$_2$**CH-), 4.44 (dd, *J*= 12, 3.5 Hz, 1H, -**CH$_2$**OOC-), 4.10 (dd, *J*= 12, 6Hz, 1H, -**CH$_2$**OOC-), 3.79-3.45 (m, 75H, dendron), 2.34 (t, *J*= 7.5 Hz, 2H, -OOC**CH$_2$**-), 2.28 (t, *J*= 7.5 Hz, 2H, -OOC**CH$_2$**-), 1.61 (m, 2H, -OOCCH_2**CH$_2$**-), 1.54 (m, 2H, -OOCCH_2**CH$_2$**-), 1.34-1.26 (m, 44H,alkylchains), 0.90 (t, *J*=7 Hz, 3H, -**CH$_3$**), 0.89 (t, *J*= 7 Hz, 3H, -**CH$_3$**). ^{13}C NMR (126 MHz, Methanol-d_4) δ 174.72, 174.06, 146.79, 126.10, 101.28, 79.83, 73.98, 73.95, 72.95, 72.43, 72.41, 72.29, 72.19, 72.17, 71.02, 64.49, 64.48, 64.44, 63.65, 51.21, 49.51, 49.34, 49.30, 49.17, 49.13, 49.00, 48.96, 48.83, 48.66, 48.49, 34.90, 34.83, 33.10, 33.06, 30.82, 30.79, 30.75, 30.68, 30.66, 30.52, 30.47, 30.22, 30.14, 25.99, 25.91, 23.76, 23.73, 14.52, 14.48.

MS (ESI) m/z = 1755.0493 $[M+Na]^+$ (calcd. for $C_{81}H_{157}N_3NaO_{35}$: 1755.0495). IR: 3389, 2921, 2853, 1742, 1464.

Compound 6:

1H NMR (500 MHz, Methanol-d_4): 8.16 (m, 1H, **CH**(Triazole)), 5.21 (m, 1H, Triazole-**CH**(CH_2O-)$_2$), 4.83 (m, 2H, -O**CH$_2$**-Triazole-), 4.61-4.57 (m, 4H, -**CH$_2$**OOC-), 3.80-3.46 (m, 75H, dendron), 2.32 (t, *J*=7.5 Hz, 4H, -OOC**CH$_2$**-), 1.57 (m, 4H, -OOCCH_2**CH$_2$**-), 1.36-1.25 (m, 56H, alkyl chains), 0.90 (t, *J*= 7

Hz, 6H, -**CH$_3$**).^{13}C NMR (126 MHz, Methanol-d$_4$) δ 174.51, 124.82, 124.81, 80.01, 79.81, 79.76, 73.98, 73.94, 72.94, 72.42, 72.39, 72.28, 72.17, 72.15, 71.01, 64.48, 64.47, 64.43, 64.41, 63.43, 60.14, 49.51, 49.34, 49.30, 49.17, 49.14, 49.13, 49.00, 48.98, 48.96, 48.96, 48.83, 48.78, 48.66, 48.65, 48.49, 34.70, 33.07, 30.81, 30.77, 30.63, 30.44, 30.14, 25.89, 23.74, 14.50. MS (ESI) m/z = 1839.1412 $[M+Na]^+$ (calcd. for $C_{87}H_{169}N_3NaO_{35}$: 1839.1434). IR: 3376, 2920, 2852, 1743, 1464.

3) Critical aggregation concentration (CAC) measurements

a) Surface tension method: The critical aggregation concentrations of the amphiphiles were determined by measuring their surface tension in Milli-Q water at different concentrations. The surface tension measurements were performed on a commercially available contact angle tensiometer OCA 20 (DataPhysics Instruments GmbH, Filderstadt, Germany) using pendant drop method. The samples were prepared in Milli-Q water 24 h before measurement. All the measurements were done at 25 ± 0.5 °C. Calculation of surface tension was done by using the Young-Laplace equation. The surface tension was measured trice per minute and the measurement was stopped when the value did not change by over more than 0.1 mN m^{-1} over 5 minutes. Equilibration time was generally between 60-90 min below the CAC and around 30 min above the CAC.

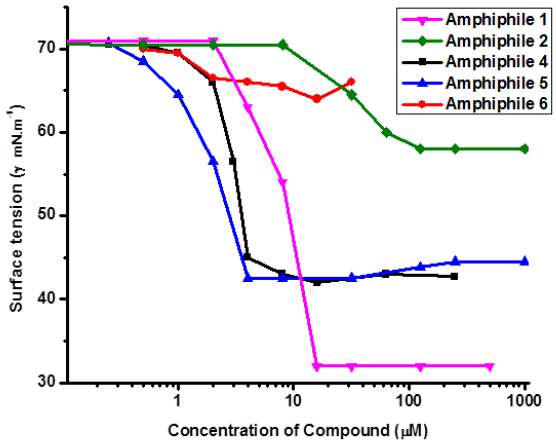


Figure S1. Surface tension measurements

b) Fluorescence method: We have reinvestigated the aggregation behavior of amphiphile **6**, which did not show a clear levelling off in the surface tension on increasing concentration, using the so-called pyrene fluorescence method. It is known that the CAC of an amphiphile depends to a certain extent on the method. We tried to confirm at first our CAC value of amphiphile **5** by the pyrene fluorescence method. Amphiphile **5** showed a well-defined break point in the surface tension measurements. The breakpoint in the semilogarithimic plot is

conventionally interpreted as the CMC.[2] The pyrene intensity ratio (I_1/I_3) shows a similar declining behavior when plotted against the concentration. The breaking points in the surface tension vs. concentration plot coincides with the inflection point of the I_1/I_3 curve. This allows us to interpret the points of inflection as the apparent cmc. This empirical procedure gives a value of 2-4 μM for amphiphile **6**.

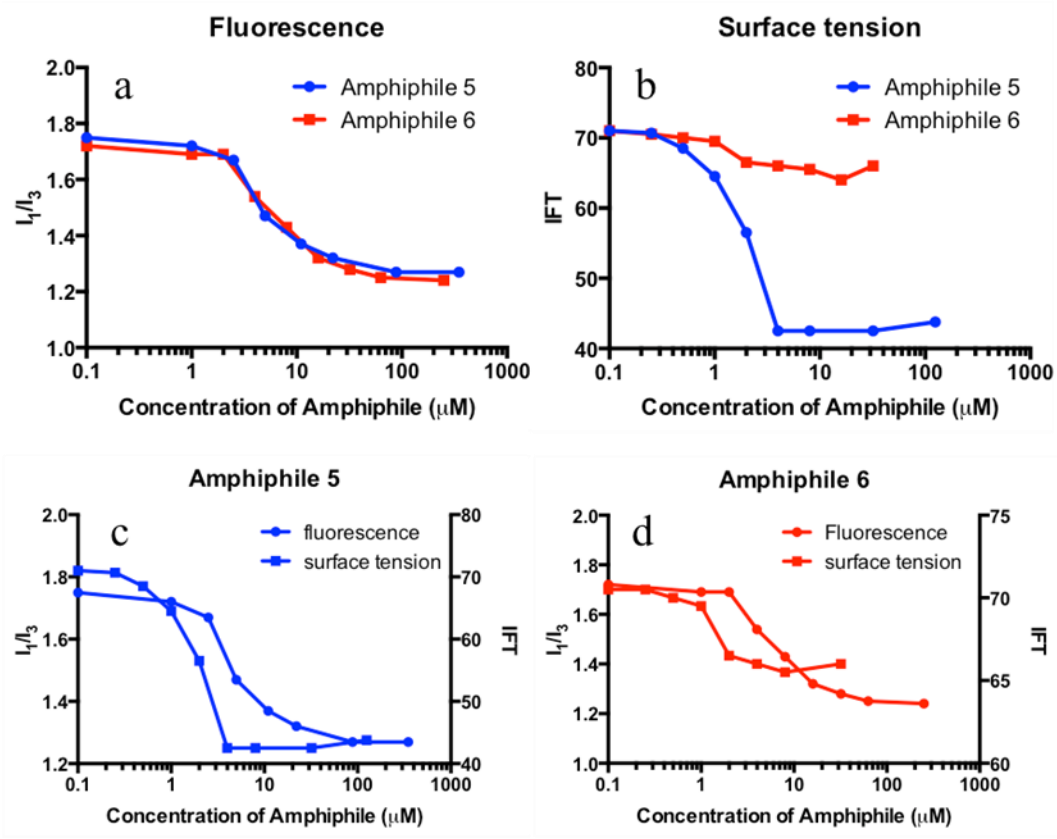


Figure S2. CAC measurement of amphiphiles (5&6) a) by pyrene fluorescence and b) by surface tension. Comparision of CAC from fluorescence and surface tension methods c) amphiphile 5 and d) amphiphile 6.

Preparation of samples for fluorescence experiments:

A stock solution of pyrene (1mM) was prepared in methanol. 50 μL of the methanolic solution of pyrene was taken in a 250 mL conical flask and the solvent was evaporated under high vacuum. 100 mL of milliQ water was added to this conical and the aqueous solution was sonicated for 1h. The aqueous pyrene solution (0.5 mM) was filtered through a membrane filter (RC, 0.45 μ) and the filtrate was used for the fluorescence studies. A stock solution of the amphiphile was prepared by dissolving required amount of the amphiphile in aqueous pyrene solution. The stock solution was further diluted to required concentrations of the amphiphile using the same aqueous

pyrene solution. All the samples were stabilized overnight and recorded their fluorescence spectra (λ_{ex}= 335 nm and λ_{em} = 350-550 nm). The ratio of first and third vibronic bands were calculated and plotted against the concentration of amphiphile as shown in the figure S2(a).

4) Dye encapsulation experiments and calculation of transport capacity

In order to test the transport capacity of the synthesized amphiphiles, two hydrophobic dyes (Nile Red and Nimodipine) were investigated as water insoluble models. A thin film of the dye (0.5 mg) was prepared in each vial by evaporating a stock solution of the dye in THF at room temperature, and then the vials were dried under high vacuum for 10-12 h. To these vials, a solution of the amphiphilic molecule (0.5% wt., 2.5 mL) was added and left stirring at 500 rpm at room temperature. All the samples were filtered through 0.45 μm RC membranes to remove the insoluble dye particles. A known volume of the filtrate (0.5 mL) was lyophilised from each sample. The lyophilised samples were dissolved in 4 mL of organic solvent (Methanol for Nile Red and Ethanol for Nimodipine) and recorded their UV-Vis spectra. The concentration of the dye molecules in the filtrate was calculated using the molar extinction coefficients of the dye molecules in corresponding solvents (45,000 $M^{-1}cm^{-1}$ for Nile Red at 552 nm in MeOH and 7,200 $M^{-1}cm^{-1}$ for Nimodipine at 356 nm in EtOH) and corresponding dilution factor.

5) Dynamic light scattering measurements

Dynamic light scattering studies were conducted using a Zetasizer Nano (Malvern Instruments Ltd.). All the samples were prepared by dissolving the compound in Milli-Q water by sonication (for 1min, get a homogeneous dispersion) and vortexing (30 min), and further tempered at 50 °C for 30 min. DLS measurements were performed before and after tempering the sample. No considerable influence of tempering was observed. All the samples were filtered through 0.45 μm RC membrane prior to measurement.

6) Cryogenic transmission electron microscopy (cryo-TEM)

The samples for cryogenic transmission electron microscopy (cryo-TEM) were prepared at room temperature by placing a droplet (6 μL) of the solution on a hydrophilized perforated carbon filmed Quantifoil grid (60 s Plasma treatment at 8 W using a BALTEC MED 020 device). The excess fluid was blotted off to create an ultra-thin layer (typical thickness of 100 nm) of the solution spanning the holes of the carbon film. The grids were immediately vitrified in liquid ethane at its freezing point (-184°C) using a standard plunging device. Ultra-fast cooling is necessary for an artifact-free thermal fixation (vitrification) of the aqueous solution avoiding crystallization of the solvent or rearrangement of the assemblies. The vitrified samples were transferred under liquid nitrogen into a Philips CM12 transmission

electron microscope using the Gatan cryoholder and -stage (Model 626). Microscopy was carried out at -175°C sample temperature using the microscopes low dose mode at a primary magnification of 58300×. Accelerating voltage was 100 kV and the defocus was chosen to be 1.2 µm.

7) Packing parameter approach

For common single-tail surfactants, the ratio of the volume of the surfactant tail, v_0, and its length, l_0, is a constant independent of tail length, equal to 21 Å^{2}.[3] [C. Tanford, *The hydrophobic Effect*: Wiley-Interscience: New York, 1973]. For double tail surfactants it is twice that value: $2v_0/l_0$ = 42 Å^2. Therefore, the chain length should not affect the molecular packing parameter, ($2v_0/al_0$), where a is the area per molecule, and consequently also not the shape of aggregate. However, if one alkyl chain contains only 2/3 of the carbon atoms of the second chain, as it is valid for the (G2-C12/18) compound **2**, the volume-to-length ratio reduces to 5/6·($2v_0/l_0$) = 35 Å^2. Hence, as compared to a symmetric double tail compounds, the volume-to-length ratio is reduced to 35 Å^2, i.e. the packing parameter is smaller, which favours an aggregate morphology with larger curvature.

References:

1. M. Wyszogrodzka and R. Haag, *Chemistry*, 2008, **14**, 9202–14.

2. J. Aguiar, P. Carpena, J. A. Molina-Bolívar, and C. Carnero Ruiz, *J. Colloid Interface Sci.*, 2003, **258**, 116–122.

3. The Hydrophobic Effect: Formation of Micelles and Biological Membranes, Charles Tanford, Wiley-Interscience, New York, 1980, 233pp.

