Electronic Supplementary Material (ESI) for ChemComm.

Supplementary Information for

Palladium-catalyzed B7–11 penta-arylation of the {CB_{11}} monocarborane cluster

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I General Information

Chemicals

If not otherwise specified, reagents and organic solvents were commercially available from the company Energy (China) and used without further purification. Acetone-d_6 and dimethyl sulfoxide- d_6 were purchased from Cambridge Isotope Laboratories**.**
The anions $[CB_{11}H_{12}]^-$, $[CB_{11}H_{11}\text{-}12\text{-}I]^-$, $[CB_{11}H_{11}\text{-}12\text{-}CN]^-$ and $[CB_{11}H_{11}\text{-}12\text{-}COOH]^-$ were prepared according to the literature.[1–3]

Characterization

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

2) 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 interpretation (where applicable). Signals were referenced against solvent peaks (^{1}H: residual C*H*D$_2$C(O)CD$_3$ = 2.05 ppm, C*H*D$_2$S(O)CD$_3$ = 2.50 ppm, ^{13}C{^{1}H}: *C*D$_3$C(O)*C*D$_3$ = 29.84 ppm, *C*D$_3$S(O)*C*D$_3$ = 39.52 ppm). ^{11}B and ^{11}B{^{1}H} NMR spectra were calibrated against external BF_3*Et_2O = 0 ppm (BF_3*Et_2O capillary in C_6D_6). Baseline correction for ^{11}B and ^{11}B{^{1}H} NMR spectra was carried out using the baseline correction function of the software TopSpin 3.5.

Additional remark about the NMR spectra:

a) In certain ^{1}H and ^{1}H{^{11}B} NMR spectra measured in acetone-d_6, double water peaks were observed. This is a result of different resonances from H_2O and HOD and has been described in the literature.[4] In our experience, the appearance of double water peaks depends on the temperature, water content and compound being measured. A spectrum of acetone-d_6 in which the distinct resonances from H_2O and HOD are visible is shown in Figure S1.

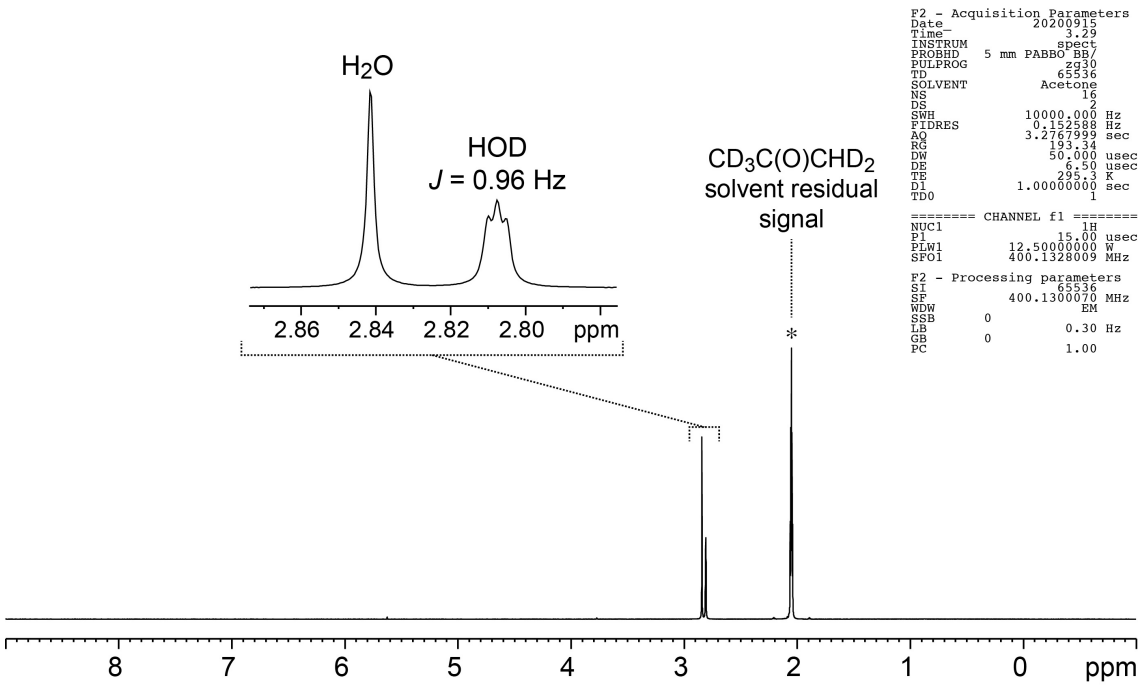

Figure S1. ^{1}H NMR spectrum of acetone-d_6 solvent as received from Cambridge Isotope Laboratories (400 MHz, 22 °C).

b) Integration of the B–H signals in the $^{1}H\{^{11}B\}$ spectra gave numbers of approximately 4–5 instead of 5 for the upper-belt hydrogen atoms. This is because coupling to ^{10}B (I = 3, 20% abundance) is still present and leads to severe broadening of the ^{10}B–H resonances.

c) Some products with an aryl *para*-substitution gave complicated ^{1}H signals for the *ortho* and *meta* positions because of magnetic inequivalence of the Ar-H hydrogen atoms ($H_AH_{A'}H_BH_{B'}$ spin system). Resonances are reported as doublets when they appeared as doublets, otherwise as multiplets.

d) For the $[Et_4N]^+$ cation, coupling to ^{14}N (I = 1) was observed in many of the ^{1}H and $^{13}C\{^{1}H\}$ spectra, leading to triplet-like splitting. Coupling is reported when it was visible.

e) In the $^{13}C\{^{1}H\}$ NMR spectra, the signals of B7–11–$\boldsymbol{C_{ipso}}$ were weak because of severe broadening and splitting by the quadrupolar nuclei ^{10}B (I = 3, 20% abundance) and ^{11}B (I = 3/2, 80% abundance).
Processing the FID with a line broadening factor of LB =20 Hz enhances the signal-to-noise ratio and can be used to improve the visibility of the $\boldsymbol{C_{ipso}}$ signal, however, at the cost of decreased resolution. This effect is illustrated in Figures S2 and S3. The spectra displayed in

Section V were processed with a line broadening factor of LB = 1 Hz.
Indirect detection of B7–11–$\boldsymbol{C_{ipso}}$ can be achieved using ^{1}H-^{13}C HMBC NMR spectroscopy. In these spectra, the correlation signal caused by $^{3}J_{H,C}$ coupling between $^{1}H_{meta}$ and $\boldsymbol{C_{ipso}}$ revealed the chemical shift of $\boldsymbol{C_{ipso}}$. An example is shown in Figures S4 and S5. Indirect detection was not applied to all of the compounds.

f) In the $^{13}C\{^{1}H\}$ NMR spectra, the signal of B12–***C*** could not detected even at sample concentrations of 30 mg/0.6 mL and using 2048 scans. The reason is severe broadening and splitting of the resonance by ^{11}B and ^{10}B.

3) High-resolution MS data were recorded using a Shimadzu IT-TOF MS instrument. The plots with a large *m/z* range demonstrate bulk purity. The zoomed-in plots show the observed isotopic pattern from the HRMS measurements.

4) Single-crystal X-ray diffraction studies were performed on a Bruker D8 Venture instrument using MoK-α radiation.

5) Elemental analysis was performed using an Elementar Vario MICRO instrument (C, H, N) in combination with pure gas carriers (helium ≥99.995%; oxygen ≥99.995%). Measurements were carried out with three randomly chosen samples in order to demonstrate agreement with bulk purity as assessed by NMR spectra and full-range mass spectra. The samples chosen were [Et_4N][**3h**], [Et_4N][**3r**] and [Et_4N][**3s**].

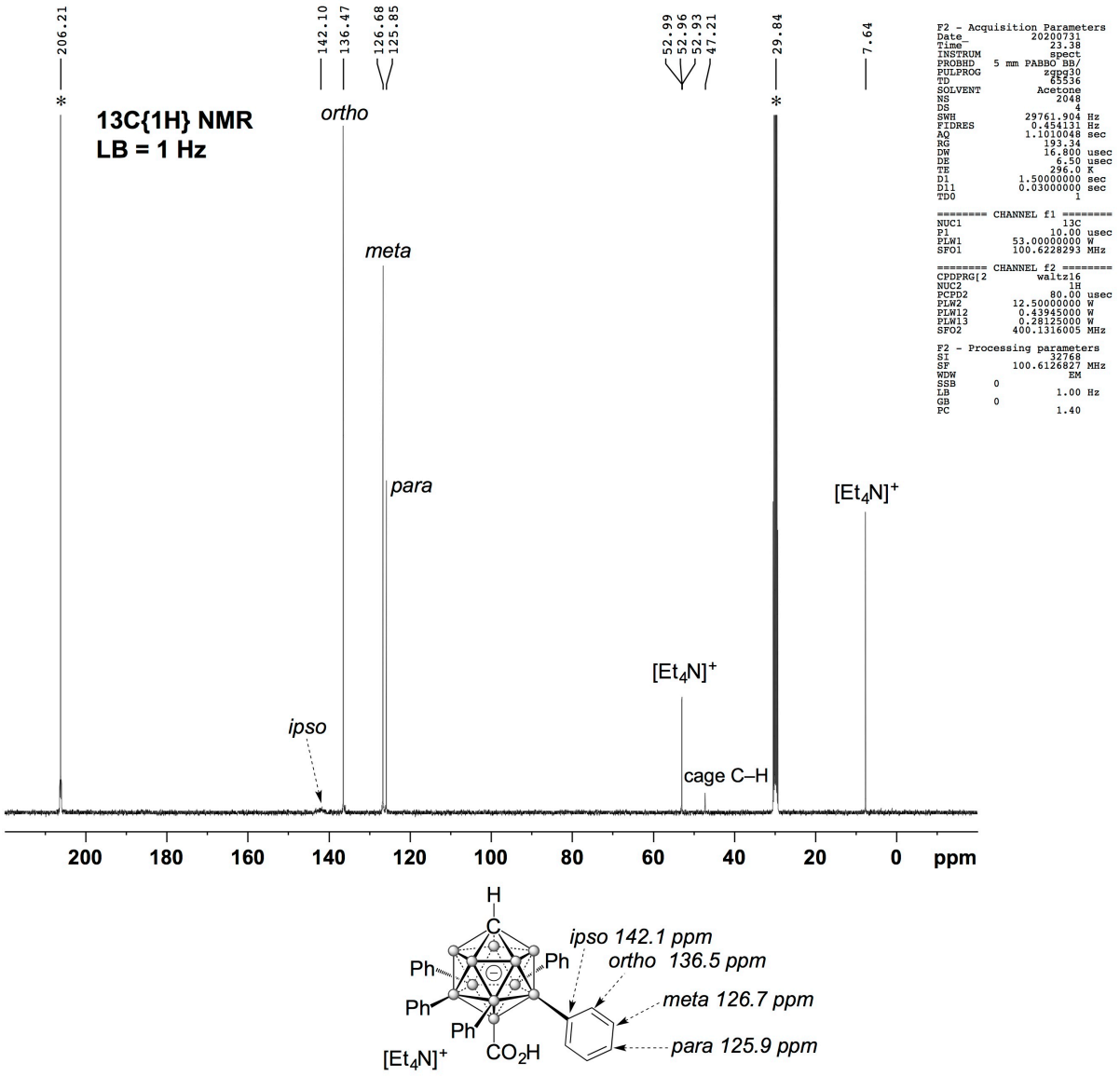


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Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of $[Et_4N][CHB_{11}\text{-}7,8,9,10,11\text{-}Ph_5\text{-}12\text{-}(CO_2H)]$ processed with a line broadening factor of LB = 1 Hz. The *ipso* signal appears as a weak and broad resonance at 142 ppm, while the B12-***C***O_2H signal is not visible. 101 MHz, acetone-d_6, 23 °C, * = solvent signals.

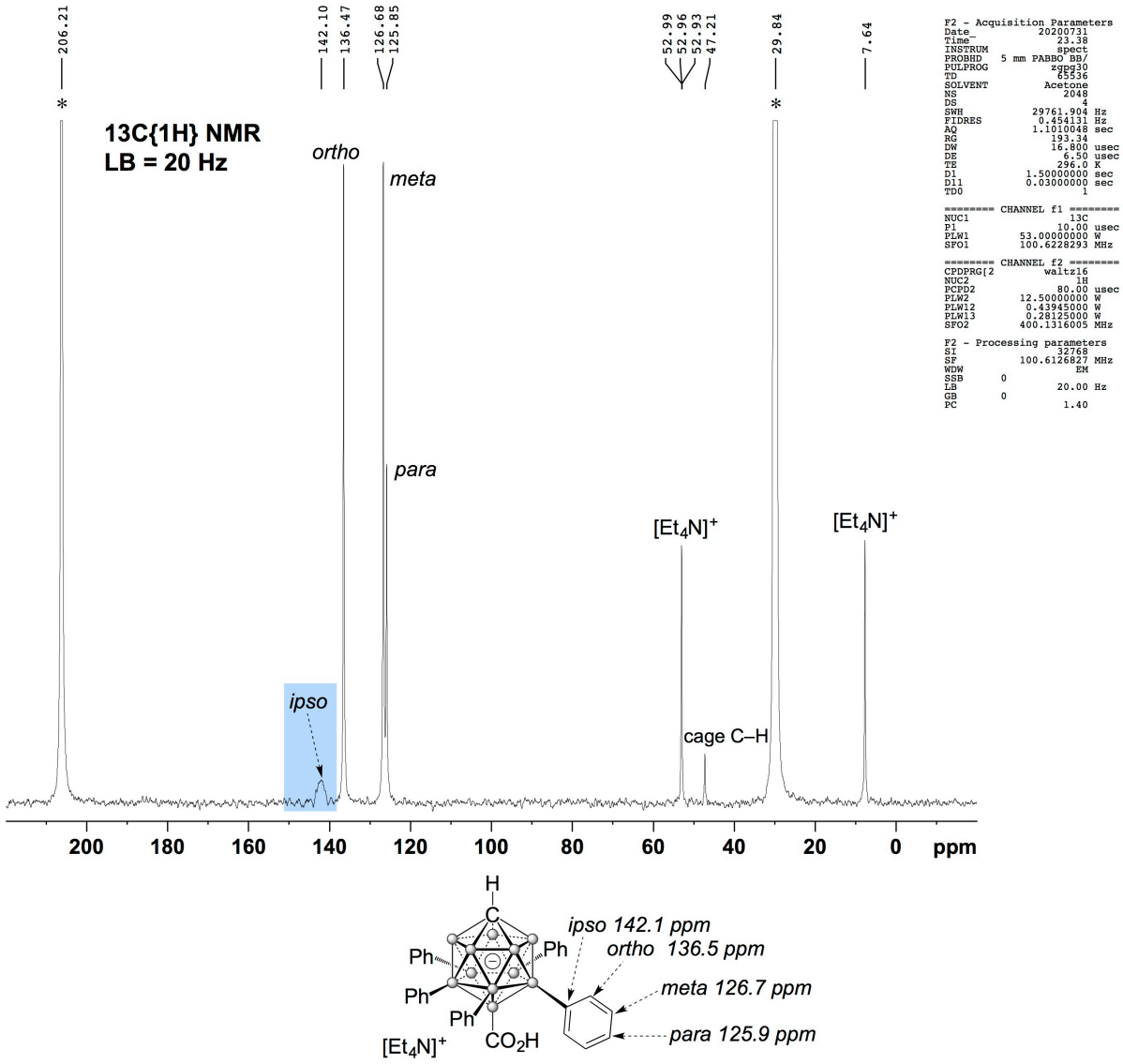


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of $[Et_4N][CHB_{11}\text{-}7,8,9,10,11\text{-}Ph_5\text{-}12\text{-}(CO_2H)]$ processed with a line broadening factor of LB = 20 Hz. The *ipso* signal appears as a resonance at 142 ppm (highlighted in blue), while the B12-***C***O_2H signal is not visible. 101 MHz, acetone-d_6, 23 °C, * = solvent signals.

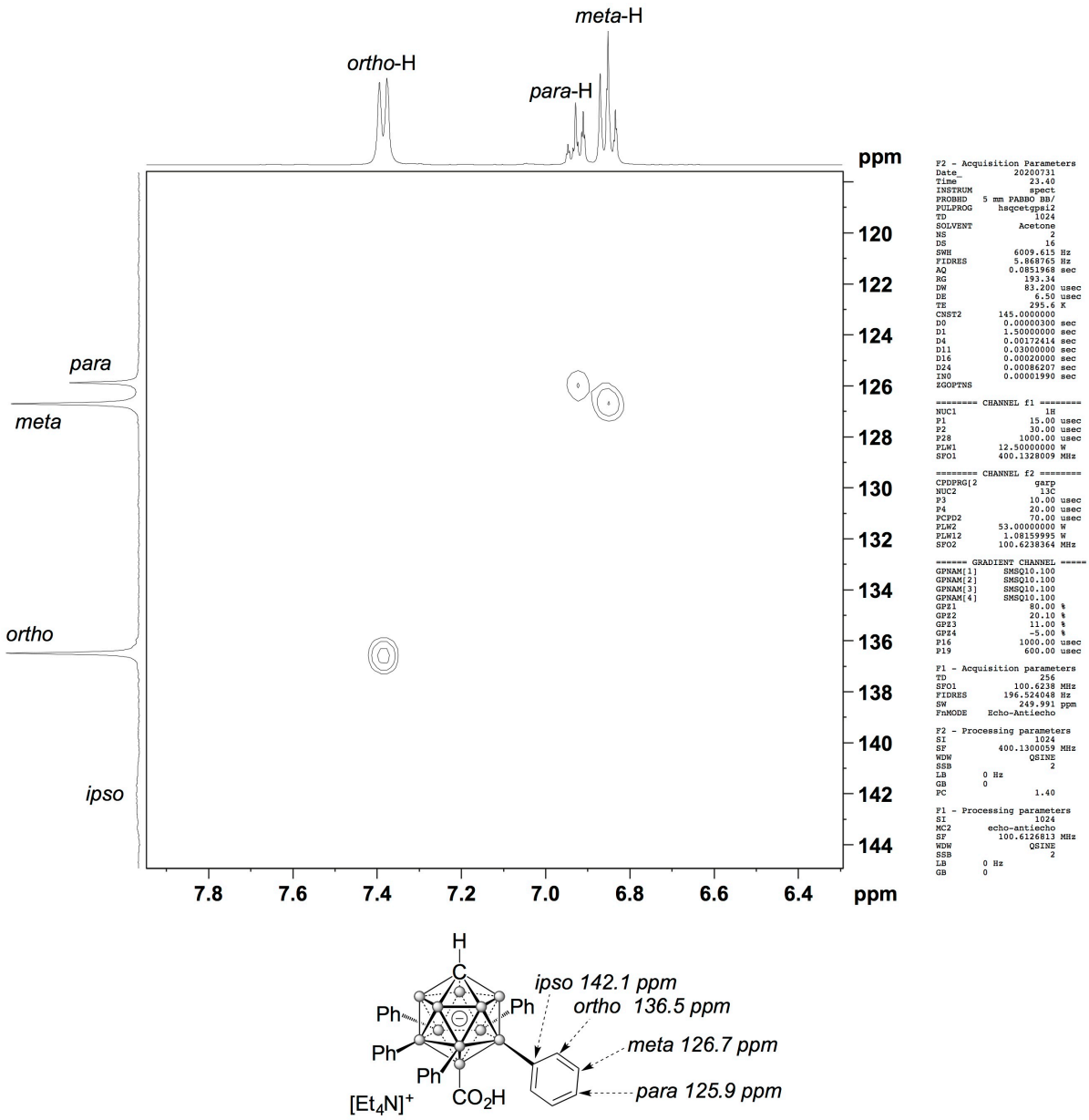


Figure S4. ^{1}H-^{13}C HSQC NMR spectrum of $[Et_4N][CHB_{11}$-7,8,9,10,11-Ph_5-12-$(CO_2H)]$ showing the direct C–H connections. 400 MHz/101 MHz, acetone-d_6, 23 °C.

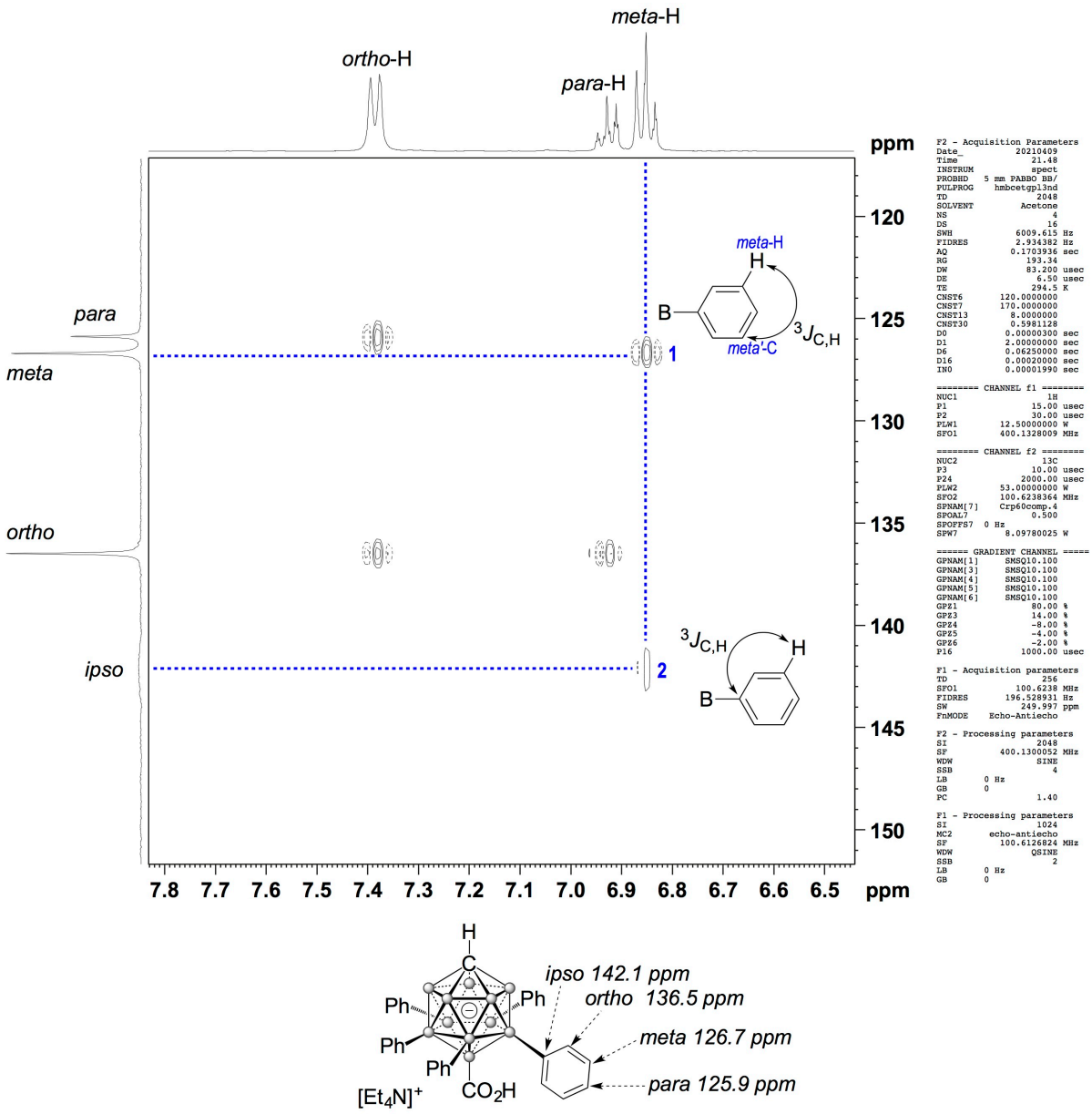


Figure S5. ^{1}H-^{13}C HSQC NMR spectrum of $[Et_4N][CHB_{11}$-7,8,9,10,11-Ph_5-12-$(CO_2H)]$ showing $^3J_{C,H}$ couplings. **1** is a correlation signal between the positions *meta*-H and *meta*'-C, and **2** shows the *meta*-H/*ipso*-C correlation. 400 MHz/101 MHz, acetone-d_6, 23 °C.

6) Regioisomeric purity

The starting material $[Et_4N][12\text{-}(COOH)\text{-}CB_{11}H_{11}]$ was prepared by the sequence $[Cs][CB_{11}H_{12}] \rightarrow [Et_4N][12\text{-}I\text{-}CB_{11}H_{11}] \rightarrow [Et_4N][12\text{-}CN\text{-}CB_{11}H_{11}] \rightarrow [Et_4N][12\text{-}(COOH)\text{-}CB_{11}H_{11}]$.[3] Monoiodination of the parent carborane, the first step, affords a crude regioisomeric mixture of *ca.* 85:15 of $[12\text{-}I\text{-}CB_{11}H_{11}]^-$ and $[7\text{-}I\text{-}CB_{11}H_{11}]^-$. Recrystallization at this stage increases the ratio to >96:4, and in our experience it is preferred over recrystallization later in the sequence. Therefore, monoiodocarborane with high regioisomeric purity gives the carborane carboxylic acid in equally high purity (Fig. S6).

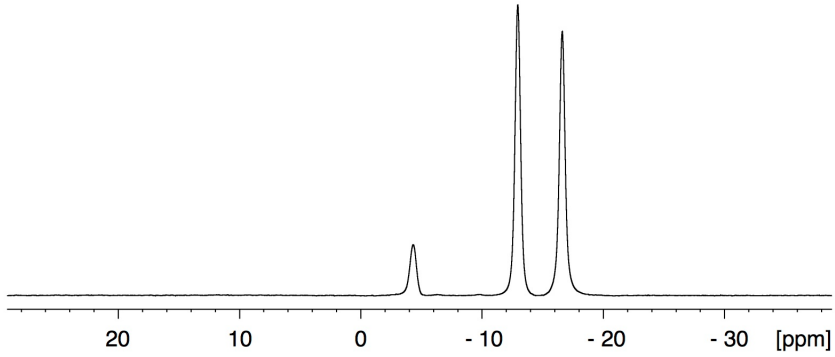


Figure S6. $^{11}B\{^1H\}$ NMR spectrum (128/400 MHz, acetone-d_6) of $[Et_4N][12\text{-}(COOH)\text{-}CB_{11}H_{11}]$.

On the other hand, ^{11}B NMR spectra of mixtures of carborane carboxylic acid with a higher amount of $[7\text{-}(COOH)\text{-}CB_{11}H_{11}]^-$ (starting from less pure monoiodocarborane) clearly show additional signals (Fig. S7). This is in agreement with the original publication describing the synthesis of $[12\text{-}(COOH)\text{-}CB_{11}H_{11}]$, for which the supporting information displays a spectrum with visible signals of $[7\text{-}(COOH)\text{-}CB_{11}H_{11}]$ (Fig. S9).[3]

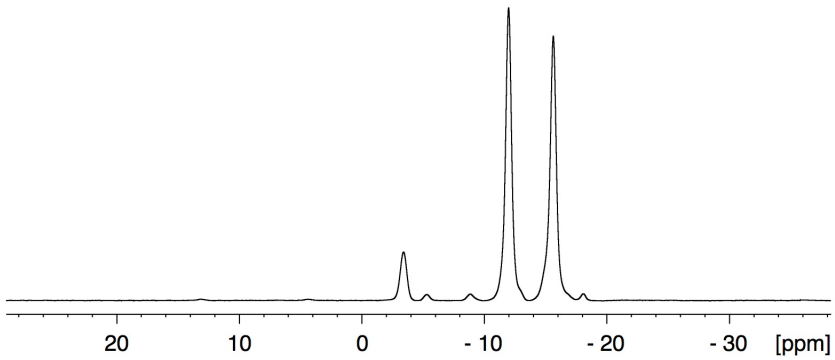


Figure S7. $^{11}B\{^1H\}$ NMR spectrum (128/400 MHz, acetone-d_6) of $[Et_4N][12\text{-}(COOH)\text{-}CB_{11}H_{11}]$ containing small amounts of $[Et_4N][7\text{-}(COOH)\text{-}CB_{11}H_{11}]$.

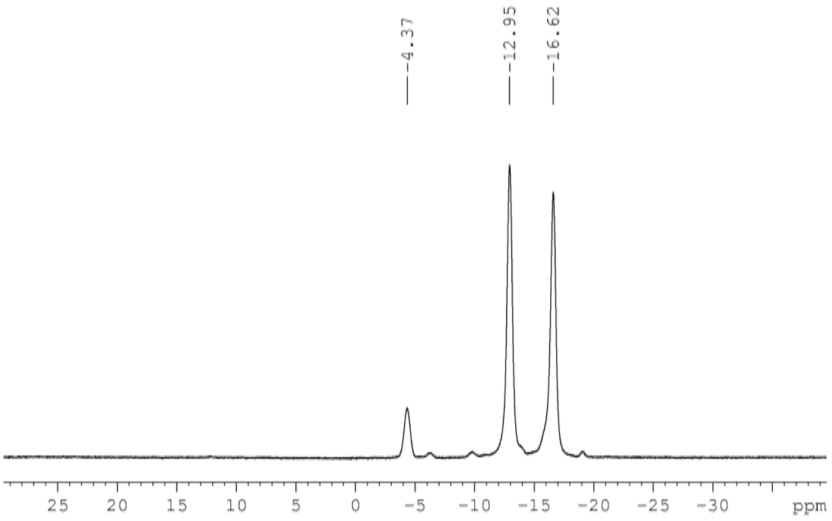


Figure S8. $^{11}B\{^{1}H\}$ NMR spectrum (128/400 MHz, acetone-d_6) of $[Et_4N][12\text{-}(COOH)\text{-}CB_{11}H_{11}]$ as reported by Juhasz and coworkers in "Copper-Promoted Cyanation of a Boron Cluster: Synthesis, X-ray Structure, and Reactivity of 12-CN-*closo*-$CHB_{11}H_{10}^-$" (p. S14 of the Supporting Information). Reprinted with permission from *Inorg. Chem.* **2013**, *52*, 10717. Copyright 2013 American Chemical Society.

For the penta-arylation reactions, we used different batches of carborane carboxylic acid with regioisomeric purity of 97:3 and higher. In some of the spectra of the final compounds **3**, the small resonance at –11.5 ppm stems from the $[7\text{-}(COOH)\text{-}2,3,8,11,12\text{-}Ar_5\text{-}CB_{11}H_6]$ isomer. This interpretation was confirmed by performing the penta-arylation using less regioisomerically pure carborane carboxylic acid. It is also consistent with the full-range mass spectra, which are devoid of signals from potential by-products with a different *m/z*.

II Experimental Section

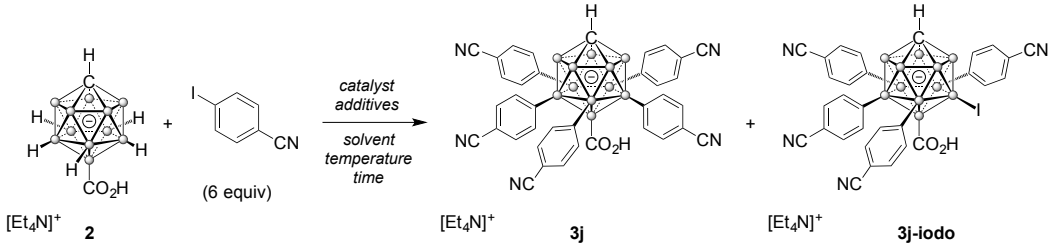
Synthesis of starting the material [Et_4N][12-COOH-$CB_{11}H_{11}$] (modified procedure of literature [3], using H_2SO_4 instead of HCl for hydrolysis)

A 35 mL microwave vial was charged with [Et_4N][12-CN-$CB_{11}H_{11}$] (400 mg, 1.34 mmol), 80 % H_2SO_4 (12 mL) and glacial acetic acid (3 mL). The vial was capped and heated to 120 ^oC for 70 minutes. The resulting mixture was extracted with dichloromethane (3 x 25 mL). The organic layers were combined and evaporated to dryness on a rotary evaporator. The residue was dissolved in 15 mL of 1 M aqueous NaOH solution. NEt_4Br (560 mg, 2.68 mmol) was added to the NaOH solution, followed by filtration. Concentrated aqueous HCl was added to the filtrate until the mixture became acidic (pH *ca.* 2) and a white precipitate had formed. The solution was cooled briefly and filtered. The collected solid was washed with 5 mL of cold water to afford [Et_4N][12-COOH-$CB_{11}H_{11}$] as a colorless solid (305.8 mg, 72%).

Optimization of Conditions for Penta-Arylation

Reaction conditions were screened using the substrate 4-iodobenzonitrile, and the outcome was assessed by ESI mass spectrometry in the negative mode (Table S1). This substrate gave clearly distinguishable *m/z* signals for the desired product **3j** and the by-product **3j-iodo** that was observed under certain conditions. In the cases where the mass spectra indicated relatively clean formation of **3j**, the product was isolated and purified by column chromatography (entries 4, 10, 11 and 18). A control experiment without Pd catalyst afforded starting materials (entry 12).

Table S1. Screening of conditions for the desired reaction **2** → **3j**.



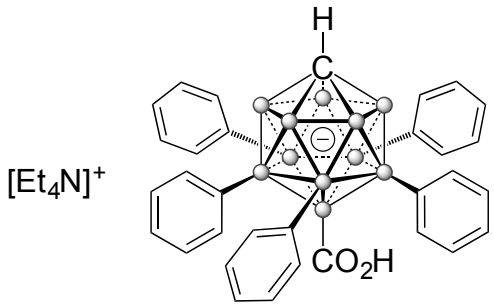
Entry	Catalyst (mol%)	Additives (equiv)	*T* / time	Solvent	Result[a]
1	$Pd(OAc)_2$ (10)	AgOAc (6), AcOH (6)	80 °C °C / 24 h	DMF	mixture[b]
2	$Pd(OAc)_2$ (10)	$AgNO_3$ (6), AcOH (6)	80 °C / 24 h	DMF	mixture
3	$Pd(OAc)_2$ (10)	$AgSbF_6$ (6), AcOH (6)	80 °C / 24 h	DMF	mixture
4	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), AcOH (6)	80 °C / 24 h	DMF	**3j** : **3j-iodo** = 100% : 15% Isolated: 52%[c]
5	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), AcOH (6)	80 °C / 24 h	Toluene	mixture
6	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), AcOH (6)	60 °C / 24 h	MeCN	mixture
7	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), AcOH (6)	80 °C / 24 h	DCE	mixture
8	$Pd(PPh_3)_2Cl_2$(10)	Ag_2CO_3 (6), AcOH (6)	80 °C / 24 h	DMF	mixture
9	$PdCl_2$(10)	Ag_2CO_3 (6), AcOH (6)	80 °C / 24 h	DMF	mixture
10	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), AcOH (6)	40 °C / 36 h	DMF	**3j** : **3j-iodo** = 100% : 13% Isolated: 63%[c]
11	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6)	40 °C / 24 h	DMF	**3j** : **3j-iodo** = 100% : 13% Isolated: 65%[c]
12	–	Ag_2CO_3 (6), AcOH 6)	40 °C / 24 h	DMF	no reaction
13	$Pd(OAc)_2$ (2.5)	Ag_2CO_3 (6)	40 °C / 36 h	DMF	**3j** : **3j-iodo** = 100% : 10%
14	$Pd(OAc)_2$ (50)	Ag_2CO_3 6)	40 °C / 24 h	DMF	**3j** : **3j-iodo** = 100% : 30%
15	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), NaOAc (6)	40 °C / 12 h	DMF	**3j** : **3j-iodo**: nbp[d] = 100% : 3% :13%
16	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), $Cu(OAc)_2$ (6)	40 °C / 48 h	DMF	mixture
17	$Pd(OAc)_2$ (10)	Ag_2CO_3 (6), LiOAc (6)	40 °C / 48 h	DMF	**3j** : **3j-iodo** = 100% : 5%
18	**$Pd(OAc)_2$ (10)**	**Ag_2CO_3 (6), NaOAc (5)**	**40 °C / 24 h**	**DMF**	**3j : 3j-iodo = 100% : 3%;** **Isolated yield 82%[c]**

[a] Ratio of **3j** and **3j-iodo** as indicated by (–)ESI-MS; [b] Mixture = complex reaction mixture with a large number of unidentified signals according to ESI-MS; [c] The reaction was set up on a 0.1 mmol scale, and the yield is the isolated yield after silica gel chromatography. [d] nbp = new unidentified by-product.

General Procedure for the Penta-Arylation

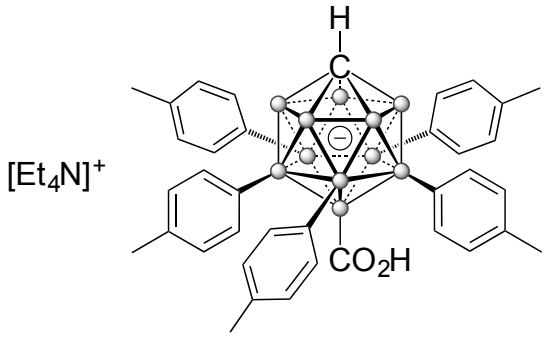
In a 10 ml vial, carborane carboxylic acid (0.1 mmol, 1 equiv), Ag_2CO_3 (0.6 mmol, 6 equiv), aryl iodide (0.6 mmol, 6 equiv), $Pd(OAc)_2$ (0.01 mmol, 10 mol%) and NaOAc (0.5 mmol, 5 equiv) were dissolved (Ag_2CO_3 and NaOAc remained partially suspended) in DMF (2 mL). The resulting mixture was stirred at 40 °C or 60 °C for 18-48 h until ESI-MS analysis showed no remaining carborane acid. The turbid reaction mixture was filtered through celite in a glass funnel, and the solid on the top of the celite was washed with MeCN (3 x 10 mL) to dissolve the crude product. The filtrate was concentrated on a rotary evaporator (40 °C, *ca.* 100 mbar). Most of the MeCN was removed under these conditions, while the DMF solvent remained. To the remaining solution, an aqueous solution of $[Et_4N]Br$ (30 mL, c = 1 g/50 mL) was added, and a colorless precipitate formed immediately. The precipitate was then collected by filtration through a fritted glass funnel (F porosity). The solid on the glass frit was washed with deionized water (3 x 10 mL, the crude product remained undissolved). The crude product was dried under vacuum at room temperature for 12 h and then purified by column chromatography using a mixture of CH_2Cl_2 and MeCN as the eluent to afford the penta-arylation product.

Spectroscopic Data



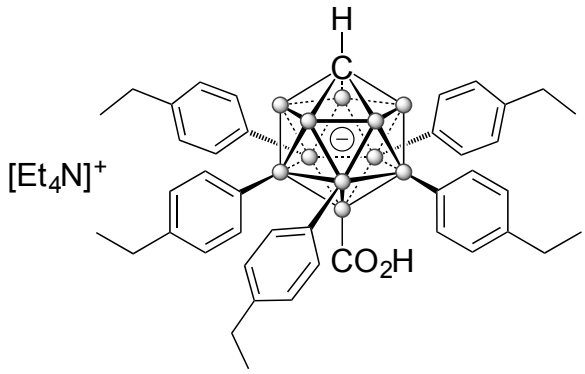
Reaction conditions: 48 h, 60 °C, 86 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 8.18 (broad signal, 1H, COOH), 7.81(d, *J* =7.1Hz, 10H, Ar-H), 6.95-6.89 (m, 5H, Ar-H), 6.89-6.81 (m, 10H, Ar-H), 3.41(q, *J* =7.3 Hz, 8H, CH_2 of cation), 2.85 (broad signal, 1H, overlapping with the signal of water, confirmed by HSQC, cage CH), 2.41 (broad signal, 5H, BH), 1.33 (tt, *J*=7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.73(5B, B-C), -5.85 (1B, B-COOH), -16.22 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 141.98 (broad signal, B-C_{aryl}), 136.47, 126.67, 125.85 (Ar-C), 52.96 (t, *J* = 2.7 Hz, CH_2 of cation), 47.21 (cage C), 7.64 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{32}B_{11}O_2]^-$: 567.3499. Found: 567.3452.



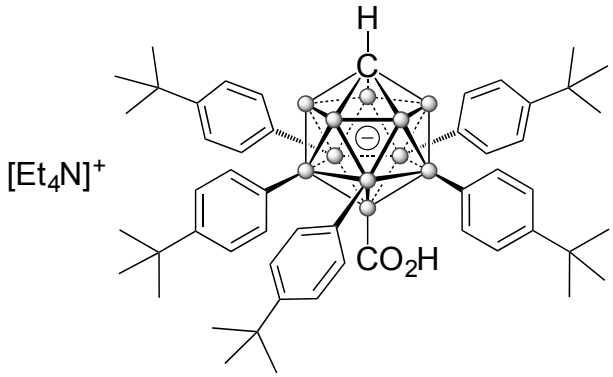
Reaction conditions: 48 h, 60 °C, 67 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 7.99 (broad signal, 1H, CO*OH*), 7.31(d, *J* = 7.9Hz, 10H, Ar-H), 6.67(d, *J* =7.9 Hz 10H, Ar-H), 3.42 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.79 (broad signal, 1H, cage CH), 2.35 (broad signal, 5H, BH), 2.13 (s, 15H, CH_3), 1.34(tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.85 (5B, B-C), -6.18 (1B, B-COOH), -16.30 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 138.74 (broad signal, B-C_{aryl}), 136.45, 134.66, 127.68 (Ar-C), 52.97(t, *J* = 2.7 Hz, CH_2 of cation), 46.93(cage C), 21.23 (CH_3), 7.67 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{37}H_{42}B_{11}O_2]^-$: 637.4281. Found: 637.4278.



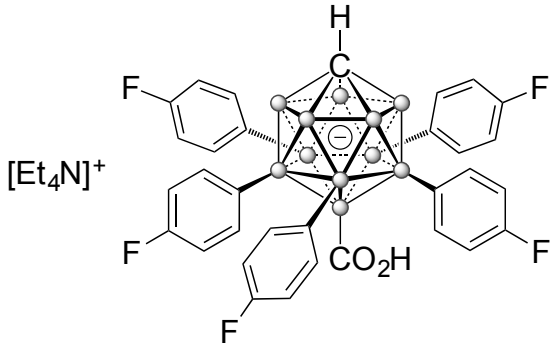
Reaction conditions: 48 h, 60 °C, 64 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 7.96 (broad signal, 1H, COOH), 7.35 (d, J = 7.6 Hz, 10 H, Ar-H), 6.72 (d, J = 7.6 Hz, 10H, Ar-H), 3.44 (m, 8H, CH_2 of cation), 2.81 (broad signal, 1H, cage CH), 2.46 (q, J = 7.5 Hz, 10H, CH_2), 2.38 (broad signal, 5H, BH), 1.34 (m, 12H, CH_3 of cation), 1.11 (t, J = 7.5 Hz, 15H, CH_3).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.89 (5B, B-C), -6.18 (1B, B-COOH), -16.24 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 141.17 (Ar-C), 139.22 (broad signal, B-C_{aryl}), 136.46, 126.36 (Ar-C), 52.96 (t, J = 2.7 Hz, CH_2 of cation), 46.99 (cage C), 29.04 (CH_2), 15.86 (CH_3), 7.62 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{42}H_{52}B_{11}O_2]^-$: 707.5064. Found: 707.5087.



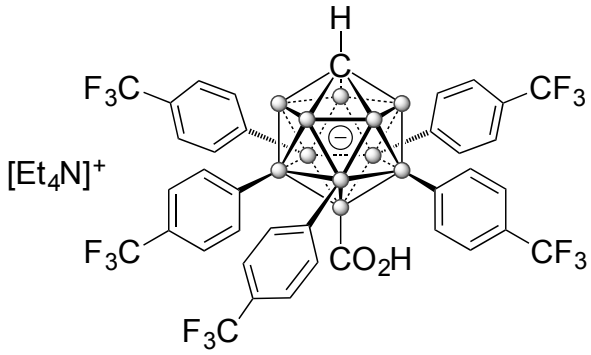
Reaction conditions: 48 h, 60 °C, 52 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 7.95 (broad signal, 1H, COOH), 7.38 (d, *J* = 8.2 Hz, 10H, Ar-H), 6.92(d, *J* = 8.2 Hz, 10H, Ar-H), 3.48 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.82 (broad signal, 1H, cage CH), 2.39 (broad signal, 5H, BH), 1.36 (tt, *J* = 7.3Hz, 1.8 Hz, 12H, CH_3 of cation), 1.19 (s, 45H, CH_3 of *t*-Bu).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.94 (5B, B-C), -6.18 (1B, B-COOH), -16.30 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 147.99 (Ar-C), 138.70 (broad signal, B-C_{aryl}), 136.25, 123.68 (Ar-C), 53.00 (t, *J* = 2.7 Hz, CH_2 of cation), 47.10 (cage C), 34.59 ($C(CH_3)_3$), 31.74 ($C(CH_3)_3$), 7.69 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{52}H_{72}B_{11}O_2]^-$: 847.6629. Found: 847.6608.



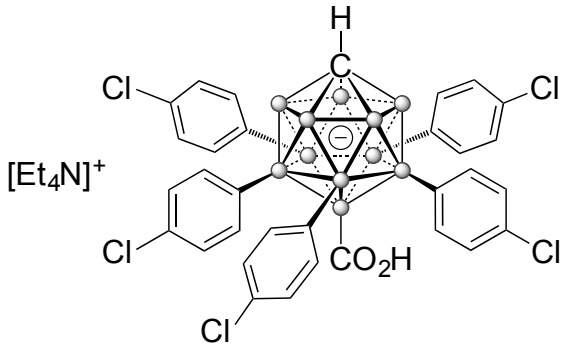
Reaction conditions: 24 h, 40 °C, 75 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*)

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 9.02(broad signal, 1H, COOH), 7.26 (dd, *J* = 6.6Hz, 8.4Hz, 10H, Ar-H), 6.65-6.58 (m, 10H, Ar-H), 3.47(q, *J* =7.3 Hz, 8H, CH_2 of cation), 2.87 (broad signal, 1H, cage C*H*), 2.35 (broad signal, 5H, BH), 1.37 (tt, *J* = 7.3Hz, 1.8 Hz, 12H, CH_3 of cation).
$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 23 °C):): δ -3.98 (5B, B-C), -5.62 (1B, B-COOH), -16.39 (5B, B-H).
$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 162.40 (d, $^1J_{C,F}$ = 241 Hz, C-F), 138.00 (d, $^3J_{C,F}$ = 6.8 Hz), 137.07 (broad signal, B-C_{aryl}), 113.09 (d, $^2J_{C,F}$ = 19.1 Hz), 52.94 (t, *J* = 2.7 Hz, CH_2 of cation), 47.07(cage C), 7.61 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}F_5O_2]^-$: 657.3027. Found: 657.3009.



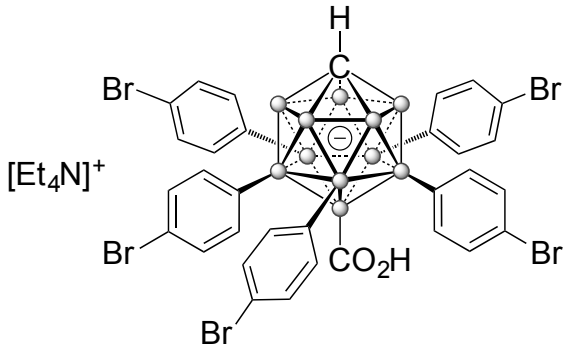
Reaction conditions: 24 h, 40 °C, 74 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d6, 23 °C): δ 9.67(broad signal, 1H, COOH), 7.43 (d, *J* = 7.9 Hz, 10H, Ar-H), 7.19 (d, *J* = 7.9Hz, 10H, Ar-H), 3.50 (q, *J* = 7.3 Hz, 8H, CH2 of cation), 3.12 (broad signal, 1H, cage CH), 2.50 (broad signal, 5H, BH), 1.39 (m, 12H, CH3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d6, 23 °C): δ -3.78 (5B, B-C), -5.24 (1B, B-COOH), -15.78 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d6, 23 °C): δ 146.75 (broad signal, B-C_{aryl}), 136.68 (Ar-C), 127.79 (q, $^{2}J_{C,F}$ = 31 Hz, Ar-C), 126.10 (q, $^{1}J_{C,F}$ = 270 Hz, CF_3), 123.16 (q, $^{3}J_{C,F}$ = 4 Hz, Ar-C), 53.01 (t, *J* = 2.7 Hz, CH_2 of cation), 47.94 (cage C), 7.64 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{37}H_{27}B_{11}F_{15}O_2]^-$: 907.2868. Found: 907.2842.



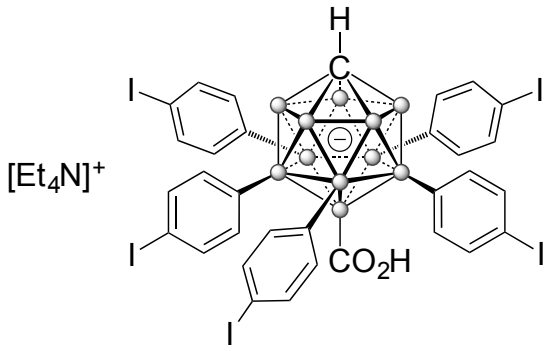
Reaction conditions: 36 h, 40 °C, 66 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*).

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 9.33 (broad signal, 1H, COOH), 7.22 (d, *J* = 8.4 Hz, 10H, Ar-H), 6.88 (d, *J* = 8.4 Hz, 10H, Ar-H), 3.48(q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.92 (broad signal, 1H, cage CH), 2.35 (broad signal, 5H, BH), 1.38 (tt, *J* = 7.3Hz, 1.8Hz, 12H, CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -4.26 (5B, B-C), -5.69 (1B, B-COOH), -16.19 (5B, B-H).
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 140.40 (broad signal, B-C_{aryl}), 137.99, 131.81, 126.61 (Ar-C), 52.98 (t, *J* = 2.7 Hz, CH_2 of cation), 47.25(cage C), 7.64 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}Cl_5O_2]^-$: 739.1520. Found: 739.1533.



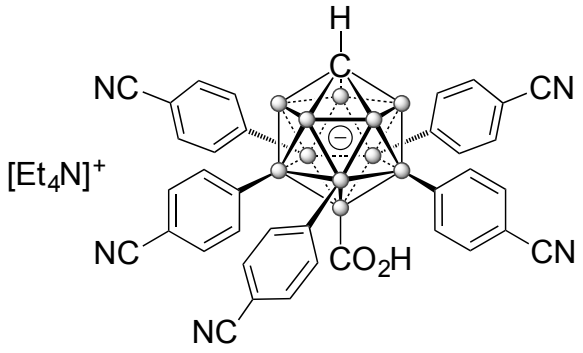
Reaction conditions: 36 h, 40 °C, 87 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 9.45 (broad signal, 1H, COOH), 7.17 (d, *J* = 8.3 Hz, 10H, Ar-H), 7.04 (d, *J* = 8.3 Hz, 10H, Ar-H), 3.47 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.92 (broad signal, 1H, cage CH), 2.35 (broad signal, 5H, BH), 1.40-1.34 (m, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.99 (5B, B-C), -5.64 (1B, B-COOH), -16.33 (5B, B-H).
13C{1H} NMR (100 MHz, acetone-d6, 23 °C): δ 141.09 (broad signal, B-C_{aryl}), 138.37, 129.58, 120.40 (Ar-C), 52.98 (t, *J* = 2.7 Hz, CH_2 of cation), 47.25 (cage C), 7.65 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}Br_5O_2]^-$: 960.8983. Found: 960.8977.
Elemental analysis: Calculated for $[Et_4N][C_{40}H_{47}B_{11}NO_2]$: C, 43.99; H, 4.34; N, 1.28; found: C, 43.55; H, 4.37; N, 1.27 (first measurement), C, 43.49; H, 4.36; N, 1.25 (second measurement).



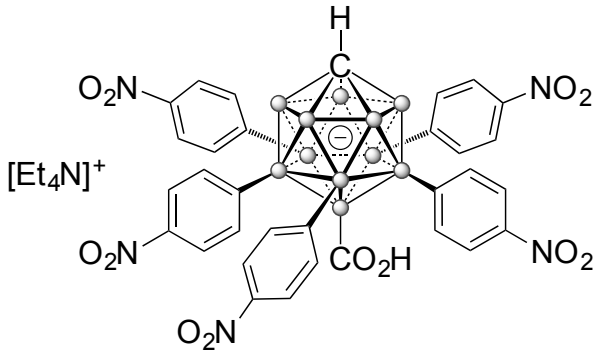
Reaction conditions: 48 h, 40 °C, 54 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 9.36 (broad signal, 1H, COOH), 7.23 (d, *J* = 8.1 Hz, 10H, Ar-H), 7.03 (d, *J* = 8.1 Hz, 10H, Ar-H), 3.47 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.91 (broad signal, 1H, cage CH), 2.33 (broad signal, 5H, BH), 1.38 (tt, *J* = 7.3Hz, 1.8Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.91 (5B, B-C), -5.71 (1B, B-COOH), -16.32 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 141.39 (broad signal, B-C_{aryl}), 138.67, 135.63, 92.25 (Ar-C), 52.97 (t, *J* = 2.7 Hz, CH_2 of cation), 47.18 (cage C), 7.67 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}I_5O_2]^-$: 1196.8331. Found: 1196.8316.



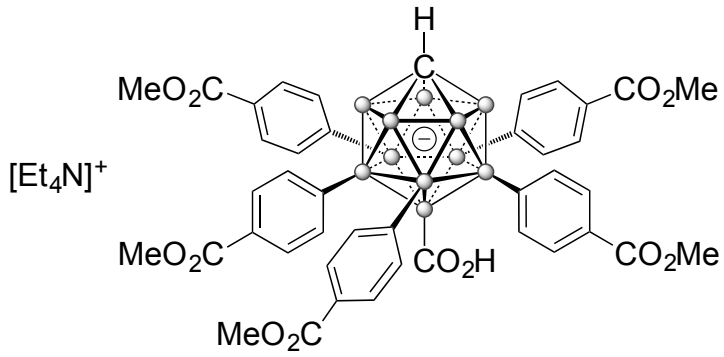
Reaction conditions: 24 h, 40 °C, 82 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*).

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d6, 23 °C): δ 9.89 (broad signal, 1H, COOH), 7.36 (d, *J* = 8.1 Hz, 10H, Ar-H), 7.27 (d, *J* = 8.1 Hz, 10H, Ar-H), 3.49 (q, *J* = 7.3Hz, 8H, CH_2 of cation), 3.17 (broad signal, 1H, cage CH), 2.48 (broad signal, 5H, BH), 1.39 (m, 12H, CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d6, 23 °C): δ -3.91 (5B, B-C), -5.32 (1B, B-COOH), -15.74 (5B, B-H).
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d6, 23 °C): δ 147.85 (broad signal, B-C_{aryl}), 136.82, 130.22, 120.13 (Ar-C), 109.98 (CN), 52.94 (t, *J* = 2.7 Hz, CH_2 of cation), 48.10 (cage C), 7.63 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{37}H_{27}B_{11}N_5O_2]^-$: 692.3261. Found: 692.3238.



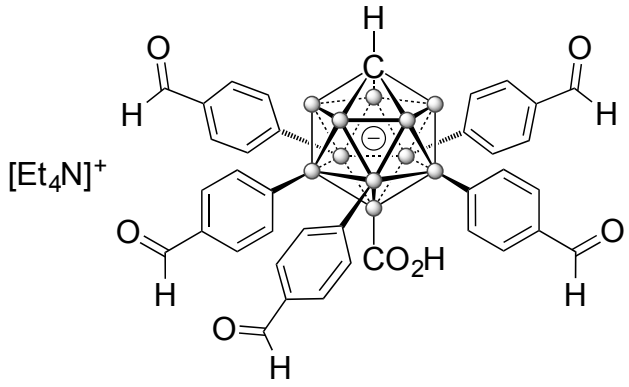
Reaction conditions: 24 h, 40 °C, 87 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 6 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 10.15(broad signal, COO*H*), 7.79 (d, *J* = 8.7 Hz, 10H, Ar-H), 7.47 (d, *J* = 8.7 Hz, 10H, Ar-H), 3.49 (q, *J* = 7.3Hz, 8H, CH_2 of cation), 3.31 (broad signal, 1H, cage CH), 2.59 (broad signal, 5H, BH), 1.39 (m, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.75 (5B, B-C), -5.08 (1B, B-COOH), -15.40 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 150.41 (broad signal, B-C_{aryl}), 147.46, 136.98, 121.61 (Ar-C), 53.00 (t, *J* = 2.7 Hz, CH_2 of cation), 48.64 (cage C), 7.66 (s, CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}N_5O_{12}]^-$: 792.2752. Found: 792.2715.



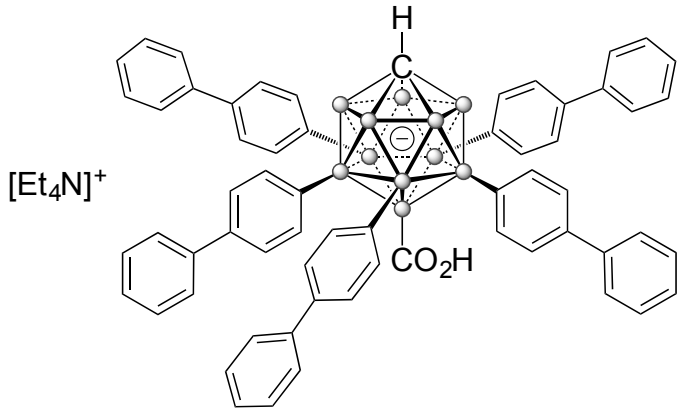
Reaction conditions: 24 h, 40 °C, 54 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 9.43 (broad signal, 1H, COO*H*), 7.51(d, *J* = 8.2 Hz, 10H, Ar-H), 7.38 (d, *J* =8.2 Hz, 10H, Ar-H), 3.78 (s, 15H, COOCH_3), 3.48 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 3.06 (broad signal, s, 1H, cage CH), 2.50 (broad signal, 5H, BH), 1.37 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.62 (5B, B-C), -5.15 (1B, B-COOH), -15.83 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 167.93 (*C*OOCH$_3$), 148.54 (broad signal, B-C_{aryl}), 136.41, 127.96, 127.46 (Ar-C), 53.00 (t, *J* = 2.7 Hz, CH_2 of cation), 51.80 (COO*C*H$_3$), 47.79 (cage CH), 7.65 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{42}H_{42}B_{11}O_{12}]^-$: 857.3773. Found: 857.3792.



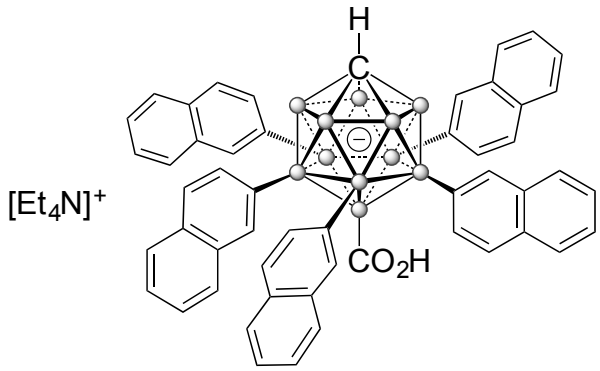
Reaction conditions: 24 h, 40 °C, 89 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*)

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 9.87(s, 5H, CHO), 9.76 (broad signal, 1H, COO*H*), 7.49 (d, *J* = 7.9 Hz, 10H, Ar-H), 7.42 (d, *J* =7.9 Hz, 10H, Ar-H), 3.48 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 3.15 (broad signal, s, 1H, cage CH), 2.54 (broad signal, 5H, BH), 1.38 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -3.59 (5B, B-C), -5.15 (1B, B-COOH), -15.62 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 193.21(s, CHO), 150.55 (broad signal, B-C_{aryl}), 136.86, 135.22, 127.73 (Ar-C), 52.98 (t, *J* = 2.7 Hz, CH_2 of cation), 48.06 (cage CH), 7.64 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{37}H_{32}B_{11}O_7]^-$: 707.3244. Found: 707.3237.



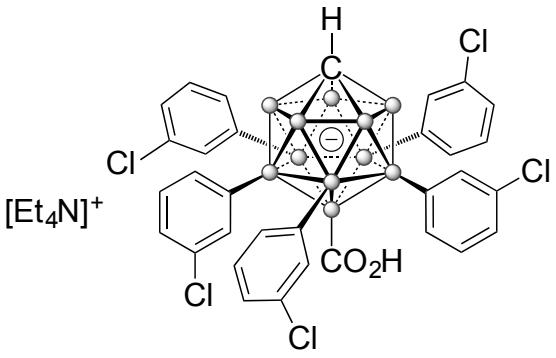
Reaction conditions: 48 h, 40 °C, 81 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*)

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 8.68 (broad signal, 1H, COOH), 7.63-7.53 (m, 20H, Ar-H), 7.40-7.31 (m, 10H, Ar-H), 7.29-7.19 (m, 15H, Ar-H), 3.39 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.99 (broad signal, 1H, cage CH), 2.55 (broad signal, 5H, BH), 1.31 (tt, *J* = 7.3Hz, 1.8Hz, 12H, CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -3.61 (5B, B-C), -5.62 (1B, B-COOH), -16.36 (5B, B-H).
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 142.45 (Ar-C), 141.95 (broad signal, B-C_{aryl}), 138.09, 137.15, 129.43, 127.29 (two overlapping signals), 125.11, (Ar-C), 52.94 (t, *J* = 2.7 Hz, CH_2 of cation), 47.37 (cage C), 7.61 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{62}H_{52}B_{11}O_2]^-$: 947.5064. Found: 947.5069.



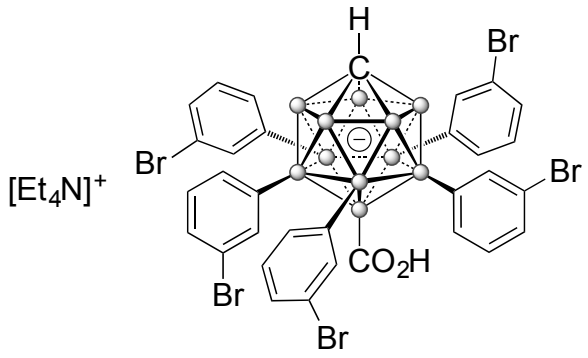
Reaction conditions: 48 h, 40 °C, 60 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*)

$^1H\{^{11}B\}$ NMR (400 MHz, DMSO-d_6, 23 °C): δ 10.61 (broad signal, 1H, COOH), 7.91 (s, 5H, Ar-H), 7.64 (d, *J* = 8.1 Hz, 5H, Ar-H), 7.56 (d, *J* = 8.5 Hz, 5H, Ar-H), 7.38-7.18 (m, 20H, Ar-H), 3.24 (broad signal, 1H, cage CH), 3.12 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.59 (broad signal, 5H, BH), 1.10 (tt, *J* = 7.3Hz, 1.8Hz, 12H, CH_3 of cation).
$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -3.21 (5B, B-C), -5.17 (1B, B-COOH), -15.76 (5B, B-H).
$^{13}C\{^1H\}$ NMR (100 MHz, DMSO-d_6, 23 °C): δ 139.53 (broad signal, B-Caryl), 134.37, 133.83, 132.22, 131.48, 127.37, 126.94, 124.51, 124.41, 123.99 (Ar-C), 51.34 (t, J = 2.7 Hz, CH2 of cation), 45.98 (cage C), 7.03 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{52}H4_{22}B_{11}O_2]^-$:817.4281. Found: 817.4299.



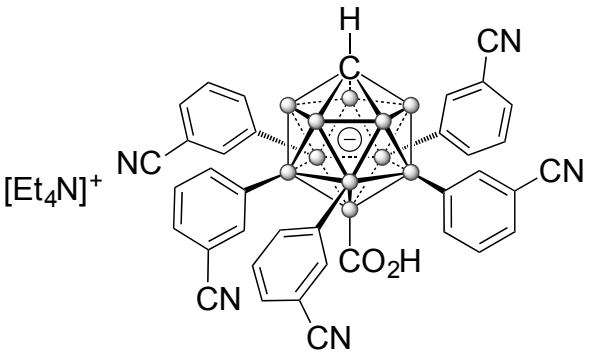
Reaction conditions: 48 h, 60 °C, 63 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

^{1}H{^{11}B} NMR (400 MHz, acetone-d_6, 23 °C): δ 9.46 (broad signal, COO*H*), 7.33 (s, 5H, Ar-H), 7.22 (d, *J* = 7.8 Hz, 5H, Ar-H), 7.02-6.96 (m, 5H, Ar-H), 6.92-6.84 (m, 5H, Ar-H), 3.45 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.99 (broad signal, 1H, cage CH), 2.40 (broad signal, 5H, BH), 1.37 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
^{11}B{^{1}H} NMR (128 MHz, acetone-d_6, 23 °C): δ -4.16 (5B, B-C), -5.69 (1B, B-COOH), -16.19 (5B, B-H).
^{13}C{^{1}H} NMR (100 MHz, acetone-d_6, 23 °C): δ 144.42 (broad signal, B-C_{aryl}), 135.98, 134.70, 132.66, 128.25, 126.05 (Ar-C), 53.00 (t, *J* = 2.7 Hz, CH_2 of cation), 47.36 (cage C), 7.69 (s, CH_3 of cation)
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}Cl_5O_2]^-$: 739.1520. Found: 739.1496.



