Supporting Information for

Natural Product-Directed Catalytic Stereoselective Synthesis of Functionalized Fused Borane Cluster–Oxazoles for the Discovery of Bactericidal Agents

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I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available and used without further purification. Anhydrous solvents were prepared by passage through activated Al_2O_3 and stored over 3 Å molecular sieves. Acetone-d_6 was purchased from Cambridge Isotope Laboratories. $[Et_3NH][B_{12}H_{11}NH_3]$ (aminododecaborate starting material) was prepared according to the literature.[1,2]

Reaction conditions

Glassware for air-sensitive reactions was dried at 150 °C and allowed to cool in a vacuum. Reactions that were carried out in a glovebox were run under a nitrogen atmosphere with O_2 <1 ppm and H_2O <1 ppm.

Characterization

Thin-layer chromatography (TLC) was carried out using silica gel 60, F254 with a thickness of 0.25 mm. Column chromatography was performed on silica gel 60 (200-300 mesh).

Low-resolution ESI-MS data were recorded on Advion Expression CMS instrument.
High-resolution MS data were recorded using IT-TOF detection (Shimadzu, Japan) equipped with an electrospray ionization source (ESI).

Single-crystal X-ray diffraction studies were performed on an Oxford Diffraction Gemini A Ultra diffractometer equipped with an 135mm Atlas CCD detector and using Mo K-α radiation.

NMR spectra were recorded on a Bruker AVANCE III 400 spectrometer (^{1}H NMR 400.13 MHz, ^{13}C NMR 100.62 MHz, ^{11}B NMR 128.38 MHz) at the temperature indicated. Data are reported as follows: Chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc.), coupling constant *J* in Hz, integration, and (where applicable) interpretation. Signals were referenced against solvent peaks (^{1}H: residual $CHD_2C(O)CD_3$ = 2.05 ppm, $^{13}C\{^1H\}$: $CD_3C(O)CD_3$ = 29.84 ppm. ^{11}B and $^{11}B\{^1H\}$ NMR spectra were calibrated against external BF_3*Et_2O = 0 ppm (BF_3*Et_2O capillary in C_6D_6). All processing was performed using the software TopSpin.

Additional remarks about the NMR spectra

a) *Double water peaks*

In certain ^{1}H and $^{1}H\{^{11}B\}$ NMR spectra measured in acetone-d_6, double water peaks were observed. This is a result of different resonances from H_2O and HOD and has been described in the literature.[3] In our experience, the appearance of double water peaks depends on the temperature, water content and compound being measured. A spectrum of acetone-d_6 solvent as received from Cambridge Isotope Laboratories in which the distinct resonances of H_2O and HOD are visible is shown in Figure S1.

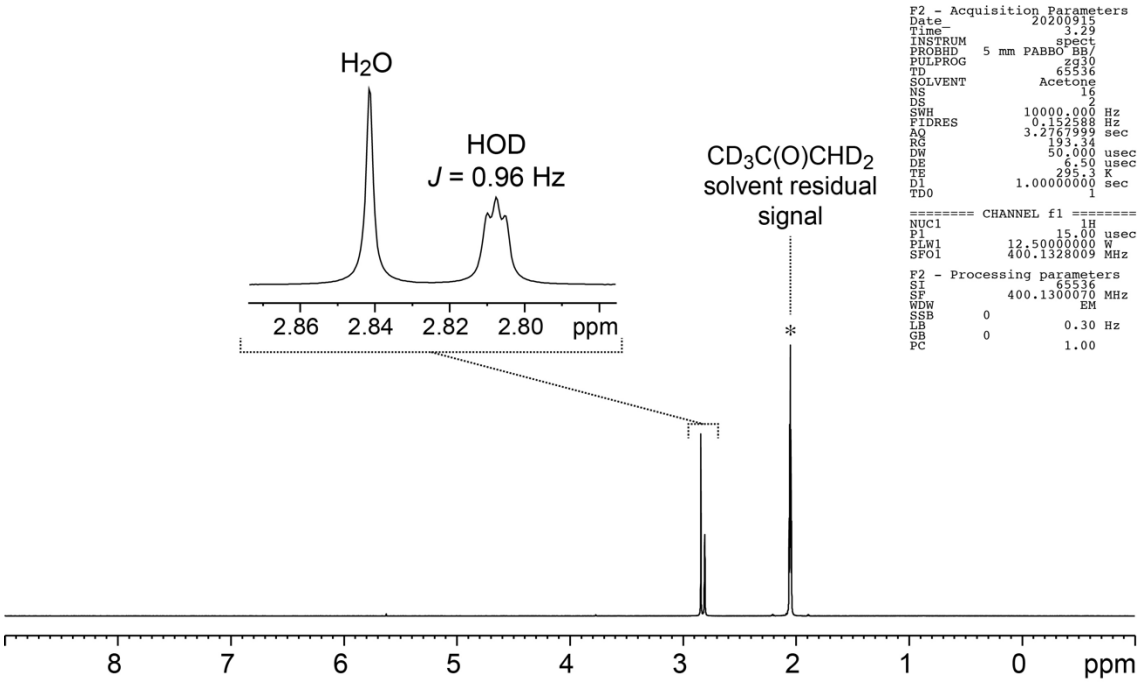


Figure S1. ^{1}H NMR spectrum of acetone-d_6 solvent as received from Cambridge Isotope Laboratories (400 MHz, 22 °C).

b) *Detection of B–**C** signals*

In the $^{13}C\{^{1}H\}$ NMR spectra of the products **13** and **14**, the B–***C*** signal appeared severely broadened because of coupling to the quadrupolar nuclei ^{10}B and ^{11}B. Therefore, only weak signals were observed, making direct detection difficult. This phenomenon is illustrated in Figure S2.

Indirect detection of the B–***C*** carbon atom was successful using ^{1}H-^{13}C HSQC NMR spectroscopy. In these spectra, the correlation signal caused by $^{1}J_{H,C}$ coupling between B–C***H₂*** and B–***C*** revealed the chemical shift of the B–***C*** position, which was uniformly observed at 19–20 ppm. This kind of detection is displayed for product **13a** in Figures S3 and S4.

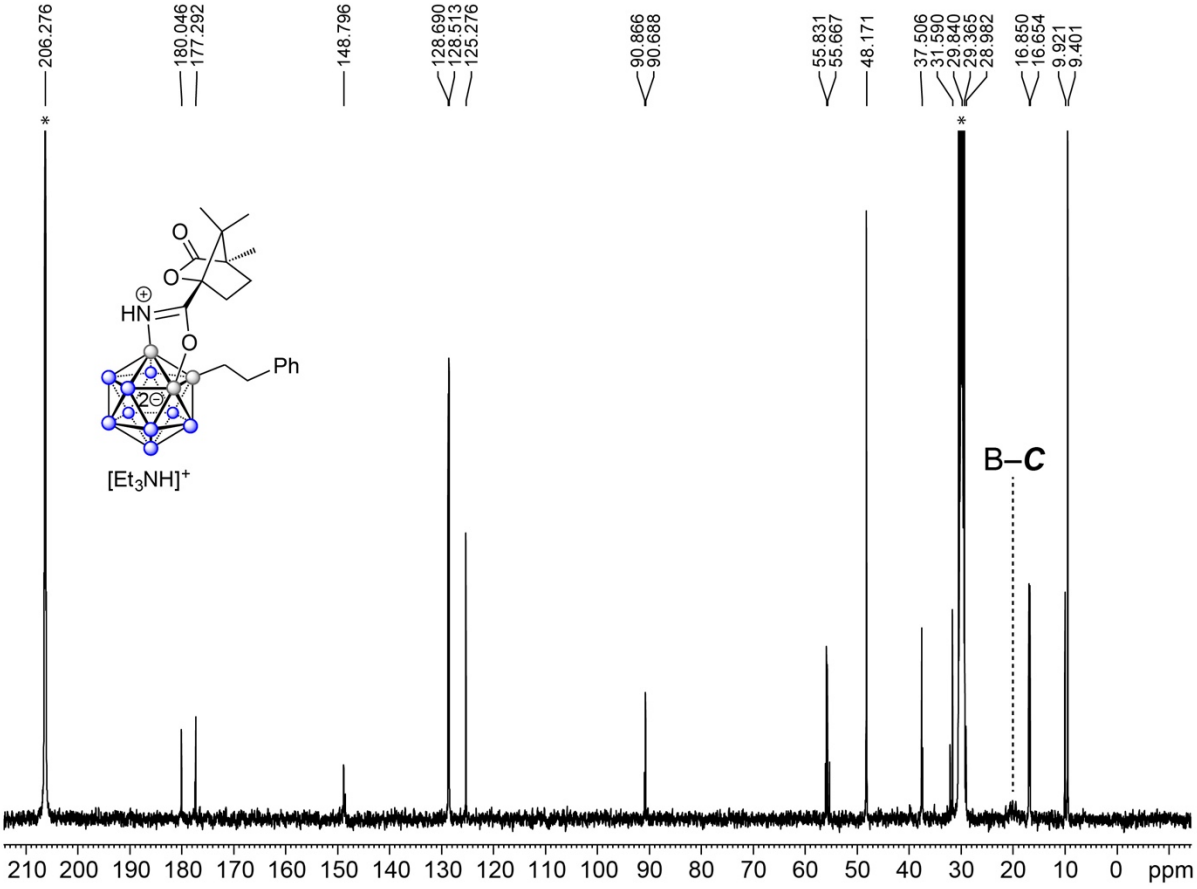


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of **13a** (acetone-d_6, 101 MHz, 23 °C). The B–***C*** signal is weak and broadened because of coupling to the quadrupolar nuclei ^{10}B and ^{11}B.

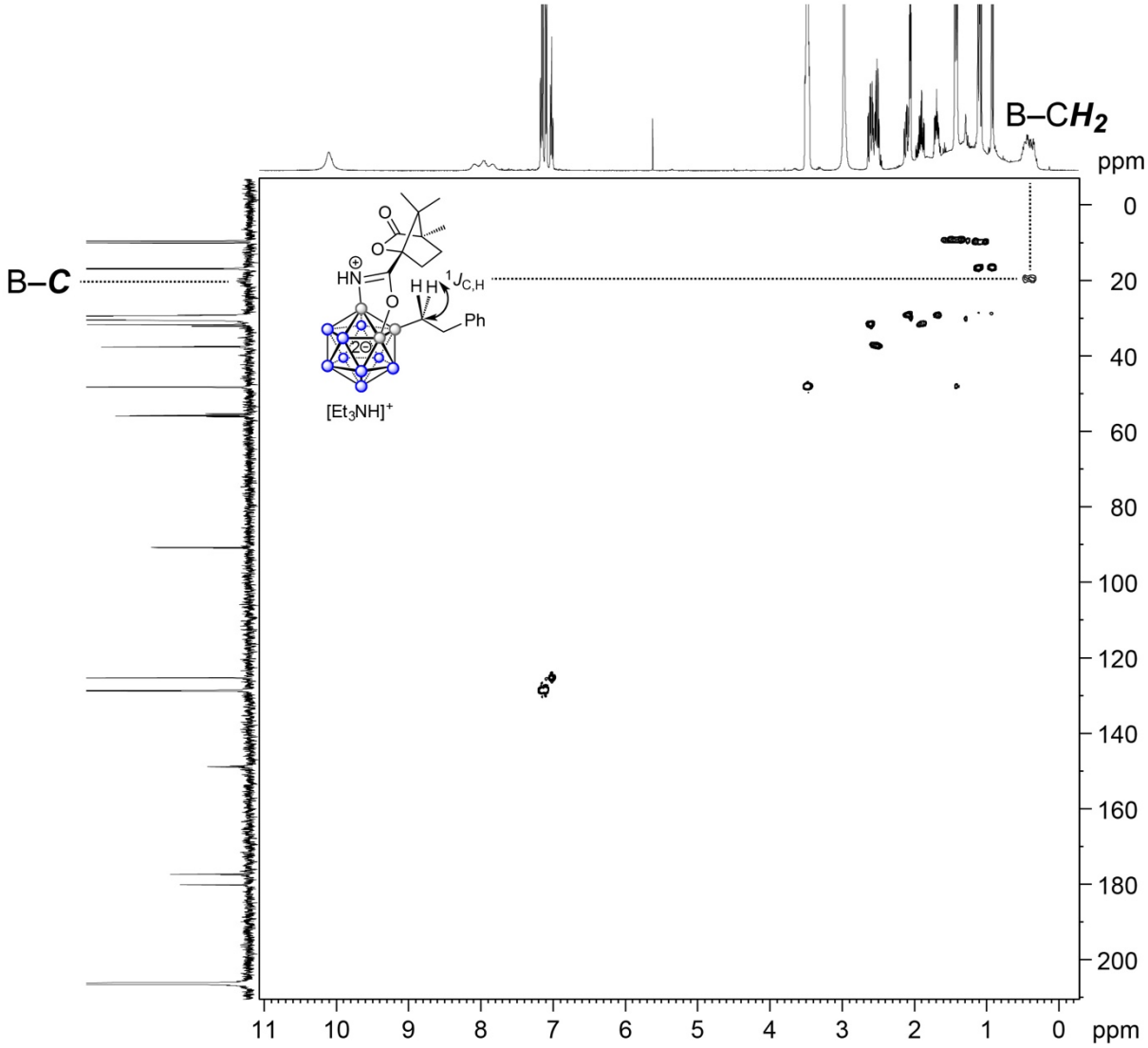


Figure S3. ^{1}H-^{13}C HSQC NMR spectrum of **13a** showing indirect detection of the B–***C*** resonance based on the correlation signal caused by $^{1}J_{H,C}$ coupling (400/101 MHz, acetone-d_6, 23 °C).

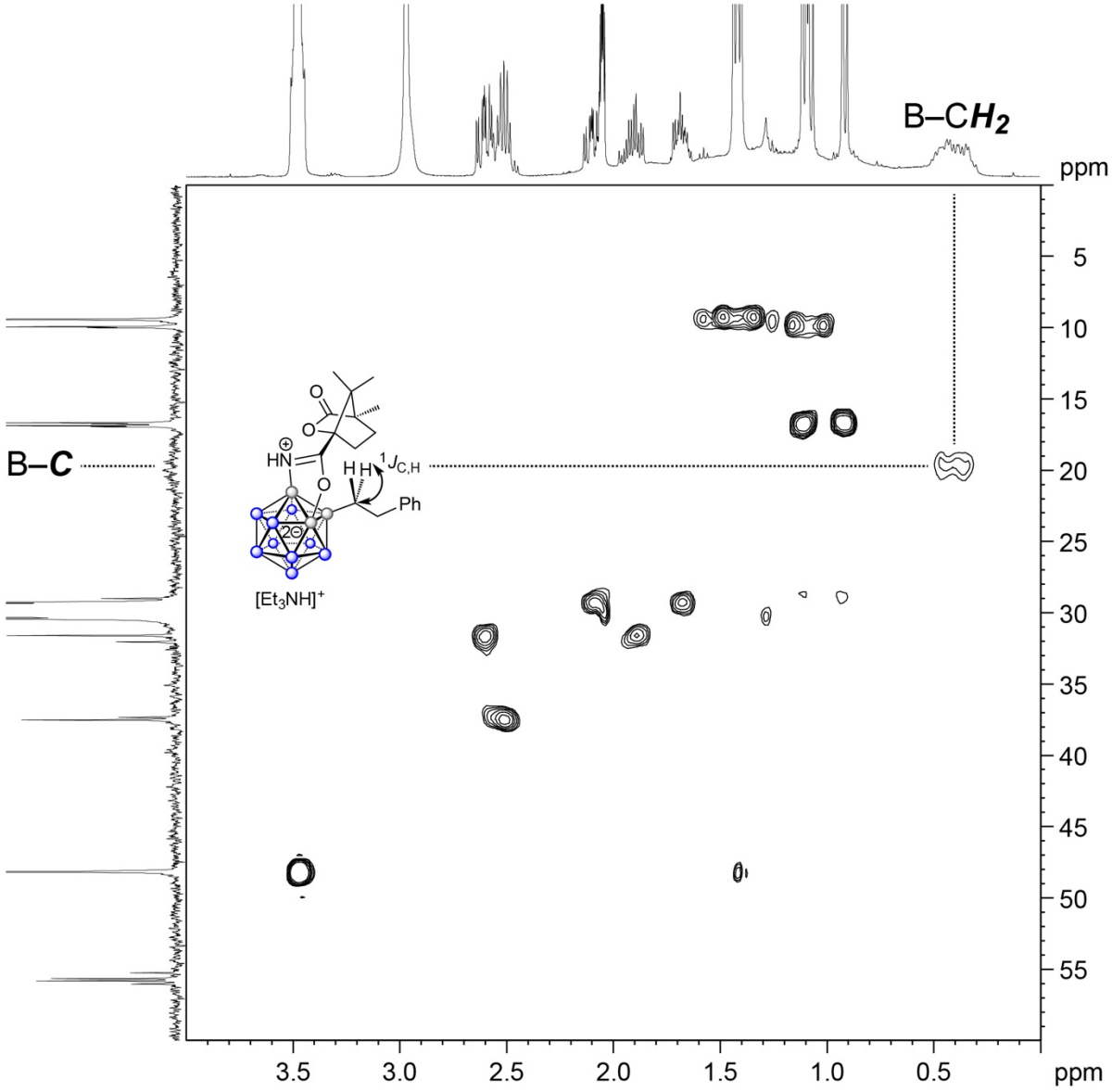


Figure S4. Detail of the ^{1}H-^{13}C HSQC NMR spectrum of **13a** displayed in Figure S3.

c) *Chemical shift assignment and determination of dr values*

A detailed assignment of ^{1}H and ^{13}C chemical shifts for **13a** and **14a** was carried out on the basis of 1D/2D NMR measurements as well as reported values for camphanic acid and menthol (Figures S5 and S6).[4]

For products **13**, resonances at δ(^{1}H) 0.93 ppm, δ(^{13}C) 32 ppm and δ(^{13}C) 37 ppm were used for the determination of diastereomeric ratios. For products **14**, resonances at δ(^{1}H) 0.79 ppm, δ(^{13}C) 21 ppm and δ(^{13}C) 82 ppm were used for the determination of diastereomeric ratios.

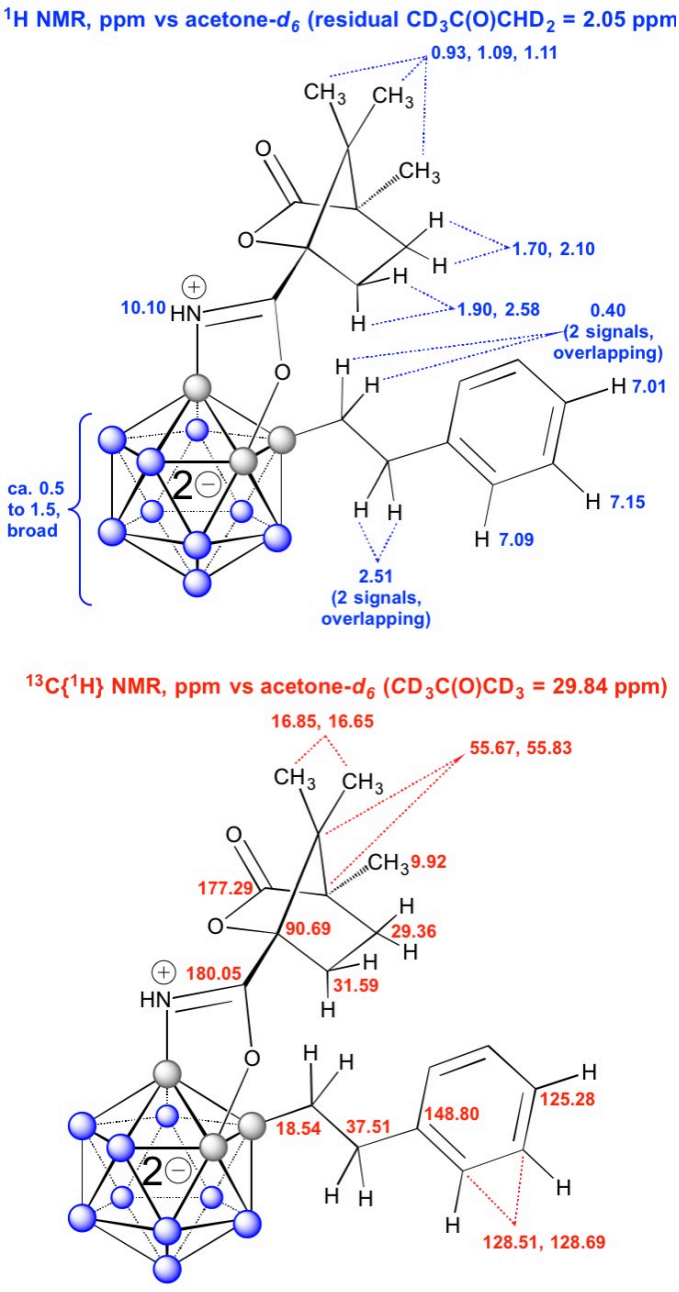


Figure S5. ^{1}H and ^{13}C NMR shifts of **13a** (400/101 MHz, acetone-d_6, 23 °C).

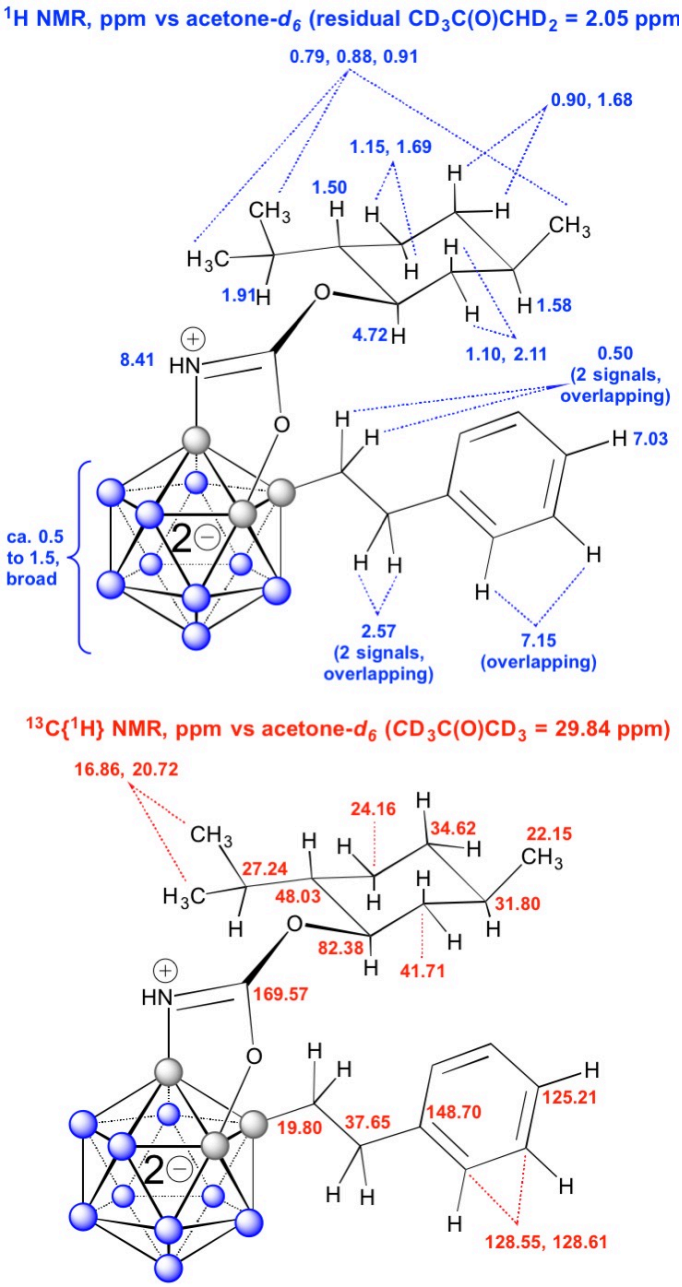
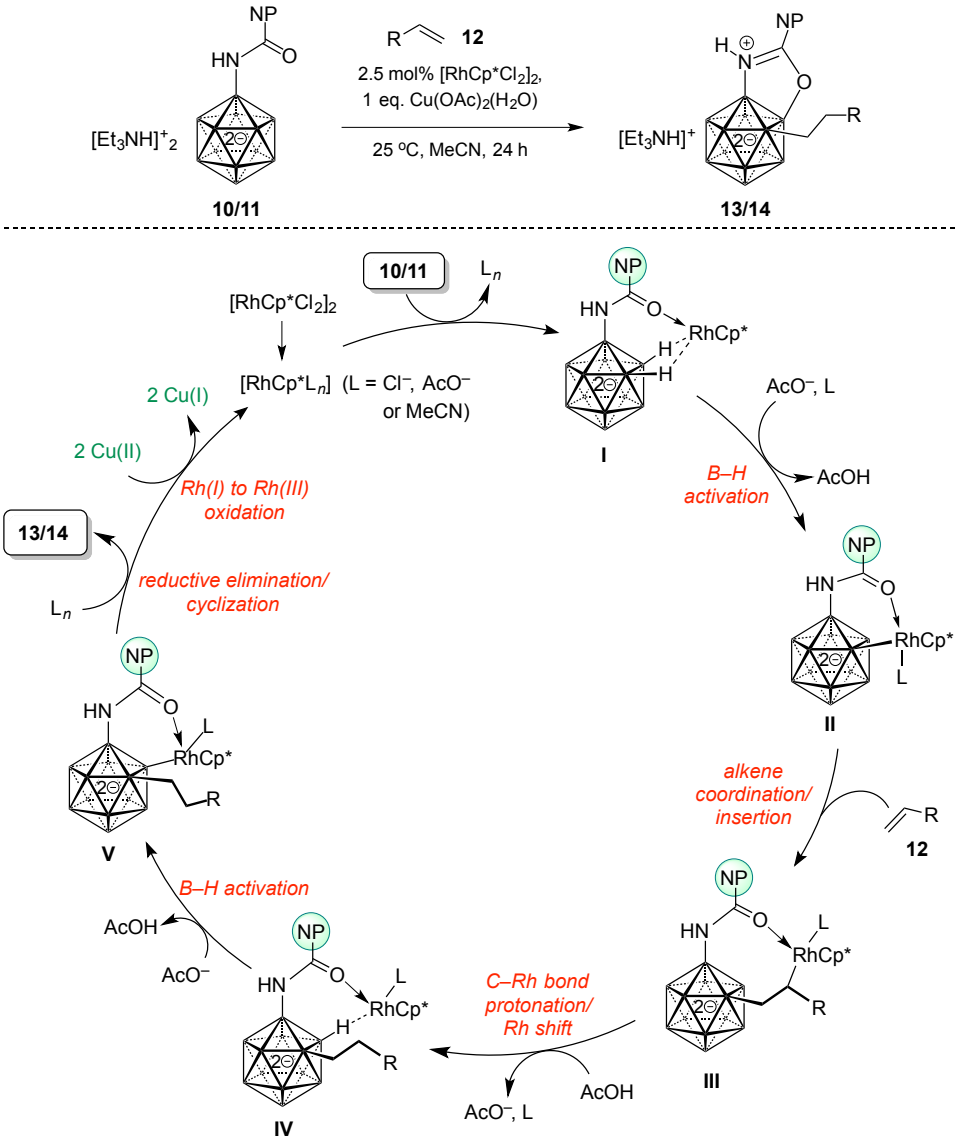


Figure S6. ^{1}H and ^{13}C NMR shifts of **14a** (400/101 MHz, acetone-d_6, 23 °C).

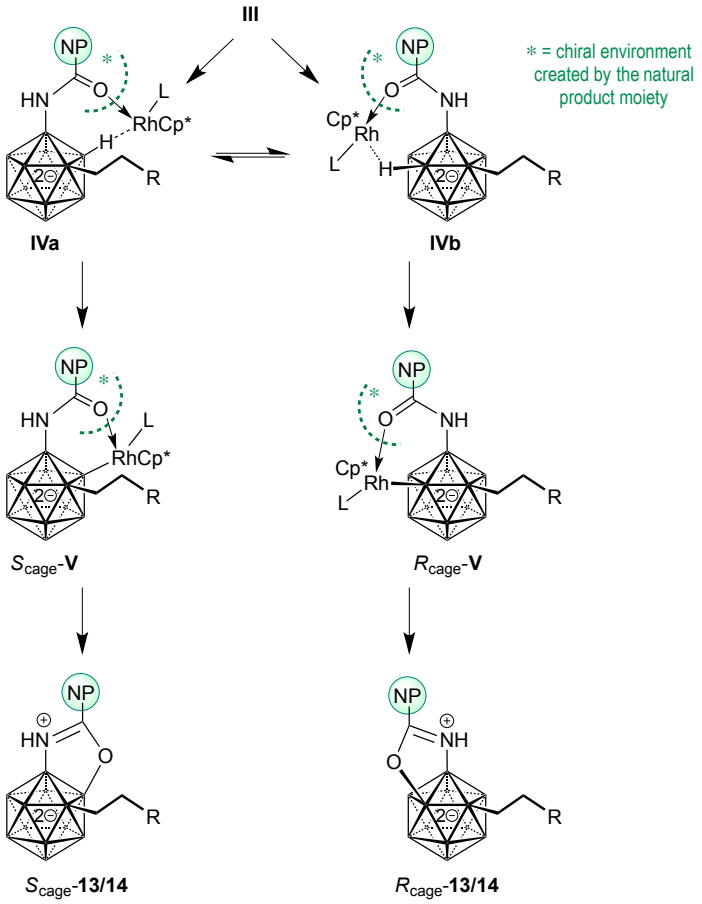
Proposed mechanism for the transformation of 10/11 to 13/14

On the basis of previously reported results, a possible mechanism of the reaction is proposed in Scheme S1.[5] The dimeric rhodium precatalyst first dissociates into a more active monomeric species [RhCp*L_n] (L = Cl^-, AcO^- or MeCN), which then forms the agostic complex **I**. Acetate-mediated B–H activation affords six-membered rhodacycle **II** with concomitant formation of acetic acid. Subsequent alkene coordination/insertion leads to intermediate **III**, which can undergo protonation of the C–Rh bond, followed by a Rh shift to give complex **IV**. A second acetate-mediated B–H activation step gives rise to rhodacycle **V**, from which the products **13/14** are released by reductive elimination/cyclization. In a final step, Cu(II) reoxidizes Rh(I) to Rh(III), which then enters a new catalytic cycle.



Scheme S1. Proposed catalytic cycle for the transformation of **10/11** to **13/14**.

Generation of R_{cage} and S_{cage} diastereoisomers begins with the formation of the two agostic-like complexes **IVa** and **IVb** from intermediate **III** (Scheme S2). The camphanic and menthyl directing groups create a chiral environment, rendering **IVa** and **IVb** diastereomeric; these two species are probably in an equilibrium on a laboratory time scale at room temperature. Subsequent B–H activation affords rhodacycles R_{cage}-**V** and S_{cage}-**V**, which upon reductive elimination/cyclization provide the final products R_{cage}-**13/14** and S_{cage}-**13/14**.



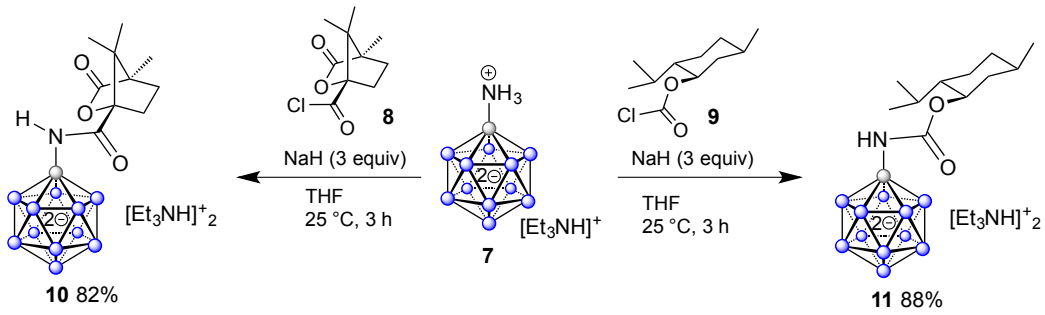
Scheme S2. Formation of diastereoisomers R_{cage}-**13/14** and S_{cage}-**13/14** induced by the chiral natural product moiety.

II Experimental Section

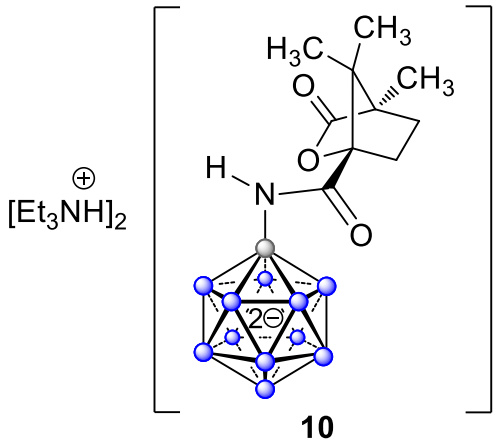
SAFETY STATEMENT:

No new or significant hazards or risks are associated with the reported work.

General procedure for the synthesis of 10 and 11



In a glovebox, a dry 20 mL vial, equipped with a stir bar, was charged with $[Et_3NH][B_{12}H_{11}NH_3]$ (**7**) (0.80 mmol, 1 equiv) and NaH (2.5 mmol, 3.1 equiv). Then anhydrous THF (6 mL) was added. The suspension was stirred at 25 °C for 30 min until hydrogen formation ceased. A solution of **8** or **9** (0.9 mmol, 1.1 equiv) in anhydrous THF (1 mL) was added dropwise by a plastic syringe over 30 min. The mixture was stirred at 25 °C for another 2 hours. The vial was transferred to a fumehood. The reaction was quenched with an aqueous $[Et_3NH]Cl$ solution (10 mL H_2O + 2 equiv $[Et_3NH]Cl$); the pH value at this point was ca. 7–8. The mixture was extracted with CH_2Cl_2/MeCN = 4 : 1 (8 x 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4, and the solution was filtered and concentrated by rotary evaporation. The cloudy residue was purified by silica gel column chromatography (eluent CH_2Cl_2/MeCN = 4 : 3, fraction size 20 mL). The combined eluates were concentrated on a rotary evaporator and dried under vacuum overnight at 60 °C to afford compounds **10** and **11** as colorless solids.



10

Product **10**: 82% yield

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.31 (br, 2H, cationic NH), 6.24 (br, 1H, NH), 3.41 (q, J = 7.3 Hz, 12H, cationic N–CH_2), 2.58-2.45 (m, 1H, camphanic CH), 1.99-1.89 (m, 1H, camphanic CH), 1.6-0.60 (broad overlapping m, 11H, BH), 1.80-.68 (m, 1H, camphanic CH), 1.62-1.50 (m, 1H, camphanic CH), 1.38 (t, J = 7.3 Hz, 18H, cationic N–CH_2–CH_3), 1.07 (s, 3H, camphanic CH_3), 1.02 (s, 3H, camphanic CH_3), 0.86 (s, 3H, camphanic CH_3).

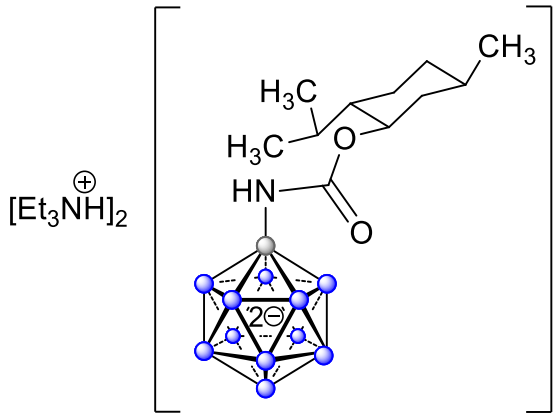
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 178.67 (C=O), 168.49 (C=O), 93.92, 55.91, 54.09 (3 camphanic C), 47.82 (cationic CH_2), 30.59, 29.92 (2 camphanic CH_2), 17.41, 17.06, 10.12 (3 camphanic CH_3), 9.17 (cationic CH_3).

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C):

δ- 5.67 (1B, B–N), -13.50 to -17.50 (10B, BH), -18.69 (1B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{11}H_{30}B_{12}NO_2]^-$: 336.2945; Found: 336.2949.

The reported signal corresponds to $[\mathbf{10}^{2-} - H^-]^-$, *i.e.*, the molecule after losing one hydride.



11

Product **11**: 88% yield

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.10 (br, 2H, cationic NH), 4.42 (s, 1H, NH), 4.29 (ddd, J = 10.8, 10.8, 4.2 Hz, 1H, menthyl CH), 3.39 (q, J = 7.3 Hz, 12H, cationic N–CH_2), 2.03-1.89 (m, 2H, 2 menthyl CH), 1.75-0.60 (broad overlapping m, 18H, 7 menthyl CH and 11 BH), 1.38 (t, J = 7.3 Hz, 18H, cationic CH_3), 0.88 (d, J = 3.7 Hz, 3H, menthyl CH_3), 0.86 (d, J = 4.4 Hz, 3H, menthyl CH_3), 0.75 (d, J = 7.0 Hz, 3H, menthyl CH_3).

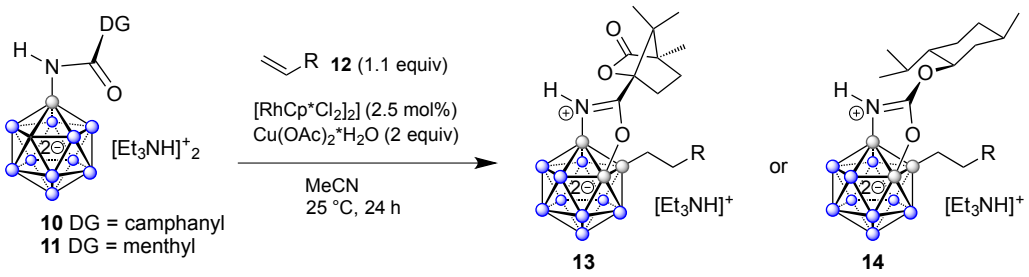
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 158.46 (C=O), 73.21 (menthyl CH), 48.05 (menthyl CH), 47.77 (cationic CH_2), 42.84, 35.15 (2 menthyl CH_2), 32.14, 26.70 (2 menthyl CH), 24.31 (menthyl CH_2), 22.48, 21.03, 16.91 (3 menthyl CH_3), 9.11 (cationic CH_3).

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -4.72 (1B, B–N), -13.48 to -17.75 (10B, BH), -19.52 (1B, BH).

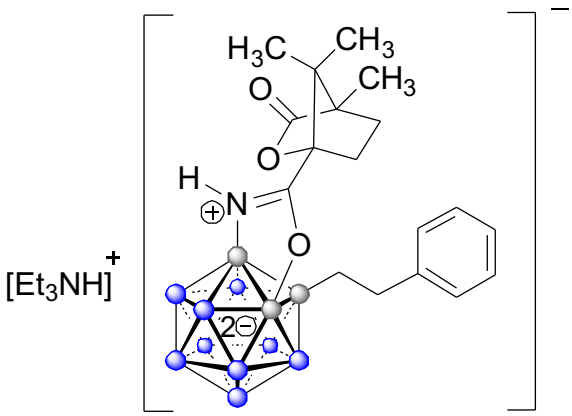
High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{11}H_{30}B_{12}NO_2]^-$: 338.3465; Found: 338.3475.

The reported signal corresponds to $[\mathbf{11}^{2-} - H^-]^-$, *i.e.*, the molecule after losing one hydride.

General Procedure for the synthesis of substituted oxazole-fused *closo*-dodecaborates



A 20 mL glass vial was charged with **10** or **11** (0.20 mmol, 1 equiv), olefin **12** (0.22 mmol, 1.1 equiv), $[RhCp^*Cl_2]_2$ (5 µmol, 2.5 mol% of Rh dimer), $Cu(OAc)_2 \cdot H_2O$ (0.40 mmol, 2 equiv) and a magnetic stir bar. Then CH_3CN (6 mL) was added, and the mixture was stirred at 25 °C for 12 hours; the reaction was monitored by TLC. After completion, the reaction mixture was extracted with hexane (4 x 10 mL) to remove excess of olefin, which facilitated separation by column chromatography. The residual solution was transferred to a 50 mL round-bottom flask and concentrated on a rotary evaporator. The residue was dissolved in CH_2Cl_2 (8 mL), transferred to a 25 mL separation funnel, and saturated aqueous $[NH_4]Cl$ solution (10 mL) was added. The CH_2Cl_2 layer was collected in a 100 mL flask. The aqueous layer was extracted with CH_2Cl_2 (5 x 10 mL). The combined organic layers were washed with brine (50 mL), and the brine layer was re-extracted with CH_2Cl_2 (40 mL). The combined organic layers were dried over anhydrous Na_2SO_4, filtered into a 200 mL one-necked round-bottom flask and concentrated on a rotary evaporator. The residue was purified by silica gel column chromatography (gradient elution with CH_2Cl_2/MeCN = 10:1 to CH_2Cl_2/MeCN = 5:1, fraction size 10–20 mL). The combined eluates were concentrated on a rotary evaporator and then dried overnight under vacuum at 60 °C to afford products **13a–k** and **14a–n** as colorless to slightly yellow solids.



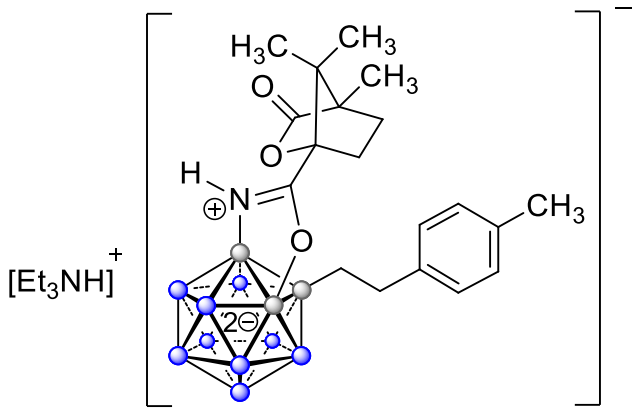
Product **13a**: 85% yield, *dr* = 73:27

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.10 (br, 1H, anionic NH), 7.94 (broad t, $^{1}J_{NH}$ = 51.4 Hz, 1H, cationic H), 7.20-7.12 (m, 2H, phenyl H), 7.12-7.05 (m, 2H, phenyl H), 7.05-6.98 (m, 1H, phenyl H), 3.55-4.00 (m, 6H, cationic N–CH_2), 2.65-2.46 (overlapping m, 3H, camphanic CH and B–CH_2–CH_2), 2.17-2.07 (m, 1H, camphanic CH), 1.97-1.82 (m, 1H, camphanic CH), 1.73–1.58 (m, 1H, camphanic CH), 1.73–0.70 (broad overlapping m, 9H, BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.11 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.93 (s, 3H, camphanic CH_3), 0.53–0.26 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.05 (C=N), 177.29 (C=O), 148.80, 128.69, 128.51, 125.28 (4 phenyl signals), 90.69, 55.83, 55.67 (3 camphanic C), 48.17, (cationic CH_2) 37.51 (B–CH_2–CH_2), 31.59, 29.36, (2 camphanic CH_2), 16.85, 16.65, 9.92 (3 camphanic CH_3), 9.40 (cationic CH_3). The B–C signal was detected indirectly at 18.54 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.56 (1B, B–O), -4.48 (1B, B–N), -10.22 (1B, B–C), -14.26 to -24.22 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{18}H_{32}B_{12}NO_3]^-$: 440.3571; Found: 440.3578.



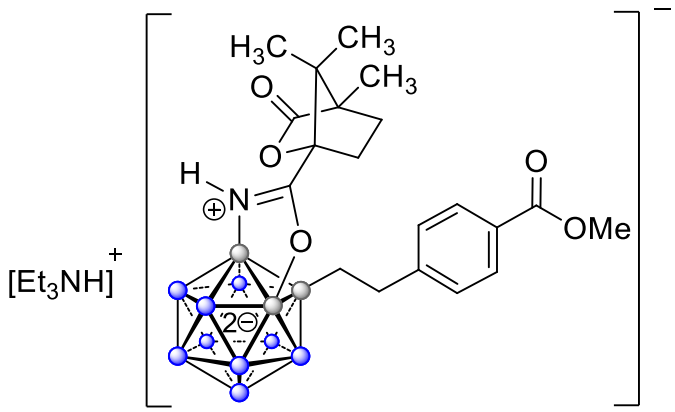
Product **13b**: 68% yield, *dr* = 66:34

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.22 (br, 1H, anionic NH), 8.15-7.66 (broad m, 1H, cationic NH), 7.04-6.90 (overlapping m, 4H, phenyl H), 3.57-3.41 (m, 6H, cationic N–CH_2), 2.61 (ddd, J = 13.6, 10.9, 4.1 Hz, 1H, camphanic CH), 2.56-2.40 (m, 2H, B–CH_2–CH_2), 2.21 (s, 3H, phenyl–CH_3), 2.16-2.07 (m, 1H, camphanic CH), 1.96-1.86 (m, 1H, camphanic CH), 1.73-0.70 (broad overlapping m 9H, BH), 1.72-1.67 (m, 1H, camphanic CH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.12 (s, 3H, camphanic CH_3), 1.10 (s, 3H, camphanic CH_3), 0.93 (s, 3H, camphanic CH_3), 0.54-0.27 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.40 (C=N), 177.19 (C=O), 145.44, 134.26, 129.35, 128.42 (4 phenyl signals), 90.65, 55.85, 55.75 (3 camphanic C), 48.19 (cationic CH_2), 36.93 (B–CH_2–CH_2), 31.61, 29.35 (2 camphanic CH_2), 20.95 (phenyl–CH_3), 16.85, 16.65, 9.92 (3 camphanic CH_3), 9.41 (cationic CH_3). The B–C signal was detected indirectly at 19.6 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.66 (1B, B–O), -4.08 (1B, B–N), -9.68 (1B, B–C), -15.12 to -24.30 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{19}H_{34}B_{12}NO_3]^-$: 454.3728; Found: 454.3731.



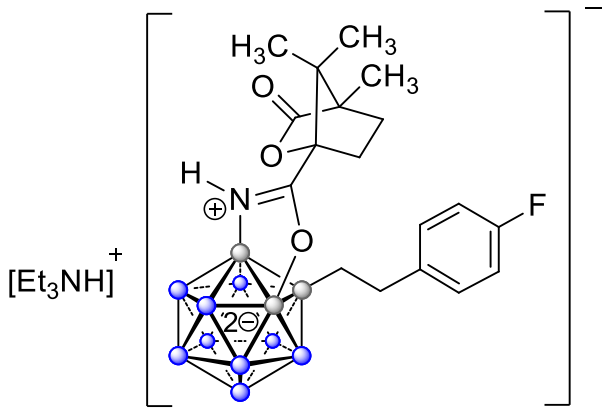
Product **13c**: 82% yield, *dr* = 60:40

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.12 (s, 1H, br, 1H, anionic NH), 7.83 (d, J = 7.9 Hz, 2H, phenyl CH), 7.22 (d, J = 7.9 Hz, 2H, phenyl CH), 3.82 (s, 3H, –COOCH_3), 3.49 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.72 – 2.50 (overlapping m, 3H, camphanic CH and B–CH_2–CH_2), 2.18 – 2.08 (m, 1H, camphanic CH), 1.99 – 1.86 (m, 1H, camphanic CH), 1.83-1.64 (m, 1H, camphanic CH), 1.83-0.70 (broad overlapping m 9H, BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.11 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.92 (s, 3H, camphanic CH_3), 0.57 – 0.27 (m, 2H, B–CH_2–CH_2). Only one N–H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.17 (C=N), 177.25 (C=O), 167.39 (C=O), 154.72, 130.05, 128.68, 127.60 (4 phenyl signals), 90.67, 55.83, 55.70 (3 camphanic C), 51.96 (–COOCH_3), 48.17 (cationic CH_2), 37.59 (B–CH_2–CH_2), 31.61, 29.36, (2 camphanic CH_2), 16.85, 16.65, 9.92 (3 camphanic CH_3), 9.40 (cationic CH_3), The B–C signal was detected indirectly at 19.5 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.53 (1B, B–O), -4.52 (1B, B–N), -10.40 (1B, B–C), -14.74 to -24.95 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{20}H_{34}B_{12}NO_5]^-$: 498.3626; Found: 498.3628.



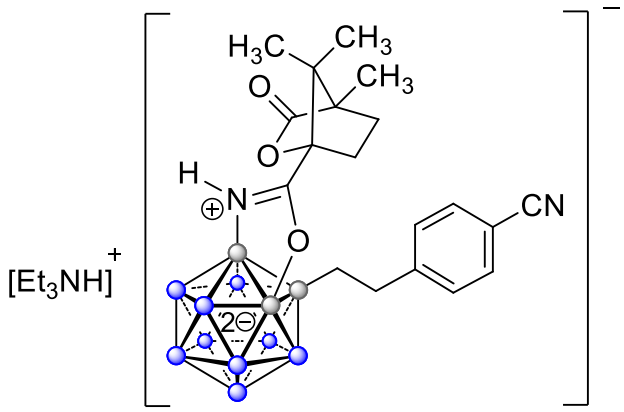
Product **13d**: 75% yield, *dr* = 84:16

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.17 (br, 1H, anionic NH), 7.98 (t, $^{1}J_{NH}$ = 49.8 Hz, 1H, cationic NH), 7.20-7.04 (m, 2H, phenyl CH), 6.99-6.85 (m, 2H, phenyl CH), 3.57-3.35 (m, 6H, cationic N–*CH*$_2$), 2.66-2.56 (m, 1H, camphanic CH), 2.55-2.42 (m, 2H, B–CH$_2$–*CH*$_2$), 2.11 (ddd, *J* = 13.2, 10.8, 4.4 Hz, 1H, camphanic CH), 1.95-1.85 (m, 1H, camphanic CH), 1.73-1.60 (m, 1H, camphanic CH), 1.73-0.70 (broad overlapping m 9H, BH), 1.41 (t, *J* = 7.3 Hz, 9H, cationic C*H*$_3$), 1.11 (s, 3H, camphanic CH$_3$), 1.09 (s, 3H, camphanic CH$_3$), 0.92 (s, 3H, camphanic CH$_3$) 0.53-0.25 (m, 2H, 2H, B–C*H*$_2$–CH$_2$)

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.25 (C=N), 177.22 (C=O), 161.35 (d, $^{1}J_{CF}$ = 239.5 Hz), 144.46, 129.89 (d, $^{3}J_{CF}$ = 7.7 Hz), 115.13 (d, $^{2}J_{CF}$ = 20.8 Hz), (4 phenyl signals), 90.63, 55.81, 55.69 (3 camphanic C), 48.13 (cationic CH$_2$), 36.47 (B–CH$_2$–*CH*$_2$), 31.57, 29.32, (2 camphanic CH$_2$) 16.82, 16.62, 9.90 (3 camphanic CH$_3$), 9.38 (cationic CH$_3$). The B–C signal was detected indirectly at 19.8 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.64 (1B, B–O), -4.33 (1B, B–N), -10.08 (1B, B–C), -15.05 to -24.40 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{18}H_{31}B_{12}FNO_3]^-$: 458.3477; Found: 458.3480.



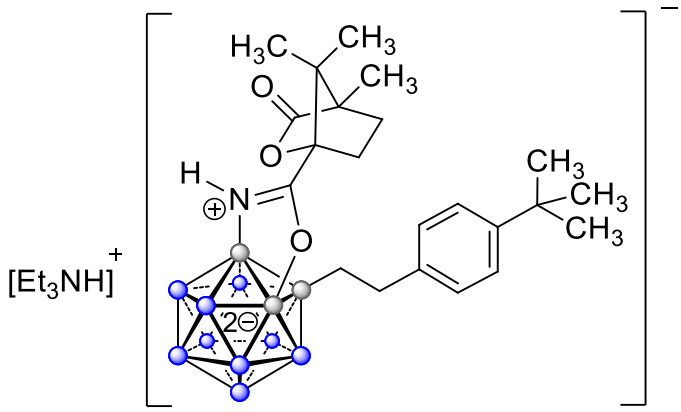
Product **13e**: 65% yield, *dr* = 52:48

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.19 (br, 1H anionic NH), 8.19-7.70 (m, 1H, cationic NH), 7.59 (d, J = 7.9 Hz, 2H, phenyl CH), 7.31 (d, J = 7.9 Hz, 2H, phenyl CH), 3.75-3.24 (m, 6H, cationic N–CH_2), 2.69-2.53 (overlapping m, 3H, camphanic CH and B–CH_2–CH_2), 2.16-2.07 (m, 1H, camphanic CH), 1.98-1.85 (m, 1H, camphanic CH), 1.76-1.59 (m, 1H, camphanic CH), 1.76-0.68 (broad overlapping m, 9H, BH) 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.10 (s, 3H, camphanic CH_3), 1.08 (s, 3H, camphanic CH_3), 0.89 (s, 3H, camphanic CH_3), 0.56-0.28 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.42 (C=N), 177.28 (C=O), 154.46, 132.71, 129.61 (3 phenyl signals), 119.76 (CN), 109.00 (phenyl signal), 90.78, 55.83, 55.29 (3 camphanic C), 48.16 (cationic CH_2), 37.44 (B–CH_2–CH_2), 31.57, 28.95, (2 camphanic CH_2) 16.91, 16.73, 9.90 (3 camphanic CH_3), 9.39 (cationic CH_3). The B-C signal was detected indirectly at 19.6 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.61 (1B, B–O), -4.27 (1B, B–N), -10.22 (1B, B–C), -13.58 to -26.34 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{19}H_{31}B_{12}N_2O_3]^-$: 465.3524; Found: 465.3531.



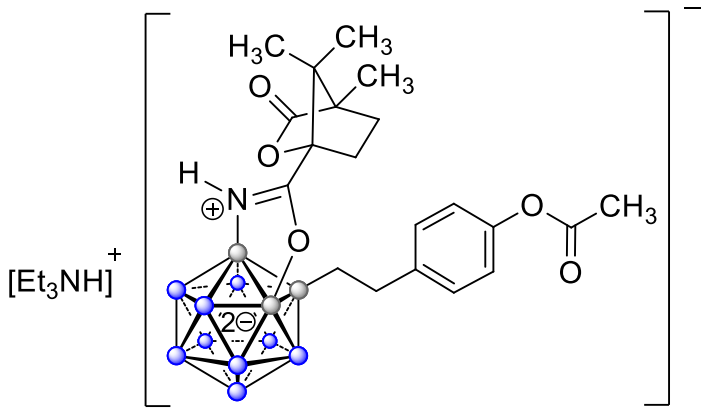
Product **13f**: 66% yield, *dr* = 91:9

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.24 (br, 1H, anionic NH), 8.23-7.97 (broad m, 1H, cationic NH), 7.21 (d, J = 8.1 Hz, 2H, phenyl CH), 7.03 (d, J = 8.1 Hz, 2H, phenyl CH), 3.68-3.35 (m, 6H, cationic N–CH_2), 2.68-2.57 (m, 1H, camphanic CH), 2.56-2.41 (m, 2H, B–CH_2–CH_2), 2.12 (ddd, J = 12.9, 10.7, 4.2 Hz, 1H, camphanic CH), 1.97-1.88 (m, 1H, camphanic CH), 1.78-1.60 (m, 1H, camphanic CH), 1.78-0.70 (broad overlapping m 9H, BH), 1.41 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.25 (s, 9H, ^{t}Bu CH_3), 1.12 (s, 3H, camphanic CH_3), 1.10 (s, 3H, camphanic CH_3), 0.93 (s, 3H, camphanic CH_3), 0.59-0.27 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.42 (C=N), 177.19 (C=O), 147.74, 145.27, 128.15, 125.47 (4 phenyl signals), 90.63, 55.83, 55.75 (3 camphanic C), 48.12 (cationic CH_2), 36.73 (B–CH_2–CH_2), 34.64 (^{t}Bu C), 31.72 (^{t}Bu CH_3), 31.57, 29.32, (2 camphanic CH_2) 16.83, 16.63, 9.90 (3 camphanic CH_3), 9.39 (cationic CH_3), The B–C signal was detected indirectly at 19.3 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.95 (1B, B–O), -4.01 (1B, B–N), -9.52 (1B, B–C), -13.60 to -25.30 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{22}H_{40}B_{12}NO_3]^-$: 496.4197; Found: 496.4202.



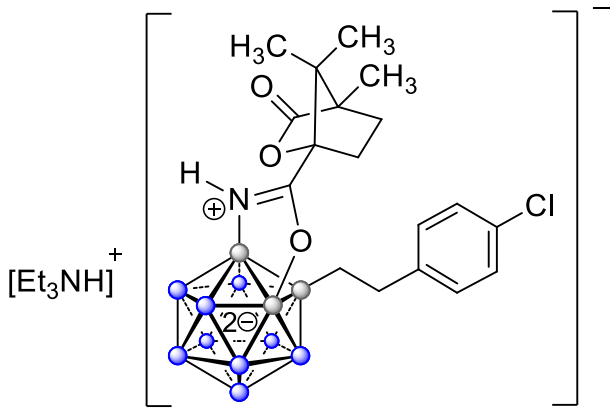
Product **13g**: 78% yield, *dr* = 90:10

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.09 (br, 1H, anionic NH), 7.11 (d, J = 8.1 Hz, 2H, phenyl CH), 6.90 (d, J = 8.4 Hz, 2H, phenyl CH), 3.43 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.64-2.44 (overlapping m, 3H, camphanic CH and B–CH_2–CH_2), 2.20 (s, 3H, O–CO–CH_3), 2.14-2.07 (m, 1H, camphanic CH), 1.90 (ddd, J = 13.5, 9.3, 4.4 Hz, 1H, camphanic CH), 1.73-1.64 (m, 1H, camphanic CH), 1.73-0.70 (broad overlapping m 9H, BH), 1.41 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.12 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.92 (s, 3H, camphanic CH_3), 0.52-0.25 (m, 2H, B–CH_2–CH_2). Only one N–H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.04 (C=N), 177.30 (C=O), 169.78 (Ph–O–*C*=O), 149.14, 146.19, 129.18, 121.87 (4 phenyl signals), 90.70, 55.83, 55.68 (3 camphanic C), 47.91 (cationic CH_2), 36.83 (B–CH_2–CH_2), 31.61, 29.39, (2 camphanic CH_2), 20.96 (CO–CH_3), 16.86, 16.67, 9.94 (3 camphanic CH_3), 9.32 (cationic CH_3), The B–C signal was detected indirectly at 19.6 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.79 (1B, B–O), -4.51 (1B, B–N), -10.30 (1B, B–C), -14.22 to -24.84 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{20}H_{34}B_{12}NO_5]^-$: 498.3626; Found: 498.3632.



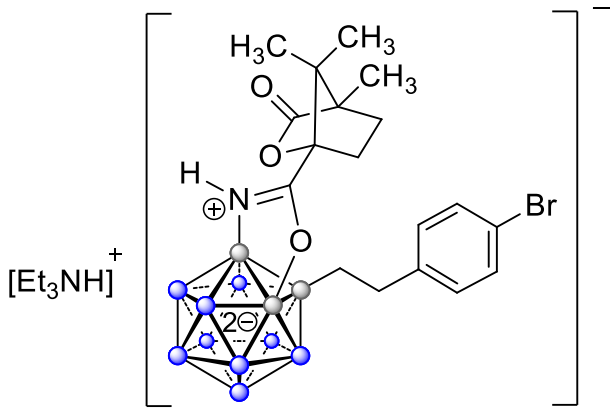
Product **13h**: 73% yield, *dr* = 72:28

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.14 (br, 1H, anionic NH), 7.99 (br, 1H, cationic NH), 7.18 (d, J = 8.3 Hz, 2H, phenyl CH), 7.10 (d, J = 8.3 Hz, 2H, phenyl CH), 3.46 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.60 (ddd, J = 13.5, 10.8, 4.3 Hz, 1H, camphanic CH), 2.55-2.42 (m, 2H, B–CH_2–CH_2), 2.18-2.08 (m, 1H, camphanic CH), 1.99-1.86 (m, 1H, camphanic CH), 1.75-1.59 (m, 1H, camphanic CH), 1.75-0.70 (broad overlapping m 9H, BH), 1.41 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.11 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.92 (s, 3H, camphanic CH_3), 0.53-0.26 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.19 (C=N), 177.22 (C=O), 147.47, 130.42, 130.16, 128.64 (4 phenyl signals), 90.61, 55.79, 55.67 (3 camphanic C), 48.11 (cationic CH_2), 36.66 (B–CH_2–CH_2), 31.56, 29.31, (2 camphanic CH_2), 16.82, 16.61, 9.89 (3 camphanic CH_3), 9.37 (cationic CH_3), The B–C signal was detected indirectly at 19.4 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.34 (1B, B–O), -4.49 (1B, B–N), -10.28 (1B, B–C), -14.44 to -24.54 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{18}H_{31}B_{12}ClNO_3]^-$: 474.3182; Found: 474.3189.



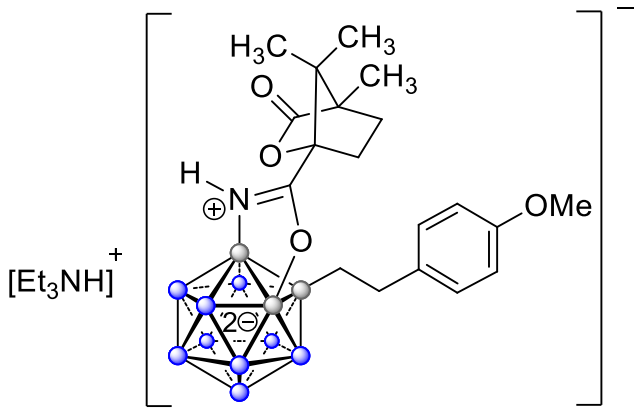
Product **13i**: 70% yield, *dr* = 74:26

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.19 (br, 1H, anionic NH), 8.00 (t, J = 49.5 Hz, 1H, cationic NH), 7.33 (d, J = 8.2 Hz, 2H, phenyl CH), 7.06 (d, J = 8.2 Hz, 2H, phenyl CH), 3.68-3-22 (m, 6H, cationic N–CH_2), 2.60 (ddd, J = 13.9, 11.0, 4.2 Hz, 1H, camphanic CH), 2.56-2.41 (m, 2H, B–CH_2-CH_2), 2.16-2.07 (m, 1H, camphanic CH), 1.97-1.76 (m, 1H, camphanic CH), 1.77-1.60 (m, 1H, camphanic CH), 1.77-0.70 (broad overlapping m 9H, BH), 1.41 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.12 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.92 (s, 3H, camphanic CH_3), 0.51-0.26 (m, 2H, B–CH_2–CH_2)

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.39 (C=N), 177.22 (C=O), 147.91, 131.61, 130.68, 118.51 (4 phenyl signals), 90.64, 55.85, 55.75 (3 camphanic C), 48.15 (cationic CH_2), 36.73 (B–CH_2–CH_2), 31.61, 29.35, (2 camphanic CH_2), 16.85, 16.65, 9.92 (3 camphanic CH_3), 9.41 (cationic CH_3), The B–C signal was detected indirectly at 19.3 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.80 (1B, B–O), -4.23 (1B, B–N), -10.04 (1B, B–C), -14.30 to -24.90 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{18}H_{31}B_{12}BrNO_3]^-$: 519.2698; Found: 519.2695.



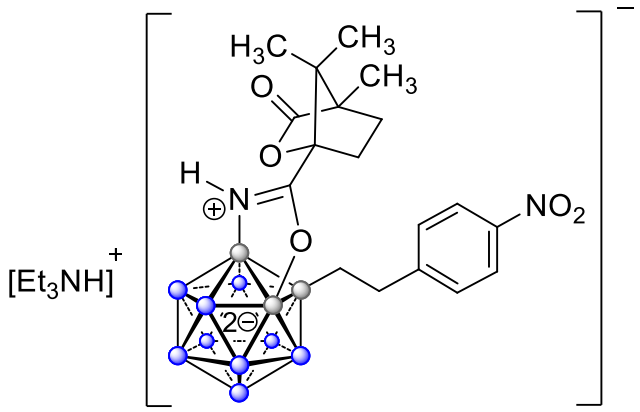
Product **13j**: 63% yield, *dr* = 66:34

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.08 (br, 1H anionic NH), 8.21-7.61 (br, 1H, cationic NH), 7.00 (d, J = 8.3 Hz, 2H, phenyl CH), 6.73 (d, J = 8.3 Hz, 2H, phenyl CH), 3.70 (s, 3H, O–CH_3), 3.48 (q, J = 7.1 Hz, 6H cationic N–CH_2), 2.60 (ddd, J = 14.1, 11.1, 4.0 Hz, 1H, camphanic CH), 2.55-2.38 (m, 2H, B–CH_2–C*H*2), 2.10 (ddd, J = 13.4, 10.9, 4.6 Hz, 1H, camphanic CH), 1.97-1.86 (m, 1H, camphanic CH), 1.73-1.55 (m, 1H, camphanic CH), 1.73-0.70 (broad overlapping m, 9H, BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.11 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.92 (s, 3H, camphanic CH_3), 0.53-0.26 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.05 (C=N), 177.29 (C=O), 157.97, 140.70, 129.25, 114.12 (4 phenyl signals), 90.69, 55.84, 55.67 (3 camphanic C), 55.28 (O–CH_3), 48.18 (cationic CH_2), 36.48 (B–CH_2–CH_2), 31.61, 29.37, (2 camphanic CH_2), 16.85, 16.66, 9.93 (3 camphanic CH_3), 9.40 (cationic CH_3), The B–C signal was detected indirectly at 19.6 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.32 (1B, B–O), -4.56 (1B, B–N), -10.21 (1B, B–C), -15.2 to -23.9 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{19}H_{34}B_{12}NO_4]^-$: 470.3677; Found: 470.3683.



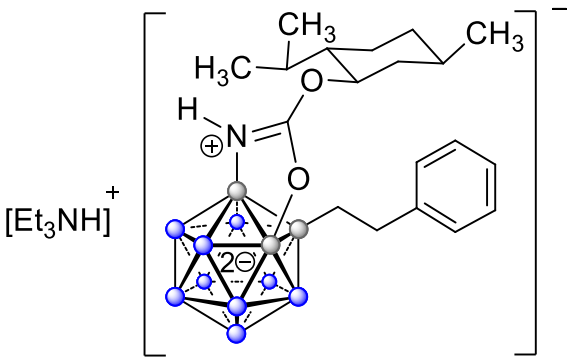
Product **13k**: 72% yield, *dr* = 55:45

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.11 (br, 1H anionic NH), 8.08 (d, J = 8.3 Hz, 2H, phenyl CH), 7.37 (d, J = 8.3 Hz, 2H, phenyl CH), 3.50 (q, J = 7.3 Hz, 6H cationic N–CH_2), 2.79-2.55 (overlapaping m, 3H, camphanic CH and B–CH_2–CH_2), 2.10 (ddd, J = 13.8, 10.0, 3.9 Hz, 1H, camphanic CH), 1.99-1.86 (m, 1H, camphanic CH), 1.77-1.58 (m, 1H, camphanic CH), 1.77-0.70 (broad overlapping m, 9H, BH), 1.43 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.12 (s, 3H, camphanic CH_3), 1.09 (s, 3H, camphanic CH_3), 0.93 (s, 3H, camphanic CH_3), 0.55-0.31 (m, 2H, B–CH_2–CH_2). Only one N-H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.21 (C=N), 177.24 (C=O), 157.29, 146.45, 129.55, 124.02 (4 phenyl signals), 90.65, 56.03, 55.72 (3 camphanic C), 48.21 (cationic CH_2), 37.47 (B–CH_2–CH_2), 31.60, 29.37, (2 camphanic CH_2), 16.96, 16.66, 9.92 (3 camphanic CH_3), 9.41 (cationic CH_3). The B–C signal was detected indirectly at 19.4 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.41 (1B, B–O), -4.59 (1B, B–N), -10.62 (1B, B–C), -14.8 to -23.9 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{18}H_{31}B_{12}N_2O_5]^-$: 485.3422; Found: 485.3431.



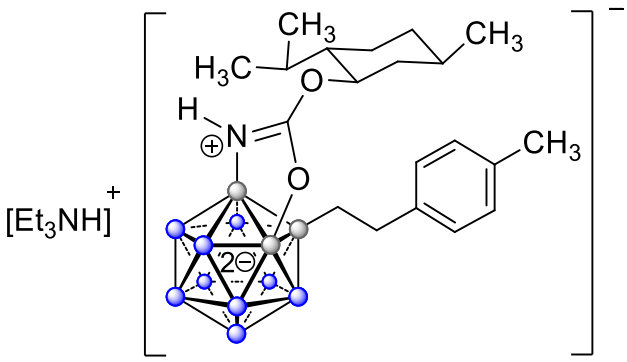
Product **14a**: 87% yield, *dr* = 75:25

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.14 (br, 1H, anionic NH), 8.06-7.48 (br, 1H cationic NH), 7.21-7.08 (m, 4H, phenyl H), 7.03 (m, 1H, phenyl H), 4.81-4.64 (m, 1H, menthyl CH), 3.50 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.63-2.51 (m, 2H, B–CH_2–CH_2), 2.16-2.08 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.93-1.86 (m, 1H, menthyl CH), 1.78-0.37 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.43 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.92 (d, J = 9.0 Hz, 3H, menthyl CH_3), 0.88 (d, J = 6.7 Hz, 3H, menthyl CH_3), 0.79 (d, J = 7.1 Hz, 3H, menthyl CH_3), 0.75-0.38 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.57 (C=N), 148.70, 128.61, 128.55, 125.21 (4 phenyl signals), 82.38 (menthyl CH), 48.21 (cationic CH_2), 48.03 (menthyl CH), 41.71 (menthyl CH_2), 37.65 (B–CH_2–CH_2), 34.62 (menthyl CH_2), 31.80, 27.24 (2 menthyl CH), 24.16 (menthyl CH_2), 22.15, 20.72, 16.86 (3 menthyl CH_3), 9.40 (cationic CH_3). The B–C signal was detected indirectly at 19.8 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 6.90 (1B, B–O), -2.78 (1B, B–N), -6.58 (1B, B–C), -13.2 to -29.9 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{19}H_{38}B_{12}NO_2]^-$: 442.4092; Found: 442.4101.



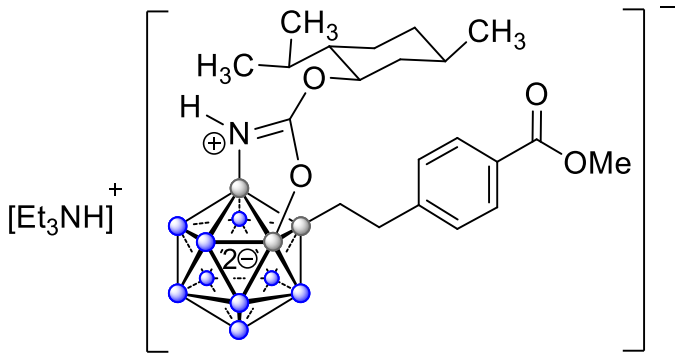
Product **14b**: 72% yield, *dr* = 73:27

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.15 (br, 1H, anionic NH), 8.09-7.70 (br, 1H, cationic NH), 7.06-6.89 (overlapping m, 4H, phenyl H), 4.78-4.66 (m, 1H, menthyl CH), 3.50 (q, J = 7.4 Hz, 6H cationic N–CH_2), 2.59-2.46 (m, 2H, B–CH_2–CH_2), 2.22 (s, 3H phenyl-CH_3), 2.14-2.08 (overlapping with solvent residual signal m, 1H, menthyl CH), 2.03-1.88 (m, 1H, menthyl CH), 1.74-0.39 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.43 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.92-0.82 (overlapping m, 6H, 2 menthyl CH_3), 0.79 (d, J = 6.9 Hz, 3H, menthyl CH_3), 0.58-0.51 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.75 (C=N), 145.47, 134.26, 129.28, 128.45 (4 phenyl signals), 82.93 (menthyl CH), 48.13 (cationic CH_2), 47.97 (menthyl CH), 41.62 (menthyl CH_2), 36.94 (B–CH_2–CH_2), 34.52 (menthyl CH_2), 31.77, 27.22 (2 menthyl CH), 24.10 (menthyl CH_2), 22.10 (1 menthyl CH_3), 20.95 (phenyl-CH_3), 20.68, 16.81 (2 menthyl CH_3), 9.39 (cationic CH_3). The B–C signal was detected indirectly at 19.3 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.82 (1B, B–O), -3.92 (1B, B–N), -7.77 (1B, B–C), -12.96 to -26.14 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{20}H_{40}B_{12}NO_2]^-$: 456.4248; Found: 456.4256.



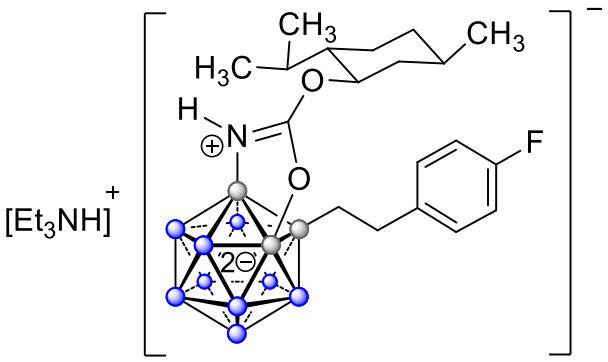
Product **14c**: 84% yield, *dr* = 71:21

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.17 (br, 1H, anionic NH), 7.85 (d, J = 7.7 Hz, 2H, phenyl H), 7.24 (d, J = 7.7 Hz, 2H, phenyl H), 4.80-4.62 (m, 1H menthyl CH), 3.83 (s, 3H, –COOCH_3), 3.48 (q, J = 7.4 Hz, 6H, cationic N–CH_2), 2.67-2.56 (m, 2H, B–CH_2–CH_2), 2.16-2.07 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.96-1.86 (m, 1H, menthyl CH), 1.77-0.41 (broad overlapping m, 16H, 7CH and 9BH), 1.42 (t, J = 7.2 Hz, 9H, cationic CH_3), 0.91 (d, J = 8.2 Hz, 3H, menthyl CH_3), 0.87 (d, J = 8.3 Hz, 3H, menthyl CH_3), 0.78 (d, J = 6.7 Hz, 3H, menthyl CH_3), 0.65-0.50 (m, 2H, B–CH_2–CH_2). Only one N-H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.59 (C=N), 167.43 (C=O), 155.05, 129.98, 128.75, 127.57 (4 phenyl signals), 82.45 (menthyl CH), 51.97 (COOCH_3), 48.11 (cationic CH_2), 47.99 (menthyl CH), 41.67 (menthyl CH_2), 37.74 (B–CH_2–CH_2), 34.57 (menthyl CH_2), 31.63, 27.23 (2 menthyl CH), 24.15 (menthyl CH_2), 22.14, 20.73, 16.85 (3 menthyl CH_3), 9.38 (cationic CH_3). The B–C signal was detected indirectly at 19.4 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.46 (1B, B–O), -4.68 (1B, B–N), -8.90 (1B, B–C), -12.90 to -22.20 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{21}H_{40}B_{12}NO_4]^-$: 500.4146; Found: 500.4149.



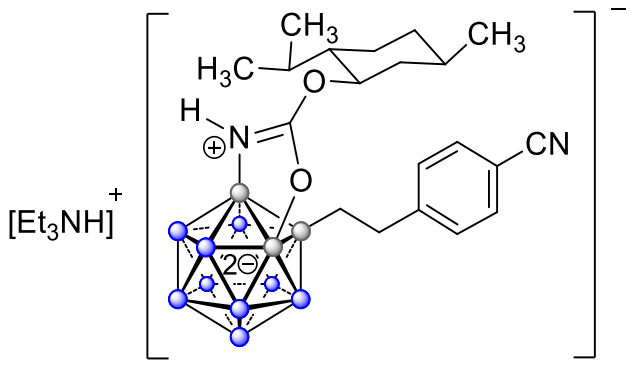
Product **14d**: 79% yield, *dr* = 79:21

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.15 (br, 1H, anionic NH), 8.08-7.56 (br, 1H, cationic NH), 7.21-7.05 (m, 2H, phenyl H), 6.98-6.86 (m, 2H, phenyl H), 4.78-4.64 (m, 1H, menthyl CH), 3.56-3.45 (m, 6H, cationic N–CH_2), 2.64-2.45 (m, 2H, B–CH_2–CH_2), 2.13-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.95-1.85(m, 1H, menthyl CH), 1.75-0.28 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.43 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.93-0.85 (overlapping m, 6H, 2 menthyl CH_3), 0.78 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.58-0.49 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.81 (C=N), 161.44 (d, $^{1}J_{CF}$ = 239.8 Hz) 144.35, 129.96 (d, $^{3}J_{CF}$ = 7.5 Hz). 115.11 (d, $^{2}J_{CF}$ = 20.9 Hz), (4 phenyl signals), 83.09 (menthyl CH), 49.17 (cationic CH_2), 47.94 (menthyl CH), 41.75 (menthyl CH_2), 36.43 (B–CH_2–CH_2), 34.48 (menthyl CH_2), 31.76, 27.23 (2 menthyl CH), 24.10 (menthyl CH_2), 22.08, 20.66, 16.80 (3 menthyl CH_3), 9.40 (cationic CH_3). The B–C signal was detected indirectly at 19.8 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.93 (1B, B–O), -3.74 (1B, B–N), -7.72 (1B, B–C), -13.47 to -25.90 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m/z* calcd for $[C_{19}H_{37}B_{12}FNO_2]^-$: 460.3998; Found: 460.4005.



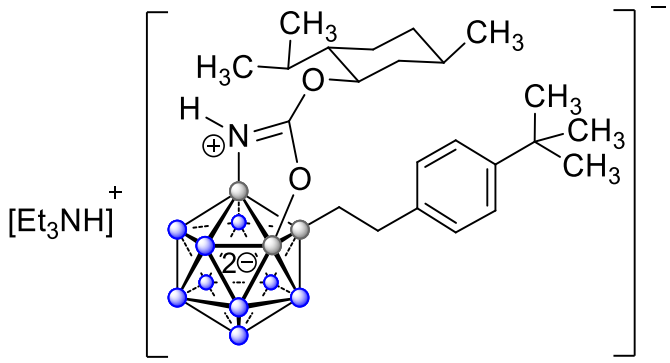
Product **14e**: 68% yield, *dr* = 72:28

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.20 (br, 1H, anionic NH), 8.14-7.65 (br, 1H, cationic NH), 7.65-7.51 (m, 2H, phenyl H), 7.40-7.20 (m, 2H, phenyl H), 4.78-4.63 (m, 1H, menthyl CH), 3.49 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.75-2.52 (m, 2H, B–CH_2–CH_2), 2.03-1.92 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.92-1.74 (m, 1H, menthyl CH), 1.74-0.39 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.93-0.83 (overlapping m, 6H, 2 menthyl CH_3), 0.77 (d, J = 6.8 Hz, 3H, menthyl CH_3), 0.62-0.49 (m, 2H, B–CH_2–CH_2). Only one N-H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.59 (C=N), 155.06, 132.58, 129.64 (3 phenyl signals), 119.85 (CN), 109.05 (phenyl signal), 82.50 (menthyl CH), 48.18 (cationic CH_2), 47.94 (menthyl CH), 41.62 (menthyl CH_2), 37.79 (B–CH_2–CH_2), 34.51 (menthyl CH_2), 31.76, 27.20 (2 menthyl CH), 24.11 (menthyl CH_2), 22.10, 20.67, 16.82 (3 menthyl CH_3), 9.39 (cationic CH_3). The B–C signal was detected indirectly at 19.7 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.32 (1B, B–O), -4.64 (1B, B–N), -8.94 (1B, B–C), -14.00 to -23.30 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{20}H_{37}B_{12}N_2O_2]^-$: 467.4044; Found: 467.4053.



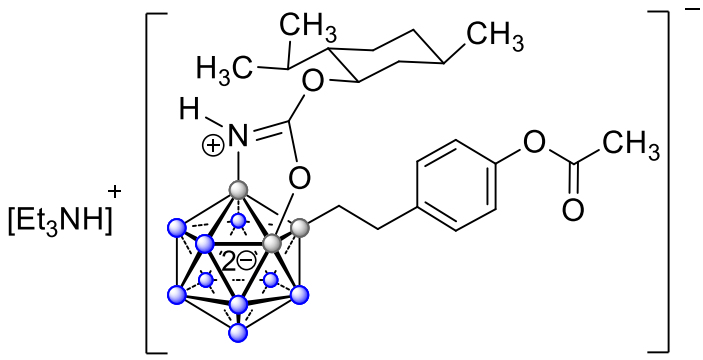
Product **14f**: 65% yield, *dr* = 85:15

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.40 (br, 1H, anionic NH), 8.32-7.72 (br, 1H, cationic NH), 7.22 (d, J = 8.1 Hz, 2H, phenyl H), 7.05 (d, J = 8.1 Hz, 2H, phenyl H), 4.82-4.71 (m, 1H, menthyl CH), 3.60-3.39 (m, 6H, cationic N–CH_2), 2.62-2.46 (m, 2H, B–CH_2–CH_2), 2.15-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.93-1.85 (m, 1H), 1.72-0.37 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.26 (s, 9H ^{t}Bu CH_3), 0.90 (d, J = 7.3 Hz, 3H, menthyl CH_3), 0.88 (d, J = 6.6 Hz, 3H, menthyl CH_3), 0.78 (d, J = 6.9 Hz, 3H, menthyl CH_3), 0.64-0.50 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.82 (C=N), 147.77, 145.37, 128.24, 125.45 (4 phenyl signals), 83.09 (menthyl CH), 48.17 (cationic CH_2), 47.98 (menthyl CH), 41.64 (menthyl CH_2), 36.78 (B–CH_2–CH_2), 34.67 (^{t}Bu C), 34.52 (menthyl CH_2), 31.79 (^{t}Bu CH_3), 31.57, 27.23 (2 menthyl CH), 24.10 (menthyl CH_2), 22.13, 20.69, 16.80 (3 menthyl CH_3), 9.40 (cationic CH_3). The B–C signal was detected indirectly at 19.7 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.99 (1B, B–O), -3.67 (1B, B–N), -7.45 (1B, B–C), -12.07 to -26.29 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{23}H_{46}B_{12}NO_2]^-$: 498.4718; Found: 498.4722.



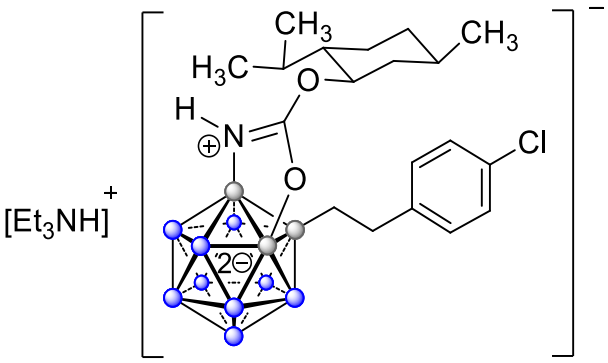
Product **14g**: 78% yield, *dr* = 85:15

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.23 (br, 1H anionic NH), 8.09-7.60 (br, 1H, cationic NH), 7.13 (d, J = 8.2 Hz, 2H, phenyl H), 6.91 (d, J = 8.2 Hz, 2H, phenyl H), 4.82-4.66 (m, 1H, menthyl CH), 3.63-3.28 (m, 6H, cationic N–CH_2), 2.67-2.48 (m, 2H, B–CH_2–CH_2), 2.20 (s, 3H, –OCOCH_3), 2.16-2.08 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.99-1.86 (m, 1H, menthyl CH), 1.73-0.29 (broad overlapping m, 16H, 7CH and 9BH), 1.41 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.90 (d, J = 5.2 Hz, 3H, menthyl CH_3), 0.88 (d, J = 4.3 Hz, 3H, menthyl CH_3), 0.79 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.60-0.50 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.75, 169.61 (C=O and C=N), 149.12, 146.08, 129.13, 121.79 (4 phenyl signals), 82.65 (menthyl CH), 48.18 (cationic CH_2), 47.92 (menthyl CH), 41.59 (menthyl CH_2), 36.79 (B–CH_2–CH_2), 34.50 (menthyl CH_2), 31.76, 27.19 (2 menthyl CH), 24.11 (menthyl CH_2), 22.11 (menthyl CH_3), 20.94 (OCOCH_3), 20.65, 16.81 (2 menthyl CH_3), 9.39 (cationic CH_3). The B–C signal was detected indirectly at 19.9 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.84 (1B, B–O), -4.26 (1B, B–N), -8.36 (1B, B–C), -13.05 to -24.94 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{21}H_{40}B_{12}NO_4]^-$: 500.4147; Found: 500.4149.



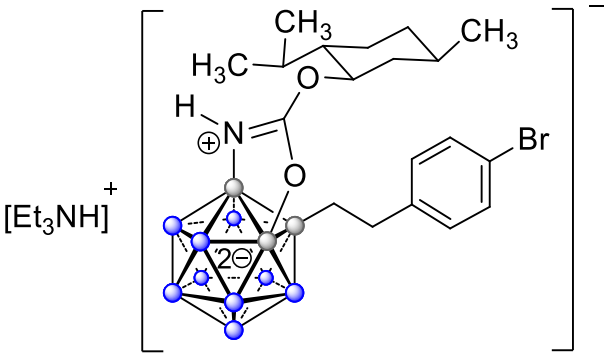
Product **14h**: 75% yield, *dr* = 68:32

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.20 (br, 1H, anionic NH), 8.11-7.59 (br, 1H, cationic NH), 7.21-7.17 (m, 2H, phenyl H), 7.17-7.08 (m, 2H, phenyl H), 4.78-4.65 (m, 1H, menthyl CH), 3.53-3.37 (m, 6H, cationic N–CH_2), 2.63-2.45 (m, 2H, B–CH_2–CH_2), 2.11-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.96-1.82 (m, 1H, menthyl CH) 1.78-0.35 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.93-0.86 (overlapping m, 6H, 2 menthyl CH_3), 0.80 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.58-0.49 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.59 (C=N), 147.79, 130.41, 130.22 128.58 (4 phenyl signals), 82.53 (menthyl CH), 48.18 (cationic CH_2), 47.95 (menthyl CH), 41.62 (menthyl CH_2), 36.82 (B–CH_2–CH_2), 34.52 (menthyl CH_2), 31.77, 27.21 (2 menthyl CH), 24.13 (menthyl CH_2), 22.10, 20.67, 16.83 (3 menthyl CH_3), 9.39 (cationic CH_3). The B–C signal was detected indirectly at 19.8 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.65 (1B, B–O), -4.50 (1B, B–N), -8.71 (1B, B–C), -113.71 to -24.55 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{19}H_{37}B_{12}ClNO_2]^-$: 476.3702; Found: 476.3707.



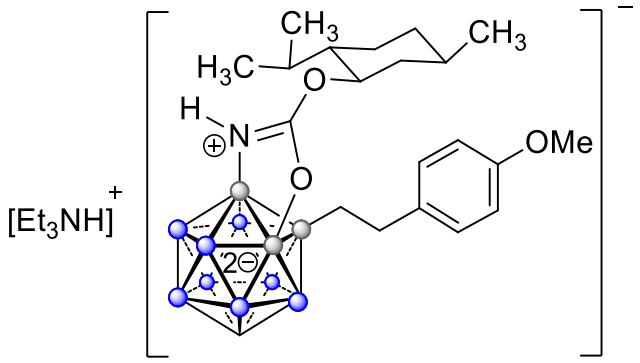
Product **14i**: 73% yield, *dr* = 71:29

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.19 (br, 1H, anionic NH), 8.07-7.49 (br, 1H, cationic NH), 7.39-7.30 (m, 2H, phenyl H), 7.13-7.01 (m, 2H, phenyl H), 4.77-4.63 (m, 1H, menthyl CH), 3.48 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.62-2.43 (m, 2H, B–CH_2–CH_2), 2.14-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.94-1.82 (m, 1H, menthyl CH) 1.77-0.34 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.90 (overlapping m, 6H, 2 menthyl CH_3), 0.80 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.58-0.46 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.56 (C=N), 148.28, 131.35, 130.68, 118.38 (4 phenyl signals), 82.48 (menthyl CH), 48.20 (cationic CH_2), 47.92 (menthyl CH), 41.61 (menthyl CH_2), 36.88 (B–CH_2–CH_2), 34.51 (menthyl CH_2), 31.76, 27.20 (2 menthyl CH), 24.13 (menthyl CH_2), 22.10, 20.66, 16.83 (3 menthyl CH_3), 9.41 (cationic CH_3). The B–C signal was detected indirectly at 19.8 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.43 (1B, B–O), -4.59 (1B, B–N), -8.79 (1B, B–C), -13.51 to -24.51 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{19}H_{37}B_{12}BrNO_2]^-$: 520.3197; Found: 520.3204.



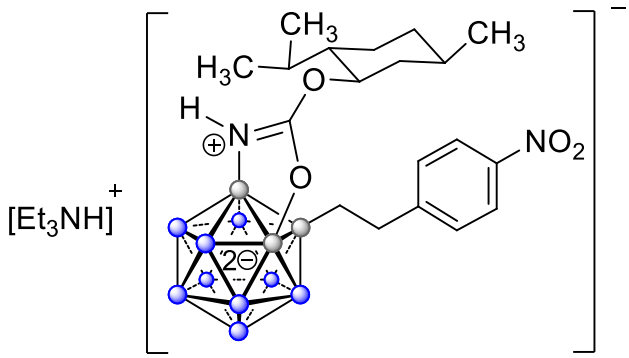
Product **14j**: 66% yield, *dr* = 70:30

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.21 (br, 1H, anionic NH), 8.10-7.64 (br, 1H, cationic NH), 7.20-6.89 (m, 2H, phenyl H), 6.81-6.67 (m, 2H, phenyl H), 4.81-4.64 (m, 1H, menthyl CH), 3.71 (s, 3H, –OCH_3), 3.56-3.40 (m, 6H, cationic N–CH_2), 2.59-2.41 (m, 2H, B–CH_2–CH_2), 2.18-2.07 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.95-1.85 (m, 1H, menthyl CH) 1.78-0.36 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.93-0.87 (overlapping m, 6H, 2 menthyl CH_3), 0.81 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.58-0.50 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.64 (C=N), 158.01, 140.84, 129.31, 114.07 (4 phenyl signals), 82.59 (menthyl CH), 55.32 (–OCH_3), 48.21 (cationic CH_2), 48.01 (menthyl CH), 41.67 (menthyl CH_2), 36.55 (B–CH_2–CH_2), 34.58 (menthyl CH_2), 31.80, 27.24 (2 menthyl CH), 24.16 (menthyl CH_2), 22.15, 20.70, 16.85 (3 menthyl CH_3), 9.41 (cationic CH_3). The B–C signal was detected indirectly at 19.9 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.52 (1B, B–O), -4.39 (1B, B–N), -8.36 (1B, B–C), -14.21 to -23.81 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{20}H_{40}B_{12}NO_3]^-$: 472.4197; Found: 472.4206.



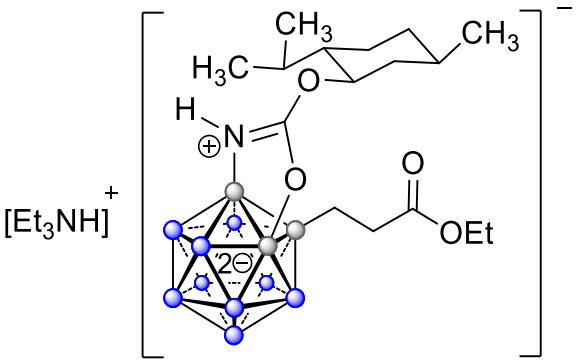
Product **14k**: 78% yield, *dr* = 72:28

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.30 (br, 1H, anionic NH), 8.19-8.06 (m, 2H, phenyl H), 8.16-7.61 (overlapping br, 1H, cationic NH), 7.59-7.30 (m, 2H, phenyl H), 4.81-4.65 (m, 1H, menthyl CH), 3.55-3.40 (m, 6H, cationic N–CH_2), 2.77-2.58 (m, 2H, B–CH_2–CH_2), 2.10-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 1.94-1.81 (m, 1H, menthyl CH), 1.76-0.35 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, *J* = 7.3 Hz, 9H, cationic CH_3), 0.93-0.84 (overlapping m, 6H, 2 menthyl CH_3), 0.78 (d, *J* = 6.9 Hz, 3H, menthyl CH_3), 0.62-0.53 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.69 (C=N), 157.31, 146.45, 129.56, 123.94 (4 phenyl signals), 82.79 (menthyl CH), 48.16 (cationic CH_2), 47.93 (menthyl CH), 41.58 (menthyl CH_2), 37.46 (B–CH_2–CH_2), 34.46 (menthyl CH_2), 31.75, 27.21 (2 menthyl CH), 24.11 (menthyl CH_2), 22.07, 20.65, 16.81 (3 menthyl CH_3), 9.39 (cationic CH_3). The B–C signal was detected indirectly at 19.0 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.60 (1B, B–O), -4.33 (1B, B–N), -8.59 (1B, B–C), -13.64 to -24.05 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{19}H_{37}B_{12}N_2O_4]^-$: 487.3943; Found: 487.3951.



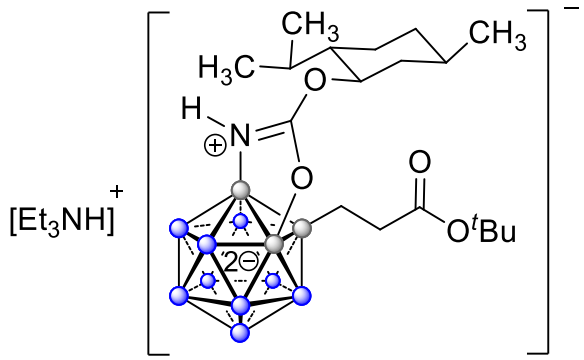
Product **14l**: 92% yield, *dr* = 50:50

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.17 (br, 1H, anionic NH), 8.10-7.71 (broad m, 1H, cationic NH), 4.78-4.65 (m, 1H, menthyl CH), 3.98 (q, J = 7.0 Hz, 2H, O–*CH*$_2$–CH$_3$), 3.47 (q, J = 7.3 Hz, 6H, cationic N–C*H*$_2$), 2.21-2.14 (m, 2H, B–CH$_2$–C*H*$_2$), 2.14-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 2.00-1.85 (m, 1H, menthyl CH), 1.76-0.30 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.41 (t, J = 7.3 Hz, 9H, cationic C*H*$_3$), 1.16 (t, J = 7.0 Hz, 3H, O–CH$_2$–*CH*$_3$), 0.95-0.89 (m, 6H, overlapping m, 6H, 2 menthyl CH$_3$), 0.80 (d, J = 6.9 Hz, 3H, menthyl CH$_3$), 0.61-0.44 (m, 2H, B–C*H*$_2$–CH$_2$).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 176.67 (C=O), 169.58 (C=N), 82.46 (menthyl CH), 59.58 (O–*CH*$_2$–CH$_3$), 48.14 (cationic CH$_2$), 47.99 (menthyl CH), 41.45 (menthyl CH$_2$), 35.81 (B–CH$_2$–*CH*$_2$), 34.56 (menthyl CH$_2$), 31.79, 27.18 (2 menthyl CH), 23.84 (menthyl CH$_2$), 22.13, 20.67, 16.80 (3 menthyl CH$_3$), 14.68 (O–CH$_2$–*CH*$_3$), 9.38 (cationic CH$_3$). The B–C signal was detected indirectly at 12.1 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.18 (1B, B–O), -4.66 (1B, B–N), -9.16 (1B, B–C), -13.70 to -23.80 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{16}H_{38}B_{12}NO_4]^-$: 438.3990; Found: 438.3998.



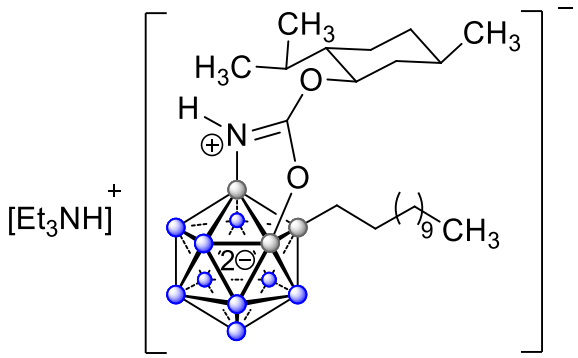
Product **14m**: 90% yield, *dr* = 51:49

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.17 (br, 1H, anionic NH), 8.08-7.69 (broad m, 1H, cationic NH), 4.80-4.64 (m, 1H, menthyl CH), 3.47 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.18-2.07 (overlapping with solvent residual signal m, 2H, B–CH_2–CH_2), 2.02-1.84 (m, 2H, 2 menthyl CH), 1.79-0.30 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 1.38 (s, 9H, CH_3 ^{t}Bu), 0.95-0.89 (overlapping m, 6H, 2 menthyl CH_3), 0.85-0.78 (m, 3H, menthyl CH_3), 0.57-0.41 (m, 2H, B–CH_2–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 176.40 (C=O), 169.57 (C=N), 82.42 (menthyl CH), 78.42 (C ^{t}Bu), 48.11 (cationic CH_2), 47.87 (menthyl CH), 41.57 (menthyl CH_2), 37.23 (B–CH_2–CH_2), 34.57 (menthyl CH_2), 31.84 (menthyl CH), 28.35 (CH_3 ^{t}Bu), 27.21, (menthyl CH), 24.13 (menthyl CH_2), 22.21, 20.86, 16.83 (3 menthyl CH_3), 9.37 (cationic CH_3). The B–C signal was detected indirectly at 11.9 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.28 (1B, B–O), -4.67 (1B, B–N), -9.11 (1B, B–C), -14.32 to -23.22 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{18}H_{42}B_{12}NO_4]^-$: 466.4303; Found: 466.4309.



Product **14n**: 85% yield, *dr* = 50:50

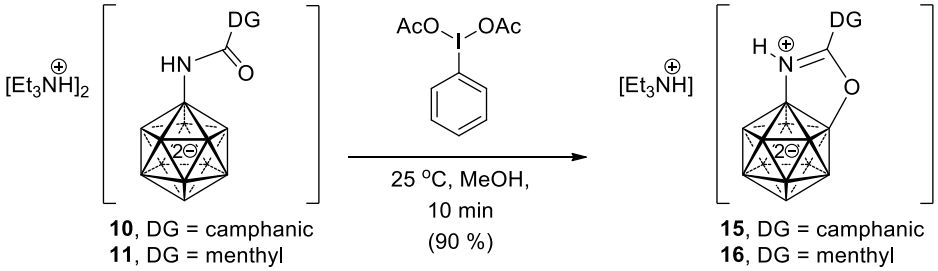
$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.11 (br, 1H, anionic NH), 8.00-7.51 (broad m, 1H, cationic NH), 4.80-4.61 (m, 1H, menthyl CH), 3.47 (q, *J* = 7.3 Hz, 6H, cationic N–C*H*$_2$), 2.17-2.06 (overlapping with solvent residual signal m, 1H, menthyl CH), 2.02-1.85 (m, 1H, menthyl CH), 1.76-0.08 (broad overlapping m, 16H, 7 menthyl CH and 9 BH), 1.41 (t, *J* = 7.3 Hz, 9H, cationic C*H*$_3$), 1.30-1.08 (overlapping m, 20H, 8 dodecyl CH_2), 0.95-0.90 (overlapping m, 6H 2 menthyl CH_3), 0.90-0.85 (m, 3H, dodecyl CH_3), 0.85-0.79 (m, 3H, menthyl CH_3), 0.33-0.10 (m, 2H, B–C*H*$_2$–CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 169.48 (C=N), 82.21 (menthyl CH), 48.18 (cationic CH_2), 47.77 (menthyl CH), 41.55 (menthyl CH_2), 34.54 (B–CH_2–*CH*$_2$), 32.57 (menthyl CH_2), 31.74 (menthyl CH), 31.11, 30.69, 30.62, 30.53, 30.49, 30.41, 30.33, 30.01 (CH_2 dodecane), 26.98 (menthyl CH), 23.94 (menthyl CH_2), 23.26 (CH_2 dodecane), 22.10, 20.65, 16.94 (3 menthyl CH_3), 14.32 (CH_3 dodecane), 9.37 (cationic CH_3). The B–C signal was detected indirectly at 16.7 ppm in the HSQC spectrum. Direct detection was not successful because of broadening due to coupling to ^{10}B and ^{11}B.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.25 (1B, B–O), -4.56 (1B, B–N), -8.26 (1B, B–C), -14.13 to -23.88 (9B, BH).

High resolution ESI-MS (negative mode, MeOH): *m*/*z* calcd for $[C_{23}H_{54}B_{12}NO_2]^-$: 506.5344; Found: 506.5353.

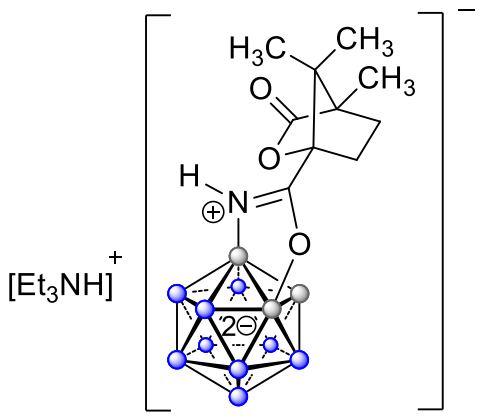
General procedure for the synthesis of cyclized compounds 15 and 16:



10, DG = camphanic
11, DG = menthyl

15, DG = camphanic
16, DG = menthyl

A 20 mL vial was charged with **10** or **11** (0.20 mmol, 1 equiv), (diacetoxy)iodobenzene (0.22 mmol, 1.1 equiv) and magnetic stir bar. Then MeOH (6 mL) was added. The reaction mixture was stirred at 25 °C for 10 min. Et_3N (0.5 mL) was added, and the solution was concentrated on a rotary evaporator. The residue was purified by silica gel column chromatography (eluent DCM/MeCN = 9 : 1, fraction size 15-20 mL). The combined eluates were concentrated on a rotary evaporator and dried under vacuum overnight at 25 °C to afford products **15** or **16** as colorless solids.



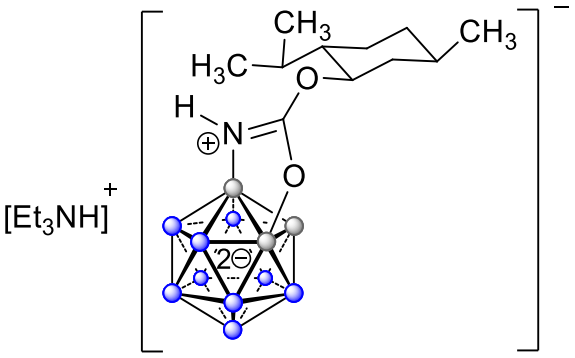
Product **15**: 90% yield.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.09 (br, 1H, cationic NH), 3.50 (q, J = 7.3 Hz, 6H, cationic N–CH), 2.58 (ddd, J = 14.7, 10.9, 4.2 Hz, 1H, camphanic CH), 2.17-2.07 (m, 1H, camphanic CH), 1.94 (ddd, J = 13.6, 9.3, 4.4 Hz, 1H, camphanic CH), 1.73-0.62 (broad overlapping m, 10H, BH), 1.73-1.63 (m, 1H, camphanic CH_2) 1.43 (t, J = 7.3 Hz, 9H, cationic N-CH_2-*CH_3*), 1.09 (overlapping s, 6H, camphanic CH_3), 0.91 (s, 3H, camphanic CH_3). Only one N-H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 180.71 (C=N), 177.33 (C=O), 90.68, 55.76, 55.75 (3 camphanic C), 48.20 (cationic CH_2), 30.98, 29.37 (2 camphanic CH_2), 16.82, 18.89, 9.95 (3 camphanic CH_3), 9.41 (cationic CH_3).

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -6.63 (1B, B–O), -4.45 (1B, B–N), -15.10 to -20.30 (overlapping signals, 8B, BH), -20.91 (1B, BH), -22.22 (1B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{10}H_{24}B_{12}NO_3]^-$: 336.2945; Found: 336.2951



Product **16**: 90% yield

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.14 (br, 1H, anionic NH), 4.69 (ddd, J = 10.9, 10.9, 4.4 Hz, 1H, menthyl CH), 3.49 (q, J = 7.3 Hz, 6H, cationic N–CH_2), 2.04-1.99 (m overlapping with solvent residual signal, 1H, menthyl CH), 1.97-1.85 (m, 1H, menthyl CH), 1.79 – 0.7 (broad overlapping m, 17H, 7 menthyl CH and 10 BH), 1.42 (t, J = 7.3 Hz, 9H, cationic CH_3), 0.93 (d, J = 6.5 Hz, 3H, menthyl CH_3), 0.90 (d, J = 7.0 Hz, 3H, menthyl CH_3), 0.79 (d, J = 6.9 Hz, 3H, menthyl CH_3). Only one N-H signal was detected clearly.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 170.15 (C=N), 82.44 (menthyl CH), 48.21 (cationic CH_2), 48.18 (menthyl CH), 41.58, 34.63 (2 menthyl CH_2), 31.88, 27.13 (2 menthyl CH), 24.09 (menthyl CH_2), 22.14, 20.75, 16.78 (3 menthyl CH_3), 9.40 (cationic CH_3).

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ 5.80 (1B, B–O), -4.36 (1B, B–N), -13.7 to -23.9 (10B, BH).

High resolution ESI-MS (negative mode, MeOH): m/z calcd for $[C_{11}H_{30}B_{12}NO_2]^-$: 338.3466; Found: 338.3471.

III X-ray Crystallography

Crystal structure of 10

$[Et_3NH]_2$[**10**] (20 mg) was dissolved in acetone (0.6 mL) in a 5 mm NMR tube. This solution was layered with hexane (1 mL) and cooled to 4 °C in a refrigerator. Crystals of the composition $[Et_3NH]_4$[**10**]$_2$·acetone suitable for X-ray diffraction were obtained within 15 days.

Bond precision: C-C = 0.0043 A Wavelength=1.54178

Cell: a=18.2099(5) b=10.1365(3) c=19.5538(5)
alpha=90 beta=103.548(1) gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	3508.90(17)	3508.90(17)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	2(C10 H25 B12 N O3), 4(C6 H16 N), C3 H6 O	2(C10 H25 B12 N O3), C3 H6 O, 4(C6 H16 N)
Sum formula	C47 H120 B24 N6 O7	C47 H120 B24 N6 O7
Mr	1140.93	1140.92
Dx,g cm-3	1.080	1.080
Z	2	2
Mu (mm-1)	0.483	0.483
F000	1240.0	1240.0
F000'	1242.97	
h,k,lmax	21,12,23	21,12,23
Nref	12912[6850]	12833
Tmin,Tmax	0.901,0.953	0.655,0.753
Tmin'	0.793	

Correction method= # Reported T Limits: Tmin=0.655 Tmax=0.753
AbsCorr = MULTI-SCAN

Data completeness= 1.87/0.99 Theta(max)= 68.452

R(reflections)= 0.0526(12514) wR2(reflections)= 0.1446(12833)

S = 1.039 Npar= 835

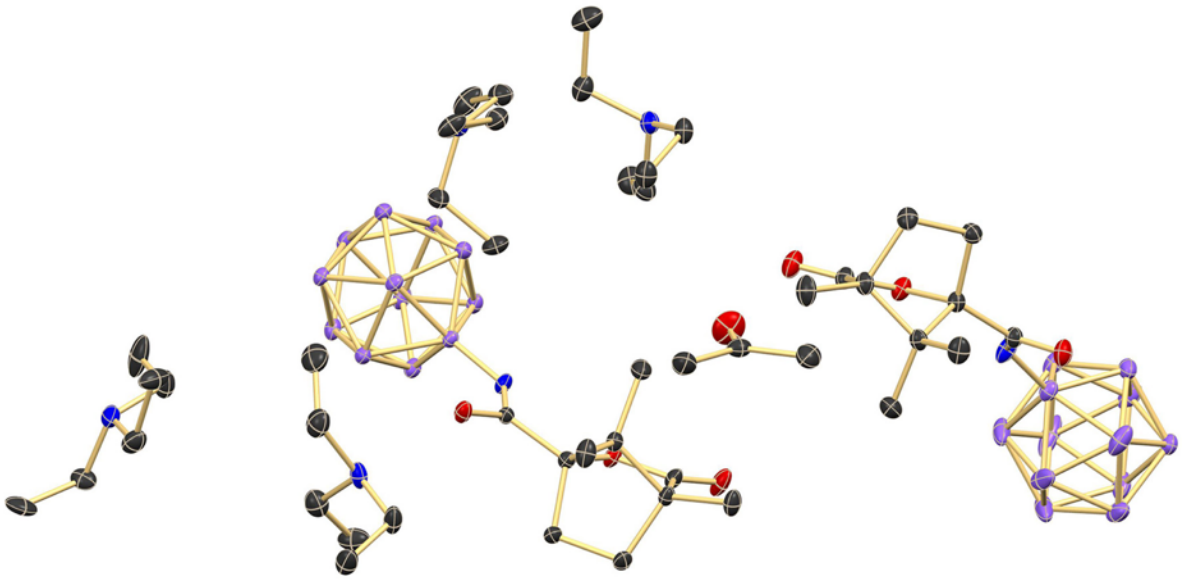


Figure S7. ORTEP representation of $[Et_3NH]_4[\mathbf{10}]_2 \cdot$acetone. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids.

Crystal structure of 13a

[Et_3NH][**13a**] (10 mg) was dissolved in ethanol (0.5 mL) in a 4 mL glass vial. Distilled water (0.2 mL) was added, resulting in a turbid mixture. Heating to 80 °C gave a clear solution. The mixture was allowed to cool to room temperature slowly. The glass vial was kept undisturbed and partially open at room temperature for 20 days, yielding a small number of crystals of the composition [Et_3NH]$_4$[**13a**]$_4$·5H_2O suitable for X-ray diffraction.

Bond precision: C-C = 0.0079 A Wavelength=0.71073

Cell: a=11.3285(9) b=29.264(2) c=20.0792(16)
alpha=90 beta=90.084(2) gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	6656.6(9)	6656.7(9)
Space group	P 21	P 1 21 1
Hall group	P 2yb	P 2yb
Moiety formula	4(C18 H32 B12 N O3), 4(C6 H16 N), 5(H2 O)	C18 H32 B12 N O3, 1.25(H2 O), C6 H16 N
Sum formula	C96 H202 B48 N8 O17	C24 H50.50 B12 N2 O4.25
Mr	2259.54	564.88
Dx,g cm-3	1.127	1.127
Z	2	8
Mu (mm-1)	0.068	0.068
F000	2420.0	2420.0
F000'	2420.80	
h,k,lmax	13,35,24	13,35,24
Nref	24487[12503]	24247
Tmin,Tmax	0.990,0.995	0.694,0.745
Tmin'	0.980	

Correction method= # Reported T Limits: Tmin=0.694 Tmax=0.745
AbsCorr = MULTI-SCAN

Data completeness= 1.94/0.99 Theta(max)= 25.385

R(reflections)= 0.0465(22184) wR2(reflections)= 0.1220(24247)

S = 1.021 Npar= 1587

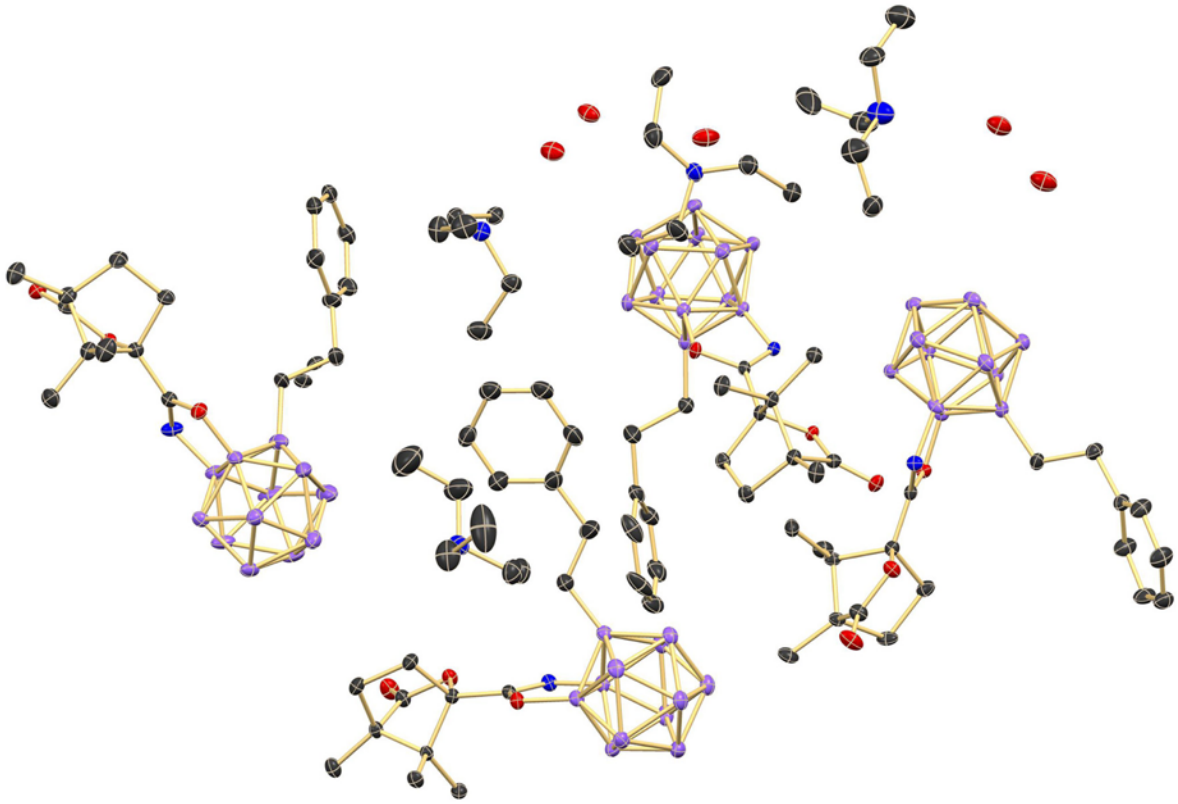


Figure S8. ORTEP representation of $[Et_3NH]_4[\mathbf{13a}]_4 \cdot 5H_2O$. Hydrogen atoms are omitted for clarity; 25% displacement ellipsoids. The ethylene group of one out of four anionic molecules in the asymmetric unit is disordered in a 71:29 ratio; otherwise there is no disorder with regard to other parts of the structure.

IV Evaluation of Antimicrobial Properties

Antimicrobial susceptibility testing

The minimal inhibitory concentrations (MICs) of compounds and antibiotics ceftriaxone, azithromycin and ciprofloxacin were determined using the agar dilution method. Bacterial suspensions (10^4 CFU) of international reference strains *Neisseria gonorrhoeae* ATCC 49226, *Staphylococcus aureus* ATCC 25923, *Enterococcus faecalis* ATCC 29212, *Acinetobacter baumannii* ATCC 19606, *Klebsiella pneumonia* ATCC 700603, *Pseudomonas aeruginosa* ATCC 27853, *Escherichia coli* ATCC 25922, *Enterobacter cloacae* ATCC 700323, *Stenotrophomonas maltophilia* ATCC 17666, *Listeria monocytogenes* EGDe and *Shigella sonnei* SD10053, and *N. gonorrhoeae* multidrug-resistant clinical isolates ZJXSH 89 and ZJXSH 86 were inoculated on the surface of agar plates containing two-fold dilution series of compounds or antibiotics. Agar plates were incubated for 24-48 h at 37 °C and 5% CO_2 and growth was determined. The MIC was defined as the lowest concentration at which no growth was observed.

Determination of bactericidal activity

N. gonorrhoeae ATCC 49226 and *S. aureus* ATCC 25923 were suspended in 12 mL GC broth (Oxoid) supplemented with 1% Vitox (Oxoid) at a concentration of 10^6-10^7 CFU/mL and incubated for 1 h at 37 °C and 200 rpm. Subsequently, compound 14k or the control antibiotics ceftriaxone (*N. gonorrhoeae*) or vancomycin (*S. aureus*) were added at 4×, 2×, 1× or 0.5× the MIC. The vehicle only was included as control. Samples were taken after 0.5, 1, 2. 4 and 8 h for CFU determination on GC agar with 1% Vitox after 24-48 h incubation at 37 °C and 5% CO_2. For live/dead staining, samples were taken after 1 h incubation, washed with PBS and incubated for 15 minutes at room temperature with SYTO 9 (1.67 μM) and propidium iodide (10 μM) stains (Thermo). After washing, fluorescence was visualized on an Olympus FV1000 confocal microscope.

Table S1. MIC data (μM) for compounds against references strains of various Gram-positive and Gram-negative species

Compound	Gram-negative								Gram-positive		
	Neisseria gonorrhoeae ATCC 49226	*Stenotrophomonas maltophilia* ATCC 17666	*Escherichia coli* ATCC 25922	*Pseudomonas aeruginosa* ATCC 27853	*Acinetobacter baumannii* ATCC 19606	*Shigella sonnei* SD10053	*Klebsiella pneumoniae* ATCC 700603	*Enterobacter cloacae* ATCC 700323	*Staphylococcus aureus* ATCC 25923	*Enterococcus faecalis* ATCC 29212	*Listeria monocytogenes* EGDe
10	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256
13a	16	>256	>256	>256	>256	>256	>256	>256	128	128	>256
13b	16	>256	>256	>256	>256	>256	>256	>256	32	64	>256
13c	16	>256	>256	>256	>256	>256	>256	>256	64	>256	>256
13d	8	>256	>256	>256	>256	>256	>256	>256	64	>256	>256
13e	16	>256	>256	>256	>256	>256	>256	>256	64	64	>256
13f	8	>256	>256	>256	>256	>256	>256	>256	8	16	>256
13g	64	>256	>256	>256	>256	>256	>256	>256	256	256	>256
13h	4	>256	>256	>256	>256	>256	>256	>256	16	32	>256
13i	4	256	>256	>256	>256	>256	>256	>256	16	16	>256
13j	32	>256	>256	>256	>256	>256	>256	>256	64	64	>256
13k	8	>256	>256	>256	>256	>256	>256	>256	64	64	>256
15	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256
11	128	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256
14a	4	64	>256	>256	>256	>256	>256	>256	4	4	8
14b	8	64	>256	>256	>256	>256	>256	>256	8	8	16
14c	16	256	>256	>256	>256	>256	>256	>256	8	16	16
14d	8	32	>256	>256	>256	>256	>256	>256	4	8	8
14e	4	128	>256	>256	>256	>256	>256	>256	4	8	16
14f	8	256	>256	>256	>256	>256	>256	>256	16	16	16
14g	4	>256	>256	>256	>256	>256	>256	>256	4	32	32
14h	4	16	>256	>256	>256	>256	>256	>256	4	4	8
14i	4	32	>256	>256	>256	>256	>256	>256	4	4	4
14j	4	64	>256	>256	>256	>256	>256	>256	4	8	8
14k	2	>256	>256	>256	>256	>256	>256	>256	4	4	32
14l	4	128	>256	>256	>256	>256	>256	>256	8	16	>256
14m	4	128	>256	>256	>256	>256	>256	>256	8	8	>256
14n	16	>256	>256	>256	>256	>256	>256	>256	>256	64	>256
16	16	>256	>256	>256	>256	>256	>256	>256	64	128	>256
(–)-Menthol	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256
(–)-Camphanic Acid	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256
$[B_{12}H_{11}\text{-}NH_3]^-$	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256	>256

Table S2. MIC data (μM) for selected compounds and marketed antibiotics against different strains of *Neisseria gonorrhoeae*

Compound	13d	13f	13h	13i	13k	14a	14b	14d	14e	14f	14g	14h	14i	14j	14k	14l	14m	Ceftriaxone	Azithromycin	Ciprofloxacin
N. gonorrhoeae ATCC 49226	8	8	4	4	8	4	8	8	4	8	4	4	4	4	**2**	4	4	0.008	0.016	0.03
N. gonorrhoeae ZJXSH 89	8	8	4	4	8	4	8	8	4	16	4	4	4	4	**2**	4	4	0.016	2048	48
N. gonorrhoeae ZJXSH 86	8	8	4	4	8	4	8	8	4	8	4	4	4	4	**2**	4	4	0.008	0.016	48

V References

[1] V. Geis, K. Guttsche, C. Knapp, H. Scherer, R. Uzun, *Dalton Trans.* **2009**, 2687–2694.

[2] O. Bondarev, A. A. Khan, X. Tu, Y. V. Sevrugina, S. S. Jalisatgi, M. F. Hawthorne, *J. Am. Chem. Soc*. **2013**, *135*, 13204–13211.

[3] J. R. Holmes D. Kivelson, W. C. Drinkard, *J. Chem. Phys.* **1962**, *37*, 150–152;
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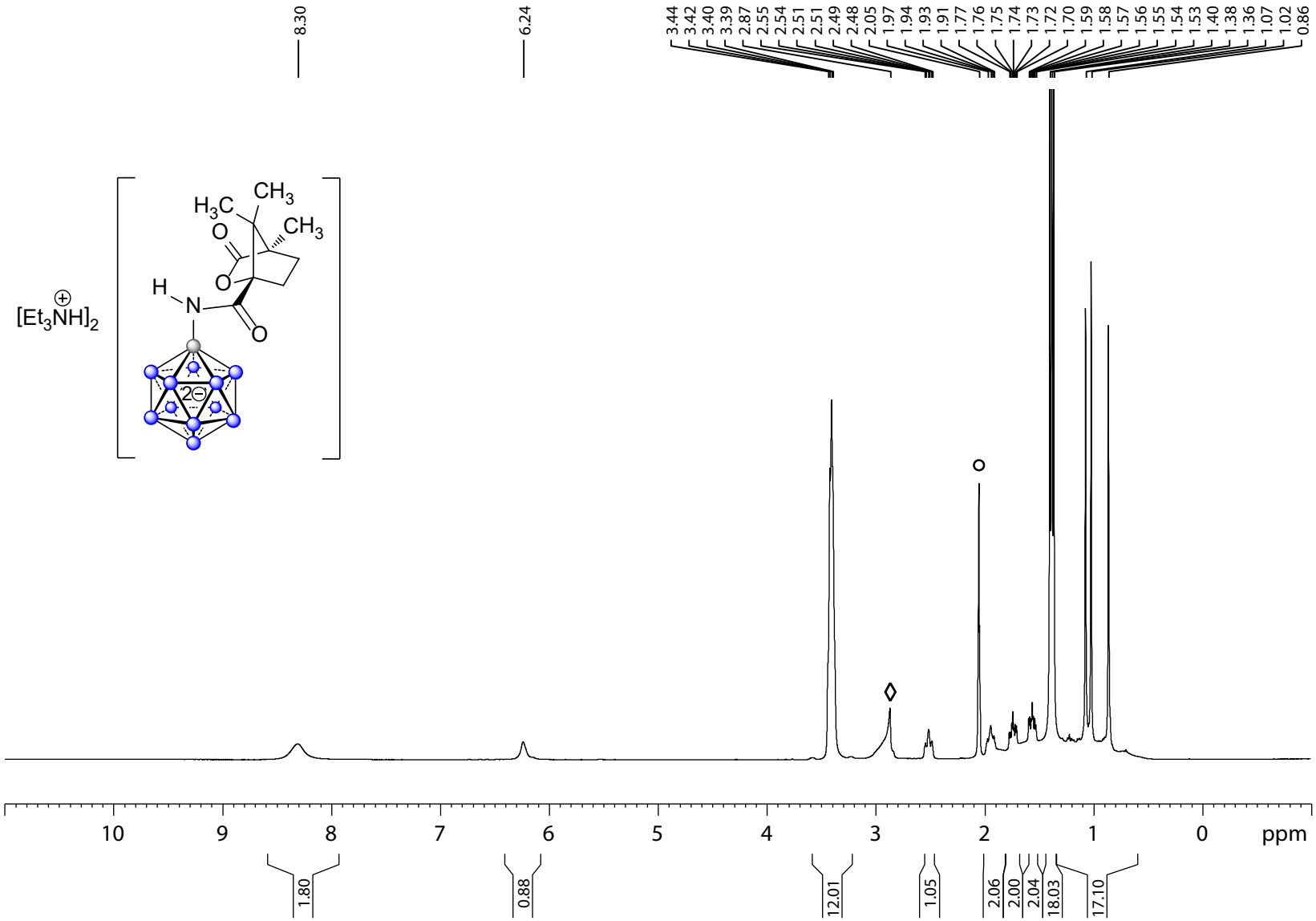
[5] Y. Zhang, Y. Sun, F. Lin, J. Liu, S Duttwyler, *Angew. Chem. Int. Ed.* **2016**, *55*, 15609–15614.

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_            20190701
Time                9.21
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ              3.2767999 sec
RG                 107.6
DW                50.000 usec
DE                 6.50 usec
TE                 296.0 K
D1             1.00000000 sec
TD0                    1

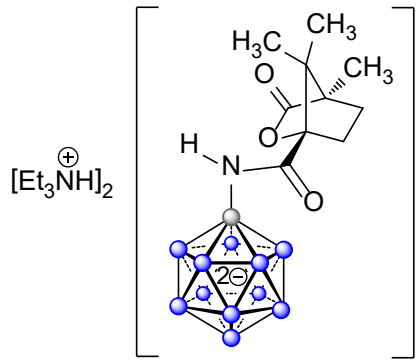
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300075 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

NMR-001

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190701
Time                 9.23
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgig30
TD                 16384
SOLVENT          Acetone
NS                    16
DS                     4
SWH             8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                   107.6
DW                  62.400 usec
DE                   6.50 usec
TE                  296.3 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1          12.50000000 W
SFO1         400.1320007 MHz

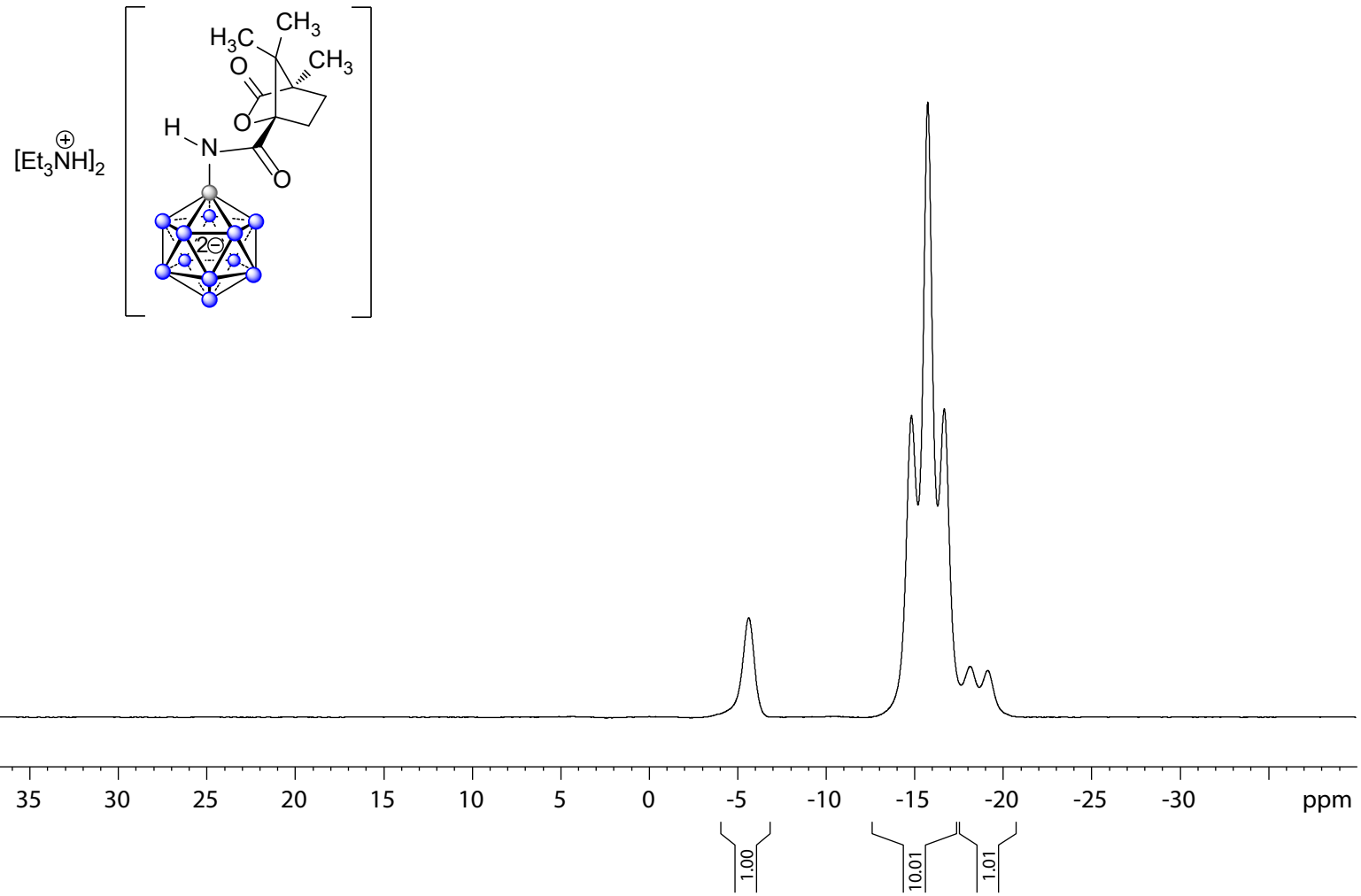
======== CHANNEL f2 ========
CPDPRG[2              garp4
NUC2                   11B
PCPD2                90.00 usec
PLW2          52.96599960 W
PLW12          0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                    32768
SF           400.1300074 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

NMR-002

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190701
Time                9.29
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE                296.3 K
D1           1.00000000 sec
TD0                     1

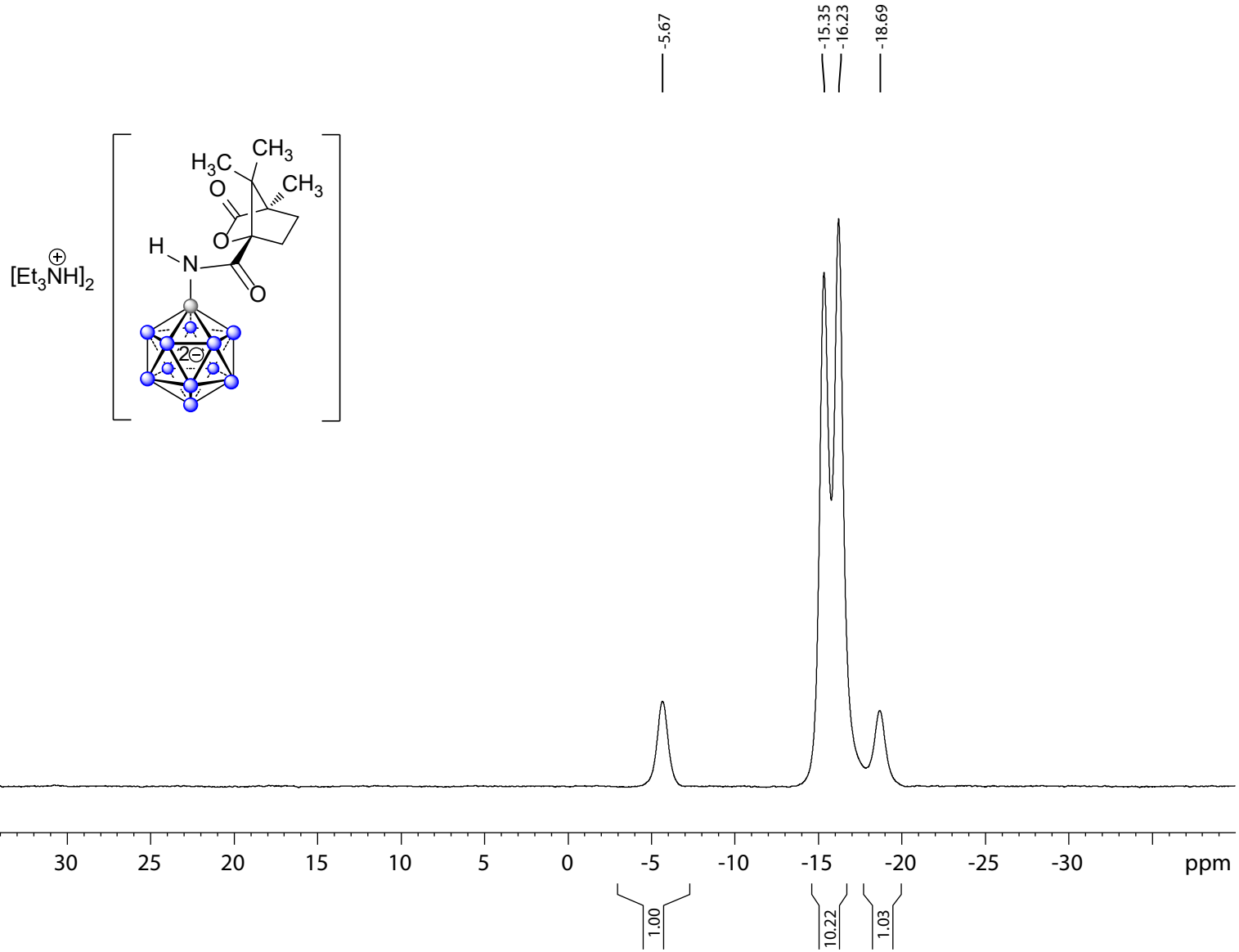
======== CHANNEL f1 ========
NUC1                  11B
P1                   9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                  32768
SF          128.3776050 MHz
WDW                    EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-003

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

$^{11}B\{^1H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190701
Time                9.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

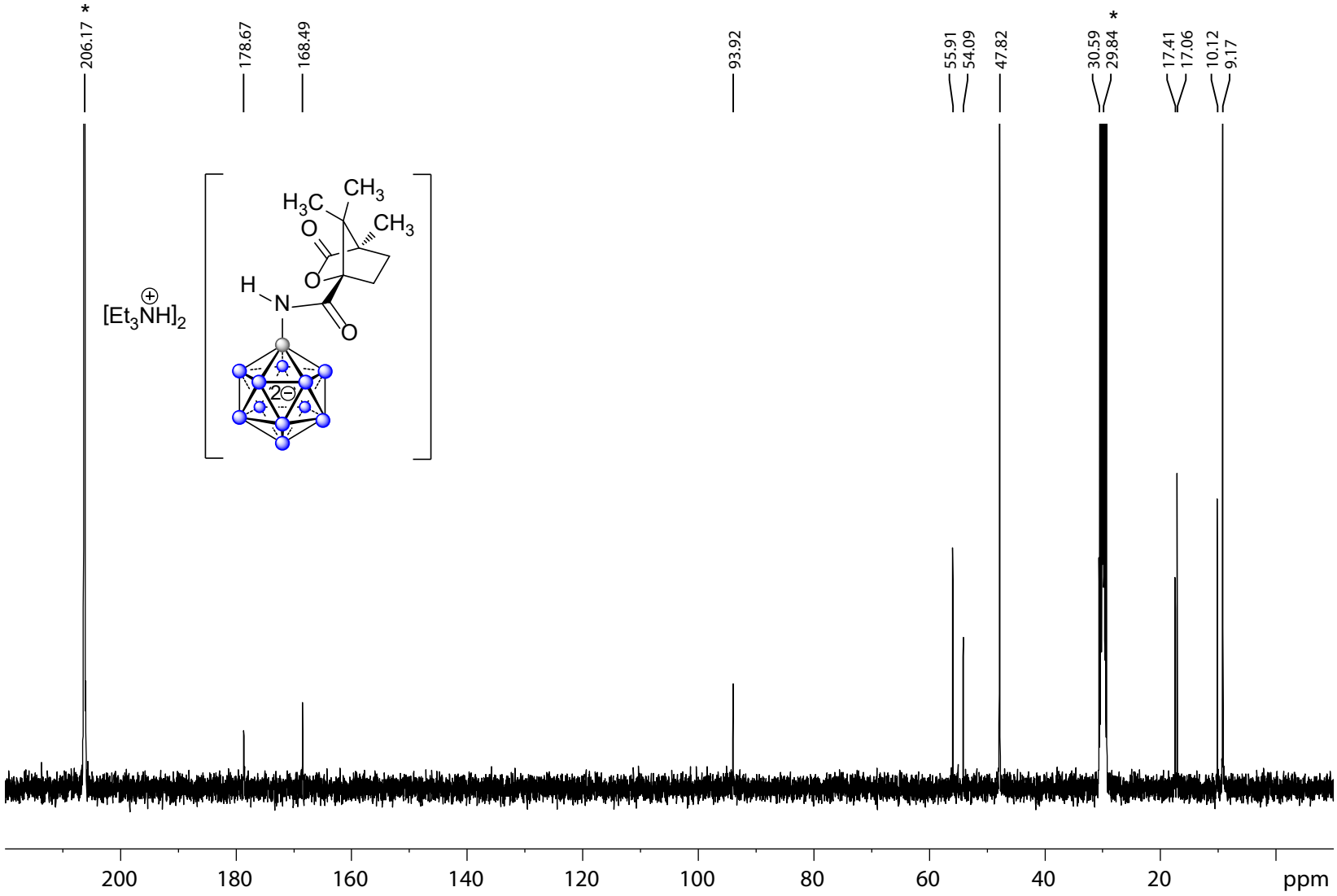
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF           128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-004

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190701
Time               11.08
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE                297.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

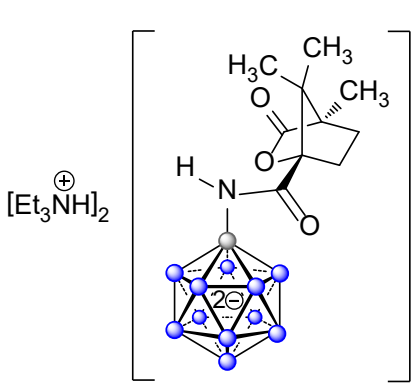
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF         100.6126798 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

^{13}CDEPT NMR 100 MHz



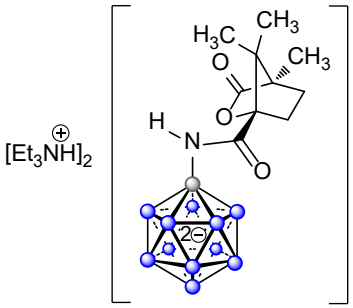

```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    6
PROCNO                   1

F2 - Acquisition Parameters
Date_           20190701
Time              12.03
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE                296.4 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

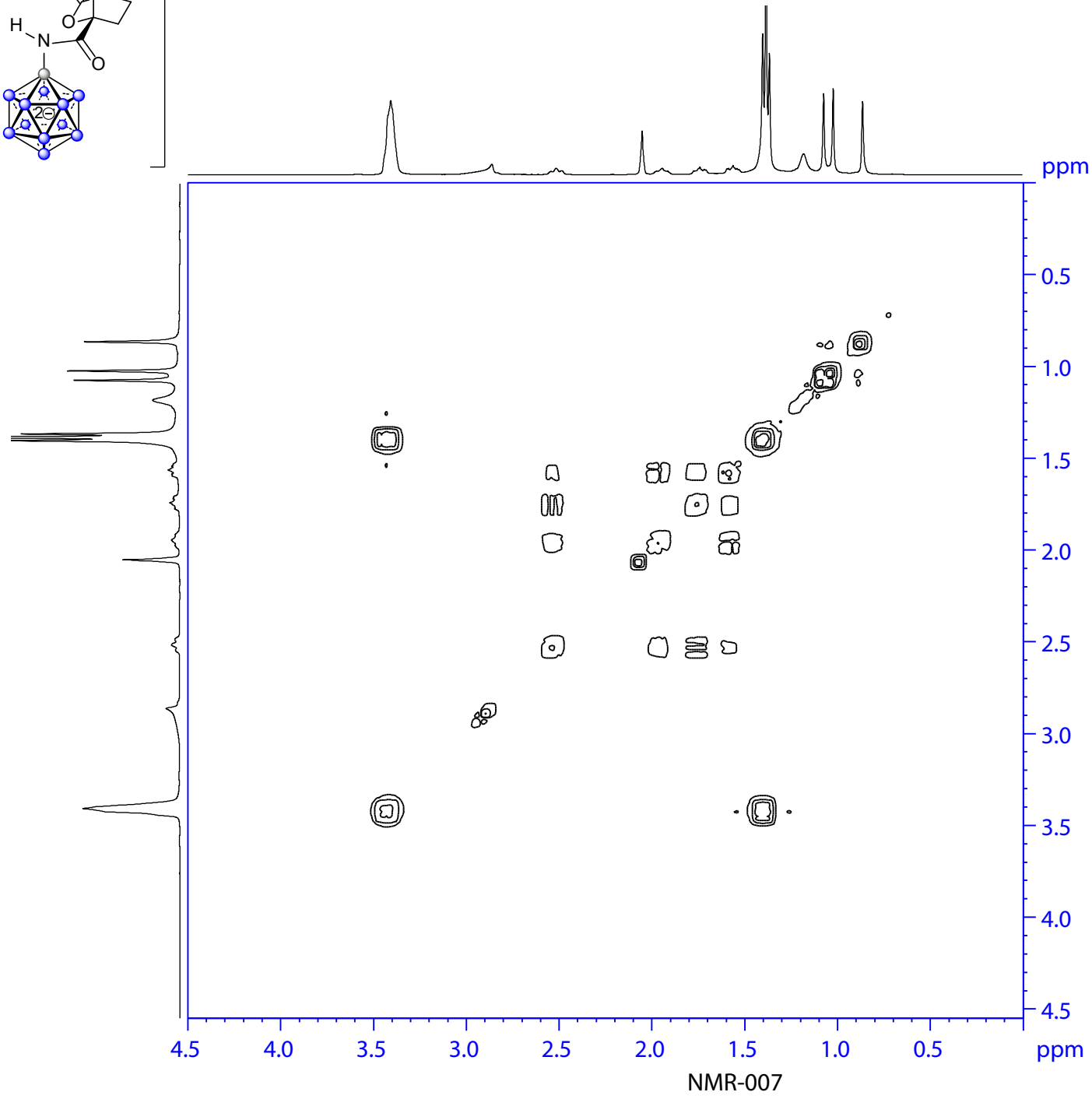
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                 15.00 usec
P4                 30.00 usec
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126795 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```



20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

^1H - ^1H COSY NMR




```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    8
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190701
Time                 12.19
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                    2048
SOLVENT           Acetone
NS                       2
DS                       8
SWH               5341.880 Hz
FIDRES            2.608340 Hz
AQ               0.1916928 sec
RG                  170.36
DW                  93.600 usec
DE                   6.50 usec
TE                  296.1 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00018720 sec

======== CHANNEL f1 ========
NUC1                     1H
P0                   15.00 usec
P1                   15.00 usec
P17                2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                10.00 %
P16               1000.00 usec

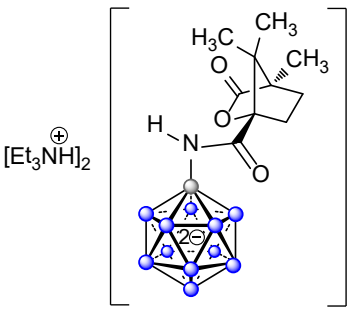
F1 - Acquisition parameters
TD                     128
SFO1            400.1324 MHz
FIDRES         83.466881 Hz
SW                  13.350 ppm
FnMODE                 QF

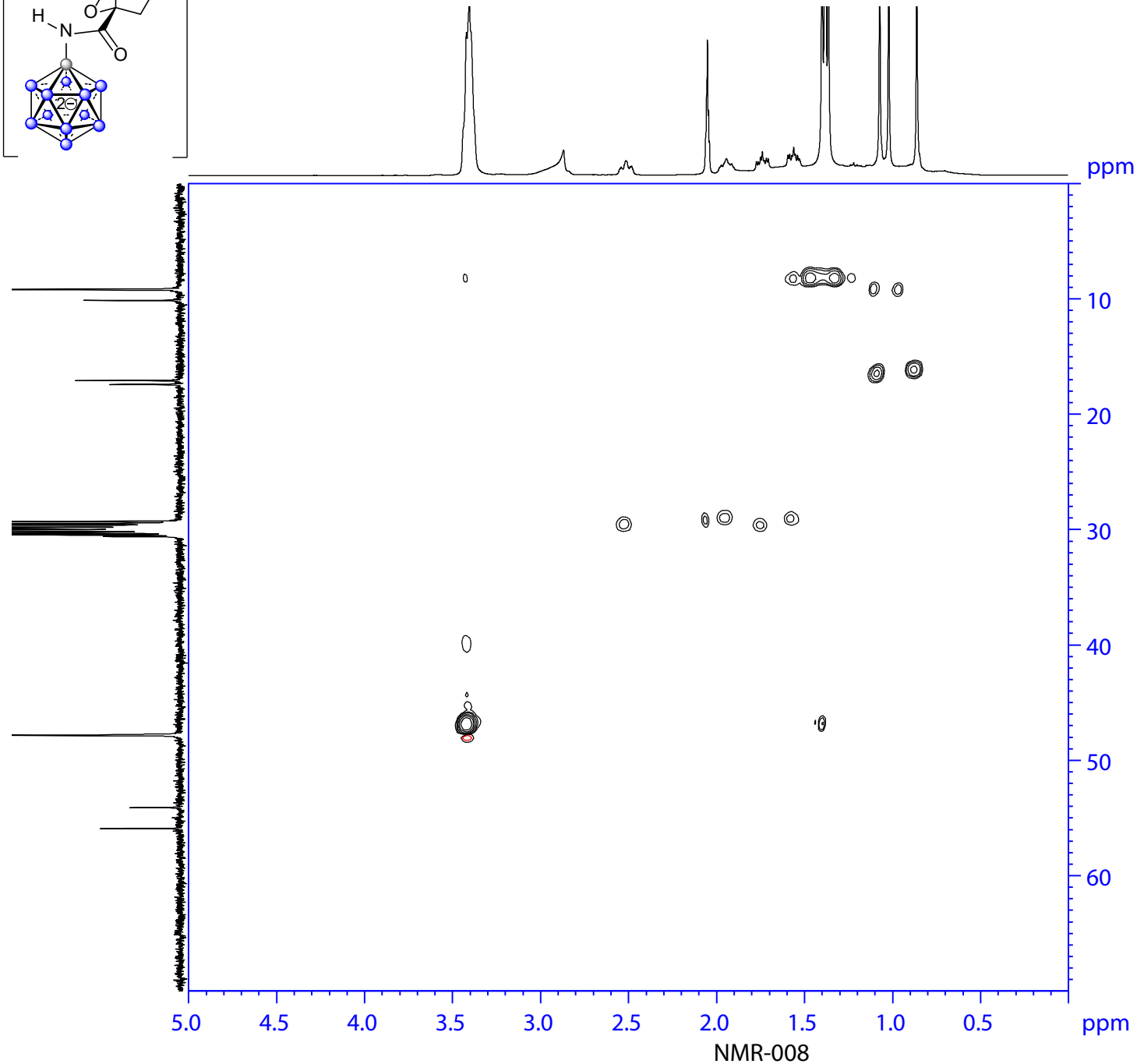
F2 - Processing parameters
SI                     1024
SF           400.1300000 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
PC                   1.40

F1 - Processing parameters
SI                     1024
MC2                    QF
SF           400.1300000 MHz
WDW                  QSINE
SSB       0
LB        0 Hz
GB        0
```

20190630-B12C 20 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCOCamphanic]$ dissolved in 0.6 mL acetone-*d*6

^1H - ^{13}C HSQC NMR






```
Current Data Parameters
NAME      20190630-RV-B12C
EXPNO                    7
PROCNO                   1

F2 - Acquisition Parameters
Date_             20190701
Time_                12.04
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                   1024
SOLVENT           Acetone
NS                      2
DS                     16
SWH              6009.615 Hz
FIDRES           5.868765 Hz
AQ               0.0851968 sec
RG                  193.34
DW                  83.200 usec
DE                    6.50 usec
TE                   296.3 K
CNST2          145.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D4              0.00172414 sec
D11             0.03000000 sec
D16             0.00020000 sec
D24             0.00086207 sec
IN0             0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
P2                   30.00 usec
P28                1000.00 usec
PLW1          12.50000000 W
SFO1          400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2              garp
NUC2                   13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                70.00 usec
PLW2          53.00000000 W
PLW12          1.08159995 W
SFO2          100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                 80.00 %
GPZ2                 20.10 %
GPZ3                 11.00 %
GPZ4                 -5.00 %
P16                1000.00 usec
P19                 600.00 usec

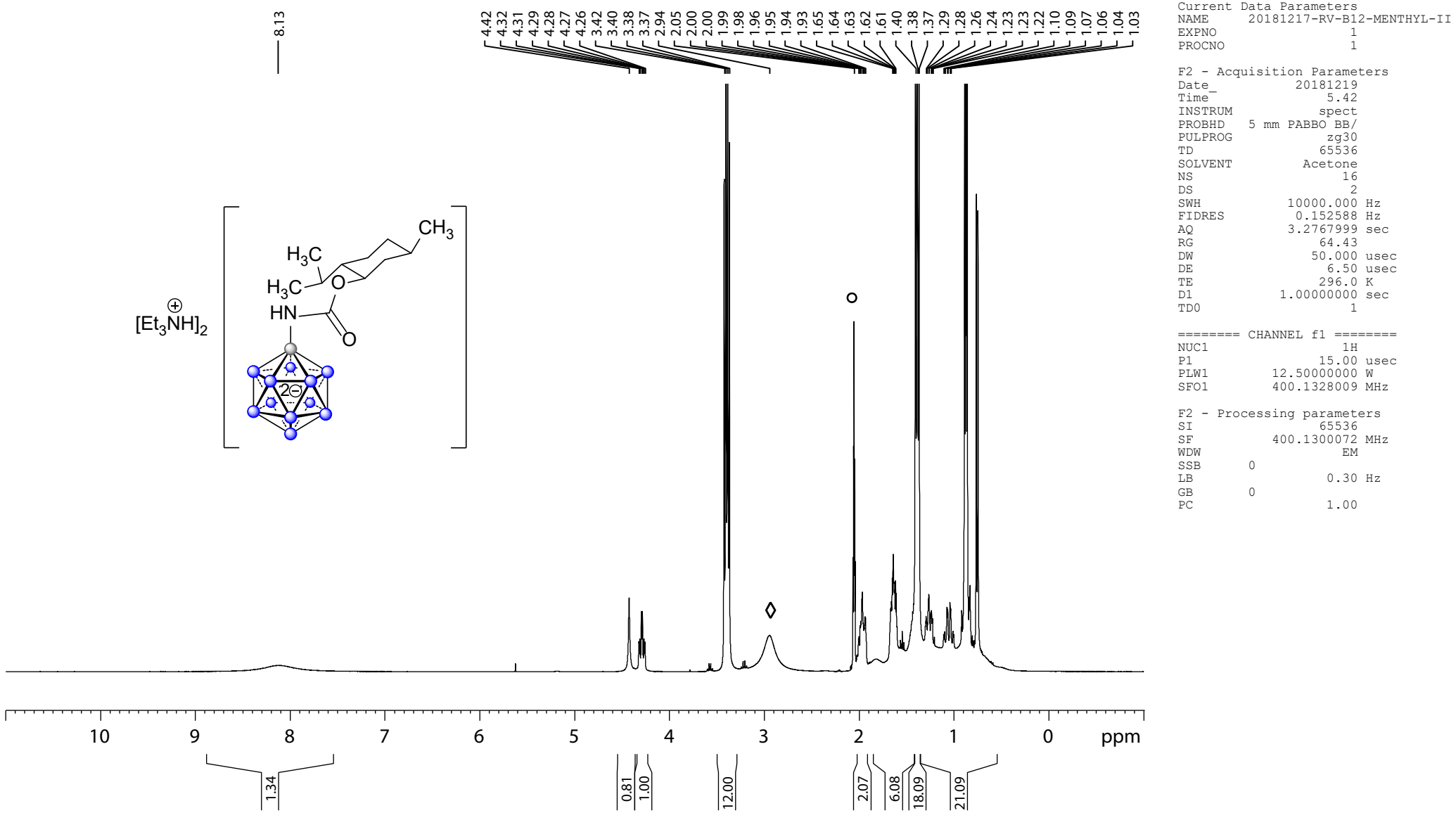
F1 - Acquisition parameters
TD                      256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW                249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                     1024
SF            400.1300000 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
PC                    1.40