8) Additional cryo-TEM images

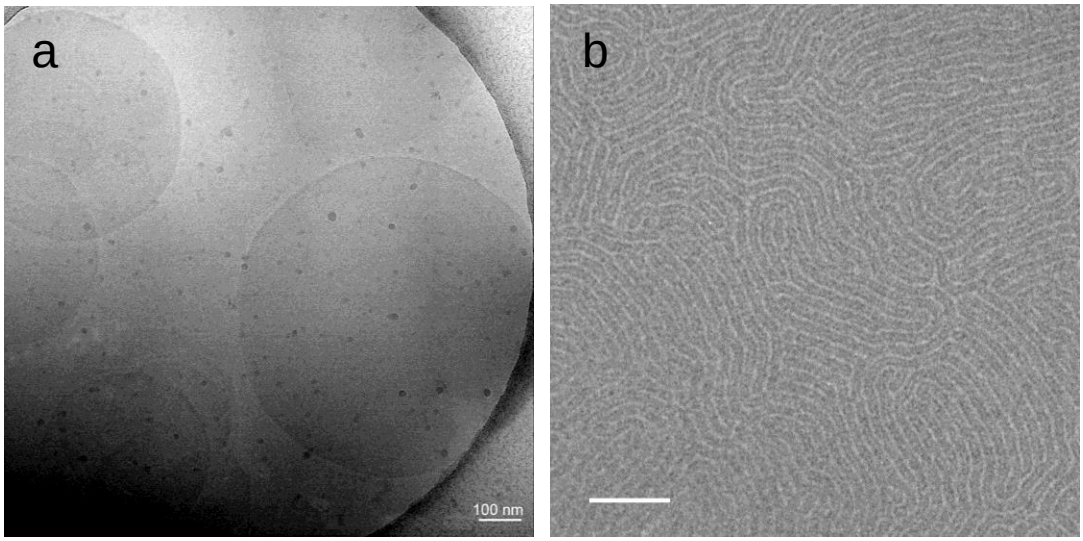


Figure S3. (a) Additional cryo-TEM image of a sample of amphiphile **3** showing large vesicles and (b) Cryo-TEM image of the amphiphile **2** after tempering at 60 °C for 3 h. It shows mainly worm-like micelles. (Scale bar 30 nm)

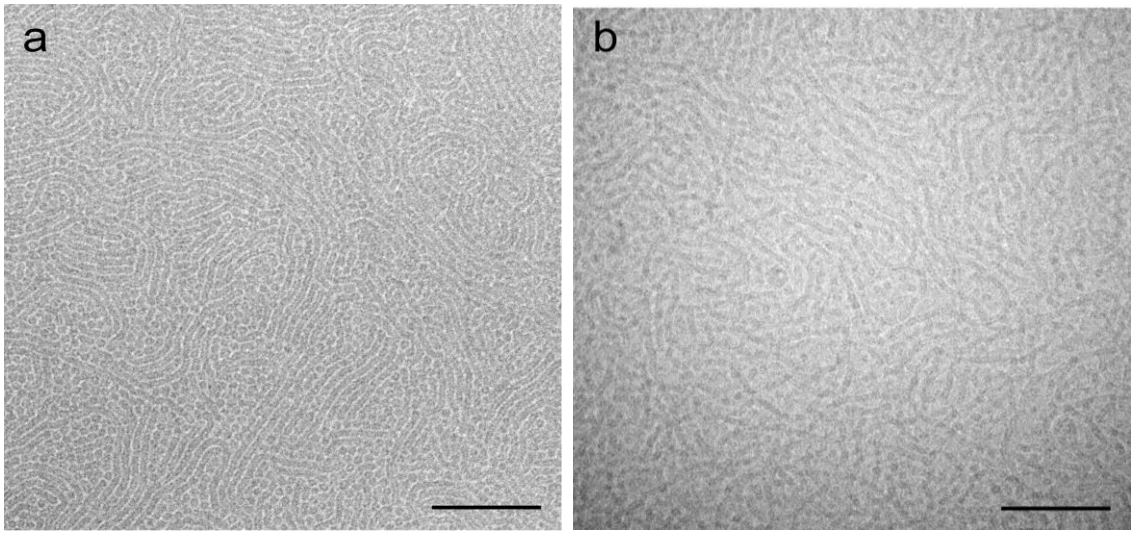
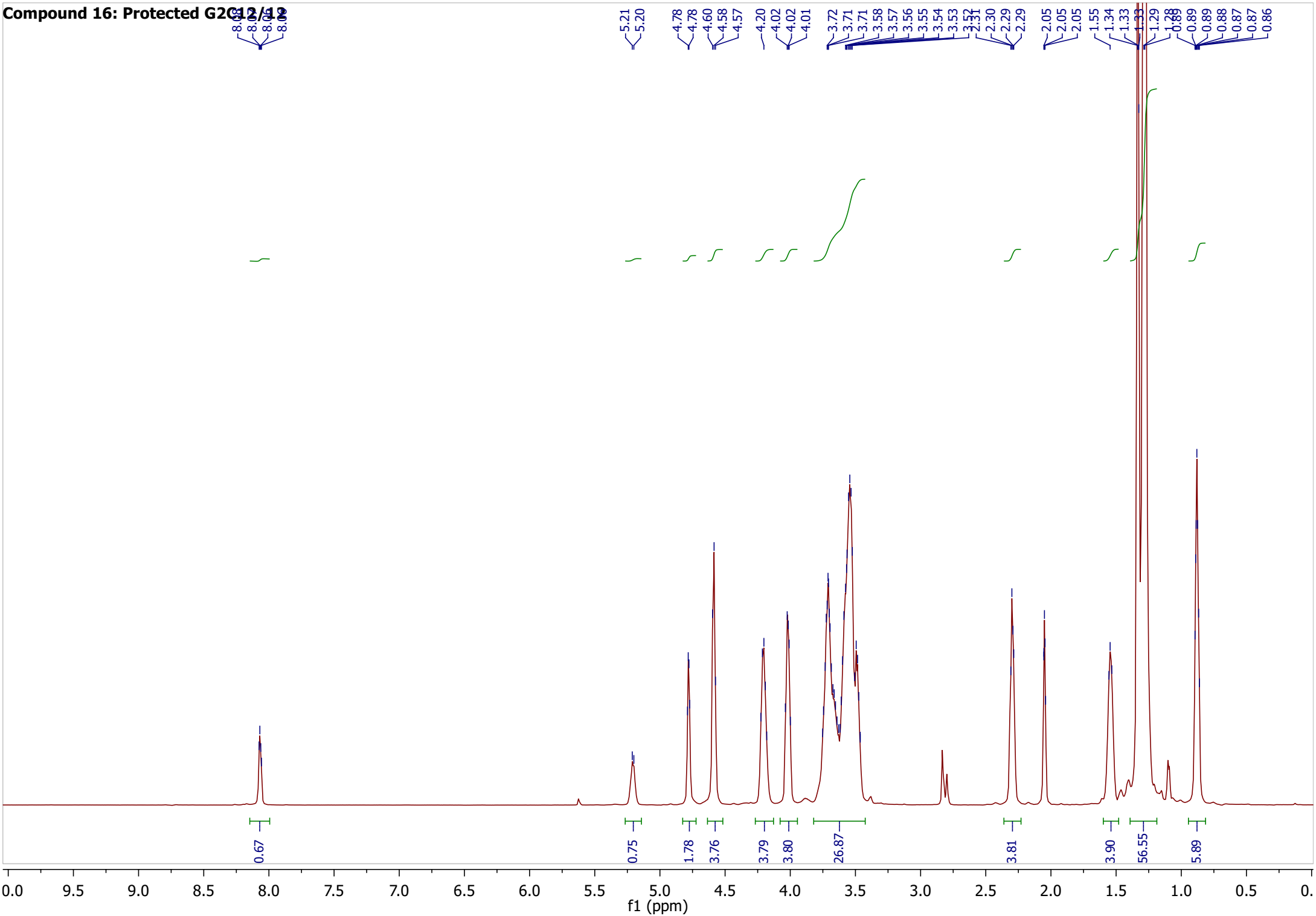
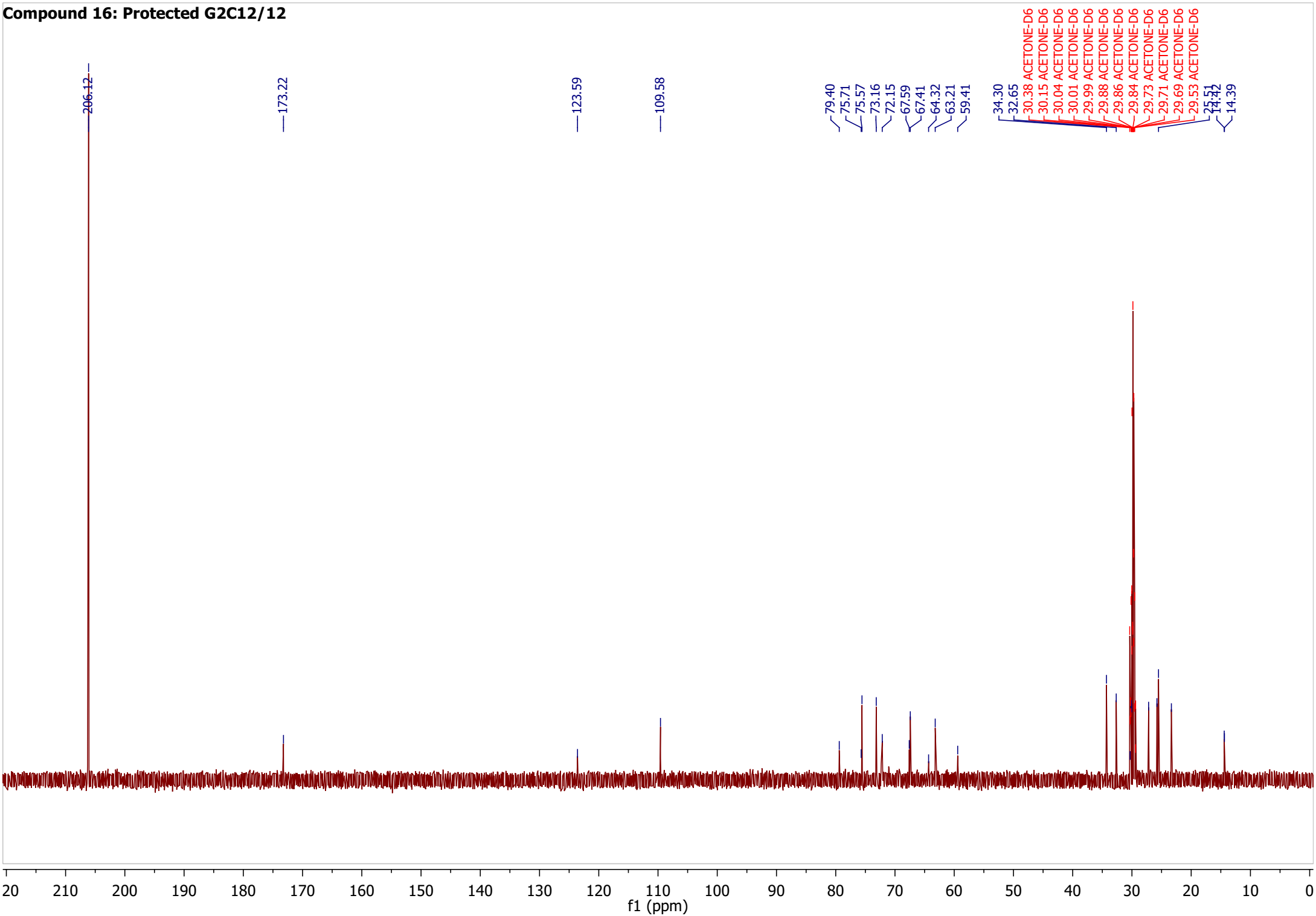


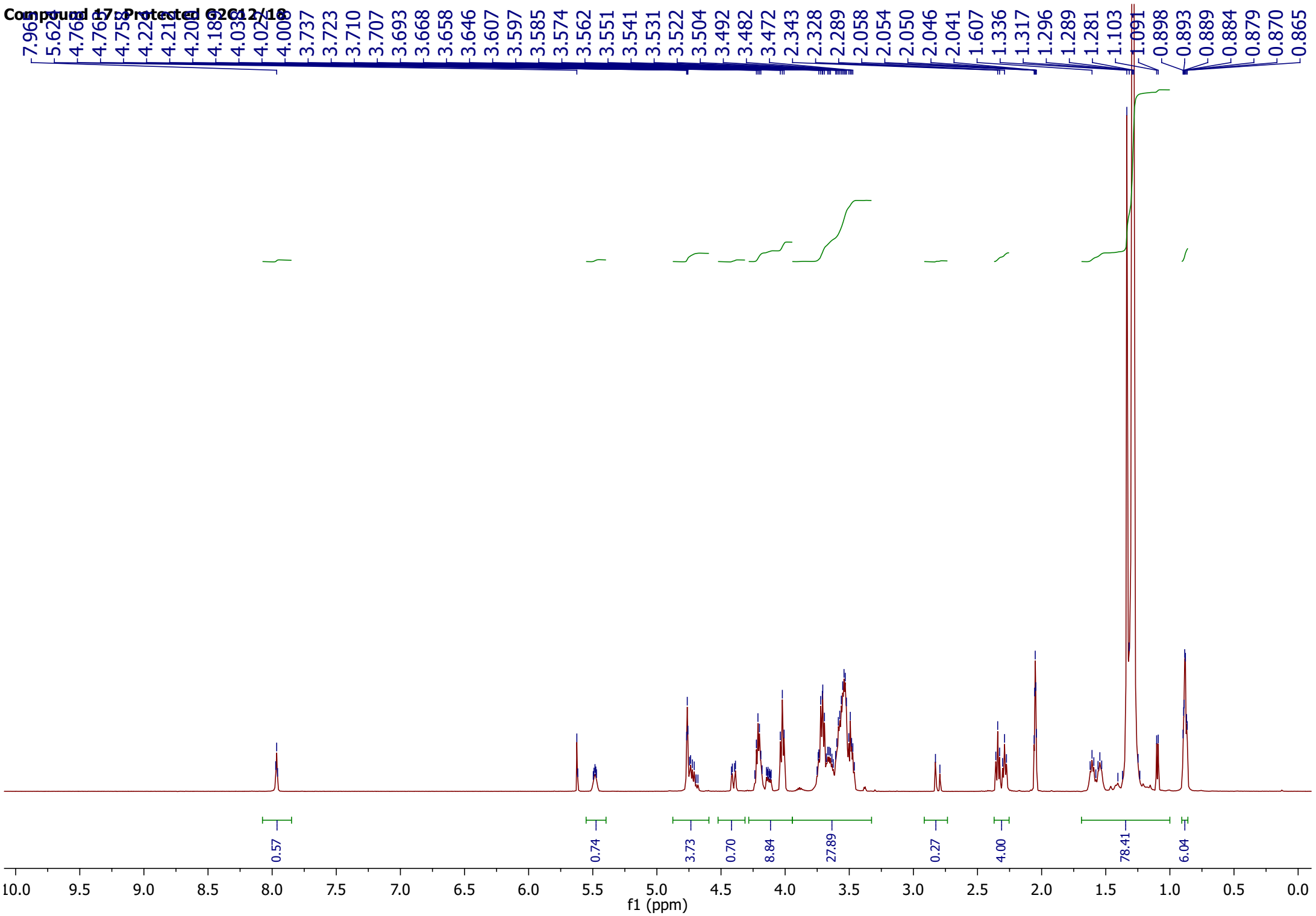
Figure S4. Cryo-TEM images of a sample of amphiphile **2** prior (a) and after (b) encapsulation of Nimodipine. The coexistence of spherical and worm-like micelles persists even after encapsulation of the guest molecule. (Scale bars 100 nm)

