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Supplementary Information for

Efficient access to amides of the carborane carboxylic acid $[1\text{-(COOH)-}CB_{11}H_{11}]^-$

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I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available and used without further purification. acetone-d_6 and CD_3CN were purchased from Cambridge Isotope Laboratories and filtered through Al_2O_3 prior to use. All carborane starting materials were prepared according to the literature.[1] Anhydrous solvents were prepared by passage through activated Al_2O_3 and stored over 3 Å molecular sieves.

Reaction Conditions

Glassware for air-sensitive reations was dried at 150 °C for at least 12 h and allowed to cool in a vacuum.

Characterization

Thin-layer chromatography (TLC) was carried out using silica gel 60, F254 with a thickness of 0.25 mm. Column chromatography was performed on silica gel 60 (200-30 mesh).

NMR spectra were recorded on a Bruker AVANCE III 500 spectrometer (^{1}H NMR 500.13 MHz, ^{13}C NMR 125.77 MHz, ^{11}B NMR 160.46 MHz) or a Bruker AVANCE III 400 spectrometer (^{1}H NMR 400.13 MHz, ^{13}C NMR 100.62 MHz, ^{11}B NMR 128.38 MHz) at the temperature indicated. Data are reported as follows: Chemical shift in ppm, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, dd = doublet of doublets, etc.), coupling constant *J* in Hz, integration, and (where applicable) interpretation. Signals were referenced against solvent peaks (^{1}H: residual $CHD_2C(O)CD_3$ = 2.05 ppm, residual CHD_2CN = 1.94 ppm, residual $^{13}C\{^1H\}$: $CD_3C(O)CD_3$ = 29.84 ppm, CD_3CN = 1.32 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 and $^1H\{^{11}B\}$ NMR spectra measured in acetone-d_6, double water peaks were observed. This is a result of different resonances from H_2O and HOD and has been described in the literature.[2]

Low-resolution ESI-MS data were recorded on Advion Expression CMS instrument.

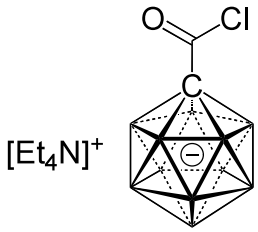
High-resolution MS data were recorded using IT-TOF detection (Shimadzu, Japan) equipped with an electrospray ionization source (ESI). Calibration to achieve accurate mass determination was carried out with sodium trifluoroacetate clusters as a reference.

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 Mo K-a radiation.

Elemental analysis of boron-containing compounds performed by our department has resulted in inconsistent C/H/N values for identical crystalline batches. The reason seems to be irreproducible formation of boron carbide and boron nitride species as a result of incomplete combustion, at least on our instrument. Other groups have observed discrepancies between calculated and found values for certain boron cage compounds as well, see references [3,4].
We therefore refrained from "submitting until the numbers are right" and focused on collecting spectroscopic data that give evidence of the purity of the isolated products. Especially the full-range mass spectra demonstrate the absence of undesired carborane by-products.

II Experimental Section

II. a) Synthesis of acid chloride 1



To a stirred suspension of carboxylic acid $[Et_4N][1\text{-}(COOH)\text{-}CB_{11}H_{11}]$ (800 mg, 2.52 mmol) in dry CH_2Cl_2 (15 mL) were added dimethylformamide (*ca.* 10 drops) and oxalyl chloride (0.234 mL, 2.77 mmol). The reaction mixture was allowed to stir for 30 min at room temperature. Isolation of the acid chloride **1** could be accomplished using the following methods:

(i) The volatiles were removed carefully under vacuum with nitrogen-cooled solvent traps. A white solid was obtained that was dried under high vacuum at 25 °C for 12 h. It was identified as acid chloride **1** in >95% purity as evidenced by NMR spectroscopy and mass spectrometry (735 mg, 87% yield).

(ii): Direct precipitation by hexane addition (10 mL), stirring at 25 °C for 1 h and collection in a glass frit. After washing with hexane (2 x 10 mL) and drying in a vacuum, **1** was obtained in identical yield.

$^1H\{^{11}B\}$ NMR (400 MHz, CD_3CN, 22 °C): δ 3.16 (q, J = 7.3 Hz, 8H, CH_2 of cation), 1.97 (broad signal, 5H, BH), 1.78 (broad signal, 1H, BH), 1.59 (broad signal, 5H, BH), 1.21 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^1H\}$ NMR (100 MHz, CD_3CN, 22 °C): δ 169.72 (CO), 75.55 (cage C), 53.02 (CH_2 of cation), 7.65 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, CD_3CN, 22 °C): δ -4.87 (1B), -12.64 (5B), -13.39 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_2H_{11}B_{11}ClO]^-$, 205.1595; found, 205.1609.

Monitoring of the hydrolysis of 1

The hydrolysis of acid chloride **1** was followed by NMR spectroscopy in CD_3CN/D_2O (5:1 *v*/*v*) at 25 °C and 50 °C. The $^{11}B\{^1H\}$ NMR spectra are shown in Figures S1 and S2. At 25 °C, hydrolysis was slow with a 52% conversion to the acid after 40 h. At 50 °C, the conversion to the acid was 83% after 20 h and >95% after 40 h.

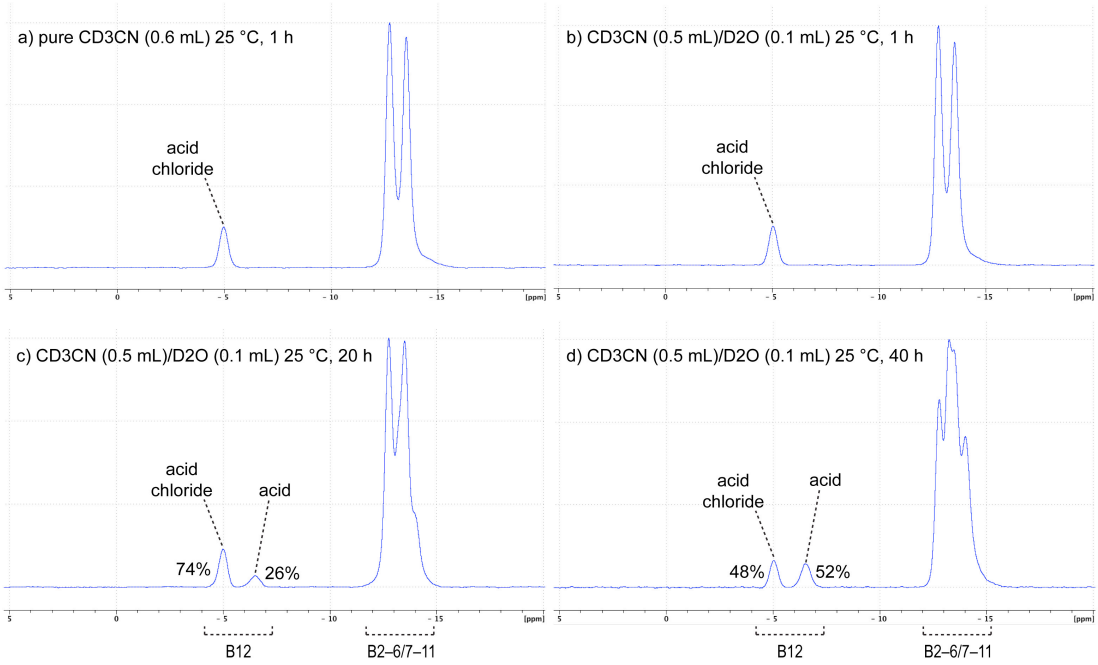


Figure S1. Monitoring of the hydrolysis of **1** at 25 °C by $^{11}B\{^1H\}$ NMR spectroscopy by integration of the resonance of the B12 position.

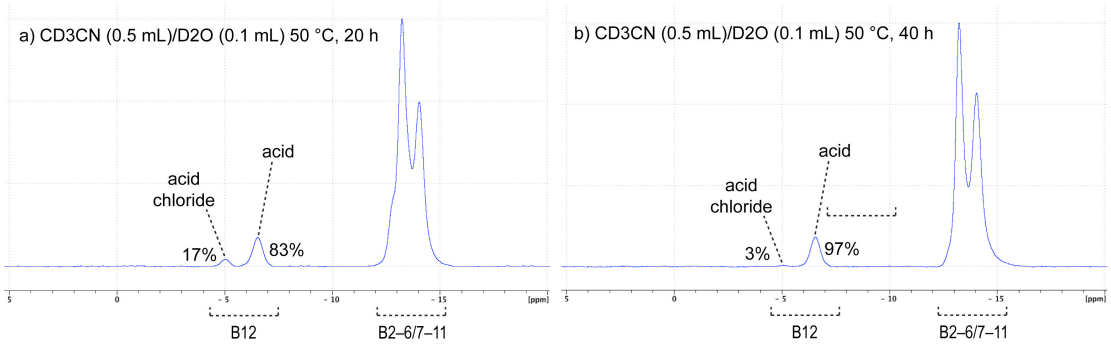


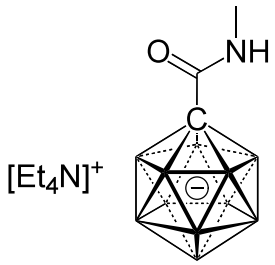
Figure S2. Monitoring of the hydrolysis of **1** at 50 °C by $^{11}B\{^1H\}$ NMR spectroscopy by integration of the resonance of the B12 position.

b) General procedure for the synthesis of carborane amides 2

Acid chloride **1** (250 mg, 0.75 mmol) was dissolved in dry CH_2Cl_2 (20 mL), amine (1.5 mmol) and Et_3N (0.10 mL, 0.75 mmol) were added, and the resulting mixture was stirred at room temperature for 20 min. All volatile components were then removed completely in a vacuum.

(i) For the synthesis of **2b**, **2d**, and **2f**–**l**, the residue was taken up in 1 M HCl (pH = 2) and extracted with diethyl ether (3 x 40 mL). The combined organic extracts were evaporated under reduced pressure, and the crude product was dissolved in water (15 mL) and filtered. $[Et_4N]^+Br^-$ (315 mg, 1.5mmol) was added to the filtrate, and the resulting white precipitate was collected in a glass frit and dried in a vacuum to give the product.

(ii) For synthesis of **2a**, **2c**, **2e and 2m**, the residue was purified by column chromatography on silica gel eluting with a mixture of CH_2Cl_2/CH_3CN to afford the desired product.



2a: Prepared following the general procedure, using methylamine as the substrate, **2a** (114 mg, 46 % yield) was obtained as a white solid. Methylamine was prepared as a 0.1 M solution in EtOAc by mixing $[MeNH_3][Cl]$ with Na_2CO_3 (1.5 equiv) in $EtOAC/H_2O$ (2:1 *v*/*v*).

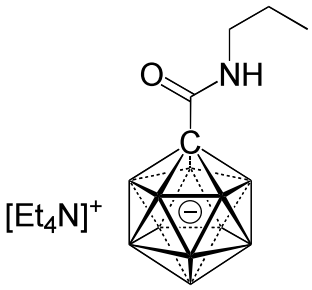
$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 6.49 (broad signal, 1H, NH), 3.47 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.60 (d, J = 6.2 Hz 3H, CH_3NH), 1.90 (broad signal, 5H, BH), 1.73 (broad signal, 1H, BH), 1.59 (broad signal, 5H, BH), 1.39 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 166.20 (CO), 71.57 (cage C), 52.62

(CH_2 of cation), 26.80, 7.30 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (160 MHz, acetone-d_6, 22 °C): δ -6.13 (1B), -12.27 (5B), -13.41 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_3H_{15}B_{11}NO]^-$, 200.2250; found, 200.2265.



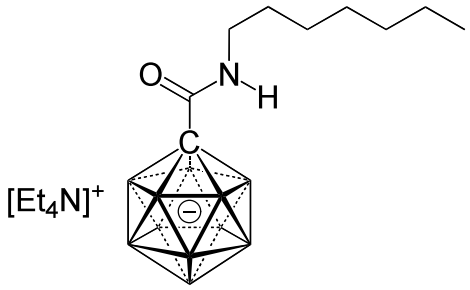
2b: Prepared following the general procedure, using propylamine as the substrate, **2b** (243 mg, 91% yield) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 6.42 (1H, NH), 3.48 (q, J = 7.3 Hz, 8H, CH_2 of cation), 3.03 (q, J = 6.3 Hz, 2H, NHCH_2), 1.92 (broad signal, 5H, BH), 1.74 (broad signal, 1H, BH), 1.60 (broad signal, 5H, BH), 1.42 (overlapping signals, 14H, CH_3 of cation and CH_2), 0.82 (t, J = 7.3 Hz, 3H, CH_3).

$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 165.93 (CO), 72.18 (cage C), 53.00 (CH_2 of cation), 42.19, 23.31, 11.46, 7.68 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.09 (1B), -13.14 (5B), -14.27 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_5H_{19}B_{11}NO]^-$, 228.2563; found, 228.2576.



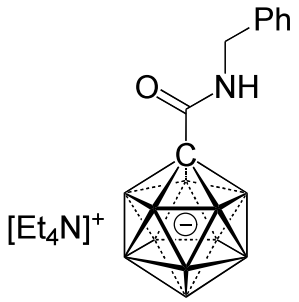
2c: Prepared following the general procedure, using *n*-heptylamine as the substrate, **2c** (280 mg, 90% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 6.51 (broad signal, 1H, NH), 3.46 (q, J = 7.3 Hz, 8H, CH_2 of cation), 3.08 (q, J = 6.7 Hz, 2H, $NHCH_2$), 1.90 (broad signal, 5H, BH), 1.73 (broad signal, 1H, BH), 1.59 (broad signal, 5H, BH), 1.38 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation), 1.26 (overlapping m, 10H, CH_2), 0.86 (t, J = 6.5 Hz, 3H, CH_3).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 166.22 (CO), 71.90 (cage C), 52.94 (CH_2 of cation), 40.55, 32.42, 29.99, 29.60 27.28, 23.14, 14.28, 7.63 (CH_3 of cation).

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.01 (1B), -13.11 (5B), -14.29 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_9H_{27}B_{11}NO]^-$, 284.3189; found, 284.3224.



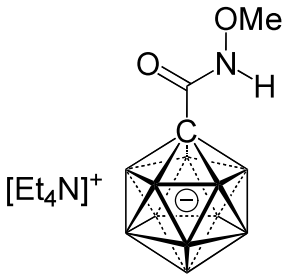
2d: Prepared following the general procedure, using benzylamine as the substrate, **2d** (265 mg, 87% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22°C): δ 7.30 (m, 2H, ArH), 7.21 (m, 3H, ArH), 7.00 (broad signal, 1H, NH), 4.31 (d, J = 6.2 Hz, 2H, $NHCH_2$), 3.44 (q, J = 7.3 Hz, 8H, CH_2 of cation), 1.98 (broad signal, 5H, BH), 1.77 (broad signal, 1H, BH), 1.63 (broad signal, 5H, BH), 1.36 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 22°C): δ 166.25 (CO), 140.72, 129.03, 127.58, 127.41 (aryl C), 71.88 (cage C), 52.95 (CH_2 of cation), 43.9, 7.64 (CH_3 of cation).

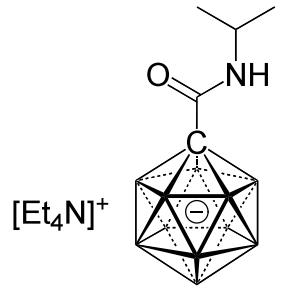
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 22°C): δ -6.85 (1B), -13.05 (5B), -14.21 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_9H_{25}B_{11}NO]^-$, 276.2563; found, 276.2576.



2e: Prepared following the general procedure b, using methoxyamine as the substrate, **2e** (130 mg, 50% yield) was obtained as a white solid. Methoxyamine was prepared as a 0.1 M solution in EtOAc by mixing [$MeONH_3$][Cl] with Na_2CO_3 (1.5 equiv) in EtOAC/H_2O (2:1 *v*/*v*).

$^1H\{^{11}B\}$ NMR (500 MHz, CD_3CN, 22 °C): δ 9.03 (broad signal, 1 H, NH), 3.55 (s, 3H, CH_3O), 3.16 (q, J = 7.3 Hz, 8H, CH_2 of cation), 1.81 (broad overlapping signals, 6H, BH), 1.52 (broad signal, 5H, BH), 1.21 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation).
$^{13}C\{^1H\}$ NMR (100 MHz, CD_3CN, 22 °C): δ 163.80 (CO), 68.91 (cage C), 63.93 (CH_3O), 53.03 (CH_2 of cation), 7.66 (CH_3 of cation).
$^{11}B\{^1H\}$ NMR (160 MHz, CD_3CN, 22 °C): δ -6.70 (1B), -13.25 (5B), -14.55 (5B).
HRMS (ESI): *m/z* Calcd. for $[C_3H_{15}B_{11}NO_2]^-$, 216.2199; found, 216.2248.



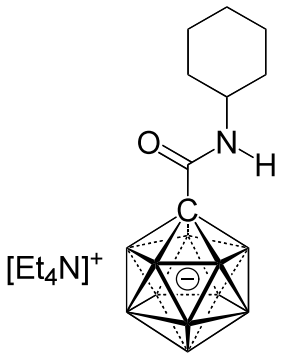
2f: Prepared following the general procedure, using isopropylamine as the substrate, **2f** (239 mg, 89% yield) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 3.78 (septet, J = 6.5 Hz, 1H, CH), 3.48 (q, J = 7.3 Hz, 8H, CH_2 of cation), 1.89 (broad signal, 5H, BH), 1.74 (broad signal, 1H, BH), 1.60 (broad signal, 5H, BH), 1.39 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation), 1.05 (d, J = 6.5 Hz, 6H, CH_3). The N-H signal could not be detected unambiguously.
$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 165.05 (CO), 72.09 (cage C), 52.98

(CH_2 of cation), 42.28, 22.36, 7.66 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.06 (1B), -13.14 (5B), -14.30 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_5H_{19}B_{11}NO]^-$, 228.2563; found, 228.2575.



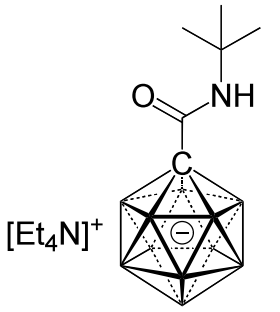
2g: Prepared following the general procedure, using cyclohexylamine as the substrate, **2g** (257 mg, 86% yield) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 3.35-3.60 (overlapping signals, 9H, CH_2 of cation and N-C*H*), 1.90 (broad signal, 5H, BH), 1.80-1.47 (overlapping signals, 11H, BH, cyclohexyl CH), 1.39 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation), 1.10-1.30 (overlapping signals, 5H, cyclohexyl CH). The N-H signal appeared as a weak signal at 6.07 ppm.

$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 164.97 (CO), 72.11 (cage C), 52.97 (CH_2 of cation), 49.13, 32.92, 26.19, 25.36, 7.66 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.06 (1B), -13.12 (5B), -14.29 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_8H_{23}B_{11}NO]^-$, 268.2876; found, 268.2890.



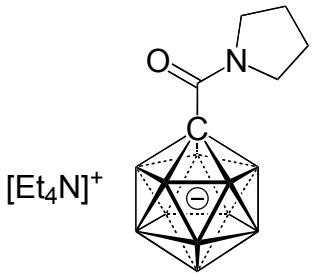
2h: Prepared following the general procedure, using *tert*-butylamine as the substrate, **2h** (251 mg, 90% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 5.91 (broad signal, 1 H, NH), 3.48 (q, J = 7.3 Hz, 8H, CH_2 of cation), 1.89 (broad signal, 5H, BH), 1.73 (broad signal, 1H, BH), 1.60 (broad signal, 5H, BH), 1.40 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation), 1.22 (s, 9H, CH_3). The N-H signal appeared as a weak signal at 5.91 ppm.

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6 22 °C): δ 165.12 (CO), 72.95 (cage C), 52.99 (CH_2 of cation), 51.13, 29.64, 7.66 (CH_3 of cation).

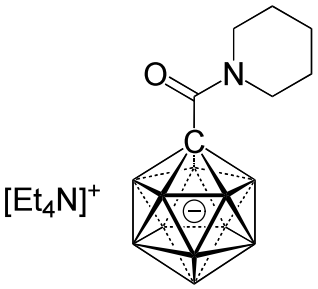
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.23 (1B), -13.14 (5B), -14.26 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_6H_{21}B_{11}NO]^-$, 242.2719; found, 242.2727.



2i: Prepared following the general procedure, using pyrrolidine as the substrate, **2i** (251 mg, 90% yield) was obtained as a white solid.

The spectroscopic data matched with those reported.[1]



2j: Prepared following the general procedure, using piperidine as the substrate, **2j** (242 mg, 84% yield) was obtained as a white solid.

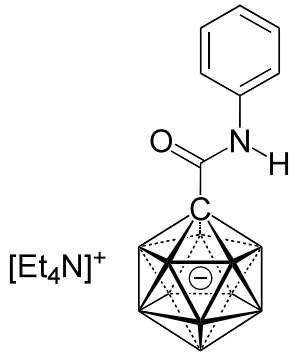
$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 3.63 (m, 4H, CH_2NCH_2), 3.48 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.05 (broad signal, overlapping with solvent residual signal, 5 H, BH), 1.84 (broad signal, 1H, BH), 1.65-1.55 (overlapping signals, 7H,

BH and CH_2), 1.45-1.30 (overlapping signals, 18H, CH_3 of cation and CH_2).

$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 164.27 (CO), 71.61 (cage C), 53.02 (CH_2 of cation), 48.15, 27.20, 25.33, 7.68 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -5.26 (1B), -13.23 (10B).

HRMS (ESI): *m/z* Calcd. for $[C_7H_{21}B_{11}NO]^-$, 254.2719; found, 254.2730.



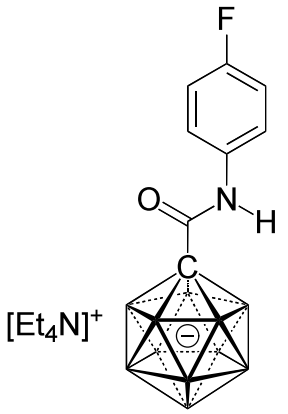
2k: Prepared following the general procedure, using aniline as the substrate, **2k** (256 mg, 87% yield) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22°C): δ 8.13 (broad signal, 1H, NH), 7.61 (d, J = 8.0 Hz, 2H, ArH), 7.29 (t, J = 8.0 Hz, 2H, ArH), 7.06 (t, J = 8.0 Hz, 1H, ArH), 3.45 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.05 (broad signal, overlapping with solvent residual signal, 5H, BH), 1.83 (broad signal, 1H, BH), 1.69 (broad signal, 5H, BH), 1.38 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 22°C): δ 164.31 (CO), 139.73, 129.42, 124.38, 120.32, 72.23 (cage C), 52.96 (CH_2 of cation), 7.63 (CH_3 of cation)

$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 22°C): δ -6.62 (1B), -12.87 (5B), -14.18 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_8H_{17}B_{11}NO]^-$, 262.2406 ; found, 262.2412.



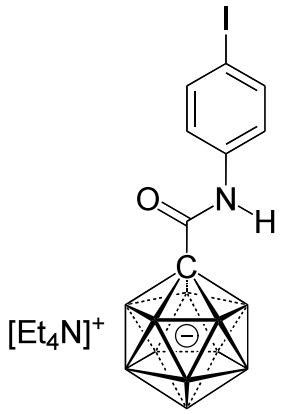
2l: Prepared following the general procedure, using 4-fluoroaniline as the substrate, **2l** (265 mg, 86% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22°C): δ 8.18 (broad signal, 1H, NH), 7.45-7.78 (m, 2H, ArH), 6.89-7.27 (m, 2H, ArH), 3.47 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.02 (broad signal, 5H, BH), 1.81 (broad signal, 1H, BH), 1.67 (broad signal, 5H, BH), 1.38 (tt, J = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^{1}H\}$ NMR (125 MHz, acetone-d_6, 22°C): δ 164.55 (CO), 159.75 (d, J = 240 Hz, C-F), 136.24 (d, J = 2.4 Hz), 122.47 (d, J = 8.0 Hz), 115.87 (d, J = 22.4 Hz), 72.06 (cage C), 53.00 (CH_2 of cation), 7.65 (CH_3 of cation).

$^{11}B\{^{1}H\}$ NMR (160 MHz, acetone-d_6, 22°C): δ -6.54 (1B), -12.87 (5B), -14.20 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_8H_{16}B_{11}FNO]^-$, 280.2312; found, 280.2325.



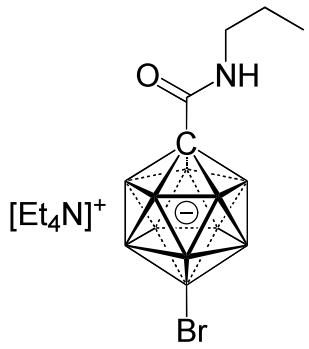
2m: Prepared following the general procedure, using 4-iodoaniline as the substrate, **2m** (357 mg, 92% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, CD_3CN, 22 °C): δ 7.97 (broad signal, 1H, NH), 7.58 (d, *J* = 7.3 Hz, 2H, ArH), 7.29 (d, *J* = 7.3, 2H, ArH), 3.12 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.20 (broad signal, 5H, BH), 1.68 (broad signal, 1 H, BH), 1.55 (broad signal, 5H, BH), 1.19 (tt, *J* = 7.3Hz, 1.9 Hz, 12H, CH_3 of cation).

$^{13}C\{^{1}H\}$ NMR (100 MHz, CD_3CN, 22 °C): δ 164.66 (CO), 139.09, 138.49, 123.14, 87.64, 72.21 (cage C), 52.98 (CH_2 of cation), 7.62 (CH_3 of cation).

$^{11}B\{^{1}H\}$ NMR (128 MHz, CD_3CN, 22 °C): δ -6.69 (1B), -12.97 (5B), -14.21 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_8H_{16}B_{11}INO]^-$, 388.1373; found, 388.1392.



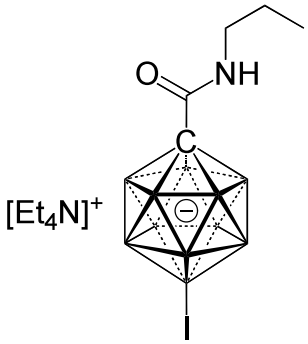
4a: The acid chloride [1-(C(O)Cl)-$CB_{11}H_{10}$-12-Br][Et_4N] was prepared in a similar manner to **1** and collected as a precipitate in a glass frit. Prepared following the general procedure for products **2**, using propylamine as the substrate, **4a** (265 mg, 81% yield with respect to the carboxylic acid) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 6.48 (broad signal, 1H, NH), 3.49 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 3.04 (m, 2H, NHCH_2), 2.00-1.80 (broad overlapping signals, 10H, BH), 1.45-1.31 (overlapping signals, 14H, CH_3 of cation, CH_3CH_2), 0.81 (t, *J* = 7.4 Hz, 3H, CH_3CH_2).

$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 22°C): δ 165.82 (CO), 66.08 (cage C), 52.99 (CH_2 of cation), 42.27 ($NHCH_2$), 23.24 (CH_3CH_2), 11.41 (CH_3CH_2), 7.67 (CH_3 of cation).

$^{11}B\{^{1}H\}$ NMR (160 MHz, acetone-d_6, 22 °C): δ -1.94 (1B), -12.37 (5B), -14.90 (5B).

HRMS (ESI): *m/z* Calcd. for $[C_5H_{18}B_{11}BrNO]^-$, 306.1668; found, 306.1707.



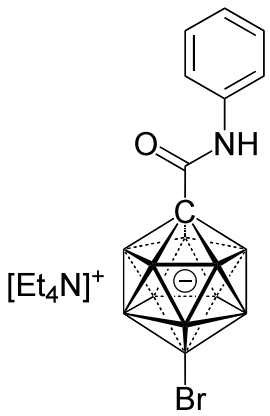
4b: The acid chloride [1-(C(O)Cl)-$CB_{11}H_{10}$-12-I][Et_4N] was prepared in a similar manner to **1** and collected as a precipitate in a glass frit. Prepared following the general procedure for products **2**, using propylamine as the substrate, **4b** (320 mg, 88% yield with respect to the carboxylic acid) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22°C): δ 6.45 (broad signal, 1H, NH), 3.49 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.95-3.09 (m, 2H, NHCH_2), 2.05 (broad signal, overlapping with solvent residual signal, 5H, BH), 1.95 (broad signal, 5H, BH), 1.50-1.32 (overlapping signals, 14H, CH_3 of cation, CH_3CH_2), 0.81 (t, J = 7.4 Hz, 3H, CH_3CH_2).

$^{13}C\{^1H\}$ NMR (125 MHz, acetone-d_6, 22°C): δ 165.96 (CO), 69.62 (cage C), 53.02 (CH_2 of cation), 42.27 ($NHCH_2$), 23.23 (CH_3CH_2), 11.40 (CH_3CH_2), 7.69 (CH_3 of cation).

$^{11}B\{^1H\}$ NMR (160 MHz, acetone-d_6, 22°C): δ -11.64 (5B), -14.08 (5B), -17.00 (1B).

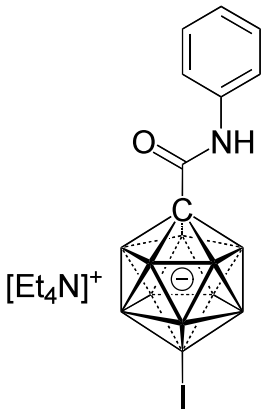
HRMS (ESI): *m/z* Calcd. for $[C_5H_{18}B_{11}INO]^-$, 354.1529; found, 354.1517.



4c: The acid chloride [1-(C(O)Cl)-$CB_{11}H_{10}$-12-Br][Et_4N] was prepared in a similar manner to **1** and collected as a precipitate in a glass frit. Prepared following the

general procedure for products **2**, using aniline as the substrate, **4c** (303 mg, 86% yield with respect to the carboxylic acid) was obtained as a white solid.

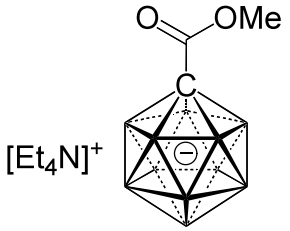
$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 22 °C): δ 8.14 (broad signal, 1H, NH), 7.66-7.55 (m, 2H, ArH), 7.33-7.23 (m, 2H, ArH), 7.10-7.00 (m, 1H, ArH), 3.47 (q, J = 7.3 Hz, 8H, CH_2 of cation), 2.05 (broad signal, overlapping with solvent residual signal, 5H, BH), 2.0 (broad signal, 5H, BH), 1.38 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 22 °C): δ 164.39 (CO), 139.57, 129.40, 124.57, 120.58, 66.30 (cage C), 52.97 (CH_2 of cation), 7.65 (CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (160 MHz, acetone-d_6, 22 °C): δ -1.57 (1B), -12.12 (5B), -14.82 (5B).
HRMS (ESI): *m/z* Calcd. for $[C_8H_{16}B_{11}BrNO]^-$, 340.1512; found, 340.1539.



4d: The acid chloride [1-(C(O)Cl)-$CB_{11}H_{10}$-12-I][Et_4N] was prepared in a similar manner to **1** and collected as a precipitate in a glass frit. Prepared following the general procedure for products **2**, using aniline as the substrate, **4d** (350 mg, 90% yield with respect to the carboxylic acid) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 22 °C): δ 8.10 (broad signal, 1H, NH), 7.65-7.55 (m, 2H, ArH), 7.30-7.18 (m, 2H, ArH), 7.10-7.00 (m, 1H, ArH), 3.47 (q, J = 7.3Hz, 8H, CH_2 of cation), 2.12 (broad signal, 5H, BH), 2.05 (broad signal, overlapping with solvent residual signal, 5H, BH), 1.38 (tt, J = 7.3Hz, 1.9Hz, 12H, CH_3 of cation).
$^{13}C\{^{1}H\}$ NMR (125 MHz, acetone-d_6, 22 °C): δ 164.50 (CO), 139.54, 129.39, 124.58, 120.61, 69.81 (cage C), 52.99 (CH_2 of cation), 7.67 (CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (160 MHz, acetone-d_6, 22 °C): δ -11.41 (5B), -13.99 (5B), -16.71 (1B).

HRMS (ESI): *m/z* Calcd. for $[C_8H_{16}B_{11}INO]^-$, 388.1373; found, 388.1385.

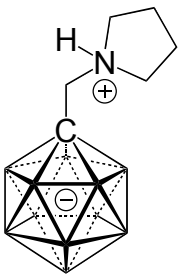


5: Prepared following the general procedure for products **2**, using methanol as the solvent. The reaction was conducted at 50 °C for 5 h. **5** (226 mg, 91% yield) was obtained as a white solid.

$^1H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 22 °C): δ 3.51 (s, 3H, OCH_3), 3.48 (q, J =7.3 Hz, 8H, CH_2 of cation), 1.93 (broad signal, 5H, BH), 1.78 (broad signal, 1H, BH), 1.60 (broad signal, 5H, BH), 1.39 (tt, J = 7.3 Hz, 1.9 Hz, 12H, CH_3 of cation).
$^{13}C\{^1H\}$ NMR (125 MHz, acetone-d_6, 22 °C): δ 167.73 (CO), 68.23 (cage C), 53.00 (CH_2 of cation), 52.81 (CO_2CH_3), 7.65 (CH_3 of cation).
$^{11}B\{^1H\}$ NMR (160 MHz, acetone-d_6, 22 °C): δ -6.10 (1B), -13.07 (5B), -14.00 (5B).
HRMS (ESI): *m/z* Calcd. for $[C_3H_{14}B_{11}O_2]^-$, 201.2090; found, 201.2095.