F1 - Processing parameters
SI                     1024
MC2         echo-antiecho
SF            100.6127690 MHz
WDW                  QSINE
SSB                      2
LB         0 Hz
GB         0
```

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20181217-RV-B12-MENTHYL-II
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20181219
Time                5.42
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ              3.2767999 sec
RG                 64.43
DW                50.000 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                    1

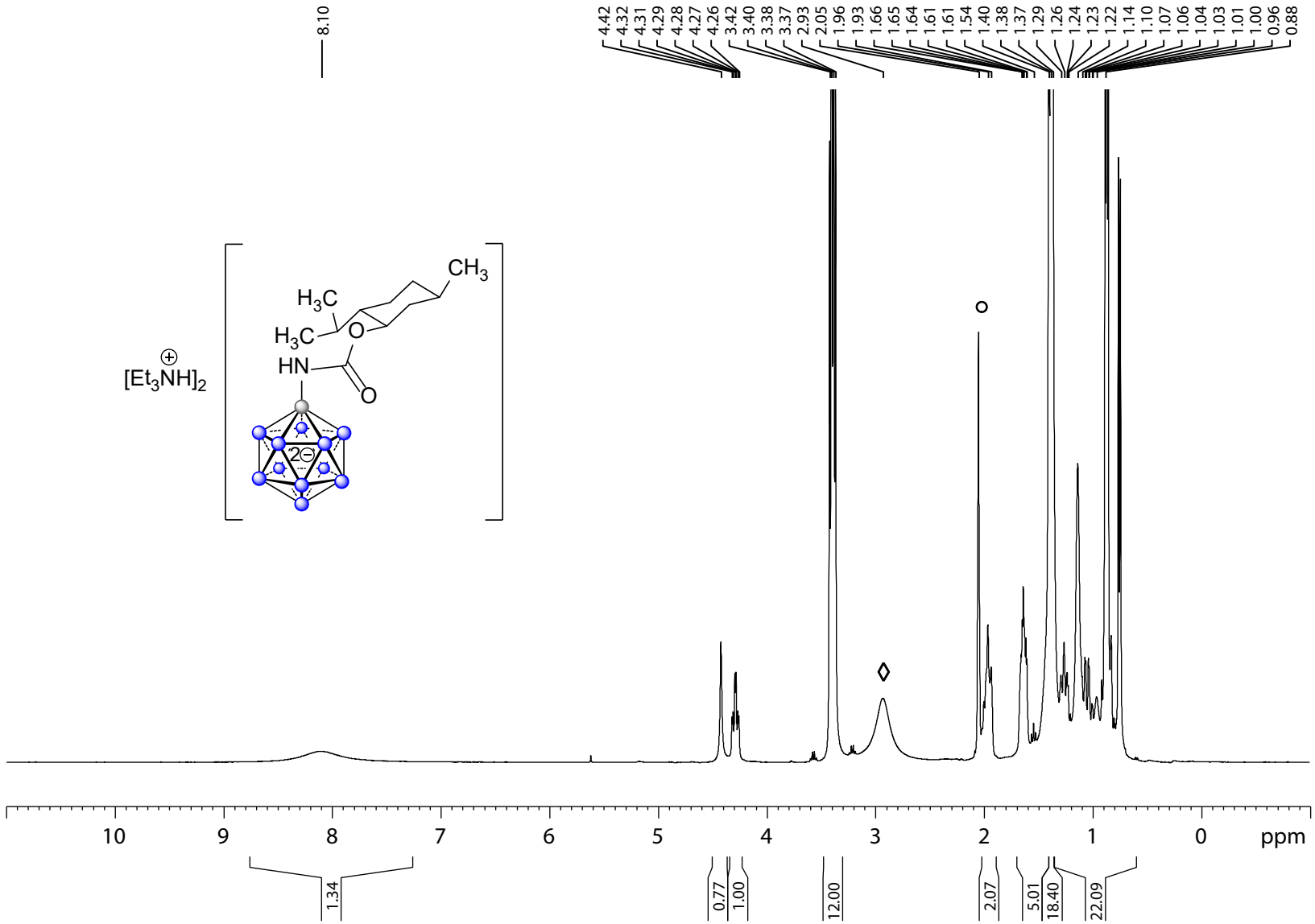
======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300072 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

NMR-009

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20181217-RV-B12-MENTHYL-II
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20181219
Time               5.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD              16384
SOLVENT       Acetone
NS                16
DS                 4
SWH          8012.820 Hz
FIDRES       0.489064 Hz
AQ           1.0223616 sec
RG              64.43
DW              62.400 usec
DE               6.50 usec
TE              296.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                1

======== CHANNEL f1 ========
NUC1               1H
P1              15.00 usec
PLW1       12.50000000 W
SFO1       400.1320007 MHz

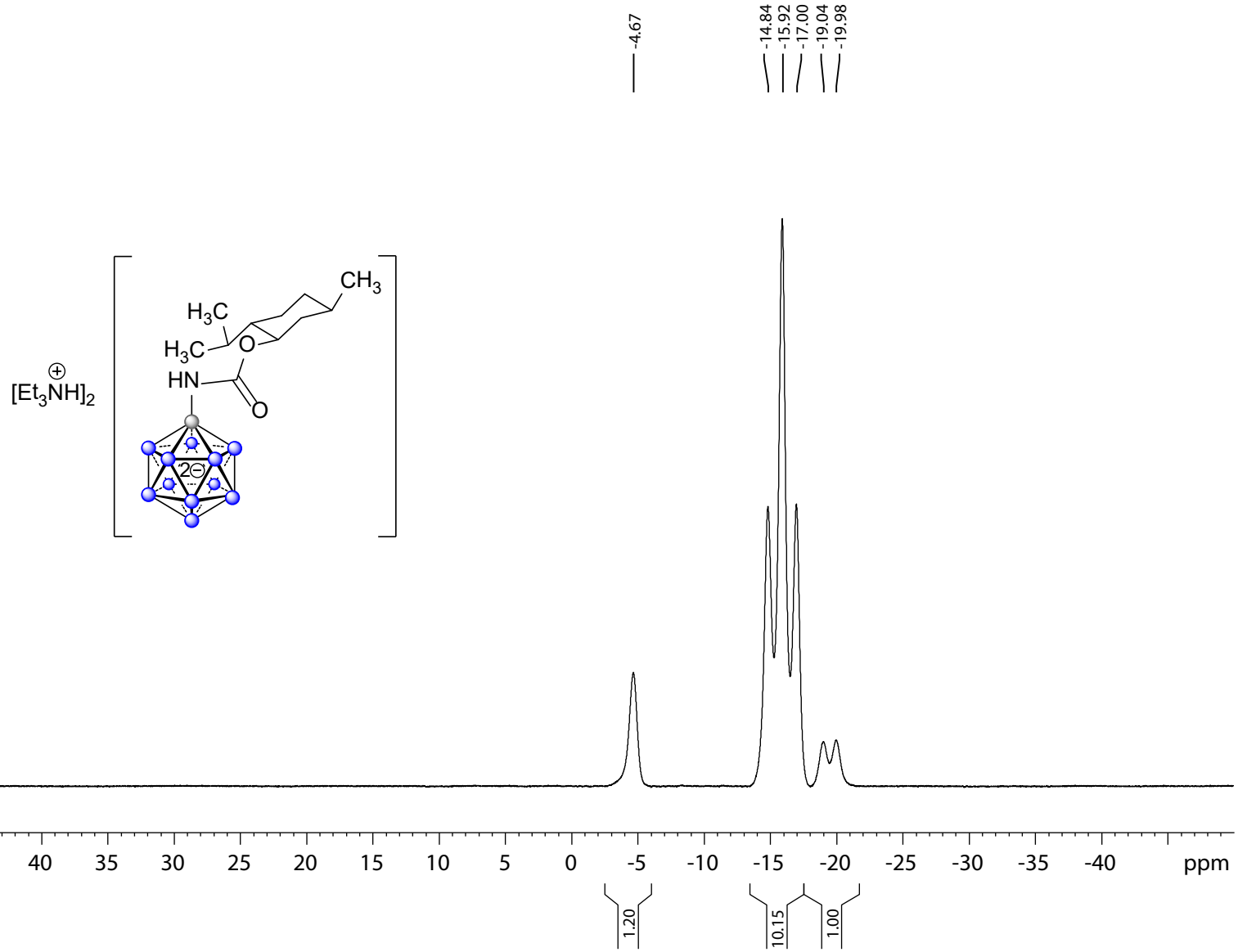
======== CHANNEL f2 ========
CPDPRG[2         garp4
NUC2              11B
PCPD2           90.00 usec
PLW2       52.96599960 W
PLW12       0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI             32768
SF         400.1300073 MHz
WDW               EM
SSB       0
LB             1.00 Hz
GB        0
PC             1.40
```

NMR-010

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20181217-RV-B12-MENTHYL-II
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20181219
Time                5.47
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                295.9 K
D1             1.00000000 sec
TD0                    1

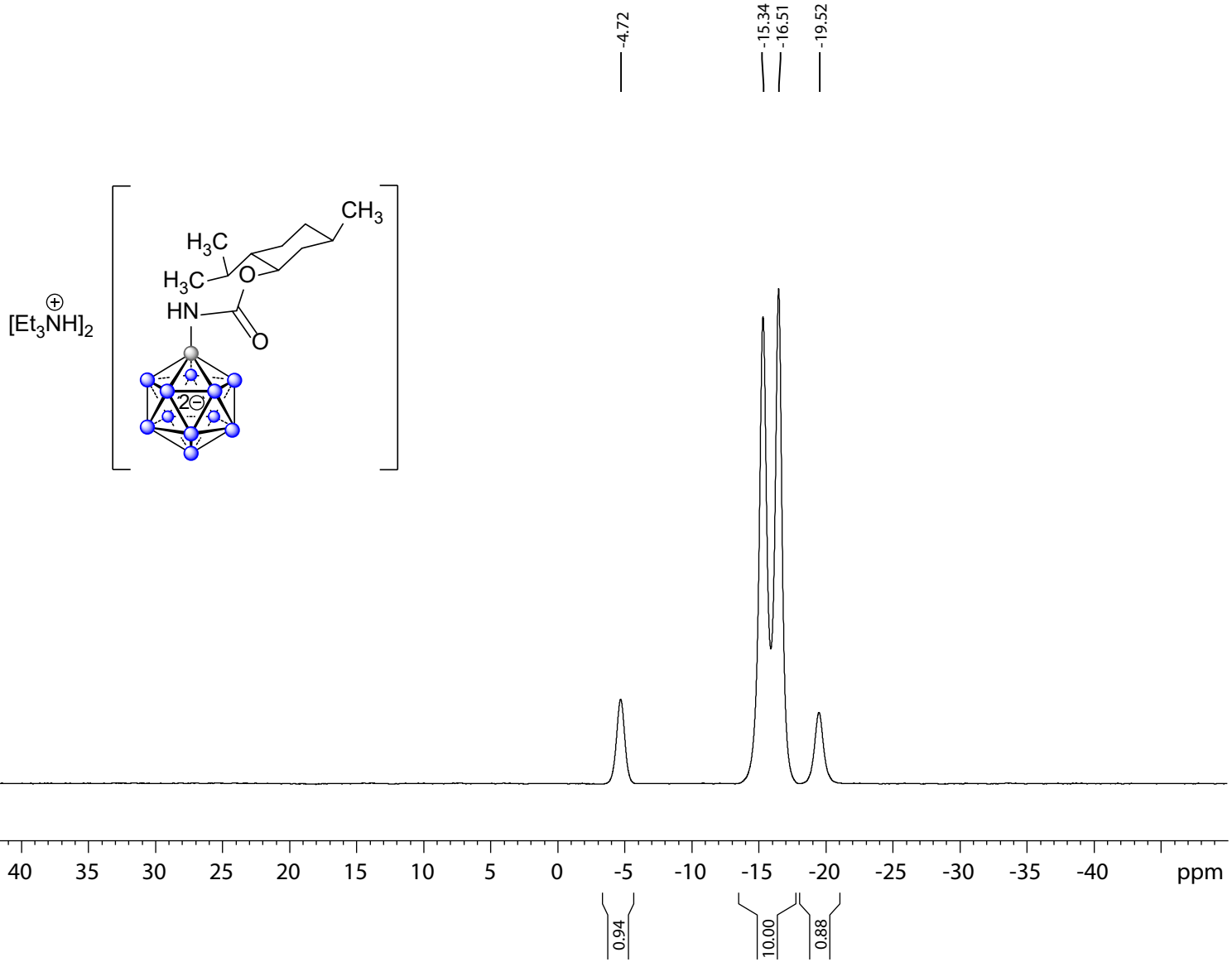
======== CHANNEL f1 ========
NUC1                  11B
P1                   9.93 usec
PLW1         52.96599960 W
SFO1         128.3776052 MHz

F2 - Processing parameters
SI                 32768
SF           128.3776050 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

NMR-011

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20181217-RV-B12-MENTHYL-II
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20181219
Time               5.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

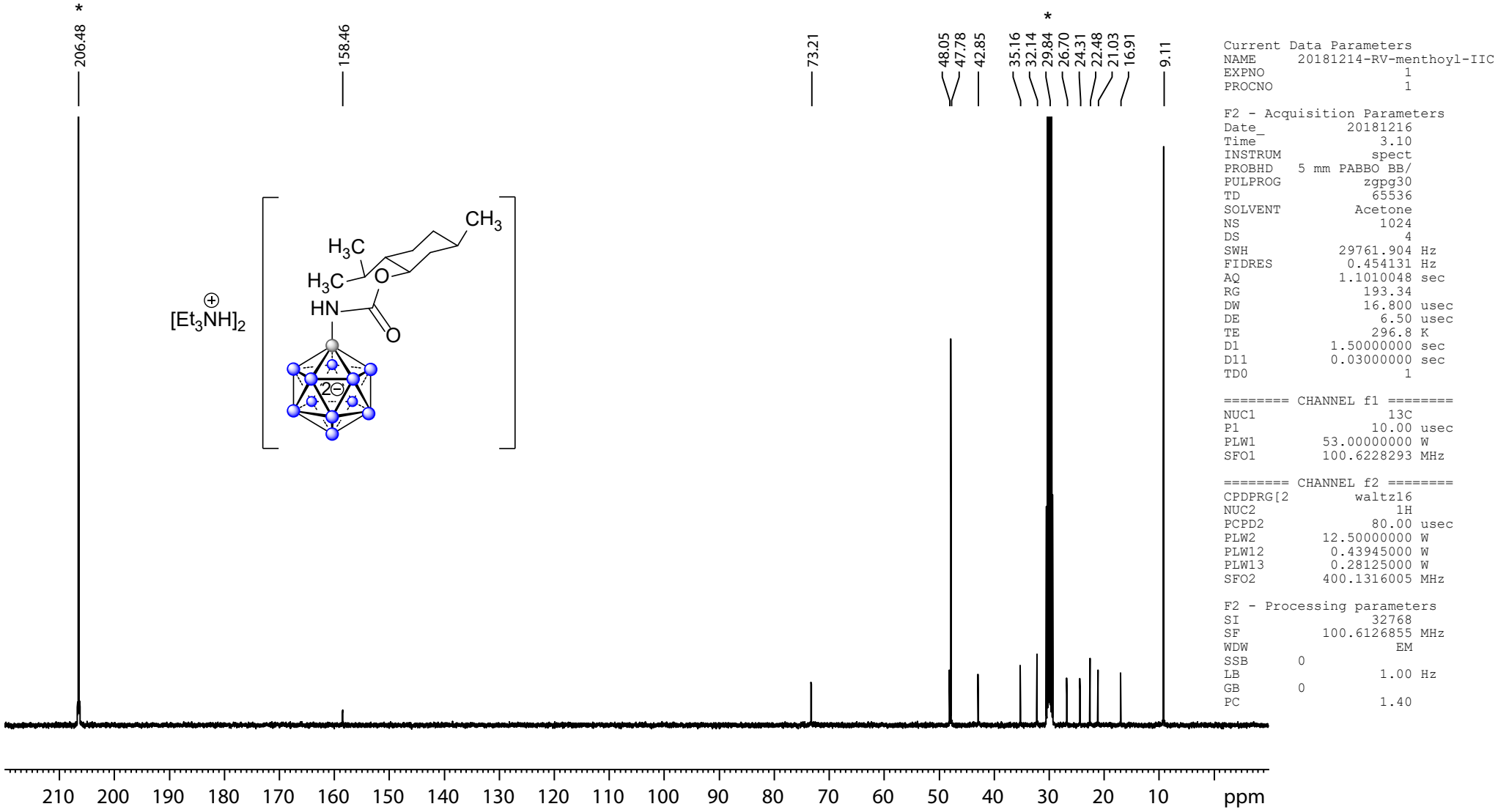
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                EM
SSB      0
LB               10.00 Hz
GB       0
PC                1.40
```

NMR-012

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20181214-RV-menthoyl-IIC
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20181216
Time               3.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW                16.800 usec
DE                 6.50 usec
TE                296.8 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

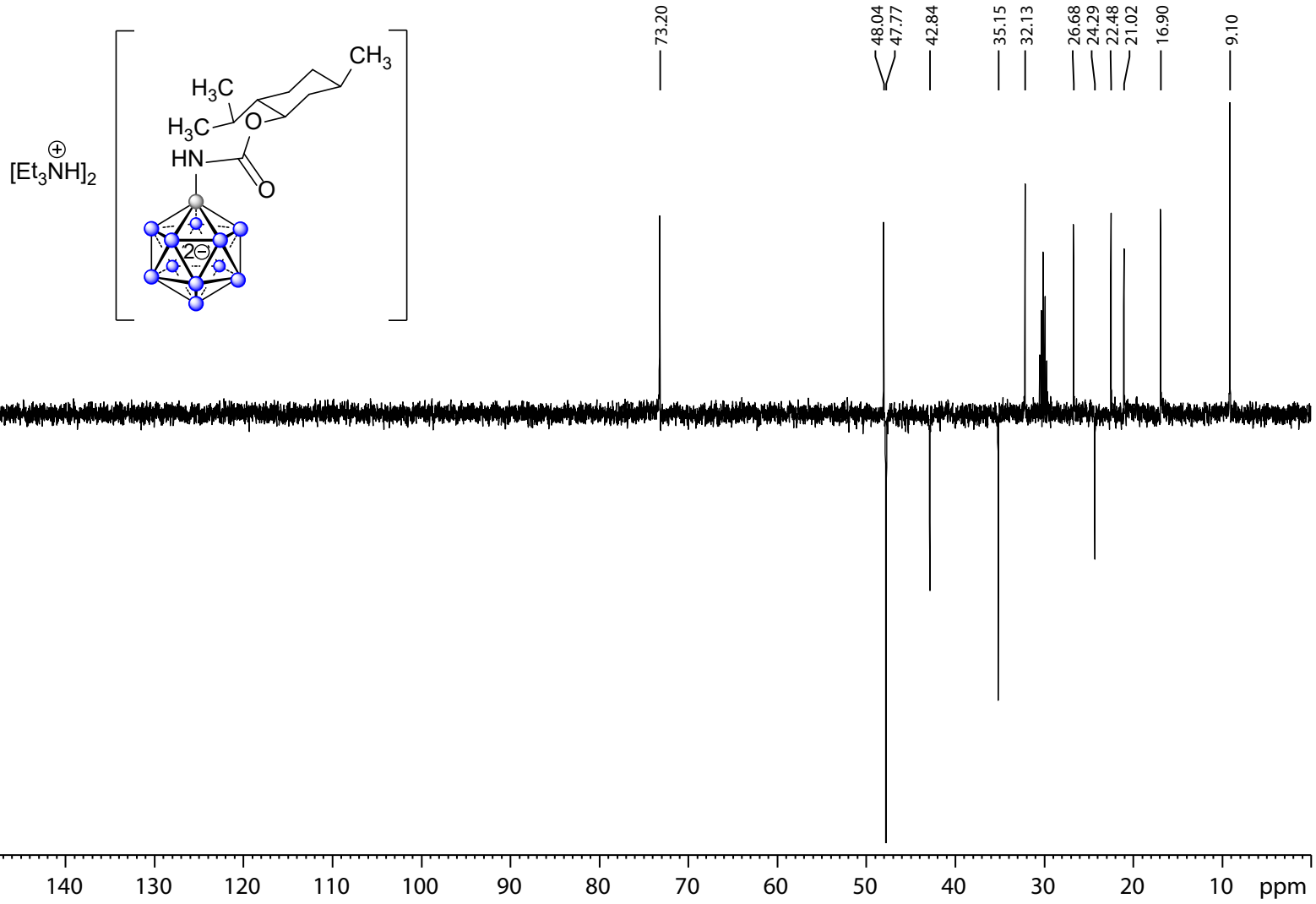
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126855 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz



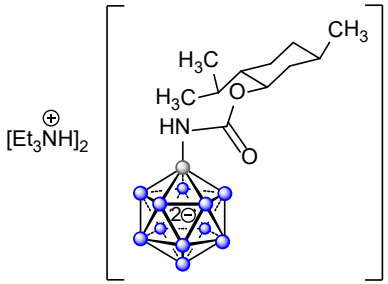

```
Current Data Parameters
NAME      20181214-RV-menthoyl-IIC
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20181216
Time               3.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  256
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG               193.34
DW               17.067 usec
DE                 6.50 usec
TE                296.0 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

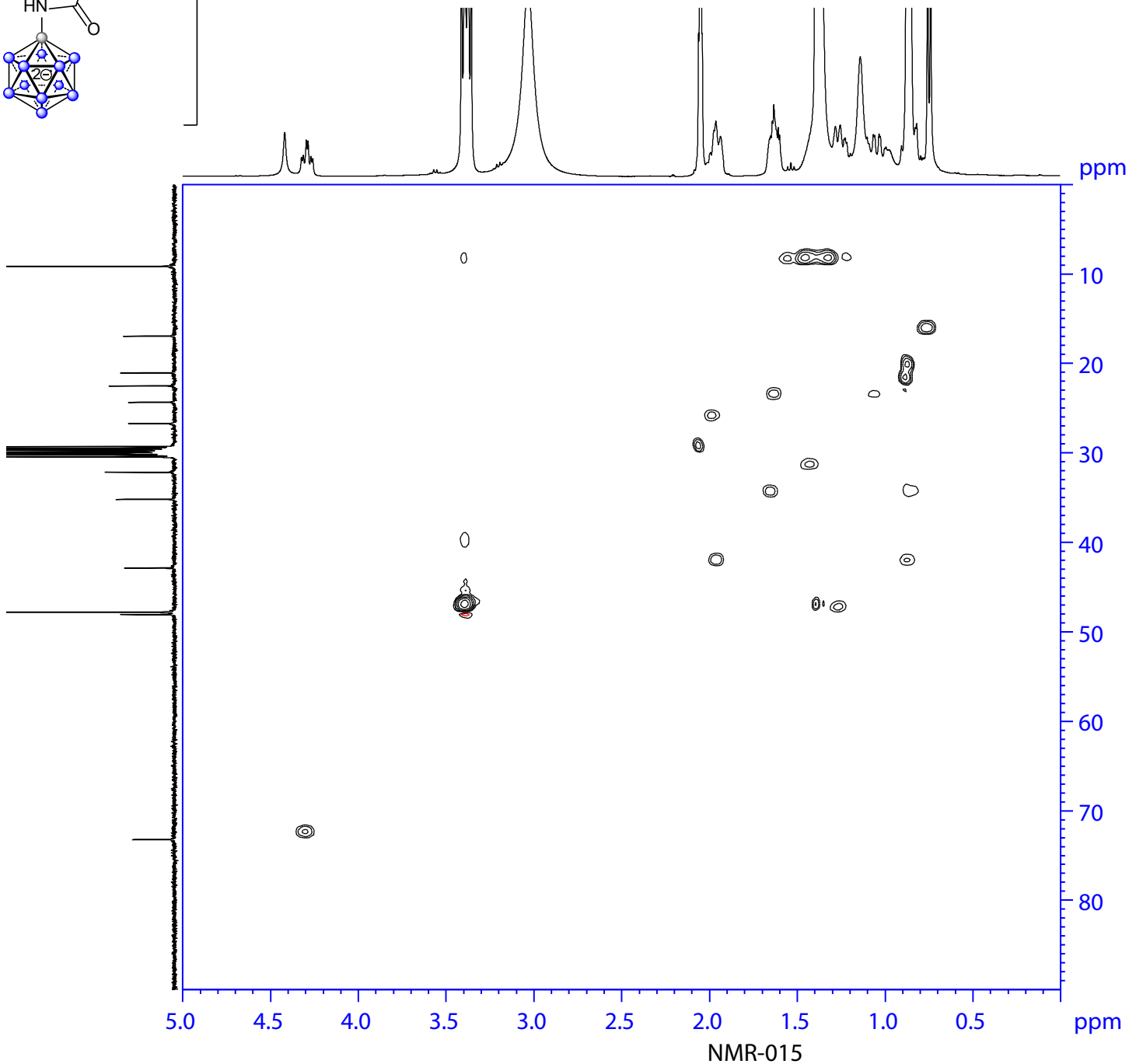
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                 15.00 usec
P4                 30.00 usec
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126862 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 4.00
```



20182117-B12M-Menthyl 10 mg white solid $[Et_3NH]_2[B_{12}H_{11}NHCO(Menthyl)]$ dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20181214-RV-menthoyl-IIC
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20181216
Time_              3.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW              83.200 usec
DE                6.50 usec
TE                295.8 K
CNST2        145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1             80.00 %
GPZ2             20.10 %
GPZ3             11.00 %
GPZ4             -5.00 %
P16            1000.00 usec
P19             600.00 usec

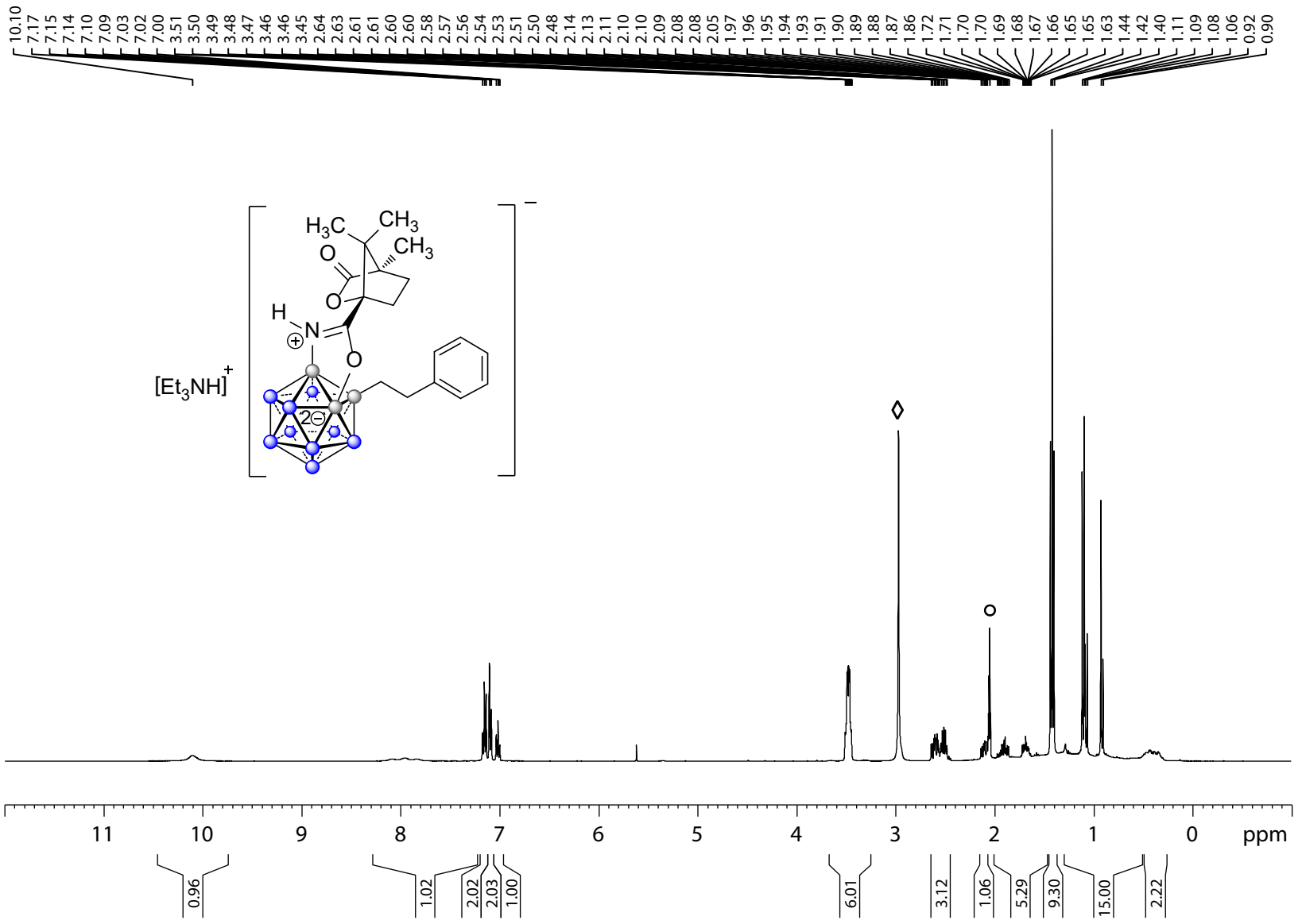
F1 - Acquisition parameters
TD                  256
SFO1          100.6238 MHz
FIDRES        196.524048 Hz
SW               249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW                QSINE
SSB                    2
LB         0 Hz
GB         0
PC                  1.40

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW                QSINE
SSB                    2
LB         0 Hz
GB         0
```

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190704-RV-B12C-Styr
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                 20.39
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT           Acetone
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ               3.2767999 sec
RG                   95.29
DW                   50.000 usec
DE                    6.50 usec
TE                   296.4 K
D1              1.00000000 sec
TD0                      1

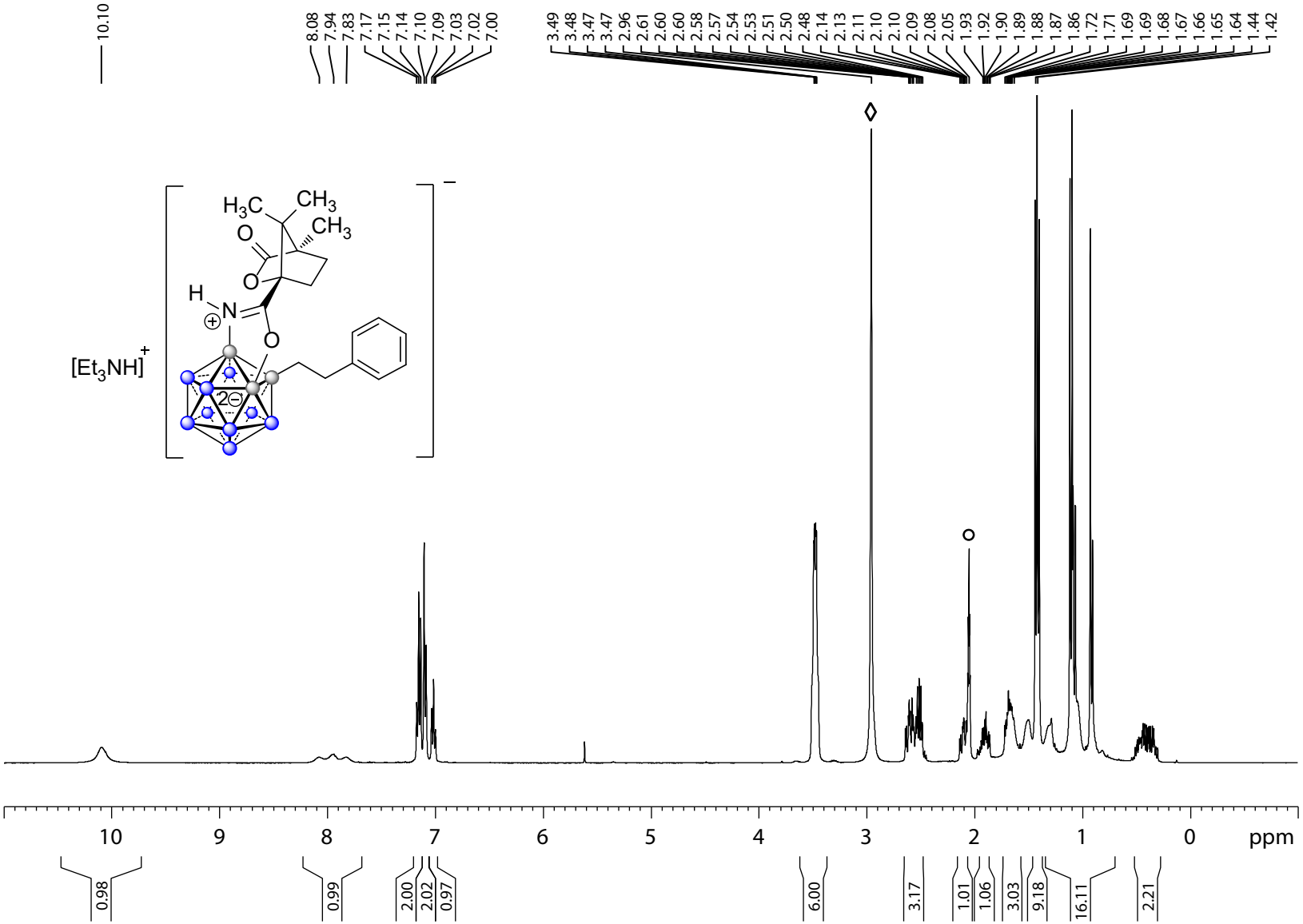
======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1           12.50000000 W
SFO1           400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF             400.1300070 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

NMR-016

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190704-RV-B12C-Styr
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                 20.41
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   296.6 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1           12.50000000 W
SFO1          400.1320007 MHz

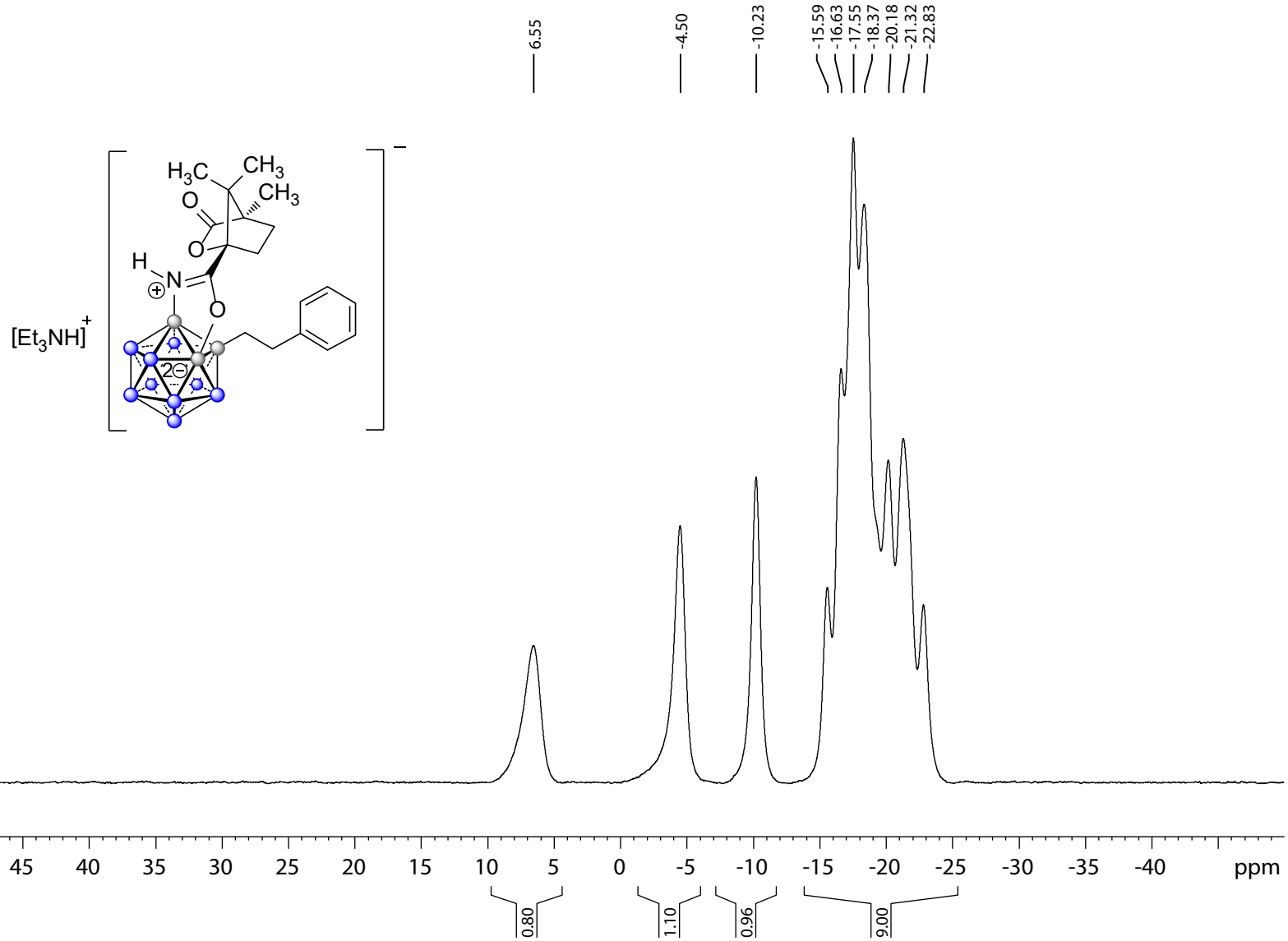
======== CHANNEL f2 ========
CPDPRG[2              garp4
NUC2                   11B
PCPD2                90.00 usec
PLW2           52.96599960 W
PLW12           0.64477998 W
SFO2          128.3776050 MHz

F2 - Processing parameters
SI                    32768
SF            400.1300070 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

NMR-017

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190703-RV-B12C-Styr
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                   4.41
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH              25510.203 Hz
FIDRES            0.389255 Hz
AQ               1.2845056 sec
RG                    193.34
DW                  19.600 usec
DE                   6.50 usec
TE                   296.1 K
D1             1.00000000 sec
TD0                        1

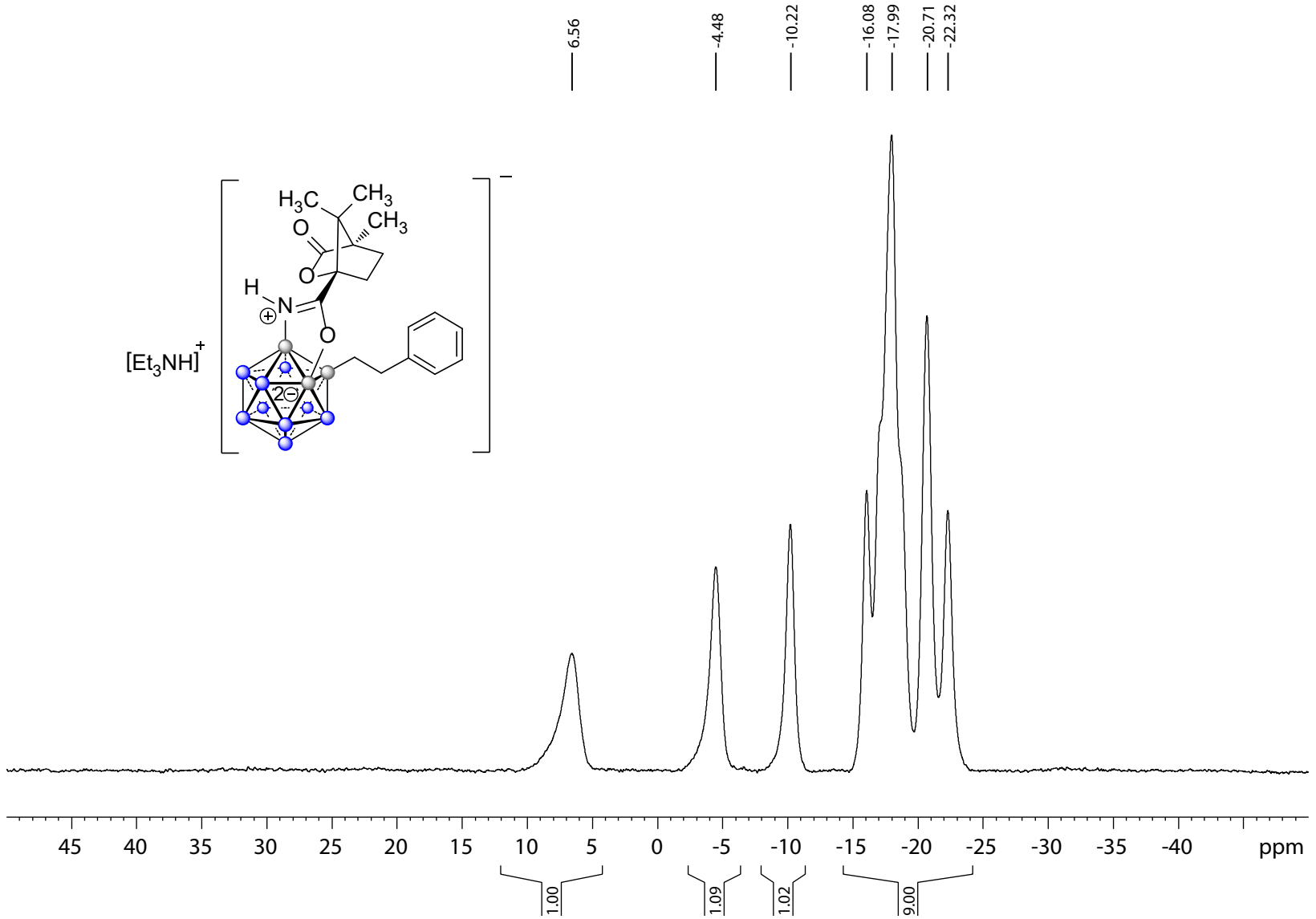
======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1           52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                       32768
SF             128.3776050 MHz
WDW                       EM
SSB          0
LB                     10.00 Hz
GB           0
PC                      1.40
```

NMR-018

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190704-RV-B12C-Styr
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                  20.53
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    296.7 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1              52.96599960 W
SFO1             128.3776050 MHz

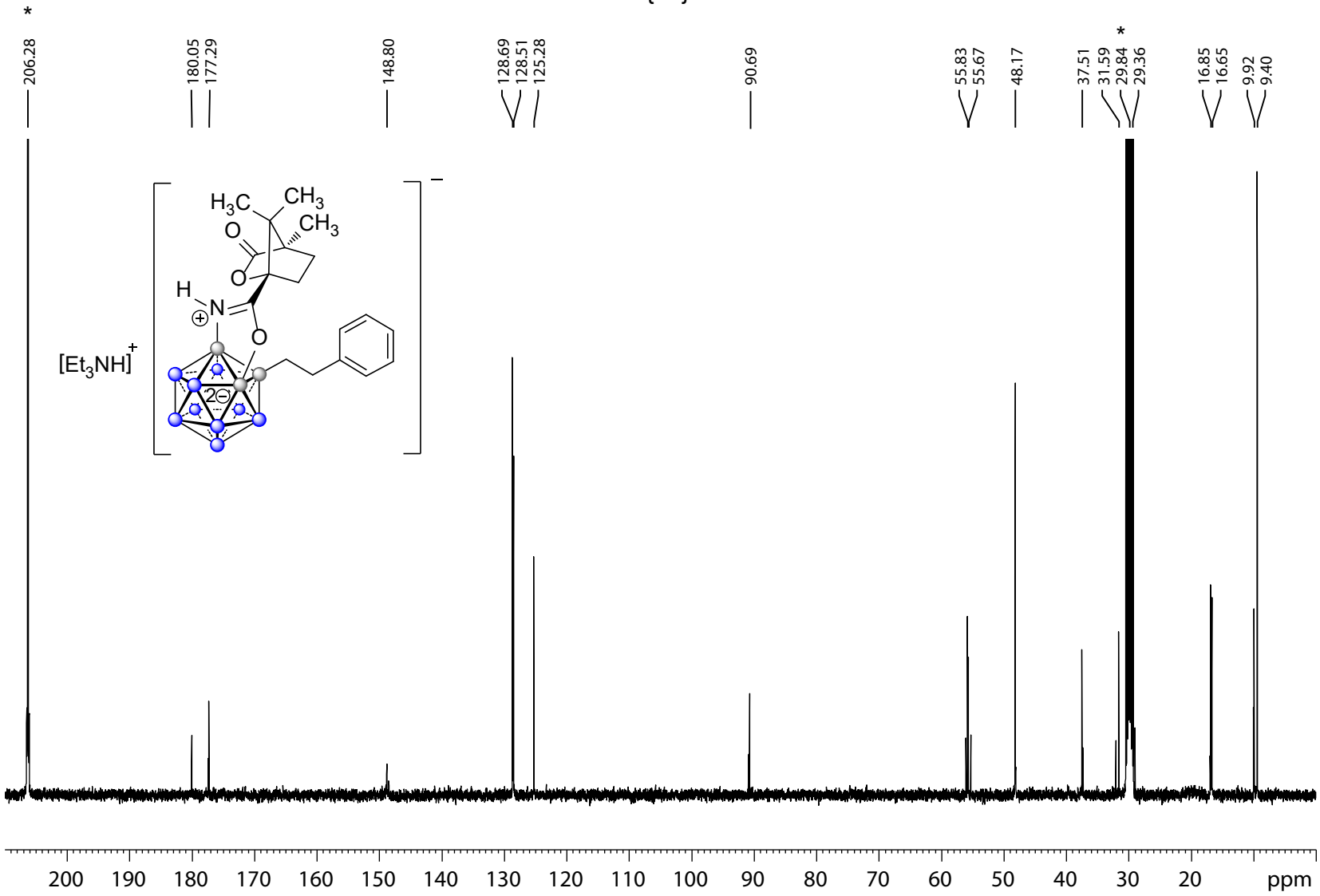
======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                       1H
PCPD2                  80.00 usec
PLW2              12.50000000 W
PLW12              0.43945000 W
PLW13              0.28125000 W
SFO2             400.1320007 MHz

F2 - Processing parameters
SI                       32768
SF               128.3776050 MHz
WDW                         EM
SSB       0
LB                     10.00 Hz
GB        0
PC                      1.40
```

NMR-019

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190704-RV-B12C-Styr
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                 22.26
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  297.2 K
D1               1.50000000 sec
D11              0.03000000 sec
TD0                      1

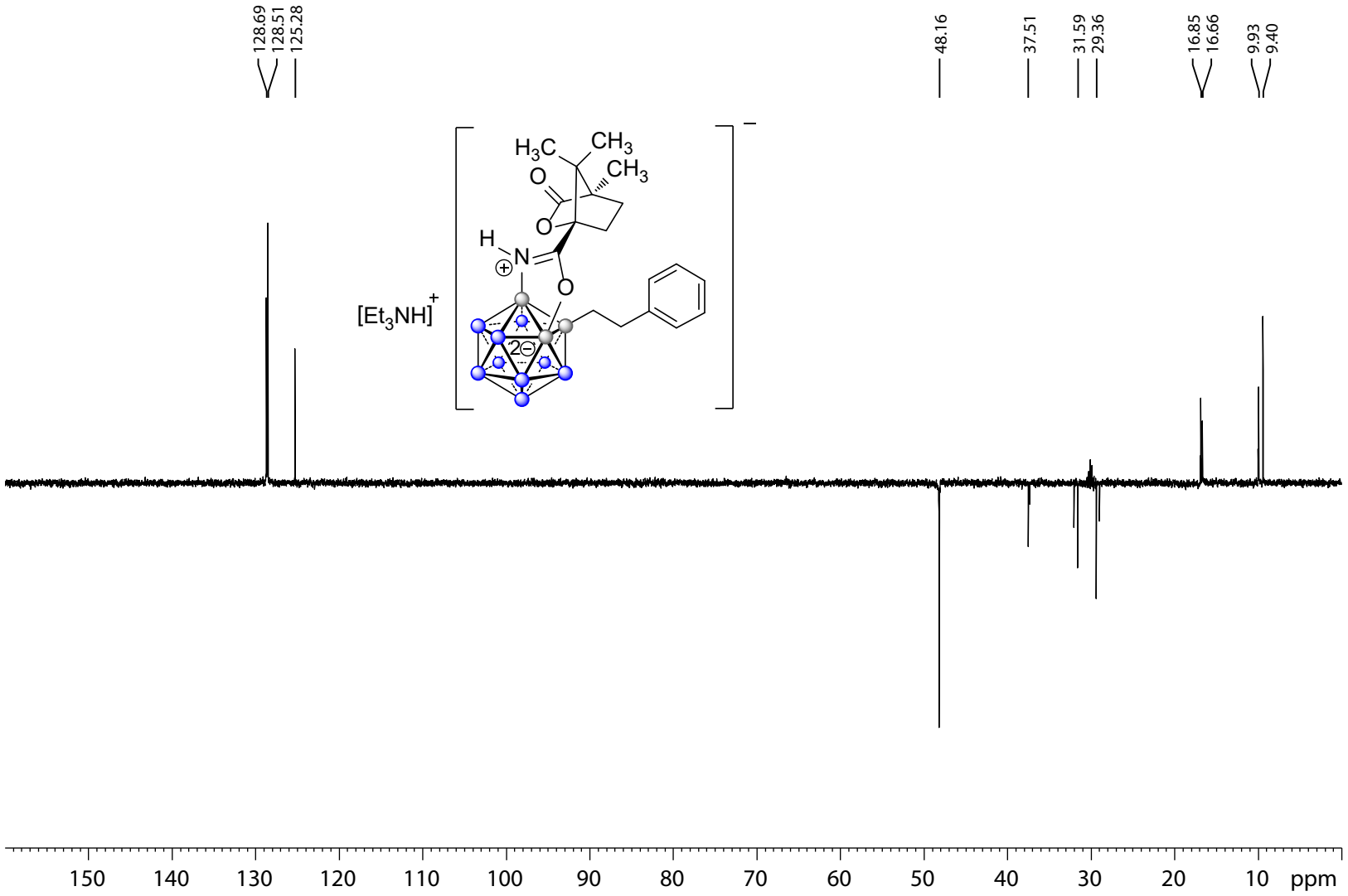
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6126830 MHz
WDW                    EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190704-RV-B12C-Styr
EXPNO                        6
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190704
Time                  22.54
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             dept135
TD                    65536
SOLVENT             Acetone
NS                        512
DS                          4
SWH               29296.875 Hz
FIDRES             0.447035 Hz
AQ                 1.1184810 sec
RG                    193.34
DW                    17.067 usec
DE                      6.50 usec
TE                     296.3 K
CNST2            145.0000000
D1                 2.00000000 sec
D2                 0.00344828 sec
D12                0.00002000 sec
TD0                         1

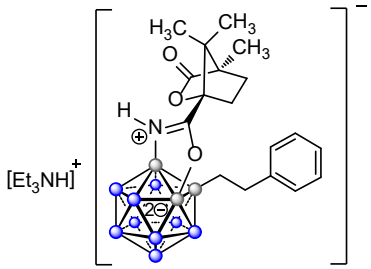
======== CHANNEL f1 ========
NUC1                      13C
P1                      10.00 usec
P2                      20.00 usec
PLW1             53.00000000 W
SFO1            100.6228293 MHz

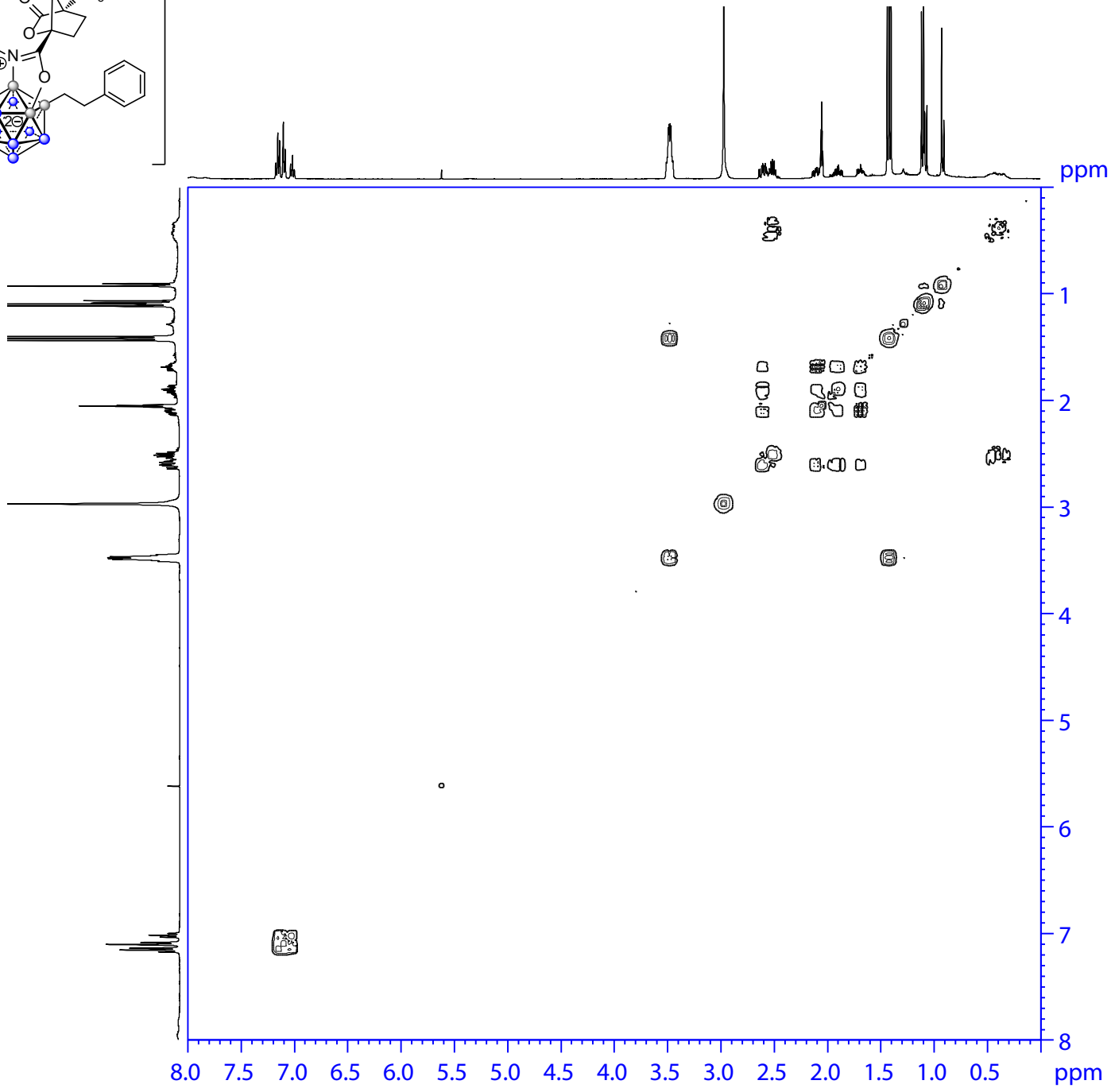
======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                      1H
P3                      15.00 usec
P4                      30.00 usec
PCPD2                   80.00 usec
PLW2             12.50000000 W
PLW12             0.43945000 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF              100.6126828 MHz
WDW                          EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       4.00
```

20190704-B12C-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d* 6*

^1H - ^1H COSY NMR





Current Data Parameters
NAME 20190704-RV-B12C-Styr
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190704
Time 22.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 170.36
DW 93.600 usec
DE 6.50 usec
TE 296.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

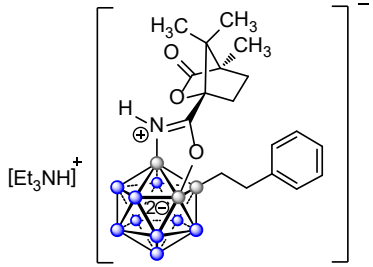
F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300072 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300074 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

20190704-B12C-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_5$] dissolved in 0.6 mL acetone-*d* 6*

^1H - ^{13}C HSQC NMR



Current Data Parameters
NAME 20190704-RV-B12C-Styr
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190704
Time 23.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgpsi2
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 296.4 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

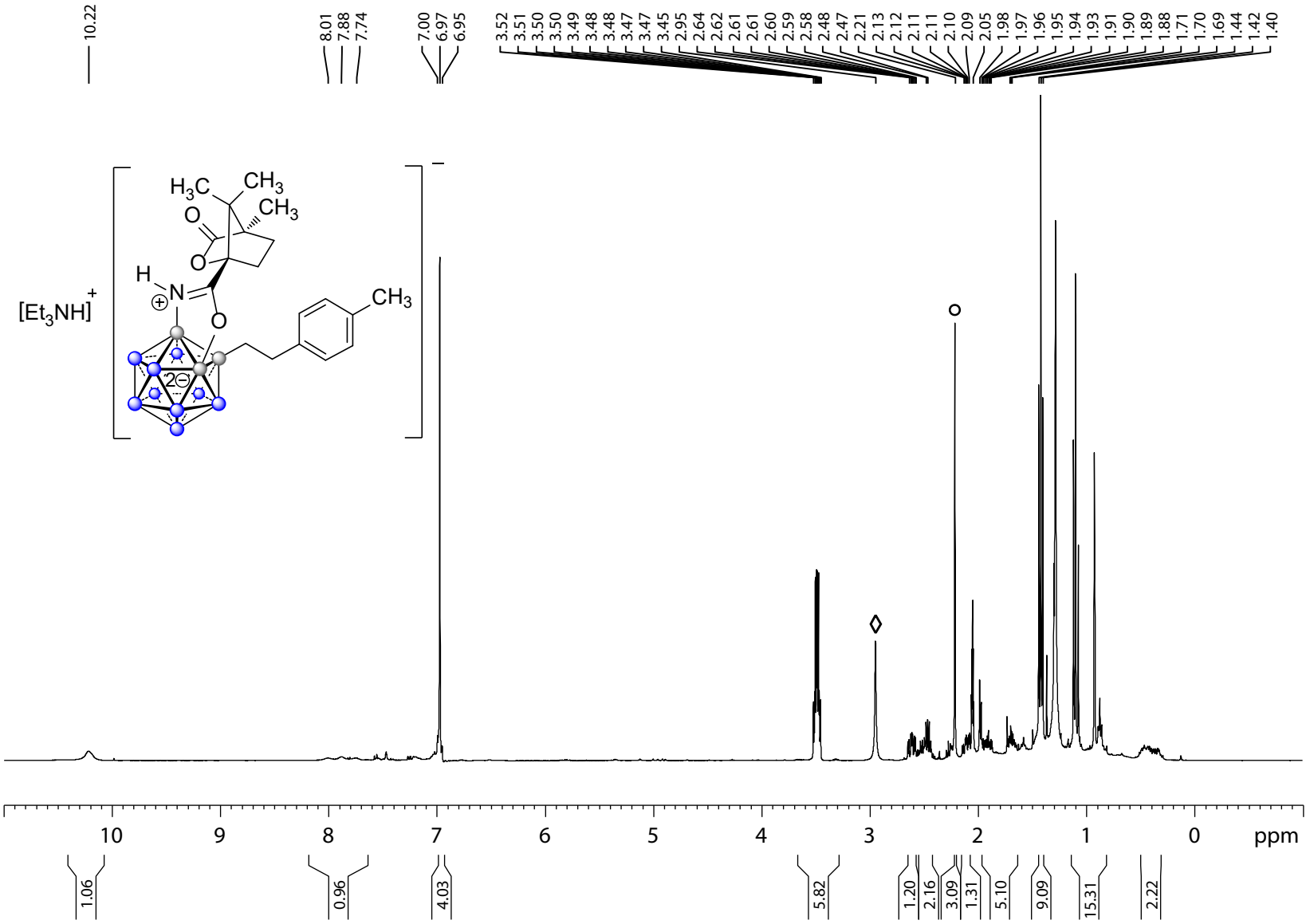
F2 - Processing parameters
SI 1024
SF 400.1300066 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126760 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

NMR-023

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20190730
Time                  11.34
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT           Acetone
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.152588 Hz
AQ                3.2767999 sec
RG                       78.69
DW                    50.000 usec
DE                     6.50 usec
TE                    294.9 K
D1               1.00000000 sec
TD0                       1

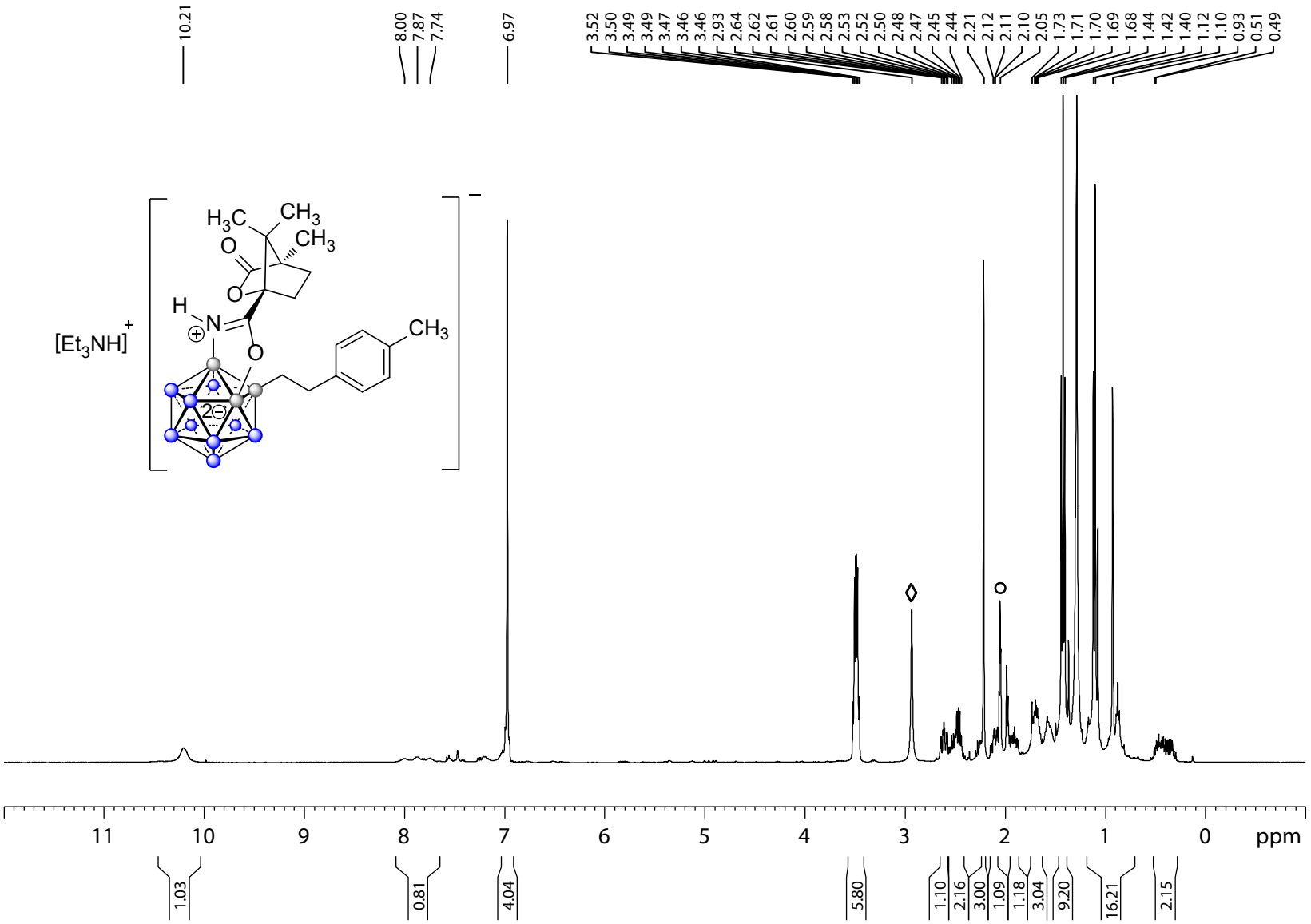
======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1            12.50000000 W
SFO1            400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF              400.1300072 MHz
WDW                      EM
SSB       0
LB                     0.30 Hz
GB        0
PC                     1.00
```

NMR-024

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190730
Time                  11.36
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                     78.69
DW                    62.400 usec
DE                     6.50 usec
TE                    295.4 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1

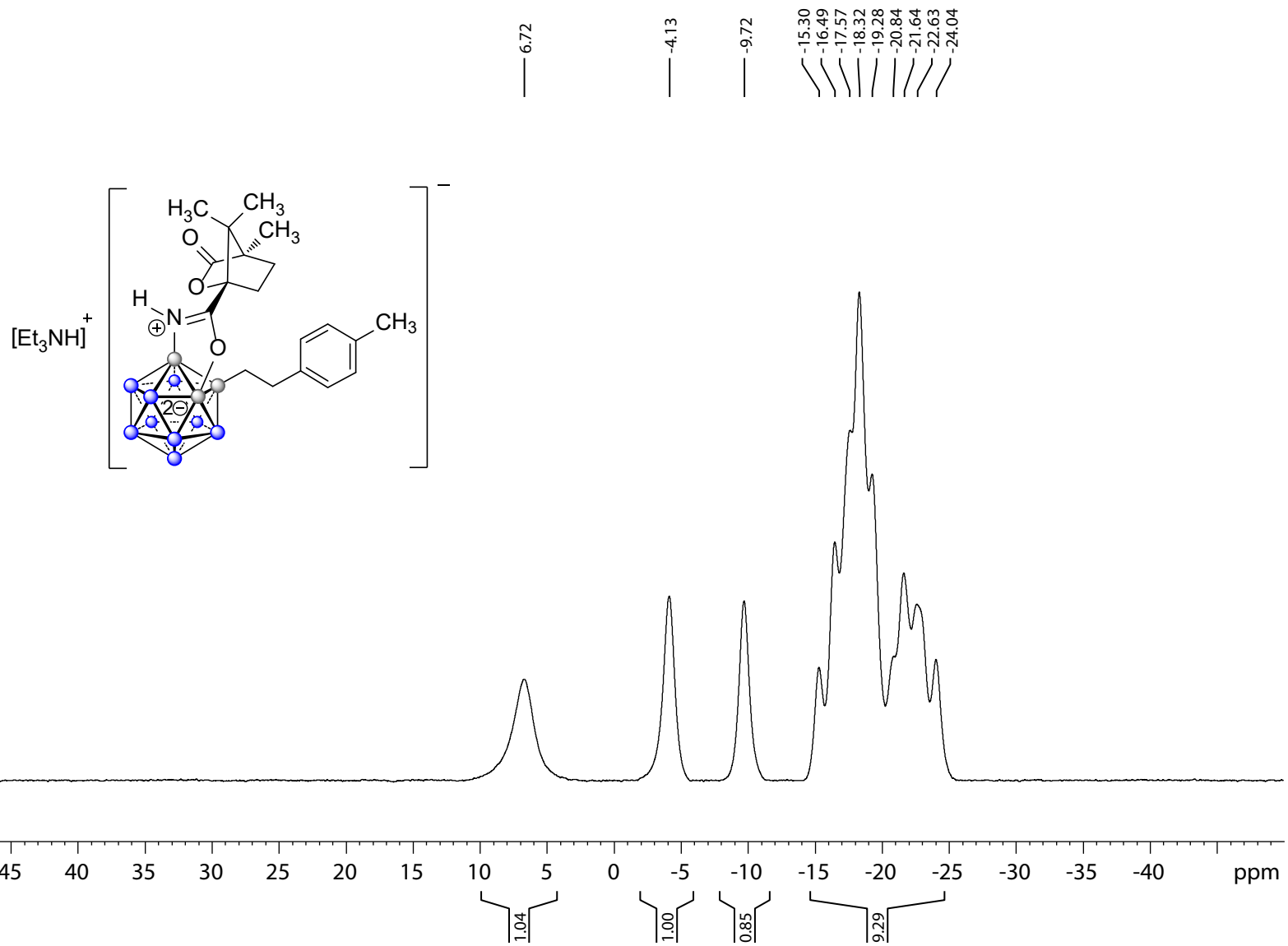
======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.50000000 W
SFO1            400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp4
NUC2                      11B
PCPD2                  90.00 usec
PLW2             52.96599960 W
PLW12             0.64477998 W
SFO2            128.3776050 MHz

F2 - Processing parameters
SI                        32768
SF              400.1300073 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190730
Time                  11.41
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH                25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   294.8 K
D1                1.00000000 sec
TD0                          1

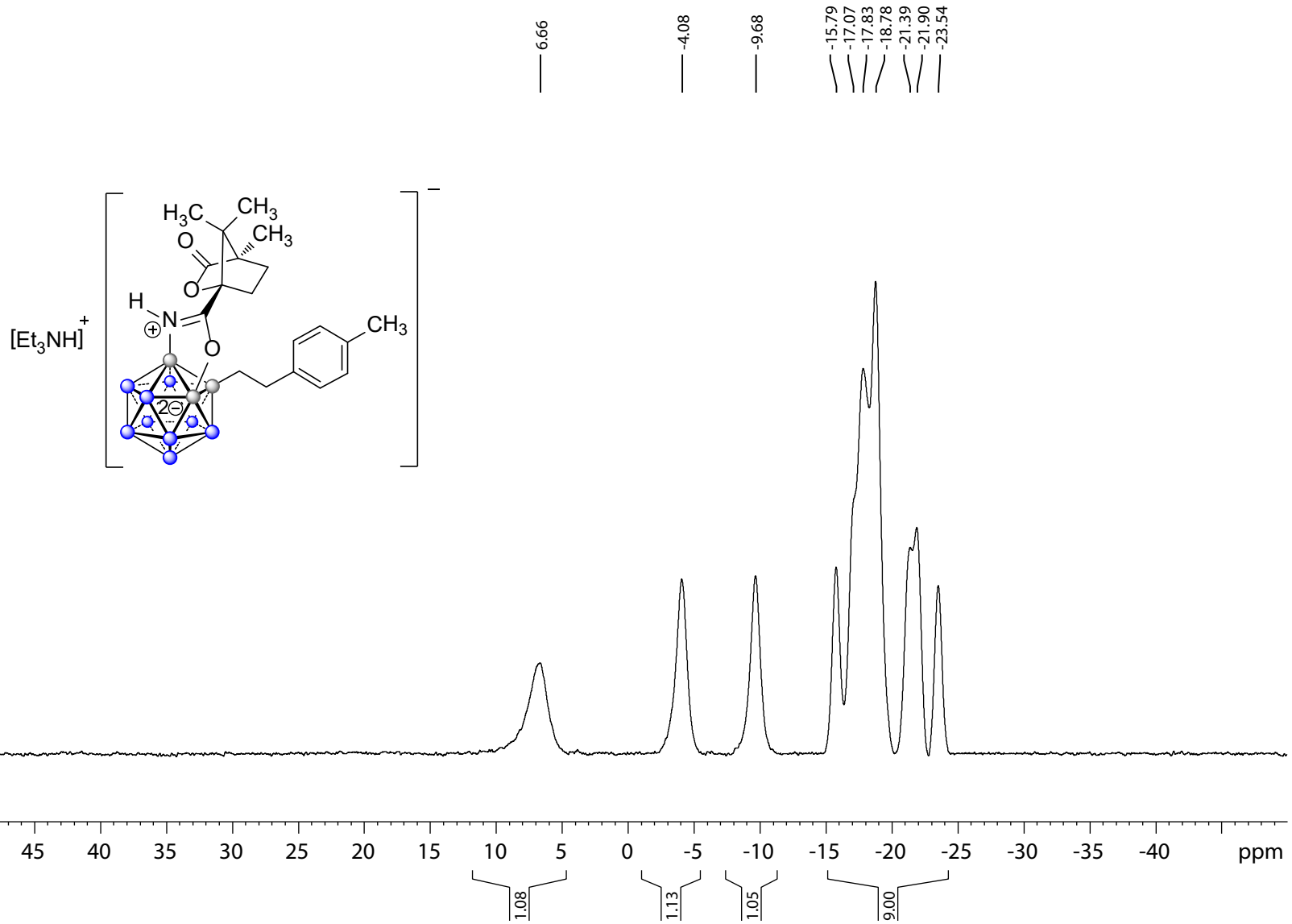
======== CHANNEL f1 ========
NUC1                      11B
P1                       9.93 usec
PLW1            52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                       32768
SF             128.3776050 MHz
WDW                        EM
SSB       0
LB                    10.00 Hz
GB        0
PC                     1.40
```

NMR-026

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_              20190730
Time                  11.48
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   296.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1             52.96599960 W
SFO1            128.3776050 MHz

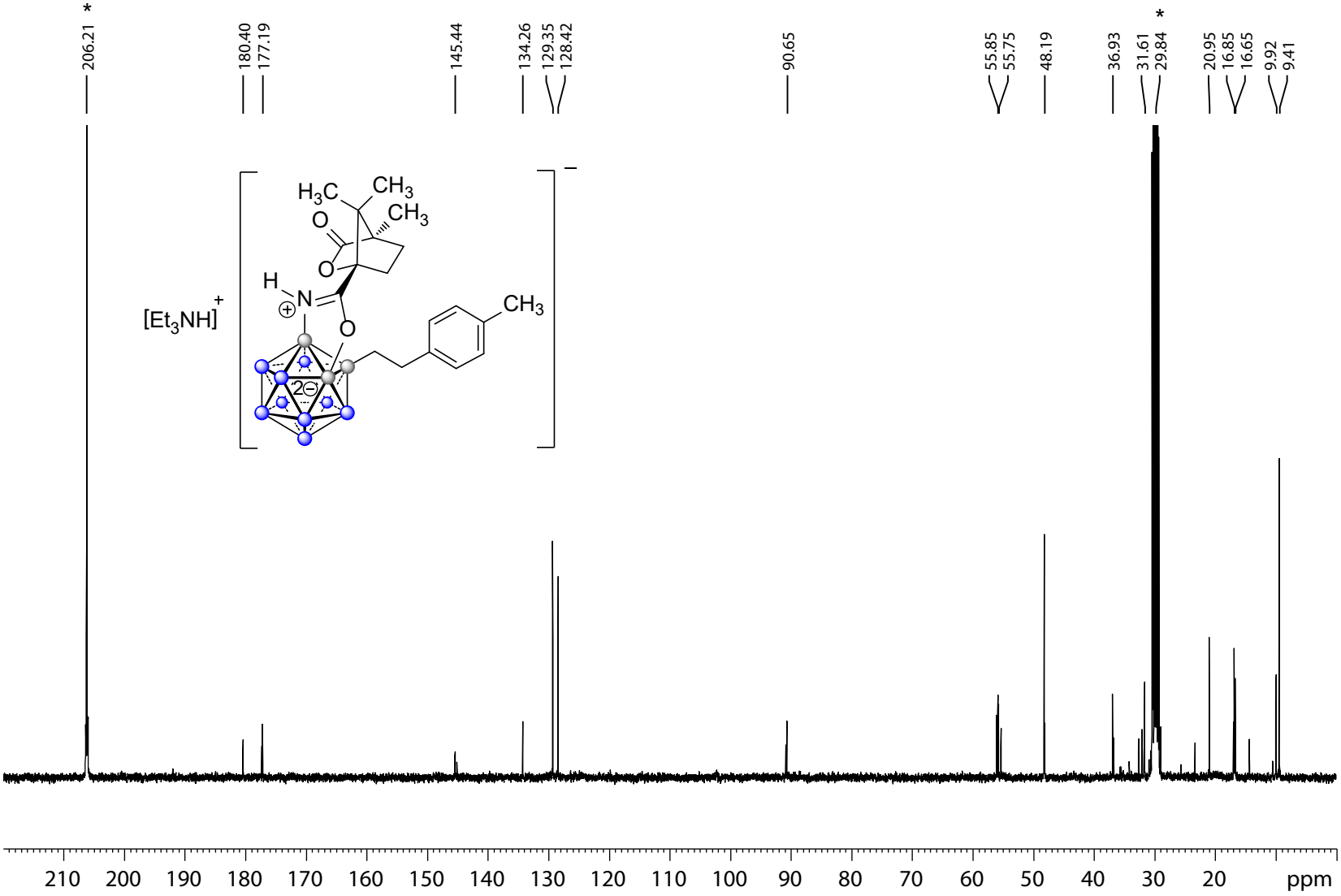
======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PLW2             12.50000000 W
PLW12             0.43945000 W
PLW13             0.28125000 W
SFO2            400.1320007 MHz

F2 - Processing parameters
SI                       32768
SF              128.3776050 MHz
WDW                         EM
SSB          0
LB                    10.00 Hz
GB           0
PC                     1.40
```

NMR-027

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_              20190730
Time                  13.20
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT             Acetone
NS                     2048
DS                        4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                    193.34
DW                    16.800 usec
DE                     6.50 usec
TE                    295.7 K
D1                1.50000000 sec
D11               0.03000000 sec
TD0                       1

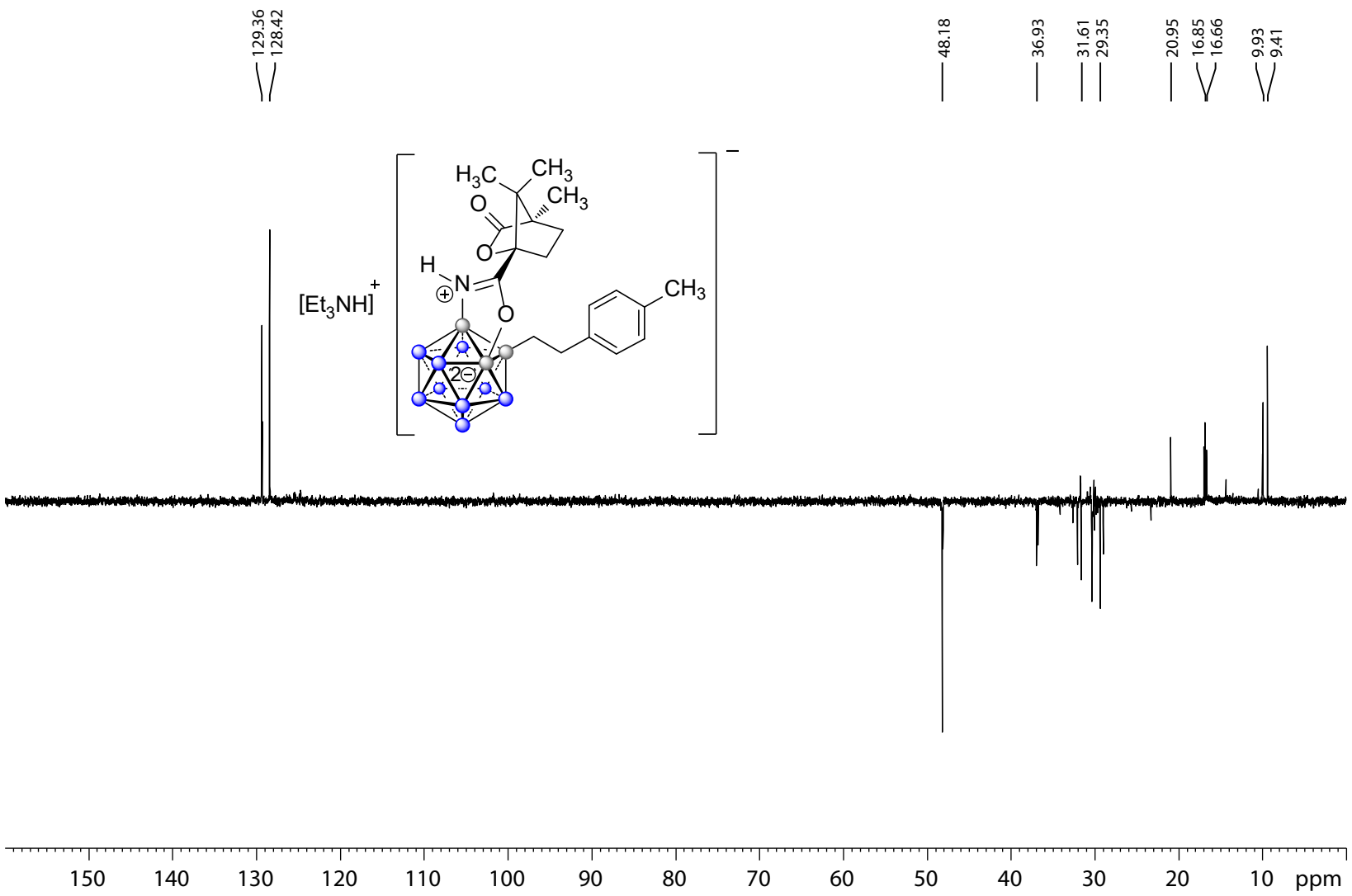
======== CHANNEL f1 ========
NUC1                     13C
P1                    10.00 usec
PLW1           53.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                     1H
PCPD2                 80.00 usec
PLW2           12.50000000 W
PLW12           0.43945000 W
PLW13           0.28125000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6126831 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

20190729-B12C-4MeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190729-B12C-4MeSTYR
EXPNO                        6
PROCNO                       1

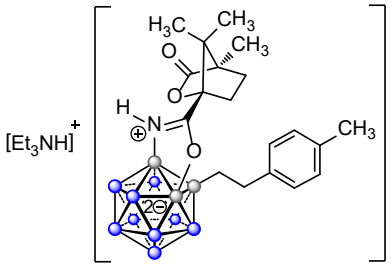
F2 - Acquisition Parameters
Date_              20190730
Time                 13.48
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            dept135
TD                   65536
SOLVENT            Acetone
NS                     512
DS                       4
SWH              29296.875 Hz
FIDRES            0.447035 Hz
AQ                1.1184810 sec
RG                   193.34
DW                   17.067 usec
DE                    6.50 usec
TE                   295.5 K
CNST2           145.0000000
D1                2.00000000 sec
D2                0.00344828 sec
D12               0.00002000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.00 usec
P2                     20.00 usec
PLW1            53.00000000 W
SFO1           100.6228293 MHz

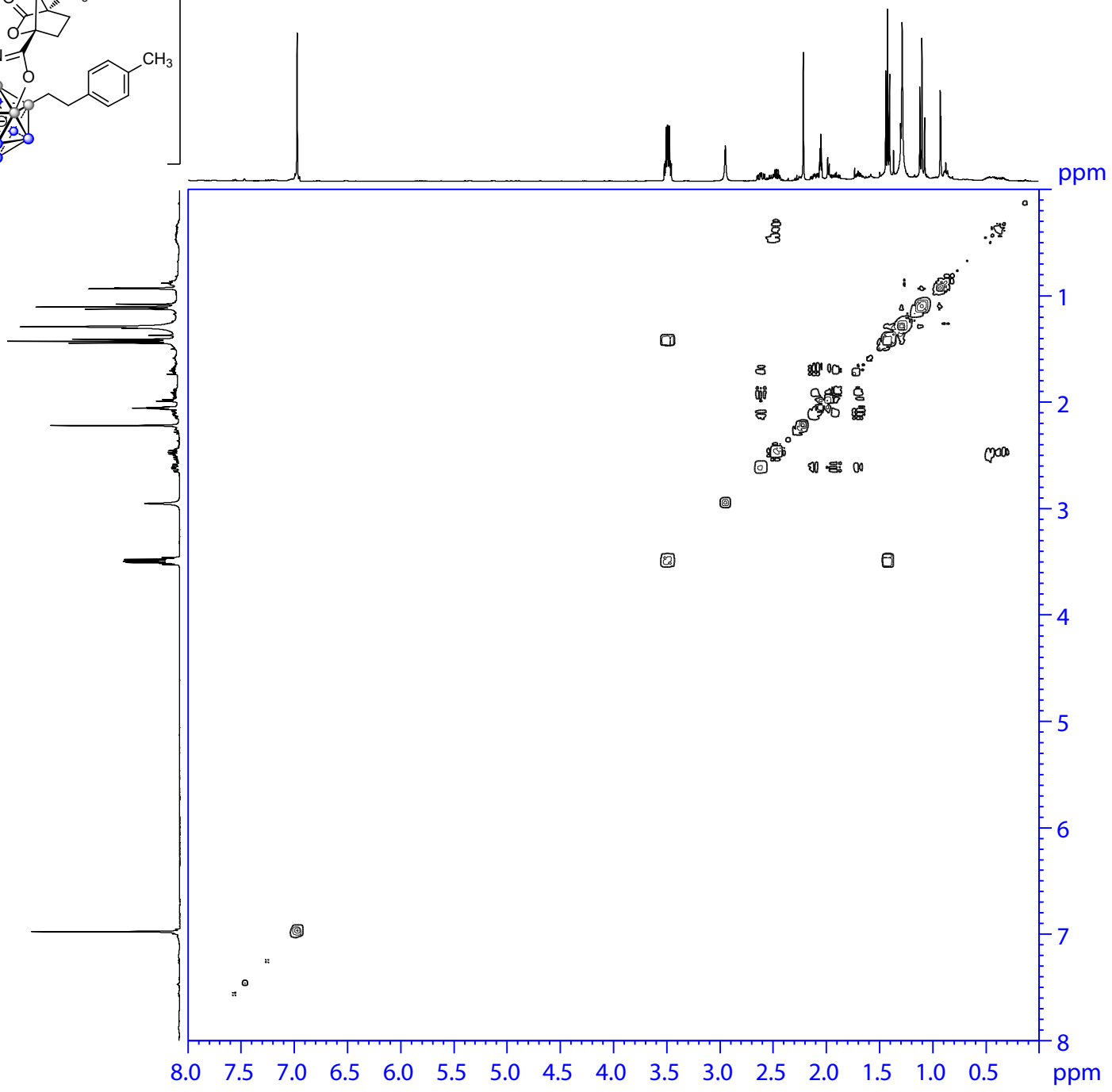
======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                     1H
P3                     15.00 usec
P4                     30.00 usec
PCPD2                  80.00 usec
PLW2            12.50000000 W
PLW12            0.43945000 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF             100.6126830 MHz
WDW                         EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     4.00
```

20190729-B12C-4MeSTYR 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4Me] dissolved in 0.6 mL acetone-*d*6*



^{1}H - ^{1}H COSY NMR



Current Data Parameters
NAME 20190729-B12C-4MeSTYR
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190730
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 138.32
DW 93.600 usec
DE 6.50 usec
TE 295.2 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

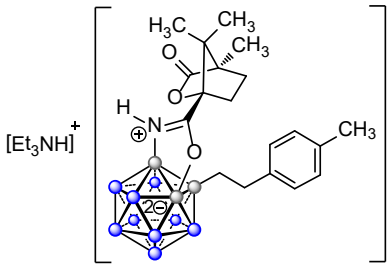
F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300082 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

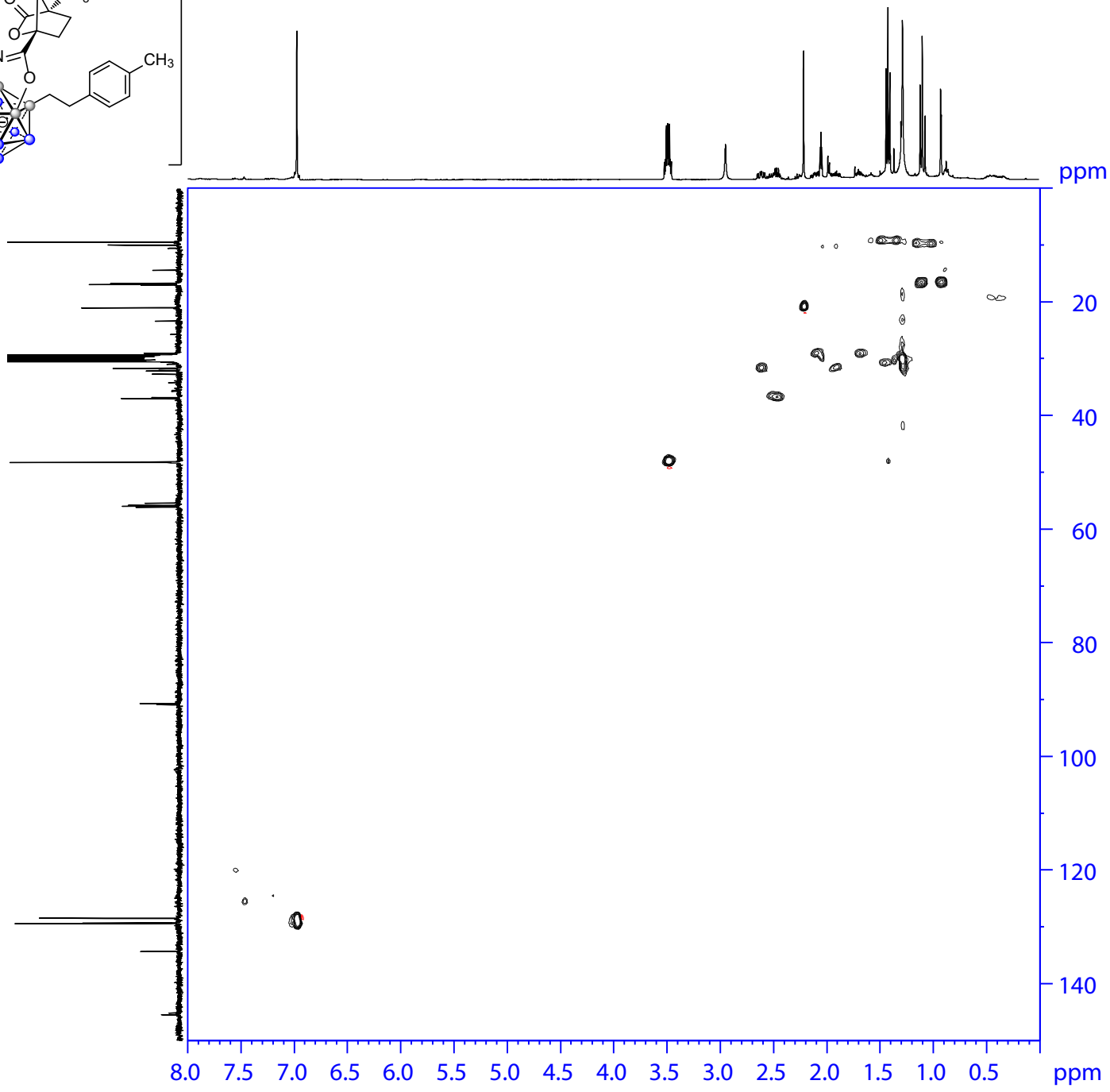
F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300082 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

NMR-030

20190729-B12C-4MeSTYR 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4Me] dissolved in 0.6 mL acetone-*d*6*



^{1}H - ^{13}C HSQC NMR



NMR-031

Current Data Parameters
NAME 20190729-B12C-4MeSTYR
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190730
Time 14.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgpsi2
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 295.1 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

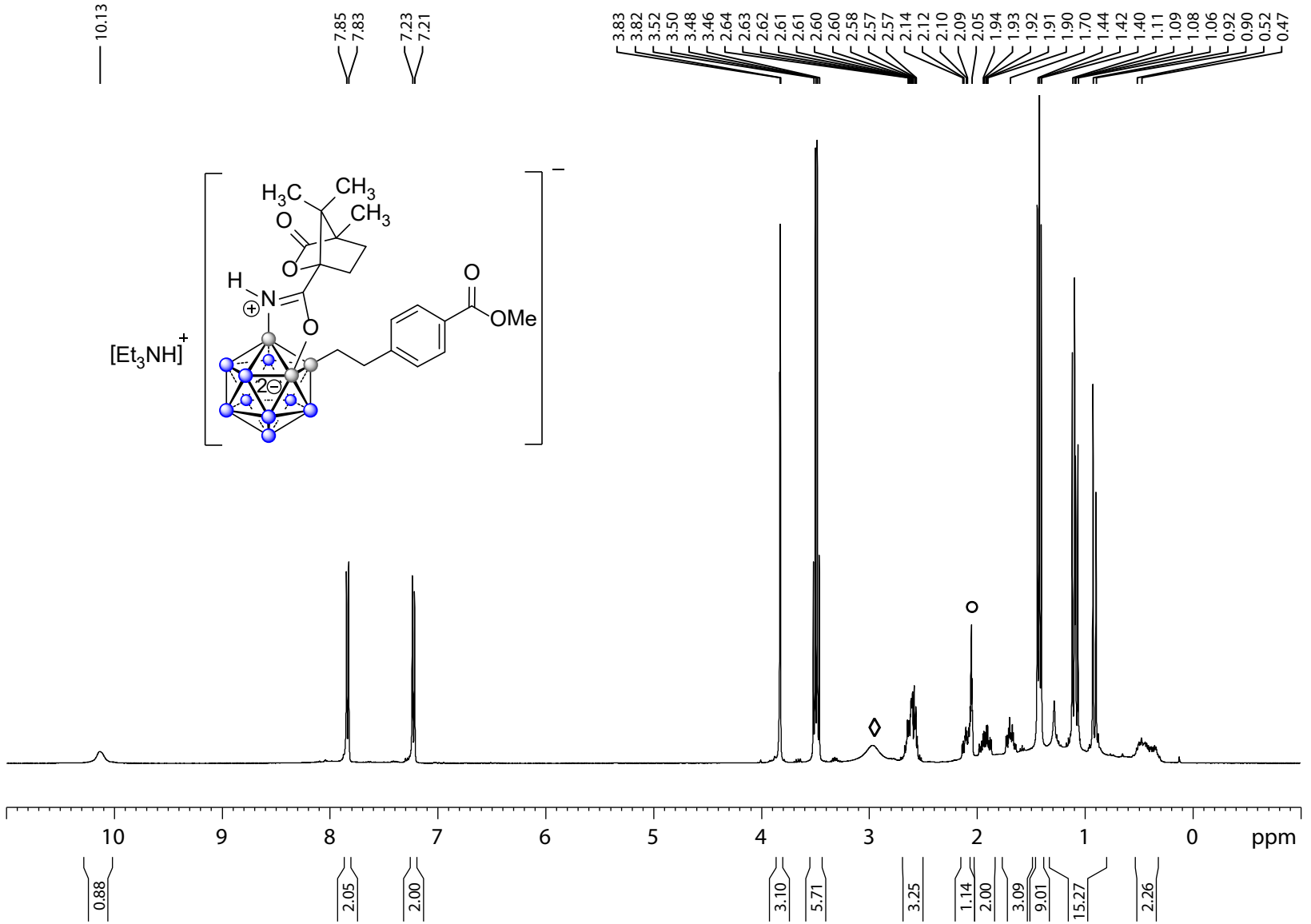
F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300079 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126742 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

20191213-B12C-4COOMeSTYR 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4COOMe]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-032

Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 1
PROCNO 1

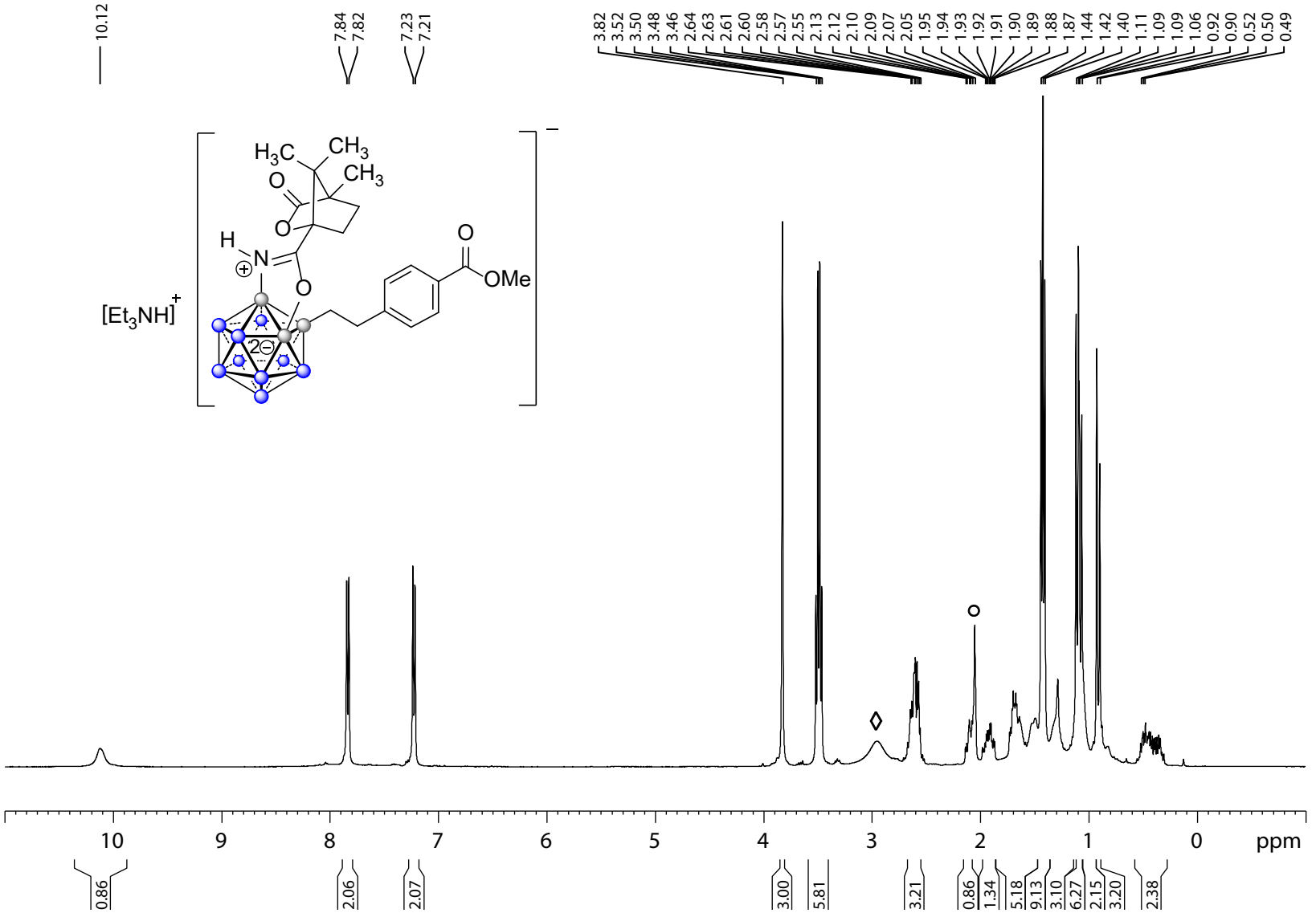
F2 - Acquisition Parameters
Date_ 20191214
Time 13.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 86.58
DW 50.000 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300075 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20191213-B12C-4COOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4COOMe] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H{B) NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 13.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgig30
TD 16384
SOLVENT Acetone
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 86.58
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.50000000 W
SFO1 400.1320007 MHz

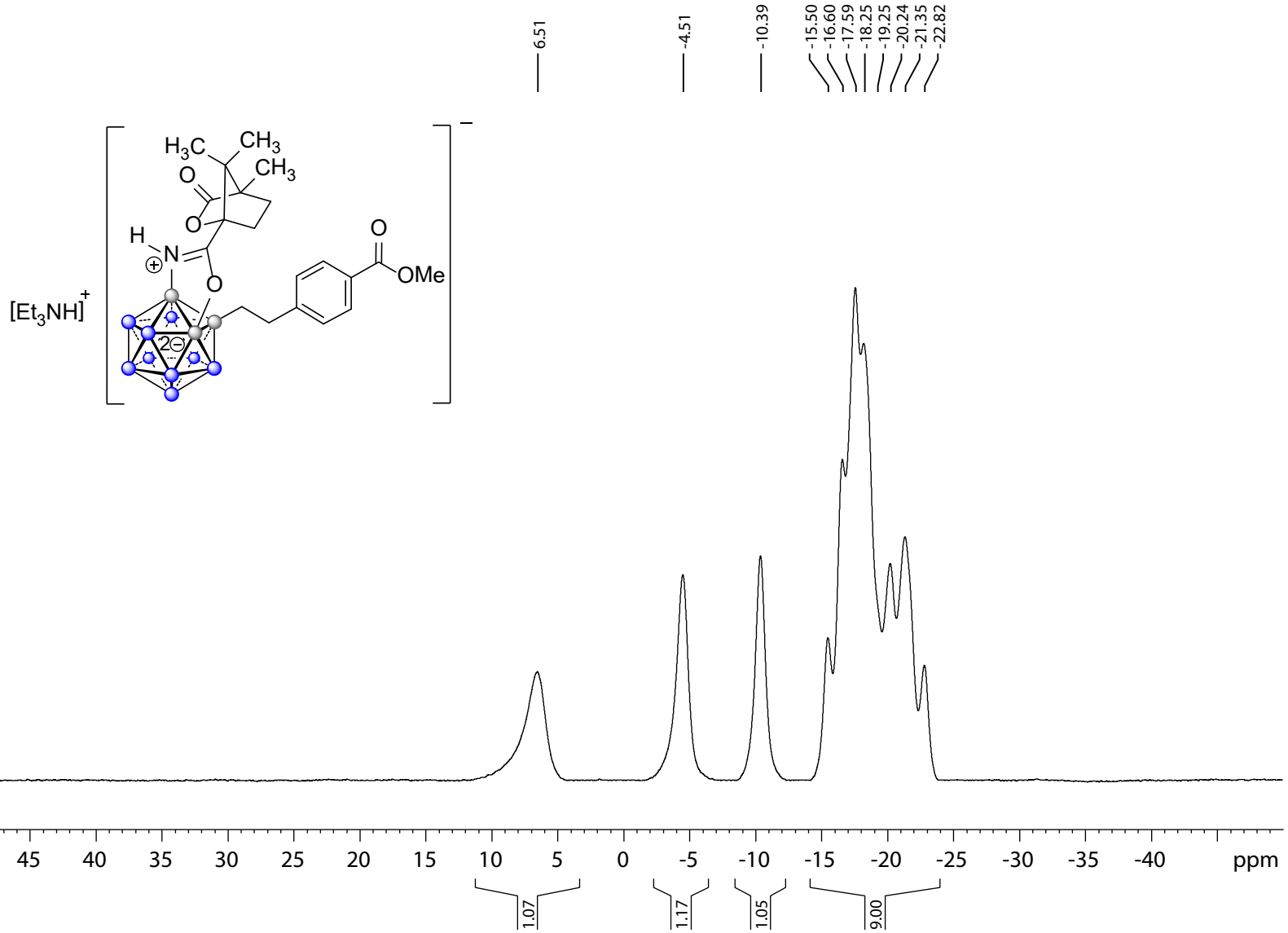
======== CHANNEL f2 ========
CPDPRG[2 garp4
NUC2 11B
PCPD2 90.00 usec
PLW2 52.96599960 W
PLW12 0.64477998 W
SFO2 128.3776050 MHz

F2 - Processing parameters
SI 32768
SF 400.1300079 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR-033

20191213-B12C-4COOMeSTYR 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4COOMe]$ dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz



Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 13.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1

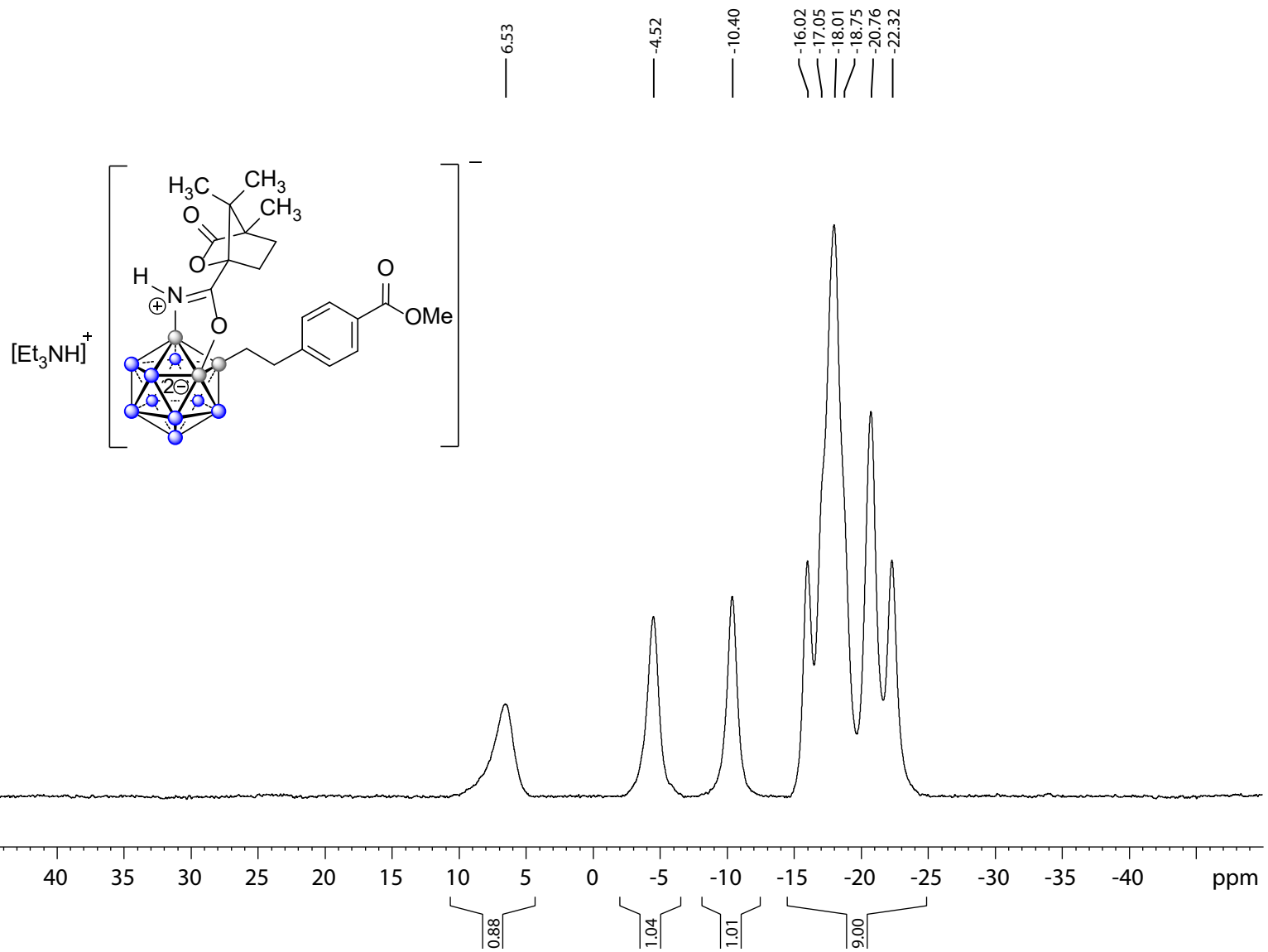
======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776052 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-034

20191213-B12C-4COOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4COOMe] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz



Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 13.51
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776050 MHz

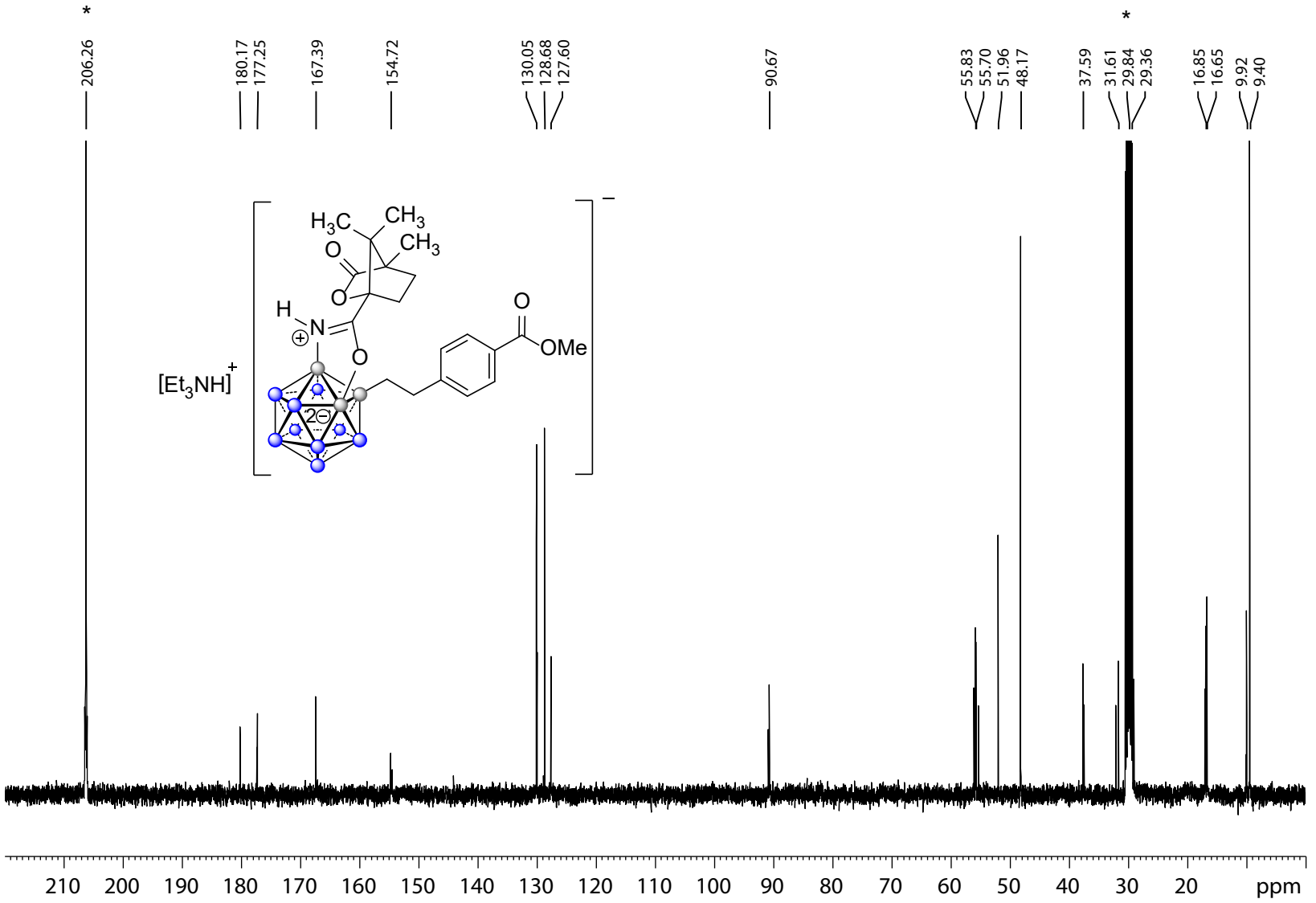
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-035

20191213-B12C-4COOMeSTYR 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4COOMe]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz



Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 14.38
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 295.9 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

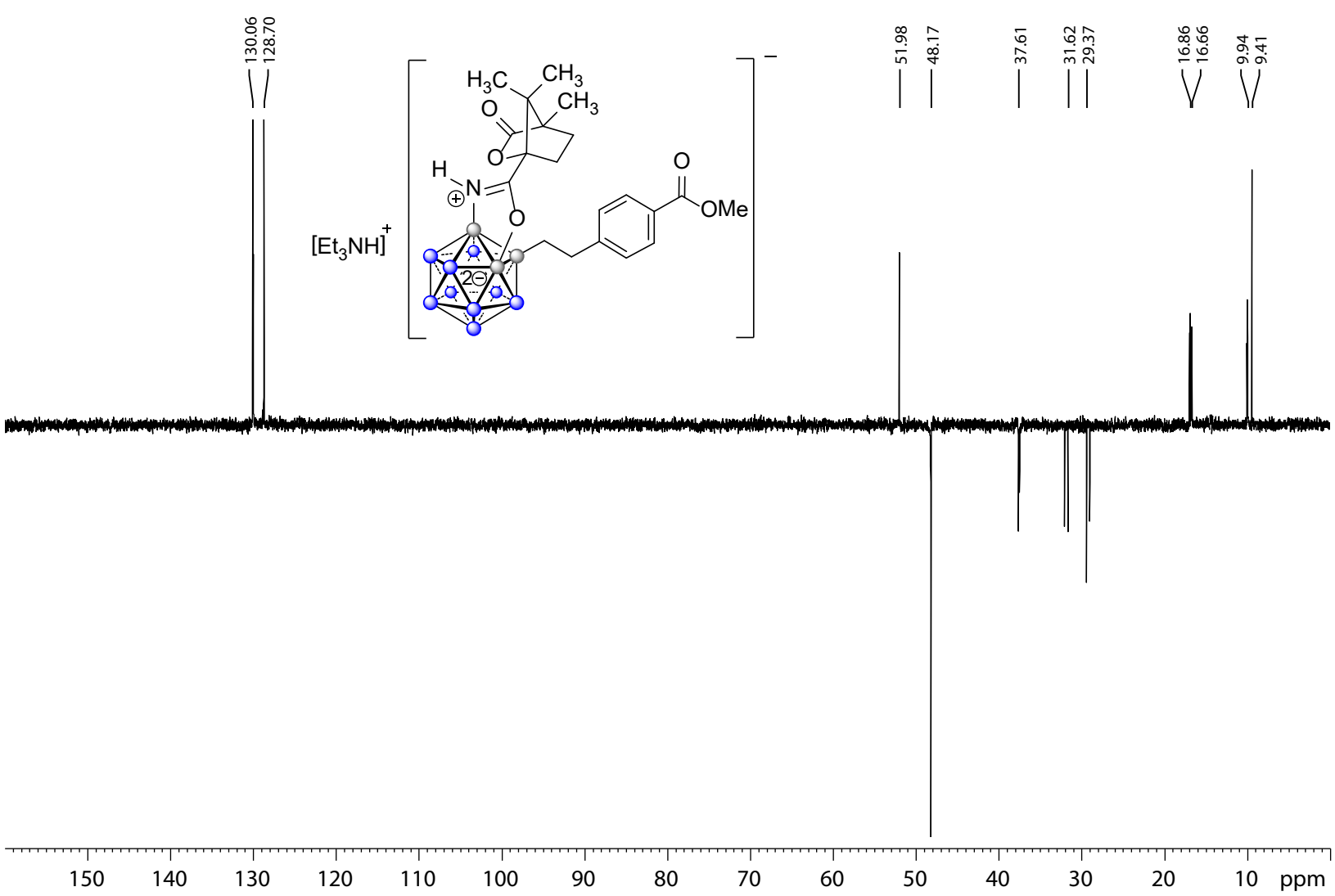
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126830 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20191213-B12C-4COOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4COOMe] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz



Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 6
PROCNO 1

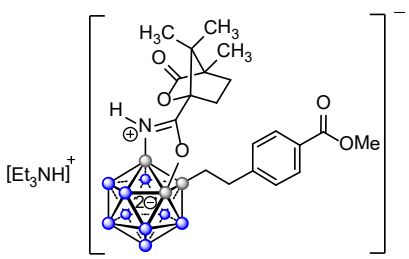
F2 - Acquisition Parameters
Date_ 20191214
Time 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG dept135
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 29296.875 Hz
FIDRES 0.447035 Hz
AQ 1.1184810 sec
RG 193.34
DW 17.067 usec
DE 6.50 usec
TE 295.3 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

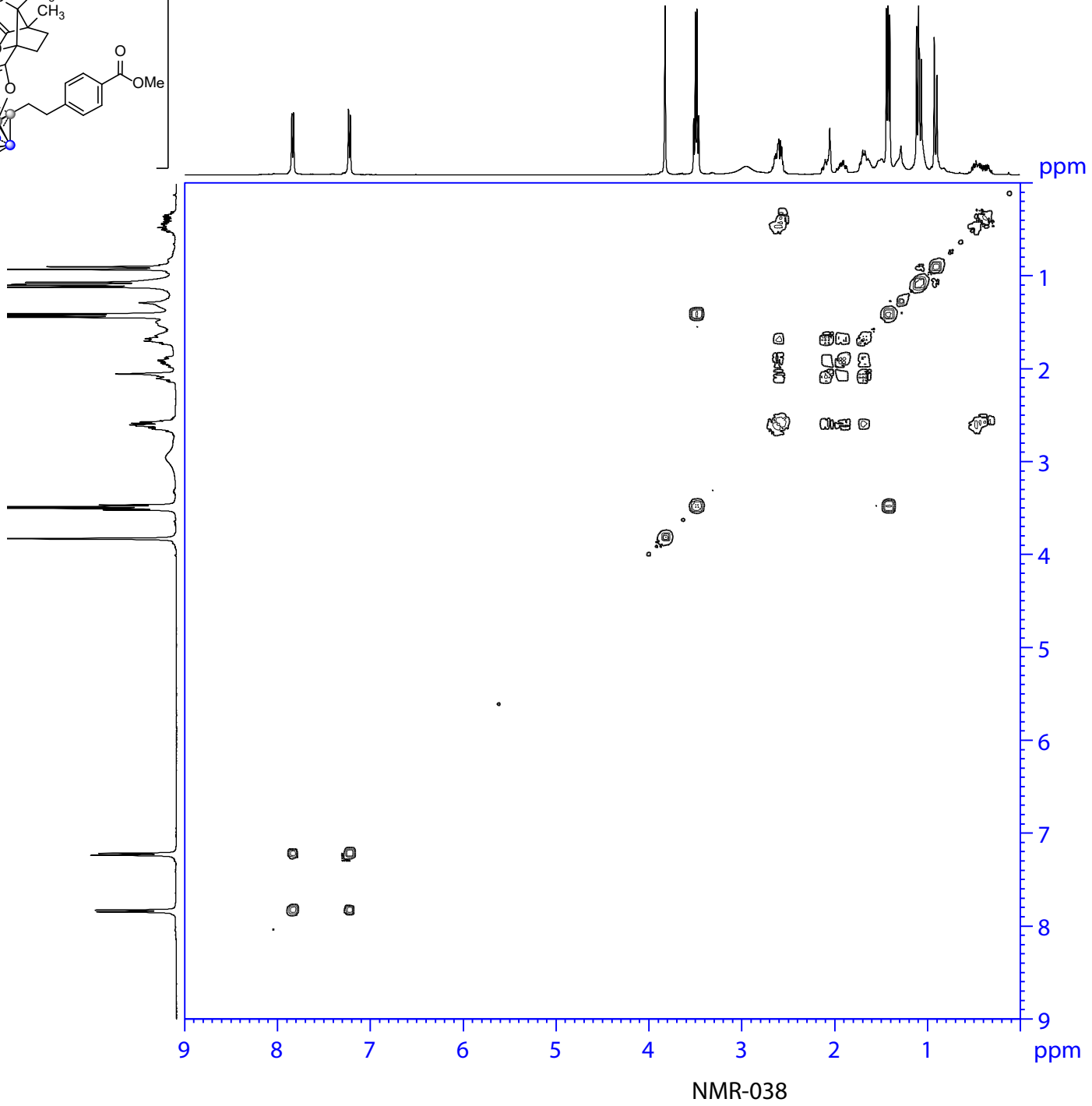
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126819 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00

20191213-B12C-4COOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4COOMe] dissolved in 0.6 mL acetone-*d6**



^1H - ^1H COSY NMR



NMR-038

Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 193.34
DW 93.600 usec
DE 6.50 usec
TE 295.1 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

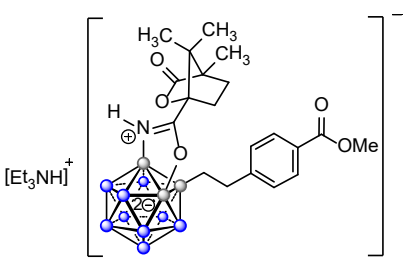
====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

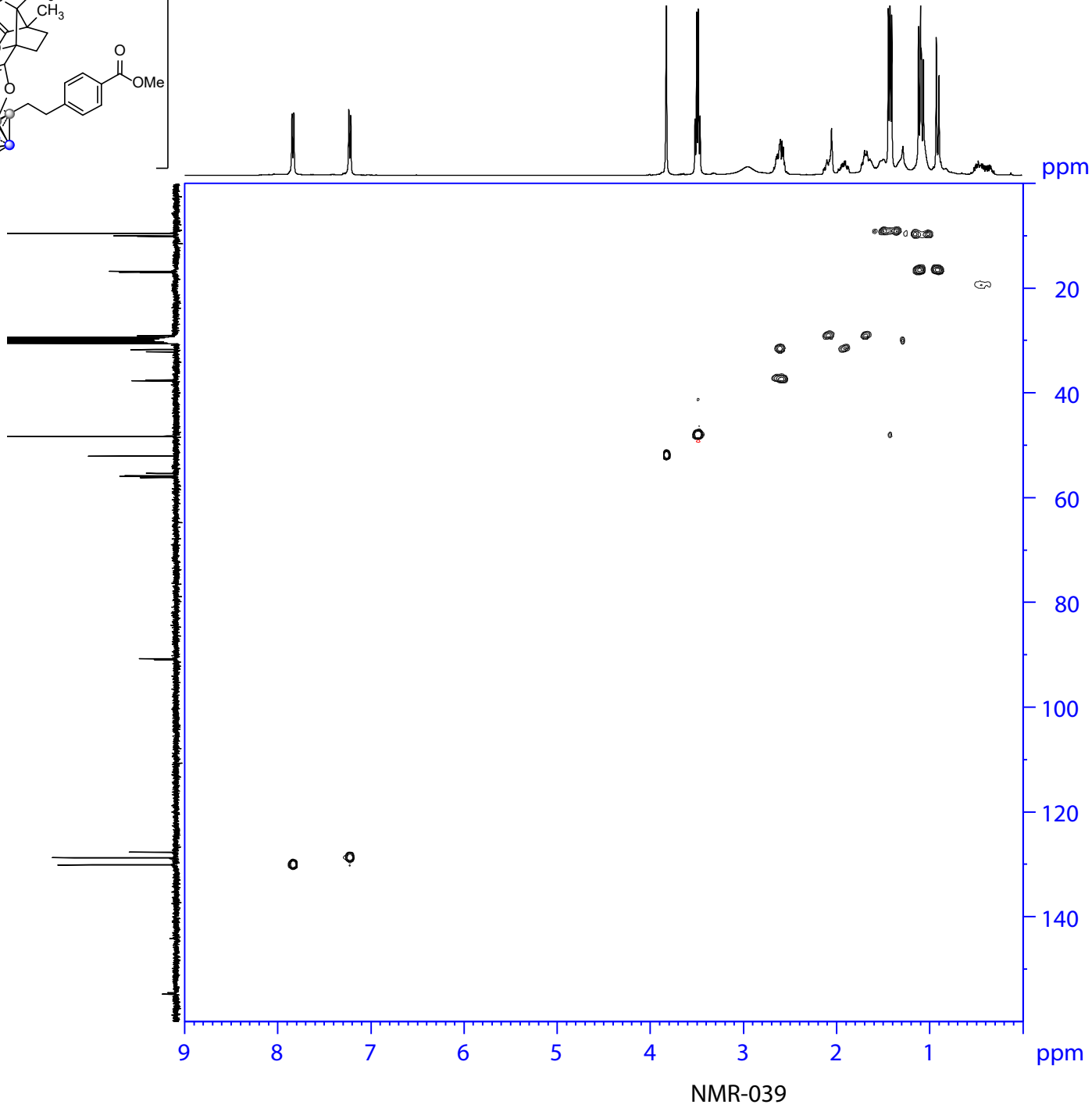
F2 - Processing parameters
SI 1024
SF 400.1300098 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300095 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

20191213-B12C-4COOMeSTYR 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4COOMe] dissolved in 0.6 mL acetone-*d*6*



^{1}H - ^{13}C HSQC NMR



NMR-039

Current Data Parameters
NAME 20191213-RV-B12C-4COOMeStyr
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191214
Time 15.18
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgpsi2
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 295.0 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

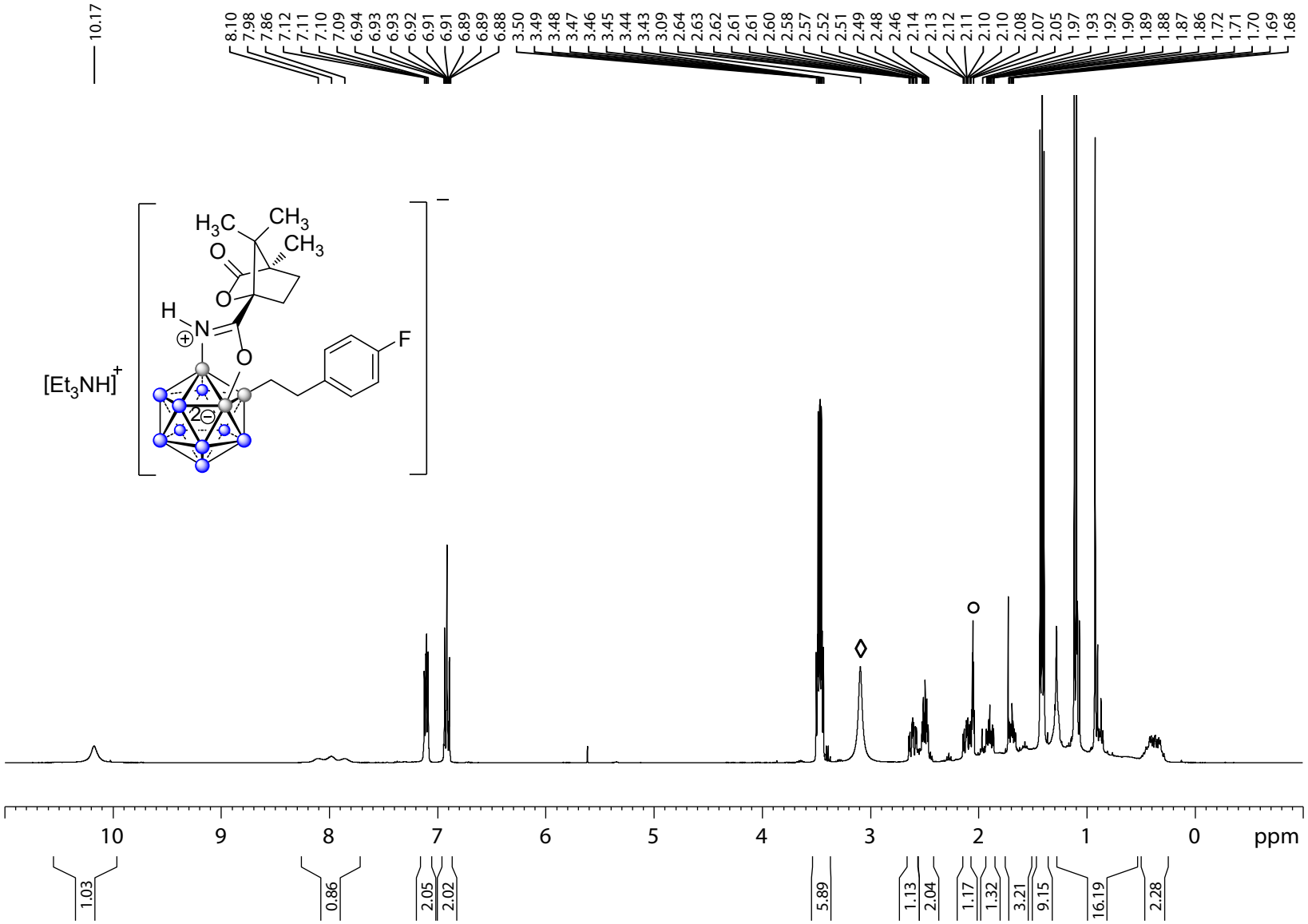
F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300092 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126866 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

20190802-B12C-4F-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4F] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20190802
Time              12.39
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ            3.2767999 sec
RG                55.74
DW                50.000 usec
DE                 6.50 usec
TE                295.2 K
D1             1.00000000 sec
TD0                  1

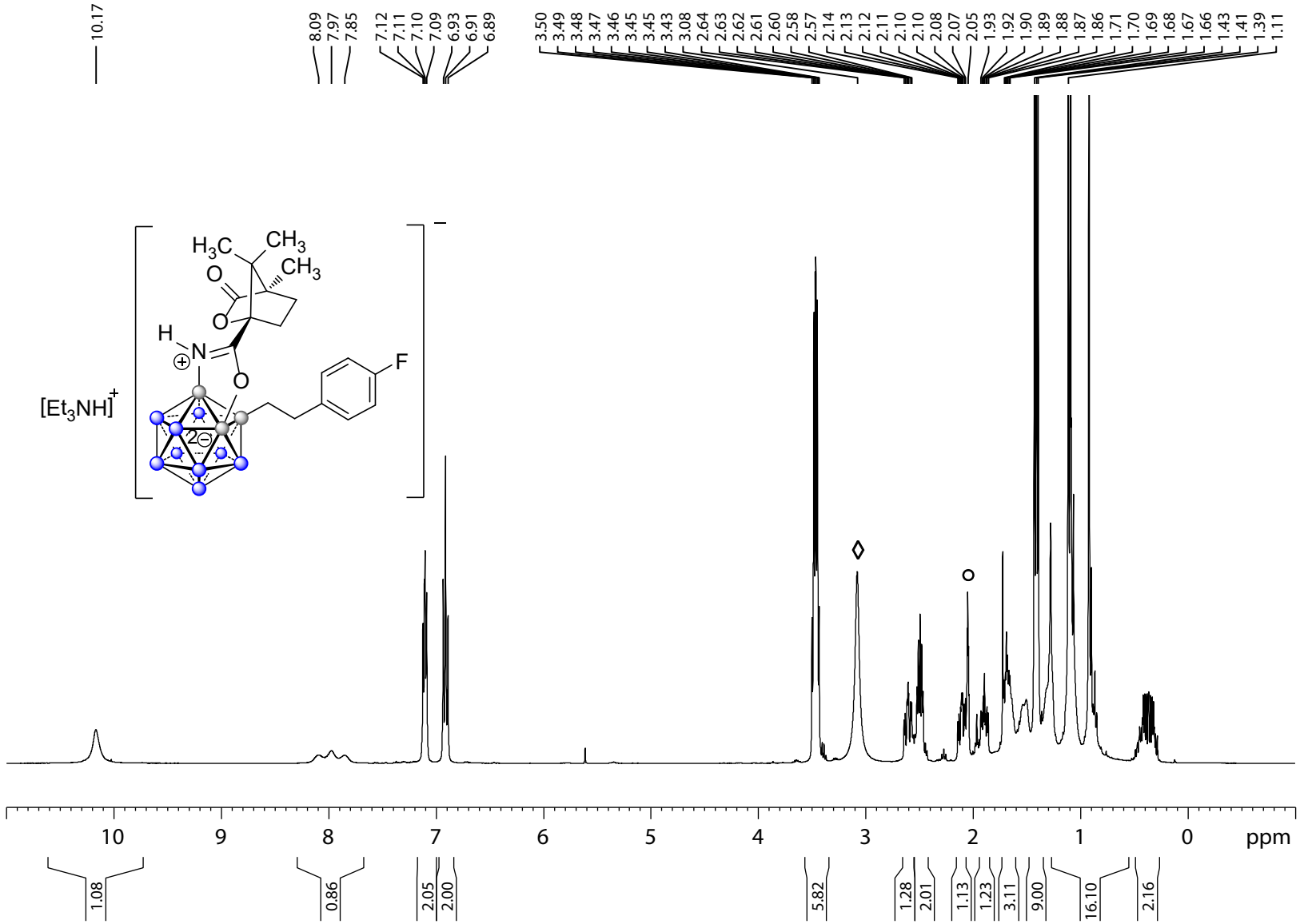
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300070 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-040

20190802-B12C-4F-Styr 20 mg white solid $[Et_3NH]_2[B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4F]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-041

```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20190802
Time              12.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ             1.0223616 sec
RG                55.74
DW                62.400 usec
DE                 6.50 usec
TE                295.3 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  1

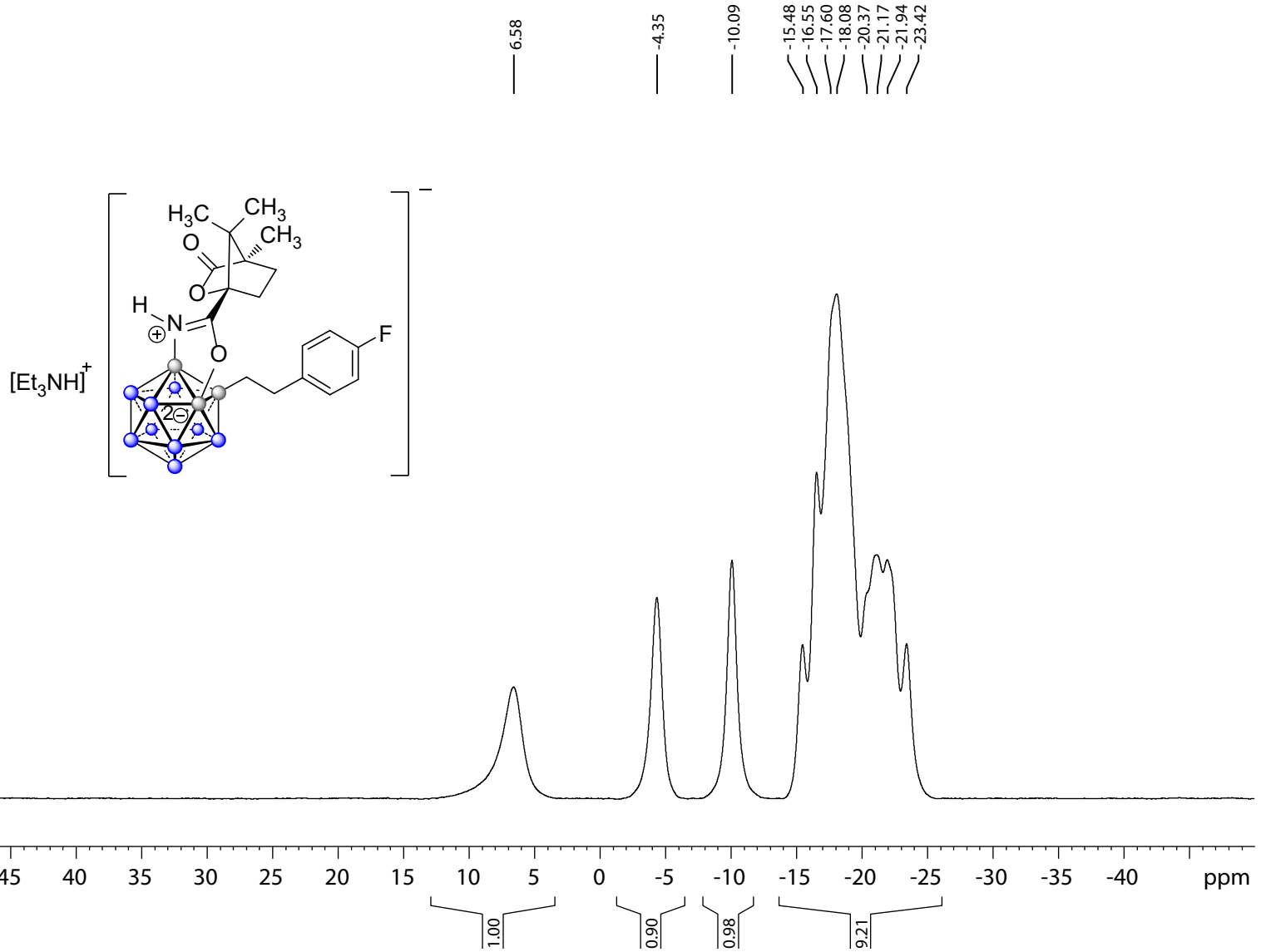
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2              90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300071 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190802-B12C-4F-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4F] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190802
Time              12.47
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.2 K
D1           1.00000000 sec
TD0                   1

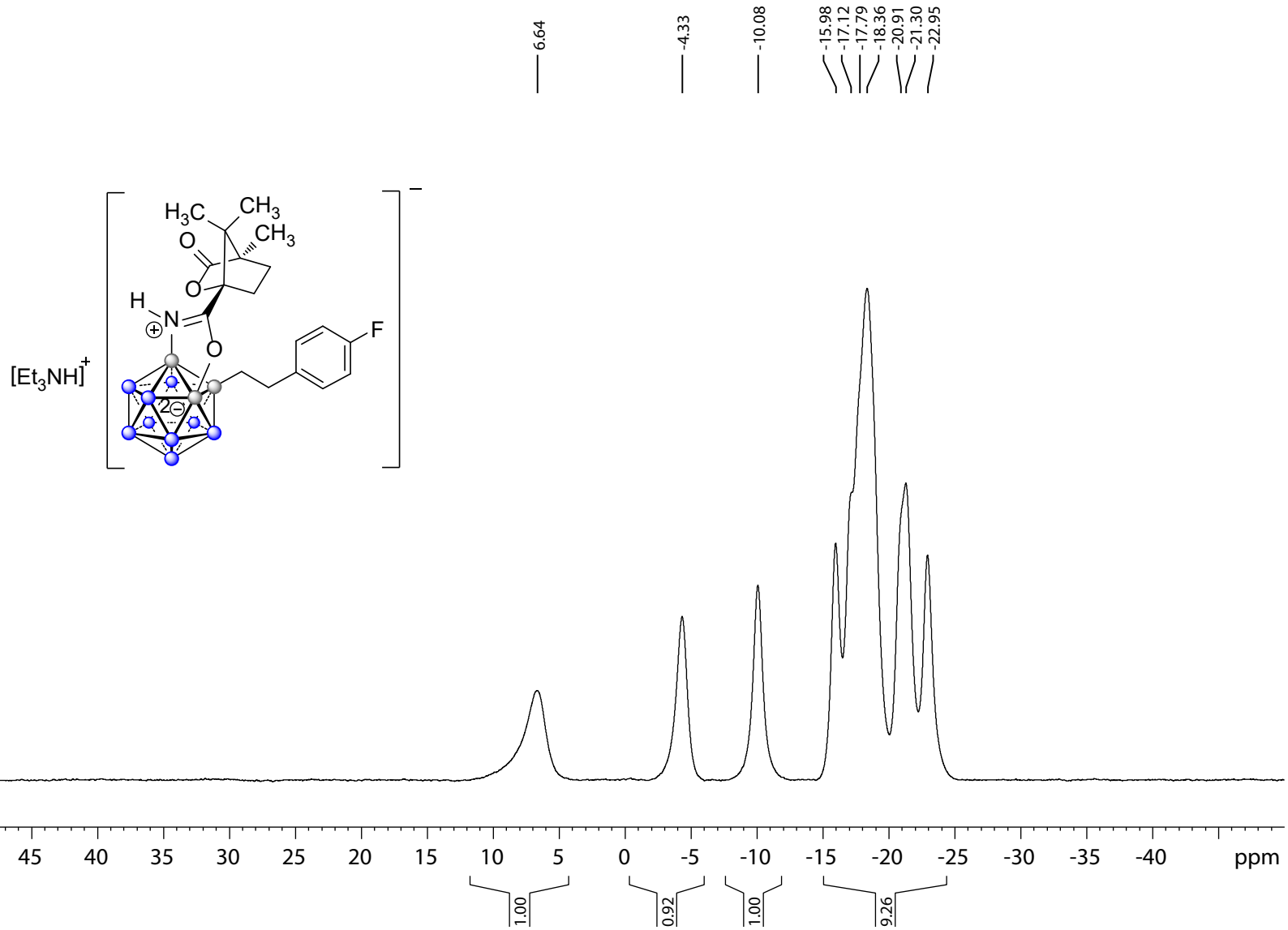
======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                 EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-042

20190802-B12C-4F-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4F] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190802
Time              12.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

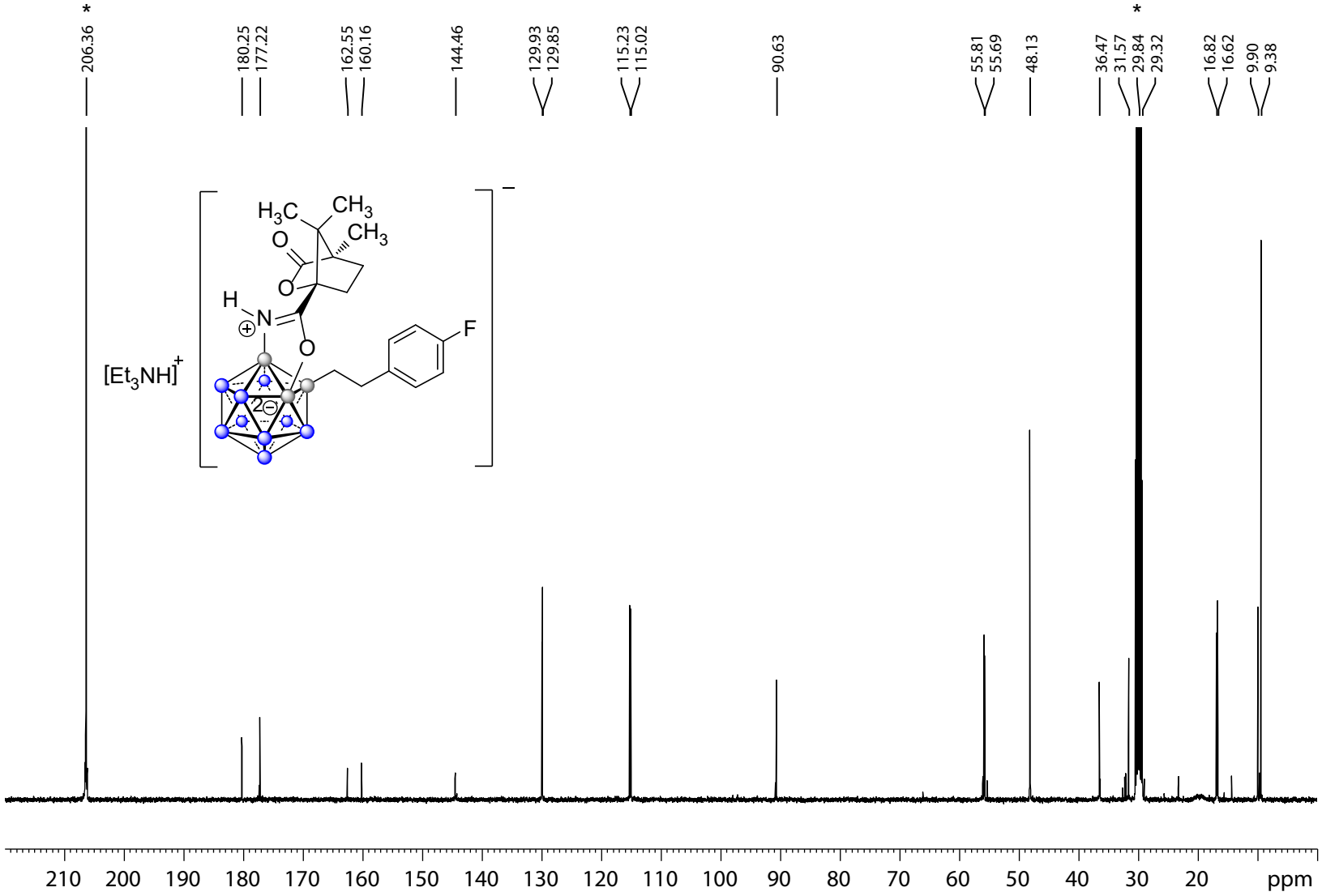
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-043

20190802-B12C-4F-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4F] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190802
Time              14.25
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                295.9 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

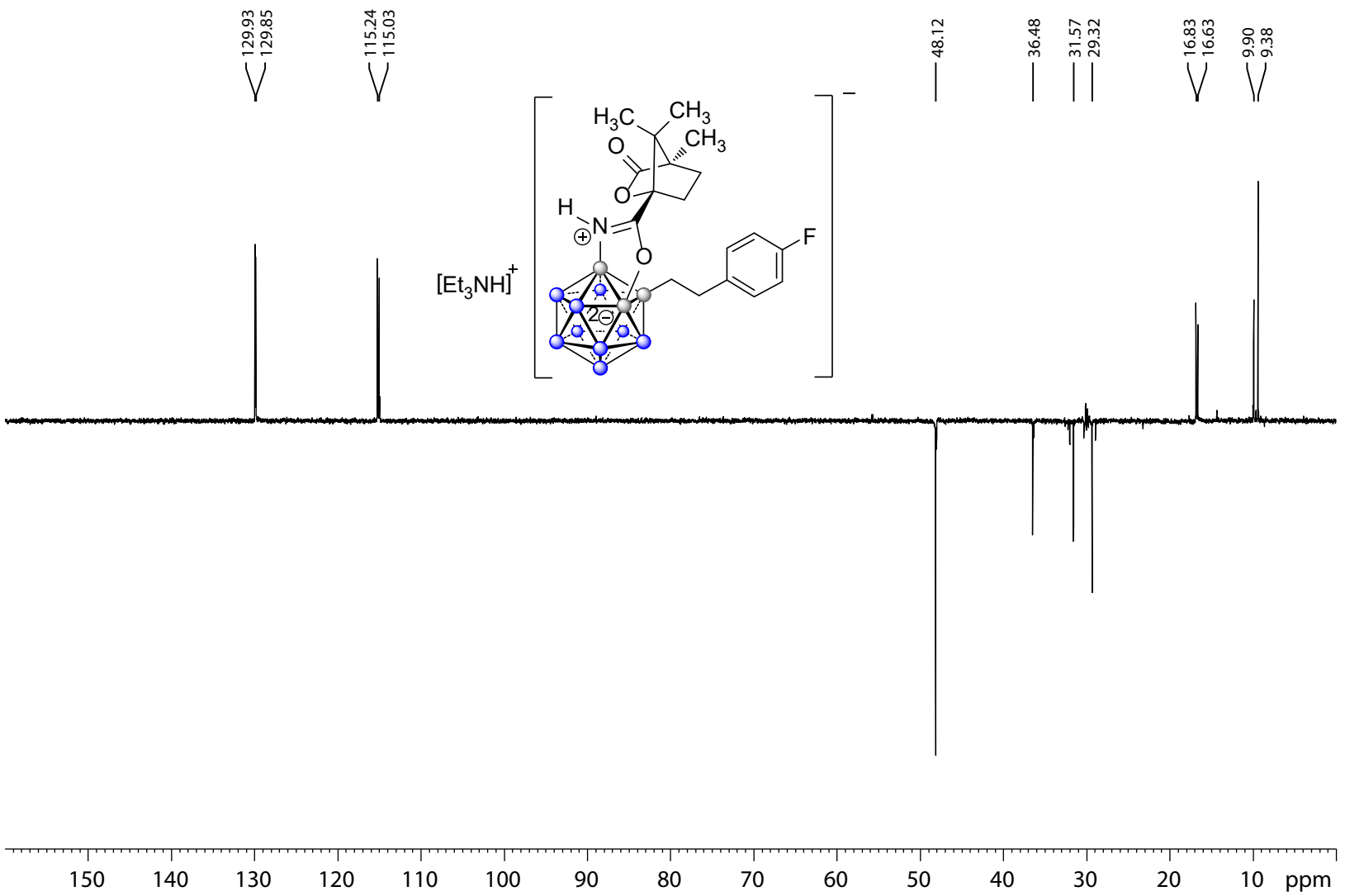
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126870 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190802-B12C-4F-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4F]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_           20190802
Time              14.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                295.5 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

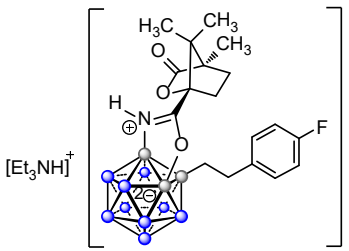
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

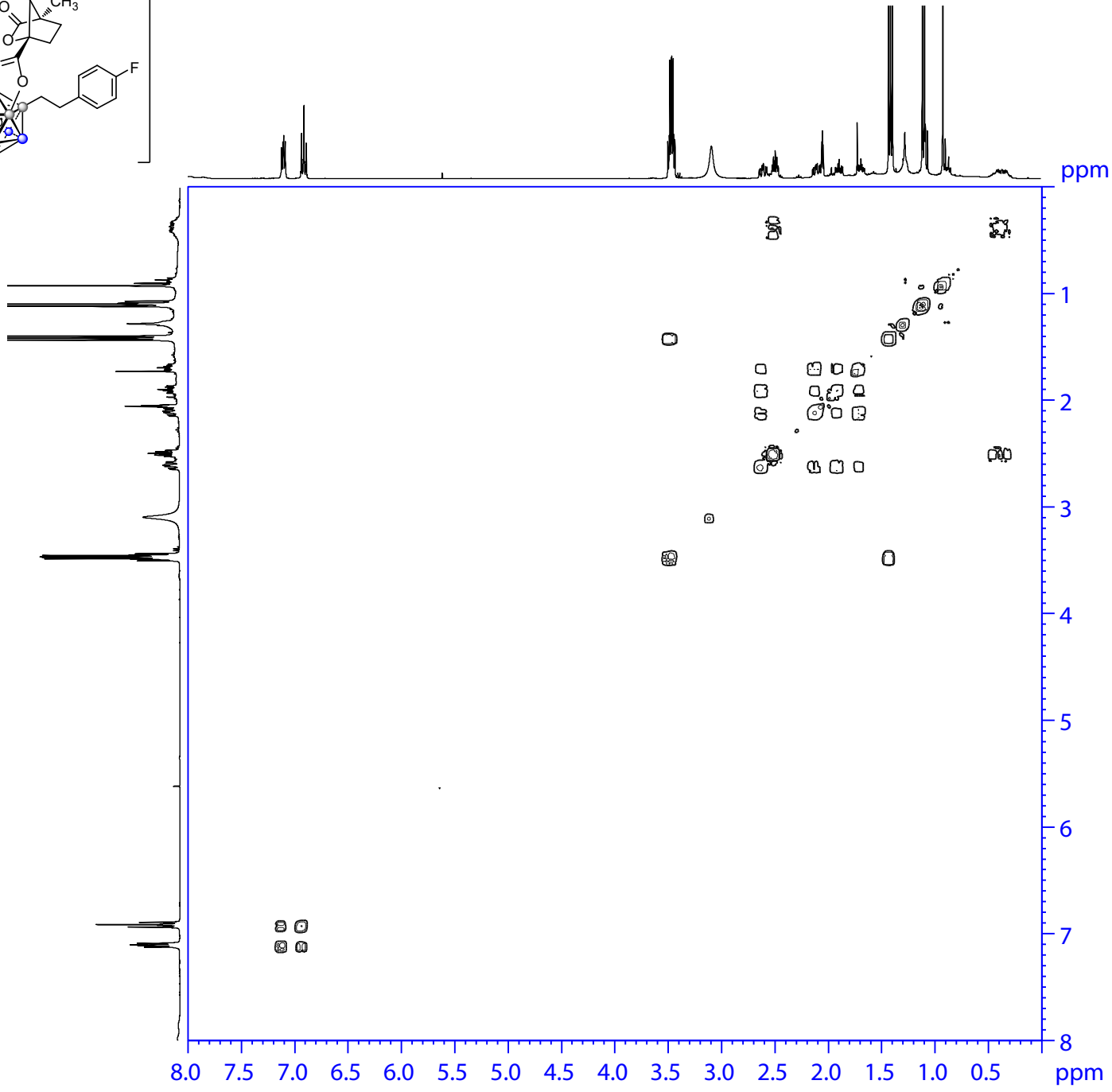
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126867 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190802-B12C-4F-Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4F]$ dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR






```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190802
Time              14.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT         Acetone
NS                   2
DS                   8
SWH           5341.880 Hz
FIDRES        2.608340 Hz
AQ            0.1916928 sec
RG               95.29
DW              93.600 usec
DE               6.50 usec
TE              295.3 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1       400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1             10.00 %
P16            1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1          400.1324 MHz
FIDRES       83.466881 Hz
SW              13.350 ppm
FnMODE               QF

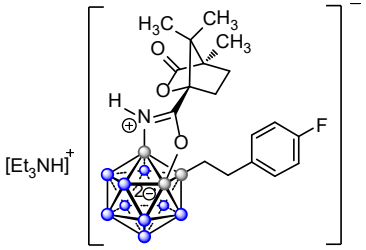
F2 - Processing parameters
SI                  1024
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
```

NMR-046

20190802-B12C-4F-Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4F] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR



NMR-047

```
Current Data Parameters
NAME      20190802-RV-B12C-4F-Styr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_            20190802
Time_              15.05
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                295.2 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

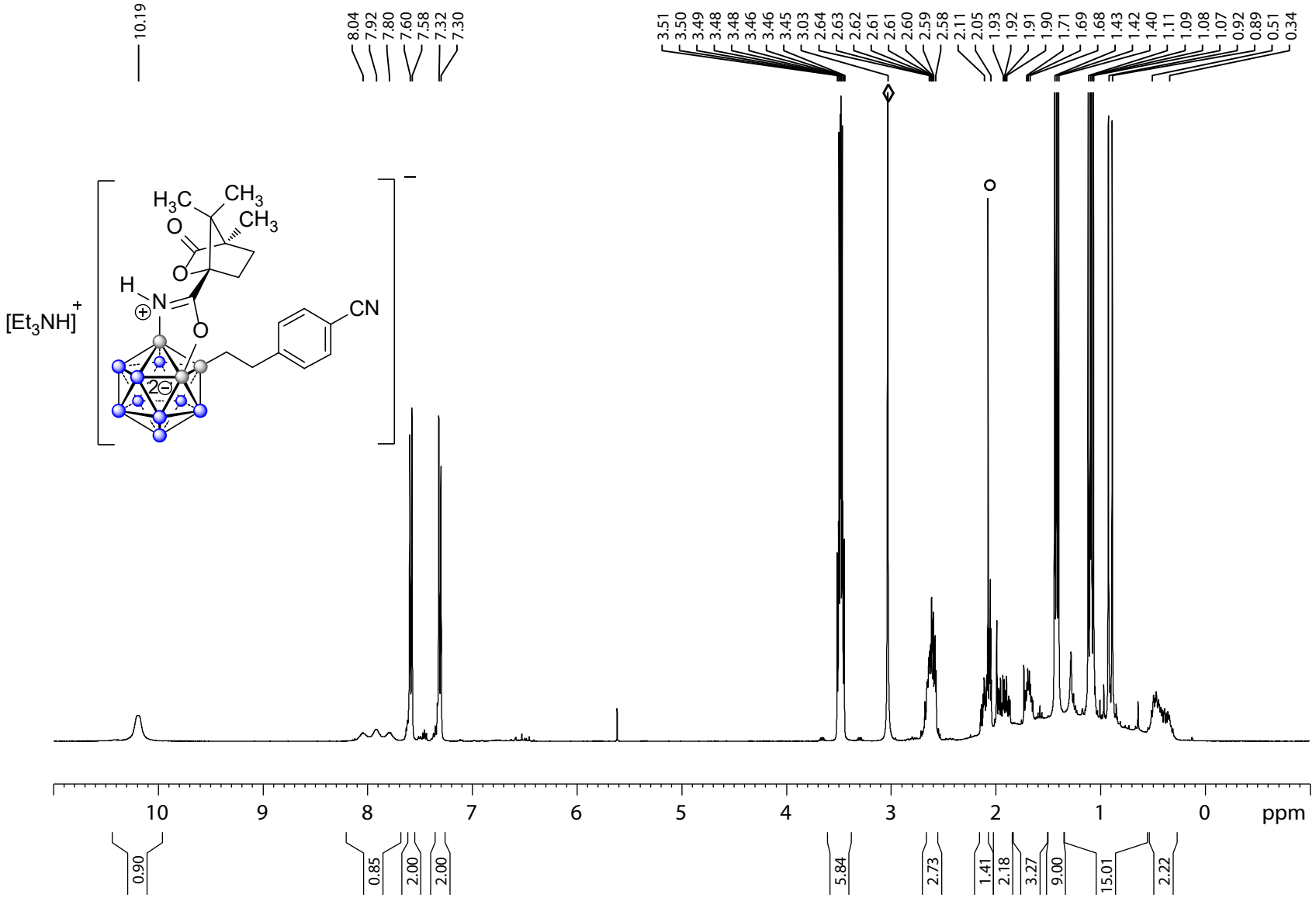
F1 - Acquisition parameters
TD                  256
SFO1            100.6238 MHz
FIDRES       196.524048 Hz
SW              249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2       echo-antiecho
SF          100.6127690 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
```

