Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

Rhodium(III)-catalyzed dehydrogenative dialkenylation of the monocarba-*closo*-decaborate cluster by regioselective B–H activation

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Table of Contents

I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available and used without further purification. Acetone-d_6 was purchased from Cambridge Isotope Laboratories. $[Et_4N][1\text{-}COOH\text{-}1\text{-}CB_9H_9]$ and alkenes **2b**, **2d**–**h**, **2j**, **2k** were prepared according to the literature.[1,2] Anhydrous dichloromethane was prepared by passage through activated Al_2O_3 and stored over 3 Å molecular sieves.

Reaction Conditions

Glassware for air-sensitive reactions was dried at 150 °C for at least 3 h and allowed to cool in a stream of nitrogen. Air-sensitive reactions were carried out under an atmosphere of dry nitrogen.

Characterization

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

NMR spectra were recorded on a Bruker AVANCE 400 spectrometer (^{1}H NMR 400 MHz, ^{13}C NMR 101 MHz, ^{11}B NMR 128 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, residual $^{13}C\{^1H\}$: $CD_3C(O)CD_3$ = 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).

In certain ^{1}H 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]

Baseline correction for ^{11}B and $^{11}B\{^{1}H\}$ NMR spectra was carried out using the baseline correction function of the software TopSpin 3.5.

Low-resolution ESI-MS data were recorded on Advion Expression CMS instrument. The full-range spectra with *m*/*z* 100–1000 demonstrated bulk purity.

High-resolution MS data were recorded using IT-TOF detection (Shimadzu, Japan) equipped with an electrospray ionization source (ESI). Calibration to achieve accurate mass determination was carried out with sodium trifluoroacetate clusters as a reference.

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 MoK-α radiation.

Additional remarks regarding the NMR characterization of the products

Assignment of ^{1}H and ^{11}B signals was made based on reported chemical shifts for [1-COOH-1-CB_9H_9]$^-$.[4] In order to obtain B–H resonances with enhanced resolution, ^{1}H NMR spectra were recorded with decoupling from ^{11}B (nuclear spin I = 3/2). The integration of B–H signals is *ca.* 15–20% lower than the expected value. The reason for this is that there is still residual coupling to ^{10}B (nuclear spin I = 3). The natural abundance of ^{11}B (80.4% *vs* 19.6% for ^{10}B) therefore leads to a sharpening of *ca.* 80% of the B–H signals and inaccurate integrals unless a very broad ppm range is chosen for integration. An example for B–H line sharpening upon decoupling is shown for [Na][**3l**] in Figure S1.

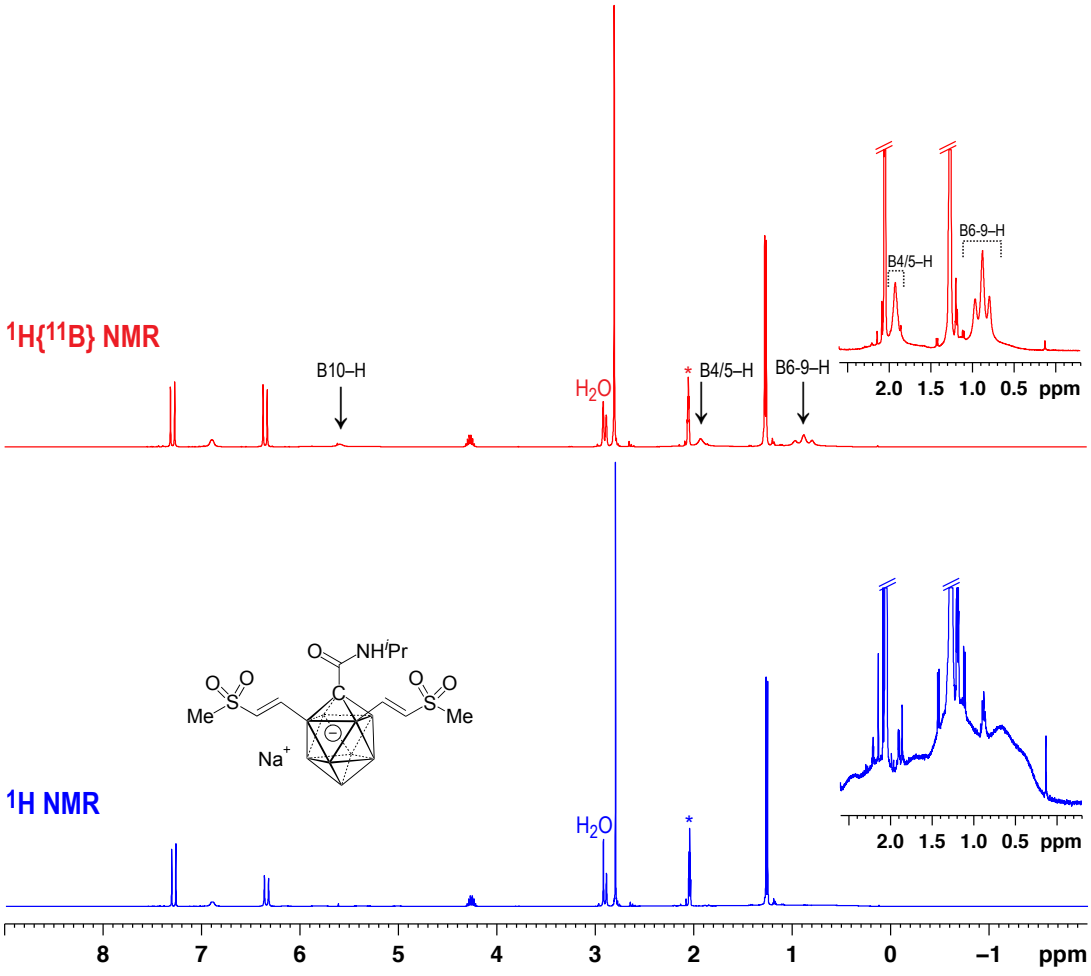


Figure S1. Comparison of ^{1}H and ^{1}H{^{11}B} NMR spectra of **3l**, showing a sharpening of the B–H resonances upon decoupling from ^{11}B. Conditions: 400 MHz, 20 mg in 0.6 mL acetone-d_6, 23 °C.

^{11}B-^{11}B COSY NMR spectra were recorded for amide **1** and selected products **3**. For **1**, clear correlation signals were obtained (Figure S2). On the other hand, for for B2/3-disubstituted **3**, only very weak or even no $^{1}J_{B\text{-}B}$ correlation signals were found, as shown for **3l** (Figure S3). A detailed study by Grimes addressed the phenomenon of weak correlation peaks,[5] and an explanatory summary is given in the following. The detection of cross peaks requires that several criteria be fulfilled: (a) Sufficient electron density must exist directly between the respective boron atoms; (b) the relaxation times T_1 and T_2 must be long enough and (c) the individual ^{11}B resonances in the 1D spectrum are fully or at partially resolved. All of these conditions influence scalar coupling and heavily depend on the number, nature and position of the cage substituents. They cannot be changed by the measurement parameters, except for (c) where recording data at a higher field is beneficial.

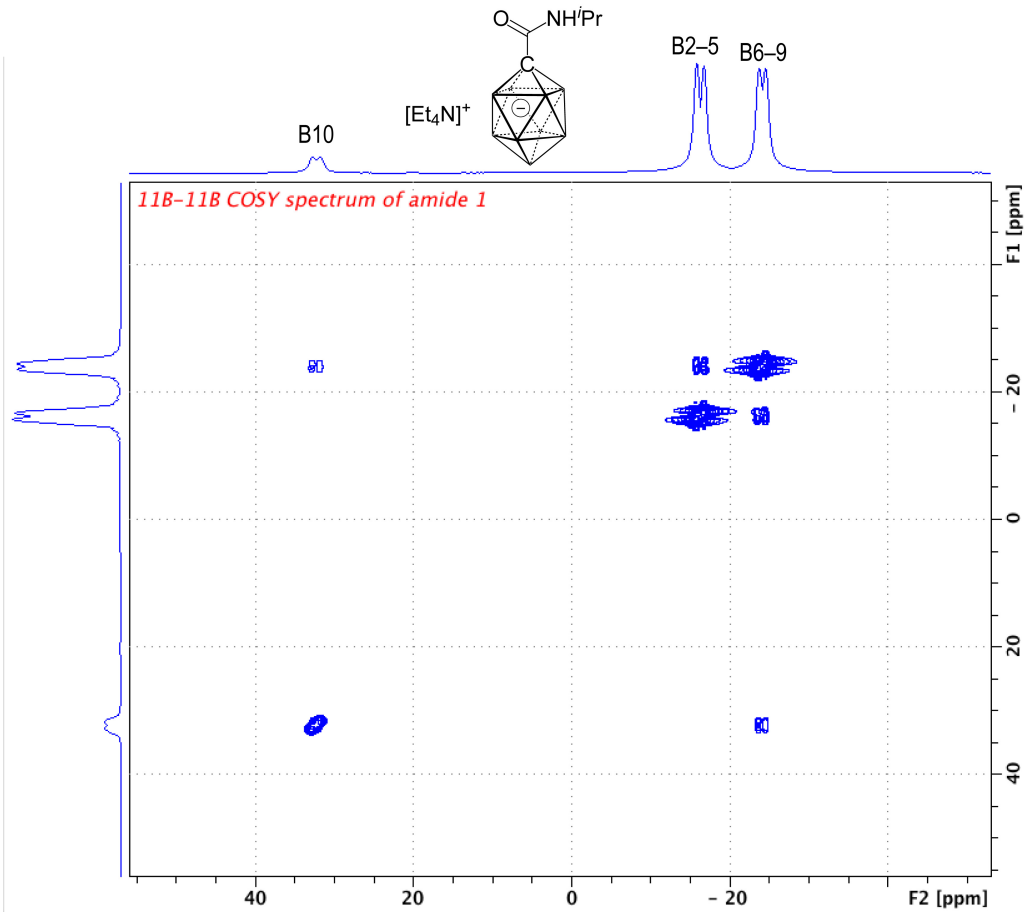


Figure S2. ^{11}B-^{11}B COSY NMR spectrum of **1**. Conditions: 160 MHz, 20 mg in 0.6 mL acetone-d_6, 23 °C.

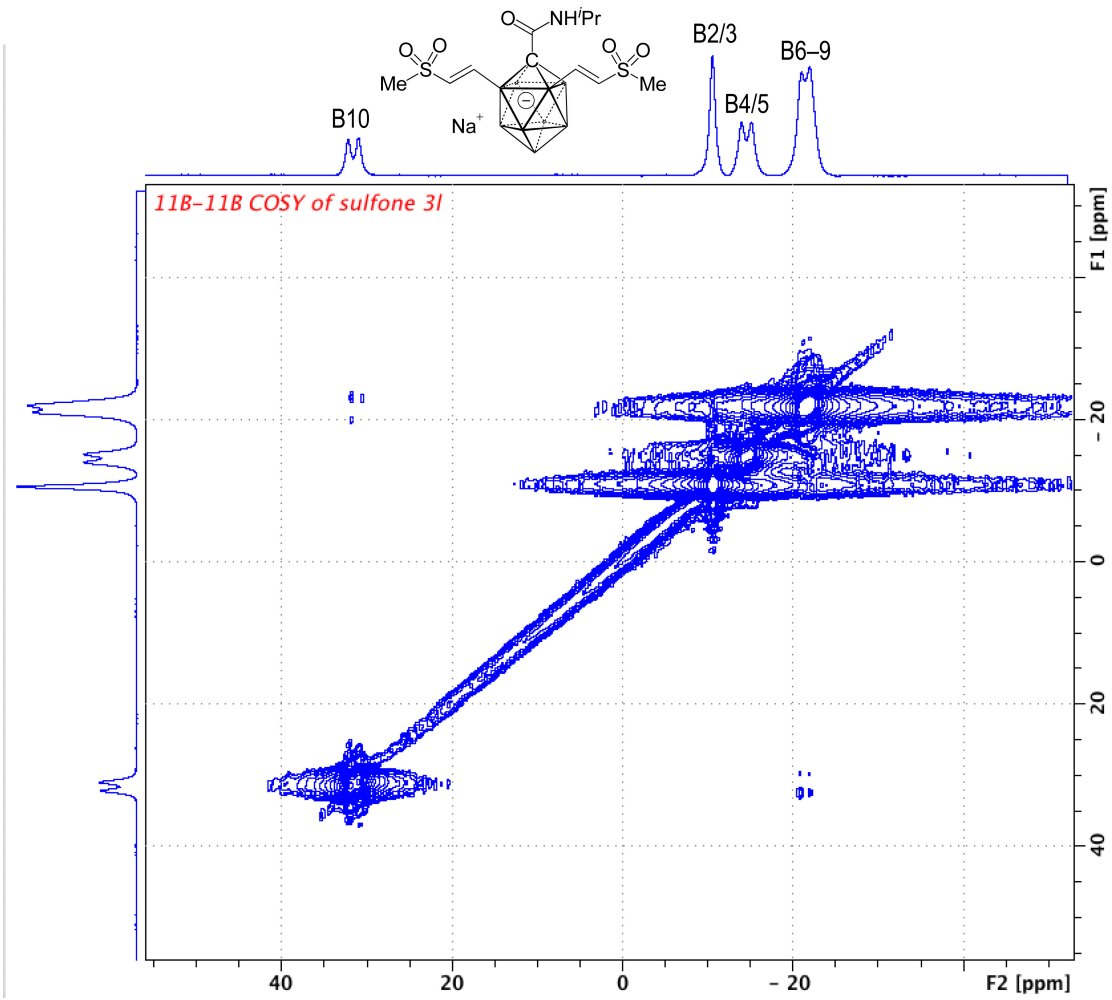


Figure S3. ^{11}B-^{11}B COSY NMR spectrum of **3l**; only very weak correlation signals are observed. Conditions: 160 MHz, 20 mg in 0.6 mL acetone-d_6, 23 °C.

II Experimental Section

Synthesis of carborane amide [Et_4N][1-(CONH*i*Pr)-1-CB_9H_9] ([Et_4N][1])

To a suspension of [Et_4N][1-COOH-1-CB_9H_9] (1.50 g, 5.1 mmol) in dichloromethane (40 mL) in a 100 mL Schlenk flask, DMF (50 μL, cat.) and oxalyl chloride (1.3 mL, 15.3 mmol, 3 equiv) were added at room temperature under air. The mixture was stirred for 30 min, and then the solvent was removed under high vacuum using a trap cooled with liquid nitrogen. The Schlenk flask was refilled with nitrogen, and then anhydrous dichloromethane was added (40 mL). To the obtained solution, isopropylamine (1.3 mL, 15.3 mmol, 3 equiv) was added. The mixture was stirred for 1 h, and then the solvent was removed using a rotary evaporator. The residue was acidified with 1 M aq. HCl (50 mL) and then extracted with Et_2O (3 x 50 mL). To the combined Et_2O layers, H_2O (100 mL) was added. The Et_2O layer was removed using a rotary evaporator. Et_4NBr (2.14 g, 10.2 mmol) was added to the residual aqueous solution. A precipitate formed immediately, which was collected by filtration through a glass frit and dried under high vacuum at 50 °C for 12 h to give product [Et_4N][**1**] as a colorless solid (1.46 g, 85% yield).

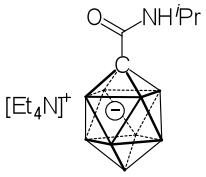
General procedure for the dialkenylation of 1

To a mixture of [Et_4N][**1**] (100 mg, 0.3 mmol), [$RhCp^*Cl_2]_2$ (18.5 mg, 0.1 equiv), $AgSbF_6$ (41 mg, 0.4 equiv.), $Cu(OAc)_2 \cdot H_2O$ (60 mg, 1 equiv.) in dimethylacetamide (8 mL) in a 20 mL glass vial, the alkene **2** (5 equiv) was added. The mixture was stirred under air atmosphere at 20–45 °C. Monitoring was carried out using (–)-ESI mass spectrometry on an Advion Expression CMS instrument. After completion of the reaction, brine (40 mL) was added. The mixture was extracted with EtOAc (3 x 50 mL), and the combined EtOAc layers were washed with brine (3 x 120 mL). The EtOAc layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography using a mixture of dichloromethane and MeCN as the eluent.

The reaction temperature, time and eluent for chromatography is given at the beginning of the peak list for each product.

To ensure isolation of the product as its $[Et_4N]^+$ salt, the following steps were carried out: The product, as obtained after column chromatography, and Et_4NBr (300 mg) were added to a biphasic mixture of 1 M aq. HCl (15 mL) dichloromethane (15 mL) in a separation funnel. The first dichloromethane extraction layer was separated, and the aqueous layer was extracted with more dichloromethane (2 x 15 mL). The combined dichloromethane layers were washed with deionized H_2O (5 x 50 mL). The dichloromethane layer was concentrated under reduced pressure and dried under high vacuum at 60 °C overnight to give $[Et_4N]$[**3**].

Starting material [Et_4N][1]



$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 6.80 (broad signal, 1H, NH), 5.59 (broad signal, 1H, BH), 4.32-4.16 (m, 1H), 3.47 (q, J = 7.2 Hz, 8H), 1.69 (broad signal, 4H, BH), 1.39 (broad signal, 12H), 1.27 (d, J = 6.5 Hz, 6H), 0.69 (broad signal, 4H, BH).

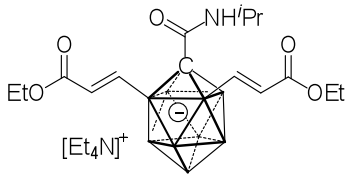
^{11}B NMR (128 MHz, acetone-d_6): δ 32.34 (d, J = 152.8 Hz, 1B), -16.23 (d, J = 151.1 Hz, 4B), -24.03 (d, J = 138.4 Hz, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 32.37 (1B), -16.17 (4B), -24.01 (4B).

$^{13}C\{1H\}$ NMR (101 MHz, acetone-d_6): δ 168.51 (C=O), 72.56 (cage C), 52.96 (t, J = 3.1 Hz, cation CH_2), 42.29 (*i*Pr CH), 22.85 (*i*Pr CH_3), 7.66 (cation CH_3).

HRMS ((–)-ESI): m/z calculated for $[C_5H_{17}B_9NO]^-$: 205.2184; found: 205.2197.

Product [Et_4N][3a]



Reaction conditions: 28 h, 40 °C; 73% yield, yellowish solid; eluent CH_2Cl_2 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.47 (d, *J* = 17.7 Hz, 2 H), 6.67 (broad d, *J* = 6.3 Hz, 1H, NH), 5.81 (d, *J* = 17.7 Hz, 2H), 5.52 (broad signal, 1H, BH), 4.30-4.20 (m, 1H), 4.06 (q, *J* = 7.1 Hz, 4H), 3.49 (q, J = 7.2 Hz, 8H), 1.90 (broad signal, 2H, BH), 1.39 (tt, *J* = 7.2 Hz, 1.8 Hz, 12H), 1.24 (d, *J* = 6.6 Hz, 6H), 1.19 (t, *J* = 7.1 Hz, 6H), 1.00-0.78 (broad overlapping signals, 4H, BH).

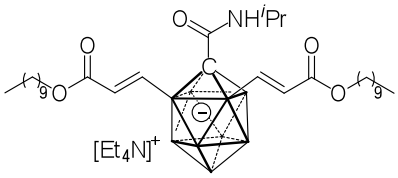
^{11}B NMR (128 MHz, acetone-d_6): δ 30.85 (d, *J* = 158.0 Hz, 1B), -9.97 (s, 2B), -14.7 (d, *J* = 142.5 Hz, 2B), *ca.* -19 to -25 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 30.89 (1B), -9.99 (2B), -14.73 (2B), *ca.* -20 to -24 (three overlapping signals from B6–9, 4B).

$^{13}C\{1H\}$ NMR (101 MHz, acetone-d_6): δ 166.72 (C=O), 166.64 (C=O), 131.17 (CH), 60.07 (CH_2), 53.01 (t, *J* = 3.1 Hz, cation CH_2), 42.37 (*i*Pr CH), 22.98 (*i*Pr CH_3), 14.66 (CH_3), 7.73 (cation CH_3). The B-C signal appeared as a very broad resonance at 150 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{15}H_{29}B_9NO]^-$: 401.2920; found: 401.2929.

Product [Et_4N][3b]



Reaction conditions: 48 h, 30 °C; 73% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.47 (d, J = 17.8 Hz, 2H), 6.63 (broad d, J = 7.0 Hz, 1H, NH), 5.83 (d, J = 17.8 Hz, 2H), 5.53 (broad signal, 1H, BH), 4.32-4.18 (m, 1H), 4.01 (t, J = 6.7 Hz, 4H), 3.49 (q, J = 7.2 Hz, 8H), 1.90 (broad signal, 2H, BH), 1.66-1.53 (m, 4H), 1.44-1.20 (overlapping signals, 46H, cation CH_3, *i*Pr CH_3, alkyl CH_2), 0.92-0.82 (broad signal, 10H, B-H overlapping with alkyl CH_3,)

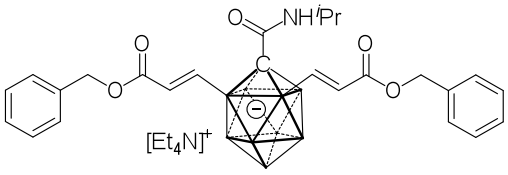
^{11}B NMR (128 MHz, acetone-d_6): δ 30.90 (d, J = 146.4 Hz, 1B), -9.90 (s, 2B), -14.66 (d, J = 131 Hz, 2B), *ca.* -17.8 to -24.9 (three overlapping d from B6–9, 4B)

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 30.95 (1B), -9.90 (2B), -14.70 (2B), *ca.* -18.5 to -24.1 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.77 (C=O), 166.60 (C=O), 131.10 (CH), 64.25 (CH_2), 53.00 (t, J = 3.1 Hz, cation CH_2), 42.34 (*i*Pr CH), 32.60 (CH_2), 30.27 (CH_2), 29.55 (CH_2), 26.72 (CH_2), 23.31 (CH_2), 23.00 (*i*Pr CH_3), 14.37 (CH_2), 7.70 (cation CH_3). Two alkyl CH_2 signals could not be observed clearly because of overlap with the solvent signal; the B-C signal appeared as a very broad resonance at 150 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{31}H_{61}B_9NO_5]^-$: 625.5424; found: 625.5443.

Product [Et_4N][3c]



Reaction conditions: 18 h, 45 °C; 76% yield, yellowish solid; eluent CH_2Cl_2 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.54 (d, *J* = 17.8 Hz, 2H), 7.39-7.26 (m, 10H), 6.66 (broad d, *J* = 6.6 Hz, 1H, NH), 5.88 (d, *J* = 17.8 Hz, 2H), 5.54 (broad signal, 1H), 5.10 (s, 4H), 4.31-4.16 (m, 1H), 3.45 (q, *J* = 7.2 Hz, 8H), 1.91 (broad signal, 2H, BH), 1.36 (tt, *J* = 7.3 Hz, 1.7 Hz, 12H), 1.21 (d, *J* = 6.6 Hz, 6H), 1.01-0.65 (broad overlapping signals, 4H, BH).

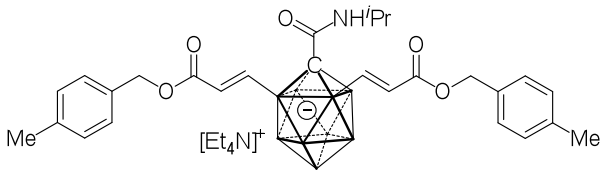
^{11}B NMR (128 MHz, acetone-d_6): δ 31.06 (d, *J* = 153.3 Hz, 1B), -10.02 (s, 2B), -14.70 (d, *J* = 147.3 Hz, 2B), *ca.* -18.3 to -24.8 (three overlapping d from B6–9, 4B)

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.00 (1B), -9.96 (2B), -14.74 (2B), *ca.* -19.4 to -24.2 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.57 (C=O), 166.50 (C=O), 137.91 (C_q), 130.69 (CH), 129.23 (CH), 128.87 (CH), 128.66 (CH), 65.92 (CH_2), 53.01 (t, *J* = 3.2 Hz, cation CH_2), 42.36 (*i*Pr CH), 22.96 (*i*Pr CH_3), 7.69 (cation CH_3). The B-C signal appeared as a very broad resonance at 151 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{25}H_{33}B_9NO_5]^-$: 525.3233; found: 525.3248.

Product [Et_4N][3d]



Reaction conditions: 18 h, 45 °C; 72% yield, yellowish solid; eluent CH_2Cl_2 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.52 (d, J = 17.7 Hz, 2H), 7.28-7.21 (m, 4H), 7.17-7.10 (m, 4H), 6.65 (broad d, J = 6.7 Hz, 1H, NH), 5.86 (d, J = 17.7 Hz, 2H), 5.53 (broad signal, 1H, BH), 5.04 (s, 4H), 4.30-4.16 (m, 1H), 3.45 (q, J = 7.3 Hz, 8H), 2.30 (s, 6H), 1.90 (broad signal, 2H, BH), 1.36 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.21 (d, J = 6.6 Hz, 6H), 1.02-0.54 (broad overlapping signals, 4H, BH).

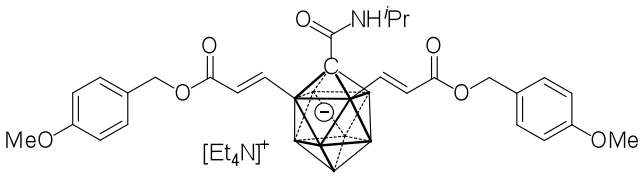
^{11}B NMR (128 MHz, acetone-d_6): δ 30.93 (d, J = 155.1 Hz, 1B), -10.02 (s, 2B), -14.78 (d, J = 136.7 Hz, 2B), *ca.* -18.4 to -26.2 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.02 (1B), -10.03 (2B), -14.67 (2B), *ca.* -18.9 to -25.4 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.58 (C=O), 166.55 (C=O), 138.32 (C_q), 134.90 (C_q), 130.81 (CH), 129.84 (CH), 129.09 (CH), 65.87 (CH_2), 53.02 (t, J = 3.1 Hz, cation CH_2), 42.37 (*i*Pr CH), 22.98 (*i*Pr CH_3), 21.17 (CH_3), 7.70 (cation CH_3). The B-C signal appeared as a very broad resonance at 151 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for [$C_{27}H_{37}B_9NO_5$]: 553.3546; found: 553.3558.

Product [Et_4N][3e]



Reaction conditions: 24 h, 30 °C; 63% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.50 (d, J = 17.8 Hz, 2H), 7.34-7.26 (m, 4H), 6.93-6.85 (m, 4H), 6.64 (broad d, J = 6.7 Hz, 1H, NH), 5.84 (d, J = 17.7 Hz, 2H), 5.52 (broad signal, 1H, BH), 5.01 (s, 4H), 4.30-4.14 (m, 1H), 3.78 (s, 6H), 3.46 (q, J = 7.2 Hz, 8H), 1.89 (broad signal, 2H, BH), 1.37 (tt, J = 7.3 Hz, 1.7 Hz, 12H), 1.20 (d, J = 6.6 Hz, 6H), 1.02-0.59 (broad overlapping signals, 4H, BH).

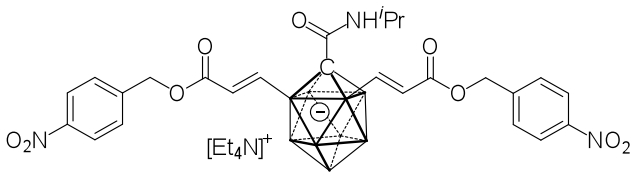
^{11}B NMR (128 MHz, acetone-d_6): δ 30.92 (d, J = 149.7 Hz, 1B), -9.97 (s, 2B), -14.64 (d, J = 150.9 Hz, 2B), *ca.* -18.5 to -25.1 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 30.96 (1B), -10.00 (2B), -14.69 (2B), *ca.* -19.0 to -25.2 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.57 (two overlapping C=O), 160.50 (C_q), 130.89 (CH), 130.80 (CH), 129.82 (C_q), 114.59 (CH), 65.75 (CH_2), 55.53 (CH_3), 53.02 (t, J = 3.2 Hz, cation CH_2), 42.35 (*i*Pr CH), 22.97 (*i*Pr CH_3), 7.69 (cation CH_3). The B-C signal appeared as a very broad resonance at 151 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{27}H_{37}B_9NO_7]^-$: 585.3444; found: 585.3446.

Product [Et_4N][3f]



Reaction conditions: 48 h, 30 °C; 70% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 10:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 8.29-8.19 (m, 4H), 7.70-7.11 (m, 4H), 7.60 (d, *J* = 17.7 Hz, 2H), 6.73 (broad d, *J* = 6.9 Hz, 1H, NH), 5.91 (d, *J* = 17.7 Hz, 2H), 5.56 (broad signal, 1H, BH), 5.26 (s, 4H), 4.32-4.18 (m, 1H), 3.48 (q, *J* = 7.2 Hz, 8H), 1.92 (broad signal, 2H, BH), 1.39 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.23 (d, *J* = 6.6 Hz, 6H), 1.07-0.70 (broad overlapping signals, 4H, BH).

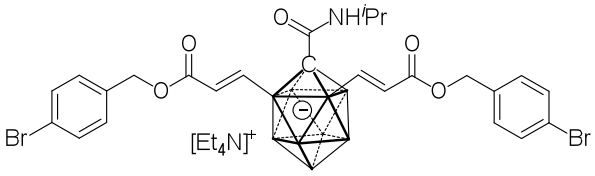
^{11}B NMR (128MHz, acetone-d_6): δ 31.06 (d, *J* = 147.8 Hz, 1B), -10.03 (s, 2B), -14.67 (d, *J* = 140.2 Hz, 2B), *ca.* -18.3 to -25.8 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.09 (1B), -9.98 (2B), -14.59 (2B), *ca.* -18.7 to -24.5 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.56 (C=O), 166.25 (C=O), 148.41 (C_q), 145.57 (C_q), 130.14 (CH), 129.34 (CH), 124.33 (CH), 64.74 (CH_2), 53.01 (t, *J* = 2.9 Hz, cation CH_2), 42.39 (*i*Pr CH), 22.95 (*i*Pr CH_3), 7.68 (cation CH_3). The B-C signal appeared as a very broad resonance at 152 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): Calculated for $[C_{25}H_{31}B_9N_3O_9]^-$: 615.2934; found: 615.2949.

Product [Et_4N][3g]



Reaction conditions: 36 h, 35 °C; 74% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.60-7.49 (overlapping signals, 6H), 7.37-7.30 (m, 4H), 6.66 (broad d, J = 6.6 Hz, 1H, NH), 5.87 (d, J =17.7 Hz, 2H), 5.54 (broad signal, 1H, BH), 5.08 (s, 4H), 4.30-4.16 (m, 1H), 3.47 (q, J = 7.2 Hz, 8H), 1.90 (broad signal, 2H, BH), 1.38 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.21 (d, J = 6.6 Hz, 6H), 1.04-0.68 (broad overlapping signals, 4H, BH).

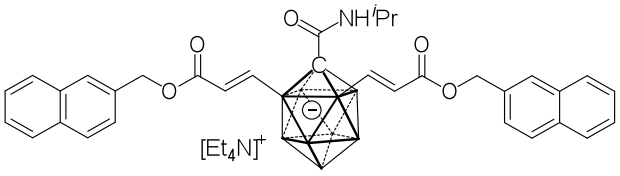
^{11}B NMR (128 MHz, acetone-d_6): δ 31.02 (d, J = 153.9 Hz, 1B), -10.04 (s, 2B), -14.63 (d, J = 133.6 Hz, 2B), -21.56 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.10 (1B), -9.93 (2B), -14.61 (2B), *ca.* -17.9 to -25.5 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.55 (C=O), 166.39 (C=O), 137.37 (C_q), 132.30 (CH), 130.92 (CH), 130.46 (CH), 122.13 (C_q), 65.14 (CH_2), 53.03 (t, J = 2.9 Hz, cation CH_2), 42.36 (*i*Pr CH), 22.96 (*i*Pr CH_3), 7.70 (cation CH_3). The B-C signal appeared as a very broad resonance at 151 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{25}H_{31}B_9Br_2NO_5]^-$: 683.1442; found: 682.1443.

Product [Et_4N][3h]



Reaction conditions: 48 h, 35 °C; 83% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.95-7.81 (overlapping signals, 8H), 7.59 (d, *J* = 17.7 Hz, 2H), 7.53-7.45 (overlapping signals, 6H), 6.68 (broad d, *J* = 6.9 Hz, 1H, NH), 5.92 (d, *J* = 17.7 Hz, 2H), 5.55 (broad signal, 1H, BH), 5.27 (s, 4H), 4.31-4.15 (m, 1H), 3.37 (q, *J* = 7.2 Hz, 8H), 1.92 (broad signal, 2H, BH), 1.30 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.20 (d, *J* = 6.6 Hz, 6H), 1.03-0.69 (broad overlapping signals, 4H, BH).

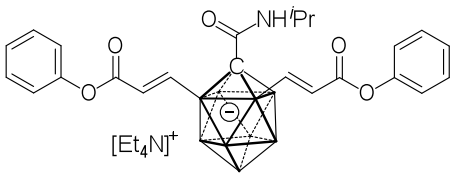
^{11}B NMR (128MHz, acetone-d_6): δ 30.98 (d, *J* = 161.1 Hz, 1B), -9.96 (s, 2B), -14.62 (d, *J* = 139.1 Hz, 2B), *ca.* -18.6 to -24.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.01 (1B), -9.98 (2B), -14.72 (2B), *ca.* -18.1 to -24.7 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.62 (C=O), 166.58 (C=O), 135.50 (C_q), 134.24 (C_q), 133.98 (C_q), 130.69 (CH), 128.99 (CH), 128.80 (CH), 128.50 (CH), 127.70 (CH), 127.08 (CH), 126.95 (CH), 126.83 (CH), 66.06 (CH_2), 52.98 (t, *J* = 2.9 Hz, cation CH_2), 42.39 (*i*Pr CH), 22.98 (*i*Pr CH_3), 7.65 (cation CH_3). The B-C signal appeared as a very broad resonance at 152 ppm; the cage C signal was not detected unambiguously.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{33}H_{37}B_9NO_5]^-$: 625.3546; found: 625.3554.

Product [Et_4N][3i]



Reaction conditions: 48 h, 45 °C; 73% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.75 (d, J = 17.7 Hz, 2H), 7.43-7.34 (m, 4H), 7.25 - 7.17 (m, 2 H), 7.16-7.08 (m, 4H), 6.83 (broad d, J = 6.9 Hz, 1H, NH), 6.05 (d, J = 17.7 Hz, 2H), 5.62 (broad signal, 1H, BH), 4.39-4.22 (m, 1H), 3.45 (q, J = 7.1 Hz, 8H), 1.99 (broad signal, 2H, BH), 1.36 (tt, J = 7.3 Hz, 1.8 Hz, 12H), 1.28 (d, J = 6.6 Hz, 6H), 1.08-0.80 (broad overlapping signals, 4H, BH).

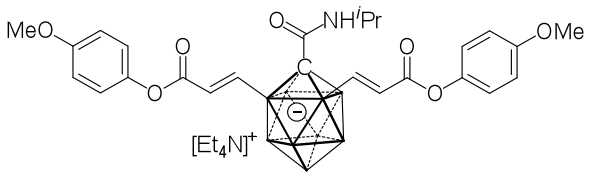
^{11}B NMR (128 MHz, acetone-d_6): δ 31.18 (d, J = 158.2 Hz, 1B), -10.01 (s, 2B), -14.52 (d, J = 132.2 Hz, 2B), *ca.* -18.8 to -24.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.27 (1B), -10.01 (2B), -14.51 (2B), *ca.* -19.3 to -25.0 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.60 (C=O), 165.12 (C=O), 152.25 (C_q), 130.12 (CH), 130.05 (CH), 126.13 (CH), 122.72 (CH), 53.00 (t, J = 2.8 Hz cation CH_2), 42.44 (*i*Pr CH), 22.98 (*i*Pr CH_3), 7.67 (cation CH_3). The B-C signal appeared as a very broad resonance at 153 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{23}H_{29}B_9NO_5]^-$: 497.2920; found: 497.2921.

Product [Et_4N][3j]



Reaction conditions: 48 h, 35 °C; 61% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*). Based on the $^1H\{^{11}B\}$ NMR spectrum, the purity of **3j** was 90%. We were not able to separate the unknown impurity from the desired product chromatographically. The yield was corrected accordingly.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.72 (d, J = 17.7 Hz, 2H), 7.07-7.00 (m, 4H), 6.94-6.87 (m, 4H), 6.83 (broad d, J = 6.5 Hz, 1H, NH), 6.02 (d, J = 17.7 Hz, 2H), 5.61 (broad signal, 1H, BH), 4.38-4.22 (m, 1H), 3.78 (s, 6H), 3.45 (q, J = 7.1 Hz, 8H), 1.97 (broad signal, 2H BH), 1.36 (tt, J = 7.3 Hz, 1.8 Hz, 12H), 1.28 (d, J = 6.5 Hz, 6H), 1.08-0.79 (broad overlapping signals, 4H, BH).

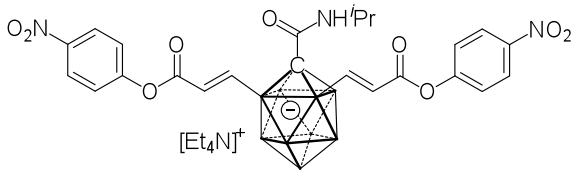
^{11}B NMR (128 MHz, acetone-d_6): δ 31.16 (d, J = 149.4 Hz, 1B), -10.03 (s, 2B), -14.44 (d, J = 100.6 Hz, 2B), *ca.* -18.8 to -24.6 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.18 (1B), -9.98 (2B), -14.62 (2B), *ca.* -17.8 to -25.2 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.59 (C=O), 165.46 (C=O), 157.99 (C_q), 145.58 (C_q), 130.22 (CH), 123.41 (CH), 114.97 (CH), 55.80 (CH_3), 52.98 (t, J = 2.8 Hz, cation CH_2), 42.42 (*i*Pr CH), 22.97 (*i*Pr CH_3), 7.67 (cation CH_3). The B-C signal appeared as a very broad resonance at 153 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{25}H_{33}B_9NO_7]^-$: 557.3131; found: 557.3142.

Product [Et_4N][3k]



Reaction conditions: 48 h, 45 °C; 43% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ (400 MHz, acetone-d_6): δ 8.33-8.24 (m, 4H), 7.82 (d, *J* = 17.7 Hz, 2H), 7.49-7.41 (m, 4H), 6.91 (broad d, *J* = 7.4 Hz, 1H, NH), 6.05 (d, *J* = 17.7 Hz, 2H), 5.63 (broad signal, 1H, BH), 4.39 - 4.20 (m, 1H), 3.49 (q, *J* = 7.3 Hz, 8H), 1.98 (broad signal, 2H, BH), 1.38 (tt, *J* = 7.2 Hz, 1.8 Hz, 12H), 1.29 (d, *J* = 6.6 Hz, 6H), 1.12 - 0.71 (broad overlapping signals, 4H, BH).

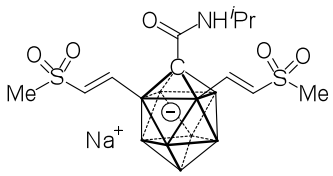
^{11}B NMR (128 MHz, acetone-d_6): δ 31.40 (d, *J* = 153.1 Hz, 1B), -10.09 (s, 2B), -14.47 (d, *J* = 132.2 Hz, 2B), *ca.* -17.9 to -25.1 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.44 (1B), -10.08 (2B), -14.52 (2B), *ca.* -18.4 to -25.1 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.51 (C=O), 164.25 (C=O), 157.16 (C_q), 146.05 (C_q), 129.18 (CH), 125.81 (CH), 123.86 (CH), 53.00 (t, *J* = 2.8 Hz, cation CH_2), 42.47 (*i*Pr CH), 22.95 (*i*Pr CH_3), 7.67 (cation CH_3). The B-C signal appeared as a very broad resonance at 155 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{23}H_{27}B_9N_3O_9]^-$: 587.2621; found: 587.2639.

Product [Na][3l]



Reaction conditions: 48 h, 45 °C; 84% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 5:1 to CH_2Cl_2:MeCN = 3:1 (*v*/*v*). This product was isolated as its Na^+ salt. Standard work-up and purification involving cation exchange to $[Et_4N]^+$ lead to a significantly decreased yield.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.29 (d, J = 17.0 Hz, 2H), 6.88 (broad d, J = 6.1 Hz, 1H, NH), 6.35 (d, J = 17.0 Hz, 2H), 5.57 (broad signal, 1H, BH), 4.33-4.20 (m, 1H), 3.48 (q, J = 7.2 Hz, 8H), 2.80 (s, 6H), 1.92 (broad signal, 2H, BH), 1.38 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.27 (d, J = 6.6 Hz, 6H), 1.04-0.54 (broad overlapping signals with peaks at 0.96, 0.88 and 0.79 ppm, 4H, BH).

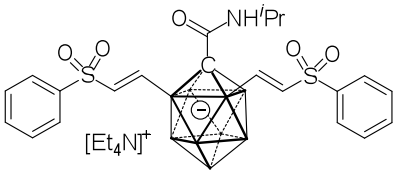
^{11}B NMR (128 MHz, acetone-d_6): δ 31.51 (d, J = 160.1 Hz, 1B), -10.64 s, 2B), -14.62 (d, J = 144.5 Hz, 2B), *ca.* -18.9 to -24.3 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.52 (1B), -10.69 (2B), -14.71 (2B), *ca.* -20.0 to -24.1 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.38 (C=O), 138.95 (CH), 42.59 (*i*Pr CH), 42.35 (CH_3), 22.90 (*i*Pr CH_3). The B-C signal appeared as a very broad resonance at 146 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{11}H_{25}B_9NO_5S_2]^-$: 413.2048; found: 413.2042.

Product [Et_4N][3m]



Reaction conditions: 48 h, 30 °C; 85% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.84-7.77 (m, 4H), 7.69-7.61 (m, 2H), 7.61-7.53 (m, 4H), 7.43 (d, *J* = 17.0 Hz, 2H), 6.89 (broad d, *J* = 6.1 Hz, 1H, NH), 6.24 (d, *J* = 17.0 Hz, 2H), 5.52 (broad signal, 1H, BH), 4.32-4.15 (m, 1H), 3.48 (q, *J* =7.2 Hz, 8H), 1.89 (broad signal, 2H, BH), 1.38 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.20 (d, *J* = 6.6Hz, 6H), 0.99-0.53 (broad overlapping signals with peaks at 0.93, 0.82 and 0.70 ppm, 4H, BH).

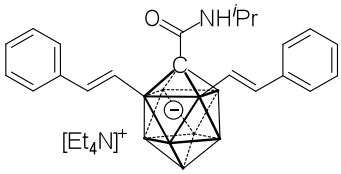
^{11}B NMR (128MHz, acetone-d_6): δ 31.40 (d, *J* = 159.6 Hz, 1B), -10.62 (s, 2B), -14.71 (d, *J* = 141.2 Hz, 2B), *ca.* -18.3 to -24.8 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 31.46 (1B), -10.60 (2B), -14.69 (2B), *ca.* -18.5 to -24.8 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 166.20 (C=O), 142.57 (C_q), 138.47 (CH), 133.68 (CH), 130.04 (CH), 128.15 (CH), 53.01 (t, *J* = 2.9 Hz, cation CH_2), 42.61 (*i*Pr CH), 22.84 (*i*Pr CH_3), 7.69 (cation CH_3). The B-C signal appeared as a very broad resonance at 148 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{29}B_9NO_5S_2]^-$: 537.2361; found: 537.2382.

Product [Et_4N][3n]



Reaction conditions: 12 h, 20 °C; 52% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.37-7.30 (m, 4H), 7.27-7.20 (m, 4H), 7.15-7.07 (m, 2H), 6.82 (d, J = 18.0 Hz, 2H), 6.58 (broad d, J = 6.8 Hz, 1H, NH), 6.49 (d, J = 18.0 Hz, 2H), 5.50 (broad signal, 1H, BH), 4.34-4.17 (m, 1H), 3.39 (q, J = 7.2 Hz, 8H), 1.94 (broad signal, 2H, BH), 1.32 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.20 (d, J = 6.6 Hz, 6H), 1.10-0.80 (broad overlapping signals, 4H, BH).

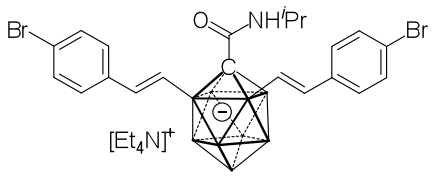
^{11}B NMR (128 MHz, acetone-d_6): δ 29.50 (d, J = 154.6 Hz, 1B), -8.71 (s, 2B), -14.91 (d, J = 144.0 Hz, 2B), *ca.* -18.4 to -24.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.55 (1B), -8.68 (2B), -14.86 (2B), *ca.* -18.9 to -24.0 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.52 (C=O), 140.90 (CH), 140.61 (C_q), 129.15 (CH), 127.34 (CH), 126.53 (CH), 52.97 (t, J = 2.8 Hz, cation CH_2), 42.10 (*i*Pr CH), 23.19 (*i*Pr CH_3), 7.65 (cation CH_3). The B-C signal appeared as a very broad resonance at 130 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{29}B_9NO]^-$: 409.3123; found: 409.3144.

Product [Et_4N][3o]



Reaction conditions: 24 h, 25 °C; 54% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ (400 MHz, acetone-d_6): δ 7.44-7.37 (m, 4H), 7.31-7.25 (m, 4H), 6.86 (d, *J* = 18.0 Hz, 2H), 6.57 (d, *J* = 7.0 Hz, 1H, NH), 6.42 (d, *J* = 8.4 Hz, 2H), 5.49 (broad signal, 1H, BH), 4.33-4.19 (m, 1H), 3.43 (q, *J* = 7.2 Hz, 8H), 1.92 (broad signal, 2H, BH), 1.35 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.20 (d, *J* = 6.6 Hz, 6H), 1.08-0.84 (broad overlapping signals, 4H, BH).

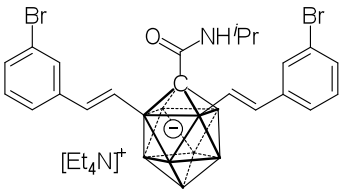
^{11}B NMR (128 MHz, acetone-d_6): δ 29.71 (d, *J* = 152.9 Hz, 1B), -8.82 (s, 2B), -14.83 (d, *J* = 131.9 Hz, 2B), *ca.* -18.3 to -25.1 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.75 (1B), -8.80 (2B), -14.89 (2B), *ca.* -19.0 to -25.0 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.49 (C=O), 139.86 (C_q), 139.45 (CH), 132.18 (CH), 128.43 (CH), 120.42 (C_q), 53.03 (t, *J* = 3.0 Hz, cation CH_2), 42.17 (*i*Pr CH), 23.19 (*i*Pr CH_3), 7.69 (cation CH_3). The B-C signal appeared as a very broad resonance at 132 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{27}B_9Br_2NO]^-$: 567.1313; found: 567.1329.

Product [Et_4N][3p]



Reaction conditions: 12 h, 25 °C; 55% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$NMR (400 MHz, acetone-d_6): δ 7.51 (s, 2H), 7.34-7.26 (m, 4H), 7.23-7.16 (m, 2H), 6.90 (d, J = 18.0 Hz, 2H), 6.61 (d, J = 6.7 Hz, 1H, NH), 6.41 (d, J =18.0 Hz, 2H), 5.50 (broad signal, 1H, BH), 4.36-4.20 (m, 1H), 3.44 (q, J = 7.2 Hz, 8H), 1.93 (broad signal, 2H, BH), 1.35 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.22 (d, J = 6.6 Hz, 6H), 1.09-0.83 (broad overlapping signals, 4H, BH).

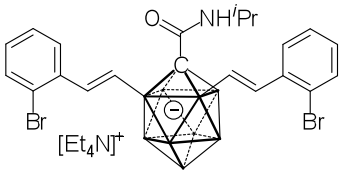
^{11}B NMR (128 MHz, acetone-d_6): δ 29.72 (d, J = 148.5 Hz, 1B), -8.93 (s, 2B), -14.81 (d, J = 141.9 Hz, 2B), *ca.* -18.3 to -25.2 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.81 (1B), -8.92 (2B), -14.77 (2B), *ca.* -18.8 to -23.9 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.41 (C=O), 143.10 (C_q), 139.09 (CH), 131.13 (CH), 130.01 (CH), 129.10 (CH), 125.51 (CH), 123.06 (C_q), 52.98 (t, J = 3.1 Hz, cation CH_2), 42.15 (*i*Pr CH), 23.14 (*i*Pr CH_3), 7.66 (cation CH_3). The B-C signal appeared as a very broad resonance at 133 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{27}B_9Br_2NO]^-$: 567.1313; found: 567.1340.

Product [Et_4N][3q]



Reaction conditions: 12 h, 25 °C; 47% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.66-7.59 (m, 2H), 7.51-7.44 (m, 2H), 7.32-7.24 (m, 2H), 7.10-7.02 (m, 2H), 6.94-6.80 (overlapping signals from which the coupling constant could not be determined because of "roof effect", 4H, alkenyl H), 6.57 (broad d, *J* = 5.9 Hz, 1H, NH), 5.53 (broad signal, 1H, BH), 4.32-4.17 (m, 1H), 3.42 (q, *J* = 7.3 Hz, 8H), 1.96 (broad signal, 2H, BH), 1.34 (tt, *J* =7.2 Hz, 1.8 Hz, 12H), 1.19 (d, *J* = 6.6 Hz, 6H), 1.14-0.8 (broad overlapping signals, 4H, BH).

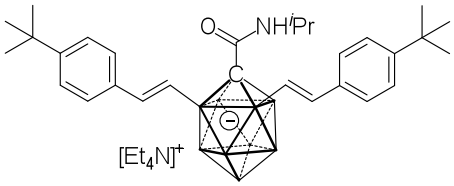
^{11}B NMR (128 MHz, acetone-d_6): δ 29.95 (d, *J* = 154.0 Hz, 1B), -8.85 (s, 2B), -14.76 (d, *J* = 142.8 Hz, 2B), *ca.* -18.1 to -24.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.97 (1B), -8.90 (2B), -14.80 (2B), *ca.* -18.7 to -24.7 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.32 (C=O), 139.93 (C_q), 138.84 (CH), 133.50 (CH), 128.91 (CH), 128.35 (CH), 127.40 (CH), 123.51 (C_q), 52.99 (t, *J* = 3.2 Hz, cation CH_2), 42.17 (*i*Pr CH), 23.16 (*i*Pr CH_3), 7.68 (cation CH_3). The B-C signal appeared as a very broad resonance at 135 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{27}B_9Br_2NO]^-$: 567.1313; found: 567.1326.

Product [Et_4N][3r]



Reaction conditions: 24 h, 25 °C; 48% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 5:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.33-7.22 (m, 8H), 6.75 (d, J = 18.0 Hz, 2H), 6.57 (broad d, J = 7.6 Hz, 1H, NH), 6.47 (d, J = 18.0 Hz, 2H), 5.49 (broad signal, 1H, BH), 4.32-4.19 (m, 1H), 3.38 (q, J = 7.3 Hz, 8H), 1.93 (broad signal, 2H, BH), 1.31 (tt, J = 7.2 Hz, 1.6 Hz, 12H), 1.26 (s, 18H), 1.21 (d, J = 6.6 Hz, 6H), 1.11-0.86 (broad overlapping signals, 4H, BH).

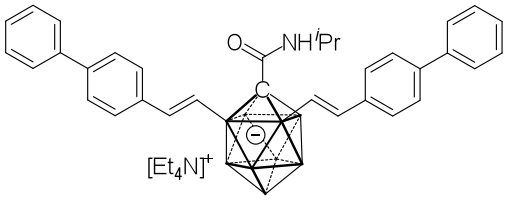
^{11}B NMR (128 MHz, acetone-d_6): δ 29.44 (d, J = 152.6 Hz, 1B), -8.55 (s, 2B), -14.81 (d, J = 124.4 Hz, 2B), *ca.* -18.2 to -24.2 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.52 (1B), -8.62 (2B), -14.89 (2B), *ca.* -19.0 to -23.6 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.59 (C=O), 150.13 (C_q), 140.75 (CH), 137.95 (C_q), 126.30 (CH), 125.96 (CH), 52.98 (t, J = 3.2 Hz, cation CH_2), 42.11 (*i*Pr CH), 34.93 (C_q), 31.61 (CH_3), 23.25 (*i*Pr CH_3), 7.66 (cation CH_3). The B-C signal appeared as a very broad resonance at 130 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{29}H_{45}B_9NO]^-$: 521.4375; found: 521.4387.

Product [Et_4N][3s]



Reaction conditions: 12 h, 30 °C; 52% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.67-7.61 (m, 4H), 7.61-7.54 (m, 4H), 7.48-7.38 (m, 8H), 7.34-7.28 (m, 2H), 6.92 (d, *J* = 18.0 Hz, 2H), 6.64 (broad d, *J* = 7.9 Hz, 1H, NH), 6.55 (d, *J* =18.0 Hz, 2H), 5.53 (broad signal, 1H, BH), 4.37-4.22 (m, 1H), 3.37 (q, *J* = 7.2 Hz, 8H), 1.97 (broad signal, 2H, BH), 1.30 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.24 (d, *J* = 6.6 Hz, 6H), 1.17-0.82 (broad overlapping signals, 4H, BH).

^{11}B NMR (128 MHz, acetone-d_6): δ 29.66 (d, *J* = 155.4 Hz, 1B), -8.53 (s, 2B), -14.72 (d, *J* = 105.3 Hz, 2B), *ca.* -18.1 to -25.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.66 (1B), -8.48 (2B), -14.69 (2B), *ca.* -18.7 to -23.5 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.59 (C=O), 141.49 (C_q), 140.39 (two overlapping quaternary C according to integration and DEPT spectra), 139.79 (CH), 129.66 (CH), 127.93 (CH), 127.61 (CH), 127.36 (CH), 127.12 (CH), 52.97 (t, *J* = 3.1 Hz, cation CH_2), 42.16 (*i*Pr CH), 23.24 (*i*Pr CH_3), 7.64 (cation CH_3). The B-C signal appeared as a very broad resonance at 131 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{33}H_{37}B_9NO]^-$: 561.3749; found: 561.3762.

With respect to UV/Vis absorption properties, a comparison of data for [Et_4N][**1**], 4-vinyl-1,1'-biphenyl and [Et_4N][**3s**] is given in Table S1 and Figure S4.

For [Et_4N][**3s**] compared to 4-vinyl-1,1'-biphenyl, the change in λ_{max} and ε ($\varepsilon_{\mathbf{3s}} > 2 \cdot \varepsilon_{alkene}$) is interpreted in terms of a certain degree of conjugation transmitted through the boron cage; see the discussion and references in the manuscript main text.

Table S1. UV/Vis properties of [Et_4N][**1**], 4-vinyl-1,1'-biphenyl and [Et_4N][**3s**].

Compound	**Solvent / concentration**	λ_{max} **(**ε**)**[a]
[Et_4N][**1**]	MeCN / $1.49 \cdot 10^{-5}$ M	– [b]
4-vinyl-1,1'-biphenyl	MeCN / $1.49 \cdot 10^{-5}$ M	290 nm ($2.14 \cdot 10^4$)[c]
[Et_4N][**3s**]	MeCN / $1.49 \cdot 10^{-5}$ M	299 nm ($6.71 \cdot 10^4$)

[a]The unit of ε is $mol^{-1}dm^3cm^{-1}$; [b]no characteristic absorption was observed in the range of 190–500 nm; [c]reported ε value for 4-vinyl-1,1'-biphenyl is $2.37 \cdot 10^4$ [6].

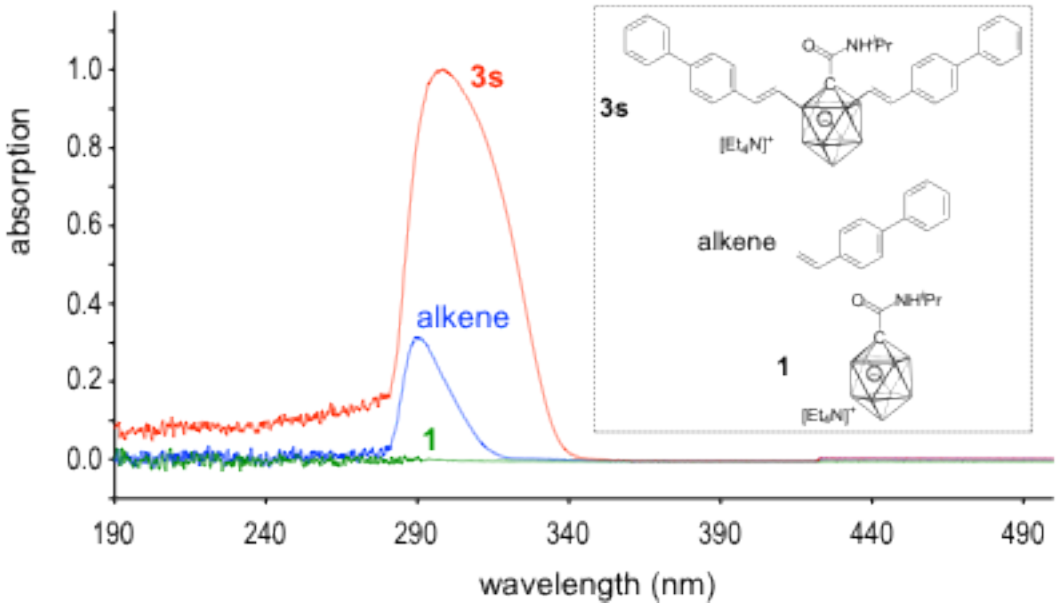
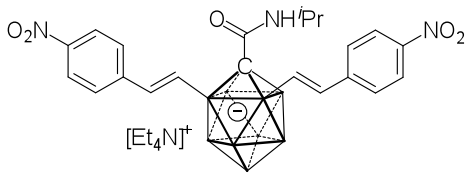


Figure S4. UV/Vis absorption spectra of [Et_4N][**1**] (green), 4-vinyl-1,1'-biphenyl (blue) and [Et_4N][**3s**] (red). Conditions: MeCN, c = $1.49 \cdot 10^{-5}$ M for all compounds.

Product [Et_4N][3t]



Reaction conditions: 24 h, 30 °C; 33% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

Based on the $^1H\{^{11}B\}$ NMR spectrum, the purity of **3t** was 96%. We were not able to separate the unknown impurity from the desired product chromatographically. The yield was corrected accordingly.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 8.18-8.11 (m, 4H), 7.62-7.53 (m, 4H), 7.18 (d, *J* = 18.0 Hz, 2H), 6.69 (d, *J* = 6.4 Hz, 1H, NH), 6.57 (d, *J* =18.0 Hz, 2H), 5.55 (broad signal, 1H, BH), 4.37-4.22 (m, 1H), 3.47 (q, *J* = 7.2 Hz, 8H), 1.96 (broad signal, 2H, BH), 1.37 (m, 12H), 1.23 (d, *J* = 6.6 Hz, 6H), 1.10-0.87 (broad overlapping signals, 4H, BH).

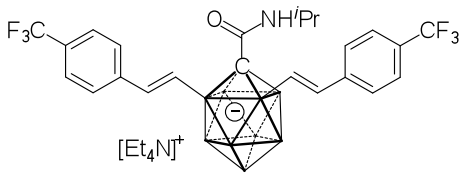
^{11}B NMR (128 MHz, acetone-d_6): δ 30.11 (d, *J* = 151.4 Hz, 1B), -9.04 (s, 2B), -14.65 (d, *J* = 131.9 Hz, 2B), *ca.* -18.2 to -24.7 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 30.19 (1B), -9.11 (2B), -14.66 (2B), *ca.* -18.6 to -24.4 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.30 (C=O), 147.07 (C_q), 146.95 (C_q), 138.73 (CH), 127.21 (CH), 124.60 (CH), 53.00 (t, *J* =2.8 Hz, cation CH_2), 42.26 (*i*Pr CH), 23.10 (*i*Pr CH_3), 7.67 (cation CH_3). The B-C signal appeared as a very broad resonance at 137 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{21}H_{27}B_9N_3O_5]^-$: 499.2825; found:499.2858.

Product [Et_4N][3u]



Reaction conditions: 16 h, 20 °C; 40% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.61-7.50 (m, 8H), 7.04 (d, J = 18.0 Hz, 2H), 6.63 (broad d, J = 6.6 Hz, 1H, NH), 6.53 (d, J =18.0 Hz, 2H), 5.53 (broad signal, 1H, BH), 4.35-4.20 (m, 1H), 3.45 (q, J = 7.2 Hz, 8H), 1.94 (broad signal, 2H, BH), 1.36 (tt, J = 7.2 Hz, 1.7 Hz, 12H), 1.22 (d, J = 6.6 Hz, 6H), 1.14-0.77 (broad overlapping signals, 4H, BH).

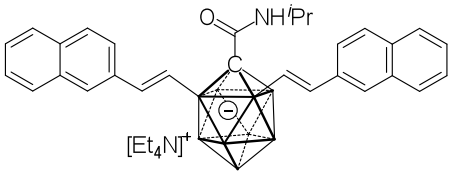
^{11}B NMR (128 MHz, acetone-d_6): δ 29.88 (d, J = 154.5 Hz, 1B), -8.90 (s, 2B), -14.75 (d, J = 137.8 Hz, 2B), *ca.* -18.2 to -24.9 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.95 (1B), -8.93 (2B), -14.76 (2B), *ca.* -18.9 to -24.0 (three overlapping signals from B6–9, 4B).

$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.38 (C=O), 144.38 (C_q), 139.24 (CH), 128.42 (q, J = 31.7 Hz, C_q), 126.96 (CH), 126.10 (q, J = 3.8 Hz, CH), 125.58 (q, J = 271 Hz, CF_3 C_q), 53.00 (t, J =2.8 Hz, cation CH_2), 42.20 (*i*Pr CH), 23.13 (*i*Pr CH_3), 7.66 (cation CH_3).
The B-C signal appeared as a very broad resonance at 134 ppm; the cage C signal was not detected unambiguously. For details, see the copy of the spectrum.