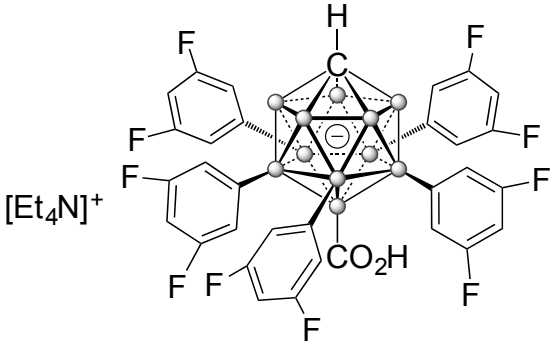
Reaction conditions: 48 h, 60 °C, 42 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 9.45 (broad signal, COO*H*), 7.49 (s, 5H, Ar-H), 7.26 (d, *J* = 7.8 Hz, 5H, Ar-H), 7.17-7.10 (m, 5H, Ar-H), 6.87-6.79 (m, 5H, Ar-H), 3.47 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 2.98 (broad signal, 1H, cage CH), 2.39 (broad signal, 5H, BH), 1.37 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -4.21 (5B, B-C), -5.44 (1B, B-COOH), -16.02 (5B, B-H).
$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 145.11 (broad signal, B-C_{aryl}), 138.87, 135.03, 128.95, 128.59, 121.51 (Ar-C), 52.97 (t, *J* = 2.7 Hz, CH_2 of cation), 47.32 (cage C), 7.66 (s, CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{27}B_{11}Br_5O_2]^-$: 960.8983. Found: 960.8918.



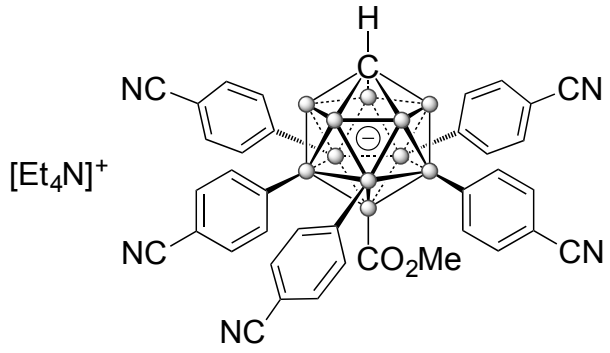
Reaction conditions: 36 h, 40 °C, 85 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 8 : 1 (*v*/*v*)

$^1H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.06 (broad signal, COO*H*), 7.53 (d, *J* = 7.8 Hz, 5H, Ar-H), 7.49 (s, 5H, Ar-H), 7.45-7.39 (m, 5H, Ar-H), 7.19-7.09 (m, 5H, Ar-H), 3.48 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 3.19 (broad signal, 1H, cage CH), 2.49 (broad signal, 5H, BH), 1.38 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
$^{11}B\{^1H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -4.21 (5B, B-C), -5.44 (1B, B-COOH), -16.02 (5B, B-H).
$^{13}C\{^1H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 142.66 (broad signal, B-C_{aryl}), 140.58, 139.50, 130.19, 127.97, 120.26 (Ar-C), 110.10 (CN), 53.03(t, *J* = 2.7 Hz, CH_2 of cation), 47.96 (cage CH), 7.69 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{37}H_{27}B_{11}N_5O_2]^-$: 692.3261. Found: 692.3236.
Elemental analysis: Calculated for $[Et_4N][C_{45}H_{47}B_{11}N_6O_2]$: C, 65.69; H, 5.76; N, 10.21; found: C, 64.92; H, 5.91; N, 9.90 (first measurement), C, 65.11; H, 5.84; N, 9.95 (second measurement).



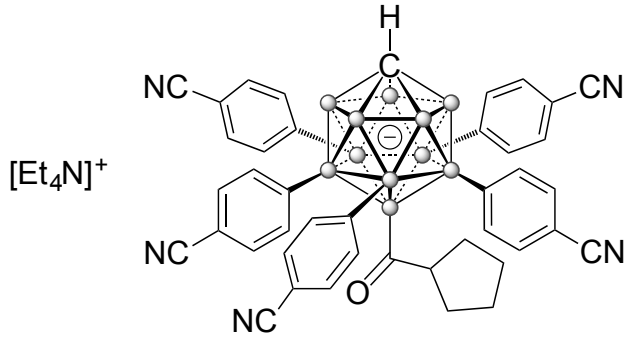
Reaction conditions: 48 h, 40 °C, 64 % yield, colorless solid;
eluent: CH_2Cl_2 : MeCN = 20 : 1 to CH_2Cl_2 : MeCN = 10 : 1 (*v*/*v*).

$^{1}H\{^{11}B\}$ NMR (400 MHz, acetone-d_6, 23 °C): δ 10.07 (broad signal, COO*H*), 6.93-6.80 (m, 10H, Ar-H), 6.67-6.56 (m, 5H, Ar-H), 3.49 (q, *J* = 7.3 Hz, 8H, CH_2 of cation), 3.13 (broad signal, 1H, cage CH), 2.42 (broad signal, 5H, BH), 1.39 (tt, *J* = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
$^{11}B\{^{1}H\}$ NMR (128 MHz, acetone-d_6, 23 °C): δ -4.41 (5B, B-C), -5.83 (1B, B-COOH), -16.00 (5B, B-H).
$^{13}C\{^{1}H\}$ NMR (100 MHz, acetone-d_6, 23 °C): δ 162.53 (dd, *J* = 245Hz, 12 Hz, Ar-C), 146.09 (broad signal, B-C_{aryl}), 118.13 (dd, *J* = 18Hz, 5Hz, Ar-C), 101.48 (t, *J* = 26 Hz, Ar-C), 52.98 (t, *J* = 2.7 Hz, CH_2 of cation), 47.52 (cage C), 7.64 (CH_3 of cation).
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{32}H_{22}B_{11}F_{10}O_2]^-$:747.2556. Found: 747.2544.
Elemental analysis: Calculated for $[Et_4N][C_{40}H_{42}B_{11}F_{10}NO_2]$: C, 54.74; H, 4.82; N, 1.60; found: C, 54.70; H, 4.96; N, 1.43 (first measurement), C, 54.70; H, 4.92; N, 1.54 (second measurement).



A 10 mL vial was charged with [Et_4N][**3j**] (82.2 mg, 0.1 mmol, 1 equiv), K_2CO_3 (27.4mg, 0.2 mmol 2 equiv) and 2 mL DMF. Then iodomethane (30 μL, 0.5 mmol 5 equiv) was added to the mixture using an Eppendorf pipet. The reaction mixture was stirred at 40 °C for 2 hours and then allowed to cool to 25 °C. 0.4 M aqueous Et_4NBr solution (10 mL) was added to the DMF solution, and a white precipitate formed immediately. The precipitate was collected by filtration through a fritted glass funnel (F porosity), followed by washing with deionized water (2 x 10 mL). The solid colorless product was dried under vacuum for 12 h to afford the esterification product (81.6 mg, 98 %).

$^1H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 23 °C): δ 7.32-7.23 (overlapping signals, 20H, Ar-H), 3.50 (q, J = 7.6 Hz, 8H, CH_2 of cation), 3.26 (s, 3H, OCH_3), 3.17 (broad signal, 1H, cage CH), 2.48 (broad signal, 5H, BH), 1.40 (tt, J = 7.3 Hz, 1.8 Hz, 12H, CH_3 of cation).
$^{11}B\{^1H\}$ NMR (160 MHz, acetone-d_6, 23 °C): δ -3.93 (5B, B-C), -5.32 (1B, B-$COOCH_3$), -15.72 (5B, B-H).
$^{13}C\{^1H\}$ NMR (125 MHz, acetone-d_6, 23 °C): δ 147.67 (broad signal, B-C_{aryl}), 136.70, 130.29, 120.11, 110.05 (Ar-C and CN), 52.98 (t, J = 2.7 Hz, CH_2 of cation), 48.33 (OCH_3), 48.09 (cage C), 7.65 (CH_3 of cation).
HRMS((-)-ESI): *m/z* calculated for $[C_{38}H_{29}B_{11}N_5O_2]^-$:706.3417. Found: 706.3403.



To a stirred suspension of [Et_4N][**3j**] (82.2 mg 0.1 mmol) in dry CH_2Cl_2 (3 mL), dimethylformamide (ca. 1 drop) and oxalyl chloride (20 μL, 0.2 mmol) were added under N_2 atmosphere. The reaction mixture was allowed to stir for 2 h at 25 °C. The volatiles were removed carefully under vacuum. The acid chloride was dissolved in a minimum amount of dry CH_2Cl_2 and added dropwise to a solution of pyrrolidine (41 μL, 0.5 mmol) and triethylamine (14 μL, 0.1 mmol) in CH_2Cl_2 (4 mL). The resulting mixture was stirred for 4 h. All volatile components were then removed completely in a vacuum, and the residue was purified by column chromatography on silica gel with CH_2Cl_2/CH_3CN (10 : 1 *v*/*v*) as the eluent to afford a yellowish solid (73.5 mg, 84 % yield).

$^1H\{^{11}B\}$ NMR (500 MHz, acetone-d_6, 23 °C): δ 7.49 (d, J = 8.1 Hz, 10H, Ar-H), 7.31 (d, J = 8.1 Hz, 10H, Ar-H), 3.49 (q, J = 7.6 Hz, 8H, CH_2 of cation), 3.35 (broad signal, 2H, CH_2 of pyrrolidine), 3.18 (broad signal, 1H, cage CH), 2.42 (broad signal, 5H, BH), 2.36 (broad signal, 2H, CH_2 of pyrrolidine), 1.53 (broad signal, 2H, CH_2 of pyrrolidine), 1.39 (tt, J = 7.3 Hz, 1.8 Hz, 12H, CH3 of cation), 1.16 (broad signal, 2H, CH_2 of pyrrolidine).
The rotation of the pyrrolidine ring about the amide bond is slow on the NMR time scale, leading to four broad CH_2 signals.
$^{11}B\{^1H\}$ NMR (160 MHz, acetone-d_6, 23 °C): δ -2.73 (1B, B-C(O)N), -4.36 (1B, B-C), -14.93 (5B, B-H).
$^{13}C\{^1H\}$ NMR (125 MHz, acetone-d_6, 23 °C): δ 150.06 (broad signal, B-Caryl), 136.55, 130.40, 120.12, 109.89 (Ar-C and CN), 52.98 (t, J = 2.7 Hz, CH2 of cation), 48.86 (cage C), 49.39, 46.64, 26.65, 23.49 (C of pyrrolidine), 7.67 (CH_3 of cation).
The rotation of the pyrrolidine ring about the amide bond is slow on the NMR time scale, leading to four broad ring signals.
HRMS ((–)-ESI): *m*/*z* calculated for $[C_{41}H_{34}B_{11}N_6O]^-$:745.3890. Found: 745.3863.

III X-ray Crystallography

*Procedure for crystal growth (identical procedure for **3a, 3b, 3h, 3q** and **5**):*
20 mg of the $[Et_4N]^+$ salt of the product was dissolved in acetone (0.6 mL) and filtered into an NMR tube (5 mm diameter, 18 cm length). The solution was layered with hexane (1.4 mL). Crystals suitable for X-ray diffraction grew within 1 month at 13 °C.

Crystal structure of 3a (CCDC 2206555)

Remark: The phenyl-group C31-C36 is occasionally replaced by iodine. The free refinement of the respective occupancies leads to a ratio phenyl:iodine of about 95:5. The reason for the presence of iodine in this structure is that the crystals were grown from a batch of **3a** that was obtained under non-optimized conditions at an early stage of the project (see above, p. S10).

Table S2. Crystal data and structure refinement for **3a**.

Identification code	200611_jyj_255_0m
Empirical formula	$C_{39.7}H_{51.76}B_{11}I_{0.05}NO_2$
Formula weight	700.29
Temperature/K	170.00
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	10.528(3)
b/Å	12.446(4)
c/Å	16.138(5)
α/°	81.066(14)
β/°	71.006(11)
γ/°	78.919(10)
Volume/Å^3	1952.3(10)
Z	2
ρ_{calc}g/cm^3	1.191
μ/mm^{-1}	0.106
F(000)	741.0
Crystal size/mm^3	0.43 × 0.26 × 0.18
Radiation	MoKα (*λ* = 0.71073)
2*Θ* range for data collection/°	4.498 to 54.262
Index ranges	-13 ≤ *h* ≤ 13, -15 ≤ *k* ≤ 15, -20 ≤ *l* ≤ 20
Reflections collected	33108
Independent reflections	8599 [R_{int} = 0.0269, R_{sigma} = 0.0327]
Data/restraints/parameters	8599/1/514
Goodness-of-fit on F^2	1.057
Final *R* indexes [*I*>=2*σ* (*I*)]	R_1 = 0.0458, wR_2 = 0.1134
Final *R* indexes [all data]	R_1 = 0.0493, wR_2 = 0.1162
Largest diff. peak/hole / e Å^{-3}	0.43/-0.29

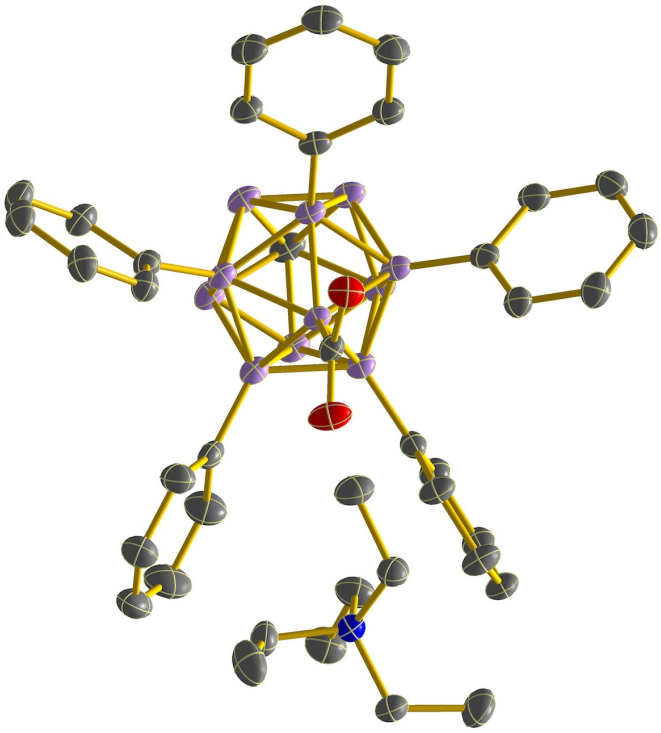


Figure S9. ORTEP representation of [Et_4N][**3a**]; minor component ([Et_4N][$CB_{11}H_6$-7,8,9,10-Ph_4-11-I-12-COOH], 5%) not shown. Hydrogen atoms omitted for clarity; 50% displacement ellipsoids.

Crystal structure of 3b (CCDC 2206556)

Remark: There is disorder about one of the cations, one of the tolyl rings and an approximate 90:10 disorder about two of the carboxyl groups.

Table S3. Crystal data and structure refinement for **3b**.

Identification code	191010_jyj_133_0m_pl
Empirical formula	$C_{45}H_{62}B_{11}NO_2$
Formula weight	767.86
Temperature/K	170.15
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	23.9942(6)
b/Å	33.9029(10)
c/Å	21.9390(7)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	17846.8(9)
Z	16
ρ_{calc}g/cm^3	1.143
μ/mm^{-1}	0.064
F(000)	6560.0
Crystal size/mm^3	0.19 × 0.1 × 0.09
Radiation	MoKα (*λ* = 0.71073)
2*Θ* range for data collection/°	4.422 to 54.66
Index ranges	-30 ≤ *h* ≤ 30, -43 ≤ *k* ≤ 43, -27 ≤ *l* ≤ 28
Reflections collected	170781
Independent reflections	39678 [R_{int} = 0.0803, R_{sigma} = 0.0687]
Data/restraints/parameters	39678/265/2284
Goodness-of-fit on F^2	1.012
Final *R* indexes [*I*>=2*σ* (*I*)]	R_1 = 0.0565, wR_2 = 0.1292
Final *R* indexes [all data]	R_1 = 0.0936, wR_2 = 0.1487
Largest diff. peak/hole / e Å^{-3}	0.34/-0.37
Flack parameter	-0.1(5)

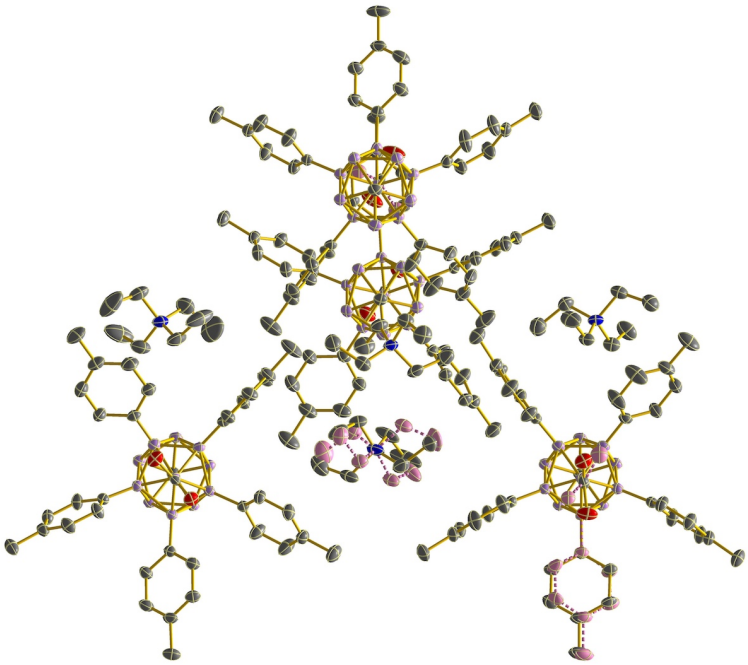


Figure S10. ORTEP representation of [Et_4N][**3b**]. Hydrogen atoms omitted for clarity; 50% displacement ellipsoids. Minor component of disordered parts shown in pink.

Crystal structure of 3h (CCDC 2206557)

Remark: This compound crystallized as $[Et_4N][\mathbf{3h}][acetone]_{0.5}$. There is disorder about the cation and the solvent molecule.

Table S4. Crystal data and structure refinement for **3h**.

Identification code	191105_jyj_160_0m
Empirical formula	$C_{41.5}H_{50}B_{11}Br_5NO_{2.5}$
Formula weight	1121.28
Temperature/K	170.00
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	11.455(2)
b/Å	12.268(2)
c/Å	17.830(3)
α/°	92.876(6)
β/°	96.299(6)
γ/°	106.337(6)
Volume/Å^3	2381.3(8)
Z	2
ρ_{calc}g/cm^3	1.564
μ/mm^{-1}	4.257
F(000)	1112.0
Crystal size/mm^3	0.16 × 0.12 × 0.08
Radiation	MoKα (*λ* = 0.71073)
2*Θ* range for data collection/°	4.614 to 55.188
Index ranges	-14 ≤ *h* ≤ 14, -15 ≤ *k* ≤ 15, -22 ≤ *l* ≤ 21
Reflections collected	45049
Independent reflections	10553 [R_{int} = 0.0969, R_{sigma} = 0.0825]
Data/restraints/parameters	10553/49/543
Goodness-of-fit on F^2	1.034
Final *R* indexes [*I*>=2*σ* (*I*)]	R_1 = 0.0701, wR_2 = 0.1957
Final *R* indexes [all data]	R_1 = 0.0952, wR_2 = 0.2141
Largest diff. peak/hole / e Å^{-3}	1.52/-1.50

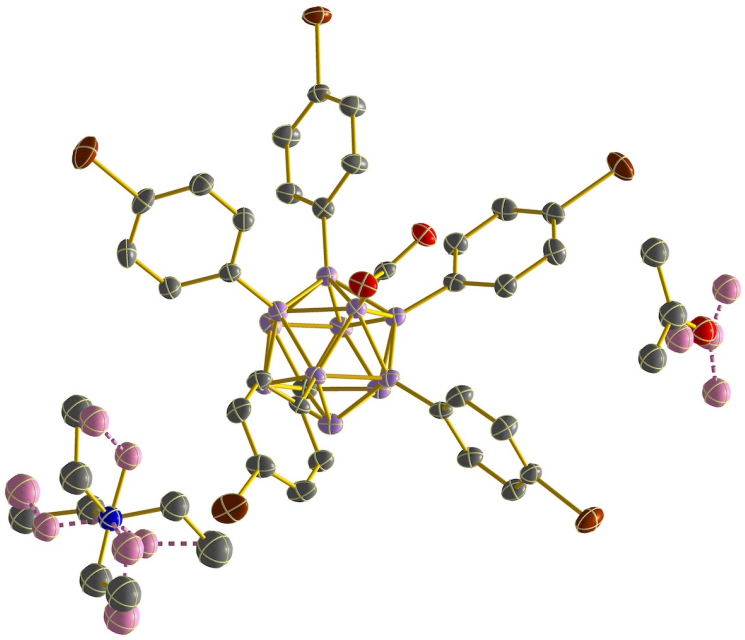


Figure S11. ORTEP representation of $[Et_4N][\mathbf{3h}][acetone]_{0.5}$. Hydrogen atoms are omitted for clarity; 50% displacement ellipsoids. Minor component of disordered parts shown in pink.

Crystal structure of 3q (CCDC 2206558)

Remark: This compound crystallized as $[Et_4N][\mathbf{3q}][acetone]_{0.5}$. There is disorder about the cation and the solvent molecule.

Table S5. Crystal data and structure refinement for **3q**.

Identification code	191101_jyj_183_0m
Empirical formula	$C_{45.51}H_{58.02}B_{11}Br_5NO_{3.83}$
Formula weight	1198.89
Temperature/K	170.00
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	12.7612(3)
b/Å	14.7509(3)
c/Å	16.4625(4)
α/°	67.0770(10)
β/°	74.7490(10)
γ/°	69.0300(10)
Volume/Å^3	2637.44(11)
Z	2
ρ_{calc}g/cm^3	1.510
μ/mm^{-1}	3.850
F(000)	1198.0
Crystal size/mm^3	0.29 × 0.23 × 0.2
Radiation	MoKα (*λ* = 0.71073)
2*Θ* range for data collection/°	4.69 to 55.742
Index ranges	-16 ≤ *h* ≤ 16, -19 ≤ *k* ≤ 18, -21 ≤ *l* ≤ 21
Reflections collected	55008
Independent reflections	12560 [R_{int} = 0.0588, R_{sigma} = 0.0559]
Data/restraints/parameters	12560/14/634
Goodness-of-fit on F^2	1.037
Final *R* indexes [*I*>=2*σ* (*I*)]	R_1 = 0.0513, wR_2 = 0.1220
Final *R* indexes [all data]	R_1 = 0.0654, wR_2 = 0.1298
Largest diff. peak/hole / e Å^{-3}	2.41/-2.15

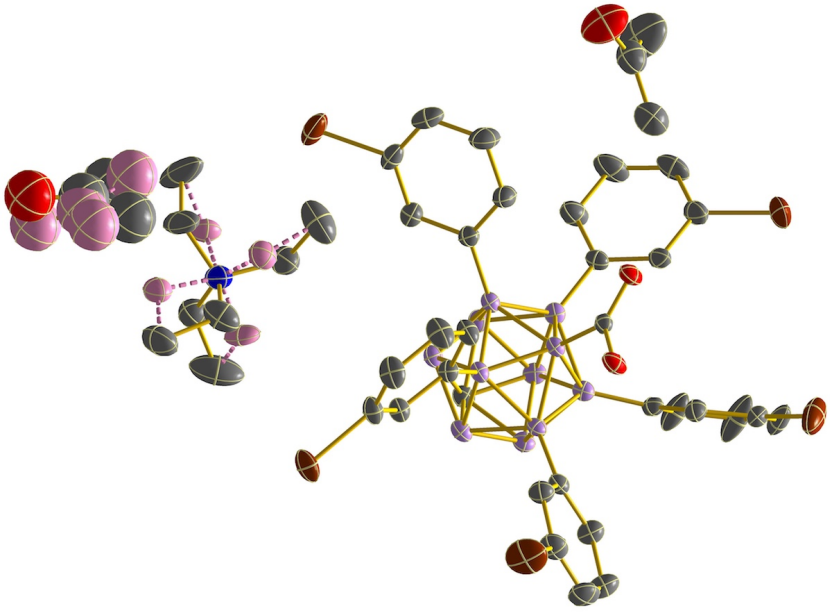


Figure S12. ORTEP representation of $[Et_4N][\mathbf{3q}][acetone]_{0.5}$. Hydrogen atoms are omitted for clarity; 50% displacement ellipsoids. Minor component of disordered parts shown in pink.

Crystal structure of 5 (CCDC 2206559)

Remark: This compound crystallized as [Et_4N][**3q**][acetone]. There is disorder about the cation and the solvent molecule.

Table S6. Crystal data and structure refinement for **5**.

Identification code	mo_220406_jyj_577_0m
Empirical formula	$C_{52}H_{60}B_{11}N_7O_2$
Formula weight	933.98
Temperature/K	170.00
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	10.7770(9)
b/Å	16.0486(13)
c/Å	16.0708(11)
α/°	100.693(3)
β/°	90.559(3)
γ/°	101.575(3)
Volume/Å^3	2672.5(4)
Z	2
ρ_{calc}g/cm^3	1.161
μ/mm^{-1}	0.068
F(000)	984.0
Crystal size/mm^3	0.10 × 0.04 × 0.02
Radiation	MoKα (*λ* = 0.71073)
2*Θ* range for data collection/°	4.54 to 53.048
Index ranges	-13 ≤ *h* ≤ 13, -20 ≤ *k* ≤ 20, -18 ≤ *l* ≤ 20
Reflections collected	44282
Independent reflections	10994 [R_{int} = 0.0834, R_{sigma} = 0.0702]
Data/restraints/parameters	10994/313/771
Goodness-of-fit on F^2	1.020
Final *R* indexes [*I*>=2*σ* (*I*)]	R_1 = 0.0594, wR_2 = 0.1323
Final *R* indexes [all data]	R_1 = 0.1176, wR_2 = 0.1628
Largest diff. peak/hole / e Å^{-3}	0.19/-0.23

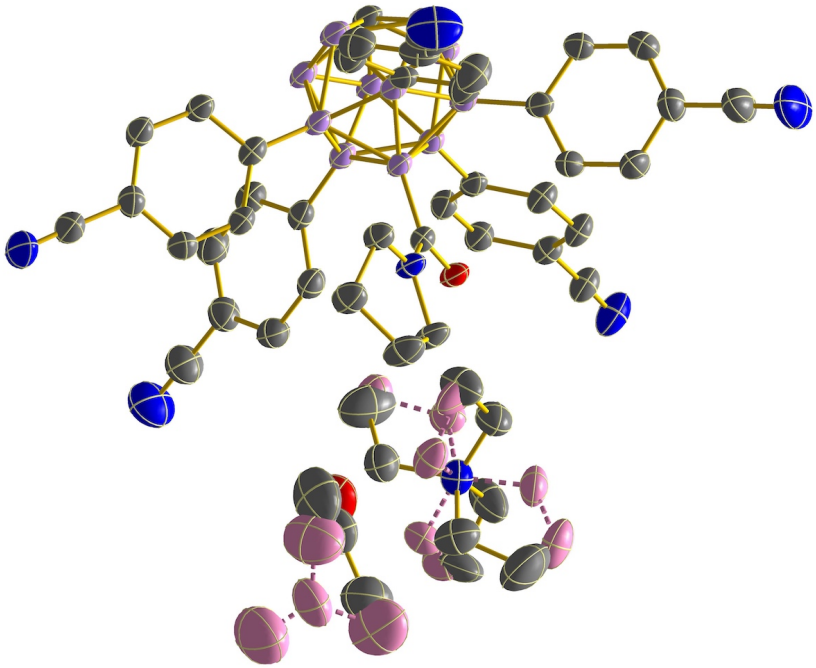


Figure S13. ORTEP representation of [Et_4N][**5**][acetone]. Hydrogen atoms are omitted for clarity; 50% displacement ellipsoids. Minor component of disordered parts shown in pink.

IV References

[1] C. A. Reed, *Acc. Chem. Res.* **2010**, *43*, 121–128.

[2] A. Himmelspach, G. J. Reiss, M. Finze, *Inorg. Chem.* **2012**, *51*, 2679–2688.

[3] A. J. Rosenbaum, D. H. Juers, M. A. Juhasz, *Inorg. Chem.* **2013**, *52*, 10717–10719.

[4] 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

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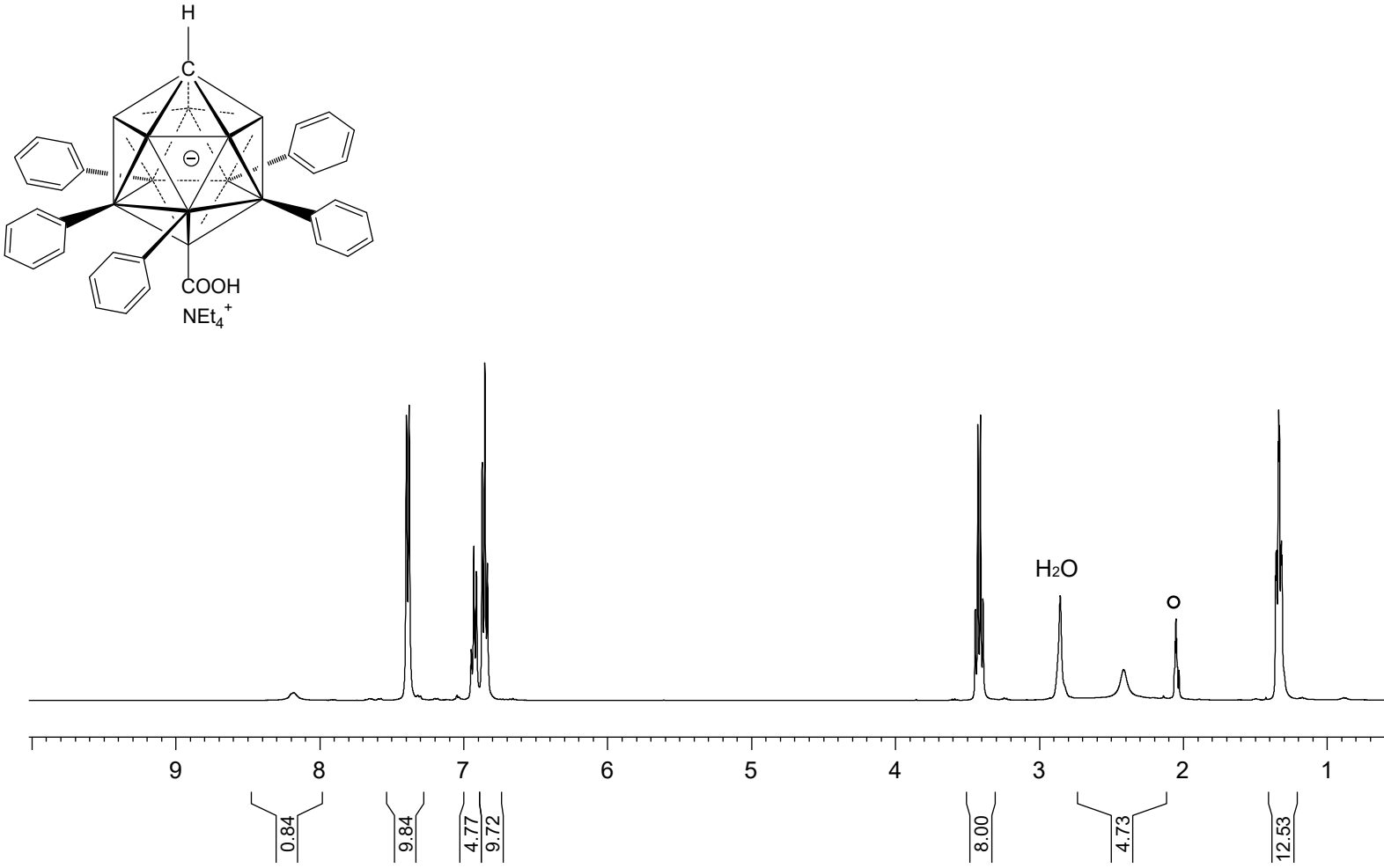


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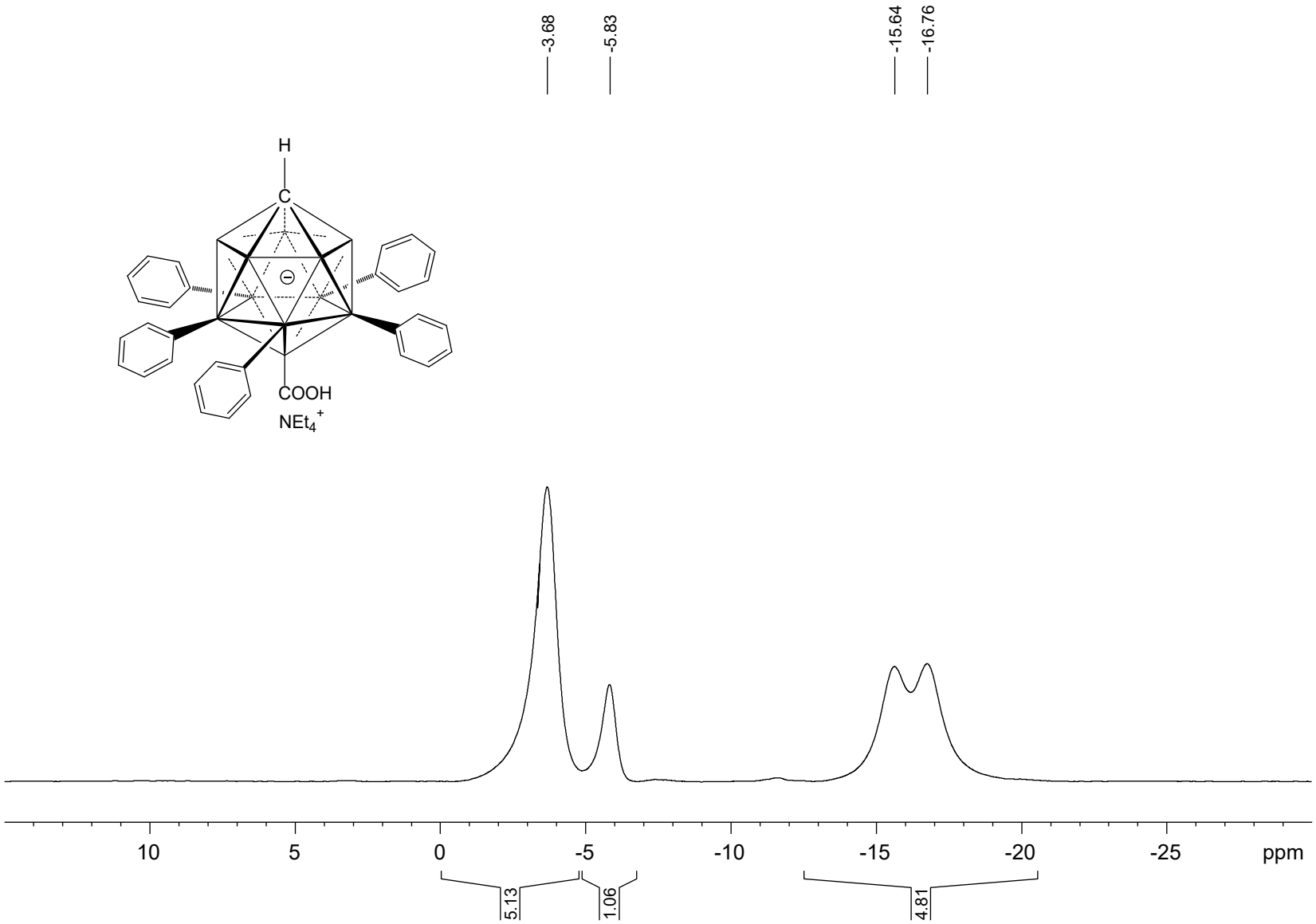


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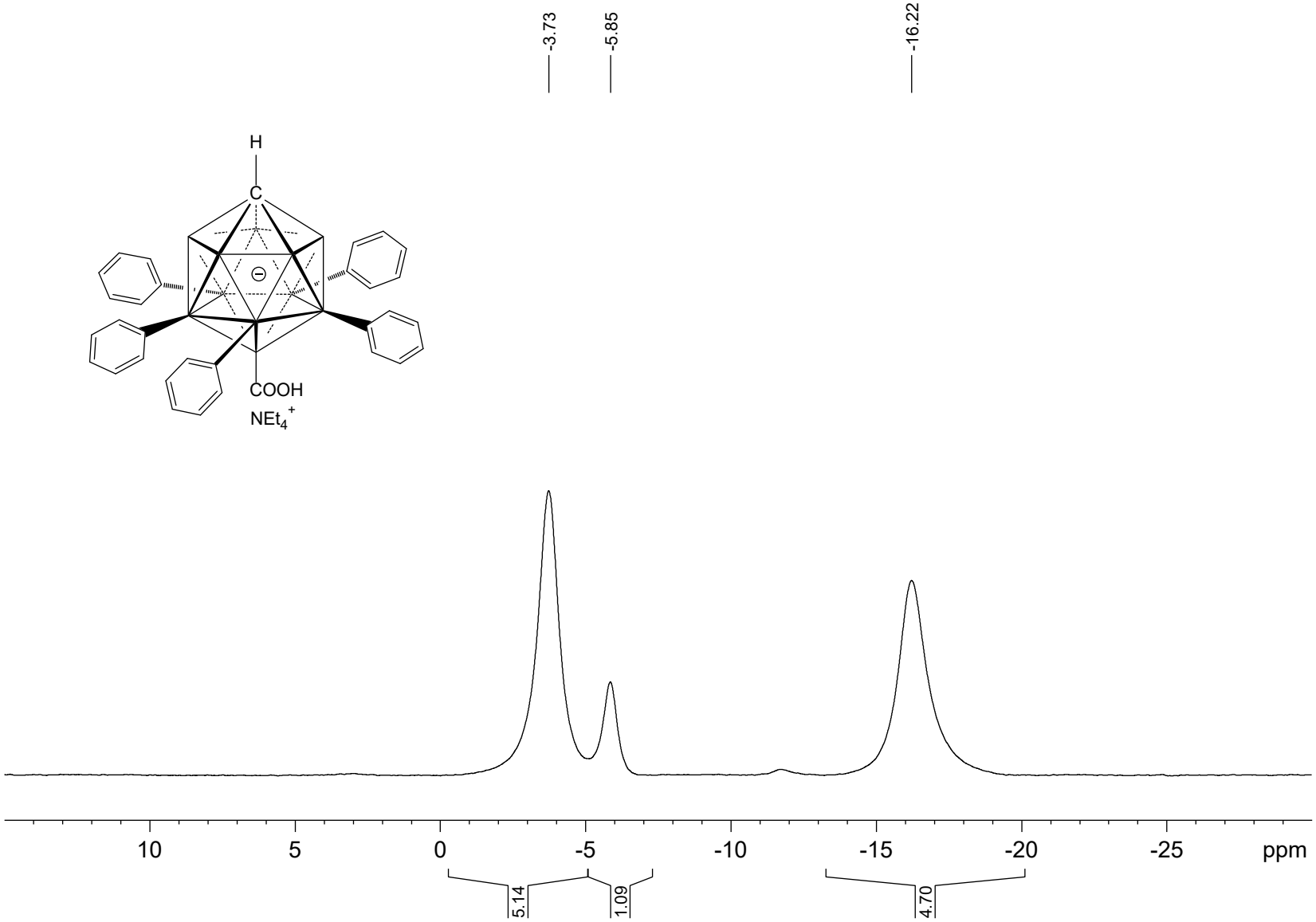
PROCNO                1

F2 - Acquisition Parameters
Date_          20200731
Time              22.00
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               295.6 K
D1            1.00000000 sec
TD0                   1

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

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

jyj-200730-255 [NEt4][12-COOH-CB11H6(C6H5)5]
11B{1H} 128MHz 20.2mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200730-255-total-C6H5
EXPNO                 4
PROCNO                1

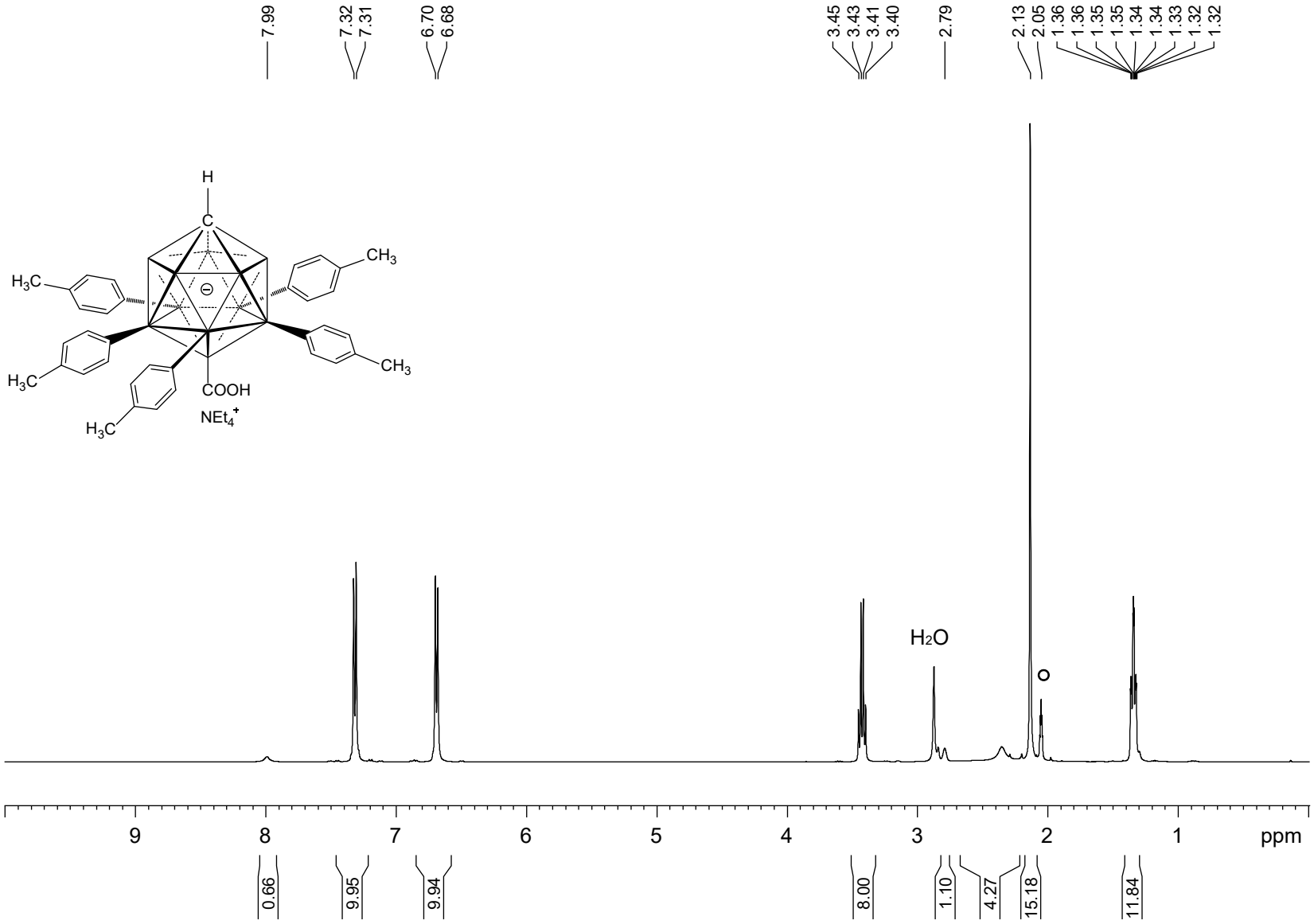
F2 - Acquisition Parameters
Date_           20200731
Time               22.06
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-200716-285-total[NEt4][12-COOH-CB11H6(4-C6H4-CH3)5]
1H{11B} 400MHz 20.8mg in acetone-d6 T= 23 C




```
Current Data Parameters
NAME      jyj-200716-285-total
EXPNO                       2
PROCNO                      1

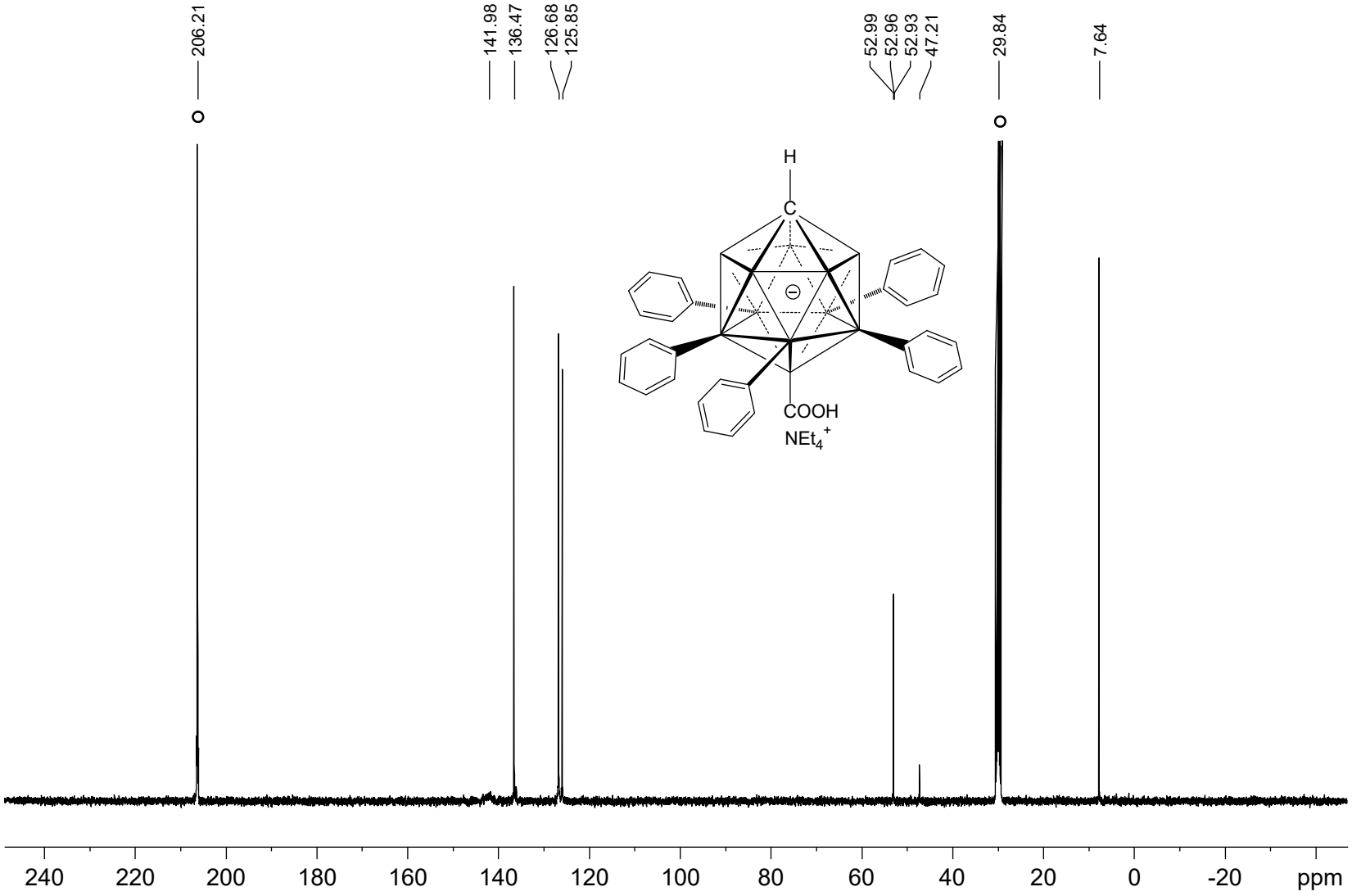
F2 - Acquisition Parameters
Date_              20200719
Time                 20.08
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   293.2 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            400.1300614 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

jyj-200730-255 [NEt4][12-COOH-CB11H6(C6H5)5]
13C 128MHz 20.2mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200730-255-total
EXPNO                    5
PROCNO                   1

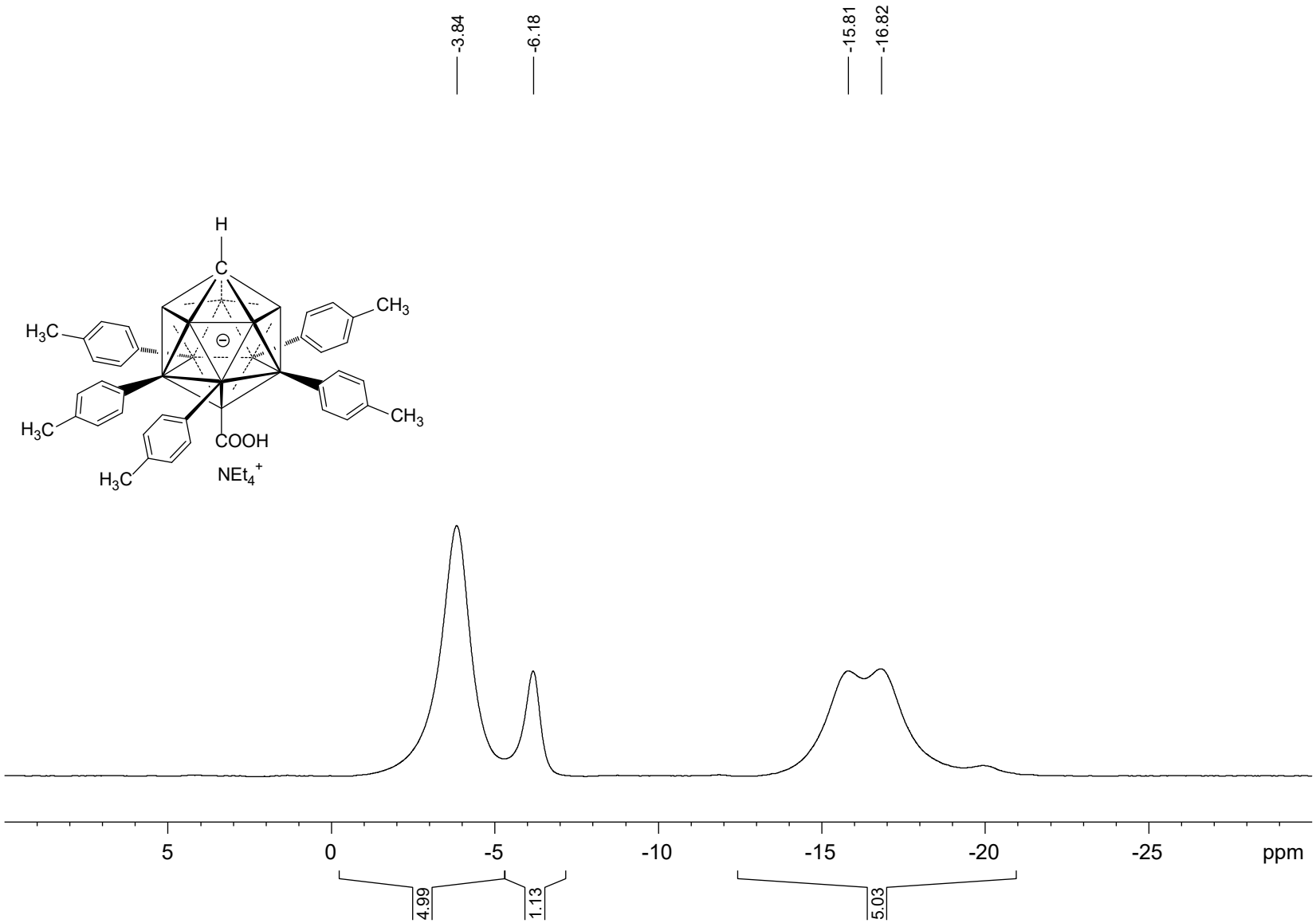
F2 - Acquisition Parameters
Date_             20200731
Time                23.38
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                  2048
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                193.34
DW               16.800 usec
DE                6.50 usec
TE               296.0 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          100.6126827 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-220914-4-CH3 [NEt4][12-COOH-CB11H6(4-C6H4-CH3)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



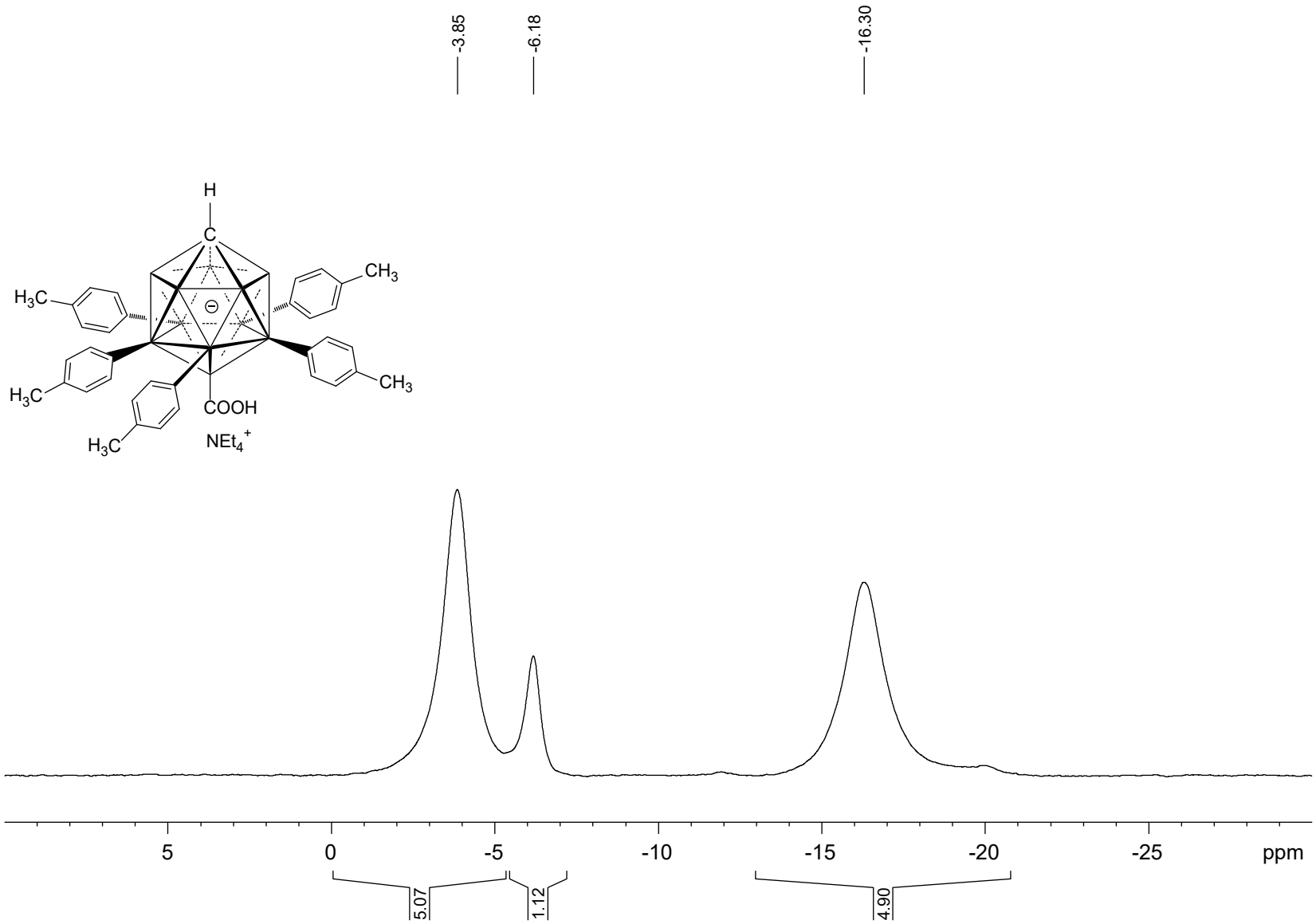

```
Current Data Parameters
NAME      jyj-220914-4-CH3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20220915
Time              10.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.3 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-4-CH3 [NEt4][12-COOH-CB11H6(4-C6H4-CH3)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-CH3
EXPNO                   2
PROCNO                  1

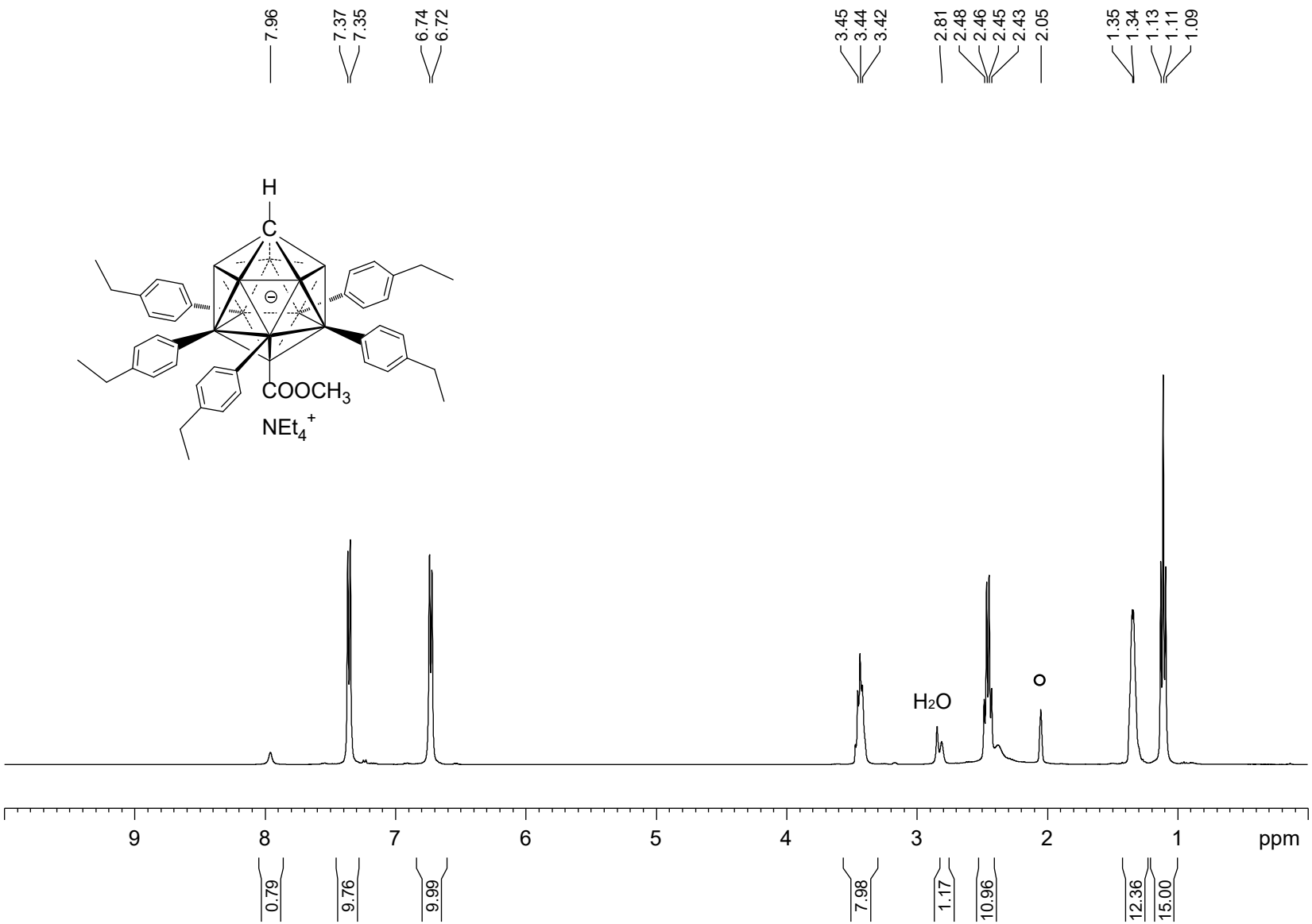
F2 - Acquisition Parameters
Date_           20220915
Time                10.34
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                297.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

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

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

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

jyj-201009-336 4-C6H4-CH2CH3
1H(11B} 400M Hz 19.8 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-201009-336
EXPNO                  1
PROCNO                 1