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-048

```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                1
PROCNO               1

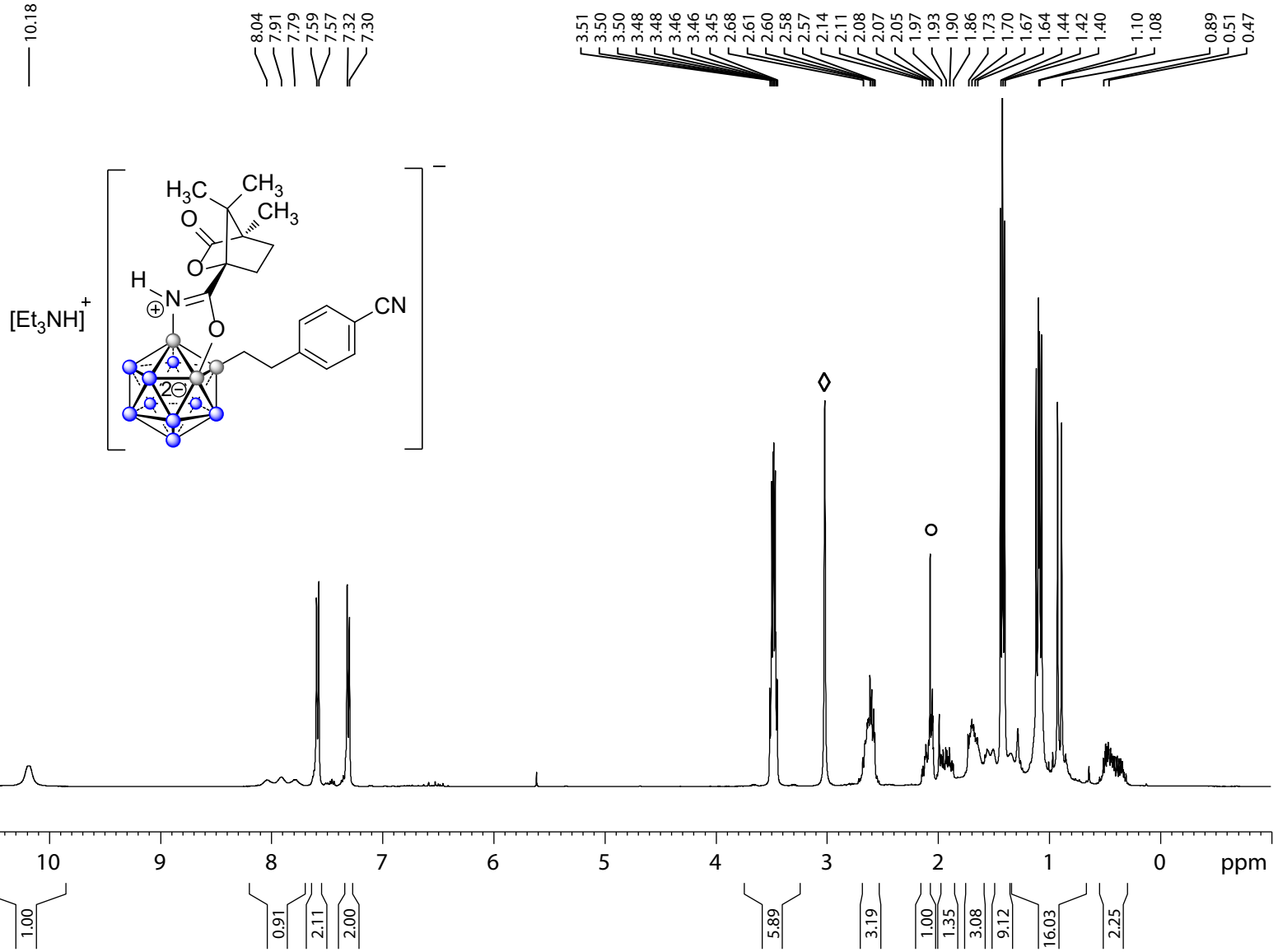
F2 - Acquisition Parameters
Date_           20190921
Time              16.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               64.43
DW               50.000 usec
DE                6.50 usec
TE               295.4 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300072 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20190921-B12C-4CNStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4CN]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-049

```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20190921
Time             16.52
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG              64.43
DW              62.400 usec
DE               6.50 usec
TE              295.8 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

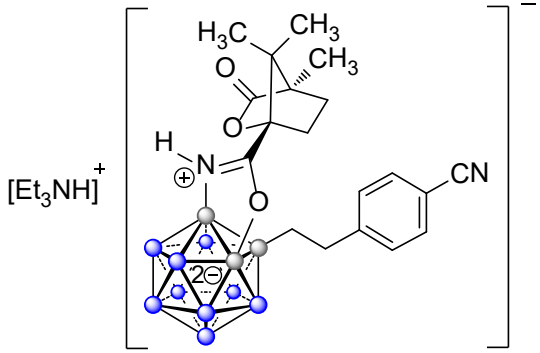
======== CHANNEL f1 ========
NUC1                1H
P1               15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2            90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF         400.1300072 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                            3
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20190921
Time                         16.58
INSTRUM                      spect
PROBHD   5 mm PABBO BB/
PULPROG                         zg
TD                           65536
SOLVENT                    Acetone
NS                               128
DS                                 4
SWH                     25510.203 Hz
FIDRES                   0.389255 Hz
AQ                       1.2845056 sec
RG                          193.34
DW                          19.600 usec
DE                           6.50 usec
TE                          295.9 K
D1                    1.00000000 sec
TD0                              1

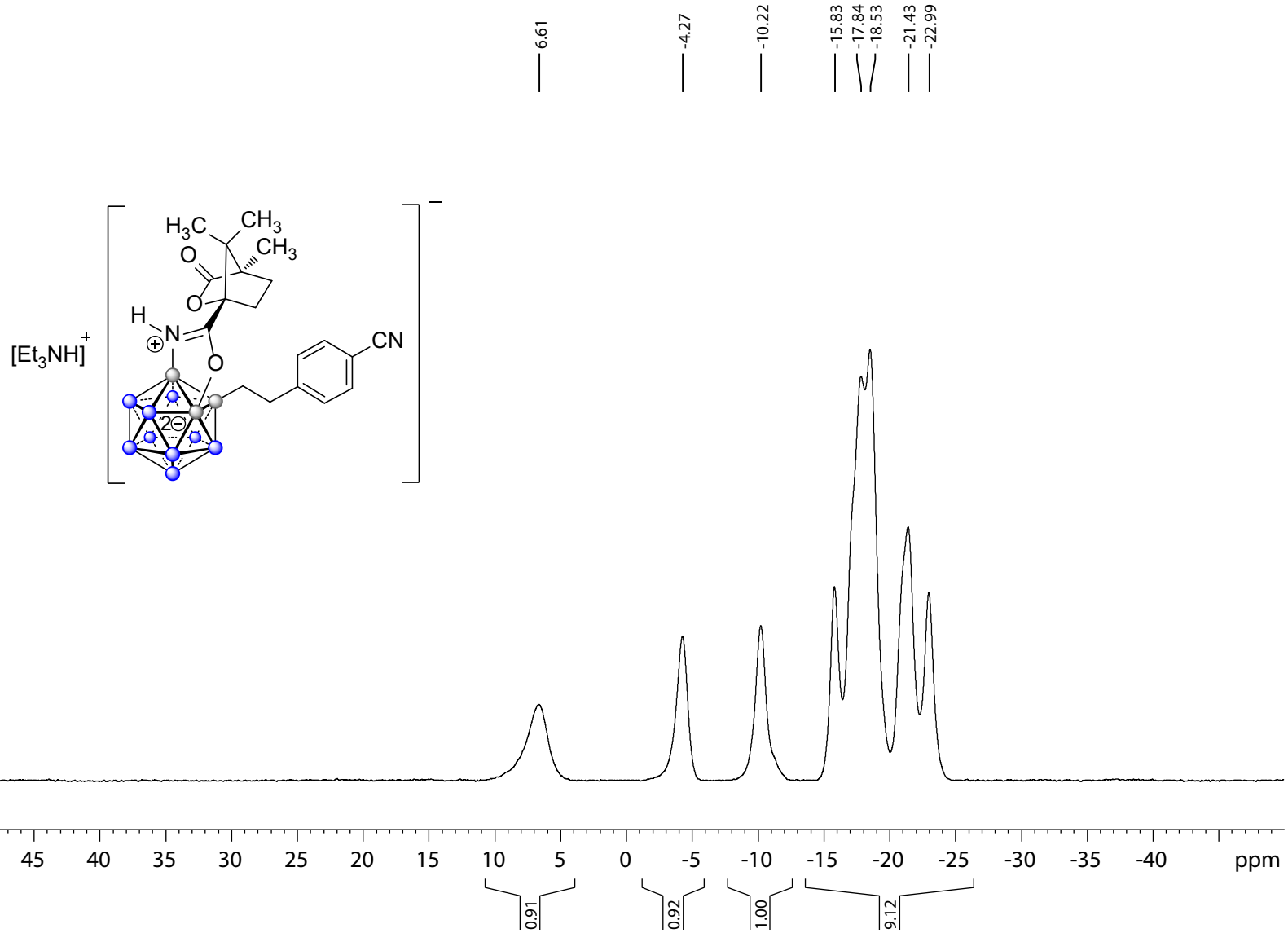
======== CHANNEL f1 ========
NUC1                           11B
P1                            9.93 usec
PLW1                 52.96599960 W
SFO1                128.3776052 MHz

F2 - Processing parameters
SI                           32768
SF                  128.3776050 MHz
WDW                             EM
SSB                 0
LB                          10.00 Hz
GB                  0
PC                           1.40
```

NMR-050

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20190921
Time              17.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE                296.9 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776050 MHz

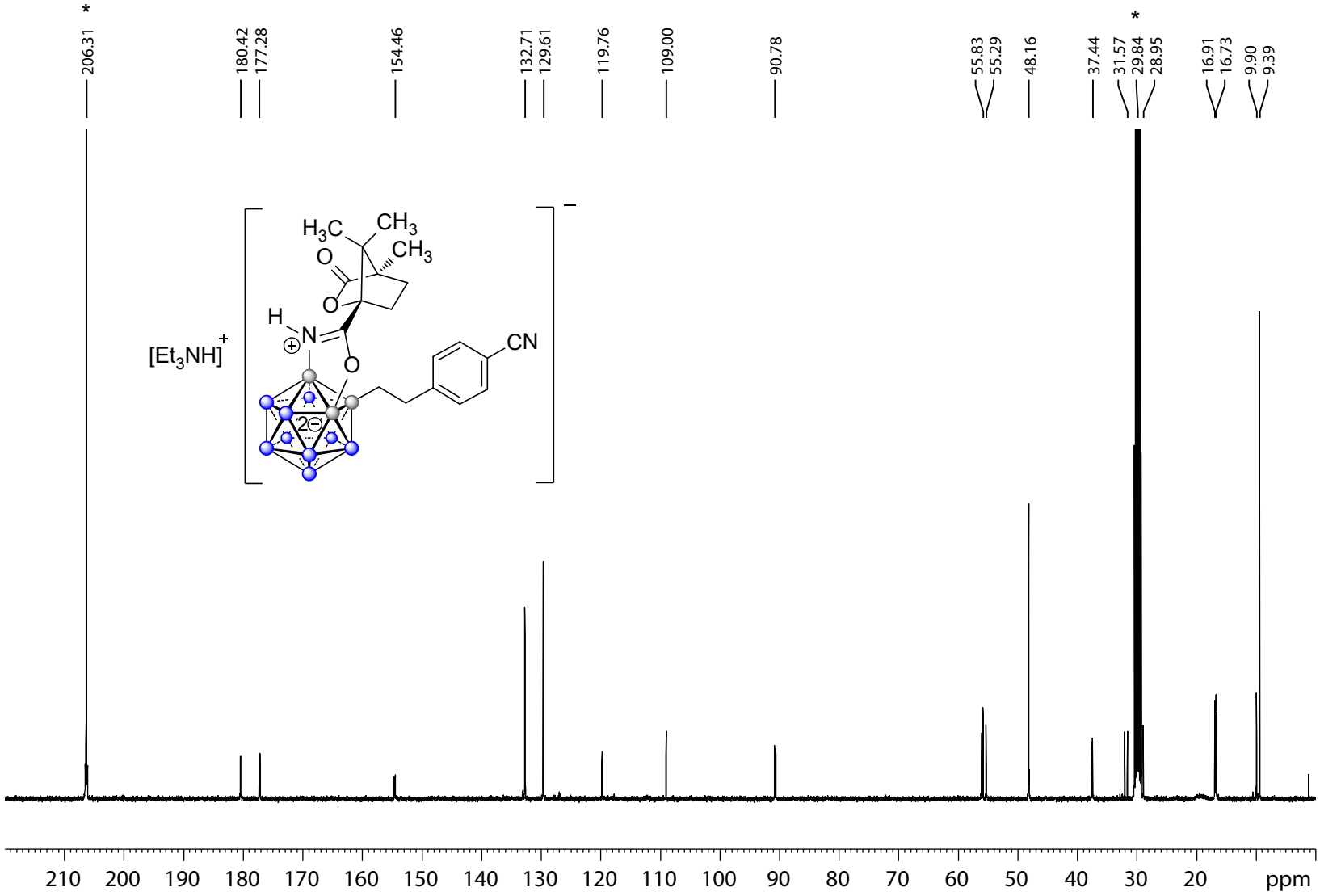
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-051

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190921
Time              18.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                296.6 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

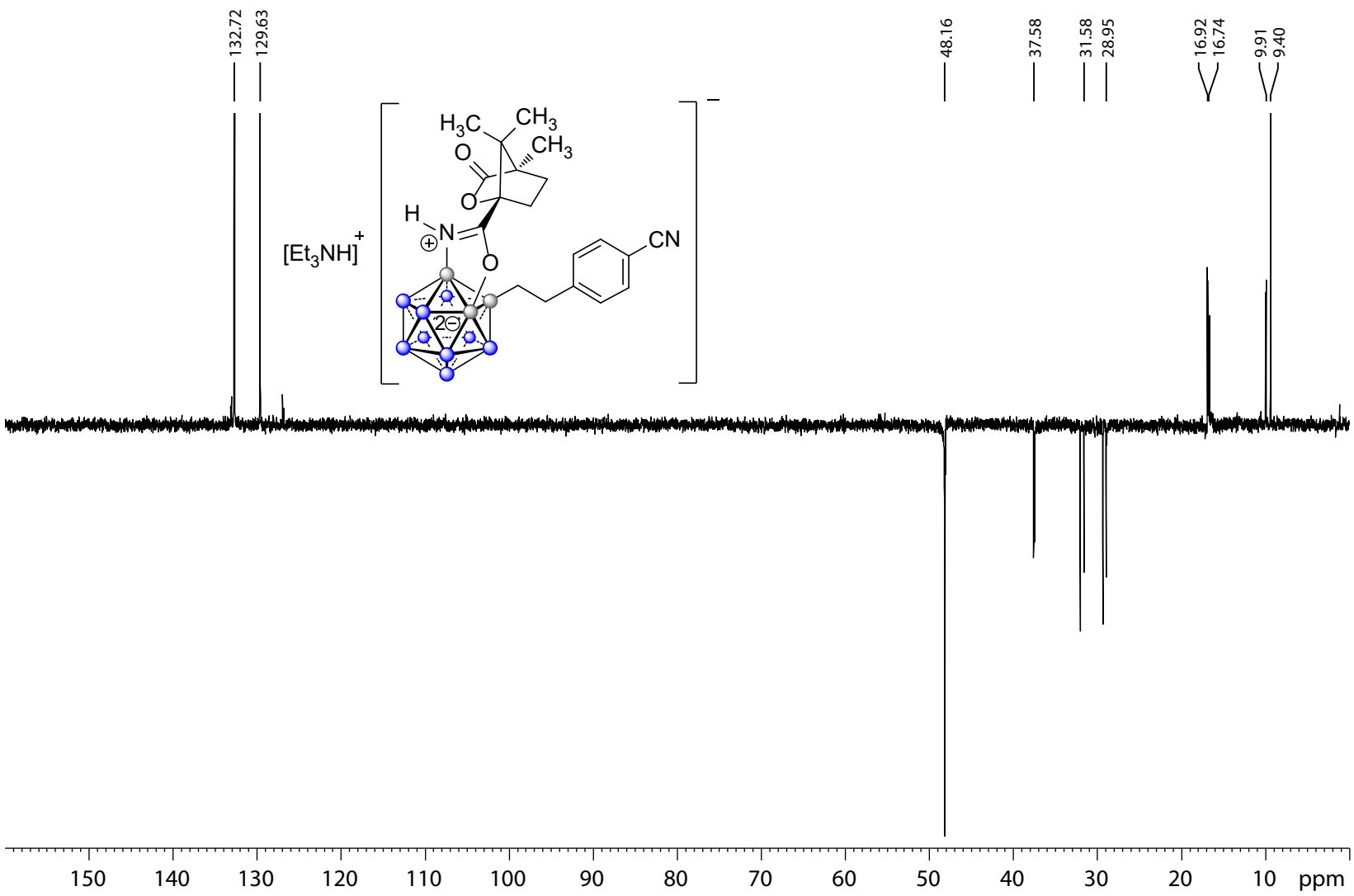
======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6126859 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_           20190921
Time              19.06
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.5 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

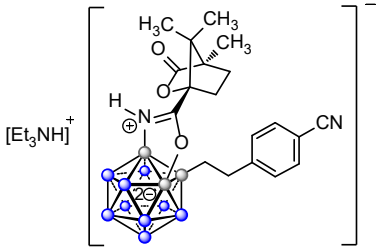
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

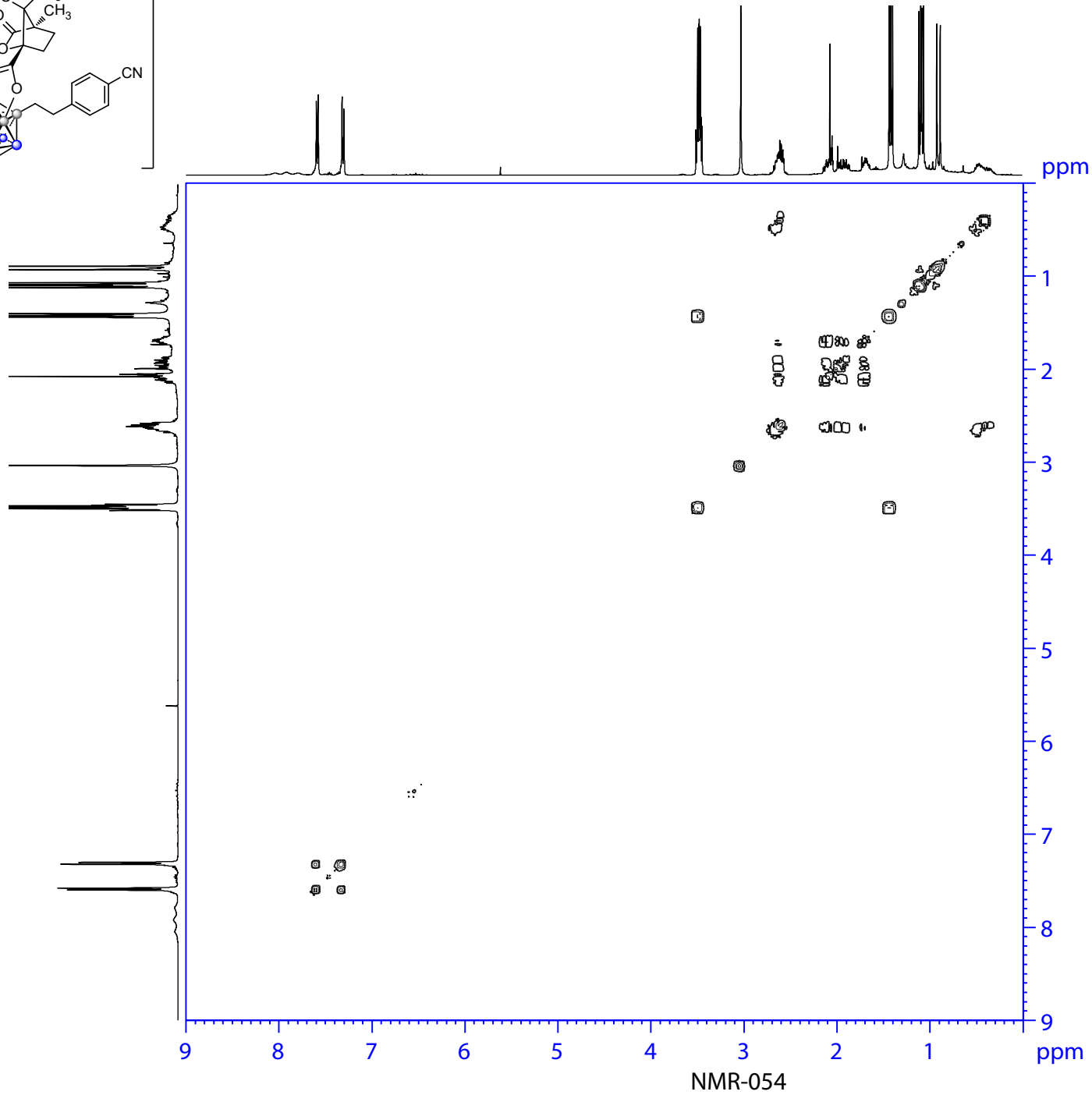
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126850 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-054

```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20190921
Time              19.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT         Acetone
NS                   2
DS                   8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG               124.48
DW                93.600 usec
DE                 6.50 usec
TE                296.0 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1        400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

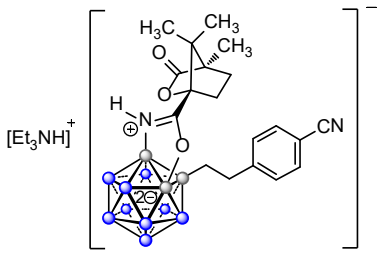
F1 - Acquisition parameters
TD                  128
SFO1           400.1324 MHz
FIDRES         83.466881 Hz
SW               13.350 ppm
FnMODE              QF

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                  QF
SF          400.1300000 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
```

20190921-B12C-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4CN] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190921-RV-B12C-4CNStyr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20190921
Time              19.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG               193.34
DW               83.200 usec
DE                6.50 usec
TE               296.4 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                 256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW              249.991 ppm
FnMODE     Echo-Antiecho

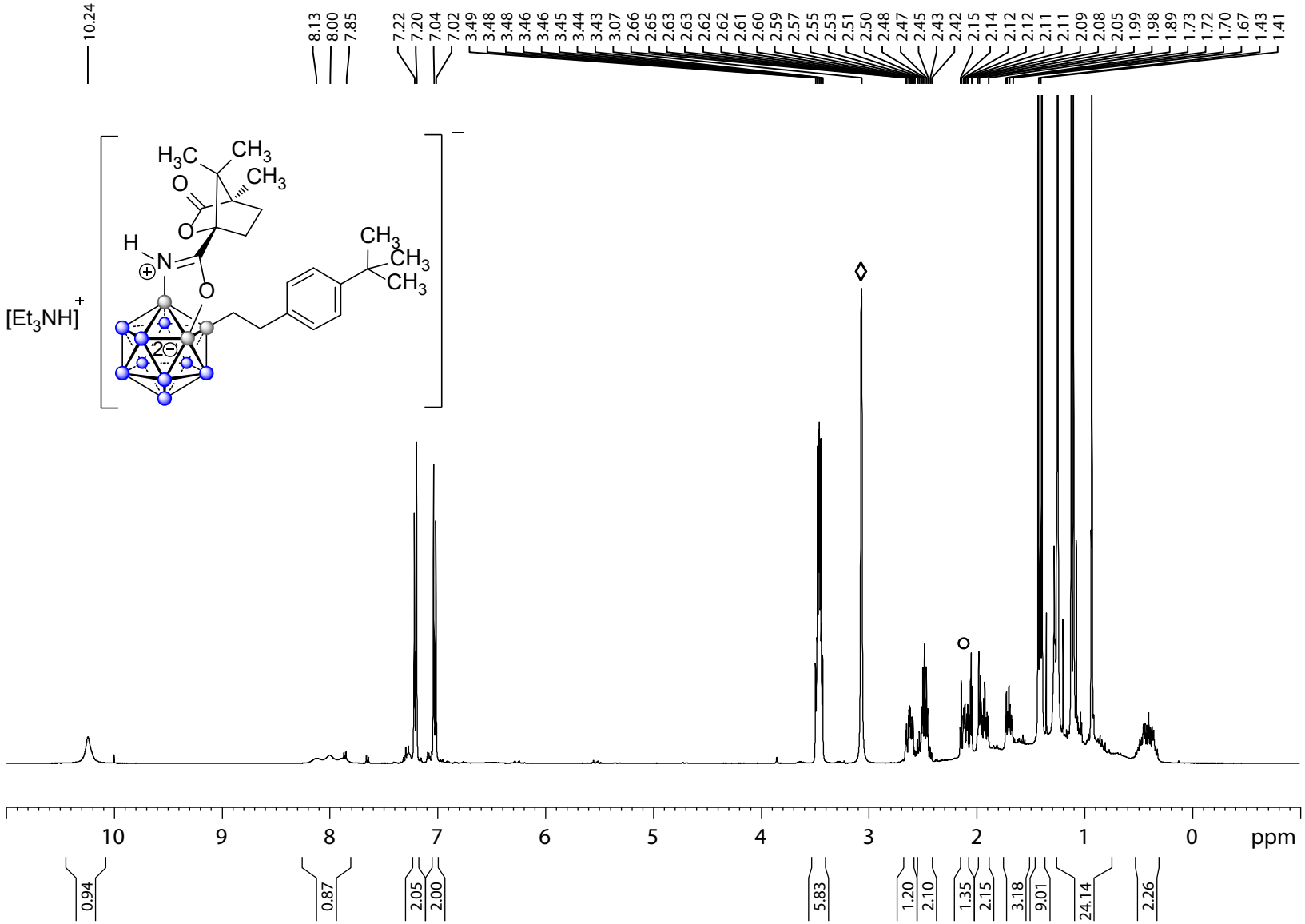
F2 - Processing parameters
SI                1024
SF          400.1300000 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

NMR-055

20191001-B12C-4tBuStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-tBu] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-056

```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                1
PROCNO               1

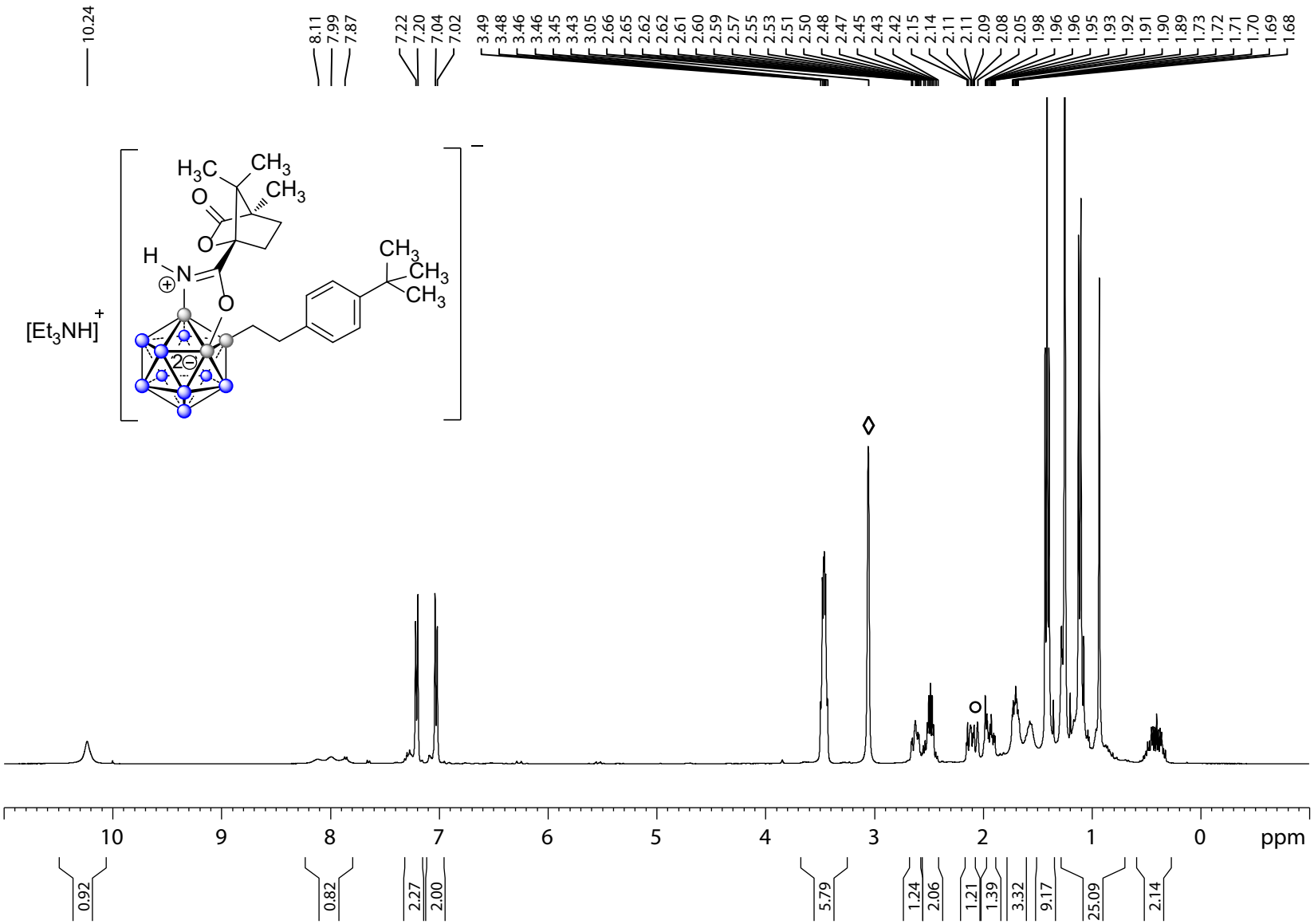
F2 - Acquisition Parameters
Date_          20191002
Time               1.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                36.87
DW                50.000 usec
DE                 6.50 usec
TE                295.8 K
D1             1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300071 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20191001-B12C-4tBuStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-tBu] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H{B) NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20191002
Time               1.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                36.87
DW               62.400 usec
DE                6.50 usec
TE               295.9 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

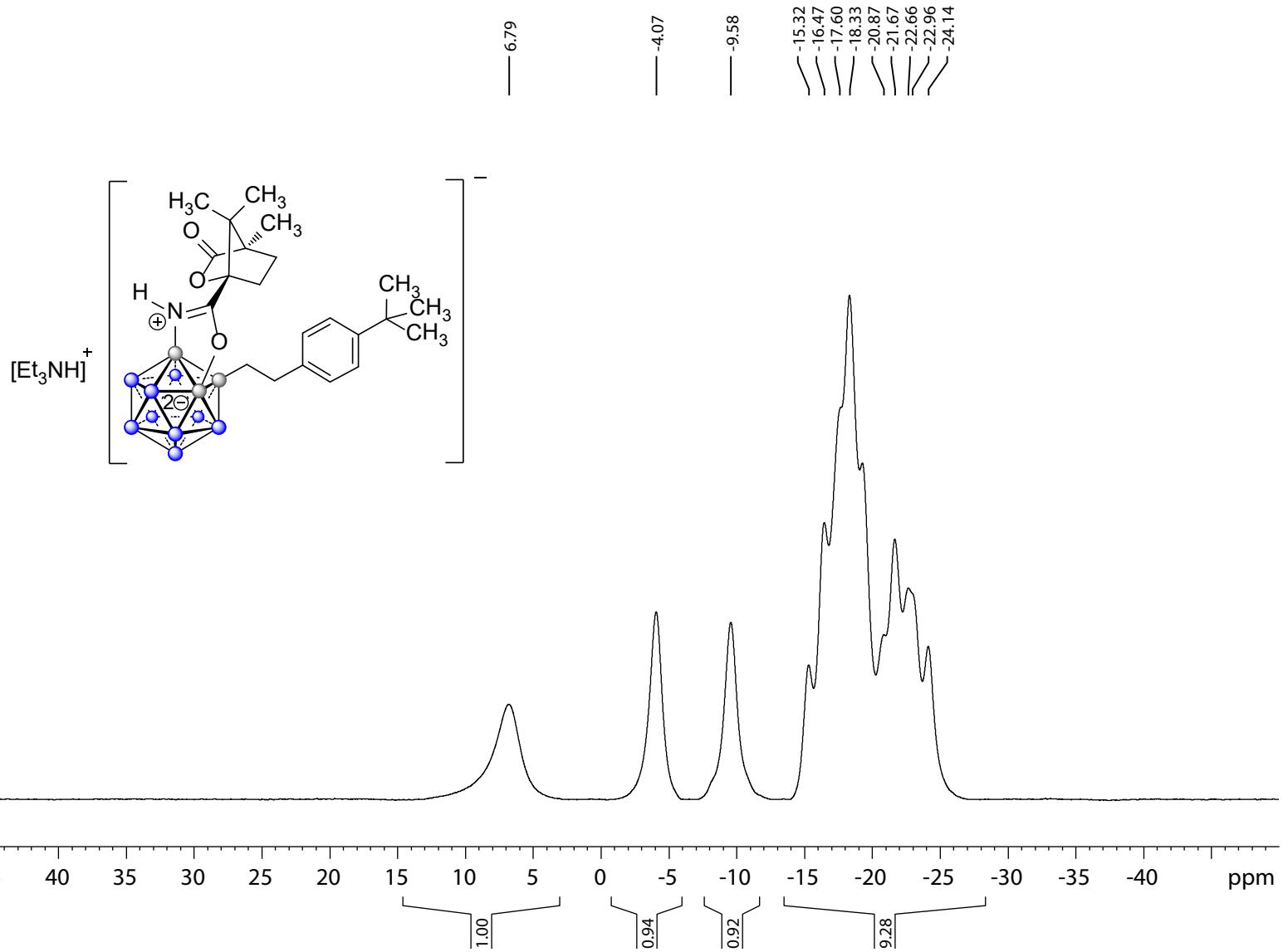
======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300074 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

NMR-057

20191001-B12C-4tBuStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-tBu] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20191002
Time               1.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.9 K
D1            1.00000000 sec
TD0                   1

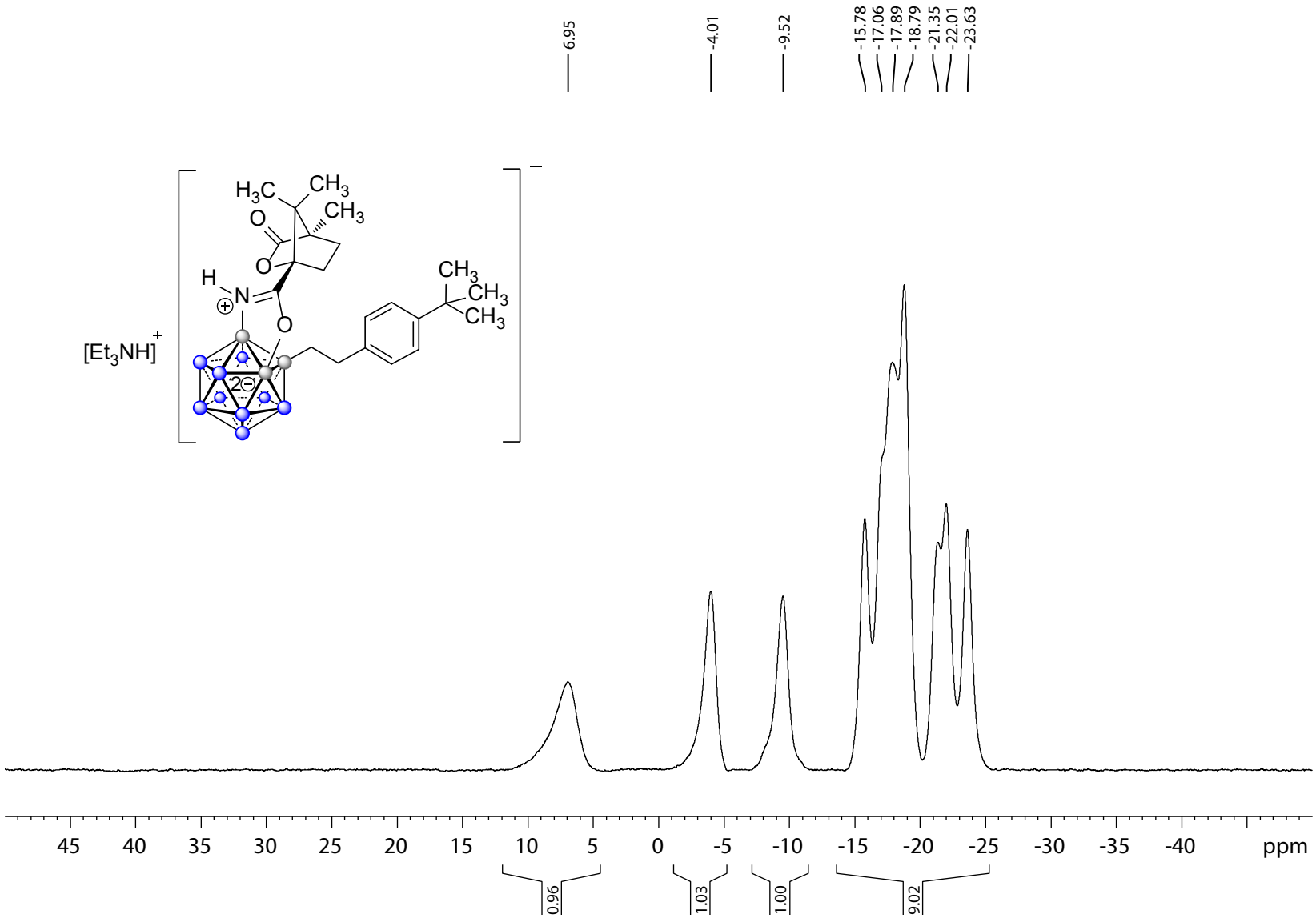
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-058

20191001-B12C-4tBuStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-tBu] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_           20191002
Time               1.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

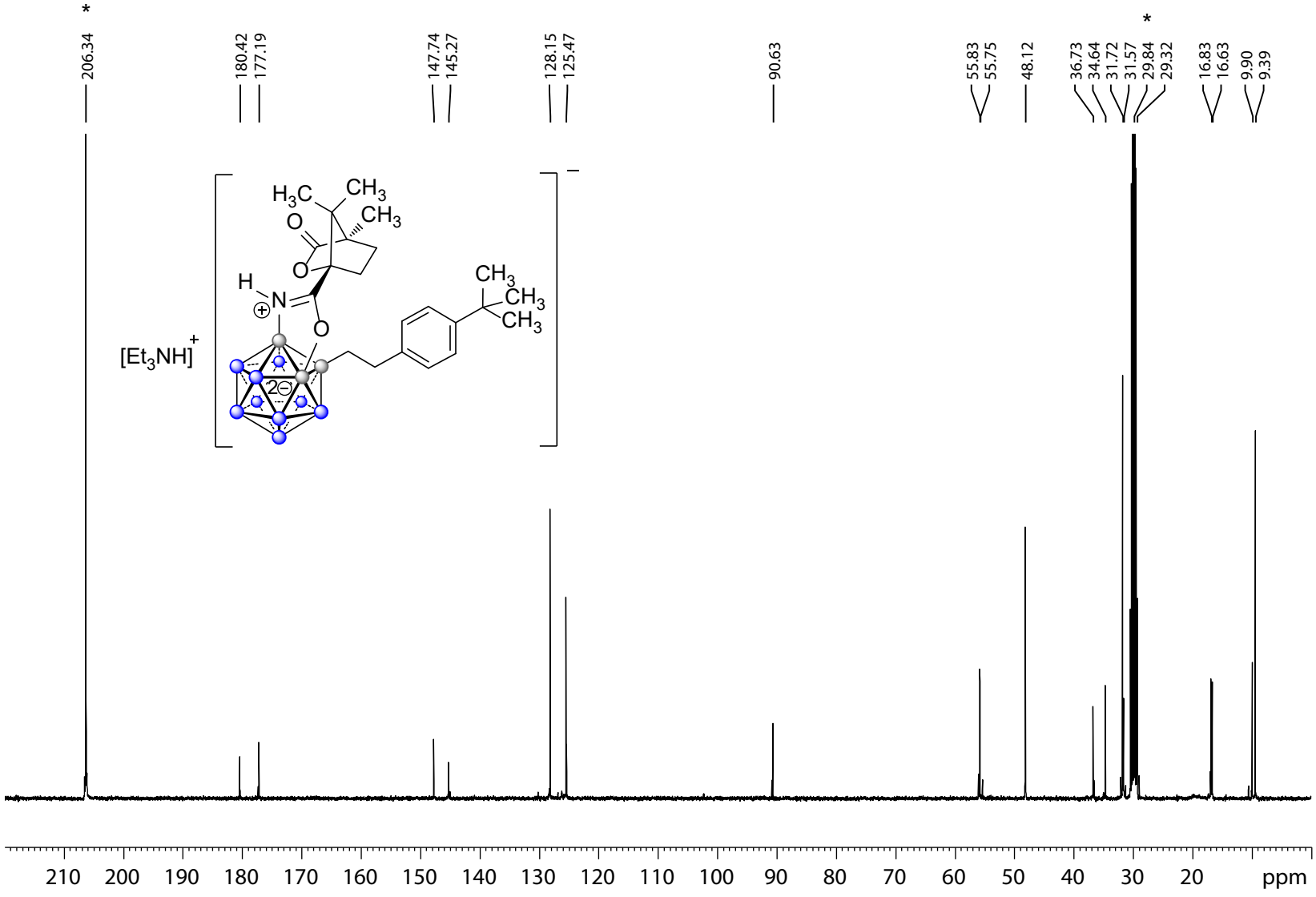
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-059

20191001-B12C-4tBuStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}tBu]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20191002
Time              3.02
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW               16.800 usec
DE                6.50 usec
TE               296.6 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

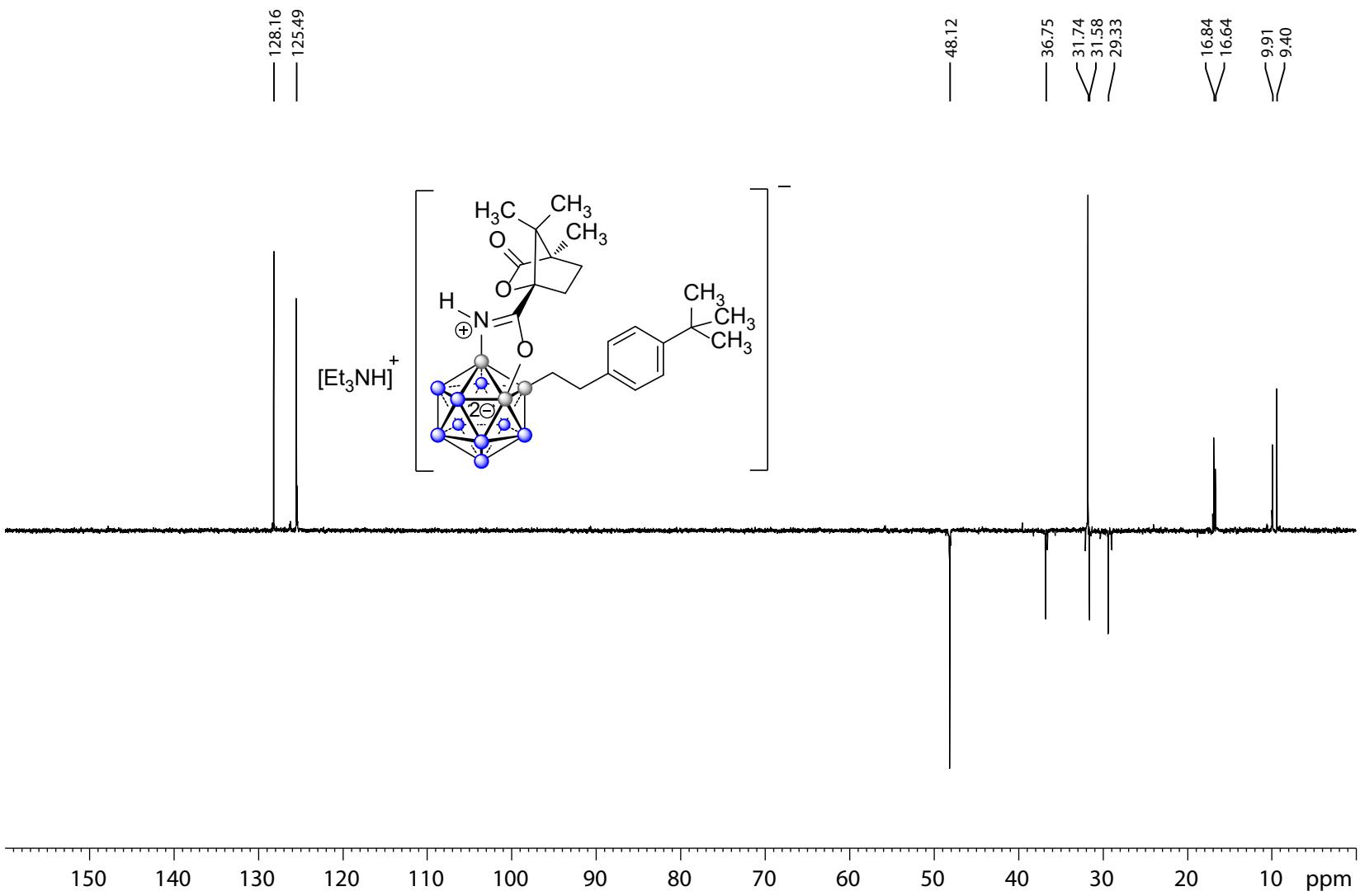
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126874 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

NMR-060

20191001-B12C-4tBuStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-tBu] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_           20191002
Time                3.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          dept135
TD                 65536
SOLVENT          Acetone
NS                   512
DS                     4
SWH            29296.875 Hz
FIDRES          0.447035 Hz
AQ              1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                296.5 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

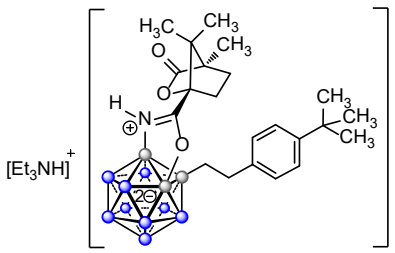
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                 15.00 usec
P4                 30.00 usec
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

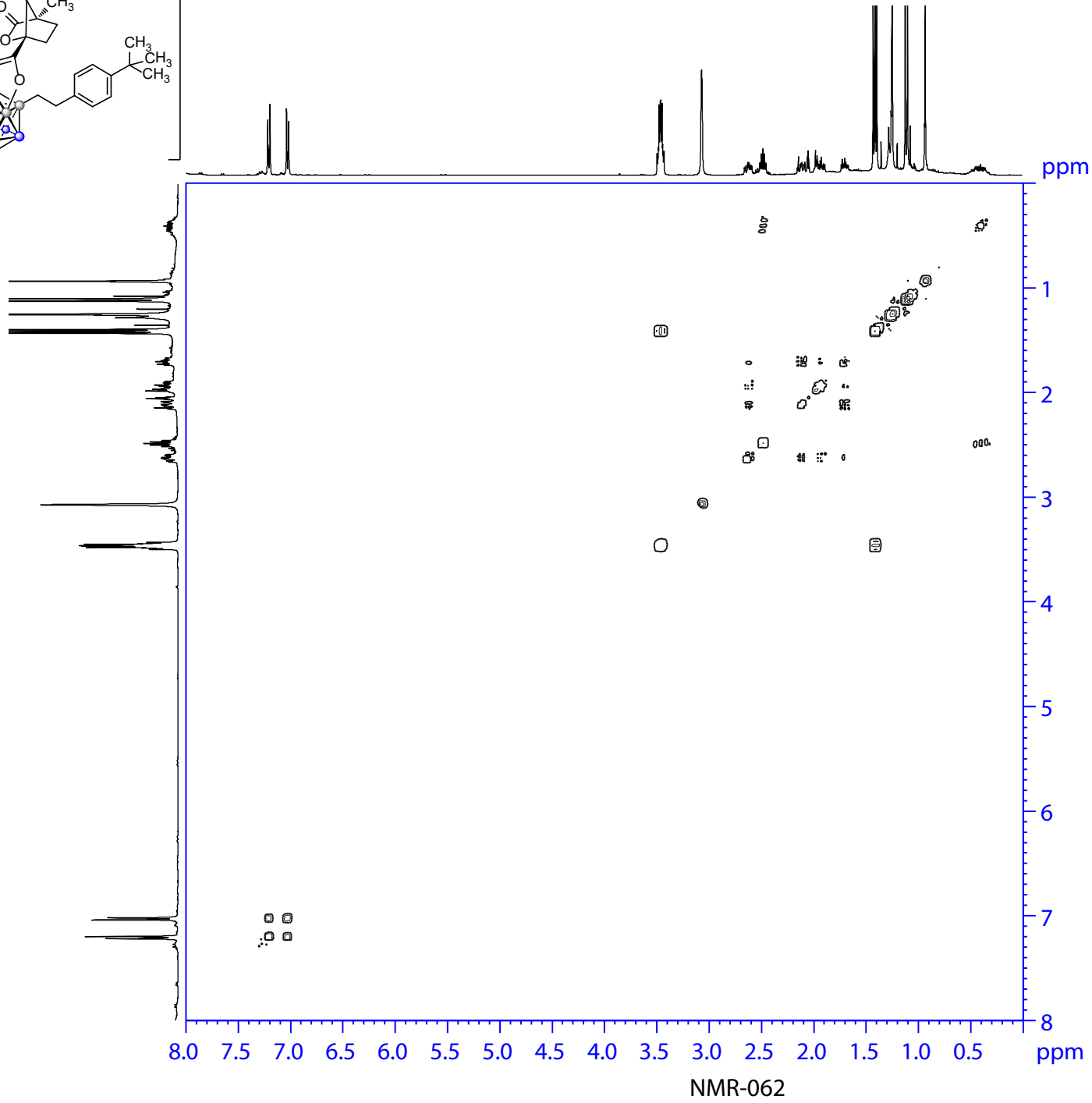
F2 - Processing parameters
SI                 32768
SF            100.6126863 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 4.00
```

NMR-061

20191001-B12C-4tBuStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-tBu] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹H COSY NMR






```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                            7
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20191002
Time                          3.31
INSTRUM                      spect
PROBHD   5 mm PABBO BB/
PULPROG              cosygpppqf
TD                           2048
SOLVENT                   Acetone
NS                               2
DS                               8
SWH                       5341.880 Hz
FIDRES                    2.608340 Hz
AQ                        0.1916928 sec
RG                           64.43
DW                          93.600 usec
DE                           6.50 usec
TE                          296.2 K
D0                        0.00000300 sec
D1                        2.00000000 sec
D11                       0.03000000 sec
D12                       0.00002000 sec
D13                       0.00000400 sec
D16                       0.00020000 sec
IN0                       0.00018720 sec

======== CHANNEL f1 ========
NUC1                             1H
P0                           15.00 usec
P1                           15.00 usec
P17                        2500.00 usec
PLW1                  12.50000000 W
PLW10                  4.16050005 W
SFO1                 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]              SMSQ10.100
GPZ1                         10.00 %
P16                        1000.00 usec

F1 - Acquisition parameters
TD                             128
SFO1                     400.1324 MHz
FIDRES                  83.466881 Hz
SW                         13.350 ppm
FnMODE                         QF

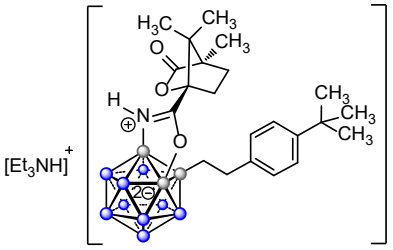
F2 - Processing parameters
SI                            1024
SF                   400.1300088 MHz
WDW                        QSINE
SSB                0
LB                 0 Hz
GB                 0
PC                           1.40

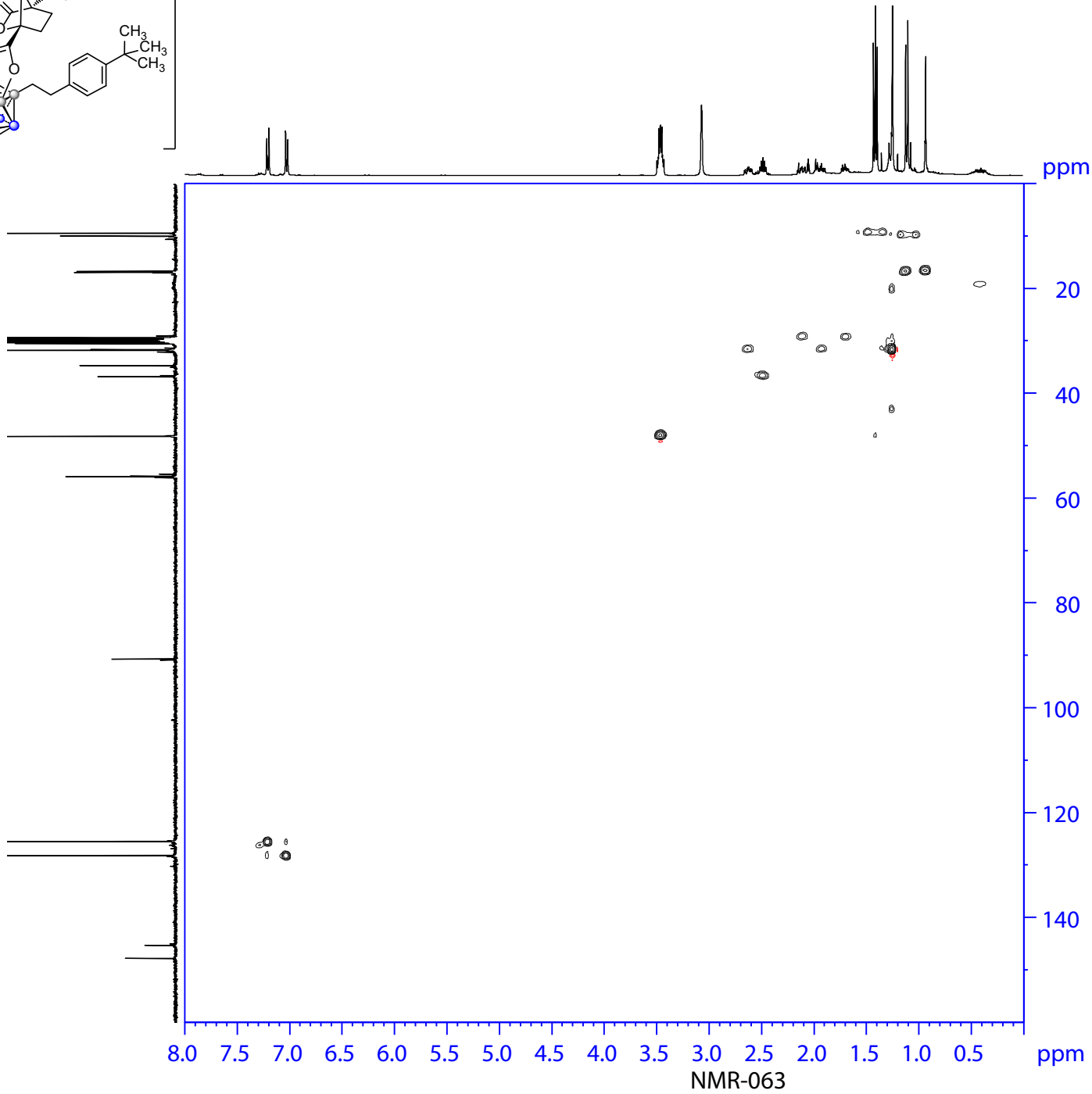
F1 - Processing parameters
SI                            1024
MC2                            QF
SF                   400.1300084 MHz
WDW                        QSINE
SSB                0
LB                 0 Hz
GB                 0
```

NMR-062

20191001-B12C-4tBuStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-tBu] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR






```
Current Data Parameters
NAME      20191001-RV-B12C-4tBuStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20191002
Time               3.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ            0.0851968 sec
RG               193.34
DW               83.200 usec
DE                6.50 usec
TE                296.1 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
P28              1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

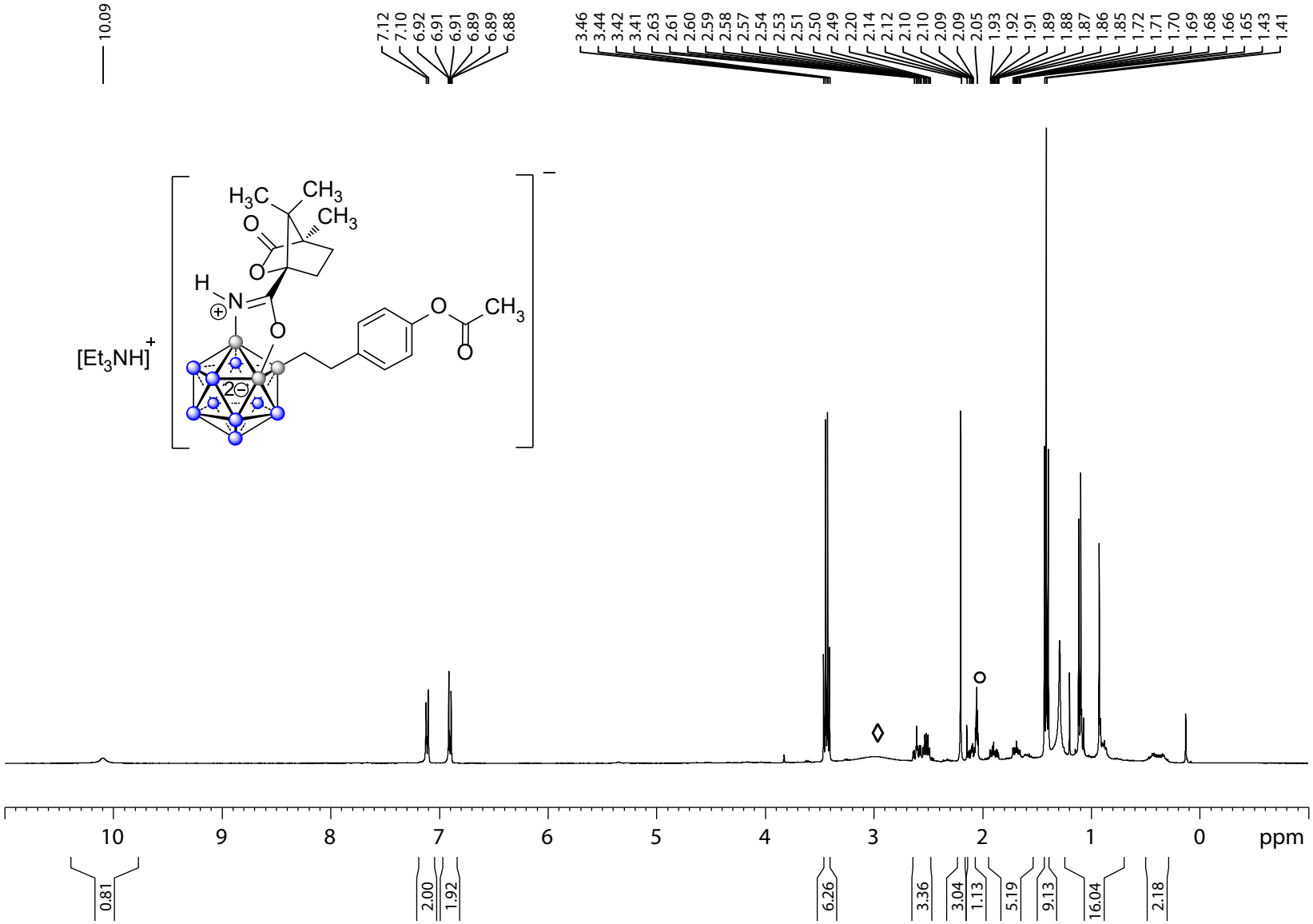
F1 - Acquisition parameters
TD                  256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300071 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2       echo-antiecho
SF          100.6126796 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
```

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-064

```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                1
PROCNO               1

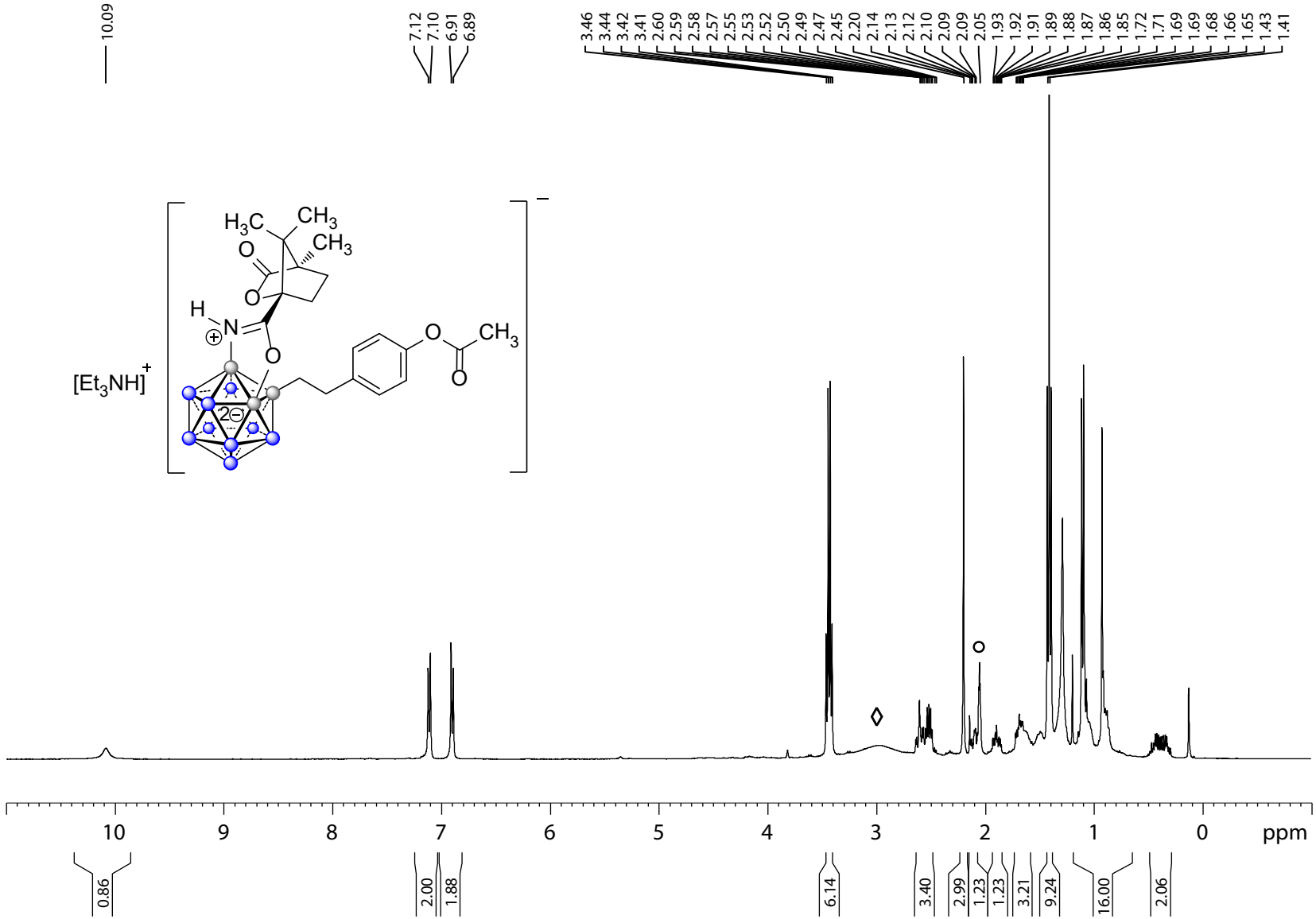
F2 - Acquisition Parameters
Date_           20190927
Time              12.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               95.29
DW               50.000 usec
DE                6.50 usec
TE               296.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300069 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20190926-B12C-4OCOMeSTYR 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4OCOMe]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{^{11}B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-065

```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20190927
Time              12.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               296.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1

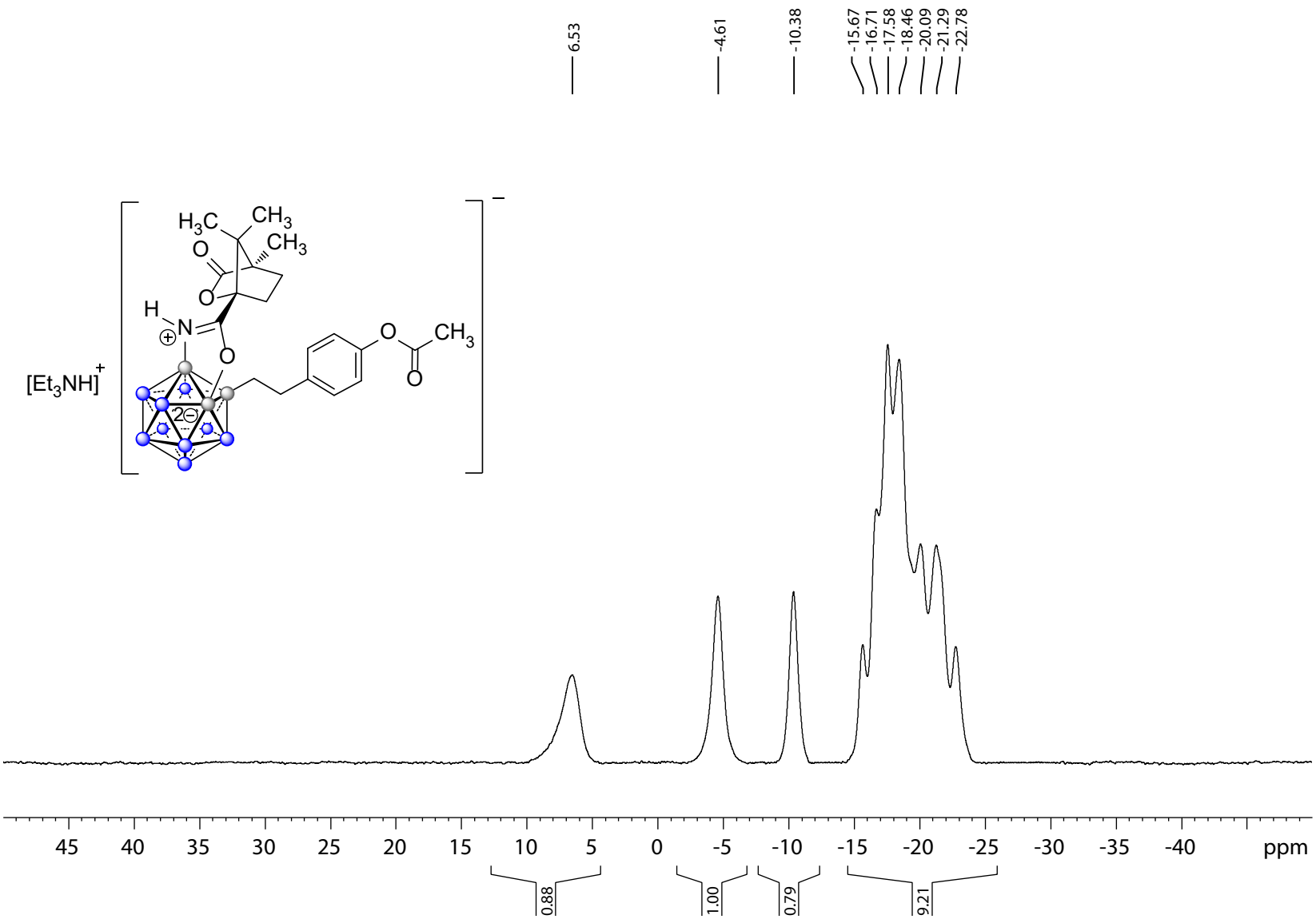
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300069 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz




```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190927
Time              12.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.4 K
D1           1.00000000 sec
TD0                   1

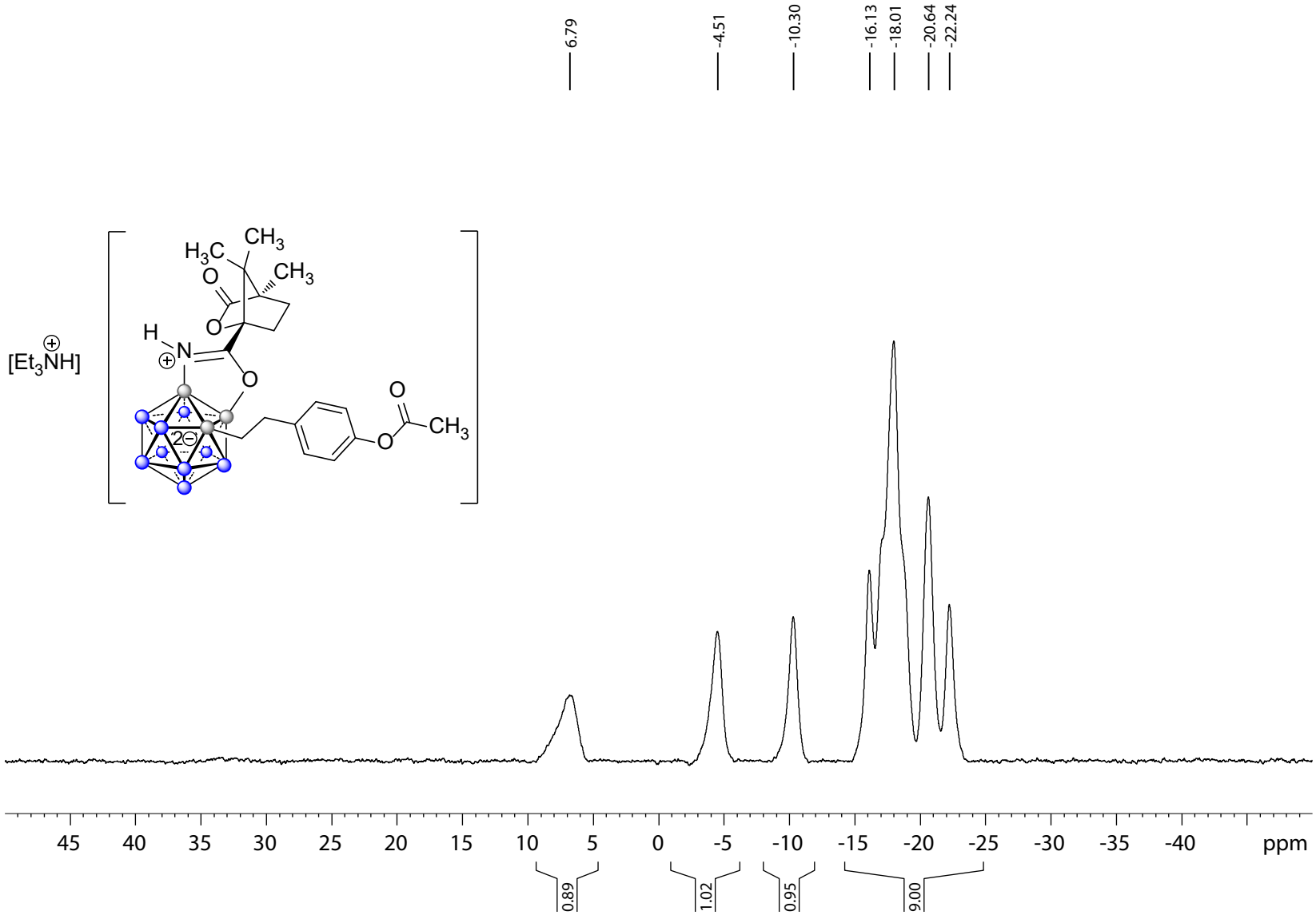
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-066

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{^1H\}$ NMR 128MHz




```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_          20190927
Time             12.38
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

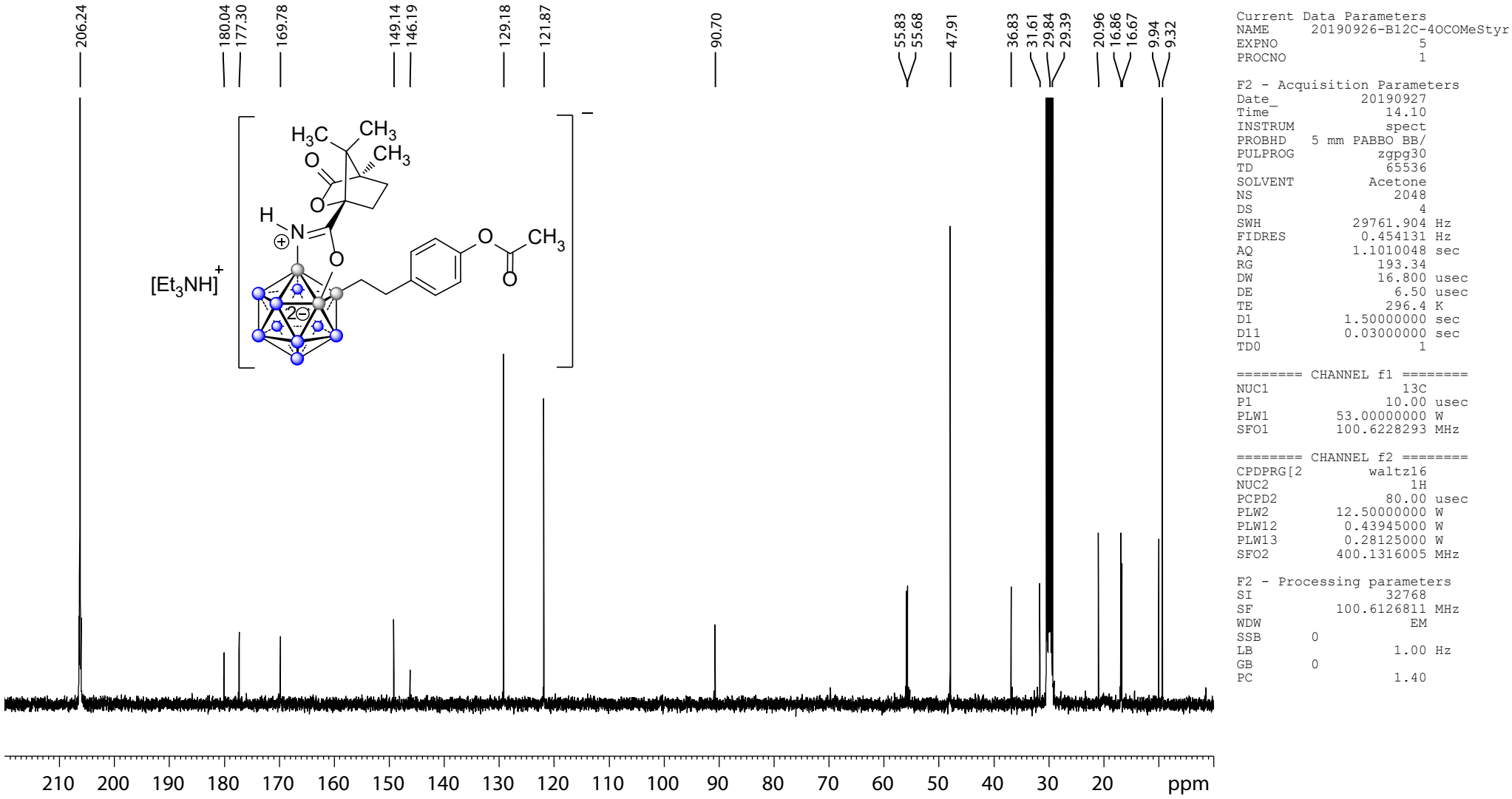
======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI               32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB              10.00 Hz
GB        0
PC               1.40
```

NMR-067

20190926-B12C-4OCOMeSTYR 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4OCOMe]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_           20190927
Time              14.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.4 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

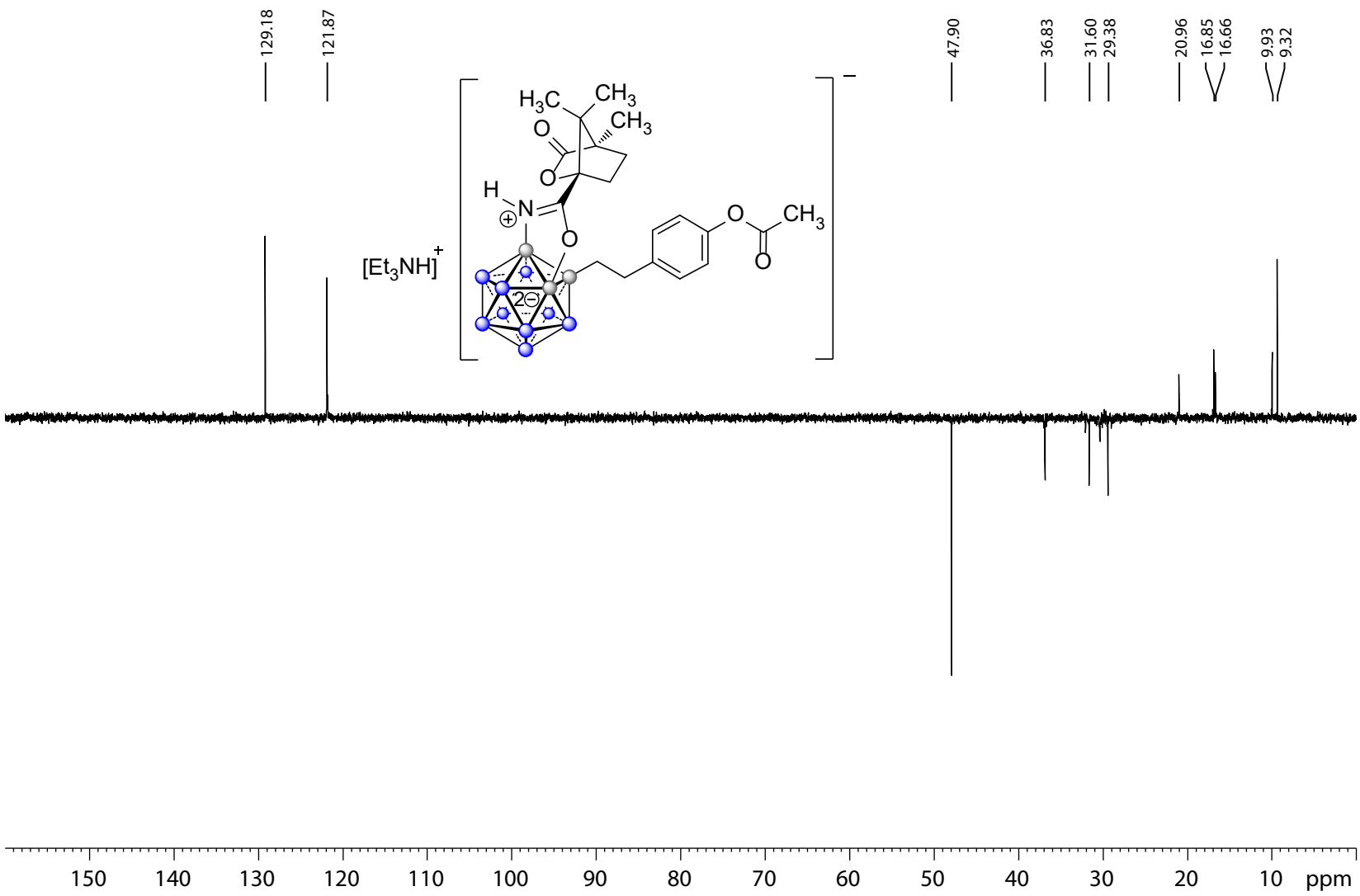
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126811 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                            6
PROCNO                           1

F2 - Acquisition Parameters
Date_                     20190927
Time                         14.38
INSTRUM                      spect
PROBHD    5 mm PABBO BB/
PULPROG                   dept135
TD                          65536
SOLVENT                   Acetone
NS                              512
DS                                4
SWH                    29296.875 Hz
FIDRES                  0.447035 Hz
AQ                      1.1184810 sec
RG                         193.34
DW                         17.067 usec
DE                           6.50 usec
TE                          296.2 K
CNST2                145.0000000
D1                     2.00000000 sec
D2                     0.00344828 sec
D12                    0.00002000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                          13C
P1                          10.00 usec
P2                          20.00 usec
PLW1                 53.00000000 W
SFO1                100.6228293 MHz

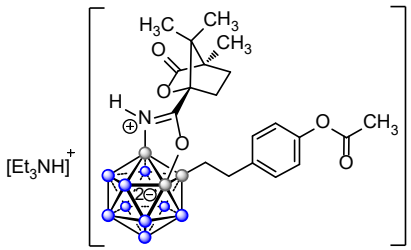
======== CHANNEL f2 ========
CPDPRG[2                 waltz16
NUC2                          1H
P3                          15.00 usec
P4                          30.00 usec
PCPD2                       80.00 usec
PLW2                 12.50000000 W
PLW12                 0.43945000 W
SFO2                400.1316005 MHz

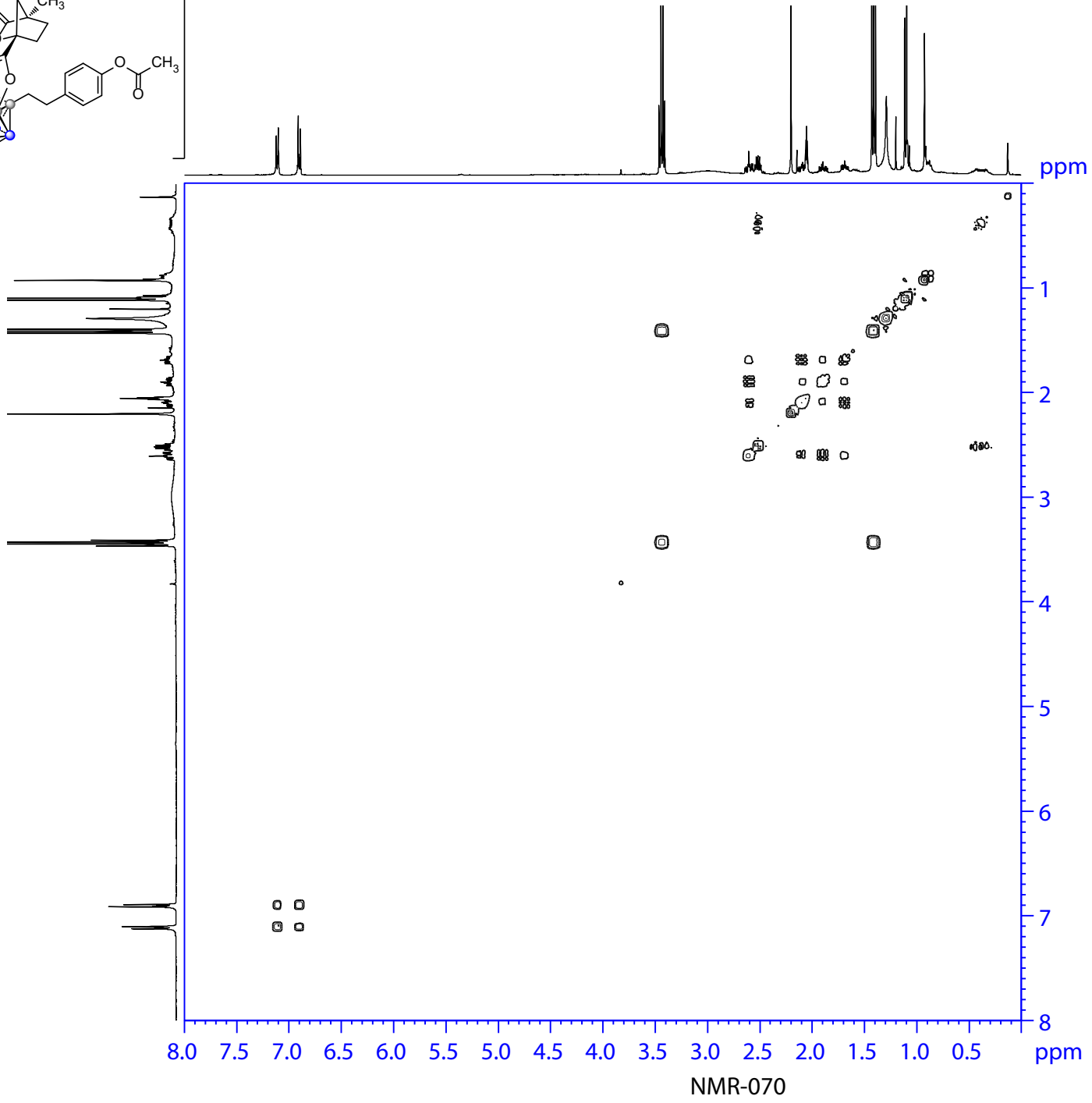
F2 - Processing parameters
SI                            32768
SF                  100.6126815 MHz
WDW                              EM
SSB               0
LB                           1.00 Hz
GB                0
PC                           4.00
```

NMR-069

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-070

Current Data Parameters
NAME 20190926-B12C-4OCOMeStyr
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190927
Time 14.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 193.34
DW 93.600 usec
DE 6.50 usec
TE 296.1 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

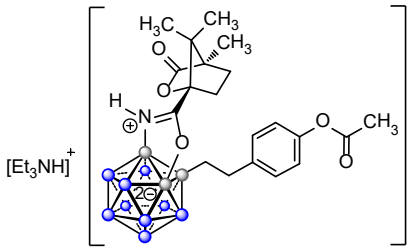
F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

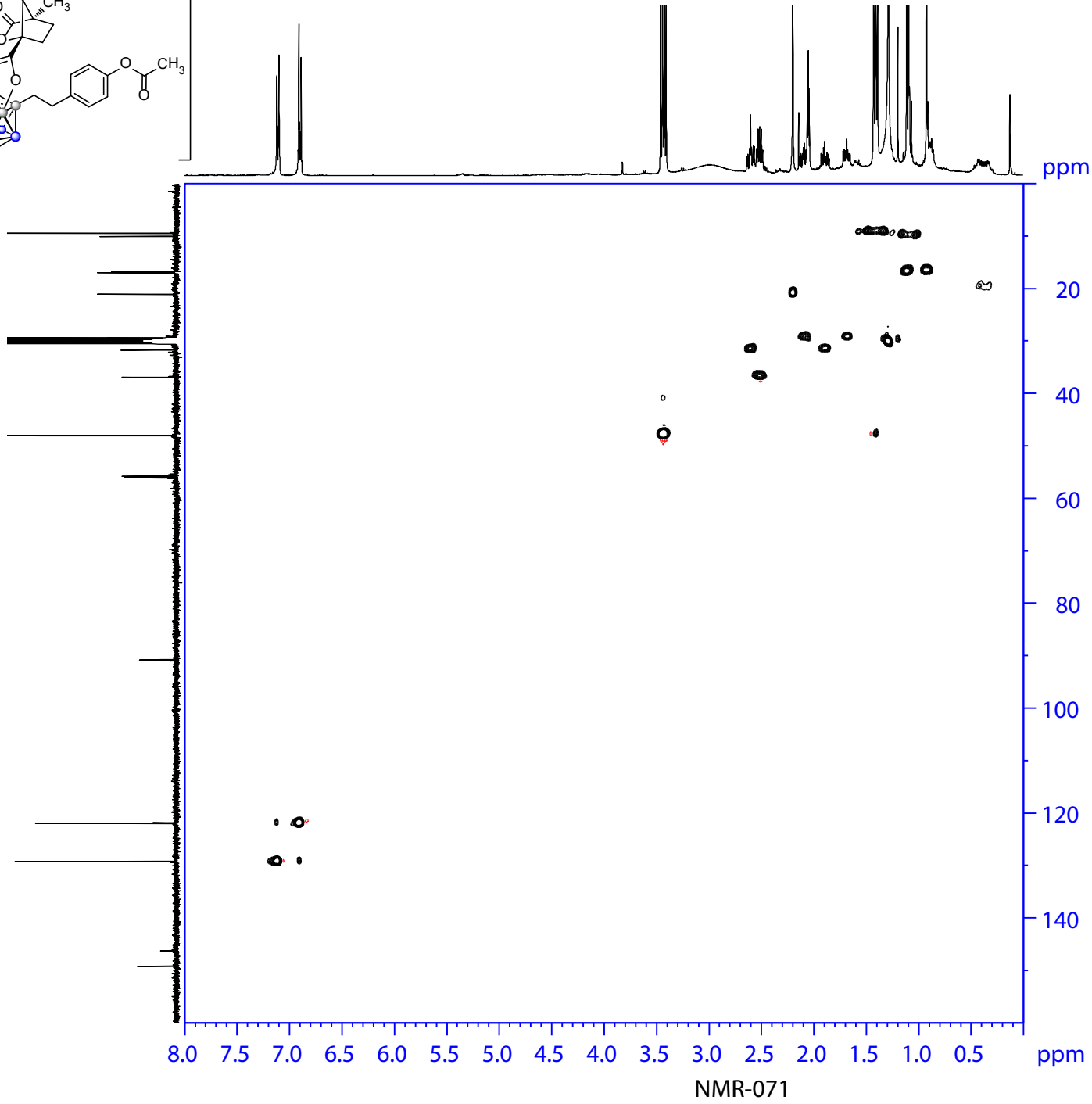
F2 - Processing parameters
SI 1024
SF 400.1300072 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300073 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

20190926-B12C-4OCOMeSTYR 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OCOMe] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR





NMR-071

```
Current Data Parameters
NAME      20190926-B12C-4OCOMeStyr
EXPNO                8
PROCNO               1

F2 - Acquisition Parameters
Date_           20190927
Time              14.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG               193.34
DW                83.200 usec
DE                 6.50 usec
TE                295.9 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2            garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

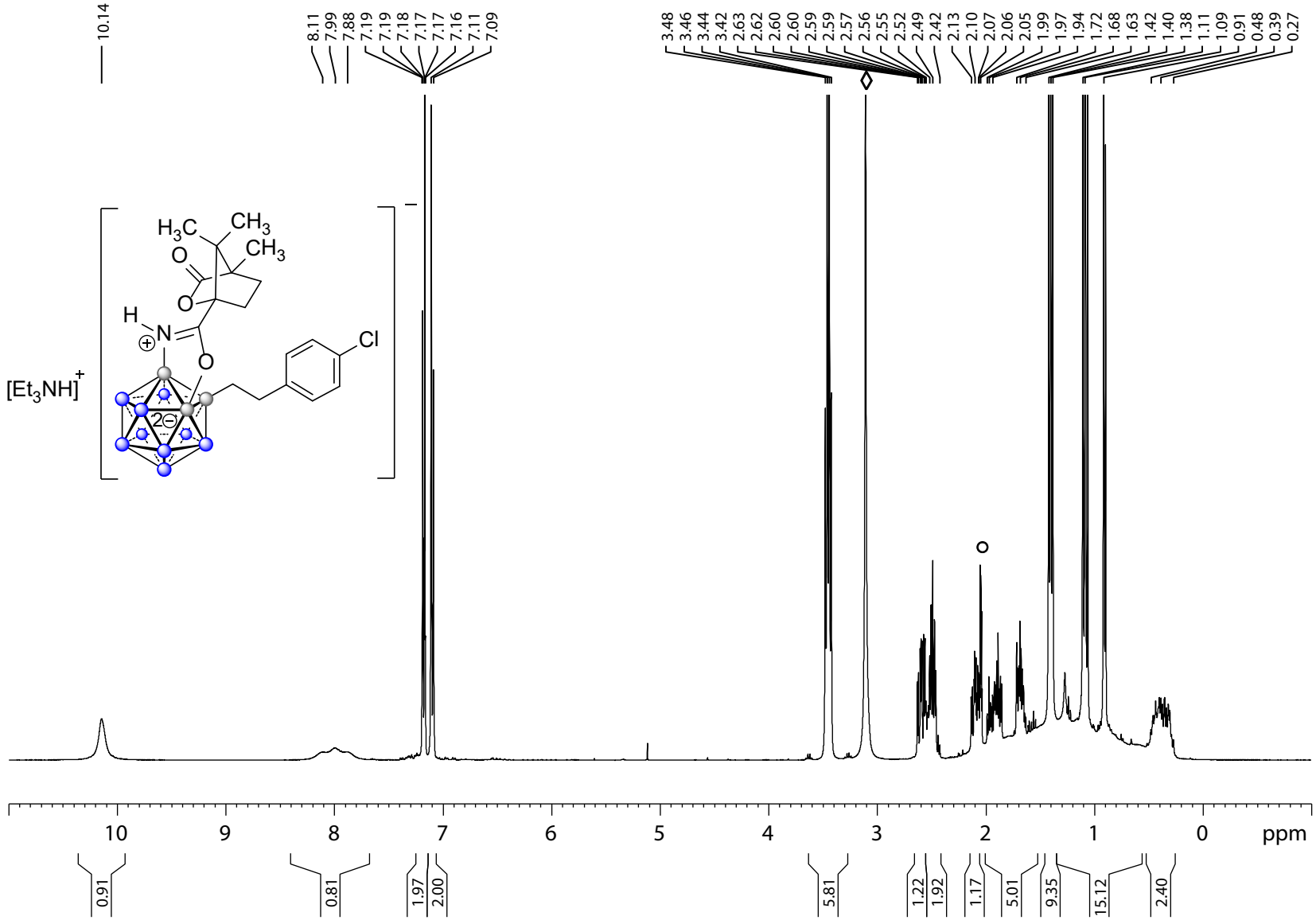
F1 - Acquisition parameters
TD                 256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300070 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126777 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

20191011-B12C-ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4Cl]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-072

```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                1
PROCNO               1

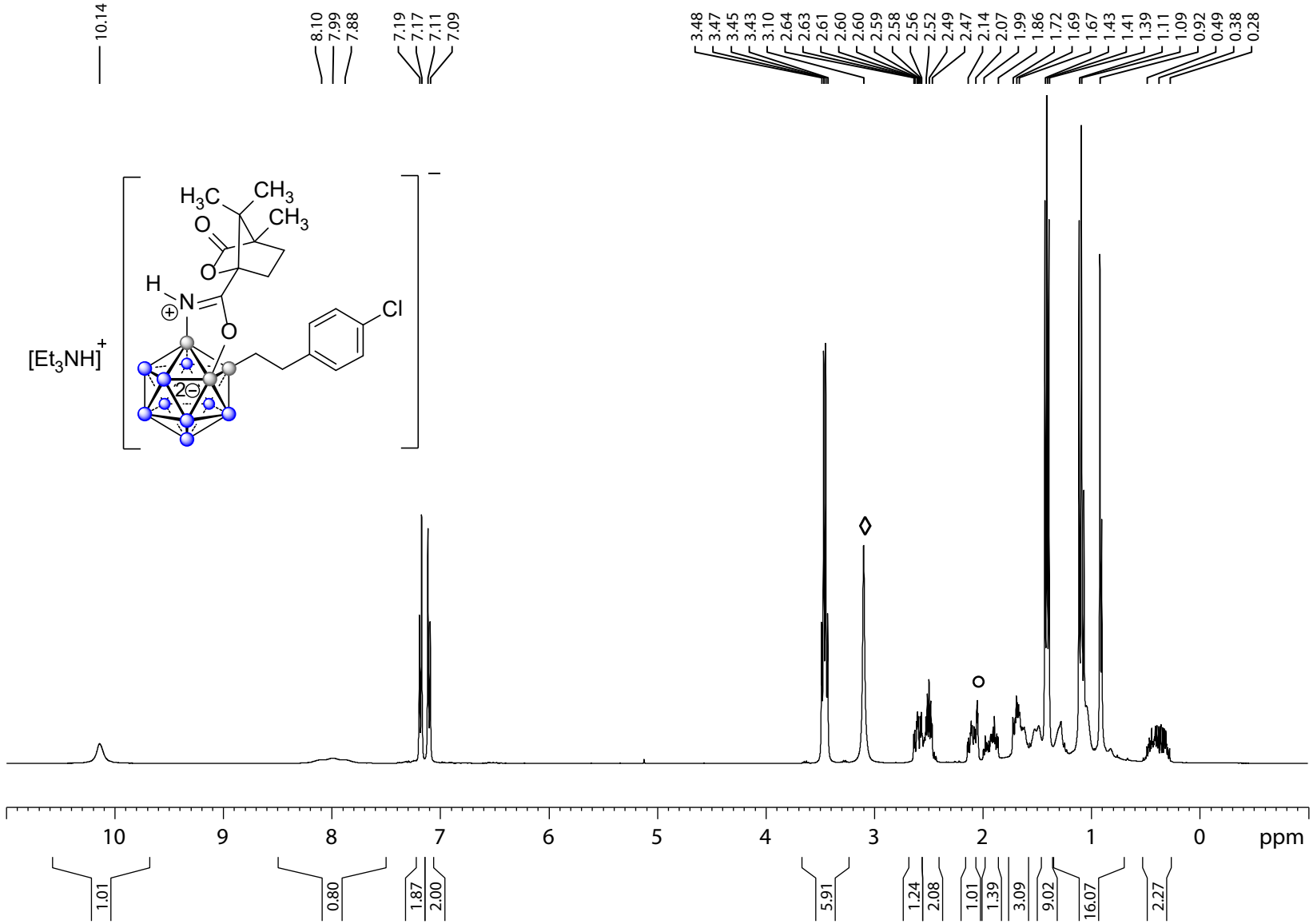
F2 - Acquisition Parameters
Date_           20191012
Time              15.03
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                52.99
DW                50.000 usec
DE                 6.50 usec
TE                295.7 K
D1             1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300092 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20191011-B12C-ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Cl] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20191012
Time              15.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ              1.0223616 sec
RG                33.25
DW                62.400 usec
DE                 6.50 usec
TE                296.1 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

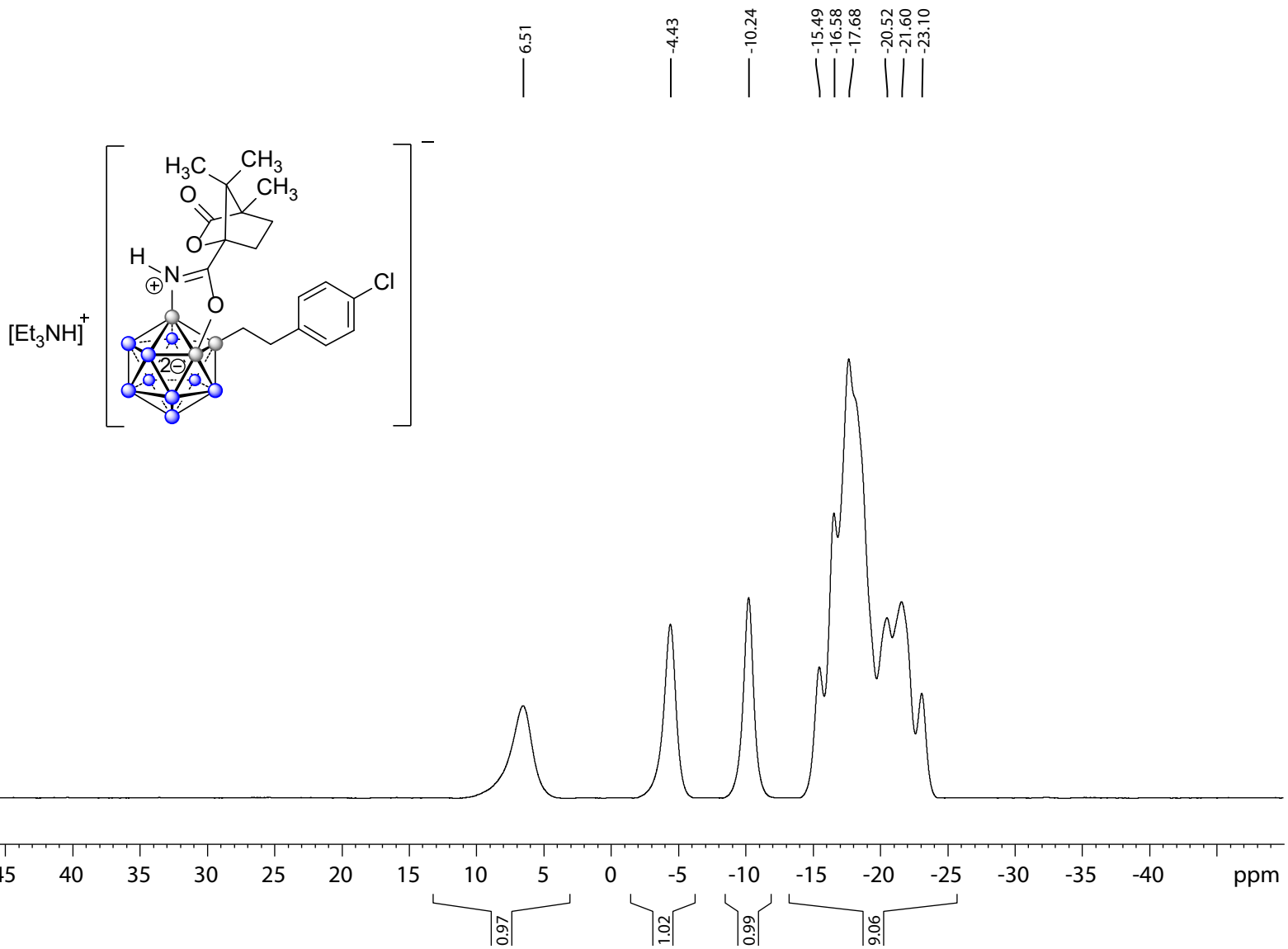
======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300074 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

NMR-073

20191011-B12C-ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4Cl]$ dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz



NMR-074

```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                3
PROCNO               1

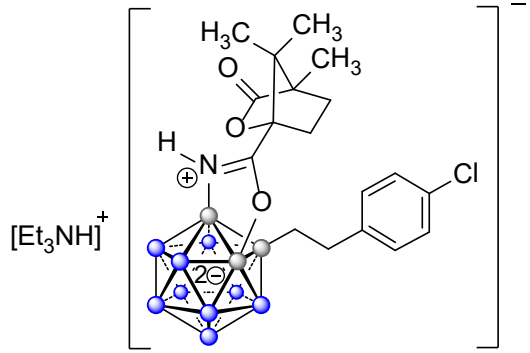
F2 - Acquisition Parameters
Date_          20191012
Time              15.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.0 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

20191011-B12C-ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Cl] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz



$[Et_3NH]^+$

NMR-075

```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20191012
Time              15.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

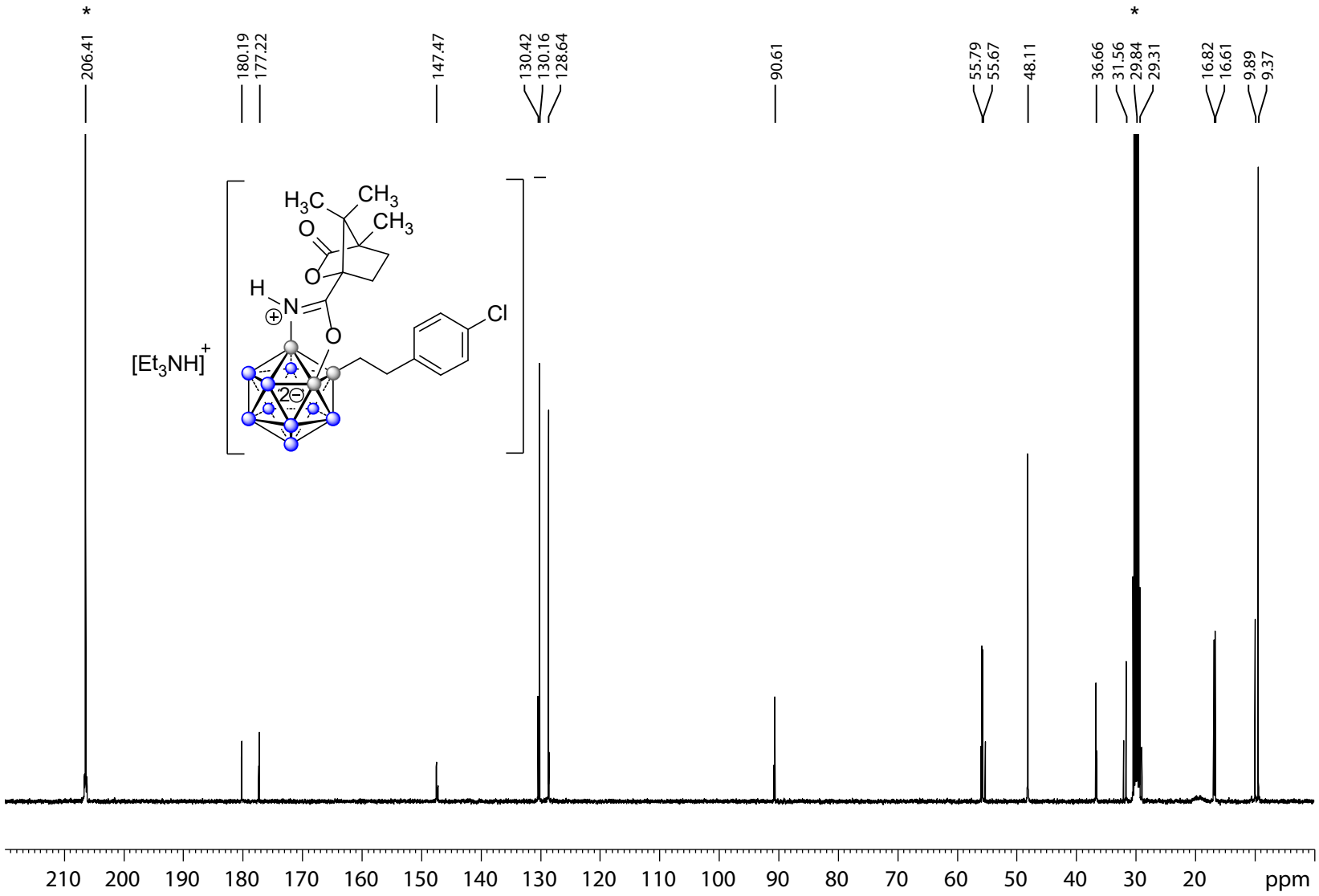
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

20191011-B12C-ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4$-4Cl] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_           20191012
Time              16.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                2048
DS                   4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG               193.34
DW                16.800 usec
DE                 6.50 usec
TE                296.6 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                  1

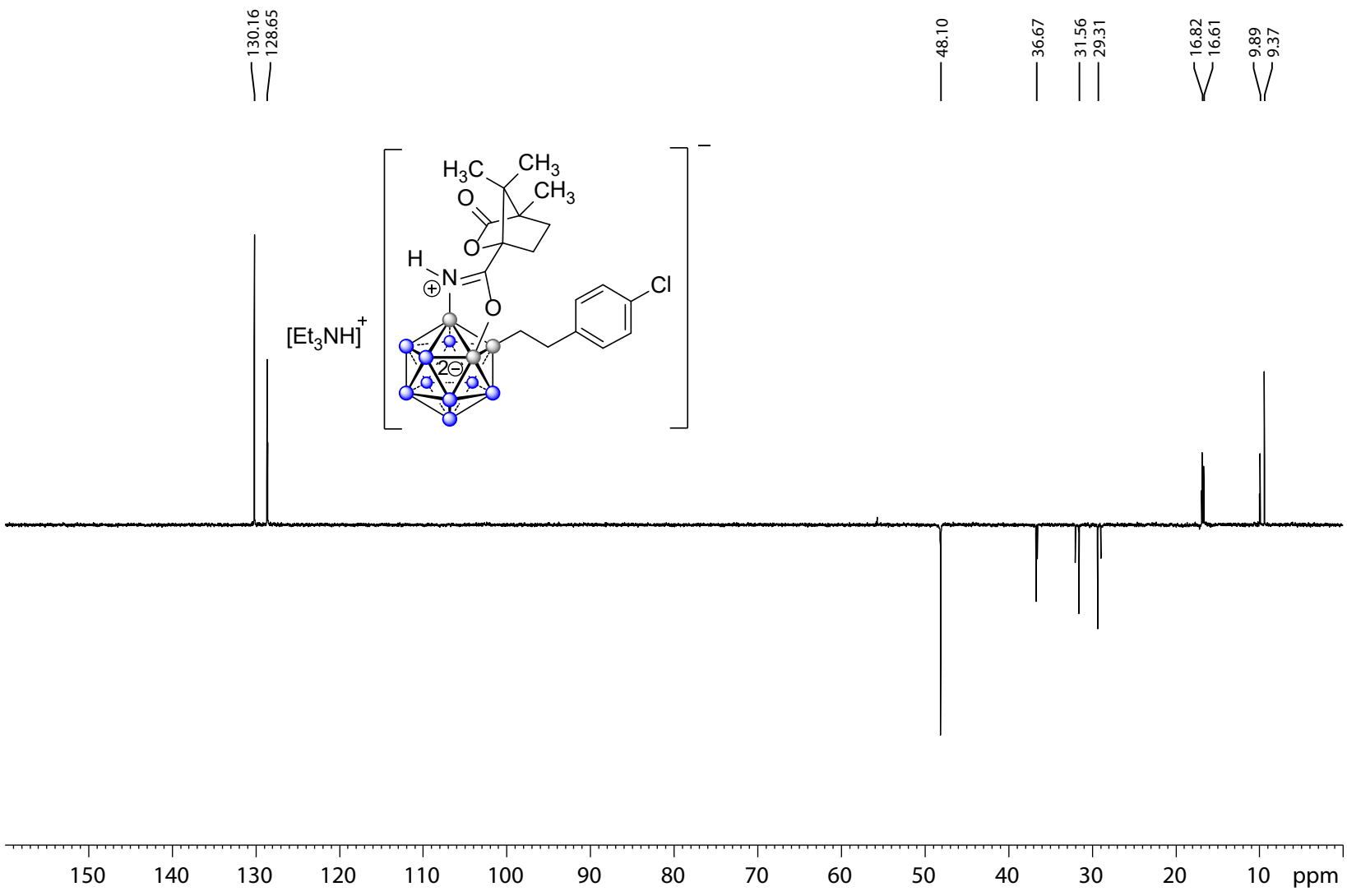
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126889 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191011-B12C-ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Me] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191012
Time               17.17
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          dept135
TD                 65536
SOLVENT          Acetone
NS                   512
DS                     4
SWH            29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                296.3 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                    1

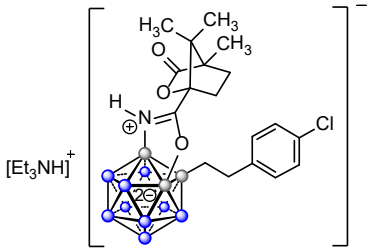
======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
P2                 20.00 usec
PLW1          53.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                  1H
P3                 15.00 usec
P4                 30.00 usec
PCPD2              80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF            100.6126887 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 4.00
```

20191011-B12C-ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4Cl$ dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR



NMR-078

```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20191012
Time              17.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT         Acetone
NS                    2
DS                    8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                95.29
DW               93.600 usec
DE                6.50 usec
TE                296.1 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1       400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

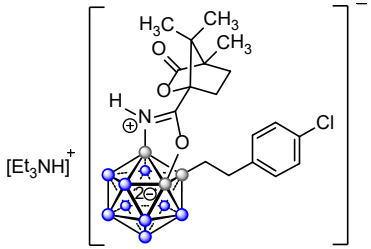
F1 - Acquisition parameters
TD                  128
SFO1          400.1324 MHz
FIDRES        83.466881 Hz
SW               13.350 ppm
FnMODE              QF

F2 - Processing parameters
SI                 1024
SF          400.1300086 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                 1024
MC2                QF
SF          400.1300080 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
```

20191011-B12C-ClStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4Cl] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR



NMR-079

```
Current Data Parameters
NAME      20191011-RV-B12C-4ClStyr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20191012
Time              17.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG               193.34
DW               83.200 usec
DE                6.50 usec
TE               296.2 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPNAM[4]     SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

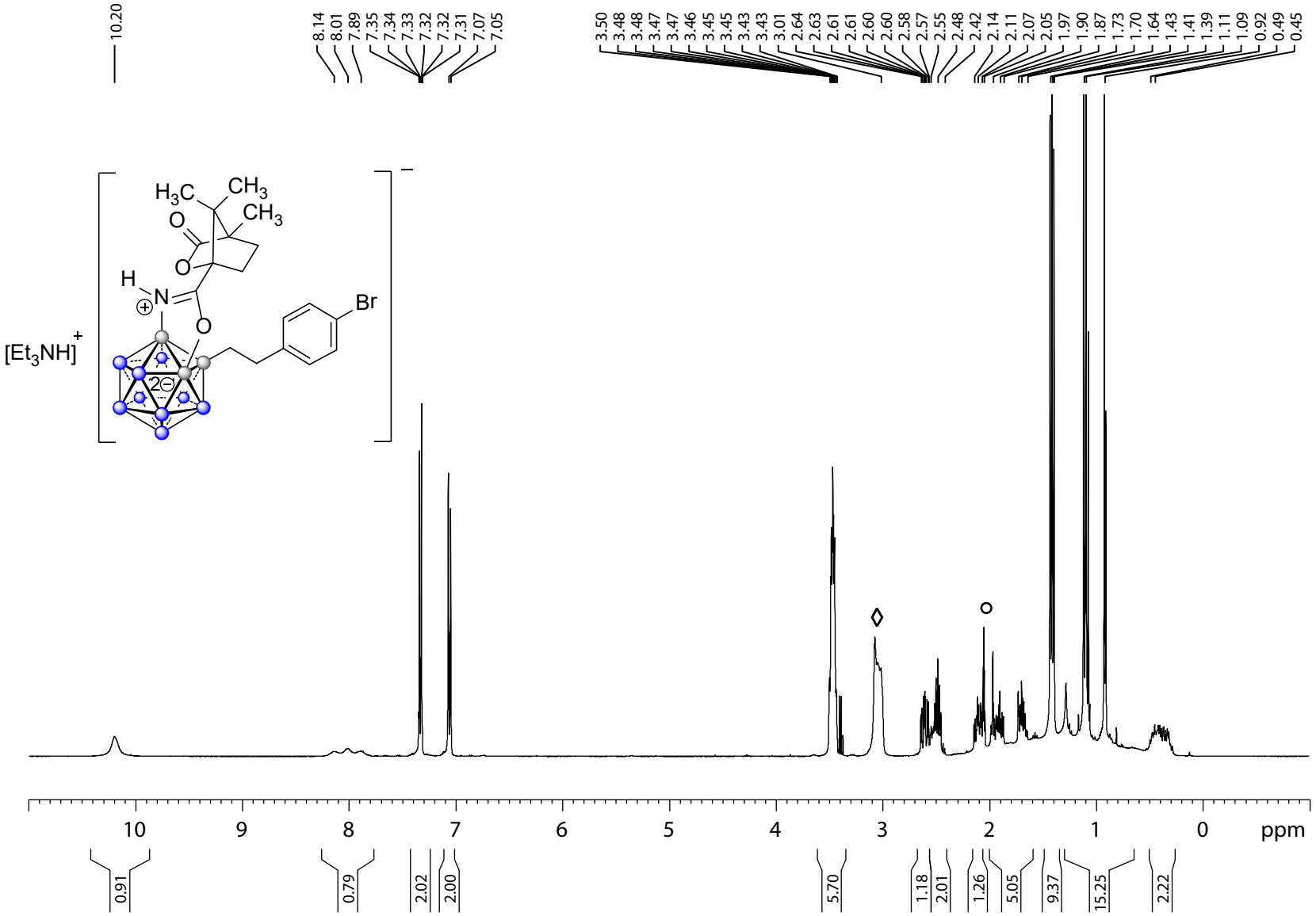
F1 - Acquisition parameters
TD                 256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300093 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126709 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

20191014-B12C-BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Br] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-080

```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                 1
PROCNO                1

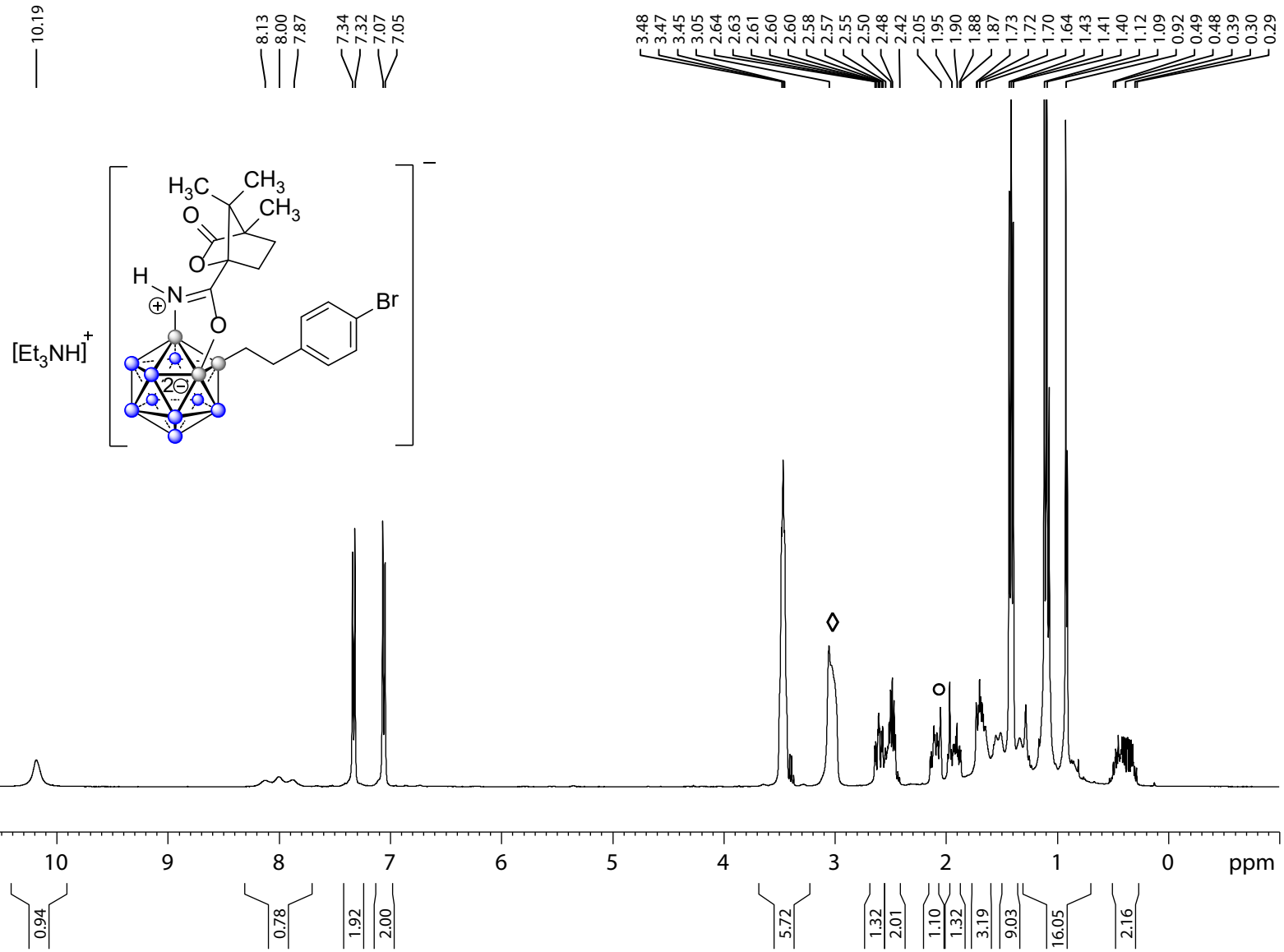
F2 - Acquisition Parameters
Date_           20191014
Time              10.06
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT        Acetone
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ             3.2767999 sec
RG                64.43
DW              50.000 usec
DE               6.50 usec
TE              296.2 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300072 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20191014-B12C-BrStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4Br]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-081

```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_           20191014
Time              10.08
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ           1.0223616 sec
RG               39.73
DW               62.400 usec
DE                6.50 usec
TE               296.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

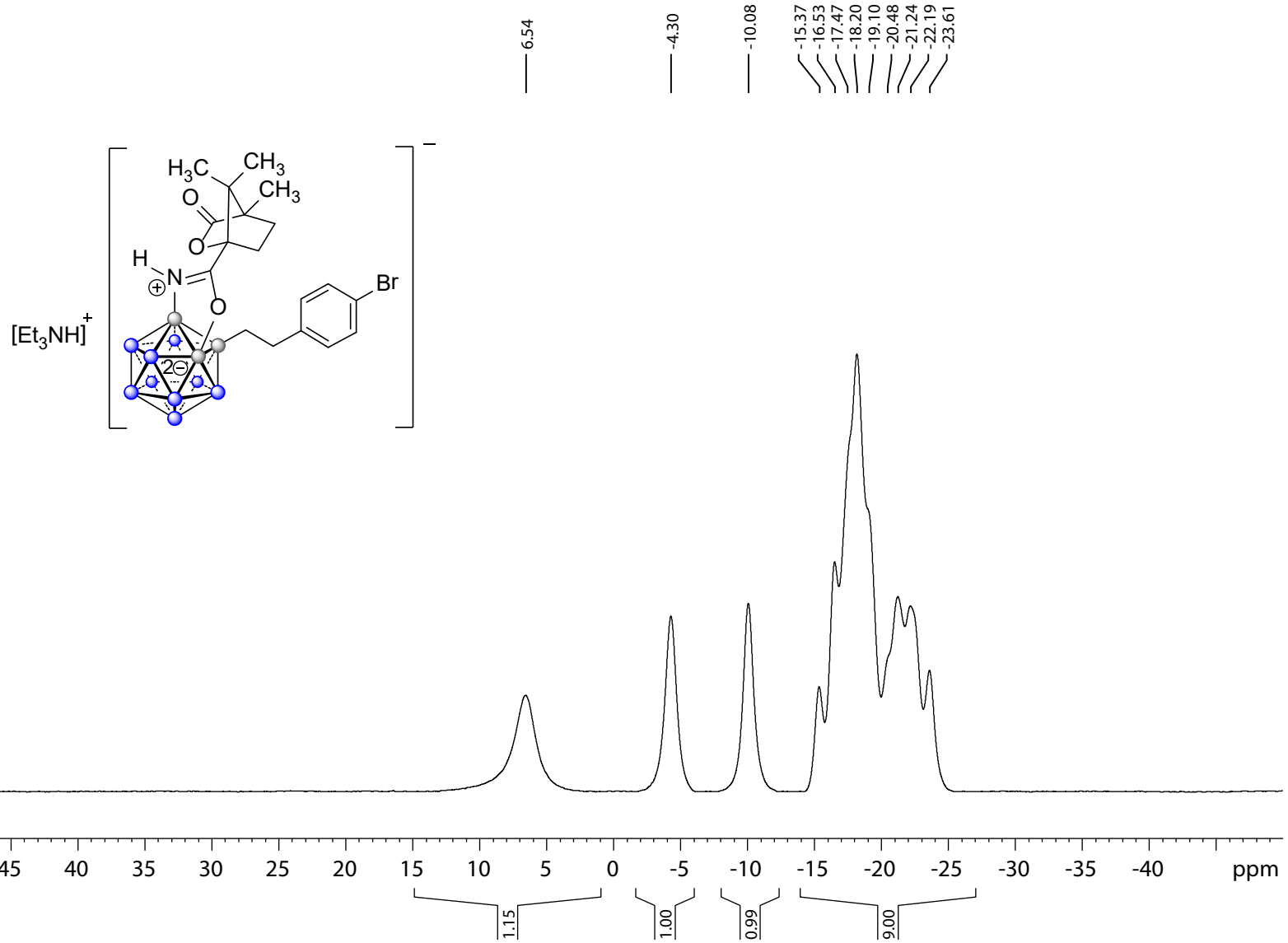
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF         400.1300073 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191014-B12C-BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Br] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                           3
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20191014
Time                        10.14
INSTRUM                     spect
PROBHD   5 mm PABBO BB/
PULPROG                        zg
TD                          65536
SOLVENT                   Acetone
NS                            128
DS                              4
SWH                     25510.203 Hz
FIDRES                   0.389255 Hz
AQ                      1.2845056 sec
RG                         193.34
DW                         19.600 usec
DE                          6.50 usec
TE                         295.7 K
D1                    1.00000000 sec
TD0                             1

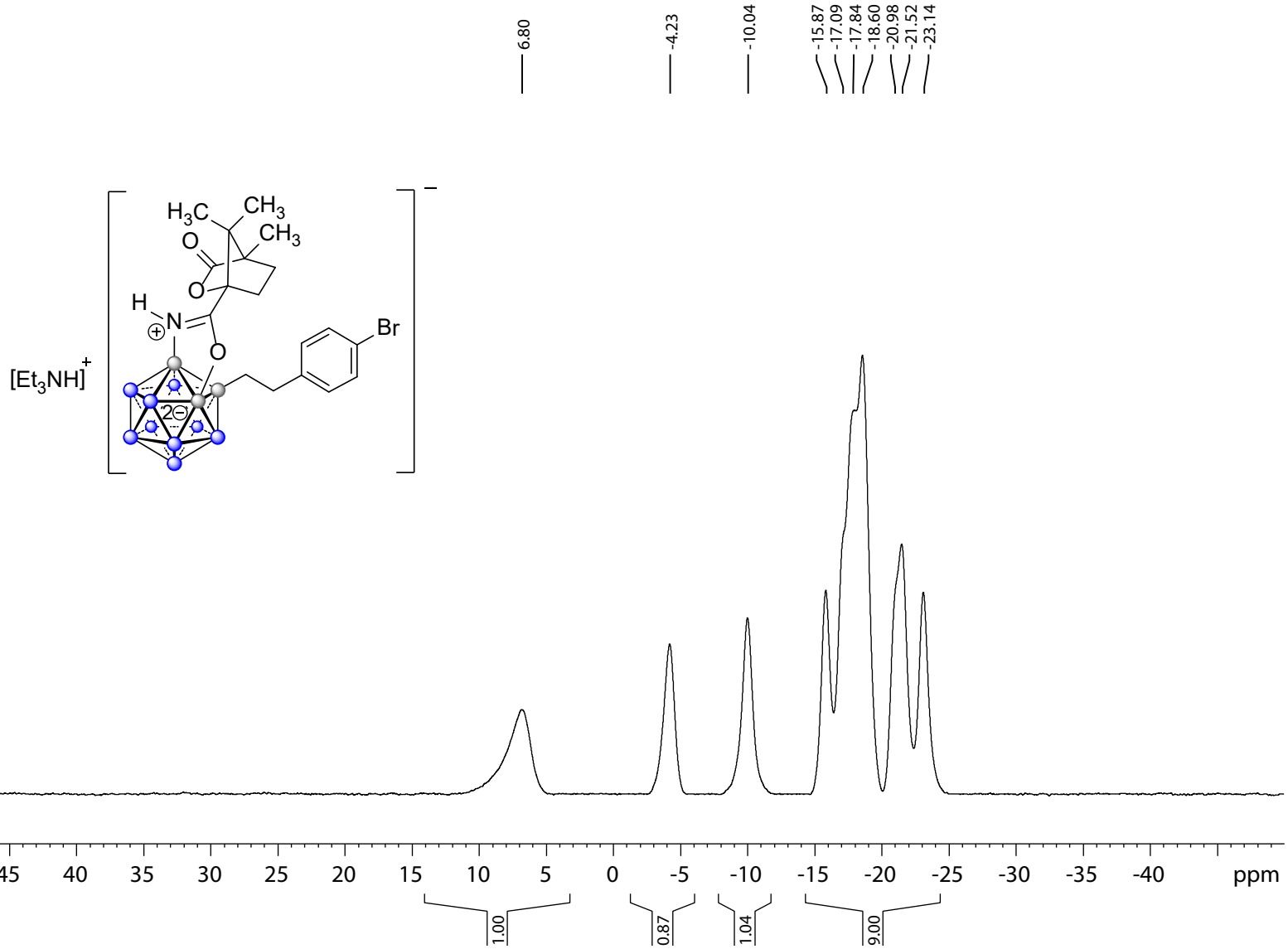
======== CHANNEL f1 ========
NUC1                          11B
P1                           9.93 usec
PLW1                52.96599960 W
SFO1               128.3776052 MHz

F2 - Processing parameters
SI                            32768
SF                 128.3776050 MHz
WDW                            EM
SSB                0
LB                          10.00 Hz
GB                 0
PC                           1.40
```

NMR-082

20191014-B12C-BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Br] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191014
Time               10.20
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

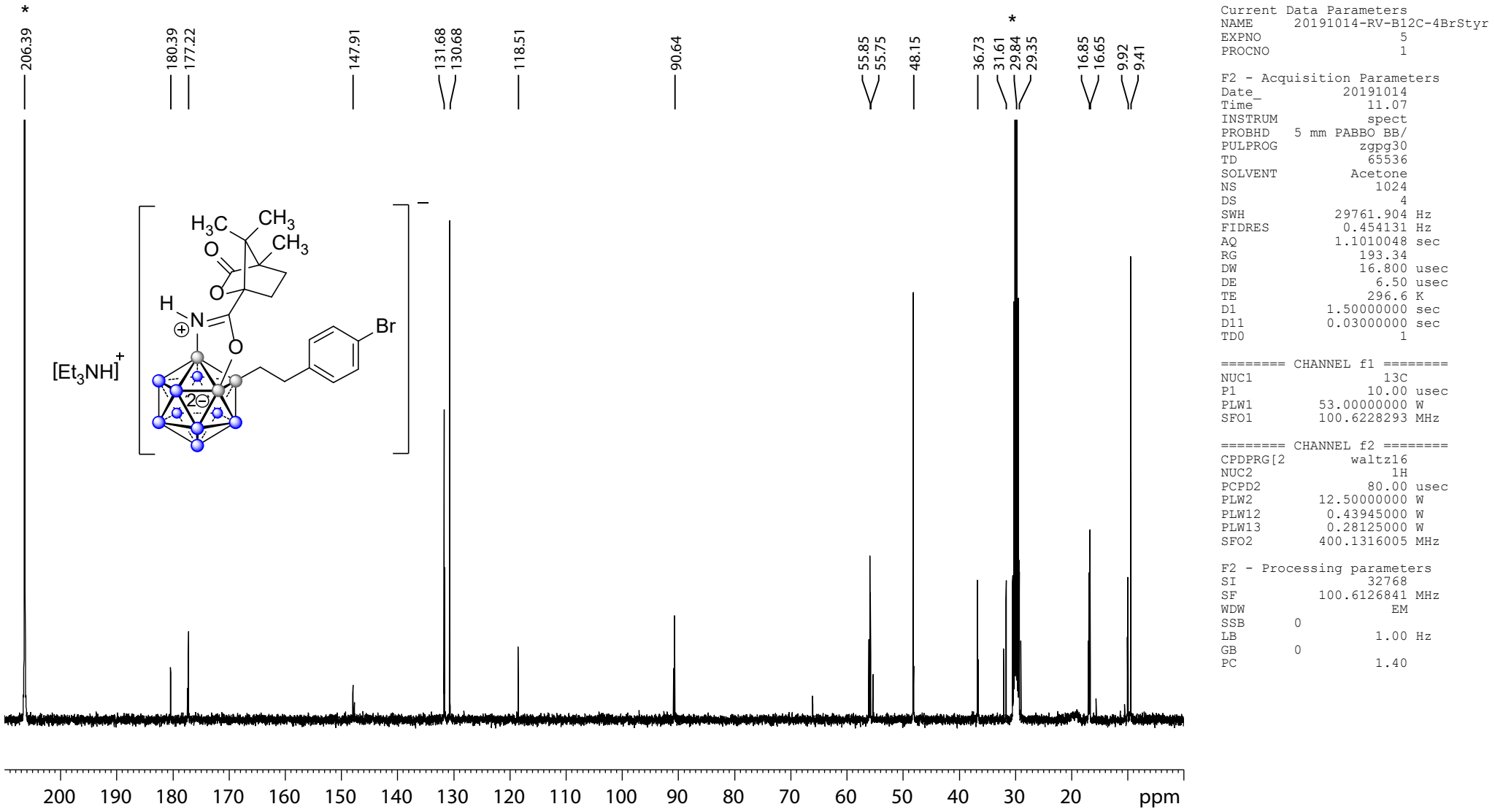
======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB               10.00 Hz
GB        0
PC                1.40
```

NMR-083

20191014-B12C-BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Br] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191014
Time              11.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE                296.6 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

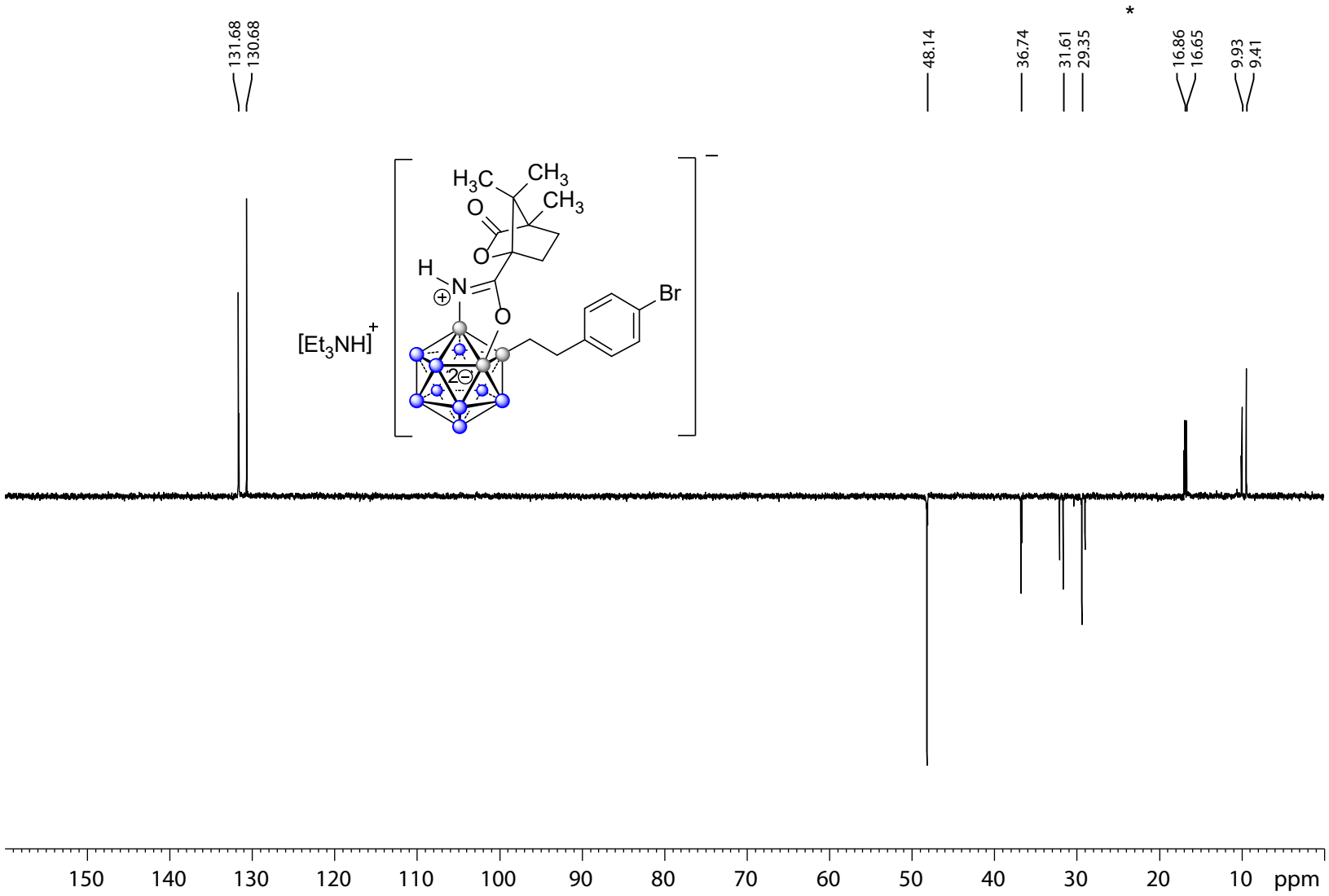
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126841 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191014-B12C-BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4Br] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191014
Time              11.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.4 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

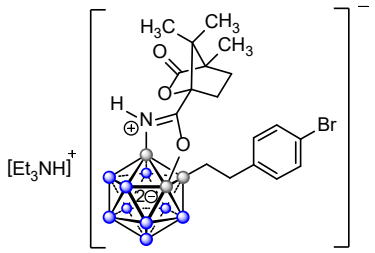
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

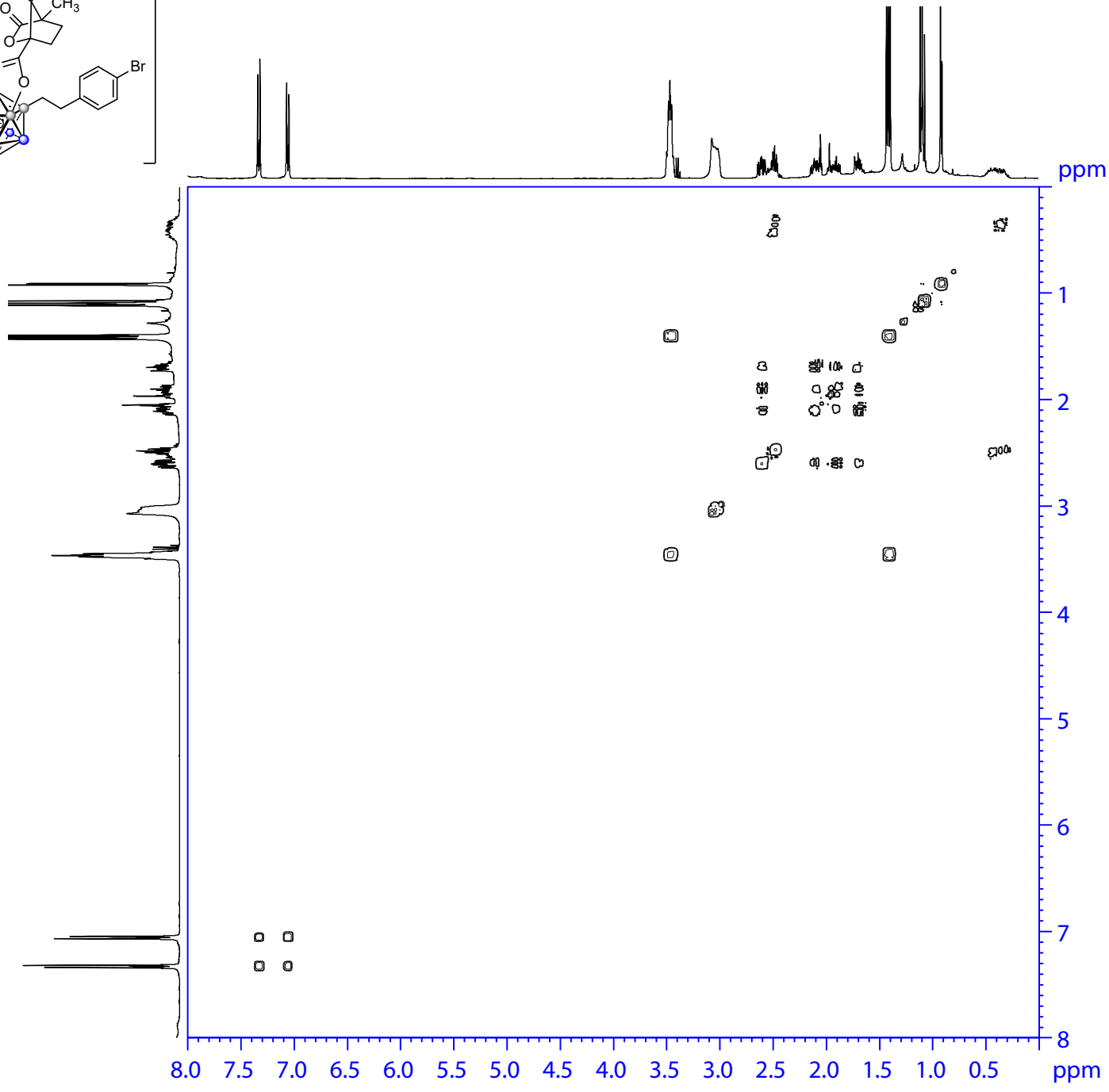
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126838 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20191014-B12C-BrStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4Br] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹H COSY NMR





NMR-086

```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20191014
Time              11.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG               124.48
DW                93.600 usec
DE                 6.50 usec
TE                295.9 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                 15.00 usec
P1                 15.00 usec
P17              2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

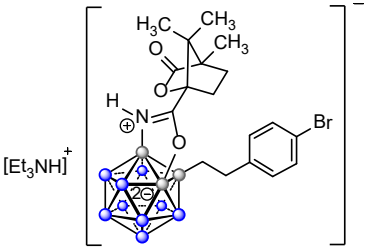
F1 - Acquisition parameters
TD                   128
SFO1            400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE               QF

F2 - Processing parameters
SI                  1024
SF           400.1300100 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300094 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
```

20191014-B12C-BrStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4Br] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR



NMR-087

```
Current Data Parameters
NAME      20191014-RV-B12C-4BrStyr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20191014
Time              11.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG               193.34
DW                83.200 usec
DE                 6.50 usec
TE                296.2 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1             80.00 %
GPZ2             20.10 %
GPZ3             11.00 %
GPZ4             -5.00 %
P16            1000.00 usec
P19             600.00 usec

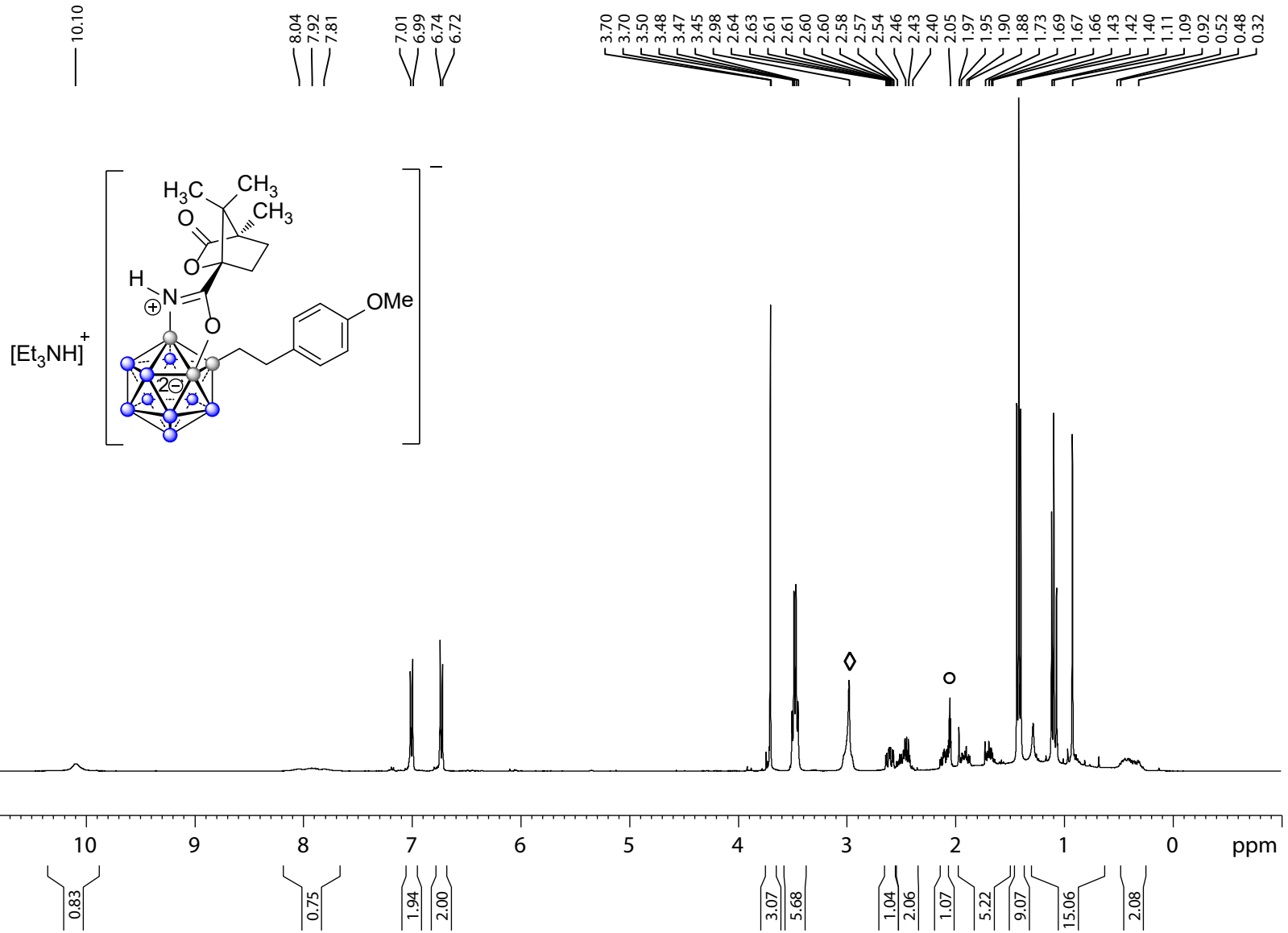
F1 - Acquisition parameters
TD                 256
SFO1          100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300024 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126691 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

20191020-B12C-OMeStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4OMe]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-088

```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 1
PROCNO                1

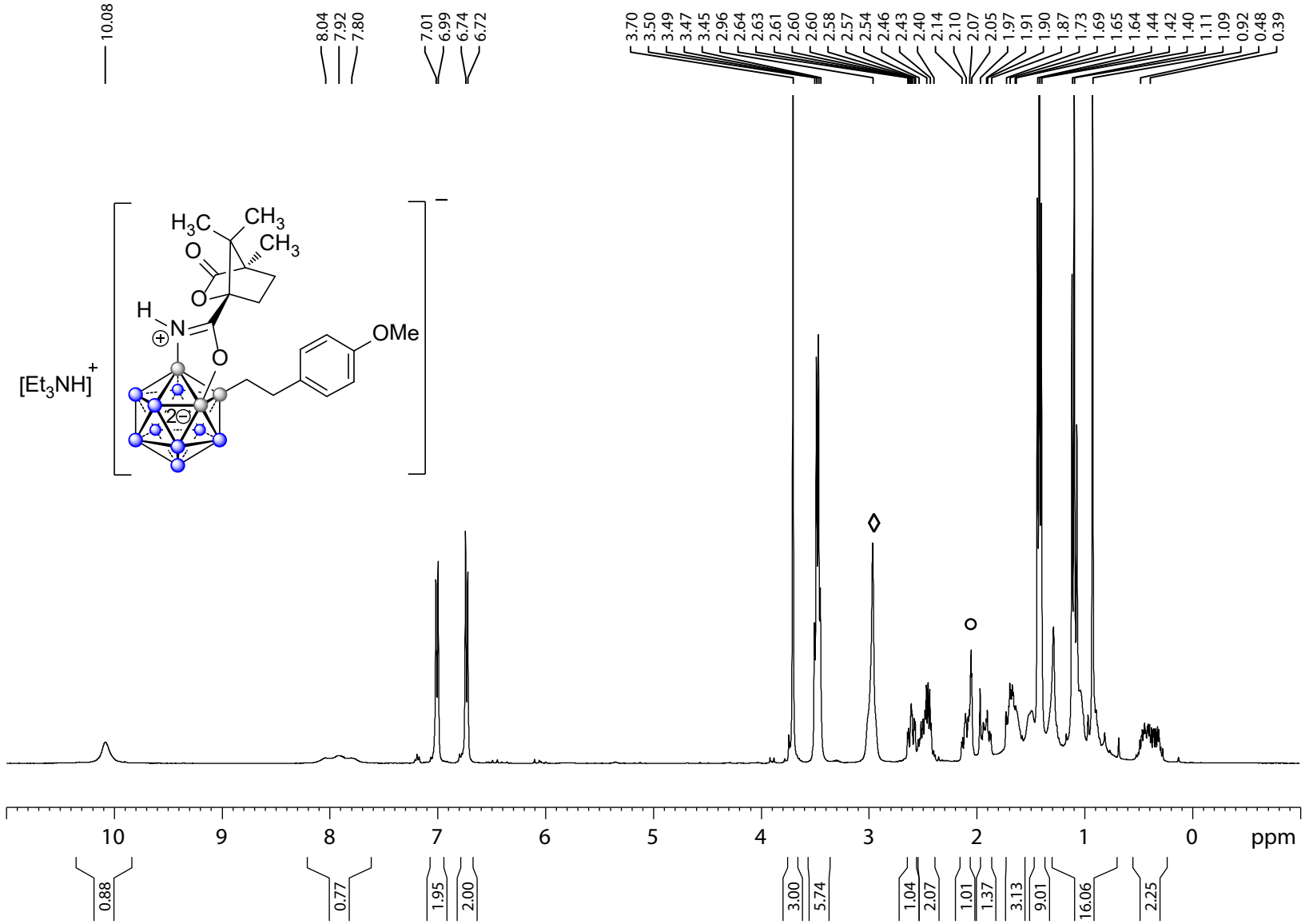
F2 - Acquisition Parameters
Date_           20191021
Time                0.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 78.69
DW                50.000 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300071 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-089

```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20191021
Time              0.38
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG               71.39
DW              62.400 usec
DE               6.50 usec
TE              296.6 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

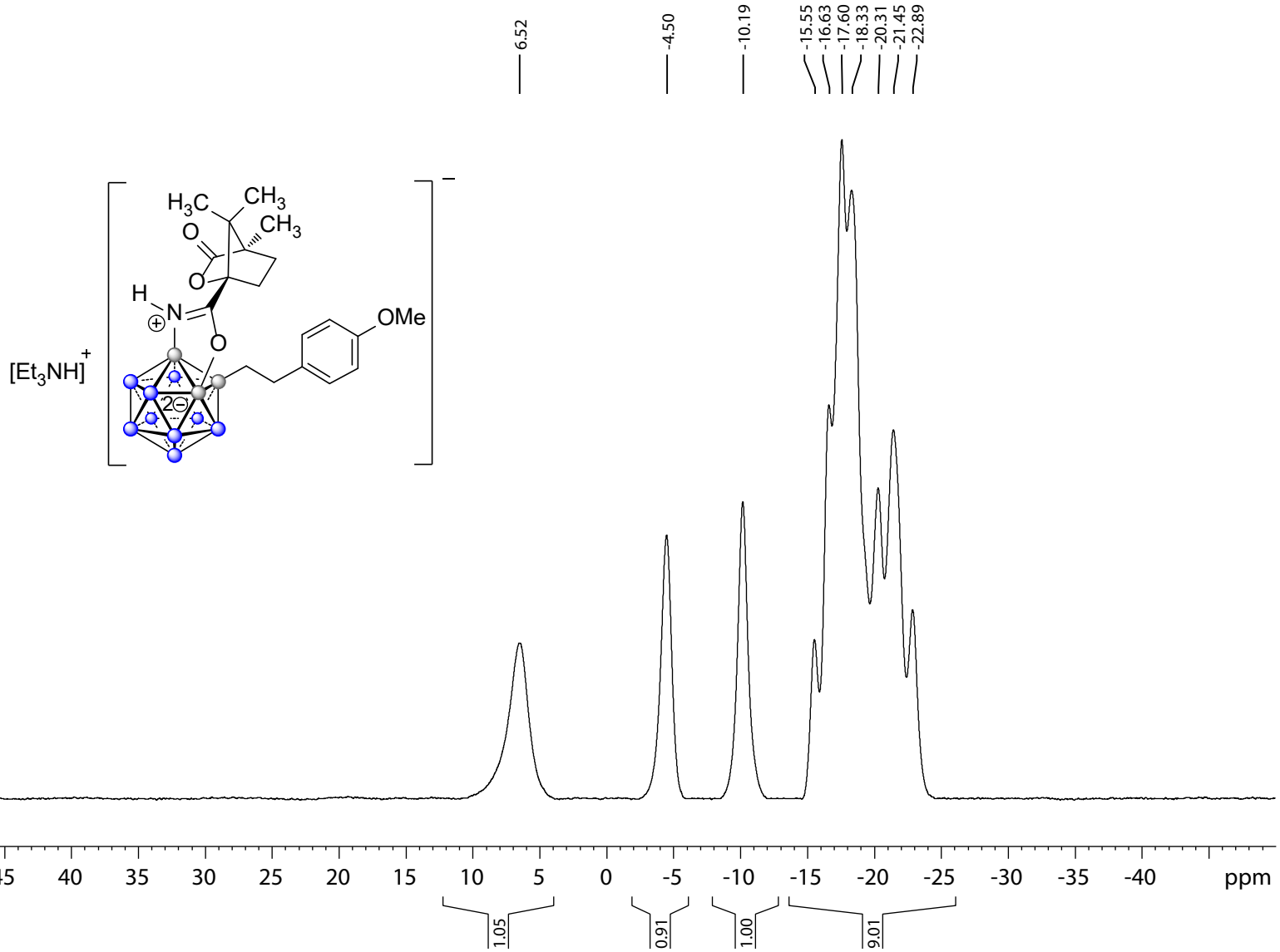
======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PLW1       12.50000000 W
SFO1      400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2           90.00 usec
PLW2       52.96599960 W
PLW12       0.64477998 W
SFO2      128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300075 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20191021
Time                0.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.6 K
D1             1.00000000 sec
TD0                    1