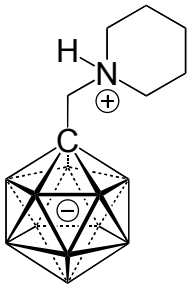
c) Reduction of carborane amides 2 to give carborane amines 6

To the amide **2** (0.5 mmol) was added a solution of lithium aluminum hydride (1 M in THF, 5 mL). The reaction mixture was then stirred for 2 h at 25 °C. Water (10 mL) was slowly added, and the aqueous solution was acidified with concentrated HCl (pH = 2), followed by extraction with Et_2O (3 x 50 mL). The combined organic layers were washed with water, dried over $MgSO_4$ and concentrated. Drying in a high vacuum at 25 °C afforded products **6.**



6a: Prepared following the above procedure, **6a** (88% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 22 °C): δ 7.82 (broad signal, 1H, NH), 4.05-3.91 (m, 2H, NCH_2CH$_2$), 3.75-3.70 (m, 2H, C(cage)CH_2N), 3.39-3.27 (m, 2H, NCH_2CH$_2$), 2.27-2.07 (overlapping m, 4 H, NCH$_2$CH_2), 1.77 (broad overlapping signals, 6H, BH), 1.66 (broad signal, 5H, BH).
$^{13}C\{^{1}H\}$ NMR (125 MHz, acetone-d_6, 22 °C): δ 63.92, 63.38 (cage C), 58.16, 23.76.
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.37 (1B), -12.39 (5B), -14.08 (5B).
HRMS (ESI): *m/z* Calcd. for $[C_6H_{21}B_{11}N]^-$, 226.2770; found, 226.2786.



6b: Prepared following the above procedure, **6b** (91% yield) was obtained as a white solid.

$^{1}H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 22 °C): δ 7.03 (broad signal, 1H, NH), 3.95-3.80 (m, 2H, NCH_2CH$_2$), 3.67-3.55 (m, 2H, C(cage)CH_2N), 3.27-3.12 (m, 2H, NCH_2CH$_2$), 2.04-1.90 (overlapping m, 4 H, NCH$_2$CH_2), 1.89-1.45 (overlapping signals, 13H, CH$_2$ and BH).
$^{13}C\{^{1}H\}$ NMR (125 MHz, acetone-d_6, 22 °C): δ 64.60, 62.61 (cage C), 56.69, 22.82, 21.98.

$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 22 °C): δ -7.21 (1B), -12.40 (5B), -14.04(5B). HRMS (ESI): *m/z* Calcd. for $[C_7H_{23}B_{11}N]^-$, 240.2927; found, 240.2952.

III X-ray Crystallography

Crystal structure of 2e (CCDC 1829932)

Compound **2e** (15 mg) was dissolved in acetonitrile (1.0 mL) in a 4 mL glass vial to give a clear colorless solution. An aqueous solution of NaCl (1 equiv in 0.1 mL) was added. Slow evaporation afforded colorless crystals of the composition $[Na][Et_4N][C_3H_{15}B_{11}NO_2]_2$ suitable for X-ray diffraction within 5 d at 25 °C.

```
Bond precision:  C-C = 0.0098 A          Wavelength=0.71073

Cell:          a=7.6610(3)       b=14.6847(11)    c=30.005(2)
               alpha=88.511(6)   beta=89.235(4)   gamma=85.054(5)
Temperature:   170 K

                Calculated                Reported
Volume          3361.6(4)                 3361.6(4)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C12 H60 B44 N4 Na2 O8,    2(C6 H30 B22 N2 Na O4),
                2(C8 H20 N)               2(C8 H20 N)
Sum formula     C28 H100 B44 N6 Na2 O8    C28 H100 B44 N6 Na2 O8
Mr              1170.76                   1170.76
Dx,g cm-3       1.157                     1.157
Z               2                         2
Mu (mm-1)       0.076                     0.076
F000            1232.0                    1232.0
F000'           1232.40
h,k,lmax        9,17,36                   9,17,36
Nref            12324                     12230
Tmin,Tmax       0.963,0.976               0.929,1.000
Tmin'           0.963

Correction method= # Reported T Limits: Tmin=0.929 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 25.350

R(reflections)= 0.1413( 9444)     wR2(reflections)= 0.3087( 12230)

S = 1.146                 Npar= 805
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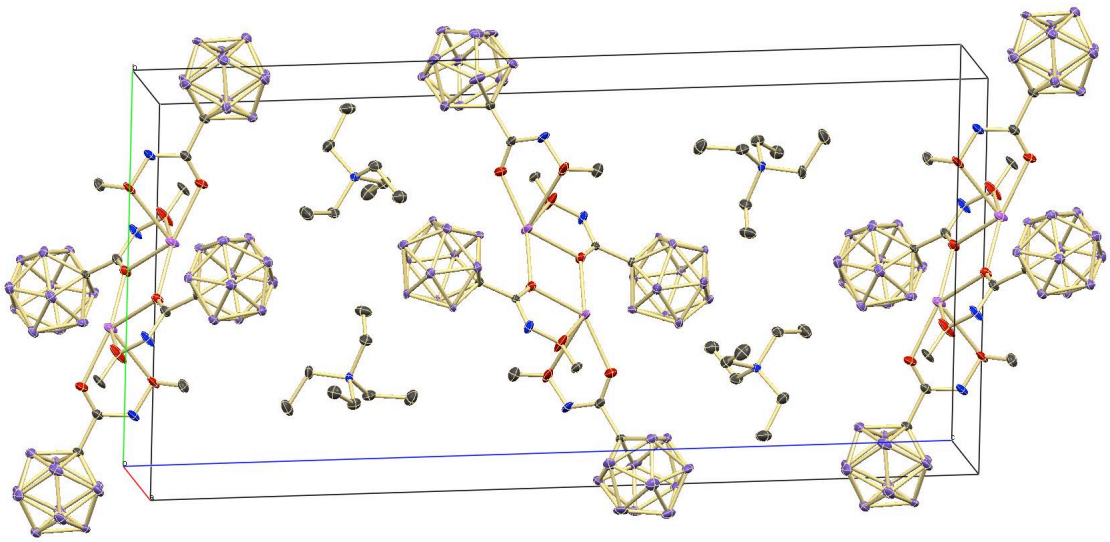


Figure S3. Unit cell of $[Na][Et_4N][C_3H_{15}B_{11}NO_2]_2$. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

The unit cell has the composition $[Na]_4[Et_4N]_4[C_3H_{15}B_{11}NO_2]_8$, whereby two similar $\{[Na][Et_4N][C_3H_{15}B_{11}NO_2]\}_2$ dimers are present (Fig. S1). O–Na coordination is observed, while the $[Et_4N]^+$ cations are well-separated from the clusters. This structure features a wR2 value of 0.3087, which is mainly attributed to the relatively large differences in anisotropic displacement parameters for the O and N atoms of the amide groups. This is most likely the result of a slight disorder or rotational flexibility of the methoxyamide group in the crystal. The connectivity of all atoms of the anions and cations is unambiguous.

Crystal structure of 2m (CCDC 1829933)

Compound **2m** (15 mg, 0.029 mmol) was dissolved in acetone (0.5 mL) a 1 mL glass vial. The resulting colorless solution was filtered into a 18 cm long NMR tube and layered with hexanes (1 mL). Colorless crystals of the composition $[Et_4N][C_8H_{16}B_{11}INO]$ suitable for X-ray diffraction grew within 5 d at 25 °C.

```
Bond precision:  C-C = 0.0095 A          Wavelength=1.34139

Cell:          a=9.1861(5)       b=11.3166(6)     c=13.6234(6)
               alpha=71.718(3)   beta=83.920(4)   gamma=72.759(4)
Temperature:   170 K

                Calculated                Reported
Volume          1284.19(12)               1284.19(12)
Space group     P -1                      P -1
Hall group      -P 1                      -P 1
Moiety formula  C8 H16 B11 I N O, C8 H20 N C8 H16 B11 I N O, C8 H20 N
Sum formula     C16 H36 B11 I N2 O        C16 H36 B11 I N2 O
Mr              518.28                    518.28
Dx,g cm-3       1.340                     1.340
Z               2                         2
Mu (mm-1)       6.759                     6.601
F000            524.0                     524.0
F000'           524.81
h,k,lmax        11,13,16                  11,13,16
Nref            4881                      4856
Tmin,Tmax       0.788,0.876               0.373,0.751
Tmin'           0.719

Correction method= # Reported T Limits: Tmin=0.373 Tmax=0.751
AbsCorr = MULTI-SCAN

Data completeness= 0.995          Theta(max)= 54.958

R(reflections)= 0.0664( 3609)     wR2(reflections)= 0.1905( 4856)

S = 1.011                 Npar= 285
```

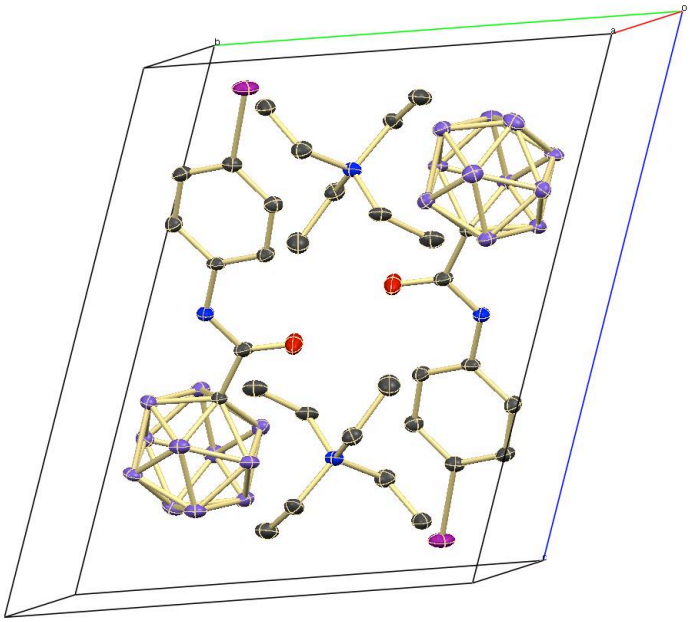


Figure S4. Unit cell of $[Et_4N][C_8H_{16}B_{11}INO]$. Hydrogen atoms are omitted for clarity; 30% displacement ellipsoids.

The unit cell has the composition $[Et_4N]_2[C_8H_{16}B_{11}INO]_2$, with a center of inversion relating the two $[Et_4N][C_8H_{16}B_{11}INO]$ units (Fig. S2). The structure was solved without any unusual features.

IV References

[1] Y. Shen, Y. Pan, K. Zhang, X. Liang, J. Liu, B. Spingler, S. Duttwyler, *Dalton Trans.* **2017**, *46*, 3135.

[2] J. R. Holmes, D. Kivelson, W. C. Drinkard, *J. Chem. Phys.* **1962**, *37*, 150–152;
a more recent summary is available online from the Sigma-Aldrich company: https://www.sigmaaldrich.com/content/dam/sigma-aldrich/docs/Aldrich/General_Information/double_water_peaks.pdf

[3] J. Kahlert, L. Böhling, A. Brockhinke, H.-G. Stammler, B. Neumann, L. M. Rendina, P. J. Low, L. Weber, M. A. Fox, *Dalton Trans.* **2015**, *44*, 9766.

[4] E. Justus, K. Rischka, J. F. Wishart, K. Werner, D. Gabel, *Chem. Eur. J.* **2008**, *14*, 1918 and references cited therein.

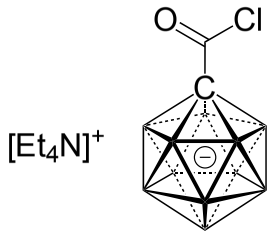
V NMR Spectra

Following on p. NMR1–NMR80

V Mass Spectra

Following on p. MS1–MS20

[Et4N][CB11H11–COCl], ca. 8mg in CD3CN *
1H{11B} NMR, 400 MHz, T = 22 C

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EXPNO                 1
PROCNO                1

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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                294.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

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

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

F2 - Processing parameters
SI                 32768
SF            400.1300560 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
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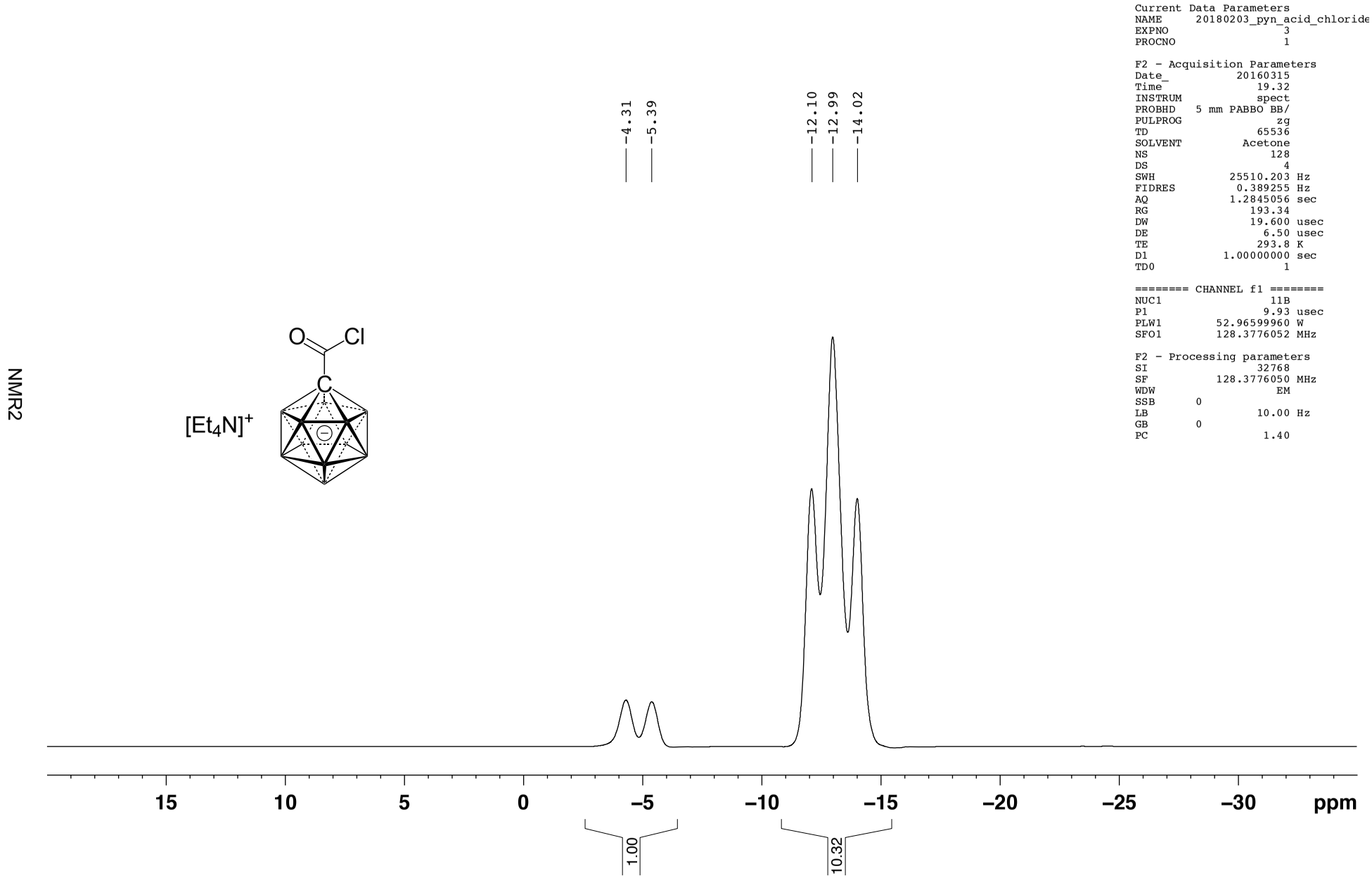
20160314_pyn-2084-0258-3 [Et4N][CB11H11-COCl], ca. 8mg in acetone-d6
11B NMR, Bruker 500MHz. T=22C

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PROCNO                1

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PULPROG             zg
TD                65536
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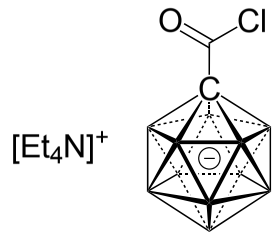
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               293.8 K
D1            1.00000000 sec
TD0                   1

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

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

[Et4N][CB11H11–COCl], ca. 8mg in CD3CN
11B{1H} NMR, 128 MHz, T = 22 C



NMR3

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PROCNO                1

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PULPROG          zgpg30
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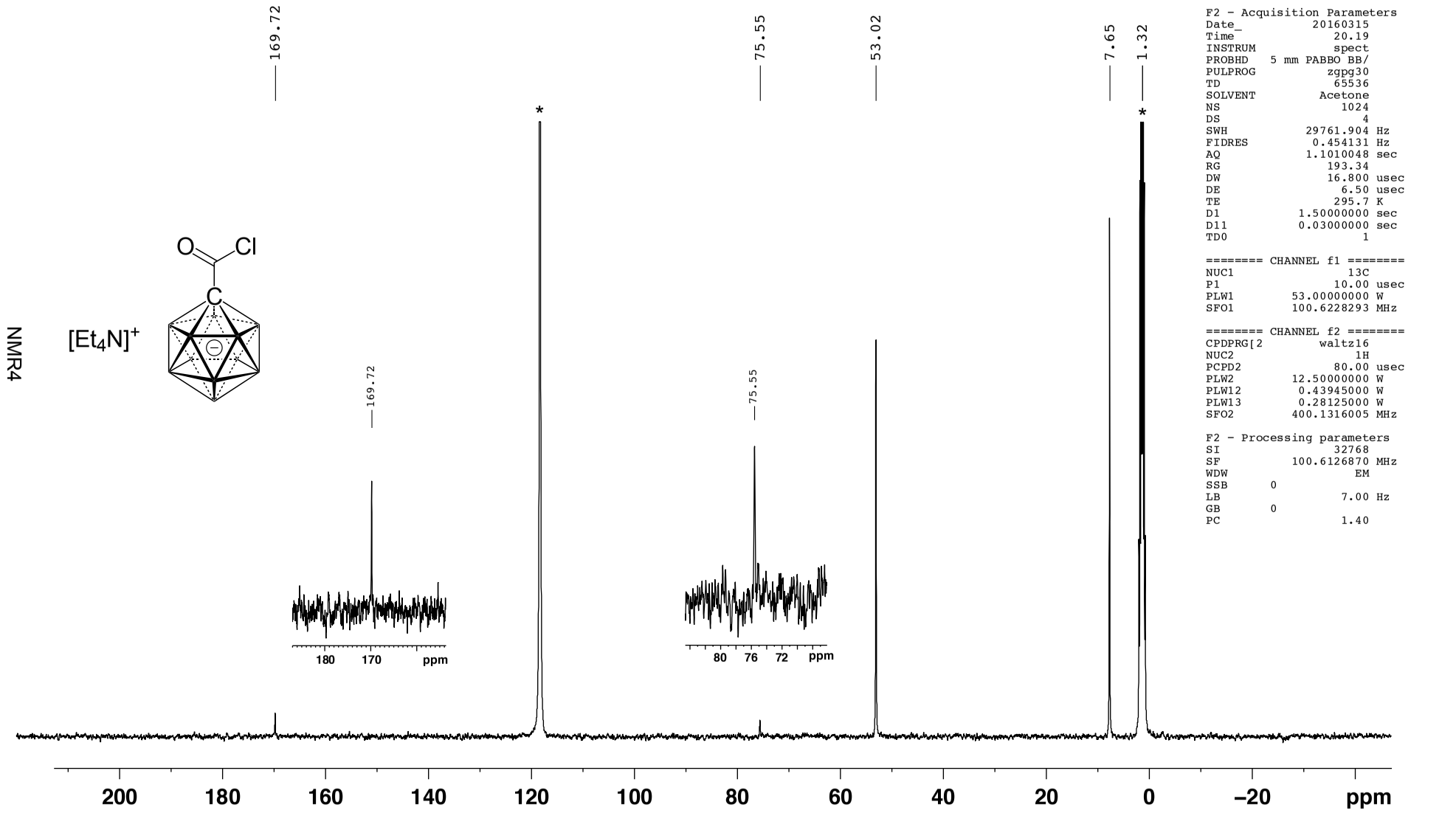
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               294.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

[Et4N][CB11H11–COCl], ca. 8mg in CD3CN*
13C{1H} NMR, 100 MHz, T = 22 C




```
Current Data Parameters
NAME      20180203_pyn_acid_chloride
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160315
Time              20.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               295.7 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

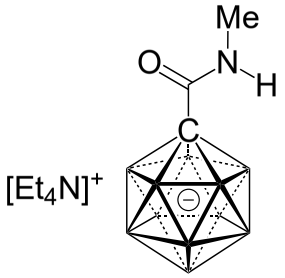
======== CHANNEL f1 ========
NUC1                 13C
P1                10.00 usec
PLW1         53.00000000 W
SFO1        100.6228293 MHz

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

F2 - Processing parameters
SI                32768
SF          100.6126870 MHz
WDW                  EM
SSB       0
LB                7.00 Hz
GB        0
PC                1.40
```

Me amide, ca. 14 mg in acetone-d6 *
1H{11B} NMR, 400 MHz, T = 22 C

NMR5




```
Current Data Parameters
NAME      20180203_20160105-pyn-Mea
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20160106
Time              15.42
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                55.74
DW              62.400 usec
DE               6.50 usec
TE              294.7 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

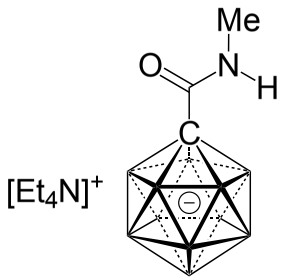
======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1         12.50000000 W
SFO1        400.1320007 MHz

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

F2 - Processing parameters
SI                32768
SF          400.1300078 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

Me amide, ca. 14 mg in acetone-d6
11B NMR, 160 MHz, T = 22 C

NMR6




```
Current Data Parameters
NAME      20180203_20160122-pyn-2-Me
EXPNO                  3
PROCNO                 1

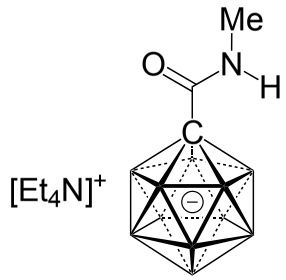
F2 - Acquisition Parameters
Date_           20160122
Time              17.50
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG              zg
TD                64098
SOLVENT            C6D6
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.500036 Hz
AQ            0.9999288 sec
RG                  203
DW               15.600 usec
DE               16.00 usec
TE               292.8 K
D1            1.00000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1               10.00 usec
PLW1        75.00000000 W
SFO1        160.4615792 MHz

F2 - Processing parameters
SI                32768
SF          160.4615993 MHz
WDW                  EM
SSB       0
LB               10.00 Hz
GB        0
PC                1.40
```

Me amide, ca. 14 mg in acetone-d6
11B{1H} NMR, 160 MHz, T = 22 C

NMR7




```
Current Data Parameters
NAME      20180203_20160122-pyn-2-Me
EXPNO                 2
PROCNO                1

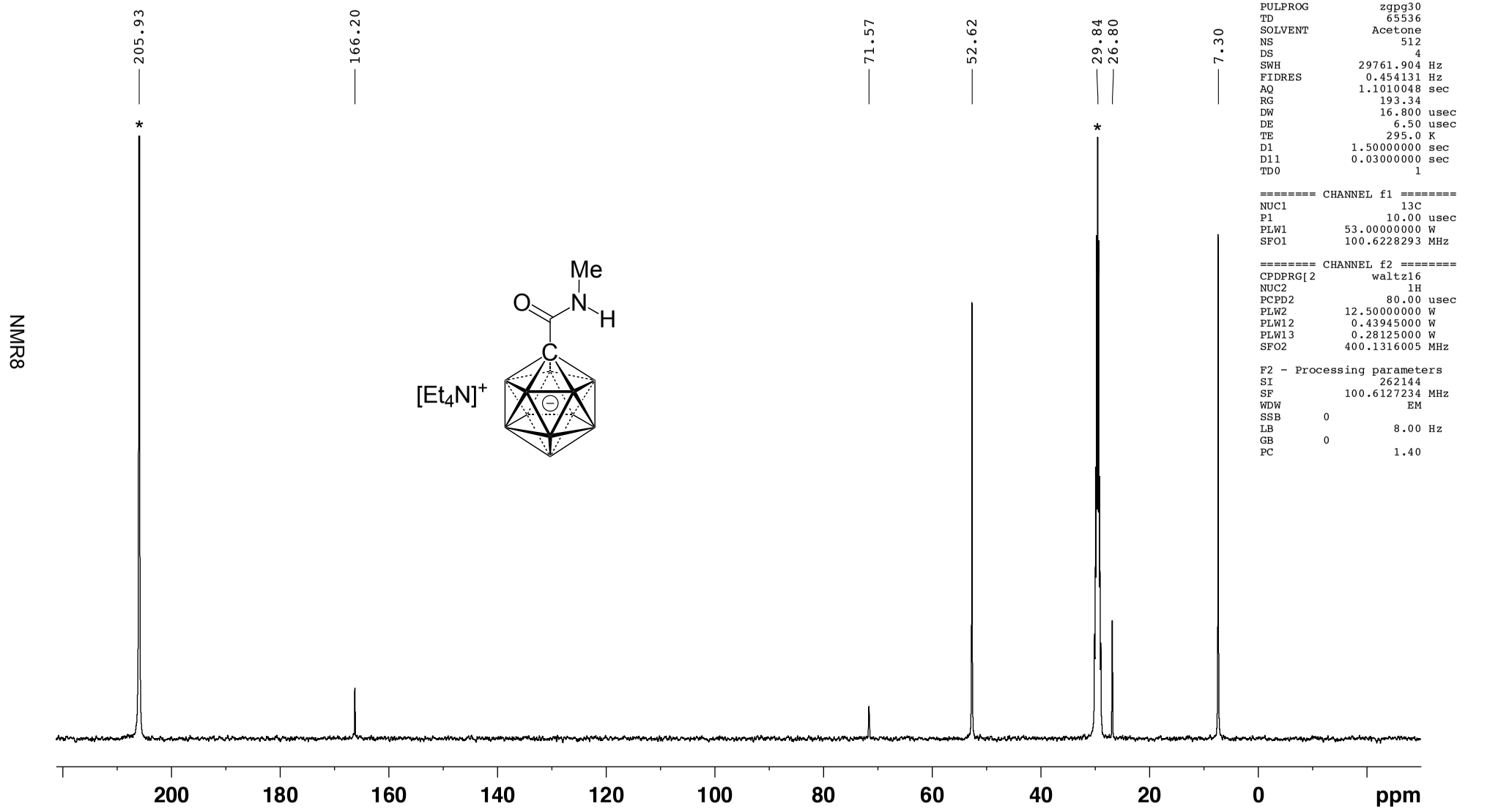
F2 - Acquisition Parameters
Date_          20160122
Time              17.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            C6D6
NS                   26
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE                293.1 K
D1           5.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                10.00 usec
PLW1        75.00000000 W
SFO1       160.4615792 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        19.00000000 W
PLW12        0.42750001 W
PLW13        0.27360001 W
SFO2       500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          160.4615993 MHz
WDW                 EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

Me amide, ca. 14 mg in acetone-d6 *
13C{1H} NMR, 101 MHz, T = 22 C




```
Current Data Parameters
NAME      20180203_20160105-pyn-Mean
EXPNO                 3
PROCNO                1

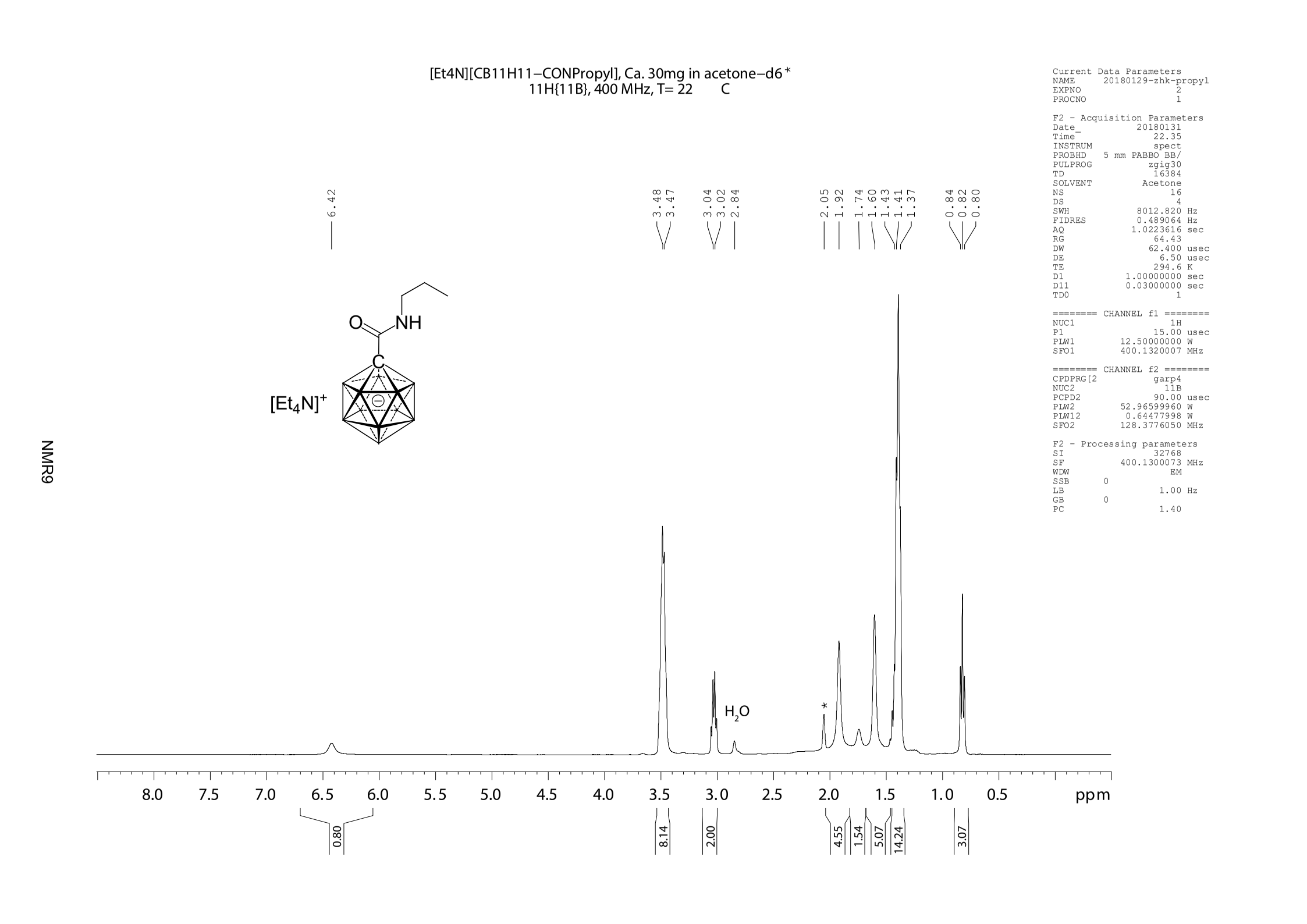
F2 - Acquisition Parameters
Date_          20160106
Time              15.40
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  512
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                295.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

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

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

F2 - Processing parameters
SI                 262144
SF          100.6127234 MHz
WDW                  EM
SSB       0
LB                 8.00 Hz
GB        0
PC                 1.40
```

[Et4N][CB11H11−CONPropyl], Ca. 30mg in acetone−d6 *
11H{11B}, 400 MHz, T= 22 C



NMR9

```
Current Data Parameters
NAME      20180129-zhk-propyl
EXPNO                       2
PROCNO                      1

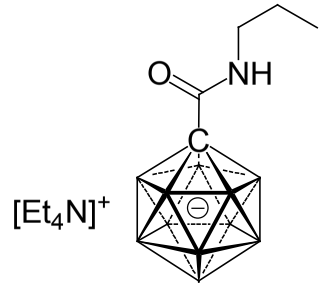
F2 - Acquisition Parameters
Date_              20180131
Time                 22.35
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH               8012.820 Hz
FIDRES               0.489064 Hz
AQ                1.0223616 sec
RG                    64.43
DW                  62.400 usec
DE                   6.50 usec
TE                  294.6 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

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

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

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

[Et4N][CB11H11-CONPropyl], Ca. 30mg in acetone-d6
11B, 128 MHz, T= 22 C



NMR10

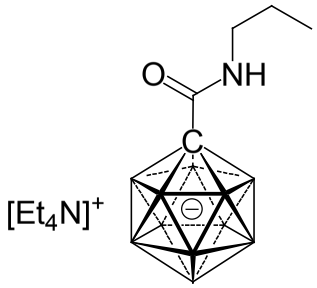
```
Current Data Parameters
NAME      20180129-zhk-propyl
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_            20180131
Time                22.41
INSTRUM             spect
PROBHD    5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                19.600 usec
DE                 6.50 usec
TE                293.9 K
D1             1.00000000 sec
TD0                     1

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

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

[Et4N][CB11H11-CONPropyl], Ca. 30mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR11


```
Current Data Parameters
NAME      20180129-zhk-propyl
EXPNO                       4
PROCNO                      1

