Supplementary Information

Rhodium Catalyzed Cascade Cyclization Featuring B-H and C-H Activation: One-Step Construction of Carborane-Fused *N*-Polyheterocycles

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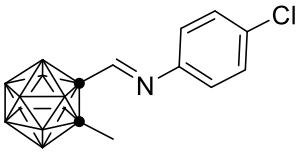
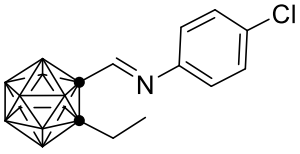
General Procedures. All reactions were carried out in flame-dried glassware using standard Schlenk techniques. All organic solvents were dried and distilled by standard methods prior to use. ^{1}H, ^{13}C, ^{11}B and ^{19}F NMR spectra were recorded on Bruker DPX 400/500 spectrometers at 400/500, 100/125, 128/160 and 376/470 MHz, respectively. All chemical shifts were reported in δ units with references to the residual solvent resonances of the deuterated solvents for proton and carbon chemical shifts, to external $BF_3 \cdot OEt_2$ (0.00 ppm) for boron chemical shifts, and to $CFCl_3$ (0.00 ppm) for fluorine chemical shifts. High resolution mass spectra (HRMS) were obtained on a Thermo Finnigan MAT 95 XL spectrometer. GC-MS analyses were performed on Agilent GC-MS 6890N. $Cu(OPiv)_2$ and *o*-carboranyl aldehydes were synthesized according to the reported procedures.[1,2] All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified.

Preparation of Starting Materials.

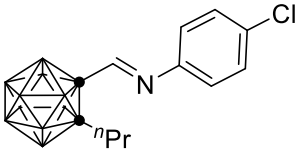
Preparation of Carboranyl *N*-Arylimines (1). A Representative Procedure. *o*-Carboranyl aldehyde (1.0 mmol) and aniline (1.5 mmol) were dissolved in toluene (3 ml) in the presence of molecular sieves (3 Å, 100 mg). The resulting solution was stirred at 100 ^{o}C for 18 h. After cooling to room temperature, the reaction mixture was filtered through a pad of Celite and concentrated. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (100 : 1 in V/V) as eluent to afford carboranyl *N*-arylimines **1**.



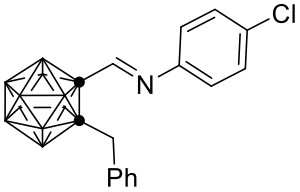
1a: Yield 93%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (s, 1H) (imine C*H*), 7.37 (d, *J* = 8.8 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H) (aryl C*H*), 2.10 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 152.3 (imine *C*H), 147.0, 134.0, 129.7, 122.3 (aryl *C*), 75.3 (cage *C*), 23.7 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.2 (1B), -5.9 (1B), -9.7 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}ClN$ $[M]^+$: 295.2125. Found: 295.2125.



1b: Yield 82%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (s, 1H) (imine C*H*), 7.36 (d, *J* = 8.8 Hz, 2H), 7.06 (d, *J* = 8.8 Hz, 2H) (aryl C*H*), 2.36 (q, *J* = 7.4 Hz, 2H), 1.15 (t, *J* = 7.4 Hz, 3H) (Et). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 152.2 (imine *C*H), 147.0, 134.0, 129.7, 122.3 (aryl *C*), 83.1, 76.6 (cage *C*), 29.2, 14.3 (Et). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -1.8 (1B), -4.4 (1B), -9.1 (2B), -10.3 (6B). HRMS: *m*/*z* calcd for $C_{11}H_{20}B_{10}ClN$ $[M]^+$: 309.2282. Found: 309.2283.

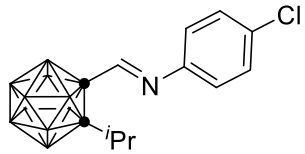


1c: Yield 86%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.78 (s, 1H) (imine C*H*), 7.37 (d, *J* = 9.0 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H) (aryl C*H*), 2.26 (m, 2H), 1.58 (m, 2H), 0.90 (t, *J* = 7.5 Hz, 3H) (^{n}Pr). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 152.2 (imine *C*H), 147.1, 134.0, 129.7, 122.3 (aryl *C*), 82.2, 76.5 (cage *C*), 37.5, 23.3, 13.9 (^{n}Pr). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -2.2 (1B), -4.7 (1B), -9.4 (2B), -10.6 (6B). HRMS: *m*/*z* calcd for $C_{12}H_{22}B_{10}ClN$ $[M]^+$: 324.2418. Found: 324.2419.

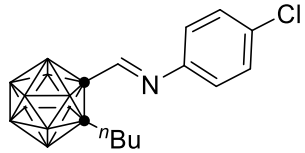


1d: Yield 89%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.87 (s, 1H) (imine C*H*), 7.42 (d, *J* = 9.0 Hz, 2H), 7.32 (m, 3H), 7.15 (m, 4H) (aryl C*H*), 3.63 (s, 2H) (CH_2). ^{13}C{^{1}H} NMR (125 MHz,

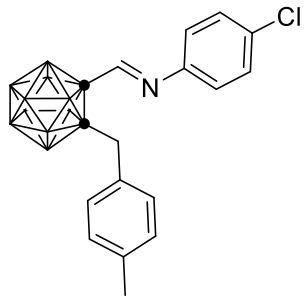
$CDCl_3$): δ 152.4 (imine *C*H), 146.8, 135.3, 134.3, 130.4, 129.8, 128.7, 128.2, 122.5 (aryl *C*), 82.2, 76.8 (cage *C*), 41.0 (*C*H_2). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.0 (1B), -4.3 (1B), -9.0 (2B), -10.4 (6B). HRMS: *m*/*z* calcd for $C_{16}H_{22}B_{10}ClN$ $[M]^+$: 371.2438. Found: 371.2436.



1e: Yield 78%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.77 (s, 1H) (imine C*H*), 7.37 (d, *J* = 9.0 Hz, 2H), 7.06 (d, *J* = 9.0 Hz, 2H) (aryl C*H*), 2.45 (m, 1H), 1.22 (d, *J* = 7.0 Hz, 6H) (^{i}Pr). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 152.0 (imine *C*H), 147.1, 134.0, 129.7, 122.3 (aryl *C*), 88.6, 78.3 (cage *C*), 32.3, 24.3 (^{i}Pr). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.6 (1B), -3.9 (1B), -9.2 (2B), -11.4 (6B). HRMS: *m*/*z* calcd for $C_{12}H_{22}B_{10}ClN$ $[M]^+$: 324.2418. Found: 324.2418.

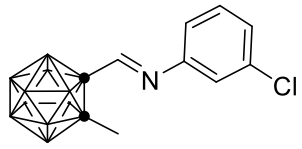


1f: Yield 87%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.78 (s, 1H) (imine C*H*), 7.37 (d, *J* = 8.5 Hz, 2H), 7.05 (d, *J* = 9.0 Hz, 2H) (aryl C*H*), 2.29 (m, 2H), 1.53 (m, 2H), 1.27 (m, 2H), 0.88 (t, *J* = 7.5 Hz, 3H) (^{n}Bu). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 152.3 (imine *C*H), 147.1, 134.0, 129.7, 122.2 (aryl *C*), 82.4, 76.5 (cage *C*), 35.3, 31.9, 22.4, 13.8 (^{n}Bu). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.2 (1B), -4.7 (1B), -9.4 (2B), -10.5 (6B). HRMS: *m*/*z* calcd for $C_{13}H_{24}B_{10}ClN$ $[M]^+$: 338.2576. Found: 338.2577.

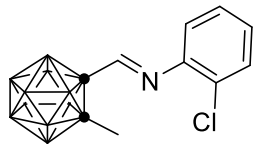


1g: Yield 86%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.87 (s, 1H) (imine C*H*), 7.43 (d, *J* = 9.0 Hz, 2H), 7.16 (m, 4H), 7.04 (d, *J* = 8.0 Hz, 2H) (aryl C*H*), 3.60 (s, 2H) (C*H*$_2$), 2.37 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 152.4 (imine *C*H), 146.8, 138.0, 134.2, 132.2, 130.2, 129.8, 129.3, 122.5 (aryl *C*), 82.4, 76.8 (cage *C*), 40.7 (*C*H_2), 21.3

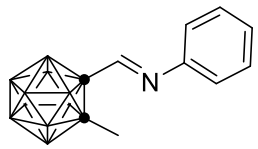
(*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.0 (1B), -4.4 (1B), -9.0 (2B), -10.4 (6B). HRMS: *m*/*z* calcd for $C_{17}H_{24}B_{10}ClN$ $[M]^+$: 386.2578. Found: 386.2578.



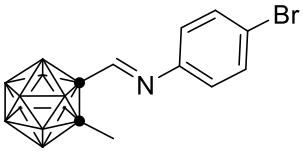
1j: Yield 77%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.81 (s, 1H) (imine C*H*), 7.30 (m, 2H), 7.10 (s, 1H), 7.00 (d, *J* = 8.0 Hz, 1H) (aryl C*H*), 2.12 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 153.3 (imine *C*H), 149.8, 135.2, 130.6, 128.0, 121.1, 119.2 (aryl *C*), 75.1 (cage *C*), 23.7 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -1.6 (1B), -5.5 (1B), -9.3 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}ClN$ $[M]^+$: 295.2134. Found: 295.2133.



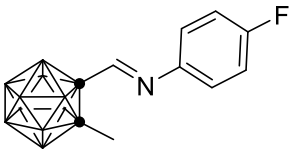
1k: Yield 70%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.80 (s, 1H) (imine C*H*), 7.44 (d, *J* = 8.0 Hz, 1H), 7.28 (m, 1H), 7.22 (m, 1H), 6.90 (d, *J* = 8.0 Hz, 1H) (aryl C*H*), 2.22 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 153.3 (imine *C*H), 149.8, 135.2, 130.6, 128.0, 121.1, 119.2 (aryl *C*), 75.1 (cage *C*), 23.7 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -1.6 (1B), -5.5 (1B), -9.3 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}ClN$ $[M]^+$: 295.2134. Found: 295.2133.



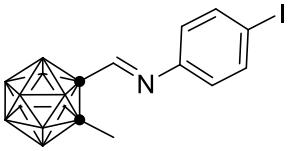
1l: Yield 90%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.82 (s, 1H) (imine C*H*), 7.41 (t, *J* = 7.5 Hz, 2H), 7.32 (t, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 7.5 Hz, 2H) (phenyl C*H*), 2.12 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 151.9 (imine *C*H), 148.7, 129.6, 128.2, 120.9 (phenyl *C*), 75.5 (cage *C*), 23.7 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -1.9 (1B), -5.5 (1B), -9.4 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{19}B_{10}N$ $[M]^+$: 261.2520. Found: 261.2521.



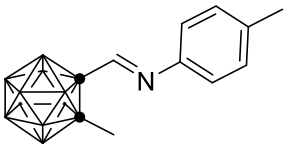
1m: Yield 91%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (s, 1H) (imine C*H*), 7.52 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H) (aryl C*H*), 2.11 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 152.4 (imine *C*H), 147.5, 132.7, 122.6, 121.9 (aryl *C*), 76.9, 75.3 (cage *C*), 23.7 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.2 (1B), -6.0 (1B), -9.8 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}BrN$ $[M]^+$: 340.1611. Found: 340.1612.



1n: Yield 83%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H) (imine C*H*), 7.13 (m, 4H) (aryl C*H*), 2.12 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 162.6 (d, $^{1}J_{C\text{-}F}$ = 247 Hz) (aryl *C*), 151.4 (imine *C*H), 144.6 (d, $^{4}J_{C\text{-}F}$ = 3 Hz), 122.8 (d, $^{3}J_{C\text{-}F}$ = 8 Hz), 116.4 (d, $^{2}J_{C\text{-}F}$ = 22 Hz) (aryl *C*), 77.0, 75.5 (cage *C*), 23.6 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.4 (1B), -6.1 (1B), -9.9 (5B), -10.9 (3B). ^{19}F NMR (376 MHz, $CDCl_3$): δ -105.5 (m, 1F). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}FN$ $[M]^+$: 279.2426. Found: 279.2426.

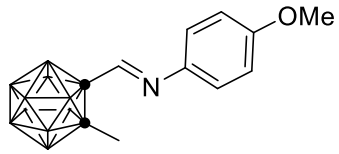


1o: Yield 80%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (s, 1H) (imine C*H*), 7.71 (d, *J* = 8.4 Hz, 2H), 6.87 (d, *J* = 8.8 Hz, 2H) (aryl C*H*), 2.11 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 152.4 (imine *C*H), 148.2, 138.6, 122.8, 93.1 (aryl *C*), 76.9, 75.2 (cage *C*), 23.7 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -2.2 (1B), -6.0 (1B), -9.9 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{18}B_{10}IN$ $[M]^+$: 387.1487. Found: 387.1486.

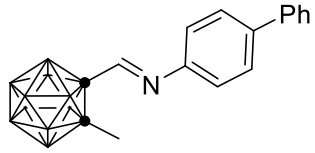


1p: Yield 86%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (s, 1H) (imine C*H*), 7.23 (d, *J* = 8.0 Hz, 2H), 7.08 (d, *J* = 8.4 Hz, 2H)

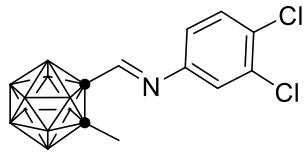
(aryl C*H*), 2.40 (s, 3H), 2.12 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 150.6 (imine *C*H), 146.0, 138.5, 130.1, 121.0 (aryl *C*), 77.0, 75.8 (cage *C*), 23.6, 21.2 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.5 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m*/*z* calcd for $C_{11}H_{21}B_{10}N$ $[M]^+$: 275.2677. Found: 275.2678.



1q: Yield 85%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H) (imine C*H*), 7.17 (d, *J* = 8.8 Hz, 2H), 6.92 (d, *J* = 8.8 Hz, 2H) (aryl C*H*), 3.83 (s, 3H) (OCH_3), 2.09 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 160.1 (aryl *C*), 148.8 (imine *C*H), 141.3, 122.8, 114.7 (aryl *C*), 77.0, 76.1 (cage *C*), 55.7 (O*C*H_3), 23.6 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.2 (1B), -5.6 (1B), -9.6 (8B). HRMS: *m*/*z* calcd for $C_{11}H_{21}B_{10}NO$ $[M]^+$: 291.2626. Found: 291.2626.

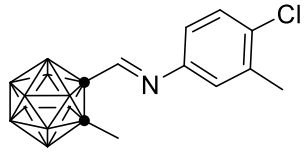


1r: Yield 82%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.90 (s, 1H) (imine C*H*), 7.62 (m, 4H), 7.48 (t, *J* = 7.6 Hz, 2H), 7.39 (m, 1H), 7.23 (dd, *J* = 1.6, 6.4 Hz, 2H) (aryl C*H*), 2.15 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 151.5 (imine *C*H), 147.6, 141.3, 140.1, 129.1, 128.2, 127.9, 127.1, 121.5 (aryl *C*), 77.0, 75.6 (cage *C*), 23.7 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.2 (1B), -5.6 (1B), -9.6 (8B). HRMS: *m*/*z* calcd for $C_{20}H_{25}B_{10}N$ $[M]^-$: 387.2998. Found: 387.3005.

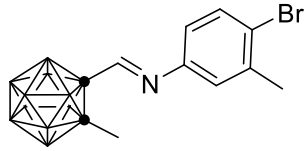


1s: Yield 77%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.81 (s, 1H) (imine C*H*), 7.47 (d, *J* = 8.5 Hz, 1H), 7.22 (d, *J* = 2.5 Hz, 1H), 6.98 (dd, *J* = 2.5, 8.5 Hz, 1H) (aryl C*H*), 2.11 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 153.6 (imine *C*H), 147.8, 133.6, 132.1, 131.2, 122.9, 120.4 (aryl *C*), 74.9 (cage *C*),

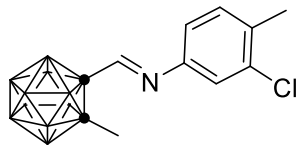
23.7 (*C*CH_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -1.7 (1B), -5.6 (1B), -9.4 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{10}B_{17}Cl_2N$ $[M-H]^+$: 329.1641. Found: 329.1641.



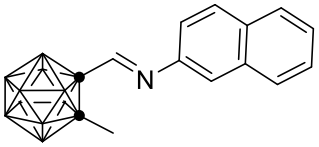
1t: Yield 76%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.81 (s, 1H) (imine C*H*), 7.35 (d, *J* = 8.4 Hz, 1H), 7.01 (s, 1H), 6.91 (d, *J* = 8.4 Hz, 1H) (aryl C*H*), 2.40, 2.11 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 151.9 (imine *C*H), 147.0, 137.5, 134.1, 130.0, 123.5, 119.4 (aryl *C*), 76.9, 75.4 (cage *C*), 23.7, 20.2 (*C*CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.4 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m*/*z* calcd for $C_{11}H_{20}B_{10}ClN$ $[M]^+$: 309.2282. Found: 309.2288.



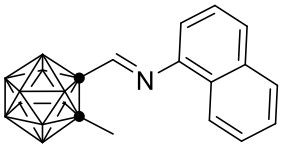
1u: Yield 79%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.81 (s, 1H) (imine C*H*), 7.53 (d, *J* = 8.5 Hz, 1H), 7.00 (s, 1H), 6.82 (d, *J* = 8.0 Hz, 1H) (aryl C*H*), 2.42, 2.11 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 152.0 (imine *C*H), 147.7, 139.4, 133.3, 124.3, 123.4, 119.6 (aryl *C*), 75.4 (cage *C*), 23.7, 23.1 (*C*CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.4 (1B), -6.1 (1B), -10.0 (8B). HRMS: *m*/*z* calcd for $C_{11}H_{20}B_{10}BrN$ $[M]^+$: 354.1768. Found: 354.1766.



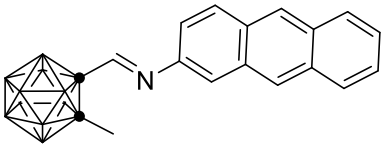
1v: Yield 75%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H) (imine C*H*), 7.26 (d, *J* = 8.0 Hz, 1H), 7.15 (s, 1H), 6.96 (d, *J* = 8.0 Hz, 1H) (aryl C*H*), 2.40, 2.11 (s, 3H) (C*H*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 152.0 (imine *C*H), 147.7, 139.4, 133.3, 124.3, 123.4, 119.6 (aryl *C*), 75.4 (cage *C*), 23.7, 23.1 (*C*CH_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -2.3 (1B), -6.1 (1B), -9.9 (8B). HRMS: *m*/*z* calcd for $C_{11}H_{20}B_{10}ClN$ $[M]^+$: 309.2282. Found: 309.2284.



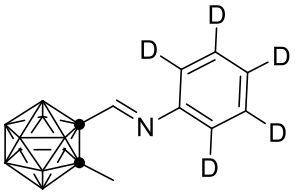
1w: Yield 82%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.97 (s, 1H) (imine C*H*), 7.87 (m, 3H), 7.53 (m, 3H), 7.32 (d, *J* = 8.5 Hz, 1H) (aryl *H*), 2.17 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 151.7 (imine *C*H), 146.0, 133.7, 133.0, 129.6, 128.3, 127.9, 127.1, 126.6, 119.7, 119.4 (aryl *C*), 77.0, 75.7 (cage *C*), 23.7 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -1.8 (1B), -5.4 (1B), -9.3 (8B). HRMS: *m*/*z* calcd for $C_{14}H_{21}B_{10}N$ $[M]^+$: 311.2679. Found: 311.2677.



1x: Yield 72%. Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.12 (t, *J* = 7.5 Hz, 1H) (aryl C*H*), 7.95 (s, 1H) (imine C*H*), 7.86 (t, *J* = 6.0 Hz, 1H), 7.81 (d, *J* = 10.0 Hz, 1H), 7.56 (m, 2H), 7.44 (t, *J* = 10.0 Hz, 1H), 6.94 (d, *J* = 9.0 Hz, 1H) (aryl C*H*), 2.20 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 152.0 (imine *C*H), 145.8, 134.1, 128.5, 128.3, 128.0, 127.1, 126.8, 125.7, 123.4, 112.7 (aryl *C*), 76.8, 75.8 (cage *C*), 23.9 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, CDCl3): δ -2.3 (1B), -5.9 (1B), -9.8 (8B). HRMS: *m*/*z* calcd for $C_{14}H_{21}B_{10}N$ $[M]^+$: 311.2672. Found: 311.2672.

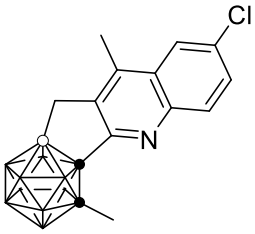


1y: Yield 70%. Yellow solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.44 (s, 1H), 8.43 (s, 1H), 8.01 (m, 4H), 7.70 (s, 1H), 7.51 (m, 2H), 7.33 (dd, *J* = 2.0, 9.0 Hz, 1H) (aryl C*H* and imine C*H*), 2.18 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 151.3 (imine *C*H), 145.3, 132.4, 132.2, 131.6, 130.9, 130.1, 128.4, 128.2, 127.1, 126.6, 126.2, 126.1, 119.9, 119.7 (aryl *C*), 77.1, 75.8 (cage *C*), 23.8 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -1.7 (1B), -5.5 (1B), -9.3 (8B). HRMS: *m*/*z* calcd for $C_{18}H_{23}B_{10}N$ $[M]^+$: 361.2837. Found: 361.2836.

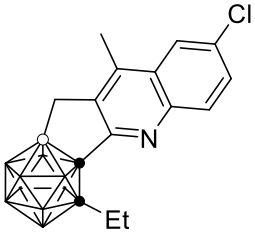


1l-d_5**:** Yield 91%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (s, 1H) (imine C*H*), 2.12 (s, 3H) (CH_3). ^{2}H NMR (61 MHz, $CDCl_3$): δ 7.47, 7.19 (aryl C*D*). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 151.9 (imine *C*H), 148.6, 129.1 (t, $J_{C\text{-}D}$ = 11.3 Hz), 127.7 (t, $J_{C\text{-}D}$ = 11.3 Hz), 120.5 (t, $J_{C\text{-}D}$ = 11.3 Hz) (aryl *C*), 75.5 (cage *C*), 23.7 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -1.9 (1B), -5.6 (1B), -9.4 (8B). HRMS: *m*/*z* calcd for $C_{10}H_{14}B_{10}ND_5$ $[M\text{-}H]^-$: 265.2764. Found: 265.2762.

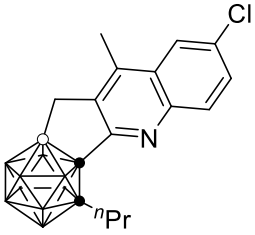
Synthesis of C,B-Substituted *o*-Carborane-Fused *N*-Polyheterocycles (3). A Representative Procedure. Carboranyl *N*-arylimine **1** (0.10 mmol), vinyl ketone (0.50 mmol, 5.0 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (34.4 or 17.2 mg, 0.10 or 0.05 mmol, 1.0 or 0.5 equiv), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^{o}C for 6 h or 10 h under argon. After cooling to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The filtrate was concentrated to dryness in vacuo, and subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **3**. It is noted that cage B(4)-H and B(5)-H are identical according to the symmetry of the cluster, which will generate a pair of enantiomers in the reactions.[3]



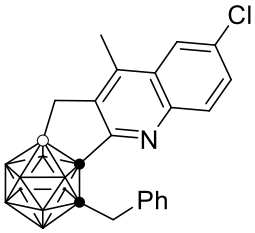
3a: Yield 70%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (m, 2H), 7.61 (dd, *J* = 2.0, 8.8 Hz, 1H) (aryl C*H*), 2.62 (s, 3H) (CH_3), 2.53 (m, 2H) (CH_2), 2.42 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.9, 144.2, 142.1, 140.7, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl *C*), 83.0, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.3 (1B) (*B*-C), -5.3 (1B), -6.5 (1B), -8.2 (2B), -9.8 (4B), -13.1 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}ClN$ $[M]^+$: 346.2263. Found: 346.2264.



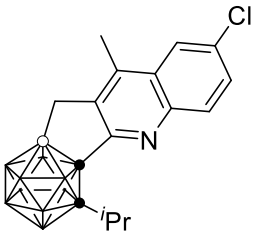
3b: Yield 72%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (m, 2H), 7.61 (dd, *J* = 2.0, 8.8 Hz, 1H) (aryl C*H*), 2.91 (m, 1H), 2.72 (m, 1H) (CH_2), 2.61 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 1.22 (t, *J* = 7.2 Hz, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.9, 144.1, 142.1, 140.8, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl *C*), 84.1, 81.7 (cage *C*), 27.9, 15.1, 14.4 (*C*H_3 and Et). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.4 (1B) (*B*-C), -5.7 (2B), -8.4 (2B), -10.5 (3B), -12.0 (1B), -14.5 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{22}B_{10}ClN$ $[M]^+$: 360.2420. Found: 360.2427.



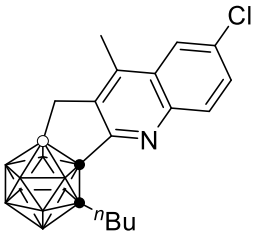
3c: Yield 74%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (m, 2H), 7.62 (dd, *J* = 2.4, 8.8 Hz, 1H) (aryl C*H*), 2.79 (m, 1H), 2.62 (m, 4H), 2.51 (m, 2H), 1.79 (m, 1H), 1.52 (m, 1H), 0.92 (t, *J* = 7.2 Hz, 3H) (CH_2, CH_3 and ^{n}Pr). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.9, 144.1, 142.1, 140.8, 133.1, 131.9, 129.9, 128.3, 122.9 (aryl *C*), 83.9, 80.8 (cage *C*), 36.2, 23.5, 15.1, 13.9 (*C*H_3 and ^{n}Pr). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.5 (1B) (*B*-C), -5.7 (2B), -10.0 (6B), -14.4 (1B). HRMS: *m*/*z* calcd for $C_{16}H_{24}B_{10}ClN$ $[M]^+$: 374.2577. Found: 374.2579.



3d: Yield 69%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.05 (d, *J* = 9.0 Hz, 1H), 8.01 (d, *J* = 2.5 Hz, 1H), 7.66 (dd, *J* = 2.0, 9.0 Hz, 1H), 7.30 (m, 5H) (aryl C*H*), 4.27 (d, *J* = 15.0 Hz, 1H), 3.96 (d, *J* = 15.0 Hz, 1H) (CH_2), 2.64 (s, 3H) (CH_3), 2.53 (m, 2H) (CH_2). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.0, 144.1, 142.4, 140.9, 136.3, 133.3, 131.8, 130.8, 130.1, 128.5, 128.4, 127.9, 123.0 (aryl *C*), 84.3, 80.2 (cage *C*), 39.4, 15.2 (*C*H_2 and *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.6 (1B) (*B*-C), -5.5 (2B), -10.1 (5B), -12.4 (1B), -14.1 (1B). HRMS: *m*/*z* calcd for $C_{20}H_{24}B_{10}ClN$ $[M]^+$: 421.2596. Found: 421.2593.

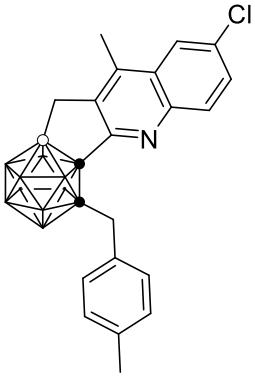


3e: Yield 64%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.95 (m, 2H), 7.61 (dd, *J* = 2.5, 9.0 Hz, 1H) (aryl C*H*), 3.39 (m, 1H) (C*H*), 2.61 (s, 3H) (CH_3), 2.50 (m, 2H) (CH_2), 1.45 (d, *J* = 6.5 Hz, 3H), 1.08 (d, *J* = 7.0 Hz, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.0, 144.1, 142.1, 140.8, 133.1, 132.0, 129.9, 128.3, 122.9 (aryl *C*), 87.1, 85.5 (cage *C*), 30.9, 24.6, 24.5, 15.1 (*C*H_3 and ^{i}Pr). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.5 (1B) (*B*-C), -5.0 (1B), -5.9 (1B), -9.6 (3B), -10.6 (3B), -15.4 (1B). HRMS: *m*/*z* calcd for $C_{16}H_{24}B_{10}ClN$ $[M]^+$: 373.2595. Found: 373.2593.

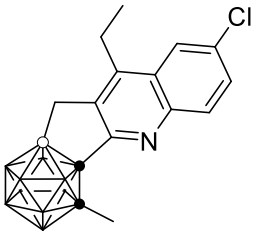


3f: Yield 74%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (m, 2H), 7.61 (dd, *J* = 2.0, 8.8 Hz, 1H) (aryl C*H*), 2.83 (m, 1H), 2.65 (m, 4H), 2.51 (m, 2H), 1.75 (m, 1H), 1.46 (m, 1H), 1.50 (m, 2H), 0.94 (t, *J* = 7.2 Hz, 3H), (CH_2, CH_3 and ^{n}Bu). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 156.9, 144.1, 142.1, 140.8, 133.1, 131.8, 129.9, 128.3, 122.9 (aryl *C*), 84.0, 80.9 (cage *C*), 33.8, 32.1, 22.5, 15.1, 13.8 (*C*H_3 and ^{n}Bu). ^{11}B{^{1}H} NMR (128 MHz, CDCl3): δ -1.9 (1B) (*B*-C), -4.0 (2B), -8.3

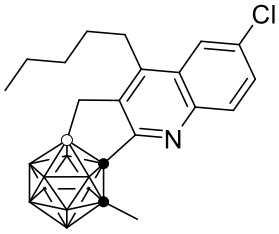
(5B), -10.3 (1B), -12.7 (1B). HRMS: *m*/*z* calcd for $C_{17}H_{26}B_{10}ClN$ $[M]^+$: 387.2751. Found: 387.2752.



3g: Yield 71%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.8 Hz, 1H), 8.00 (d, *J* = 2.0 Hz, 1H), 7.66 (dd, *J* = 2.4, 8.8 Hz, 1H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H) (aryl C*H*), 4.21 (d, *J* = 15.2 Hz, 1H), 3.92 (d, *J* = 15.2 Hz, 1H) (CH_2), 2.64 (s, 3H) (CH_3), 2.52 (m, 2H) (CH_2), 2.33 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.0, 144.1, 142.3, 140.9, 137.5, 133.3, 133.3, 131.8, 130.7, 130.1, 129.2, 128.4, 123.0 (aryl *C*), 84.2, 80.5 (cage *C*), 39.0, 12.3, 15.2 (*C*H_2 and *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -4.1 (1B) (*B*-C), -6.1 (2B), -10.7 (5B), -13.0 (1B), -14.6 (1B). HRMS: *m*/*z* calcd for $C_{21}H_{26}B_{10}ClN$ $[M]^+$: 435.2751. Found: 435.2739.

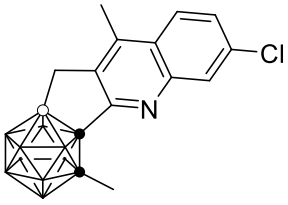


3h: Yield 63%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (m, 2H), 7.62 (dd, *J* = 2.0, 8.8 Hz, 1H) (aryl C*H*), 3.06 (q, *J* = 7.6 Hz, 2H), 2.53 (m, 2H) (CH_2), 2.42 (s, 3H), 1.30 (t, *J* = 7.6 Hz, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.1, 147.9, 144.7, 139.9, 133.2, 132.1, 129.9, 127.3, 122.7 (aryl *C*), 83.0, 75.4 (cage *C*), 22.5, 22.3, 13.9 (*C*H_2 and *C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.5 (1B) (*B*-C), -5.5 (1B), -6.7 (3B), -9.9 (2B), -10.7 (2B), -13.2 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{22}B_{10}ClN$ $[M]^+$: 360.2420. Found: 360.2424.

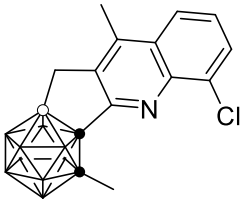


3i: Yield 35%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.96 (m, 2H), 7.61 (dd, *J* = 2.5, 9.0 Hz, 1H) (aryl C*H*), 3.01 (t, *J* = 8.0 Hz, 2H), 2.53 (m, 2H) (CH_2), 2.42 (s, 3H) (CH_3), 1.64 (m, 2H), 1.48 (m,

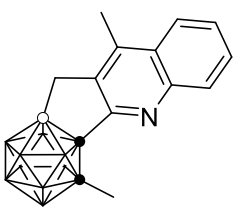
2H), 1.42 (m, 2H) (CH_2), 0.94 (t, J = 7.5 Hz, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 157.0, 146.8, 144.6, 140.2, 133.1, 132.1, 129.9, 127.6, 122.8 (aryl *C*), 83.0, 75.4 (cage *C*), 32.4, 29.5, 29.3, 22.6, 22.3, 14.2 (*C*H_2 and *C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.9 (1B) (*B*-C), -4.8 (1B), -5.9 (1B), -7.6 (2B), -9.9 (4B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{18}H_{28}B_{10}ClN$ $[M]^+$: 402.2892. Found: 402.2893.



3j: Yield 68%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, J = 2.0 Hz, 1H), 7.94 (d, J = 8.8 Hz, 1H), 7.53 (dd, J = 2.0, 9.2 Hz, 1H) (aryl C*H*), 2.64 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 157.7, 146.3, 143.1, 140.1, 135.1, 129.2, 128.1, 126.0, 125.1 (aryl *C*), 82.9, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.2 (1B) (*B*-C), -5.3 (1B), -6.4 (1B), -8.2 (2B), -9.7 (2B), -10.4 (2B), -12.9 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}ClN$ $[M]^+$: 345.2282. Found: 345.2287.

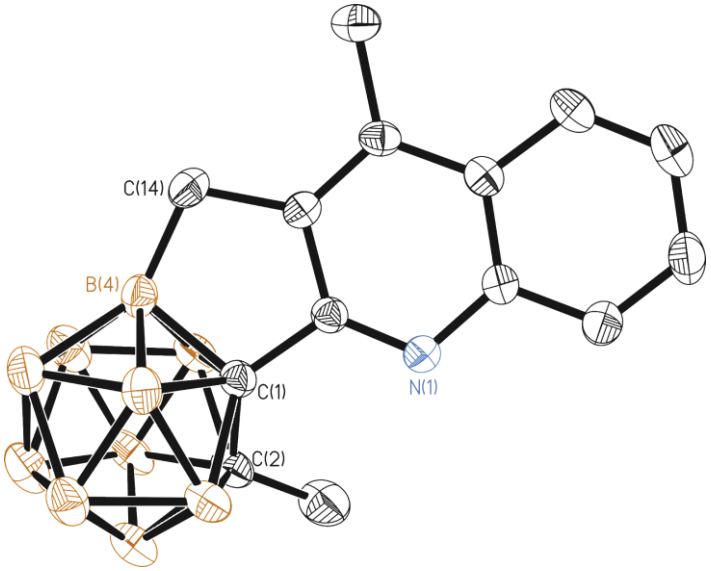


3k: Yield 39%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 7.94 (dd, J = 1.2, 8.4 Hz, 1H), 7.80 (dd, J = 1.2, 7.6 Hz, 1H), 7.49 (dd, J = 7.6, 8.4 Hz, 1H) (aryl C*H*), 2.67 (s, 3H) (CH_3), 2.54 (m, 2H) (CH_2), 2.49 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 157.0, 143.5, 142.2, 140.6, 134.8, 129.4, 128.9, 127.0, 122.8 (aryl *C*), 82.8, 75.4 (cage *C*), 22.2, 15.4 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.5 (1B) (*B*-C), -5.3 (1B), -6.5 (1B), -8.2 (2B), -9.8 (2B), -10.5 (2B), -12.9 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}ClN$ $[M]^+$: 346.2263. Found: 346.2264.

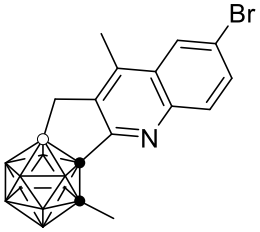


3l: Yield 62%. Colorless crystals. ^1H NMR (400 MHz, $CDCl_3$): δ 8.03 (m, 2H), 7.69 (t, J = 7.2 Hz, 1H), 7.59 (t, J = 6.8 Hz, 1H) (aryl C*H*), 2.67

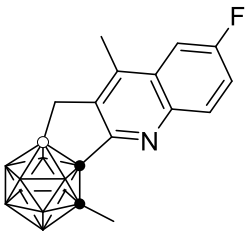
(s, 3H) (CH_3), 2.54 (m, 2H) (CH_2), 2.45 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 156.5, 145.7, 143.0, 139.8, 130.3, 129.1, 127.5, 127.3, 123.7 (aryl *C*), 83.3, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.6 (1B) (*B*-C), -5.9 (1B), -6.9 (1B), -8.5 (2B), -10.8 (4B), -13.4 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{21}B_{10}N$ $[M]^+$: 311.2672. Found: 311.2675.



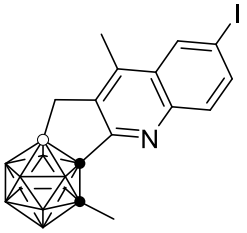
Supplementary Figure 1. Molecular structure of **3l** drawn with 30% probability ellipsoids.



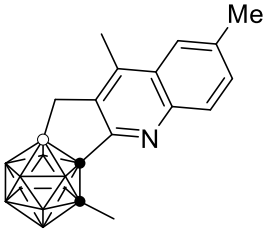
3m: Yield 67%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 8.15 (d, *J* = 2.0 Hz, 1H), 7.89 (d, *J* = 8.8 Hz, 1H), 7.74 (dd, *J* = 2.0, 8.8 Hz, 1H) (aryl C*H*), 2.62 (s, 3H) (CH_3), 2.54 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 157.0, 144.4, 142.1, 140.7, 132.5, 132.0, 128.8, 126.3, 121.4 (aryl *C*), 83.0, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.3 (1B) (*B*-C), -5.3 (1B), -6.4 (1B), -8.3 (2B), -9.7 (2B), -10.4 (2B), -13.1 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}BrN$ $[M-H]^-$: 390.1696. Found: 390.1691.



3n: Yield 58%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.02 (dd, *J* = 6.0, 9.2 Hz, 1H), 7.59 (dd, *J* = 2.4, 10.0 Hz, 1H), 7.45 (t, *J* = 9.2 Hz, 1H) (aryl C*H*), 2.61 (s, 3H) (CH_3), 2.53 (m, 2H) (CH_2), 2.42 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 161.1 (d, $^{1}J_{C\text{-}F}$ = 247 Hz), 156.0, 142.8, 142.3 (d, $^{4}J_{C\text{-}F}$ = 6 Hz), 140.5, 132.8 (d, $^{3}J_{C\text{-}F}$ = 10 Hz), 128.6 (d, $^{3}J_{C\text{-}F}$ = 10 Hz), 119.1 (d, $^{2}J_{C\text{-}F}$ = 25 Hz), 107.5 (d, $^{2}J_{C\text{-}F}$ = 22 Hz) (aryl *C*), 83.1, 75.4 (cage *C*), 22.3, 15.2 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.3 (1B) (*B*-C), -5.4 (1B), -6.5 (1B), -8.1 (2B), -9.8 (2B), -10.5 (1B), -11.3 (1B), -13.0 (1B). ^{19}F NMR (376 MHz, $CDCl_3$): δ -111.4 (m, 1F). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}FN$ $[M]^+$: 329.2584. Found: 329.2585.

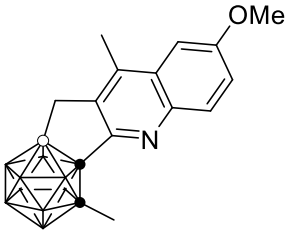


3o: Yield 42%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.37 (d, *J* = 1.6 Hz, 1H), 7.91 (dd, *J* = 1.6, 8.8 Hz, 1H), 7.74 (d, *J* = 8.8 Hz, 1H) (aryl C*H*), 2.61 (s, 3H) (CH_3), 2.52 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.1, 144.8, 141.8, 140.6, 137.9, 133.0, 131.9, 129.3, 93.2 (aryl *C*), 83.0, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.2 (1B) (*B*-C), -5.2 (1B), -6.4 (1B), -8.1 (2B), -9.7 (2B), -10.3 (2B), -13.0 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{20}B_{10}IN$ $[M]^+$: 437.1638. Found: 437.1639.

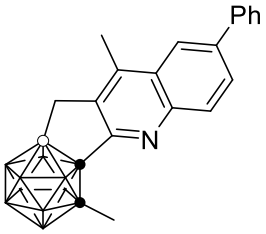


3p: Yield 53%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 8.8 Hz, 1H), 7.76 (s, 1H), 7.51 (dd, *J* = 1.2, 8.8 Hz, 1H) (aryl C*H*), 2.63 (s, 3H), 2.57 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 2.43 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 155.7, 144.3, 142.2, 139.7, 137.2, 131.3, 130.0, 127.5, 122.8 (aryl *C*), 83.4, 75.3 (cage *C*), 22.3, 22.1, 15.0 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz,

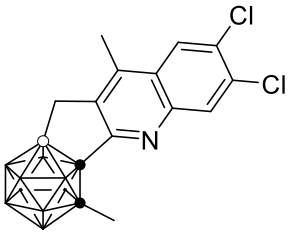
$CDCl_3$): δ -3.1 (1B) (*B*-C), -5.6 (1B), -6.6 (1B), -8.1 (2B), -9.9 (2B), -10.5 (2B), -13.1 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{23}B_{10}N$ $[M]^+$: 325.2836. Found: 325.2837.



3q: Yield 32%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.92 (d, *J* = 9.2 Hz, 1H), 7.34 (dd, *J* = 2.8, 9.2 Hz, 1H), 7.19 (d, *J* = 1.2 Hz, 1H) (aryl C*H*), 3.96 (s, 3H) (OCH_3), 2.60 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 2.42 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 158.5, 154.2, 141.6, 141.4, 140.1, 131.8, 128.6, 121.2, 102.1 (aryl *C*), 83.5, 75.2 (cage *C*), 55.7 (O*C*H_3), 22.3, 15.2 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.2 (1B) (*B*-C), -5.7 (1B), -6.6 (3B), -10.0 (4B), -13.0 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{23}B_{10}NO$ $[M]^-$: 341.2790. Found: 341.2796.

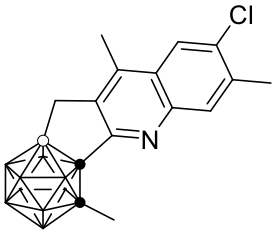


3r: Yield 56%. White solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16 (d, *J* = 1.6 Hz, 1H), 8.10 (d, *J* = 8.8 Hz, 1H), 7.94 (dd, *J* = 1.2, 8.8 Hz, 1H), 7.72 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.6 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H) (aryl C*H*), 2.71 (s, 3H) (CH_3), 2.55 (m, 2H) (CH_2), 2.45 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 156.5, 145.1, 143.0, 140.8, 140.2, 140.1, 130.8, 129.2, 128.9, 128.0, 127.7, 127.7, 121.7 (aryl *C*), 83.3, 75.4 (cage *C*), 22.3, 15.2 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.1 (1B) (*B*-C), -6.5 (4B), -9.8 (2B), -10.4 (2B), -12.9 (1B). HRMS: *m*/*z* calcd for $C_{20}H_{25}B_{10}N$ $[M]^-$: 387.2998. Found: 387.3005.

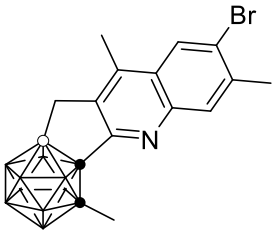


3s: Yield 63%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.16 (s, 1H), 8.09 (s, 1H) (aryl C*H*), 2.62 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 2.40 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 158.0, 144.6, 142.2, 140.9, 133.6, 131.8, 131.2, 126.9, 124.8 (aryl *C*), 82.7, 75.5 (cage *C*), 22.3, 15.2

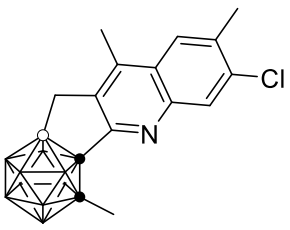
(*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.8 (1B) (*B*-C), -4.6 (1B), -5.9 (1B), -7.7 (2B), -9.9 (4B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{19}B_{10}Cl_2N$ $[M]^-$: 379.1804. Found: 379.1811.



3t: Yield 70%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 7.98 (s, 1H), 7.89 (s, 1H) (aryl C*H*), 2.60 (s, 3H), 2.55 (s, 3H) (CH_3), 2.50 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 156.8, 144.5, 141.9, 139.8, 137.8, 134.5, 131.4, 126.8, 123.2 (aryl *C*), 83.1, 75.3 (cage *C*), 22.3, 20.6, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.8 (1B) (*B*-C), -4.9 (1B), -6.0 (1B), -7.1 (2B), -9.9 (3B), -10.9 (1B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{22}B_{10}ClN$ $[M]^+$: 360.2420. Found: 360.2423.

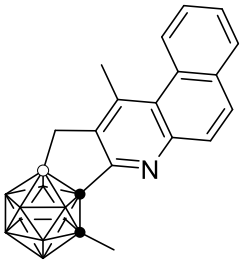


3u: Yield 66%. White solid. ^1H NMR (500 MHz, $CDCl_3$): δ 8.19 (s, 1H), 7.89 (s, 1H) (aryl C*H*), 2.60 (s, 3H), 2.58 (s, 3H) (CH_3), 2.51 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 157.0, 144.9, 141.8, 139.8, 139.2, 131.1, 127.1, 126.9, 125.1 (aryl *C*), 83.1, 75.3 (cage *C*), 22.3, 20.6, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.6 (1B) (*B*-C), -4.8 (1B), -5.9 (1B), -7.6 (2B), -9.9 (4B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{22}B_{10}BrN$ $[M-H]^-$: 404.1849. Found: 404.1849.

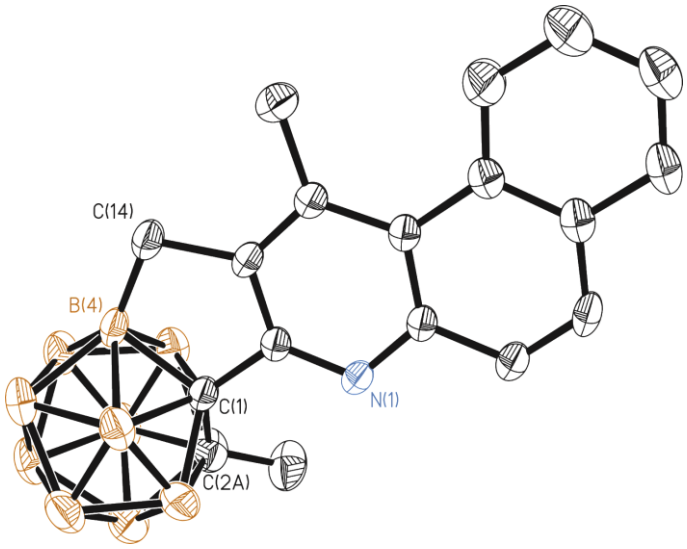


3v: Yield 64%. White solid. ^1H NMR (400 MHz, $CDCl_3$): δ 8.05 (s, 1H), 7.82 (s, 1H) (aryl C*H*), 2.62 (s, 3H), 2.58 (s, 3H) (CH_3), 2.50 (m, 2H) (CH_2), 2.41 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 156.8, 145.0, 142.3, 140.0, 136.4, 135.7, 129.4, 126.3, 124.6 (aryl *C*), 83.1, 75.4 (cage *C*), 22.3, 21.0, 15.1 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.9 (1B) (*B*-C), -5.0

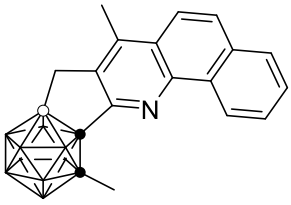
(1B), -6.2 (1B), -7.8 (2B), -10.1 (4B), -12.7 (1B). HRMS: *m*/*z* calcd for $C_{15}H_{22}B_{10}ClN$ $[M]^+$: 360.2420. Found: 360.2420.



3w: Yield 50%. Colorless crystals. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, *J* = 9.2 Hz, 1H), 7.94 (m, 3H), 7.67 (m, 2H) (aryl C*H*), 3.06 (s, 3H) (CH_3), 2.61 (m, 2H) (CH_2), 2.46 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 154.8, 147.3, 144.2, 142.5, 133.5, 131.0, 130.5, 129.1, 129.0, 128.1, 127.0, 126.3, 125.7 (aryl *C*), 83.5, 75.1 (cage *C*), 22.3, 22.0 (*C*H_3). ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ -3.3 (1B) (*B*-C), -6.5 (4B), -10.3 (4B), -12.9 (1B). HRMS: *m*/*z* calcd for $C_{18}H_{23}B_{10}N$ $[M-H]^-$: 360.2769. Found: 360.2770.

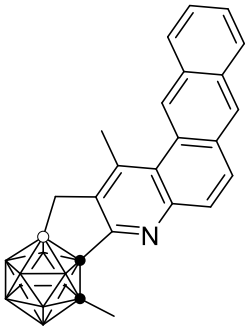


Supplementary Figure 2. Molecular structure of **3w** drawn with 30% probability ellipsoids.

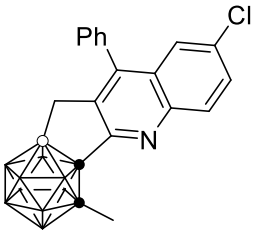


3x: Yield 37%. White solid. ^{1}H NMR (500 MHz, $CDCl_3$): δ 9.17 (d, *J* = 7.5 Hz, 1H), 7.90 (m, 3H), 7.70 (m, 2H) (aryl C*H*), 2.72 (s, 3H) (CH_3), 2.58 (m, 2H) (CH_2), 2.55 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 154.8, 143.7, 143.3, 141.2, 133.3, 131.9, 128.3, 128.3, 127.9, 127.3, 125.3, 124.6, 121.3 (aryl *C*), 83.8, 74.8 (cage *C*), 22.4, 15.4 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz,

$CDCl_3$): δ -2.6 (1B) (*B*-C), -5.1 (1B), -6.0 (3B), -9.9 (4B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{18}H_{23}B_{10}N$ $[M]^-$: 361.2835. Found: 361.2850.



3y: Yield 29%. White solid. ^1H NMR (400 MHz, CD_2Cl_2): δ 9.26 (s, 1H), 8.45 (s, 1H), 8.16 (m, 1H), 8.09 (m, 1H), 8.00 (d, *J* = 9.2 Hz, 1H), 7.73 (d, *J* = 9.2 Hz, 1H), 7.63 (t, *J* = 8.8 Hz, 2H) (aryl C*H*), 3.16 (s, 3H) (CH_3), 2.65 (m, 2H) (CH_2), 2.47 (s, 3H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, CD_2Cl_2): δ 154.6, 148.3, 145.0, 143.4, 132.0, 131.9, 131.8, 131.8, 129.2, 129.0, 128.8, 128.7, 127.8, 127.4, 127.2, 126.6, 126.3 (aryl *C*), 84.1, 75.6 (cage *C*), 22.4, 22.0 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, CD_2Cl_2): δ -3.1 (1B) (*B*-C), -6.6 (4B), -10.4 (4B), -13.0 (1B). HRMS: *m*/*z* calcd for $C_{22}H_{25}B_{10}N$ $[M-H]^-$: 410.2921. Found: 410.2928.

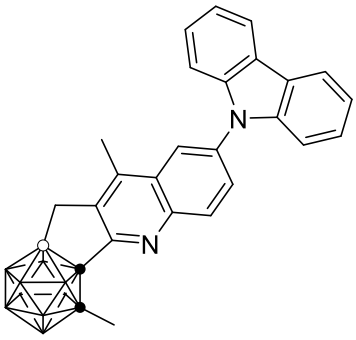


3z: Yield 38%. Colorless oil. ^1H NMR (400 MHz, $CDCl_3$): δ 8.03 (d, *J* = 8.8 Hz, 1H), 7.60 (d, *J* = 8.8 Hz, 1H), 7.54 (m, 4H), 7.30 (m, 2H), (aryl C*H*), 2.47 (s, 3H) (CH_3), 2.34 (m, 2H) (CH_2). $^{13}C\{^1H\}$ NMR (100 MHz, $CDCl_3$): δ 157.1, 146.8, 144.6, 140.5, 135.4, 133.4, 131.4, 130.3, 129.1, 129.1, 128.8, 128.9, 124.9 (aryl *C*), 82.8, 75.4 (cage *C*), 22.3 (*C*H_3). $^{11}B\{^1H\}$ NMR (128 MHz, $CDCl_3$): δ -3.0 (1B) (*B*-C), -6.3 (4B), -9.5 (4B), -12.9 (1B). HRMS: *m*/*z* calcd for $C_{19}H_{22}B_{10}ClN$ $[M+H]^+$: 408.2529. Found: 408.2520.

Transformations of 3m.

Reaction of 3m with Carbazole. Compound **3m** (39.0 mg, 0.10 mmol), carbazole (20.0 mg, 0.12 mmol, 1.2 equiv), $Pd_2(dba)_3$ (4.6 mg, 0.005 mmol, 5 mol%), lithium tert-butoxide (36.0

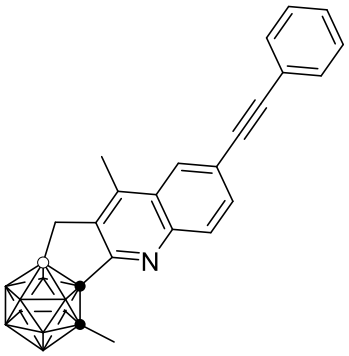
mg, 0.45 mmol, 4.5 equiv) and tri-tert-butylphosphine (1M in toluene, 8.0 μL, 8 mol%) were mixed in *o*-xylene (2 mL). The resultant mixture was stirred at 140 ^{o}C for 24 h under argon, and then cooled down to room temperature. After filtration through a Celite pad, the filtrate was concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **4m** as a white solid (45.0 mg, 95%).



4m. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.27 (d, *J* =8.5 Hz, 1H), 8.23 (s, 1H), 8.20 (d, *J* = 8.0 Hz, 2H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.45 (m, 4H), 7.34 (t, *J* = 7.0 Hz, 2H) (aryl C*H*), 2.66 (s, 3H) (CH_3), 2.59 (m, 2H) (CH_2), 2.49 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (125 MHz, $CDCl_3$): δ 157.1, 144.6, 142.8, 140.9, 140.7, 136.4, 132.3, 128.5, 128.4, 126.3, 123.7, 121.5, 120.7, 120.5, 109.6 (aryl *C*), 83.1, 75.4 (cage *C*), 22.3, 15.3 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -2.6 (1B) (*B*-C), -5.9 (4B), -9.8 (4B), -12.4 (1B). HRMS: *m*/*z* calcd for $C_{26}H_{28}B_{10}N_2$ [M-H]$^{-}$: 475.3179. Found: 475.3195.

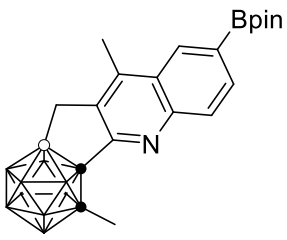
Reaction of 3m with Phenylacetylene. Compound **3m** (39.0 mg, 0.10 mmol), $PdCl_2(PPh_3)_2$ (3.5 mg, 0.005 mmol, 5 mol%), CuI (1.9 mg, 0.01 mmol, 10 mol%), phenylacetylene (13.2 μL, 0.12 mmol, 1.2 equiv), and triethylamine (70.0 μL, 0.50 mmol, 5.0 equiv) were dissolved in DMF (2 mL). The resultant mixture was stirred at 60 ^{o}C for 16 h under argon. The reaction was quenched with water, and extracted with diethyl ether (5 mL x 3). The organic portions were combined, washed with water (5 mL x 3), dried with $MgSO_4$, and concentrated to dryness in vacuo. Then, the obtained residue was subjected to flash column chromatography

on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **5m** as a white solid (39.5 mg, 96%).



5m. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.19 (d, *J* =1.2 Hz, 1H), 7.99 (d, *J* =8.4 Hz, 1H), 7.78 (dd, *J* =1.6, 8.8 Hz, 1H), 7.60 (m, 2H), 7.39 (m, 3H) (aryl C*H*), 2.67 (s, 3H) (CH_3), 2.53 (m, 2H) (CH_2), 2.44 (s, 3H) (CH_3). ^{13}C{^{1}H} NMR (100 MHz, $CDCl_3$): δ 157.1, 145.2, 142.7, 140.5, 131.9, 131.8, 130.5, 128.8, 128.6, 127.4, 127.3, 123.0, 122.2 (aryl *C*), 91.0, 89.4 (alkynyl *C*), 83.1, 75.4 (cage *C*), 22.3, 15.1 (*C*H_3). ^{11}B{^{1}H} NMR (160 MHz, $CDCl_3$): δ -2.6 (1B) (*B*-C), -4.7 (1B), -5.9 (3B), -9.2 (2B), -9.9 (2B), -12.5 (1B). HRMS: *m*/*z* calcd for $C_{22}H_{25}B_{10}N$ $[M-H]^-$: 410.2927. Found: 410.2928.

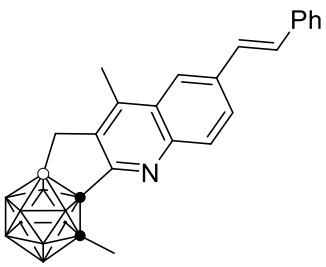
Reaction of 3m with B_2pin_2. Compound **3m** (39.0 mg, 0.10 mmol), bis(pinacolato)diboron (28.0 mg, 0.11 mmol, 1.1 equiv), Pd(dppf)Cl_2 (dppf = 1,1'-bis(diphenylphosphino)ferrocene) (7.3 mg, 0.01 mmol, 10 mol%), and potassium acetate (29.4 mg, 0.30 mmol, 3.0 equiv) were mixed in toluene (2 mL). The resultant mixture was stirred at 90 ^{o}C under Ar for 18 h. The reaction mixture was allowed to cool to room temperature before filtered through a pad of Celite and washed with diethyl ether. The filtrate was concentrated to dryness in vacuo and subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and ethyl acetate (10 : 1 in V/V) as eluent to give the product **6m** as a white solid (39.0 mg, 89%).



6m. ^{1}H NMR (500 MHz, $CDCl_3$): δ 8.50 (s, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H) (aryl C*H*), 2.71 (s, 3H) (CH_3), 2.52 (m, 2H) (CH_2), 2.44 (s, 3H) (CH_3), 1.40 (s, 12H) (pinacolato CH_3).

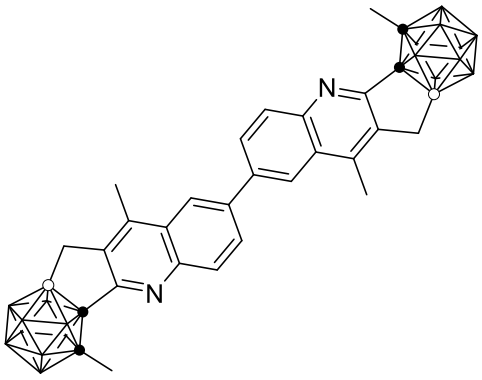
$^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 157.4, 147.4, 143.8, 139.8, 134.0, 131.8, 129.4, 126.8 (aryl *C*), 84.4 (pinacolato *C*), 83.3, 75.4 (cage *C*), 25.1 (pinacolato *C*H_3), 22.3, 15.2 (*C*H_3). $^{11}B\{^{1}H\}$ NMR (160 MHz, $CDCl_3$): δ -31.6 (1B) (*B*pin), -2.7 (1B) (*B*-C), -4.9 (1B), -6.0 (3B), -10.0 (4B), -12.6 (1B). HRMS: *m*/*z* calcd for $C_{20}H_{32}B_{11}NO_2$ $[M+H]^+$: 438.3608. Found: 438.3613.

Reaction of 3m with Styrene. Compound **3m** (39.0 mg, 0.10 mmol), styrene (12.5 mg, 0.12 mmol, 1.2 equiv), $PdCl_2(PPh_3)_2$ (7.0 mg, 0.01 mmol, 10 mol%), and potassium carbonate (55.0 mg, 0.40 mmol, 4.0 equiv) were mixed in toluene (2 mL). The resultant mixture was stirred at 130 ^{o}C under Ar for 12 h. The reaction mixture was allowed to cool to room temperature and filtered through a pad of Celite. The filtrate was then concentrated in vacuo, and purified by column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **7m** as a white solid (29.0 mg, 70%).



7m. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (m, 3H), 7.58 (d, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.30 (m, 3H) (aryl C*H* and alkenyl C*H*), 2.68 (s, 3H) (CH_3), 2.53 (m, 2H) (CH_2), 2.44 (s, 3H) (CH_3). $^{13}C\{^{1}H\}$ NMR (125 MHz, $CDCl_3$): δ 156.2, 145.6, 142.7, 140.3, 137.1, 136.2, 130.7, 130.5, 129.0, 128.3, 128.2, 127.8, 126.8, 126.6, 122.3 (aryl *C* and alkenyl *C*), 83.4, 75.3 (cage *C*), 22.3, 15.1 (*C*H_3). $^{11}B\{^{1}H\}$ NMR (128 MHz, $CDCl_3$): δ -3.1 (1B) (*B*-C), -6.5 (4B), -10.4 (4B), -13.0 (1B). HRMS: *m*/*z* calcd for $C_{22}H_{27}B_{10}N$ $[M-H]^-$: 412.3083. Found: 412.3085.

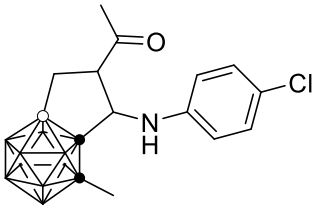
Homo-coupling Reaction of 3m. A solution of $NiCl_2$ (13.0 mg, 0.10 mmol, 1.0 equiv) and PPh_3 (105.0 mg, 0.40 mmol, 4.0 equiv) in DMF (3 mL) was stirred at 50 ^oC under Ar for 0.5 h. The resulting blue suspension was treated with Zn dust (6.5 mg, 0.10 mmol, 1.0 equiv) to produce a red-brown suspension, which was stirred for another 0.5 h. To which was added a solution of **3a** (39.0 mg, 0.10 mmol) in DMF (2 mL), and the resulting mixture was stirred at 50 ^oC under Ar overnight. The reaction was quenched by aqueous ammonia solution (2 M, 5 mL) and extracted with diethyl ether (5 mL x 3). The organic portions were combined, washed with water (5 mL x 3), dried with $MgSO_4$ and evaporated to dryness. The residue was purified by column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give the product **8m** as a white solid (25.5 mg, 83%).



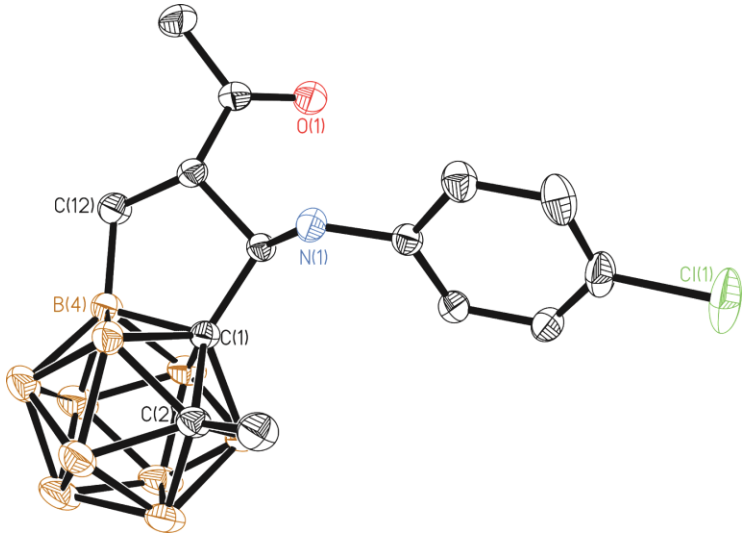
8m. ^1H NMR (500 MHz, $CDCl_3$): δ 8.26 (s, 2H), 8.16 (d, *J* = 8.5 Hz, 2H), 8.05 (d, *J* = 8.5 Hz, 2H) (aryl C*H*), 2.75 (s, 6H) (CH_3), 2.57 (m, 4H) (CH_2), 2.46 (s, 6H) (CH_3). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 156.9, 145.3, 143.1, 140.5, 139.6, 131.1, 128.9, 127.8, 122.3 (aryl *C*), 83.2, 75.4 (cage *C*), 22.3, 15.2 (*C*H_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -2.7 (2B) (*B*-C), -5.9 (8B), -9.9 (8B), -12.2 (2B). HRMS: *m*/*z* calcd for $C_{28}H_{40}B_{20}N_2$ $[M-H]^-$: 619.5142. Found: 619.5142.

Supplementary Discussion

Control Experiments. **Isolation of the Reaction Intermediate D**. Carboranyl *N*-4-chlorophenylimine **1a** (29.5 mg, 0.10 mmol), 2-butenone (42.0 μL, 0.50 mmol, 5.0 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (34.4 mg, 0.10 mmol, 1.0 equiv) and $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 30 min under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The obtained filtrate was concentrated to dryness in vacuo and subjected to column chromatography on silica gel (230-400 mesh) using *n*-hexane and ether acetate (100 : 1 to 5 : 1 in V/V) as eluent to give intermediate **D** (10.5 mg, 28%) and **3a** (5.2 mg, 15%).



D. Colorless crystals. ^1H NMR (500 MHz, $CDCl_3$): δ 7.14 (d, *J* = 8.5 Hz, 2H), 6.58 (d, *J* = 8.0 Hz, 2H) (aryl C*H*), 5.21 (t, *J* = 9.0 Hz, 1H) (C*H*), 3.48 (d, *J* = 8.5 Hz, 1H) (N*H*), 3.23 (m, 1H) (C*H*), 2.19 (s, 3H), 1.95 (s, 3H) (CH_3), 1.73 (dd, *J* = 10.0, 14.0 Hz, 1H), 1.23 (t, *J* = 13.5 Hz, 1H) (CH_2). $^{13}C\{^1H\}$ NMR (125 MHz, $CDCl_3$): δ 205.5 (carbonyl *C*), 143.9, 129.8, 124.0, 114.0 (aryl *C*), 82.8, 77.8 (cage *C*), 67.4, 61.0 (*C*H), 28.6, 23.5 (CH_3). $^{11}B\{^1H\}$ NMR (160 MHz, $CDCl_3$): δ -1.2 (1B) (*B*-C), -5.3 (2B), -7.5 (2B), -11.5 (3B), -12.5 (1B), -13.5 (1B). HRMS: *m*/*z* calcd for $C_{14}H_{24}B_{10}ClNO$ $[M+H]^+$: 366.2626. Found: 366.2633.



Supplementary Figure 3. Molecular structure of **D** drawn with 30% probability ellipsoids.

Further Transformation of Intermediate D. Compound **D** (36.5 mg, 0.10 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (34.4 mg, 0.10 mmol, 1.0 equiv), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was concentrated to dryness in vacuo and analyzed by ^1H NMR spectroscopy. Product **3a** was detected in 95% yield using dibromomethane as an internal standard.

Compound **D** (36.5 mg, 0.10 mmol), $AgSbF_6$ (34.4 mg, 0.10 mmol, 1.0 equiv), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was diluted

with ethyl acetate and subjected to GC-MS analysis. Only trace amount of product **3a** was detected.

Compound **D** (36.5 mg, 0.10 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was diluted with ethyl acetate and subjected to GC-MS analysis. Only trace amount of product **3a** was detected.

Compound **D** (36.5 mg, 0.10 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (34.4 mg, 0.10 mmol, 1.0 equiv), and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was concentrated to dryness in vacuo and analyzed by ^1H NMR spectroscopy. Product **3a** was detected in 43% yield using dibromomethane as an internal standard.

Compound **D** (36.5 mg, 0.10 mmol), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (68.8 mg, 0.20 mmol, 2.0 equiv), and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^oC for 6 h under argon. After cooling to room temperature and the addition of 0.1 mL of pyridine, the reaction mixture was filtered through a pad of Celite. The filtrate was

concentrated to dryness in vacuo and analyzed by ^{1}H NMR spectroscopy. Product **3a** was detected in 84% yield using dibromomethane as an internal standard.

Kinetic Isotope Experiment. Compounds **1l** (26.1 mg, 0.10 mmol, 1.0 equiv), **1l**-d_5 (26.6 mg, 0.10 mmol, 1.0 equiv), 2-butenone (42.0 μL, 0.50 mmol, 5.0 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (17.2 mg, 0.05 mmol, 0.5 equiv), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv) and 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^{o}C for 1 h under argon. After cooling to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The filtrate was concentrated to dryness in vacuo and subjected to flash column chromatography on silica gel (230-400 mesh) using *n*-hexane and dichloromethane (10 : 1 in V/V) as eluent to give **3l / 3l**-d_4 as a white solid (6.0 mg, 19%). The KIE value k_H/k_D = 1.7 was measured according to ^{1}H NMR spectroscopy.

Radical Scavenger Experiment. Compounds **1a** (29.5 mg, 0.10 mmol), 2-butenone (42.0 μL, 0.50 mmol, 5.0 equiv), $[Cp^*RhCl_2]_2$ (3.1 mg, 0.005 mmol, 5 mol%), $AgSbF_6$ (34.4 mg, 0.10 mmol, 1.0 equiv), $Cu(OPiv)_2$ (66.0 mg, 0.25 mmol, 2.5 equiv), 2,4,6-trimethylbenzoic acid (8.2 mg, 0.05 mmol, 0.5 equiv) and 1,1-diphenylethene (18.0 mg, 0.10 mmol, 1.0 equiv) were mixed in 1,4-dichlorobutane (2 mL). The resulting mixture was stirred at 90 ^{o}C for 6 h under argon. After cooling to room temperature and the addition of pyridine (0.1 mL), the reaction mixture was filtered through a pad of Celite and washed with dichloromethane. The filtrate

was concentrated to dryness in vacuo and analyzed by ^{1}H NMR spectroscopy. Product **3a** was detected in 73% yield using dibromomethane as an internal standard.

X-ray Structure Determination. X-ray data of **3l**, **3w**, and **D** were collected at 293 K on a Bruker SMART 1000 CCD diffractometer using Cu-Kα radiation. An empirical absorption correction was applied using the SADABS program.[4] All structures were solved by direct methods and subsequent Fourier difference techniques and refined anisotropically for all non-hydrogen atoms by full-matrix least squares calculations on F^2 using the SHELXTL program package.[5] All hydrogen atoms were geometrically fixed using the riding model.