9) Representation NMR spectra for final compounds

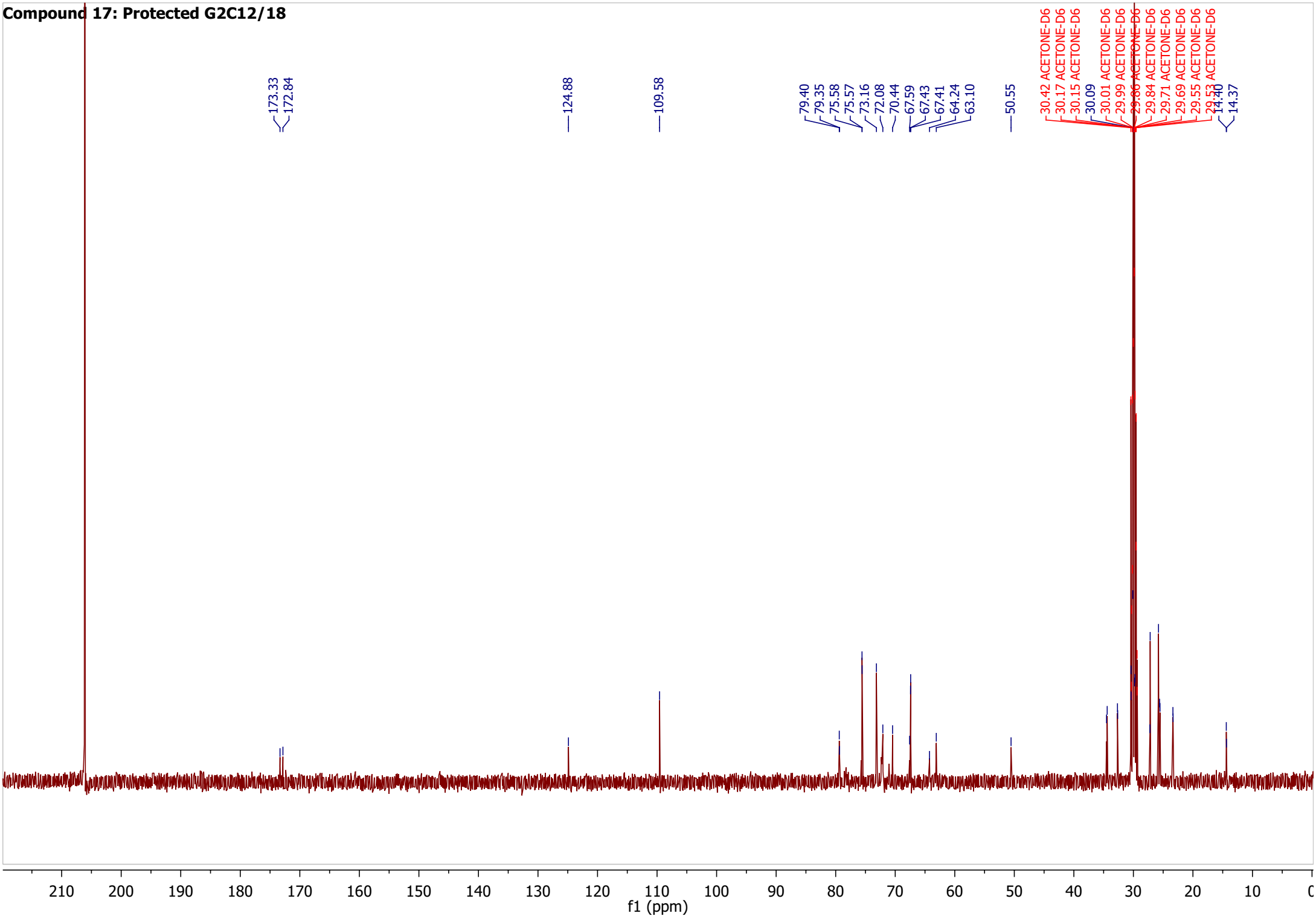

Compound 16: Protected G2C12/12
8.07
8.07
8.06
8.06
5.21
5.20
4.78
4.78
4.60
4.58
4.57
4.20
4.02
4.02
4.01
3.72
3.71
3.71
3.58
3.57
3.56
3.55
3.54
3.53
3.52
3.51
2.30
2.29
2.29
2.05
2.05
2.05
1.55
1.34
1.33
1.33
1.29
1.28
0.89
0.89
0.89
0.88
0.87
0.87
0.86
0.67
0.75
1.78
3.76
3.79
3.80
26.87
3.81
3.90
56.55
5.89
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.
f1 (ppm)

Compound 16: Protected G2C12/12

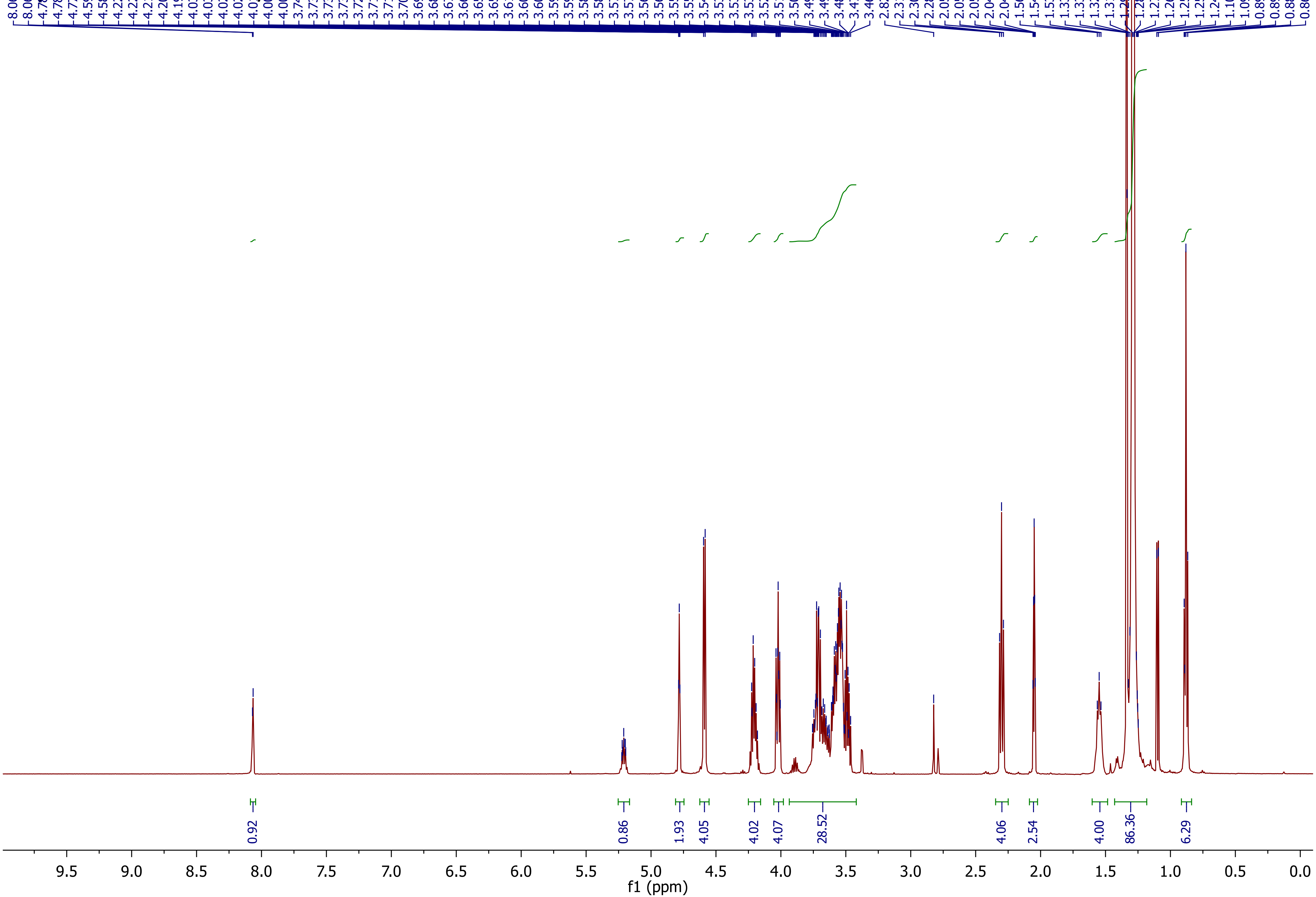



Compound 17 Protected G2C12/18
7.962
5.622
4.767
4.761
4.758
4.224
4.216
4.205
4.187
4.039
4.027
4.008
3.737
3.723
3.710
3.707
3.693
3.668
3.658
3.646
3.607
3.597
3.585
3.574
3.562
3.551
3.541
3.531
3.522
3.504
3.492
3.482
3.472
2.343
2.328
2.289
2.058
2.054
2.050
2.046
2.041
1.607
1.336
1.317
1.296
1.289
1.281
1.103
1.091
0.898
0.893
0.889
0.884
0.879
0.870
0.865
0.57
0.74
3.73
0.70
8.84
27.89
0.27
4.00
78.41
6.04
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