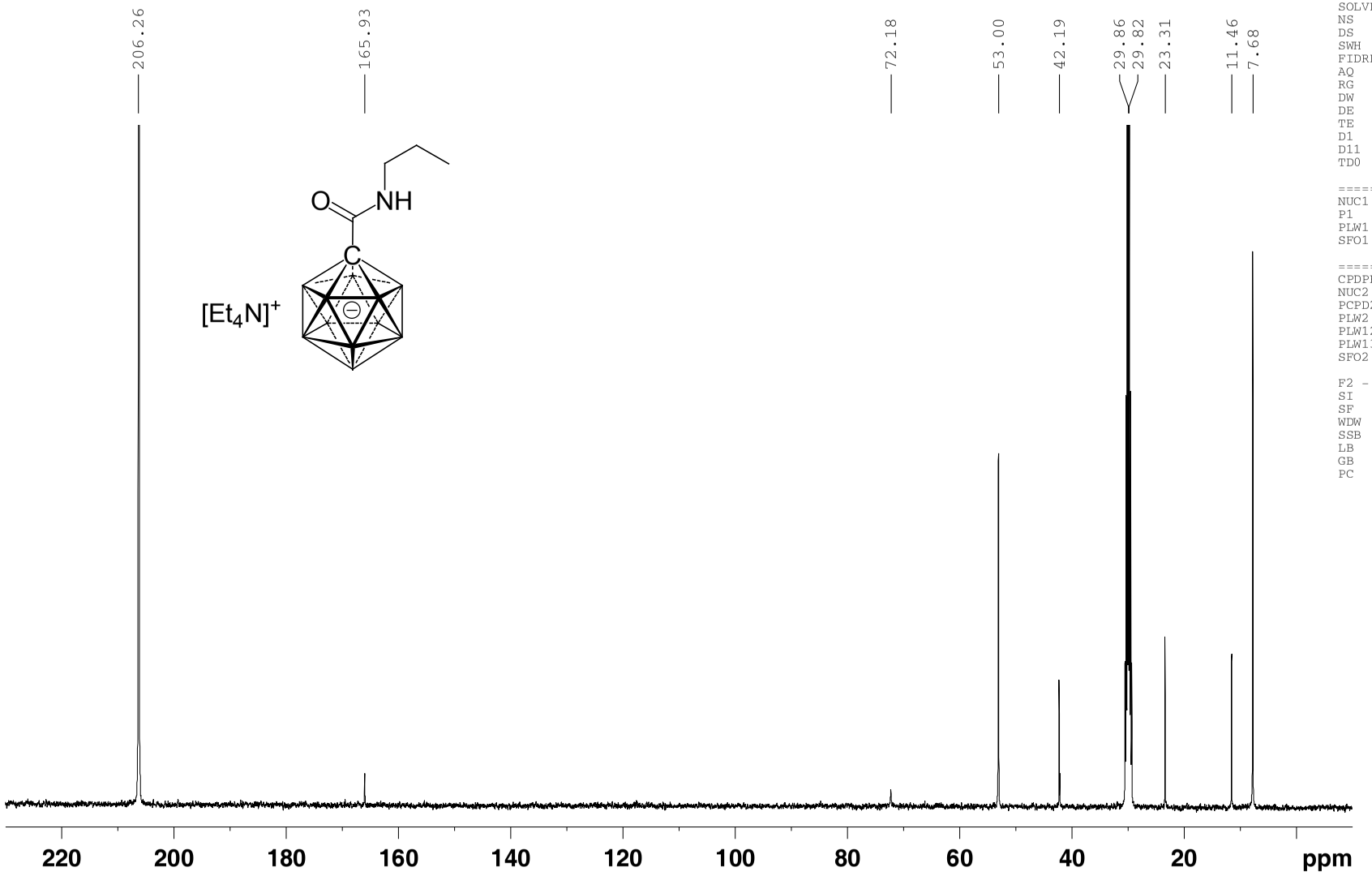
F2 - Acquisition Parameters
Date_              20180131
Time                  22.47
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   294.6 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

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

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

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

[Et4N][CB11H11−CONPropyl], Ca. 30mg in acetone−d6
13C{1H}, 100 MHz, T= 22 C



NMR12

```
Current Data Parameters
NAME      20180129-zhk-propyl
EXPNO                       5
PROCNO                      1

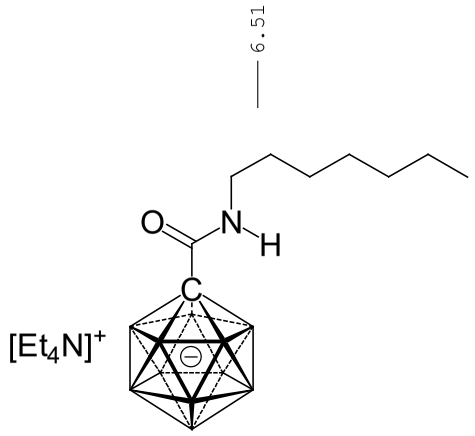
F2 - Acquisition Parameters
Date_              20180131
Time                 23.34
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                   1024
DS                      4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  295.1 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                     1

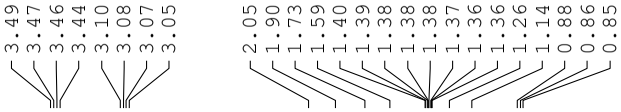
======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PLW1           53.00000000 W
SFO1          100.6228293 MHz

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

F2 - Processing parameters
SI                  32768
SF            100.6126846 MHz
WDW                    EM
SSB          0
LB                   3.00 Hz
GB           0
PC                   1.40
```

[Et4N][CB11H11–CONHC7H15], Ca. 30mg in acetone–d6 *
1H{11B}, 400 MHz, T= 22 C






```
Current Data Parameters
NAME      21080106-zhk-C7H15NH2
EXPNO                         1
PROCNO                        1

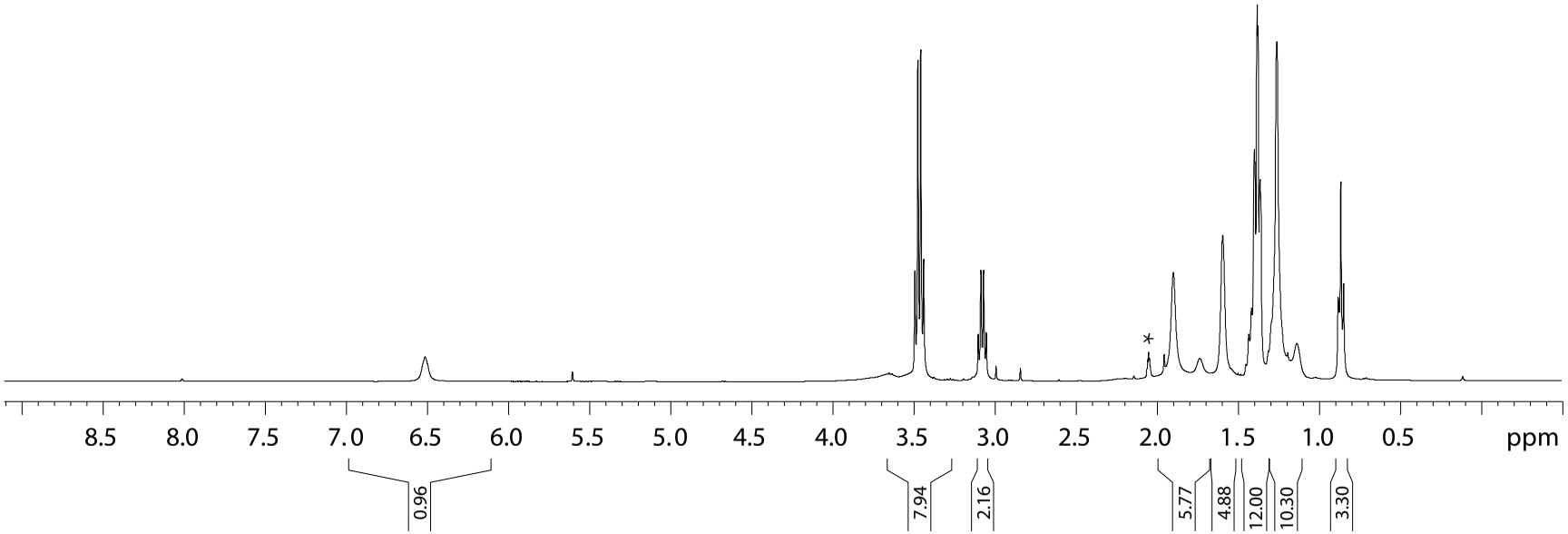
F2 - Acquisition Parameters
Date_              20180107
Time                   15.48
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT             Acetone
NS                         16
DS                          4
SWH                 8012.820 Hz
FIDRES              0.489064 Hz
AQ                 1.0223616 sec
RG                     24.52
DW                    62.400 usec
DE                     6.50 usec
TE                    294.4 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                         1

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

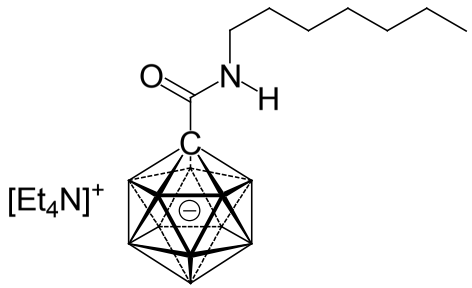
======== CHANNEL f2 ========
CPDPRG[2                garp4
NUC2                      11B
PCPD2                   90.00 usec
PLW2           52.96599960 W
PLW12           0.64477998 W
SFO2           128.3776050 MHz

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

NMR13



[Et4N][CB11H11-CONHC7H15], Ca. 30mg in acetone-d6
11B, 128 MHz, T= 22 C



NMR14

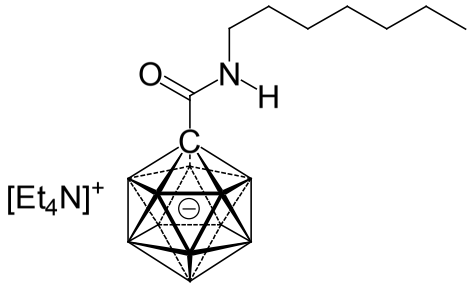
```
Current Data Parameters
NAME      21080106-zhk-C7H15NH2
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_              20180107
Time                  16.00
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   293.8 K
D1             1.00000000 sec
TD0                        1

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

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

[Et4N][CB11H11-CONHC7H15], Ca. 30mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR15


```
Current Data Parameters
NAME      21080106-zhk-C7H15NH2
EXPNO                         2
PROCNO                        1

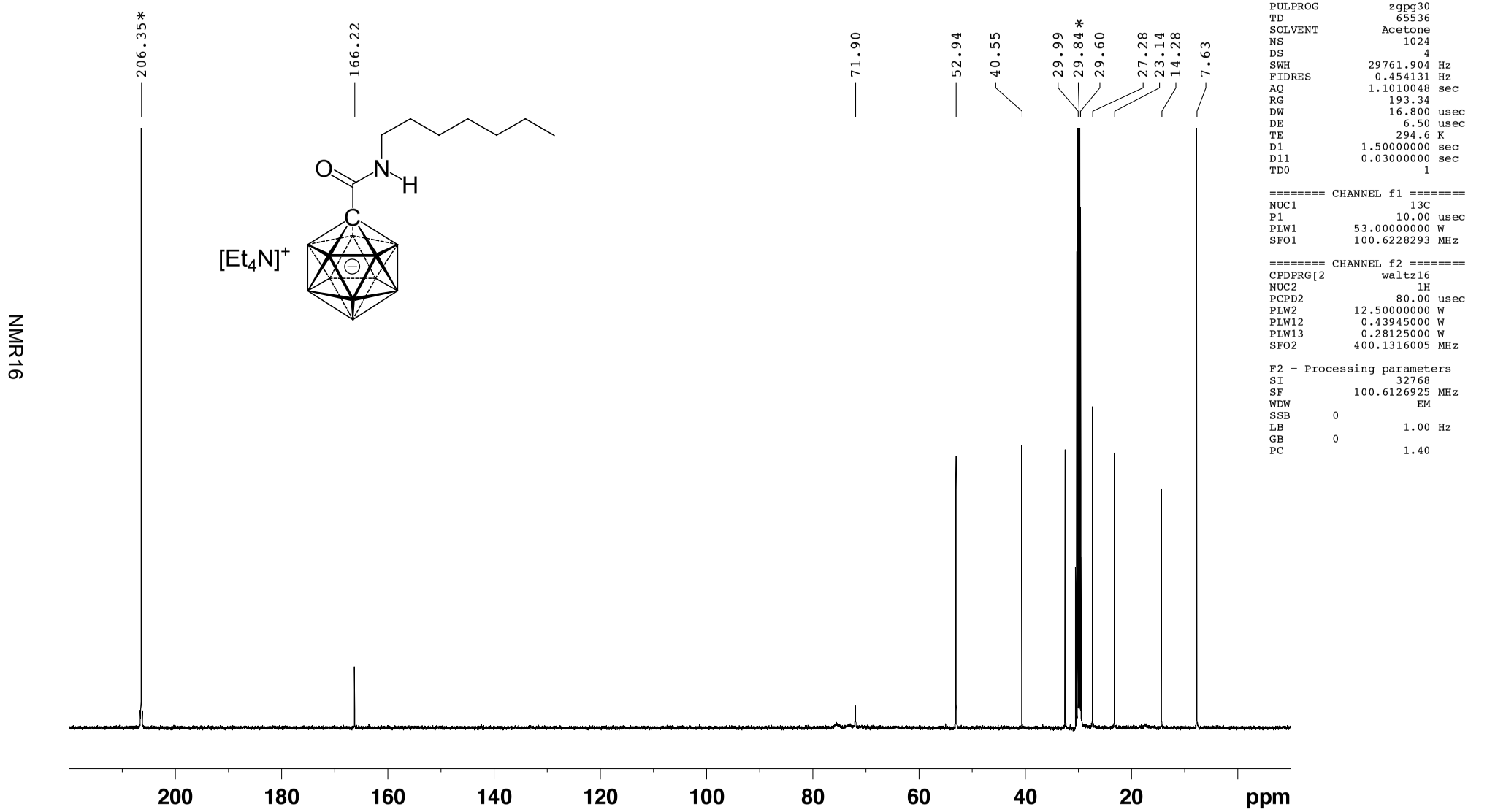
F2 - Acquisition Parameters
Date_              20180107
Time                   15.54
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT              Acetone
NS                         128
DS                           4
SWH                25510.203 Hz
FIDRES             0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    294.7 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                          1

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

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

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

[Et4N][CB11H11–CONHC7H15], Ca. 30mg in acetone–d6*
13C{1H}, 100 MHz, T= 22 C



NMR16

```
Current Data Parameters
NAME      21080106-zhk-C7H15NH2
EXPNO                         4
PROCNO                        1

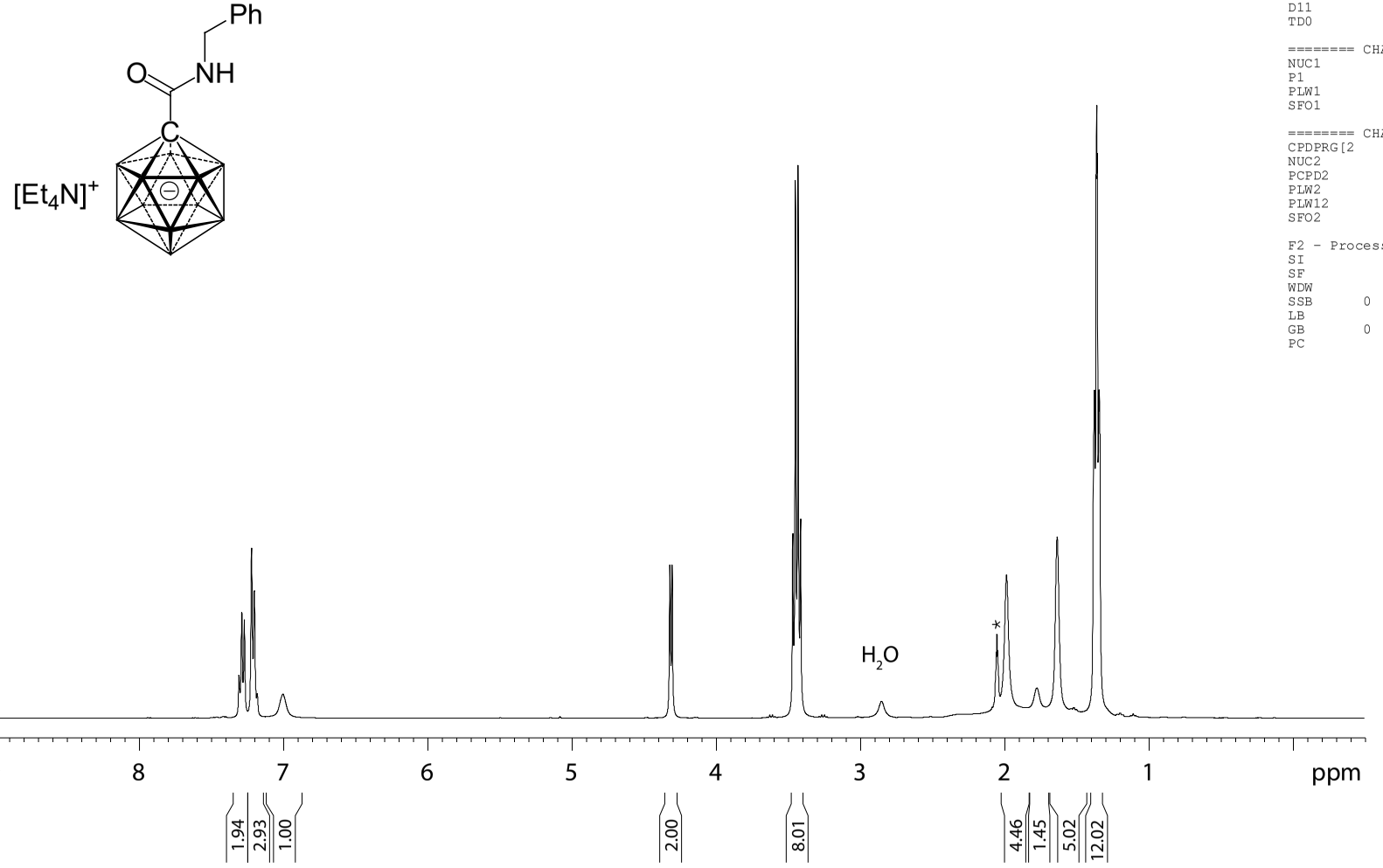
F2 - Acquisition Parameters
Date_              20180107
Time                  16.47
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1024
DS                       4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                    193.34
DW                   16.800 usec
DE                    6.50 usec
TE                   294.6 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                    32768
SF            100.6126925 MHz
WDW                     EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

[Et4N][CB11H11–CONHBn], Ca. 20mg in acetone–d6 *
11H{11B}, 400 MHz, T= 22 C



NMR17

```
Current Data Parameters
NAME      20180119-zhk-benzyl
EXPNO                       2
PROCNO                      1

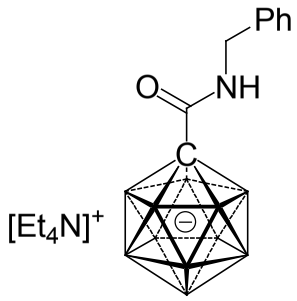
F2 - Acquisition Parameters
Date_              20180120
Time                  14.59
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT             Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                    1.0223616 sec
RG                       78.69
DW                    62.400 usec
DE                     6.50 usec
TE                     294.9 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                          1

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

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

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

[Et4N][CB11H11-CONHBn], Ca. 20mg in acetone-d6
11B, 128 MHz, T= 22 C



NMR18

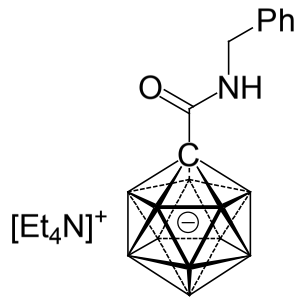
```
Current Data Parameters
NAME      20180119-zhk-benzyl
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180120
Time                  15.05
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                   294.5 K
D1              1.00000000 sec
TD0                        1

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

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

[Et4N][CB11H11-CONHBn], Ca. 20mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR19


```
Current Data Parameters
NAME      20180119-zhk-benzyl
EXPNO                       4
PROCNO                      1

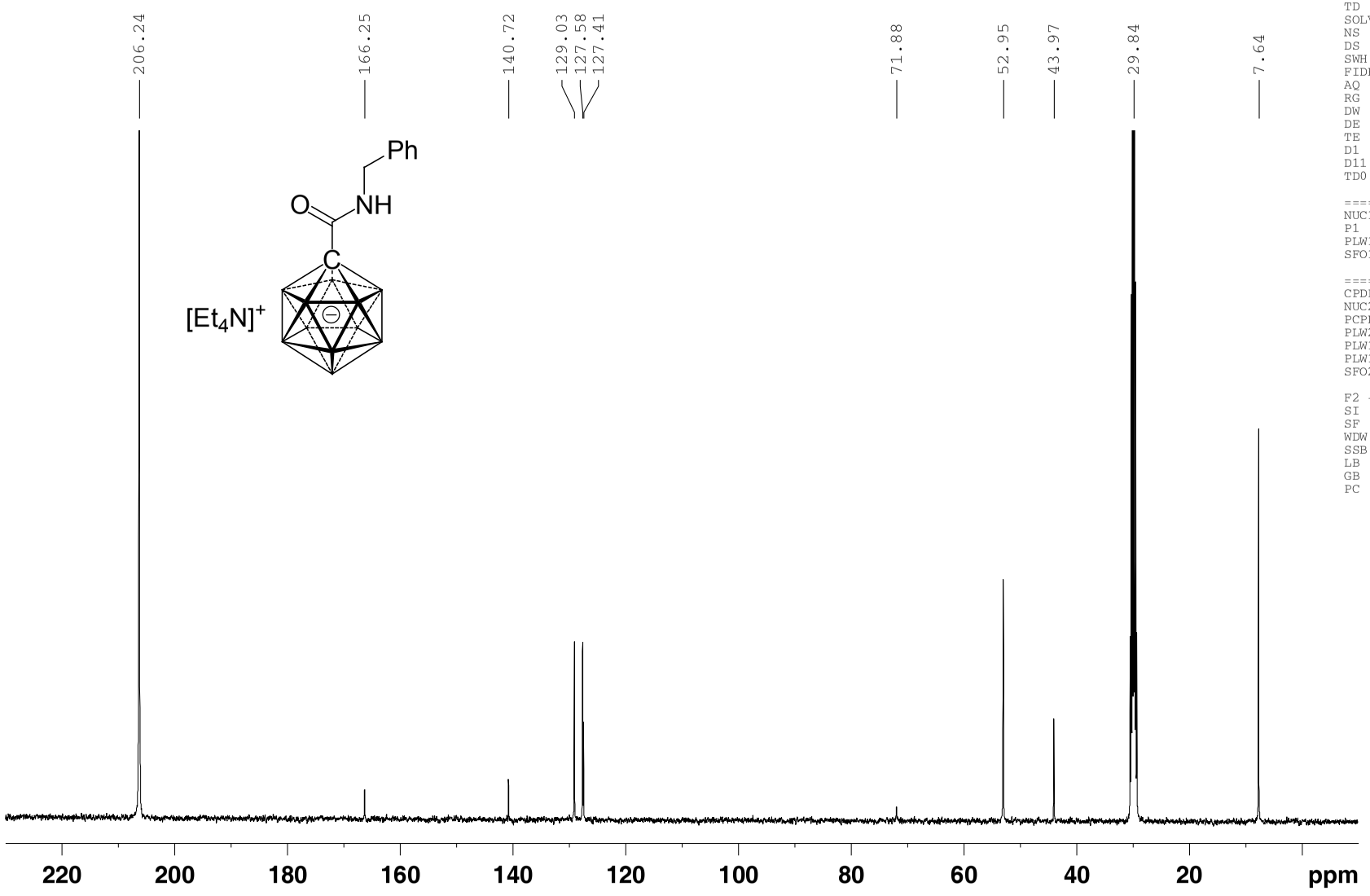
F2 - Acquisition Parameters
Date_              20180120
Time                  15.11
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    295.3 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

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

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

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

[Et4N][CB11H11-CONHBn], Ca. 20mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C



NMR20

```
Current Data Parameters
NAME      20180119-zhk-benzyl
EXPNO                      5
PROCNO                     1

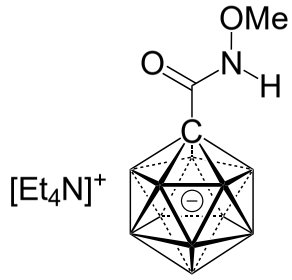
F2 - Acquisition Parameters
Date_              20180120
Time                  15.35
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                     512
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  295.4 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   32768
SF           100.6126854 MHz
WDW                     EM
SSB       0
LB                   4.00 Hz
GB        0
PC                   1.40
```

OMe amide, ca. 24 mg in CD3CN *
1H{11B} NMR, 500 MHz, T = 22 C



NMR21


```
Current Data Parameters
NAME      20180203_pyn_OMe amide_201
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20150127
Time              17.56
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgig30
TD                65536
SOLVENT           CD3CN
NS                   16
DS                    0
SWH           14097.744 Hz
FIDRES         0.215115 Hz
AQ             2.3243434 sec
RG                 50.8
DW               35.467 usec
DE                6.50 usec
TE               296.0 K
D1            5.00000000 sec
D11           0.03000000 sec

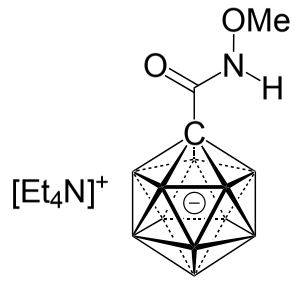
======== CHANNEL f1 ========
NUC1                  1H
P1                12.00 usec
PLW1         19.00000000 W
SFO1         500.1310003 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 11B
PCPD2             60.00 usec
PLW2         75.00000000 W
PLW12         2.08330011 W
SFO2         160.4615690 MHz

F2 - Processing parameters
SI                65536
SF           500.1300156 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                1.00
```

NMR22

OMe amide, ca. 24 mg in CD3CN
11B NMR, 160 MHz, T = 22 C




```
Current Data Parameters
NAME      20180203_pyn_OMe amide_201
EXPNO                 3
PROCNO                1

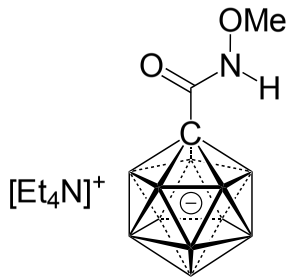
F2 - Acquisition Parameters
Date_           20150127
Time              17.59
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG              zg
TD                64098
SOLVENT           CD3CN
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.500036 Hz
AQ            0.9999288 sec
RG                  203
DW               15.600 usec
DE                16.00 usec
TE                295.9 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                10.00 usec
PLW1        75.00000000 W
SFO1        160.4615792 MHz

F2 - Processing parameters
SI                32768
SF          160.4615993 MHz
WDW                  EM
SSB       0
LB              10.00 Hz
GB        0
PC                 1.40
```

NMR23

OMe amide, ca. 24 mg in CD3CN
11B NMR, 160 MHz, T = 22 C




```
Current Data Parameters
NAME      20180203_pyn_OMe amide_201
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_           20150127
Time              18.03
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CD3CN
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               295.9 K
D1           2.00000000 sec
D11          0.03000000 sec

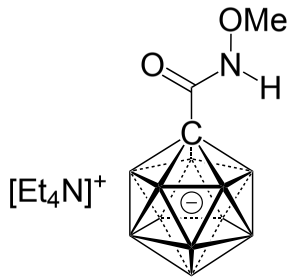
======== CHANNEL f1 ========
NUC1                11B
P1                10.00 usec
PLW1        75.00000000 W
SFO1       160.4615792 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2        19.00000000 W
PLW12        0.42750001 W
PLW13        0.27360001 W
SFO2       500.1330885 MHz

F2 - Processing parameters
SI                32768
SF          160.4615993 MHz
WDW                 EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

OMe amide, ca. 24 mg in CD3CN*
13C{1H} NMR, 101 MHz, T = 22 C

NMR24




```
Current Data Parameters
NAME     20180203_pyn_OMe amide_201
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_           20150128
Time              3.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CD3CN
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                295.6 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

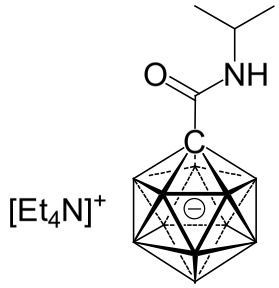
======== CHANNEL f1 ========
NUC1                 13C
P1                 10.00 usec
PLW1        53.00000000 W
SFO1        100.6228293 MHz

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

F2 - Processing parameters
SI                32768
SF          100.6126733 MHz
WDW                  EM
SSB       0
LB                 8.00 Hz
GB        0
PC                 1.40
```

[Et4N][CB11H11−CONHisopropyl], Ca. 30mg in acetone−d6 *
11H{11B}, 400 MHz, T= 22 C

NMR25




```
Current Data Parameters
NAME      20180129-zhk-isopropyl
EXPNO                          2
PROCNO                         1

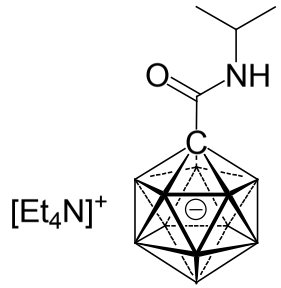
F2 - Acquisition Parameters
Date_              20180131
Time                  23.41
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                    64.43
DW                    62.400 usec
DE                     6.50 usec
TE                    294.2 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                        1

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

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

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

[Et4N][CB11H11–CONHisopropyl], Ca. 30mg in acetone–d6
11B, 128 MHz, T= 22 C



NMR26

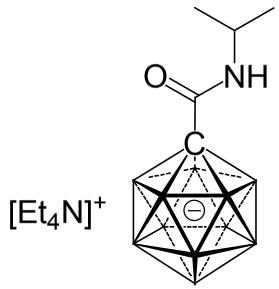
```
Current Data Parameters
NAME      20180129-zhk-isopropyl
EXPNO                          3
PROCNO                         1

F2 - Acquisition Parameters
Date_               20180131
Time                   23.46
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                     294.1 K
D1                1.00000000 sec
TD0                          1

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

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

[Et4N][CB11H11–CONHisopropyl], Ca. 30mg in acetone–d6
11B{1H}, 128 MHz, T= 22 C



NMR27

```
Current Data Parameters
NAME      20180129-zhk-isopropyl
EXPNO                          4
PROCNO                         1

F2 - Acquisition Parameters
Date_               20180131
Time                   23.53
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zgpg30
TD                     65536
SOLVENT              Acetone
NS                         128
DS                           4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    294.9 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                          1

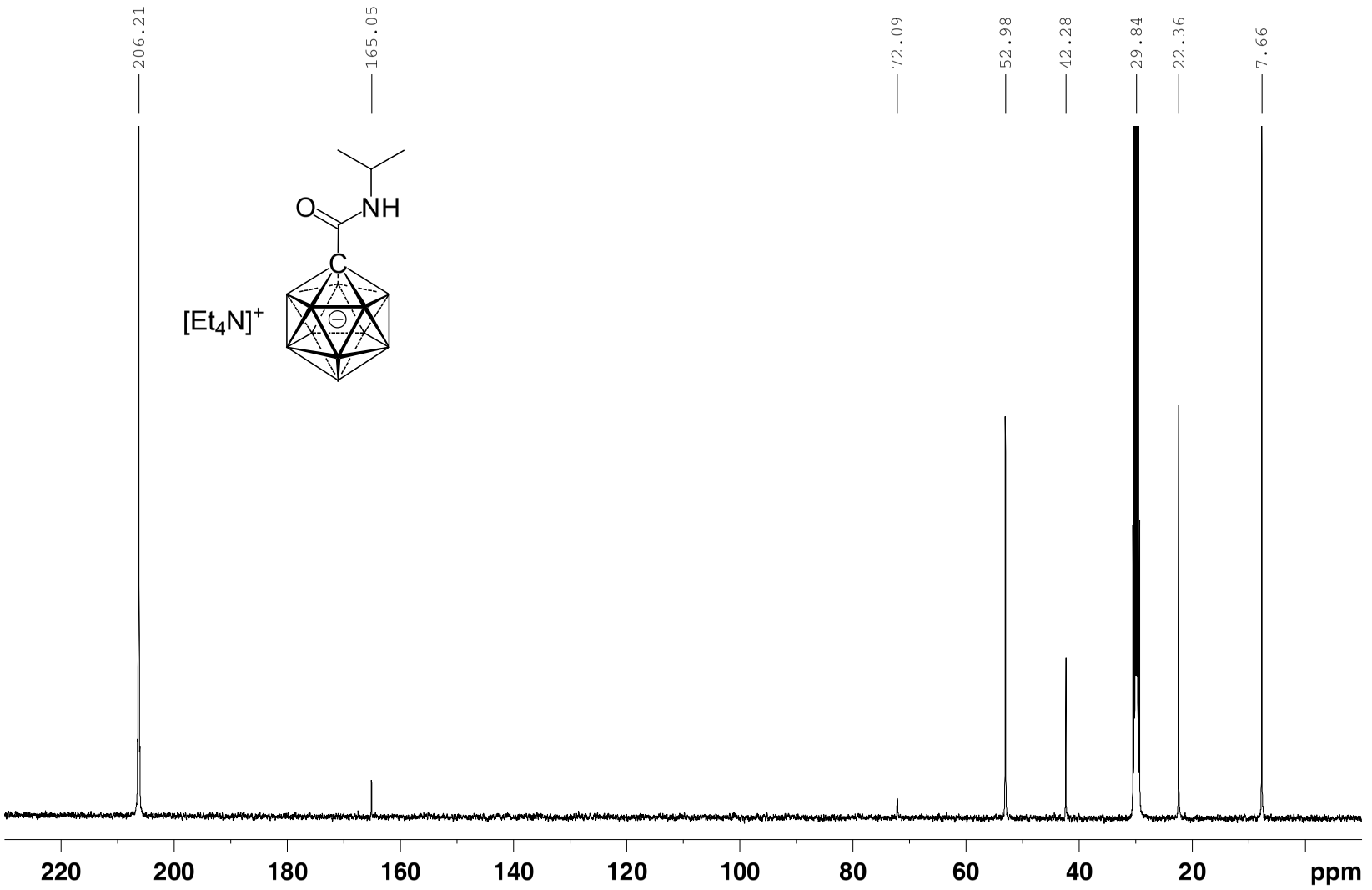
======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1              52.96599960 W
SFO1             128.3776050 MHz

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

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

[Et4N][CB11H11–CONHisopropyl], Ca. 30mg in acetone–d6
13C{1H}, 100 MHz, T= 22 C

NMR28