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{23}H_{27}B_9F_6NO]^-$: 545.2871, found: 545.2870.

Product [Et_4N][3v]



Reaction conditions: 36 h, 30 °C; 54% yield, yellowish solid; eluent CH_2Cl_2:MeCN = 20:1 to CH_2Cl_2:MeCN = 10:1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6): δ 7.84-7.76 (m, 6H), 7.72-7.64 (m, 4H), 7.40 (m, 4H), 7.02 (d, *J* = 18.0 Hz, 2H), 6.70 (d, *J* =18.0 Hz, 2H), 6.65 (broad siganl, overlapping with doublet at 6.70 ppm, 1H, NH), 5.56 (broad signal, 1H, BH), 4.36-4.24 (m, 1H), 3.33 (q, *J* = 7.2 Hz, 8H), 2.00 (broad signal, 2H, BH), 1.27 (tt, *J* = 7.2 Hz, 1.7 Hz, 12H), 1.22 (d, *J* = 6.6 Hz, 6H), 1.18-0.92 (broad overlapping signals, 4H, BH).

^{11}B NMR (128 MHz, acetone-d_6): δ 29.62 (d, *J* = 156.5 Hz, 1B), -8.49 (s, 2B), -14.74 (d, *J* = 133.3 Hz, 2B), *ca.* -18.2 to -24.4 (three overlapping d from B6–9, 4B).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6): δ 29.71 (1B), -8.64 (2B), -14.71 (2B), *ca.* -18.5 to -24.5 (three overlapping signals from B6–9, 4B).

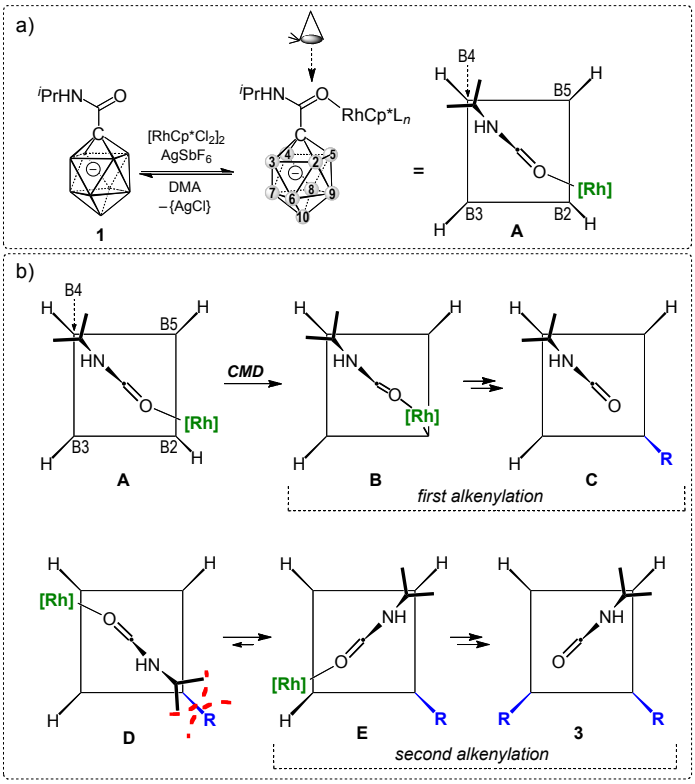
$^{13}C\{^1H\}$ NMR (101 MHz, acetone-d_6): δ 167.64 (C=O), 140.99 (CH), 138.20 (C_q), 134.86 (C_q), 133.68 (C_q), 128.75 (CH), 128.70 (CH), 128.38 (CH), 126.88 (CH), 126.18 (CH), 125.99 (CH), 124.38 (CH), 52.98 (t, *J* = 2.9 Hz, cation CH_2), 42.20 (*i*Pr CH), 23.26 (*i*Pr CH_3), 7.64 (cation CH_3). The B-C signal appeared as a very broad resonance at 131 ppm; the cage C signal was not detected unambiguously

HRMS ((–)-ESI): *m*/*z* calculated for $[C_{29}H_{33}B_9NO]^-$: 509.3436; found: 509.3452.

Proposed model to account for the observed B2/3 regioselectivity

A plausible mechanism accounting for the regioselectivity is shown in Scheme S1. Based on previous mechanistic studies on transition metal-mediated B–H activation [references 11e, 11m, 11n, 12 and 14 in the main text], the transformation starts with coordination of the metal center by the oxygen atom of **1**, giving complex **A**, followed by cyclometalation–deprotonation affording five-membered rhodacycle **B**. Alkene coordination, insertion (to form the B–C bond), beta-hydride elimination (to give a rhodium hydride complex) and oxidation of the formal Rh(I) lead to mono-substituted **C**. For the second coupling, initial coordination of the Rh(III) can occur in a Rh–B4-eclipsed or Rh–B3-eclipsed geometry (species **D** and **E**). Because of steric repulsion between the amide isopropyl group and the substituent at B2, **E** is lower in energy and preferentially undergoes cyclometalation and subsequent steps to furnish observed regioisomer **3**.

The Cu(II) additive improves the amount of di-substituted product that is formed. Control experiments using standard conditions but 10 mol% copper instead of a stoichiometric amount showed that the di-substitution/mono-substitution ratio is better than without any copper, but worse than with 1 equiv of copper. Oxidative coupling to give the vinylic products takes place also in the absence of Cu(II), so it is likely that the rhodium hydride species reacts with protons in the reaction system (e.g. from residual H_2O) to give H_2 and Rh(III).



Scheme S1. Coordination of the rhodium center by **1** (a); proposed sequence to explain the B2/3 regioselectivity (b); DMA = dimethyl acetamide, Cp* = pentamethylcyclopentadienyl, L_n = additional ligands at Rh, CMD = cyclometalation– deprotonation.

III X-ray Crystallography

Crystal structure of 1 (CCDC 1854824)

Compound **1** (11 mg) was dissolved in dichloromethane (0.4 mL) in an NMR tube (5 mm diameter). Layering with hexane afforded colorless crystals of the composition $[Et_4N][C_5H_{17}B_9NO]$ suitable for X-ray diffraction within 2 d at 12 °C.

```
Bond precision:  C-C = 0.0060 A          Wavelength=0.71073

Cell:            a=31.845(4)    b=10.2834(6)          c=15.723(2)
                 alpha=90       beta=118.864(19)      gamma=90
Temperature:     293 K

                 Calculated                Reported
Volume           4509.2(12)                4509.1(12)
Space group      C 2/c                     C 1 2/c 1
Hall group       -C 2yc                    -C 2yc
Moiety formula   C5 H17 B9 N O, 0.5(C8 N), C5 H17 B9 N O, C4 H10
                 0.5(C8 H20 N)             N0.5, C4 N0.5
Sum formula      C13 H27 B9 N2 O           C13 H27 B9 N2 O
Mr               324.66                    324.65
Dx,g cm-3        0.956                     0.956
Z                8                         8
Mu (mm-1)        0.053                     0.053
F000             1376.0                    1376.0
F000'            1376.33
h,k,lmax         38,12,18                  38,12,18
Nref             4141                      4123
Tmin,Tmax        0.977,0.989               0.858,1.000
Tmin'            0.975

Correction method= # Reported T Limits: Tmin=0.858 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.349

R(reflections)= 0.0823( 2517)     wR2(reflections)= 0.2862( 4123)

S = 1.051                 Npar= 254
```

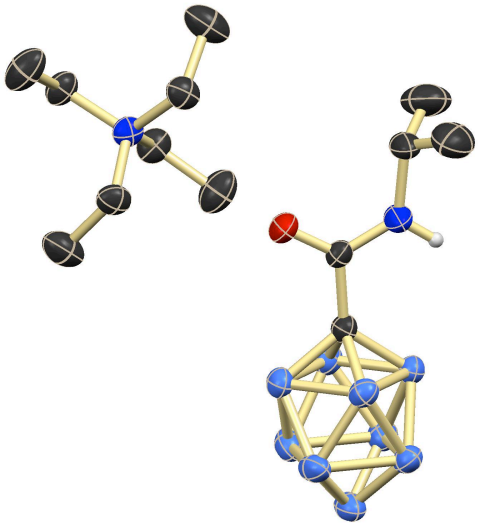


Figure S5. ORTEP representation of **1**. The disordered $[Et_4N]^+$ cation is not shown. H atoms except for NH are omitted for clarity; 25% displacement ellipsoids.

Two types of $[Et_4N]^+$ cations are present in this structure. One was refined, and the other one is heavily disordered, and its hydrogen positions were not calculated. The structure features a wR2 value of 0.2862, which is mainly attributed to the disordered cation and the fact that the crystal was measured at 293 K (our department does not routinely offer low-temperature measurements); connectivity, distances and angles for the anion could still be determined reliably.

Crystal structure of 3a (CCDC 1854825)

Compound **3a** (15 mg) was dissolved in a mixture of dichloromethane (0.3 mL) and acetone (0.05 mL) in an NMR tube (5 mm diameter). Layering with hexane afforded colorless crystals of the composition [Na][$C_{15}H_{29}B_9NO_5$][C_4H_9NO] suitable for X-ray diffraction within 20 d at 12 °C (C_4H_9NO is dimethyl acetamide solvent from the reaction).

```
Bond precision:  C-C = 0.0076 A          Wavelength=0.71073

Cell:           a=11.6821(10)    b=16.6672(16)      c=16.3779(11)
                alpha=90         beta=110.407(9)    gamma=90
Temperature:    150 K

                Calculated                Reported
Volume          2988.8(5)                 2988.8(5)
Space group     P 21/n                    P 1 21/n 1
Hall group      -P 2yn                    -P 2yn
Moiety formula  C19 H38 B9 N2 Na O6       C19 H38 B9 N2 Na O6
Sum formula     C19 H38 B9 N2 Na O6       C19 H38 B9 N2 Na O6
Mr              510.79                    510.79
Dx,g cm-3       1.135                     1.135
Z               4                         4
Mu (mm-1)       0.087                     0.087
F000            1080.0                    1080.0
F000'           1080.54
h,k,lmax        14,20,19                  14,20,19
Nref            5466                      5444
Tmin,Tmax       0.959,0.969               0.903,1.000
Tmin'           0.959

Correction method= # Reported T Limits: Tmin=0.903 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.996          Theta(max)= 25.342

R(reflections)= 0.0971( 3810)     wR2(reflections)= 0.2820( 5444)

S = 1.044                 Npar= 358
```

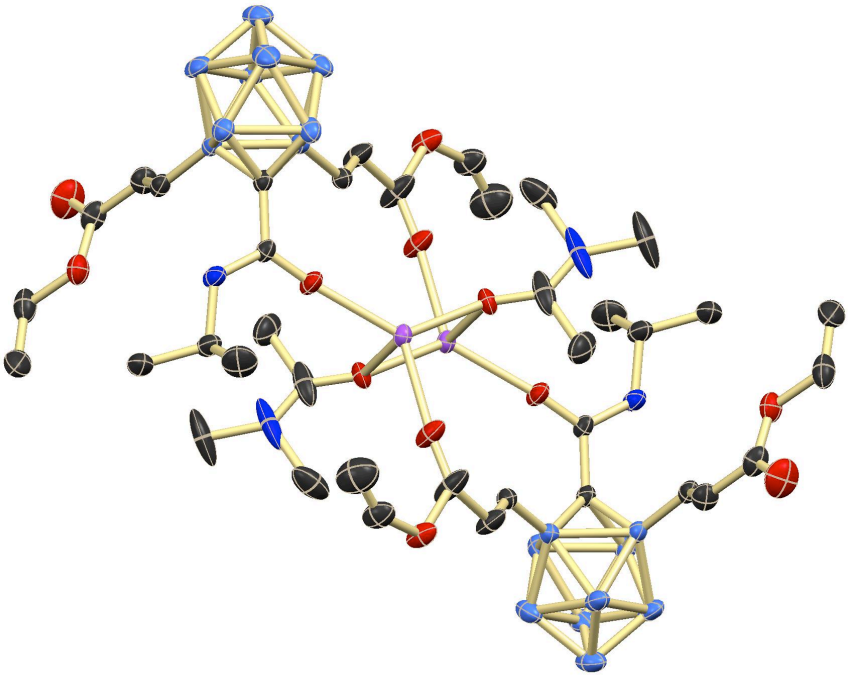


Figure S6. ORTEP representation of **3a**, showing two anions, two Na^+ and coordination by dimethyl acetamide. H atoms are omitted for clarity; 25% displacement ellipsoids.

Crystals of **3a** were obtained after purification by column chromatography before addition of Et_4NBr (see the general procedure on p. S4). Dimethylacetamide stems from the reaction mixture and co-eluted on the column; the presence of Na^+ results from the use of NaCl during the extraction. The structure features a wR2 value of 0.2820, which is mainly attributed to some disorder of one of the ethyl groups of the anion and disorder of the coordinating dimethylacetamide (relatively large differences in anisotropic displacement parameters were observed for dimethylacetamide).

Crystal structure of 3l (CCDC 1854826)

Compound **3a** (24 mg) was dissolved in a mixture of dichloromethane (0.3 mL) and acetone (0.05 mL) in an NMR tube (5 mm diameter). Layering with hexane afforded colorless crystals of the composition $[Na][C_{11}H_{25}B_9NO_5S_2]$ suitable for X-ray diffraction within 5 d at 12 °C.

Bond precision: C-C = 0.0150 A Wavelength=1.34139

Cell: a=14.3755(8) b=11.2861(6) c=51.571(3)
alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	8367.1(8)	8367.1(8)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C11 H25 B9 N Na O5 S2 [+ solvent]	C11 H25 B9 N Na O5 S2
Sum formula	C11 H25 B9 N Na O5 S2 [+ solvent]	C11 H25 B9 N Na O5 S2
Mr	435.72	435.72
Dx,g cm-3	0.692	0.692
Z	8	8
Mu (mm-1)	0.887	0.879
F000	1808.0	1808.0
F000'	1816.73	
h,k,lmax	17,13,63	17,13,63
Nref	8025	7759
Tmin,Tmax	0.949,0.974	0.493,0.743
Tmin'	0.932	

Correction method= # Reported T Limits: Tmin=0.493 Tmax=0.743
AbsCorr = MULTI-SCAN

Data completeness= 0.967 Theta(max)= 55.138

R(reflections)= 0.1650(5190) wR2(reflections)= 0.3961(7759)

S = 0.924 Npar= 271

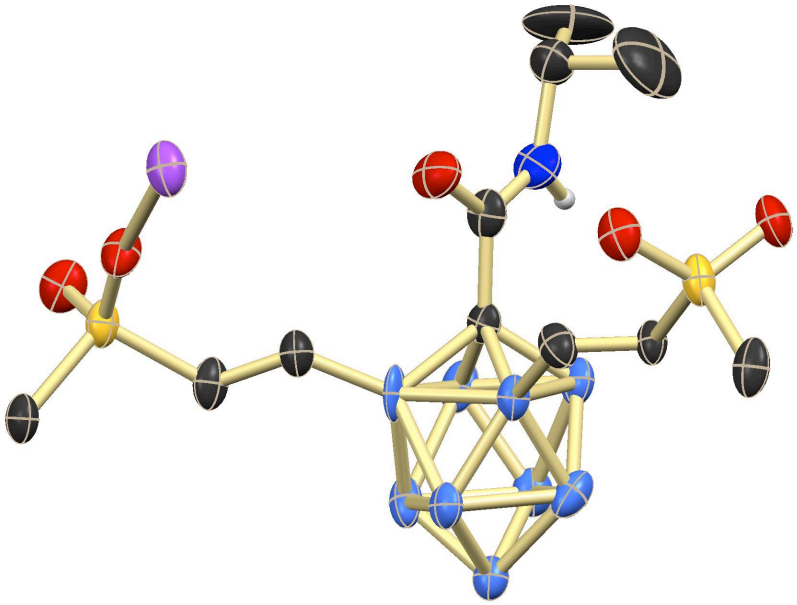


Figure S7. ORTEP representation of **3l**; H atoms except for NH are omitted for clarity; 25% displacement ellipsoids.

Crystals of **3l** were obtained after purification by column chromatography before addition of Et_4NBr (see the general procedure on p. S4). The presence of Na^+ results from the use of NaCl during the extraction. The structure features a wR2 value of 0.3961, which is mainly attributed to limited crystal quality. The connectivity, in particular the substitution pattern of the cage, can be inferred from the data, while distances and angles are associated with large standard uncertainties.

Crystal structure of 3n (CCDC 1854827)

Compound **3n** (12 mg) was dissolved in dichloromethane (0.4 mL) in an NMR tube (5 mm diameter). Layering with hexane afforded colorless crystals of the composition $[Et_4N][C_{21}H_{29}B_9NO]$ suitable for X-ray diffraction within 10 d at 12 °C.

```
Bond precision:  C-C = 0.0031 A          Wavelength=1.34139

Cell:            a=7.9588(2)     b=22.6600(4)       c=18.5609(3)
                 alpha=90        beta=90.433(1)     gamma=90
Temperature:     170 K

                 Calculated                  Reported
Volume           3347.30(12)                 3347.30(12)
Space group      C c                         C 1 c 1
Hall group       C -2yc                      C -2yc
Moiety formula   C21 H29 B9 N O, C8 H20 N    C21 H29 B9 N O, C8 H20 N
Sum formula      C29 H49 B9 N2 O             C29 H49 B9 N2 O
Mr               538.99                      538.99
Dx,g cm-3        1.070                       1.070
Z                4                           4
Mu (mm-1)        0.279                       0.283
F000             1160.0                      1160.0
F000'            1161.99
h,k,lmax         9,27,22                     9,27,22
Nref             6387[ 3200]                 5310
Tmin,Tmax        0.980,0.992                 0.514,0.751
Tmin'            0.967

Correction method= # Reported T Limits: Tmin=0.514 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 1.66/0.83      Theta(max)= 55.017

R(reflections)= 0.0333( 5165)     wR2(reflections)= 0.0857( 5310)

S = 1.063                 Npar= 380
```

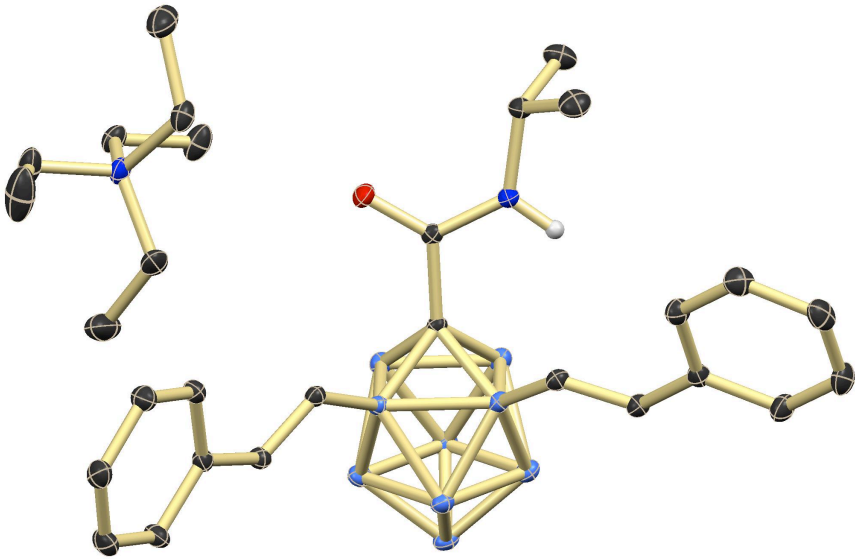


Figure S8. ORTEP representation of **3n**; H atoms except for NH are omitted for clarity; 25% displacement ellipsoids.

IV References

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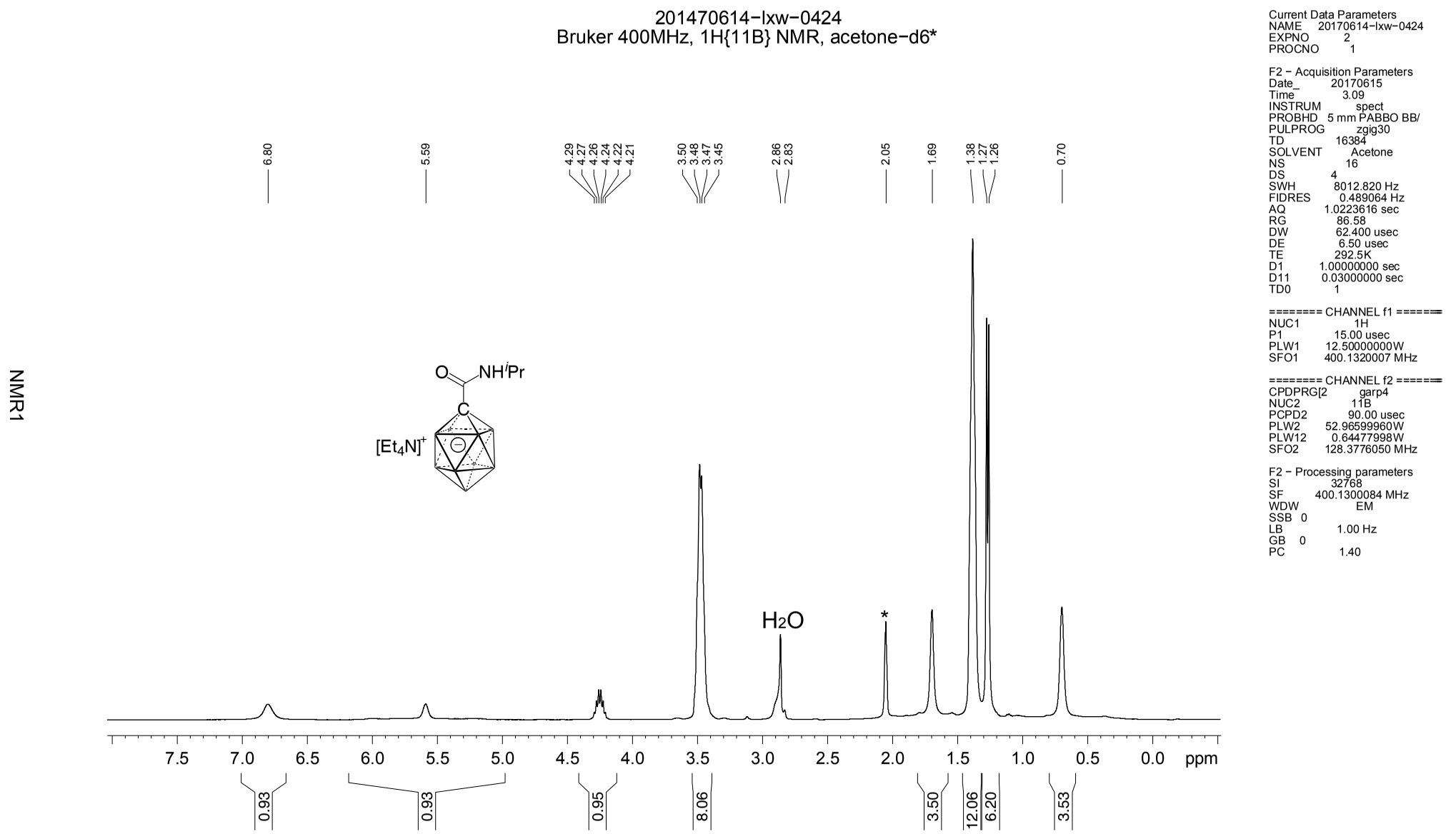

Current Data Parameters
NAME 20170614-lxw-0424
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170615
Time 3.09
INSTRUM spect
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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 292.5K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

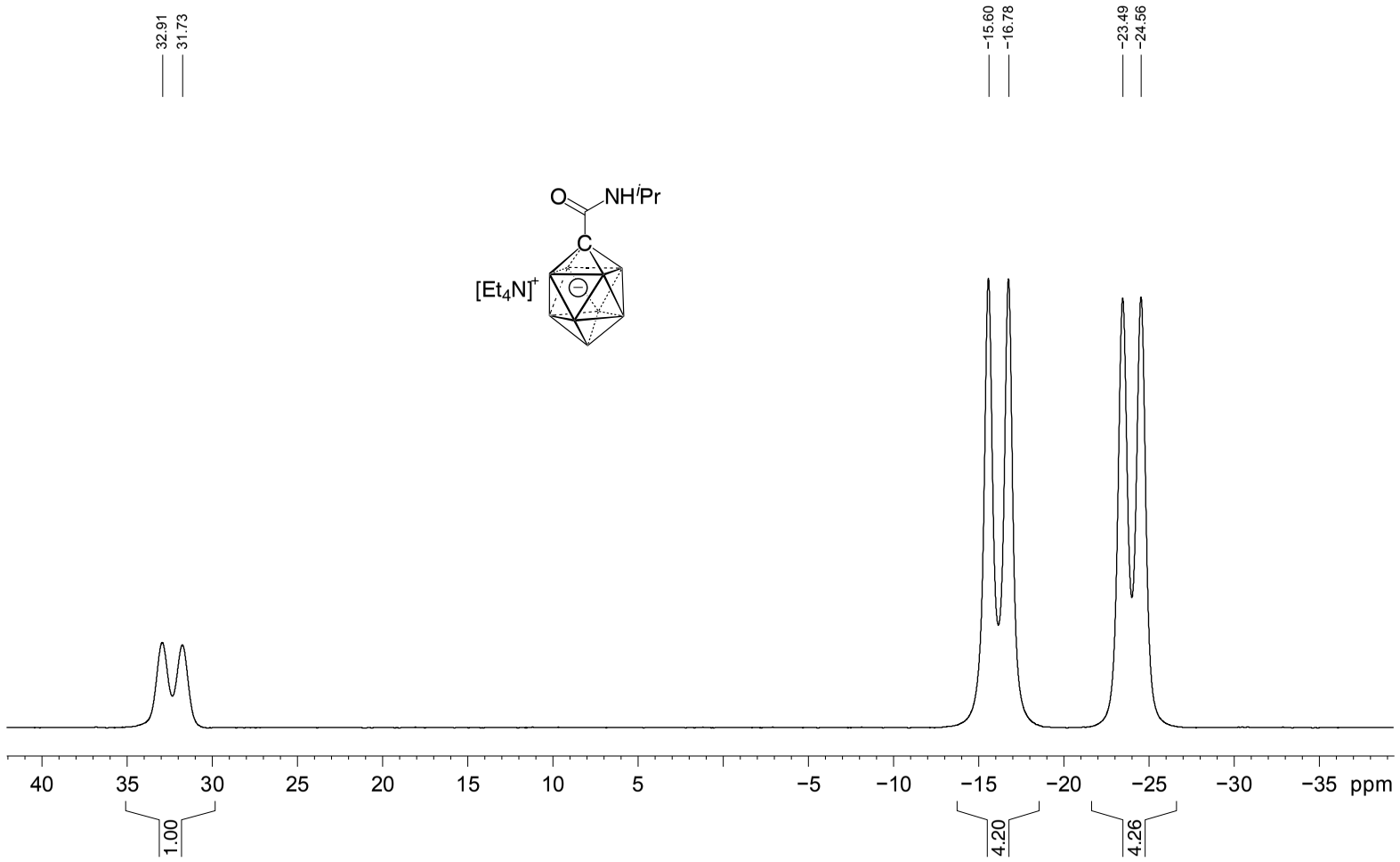
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

F2 - Processing parameters
SI 32768
SF 400.1300084 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR2

201470614-lxw-0424
Bruker 128MHz, 11B NMR acetone-d6



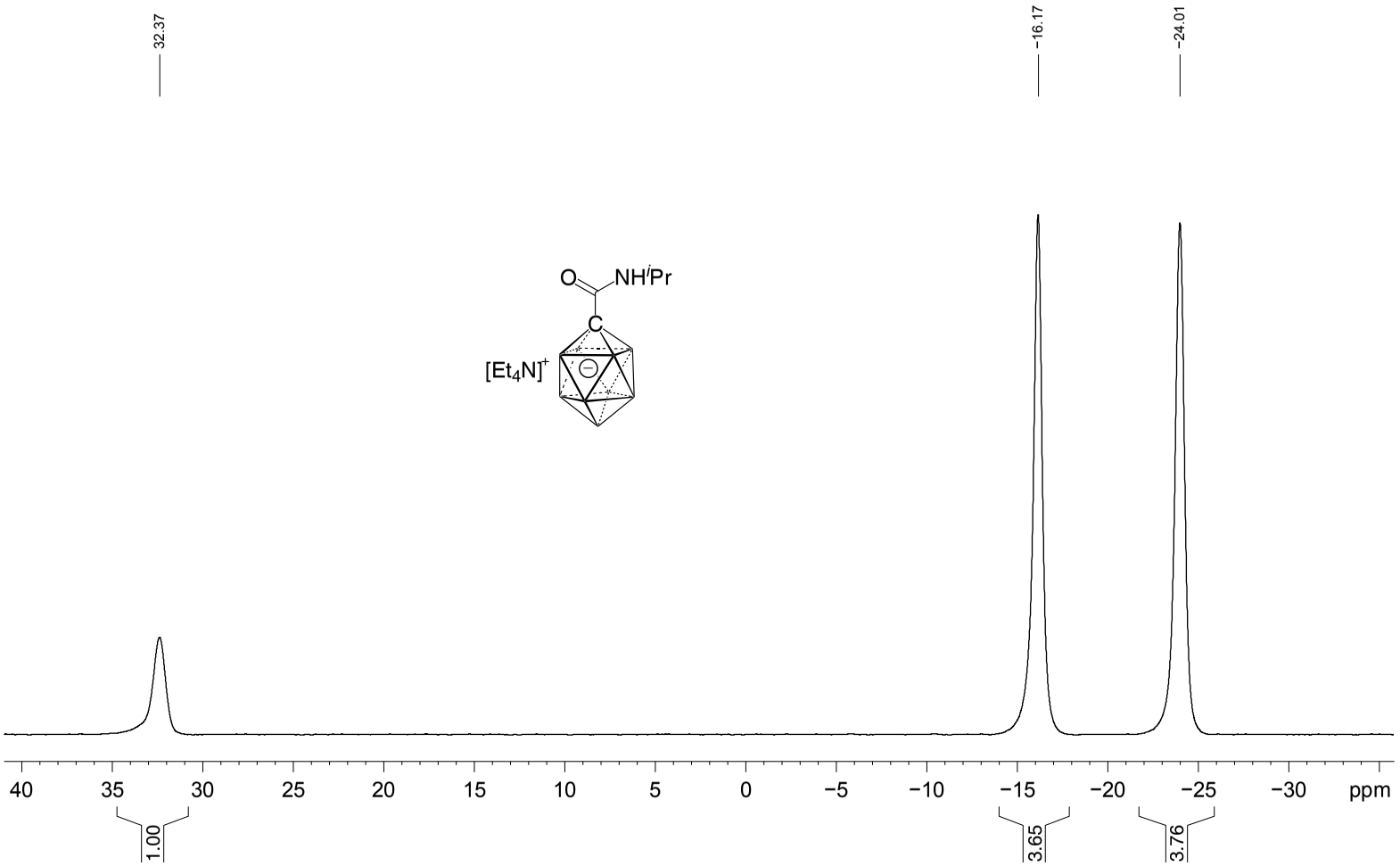
Current Data Parameters
NAME 20170614-lxw-0424
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170615
Time 3.21
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 292.0K
D1 1.00000000 sec
TD0 1

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

201470614-lxw
Bruker 128MHz, 11B{1H} NMR acetone-d6



NMR3

Current Data Parameters
NAME 20170614-lxw-0424
EXPNO 3
PROCNO 1

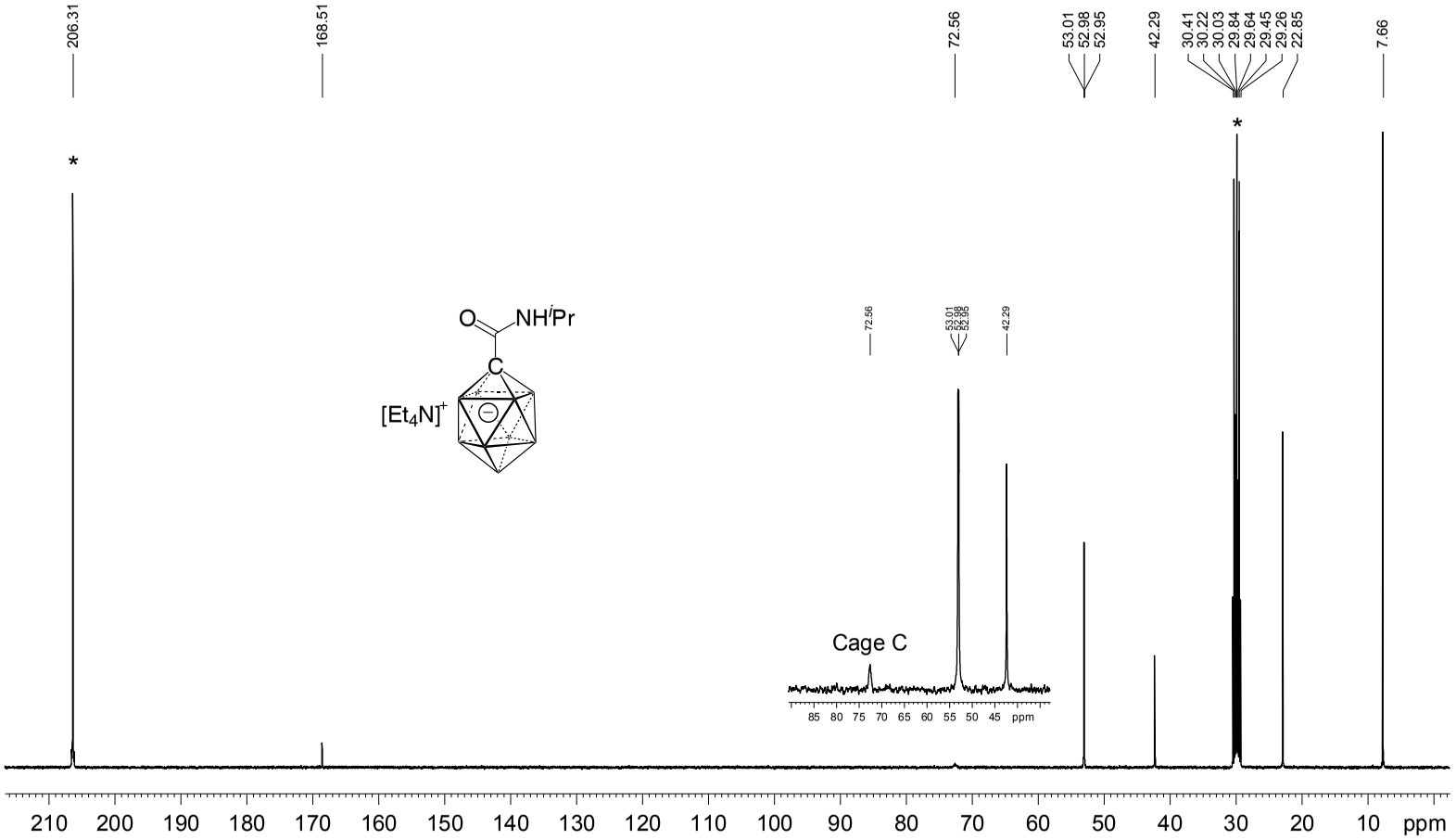
F2 - Acquisition Parameters
Date_ 20170615
Time 3.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 292.6K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20180709-lxw-CONHiPr
Bruker 101 MHz, acetone-d6*



NMR4

Current Data Parameters
NAME 20180709-lxw-CONHiPr
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180710
Time 15.40
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 408.5K
D1 1.10000002 sec
D11 0.03000000 sec
TD0 1

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

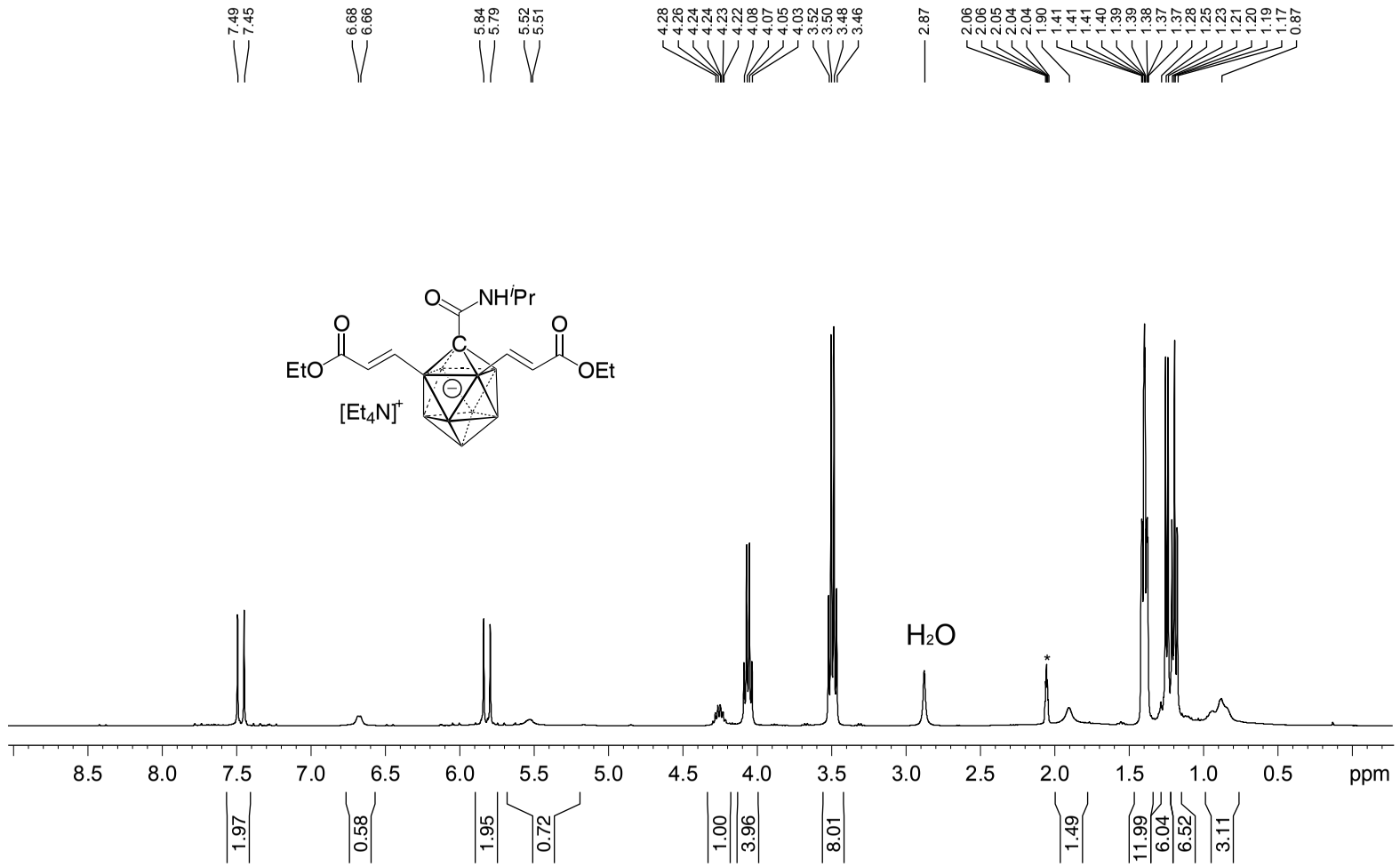
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000W
PLW12 0.43945000W
PLW13 0.28125000W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR5

20171023-lxw-0479-4

Bruker 400MHz, 1H{11B} NMR, acetone-d6*



Current Data Parameters
NAME 20171023-lxw-0479-4
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171024
Time 10.50
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 292.8K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

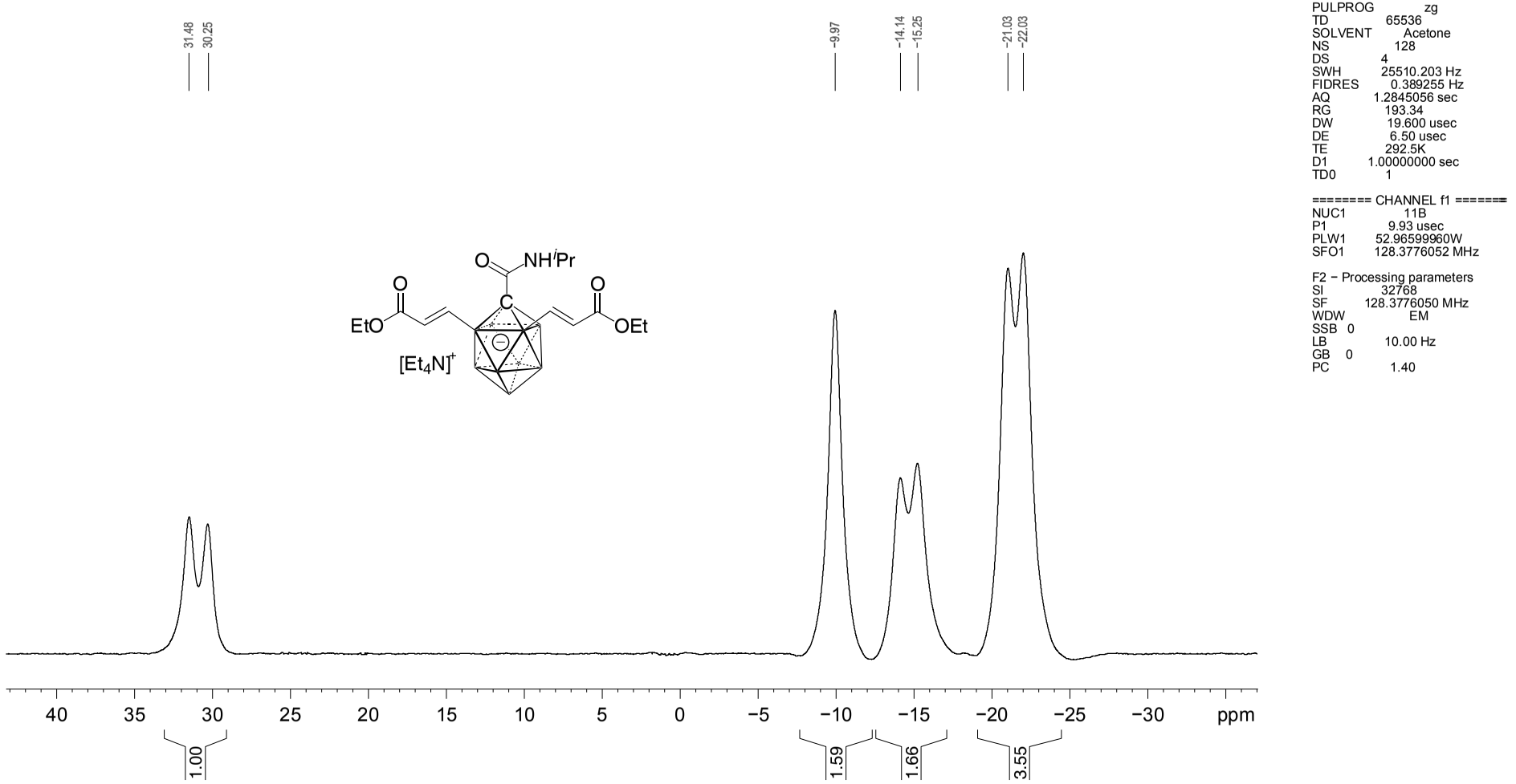
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

20171023-lxw-0479-4
Bruker 128MHz, 11B NMR, acetone-d6

NMR6



Current Data Parameters
NAME 20171023-lxw-0479-4
EXPNO 5
PROCNO 1

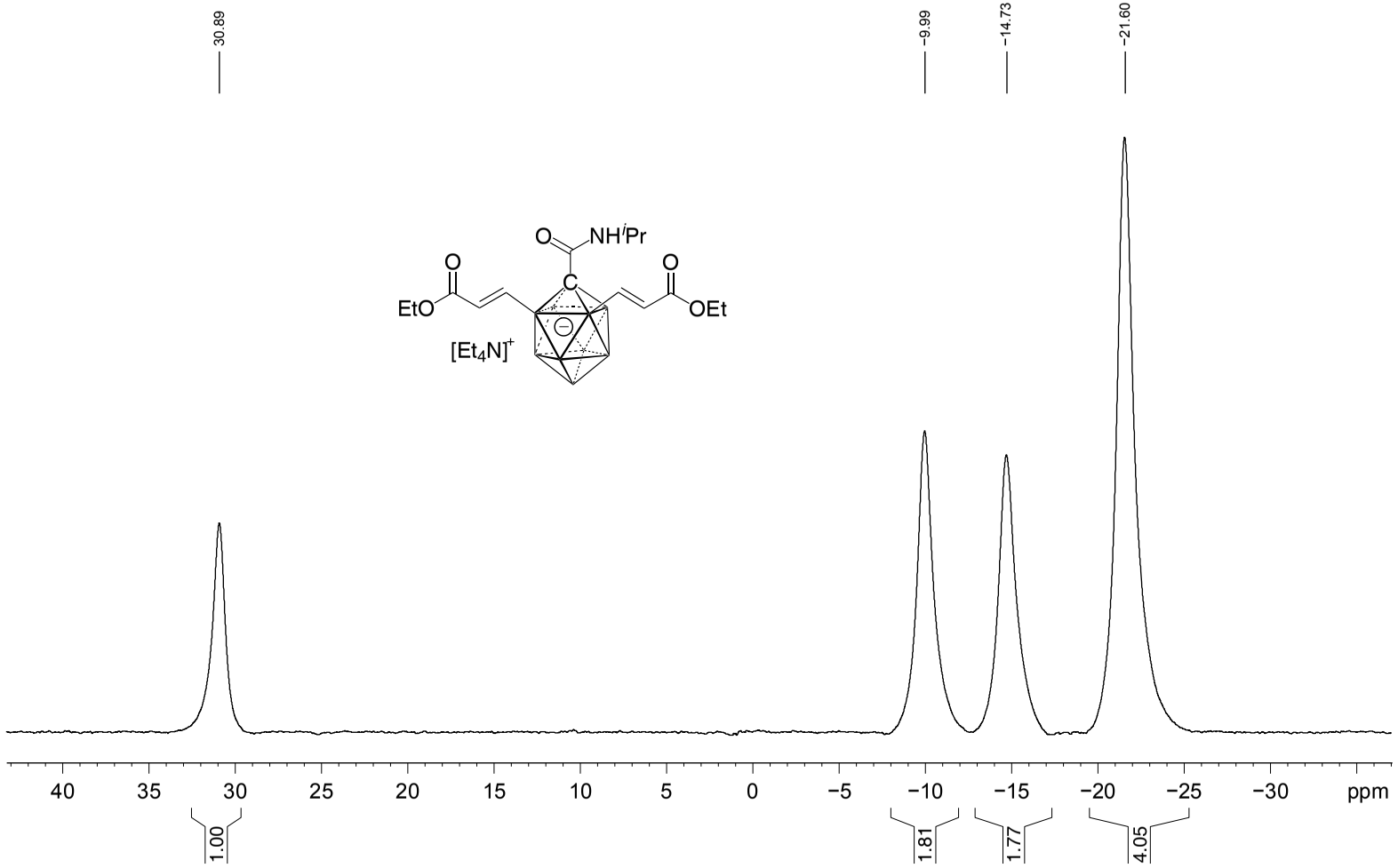
F2 - Acquisition Parameters
Date_ 20171024
Time 11.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 292.5K
D1 1.00000000 sec
TD0 1

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

NMR7

20171023-lxw-0479-4
Bruker 128MHz, 11B{1H} NMR, acetone-d6



Current Data Parameters
NAME 20171023-lxw-0479-4
EXPNO 4
PROCNO 1

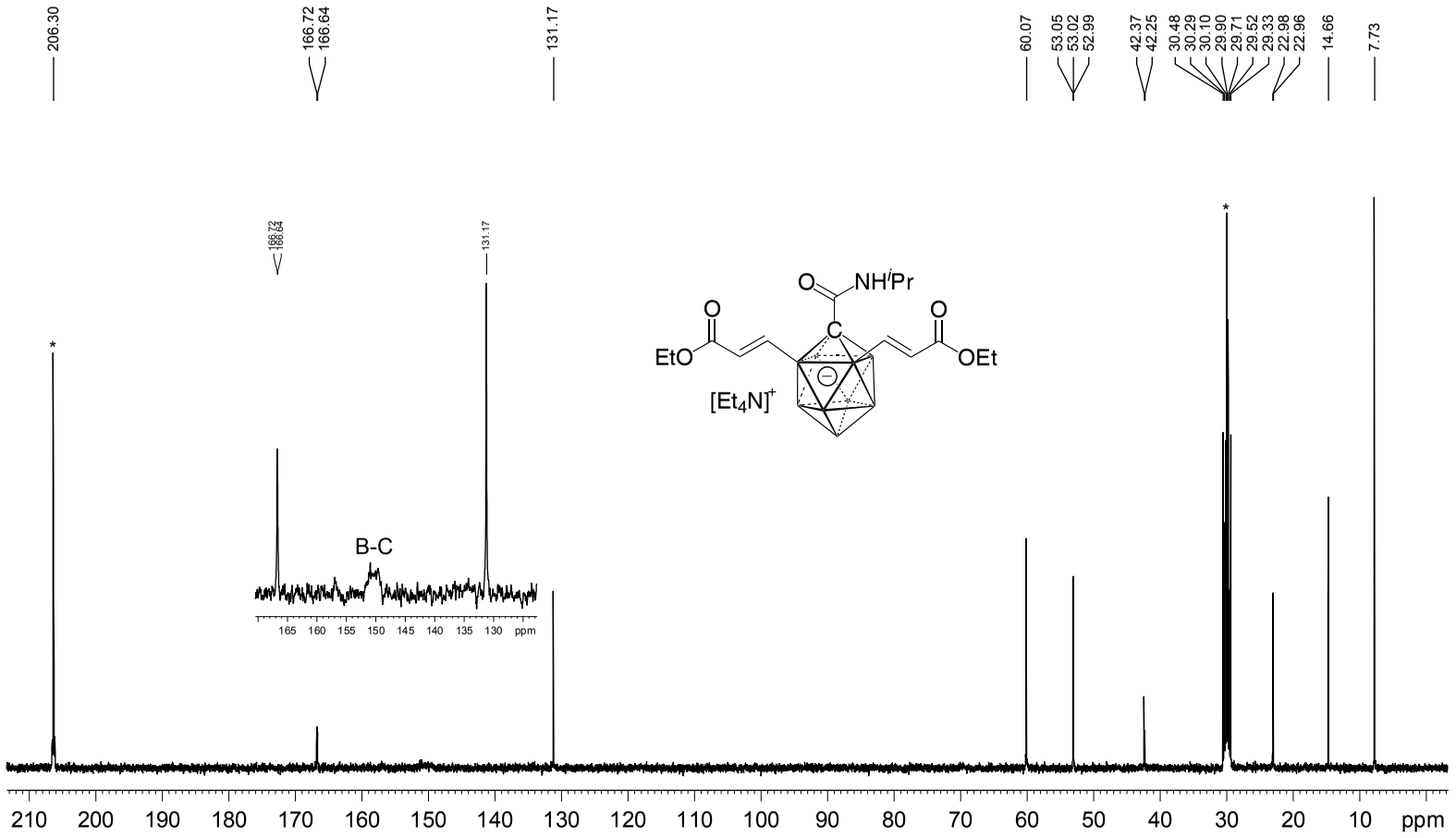
F2 - Acquisition Parameters
Date_ 20171024
Time 11.21
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 29[illegible].3
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171023-lxw-0479-4
Bruker 4101MHz, 13C NMR, acetone-d6*



NMR8

Current Data Parameters
NAME 20171023-lxw-0479-4
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171024
Time 11.14
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 293.7K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

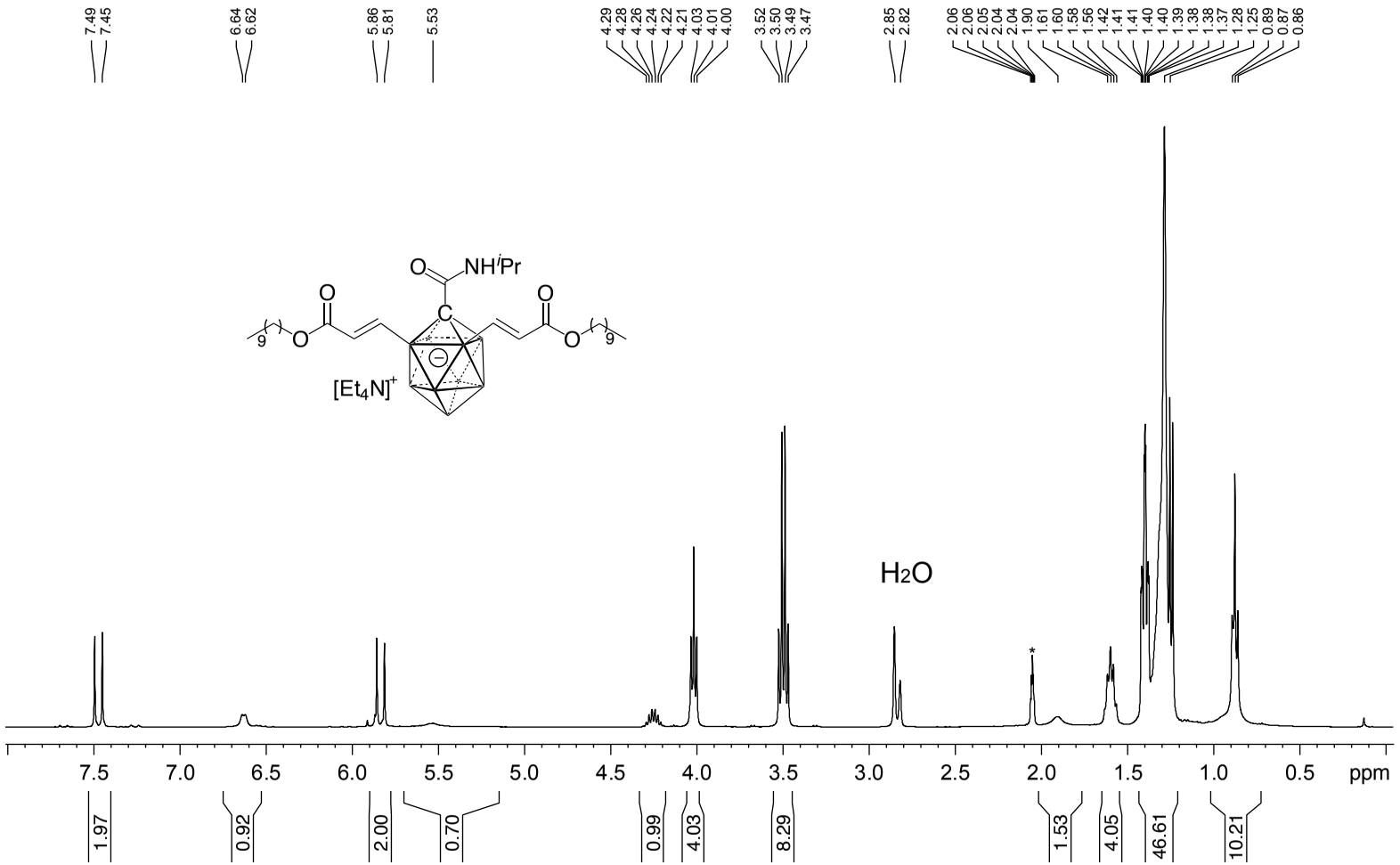
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR9

20171108-lxw-0486
Bruker 400Hz, 1H{11B} NMR, acetone-d6*



Current Data Parameters
NAME 20171108-lxw-0486
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 6.40
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 295.8K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

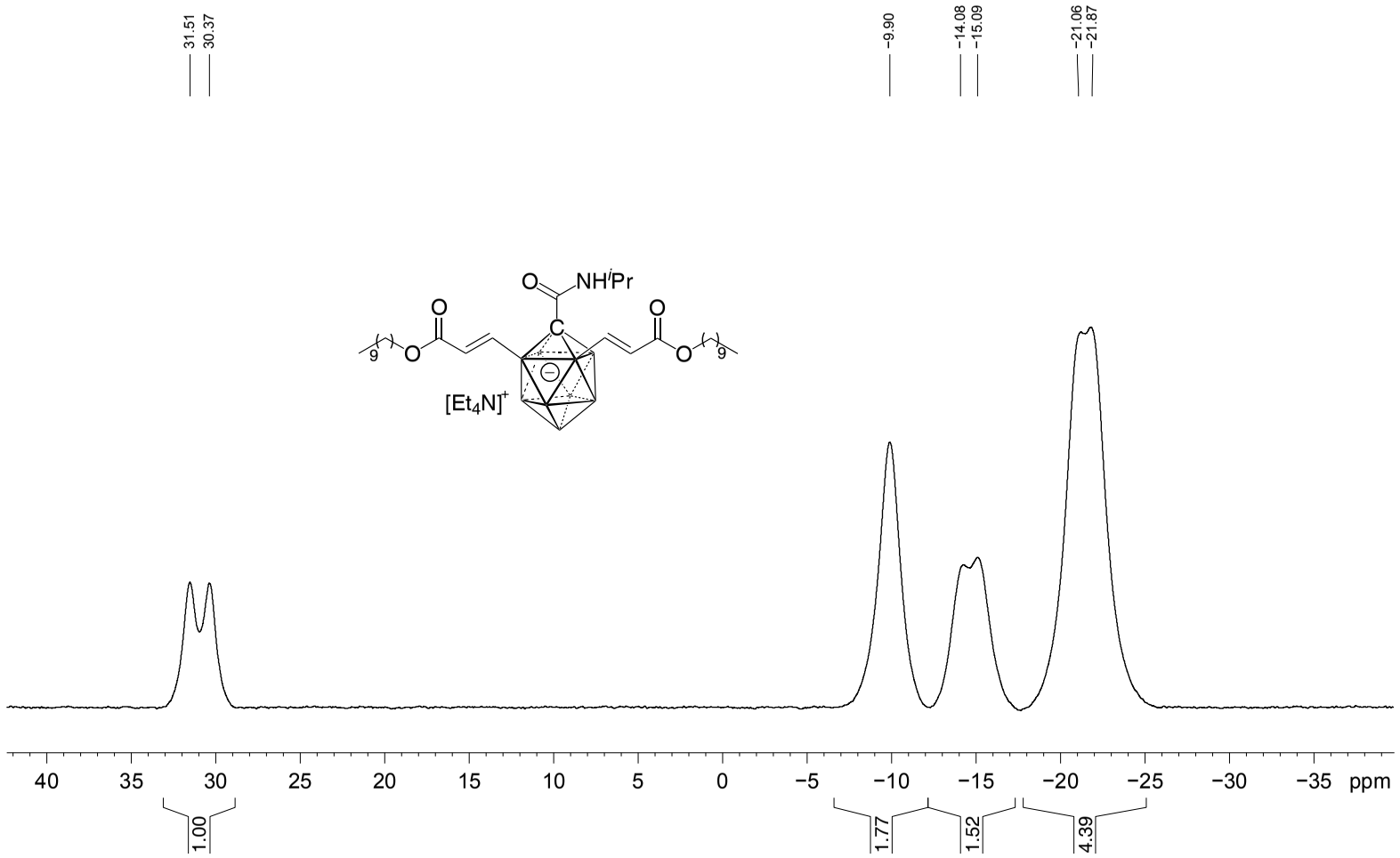
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR10

20171108-lxw-0486
Bruker 128MHz, 11B NMR, acetone-d6



Current Data Parameters
NAME 20171108-lxw-0486
EXPNO 4
PROCNO 1

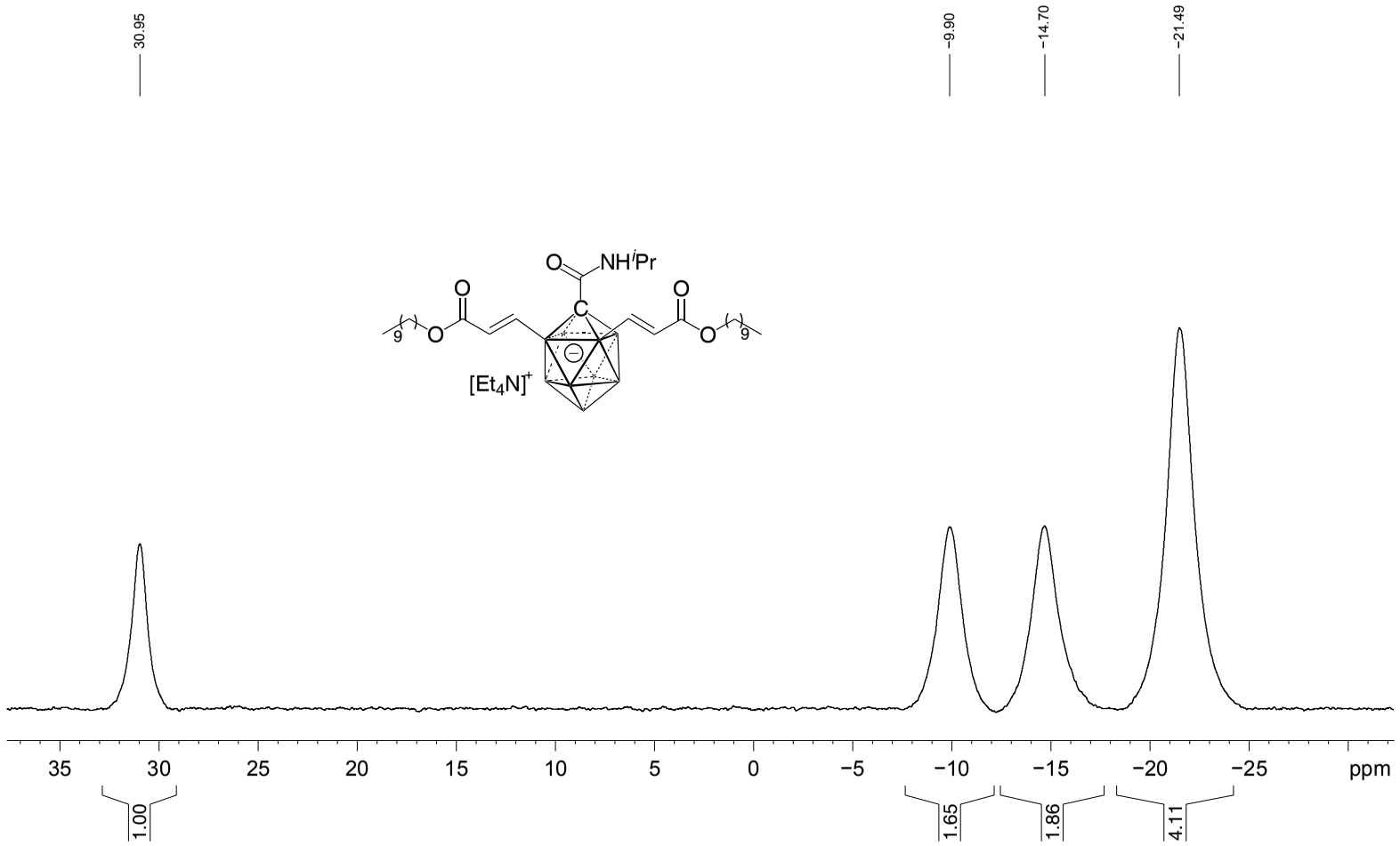
F2 - Acquisition Parameters
Date_ 20171109
Time 6.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.0K
D1 1.00000000 sec
TD0 1