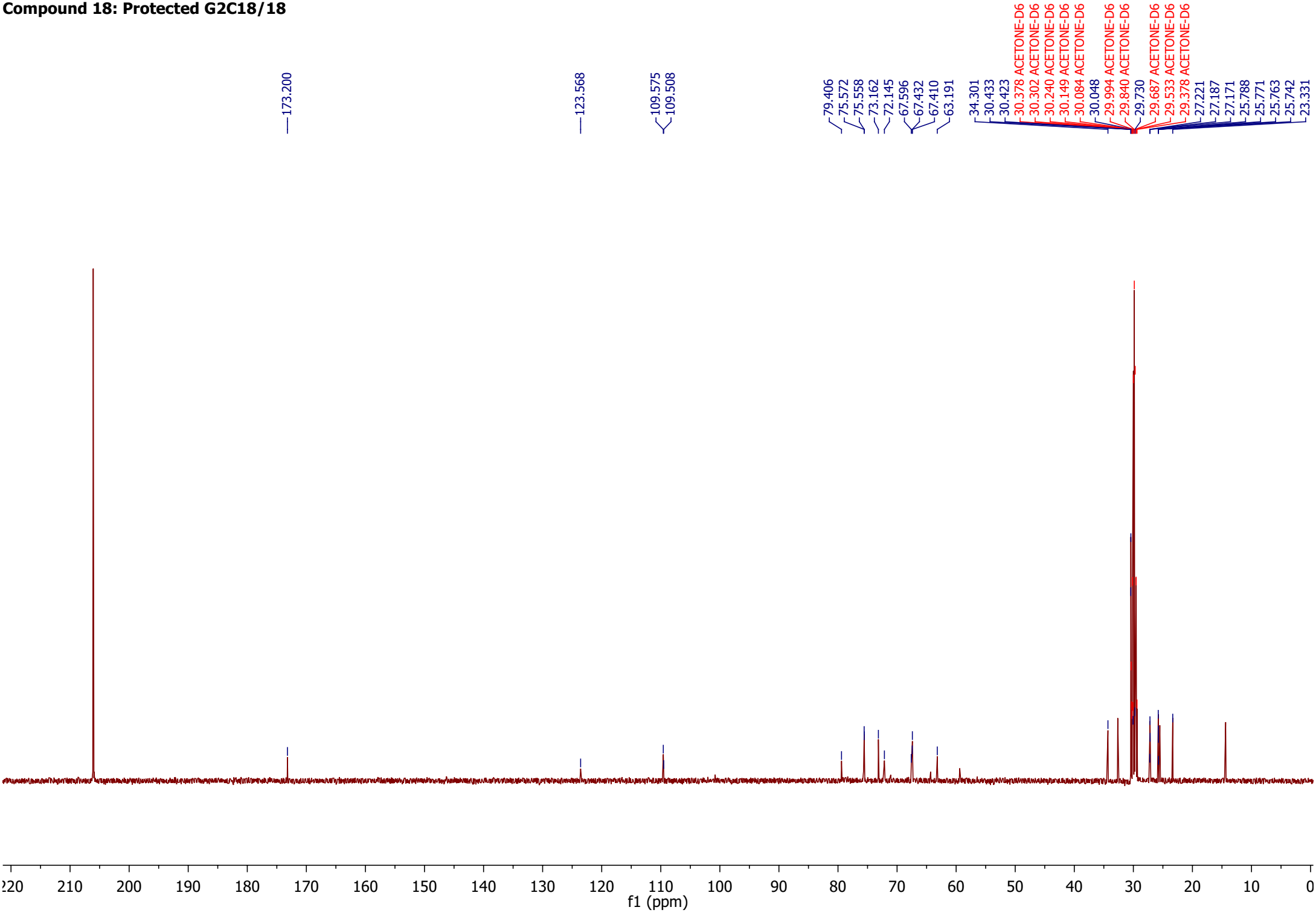
Compound 17: Protected G2C12/18



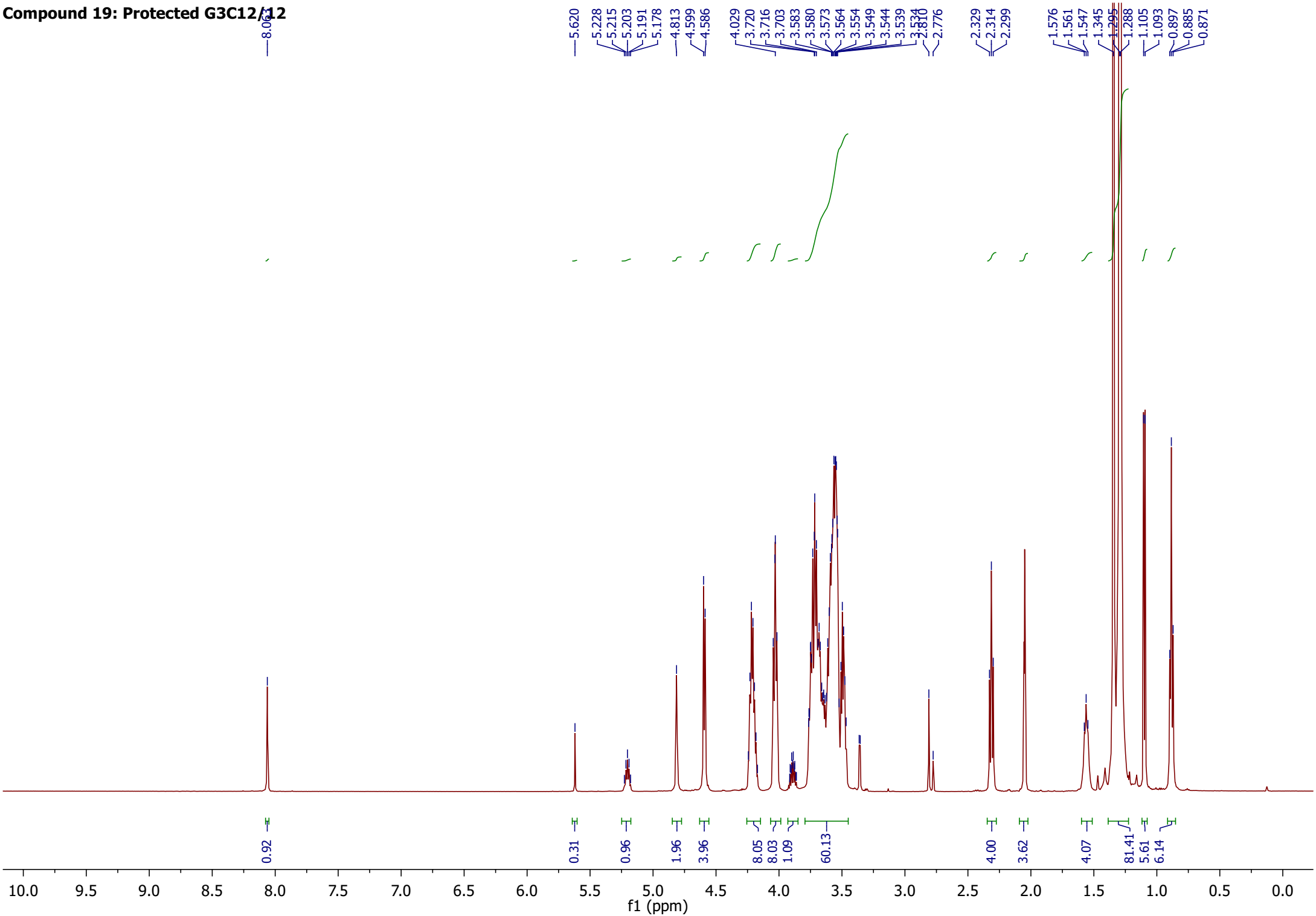
Compound 18: Protected G2C18/18



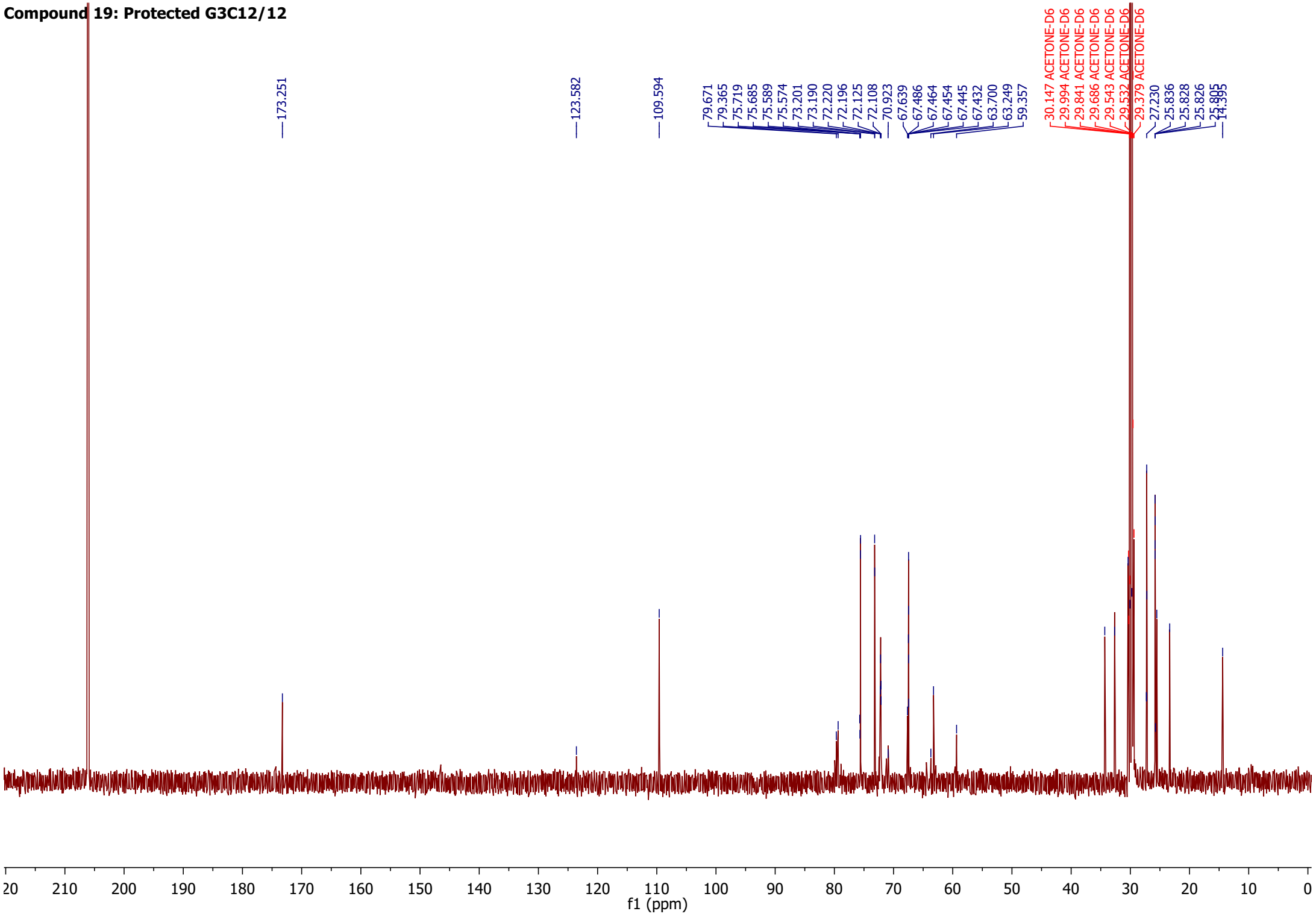
Compound 18: Protected G2C18/18

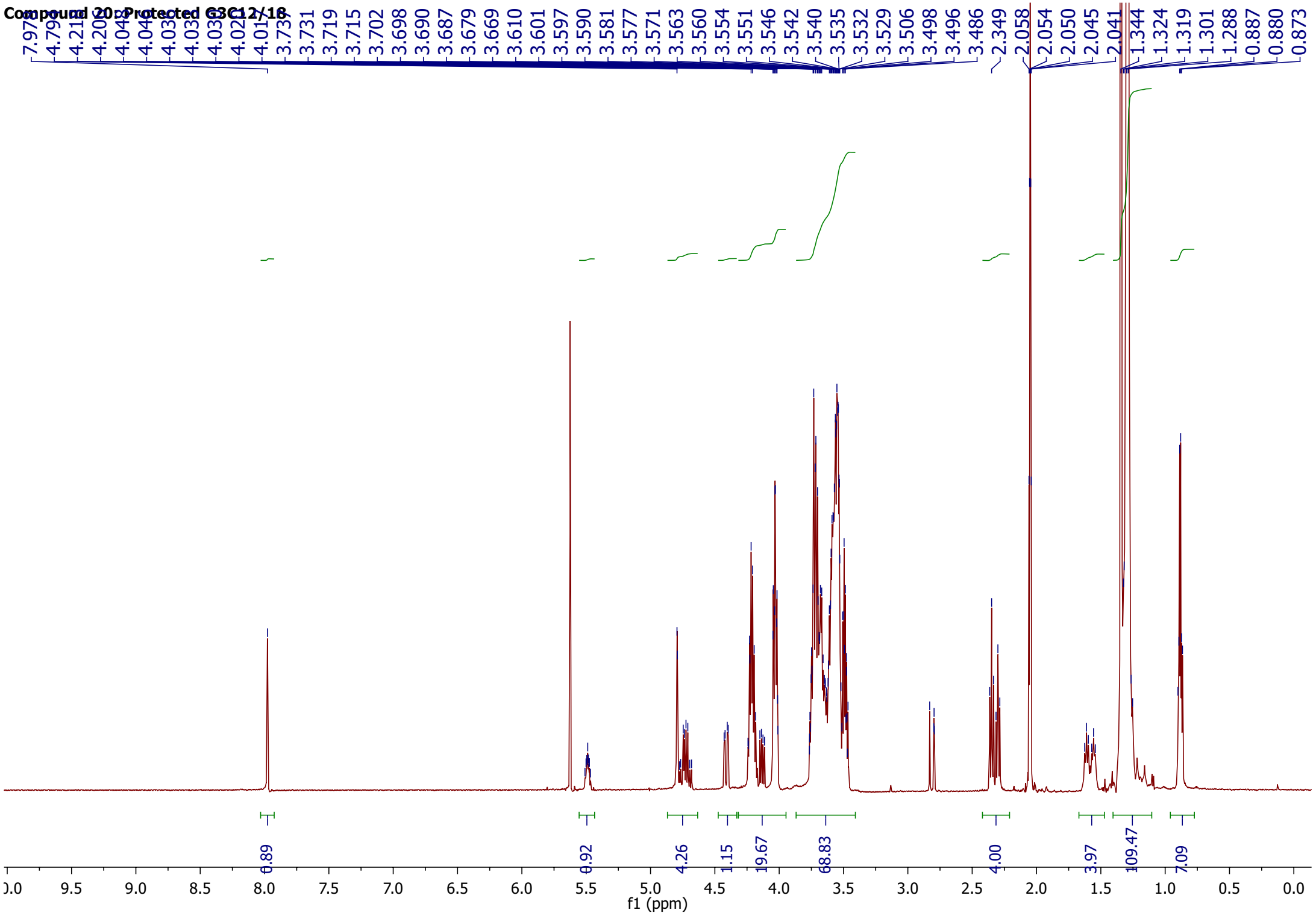


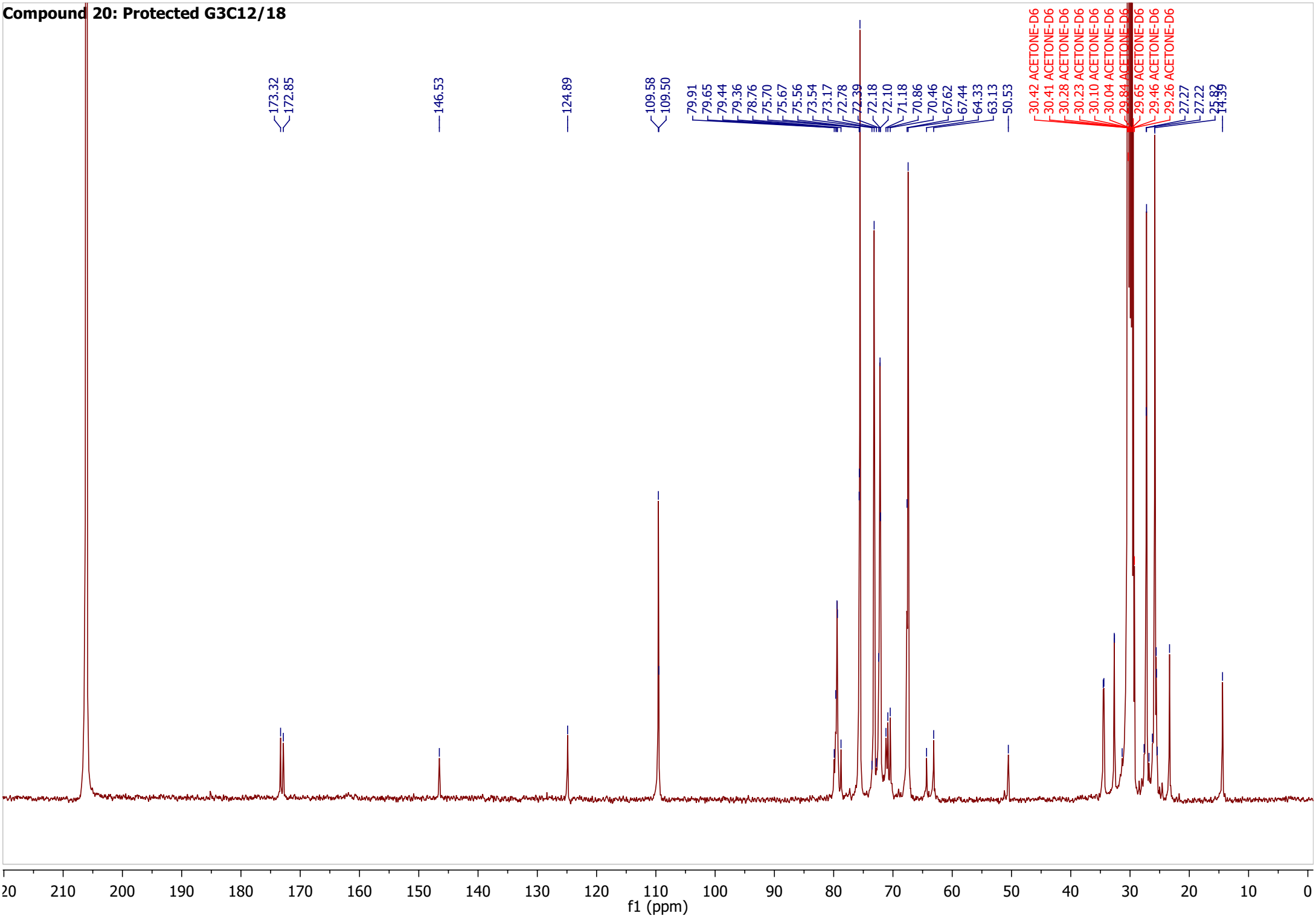
Compound 19: Protected G3C12/12



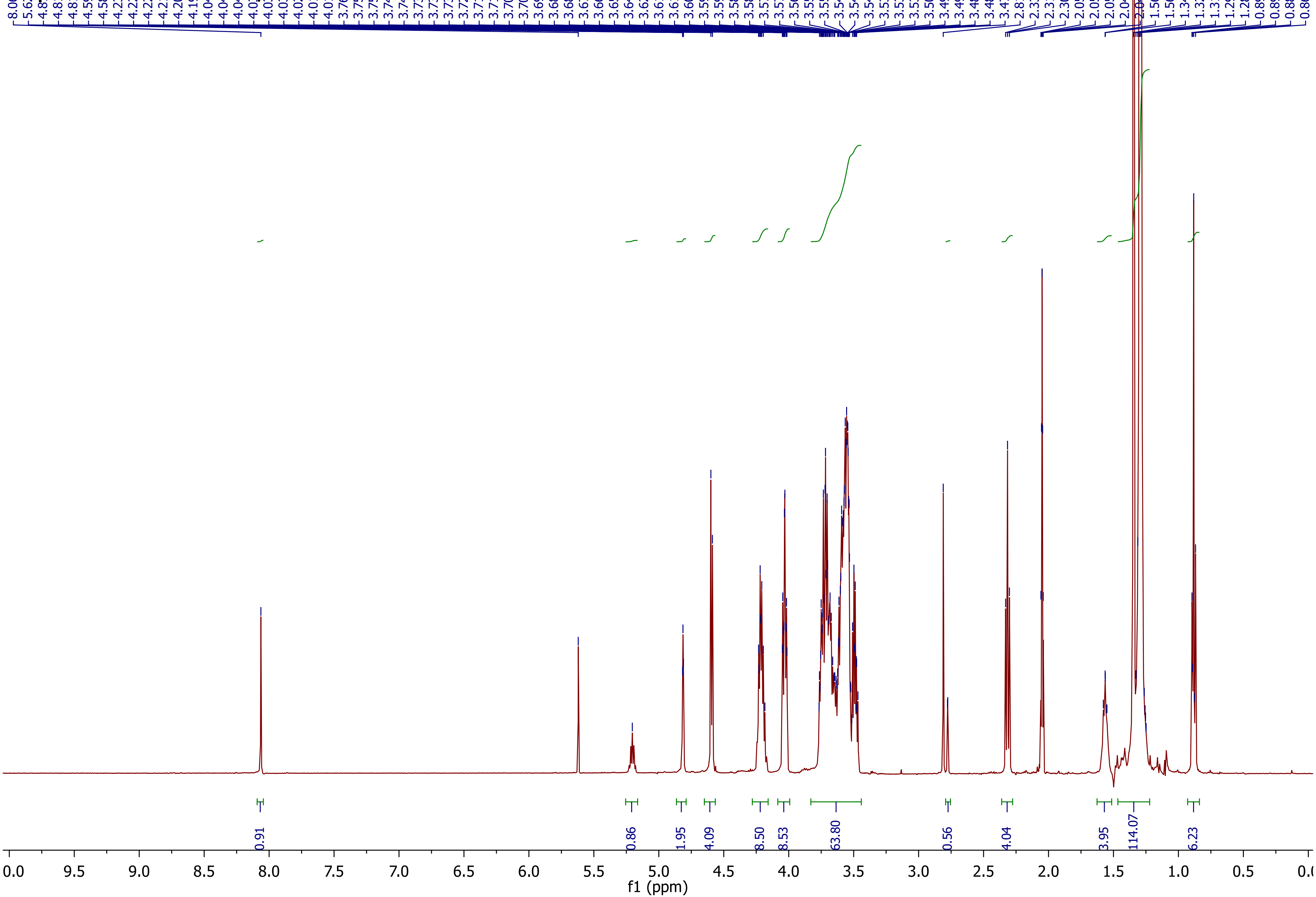
Compound 19: Protected G3C12/12



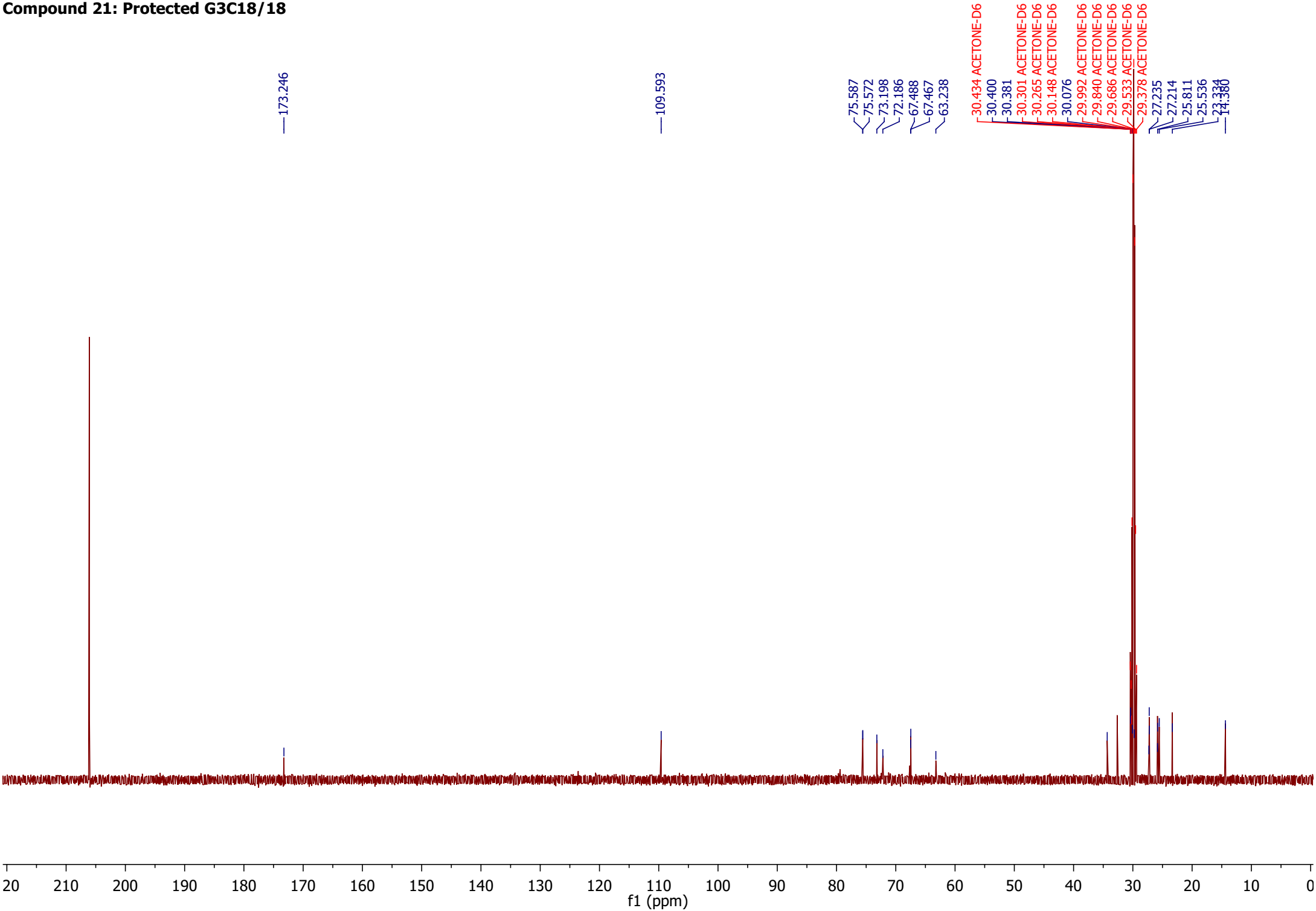

Compound 20 Protected G3C12/18
7.970
4.791
4.213
4.204
4.048
4.041
4.036
4.031
4.027
4.017
3.739
3.731
3.719
3.715
3.702
3.698
3.690
3.687
3.679
3.669
3.610
3.601
3.597
3.590
3.581
3.577
3.571
3.563
3.560
3.554
3.551
3.546
3.542
3.540
3.535
3.532
3.529
3.506
3.498
3.496
3.486
2.349
2.058
2.054
2.050
2.045
2.041
1.344
1.324
1.319
1.301
1.288
0.887
0.880
0.873
0.89
0.92
4.26
1.15
19.67
68.83
4.00
3.97
109.47
7.09
f1 (ppm)


Compound 20: Protected G3C12/18
173.32
172.85
146.53
124.89
109.58
109.50
79.91
79.65
79.44
79.36
78.76
75.70
75.67
75.56
73.54
73.17
72.78
72.39
72.18
72.10
71.18
70.86
70.46
67.62
67.44
64.33
63.13
50.53
30.42 ACETONE-D6
30.41 ACETONE-D6
30.28 ACETONE-D6
30.23 ACETONE-D6
30.10 ACETONE-D6
30.04 ACETONE-D6
29.84 ACETONE-D6
29.65 ACETONE-D6
29.46 ACETONE-D6
29.26 ACETONE-D6
27.27
27.22
25.82
14.39
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