```
Current Data Parameters
NAME      20180129-zhk-isopropyl
EXPNO                          5
PROCNO                         1

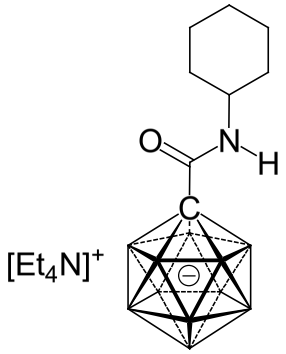
F2 - Acquisition Parameters
Date_                   20180201
Time                        0.39
INSTRUM                    spect
PROBHD    5 mm PABBO BB/
PULPROG                   zgpg30
TD                         65536
SOLVENT                  Acetone
NS                          1024
DS                             4
SWH                    29761.904 Hz
FIDRES                  0.454131 Hz
AQ                     1.1010048 sec
RG                        193.34
DW                        16.800 usec
DE                         6.50 usec
TE                        295.0 K
D1                   1.50000000 sec
D11                  0.03000000 sec
TD0                            1

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

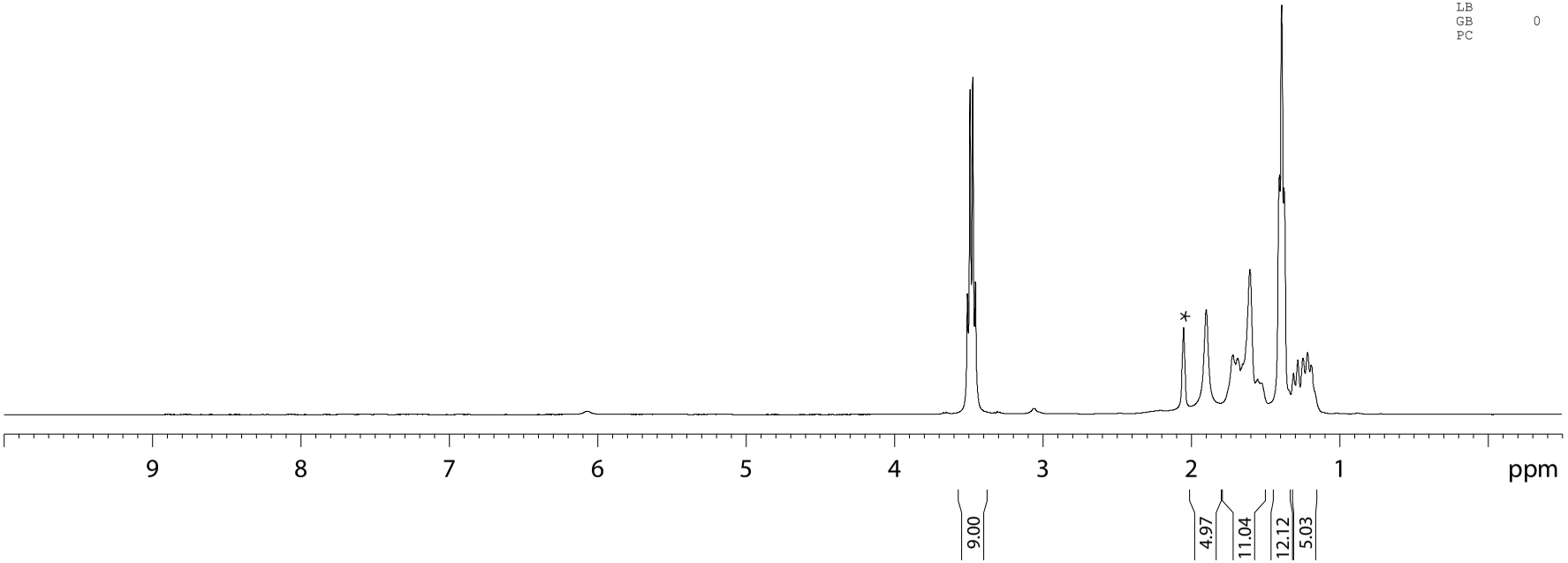
======== CHANNEL f2 ========
CPDPRG[2                waltz16
NUC2                         1H
PCPD2                     80.00 usec
PLW2                12.50000000 W
PLW12                0.43945000 W
PLW13                0.28125000 W
SFO2               400.1316005 MHz

F2 - Processing parameters
SI                         32768
SF                 100.6126858 MHz
WDW                           EM
SSB       0
LB                         3.00 Hz
GB        0
PC                         1.40
```

[Et4N][CB11H11–CONHCyclohex], Ca. 20mg in acetone–d6 *
11H{11B}, 400 MHz, T= 22 C



NMR29




```
Current Data Parameters
NAME      20180110-zhk-cyclohex
EXPNO                         1
PROCNO                        1

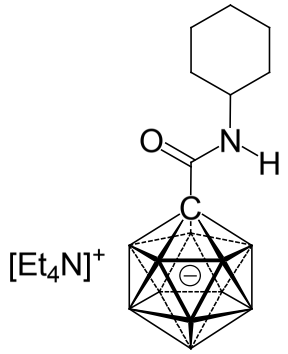
F2 - Acquisition Parameters
Date_              20180111
Time                   22.15
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT           Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES            0.489064 Hz
AQ                1.0223616 sec
RG                    52.99
DW                   62.400 usec
DE                    6.50 usec
TE                   293.7 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                       1

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

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

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

[Et4N][CB11H11-CONHCyclohex], Ca. 20mg in acetone-d6
11B, 128 MHz, T= 22 C



-6.56
-7.60
-12.59
-13.68
-14.88

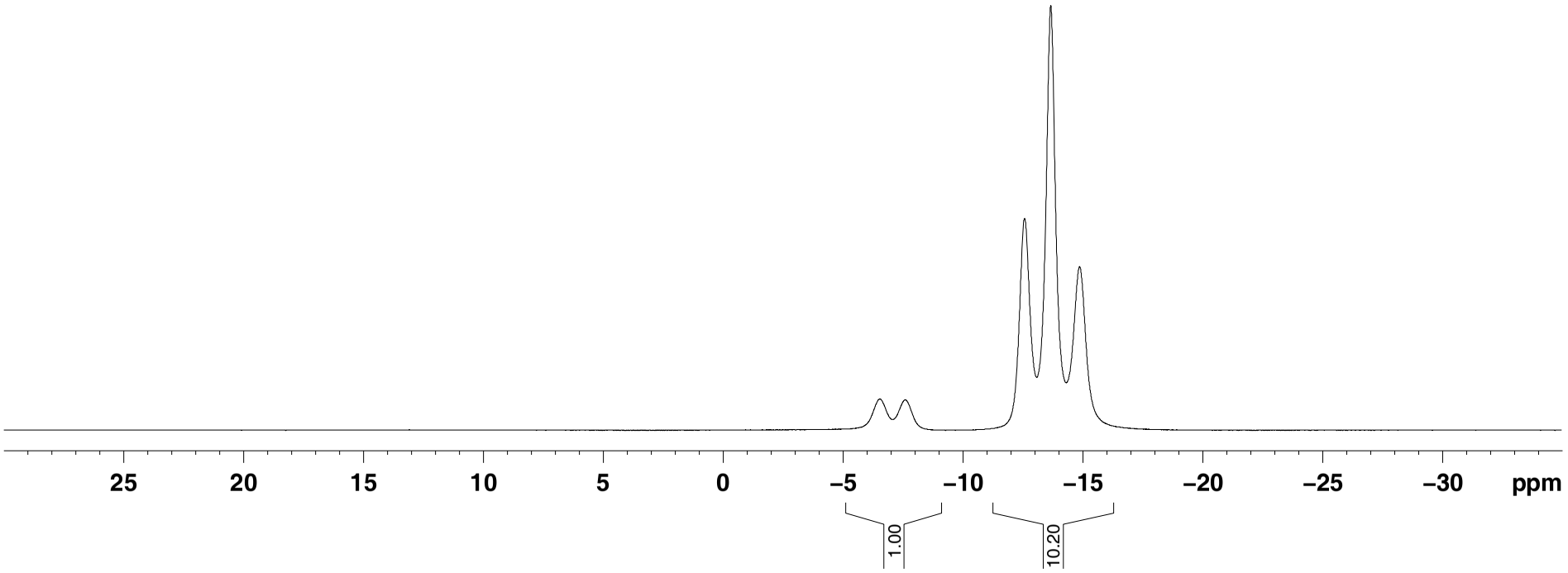
```
Current Data Parameters
NAME      20180110-zhk-cyclohex
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_              20180111
Time                   22.27
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                    293.9 K
D1              1.00000000 sec
TD0                          1

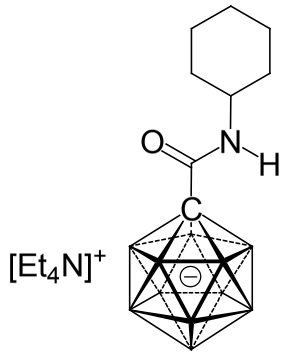
======== CHANNEL f1 ========
NUC1                       11B
P1                        9.93 usec
PLW1              52.96599960 W
SFO1             128.3776052 MHz

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

NMR30



[Et4N][CB11H11-CONHCyclohex], Ca. 20mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR31

```
Current Data Parameters
NAME      20180110-zhk-cyclohex
EXPNO                         2
PROCNO                        1

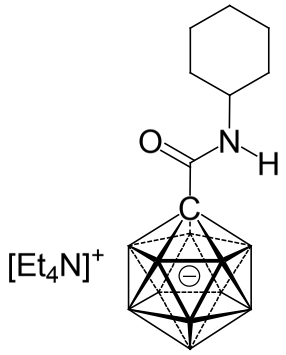
F2 - Acquisition Parameters
Date_              20180111
Time                  22.22
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT             Acetone
NS                      128
DS                        4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   294.4 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                       1

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

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

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

[Et4N][CB11H11-CONHCyclohex], Ca. 20mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C



NMR32

```
Current Data Parameters
NAME      20180110-zhk-cyclohex
EXPNO                         4
PROCNO                        1

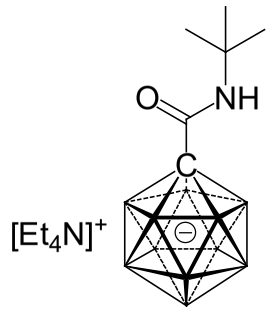
F2 - Acquisition Parameters
Date_              20180111
Time                  23.14
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1024
DS                       4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                1.1010048 sec
RG                   193.34
DW                   16.800 usec
DE                    6.50 usec
TE                   294.3 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

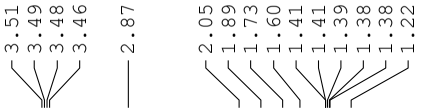
======== CHANNEL f1 ========
NUC1                    13C
P1                    10.00 usec
PLW1          53.00000000 W
SFO1          100.6228293 MHz

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

F2 - Processing parameters
SI                   32768
SF            100.6126863 MHz
WDW                     EM
SSB       0
LB                    3.00 Hz
GB        0
PC                    1.40
```

[Et4N][CB11H11–CONHtBu], Ca. 20mg in acetone–d6 *
11H{11B}, 400 MHz, T= 22 C





NMR33

```
Current Data Parameters
NAME      20180119-zhk-t-butyl
EXPNO                        2
PROCNO                       1

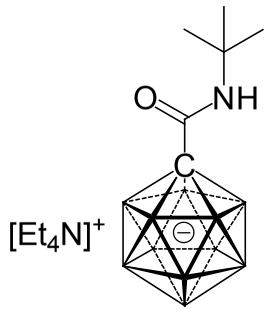
F2 - Acquisition Parameters
Date_              20180120
Time                  14.16
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES            0.489064 Hz
AQ                1.0223616 sec
RG                    64.43
DW                   62.400 usec
DE                    6.50 usec
TE                   294.8 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

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

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

F2 - Processing parameters
SI                     32768
SF             400.1300075 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

[Et4N][CB11H11-CONHtBu], Ca. 20mg in acetone-d6
11B, 128 MHz, T= 22 C



NMR34

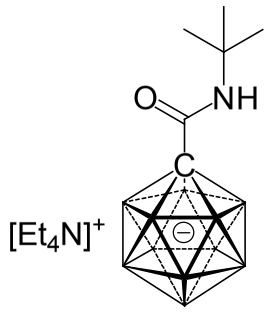
```
Current Data Parameters
NAME      20180119-zhk-t-butyl
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180120
Time                  14.22
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                 zg
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                    19.600 usec
DE                     6.50 usec
TE                    295.0 K
D1              1.00000000 sec
TD0                        1

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

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

[Et4N][CB11H11-CONHtBu], Ca. 20mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR35

```
Current Data Parameters
NAME      20180119-zhk-t-butyl
EXPNO                        4
PROCNO                       1

F2 - Acquisition Parameters
Date_              20180120
Time                  14.28
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       128
DS                         4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   295.6 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

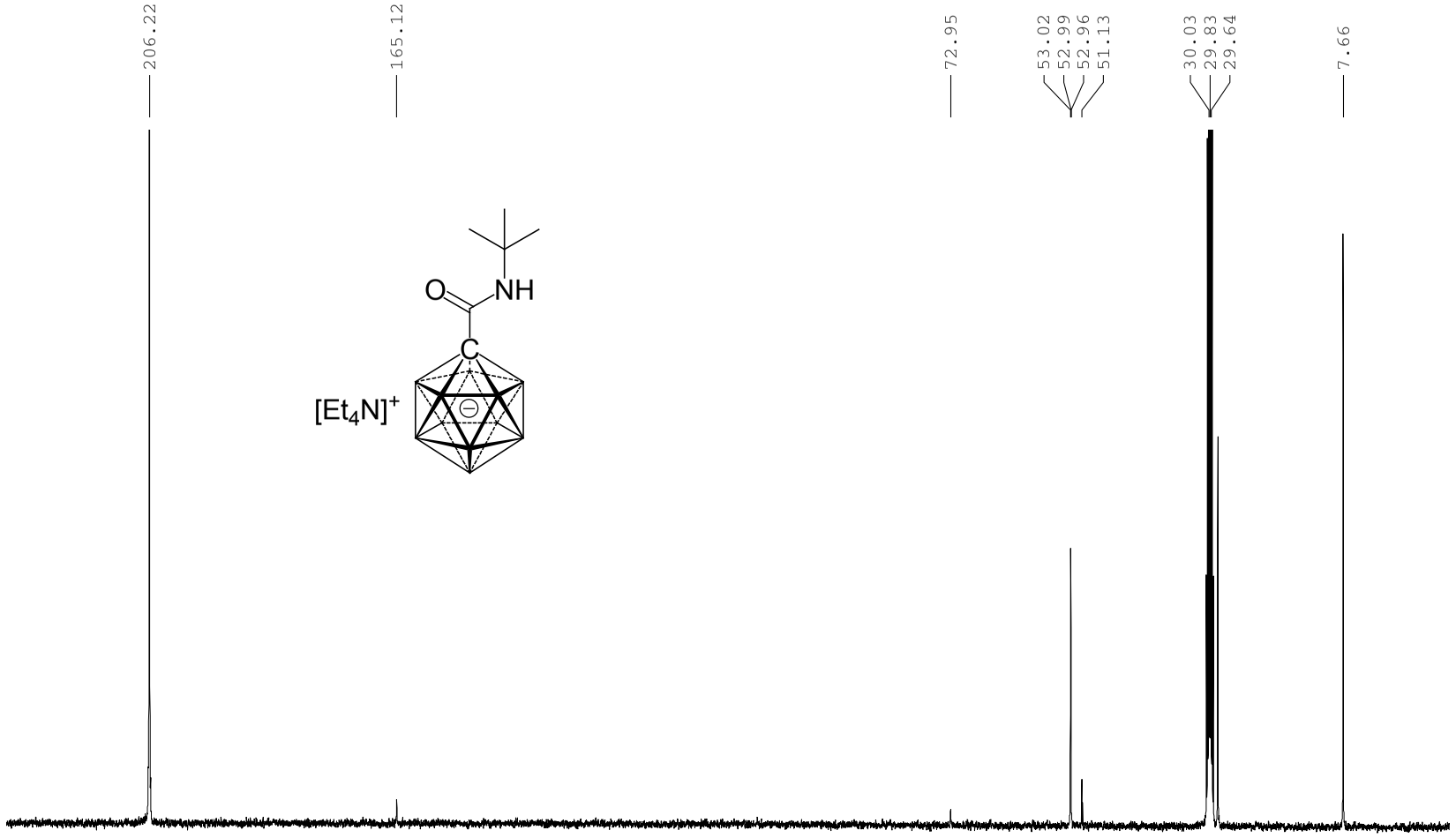
======== CHANNEL f1 ========
NUC1                     11B
P1                      9.93 usec
PLW1           52.96599960 W
SFO1          128.3776050 MHz

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

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

[Et4N][CB11H11-CONHtBu], Ca. 20mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C

NMR36




```
Current Data Parameters
NAME      20180119-zhk-t-butyl
EXPNO                        5
PROCNO                       1

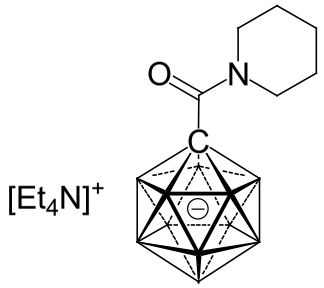
F2 - Acquisition Parameters
Date_              20180120
Time                  14.53
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       512
DS                         4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                    193.34
DW                    16.800 usec
DE                     6.50 usec
TE                    295.5 K
D1              1.50000000 sec
D11             0.03000000 sec
TD0                        1

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

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

F2 - Processing parameters
SI                       32768
SF             100.6126855 MHz
WDW                         EM
SSB          0
LB                      2.00 Hz
GB           0
PC                      1.40
```

[Et4N][CB11H11–CONPip], Ca. 30mg in acetone–d6 *
1H{11B}, 400 MHz, T= 22 C



NMR37


```
Current Data Parameters
NAME      20171214-zhk-C5H11N
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20171216
Time                  22.42
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                    71.39
DW                  62.400 usec
DE                    6.50 usec
TE                   296.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                        1

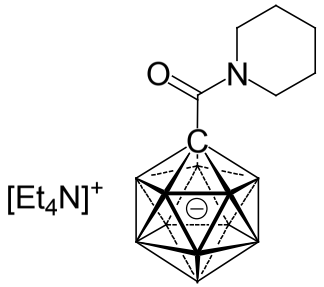
======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1           12.50000000 W
SFO1           400.1320007 MHz

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

F2 - Processing parameters
SI                        32768
SF             400.1300093 MHz
WDW                          EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

[Et4N][CB11H11-CONPip], Ca. 30mg in acetone-d6
11B, 128 MHz, T= 22 C

NMR38



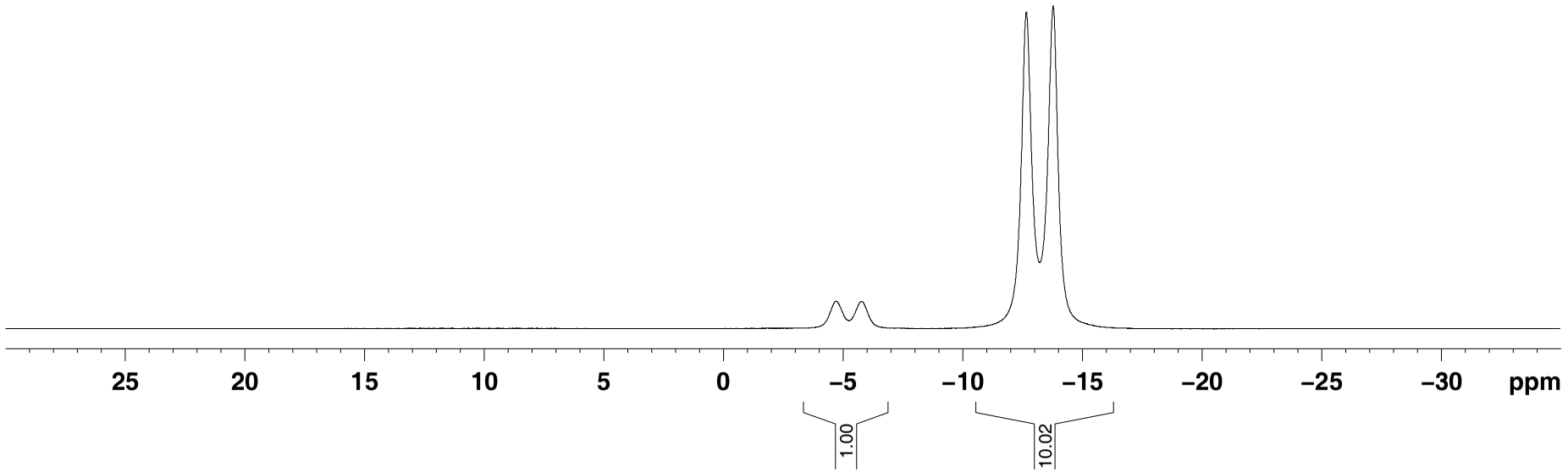
-4.73
-5.78
-12.68
-13.80

```
Current Data Parameters
NAME      20171214-zhk-C5H11N
EXPNO                      2
PROCNO                     1

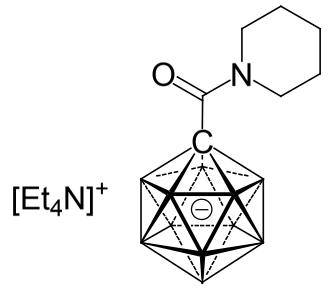
F2 - Acquisition Parameters
Date_            20171216
Time                22.47
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 295.5 K
D1              1.00000000 sec
TD0                    1

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

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



[Et4N][CB11H11-CONPip], Ca. 30mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR39


```
Current Data Parameters
NAME      20171214-zhk-C5H11N
EXPNO                      3
PROCNO                     1

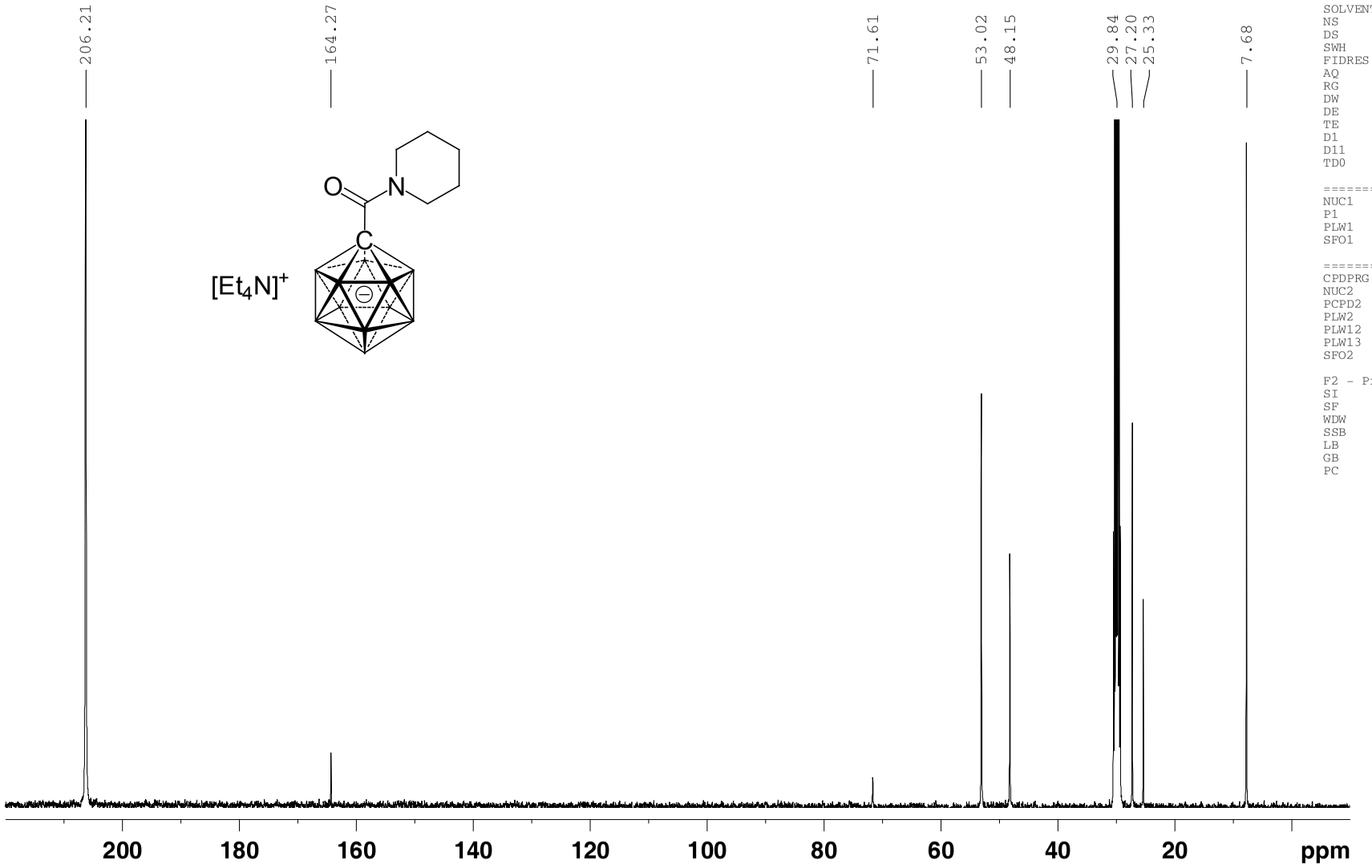
F2 - Acquisition Parameters
Date_            20171216
Time                22.54
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 296.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     1

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

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

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

[Et4N][CB11H11-CONPip], Ca. 30mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C



NMR40

```
Current Data Parameters
NAME      20171214-zhk-C5H11N
EXPNO                      4
PROCNO                     1

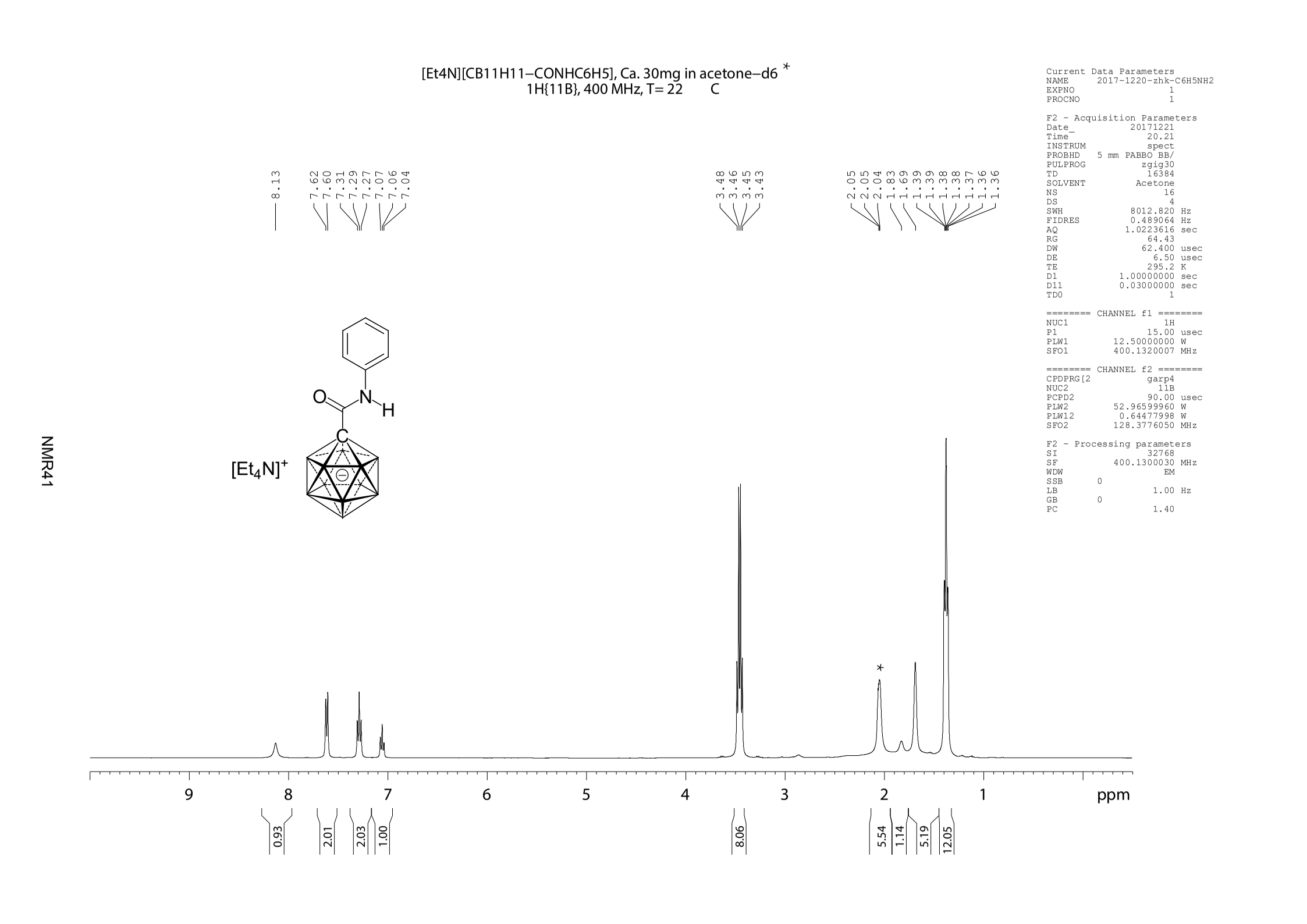
F2 - Acquisition Parameters
Date_              20171216
Time                  23.40
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                 296.3 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   32768
SF           100.6126835 MHz
WDW                     EM
SSB       0
LB                   3.00 Hz
GB        0
PC                   1.40
```

[Et4N][CB11H11–CONHC6H5], Ca. 30mg in acetone–d6 *
1H{11B}, 400 MHz, T= 22 C



NMR41

```
Current Data Parameters
NAME      2017-1220-zhk-C6H5NH2
EXPNO                        1
PROCNO                       1

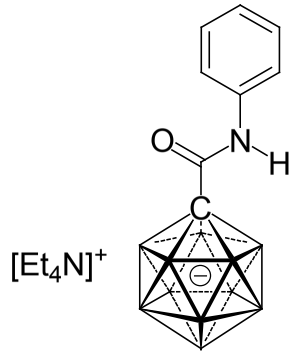
F2 - Acquisition Parameters
Date_              20171221
Time                  20.21
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT           Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                    64.43
DW                    62.400 usec
DE                     6.50 usec
TE                    295.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                       1

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

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

F2 - Processing parameters
SI                    32768
SF             400.1300030 MHz
WDW                      EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

[Et4N][CB11H11-CONHC6H5], Ca. 30mg in acetone-d6
11B, 128 MHz, T= 22 C



NMR42

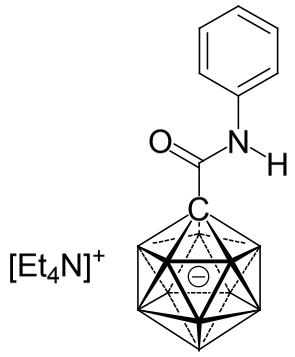
```
Current Data Parameters
NAME      2017-1220-zhk-C6H5NH2
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171221
Time                  20.33
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                   294.3 K
D1              1.00000000 sec
TD0                        1

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

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

[Et4N][CB11H11-CONHC6H5], Ca. 30mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C