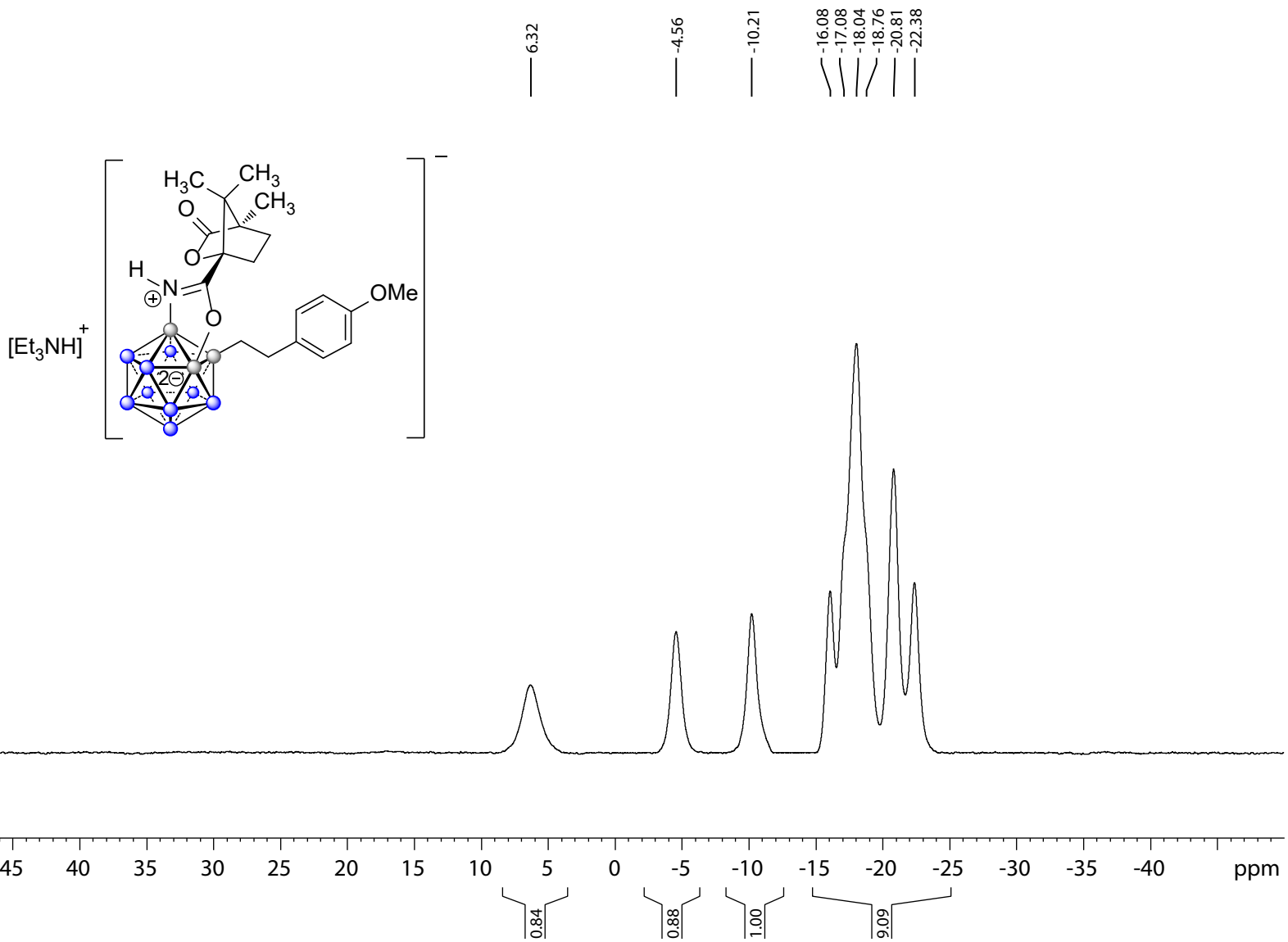
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1         128.3776052 MHz

F2 - Processing parameters
SI                 32768
SF           128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-090

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20191021
Time               0.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

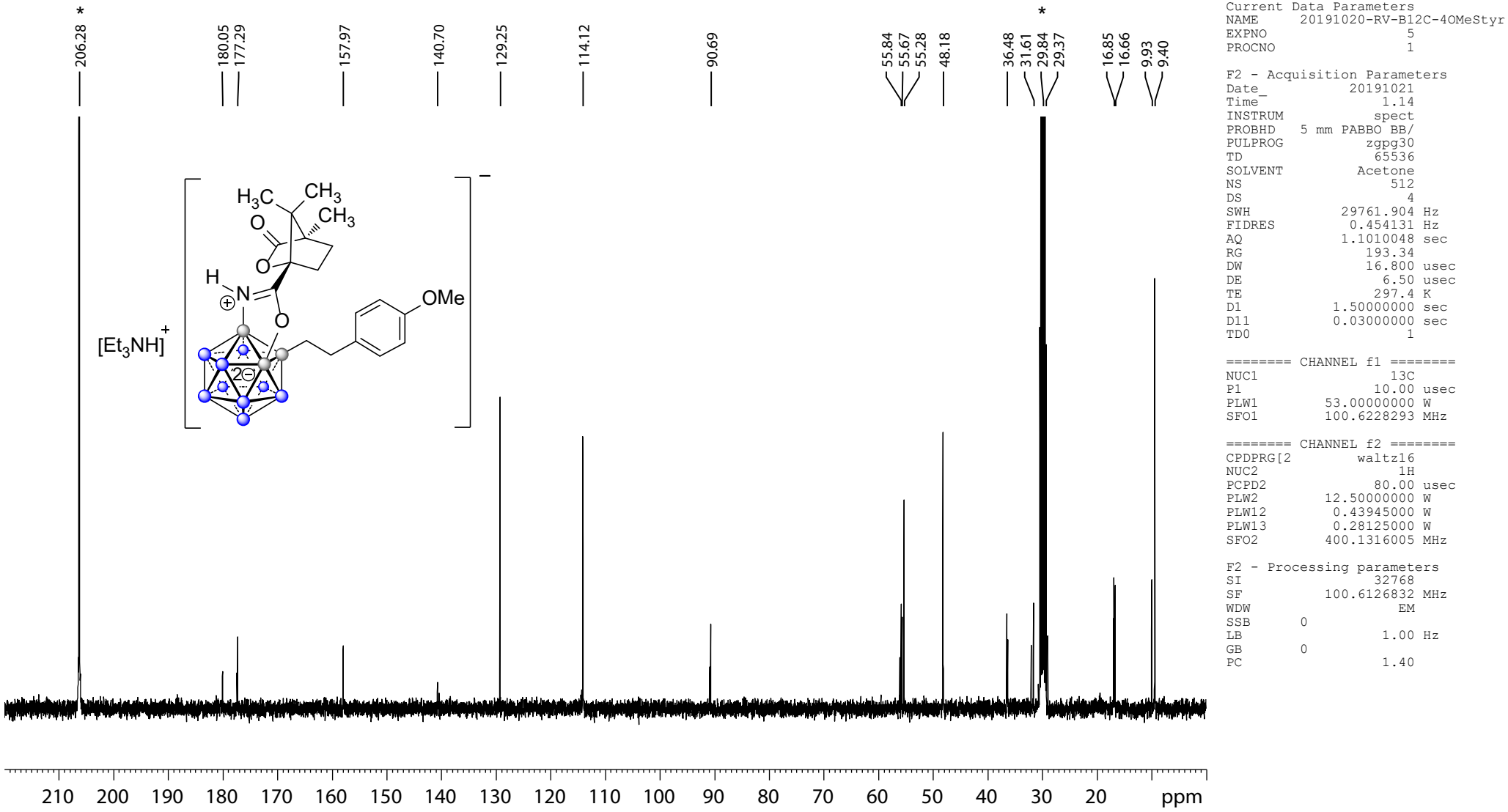
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-091

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20191021
Time_              1.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               297.4 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

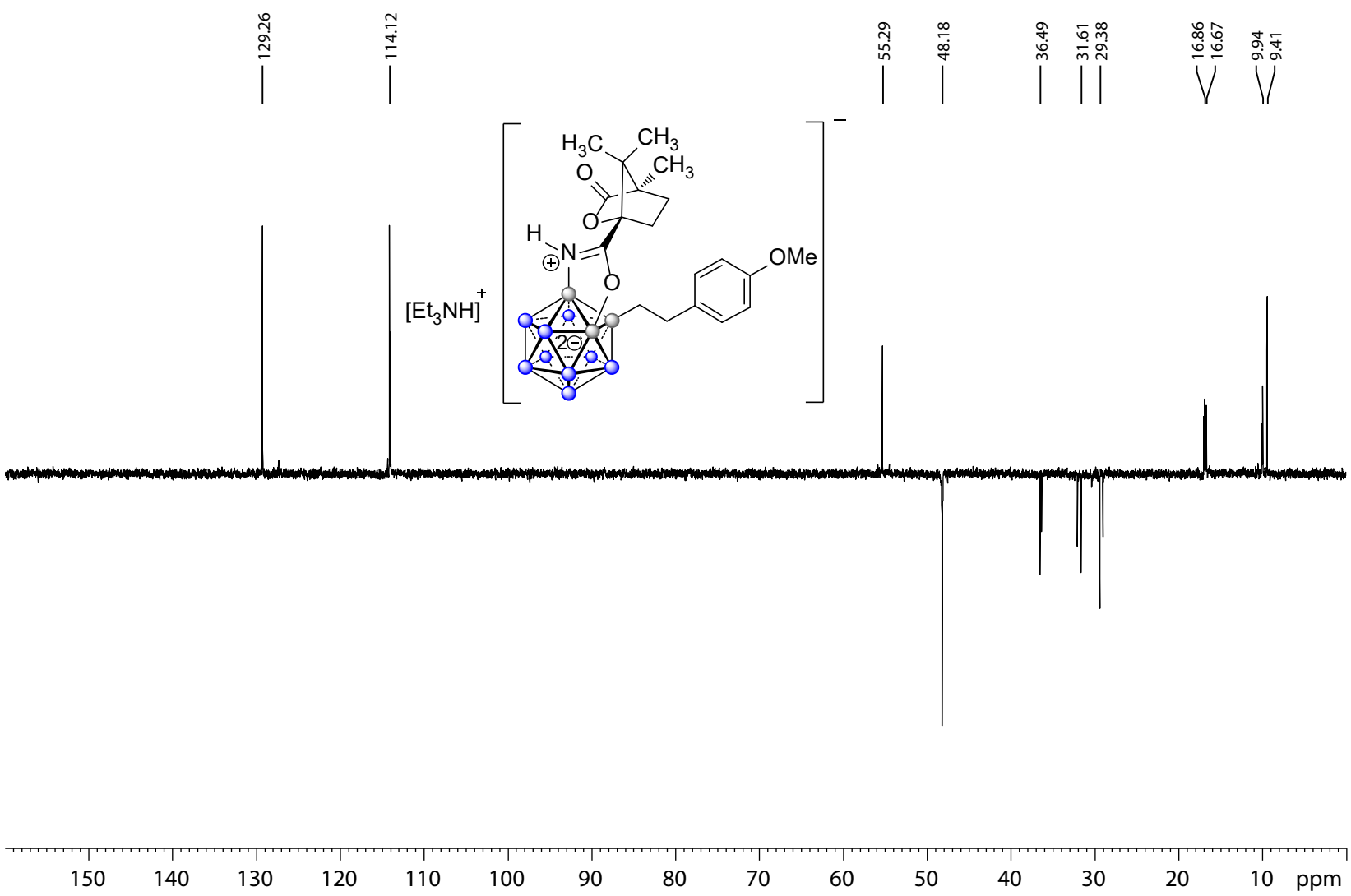
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126832 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20191021
Time               1.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.9 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

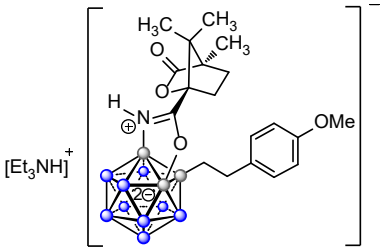
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126823 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20191020-B12C-OMeStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHCO(Camphanic)CH₂CH₂C₆H₄-4OMe] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹H COSY NMR




```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20191021
Time              1.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH           5341.880 Hz
FIDRES        2.608340 Hz
AQ            0.1916928 sec
RG               152.18
DW                93.600 usec
DE                 6.50 usec
TE                296.7 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1        400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1             10.00 %
P16            1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1          400.1324 MHz
FIDRES        83.466881 Hz
SW               13.350 ppm
FnMODE              QF

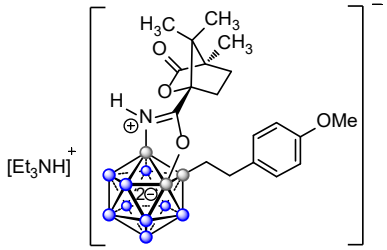
F2 - Processing parameters
SI                 1024
SF          400.1300082 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

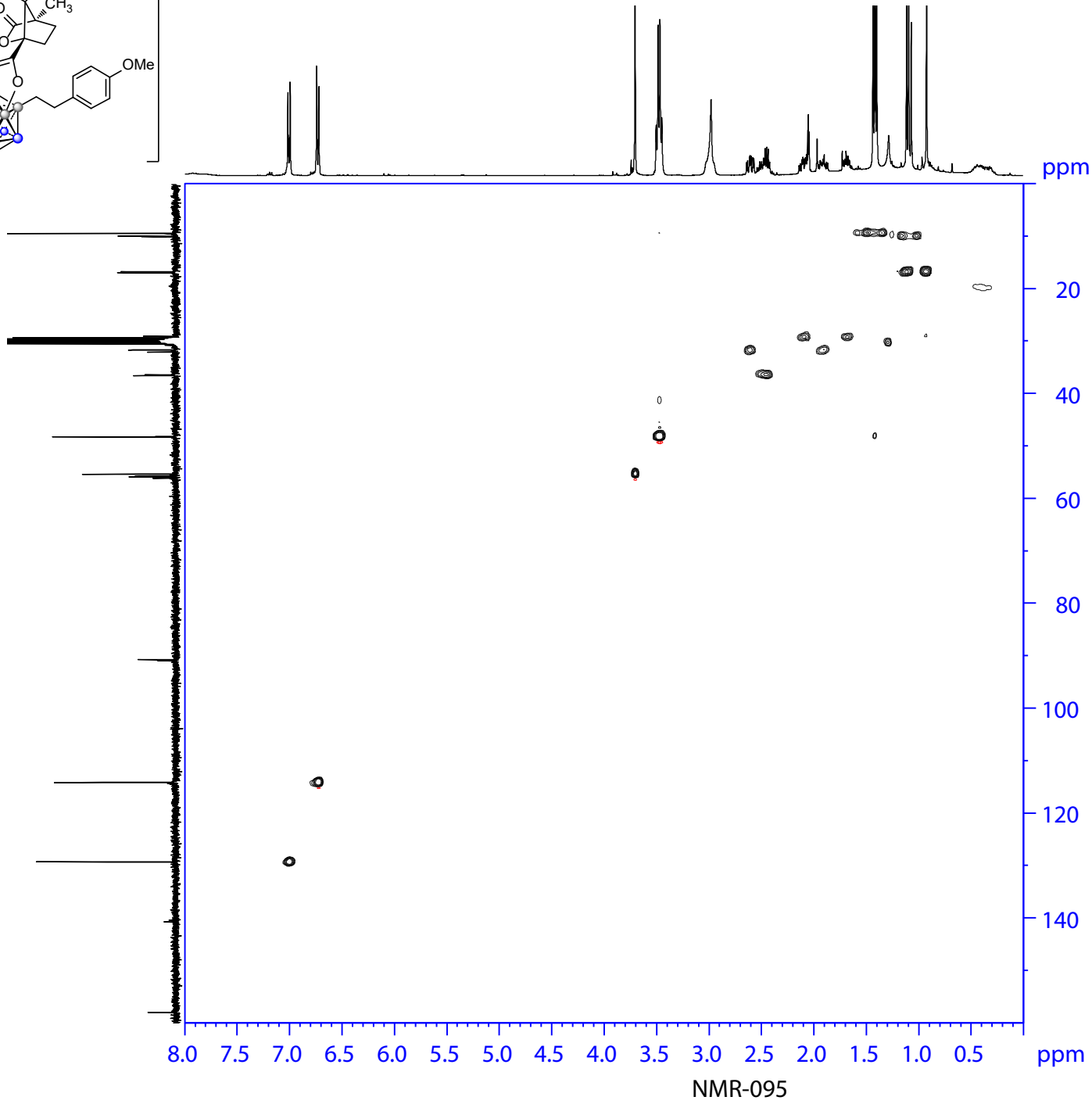
F1 - Processing parameters
SI                 1024
MC2                 QF
SF          400.1300071 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
```

NMR-094

20191020-B12C-OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4OMe] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR





NMR-095

```
Current Data Parameters
NAME      20191020-RV-B12C-4OMeStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20191021
Time               1.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                296.7 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
P28              1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

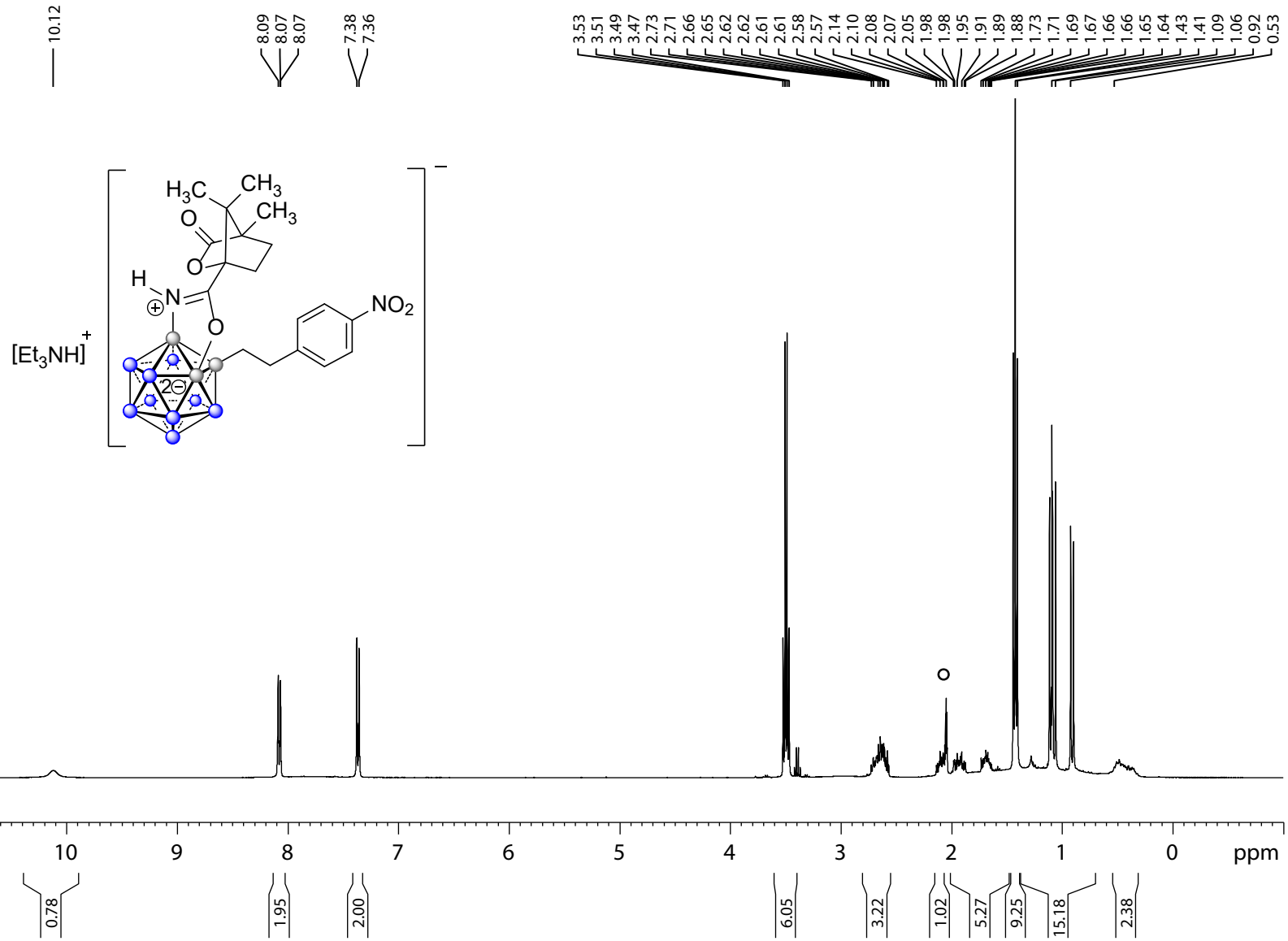
F1 - Acquisition parameters
TD                  256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300085 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2       echo-antiecho
SF          100.6126714 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
```

20191020-B12C-NO2Styr 40 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-096

```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                1
PROCNO               1

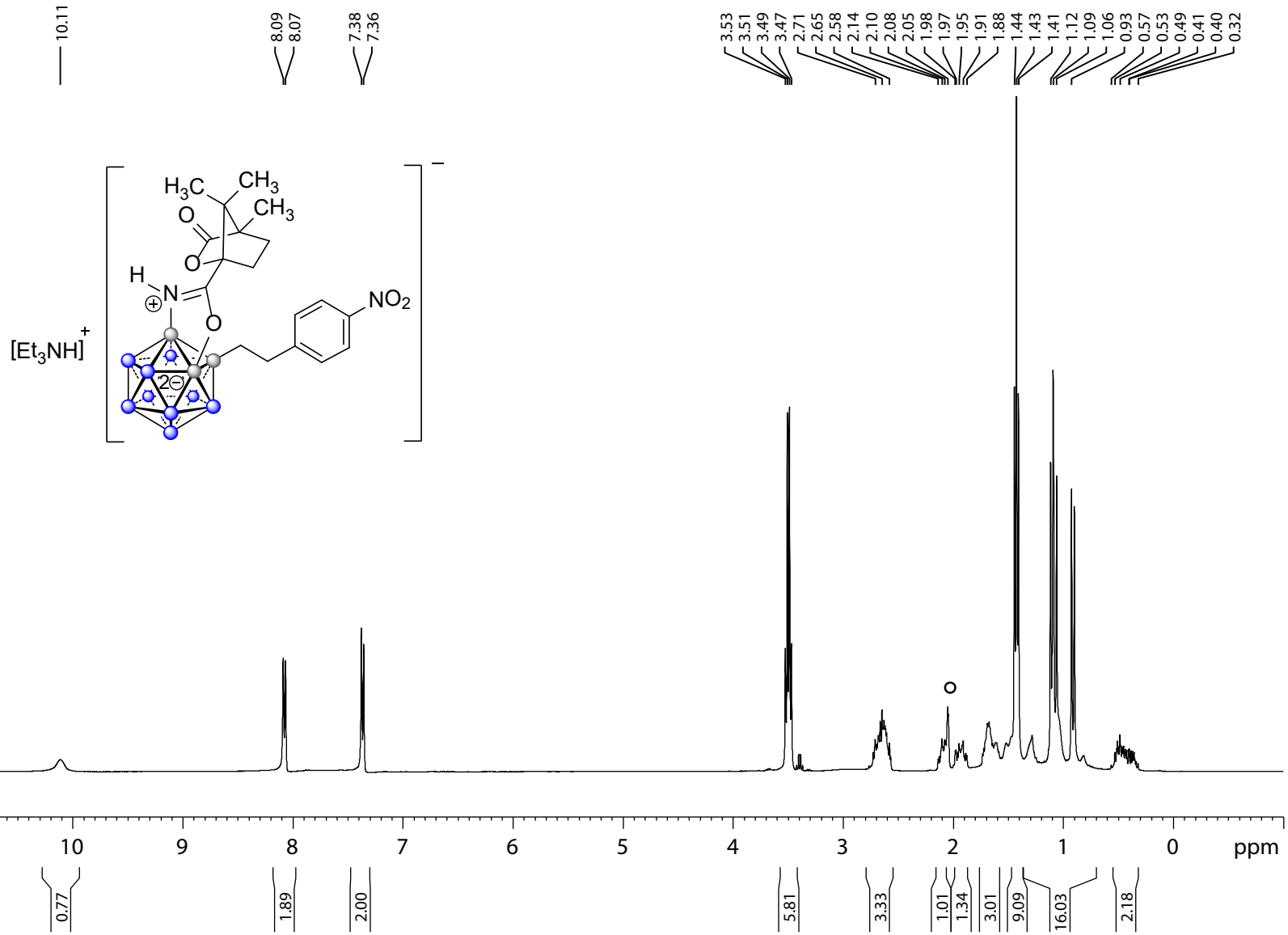
F2 - Acquisition Parameters
Date_           20191024
Time              14.36
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                86.58
DW               50.000 usec
DE                6.50 usec
TE                295.8 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300071 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20191020-B12C-NO2Styr 40 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-097

```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                2
PROCNO               1

F2 - Acquisition Parameters
Date_          20191024
Time              14.38
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG              86.58
DW              62.400 usec
DE               6.50 usec
TE              296.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

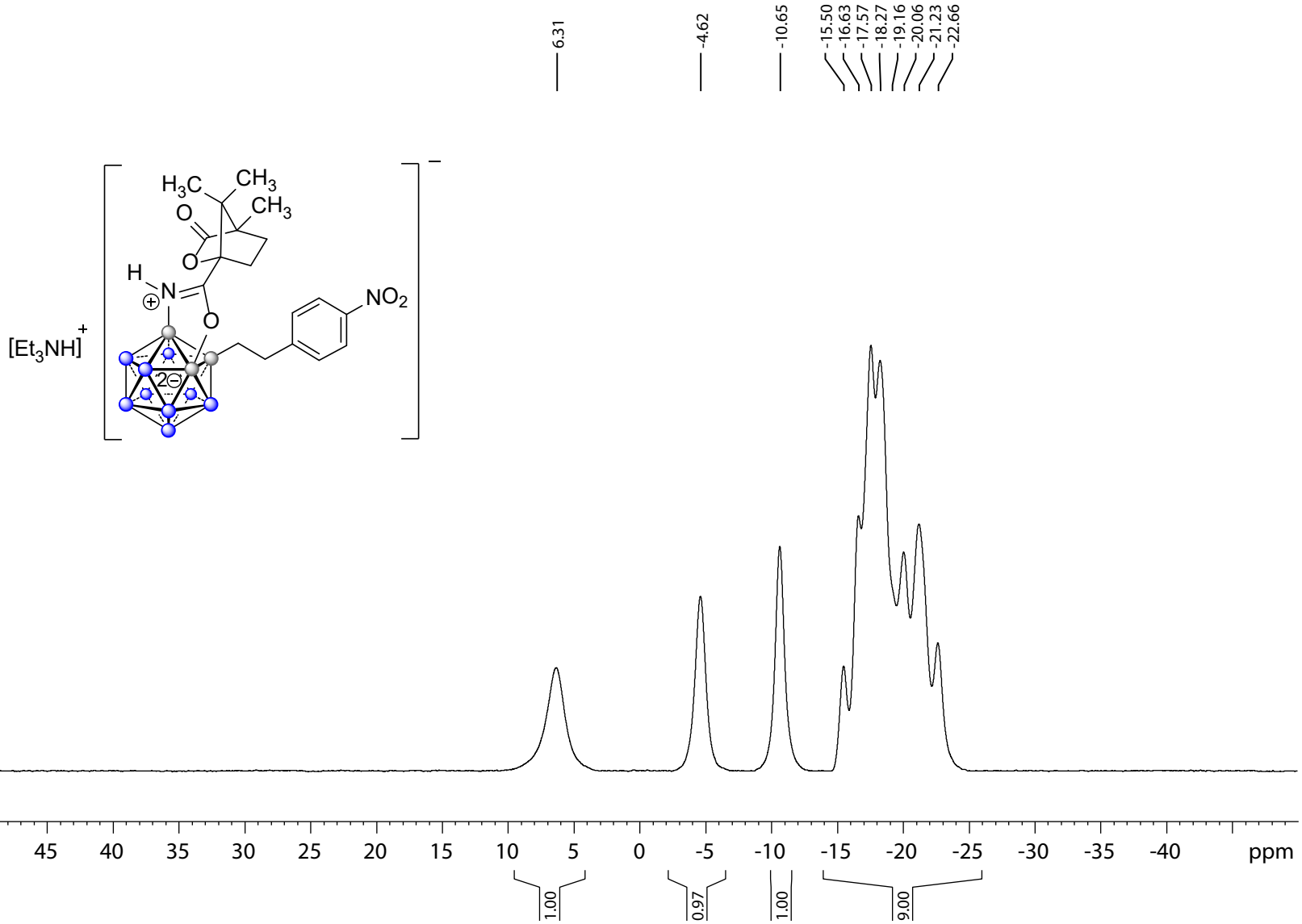
======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2           90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300075 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

20191020-B12C-NO2Styr 40 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4NO_2] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_          20191024
Time             14.44
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.2 K
D1           1.00000000 sec
TD0                  1

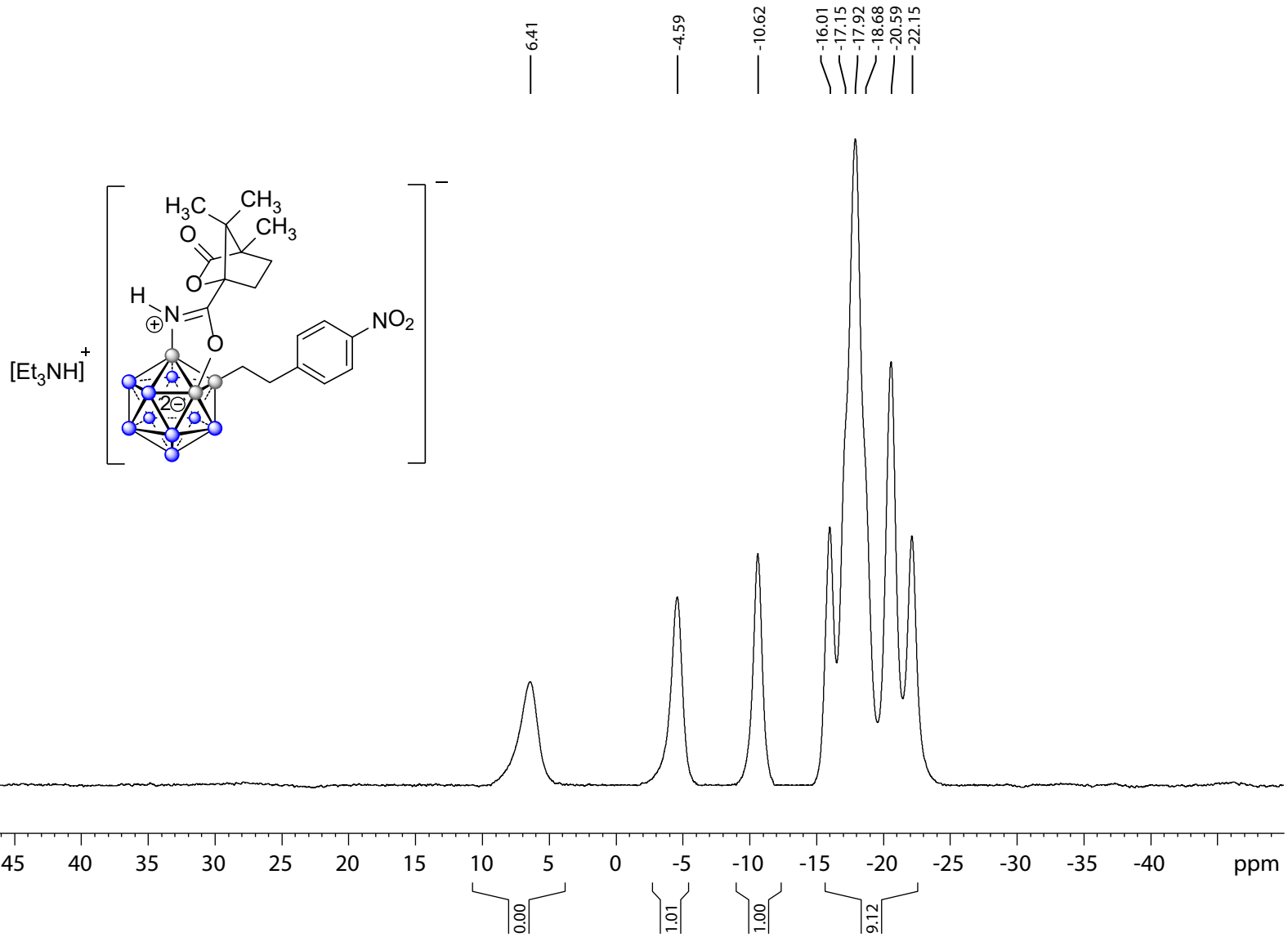
======== CHANNEL f1 ========
NUC1                11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI               32768
SF          128.3776050 MHz
WDW                 EM
SSB       0
LB              10.00 Hz
GB        0
PC               1.40
```

NMR-098

20191020-B12C-NO2Styr 40 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4NO_2] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz



NMR-099

```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191024
Time              14.51
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG               193.34
DW                19.600 usec
DE                 6.50 usec
TE                297.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

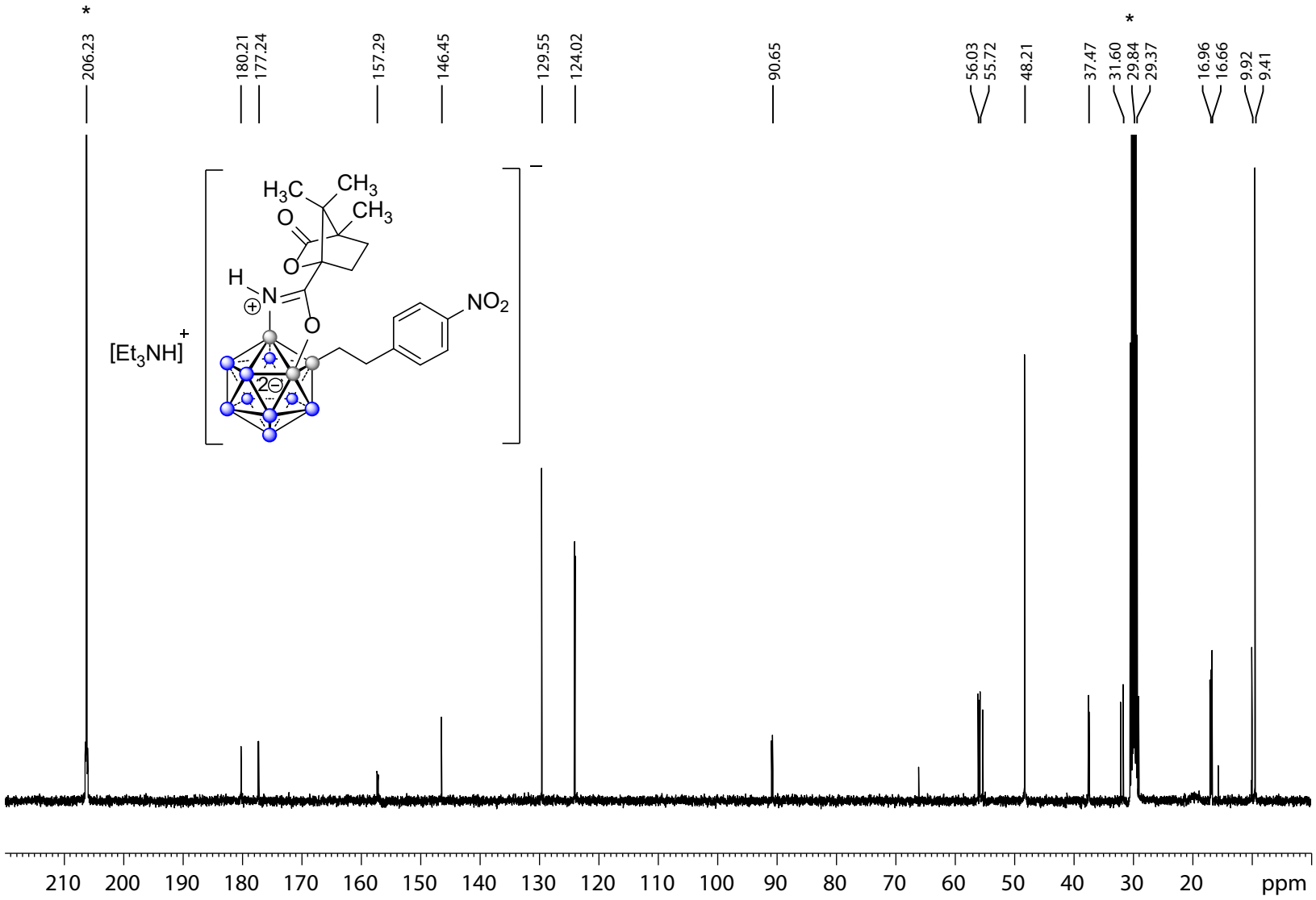
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191020-B12C-NO2Styr 40 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20191024
Time              16.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.5 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

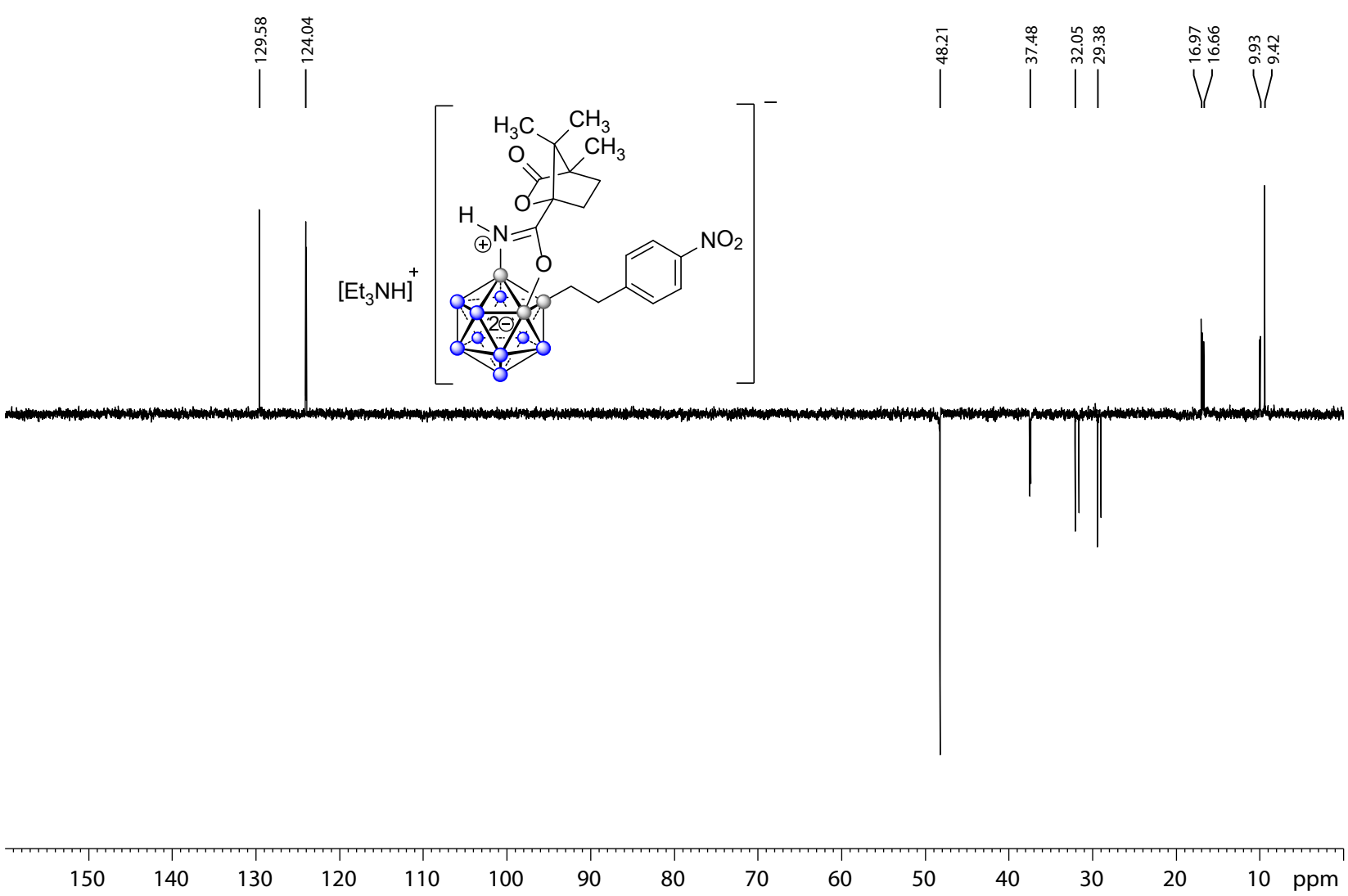
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126827 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

NMR-100

20191020-B12C-NO2Styr 40 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Camphanic)CH_2CH_2C_6H_4\text{-}4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                 6
PROCNO                1

F2 - Acquisition Parameters
Date_          20191024
Time              16.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.2 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

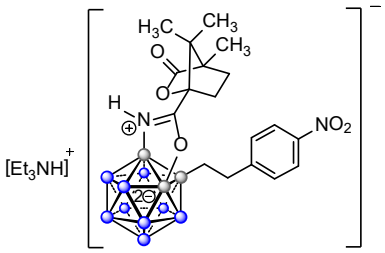
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

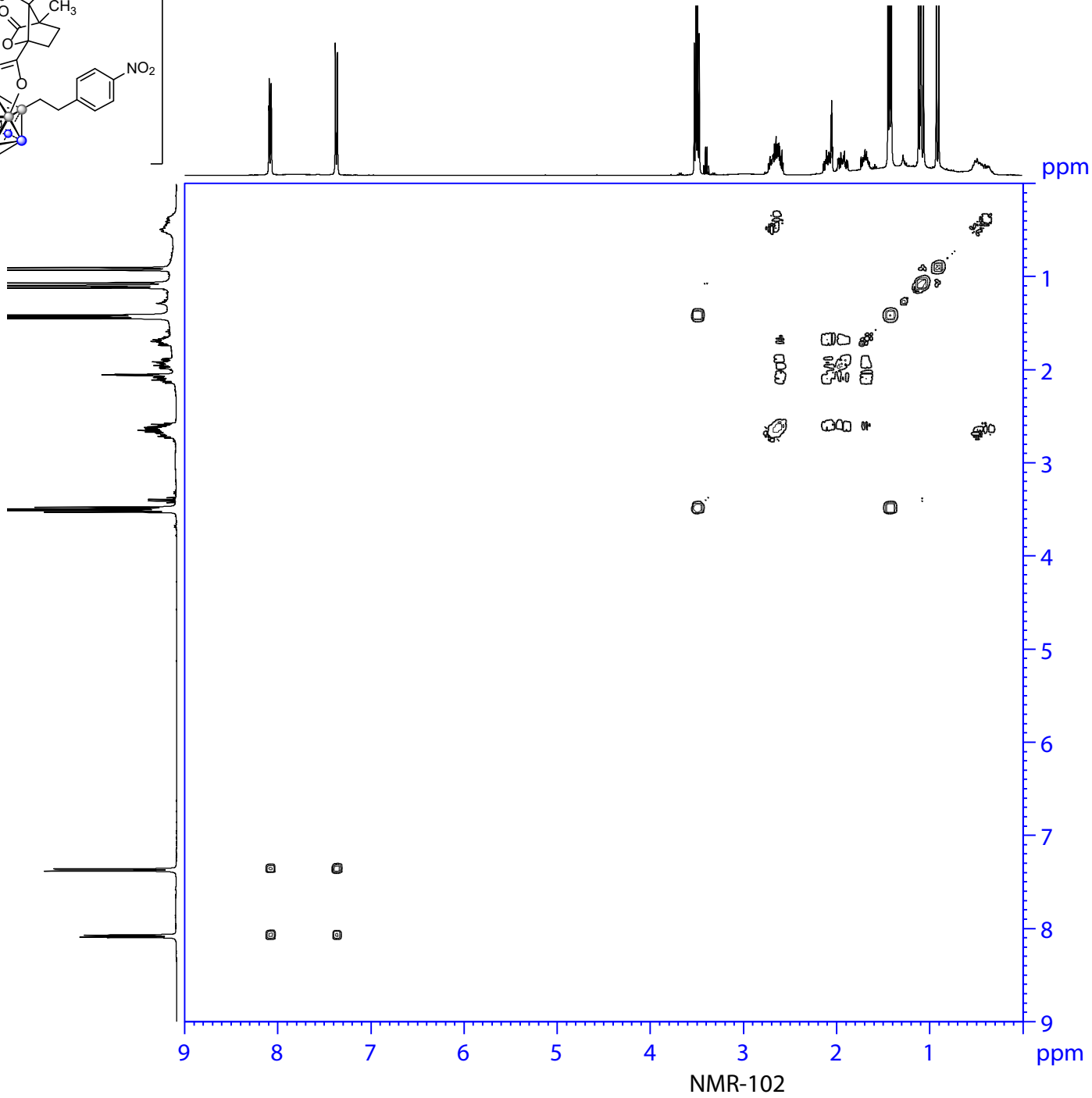
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126819 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20191020-B12C-NO2Styr 40 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4NO_2] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-102

Current Data Parameters
NAME 20191024-RV-B12C-4NO2Styr
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191024
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 193.34
DW 93.600 usec
DE 6.50 usec
TE 295.9 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

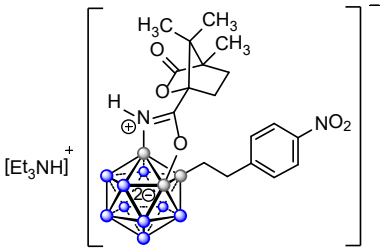
F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300095 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300096 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

20191020-B12C-NO2Styr 40 mg white solid [Et_3NH][$B_{12}H_{10}NHCO$(Camphanic)$CH_2CH_2C_6H_4$-4NO_2] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR



NMR-103

```
Current Data Parameters
NAME      20191024-RV-B12C-4NO2Styr
EXPNO                8
PROCNO               1

F2 - Acquisition Parameters
Date_           20191024
Time              17.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT        Acetone
NS                   2
DS                  16
SWH           6009.615 Hz
FIDRES        5.868765 Hz
AQ           0.0851968 sec
RG              193.34
DW               83.200 usec
DE                6.50 usec
TE               296.2 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPNAM[4]     SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

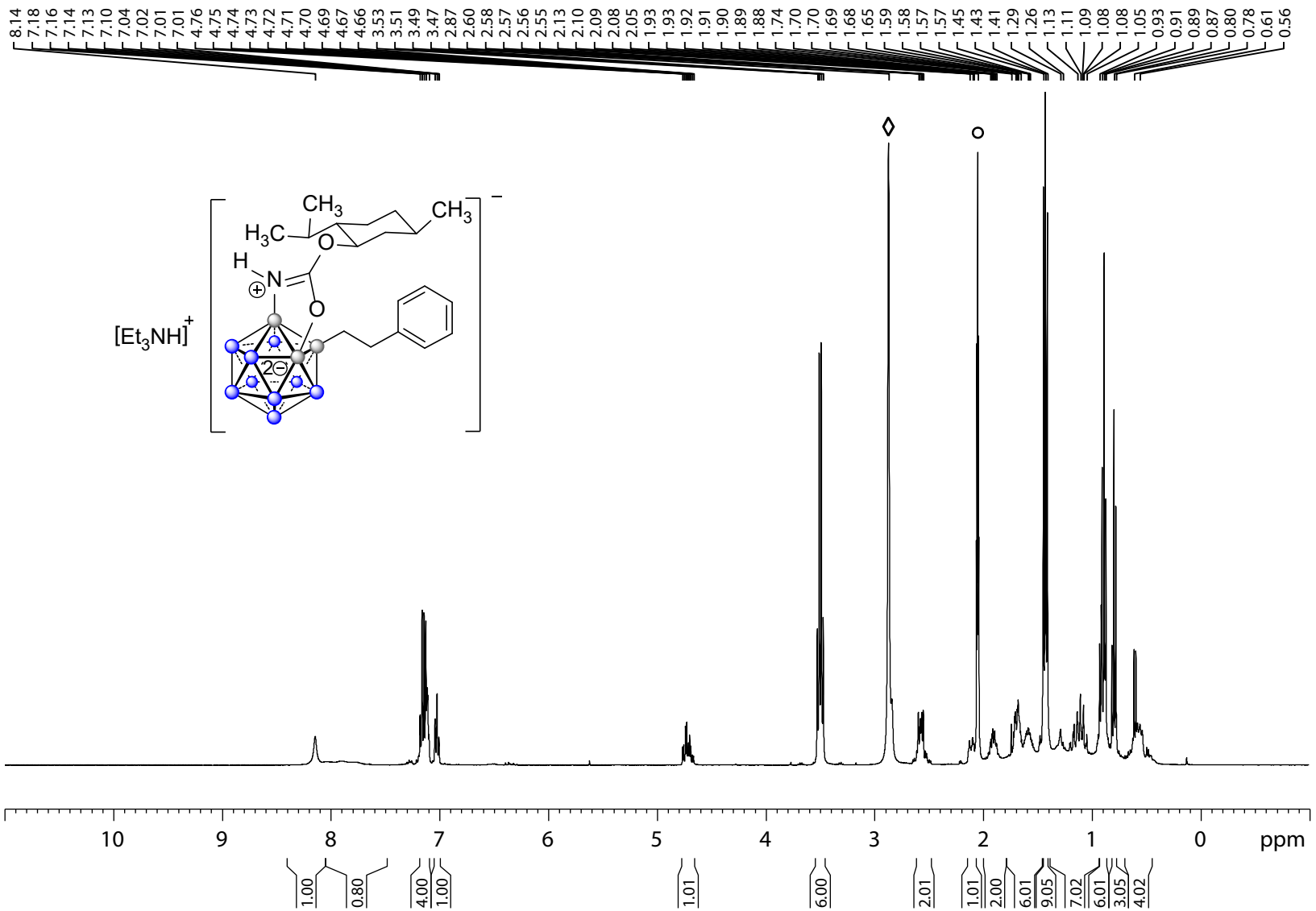
F1 - Acquisition parameters
TD                 256
SFO1          100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300043 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126709 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

20190110-B12M-Styr 10 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190110-RV-B12-MENTH-STYR-1Cu
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190111
Time                19.19
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     2
SWH            10000.000 Hz
FIDRES          0.152588 Hz
AQ              3.2767999 sec
RG                193.34
DW                50.000 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
TD0                    1

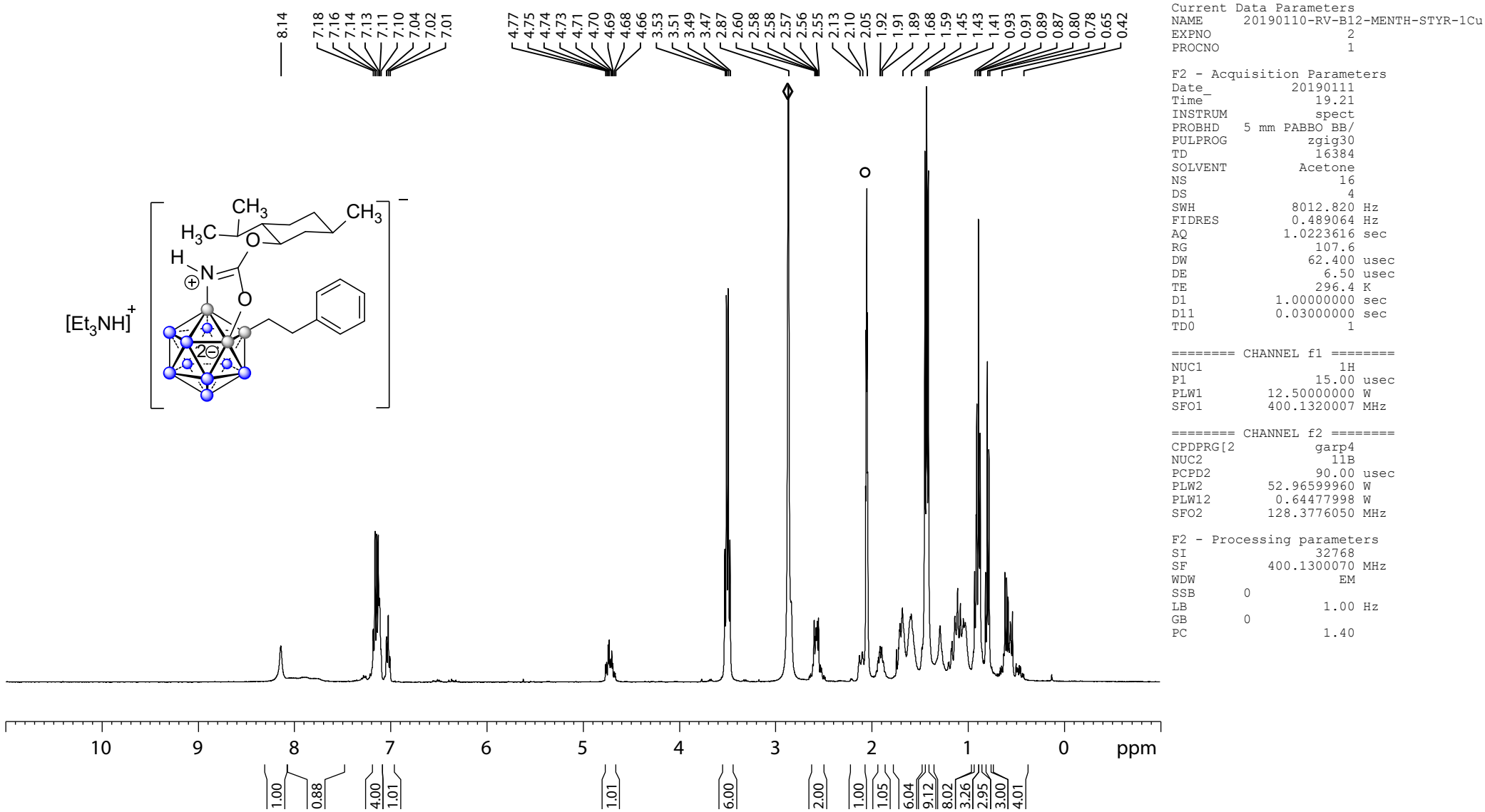
======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                 65536
SF           400.1300069 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

NMR-104

20190110-B12M-Styr 10 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, o deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190110-RV-B12-MENTH-STYR-1Cu
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190111
Time              19.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES          0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               296.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

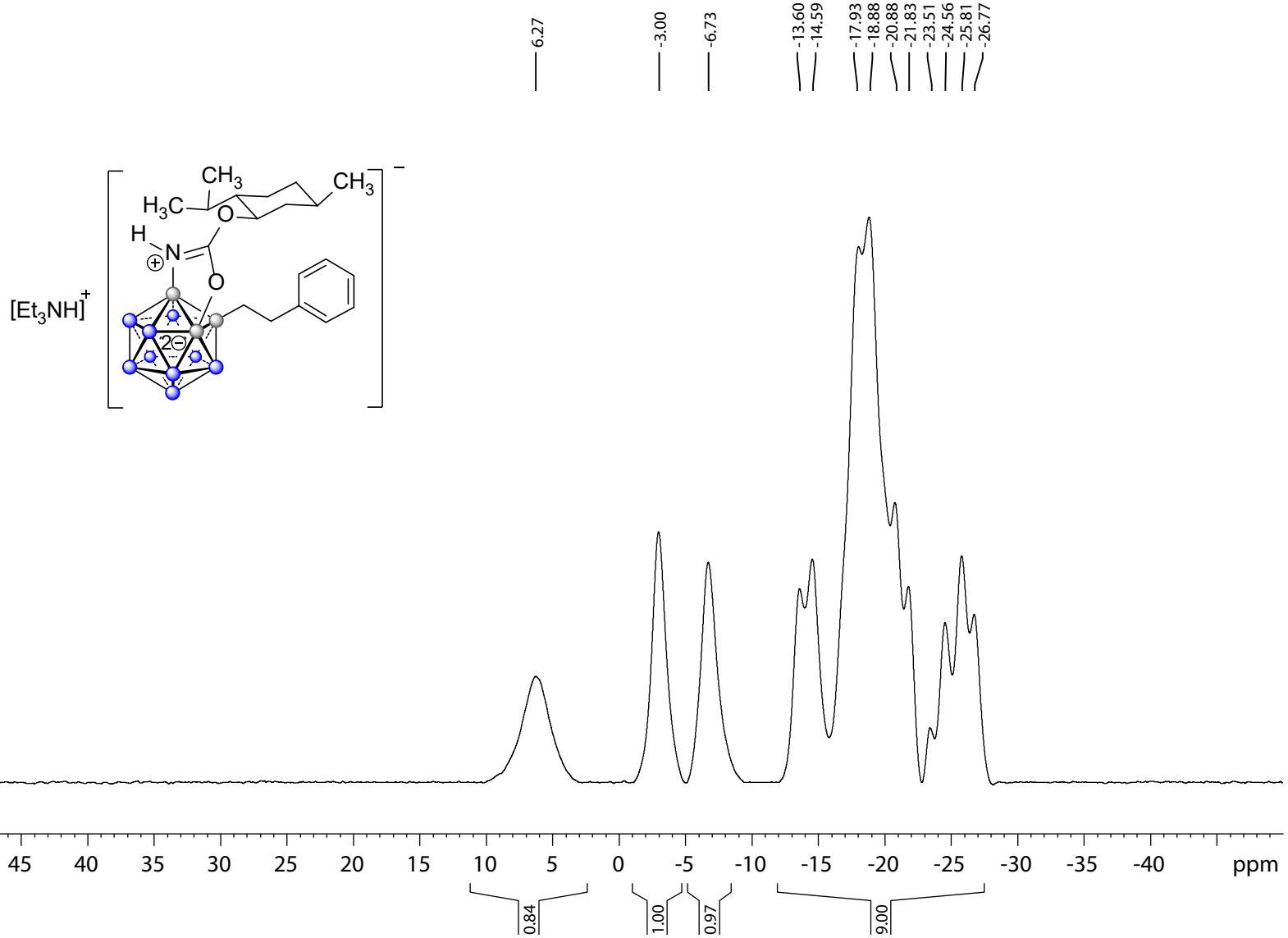
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2            90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300070 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190110-B12M-Styr 10 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190622-B12M-Styr-B
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_           20190623
Time      0
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       640
DS                         4
SWH              25510.203 Hz
FIDRES            0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   296.1 K
D1              1.00000000 sec
TD0                        1

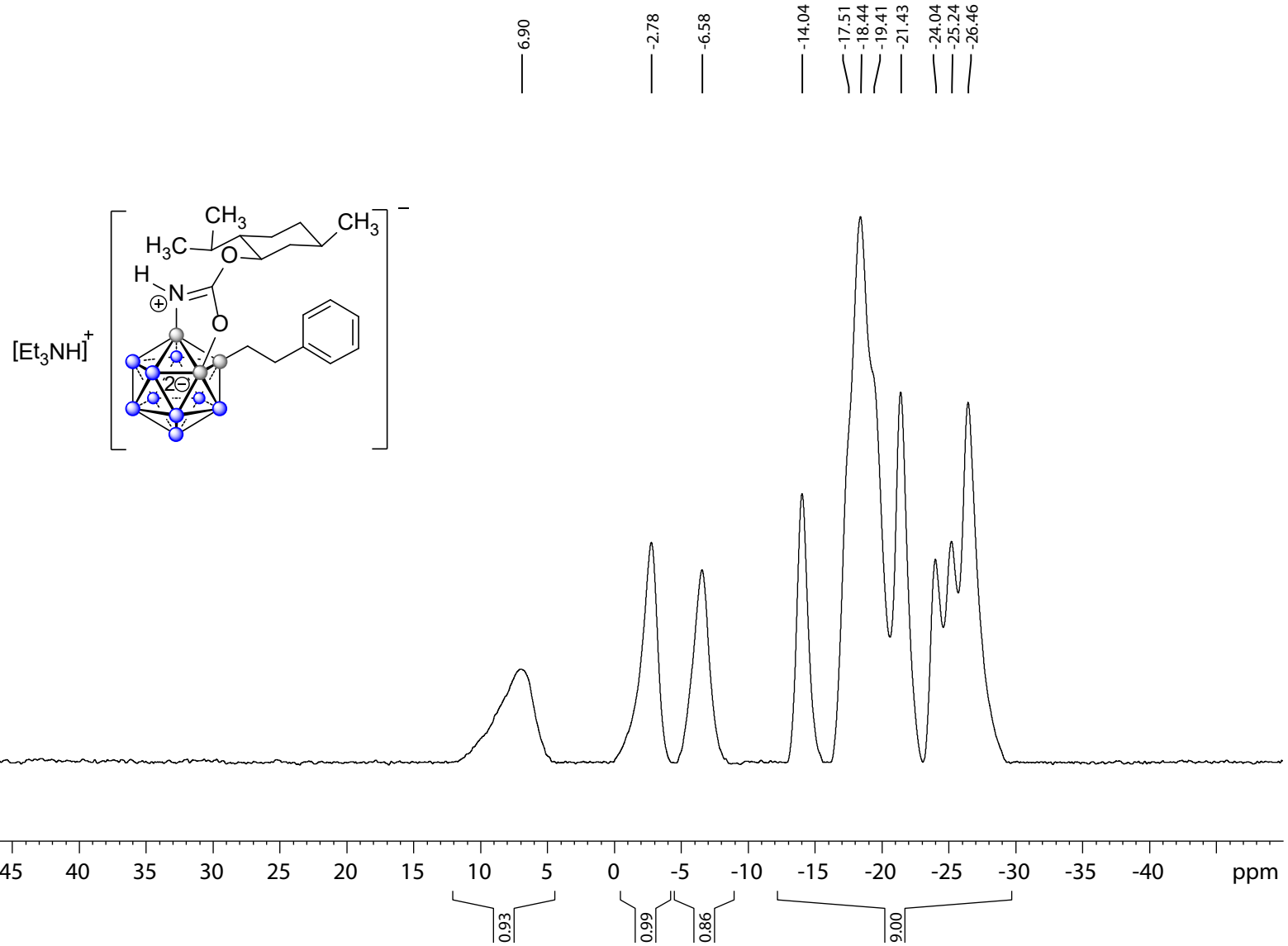
======== CHANNEL f1 ========
NUC1                    11B
P1                     9.93 usec
PLW1           52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                     32768
SF             128.3776050 MHz
WDW                      EM
SSB       0
LB                    20.00 Hz
GB        0
PC                     1.40
```

NMR-106

20190110-B12M-Styr 10 mg white solid $[Et_3NH][B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz



NMR-107

```
Current Data Parameters
NAME      20190622-B12M-Styr-B
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190623
Time                   0.26
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       640
DS                         4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    297.3 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1

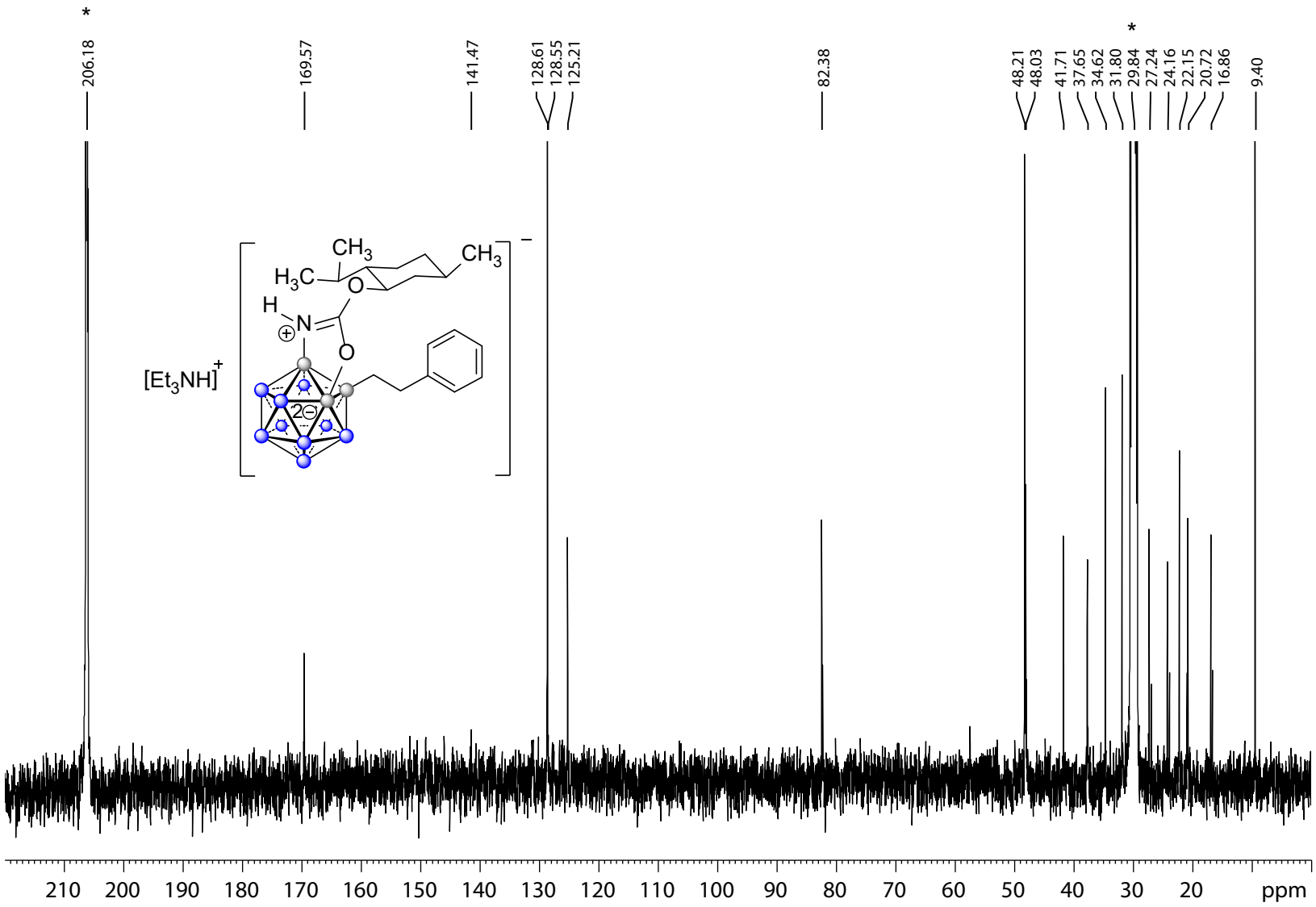
======== CHANNEL f1 ========
NUC1                      11B
P1                       9.93 usec
PLW1              52.96599960 W
SFO1             128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PLW2              12.50000000 W
PLW12              0.43945000 W
PLW13              0.28125000 W
SFO2             400.1320007 MHz

F2 - Processing parameters
SI                       32768
SF               128.3776050 MHz
WDW                         EM
SSB          0
LB                     20.00 Hz
GB           0
PC                      1.40
```

20190110-B12M-Styr 10 mg white solid $[Et_3NH]_2[B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190110-RV-B12-MENTH-STYR-1Cu
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20190111
Time_             21.06
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                297.1 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

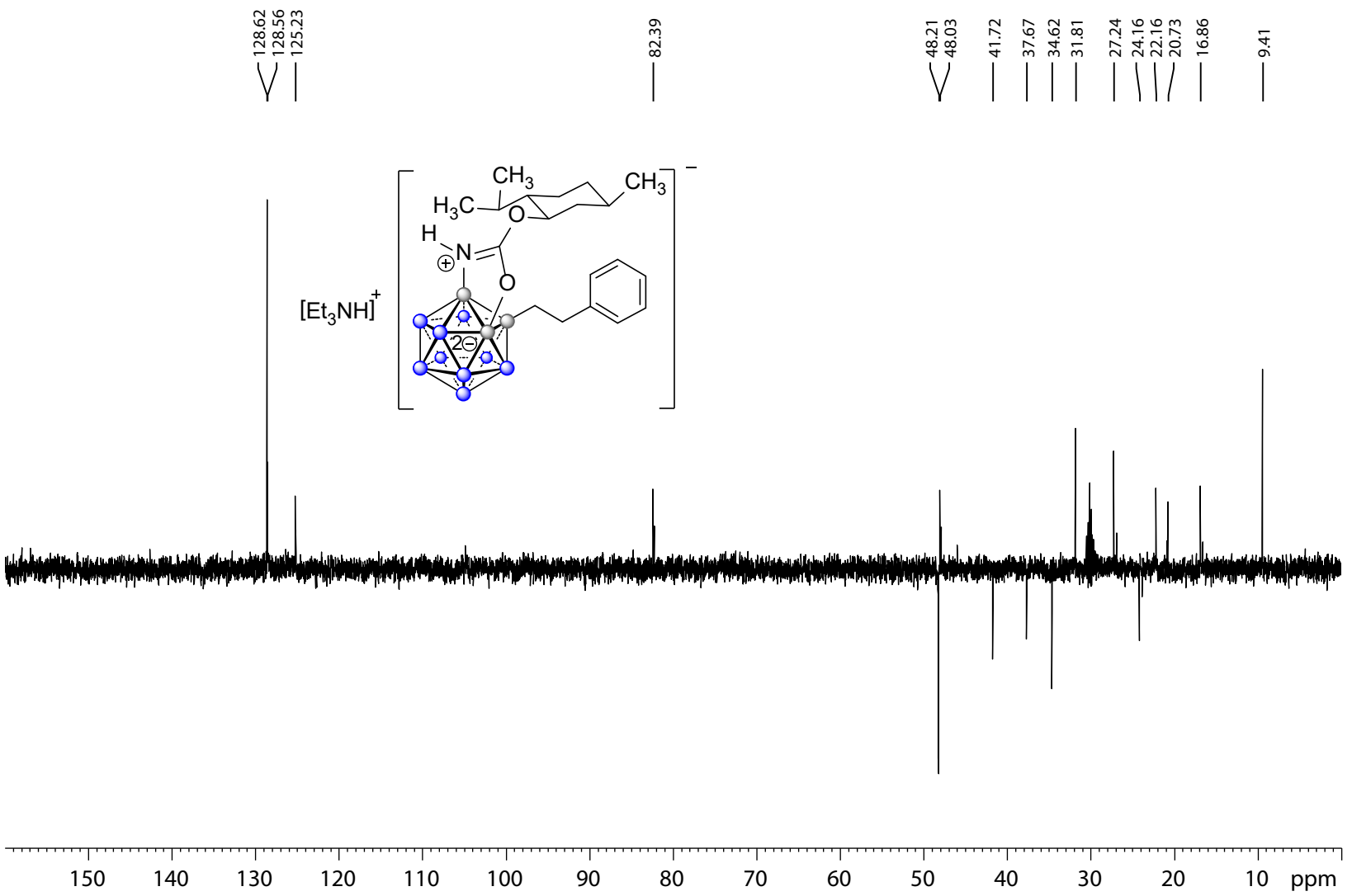
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126794 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

20190110-B12M-Styr 10 mg white solid [Et_3NH][$B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190110-RV-B12-MENTH-STYR-1Cu
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190111
Time              21.34
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW              17.067 usec
DE                6.50 usec
TE               296.7 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

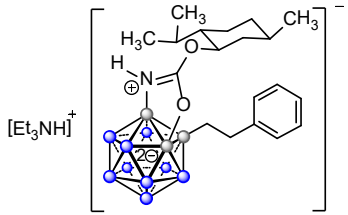
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126793 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190110-B12M-Styr 10 mg white solid [Et_3NH][$B_{12}H_{10}NHCO(Menthyl)CH_2CH_2C_6H_5$] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190110-RV-B12-MENTH-STYR-1Cu
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_            20190111
Time             21.35
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                  1024
SOLVENT          Acetone
NS                     2
DS                    16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ              0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                296.4 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1          12.50000000 W
SFO1          400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2          53.00000000 W
PLW12          1.08159995 W
SFO2          100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

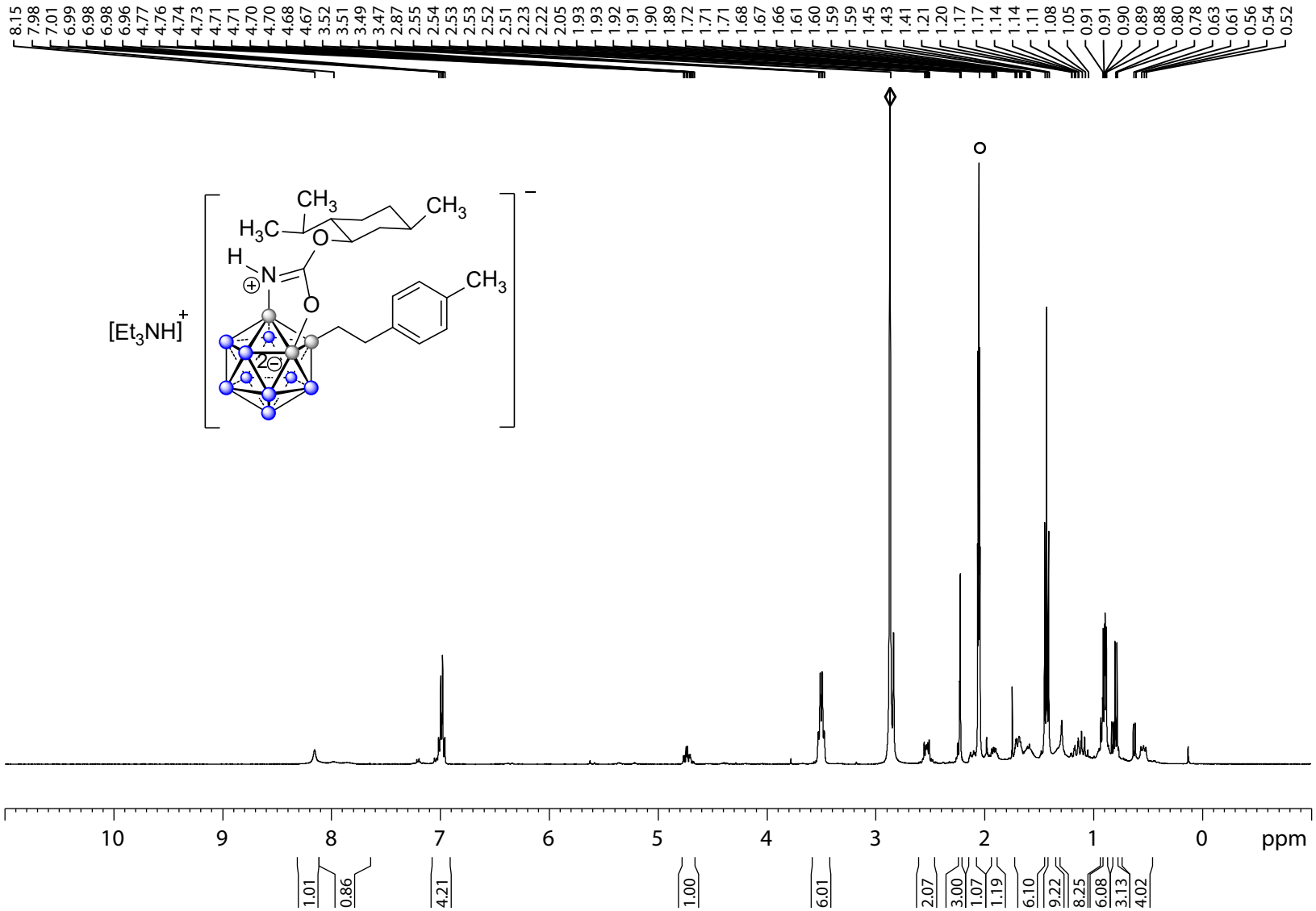
F1 - Acquisition parameters
TD                   256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW              249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW                 QSINE
SSB                    2
LB        0 Hz
GB        0
```

20190122-B12M-4MeStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Me]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190122-RV-B12M-4MeSTYR-I
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190123
Time               4.26
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   64
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                193.34
DW                50.000 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
TD0                   1

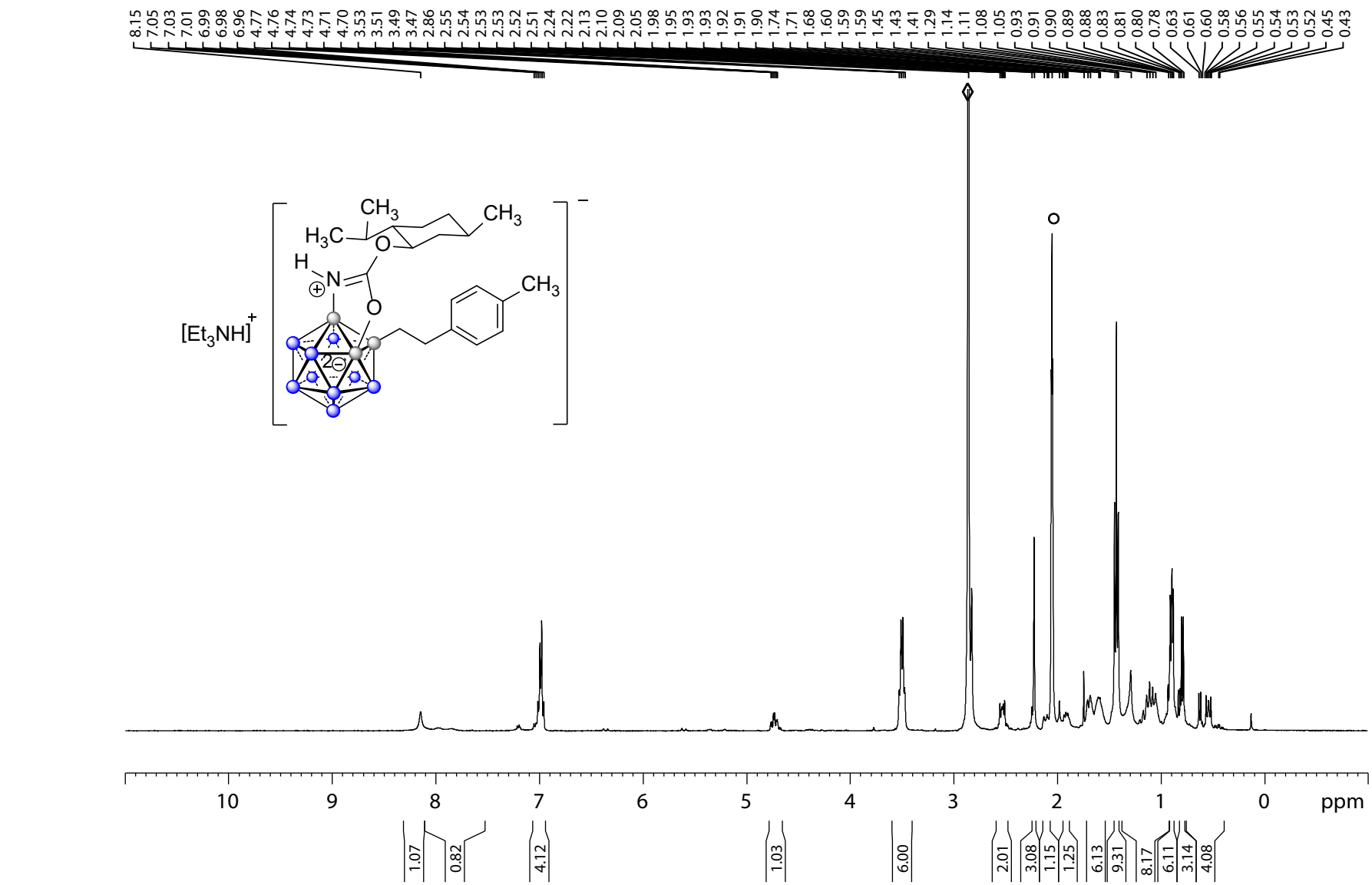
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300069 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-111

20190122-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-112

```
Current Data Parameters
NAME      20190122-RV-B12M-4MeSTYR-I
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190123
Time              4.28
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT        Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG              193.34
DW              62.400 usec
DE               6.50 usec
TE              296.5 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

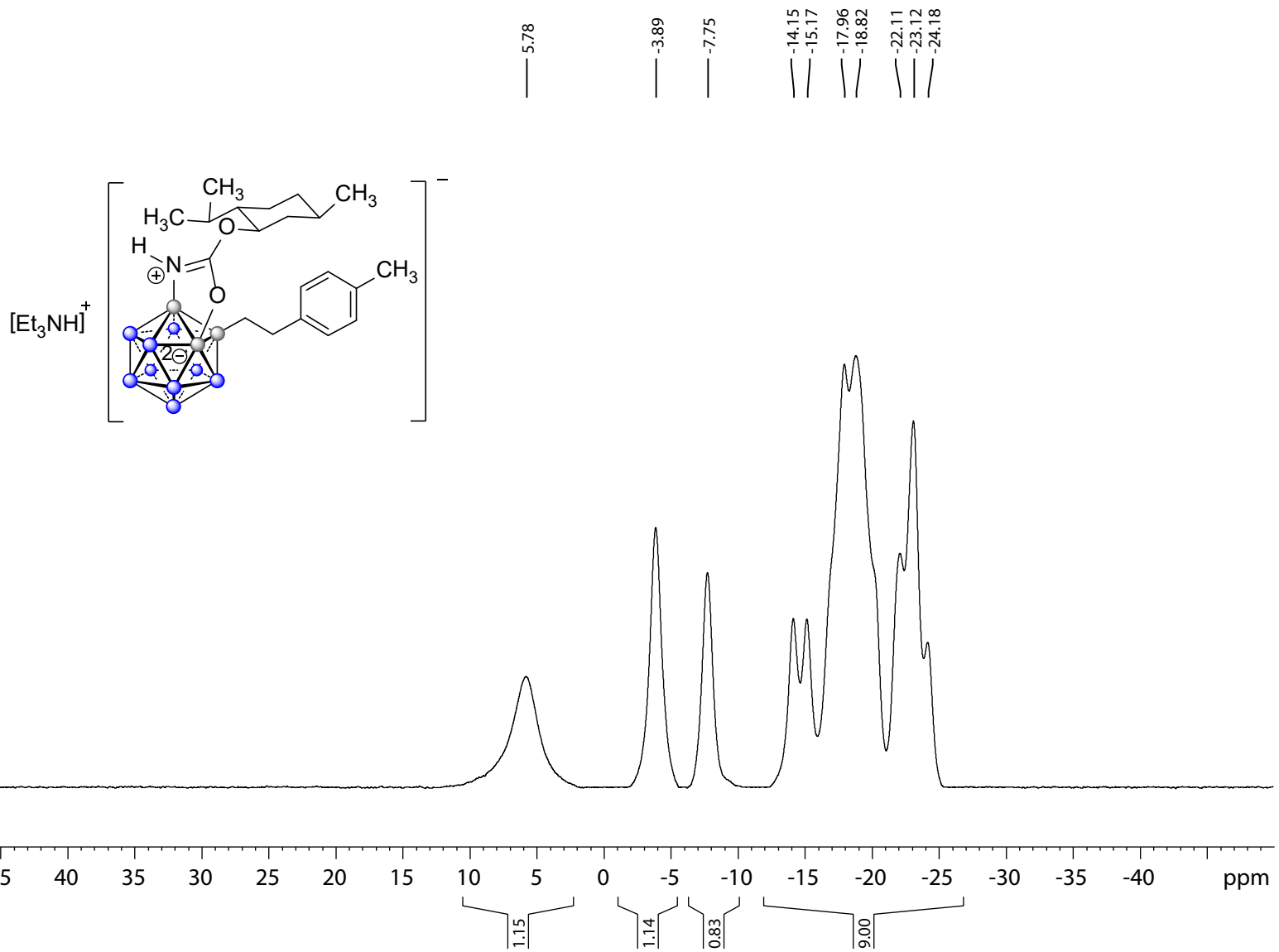
======== CHANNEL f1 ========
NUC1                1H
P1               15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2            90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300069 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_          20190725
Time              18.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                295.1 K
D1           1.00000000 sec
TD0                   1

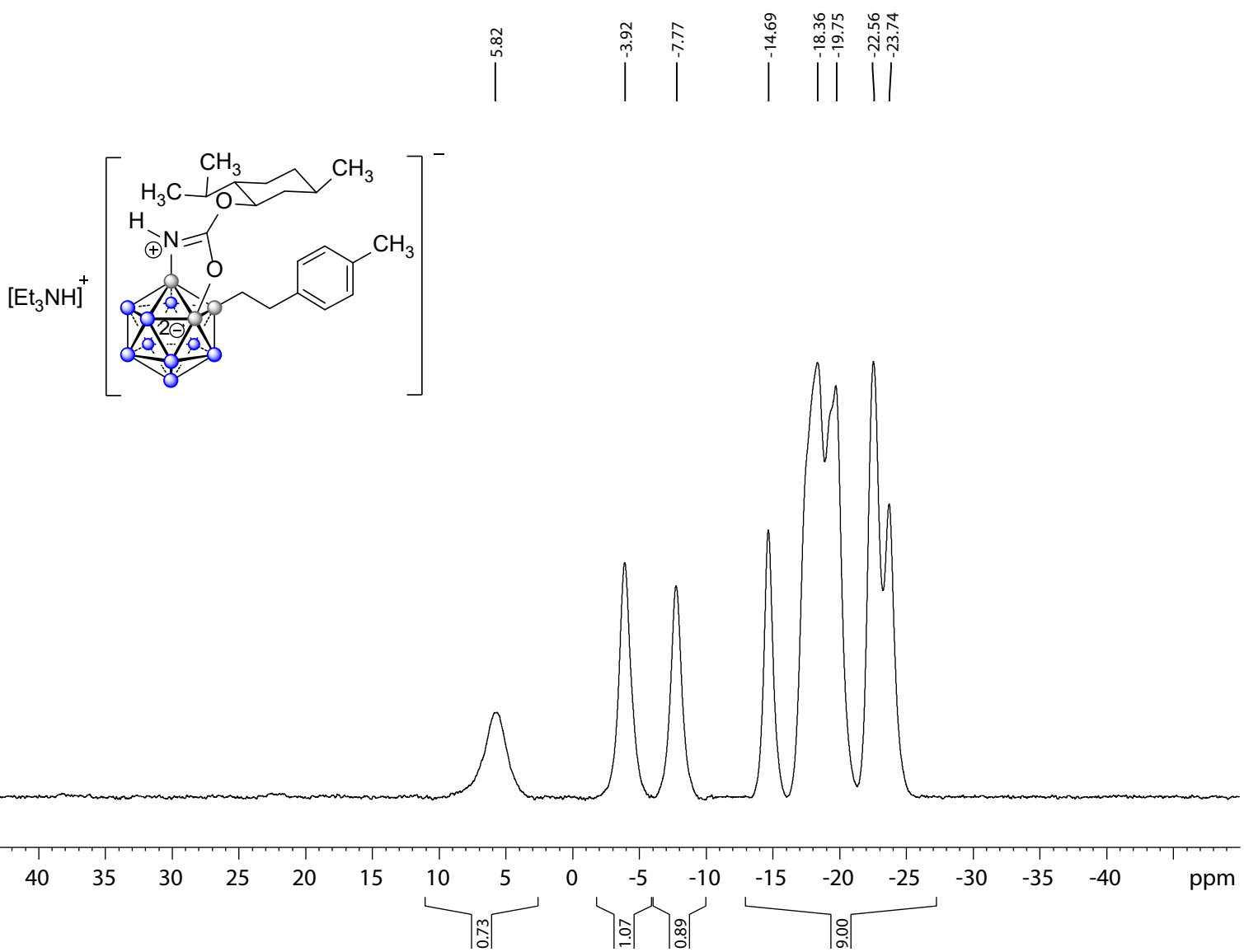
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB              10.00 Hz
GB        0
PC                1.40
```

NMR-113

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190725
Time              18.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

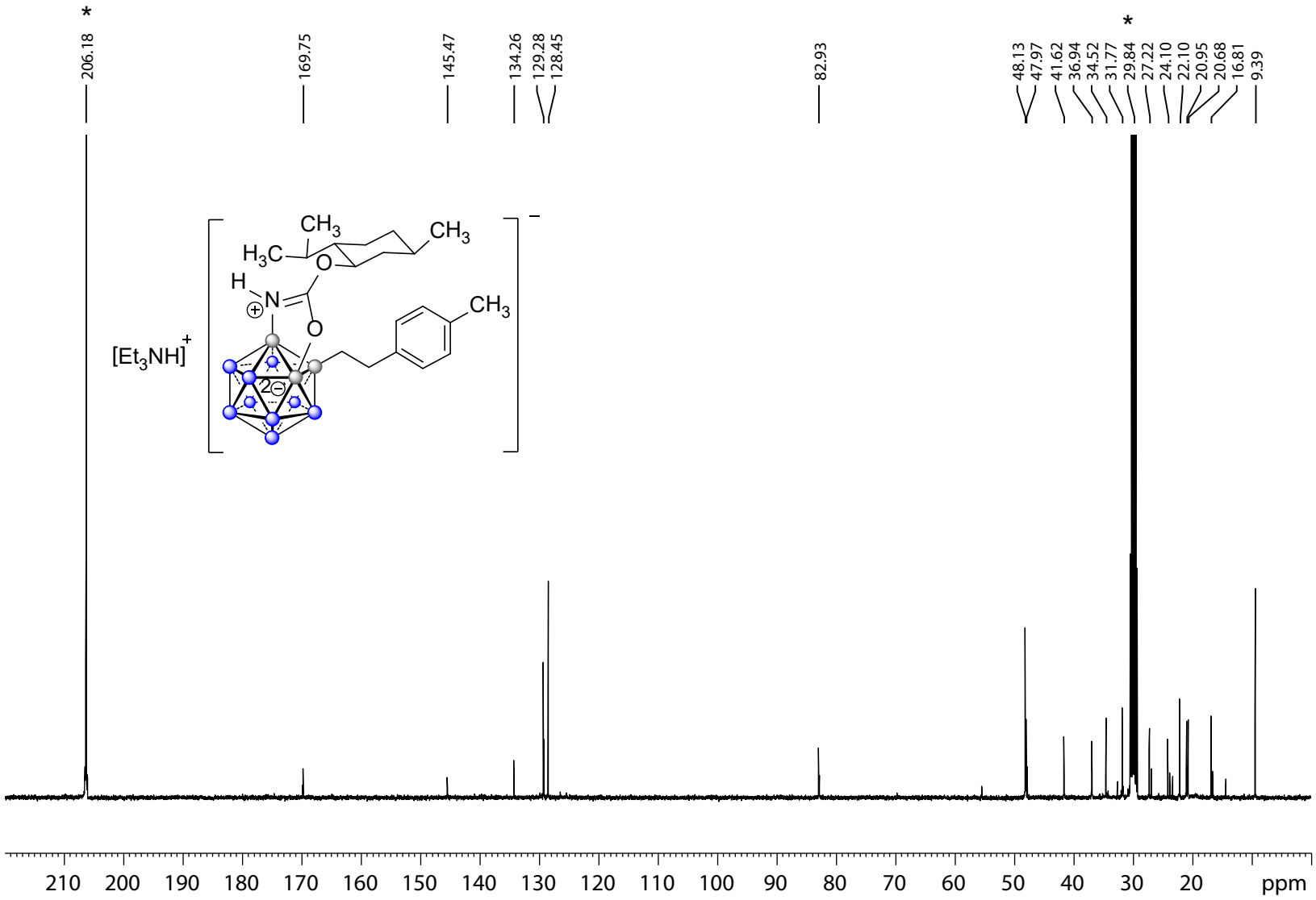
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-114

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190725
Time              20.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.0 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

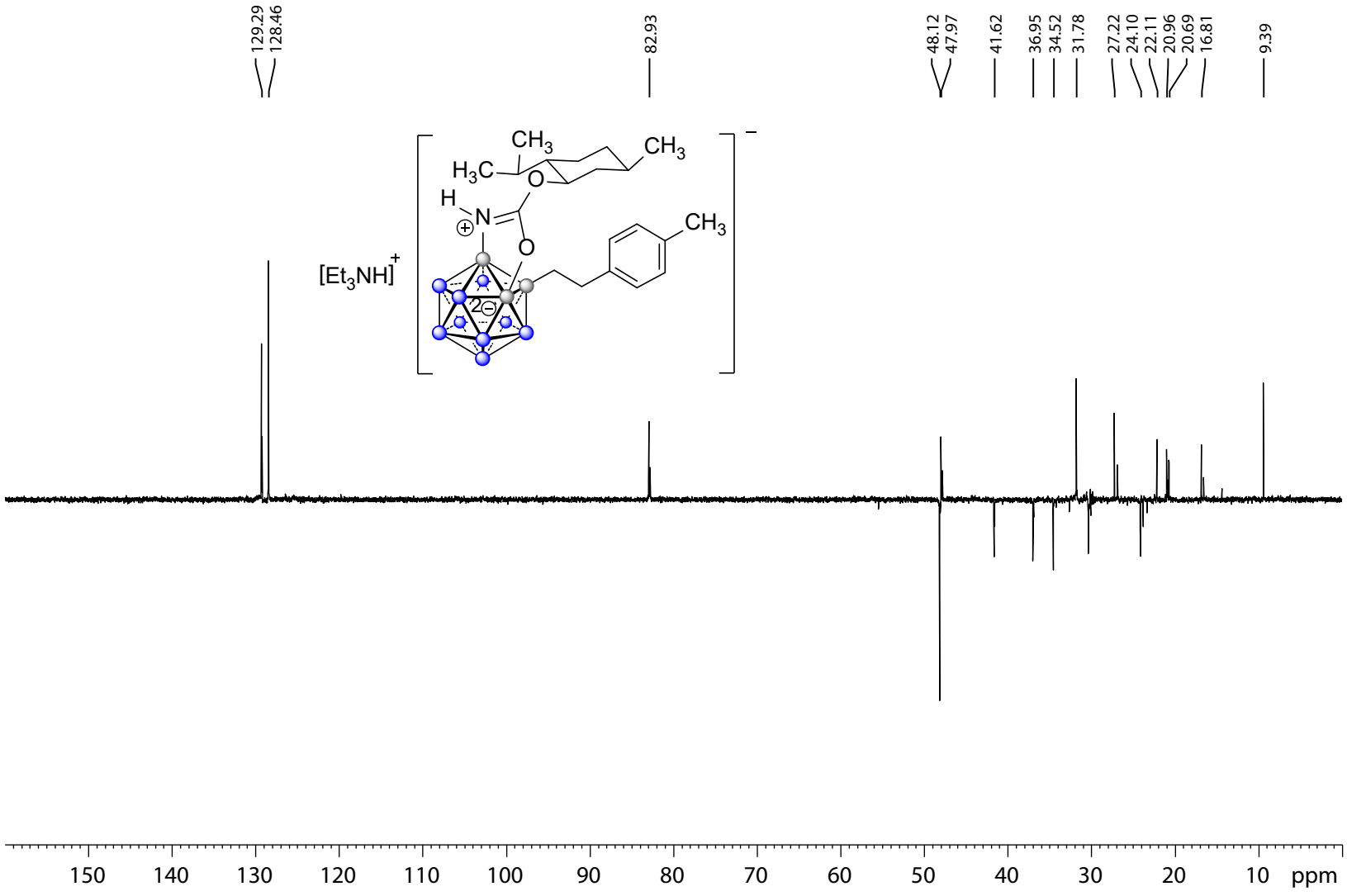
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126842 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190725
Time              20.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          dept135
TD                65536
SOLVENT          Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG               193.34
DW                17.067 usec
DE                 6.50 usec
TE                295.4 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

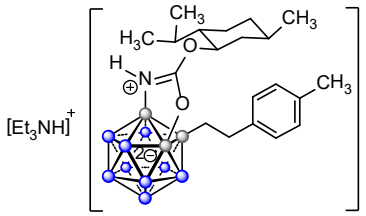
======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
P2                 20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

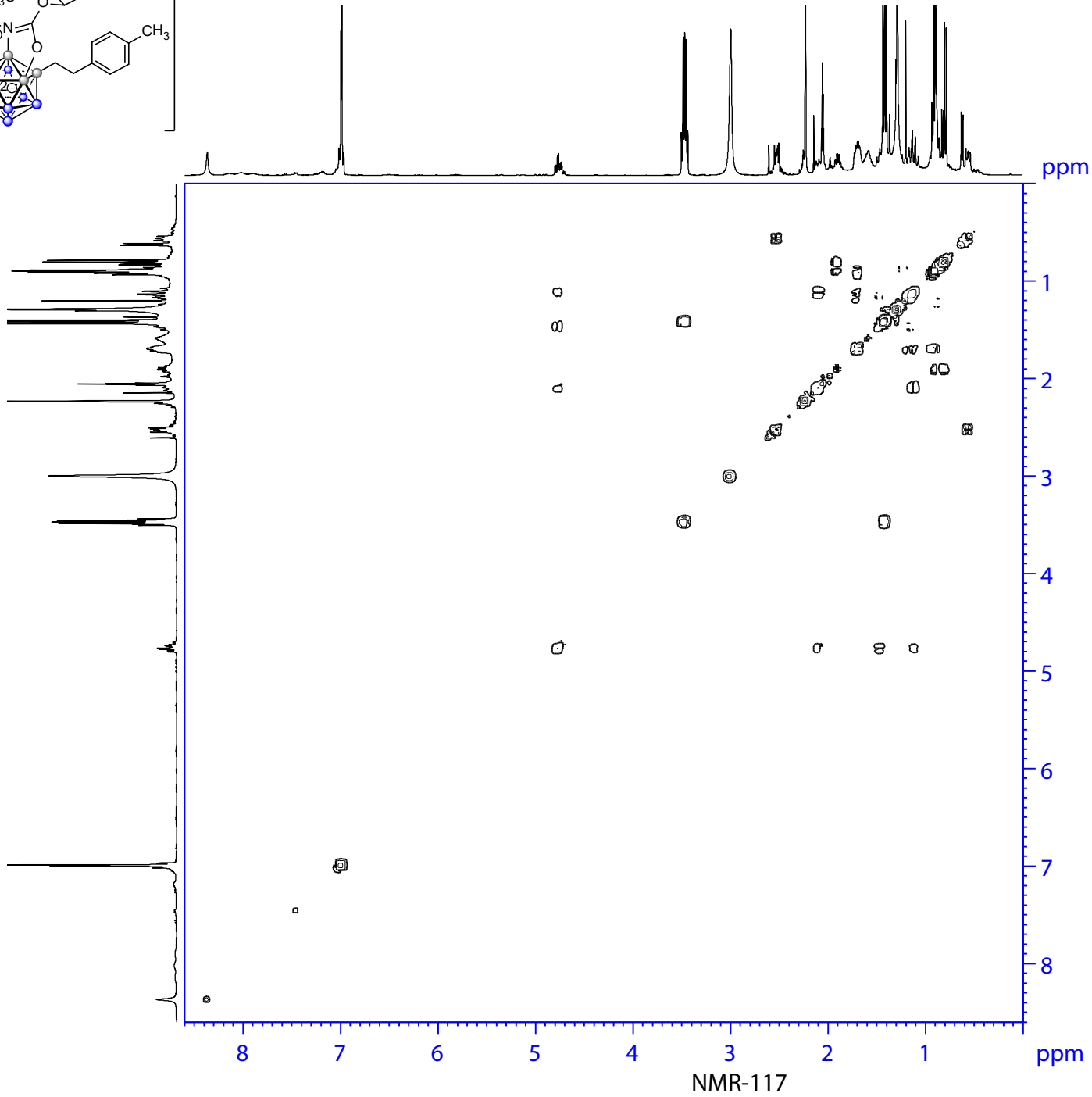
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                 15.00 usec
P4                 30.00 usec
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126836 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 4.00
```

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-117

```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                   8
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190725
Time              20.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                107.6
DW               93.600 usec
DE                6.50 usec
TE                294.9 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

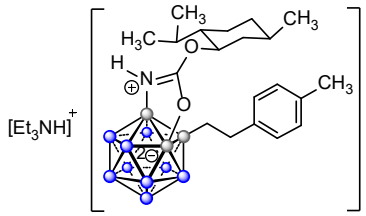
F1 - Acquisition parameters
TD                  128
SFO1           400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE               QF

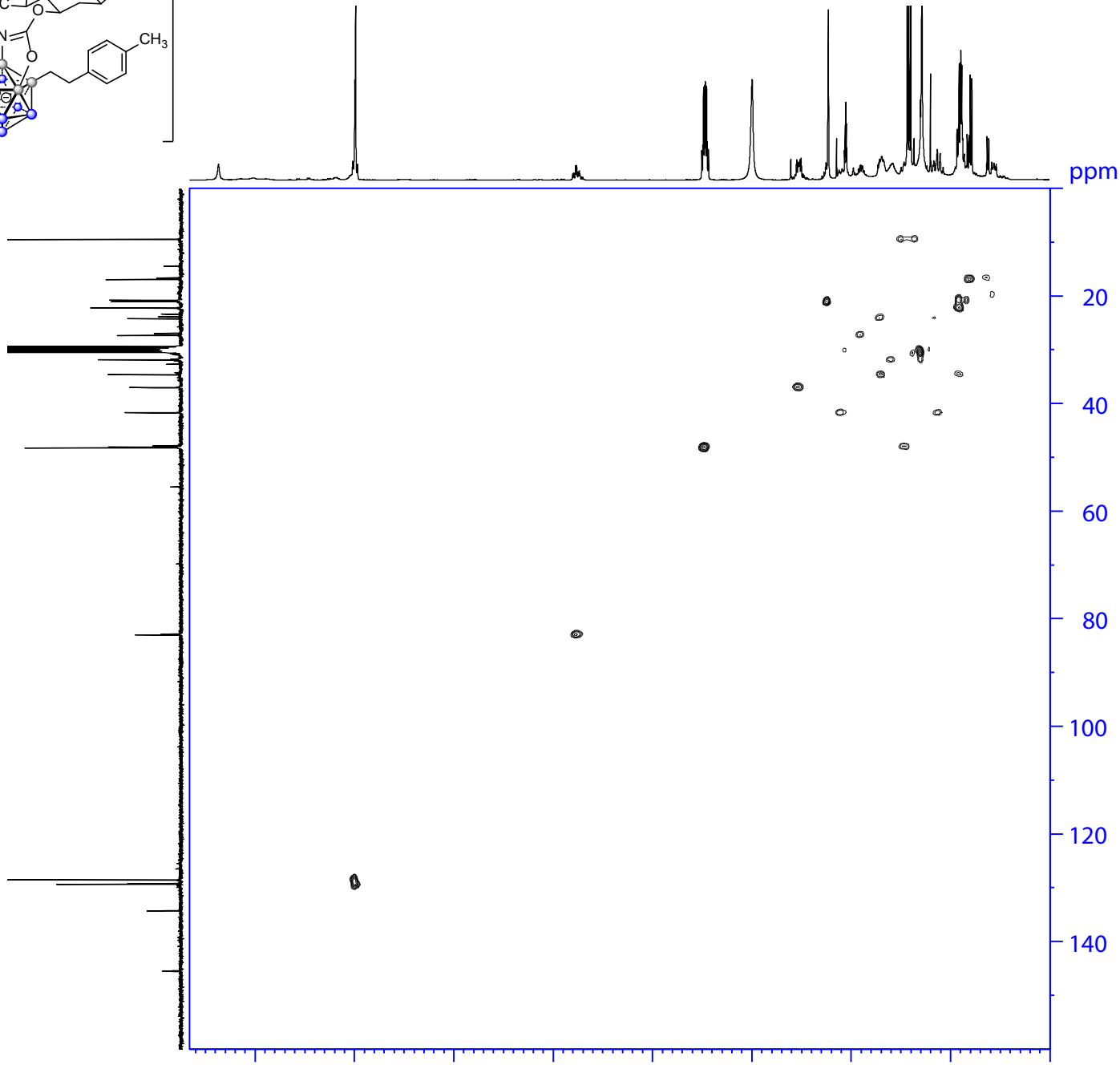
F2 - Processing parameters
SI                  1024
SF           400.1300073 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300074 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

20190725-B12M-4MeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Me$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR





NMR-118

```
Current Data Parameters
NAME      20190725-RV-B12M-4MeSTYR
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_            20190725
Time                20.44
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                  1024
SOLVENT          Acetone
NS                     2
DS                    16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                295.3 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
P2                  30.00 usec
P28               1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

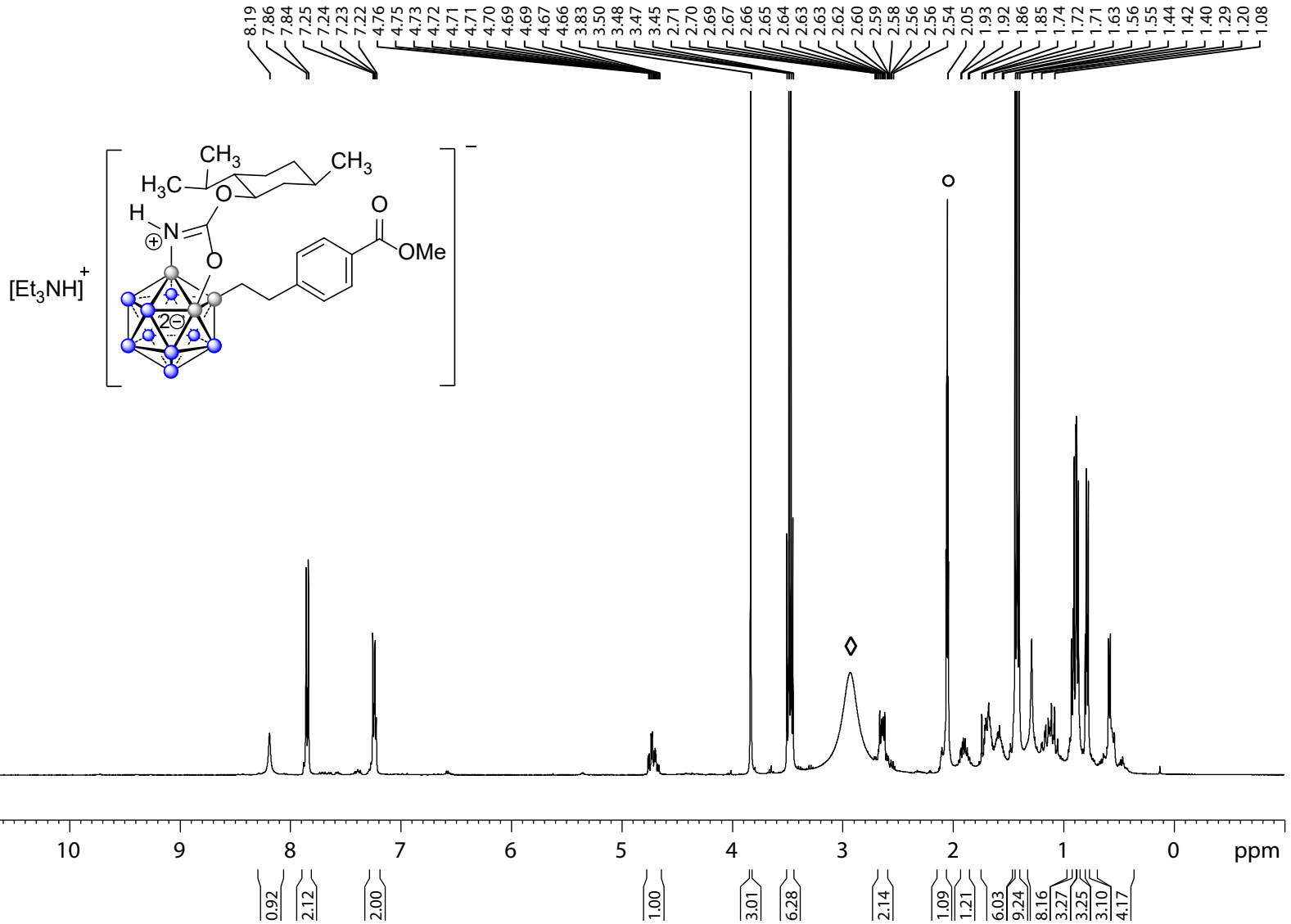
F1 - Acquisition parameters
TD                   256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW              249.991 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300034 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6126680 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
```

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190129
Time              15.29
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  64
DS                   2
SWH          10000.000 Hz
FIDRES         0.152588 Hz
AQ           3.2767999 sec
RG              124.48
DW               50.000 usec
DE                6.50 usec
TE              296.0 K
D1           1.00000000 sec
TD0                  1

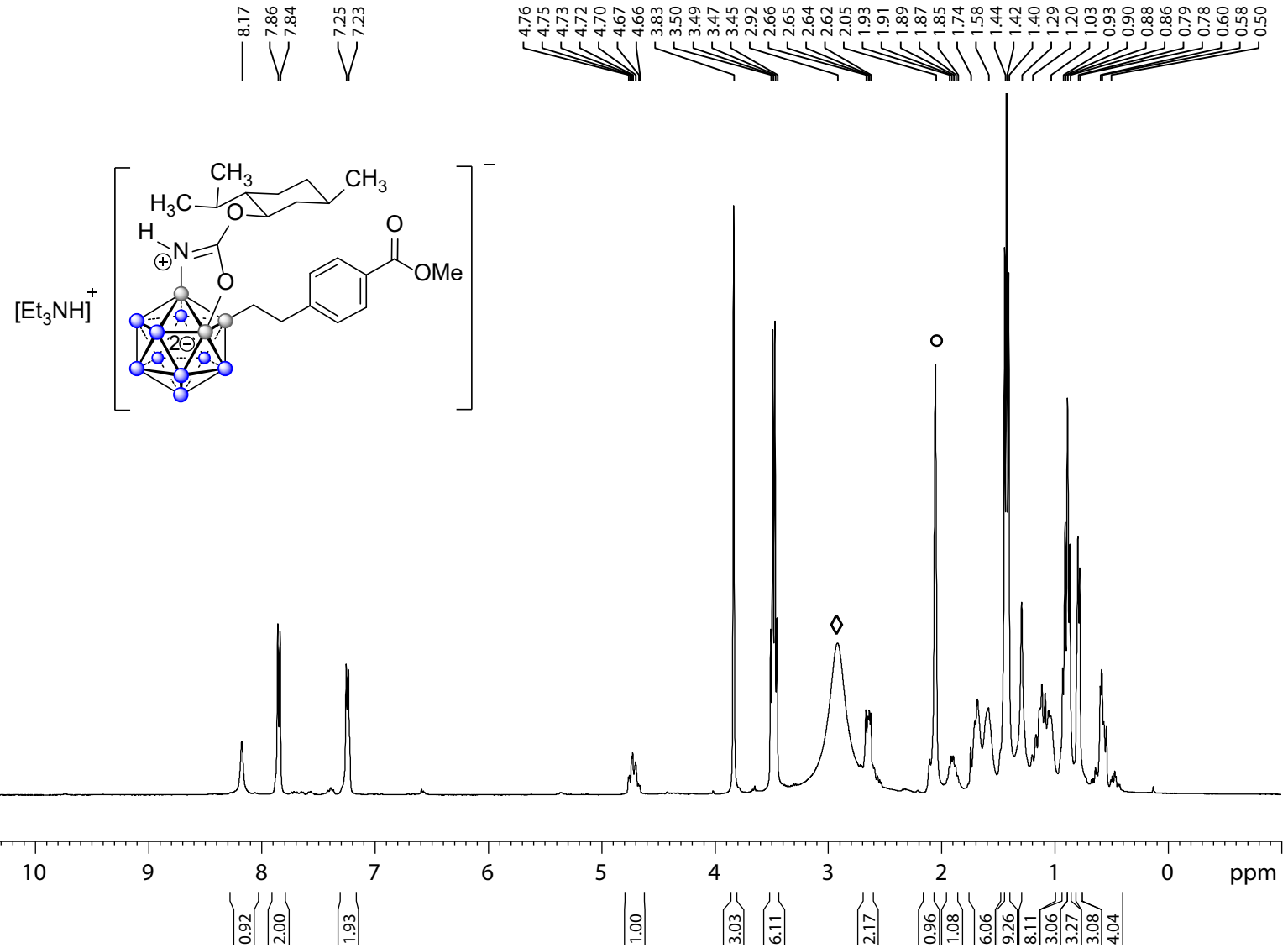
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI               65536
SF          400.1300069 MHz
WDW                 EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-119

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              15.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   64
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ              1.0223616 sec
RG                 107.6
DW                62.400 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

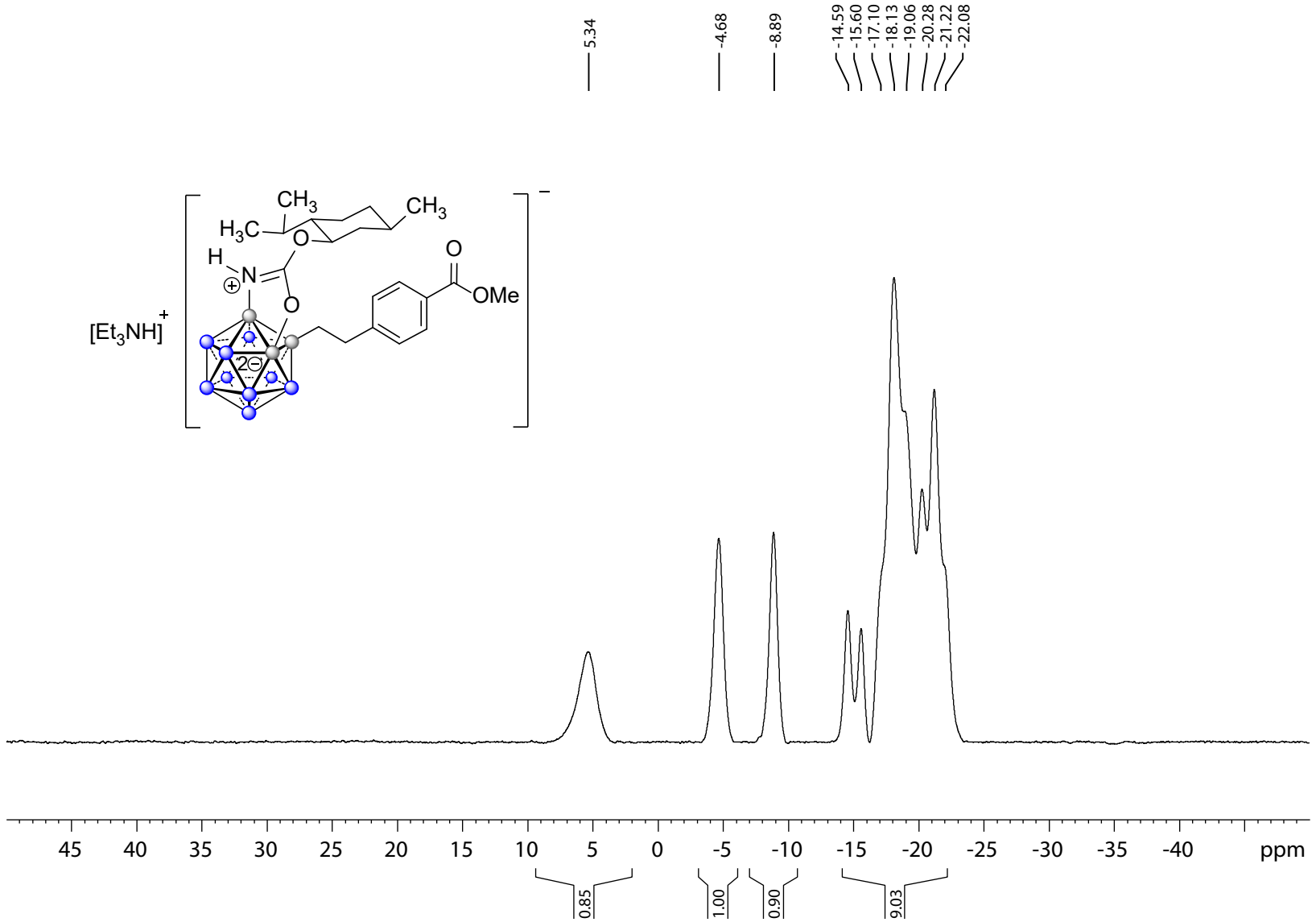
======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                 11B
PCPD2              90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                32768
SF           400.1300068 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              15.53
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.8 K
D1           1.00000000 sec
TD0                   1

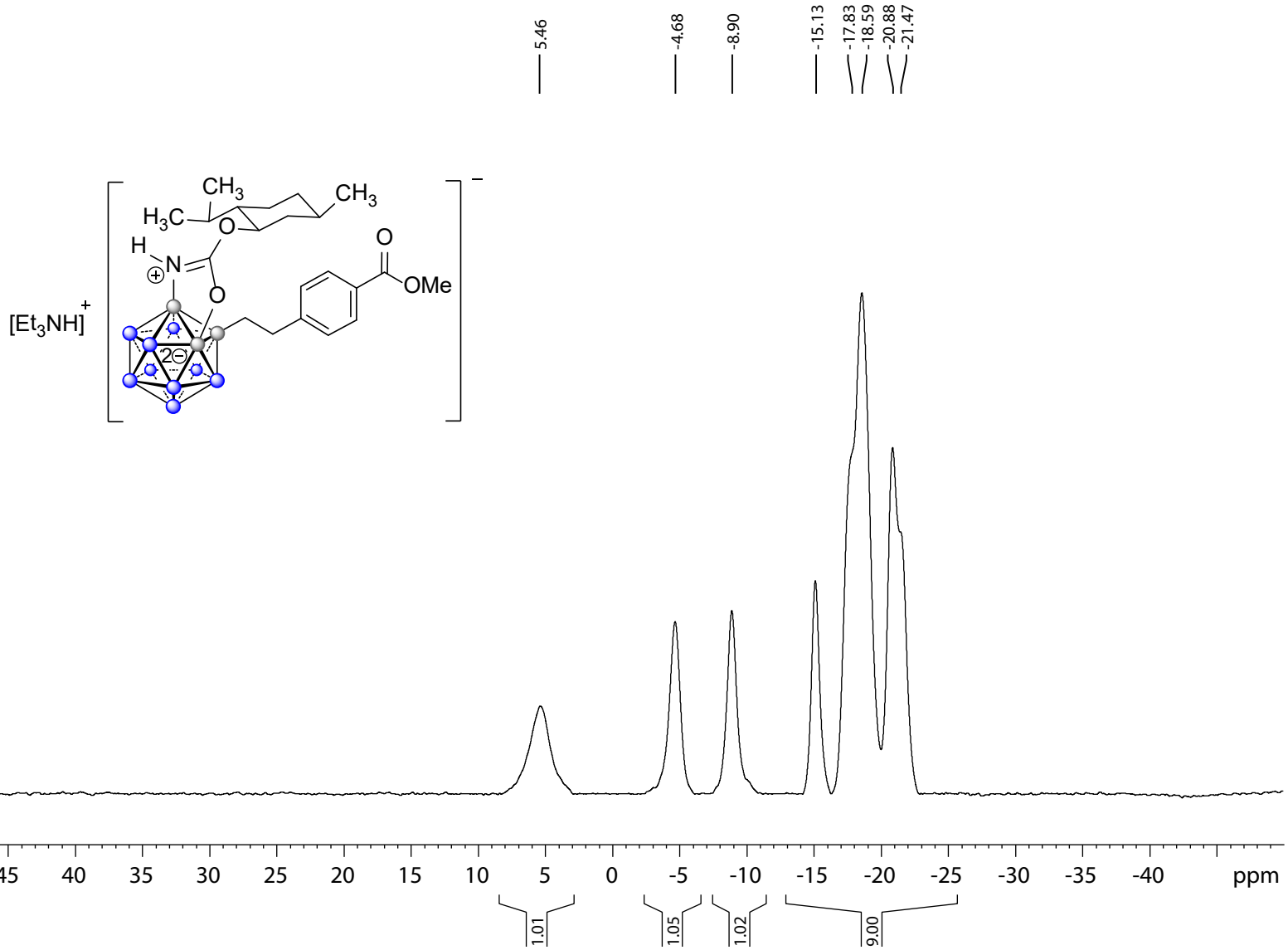
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-121

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190129
Time              16.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE                6.50 usec
TE               296.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

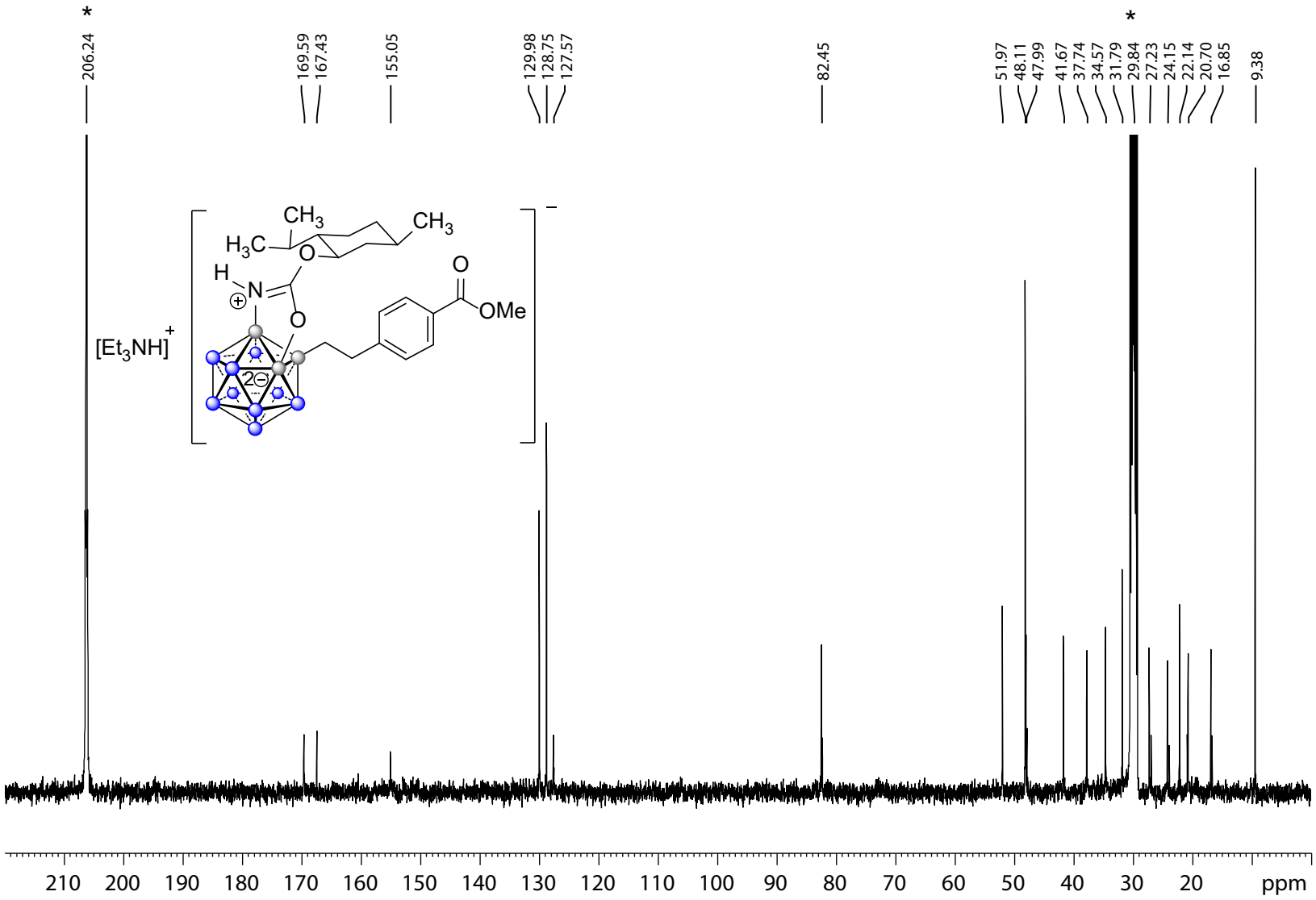
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB                20.00 Hz
GB        0
PC                 1.40
```

NMR-122

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              19.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 4098
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.8 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

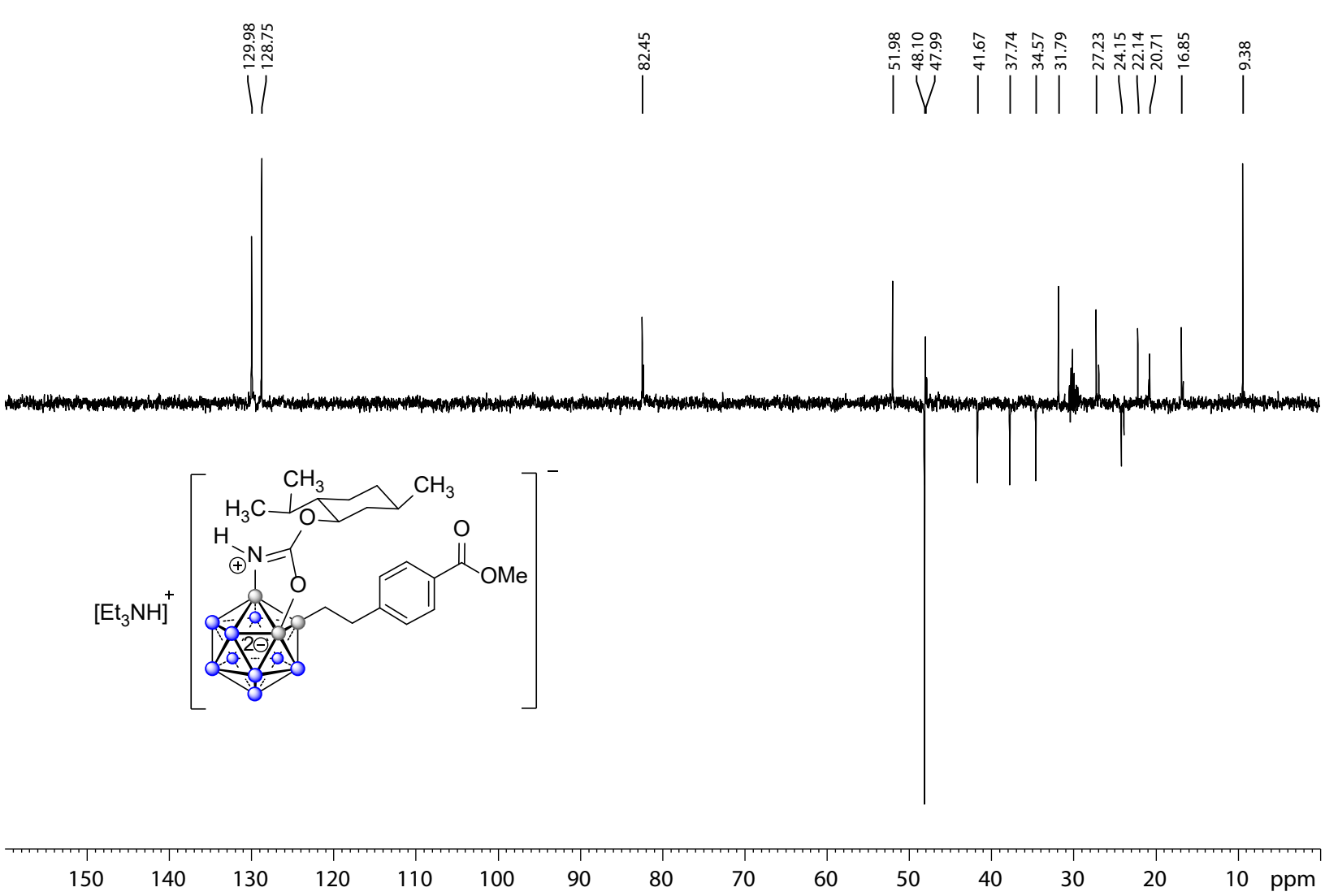
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126805 MHz
WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

20190128-B12M-4COOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4COOMe$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                  6
PROCNO                 1

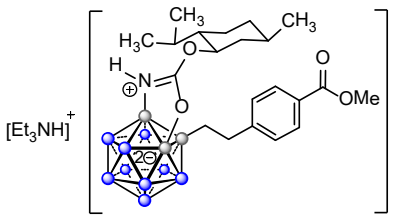
F2 - Acquisition Parameters
Date_           20190129
Time              20.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                296.2 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

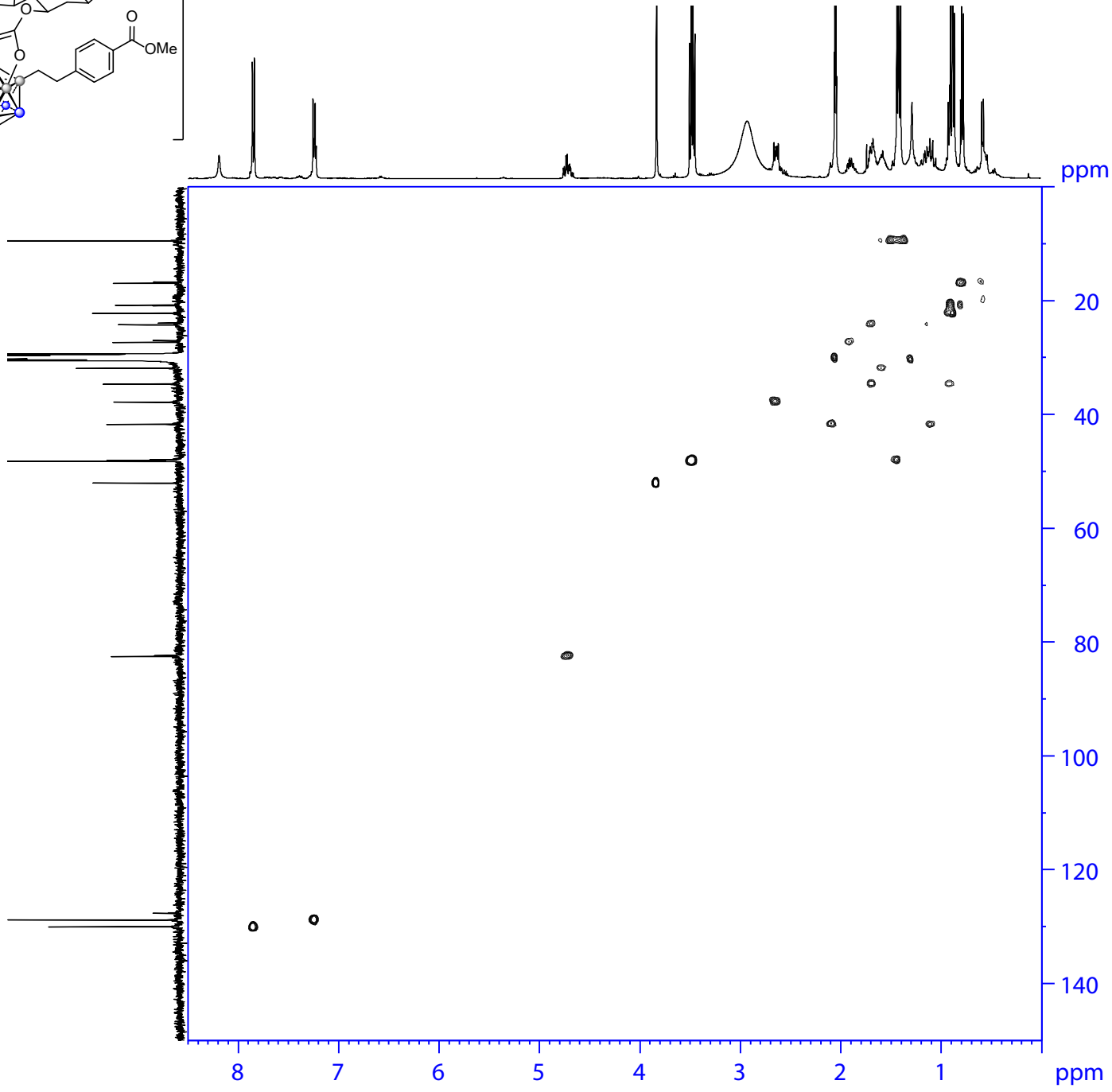
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126805 MHz
WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                4.00
```

20190128-B12M-4COOMeStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)OCH₂CH₂C₆H₄COOMe] dissolved in 0.6 mL acetone-*d*6*



^{1}H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190128-RV-B12M-4COMe-STYR-II
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20190129
Time              20.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ            0.0851968 sec
RG               193.34
DW               83.200 usec
DE                6.50 usec
TE               296.5 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPNAM[4]     SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                 256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

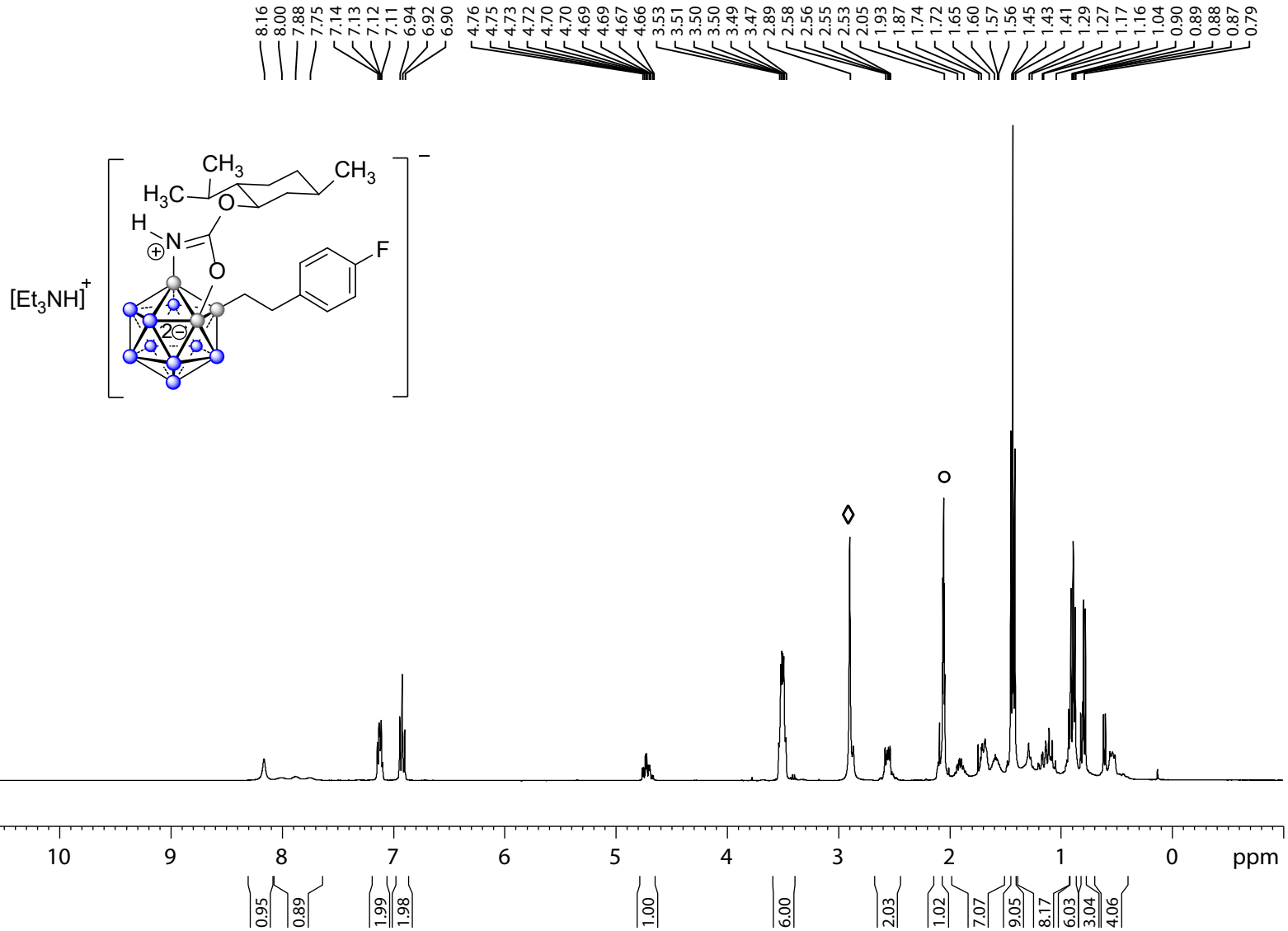
F2 - Processing parameters
SI                1024
SF          400.1300039 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126679 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

NMR-125

20190118-B12M-4FStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190118-RV-B12M-4FSTYR-I
EXPNO                 1
PROCNO                1

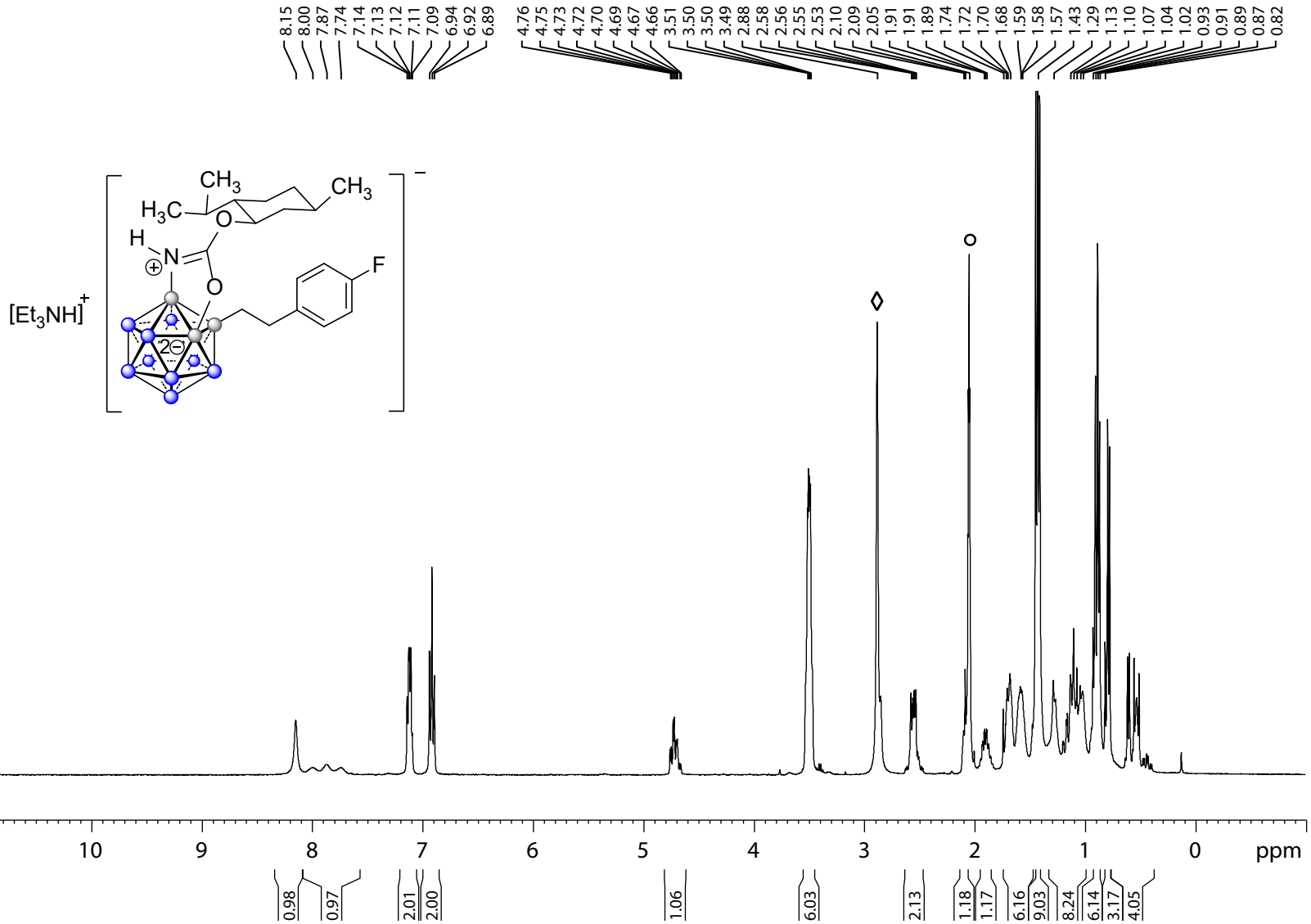
F2 - Acquisition Parameters
Date_           20190119
Time              18.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   64
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                193.34
DW                50.000 usec
DE                 6.50 usec
TE                295.8 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300068 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20190118-B12M-4FStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190118-RV-B12M-4FSTYR-I
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190119
Time              18.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgig30
TD               16384
SOLVENT         Acetone
NS                  16
DS                   4
SWH           8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG               107.6
DW              62.400 usec
DE               6.50 usec
TE              296.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

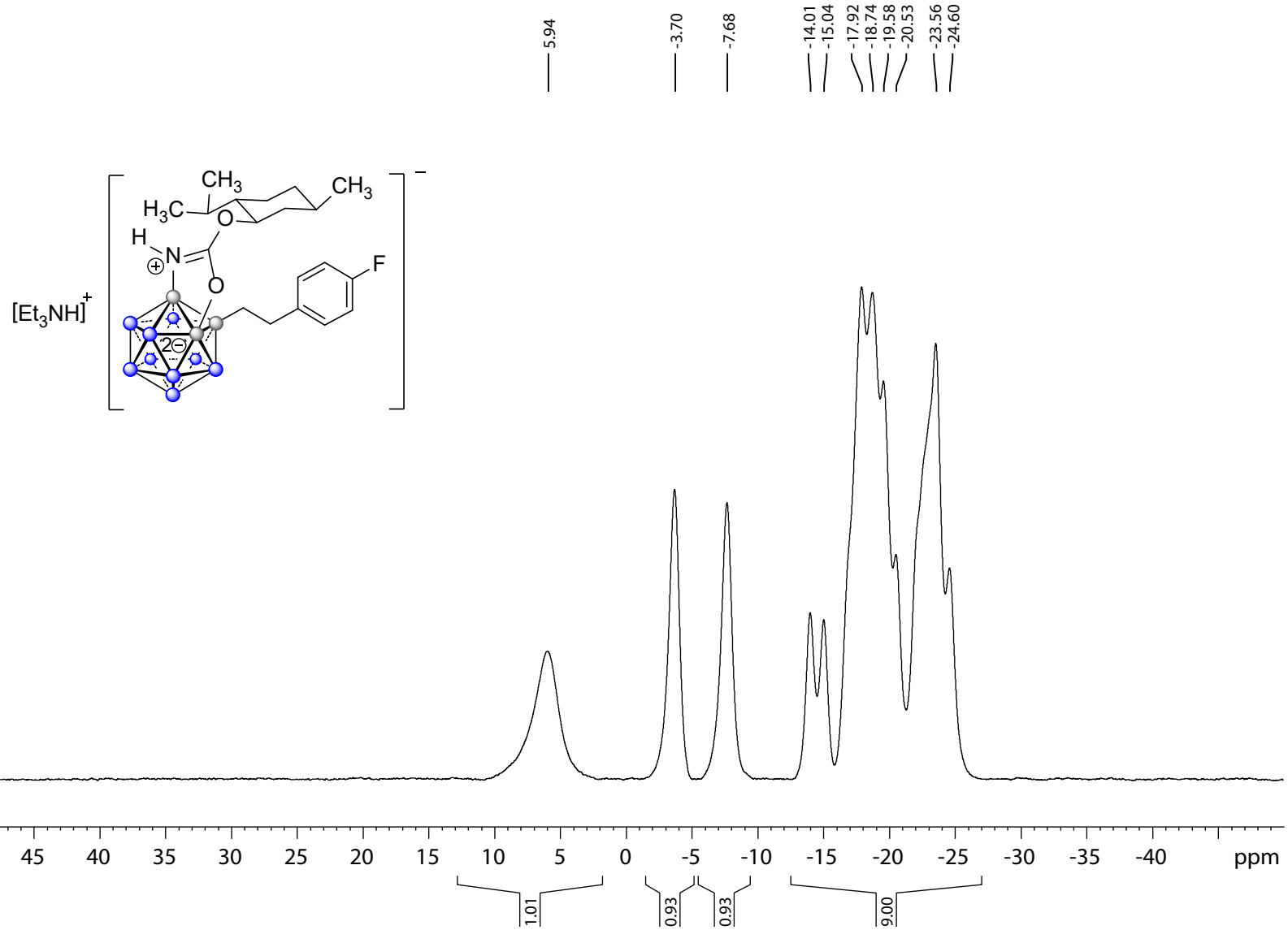
======== CHANNEL f1 ========
NUC1                1H
P1              15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2               11B
PCPD2           90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                32768
SF         400.1300069 MHz
WDW                EM
SSB       0
LB              1.00 Hz
GB        0
PC              1.40
```

20190717-B12M-4FStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190717
Time                   17.15
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                   zg
TD                     65536
SOLVENT              Acetone
NS                         128
DS                           4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                     295.0 K
D1                 1.00000000 sec
TD0                          1

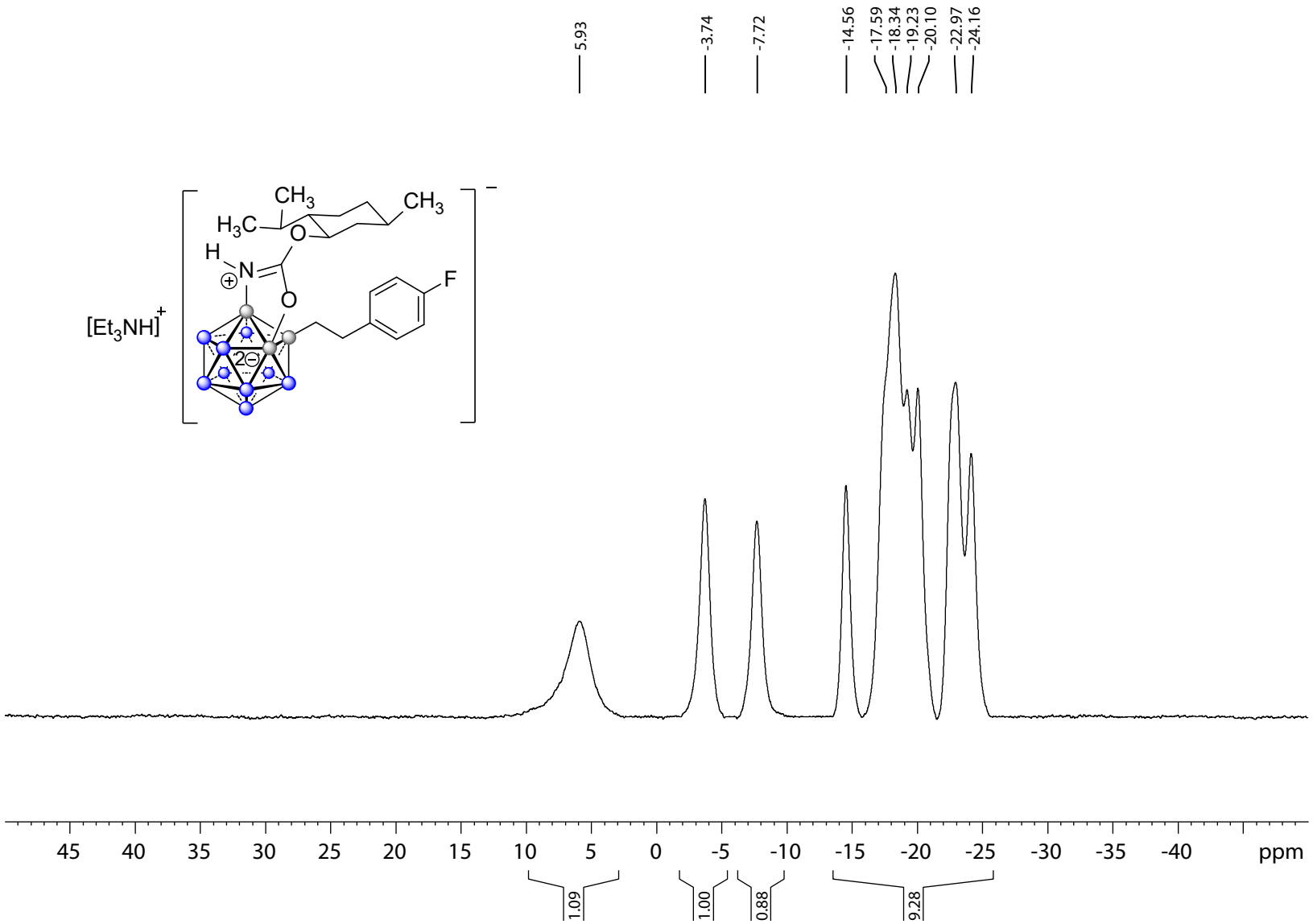
======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1              52.96599960 W
SFO1             128.3776052 MHz

F2 - Processing parameters
SI                         32768
SF               128.3776050 MHz
WDW                           EM
SSB          0
LB                       10.00 Hz
GB           0
PC                        1.40
```

NMR-128

20190717-B12M-4FStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190717
Time                   17.21
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT             Acetone
NS                        128
DS                          4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                     295.6 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                         1

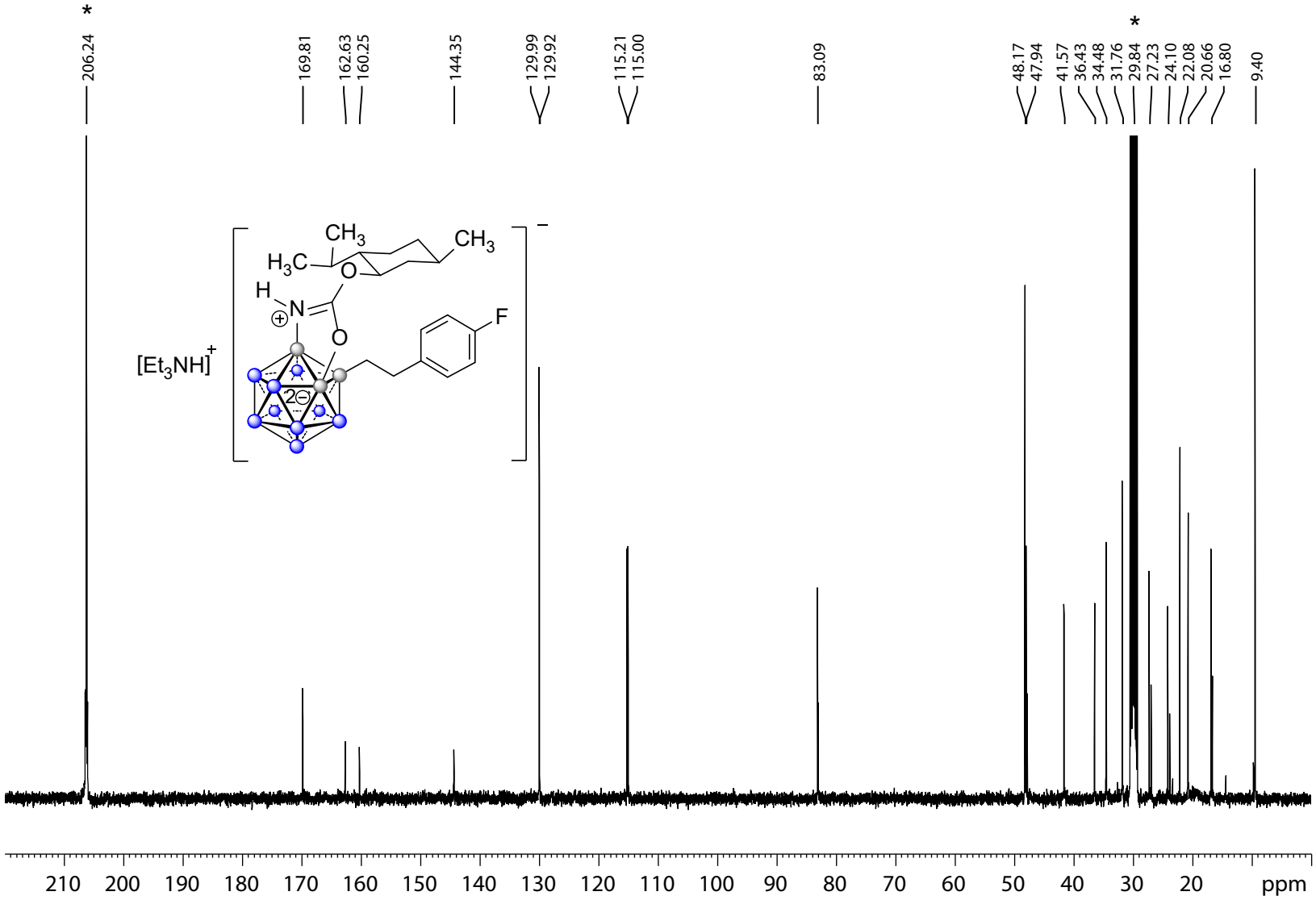
======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1               52.96599960 W
SFO1              128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2               waltz16
NUC2                       1H
PCPD2                  80.00 usec
PLW2               12.50000000 W
PLW12               0.43945000 W
PLW13               0.28125000 W
SFO2              400.1320007 MHz

F2 - Processing parameters
SI                        32768
SF                128.3776050 MHz
WDW                          EM
SSB       0
LB                     10.00 Hz
GB        0
PC                      1.40
```

20190717-B12M-4FStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4F$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                          5
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190717
Time                   18.55
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT             Acetone
NS                       2048
DS                          4
SWH                29761.904 Hz
FIDRES              0.454131 Hz
AQ                  1.1010048 sec
RG                     193.34
DW                     16.800 usec
DE                      6.50 usec
TE                     296.1 K
D1                  1.50000000 sec
D11                 0.03000000 sec
TD0                         1