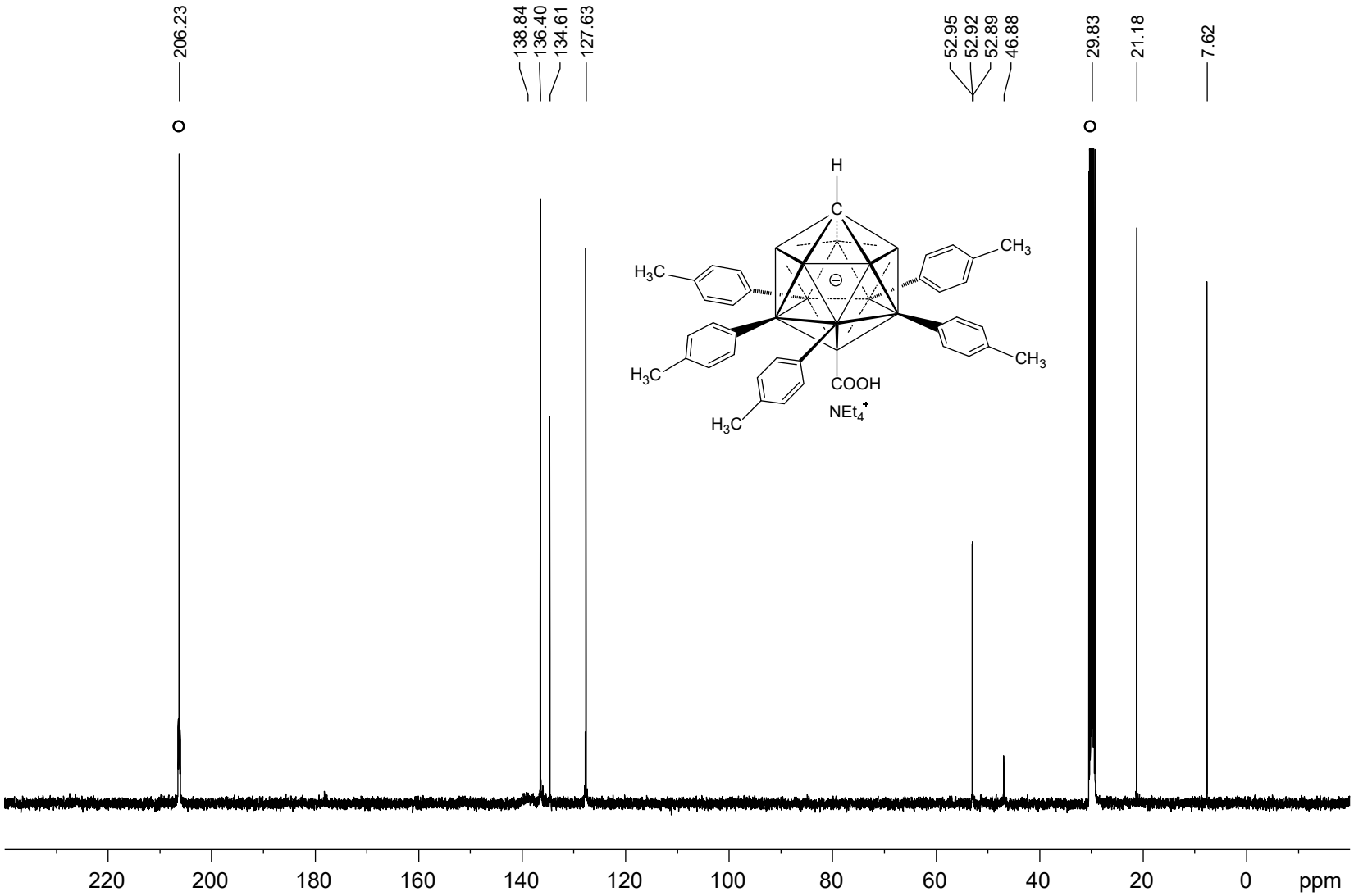
F2 - Acquisition Parameters
Date_           20201010
Time                3.01
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgig30
TD                 16384
SOLVENT          Acetone
NS                    16
DS                     4
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                 78.69
DW                62.400 usec
DE                 6.50 usec
TE                294.0 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          400.1300075 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200716-285-total[NEt4][12-COOH-CB11H6(4-C6H4-CH3)5]
13C 100MHz 20.8mg in acetone-d6 T= 23 C




```
Current Data Parameters
NAME      jyj-200716-285-total
EXPNO                       5
PROCNO                      1

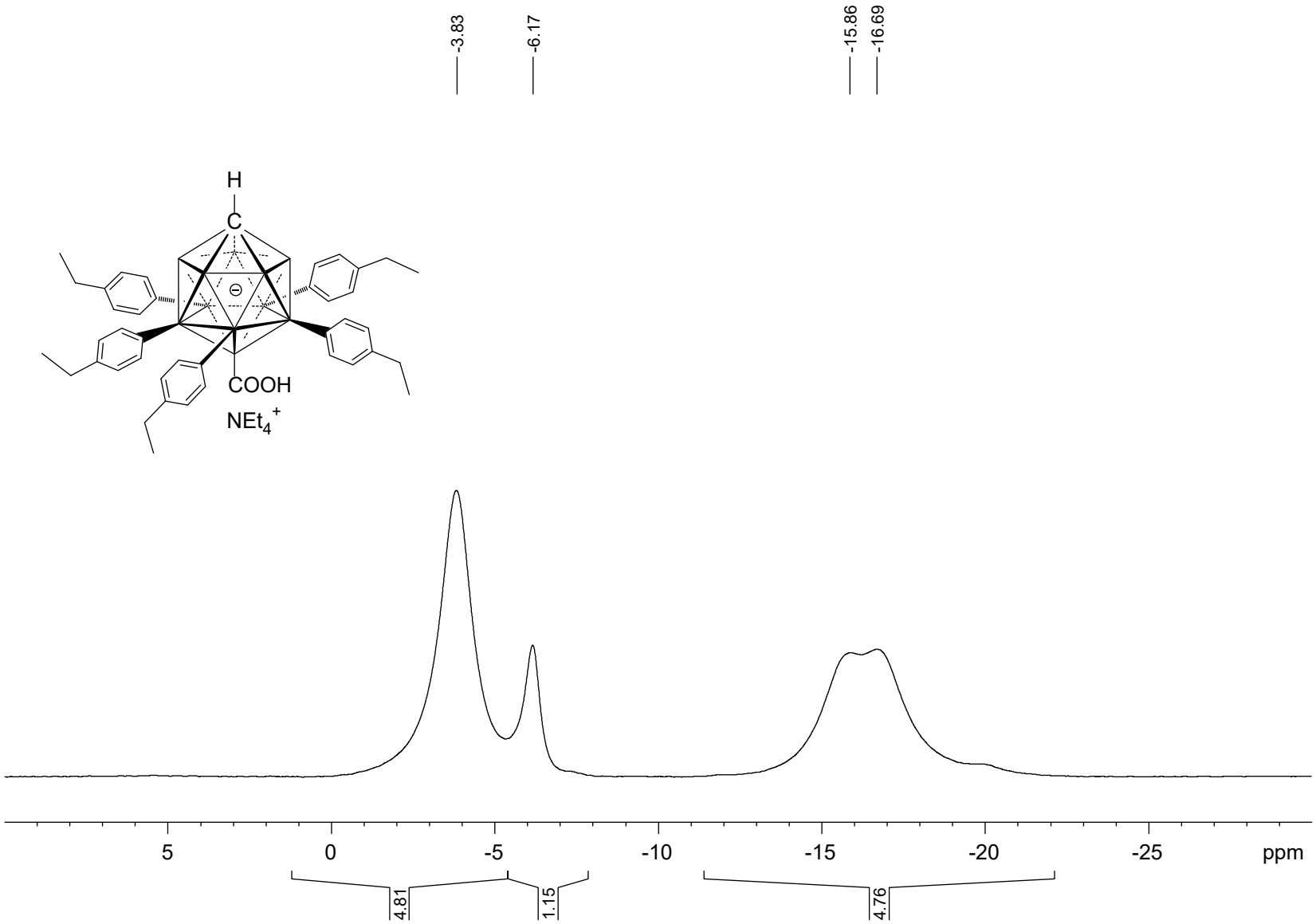
F2 - Acquisition Parameters
Date_            20200719
Time                21.53
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                293.6 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            100.6126836 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

jyj-220914-4-Et [NEt4][12-COOH-CB11H6(4-C6H4-Et)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



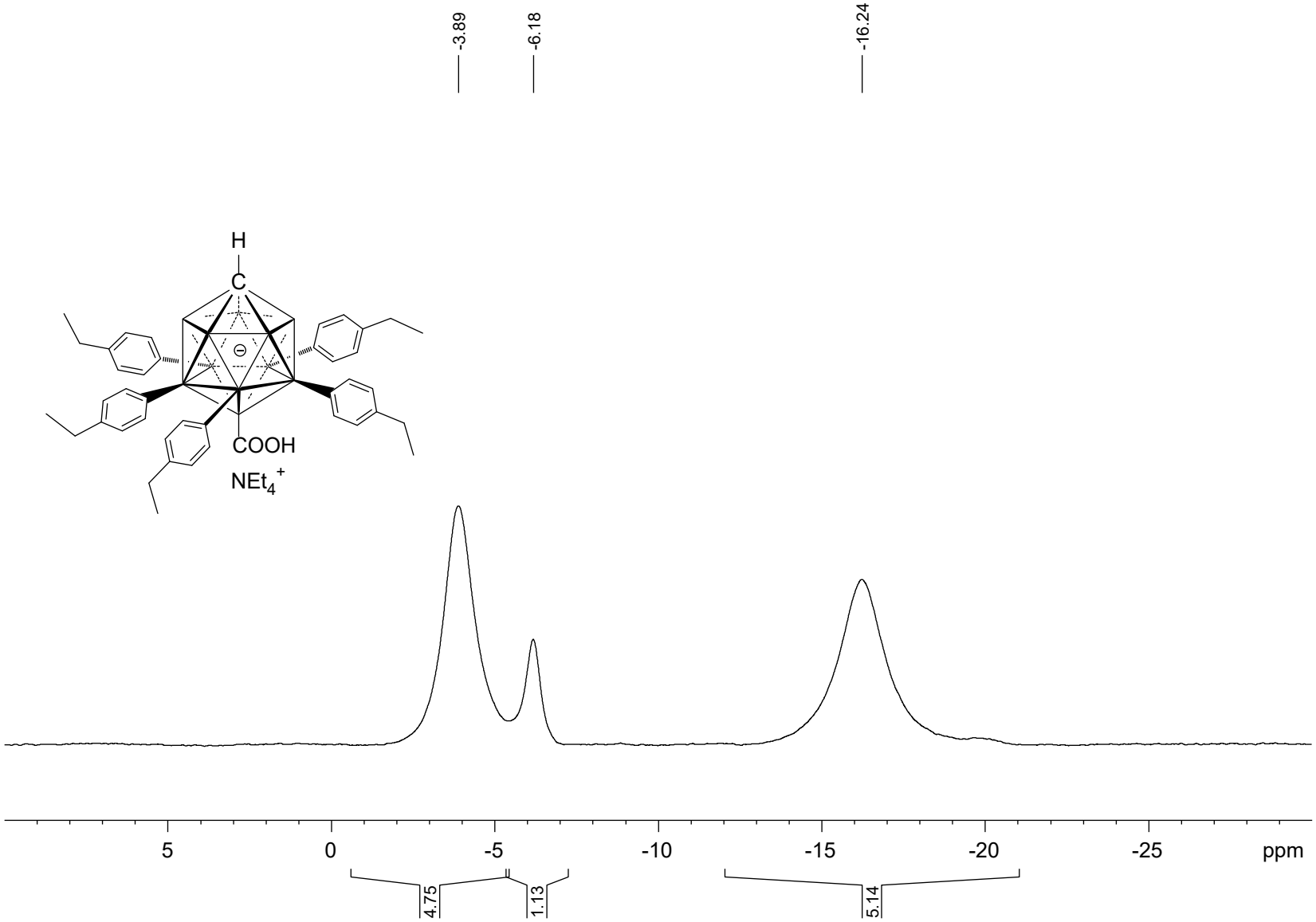

```
Current Data Parameters
NAME      jyj-220914-4-Et
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time              10.43
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.1 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-4-Et [NEt4][12-COOH-CB11H6(4-C6H4-Et)5]
11B{1H] 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-Et
EXPNO                  2
PROCNO                 1

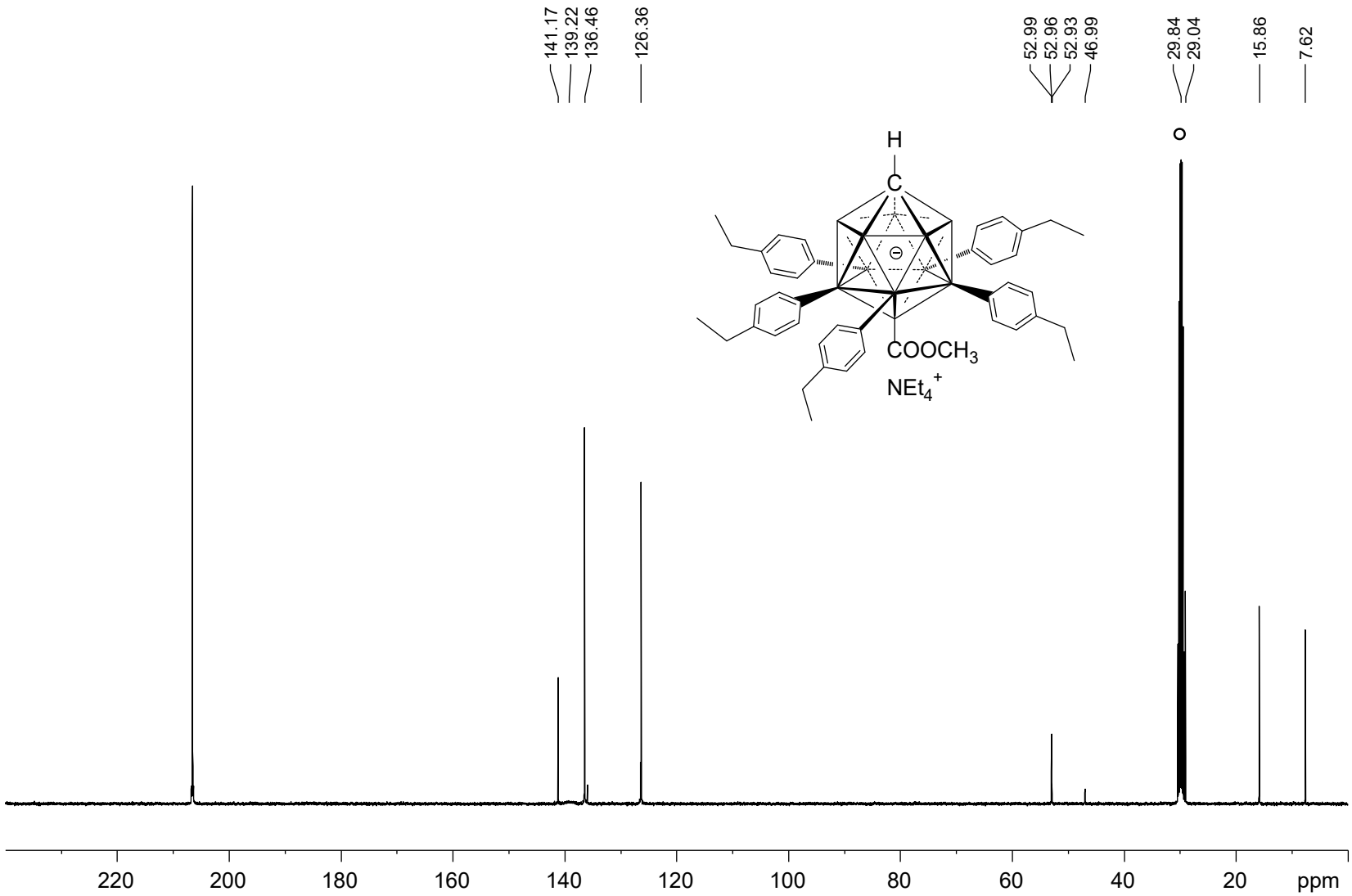
F2 - Acquisition Parameters
Date_           20220915
Time               10.49
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-201009-336 4-C6H4-CH2CH3
13C 100M Hz 19.8 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-211029-336
EXPNO                  1
PROCNO                 1

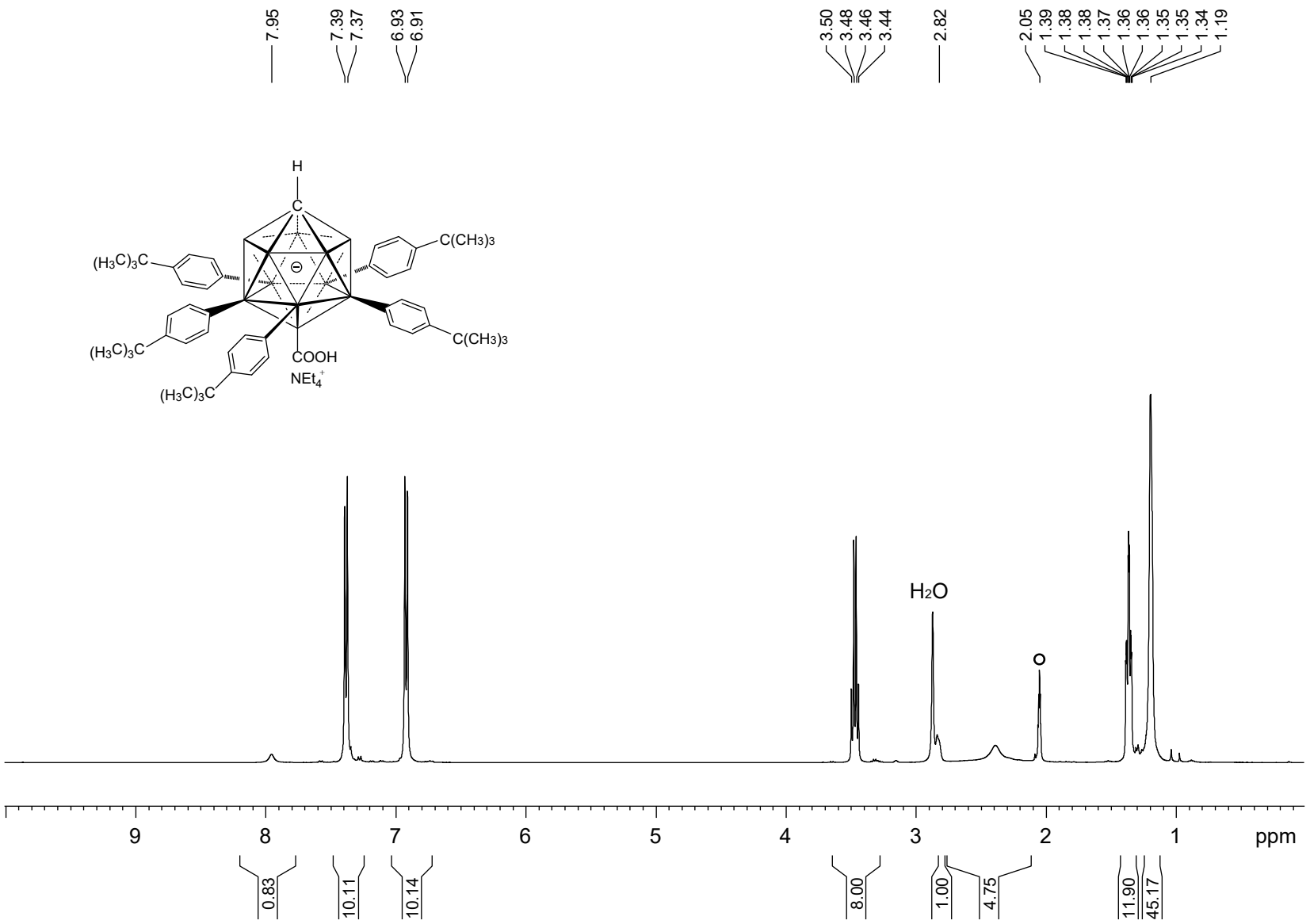
F2 - Acquisition Parameters
Date_           20211030
Time              15.42
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT        Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              297.1 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                  1

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

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

F2 - Processing parameters
SI                 32768
SF         100.6126845 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200619-237-total [NEt4][12-COOH-CB11H6(4-C6H4(C(CH3)3))5]
1H{11B} 400M Hz 16.8mg in Acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200619-237-total
EXPNO                        2
PROCNO                       1

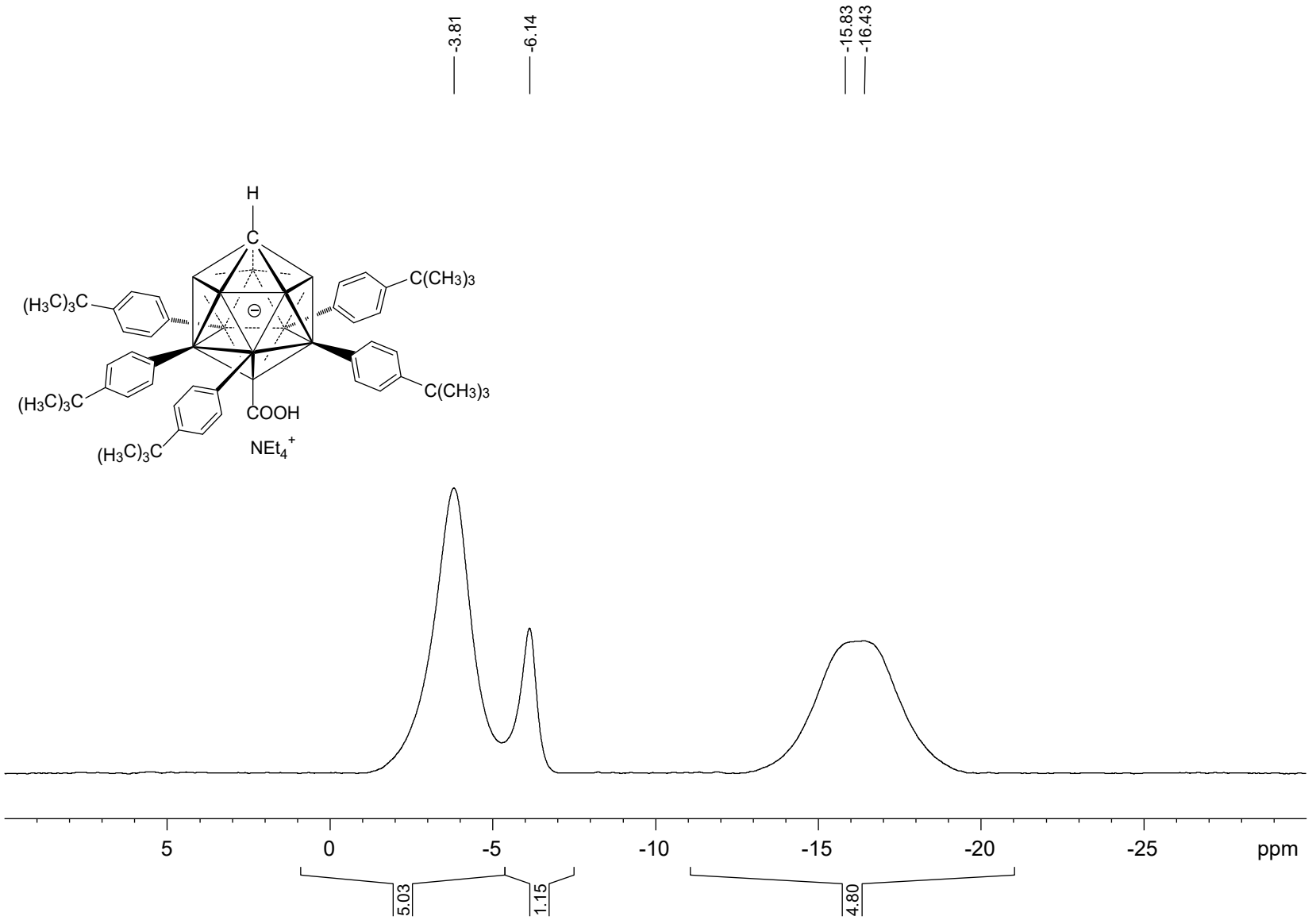
F2 - Acquisition Parameters
Date_              20200622
Time                   3.46
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                        16
DS                         4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                      86.58
DW                     62.400 usec
DE                      6.50 usec
TE                     291.9 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
```

jyj-220914-4-t-Bu [NEt4][12-COOH-CB11H6(4-C6H4-t-Bu)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



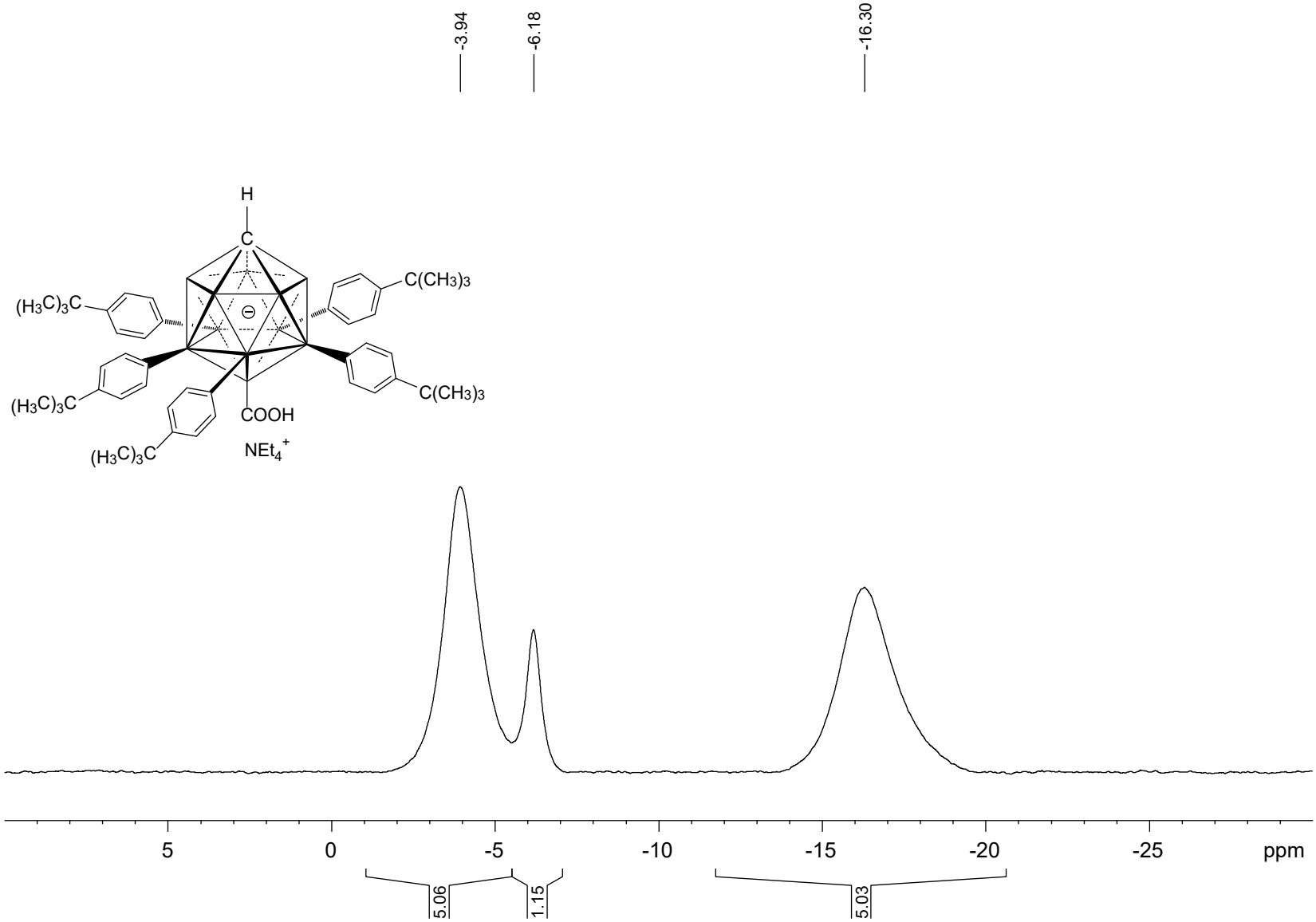

```
Current Data Parameters
NAME      jyj-220914-4-t-Bu
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20220915
Time              10.58
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.1 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-4-t-Bu [NEt4][12-COOH-CB11H6(4-C6H4-t-Bu)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-t-Bu
EXPNO                    2
PROCNO                   1

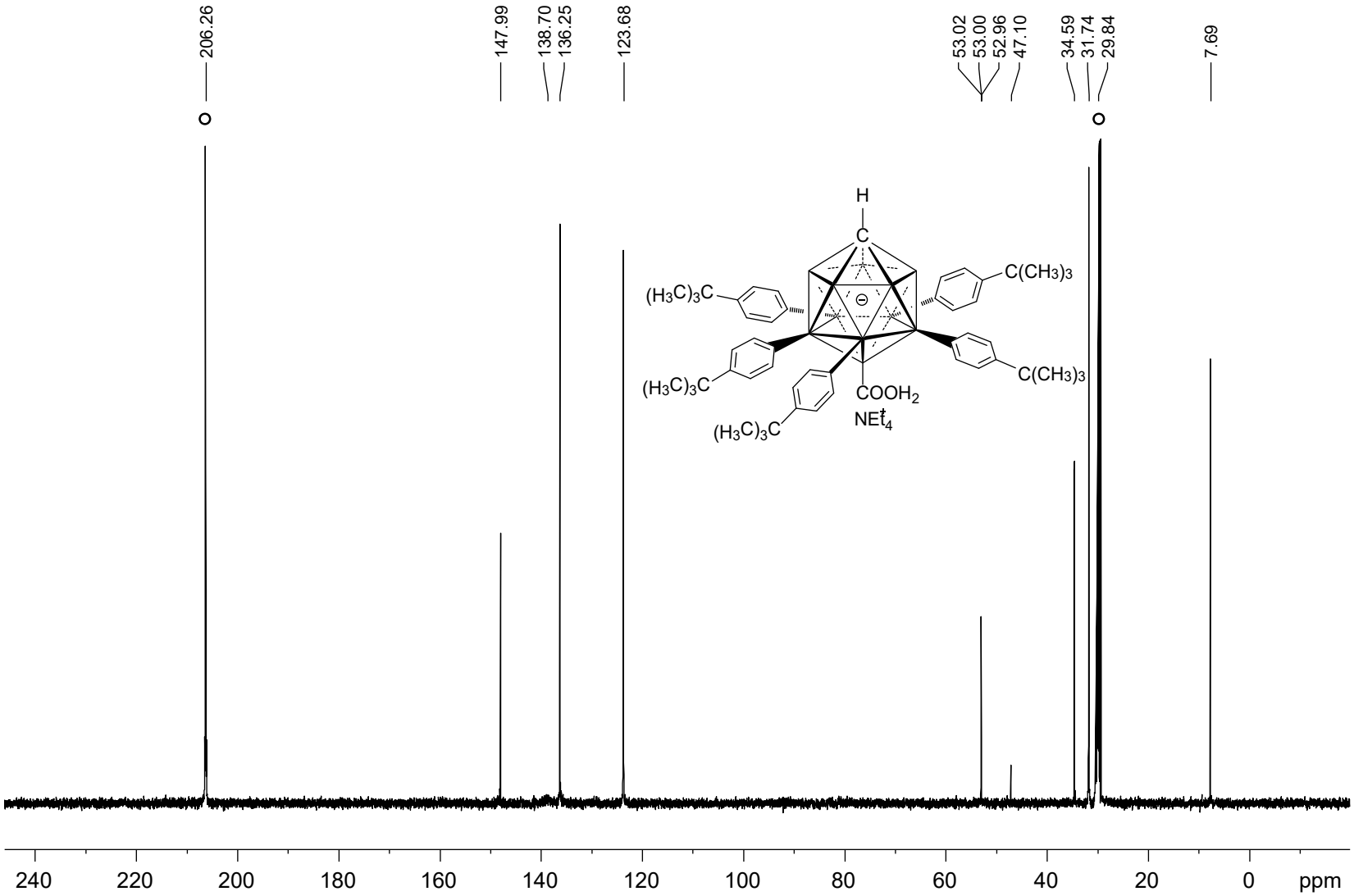
F2 - Acquisition Parameters
Date_            20220915
Time                11.04
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                  65536
SOLVENT           Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                19.600 usec
DE                 6.50 usec
TE                297.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                     1

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

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

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

jyj-200619-237-total [NEt4][12-COOH-CB11H6(4-C6H4(C(CH3)3))5]
13C 100M Hz 16.8mg in Acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200619-237-total
EXPNO                        5
PROCNO                       1

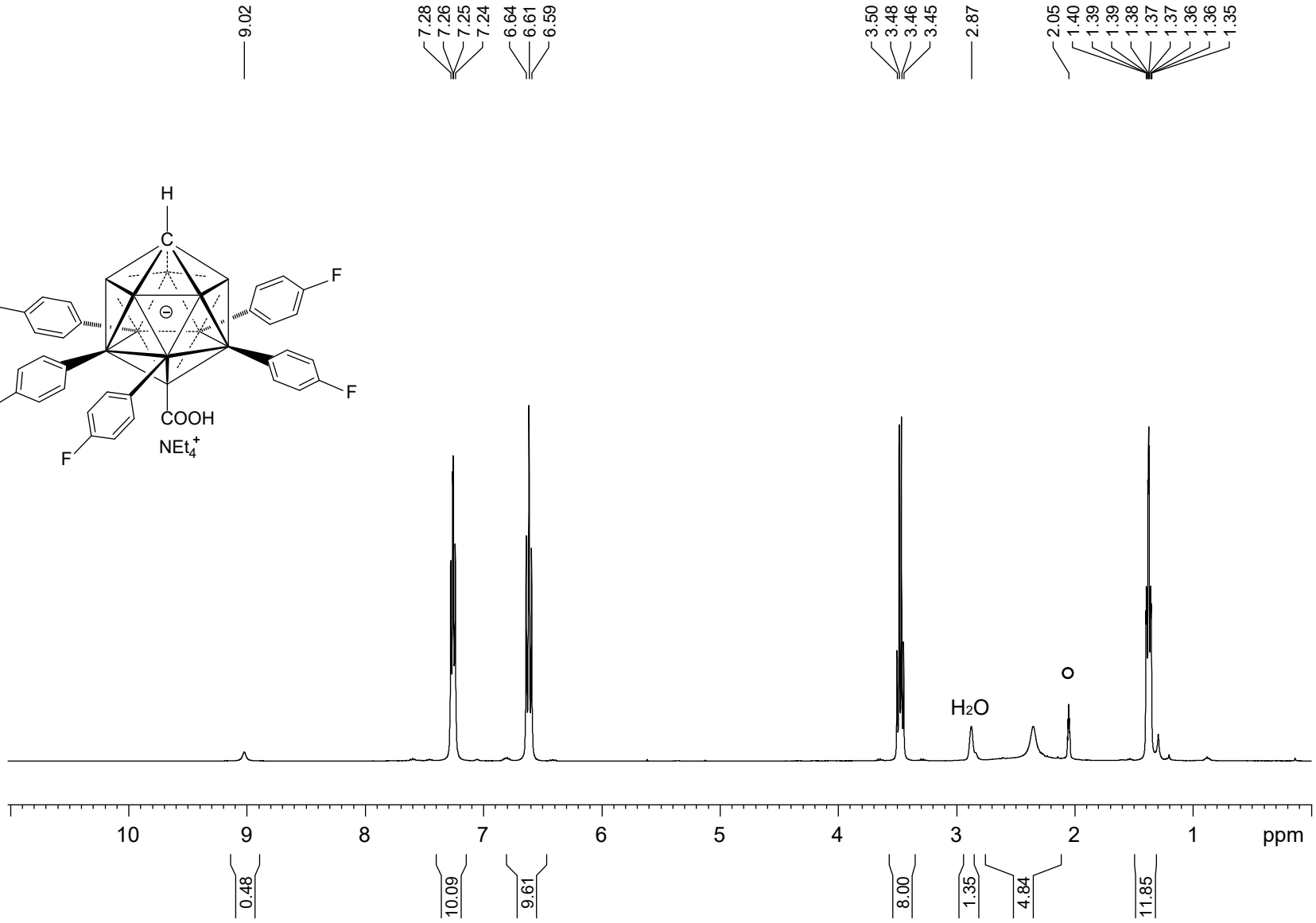
F2 - Acquisition Parameters
Date_              20200622
Time                   5.31
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT           Acetone
NS                     2048
DS                        4
SWH               29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                    193.34
DW                  16.800 usec
DE                   6.50 usec
TE                  292.7 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            100.6126784 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

jyj-200611-263 [NEt4][12-COOH-CB11H6(4-C6H4-F)5]
1H{11B} 400MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200611-263
EXPNO                  2
PROCNO                 1

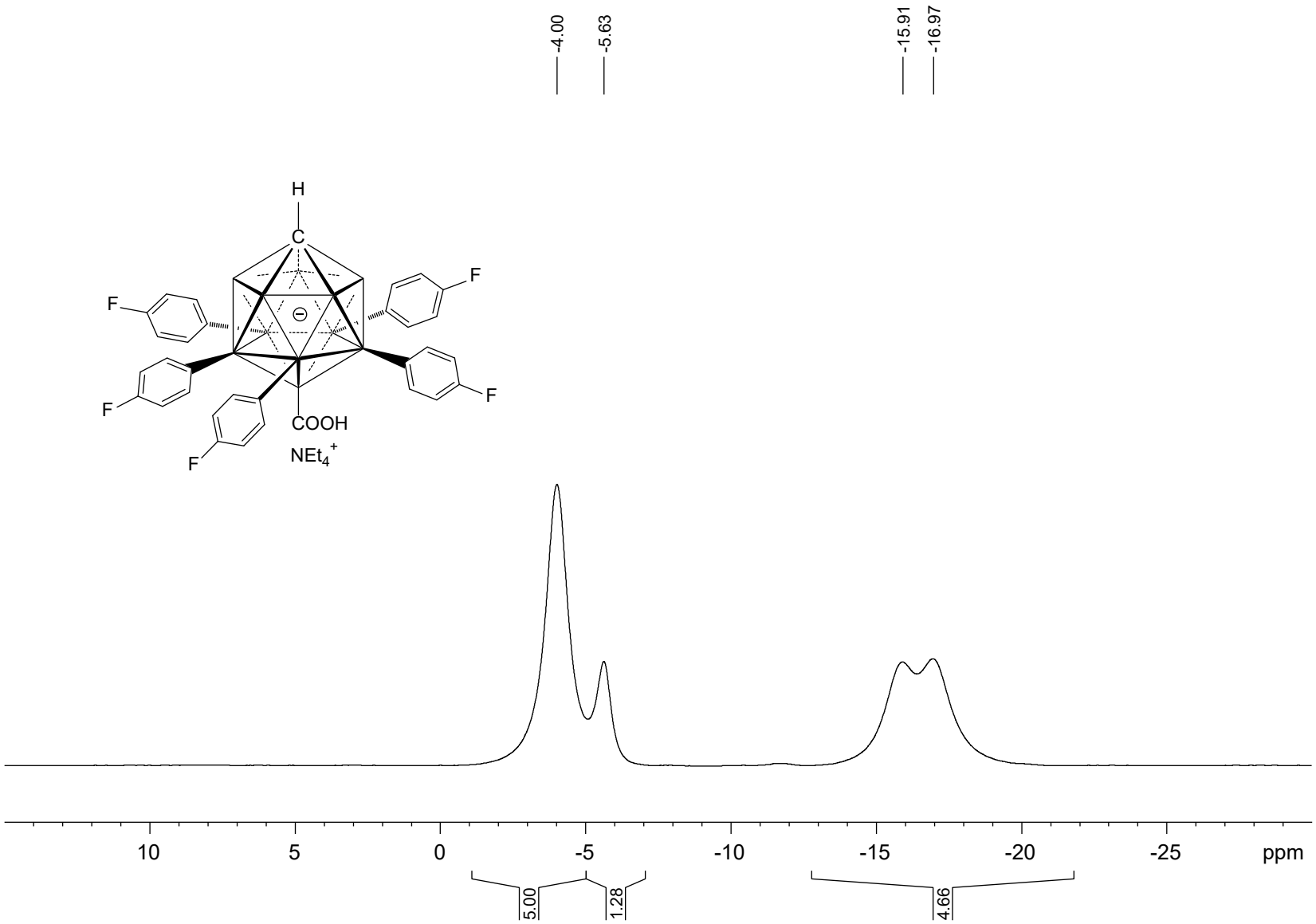
F2 - Acquisition Parameters
Date_           20200612
Time                19.15
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ             1.0223616 sec
RG                95.29
DW                62.400 usec
DE                 6.50 usec
TE                293.2 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
```

jyj-200611-263 [NEt4][12-COOH-CB11H6(4-C6H4-F)5]
11B 128MHz 20.5mg in acetone-d6 T=23 C



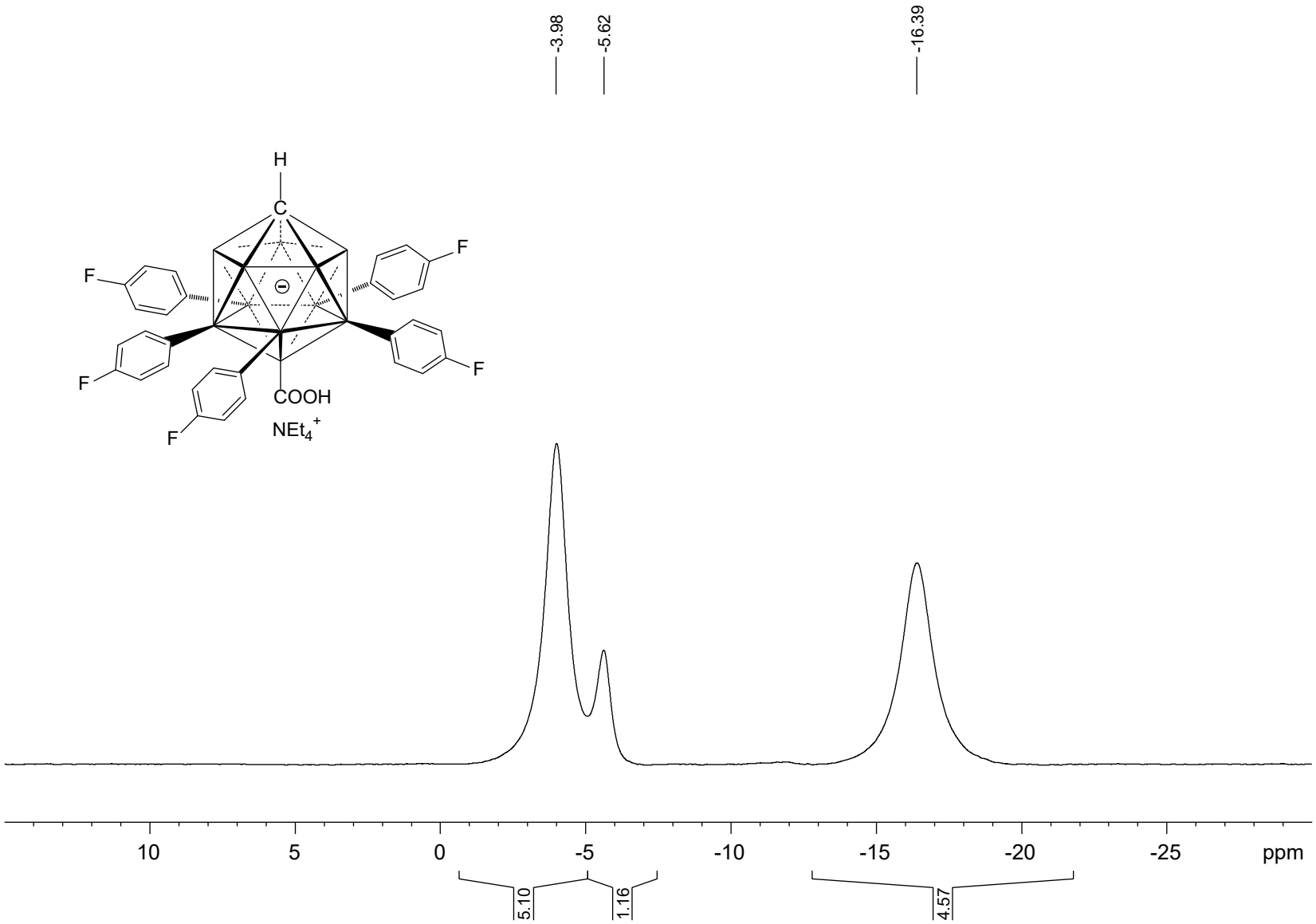

```
Current Data Parameters
NAME      jyj-200611-263-total
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_              20200612
Time                  19.21
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                  zg
TD                    65536
SOLVENT           Acetone
NS                      128
DS                        4
SWH               25510.203 Hz
FIDRES             0.389255 Hz
AQ                1.2845056 sec
RG                   193.34
DW                   19.600 usec
DE                    6.50 usec
TE                   293.2 K
D1              1.00000000 sec
TD0                       1

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

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

jyj-200611-263 [NEt4][12-COOH-CB11H6(4-C6H4-F)5]
11B{1H} 128MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200611-263-total
EXPNO                    4
PROCNO                   1

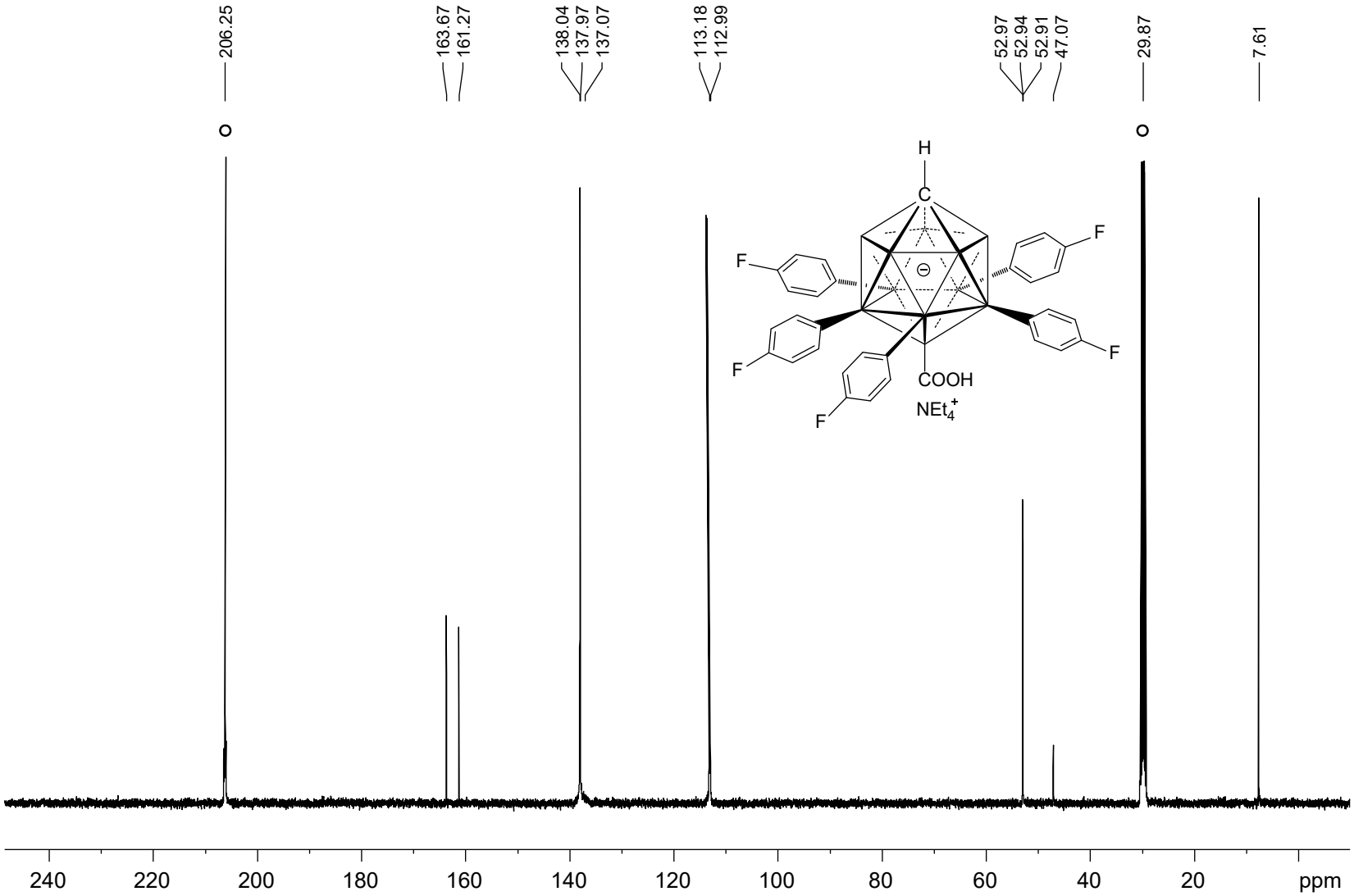
F2 - Acquisition Parameters
Date_             20200612
Time                 19.27
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW               19.600 usec
DE                6.50 usec
TE                293.8 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
```

jyj-200611-263 [NEt4][12-COOH-CB11H6(4-C6H4-F)5]
13C 100MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200611-263
EXPNO                  5
PROCNO                 1

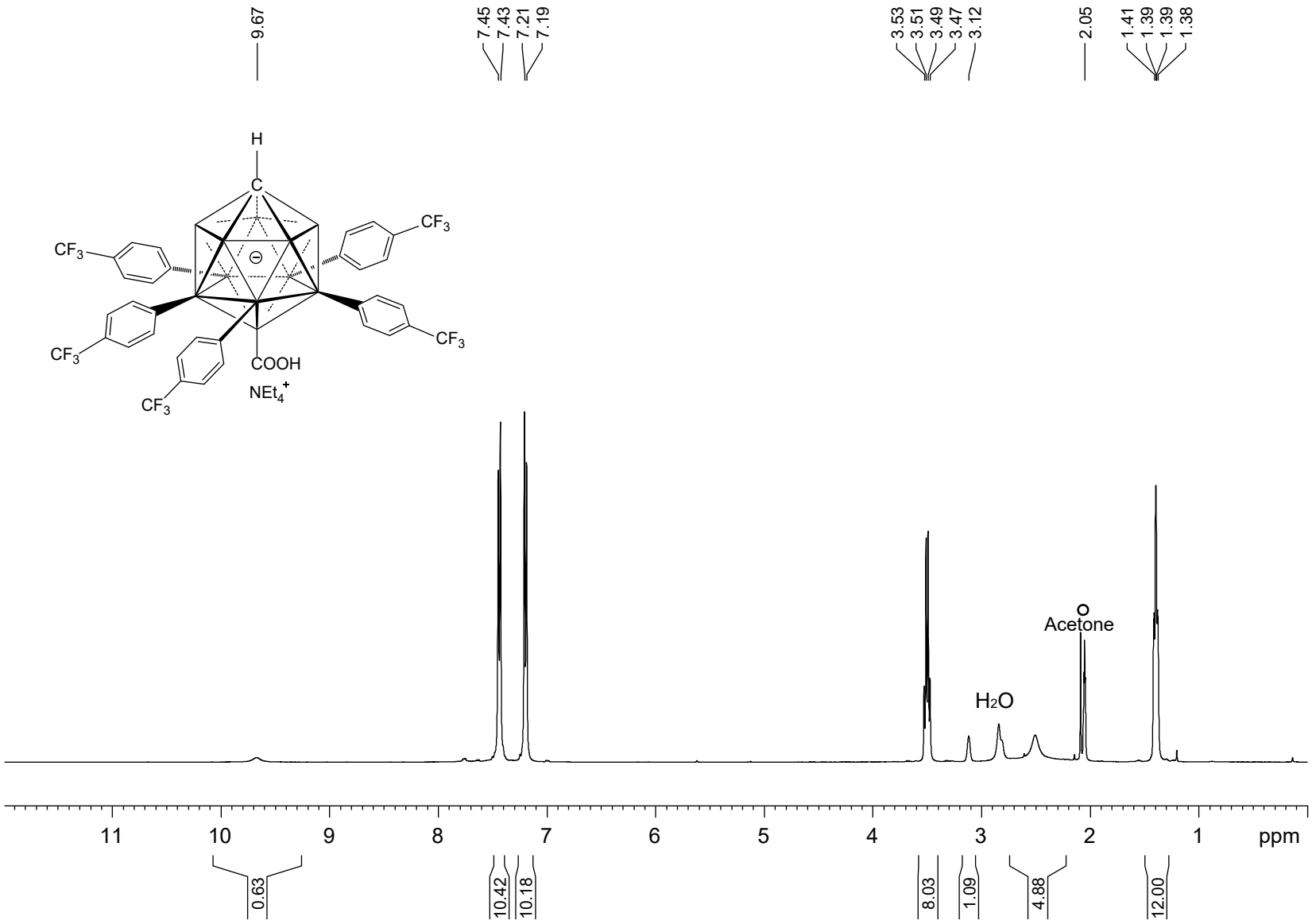
F2 - Acquisition Parameters
Date_           20200612
Time              21.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT         Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ           1.1010048 sec
RG              193.34
DW              16.800 usec
DE               6.50 usec
TE              294.1 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          100.6126831 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200506-139 [NEt4][12-COOH-CB11H6(4-C6H4CF3)5]
1H{11B} 400MHz 20.2mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-190511-139
EXPNO                 1
PROCNO                1

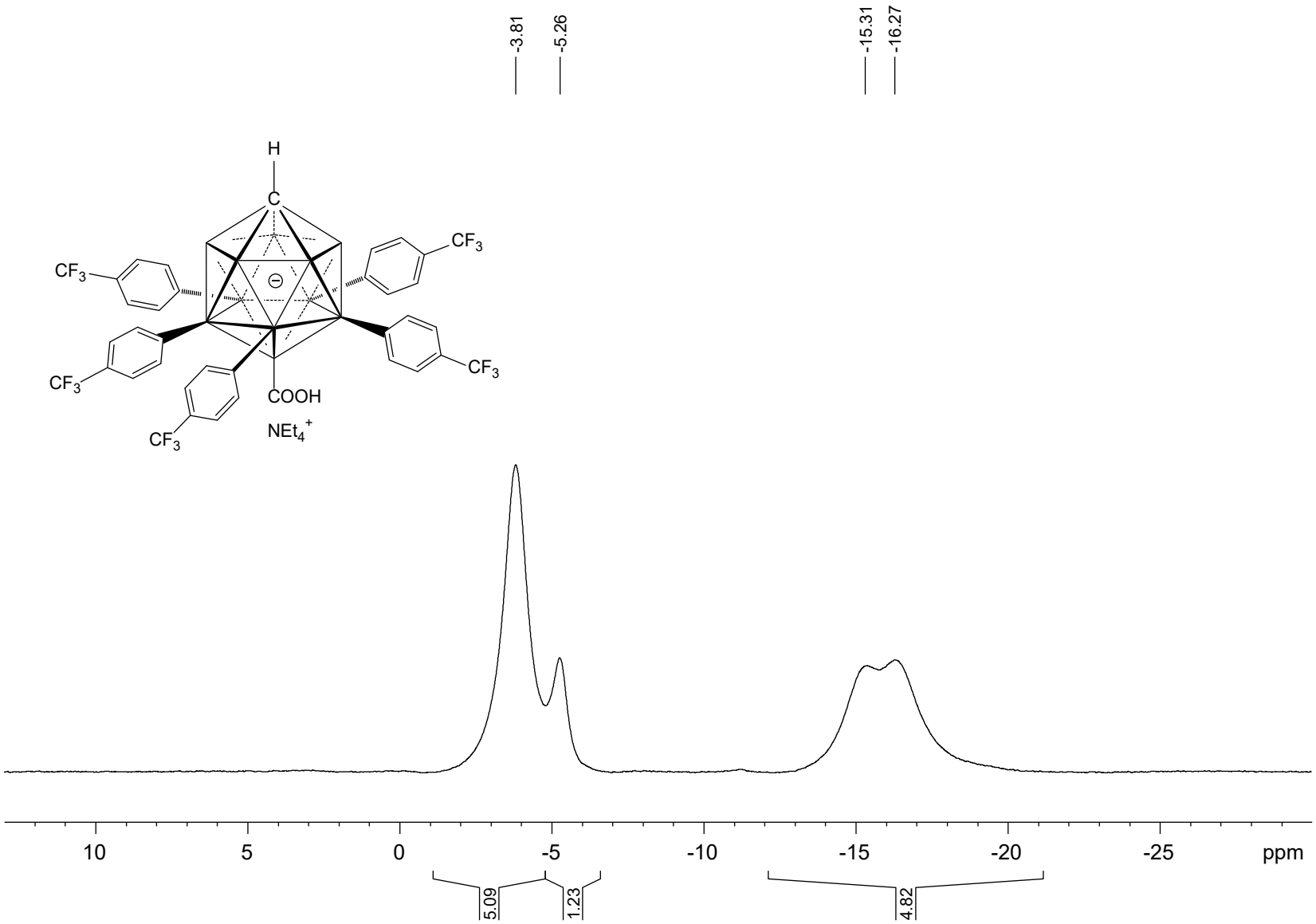
F2 - Acquisition Parameters
Date_          20190512
Time              21.27
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES            0.489064 Hz
AQ             1.0223616 sec
RG                 107.6
DW                62.400 usec
DE                 6.50 usec
TE                296.3 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   1

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

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

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

jyj-200506-139 [NEt4][12-COOH-CB11H6(4-C6H4CF3)5]
11B 128MHz 20.2mg in acetone-d6 T=23 C



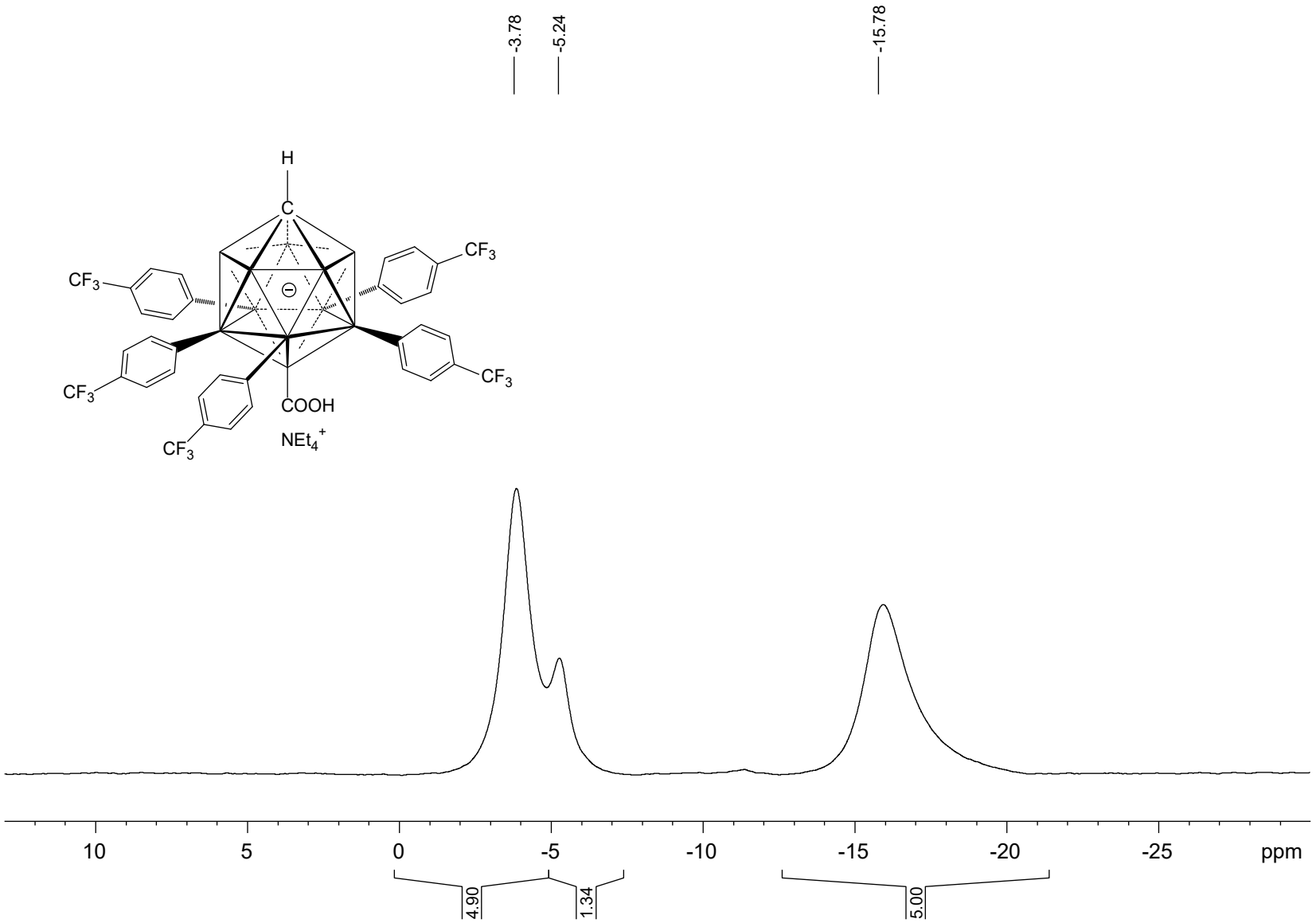

```
Current Data Parameters
NAME      jyj-190511-139-4-CF3 total
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_           20190512
Time              21.33
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                 5.00 Hz
GB                    0
PC                 1.40
```

jyj-200506-139 [NEt4][12-COOH-CB11H6(4-C6H4CF3)5]
11B{1H} 128MHz 20.2mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-190511-139-4-CF3 total
EXPNO                 3
PROCNO                1

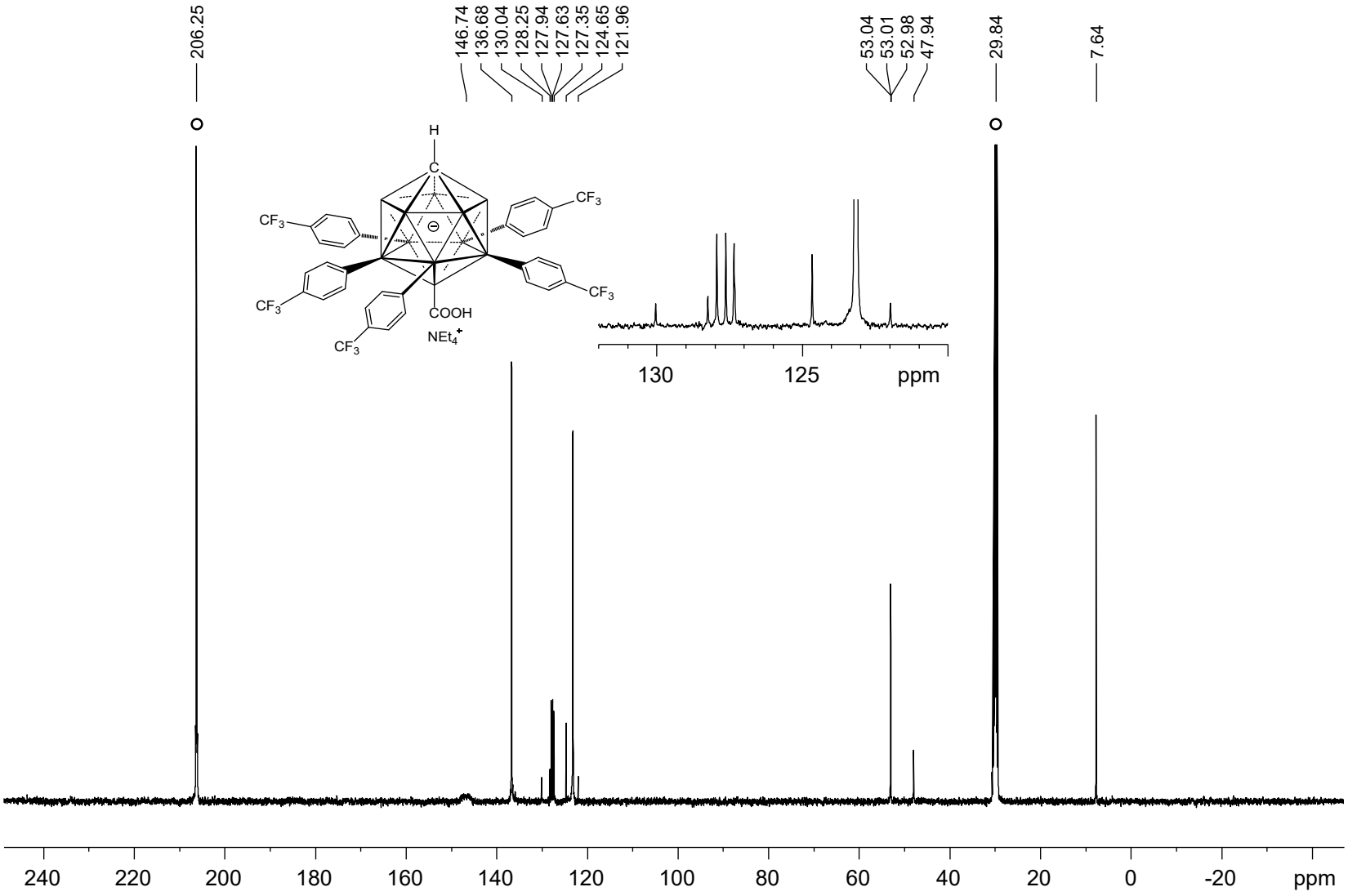
F2 - Acquisition Parameters
Date_          20190512
Time              21.39
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              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              20.00 Hz
GB                  0
PC                1.40
```

jyj-200506-139 [NEt4][12-COOH-CB11H6(4-C6H4CF3)5]
13C 100MHz 20.2mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200506-139
EXPNO                 3
PROCNO                1