NMR43

```
Current Data Parameters
NAME      2017-1220-zhk-C6H5NH2
EXPNO                        2
PROCNO                       1

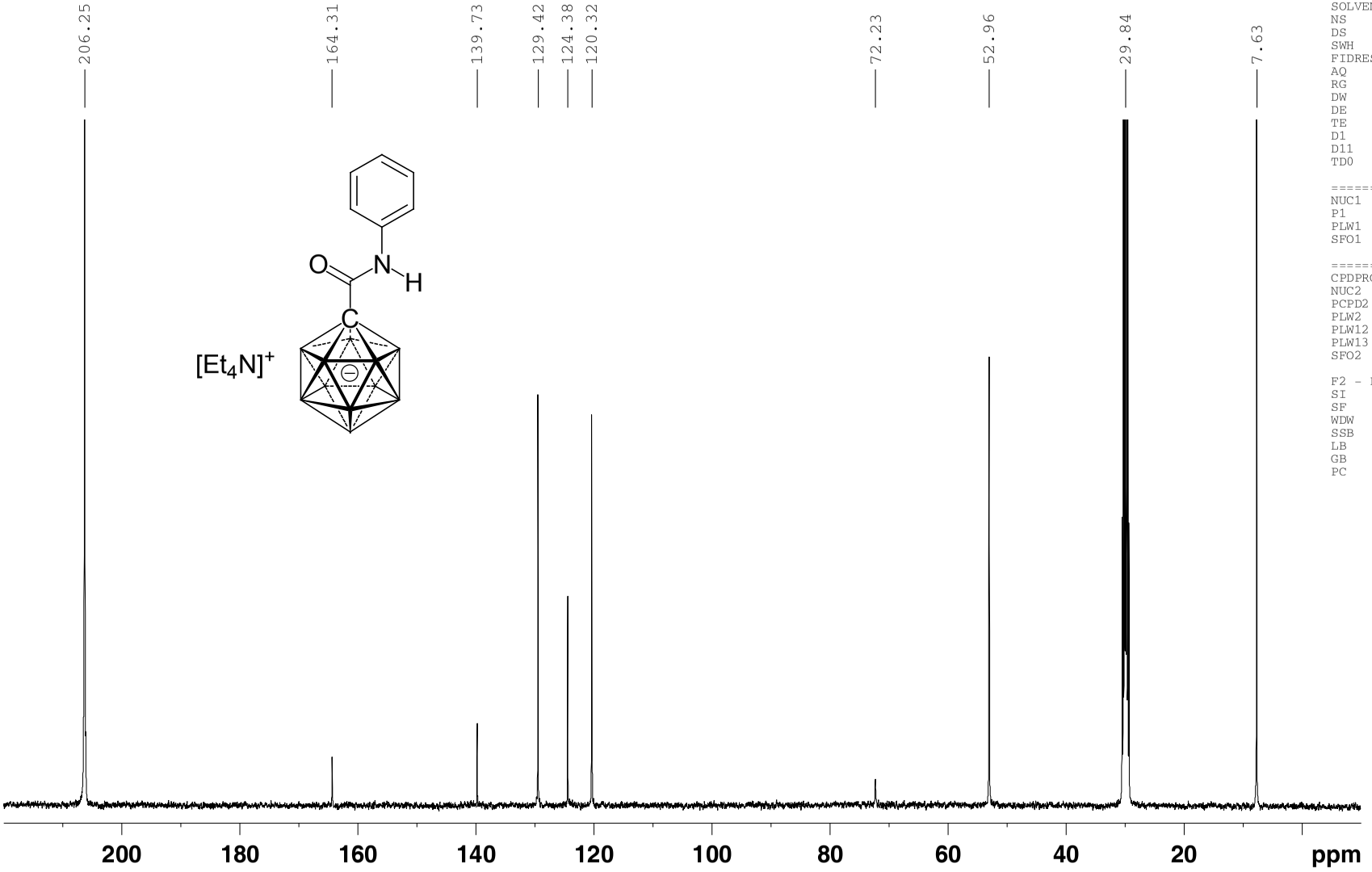
F2 - Acquisition Parameters
Date_              20171221
Time                  20.28
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT           Acetone
NS                      128
DS                        4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   295.3 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                       1

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

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

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

[Et4N][CB11H11–CONHC6H5], Ca. 30mg in acetone–d6
13C{1H}, 100 MHz, T= 22 C



NMR44

```
Current Data Parameters
NAME      2017-1220-zhk-C6H5NH2
EXPNO                        4
PROCNO                       1

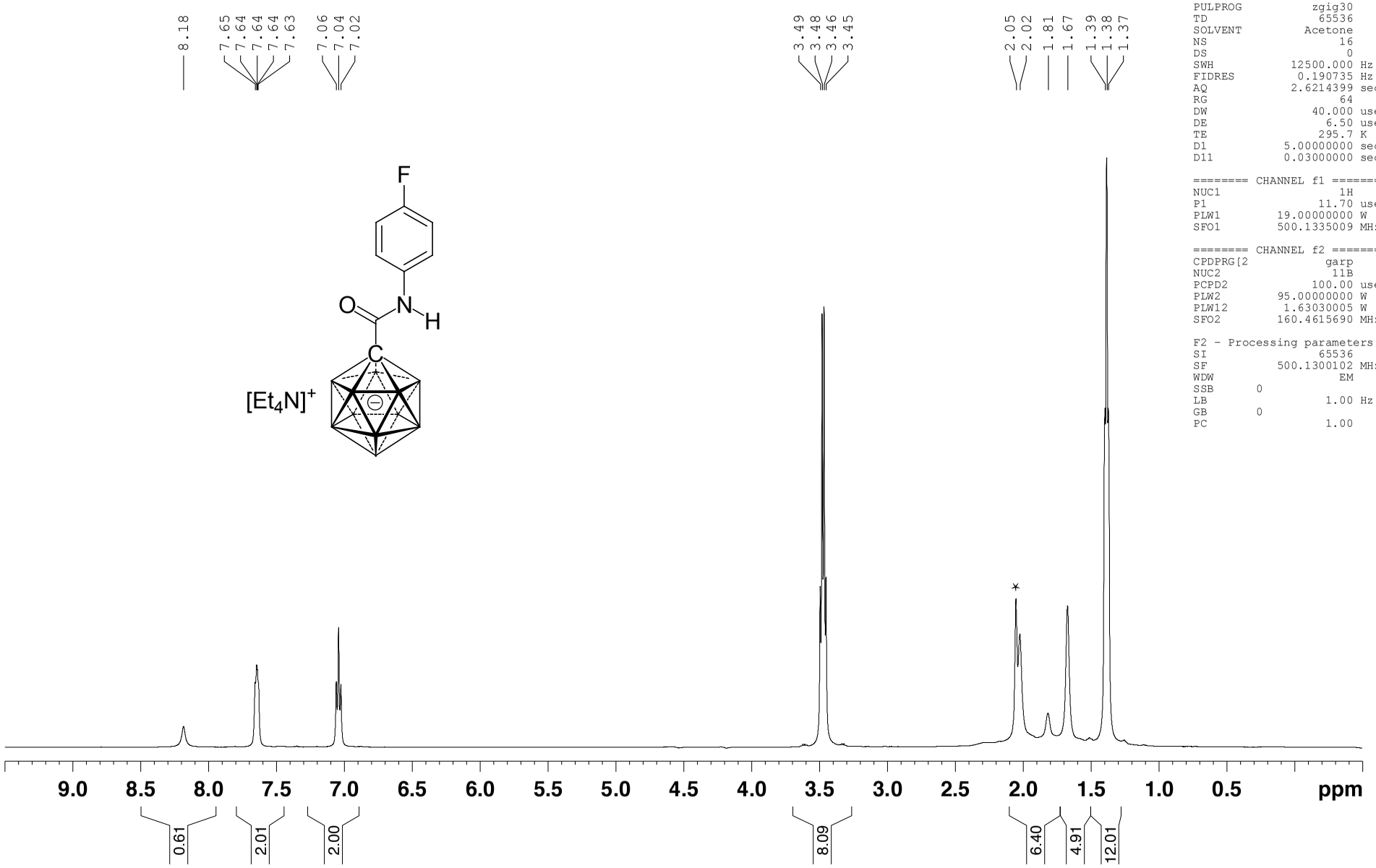
F2 - Acquisition Parameters
Date_              20171221
Time                 21.20
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                   193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  295.3 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                   32768
SF           100.6126866 MHz
WDW                     EM
SSB       0
LB                    3.00 Hz
GB        0
PC                    1.40
```

[Et4N][CB11H11–CONHC6H4F], Ca. 30mg in acetone–d6*
1H{11B}, 500 MHz, T= 22 C



NMR45

```
Current Data Parameters
NAME                  1062-FB
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20180201
Time                    12.33
INSTRUM                 spect
PROBHD    5 mm PABBO BB-
PULPROG                zgig30
TD                      65536
SOLVENT               Acetone
NS                         16
DS                          0
SWH                 12500.000 Hz
FIDRES                0.190735 Hz
AQ                    2.6214399 sec
RG                         64
DW                    40.000 usec
DE                     6.50 usec
TE                     295.7 K
D1                 5.00000000 sec
D11                0.03000000 sec

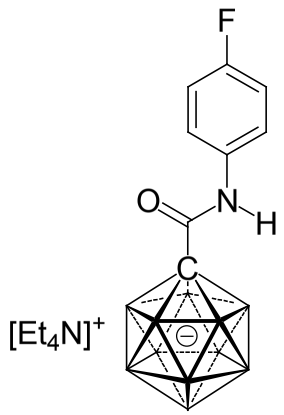
======== CHANNEL f1 ========
NUC1                       1H
P1                     11.70 usec
PLW1              19.00000000 W
SFO1             500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2                 garp
NUC2                      11B
PCPD2                 100.00 usec
PLW2              95.00000000 W
PLW12              1.63030005 W
SFO2             160.4615690 MHz

F2 - Processing parameters
SI                        65536
SF               500.1300102 MHz
WDW                          EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.00
```

[Et4N][CB11H11-CONHC6H4F], Ca. 30mg in acetone-d6
11B, 160 MHz, T= 22 C

NMR46




```
Current Data Parameters
NAME                  1062-FB
EXPNO                       2
PROCNO                      1

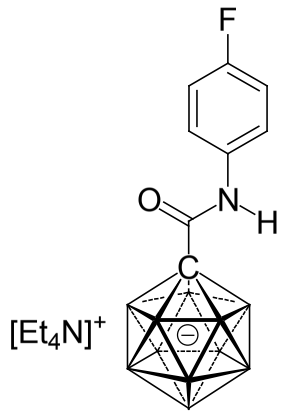
F2 - Acquisition Parameters
Date_              20180201
Time                   12.35
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    64098
SOLVENT             Acetone
NS                         32
DS                          0
SWH               32051.281 Hz
FIDRES             0.500036 Hz
AQ                0.9999288 sec
RG                       203
DW                  15.600 usec
DE                   6.50 usec
TE                   295.4 K
D1              1.00000000 sec

======== CHANNEL f1 ========
NUC1                     11B
P1                   13.10 usec
PLW1           95.00000000 W
SFO1           160.4615792 MHz

F2 - Processing parameters
SI                       32768
SF             160.4615790 MHz
WDW                         EM
SSB         0
LB                   10.00 Hz
GB          0
PC                    1.40
```

[Et4N][CB11H11-CONHC6H4F], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C

NMR47




```
Current Data Parameters
NAME                  1062-FB
EXPNO                       3
PROCNO                      1

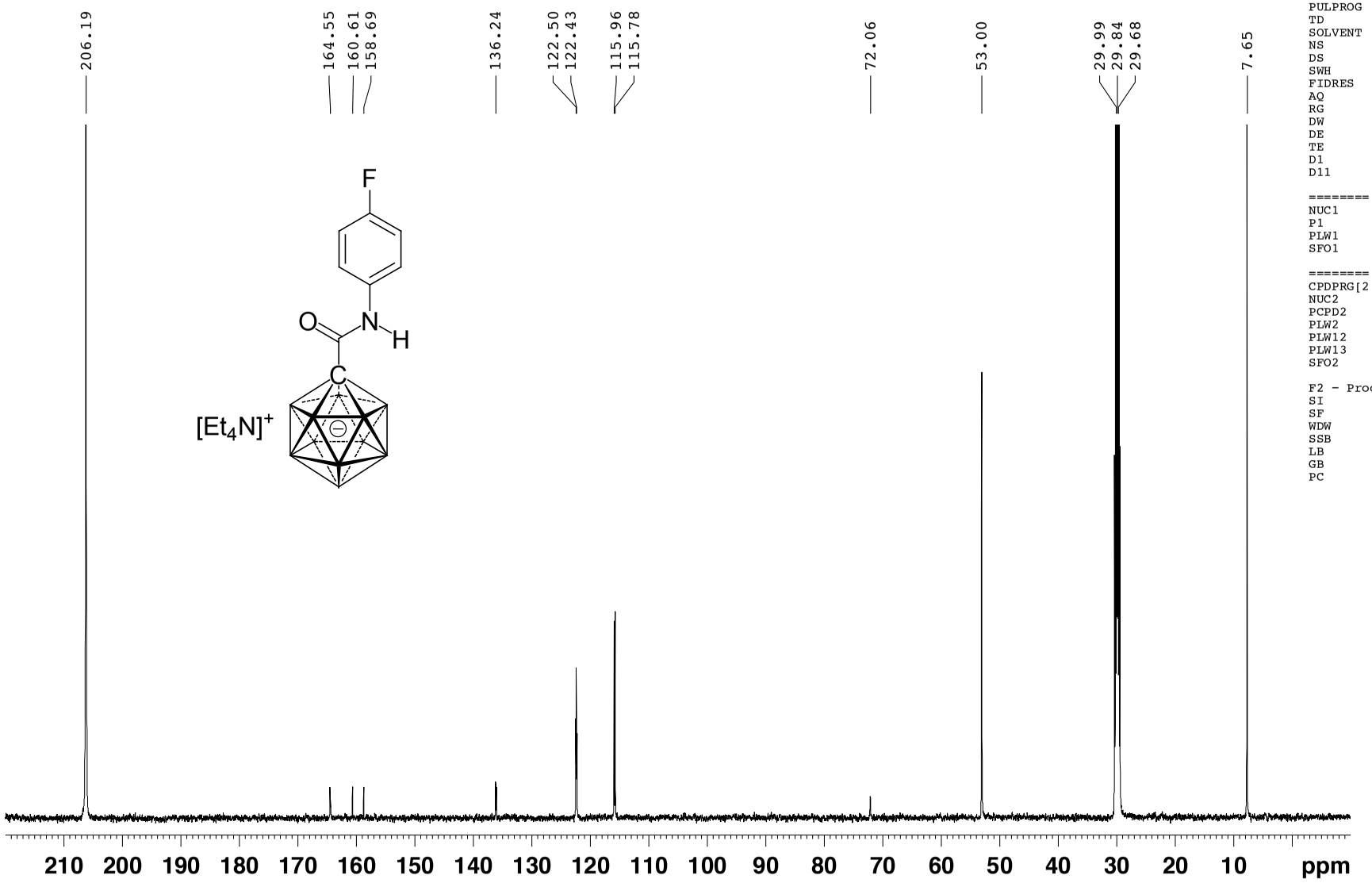
F2 - Acquisition Parameters
Date_              20180201
Time                   12.37
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zgpg30
TD                      65536
SOLVENT              Acetone
NS                         32
DS                          0
SWH                32051.281 Hz
FIDRES              0.489064 Hz
AQ                 1.0223616 sec
RG                       203
DW                    15.600 usec
DE                     6.50 usec
TE                    295.6 K
D1                 1.00000000 sec
D11                0.03000000 sec

======== CHANNEL f1 ========
NUC1                      11B
P1                      13.10 usec
PLW1              95.00000000 W
SFO1             160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2               waltz16
NUC2                       1H
PCPD2                   80.00 usec
PLW2              19.00000000 W
PLW12              0.40639001 W
PLW13              0.26008999 W
SFO2             500.1325007 MHz

F2 - Processing parameters
SI                       32768
SF               160.4615790 MHz
WDW                         EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```

[Et4N][CB11H11-CONHC6H4F], Ca. 30mg in acetone-d6
13C{1H}, 125 MHz, T= 22 C



NMR48

```
Current Data Parameters
NAME                 1062-FB
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_               20180201
Time                   13.20
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT              Acetone
NS                        1024
DS                           4
SWH                37878.789 Hz
FIDRES             0.577984 Hz
AQ                 0.8650752 sec
RG                       203
DW                    13.200 usec
DE                     6.50 usec
TE                    296.4 K
D1                 1.50000000 sec
D11                0.03000000 sec

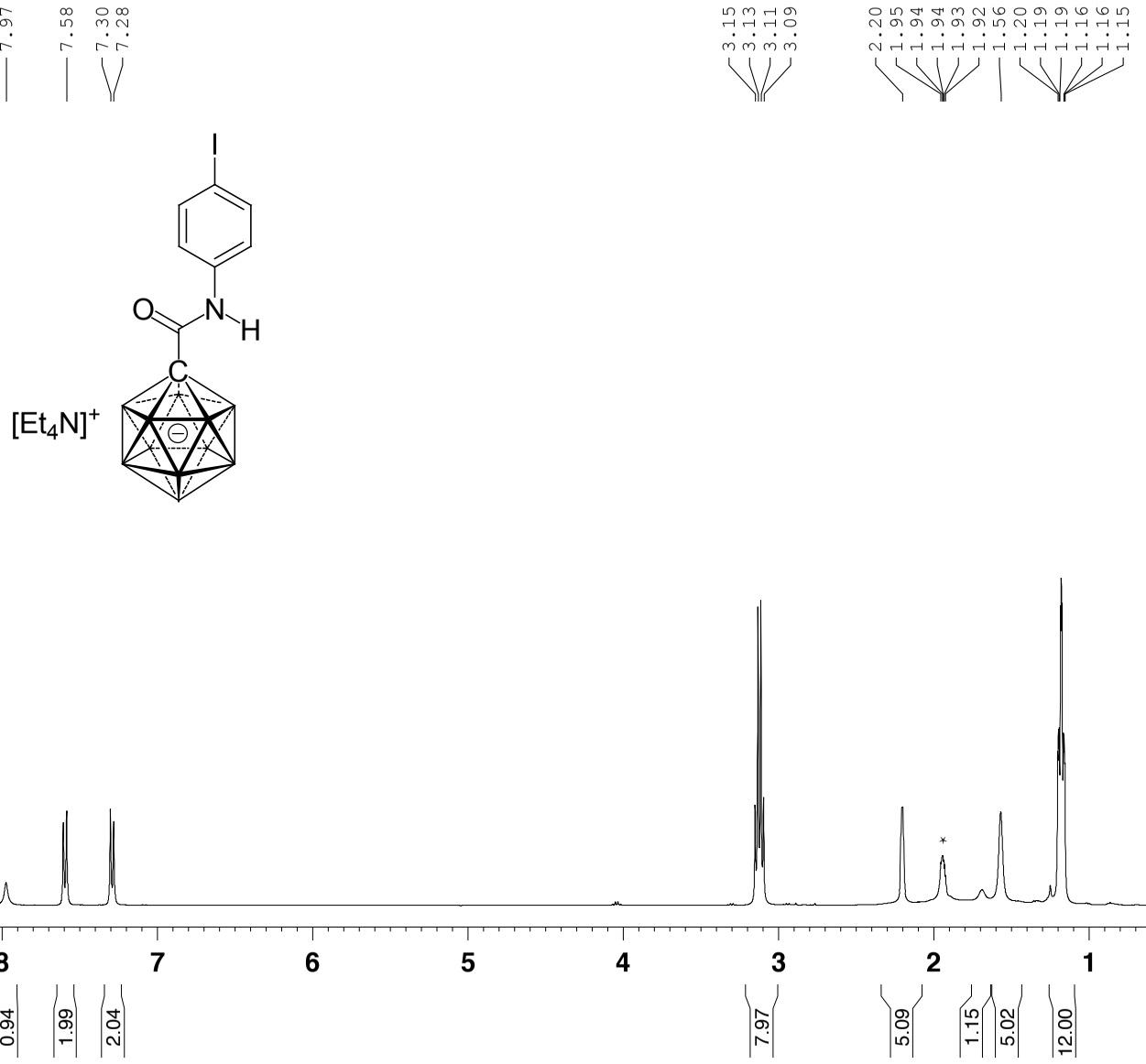
======== CHANNEL f1 ========
NUC1                      13C
P1                     10.50 usec
PLW1              95.00000000 W
SFO1             125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG[2               waltz16
NUC2                       1H
PCPD2                  80.00 usec
PLW2              19.00000000 W
PLW12              0.40639001 W
PLW13              0.26008999 W
SFO2             500.1320005 MHz

F2 - Processing parameters
SI                       32768
SF               125.7576822 MHz
WDW                         EM
SSB          0
LB                      3.00 Hz
GB           0
PC                      1.40
```

[Et4N][CB11H11–CONHC6H4I], Ca. 30mg in acetonitrile–d3 *
1H{11B}, 400 MHz, T= 22 C

NMR49




```
Current Data Parameters
NAME      20171227-zhk-IC6H4NH2
EXPNO                         1
PROCNO                        1

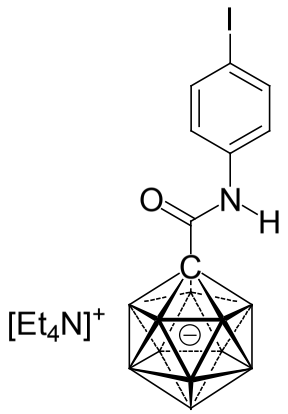
F2 - Acquisition Parameters
Date_              20171230
Time                  16.42
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT               CD3CN
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES            0.489064 Hz
AQ               1.0223616 sec
RG                    71.39
DW                   62.400 usec
DE                    6.50 usec
TE                   294.7 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                       1

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

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

F2 - Processing parameters
SI                        32768
SF             400.1300179 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

[Et4N][CB11H11-CONHC6H4I], Ca. 30mg in acetonitrile-d3
11B, 128 MHz, T= 22 C



NMR50

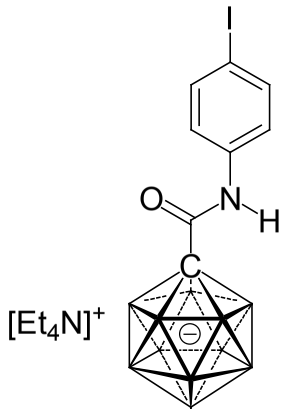

```
Current Data Parameters
NAME      20171227-zhk-IC6H4NH2
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171230
Time                  16.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                   zg
TD                     65536
SOLVENT                CD3CN
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                    294.5 K
D1              1.00000000 sec
TD0                        1

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

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

[Et4N][CB11H11-CONHC6H4I], Ca. 30mg in acetonitrile-d3
11B{1H}, 128 MHz, T= 22 C



NMR51


```
Current Data Parameters
NAME      20171227-zhk-IC6H4NH2
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171230
Time                  16.48
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CD3CN
NS                     128
DS                       4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   295.2 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

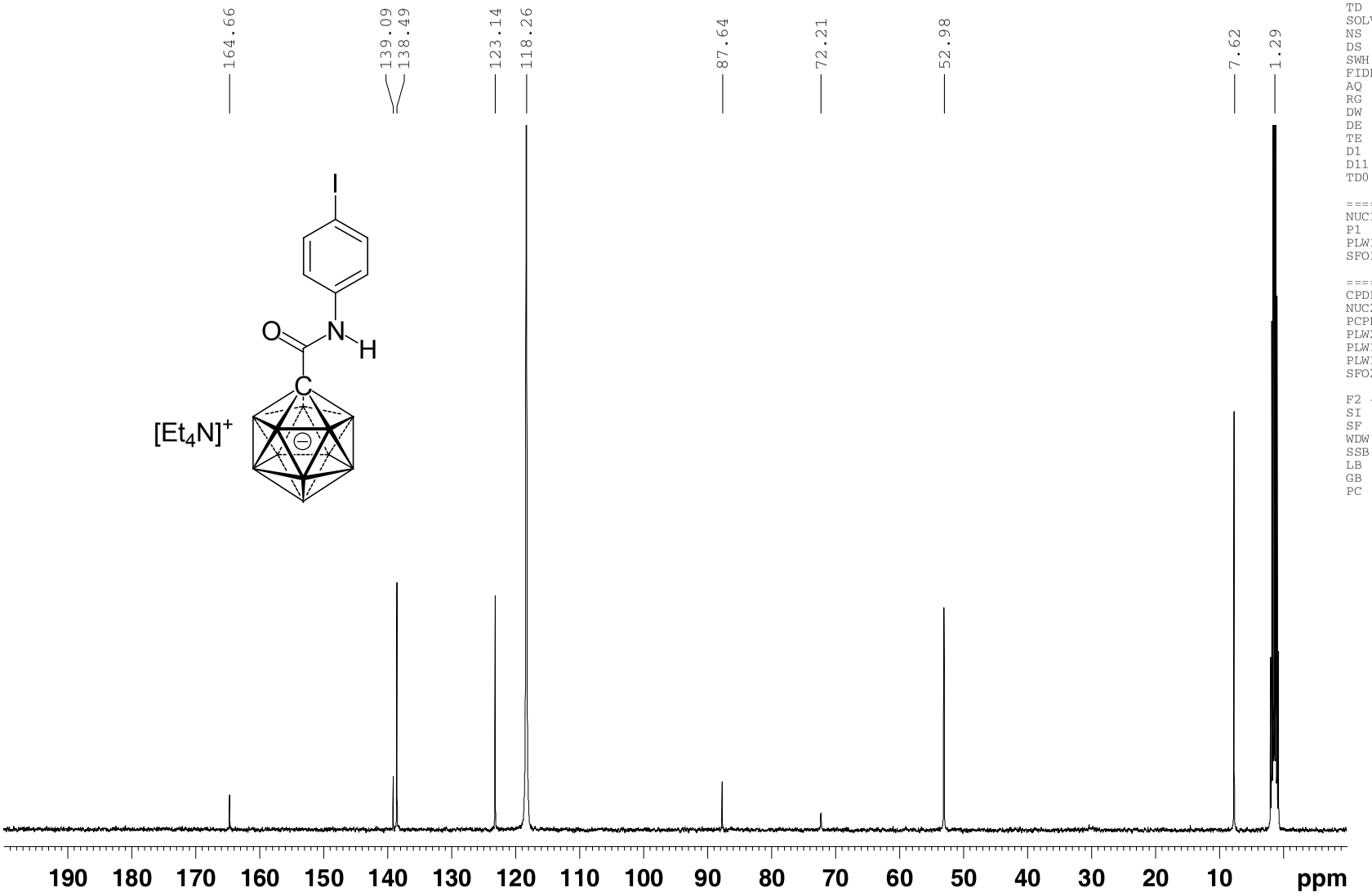
======== CHANNEL f1 ========
NUC1                    11B
P1                     9.93 usec
PLW1          52.96599960 W
SFO1         128.3776050 MHz

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

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

[Et4N][CB11H11-CONHC6H4I], Ca. 30mg in acetonitrile-d3
13C{1H}, 100 MHz, T= 22 C

NMR52




```
Current Data Parameters
NAME      20171227-zhk-IC6H4NH2
EXPNO                         4
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171230
Time                  17.41
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CD3CN
NS                    1024
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                 295.4 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

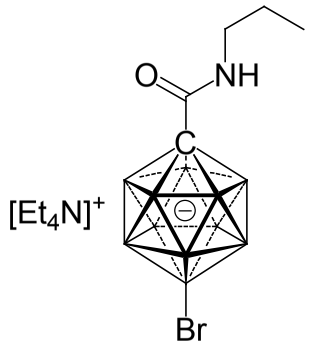
======== CHANNEL f1 ========
NUC1                   13C
P1                  10.00 usec
PLW1          53.00000000 W
SFO1         100.6228293 MHz

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

F2 - Processing parameters
SI                   32768
SF           100.6126793 MHz
WDW                     EM
SSB       0
LB                   3.00 Hz
GB        0
PC                   1.40
```

[Et4N][12–Br–CB11H10–CONPropyl], Ca. 30mg in acetone–d6 *
1H{11B}, 128 MHz, T= 22 C

NMR53




```
Current Data Parameters
NAME      20180201-ZHK-Br-SS-propyl
EXPNO                 1
PROCNO                1

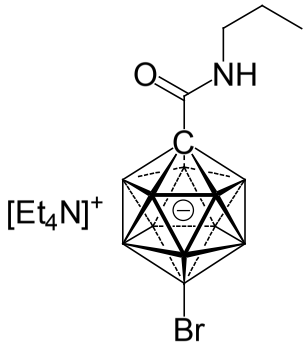
F2 - Acquisition Parameters
Date_          20180203
Time               3.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES        0.489064 Hz
AQ            1.0223616 sec
RG                86.58
DW               62.400 usec
DE                6.50 usec
TE               294.4 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

[Et4N][12-Br-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
11B, 160 MHz, T= 22 C




```
Current Data Parameters
NAME         1802-br-pro
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180323
Time               18.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 64098
SOLVENT          Acetone
NS                    32
DS                     0
SWH            32051.281 Hz
FIDRES          0.500036 Hz
AQ             0.9999288 sec
RG                   203
DW                15.600 usec
DE                 6.50 usec
TE                295.4 K
D1           1.00000000 sec

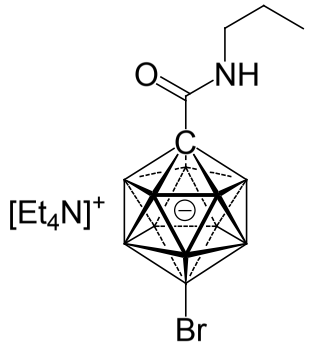
======== CHANNEL f1 ========
NUC1                 11B
P1                13.10 usec
PLW1         95.00000000 W
SFO1         160.4615792 MHz

F2 - Processing parameters
SI                   32768
SF           160.4615790 MHz
WDW                  EM
SSB       0
LB                10.00 Hz
GB        0
PC                 1.40
```

NMR54

[Et4N][12-Br-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C

NMR55




```
Current Data Parameters
NAME         1802-br-pro
EXPNO                  2
PROCNO                 1

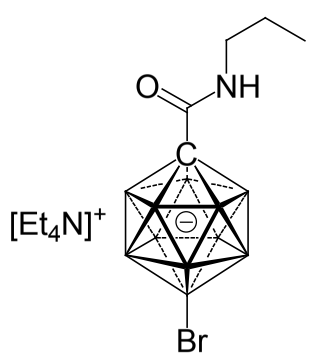
F2 - Acquisition Parameters
Date_           20180323
Time               19.01
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE                295.8 K
D1           1.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                13.10 usec
PLW1        95.00000000 W
SFO1       160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        19.00000000 W
PLW12        0.40639001 W
PLW13        0.26008999 W
SFO2       500.1325007 MHz

F2 - Processing parameters
SI                 32768
SF         160.4615790 MHz
WDW                   EM
SSB       0
LB                 5.00 Hz
GB        0
PC                 1.40
```

[Et4N][12-Br-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C



NMR56

206.19
165.82
66.08
53.02
52.99
52.96
42.27
30.03
29.84
29.64
23.24
7.67

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

```
Current Data Parameters
NAME      20180201-ZHK-Br-SS-propyl
EXPNO                 4
PROCNO                1

F2 - Acquisition Parameters
Date_          20180203
Time               4.20
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT       Acetone
NS               1024
DS                  4
SWH         29761.904 Hz
FIDRES       0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              295.2 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                 1

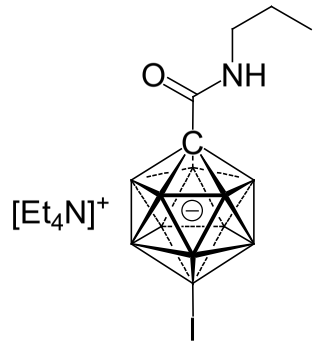
======== CHANNEL f1 ========
NUC1               13C
P1               10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

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

F2 - Processing parameters
SI               32768
SF         100.6126845 MHz
WDW                EM
SSB       0
LB               3.00 Hz
GB        0
PC               1.40
```

[Et4N][12–I–CB11H10–CONPropyl], Ca. 30mg in acetone–d6 *
1H{11B}, 500 MHz, T= 22 C

NMR57




```
Current Data Parameters
NAME       1094-I-Propyl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180202
Time               12.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgig30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    0
SWH           12500.000 Hz
FIDRES            0.190735 Hz
AQ               2.6214399 sec
RG                   64
DW                40.000 usec
DE                 6.50 usec
TE                295.9 K
D1             5.00000000 sec
D11            0.03000000 sec

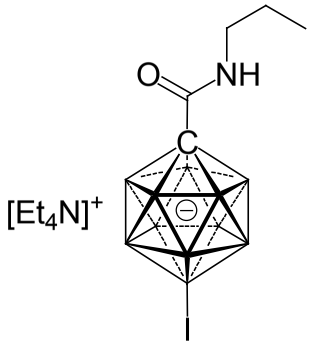
======== CHANNEL f1 ========
NUC1                  1H
P1                 11.70 usec
PLW1          19.00000000 W
SFO1         500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2             garp
NUC2                 11B
PCPD2             100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2         160.4615690 MHz

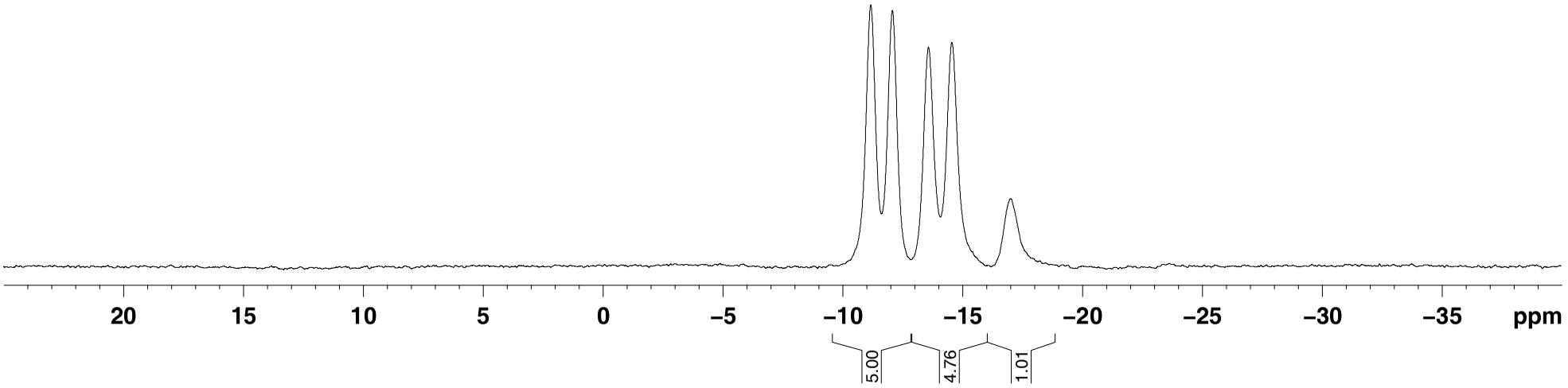
F2 - Processing parameters
SI                 65536
SF           500.1300105 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```

[Et4N][12-I-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
11B, 160 MHz, T= 22 C

NMR58



-11.18
-12.08
-13.58
-14.54
-16.97




```
Current Data Parameters
NAME      1568-I-SS-propyl
EXPNO                    1
PROCNO                   1