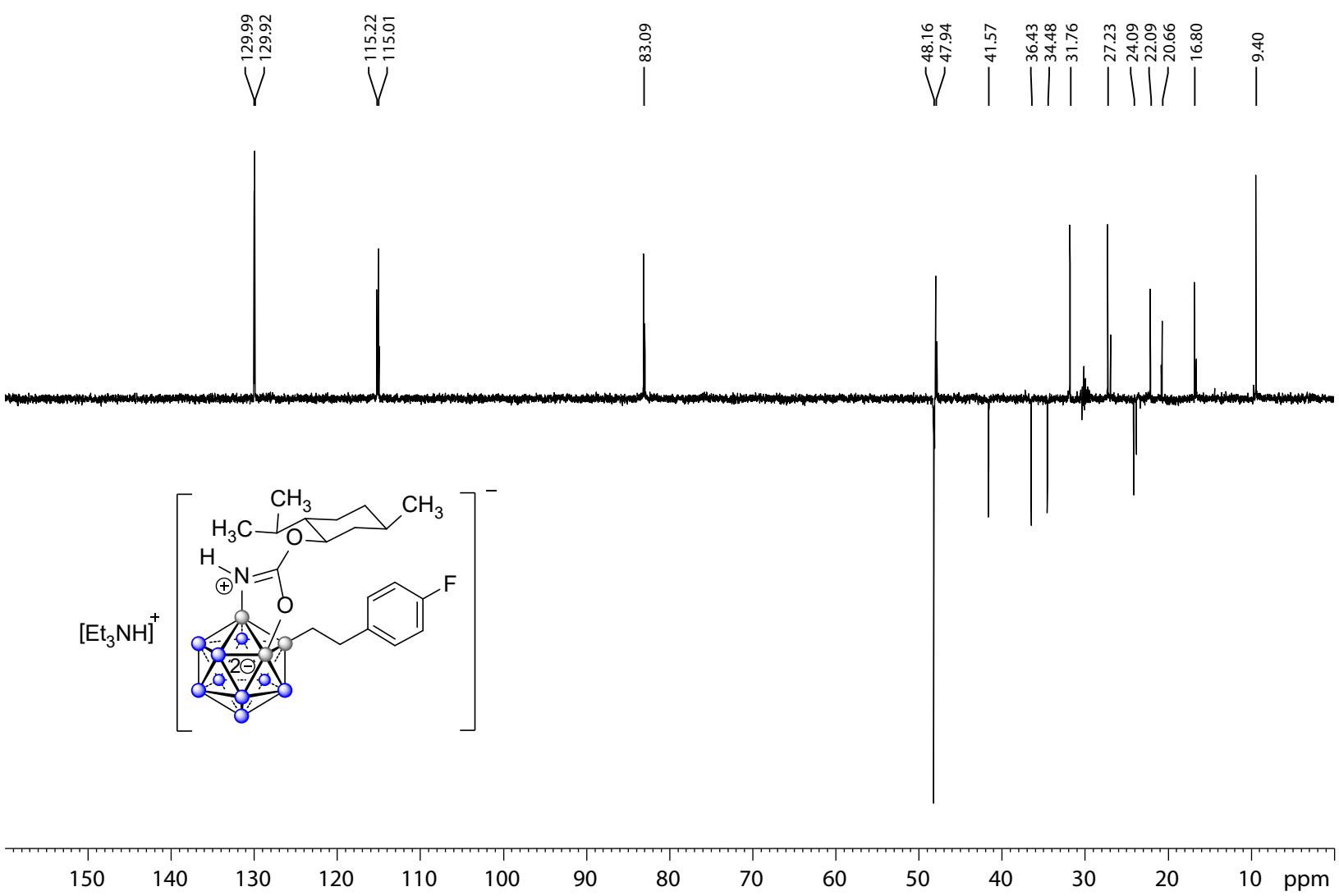
======== CHANNEL f1 ========
NUC1                      13C
P1                      10.00 usec
PLW1               53.00000000 W
SFO1              100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                      1H
PCPD2                  80.00 usec
PLW2               12.50000000 W
PLW12               0.43945000 W
PLW13               0.28125000 W
SFO2              400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF                100.6126839 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

20190118-B12M-4FStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz



$[Et_3NH]^+$

```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                          6
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190717
Time                   19.23
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              dept135
TD                     65536
SOLVENT              Acetone
NS                         512
DS                           4
SWH                29296.875 Hz
FIDRES              0.447035 Hz
AQ                  1.1184810 sec
RG                     193.34
DW                     17.067 usec
DE                       6.50 usec
TE                      295.5 K
CNST2             145.0000000
D1                  2.00000000 sec
D2                  0.00344828 sec
D12                 0.00002000 sec
TD0                          1

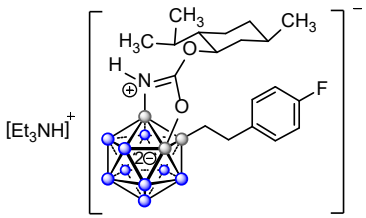
======== CHANNEL f1 ========
NUC1                       13C
P1                       10.00 usec
P2                       20.00 usec
PLW1              53.00000000 W
SFO1             100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                       1H
P3                       15.00 usec
P4                       30.00 usec
PCPD2                    80.00 usec
PLW2              12.50000000 W
PLW12              0.43945000 W
SFO2             400.1316005 MHz

F2 - Processing parameters
SI                       32768
SF                100.6126837 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        4.00
```

20190118-B12M-4FStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)OCH₂CH₂C₆H₄F] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹H COSY NMR



NMR-132

```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                          8
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190717
Time                   19.39
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG        cosygpppqf
TD                     2048
SOLVENT             Acetone
NS                           2
DS                           8
SWH                 5341.880 Hz
FIDRES              2.608340 Hz
AQ                  0.1916928 sec
RG                     124.48
DW                     93.600 usec
DE                      6.50 usec
TE                     295.3 K
D0                  0.00000300 sec
D1                  2.00000000 sec
D11                 0.03000000 sec
D12                 0.00002000 sec
D13                 0.00000400 sec
D16                 0.00020000 sec
IN0                 0.00018720 sec

======== CHANNEL f1 ========
NUC1                         1H
P0                       15.00 usec
P1                       15.00 usec
P17                    2500.00 usec
PLW1                12.50000000 W
PLW10                4.16050005 W
SFO1               400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                    10.00 %
P16                   1000.00 usec

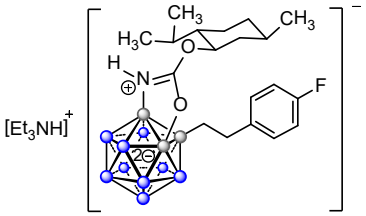
F1 - Acquisition parameters
TD                           128
SFO1                  400.1324 MHz
FIDRES               83.466881 Hz
SW                       13.350 ppm
FnMODE                       QF

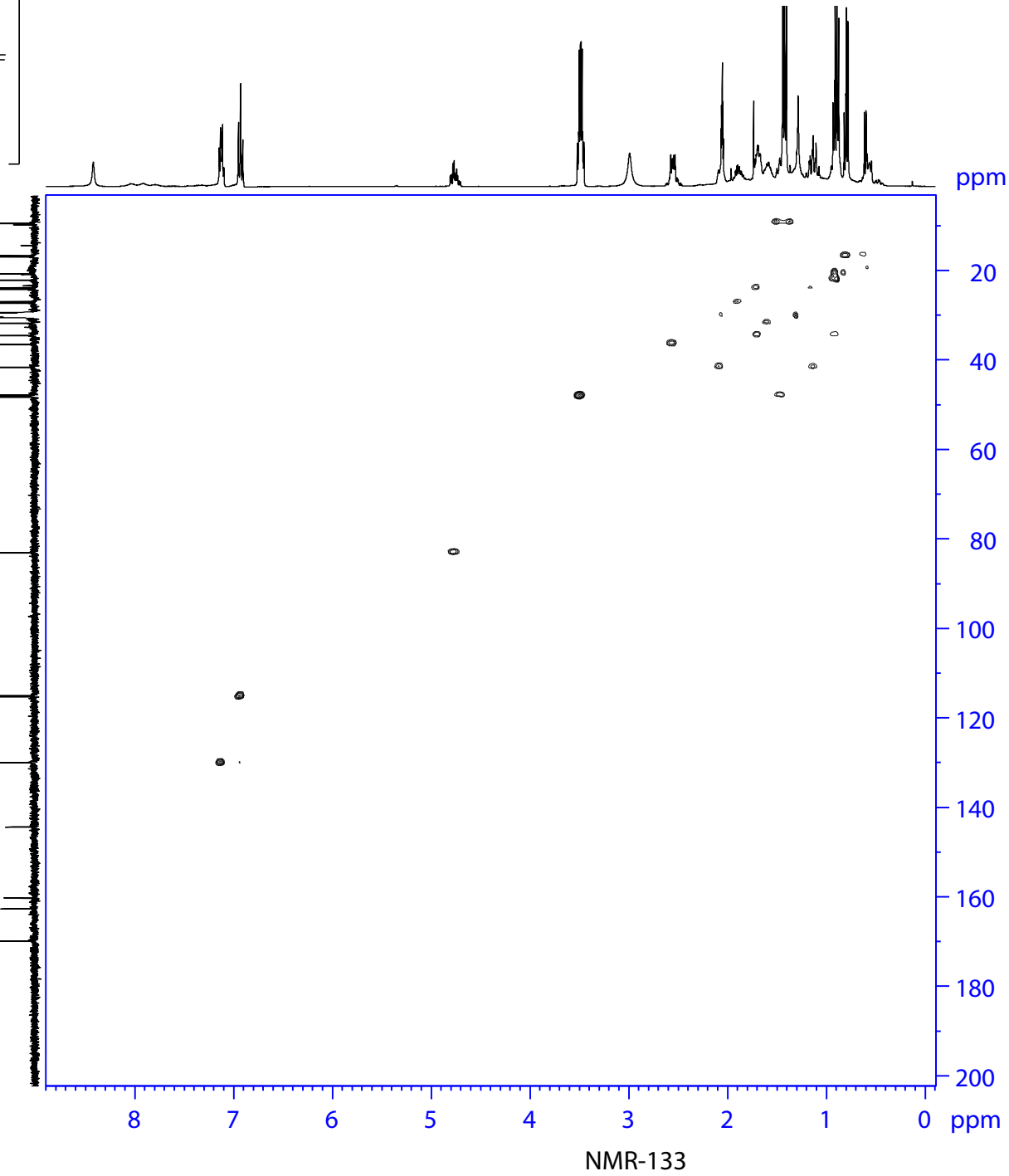
F2 - Processing parameters
SI                          1024
SF                 400.1300096 MHz
WDW                       QSINE
SSB       0
LB        0 Hz
GB        0
PC                        1.40

F1 - Processing parameters
SI                          1024
MC2                           QF
SF                 400.1300095 MHz
WDW                       QSINE
SSB       0
LB        0 Hz
GB        0
```

20190118-B12M-4FStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4F$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR






```
Current Data Parameters
NAME      20190717-RV-B12M4FStyr
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_            20190717
Time                19.25
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                  1024
SOLVENT          Acetone
NS                     2
DS                    16
SWH              6009.615 Hz
FIDRES           5.868765 Hz
AQ               0.0851968 sec
RG                 193.34
DW                  83.200 usec
DE                   6.50 usec
TE                  295.4 K
CNST2          145.0000000
D0              0.00000300 sec
D1              1.50000000 sec
D4              0.00172414 sec
D11             0.03000000 sec
D16             0.00020000 sec
D24             0.00086207 sec
IN0             0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
P2                  30.00 usec
P28               1000.00 usec
PLW1           12.50000000 W
SFO1          400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                  10.00 usec
P4                  20.00 usec
PCPD2               70.00 usec
PLW2           53.00000000 W
PLW12           1.08159995 W
SFO2          100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

F1 - Acquisition parameters
TD                    256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW              249.991 ppm
FnMODE     Echo-Antiecho

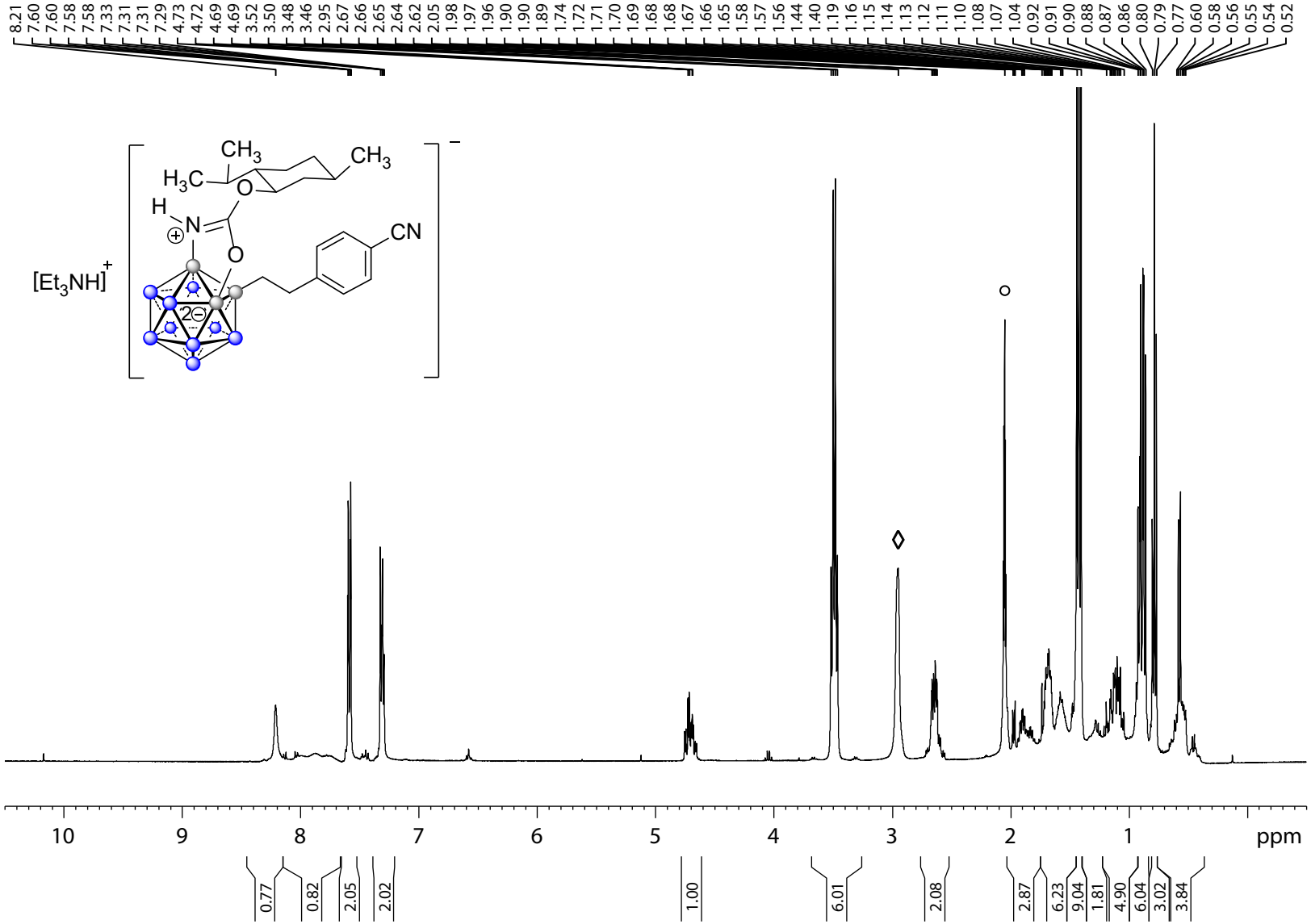
F2 - Processing parameters
SI                   1024
SF           400.1300020 MHz
WDW                  QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF           100.6126718 MHz
WDW                  QSINE
SSB                     2
LB         0 Hz
GB         0
```

NMR-133

20190310-B12M-4CNStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   6.13
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT           Acetone
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2767999 sec
RG                     86.58
DW                    50.000 usec
DE                     6.50 usec
TE                    294.3 K
D1               1.00000000 sec
TD0                       1

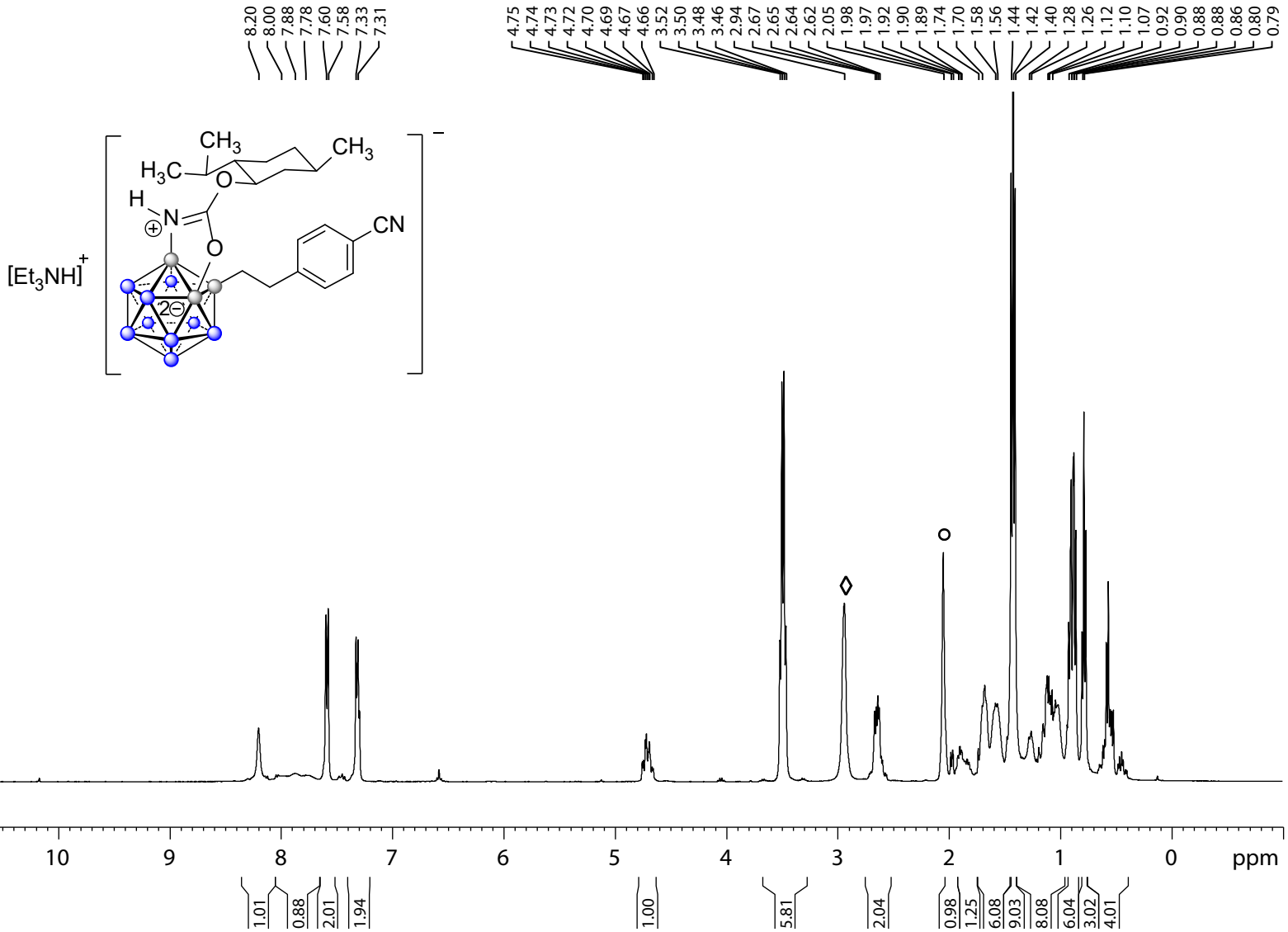
======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1            12.50000000 W
SFO1            400.1328009 MHz

F2 - Processing parameters
SI                    65536
SF              400.1300069 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

NMR-134

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   6.15
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                     107.6
DW                    62.400 usec
DE                     6.50 usec
TE                    294.5 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1          12.50000000 W
SFO1          400.1320007 MHz

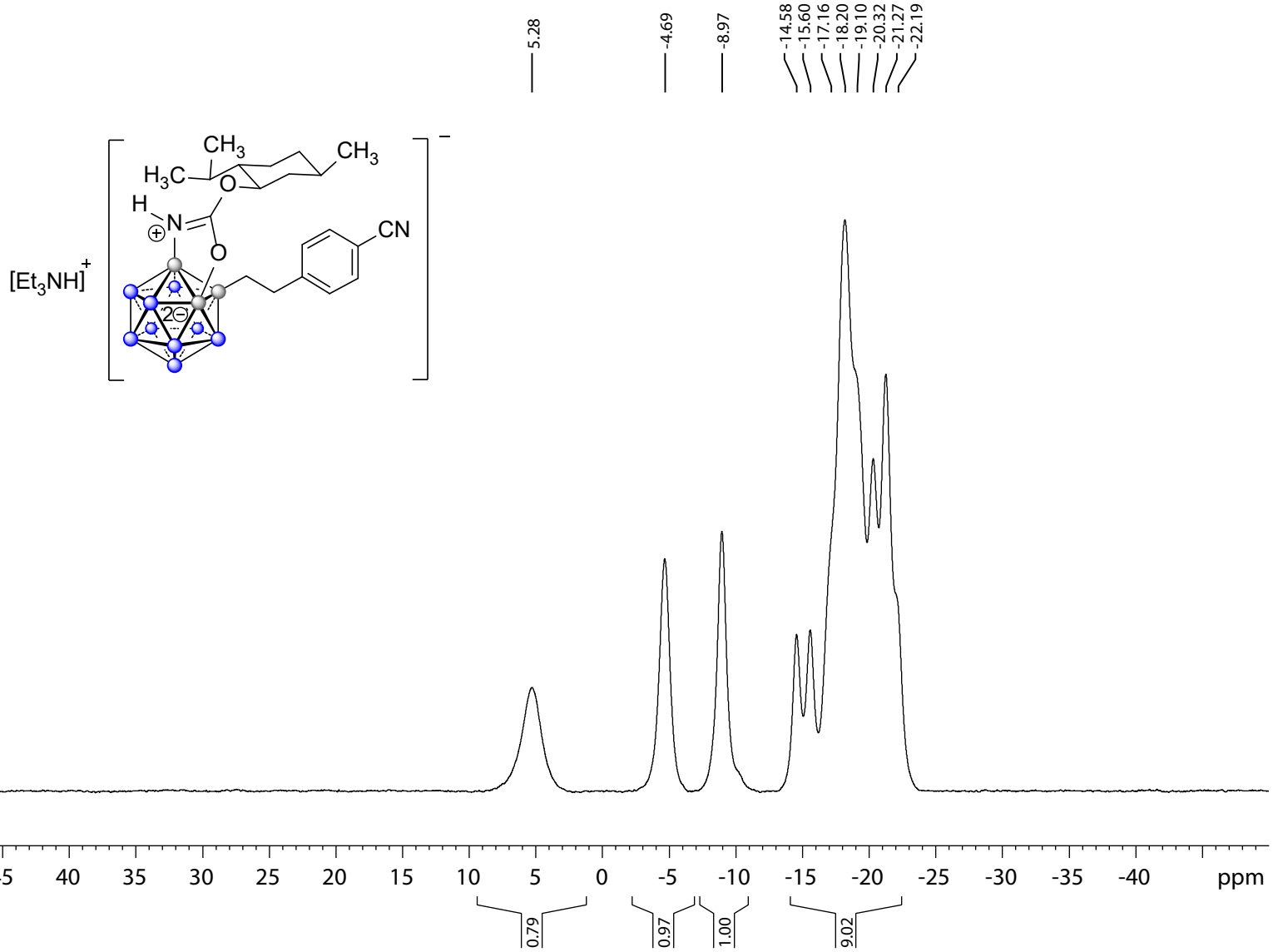
======== CHANNEL f2 ========
CPDPRG[2                garp4
NUC2                     11B
PCPD2                  90.00 usec
PLW2          52.96599960 W
PLW12          0.64477998 W
SFO2          128.3776050 MHz

F2 - Processing parameters
SI                     32768
SF            400.1300070 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

NMR-135

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   6.21
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg
TD                    65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   294.2 K
D1              1.00000000 sec
TD0                        1

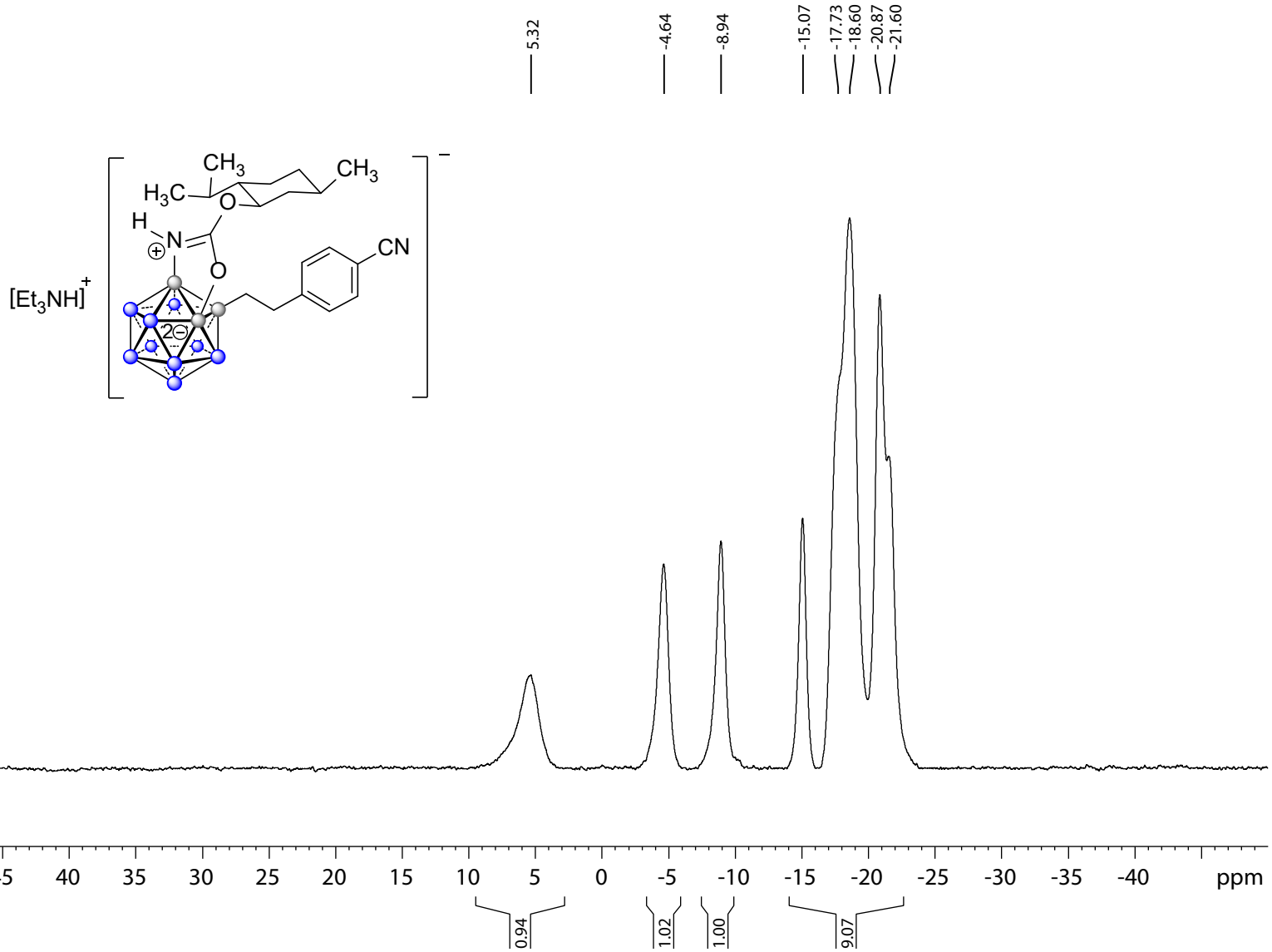
======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1           52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                       32768
SF             128.3776050 MHz
WDW                        EM
SSB         0
LB                    10.00 Hz
GB          0
PC                     1.40
```

NMR-136

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

11B{^{1}H} NMR 128MHz




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   6.27
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH              25510.203 Hz
FIDRES            0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   295.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

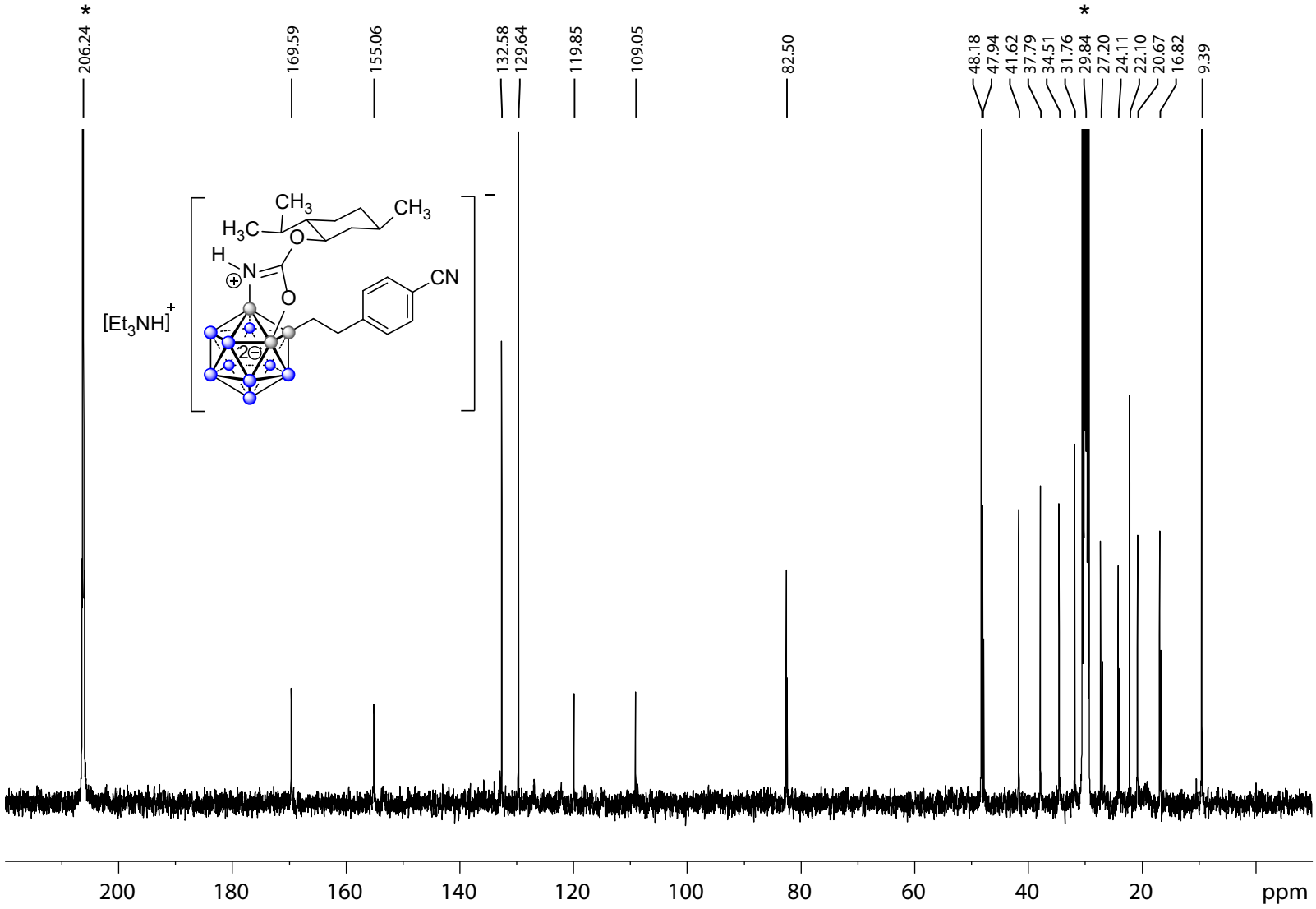
======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1          52.96599960 W
SFO1          128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                     1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2          400.1320007 MHz

F2 - Processing parameters
SI                       32768
SF            128.3776050 MHz
WDW                       EM
SSB       0
LB                   10.00 Hz
GB        0
PC                    1.40
```

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        5
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   8.00
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  295.0 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1

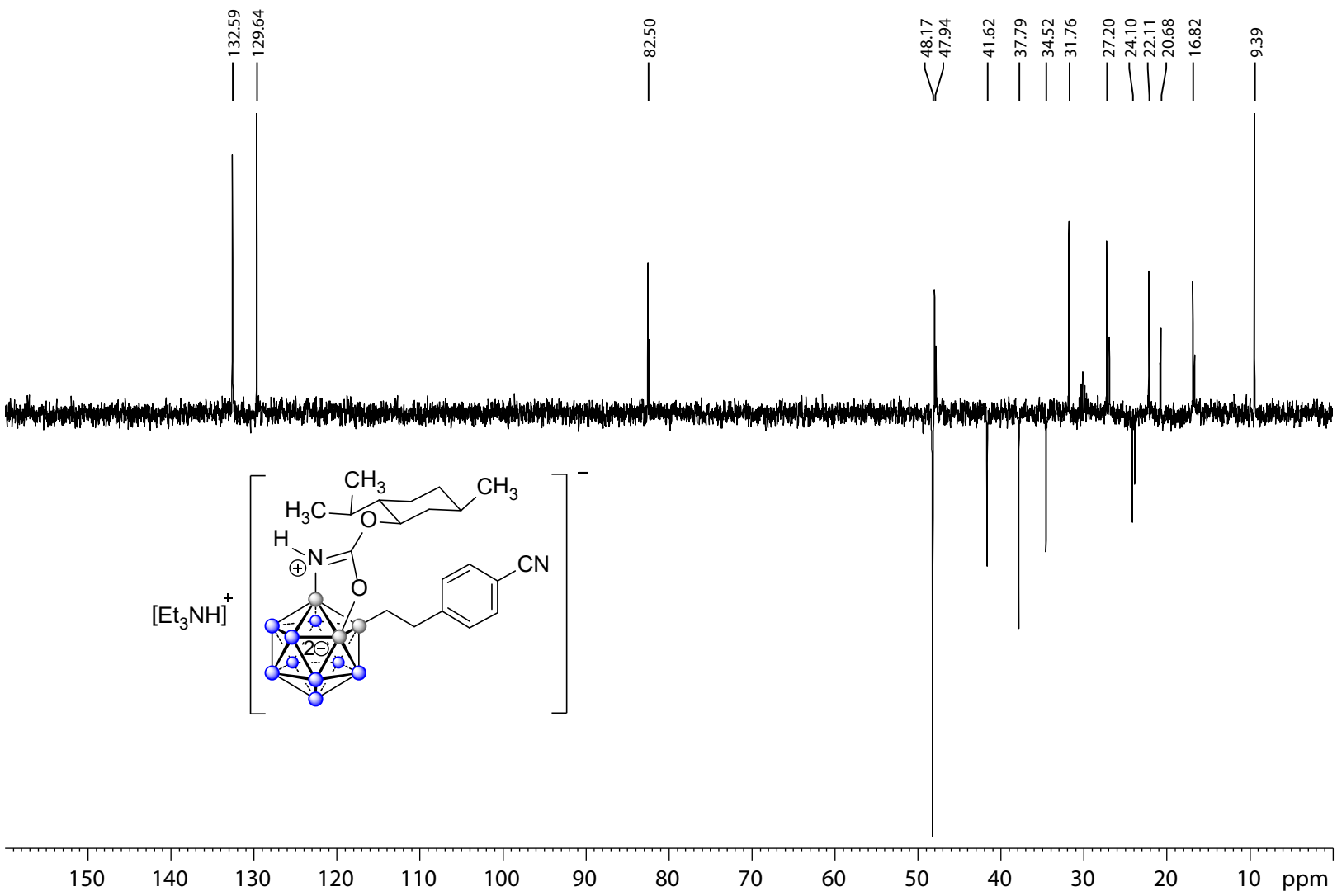
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6126831 MHz
WDW                    EM
SSB       0
LB                   2.00 Hz
GB        0
PC                   1.40
```

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz



[Et_3NH]$^+$

```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        6
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   8.14
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG           dept135
TD                  65536
SOLVENT           Acetone
NS                    256
DS                      4
SWH             29296.875 Hz
FIDRES           0.447035 Hz
AQ               1.1184810 sec
RG                 193.34
DW                 17.067 usec
DE                  6.50 usec
TE                 294.4 K
CNST2         145.0000000
D1              2.00000000 sec
D2              0.00344828 sec
D12             0.00002000 sec
TD0                     1

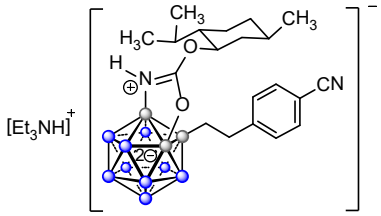
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
P2                   20.00 usec
PLW1          53.00000000 W
SFO1          100.6228293 MHz

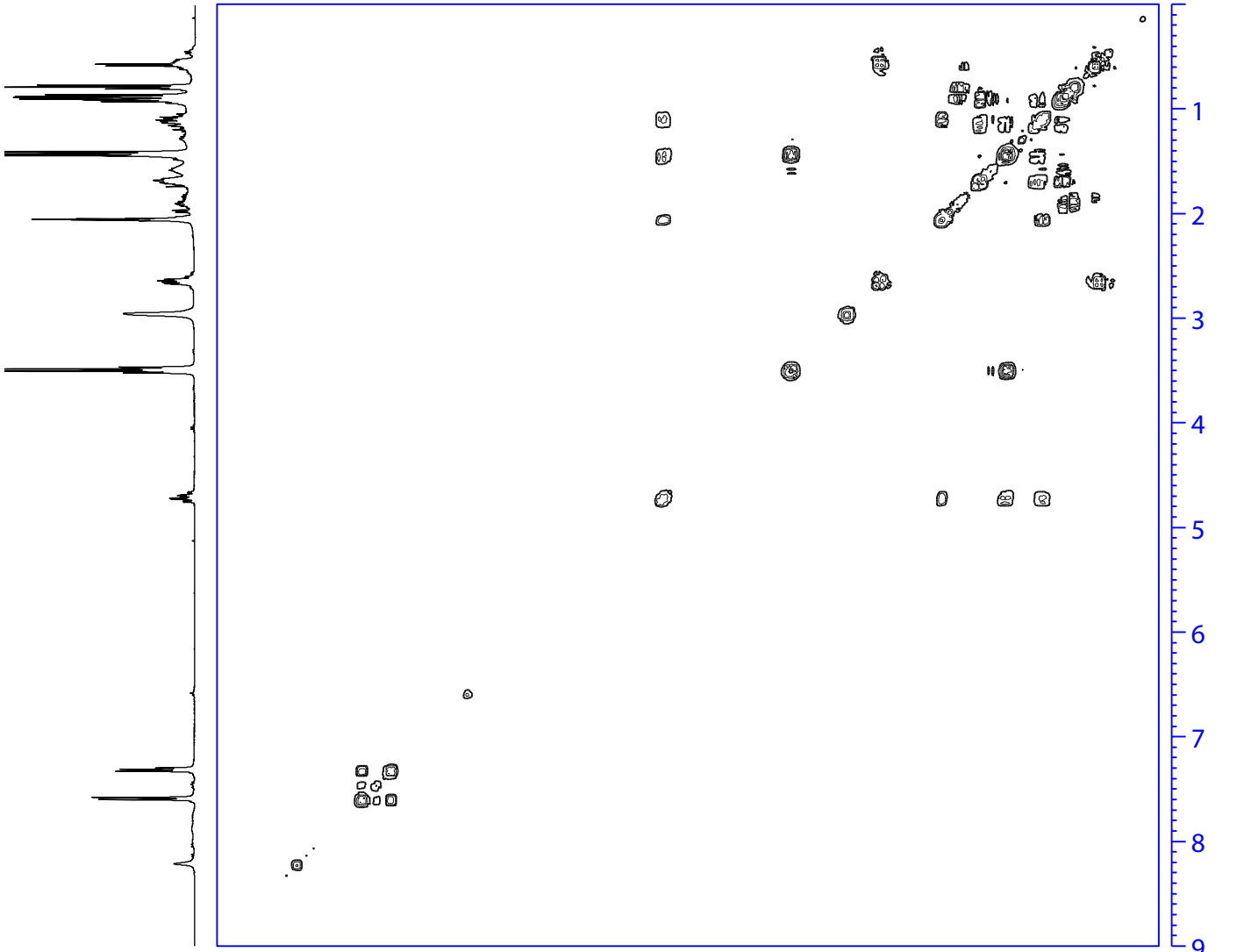
======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
P3                   15.00 usec
P4                   30.00 usec
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                    32768
SF            100.6126829 MHz
WDW                     EM
SSB       0
LB                    2.00 Hz
GB        0
PC                    4.00
```

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-140

```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        7
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   8.15
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG       cosygpppqf
TD                     2048
SOLVENT          Acetone
NS                        2
DS                        8
SWH              5341.880 Hz
FIDRES           2.608340 Hz
AQ               0.1916928 sec
RG                  170.36
DW                  93.600 usec
DE                   6.50 usec
TE                  294.2 K
D0               0.00000300 sec
D1               2.00000000 sec
D11              0.03000000 sec
D12              0.00002000 sec
D13              0.00000400 sec
D16              0.00020000 sec
IN0              0.00018720 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                    15.00 usec
P1                    15.00 usec
P17                 2500.00 usec
PLW1             12.50000000 W
PLW10             4.16050005 W
SFO1            400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                  10.00 %
P16                 1000.00 usec

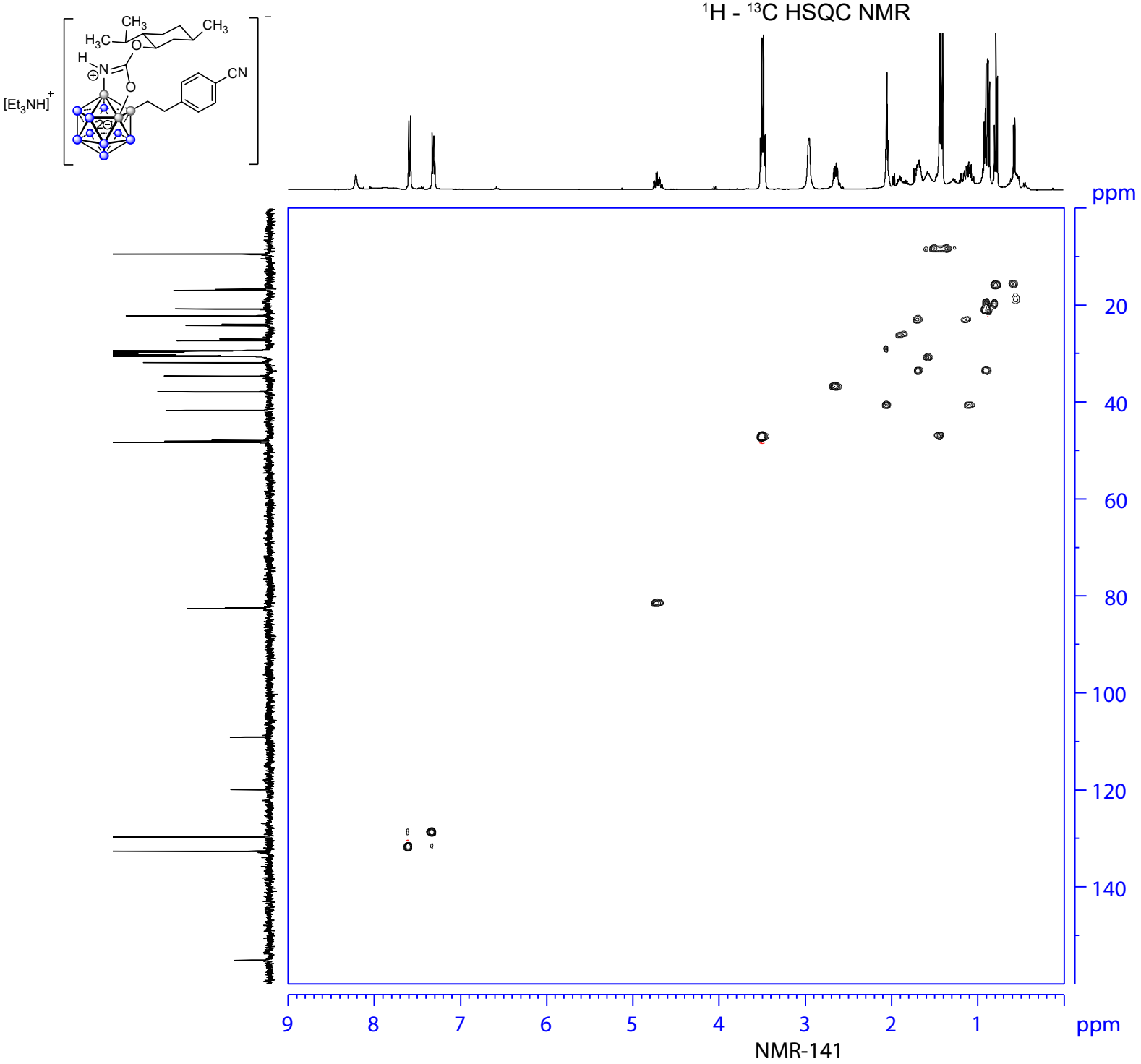
F1 - Acquisition parameters
TD                       128
SFO1              400.1324 MHz
FIDRES           83.466881 Hz
SW                  13.350 ppm
FnMODE                   QF

F2 - Processing parameters
SI                       1024
SF              400.1300000 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
GB           0
PC                       1.40

F1 - Processing parameters
SI                       1024
MC2                        QF
SF              400.1300000 MHz
WDW                    QSINE
SSB          0
LB           0 Hz
GB           0
```

20190310-B12M-4CNStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4CN$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      B12-MENTH-4CN-STYR-II
EXPNO                        8
PROCNO                       1

F2 - Acquisition Parameters
Date_              20190310
Time                   8.26
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                     1024
SOLVENT           Acetone
NS                       2
DS                      16
SWH                6009.615 Hz
FIDRES             5.868765 Hz
AQ                 0.0851968 sec
RG                    193.34
DW                  83.200 usec
DE                   6.50 usec
TE                  294.6 K
CNST2            145.0000000
D0                 0.00000300 sec
D1                 1.50000000 sec
D4                 0.00172414 sec
D11                0.03000000 sec
D16                0.00020000 sec
D24                0.00086207 sec
IN0                0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
P2                     30.00 usec
P28                  1000.00 usec
PLW1             12.50000000 W
SFO1            400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp
NUC2                     13C
P3                     10.00 usec
P4                     20.00 usec
PCPD2                  70.00 usec
PLW2             53.00000000 W
PLW12             1.08159995 W
SFO2            100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]       SMSQ10.100
GPNAM[2]       SMSQ10.100
GPNAM[3]       SMSQ10.100
GPNAM[4]       SMSQ10.100
GPZ1                   80.00 %
GPZ2                   20.10 %
GPZ3                   11.00 %
GPZ4                   -5.00 %
P16                  1000.00 usec
P19                   600.00 usec

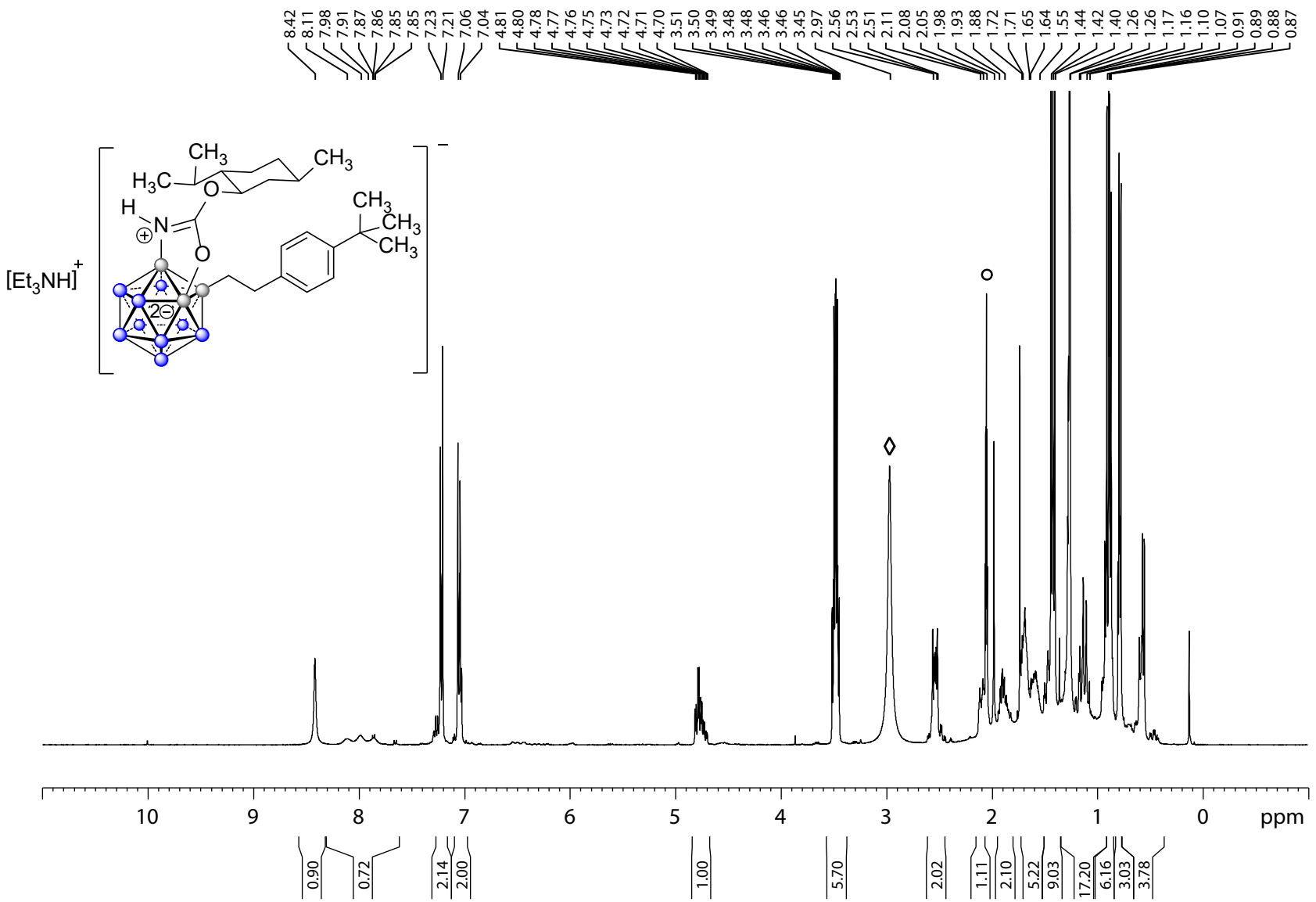
F1 - Acquisition parameters
TD                       256
SFO1               100.6238 MHz
FIDRES           196.524048 Hz
SW                  249.991 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                      1024
SF             400.1300000 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
PC                      1.40

F1 - Processing parameters
SI                      1024
MC2         echo-antiecho
SF              100.6127690 MHz
WDW                    QSINE
SSB                        2
LB         0 Hz
GB         0
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190324
Time               6.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ              3.2767999 sec
RG                71.39
DW                50.000 usec
DE                 6.50 usec
TE                295.7 K
D1            1.00000000 sec
TD0                   1

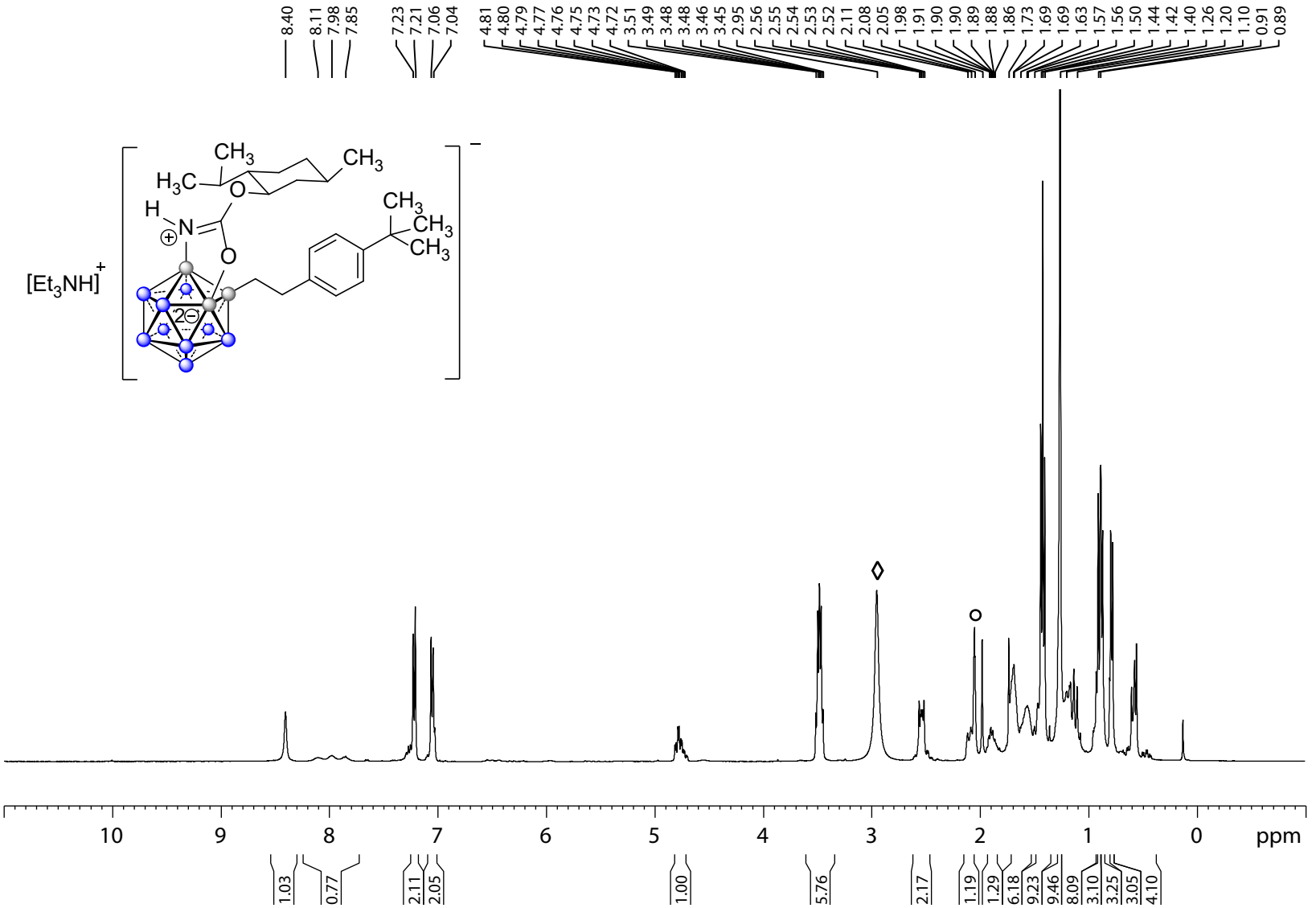
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300070 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-142

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190324
Time                6.35
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                78.69
DW               62.400 usec
DE                6.50 usec
TE                296.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

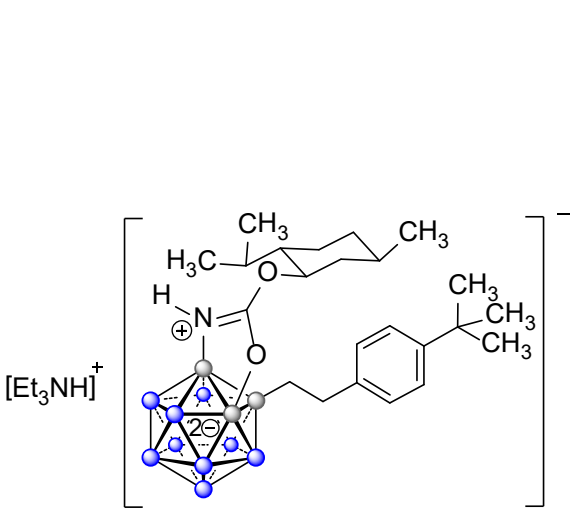
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300071 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20190324
Time              6.41
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               295.7 K
D1           1.00000000 sec
TD0                   1

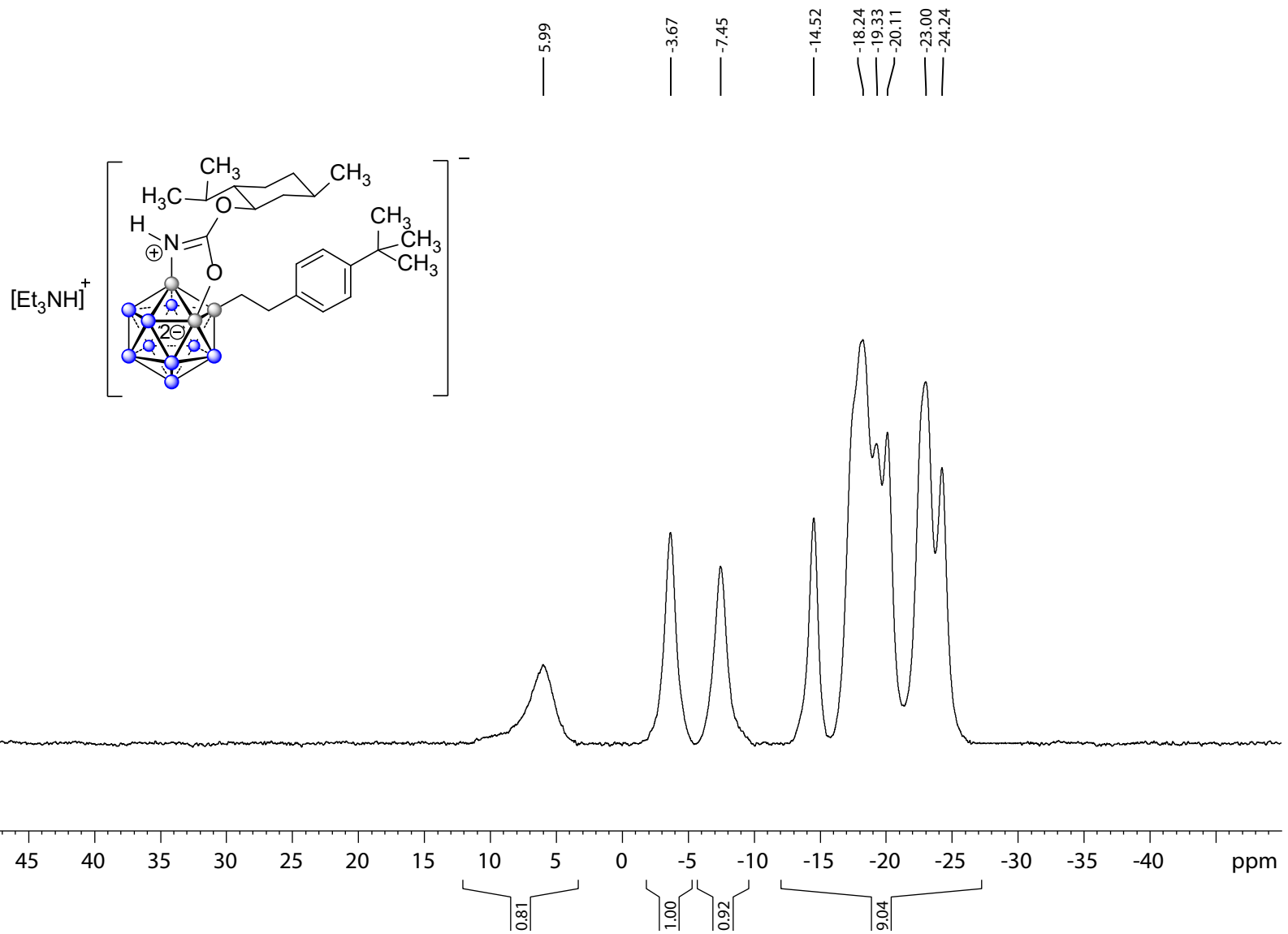
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                1.40
```

NMR-144

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20190324
Time              6.47
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

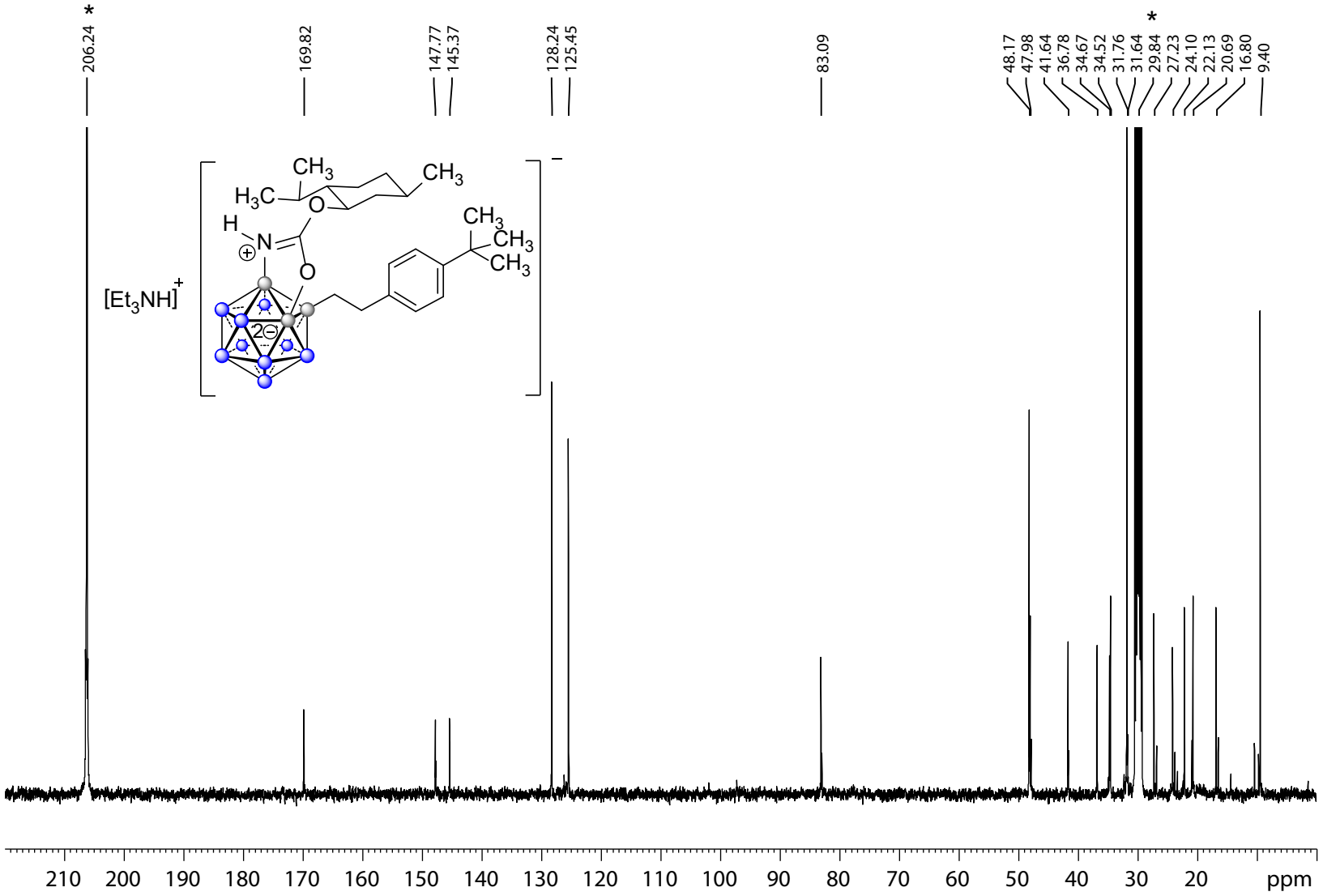
======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB              10.00 Hz
GB        0
PC               1.40
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20190324
Time               8.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.8 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

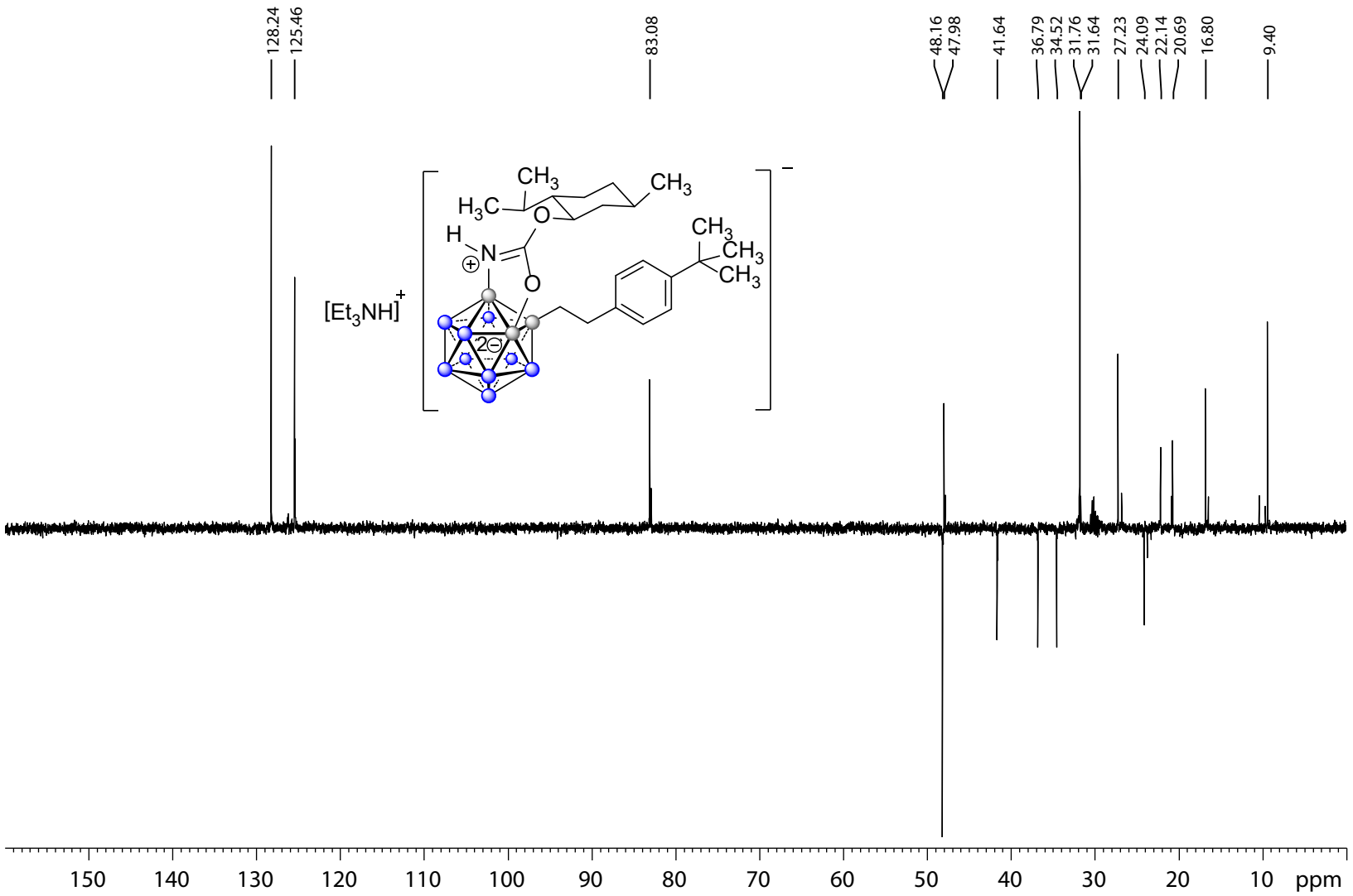
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126829 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                   6
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190324
Time                8.47
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          dept135
TD                 65536
SOLVENT          Acetone
NS                   512
DS                     4
SWH            29296.875 Hz
FIDRES          0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                296.3 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                    1

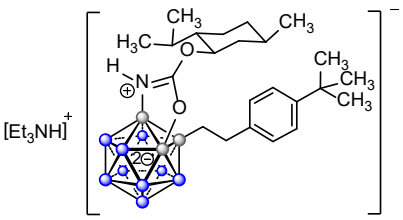
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126827 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et$_3$NH][B$_{12}$H$_{10}$NHC(Menthyl)OCH$_2$CH$_2$C$_6$H$_4$Bu] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{1}H COSY NMR




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20190324
Time              9.04
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH           5341.880 Hz
FIDRES        2.608340 Hz
AQ            0.1916928 sec
RG               124.48
DW               93.600 usec
DE                6.50 usec
TE                296.0 K
D0           0.00000300 sec
D1           2.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
D13          0.00000400 sec
D16          0.00020000 sec
IN0          0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1        400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

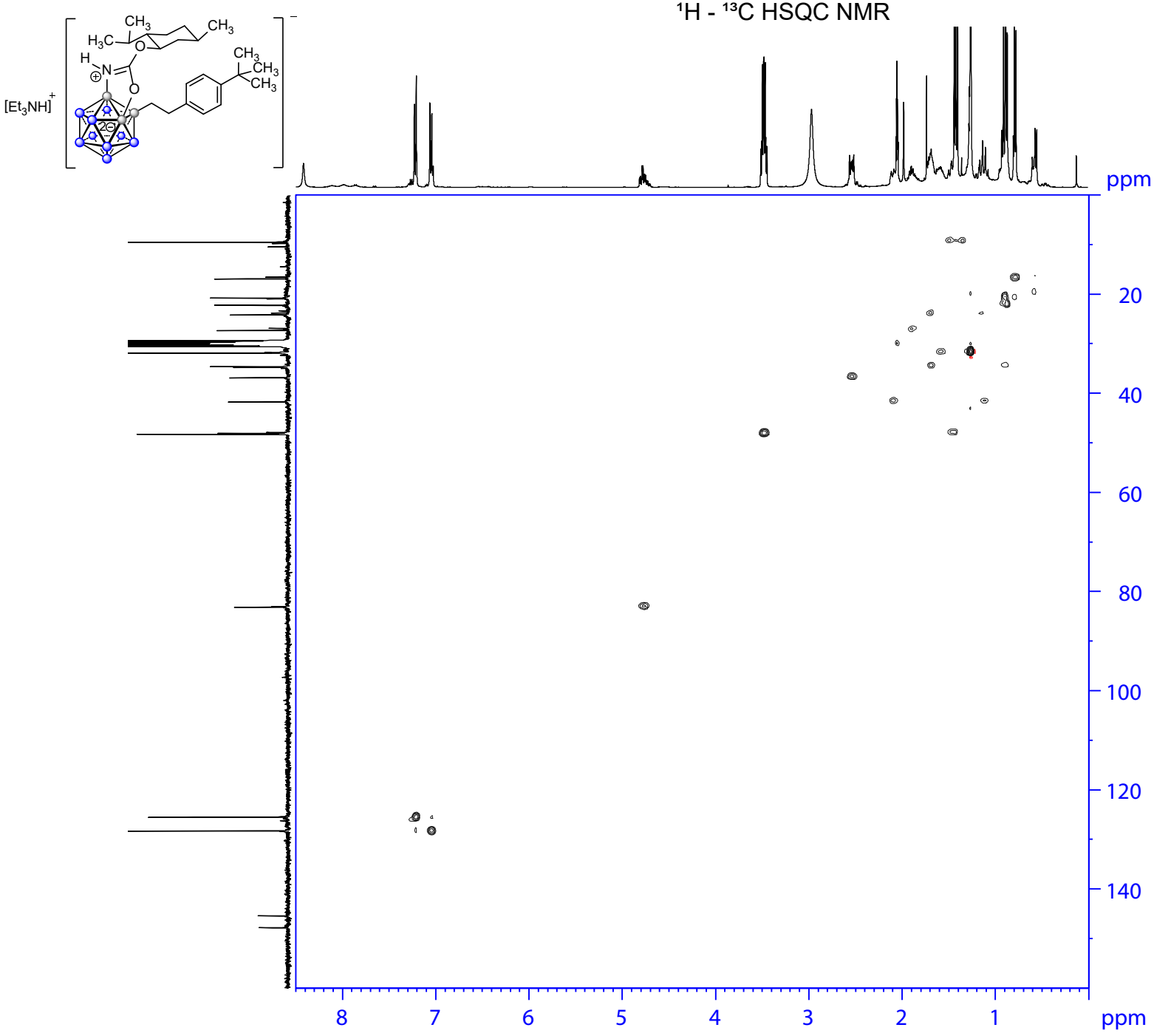
F1 - Acquisition parameters
TD                  128
SFO1          400.1324 MHz
FIDRES       83.466881 Hz
SW              13.350 ppm
FnMODE               QF

F2 - Processing parameters
SI                 1024
SF          400.1300068 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                 1024
MC2                  QF
SF          400.1300067 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
```

20190323-B12M-4tBuMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Bu$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190323-RV-B12Menth-4BuStyr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_           20190324
Time               8.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH           6009.615 Hz
FIDRES        5.868765 Hz
AQ           0.0851968 sec
RG              193.34
DW               83.200 usec
DE                6.50 usec
TE               296.1 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPNAM[4]     SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

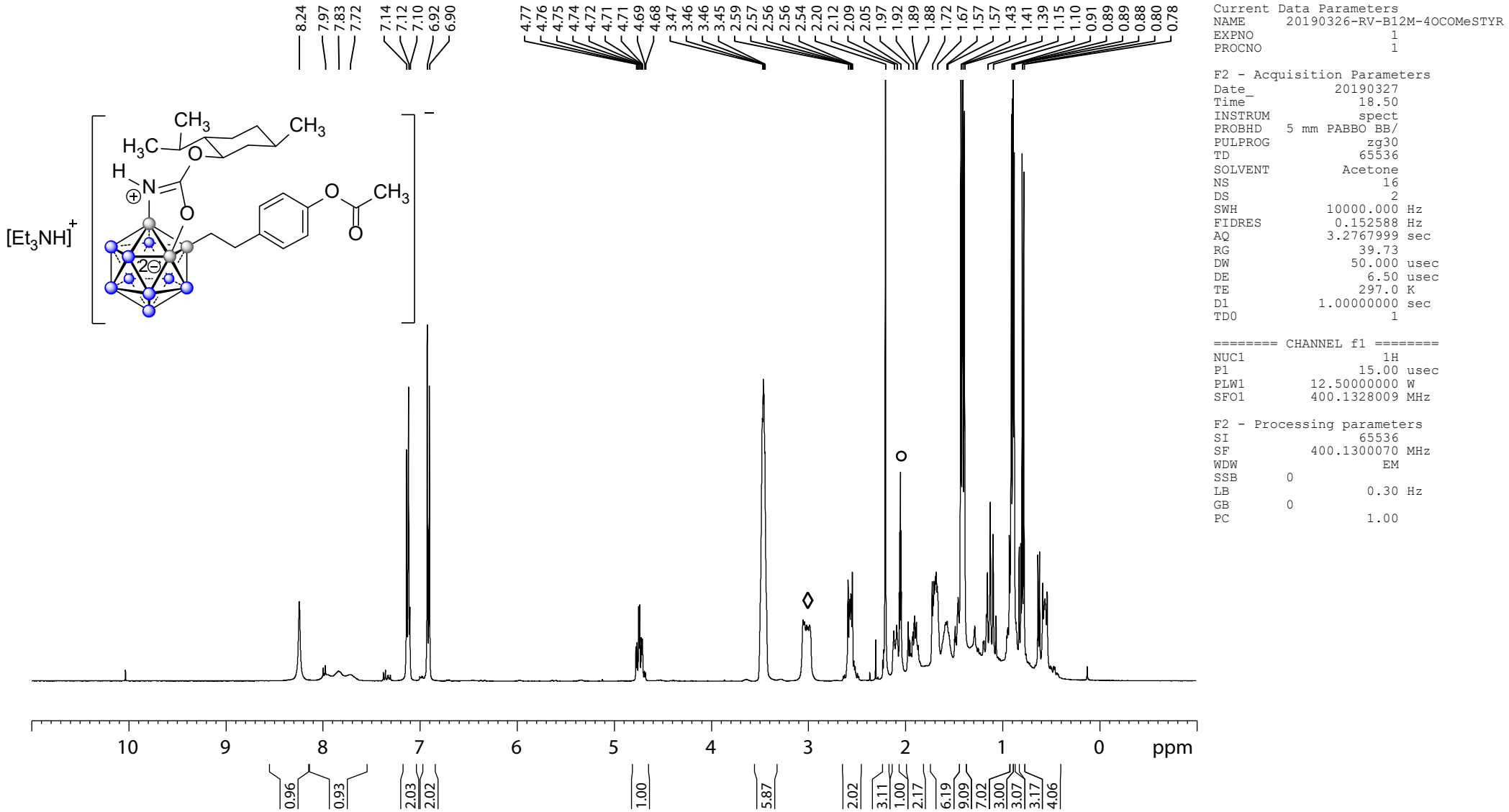
F2 - Processing parameters
SI                  1024
SF          400.1300092 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2       echo-antiecho
SF          100.6126749 MHz
WDW                QSINE
SSB                    2
LB        0 Hz
GB        0
```

NMR-149

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190326-RV-B12M-4OCOMeSTYR
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190327
Time              18.50
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                39.73
DW               50.000 usec
DE                6.50 usec
TE                297.0 K
D1           1.00000000 sec
TD0                   1

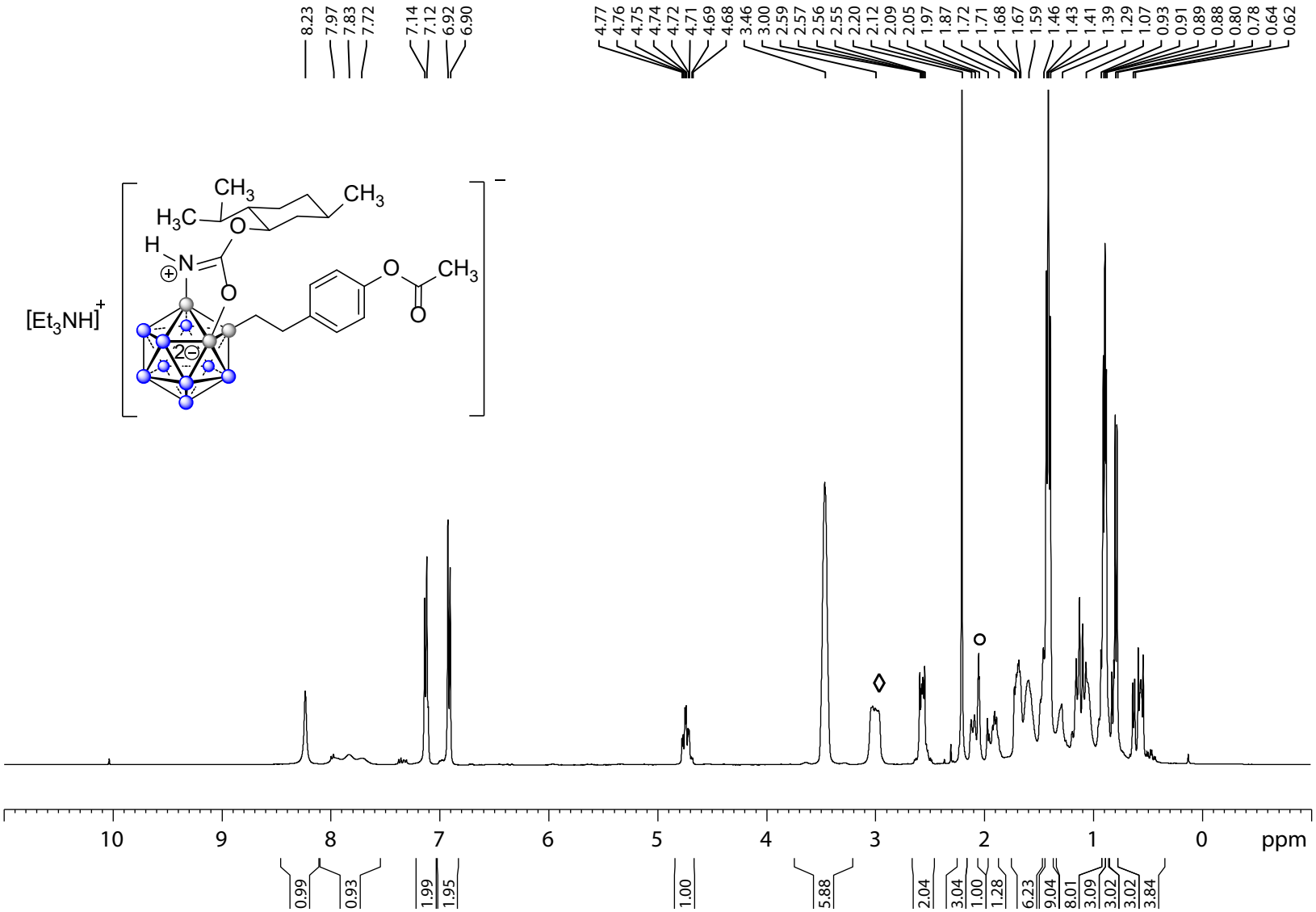
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300070 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-150

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190326-RV-B12M-4OCOMeSTYR
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190327
Time              18.51
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES          0.489064 Hz
AQ            1.0223616 sec
RG                39.73
DW                62.400 usec
DE                 6.50 usec
TE                297.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

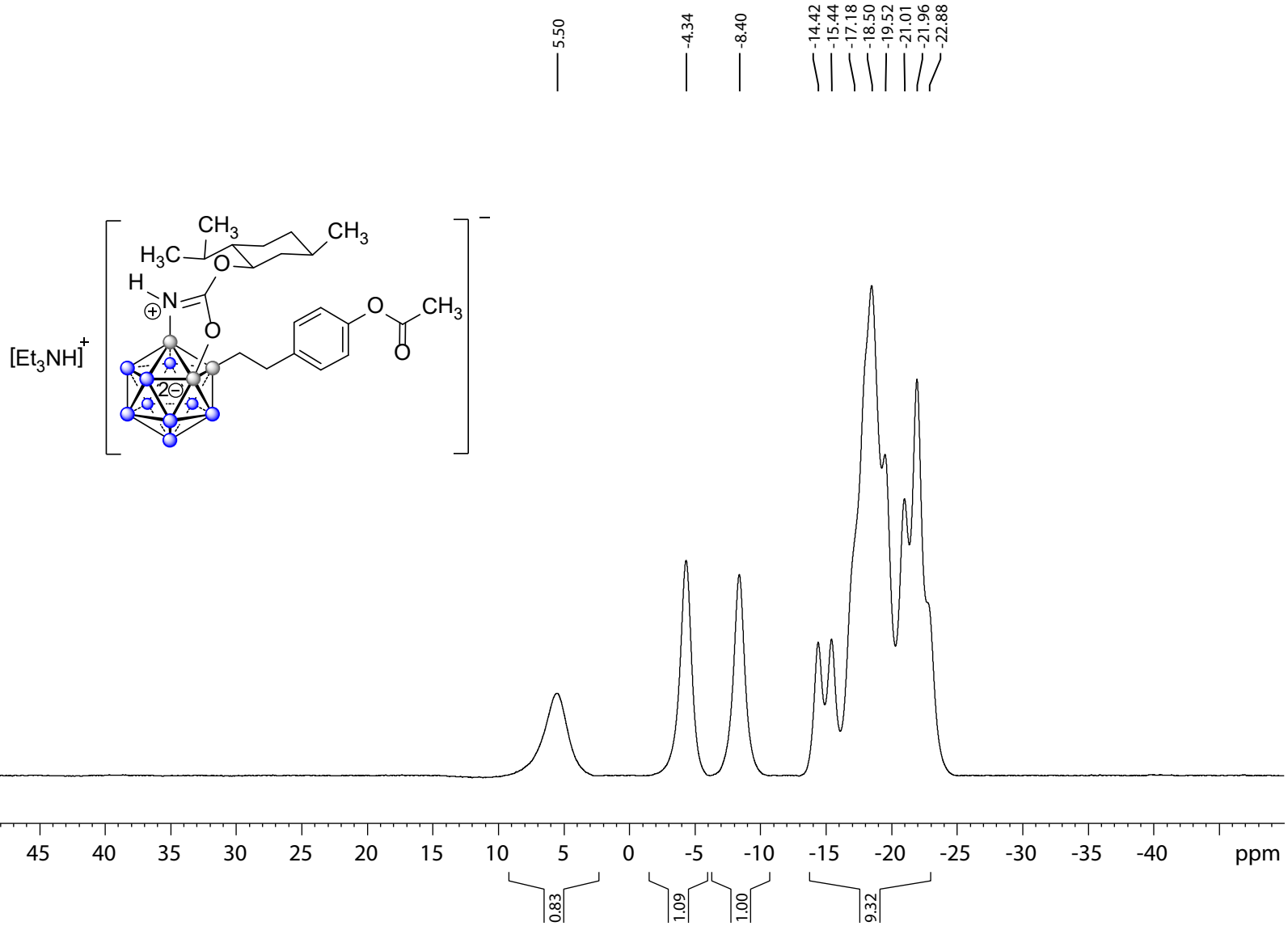
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2          garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300071 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190326-RV-B12M-4OCOMeSTYR
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20190327
Time              18.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG               193.34
DW              19.600 usec
DE               6.50 usec
TE              296.9 K
D1           1.00000000 sec
TD0                   1

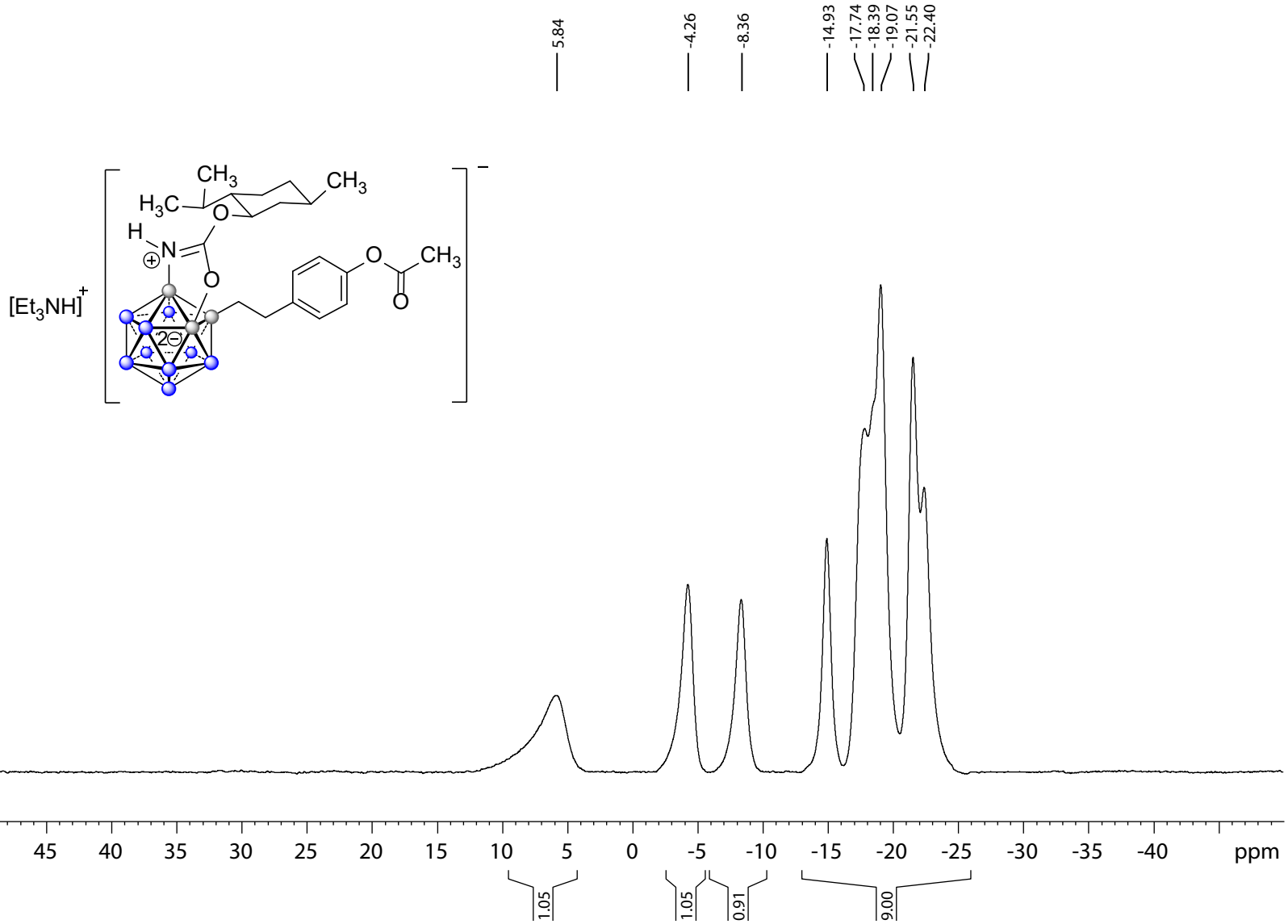
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-152

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190326-RV-B12M-4OCOMeSTYR
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20190327
Time             19.03
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              297.7 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

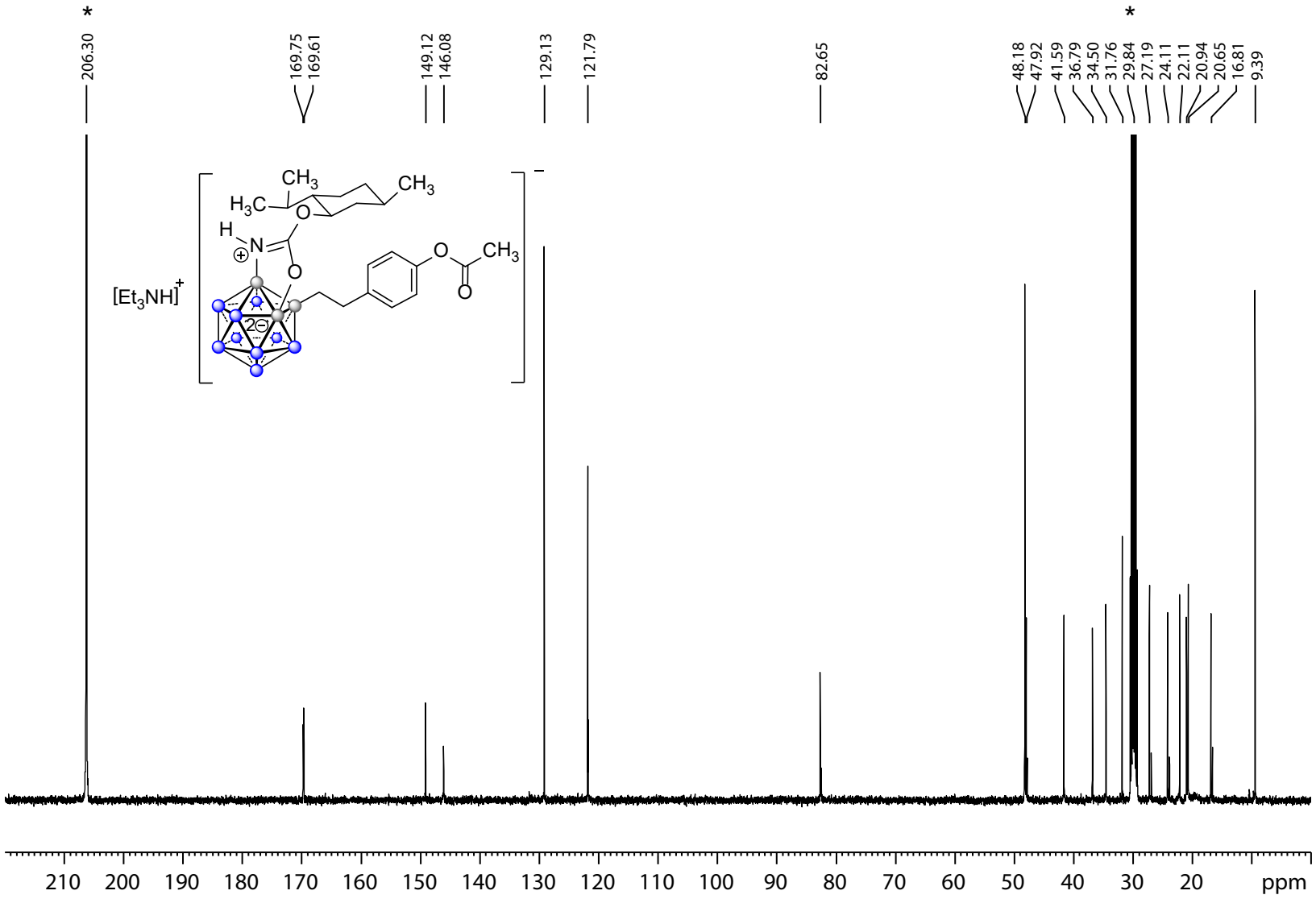
======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB              10.00 Hz
GB        0
PC               1.40
```

NMR-153

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz



Current Data Parameters
NAME 20190326-RV-B12M-4OCOMeSTYR
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190327
Time 20.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 297.8 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

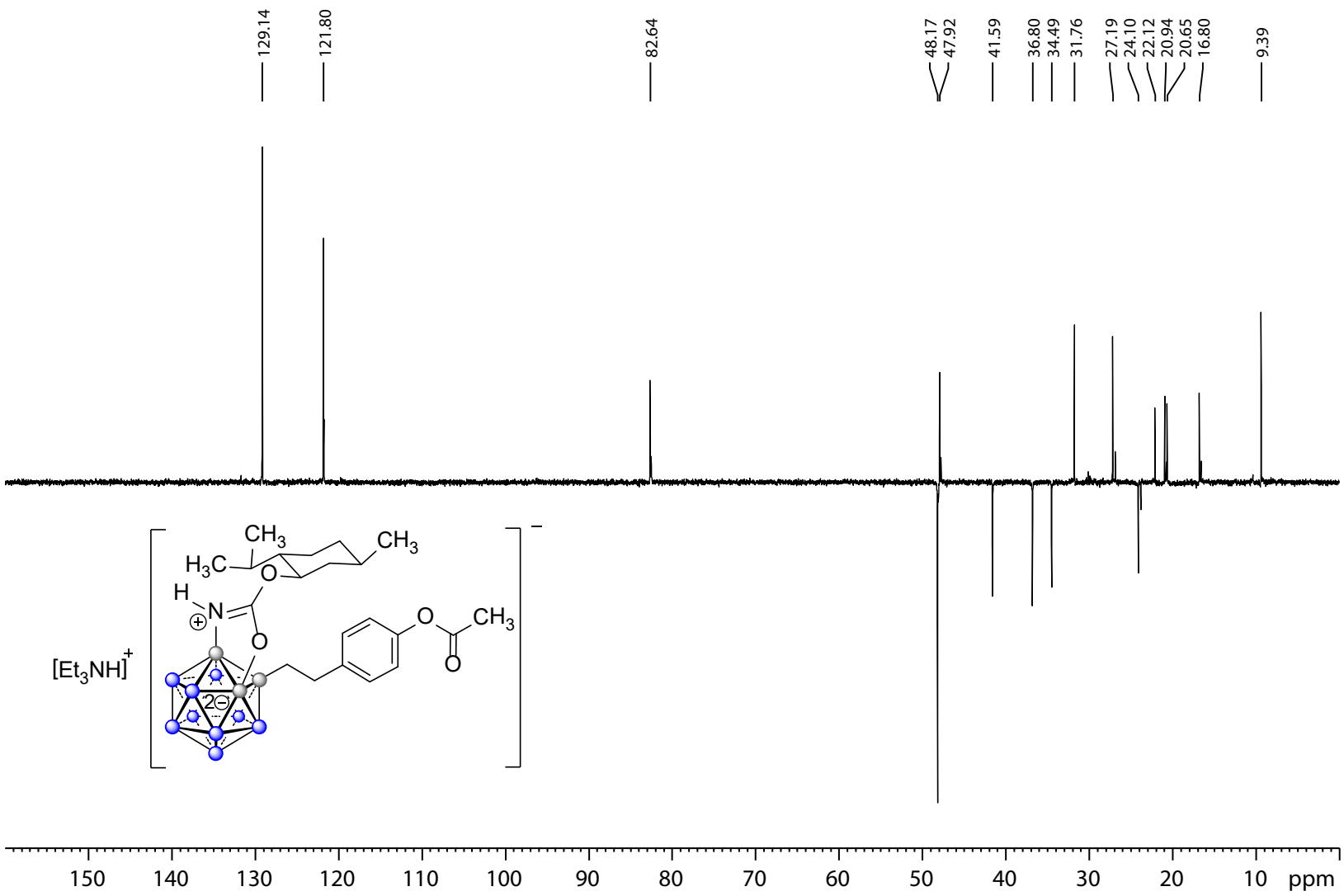
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126875 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190326-B12M-4OCOMeSTYR
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_           20190327
Time              21.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW              17.067 usec
DE                6.50 usec
TE               297.3 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

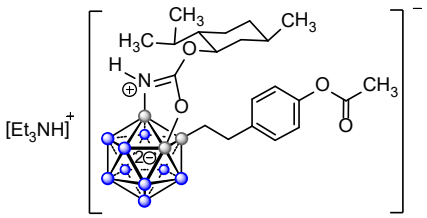
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126873 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR



NMR-156

```
Current Data Parameters
NAME      20190326-RV-B12-MENTH-4OCOMeSTYR
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20190327
Time             21.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH           5341.880 Hz
FIDRES        2.608340 Hz
AQ            0.1916928 sec
RG               64.43
DW              93.600 usec
DE               6.50 usec
TE              297.1 K
D0          0.00000300 sec
D1          2.00000000 sec
D11         0.03000000 sec
D12         0.00002000 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0              15.00 usec
P1              15.00 usec
P17           2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1       400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1             10.00 %
P16            1000.00 usec

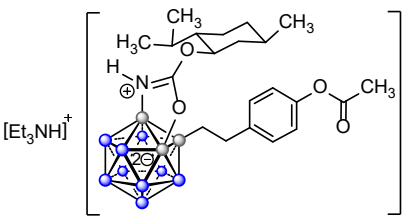
F1 - Acquisition parameters
TD                  128
SFO1          400.1324 MHz
FIDRES        83.466881 Hz
SW              13.350 ppm
FnMODE               QF

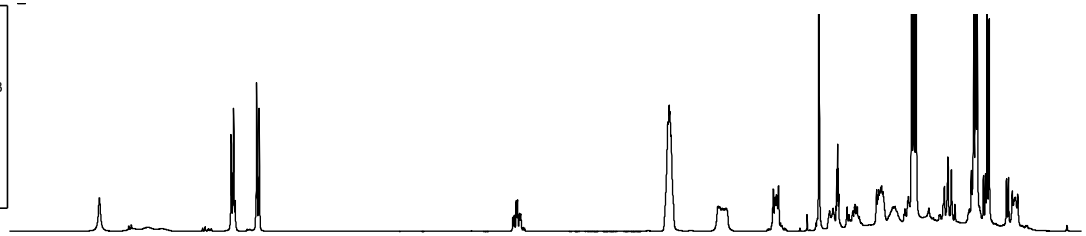
F2 - Processing parameters
SI                  1024
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

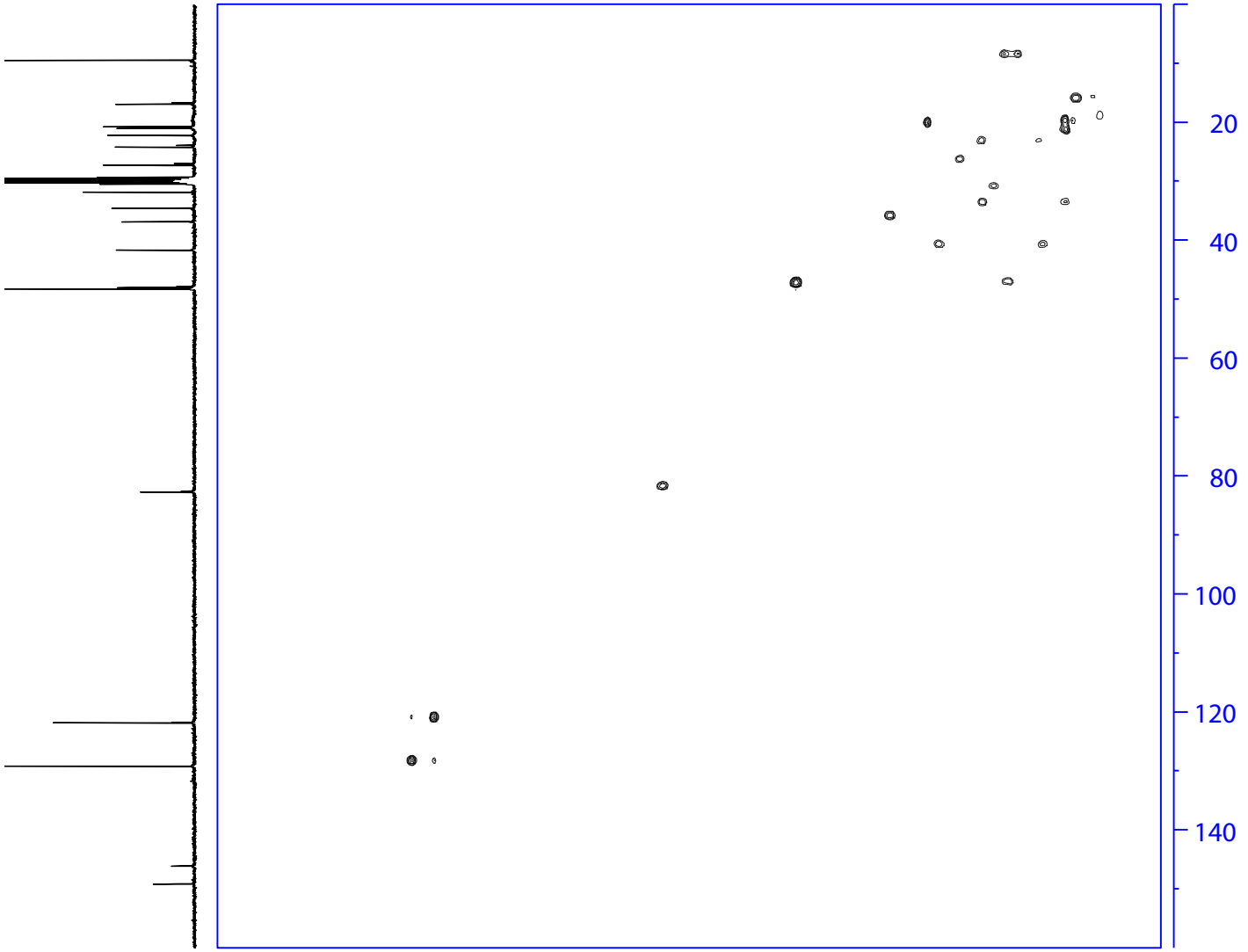
F1 - Processing parameters
SI                  1024
MC2                 QF
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
```

20190326-B12M-4OOMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4OCOMe$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR







NMR-157

```
Current Data Parameters
NAME      20190326-RV-B12-MENTH-4OCOMeSTYR
EXPNO                   8
PROCNO                  1

F2 - Acquisition Parameters
Date_           20190327
Time              21.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                297.0 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
P28              1000.00 usec
PLW1          12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              70.00 usec
PLW2          53.00000000 W
PLW12          1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

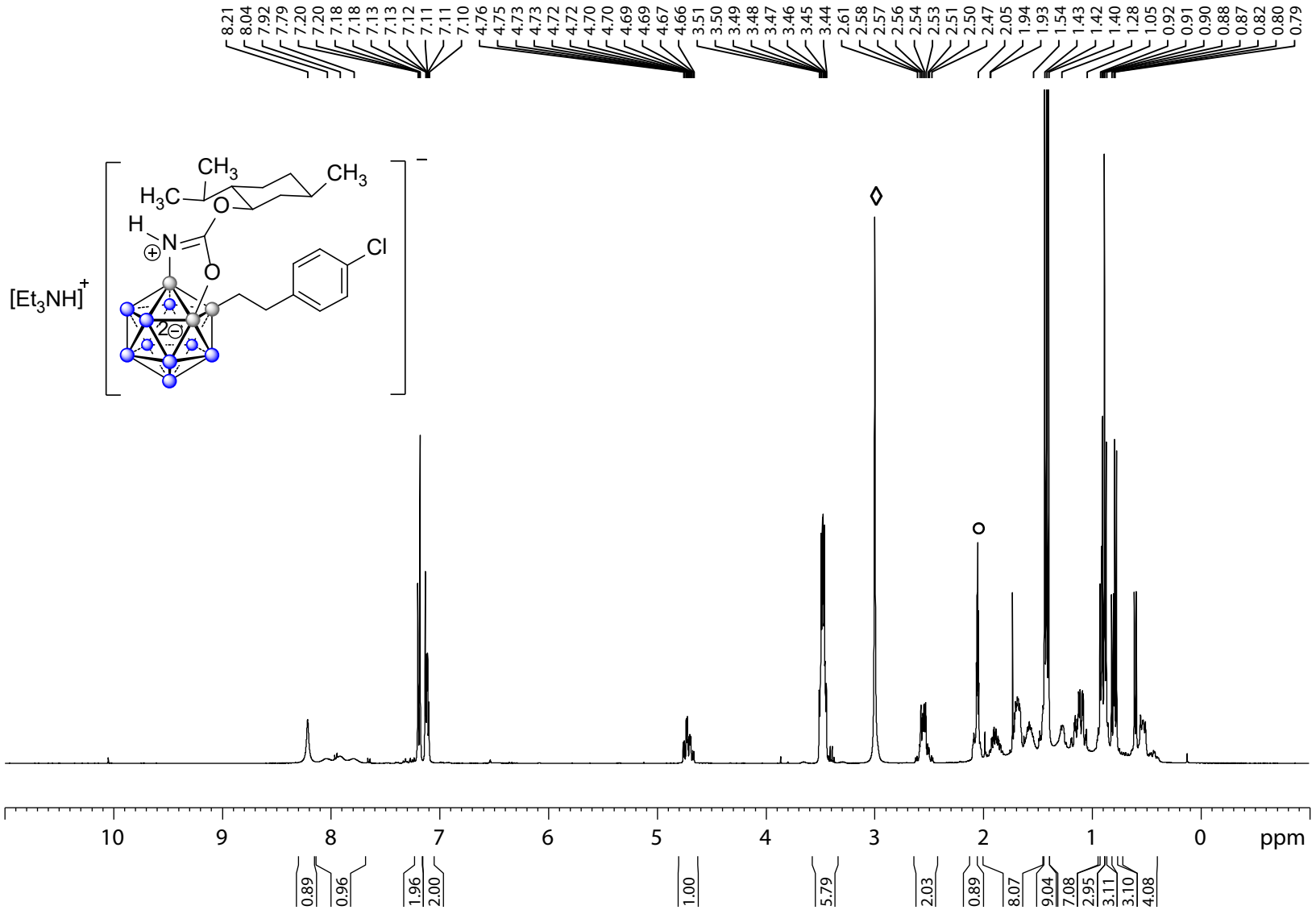
F1 - Acquisition parameters
TD                  256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW              249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
```

20190401-B12M-4ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



Current Data Parameters
NAME 20190401-B12M-4Cl-STYR
EXPNO 1
PROCNO 1

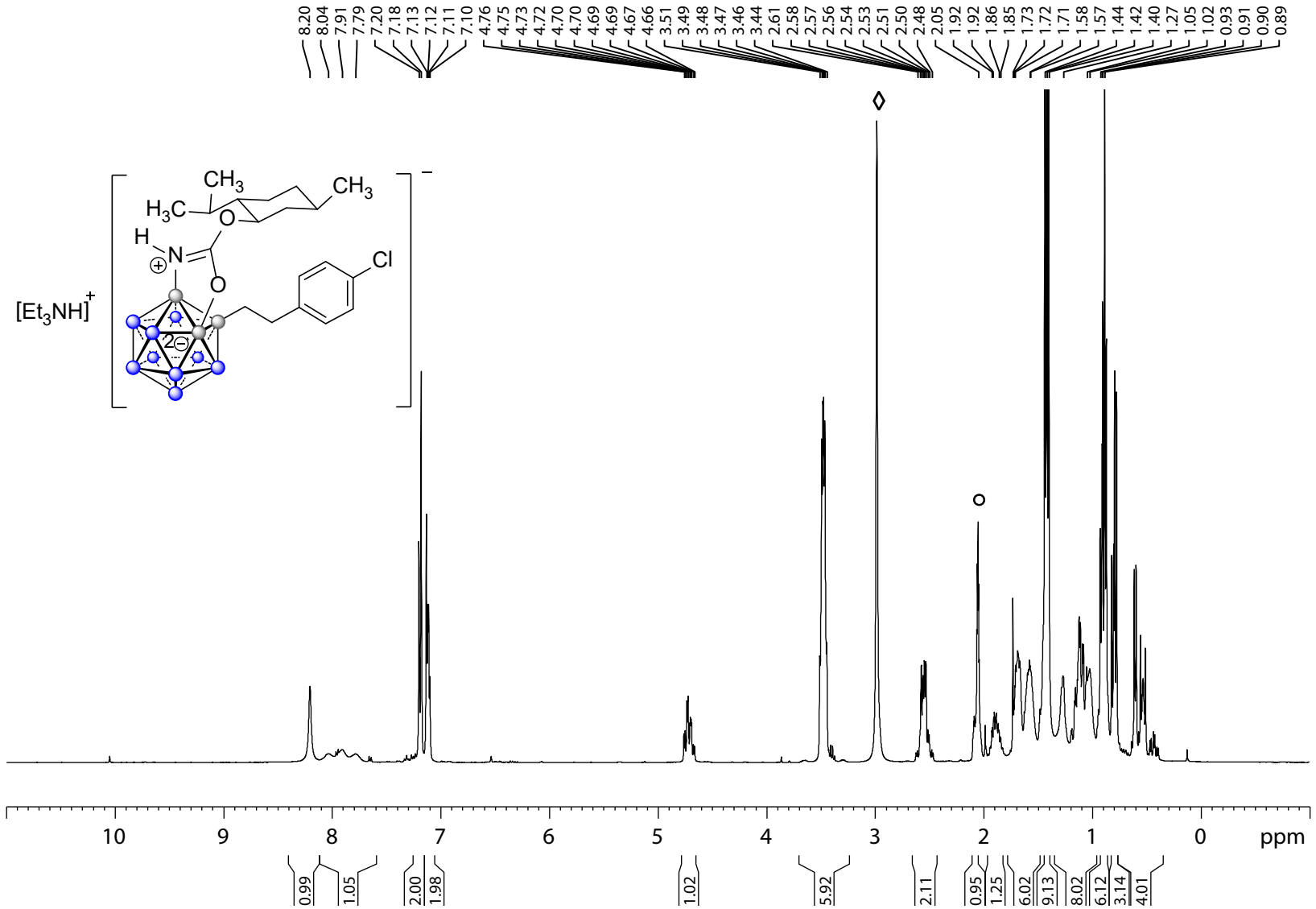
F2 - Acquisition Parameters
Date_ 20190402
Time 21.01
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 64.43
DW 50.000 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

F2 - Processing parameters
SI 65536
SF 400.1300070 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

20190401-B12M-4ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



Current Data Parameters
NAME 20190401-B12M-4Cl-STYR
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 21.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgig30
TD 16384
SOLVENT Acetone
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.39
DW 62.400 usec
DE 6.50 usec
TE 296.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

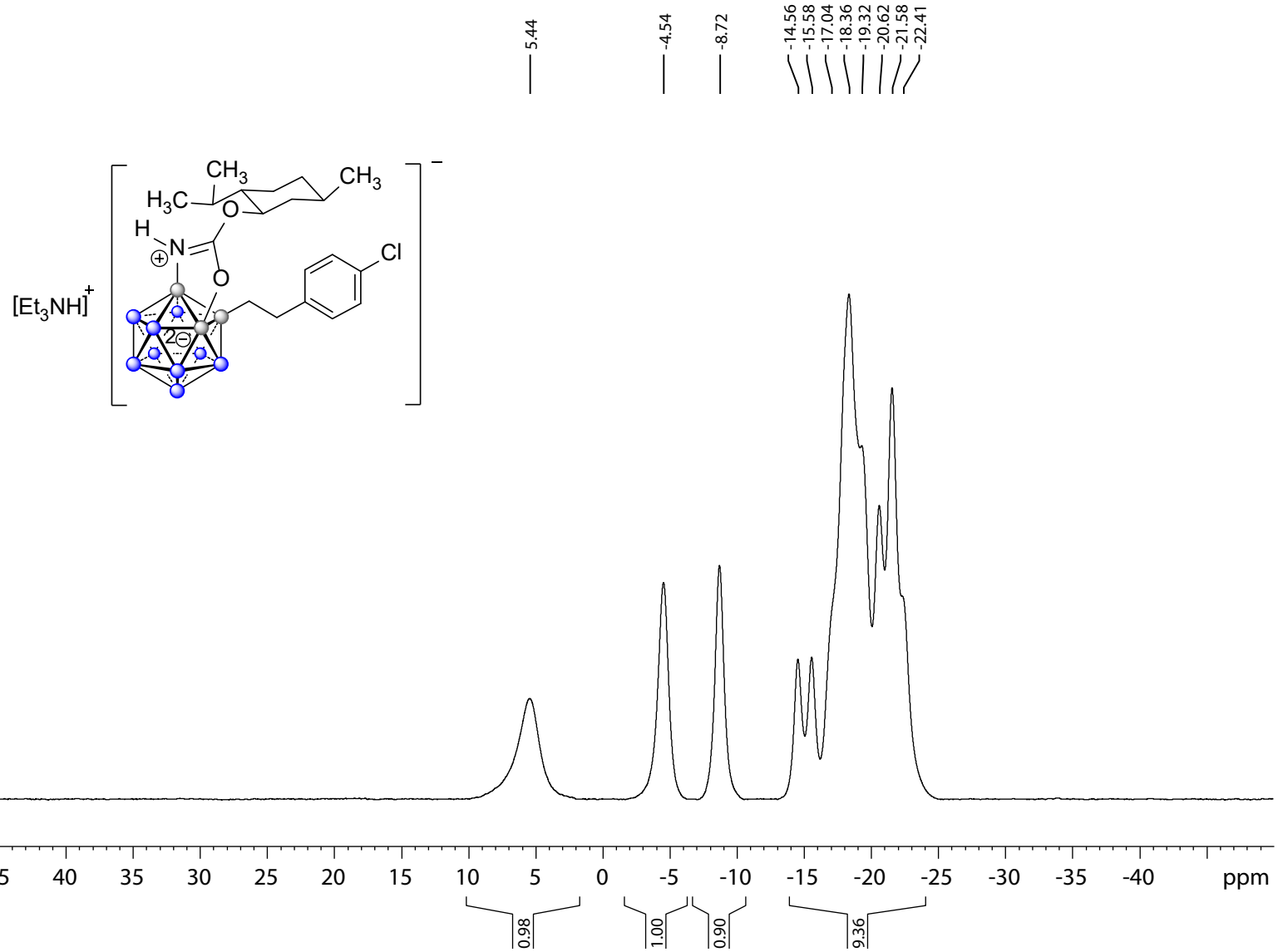
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 12.50000000 W
SFO1 400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp4
NUC2 11B
PCPD2 90.00 usec
PLW2 52.96599960 W
PLW12 0.64477998 W
SFO2 128.3776050 MHz

F2 - Processing parameters
SI 32768
SF 400.1300071 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20190401-B12M-4ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz



Current Data Parameters
NAME 20190401- RD-B12M-4Cl-STYR
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 21.09
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1

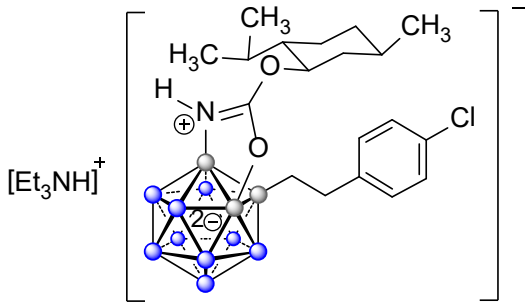
======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776052 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-160

20190401-B12M-4ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{^1H\}$ NMR 128MHz



$[Et_3NH]^+$

Current Data Parameters
NAME 20190401 RD--B12M-4Cl-STYR
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 21.15
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776050 MHz

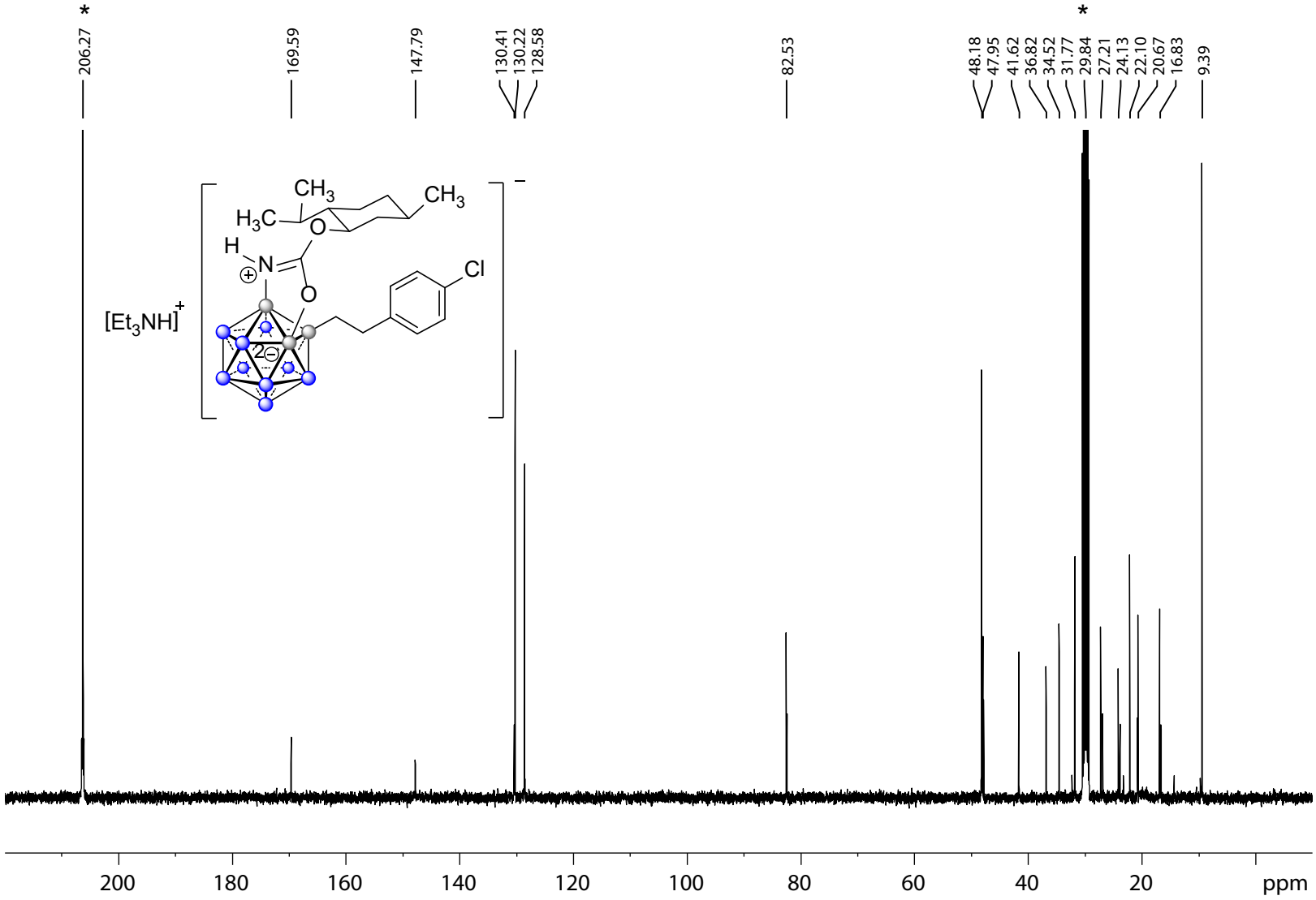
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-161

20190401-B12M-4ClStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)OCH₂CH₂C₆H₄Cl] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^{1}H\}$ NMR 100 MHz



Current Data Parameters
NAME 20190401-RD--B12M-4Cl-STYR
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

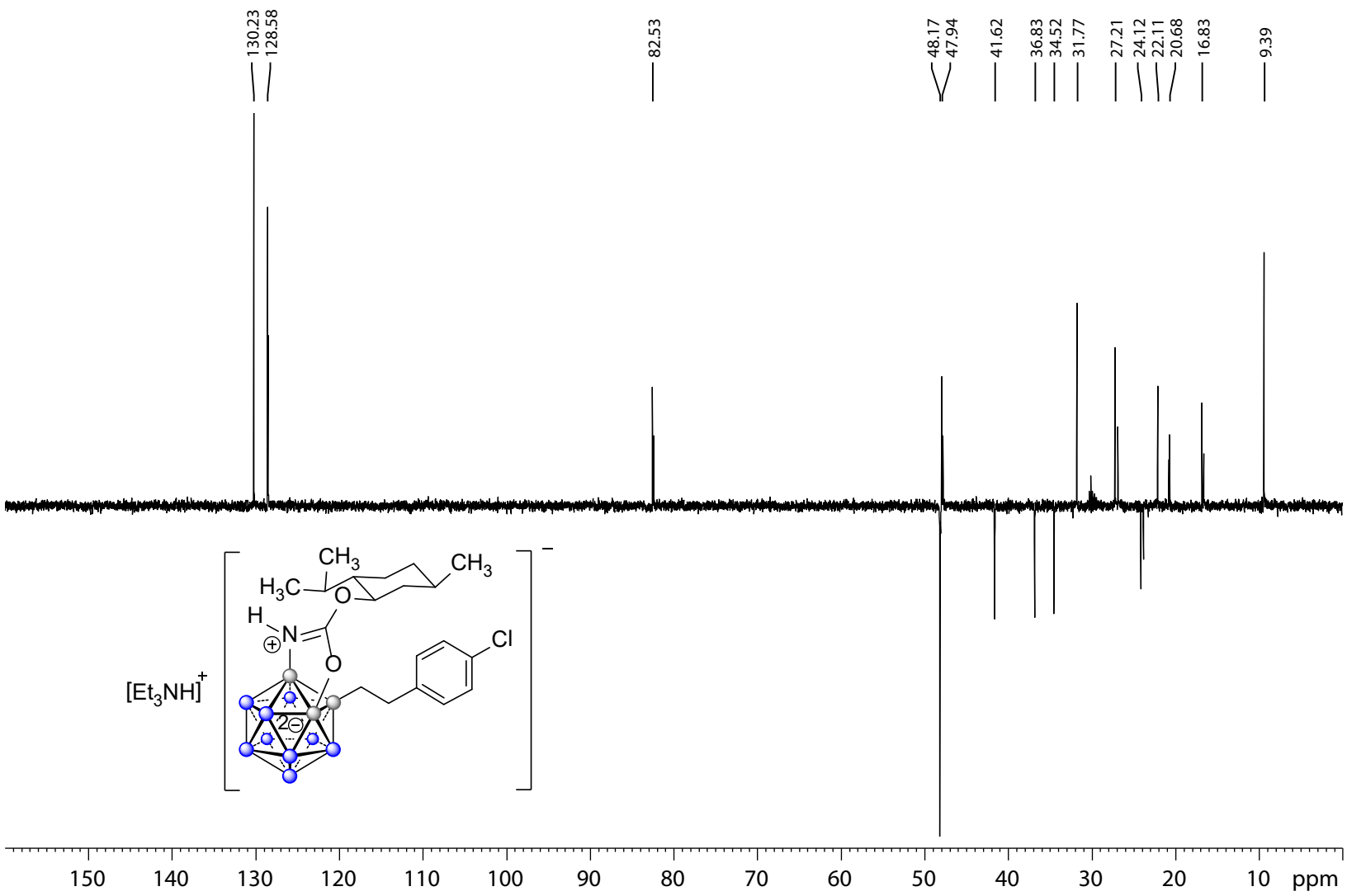
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126841 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20190401-B12M-4ClStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl]$ dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz



$[Et_3NH]^+$

Current Data Parameters
NAME 20190401-RD-B12M-4Cl-STYR
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 22.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG dept135
TD 65536
SOLVENT Acetone
NS 256
DS 4
SWH 29296.875 Hz
FIDRES 0.447035 Hz
AQ 1.1184810 sec
RG 193.34
DW 17.067 usec
DE 6.50 usec
TE 296.5 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1

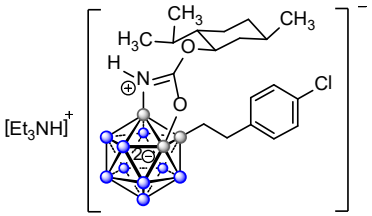
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
P2 20.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

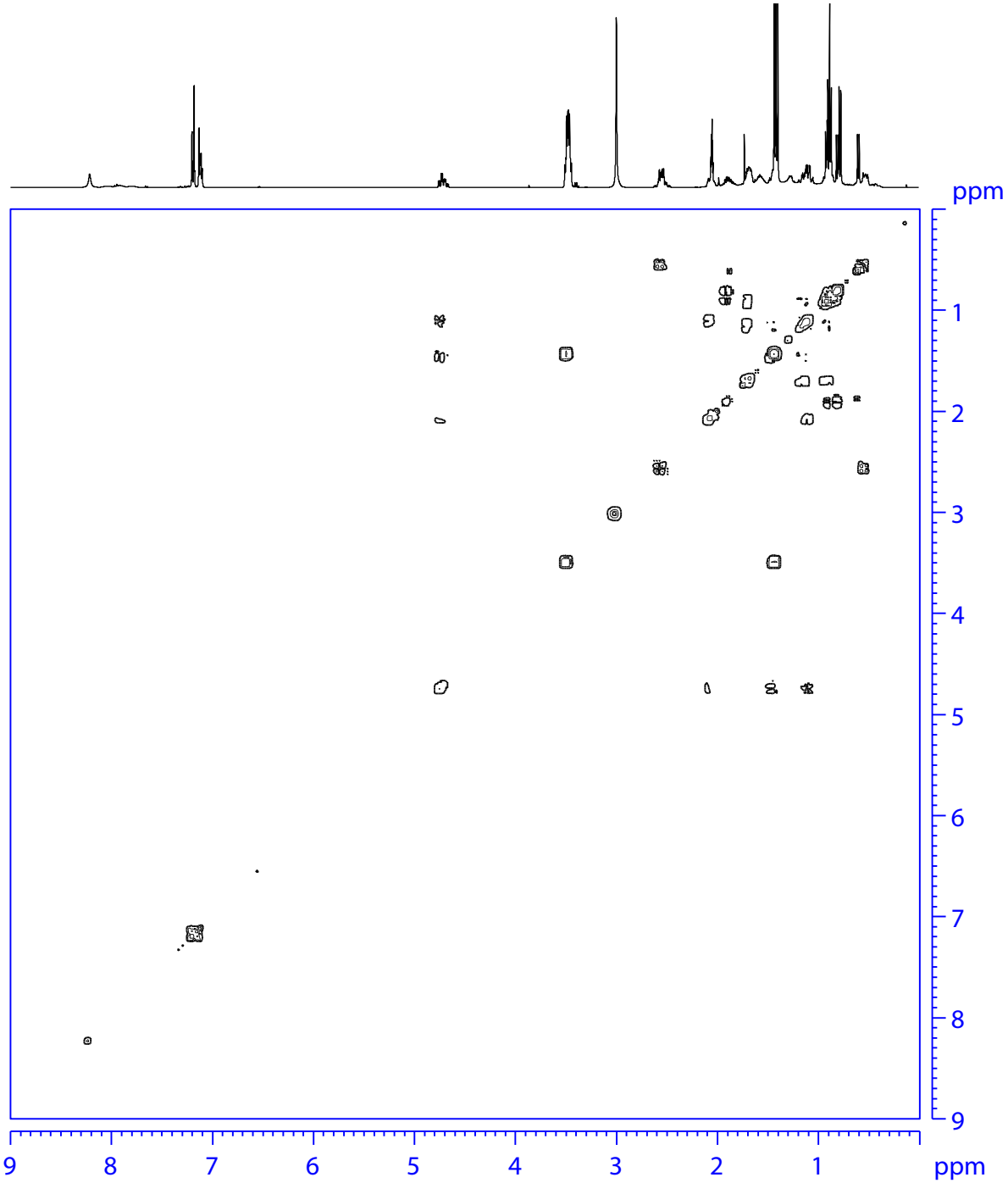
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
P3 15.00 usec
P4 30.00 usec
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126839 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 4.00

20190401-B12M-4ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-164

Current Data Parameters
NAME 20190401- RD- -B12M-4Cl-STYR
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 124.48
DW 93.600 usec
DE 6.50 usec
TE 296.3 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

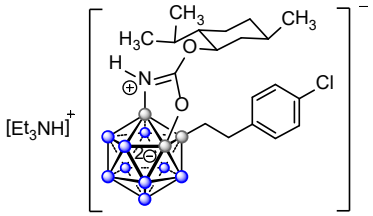
F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300000 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

20190401-B12M-4ClStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Cl$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR



NMR-165

Current Data Parameters
NAME 20190401-B12M-4Cl-STYR
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 22.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgpsi2
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 296.2 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

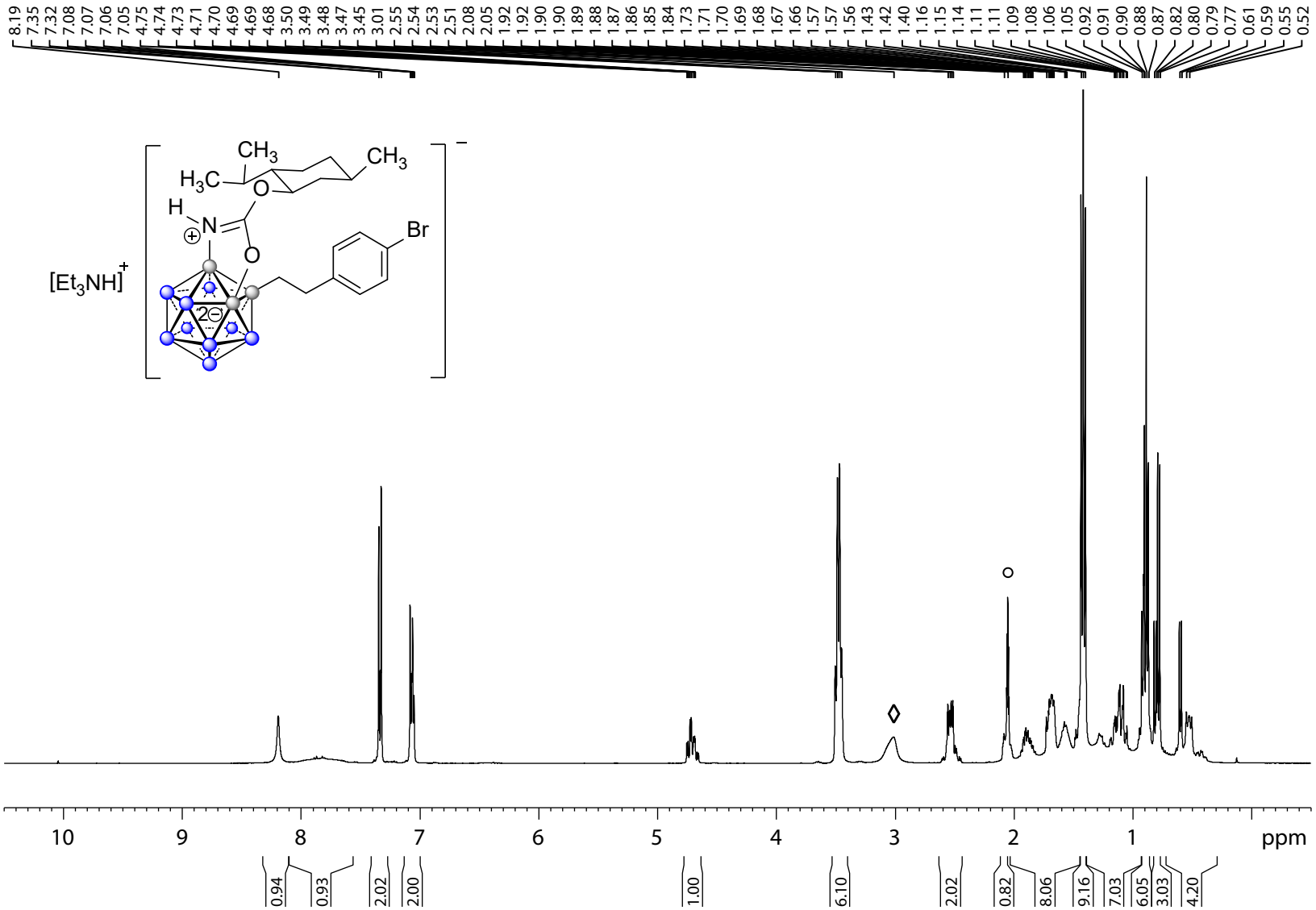
F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300000 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190401-RV-B12M-4-BrSTYR
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20190402
Time              12.52
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT         Acetone
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                55.74
DW                50.000 usec
DE                 6.50 usec
TE                296.2 K
D1           1.00000000 sec
TD0                  1

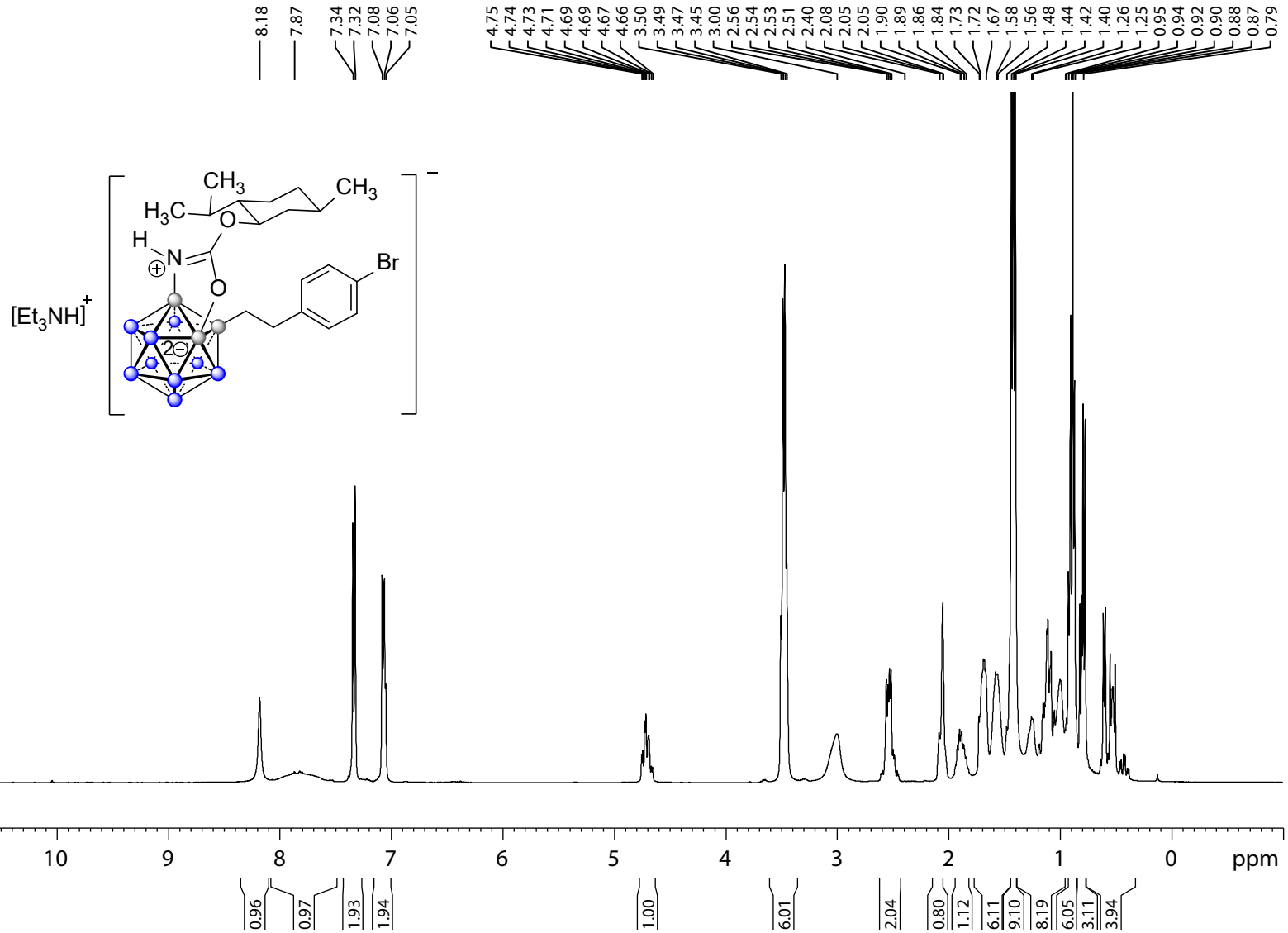
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300071 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-166

20190401-B12M-4BrStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Br]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190401-RV-B12M-4-BrSTYR
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190402
Time              12.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ              1.0223616 sec
RG                55.74
DW                62.400 usec
DE                 6.50 usec
TE                296.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

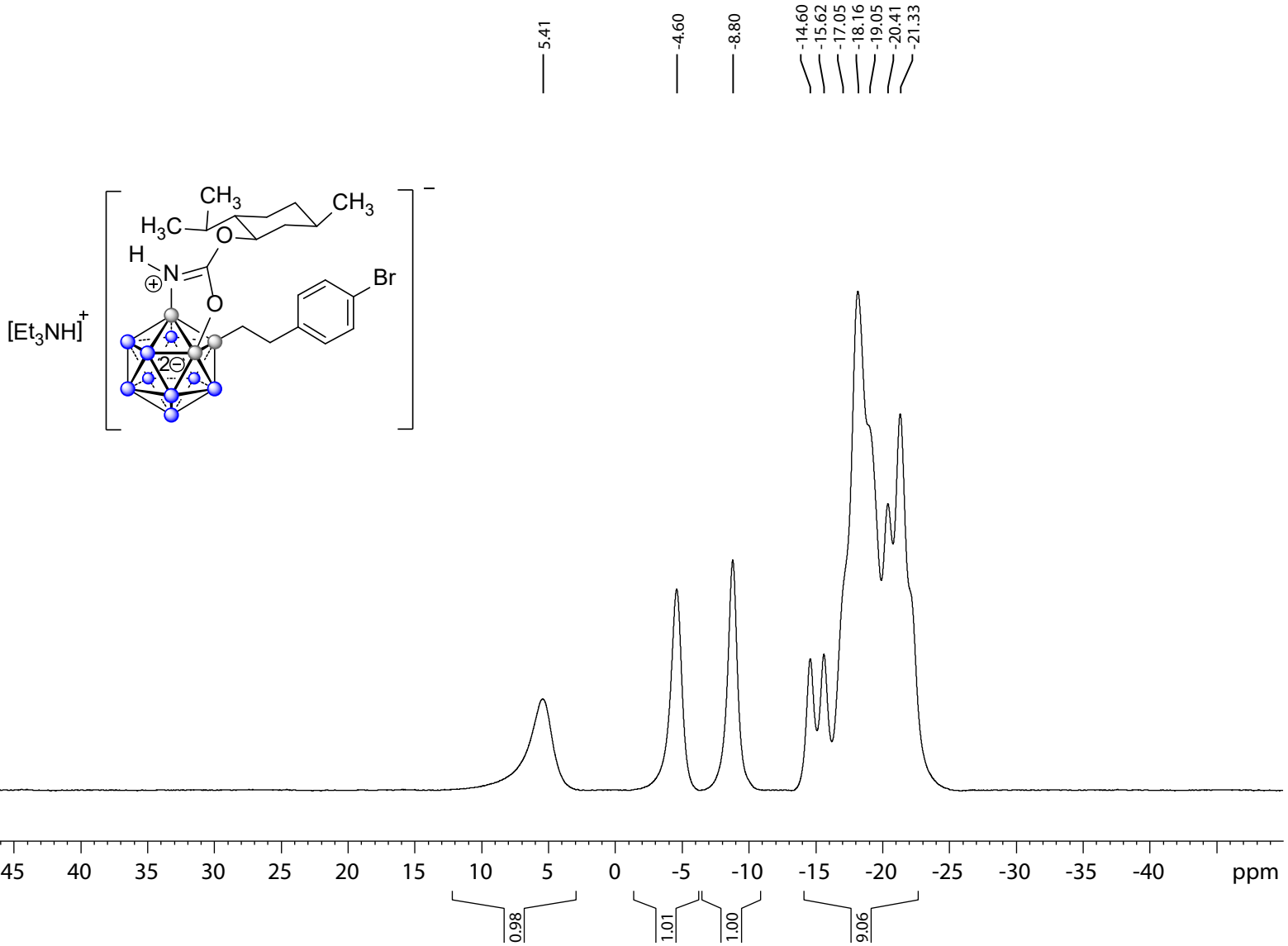
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2              90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300074 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz



Current Data Parameters
NAME 20190401-RV-B12M-4-BrSTYR
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

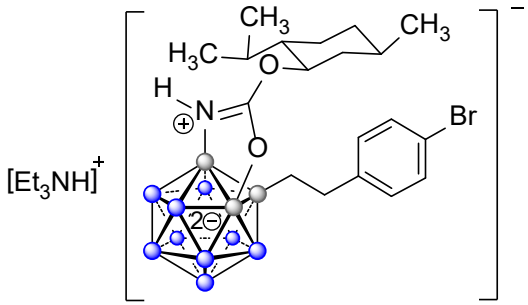
======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776052 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-168

20190401-B12M-4BrStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Br]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{^1H\}$ NMR 128MHz



$[Et_3NH]^+$

Current Data Parameters
NAME 20190401-RV-B12M-4-BrSTYR
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 13.06
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 297.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 9.93 usec
PLW1 52.96599960 W
SFO1 128.3776050 MHz

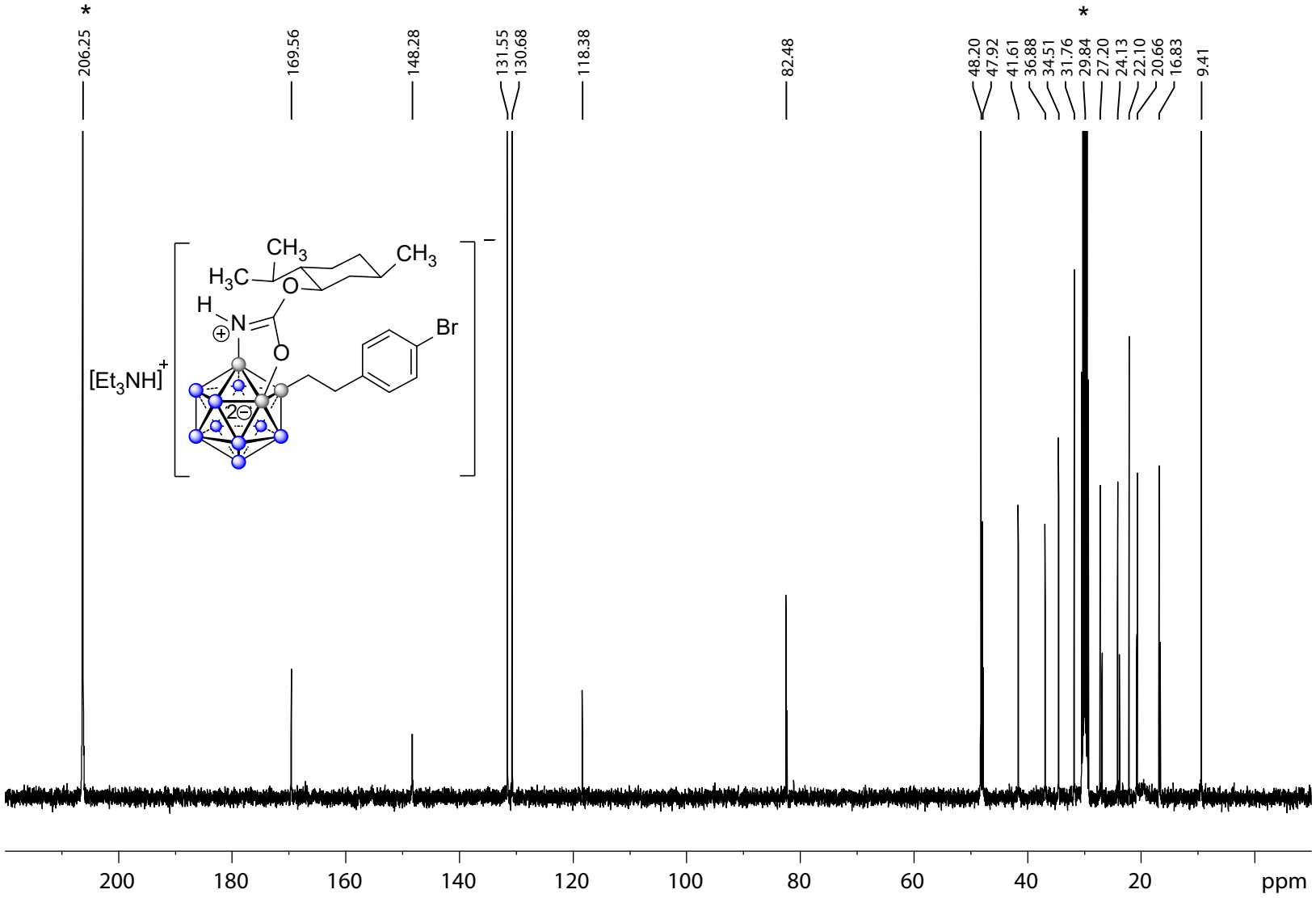
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1320007 MHz

F2 - Processing parameters
SI 32768
SF 128.3776050 MHz
WDW EM
SSB 0
LB 10.00 Hz
GB 0
PC 1.40

NMR-169

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz



Current Data Parameters
NAME 20190401-RV-B12M-4-BrSTYR
EXPNO 6
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

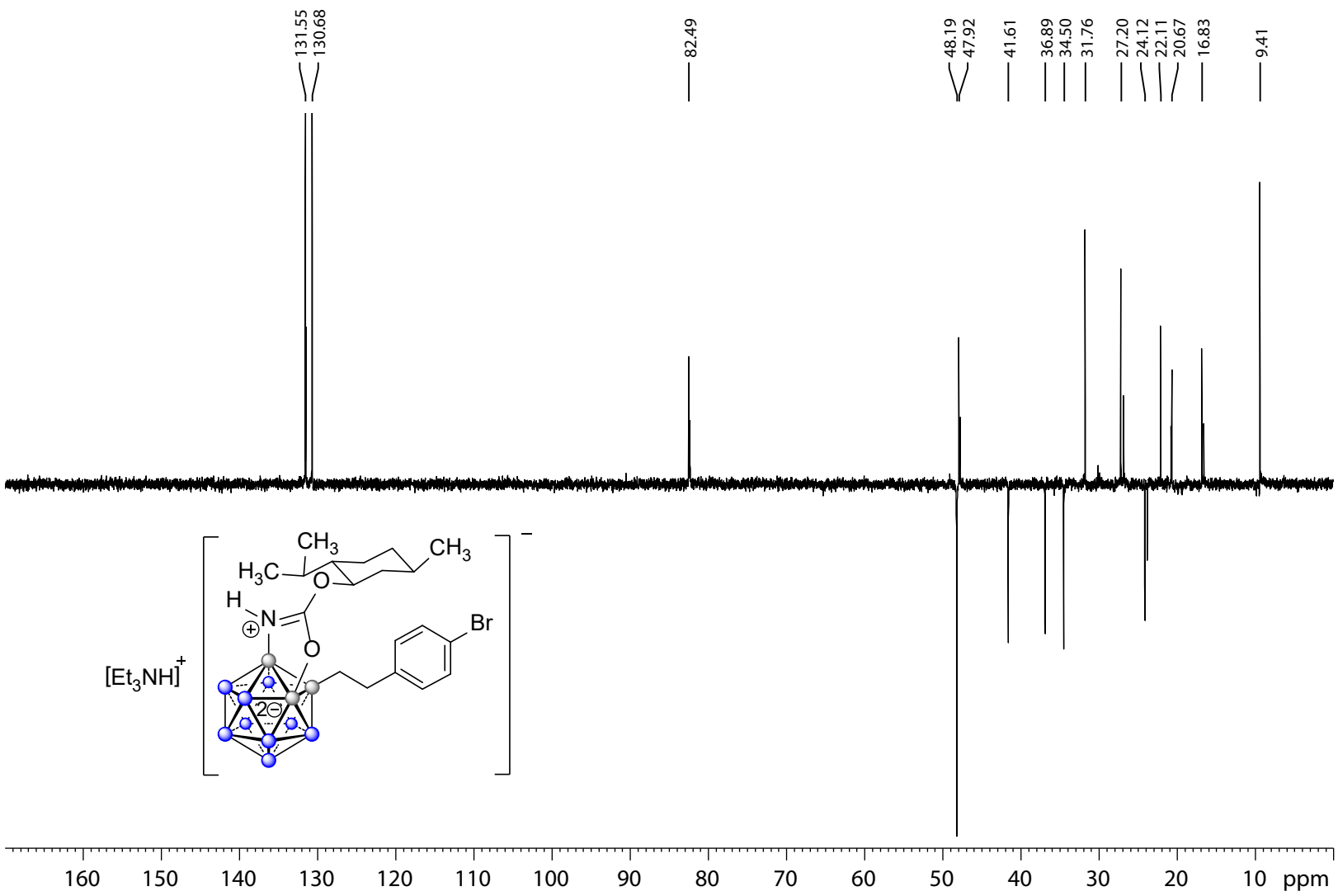
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000 W
SFO1 100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000 W
PLW12 0.43945000 W
PLW13 0.28125000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126858 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz



[Et_3NH]$^+$

```
Current Data Parameters
NAME      20190401-RV-B12M-4-BrSTYR
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20190402
Time              20.31
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  256
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW                17.067 usec
DE                 6.50 usec
TE                296.6 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

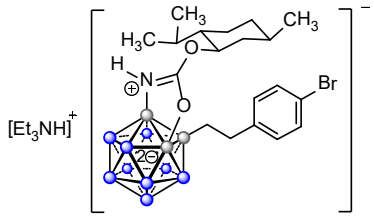
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

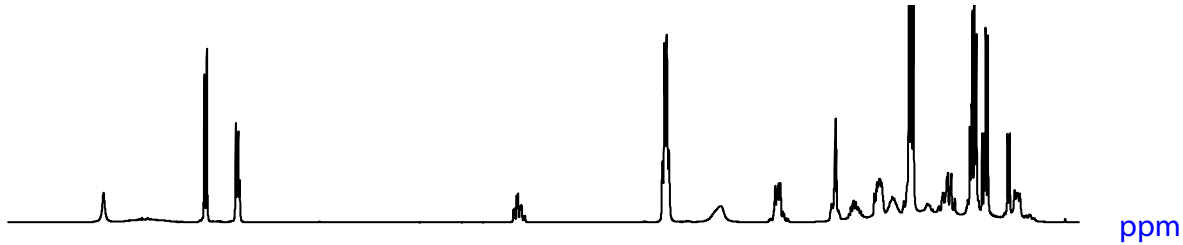
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

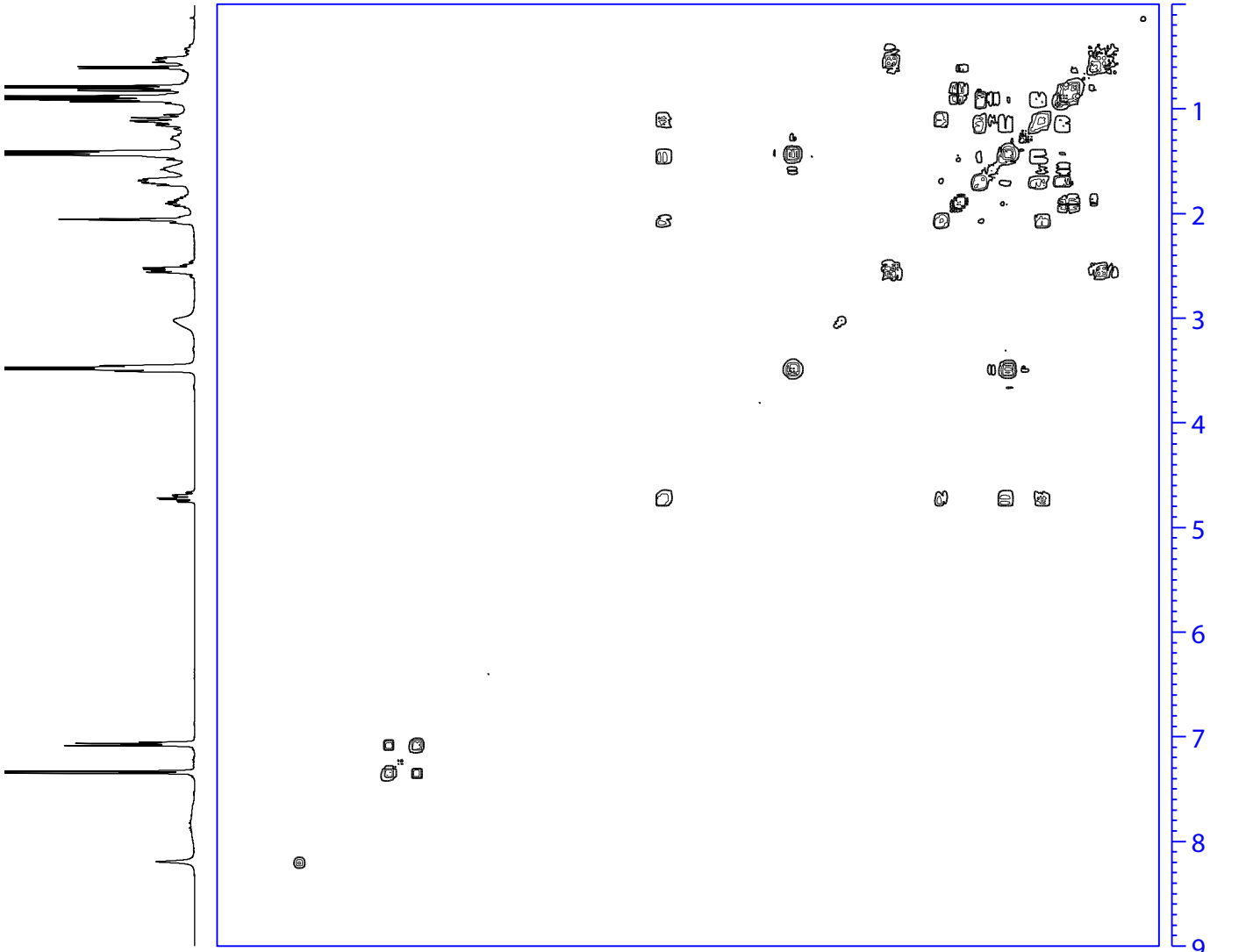
F2 - Processing parameters
SI                32768
SF           100.6126857 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 4.00
```

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR







NMR-172

```
Current Data Parameters
NAME      20190401-RV-B12M-4-BrSTYR
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20190402
Time              20.32
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT         Acetone
NS                    2
DS                    8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                64.43
DW               93.600 usec
DE                6.50 usec
TE               296.4 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

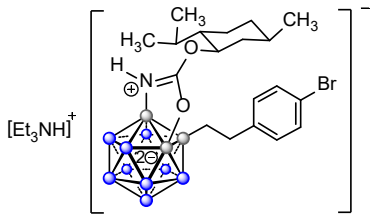
F1 - Acquisition parameters
TD                  128
SFO1           400.1324 MHz
FIDRES         83.466881 Hz
SW               13.350 ppm
FnMODE              QF