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

NMR11

20171108-lxw-0486
Bruker 128MHz, 11B{1H} NMR, acetone-d6



Current Data Parameters
NAME 20171108-lxw-0486
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
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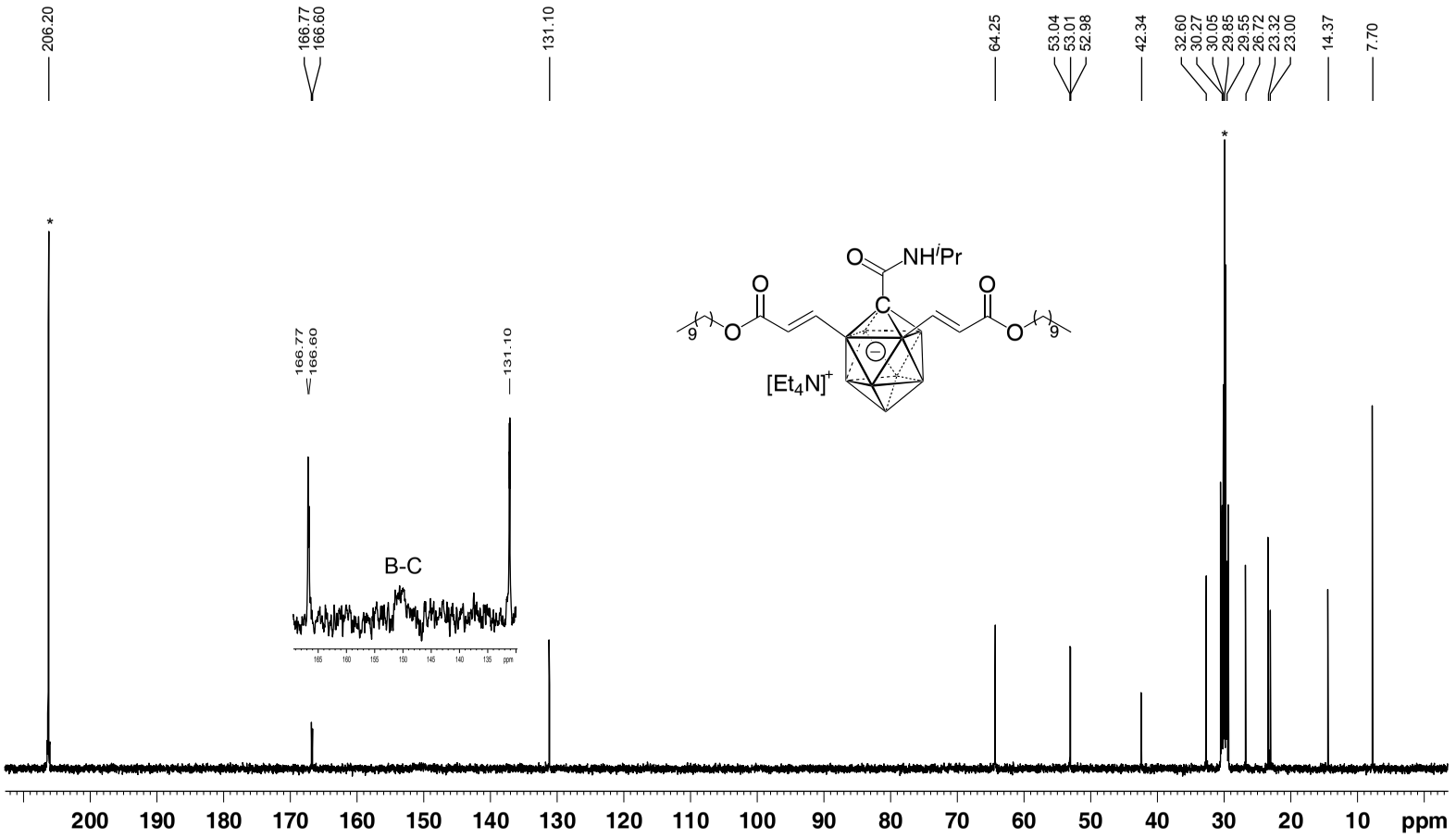
Time 6.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.0K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171108-lxw-0486
Bruker 101MHz, 13C NMR, acetone-d6*



NMR12

Current Data Parameters
NAME 20171108-lxw-0486
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 7.16
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 296.0K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

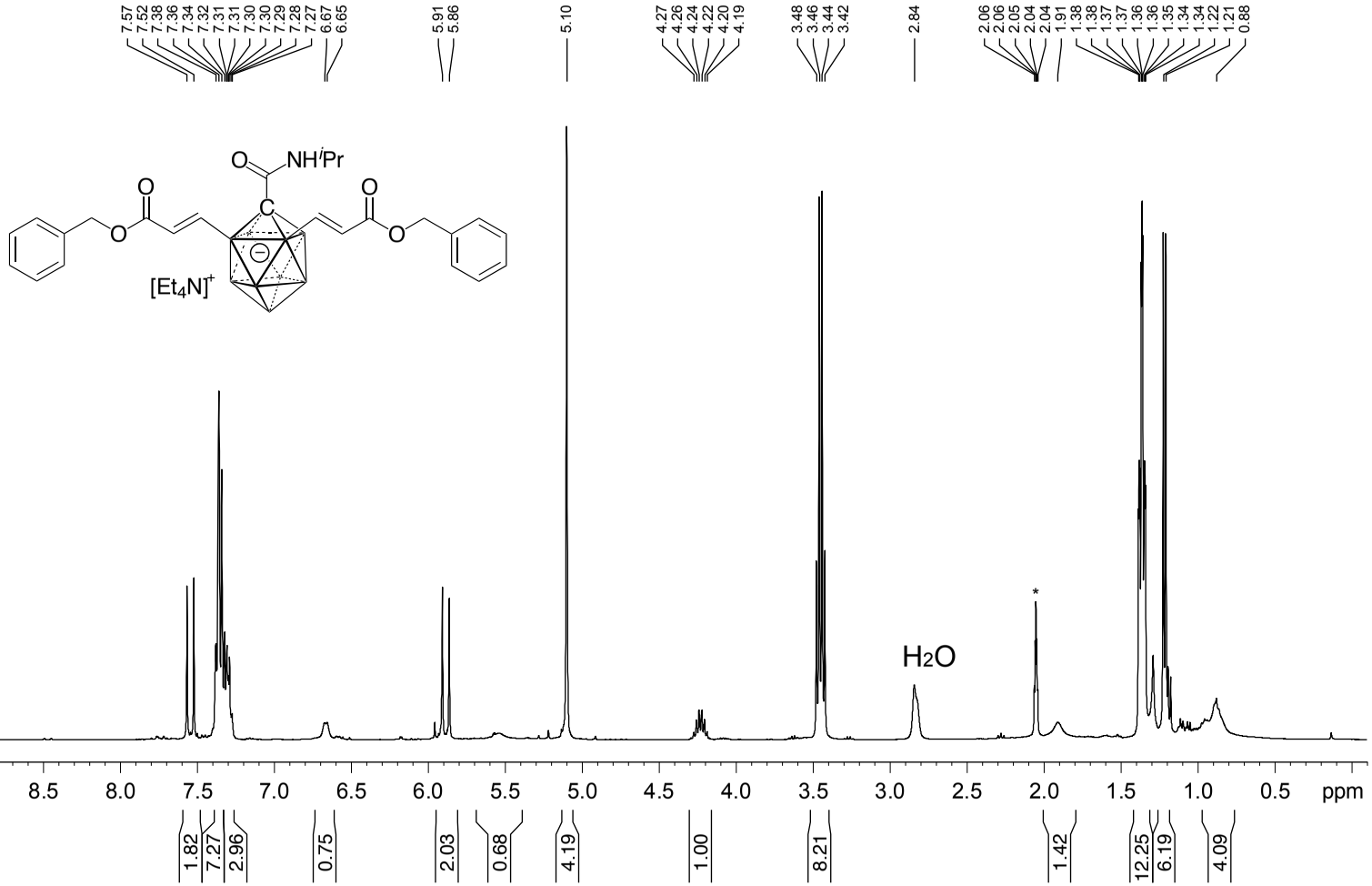
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126809 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR13

20171115-lxw-446
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171115-lxw-446
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 18.25
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 296.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

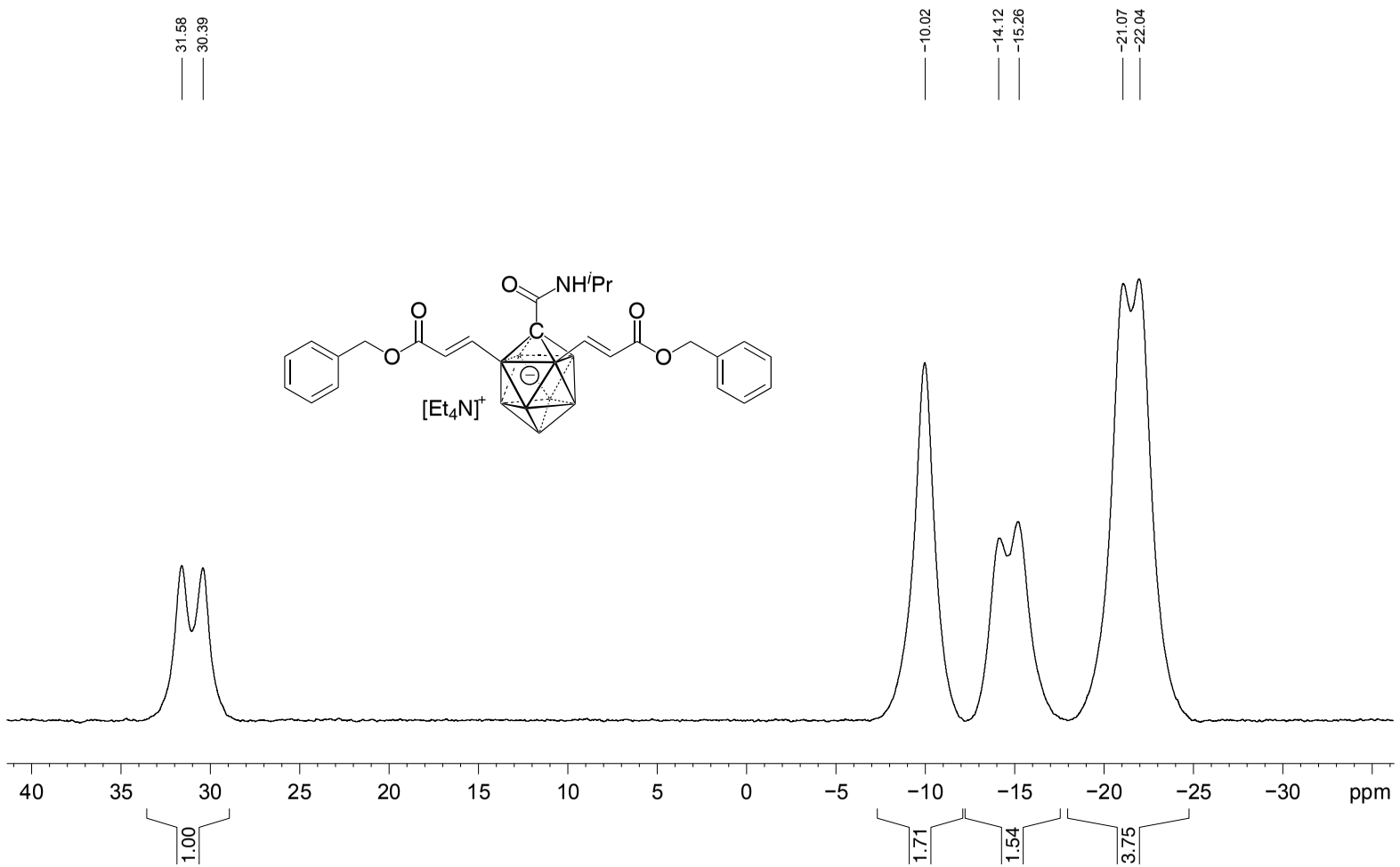
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR14

20171115-lxw-446
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171115-lxw-446
EXPNO 4
PROCNO 1

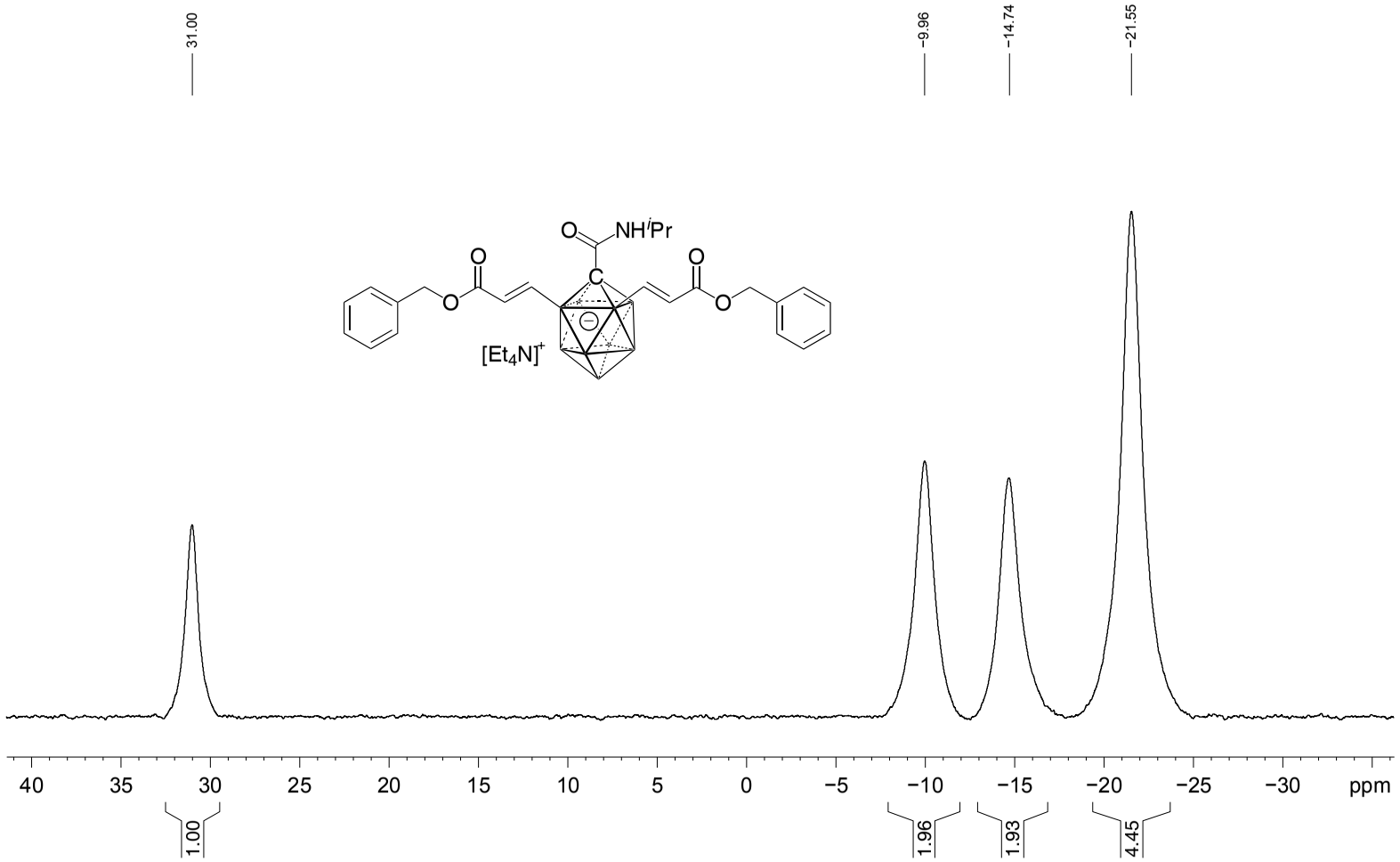
F2 - Acquisition Parameters
Date_ 20171116
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.7K
D1 1.00000000 sec
TD0 1

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

NMR15

20171115-lxw-446
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171115-lxw-446
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 18.31
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 297.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

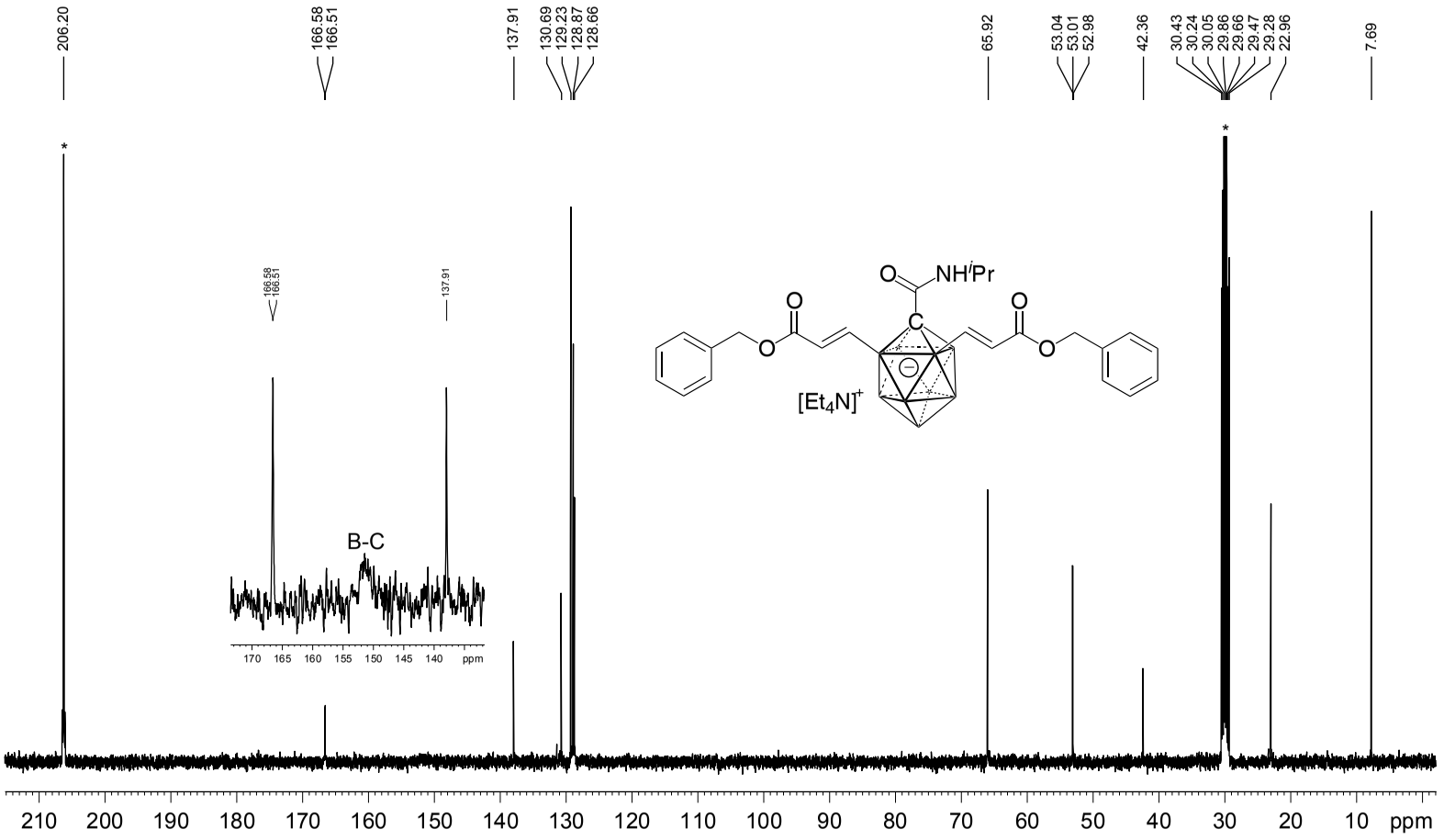
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR16

20171115-lxw-446
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171115-lxw-446
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 19.01
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 297.6K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

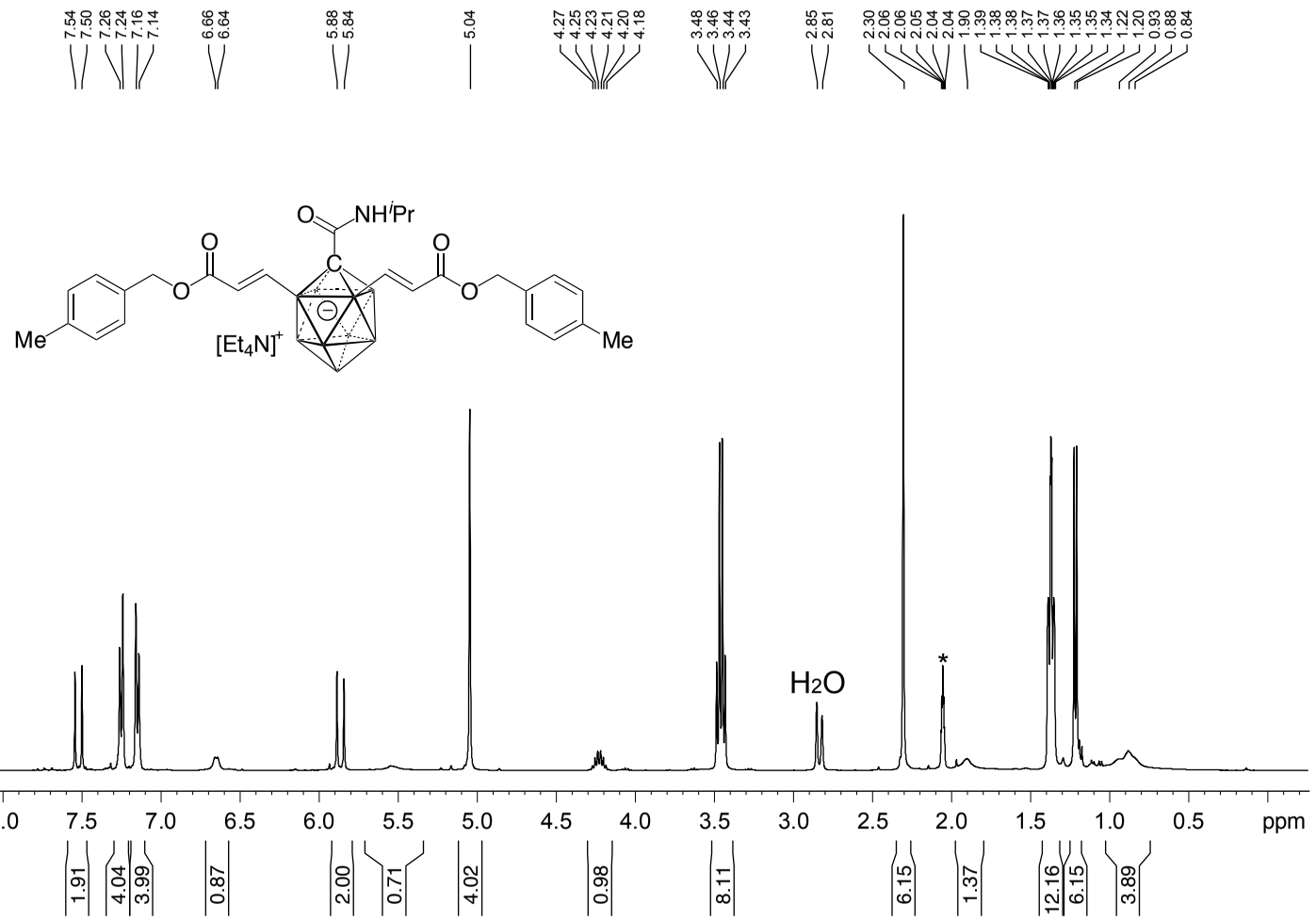
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126804 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR17

20171201-lxw-0495
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171201-lxw-0495
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 19.50
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 95.29
DW 62.400 usec
DE 6.50 usec
TE 295.8K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

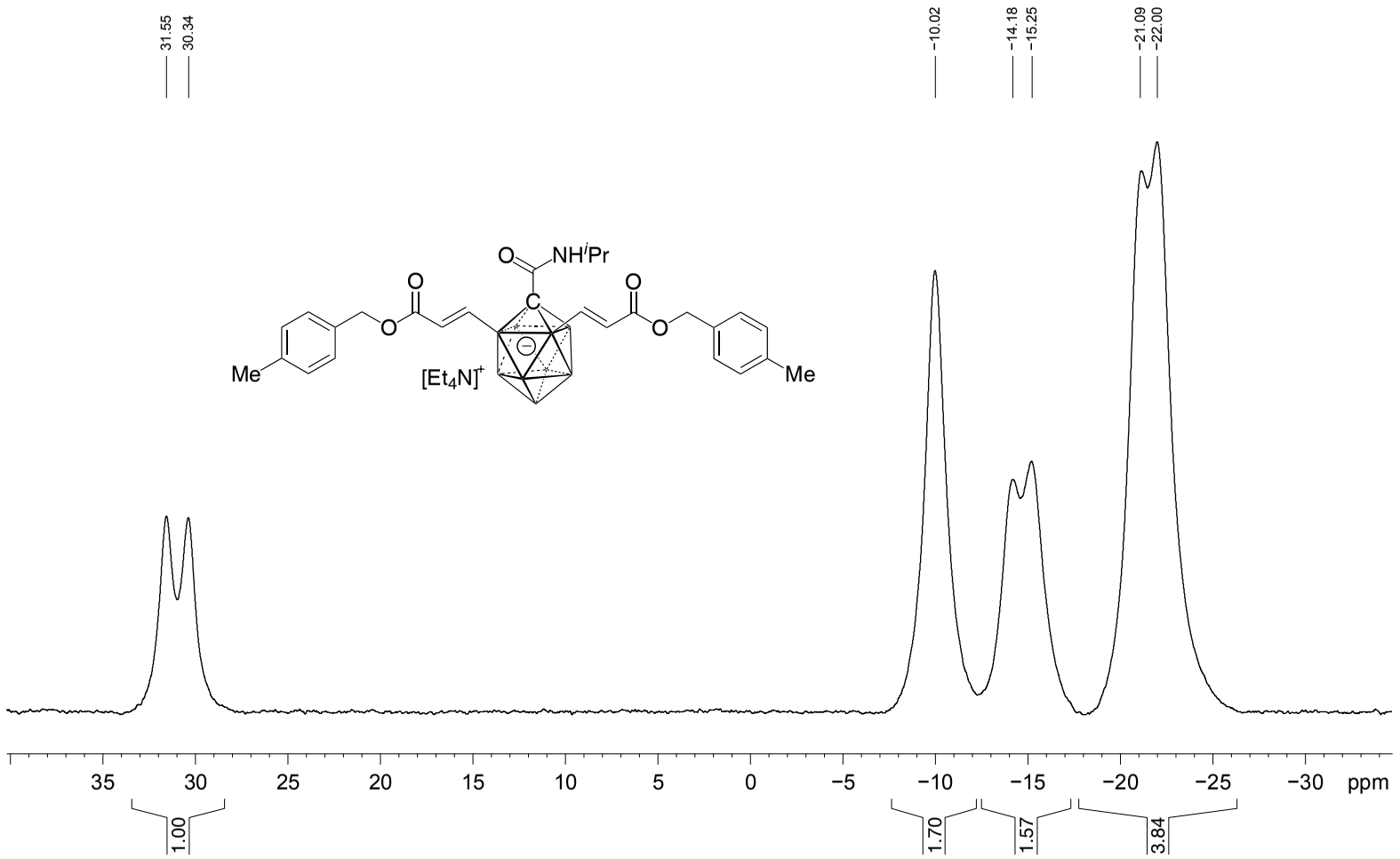
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR18

20171201-lxw-0495
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0495
EXPNO 4
PROCNO 1

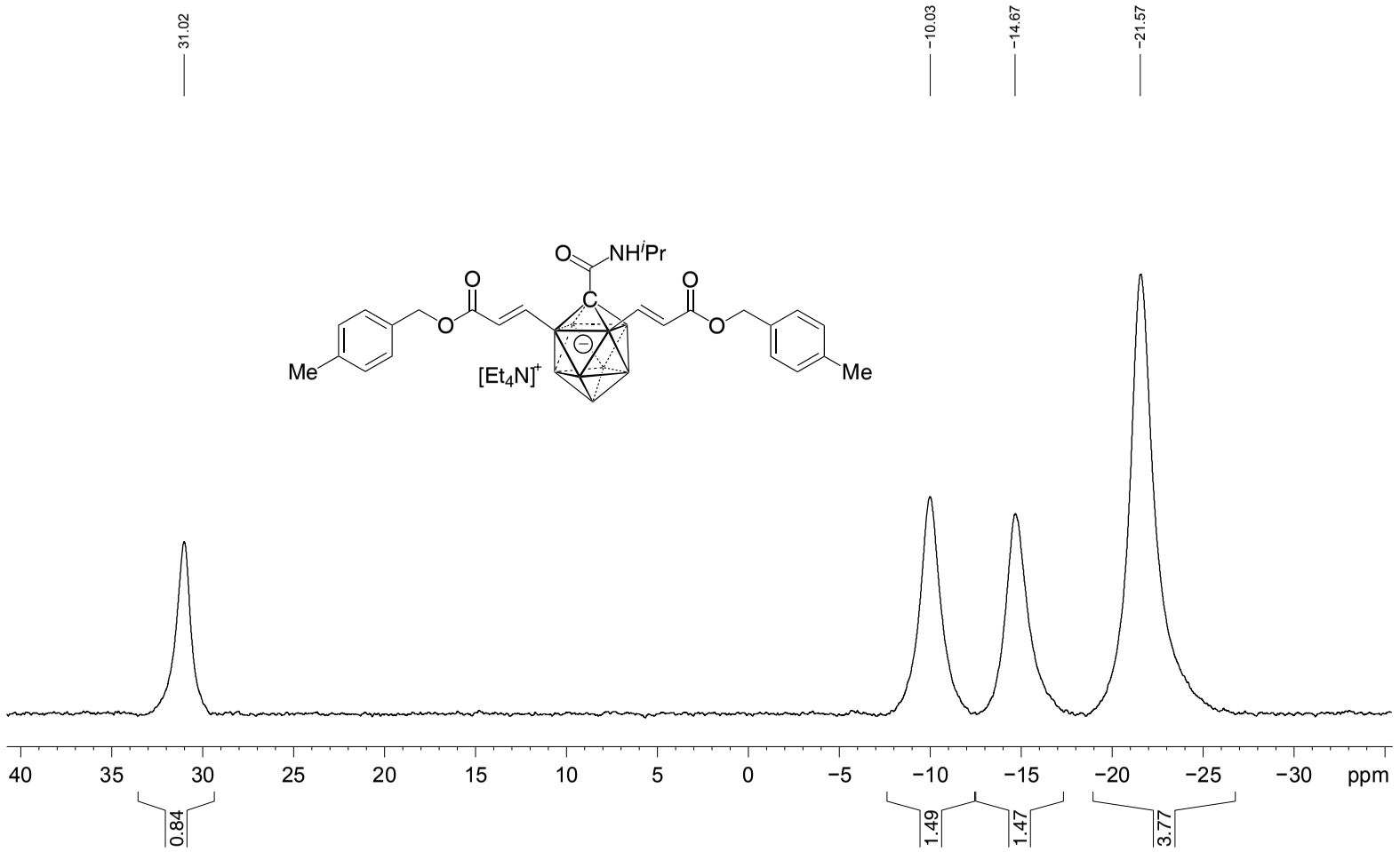
F2 - Acquisition Parameters
Date_ 20171202
Time 20.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.5K
D1 1.00000000 sec
TD0 1

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

NMR19

20171201-lxw-0495
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0495
EXPNO 3
PROCNO 1

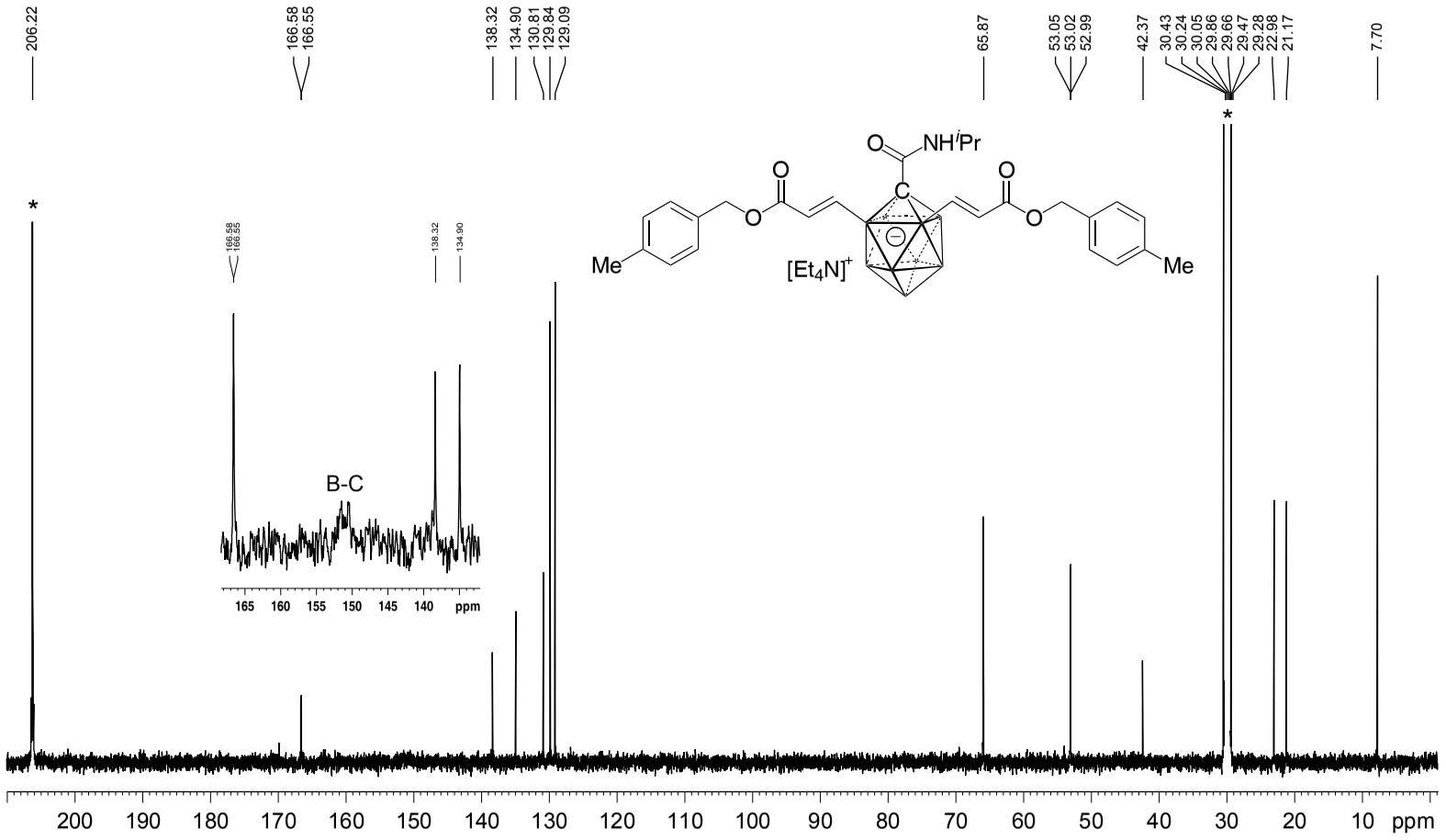
F2 - Acquisition Parameters
Date_ 20171202
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171201-lxw-0495
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



NMR20

Current Data Parameters
NAME 20171201-lxw-0495
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 20.26
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 296.4K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

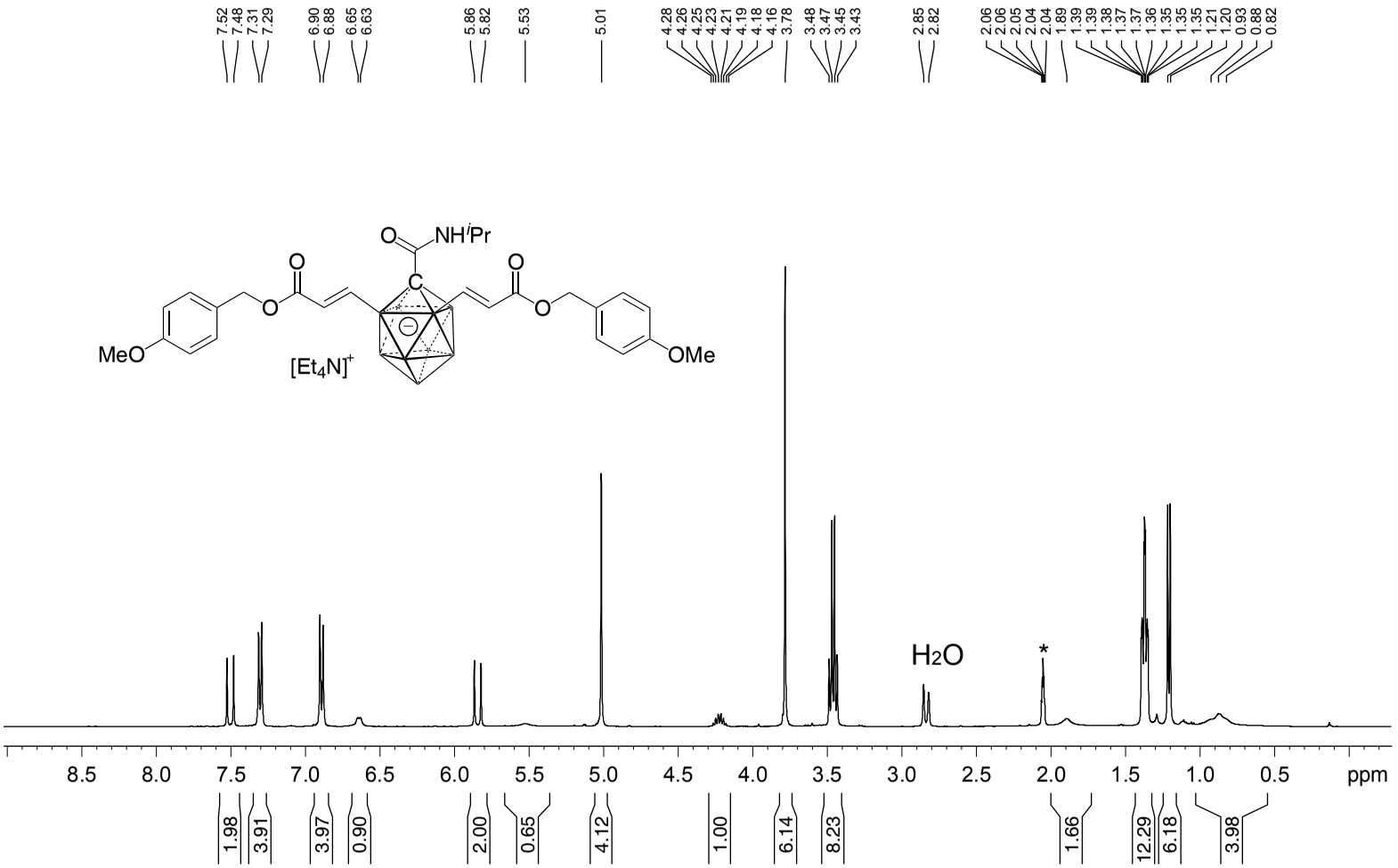
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR21

20171113-lxw-0490
Bruker 400MHz, 1H{11B} NMR, acetone-d6*



Current Data Parameters
NAME 20171113-lxw-0490
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171114
Time 15.07
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 295.8K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

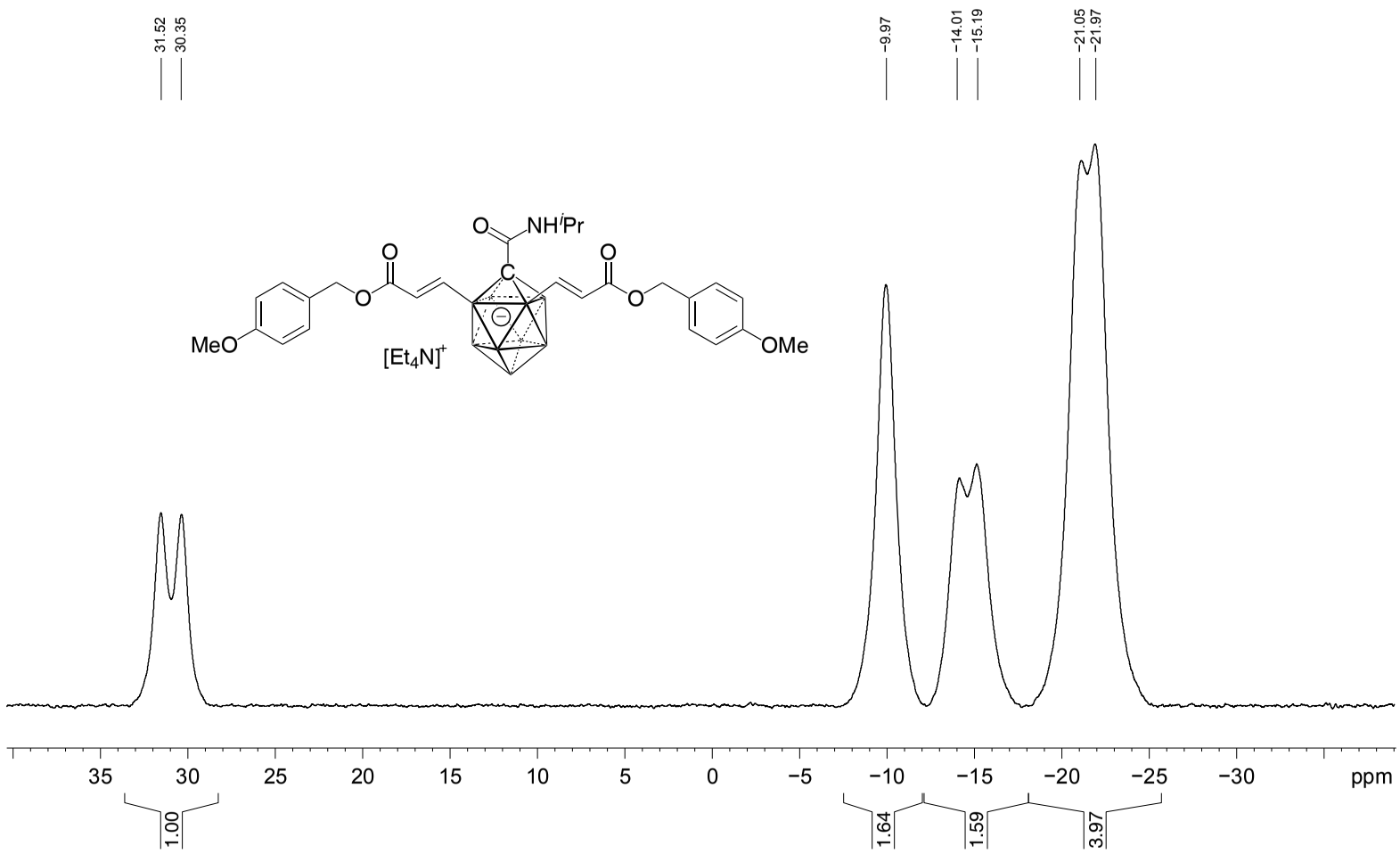
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR22

20171113-lxw-0490
Bruker 128MHz, 11B NMR, acetone-d6



Current Data Parameters
NAME 20171113-lxw-0490
EXPNO 3
PROCNO 1

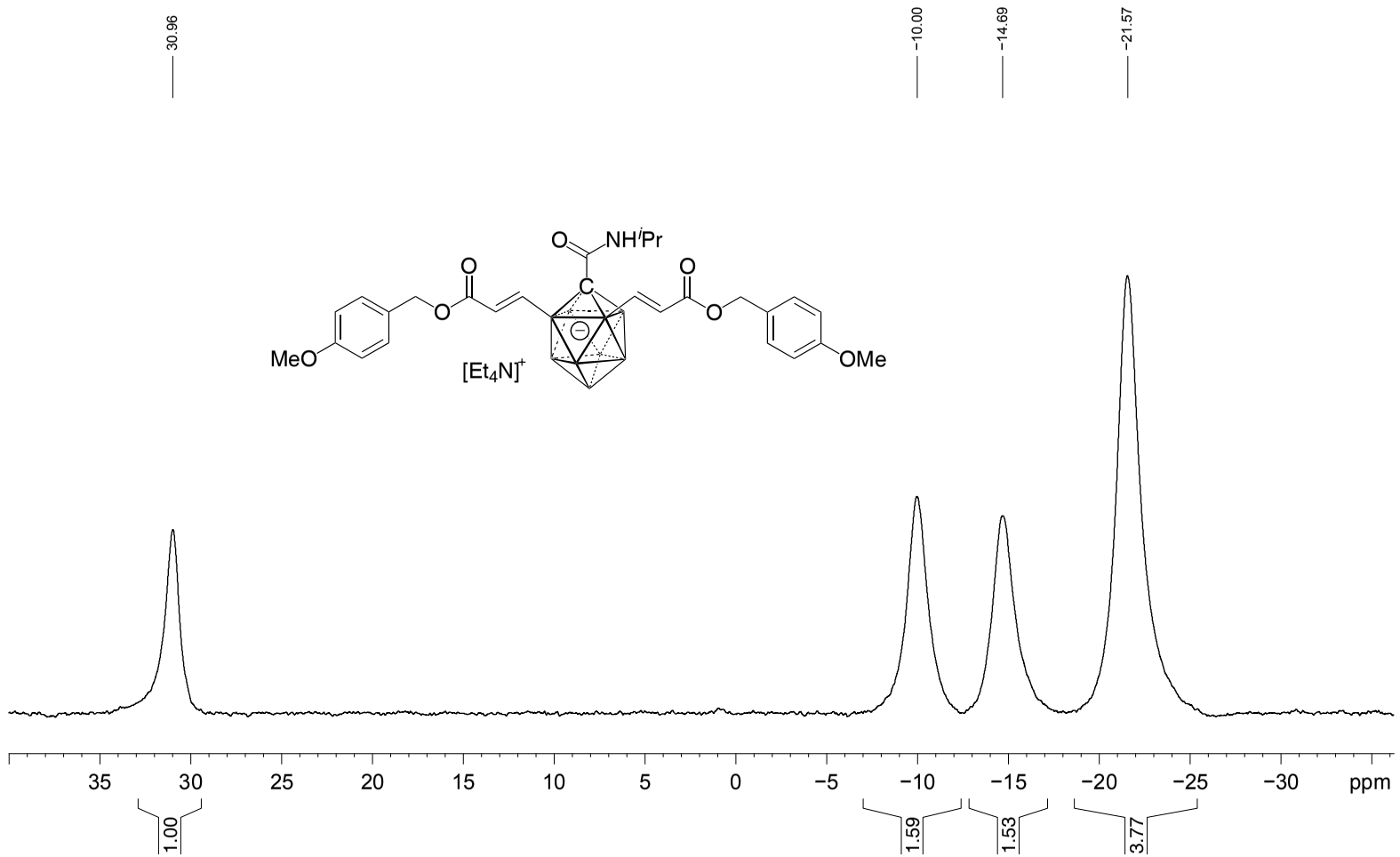
F2 - Acquisition Parameters
Date_ 20171114
Time 15.20
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.0K
D1 1.00000000 sec
TD0 1

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

NMR23

20171113-lxw-0490
Bruker 128MHz, 11B{1H} NMR, acetone-d6



Current Data Parameters
NAME 20171113-lxw-0490
EXPNO 2
PROCNO 1

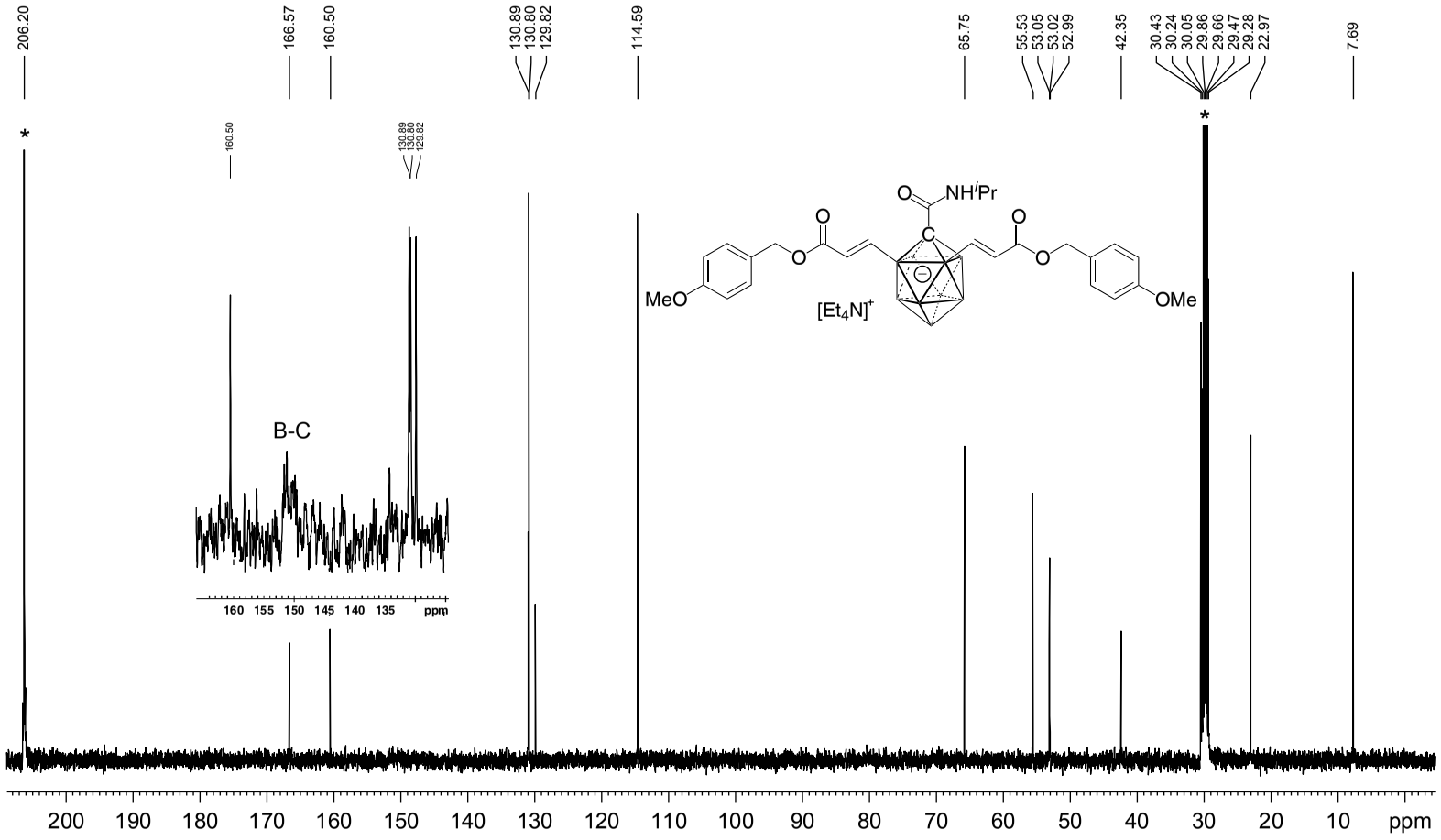
F2 - Acquisition Parameters
Date_ 20171114
Time 15.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.6K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171113-lxw-0490
Bruker 101MHz, 13C NMR, acetone-d6*



NMR24

Current Data Parameters
NAME 20171113-lxw-0490
EXPNO 5
PROCNO 1

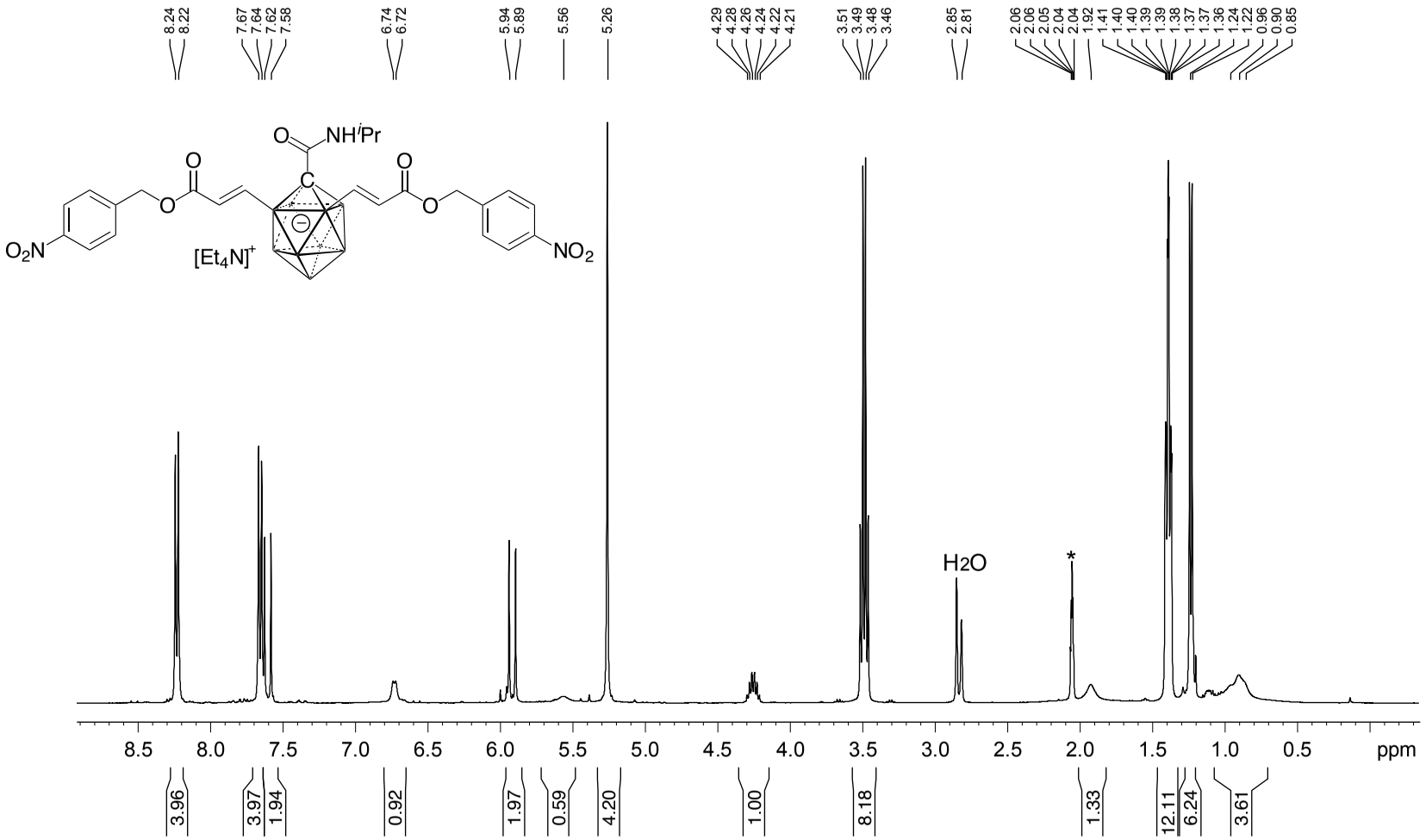
F2 - Acquisition Parameters
Date_ 20171114
Time 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 297.2K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6126797 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20171114-lxw-0487
Bruker 400MHz, 1H{11B} NMR, acetone-d6*



NMR25

Current Data Parameters
NAME 20171114-lxw-0487
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 6.30
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 296.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

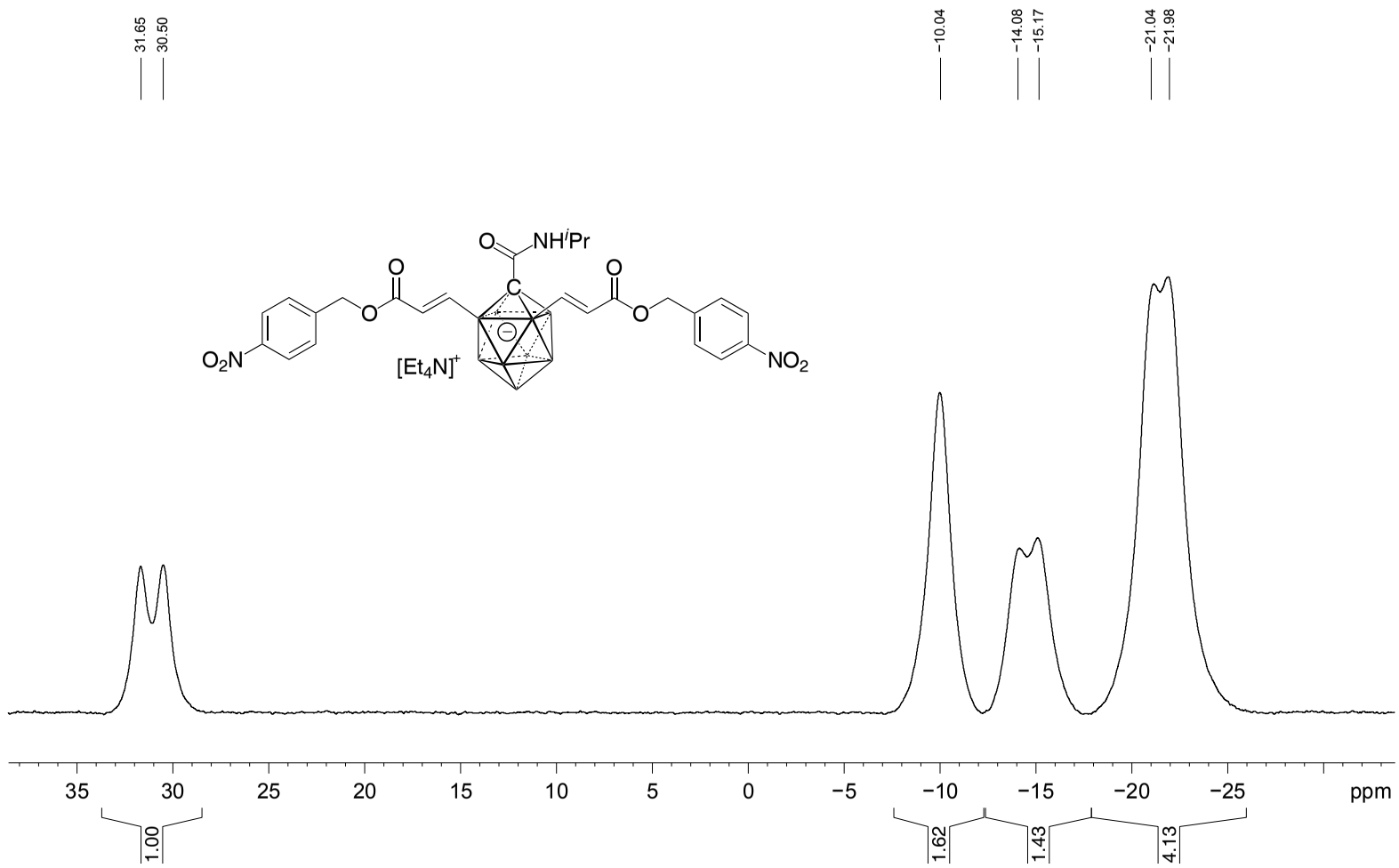
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR26