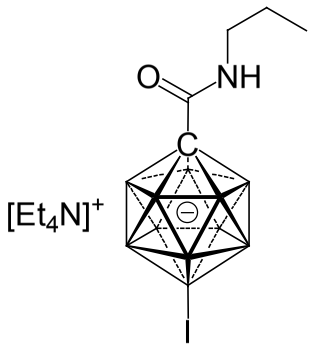
F2 - Acquisition Parameters
Date_           20180316
Time               22.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 64098
SOLVENT          Acetone
NS                    32
DS                     0
SWH            32051.281 Hz
FIDRES          0.500036 Hz
AQ             0.9999288 sec
RG                   203
DW                15.600 usec
DE                 6.50 usec
TE                296.9 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                 11B
P1                 13.10 usec
PLW1         95.00000000 W
SFO1         160.4615792 MHz

F2 - Processing parameters
SI                   32768
SF          160.4615790 MHz
WDW                     EM
SSB       0
LB                 10.00 Hz
GB        0
PC                  1.40
```

[Et4N][12-I-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C

NMR59




```
Current Data Parameters
NAME      1568-I-SS-propyl
EXPNO                    2
PROCNO                   1

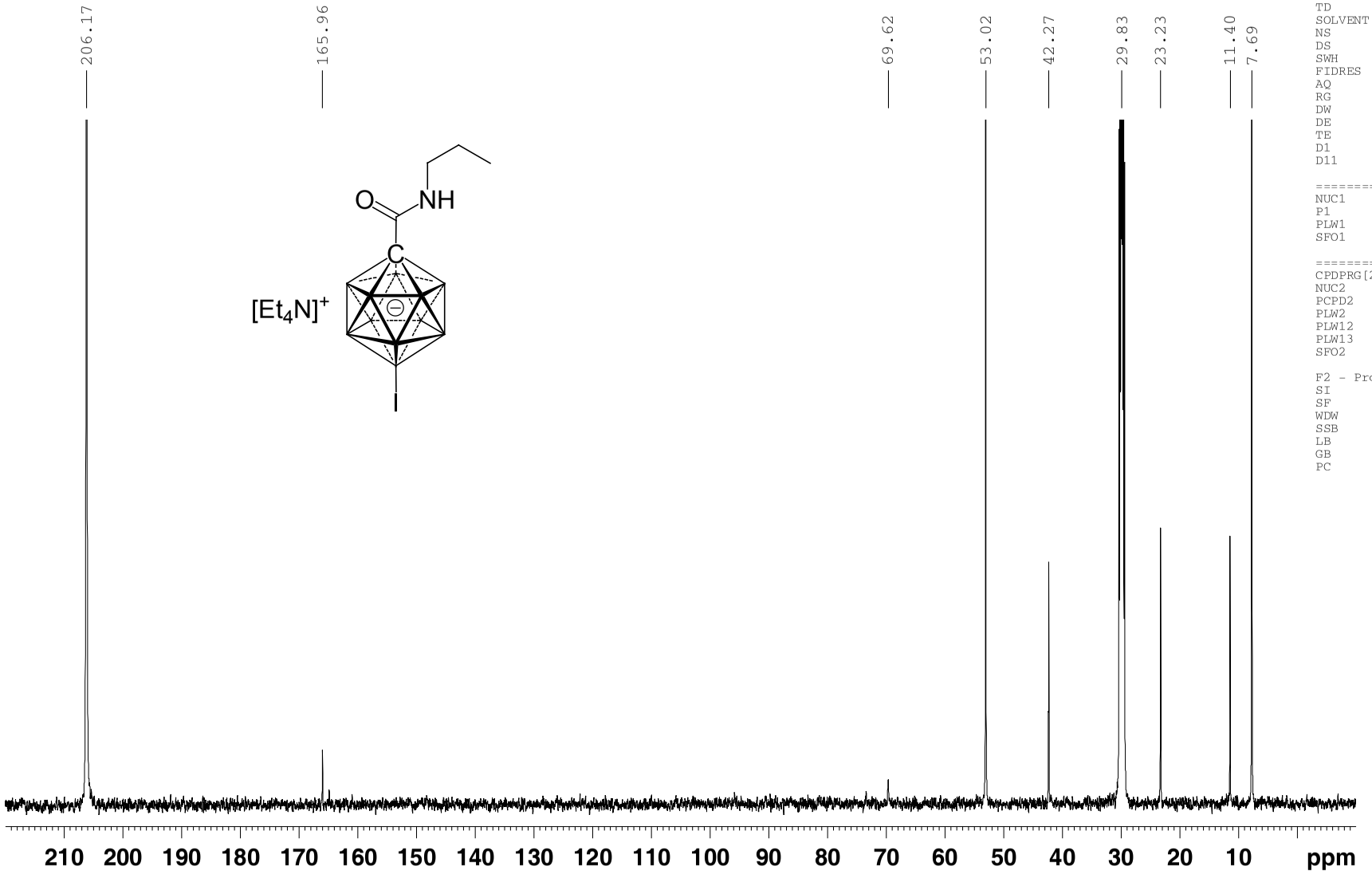
F2 - Acquisition Parameters
Date_           20180316
Time               22.58
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               297.0 K
D1            1.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                13.10 usec
PLW1         95.00000000 W
SFO1        160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2             80.00 usec
PLW2         19.00000000 W
PLW12         0.40639001 W
PLW13         0.26008999 W
SFO2         500.1325007 MHz

F2 - Processing parameters
SI                32768
SF          160.4615790 MHz
WDW                 EM
SSB       0
LB                5.00 Hz
GB        0
PC                1.40
```

[Et4N][12-I-CB11H10-CONPropyl], Ca. 30mg in acetone-d6
13C{1H}, 125 MHz, T= 22 C



NMR60

```
Current Data Parameters
NAME       1094-I-Propyl
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180202
Time               12.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 1024
DS                    4
SWH           37878.789 Hz
FIDRES         0.577984 Hz
AQ             0.8650752 sec
RG                  203
DW               13.200 usec
DE                6.50 usec
TE                296.2 K
D1           1.50000000 sec
D11          0.03000000 sec

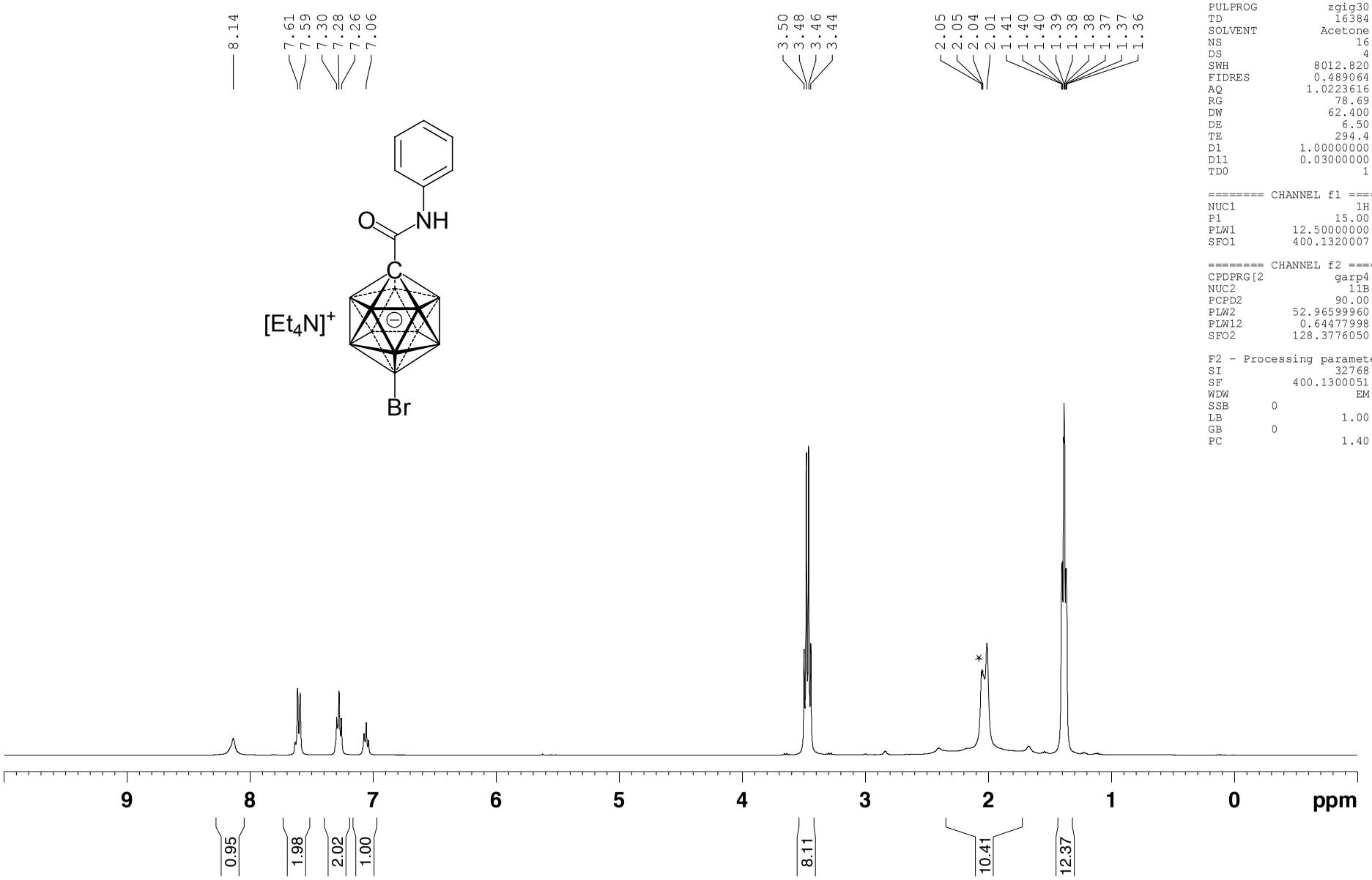
======== CHANNEL f1 ========
NUC1               13C
P1               10.50 usec
PLW1        95.00000000 W
SFO1       125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2        19.00000000 W
PLW12        0.40639001 W
PLW13        0.26008999 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF         125.7576832 MHz
WDW                   EM
SSB       0
LB                4.00 Hz
GB        0
PC                1.40
```

[Et4N][12−Br−CB11H10−CONHC6H5], Ca. 30mg in acetone−d6 *
1H{11B}, 400 MHz, T= 22 C

NMR61




```
Current Data Parameters
NAME      20180201-ZHK-Br-SS-phenyl
EXPNO                             1
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20180203
Time                           5.21
INSTRUM                       spect
PROBHD    5 mm PABBO BB/
PULPROG                     zgig30
TD                           16384
SOLVENT                    Acetone
NS                              16
DS                               4
SWH                       8012.820 Hz
FIDRES                    0.489064 Hz
AQ                       1.0223616 sec
RG                            78.69
DW                           62.400 usec
DE                            6.50 usec
TE                           294.4 K
D1                     1.00000000 sec
D11                    0.03000000 sec
TD0                               1

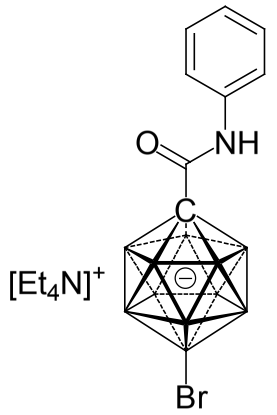
======== CHANNEL f1 ========
NUC1                             1H
P1                           15.00 usec
PLW1                  12.50000000 W
SFO1                 400.1320007 MHz

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

F2 - Processing parameters
SI                            32768
SF                   400.1300051 MHz
WDW                              EM
SSB                 0
LB                            1.00 Hz
GB                  0
PC                            1.40
```

[Et4N][12-Br-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
11B, 160 MHz, T= 22 C

NMR62




```
Current Data Parameters
NAME          1801-br-ph
EXPNO                  1
PROCNO                 1

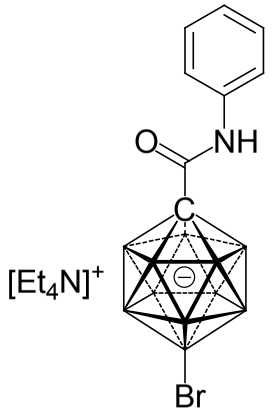
F2 - Acquisition Parameters
Date_           20180323
Time               18.52
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 64098
SOLVENT          Acetone
NS                    32
DS                     0
SWH            32051.281 Hz
FIDRES          0.500036 Hz
AQ             0.9999288 sec
RG                   203
DW                15.600 usec
DE                 6.50 usec
TE                295.4 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                  11B
P1                 13.10 usec
PLW1         95.00000000 W
SFO1         160.4615792 MHz

F2 - Processing parameters
SI                 32768
SF           160.4615790 MHz
WDW                   EM
SSB       0
LB                 10.00 Hz
GB        0
PC                  1.40
```

[Et4N][12-Br-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C

NMR63




```
Current Data Parameters
NAME          1801-br-ph
EXPNO                  2
PROCNO                 1

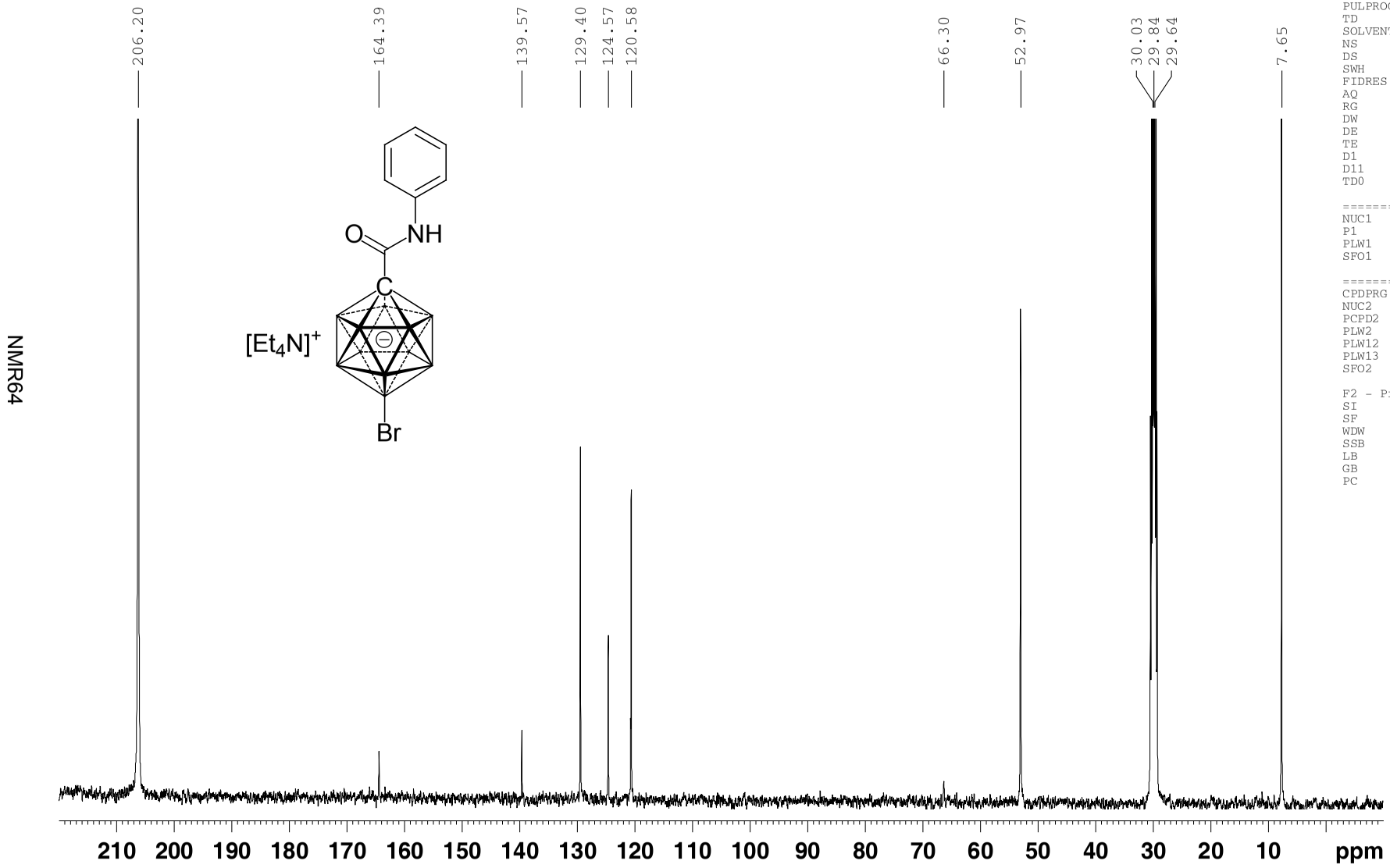
F2 - Acquisition Parameters
Date_           20180323
Time               18.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               295.8 K
D1            1.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                13.10 usec
PLW1         95.00000000 W
SFO1        160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2         19.00000000 W
PLW12         0.40639001 W
PLW13         0.26008999 W
SFO2        500.1325007 MHz

F2 - Processing parameters
SI                 32768
SF          160.4615790 MHz
WDW                   EM
SSB       0
LB                5.00 Hz
GB        0
PC                1.40
```

[Et4N][12-Br-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
13C{1H}, 100 MHz, T= 22 C



NMR64

```
Current Data Parameters
NAME      20180201-ZHK-Br-SS-phenyl
EXPNO                             4
PROCNO                            1

F2 - Acquisition Parameters
Date_                      20180203
Time                           5.58
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                          294.9 K
D1                    1.50000000 sec
D11                   0.03000000 sec
TD0                              1

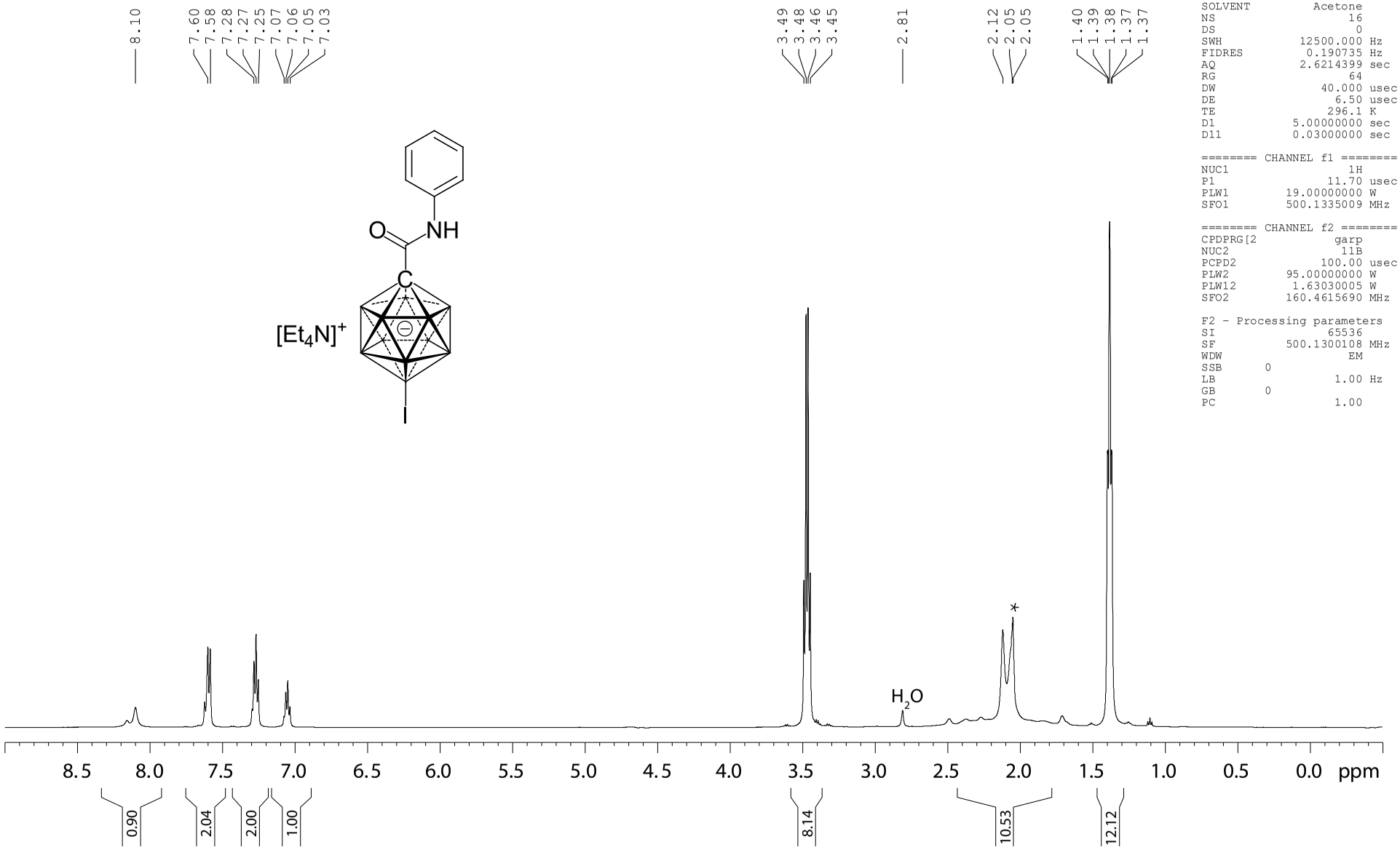
======== CHANNEL f1 ========
NUC1                            13C
P1                           10.00 usec
PLW1                  53.00000000 W
SFO1                 100.6228293 MHz

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

F2 - Processing parameters
SI                           32768
SF                  100.6126853 MHz
WDW                             EM
SSB                 0
LB                            5.00 Hz
GB                  0
PC                            1.40
```

[Et4N][12–I–CB11H10–CONHC6H5], Ca. 30mg in acetone–d6 *
1H{11B}, 500 MHz, T= 22 C

NMR65




```
Current Data Parameters
NAME       1095-I-Phenyl
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180202
Time              12.54
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgig30
TD               65536
SOLVENT        Acetone
NS                  16
DS                   0
SWH          12500.000 Hz
FIDRES        0.190735 Hz
AQ            2.6214399 sec
RG                  64
DW               40.000 usec
DE                6.50 usec
TE               296.1 K
D1           5.00000000 sec
D11          0.03000000 sec

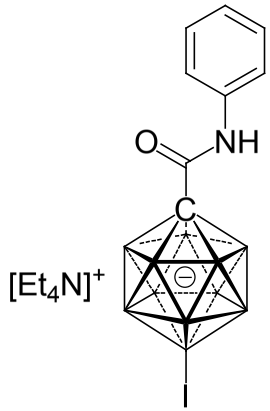
======== CHANNEL f1 ========
NUC1                1H
P1               11.70 usec
PLW1        19.00000000 W
SFO1       500.1335009 MHz

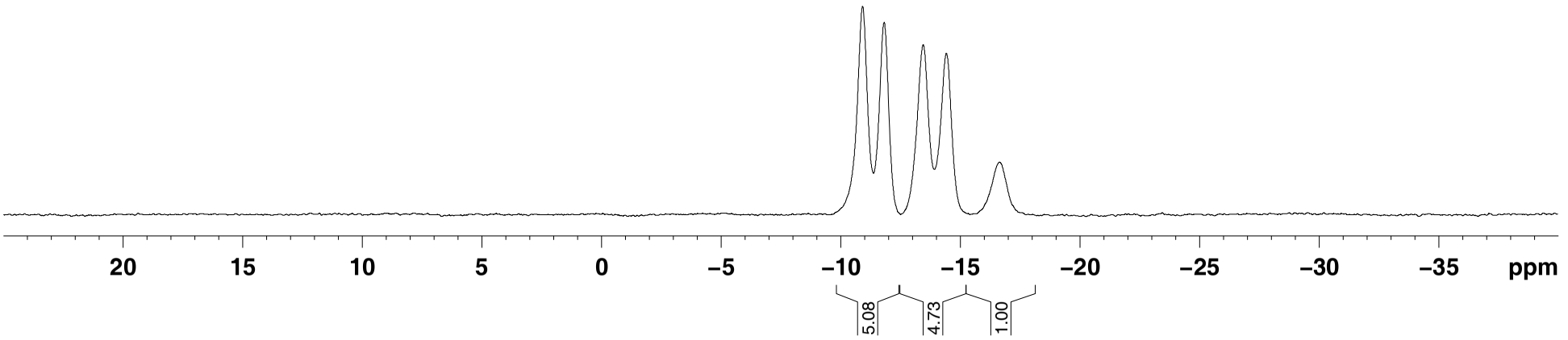
======== CHANNEL f2 ========
CPDPRG[2          garp
NUC2               11B
PCPD2           100.00 usec
PLW2        95.00000000 W
PLW12        1.63030005 W
SFO2       160.4615690 MHz

F2 - Processing parameters
SI               65536
SF          500.1300108 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.00
```

[Et4N][12-I-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
11B, 160 MHz, T= 22 C

NMR66






```
Current Data Parameters
NAME      1569-I-SS-phenyl
EXPNO                    1
PROCNO                   1

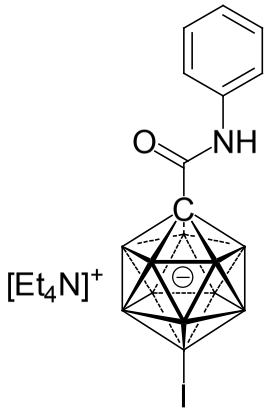
F2 - Acquisition Parameters
Date_             20180316
Time                 23.02
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  64098
SOLVENT           Acetone
NS                       32
DS                        0
SWH              32051.281 Hz
FIDRES            0.500036 Hz
AQ               0.9999288 sec
RG                     203
DW                  15.600 usec
DE                   6.50 usec
TE                  296.9 K
D1             1.00000000 sec

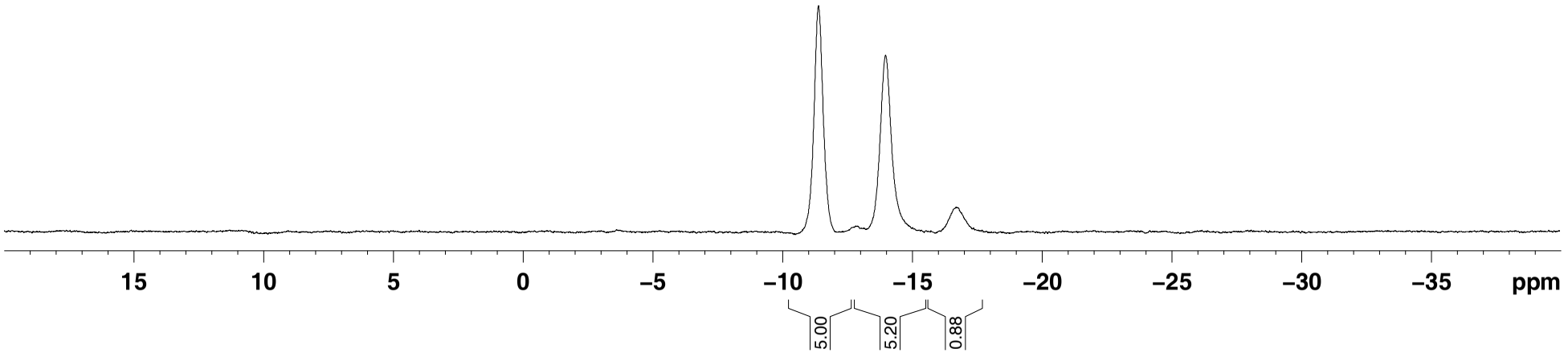
======== CHANNEL f1 ========
NUC1                   11B
P1                  13.10 usec
PLW1          95.00000000 W
SFO1          160.4615792 MHz

F2 - Processing parameters
SI                     32768
SF            160.4615790 MHz
WDW                    EM
SSB       0
LB                  10.00 Hz
GB        0
PC                   1.40
```

[Et4N][12-I-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C

NMR67






```
Current Data Parameters
NAME      1569-I-SS-phenyl
EXPNO                    2
PROCNO                   1

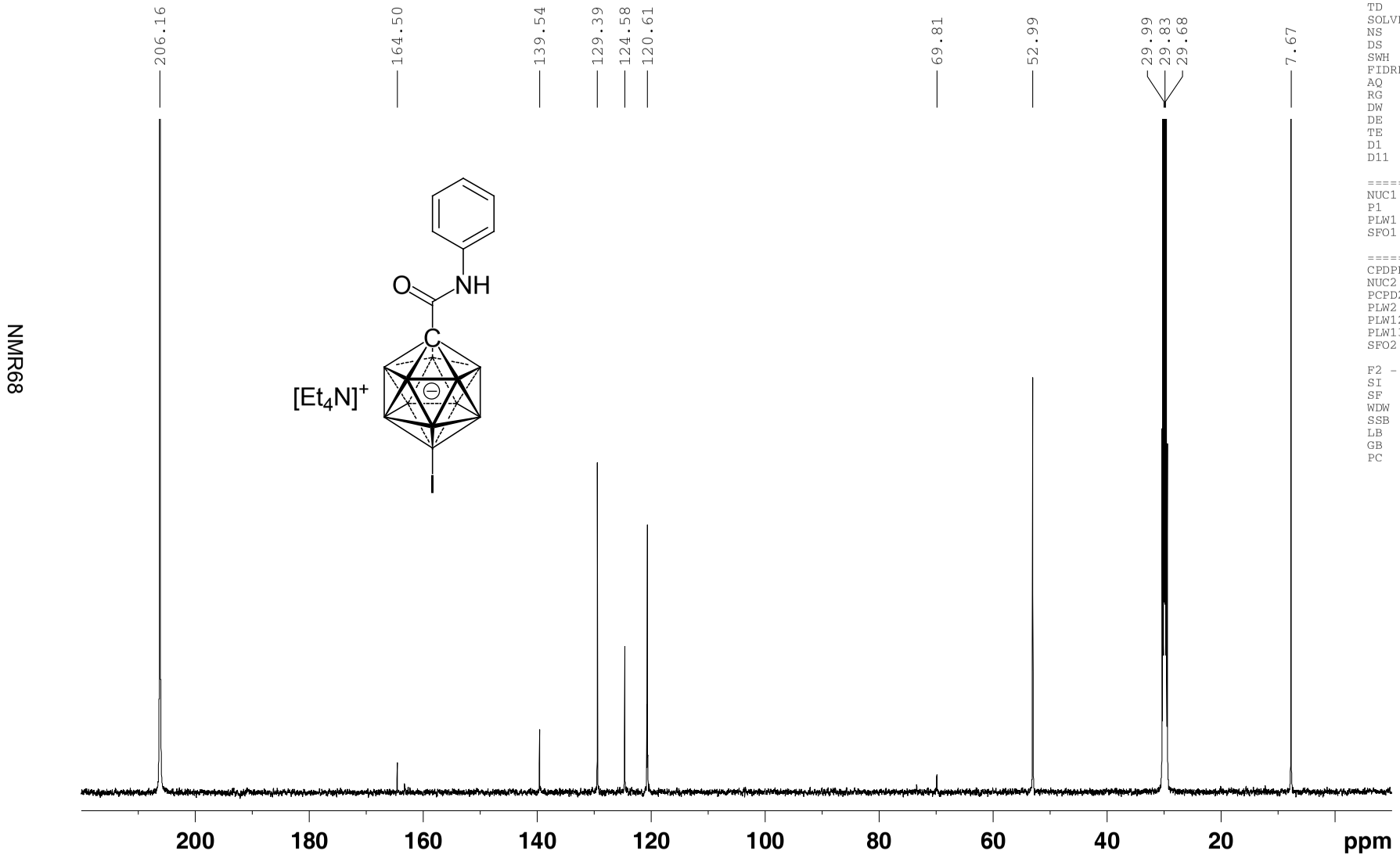
F2 - Acquisition Parameters
Date_           20180316
Time               23.04
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   32
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               297.0 K
D1            1.00000000 sec
D11           0.03000000 sec

======== CHANNEL f1 ========
NUC1                11B
P1                13.10 usec
PLW1         95.00000000 W
SFO1        160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2         19.00000000 W
PLW12         0.40639001 W
PLW13         0.26008999 W
SFO2        500.1325007 MHz

F2 - Processing parameters
SI                  32768
SF          160.4615790 MHz
WDW                    EM
SSB       0
LB                 3.00 Hz
GB        0
PC                 1.40
```

[Et4N][12-I-CB11H10-CONHC6H5], Ca. 30mg in acetone-d6
13C{1H}, 125 MHz, T= 22 C



NMR68

```
Current Data Parameters
NAME      1095-I-Phenyl
EXPNO                 4
PROCNO                1

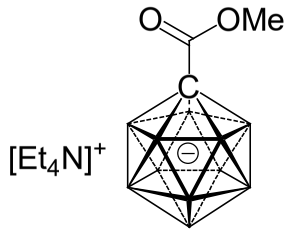
F2 - Acquisition Parameters
Date_          20180202
Time              13.41
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                1024
DS                   4
SWH          37878.789 Hz
FIDRES        0.577984 Hz
AQ            0.8650752 sec
RG                 203
DW              13.200 usec
DE               6.50 usec
TE              295.8 K
D1          1.50000000 sec
D11         0.03000000 sec

======== CHANNEL f1 ========
NUC1               13C
P1               10.50 usec
PLW1        95.00000000 W
SFO1       125.7716224 MHz

======== CHANNEL f2 ========
CPDPRG[2        waltz16
NUC2               1H
PCPD2            80.00 usec
PLW2        19.00000000 W
PLW12        0.40639001 W
PLW13        0.26008999 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                32768
SF         125.7576846 MHz
WDW                EM
SSB       0
LB               3.00 Hz
GB        0
PC               1.40
```

[Et4N][CB11H11–COOMe], Ca. 30mg in acetone–d6 *
1H{11B}, 500 MHz, T= 22 C



NMR69


```
Current Data Parameters
NAME              1061-MeOH
EXPNO                     1
PROCNO                    1