F2 - Processing parameters
SI                 1024
SF           400.1300000 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                  QF
SF           400.1300000 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
```

20190401-B12M-4BrStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4Br$] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190401-RV-B12M-4-BrSTYR
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20190402
Time               20.43
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ              0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                296.2 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
P28              1000.00 usec
PLW1          12.50000000 W
SFO1          400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              70.00 usec
PLW2          53.00000000 W
PLW12          1.08159995 W
SFO2          100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

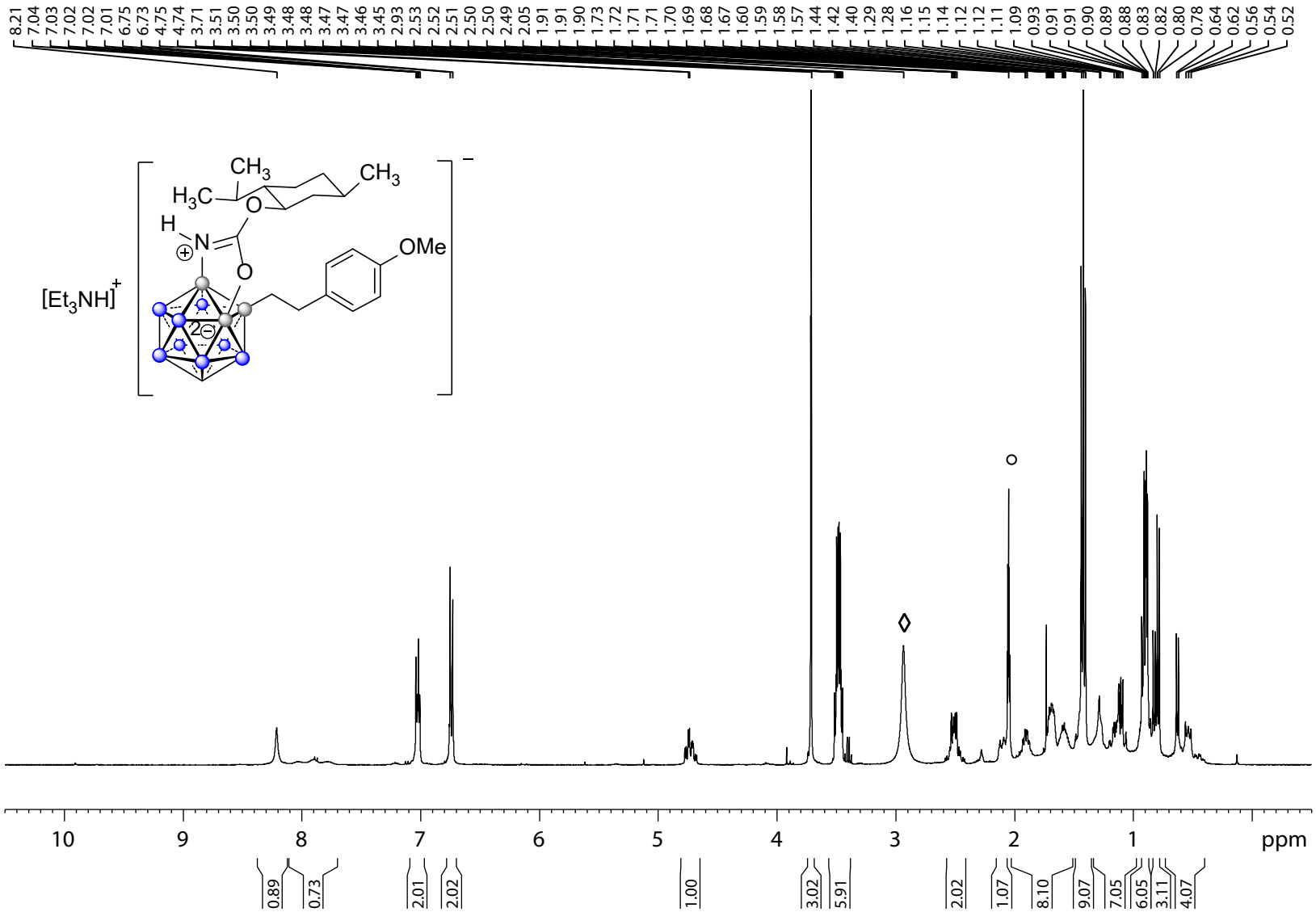
F1 - Acquisition parameters
TD                   256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW               249.991 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2         echo-antiecho
SF           100.6127690 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
```

20190410-B12M-4OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OMe$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 1
PROCNO                1

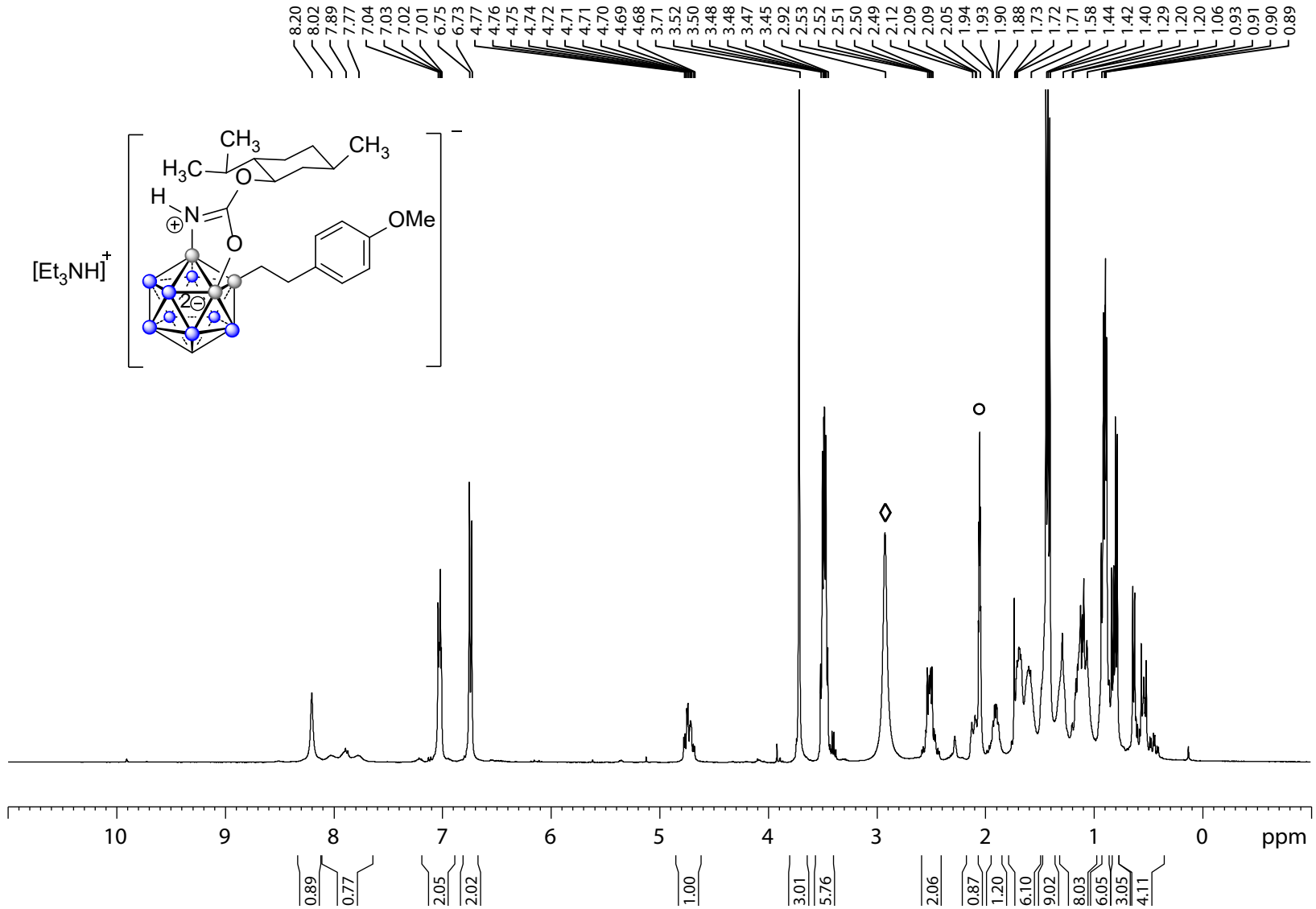
F2 - Acquisition Parameters
Date_           20190411
Time              17.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG                95.29
DW                50.000 usec
DE                 6.50 usec
TE                297.6 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300069 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20190410-B12M-4OMeStyr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4OMe]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190411
Time              17.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE                297.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1       400.1320007 MHz

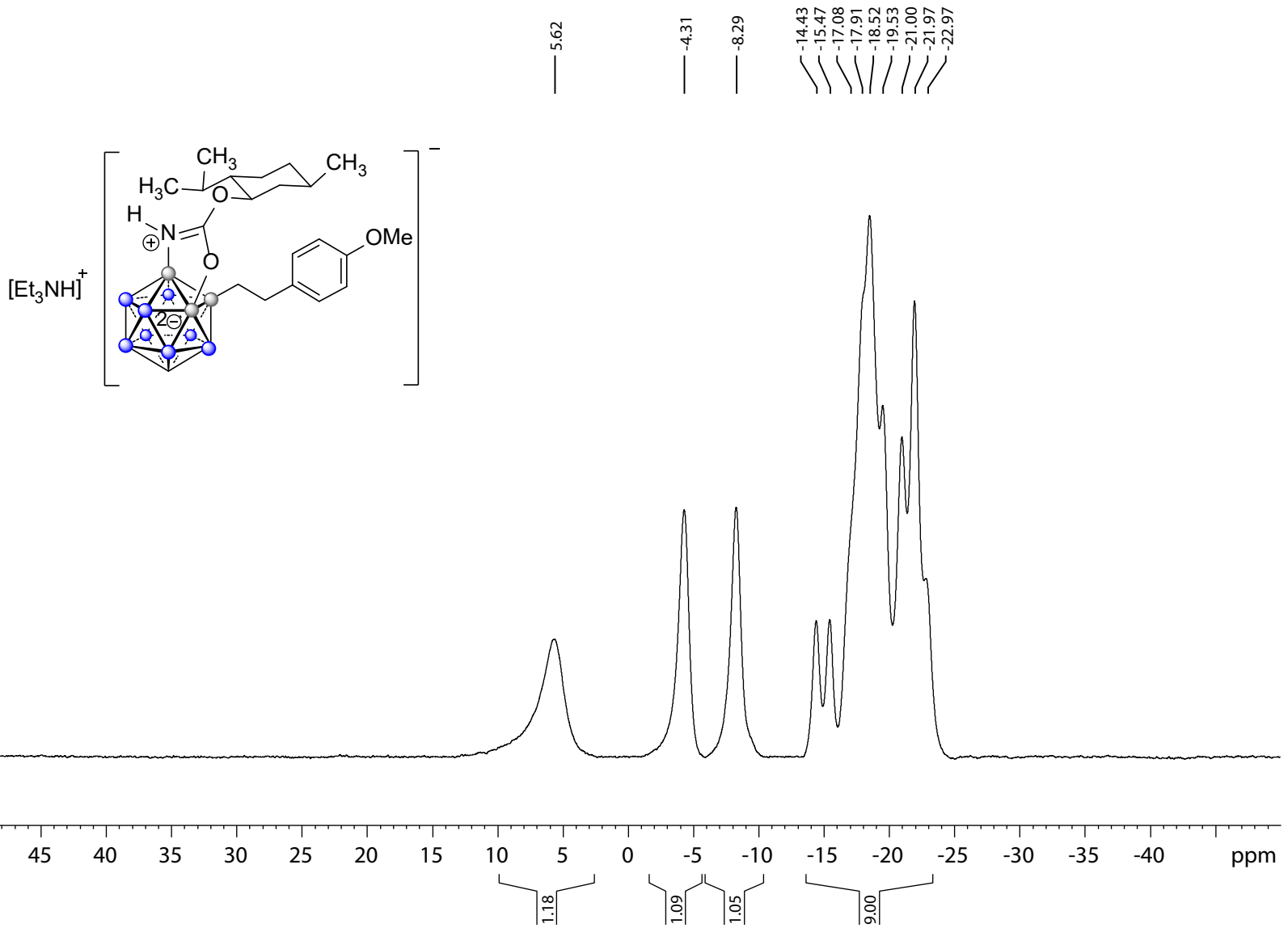
======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2       128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF         400.1300070 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

NMR-175

20190410-B12M-4OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OMe$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190411
Time              18.04
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.5 K
D1            1.00000000 sec
TD0                   1

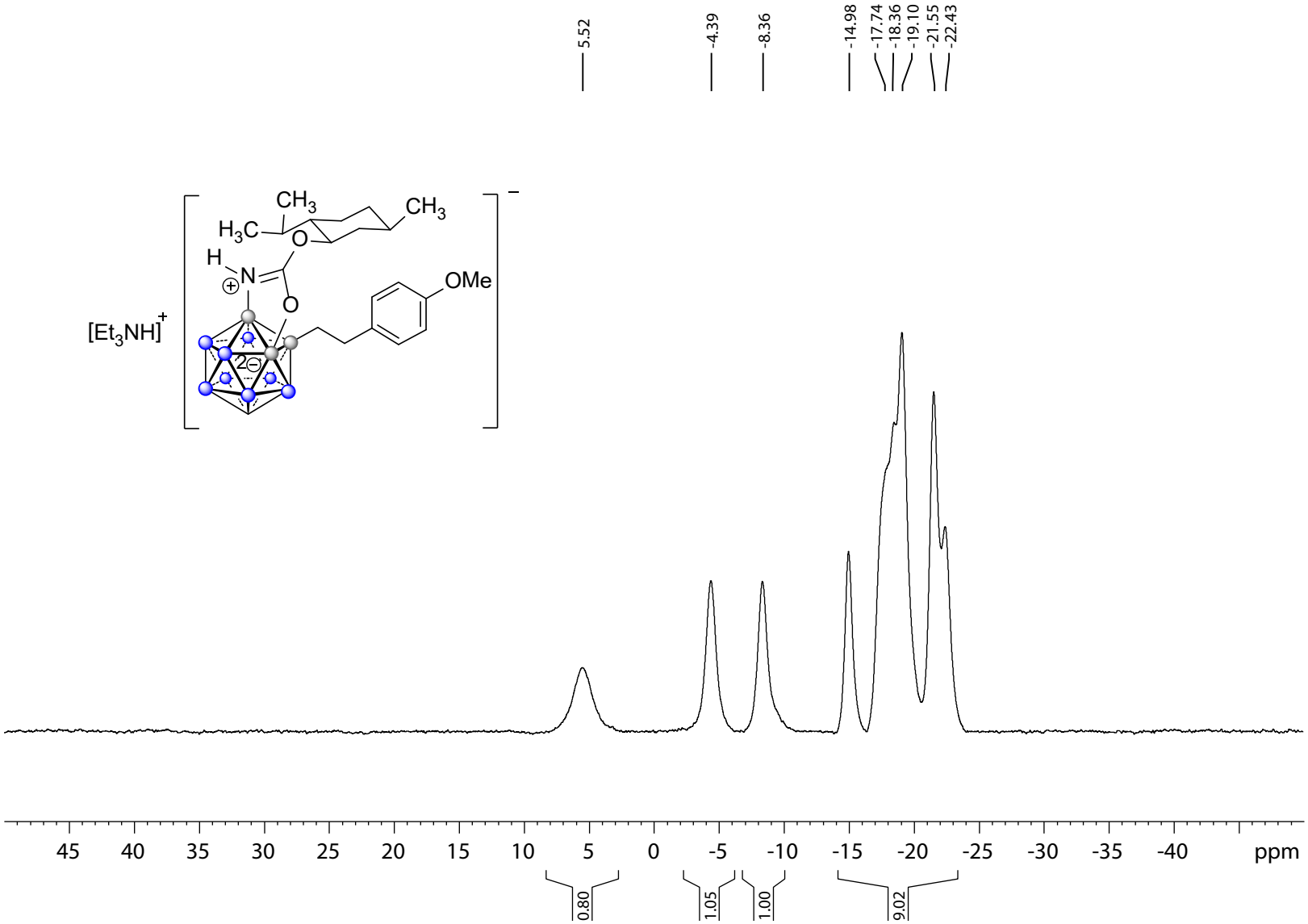
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-176

20190410-B12M-4OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OMe$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{^1H\}$ NMR 128MHz




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_           20190411
Time              18.10
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ            1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              298.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               11B
P1                9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

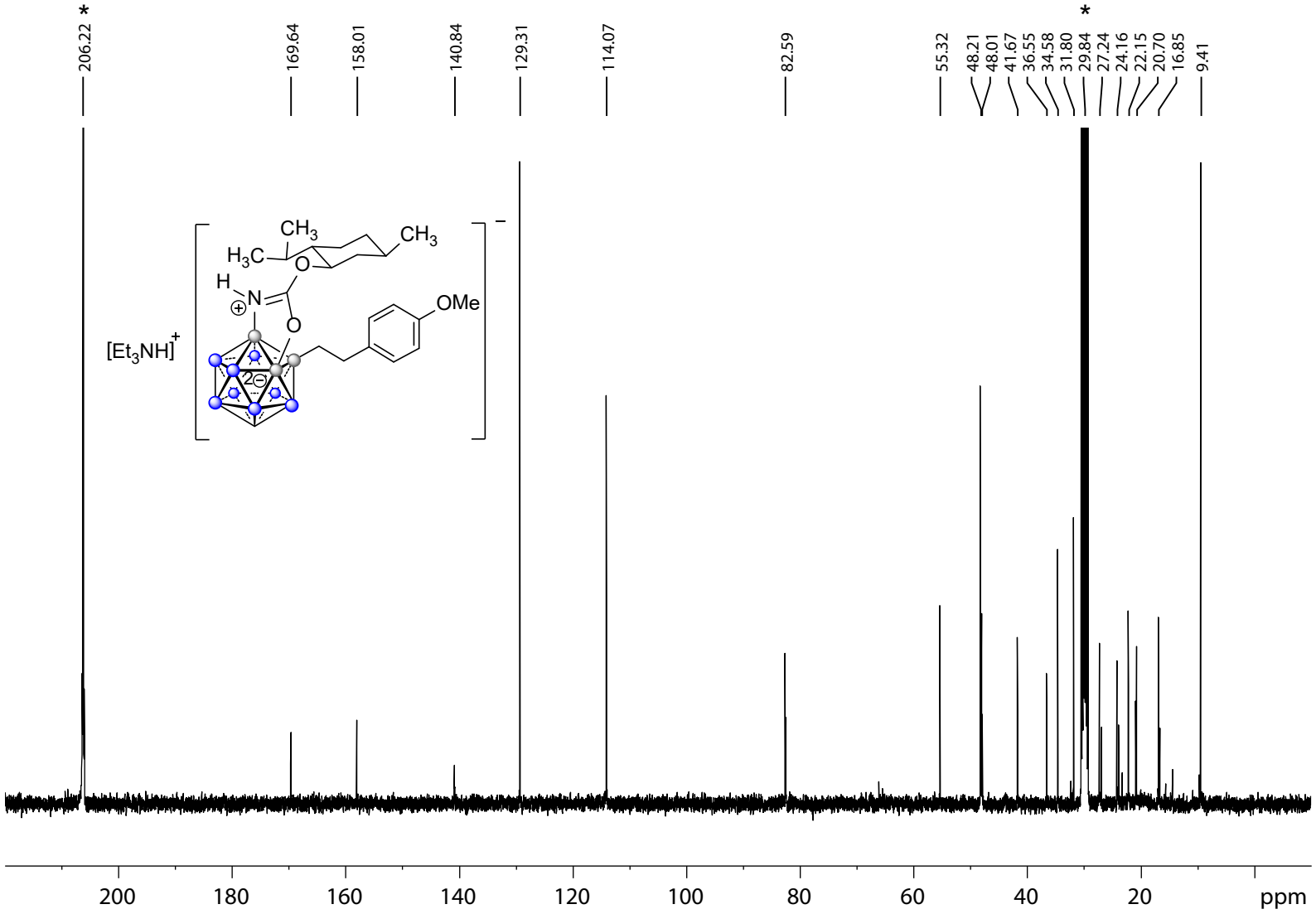
======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI               32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB              10.00 Hz
GB        0
PC               1.40
```

NMR-177

20190410-B12M-4OMeStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)OCH₂CH₂C₆H₄OMe] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^{1}H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20190411
Time              19.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                298.4 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

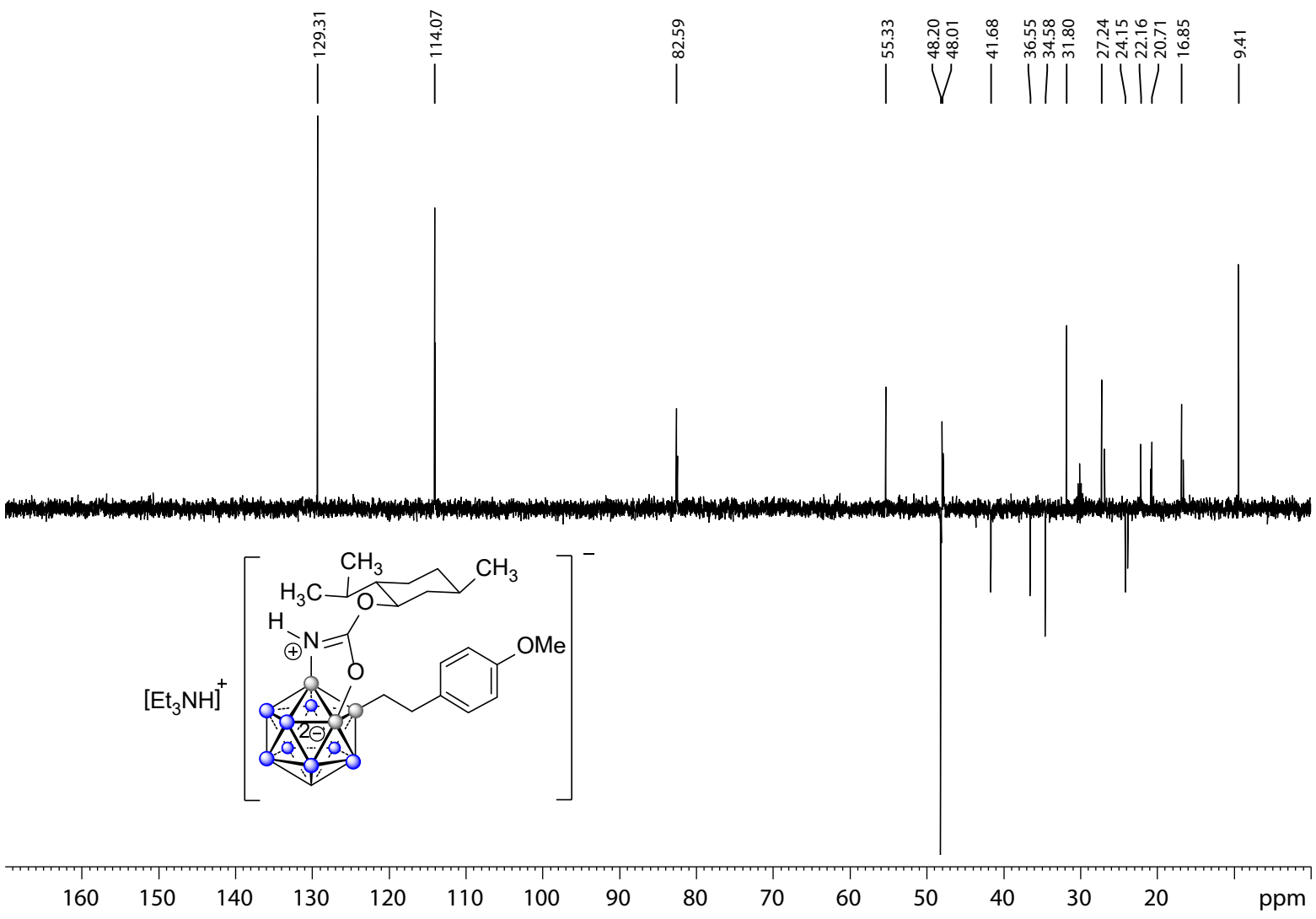
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126813 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190410-B12M-4OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4OMe$] dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                  6
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190411
Time              19.57
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  256
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ             1.1184810 sec
RG                193.34
DW              17.067 usec
DE                6.50 usec
TE                297.9 K
CNST2        145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                   1

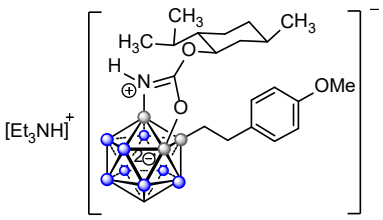
======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
P2               20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

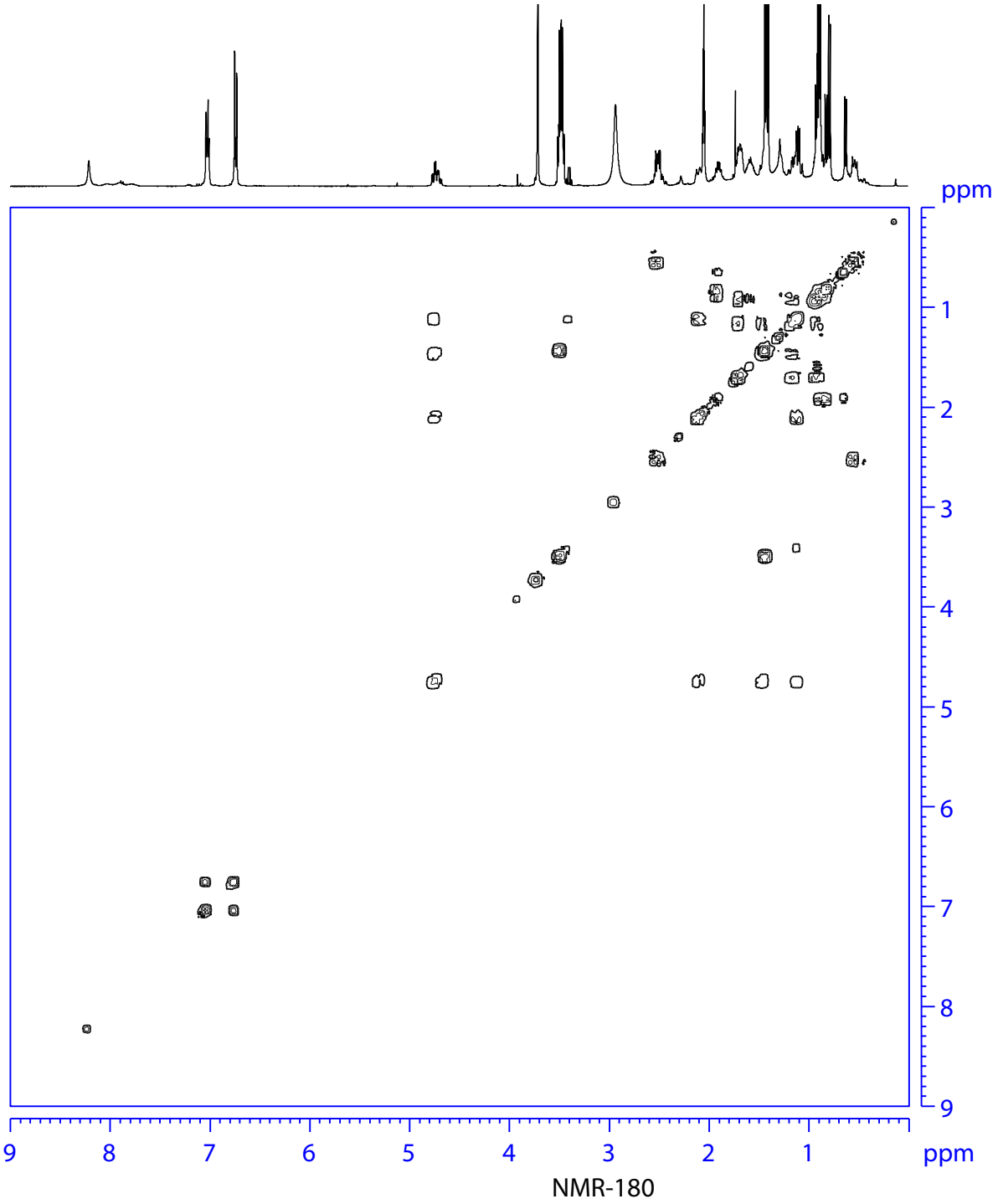
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
P3               15.00 usec
P4               30.00 usec
PCPD2            80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF          100.6126811 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190410-B12M-4OMeStyr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4OMe$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





NMR-180

```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20190411
Time              20.14
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                2048
SOLVENT        Acetone
NS                   2
DS                   8
SWH           5341.880 Hz
FIDRES        2.608340 Hz
AQ           0.1916928 sec
RG              170.36
DW               93.600 usec
DE                6.50 usec
TE               297.5 K
D0          0.00000300 sec
D1          2.00000000 sec
D11         0.03000000 sec
D12         0.00002000 sec
D13         0.00000400 sec
D16         0.00020000 sec
IN0         0.00018720 sec

======== CHANNEL f1 ========
NUC1                 1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1        12.50000000 W
PLW10        4.16050005 W
SFO1       400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

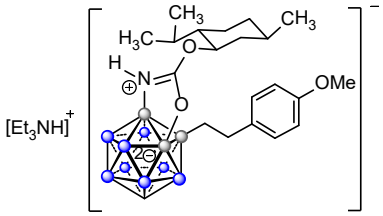
F1 - Acquisition parameters
TD                 128
SFO1          400.1324 MHz
FIDRES       83.466881 Hz
SW             13.350 ppm
FnMODE               QF

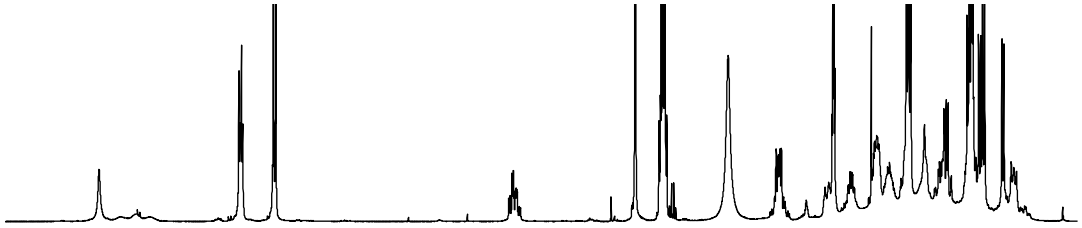
F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
PC                1.40

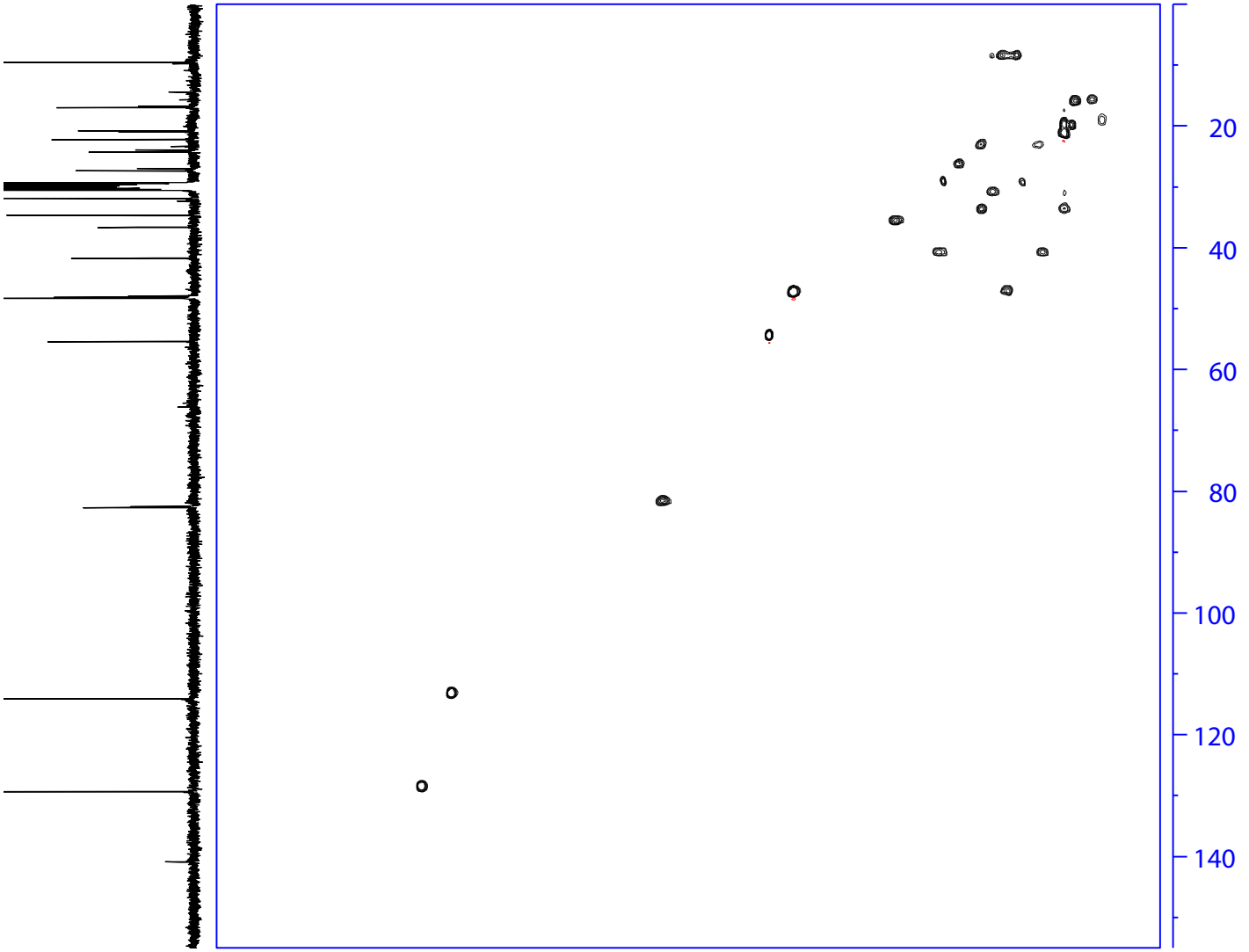
F1 - Processing parameters
SI                 1024
MC2                  QF
SF          400.1300000 MHz
WDW              QSINE
SSB       0
LB        0 Hz
GB        0
```

20190410-B12M-4OMeStyr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(MenthyI)OCH₂CH₂C₆H₄OMe] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR







NMR-181

```
Current Data Parameters
NAME      20190410-RV-B12M-4OME-Styr
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20190411
Time              19.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT          Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE               297.6 K
CNST2        145.0000000
D0            0.00000300 sec
D1            1.50000000 sec
D4            0.00172414 sec
D11           0.03000000 sec
D16           0.00020000 sec
D24           0.00086207 sec
IN0           0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2            garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

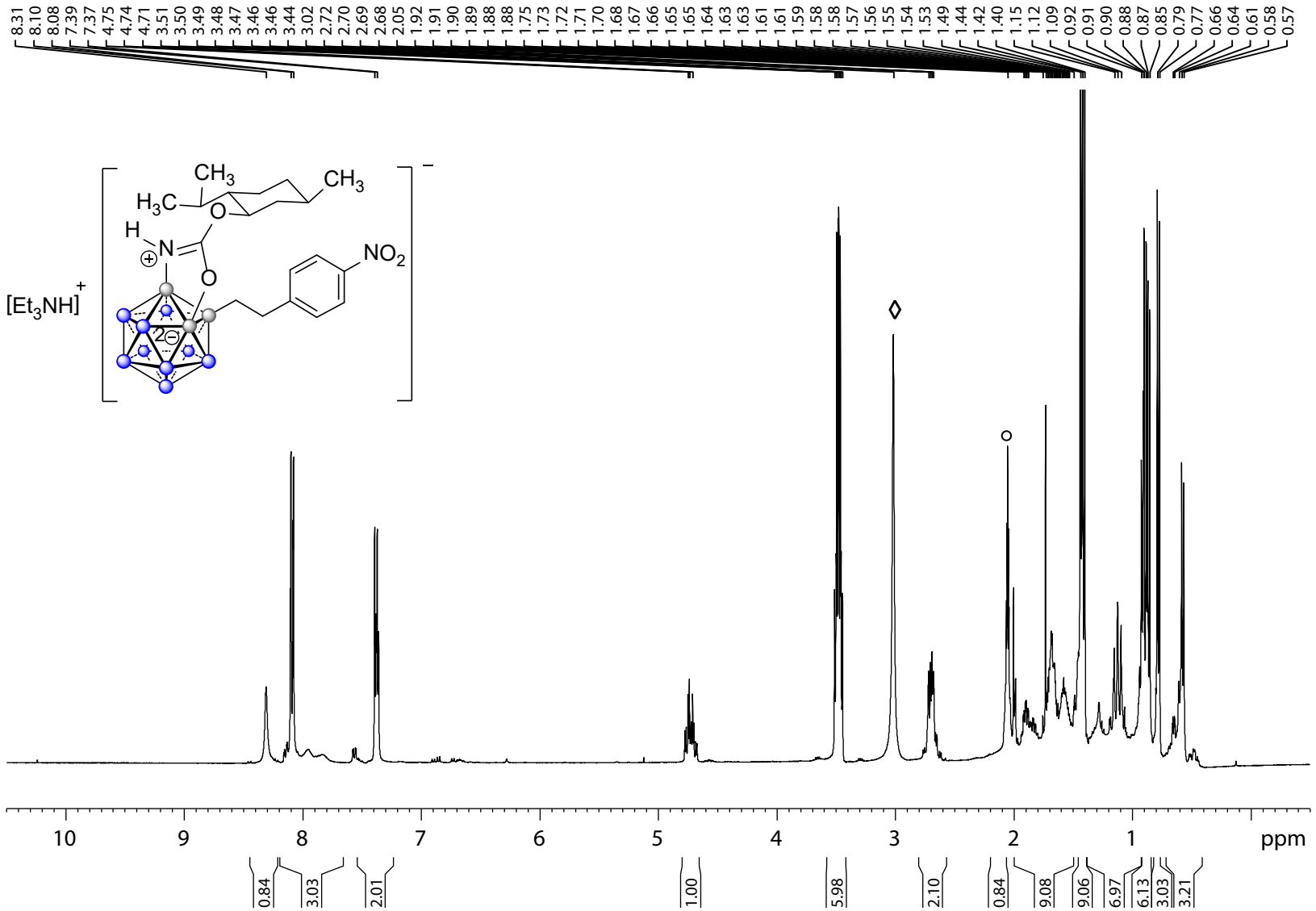
F1 - Acquisition parameters
TD                 256
SFO1          100.6238 MHz
FIDRES       196.524048 Hz
SW              249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300000 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6127690 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

20190420-B12M-4COONO2Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                 1
PROCNO                1

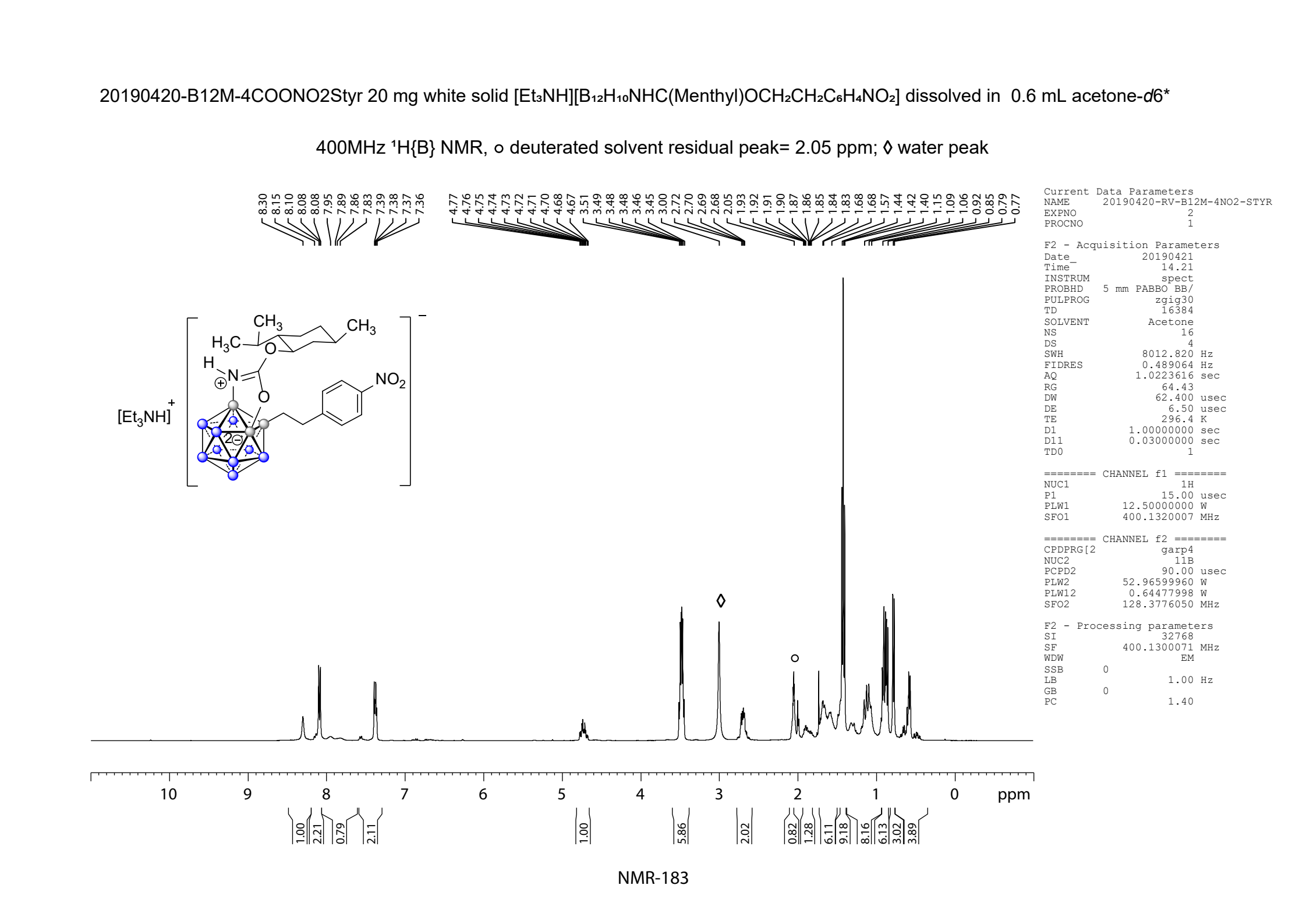
F2 - Acquisition Parameters
Date_          20190421
Time              14.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                71.39
DW                50.000 usec
DE                 6.50 usec
TE                296.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300070 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20190420-B12M-4COONO2Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4NO_2]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190420-RV-B12M-4NO2-STYR
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190421
Time                14.21
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgig30
TD                 16384
SOLVENT          Acetone
NS                    16
DS                     4
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ             1.0223616 sec
RG                 64.43
DW                62.400 usec
DE                 6.50 usec
TE                296.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

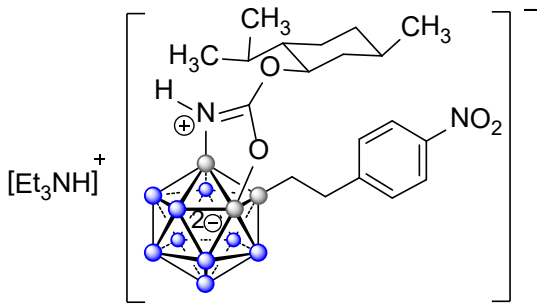
======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
PLW1         12.50000000 W
SFO1         400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2            garp4
NUC2                 11B
PCPD2              90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2         128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF           400.1300071 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190420-B12M-4COONO2Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4NO_2$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128MHz




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190421
Time              14.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.2 K
D1           1.00000000 sec
TD0                   1

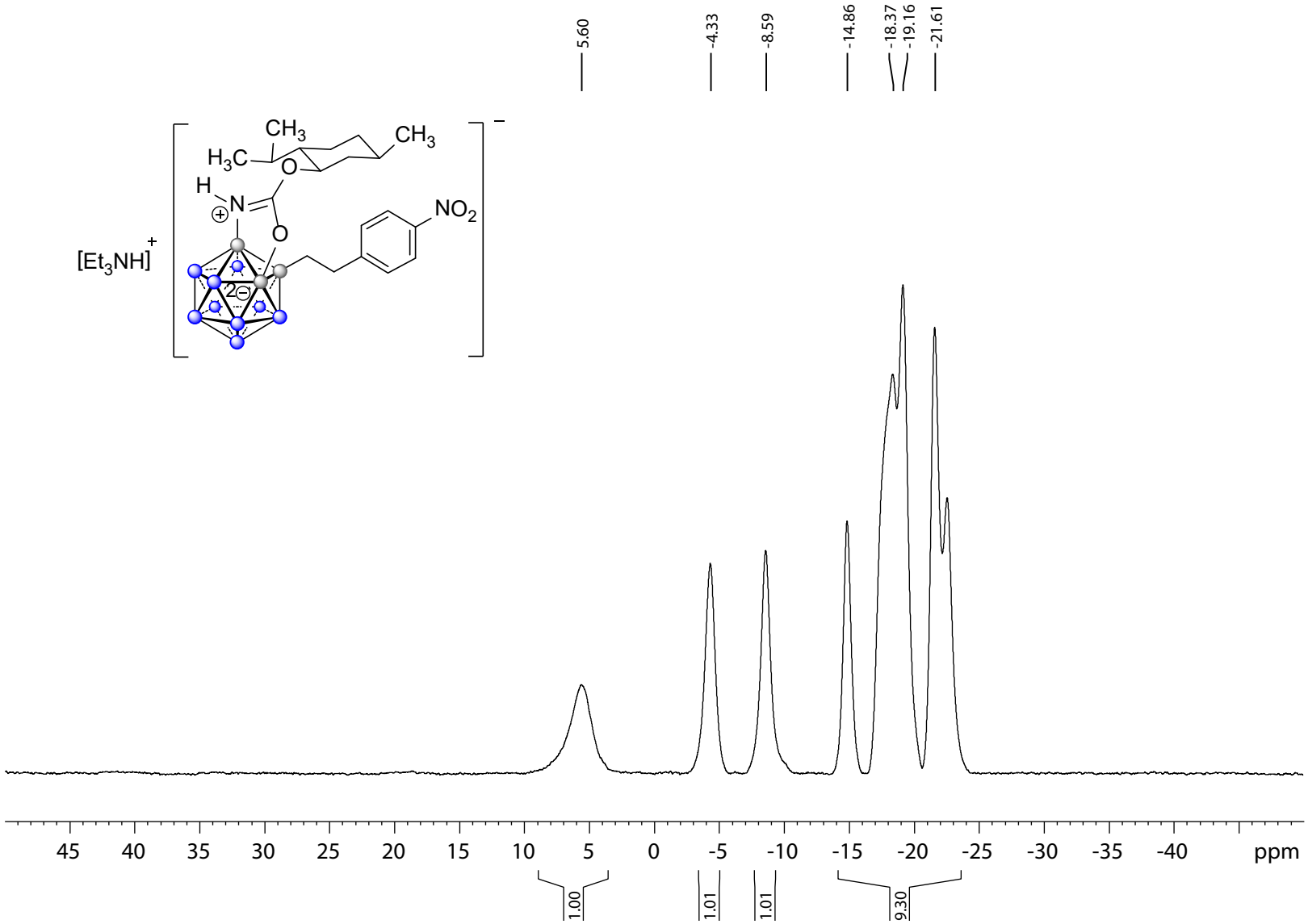
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-184

20190420-B12M-4COONO2Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4NO_2$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{^1H\}$ NMR 128MHz




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190421
Time               14.33
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.5 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776050 MHz

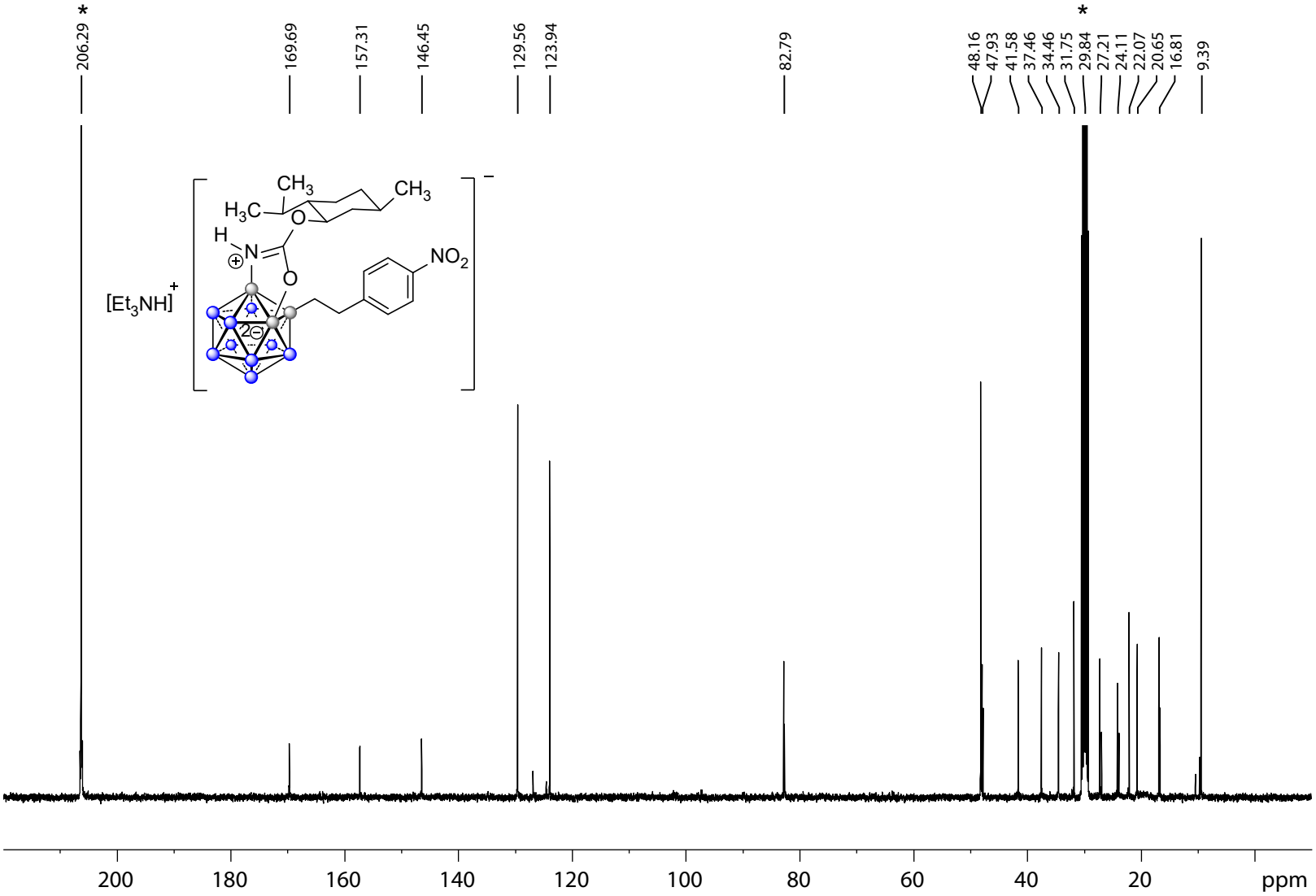
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                  32768
SF          128.3776050 MHz
WDW                    EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-185

20190420-B12M-4COONO2Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4NO_2$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190421
Time              16.05
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               296.9 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

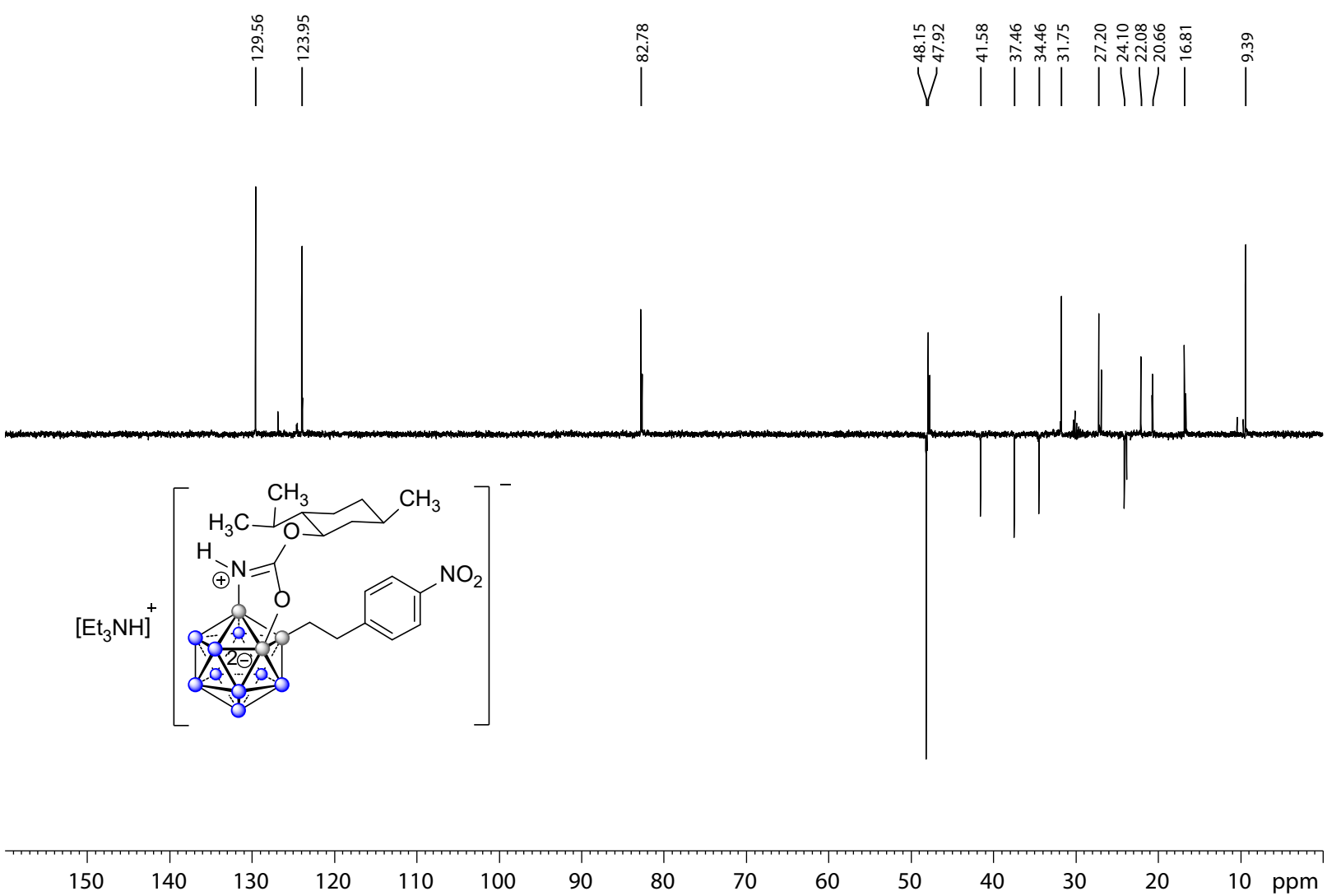
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126849 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190420-B12M-4COONO2Styr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2C_6H_4NO_2$] dissolved in 0.6 mL acetone-*d*6*

^{13}C DEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                  6
PROCNO                 1

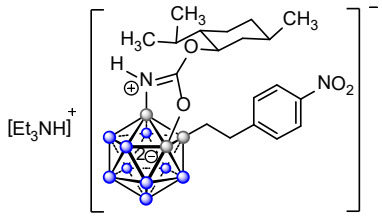
F2 - Acquisition Parameters
Date_           20190421
Time              16.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.4 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126847 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190420-B12M-4COONO2Styr 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)OCH₂CH₂C₆H₄NO₂] dissolved in 0.6 mL acetone-*d*6*



^{1}H - ^{1}H COSY NMR

NMR-188

```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_          20190421
Time              16.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT         Acetone
NS                    2
DS                    8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                107.6
DW               93.600 usec
DE                6.50 usec
TE                296.0 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

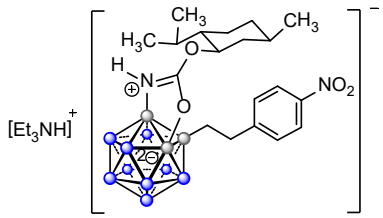
====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

F1 - Acquisition parameters
TD                  128
SFO1           400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE              QF

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2                 QF
SF          400.1300000 MHz
WDW               QSINE
SSB       0
LB        0 Hz
GB        0
```

20190420-B12M-4COONO2Styr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2C_6H_4NO_2]$ dissolved in 0.6 mL acetone-*d*6*




```
Current Data Parameters
NAME      20190420-RD-B12M-4NO2-STYR
EXPNO                  7
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190421
Time              16.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT          Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG               193.34
DW               83.200 usec
DE                6.50 usec
TE               296.2 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

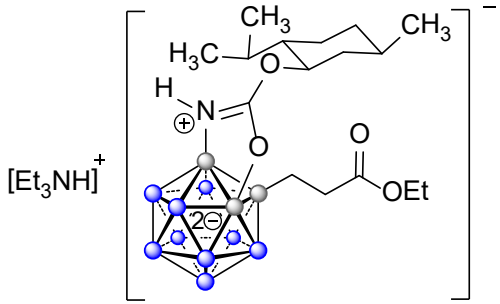
F1 - Acquisition parameters
TD                256
SFO1           100.6238 MHz
FIDRES        196.524048 Hz
SW              249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300000 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                1024
MC2        echo-antiecho
SF          100.6127690 MHz
WDW               QSINE
SSB                   2
LB        0 Hz
GB        0
```

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)OCH_2CH_2COOEt] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20190502
Time                 14.32
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT            Acetone
NS                      16
DS                       2
SWH              10000.000 Hz
FIDRES               0.152588 Hz
AQ                3.2767999 sec
RG                    55.74
DW                   50.000 usec
DE                    6.50 usec
TE                   295.3 K
D1              1.00000000 sec
TD0                      1

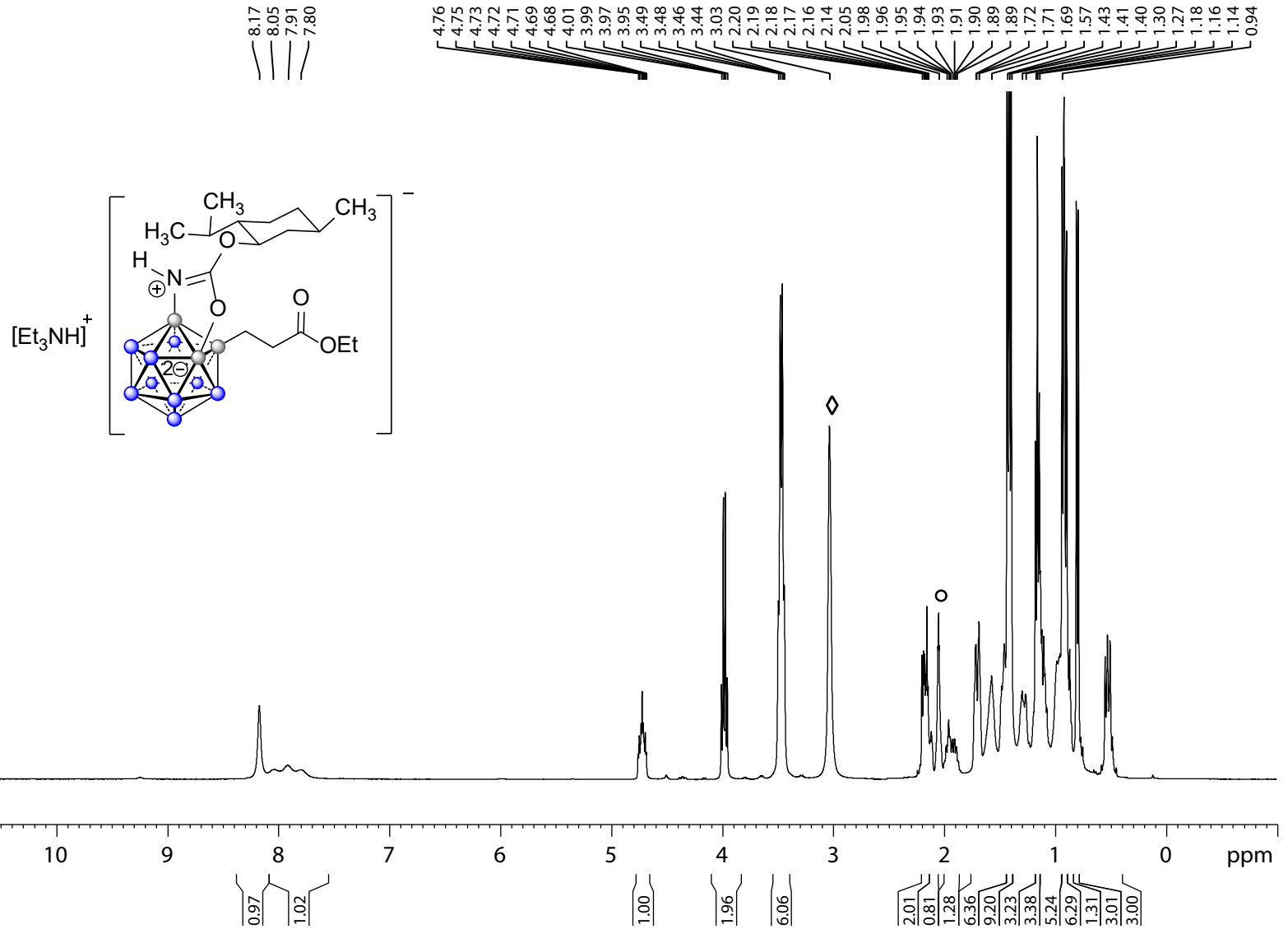
======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
PLW1          12.50000000 W
SFO1          400.1328009 MHz

F2 - Processing parameters
SI                   65536
SF            400.1300071 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

NMR-190

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-191

```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                          2
PROCNO                         1

F2 - Acquisition Parameters
Date_              20190502
Time                  14.34
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                    1.0223616 sec
RG                       55.74
DW                     62.400 usec
DE                      6.50 usec
TE                     295.6 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                           1

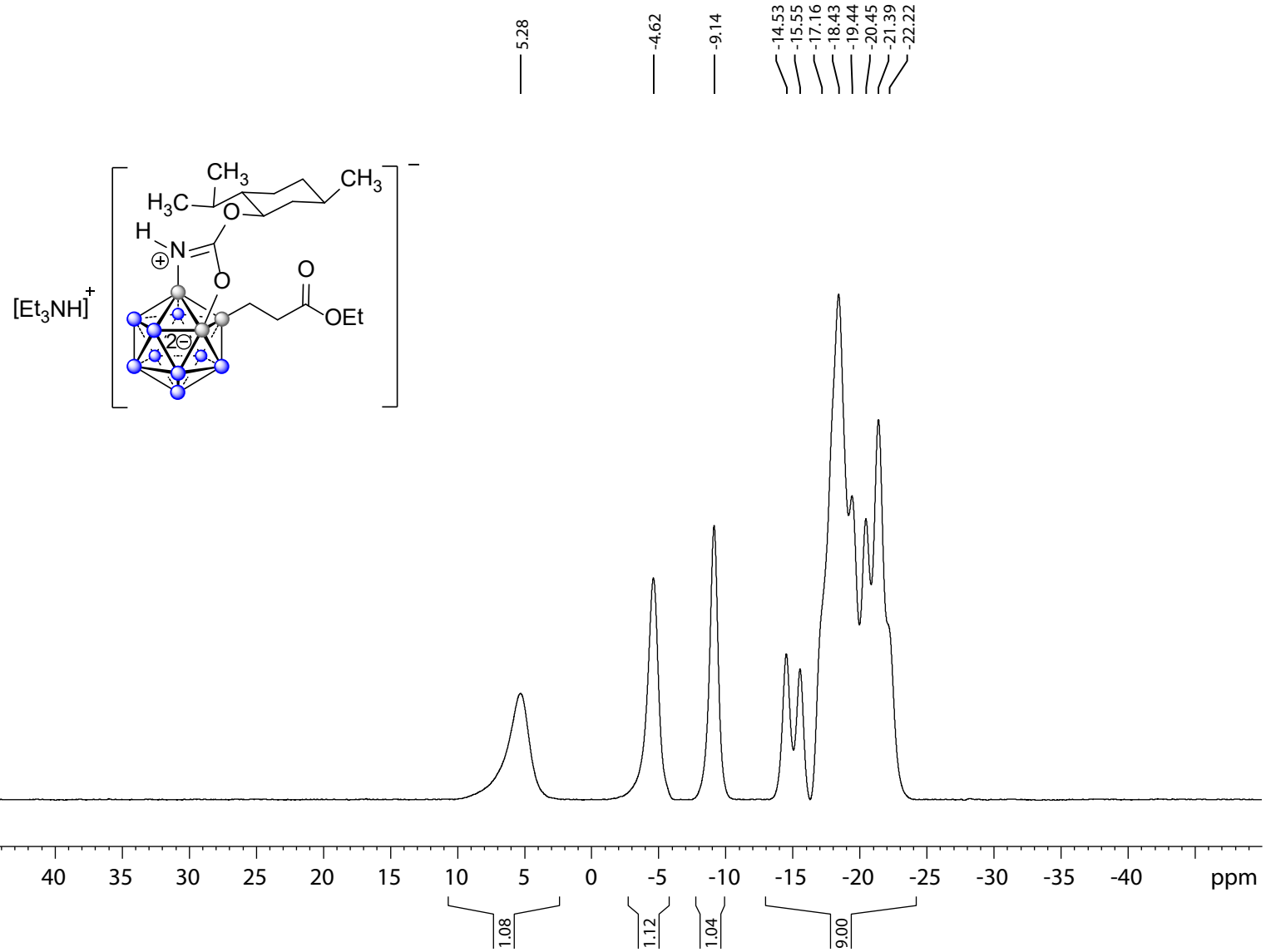
======== CHANNEL f1 ========
NUC1                         1H
P1                       15.00 usec
PLW1              12.50000000 W
SFO1              400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2                 garp4
NUC2                        11B
PCPD2                    90.00 usec
PLW2              52.96599960 W
PLW12              0.64477998 W
SFO2              128.3776050 MHz

F2 - Processing parameters
SI                       32768
SF                400.1300073 MHz
WDW                         EM
SSB          0
LB                        1.00 Hz
GB           0
PC                        1.40
```

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190502
Time                   14.40
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                   zg
TD                     65536
SOLVENT              Acetone
NS                         128
DS                           4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                  1.2845056 sec
RG                     193.34
DW                     19.600 usec
DE                      6.50 usec
TE                     295.3 K
D1                 1.00000000 sec
TD0                          1

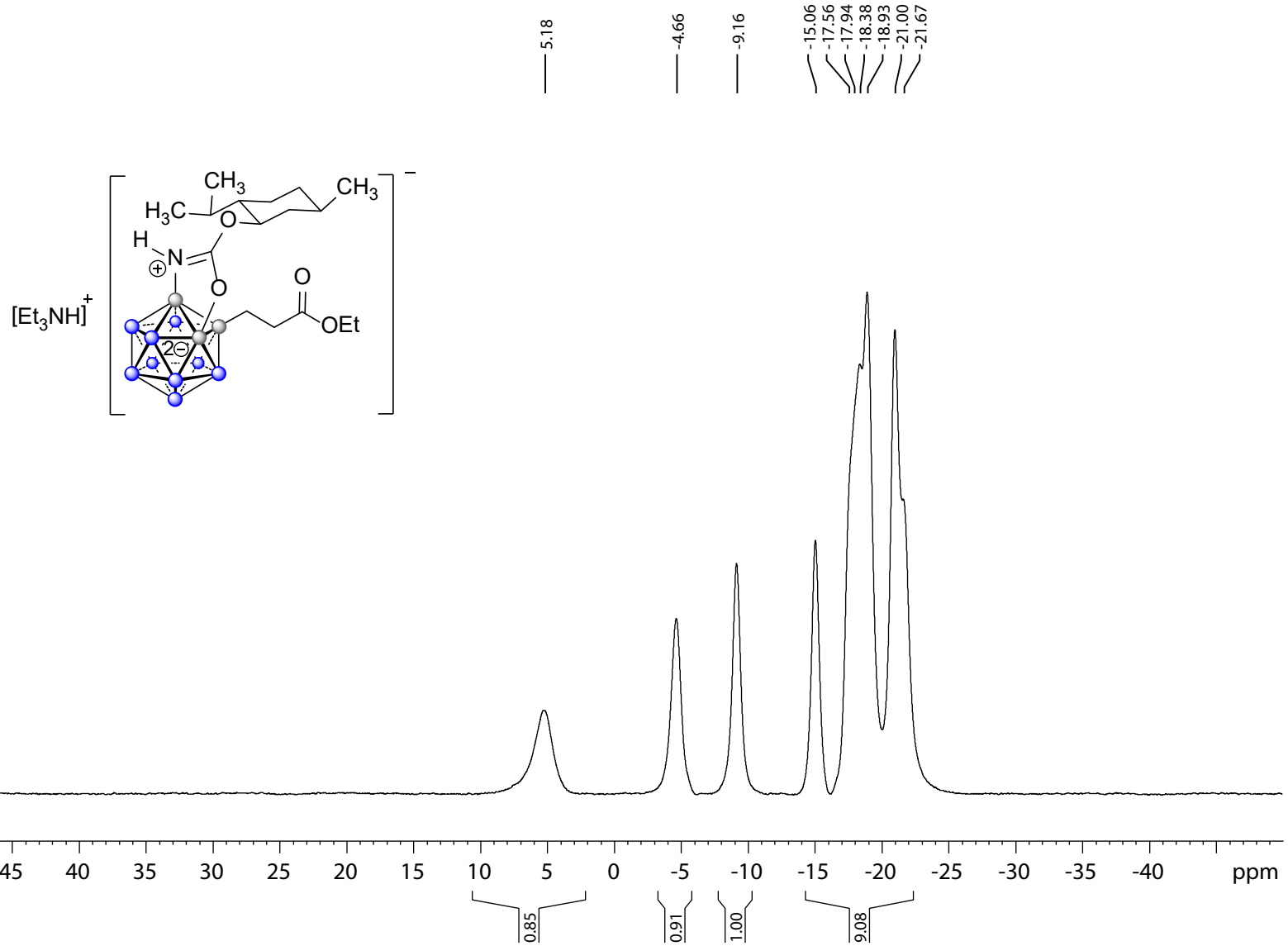
======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1              52.96599960 W
SFO1             128.3776052 MHz

F2 - Processing parameters
SI                         32768
SF                128.3776050 MHz
WDW                           EM
SSB       0
LB                     10.00 Hz
GB        0
PC                        1.40
```

NMR-192

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_              20190502
Time                 14.47
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                     128
DS                       4
SWH              25510.203 Hz
FIDRES            0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   296.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

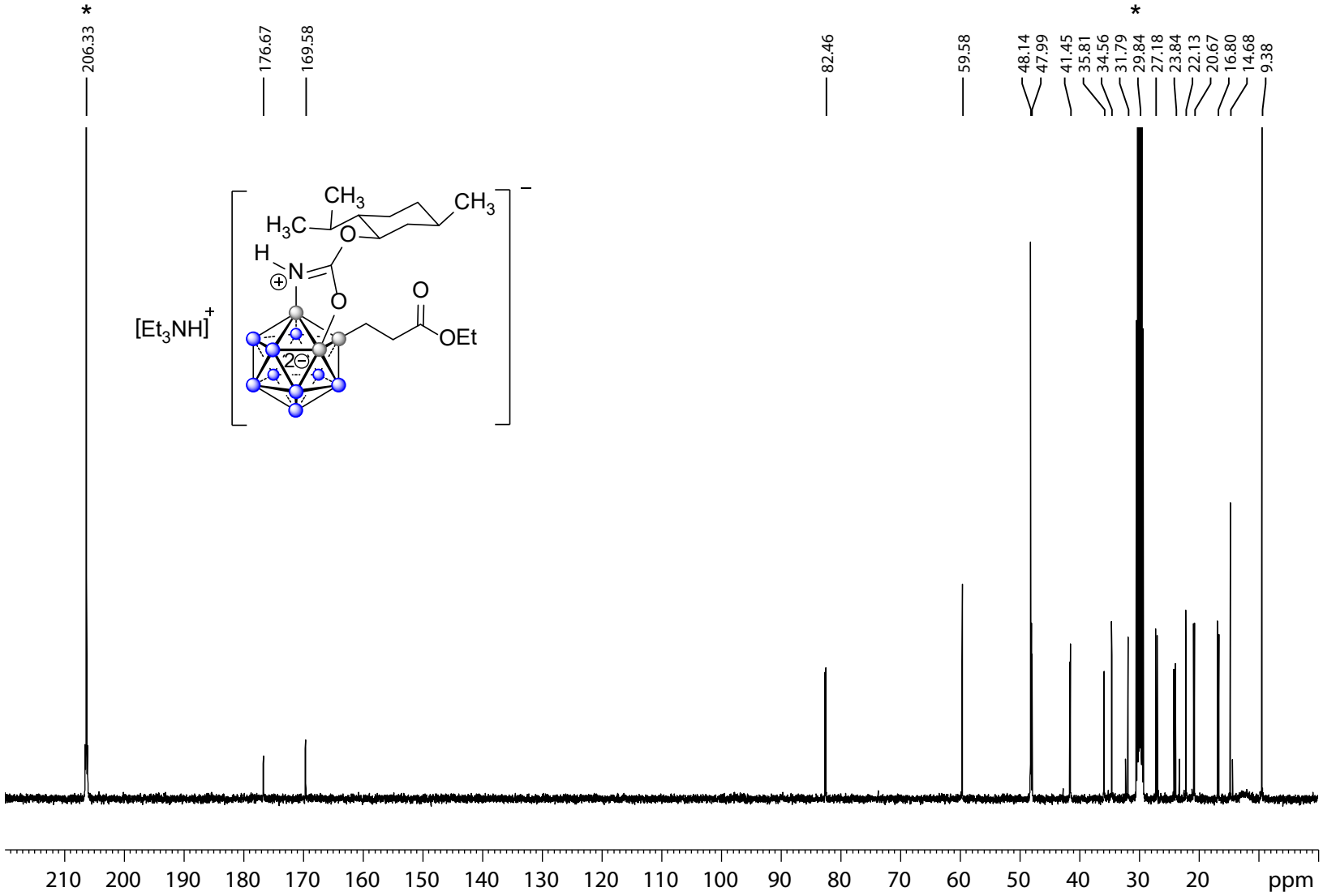
======== CHANNEL f1 ========
NUC1                   11B
P1                    9.93 usec
PLW1          52.96599960 W
SFO1         128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1320007 MHz

F2 - Processing parameters
SI                   32768
SF           128.3776050 MHz
WDW                     EM
SSB       0
LB                   10.00 Hz
GB        0
PC                    1.40
```

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                          5
PROCNO                         1

F2 - Acquisition Parameters
Date_               20190502
Time                   16.20
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  296.2 K
D1               1.50000000 sec
D11              0.03000000 sec
TD0                      1

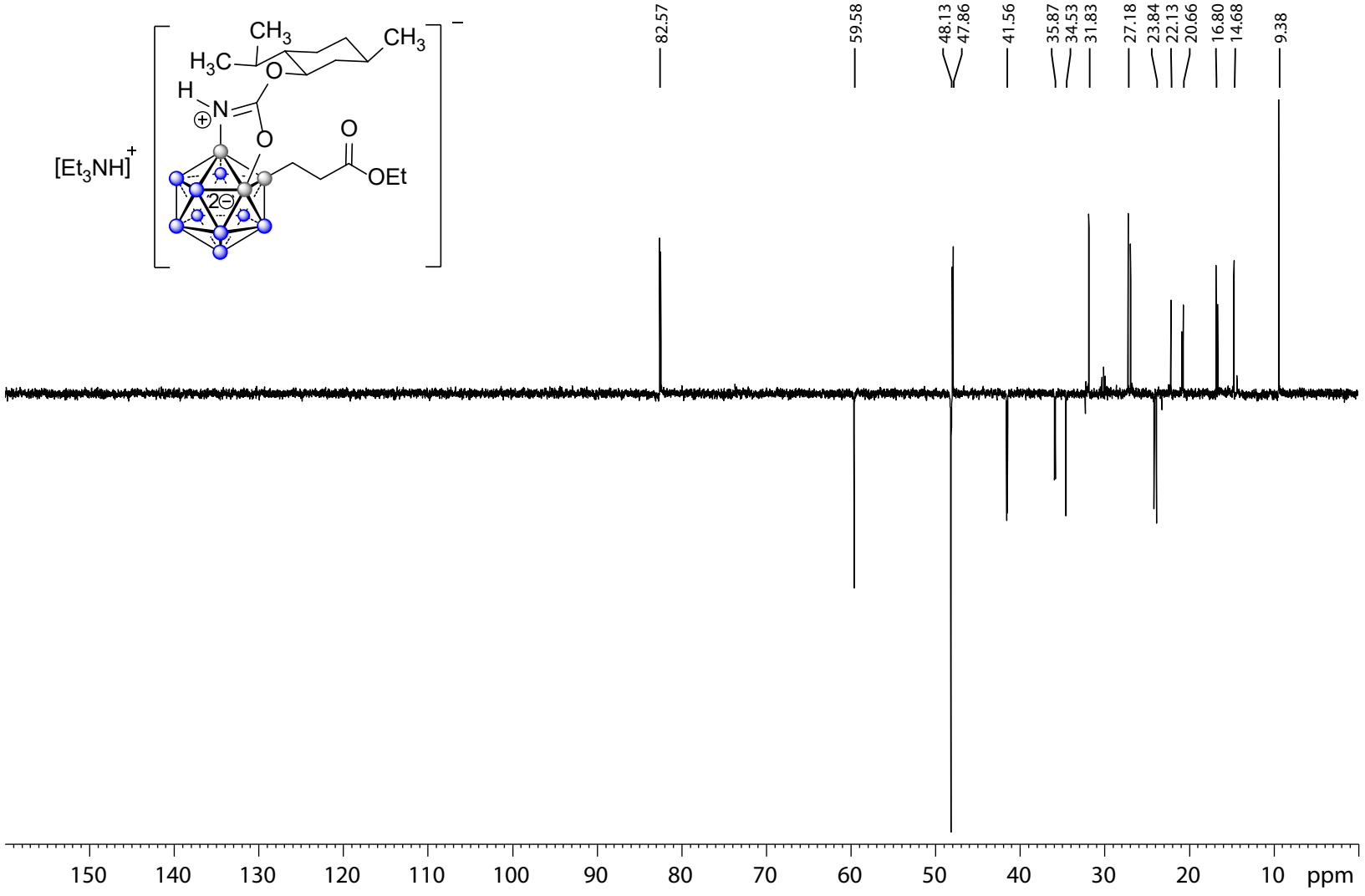
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6126860 MHz
WDW                    EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

20190501-B12M-EtAcr 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt]$ dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190501-RV-B12M-EtHcr
EXPNO                         6
PROCNO                        1

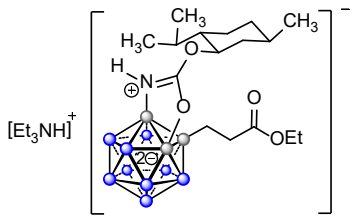
F2 - Acquisition Parameters
Date_              20190502
Time                 16.48
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            dept135
TD                   65536
SOLVENT            Acetone
NS                     512
DS                       4
SWH              29296.875 Hz
FIDRES            0.447035 Hz
AQ                1.1184810 sec
RG                   193.34
DW                  17.067 usec
DE                   6.50 usec
TE                  296.1 K
CNST2           145.0000000
D1               2.00000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
P2                   20.00 usec
PLW1           53.00000000 W
SFO1           100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
P3                   15.00 usec
P4                   30.00 usec
PCPD2                80.00 usec
PLW2           12.50000000 W
PLW12           0.43945000 W
SFO2           400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF              100.6126862 MHz
WDW                     EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    4.00
```

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*



^1H - ^1H COSY NMR

NMR-196

```
Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190502
Time               17.04
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                  2048
SOLVENT          Acetone
NS                     2
DS                     8
SWH             5341.880 Hz
FIDRES          2.608340 Hz
AQ              0.1916928 sec
RG                 64.43
DW                 93.600 usec
DE                  6.50 usec
TE                295.0 K
D0              0.00000300 sec
D1              2.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
D13             0.00000400 sec
D16             0.00020000 sec
IN0             0.00018720 sec

======== CHANNEL f1 ========
NUC1                   1H
P0                  15.00 usec
P1                  15.00 usec
P17               2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1               10.00 %
P16              1000.00 usec

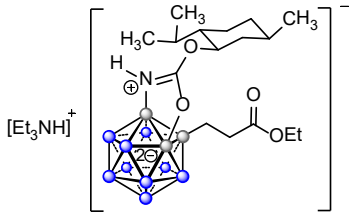
F1 - Acquisition parameters
TD                   128
SFO1            400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE                QF

F2 - Processing parameters
SI                   1024
SF           400.1300045 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                   1024
MC2                    QF
SF           400.1300041 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

20190501-B12M-EtAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOEt$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR

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Current Data Parameters
NAME      20190501-RV-B12M-EtAcr
EXPNO                          7
PROCNO                         1

F2 - Acquisition Parameters
Date_              20190502
Time               16.50
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG      hsqcetgpsi2
TD                 1024
SOLVENT          Acetone
NS                    2
DS                   16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                 83.200 usec
DE                  6.50 usec
TE                295.9 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                    1H
P1                   15.00 usec
P2                   30.00 usec
P28                1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                  13C
P3                   10.00 usec
P4                   20.00 usec
PCPD2                70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1                80.00 %
GPZ2                20.10 %
GPZ3                11.00 %
GPZ4                -5.00 %
P16               1000.00 usec
P19                600.00 usec

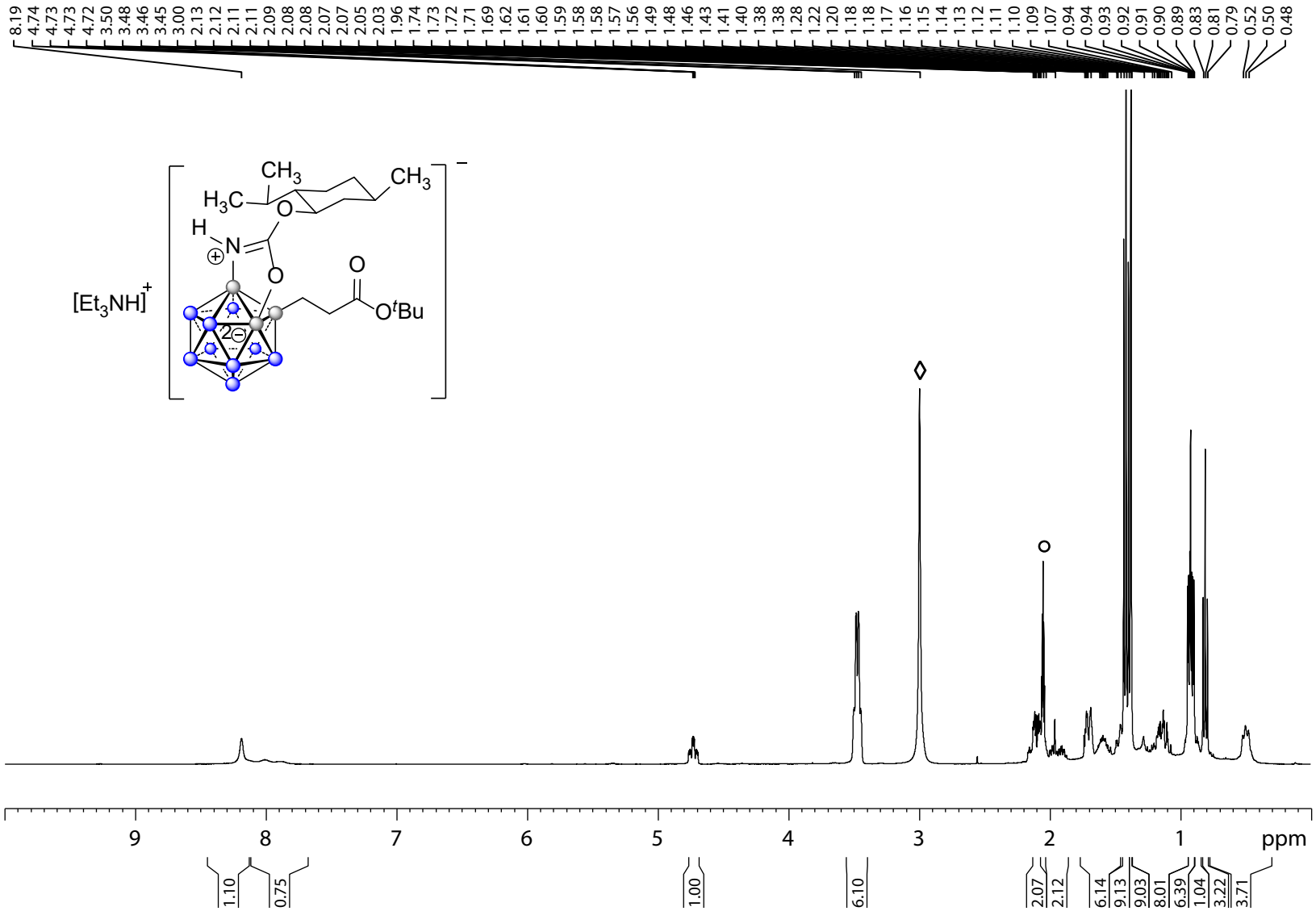
F1 - Acquisition parameters
TD                    256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW              249.991 ppm
FnMODE     Echo-Antiecho

F2 - Processing parameters
SI                   1024
SF           400.1300054 MHz
WDW                  QSINE
SSB                     2
LB         0 Hz
GB         0
PC                   1.40

F1 - Processing parameters
SI                   1024
MC2        echo-antiecho
SF           100.6126811 MHz
WDW                  QSINE
SSB                     2
LB         0 Hz
GB         0
```

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_          20190608
Time               5.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                78.69
DW                50.000 usec
DE                 6.50 usec
TE                293.3 K
D1             1.00000000 sec
TD0                  1

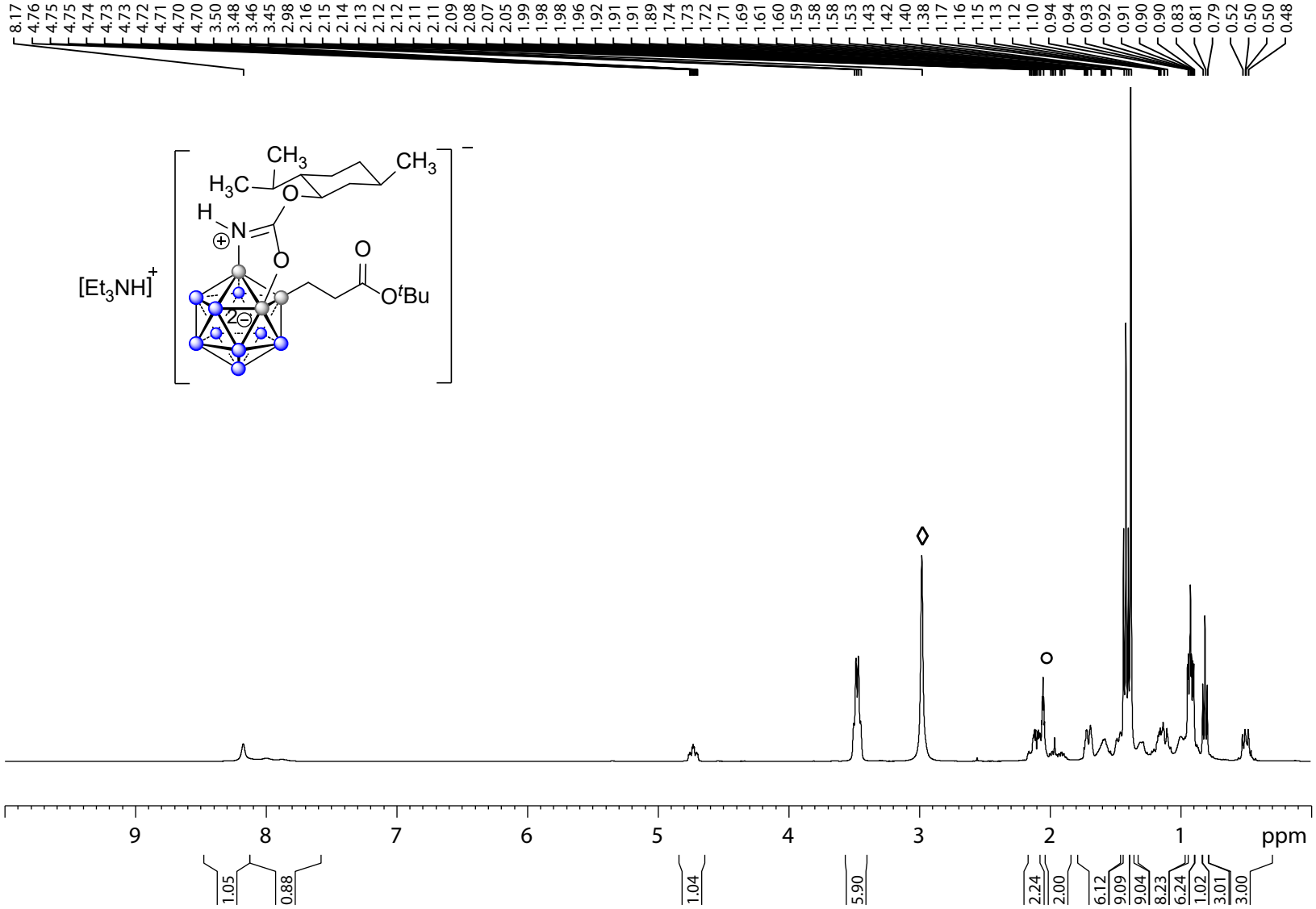
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF           400.1300071 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-198

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190608
Time                5.46
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgig30
TD                 16384
SOLVENT          Acetone
NS                    16
DS                     4
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                 78.69
DW                62.400 usec
DE                 6.50 usec
TE                293.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

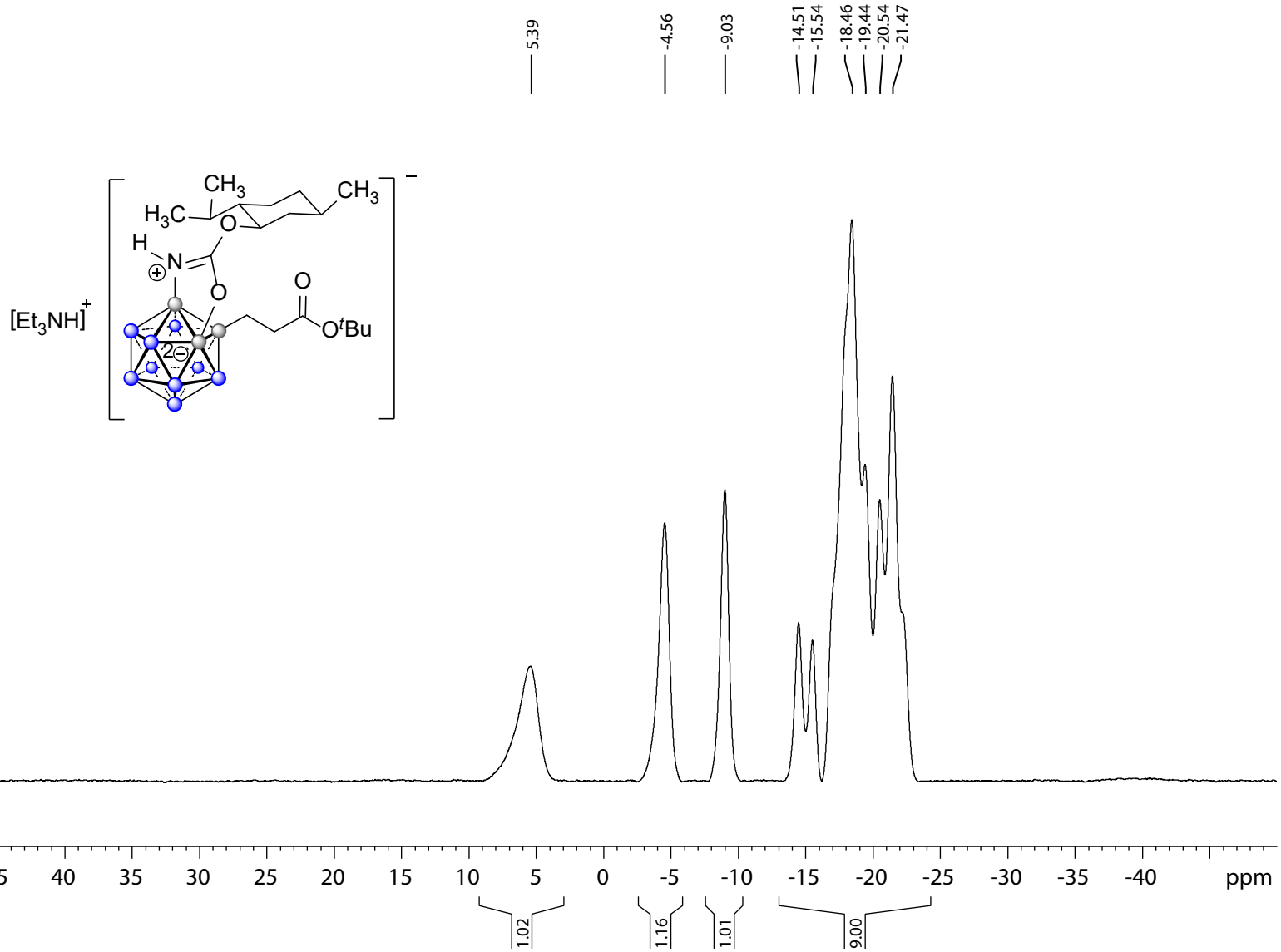
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                 11B
PCPD2             90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300072 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                3
PROCNO               1

F2 - Acquisition Parameters
Date_           20190608
Time                5.52
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                293.3 K
D1             1.00000000 sec
TD0                    1

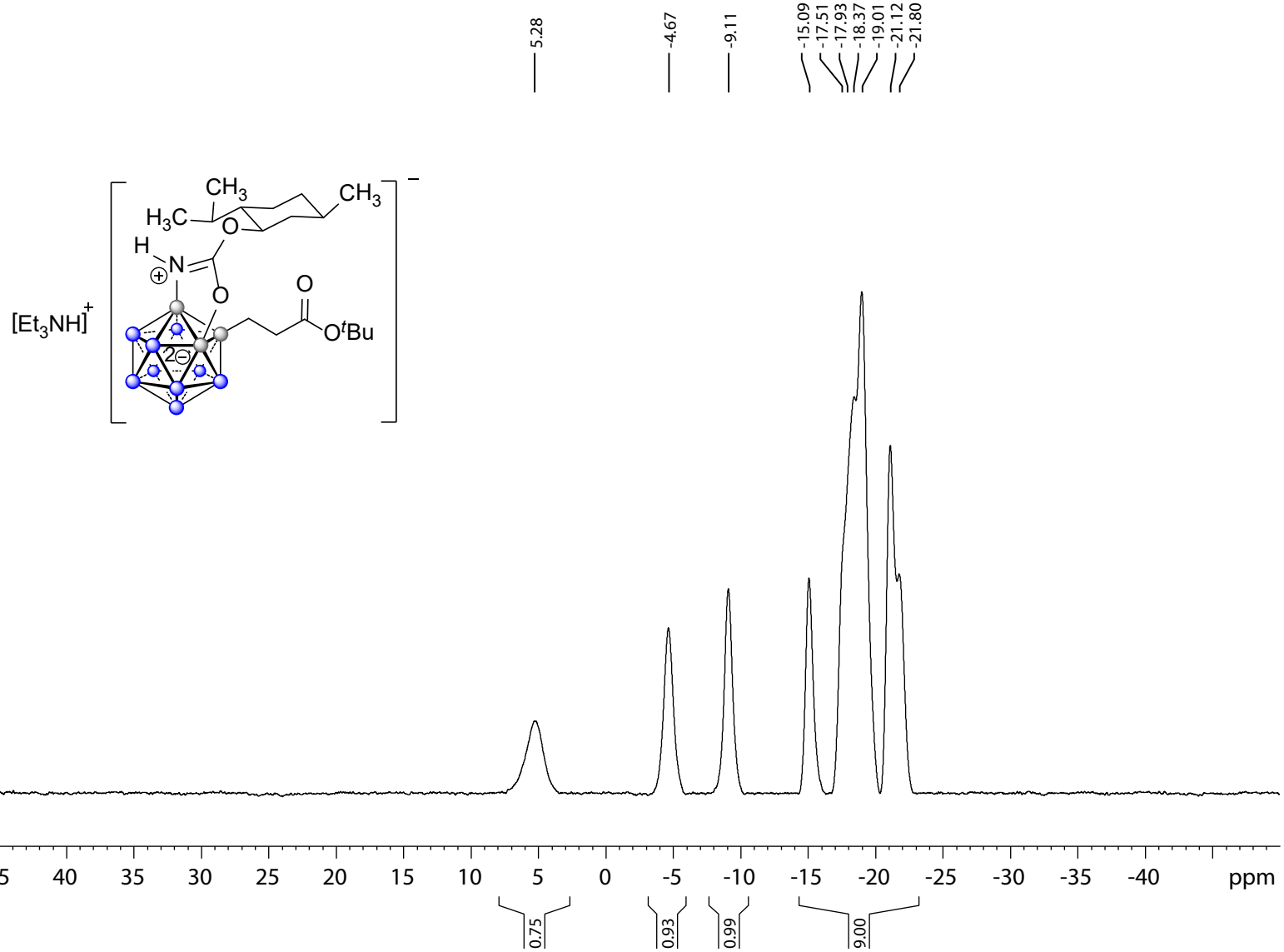
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-200

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                4
PROCNO               1

F2 - Acquisition Parameters
Date_           20190608
Time               5.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                294.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776050 MHz

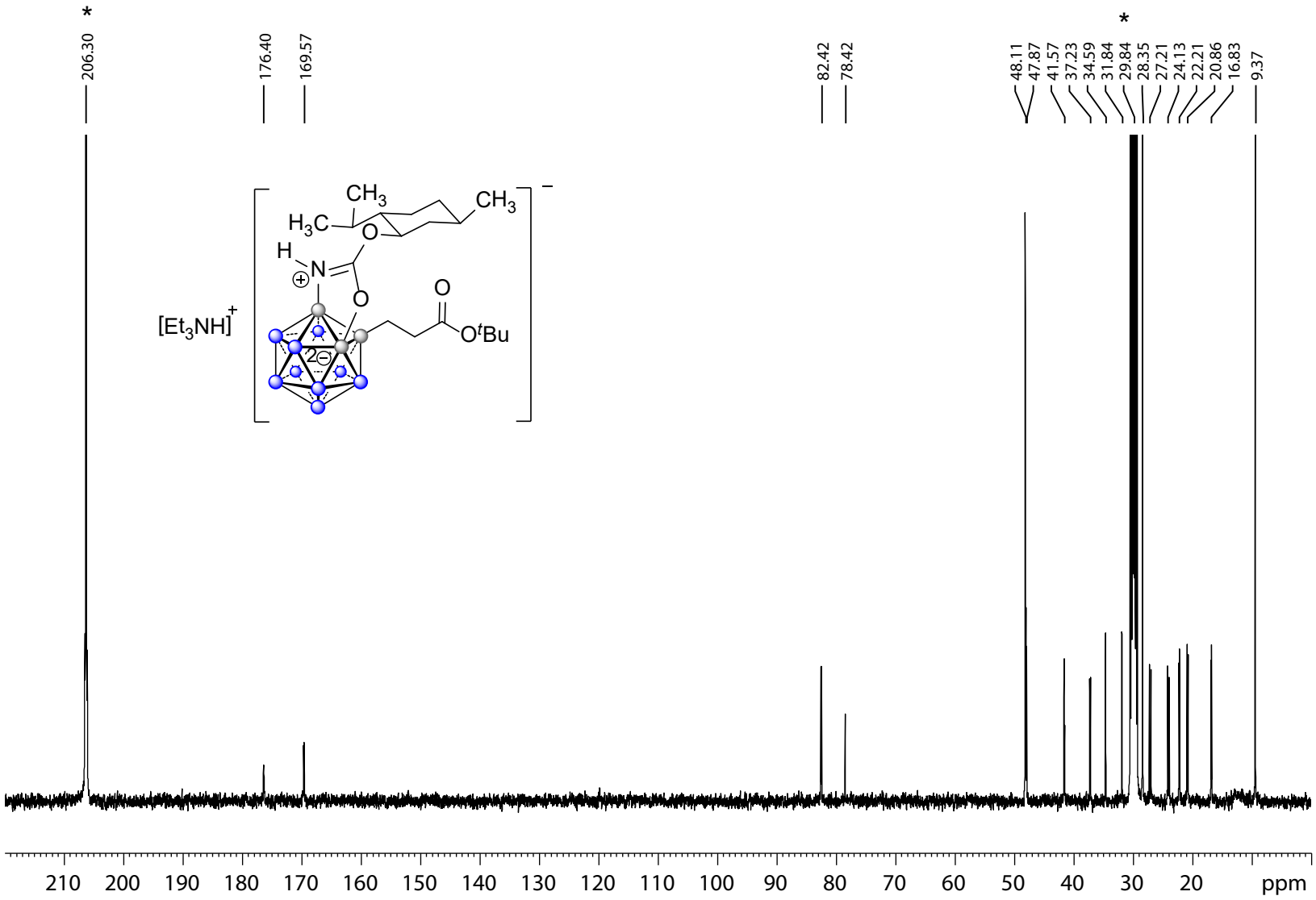
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1320007 MHz

F2 - Processing parameters
SI                32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-201

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                5
PROCNO               1

F2 - Acquisition Parameters
Date_           20190608
Time              7.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT         Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              294.4 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                  1

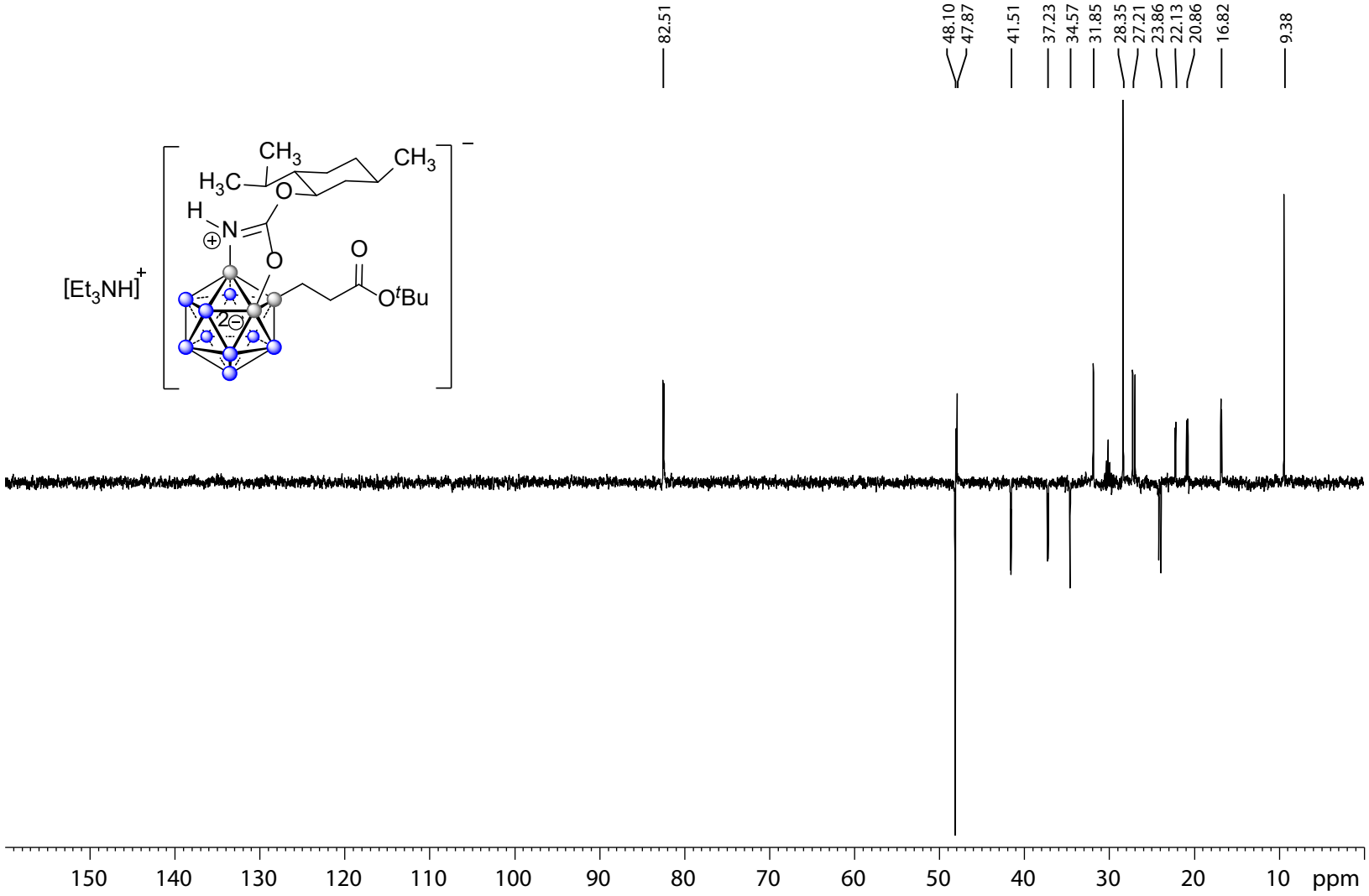
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126841 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)$OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                6
PROCNO               1

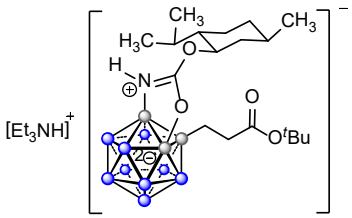
F2 - Acquisition Parameters
Date_           20190608
Time               7.59
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               293.6 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

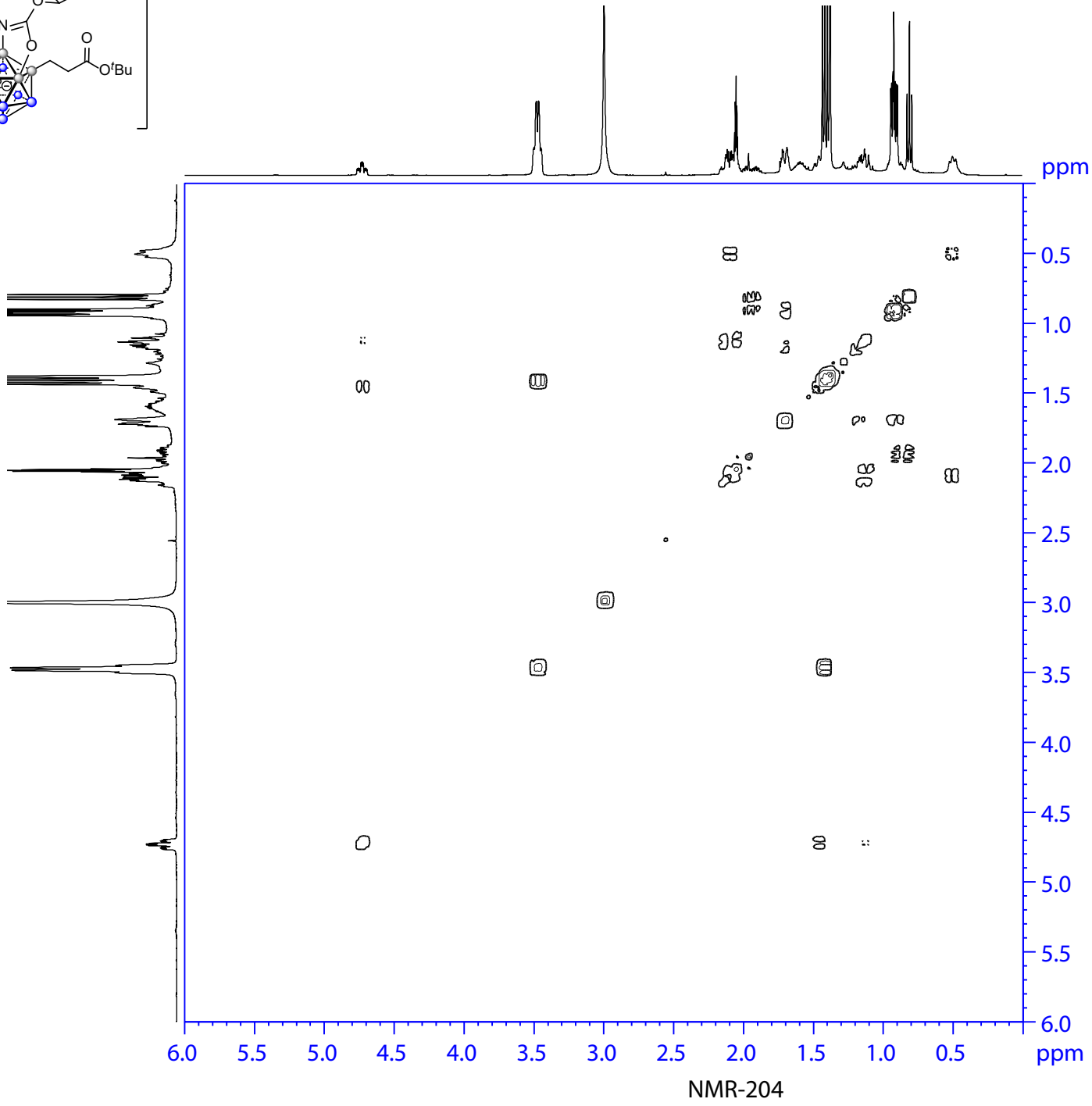
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126839 MHz
WDW                EM
SSB       0
LB                2.00 Hz
GB        0
PC                4.00
```

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OCH_2CH_2COOtBu$] dissolved in 0.6 mL acetone-*d*6*



^1H - ^1H COSY NMR



NMR-204

```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20190608
Time               8.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT         Acetone
NS                    2
DS                    8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                138.32
DW                93.600 usec
DE                 6.50 usec
TE                293.7 K
D0             0.00000300 sec
D1             2.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1         400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

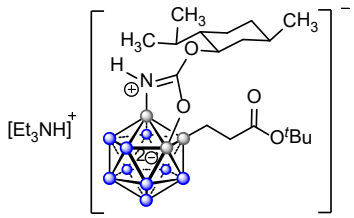
F1 - Acquisition parameters
TD                   128
SFO1            400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE               QF

F2 - Processing parameters
SI                  1024
SF           400.1300077 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300077 MHz
WDW                QSINE
SSB       0
LB        0 Hz
GB        0
```

20190607-B12M-tBuAcr 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)$OCH_2CH_2COO^tBu$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^{13}C HSQC NMR




```
Current Data Parameters
NAME      20190607-RV-B12M-tBuAcry
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20190608
Time_              8.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                 1024
SOLVENT         Acetone
NS                    2
DS                   16
SWH             6009.615 Hz
FIDRES          5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                293.5 K
CNST2         145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                 15.00 usec
P2                 30.00 usec
P28              1000.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                 10.00 usec
P4                 20.00 usec
PCPD2              70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2         100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16              1000.00 usec
P19               600.00 usec

F1 - Acquisition parameters
TD                   256
SFO1            100.6238 MHz
FIDRES        196.524048 Hz
SW               249.991 ppm
FnMODE     Echo-Antiecho

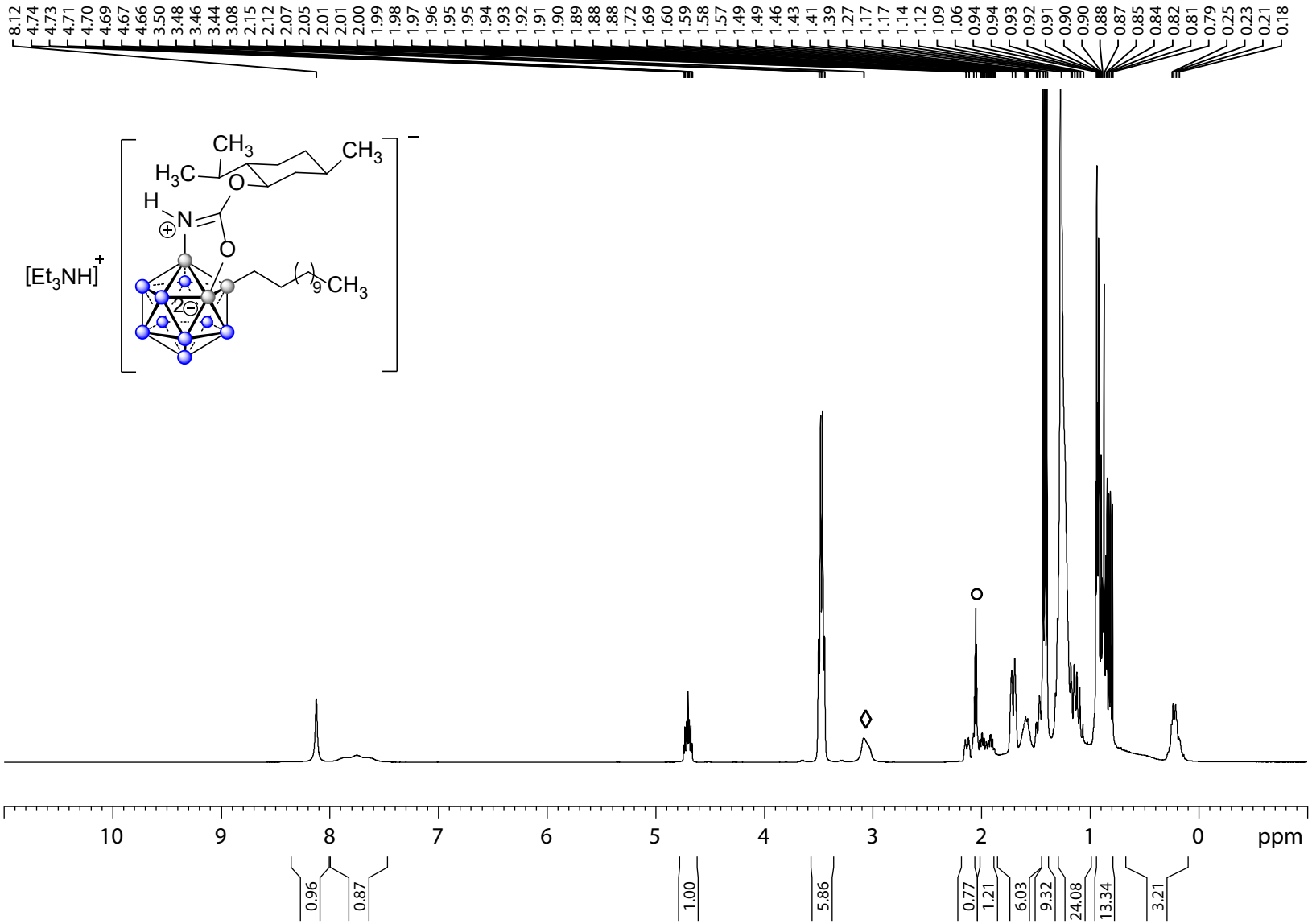
F2 - Processing parameters
SI                  1024
SF           400.1300052 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2        echo-antiecho
SF           100.6126833 MHz
WDW                 QSINE
SSB                    2
LB         0 Hz
GB         0
```

NMR-205

20190507-B12M-Dodecane 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20190508
Time              5.38
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT        Acetone
NS                  16
DS                   2
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ               3.2767999 sec
RG                  39.73
DW                50.000 usec
DE                 6.50 usec
TE                294.1 K
D1             1.00000000 sec
TD0                  1

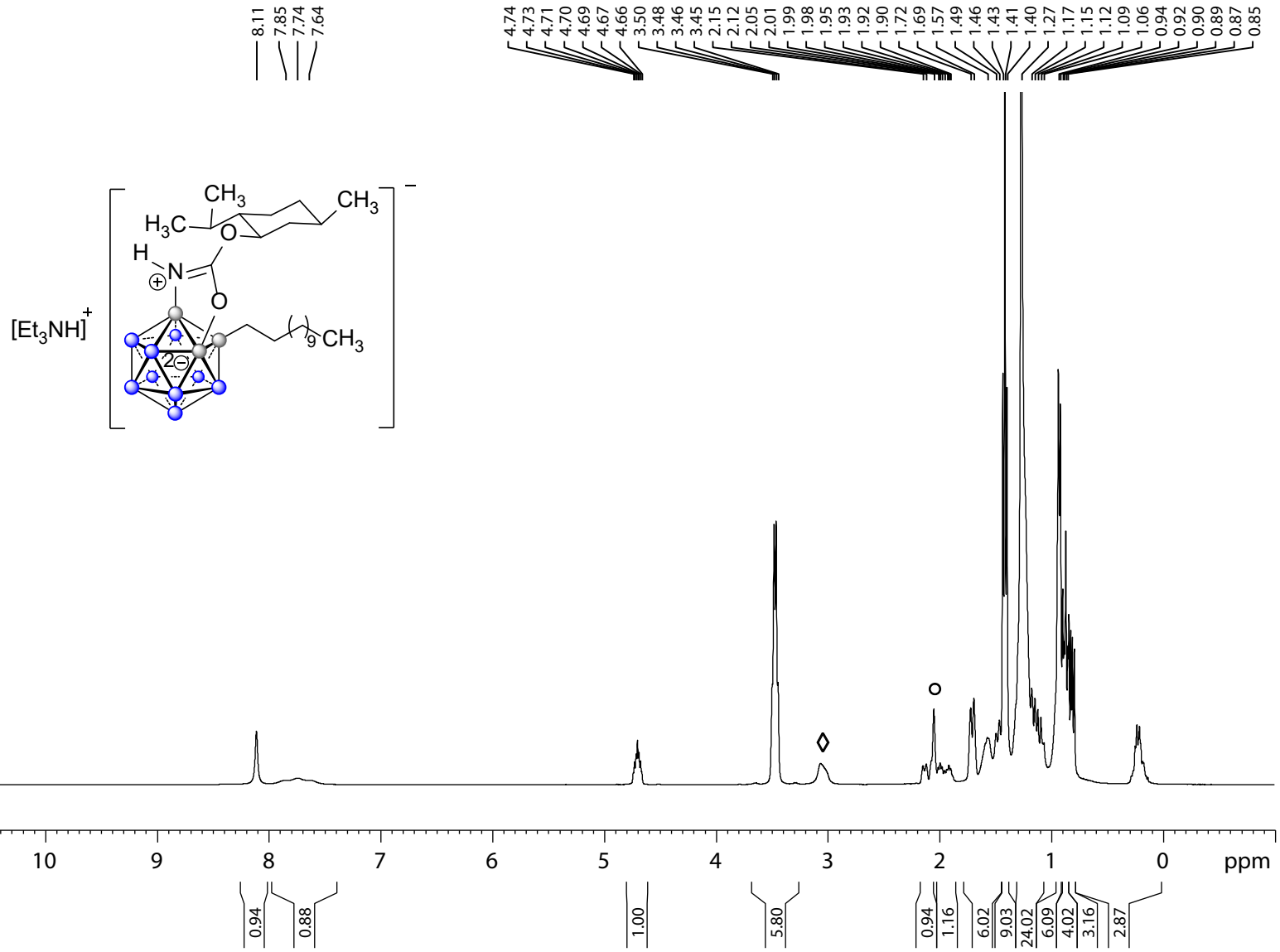
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1         400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300071 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-206

20190507-B12M-Dodecane 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}]$ dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-207

```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20190508
Time               5.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                39.73
DW               62.400 usec
DE                6.50 usec
TE               294.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

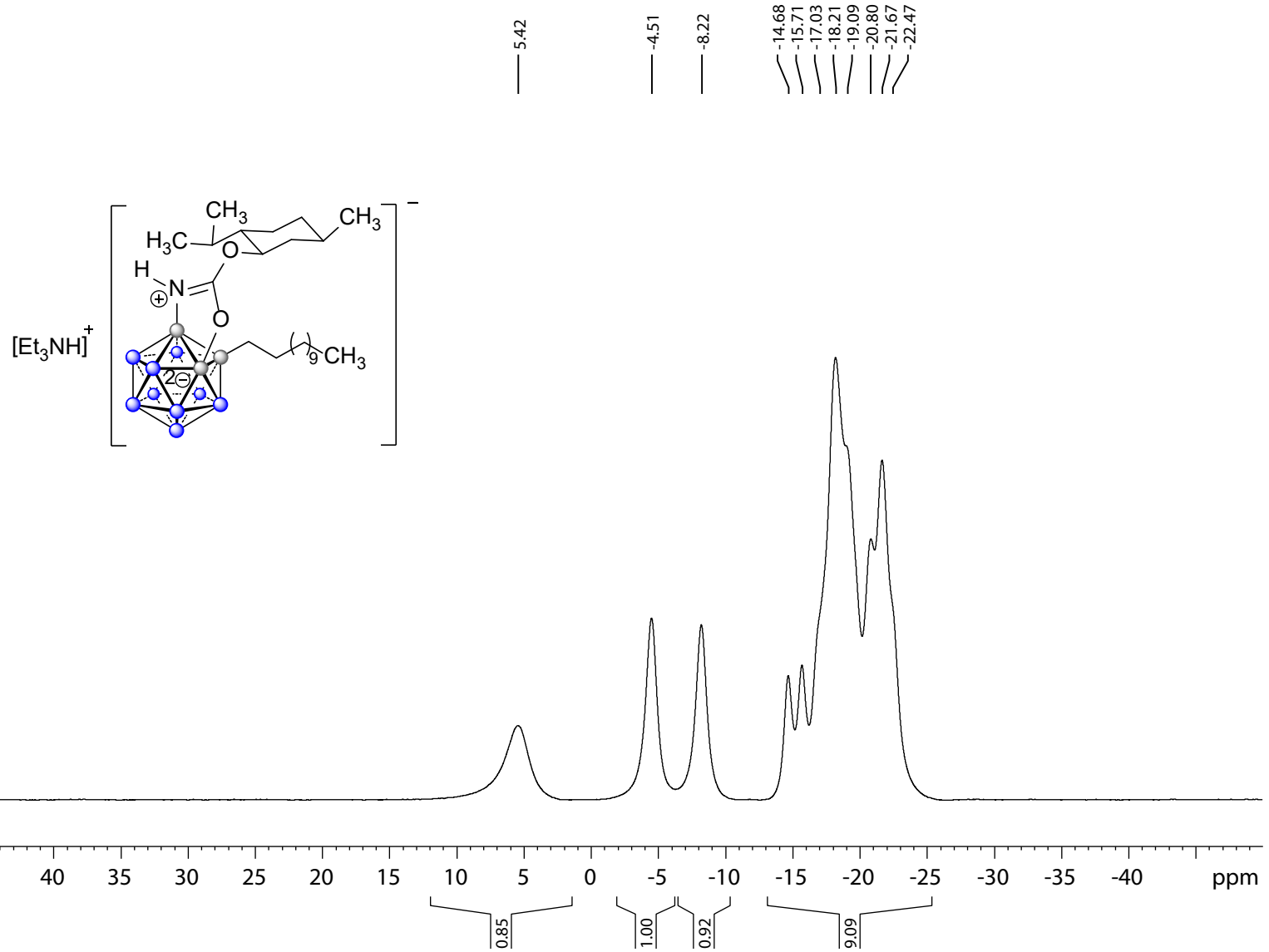
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2              90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                32768
SF          400.1300072 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190507-B12M-Dodecane 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}]$ dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20190508
Time                5.46
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                294.4 K
D1            1.00000000 sec
TD0                    1

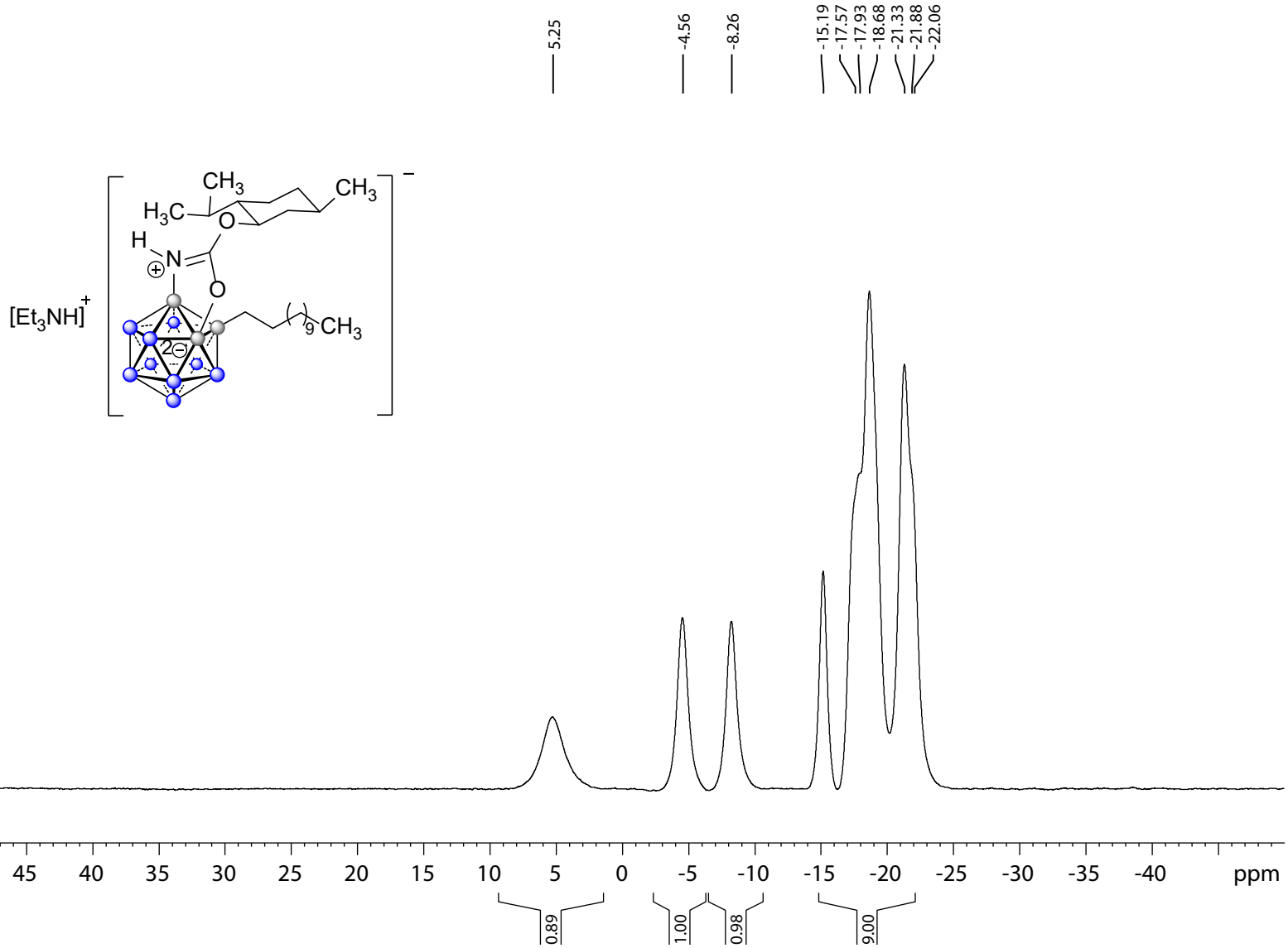
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1         52.96599960 W
SFO1        128.3776052 MHz

F2 - Processing parameters
SI                 32768
SF          128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR-208

20190507-B12M-Dodecane 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}]$ dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20190508
Time              5.52
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE                6.50 usec
TE               294.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  1

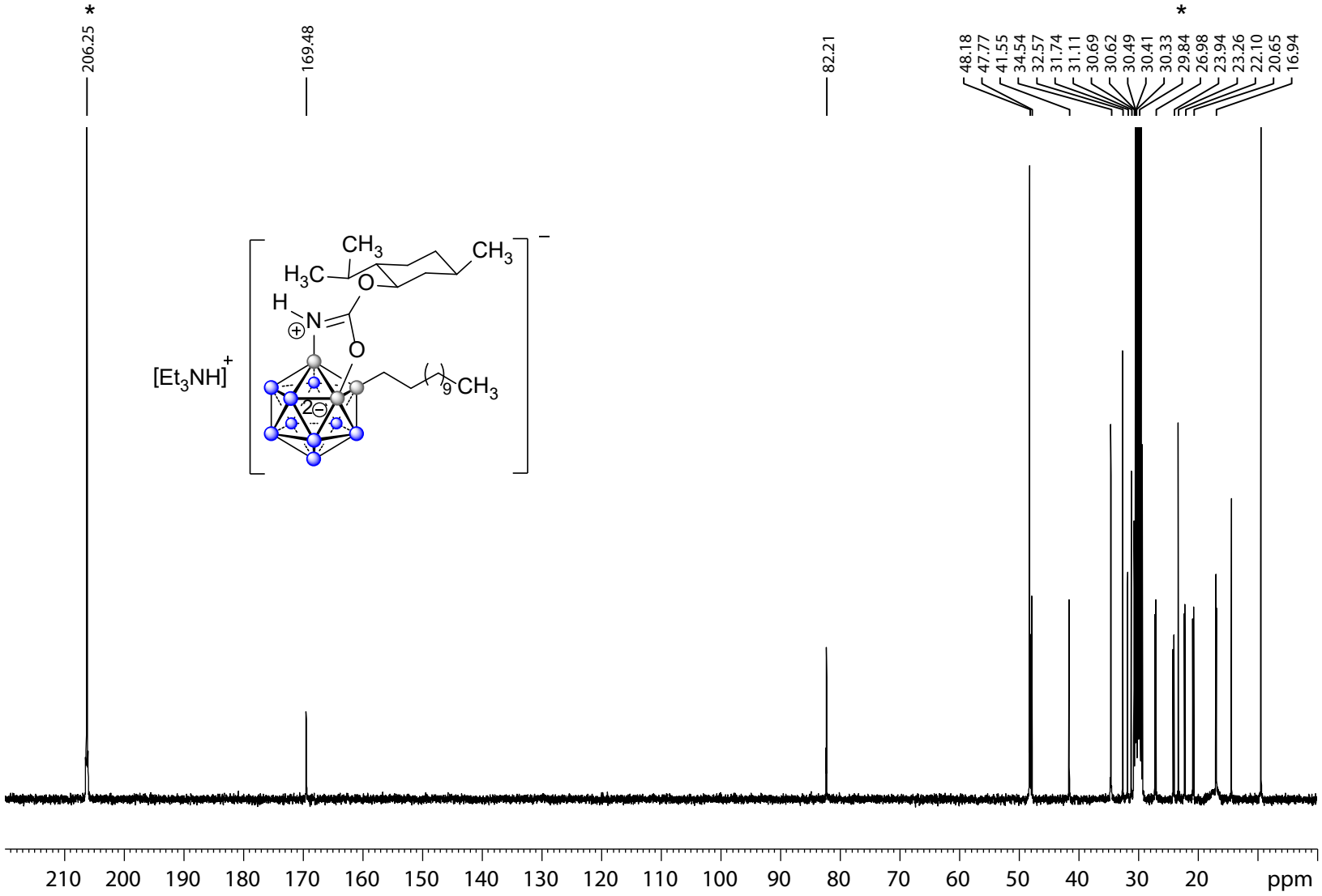
======== CHANNEL f1 ========
NUC1                11B
P1                 9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                EM
SSB       0
LB               10.00 Hz
GB        0
PC                1.40
```

20190507-B12M-Dodecane 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190508
Time              18.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                295.5 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

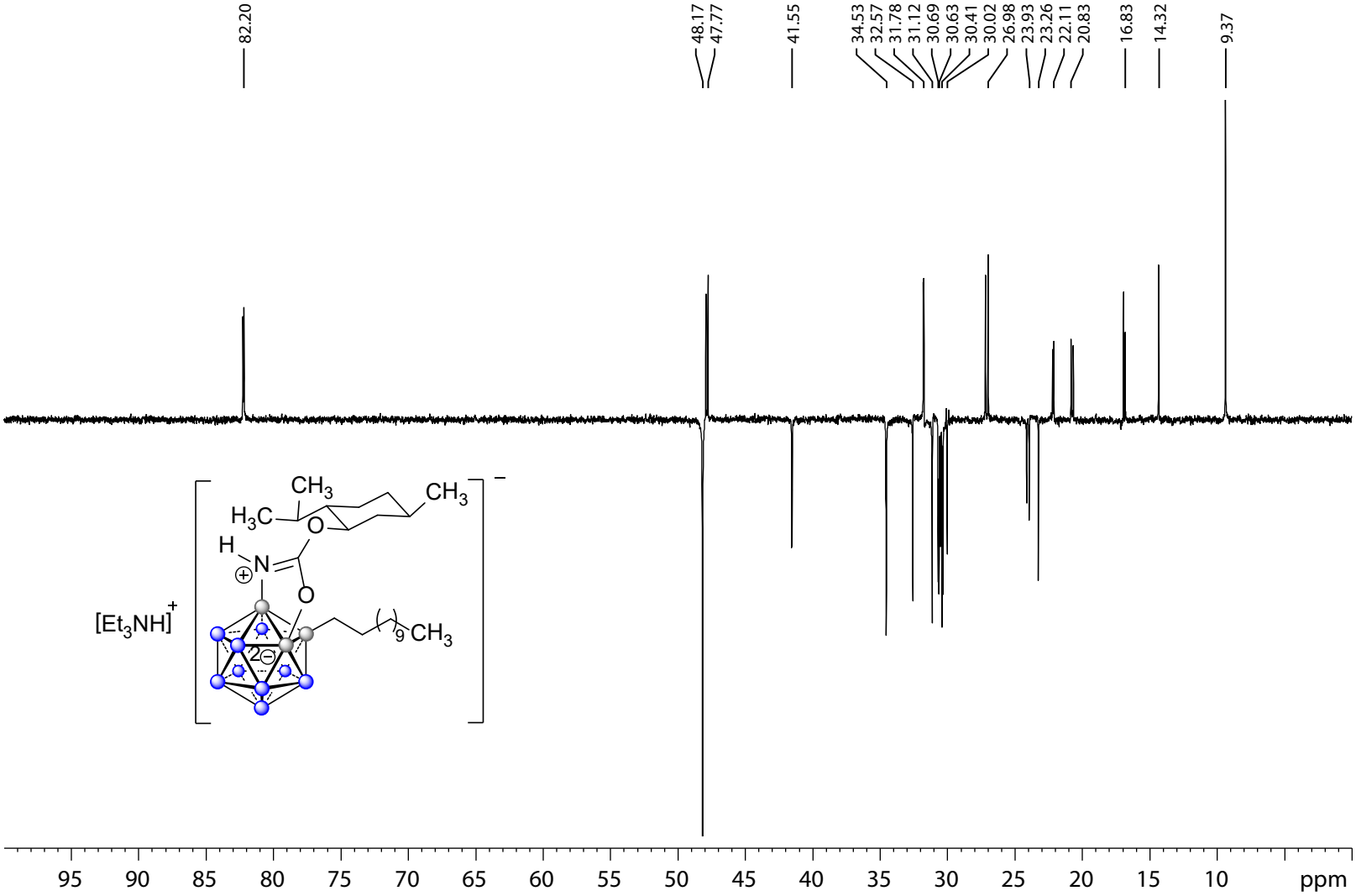
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6126885 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190507-B12M-Dodecane 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}$] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz



[Et_3NH]$^+$

```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_            20190508
Time                19.23
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           dept135
TD                  65536
SOLVENT           Acetone
NS                    512
DS                      4
SWH             29296.875 Hz
FIDRES          0.447035 Hz
AQ              1.1184810 sec
RG                 193.34
DW                 17.067 usec
DE                  6.50 usec
TE                 294.8 K
CNST2         145.0000000
D1             2.00000000 sec
D2             0.00344828 sec
D12            0.00002000 sec
TD0                     1

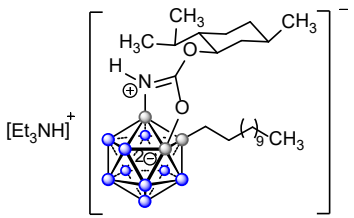
======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
P2                  20.00 usec
PLW1          53.00000000 W
SFO1          100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
P3                  15.00 usec
P4                  30.00 usec
PCPD2               80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
SFO2          400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF            100.6126883 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  4.00
```

20190507-B12M-Dodecane 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}$] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR



NMR-212

```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20190508
Time              19.24
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG      cosygpppqf
TD                 2048
SOLVENT         Acetone
NS                    2
DS                    8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1916928 sec
RG                64.43
DW                93.600 usec
DE                 6.50 usec
TE                294.6 K
D0            0.00000300 sec
D1            2.00000000 sec
D11           0.03000000 sec
D12           0.00002000 sec
D13           0.00000400 sec
D16           0.00020000 sec
IN0           0.00018720 sec

======== CHANNEL f1 ========
NUC1                  1H
P0                15.00 usec
P1                15.00 usec
P17             2500.00 usec
PLW1         12.50000000 W
PLW10         4.16050005 W
SFO1        400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1              10.00 %
P16             1000.00 usec

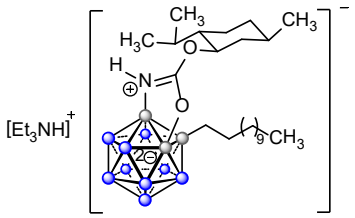
F1 - Acquisition parameters
TD                  128
SFO1           400.1324 MHz
FIDRES         83.466881 Hz
SW                13.350 ppm
FnMODE               QF

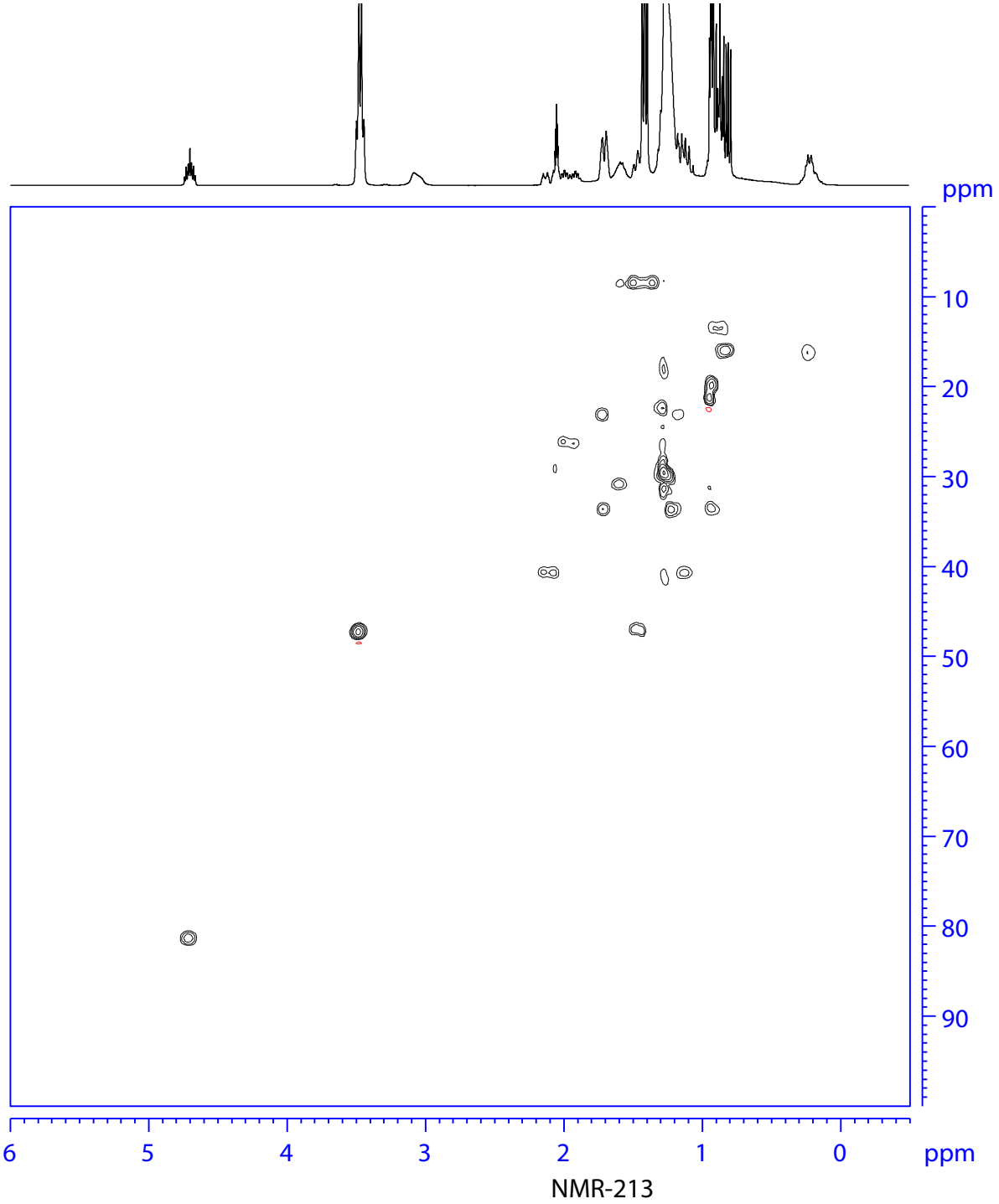
F2 - Processing parameters
SI                  1024
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
PC                  1.40

F1 - Processing parameters
SI                  1024
MC2                   QF
SF           400.1300000 MHz
WDW                 QSINE
SSB       0
LB        0 Hz
GB        0
```

20190507-B12M-Dodecane 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Menthyl)OC_{10}H_{21}]$ dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR





NMR-213

```
Current Data Parameters
NAME      20190507-RV-B12M-Dodecene
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190508
Time              19.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ             0.0851968 sec
RG                193.34
DW                83.200 usec
DE                 6.50 usec
TE                295.0 K
CNST2       145.0000000
D0             0.00000300 sec
D1             1.50000000 sec
D4             0.00172414 sec
D11            0.03000000 sec
D16            0.00020000 sec
D24            0.00086207 sec
IN0            0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1         12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2         53.00000000 W
PLW12         1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPNAM[2]      SMSQ10.100
GPNAM[3]      SMSQ10.100
GPNAM[4]      SMSQ10.100
GPZ1               80.00 %
GPZ2               20.10 %
GPZ3               11.00 %
GPZ4               -5.00 %
P16             1000.00 usec
P19              600.00 usec

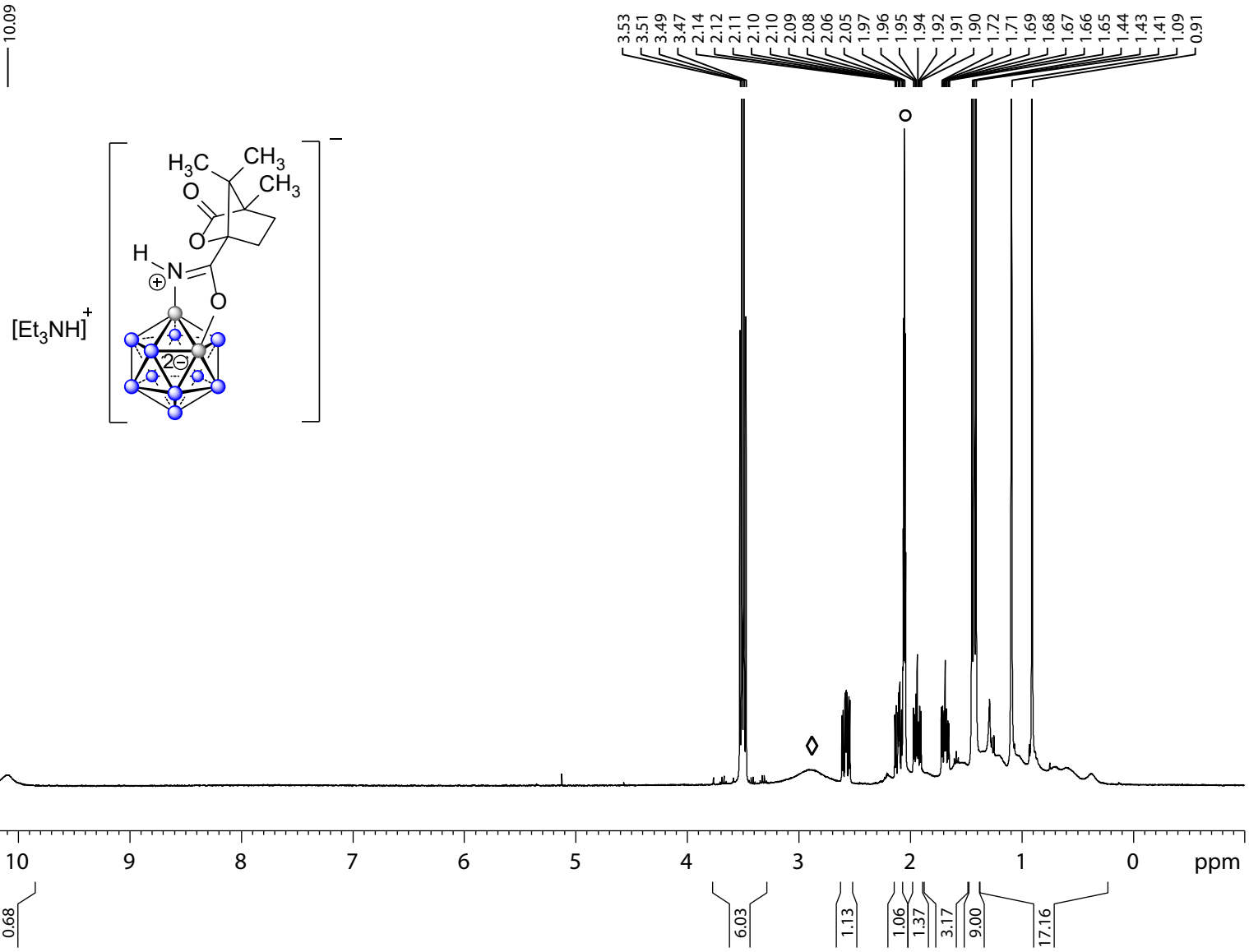
F1 - Acquisition parameters
TD                  256
SFO1           100.6238 MHz
FIDRES        196.524048 Hz
SW               249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                 1024
SF          400.1300000 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
PC                 1.40

F1 - Processing parameters
SI                 1024
MC2        echo-antiecho
SF           100.6127690 MHz
WDW                QSINE
SSB                   2
LB        0 Hz
GB        0
```

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

400MHz ^{1}H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                1
PROCNO               1

F2 - Acquisition Parameters
Date_           20191027
Time              20.44
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                193.34
DW                50.000 usec
DE                 6.50 usec
TE                297.1 K
D1           1.00000000 sec
TD0                  1

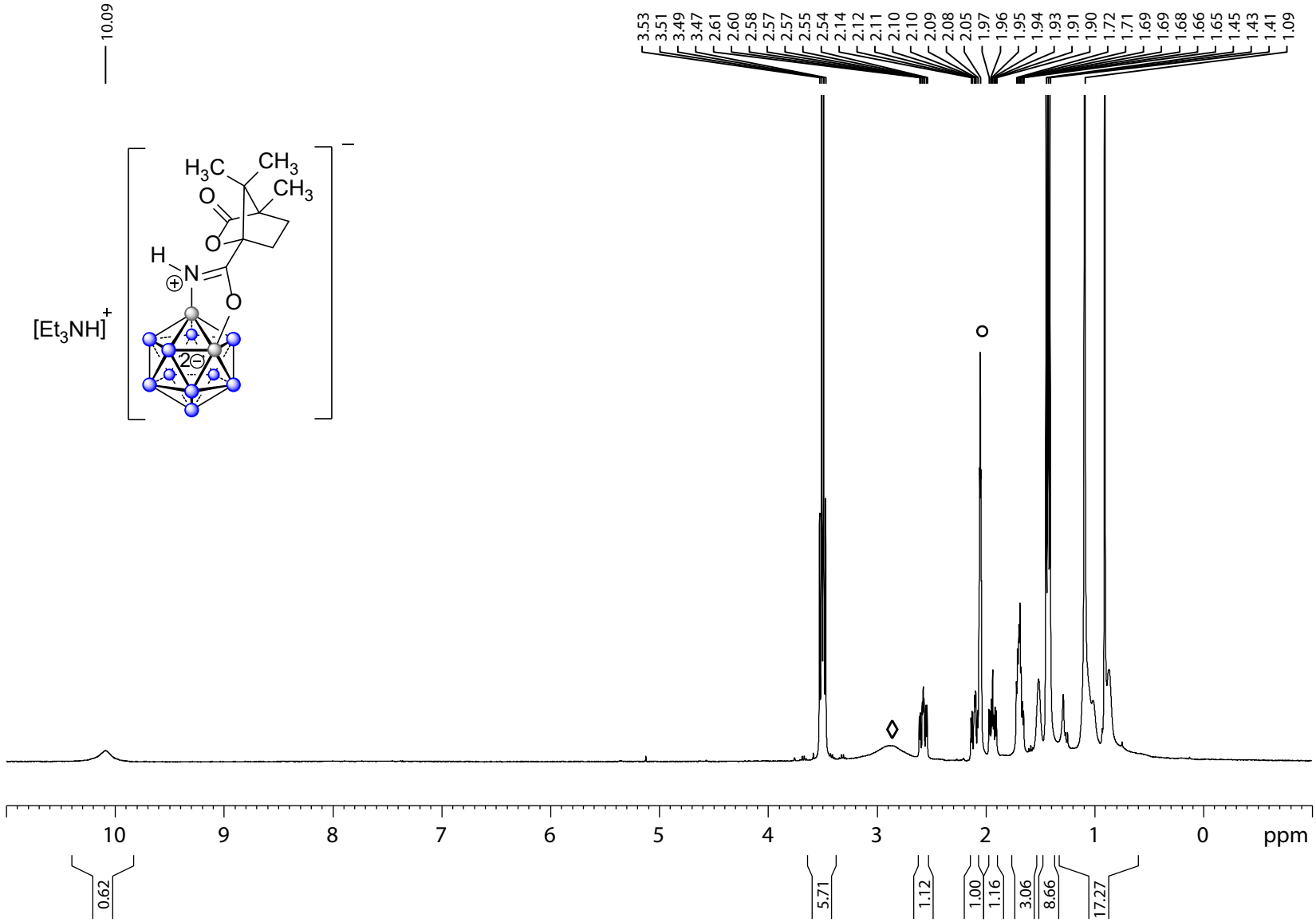
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300069 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

NMR-214

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

400MHz $^1H\{B\}$ NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191027
Time              20.46
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ           1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               297.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

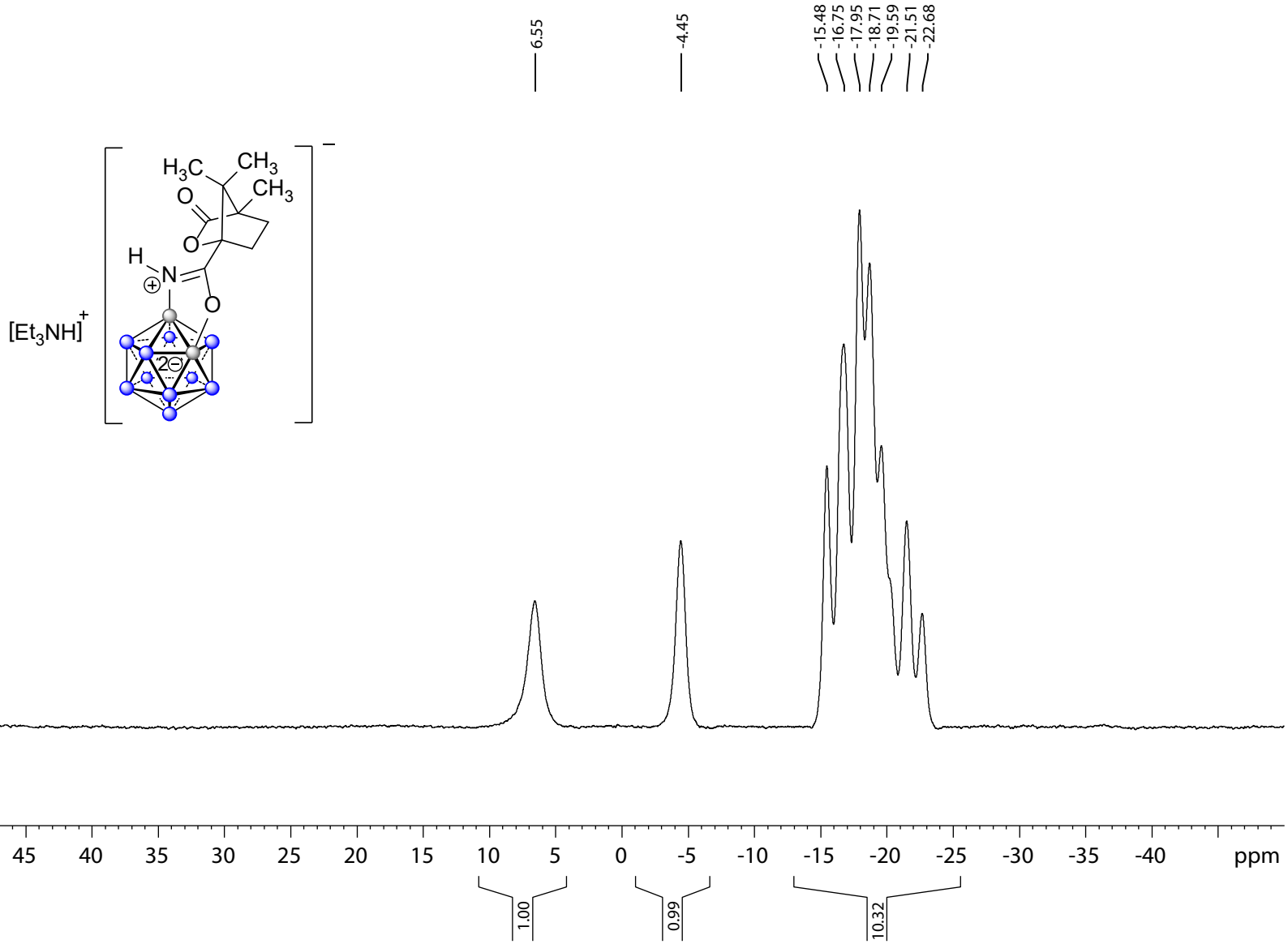
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2             90.00 usec
PLW2        52.96599960 W
PLW12        0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300071 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20191027
Time                20.52
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 296.2 K
D1             1.00000000 sec
TD0                     1