CCDC 1823584-1823586 (**3l**, **3w**, and **D**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Supplementary References

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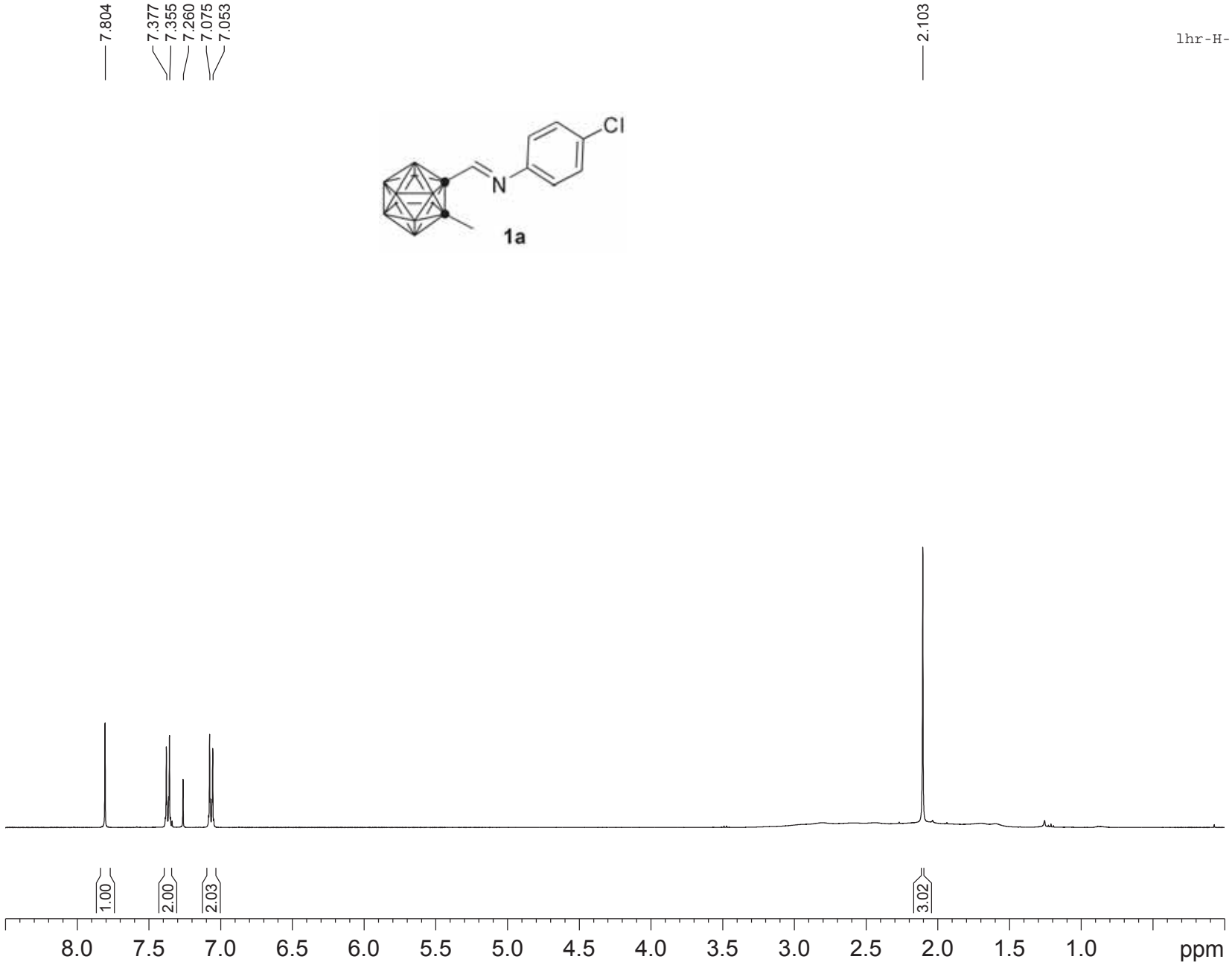
4. G. M. Sheldrick, SADABS: Program for Empirical Absorption Correction of Area Detector Data. University of Göttingen: Germany, 1996.
5. G. M. Sheldrick, SHELXTL 5.10 for Windows NT: Structure Determination Software Programs. Bruker Analytical X-ray Systems, Inc., Madison, Wisconsin, USA, 1997.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7.355
7.260
7.075
7.053
2.103
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N
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PROCNO 1
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Date_ 20160622
Time 20.20 h
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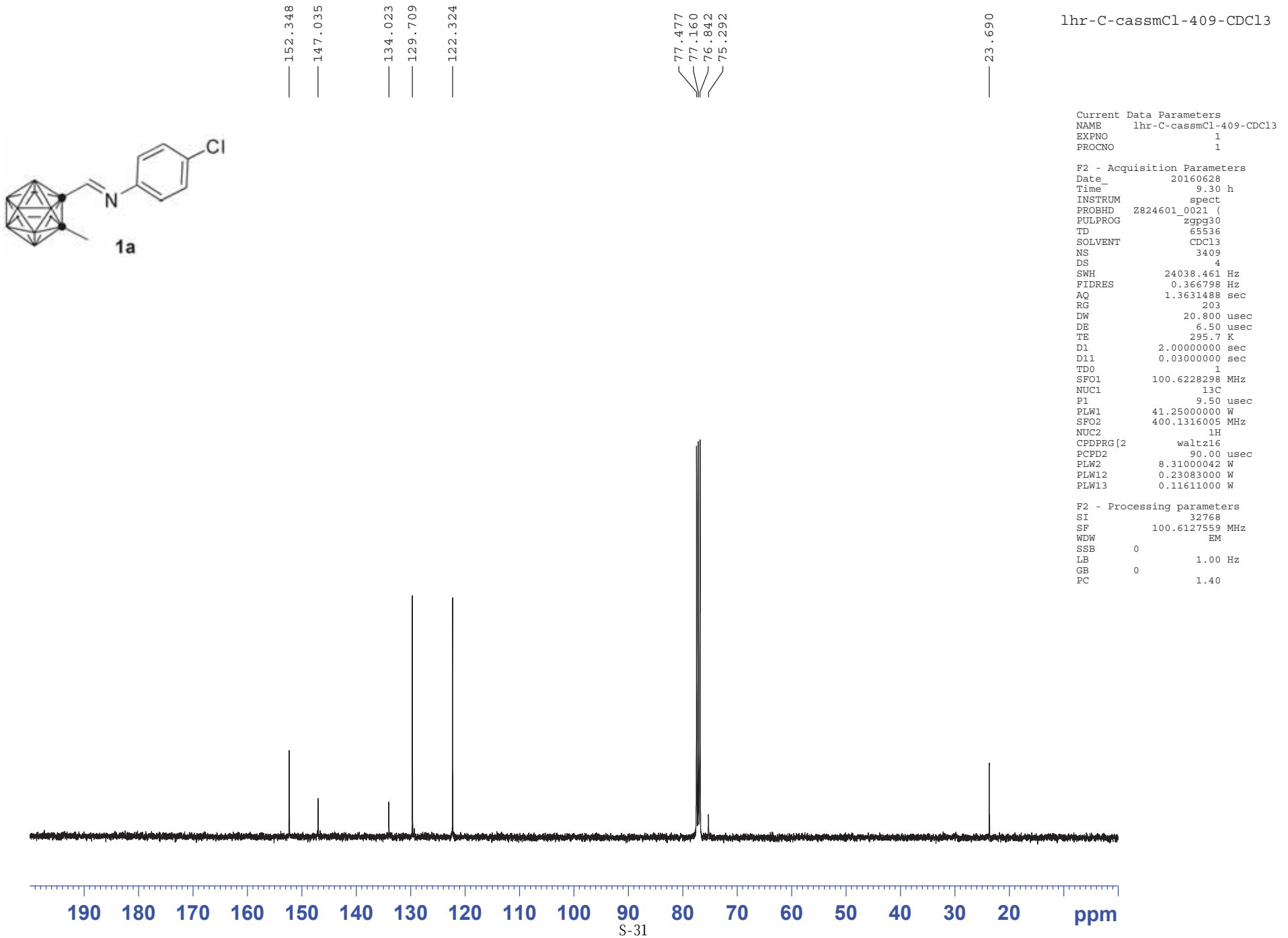
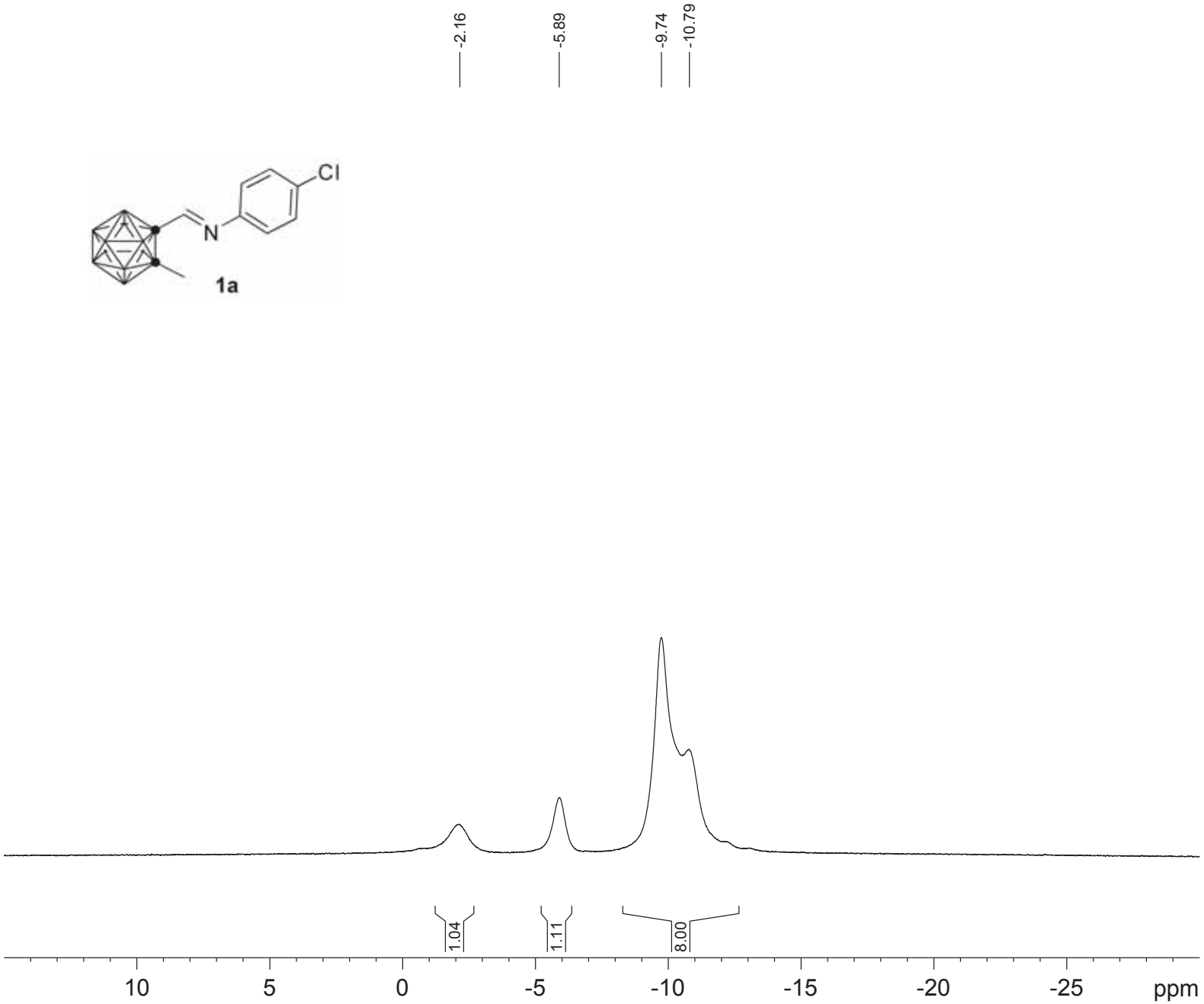
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.00
2.00
2.03
3.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

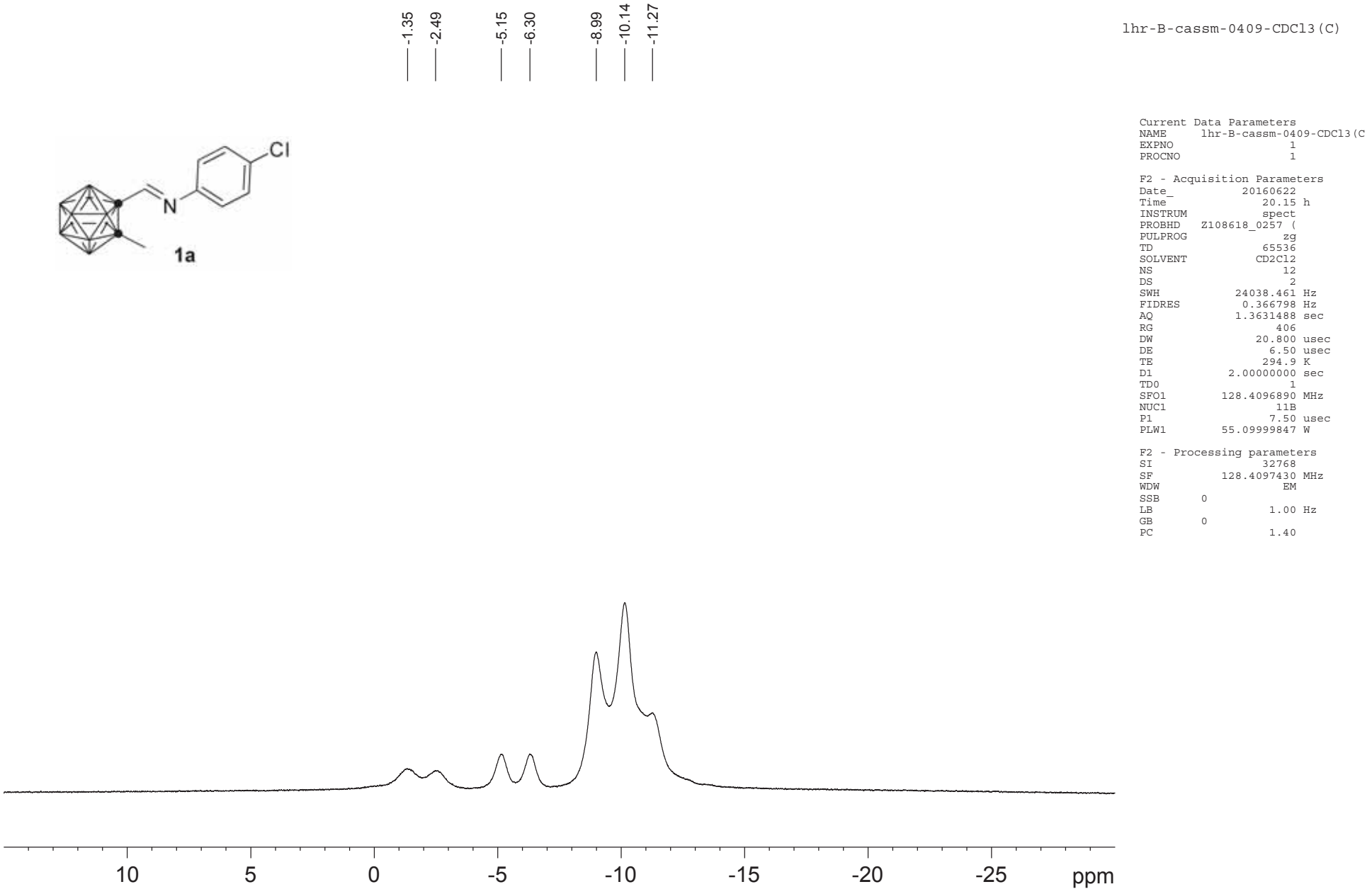

152.348
147.035
134.023
129.709
122.324
77.477
77.160
76.842
75.292
23.690
lhr-C-cassmCl-409-CDCl3
Cl
N
1a
Current Data Parameters
NAME lhr-C-cassmCl-409-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160628
Time 9.30 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 3409
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W
F2 - Processing parameters
SI 32768
SF 100.6127559 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

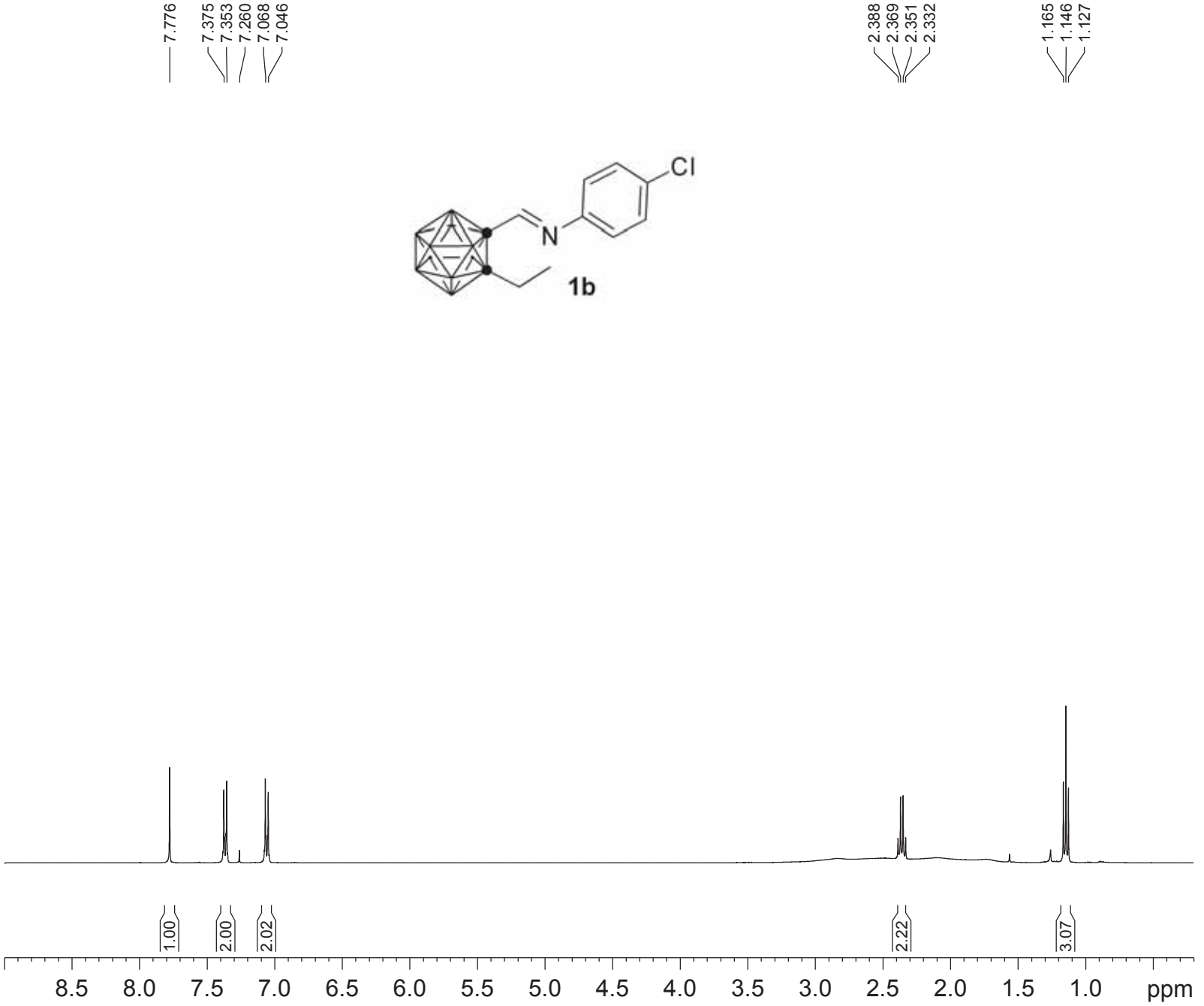
1a



lhr-B-cassm-0409-CDCl3

```
Current Data Parameters
NAME      lhr-B-cassm-0409-CDCl
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160622
Time                 20.14 h
INSTRUM                spect
PROBHD   Z108618_0257 (
PULPROG                zgdc
TD                    65536
SOLVENT             CD2Cl2
NS                        12
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                      287
DW                   20.800 usec
DE                    6.50 usec
TE                   295.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1            128.4096890 MHz
NUC1                    11B
P1                    7.50 usec
PLW1            55.09999847 W
SFO2            400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2            13.56000042 W
PLW12            0.27428001 W

F2 - Processing parameters
SI                     32768
SF              128.4097615 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


-1.35
-2.49
-5.15
-6.30
-8.99
-10.14
-11.27
lhr-B-cassm-0409-CDCl3(C)
Current Data Parameters
NAME lhr-B-cassm-0409-CDCl3(C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160622
Time 20.15 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CD2Cl2
NS 12
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 406
DW 20.800 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
TD0 1
SFO1 128.4096890 MHz
NUC1 11B
P1 7.50 usec
PLW1 55.09999847 W
F2 - Processing parameters
SI 32768
SF 128.4097430 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
N
1a
10
5
0
-5
-10
-15
-20
-25
ppm

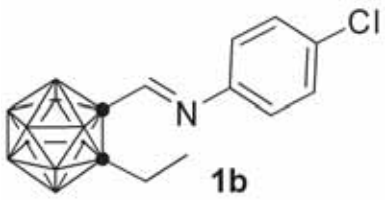


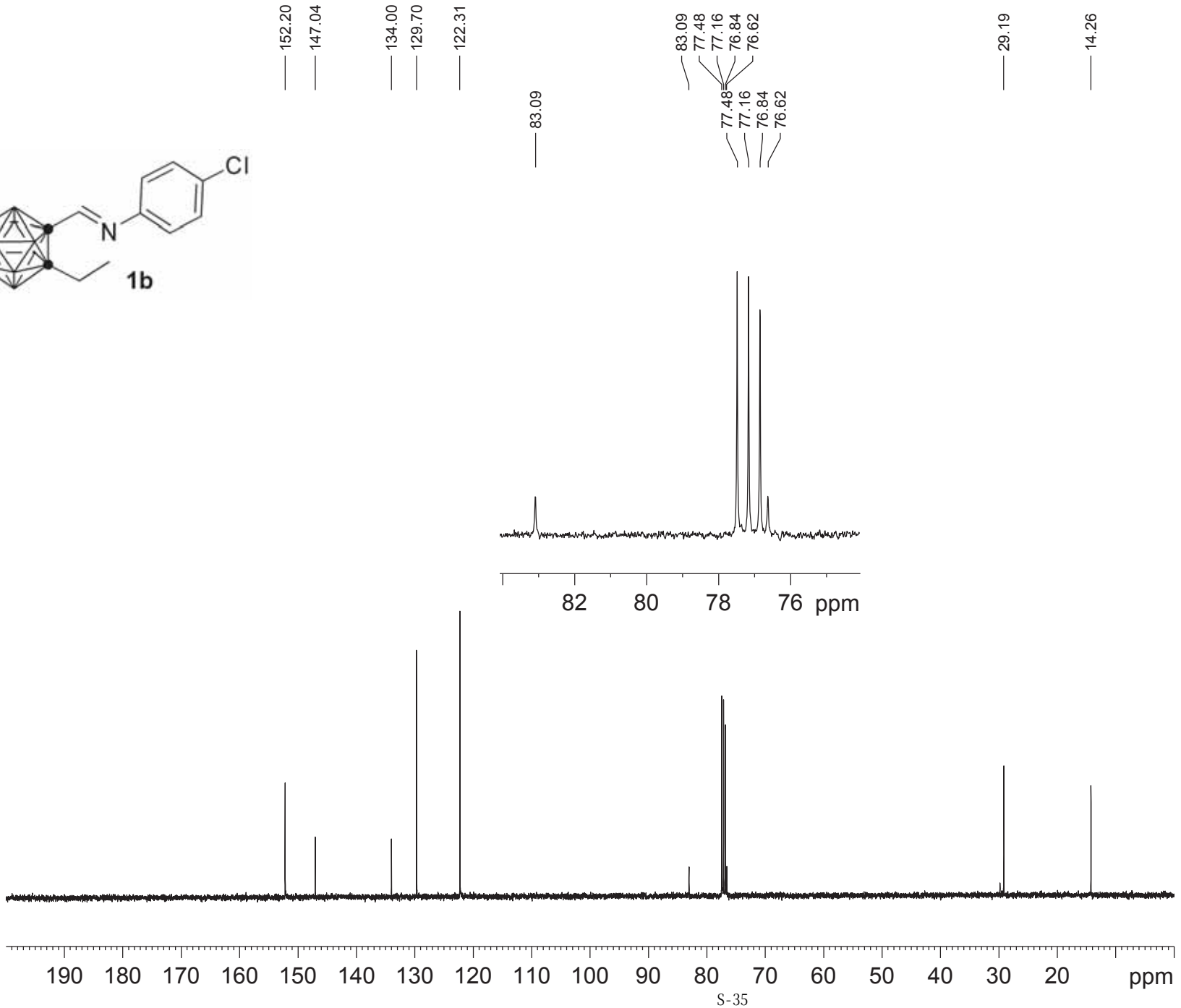
lhr-H-cassm716-CDCl3

Current Data Parameters
NAME lhr-H-cassm716-CDCl3et
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170814
Time 10.36 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

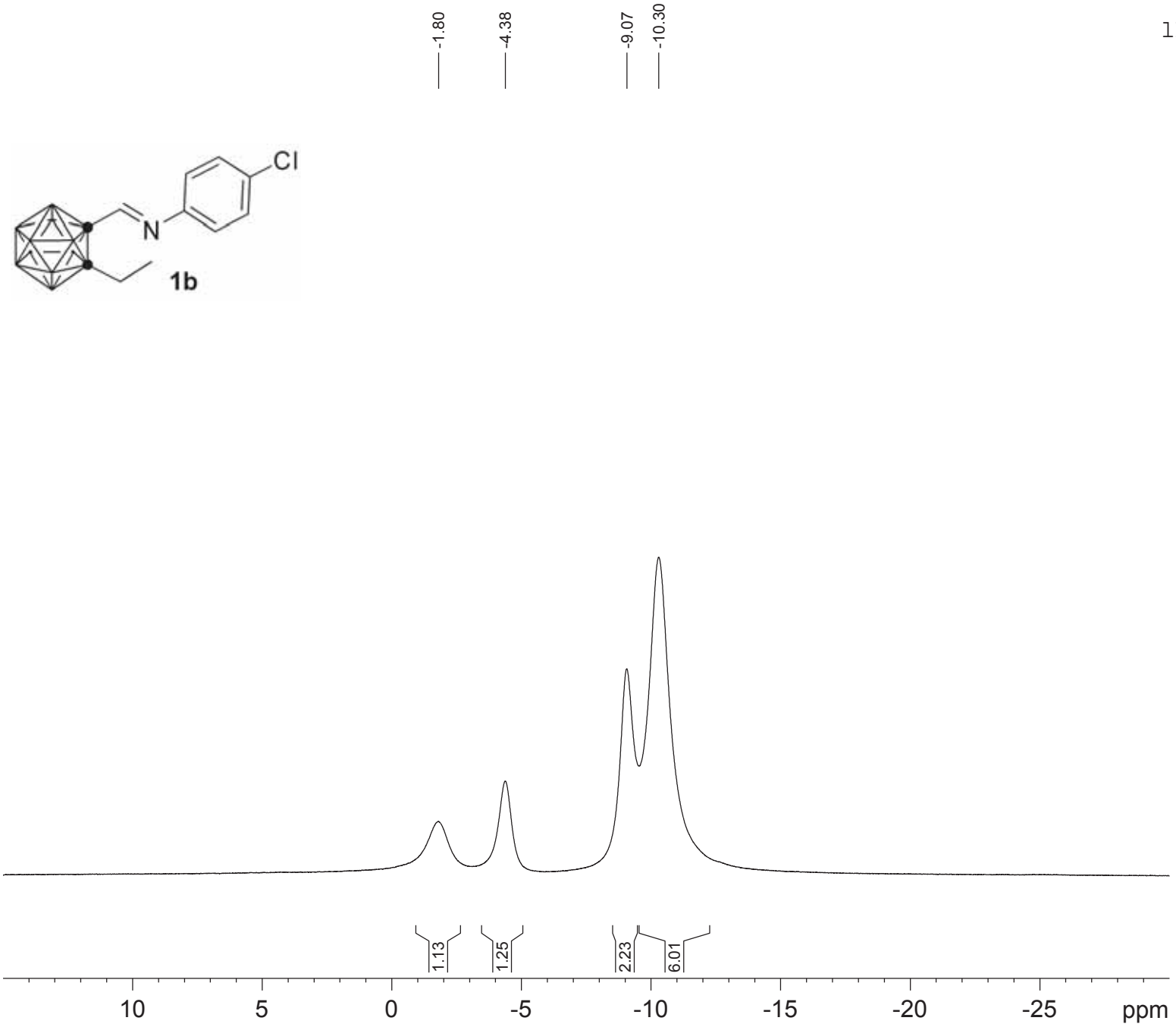
F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





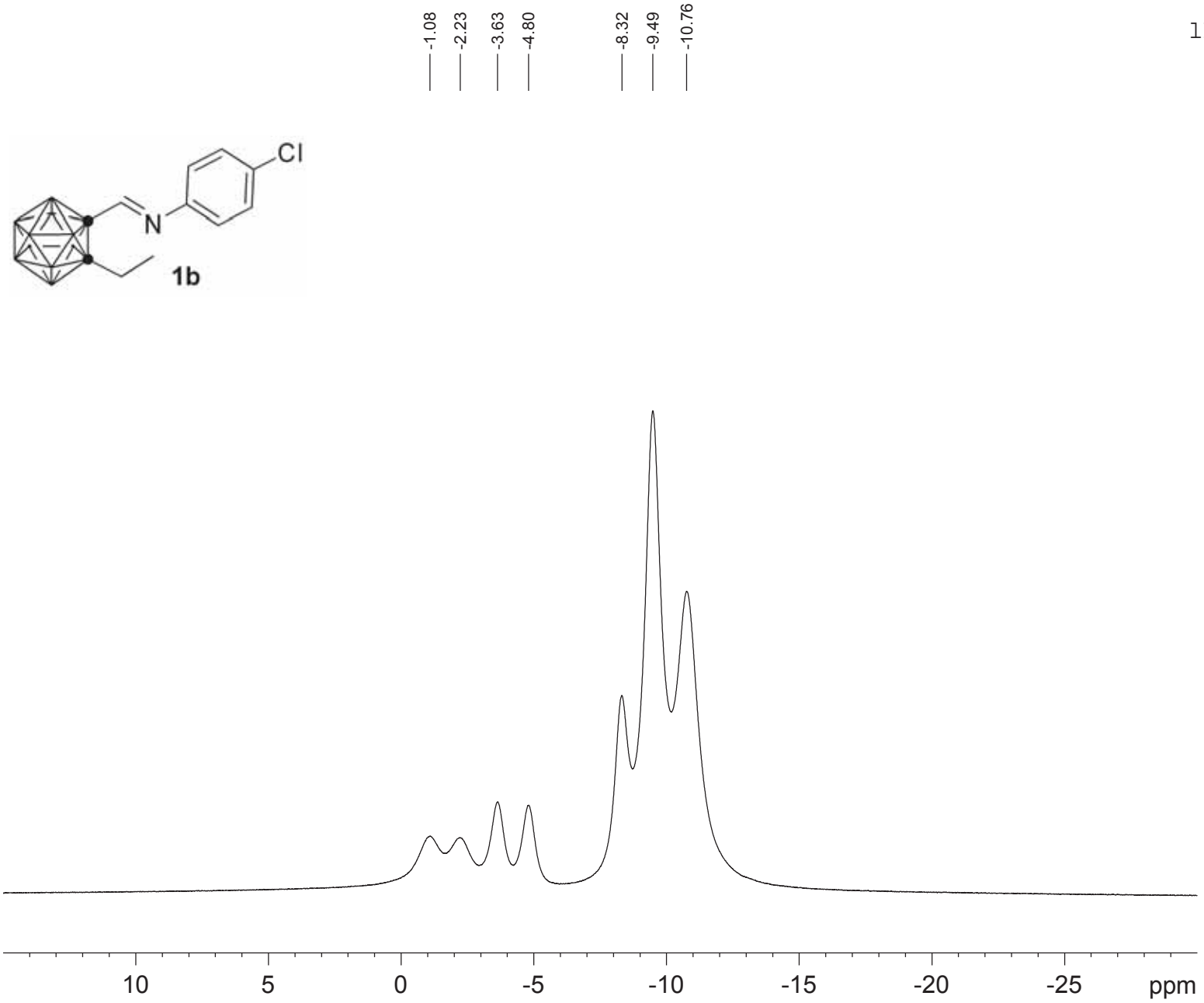
lhr-C-cassm716-CDC

```
Current Data Parameters
NAME      lhr-C-cassm716-CDCl3et
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20170814
Time                   10.39 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        80
DS                         4
SWH                40760.871 Hz
FIDRES              0.621962 Hz
AQ                  0.8039083 sec
RG                       161
DW                    12.267 usec
DE                     6.50 usec
TE                     295.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1             100.6479773 MHz
NUC1                     13C
P1                     9.50 usec
PLW1             55.34000015 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             13.56000042 W
PLW12             0.27428001 W
PLW13             0.13796000 W

F2 - Processing parameters
SI                     32768
SF               100.6379029 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



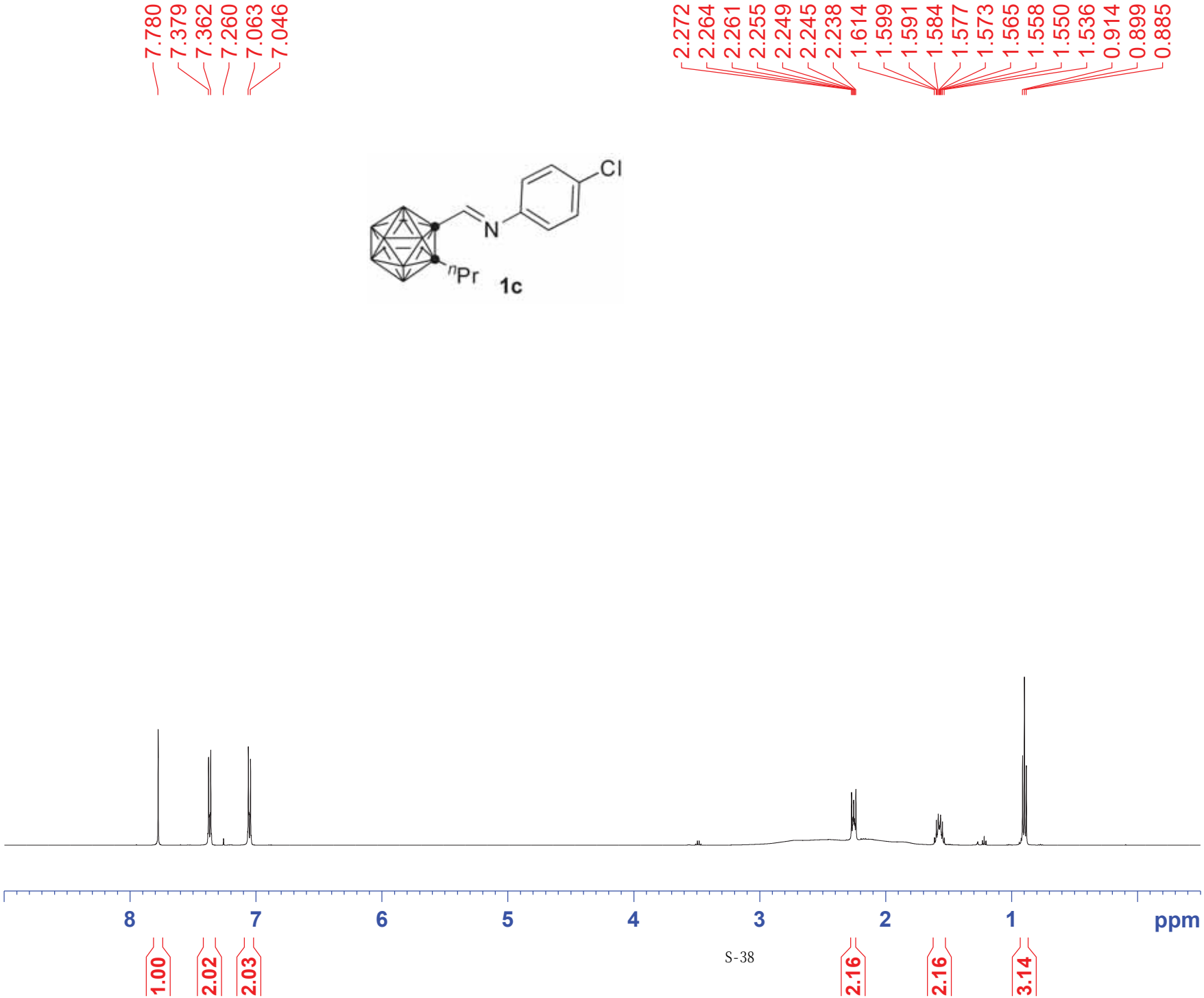
lhr-B-cassm716-CDCl3et

```
Current Data Parameters
NAME      lhr-B-cassm716-CDCl3et
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20170814
Time                       10.29 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                     zgdc
TD                         65536
SOLVENT                     C6D6
NS                            15
DS                             4
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3631488 sec
RG                           203
DW                        20.800 usec
DE                         6.50 usec
TE                        295.3 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                            1
SFO1                128.4096890 MHz
NUC1                        11B
P1                         7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

F2 - Processing parameters
SI                         32768
SF                  128.4097615 MHz
WDW                           EM
SSB               0
LB                         1.00 Hz
GB                0
PC                         1.40
```



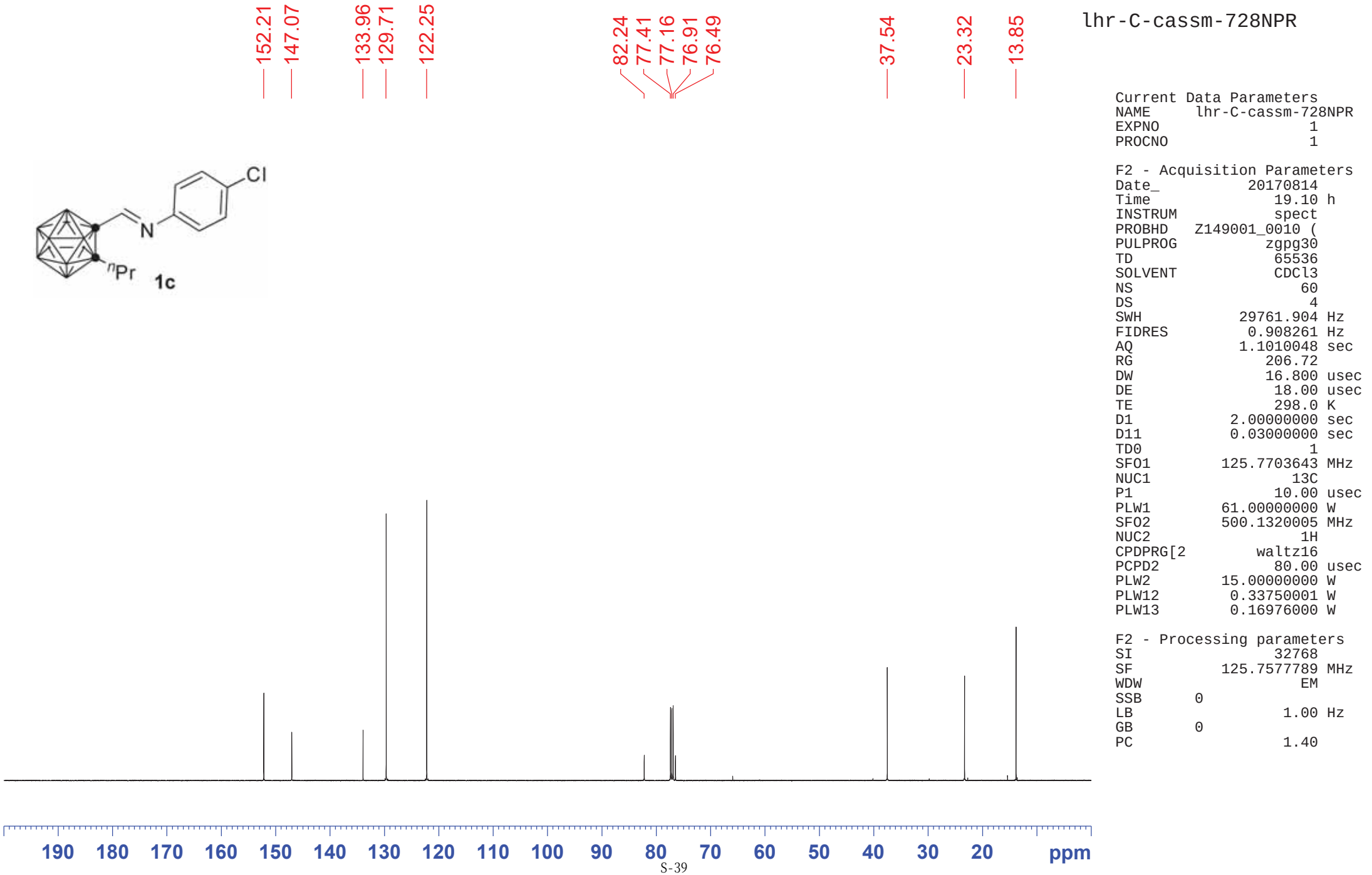
lhr-B-cassm716-CDCl3et(C)

```
Current Data Parameters
NAME      lhr-B-cassm716-CDCl3et(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170814
Time              10.31 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                 65536
SOLVENT             C6D6
NS                    28
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1           2.00000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                 32768
SF          128.4097430 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



lhr-H-cassm-728NPR

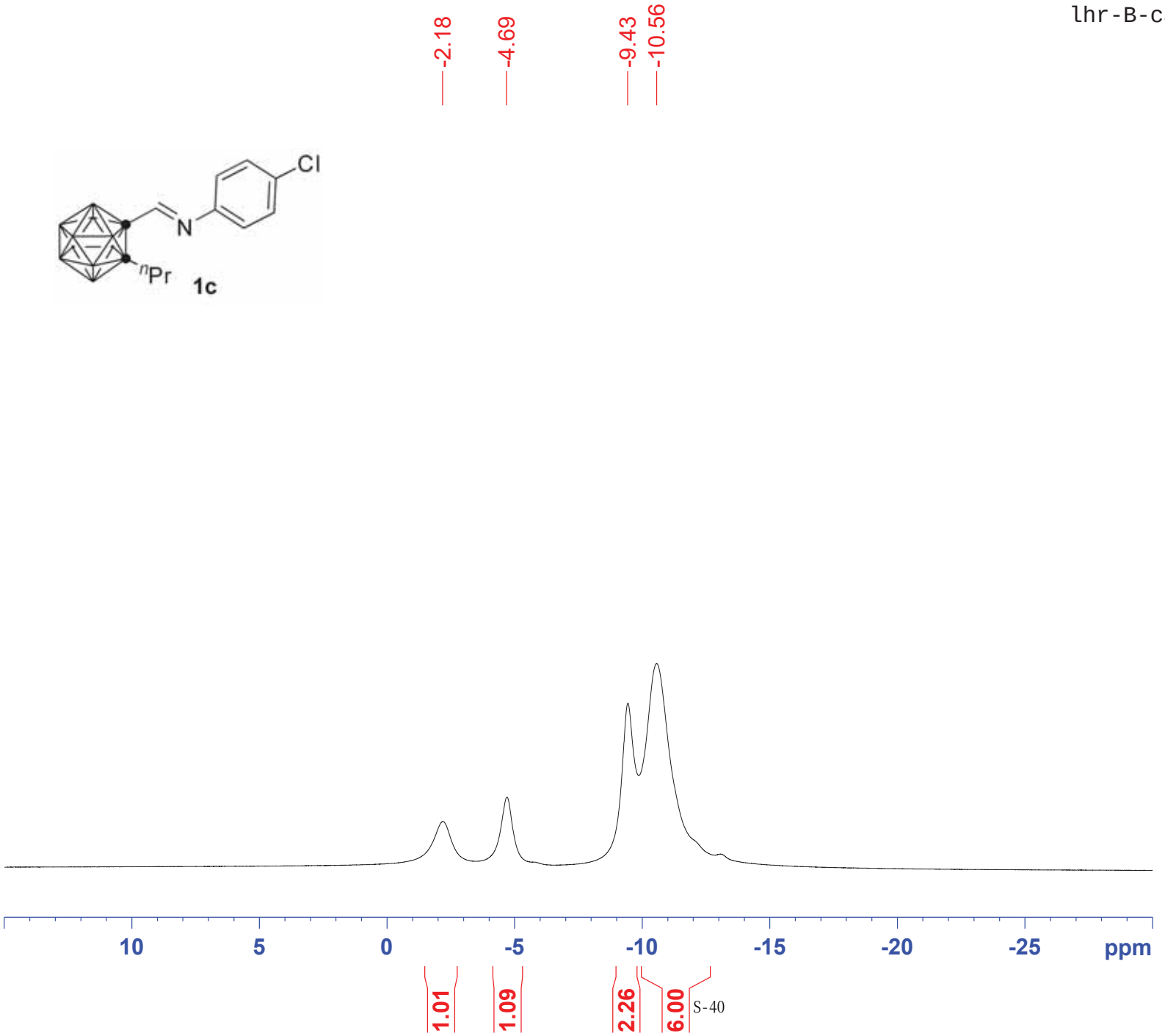
```
Current Data Parameters
NAME      lhr-H-cassm-728
EXPNO                   1
PROCNO                  1

F2 - Acquisition Paramet
Date_            20170814
Time                19.04
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 14.97
DW                 50.000
DE                 10.00
TE                 298.0
D1            1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1         15.00000000

F2 - Processing paramete
SI                 65536
SF         500.1300127
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```



lhr-C-cassm-728NPR

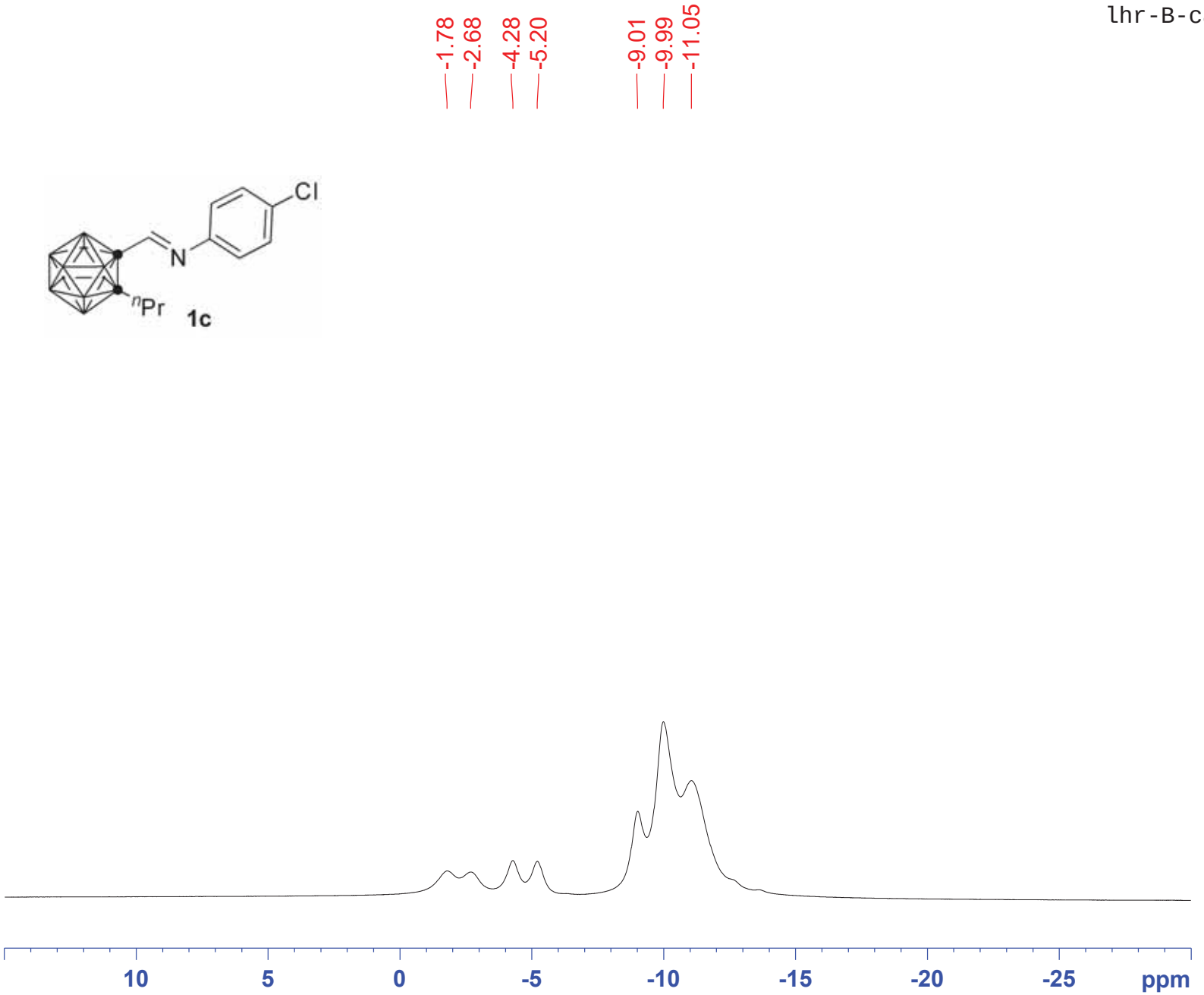
```
Current Data Parameters
NAME      lhr-C-cassm-728NPR
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20170814
Time              19.10 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577789 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-cassm-728NPR

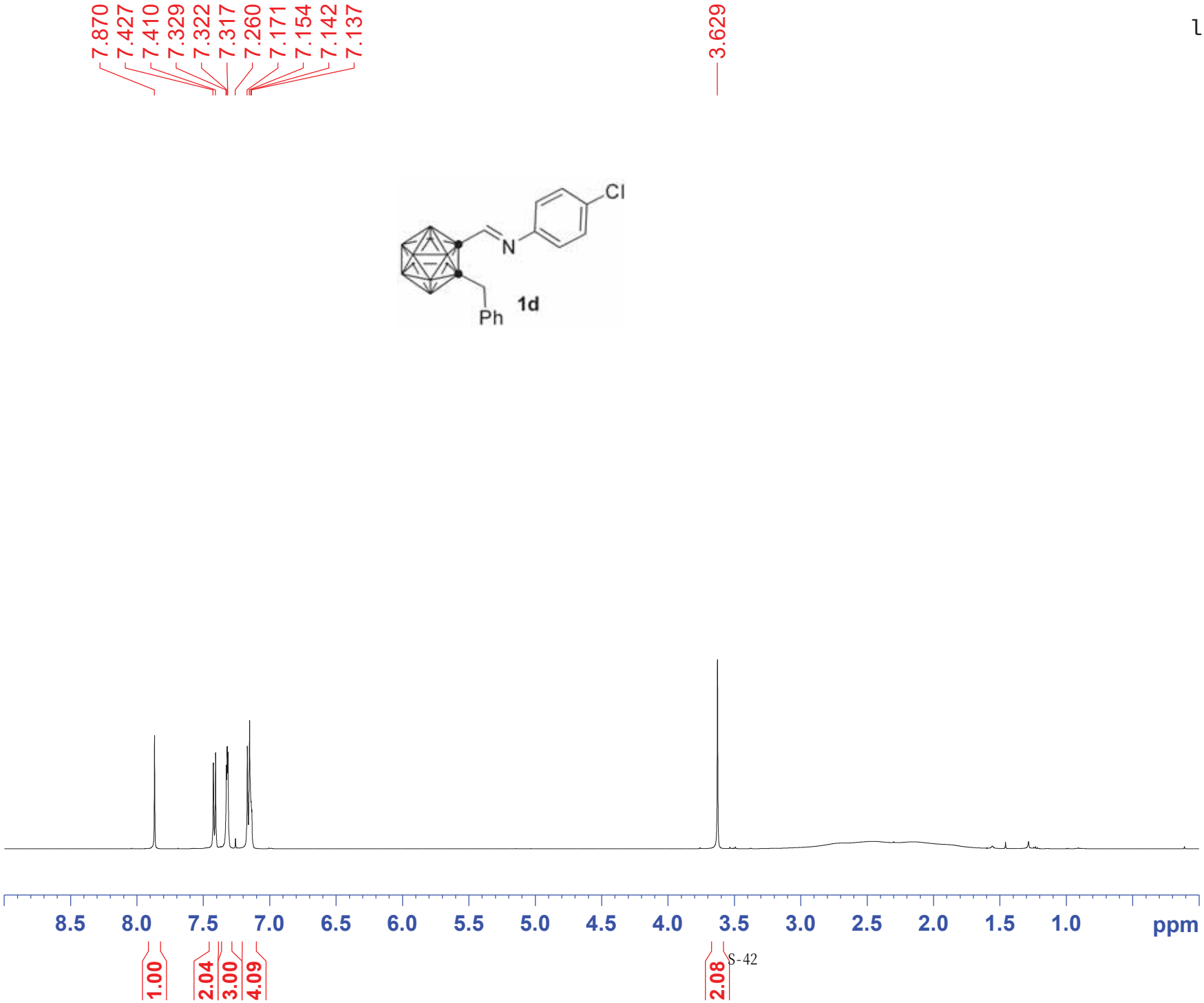



```
Current Data Parameters
NAME      lhr-B-cassm-728NPR
EXPNO                     2
PROCNO                    1

F2 - Acquisition Parameters
Date_            20170814
Time                19.13 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3762560 sec
RG                   50.6
DW                 21.000 usec
DE                 18.00 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          160.4599621 MHz
NUC1                11B
P1                 10.00 usec
PLW1           50.00000000 W
SFO2           500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W

F2 - Processing parameters
SI                    32768
SF            160.4615719 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-cassm-728NPR(c)

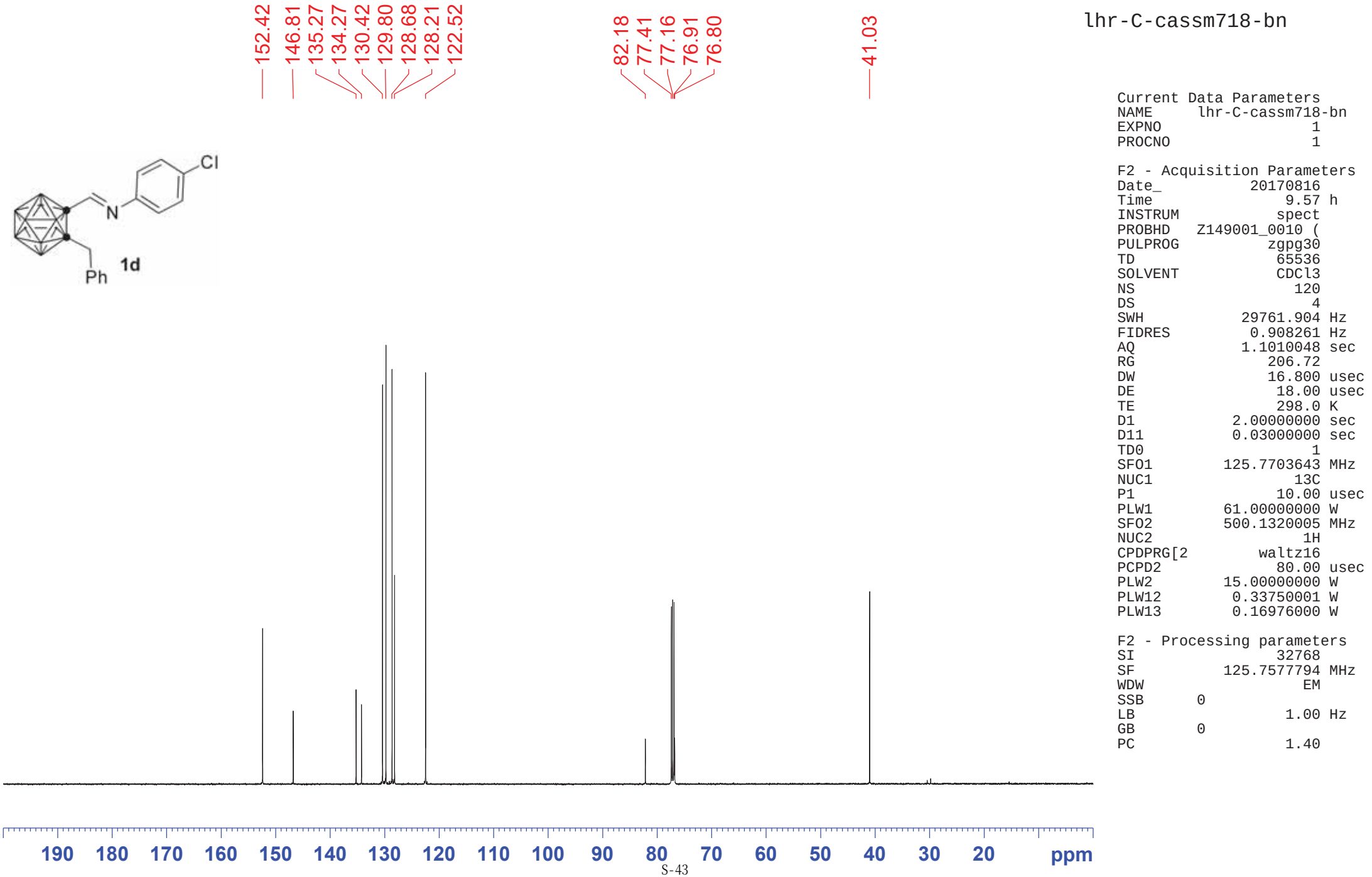



```
Current Data Parameters
NAME      lhr-B-cassm-728NPR(c)
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170814
Time                   19.14 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        12
DS                         4
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                 0.6815744 sec
RG                     56.83
DW                    20.800 usec
DE                    18.00 usec
TE                    298.0 K
D1               1.00000000 sec
TD0                        1
SFO1             160.4615792 MHz
NUC1                     11B
P1                    10.00 usec
PLW1            50.00000000 W

F2 - Processing parameters
SI                     16384
SF               160.4615792 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



lhr-H-cassm718-bn

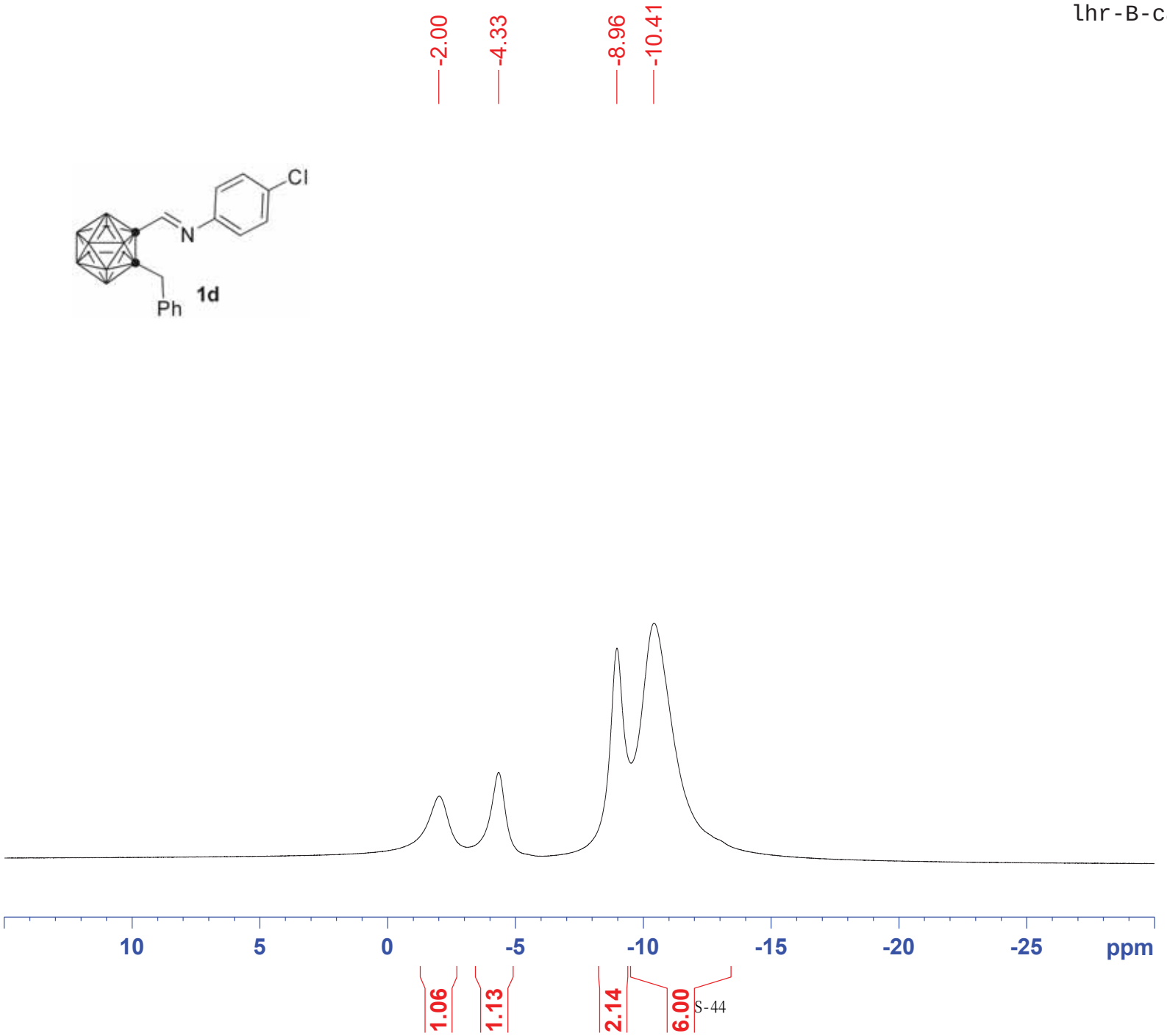
```
Current Data Parameters
NAME      lhr-H-cassm718-bn
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170816
Time                 9.49 h
INSTRUM              spect
PROBHD    Z149001_0010 (
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      12
DS                       2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ               3.2767999 sec
RG                   17.56
DW                   50.000 usec
DE                   10.00 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                      1
SFO1           500.1330883 MHz
NUC1                    1H
P1                   12.00 usec
PLW1           15.00000000 W

F2 - Processing parameters
SI                   65536
SF             500.1300127 MHz
WDW                     EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```



lhr-C-cassm718-bn

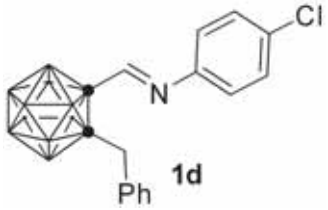
```
Current Data Parameters
NAME      lhr-C-cassm718-bn
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170816
Time                 9.57 h
INSTRUM              spect
PROBHD    Z149001_0010 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     120
DS                       4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                   13C
P1                  10.00 usec
PLW1           61.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W
PLW13           0.16976000 W

F2 - Processing parameters
SI                   32768
SF             125.7577794 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

lhr-B-cassm718-bn

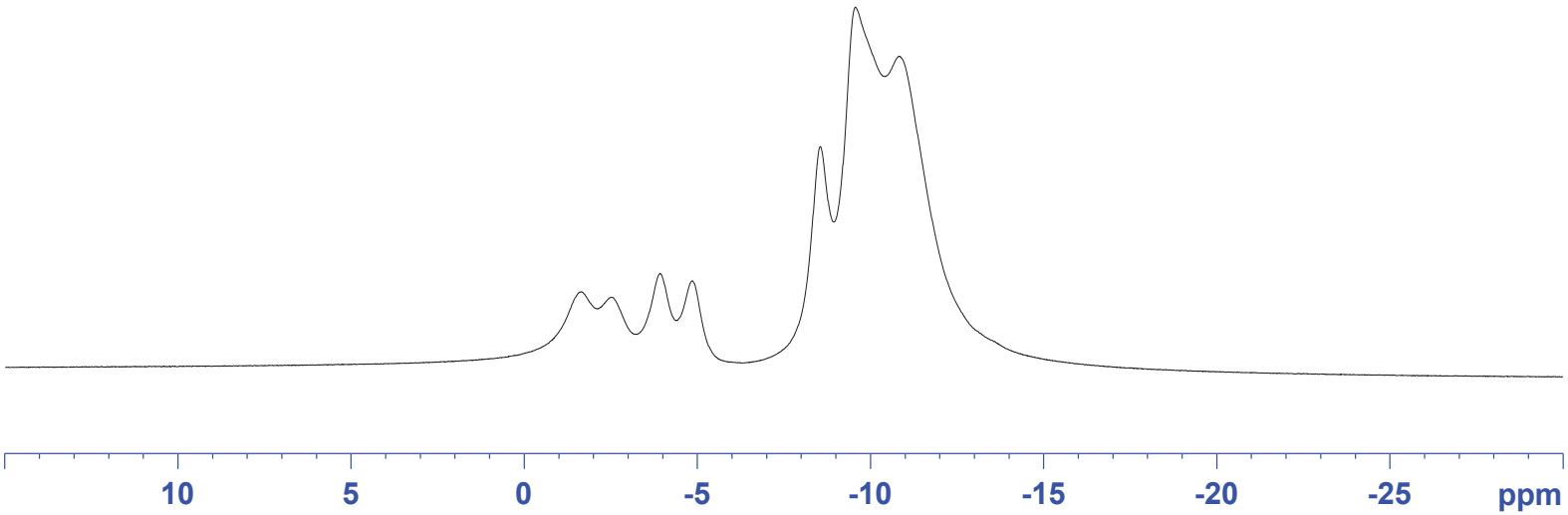


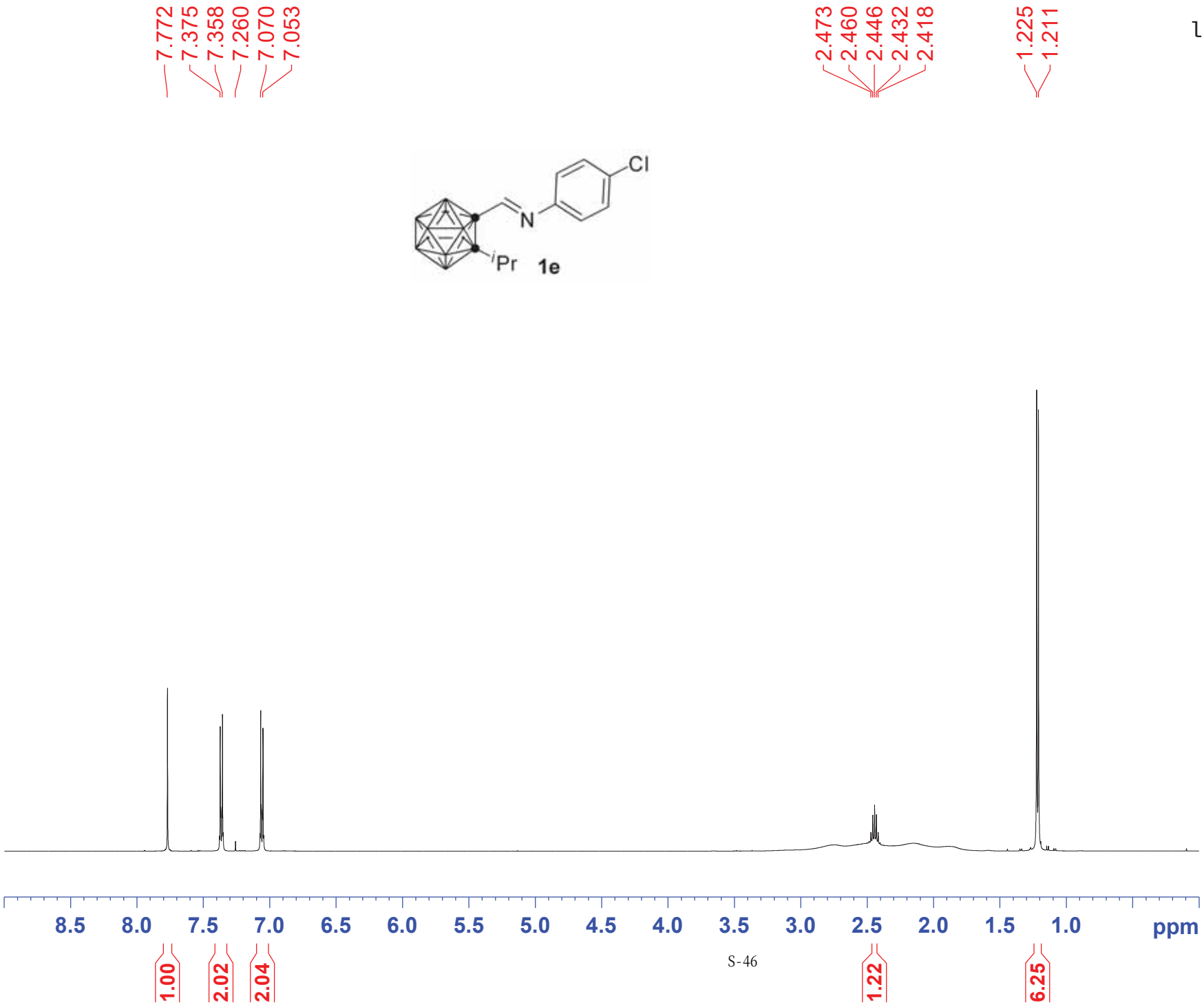

```
Current Data Parameters
NAME      lhr-B-cassm718-bn
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170816
Time                10.00 h
INSTRUM              spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3762560 sec
RG                  102.6
DW                 21.000 usec
DE                 18.00 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          160.4599621 MHz
NUC1                 11B
P1                 10.00 usec
PLW1           50.00000000 W
SFO2           500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W

F2 - Processing parameters
SI                   32768
SF            160.4615719 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-cassm718-bn(C)



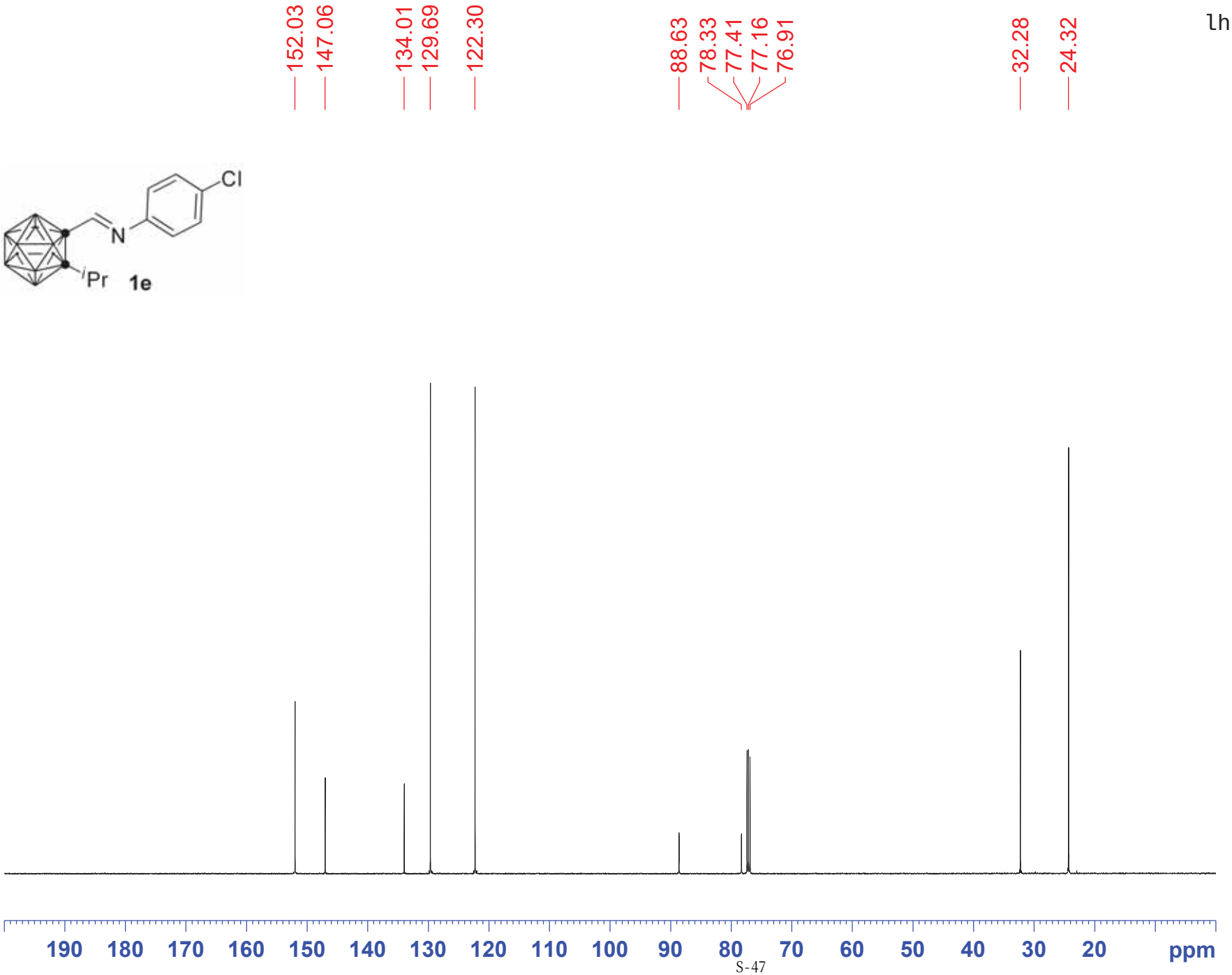

```
Current Data Parameters
NAME      lhr-B-cassm718-bn(C)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20170816
Time                10.01 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      12
DS                       4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                   102.6
DW                  20.800 usec
DE                  18.00 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                      1
SFO1          160.4615792 MHz
NUC1                  11B
P1                  10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                   16384
SF            160.4615792 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```





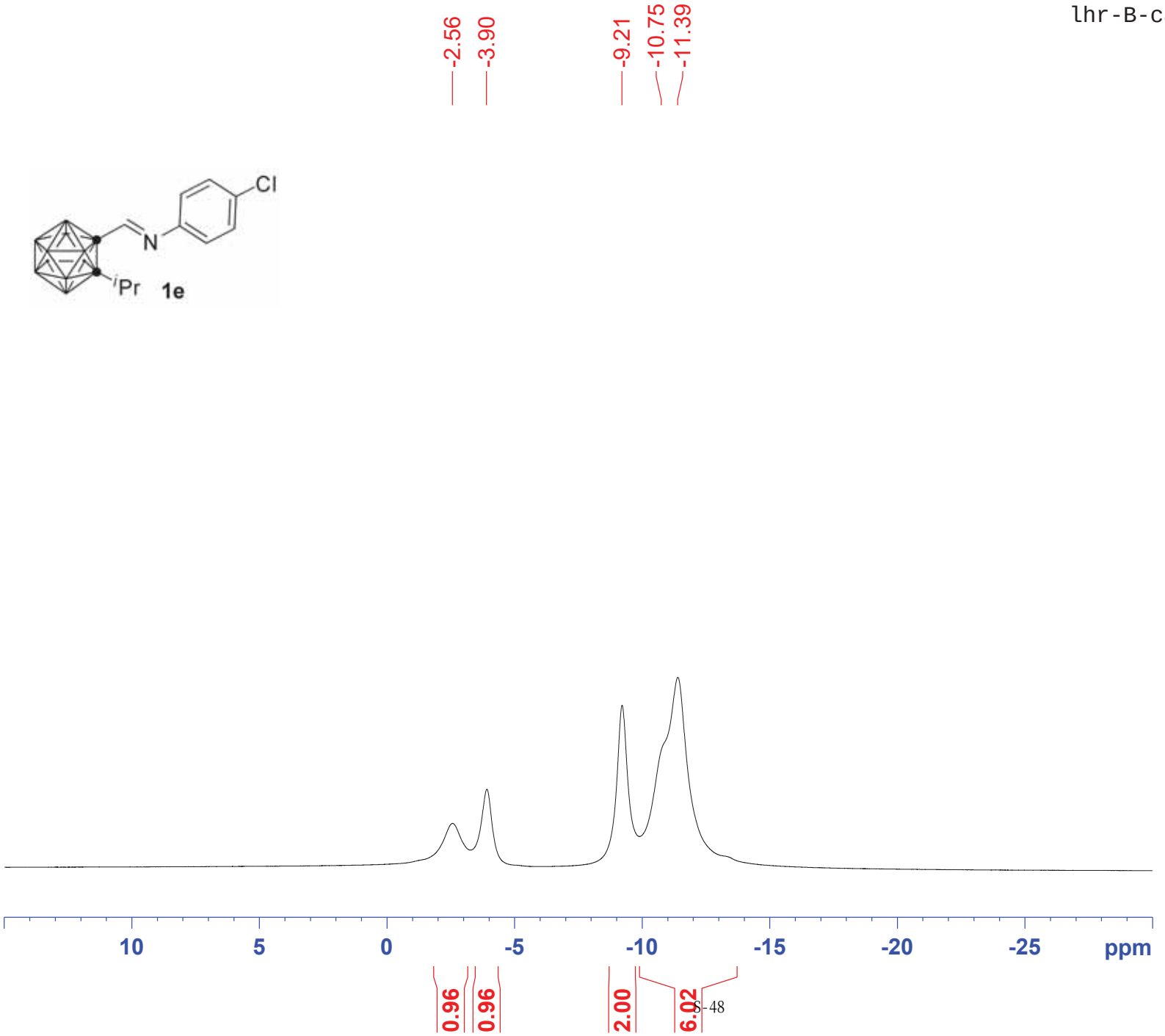
lhr-H-cassm734-ipr