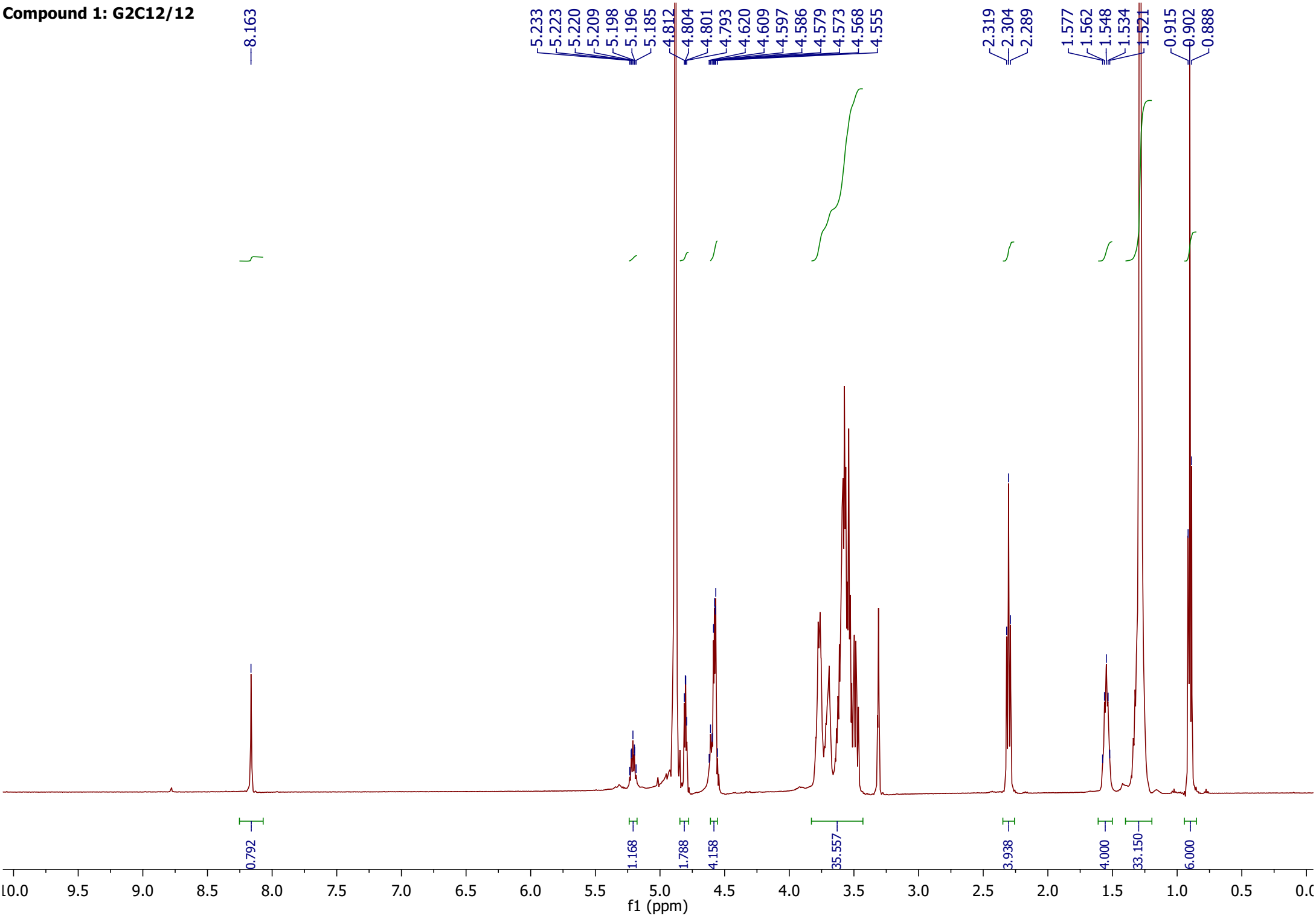
Compound 21: Protected G3C18/18



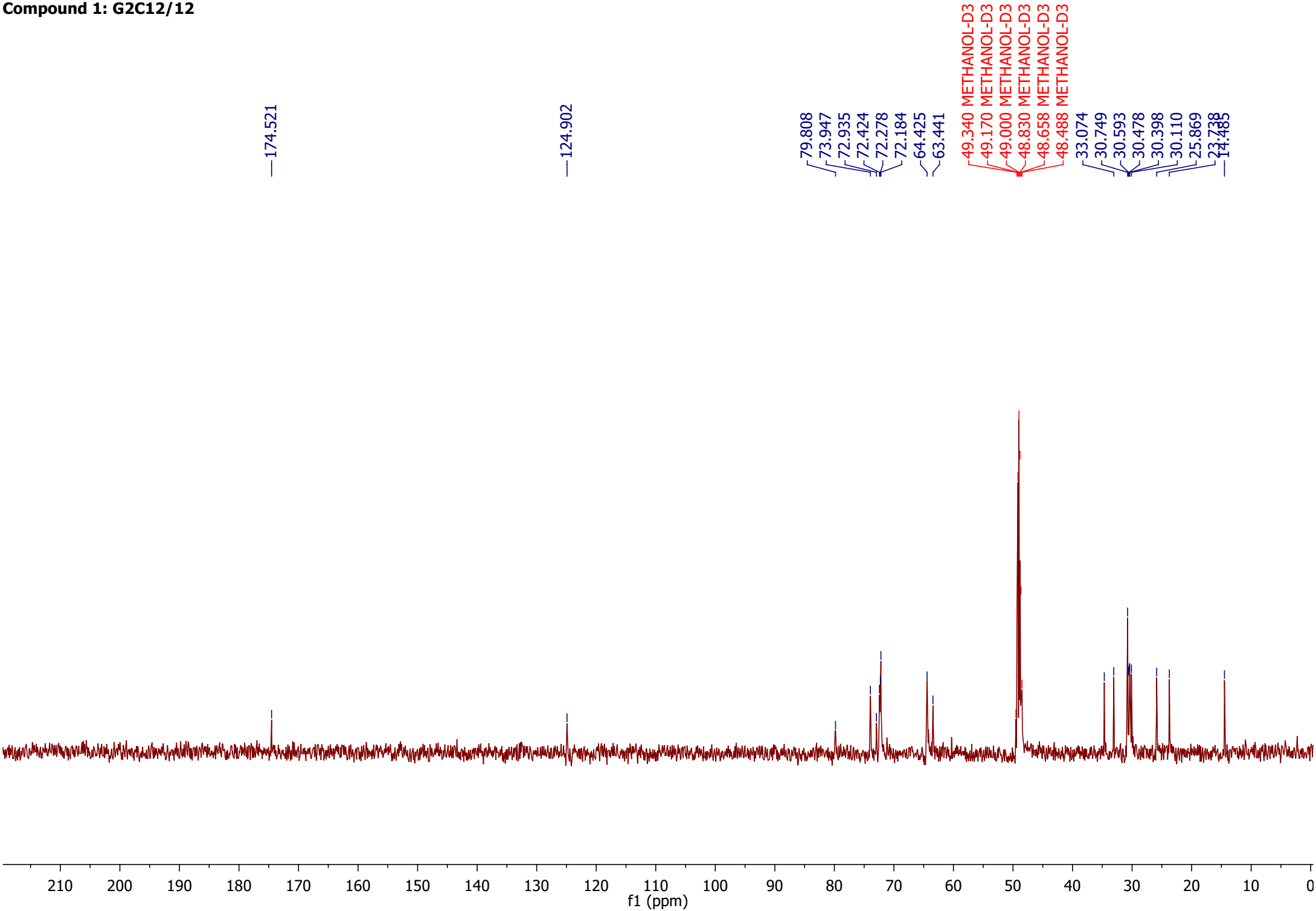
Compound 21: Protected G3C18/18

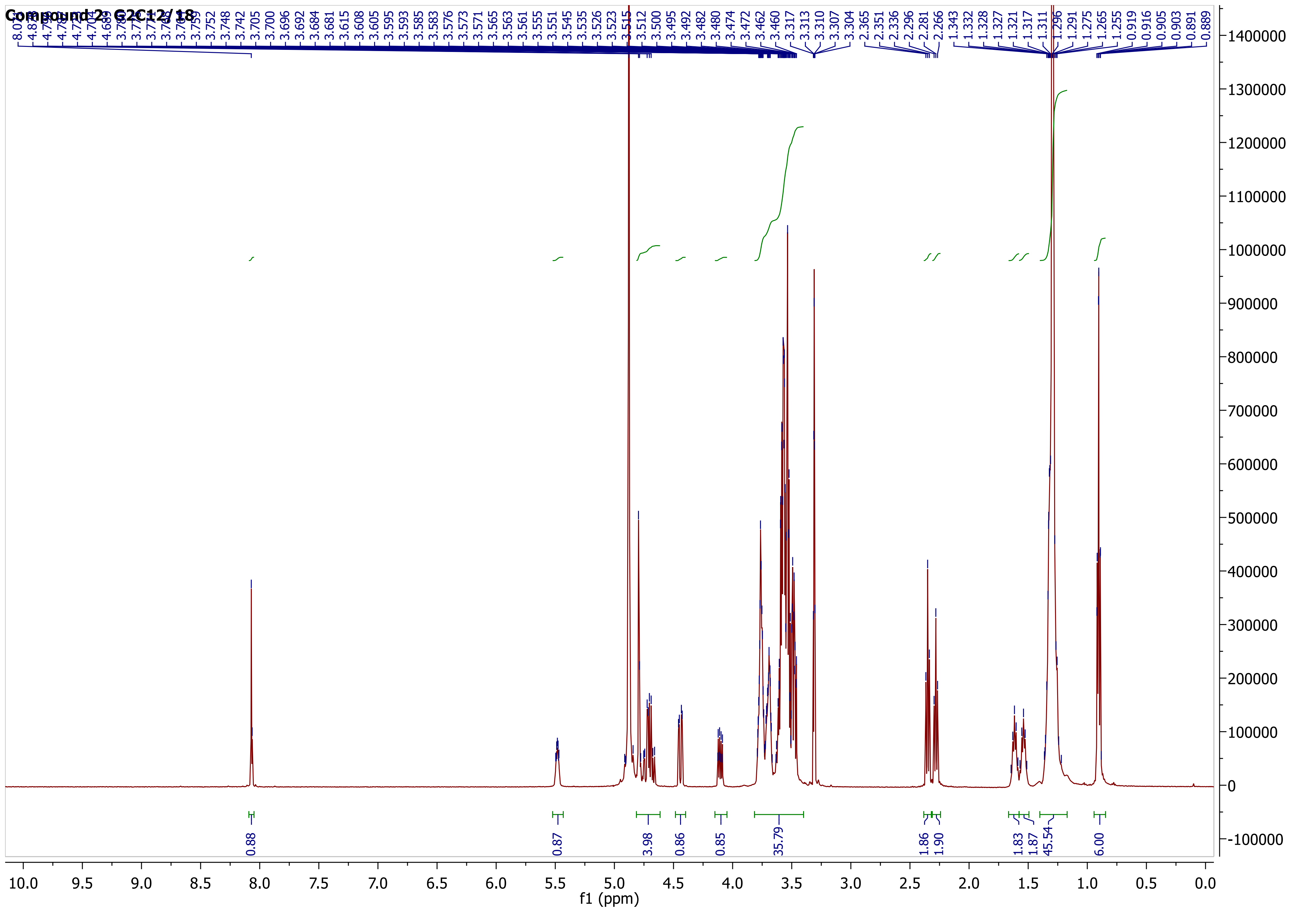


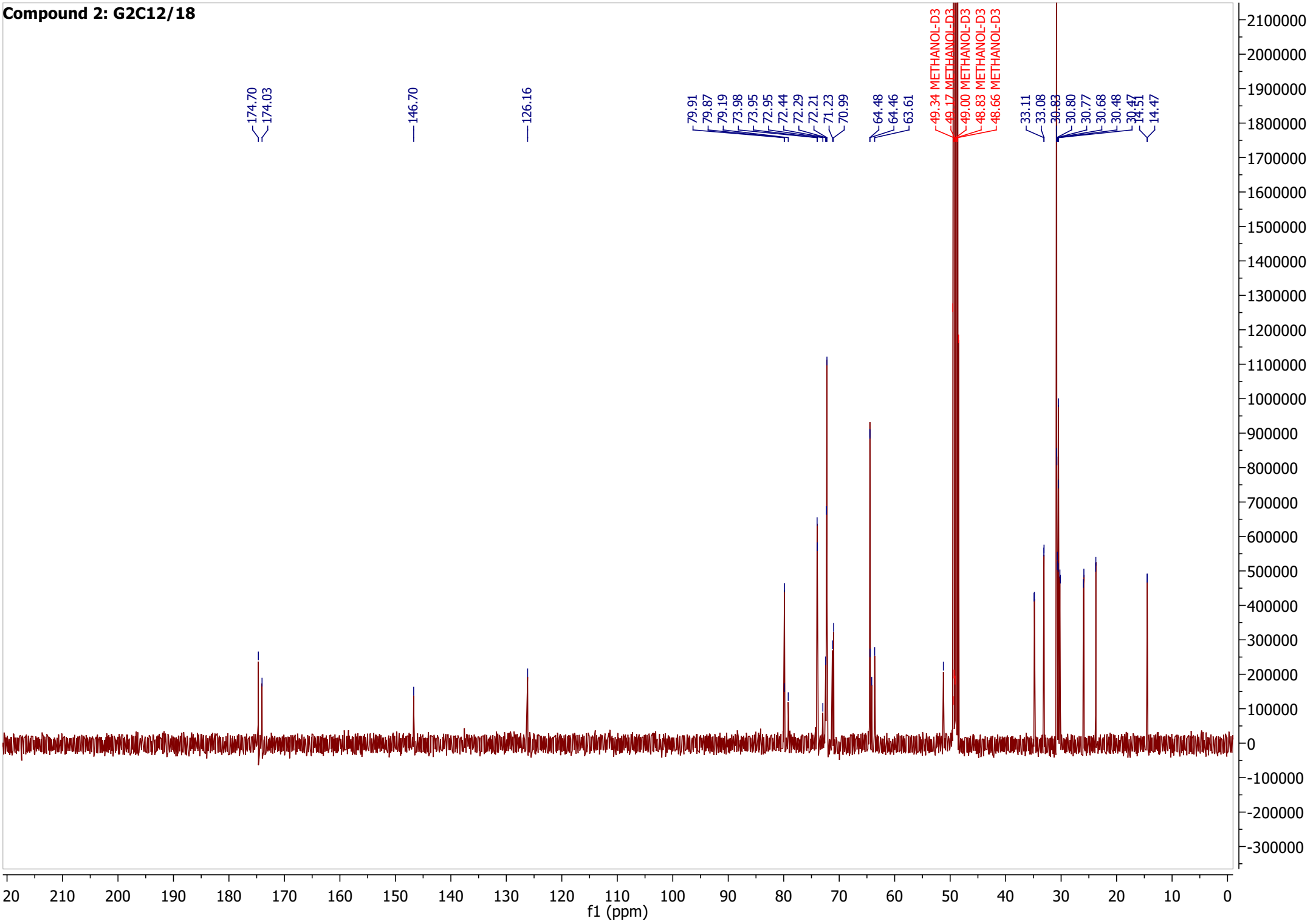
Compound 1: G2C12/12



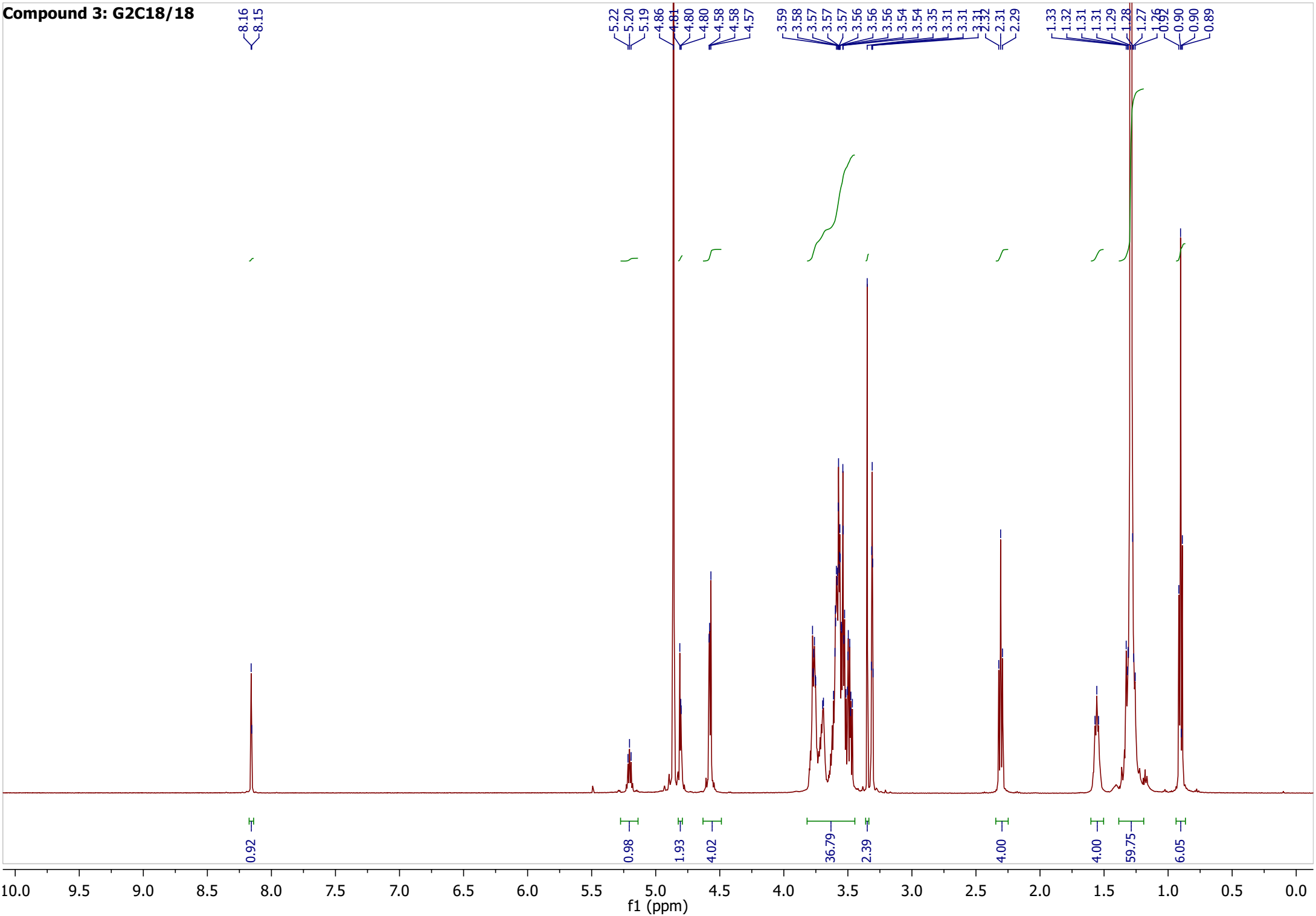
Compound 1: G2C12/12