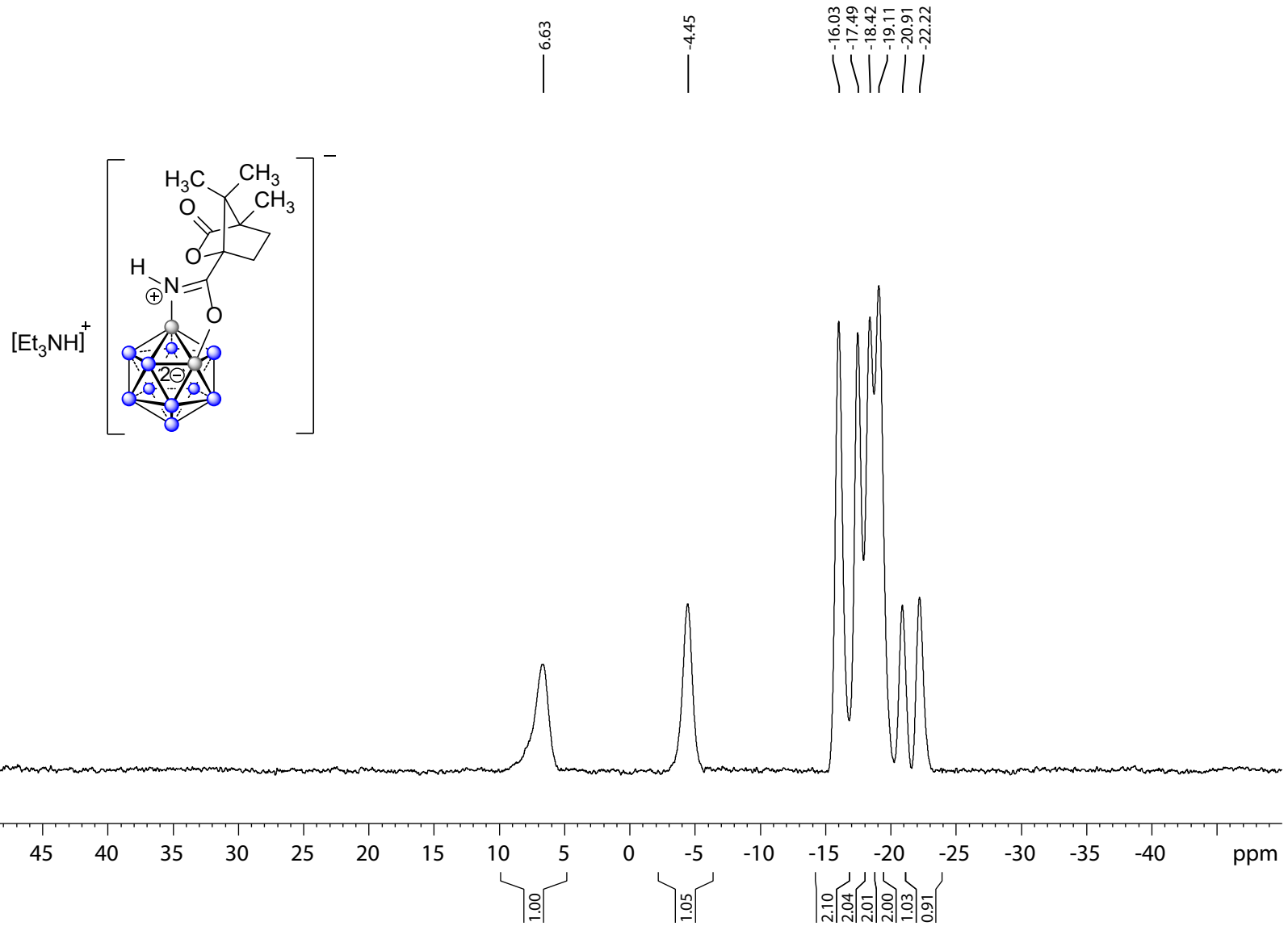
======== CHANNEL f1 ========
NUC1                  11B
P1                   9.93 usec
PLW1          52.96599960 W
SFO1          128.3776052 MHz

F2 - Processing parameters
SI                    32768
SF            128.3776050 MHz
WDW                     EM
SSB       0
LB                 10.00 Hz
GB        0
PC                    1.40
```

NMR-216

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

^{11}B{H} NMR 128 MHz




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191027
Time              20.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW                19.600 usec
DE                 6.50 usec
TE                297.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

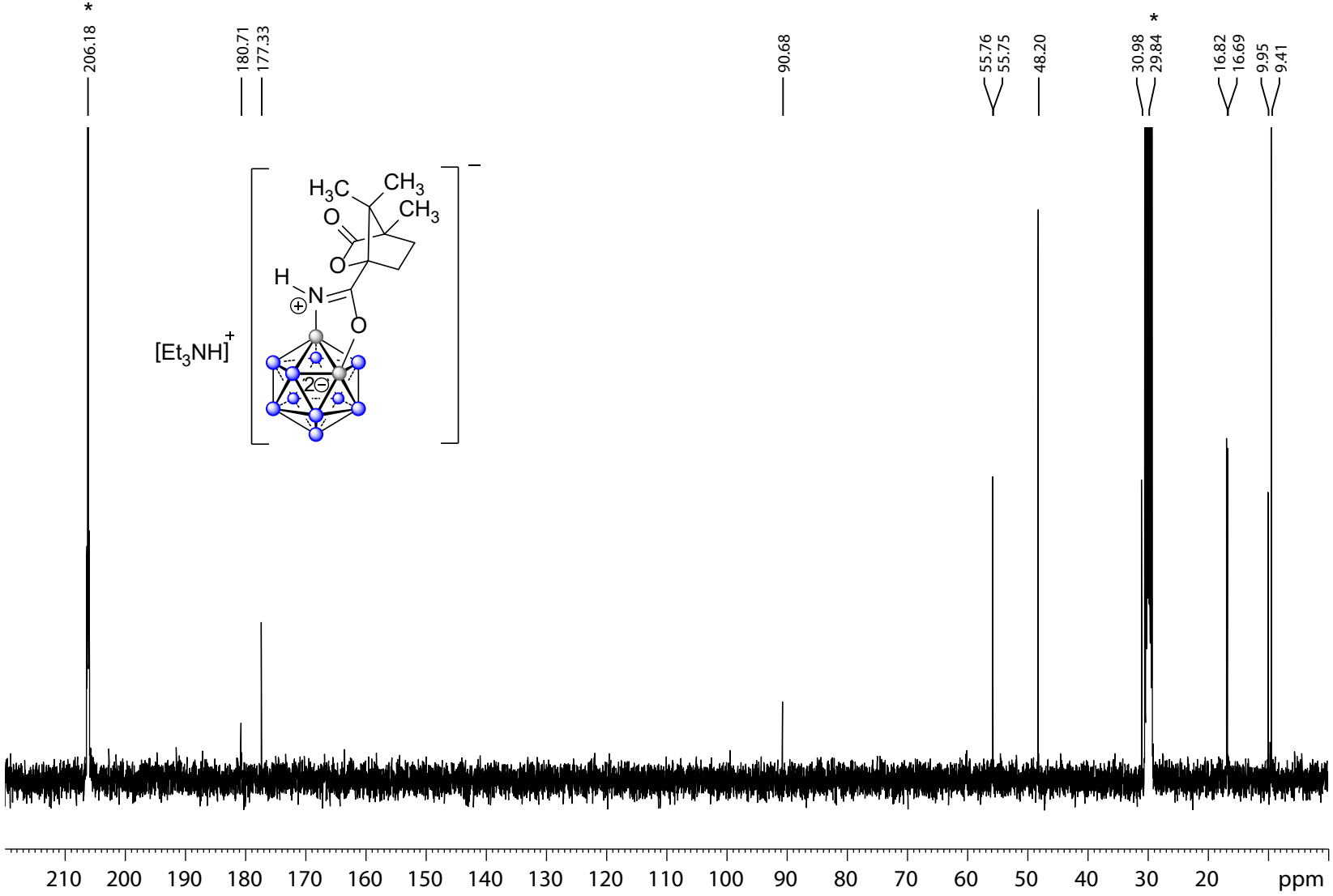
======== CHANNEL f1 ========
NUC1                 11B
P1                  9.93 usec
PLW1        52.96599960 W
SFO1       128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2        12.50000000 W
PLW12        0.43945000 W
PLW13        0.28125000 W
SFO2       400.1320007 MHz

F2 - Processing parameters
SI                 32768
SF         128.3776050 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

20190226-B12C-cyclizn 20 mg white solid $[Et_3NH][B_{12}H_{10}NHC(Camphanic)O]$ dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_           20191027
Time              22.30
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                297.8 K
D1            1.50000000 sec
D11           0.03000000 sec
TD0                   1

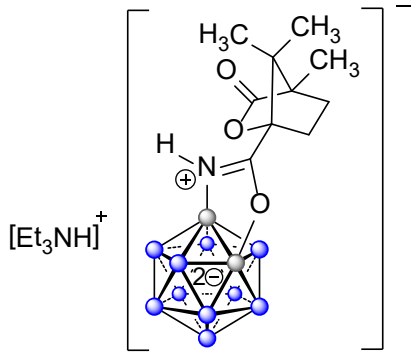
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
PLW13         0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF           100.6126789 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191026-RV-B12C-Cyclizn
EXPNO                6
PROCNO               1

F2 - Acquisition Parameters
Date_           20191027
Time              22.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         dept135
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29296.875 Hz
FIDRES         0.447035 Hz
AQ            1.1184810 sec
RG               193.34
DW               17.067 usec
DE                6.50 usec
TE               296.8 K
CNST2        145.0000000
D1            2.00000000 sec
D2            0.00344828 sec
D12           0.00002000 sec
TD0                   1

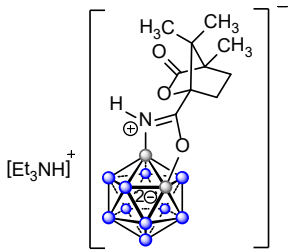
======== CHANNEL f1 ========
NUC1                13C
P1                10.00 usec
P2                20.00 usec
PLW1         53.00000000 W
SFO1         100.6228293 MHz

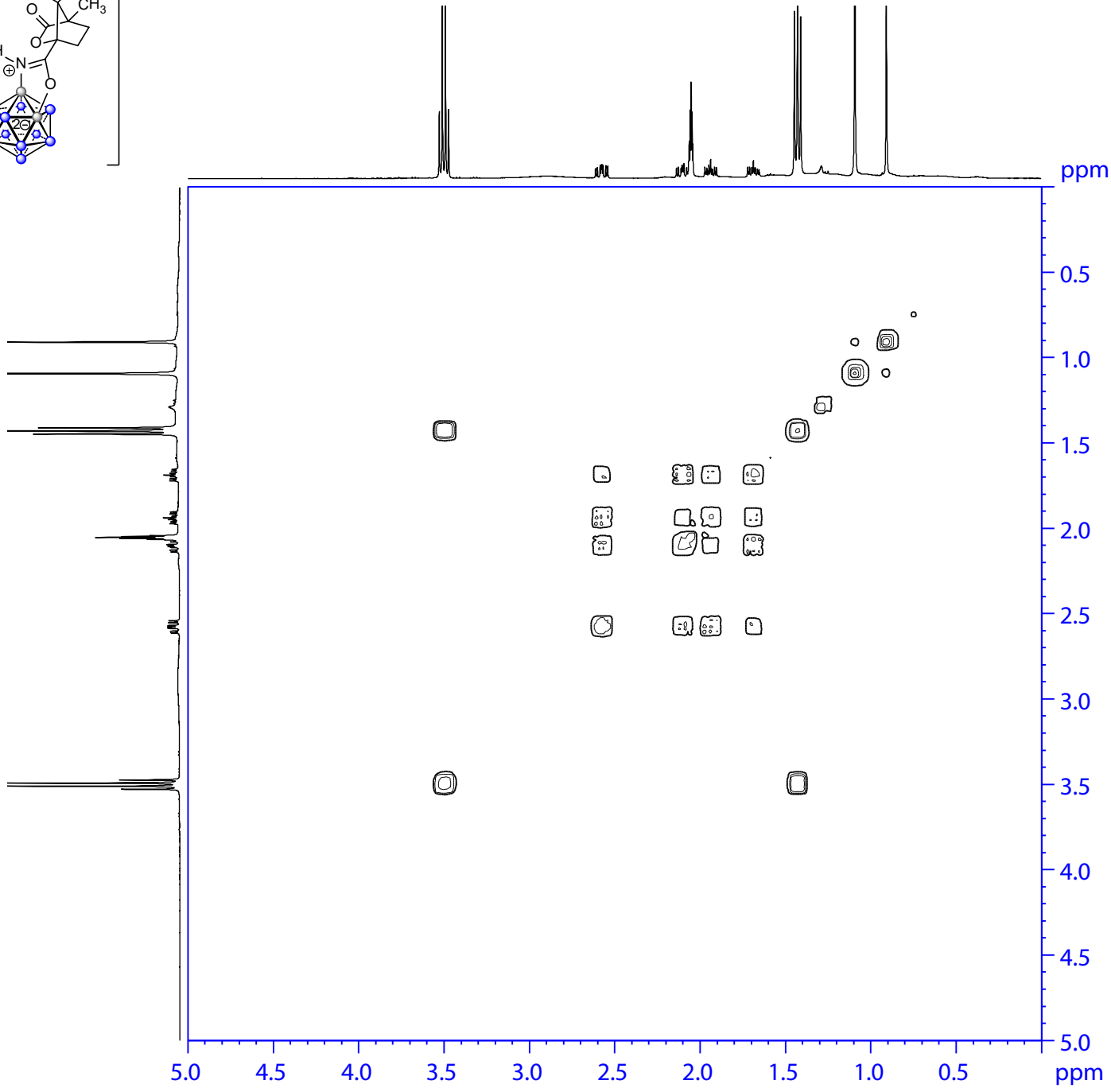
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
P3                15.00 usec
P4                30.00 usec
PCPD2             80.00 usec
PLW2         12.50000000 W
PLW12         0.43945000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                32768
SF           100.6126786 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                4.00
```

20190226-B12C-cyclizn 20 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

^1H - ^1H COSY NMR





Current Data Parameters
NAME 20191026-RV-B12C-Cyclizn
EXPNO 8
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191027
Time 23.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG cosygpppqf
TD 2048
SOLVENT Acetone
NS 2
DS 8
SWH 5341.880 Hz
FIDRES 2.608340 Hz
AQ 0.1916928 sec
RG 193.34
DW 93.600 usec
DE 6.50 usec
TE 297.0 K
D0 0.00000300 sec
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00000400 sec
D16 0.00020000 sec
IN0 0.00018720 sec

======== CHANNEL f1 ========
NUC1 1H
P0 15.00 usec
P1 15.00 usec
P17 2500.00 usec
PLW1 12.50000000 W
PLW10 4.16050005 W
SFO1 400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPZ1 10.00 %
P16 1000.00 usec

F1 - Acquisition parameters
TD 128
SFO1 400.1324 MHz
FIDRES 83.466881 Hz
SW 13.350 ppm
FnMODE QF

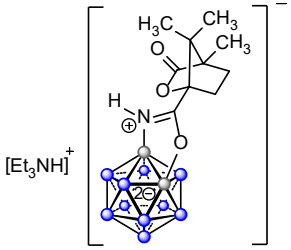
F2 - Processing parameters
SI 1024
SF 400.1300075 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 400.1300078 MHz
WDW QSINE
SSB 0
LB 0 Hz
GB 0

NMR-220

20190226-B12C-cyclizn 20 mg white solid [Et₃NH][B₁₂H₁₀NHC(Camphanic)O] dissolved in 0.6 mL acetone-*d*6*

^{1}H - ^{13}C HSQC NMR



NMR-221

Current Data Parameters
NAME 20191026-RV-B12C-Cyclizn
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191027
Time 23.00
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG hsqcetgpsi2
TD 1024
SOLVENT Acetone
NS 2
DS 16
SWH 6009.615 Hz
FIDRES 5.868765 Hz
AQ 0.0851968 sec
RG 193.34
DW 83.200 usec
DE 6.50 usec
TE 296.7 K
CNST2 145.0000000
D0 0.00000300 sec
D1 1.50000000 sec
D4 0.00172414 sec
D11 0.03000000 sec
D16 0.00020000 sec
D24 0.00086207 sec
IN0 0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
P2 30.00 usec
P28 1000.00 usec
PLW1 12.50000000 W
SFO1 400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2 garp
NUC2 13C
P3 10.00 usec
P4 20.00 usec
PCPD2 70.00 usec
PLW2 53.00000000 W
PLW12 1.08159995 W
SFO2 100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1] SMSQ10.100
GPNAM[2] SMSQ10.100
GPNAM[3] SMSQ10.100
GPNAM[4] SMSQ10.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
P16 1000.00 usec
P19 600.00 usec

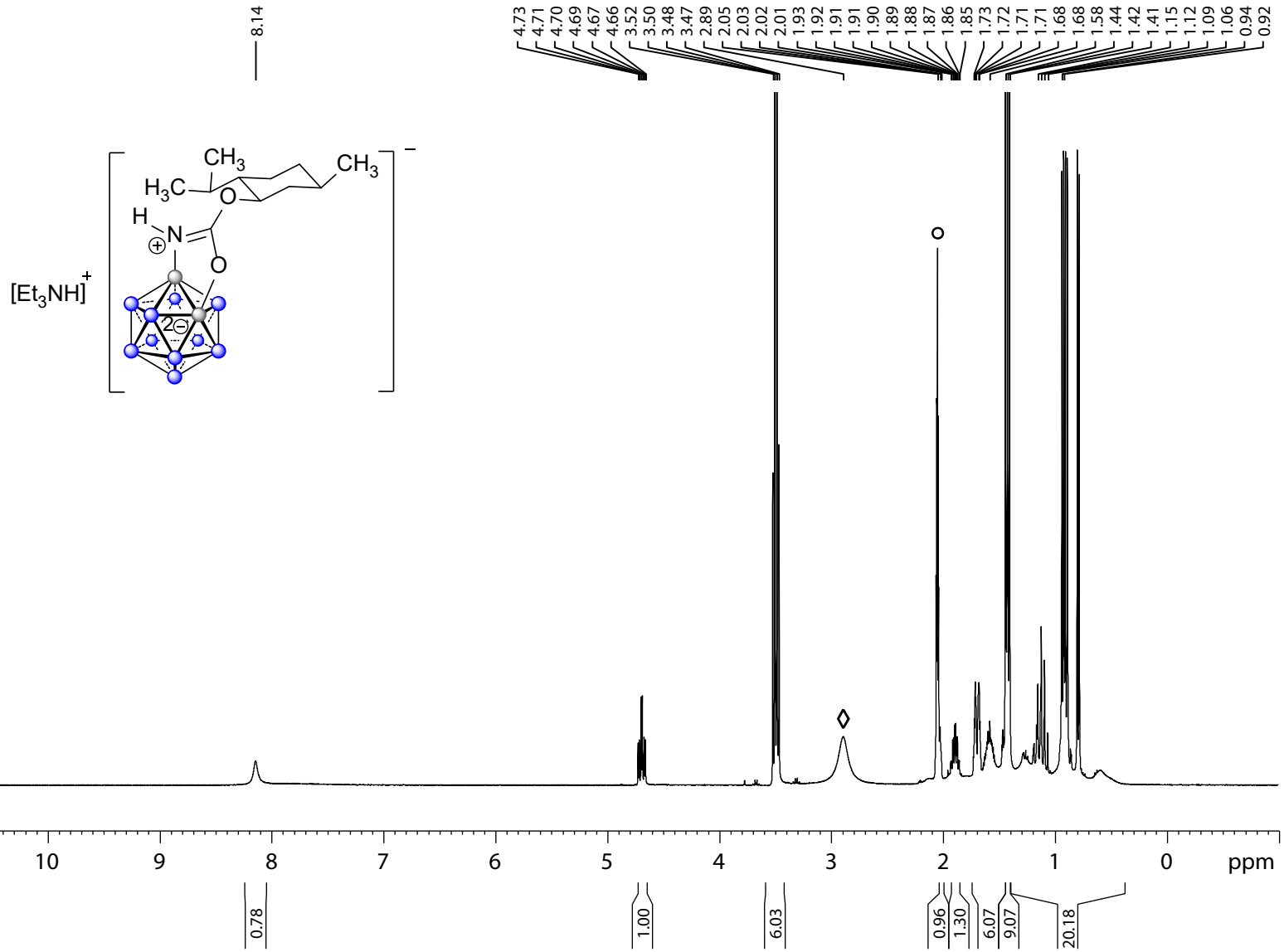
F1 - Acquisition parameters
TD 256
SFO1 100.6238 MHz
FIDRES 196.524048 Hz
SW 249.991 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 1024
SF 400.1300041 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6126732 MHz
WDW QSINE
SSB 2
LB 0 Hz
GB 0

20191104-B12M-Cycl 10 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)O$] dissolved in 0.6 mL acetone-*d*6*

400MHz ^1H NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-222

```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                 1
PROCNO                1

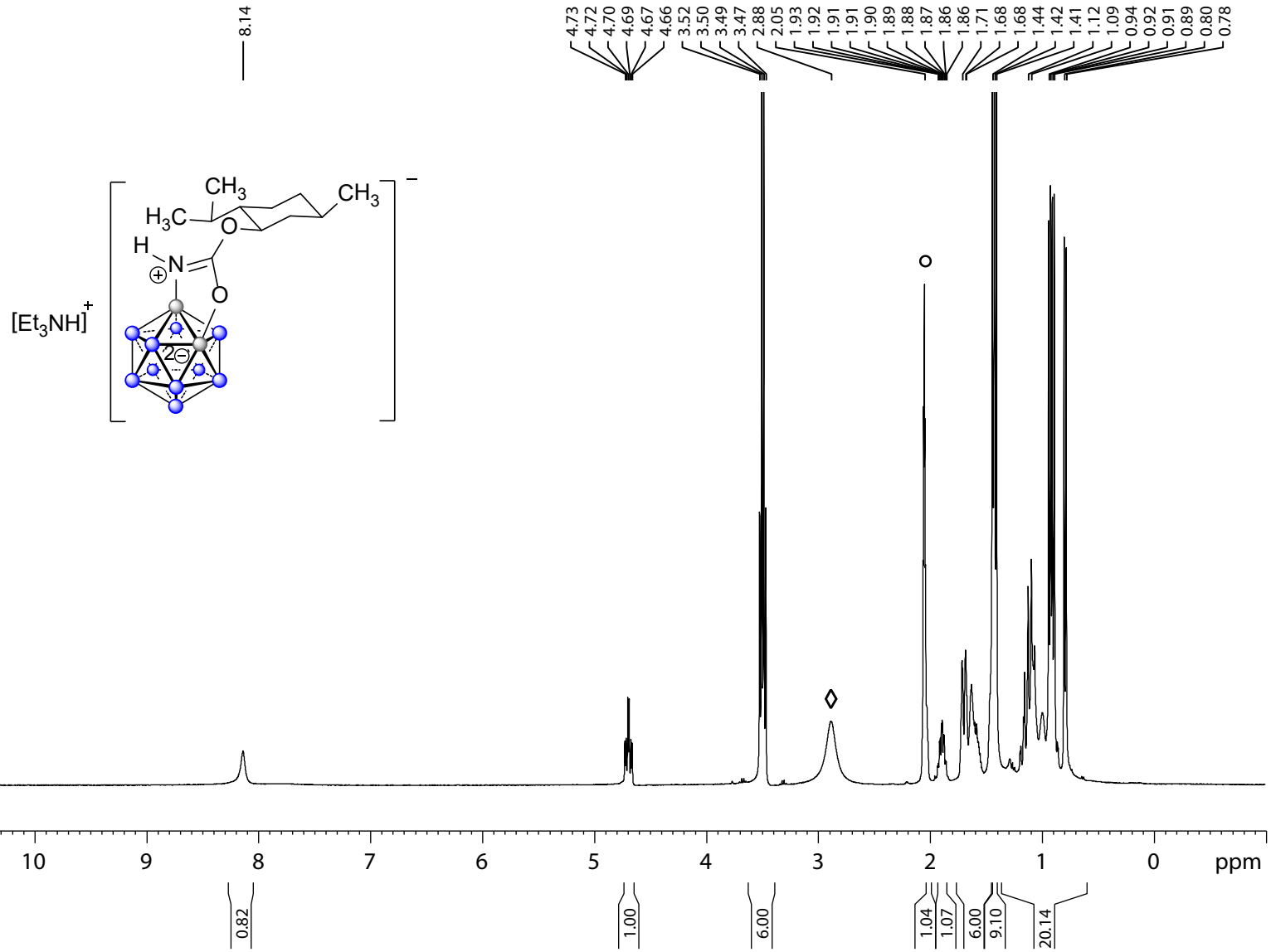
F2 - Acquisition Parameters
Date_           20191105
Time              16.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG               152.18
DW                50.000 usec
DE                 6.50 usec
TE                296.0 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

F2 - Processing parameters
SI                65536
SF          400.1300072 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

20191104-B12M-Cycl 10 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

400MHz ¹H{B} NMR, ○ deuterated solvent residual peak= 2.05 ppm; ◊ water peak



NMR-223

```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20191105
Time              16.16
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ              1.0223616 sec
RG                107.6
DW                62.400 usec
DE                 6.50 usec
TE                296.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

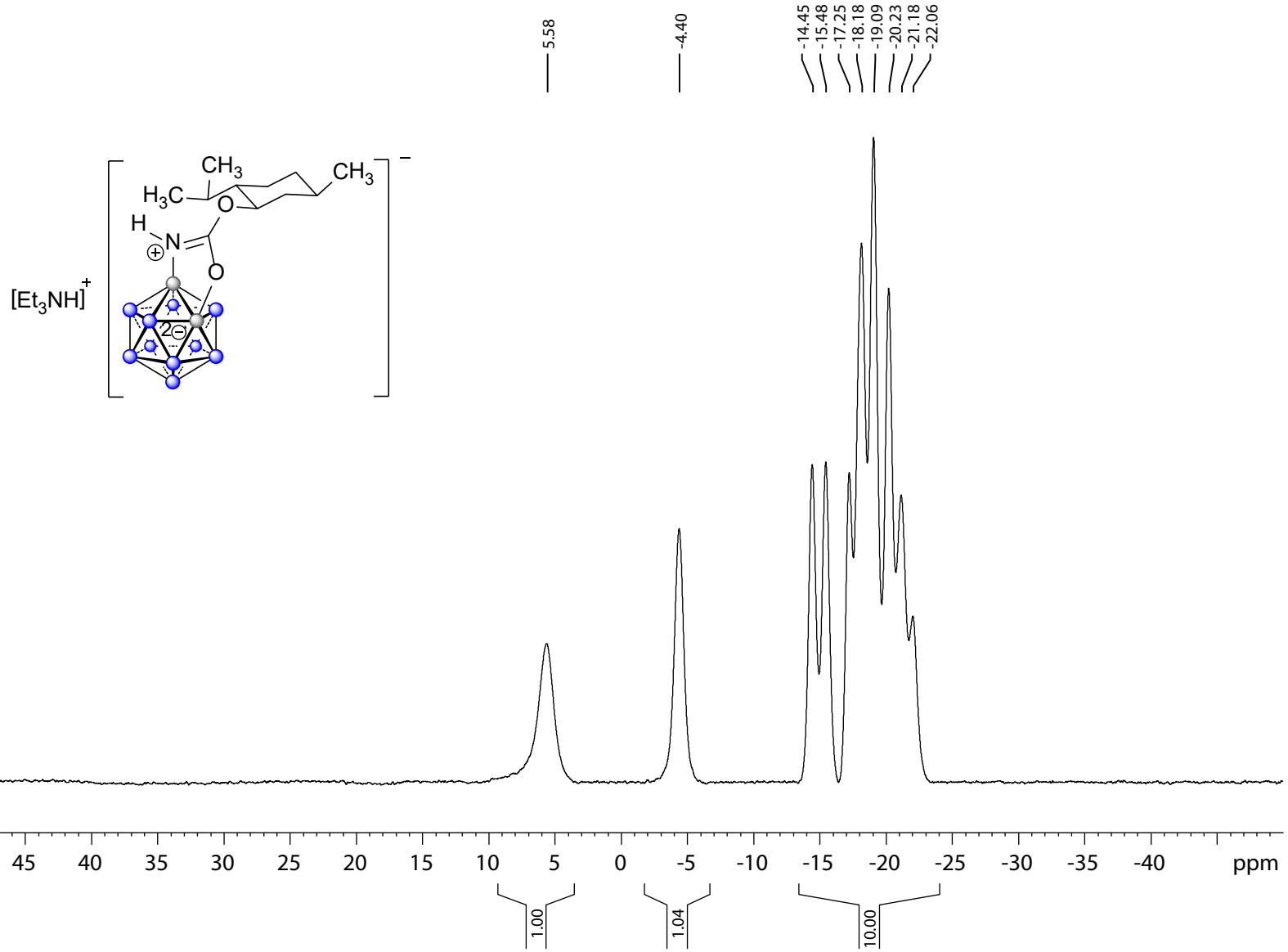
======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp4
NUC2                11B
PCPD2              90.00 usec
PLW2         52.96599960 W
PLW12         0.64477998 W
SFO2        128.3776050 MHz

F2 - Processing parameters
SI                 32768
SF          400.1300073 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

20191104-B12M-Cycl 10 mg white solid [Et_3NH][$B_{12}H_{10}NHC(Menthyl)O$] dissolved in 0.6 mL acetone-*d*6*

^{11}B NMR 128 MHz




```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20191105
Time                 16.21
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH              25510.203 Hz
FIDRES            0.389255 Hz
AQ               1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   296.2 K
D1               1.00000000 sec
TD0                        1

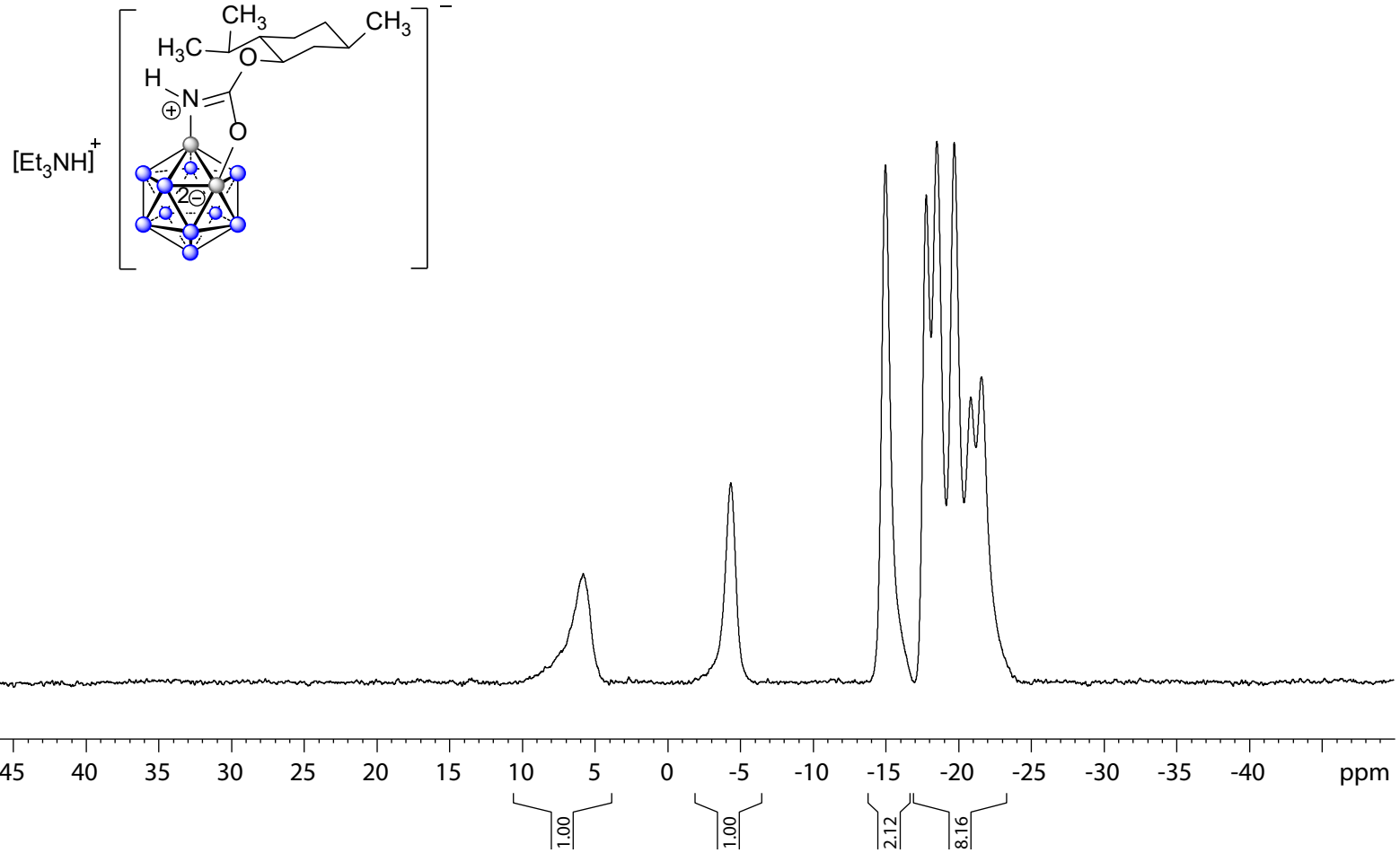
======== CHANNEL f1 ========
NUC1                    11B
P1                     9.93 usec
PLW1           52.96599960 W
SFO1           128.3776052 MHz

F2 - Processing parameters
SI                     32768
SF             128.3776050 MHz
WDW                       EM
SSB       0
LB                    10.00 Hz
GB        0
PC                     1.40
```

NMR-224

20191104-B12M-Cycl 10 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

$^{11}B\{H\}$ NMR 128 MHz




```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_              20191105
Time                  16.27
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   297.2 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                        1

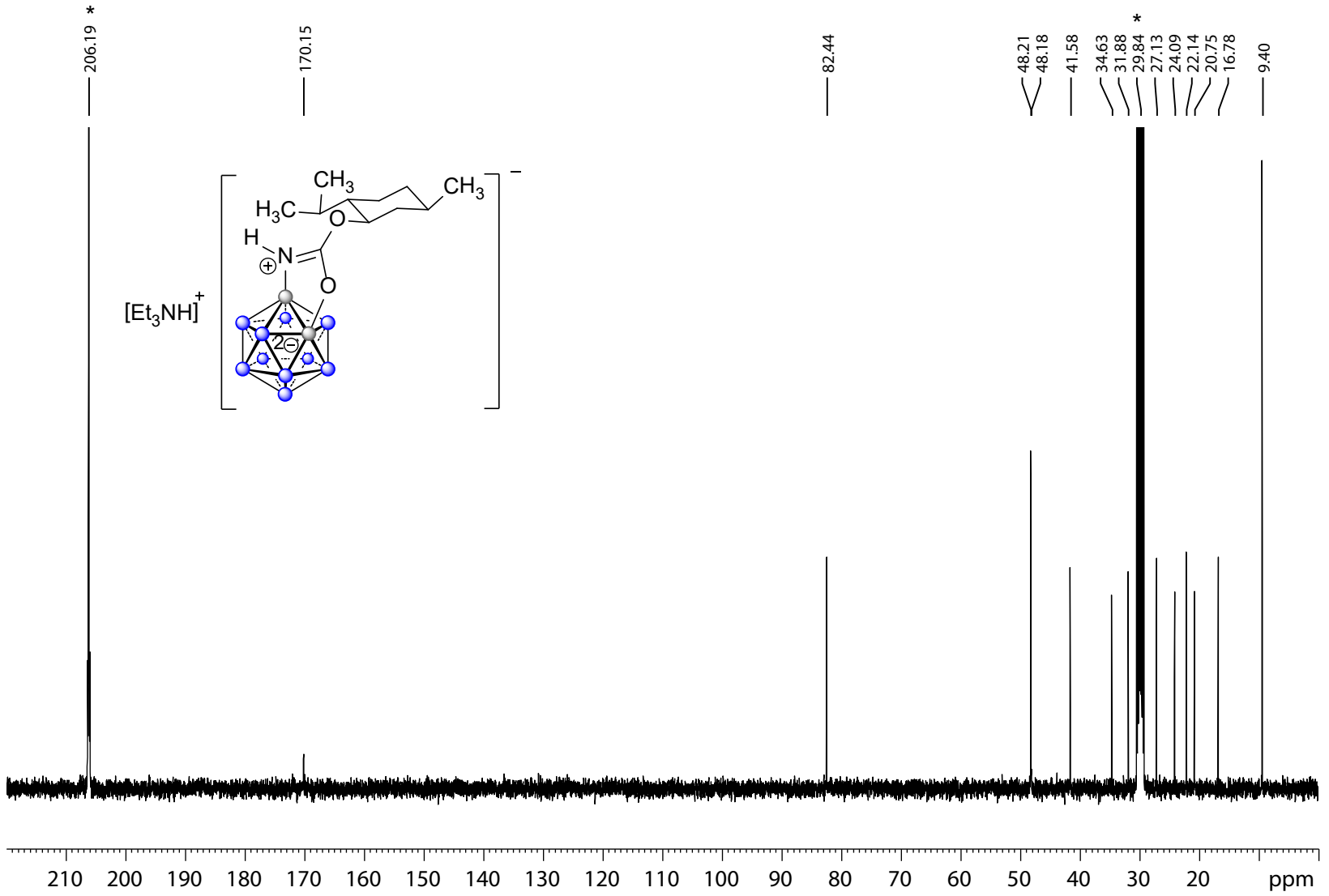
======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1            52.96599960 W
SFO1           128.3776050 MHz

======== CHANNEL f2 ========
CPDPRG[2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PLW2            12.50000000 W
PLW12            0.43945000 W
PLW13            0.28125000 W
SFO2           400.1320007 MHz

F2 - Processing parameters
SI                       32768
SF             128.3776050 MHz
WDW                         EM
SSB          0
LB                    10.00 Hz
GB           0
PC                     1.40
```

20191104-B12M-Cycl 10 mg white solid [Et_3NH][$B_{12}H_{10}NHC$(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

$^{13}C\{^1H\}$ NMR 100 MHz




```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                         5
PROCNO                        1

F2 - Acquisition Parameters
Date_              20191105
Time                 18.00
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                   2048
DS                      4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  297.6 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                     1

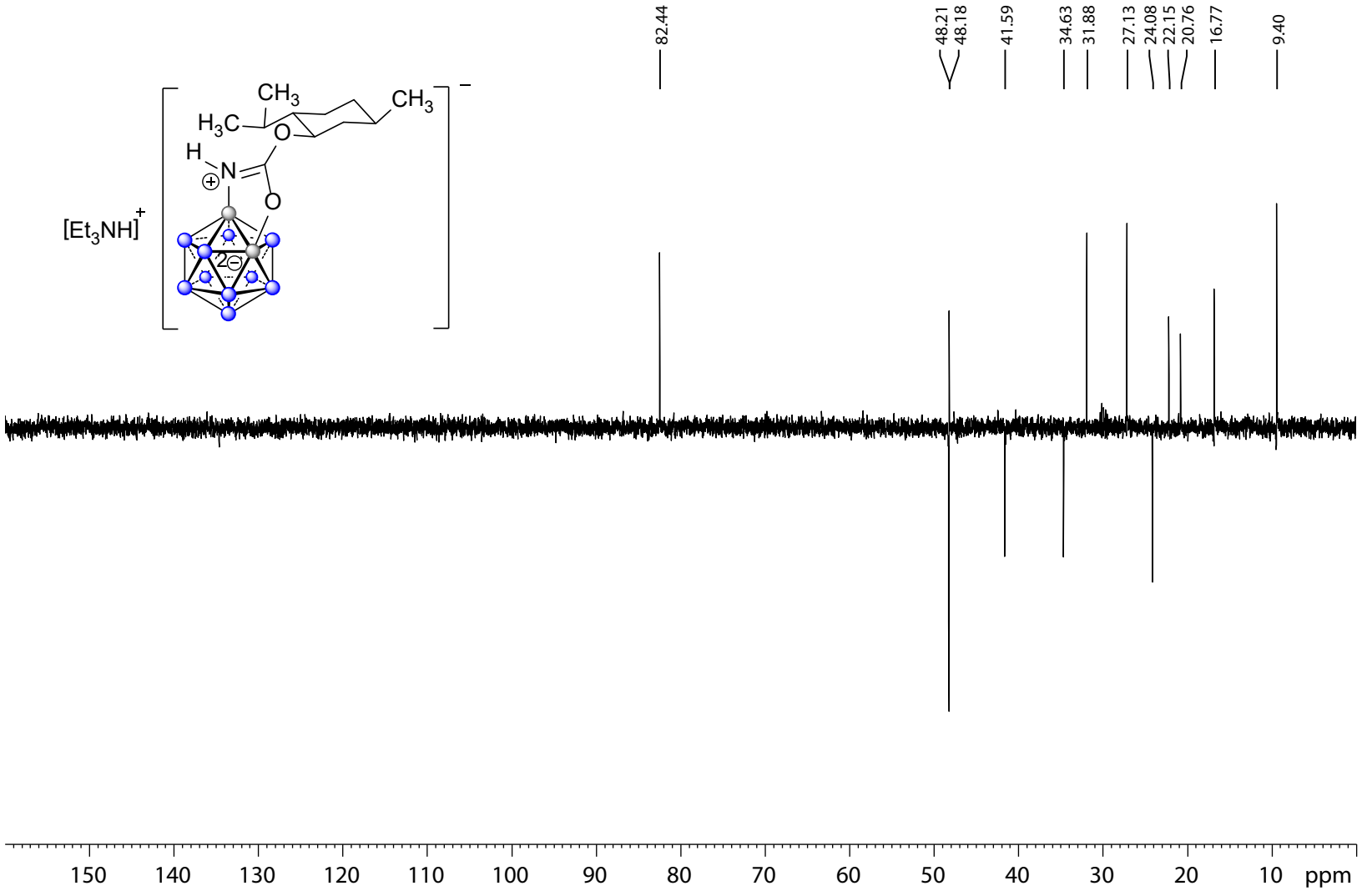
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2           waltz16
NUC2                   1H
PCPD2                80.00 usec
PLW2          12.50000000 W
PLW12          0.43945000 W
PLW13          0.28125000 W
SFO2         400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF           100.6126795 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

20191104-B12M-Cycl 10 mg white solid [Et_3NH][$B_{12}H_{10}$NHC(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

^{13}CDEPT NMR 100 MHz




```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                        6
PROCNO                       1

F2 - Acquisition Parameters
Date_              20191105
Time                 18.28
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            dept135
TD                   65536
SOLVENT            Acetone
NS                     512
DS                       4
SWH              29296.875 Hz
FIDRES            0.447035 Hz
AQ                1.1184810 sec
RG                   193.34
DW                   17.067 usec
DE                     6.50 usec
TE                    297.1 K
CNST2           145.0000000
D1               2.00000000 sec
D2               0.00344828 sec
D12              0.00002000 sec
TD0                      1

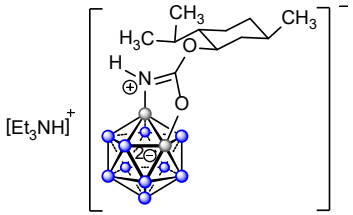
======== CHANNEL f1 ========
NUC1                   13C
P1                   10.00 usec
P2                   20.00 usec
PLW1            53.00000000 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2            waltz16
NUC2                   1H
P3                   15.00 usec
P4                   30.00 usec
PCPD2                80.00 usec
PLW2            12.50000000 W
PLW12            0.43945000 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                   32768
SF              100.6126792 MHz
WDW                     EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    4.00
```

20191104-B12M-Cycl 10 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹H COSY NMR



NMR-228

```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                        7
PROCNO                       1

F2 - Acquisition Parameters
Date_              20191105
Time                 18.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG       cosygpppqf
TD                   2048
SOLVENT           Acetone
NS                      2
DS                      8
SWH               5341.880 Hz
FIDRES            2.608340 Hz
AQ                0.1916928 sec
RG                   193.34
DW                  93.600 usec
DE                   6.50 usec
TE                  297.0 K
D0                0.00000300 sec
D1                2.00000000 sec
D11               0.03000000 sec
D12               0.00002000 sec
D13               0.00000400 sec
D16               0.00020000 sec
IN0               0.00018720 sec

======== CHANNEL f1 ========
NUC1                      1H
P0                     15.00 usec
P1                     15.00 usec
P17                  2500.00 usec
PLW1           12.50000000 W
PLW10           4.16050005 W
SFO1           400.1324057 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]      SMSQ10.100
GPZ1                  10.00 %
P16                 1000.00 usec

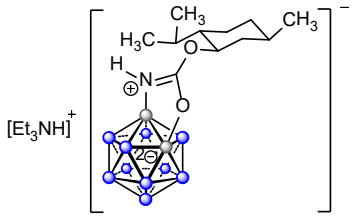
F1 - Acquisition parameters
TD                       128
SFO1              400.1324 MHz
FIDRES           83.466881 Hz
SW                  13.350 ppm
FnMODE                   QF

F2 - Processing parameters
SI                      1024
SF             400.1300094 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
PC                     1.40

F1 - Processing parameters
SI                      1024
MC2                       QF
SF             400.1300097 MHz
WDW                   QSINE
SSB          0
LB           0 Hz
GB           0
```

20191104-B12M-Cycl 10 mg white solid [Et₃NH][B₁₂H₁₀NHC(Menthyl)O] dissolved in 0.6 mL acetone-*d*6*

¹H - ¹³C HSQC NMR



NMR-229

```
Current Data Parameters
NAME      20191104-RV-B12M-Cycl
EXPNO                 8
PROCNO                1

F2 - Acquisition Parameters
Date_           20191105
Time              18.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG     hsqcetgpsi2
TD                1024
SOLVENT         Acetone
NS                   2
DS                  16
SWH            6009.615 Hz
FIDRES         5.868765 Hz
AQ            0.0851968 sec
RG              193.34
DW               83.200 usec
DE                6.50 usec
TE               297.0 K
CNST2       145.0000000
D0           0.00000300 sec
D1           1.50000000 sec
D4           0.00172414 sec
D11          0.03000000 sec
D16          0.00020000 sec
D24          0.00086207 sec
IN0          0.00001990 sec
ZGOPTNS

======== CHANNEL f1 ========
NUC1                 1H
P1                15.00 usec
P2                30.00 usec
P28             1000.00 usec
PLW1        12.50000000 W
SFO1        400.1328009 MHz

======== CHANNEL f2 ========
CPDPRG[2           garp
NUC2                13C
P3                10.00 usec
P4                20.00 usec
PCPD2             70.00 usec
PLW2        53.00000000 W
PLW12        1.08159995 W
SFO2        100.6238364 MHz

====== GRADIENT CHANNEL =====
GPNAM[1]     SMSQ10.100
GPNAM[2]     SMSQ10.100
GPNAM[3]     SMSQ10.100
GPNAM[4]     SMSQ10.100
GPZ1              80.00 %
GPZ2              20.10 %
GPZ3              11.00 %
GPZ4              -5.00 %
P16             1000.00 usec
P19              600.00 usec

F1 - Acquisition parameters
TD                 256
SFO1           100.6238 MHz
FIDRES       196.524048 Hz
SW             249.991 ppm
FnMODE    Echo-Antiecho

F2 - Processing parameters
SI                1024
SF          400.1300061 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
PC                1.40