20171114-lxw-0487
Bruker 128MHz, 11B NMR, acetone-d6



Current Data Parameters
NAME 20171114-lxw-0487
EXPNO 4
PROCNO 1

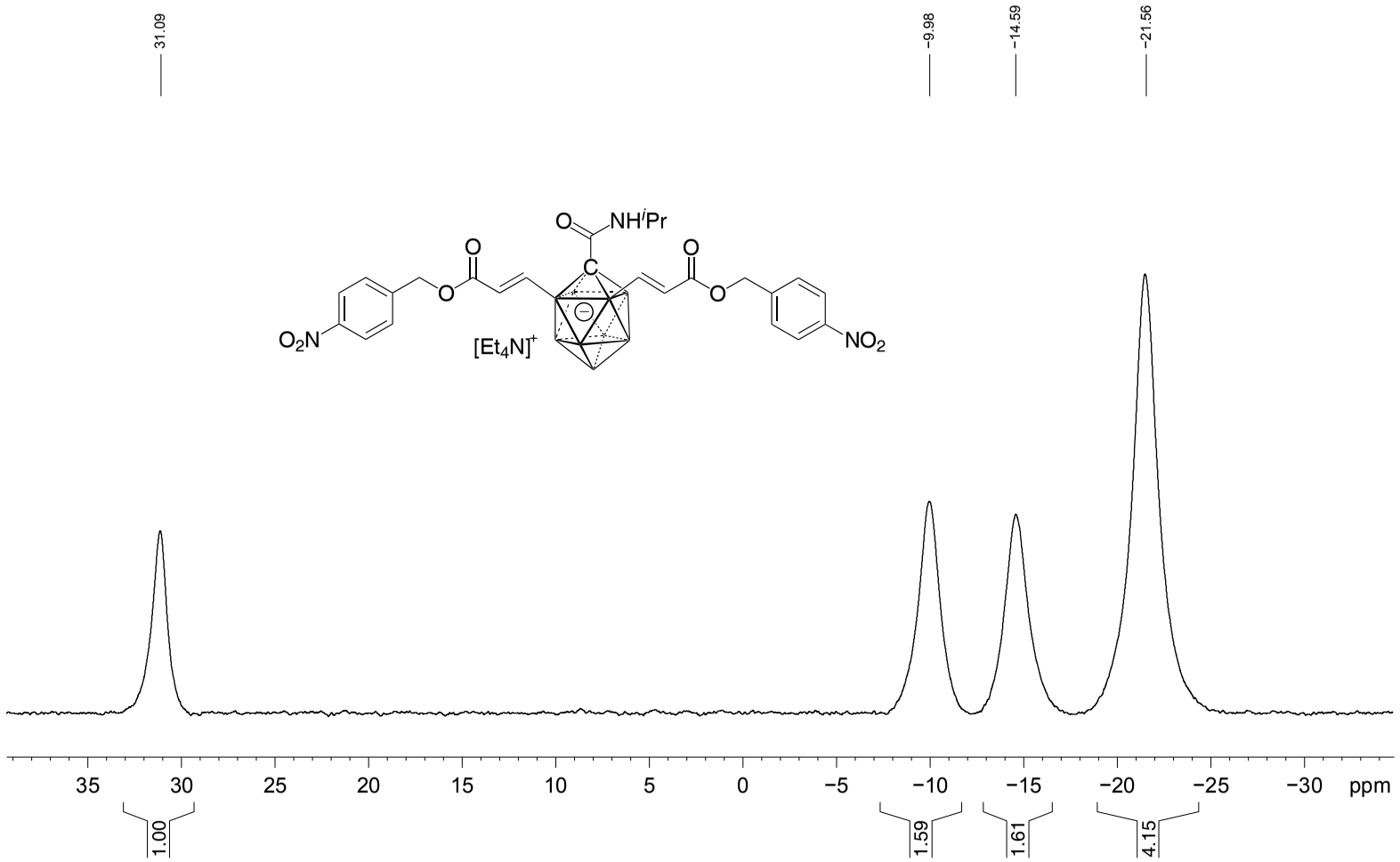
F2 - Acquisition Parameters
Date_ 20171115
Time 6.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.5K
D1 1.00000000 sec
TD0 1

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

NMR27

20171114-lxw-0487
Bruker 128MHz, 11B{1H} NMR, acetone-d6



Current Data Parameters
NAME 20171114-lxw-0487
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 6.37
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 297.2K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

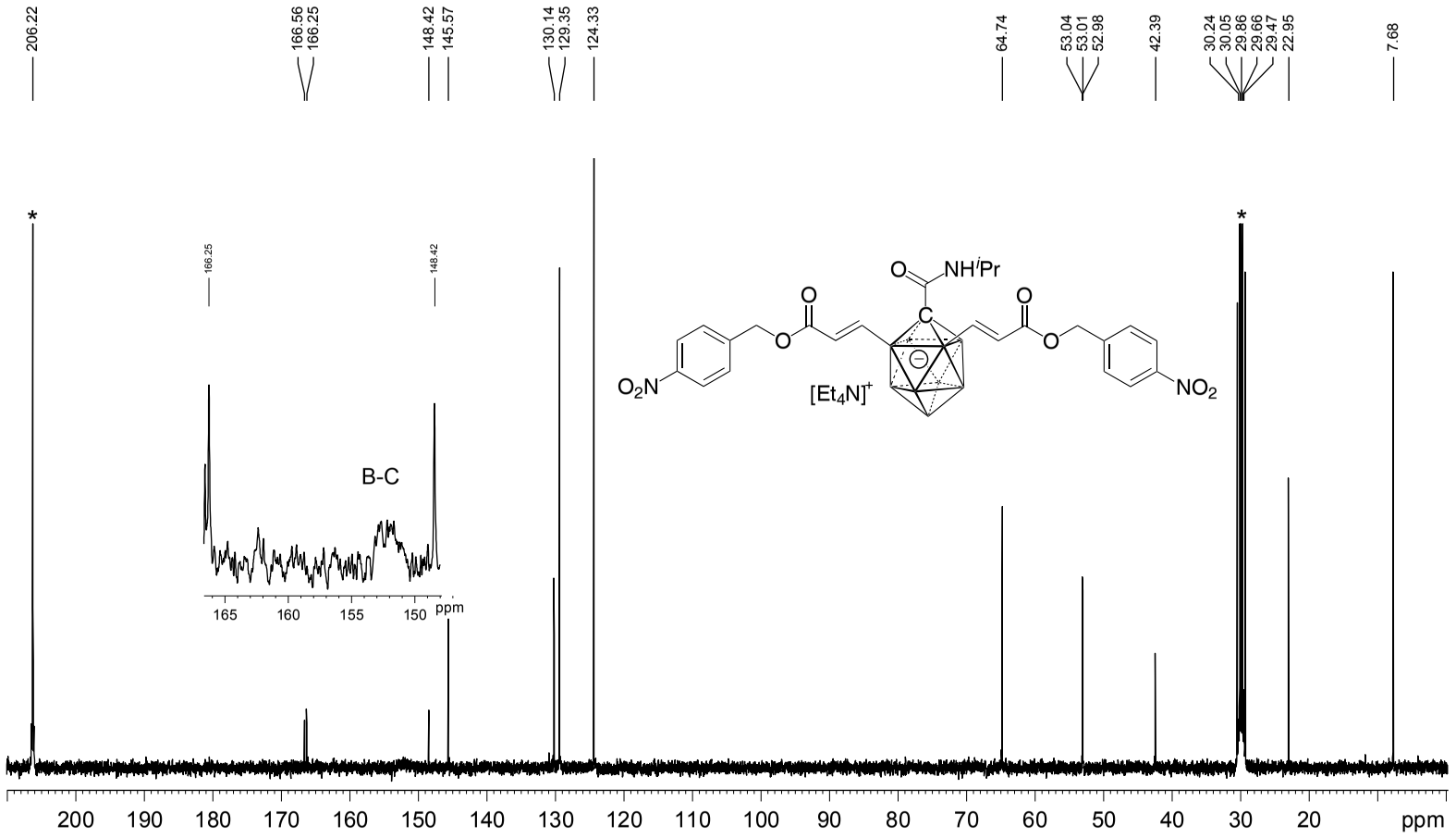
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR28

20171114-lxw-0487
Bruker 101MHz, 13C NMR, acetone-d6*



Current Data Parameters
NAME 20171114-lxw-0487
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 7.07
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 297.0K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

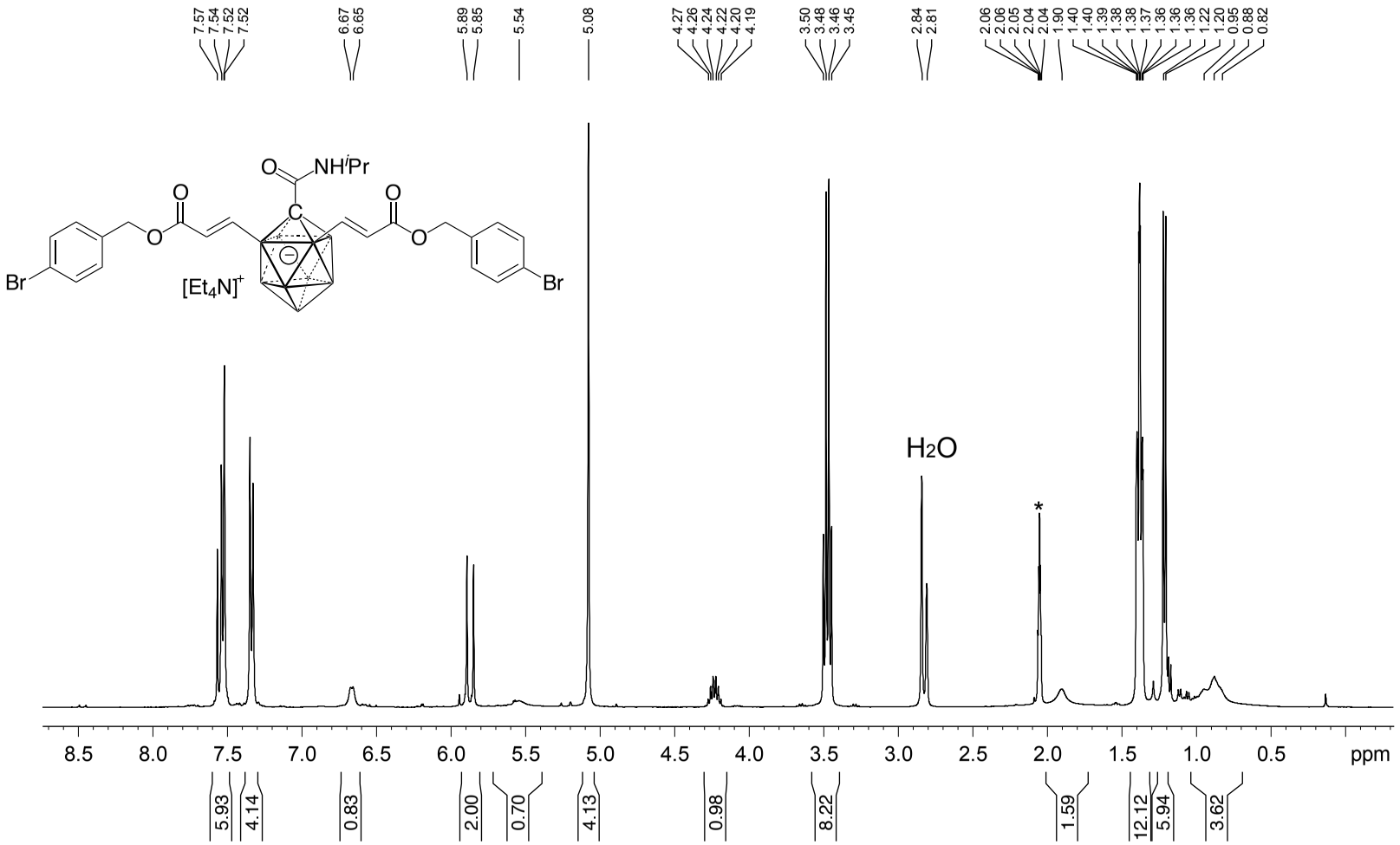
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126805 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR29

20171102-lxw-0483
Bruker 400MHz, 1H{11B} NMR,17mg in acetone-d6*



Current Data Parameters
NAME 20171102-lxw-0483
EXPNO 2
PROCNO 1

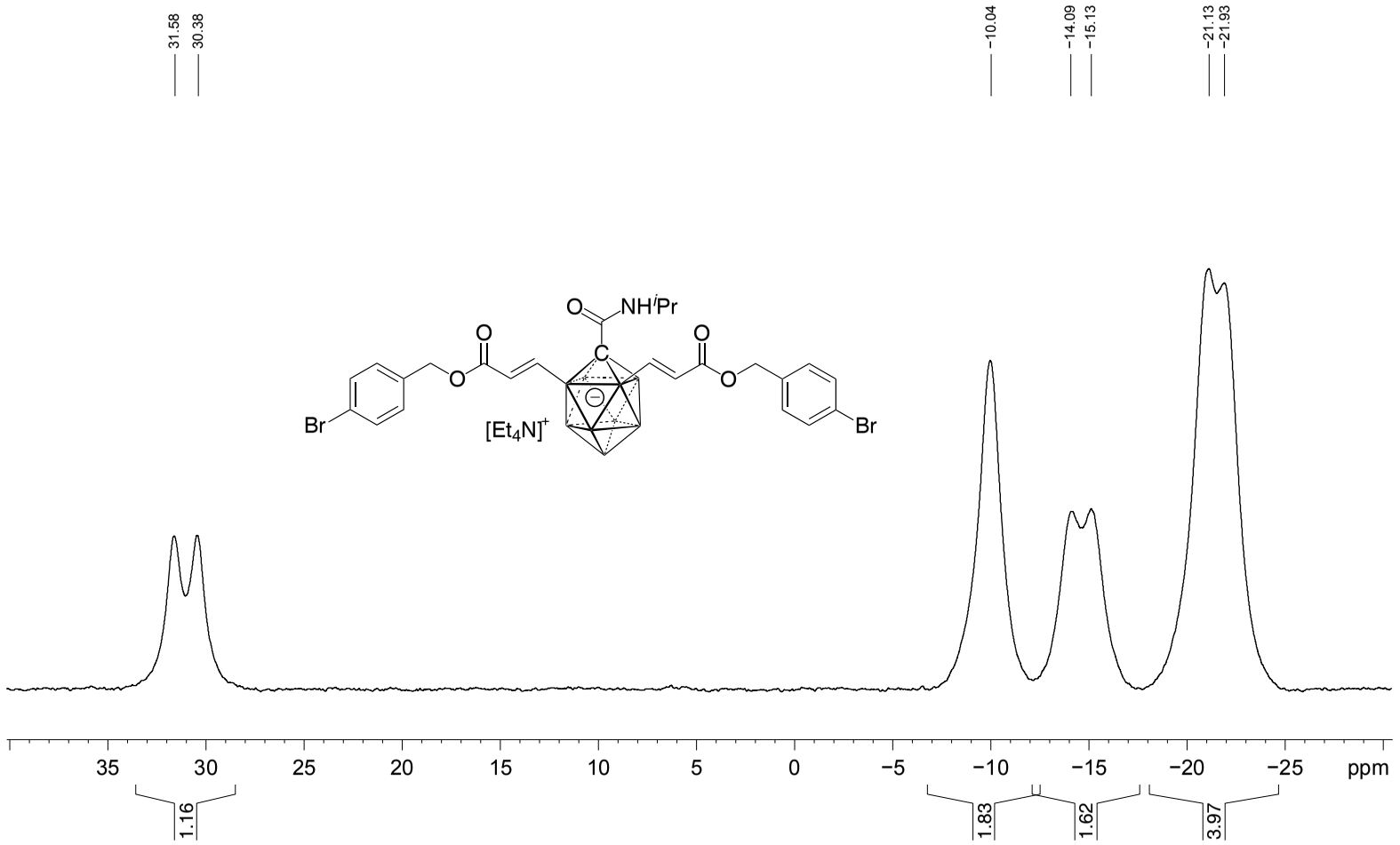
F2 - Acquisition Parameters
Date_ 20171103
Time 13.55
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgig30
TD 16384
SOLVENT Acetone
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 107.6
DW 62.400 usec
DE 6.50 usec
TE 297.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171102-lxw-0483
Bruker 128MHz, 11B NMR,17mg in acetone-d6



NMR30

Current Data Parameters
NAME 20171102-lxw-0483
EXPNO 4
PROCNO 1

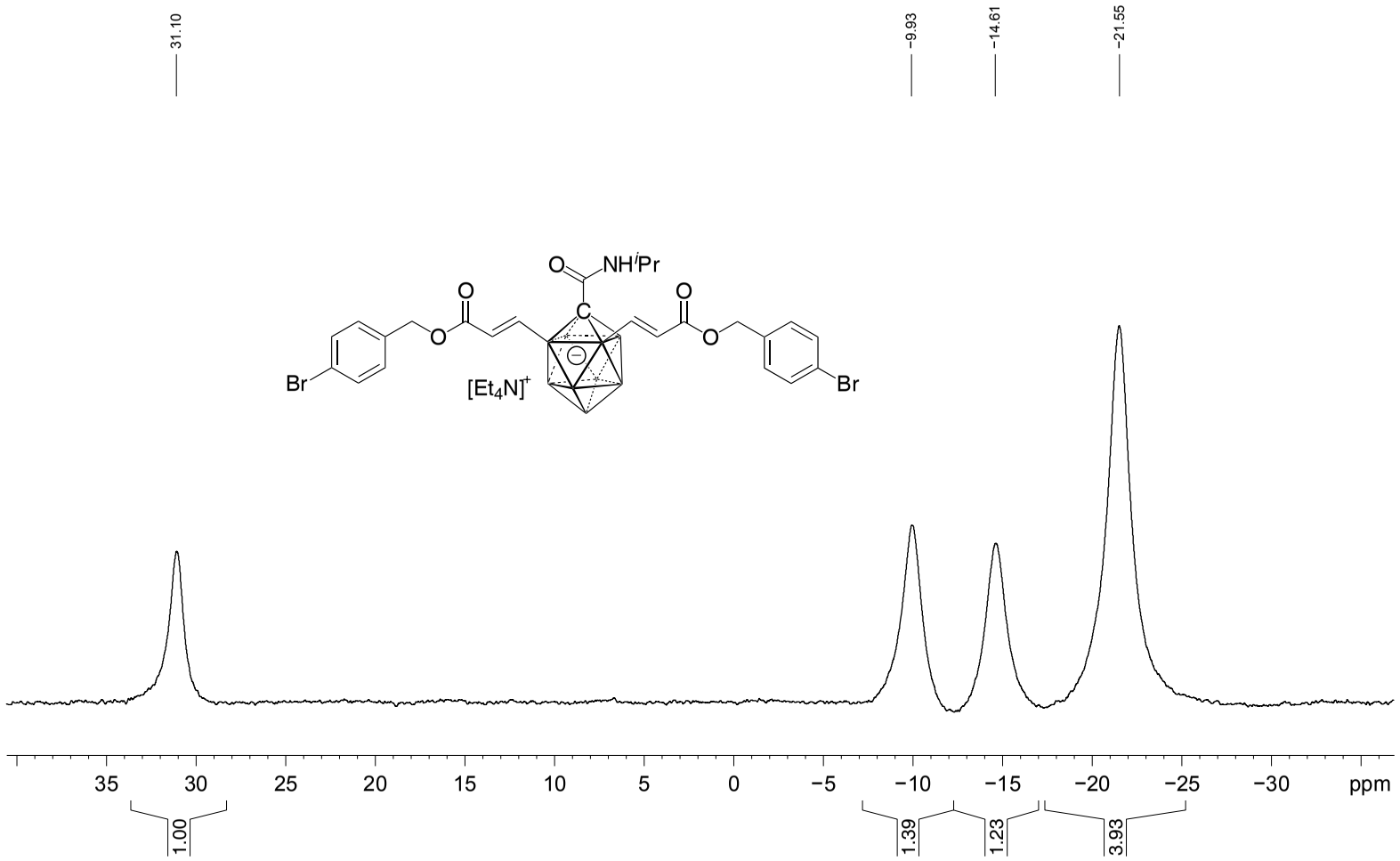
F2 - Acquisition Parameters
Date_ 20171103
Time 14.07
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 297.3K
D1 1.00000000 sec
TD0 1

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

NMR31

20171102-lxw-0483
Bruker 128MHz, 11B{1H} NMR,17mg in acetone-d6



Current Data Parameters
NAME 20171102-lxw-0483
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171103
Time 14.01
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 298.0K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

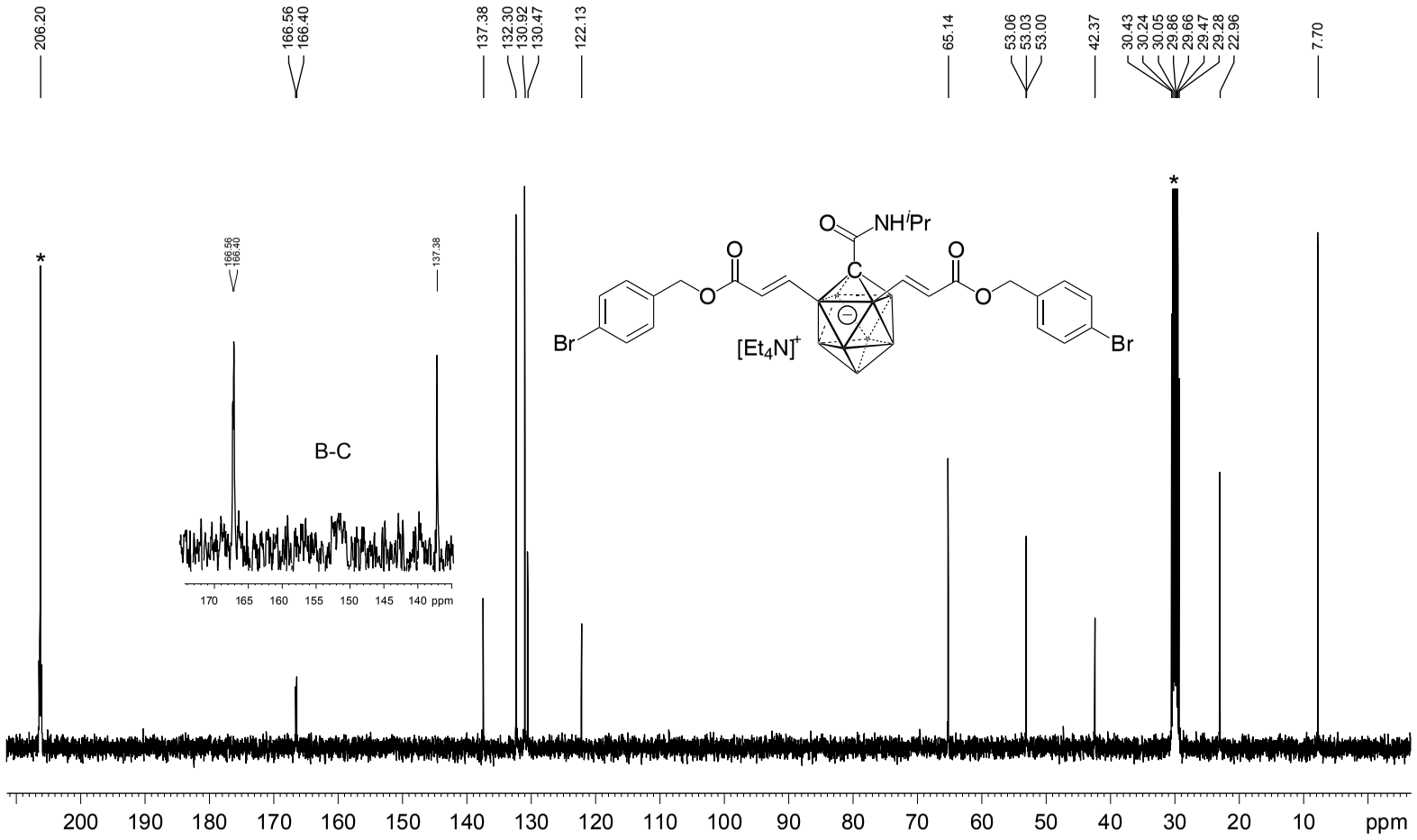
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR32

20171102-lxw-0483
Bruker 101MHz, 13C NMR,17mg in acetone-d6 *



Current Data Parameters
NAME 20171102-lxw-0483
EXPNO 5
PROCNO 1

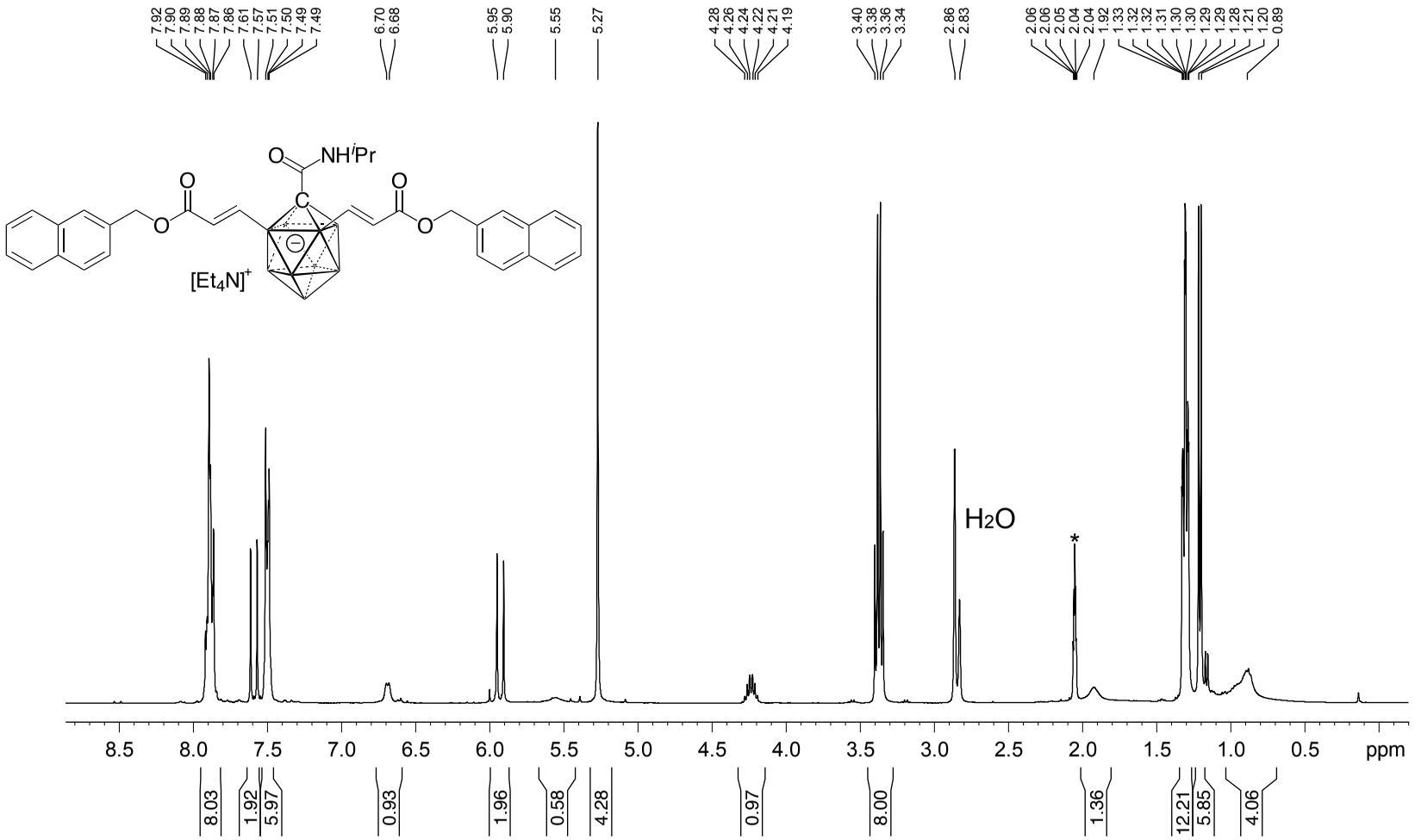
F2 - Acquisition Parameters
Date_ 20171103
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 193.34
DW 16.800 usec
DE 6.50 usec
TE 298.3K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

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

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

F2 - Processing parameters
SI 32768
SF 100.6126791 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

20171114-lxw-0485
Bruker 400MHz, 1H{11B} NMR,acetone-d6*



NMR33

Current Data Parameters
NAME 20171114-lxw-0485
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171115
Time 6.24
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 296.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

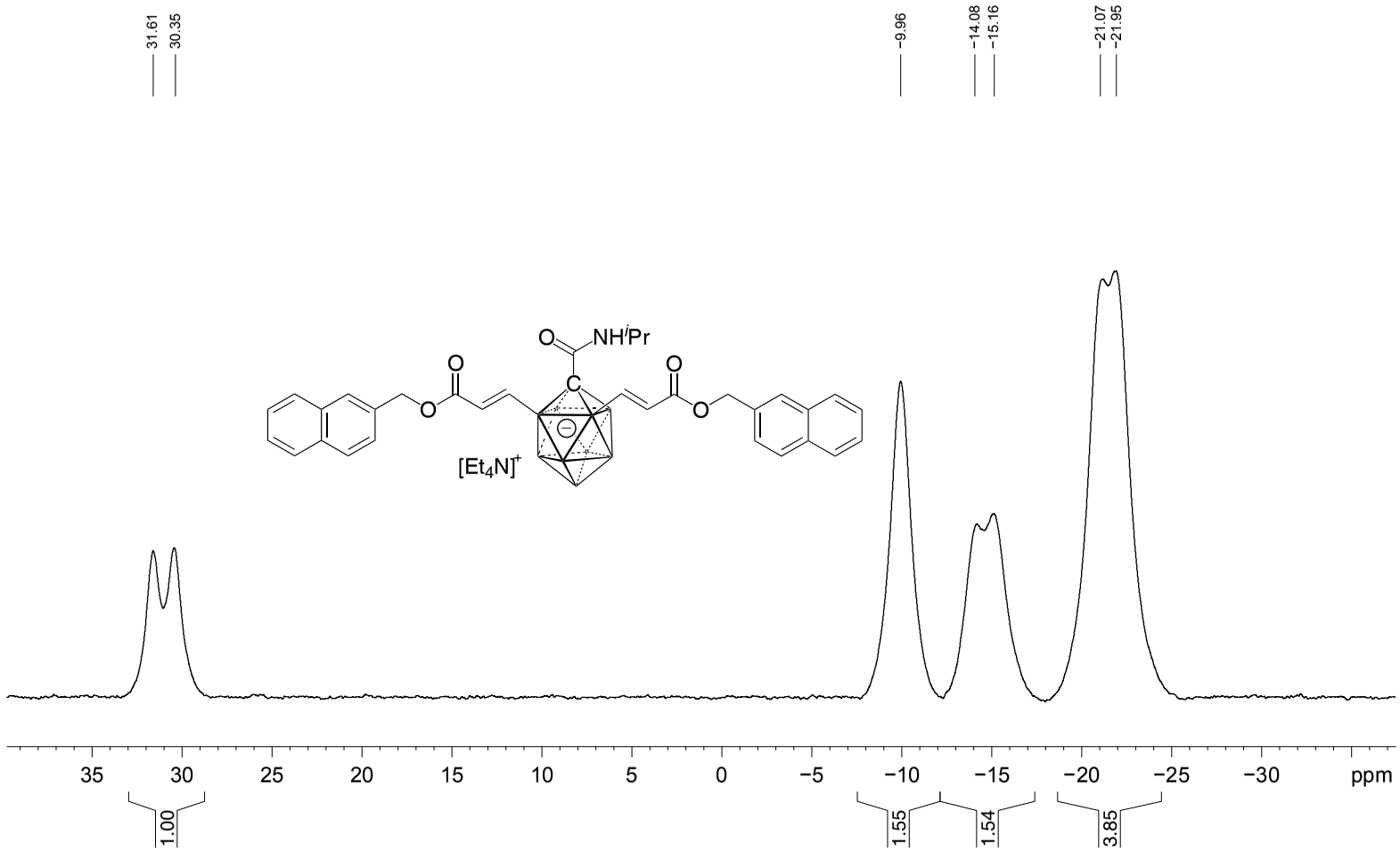
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR34

20171114-lxw-0485
Bruker 128MHz, 11B NMR,acetone-d6



Current Data Parameters
NAME 20171114-lxw-0485
EXPNO 4
PROCNO 1

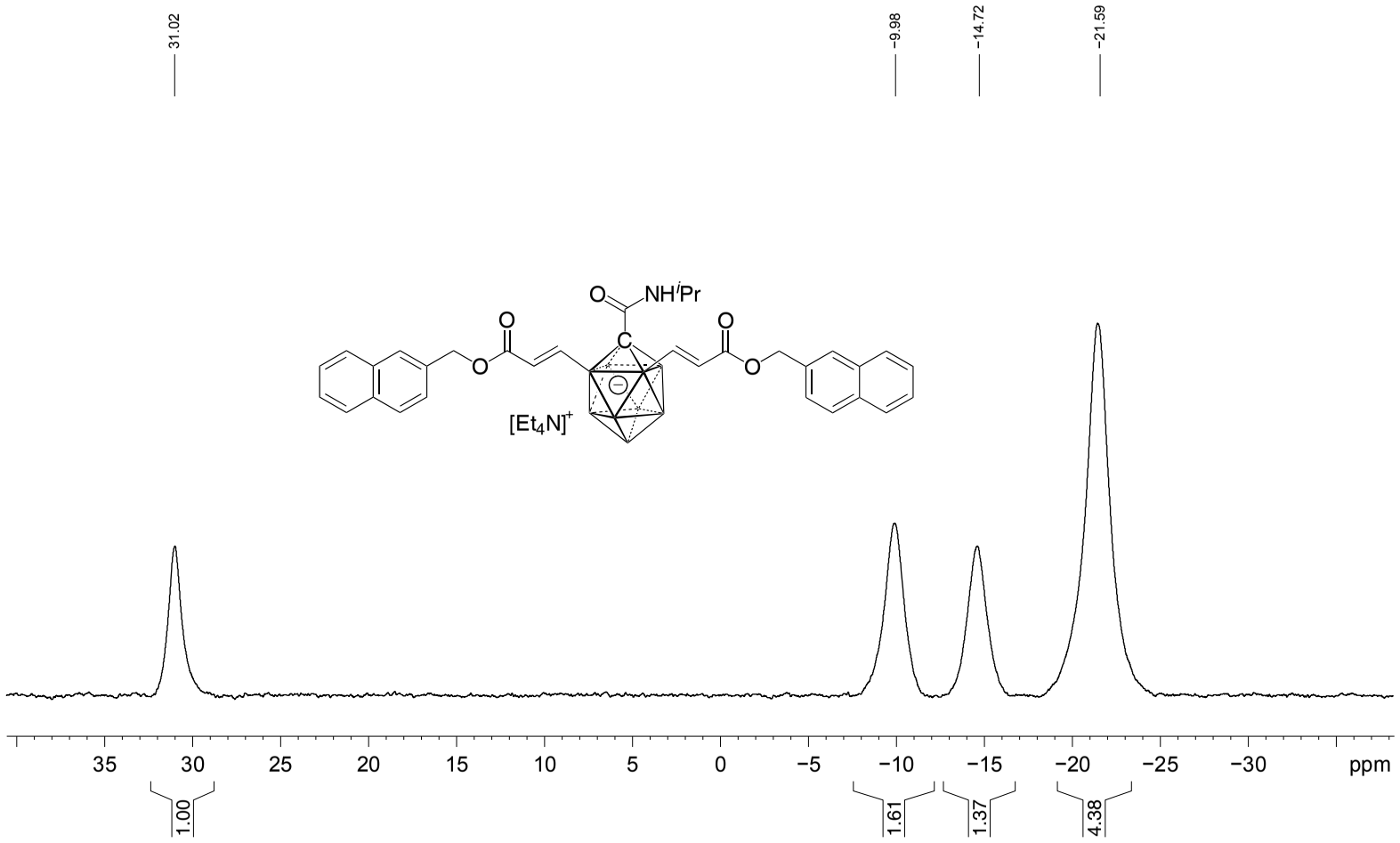
F2 - Acquisition Parameters
Date_ 20171109
Time 18.25
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.5K
D1 1.00000000 sec
TD0 1

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

NMR35

20171114-lxw-0485
Bruker 128MHz, 11B{1H} NMR,acetone-d6



Current Data Parameters
NAME 20171114-lxw-0485
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 18.19
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 297.2K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

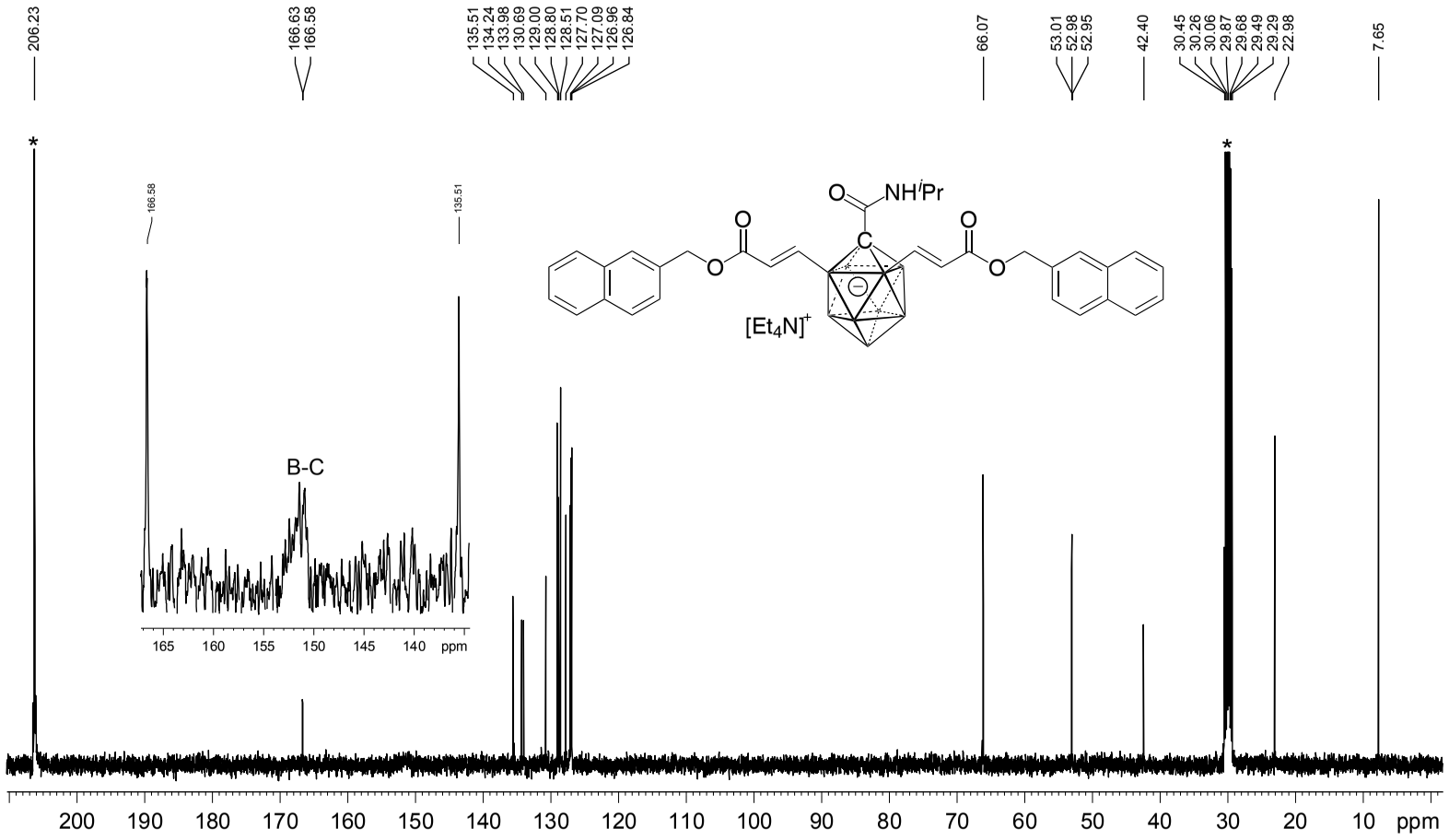
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR36

20171114-lxw-0485
Bruker 101MHz, 13C NMR,acetone-d6*



Current Data Parameters
NAME 20171114-lxw-0485
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 18.49
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 297.5K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

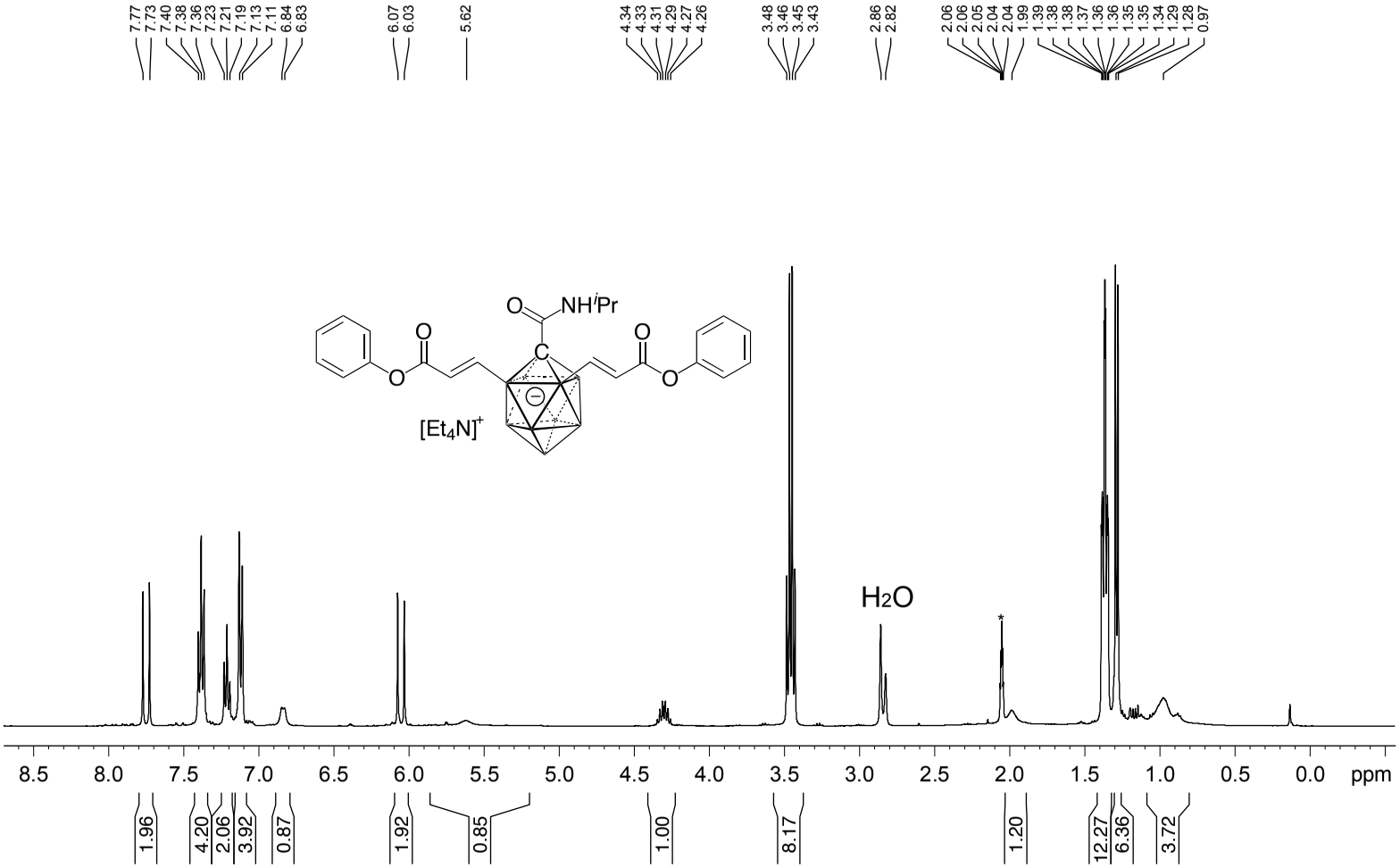
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR37

20171115-lxw-445
Bruker 400Mhz, 1H {11B} NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171115-lxw-445
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 17.42
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 296.1K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

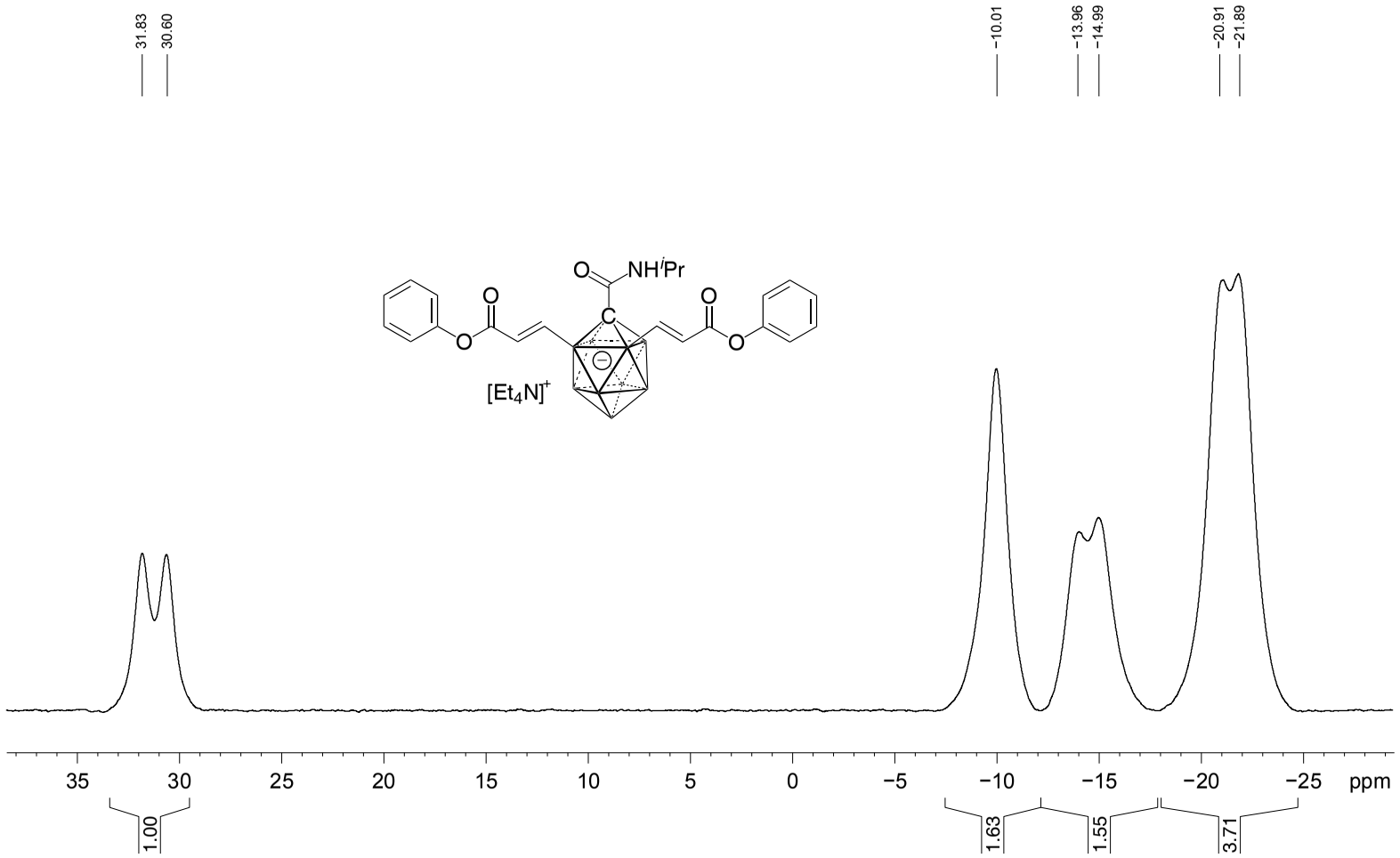
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR38

20171115-lxw-445
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171115-lxw-445
EXPNO 4
PROCNO 1

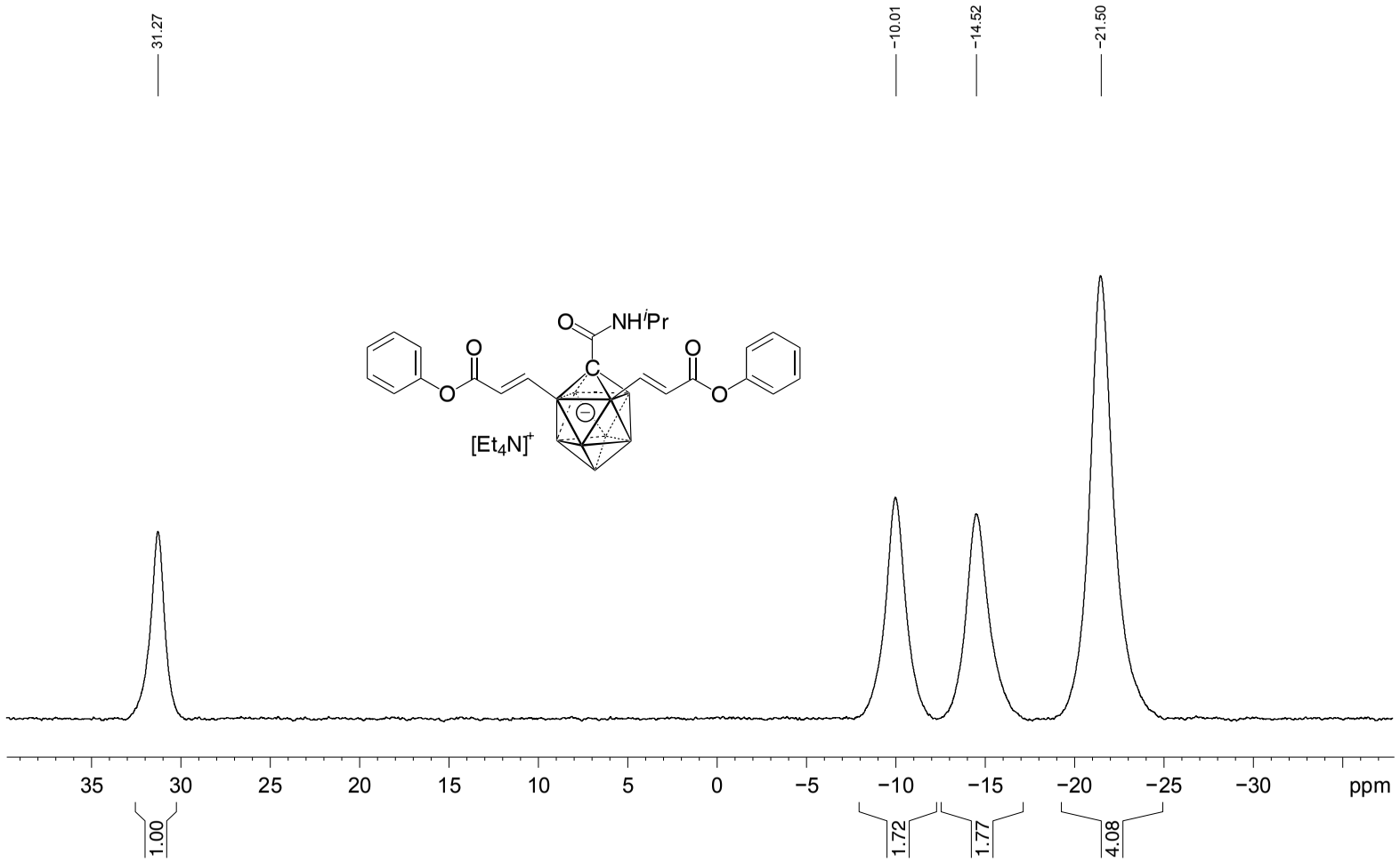
F2 - Acquisition Parameters
Date_ 20171116
Time 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.2K
D1 1.00000000 sec
TD0 1

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

NMR39

20171115-lxw-445
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171115-lxw-445
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 17.48
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 296.8K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

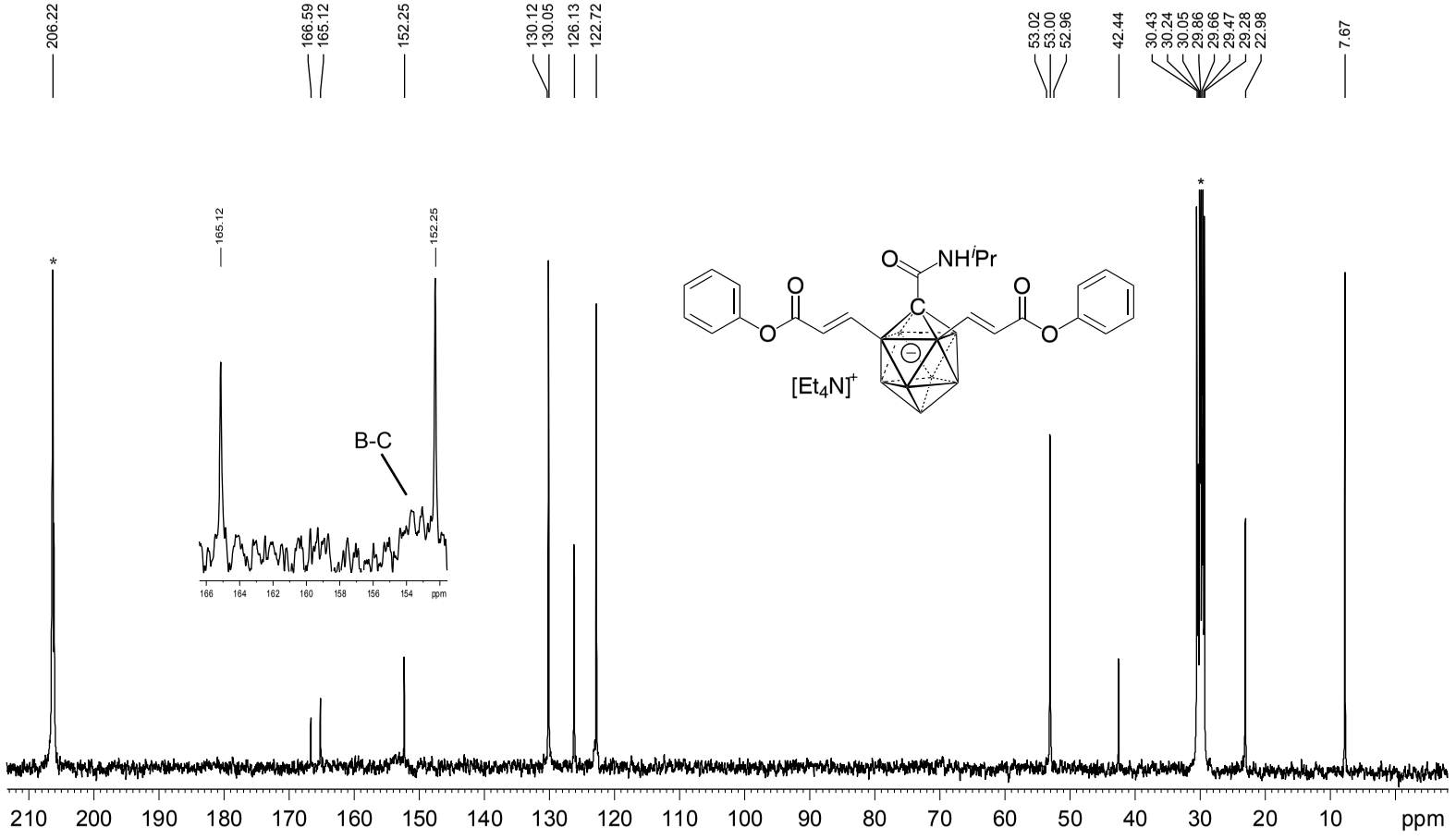
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

20171115-lxw-445
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*

NMR40



Current Data Parameters
NAME 20171115-lxw-445
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 18.18
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 297.3K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

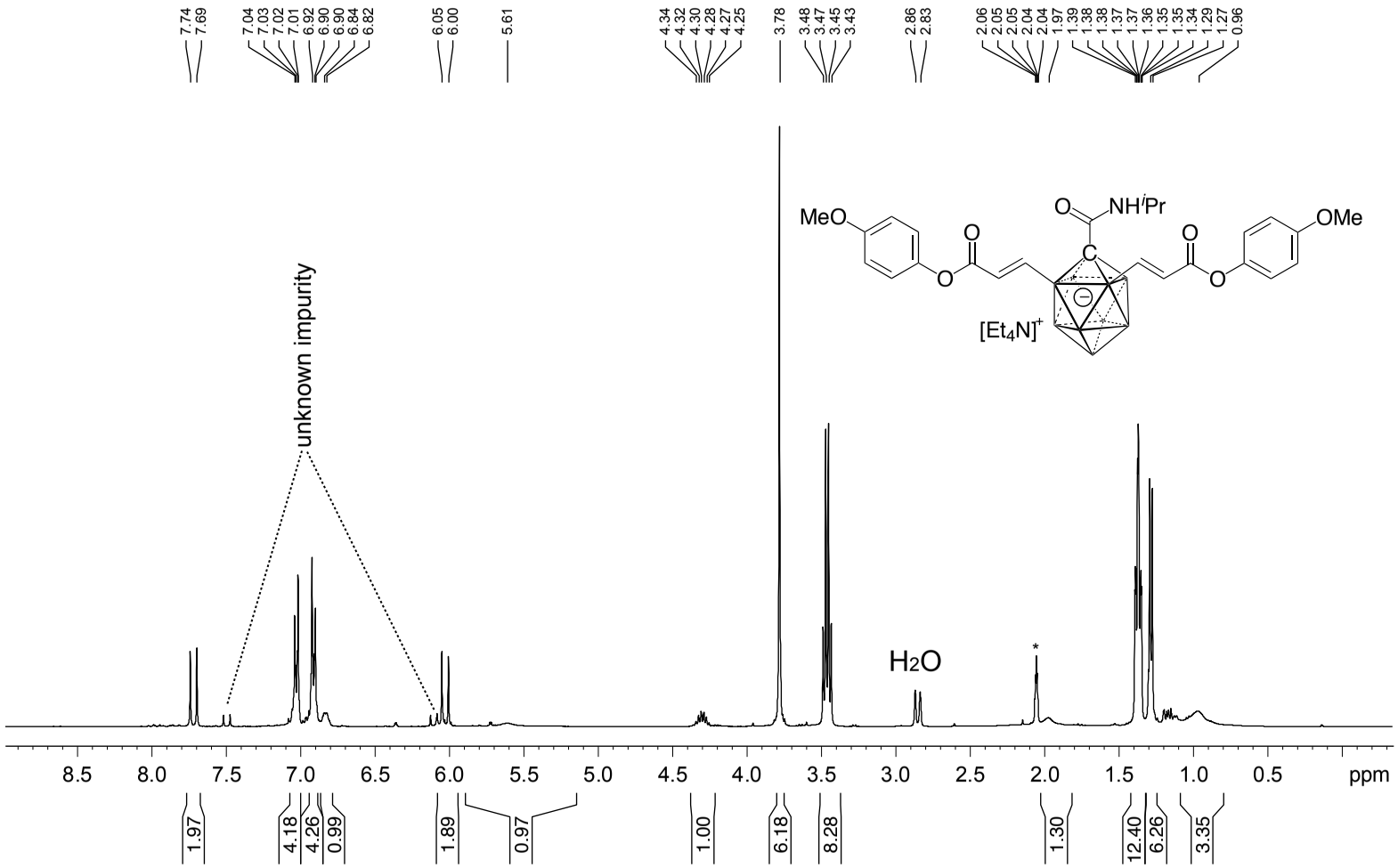
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126810 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

NMR41

20171203-lxw-0499
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171203-lxw-0499
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171204
Time 4.34
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 78.69
DW 62.400 usec
DE 6.50 usec
TE 293.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

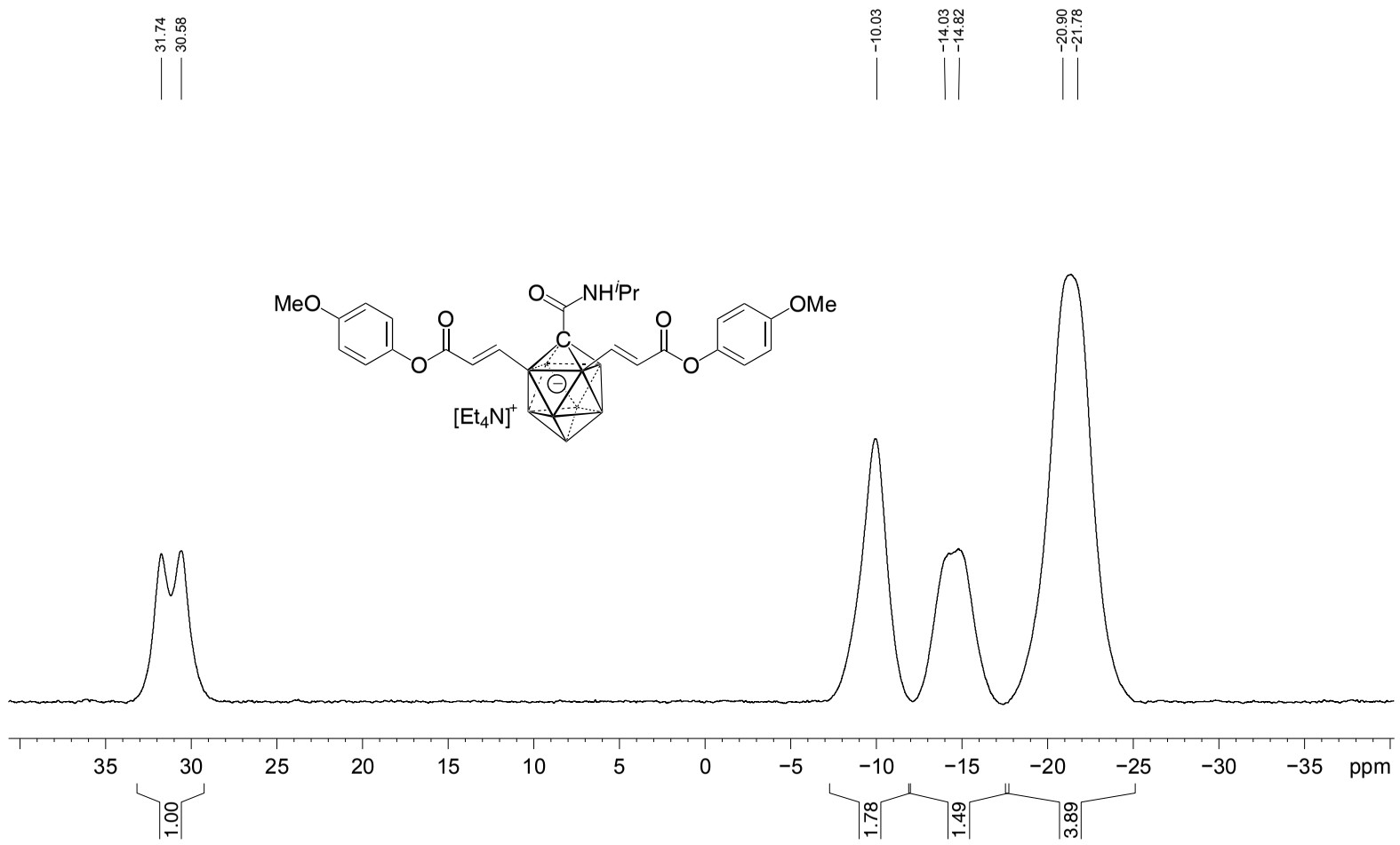
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR42