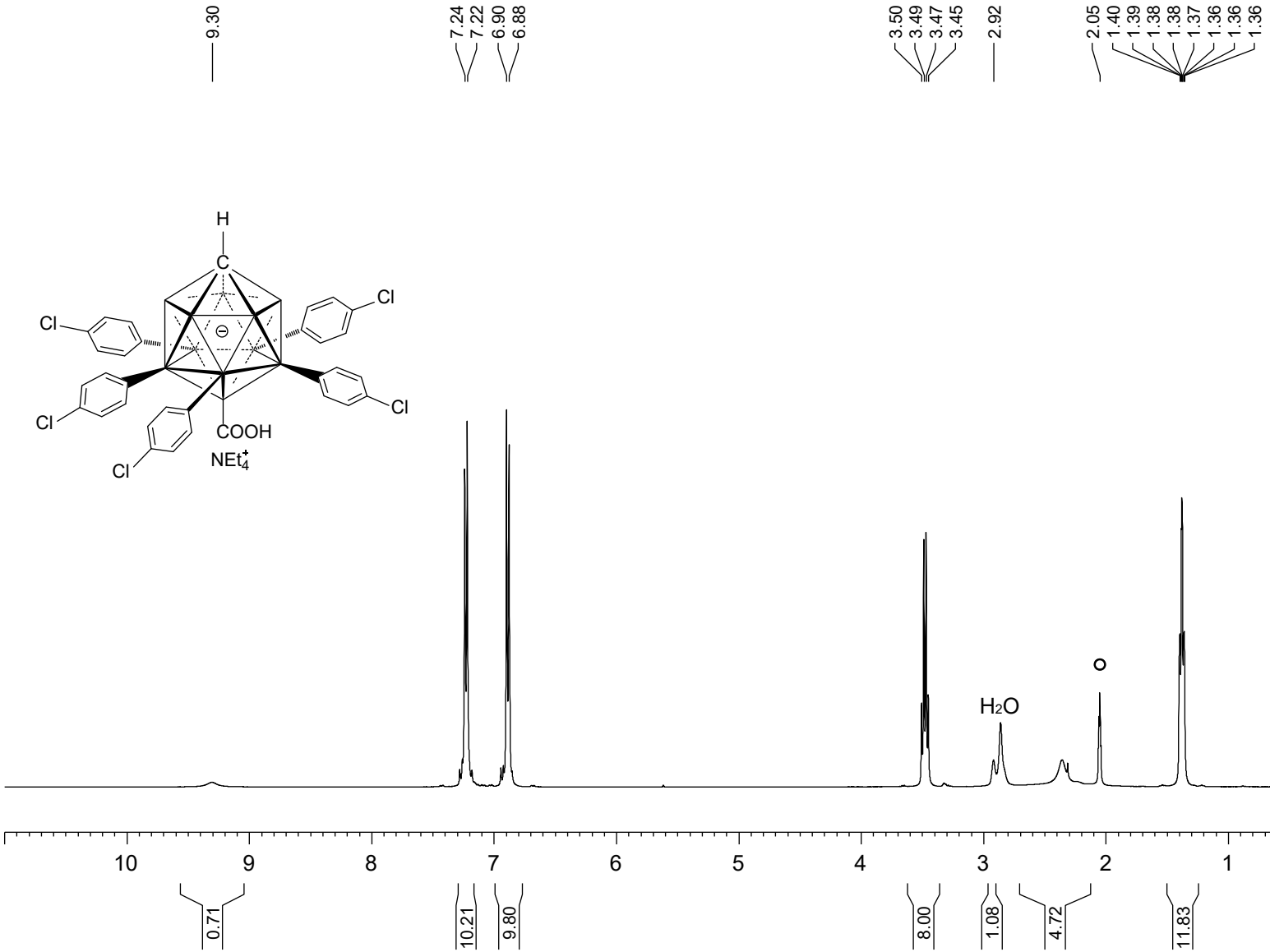
F2 - Acquisition Parameters
Date_          20200512
Time              15.33
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT       Acetone
NS               2048
DS                  4
SWH          29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                193.34
DW              16.800 usec
DE               6.50 usec
TE              296.3 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          100.6126784 MHz
WDW                  EM
SSB                   0
LB                 2.00 Hz
GB                    0
PC                 1.40
```

jyj-200712-283-total [NEt4][12-COOH-CB11H6(4-C6H4-Cl)5]
1H{11B} 400MHz 23.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200712-283-total
EXPNO                        2
PROCNO                       1

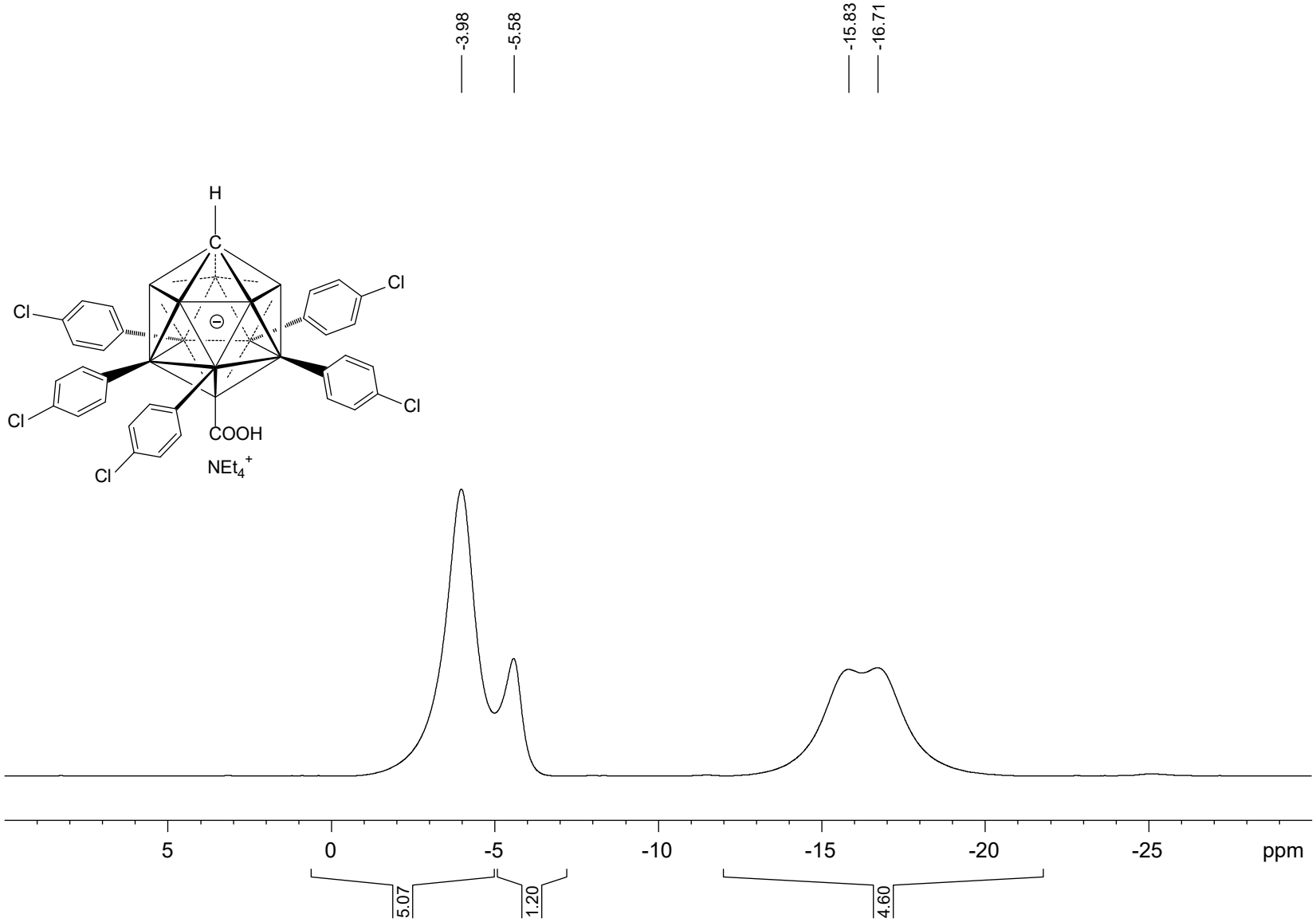
F2 - Acquisition Parameters
Date_              20200713
Time                  11.28
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT           Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                      107.6
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                400.1300072 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

jyj-220914-4-Cl [NEt4][12-COOH-CB11H6(4-C6H4-Cl)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



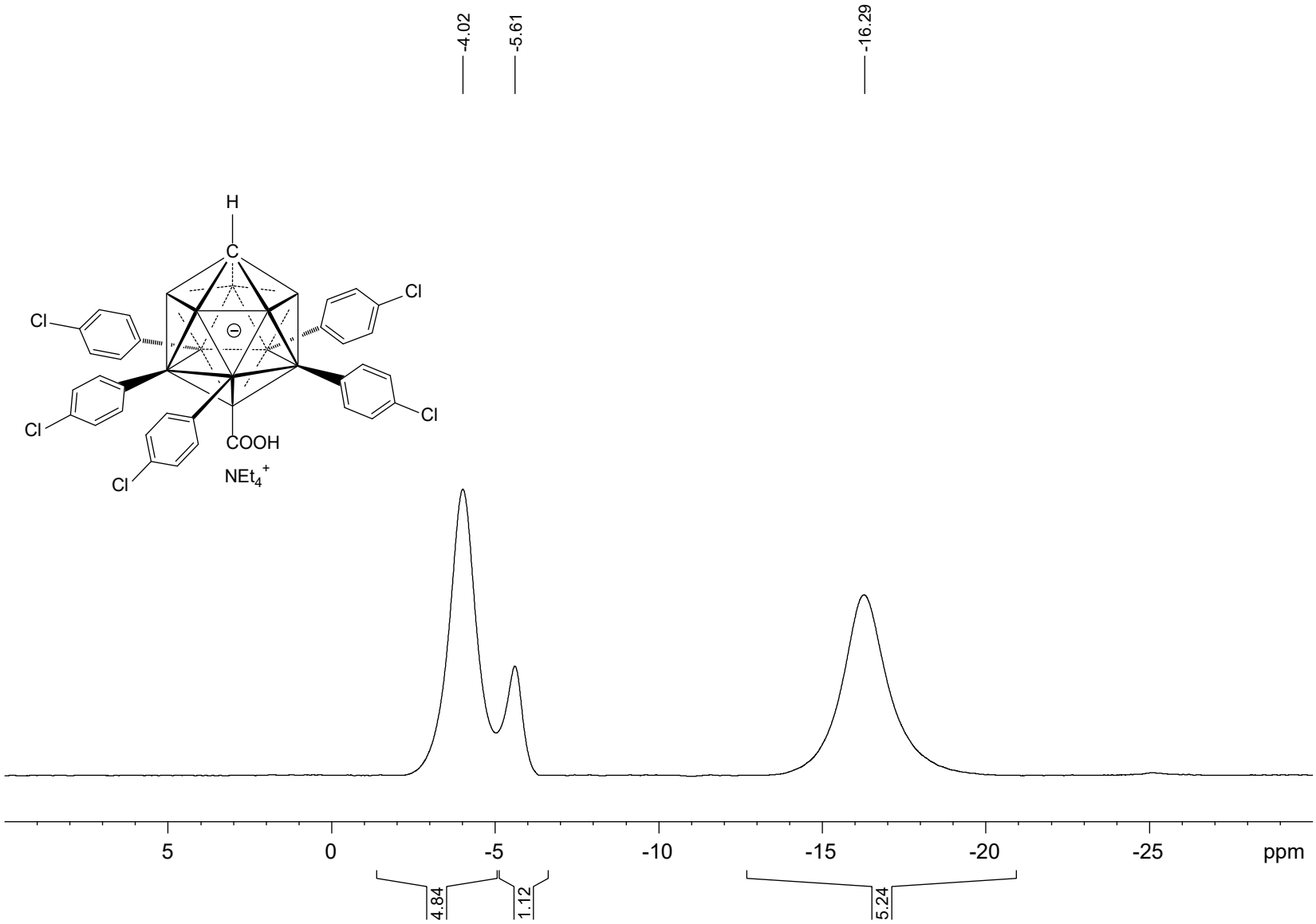

```
Current Data Parameters
NAME      jyj-220914-4-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time                2.48
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.2 K
D1            1.00000000 sec
TD0                    1

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

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

jyj-220914-4-Cl [NEt4][12-COOH-CB11H6(4-C6H4-Cl)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-Cl
EXPNO                  2
PROCNO                 1

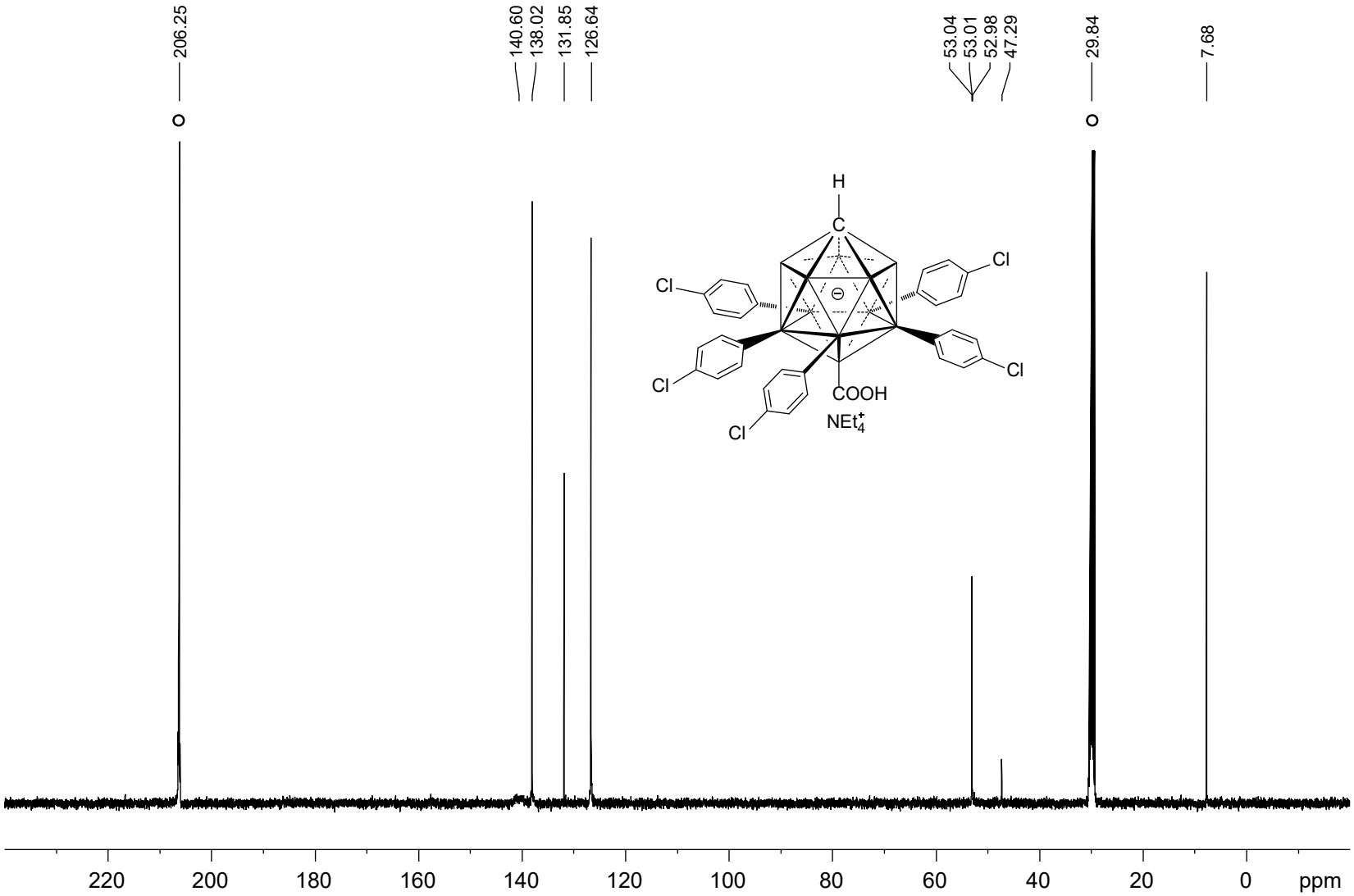
F2 - Acquisition Parameters
Date_           20220915
Time                2.54
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-200712-283-total [NEt4][12-COOH-CB11H6(4-C6H4-Cl)5]
11C 100MHz 23.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200712-283-total
EXPNO                       5
PROCNO                      1

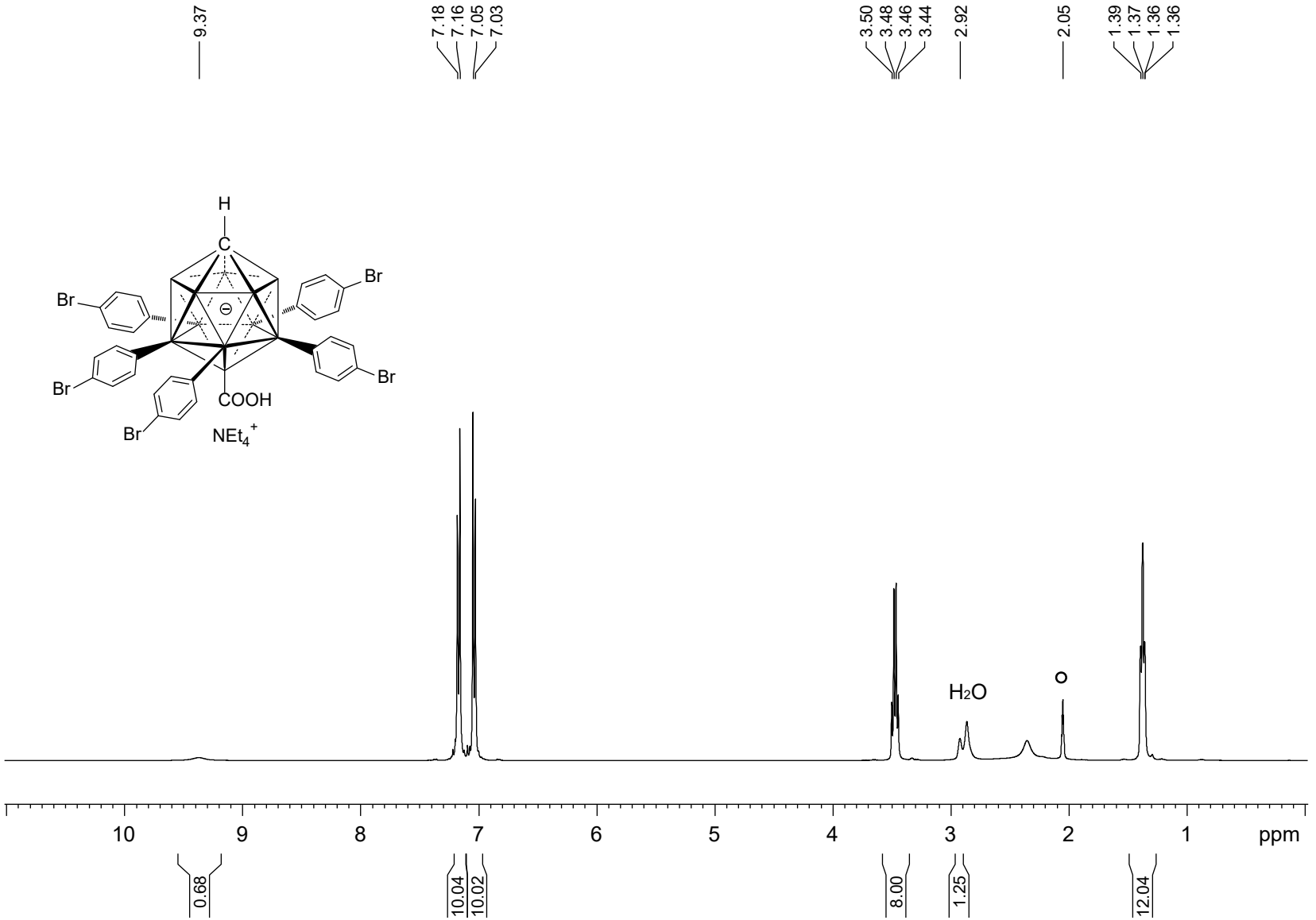
F2 - Acquisition Parameters
Date_            20200713
Time                13.12
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               295.3 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          100.6126784 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200825-284-total [NEt4][12-COOH-CB11H6(C6H4Br)5]
1H{11B} 400MHz 32.2mg in acetone-d6 T =23C




```
Current Data Parameters
NAME      jyj-200825-284-total
EXPNO                        2
PROCNO                       1

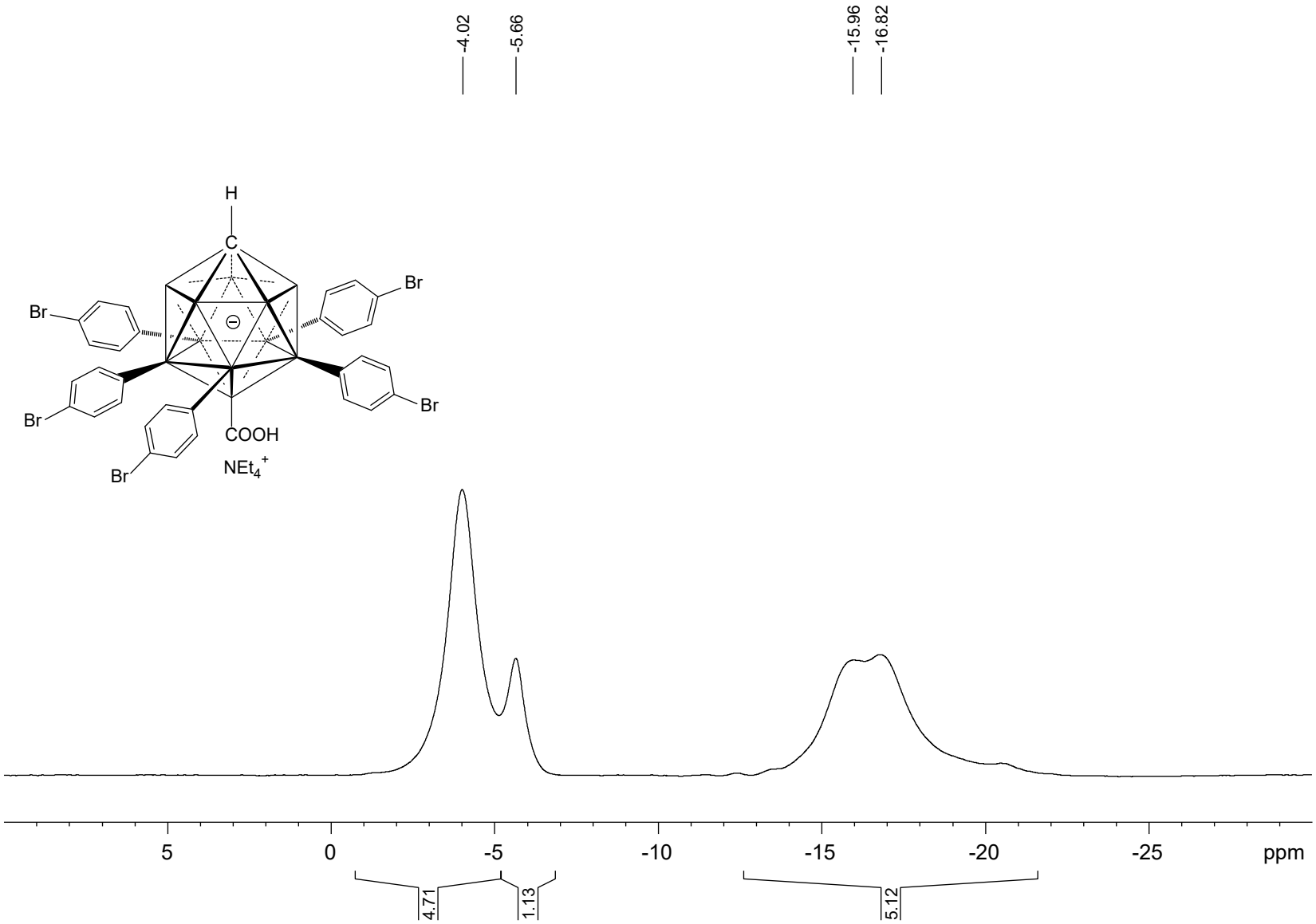
F2 - Acquisition Parameters
Date_              20200826
Time                  15.53
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT            Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES            0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   295.9 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             400.1300072 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

jyj-220914-4-Br [NEt4][12-COOH-CB11H6(4-C6H4-Br)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



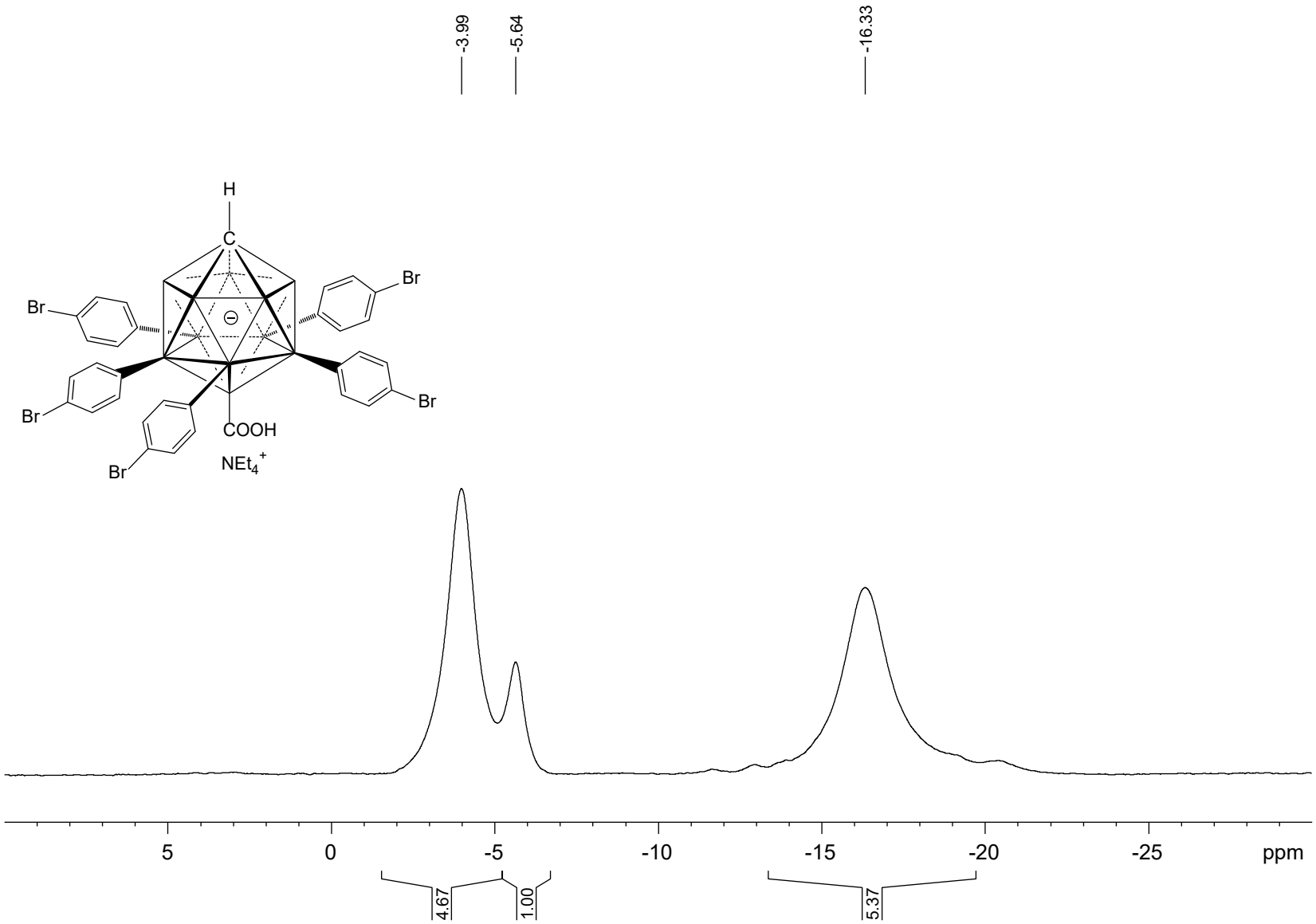

```
Current Data Parameters
NAME      jyj-220914-4-Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time                3.03
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.2 K
D1            1.00000000 sec
TD0                    1

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

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

jyj-220914-4-Br [NEt4][12-COOH-CB11H6(4-C6H4-Br)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-Br
EXPNO                  2
PROCNO                 1

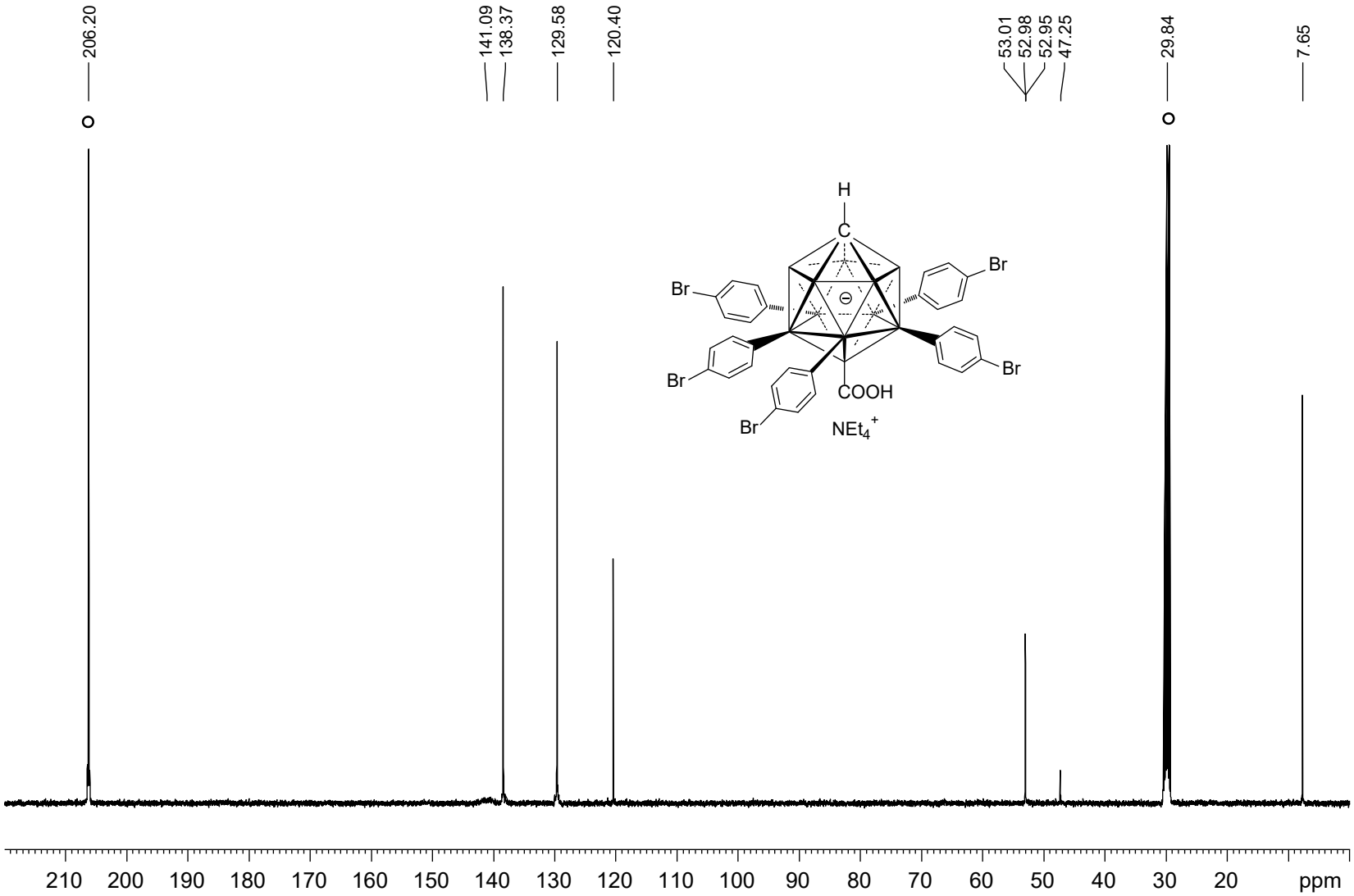
F2 - Acquisition Parameters
Date_           20220915
Time                3.09
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               297.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-200825-284-total [NEt4][12-COOH-CB11H6(C6H4Br)5]
13C 100MHz 32.2mg in acetone-d6 T =23C




```
Current Data Parameters
NAME      jyj-200825-284-total
EXPNO                        5
PROCNO                       1

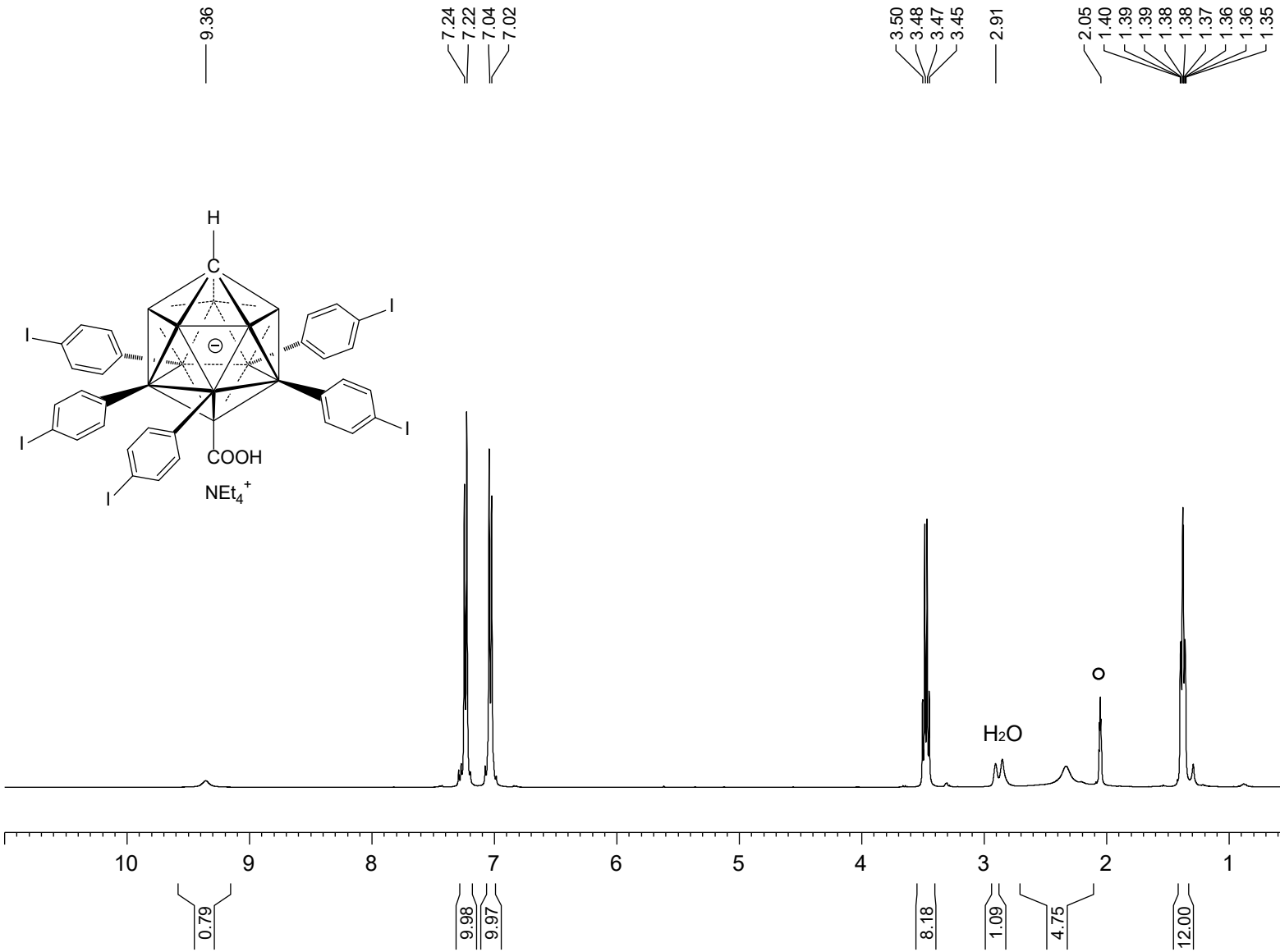
F2 - Acquisition Parameters
Date_              20200826
Time                 17.37
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                296.7 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            100.6126836 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

jyj-201006-335 [NEt4][12-COOH-CB11H6(4-I-C6H4)5]
1H{11B} 400 MHz NMR 29.6mg dissolved in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-201006-335
EXPNO                  1
PROCNO                 1

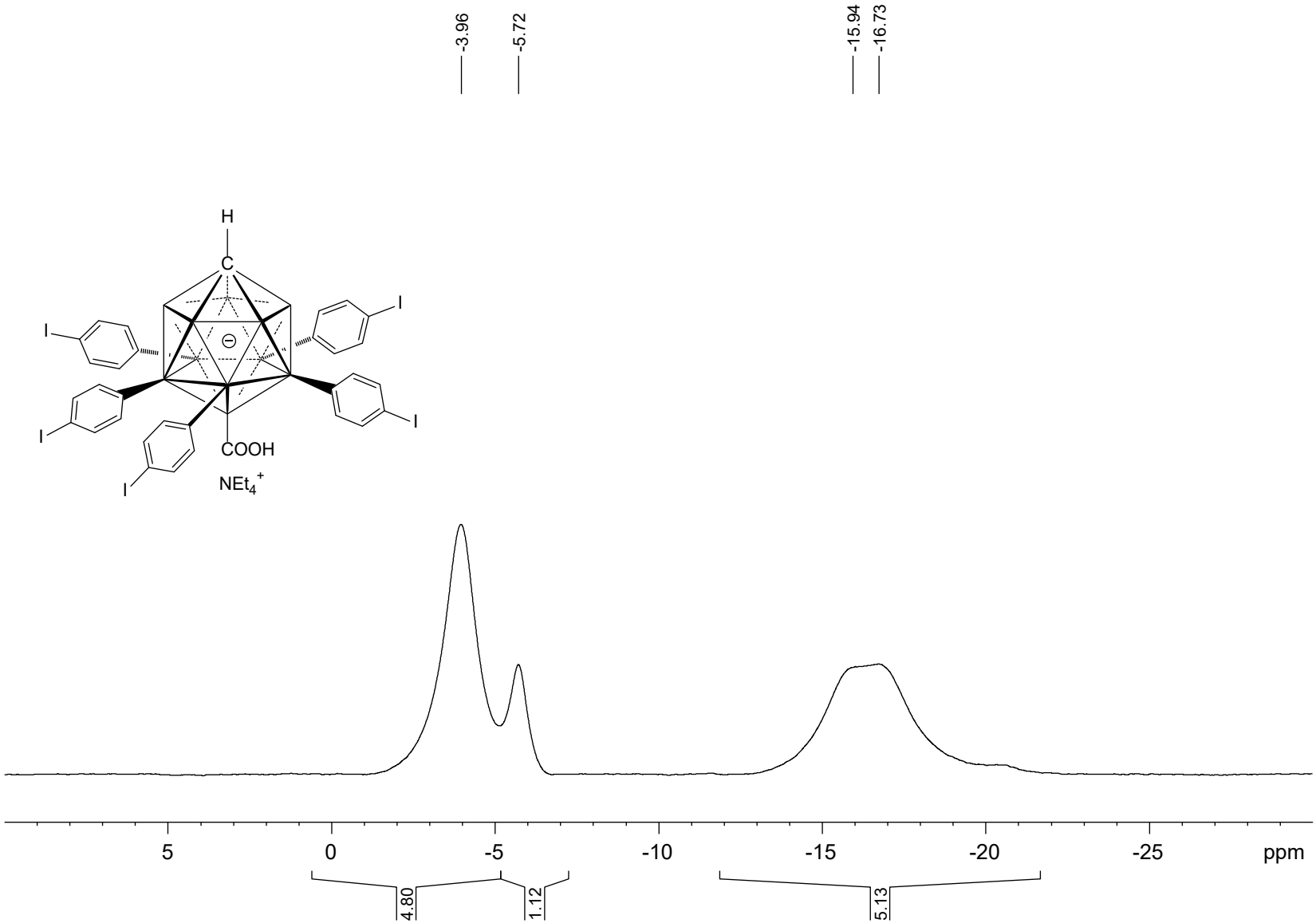
F2 - Acquisition Parameters
Date_           20201007
Time                5.07
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgig30
TD                 16384
SOLVENT          Acetone
NS                    16
DS                     4
SWH             8012.820 Hz
FIDRES          0.489064 Hz
AQ             1.0223616 sec
RG                 107.6
DW                62.400 usec
DE                 6.50 usec
TE                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         400.1300072 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-220914-4-I [NEt4][12-COOH-CB11H6(4-C6H4-I)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



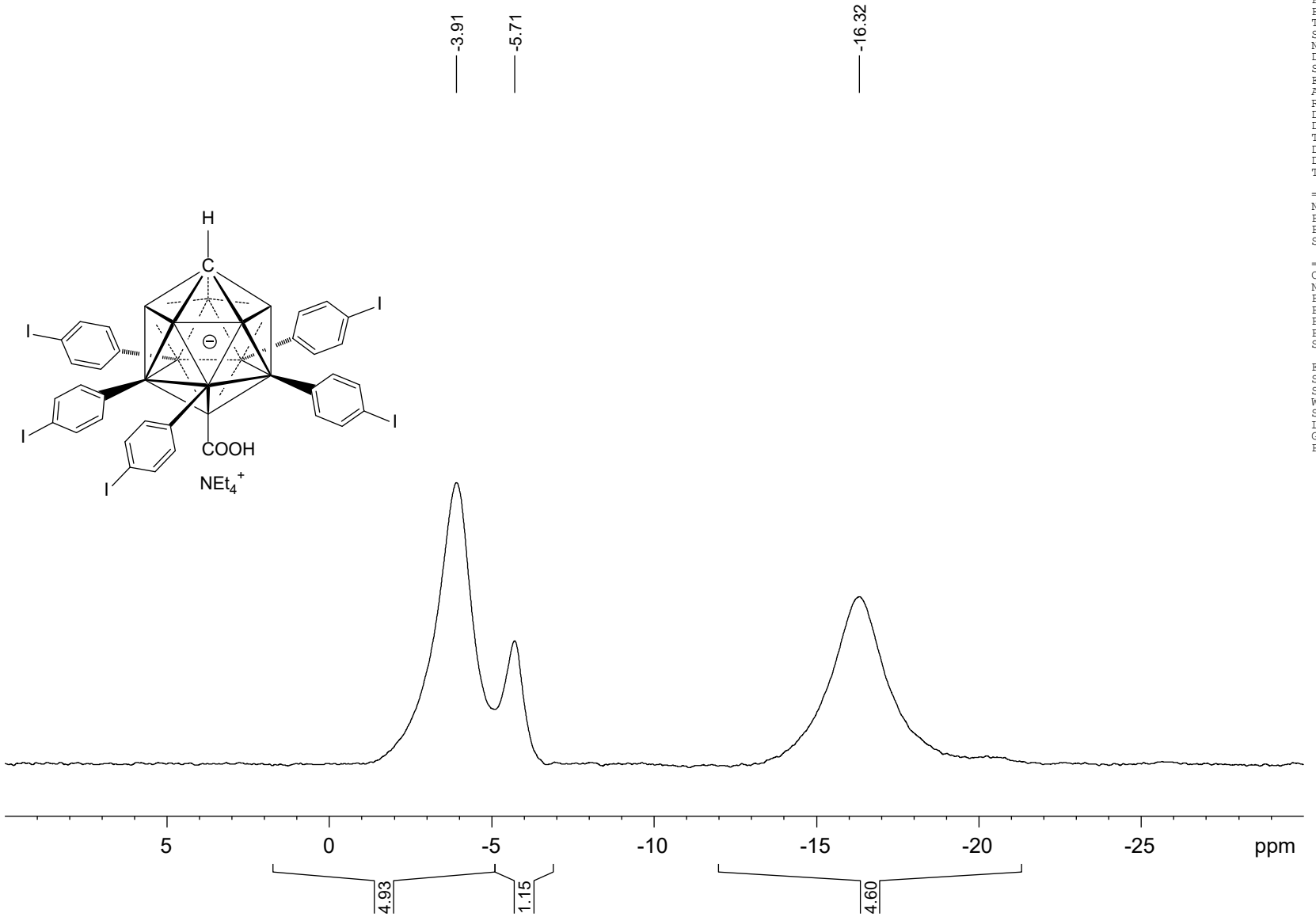

```
Current Data Parameters
NAME      jyj-220914-4-I
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20220915
Time               3.18
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.2 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-4-I [NEt4][12-COOH-CB11H6(4-C6H4-I)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-I
EXPNO                 2
PROCNO                1

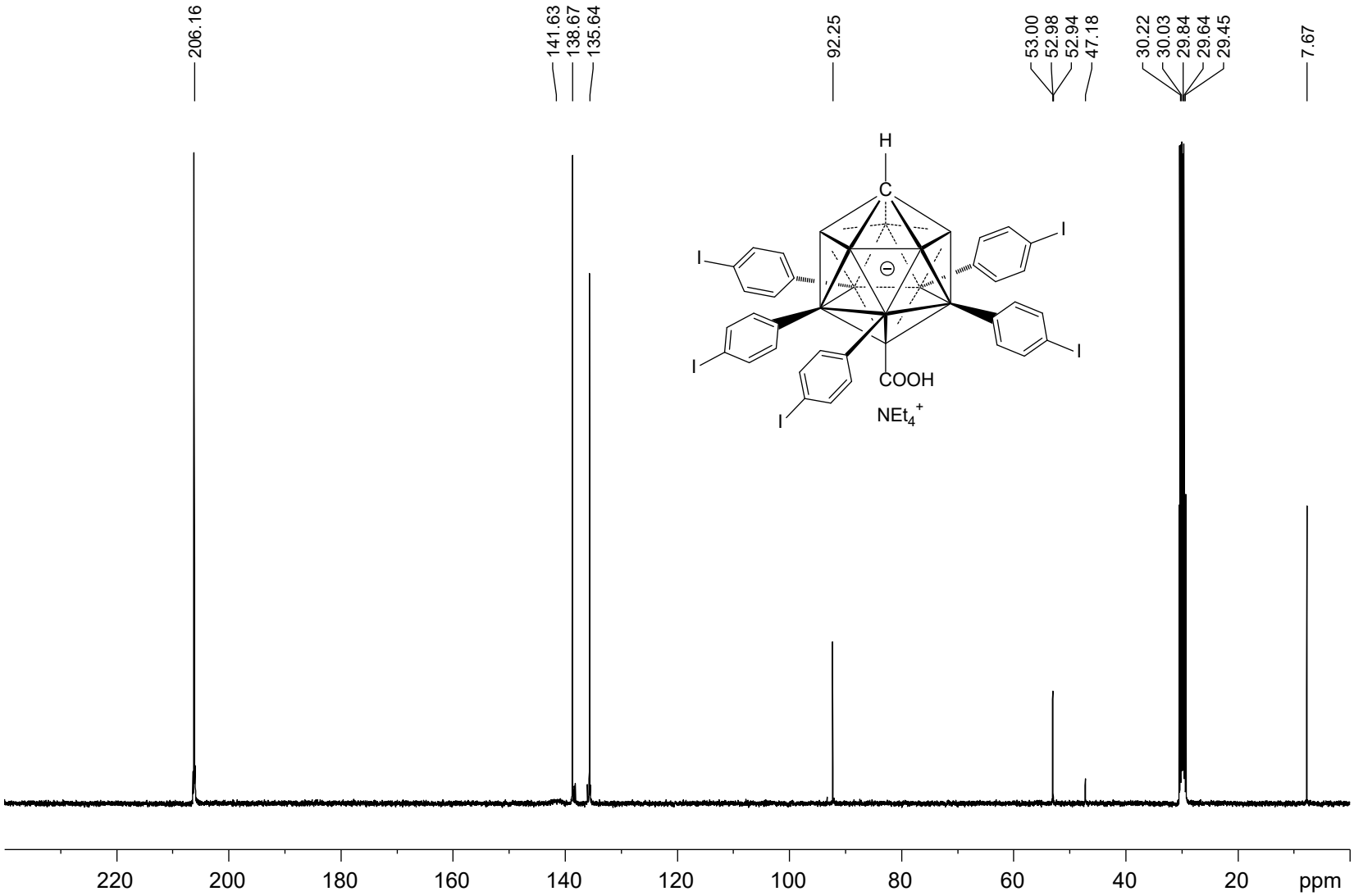
F2 - Acquisition Parameters
Date_          20220915
Time              3.25
INSTRUM          spect
PROBHD   5 mm PABBO BB/
PULPROG       zgpg30
TD             65536
SOLVENT       Acetone
NS                128
DS                  4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW             19.600 usec
DE              6.50 usec
TE              296.9 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                   1

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

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

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

jyj-201006-335 [NEt4][12-COOH-CB11H6(4-I-C6H4)5]
13C 100MHz NMR 29.6mg dissolved in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-201006-335-C
EXPNO                   1
PROCNO                  1

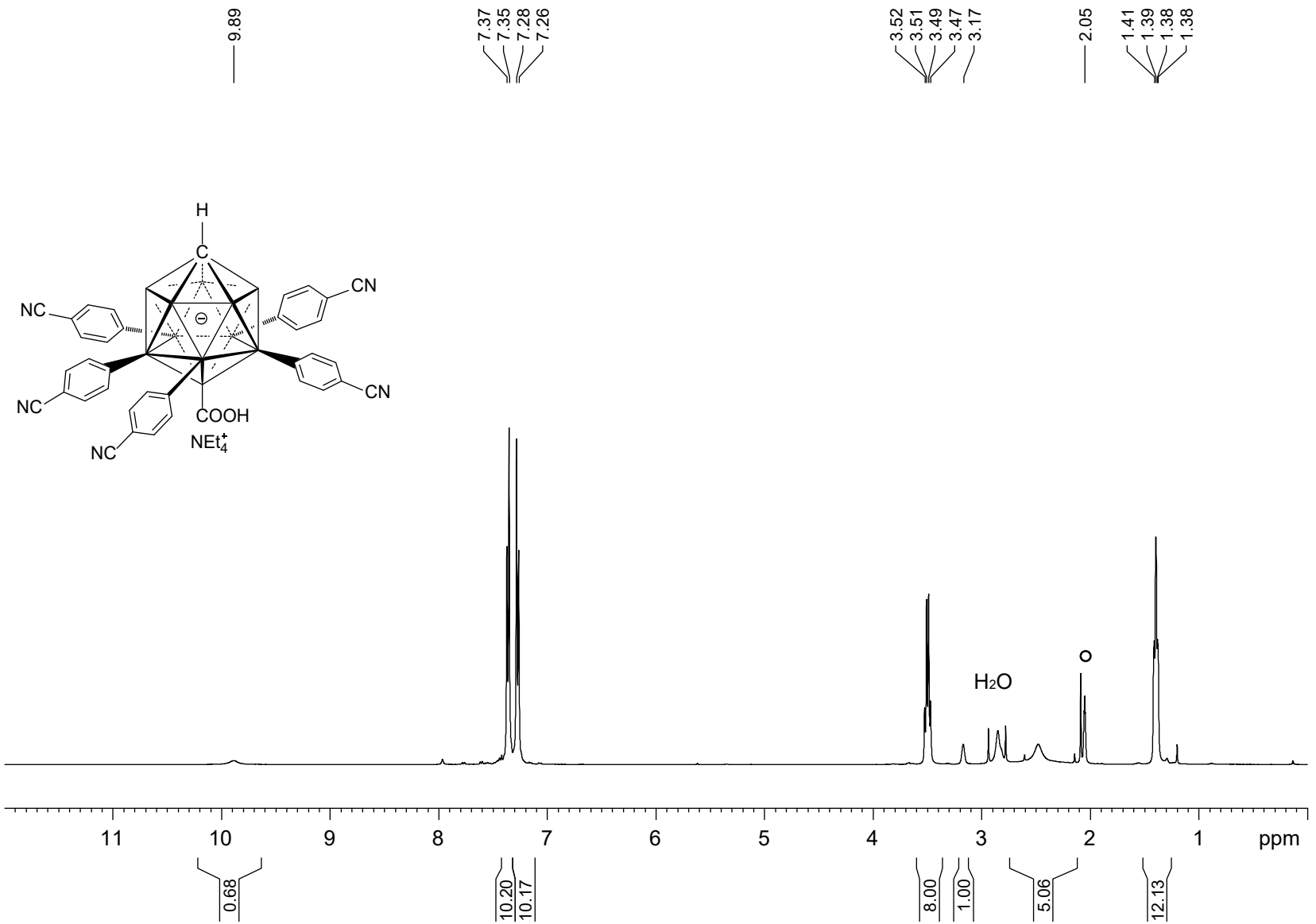
F2 - Acquisition Parameters
Date_            20201007
Time                18.24
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                193.34
DW              16.800 usec
DE               6.50 usec
TE               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           100.6126850 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

jyj-190511-140 [NEt4][12-COOH-CB11H6(4-C6H4-CN)5]
1H{11B} 400MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-190511-140
EXPNO                  1
PROCNO                 1

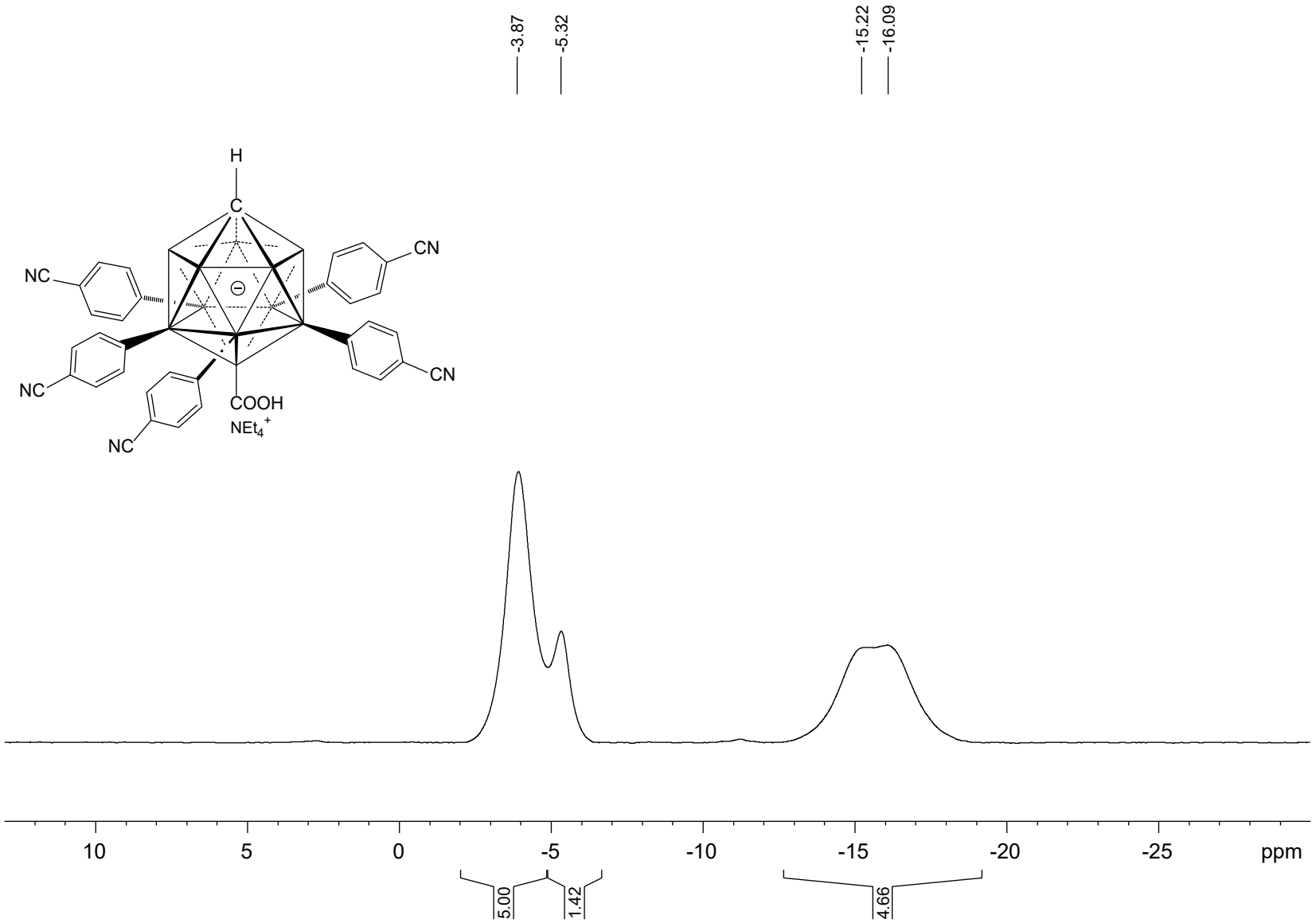
F2 - Acquisition Parameters
Date_           20190512
Time              22.07
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES        0.489064 Hz
AQ           1.0223616 sec
RG               107.6
DW              62.400 usec
DE               6.50 usec
TE              295.9 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         400.1300075 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-190511-140 [NEt4][12-COOH-CB11H6(4-C6H4-CN)5]
11B 128MHz 20.5mg in acetone-d6 T=23 C



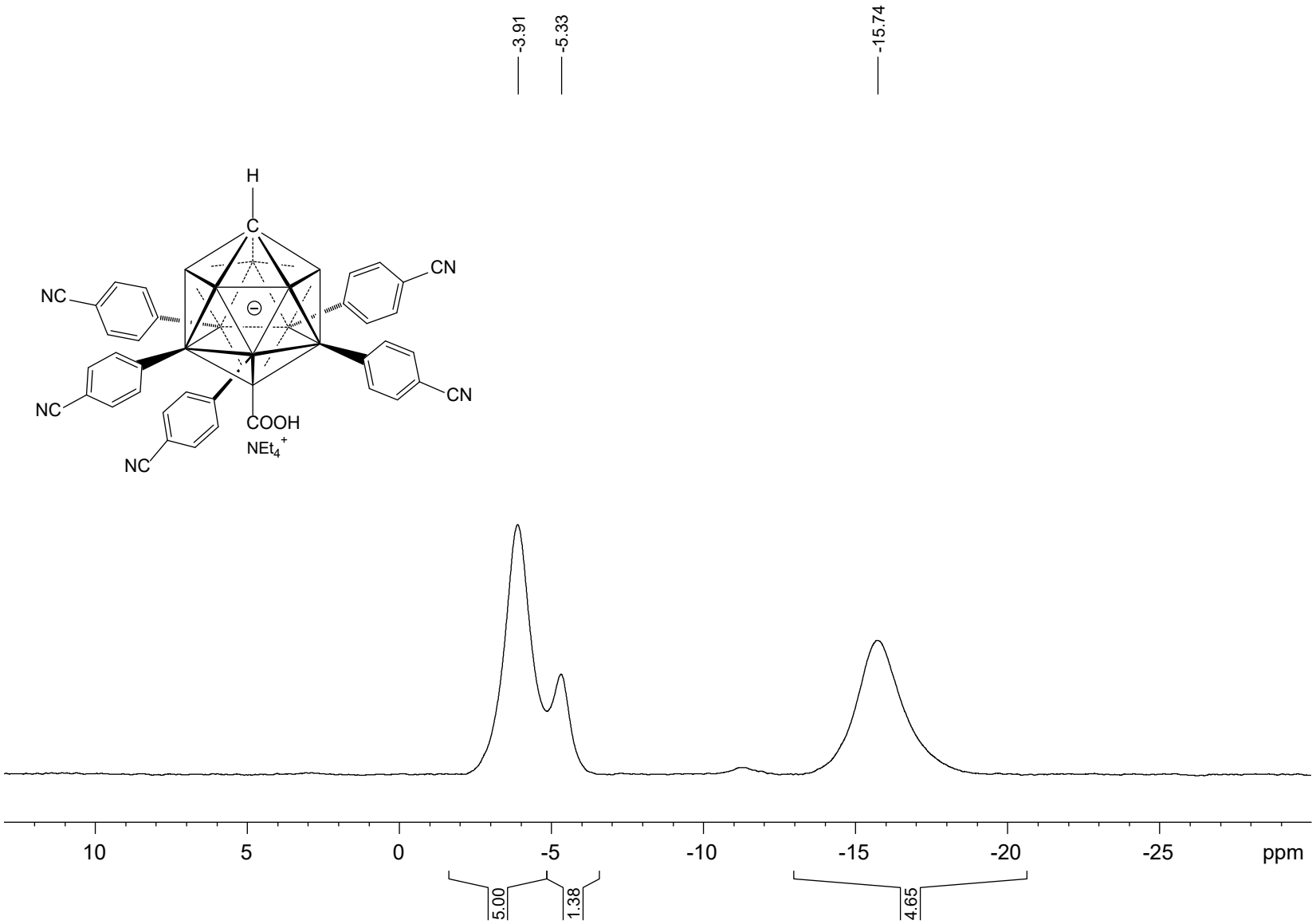

```
Current Data Parameters
NAME      jyj-190511-140
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190512
Time              22.13
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               295.8 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
```

jyj-190511-140 [NEt4][12-COOH-CB11H6(4-C6H4-CN)5]
11B{1H} 128MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-190511-140
EXPNO                  3
PROCNO                 1

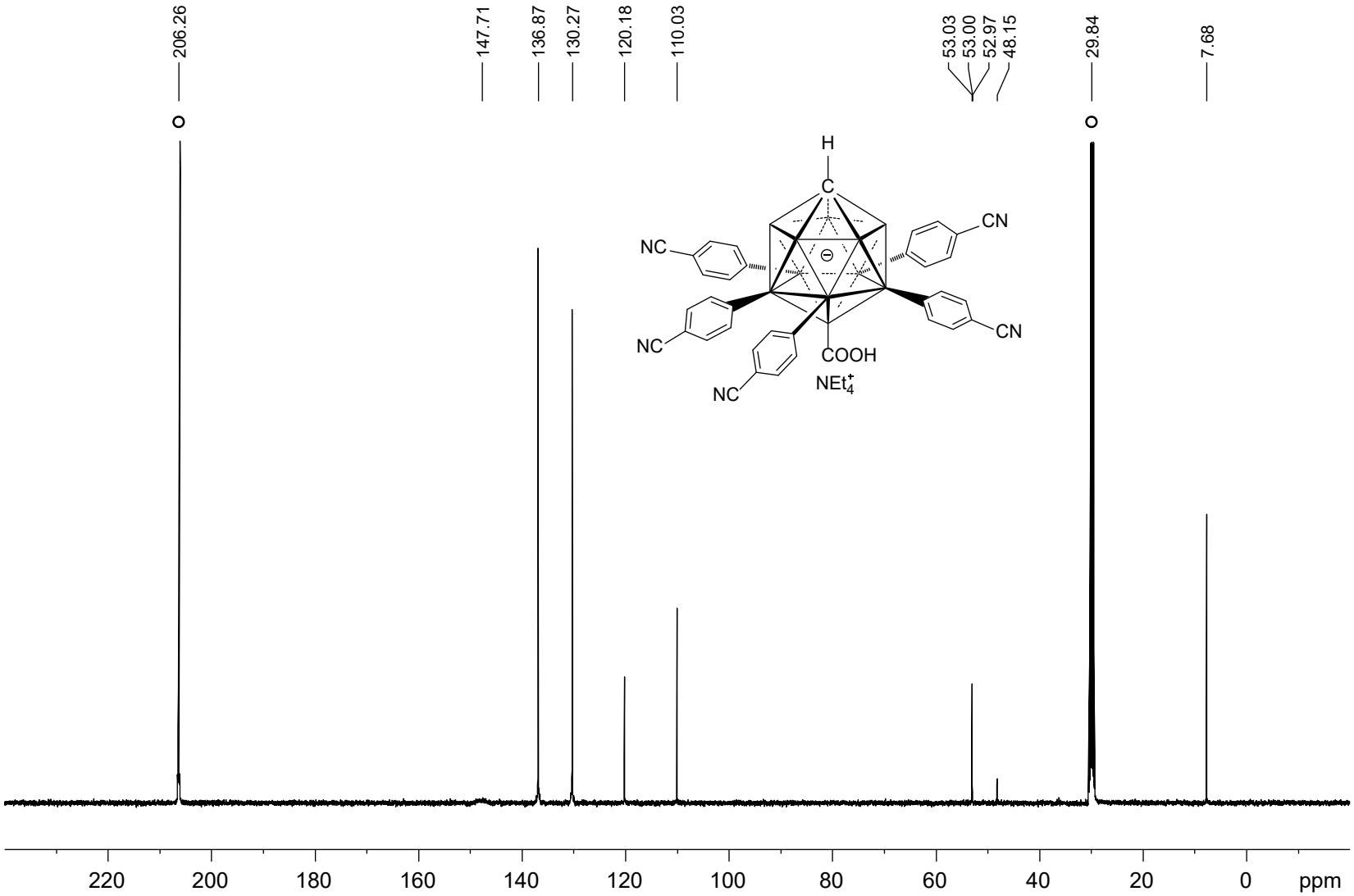
F2 - Acquisition Parameters
Date_           20190512
Time               22.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-190511-140 [NEt4][12-COOH-CB11H6(4-C6H4-CN)5]
13C 100MHz 20.5mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200718-140-C
EXPNO                   1
PROCNO                  1

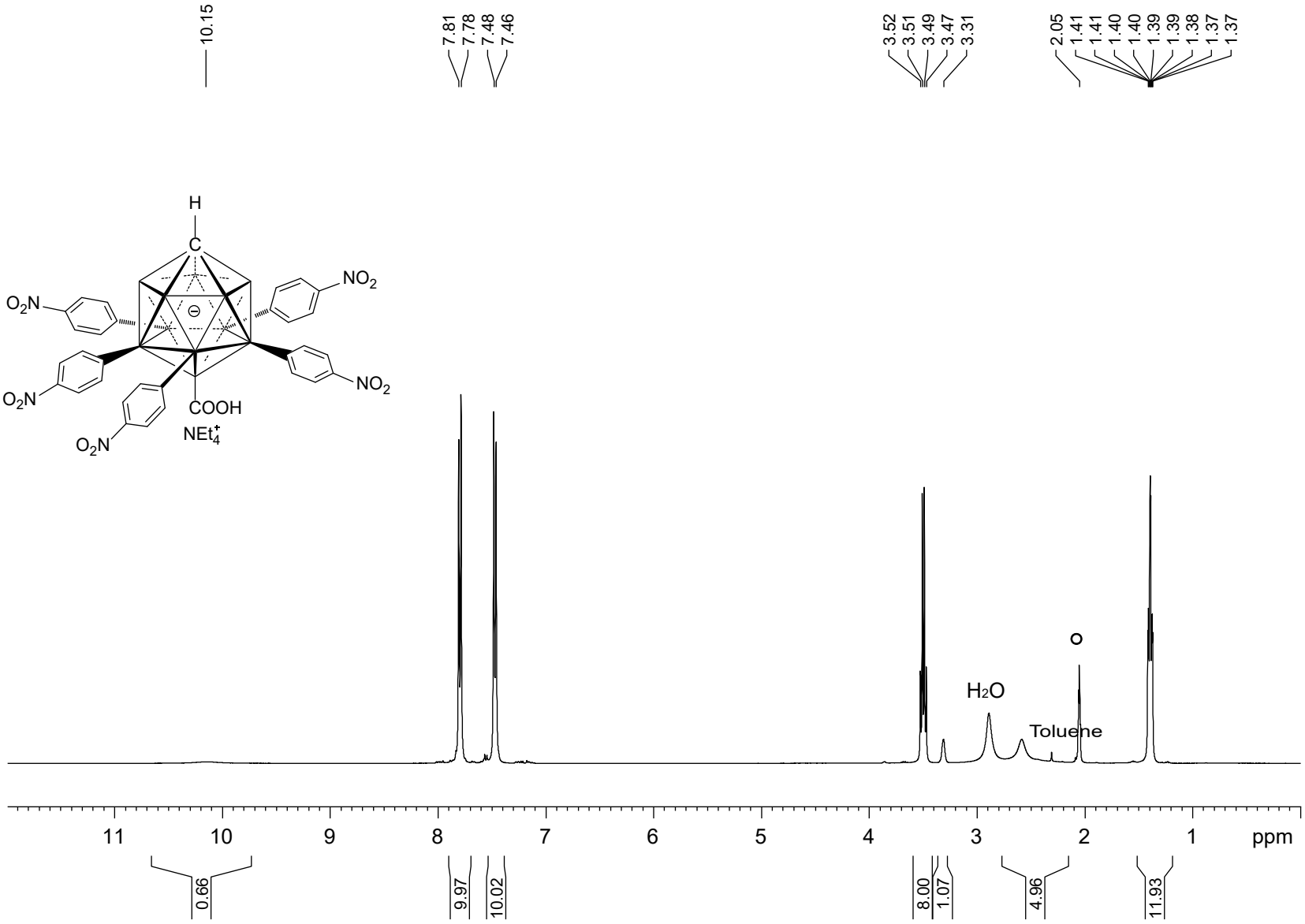
F2 - Acquisition Parameters
Date_            20200719
Time                23.27
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                 294.4 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

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

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

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

jyj-200709-281-total [NEt4][12-COOH-CB11H6(4-C6H4-NO2)5]
1H{11B} 400MHz 22.2mg dissolved in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200709-281-total
EXPNO                       2
PROCNO                      1