F1 - Processing parameters
SI                1024
MC2       echo-antiecho
SF          100.6126725 MHz
WDW               QSINE
SSB                  2
LB        0 Hz
GB        0
```

Determination of Diastereomeric Ratios

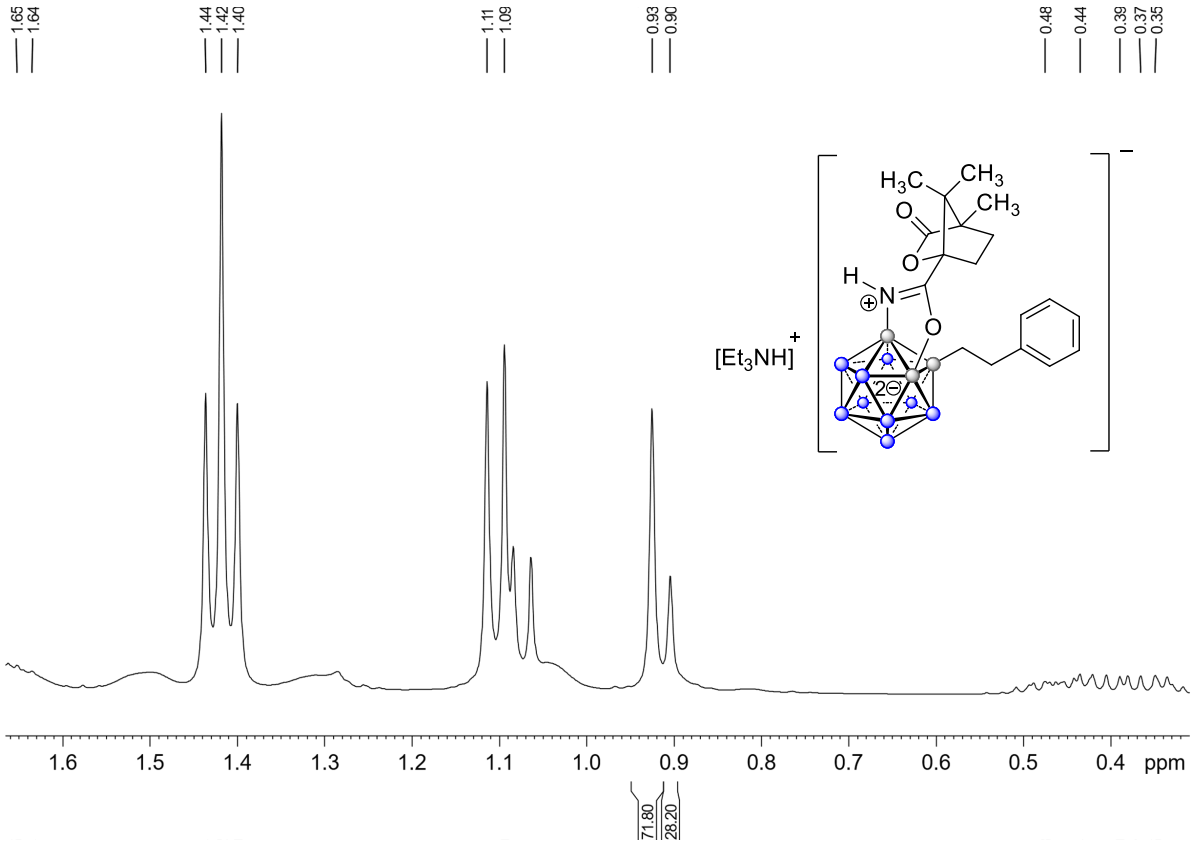
Diastereomeric ratios *dr* of the products **13** and **14** were determined using the NMR integrals of three signals for which the compounds showed distinct resonances: For **13**, δ(^{1}H) 0.92 ppm, δ(^{13}C) 32 ppm and δ(^{13}C) 37 ppm; for **14**, δ(^{1}H) 0.79 ppm, δ(^{13}C) 21 ppm and δ(^{13}C) 82 ppm The data are shown in Table S3, and details of the spectra are displayed following Table S3.

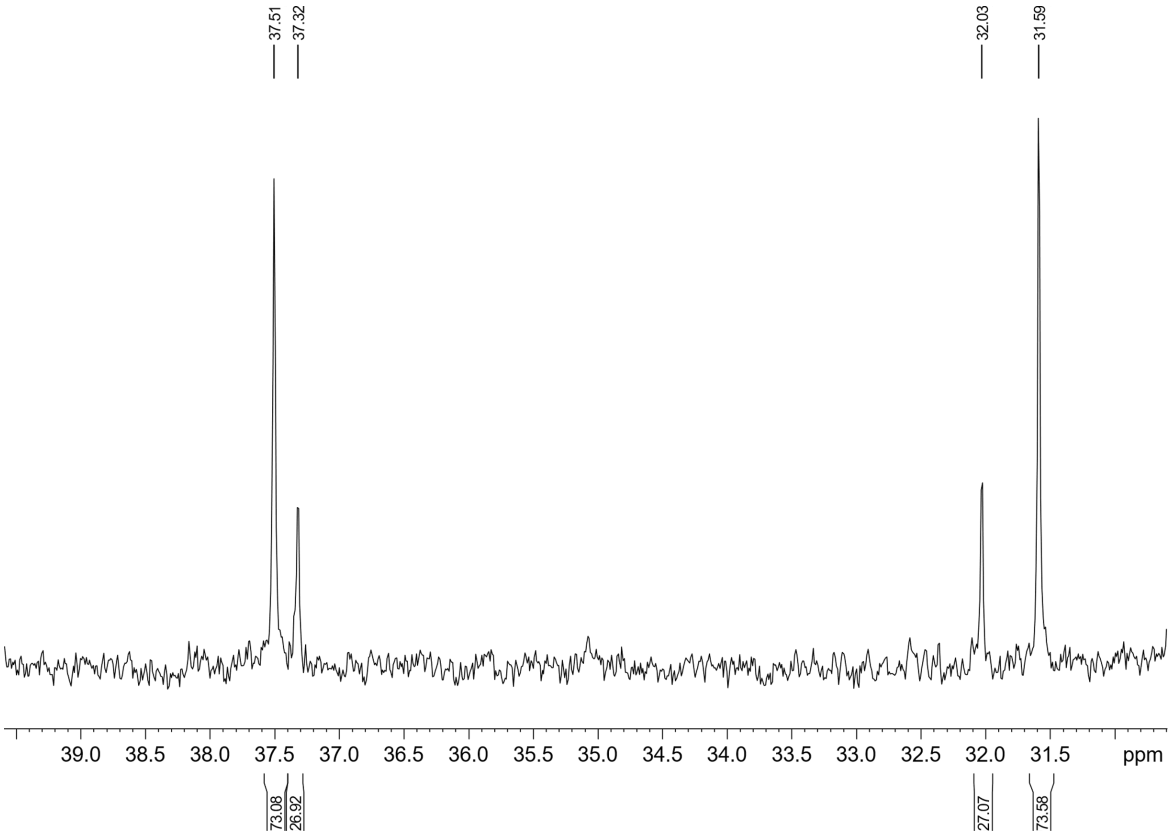
Table S3. Data of relative integration for products **13** and **14** and the resulting average *dr*.

	^{1}H relative integration			^{13}C relative integration			^{13}C relative integration			
	δ 0.92	**δ 0.90**	***dr***	**δ 37.5**	**δ 37.3**	***dr***	**δ 32.0**	**δ 31.5**	***dr***	**Average *dr***
13a	72	28	72:28	73	27	73:27	27	73	73:27	**73:27**
13b	66	34	66:34	66	34	66:34	33	67	67:33	**66:34**
13c	60	40	60:40	60	40	60:40	40	60	60:40	**60:40**
13d	83	17	83:17	83	17	83:17	13	87	87:13	**84:16**
13e	55	45	55:45	55	45	55:45	47	53	53:47	**52:48**
13f	92	8	92:8	92	8	92:8	10	90	90:10	**91:09**
13g	88	12	88:12	89	11	89:11	8	92	92:8	**90:10**
13h	72	28	72:28	72	28	72:28	28	72	72:28	**72:28**
13i	75	25	75:25	74	26	74:26	28	72	72:28	**74:26**
13j*	-	-	-	66	34	66:34	34	66	66:34	**66:34**
13k	55	45	55:45	55	45	55:45	45	55	55:45	**55:45**
	^{1}H relative integration			^{13}C relative integration			^{13}C relative integration			
	δ 0.82	**δ 0.78**	***dr***	**δ 82.4**	**δ 82.2**	***dr***	**δ 20.8**	**δ 20.7**	***dr***	**Average *dr***
14a	25	75	75:25	74	26	74:26	24	76	76:24	**75:25**
14b	27	73	73:27	72	28	72:28	26	74	74:26	**73:27**
14c*	-	-	-	78	22	78:22	20	80	80:20	**79:21**
14d	22	78	78:22	79	21	79:21	21	79	79:21	**79:21**
14e*	32	68	68:32	72	28	72:28	28	72	72:28	**72:28**
14f**	15	85	85:15	85	15	85:15	14	86	86:14	**85:15**
14g	15	85	85:15	84	16	84:16	15	85	85:15	**85:15**
14h	31	69	69:31	68	32	68:32	32	68	68:32	**68:32**
14i	29	71	71:29	71	29	71:29	29	71	71:29	**71:29**
14j	29	71	71:29	70	30	70:30	30	70	70:30	**70:30**
14k*	-	-	-	72	28	72:28	28	72	72:28	**72:28**
14l*	-	-	-	50	50	50:50	50	50	50:50	**50:50**
14m*	-	-	-	50	50	50:50	52	48	52:48	**51:49**
14n*	-	-	-	50	50	50:50	50	50	50:50	**50:50**

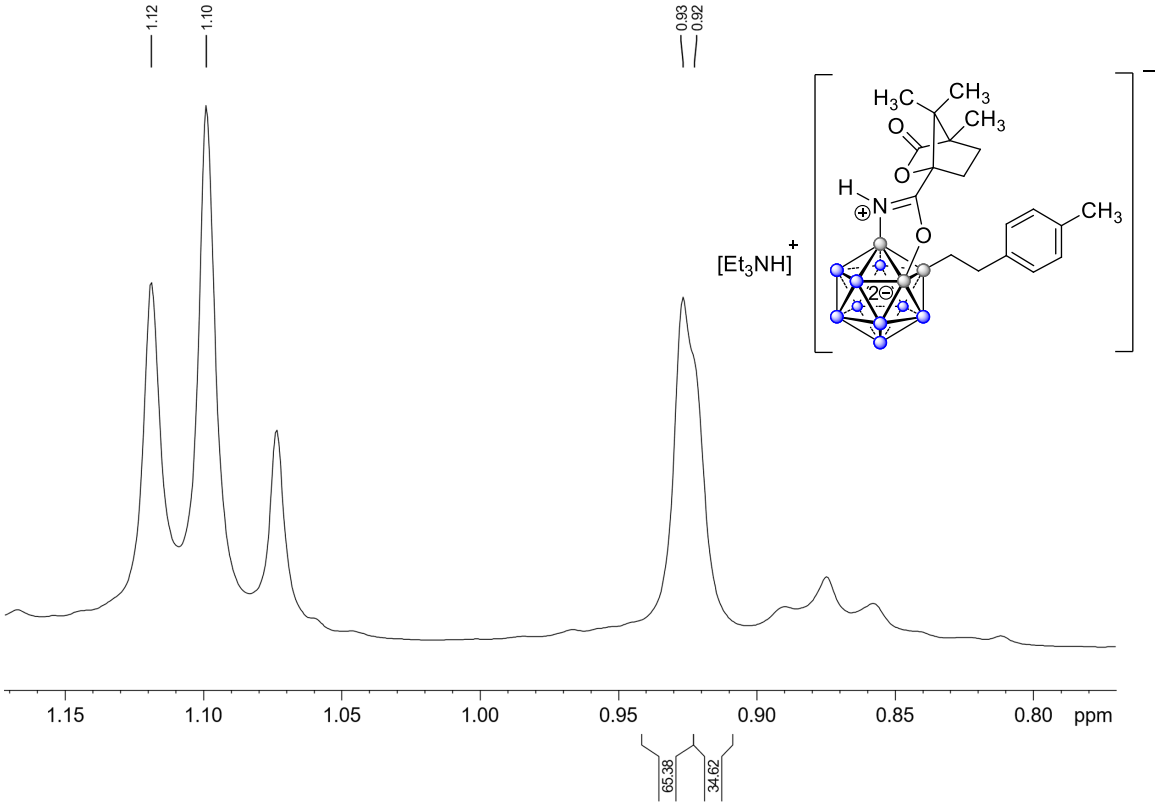
* Signal overlap did not allow for accurate determination of relative ^{1}H integrals.
** ^{1}H signals at δ 7.26 and δ 7.22 were used.

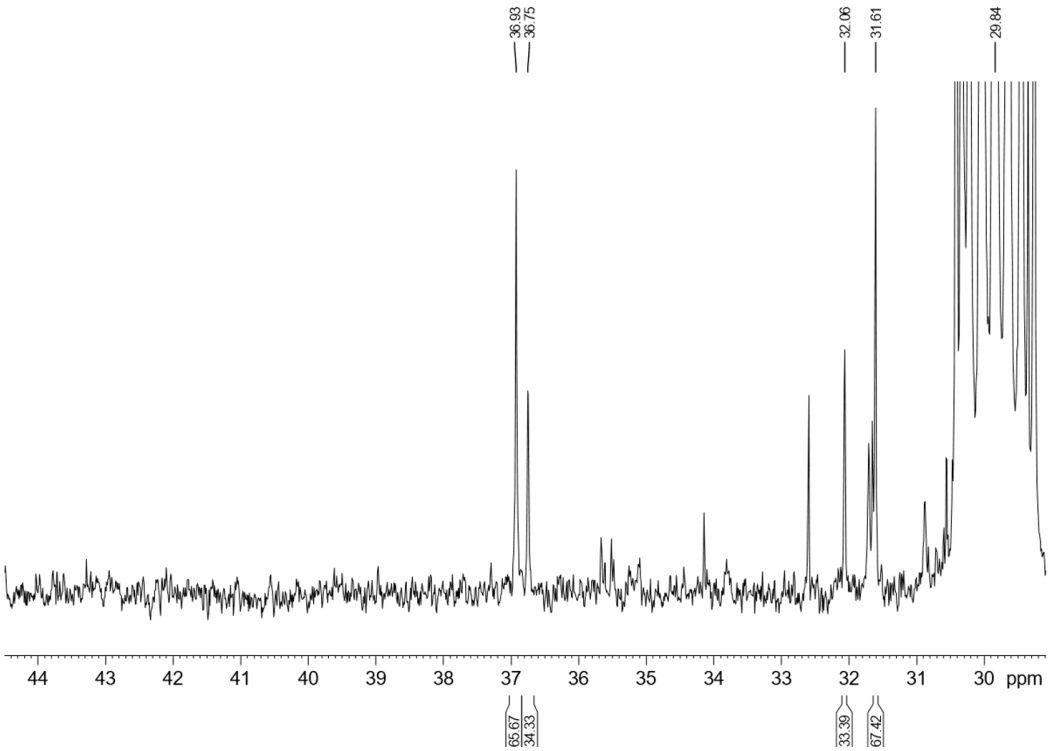
Product **13a**


1.65
1.64
1.44
1.42
1.40
1.11
1.09
0.93
0.90
0.48
0.44
0.39
0.37
0.35
[Et3NH]+
2⊖
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
ppm
71.80
28.20

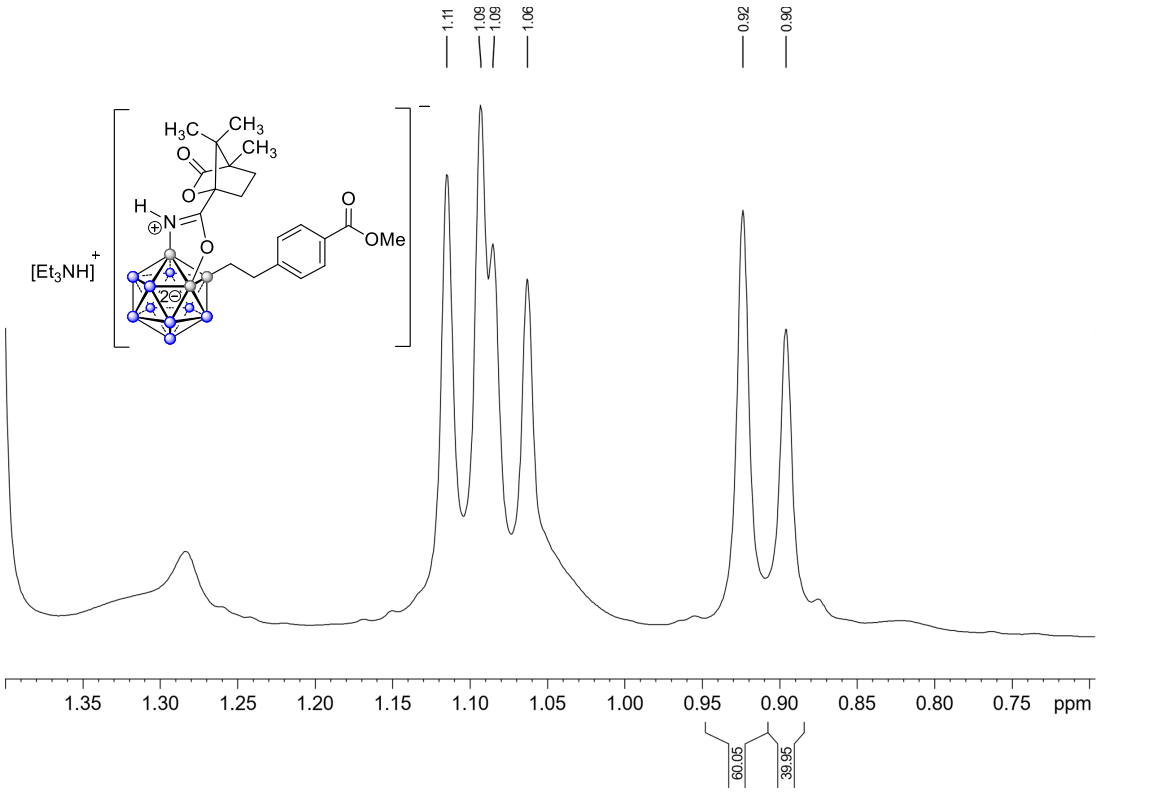

37.51
37.32
32.03
31.59
39.0
38.5
38.0
37.5
37.0
36.5
36.0
35.5
35.0
34.5
34.0
33.5
33.0
32.5
32.0
31.5
ppm
73.08
26.92
27.07
73.58

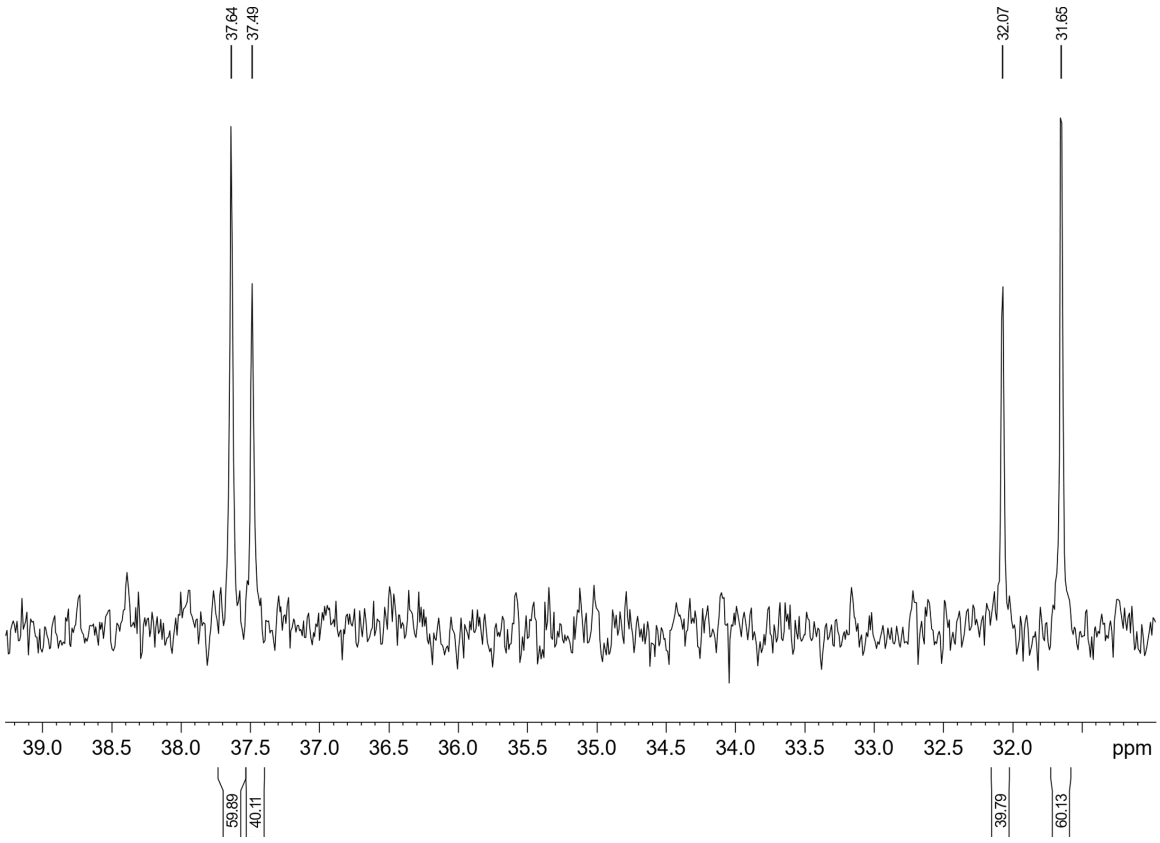
Product **13b**


1.12
1.10
0.93
0.92
[Et3NH]+
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
ppm
65.38
34.62

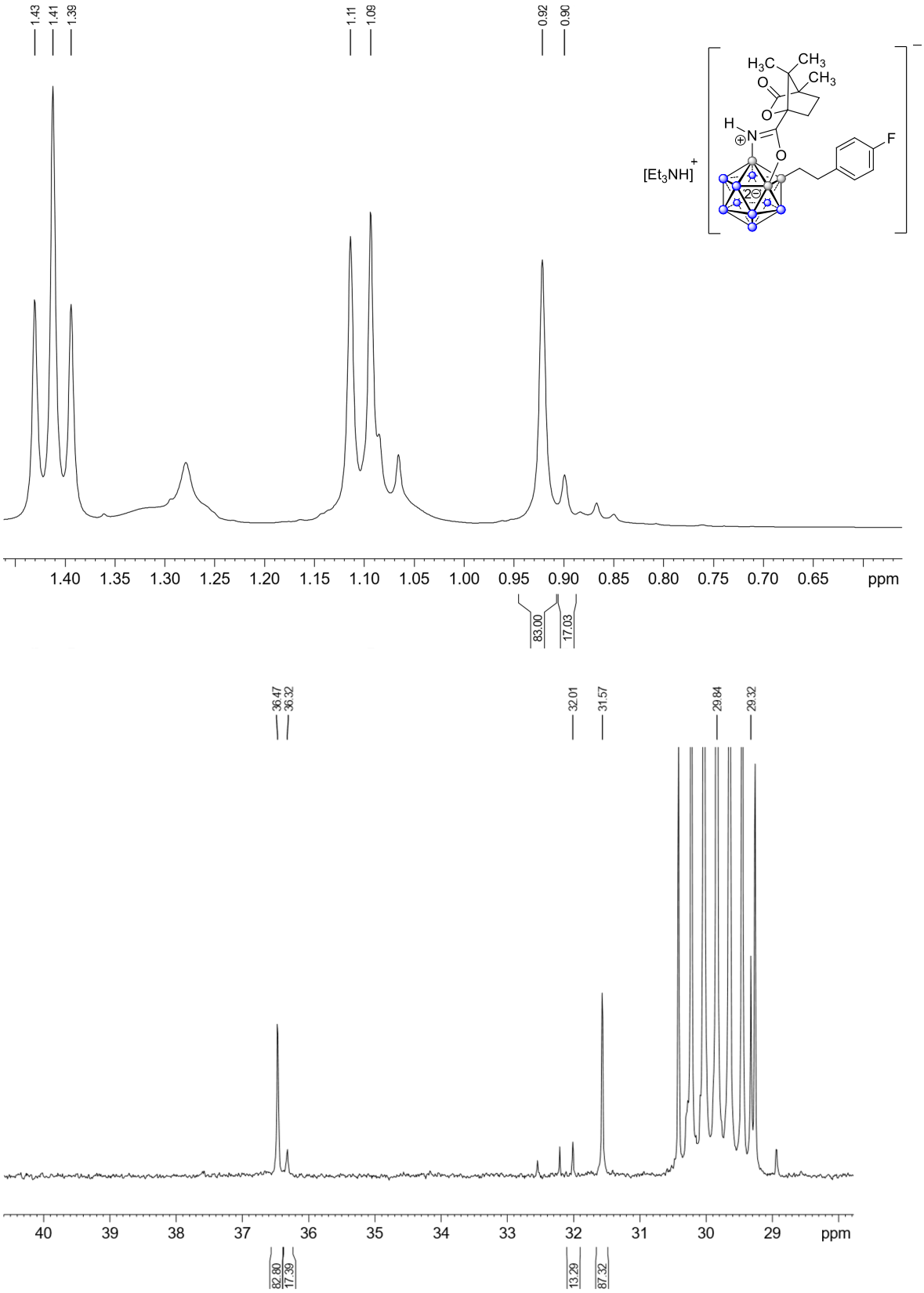

36.93
36.75
32.06
31.61
29.84
44
43
42
41
40
39
38
37
36
35
34
33
32
31
30
ppm
65.67
34.33
33.39
67.42

Product **13c**

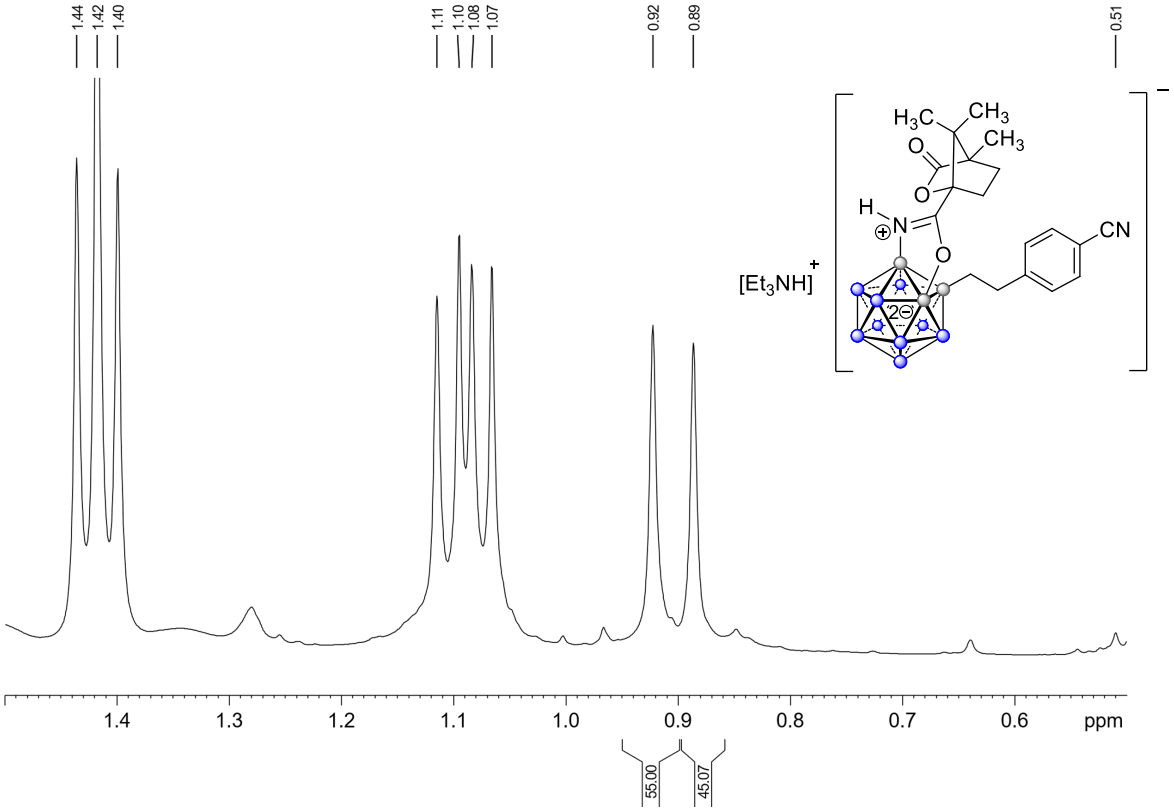

1.11
1.09
1.09
1.06
0.92
0.90
[Et3NH]+
OMe
1.35 1.30 1.25 1.20 1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 ppm
60.05
39.95

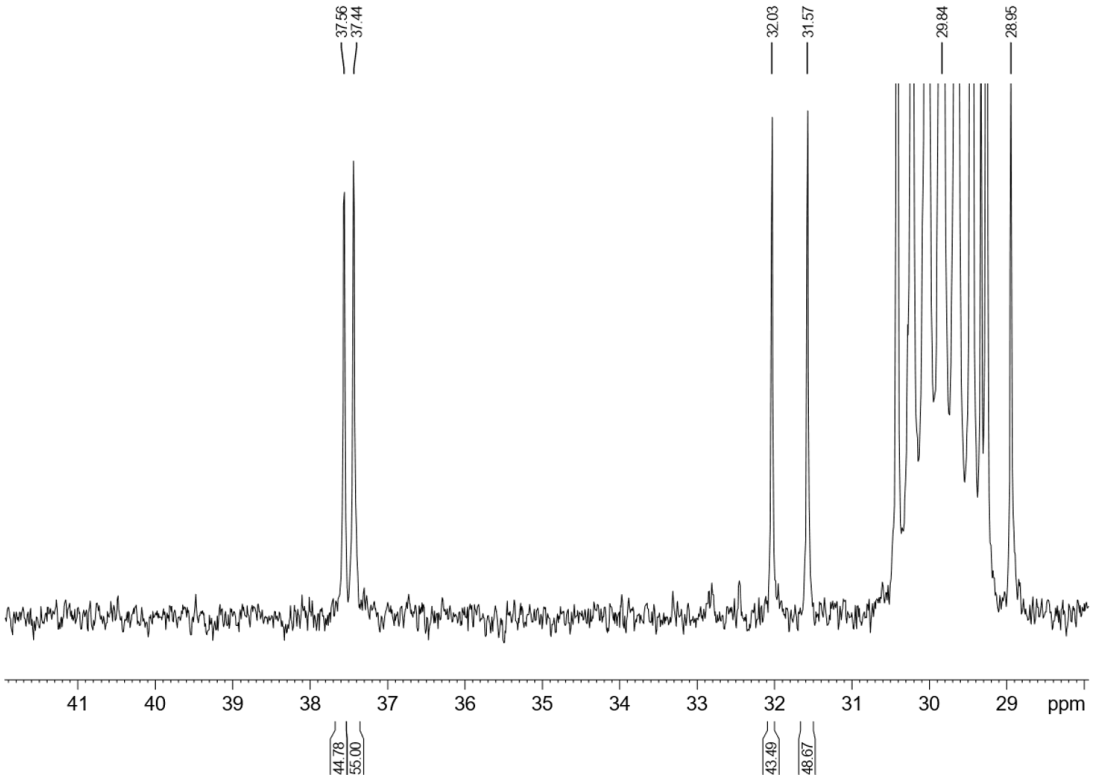

37.64
37.49
32.07
31.65
39.0 38.5 38.0 37.5 37.0 36.5 36.0 35.5 35.0 34.5 34.0 33.5 33.0 32.5 32.0 ppm
59.89
40.11
39.79
60.13

Product **13d**

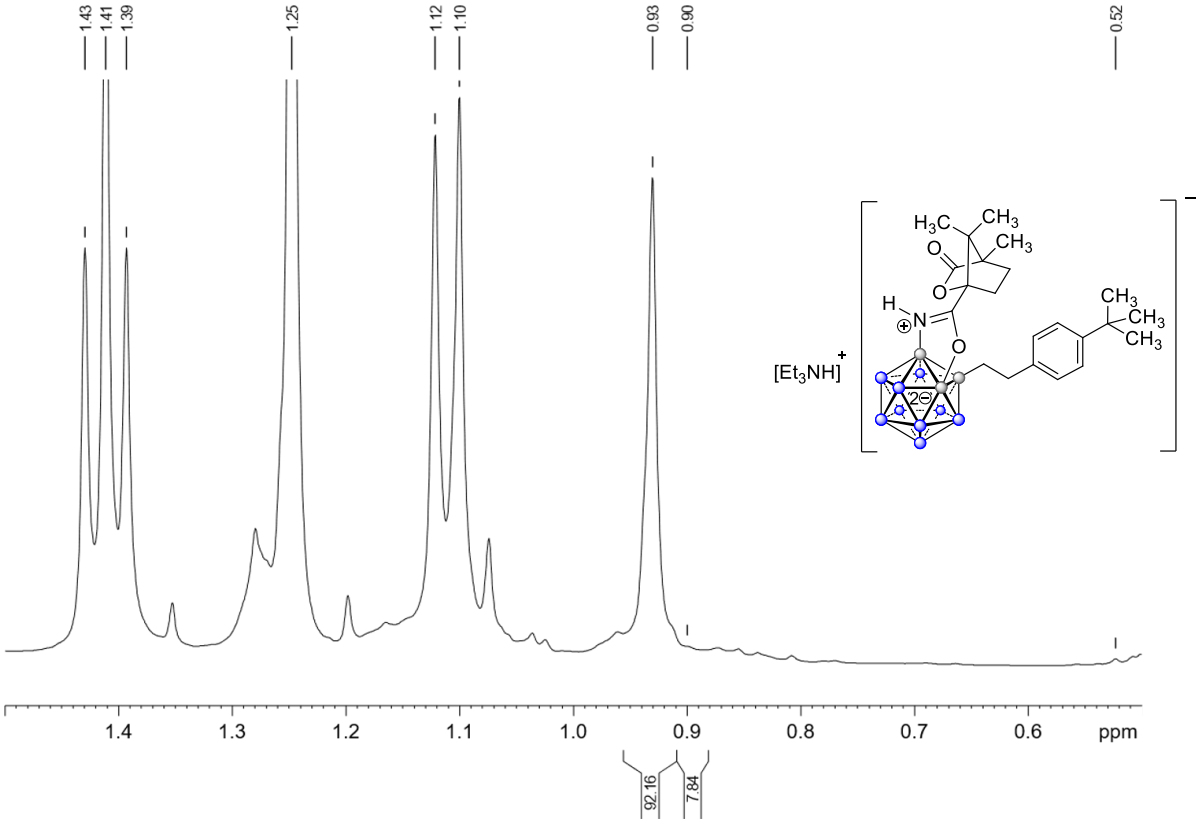

1.43
1.41
1.39
1.11
1.09
0.92
0.90
[Et3NH]+
1.40 1.35 1.30 1.25 1.20 1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 0.70 0.65 ppm
83.00
17.03
36.47
36.32
32.01
31.57
29.84
29.32
40 39 38 37 36 35 34 33 32 31 30 29 ppm
82.80
17.39
13.29
87.32

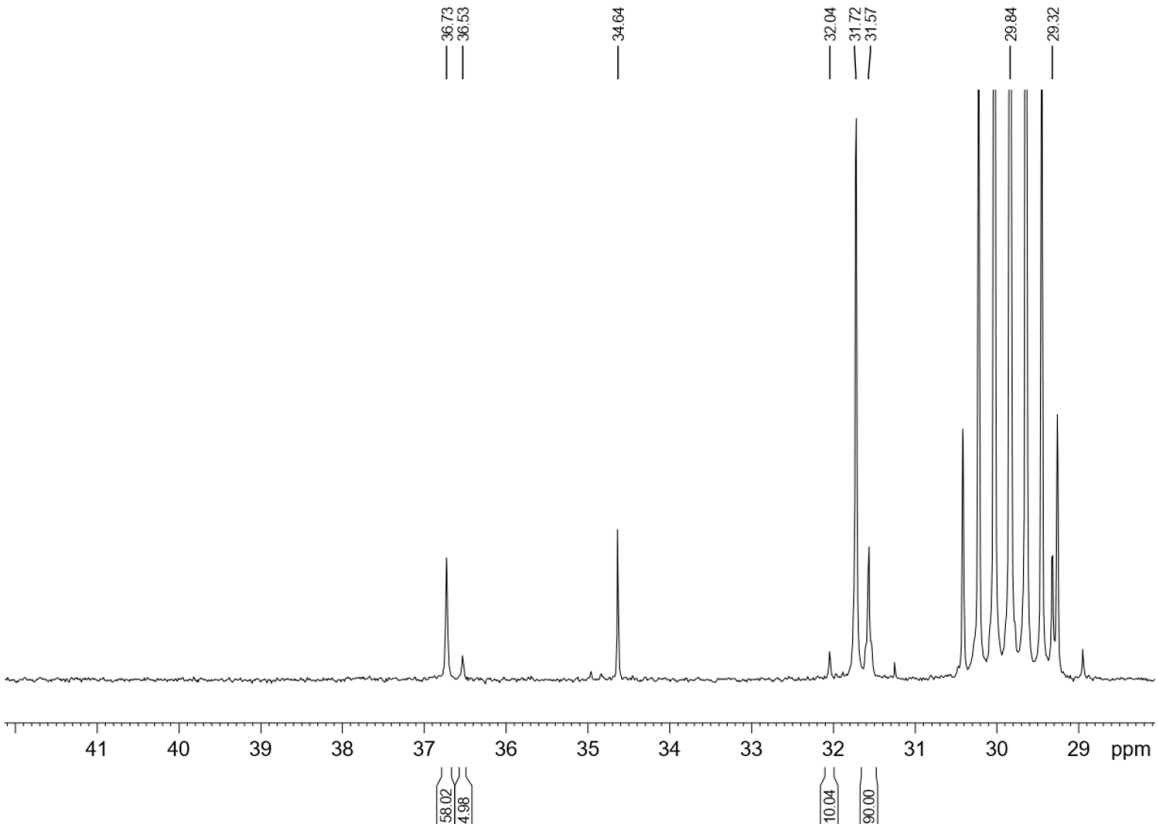
Product **13e**


1.44
1.42
1.40
1.11
1.10
1.08
1.07
0.92
0.89
0.51
[Et3NH]+
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
ppm
55.00
45.07

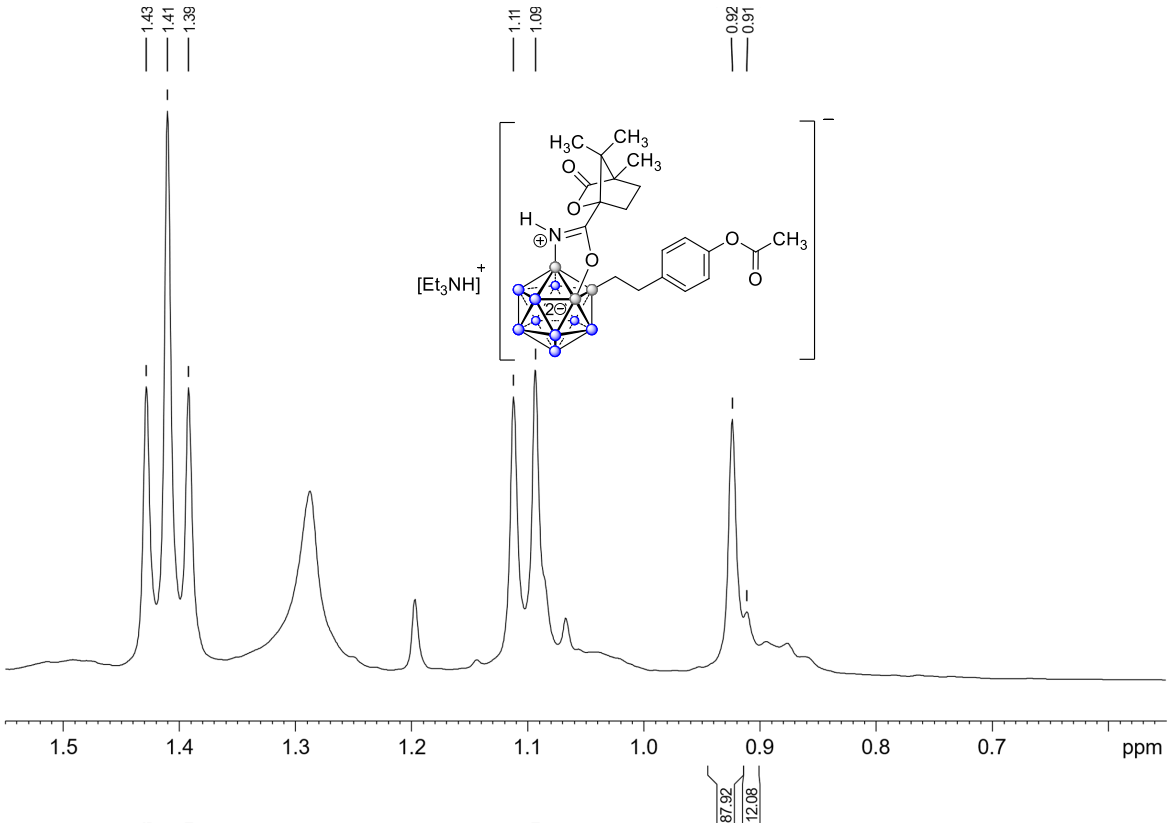

37.56
37.44
32.03
31.57
29.84
28.95
41
40
39
38
37
36
35
34
33
32
31
30
29
ppm
44.78
55.00
43.49
48.67

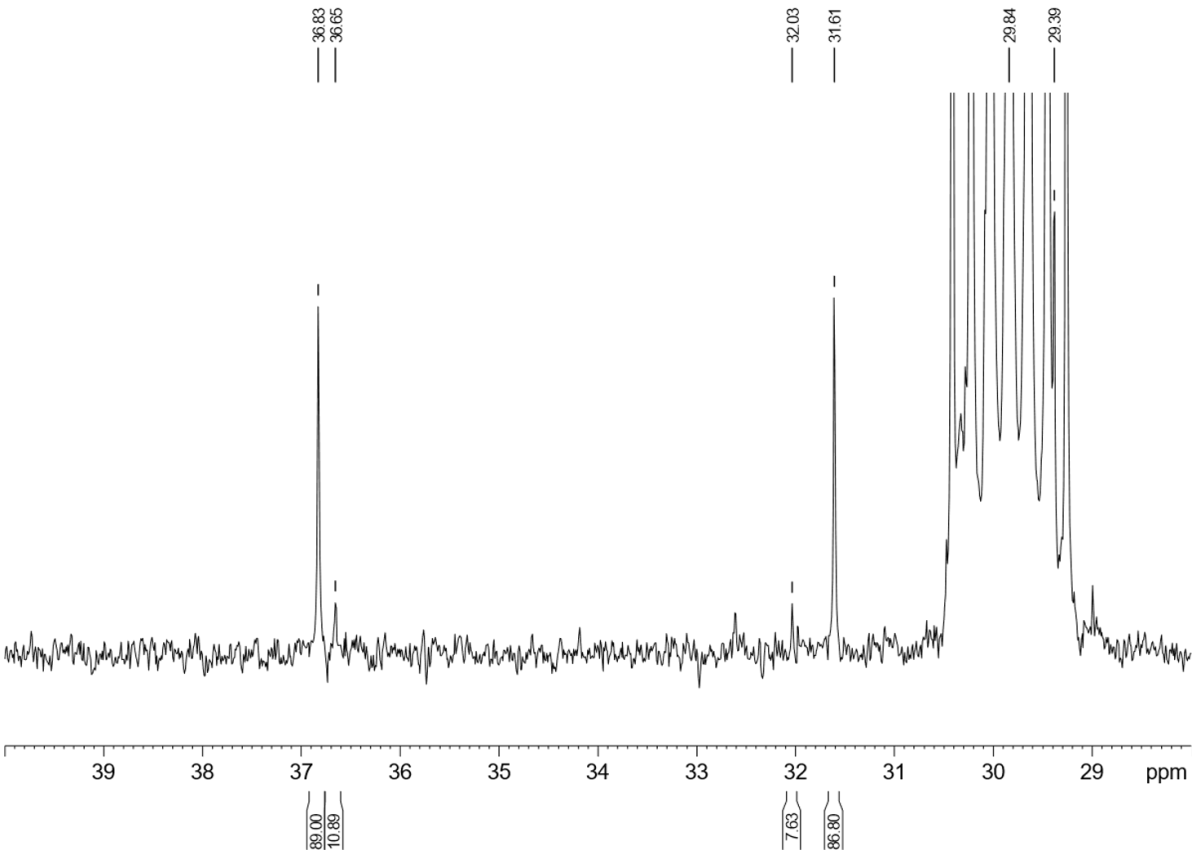
Product **13f**


1.43
1.41
1.39
1.25
1.12
1.10
0.93
0.90
0.52
[Et3NH]+
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
ppm
92.16
7.84

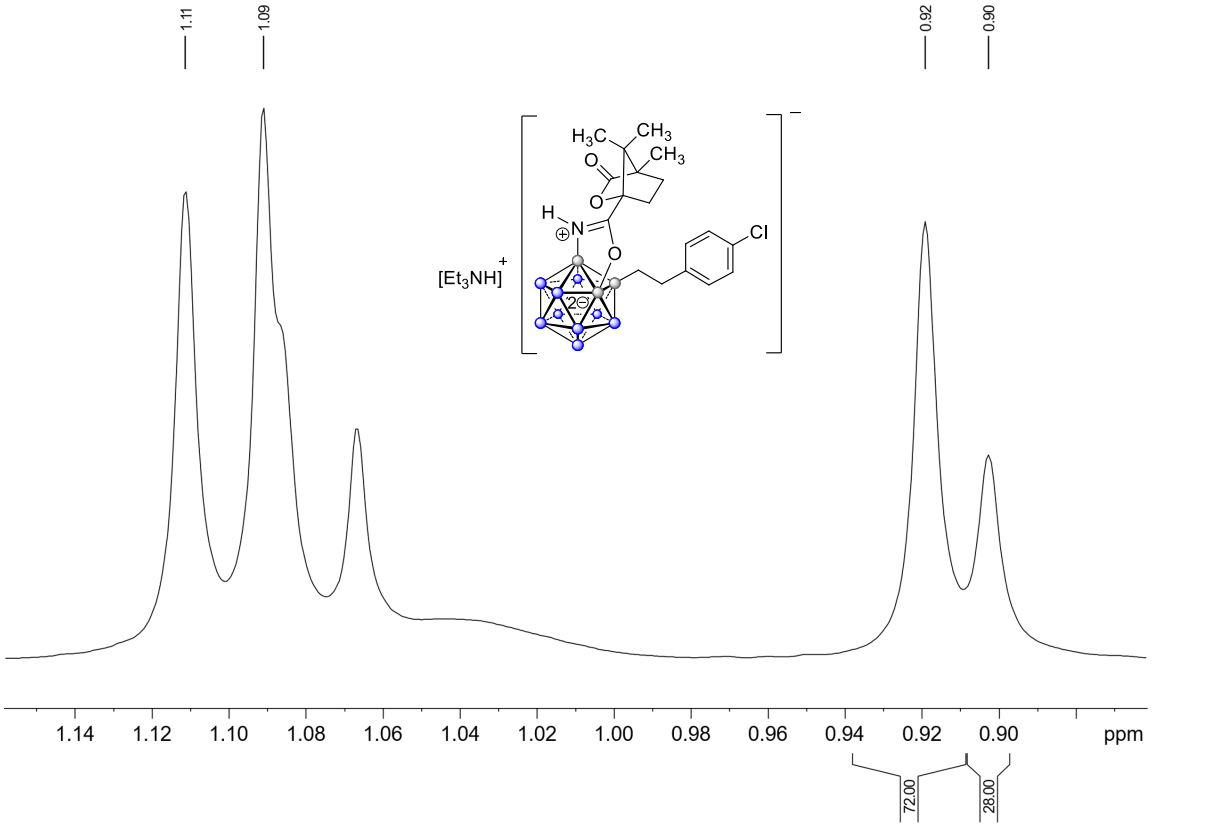

36.73
36.53
34.64
32.04
31.72
31.57
29.84
29.32
41
40
39
38
37
36
35
34
33
32
31
30
29
ppm
58.02
4.98
10.04
90.00

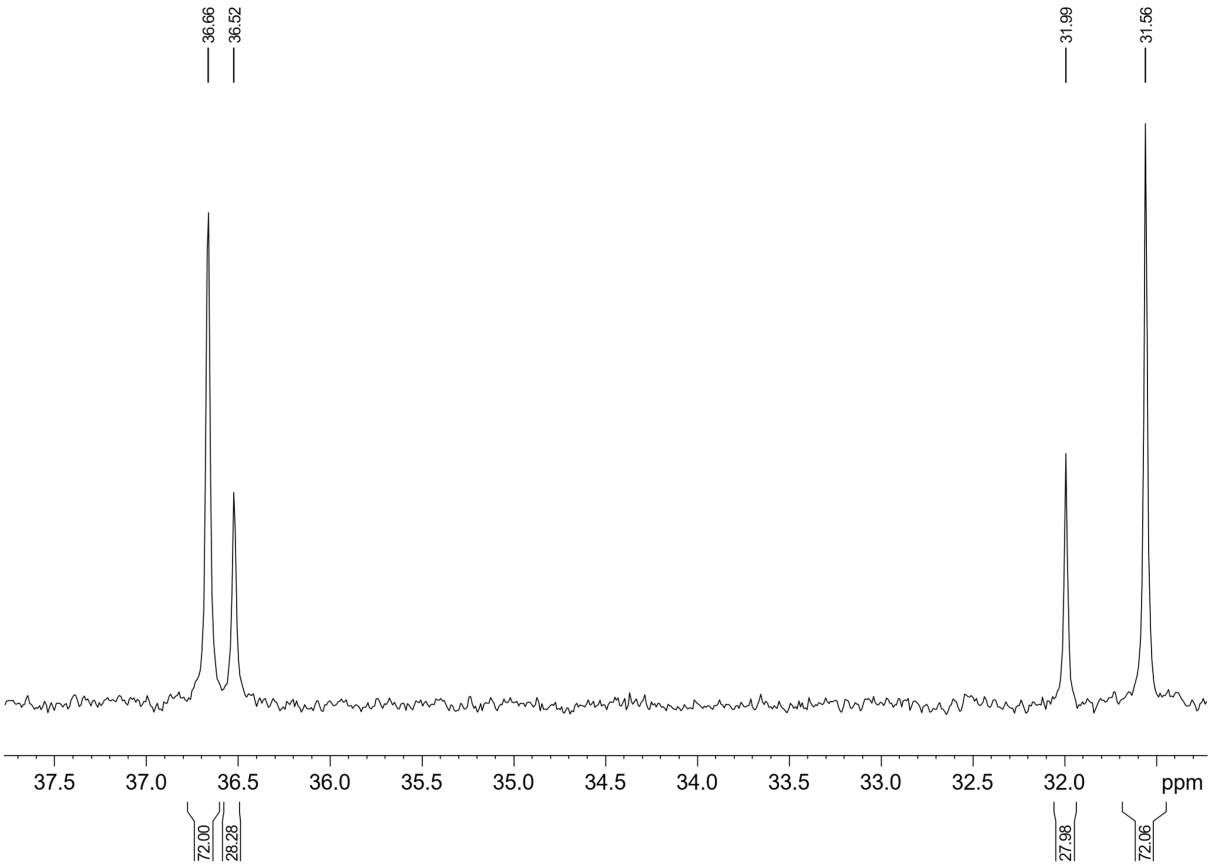
Product **13g**


1.43
1.41
1.39
1.11
1.09
0.92
0.91
[Et3NH]+
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
ppm
87.92
12.08

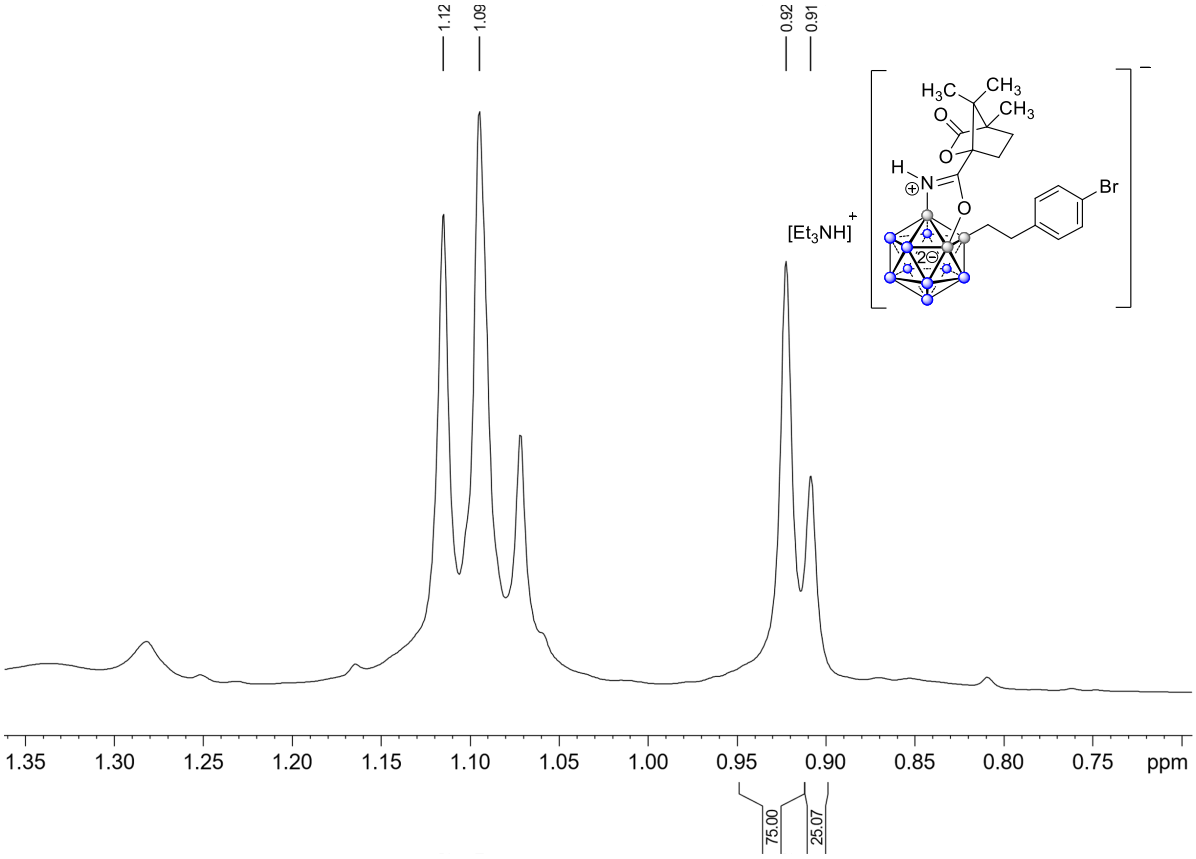

36.83
36.65
32.03
31.61
29.84
29.39
39
38
37
36
35
34
33
32
31
30
29
ppm
89.00
10.89
7.63
86.80

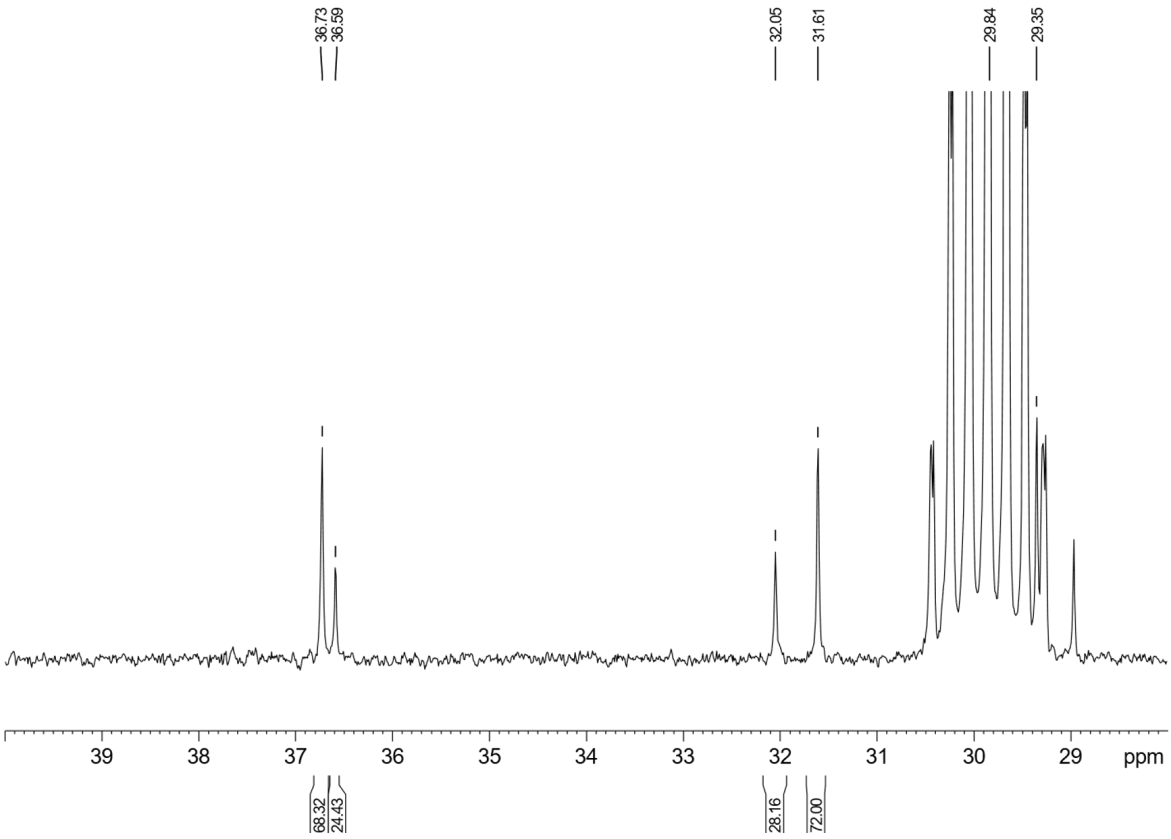
Product **13h**


1.11
1.09
0.92
0.90
[Et3NH]+
H3C
CH3
CH3
O
O
H
N
O
Cl
2⊖
1.14
1.12
1.10
1.08
1.06
1.04
1.02
1.00
0.98
0.96
0.94
0.92
0.90
ppm
72.00
28.00

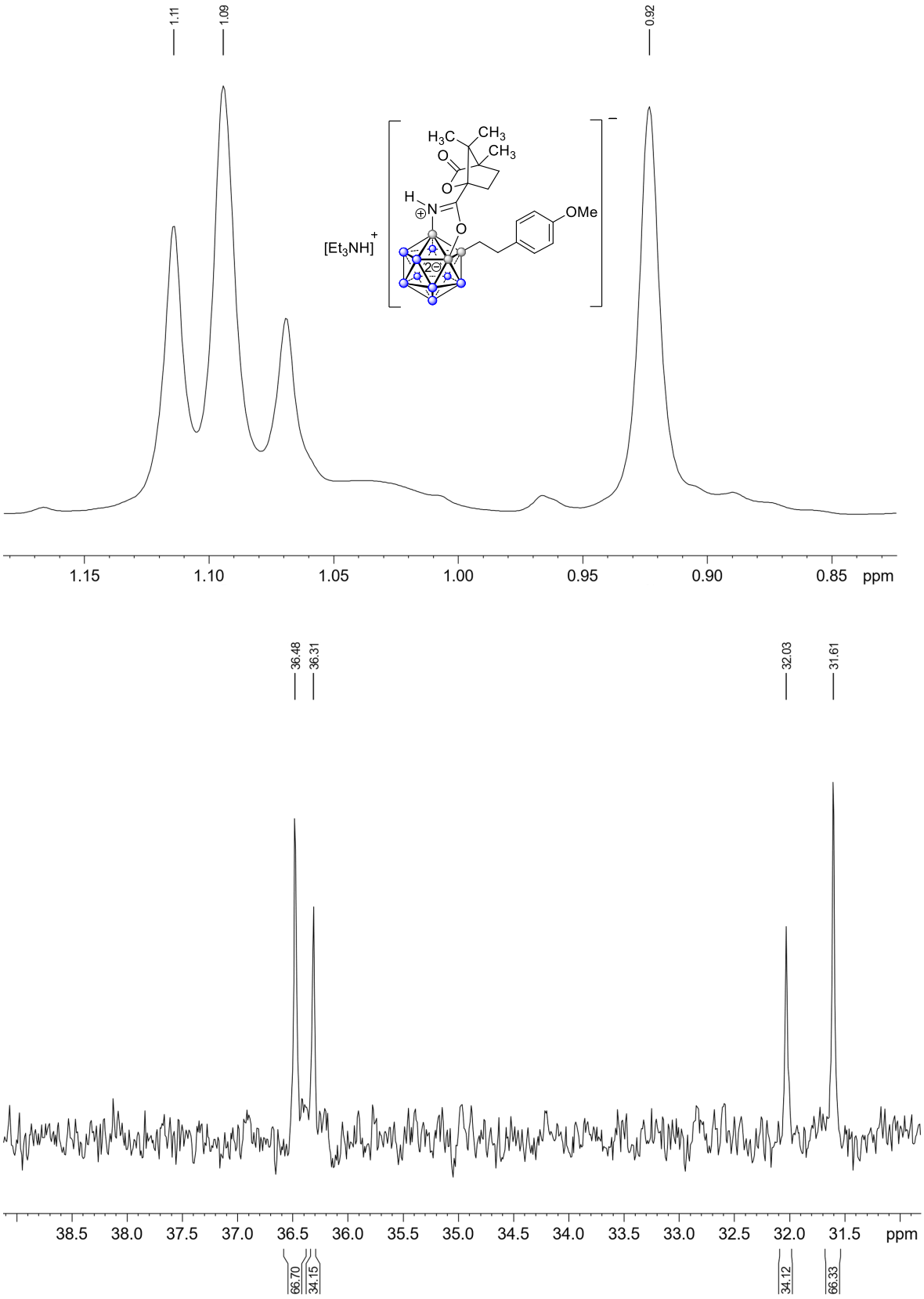

36.66
36.52
31.99
31.56
37.5
37.0
36.5
36.0
35.5
35.0
34.5
34.0
33.5
33.0
32.5
32.0
ppm
72.00
28.28
27.98
72.06

Product **13i**

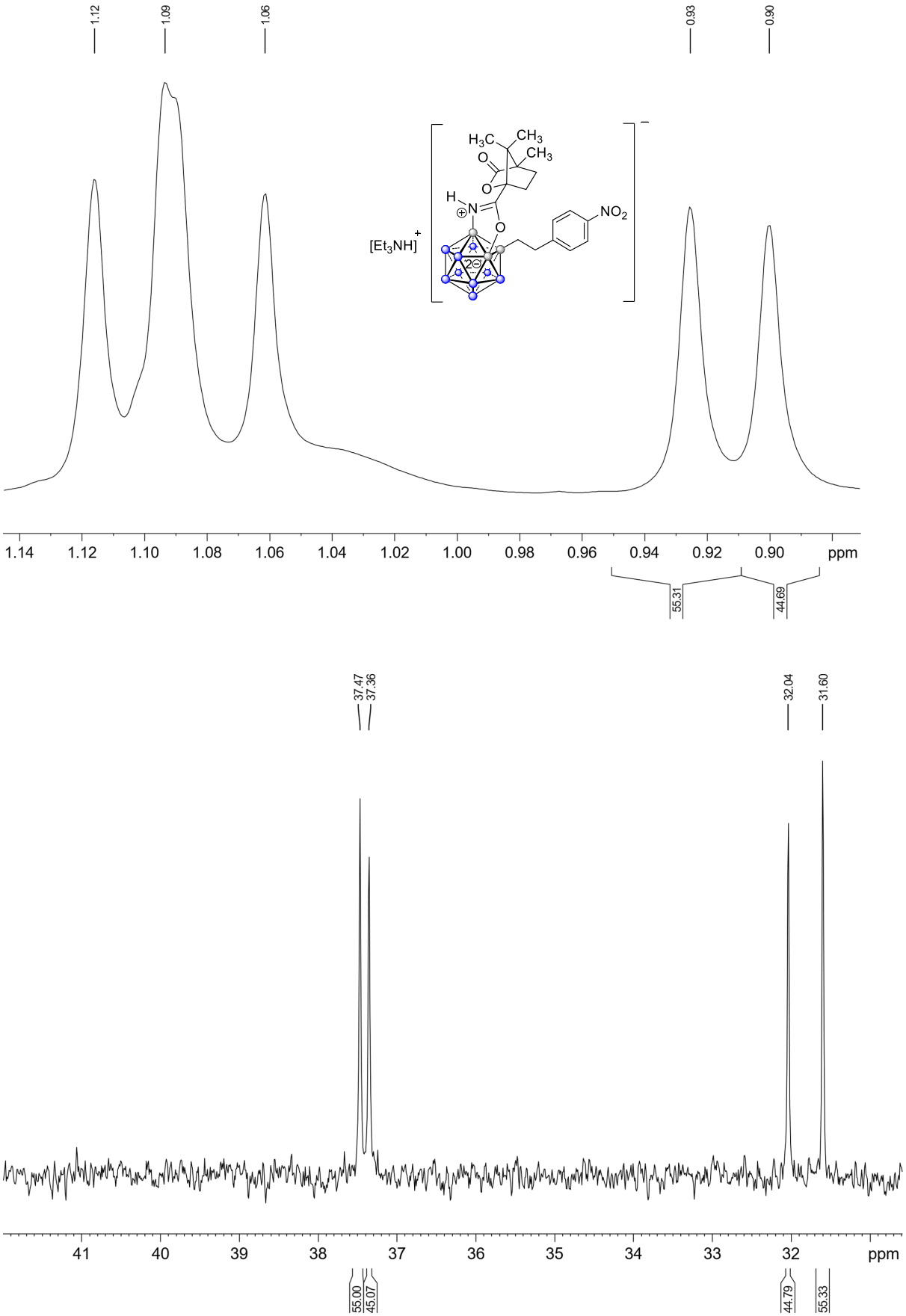

1.12
1.09
0.92
0.91
[Et3NH]+
1.35 1.30 1.25 1.20 1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 ppm
75.00
25.07


36.73
36.59
32.05
31.61
29.84
29.35
39 38 37 36 35 34 33 32 31 30 29 ppm
68.32
24.43
28.16
72.00

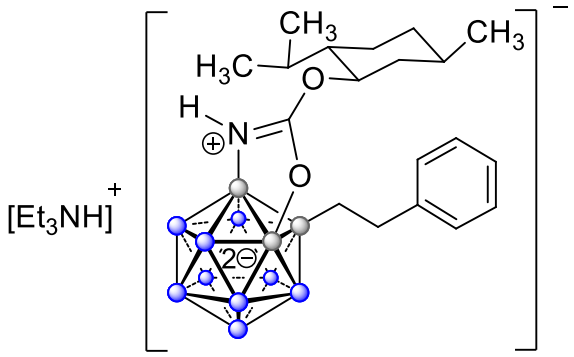
Product **13j**

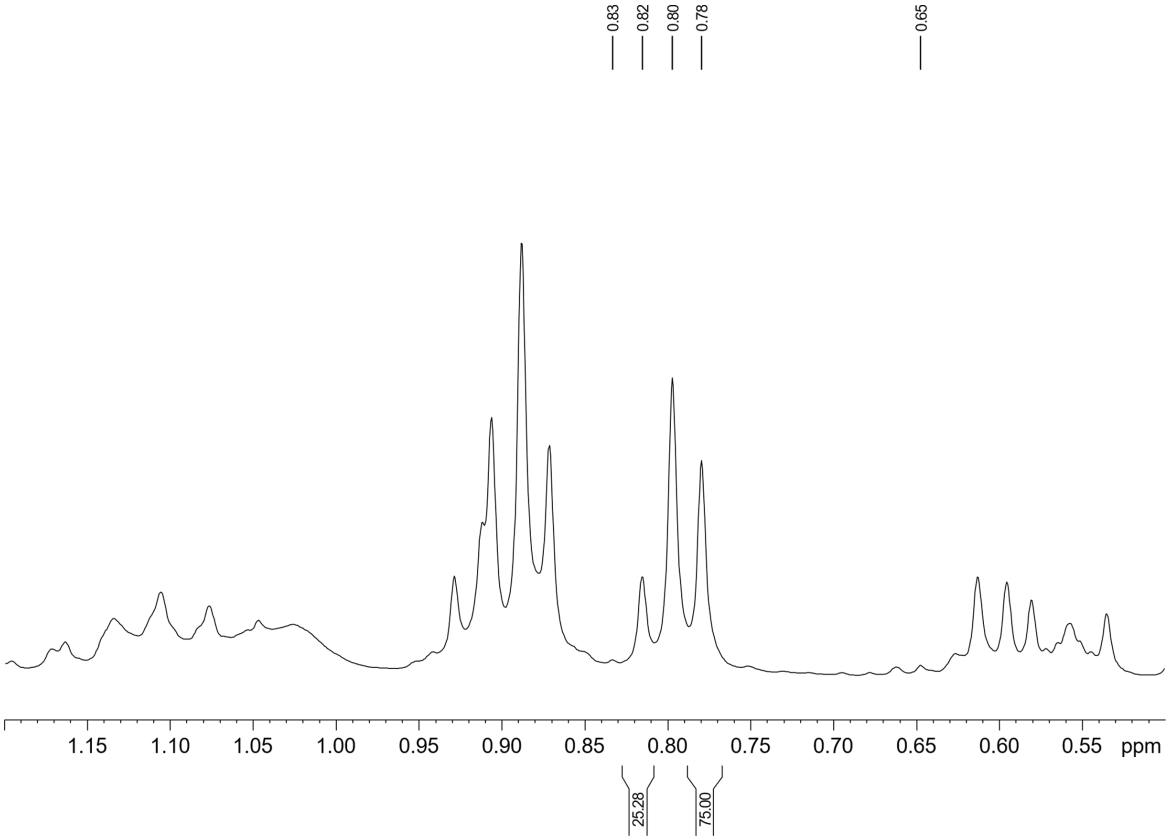

1.11
1.09
0.92
[Et3NH]+
H3C
CH3
CH3
O
O
H
N
O
OMe
2⊖
1.15
1.10
1.05
1.00
0.95
0.90
0.85
ppm
36.48
36.31
32.03
31.61
38.5
38.0
37.5
37.0
36.5
36.0
35.5
35.0
34.5
34.0
33.5
33.0
32.5
32.0
31.5
ppm
66.70
34.15
34.12
66.33

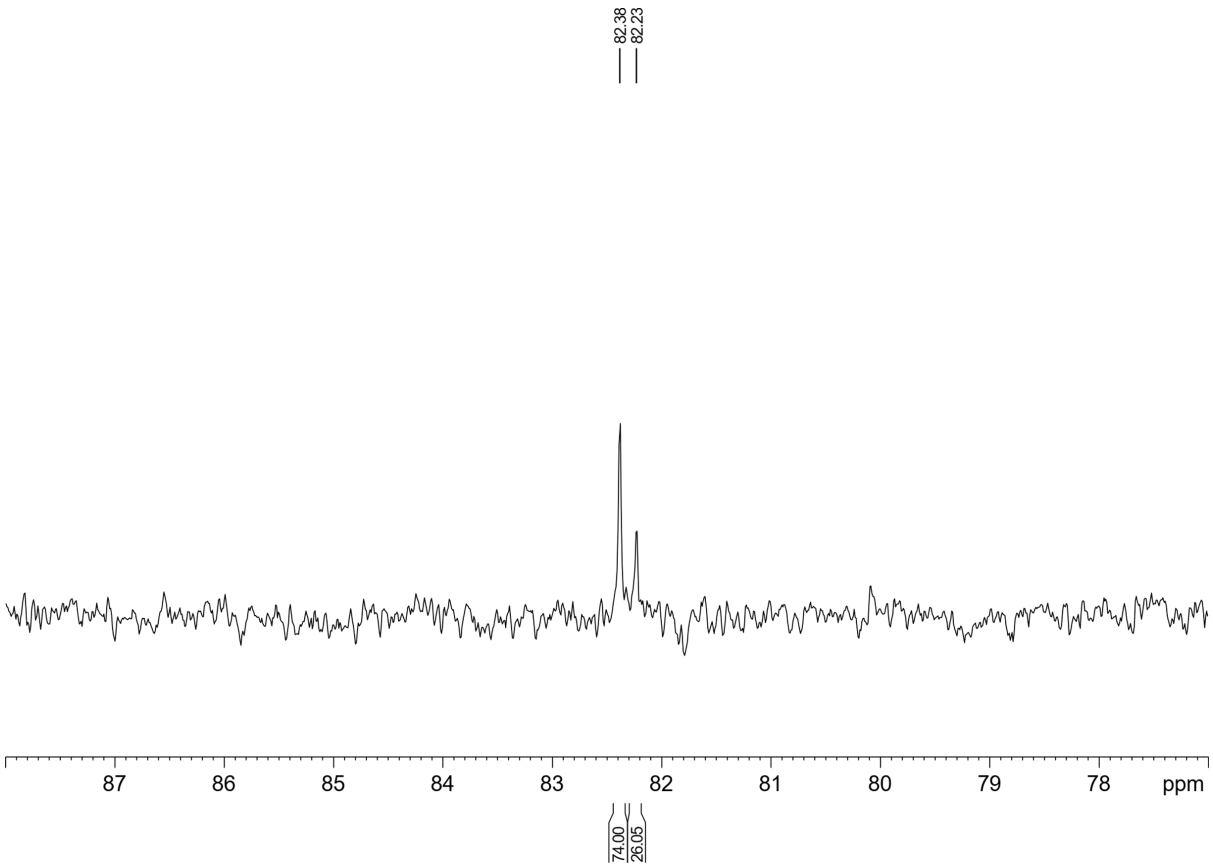
Product **13k**

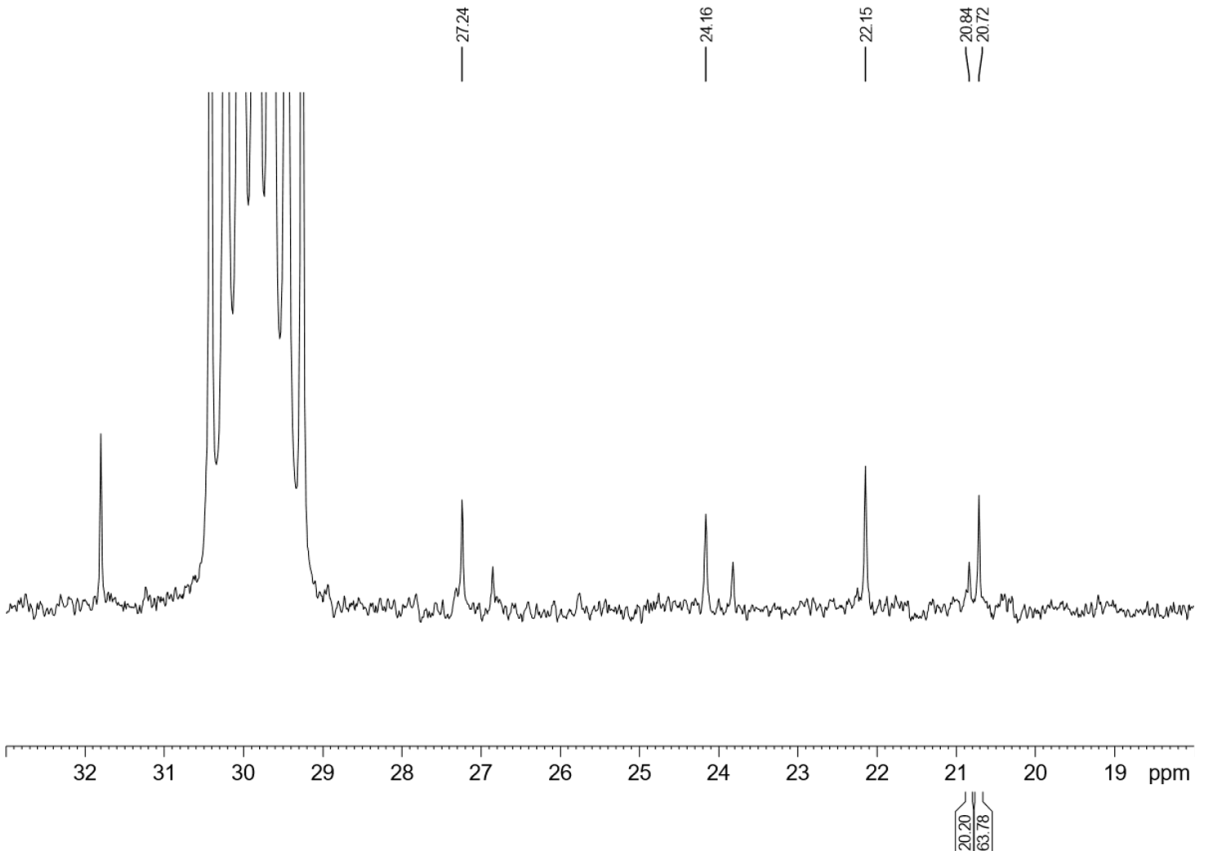

1.12
1.09
1.06
0.93
0.90
[Et3NH]+
2⊖
NO2
1.14 1.12 1.10 1.08 1.06 1.04 1.02 1.00 0.98 0.96 0.94 0.92 0.90 ppm
55.31
44.69
37.47
37.36
32.04
31.60
41 40 39 38 37 36 35 34 33 32 ppm
55.00
45.07
44.79
55.33

Product **14a**

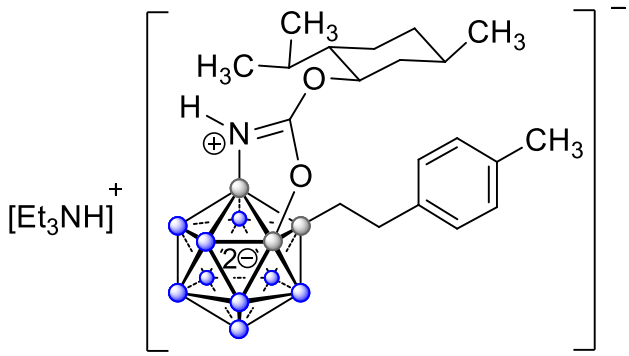

[Et3NH]+
CH3
CH3
H3C
O
H
N
O
2⊖

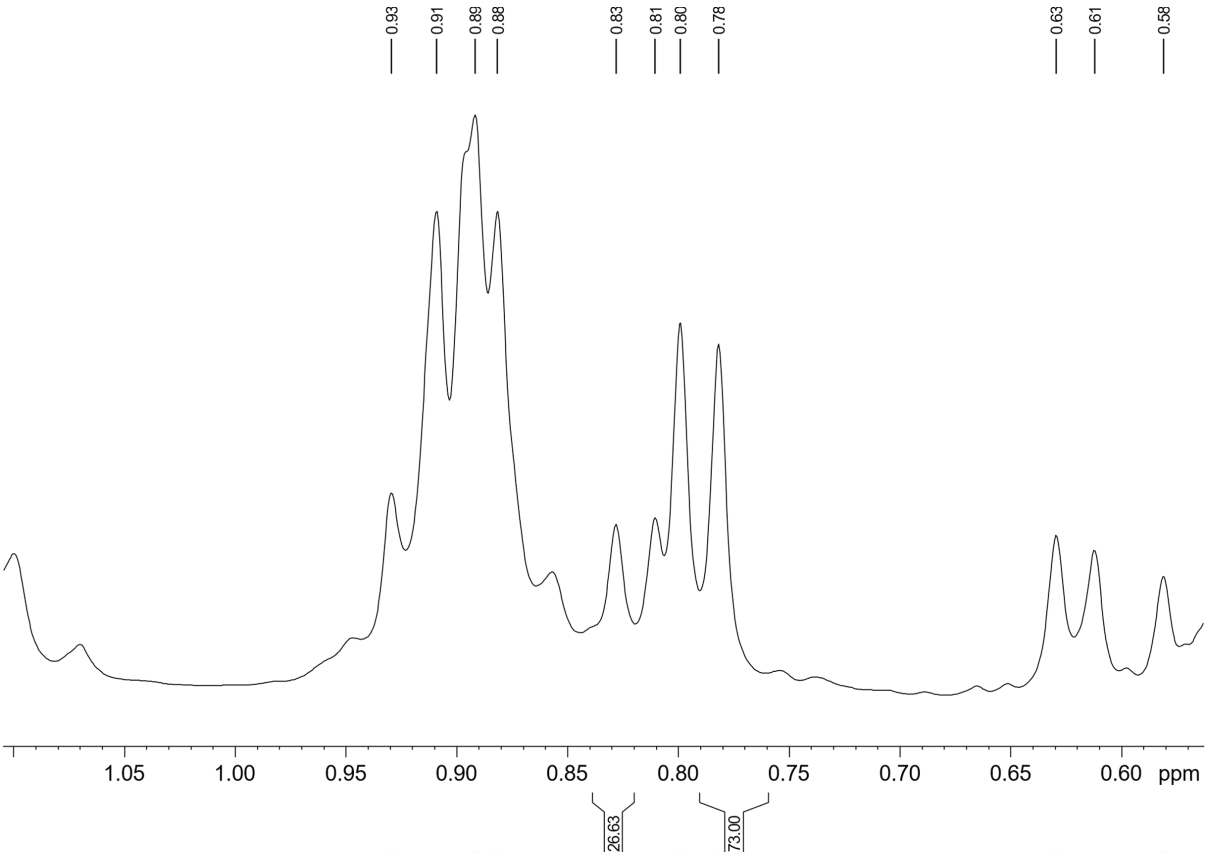

0.83
0.82
0.80
0.78
0.65
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
ppm
25.28
75.00

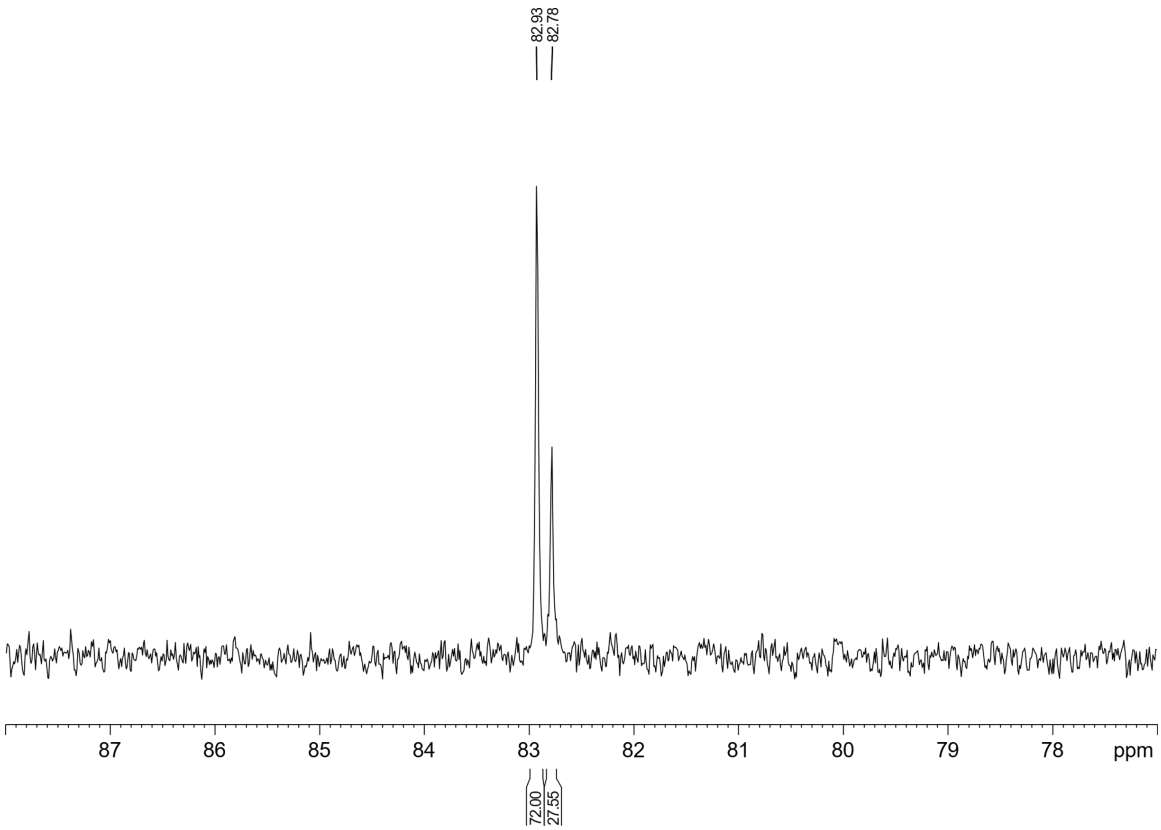

82.38
82.23
87
86
85
84
83
82
81
80
79
78
ppm
74.00
26.05

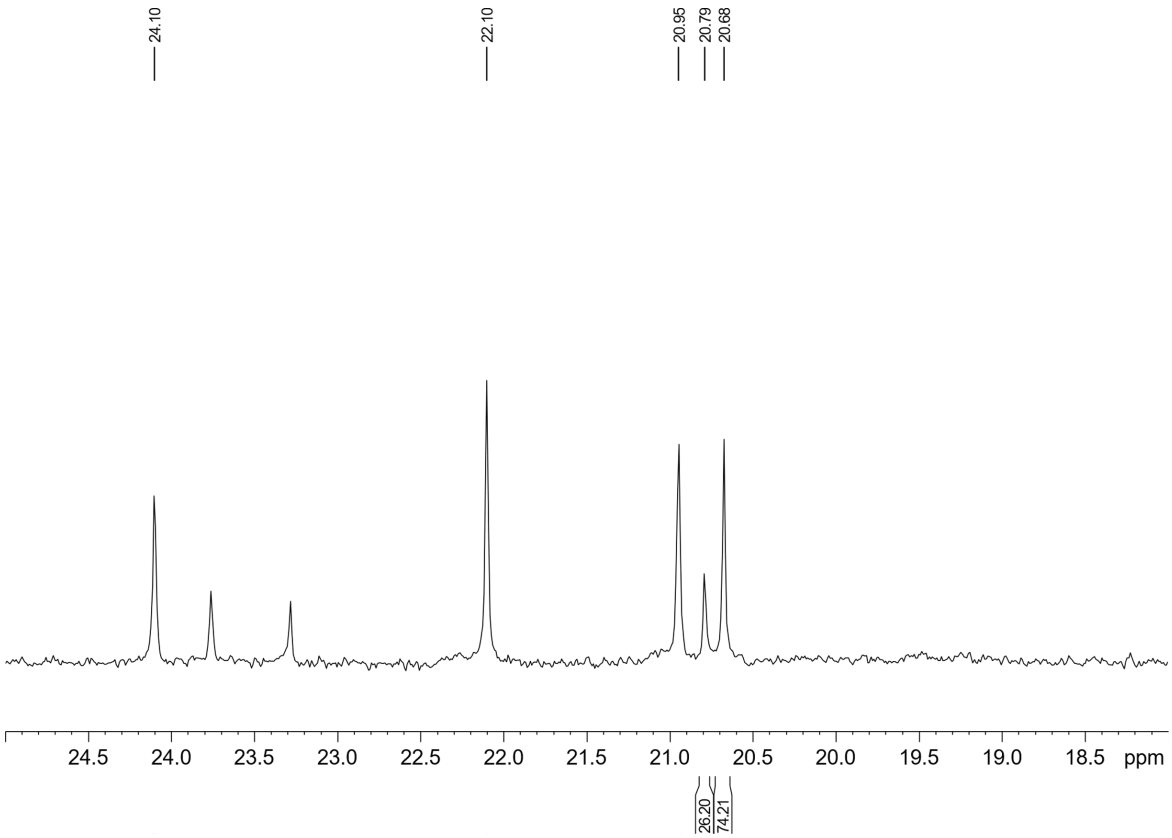

27.24
24.16
22.15
20.84
20.72
32
31
30
29
28
27
26
25
24
23
22
21
20
19
ppm
20.20
63.78

Product **14b**

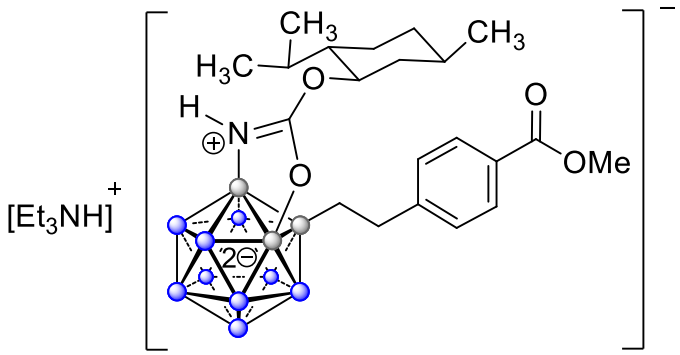

[Et3NH]+
CH3
CH3
H3C
O
H
N
CH3
O
2⊖

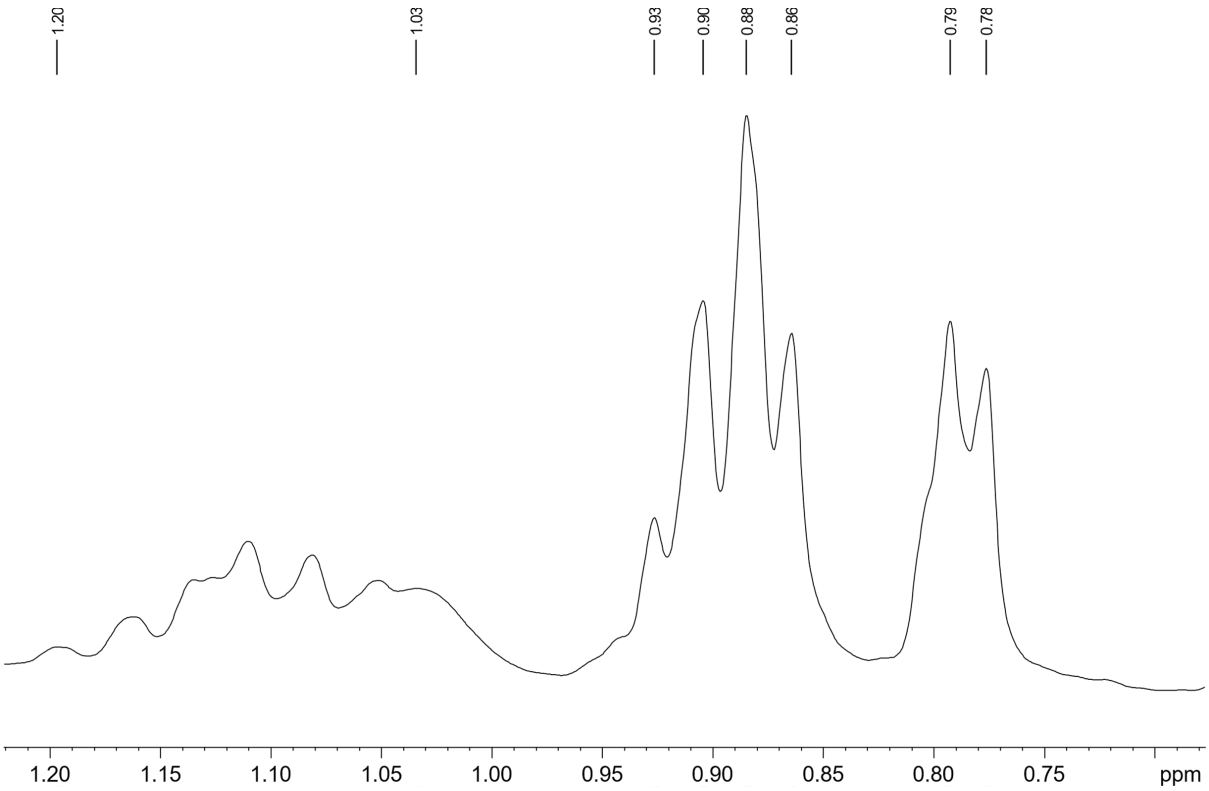

0.93
0.91
0.89
0.88
0.83
0.81
0.80
0.78
0.63
0.61
0.58
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
ppm
26.63
73.00

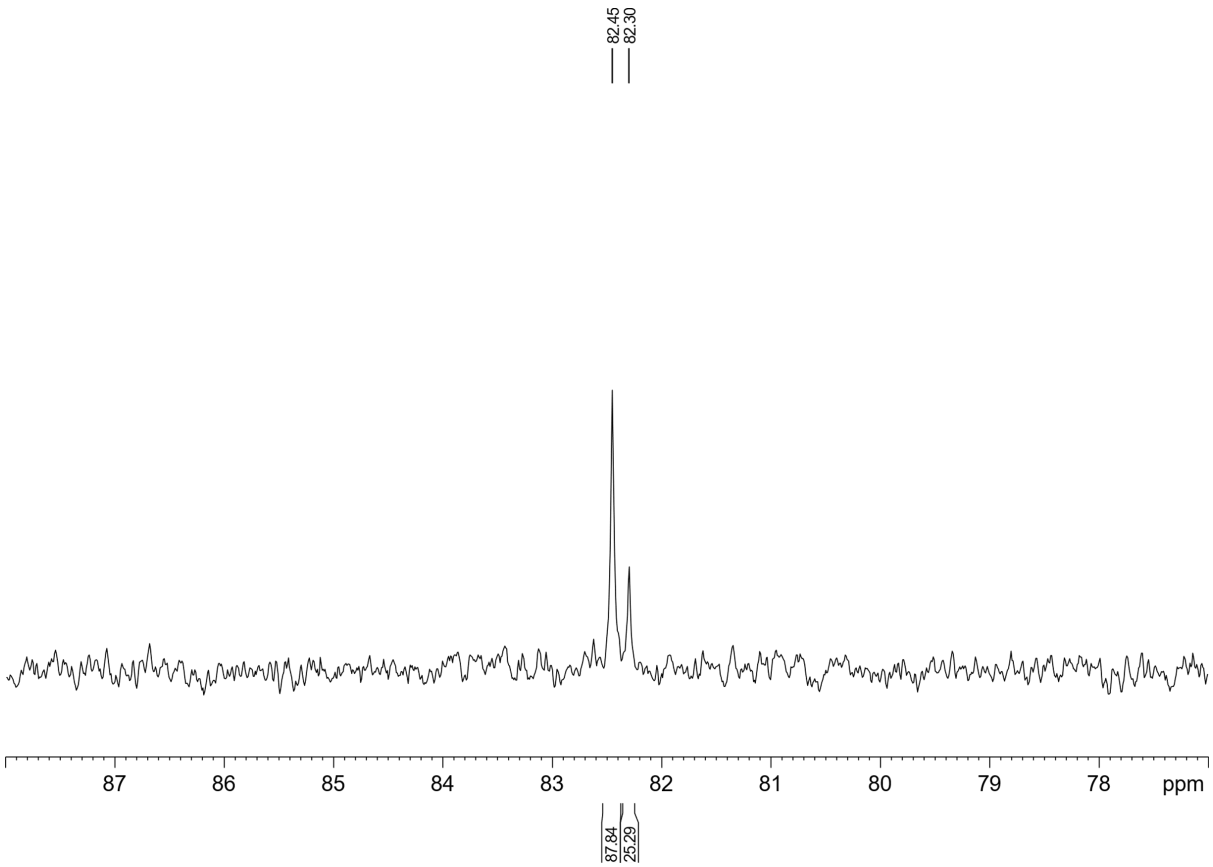

82.93
82.78
87
86
85
84
83
82
81
80
79
78
ppm
72.00
27.55

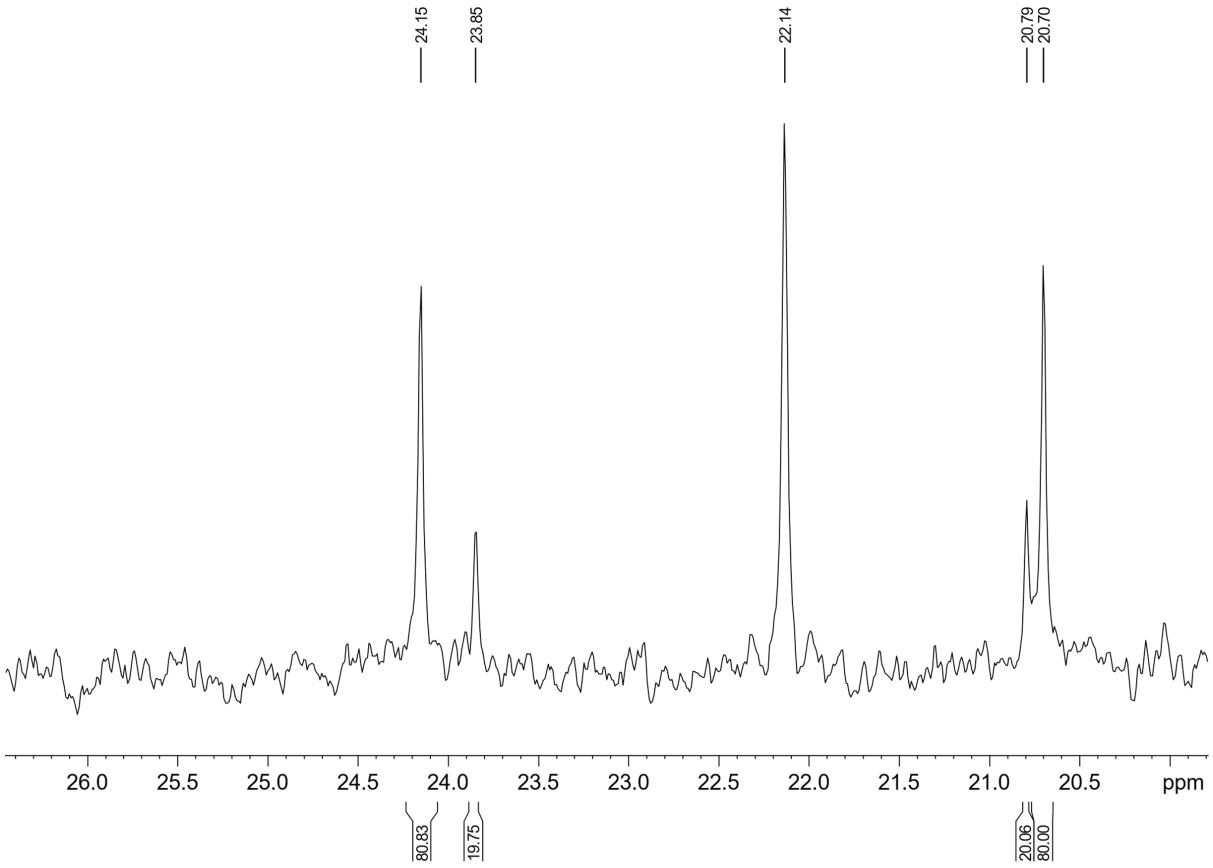

24.10
22.10
20.95
20.79
20.68
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
20.0
19.5
19.0
18.5
ppm
26.20
74.21

Product **14c**

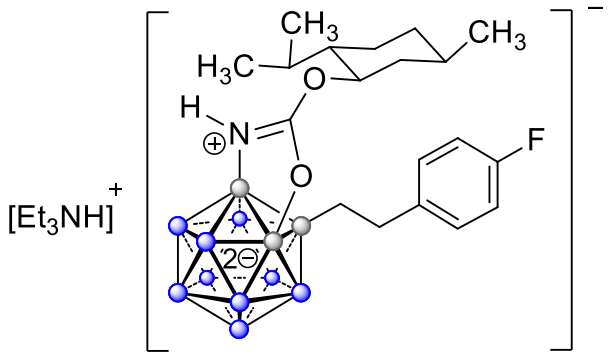

[Et3NH]+
CH3
CH3
H3C
O
H
N
O
O
OMe
2⊖

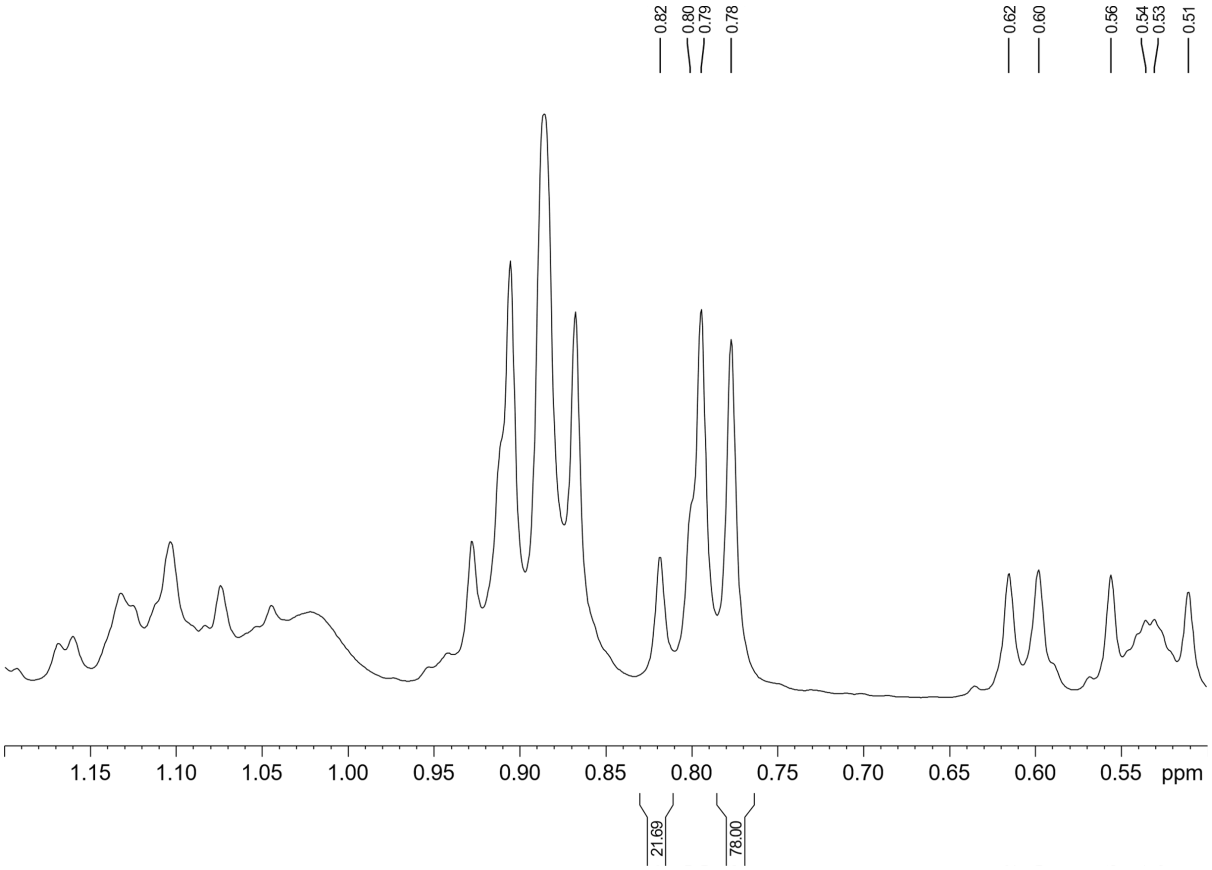

1.20
1.03
0.93
0.90
0.88
0.86
0.79
0.78
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
ppm

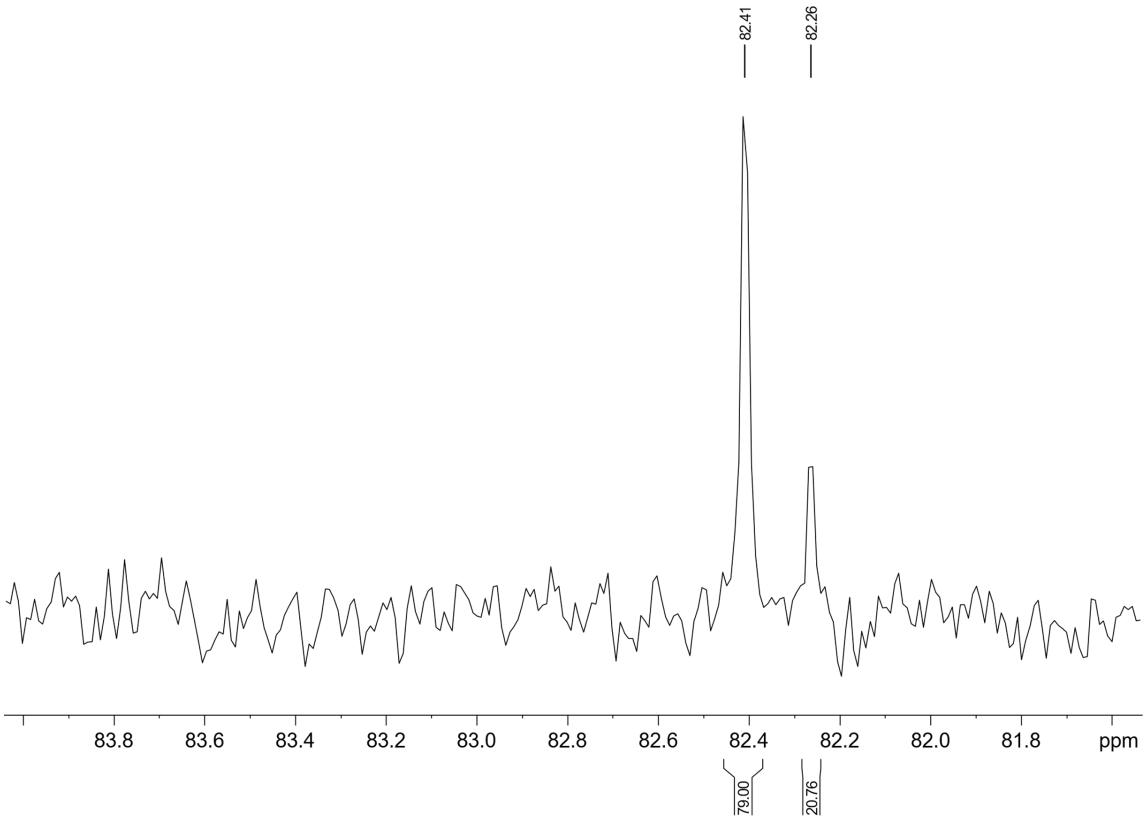

82.45
82.30
87
86
85
84
83
82
81
80
79
78
ppm
87.84
25.29

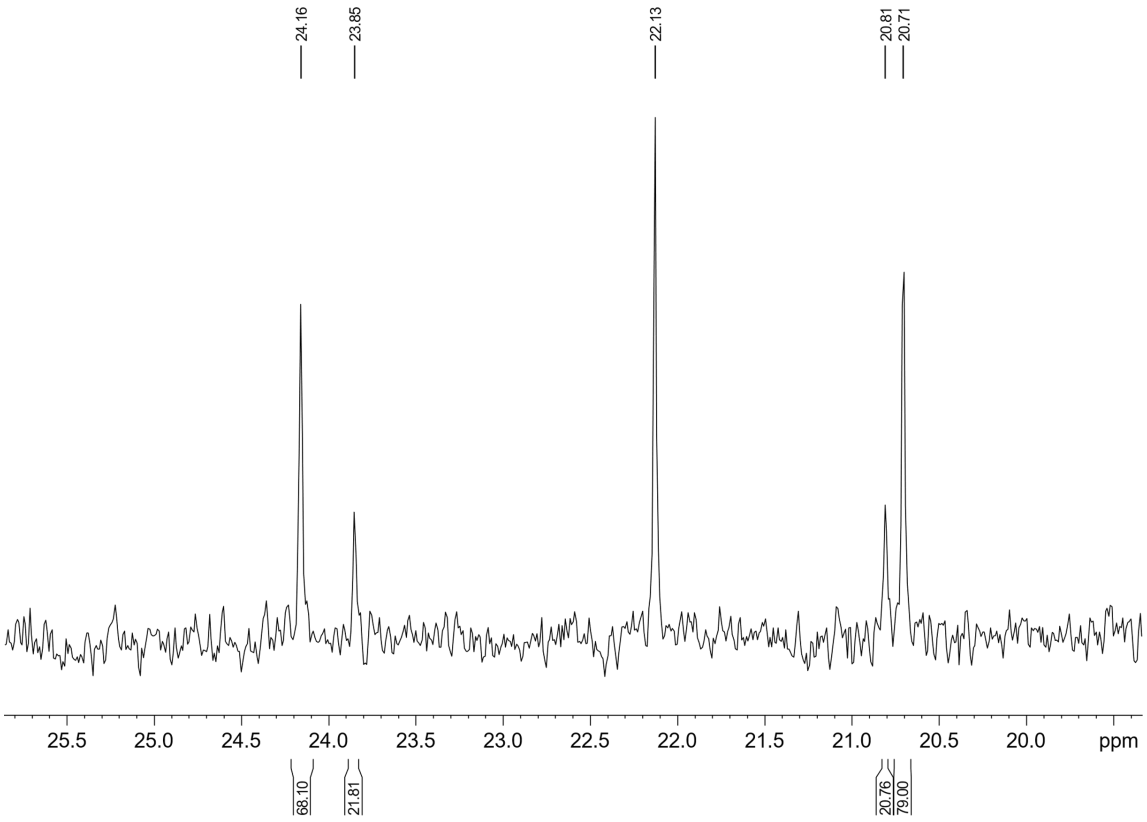

24.15
23.85
22.14
20.79
20.70
26.0
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
80.83
19.75
20.06
80.00

Product **14d**

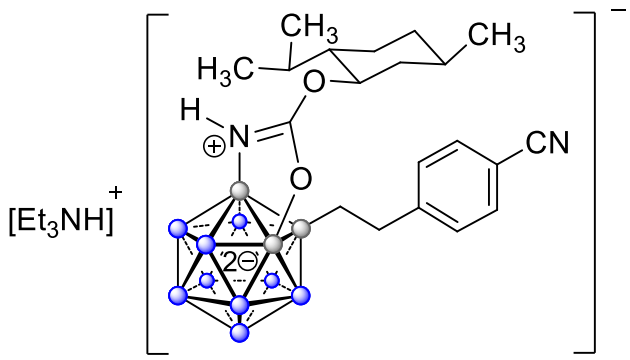

[Et3NH]+
CH3
CH3
H3C
O
H
N
F
O
2⊖

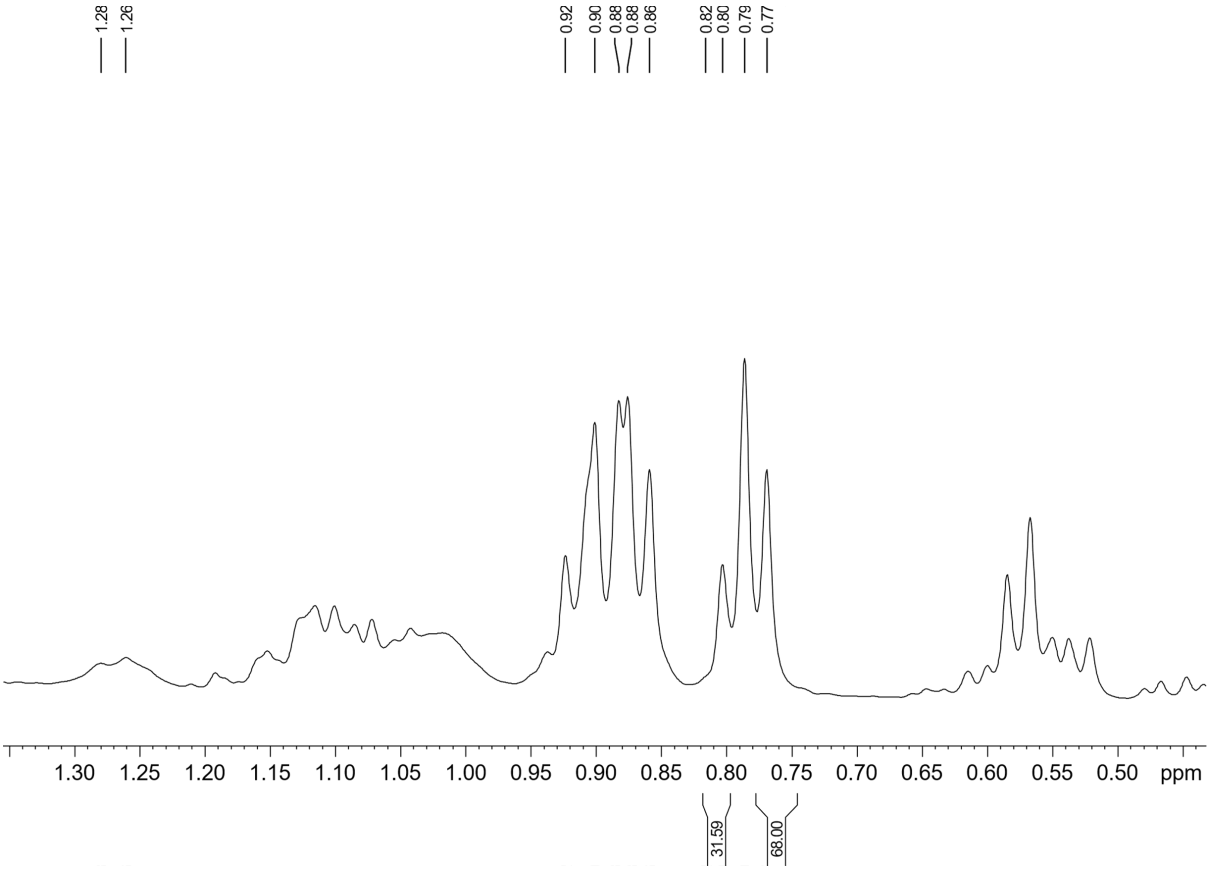

0.82
0.80
0.79
0.78
0.62
0.60
0.56
0.54
0.53
0.51
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
ppm
21.69
78.00

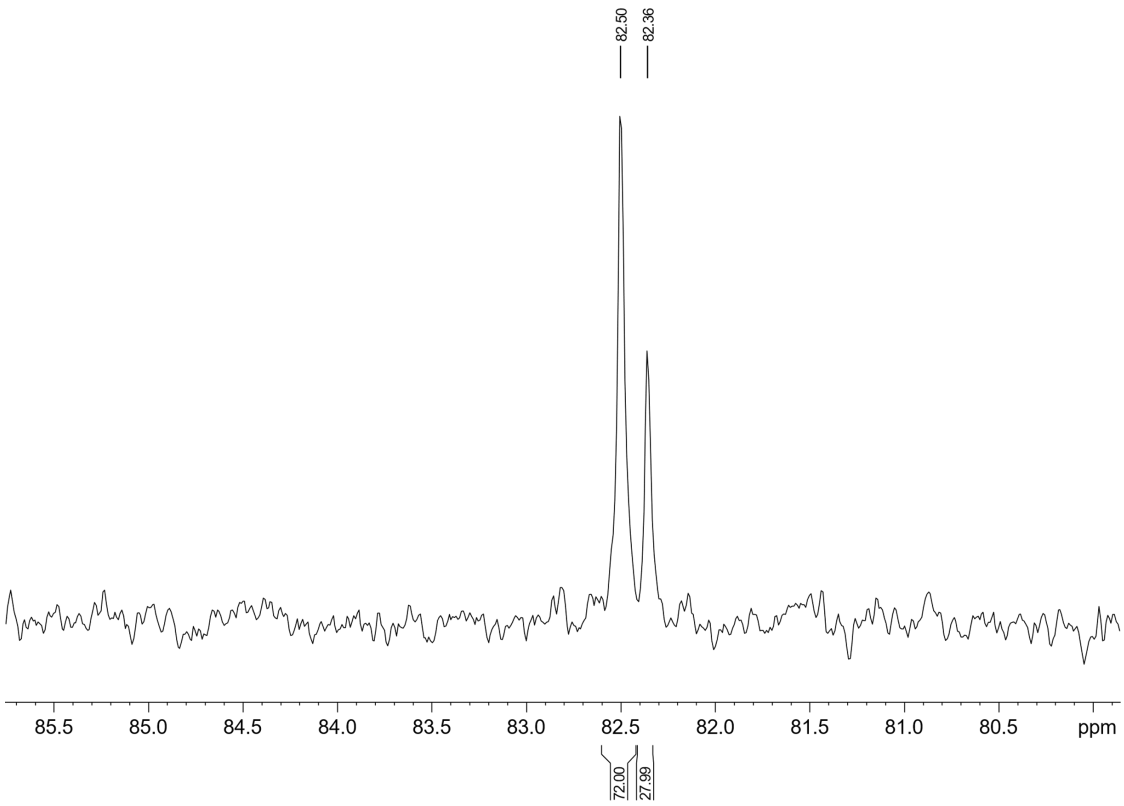

82.41
82.26
83.8
83.6
83.4
83.2
83.0
82.8
82.6
82.4
82.2
82.0
81.8
ppm
79.00
20.76

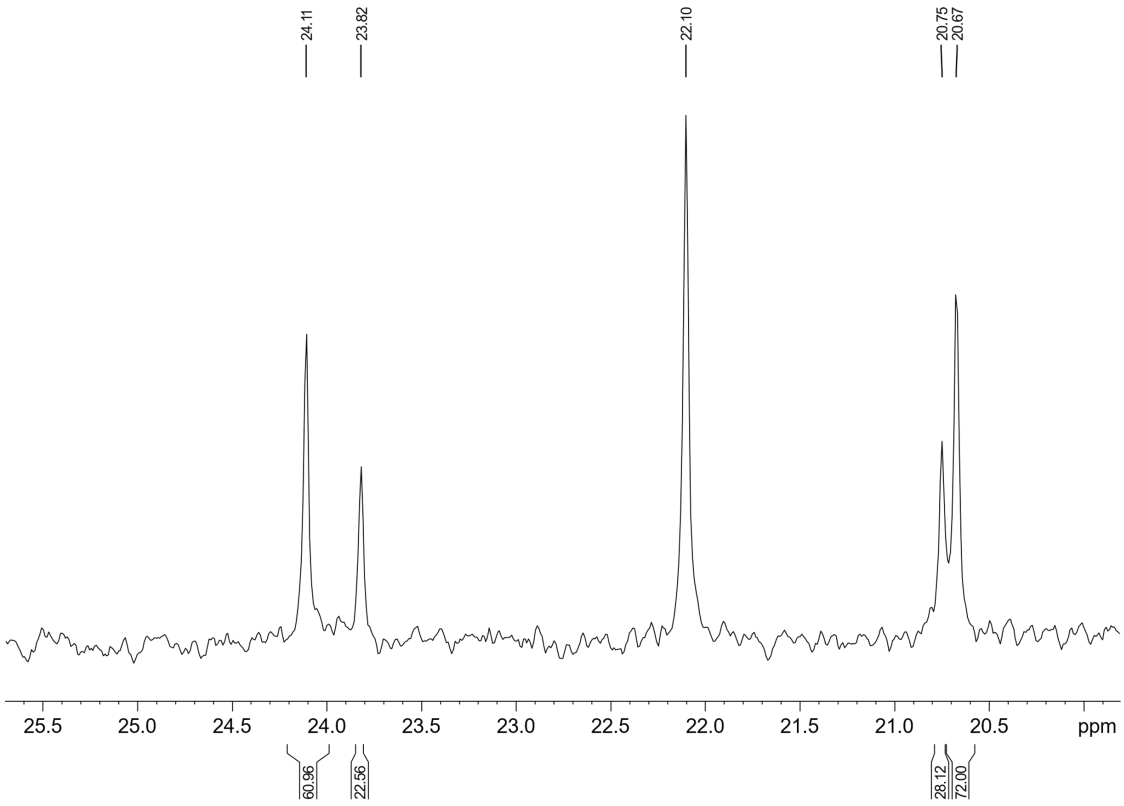

24.16
23.85
22.13
20.81
20.71
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
20.0
ppm
68.10
21.81
20.76
79.00

Product **14e**

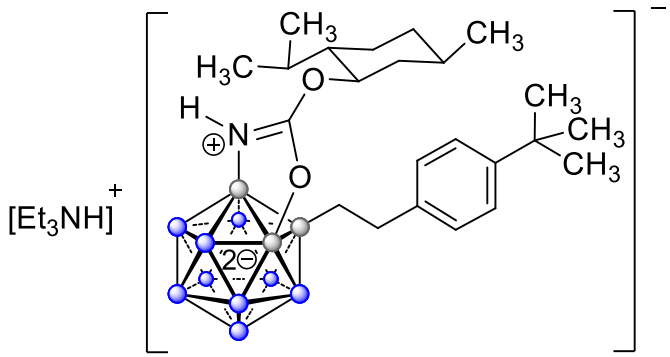

[Et3NH]+
CH3
CH3
H3C
O
H
N
CN
O
2⊖

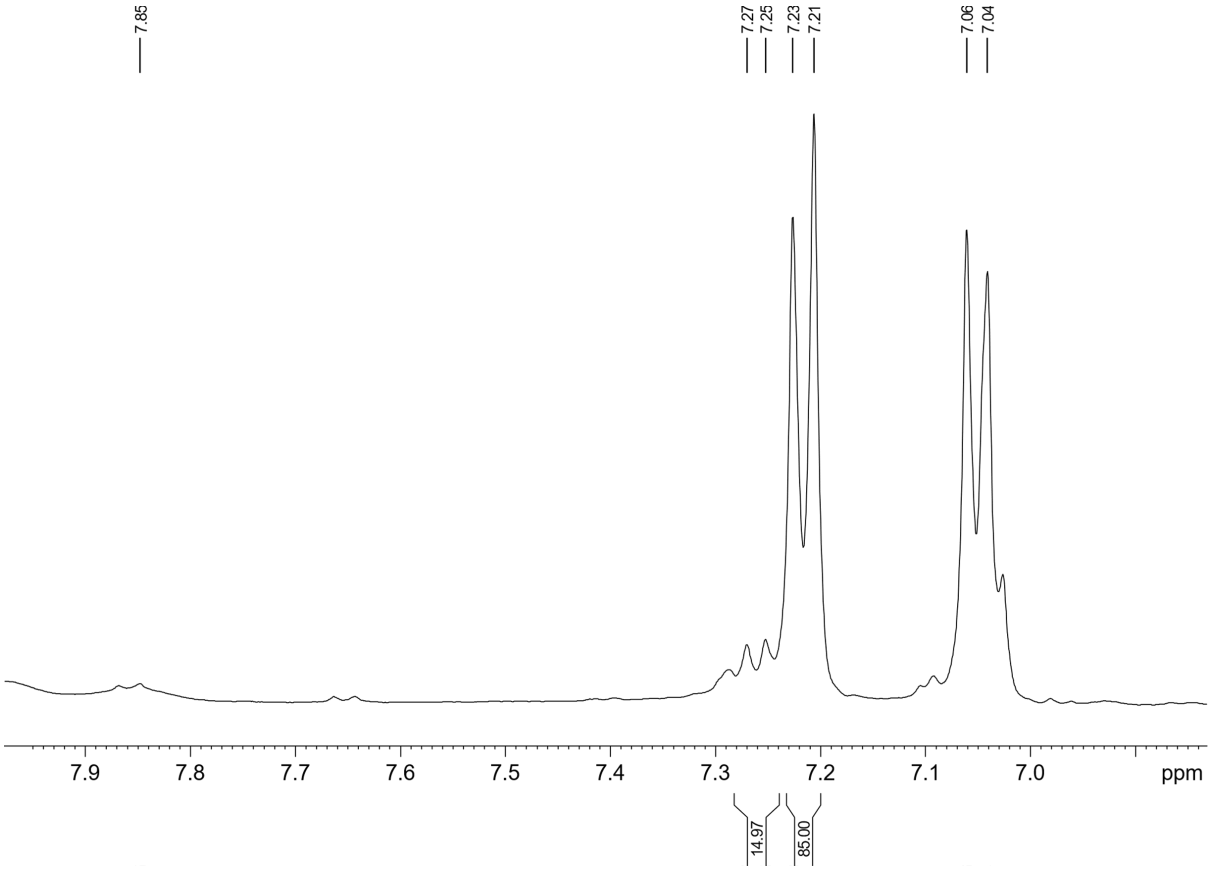

1.28
1.26
0.92
0.90
0.88
0.88
0.86
0.82
0.80
0.79
0.77
1.30 1.25 1.20 1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 0.70 0.65 0.60 0.55 0.50 ppm
31.59
68.00

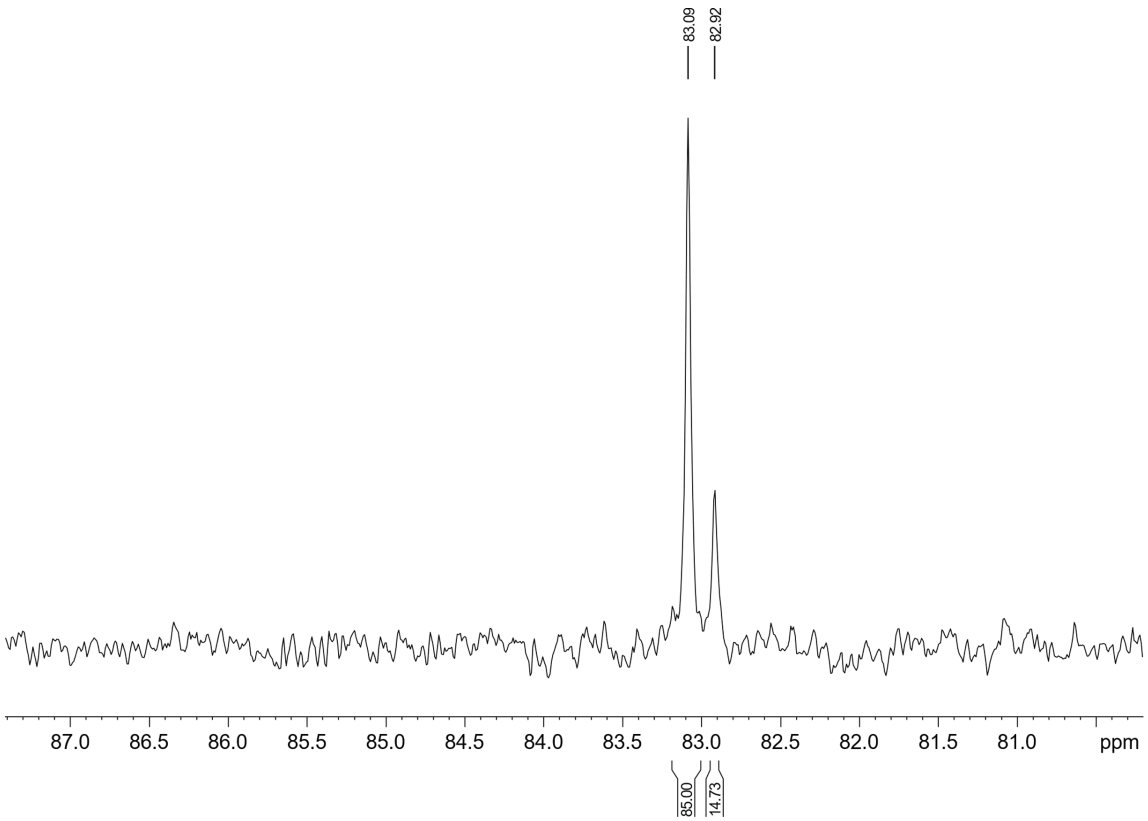

82.50
82.36
85.5
85.0
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
80.5
ppm
72.00
27.99

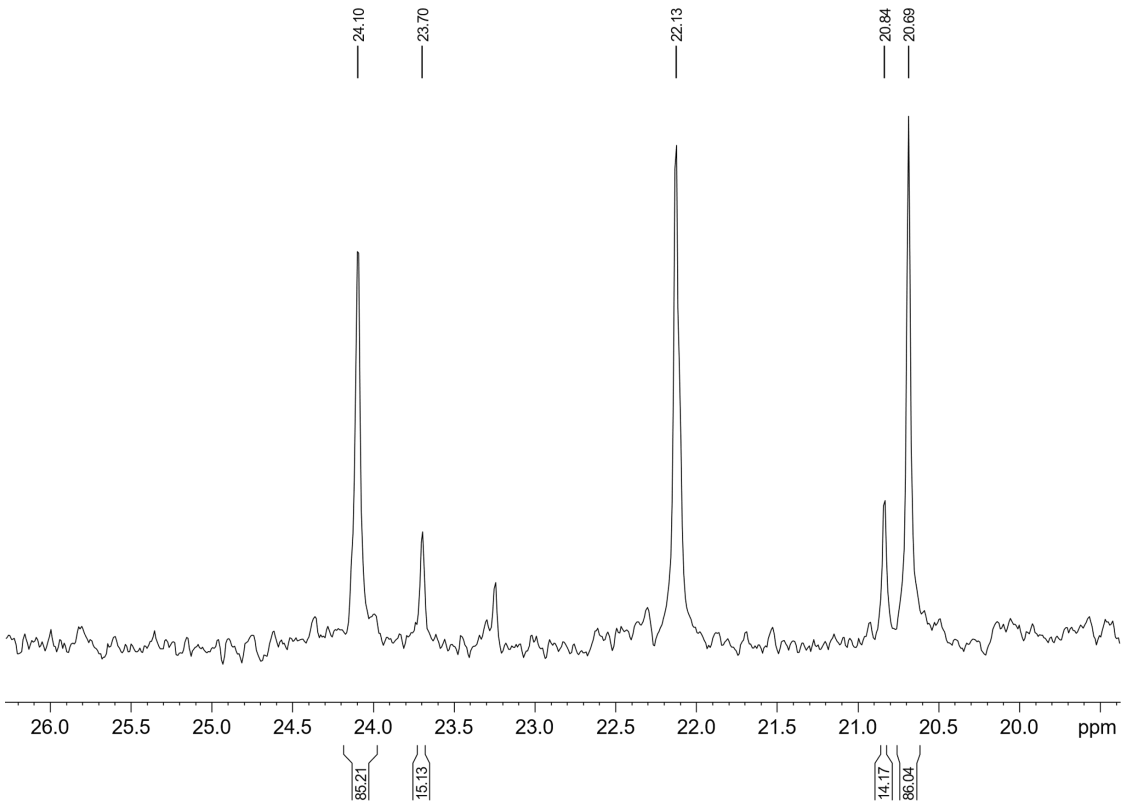

24.11
23.82
22.10
20.75
20.67
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
60.96
22.56
28.12
72.00

Product **14f**

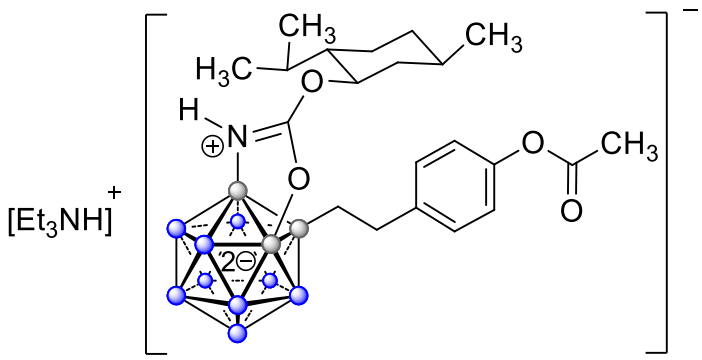

[Et3NH]+
CH3
CH3
H3C
O
H
N
O
CH3
CH3
CH3
2⊖

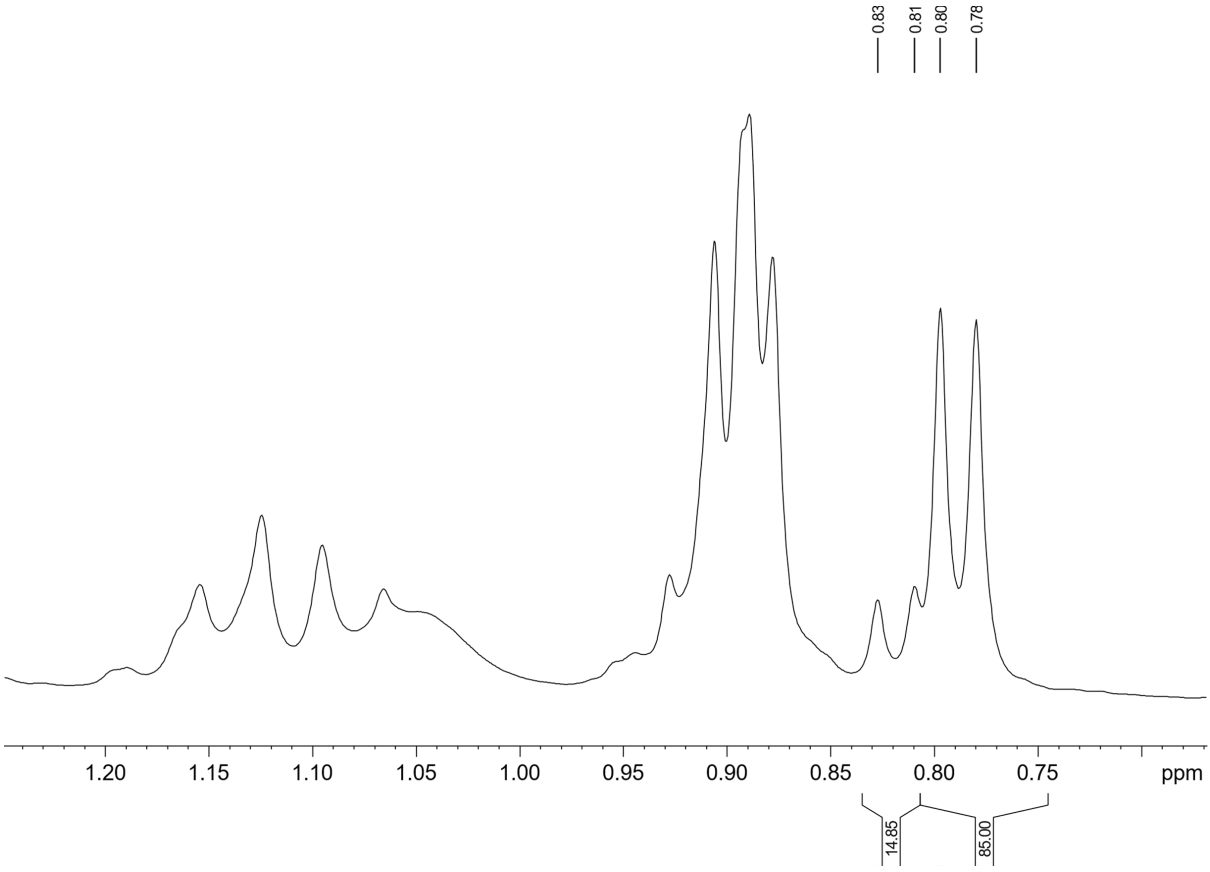

7.85
7.27
7.25
7.23
7.21
7.06
7.04
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
ppm
14.97
85.00

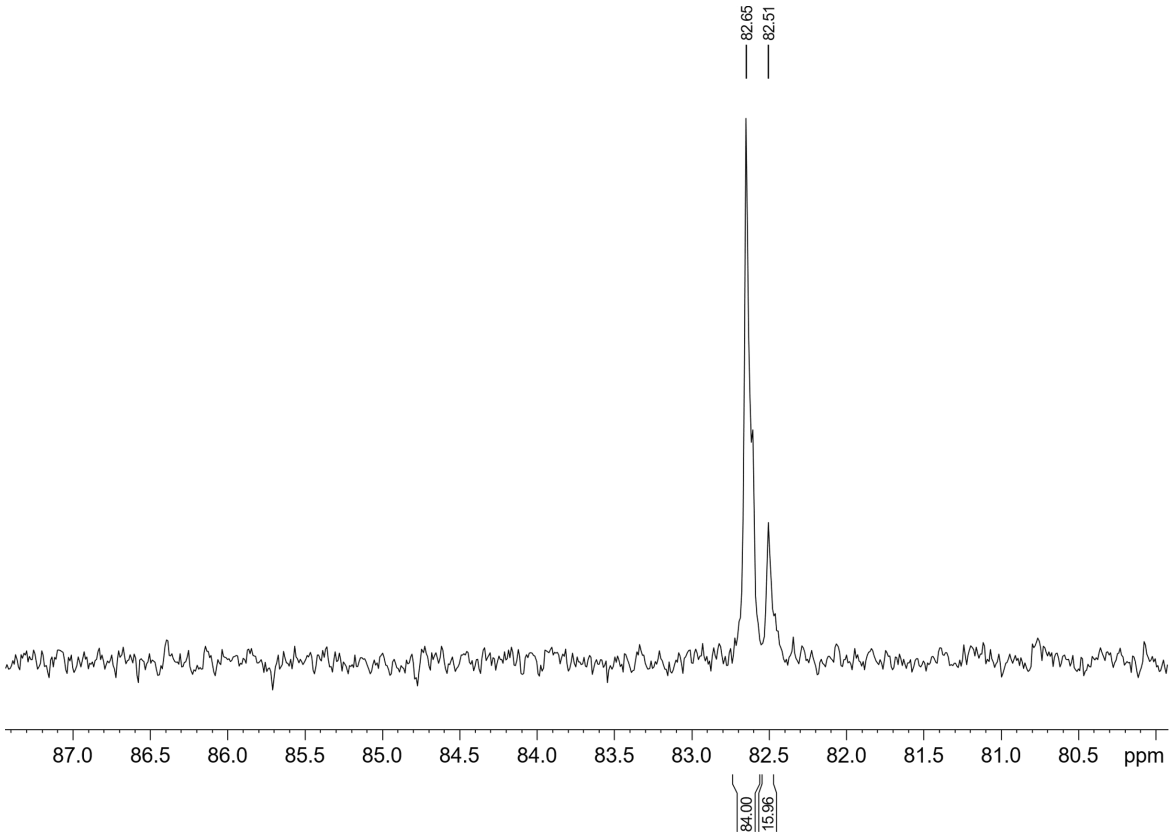

83.09
82.92
87.0
86.5
86.0
85.5
85.0
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
ppm
85.00
14.73

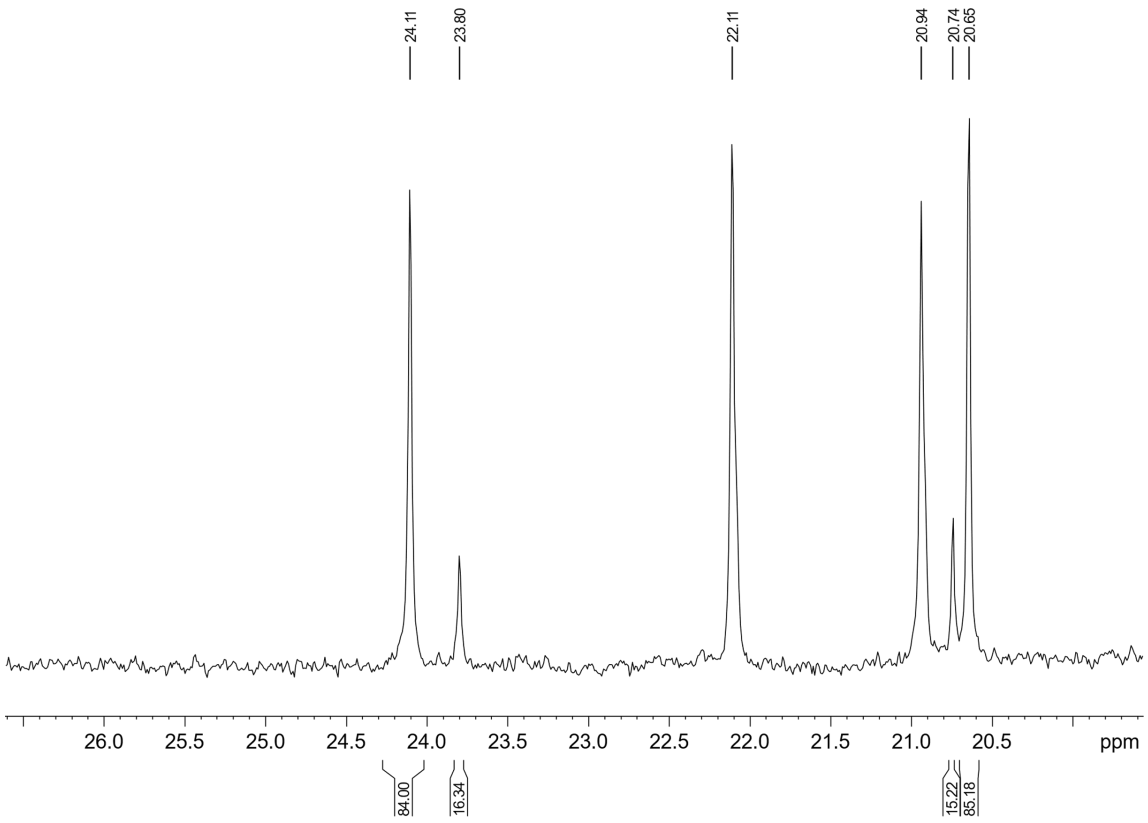

24.10
23.70
22.13
20.84
20.69
26.0
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
20.0
ppm
85.21
15.13
14.17
86.04

Product **14g**

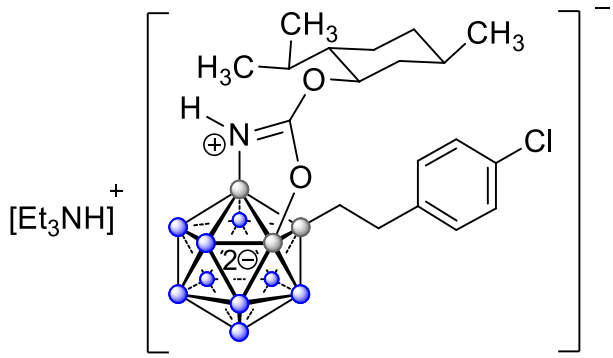

[Et3NH]+
CH3
CH3
H3C
O
H
N
O
O
CH3
O
2⊖

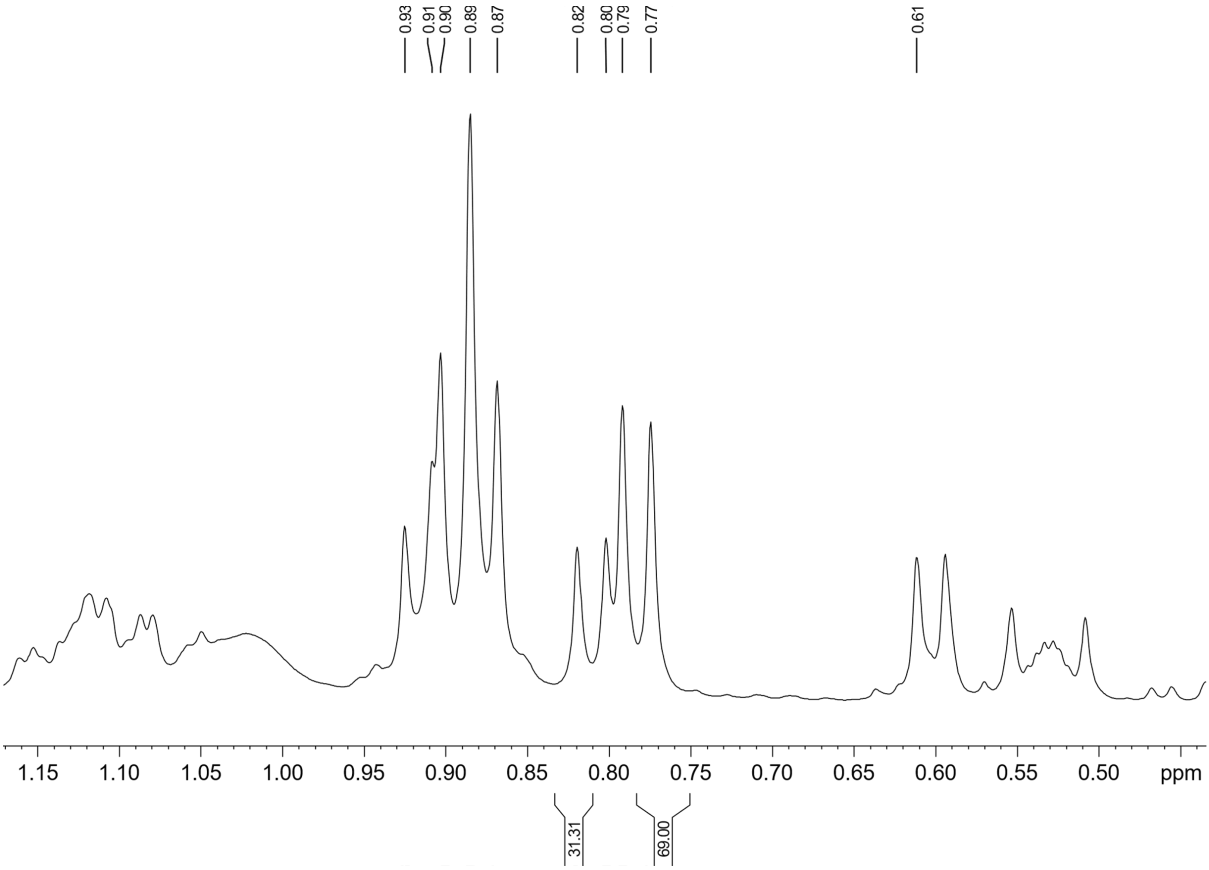

0.83
0.81
0.80
0.78
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
ppm
14.85
85.00

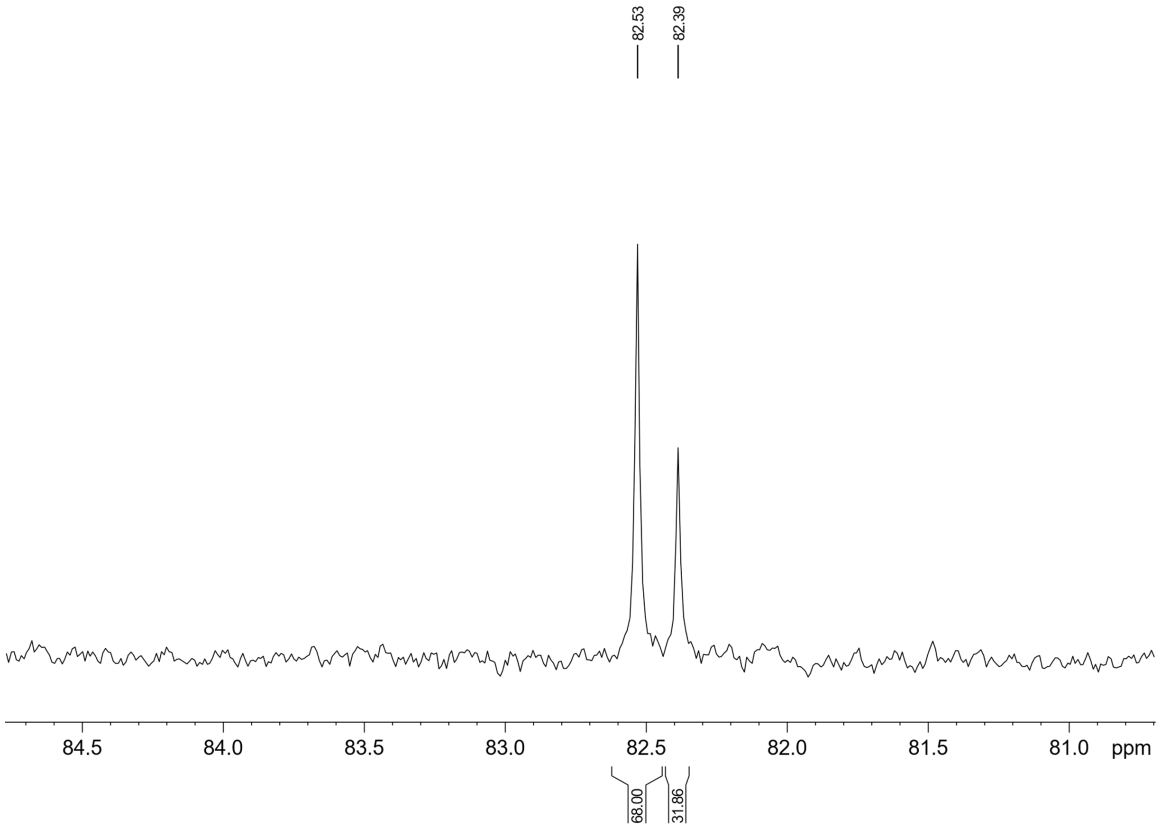

82.65
82.51
87.0
86.5
86.0
85.5
85.0
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
80.5
ppm
84.00
15.96

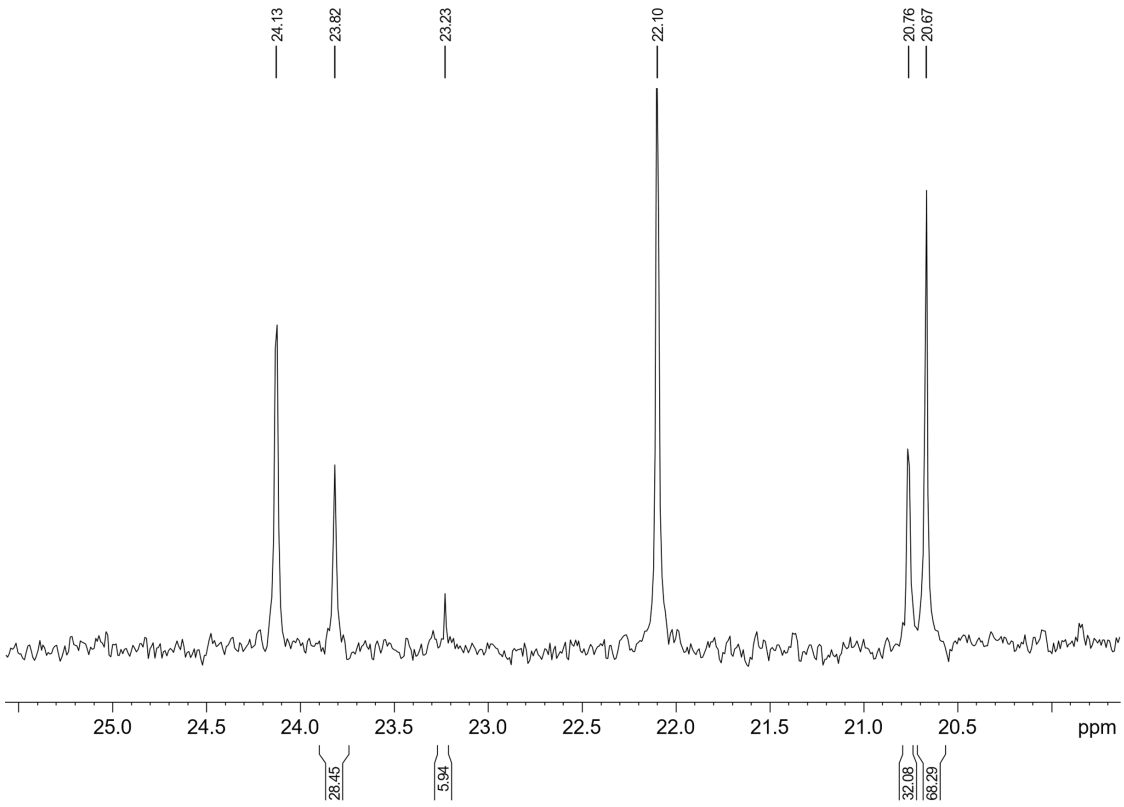

24.11
23.80
22.11
20.94
20.74
20.65
26.0
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
84.00
16.34
15.22
85.18

Product **14h**

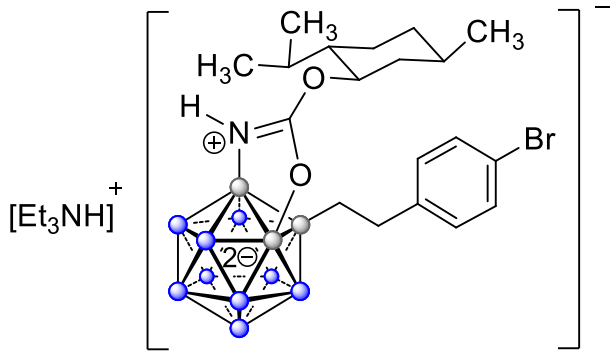

[Et3NH]+
CH3
CH3
H3C
O
H
N
O
Cl
2⊖

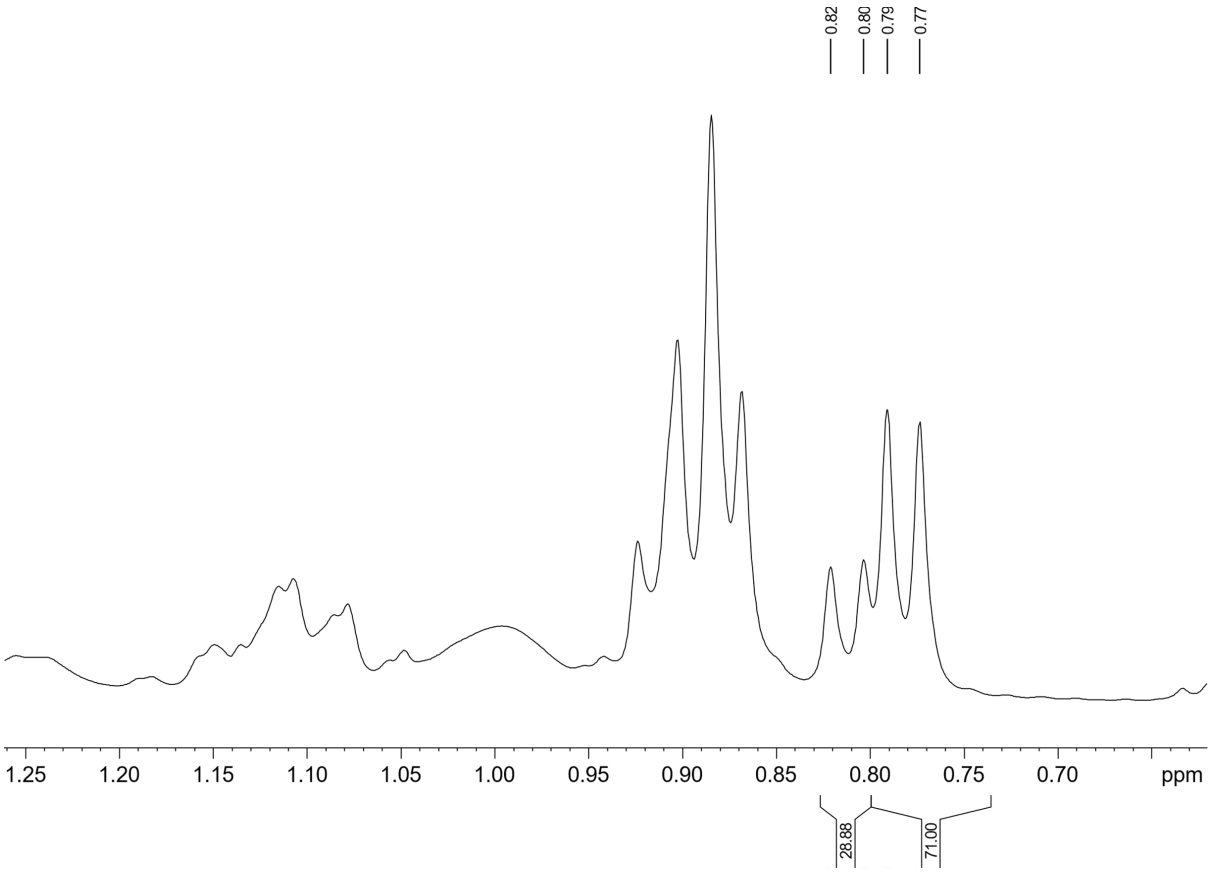

0.93
0.91
0.90
0.89
0.87
0.82
0.80
0.79
0.77
0.61
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
ppm
31.31
69.00

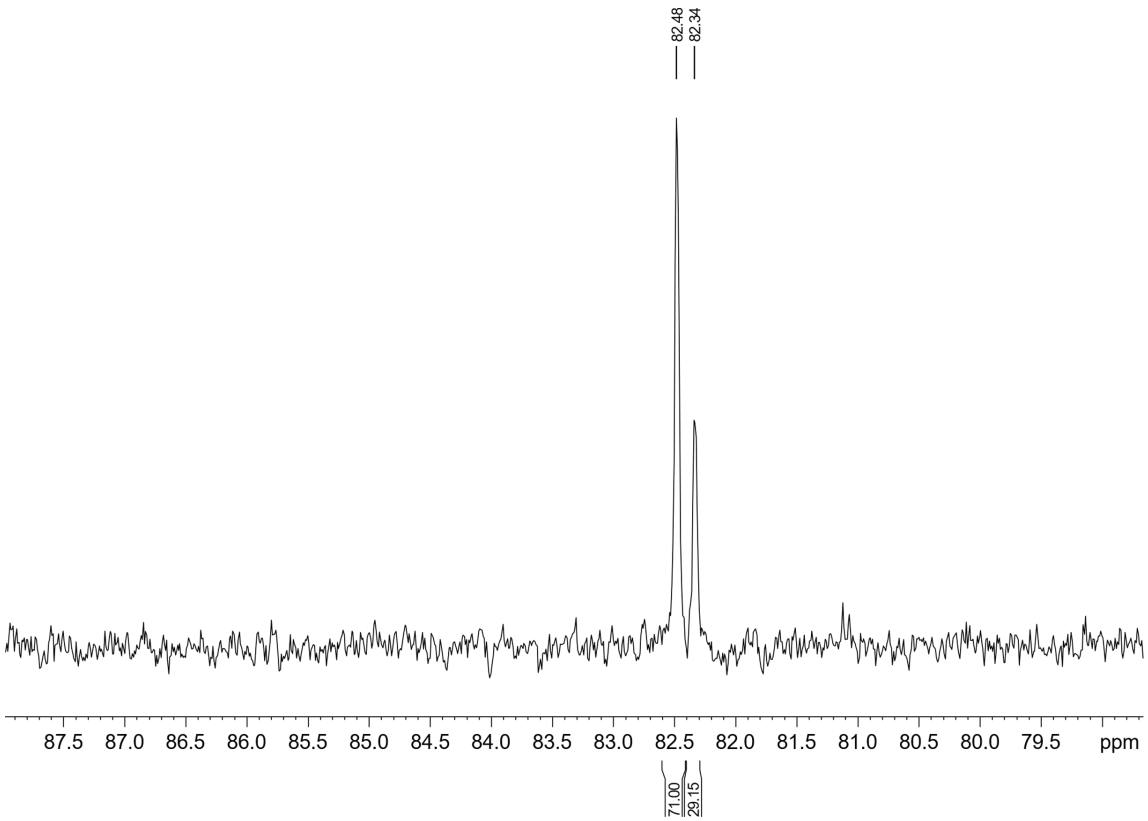

82.53
82.39
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
ppm
68.00
31.86

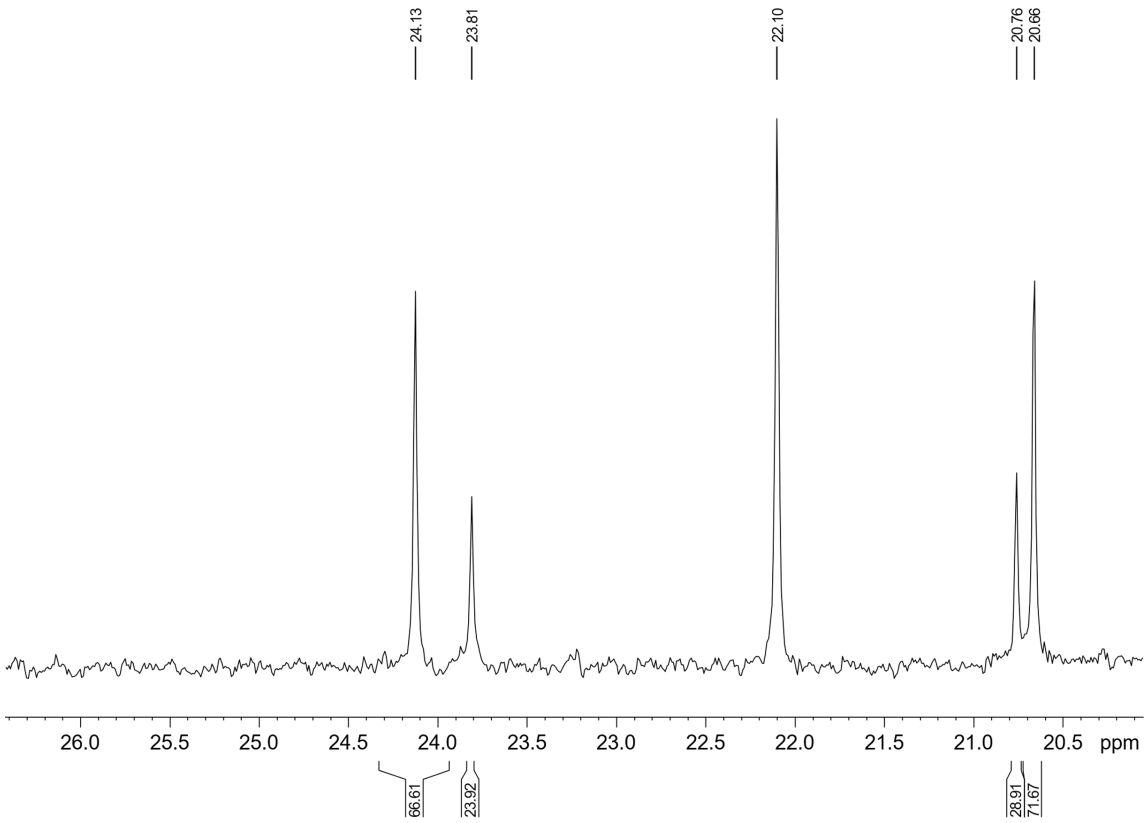

24.13
23.82
23.23
22.10
20.76
20.67
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
28.45
5.94
32.08
68.29

Product **14i**

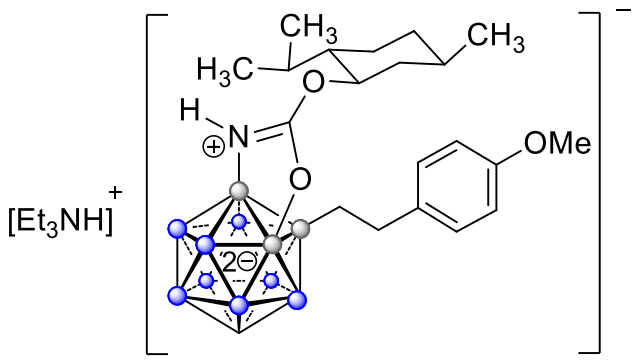

CH3
CH3
H3C
O
H
N
Br
O
2⊖
[Et3NH]+
−

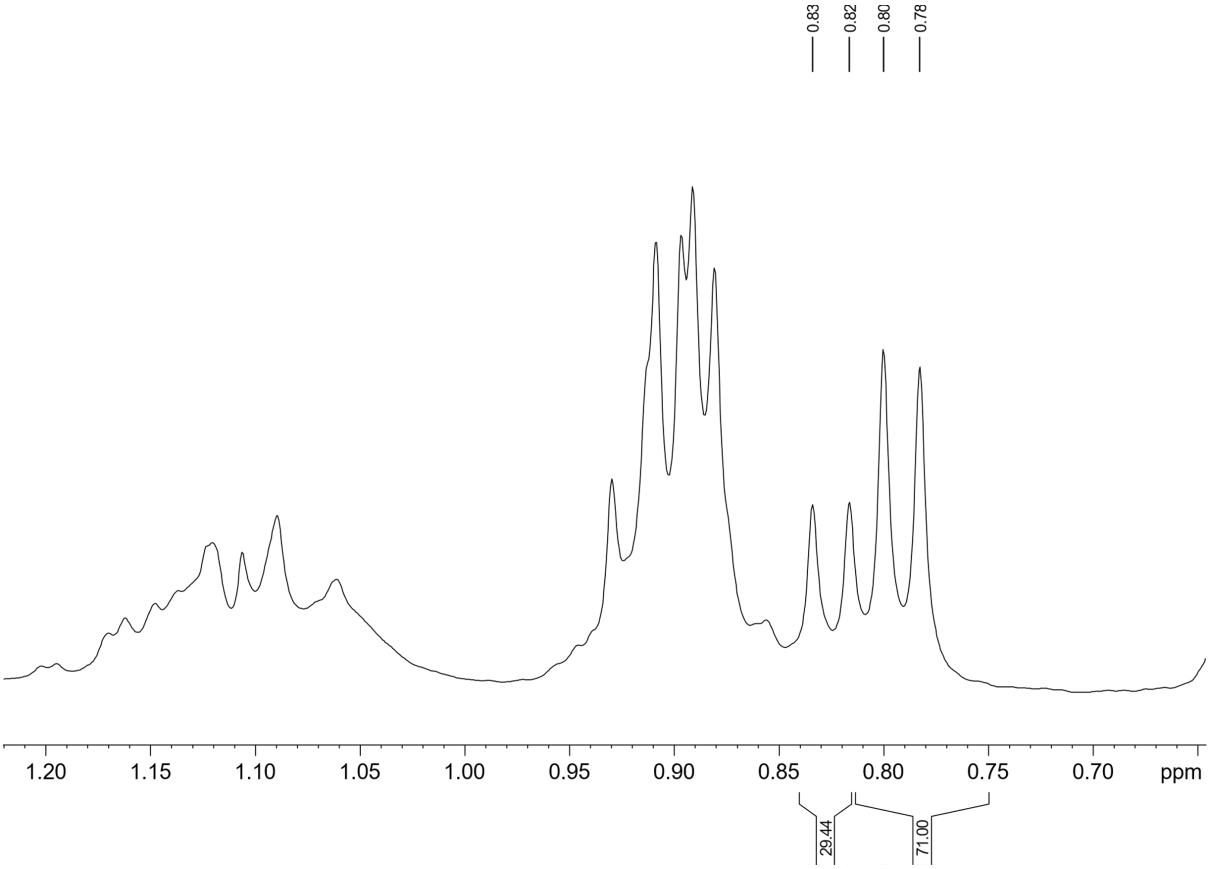

0.82
0.80
0.79
0.77
1.25
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
ppm
28.88
71.00

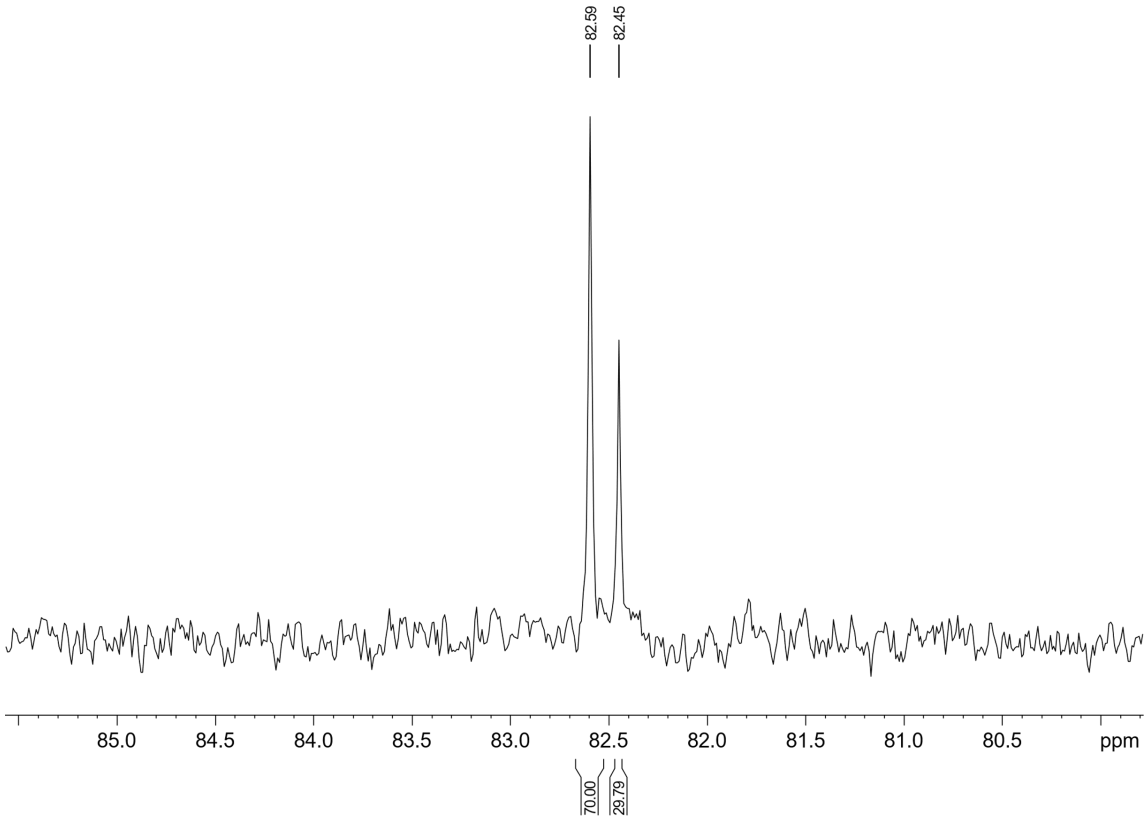

82.48
82.34
87.5 87.0 86.5 86.0 85.5 85.0 84.5 84.0 83.5 83.0 82.5 82.0 81.5 81.0 80.5 80.0 79.5 ppm
71.00
29.15

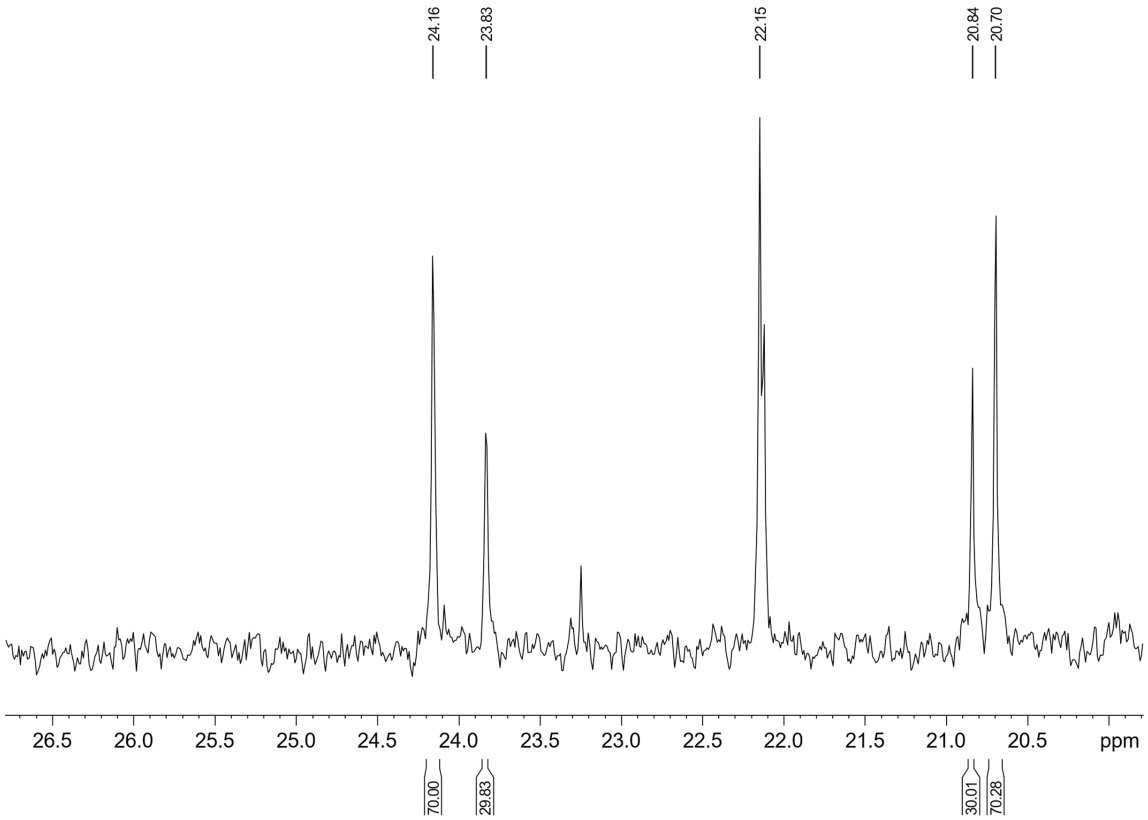

24.13
23.81
22.10
20.76
20.66
26.0 25.5 25.0 24.5 24.0 23.5 23.0 22.5 22.0 21.5 21.0 20.5 ppm
66.61
23.92
28.91
71.67

Product **14j**

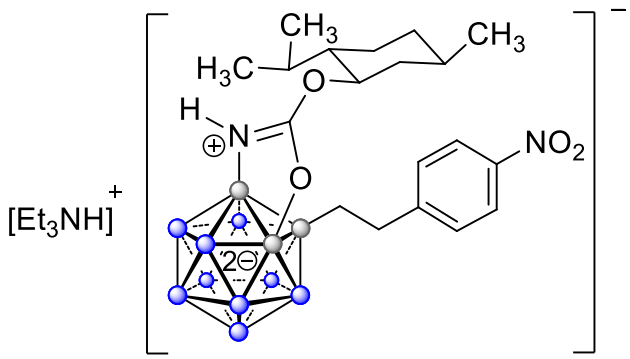

[Et3NH]+
CH3
CH3
H3C
O
H
N
OMe
O
2⊖

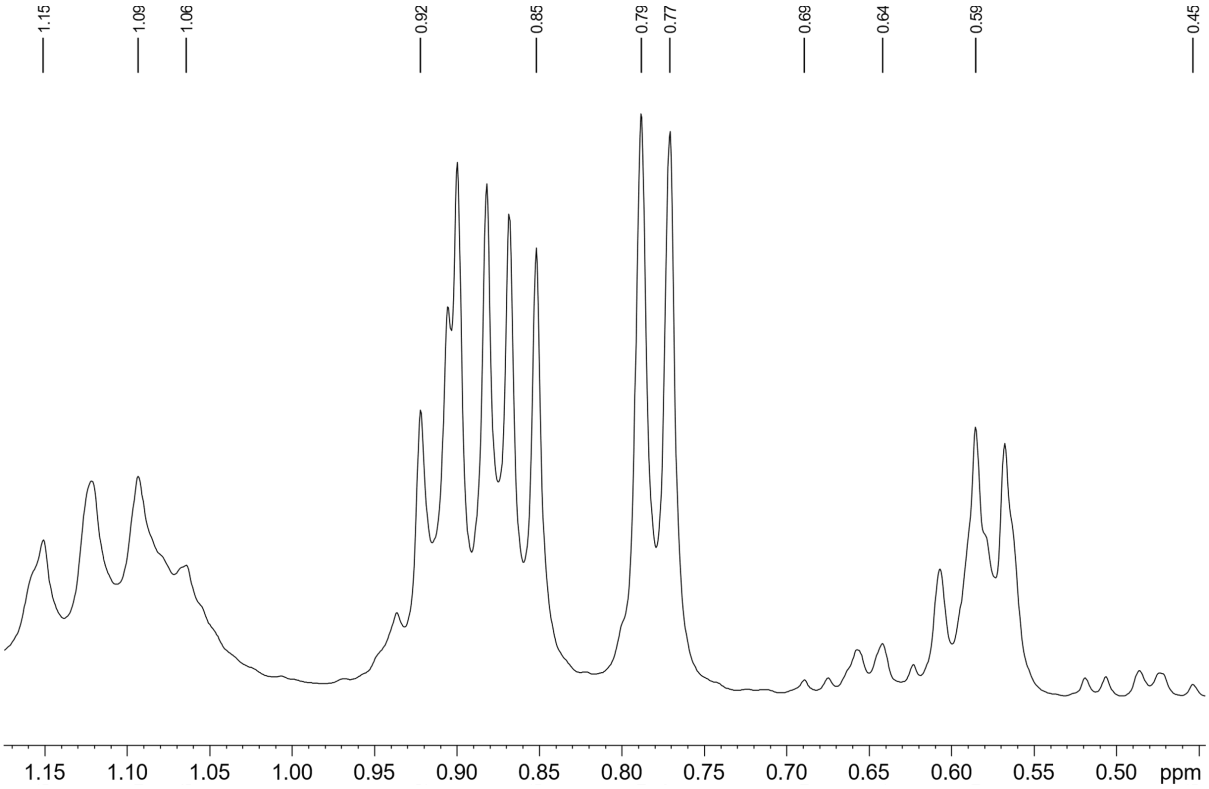

0.83
0.82
0.80
0.78
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
ppm
29.44
71.00

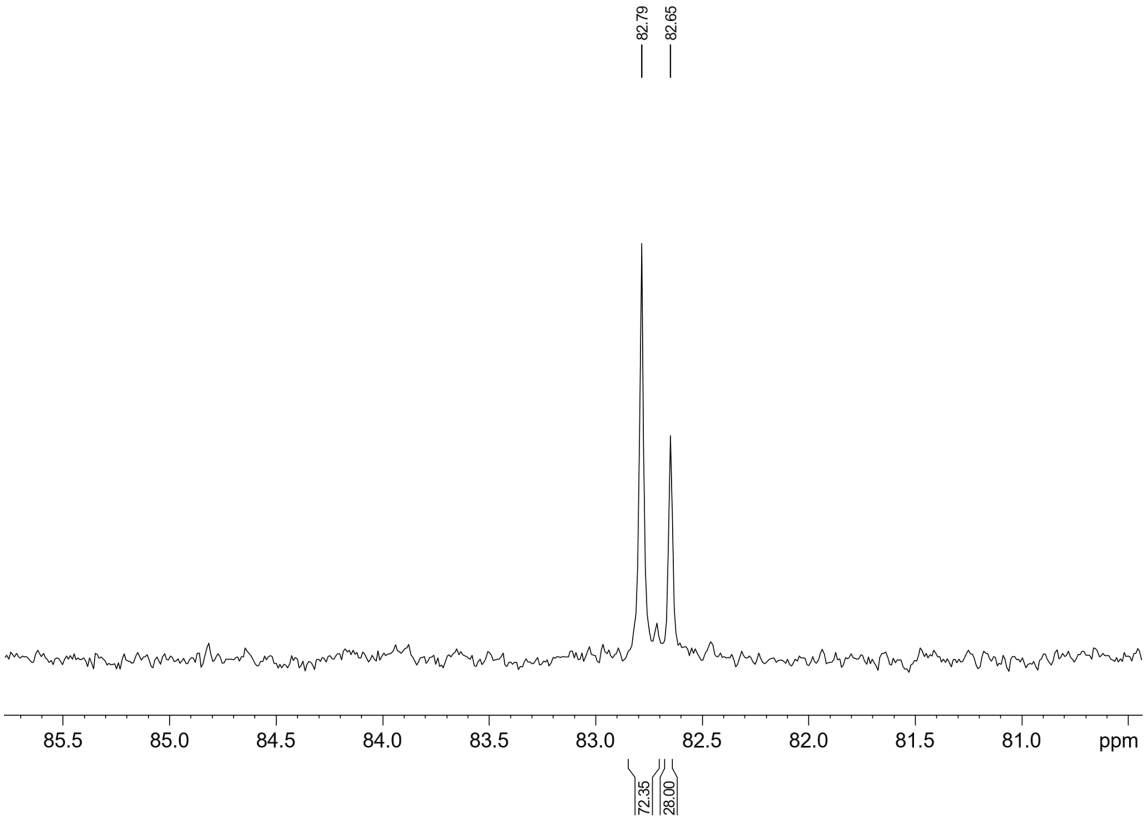

82.59
82.45
85.0
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
80.5
ppm
70.00
29.79

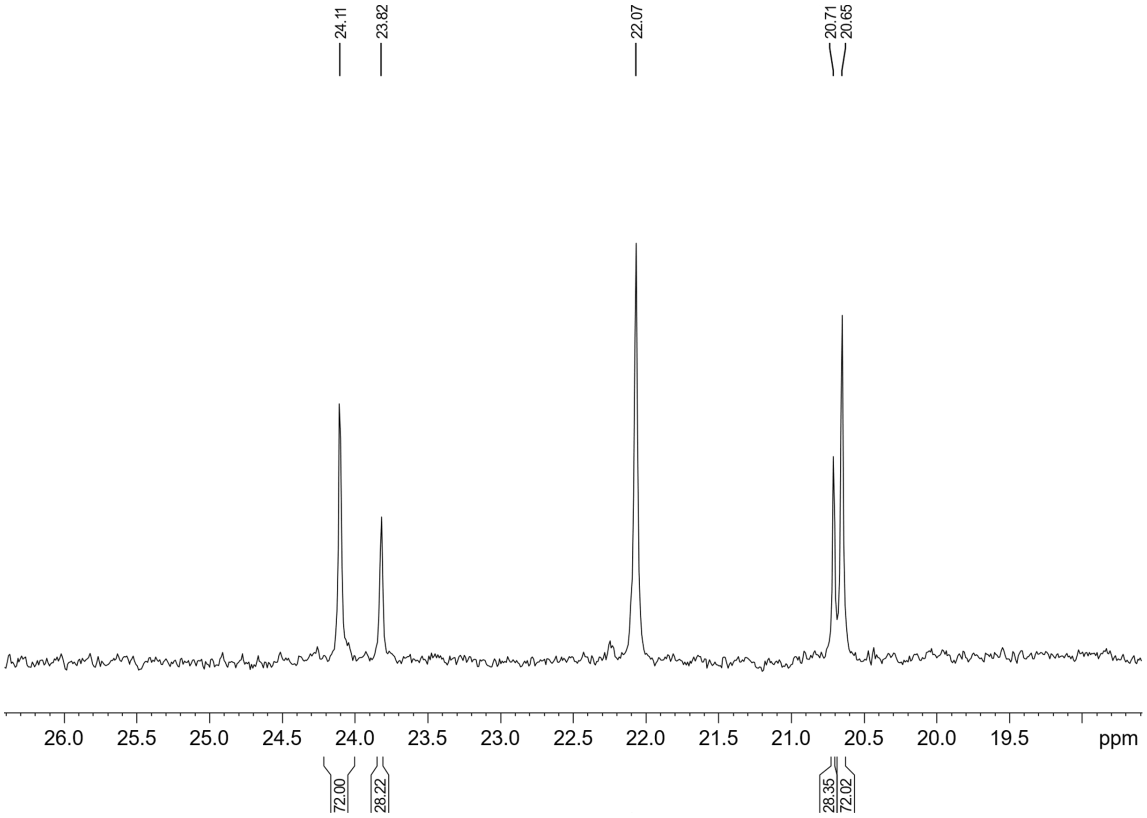

24.16
23.83
22.15
20.84
20.70
26.5
26.0
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
70.00
29.83
30.01
70.28

Product **14k**

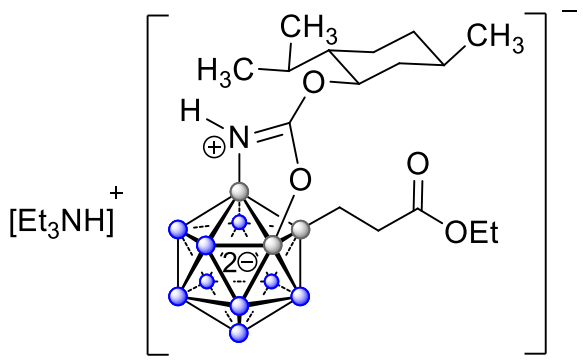

CH3
CH3
H3C
O
H
N
O
NO2
O
2⊖
[Et3NH]+
−

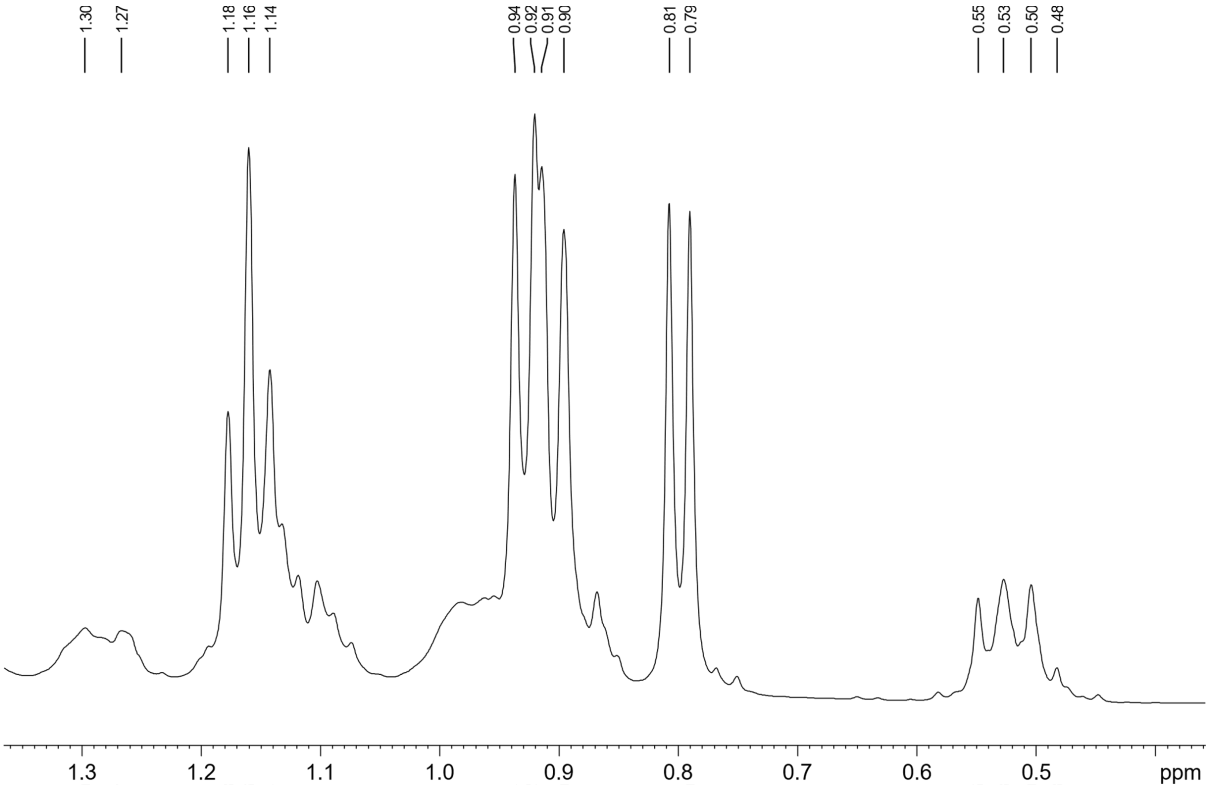

1.15
1.09
1.06
0.92
0.85
0.79
0.77
0.69
0.64
0.59
0.45
1.15 1.10 1.05 1.00 0.95 0.90 0.85 0.80 0.75 0.70 0.65 0.60 0.55 0.50 ppm

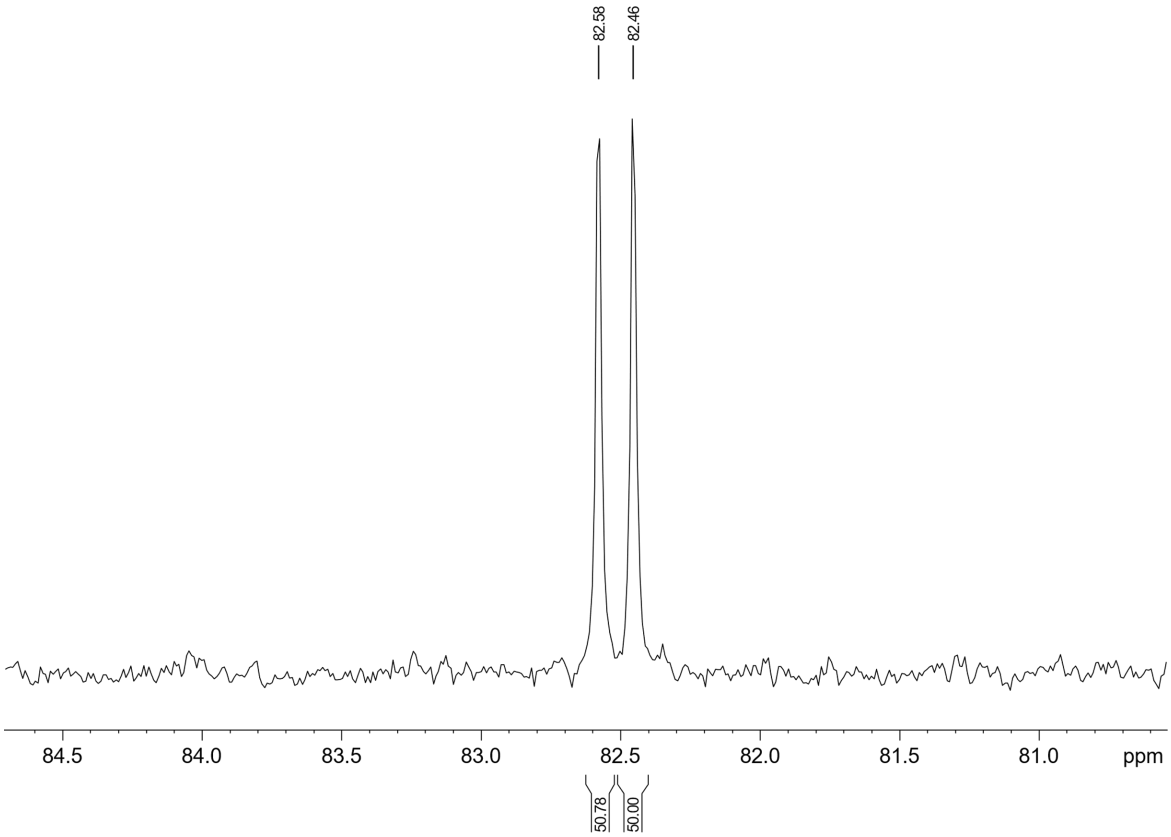

82.79
82.65
85.5
85.0
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
ppm
72.35
28.00

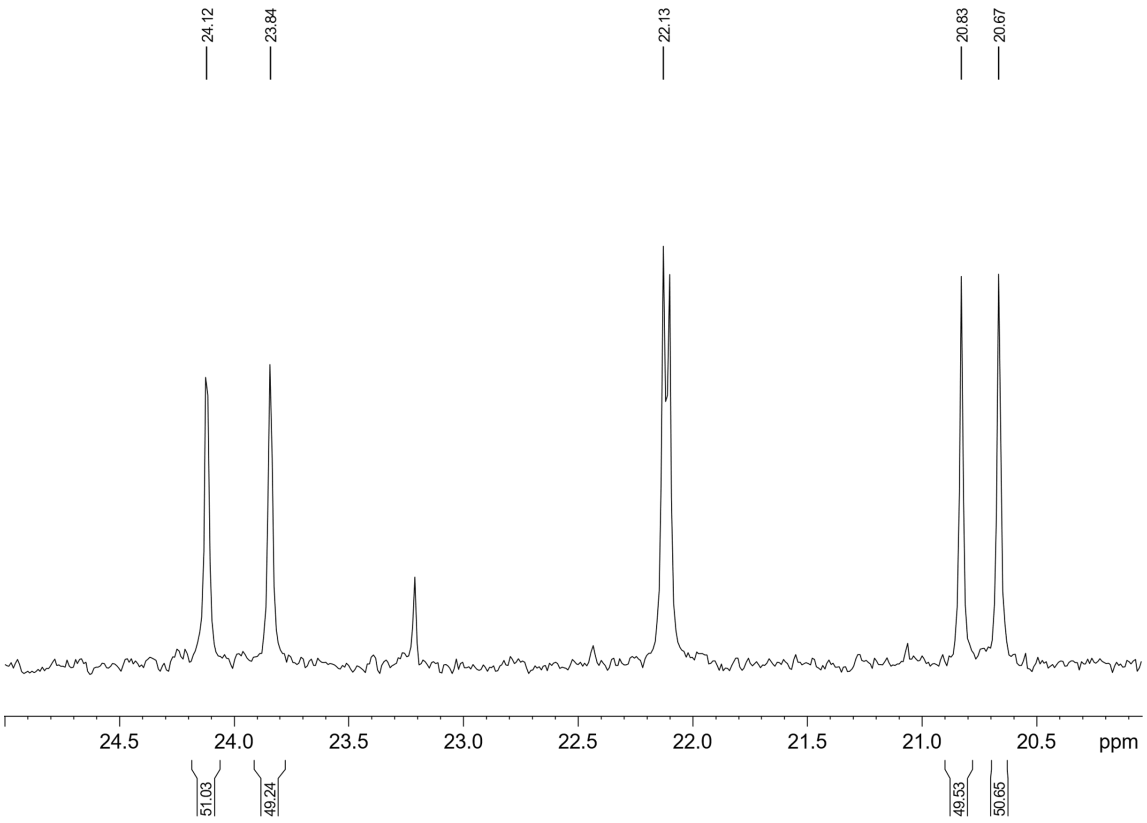

24.11
23.82
22.07
20.71
20.65
26.0
25.5
25.0
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
20.0
19.5
ppm
72.00
28.22
28.35
72.02

Product **14l**

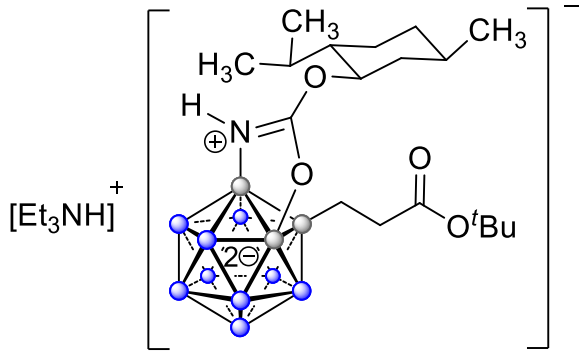

CH3
CH3
H3C
O
H
N
O
O
OEt
2⊖
[Et3NH]+
−

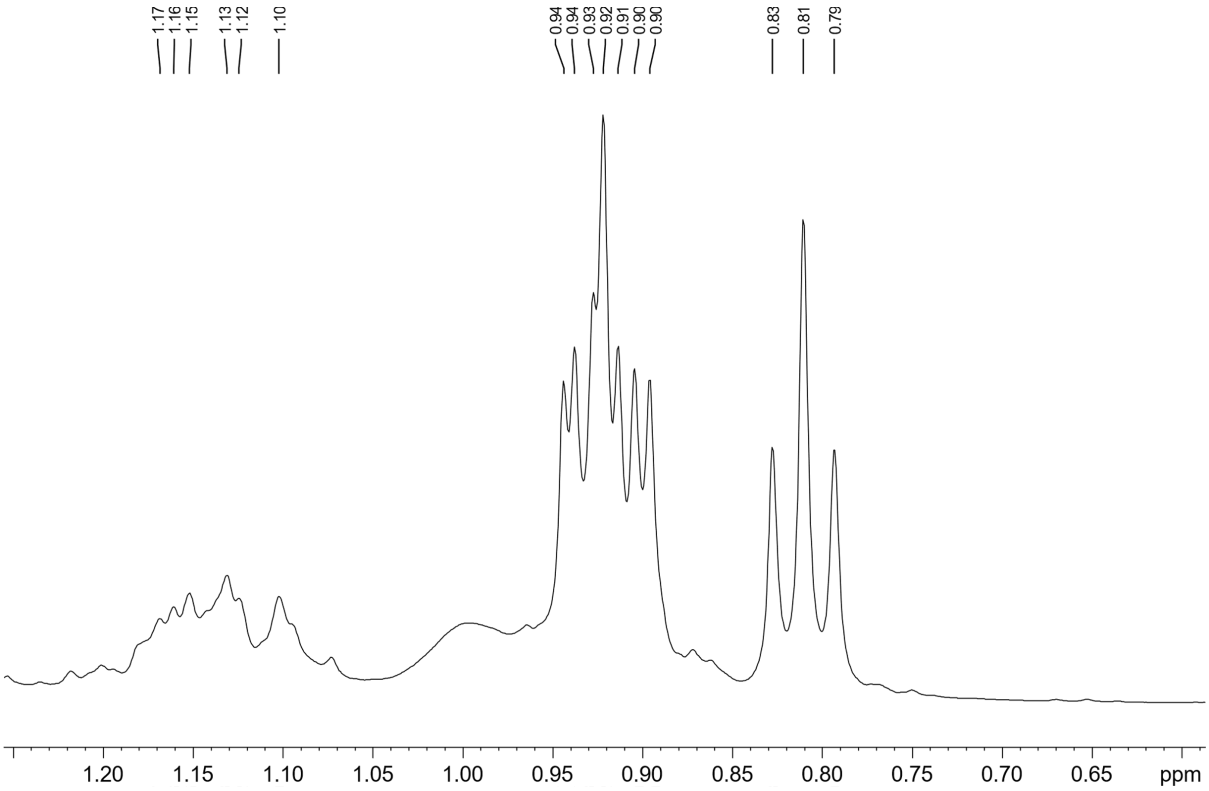

1.30
1.27
1.18
1.16
1.14
0.94
0.92
0.91
0.90
0.81
0.79
0.55
0.53
0.50
0.48
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0.6
0.5
ppm


82.58
82.46
84.5
84.0
83.5
83.0
82.5
82.0
81.5
81.0
ppm
50.78
50.00


24.12
23.84
22.13
20.83
20.67
24.5
24.0
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
51.03
49.24
49.53
50.65

Product **14m**


[Et3NH]+
CH3
CH3
H3C
O
H
N
O
O
OtBu
2⊖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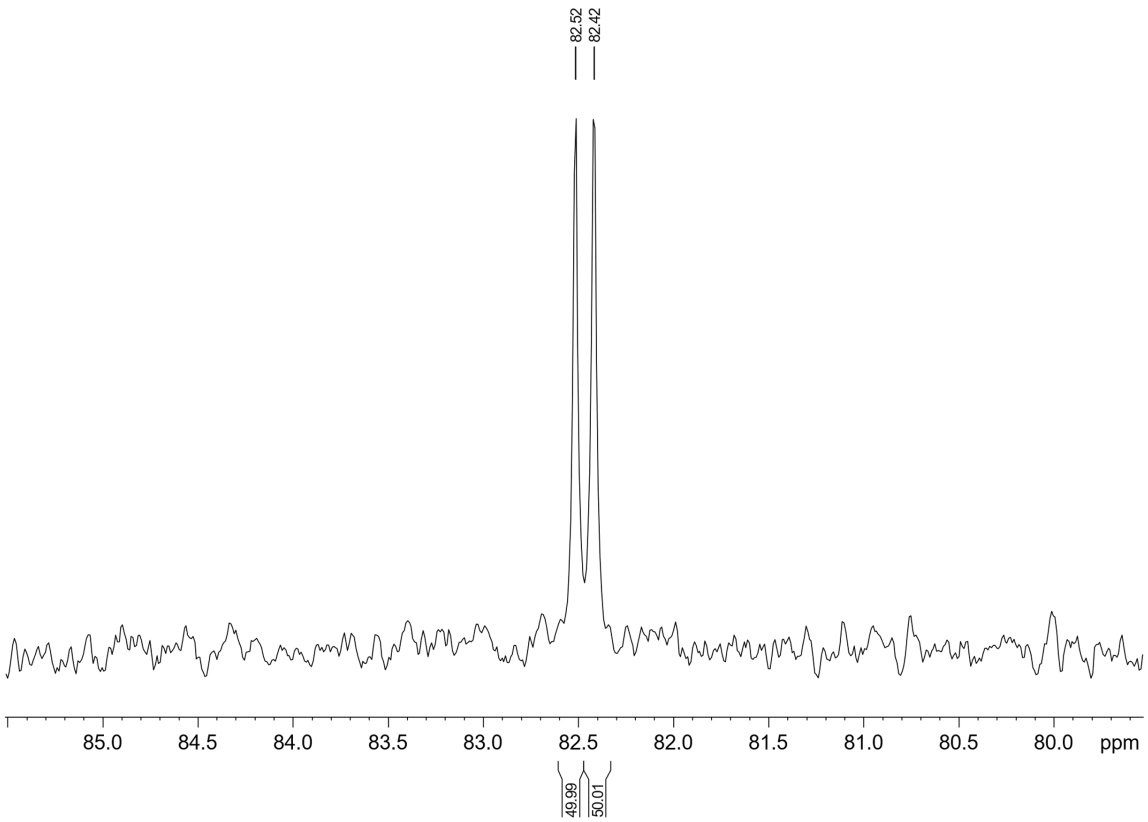
1.16
1.15
1.13
1.12
1.10
0.94
0.94
0.93
0.92
0.91
0.90
0.90
0.83
0.81
0.79
1.20
1.15
1.10
1.05
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
ppm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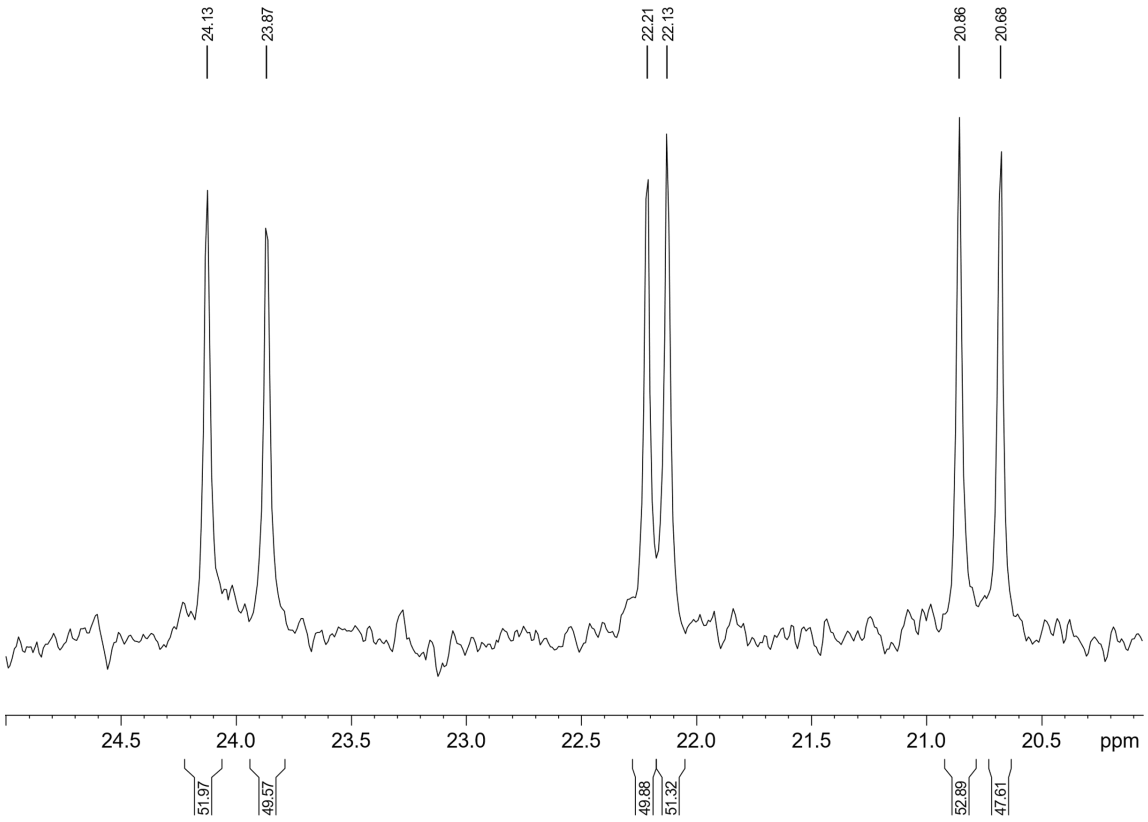
82.5
82.0
81.5
81.0
80.5
80.0
ppm
49.99
50.01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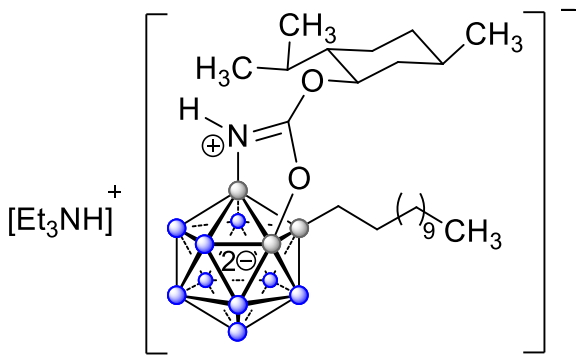
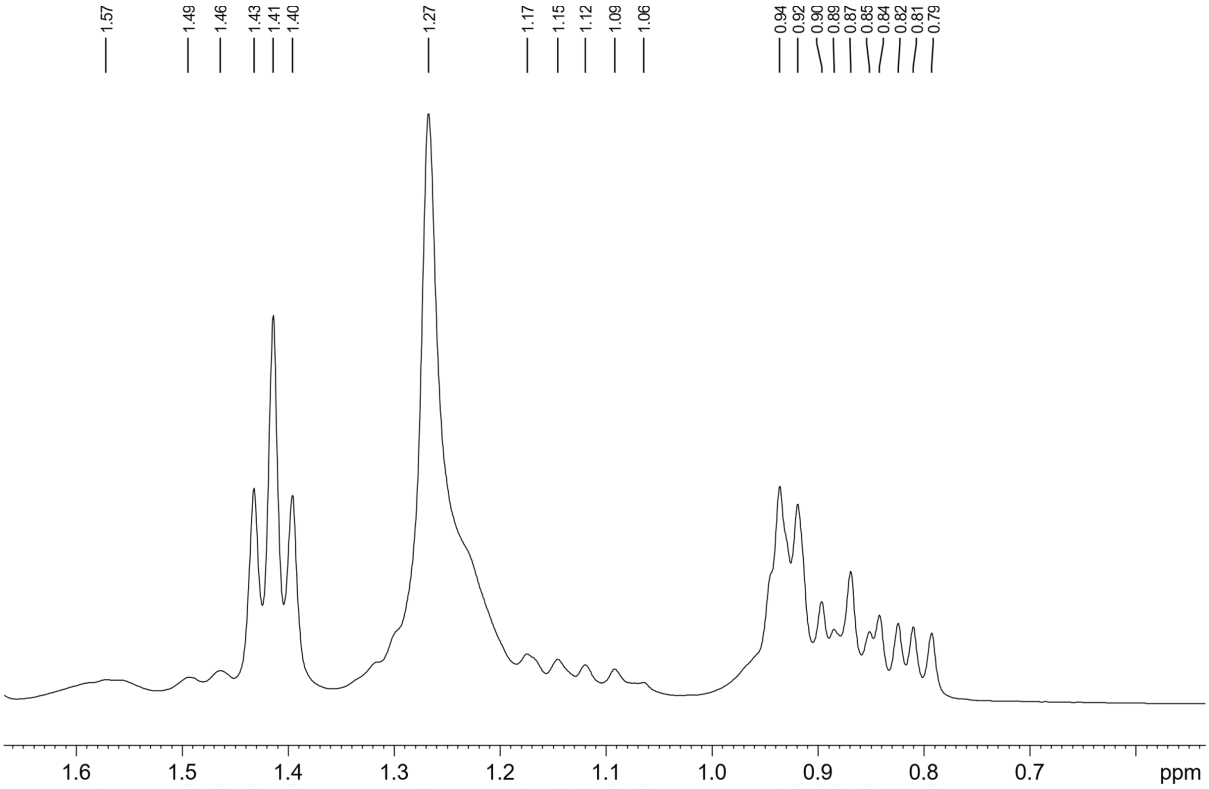
23.5
23.0
22.5
22.0
21.5
21.0
20.5
ppm
51.97
49.57
49.88
51.32
52.89
47.61

Product **14n**


CH3
CH3
H3C
O
H
N
O
9
CH3
2⊖
[Et3NH]+
−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1.43
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1.27
1.17
1.15
1.12
1.09
1.06
0.94
0.92
0.90
0.89
0.87
0.85
0.84
0.82
0.81
0.79
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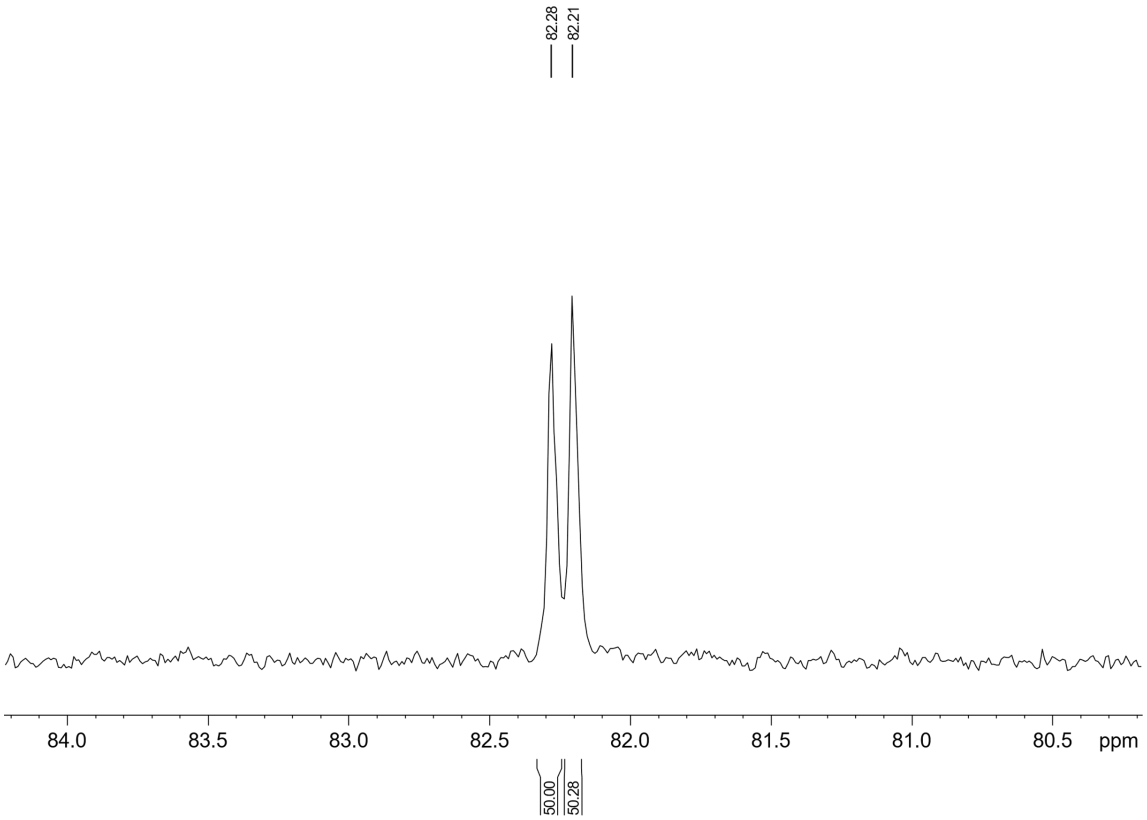
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
ppm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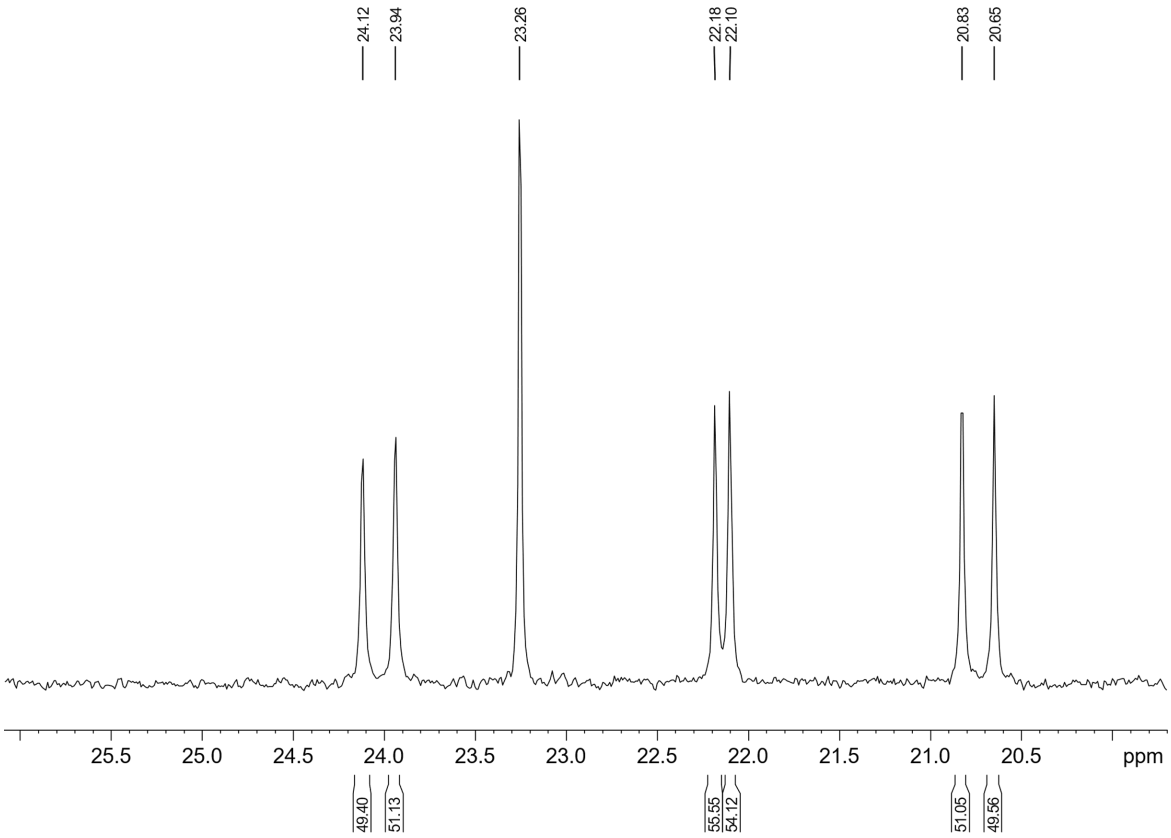
82.5
82.0
81.5
81.0
80.5
ppm
50.00
50.28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20.65
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24.0
23.5
23.0
22.5
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21.5
21.0
20.5
ppm
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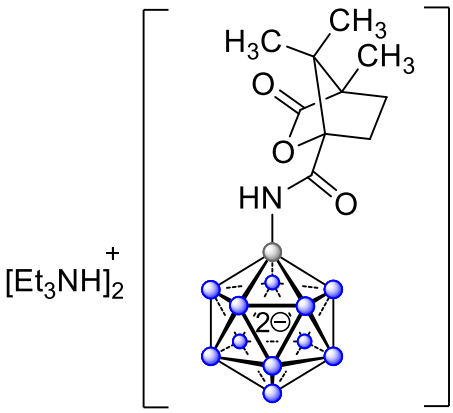
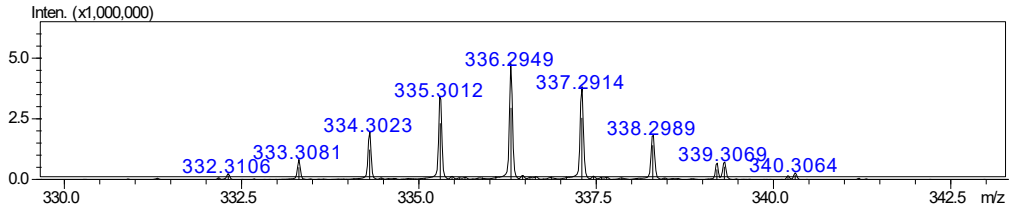
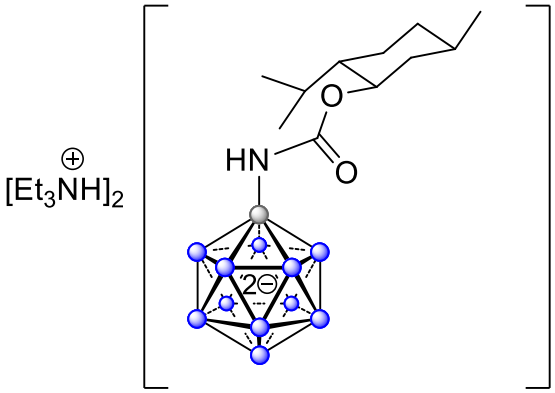
51.13
55.55
54.12
51.05
49.56



High resolution ESI-MS (negative mode, MeOH):

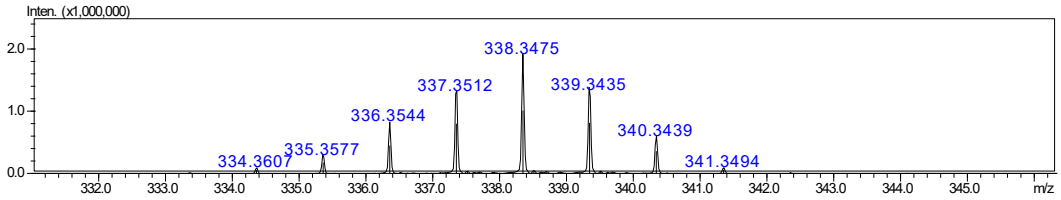
for $[C_{10}H_{25}B_{12}NO_3 - H]^-$: 336.2945; Found: 336.2949.

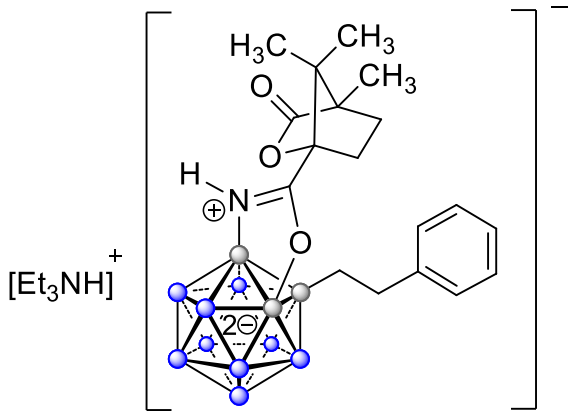




High resolution ESI-MS (negative mode, MeOH):

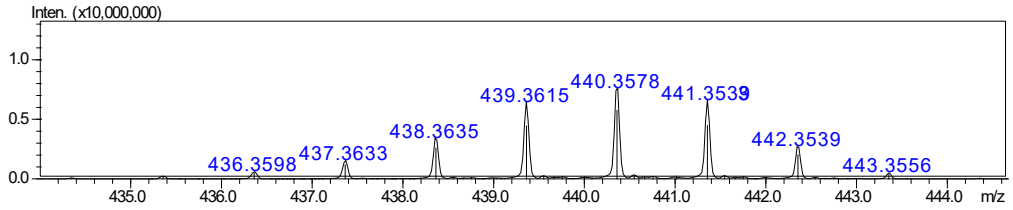
m/*z* calcd for $[C_{11}H_{31}B_{12}NO_2 - H]^-$: 338.3465; Found: 338.3475

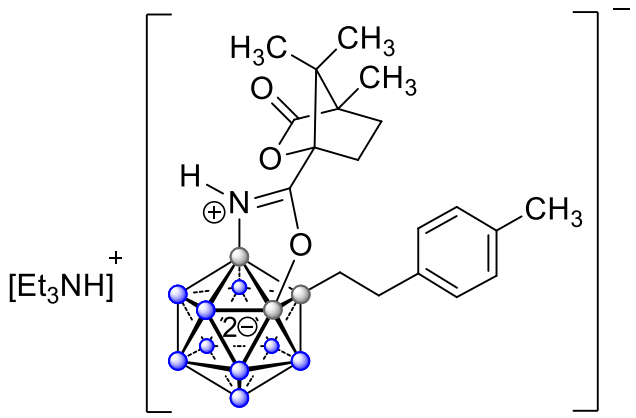




High resolution ESI-MS (negative mode, MeOH):

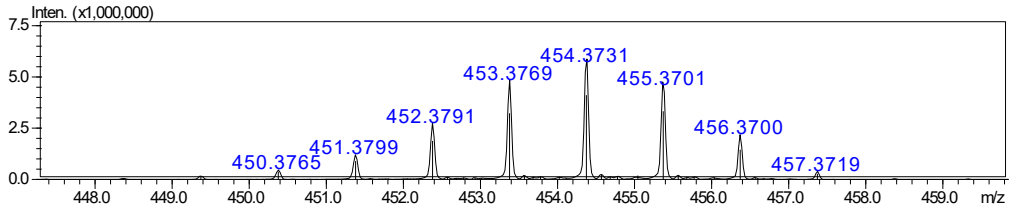
for $[C_{18}H_{32}B_{12}NO_3]^-$: 440.3571; Found: 440.3578.

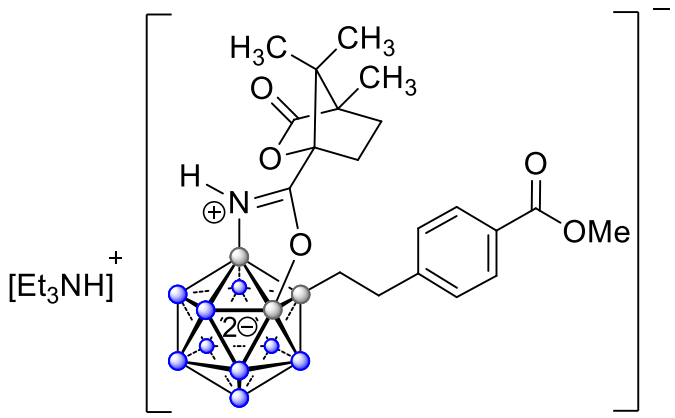




High resolution ESI-MS (negative mode, MeOH):

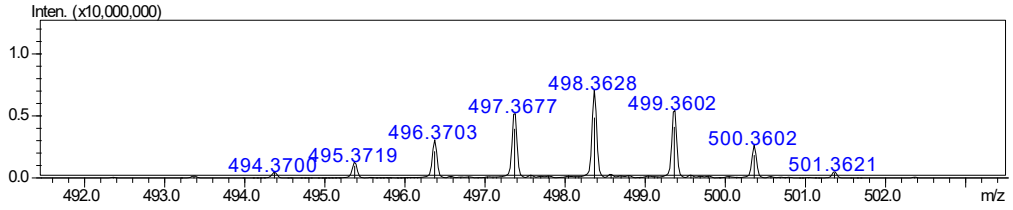
for $[C_{19}H_{34}B_{12}NO_3]^-$: 454.3728; Found: 454.3731.

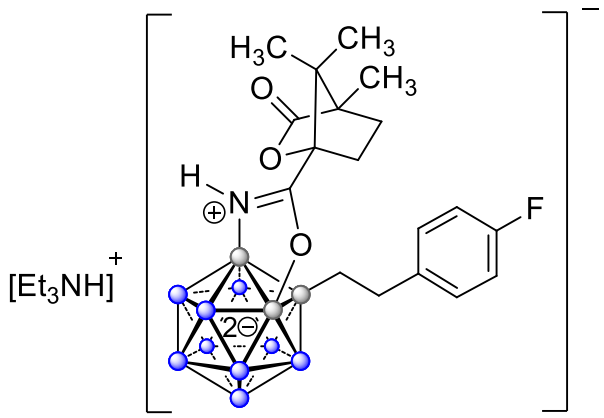




High resolution ESI-MS (negative mode, MeOH):

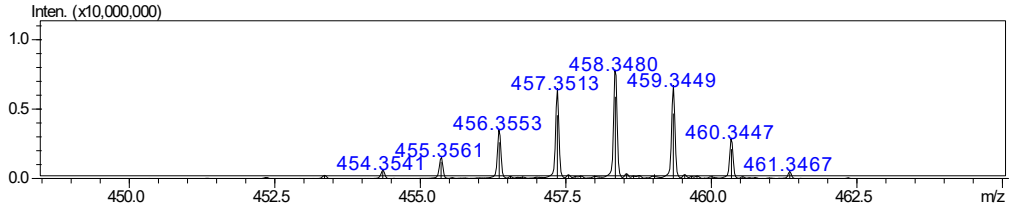
for $[C_{20}H_{34}B_{12}NO_5]^-$: 498.3626; Found: 498.3628.

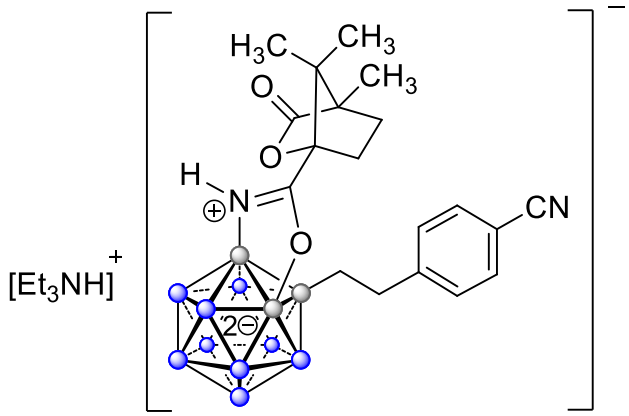




High resolution ESI-MS (negative mode, MeOH):

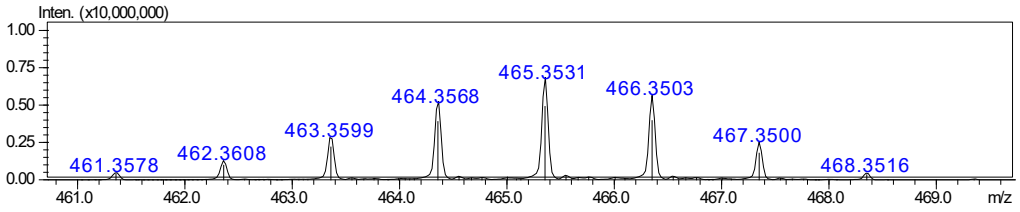
for $[C_{18}H_{31}B_{12}FNO_3]^-$: 458.3477; Found: 458.3480.

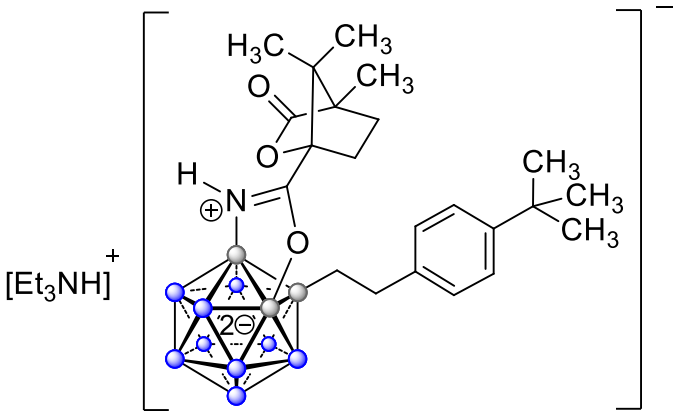




High resolution ESI-MS (negative mode, MeOH):

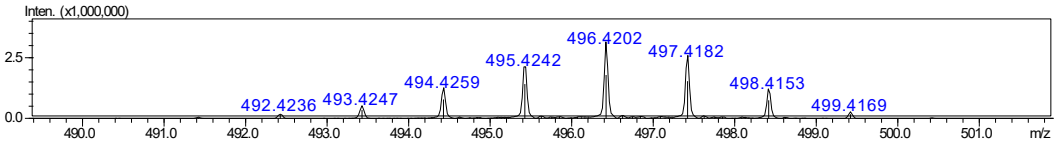
for $[C_{19}H_{31}B_{12}N_2O_3]^-$: 465.3524; Found: 465.3531.

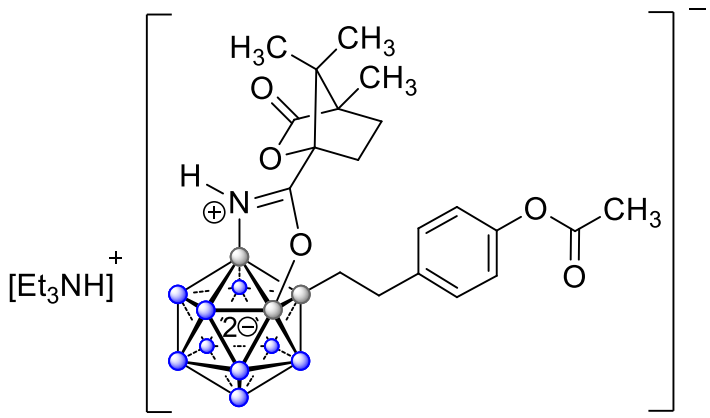




High resolution ESI-MS (negative mode, MeOH):

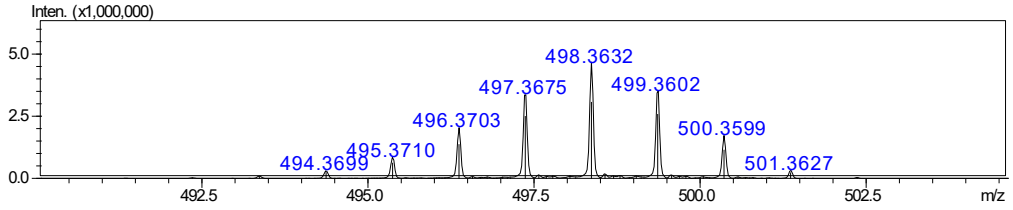
for $[C_{22}H_{40}B_{12}NO_3]^-$: 496.4197; Found: 496.4202.

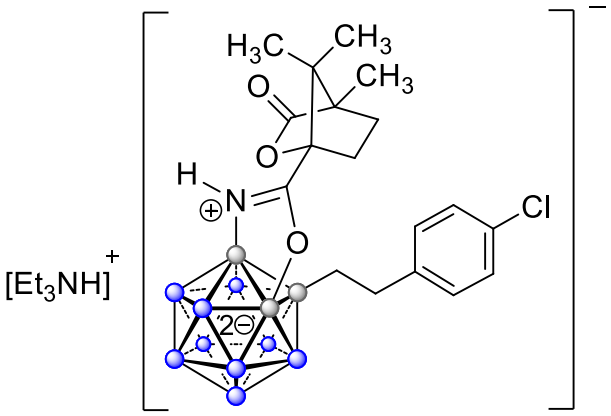




High resolution ESI-MS (negative mode, MeOH):

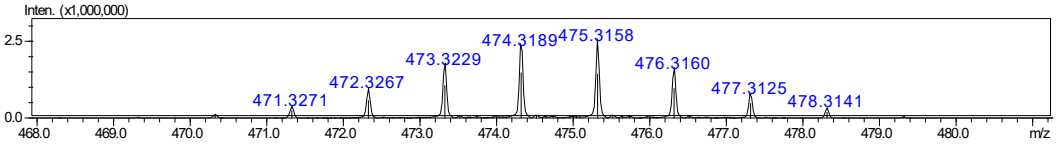
for $[C_{20}H_{34}B_{12}NO_5]^-$: 498.3626; Found: 498.3632.

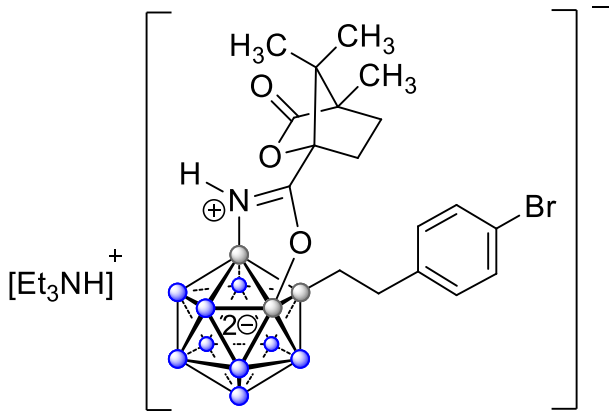




High resolution ESI-MS (negative mode, MeOH):

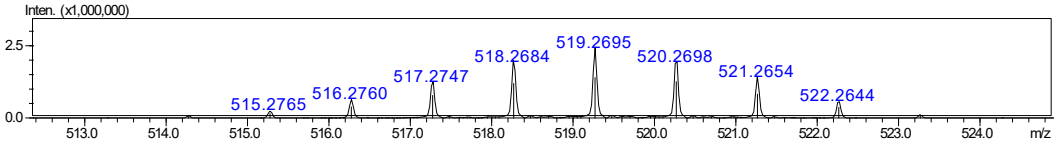
for $[C_{18}H_{31}B_{12}ClNO_3]^-$: 474.3182; Found: 474.3189.

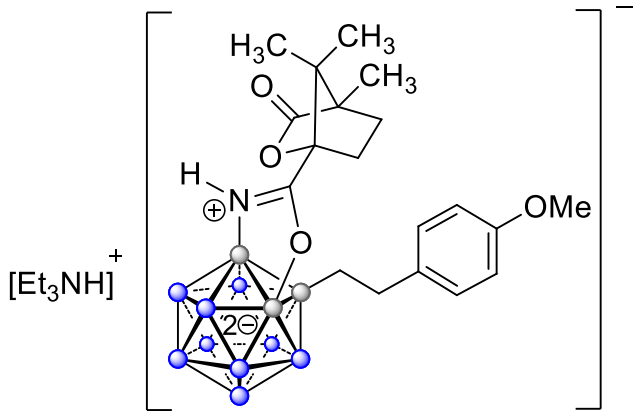




High resolution ESI-MS (negative mode, MeOH):

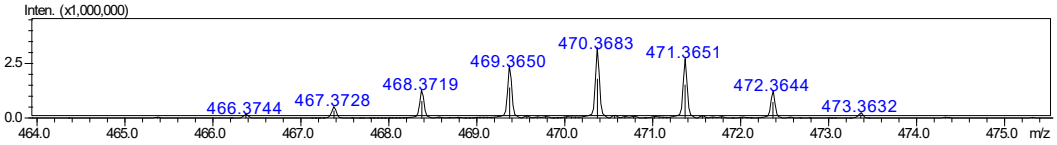
for $[C_{18}H_{31}B_{12}BrNO_3]^-$: 518.2677; Found: 518.2684.

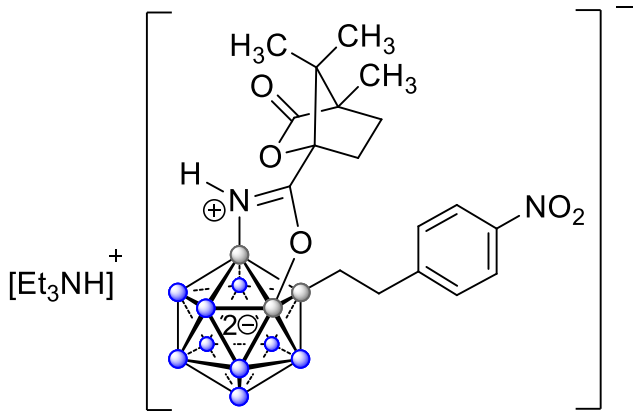




High resolution ESI-MS (negative mode, MeOH):

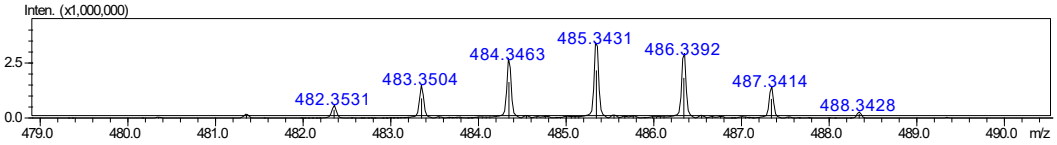
for $[C_{19}H_{34}B_{12}NO_4]^-$: 470.3677; Found: 470.3683.

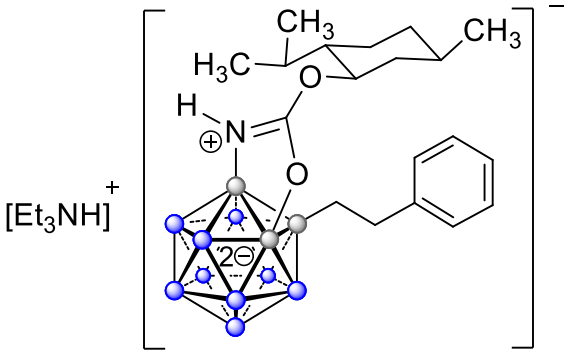




High resolution ESI-MS (negative mode, MeOH):

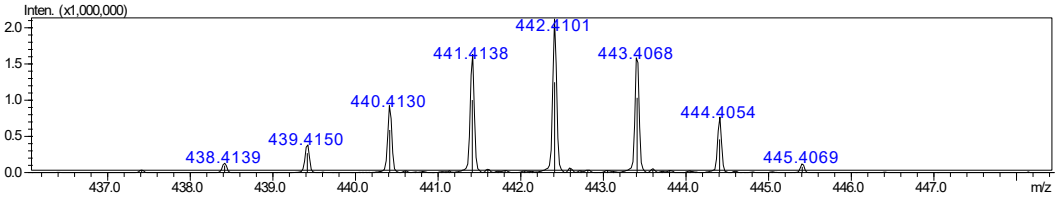
for $[C_{18}H_{31}B_{12}N_2O_5]^-$: 485.3422; Found: 485.3431.

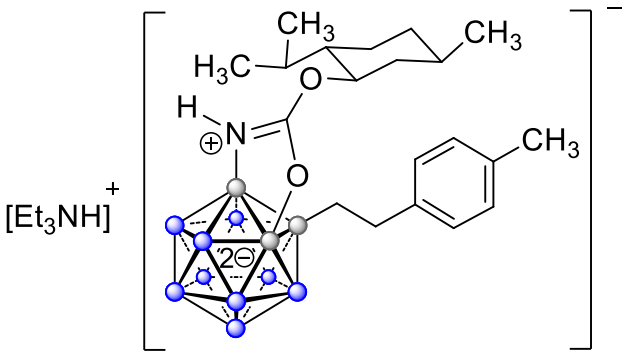




High resolution ESI-MS (negative mode, MeOH):

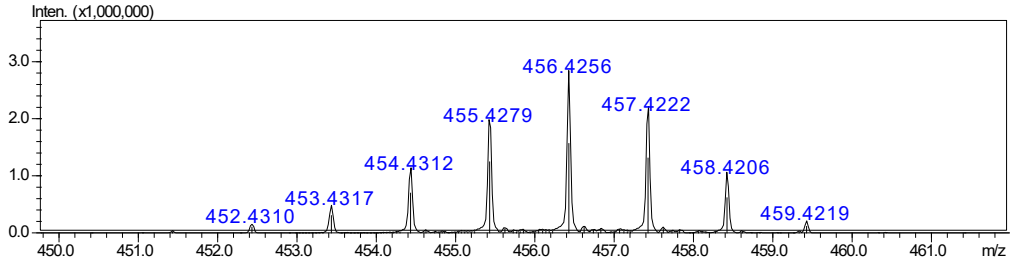
$[C_{19}H_{38}B_{12}NO_2]^-$: 442.4092; Found: 442.4101.

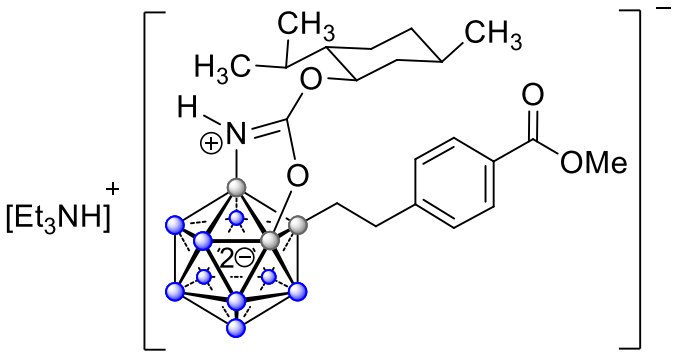




High resolution ESI-MS (negative mode, MeOH):

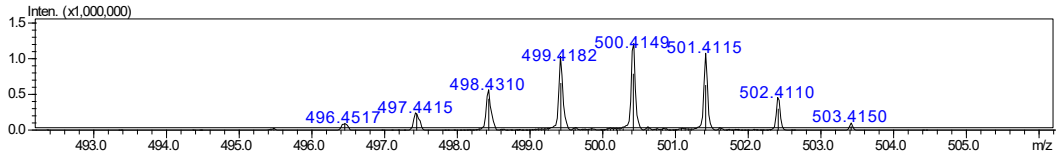
$[C_{20}H_{40}B_{12}NO_2]^-$: 456.4248; Found: 456.4256.

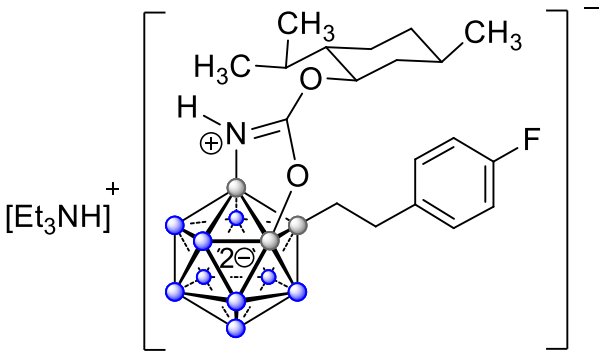




High resolution ESI-MS (negative mode, MeOH):

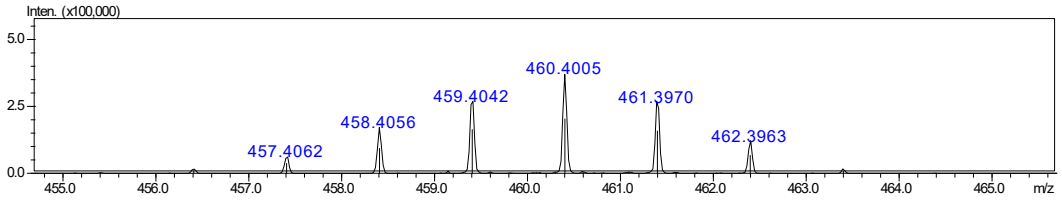
$[C_{21}H_{40}B_{12}NO_4]^-$: 500.4146 ; Found: 500.4149

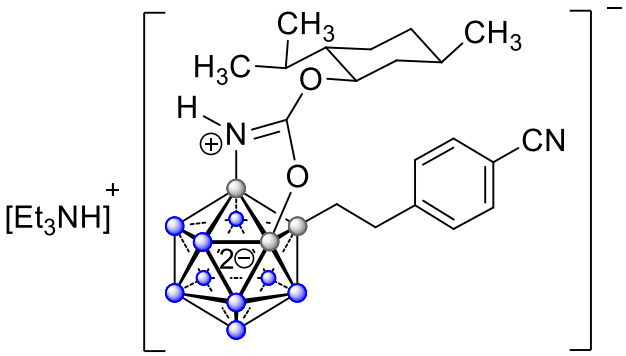




High resolution ESI-MS (negative mode, MeOH):

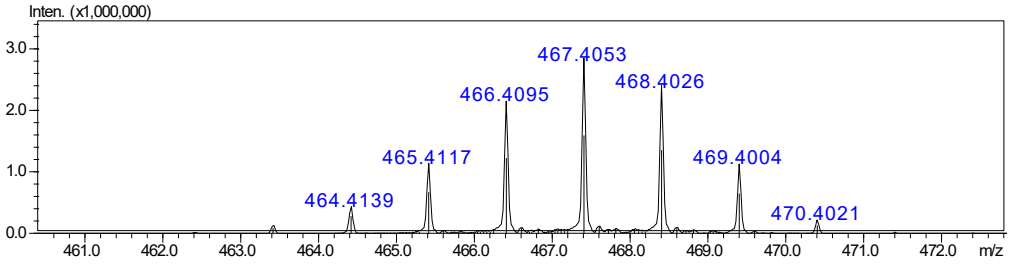
$[C_{19}H_{37}B_{12}FNO_2]^-$: 460.3998; Found: 460.4005.

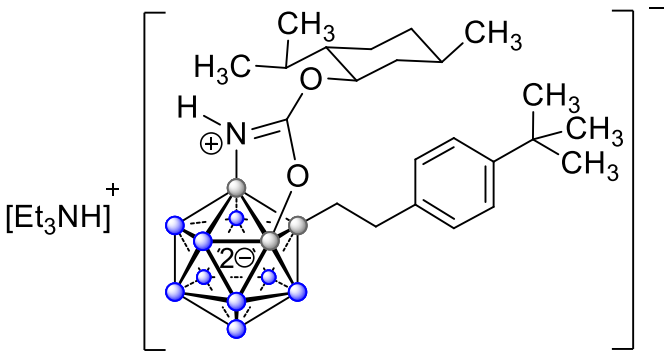




High resolution ESI-MS (negative mode, MeOH):

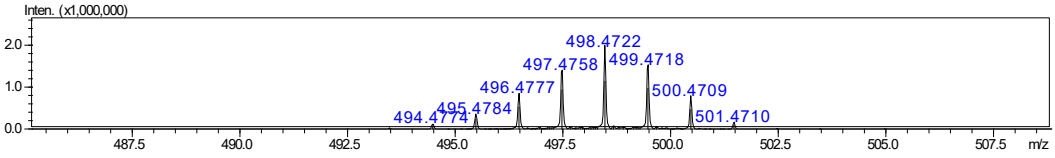
$[C_{20}H_{37}B_{12}N_2O_2]^-$: 467.4044; Found: 467.4053.

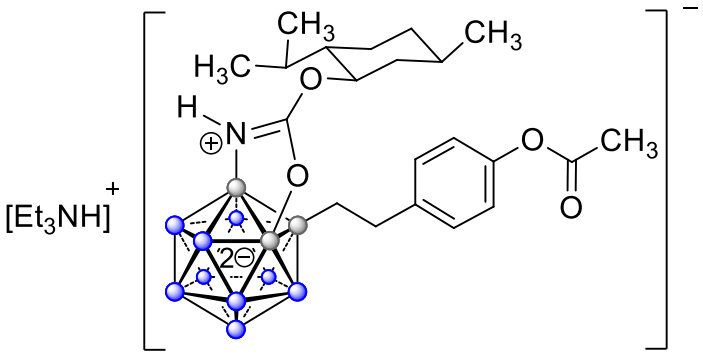




High resolution ESI-MS (negative mode, MeOH):

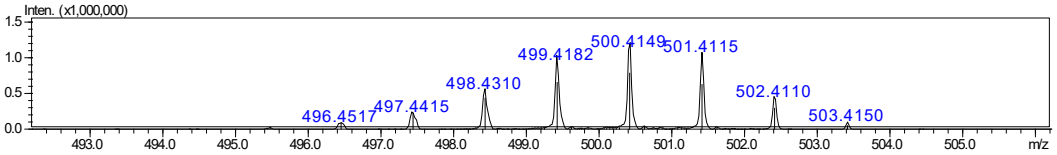
$[C_{23}H_{46}B_{12}NO_2]^-$: 498.4718; Found: 498.4722.

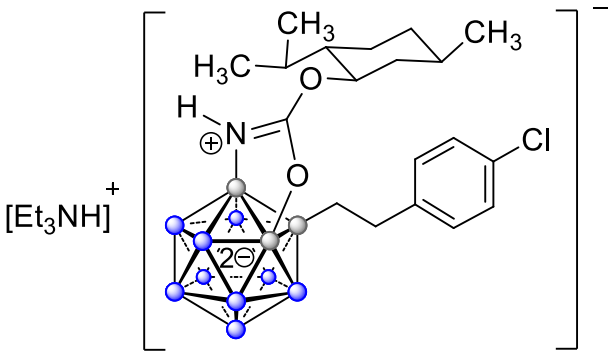




High resolution ESI-MS (negative mode, MeOH):

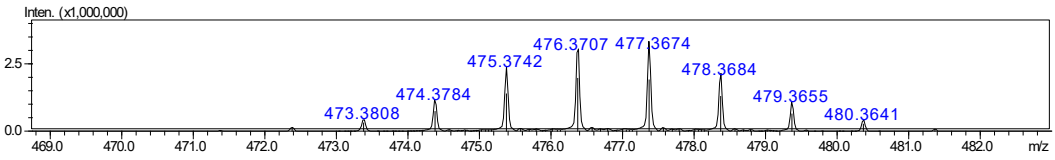
for $[C_{21}H_{40}B_{12}NO_4]^-$: 500.4147; Found: 500.4149.

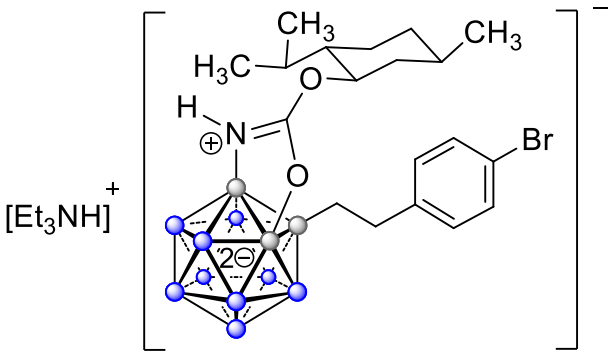




High resolution ESI-MS (negative mode, MeOH):

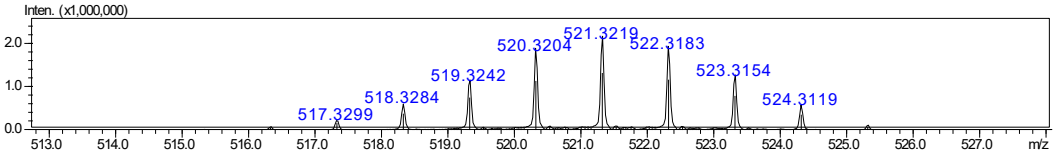
for $[C_{19}H_{37}B_{12}ClNO_2]^-$: 476.3702; Found: 476.3707.

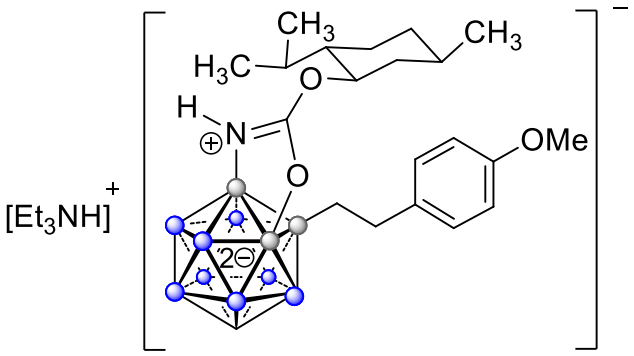




High resolution ESI-MS (negative mode, MeOH):

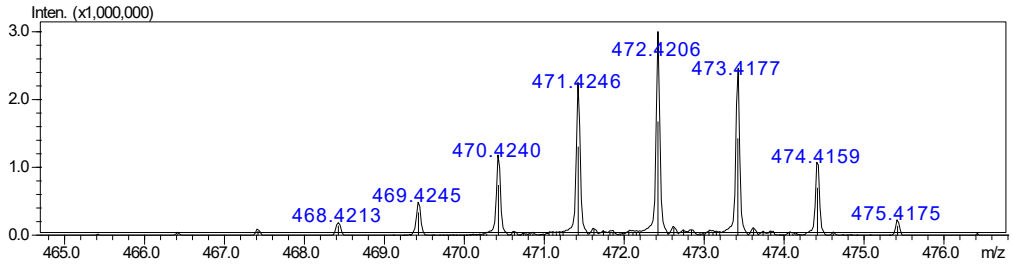
for $[C_{19}H_{37}B_{12}BrNO_2]^-$: 520.3197; Found: 520.3204.

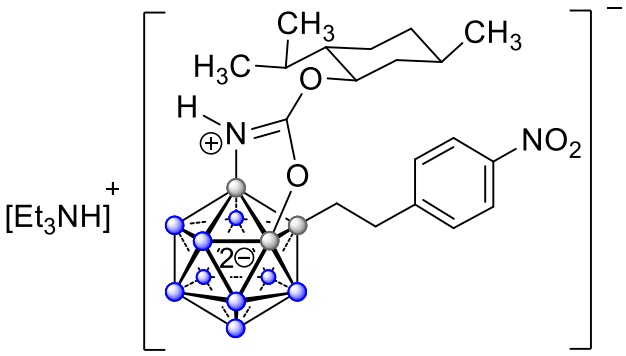




High resolution ESI-MS (negative mode, MeOH):

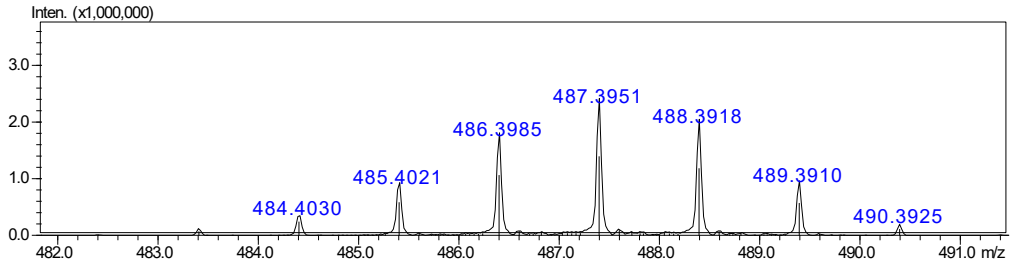
for $[C_{20}H_{40}B_{12}NO_3]^-$: 472.4197; Found: 472.4206.

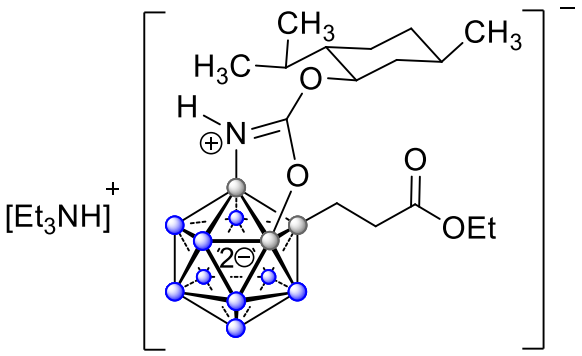




High resolution ESI-MS (negative mode, MeOH):

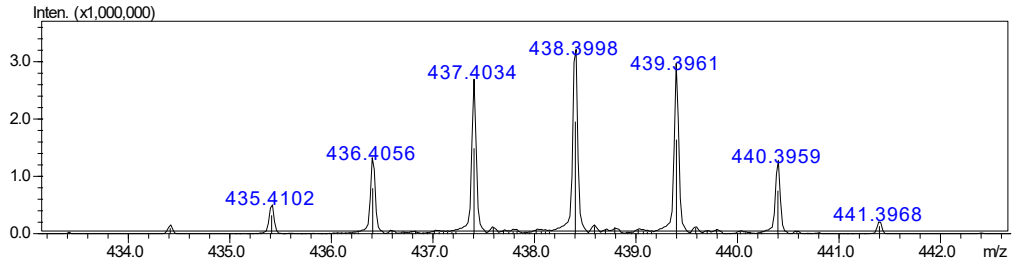
for $[C_{19}H_{37}B_{12}N_2O_4]^-$: 487.3943; Found: 487.3951.

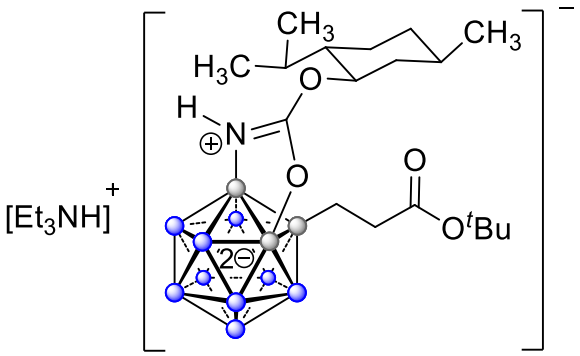




High resolution ESI-MS (negative mode, MeOH):

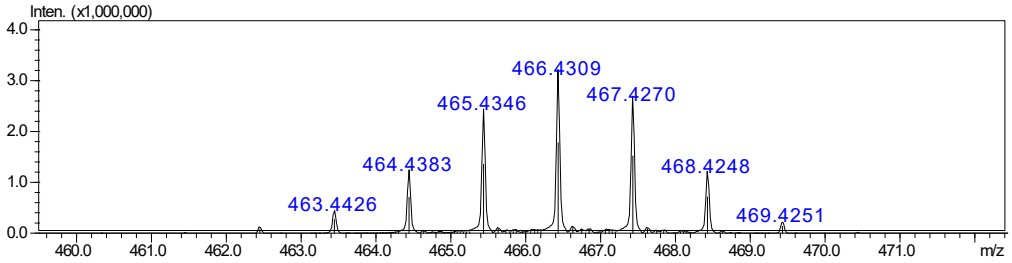
for $[C_{16}H_{38}B_{12}NO_4]^-$: 438.3990; Found: 438.3998.

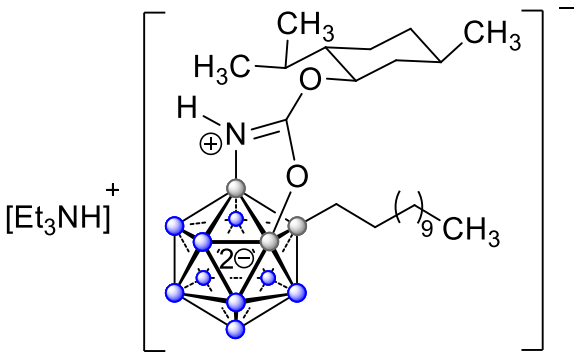




High resolution ESI-MS (negative mode, MeOH):

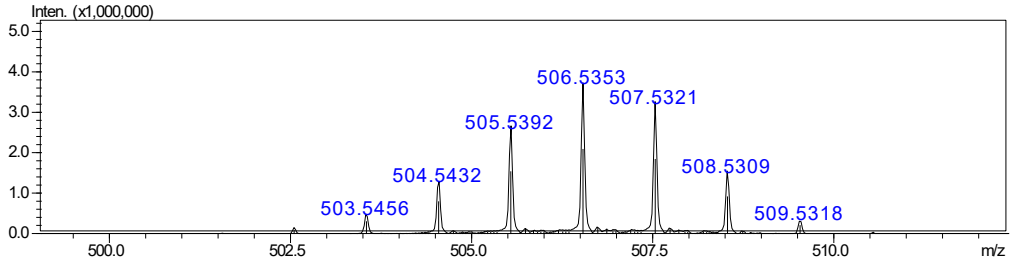
for $[C_{18}H_{42}B_{12}NO_4]^-$: 466.4303; Found: 466.4309.

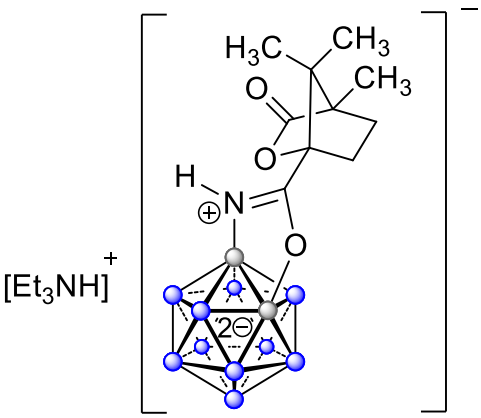




High resolution ESI-MS (negative mode, MeOH):

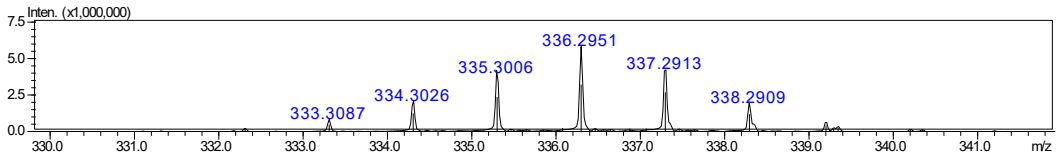
for $[C_{23}H_{54}B_{12}NO_2]^-$: 506.5344; Found: 506.5353.

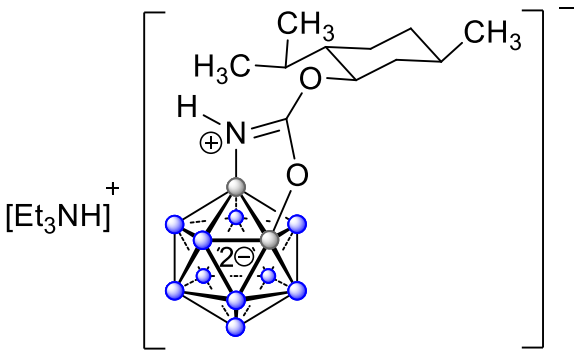




High resolution ESI-MS (negative mode, MeOH):

for $[C_{10}H_{24}B_{12}NO_3]^-$: 336.2945; Found: 336.2951.





High resolution ESI-MS (negative mode, MeOH):

for $[C_{11}H_{30}B_{12}NO_2]^-$: 338.3466; Found: 338.3471.