20171203-lxw-0499
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171203-lxw-0499
EXPNO 4
PROCNO 1

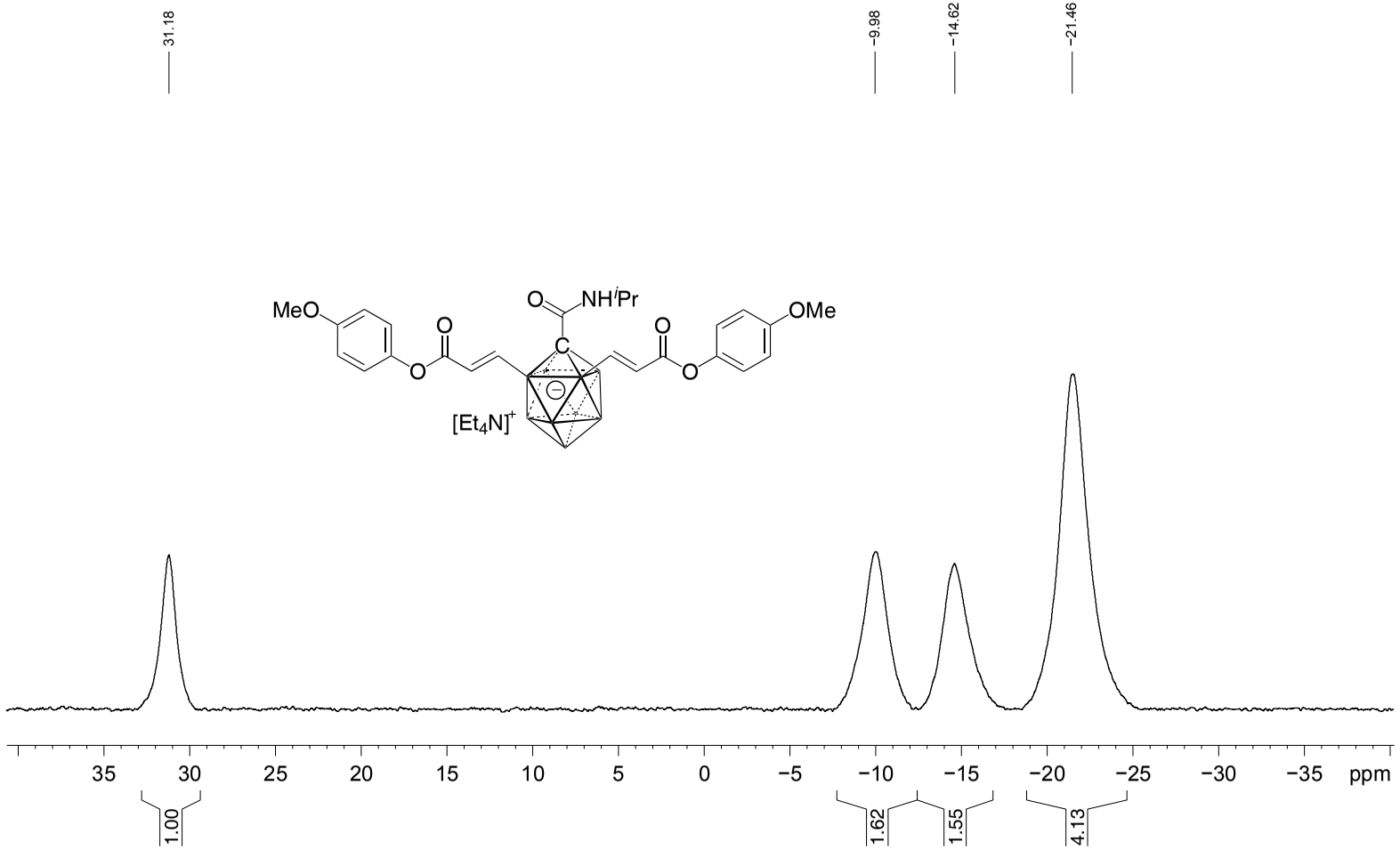
F2 - Acquisition Parameters
Date_ 20171204
Time 4.46
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 294.5K
D1 1.00000000 sec
TD0 1

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

NMR43

20171203-lxw-0499
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171203-lxw-0499
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171204
Time 4.40
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 295.0K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

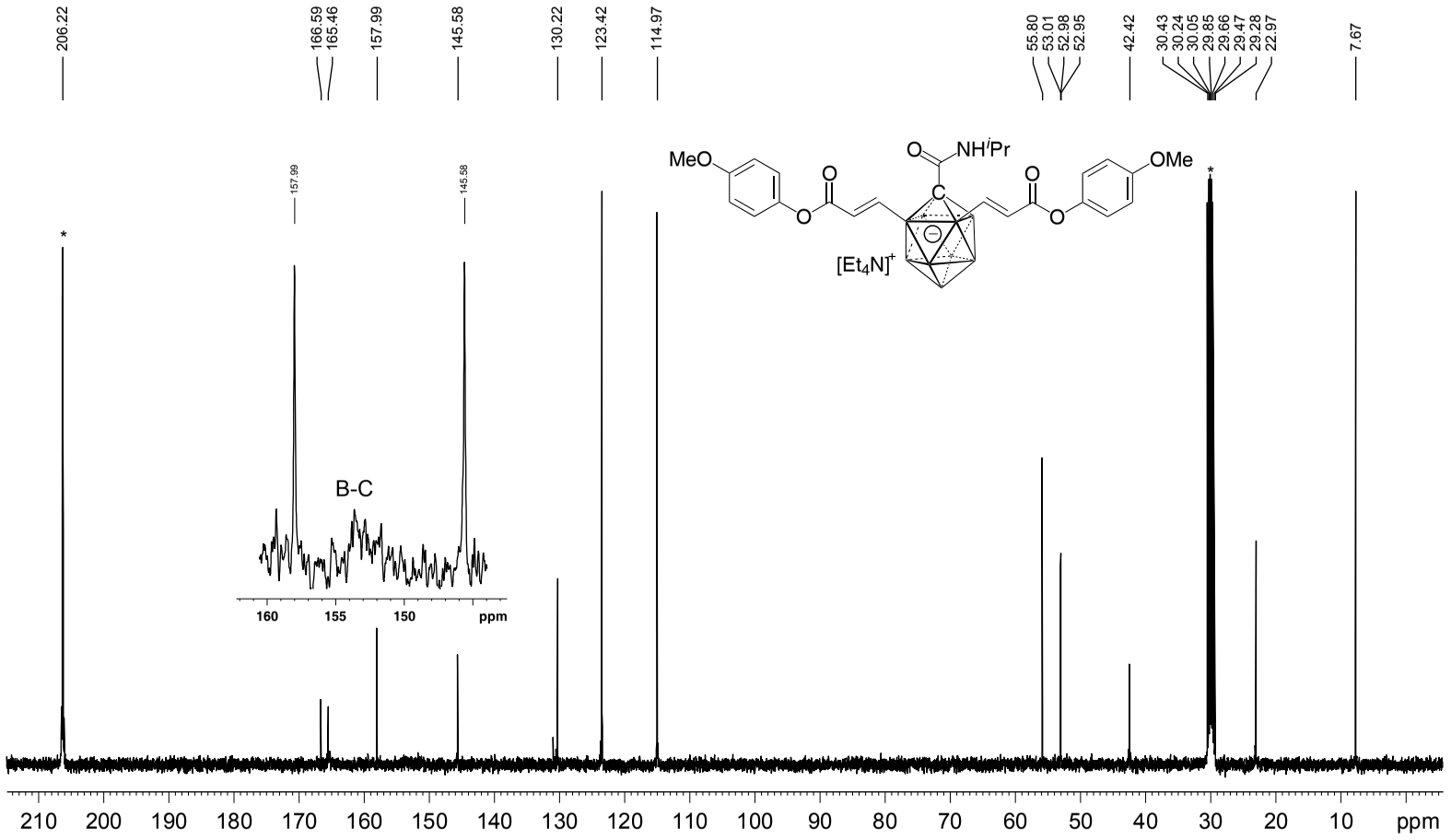
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR44

20171203-lxw-0499
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171203-lxw-0499
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171204
Time 5.10
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 295.7K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

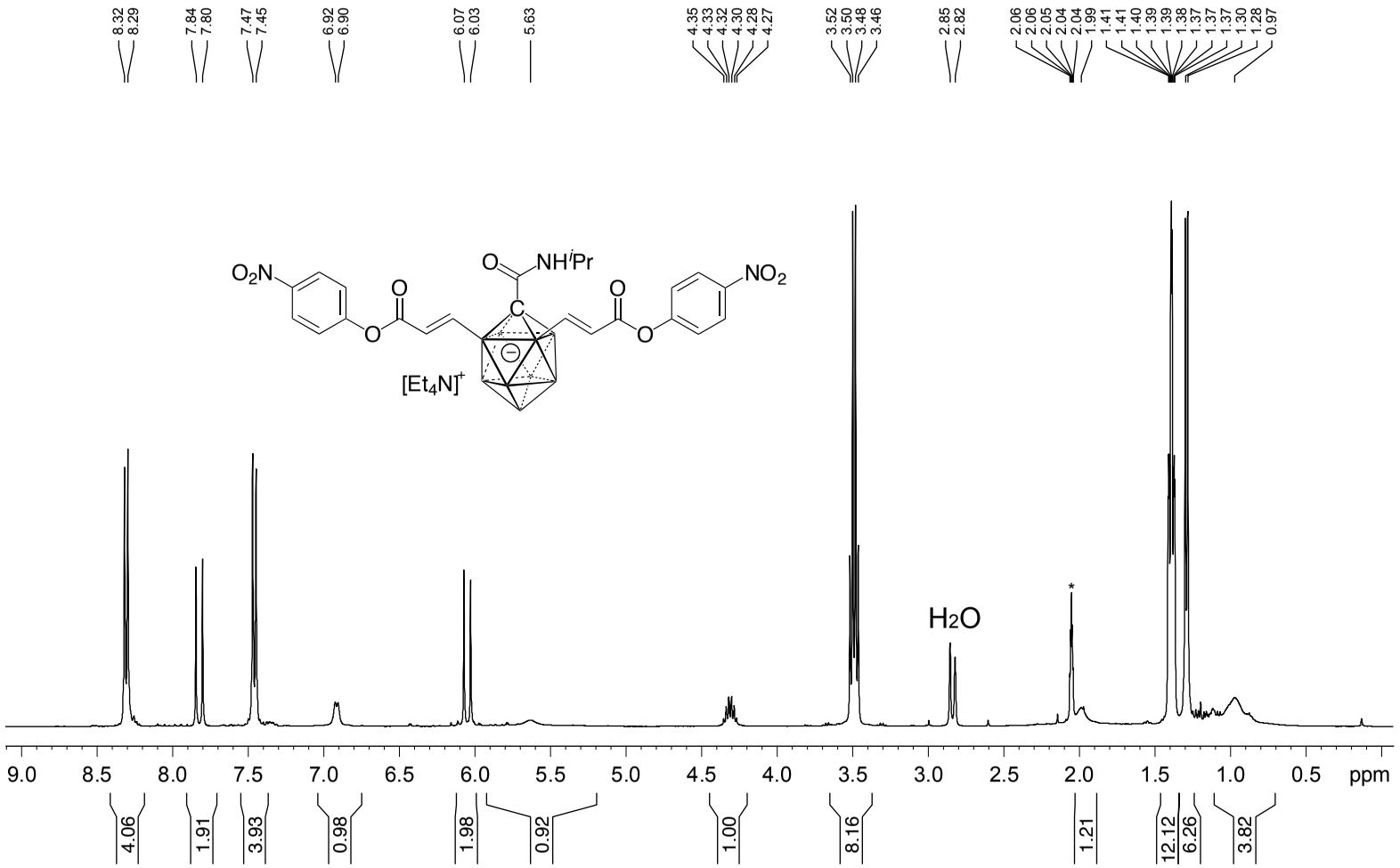
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126815 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR45

20171203−lxw−0499
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone−d6*



Current Data Parameters
NAME 20171203−lxw−0493
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20171204
Time 3.51
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 86.58
DW 62.400 usec
DE 6.50 usec
TE 295.0K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

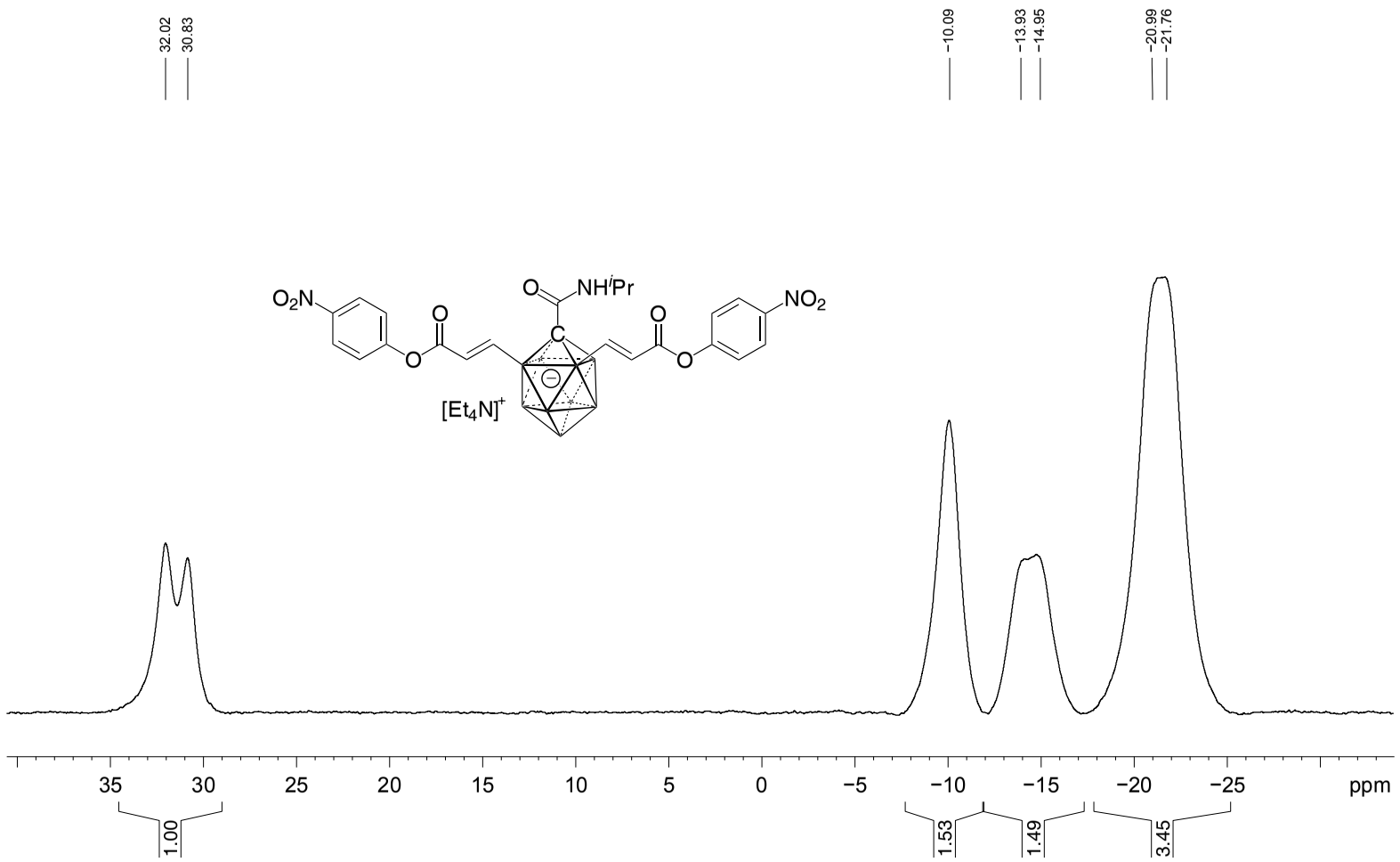
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR46

20171203-lxw-0499
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171203-lxw-0493
EXPNO 4
PROCNO 1

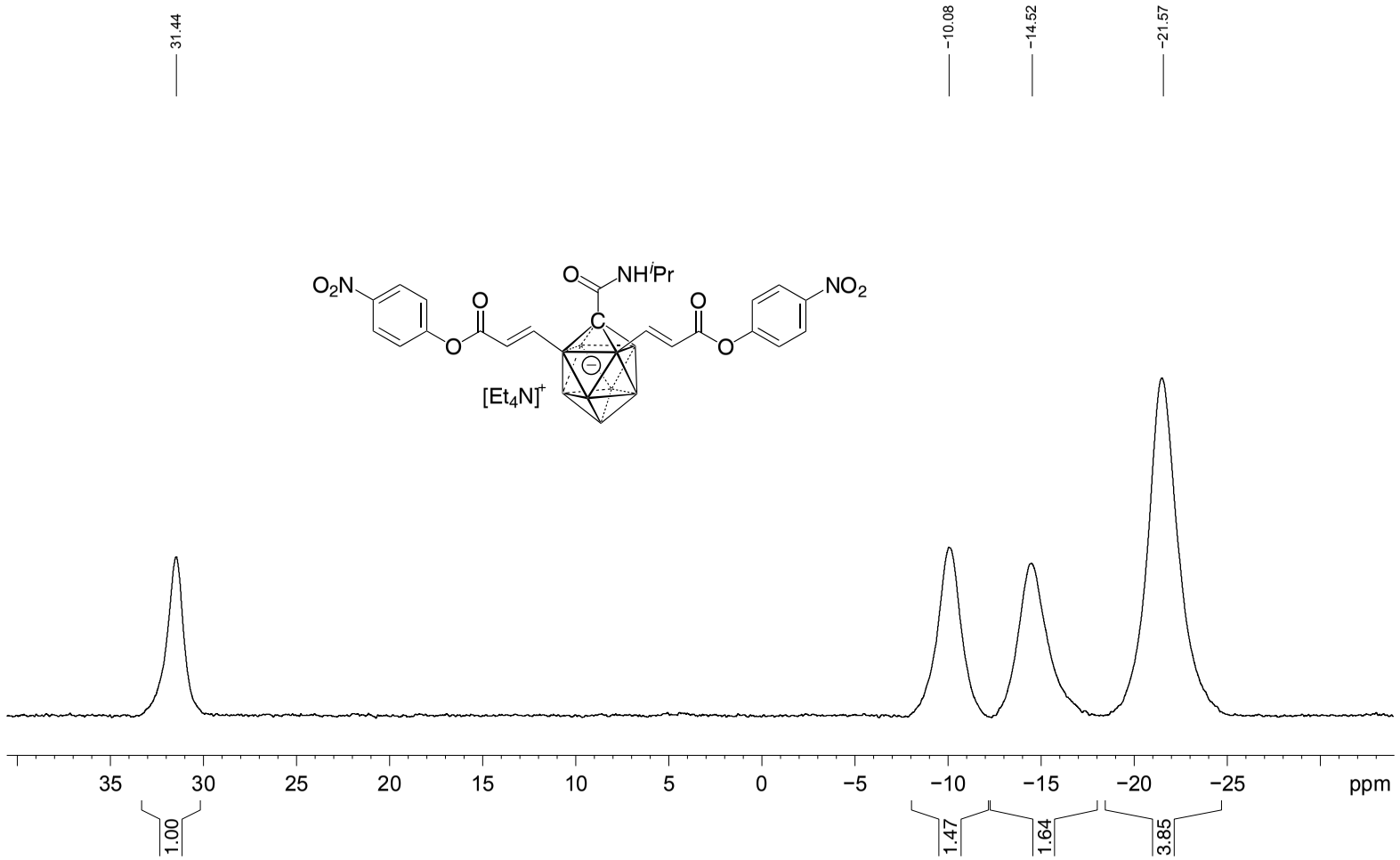
F2 - Acquisition Parameters
Date_ 20171204
Time 4.03
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.0K
D1 1.00000000 sec
TD0 1

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

NMR47

20171203-lxw-0499
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171203-lxw-0493
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171204
Time 3.57
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 295.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

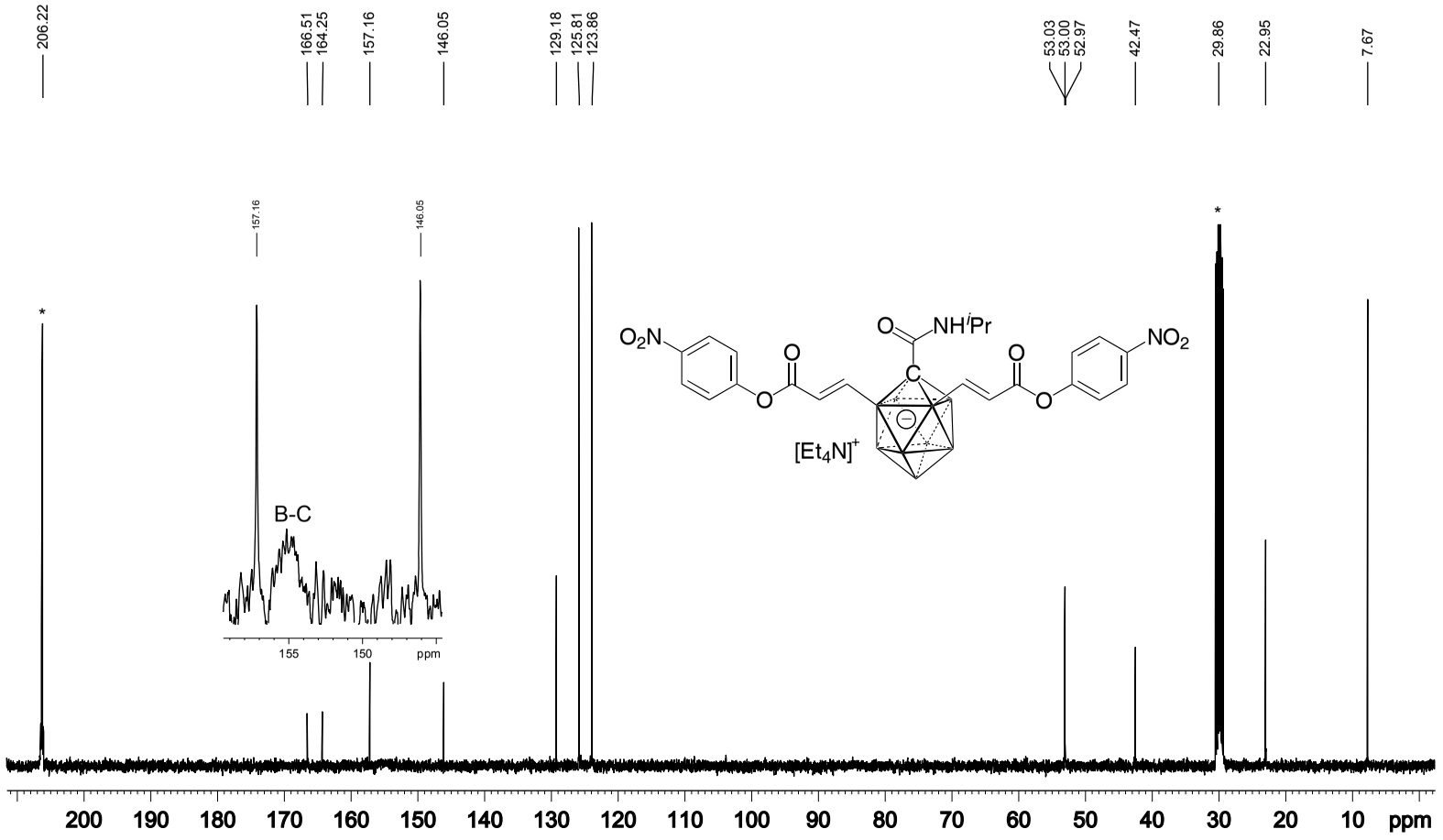
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR48

20171203-lxw-0499
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171203-lxw-0493
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171204
Time 4.27
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 295.6K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

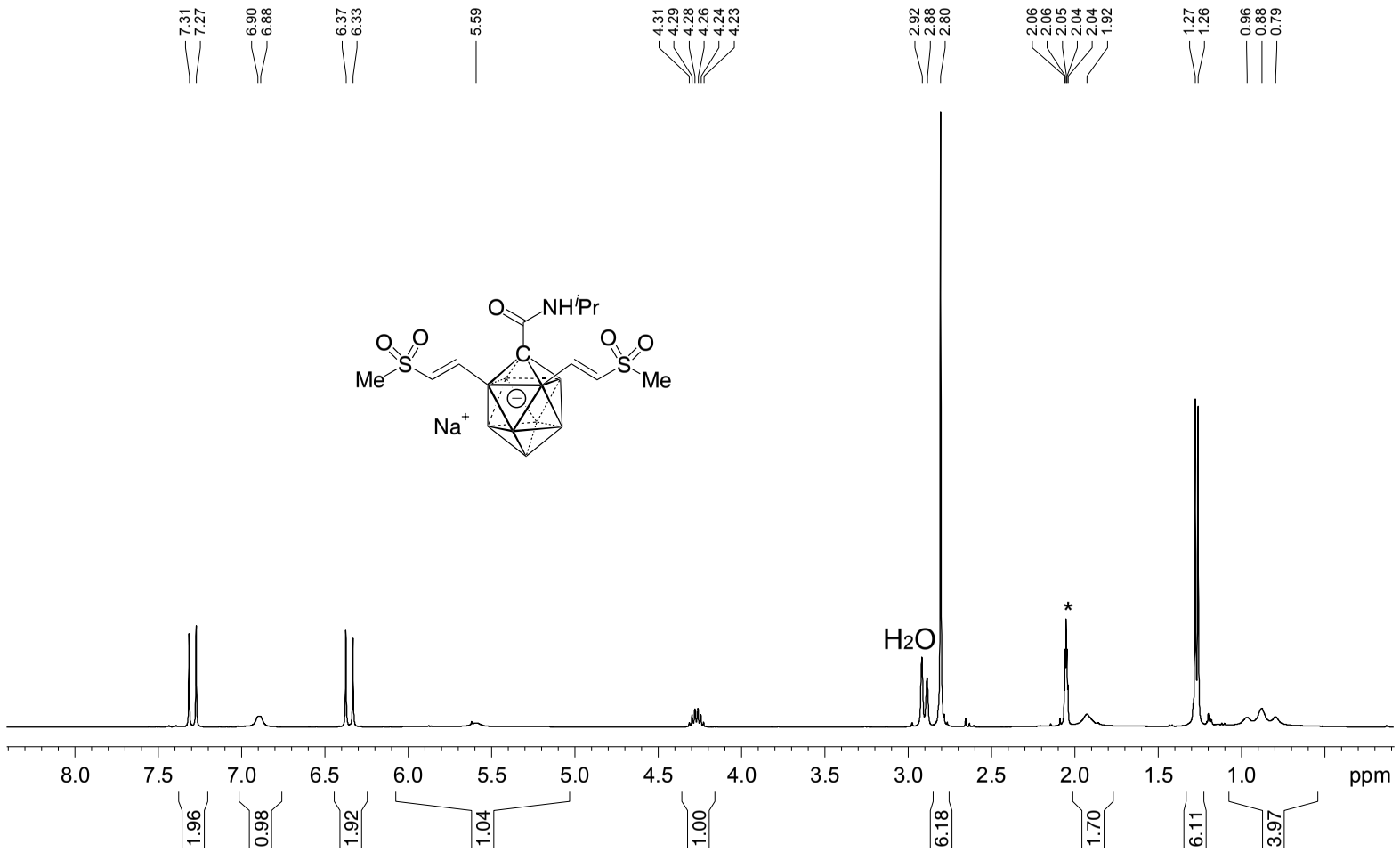
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126808 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR49

20171115-lxw-491-Na
Bruker 400MHz, 1H{11B} NMR, acetone-d6 *



Current Data Parameters
NAME 20171115-lxw-491-Na
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 19.51
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 107.6
DW 62.400 usec
DE 6.50 usec
TE 296.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

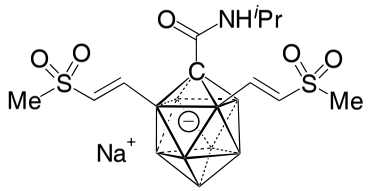
======== CHANNEL f1 =======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR50

20171115-lxw-491-Na
Bruker 128MHz, 11B NMR, in acetone-d6



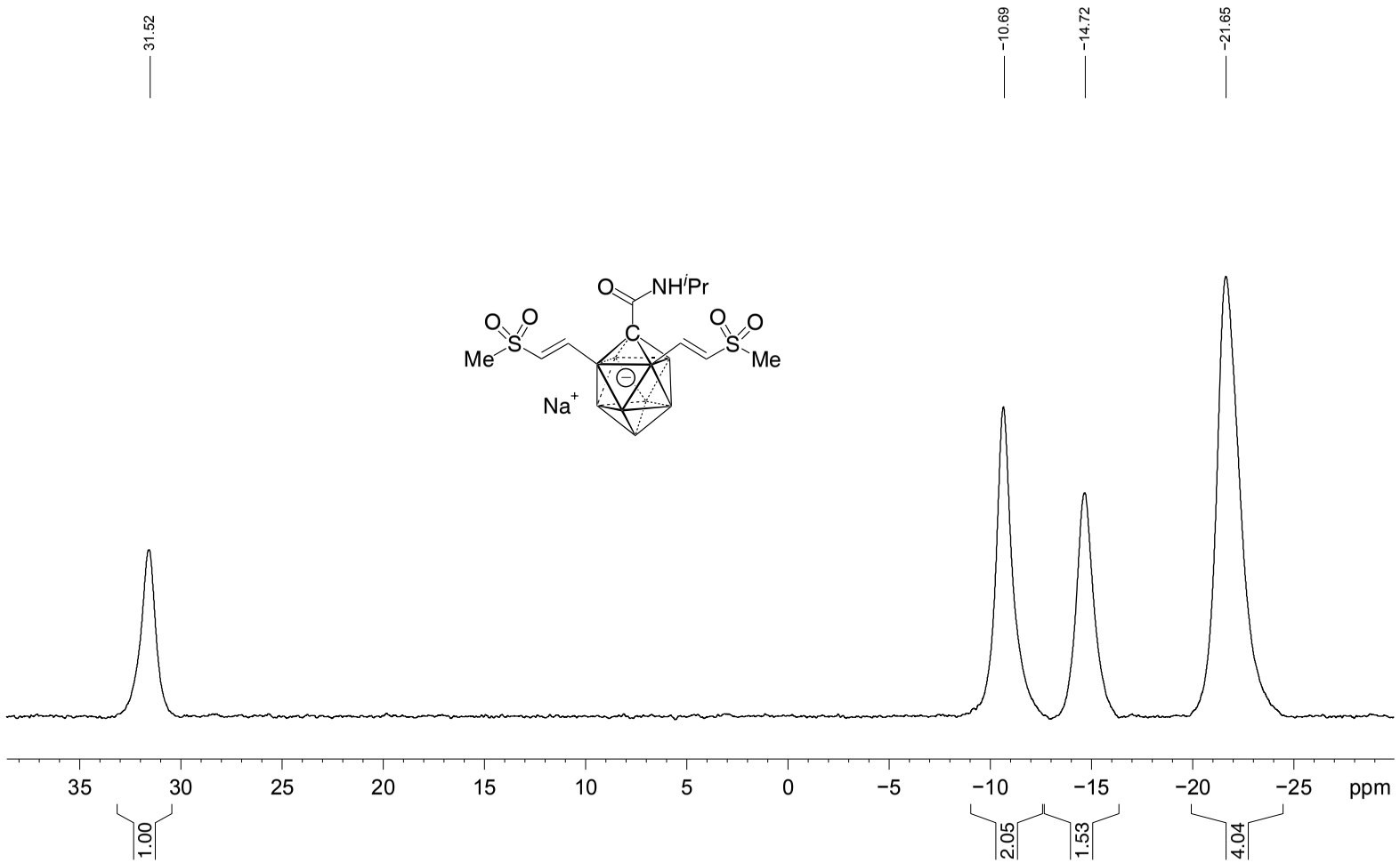
Current Data Parameters
NAME 20171115-lxw-491-Na
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 20.03
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 296.7K
D1 1.00000000 sec
TD0 1

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

20171115-lxw-491-Na
Bruker 128MHz, 11B {1H}NMR, in acetone-d6



NMR51

Current Data Parameters
NAME 20171115-lxw-491-Na
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 19.57
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 297.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

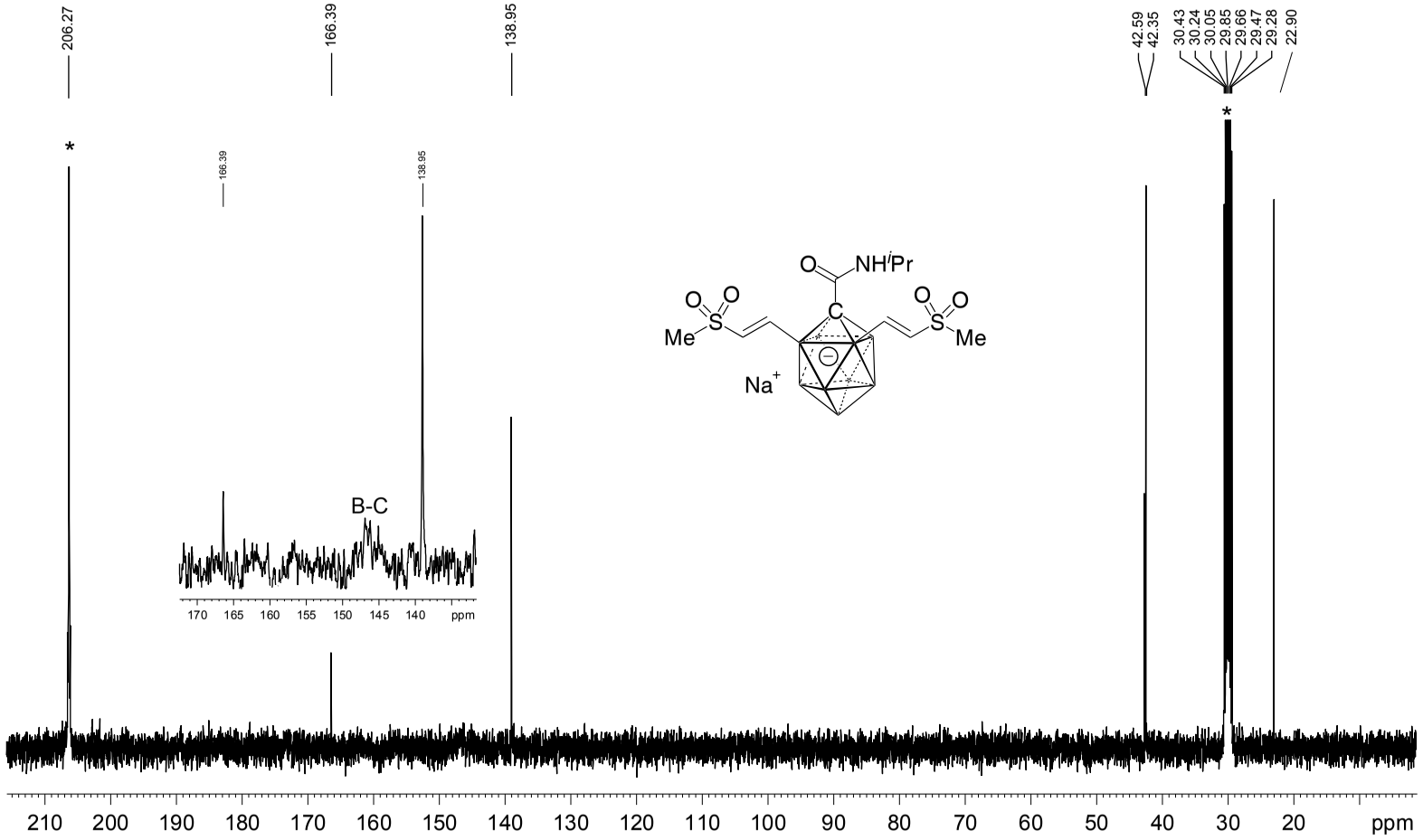
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR52

20171115-lxw-491-Na
Bruker 101MHz, 13C NMR, in acetone-d6*



Current Data Parameters
NAME 20171115-lxw-491-Na
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171116
Time 20.27
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 296.8K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

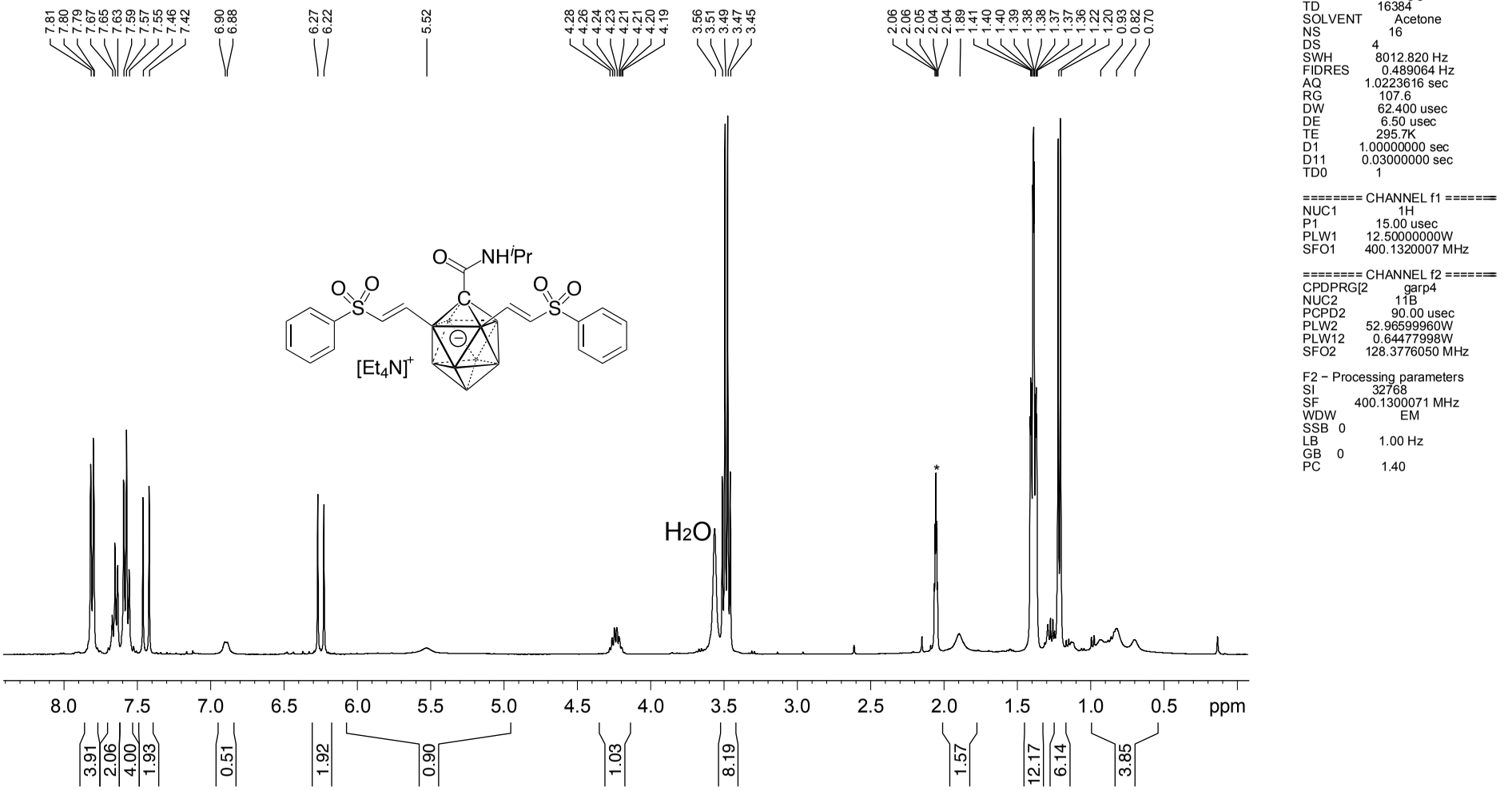
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126797 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR53

20171201−lxw−0492
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone−d6*



Current Data Parameters
NAME 20171201−lxw−0492
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20171202
Time 19.08
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 107.6
DW 62.400 usec
DE 6.50 usec
TE 295.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

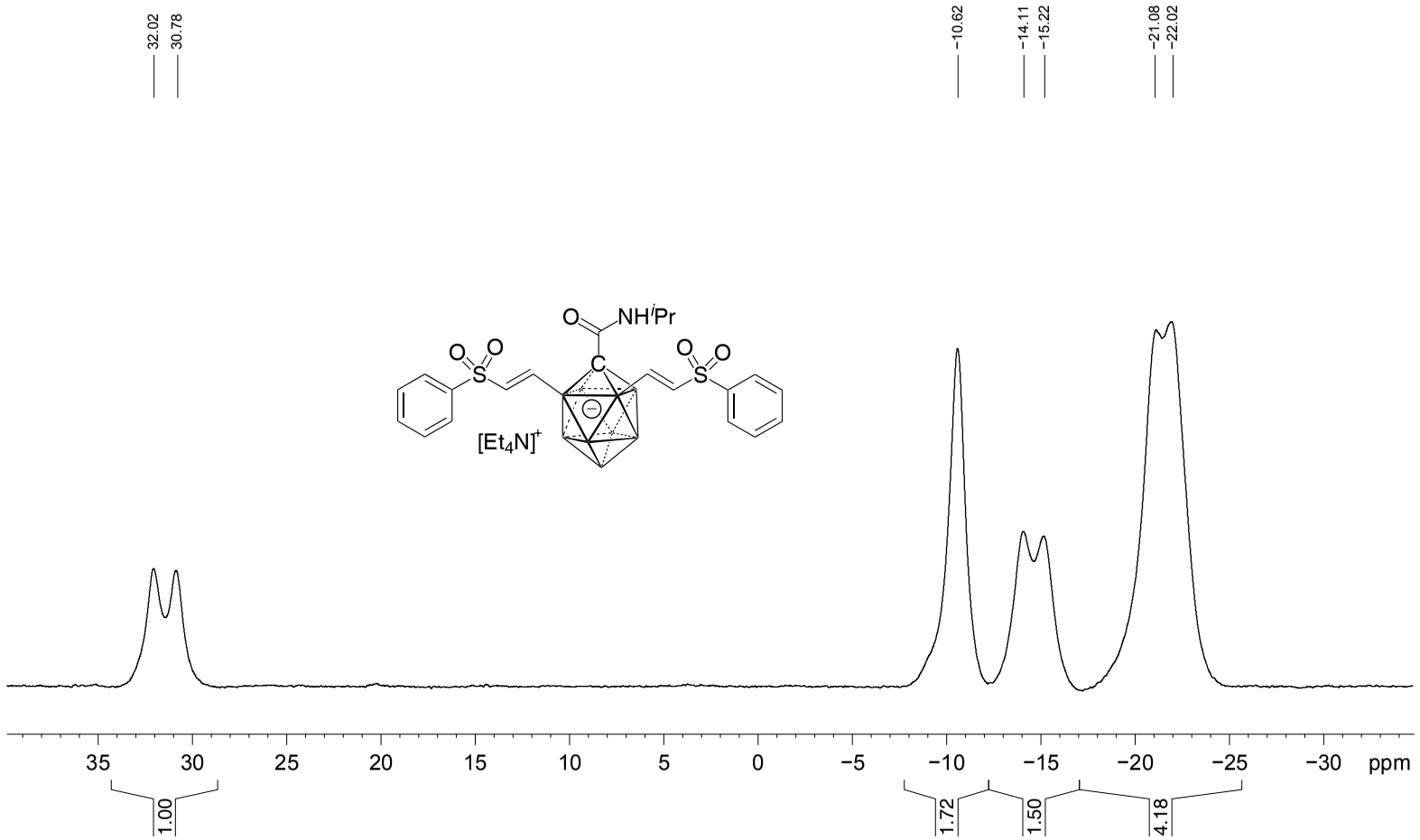
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR54

20171201-lxw-0492
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0492
EXPNO 4
PROCNO 1

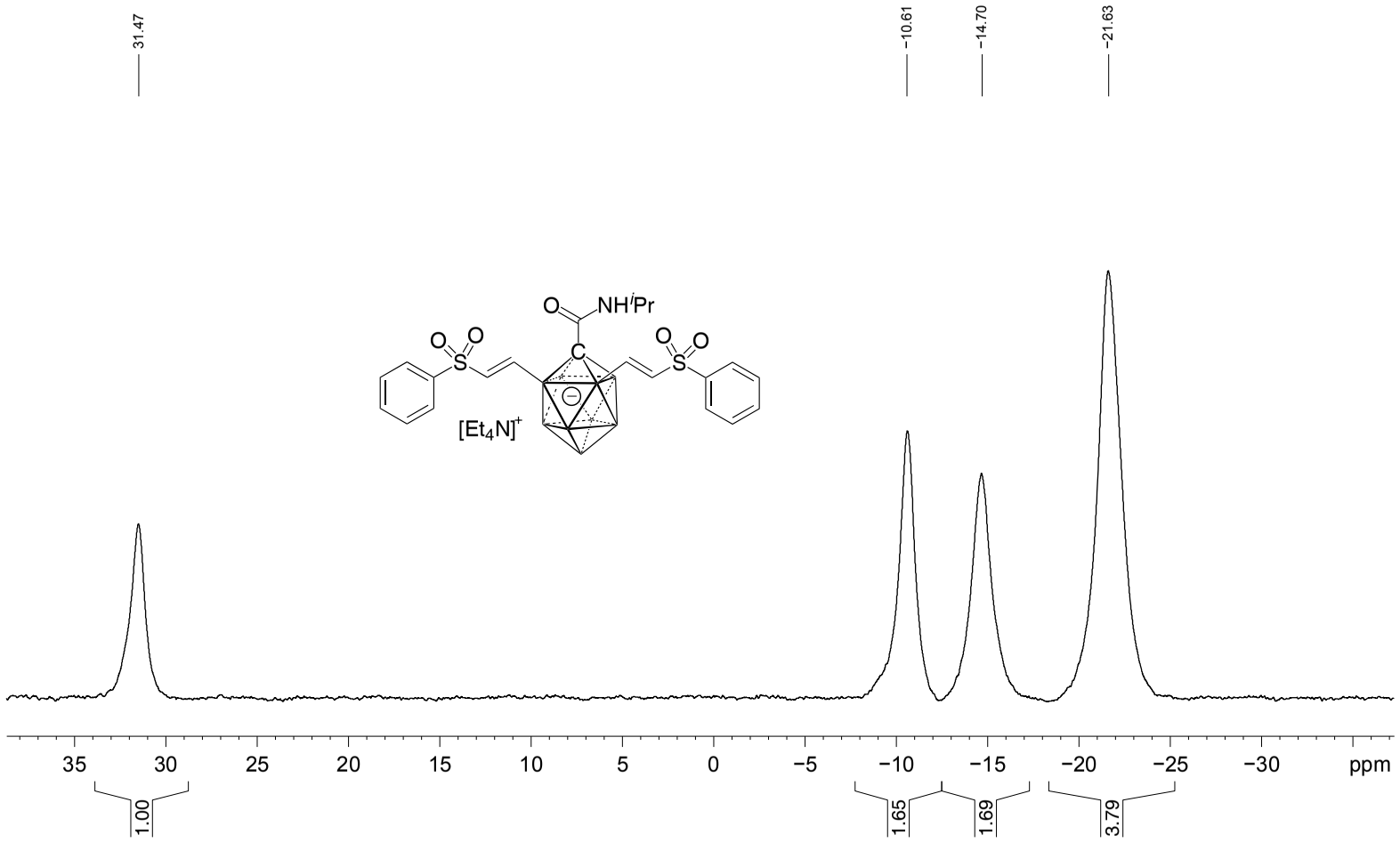
F2 - Acquisition Parameters
Date_ 20171202
Time 19.19
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.5K
D1 1.00000000 sec
TD0 1

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

NMR55

20171201-lxw-0492
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0492
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 19.14
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 296.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

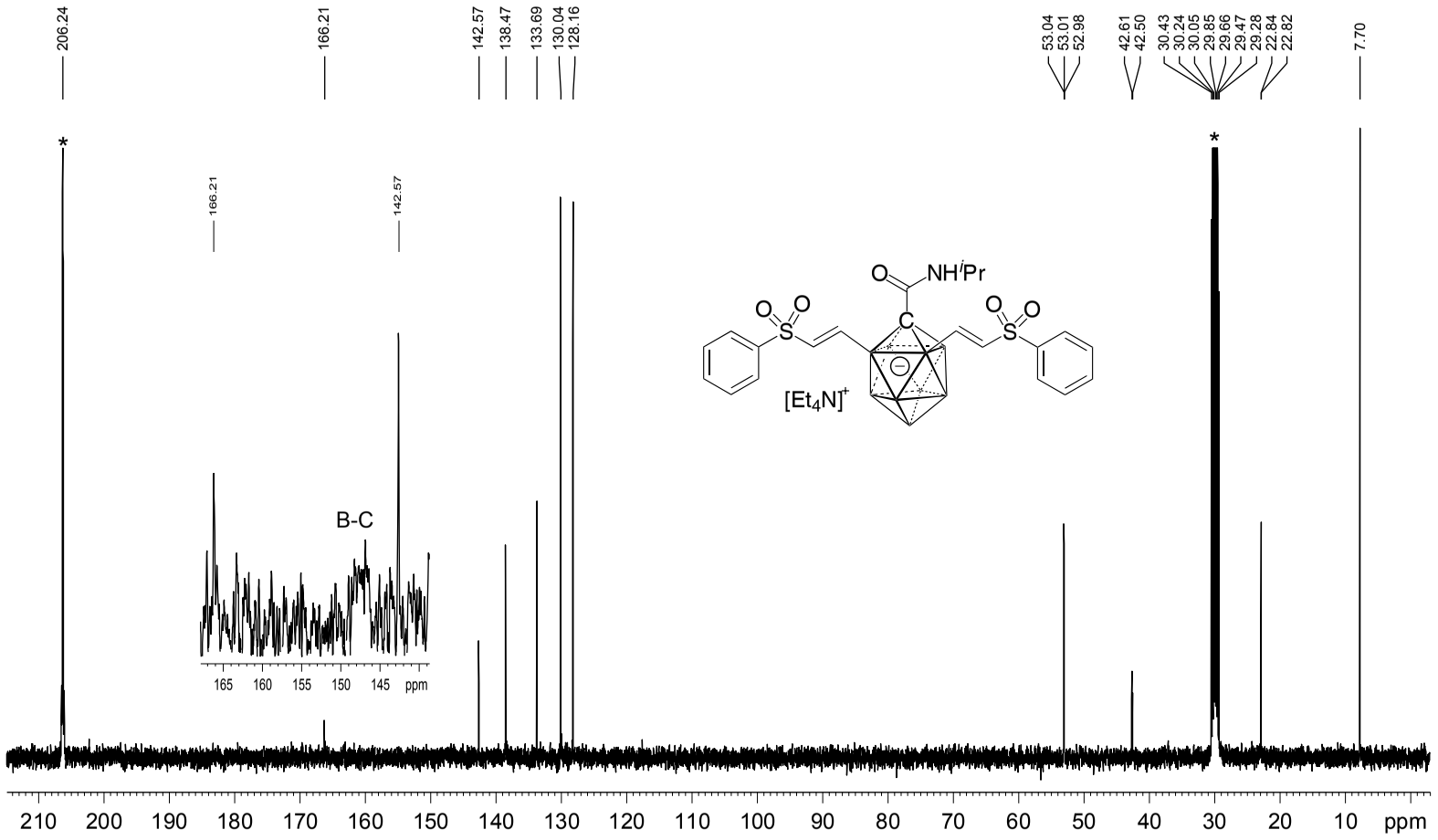
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR56

20171201-lxw-0492
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171201-lxw-0492
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 19.43
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 296.4K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

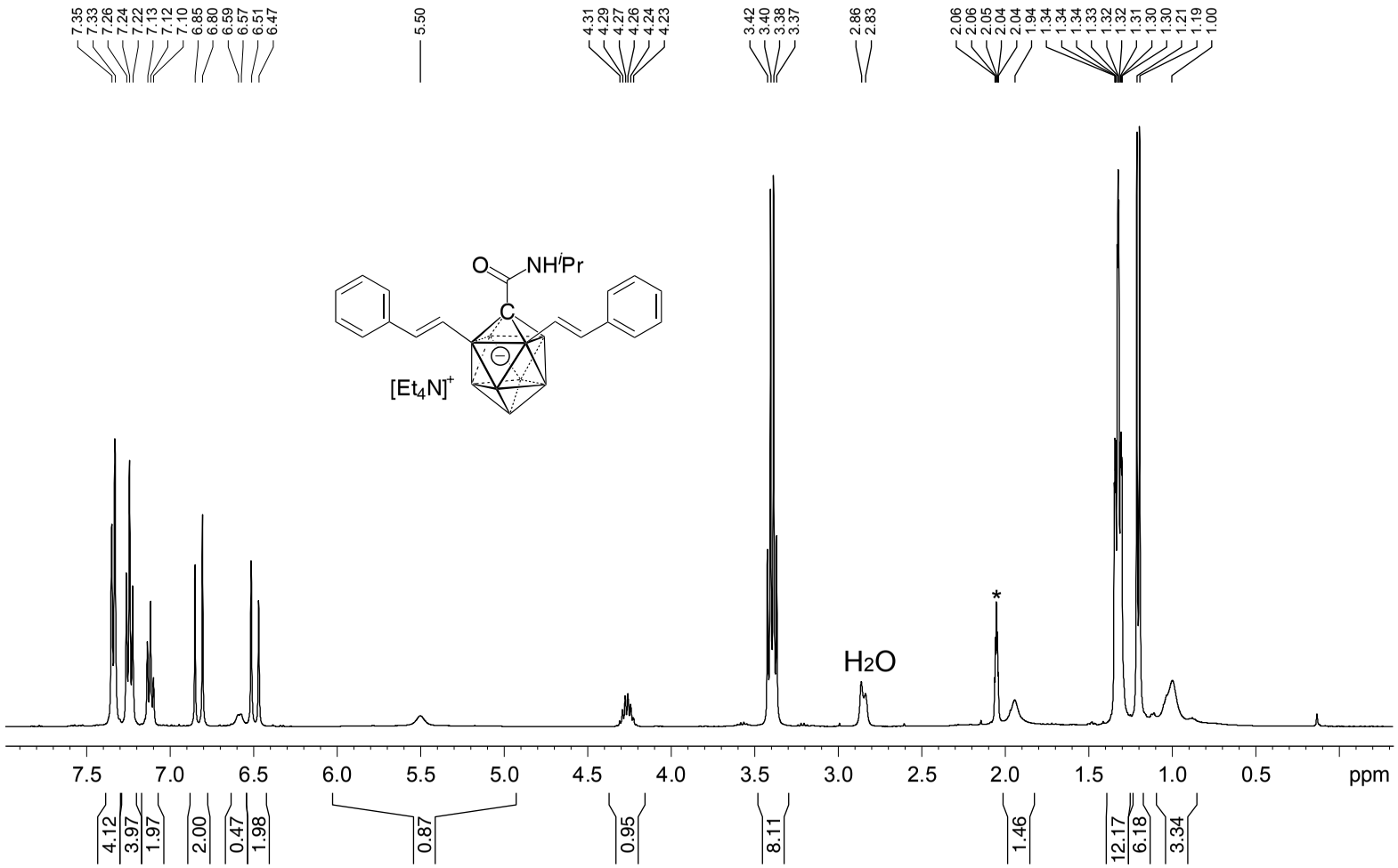
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126805 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR57

20171209-lxw-0500
Bruker 400MHz, 1H{11B} NMR, acetone-d6 *



Current Data Parameters
NAME 20171209-lxw-0500
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time 9.02
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 294.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

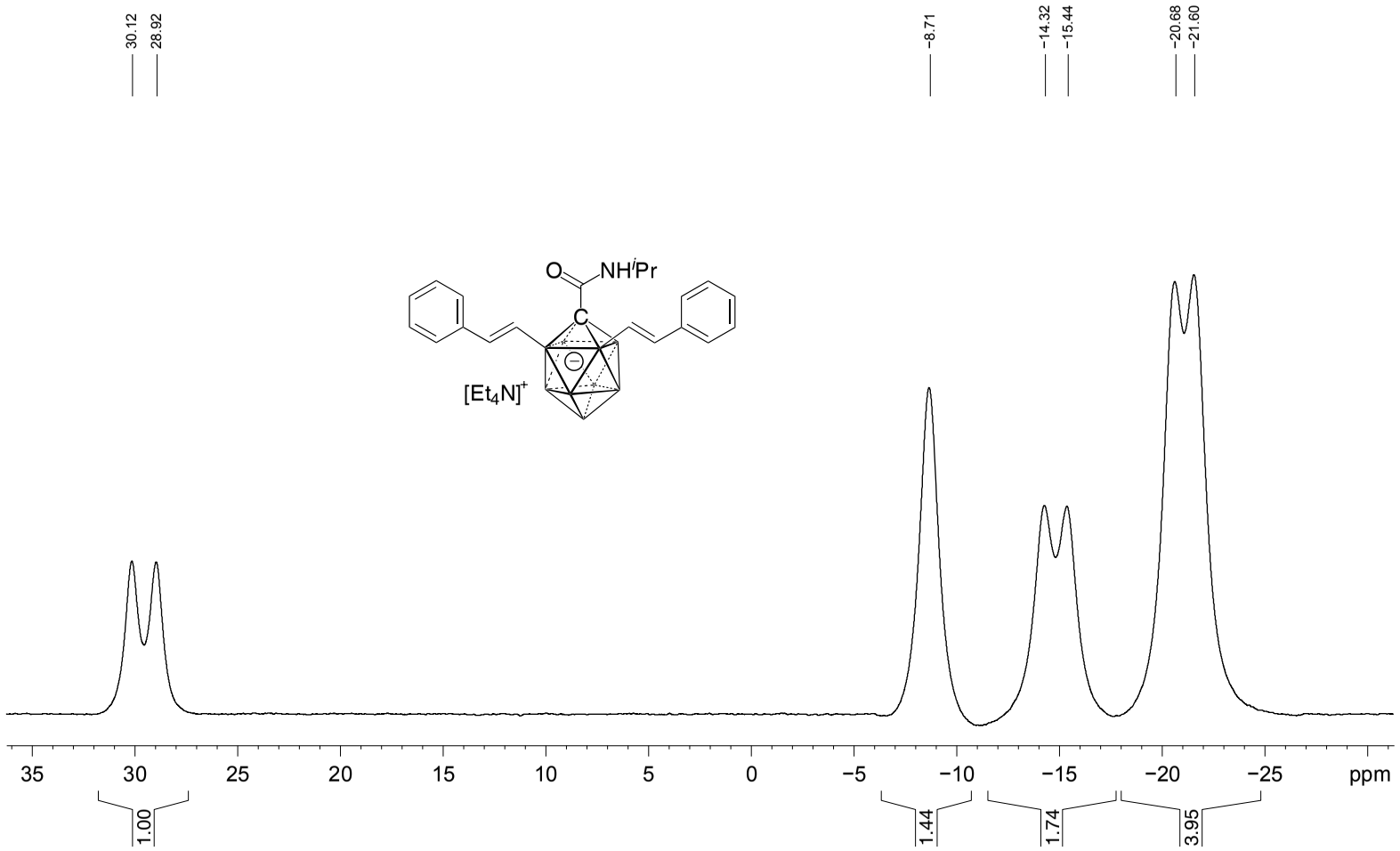
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR58

20171209-lxw-0500
Bruker 128MHz, 11B NMR, in acetone-d6



Current Data Parameters
NAME 20171209-lxw-0500
EXPNO 4
PROCNO 1

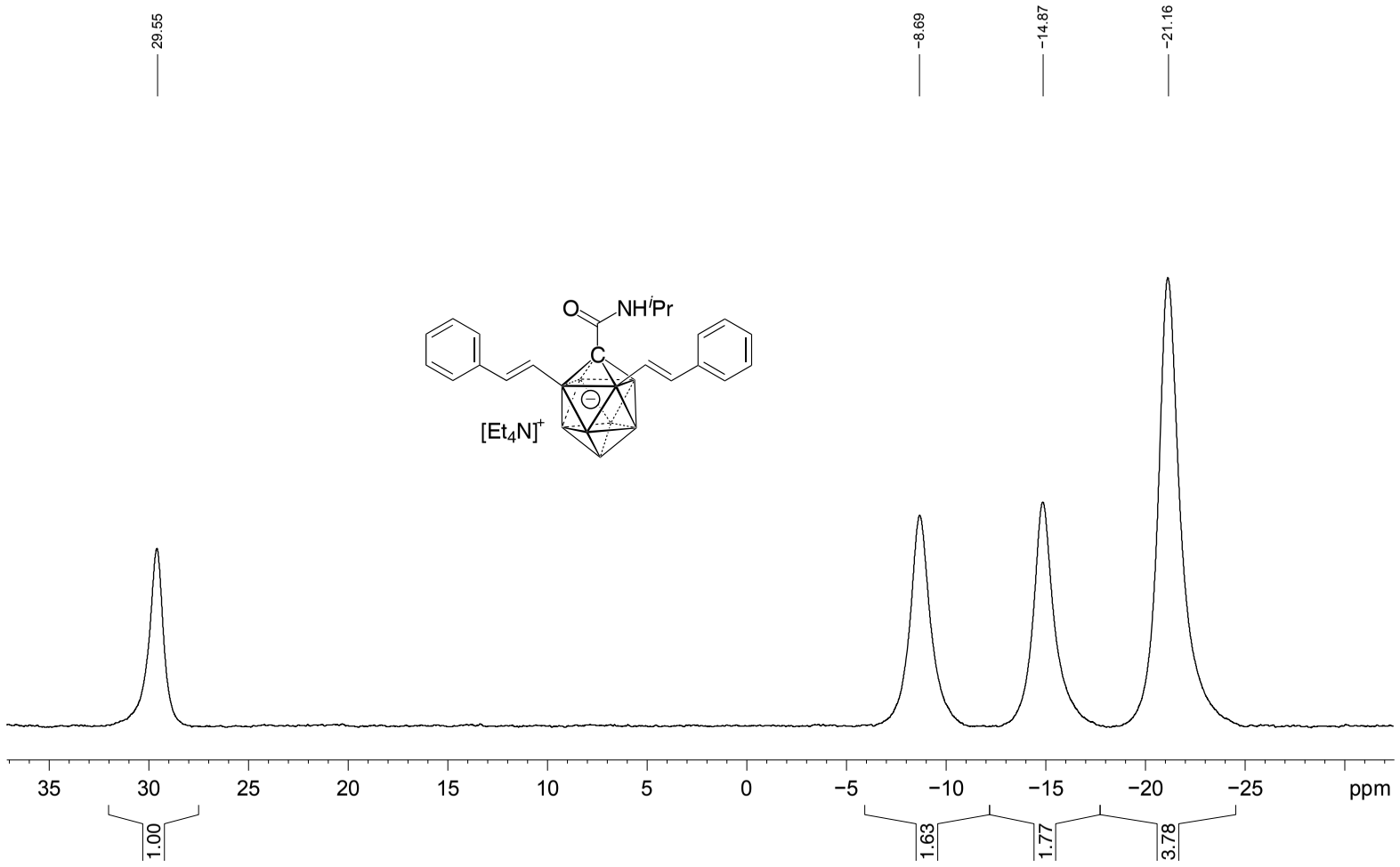
F2 - Acquisition Parameters
Date_ 20171210
Time 9.14
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 294.1K
D1 1.00000000 sec
TD0 1