```
Current Data Parameters
NAME      lhr-H-cassm734-ipr
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20170816
Time              10.06 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                 14.97
DW                50.000 usec
DE                10.00 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                  1H
P1                12.00 usec
PLW1         15.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300125 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



lhr-C-cassm734-ipr

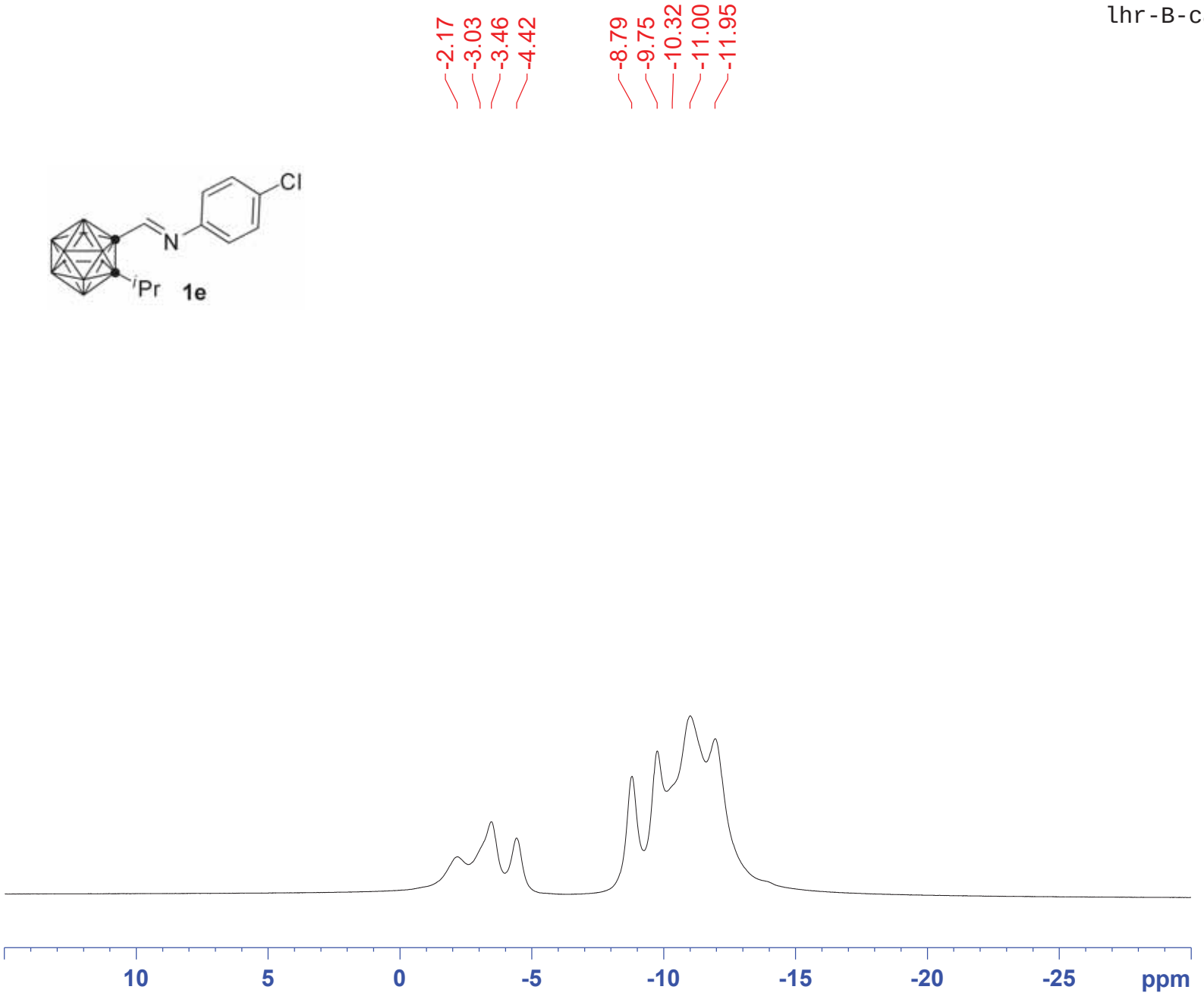
```
Current Data Parameters
NAME      lhr-C-cassm734-ipr
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20170816
Time              10.14 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   120
DS                     4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                 32768
SF          125.7577792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



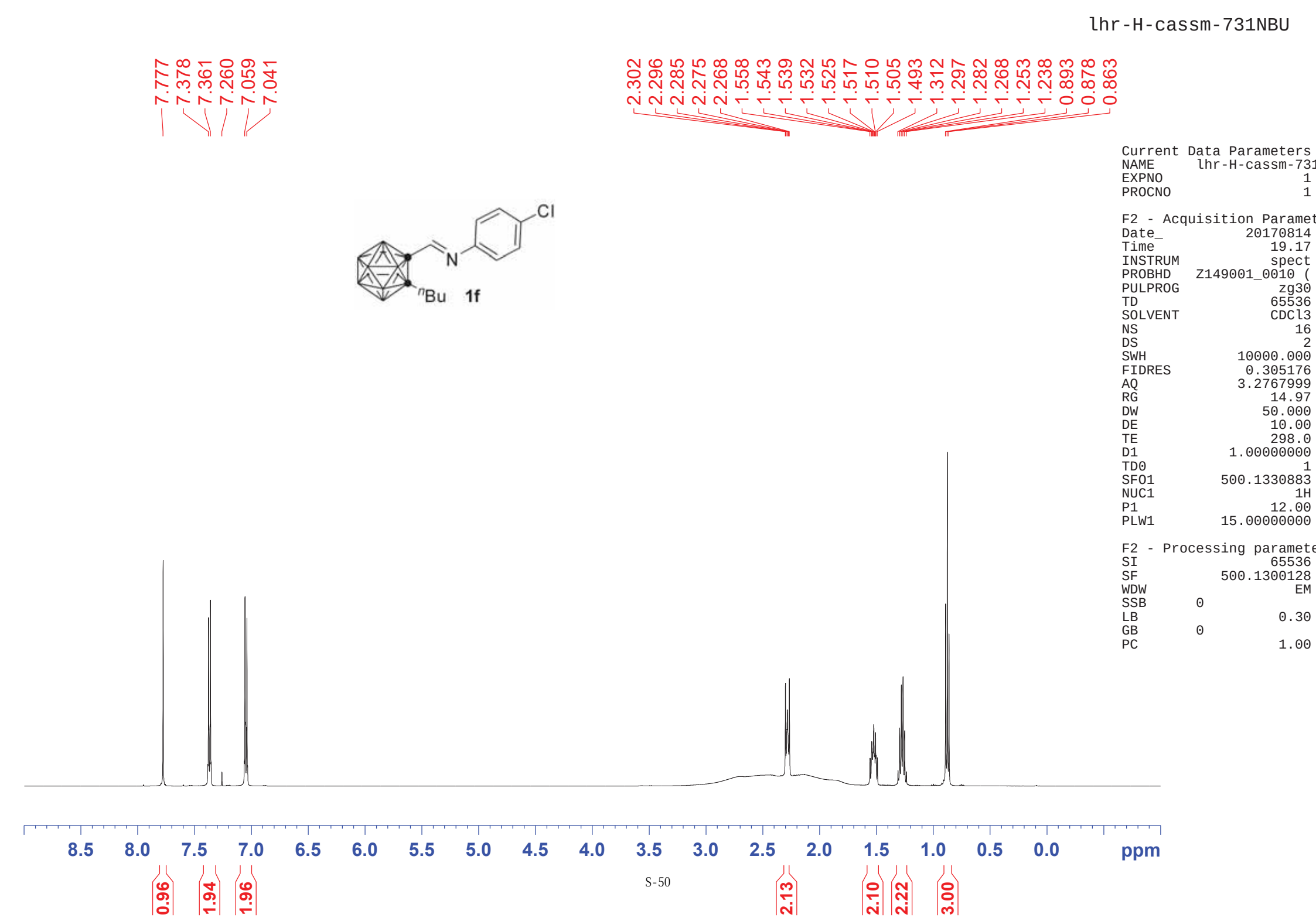
lhr-B-cassm734-ipr

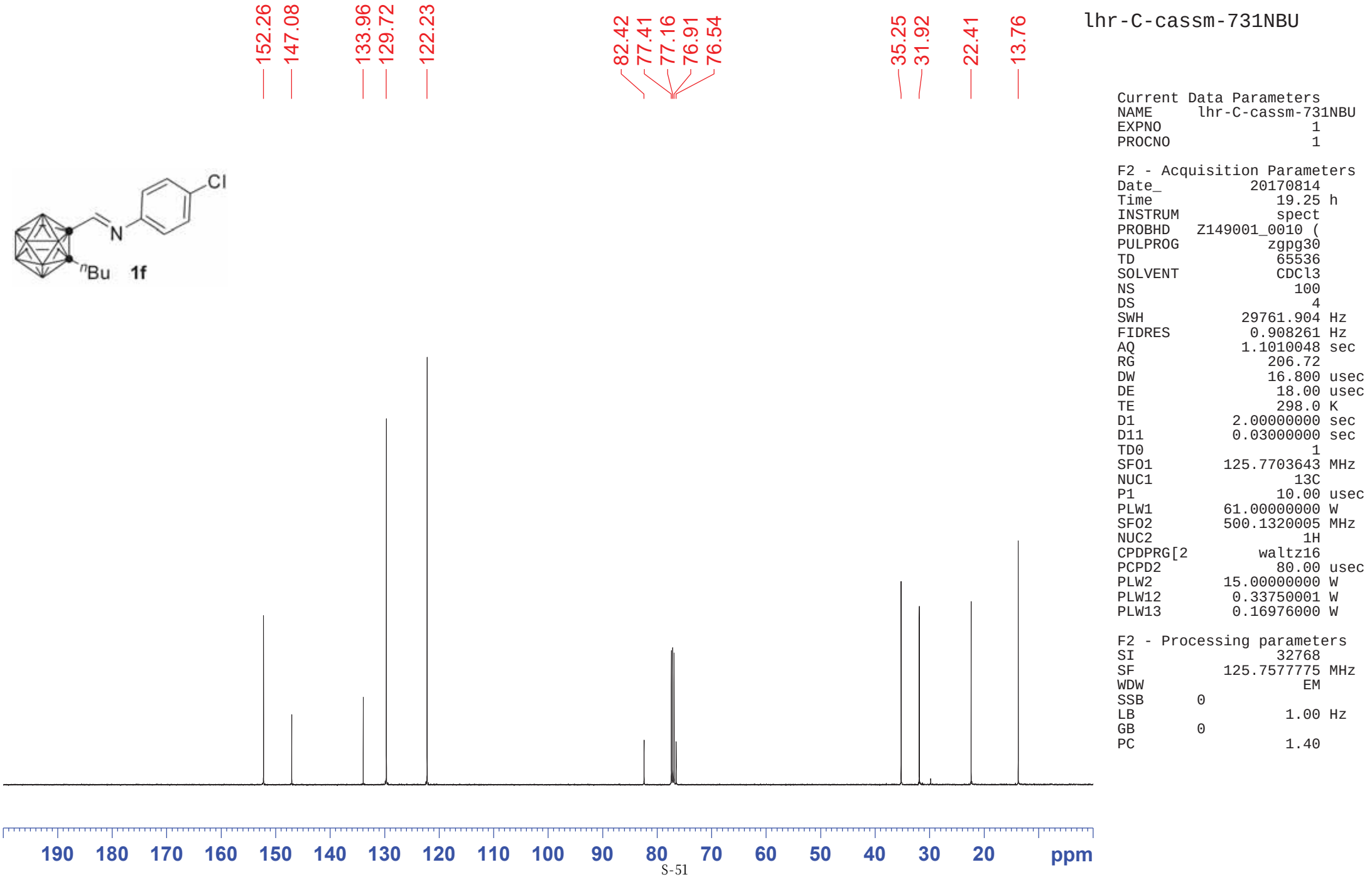
```
Current Data Parameters
NAME      lhr-B-cassm734-ipr
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20170816
Time                10.17 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3762560 sec
RG                   50.6
DW                 21.000 usec
DE                 18.00 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         160.4599621 MHz
NUC1                11B
P1                 10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                  32768
SF           160.4615719 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-cassm734-ipr(C)



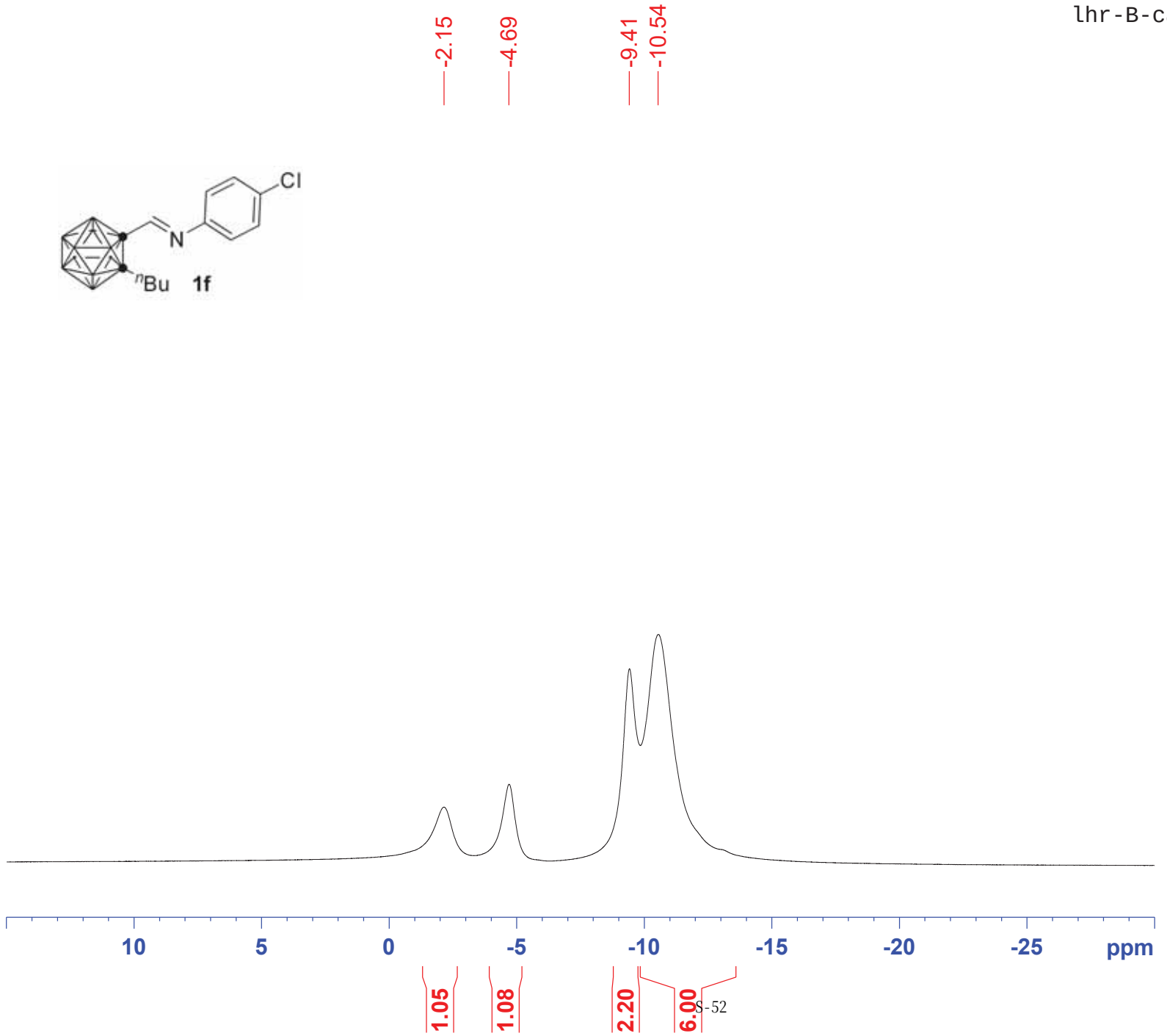

```
Current Data Parameters
NAME      lhr-B-cassm734-ipr(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170816
Time                  10.18 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        12
DS                         4
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                    56.83
DW                   20.800 usec
DE                   18.00 usec
TE                   298.0 K
D1             1.00000000 sec
TD0                        1
SFO1            160.4615792 MHz
NUC1                    11B
P1                   10.00 usec
PLW1           50.00000000 W

F2 - Processing parameters
SI                     16384
SF              160.4615792 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```


7.777
7.378
7.361
7.260
7.059
7.041
2.302
2.296
2.285
2.275
2.268
1.558
1.543
1.539
1.532
1.525
1.517
1.510
1.505
1.493
1.312
1.297
1.282
1.268
1.253
1.238
0.893
0.878
0.863
Cl
N
nBu
1f
Current Data Parameters
NAME lhr-H-cassm-731
EXPNO 1
PROCNO 1
F2 - Acquisition Paramet
Date_ 20170814
Time 19.17
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 3.2767999
RG 14.97
DW 50.000
DE 10.00
TE 298.0
D1 1.00000000
TD0 1
SFO1 500.1330883
NUC1 1H
P1 12.00
PLW1 15.00000000
F2 - Processing paramete
SI 65536
SF 500.1300128
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
ppm
0.96
1.94
1.96
2.13
2.10
2.22
3.00



lhr-C-cassm-731NBU

```
Current Data Parameters
NAME      lhr-C-cassm-731NBU
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170814
Time                 19.25 h
INSTRUM              spect
PROBHD    Z149001_0010 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    100
DS                      4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          125.7703643 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          61.00000000 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          15.00000000 W
PLW12          0.33750001 W
PLW13          0.16976000 W

F2 - Processing parameters
SI                    32768
SF            125.7577775 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

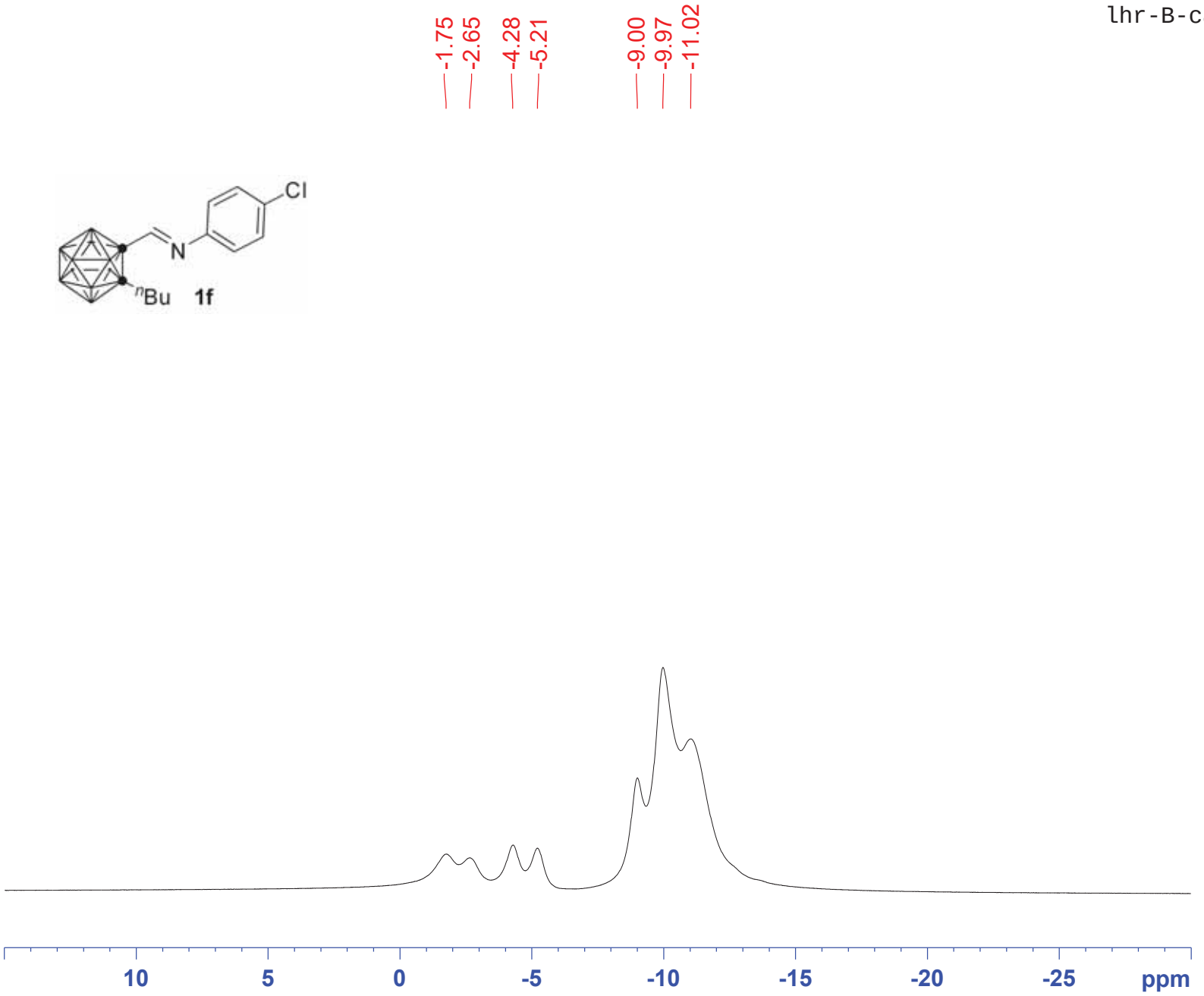


Current Data Parameters
NAME lhr-B-cassm-731NBU
EXPNO 1
PROCNO 1

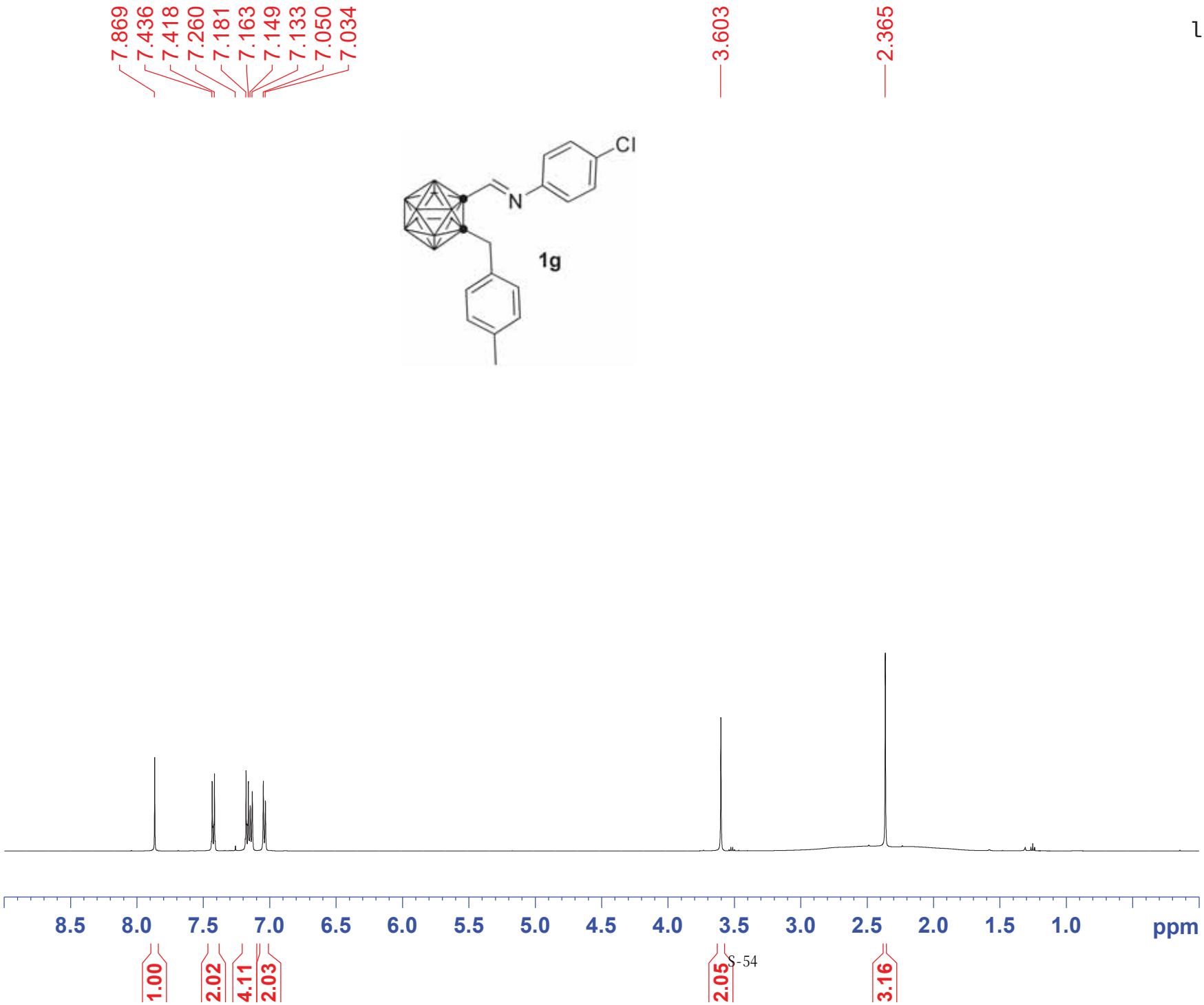
F2 - Acquisition Parameters
Date_ 20170814
Time 19.28 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 12
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 83.35
DW 21.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 160.4599621 MHz
NUC1 11B
P1 10.00 usec
PLW1 50.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W

F2 - Processing parameters
SI 32768
SF 160.4615719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

lhr-B-cassm-731NBU(c)

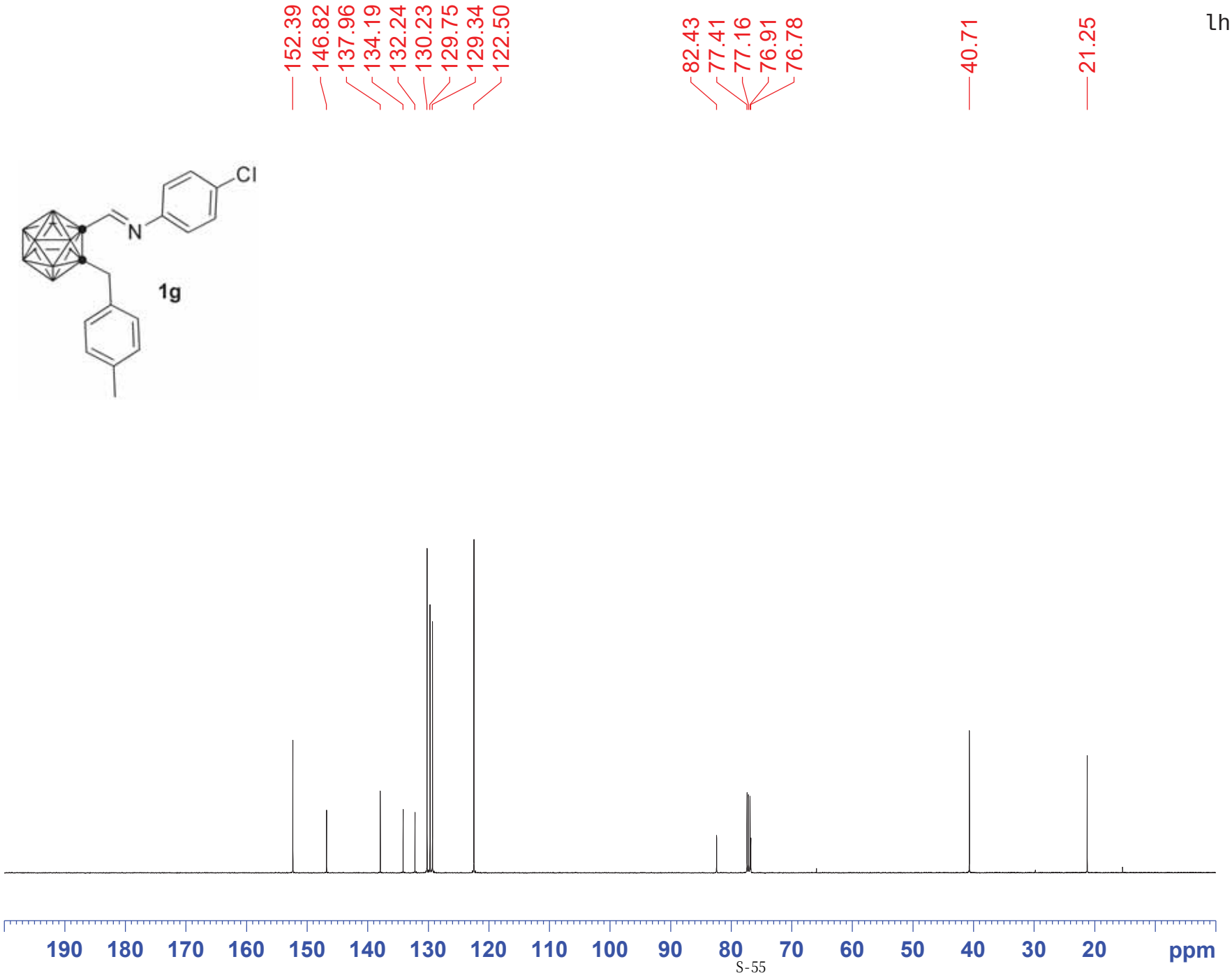



```
Current Data Parameters
NAME      lhr-B-cassm-731NBU(c)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170814
Time                   19.29 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        12
DS                         4
SWH                24038.461 Hz
FIDRES              1.467191 Hz
AQ                 0.6815744 sec
RG                     56.83
DW                    20.800 usec
DE                    18.00 usec
TE                    298.0 K
D1              1.00000000 sec
TD0                        1
SFO1             160.4615792 MHz
NUC1                     11B
P1                    10.00 usec
PLW1            50.00000000 W

F2 - Processing parameters
SI                     16384
SF               160.4615792 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



lhr-H-cassm-740-bnme

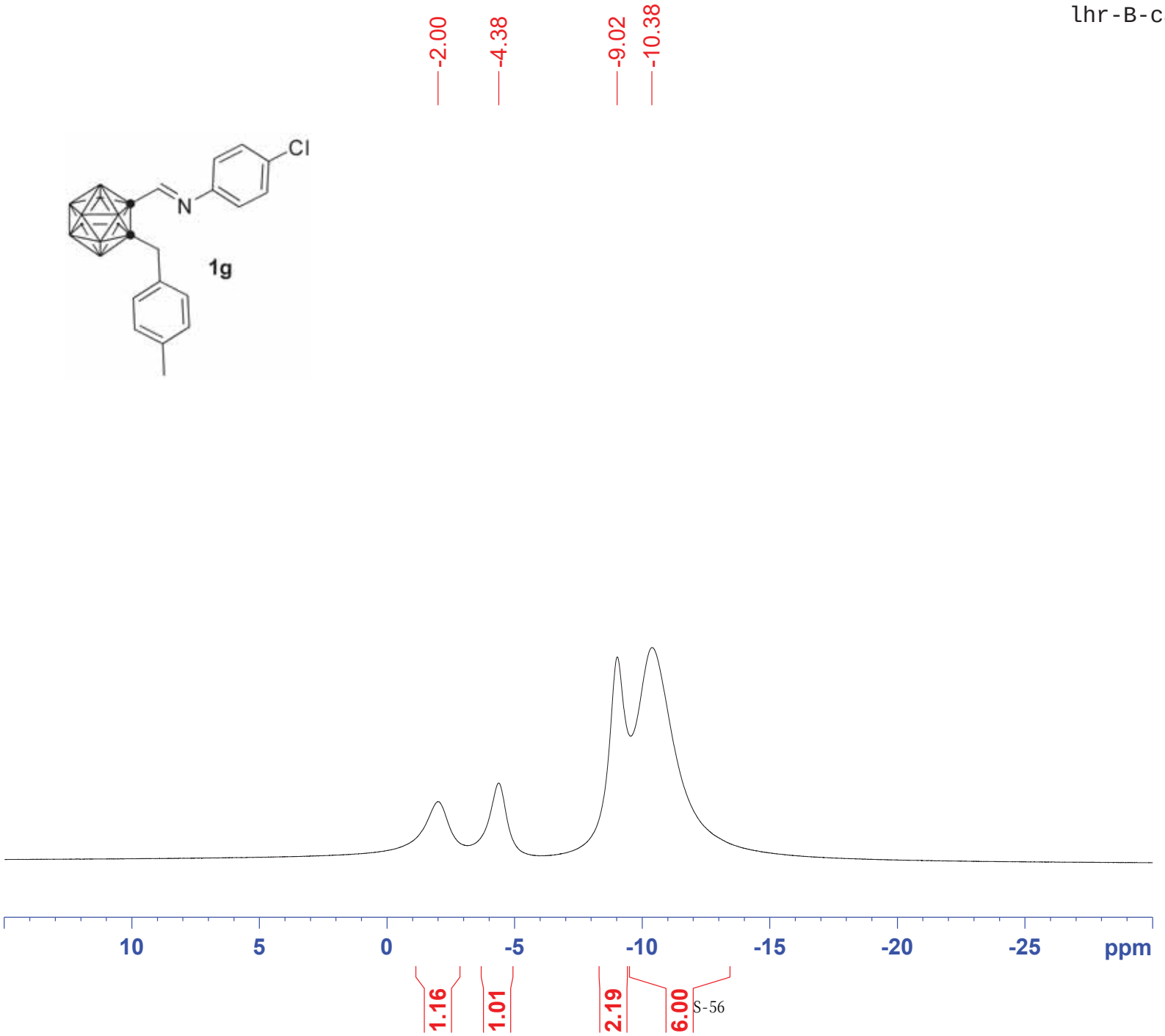
```
Current Data Parameters
NAME      lhr-H-cassm-740-bnme
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170815
Time                  15.07 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH              10000.000 Hz
FIDRES               0.305176 Hz
AQ                3.2767999 sec
RG                   13.21
DW                   50.000 usec
DE                   10.00 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                      1

SFO1            500.1330883 MHz
NUC1                    1H
P1                   12.00 usec
PLW1            15.00000000 W

F2 - Processing parameters
SI                    65536
SF              500.1300124 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```



lhr-C-cassm-740-bnme

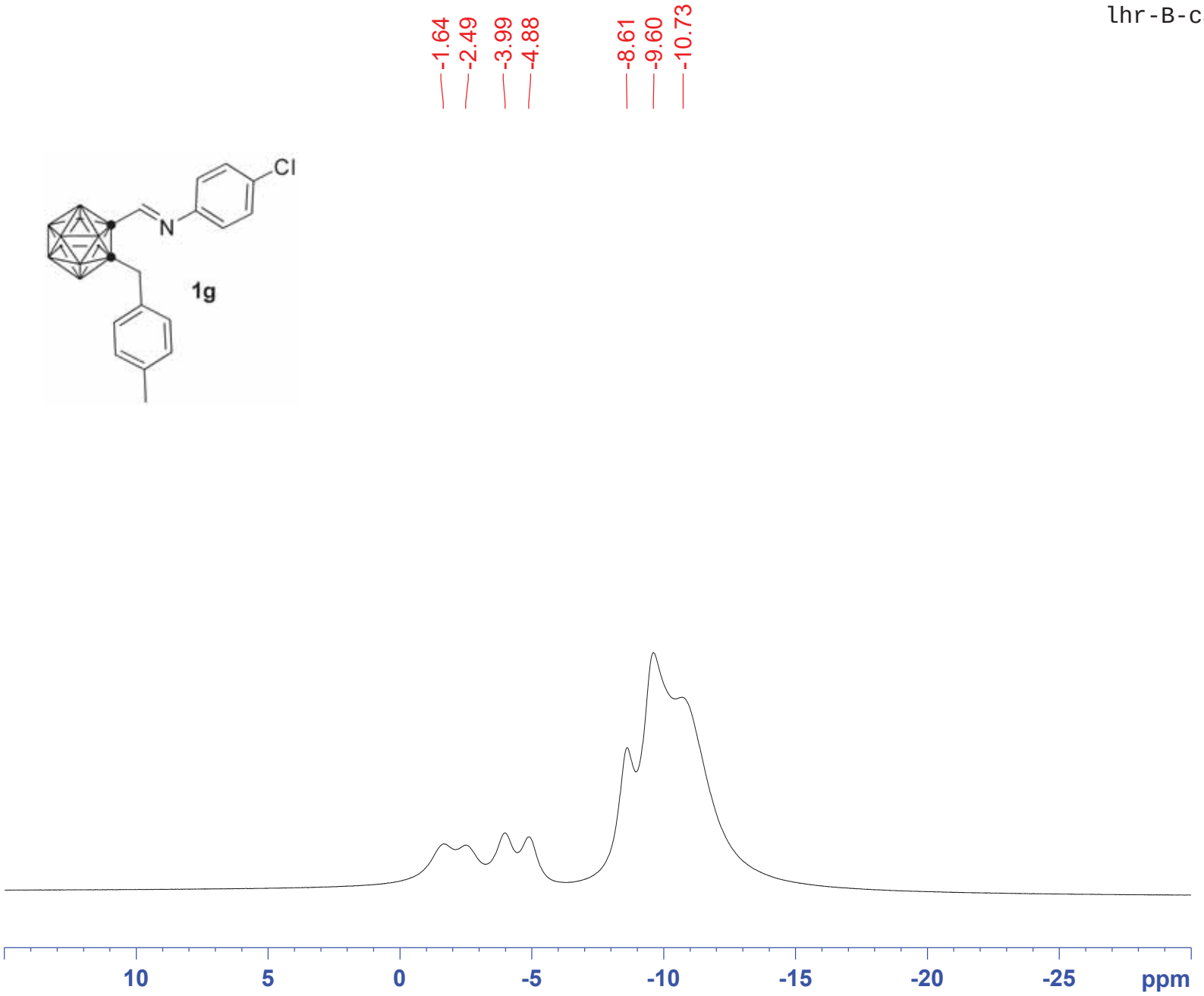
```
Current Data Parameters
NAME      lhr-C-cassm-740-bnme
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170815
Time                  15.14 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       120
DS                         4
SWH               29761.904 Hz
FIDRES             0.908261 Hz
AQ                1.1010048 sec
RG                   206.72
DW                   16.800 usec
DE                   18.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1            125.7703643 MHz
NUC1                    13C
P1                   10.00 usec
PLW1            61.00000000 W
SFO2            500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                80.00 usec
PLW2            15.00000000 W
PLW12            0.33750001 W
PLW13            0.16976000 W

F2 - Processing parameters
SI                     32768
SF              125.7577854 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

lhr-B-cassm-740-bnme

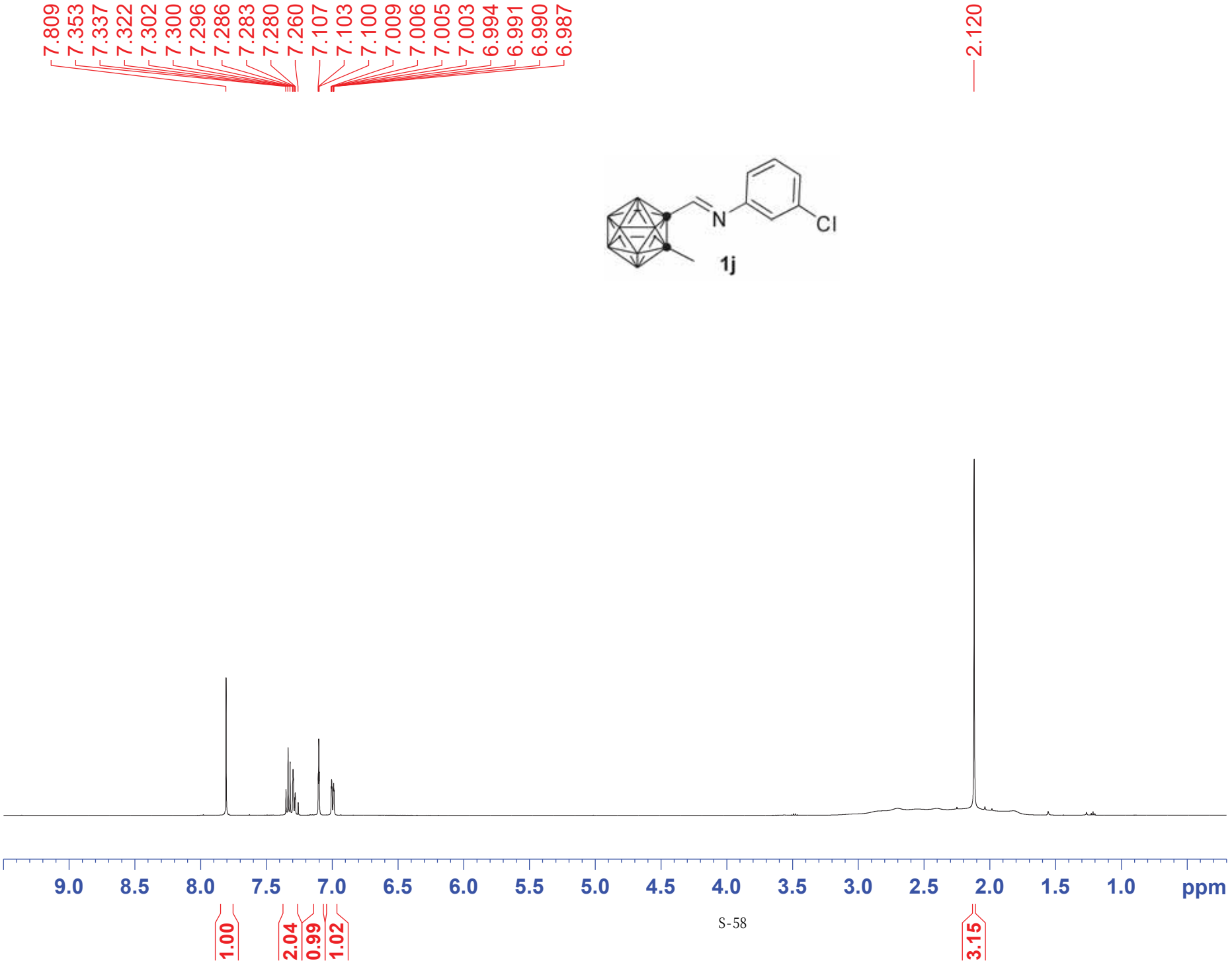



```
Current Data Parameters
NAME      lhr-B-cassm-740-bnme
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170815
Time                  15.18 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        4
SWH               23809.523 Hz
FIDRES             0.726609 Hz
AQ                1.3762560 sec
RG                     50.6
DW                   21.000 usec
DE                   18.00 usec
TE                   298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1            160.4599621 MHz
NUC1                   11B
P1                   10.00 usec
PLW1            50.00000000 W
SFO2            500.1320005 MHz
NUC2                   1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2            15.00000000 W
PLW12            0.33750001 W

F2 - Processing parameters
SI                    32768
SF              160.4615719 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

lhr-B-cassm-740-bnme(C)

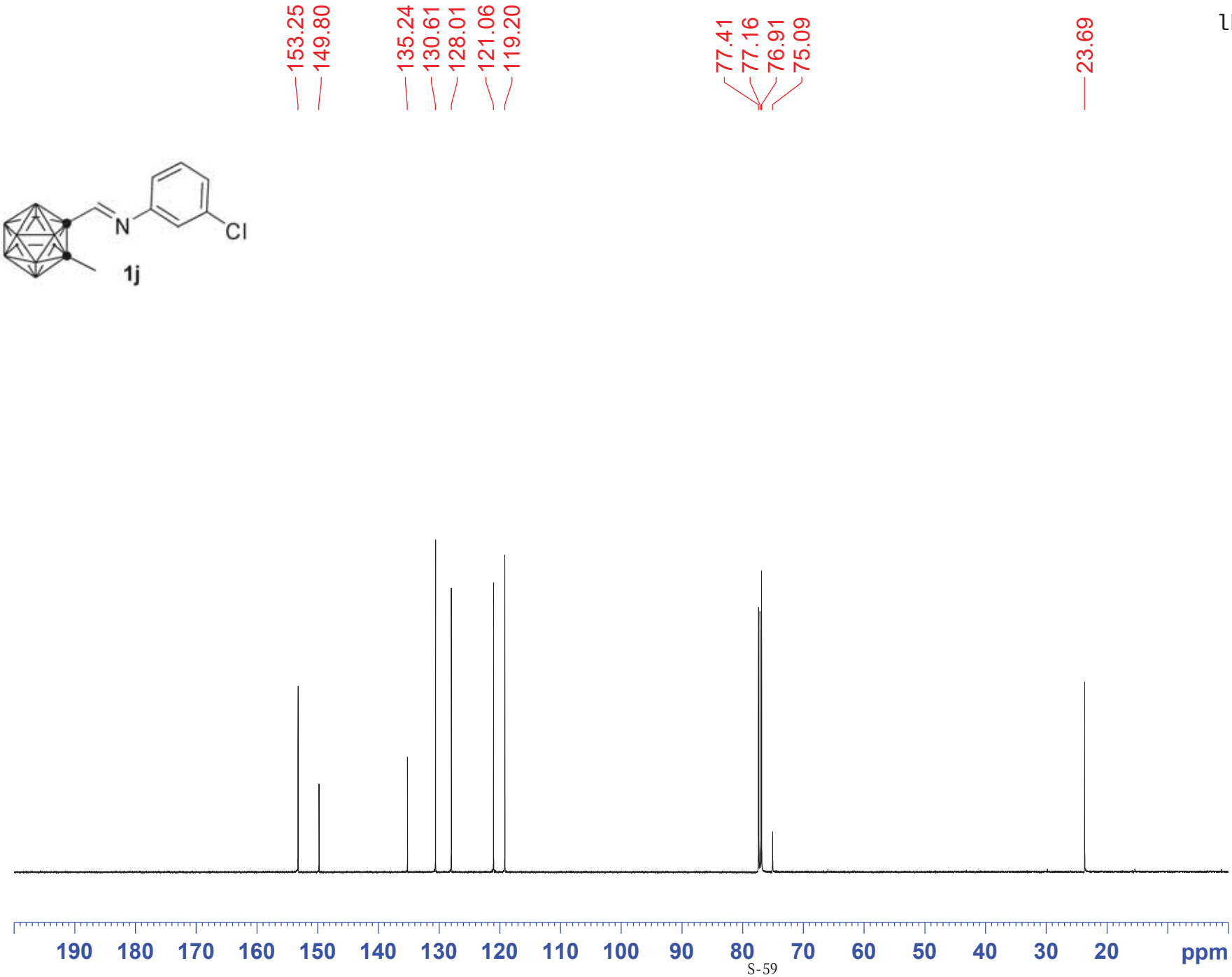



```
Current Data Parameters
NAME      lhr-B-cassm-740-bnme(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170815
Time               15.19 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   12
DS                    4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                56.83
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1          1.00000000 sec
TD0                   1
SFO1         160.4615792 MHz
NUC1              11B
P1               10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                16384
SF           160.4615792 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-H-cassm-m-cl-71

```
Current Data Parameters
NAME      lhr-H-cassm-m-cl
EXPNO                    1
PROCNO                   1

F2 - Acquisition Paramete
Date_             20170815
Time                15.23 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH             10000.000 H
FIDRES              0.305176 H
AQ                3.2767999 s
RG                    17.56
DW                   50.000 u
DE                   10.00 u
TE                   298.0 K
D1             1.00000000 s
TD0                     1
SFO1           500.1330883 M
NUC1                   1H
P1                   12.00 u
PLW1           15.00000000 W

F2 - Processing parameter
SI                   65536
SF             500.1300126 M
WDW                    EM
SSB       0
LB                    0.30 H
GB        0
PC                    1.00
```

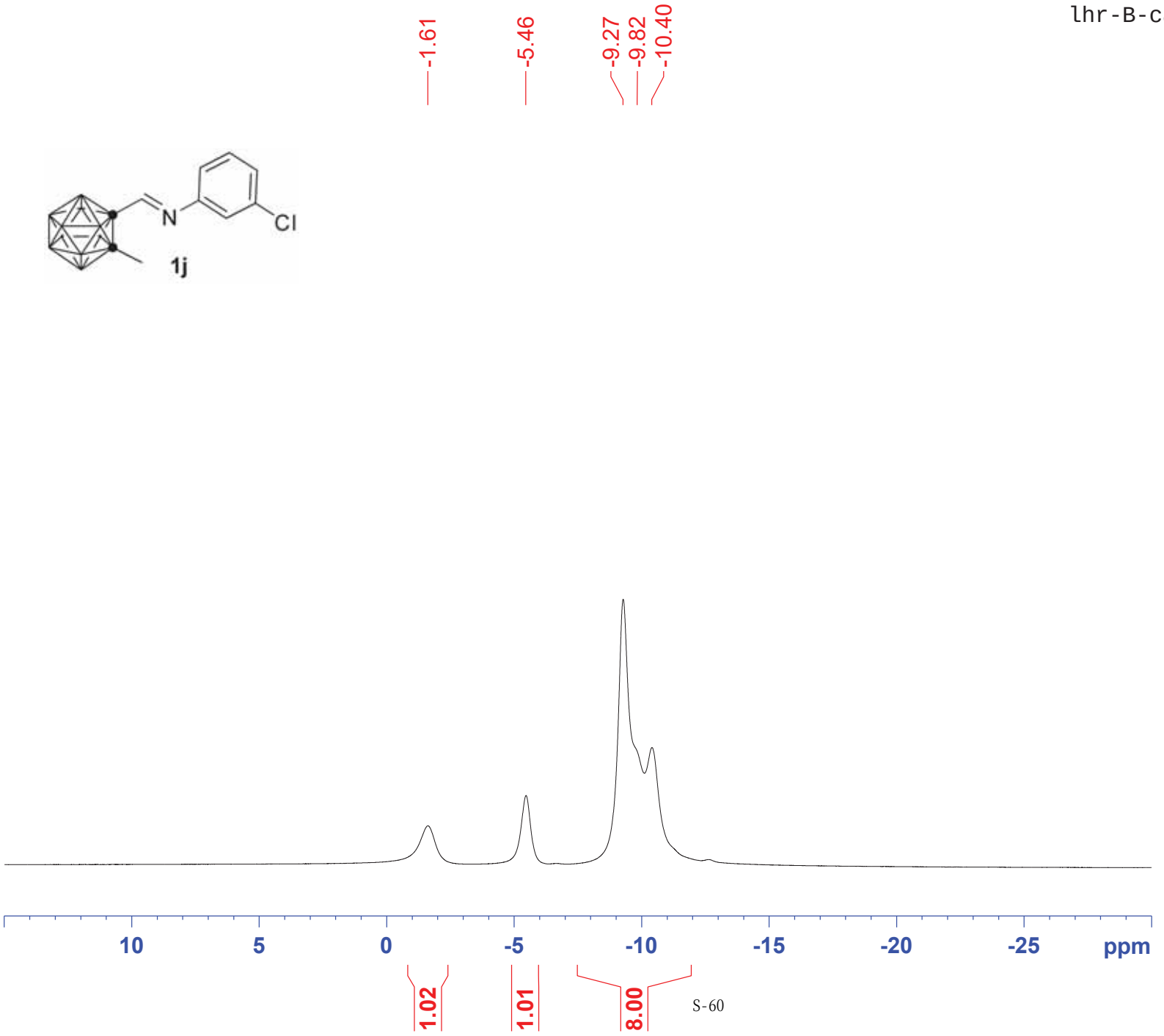


lhr-C-cassm-m-cl-712

```
Current Data Parameters
NAME      lhr-C-cassm-m-cl-712
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20170815
Time                15.32 h
INSTRUM              spect
PROBHD   Z149001_0010 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     120
DS                       4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                   13C
P1                  10.00 usec
PLW1           61.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W
PLW13           0.16976000 W

F2 - Processing parameters
SI                   32768
SF             125.7577763 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

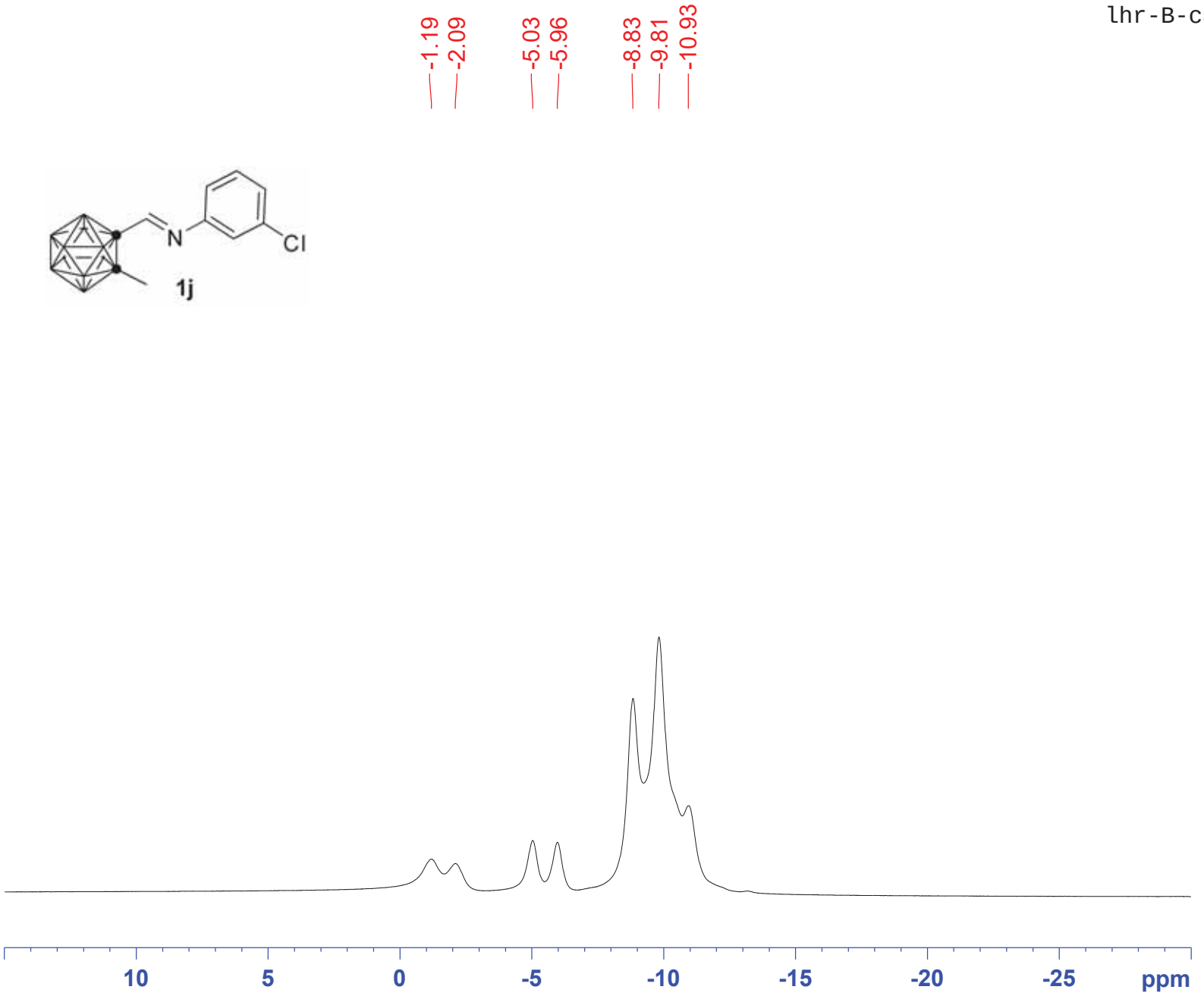
lhr-B-cassm-m-cl-712

1j

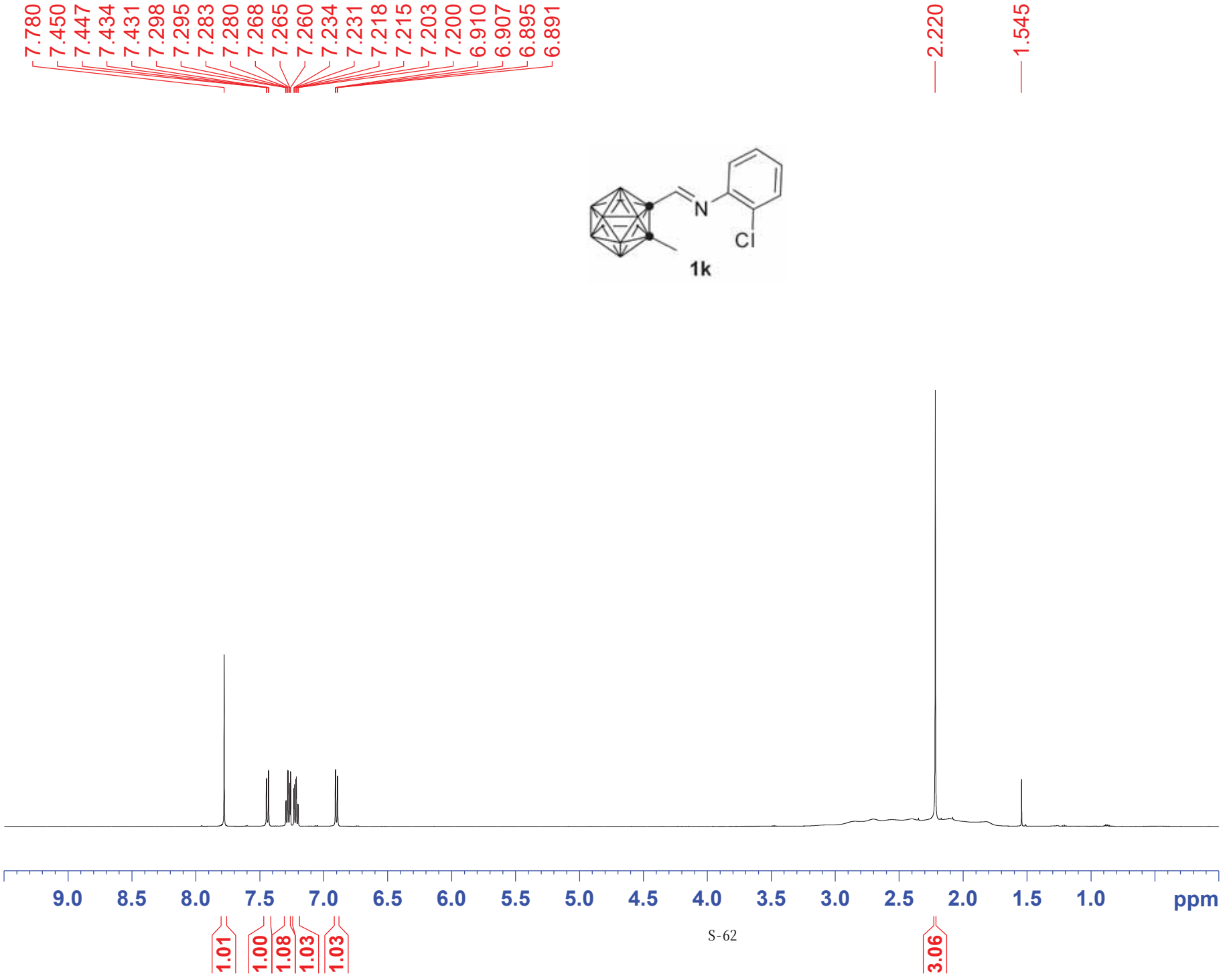



```
Current Data Parameters
NAME      lhr-B-cassm-m-cl-712
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170815
Time                  15.35 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                       12
DS                        4
SWH              23809.523 Hz
FIDRES            0.726609 Hz
AQ                1.3762560 sec
RG                   93.28
DW                  21.000 usec
DE                  18.00 usec
TE                  298.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                       1
SFO1           160.4599621 MHz
NUC1                   11B
P1                  10.00 usec
PLW1           50.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W

F2 - Processing parameters
SI                    32768
SF             160.4615719 MHz
WDW                      EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

lhr-B-cassm-m-cl-712(c)

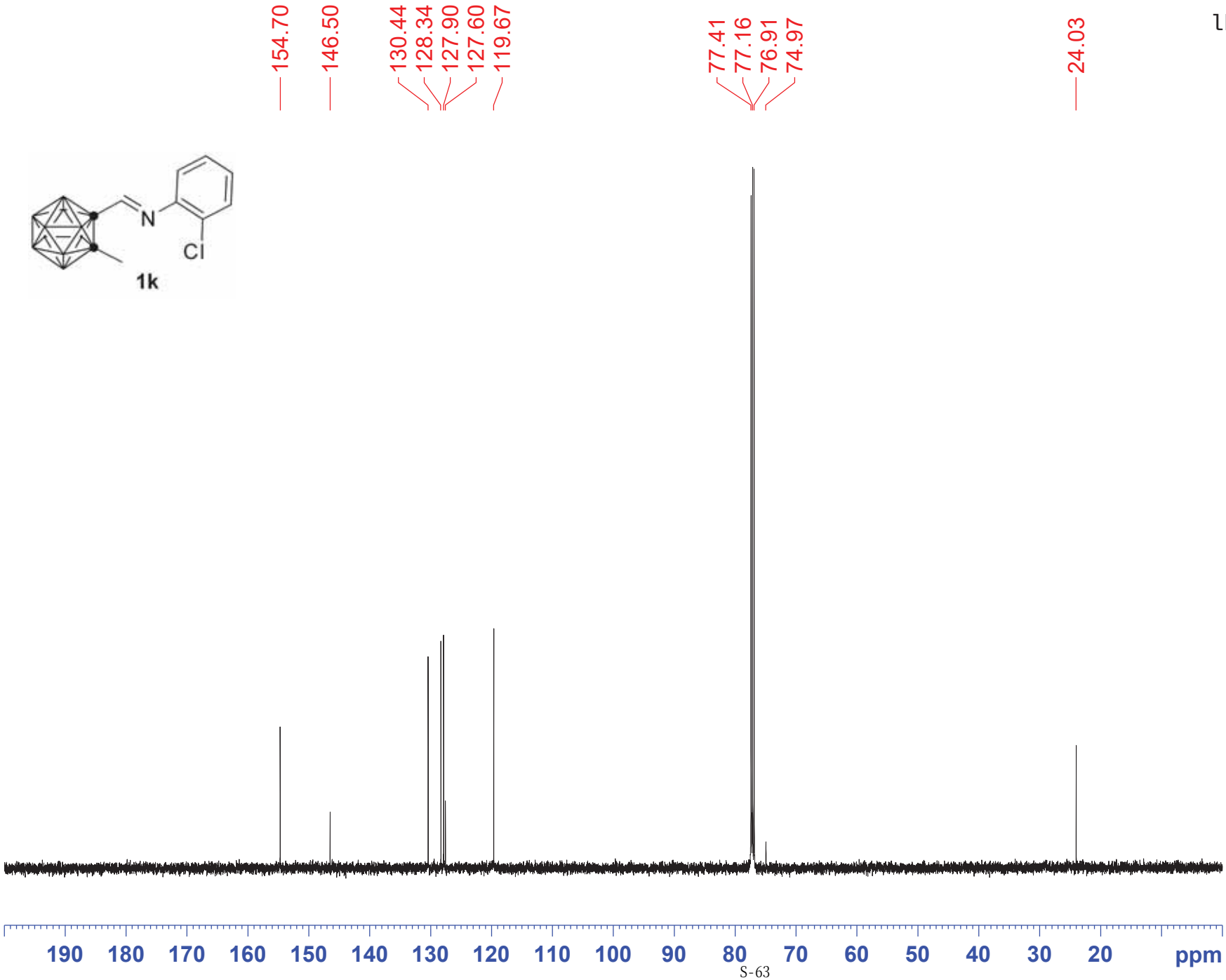



```
Current Data Parameters
NAME      lhr-B-cassm-m-cl-712(c)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170815
Time               15.36 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG              zg
TD                32768
SOLVENT           CDCl3
NS                   12
DS                    4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                 102.6
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                   1
SFO1         160.4615792 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                16384
SF           160.4615792 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



lhr-Hcassm-ocl

```
Current Data Parameters
NAME      lhr-Hcassm-ocl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Paramet
Date_            20170819
Time                13.00
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 30.85
DW                 50.000
DE                 10.00
TE                 298.0
D1            1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1         15.00000000

F2 - Processing paramete
SI                 65536
SF          500.1300126
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```

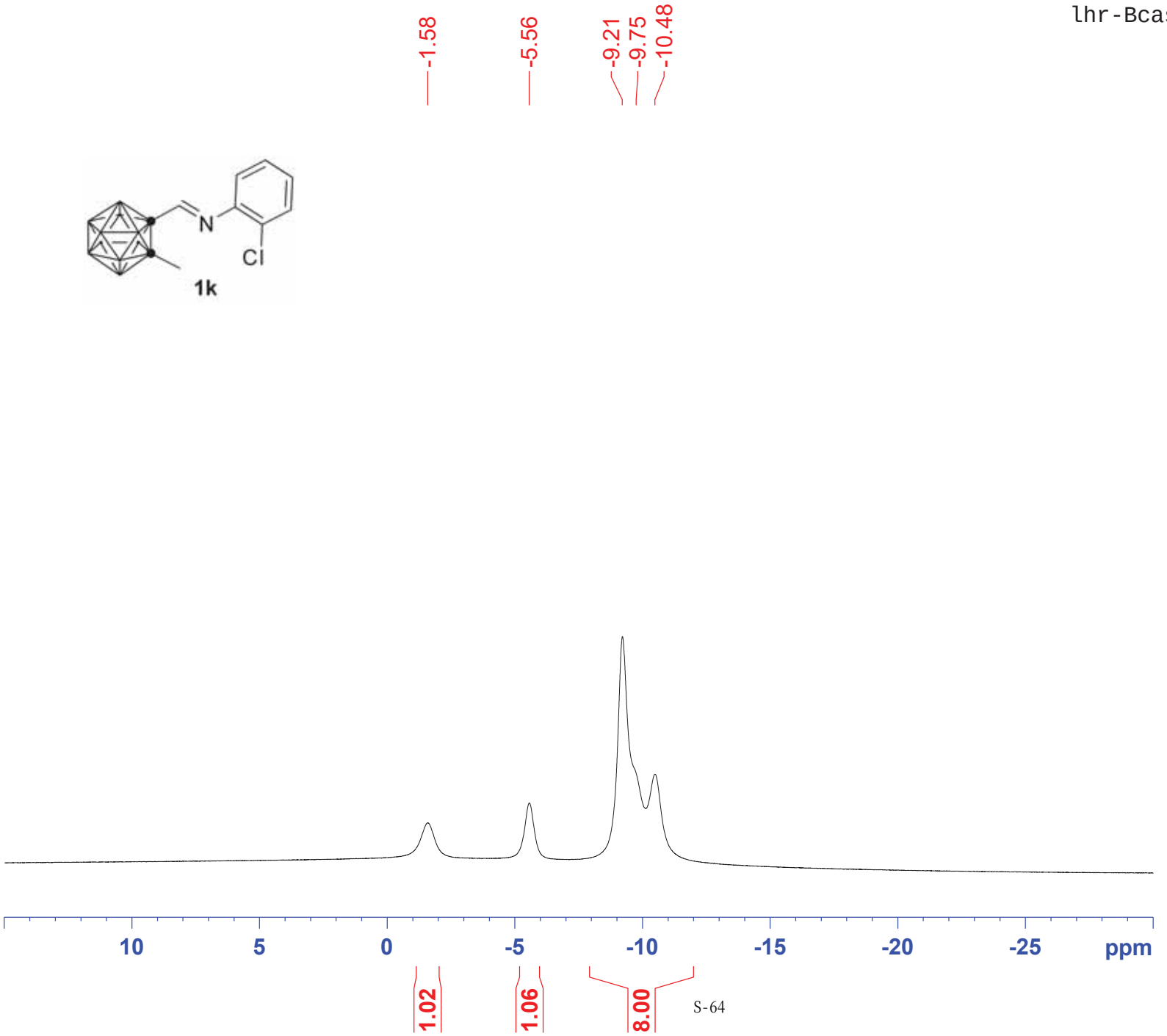


lhr-Ccassm-ocl

```
Current Data Parameters
NAME      lhr-Ccassm-ocl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170819
Time              13.21 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  360
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577722 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

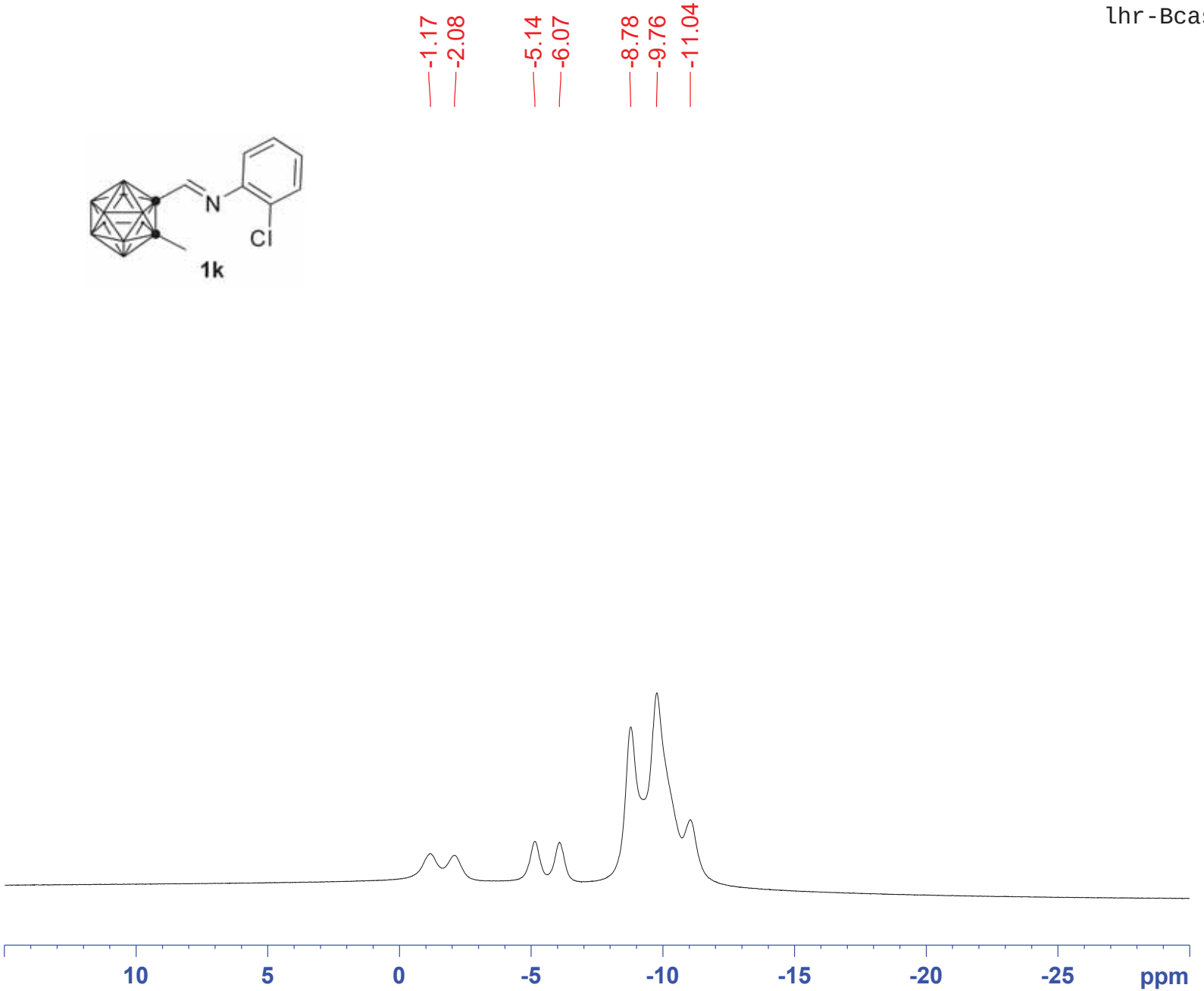
lhr-Bcassm-ocl

1k




```
Current Data Parameters
NAME      lhr-Bcassm-ocl
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170819
Time                13.24 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             1.3762560 sec
RG                 142.5
DW                21.000 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         160.4599621 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                 32768
SF          160.4615719 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

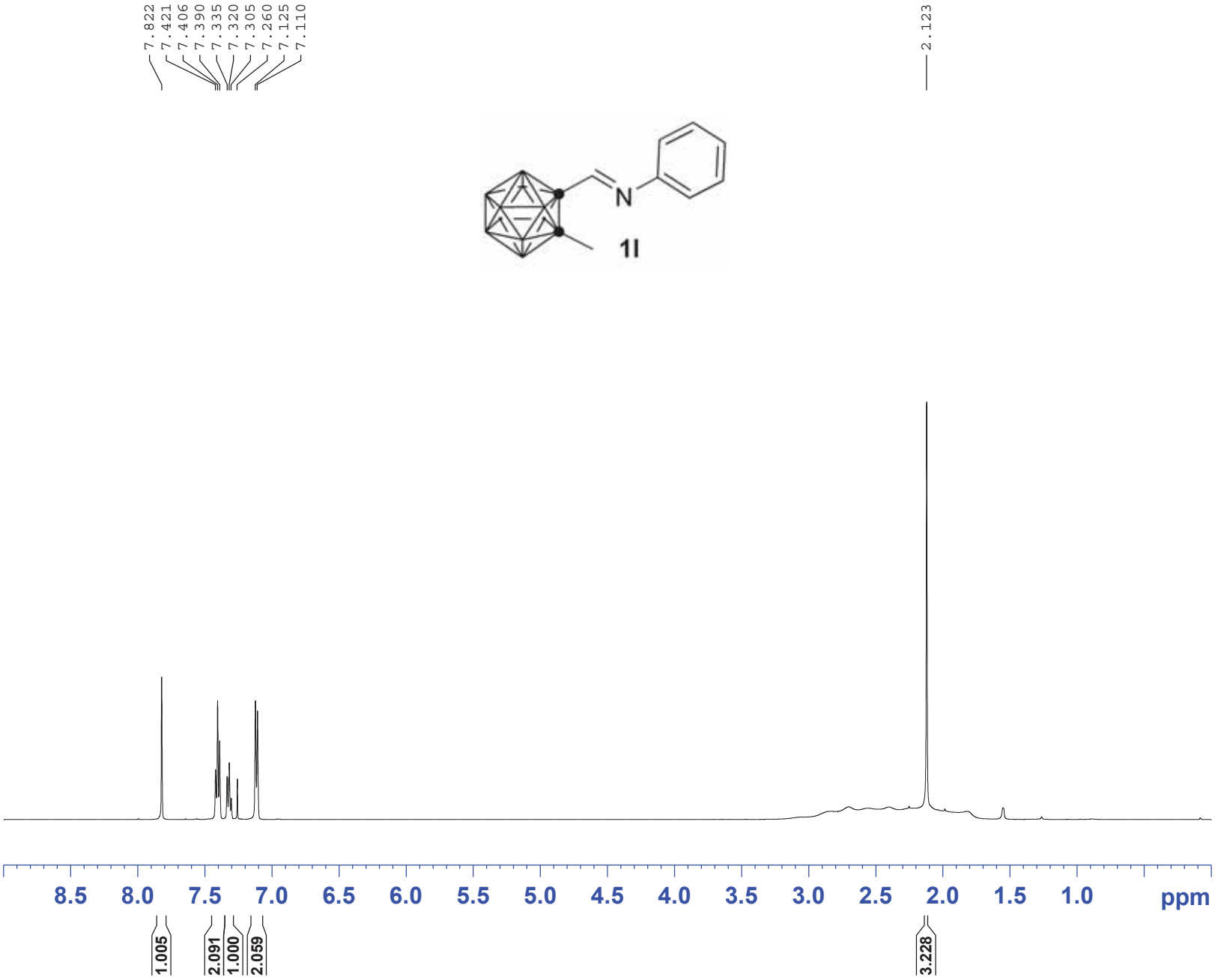
1k



lhr-Bcassm-ocl(c)

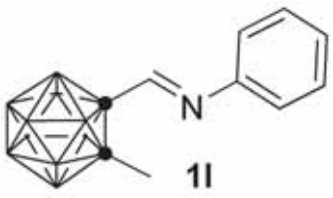
```
Current Data Parameters
NAME      lhr-Bcassm-ocl(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170819
Time                13.25 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     12
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                  142.5
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1             1.00000000 sec
TD0                     1
SFO1          160.4615792 MHz
NUC1                  11B
P1                 10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                  16384
SF            160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-H-cassm708