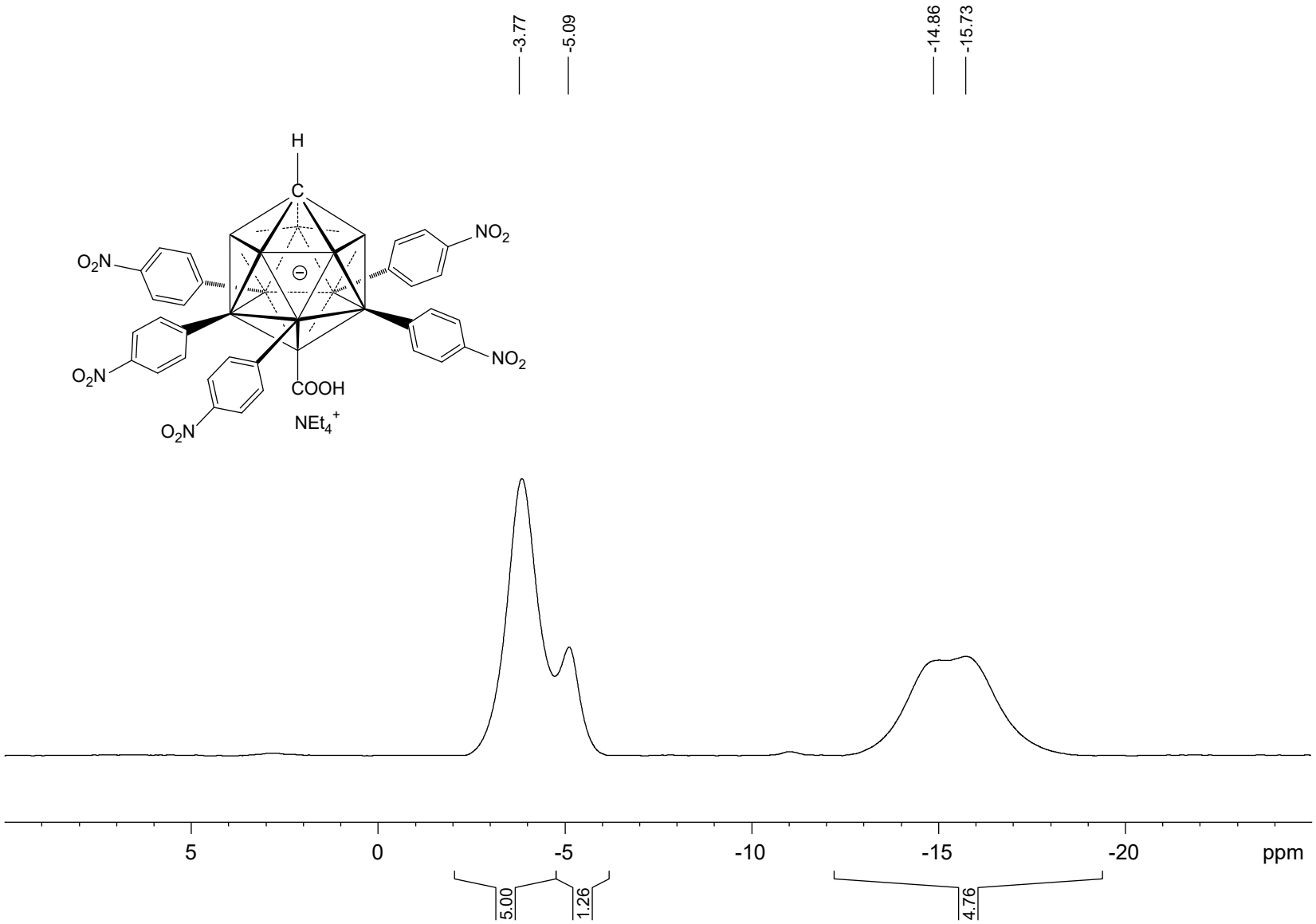
F2 - Acquisition Parameters
Date_              20200712
Time                 18.03
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH               8012.820 Hz
FIDRES               0.489064 Hz
AQ                1.0223616 sec
RG                     107.6
DW                    62.400 usec
DE                     6.50 usec
TE                    293.5 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                      1

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

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

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

jyj-200709-281-total [NEt4][12-COOH-CB11H6(4-C6H4-NO2)5]
11B 128MHz 22.2mg dissolved in acetone-d6 T=23 C



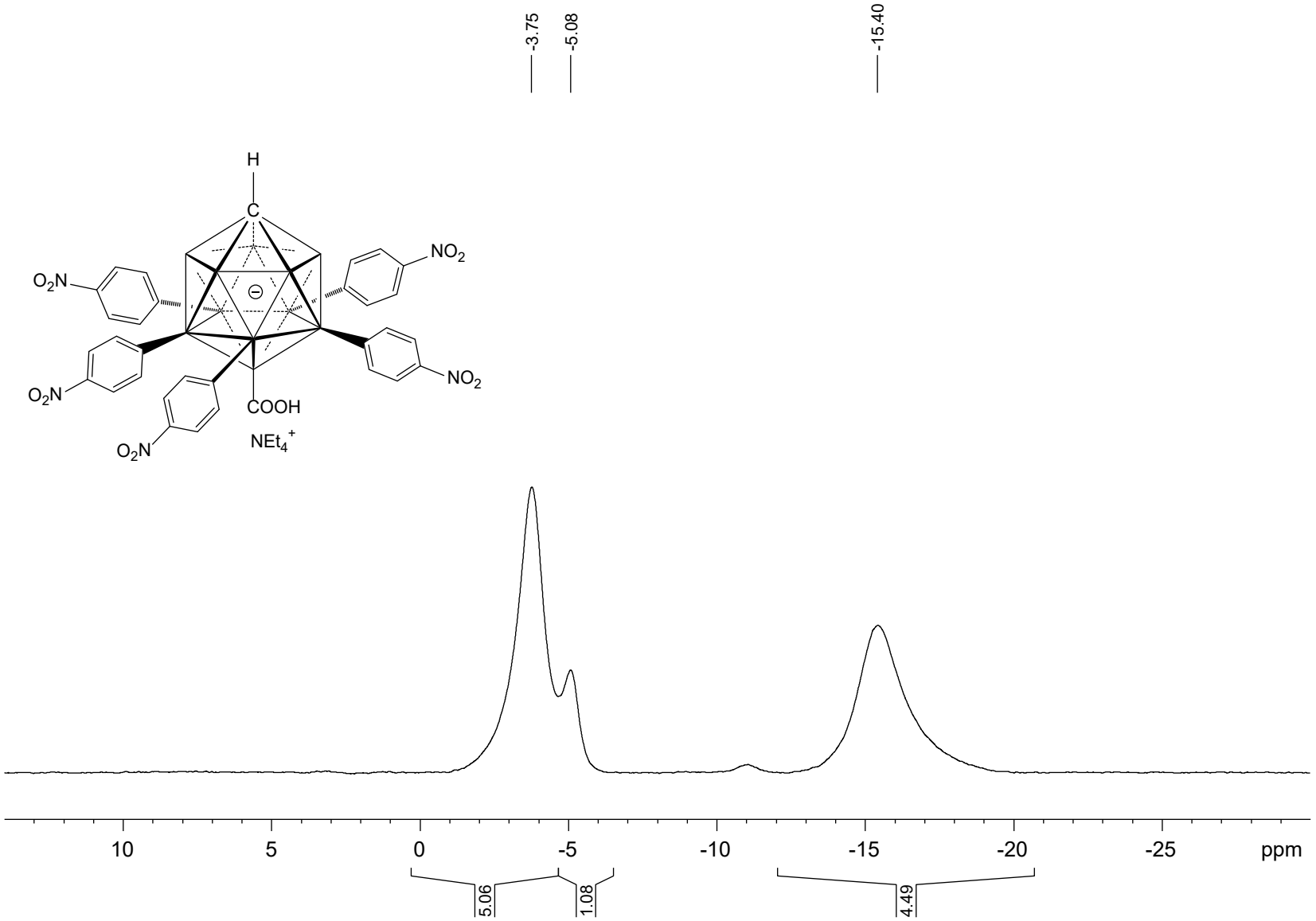

```
Current Data Parameters
NAME      jyj-200709-281-total-4-NO2
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20200712
Time              18.09
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               293.6 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-200709-281-total [NEt4][12-COOH-CB11H6(4-C6H4-NO2)5]
11B{1H} 128MHz 22.2mg dissolved in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200709-281-total-4-NO2
EXPNO                 4
PROCNO                1

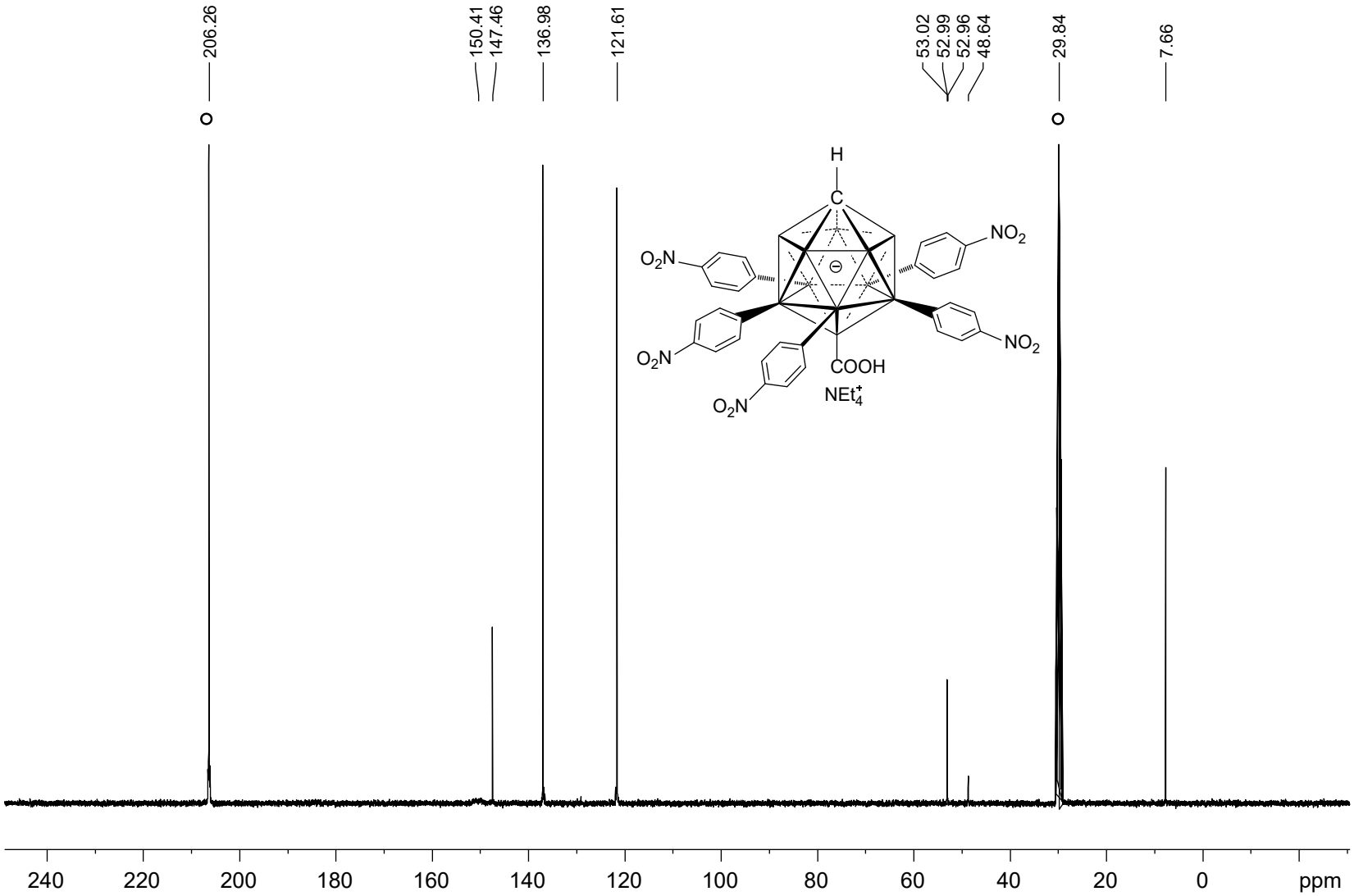
F2 - Acquisition Parameters
Date_           20200712
Time              18.15
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              294.1 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

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

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

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

jyj-200709-281-total [NEt4][12-COOH-CB11H6(4-C6H4-NO2)5]
13C 100MHz 22.2mg dissolved in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200709-281-total-C
EXPNO                  1
PROCNO                 1

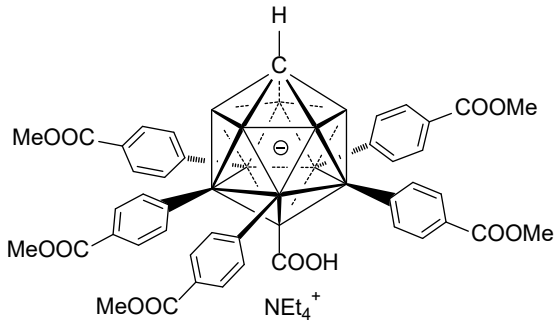
F2 - Acquisition Parameters
Date_           20200712
Time              21.41
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT         Acetone
NS                2048
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW             16.800 usec
DE              6.50 usec
TE              293.9 K
D1          1.50000000 sec
D11         0.03000000 sec
TD0                  1

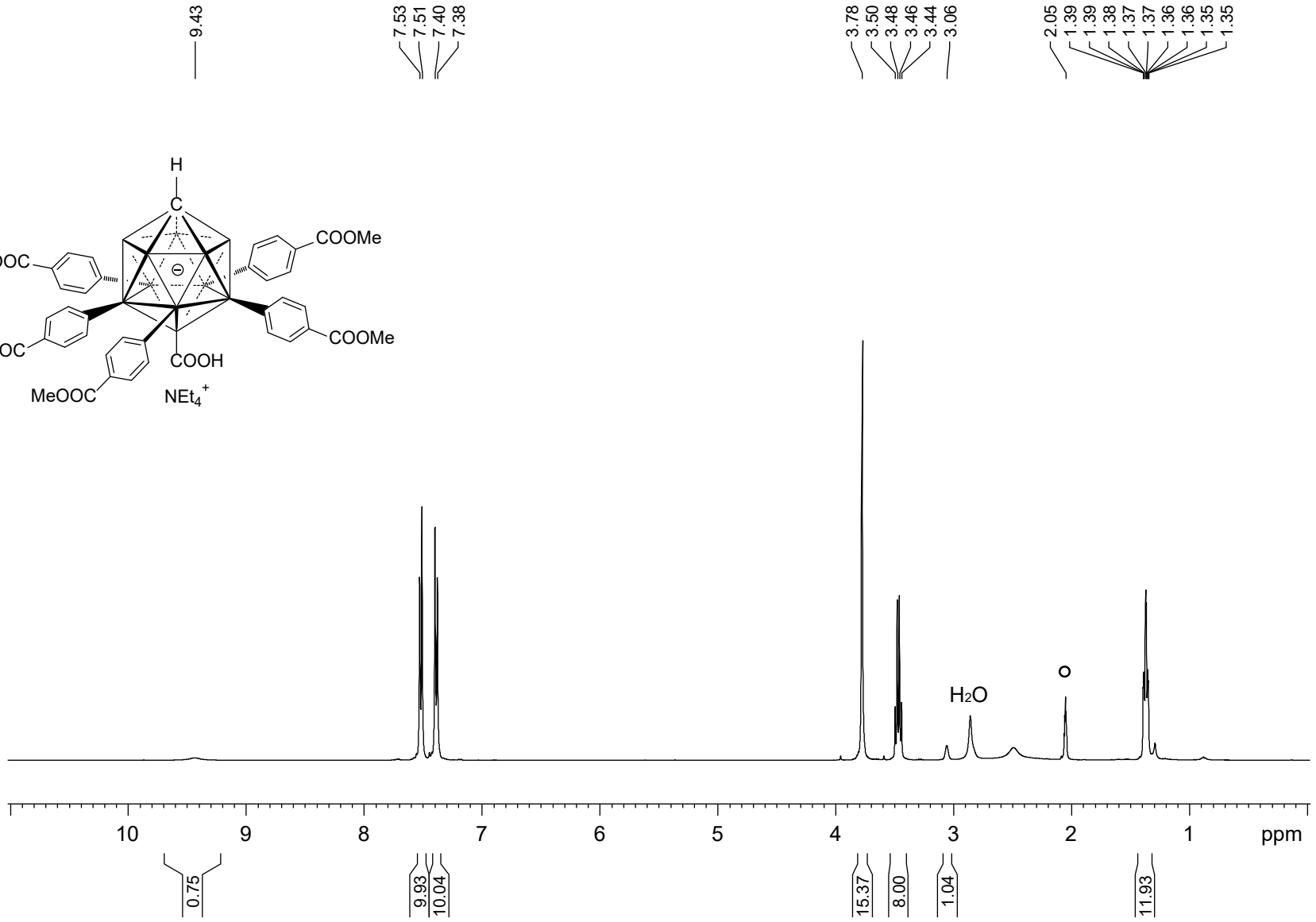
======== CHANNEL f1 ========
NUC1                13C
P1               10.00 usec
PLW1        53.00000000 W
SFO1       100.6228293 MHz

======== 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          100.6126784 MHz
WDW                EM
SSB                 0
LB               1.00 Hz
GB                  0
PC               1.40
```

jyj-200812-308-total [NEt4][12-COOH-CB11H6(C6H4COOCH3)5]
1H{11B} 400MHz 23.4mg in acetone-d6 T =23C






```
Current Data Parameters
NAME      jyj-200812-308-total
EXPNO                        2
PROCNO                       1

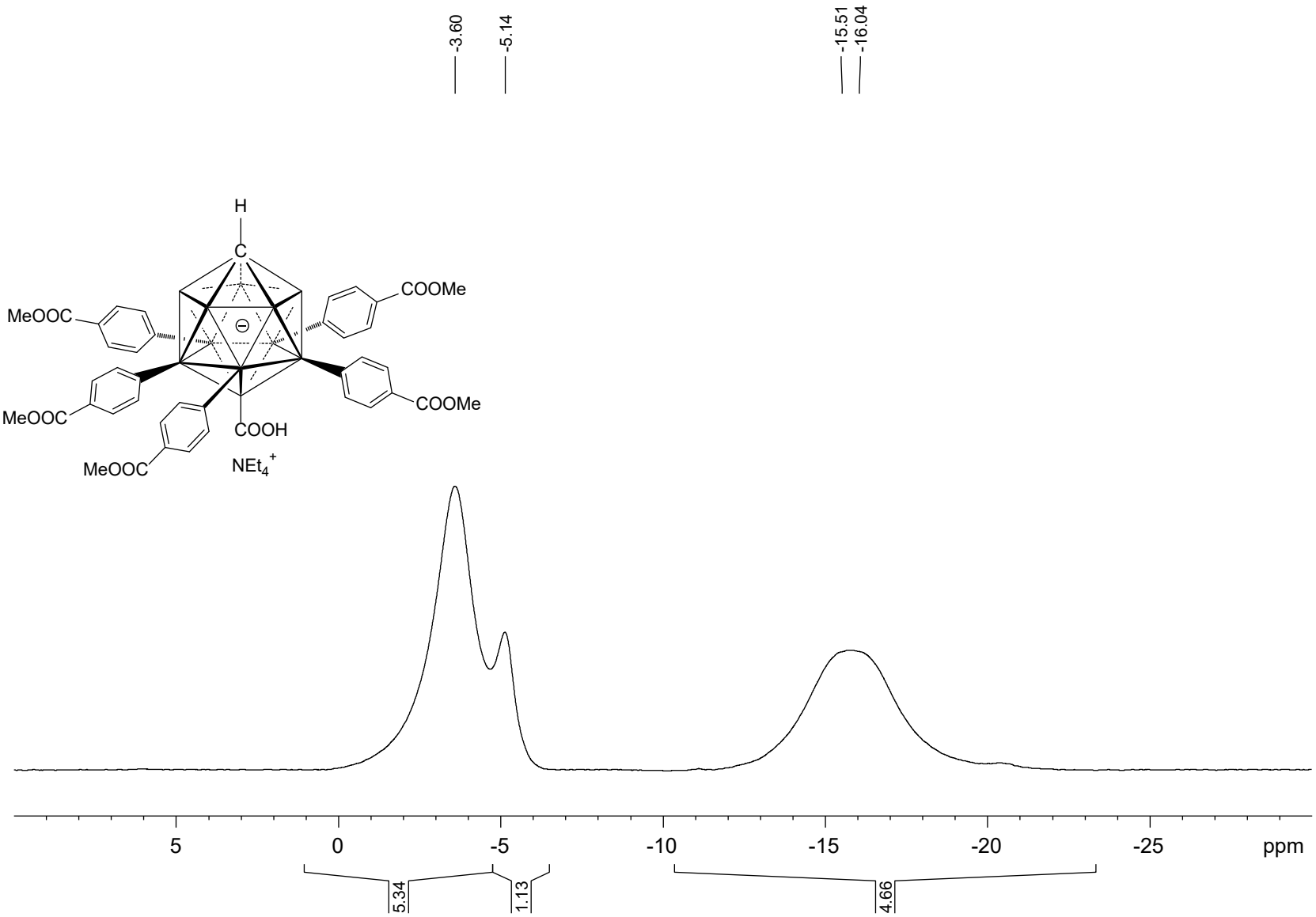
F2 - Acquisition Parameters
Date_              20200814
Time                 13.58
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   296.5 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

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

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

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

jyj-220914-4-COOMe [NEt4][12-COOH-CB11H6(4-C6H4-COOMe)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



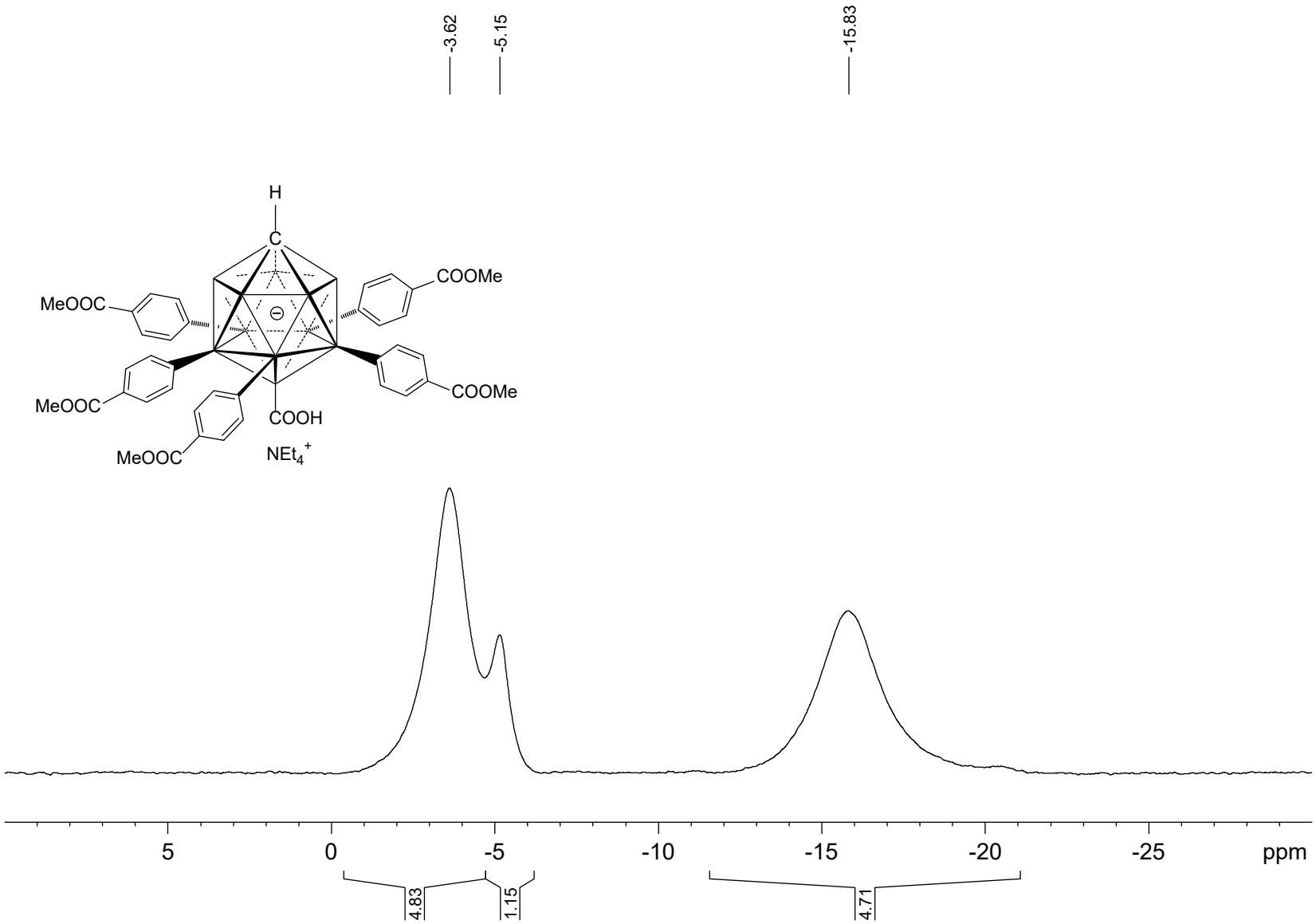

```
Current Data Parameters
NAME      jyj-220914-4-COOMe
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_            20220915
Time                9.58
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG                zg
TD                  65536
SOLVENT          Acetone
NS                    128
DS                      4
SWH             25510.203 Hz
FIDRES          0.389255 Hz
AQ              1.2845056 sec
RG                 193.34
DW                 19.600 usec
DE                  6.50 usec
TE                 296.2 K
D1             1.00000000 sec
TD0                    1

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

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

jyj-220914-4-COOMe [NEt4][12-COOH-CB11H6(4-C6H4-COOMe)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-COOMe
EXPNO                      2
PROCNO                     1

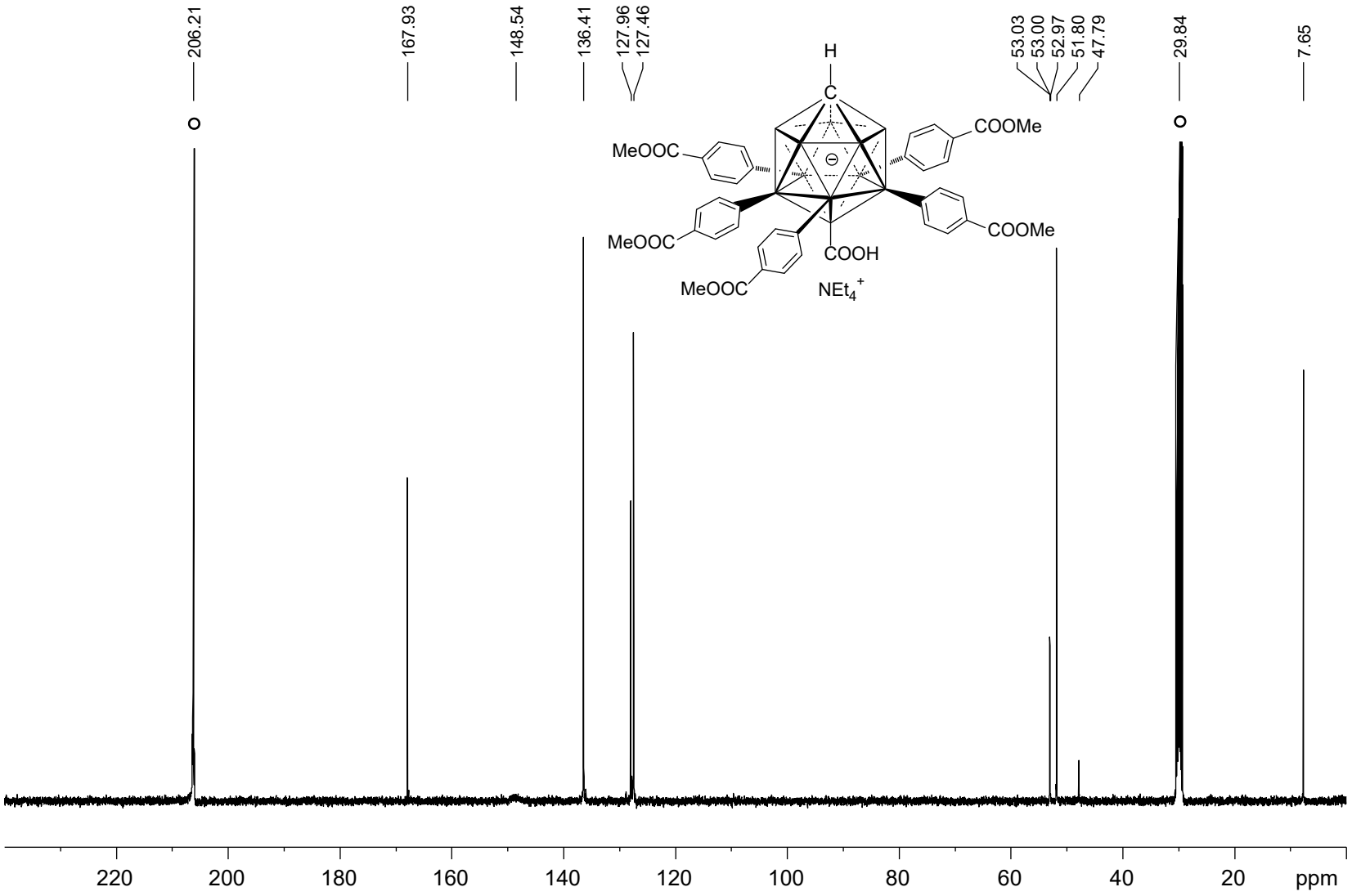
F2 - Acquisition Parameters
Date_            20220915
Time                10.04
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW              19.600 usec
DE               6.50 usec
TE              296.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

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

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

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

jyj-200812-308-total [NEt4][12-COOH-CB11H6(C6H4COOCH3)5]
13C 100MHz 23.4mg in acetone-d6 T =23C




```
Current Data Parameters
NAME      jyj-200812-308-total
EXPNO                       5
PROCNO                      1

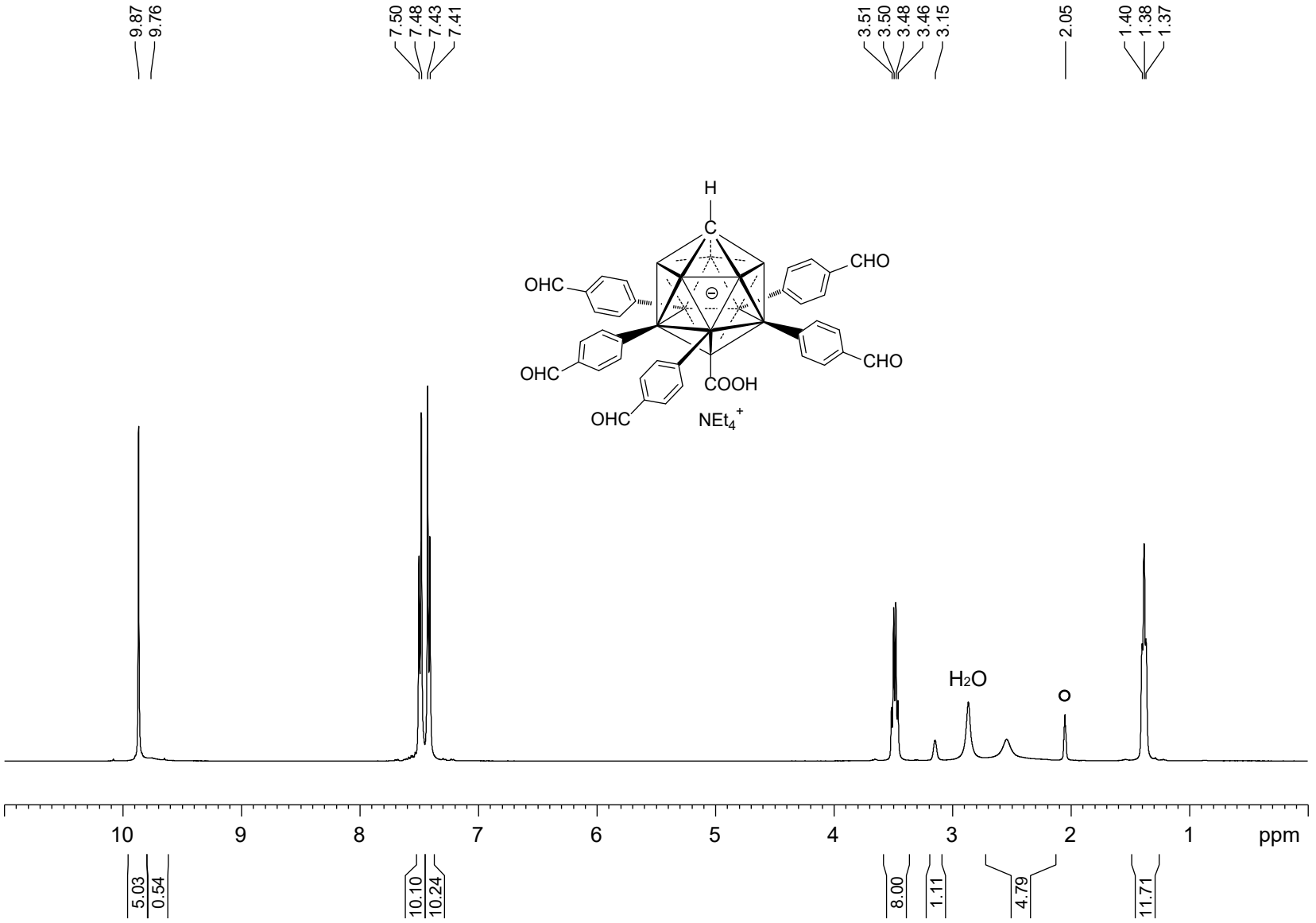
F2 - Acquisition Parameters
Date_            20200814
Time                15.42
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT          Acetone
NS                  2048
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                193.34
DW                16.800 usec
DE                 6.50 usec
TE                297.2 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                    1

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

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

F2 - Processing parameters
SI                 32768
SF          100.6126803 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200831-314 [NEt4][12-COOH-CB11H6(C6H5CHO)5]
1H{11B} 400MHz 16.8mg in acetone-d6 T=23




```
Current Data Parameters
NAME      jyj-200831-314-2
EXPNO                    1
PROCNO                   1

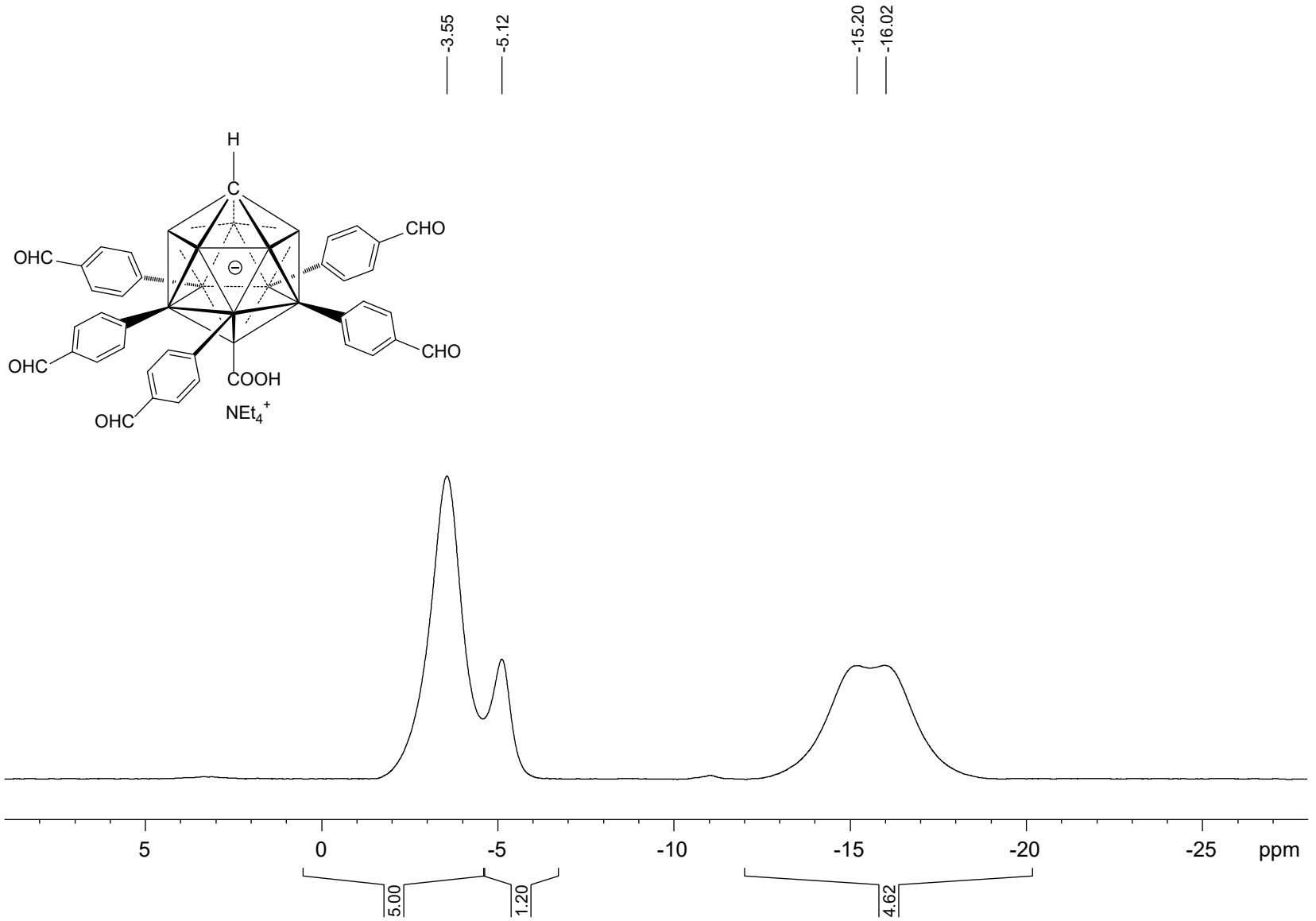
F2 - Acquisition Parameters
Date_             20200901
Time                  9.17
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH                8012.820 Hz
FIDRES            0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   295.6 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                      1

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

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

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

jyj-200831-314 [NEt4][12-COOH-CB11H6(C6H5CHO)5]
11B 128MHz 16.8mg in acetone-d6 T=23



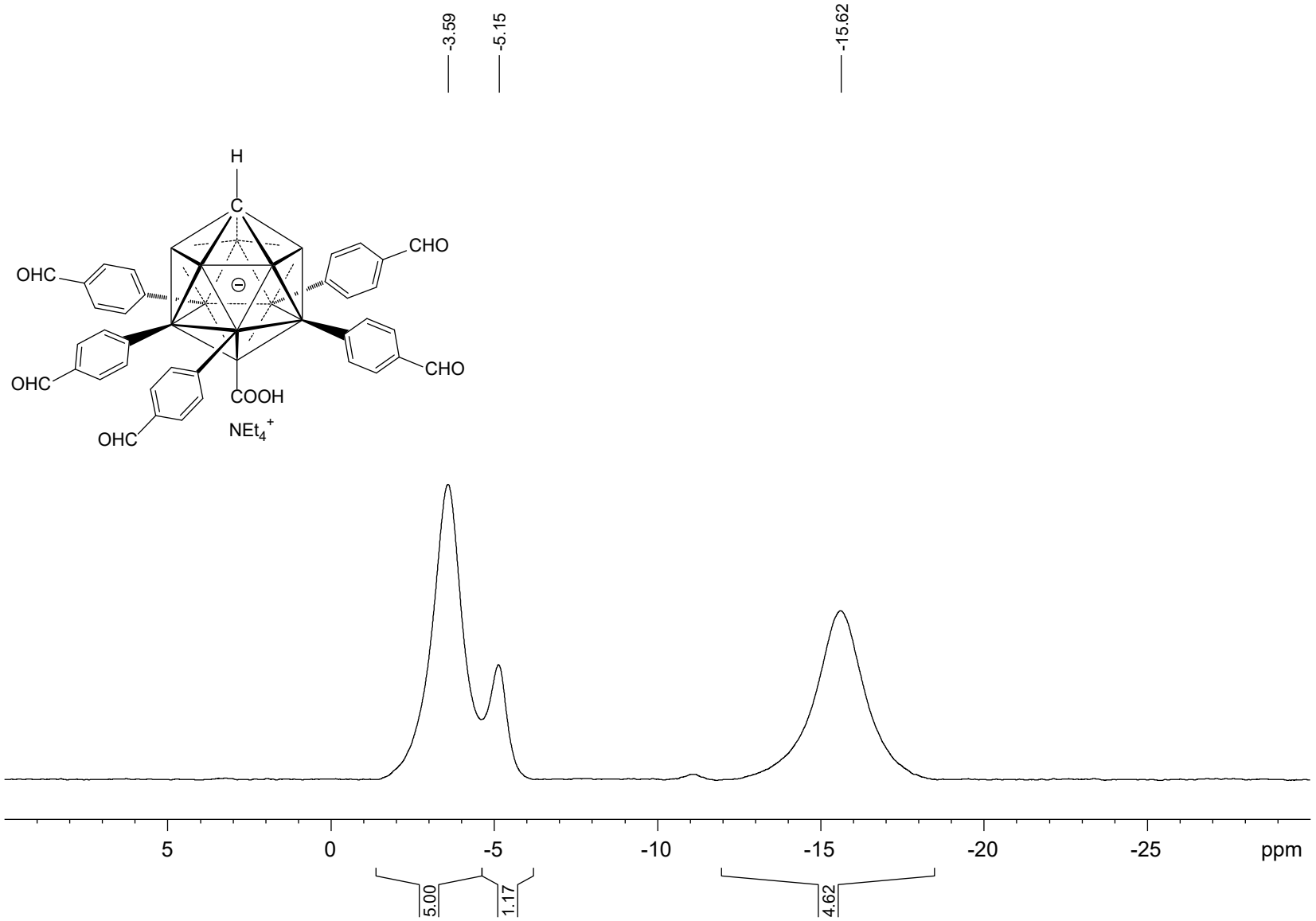

```
Current Data Parameters
NAME      jyj-200827-314-C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200828
Time               13.28
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                295.6 K
D1            1.00000000 sec
TD0                    1

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

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

jyj-200831-314 [NEt4][12-COOH-CB11H6(C6H5CHO)5]
11B{1H} 128MHz 16.8mg in acetone-d6 T=23




```
Current Data Parameters
NAME      jyj-200827-314
EXPNO                 2
PROCNO                1

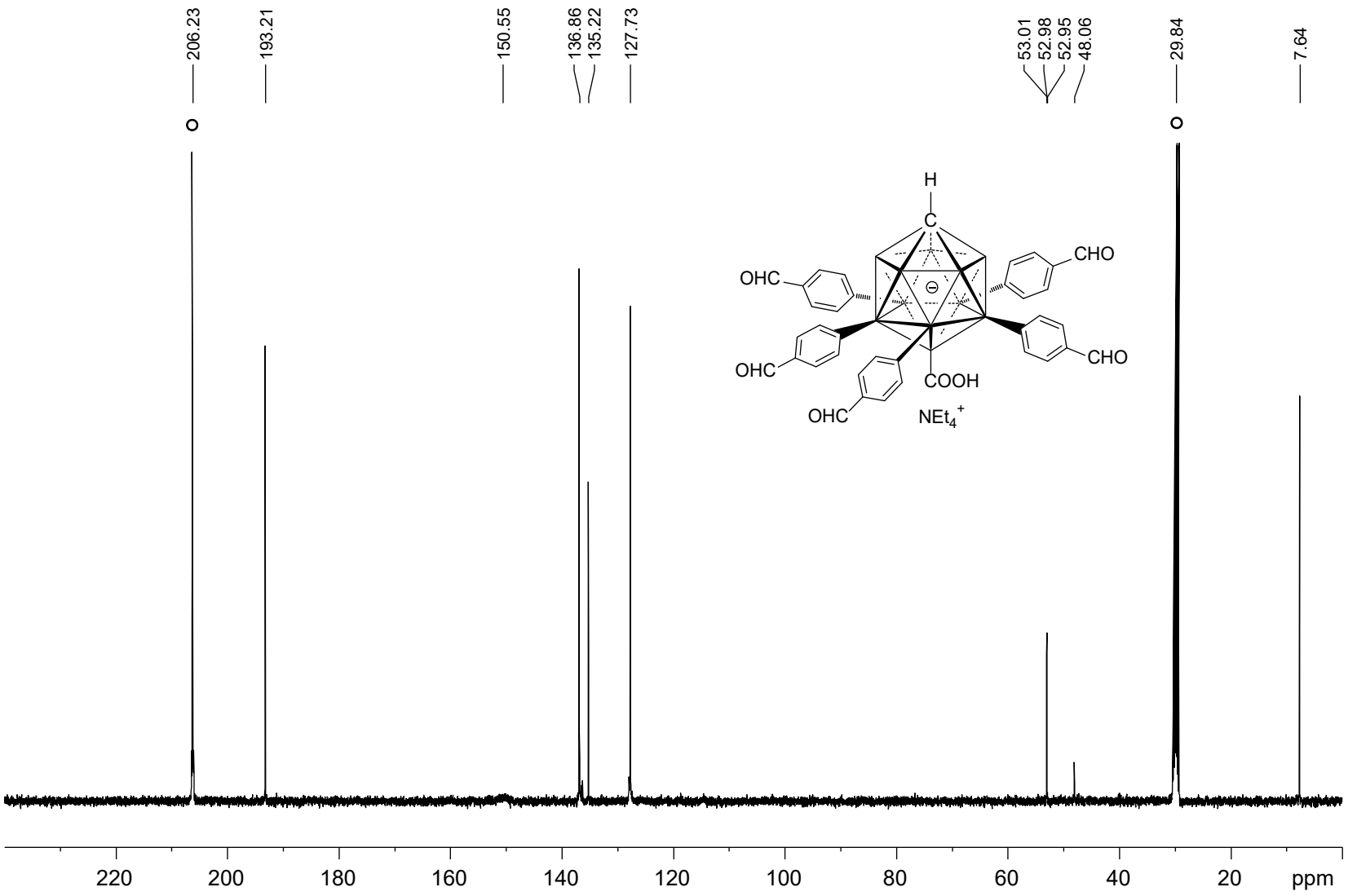
F2 - Acquisition Parameters
Date_          20200828
Time               8.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT         Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              296.3 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

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

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

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

jyj-200831-314 [NEt4][12-COOH-CB11H6(C6H5CHO)5]
13C 100MHz 16.8mg in acetone-d6 T=23




```
Current Data Parameters
NAME      jyj-200831-314-HC
EXPNO                    2
PROCNO                   1

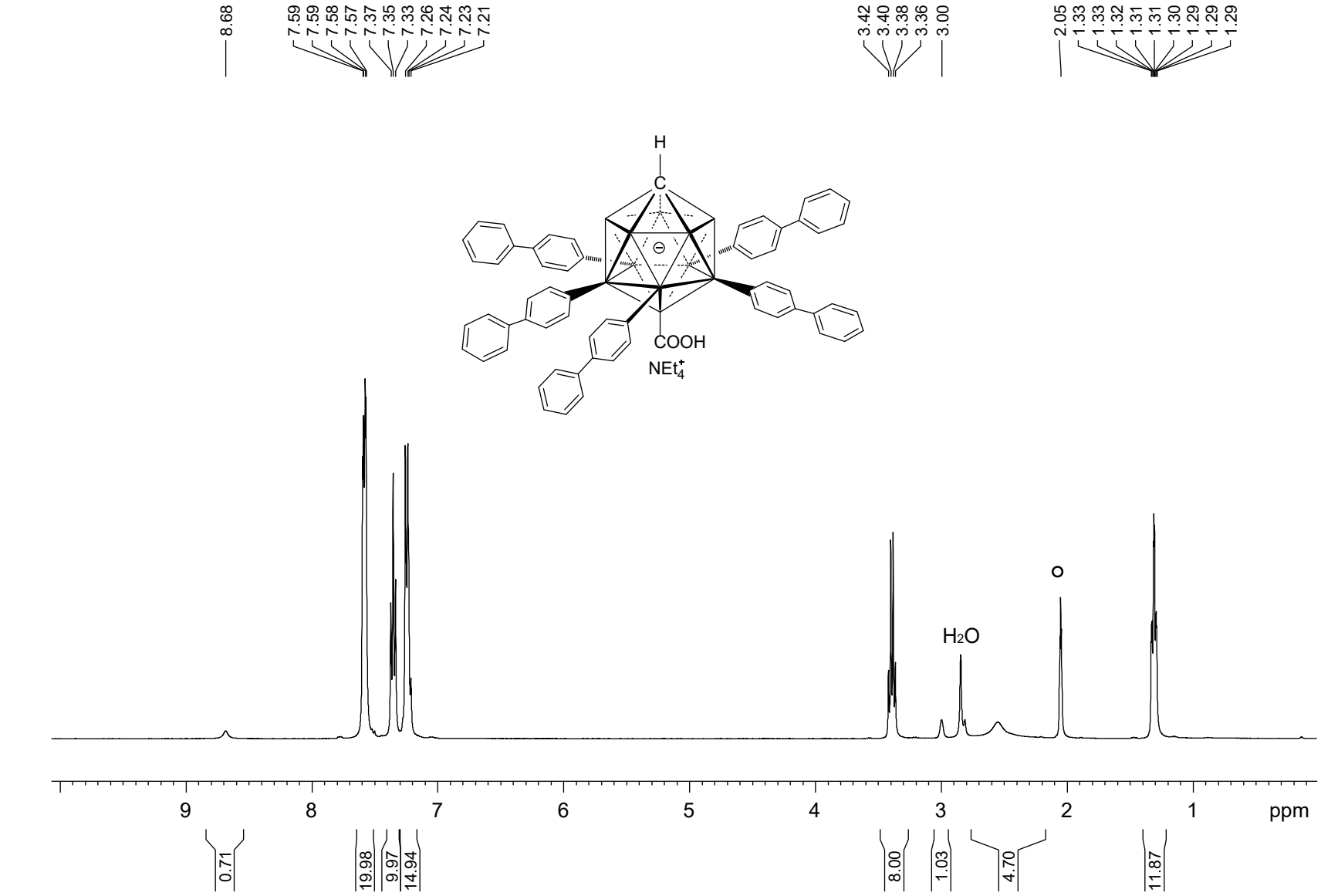
F2 - Acquisition Parameters
Date_             20200901
Time                 17.11
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                    2048
DS                       4
SWH              29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                  193.34
DW                16.800 usec
DE                 6.50 usec
TE                296.2 K
D1             1.50000000 sec
D11            0.03000000 sec
TD0                      1

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

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

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

jyj-200929-305 [NEt4][12-COOH-CB11H6(4-C6H4-Ph)]
1H{11B} 400MHz around 20mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200929-305
EXPNO                  2
PROCNO                 1

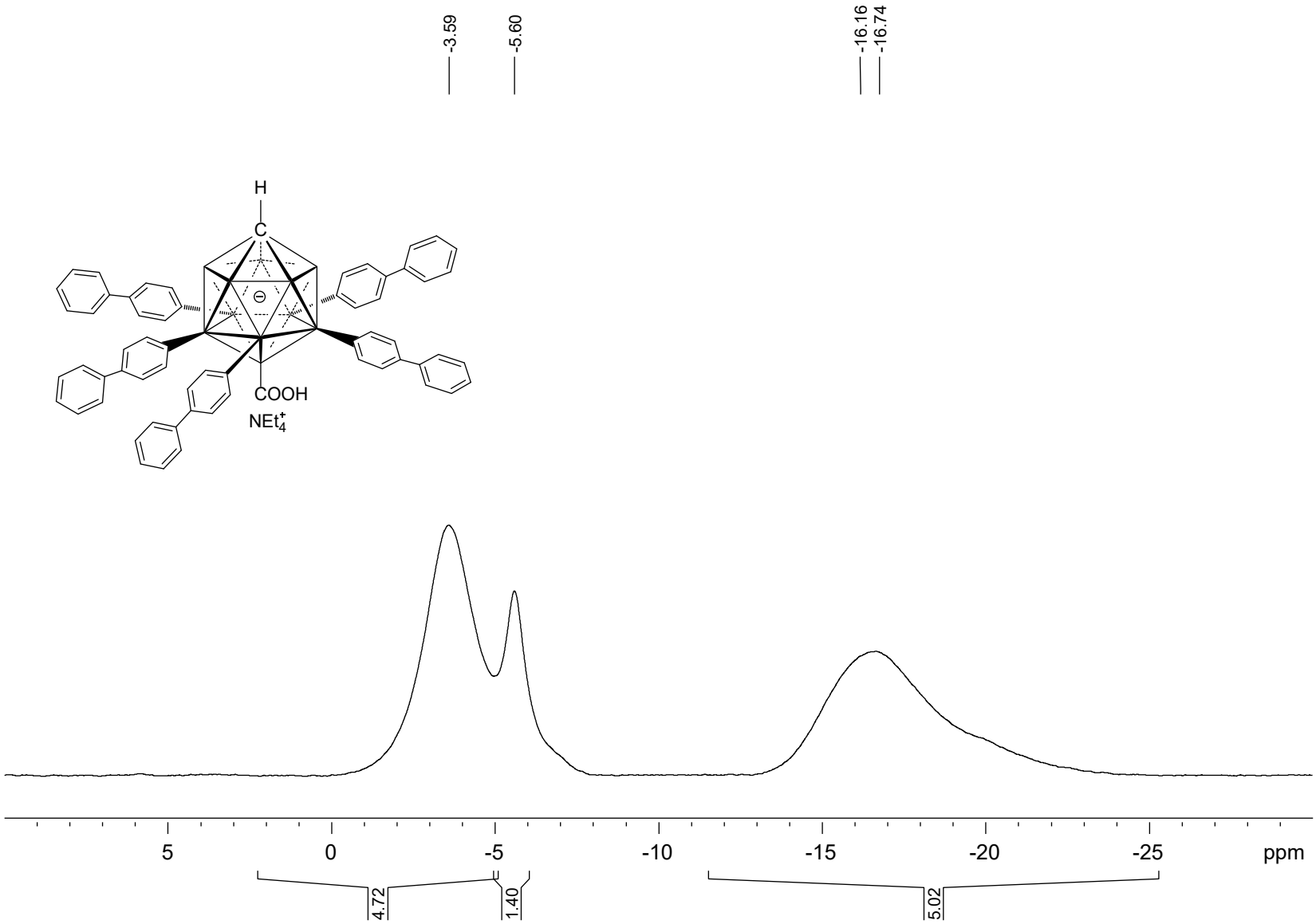
F2 - Acquisition Parameters
Date_           20200930
Time                14.12
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgig30
TD                  16384
SOLVENT           Acetone
NS                     16
DS                      4
SWH              8012.820 Hz
FIDRES           0.489064 Hz
AQ              1.0223616 sec
RG                  107.6
DW                 62.400 usec
DE                  6.50 usec
TE                 294.5 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                     1

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

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

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

jyj-220914-4-Ph [NEt4][12-COOH-CB11H6(4-C6H4-Ph)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



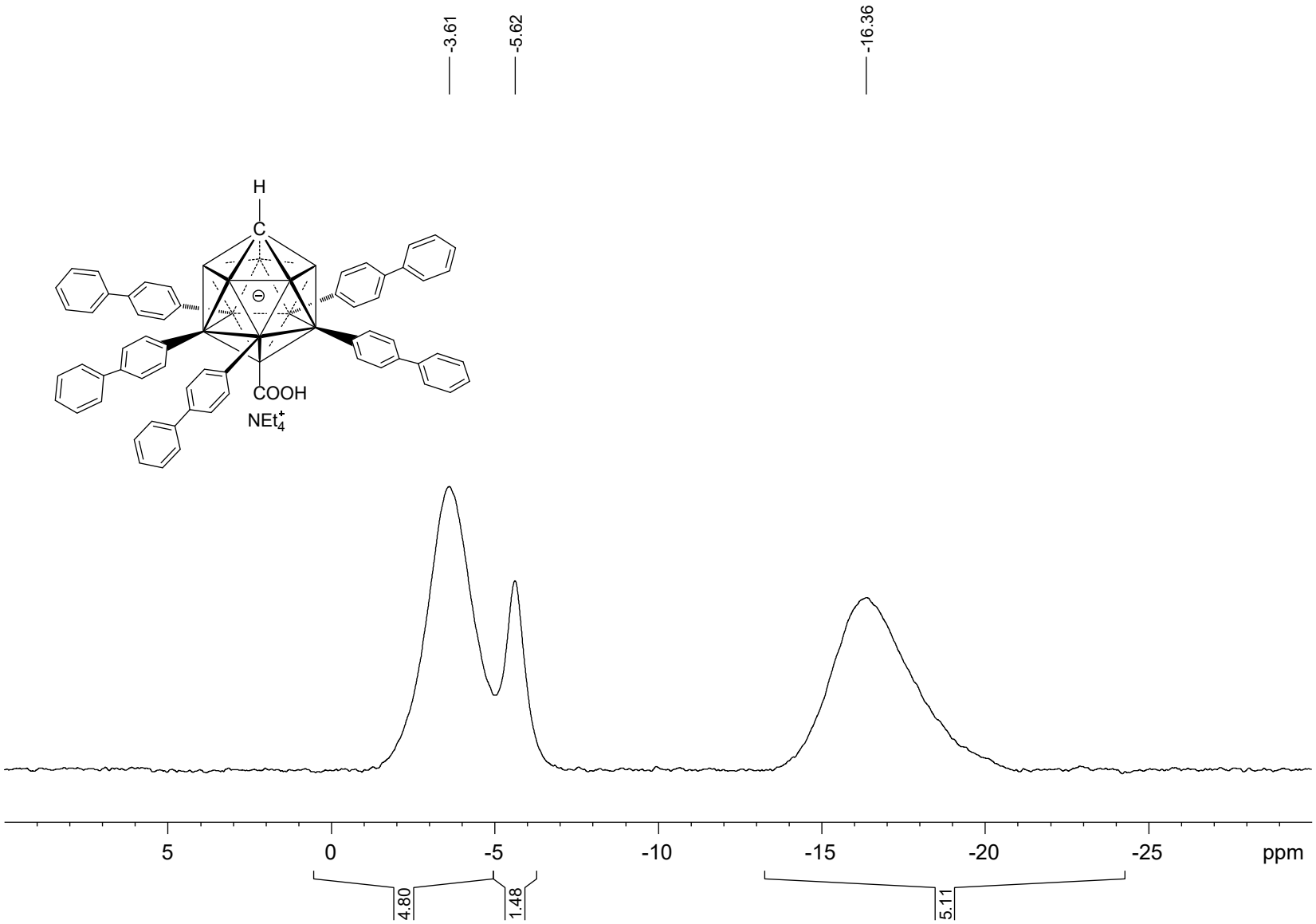

```
Current Data Parameters
NAME      jyj-220914-4-Ph
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time              10.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG              zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.3 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-4-Ph [NEt4][12-COOH-CB11H6(4-C6H4-Ph)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-4-Ph
EXPNO                  2
PROCNO                 1

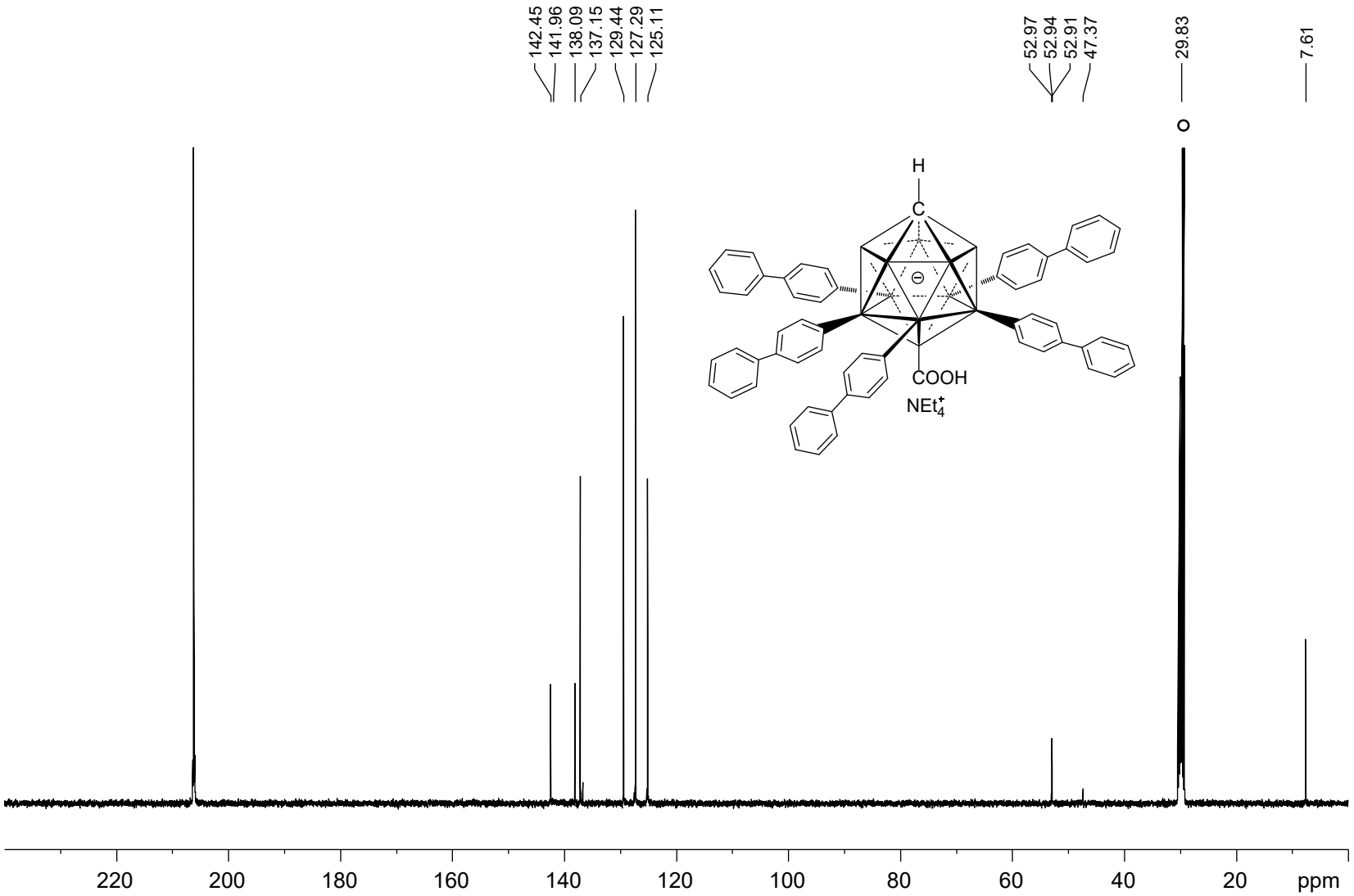
F2 - Acquisition Parameters
Date_           20220915
Time                10.19
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-200929-305 [NEt4][12-COOH-CB11H6(4-C6H4-Ph)]
13C 100MHz around 20mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-201001-305-C
EXPNO                   1
PROCNO                  1