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

NMR59

20171209-lxw-0500
Bruker 128 MHz, 11B{1H} NMR, in acetone-d6



Current Data Parameters
NAME 20171209-lxw-0500
EXPNO 3
PROCNO 1

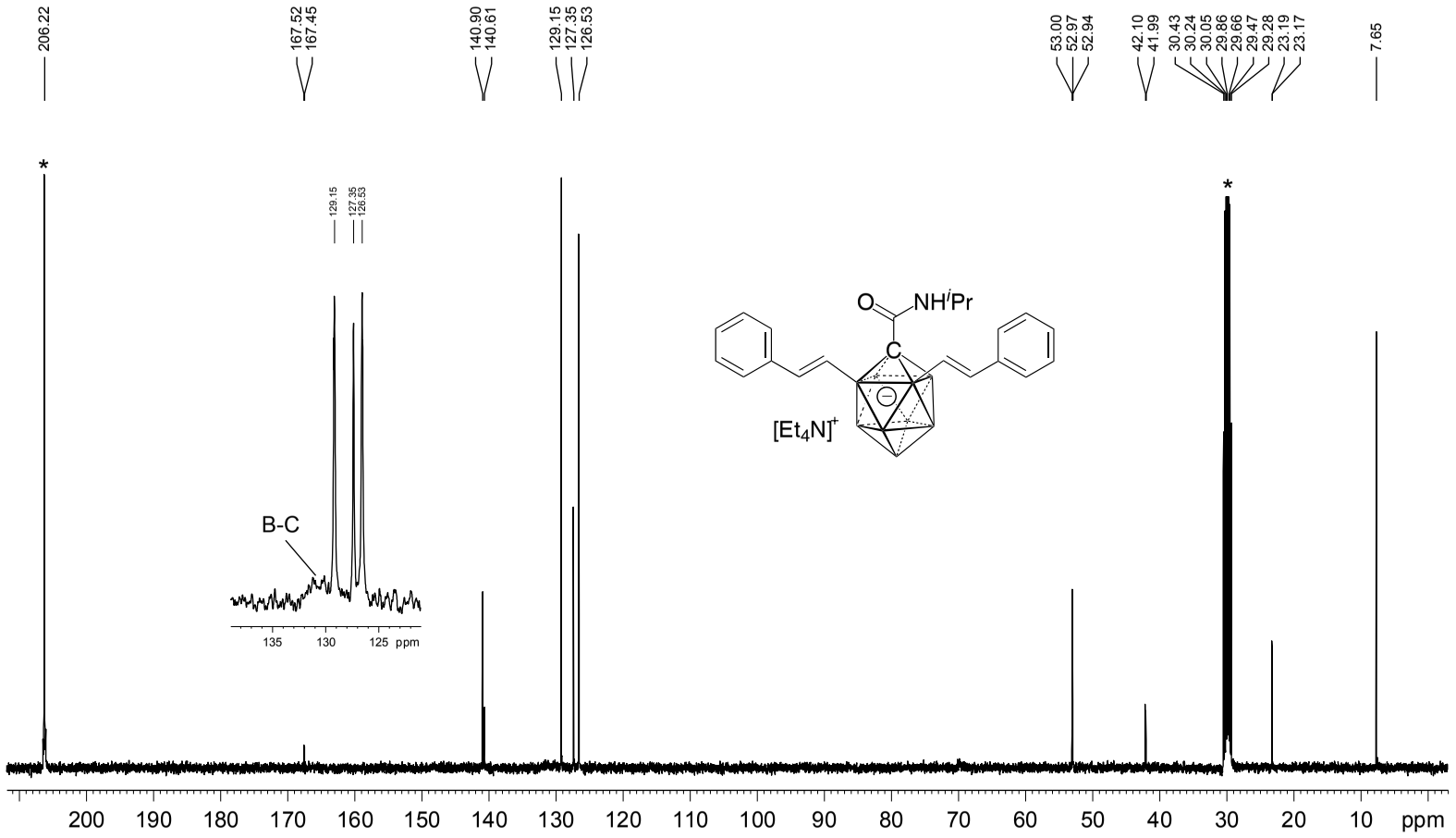
F2 - Acquisition Parameters
Date_ 20171210
Time 9.08
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 294.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171209-lxw-0500
Bruker 101MHz, 13C NMR, in acetone-d6*



NMR60

Current Data Parameters
NAME 20171209-lxw-0500
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time 9.38
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 294.9K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

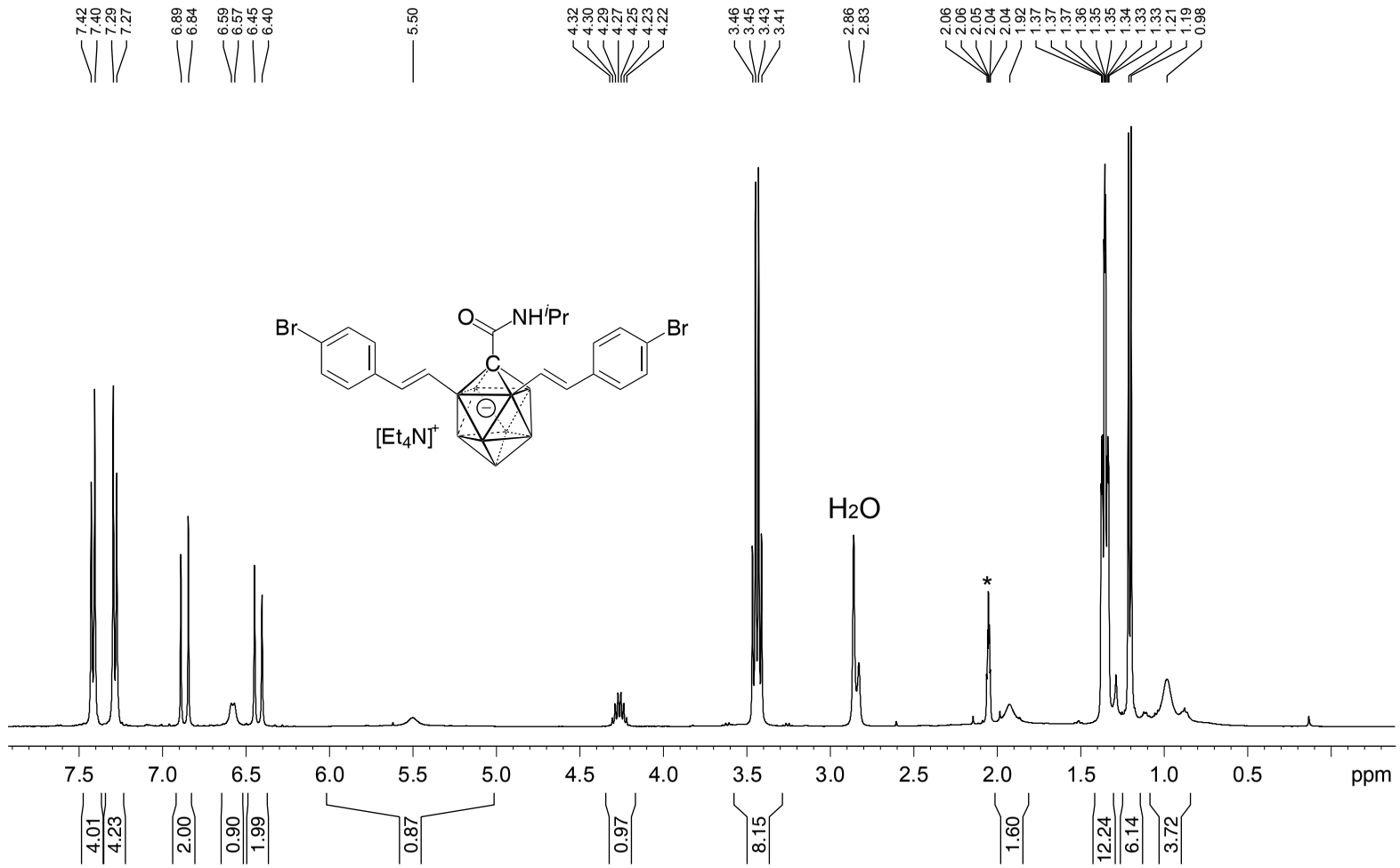
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126820 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR61

20171108-lxw-0484
Bruker 400MHz, 1H{11B} NMR,acetone-d6*



Current Data Parameters
NAME 20171108-lxw-0484
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 17.30
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 296.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

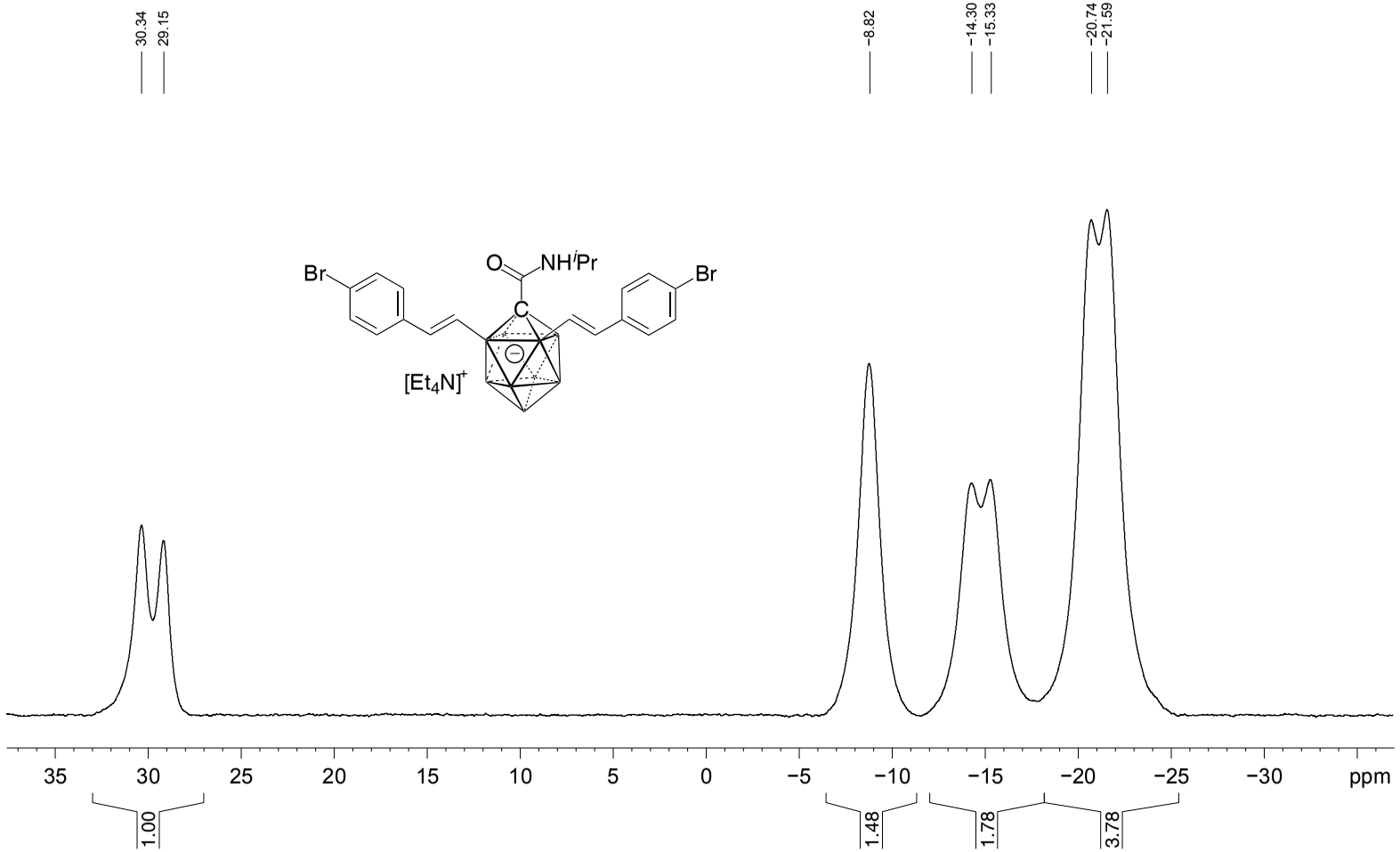
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR62

20171108-lxw-0484
Bruker 128MHz, 11B NMR,acetone-d6



Current Data Parameters
NAME 20171108-lxw-0484
EXPNO 4
PROCNO 1

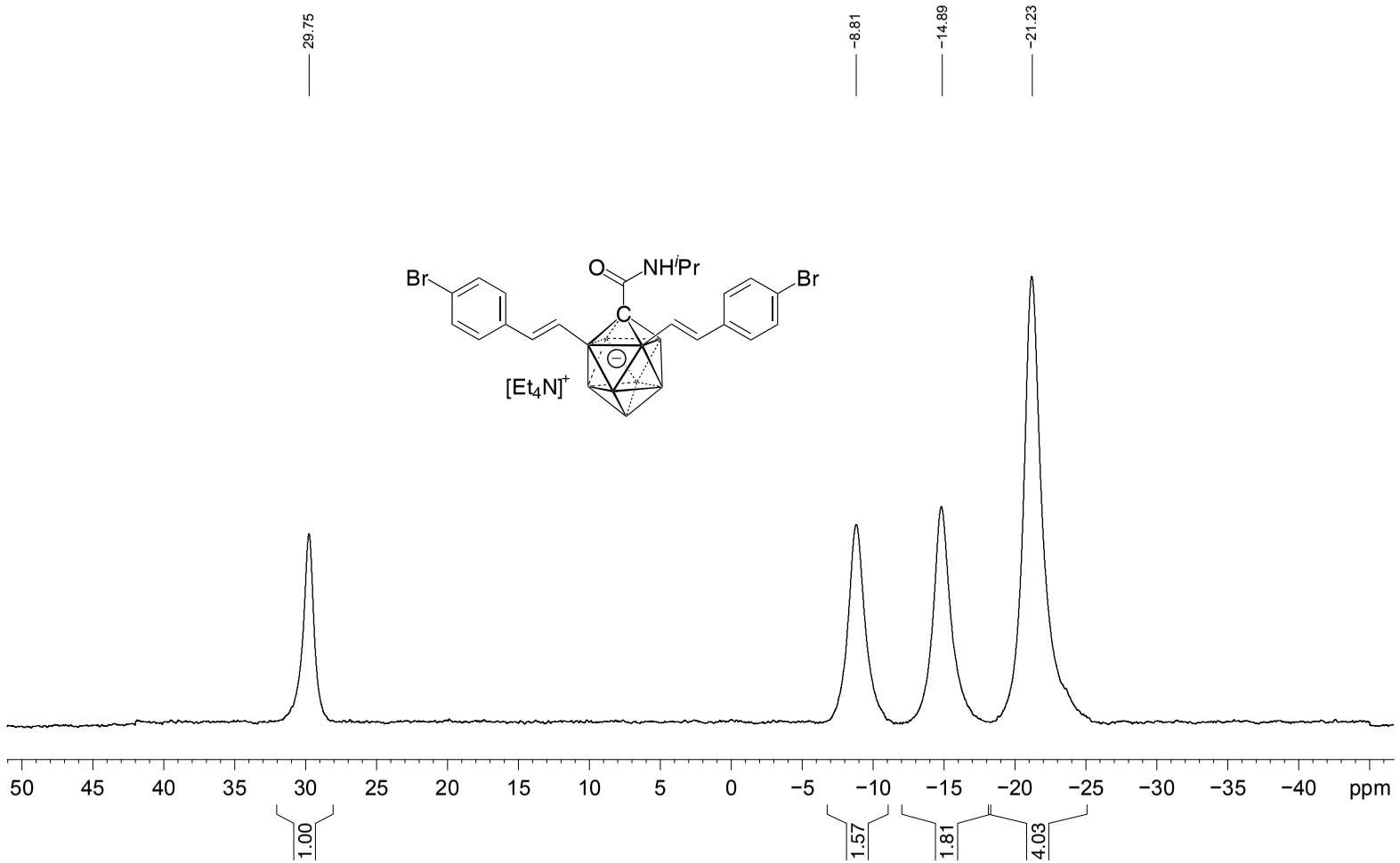
F2 - Acquisition Parameters
Date_ 20171109
Time 17.42
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 296.6K
D1 1.00000000 sec
TD0 1

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

NMR63

20171108-lxw-0484
Bruker 128MHz, 11B{1H} NMR,acetone-d6



Current Data Parameters
NAME 20171108-lxw-0484
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 17.37
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 297.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

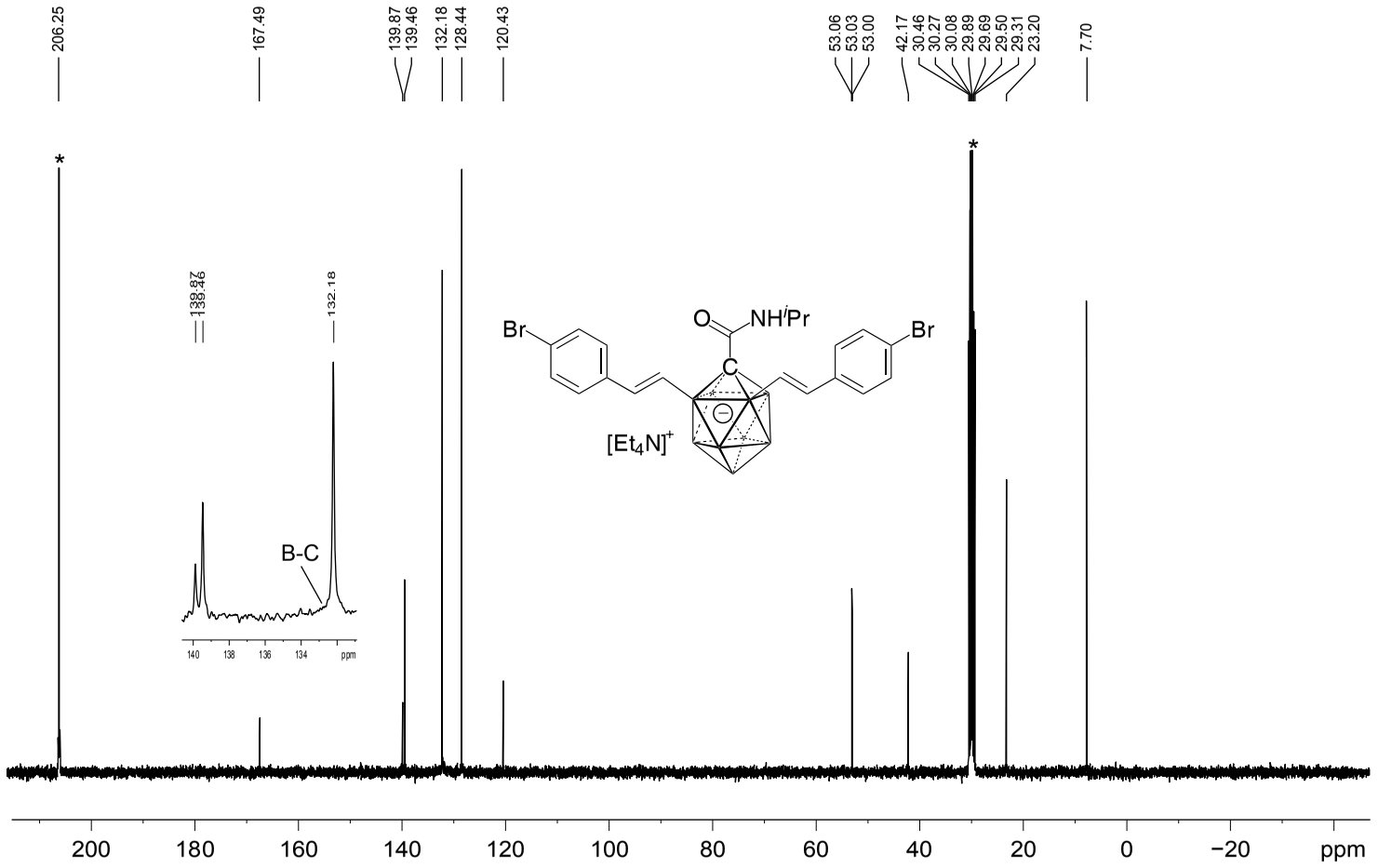
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR64

20171108-lxw-0484
Bruker 101MHz, 13C NMR,acetone-d6*



Current Data Parameters
NAME 20171108-lxw-0484
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171109
Time 18.07
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 297.0 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

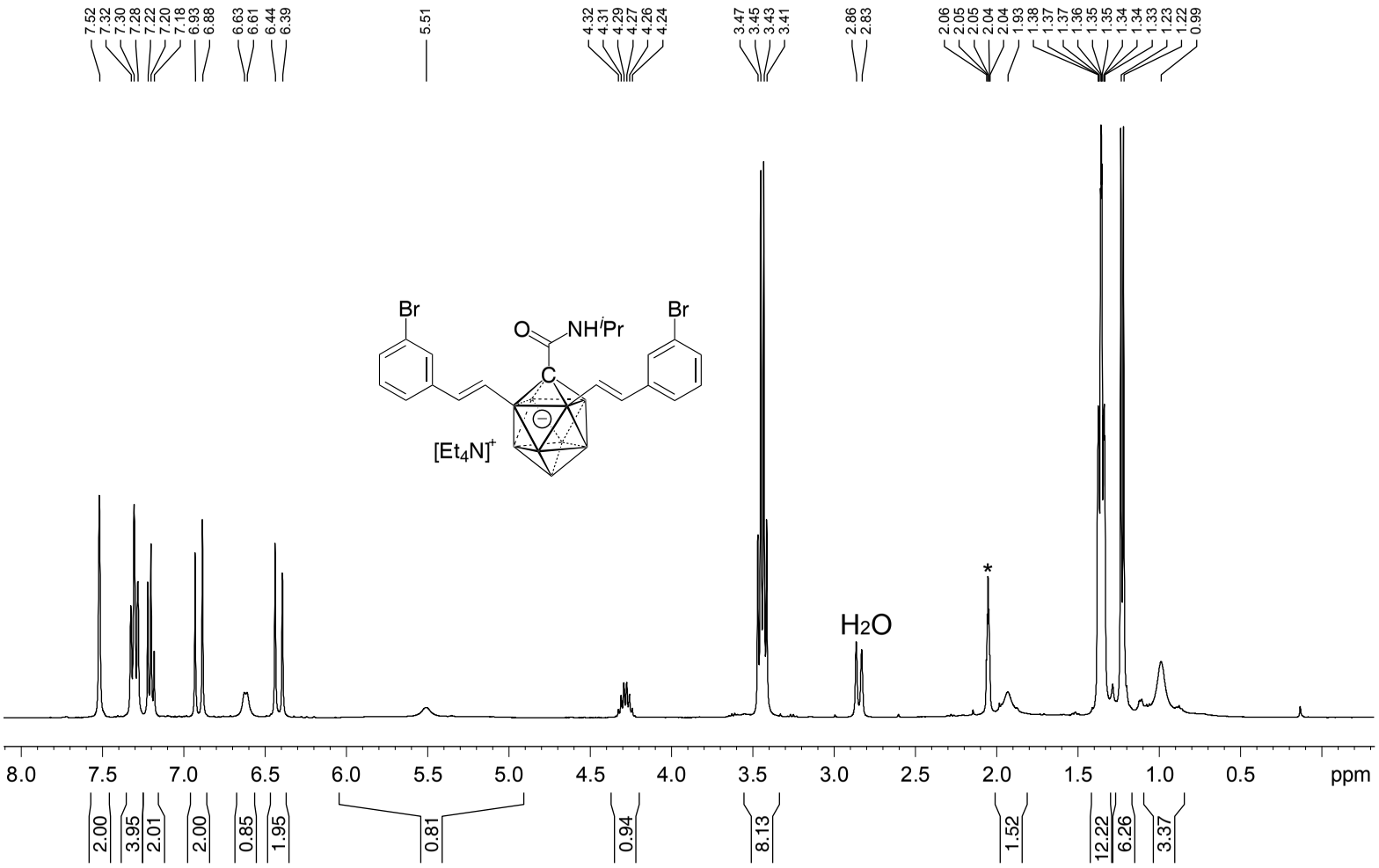
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR65

20171209-lxw-0502
Bruker 400MHz, 1H{11B} NMR, in acetone-d6*



Current Data Parameters
NAME 20171209-lxw-0502
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time 9.45
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 95.29
DW 62.400 usec
DE 6.50 usec
TE 294.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

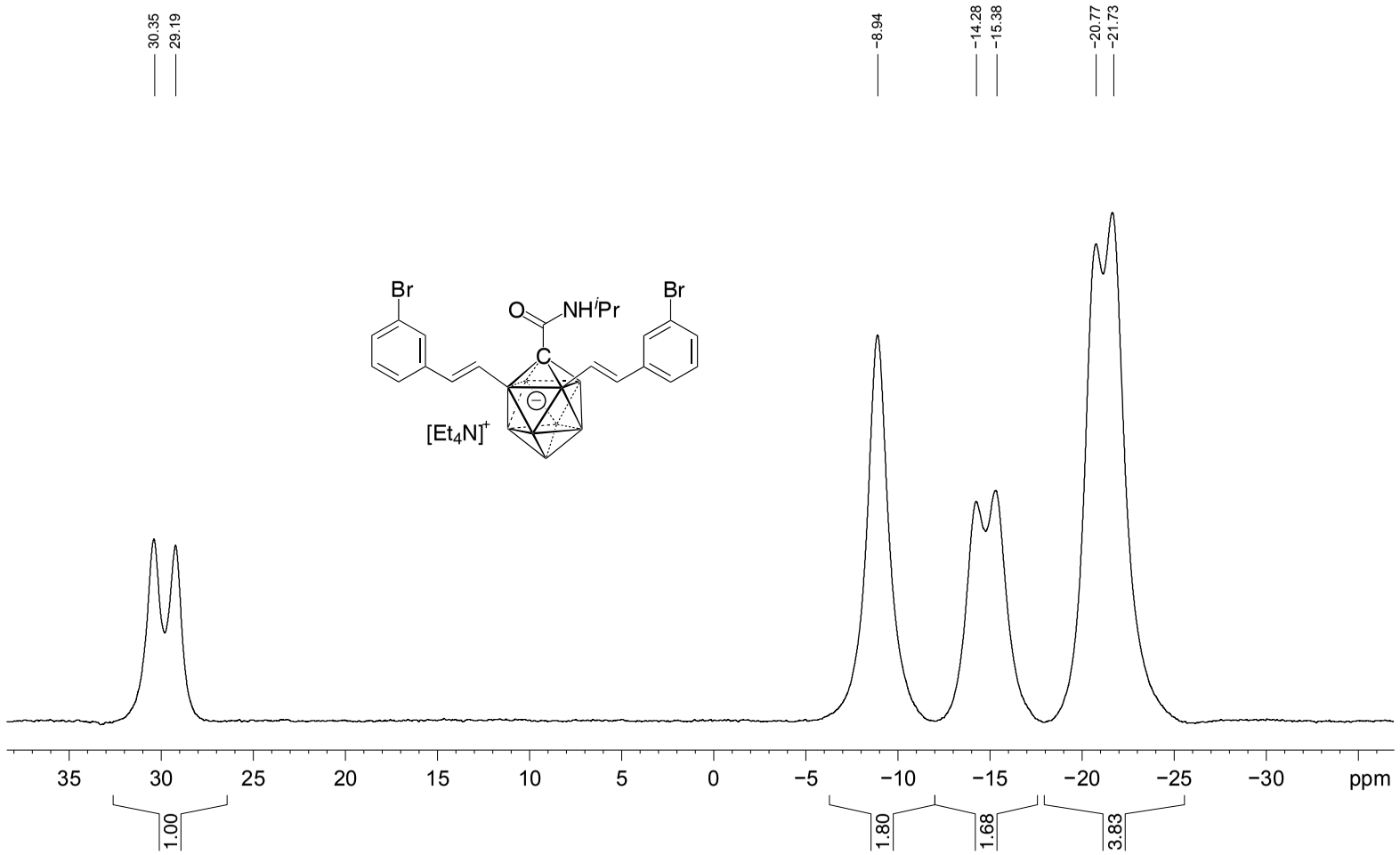
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR66

20171209-lxw-0502
Bruker 128MHz, 11B NMR, in acetone-d6



Current Data Parameters
NAME 20171209-lxw-0502
EXPNO 4
PROCNO 1

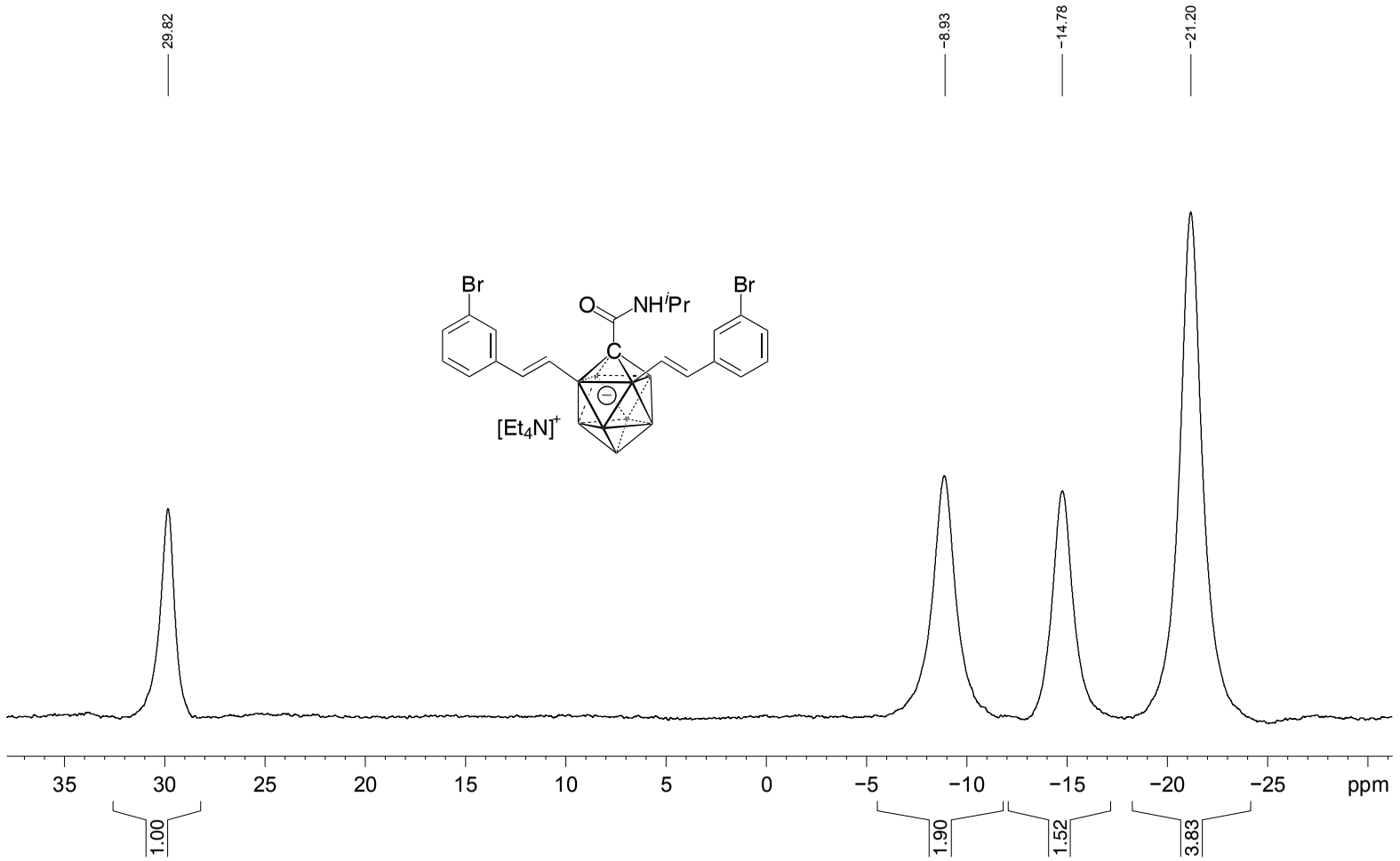
F2 - Acquisition Parameters
Date_ 20171210
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 294.0K
D1 1.00000000 sec
TD0 1

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

NMR67

20171209-lxw-0502
Bruker 128MHz, 11B{1H} NMR, in acetone-d6



Current Data Parameters
NAME 20171209-lxw-0502
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time 9.51
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 294.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

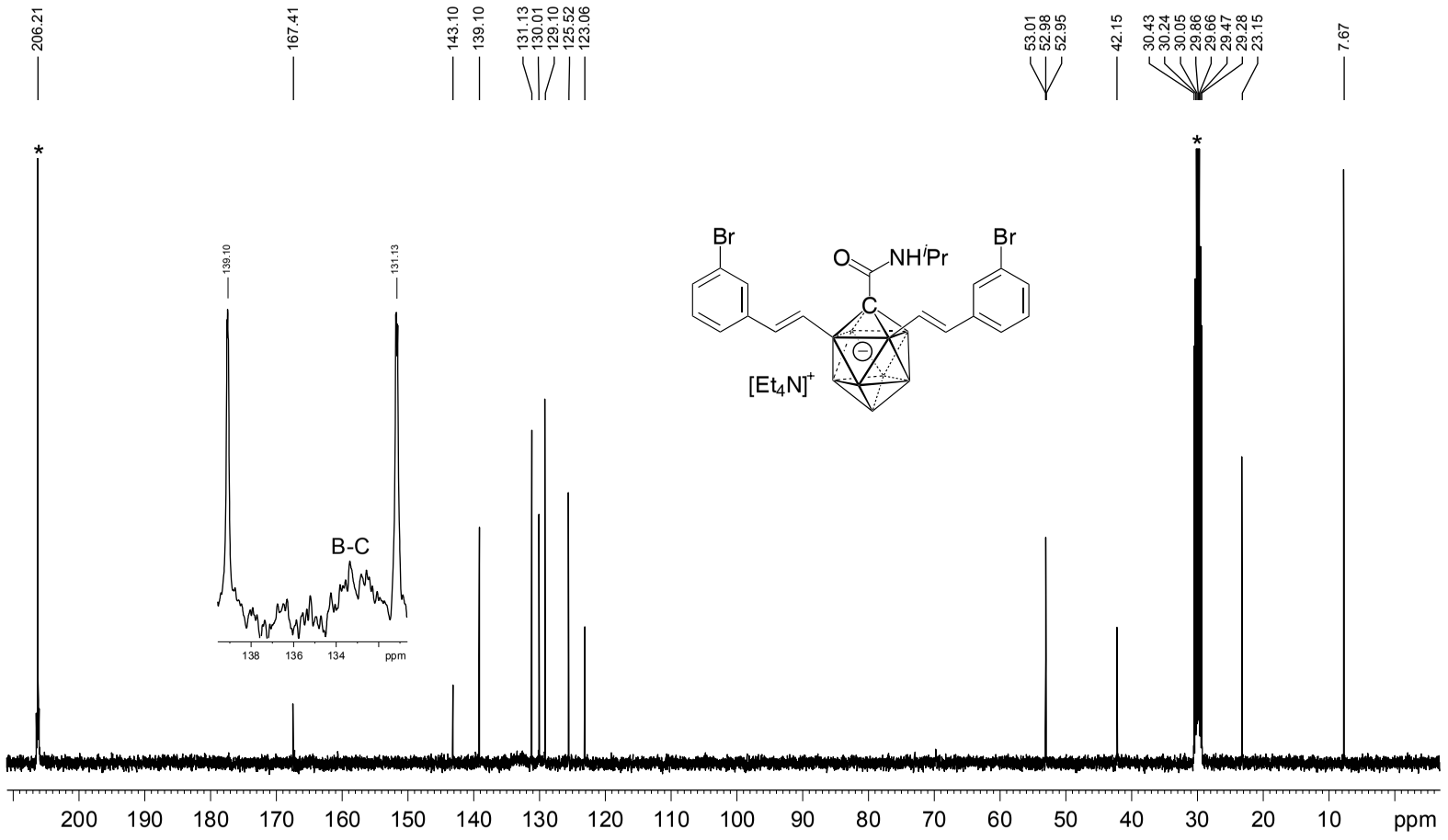
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR68

20171209-lxw-0502
Bruker 101MHz, 13C NMR, in acetone-d6*



Current Data Parameters
NAME 20171209-lxw-0502
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171210
Time 10.21
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 294.8 K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

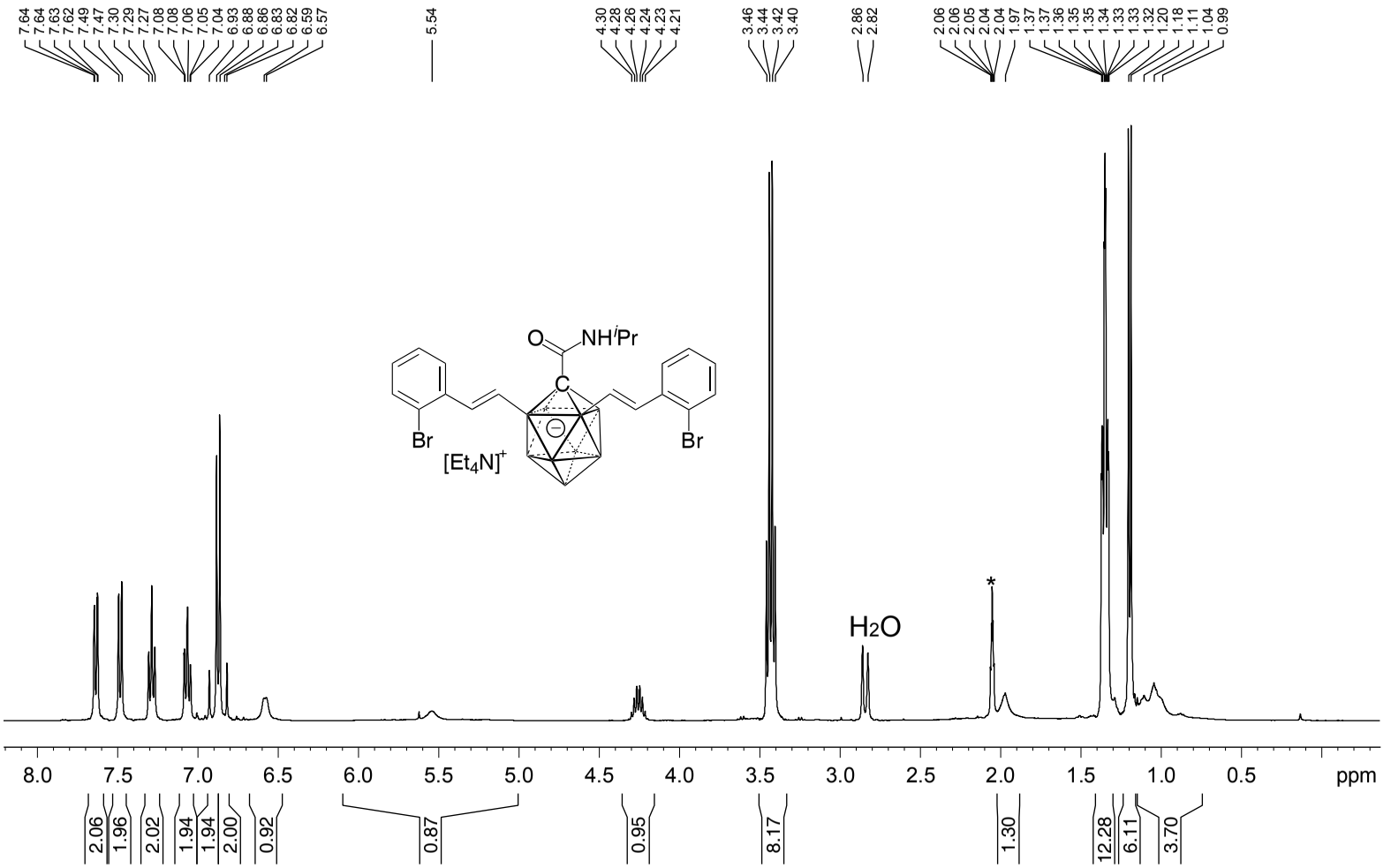
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126821 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR69

20171223-lxw-0508
Bruker 400MHz, 1H{11B} NMR, in acetone-d6*



Current Data Parameters
NAME 20171223-lxw-0508
EXPNO 2
PROCNO 1

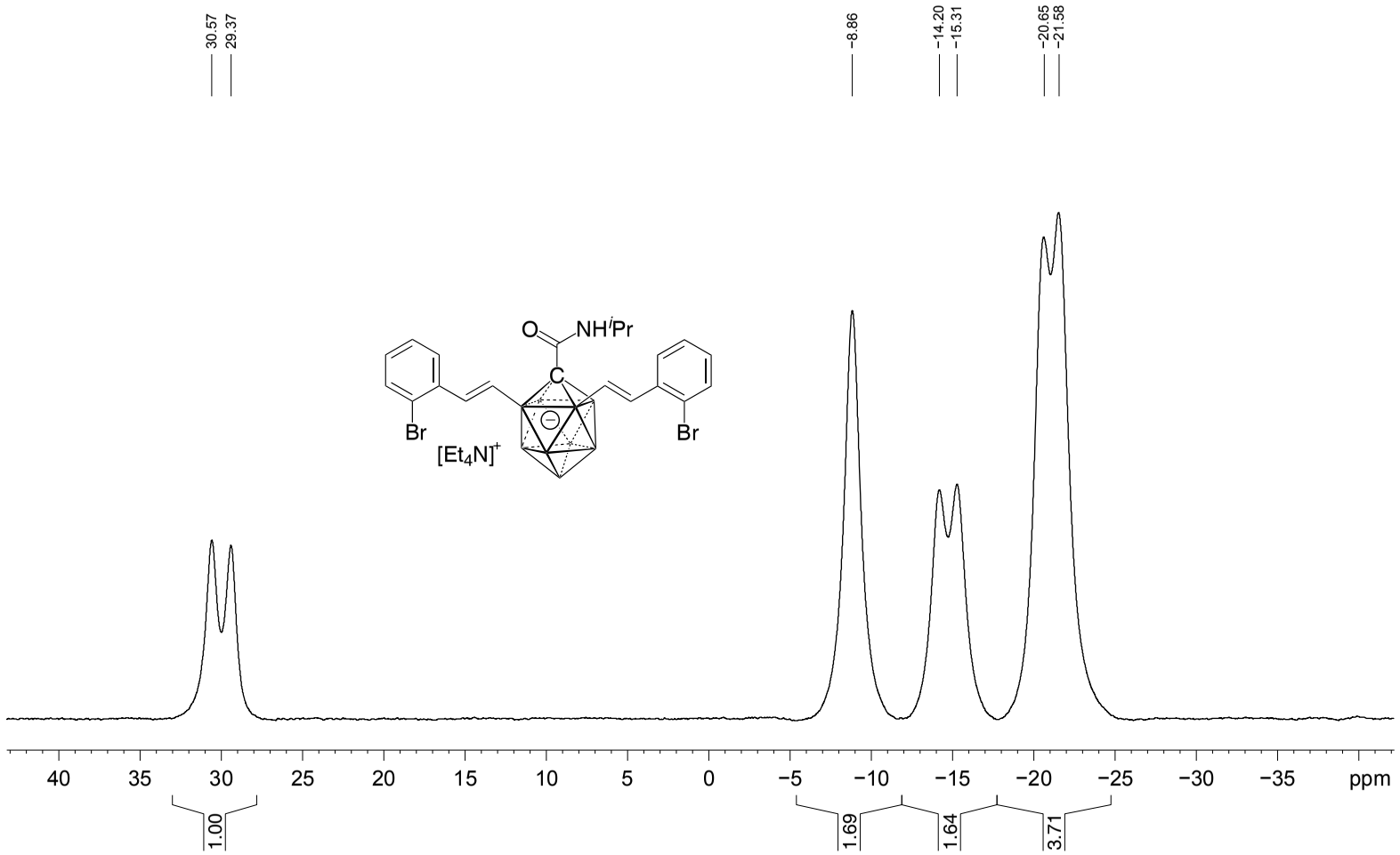
F2 - Acquisition Parameters
Date_ 20171224
Time 15.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgig30
TD 16384
SOLVENT Acetone
NS 16
DS 4
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 86.58
DW 62.400 usec
DE 6.50 usec
TE 295.2K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171223-lxw-0508
Bruker 128MHz, 11B NMR, in acetone-d6



NMR70

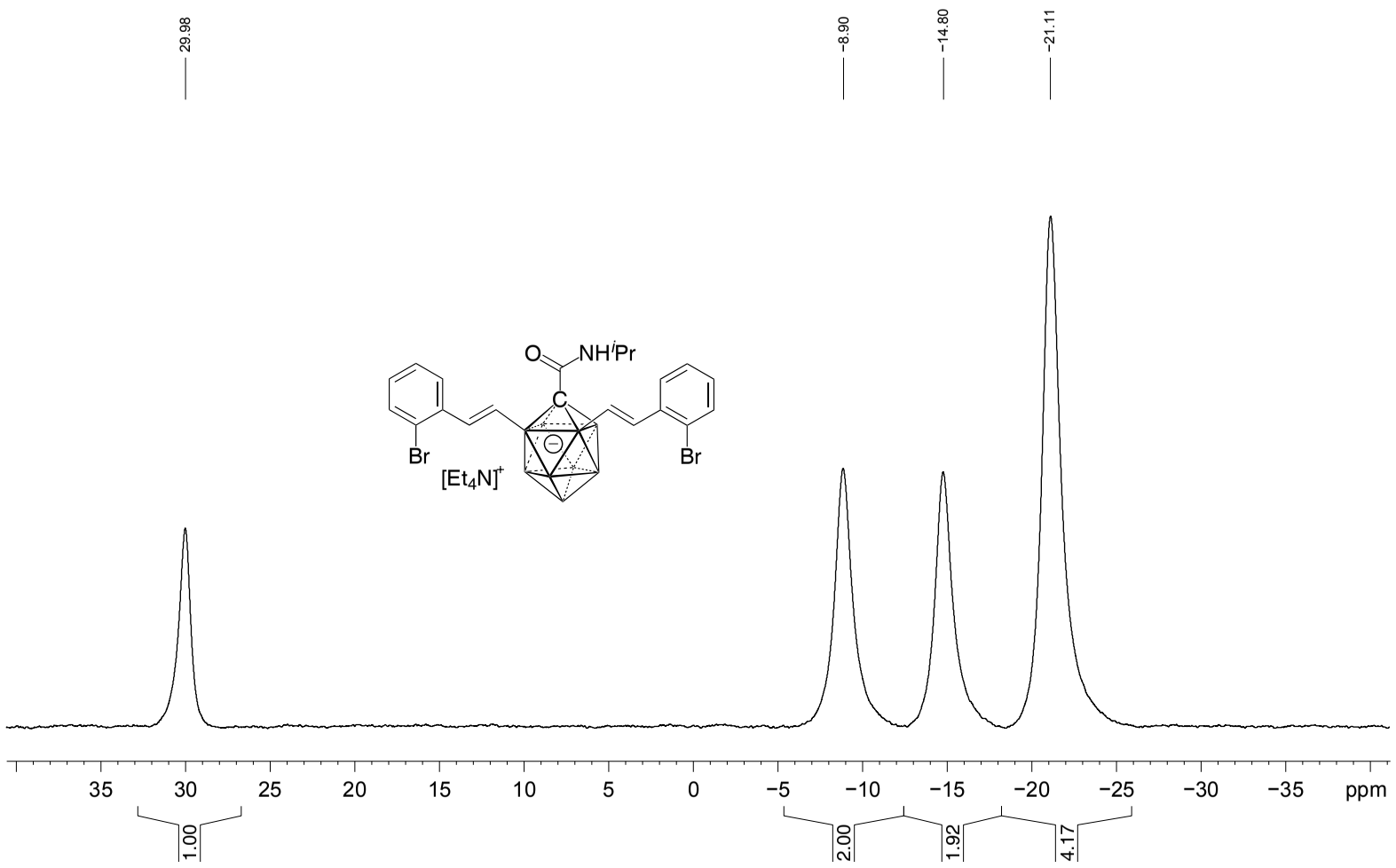
Current Data Parameters
NAME 20171223-lxw-0508
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171224
Time 16.10
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 294.9K
D1 1.00000000 sec
TD0 1

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

20171223−lxw−0508
Bruker 128MHz, 11B{1H} NMR, in acetone−d6



NMR71

Current Data Parameters
NAME 20171223−lxw−0508
EXPNO 3
PROCNO 1

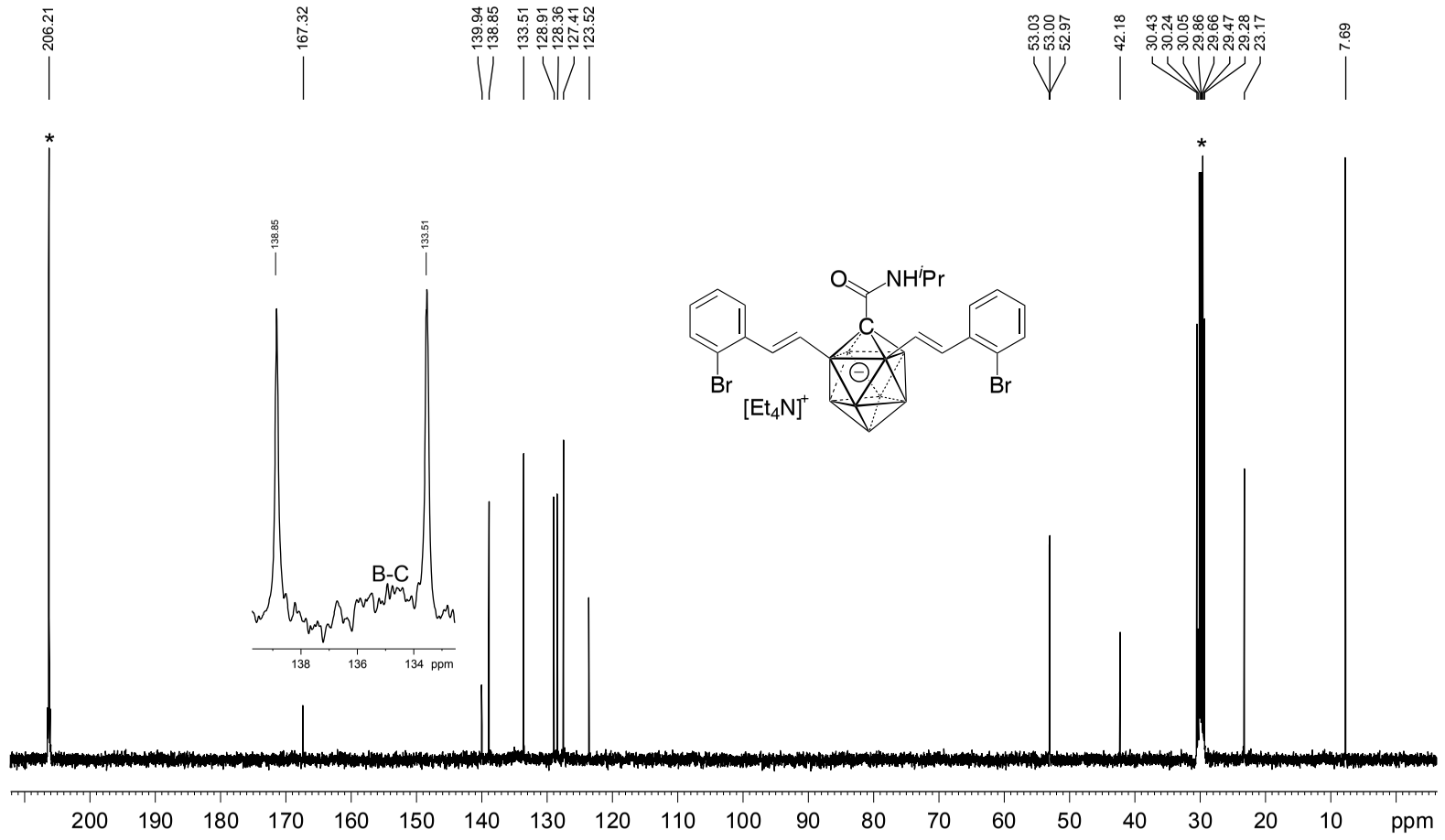
F2 − Acquisition Parameters
Date_ 20171224
Time 16.04
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171223-lxw-0508
Bruker 128MHz, 13C NMR, in acetone-d6*



NMR72

Current Data Parameters
NAME 20171223-lxw-0508
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171224
Time 16.34
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 295.7K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

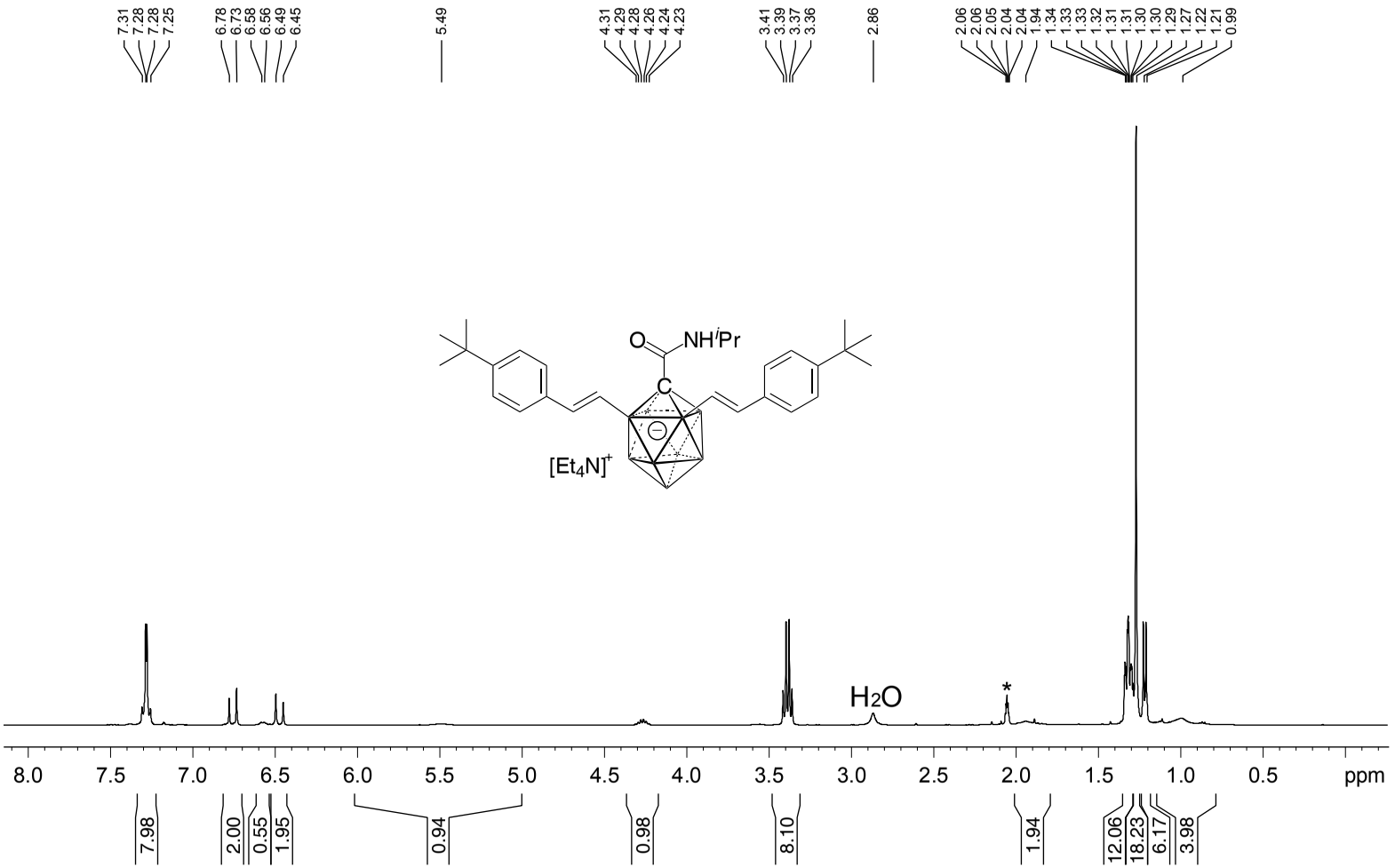
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126821 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR73

20171201-lxw-0482
Bruker 400MHz, 1H{11B} NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171201-lxw-0482
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 18.25
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 295.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

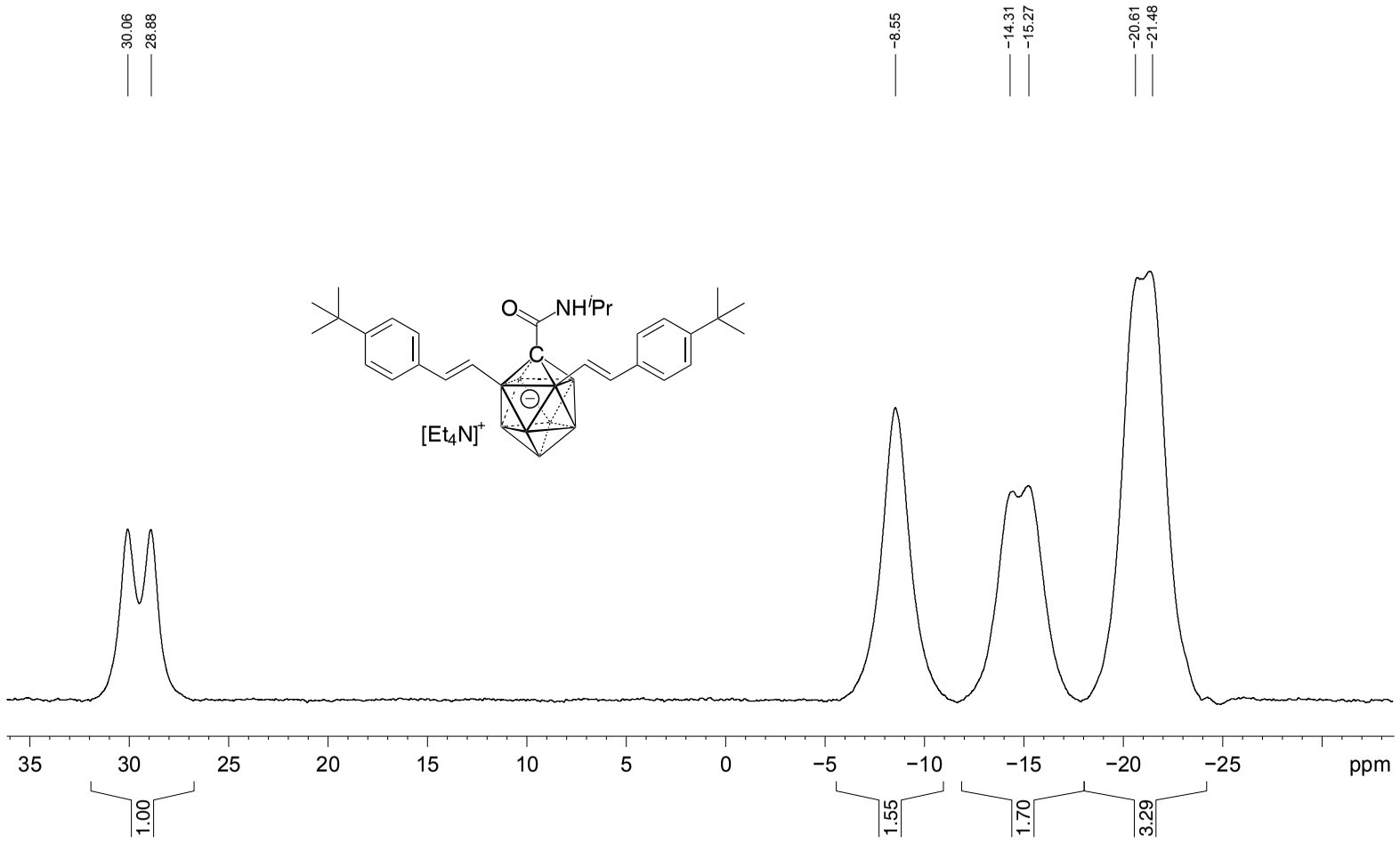
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR74

20171201-lxw-0482
Bruker 128MHz, 11B NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0482
EXPNO 4
PROCNO 1