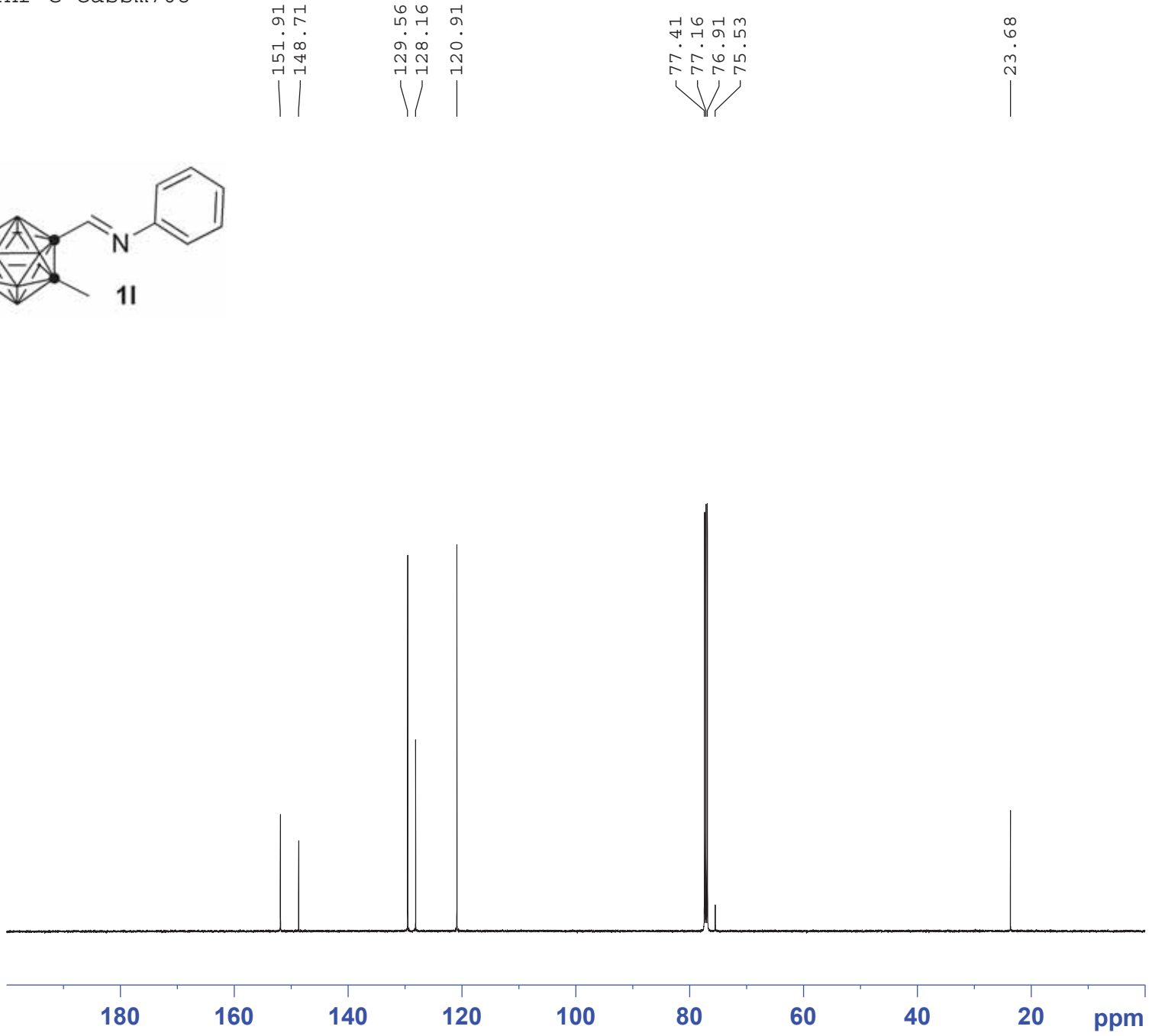



```
Current Data Parameters
NAME      lhr-H-cassm708
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171214
Time               11.51 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES          0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 usec
DE                10.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                12.00 usec
PLW1          15.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300125 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

lhr-C-cassm708

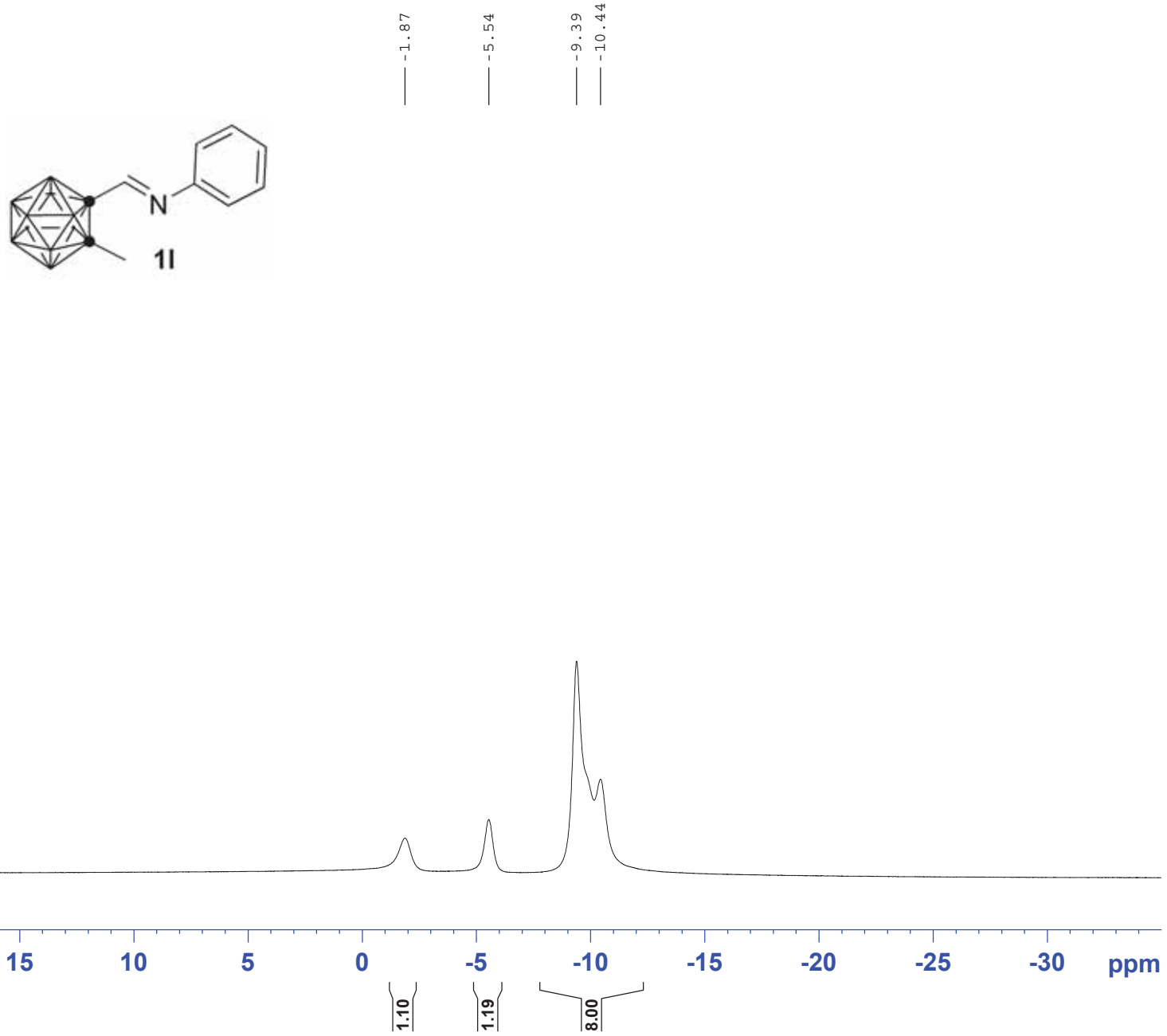


1l




```
Current Data Parameters
NAME      lhr-C-cassm708
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171214
Time              12.18 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  500
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577738 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

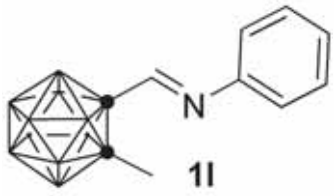
lhr-B-cassm708



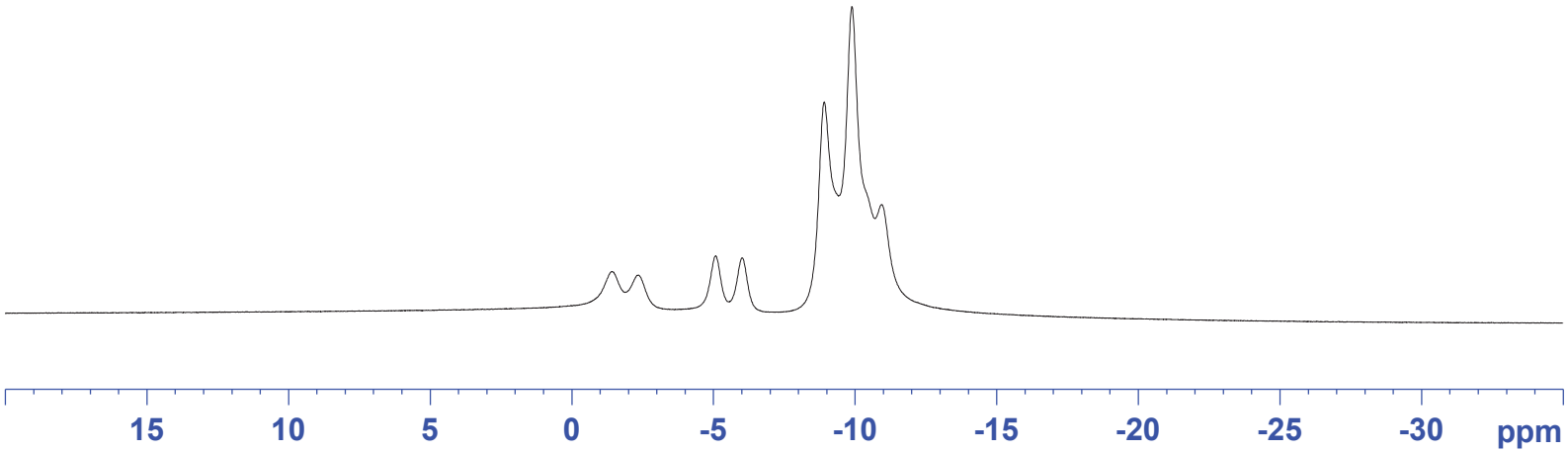

```
Current Data Parameters
NAME      lhr-B-cassm708
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171214
Time               12.21 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zgig
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                 142.5
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         160.4615790 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                 16384
SF           160.4615792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

lhr-B-cassm708(C)

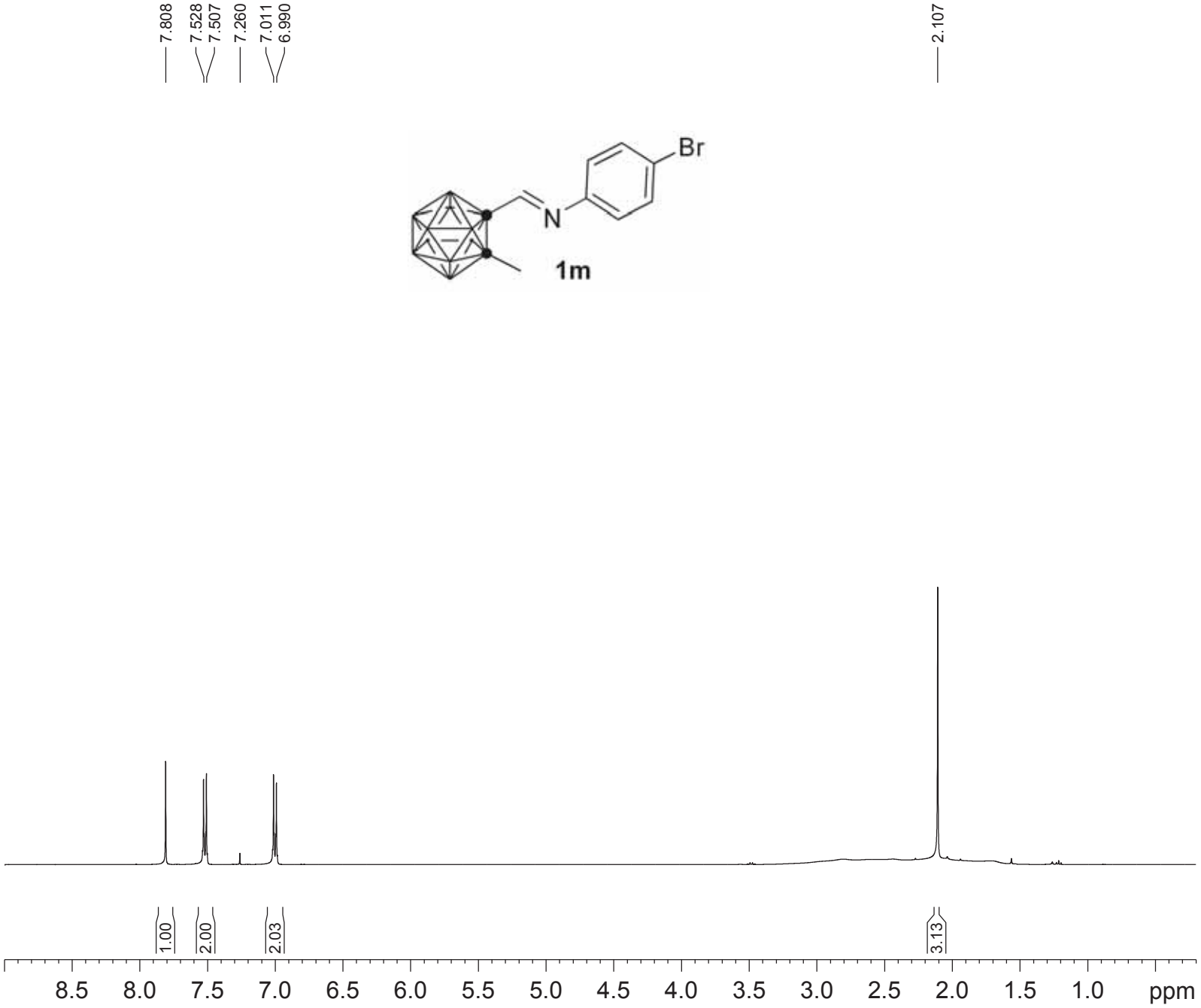
-1.42
-2.35
-5.07
-6.01
-8.91
-9.89
-10.94



1l




```
Current Data Parameters
NAME      lhr-B-cassm708(C)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_           20171214
Time               12.22 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                  142.5
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                     1
SFO1          160.4615792 MHz
NUC1                  11B
P1                 10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                  16384
SF            160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

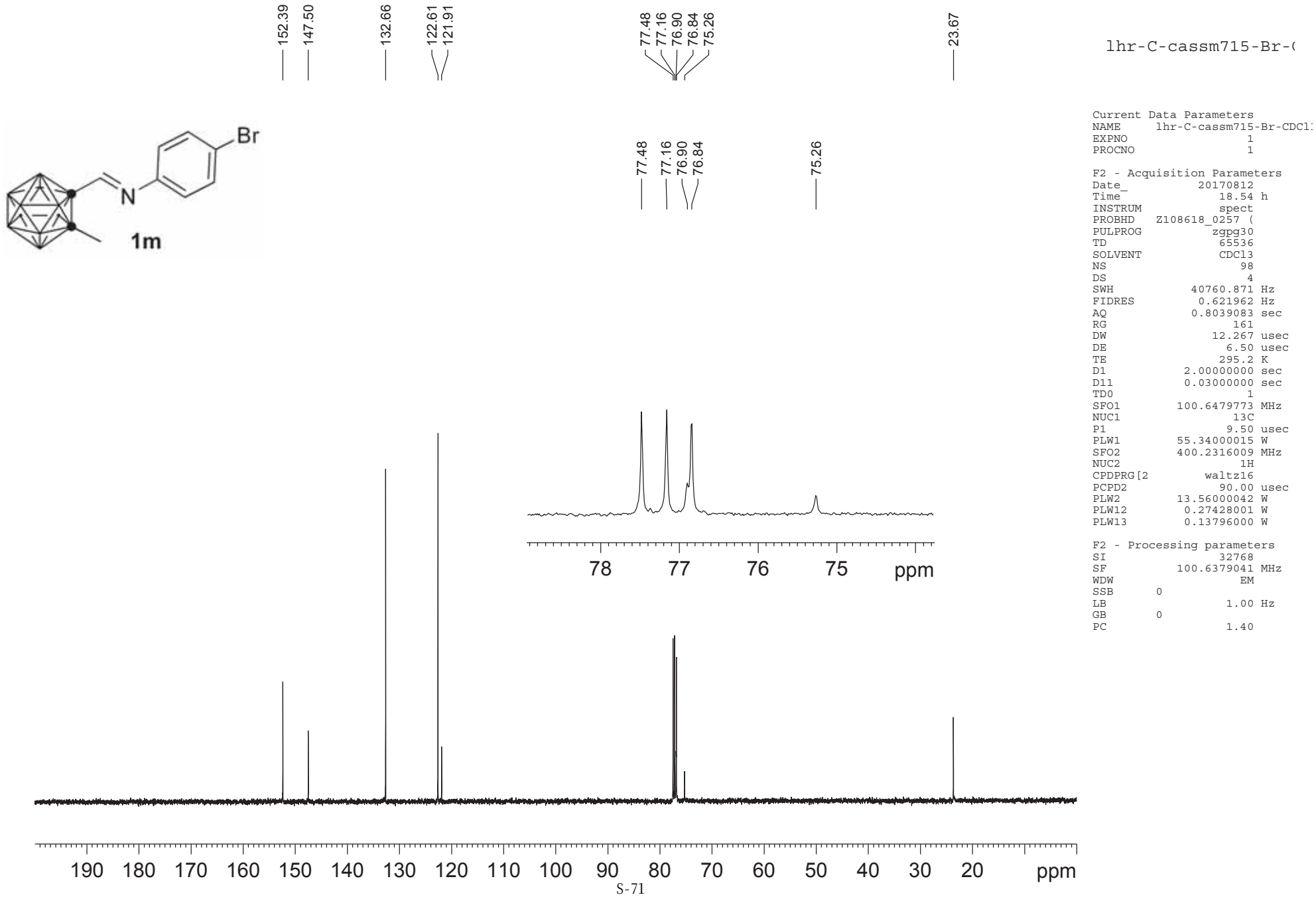


lhr-H-cassm715-Br-CI

Current Data Parameters
NAME lhr-H-cassm715-Br-CDCl3
EXPNO 1
PROCNO 1

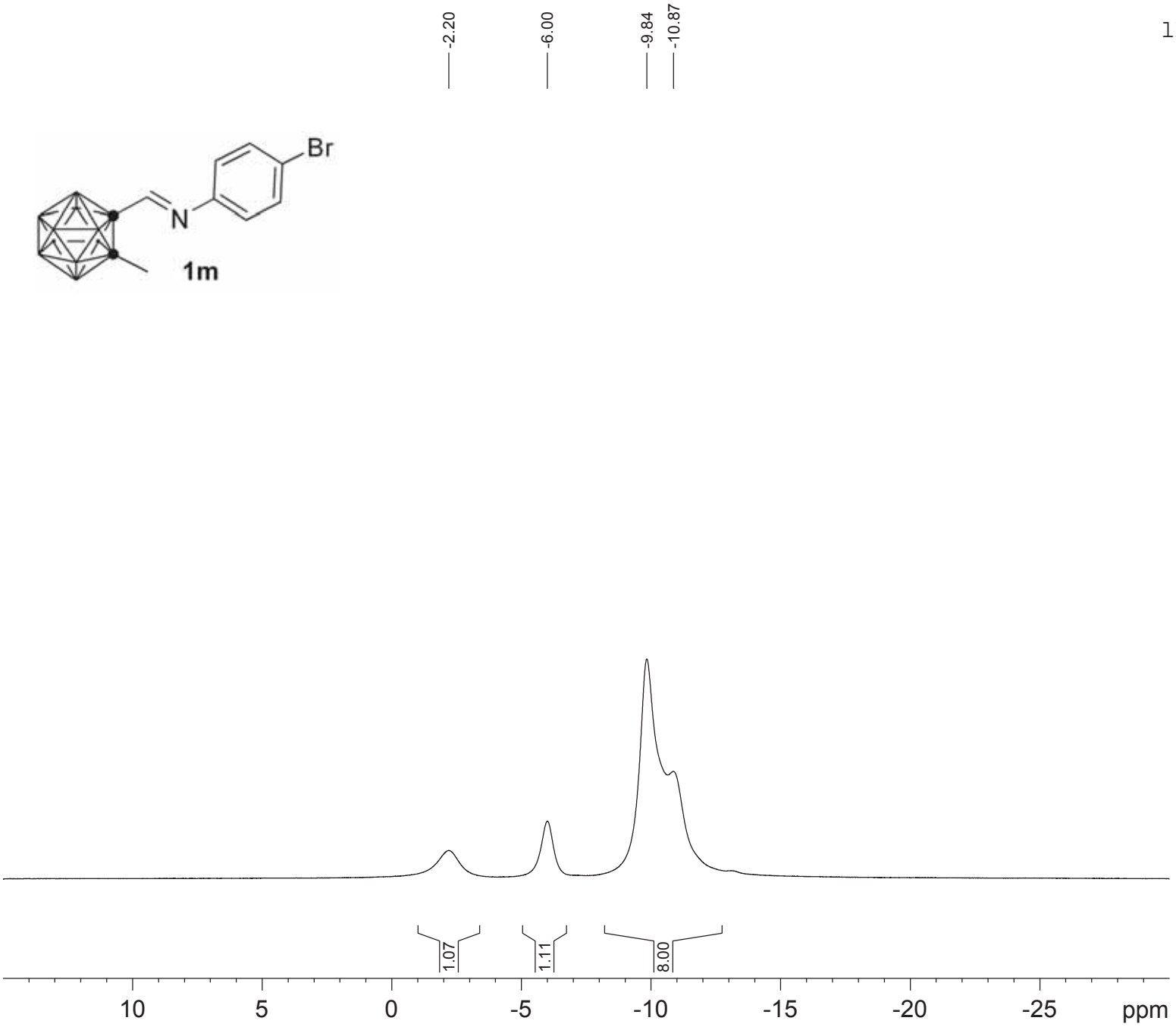
F2 - Acquisition Parameters
Date_ 20170812
Time 18.51 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



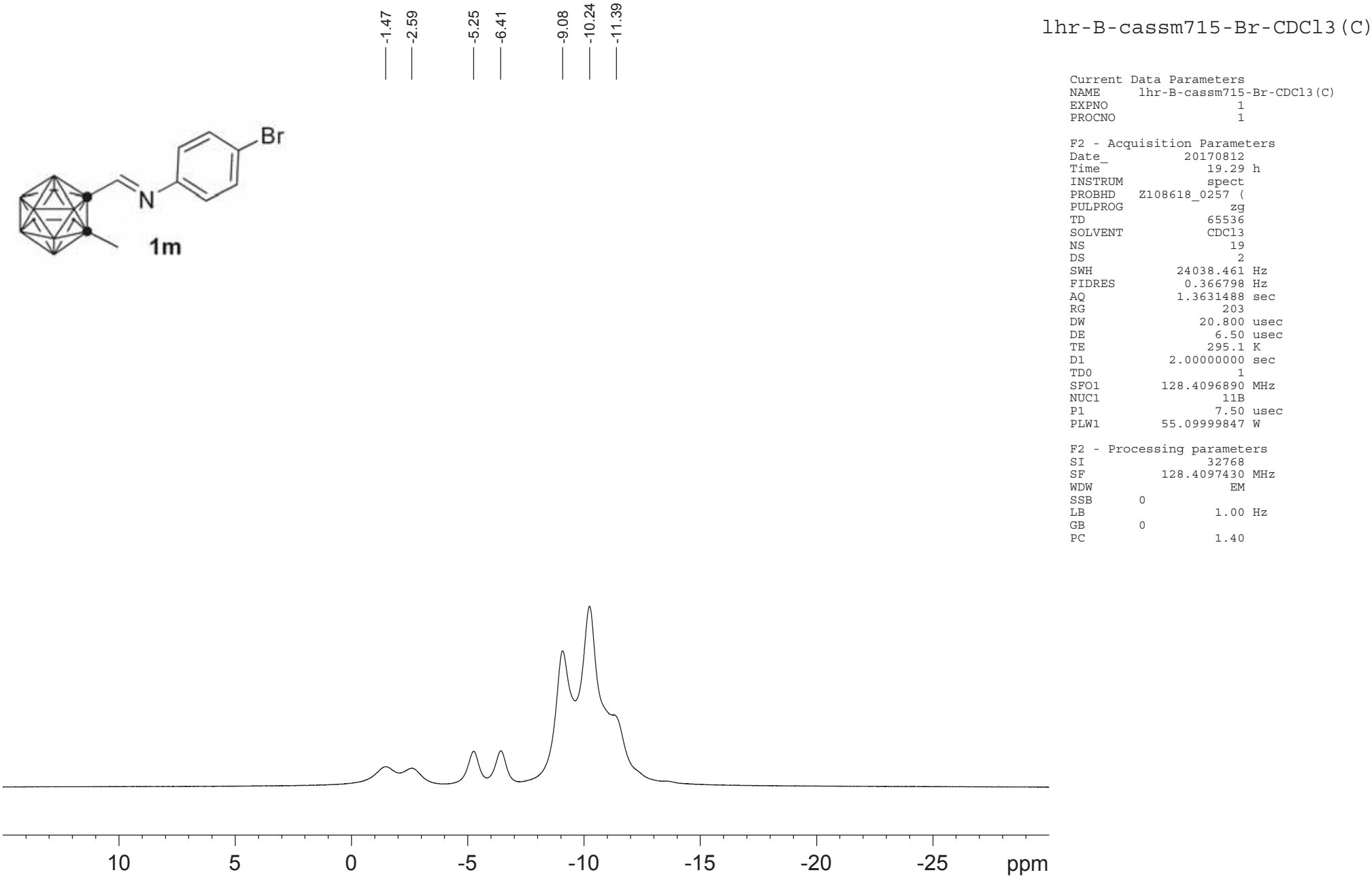
lhr-C-cassm715-Br-(

```
Current Data Parameters
NAME      lhr-C-cassm715-Br-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170812
Time              18.54 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   98
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  161
DW               12.267 usec
DE                6.50 usec
TE                295.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                 32768
SF           100.6379041 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



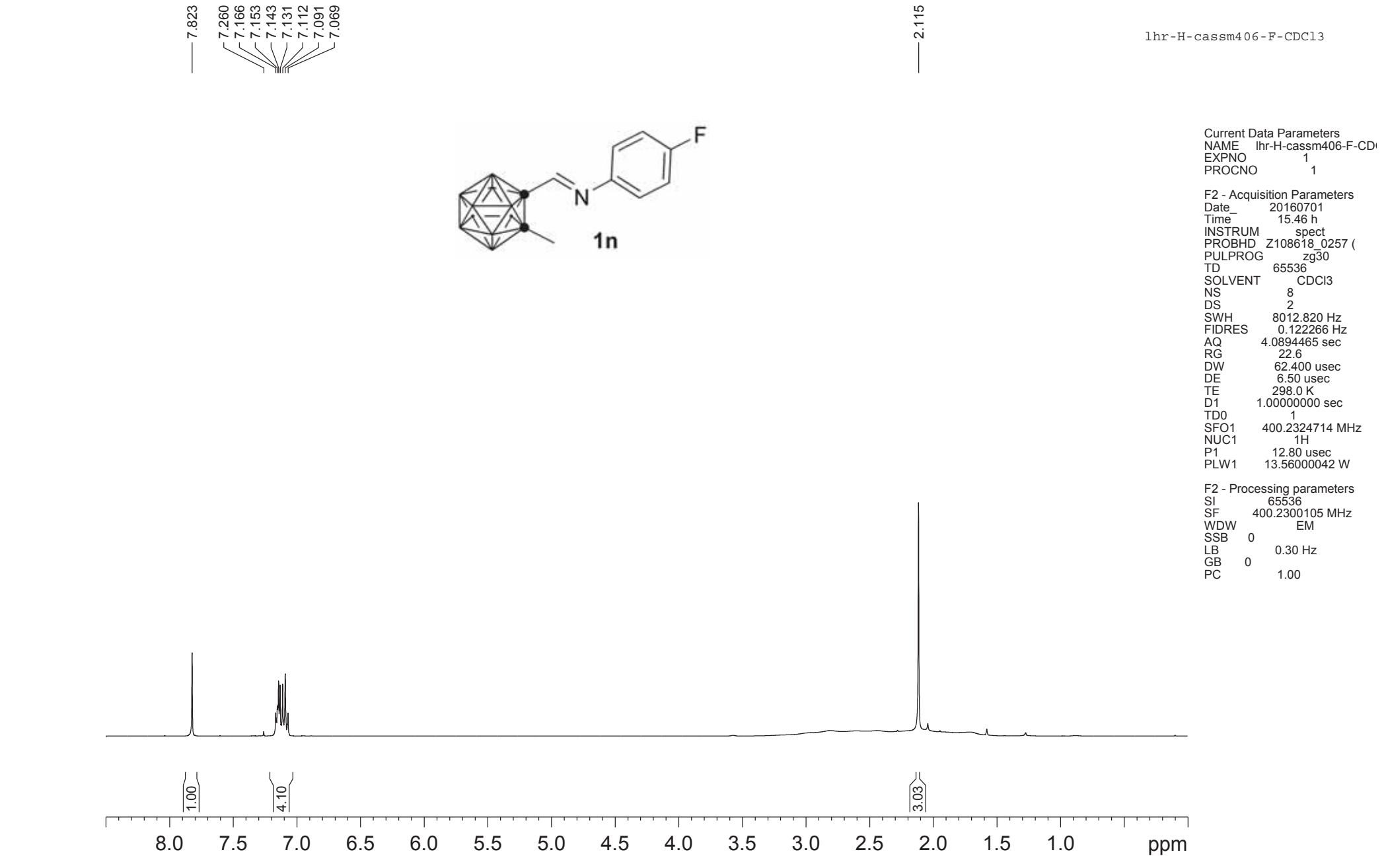
lhr-B-cassm715-Br-CDCl3

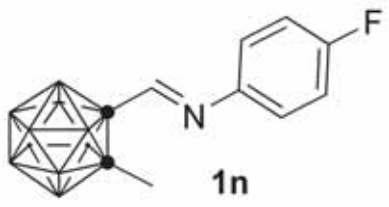
```
Current Data Parameters
NAME      lhr-B-cassm715-Br-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170812
Time               19.27 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     17
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 295.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

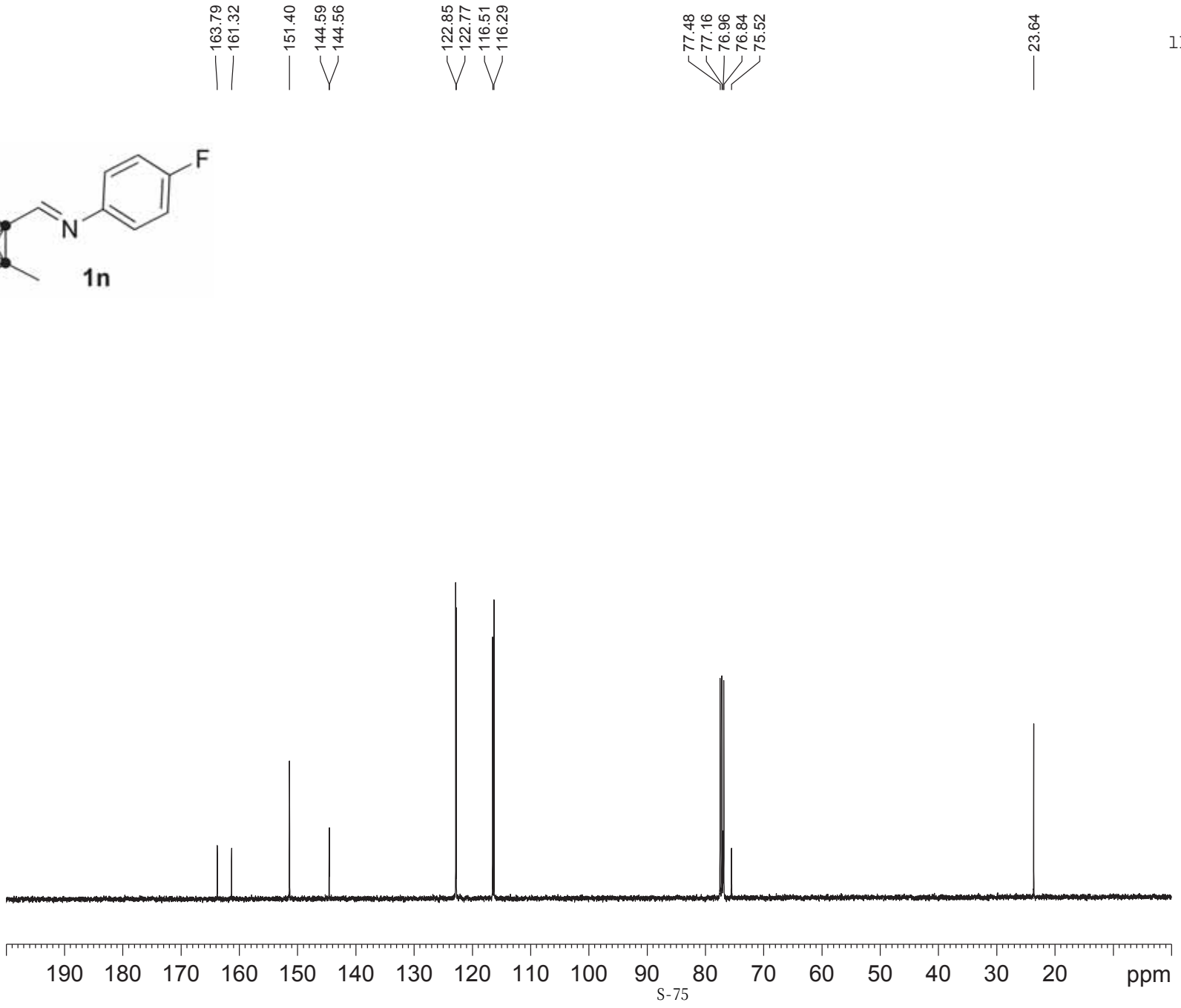


lhr-B-cassm715-Br-CDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm715-Br-CDCl3(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170812
Time              19.29 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   19
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  203
DW                20.800 usec
DE                 6.50 usec
TE                295.1 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

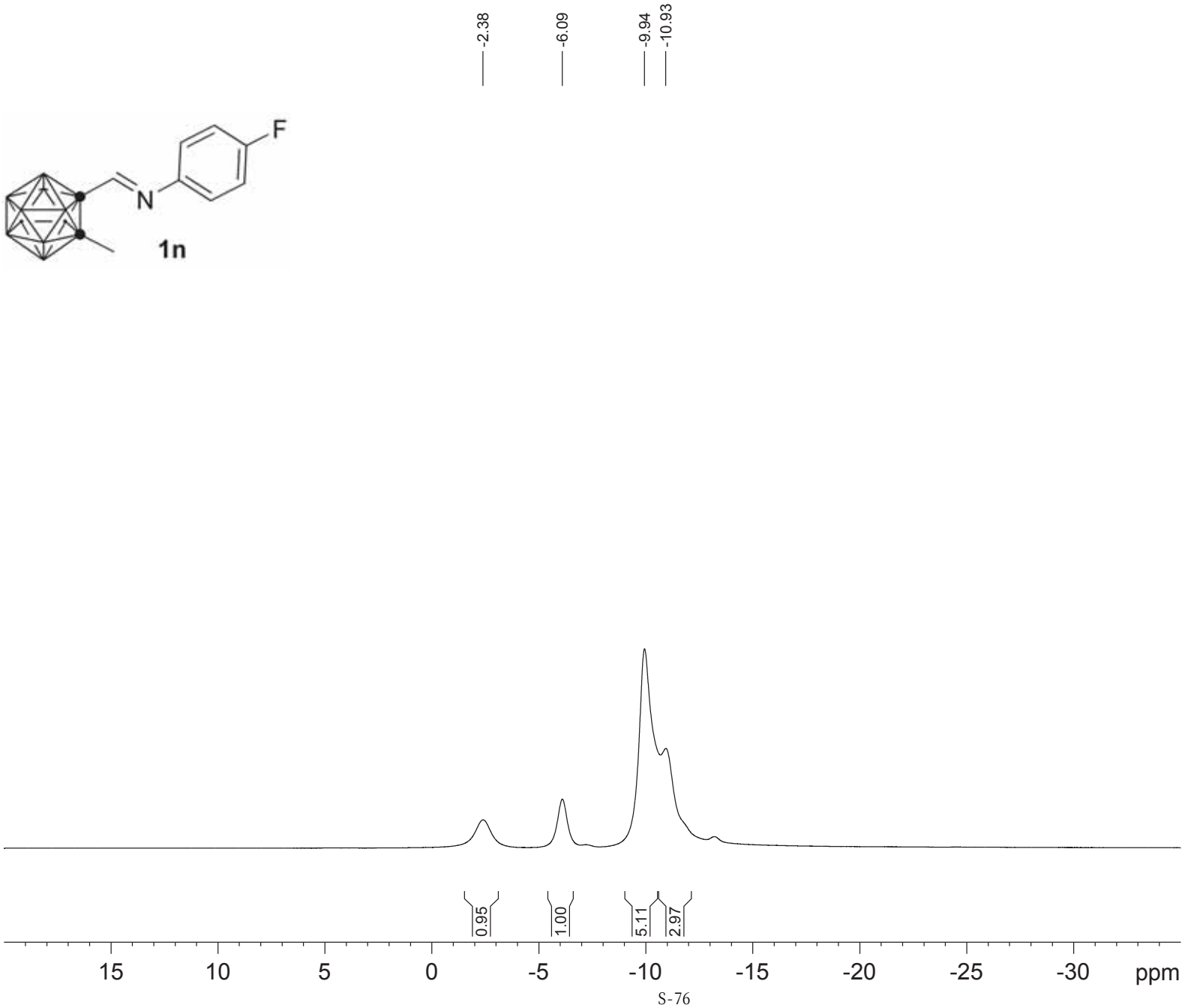

7.823
7.260
7.166
7.153
7.143
7.131
7.112
7.091
7.069
2.115
lhr-H-cassm406-F-CDCl3
F
N
1n
Current Data Parameters
NAME lhr-H-cassm406-F-CD
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160701
Time 15.46 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 22.6
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.00
4.10
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm





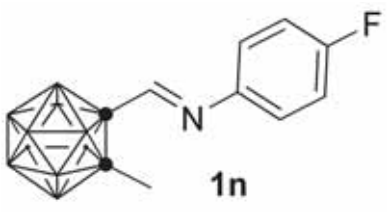
lhr-C-cassm406-F-CDCl3

```
Current Data Parameters
NAME      lhr-C-cassm406-F-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160701
Time              15.50 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                    99
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                   128
DW                16.800 usec
DE                 6.50 usec
TE                298.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                 32768
SF           100.6379046 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



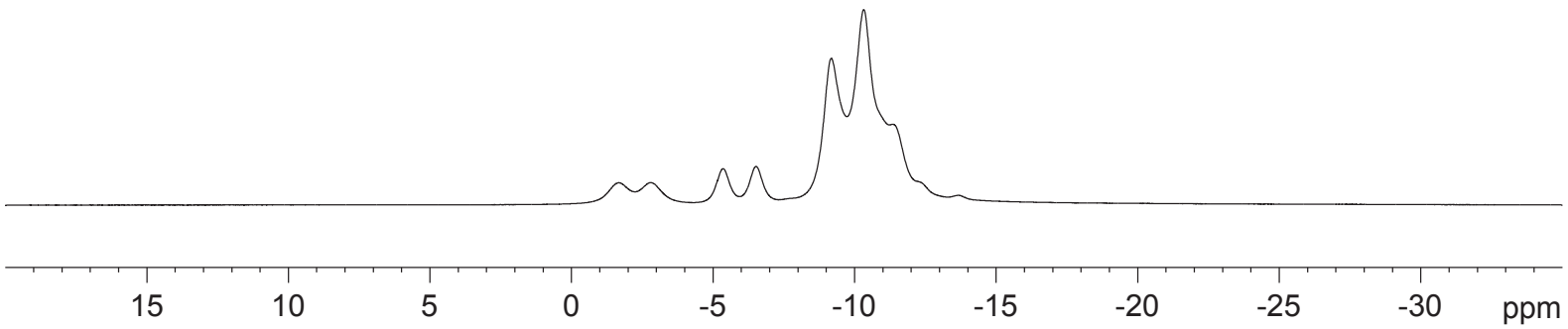
lhr-B-cassm406-F-CDCl3

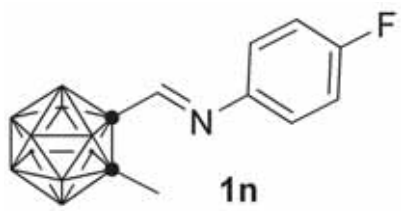
```
Current Data Parameters
NAME      lhr-B-cassm406-F-CDCl
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160701
Time                 15.58 h
INSTRUM                spect
PROBHD   Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                        19
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                      80.6
DW                    20.800 usec
DE                     6.50 usec
TE                    298.3 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                     32768
SF               128.4097615 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



lhr-B-cassm406-F-CDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm406-F-CDCl3(C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160701
Time              16.00 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   26
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                80.6
DW               20.800 usec
DE                6.50 usec
TE                297.8 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





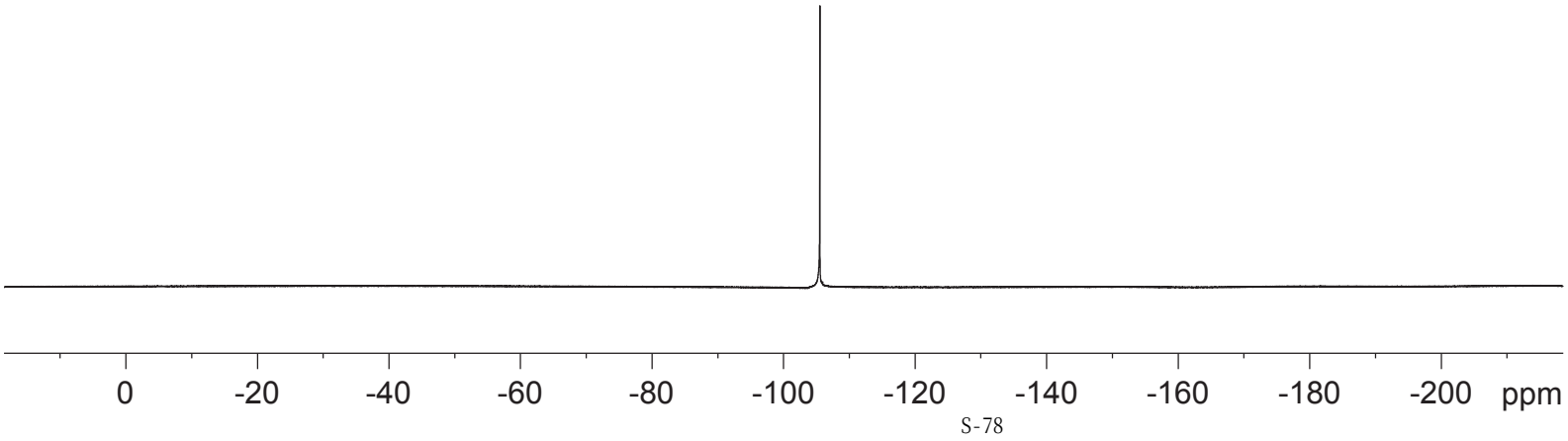
-105.51

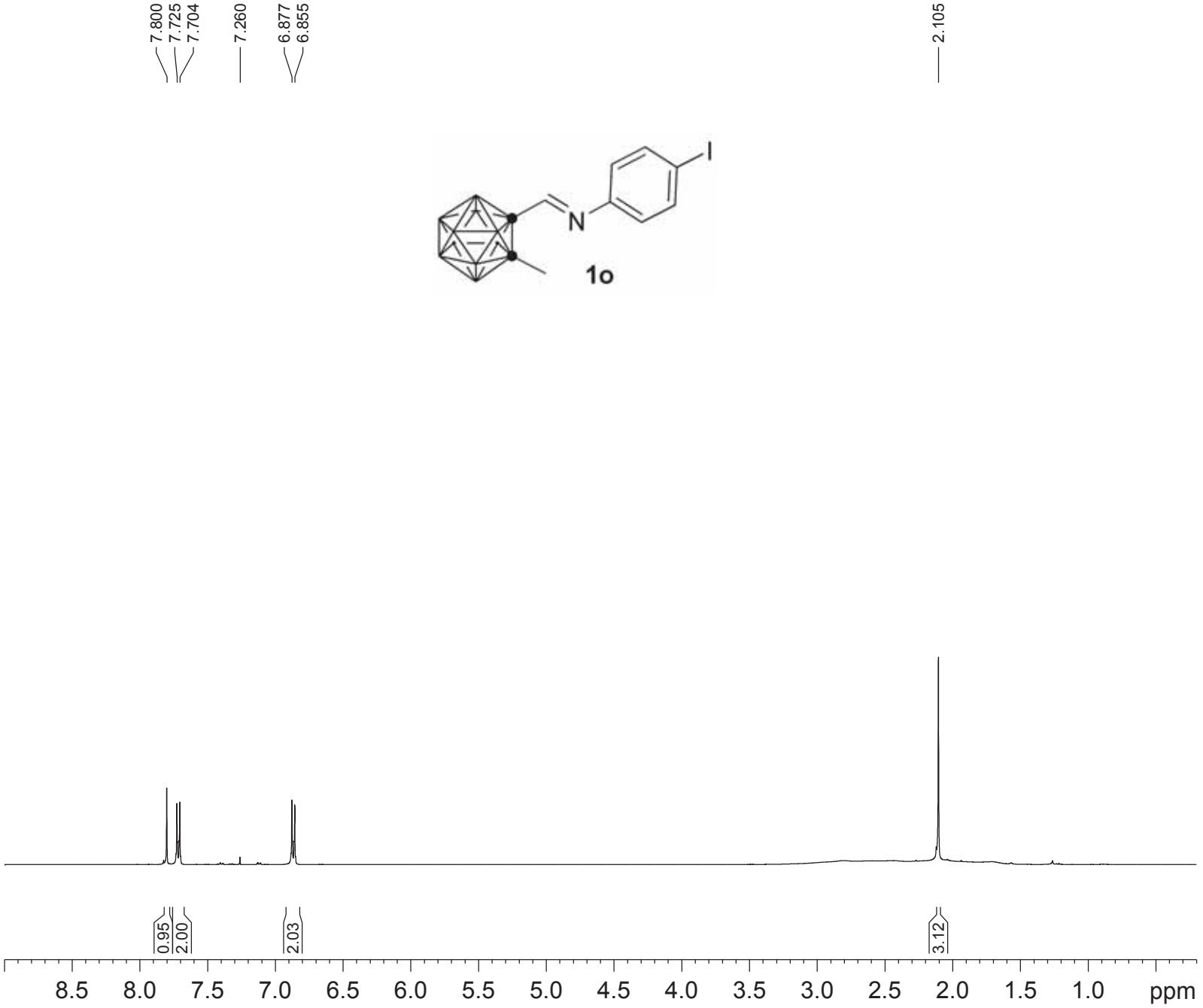
lhr-F-0704-smcascdcl3

Current Data Parameters
NAME lhr-F-0704-smcascdcl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180120
Time 9.30 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT D2O
NS 32
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 645
DW 5.600 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 376.5548010 MHz
NUC1 19F
P1 14.70 usec
PLW1 18.36000061 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.56000042 W
PLW12 0.27428001 W

F2 - Processing parameters
SI 65536
SF 376.5924602 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



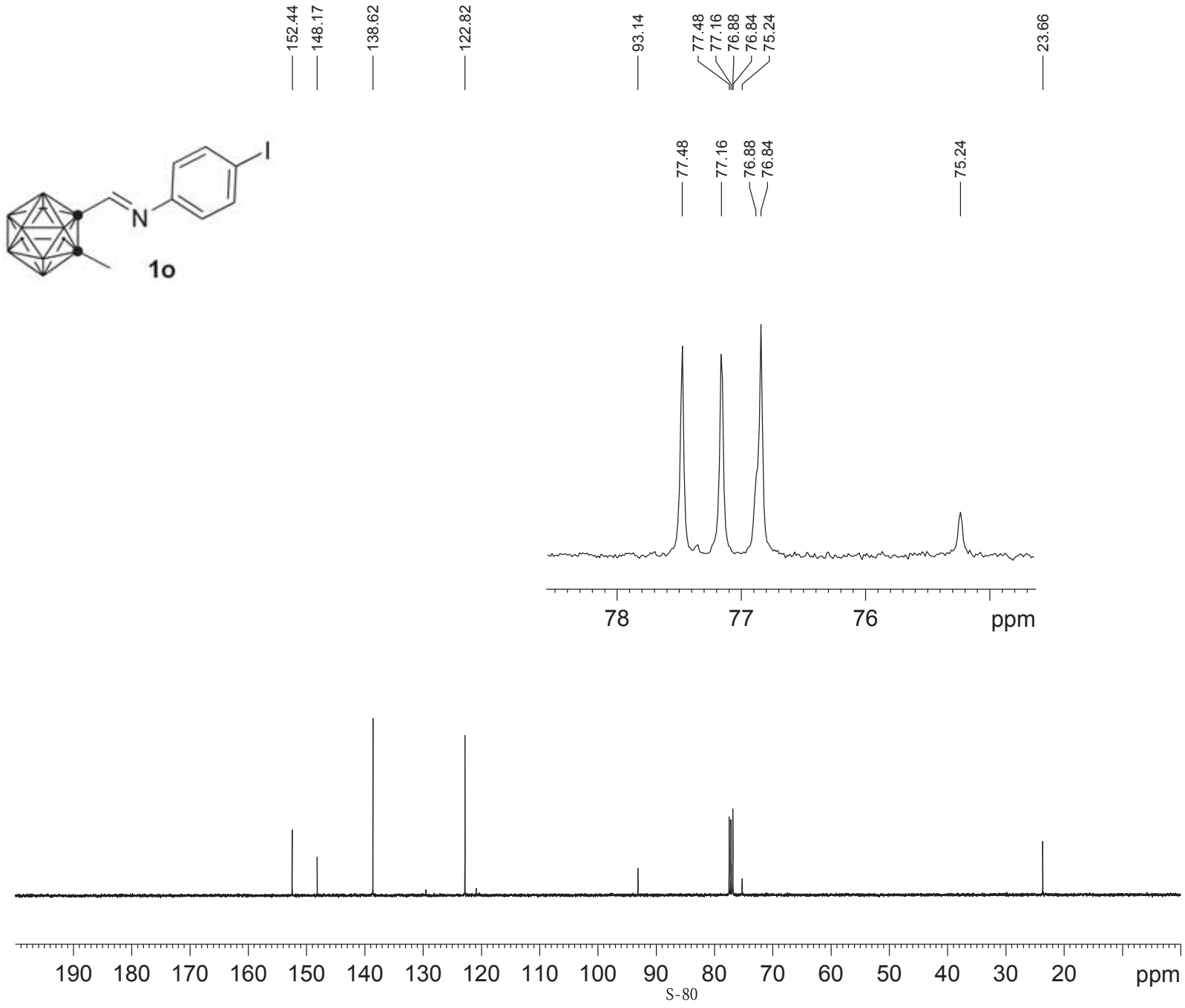


lhr-H-cassm739-I-CDC

Current Data Parameters
NAME lhr-H-cassm739-I-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170812
Time 19.38 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

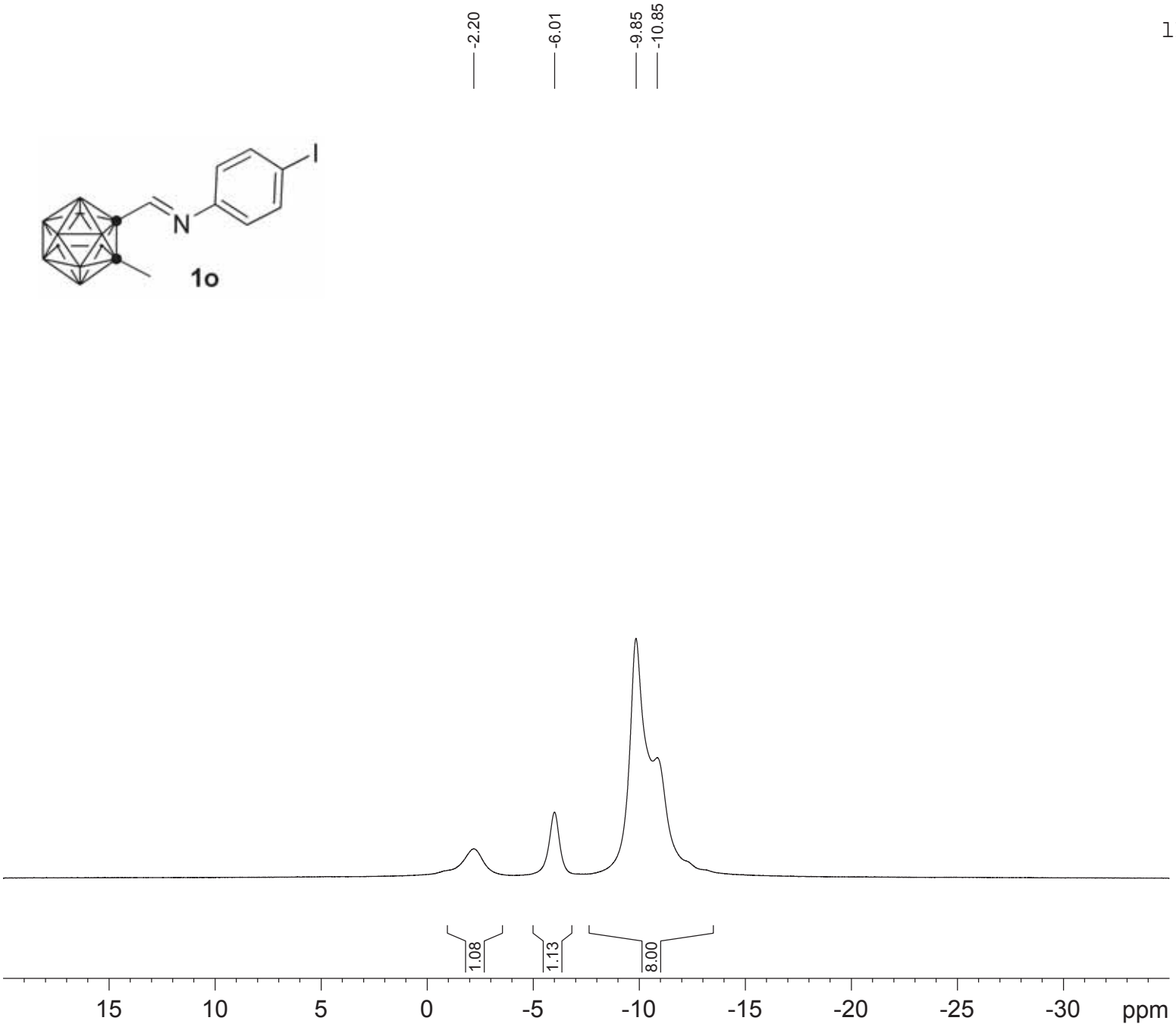
F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



lhr-C-cassm739-I-Cl

```
Current Data Parameters
NAME      lhr-C-cassm739-I-CDCl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20170812
Time                   19.41 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                        64
DS                         4
SWH                40760.871 Hz
FIDRES              0.621962 Hz
AQ                  0.8039083 sec
RG                       203
DW                    12.267 usec
DE                     6.50 usec
TE                    295.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1              100.6479773 MHz
NUC1                     13C
P1                     9.50 usec
PLW1              55.34000015 W
SFO2              400.2316009 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W
PLW13              0.13796000 W

F2 - Processing parameters
SI                     32768
SF                100.6379061 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

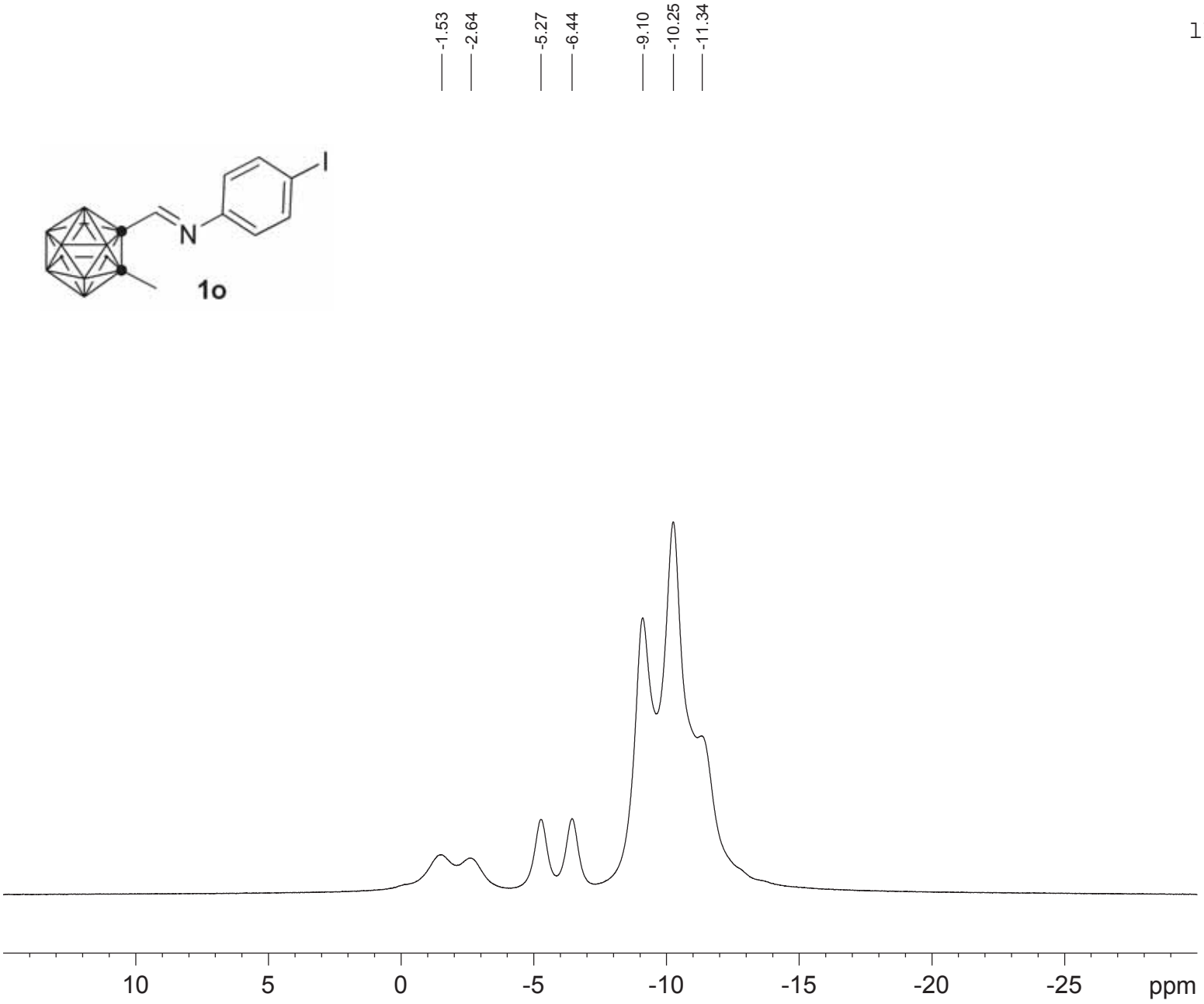
1o



lhr-B-cassm739-I-CDCl3

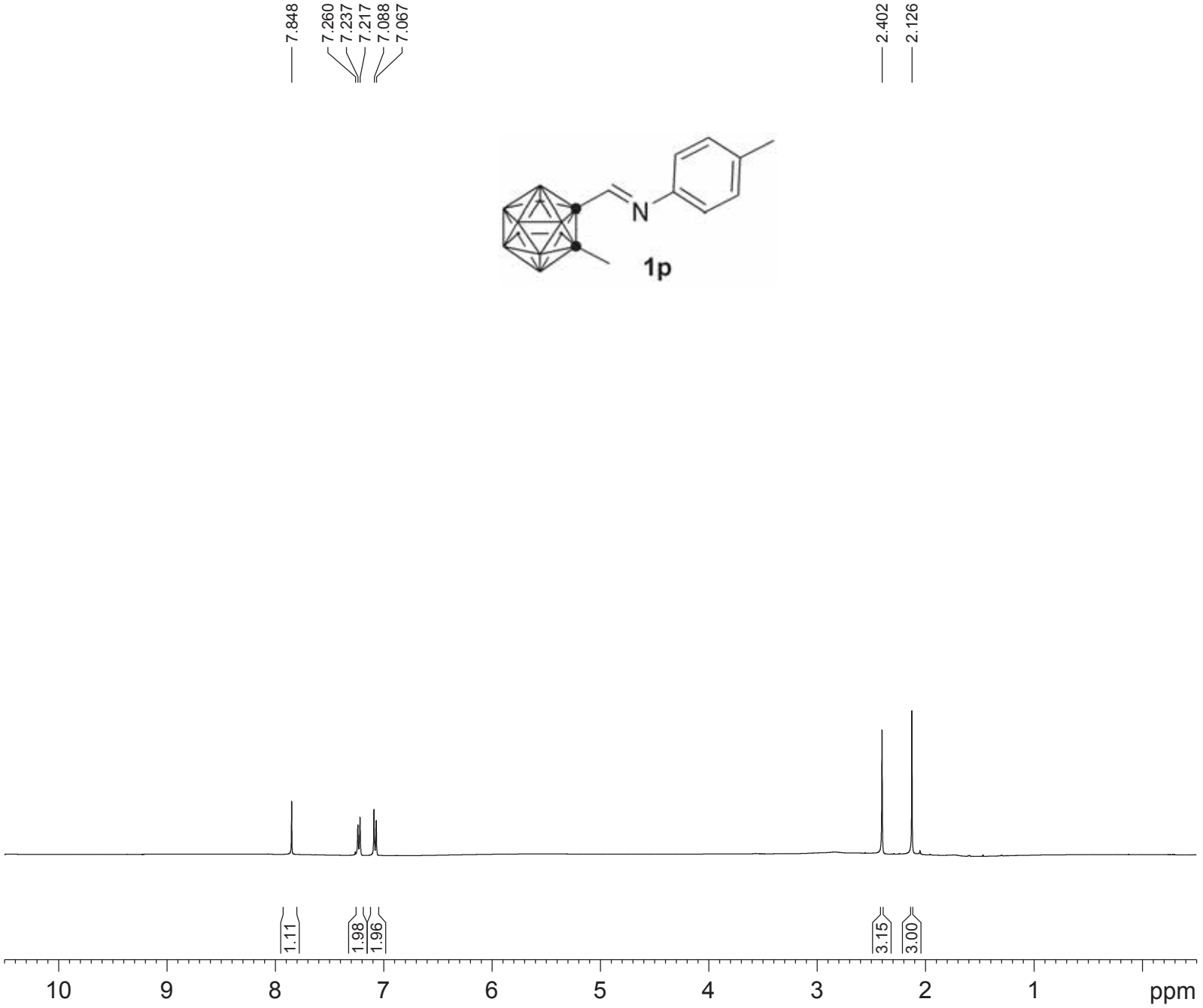
```
Current Data Parameters
NAME      lhr-B-cassm739-I-CDCl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20170812
Time                       19.32 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                     zgdc
TD                         65536
SOLVENT                    CDCl3
NS                            12
DS                             4
SWH                    24038.461 Hz
FIDRES                   0.366798 Hz
AQ                     1.3631488 sec
RG                           203
DW                        20.800 usec
DE                         6.50 usec
TE                        295.2 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1
SFO1                 128.4096890 MHz
NUC1                         11B
P1                         7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

F2 - Processing parameters
SI                         32768
SF                   128.4097615 MHz
WDW                           EM
SSB               0
LB                         1.00 Hz
GB                0
PC                         1.40
```

1o



lhr-B-cassm739-I-CDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm739-I-CDCl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170812
Time              19.34 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     17
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    203
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



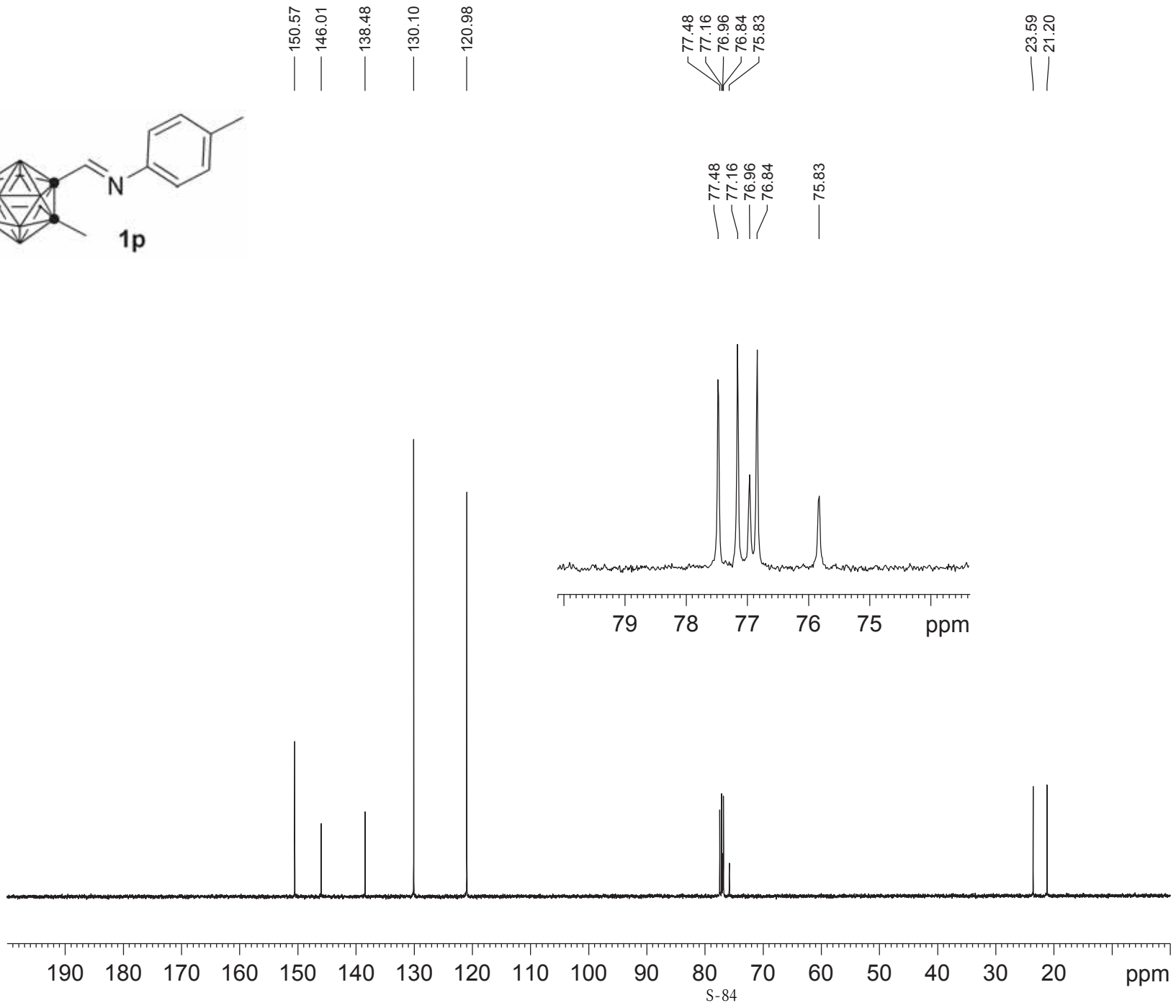
lhr-H-0732-cassm-cdc

Current Data Parameters
NAME lhr-H-0732-cassm-cdcl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170818
Time 19.05 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 17
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

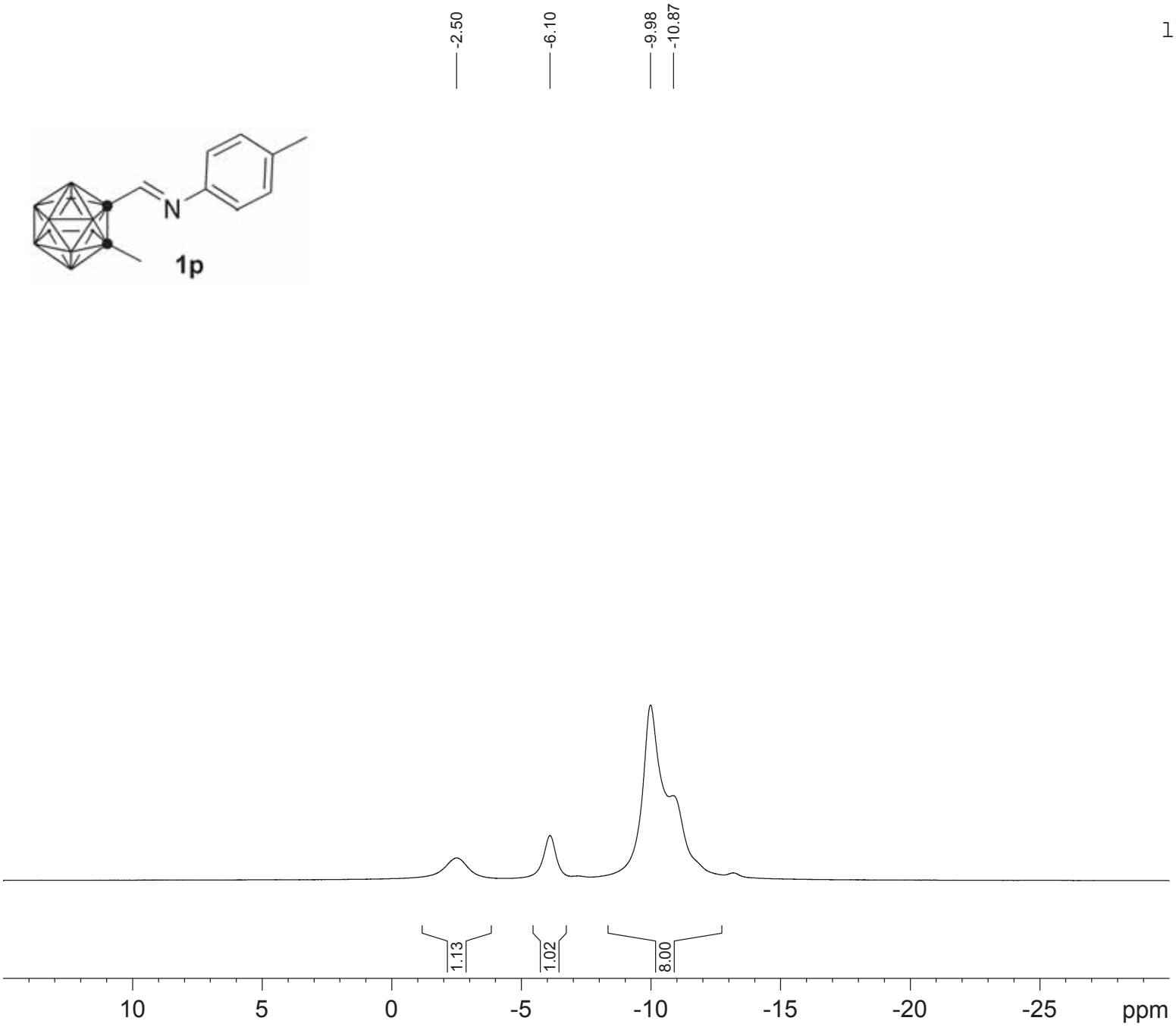
F2 - Processing parameters
SI 65536
SF 400.2300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1p



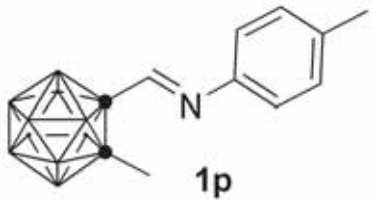
lhr-C-0732-cassm-c

```
Current Data Parameters
NAME      lhr-C-0732-cassm-cdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20170818
Time                   19.11 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       78
DS                        4
SWH                40760.871 Hz
FIDRES              0.621962 Hz
AQ                  0.8039083 sec
RG                      203
DW                     12.267 usec
DE                      6.50 usec
TE                     295.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1             100.6479773 MHz
NUC1                     13C
P1                      9.50 usec
PLW1             55.34000015 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2             13.56000042 W
PLW12             0.27428001 W
PLW13             0.13796000 W

F2 - Processing parameters
SI                       32768
SF               100.6379089 MHz
WDW                        EM
SSB          0
LB                      1.00 Hz
GB           0
PC                      1.40
```



lhr-B-0732-cassm-cdcl3

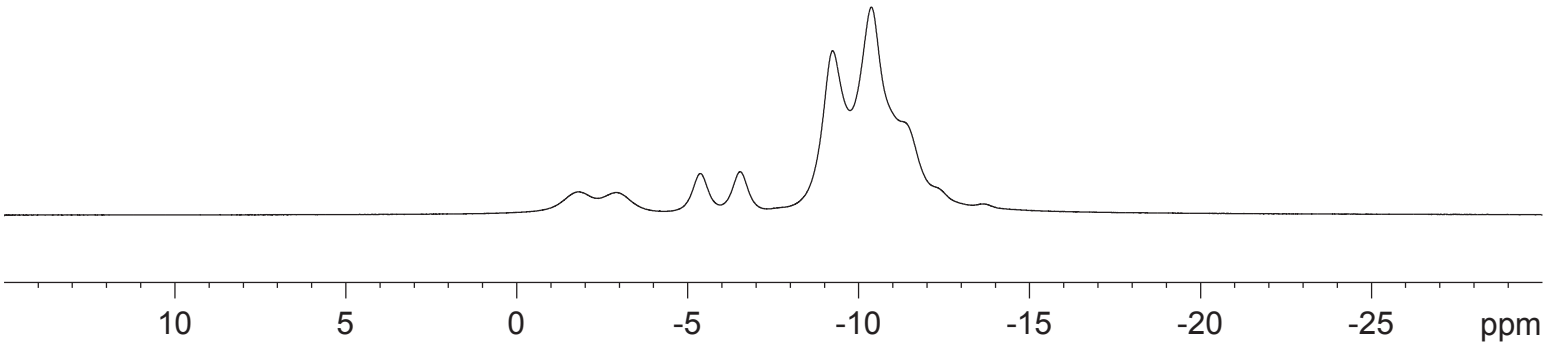
```
Current Data Parameters
NAME      lhr-B-0732-cassm-cdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170818
Time              19.14 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  50.8
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