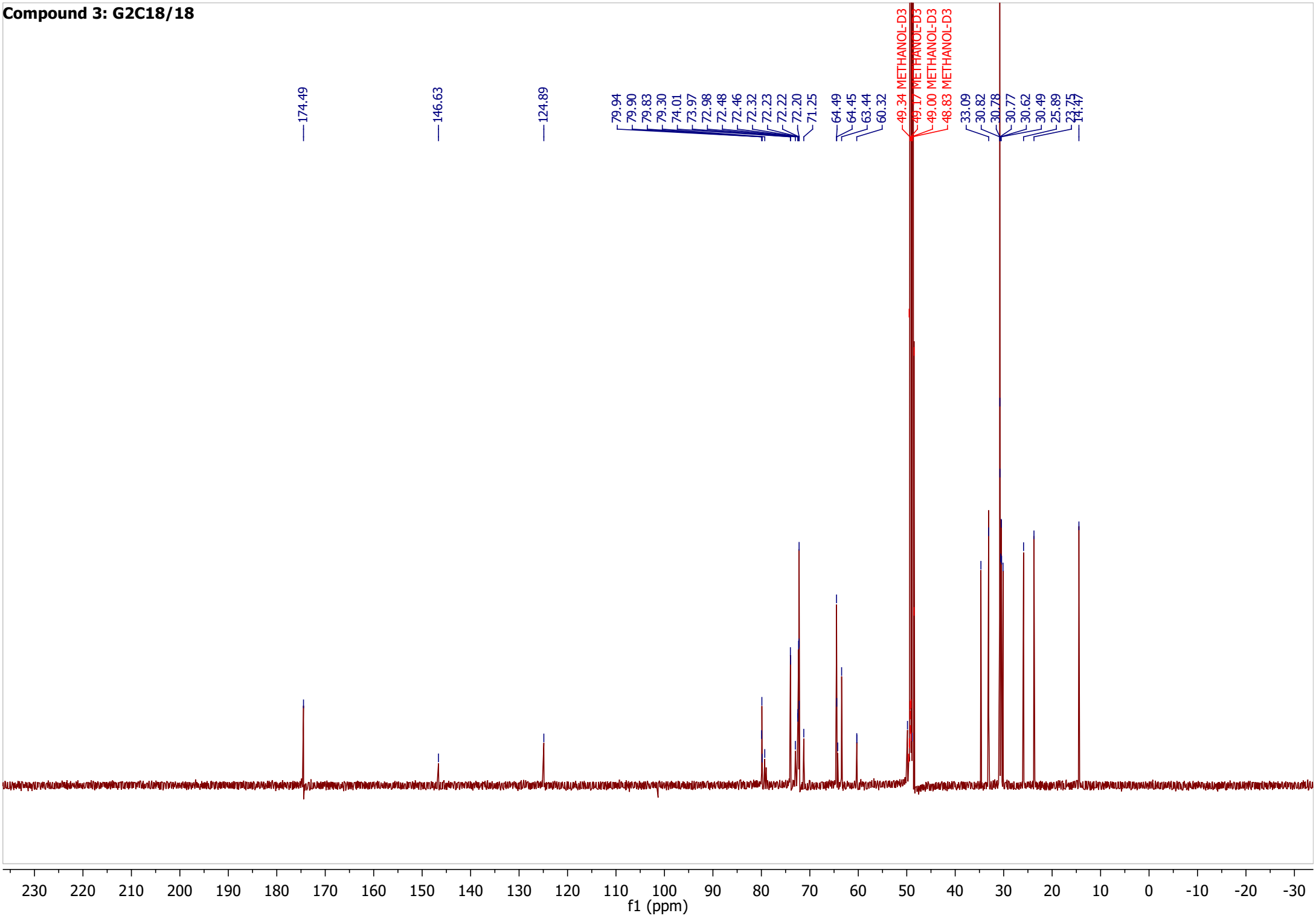

Compound 2: G2C12/18
f1 (ppm)


Compound 2: G2C12/18
174.70
174.03
146.70
126.16
79.91
79.87
79.19
73.98
73.95
72.95
72.44
72.29
72.21
71.23
70.99
64.48
64.46
63.61
49.34 METHANOL-D3
49.17 METHANOL-D3
49.00 METHANOL-D3
48.83 METHANOL-D3
48.66 METHANOL-D3
33.11
33.08
30.83
30.80
30.77
30.68
30.48
14.51
14.47
f1 (ppm)