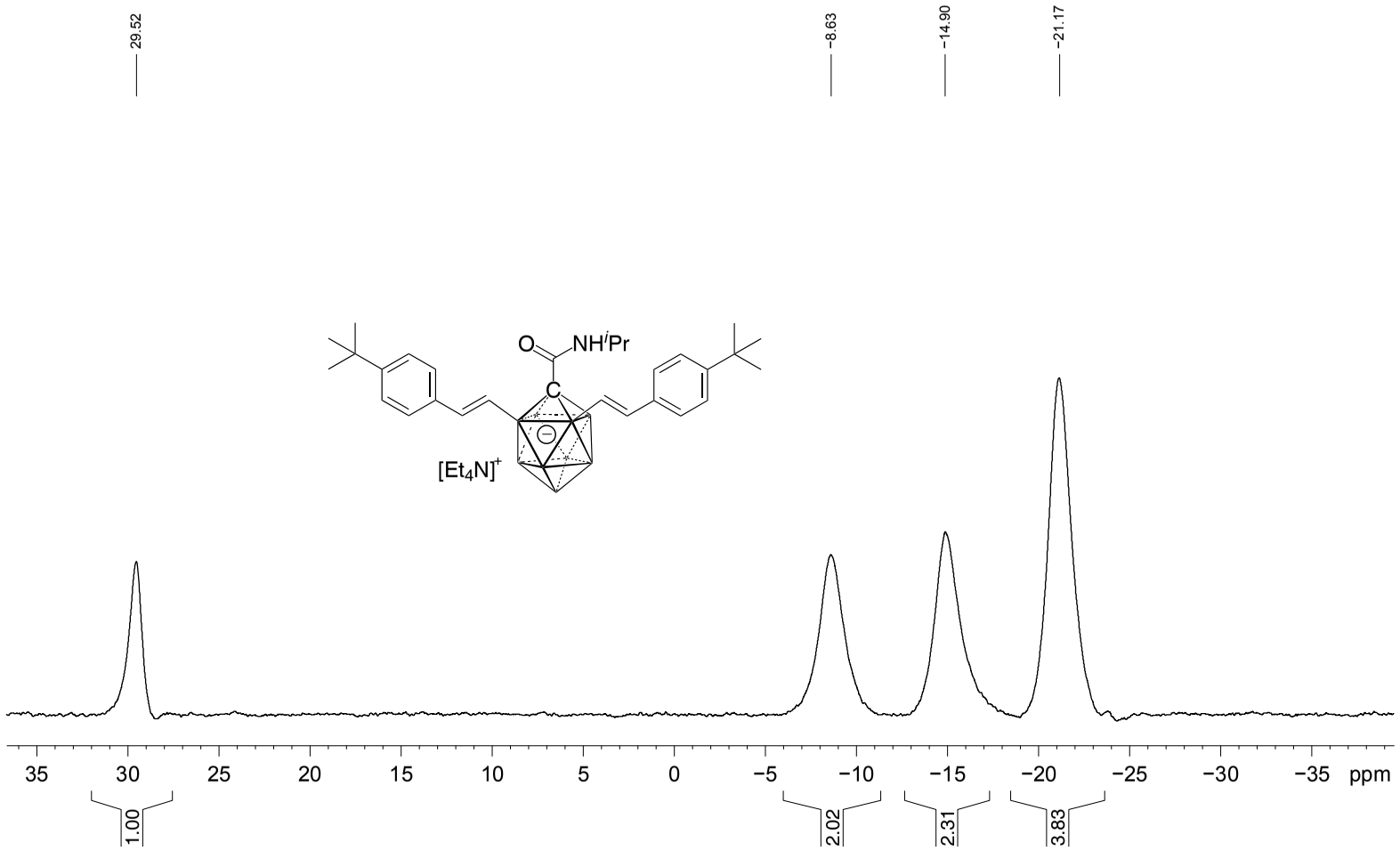
F2 - Acquisition Parameters
Date_ 20171202
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.4K
D1 1.00000000 sec
TD0 1

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

NMR75

20171201-lxw-0482
Bruker 128MHz, 11B{1H} NMR, 20mg in acetone-d6



Current Data Parameters
NAME 20171201-lxw-0482
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 18.31
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 296.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

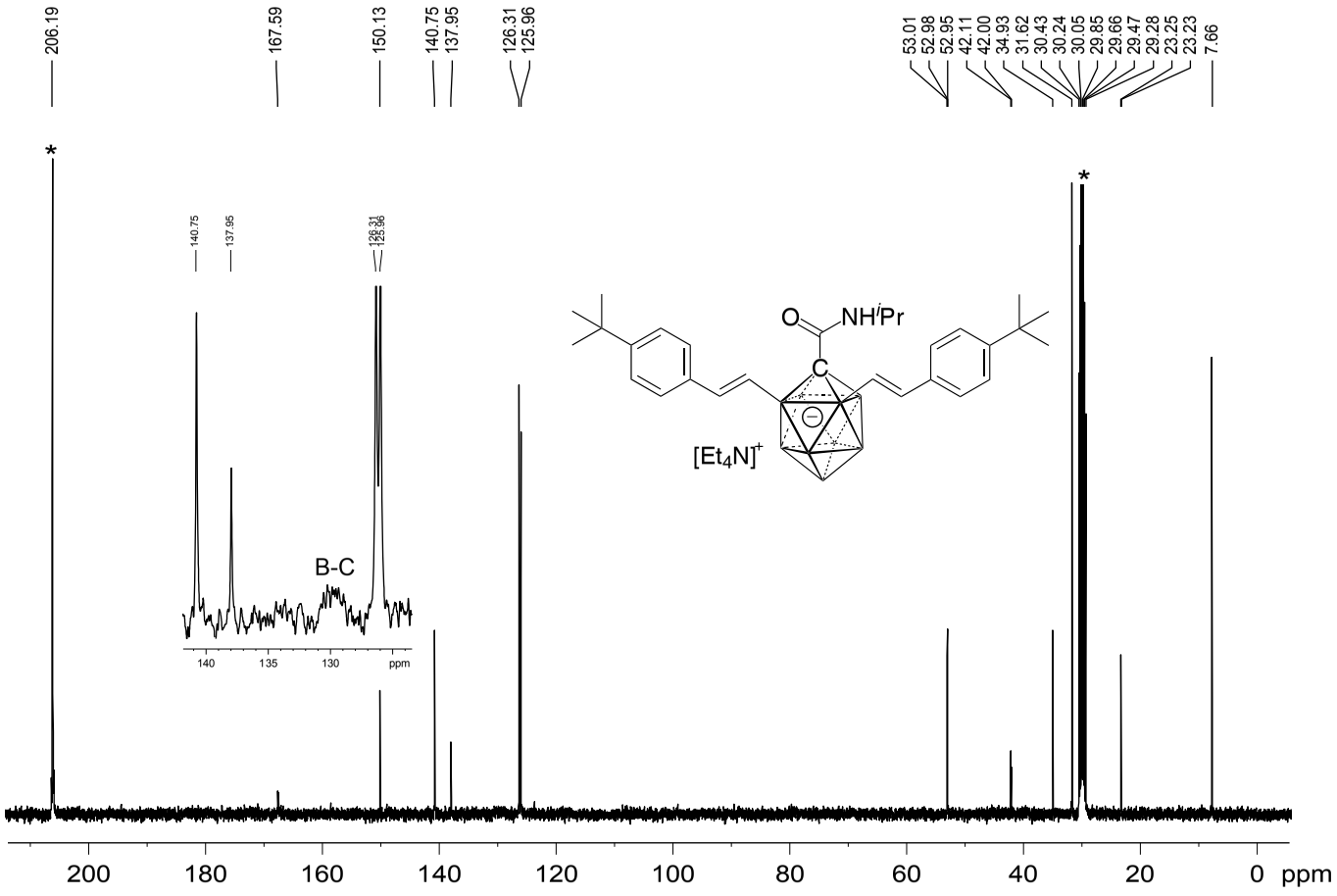
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR76

20171201-lxw-0482
Bruker 101MHz, 13C NMR, 20mg in acetone-d6*



Current Data Parameters
NAME 20171201-lxw-0482
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171202
Time 19.01
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 296.3K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

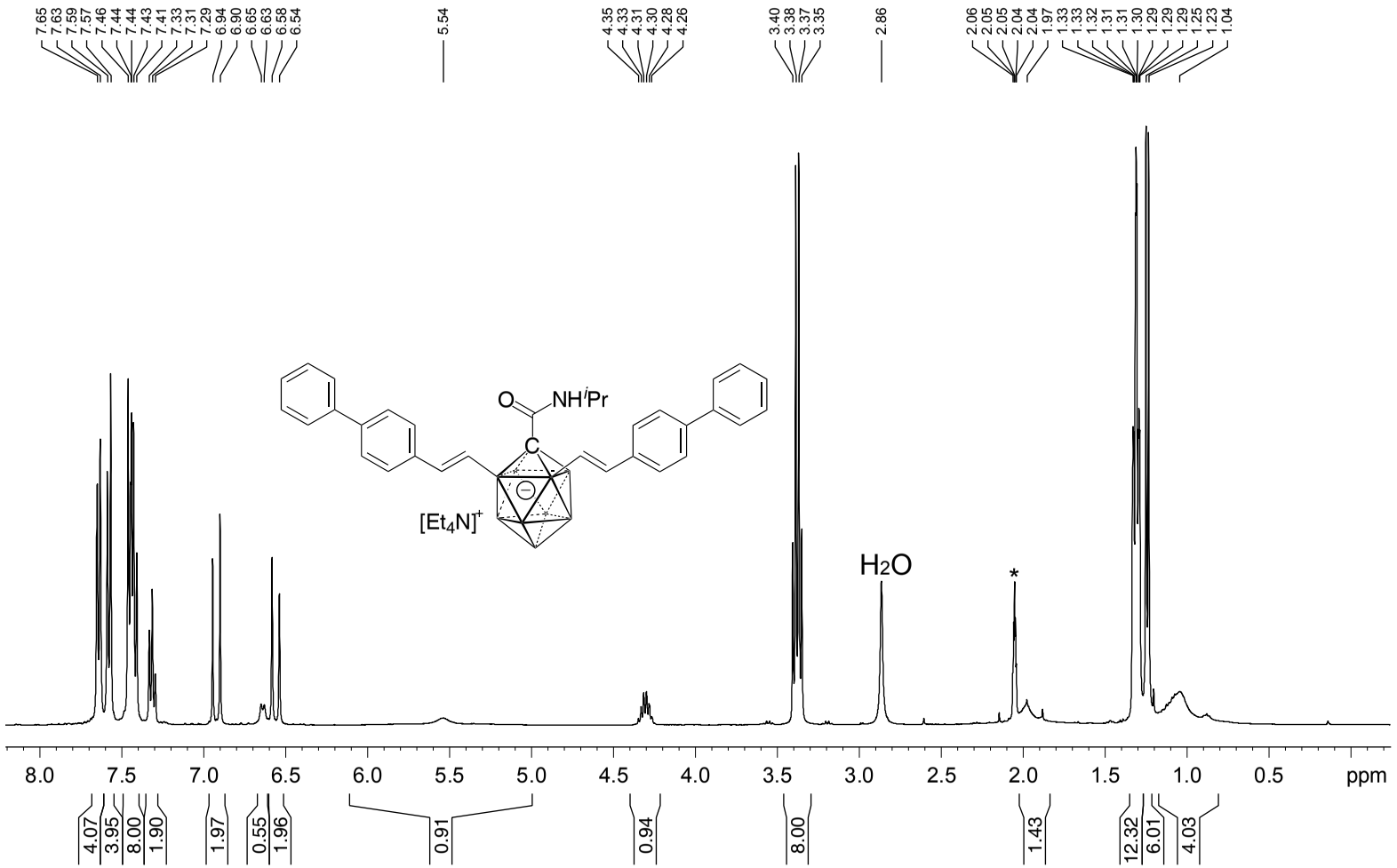
======== CHANNEL f1 ========
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126810 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR77

20171125-lxw-0494
Bruker 400MHz, 1H{11B} NMR, acetone-d6*



Current Data Parameters
NAME 20171125-lxw-0494
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171126
Time 7.16
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 78.69
DW 62.400 usec
DE 6.50 usec
TE 295.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

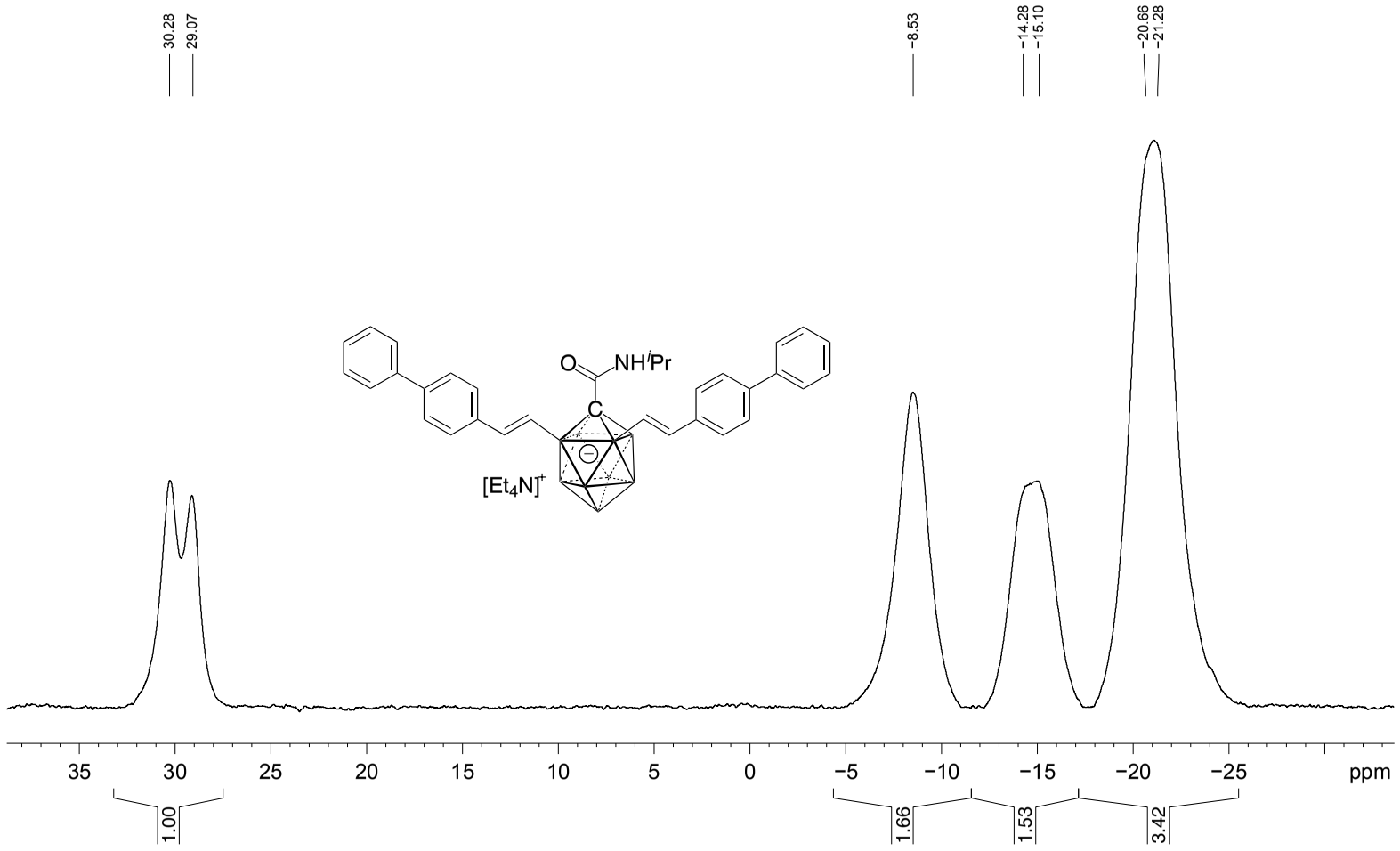
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR78

20171125-lxw-0494
Bruker 128MHz, 11B NMR, acetone-d6



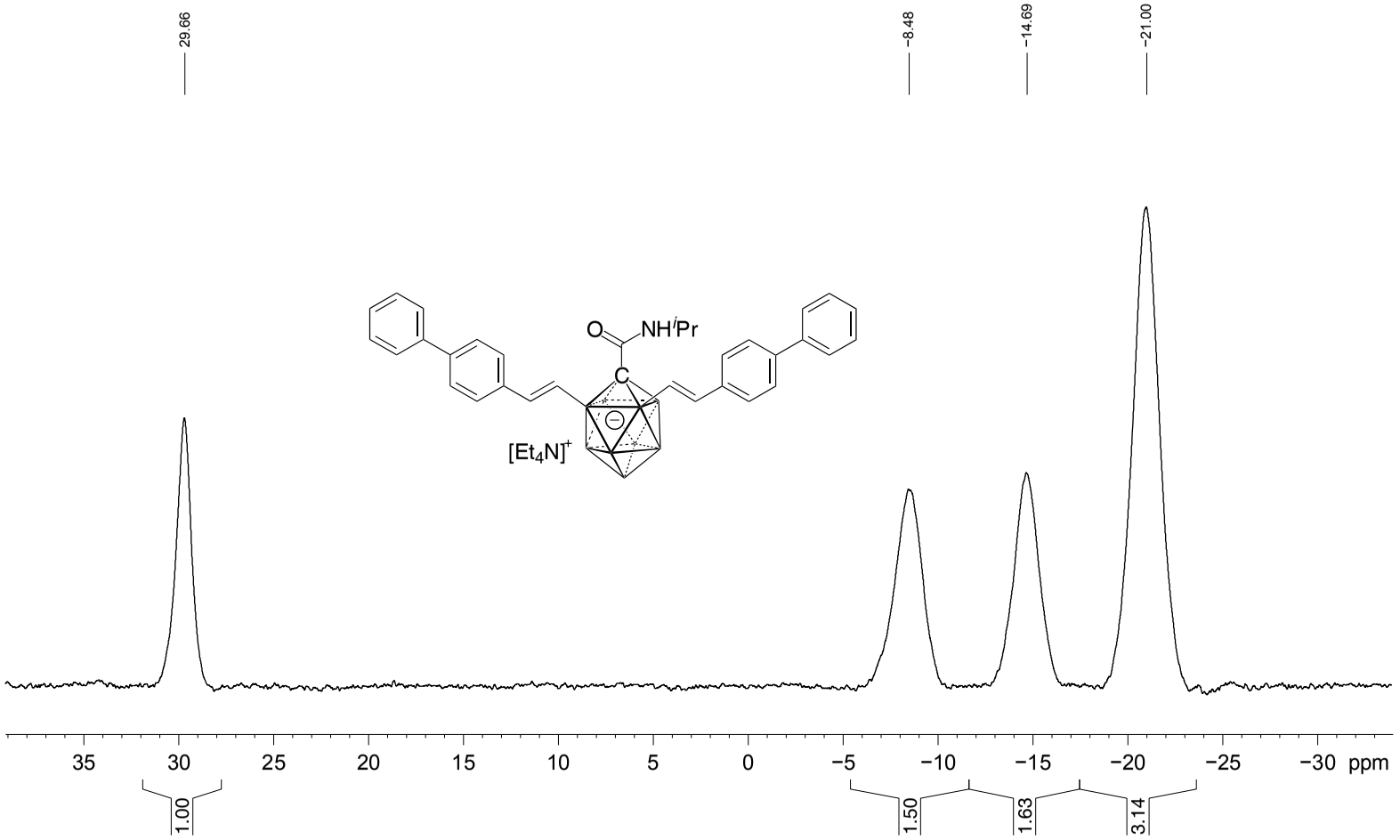
Current Data Parameters
NAME 20171125-lxw-0494
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171126
Time 7.27
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 295.2K
D1 1.00000000 sec
TD0 1

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

20171125-lxw-0494
Bruker 128MHz, 11B{1H} NMR, acetone-d6



NMR79

Current Data Parameters
NAME 20171125-lxw-0494
EXPNO 3
PROCNO 1

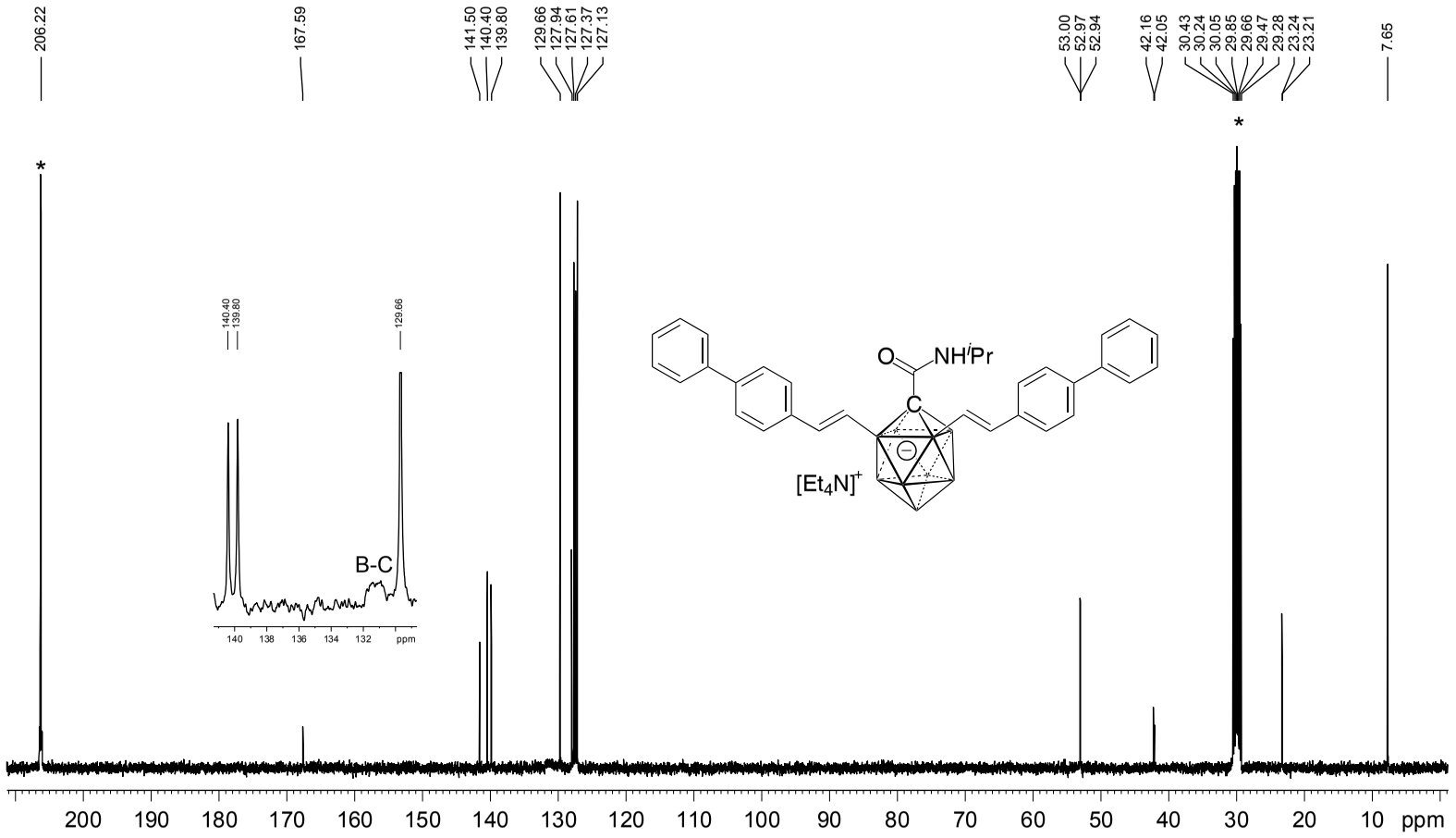
F2 - Acquisition Parameters
Date_ 20171126
Time 7.22
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

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

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

20171125-lxw-0494
Bruker 101MHz, 13C NMR, acetone-d6*



NMR80

Current Data Parameters
NAME 20171125-lxw-0494
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171126
Time 7.52
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 295.6K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

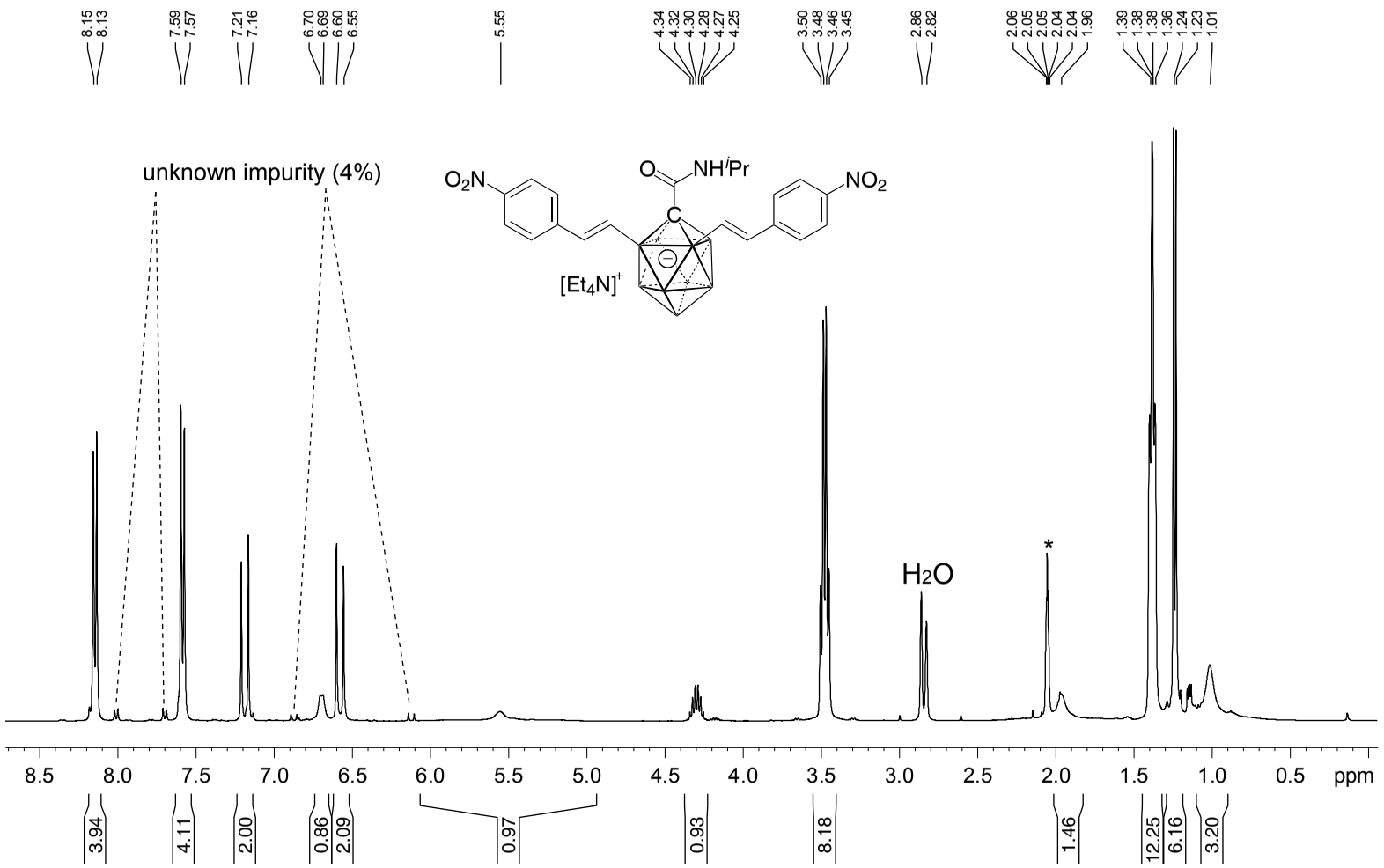
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126824 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR81

20171217−lxw−0504
Bruker 400MHz, 1H{11B} NMR, in acetone−d6*



Current Data Parameters
NAME 20171217−lxw−0504
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20171218
Time 9.53
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 295.6K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

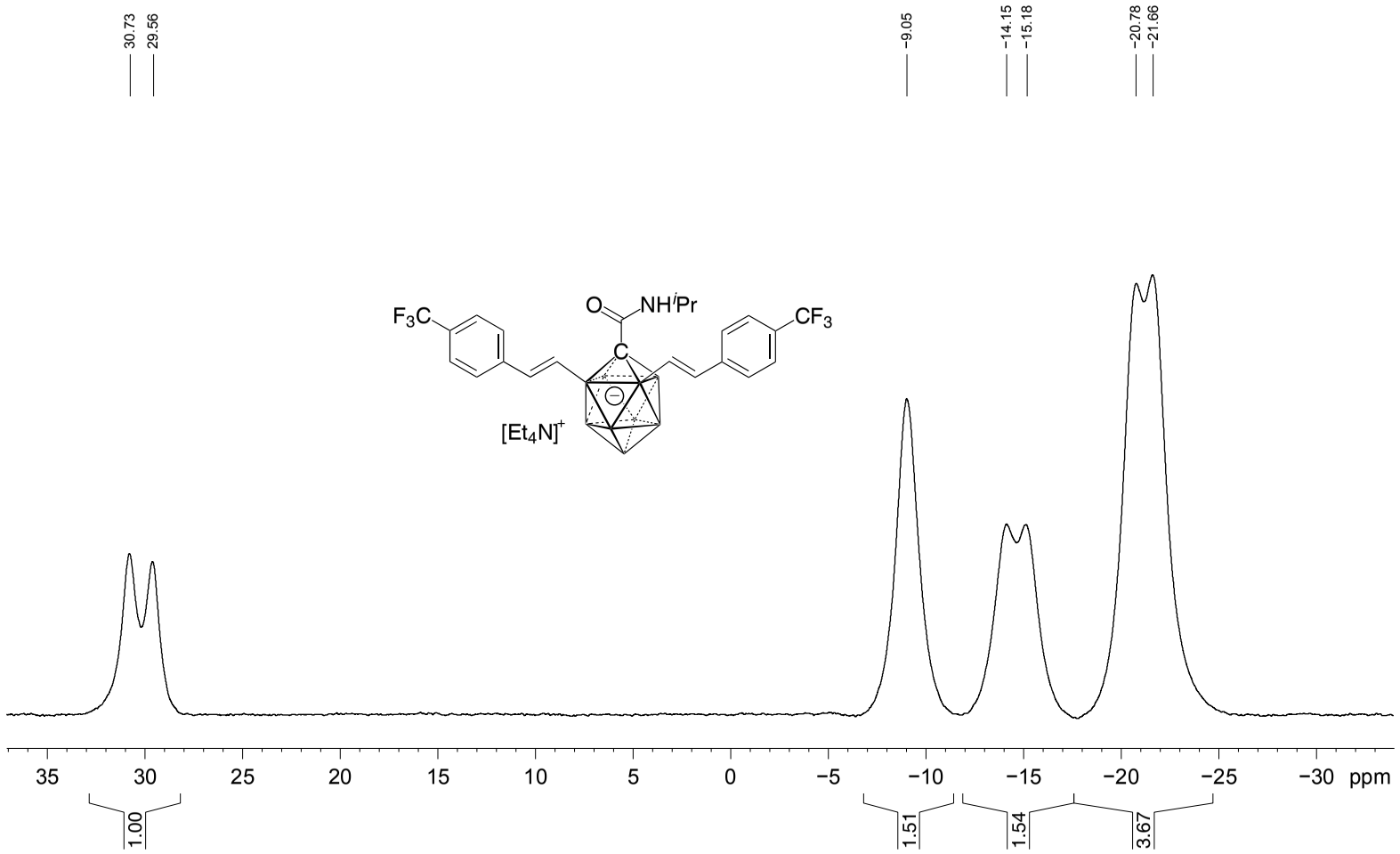
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR82

20171217-lxw-0504
Bruker 128MHz, 11B NMR, in acetone-d6



Current Data Parameters
NAME 20171217-lxw-0504
EXPNO 4
PROCNO 1

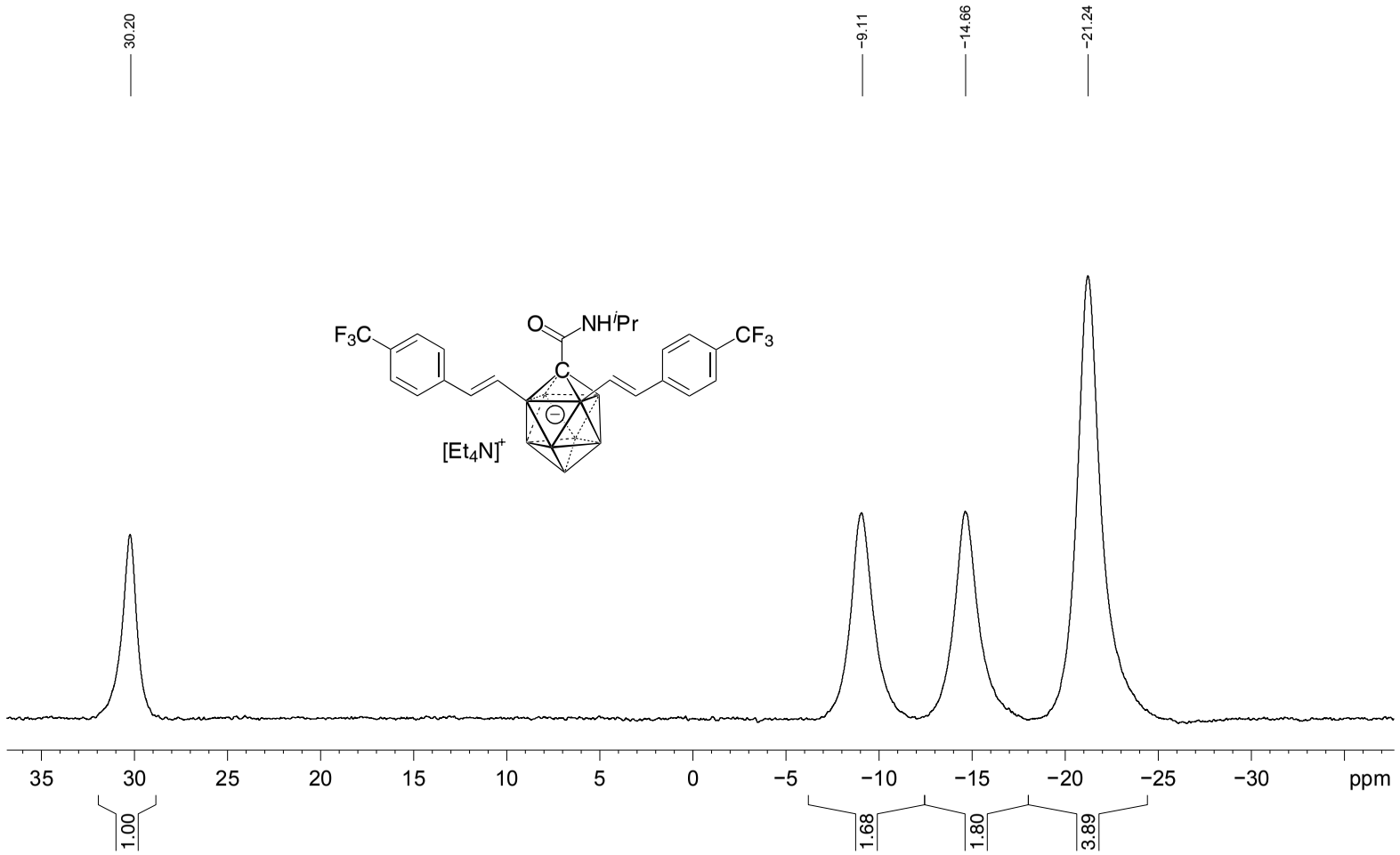
F2 - Acquisition Parameters
Date_ 20171218
Time 10.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.1K
D1 1.00000000 sec
TD0 1

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

NMR83

20171217−lxw−0504
Bruker 128MHz, 11B{1H} NMR, in acetone−d6



Current Data Parameters
NAME 20171217−lxw−0504
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20171218
Time 9.59
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 296.1K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

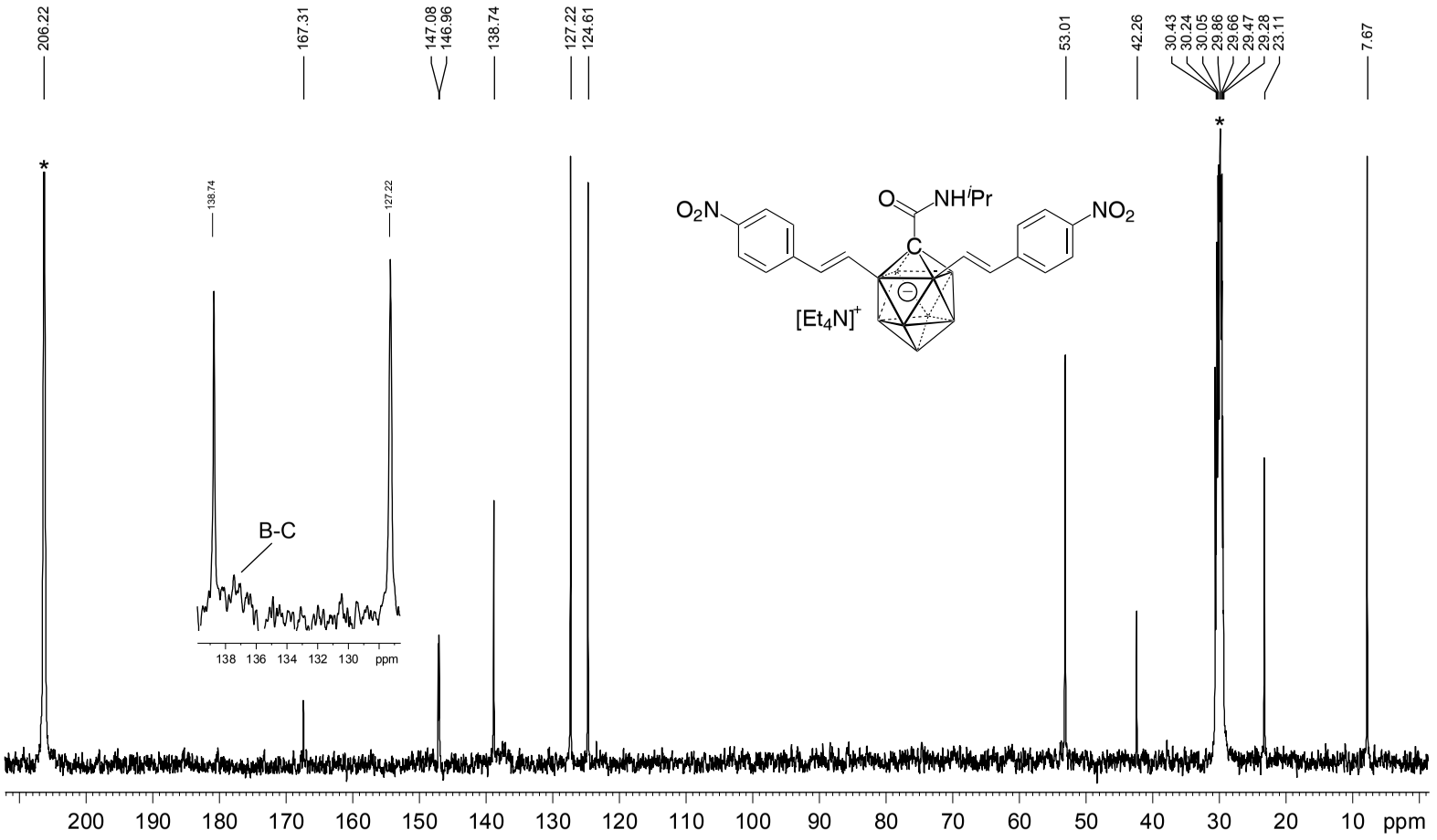
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR84

20171217-lxw-0504
Bruker 128MHz, 13C NMR, in acetone-d6*



Current Data Parameters
NAME 20171217-lxw-0504
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171218
Time 10.29
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 296.2K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

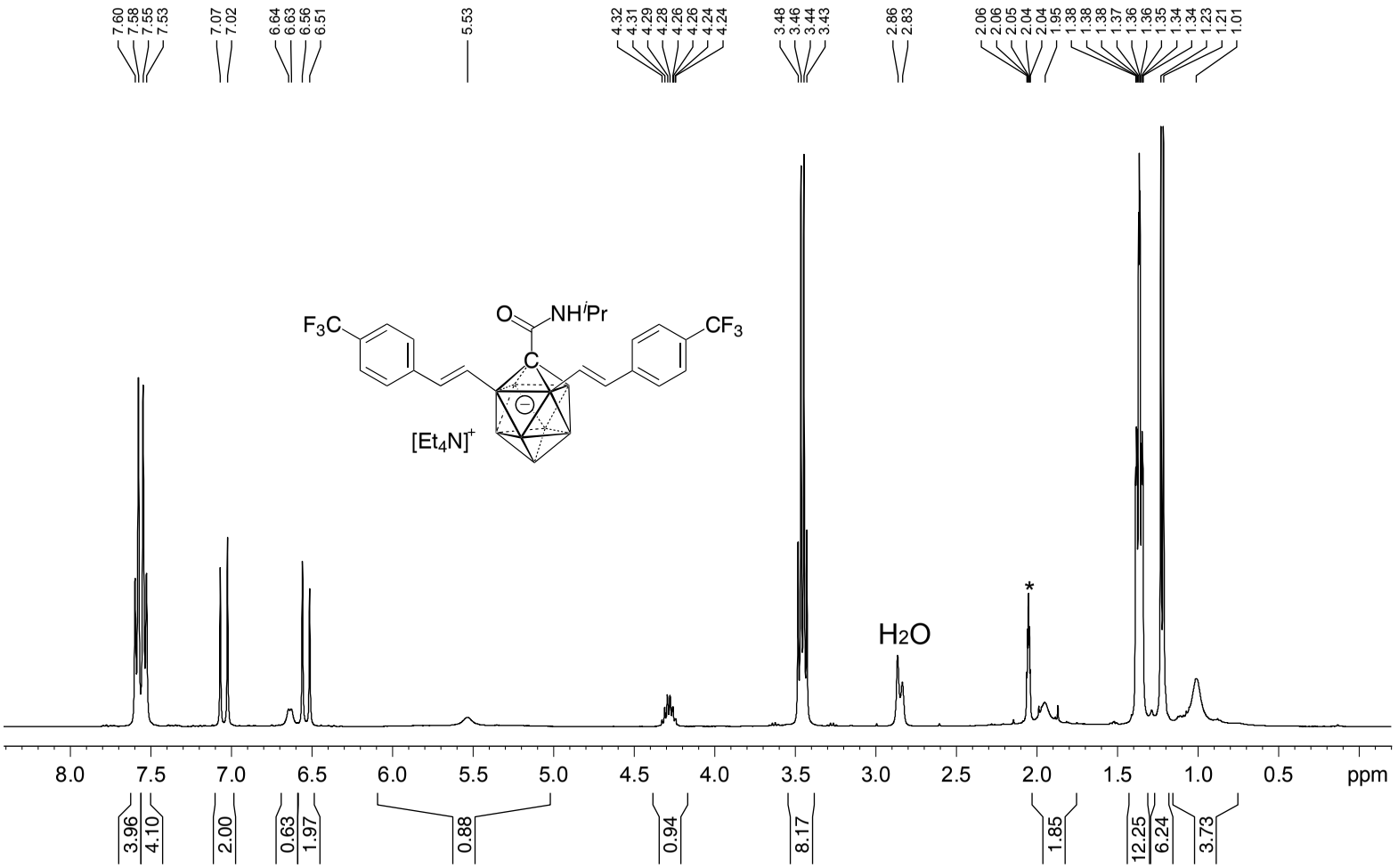
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

F2 - Processing parameters
SI 32768
SF 100.6126802 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40

NMR85

20171218-lxw-0505
Bruker 400MHz, 1H{11B} NMR, in acetone-d6*



Current Data Parameters
NAME 20171218-lxw-0505
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171220
Time 0.33
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 294.9K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

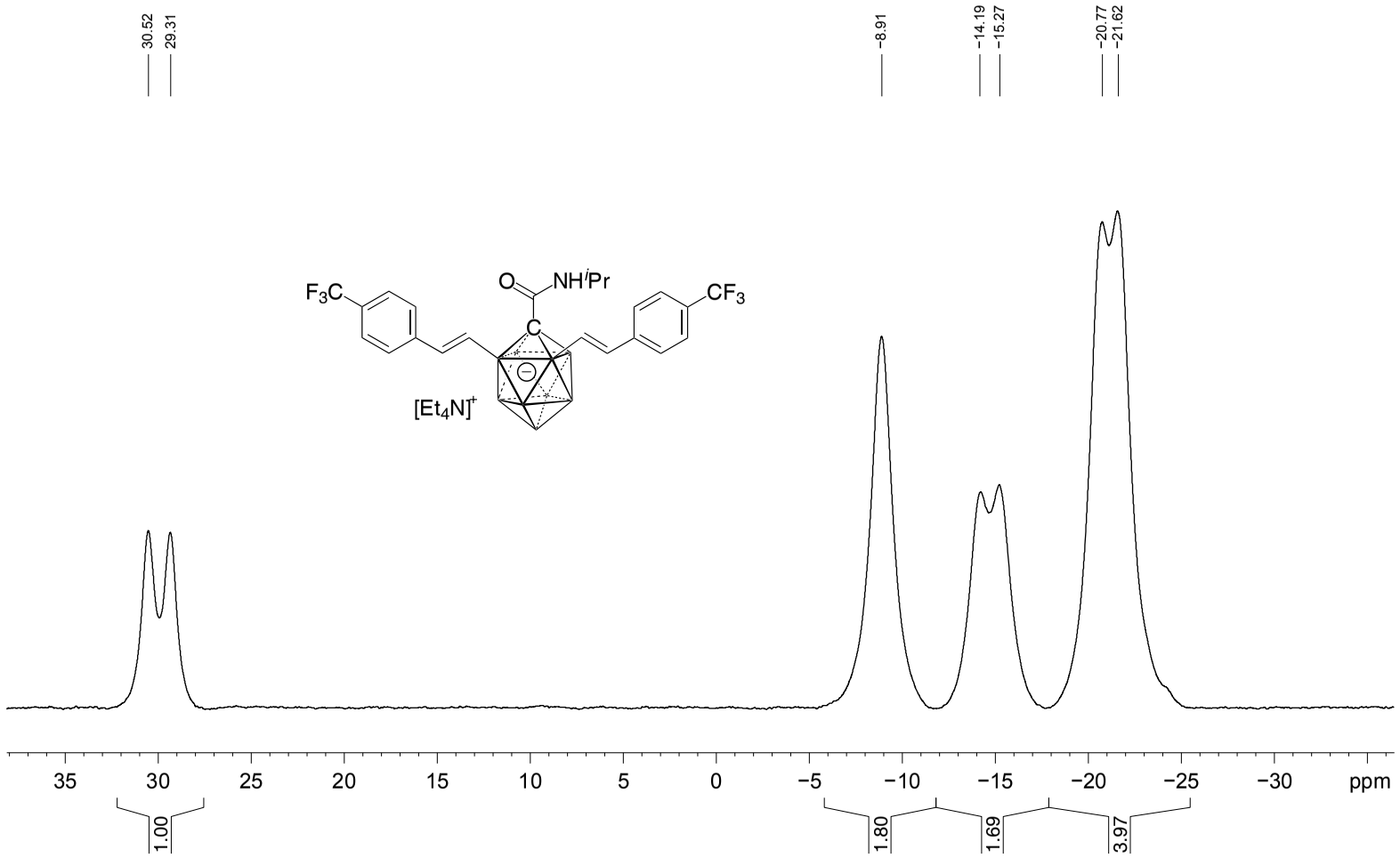
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR86

20171218-lxw-0505
Bruker 128 MHz, 11B NMR, in acetone-d6



Current Data Parameters
NAME 20171218-lxw-0505
EXPNO 4
PROCNO 1

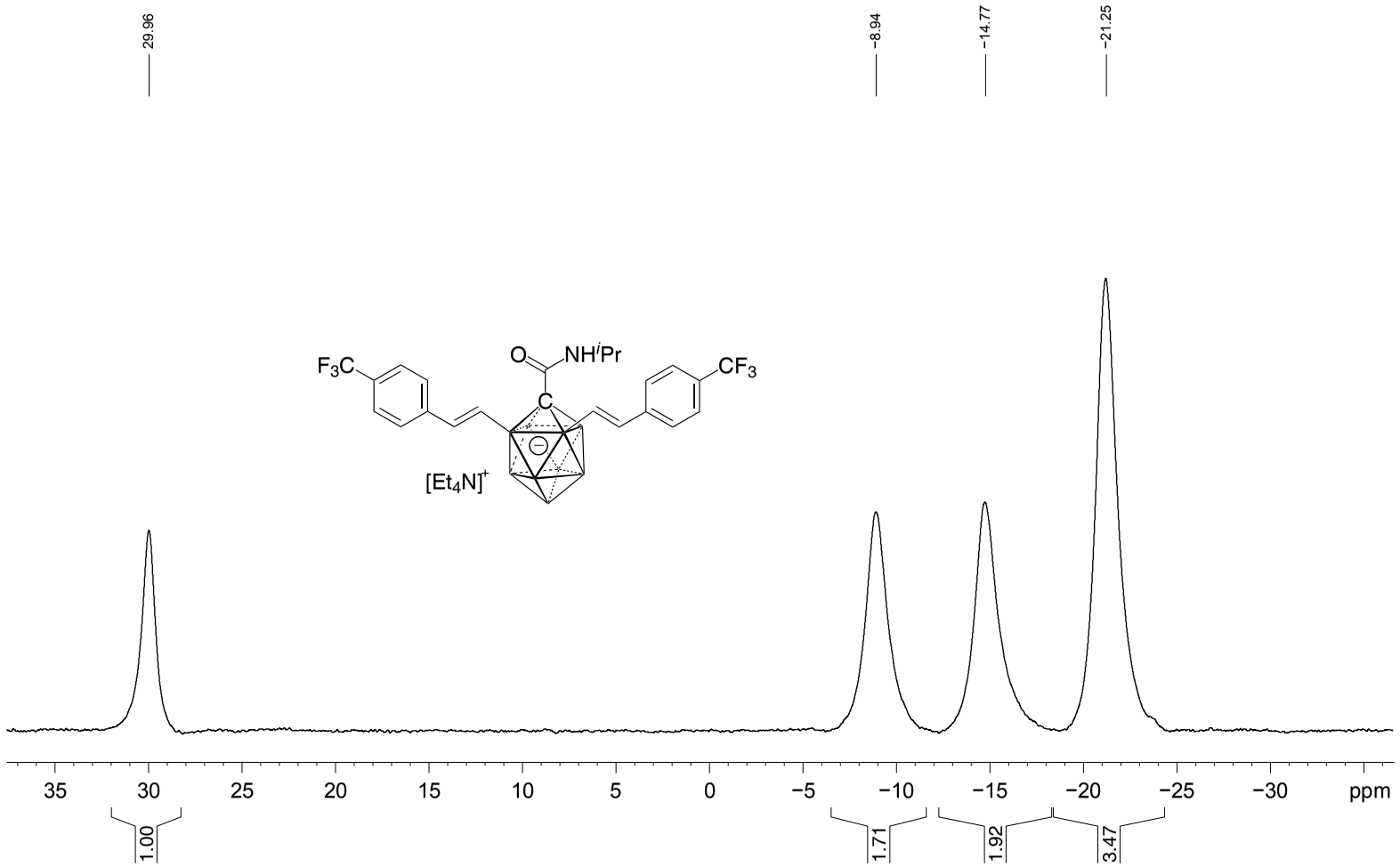
F2 - Acquisition Parameters
Date_ 20171220
Time 0.45
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 294.8K
D1 1.00000000 sec
TD0 1

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

NMR87

20171218-lxw-0505
Bruker 128 MHz, 11B{1H} NMR, in acetone-d6



Current Data Parameters
NAME 20171218-lxw-0505
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171220
Time 0.39
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 295.7K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

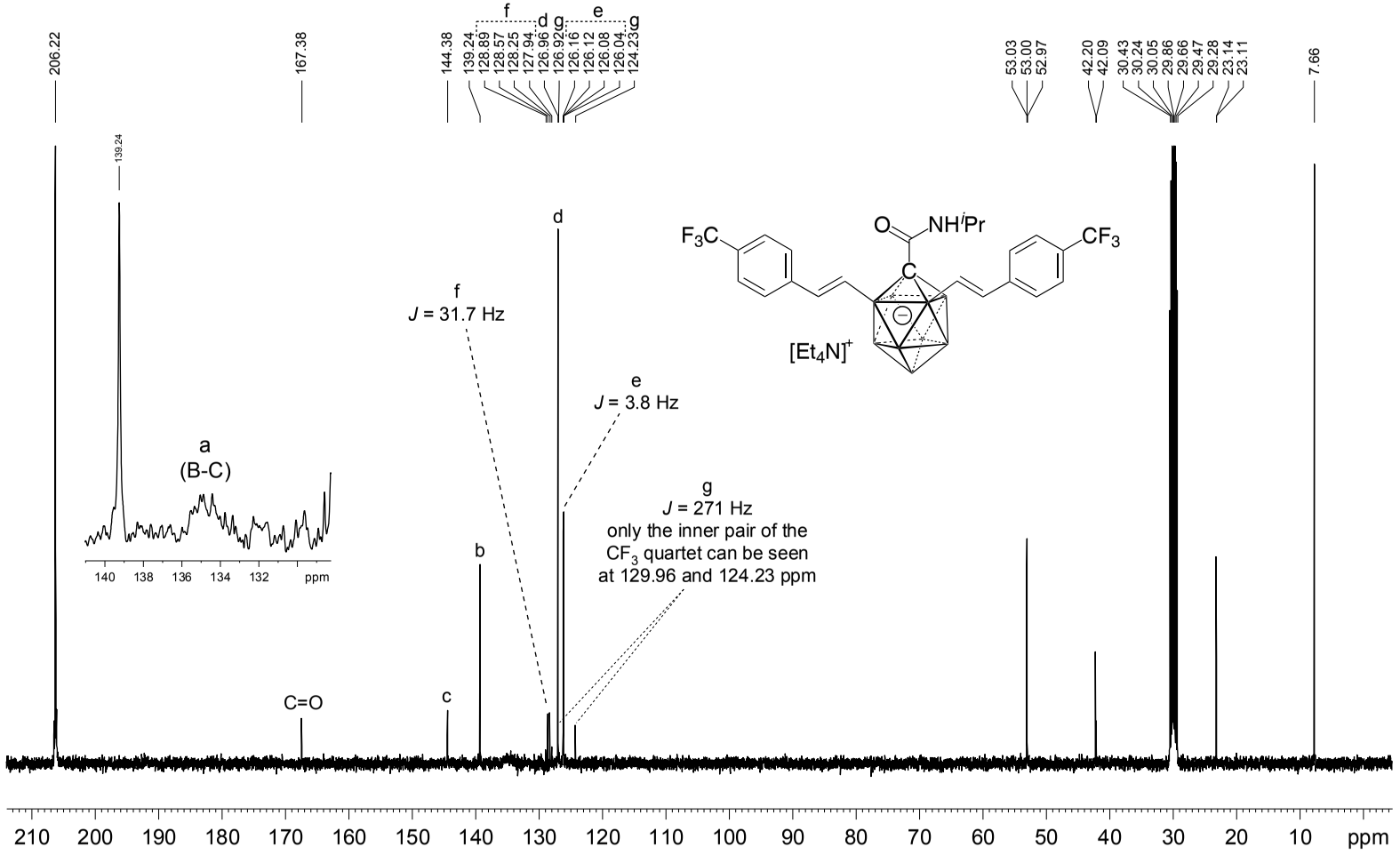
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR88

20171218-lxw-0505
Bruker 101MHz, 13C NMR, in acetone-d6



Current Data Parameters
NAME 20171218-lxw-0505
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171220
Time 1.09
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 295.2K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

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

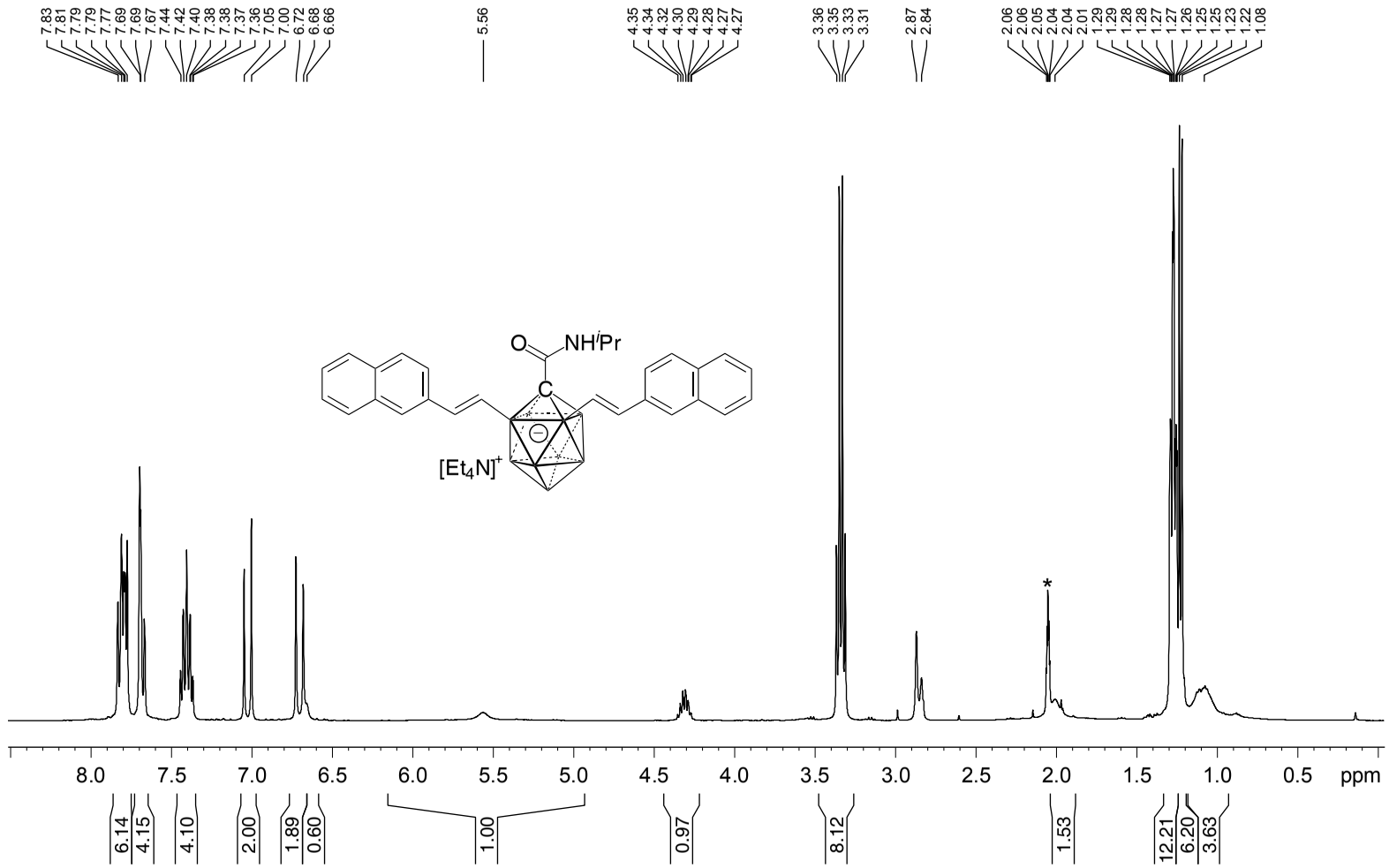
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.50000000W
PLW12 0.43945000W
PLW13 0.28125000W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6126804 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

NMR89

20171217-lxw-0501

Bruker 400MHz, 1H{11B} NMR, in acetone-d6*



Current Data Parameters
NAME 20171217-lxw-0501
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171218
Time 8.28
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 78.69
DW 62.400 usec
DE 6.50 usec
TE 295.4K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

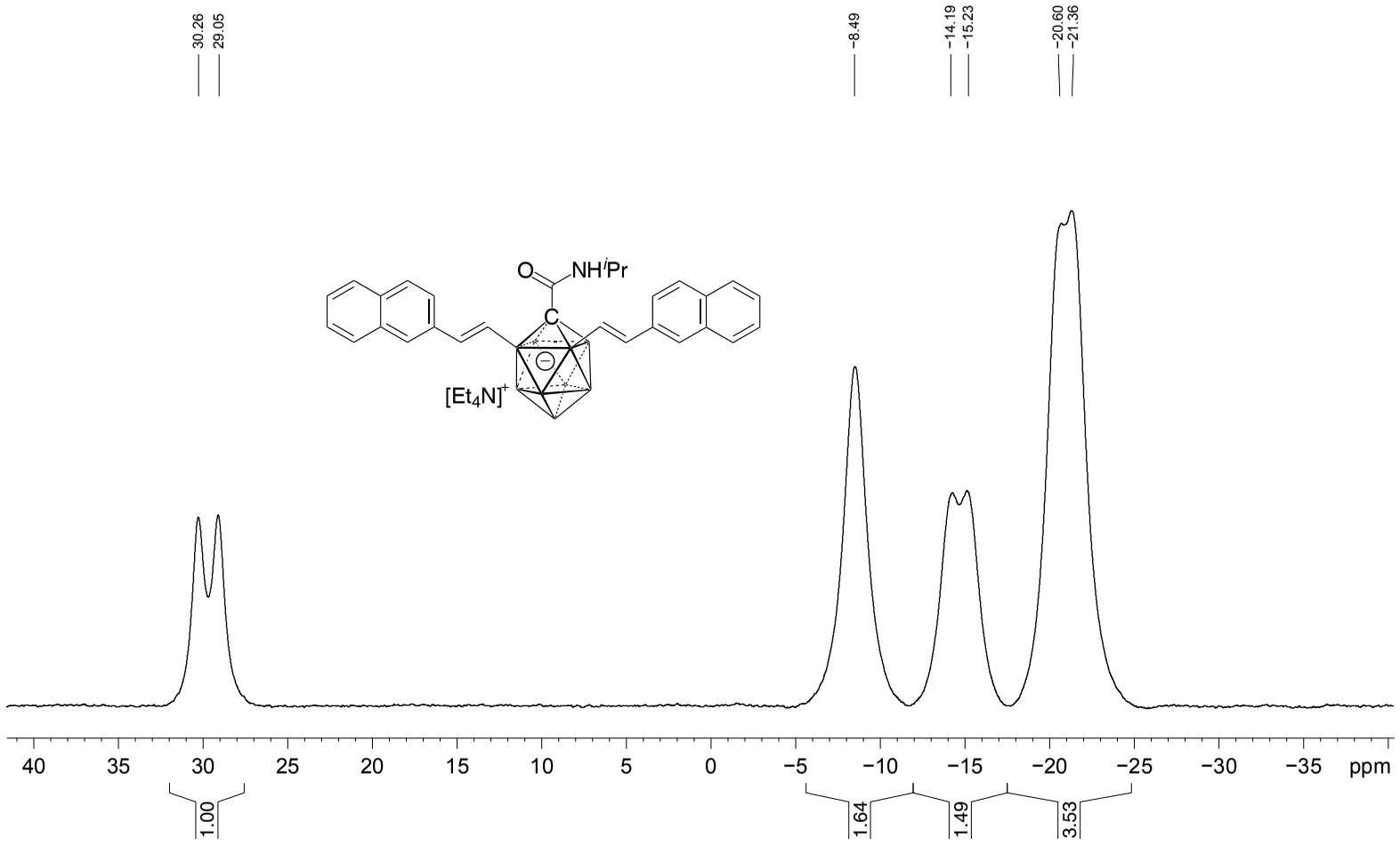
======== CHANNEL f1 ======
NUC1 1H
P1 15.00 usec
PLW1 12.50000000W
SFO1 400.1320007 MHz