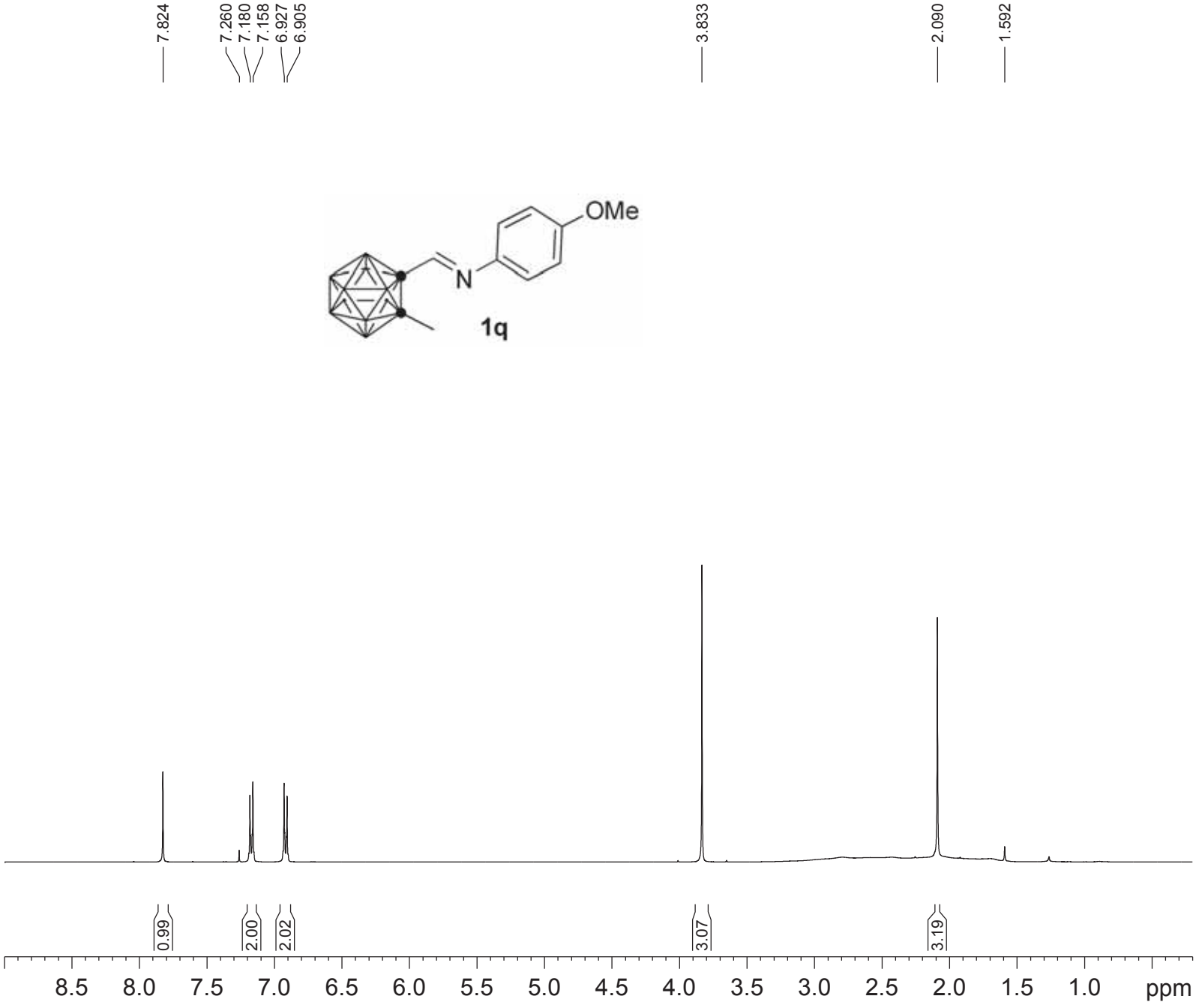


1p

lhr-B-0732-cassm-cdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0732-cassm-cdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170818
Time              19.16 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   11
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   57
DW               20.800 usec
DE                6.50 usec
TE               295.1 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



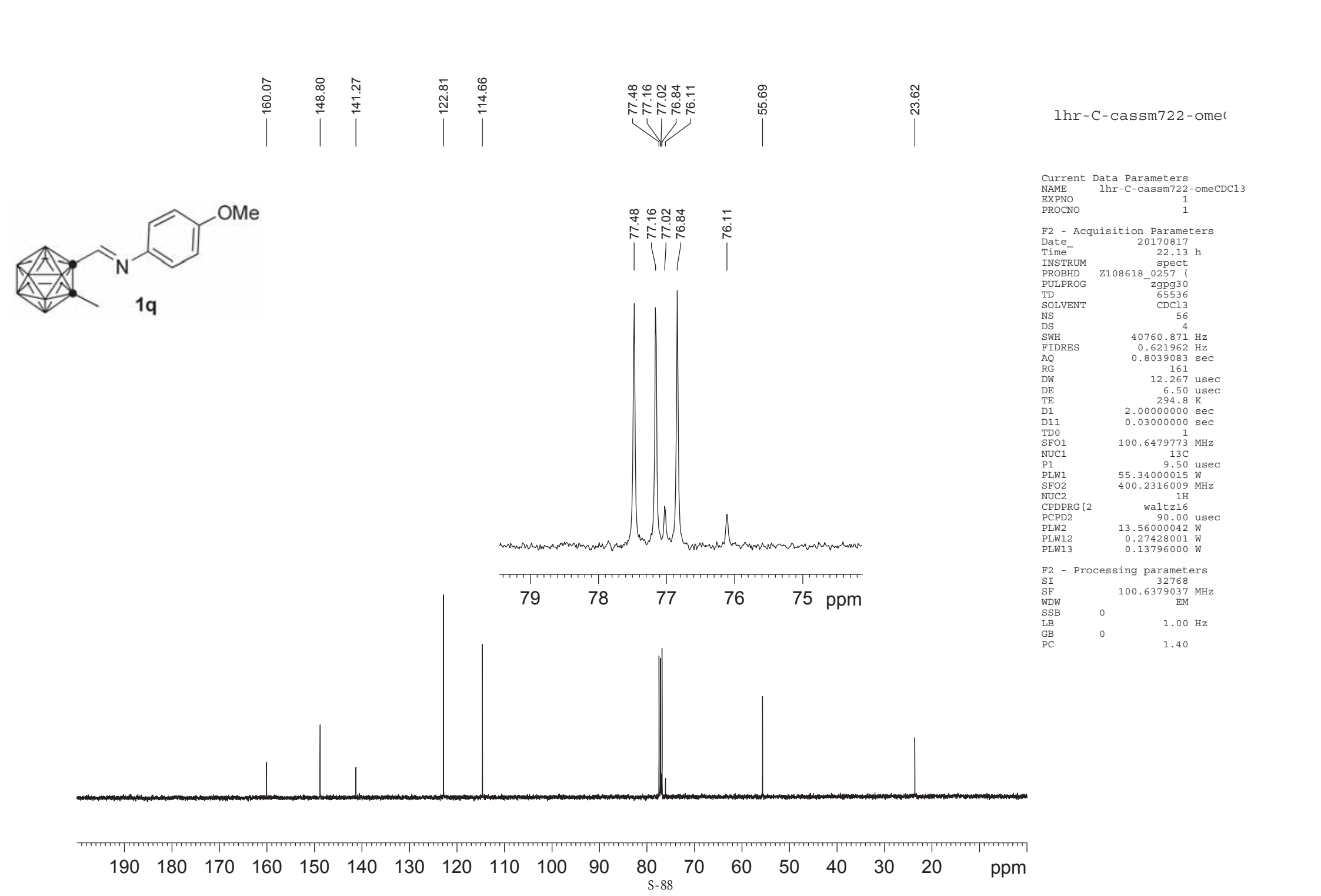


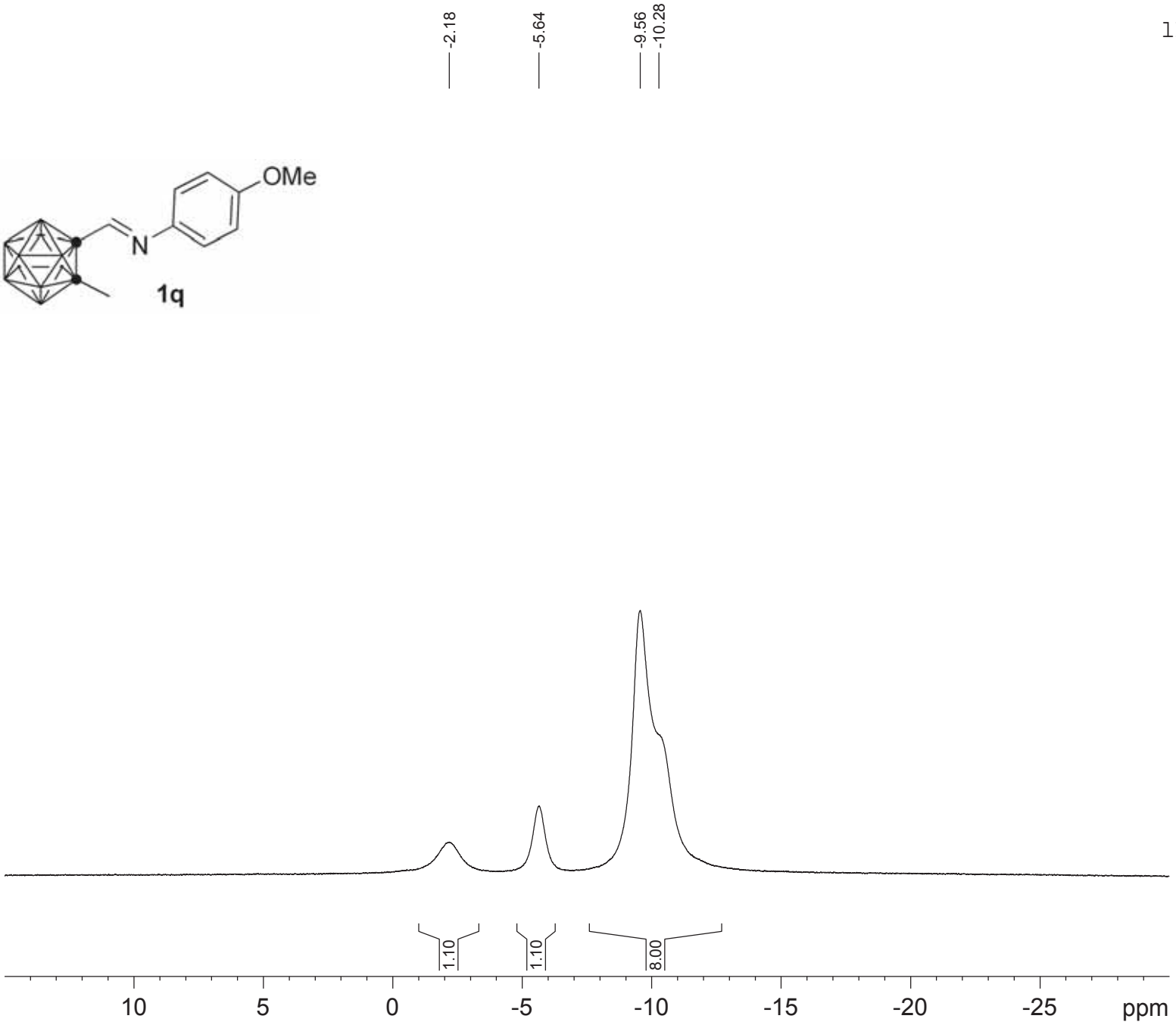
lhr-H-cassm722-omeCl

Current Data Parameters
NAME lhr-H-cassm722-omeCDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170817
Time 22.09 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

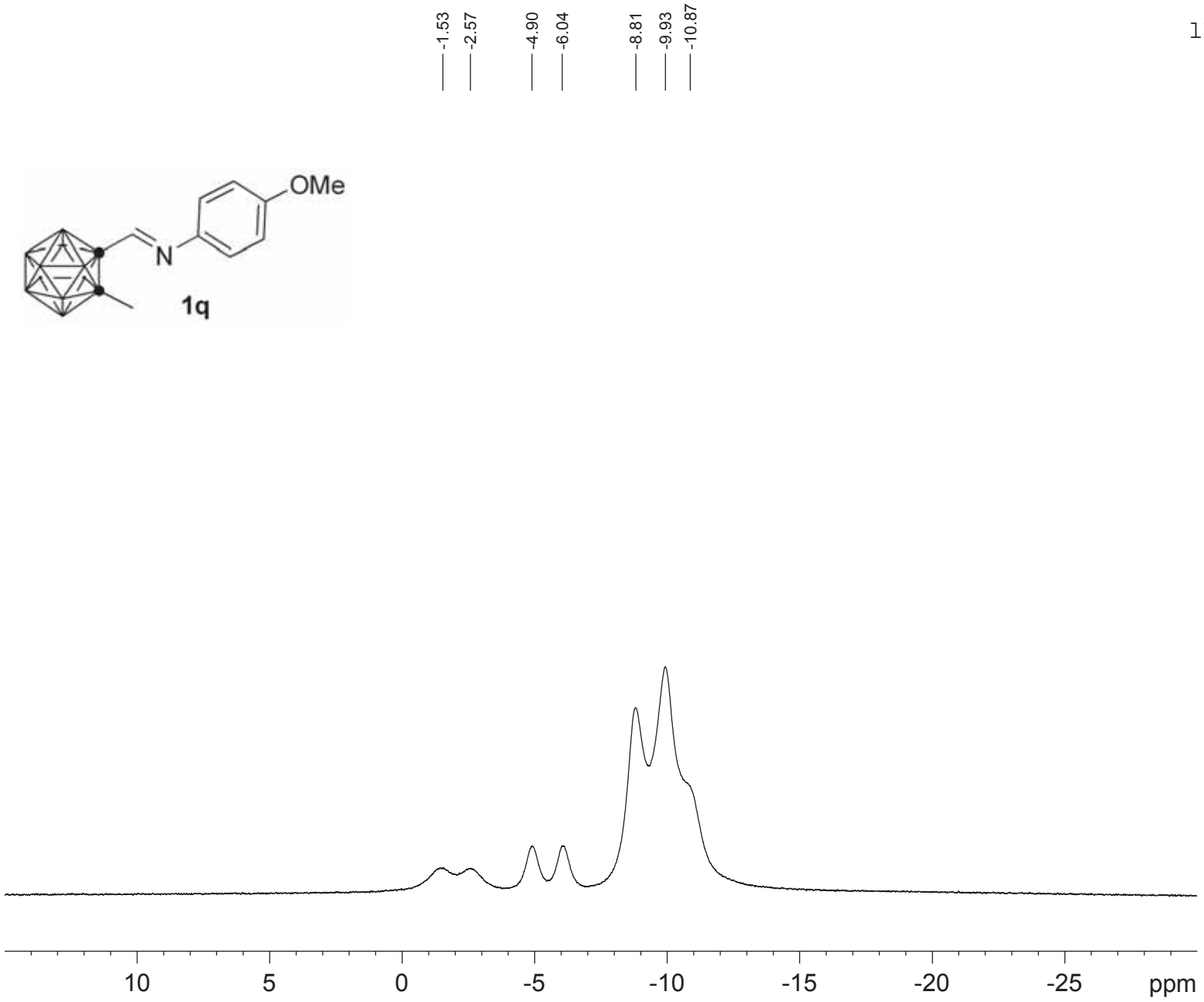

160.07
148.80
141.27
122.81
114.66
77.48
77.16
77.02
76.84
76.11
55.69
23.62
lhr-C-cassm722-ome(
OMe
N
1q
Current Data Parameters
NAME lhr-C-cassm722-omeCDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170817
Time 22.13 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 56
DS 4
SWH 40760.871 Hz
FIDRES 0.621962 Hz
AQ 0.8039083 sec
RG 161
DW 12.267 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6479773 MHz
NUC1 13C
P1 9.50 usec
PLW1 55.34000015 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.56000042 W
PLW12 0.27428001 W
PLW13 0.13796000 W
F2 - Processing parameters
SI 32768
SF 100.6379037 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
79 78 77 76 75 ppm
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



lhr-B-cassm722-omeCDCl3

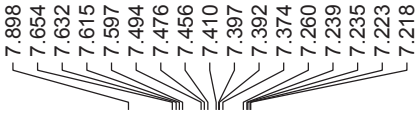
```
Current Data Parameters
NAME      lhr-B-cassm722-omeCDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170817
Time               22.03 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     11
DS                      4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    203
DW                 20.800 usec
DE                  6.50 usec
TE                 295.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

1q

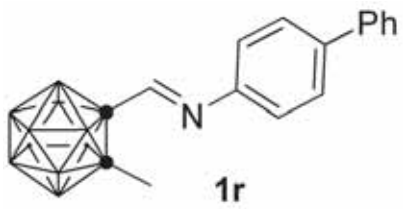


lhr-B-cassm722-omeCDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm722-omeCDCl3(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170817
Time              22.04 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE                295.0 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-H-cassm746-ph-CI

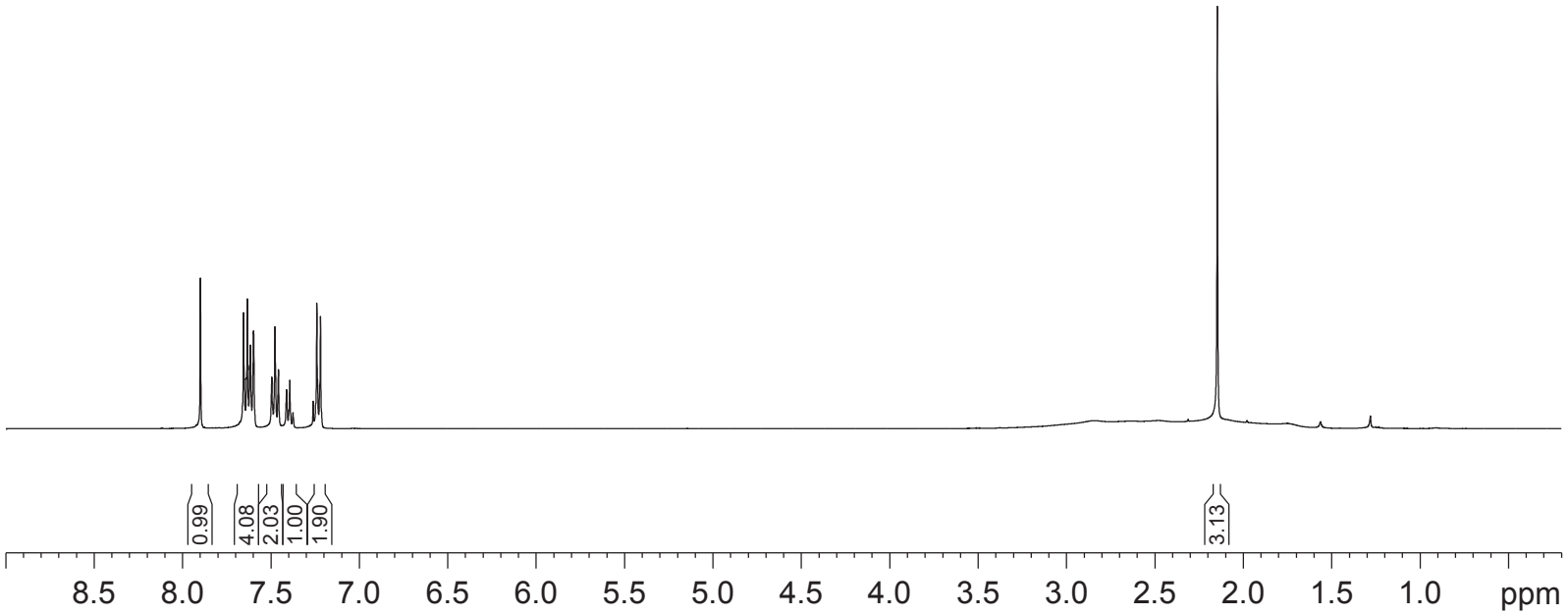


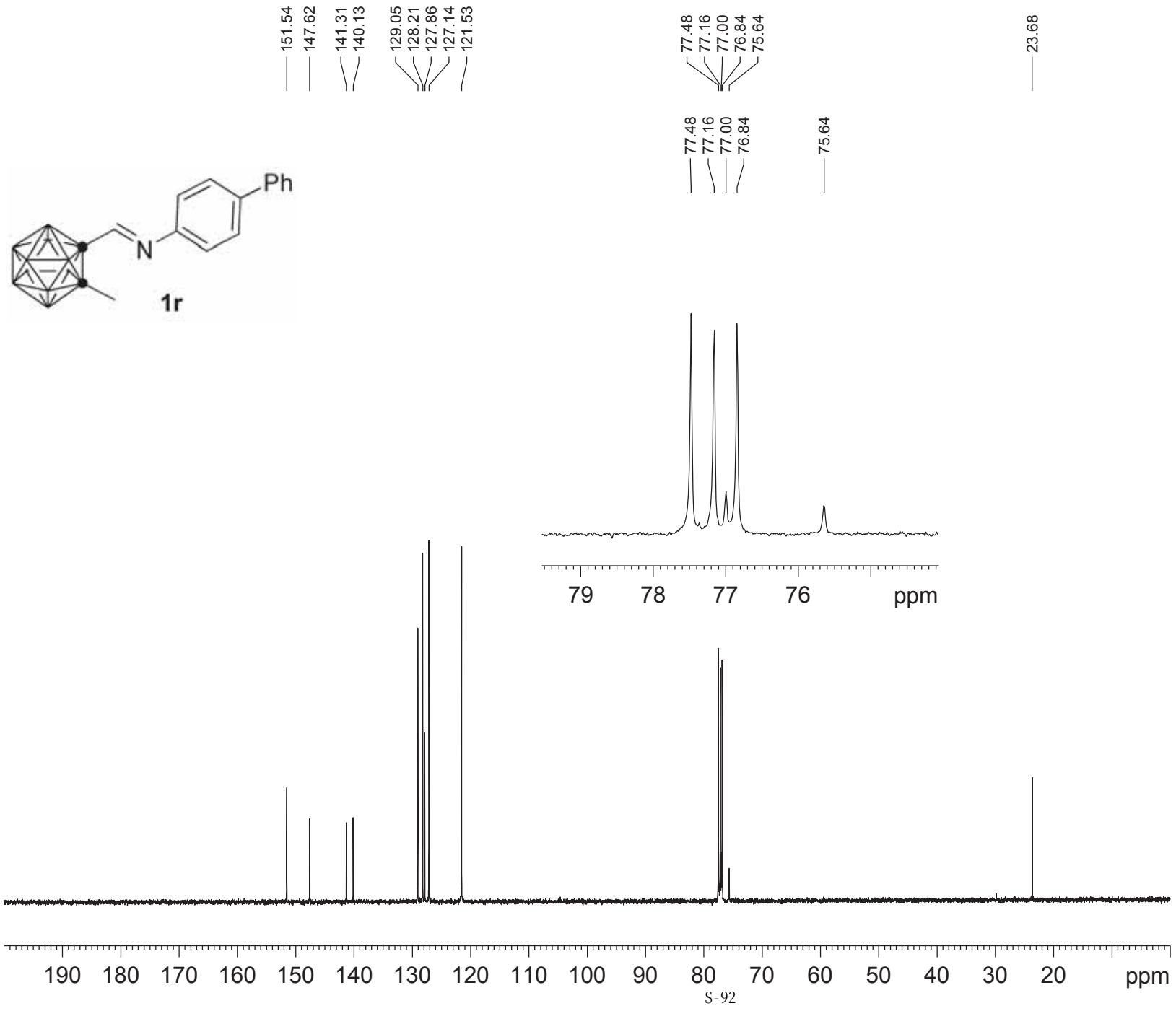
1r

Current Data Parameters
NAME lhr-H-cassm746-ph-CDCl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170812
Time 19.02 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

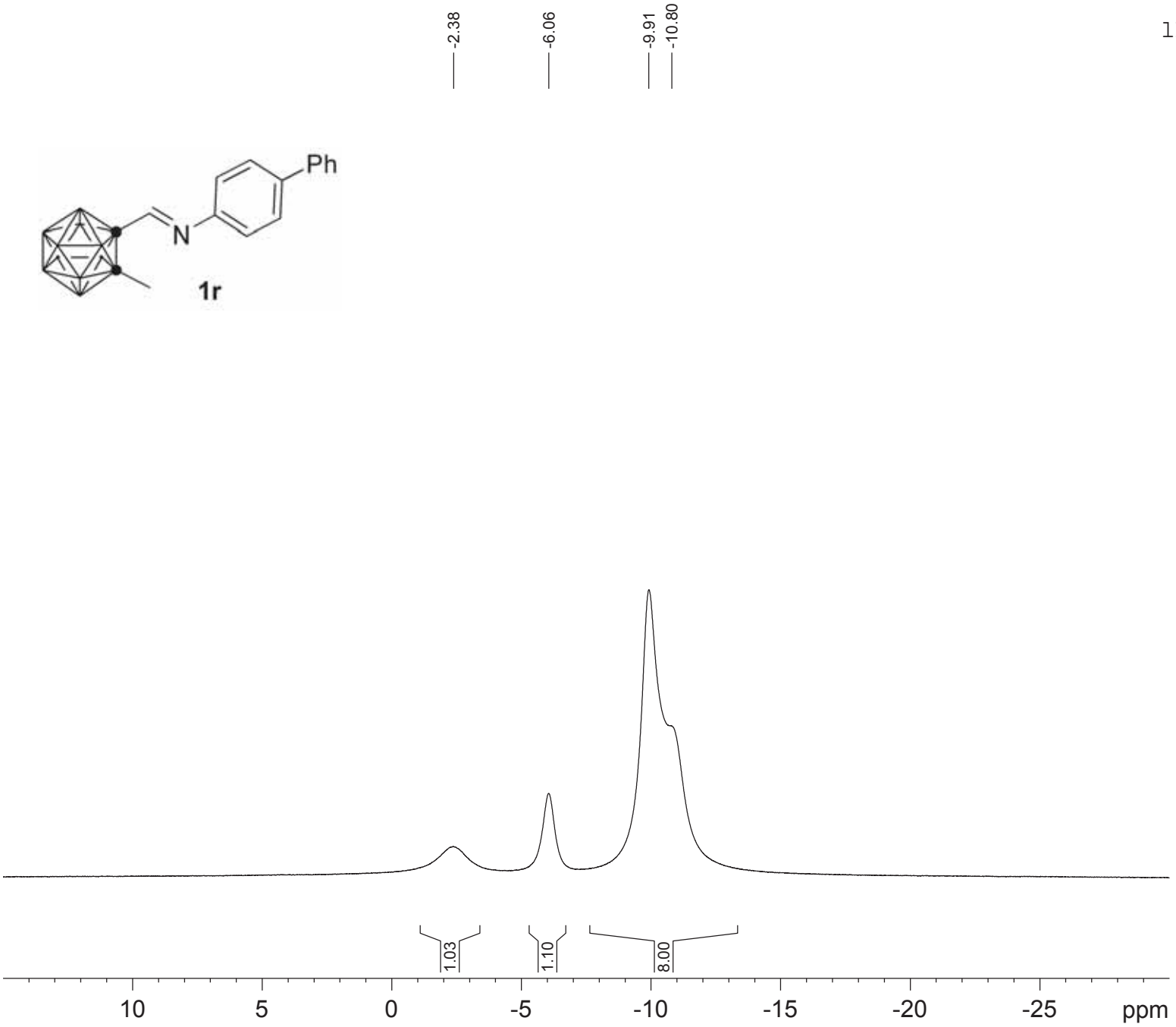
F2 - Processing parameters
SI 65536
SF 400.2300105 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





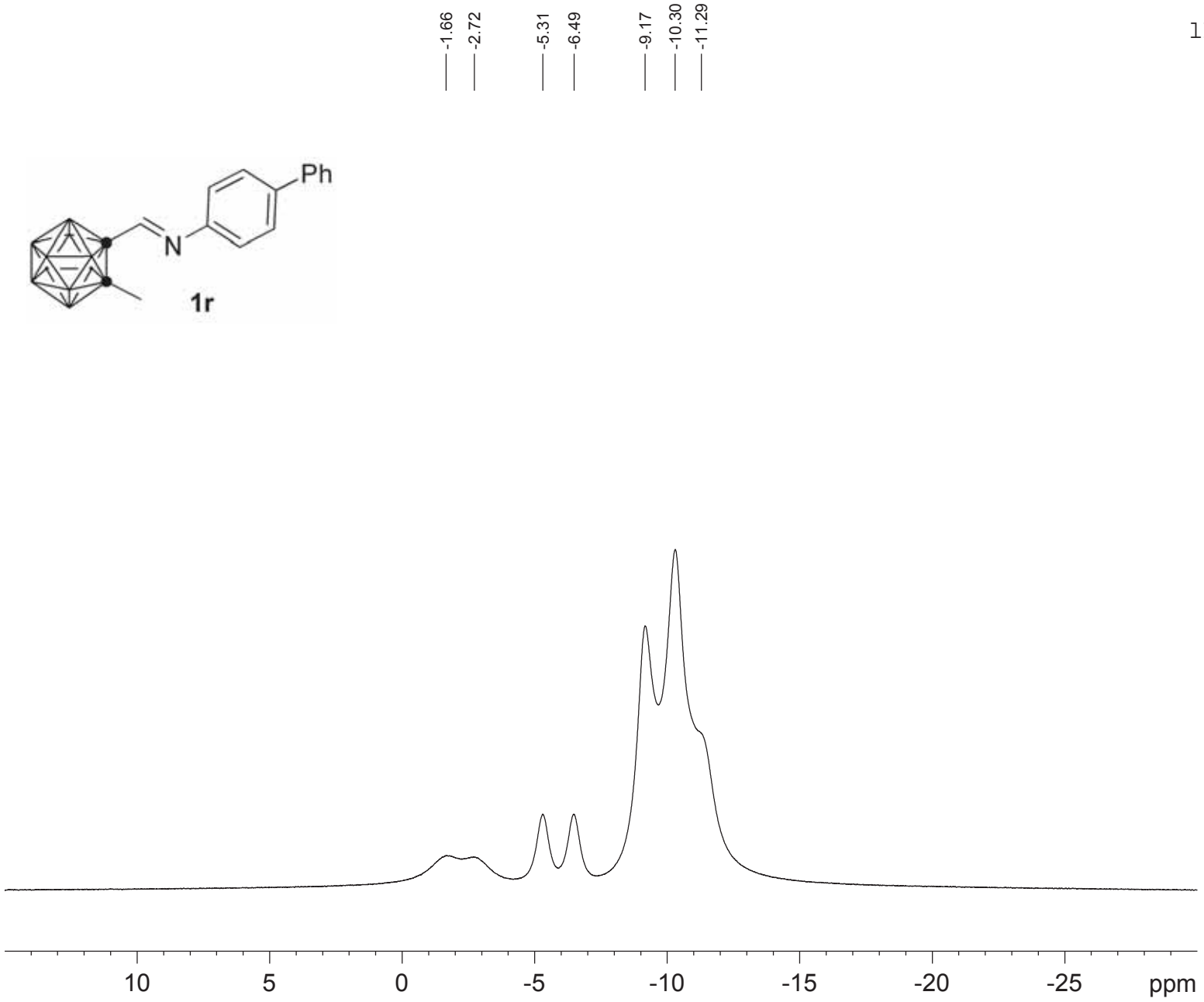
lhr-C-cassm746-Ph-(

```
Current Data Parameters
NAME      lhr-C-cassm746-Ph-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170812
Time              19.06 h
INSTRUM            spect
PROBHD    Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  349
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  161
DW                12.267 usec
DE                 6.50 usec
TE                295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6479773 MHz
NUC1               13C
P1                9.50 usec
PLW1         55.34000015 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                32768
SF          100.6379044 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



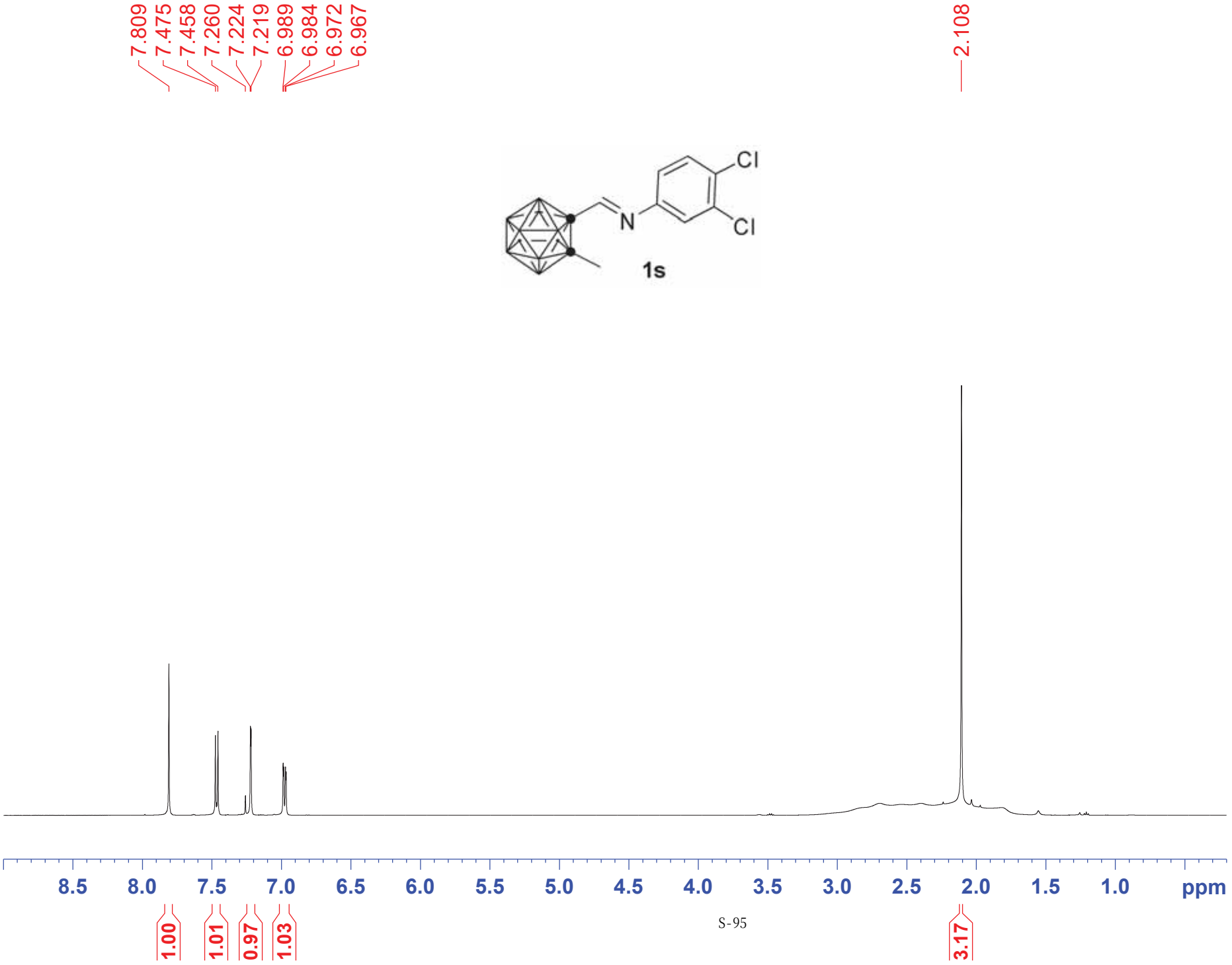
lhr-B-cassm746-ph-CDCl3

```
Current Data Parameters
NAME      lhr-B-cassm746-ph-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170812
Time               19.23 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    15
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   203
DW                20.800 usec
DE                 6.50 usec
TE                295.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                 32768
SF          128.4097615 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



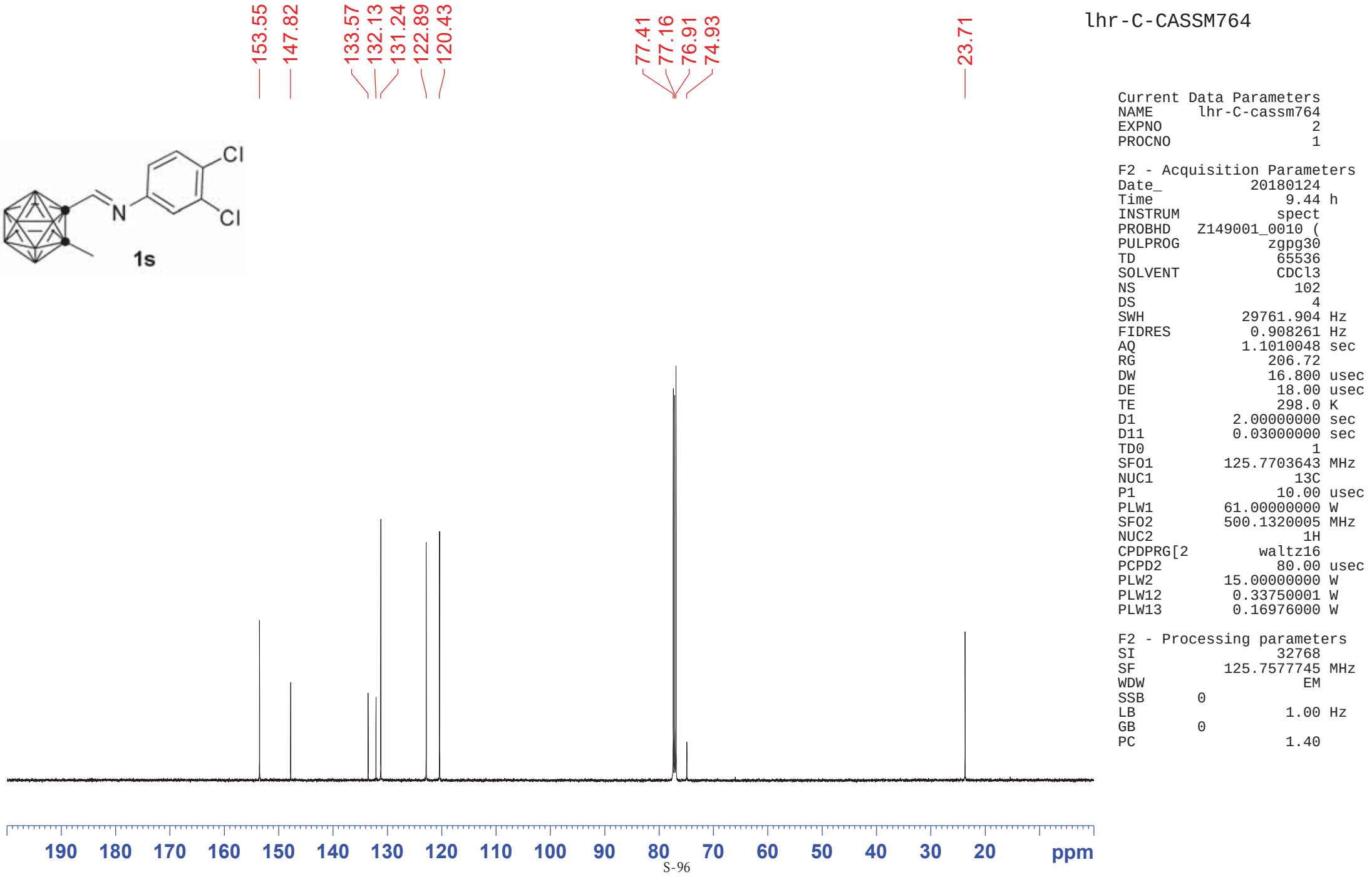
lhr-B-cassm746-ph-CDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm746-ph-CDCl3(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170812
Time              19.25 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   23
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  203
DW               20.800 usec
DE                6.50 usec
TE               295.0 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-H-CASSM764

```
Current Data Parameters
NAME      lhr-H-cassm764
EXPNO                  2
PROCNO                 1

F2 - Acquisition Paramet
Date_           20180124
Time                9.38
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 30.85
DW                 50.000
DE                 10.00
TE                298.0
D1            1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1         15.00000000

F2 - Processing paramete
SI                 65536
SF         500.1300116
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```

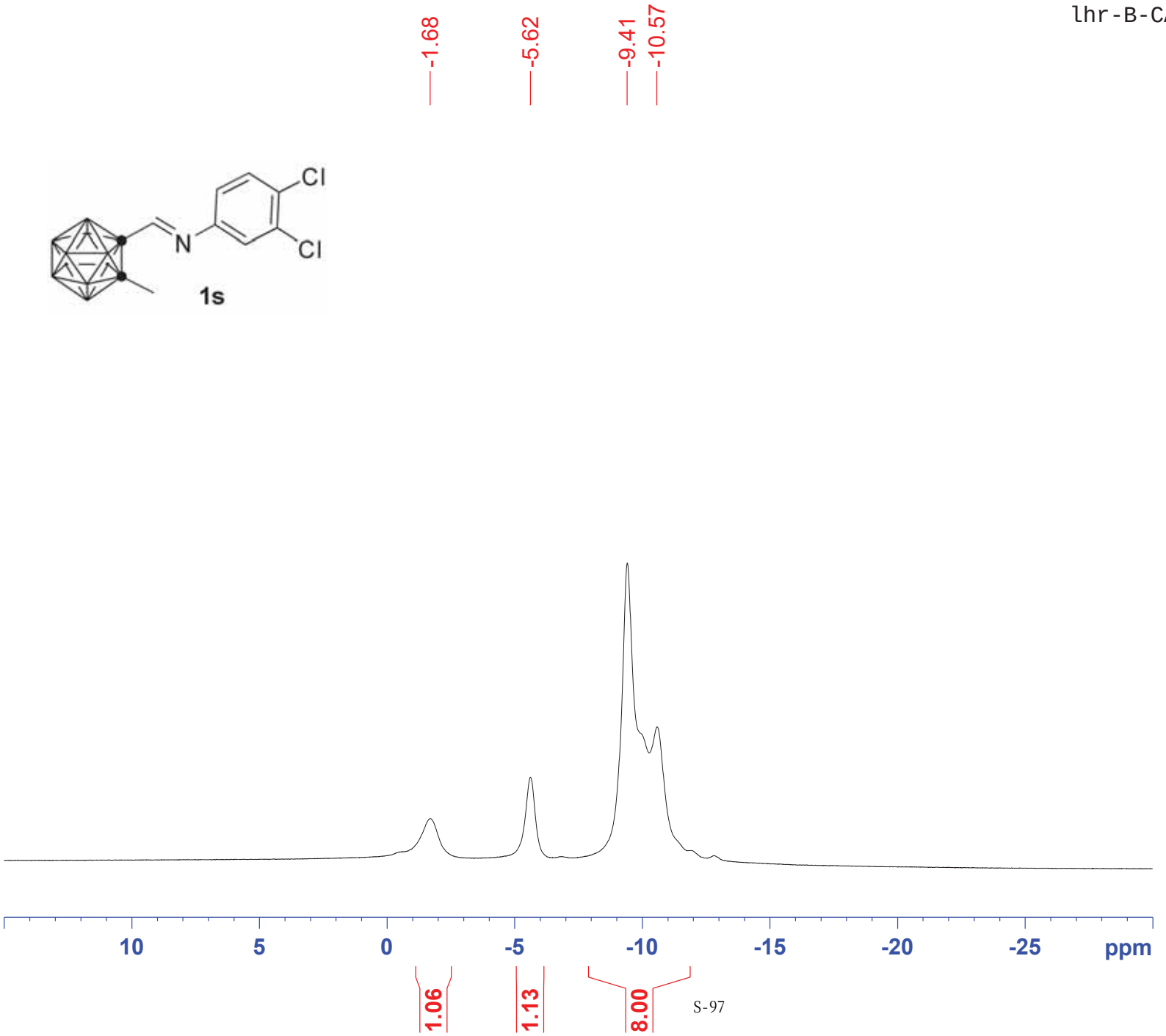


lhr-C-CASSM764

```
Current Data Parameters
NAME      lhr-C-cassm764
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180124
Time               9.44 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  102
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577745 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

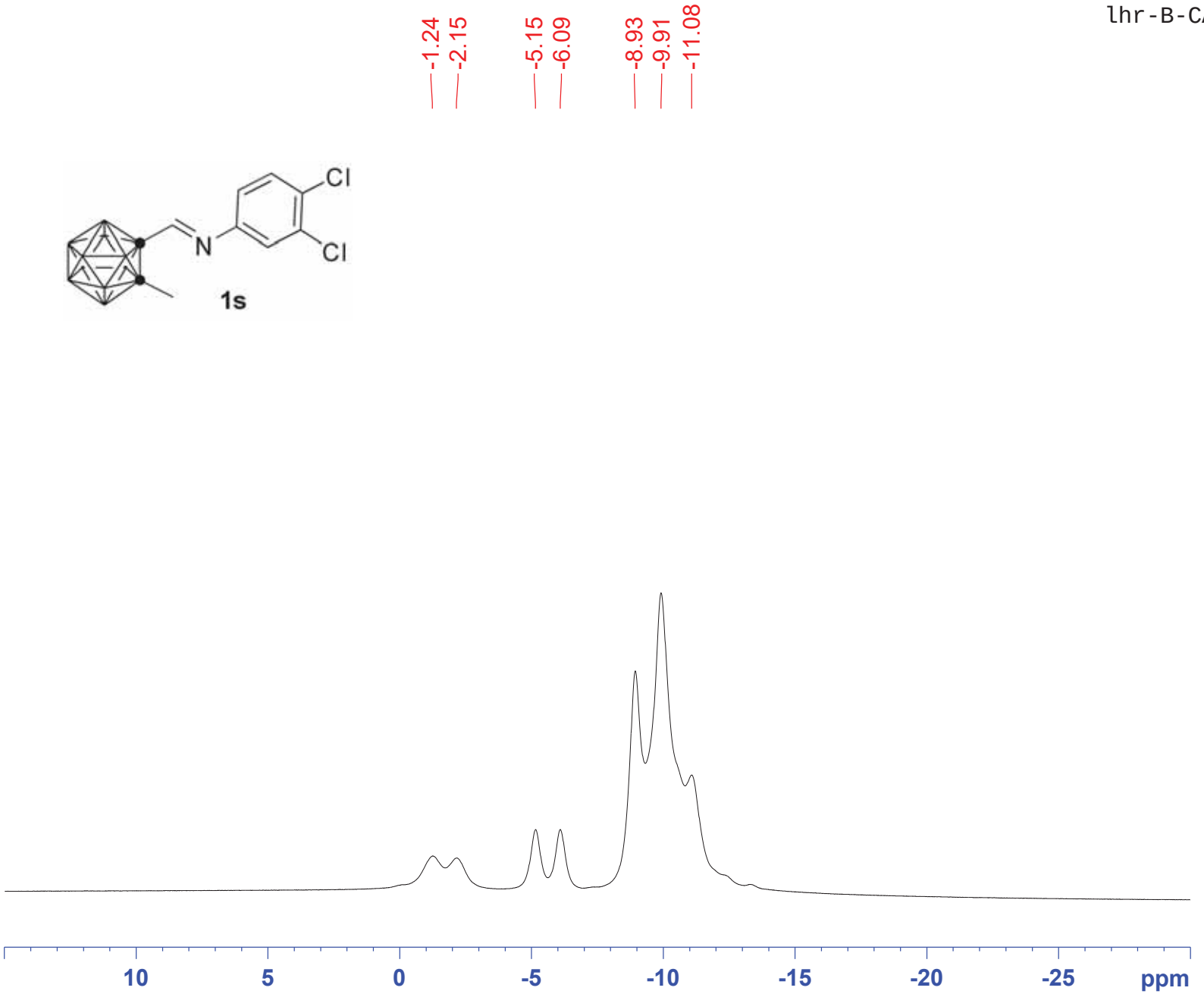
lhr-B-CASSM764

1s

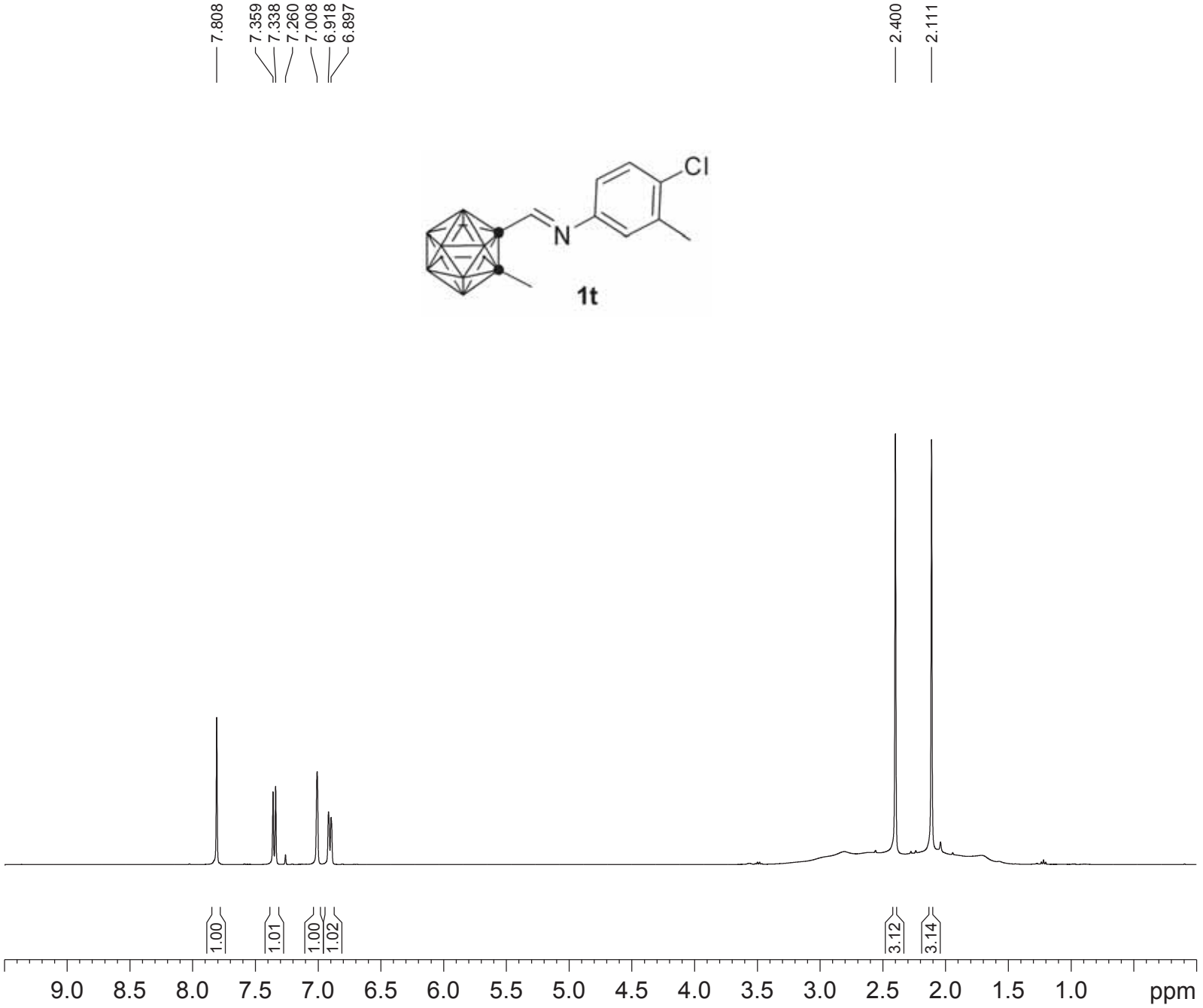



```
Current Data Parameters
NAME      lhr-B-cassm764
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180124
Time               9.48 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   20
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ             0.6815744 sec
RG                206.72
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        160.4615790 MHz
NUC1                11B
P1                10.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                16384
SF          160.4615999 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-CASSM764(C)



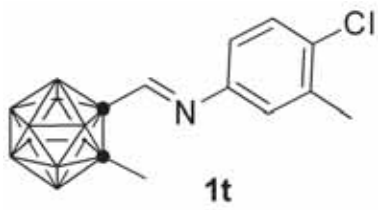

```
Current Data Parameters
NAME      lhr-B-cassm764(c)
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20180124
Time                9.49 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                  142.5
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1             1.00000000 sec
TD0                     1
SFO1         160.4615792 MHz
NUC1                 11B
P1                 10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                  16384
SF           160.4615997 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



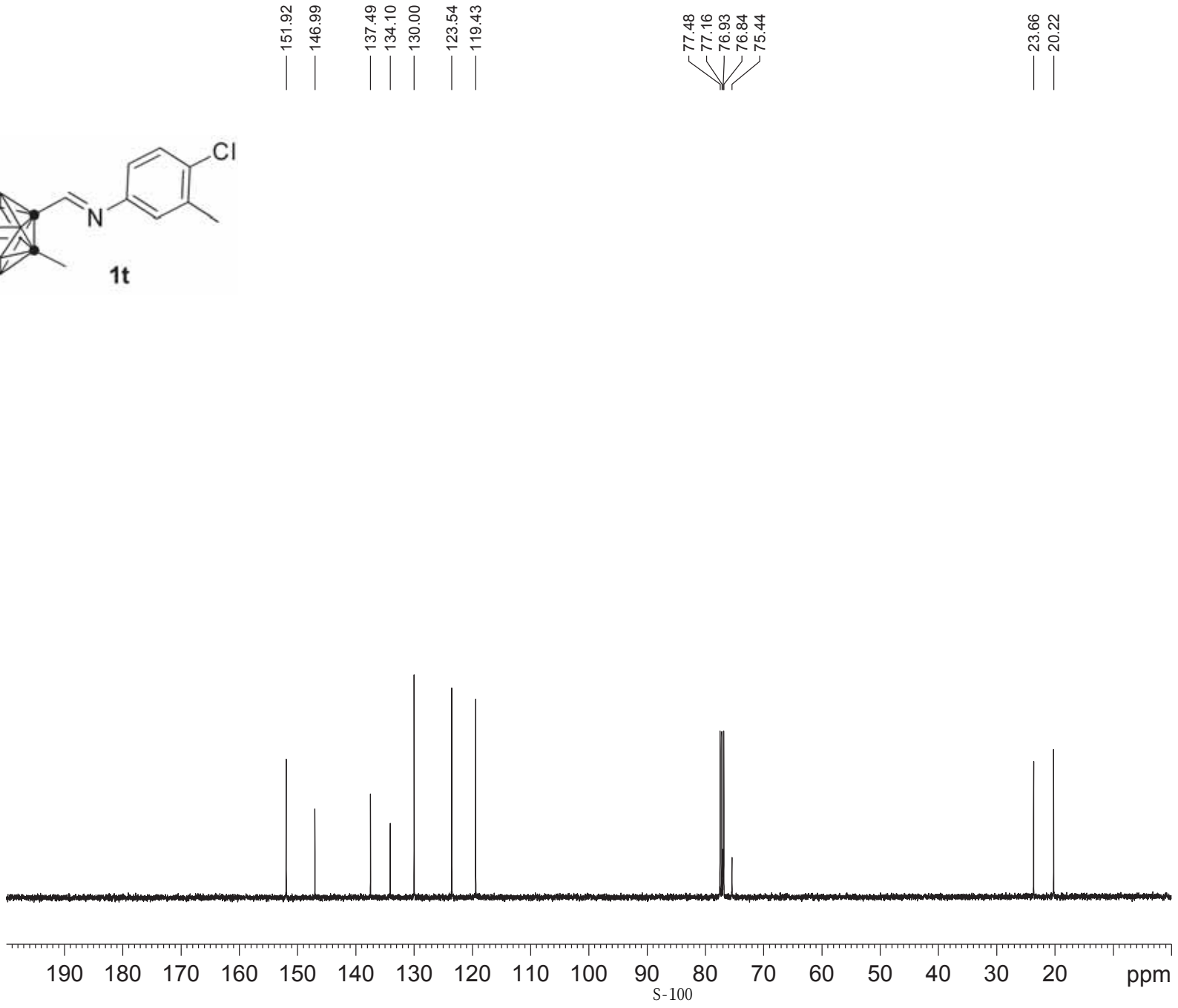
Current Data Parameters
NAME lhr-H-cassm-783-cdcl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171209
Time 16.38 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 28.5
DW 62.400 usec
DE 6.50 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



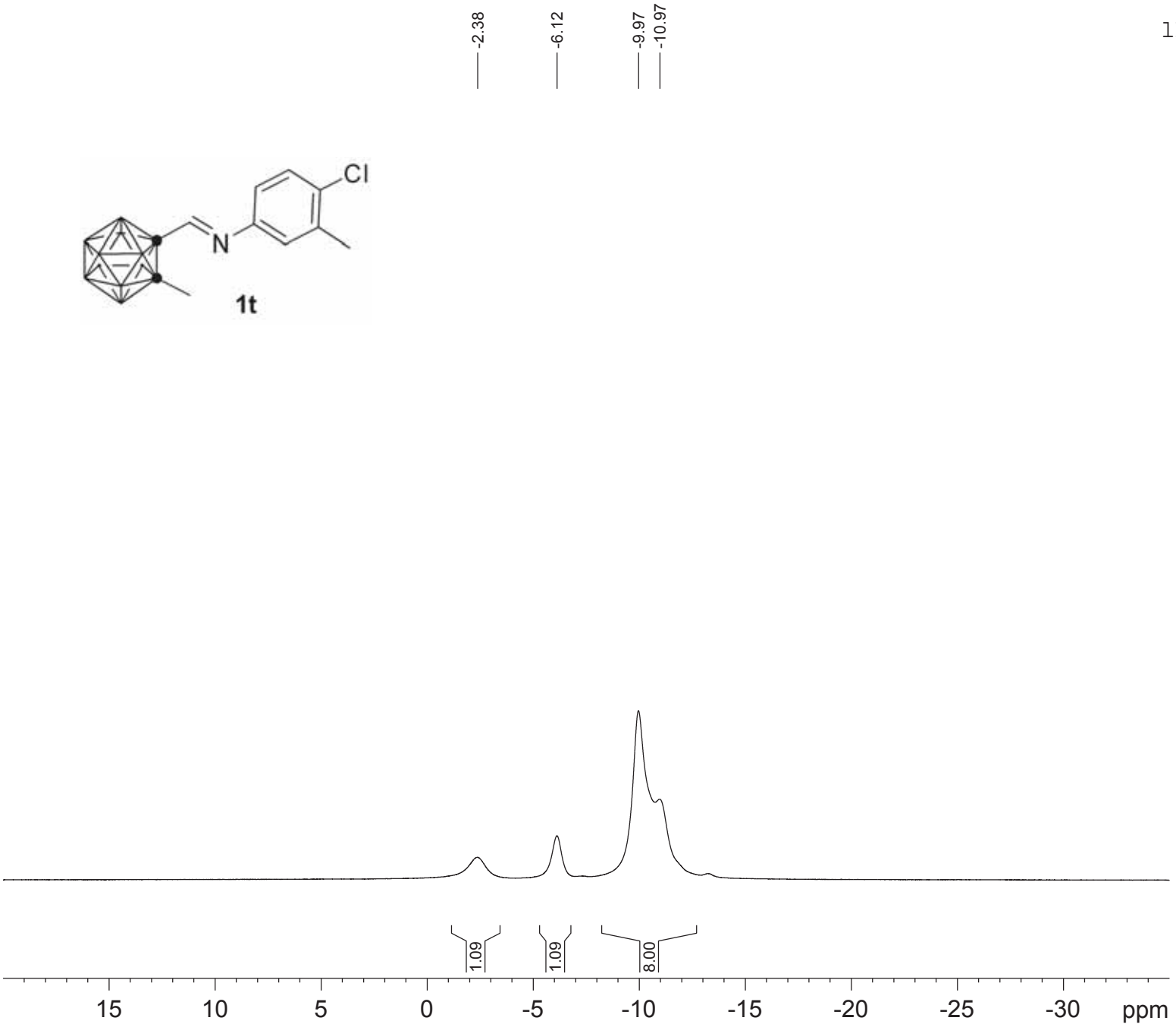
1t



lhr-C-cassm-783-cd(

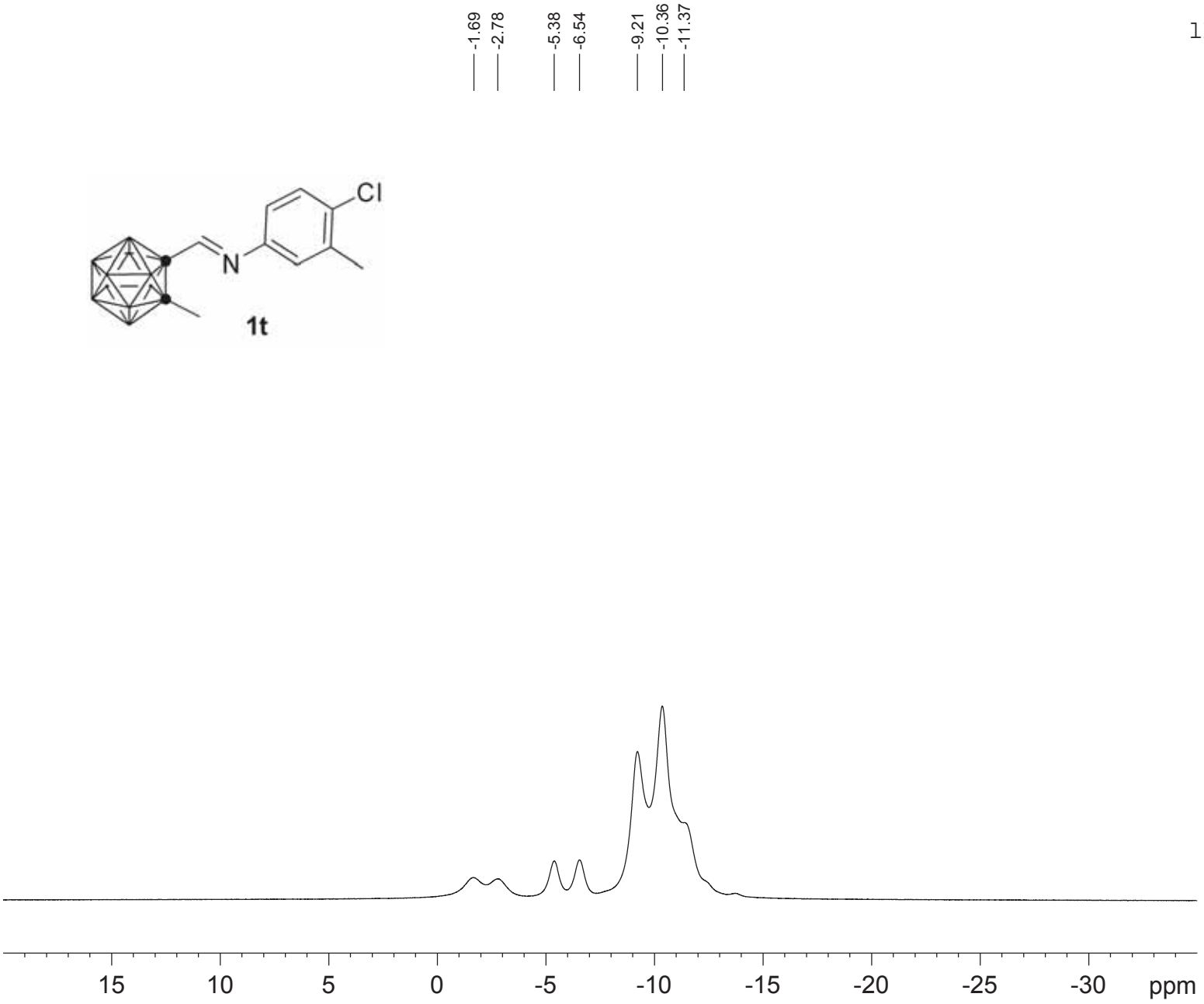
```
Current Data Parameters
NAME      lhr-C-cassm-783-cdcl3
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20171209
Time              16.41 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  203
DW                16.800 usec
DE                 6.50 usec
TE                297.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        100.6479773 MHz
NUC1               13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                32768
SF          100.6379043 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

1t



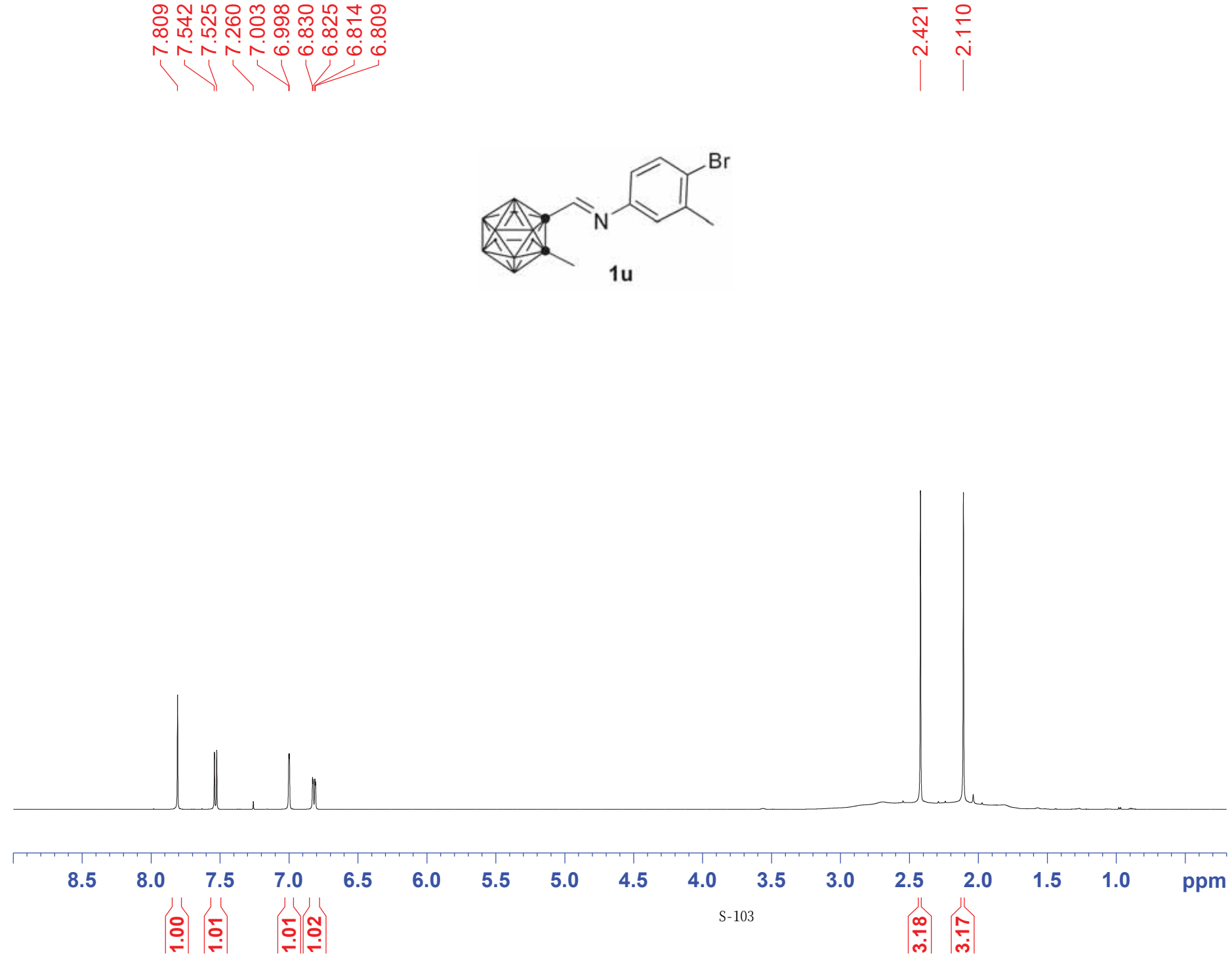
lhr-B-cassm-783-cdcl3

```
Current Data Parameters
NAME      lhr-B-cassm-783-cdcl3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171209
Time                   17.00 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                         6
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       203
DW                    20.800 usec
DE                     6.50 usec
TE                    297.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                     32768
SF               128.4097615 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



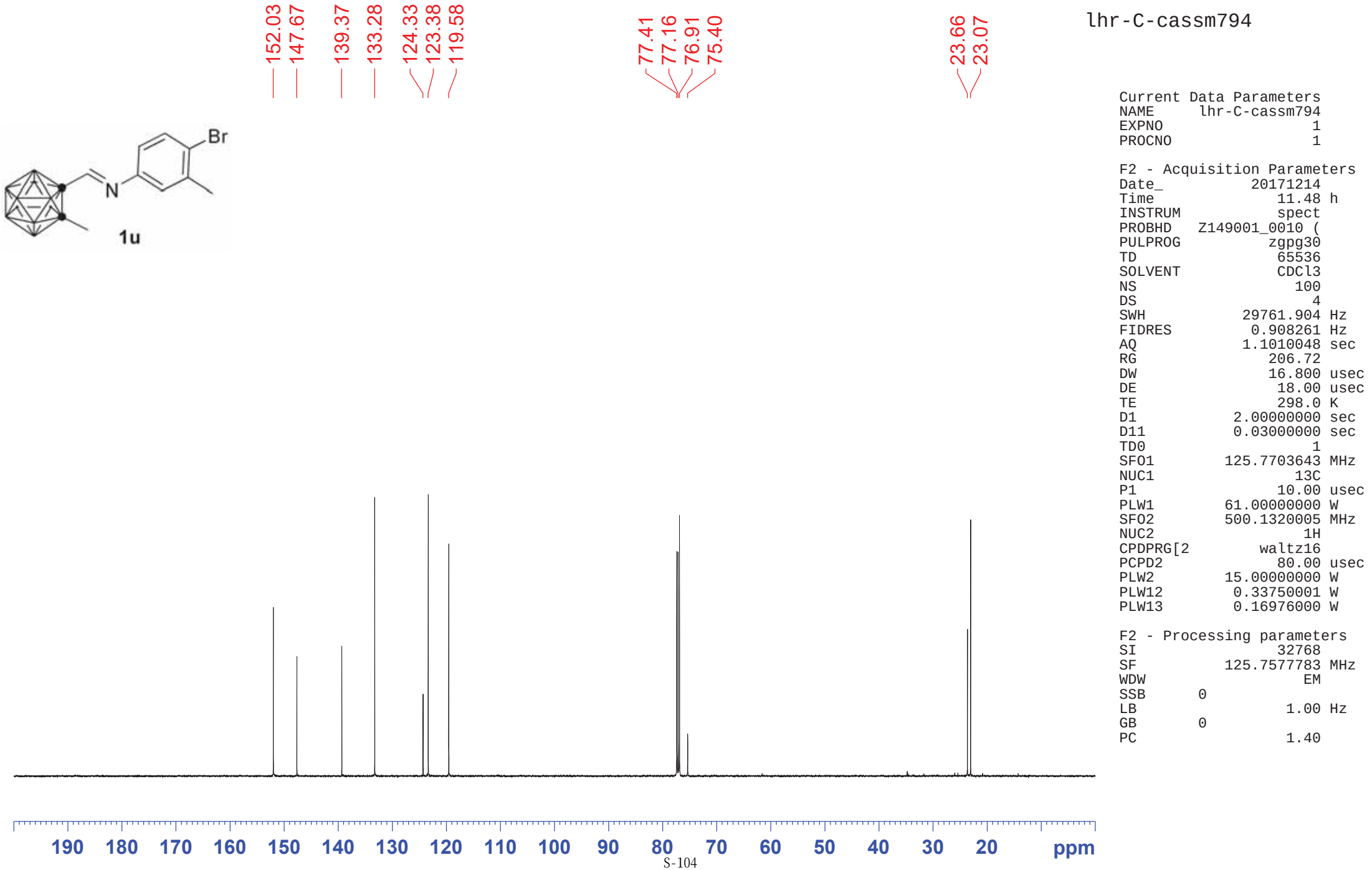
lhr-B-cassm-783-cdcl3(c)

```
Current Data Parameters
NAME      lhr-B-cassm-783-cdcl3(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20171209
Time                17.01 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      10
DS                       2
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                     203
DW                  20.800 usec
DE                   6.50 usec
TE                  296.8 K
D1              2.00000000 sec
TD0                     1
SFO1           128.4096890 MHz
NUC1                   11B
P1                   7.50 usec
PLW1           55.09999847 W

F2 - Processing parameters
SI                   32768
SF             128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