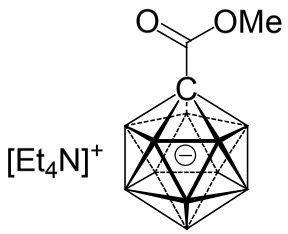
F2 - Acquisition Parameters
Date_              20180201
Time                 11.41
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgig30
TD                   65536
SOLVENT            Acetone
NS                        16
DS                         0
SWH              12500.000 Hz
FIDRES               0.190735 Hz
AQ                2.6214399 sec
RG                     50.8
DW                   40.000 usec
DE                    6.50 usec
TE                   295.7 K
D1             5.00000000 sec
D11            0.03000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    11.70 usec
PLW1          19.00000000 W
SFO1          500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp
NUC2                     11B
PCPD2                100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI                       65536
SF            500.1300104 MHz
WDW                        EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

[Et4N][CB11H11−COOMe], Ca. 30mg in acetone−d6
11B, 160 MHz, T= 22 C



NMR70

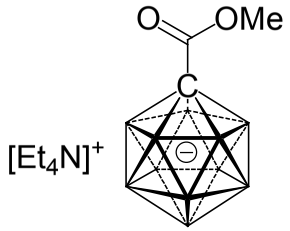
```
Current Data Parameters
NAME            1061-MeOH
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180201
Time                11.43
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  64098
SOLVENT           Acetone
NS                     32
DS                      0
SWH             32051.281 Hz
FIDRES          0.500036 Hz
AQ              0.9999288 sec
RG                    203
DW                15.600 usec
DE                 6.50 usec
TE                295.3 K
D1           1.00000000 sec

======== CHANNEL f1 ========
NUC1                  11B
P1                  13.10 usec
PLW1         95.00000000 W
SFO1         160.4615792 MHz

F2 - Processing parameters
SI                    32768
SF           160.4615790 MHz
WDW                     EM
SSB       0
LB                  10.00 Hz
GB        0
PC                    1.40
```

[Et4N][CB11H11-COOMe], Ca. 30mg in acetone-d6
11B{1H}, 160 MHz, T= 22 C



NMR71


```
Current Data Parameters
NAME            1061-MeOH
EXPNO                   3
PROCNO                  1

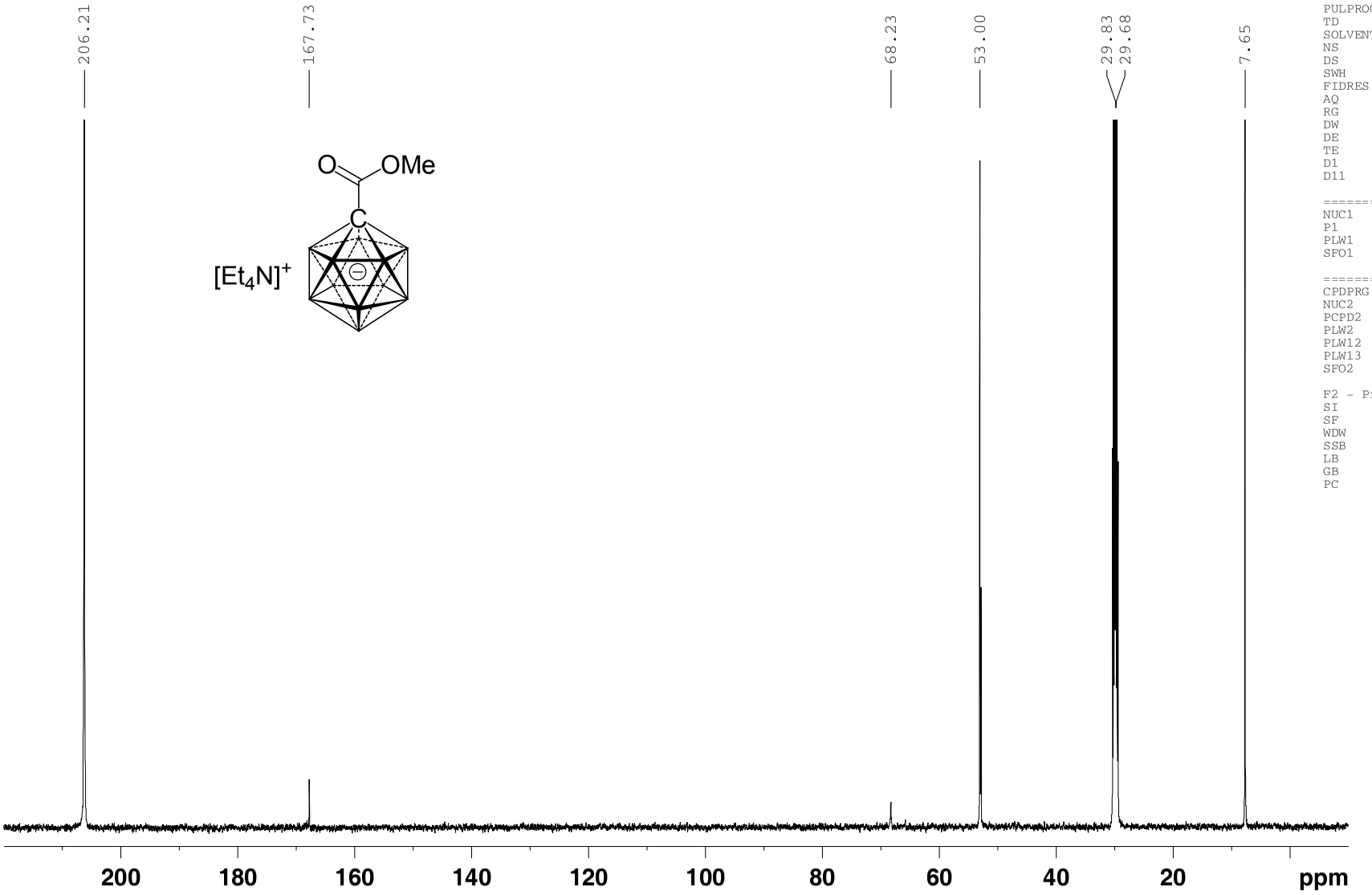
F2 - Acquisition Parameters
Date_            20180201
Time                11.45
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    32
DS                     0
SWH            32051.281 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                   203
DW                15.600 usec
DE                 6.50 usec
TE                295.6 K
D1           1.00000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                 11B
P1                 13.10 usec
PLW1         95.00000000 W
SFO1        160.4615790 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PLW2         19.00000000 W
PLW12         0.40639001 W
PLW13         0.26008999 W
SFO2        500.1325007 MHz

F2 - Processing parameters
SI                  32768
SF          160.4615790 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

[Et4N][CB11H11−COOMe], Ca. 30mg in acetone−d6
13C{1H}, 125 MHz, T= 22 C



NMR72

```
Current Data Parameters
NAME            1061-MeOH
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180201
Time                12.27
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                   1024
DS                      4
SWH             37878.789 Hz
FIDRES          0.577984 Hz
AQ              0.8650752 sec
RG                    203
DW                13.200 usec
DE                 6.50 usec
TE                296.0 K
D1           1.50000000 sec
D11          0.03000000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                10.50 usec
PLW1         95.00000000 W
SFO1        125.7716224 MHz

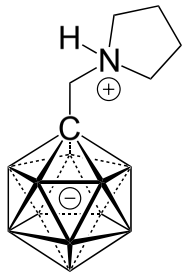
======== CHANNEL f2 ========
CPDPRG[2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PLW2         19.00000000 W
PLW12         0.40639001 W
PLW13         0.26008999 W
SFO2        500.1320005 MHz

F2 - Processing parameters
SI                  32768
SF          125.7576844 MHz
WDW                    EM
SSB       0
LB                 3.00 Hz
GB        0
PC                 1.40
```

[Et4N][CB11H11–CH2–N(pyrrolidine)] in acetone-d6*

1H{11B} NMR, 500 MHz, T = 22

NMR73




```
Current Data Parameters
NAME      20180317_1566-PY
EXPNO                    1
PROCNO                   1

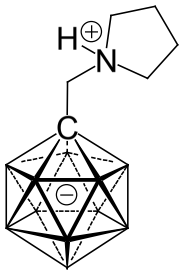
F2 - Acquisition Parameters
Date_             20180316
Time                 22.43
INSTRUM              spect
PROBHD    5 mm PABBO BB-
PULPROG             zgig30
TD                   65536
SOLVENT            Acetone
NS                      16
DS                       0
SWH              12500.000 Hz
FIDRES               0.190735 Hz
AQ                2.6214399 sec
RG                      64
DW                  40.000 usec
DE                   6.50 usec
TE                  296.9 K
D1               5.00000000 sec
D11              0.03000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.70 usec
PLW1           19.00000000 W
SFO1           500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp
NUC2                    11B
PCPD2                100.00 usec
PLW2           95.00000000 W
PLW12           1.63030005 W
SFO2           160.4615690 MHz

F2 - Processing parameters
SI                      65536
SF             500.1300101 MHz
WDW                        EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.00
```

[H][CB11H11-CH2NC4H8], Ca. 30mg in acetone-d6
11B, 128 MHz, T= 22 C




```
Current Data Parameters
NAME      20180405-zhk-Py-re
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180407
Time                   0.33
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                  zg
TD                    65536
SOLVENT             Acetone
NS                        128
DS                          4
SWH                25510.203 Hz
FIDRES              0.389255 Hz
AQ                 1.2845056 sec
RG                    193.34
DW                  19.600 usec
DE                   6.50 usec
TE                   296.1 K
D1                1.00000000 sec
TD0                        1

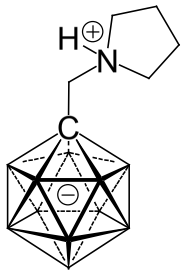
======== CHANNEL f1 ========
NUC1                      11B
P1                       9.93 usec
PLW1            52.96599960 W
SFO1           128.3776052 MHz

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

NMR74

[H][CB11H11-CH2NC4H8], Ca. 30mg in acetone-d6
11B{1H}, 128 MHz, T= 22 C

NMR75




```
Current Data Parameters
NAME      20180405-zhk-Py-re
EXPNO                      1
PROCNO                     1

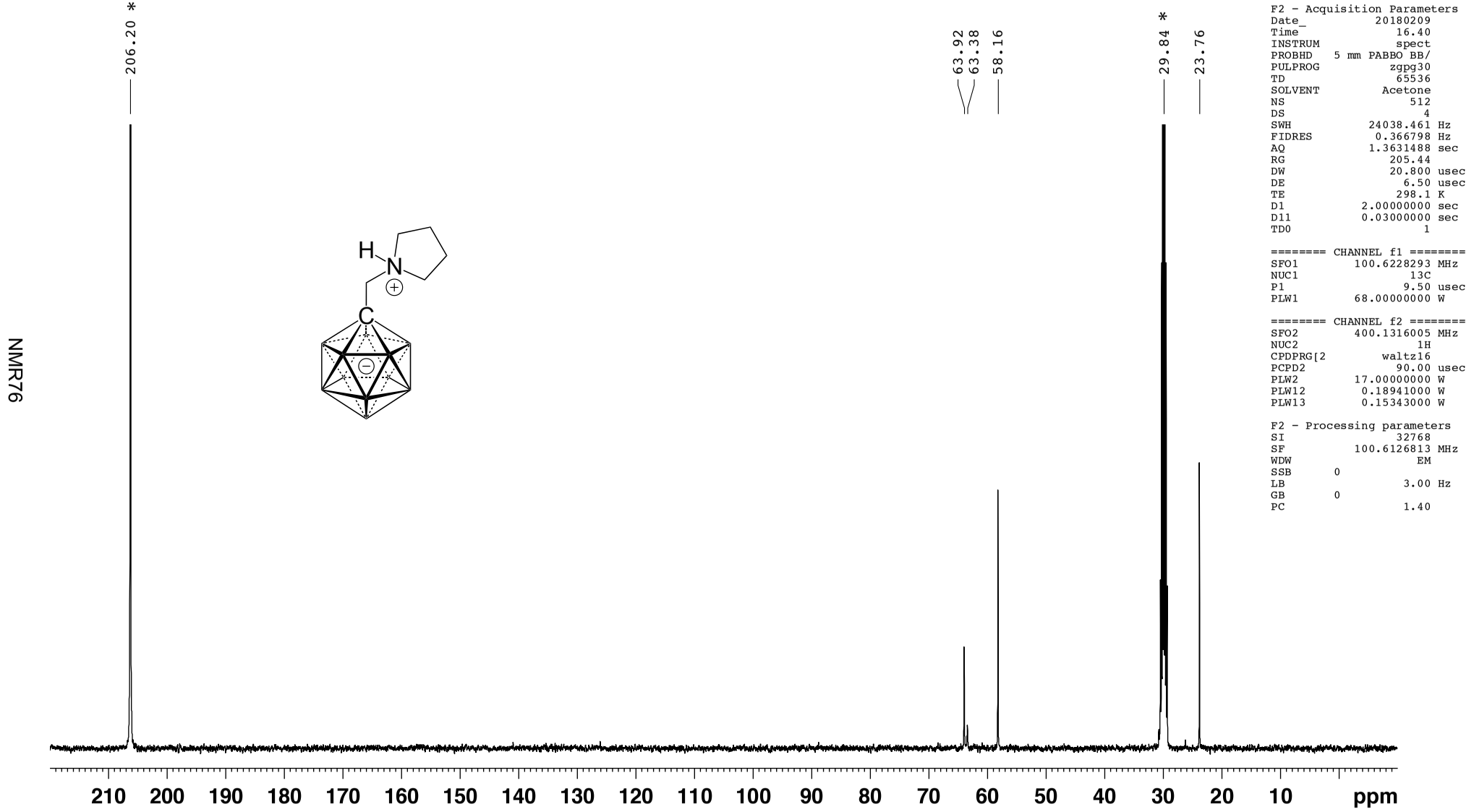
F2 - Acquisition Parameters
Date_            20180407
Time                 0.27
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW              19.600 usec
DE               6.50 usec
TE               296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

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

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

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

[Et4N][CB11H11–CH2–N(pyrrolidine)] in acetone-d6*
13C{1H} NMR, 500 MHz, T = 22




```
Current Data Parameters
NAME      20180209-zhk-py-re
EXPNO                      4
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180209
Time                  16.40
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       512
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                    205.44
DW                  20.800 usec
DE                   6.50 usec
TE                   298.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1            100.6228293 MHz
NUC1                    13C
P1                    9.50 usec
PLW1           68.00000000 W

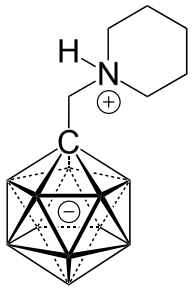
======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2           17.00000000 W
PLW12           0.18941000 W
PLW13           0.15343000 W

F2 - Processing parameters
SI                     32768
SF              100.6126813 MHz
WDW                       EM
SSB          0
LB                    3.00 Hz
GB           0
PC                    1.40
```

[Et4N][CB11H11–CH2–N(piperidine)] in acetone-d6*

1H{11B} NMR, 500 MHz, T = 22

NMR77

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Current Data Parameters
NAME      20180317_1567-PI
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180316
Time                 22.51
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG             zgig30
TD                   65536
SOLVENT            Acetone
NS                      16
DS                       0
SWH              12500.000 Hz
FIDRES           0.190735 Hz
AQ               2.6214399 sec
RG                    45.2
DW                 40.000 usec
DE                  6.50 usec
TE                 296.9 K
D1              5.00000000 sec
D11             0.03000000 sec

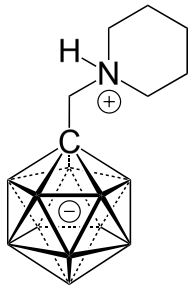
======== CHANNEL f1 ========
NUC1                     1H
P1                   11.70 usec
PLW1          19.00000000 W
SFO1          500.1335009 MHz

======== CHANNEL f2 ========
CPDPRG[2                garp
NUC2                    11B
PCPD2              100.00 usec
PLW2          95.00000000 W
PLW12          1.63030005 W
SFO2          160.4615690 MHz

F2 - Processing parameters
SI                   65536
SF            500.1300101 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.00
```

20180316-zhk-PI-re
11B, 128 MHz, T= 22 C

NMR78

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Current Data Parameters
NAME      20180316-zhk-PI-re
EXPNO                      2
PROCNO                     1

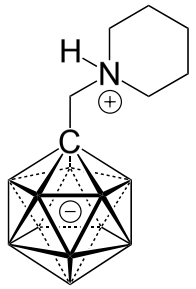
F2 - Acquisition Parameters
Date_              20180321
Time                  13.54
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg
TD                    65536
SOLVENT           Acetone
NS                      128
DS                        4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                     6.50 usec
TE                    294.1 K
D1                1.00000000 sec
TD0                       1

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

F2 - Processing parameters
SI                    32768
SF            128.3776050 MHz
WDW                      EM
SSB       0
LB                     5.00 Hz
GB        0
PC                     1.40
```

20180316-zhk-PI-re
11B{1H}, 128 MHz, T=22

NMR79




```
Current Data Parameters
NAME      20180316-zhk-PI-re
EXPNO                      1
PROCNO                     1

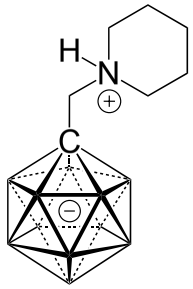
F2 - Acquisition Parameters
Date_            20180321
Time                13.48
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES           0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 294.8 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                     1

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

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

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

[Et4N][CB11H11–CH2–N(piperidine)] in acetone-d6*
13C{1H} NMR, 500 MHz, T = 22



64.60
62.61
56.69
29.84*
22.82
21.98
*

NMR80

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

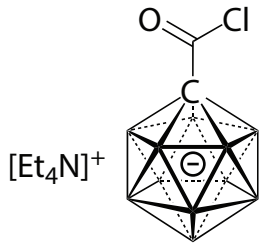
```
Current Data Parameters
NAME      20180209-zhk-pi-re
EXPNO                      4
PROCNO                     1

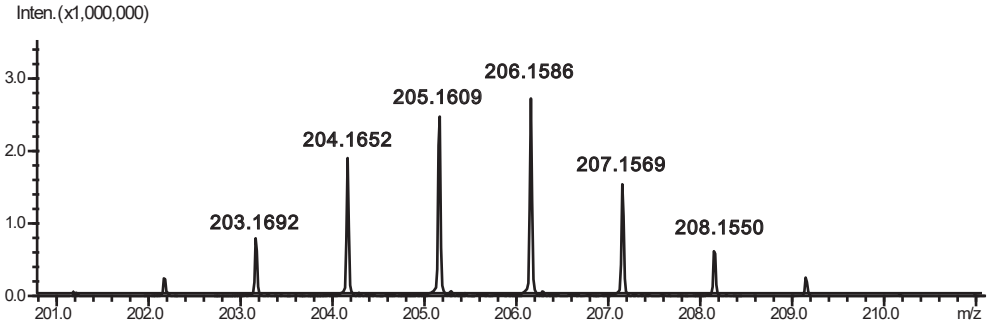
F2 - Acquisition Parameters
Date_              20180209
Time                  15.54
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT            Acetone
NS                       512
DS                         4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   205.44
DW                   20.800 usec
DE                    6.50 usec
TE                   298.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                    13C
P1                     9.50 usec
PLW1          68.00000000 W

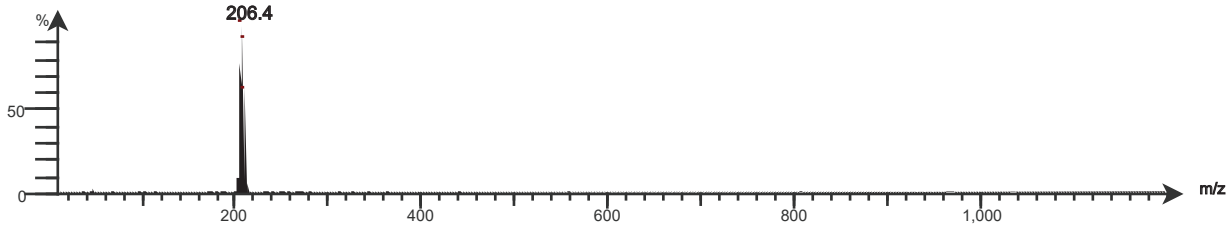
======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                 90.00 usec
PLW2          17.00000000 W
PLW12          0.18941000 W
PLW13          0.15343000 W

F2 - Processing parameters
SI                     32768
SF            100.6126836 MHz
WDW                       EM
SSB       0
LB                     3.00 Hz
GB        0
PC                     1.40
```

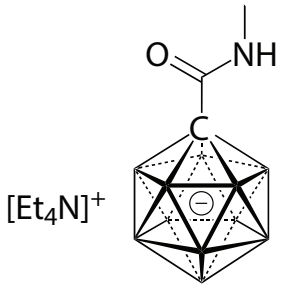


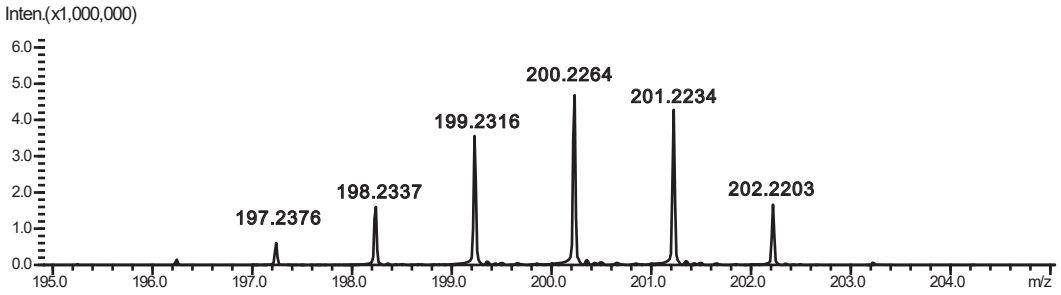


(–)-ESI-HRMS Shimadzu IT-TOF

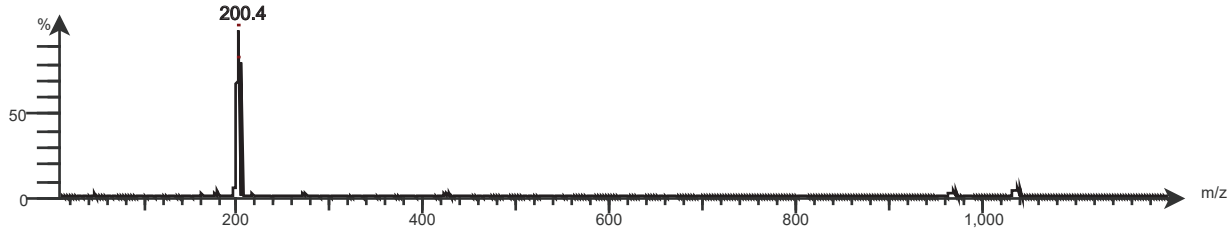


Full-range (–)-ESI-MS Expression CMS

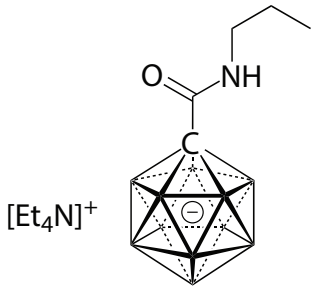


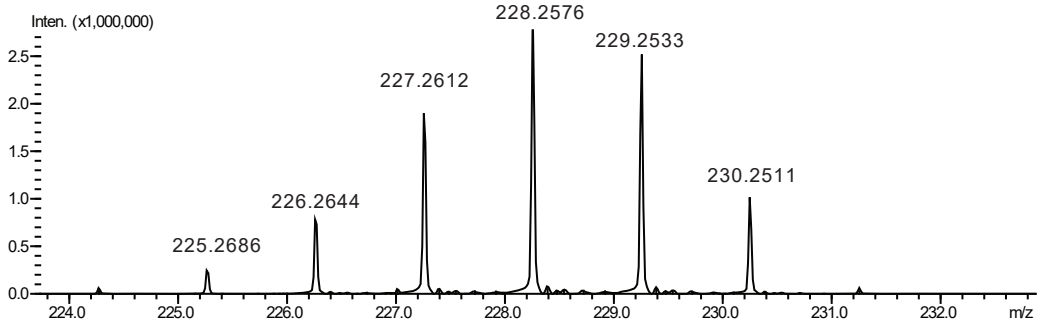


(–)-ESI-HRMS Shimadzu IT-TOF

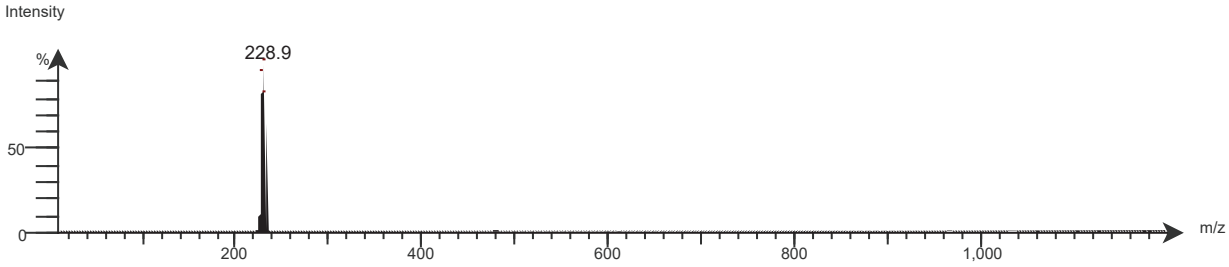


Full-range (–)-ESI-MS Expression CMS

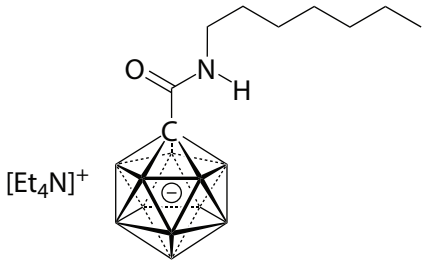


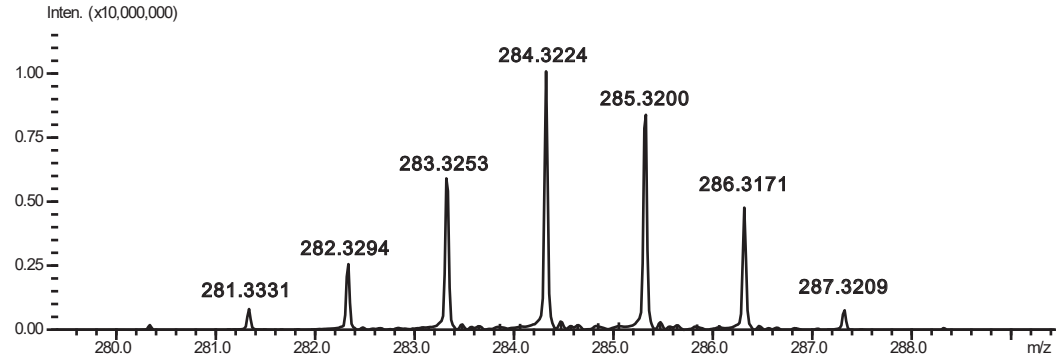


(–)-ESI-HRMS Shimadzu IT-TOF

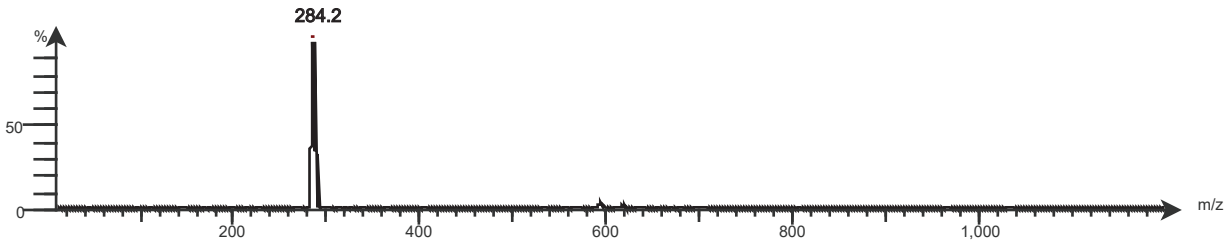


Full-range (–)-ESI-MS Expression CMS

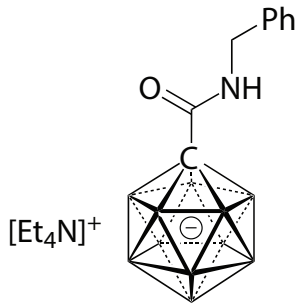


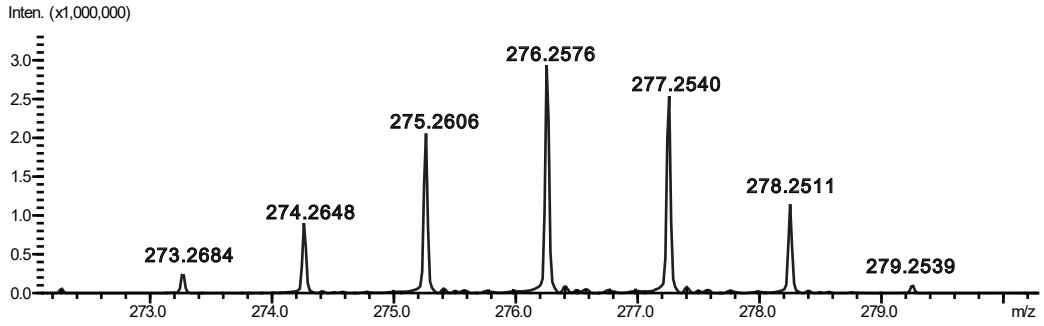


(–)-ESI-HRMS Shimadzu IT-TOF



Full-range (–)-ESI-MS Expression CMS





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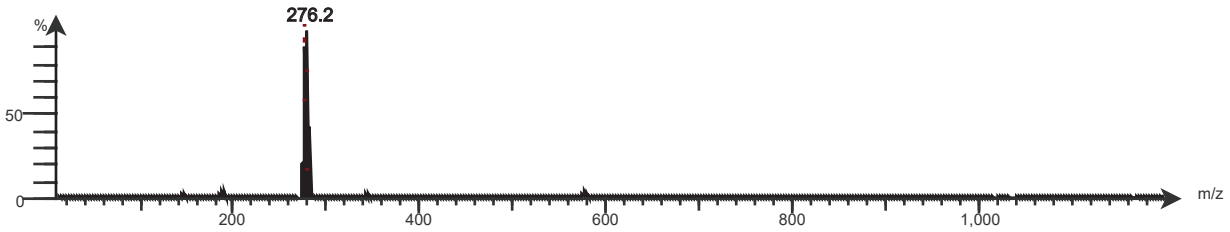
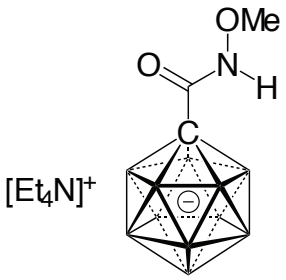
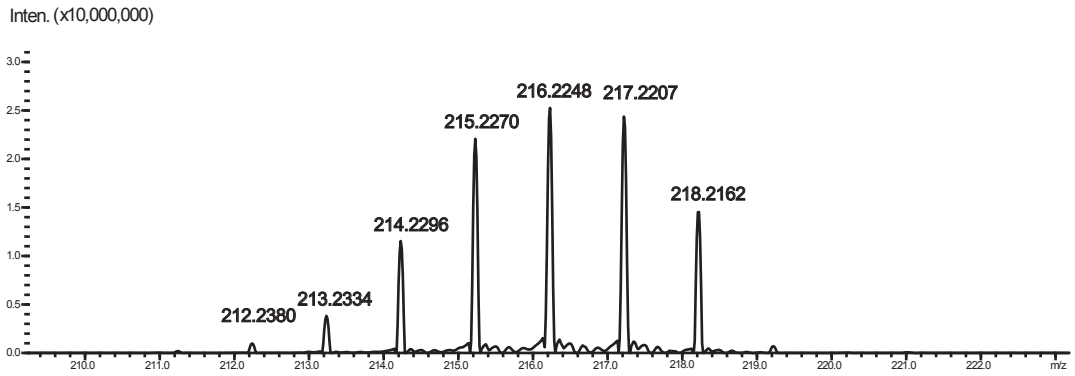
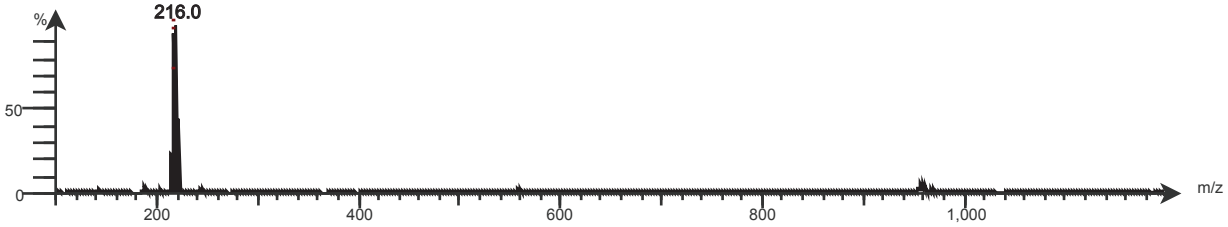