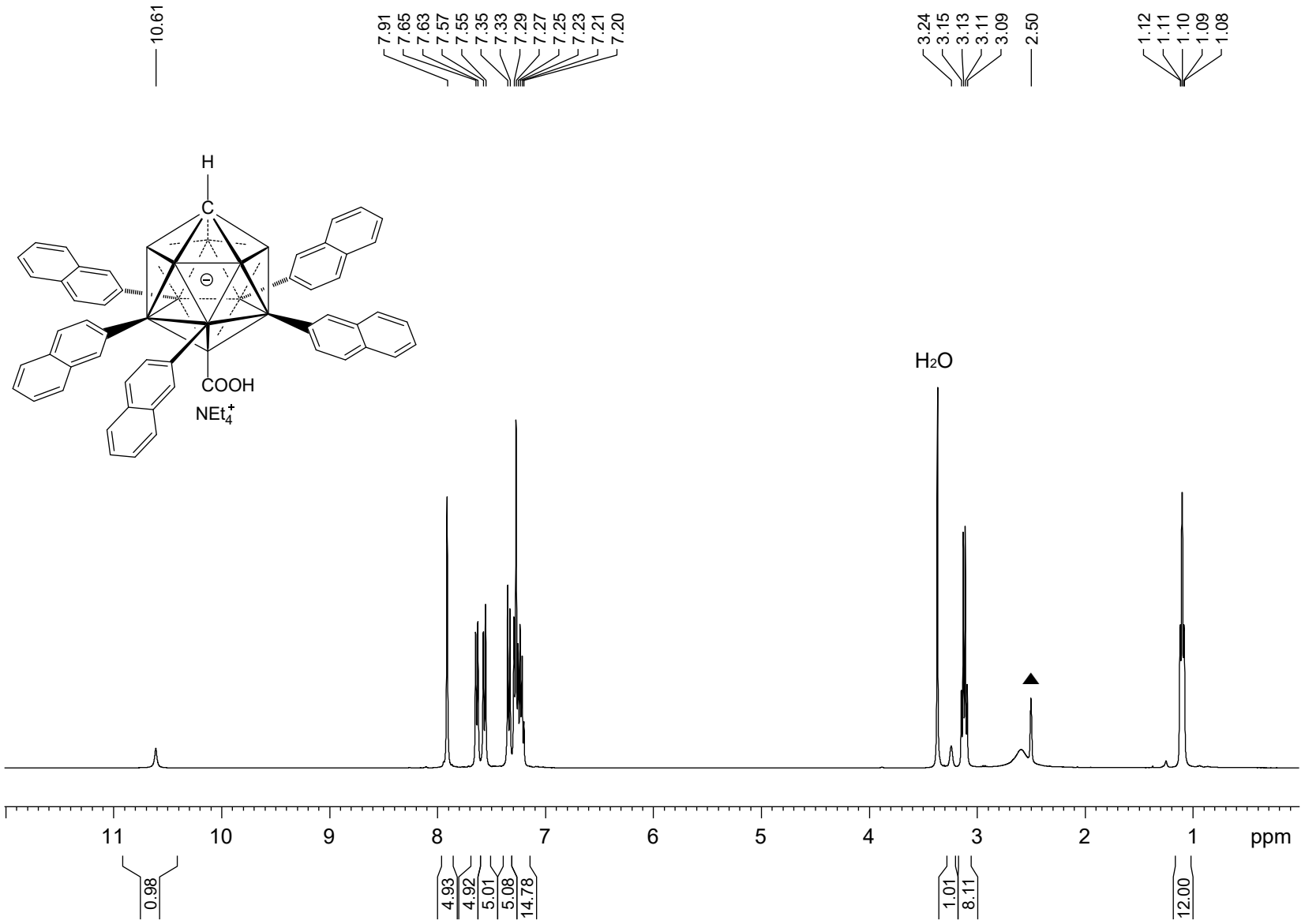
F2 - Acquisition Parameters
Date_            20201002
Time                21.10
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG                193.34
DW              16.800 usec
DE               6.50 usec
TE               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           100.6126817 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

jyj-200807-301-DMSO [NEt4][12-COOH-CB11H6(2-C10H7)5]
1H{11B} 400MHz 21.8mg in DMSO-d6 T = 23C




```
Current Data Parameters
NAME      jyj-200807-301-DMSO
EXPNO                      2
PROCNO                     1

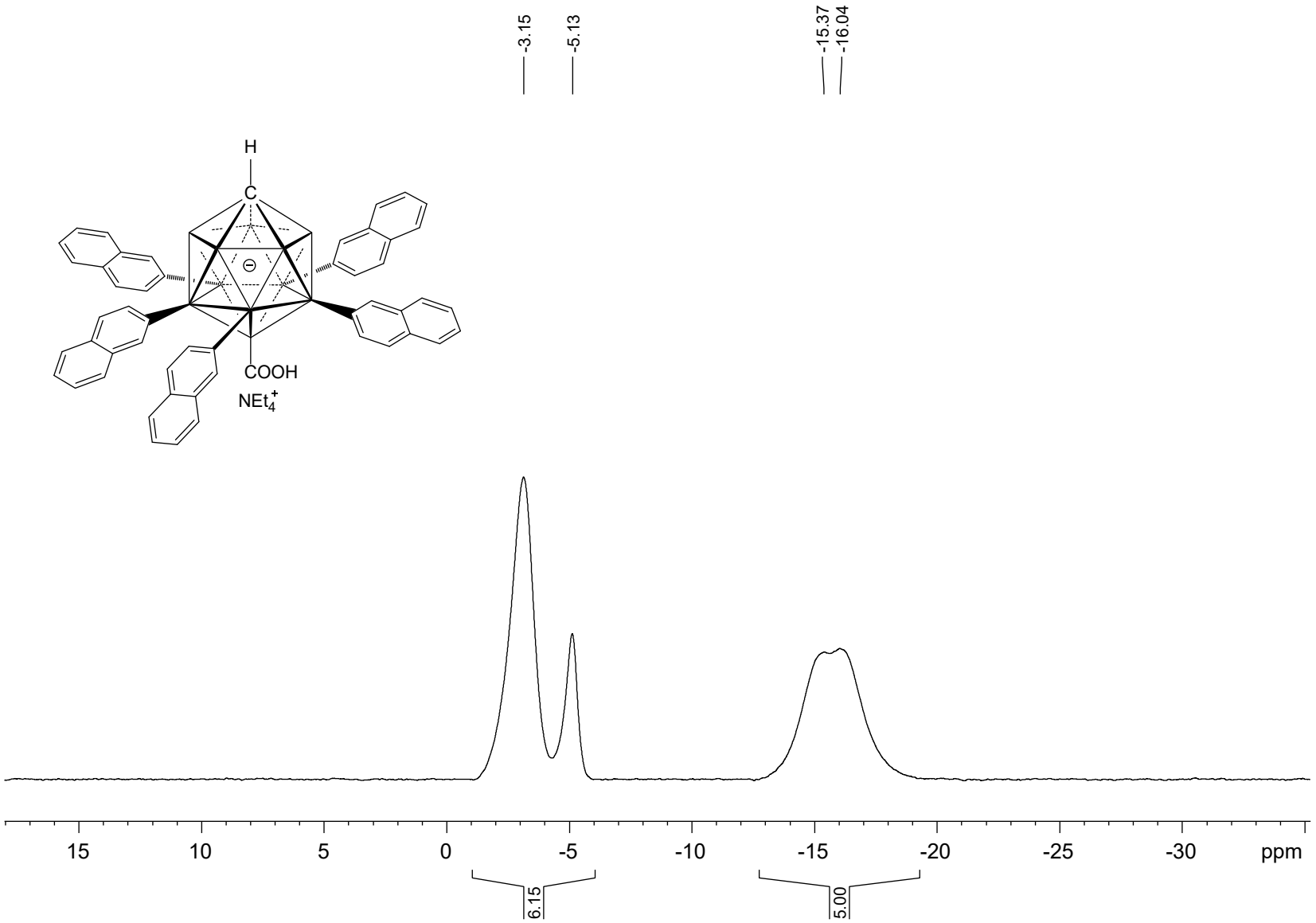
F2 - Acquisition Parameters
Date_              20200808
Time                 20.03
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT               DMSO
NS                      16
DS                       4
SWH               8012.820 Hz
FIDRES            0.489064 Hz
AQ               1.0223616 sec
RG                   78.69
DW                 62.400 usec
DE                  6.50 usec
TE                 296.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                      1

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

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

F2 - Processing parameters
SI                     32768
SF           400.1300034 MHz
WDW                       EM
SSB                        0
LB                    1.00 Hz
GB                         0
PC                    1.40
```

jyj-200807-301-acetone-d6 [NEt4][12-COOH-CB11H6(2-C10H7)5]
11B 128MHz 34.8mg partial dissolved in acetone-d6 T = 23C



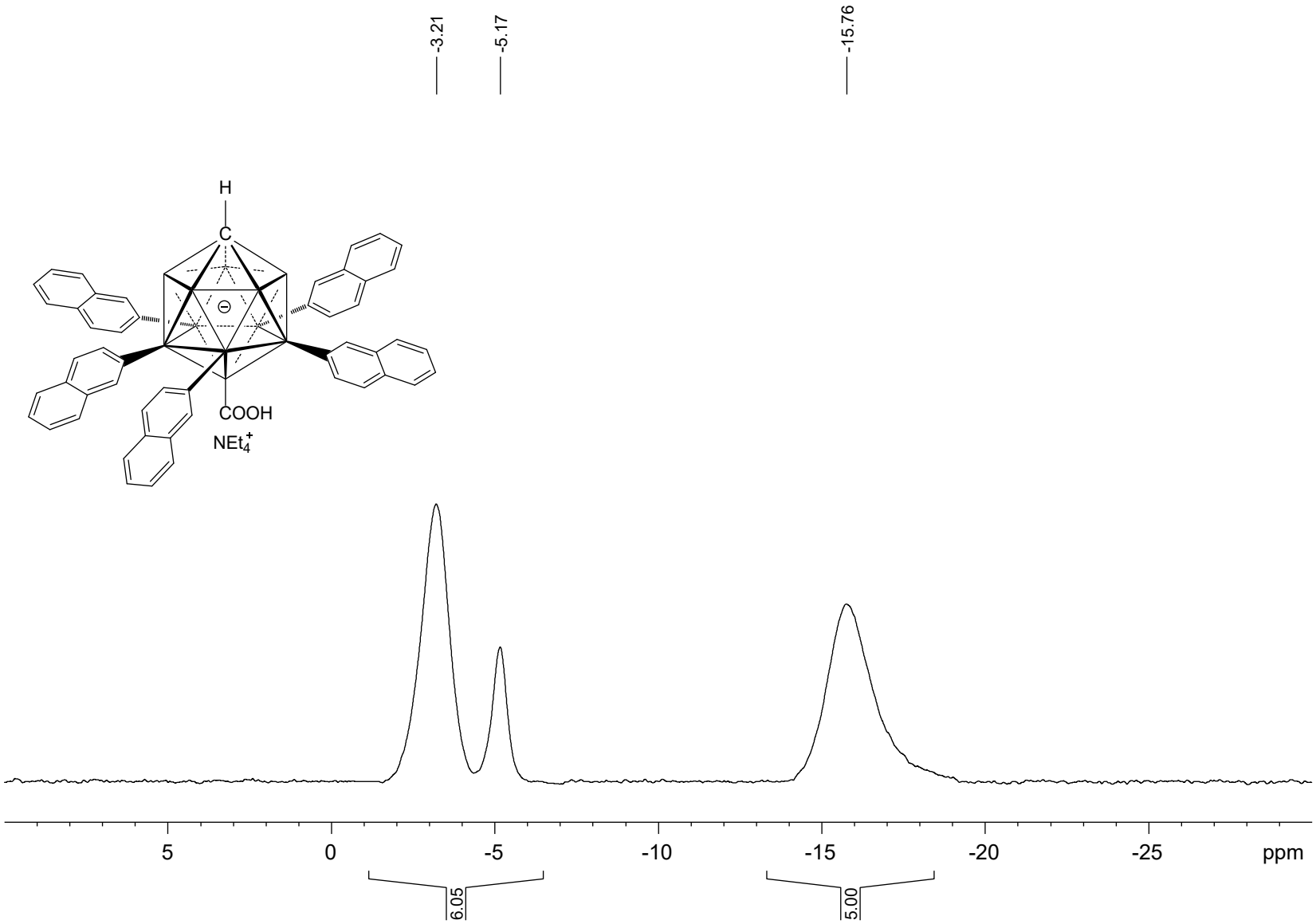

```
Current Data Parameters
NAME      jyj-200807-301-HB
EXPNO                    3
PROCNO                   1

F2 - Acquisition Parameters
Date_           20200808
Time               10.23
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG               zg
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                295.8 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
```

jyj-200807-301-acetone-d6 [NEt4][12-COOH-CB11H6(2-C10H7)5]
11B 128MHz 34.8mg partial dissolved in acetone-d6 T = 23C



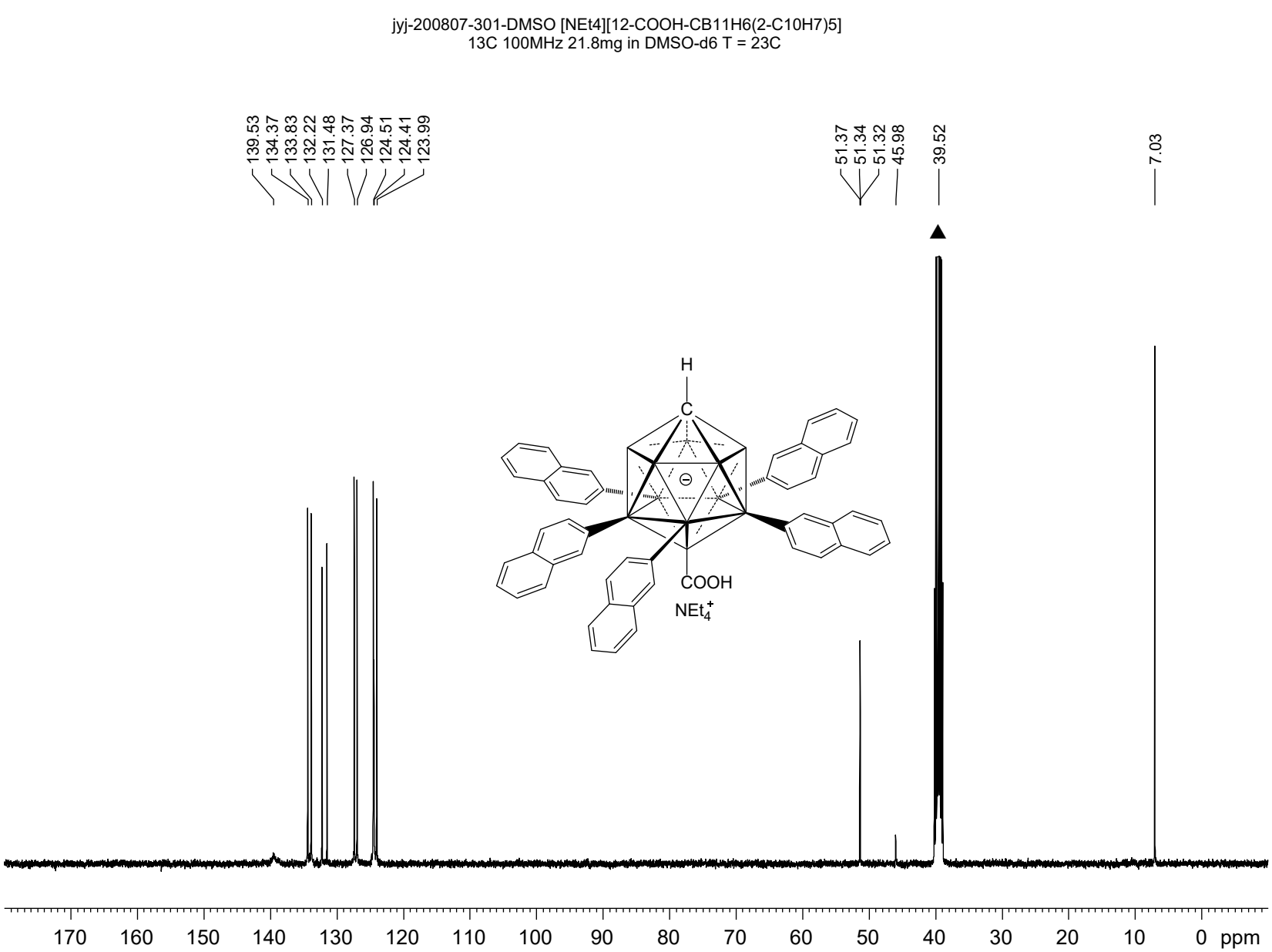

```
Current Data Parameters
NAME      jyj-200807-301-HB
EXPNO                    4
PROCNO                   1

F2 - Acquisition Parameters
Date_             20200808
Time                 10.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT          Acetone
NS                   128
DS                     4
SWH            25510.203 Hz
FIDRES          0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW                19.600 usec
DE                 6.50 usec
TE                296.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1

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

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

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




```
Current Data Parameters
NAME      jyj-200807-301-DMSO
EXPNO                      5
PROCNO                     1

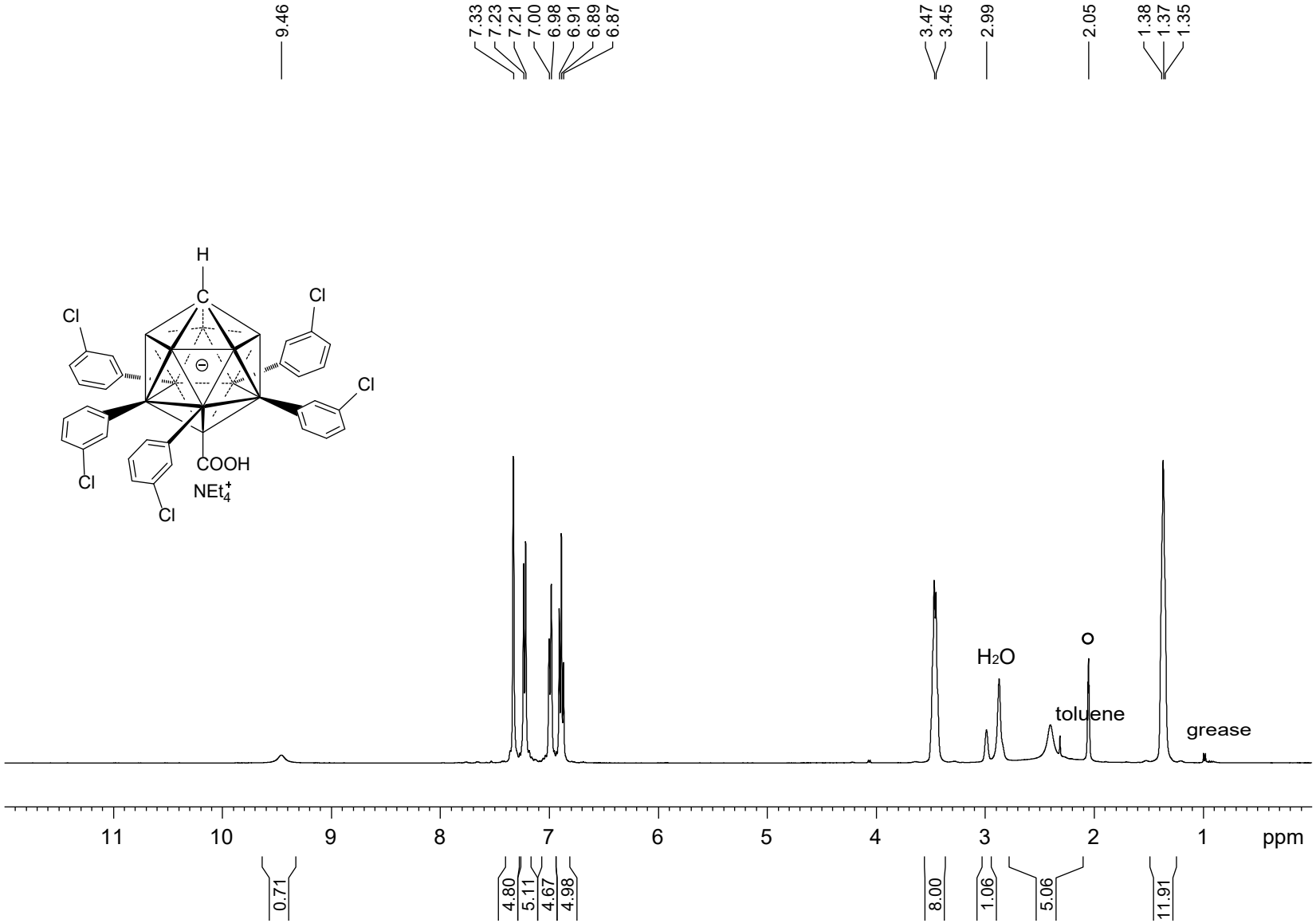
F2 - Acquisition Parameters
Date_            20200808
Time                21.43
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               170.36
DW               16.800 usec
DE                6.50 usec
TE               296.4 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

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

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

F2 - Processing parameters
SI                32768
SF          100.6128157 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

jyj-200706-273-total [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
1H{11B} 400MHz 21.3mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-200706-273-total
EXPNO                        2
PROCNO                       1

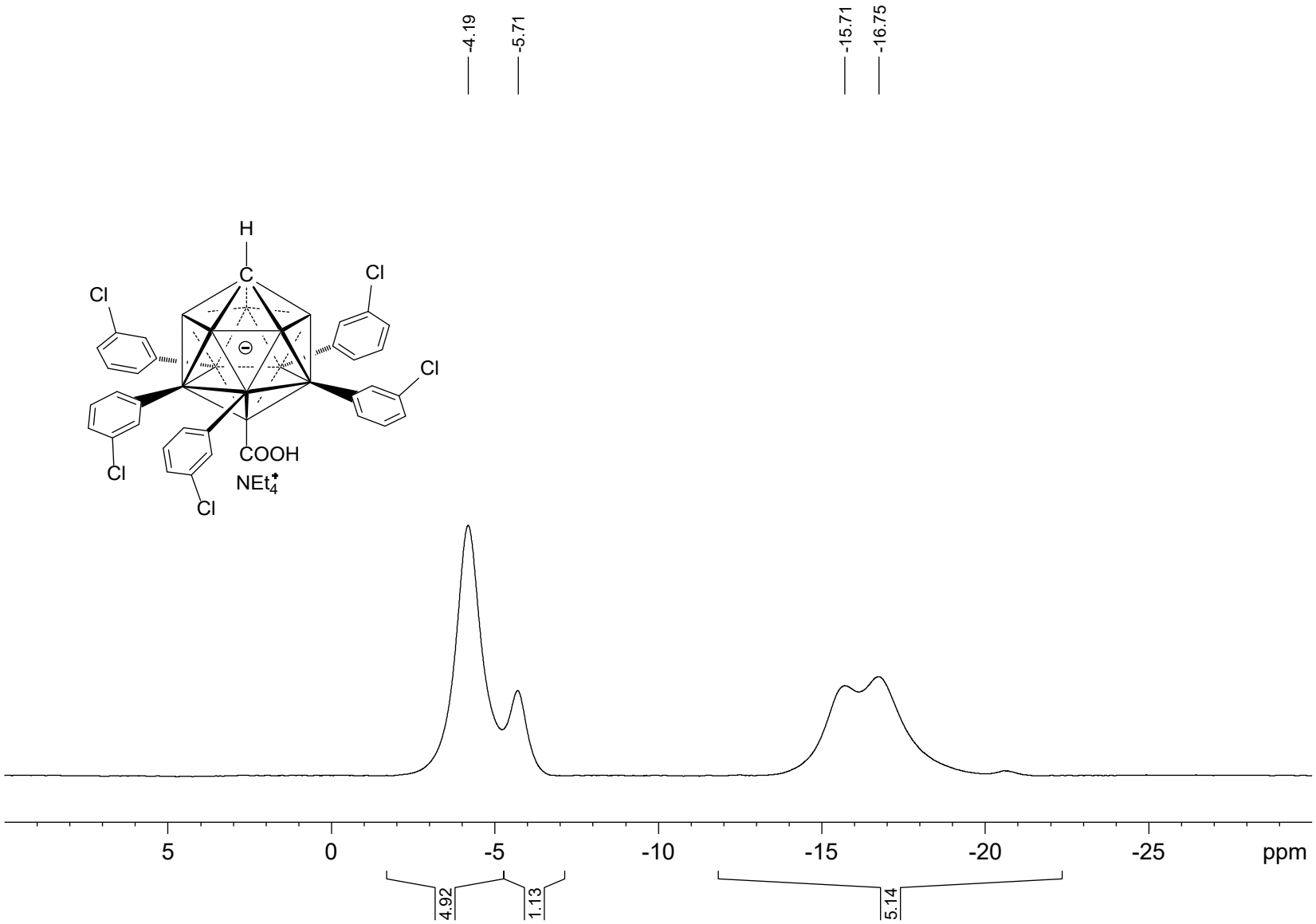
F2 - Acquisition Parameters
Date_              20200707
Time                 19.21
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG            zgig30
TD                  16384
SOLVENT           Acetone
NS                     16
DS                      4
SWH               8012.820 Hz
FIDRES               0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
DW                   62.400 usec
DE                    6.50 usec
TE                   293.8 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                     1

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

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

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

jyj-220914-3-Cl [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
11B128MHz 20mg in 0.6ml acetone-d6 23C



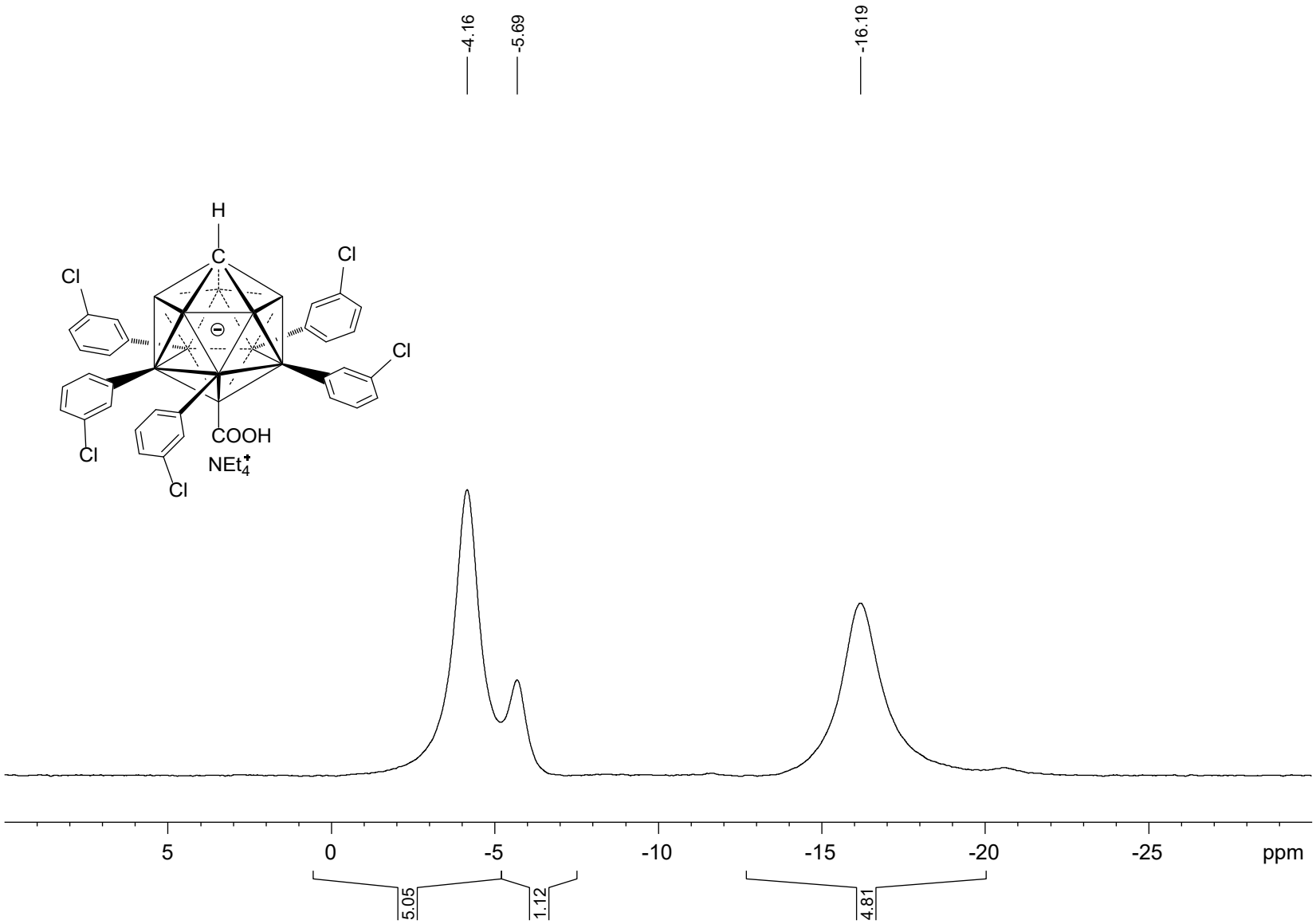

```
Current Data Parameters
NAME      jyj-220914-3-Cl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time              11.13
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.2 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-220914-3-Cl [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-3-Cl
EXPNO                  2
PROCNO                 1

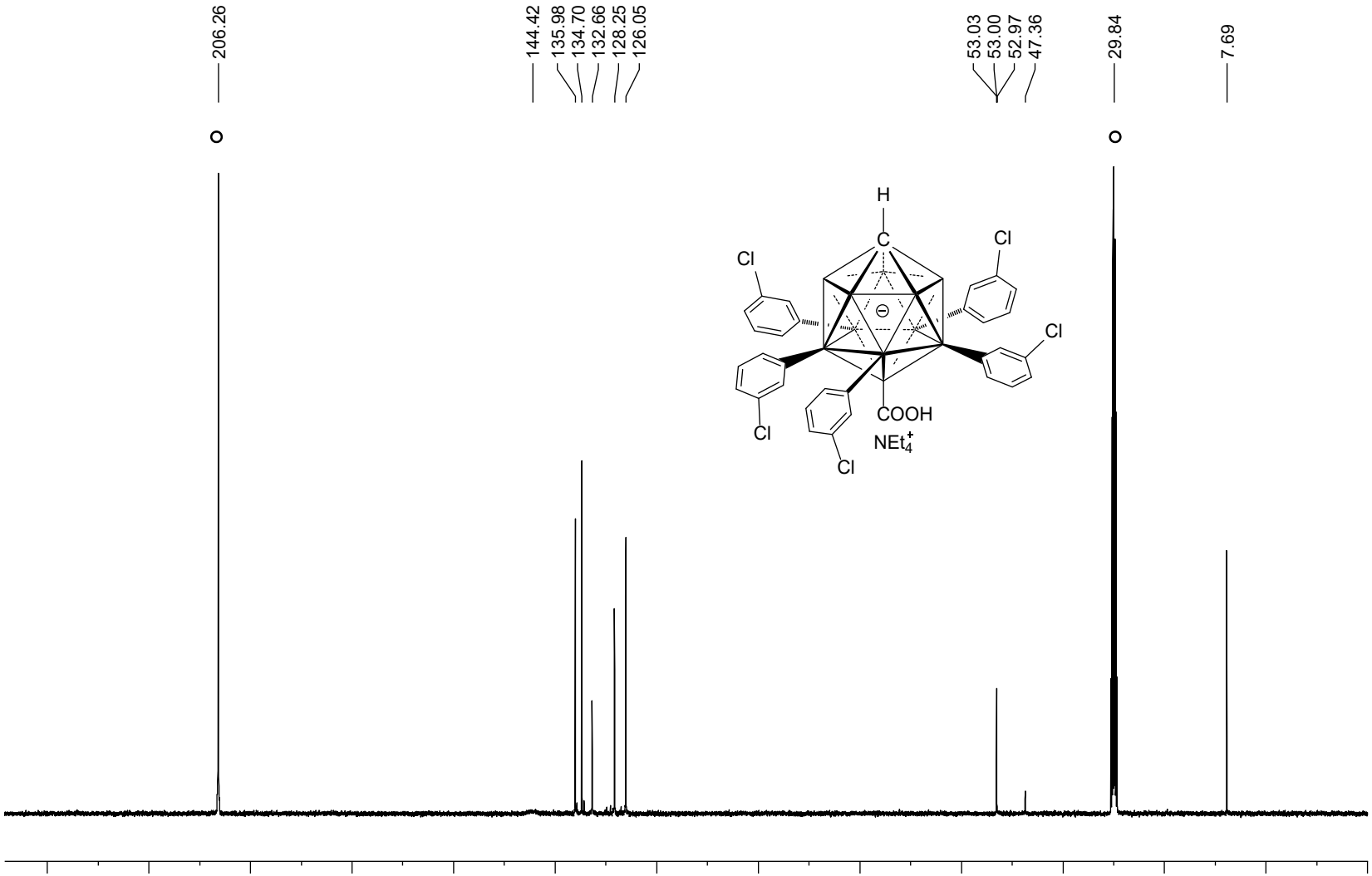
F2 - Acquisition Parameters
Date_           20220915
Time               11.19
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE              297.2 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-200706-273-total [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
13C 100MHz 21.3mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-200706-273-total
EXPNO                       5
PROCNO                      1

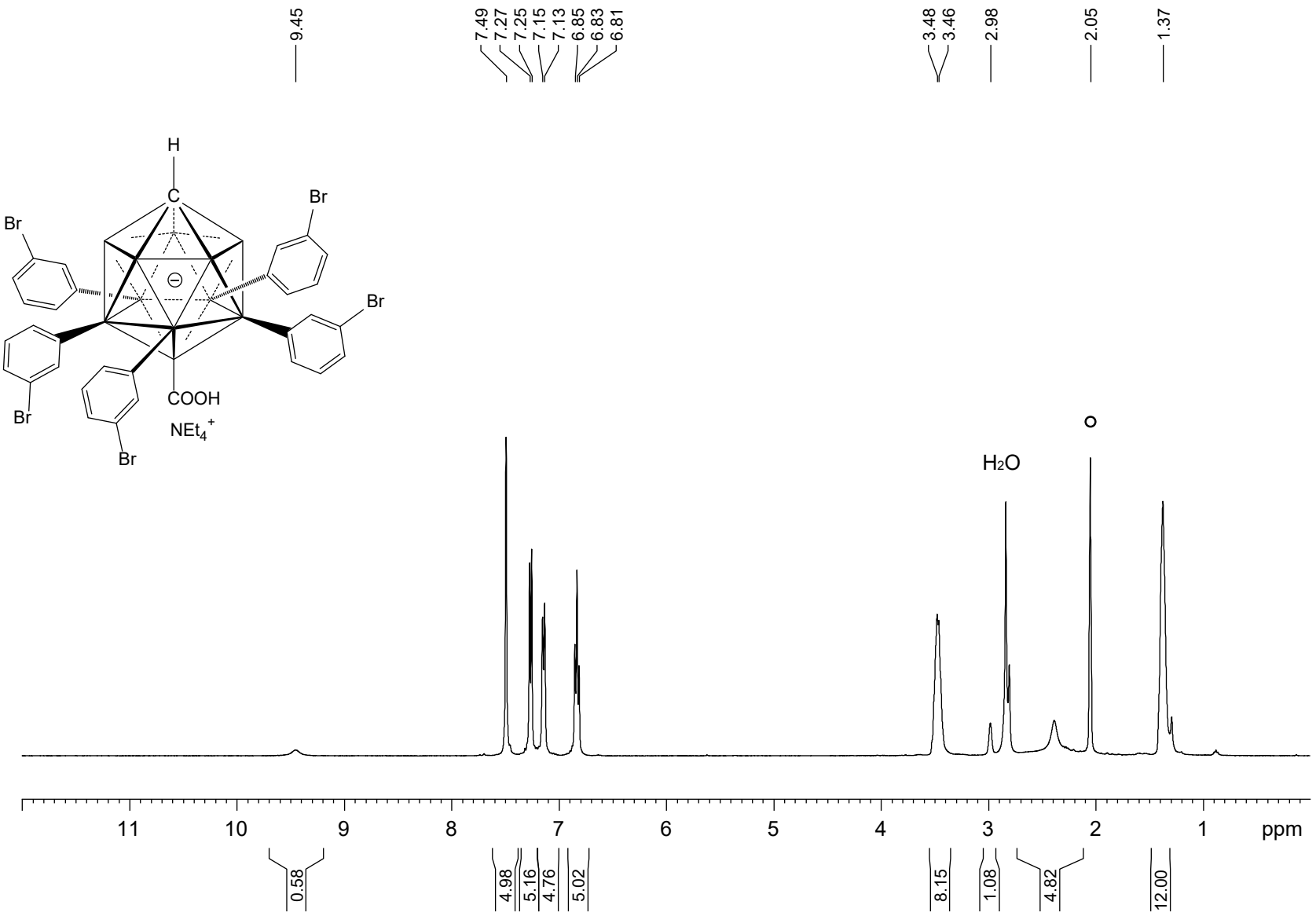
F2 - Acquisition Parameters
Date_            20200707
Time                21.07
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   2048
DS                      4
SWH             29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 193.34
DW                16.800 usec
DE                 6.50 usec
TE                293.6 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          100.6126784 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

jyj-190903-183 [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
1H{11B} 400MHz 16.4mg in acetone-d6 T= 23 C




```
Current Data Parameters
NAME      jyj-190903-183
EXPNO                 1
PROCNO                1

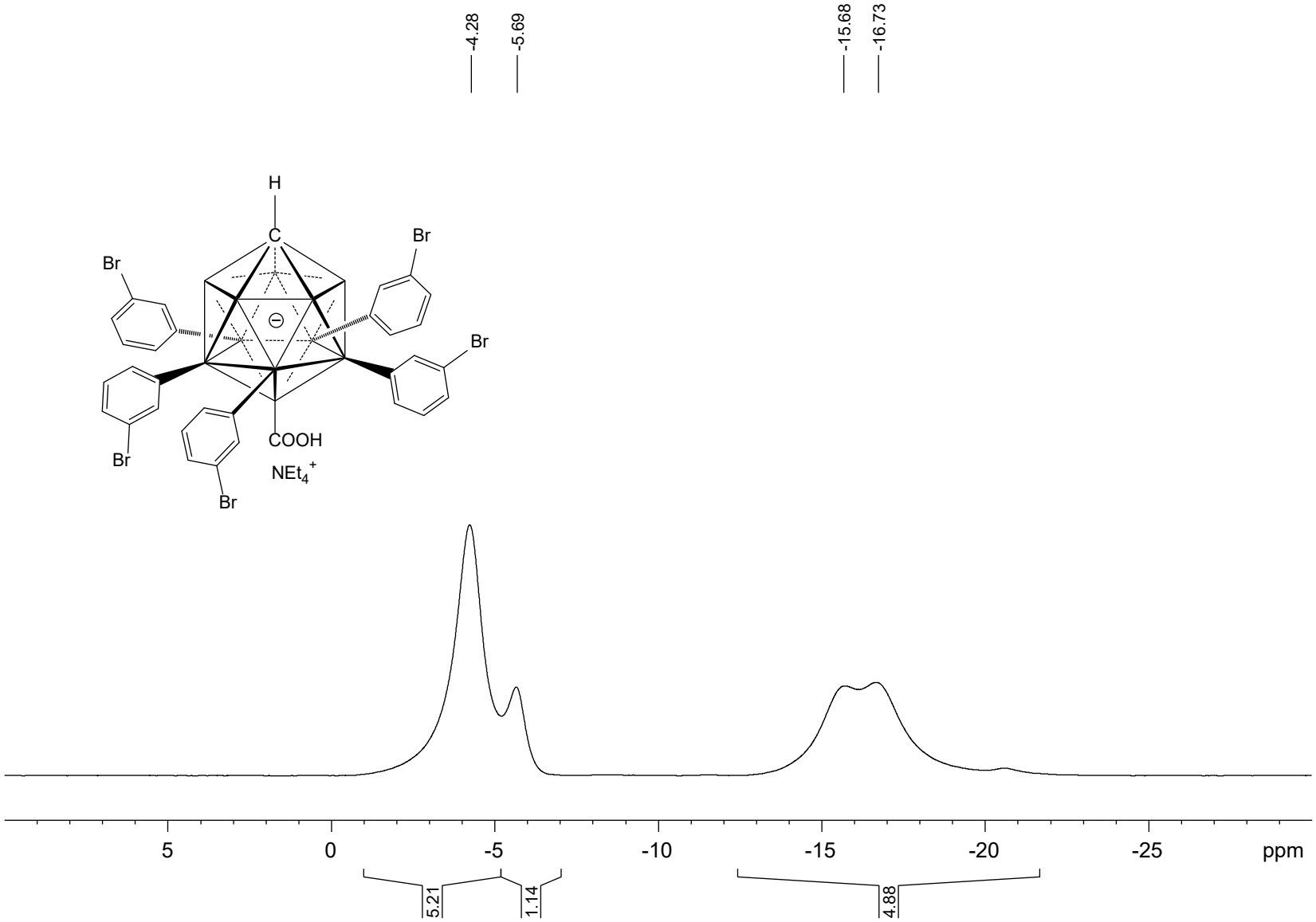
F2 - Acquisition Parameters
Date_          20190904
Time              12.03
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgig30
TD                16384
SOLVENT         Acetone
NS                   16
DS                    4
SWH            8012.820 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                107.6
DW               62.400 usec
DE                6.50 usec
TE               296.2 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                   1

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

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

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

jyj-220914-3-Br [NEt4][12-COOH-CB11H6(3-C6H4-Br)5]
11B 128MHz 20mg in 0.6ml acetone-d6 23C



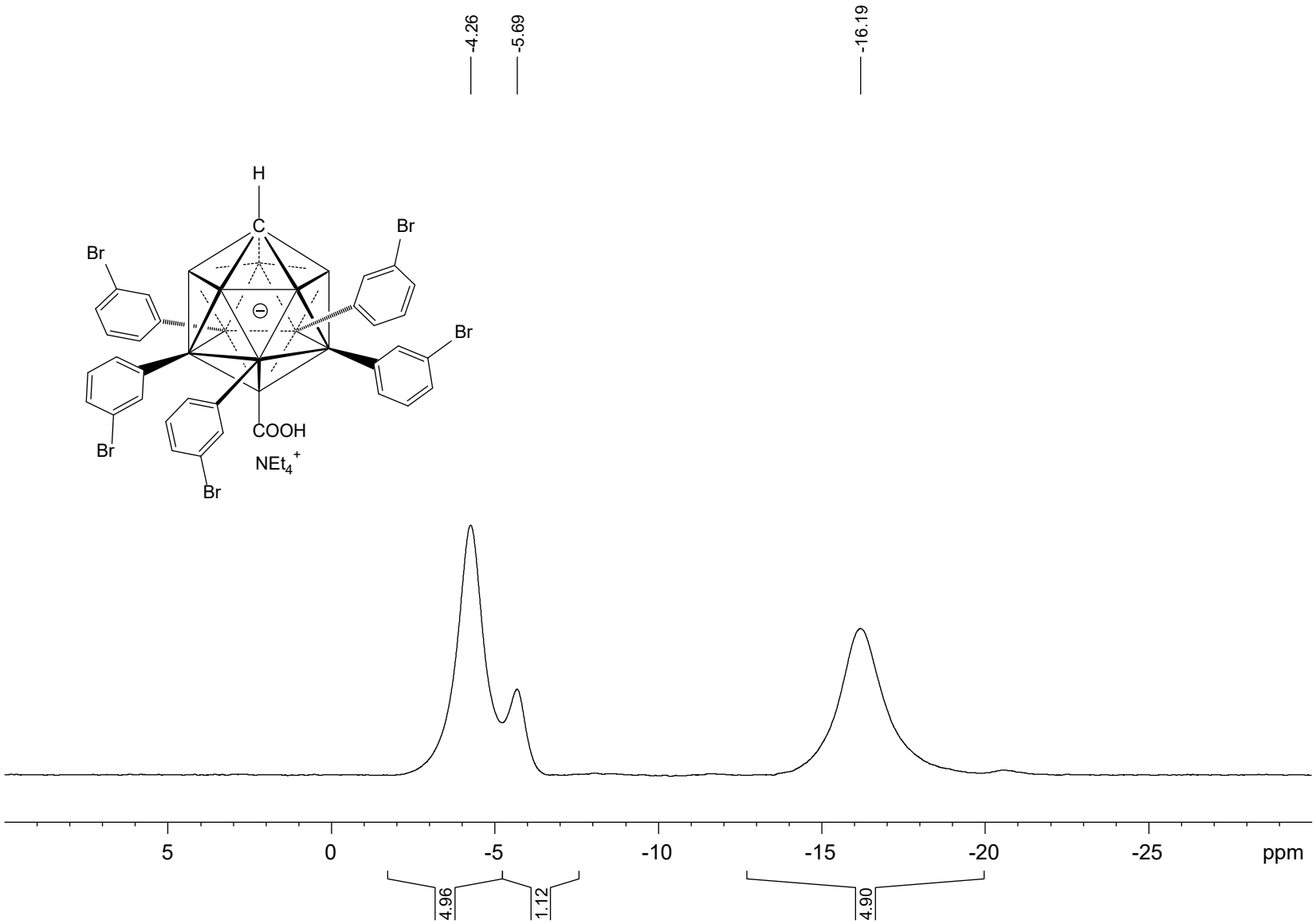

```
Current Data Parameters
NAME      jyj-220914-3-Br
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20220915
Time                3.33
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                296.2 K
D1            1.00000000 sec
TD0                    1

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

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

jyj-220914-3-Br [NEt4][12-COOH-CB11H6(3-C6H4-Br)5]
11B{1H} 128MHz 20mg in 0.6ml acetone-d6 23C




```
Current Data Parameters
NAME      jyj-220914-3-Br
EXPNO                  2
PROCNO                 1

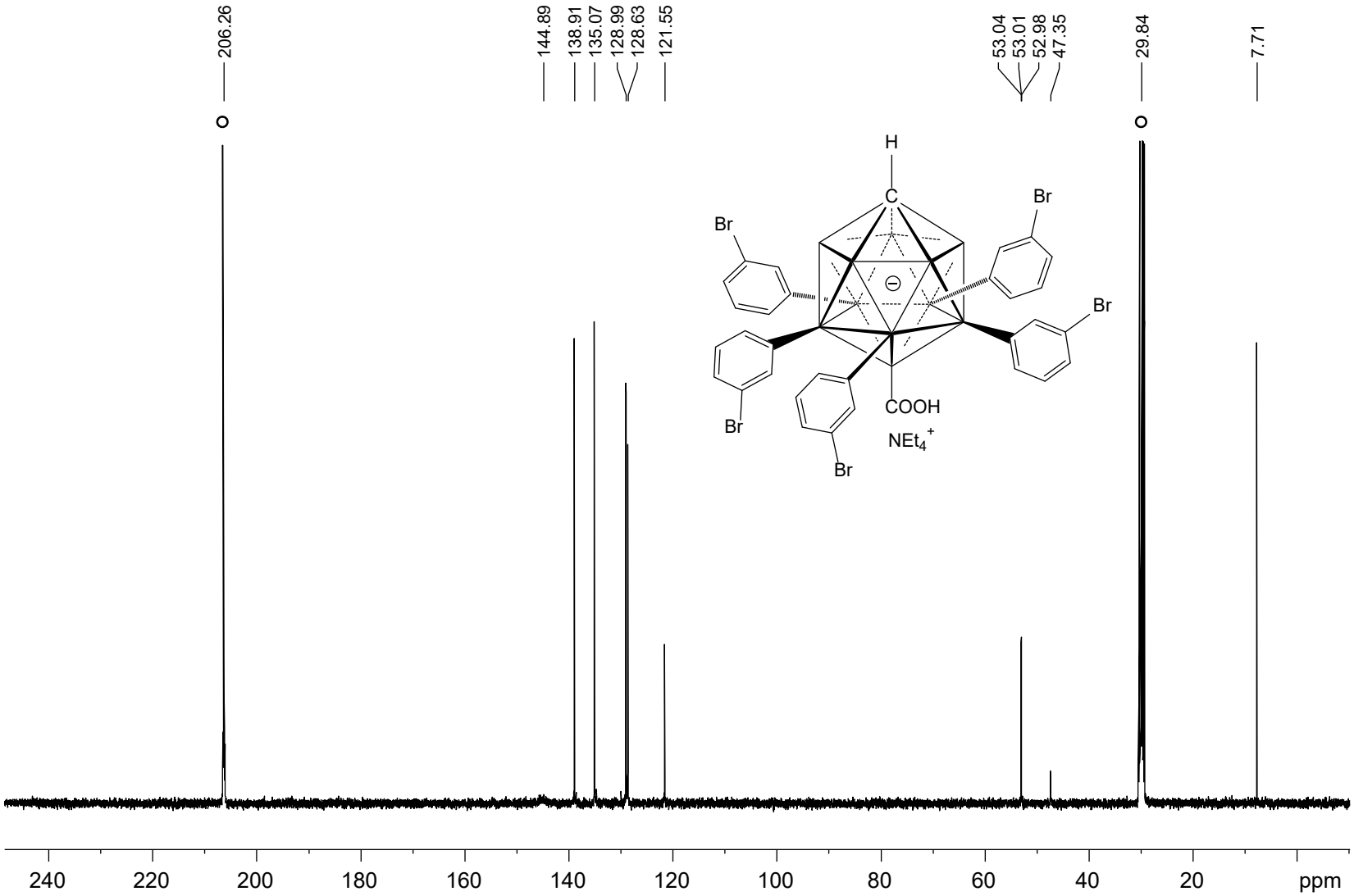
F2 - Acquisition Parameters
Date_           20220915
Time                3.39
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               296.9 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

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

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

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

jyj-190903-183 [NEt4][12-COOH-CB11H6(3-C6H4-Cl)5]
13C 100MHz 16.4mg in acetone-d6 T= 23 C




```
Current Data Parameters
NAME      jyj-200718-183-C
EXPNO                   1
PROCNO                  1

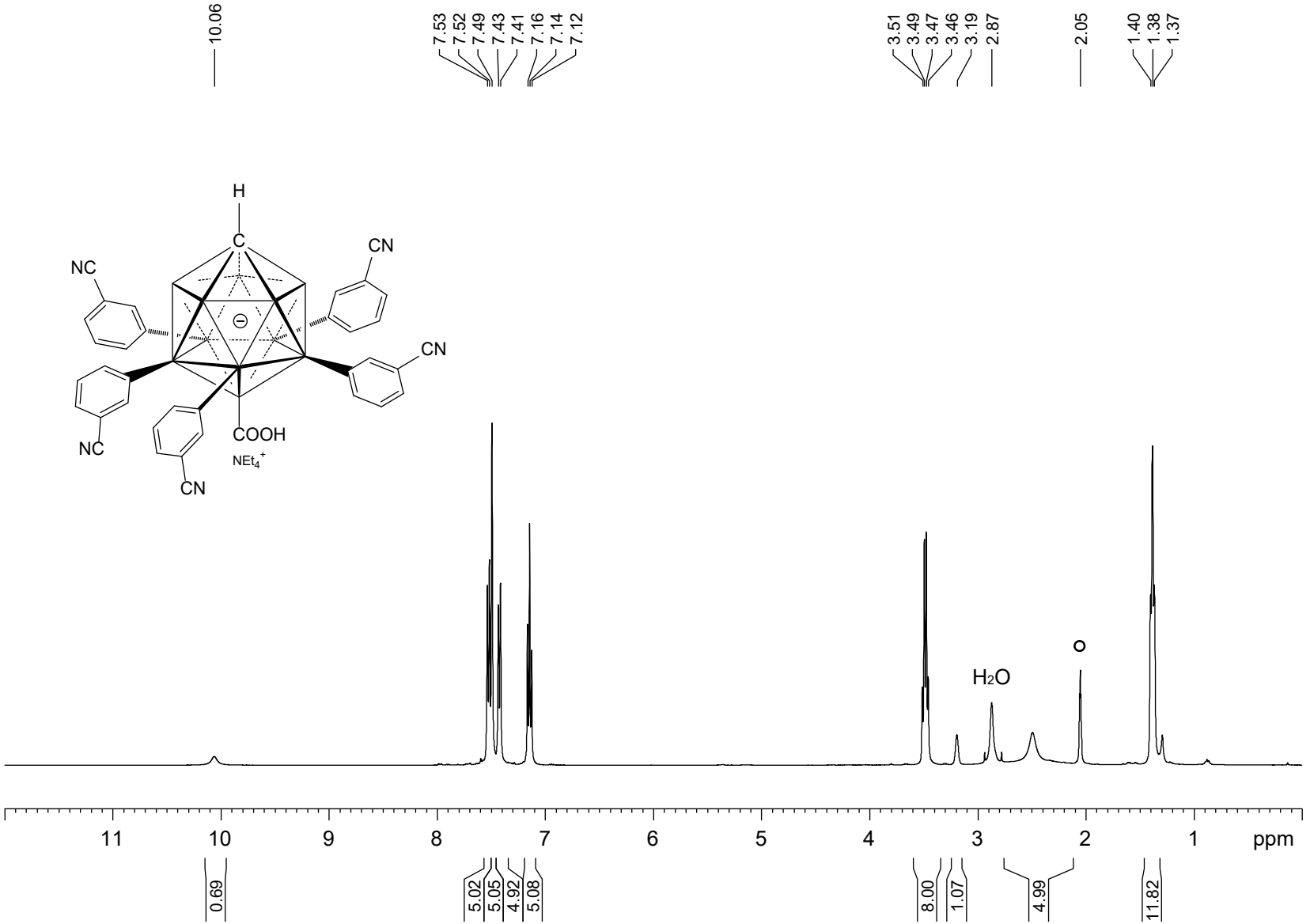
F2 - Acquisition Parameters
Date_            20200720
Time                1.02
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2048
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010048 sec
RG               193.34
DW               16.800 usec
DE                6.50 usec
TE               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          100.6126784 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

jyj-200701-275-total [NEt4+][12-COOH-CB11H6(3-C6H4-CN)5]
1H{11B} 400MHz 20.4mg in Acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200701-275-total
EXPNO                        2
PROCNO                       1

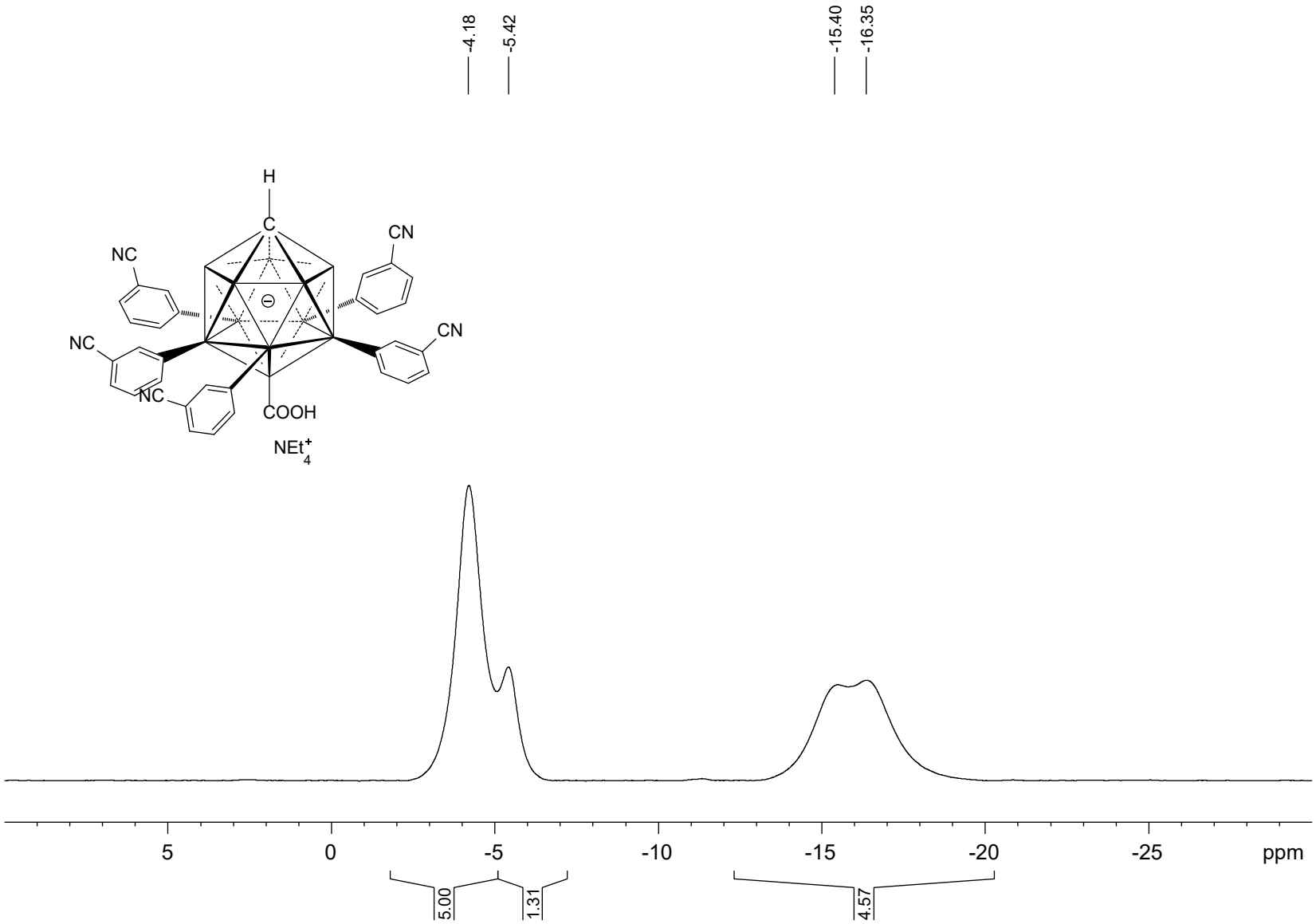
F2 - Acquisition Parameters
Date_              20200702
Time                 16.49
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG             zgig30
TD                   16384
SOLVENT            Acetone
NS                      16
DS                       4
SWH                8012.820 Hz
FIDRES             0.489064 Hz
AQ                1.0223616 sec
RG                    107.6
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           400.1300073 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

jyj-200701-275-total [NEt4+][12-COOH-CB11H6(3-C6H4-CN)5]
11B 128MHz 20.4mg in Acetone-d6 T=23 C



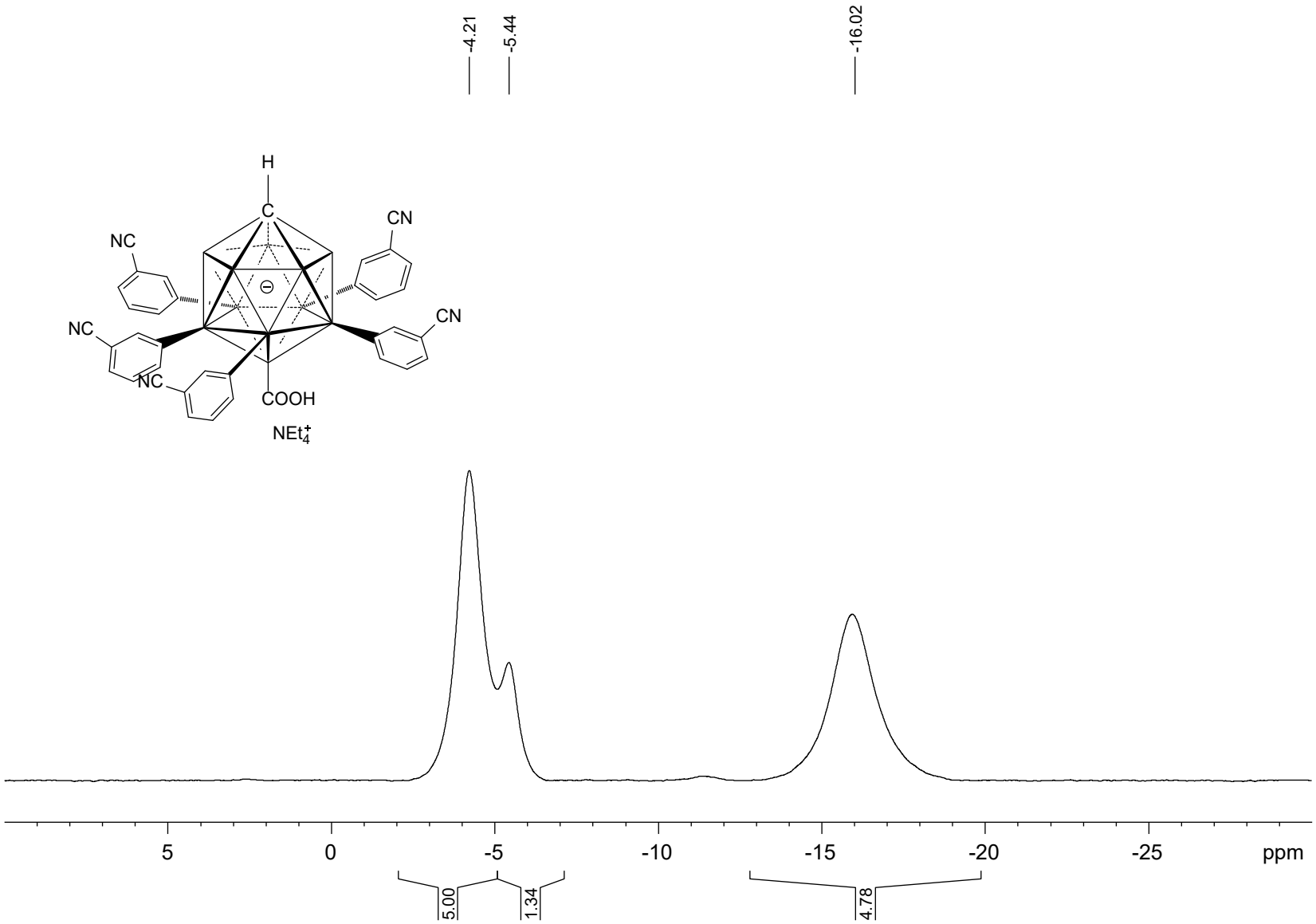

```
Current Data Parameters
NAME      jyj-200701-275-total-3-CN
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20200702
Time              16.55
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               293.6 K
D1            1.00000000 sec
TD0                   1

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

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

jyj-200701-275-total [NEt4+][12-COOH-CB11H6(3-C6H4-CN)5]
11B{1H} 128MHz 20.4mg in Acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200701-275-total-3-CN
EXPNO                 4
PROCNO                1

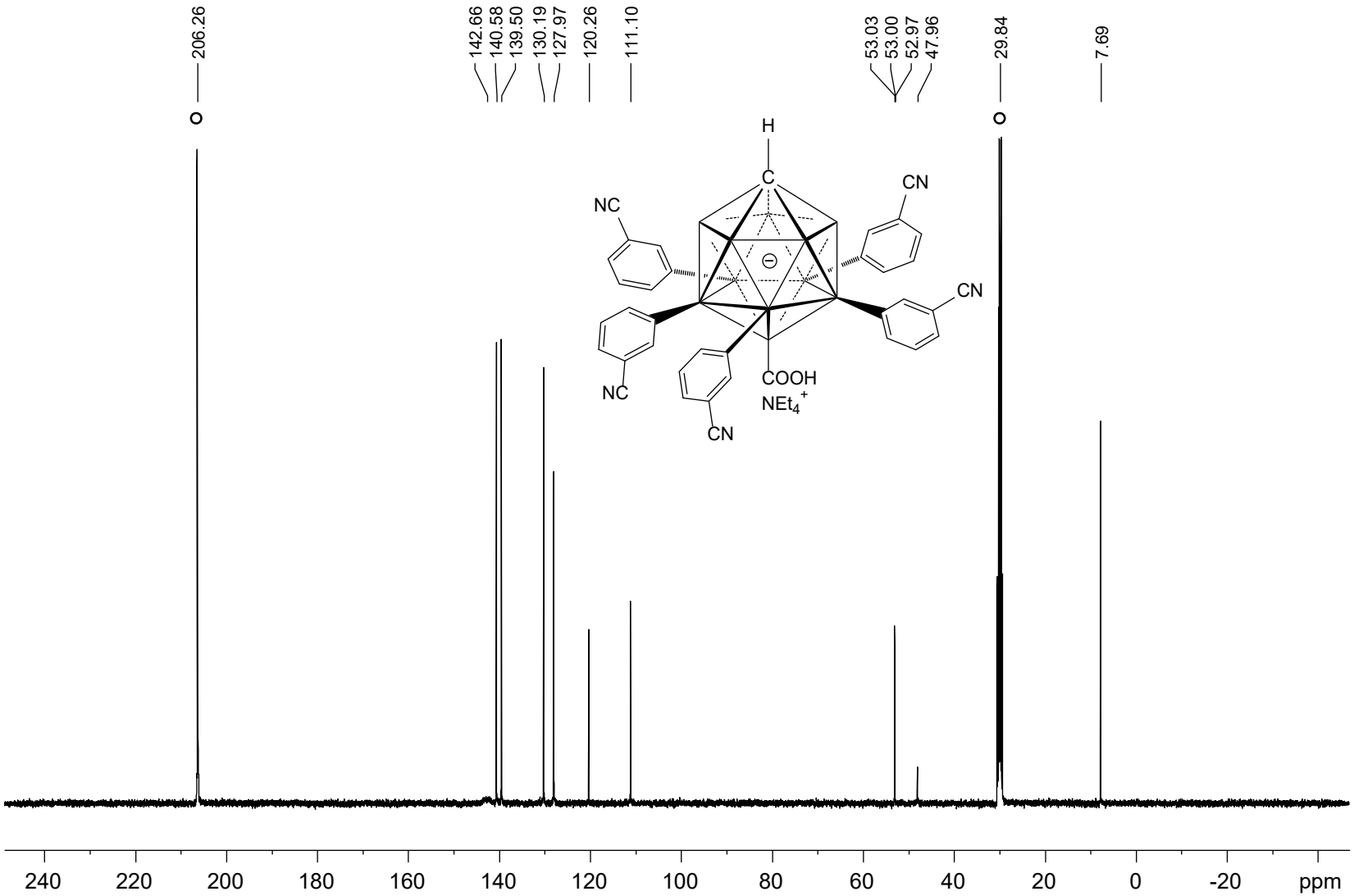
F2 - Acquisition Parameters
Date_          20200702
Time              17.01
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT        Acetone
NS                 128
DS                   4
SWH          25510.203 Hz
FIDRES        0.389255 Hz
AQ           1.2845056 sec
RG              193.34
DW              19.600 usec
DE               6.50 usec
TE              294.3 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1

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

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

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

jyj-200701-275-total [NEt4+][12-COOH-CB11H6(3-C6H4-CN)5]
13C 100MHz 20.4mg in Acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200701-275-total
EXPNO                       5
PROCNO                      1