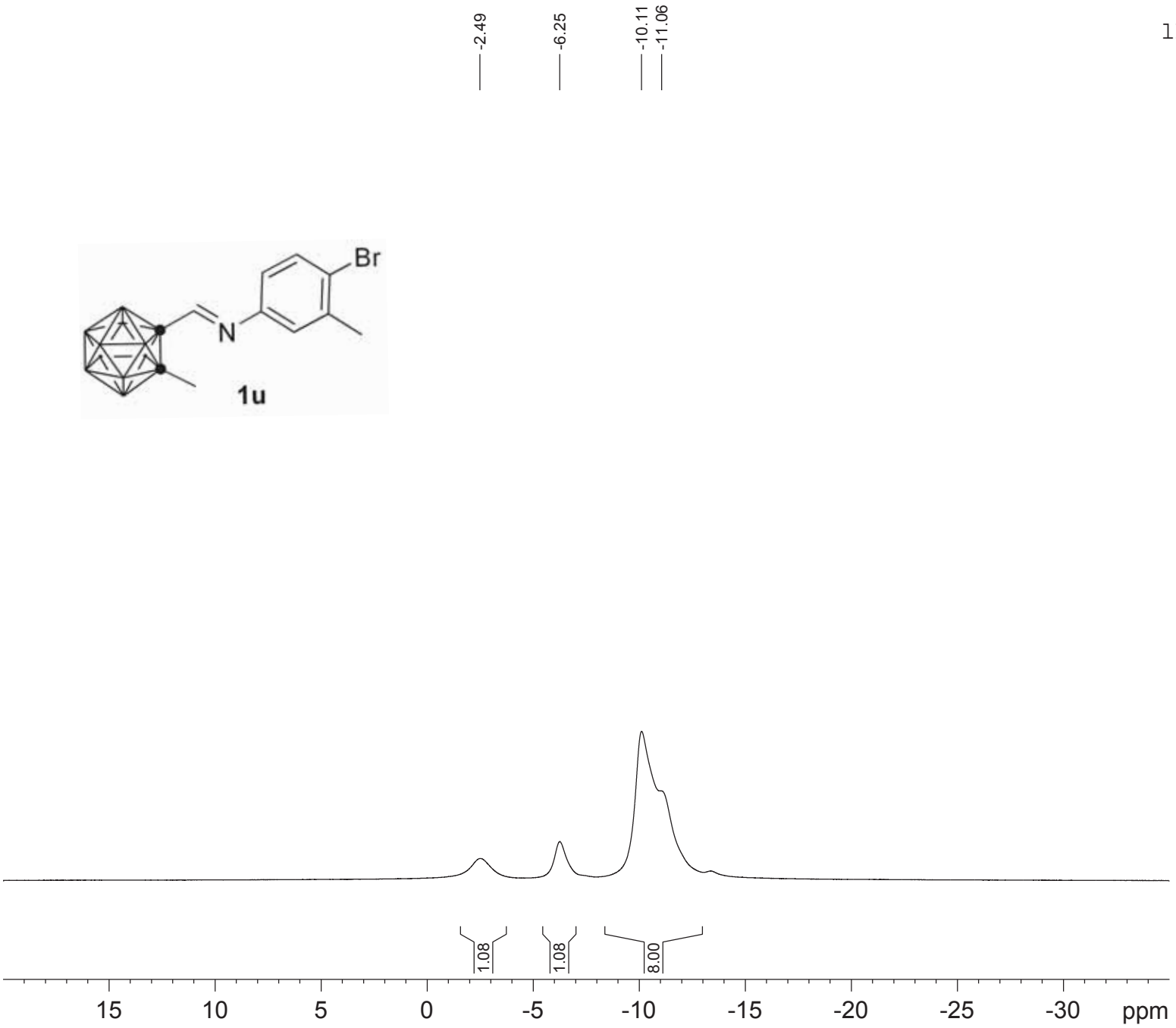
lhr-H-cassm794

```
Current Data Parameters
NAME      lhr-H-cassm794
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20171214
Time               11.42
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                  16.5
DW                50.000
DE                10.00
TE                298.0
D1           1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1        15.00000000

F2 - Processing paramete
SI                 65536
SF         500.1300126
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```



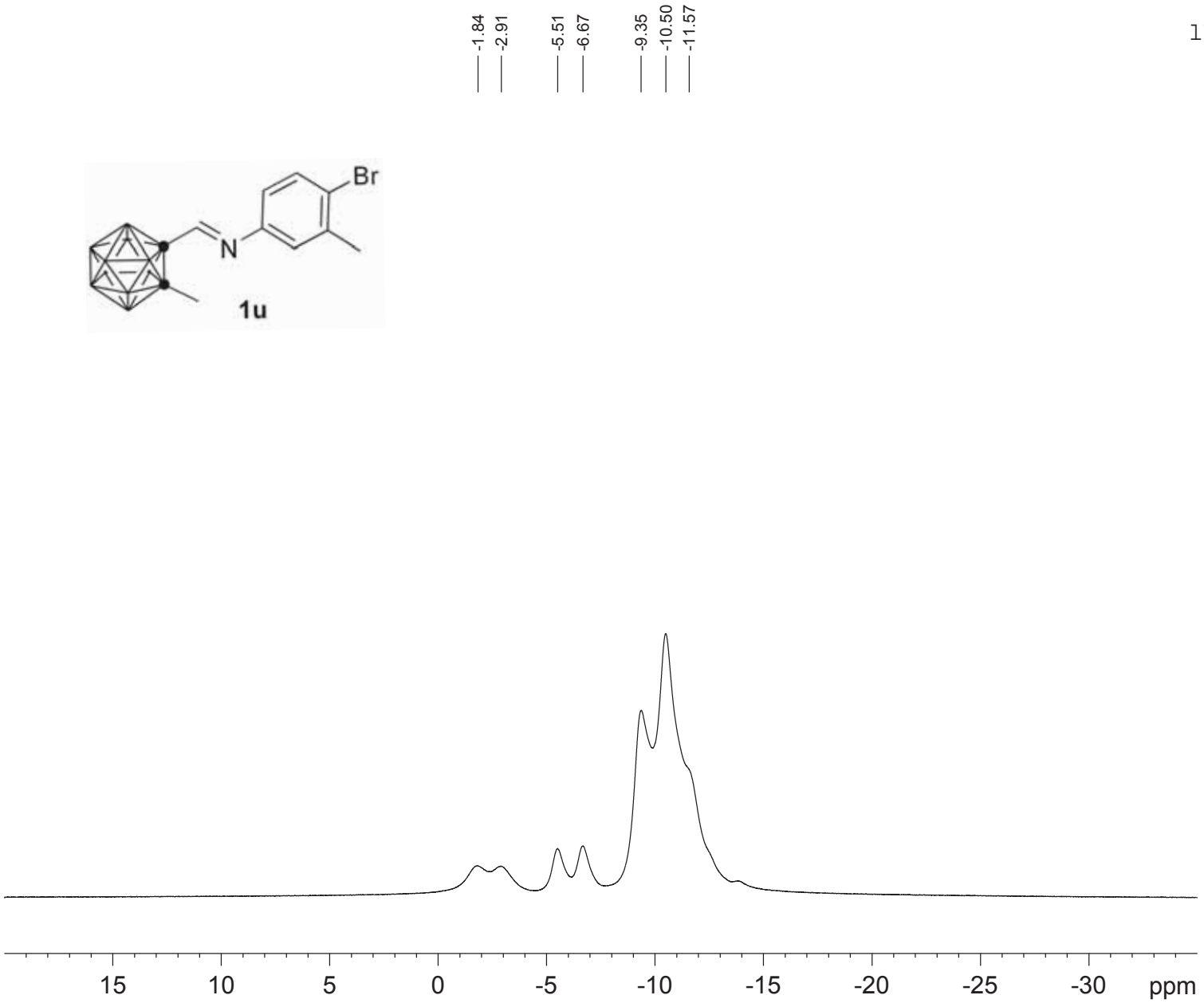
lhr-C-cassm794

```
Current Data Parameters
NAME      lhr-C-cassm794
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171214
Time              11.48 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577783 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



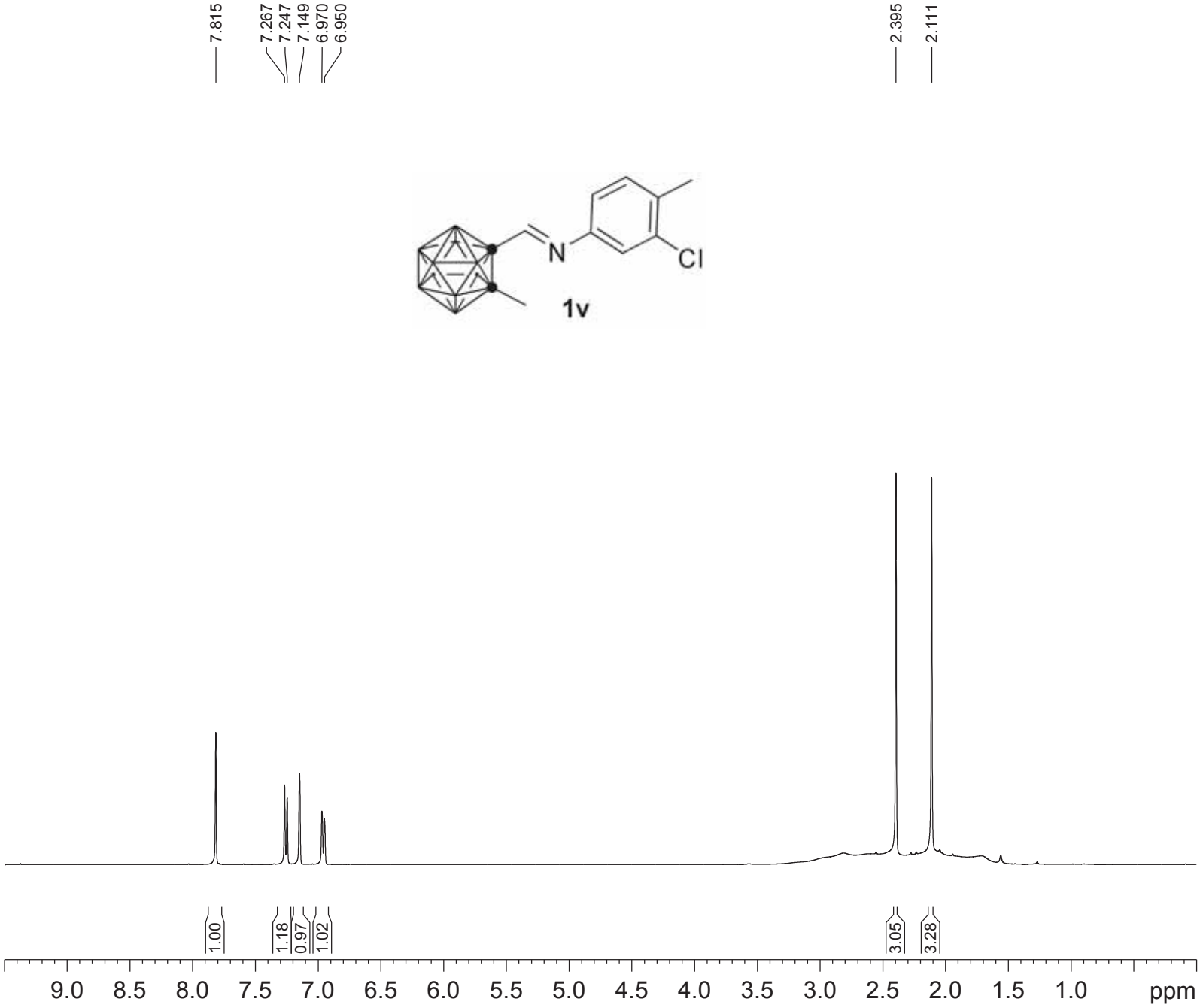
lhr-B-cassm-794-cdcl3

```
Current Data Parameters
NAME      lhr-B-cassm-794-cdcl3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171214
Time                   11.37 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                  THF
NS                        36
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                        181
DW                     20.800 usec
DE                      6.50 usec
TE                     296.5 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                      7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                     32768
SF               128.4097615 MHz
WDW                       EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



lhr-B-cassm-794-cdcl3(C)

```
Current Data Parameters
NAME      lhr-B-cassm-794-cdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171214
Time              11.38 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT               THF
NS                     16
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    181
DW                20.800 usec
DE                 6.50 usec
TE                296.0 K
D1             2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

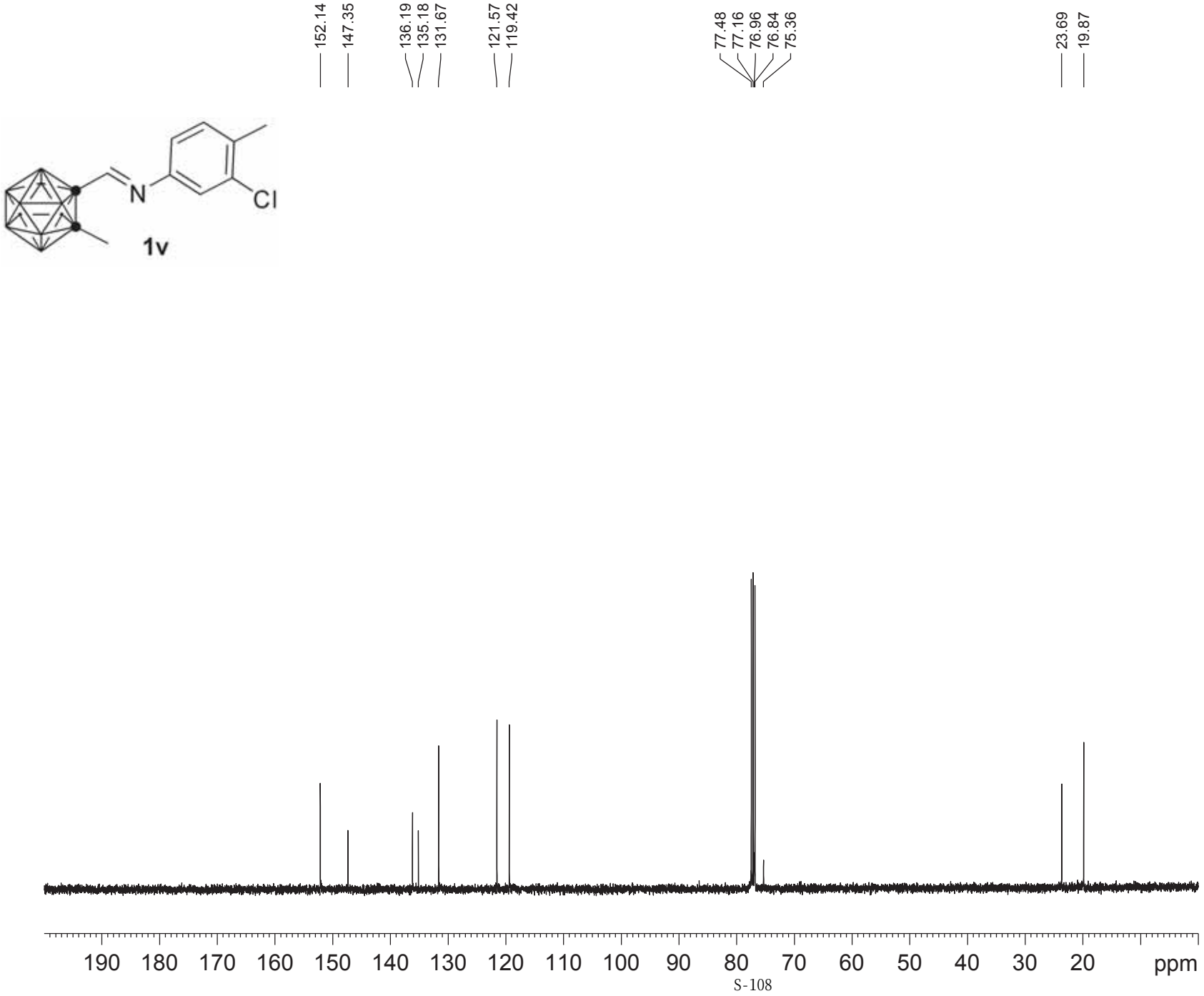


lhr-H-cassm-795-cdcl

Current Data Parameters
NAME lhr-H-cassm-795-cdcl3
EXPNO 1
PROCNO 1

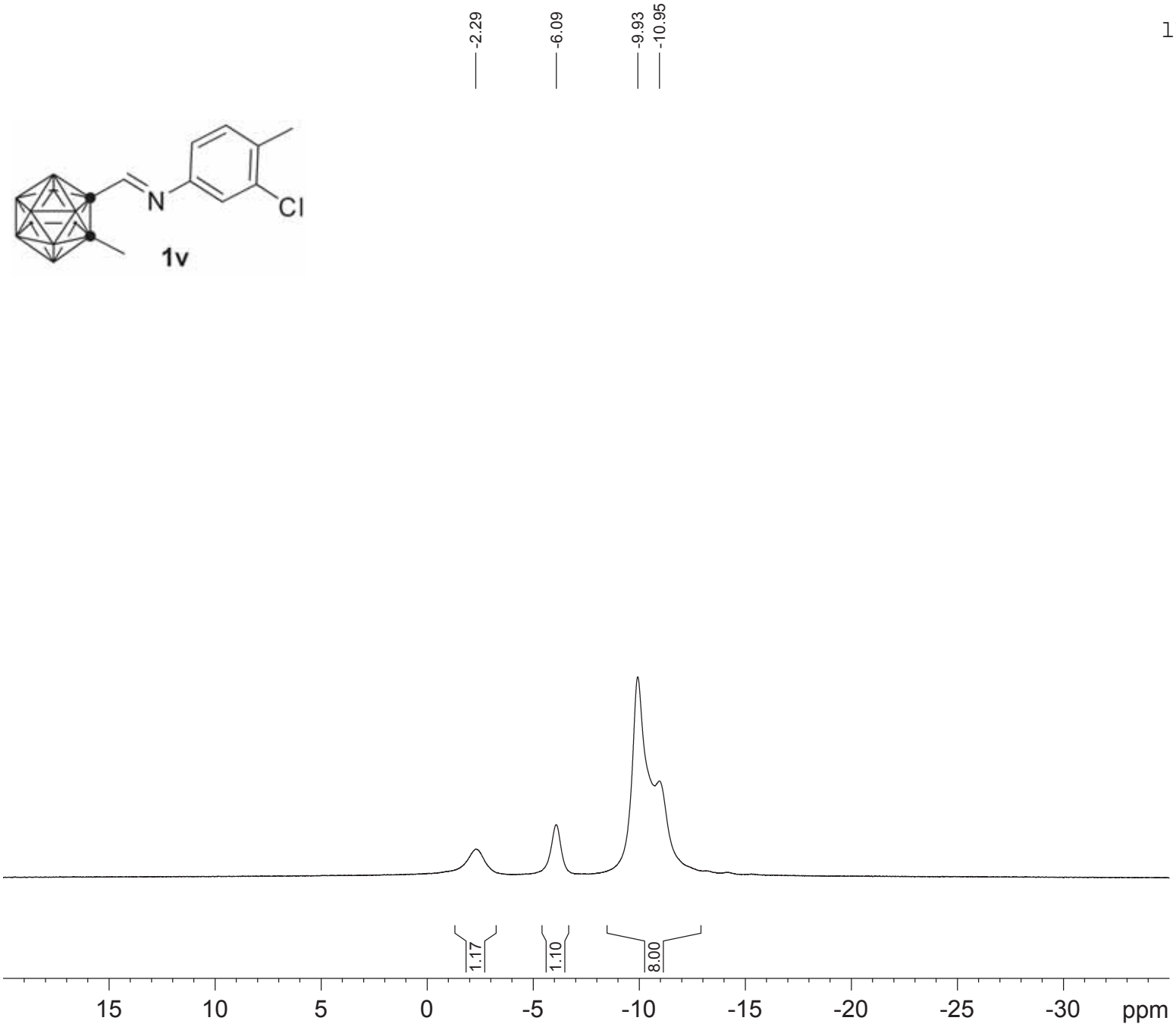
F2 - Acquisition Parameters
Date_ 20171209
Time 16.48 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300068 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



lhr-C-cassm-795-cd

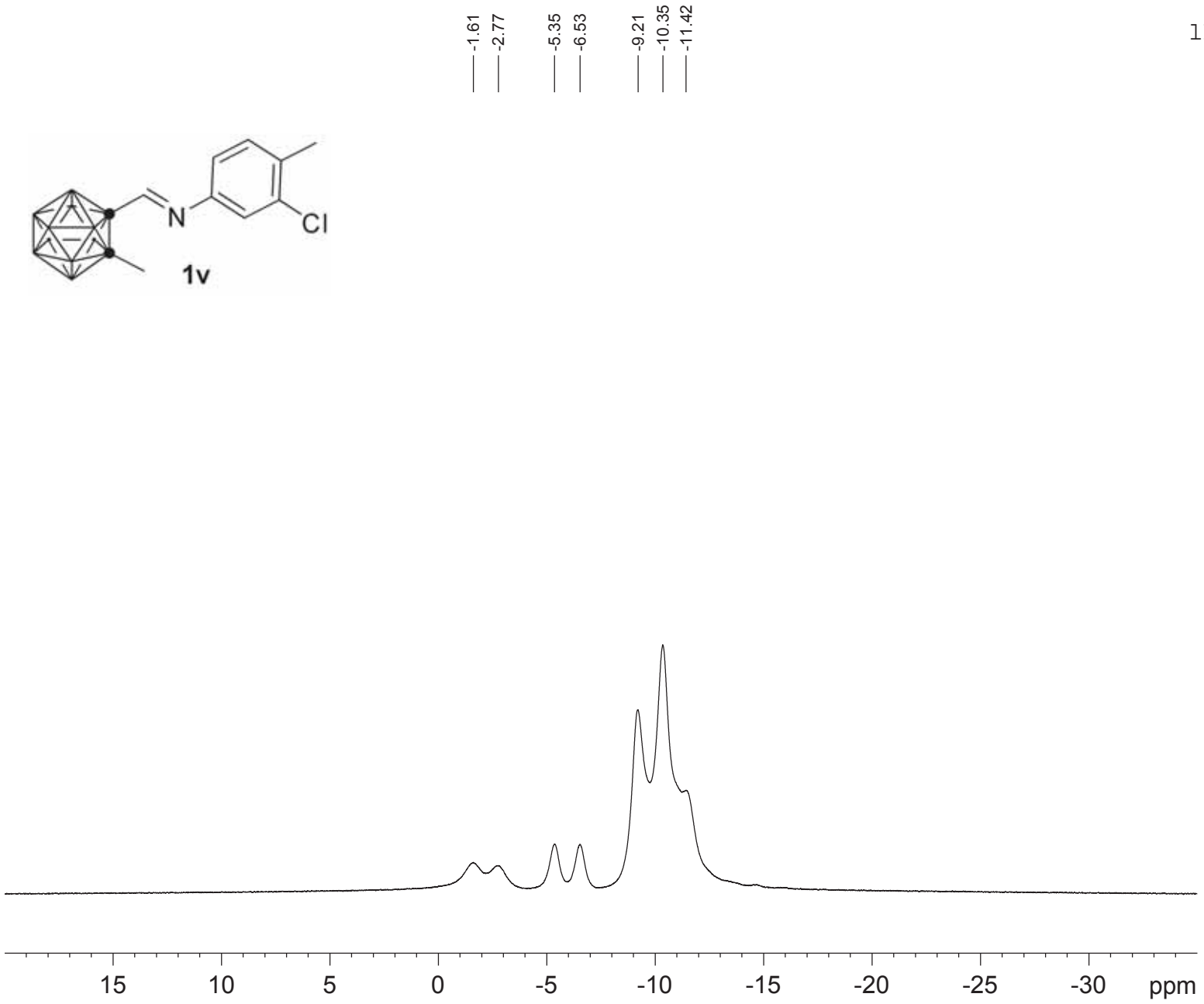
```
Current Data Parameters
NAME      lhr-C-cassm-795-cdcl3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20171209
Time                   16.53 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      100
DS                        4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                      203
DW                   16.800 usec
DE                    6.50 usec
TE                    297.3 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                           1
SFO1             100.6479773 MHz
NUC1                     13C
P1                    9.50 usec
PLW1             55.34000015 W
SFO2             400.2316009 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                90.00 usec
PLW2             13.56000042 W
PLW12             0.27428001 W
PLW13             0.13796000 W

F2 - Processing parameters
SI                        32768
SF               100.6379010 MHz
WDW                        EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



lhr-B-cassm-795-cdcl3

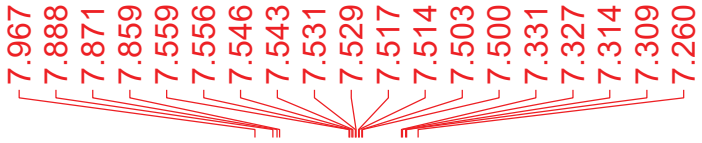
```
Current Data Parameters
NAME      lhr-B-cassm-795-cdcl3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20171209
Time                   16.57 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                zgdc
TD                     65536
SOLVENT                CDCl3
NS                         8
DS                         4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                1.3631488 sec
RG                       228
DW                    20.800 usec
DE                     6.50 usec
TE                    297.1 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1
SFO1            128.4096890 MHz
NUC1                    11B
P1                     7.50 usec
PLW1            55.09999847 W
SFO2            400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 90.00 usec
PLW2            13.56000042 W
PLW12            0.27428001 W

F2 - Processing parameters
SI                     32768
SF              128.4097615 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

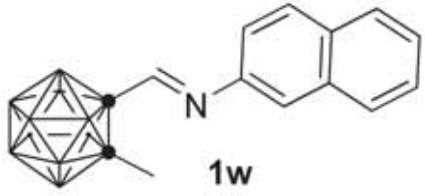
1v



lhr-B-cassm-795-cdcl3(c)

```
Current Data Parameters
NAME      lhr-B-cassm-795-cdcl3(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171209
Time              16.58 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    228
DW                 20.800 usec
DE                  6.50 usec
TE                 297.0 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

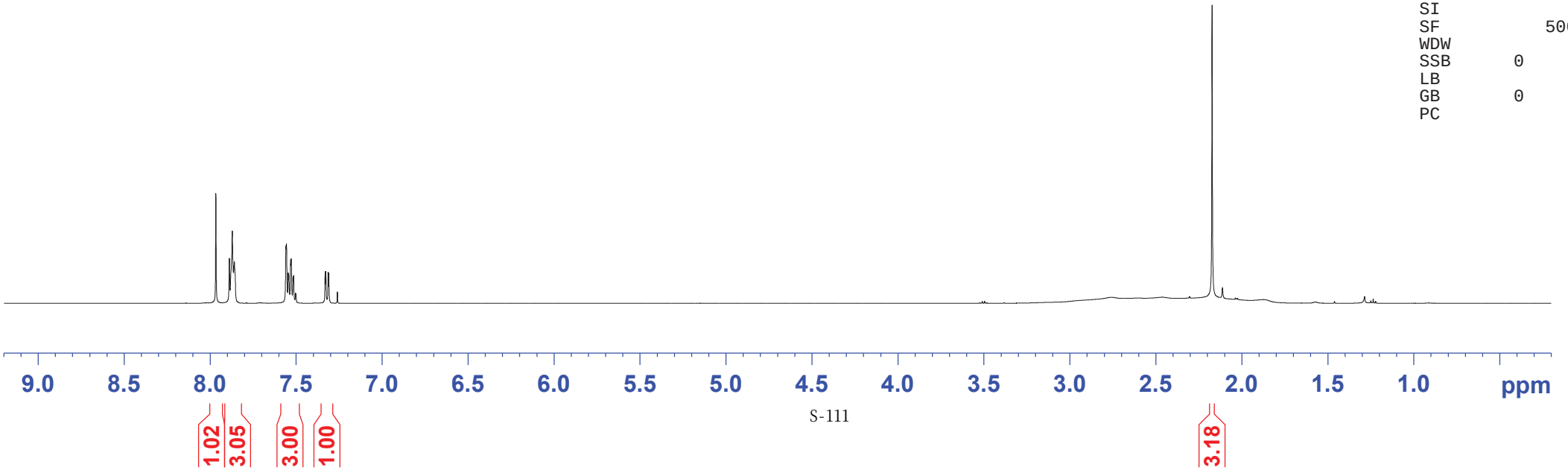


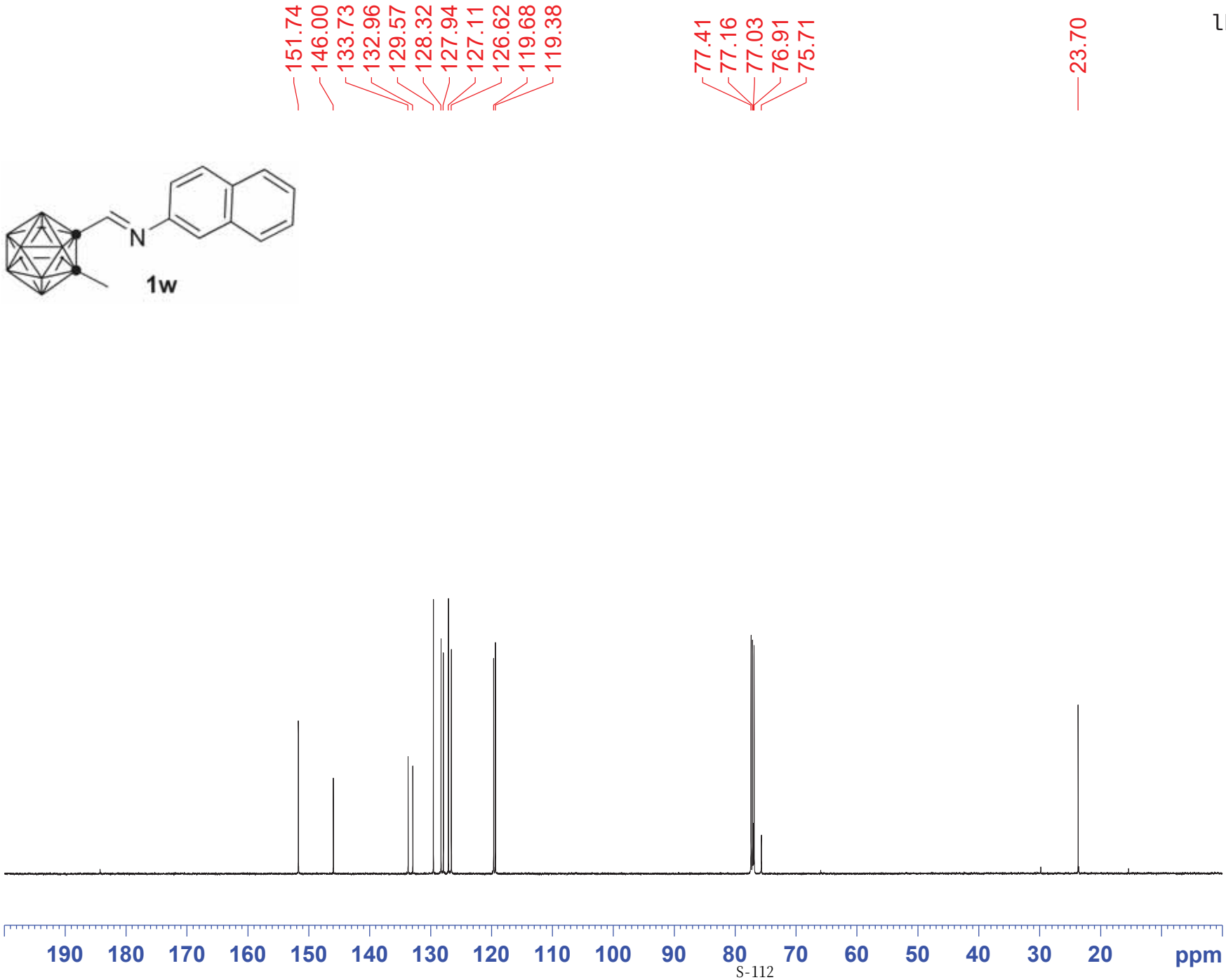


1w

lhr-H-cassm735-nap

```
Current Data Parameters
NAME      lhr-H-cassm735-
EXPNO                   1
PROCNO                  1

F2 - Acquisition Paramet
Date_            20170816
Time                10.22
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     12
DS                      2
SWH             10000.000
FIDRES          0.305176
AQ              3.2767999
RG                  17.56
DW                 50.000
DE                 10.00
TE                 298.0
D1             1.00000000
TD0                     1
SFO1          500.1330883
NUC1                   1H
P1                  12.00
PLW1          15.00000000

F2 - Processing paramete
SI                  65536
SF            500.1300125
WDW                    EM
SSB       0
LB                  0.30
GB        0
PC                  1.00
```

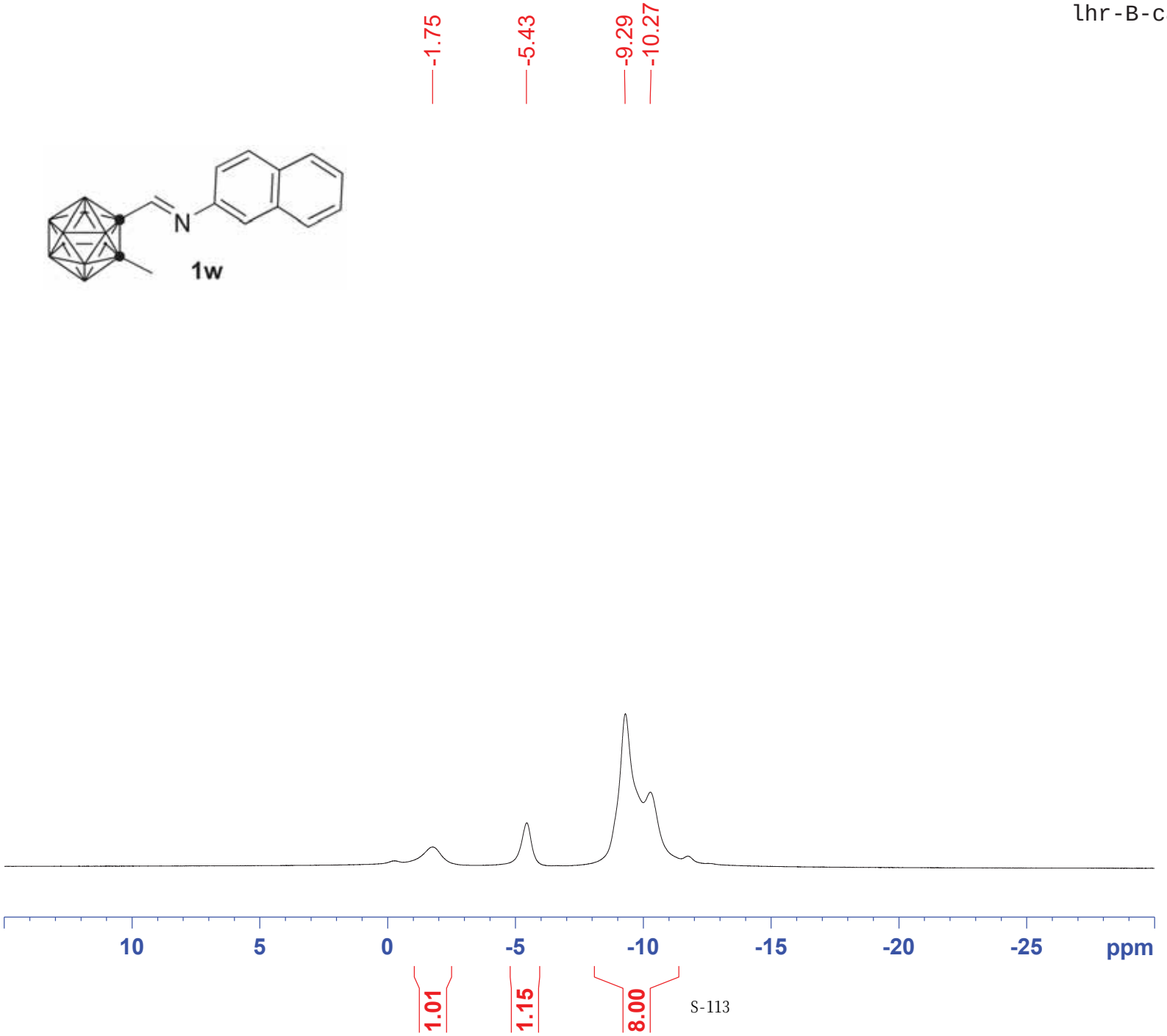




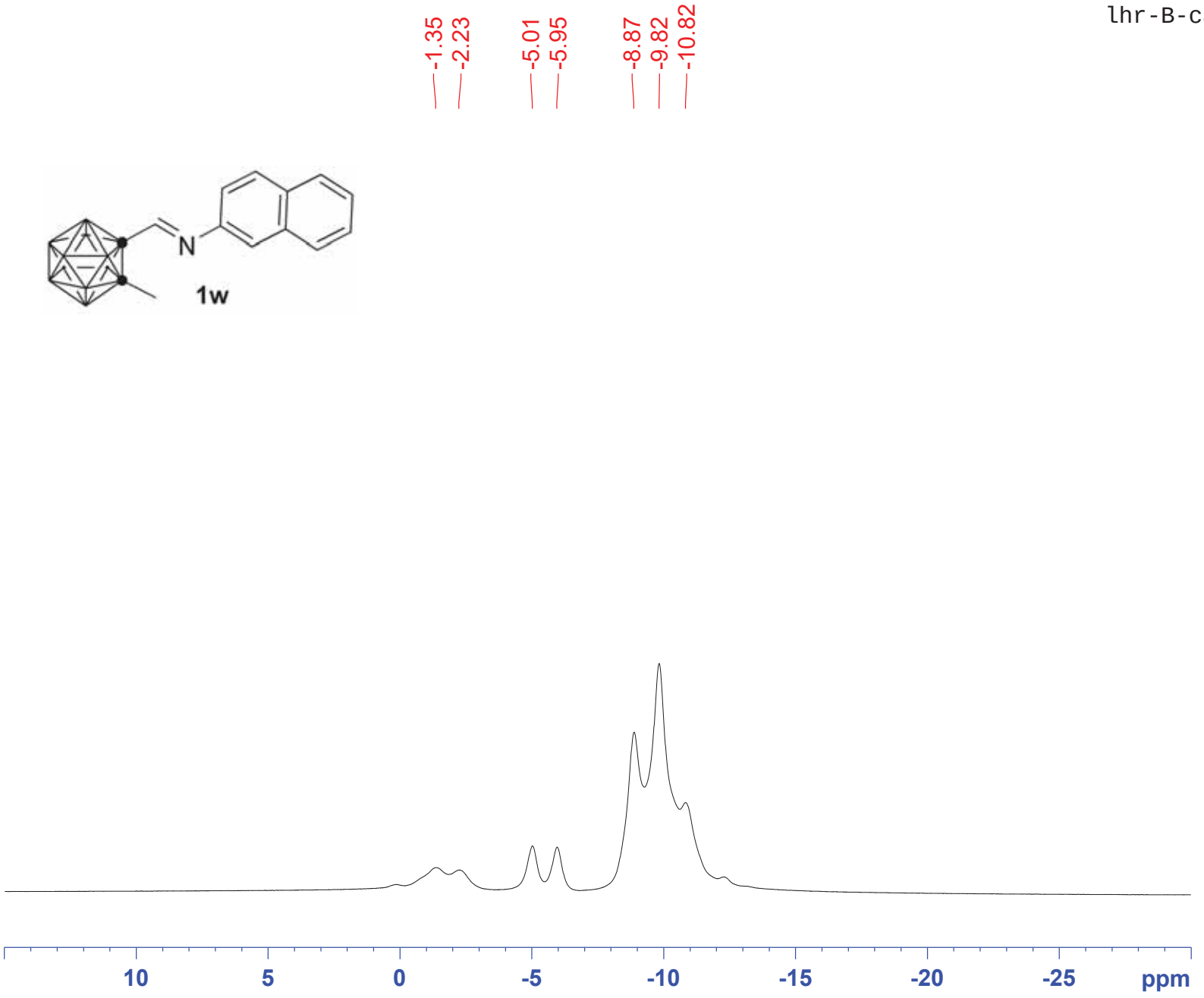
lhr-C-cassm735-nap

```
Current Data Parameters
NAME      lhr-C-cassm735-nap
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170816
Time                 10.30 h
INSTRUM              spect
PROBHD    Z149001_0010 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    120
DS                      4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1           125.7703643 MHz
NUC1                  13C
P1                  10.00 usec
PLW1           61.00000000 W
SFO2           500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2           15.00000000 W
PLW12           0.33750001 W
PLW13           0.16976000 W

F2 - Processing parameters
SI                    32768
SF             125.7577791 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

lhr-B-cassm735-nap

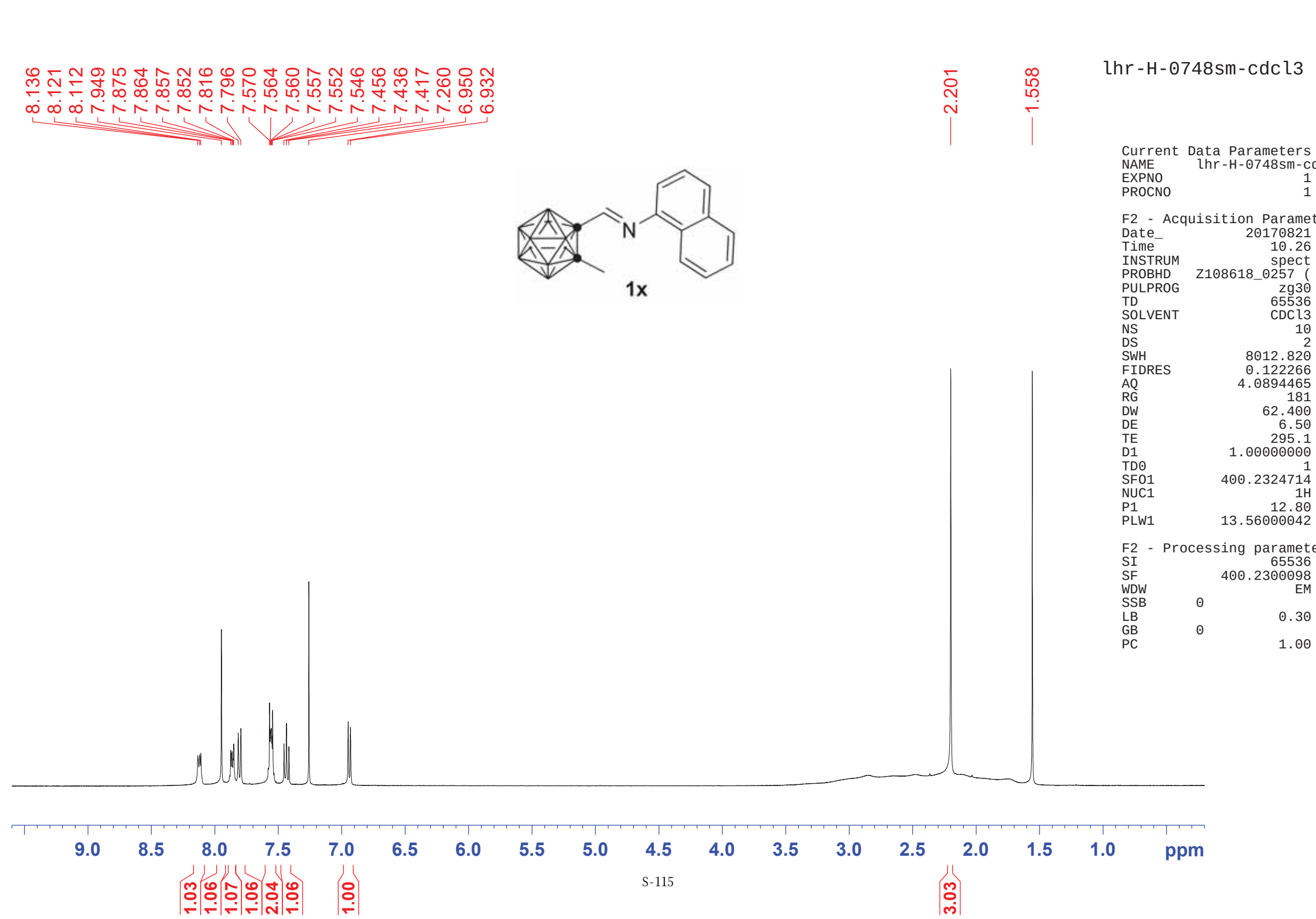


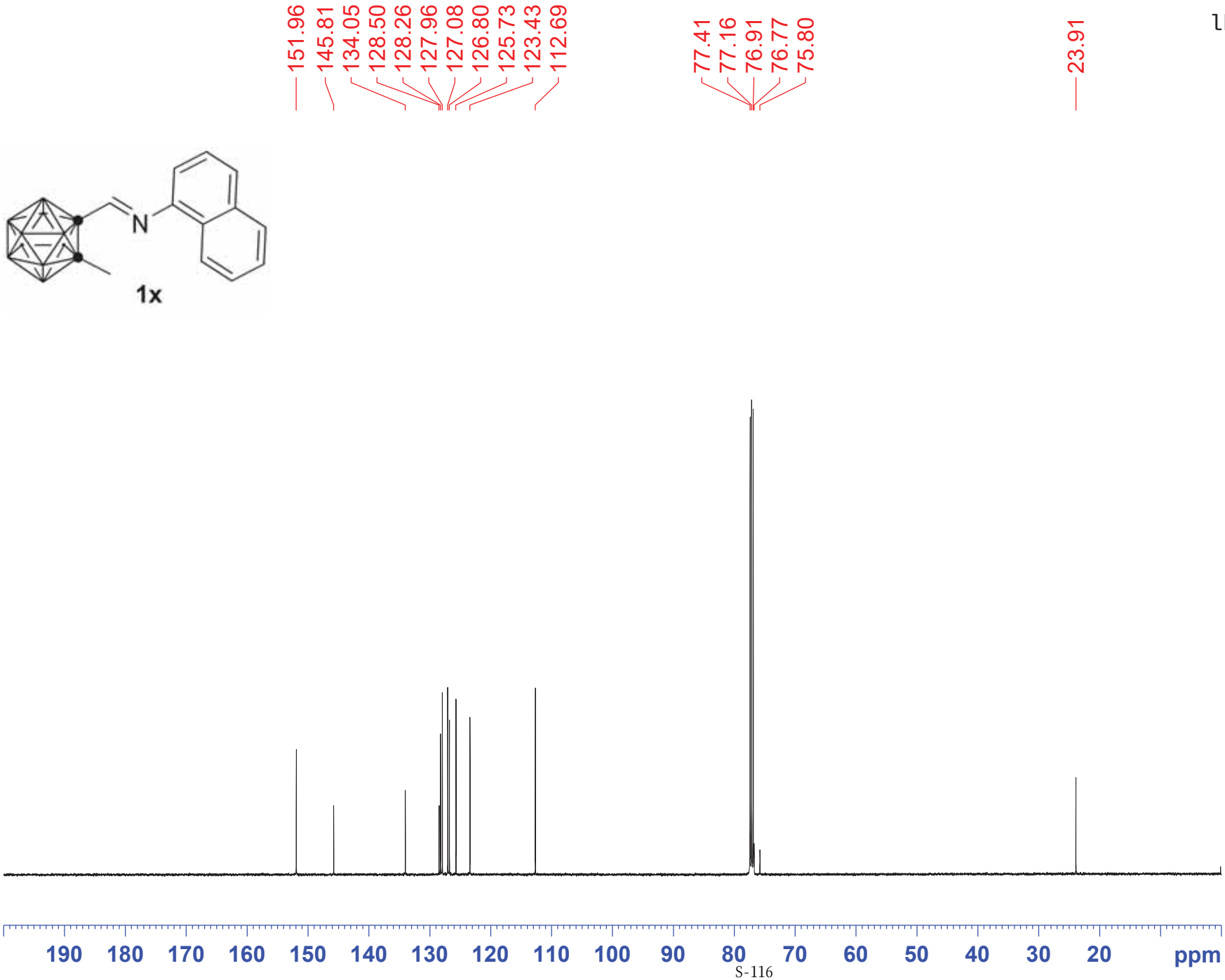

```
Current Data Parameters
NAME      lhr-B-cassm735-nap
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20170816
Time                10.33 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                      4
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3762560 sec
RG                  102.6
DW                 21.000 usec
DE                 18.00 usec
TE                 298.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          160.4599621 MHz
NUC1                11B
P1                 10.00 usec
PLW1          50.00000000 W
SFO2          500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          15.00000000 W
PLW12          0.33750001 W

F2 - Processing parameters
SI                  32768
SF            160.4615719 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



lhr-B-cassm735-nap(C)

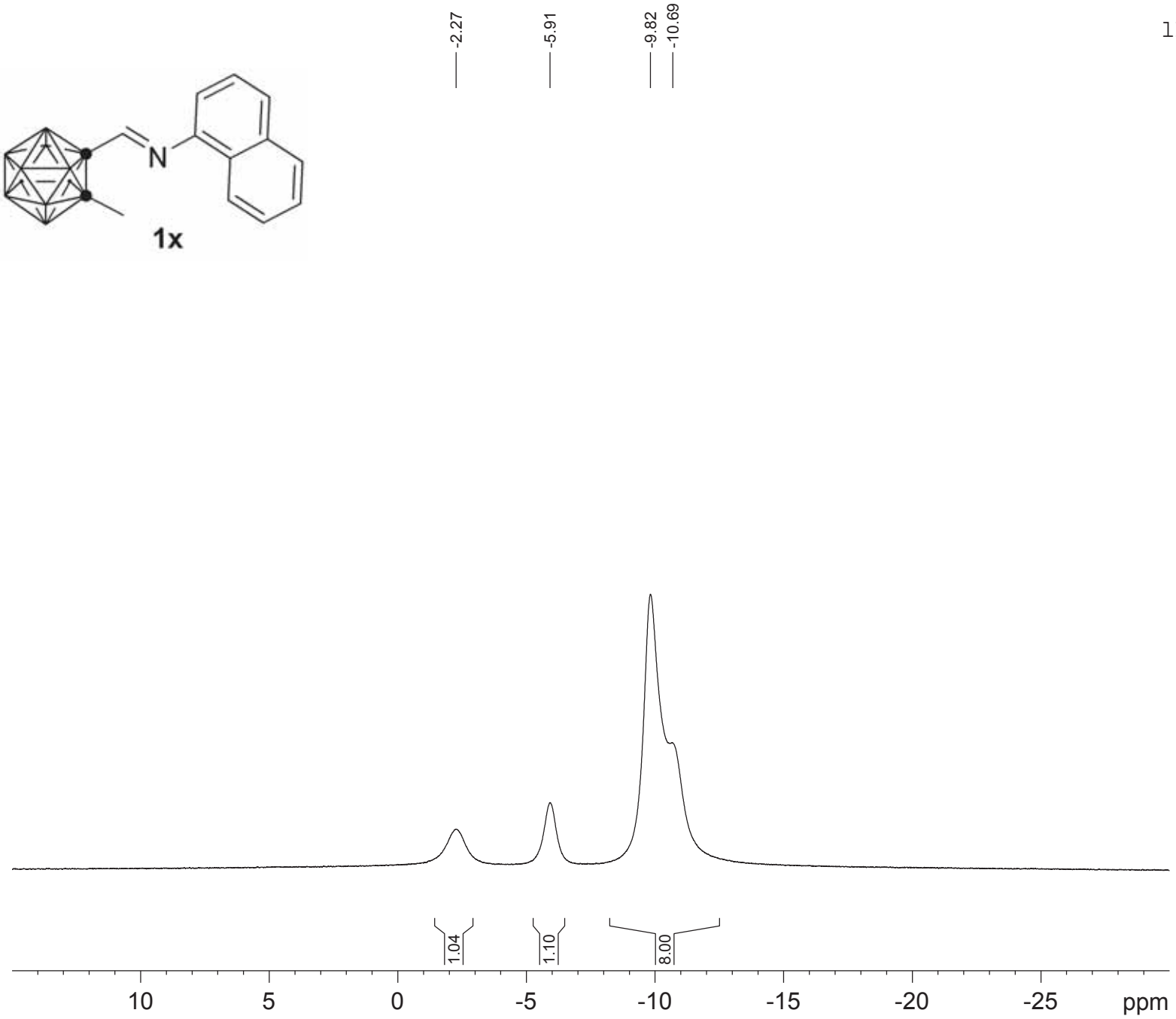
```
Current Data Parameters
NAME      lhr-B-cassm735-nap(C)
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170816
Time                  10.34 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        12
DS                         4
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                    102.6
DW                   20.800 usec
DE                   18.00 usec
TE                   298.0 K
D1             1.00000000 sec
TD0                        1
SFO1            160.4615792 MHz
NUC1                    11B
P1                   10.00 usec
PLW1           50.00000000 W

F2 - Processing parameters
SI                     16384
SF              160.4615792 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


lhr-H-0748sm-cdcl3
8.136
8.121
8.112
7.949
7.875
7.864
7.857
7.852
7.816
7.796
7.570
7.564
7.560
7.557
7.552
7.546
7.456
7.436
7.417
7.260
6.950
6.932
2.201
1.558
N
1x
Current Data Parameters
NAME lhr-H-0748sm-cd
EXPNO 1
PROCNO 1
F2 - Acquisition Paramet
Date_ 20170821
Time 10.26
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 10
DS 2
SWH 8012.820
FIDRES 0.122266
AQ 4.0894465
RG 181
DW 62.400
DE 6.50
TE 295.1
D1 1.00000000
TD0 1
SFO1 400.2324714
NUC1 1H
P1 12.80
PLW1 13.56000042
F2 - Processing paramete
SI 65536
SF 400.2300098
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.03
1.06
1.07
1.06
2.04
1.06
1.00
3.03



lhr-0748-cassm-C

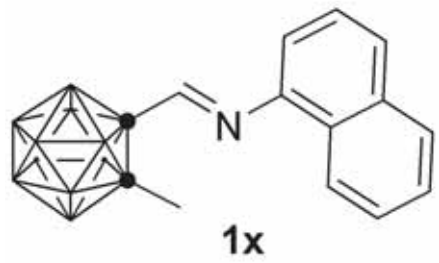
```
Current Data Parameters
NAME      lhr-0748-cassm-C
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170821
Time                19.10 h
INSTRUM              spect
PROBHD    Z149001_0010 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     300
DS                       4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                  18.00 usec
TE                  298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1          125.7703643 MHz
NUC1                  13C
P1                  10.00 usec
PLW1          61.00000000 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2          15.00000000 W
PLW12          0.33750001 W
PLW13          0.16976000 W

F2 - Processing parameters
SI                   32768
SF            125.7577740 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



lhr-B-0748-2napcassm-cdcl3

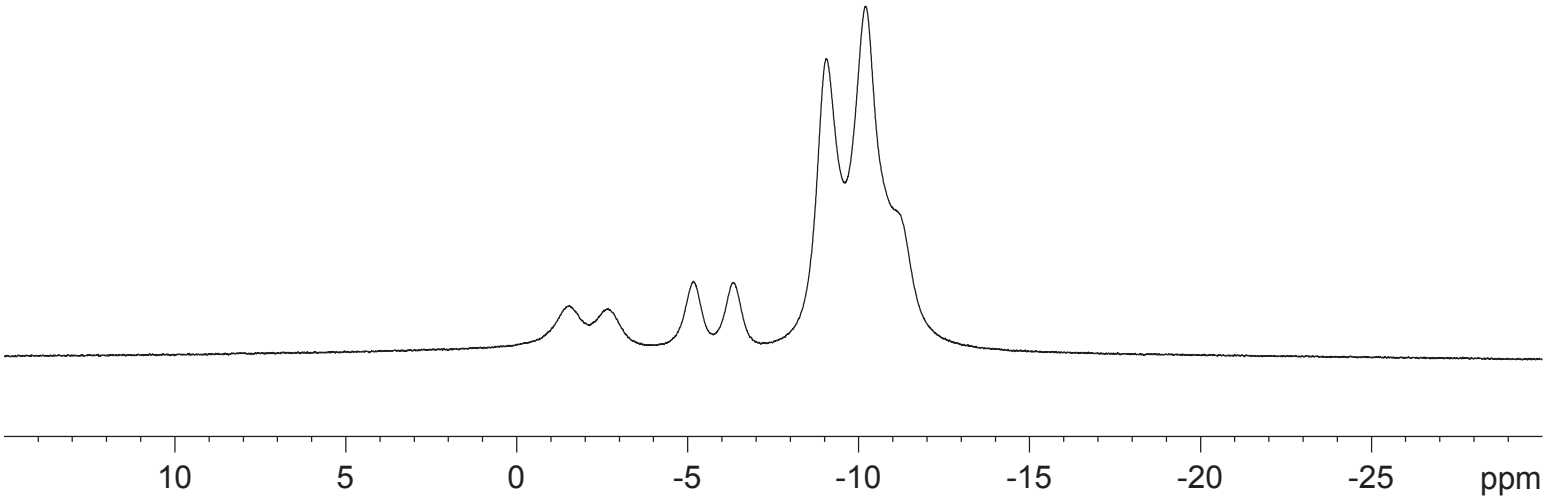
```
Current Data Parameters
NAME      lhr-B-0748-2napcassm-cdcl3
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170822
Time              9.48 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zgdc
TD               65536
SOLVENT          CDCl3
NS                  12
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG                 228
DW               20.800 usec
DE                6.50 usec
TE               295.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                32768
SF          128.4097615 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-0748-2napcassm-cdcl3(C)

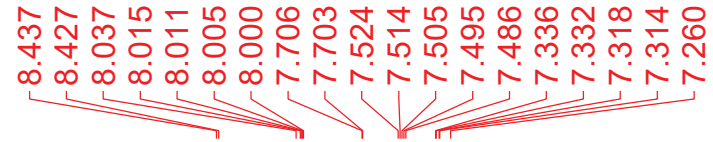


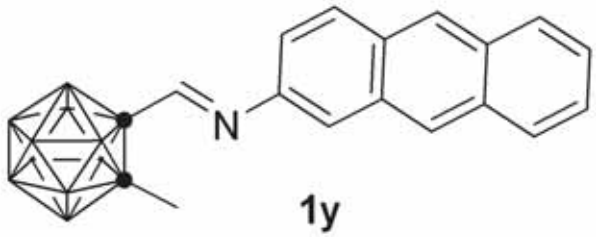
1x

-1.54
-2.67
-5.17
-6.35
-9.05
-10.21
-11.14



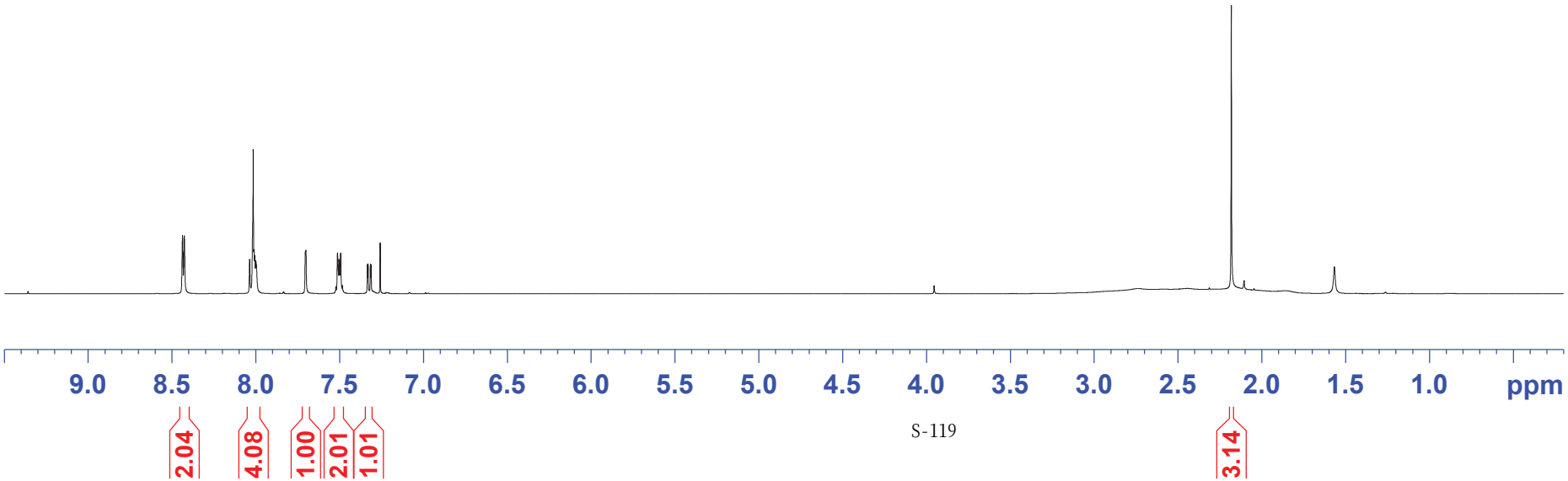

```
Current Data Parameters
NAME      lhr-B-0748-2napcassm-cdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170822
Time                9.50 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     15
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    228
DW                20.800 usec
DE                 6.50 usec
TE                295.1 K
D1           2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

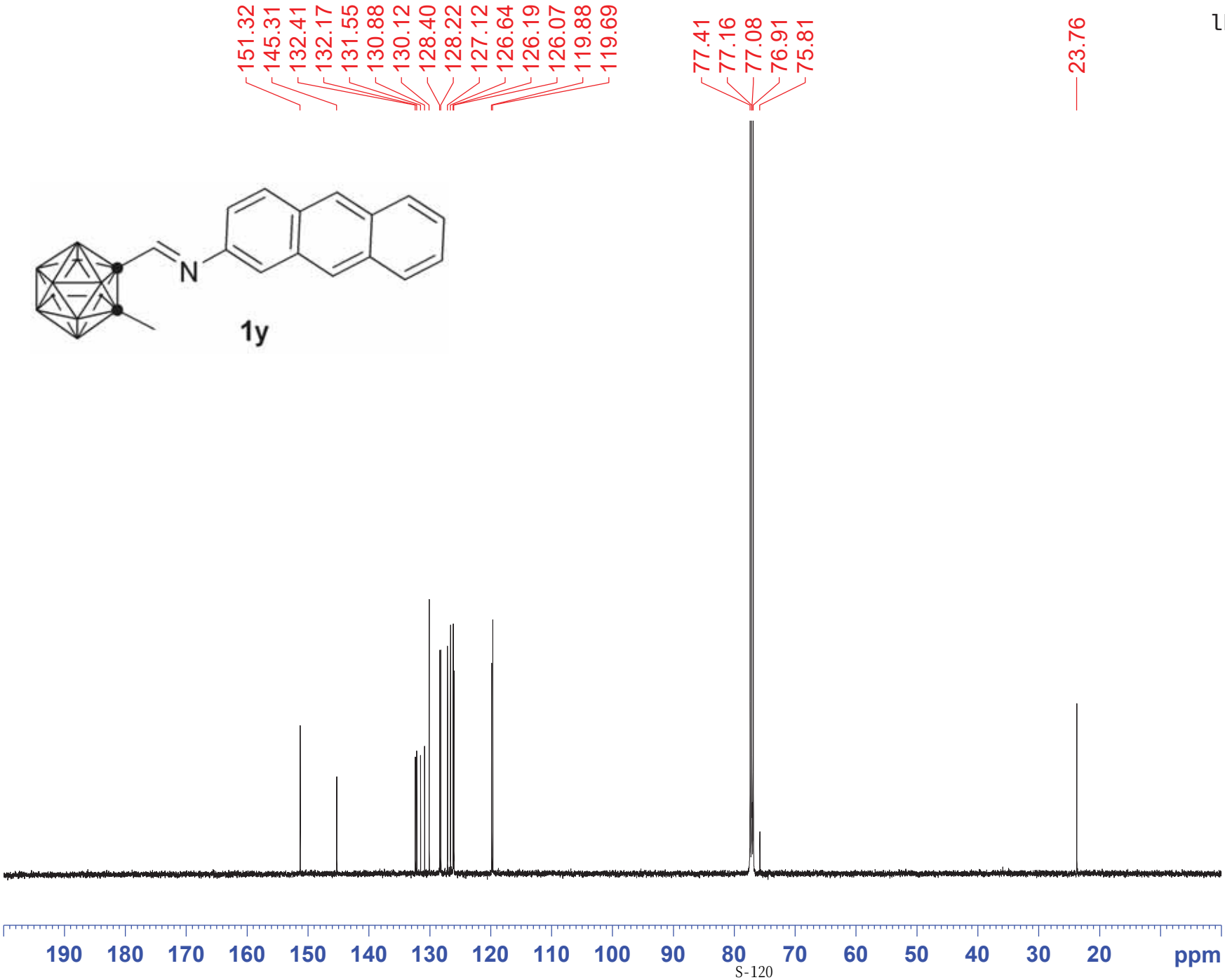




lhr-H-756cassm

```
Current Data Parameters
NAME      lhr-H-756cassm
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20170907
Time               11.03
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 30.85
DW                50.000
DE                10.00
TE                298.0
D1           1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1        15.00000000

F2 - Processing paramete
SI                 65536
SF          500.1300125
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```

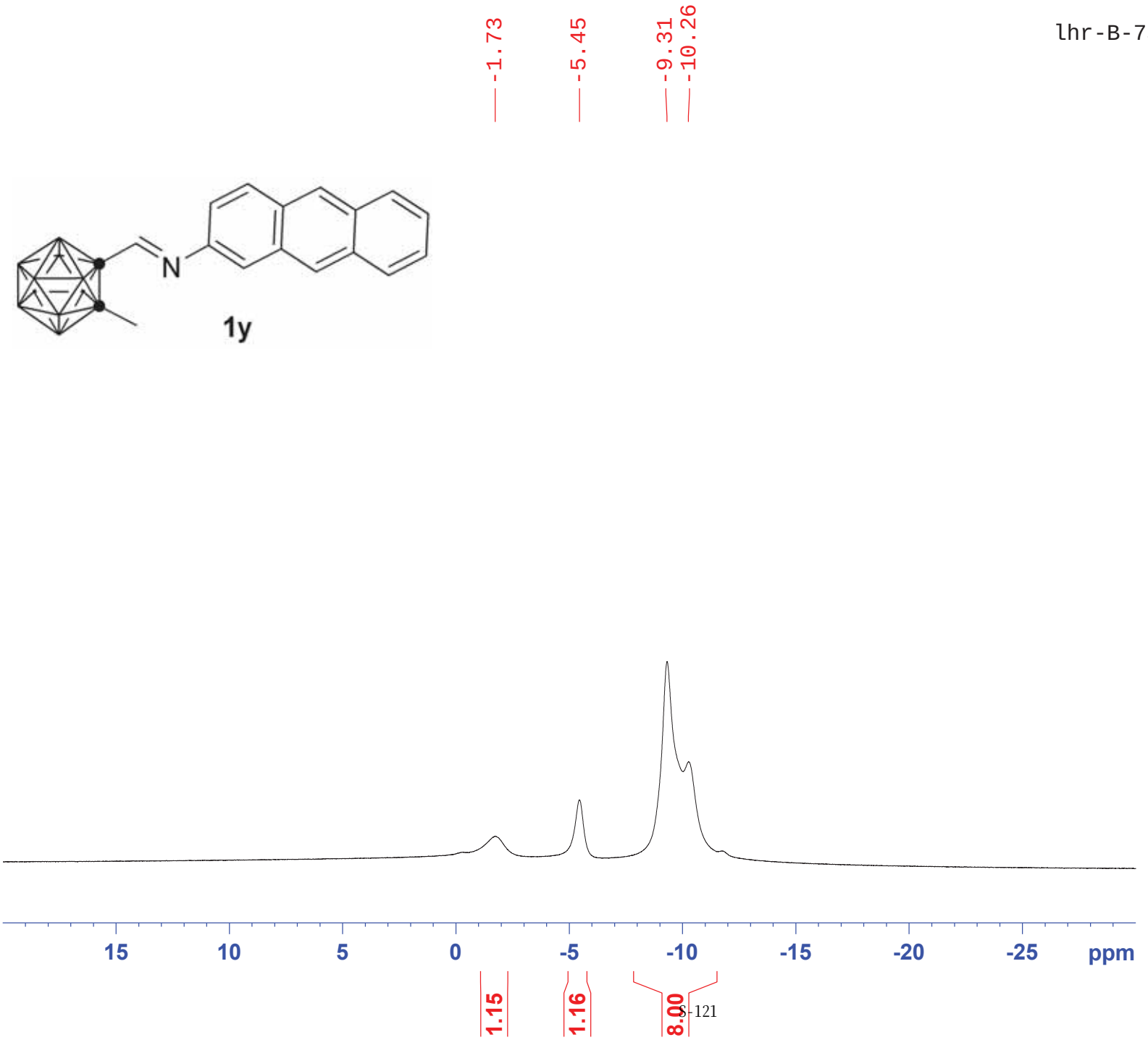




lhr-C-756cassm

```
Current Data Parameters
NAME      lhr-C-756cassm
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170907
Time              11.15 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  200
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577736 MHz
WDW                 EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

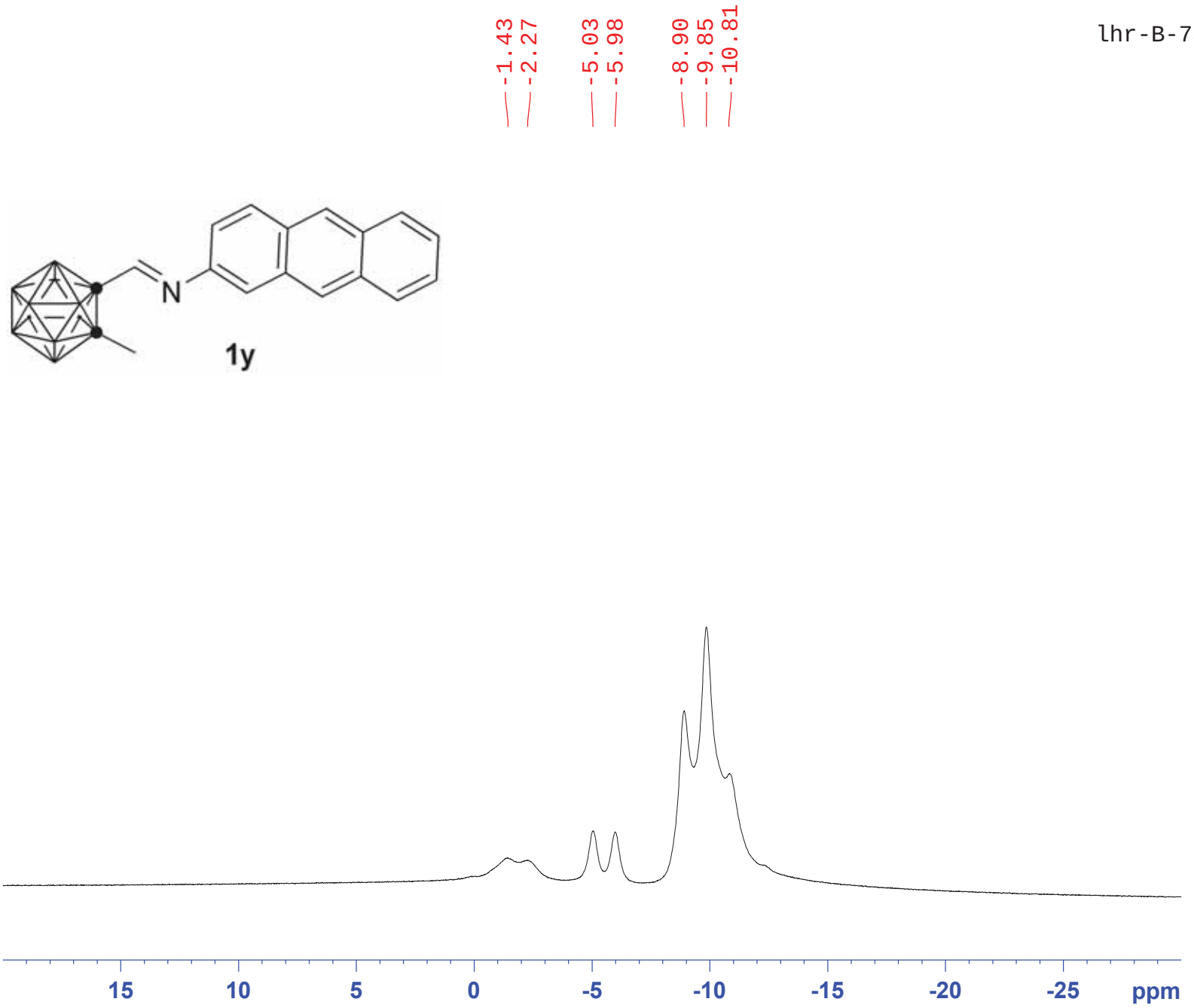
1y



lhr-B-756cassm

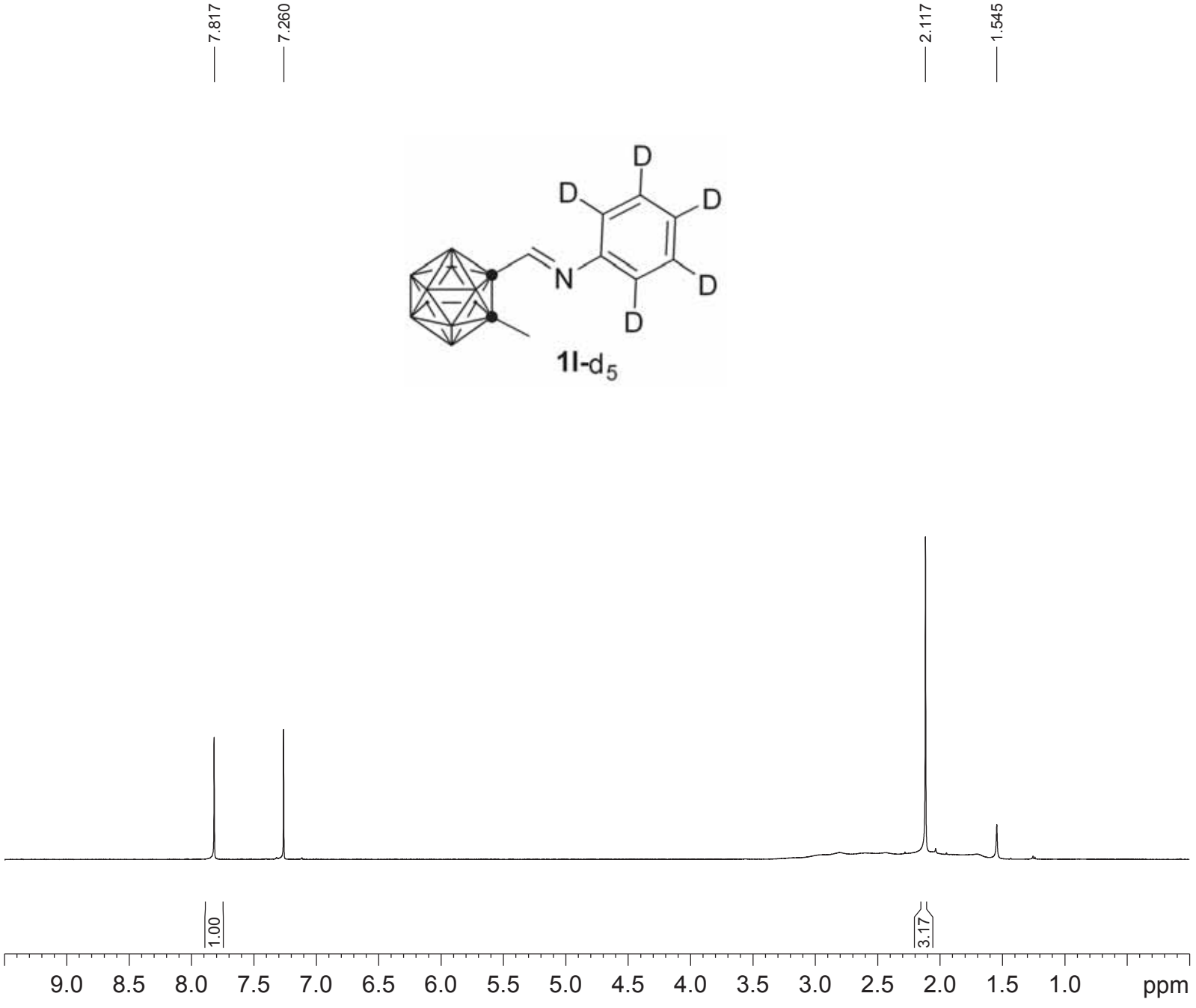
```
Current Data Parameters
NAME      lhr-B-756cassm
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170907
Time              11.19 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ             1.3762560 sec
RG                163.99
DW                21.000 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         160.4599621 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                 32768
SF           160.4615719 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