Full-range (–)-ESI-MS Expression CMS

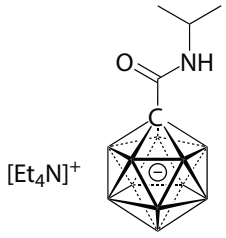


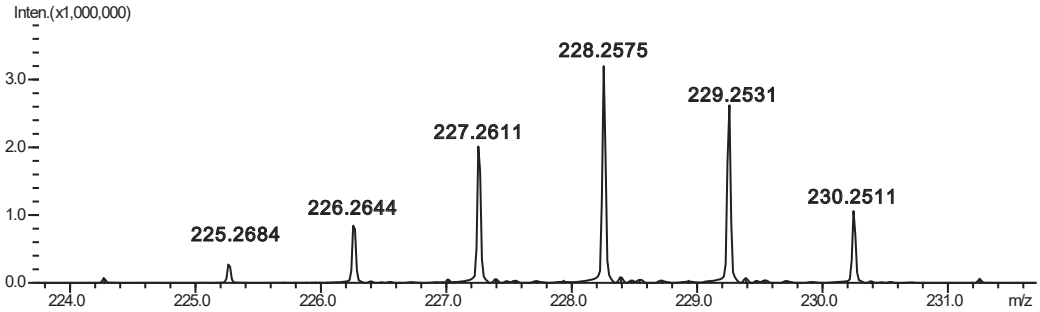


(–)-ESI-HRMS Shimadzu IT-TOF

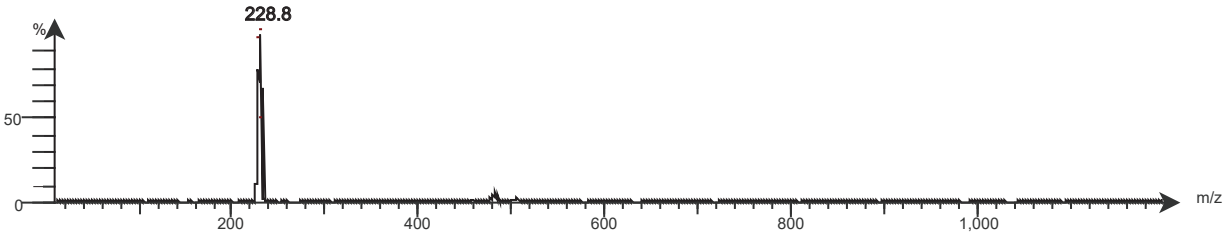


Full-range (–)-ESI-MS Expression CMS

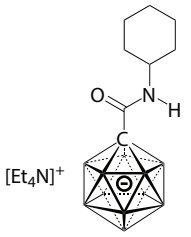


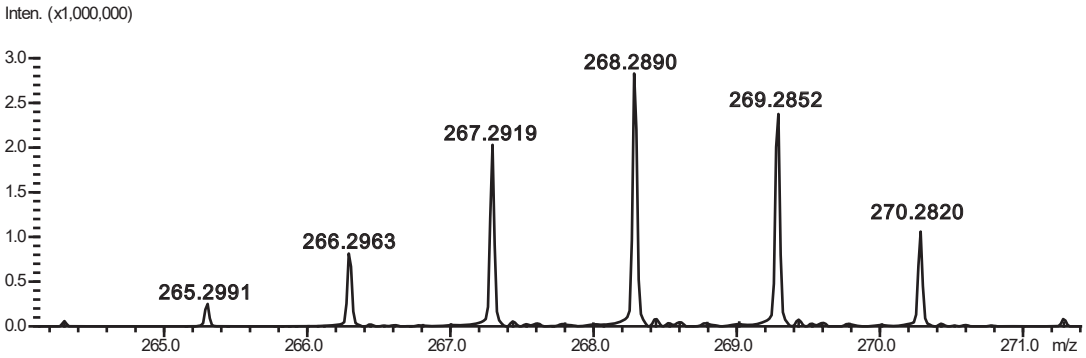


(–)-ESI-HRMS Shimadzu IT-TOF



Full-range (–)-ESI-MS Expression CMS





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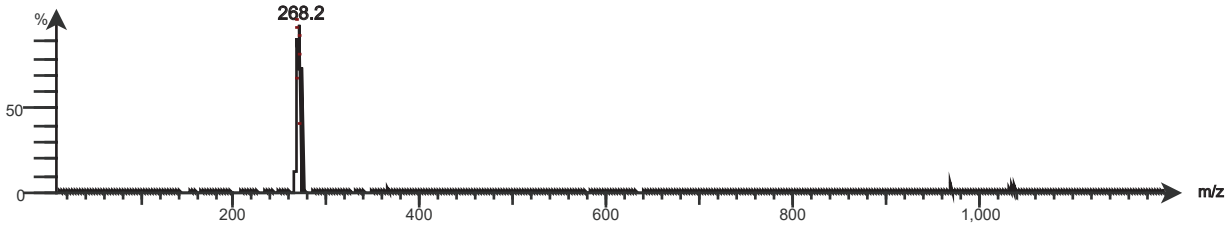
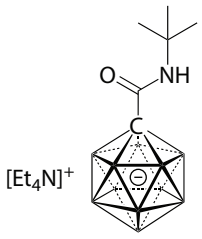
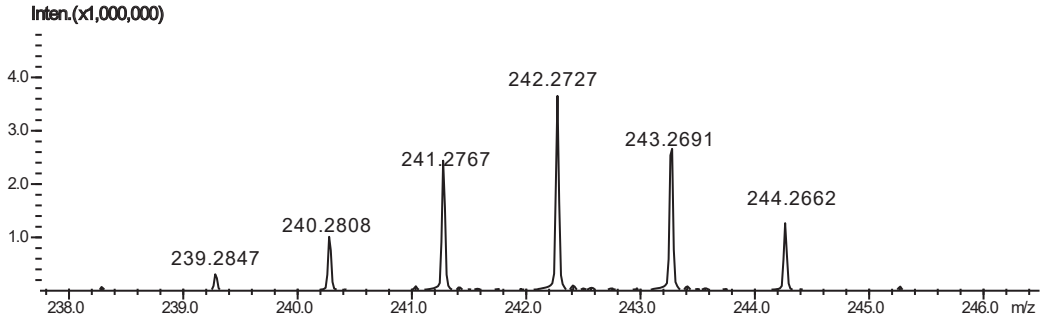


Full-range (–)-ESI-MS Expression CMS





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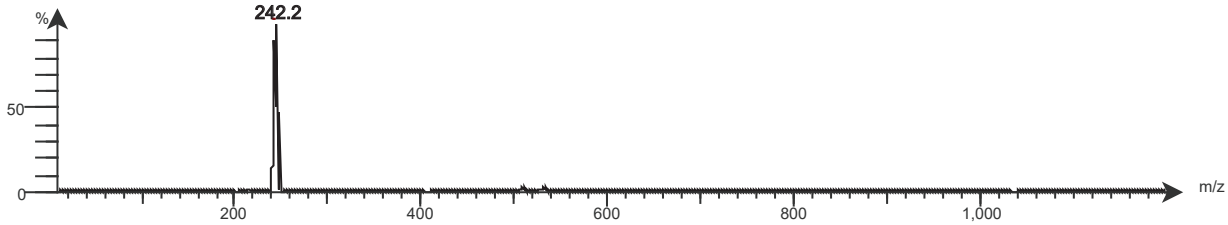

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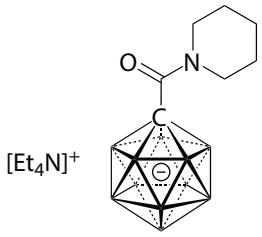

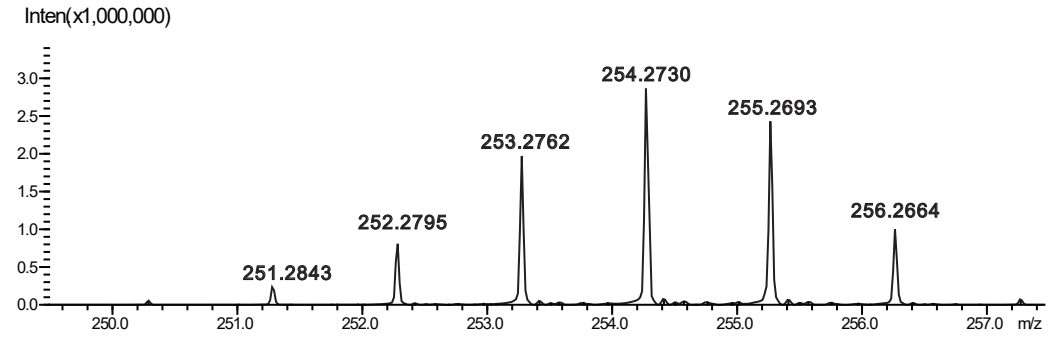

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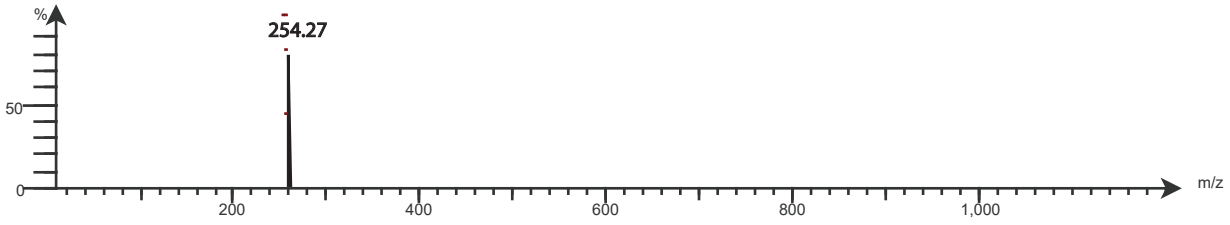
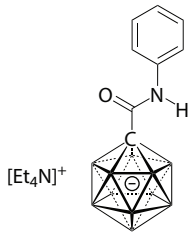
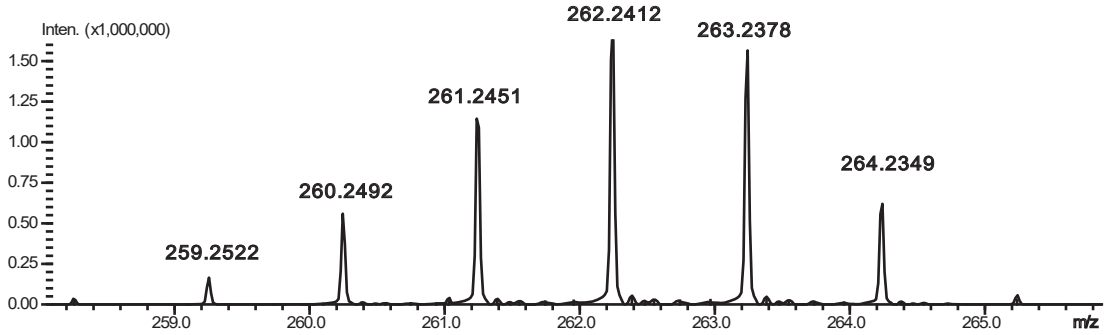
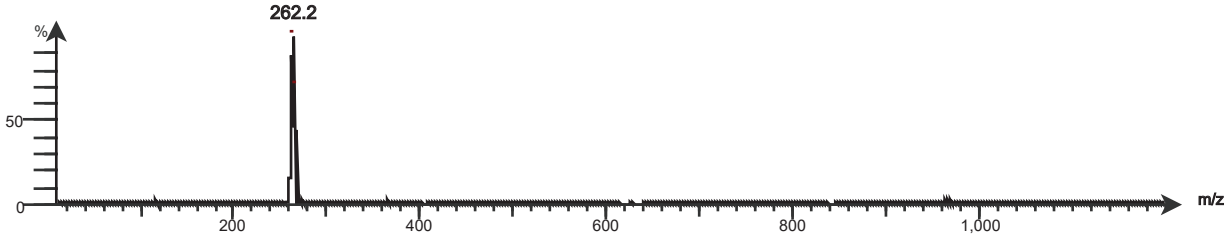


Full-range (–)-ESI-MS Expression CMS

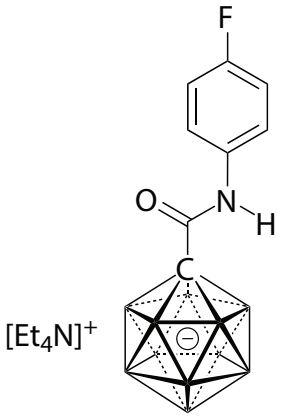


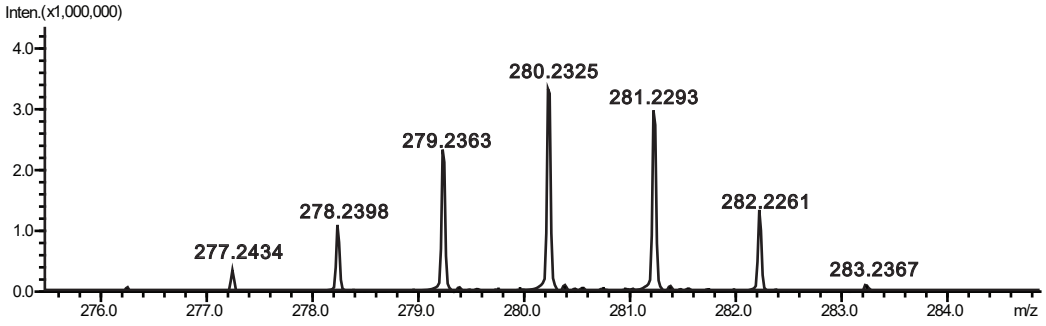


(–)-ESI-HRMS Shimadzu IT-TOF

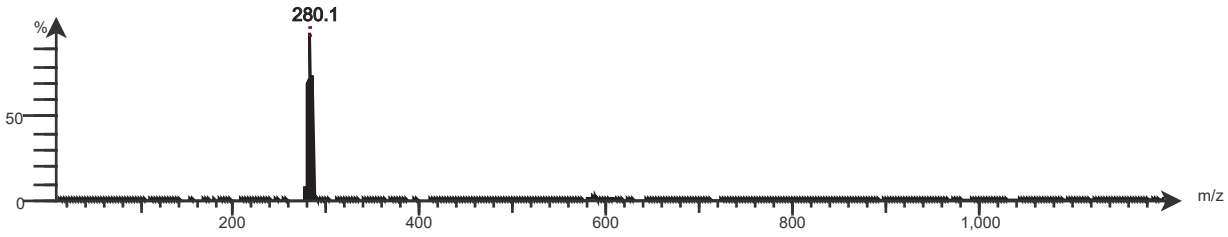


Full-range (–)-ESI-MS Expression CMS

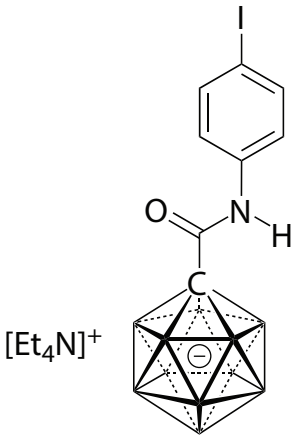


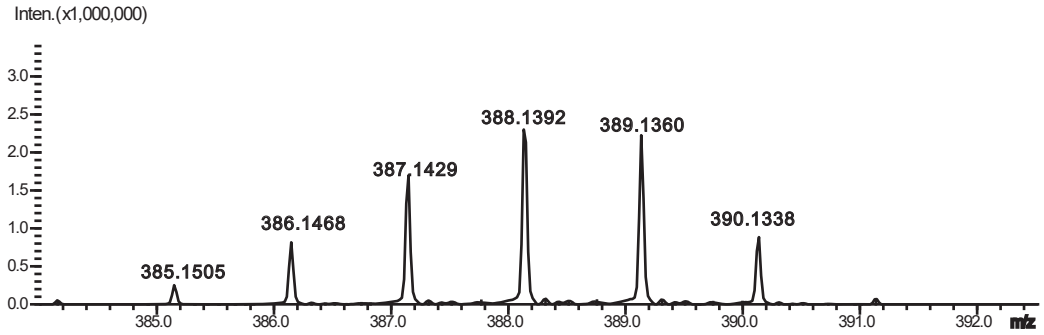


(–)-ESI-HRMS Shimadzu IT-TOF

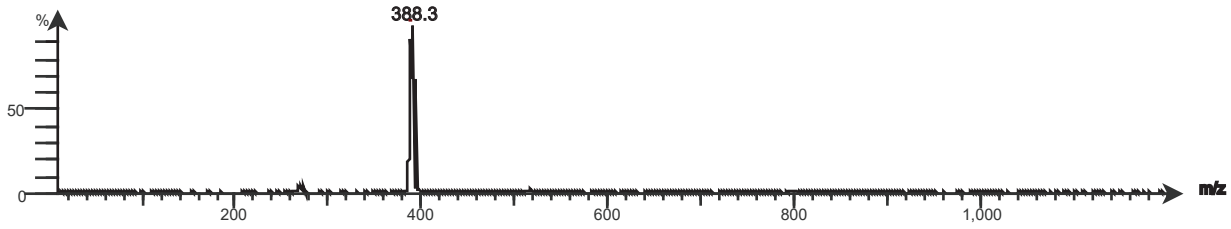


Full-range (–)-ESI-MS Expression CMS

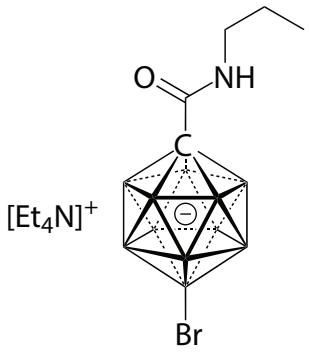


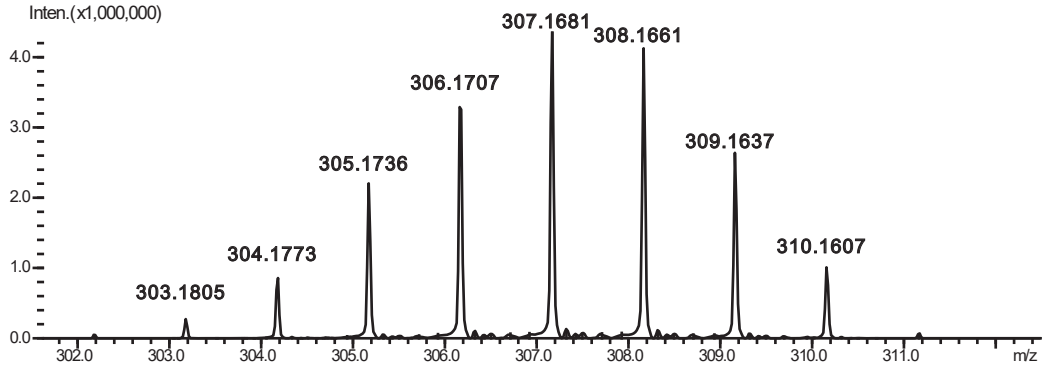


(–)-ESI-HRMS Shimadzu IT-TOF



Full-range (–)-ESI-MS Expression CMS





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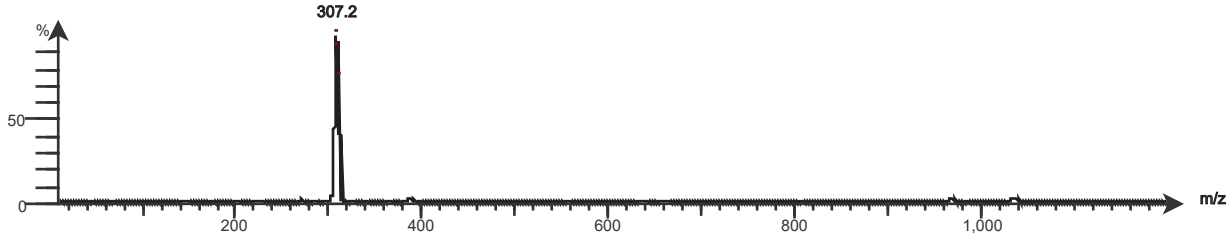
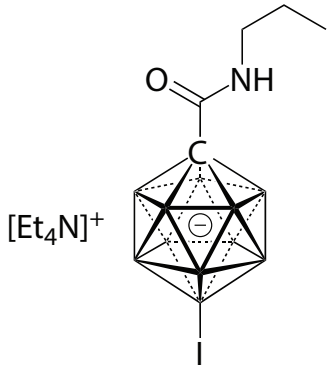
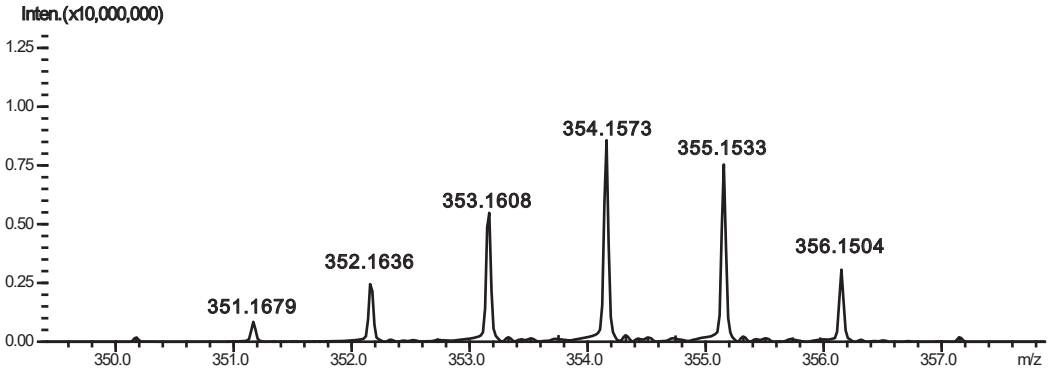
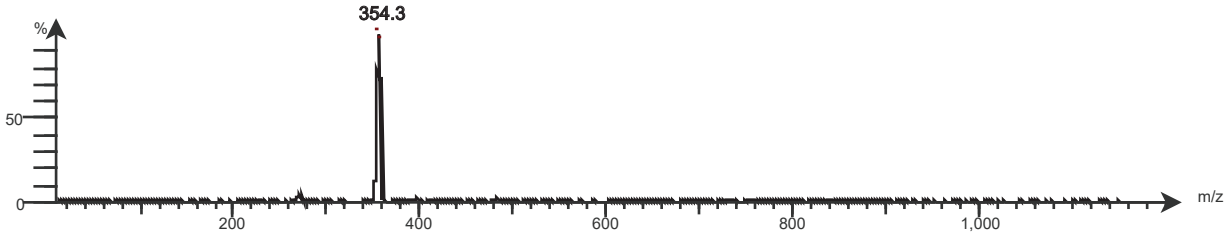


Full-range (–)-ESI-MS Expression CMS





(–)-ESI-HRMS Shimadzu IT-TOF



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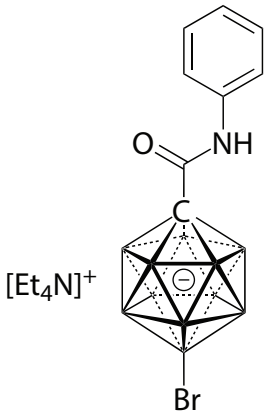

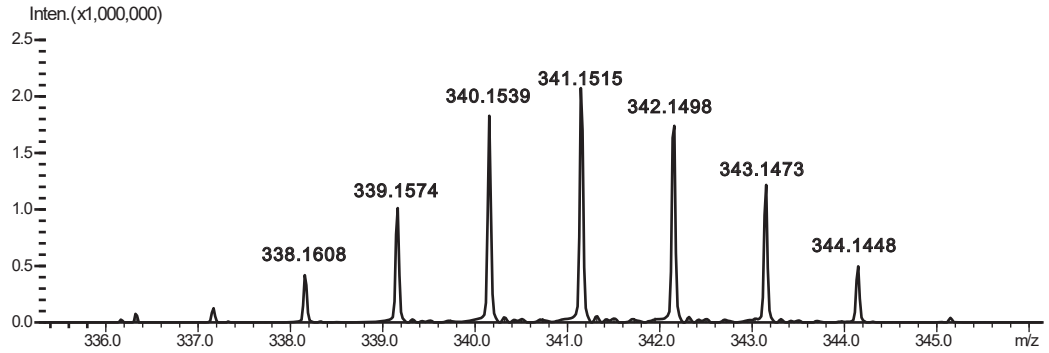

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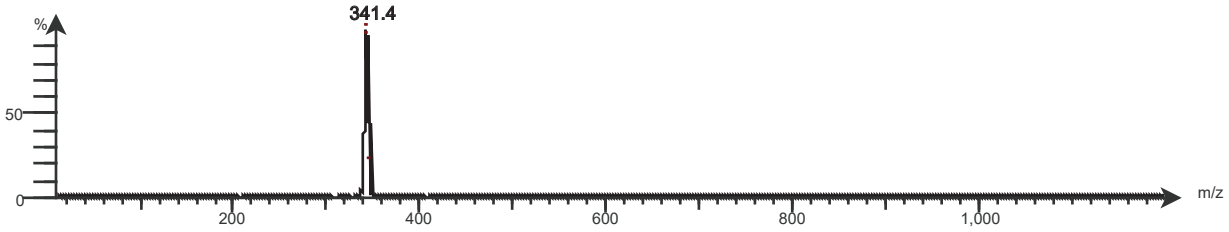

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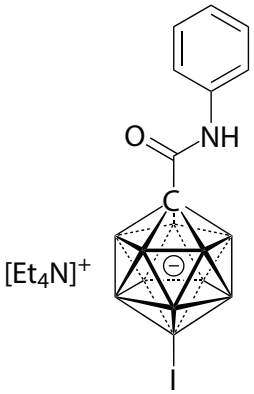

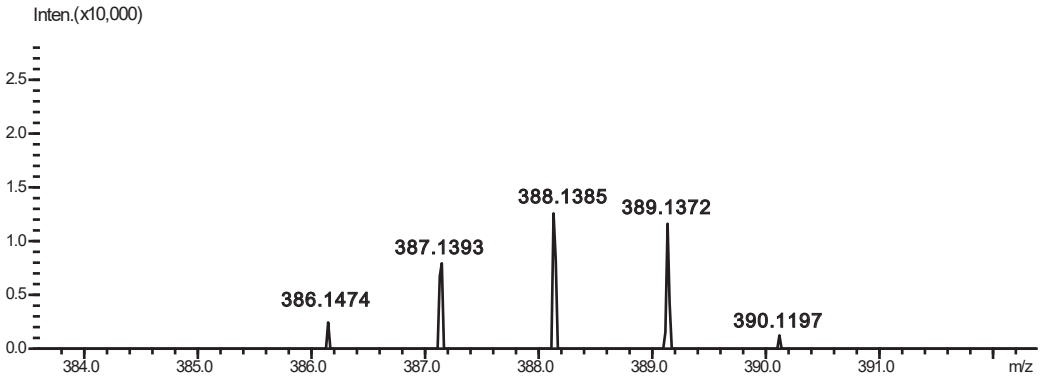

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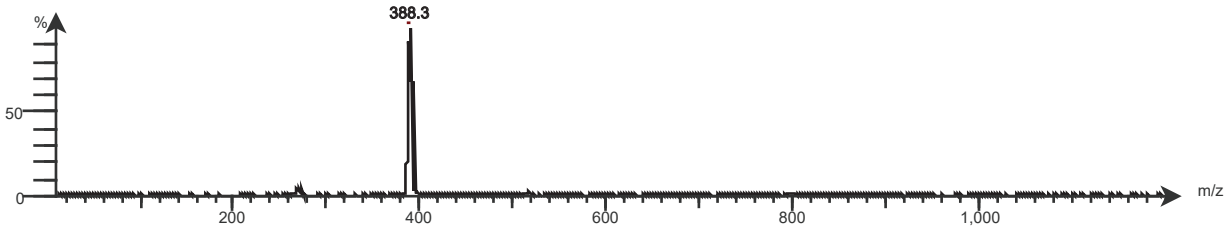

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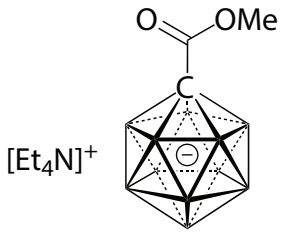

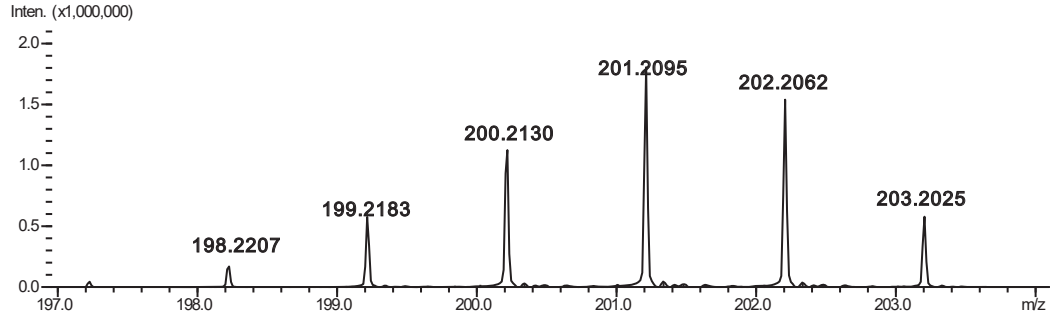

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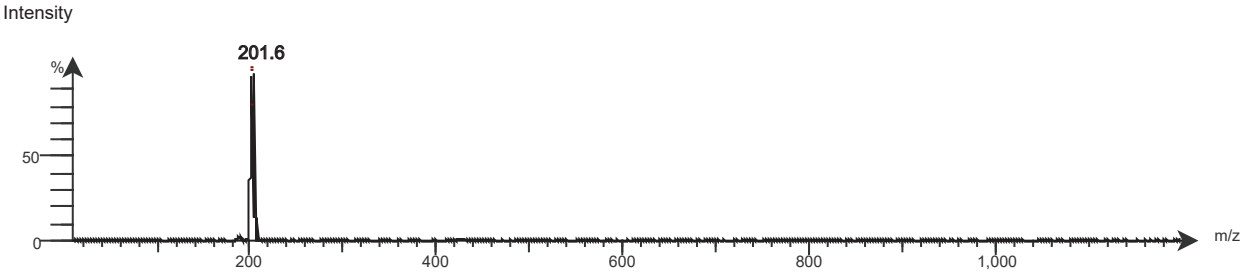

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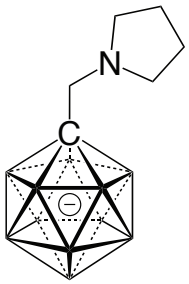

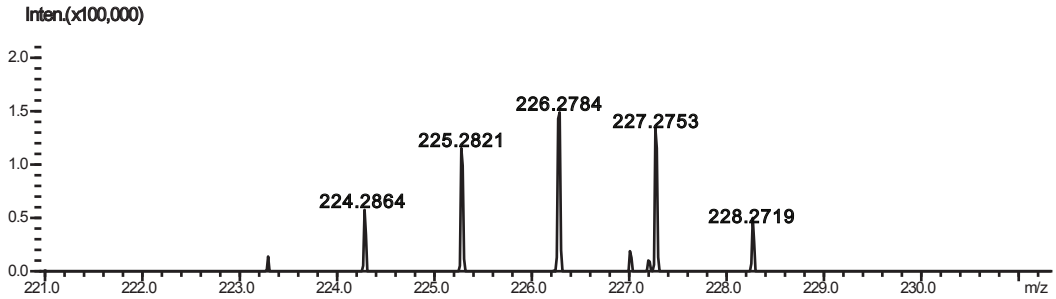

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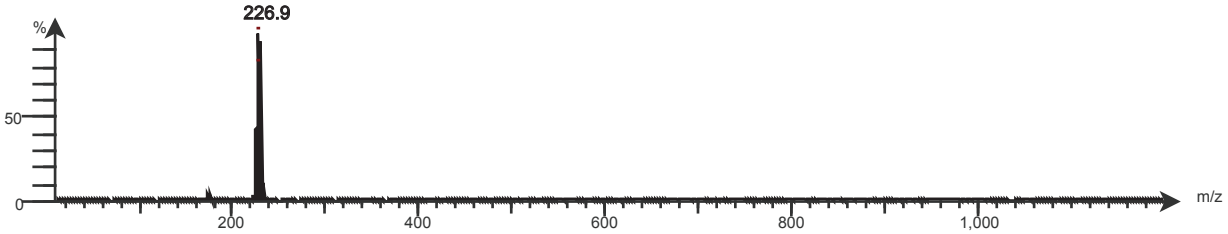

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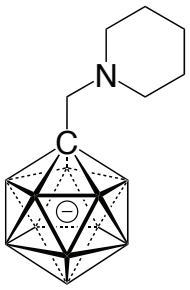

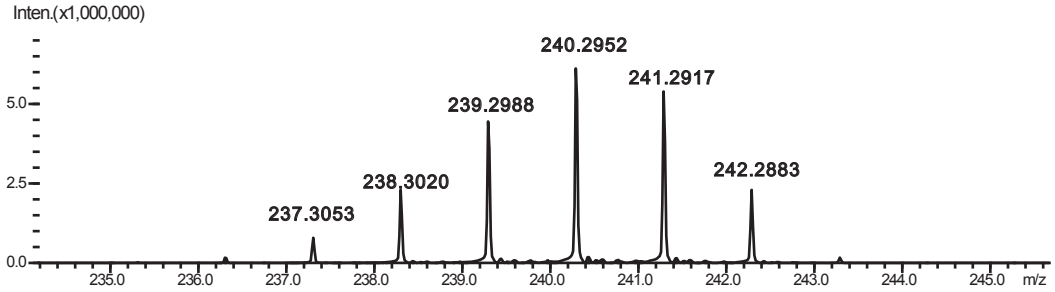

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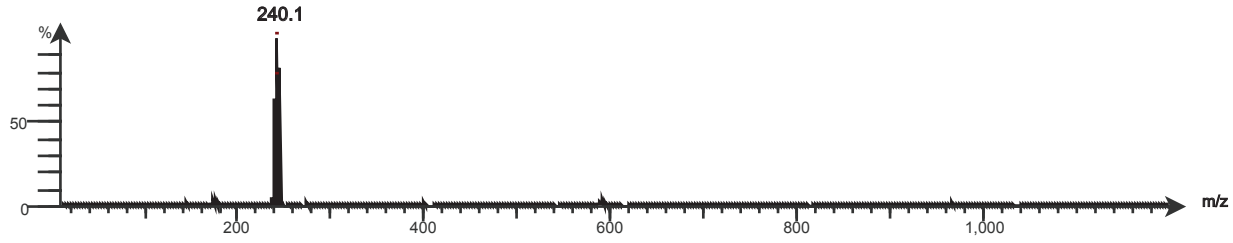

Full-range (–)-ESI-MS Expression CMS