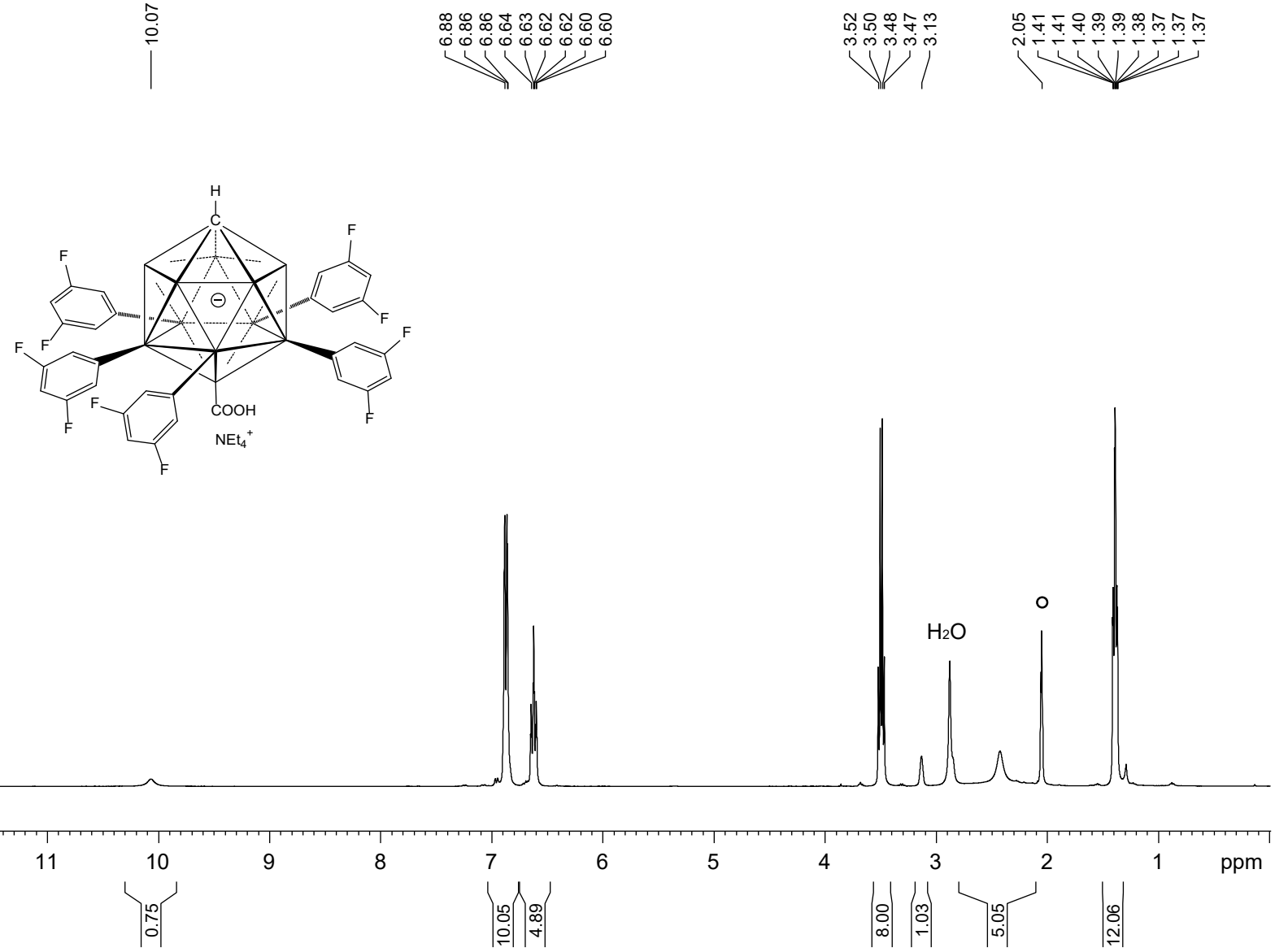
F2 - Acquisition Parameters
Date_            20200702
Time                18.33
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   2048
DS                      4
SWH             29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 193.34
DW                16.800 usec
DE                 6.50 usec
TE                293.9 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           100.6126784 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

jyj-200715-287-total [NEt4][12-COOH-CB11H6(3,5-C6H3-F2)5]
1H{11B} 400MHz 19.9mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200715-287-total
EXPNO                       2
PROCNO                      1

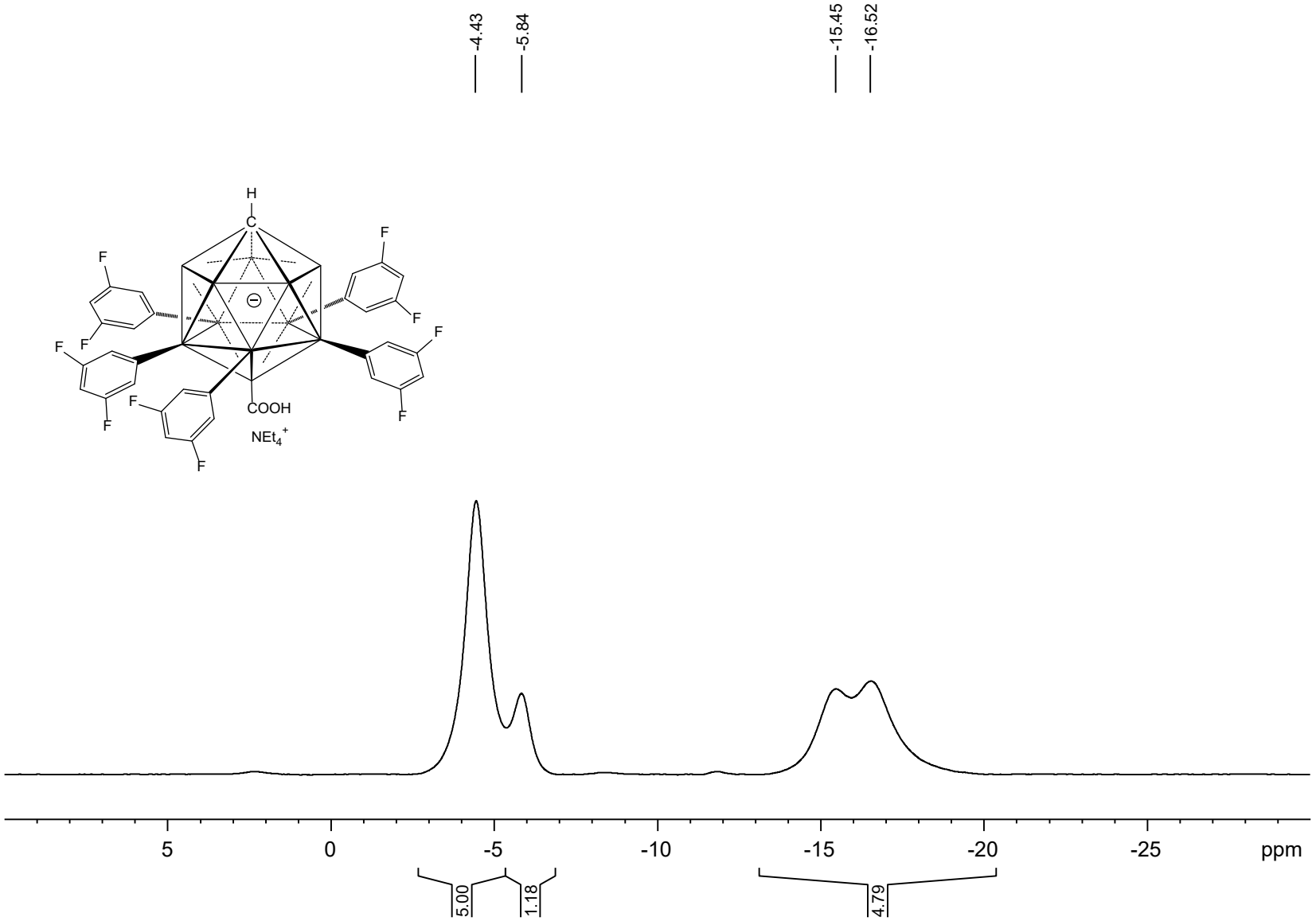
F2 - Acquisition Parameters
Date_              20200717
Time                  19.07
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgig30
TD                    16384
SOLVENT             Acetone
NS                       16
DS                        4
SWH                8012.820 Hz
FIDRES                0.489064 Hz
AQ                 1.0223616 sec
RG                      107.6
DW                     62.400 usec
DE                      6.50 usec
TE                     293.2 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
```

jyj-200715-287-total [NEt4][12-COOH-CB11H6(3,5-C6H3-F2)5]
11B 128MHz 19.9mg in acetone-d6 T=23 C



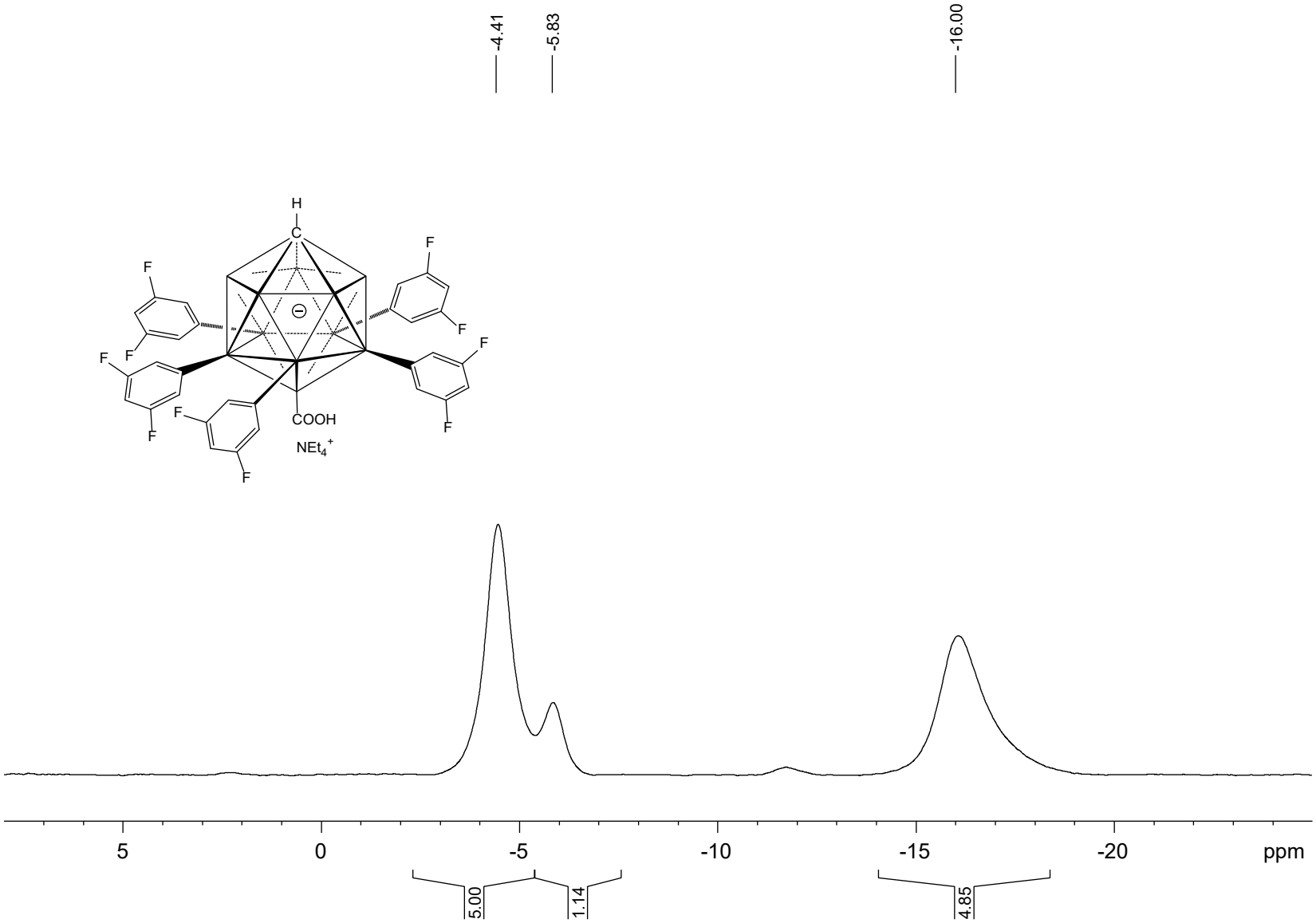

```
Current Data Parameters
NAME      jyj-200715-287-total-3,5-2F
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20200717
Time              19.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG             zg
TD                65536
SOLVENT         Acetone
NS                  128
DS                    4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ            1.2845056 sec
RG               193.34
DW               19.600 usec
DE                6.50 usec
TE               292.6 K
D1           1.00000000 sec
TD0                   1

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

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

jyj-200715-287-total [NEt4][12-COOH-CB11H6(3,5-C6H3-F2)5]
11B{1H} 128MHz 19.9mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200715-287-total-3,5-2F
EXPNO                 4
PROCNO                1

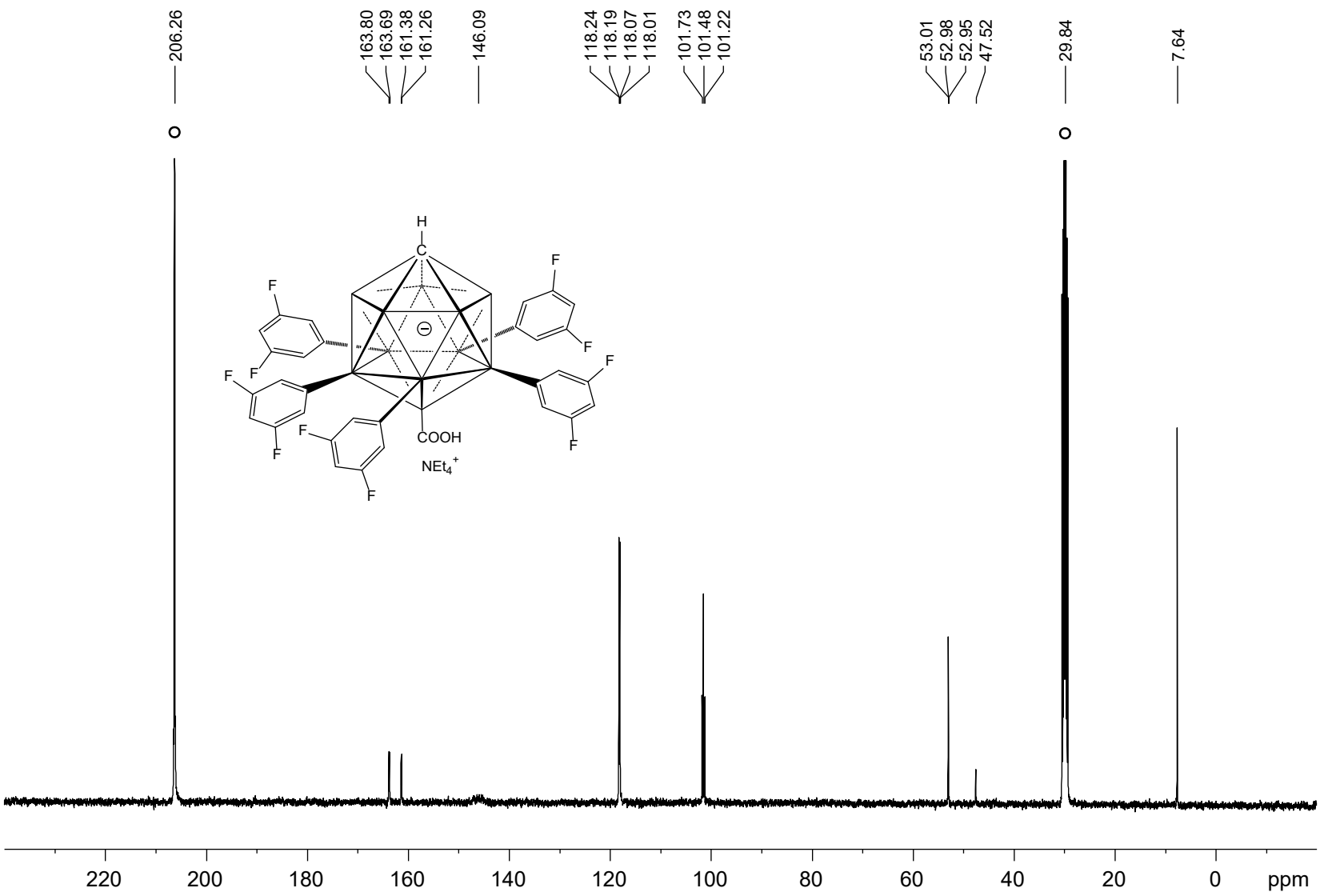
F2 - Acquisition Parameters
Date_          20200717
Time              19.19
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT       Acetone
NS                128
DS                  4
SWH           25510.203 Hz
FIDRES         0.389255 Hz
AQ             1.2845056 sec
RG                193.34
DW              19.600 usec
DE               6.50 usec
TE              293.6 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
```

jyj-200715-287-total [NEt4][12-COOH-CB11H6(3,5-C6H3-F2)5]
13C 100MHz 19.9mg in acetone-d6 T=23 C




```
Current Data Parameters
NAME      jyj-200715-287-total
EXPNO                       5
PROCNO                      1

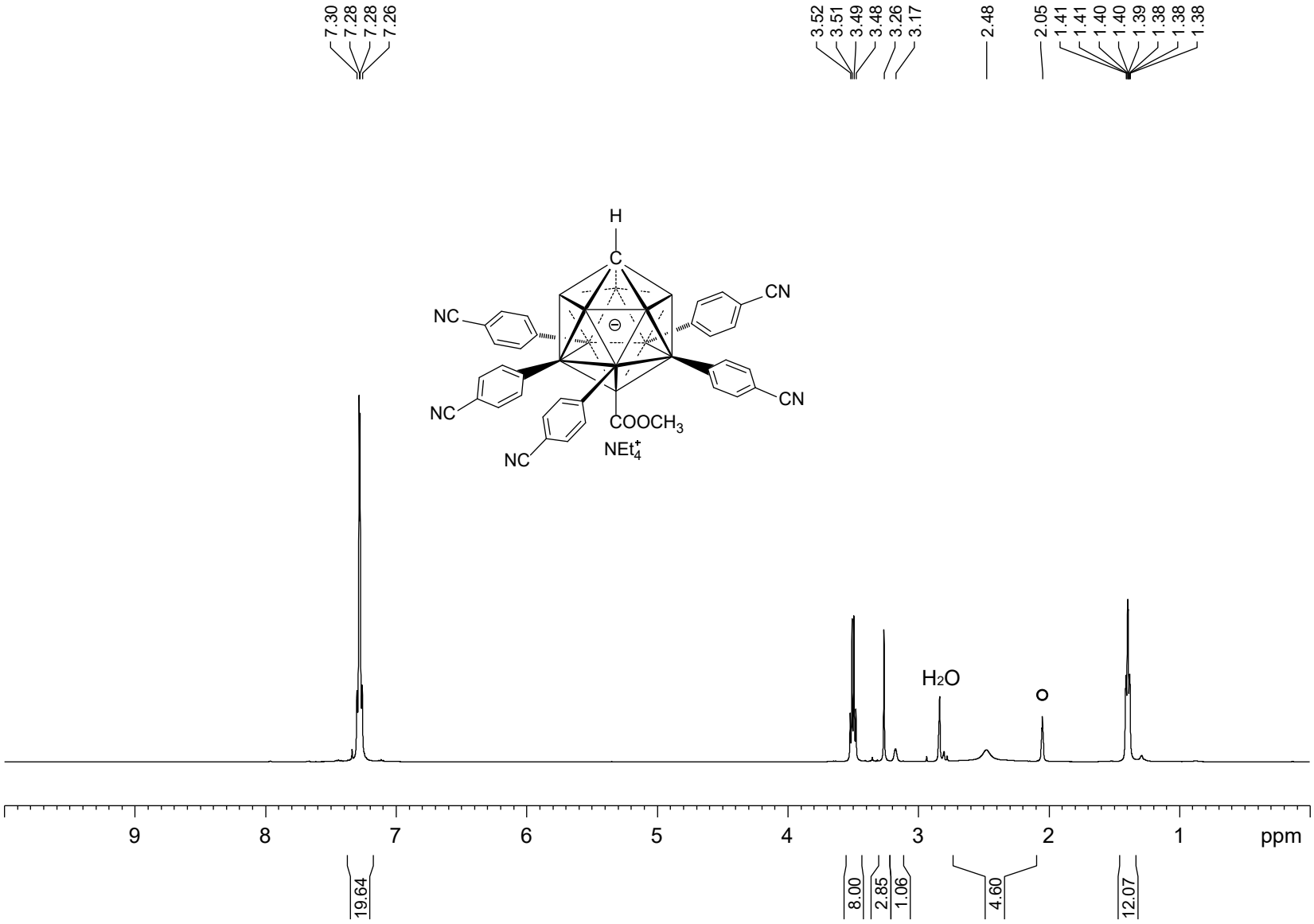
F2 - Acquisition Parameters
Date_            20200717
Time                20.51
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT          Acetone
NS                   2048
DS                      4
SWH             29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 193.34
DW                16.800 usec
DE                 6.50 usec
TE                293.7 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          100.6126784 MHz
WDW                    EM
SSB                     0
LB                   2.00 Hz
GB                      0
PC                   1.40
```

jyj-220305-578-500M 12-COOCH3-CB11H6(C6H4CN)5
1H{11b} 500M Hz 24.2 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-220308-578-total-500M
EXPNO                 2
PROCNO                1

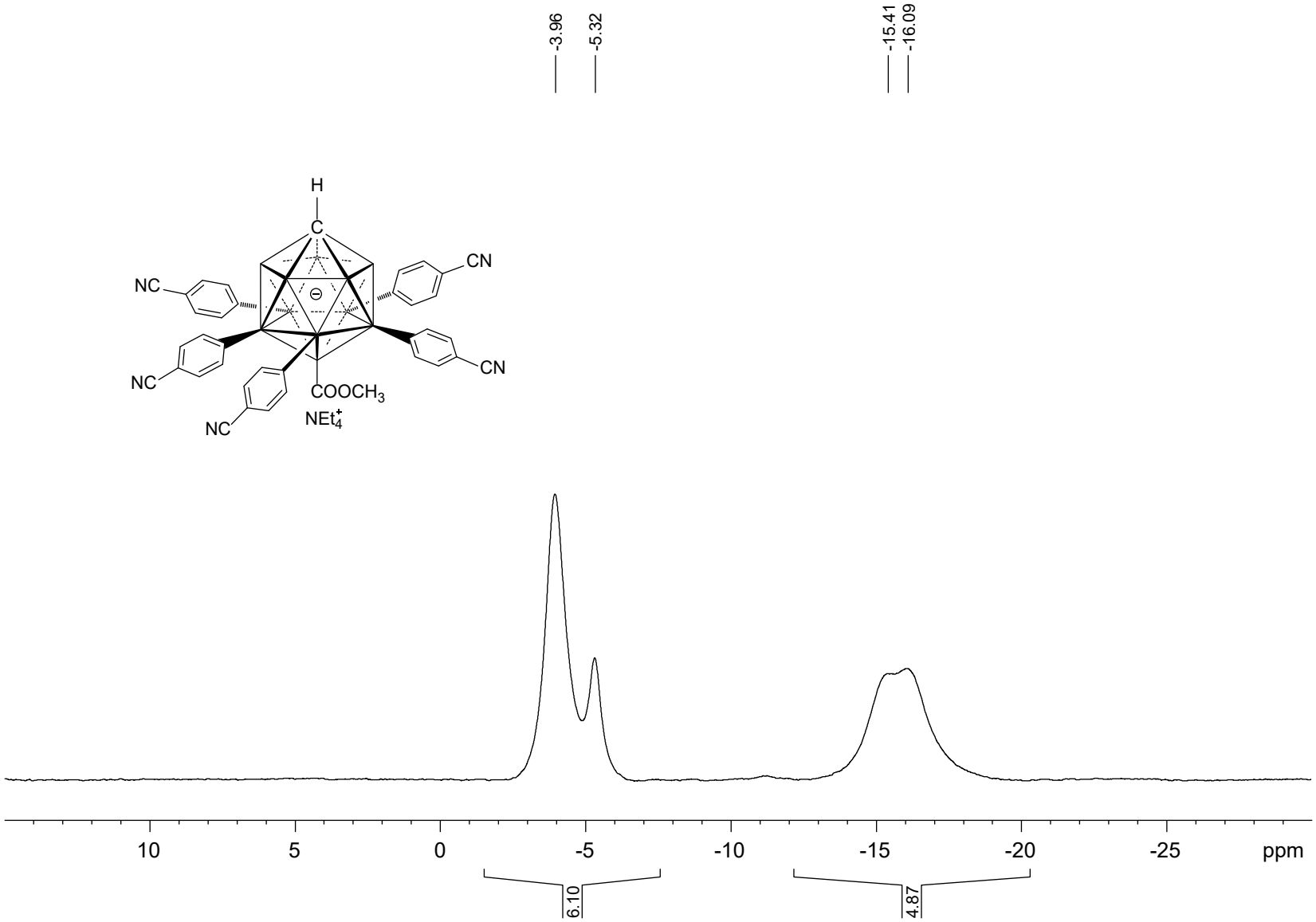
F2 - Acquisition Parameters
Date_          20220308
Time              12.44
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgig30
TD                65536
SOLVENT         Acetone
NS                   16
DS                    0
SWH           12500.000 Hz
FIDRES            0.190735 Hz
AQ             2.6214399 sec
RG                  114
DW                 40.000 usec
DE                  6.50 usec
TE                295.4 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
```

jyj-220305-578-500M 12-COOCH3-CB11H6(C6H4CN)5
11b 150M Hz 24.2 mg in acetone-d6



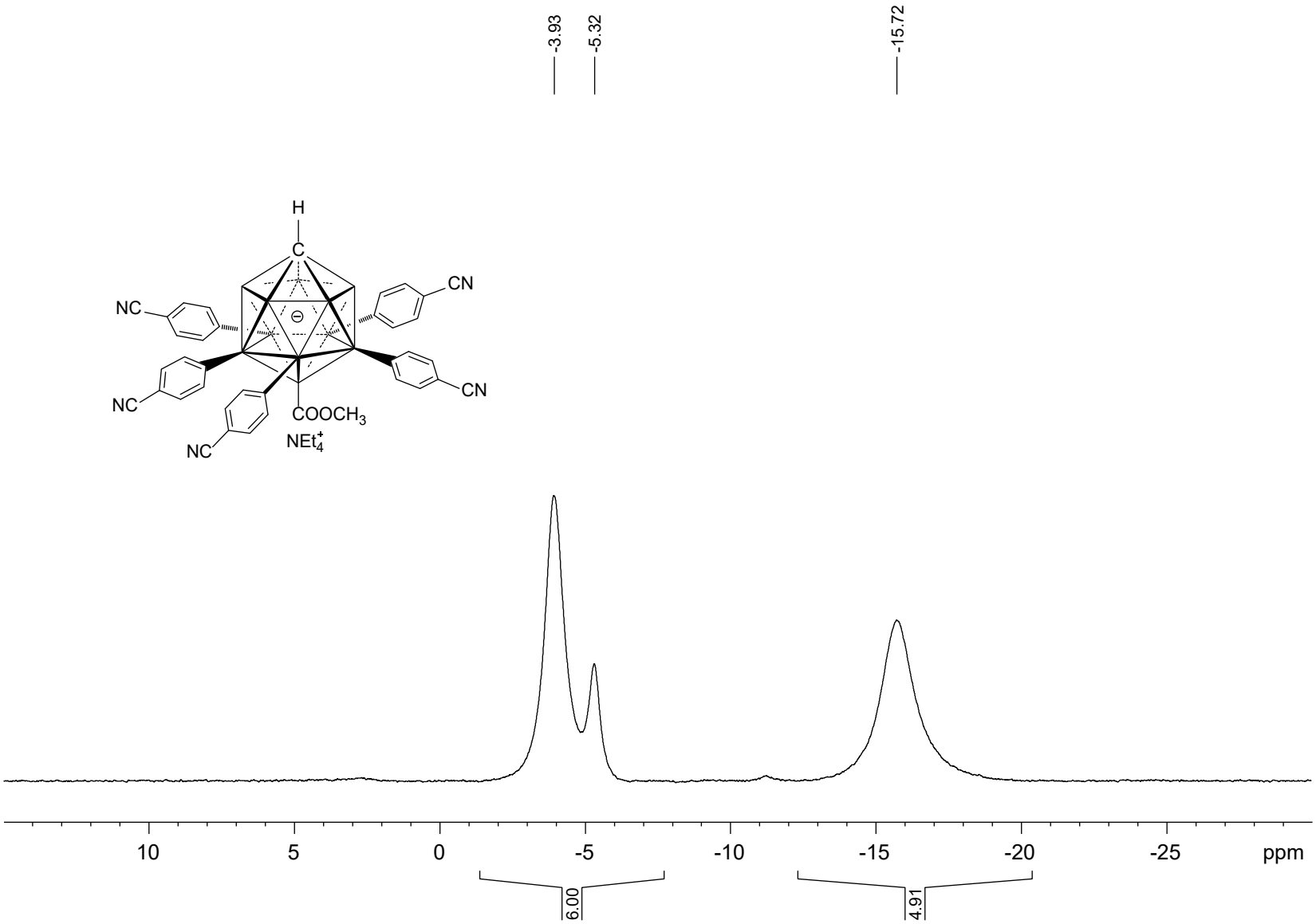

```
Current Data Parameters
NAME      jyj-220308-578-total-500M
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_           20220308
Time              12.48
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               64098
SOLVENT         Acetone
NS                  80
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              295.1 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
```

jyj-220305-578-500M 12-COOCH3-CB11H6(C6H4CN)5
11b{1H} 150M Hz 24.2 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-220308-578-total-500M
EXPNO                 4
PROCNO                1

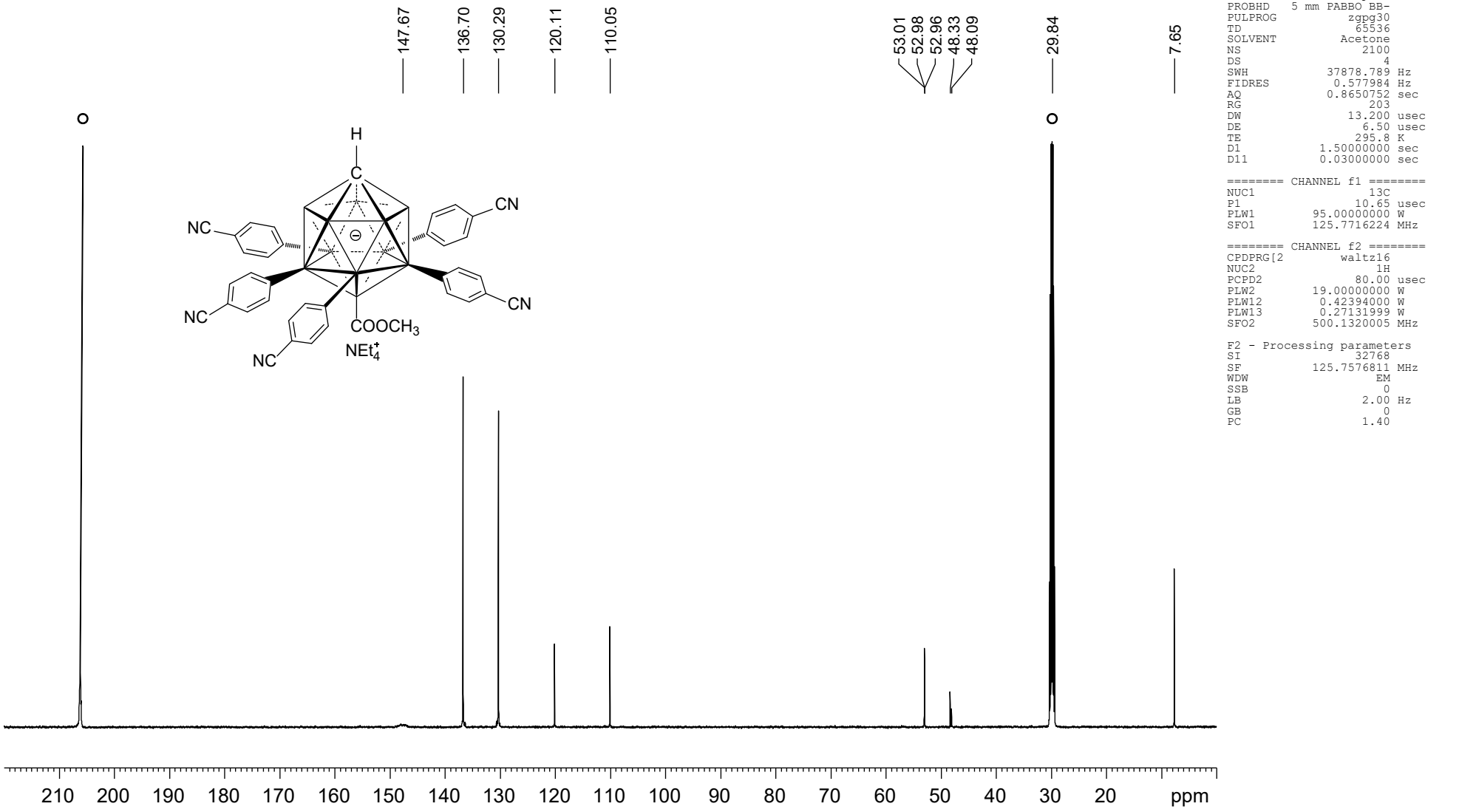
F2 - Acquisition Parameters
Date_          20220308
Time              12.51
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   80
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            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         0.42394000 W
PLW13         0.27131999 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
```

jyj-220305-578-500M 12-COOCH3-CB11H6(C6H4CN)5
13c 125M Hz 24.2 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-220308-578-total-500M
EXPNO                 5
PROCNO                1

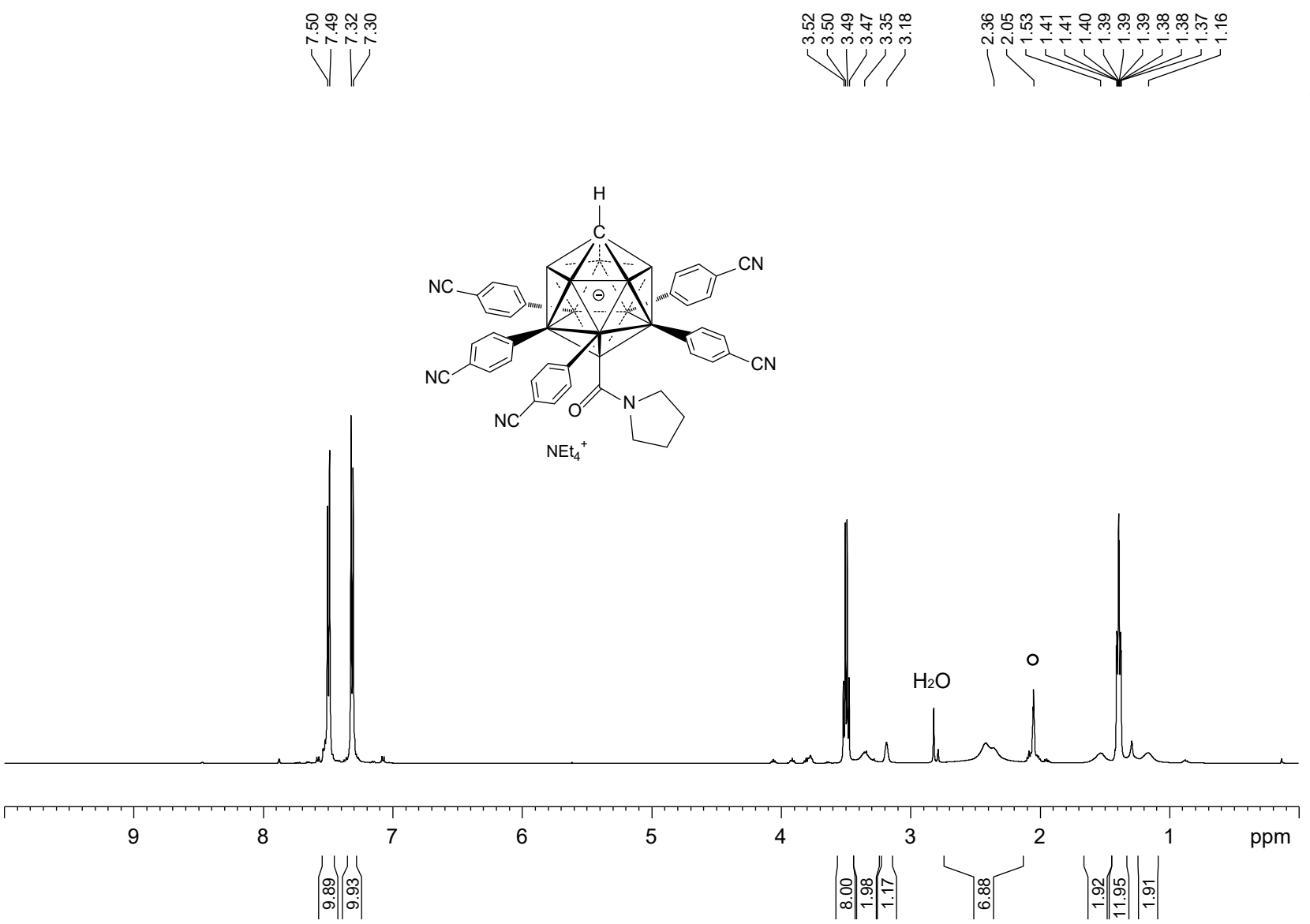
F2 - Acquisition Parameters
Date_          20220308
Time              14.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2100
DS                    4
SWH           37878.789 Hz
FIDRES         0.577984 Hz
AQ             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               10.65 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        0.42394000 W
PLW13        0.27131999 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7576811 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

jyj-220305-577-500M 12-CONC4H8-CB11H6(C6H4CN)5
1H{11B} 500M Hz 25 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-220308-577-total-500M
EXPNO                  2
PROCNO                 1

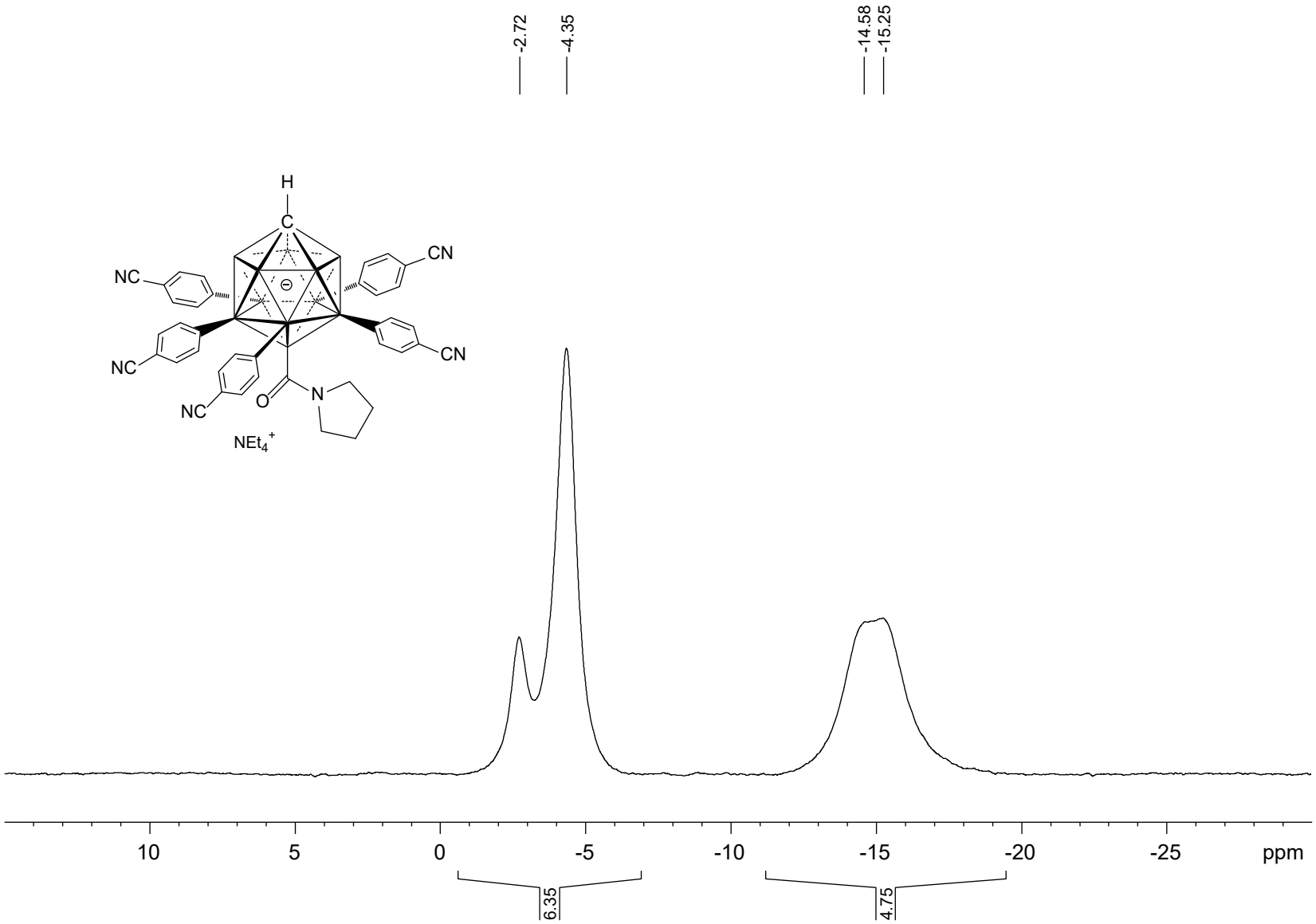
F2 - Acquisition Parameters
Date_           20220307
Time                21.14
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgig30
TD                 65536
SOLVENT          Acetone
NS                    16
DS                     0
SWH            12500.000 Hz
FIDRES             0.190735 Hz
AQ                 2.6214399 sec
RG                    71.8
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            500.1300100 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.00
```

jyj-220305-577-500M 12-CONC4H8-CB11H6(C6H4CN)5
11B 150M Hz 25 mg in acetone-d6



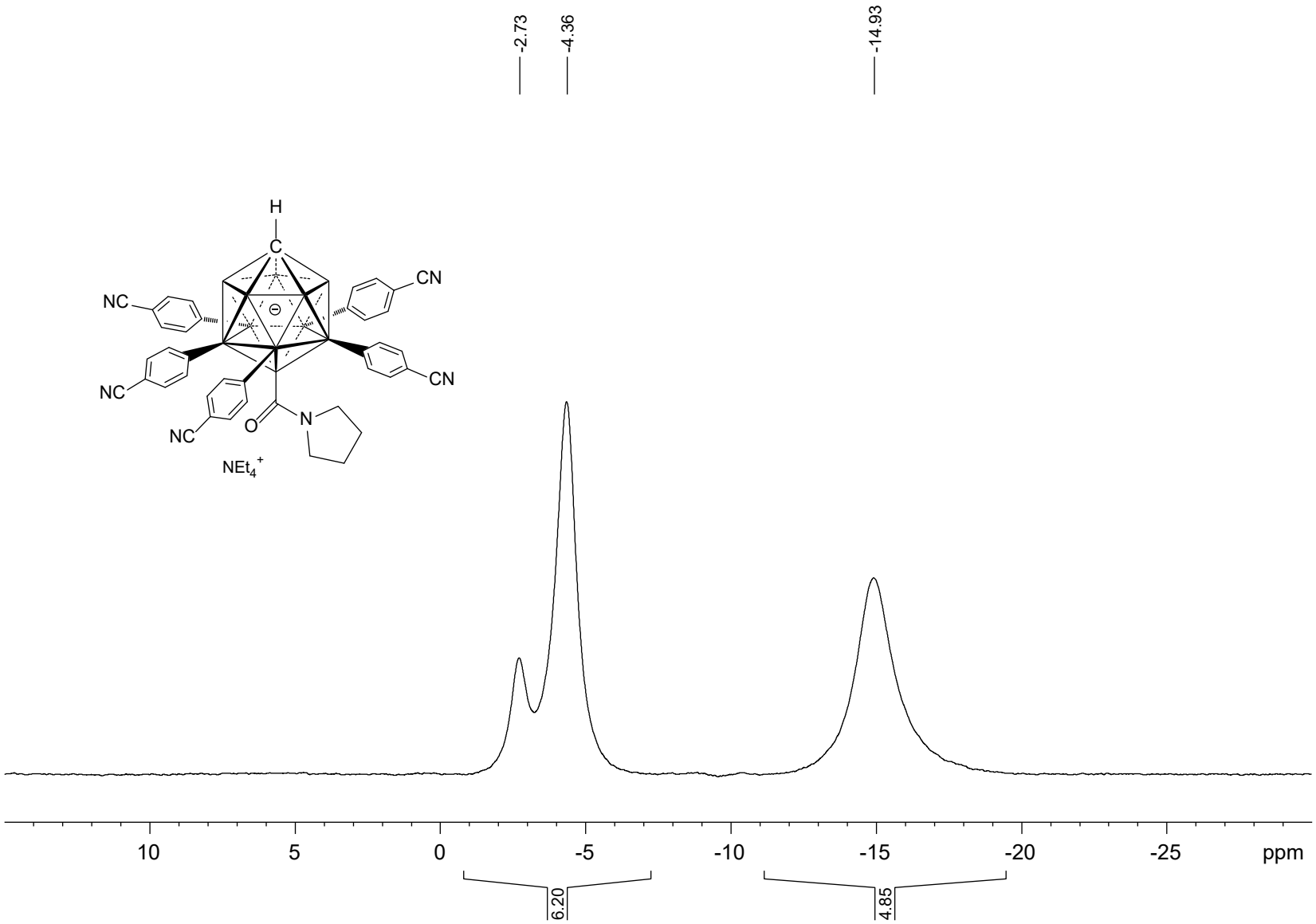

```
Current Data Parameters
NAME      jyj-220308-577-total-500M
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_          20220307
Time              21.18
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                64098
SOLVENT         Acetone
NS                   80
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
```

jyj-220305-577-500M 12-CONC4H8-CB11H6(C6H4CN)5
11B{1H} 150M Hz 25 mg in acetone-d6




```
Current Data Parameters
NAME      jyj-220308-577-total-500M
EXPNO                 4
PROCNO                1

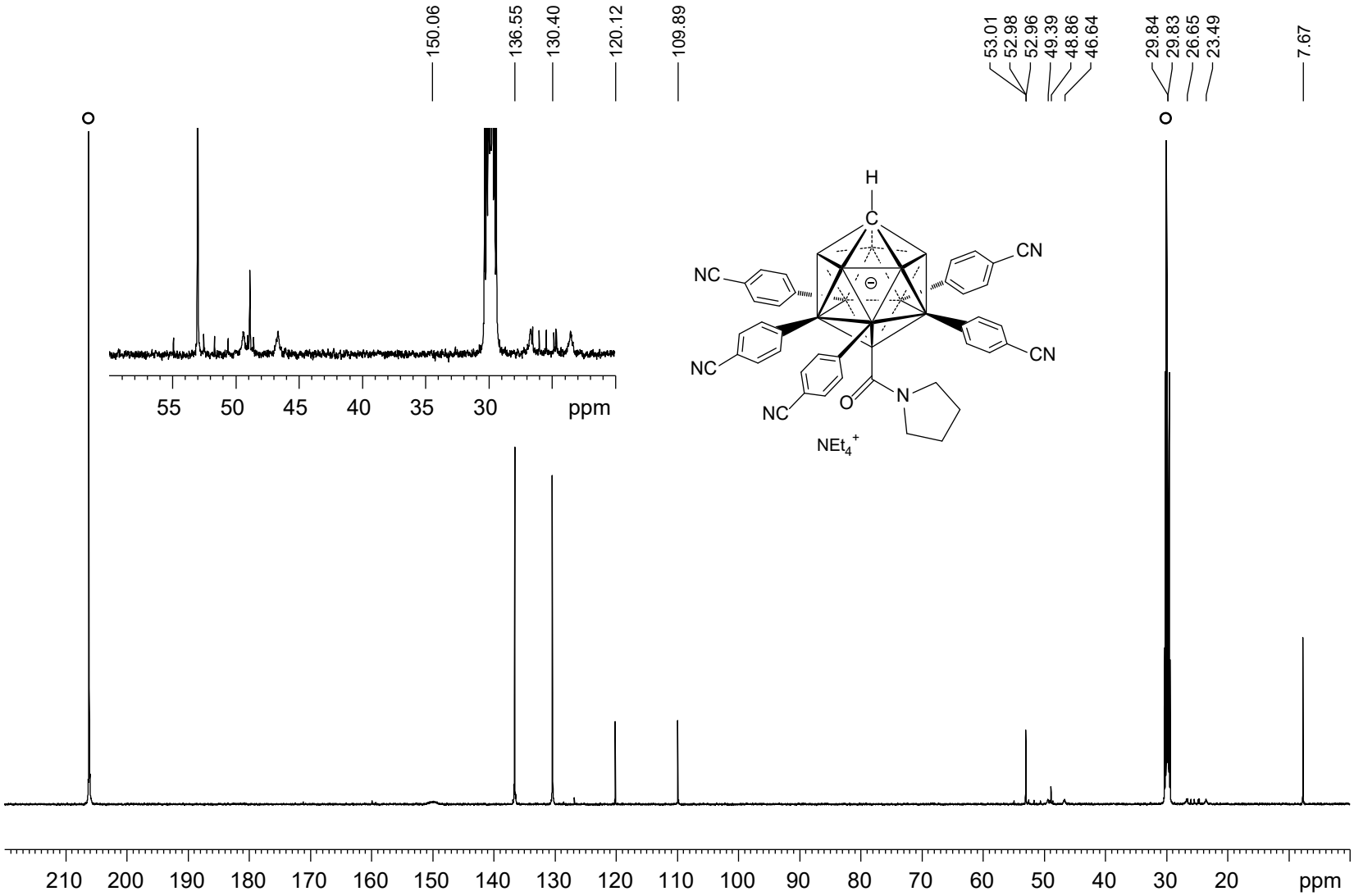
F2 - Acquisition Parameters
Date_          20220307
Time              21.22
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                   80
DS                    0
SWH           32051.281 Hz
FIDRES         0.489064 Hz
AQ            1.0223616 sec
RG                  203
DW               15.600 usec
DE                6.50 usec
TE               296.9 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         0.42394000 W
PLW13         0.27131999 W
SFO2        500.1325007 MHz

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

jyj-220305-577-500M 12-CONC4H8-CB11H6(C6H4CN)5
13C 125M Hz 25 mg in acetone-d6



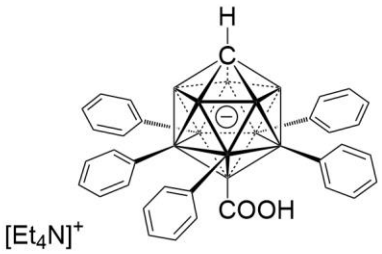

```
Current Data Parameters
NAME      jyj-220308-577-total-500M
EXPNO                 5
PROCNO                1

F2 - Acquisition Parameters
Date_          20220308
Time              15.46
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT         Acetone
NS                 2100
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               295.4 K
D1            1.50000000 sec
D11           0.03000000 sec

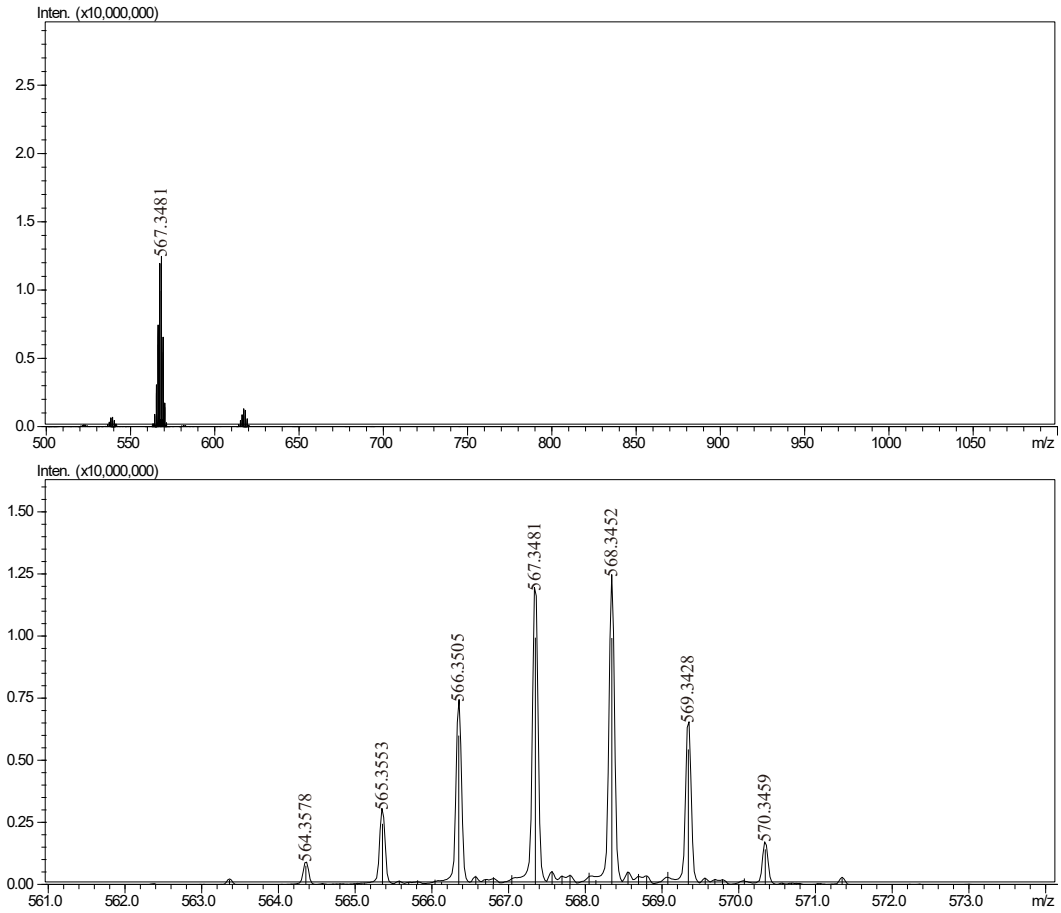
======== CHANNEL f1 ========
NUC1                13C
P1               10.65 usec
PLW1         95.00000000 W
SFO1        125.7716224 MHz

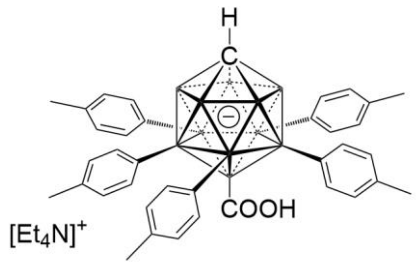
======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                1H
PCPD2            80.00 usec
PLW2         19.00000000 W
PLW12         0.42394000 W
PLW13         0.27131999 W
SFO2        500.1320005 MHz