1y



lhr-B-756cassm(c)

```
Current Data Parameters
NAME      lhr-B-756cassm(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170907
Time                11.20 h
INSTRUM              spect
PROBHD   Z149001_0010 (
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      16
DS                       4
SWH              24038.461 Hz
FIDRES            1.467191 Hz
AQ               0.6815744 sec
RG                  163.99
DW                  20.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              1.00000000 sec
TD0                      1
SFO1          160.4615792 MHz
NUC1                  11B
P1                  10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                   16384
SF            160.4615792 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



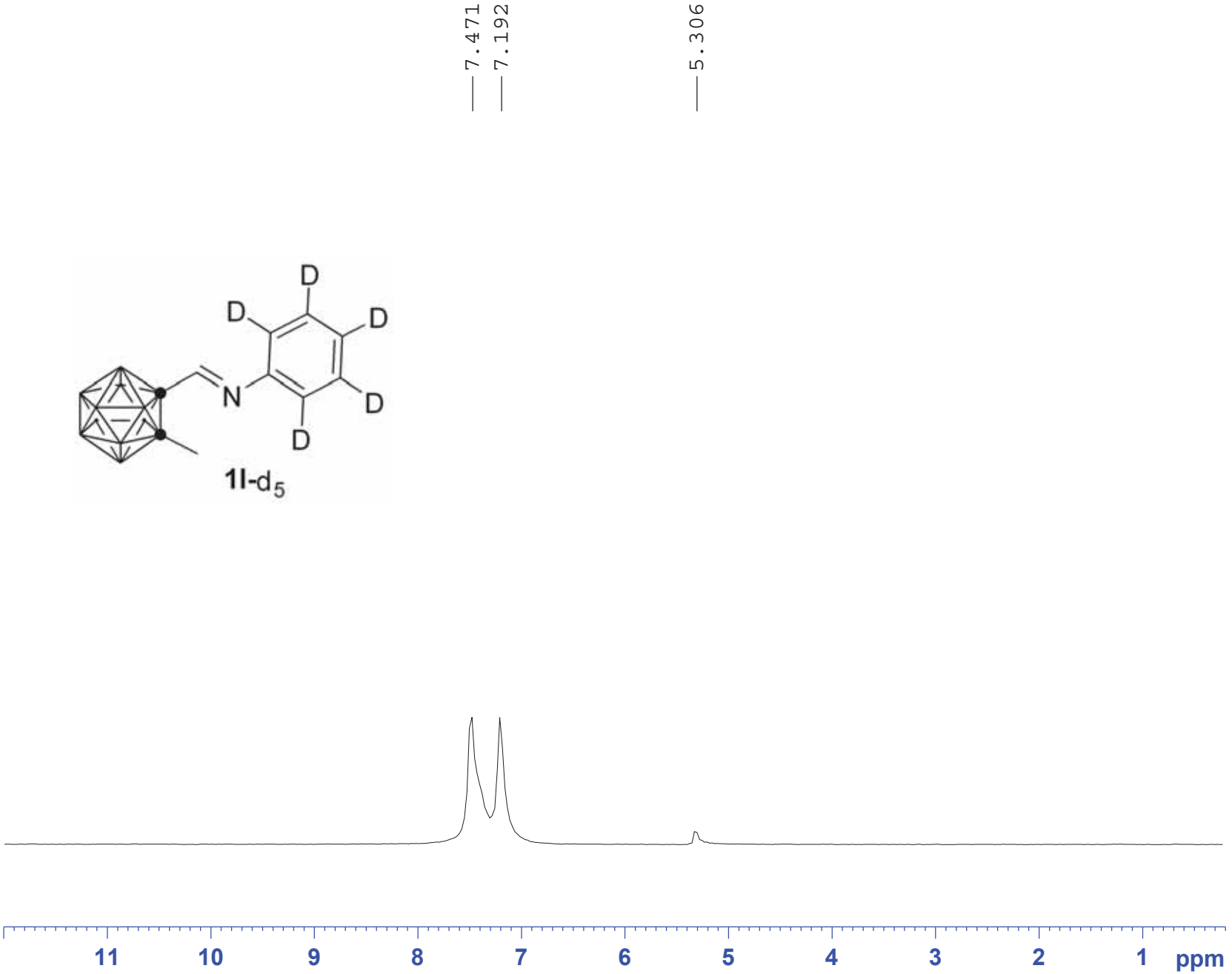
lhr-H-d5-cassmcdcl3

Current Data Parameters
NAME lhr-H-d5-cassmcdcl3
EXPNO 1
PROCNO 1

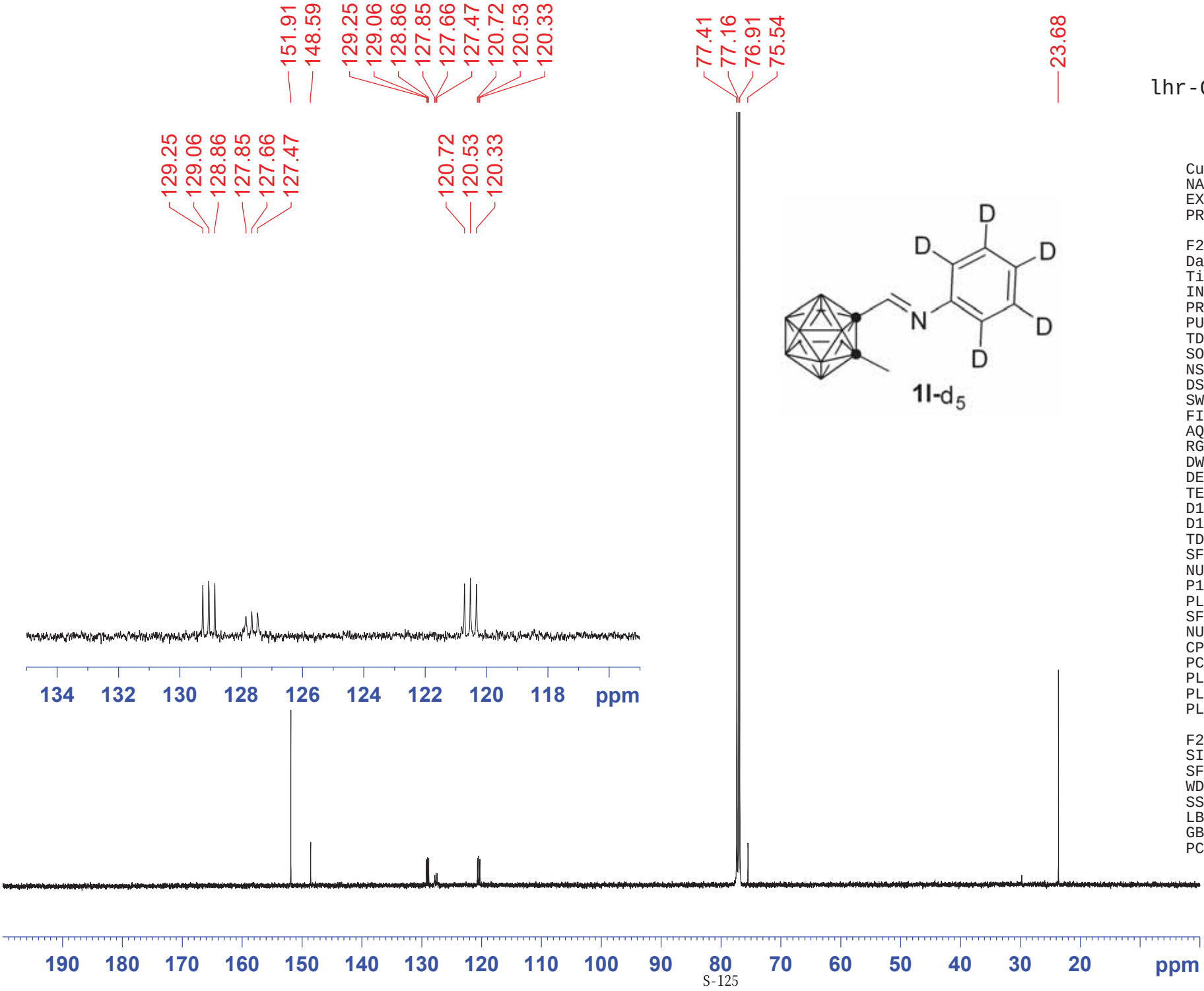
F2 - Acquisition Parameters
Date_ 20171110
Time 19.45 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1l-d_5




```
Current Data Parameters
NAME      lhr-2H-cassmd5-chloroform
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180602
Time              15.47 h
INSTRUM             spect
PROBHD    Z824601_0021 (
PULPROG             zg2h
TD                  4096
SOLVENT             CDCl3
NS                   420
DS                     0
SWH             6142.506 Hz
FIDRES          2.999271 Hz
AQ              0.3334144 sec
RG                   0.5
DW                81.400 usec
DE                 6.50 usec
TE                297.3 K
D1           0.05000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         61.4226981 MHz
NUC1                  2H
P1                300.00 usec
PLW1         3.00000000 W

F2 - Processing parameters
SI                  4096
SF           61.4223850 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.00
```



Current Data Parameters
NAME lhr-C-d5cassm-r
EXPNO 1
PROCNO 1

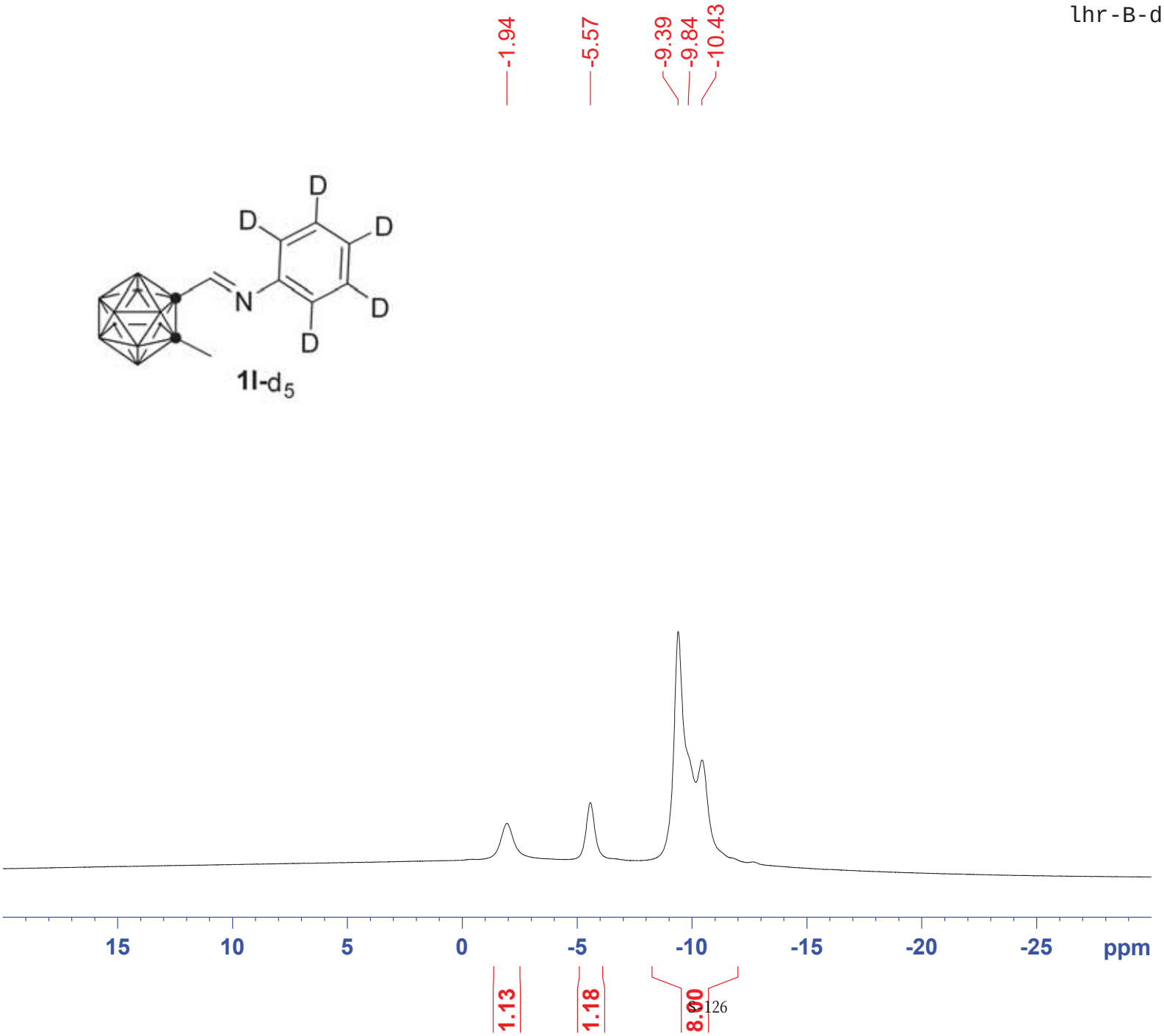
F2 - Acquisition Parameters

Date_	20171111
Time	10.30 h
INSTRUM	spect
PROBHD	Z149001_0010 (
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	300
DS	4
SWH	29761.904 Hz
FIDRES	0.908261 Hz
AQ	1.1010048 sec
RG	206.72
DW	16.800 usec
DE	18.00 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
SFO1	125.7703643 MHz
NUC1	13C
P1	10.00 usec
PLW1	61.00000000 W
SFO2	500.1320005 MHz
NUC2	1H
CPDPRG[2	waltz16
PCPD2	80.00 usec
PLW2	15.00000000 W
PLW12	0.33750001 W
PLW13	0.16976000 W

F2 - Processing parameters

SI	32768
SF	125.7577728 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

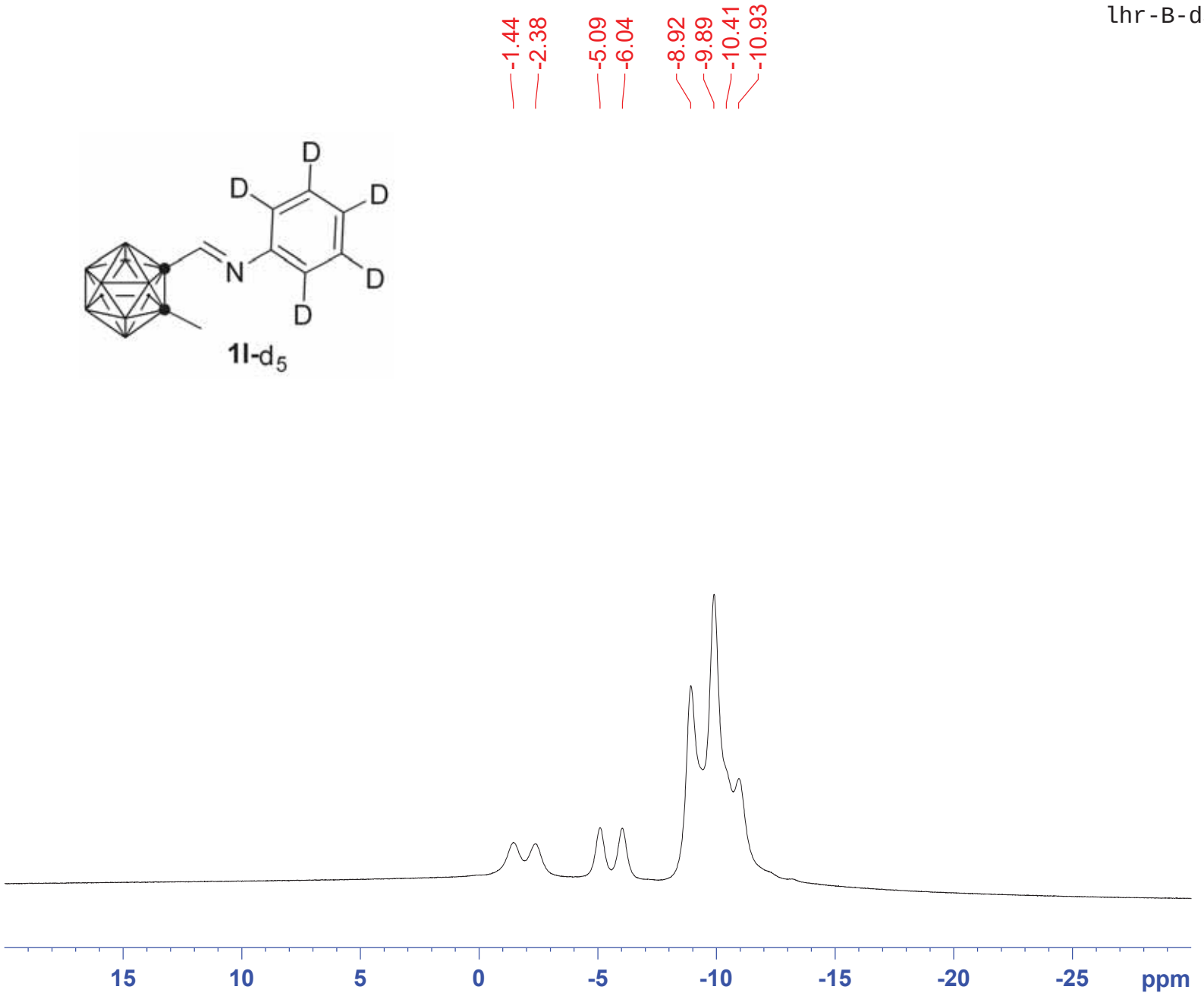
1l-d$_5$



lhr-B-d5cassm-r

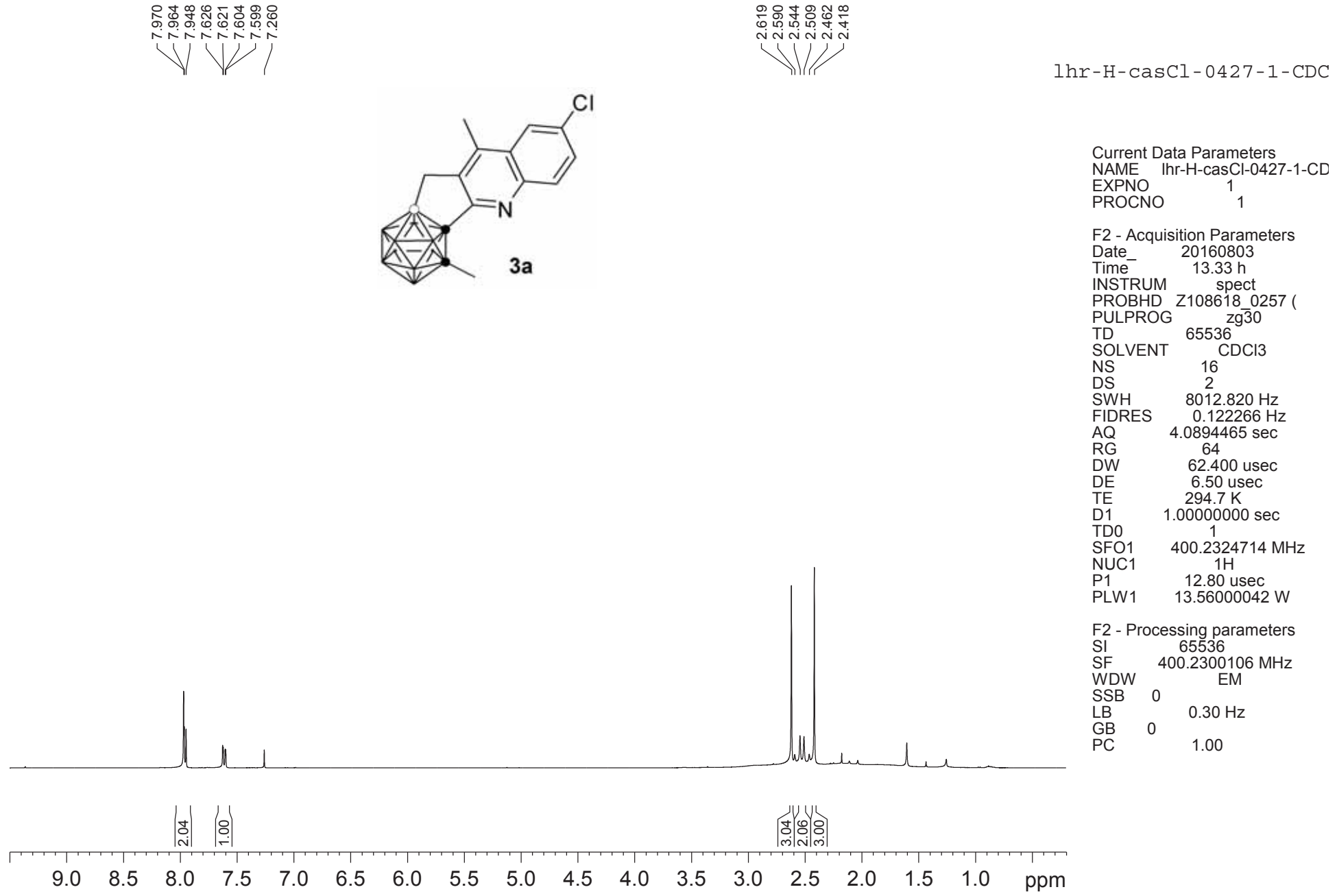
```
Current Data Parameters
NAME      lhr-B-d5cassm-r
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20171111
Time                11.12 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgig
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                 163.99
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         160.4615790 MHz
NUC1                11B
P1                 10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                  16384
SF          160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

1l-d_5



lhr-B-d5cassm-r(C)

```
Current Data Parameters
NAME      lhr-B-d5cassm-r(C)
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_            20171111
Time                11.14 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     17
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                 163.99
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                     1
SFO1         160.4615792 MHz
NUC1                 11B
P1                 10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                  16384
SF           160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

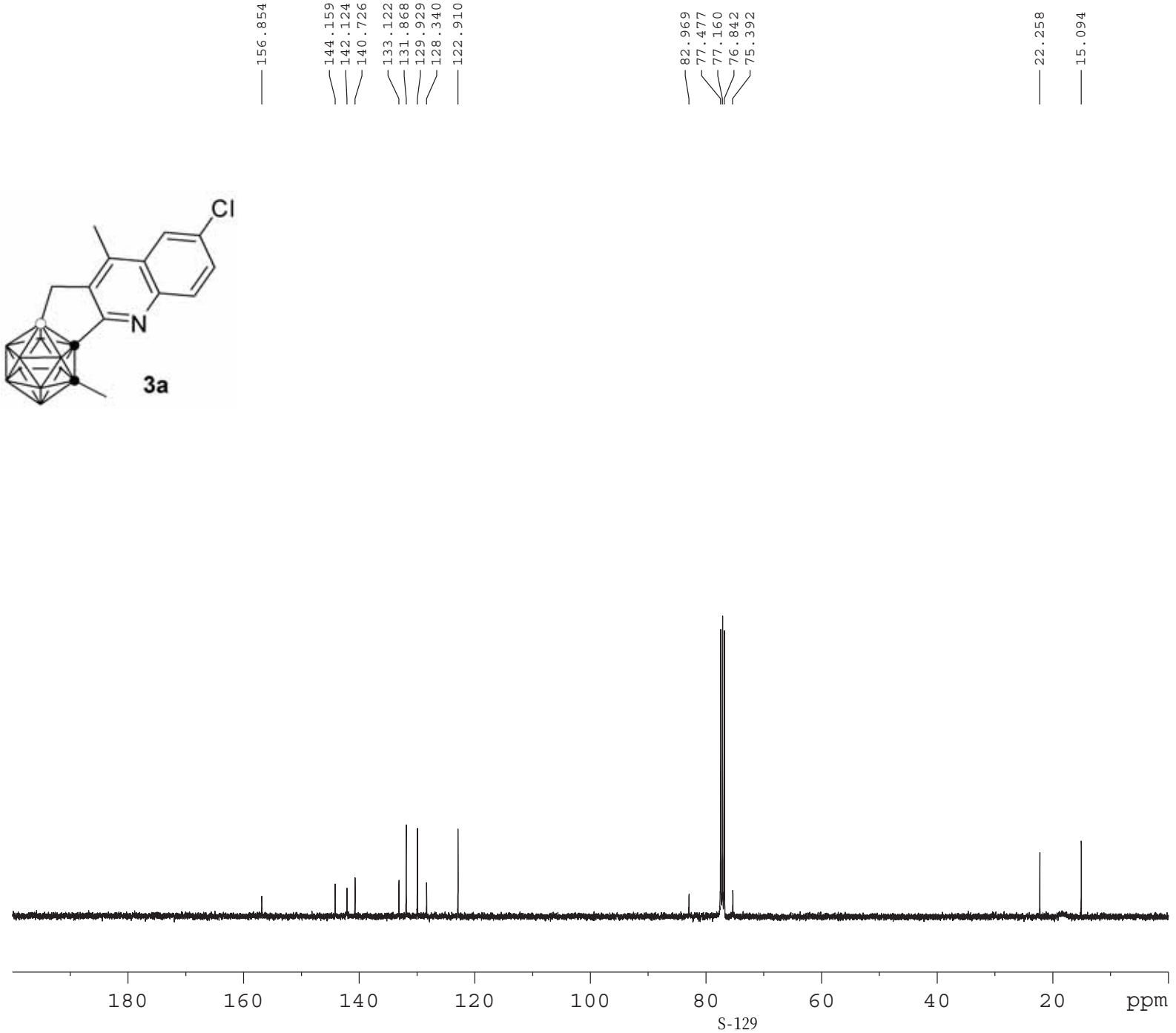


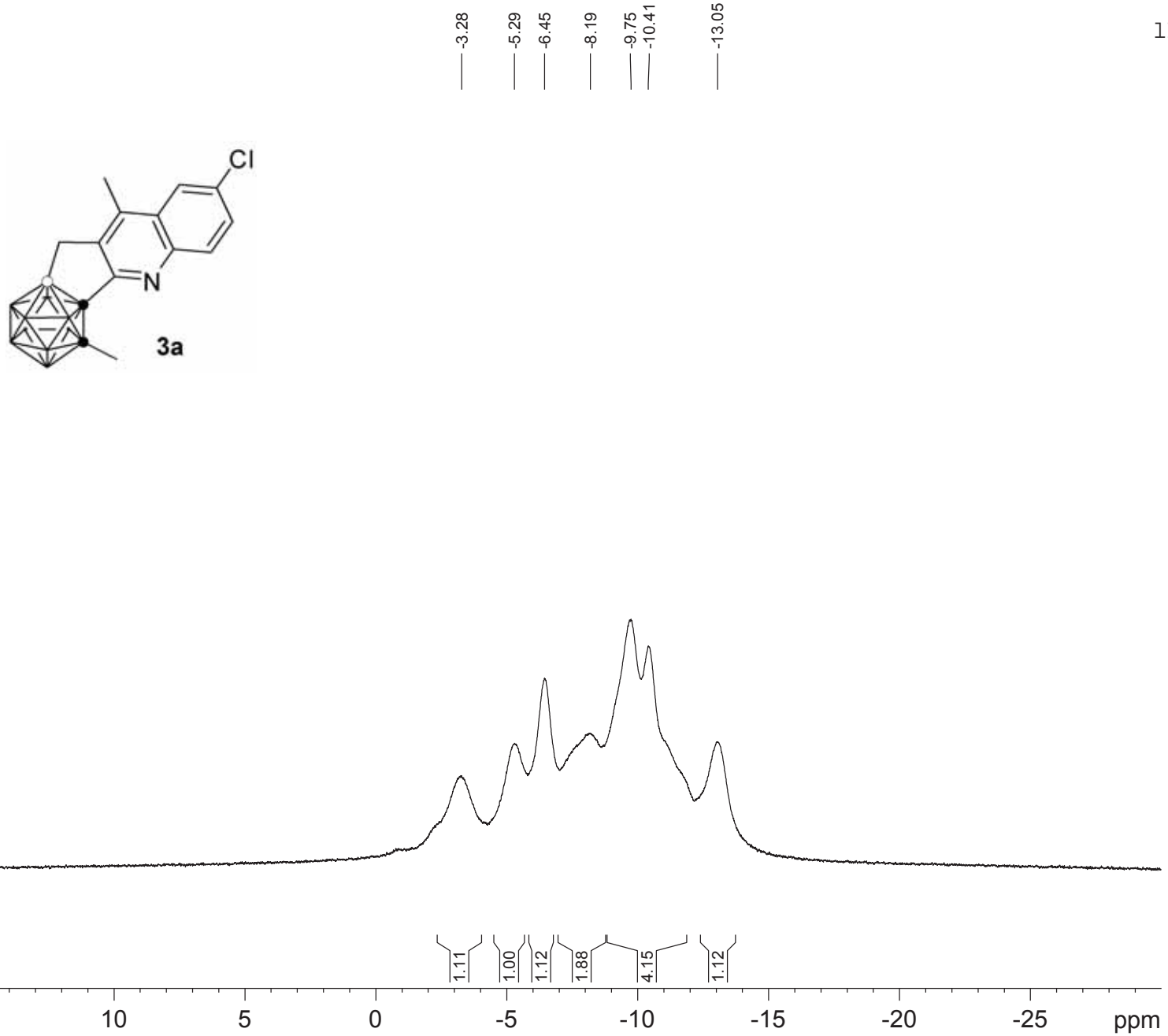
lhr-H-casCl-0427-1-CDC

Current Data Parameters
NAME lhr-H-casCl-0427-1-CD
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160803
Time 13.33 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

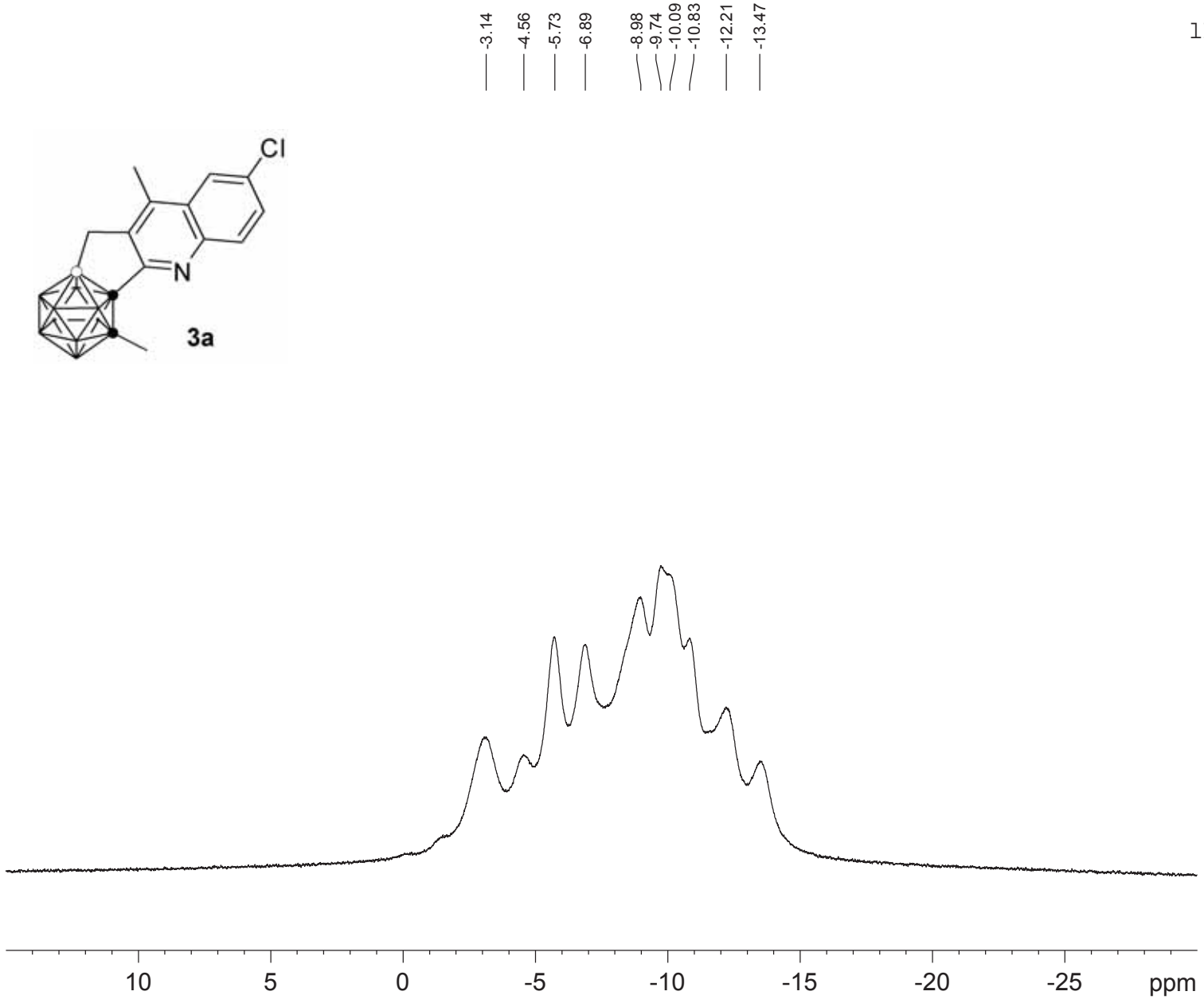
F2 - Processing parameters
SI 65536
SF 400.2300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


156.854
144.159
142.124
140.726
133.122
131.868
129.929
128.340
122.910
82.969
77.477
77.160
76.842
75.392
22.258
15.094
lhr-C-casCl-0427-1-CDCl3
Bruker Advance III 400
Current Data Parameters
NAME lhr-C-casCl-0427-1-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160803
Time 12.41 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 438
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W
F2 - Processing parameters
SI 32768
SF 100.6127568 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
N
3a
180
160
140
120
100
80
60
40
20
ppm



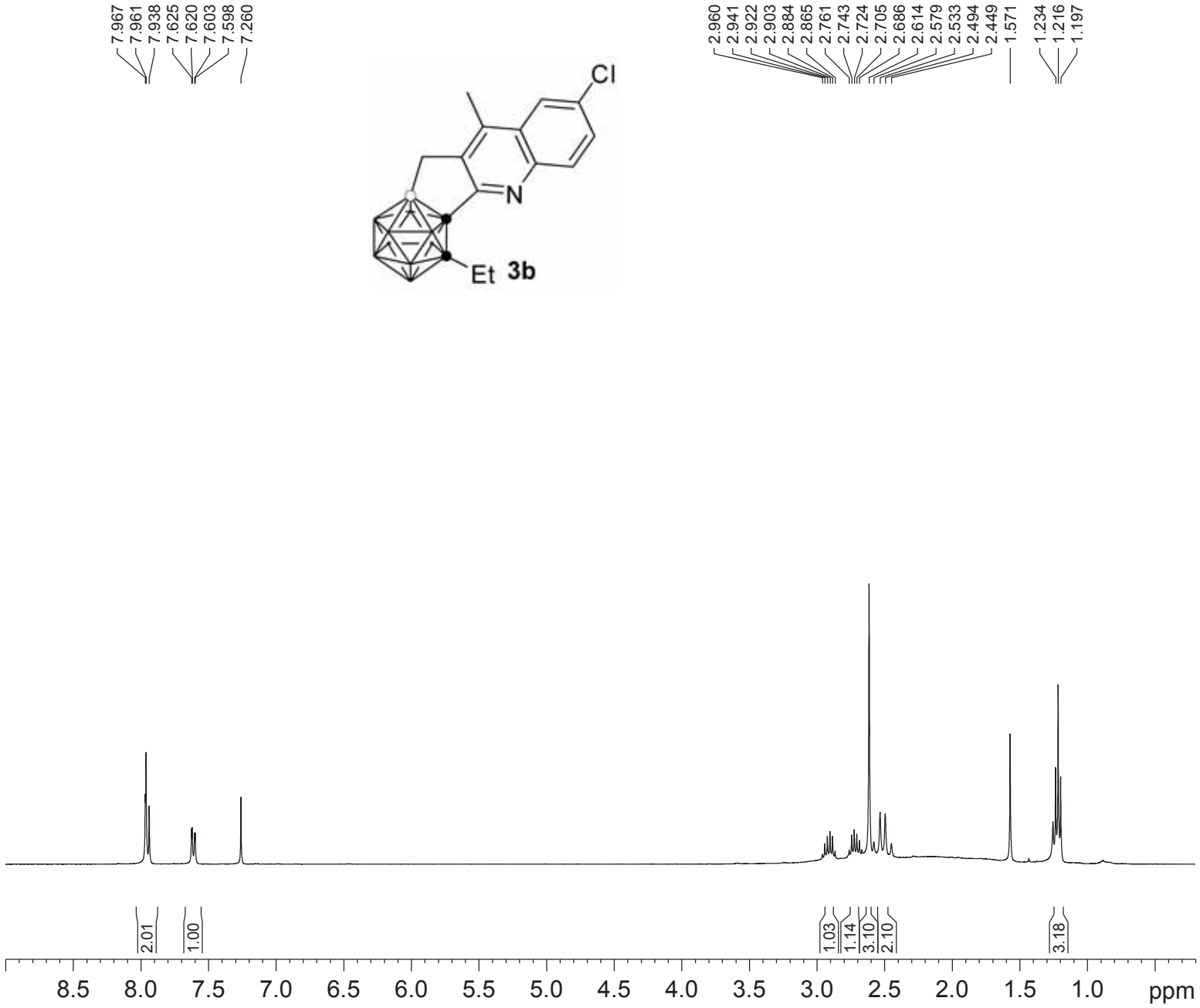
lhr-B-casCl-0427-1-CDCl3

```
Current Data Parameters
NAME      lhr-B-casCl-0427-1-CDCl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160803
Time              13.35 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG            zgdc
TD                65536
SOLVENT           CDCl3
NS                    9
DS                    4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  287
DW               20.800 usec
DE                6.50 usec
TE               295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                32768
SF          128.4097615 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-B-casCl-0427-1-CDCl3

```
Current Data Parameters
NAME      lhr-B-casCl-0427-1-CDCl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160803
Time              13.37 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG               zg
TD                 65536
SOLVENT            CDCl3
NS                    17
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   287
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1             2.00000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                 32768
SF           128.4097430 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



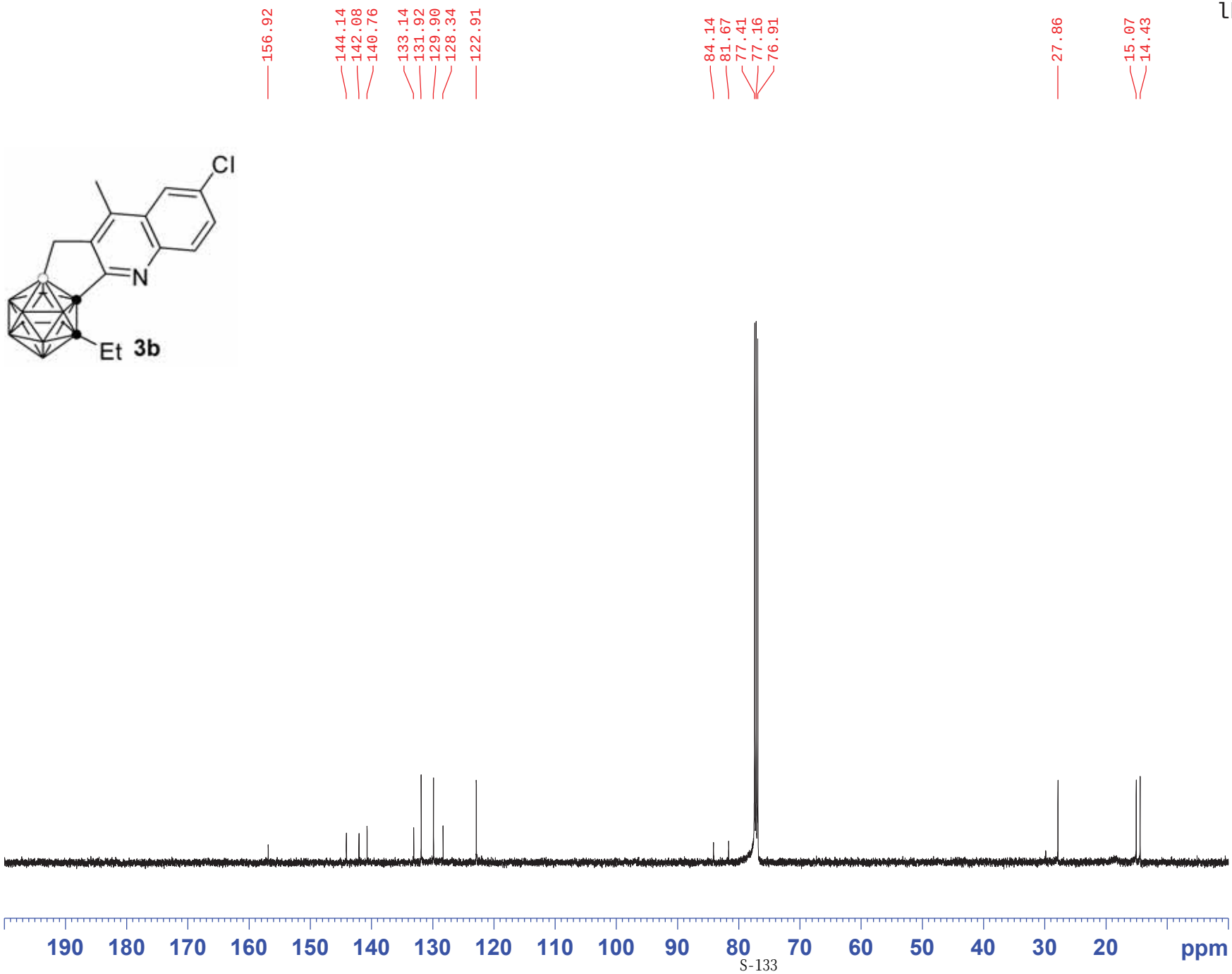
lhr-H-0716-cascdcl3

Current Data Parameters
NAME lhr-H-0716-cascdcl
EXPNO 1
PROCNO 1

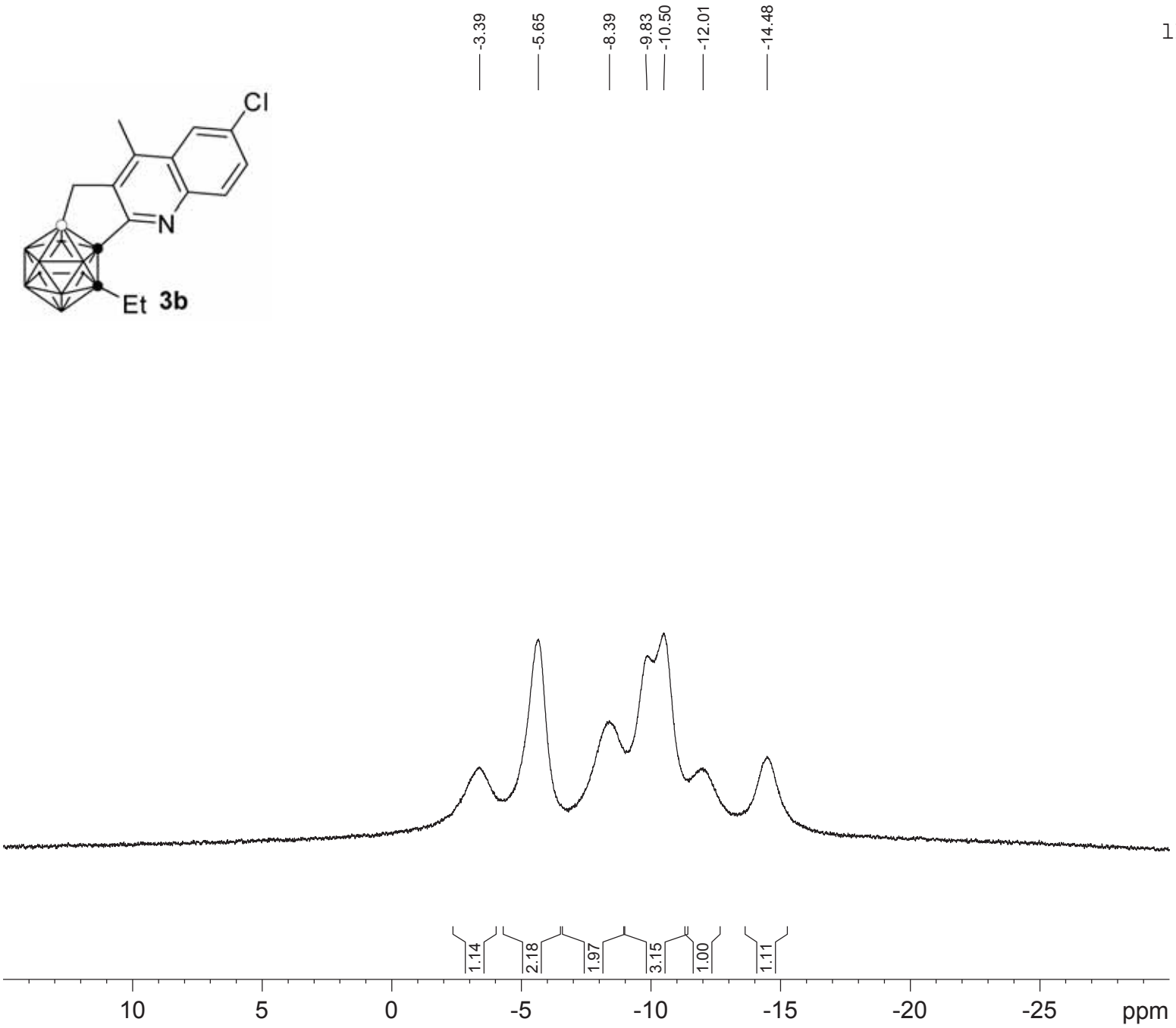
F2 - Acquisition Parameters
Date_ 20170704
Time 22.06 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH:
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

lhr-0716-4clcetcascdcl3

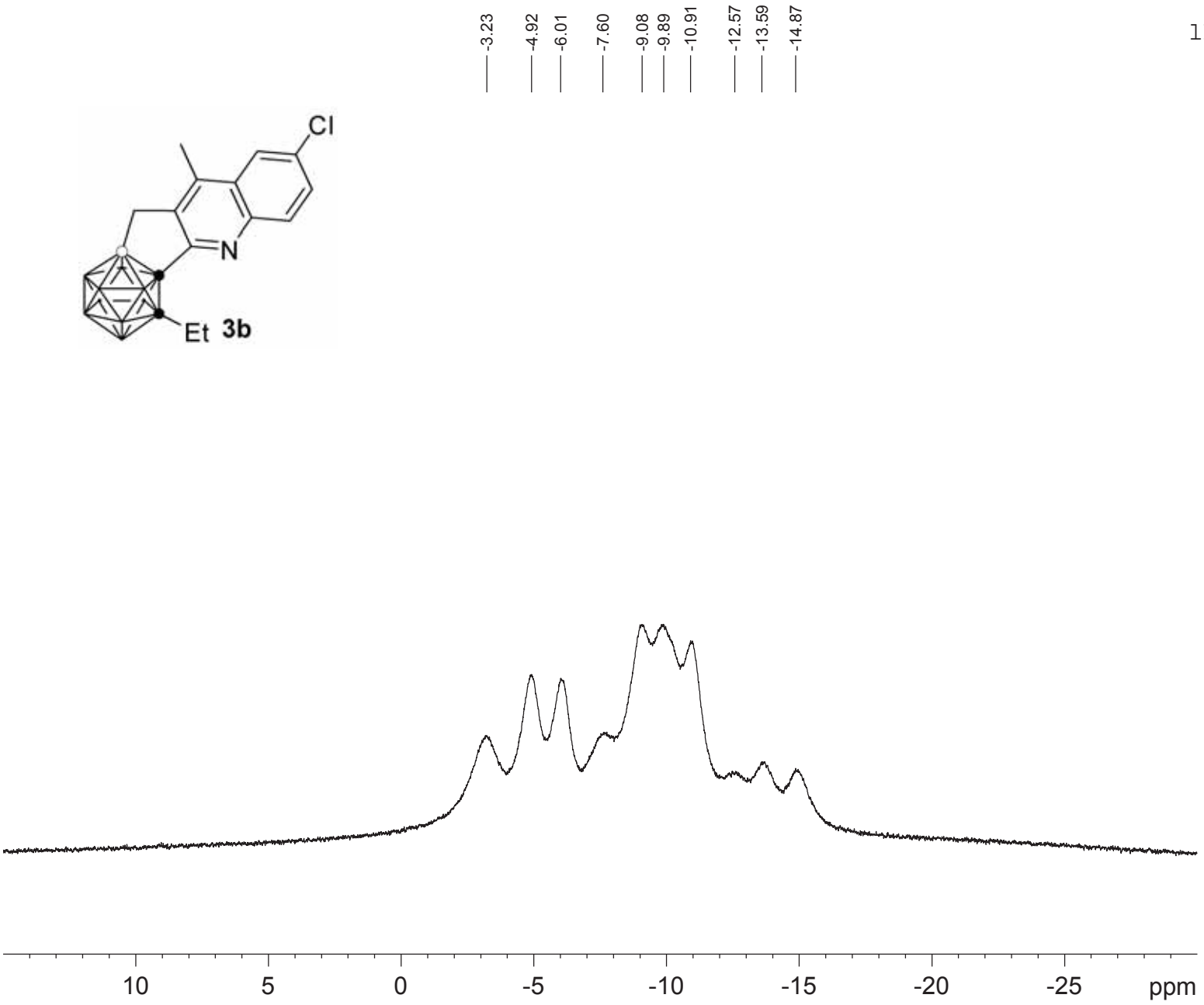



```
Current Data Parameters
NAME      lhr-0716-4clcetcascdcl3
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_               20170705
Time                   20.33 h
INSTRUM                spect
PROBHD    Z119470_0283 (
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       647
DS                         4
SWH                29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                    206.72
DW                    16.800 usec
DE                     6.50 usec
TE                    299.1 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             125.7703643 MHz
NUC1                     13C
P1                    10.00 usec
PLW1              94.00000000 W
SFO2              500.1320005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              25.00000000 W
PLW12              0.39063001 W
PLW13              0.19648001 W

F2 - Processing parameters
SI                       32768
SF                125.7577711 MHz
WDW                         EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



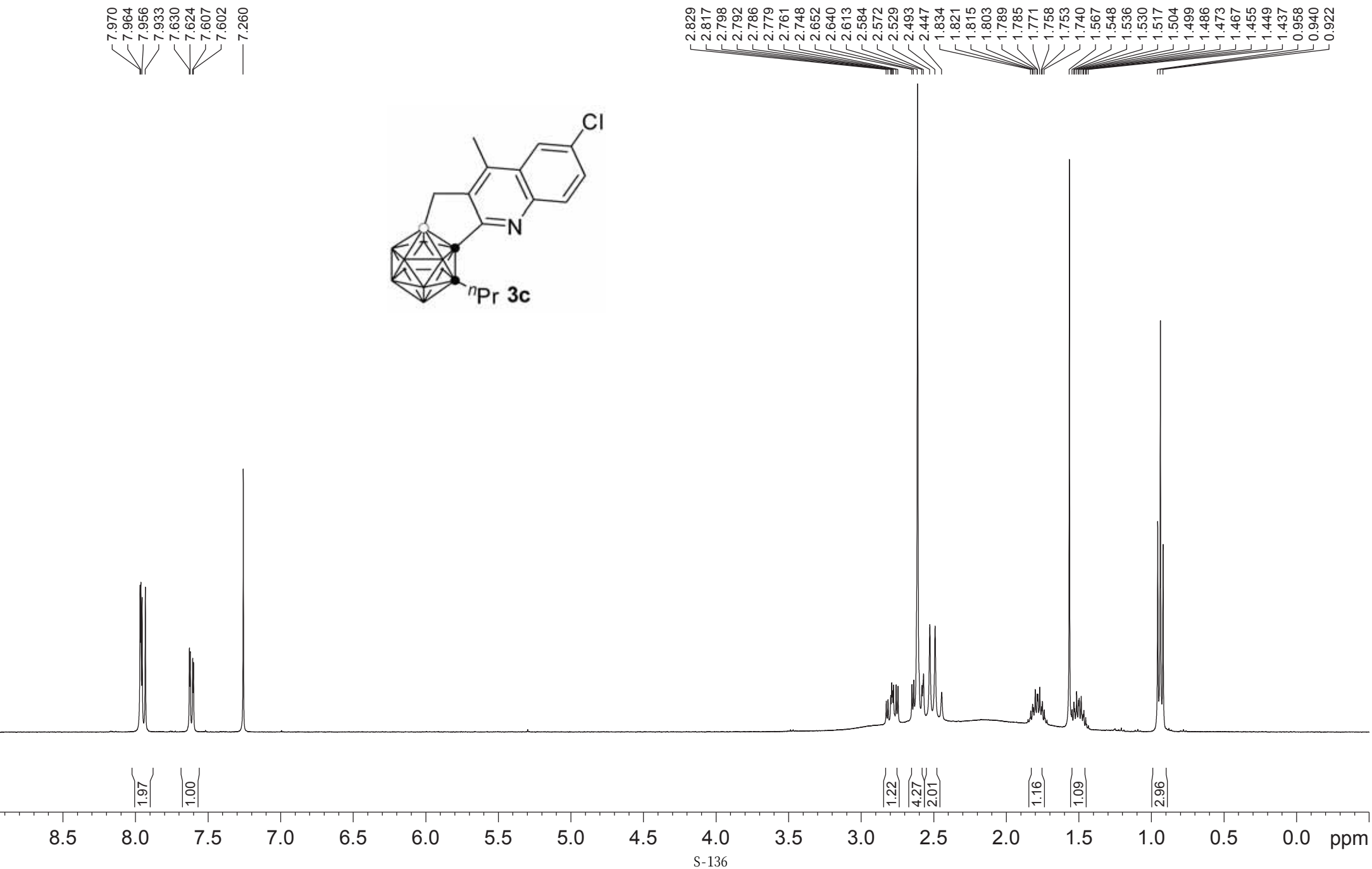
lhr-B-0716-cascdcl3

```
Current Data Parameters
NAME      lhr-B-0716-cascdcl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170705
Time                  20.58 h
INSTRUM               spect
PROBHD    Z108618_0257 (
PULPROG                zgdc
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        4
SWH              24038.461 Hz
FIDRES            0.366798 Hz
AQ               1.3631488 sec
RG                      362
DW                 20.800 usec
DE                  6.50 usec
TE                  295.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                       1
SFO1           128.4096890 MHz
NUC1                   11B
P1                    7.50 usec
PLW1           55.09999847 W
SFO2           400.2316009 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           13.56000042 W
PLW12           0.27428001 W

F2 - Processing parameters
SI                    32768
SF             128.4097615 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



lhr-B-0716-cascdcl3(C)

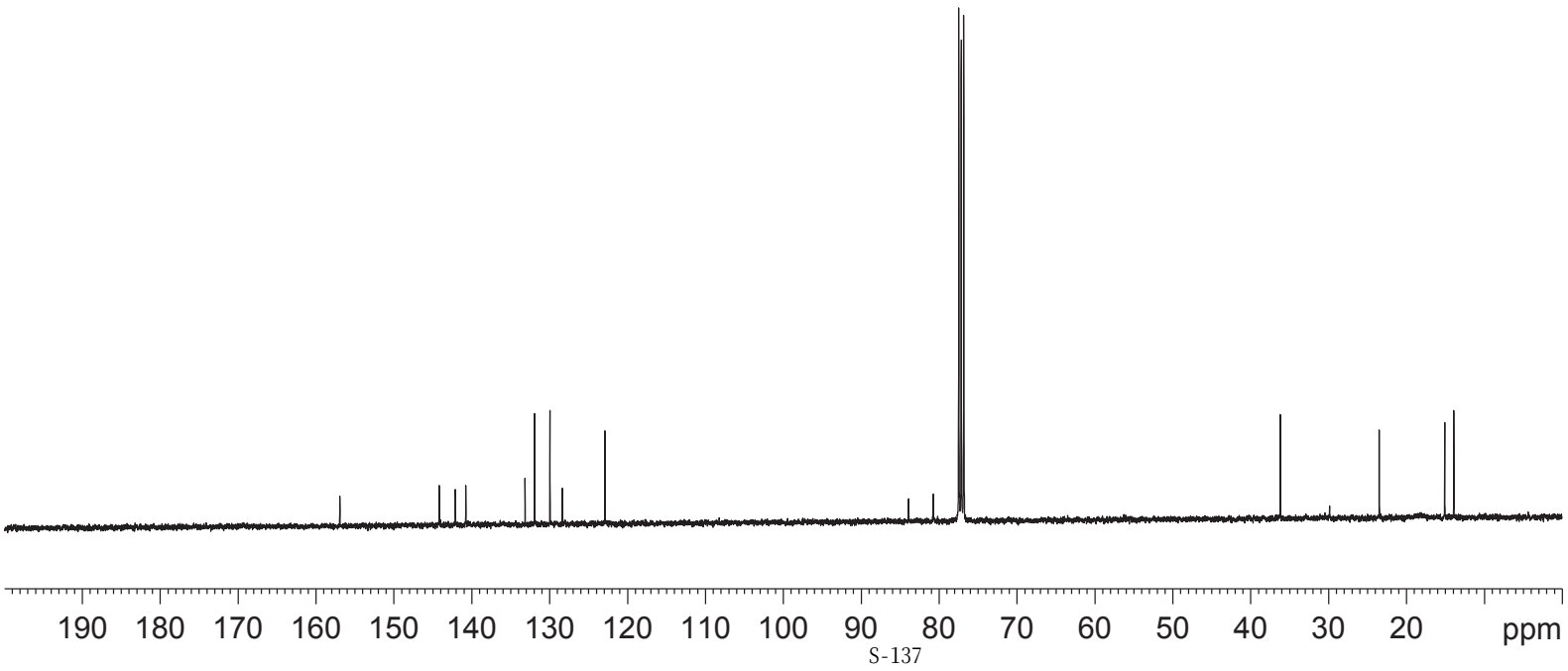
```
Current Data Parameters
NAME      lhr-B-0716-cascdcl3(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170705
Time              21.00 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   24
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  362
DW               20.800 usec
DE                6.50 usec
TE               295.4 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


7.970
7.964
7.956
7.933
7.630
7.624
7.607
7.602
7.260
2.829
2.817
2.798
2.792
2.786
2.779
2.761
2.748
2.652
2.640
2.613
2.584
2.572
2.529
2.493
2.447
1.834
1.821
1.815
1.803
1.789
1.785
1.771
1.758
1.753
1.740
1.567
1.548
1.536
1.530
1.517
1.504
1.499
1.486
1.473
1.467
1.455
1.449
1.437
0.958
0.940
0.922
Cl
N
nPr 3c
1.97
1.00
1.22
4.27
2.01
1.16
1.09
2.96
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm

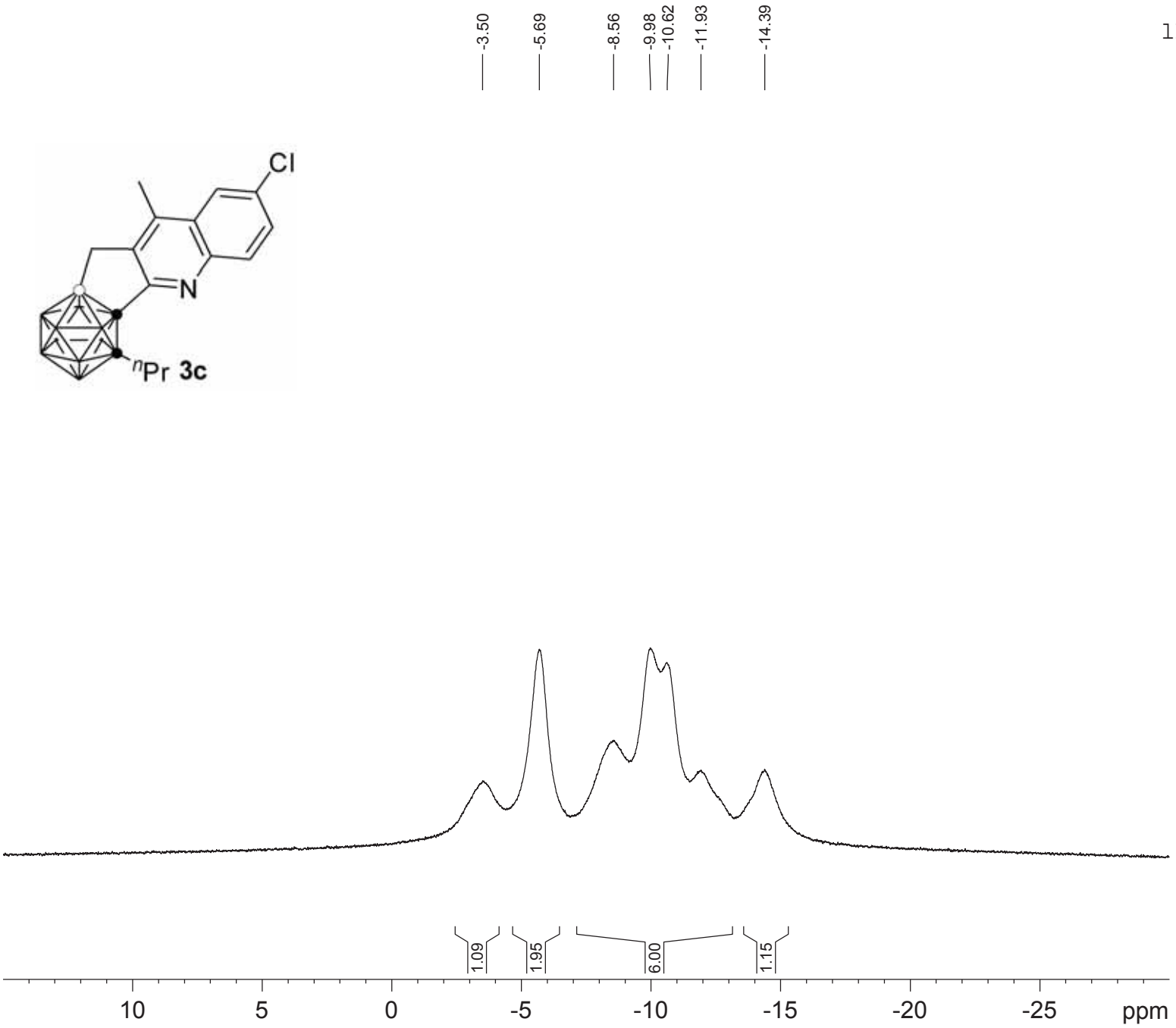
156.92
144.14
142.07
140.75
133.12
131.90
129.92
128.34
122.91
83.92
80.75
77.48
77.16
76.84
36.18
23.49
15.08
13.92

lhr-C-0728-4cl-ccc

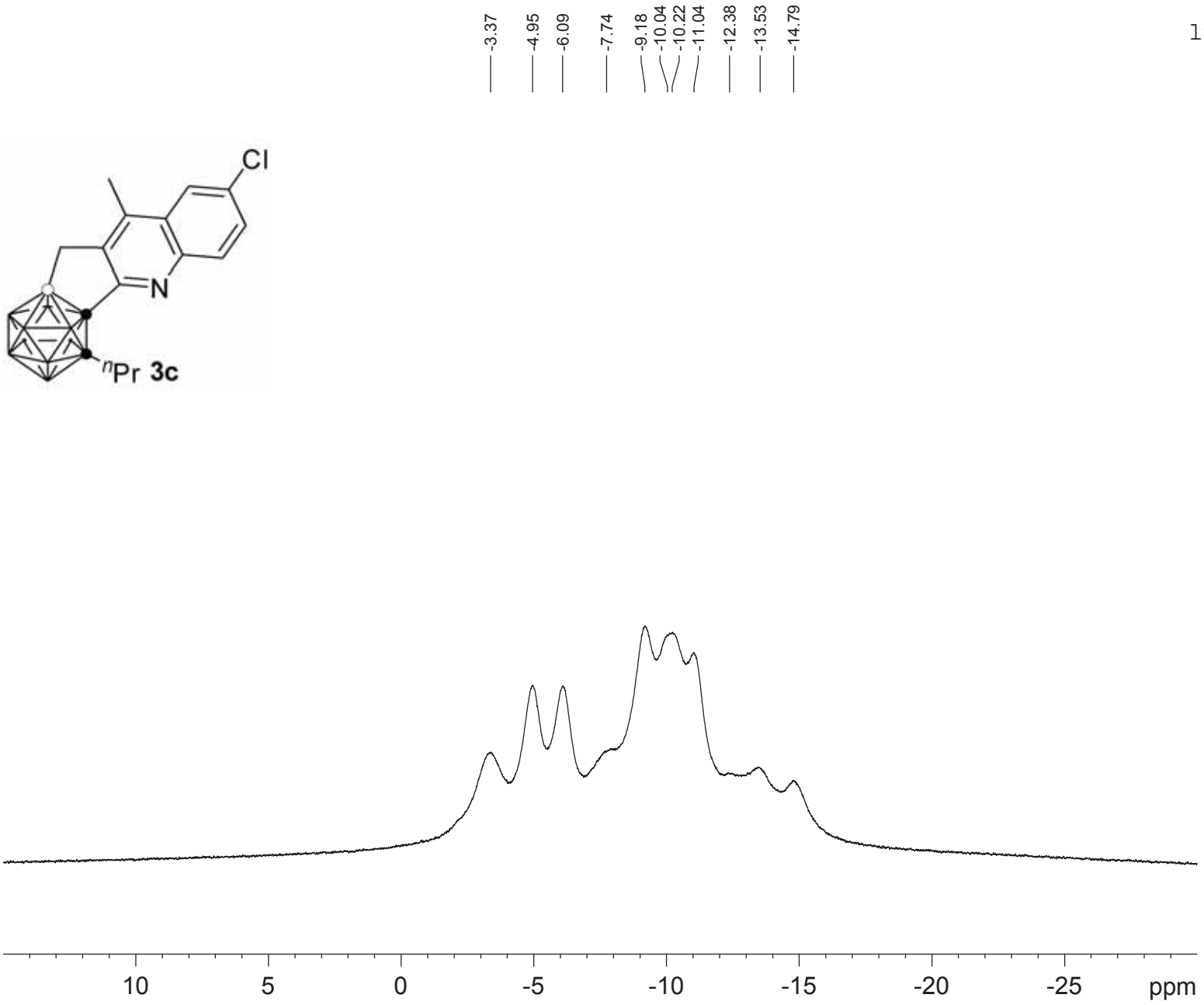
```
Current Data Parameters
NAME      lhr-C-0728-4cl-cccascdcl3-NPR
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20170716
Time              16.27 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  900
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW               12.267 usec
DE                6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                32768
SF           100.6379007 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-B-0728-4cl-cccascdcl3-NPR

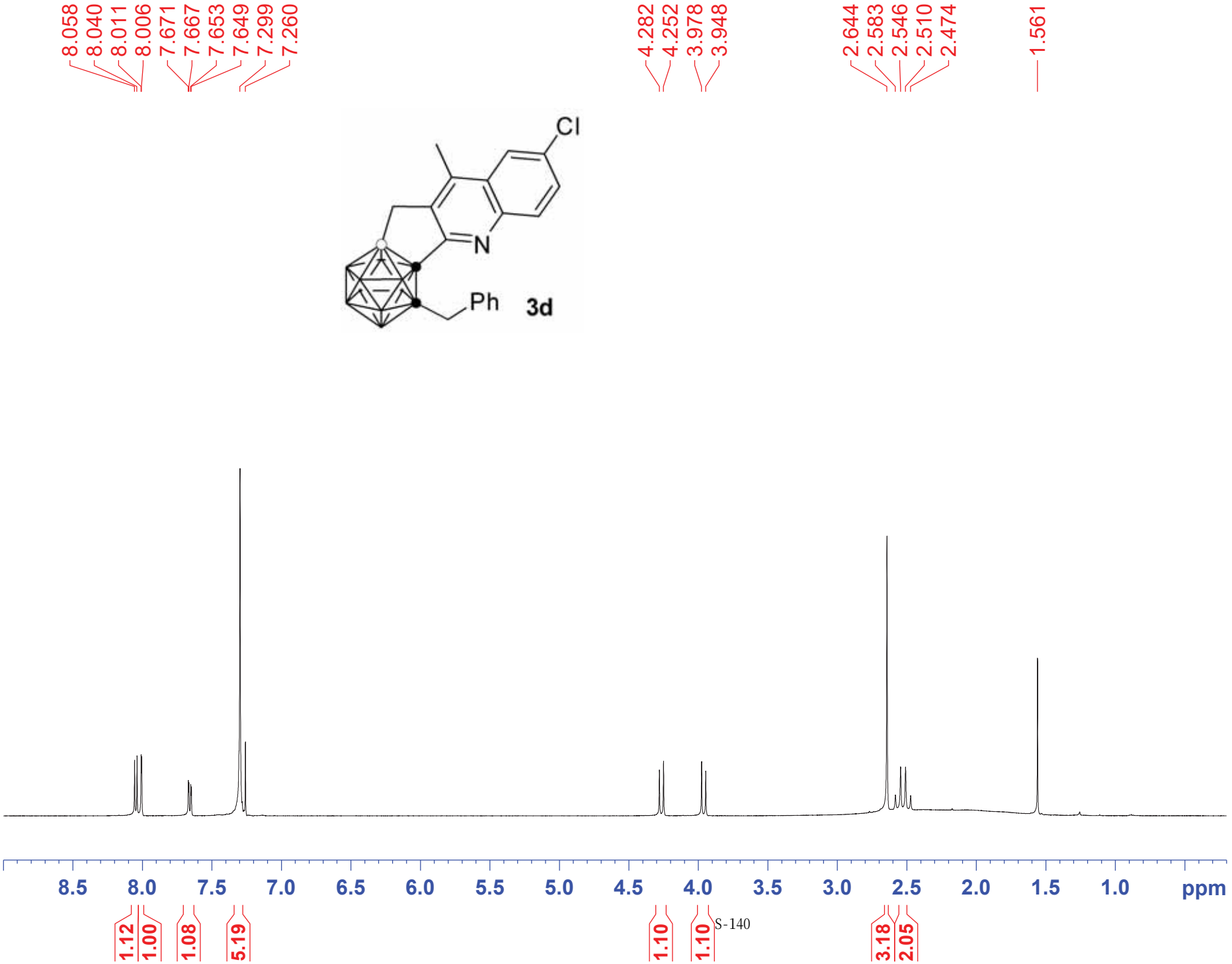



```
Current Data Parameters
NAME      lhr-B-0728-4cl-cccascdcl3-NPR
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170716
Time              17.12 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    24
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



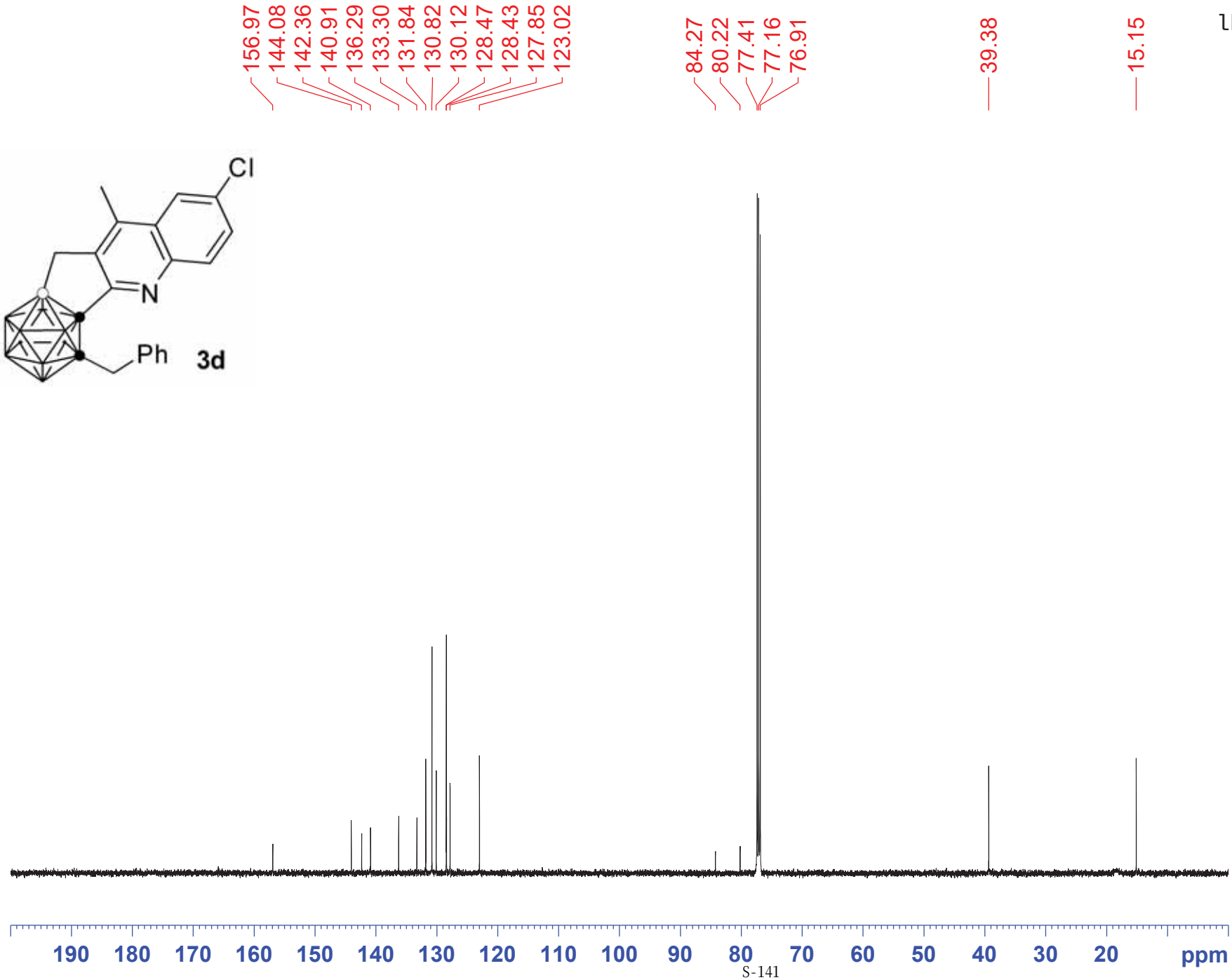
lhr-B-0728-4cl-cccascdcl3-NPR(C

```
Current Data Parameters
NAME      lhr-B-0728-4cl-cccascdcl3-NPR(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170716
Time              17.18 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     63
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    362
DW                20.800 usec
DE                 6.50 usec
TE                294.9 K
D1             2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



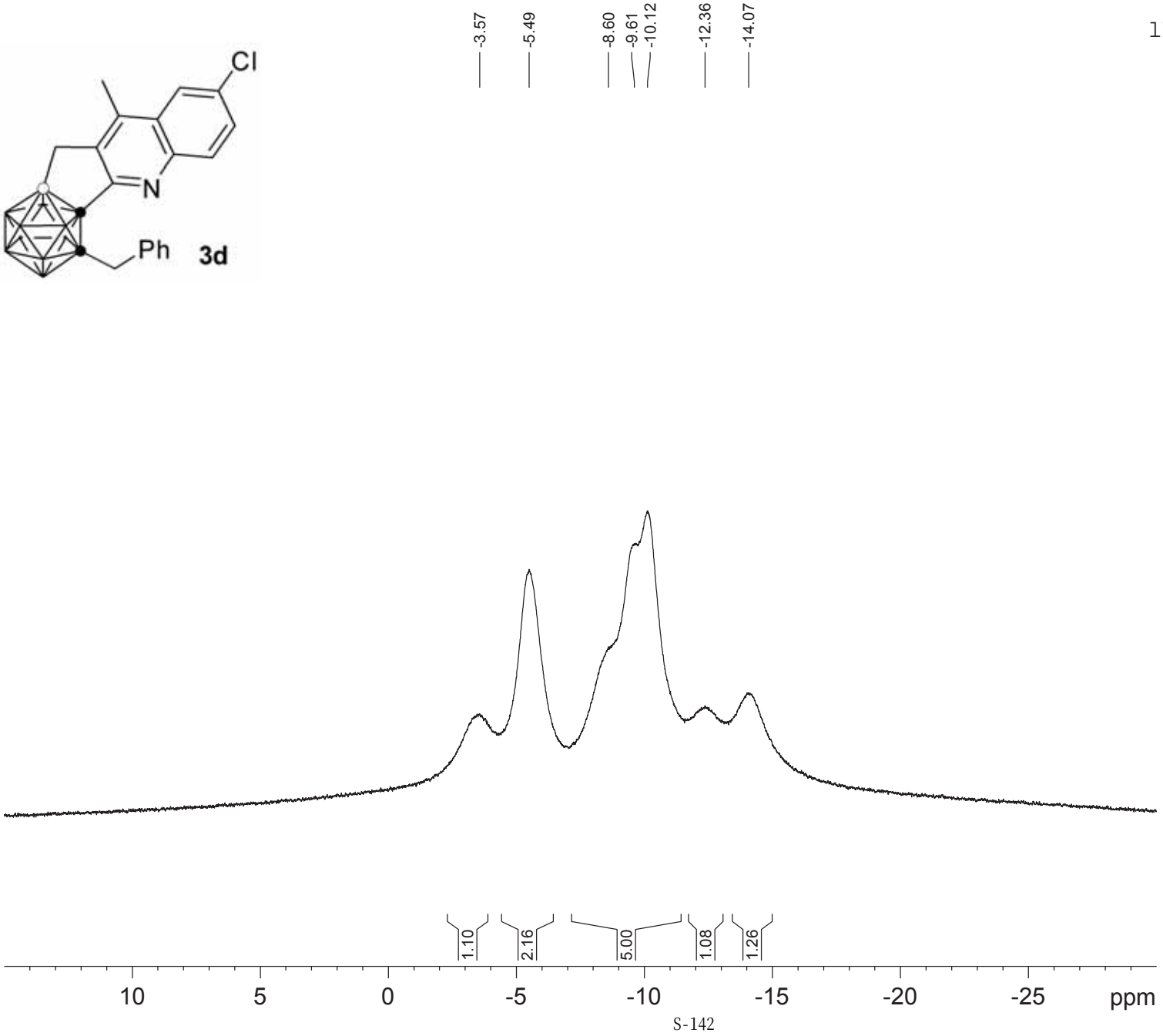
lhr-H-0723-RE