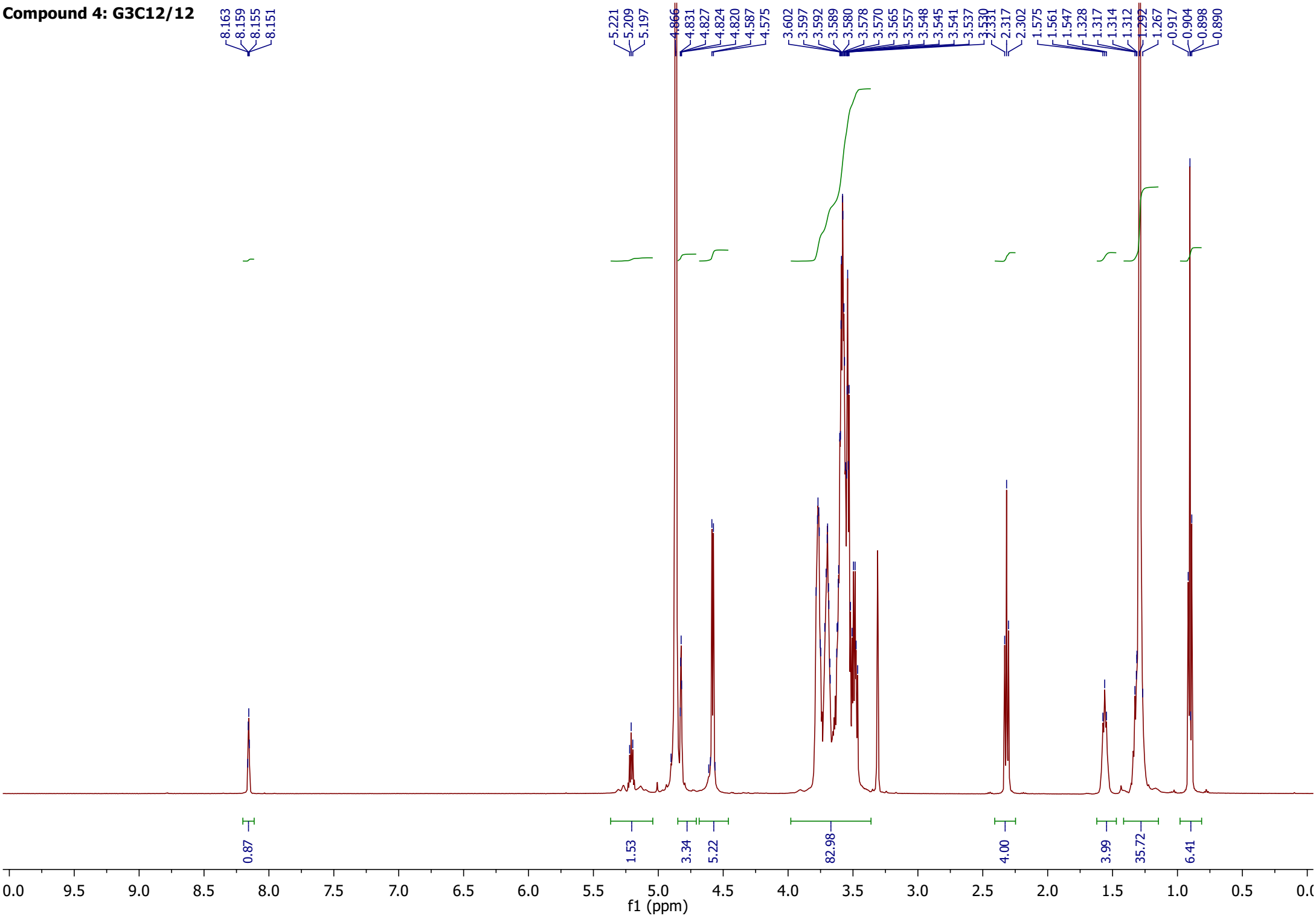
Compound 3: G2C18/18



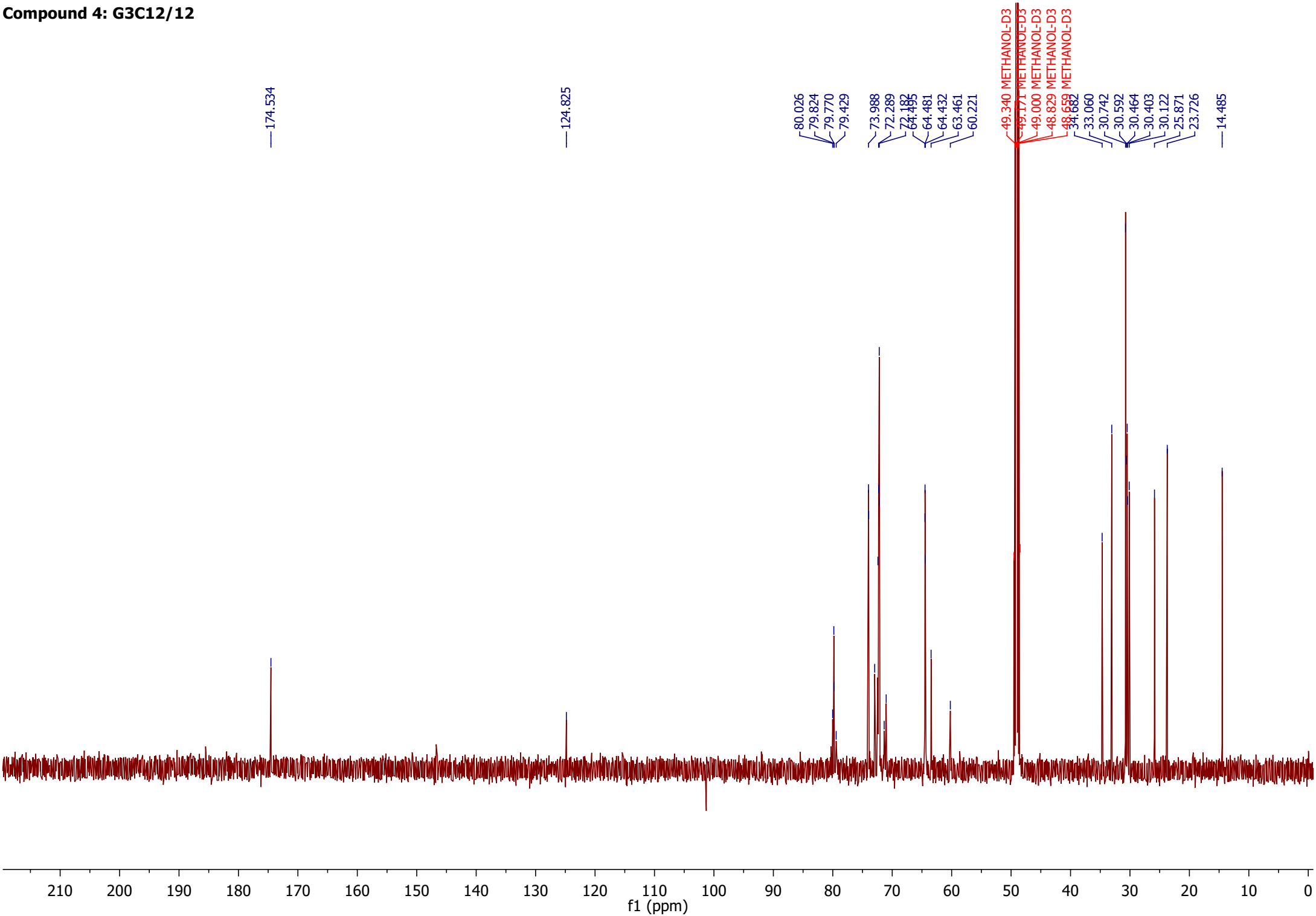
Compound 3: G2C18/18

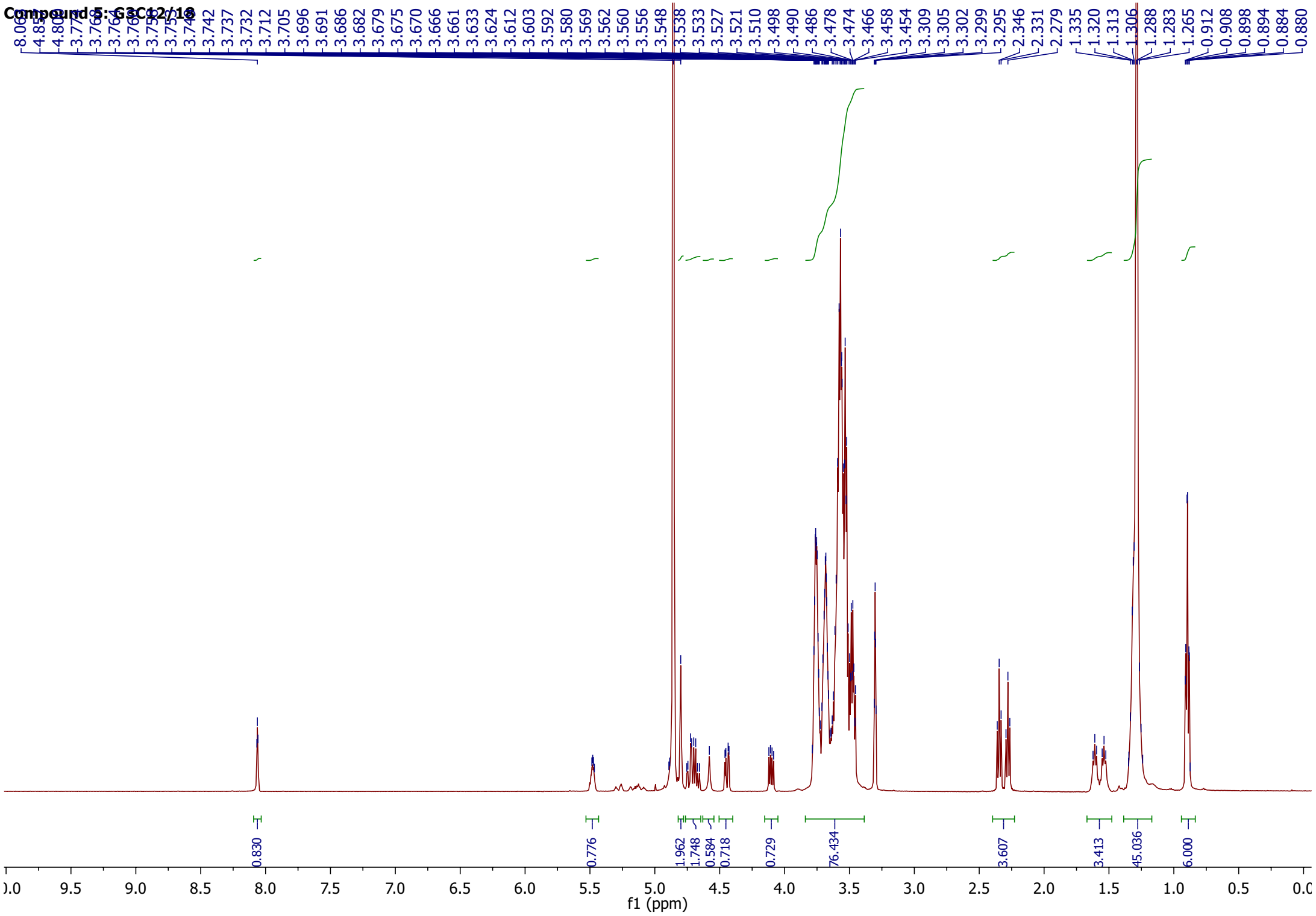


Compound 4: G3C12/12

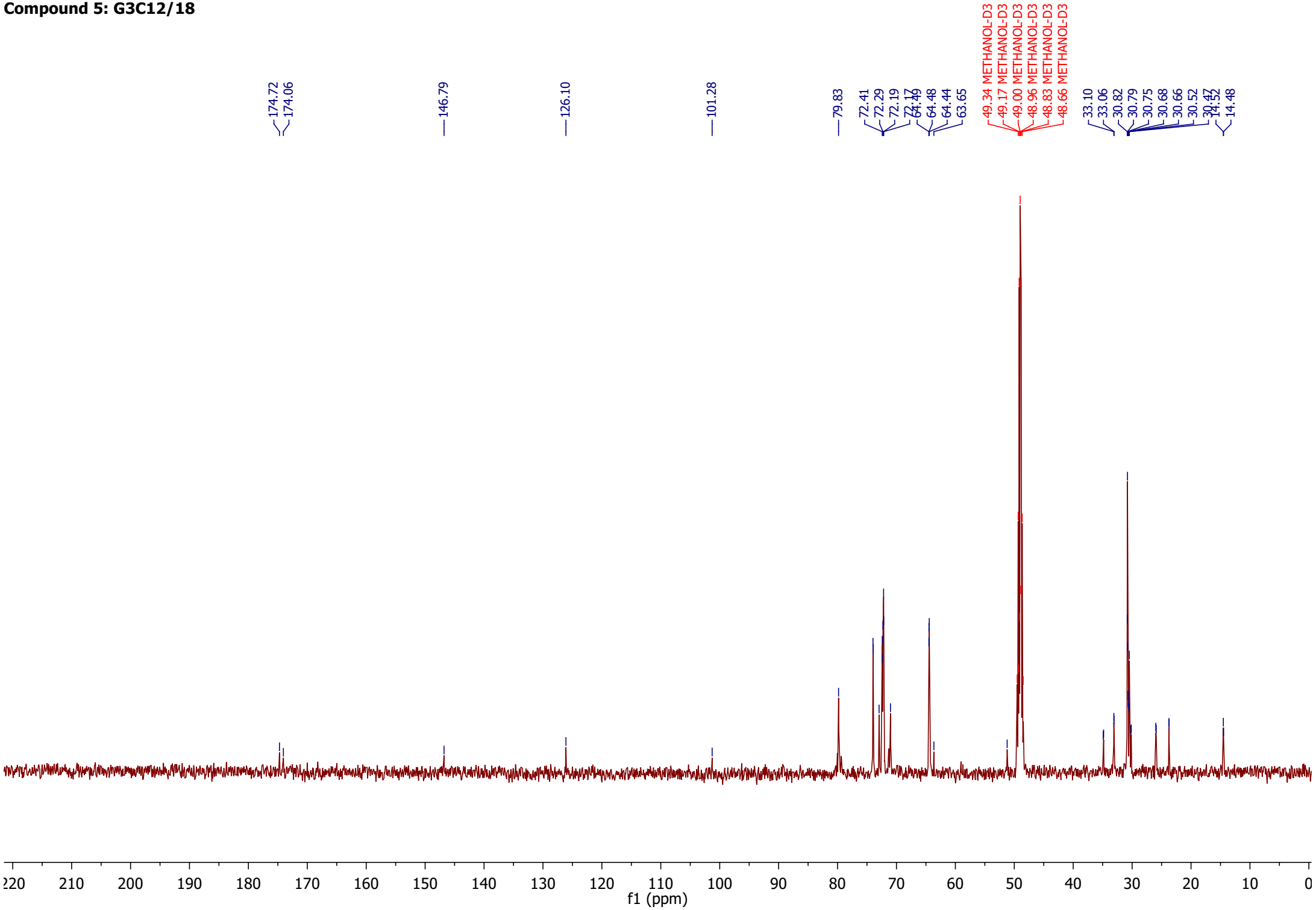


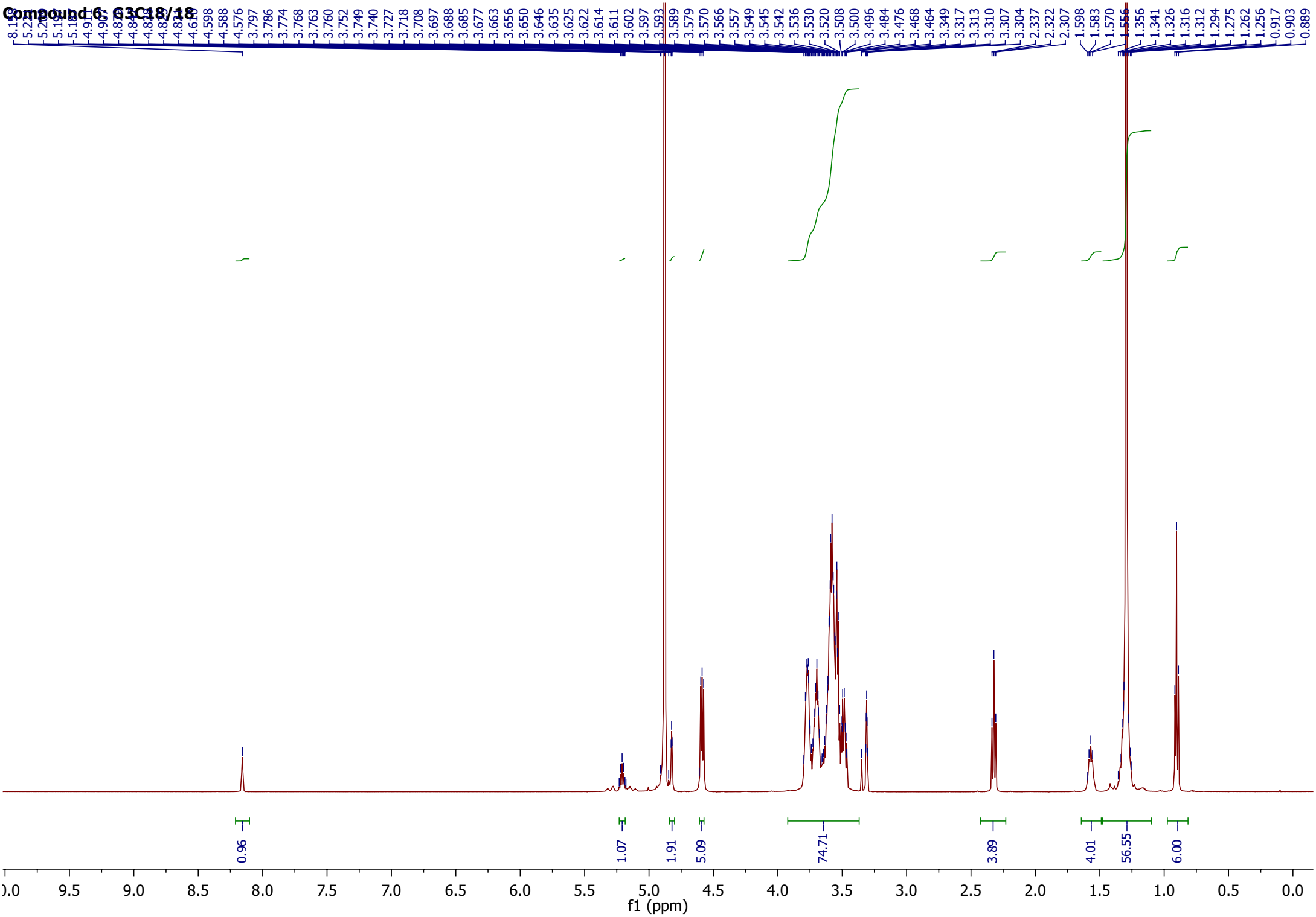
Compound 4: G3C12/12




Compound 5: G3C12/13
8.06
4.85
4.80
3.77
3.76
3.76
3.76
3.75
3.75
3.74
3.74
3.73
3.73
3.71
3.70
3.69
3.69
3.68
3.68
3.67
3.67
3.67
3.66
3.66
3.63
3.62
3.61
3.60
3.59
3.58
3.56
3.56
3.55
3.54
3.53
3.53
3.52
3.51
3.49
3.49
3.48
3.47
3.46
3.45
3.45
3.30
3.30
3.30
3.29
3.29
2.34
2.33
2.27
1.33
1.32
1.31
1.30
1.28
1.28
1.26
0.91
0.90
0.89
0.89
0.88
0.83
0.78
1.96
1.75
0.58
0.72
0.73
76.43
3.61
3.41
45.04
6.00
f1 (ppm)

Compound 5: G3C12/18




Compound 6: 63C18/18
8.194
5.224
5.205
5.190
5.180
4.918
4.907
4.875
4.847
4.844
4.837
4.830
4.611
4.598
4.588
4.576
3.797
3.786
3.774
3.768
3.763
3.760
3.752
3.749
3.740
3.727
3.718
3.708
3.697
3.688
3.685
3.677
3.663
3.656
3.650
3.646
3.635
3.625
3.622
3.614
3.611
3.602
3.597
3.593
3.589
3.579
3.570
3.566
3.557
3.549
3.545
3.542
3.536
3.530
3.520
3.508
3.500
3.496
3.484
3.476
3.468
3.464
3.349
3.317
3.313
3.310
3.307
3.304
2.337
2.322
2.307
1.598
1.583
1.570
1.556
1.356
1.341
1.326
1.316
1.312
1.294
1.275
1.262
1.256
0.917
0.903
0.889
0.96
1.07
1.91
5.09
74.71
3.89
4.01
56.55
6.00
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

Compound 6: G3C18/18