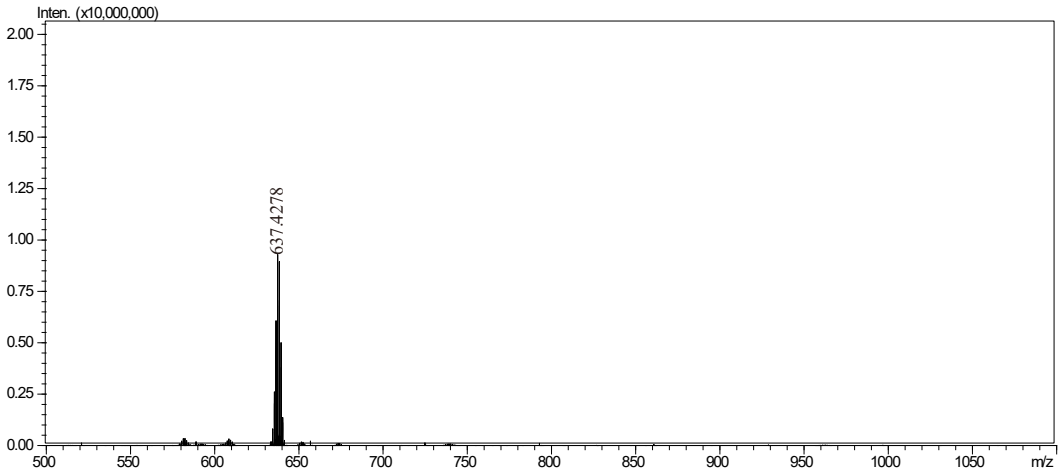
F2 - Processing parameters
SI                 32768
SF          125.7576822 MHz
WDW                   EM
SSB                    0
LB                2.00 Hz
GB                     0
PC                1.40
```

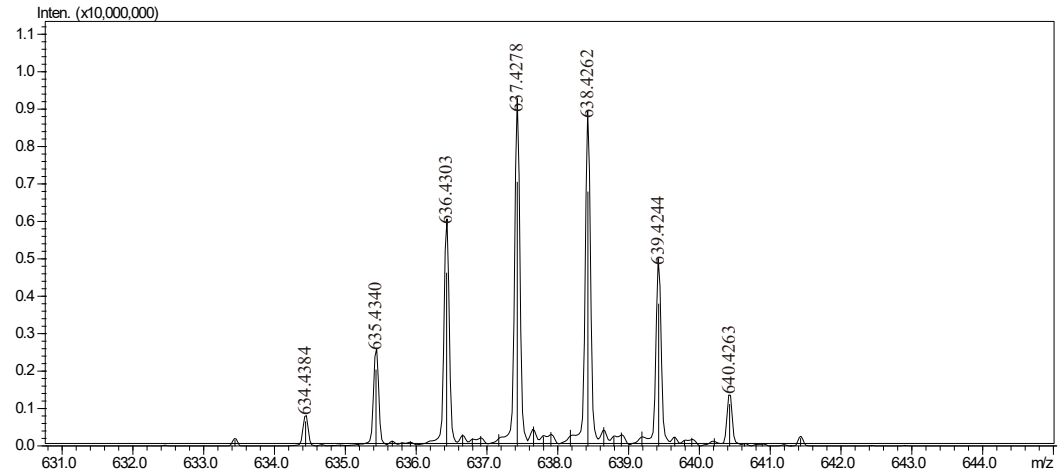

H
C
COOH

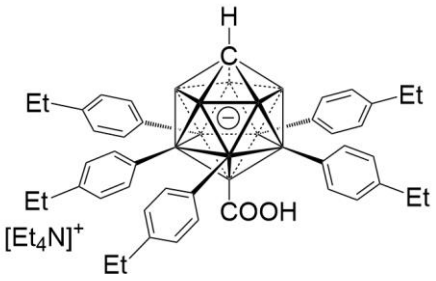
$[Et_4N]^+$

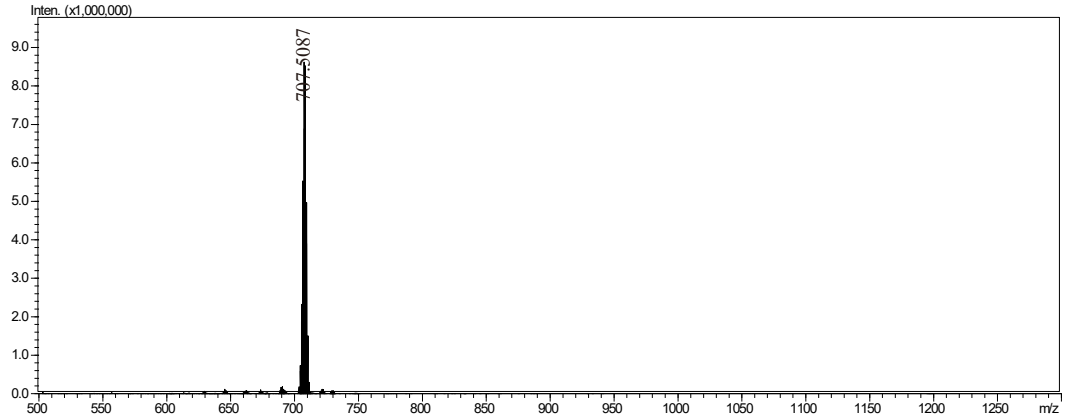

Inten. (x10,000,000)
567.3481
m/z
Inten. (x10,000,000)
564.3578
565.3553
566.3505
567.3481
568.3452
569.3428
570.3459
m/z

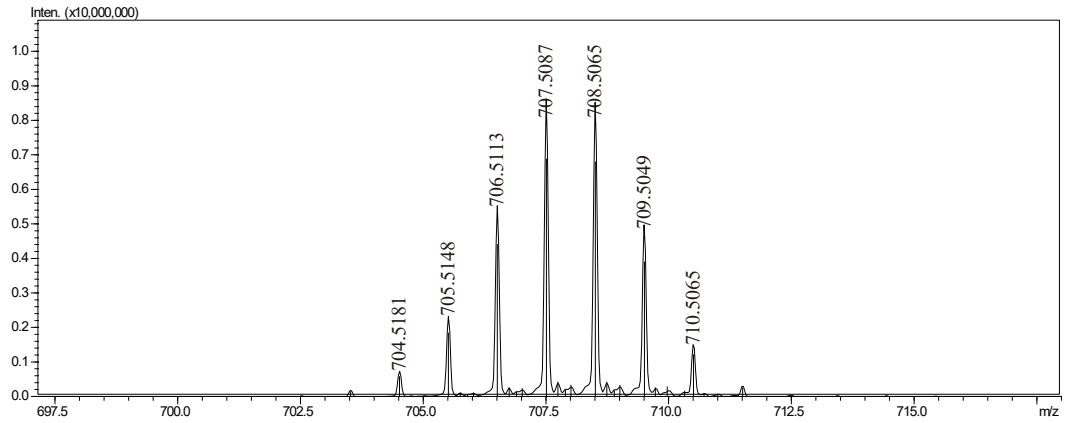

H
C
COOH
[Et4N]+

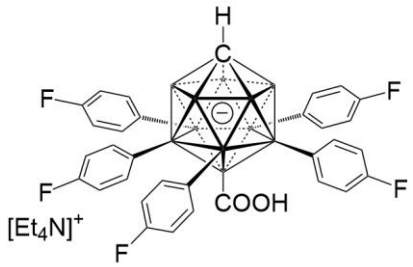

Inten. (x10,000,000)
637.4278
m/z

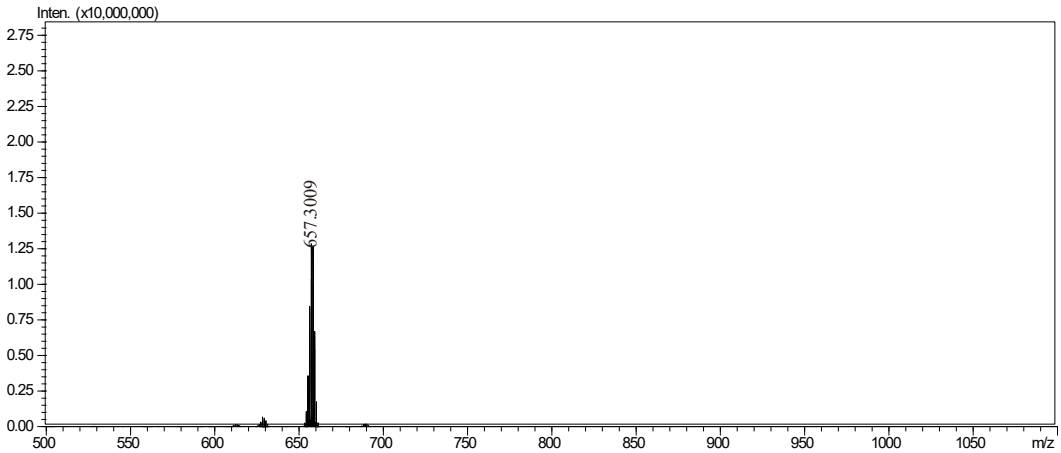

Inten. (x10,000,000)
634.4384
635.4340
636.4303
637.4278
638.4262
639.4244
640.4263
m/z

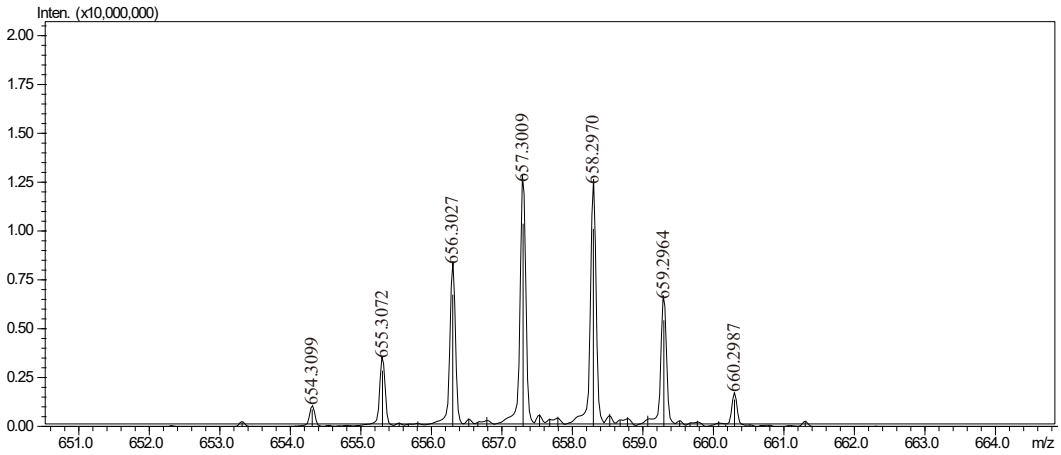

H
C
Et
Et
Et
Et
Et
COOH
[Et4N]+

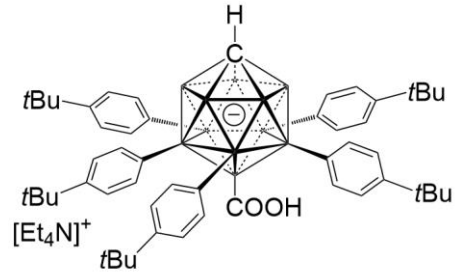

Inten. (x1,000,000)
707.5087
m/z

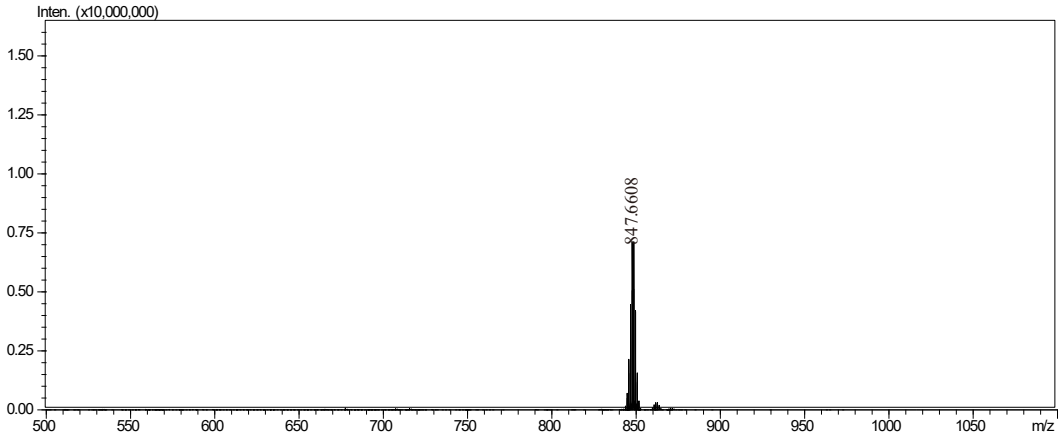

Inten. (x10,000,000)
704.5181
705.5148
706.5113
707.5087
708.5065
709.5049
710.5065
m/z

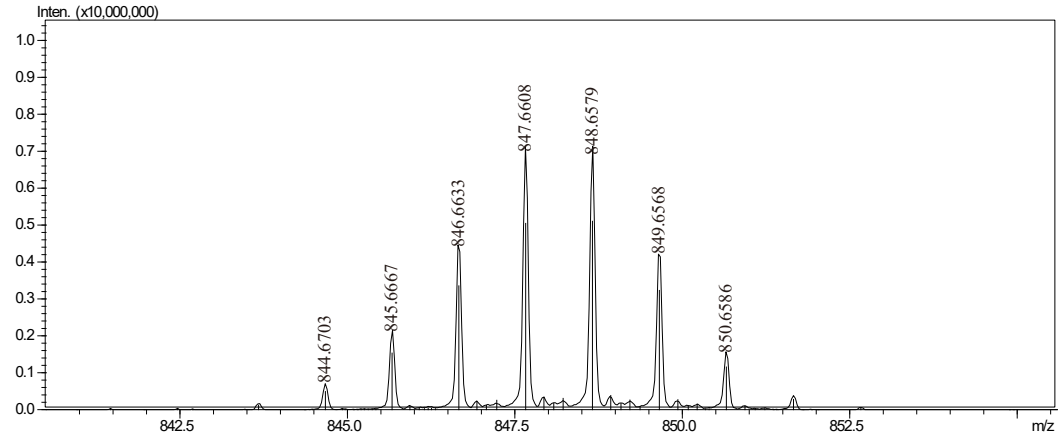

H
C
F
F
F
F
F
COOH
[Et4N]+

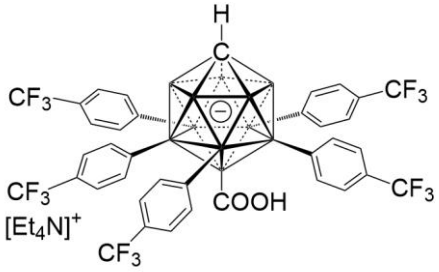

Inten. (x10,000,000)
657.3009
m/z

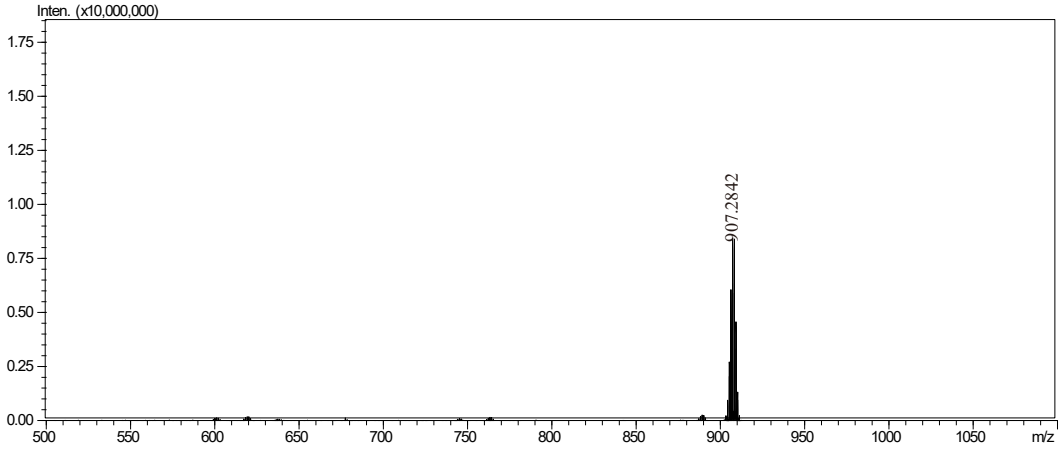

Inten. (x10,000,000)
654.3099
655.3072
656.3027
657.3009
658.2970
659.2964
660.2987
m/z

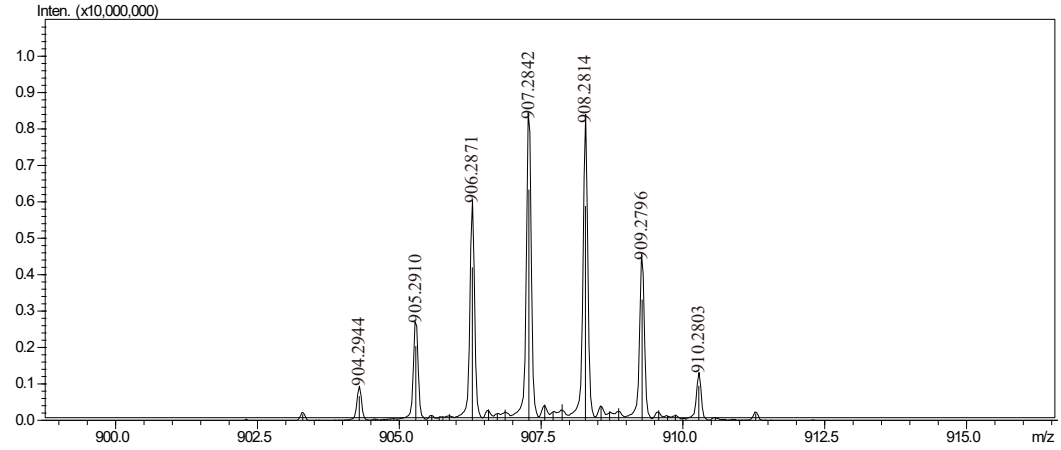

H
C
tBu
tBu
tBu
tBu
COOH
[Et4N]+
tBu

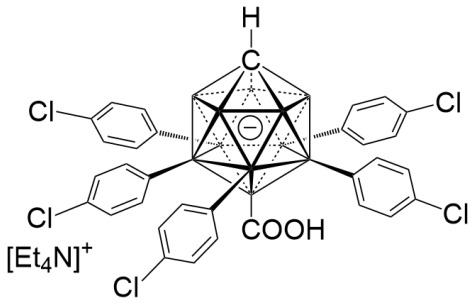

Inten. (x10,000,000)
1.50
1.25
1.00
0.75
0.50
0.25
0.00
847.6608
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z

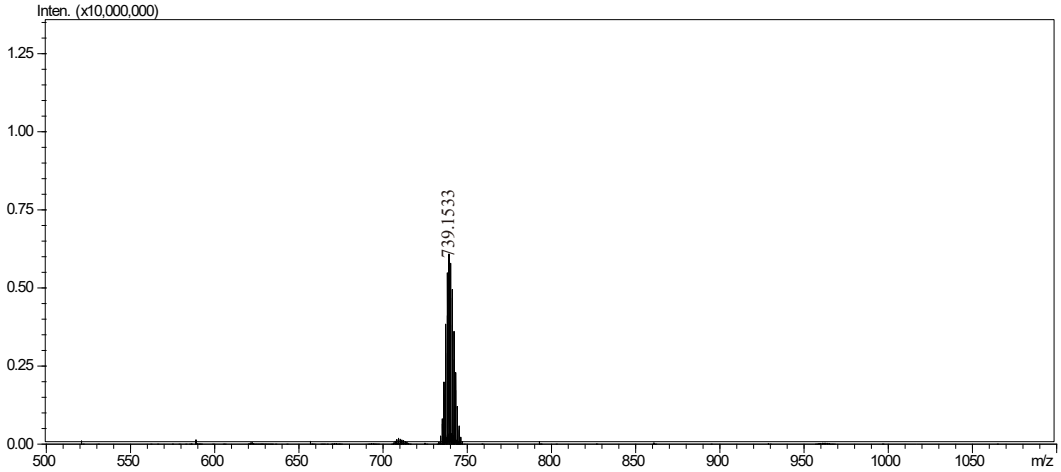

Inten. (x10,000,000)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
844.6703
845.6667
846.6633
847.6608
848.6579
849.6568
850.6586
842.5
845.0
847.5
850.0
852.5
m/z

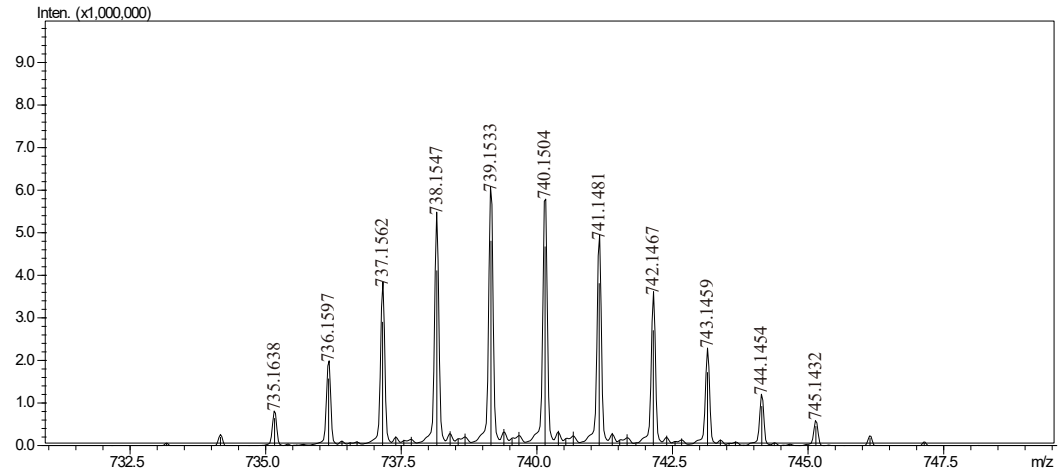

H
C
CF3
CF3
CF3
CF3
COOH
[Et4N]+
CF3

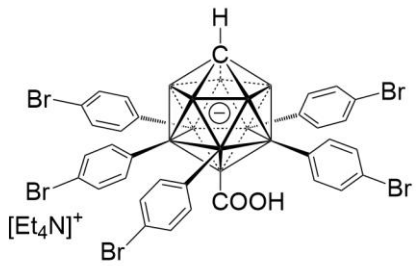

Inten. (x10,000,000)
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
907.2842
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z

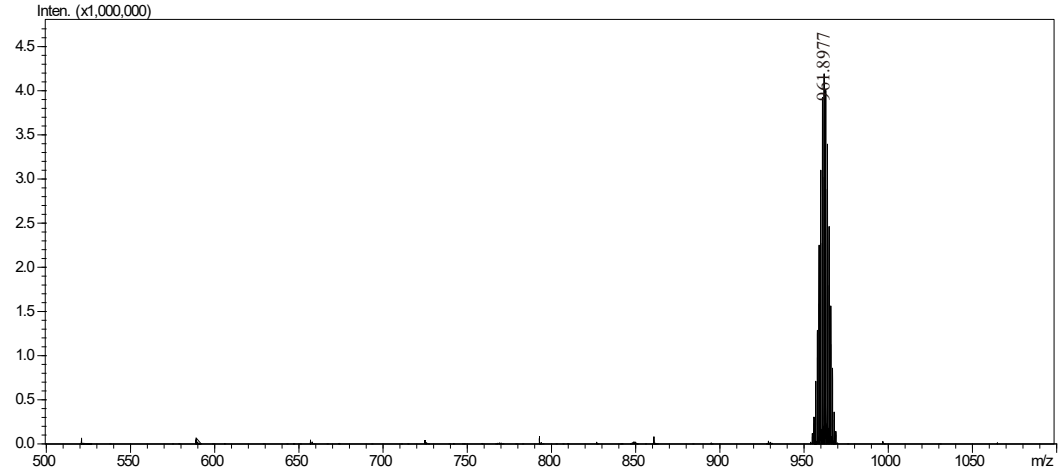

Inten. (x10,000,000)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
904.2944
905.2910
906.2871
907.2842
908.2814
909.2796
910.2803
900.0
902.5
905.0
907.5
910.0
912.5
915.0
m/z

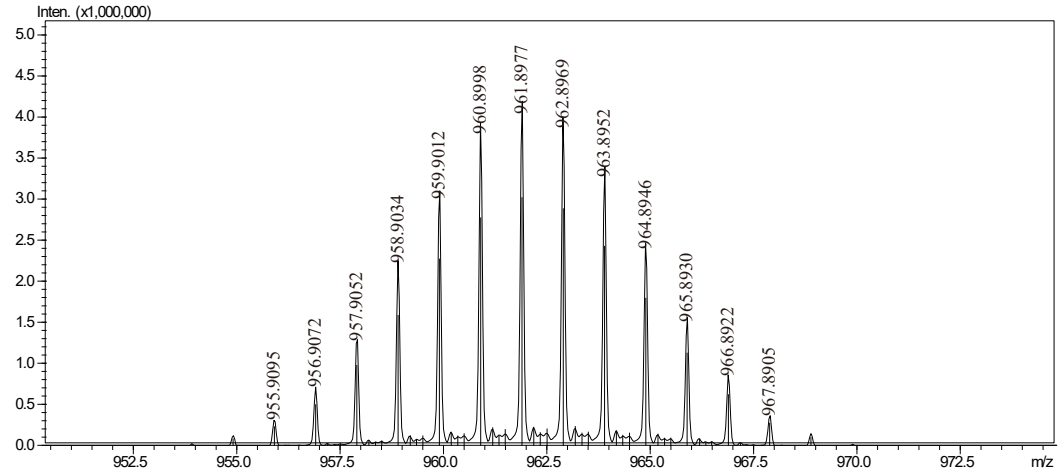

H
C
Cl
Cl
Cl
Cl
COOH
[Et4N]+
Cl


Inten. (x10,000,000)
1.25
1.00
0.75
0.50
0.25
0.00
739.1533
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z


Inten. (x1,000,000)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
735.1638
736.1597
737.1562
738.1547
739.1533
740.1504
741.1481
742.1467
743.1459
744.1454
745.1432
732.5
735.0
737.5
740.0
742.5
745.0
747.5
m/z


H
C
Br
Br
Br
Br
COOH
[Et4N]+
Br


Inten. (x1,000,000)
961.8977
m/z


Inten. (x1,000,000)
955.9095
956.9072
957.9052
958.9034
959.9012
960.8998
961.8977
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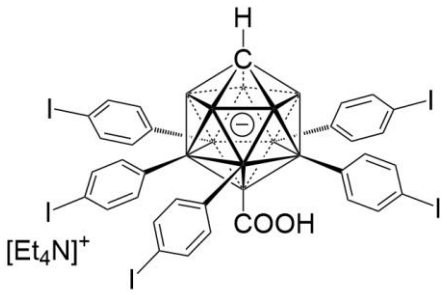
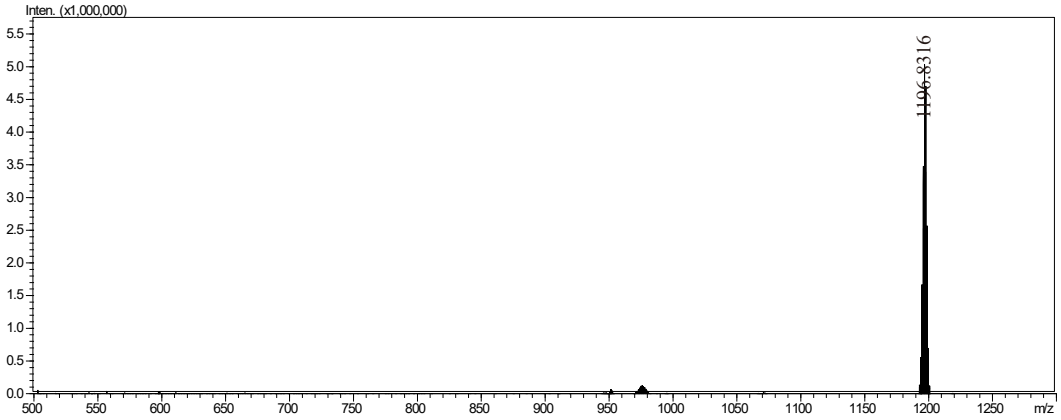
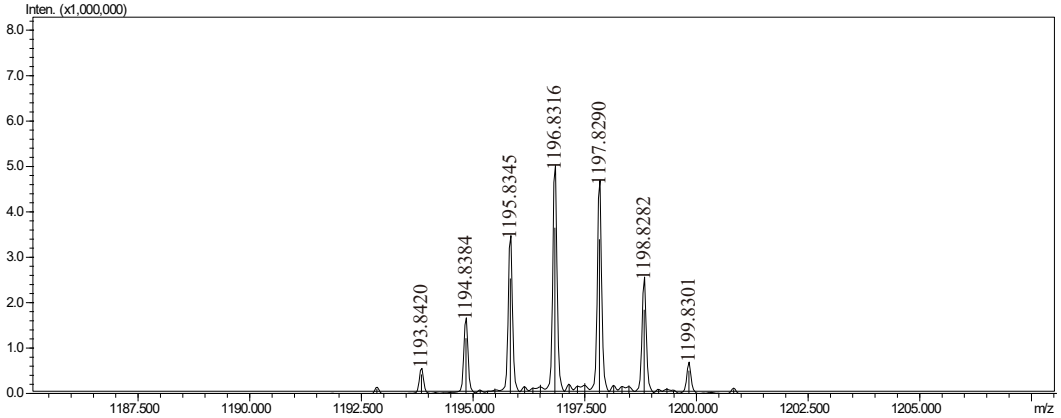
964.8946
965.8930
966.8922
967.8905
m/z


H
C
I
I
I
I
COOH
[Et4N]+


Inten. (x1,000,000)
1196.8316
m/z


Inten. (x1,000,000)
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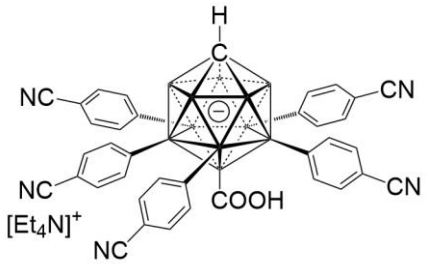
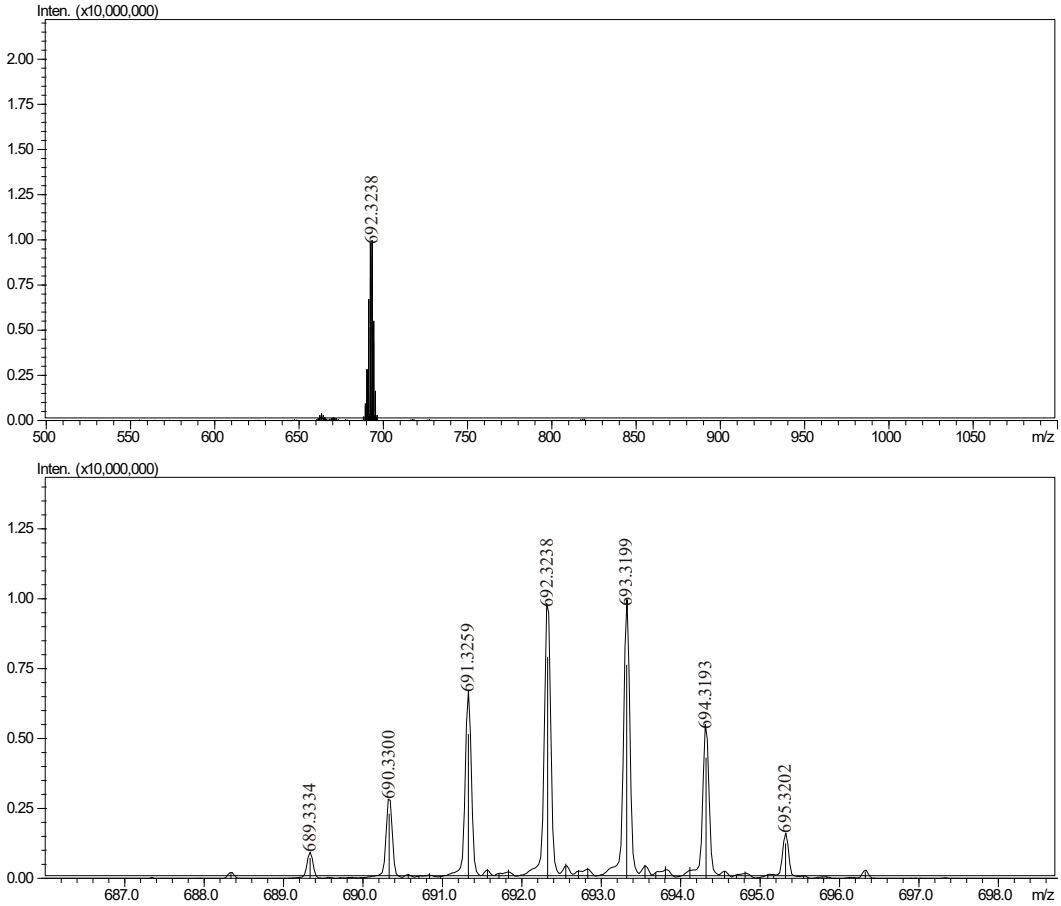
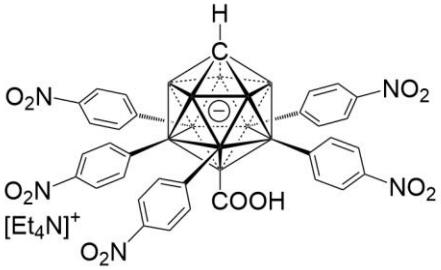
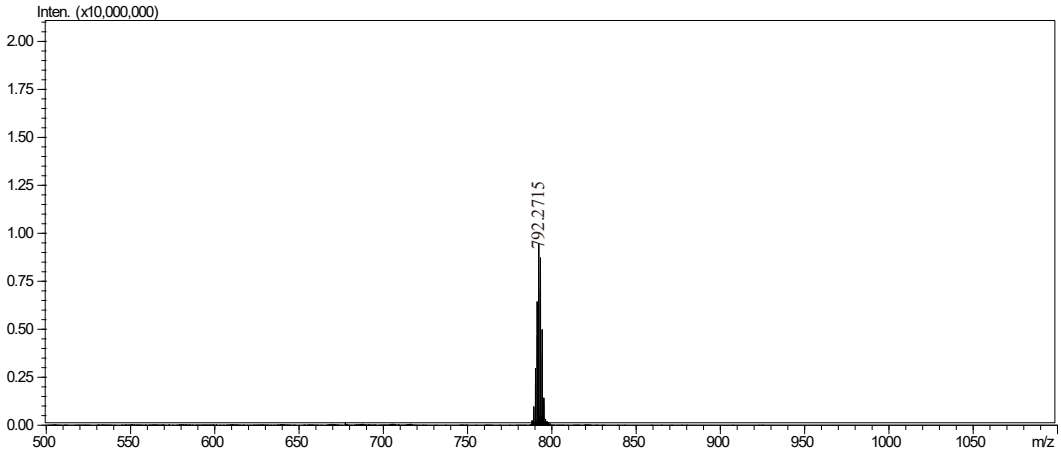
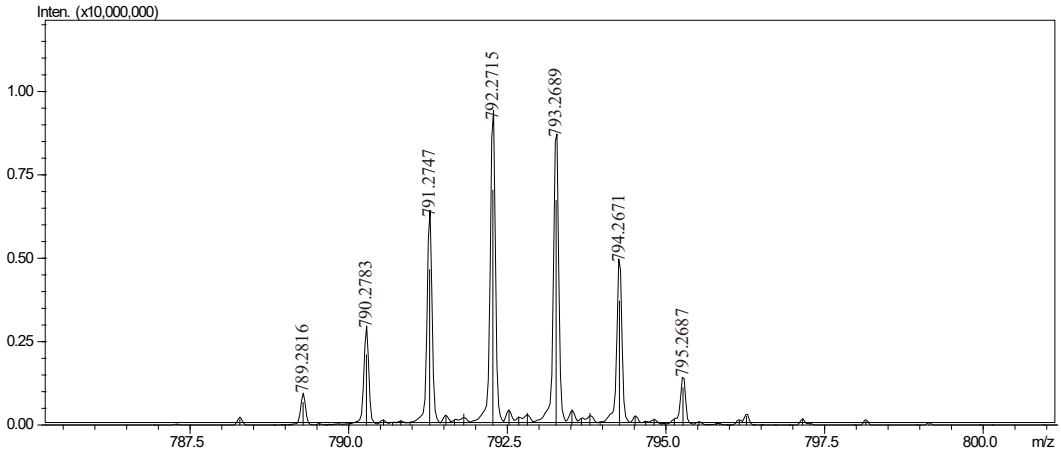
1194.8384
1195.8345
1196.8316
1197.8290
1198.8282
1199.8301
m/z

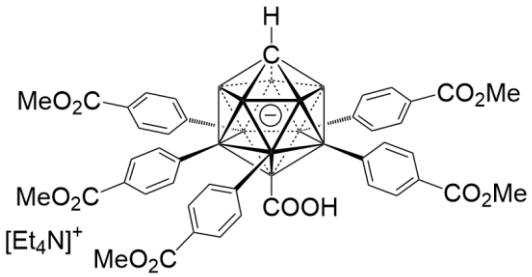

H
C
NC
CN
NC
CN
COOH
[Et4N]+
NC

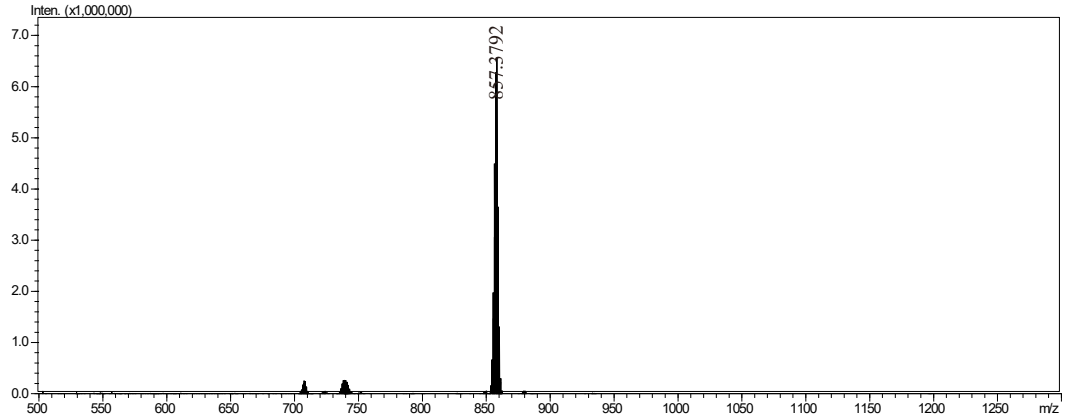

Inten. (x10,000,000)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
692.3238
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z
Inten. (x10,000,000)
1.25
1.00
0.75
0.50
0.25
0.00
689.3334
690.3300
691.3259
692.3238
693.3199
694.3193
695.3202
687.0
688.0
689.0
690.0
691.0
692.0
693.0
694.0
695.0
696.0
697.0
698.0
m/z

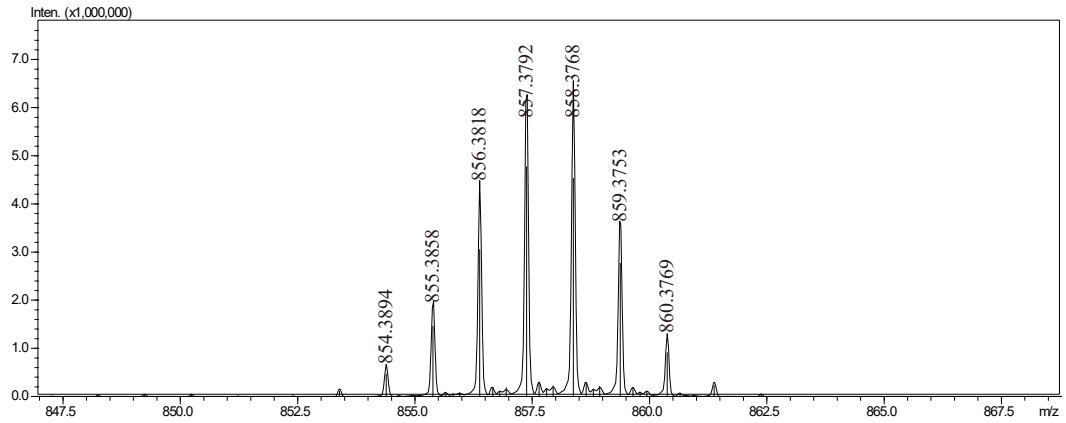

H
C
O2N
NO2
O2N
NO2
COOH
[Et4N]+
O2N

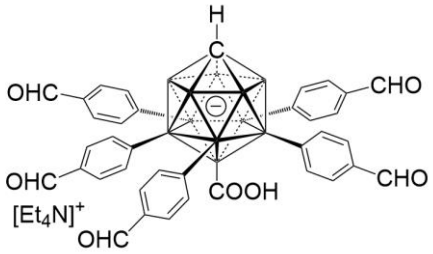

Inten. (x10,000,000)
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
792.2715
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z

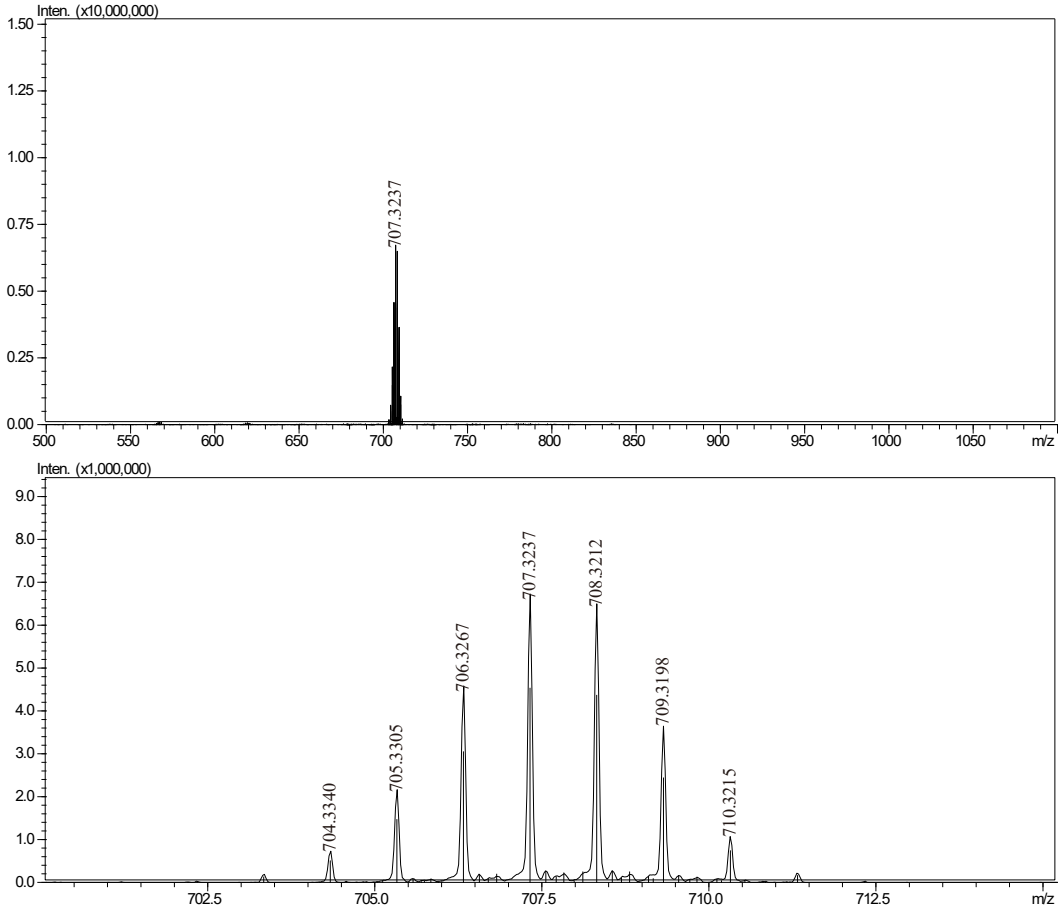

Inten. (x10,000,000)
1.00
0.75
0.50
0.25
0.00
789.2816
790.2783
791.2747
792.2715
793.2689
794.2671
795.2687
787.5
790.0
792.5
795.0
797.5
800.0
m/z

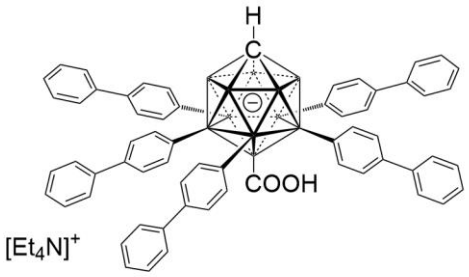

H
C
MeO2C
CO2Me
MeO2C
CO2Me
COOH
[Et4N]+
MeO2C

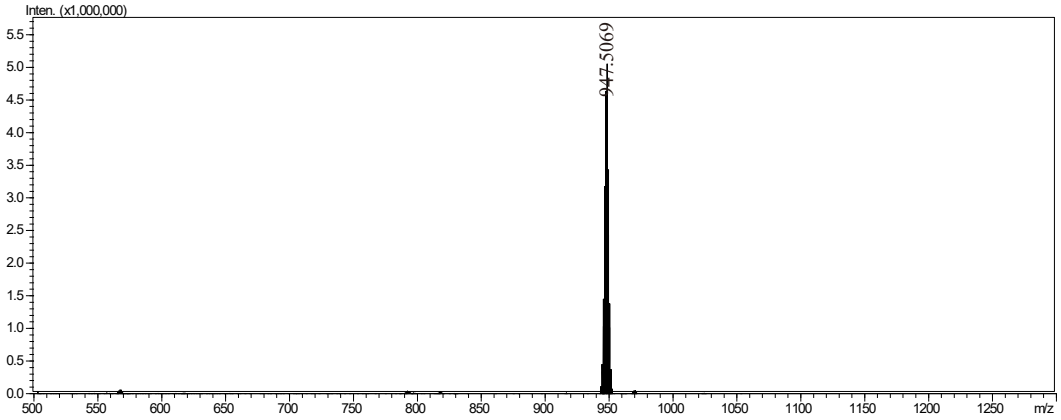

Inten. (x1,000,000)
857.3792
m/z

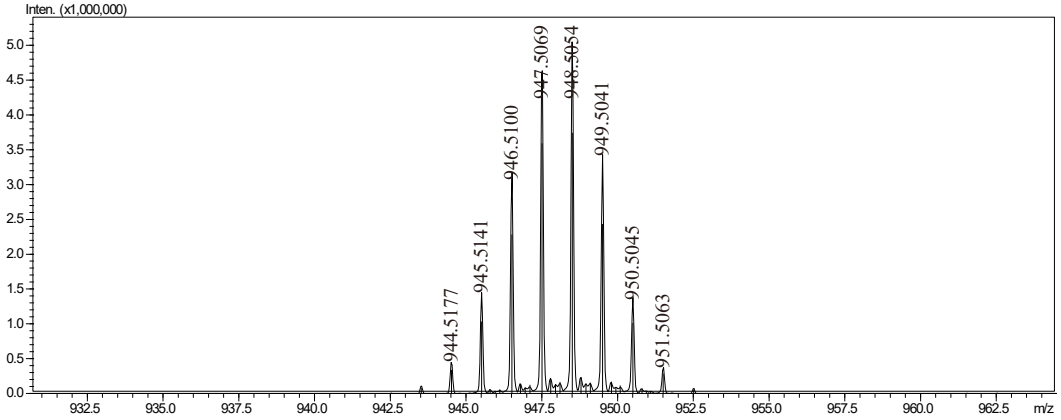

Inten. (x1,000,000)
854.3894
855.3858
856.3818
857.3792
858.3768
859.3753
860.3769
m/z


H
C
OHC
CHO
OHC
CHO
COOH
[Et4N]+
OHC


Inten. (x10,000,000)
1.50
1.25
1.00
0.75
0.50
0.25
0.00
707.3237
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z
Inten. (x1,000,000)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
704.3340
705.3305
706.3267
707.3237
708.3212
709.3198
710.3215
702.5
705.0
707.5
710.0
712.5
m/z


H
C
COOH
[Et4N]+


Inten. (x1,000,000)
947.5069
m/z


Inten. (x1,000,000)
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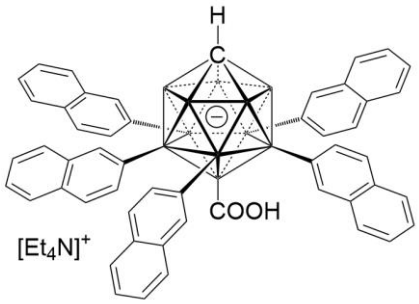
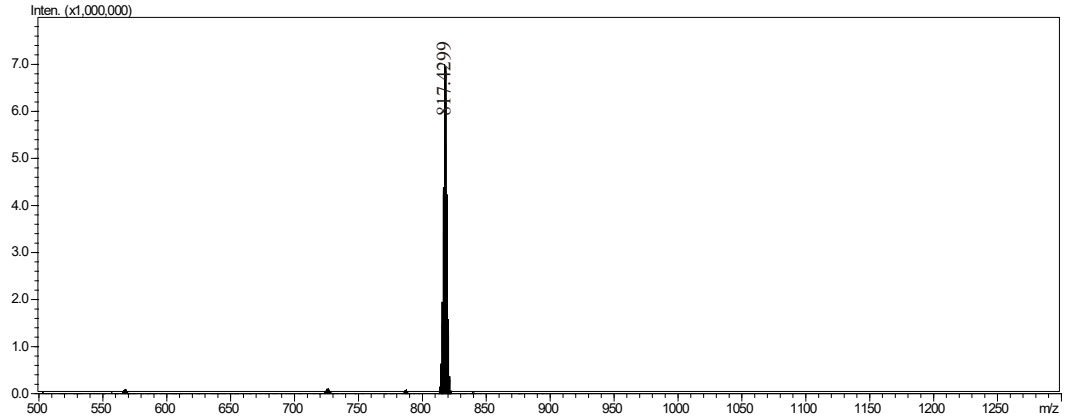
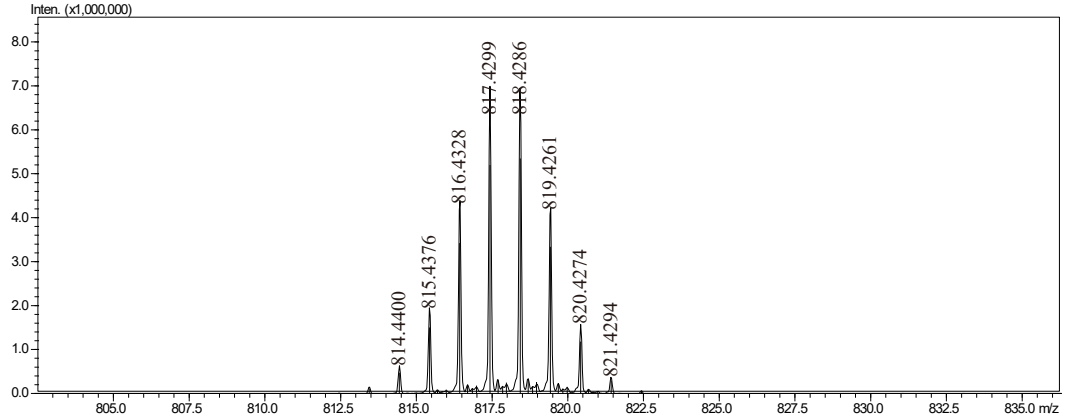
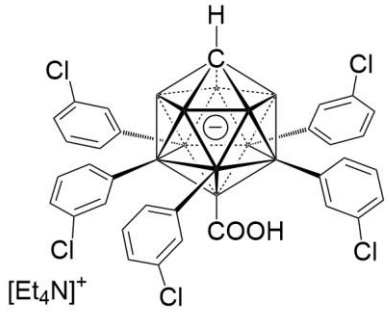
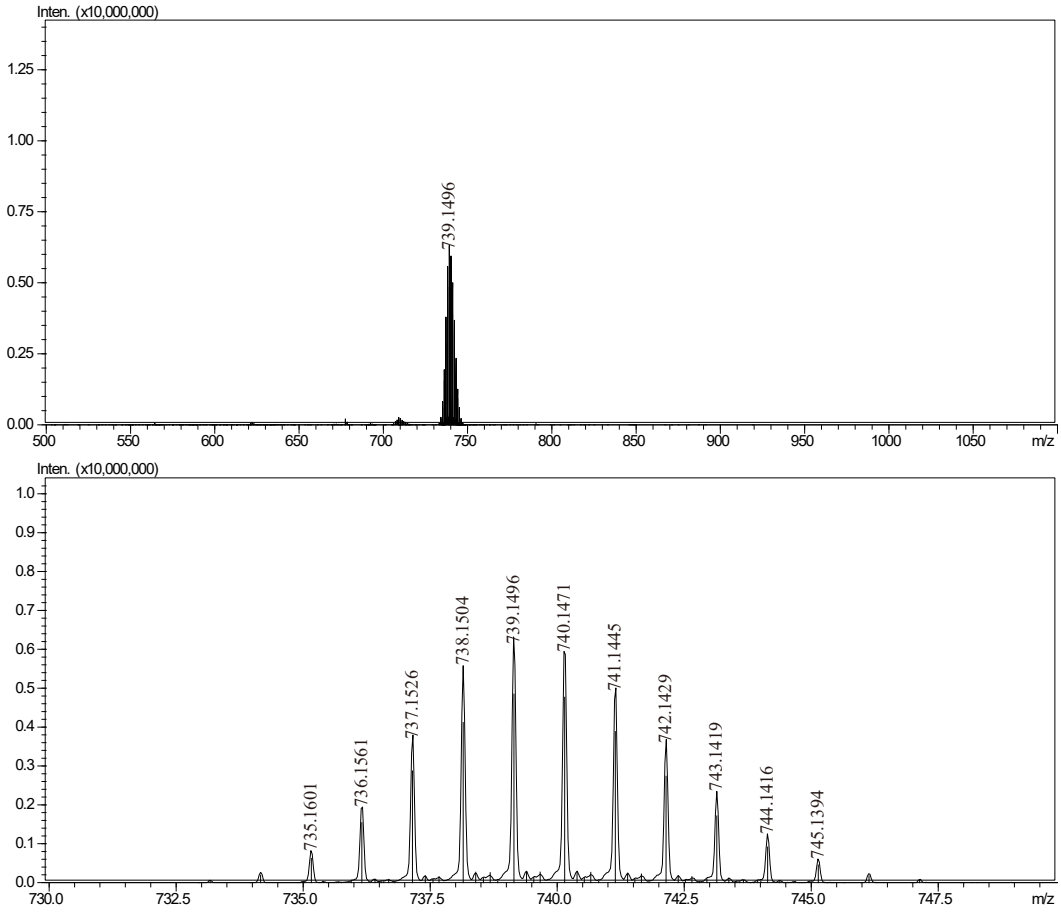
945.5141
946.5100
947.5069
948.5054
949.5041
950.5045
951.5063
m/z

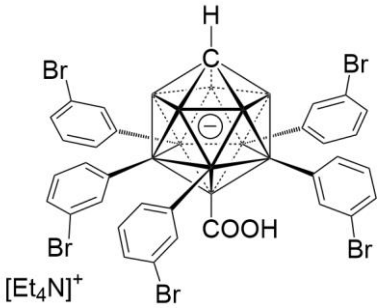

H
C
COOH
[Et4N]+

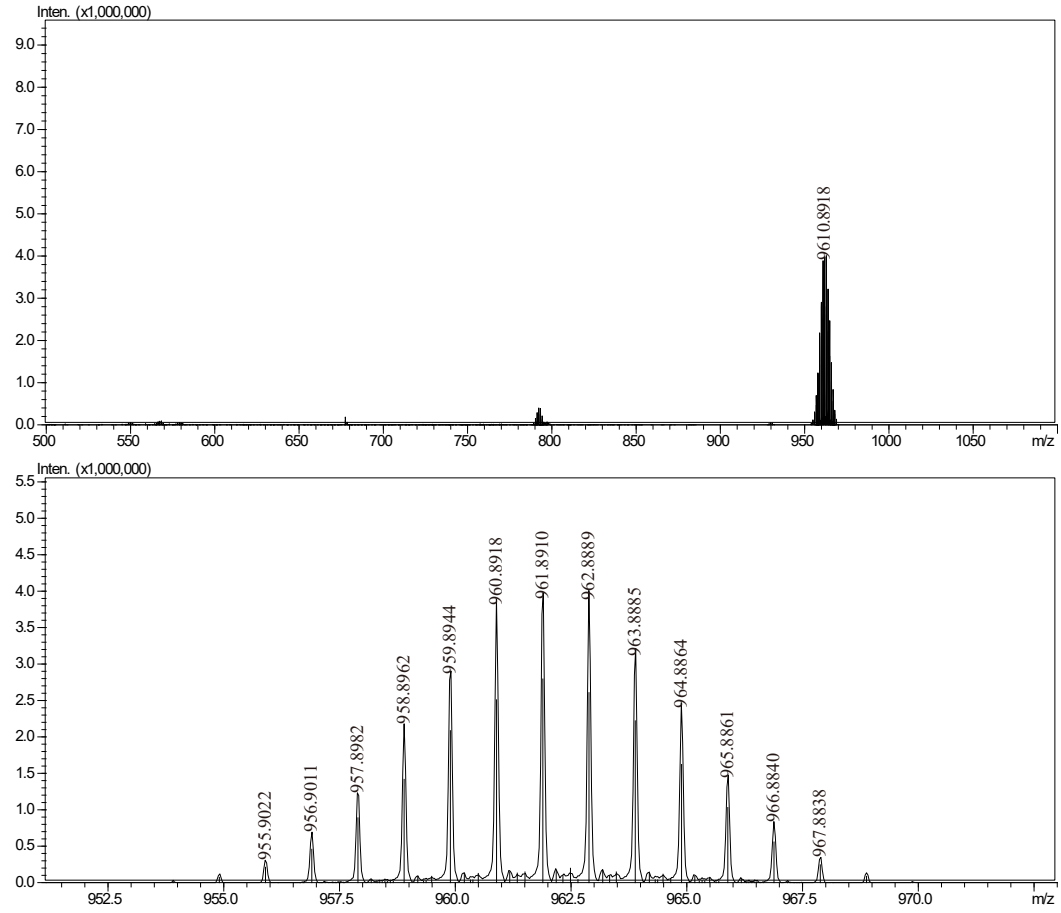

Inten. (x1,000,000)
817.4299
m/z

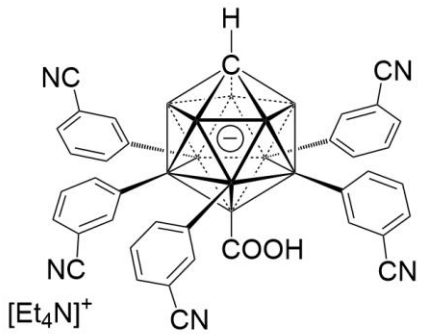

Inten. (x1,000,000)
814.4400
815.4376
816.4328
817.4299
818.4286
819.4261
820.4274
821.4294
m/z

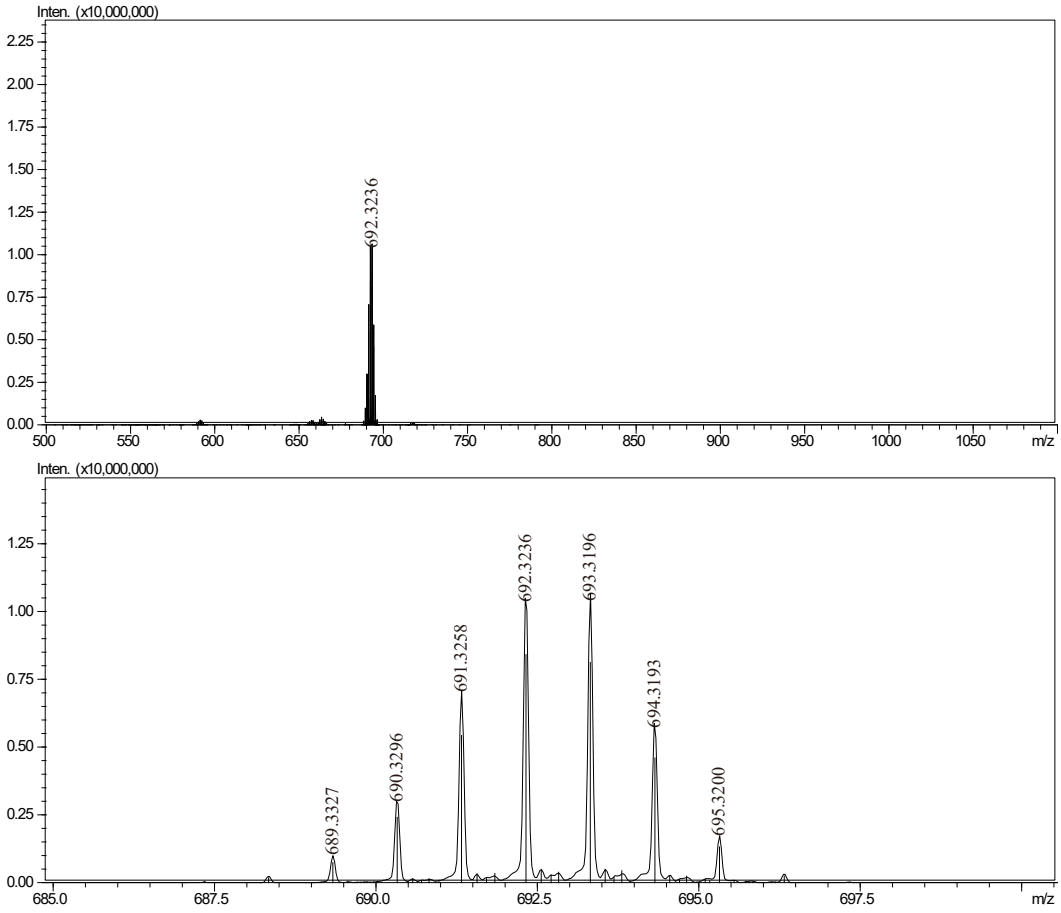

H
C
Cl
Cl
COOH
Cl
Cl
Cl
[Et4N]+

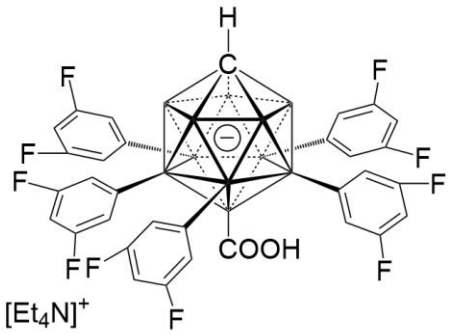

Inten. (x10,000,000)
1.25
1.00
0.75
0.50
0.25
0.00
739.1496
500
550
600
650
700
750
800
850
900
950
1000
1050
m/z
Inten. (x10,000,000)
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
735.1601
736.1561
737.1526
738.1504
739.1496
740.1471
741.1445
742.1429
743.1419
744.1416
745.1394
730.0
732.5
735.0
737.5
740.0
742.5
745.0
747.5
m/z

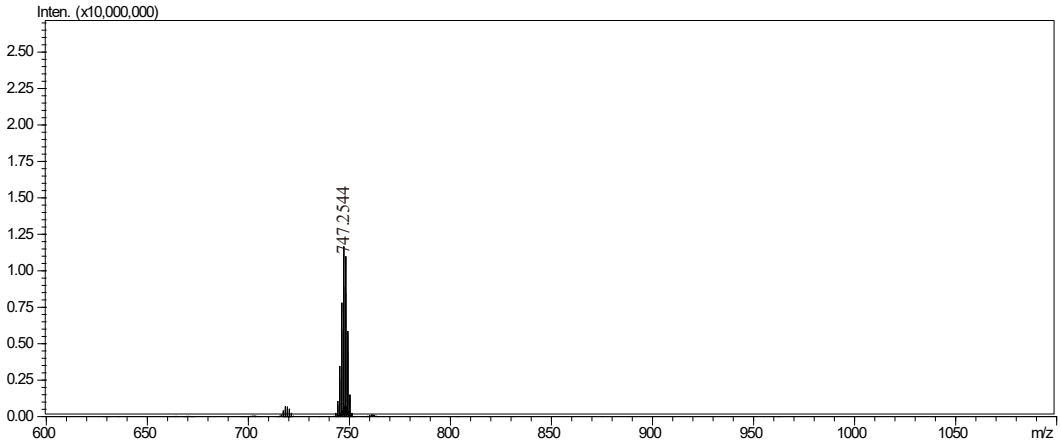

H
C
Br
Br
Br
Br
Br
COOH
[Et4N]+

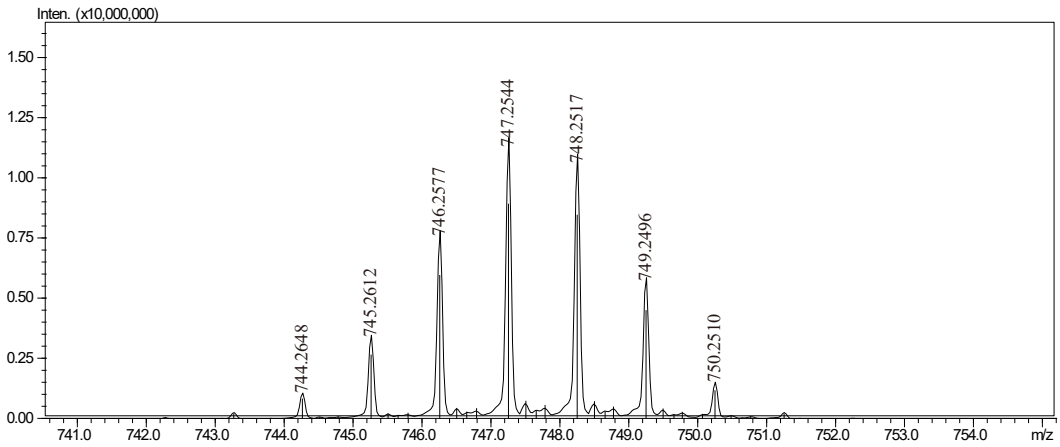

Inten. (x1,000,000)
9610.8918
m/z
Inten. (x1,000,000)
955.9022
956.9011
957.8982
958.8962
959.8944
960.8918
961.8910
962.8889
963.8885
964.8864
965.8861
966.8840
967.8838
m/z


H
C
NC
CN
COOH
NC
CN
CN
[Et4N]+


Inten. (x10,000,000)
692.3236
m/z
Inten. (x10,000,000)
689.3327
690.3296
691.3258
692.3236
693.3196
694.3193
695.3200
m/z


H
C
F
F
F
F
F
F
F
F
F
COOH
F
[Et4N]+


Inten. (x10,000,000)
2.50
2.25
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
747.2544
600
650
700
750
800
850
900
950
1000
1050
m/z


Inten. (x10,000,000)
1.50
1.25
1.00
0.75
0.50
0.25
0.00
744.2648
745.2612
746.2577
747.2544
748.2517
749.2496
750.2510
741.0
742.0
743.0
744.0
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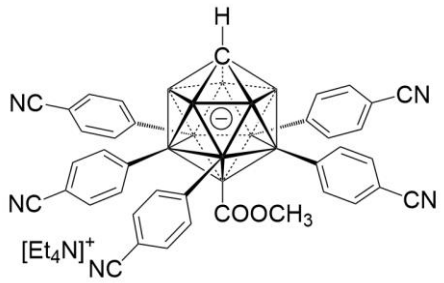
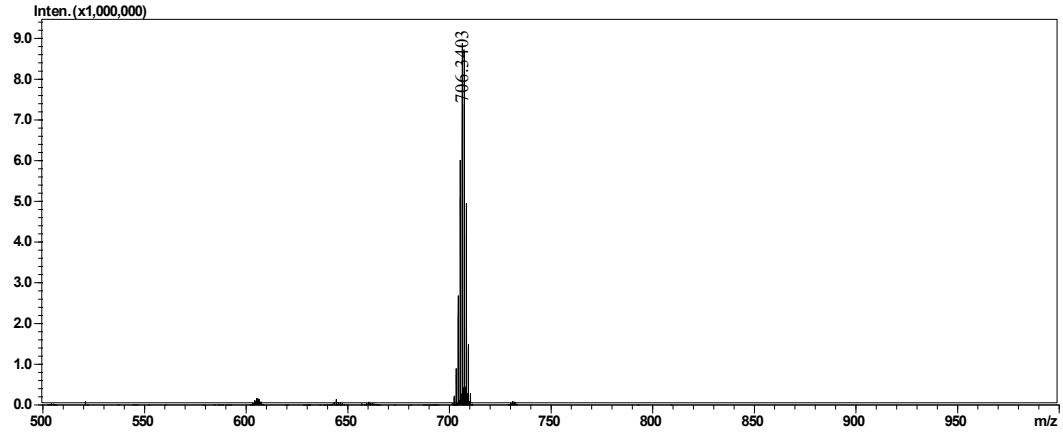
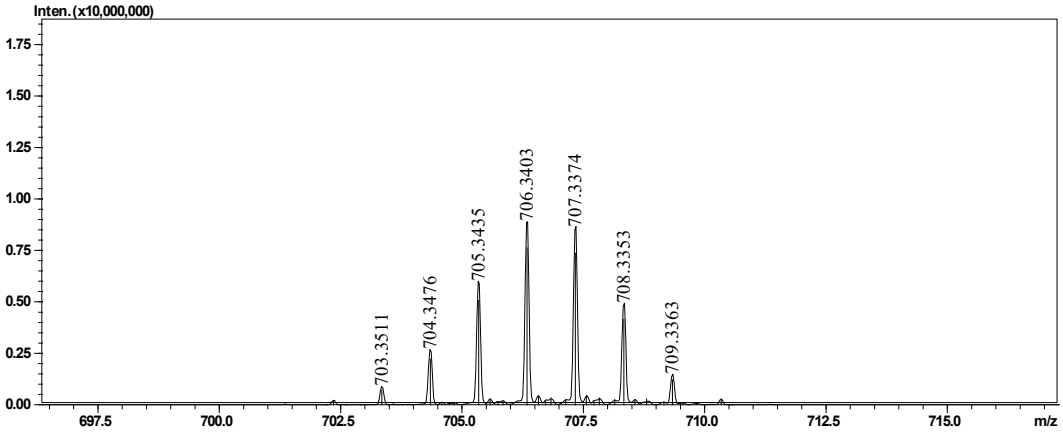
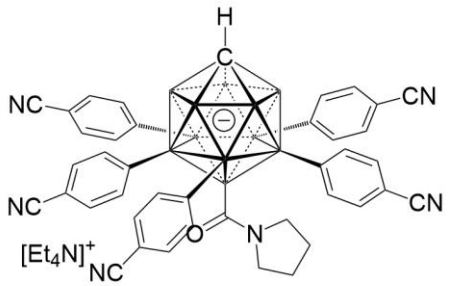
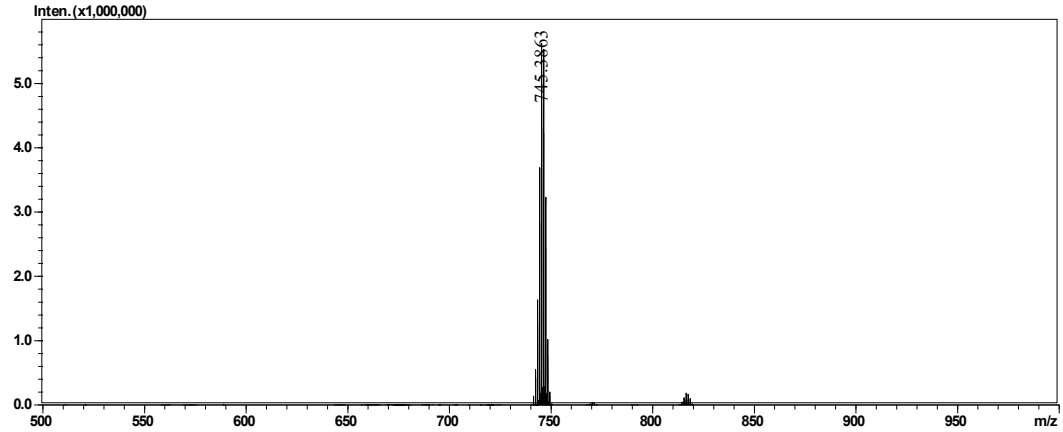
750.0
751.0
752.0
753.0
754.0
m/z

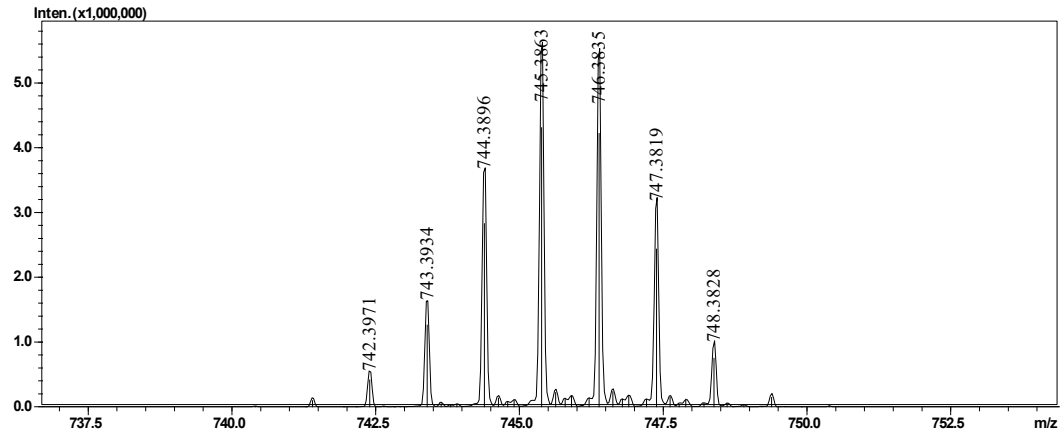

H
C
NC
CN
NC
CN
COOCH3
[Et4N]+
NC


Inten.(x1,000,000)
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
706.3403
500
550
600
650
700
750
800
850
900
950
m/z


Inten.(x10,000,000)
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
703.3511
704.3476
705.3435
706.3403
707.3374
708.3353
709.3363
697.5
700.0
702.5
705.0
707.5
710.0
712.5
715.0
m/z


H
C
NC
CN
NC
CN
O
N
[Et4N]+
NC


Inten.(x1,000,000)
745.3863
5.0
4.0
3.0
2.0
1.0
0.0
500
550
600
650
700
750
800
850
900
950
m/z


Inten.(x1,000,000)
742.3971
743.3934
744.3896
745.3863
746.3835
747.3819
748.3828
5.0
4.0
3.0
2.0
1.0
0.0
737.5
740.0
742.5
745.0
747.5
750.0
752.5
m/z

Document: 2021-11-24 (VarioMICRO) from: 2021-11-25 14:57:58

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Text report

Name	Method	Weight [mg]	N Area	C Area	H Area	N [%]	C [%]	H [%]
JYJ-3-CN	2mgChem70s	1.826	5 383	25 058	8 017	9.90	64.92	5.91
JYJ-3-CN	2mgChem70s	1.881	5 572	25 898	8 153	9.95	65.11	5.84

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2021-12-2

Text report

Name	Method	Weight [mg]	N Area	C Area	H Area	N [%]	C [%]	H [%]
JYJ-2F	2mgChem80s	1.828	816	21 197	6 806	1.43	54.70	4.96
JYJ-2F	2mgChem80s	1.816	871	21 057	6 712	1.54	54.70	4.92
JYJ-Br	2mgChem70s	1.926	760	17 790	6 347	1.27	43.55	4.37
JYJ-Br	2mgChem70s	1.838	714	16 956	6 059	1.25	43.49	4.36

Name: eassuperuser, Access: VarioMICRO superuser

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