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

NMR90

20171217−lxw−0501
Bruker 128MHz, 11B NMR, in acetone−d6



Current Data Parameters
NAME 20171217−lxw−0501
EXPNO 4
PROCNO 1

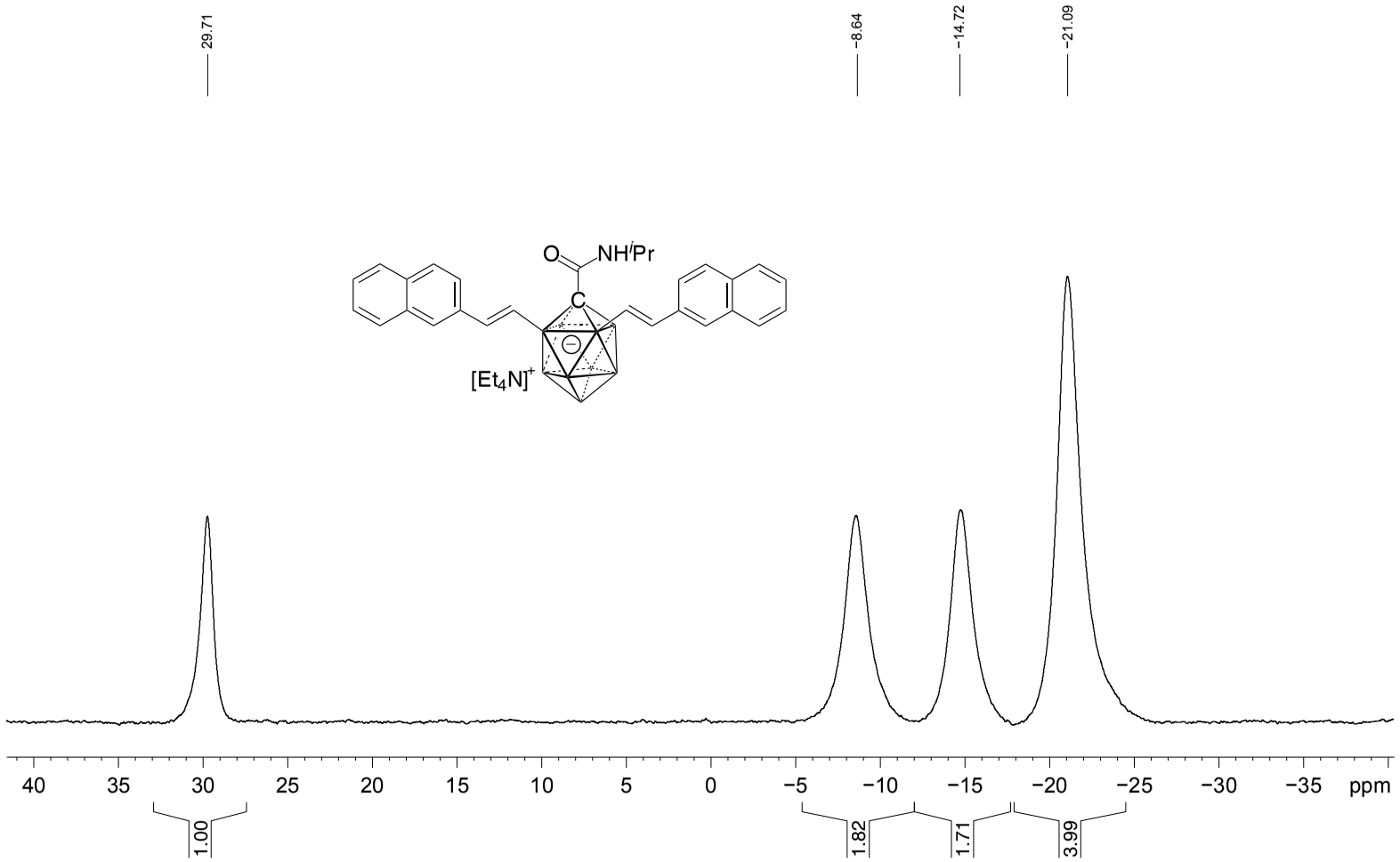
F2 − Acquisition Parameters
Date_ 20171218
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg
TD 65536
SOLVENT Acetone
NS 128
DS 4
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845056 sec
RG 193.34
DW 19.600 usec
DE 6.50 usec
TE 295.4K
D1 1.00000000 sec
TD0 1

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

NMR91

20171217−lxw−0501
Bruker 128MHz, 11B{1H} NMR, in acetone−d6



Current Data Parameters
NAME 20171217−lxw−0501
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20171218
Time 8.34
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 296.3K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1

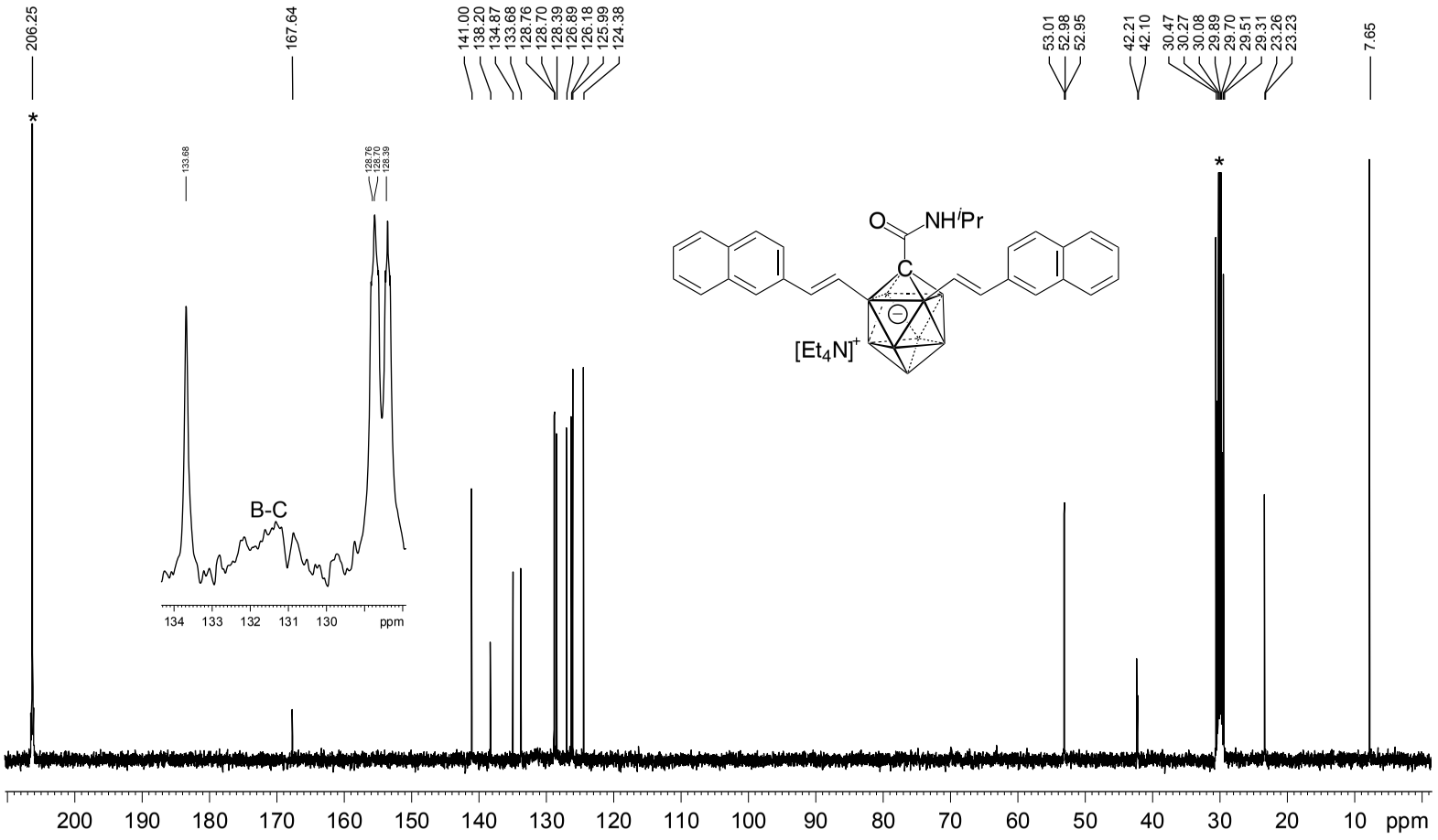
======== CHANNEL f1 =======
NUC1 11B
P1 9.93 usec
PLW1 52.96599960W
SFO1 128.3776050 MHz

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

NMR92

20171217-lxw-0501
Bruker 101MHz, 13C NMR, in acetone-d6*



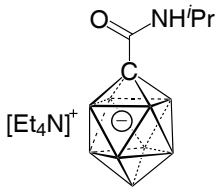
Current Data Parameters
NAME 20171217-lxw-0501
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171218
Time 9.04
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 296.1K
D1 1.50000000 sec
D11 0.03000000 sec
TD0 1

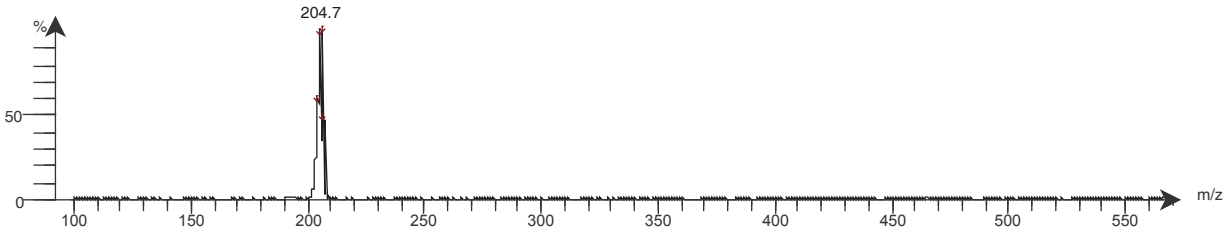
======== CHANNEL f1 =======
NUC1 13C
P1 10.00 usec
PLW1 53.00000000W
SFO1 100.6228293 MHz

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

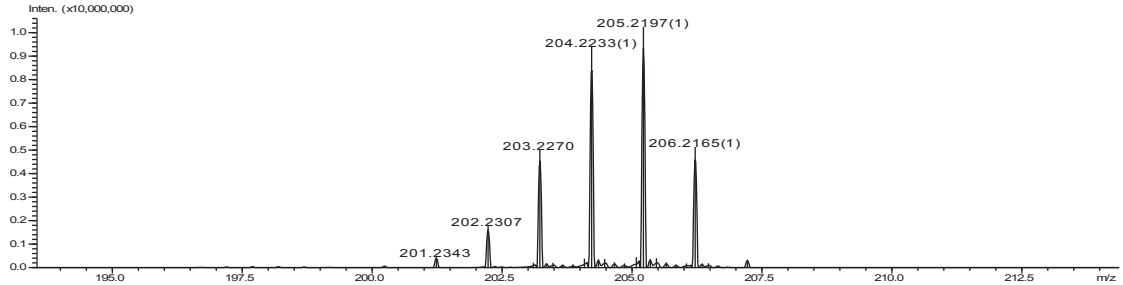
F2 - Processing parameters
SI 32768
SF 100.6126784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

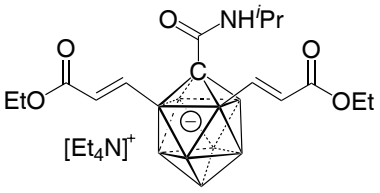


Low-resolution MS

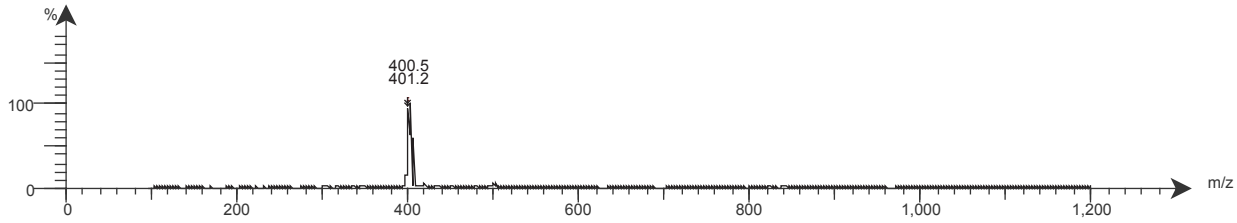


High-resolution MS

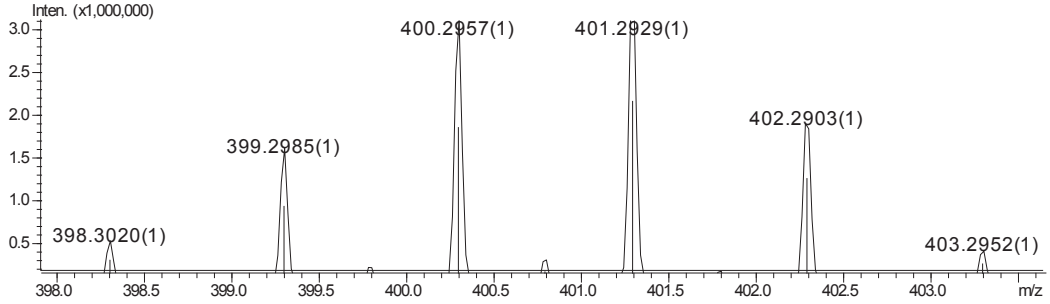


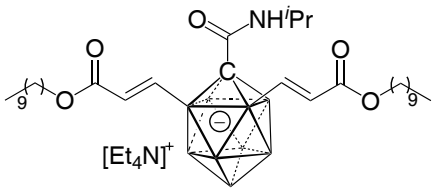


Low-resolution MS

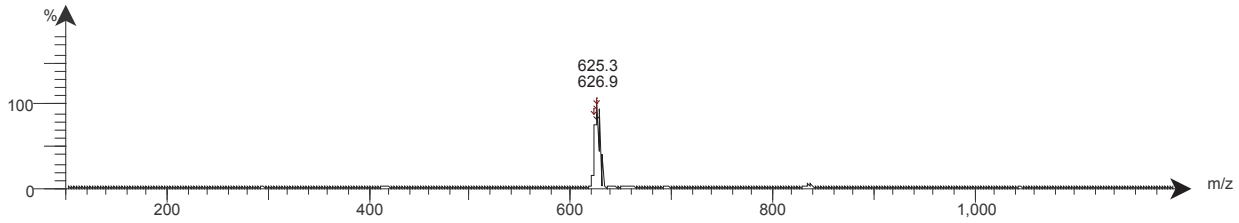


High-resolution MS

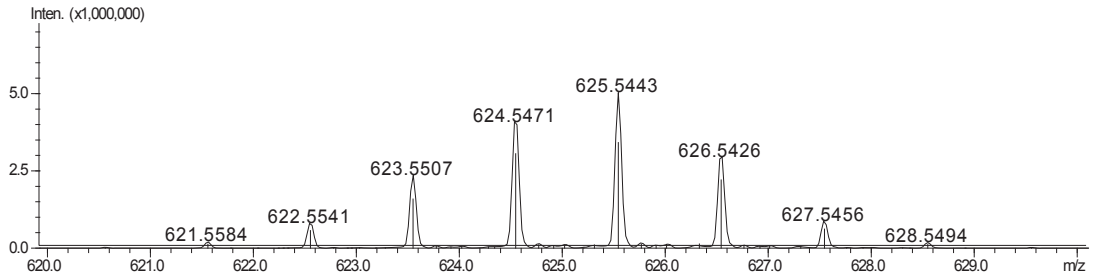


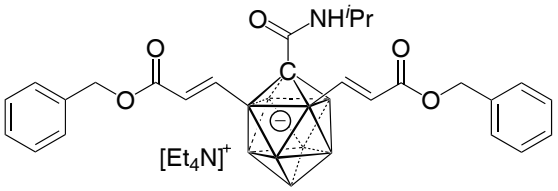


Low-resolution MS

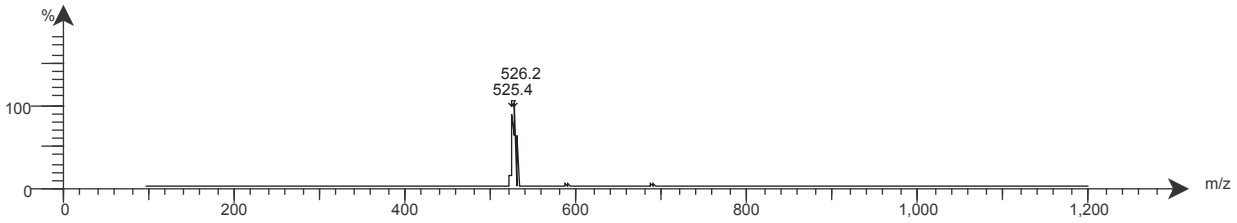


High-resolution MS

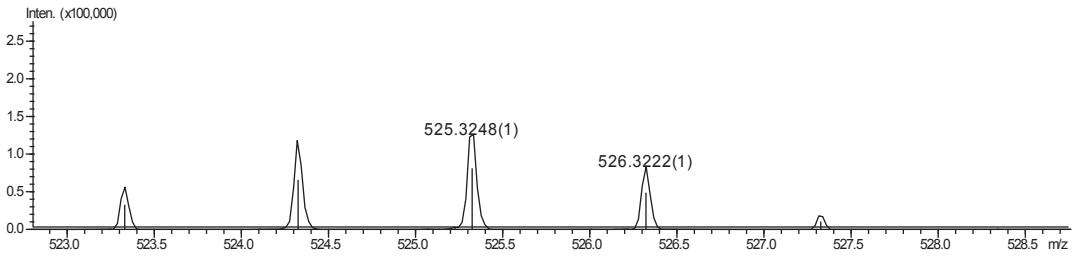


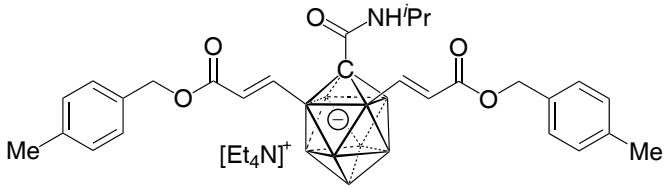


Low-resolution MS

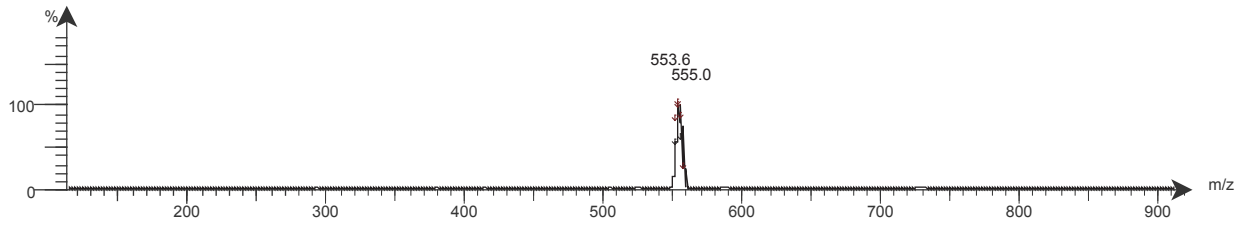


High-resolution MS

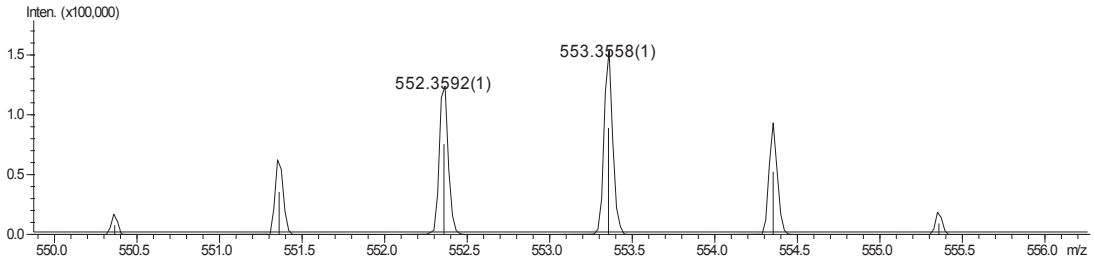


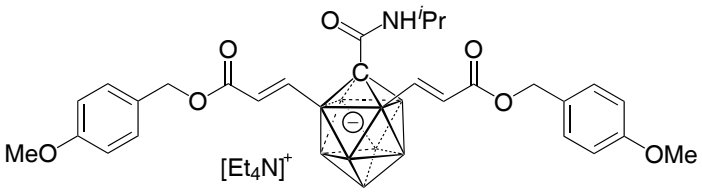


Low-resolution MS

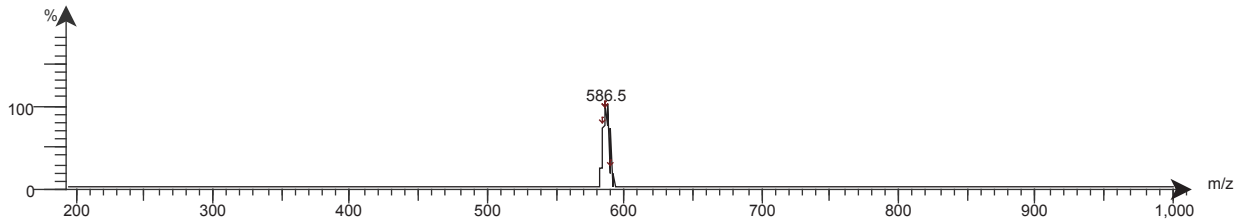


High-resolution MS





Low-resolution MS



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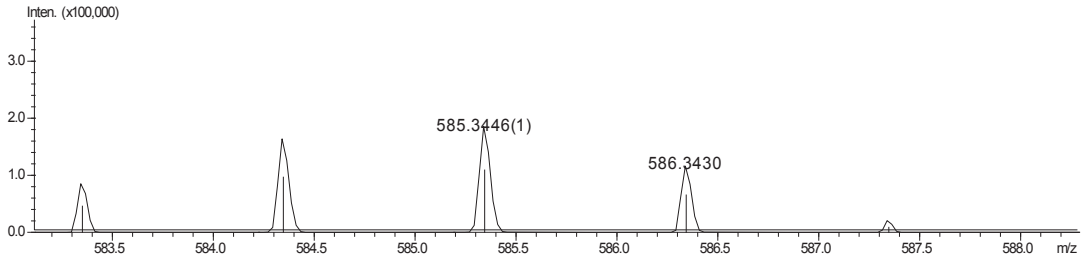

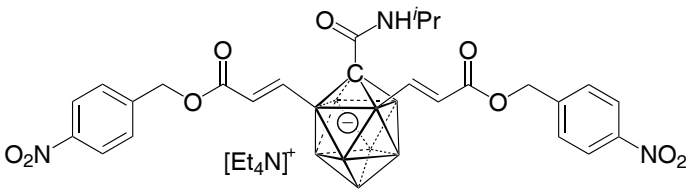

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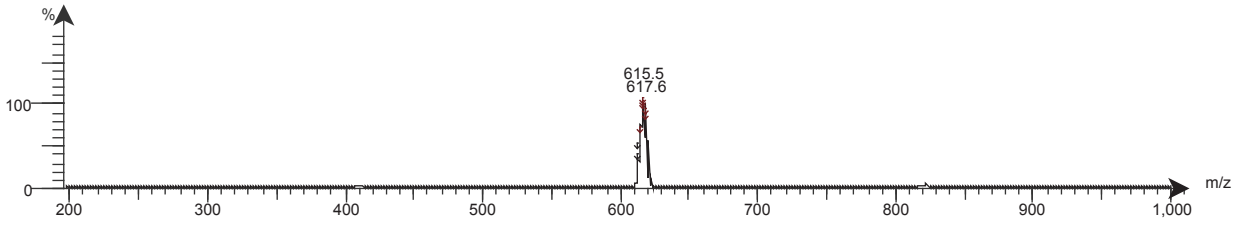

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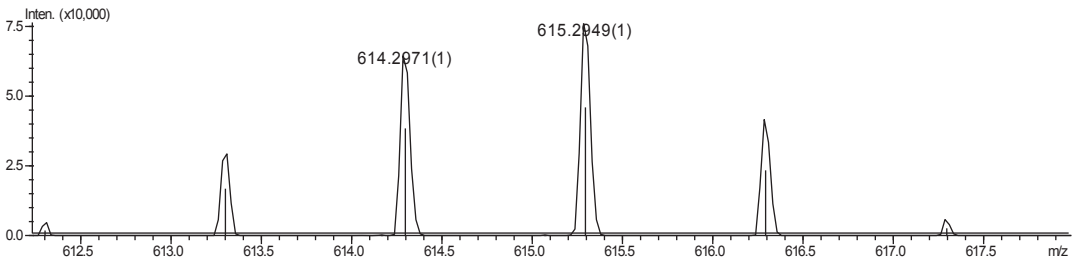

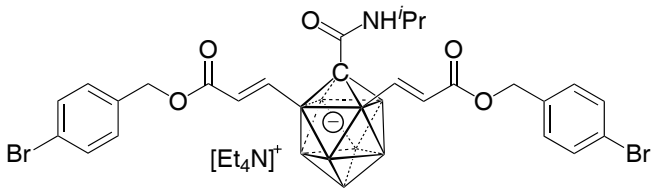

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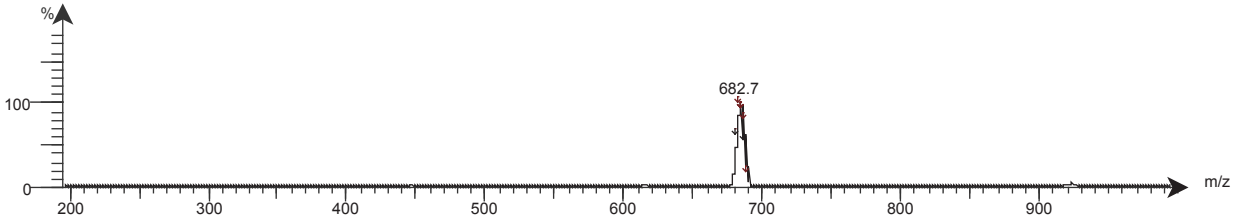

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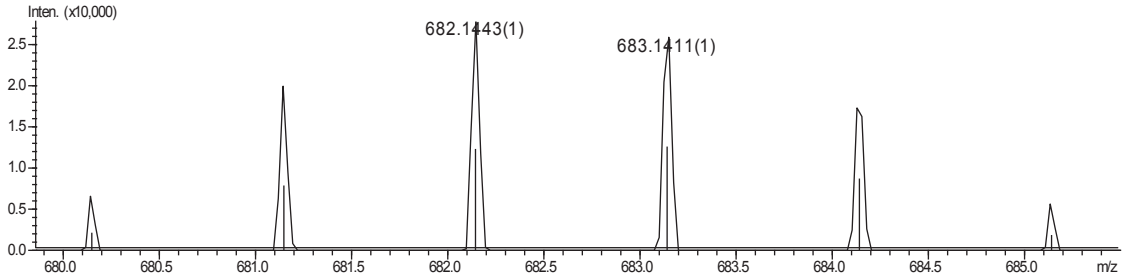

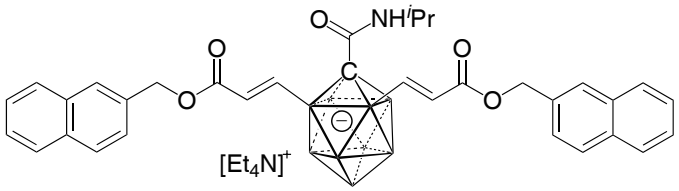

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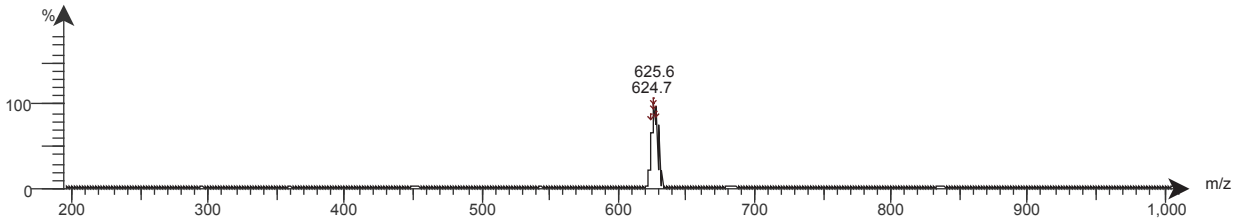

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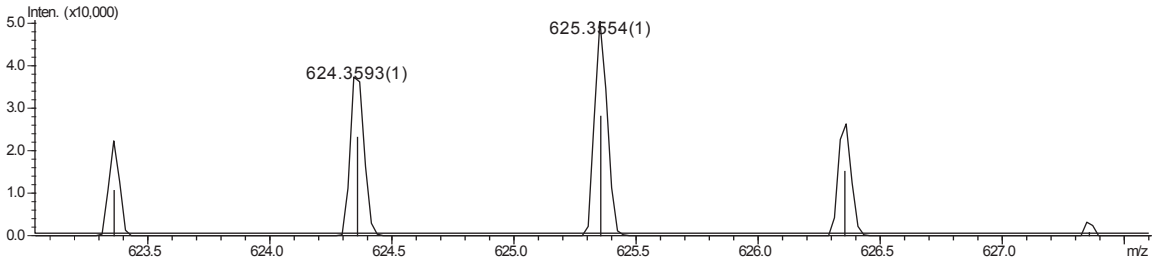

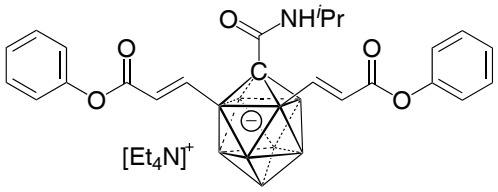

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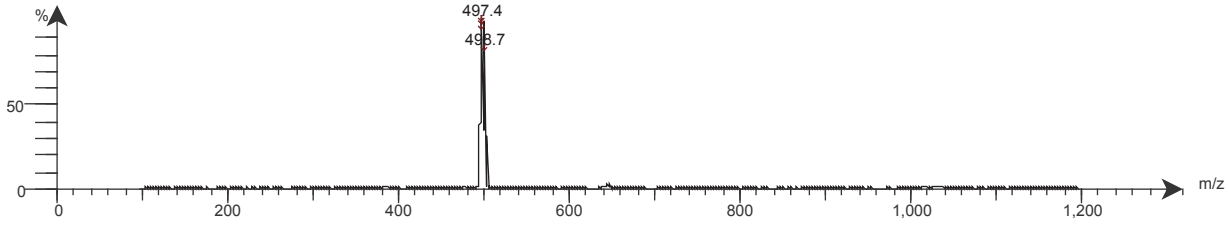

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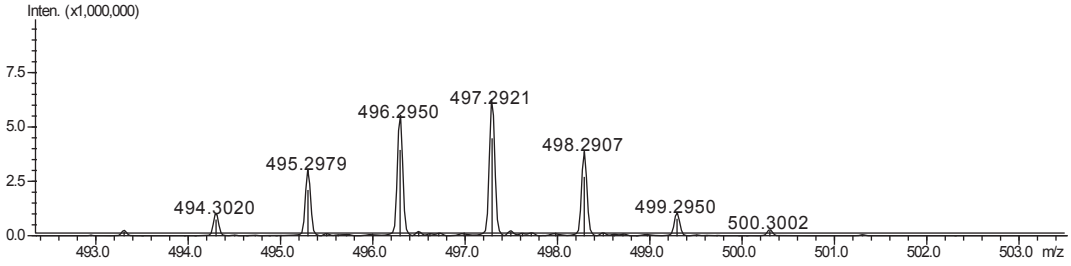

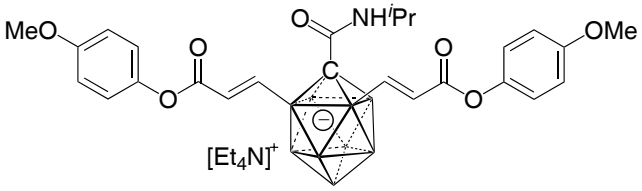

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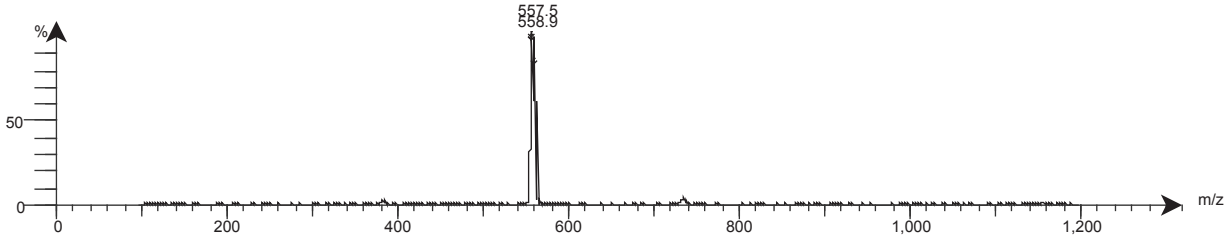

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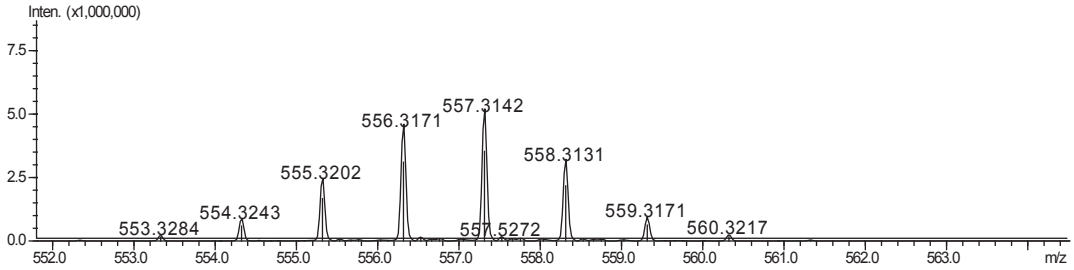

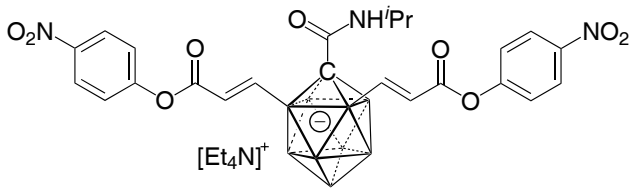

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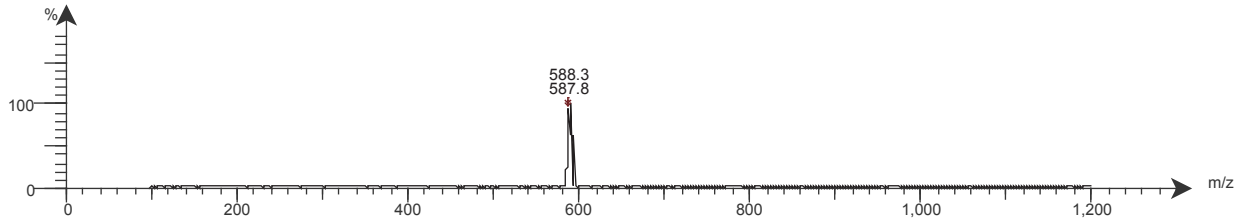

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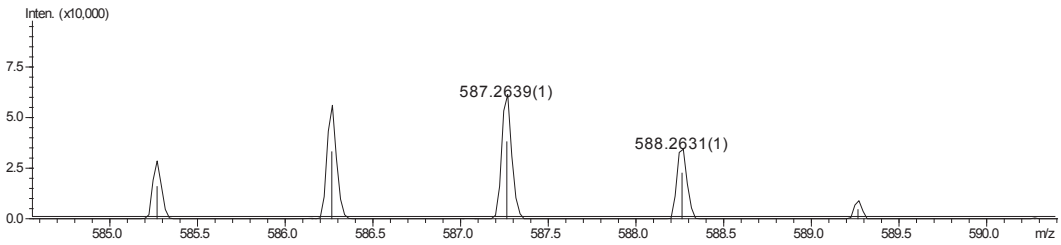

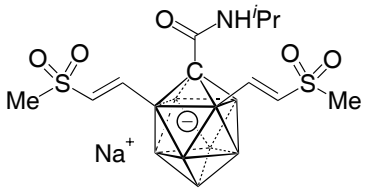

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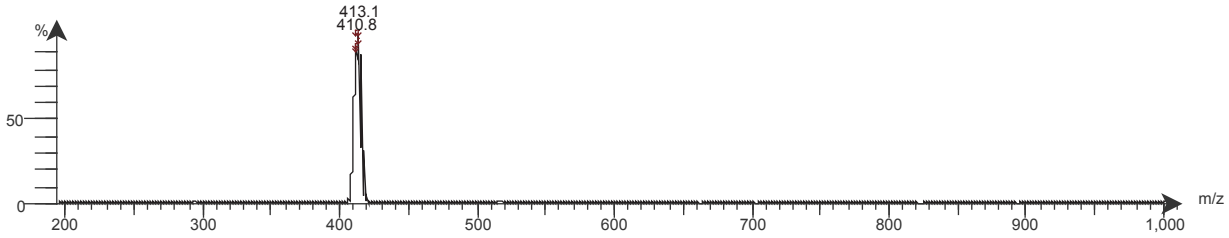

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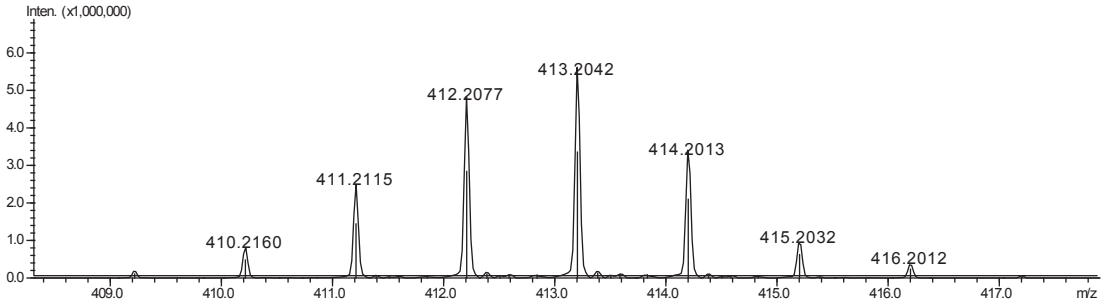

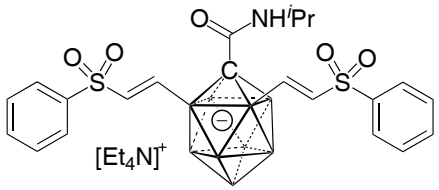

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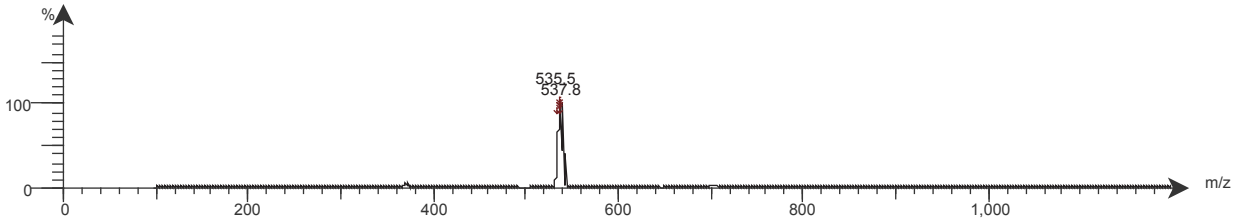

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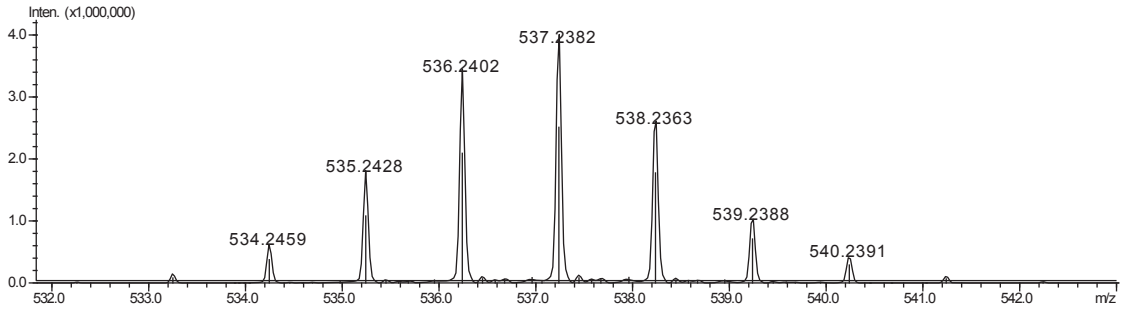

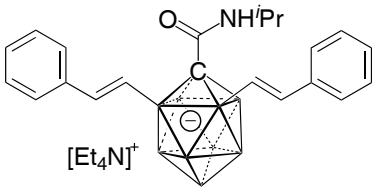

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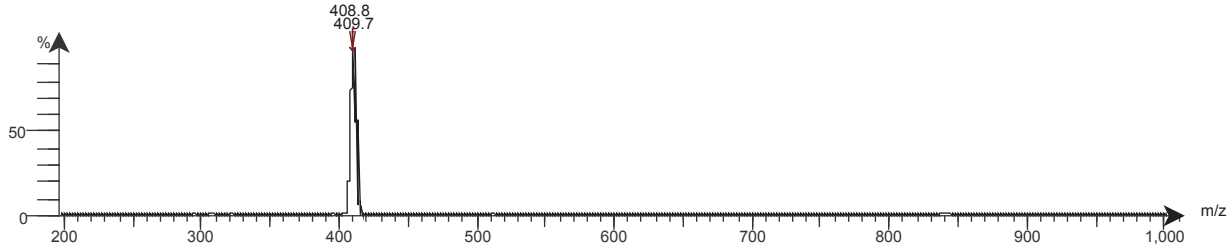

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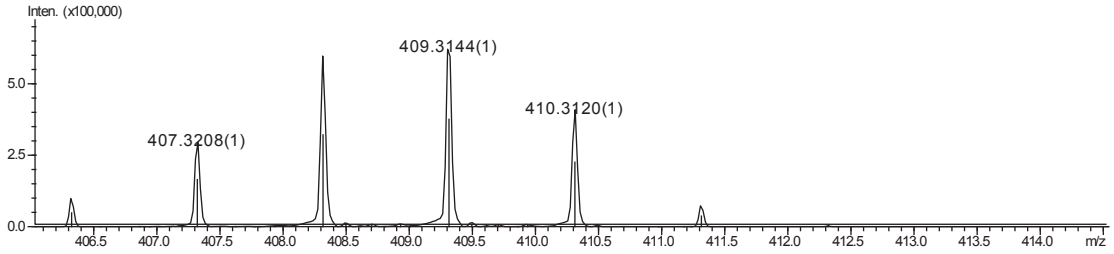

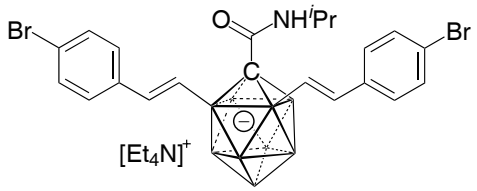

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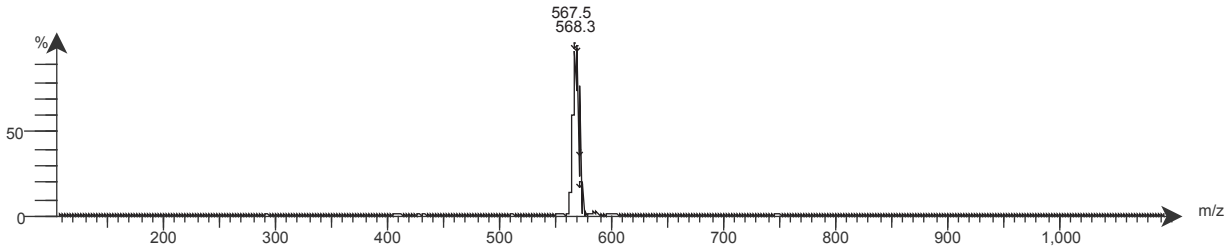

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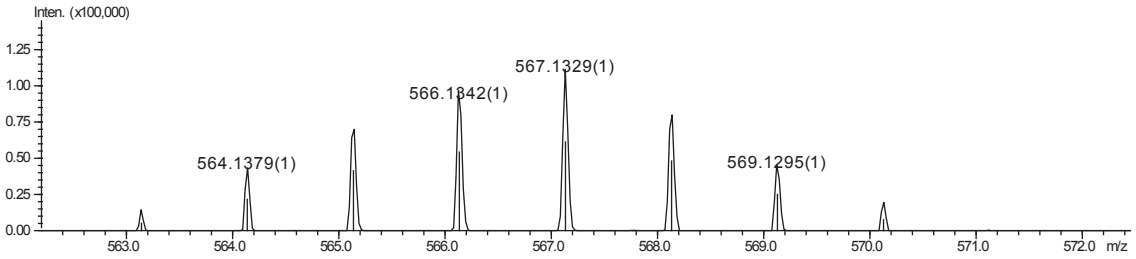

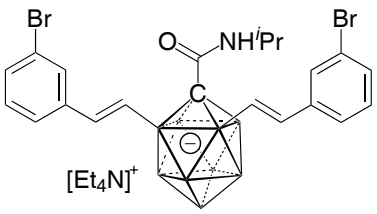

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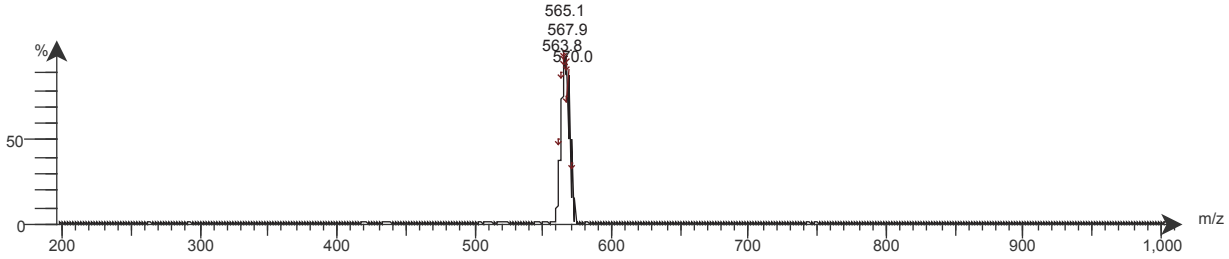

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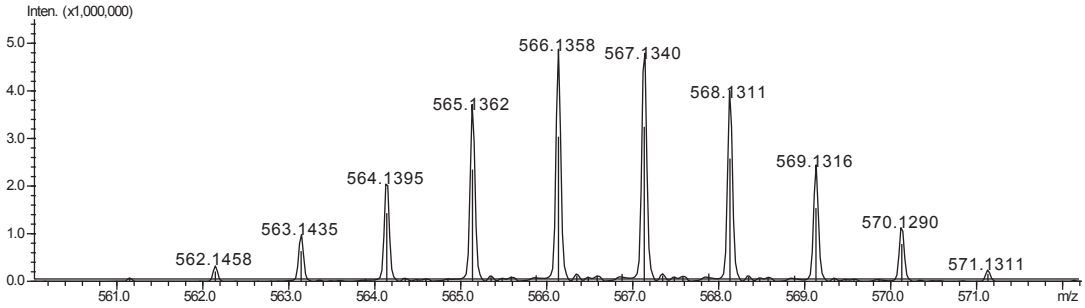

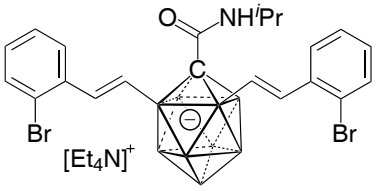

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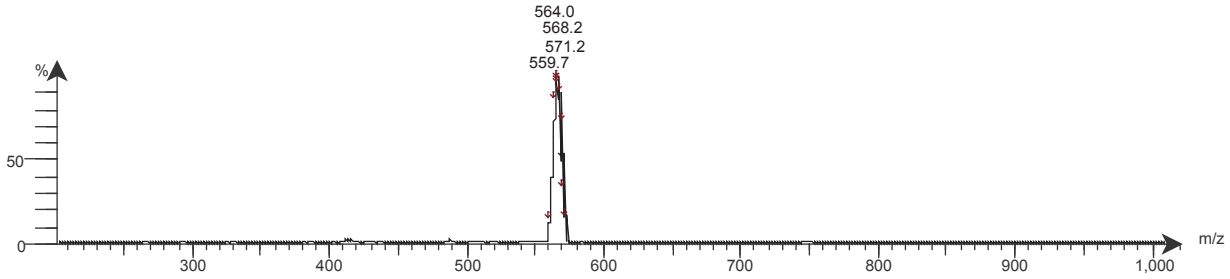

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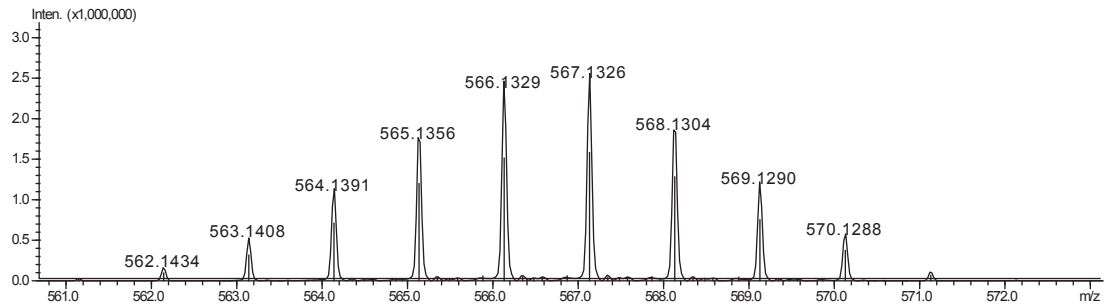

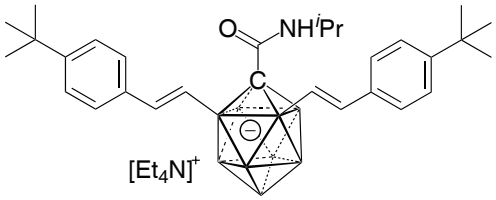

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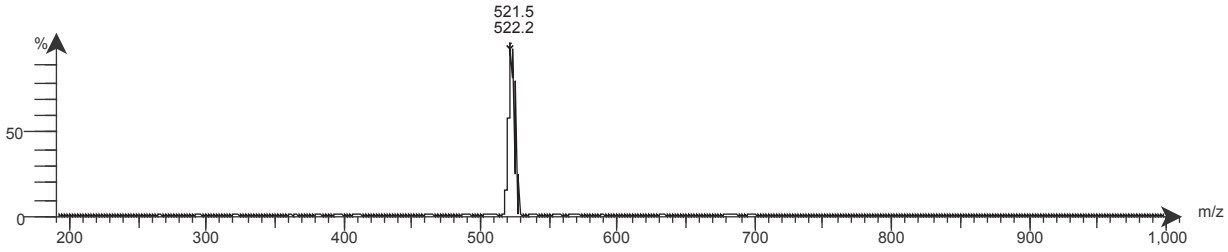

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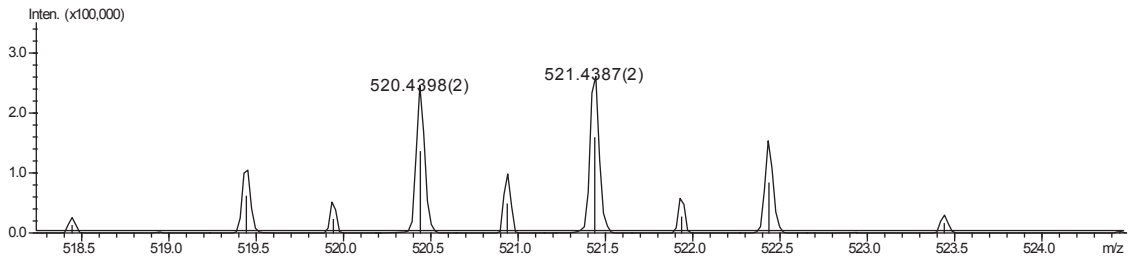

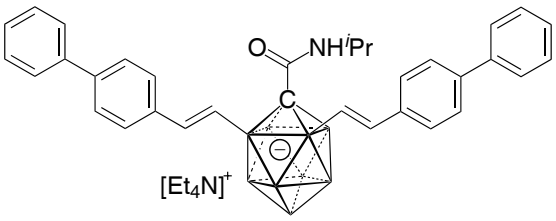

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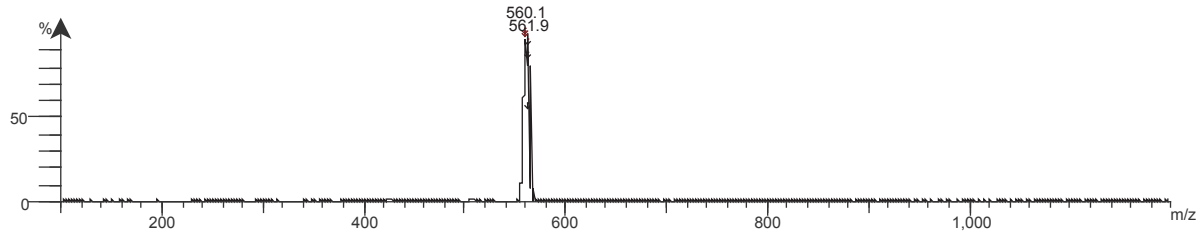

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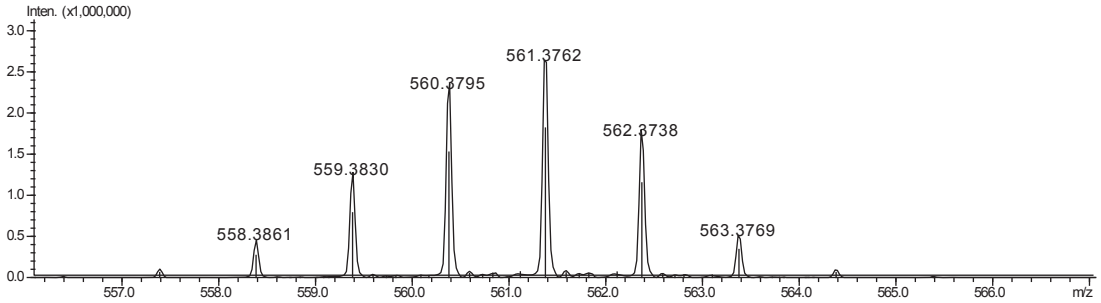

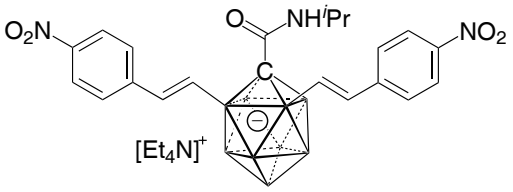

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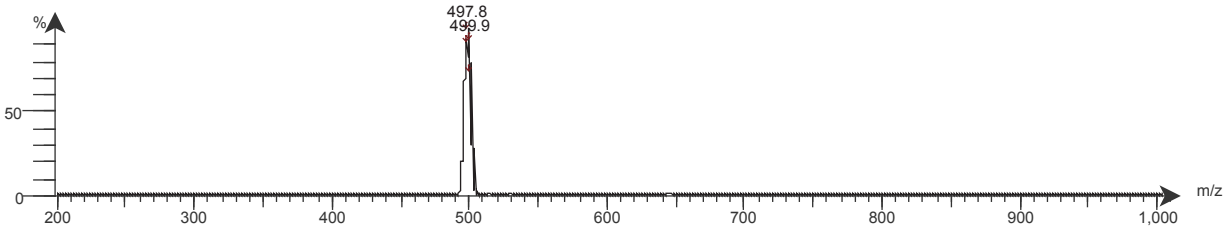

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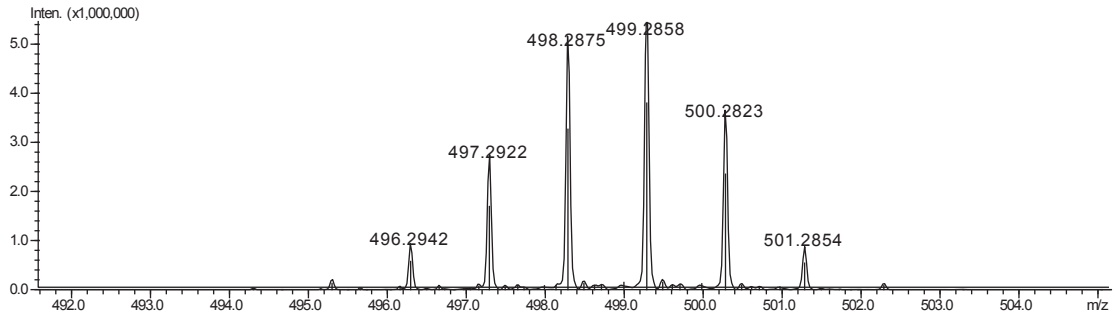

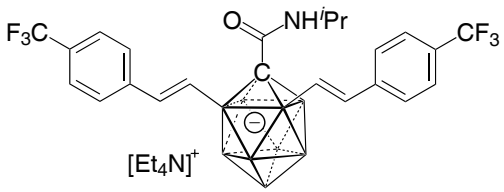

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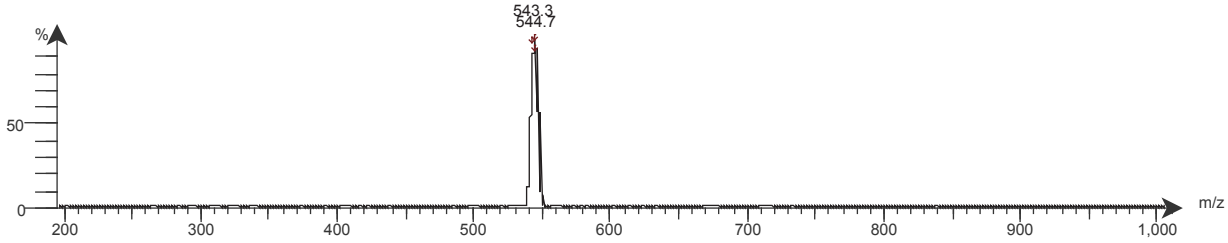

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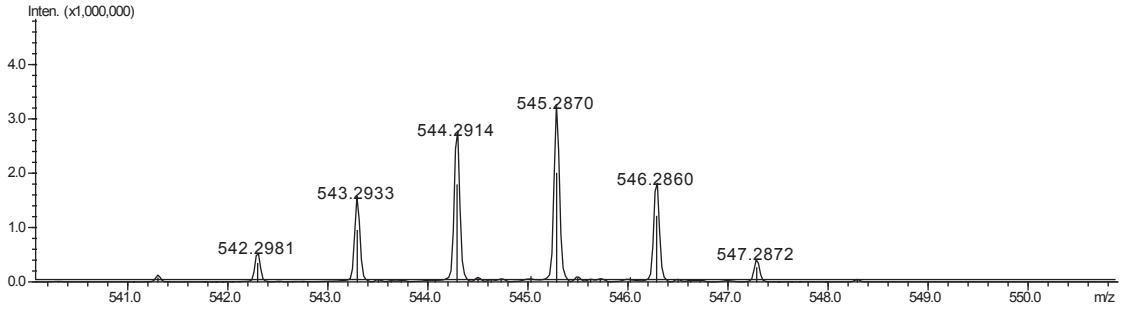

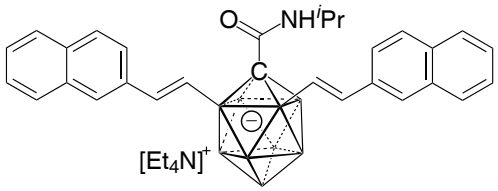

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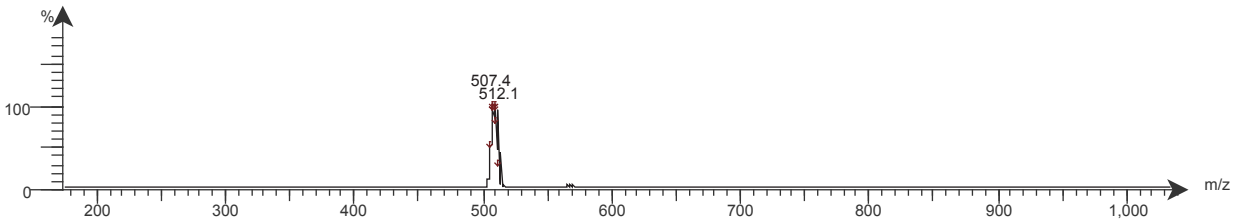

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