```
Current Data Parameters
NAME      lhr-H-0723-RE
EXPNO                 1
PROCNO                1

F2 - Acquisition Paramet
Date_          20170719
Time              19.36
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000
FIDRES        0.305176
AQ            3.2767999
RG               117.01
DW               50.000
DE                6.50
TE               297.0
D1           1.00000000
TD0                  1
SFO1         500.1330883
NUC1                1H
P1                10.00
PLW1         25.00000000

F2 - Processing paramete
SI               65536
SF          500.1300126
WDW                 EM
SSB      0
LB               0.30
GB       0
PC               1.00
```



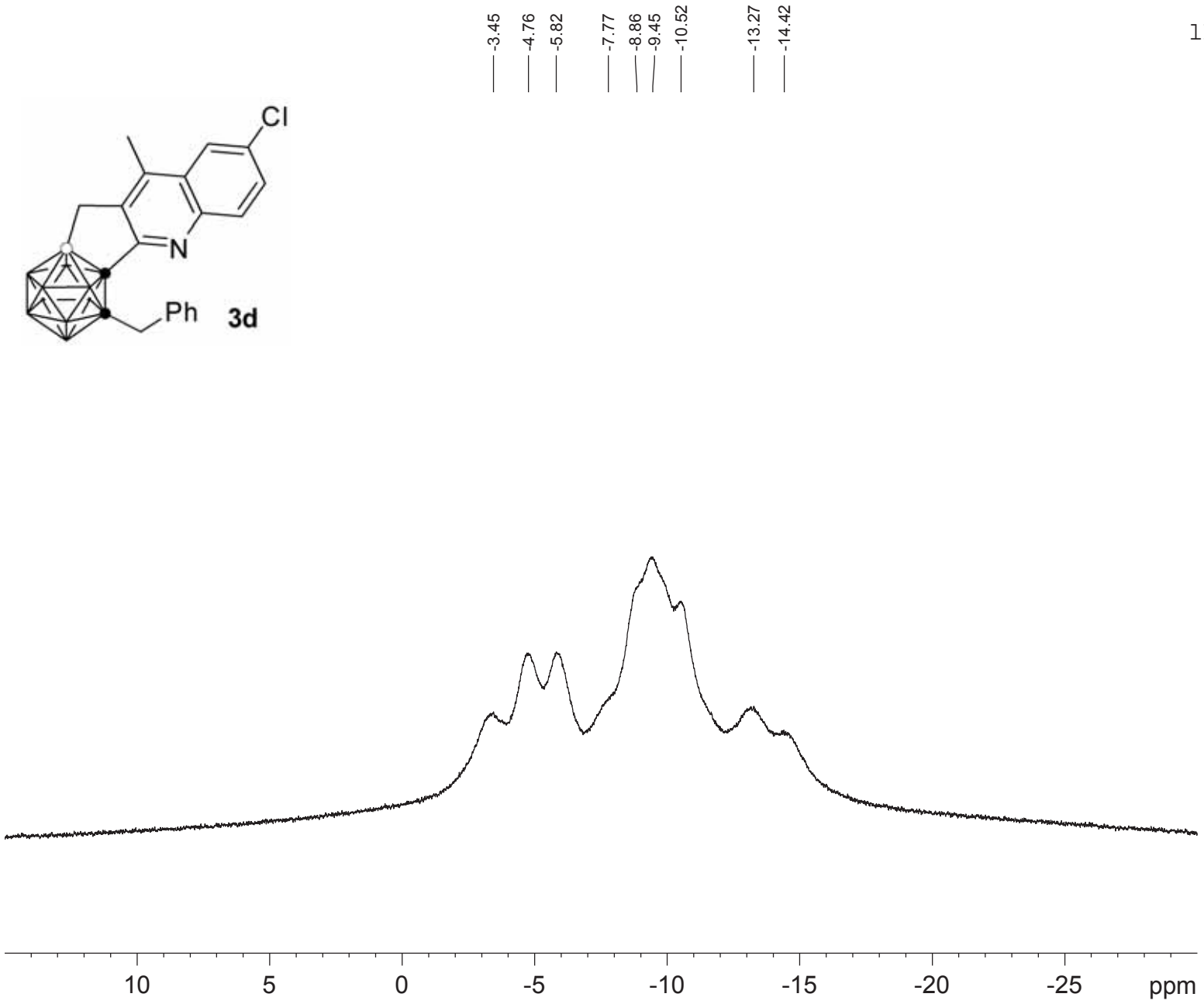
lhr-C-0723-RE

```
Current Data Parameters
NAME       lhr-C-0723-RE
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170719
Time              20.11 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  636
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE                297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        25.00000000 W
PLW12        0.39063001 W
PLW13        0.19648001 W

F2 - Processing parameters
SI                32768
SF          125.7577719 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



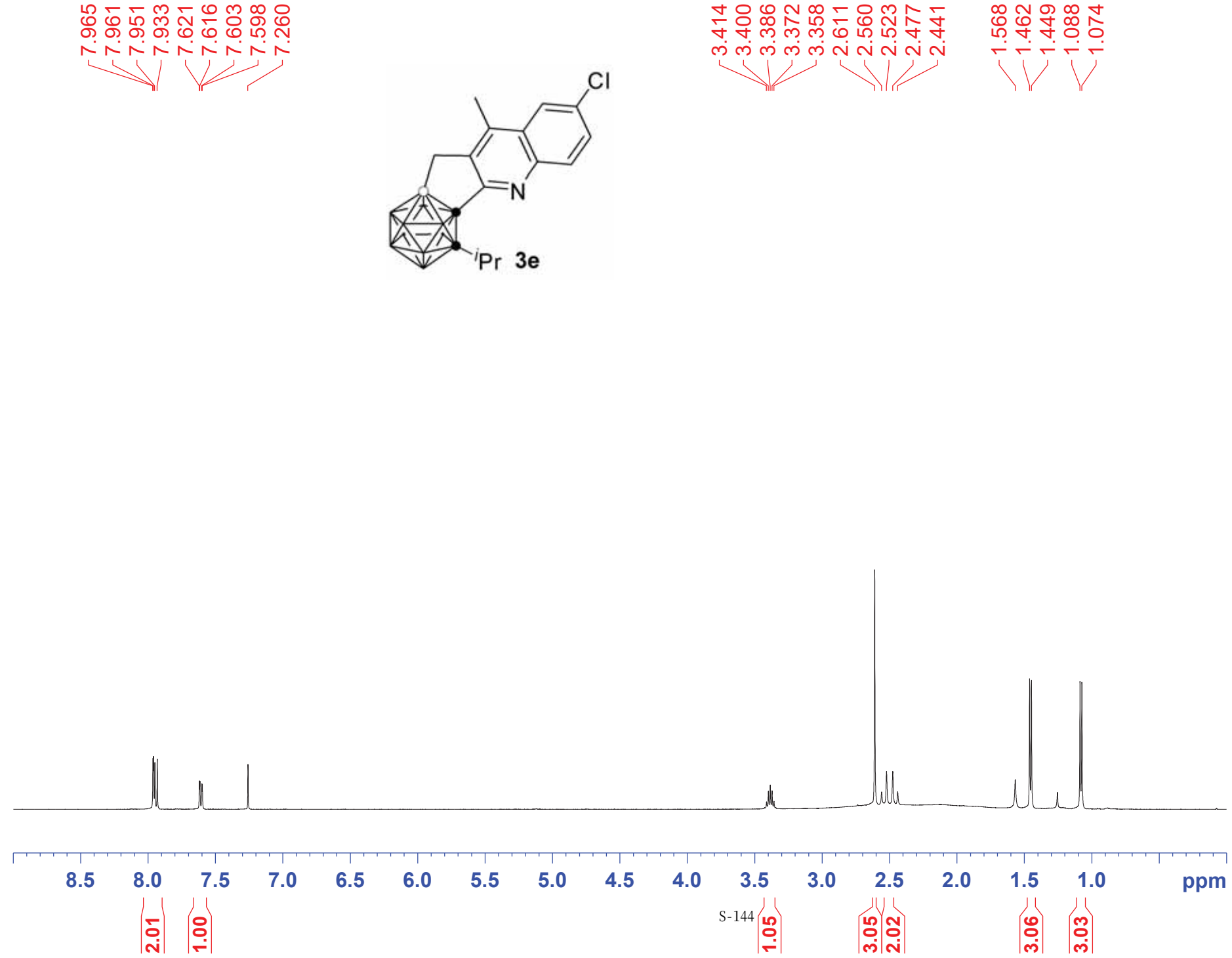
lhr-B-0723-4cl-cccascdcl

```
Current Data Parameters
NAME      lhr-B-0723-4cl-cccascdcl3-bn
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170714
Time              18.33 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    44
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   406
DW                20.800 usec
DE                 6.50 usec
TE                295.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



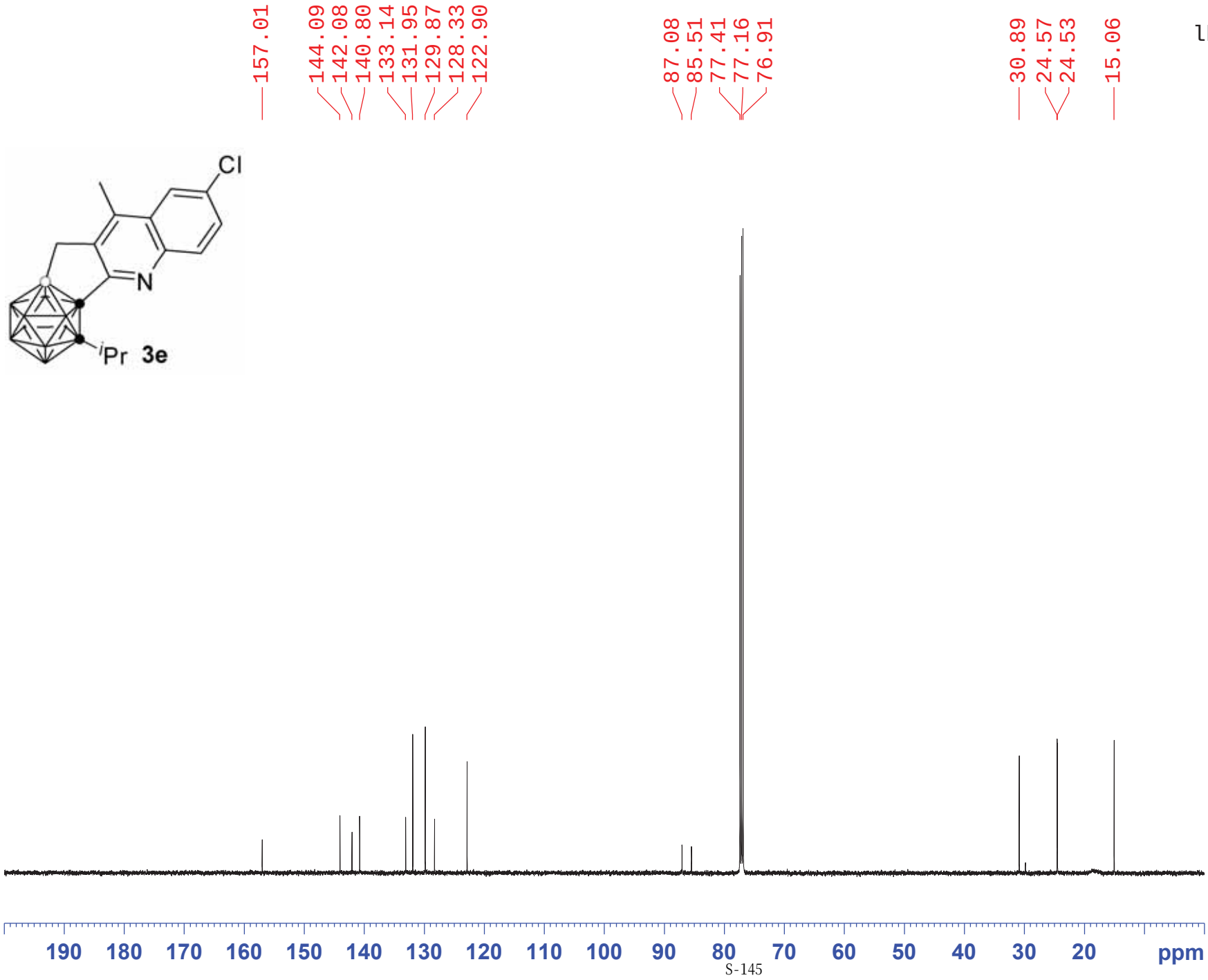
lhr-B-0723-4cl-cccascdcl3-bn(C)

```
Current Data Parameters
NAME      lhr-B-0723-4cl-cccascdcl3-bn(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170714
Time              18.35 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     37
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    362
DW                20.800 usec
DE                 6.50 usec
TE                295.1 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



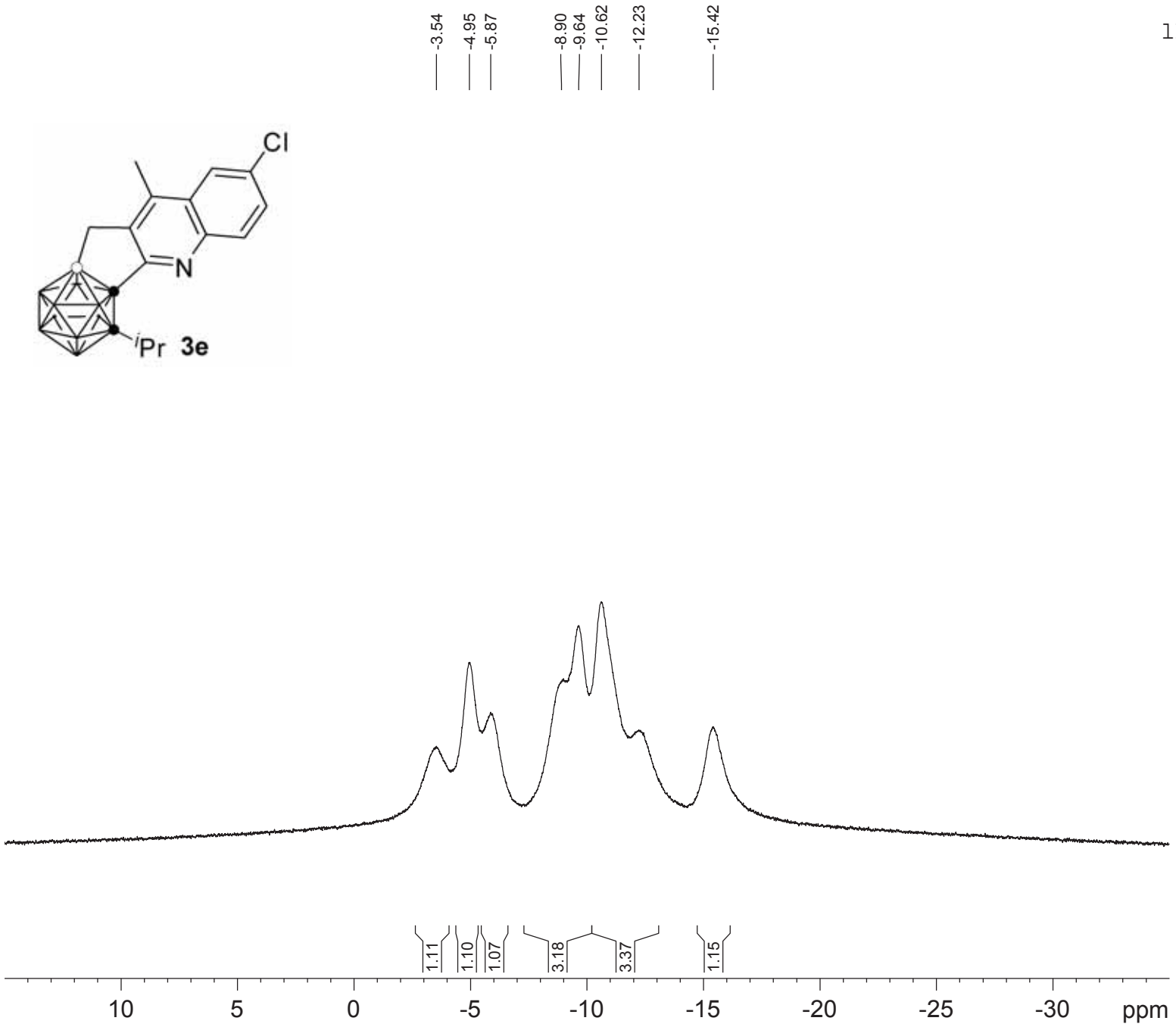
lhr-0734-casH

```
Current Data Parameters
NAME      lhr-0734-casH
EXPNO                 1
PROCNO                1

F2 - Acquisition Paramet
Date_          20170729
Time              18.28
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                  16
DS                   2
SWH          10000.000
FIDRES        0.305176
AQ           3.2767999
RG               102.6
DW              50.000
DE                6.50
TE               297.3
D1          1.00000000
TD0                  1
SFO1       500.1330883
NUC1              1H
P1               10.00
PLW1       25.00000000

F2 - Processing paramete
SI               65536
SF       500.1300127
WDW                EM
SSB      0
LB              0.30
GB       0
PC              1.00
```



lhr-0734-casC

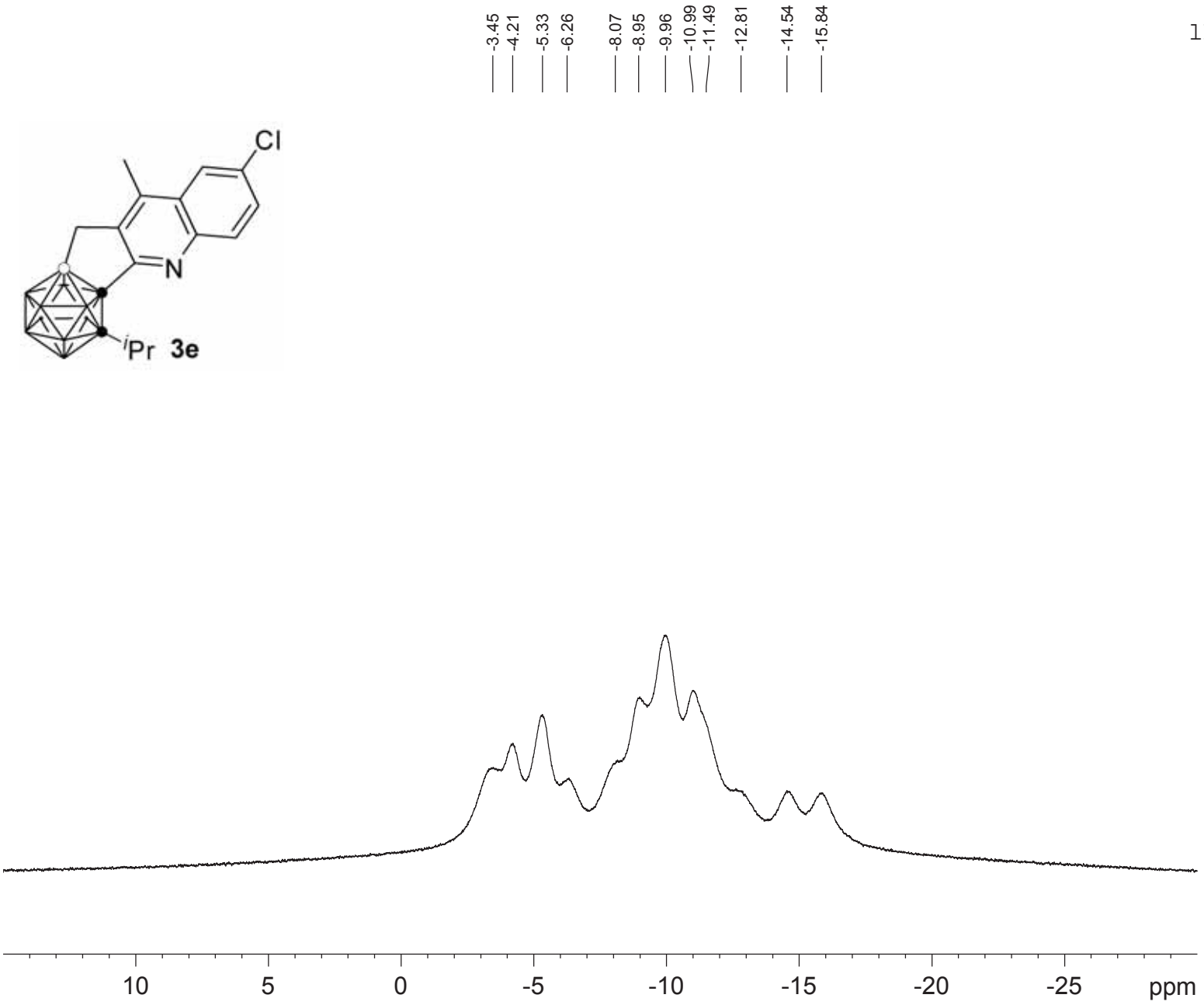
```
Current Data Parameters
NAME      lhr-0734-casC
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170729
Time             19.10 h
INSTRUM            spect
PROBHD   Z119470_0283 (
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                 800
DS                   4
SWH          29761.904 Hz
FIDRES        0.908261 Hz
AQ           1.1010048 sec
RG              206.72
DW              16.800 usec
DE               6.50 usec
TE              298.3 K
D1          2.00000000 sec
D11         0.03000000 sec
TD0                  1
SFO1       125.7703643 MHz
NUC1              13C
P1              10.00 usec
PLW1       94.00000000 W
SFO2       500.1320005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           80.00 usec
PLW2       25.00000000 W
PLW12       0.39063001 W
PLW13       0.19648001 W

F2 - Processing parameters
SI               32768
SF         125.7577714 MHz
WDW                EM
SSB      0
LB              1.00 Hz
GB       0
PC              1.40
```



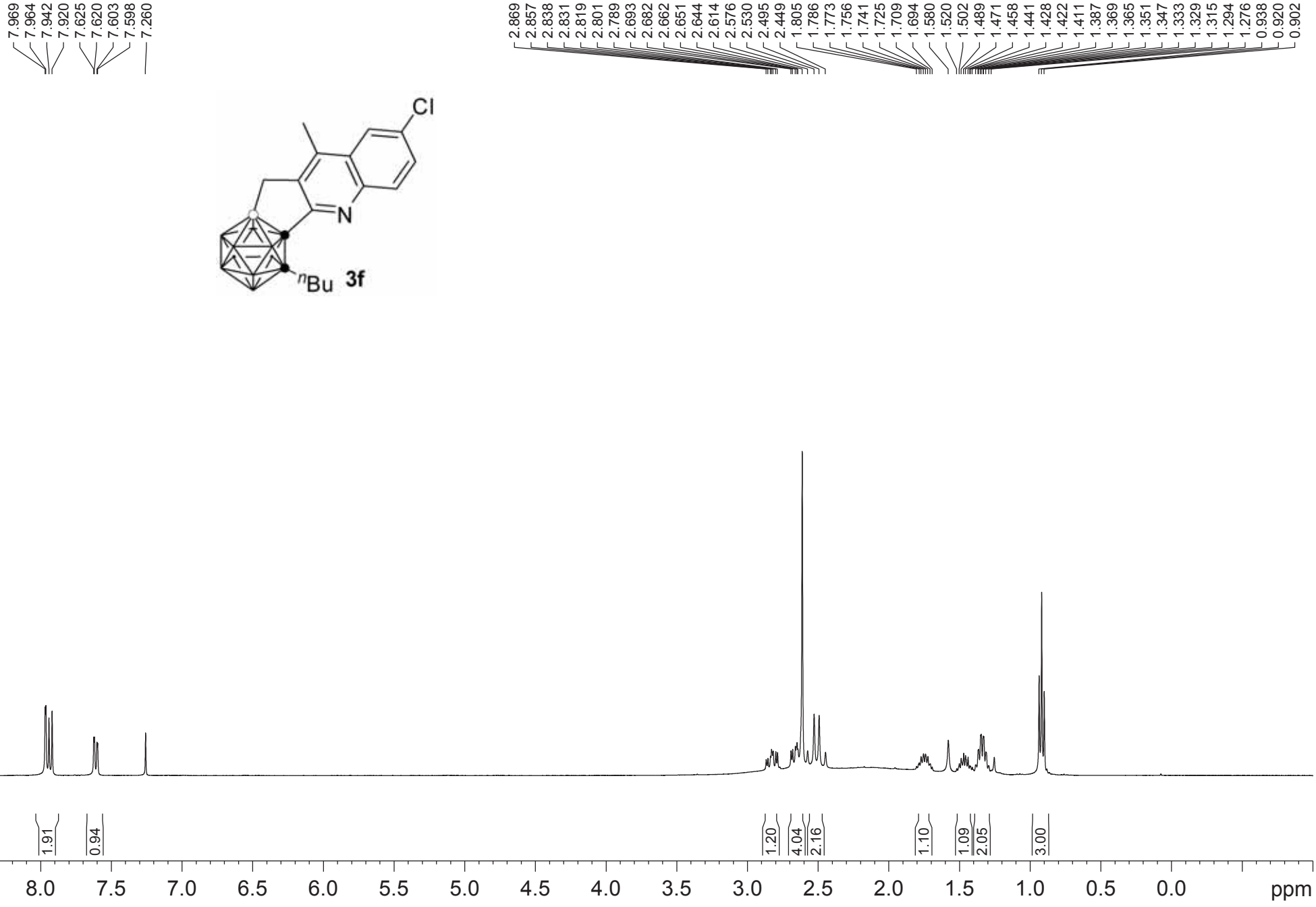
lhr-B-0734-cascdcl3-IPR

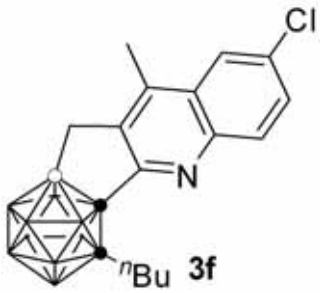
```
Current Data Parameters
NAME      lhr-B-0734-cascdcl3-IPR
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170729
Time              19.55 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    24
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                 32768
SF          128.4097615 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

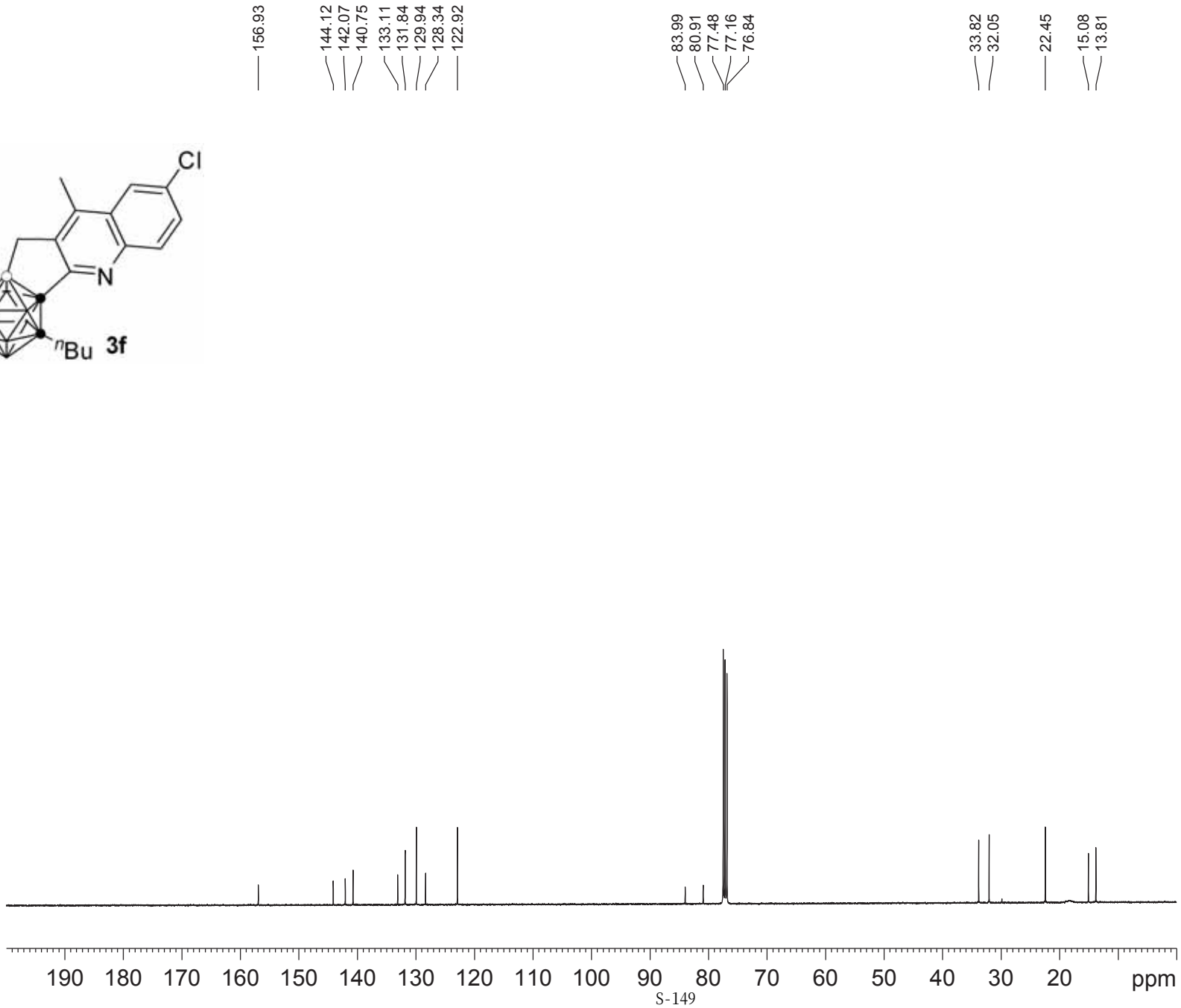
lhr-B-0734-cascdcl3-IPR(C)




```
Current Data Parameters
NAME      lhr-B-0734-cascdcl3-IPR(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170729
Time              19.58 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   36
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  362
DW               20.800 usec
DE                6.50 usec
TE               294.8 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

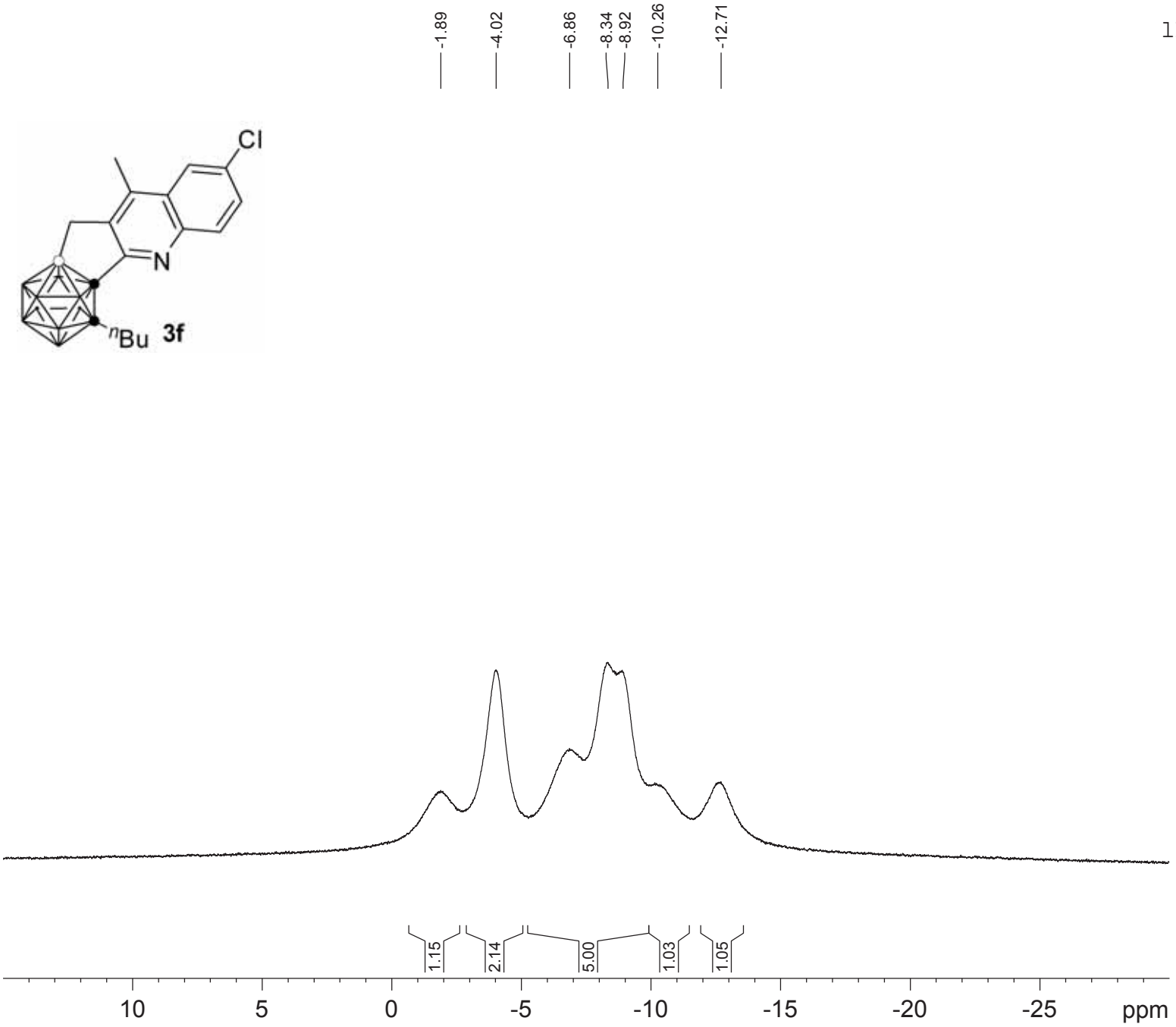

7.969
7.964
7.942
7.920
7.625
7.620
7.603
7.598
7.260
2.869
2.857
2.838
2.831
2.819
2.801
2.789
2.693
2.682
2.662
2.651
2.644
2.614
2.576
2.530
2.495
2.449
1.805
1.786
1.773
1.756
1.741
1.725
1.709
1.694
1.580
1.520
1.502
1.489
1.471
1.458
1.441
1.428
1.422
1.411
1.387
1.369
1.365
1.351
1.347
1.333
1.329
1.315
1.294
1.276
0.938
0.920
0.902
Cl
N
nBu
3f
1.91
0.94
1.20
4.04
2.16
1.10
1.09
2.05
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm





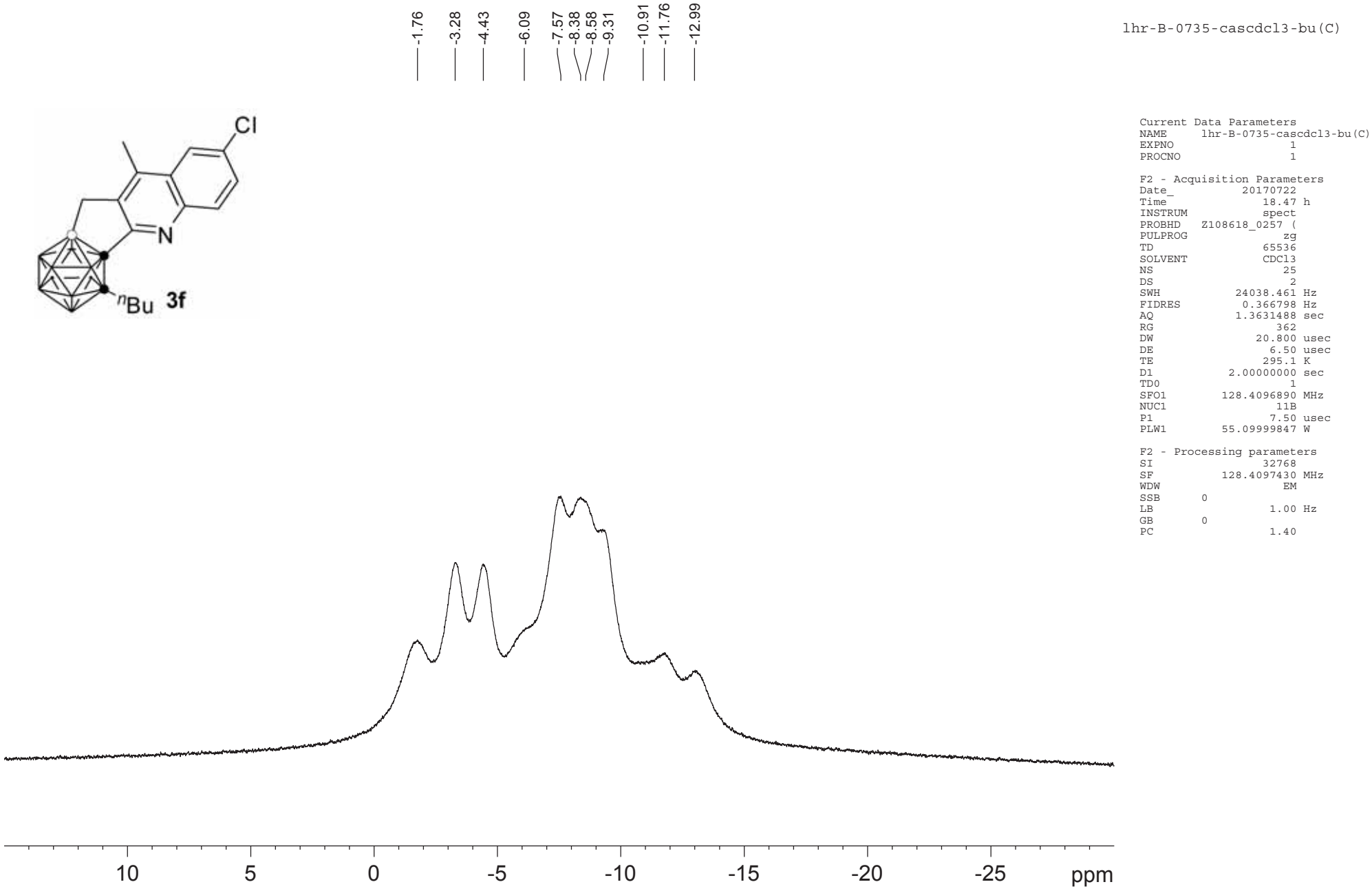
lhr-C-0731-cascdcl

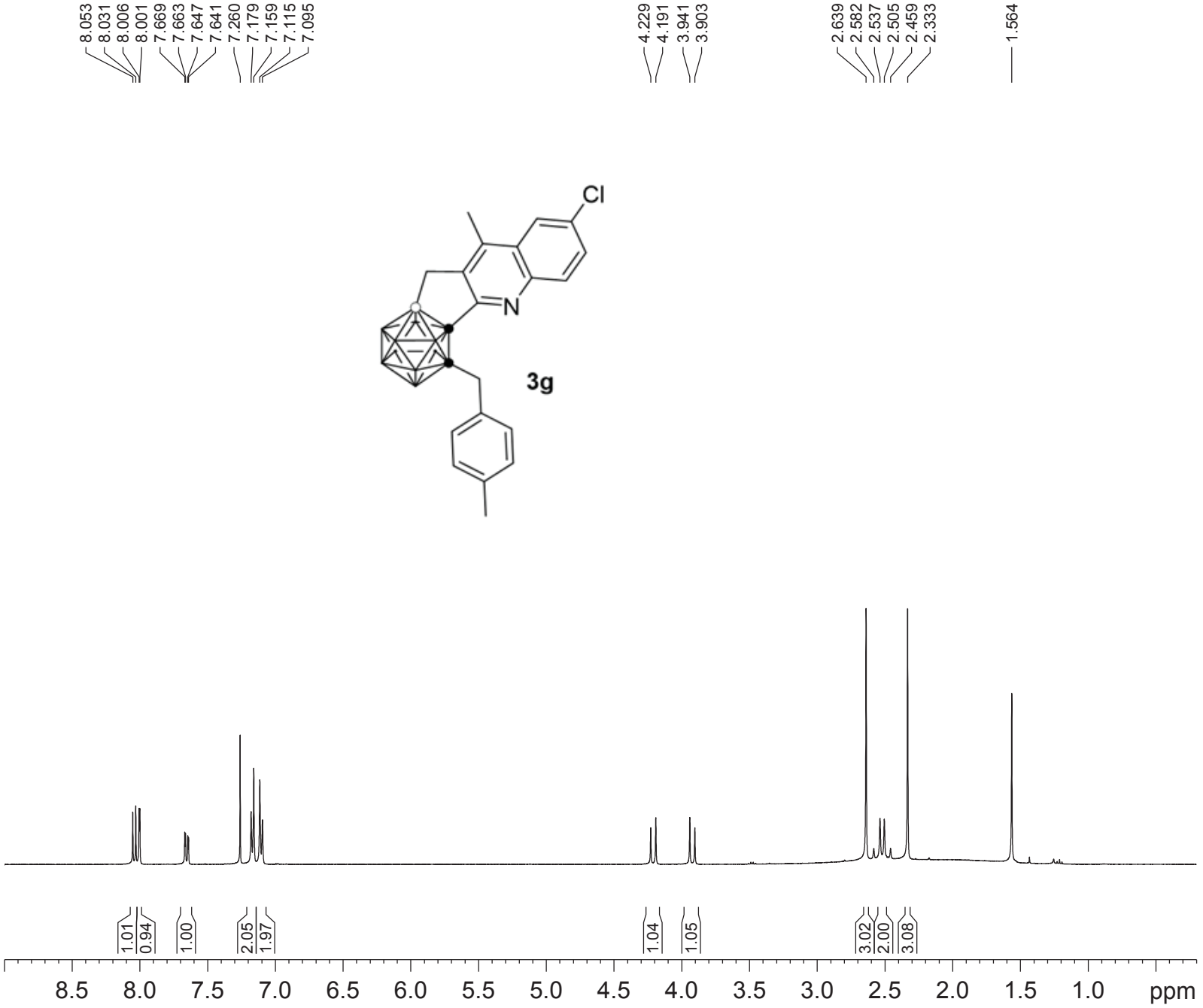
```
Current Data Parameters
NAME      lhr-C-0731-cascdcl3-bu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170722
Time              18.56 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW                12.267 usec
DE                 6.50 usec
TE                295.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                32768
SF           100.6379005 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



lhr-B-0735-cascdcl3-bu

```
Current Data Parameters
NAME      lhr-B-0735-cascdcl3-bu
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170722
Time              18.45 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   287
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

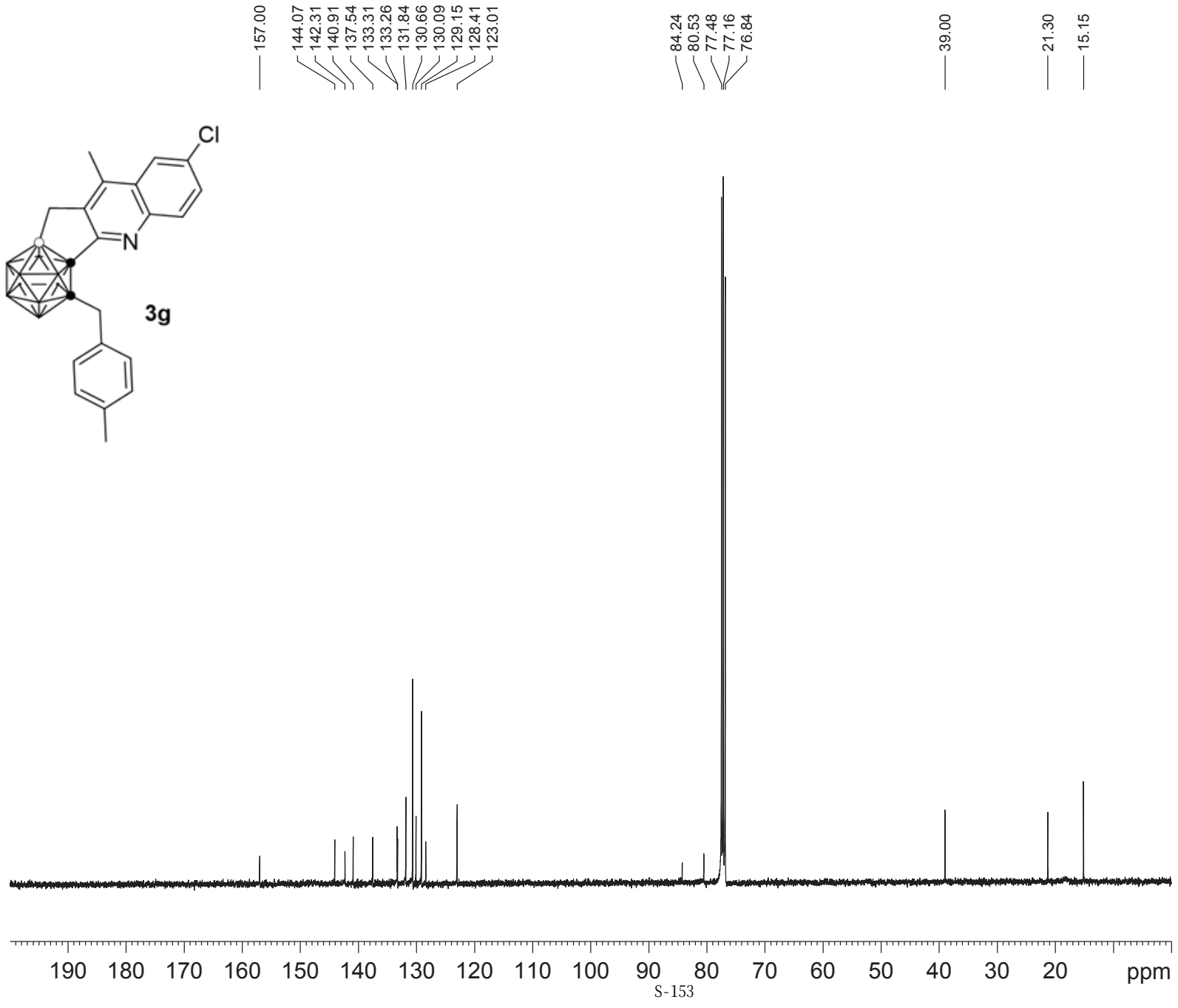

-1.76
-3.28
-4.43
-6.09
-7.57
-8.38
-8.58
-9.31
-10.91
-11.76
-12.99
lhr-B-0735-cascdcl3-bu(C)
Cl
N
nBu 3f
Current Data Parameters
NAME lhr-B-0735-cascdcl3-bu(C)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170722
Time 18.47 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 25
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
TD0 1
SFO1 128.4096890 MHz
NUC1 11B
P1 7.50 usec
PLW1 55.09999847 W
F2 - Processing parameters
SI 32768
SF 128.4097430 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
10
5
0
-5
-10
-15
-20
-25
ppm



Current Data Parameters
NAME lhr-H-0740-cascdcl3-bnch3
EXPNO 2
PROCNO 1

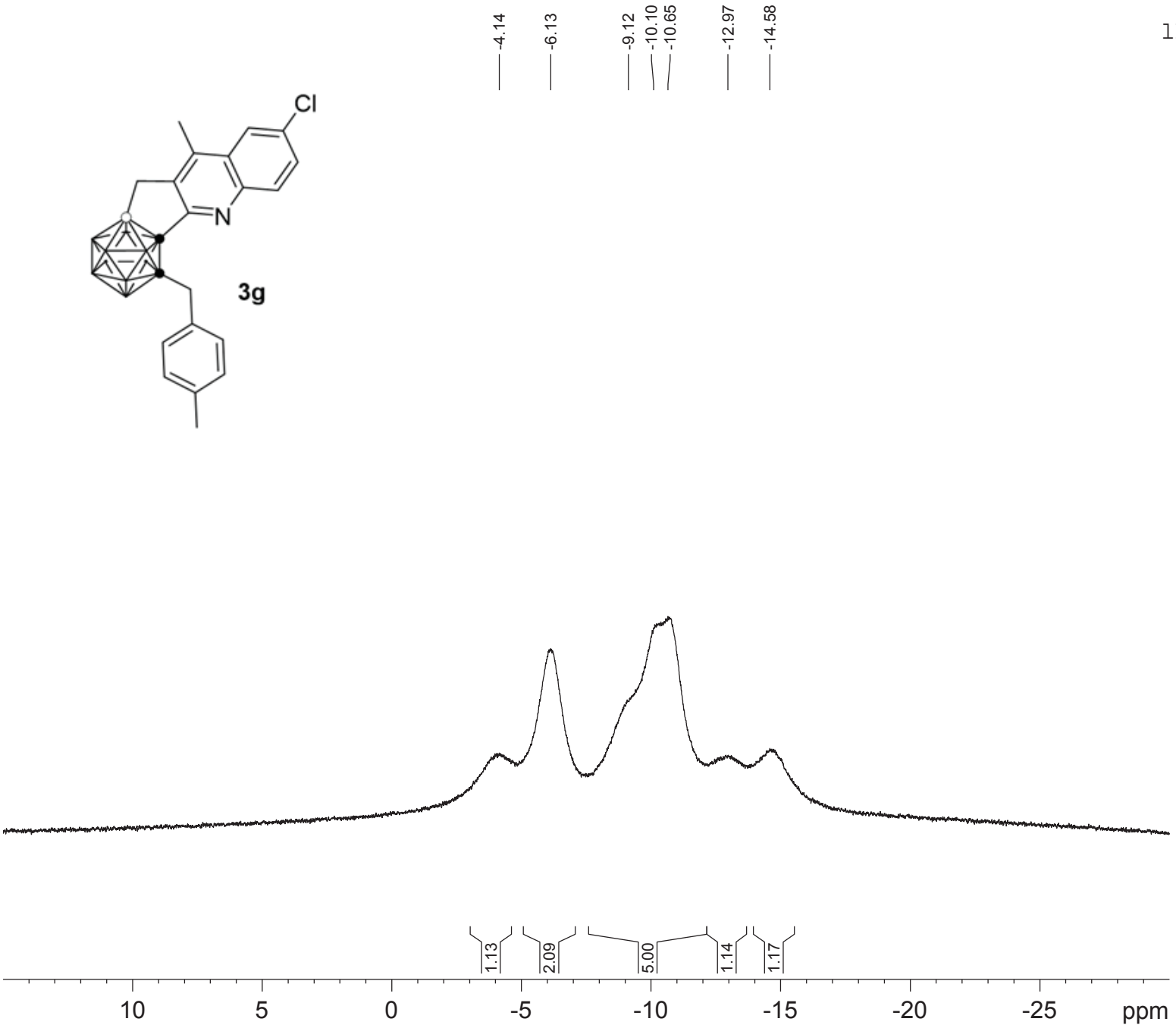
F2 - Acquisition Parameters
Date_ 20170809
Time 16.49 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



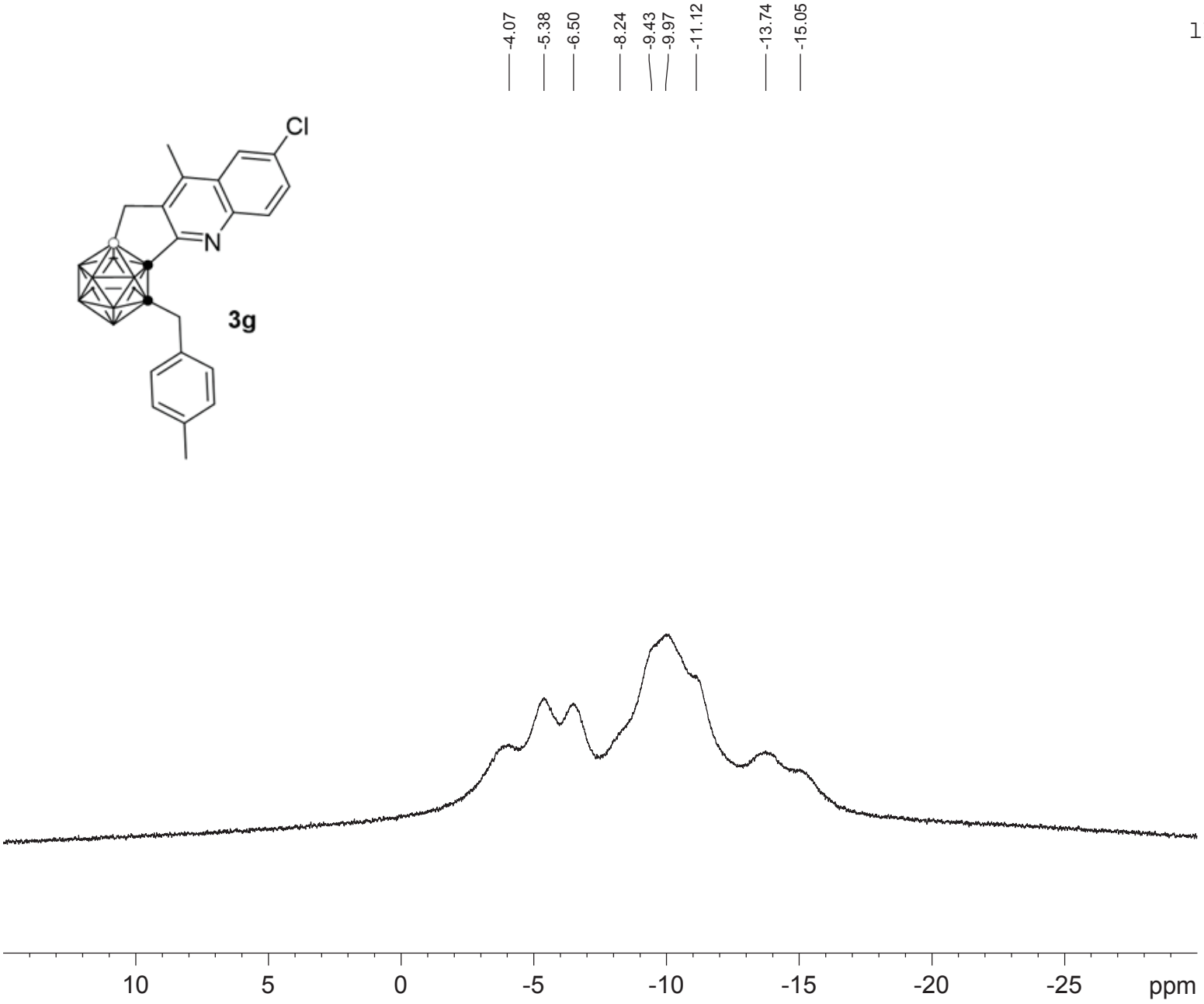
lhr-c-0740-cascdcl3

```
Current Data Parameters
NAME      lhr-C-0740-cascdcl3-bnch1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170804
Time              17.45 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1486
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW                12.267 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1        55.34000015 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W
PLW13        0.13796000 W

F2 - Processing parameters
SI                32768
SF          100.6379004 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



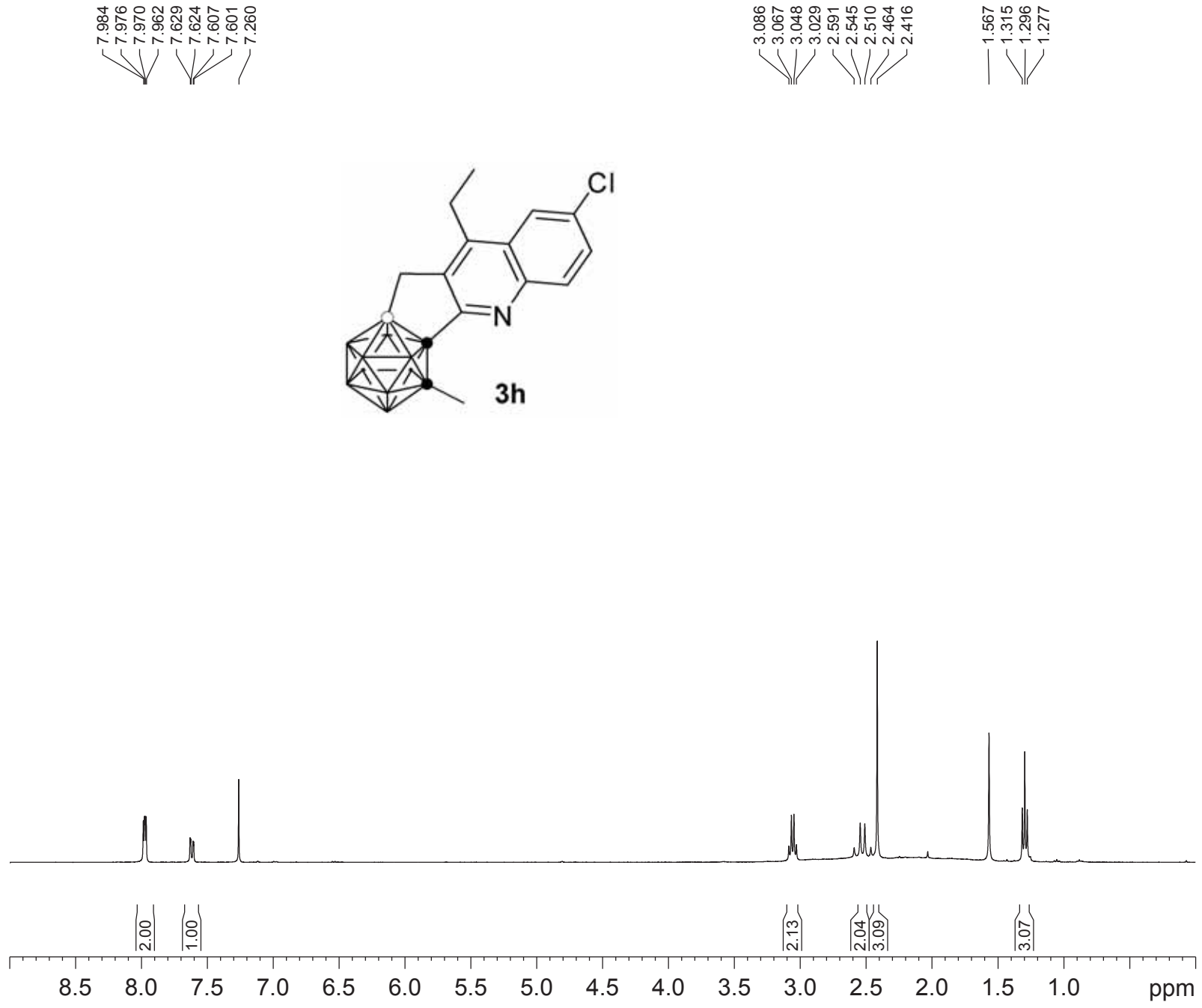
lhr-B-0740-cascdcl3-bnch3

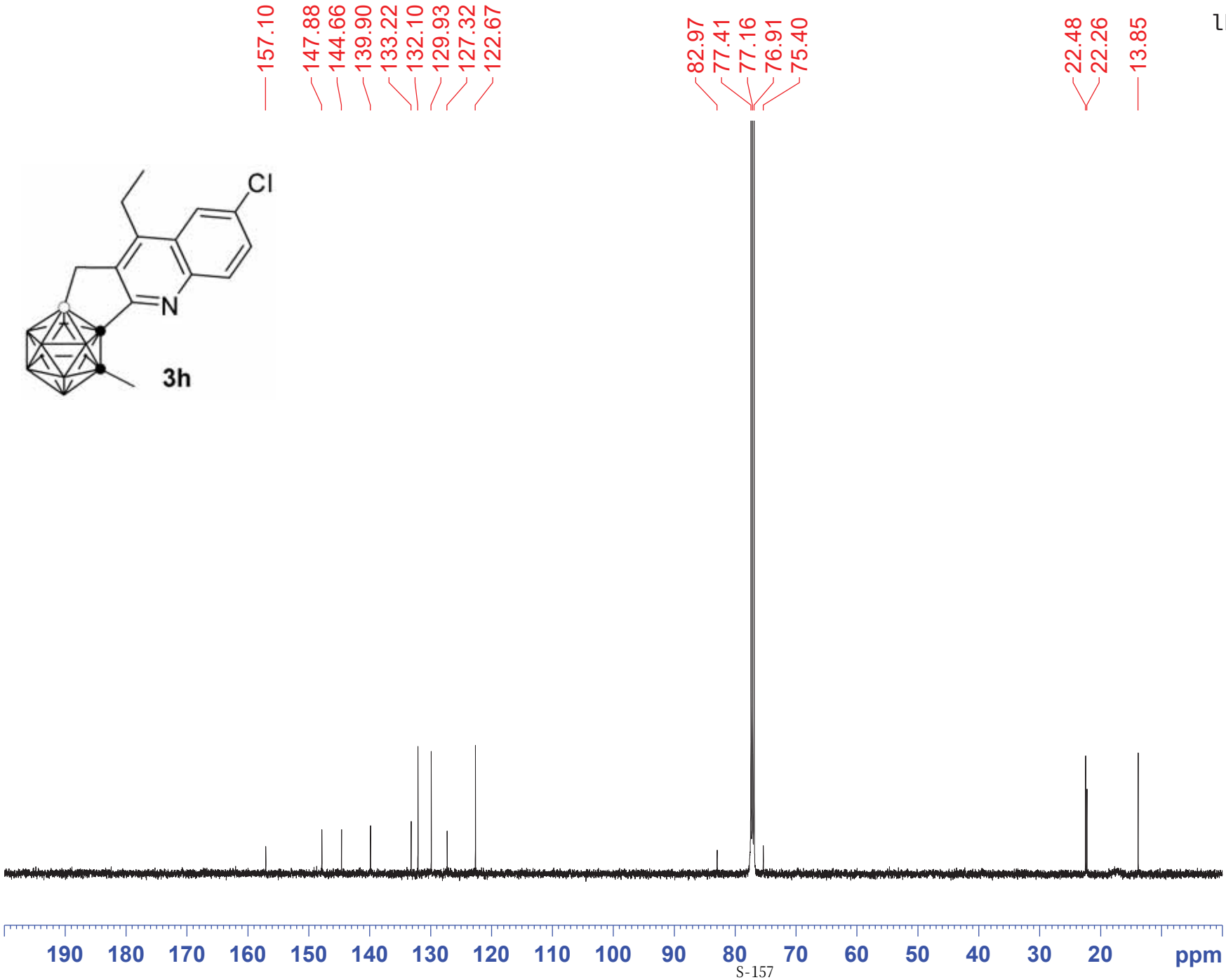
```
Current Data Parameters
NAME      lhr-B-0740-cascdcl3-bnch3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170804
Time              17.33 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CD3CN
NS                    32
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                 32768
SF          128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



lhr-B-0740-cascdcl3-bnch3(C)

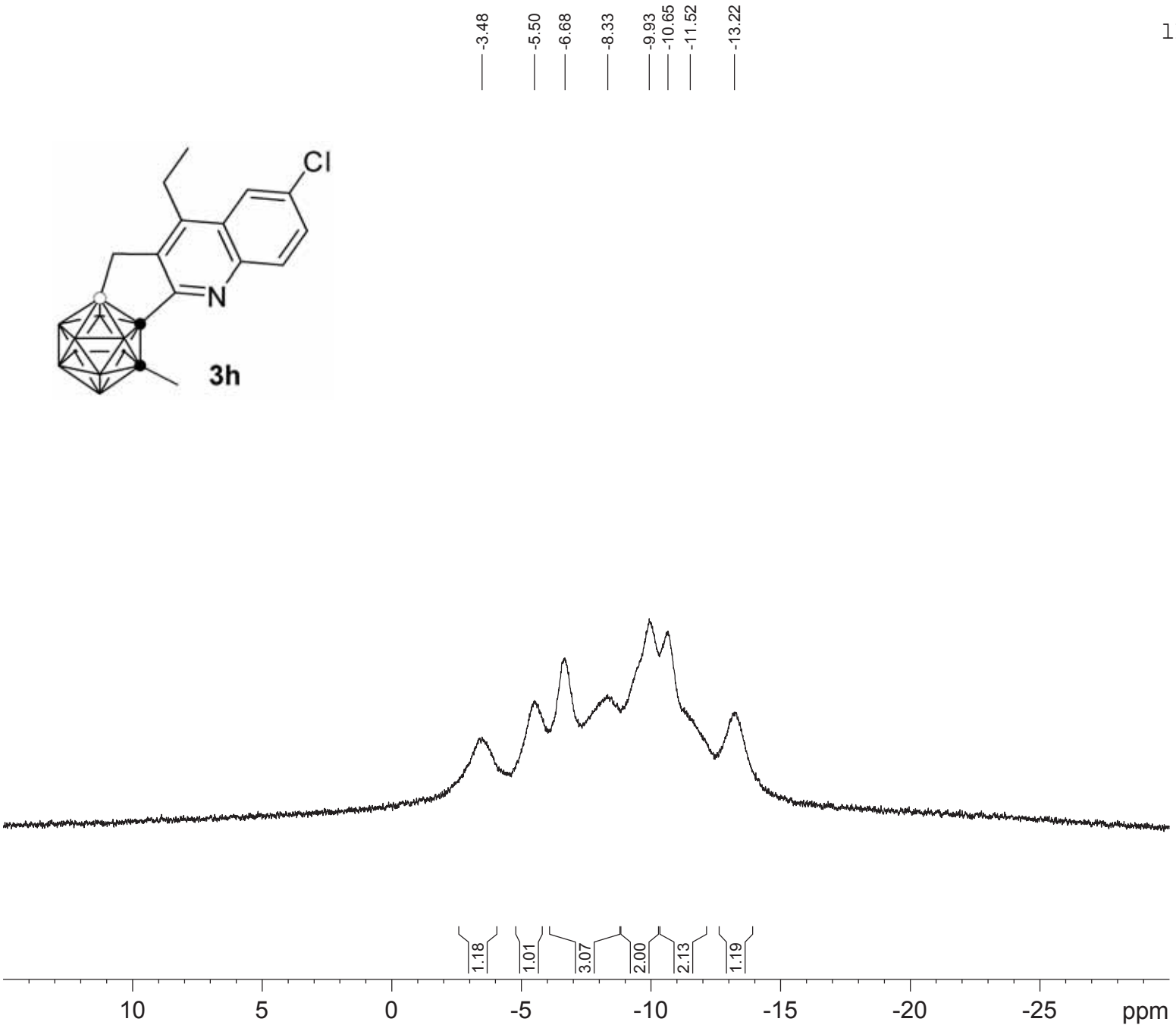
```
Current Data Parameters
NAME      lhr-B-0740-cascdcl3-bnch3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170804
Time              17.37 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CD3CN
NS                   44
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 322
DW                20.800 usec
DE                 6.50 usec
TE                294.7 K
D1            2.00000000 sec
TD0                   1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                32768
SF           128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


7.984
7.976
7.970
7.962
7.629
7.624
7.607
7.601
7.260
3.086
3.067
3.048
3.029
2.591
2.545
2.510
2.464
2.416
1.567
1.315
1.296
1.277
lhr-H-0710-pclet-cas
Cl
N
3h
Current Data Parameters
NAME lhr-H-0710-pclet-cascdcl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170702
Time 19.53 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.00
1.00
2.13
2.04
3.09
3.07
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm



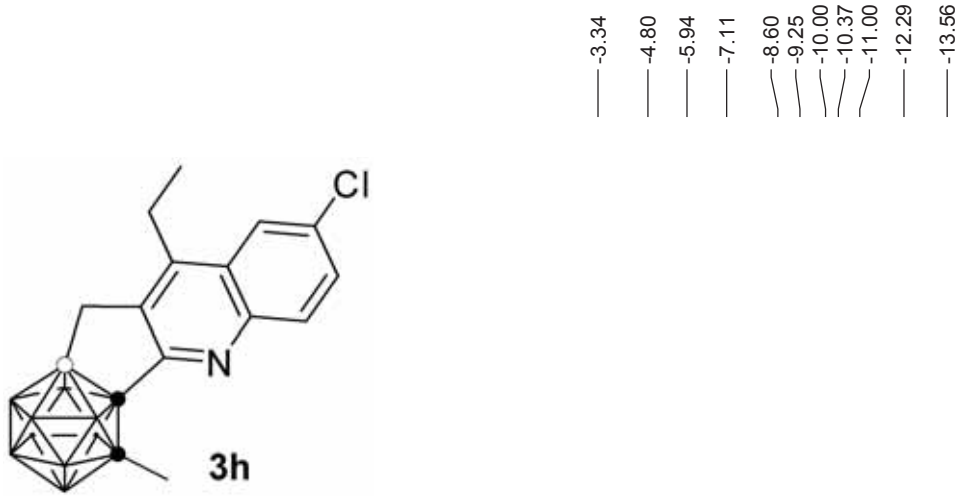
lhr-C-0710

```
Current Data Parameters
NAME      lhr-C-0710cas
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170703
Time              20.26 h
INSTRUM           spect
PROBHD   Z119470_0283 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1005
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               297.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                10.00 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.39063001 W
PLW13        0.19648001 W

F2 - Processing parameters
SI                32768
SF          125.7577709 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



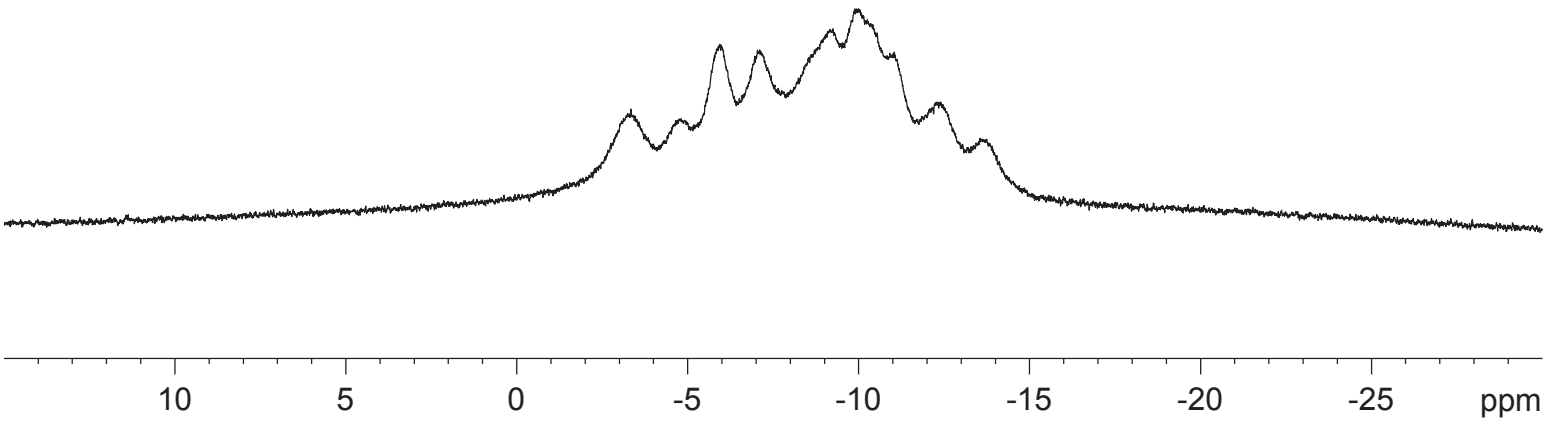
lhr-B-0710-pclet-cascdcl3

```
Current Data Parameters
NAME      lhr-B-0710-pclet-cascdcl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170702
Time                19.40 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT               THF
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                    287
DW                 20.800 usec
DE                  6.50 usec
TE                 295.8 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W
SFO2          400.2316009 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2          13.56000042 W
PLW12          0.27428001 W

F2 - Processing parameters
SI                    32768
SF            128.4097615 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```



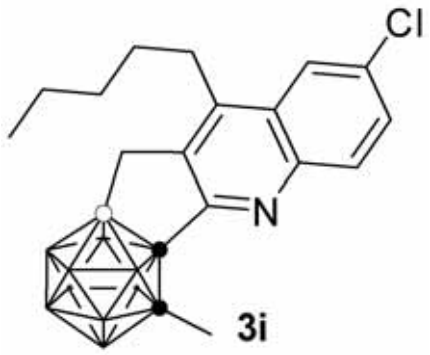
lhr-B-0710-pclet-cascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0710-pclet-cascdcl3(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170702
Time              19.42 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT             THF
NS                   28
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                  287
DW               20.800 usec
DE                6.50 usec
TE                295.4 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

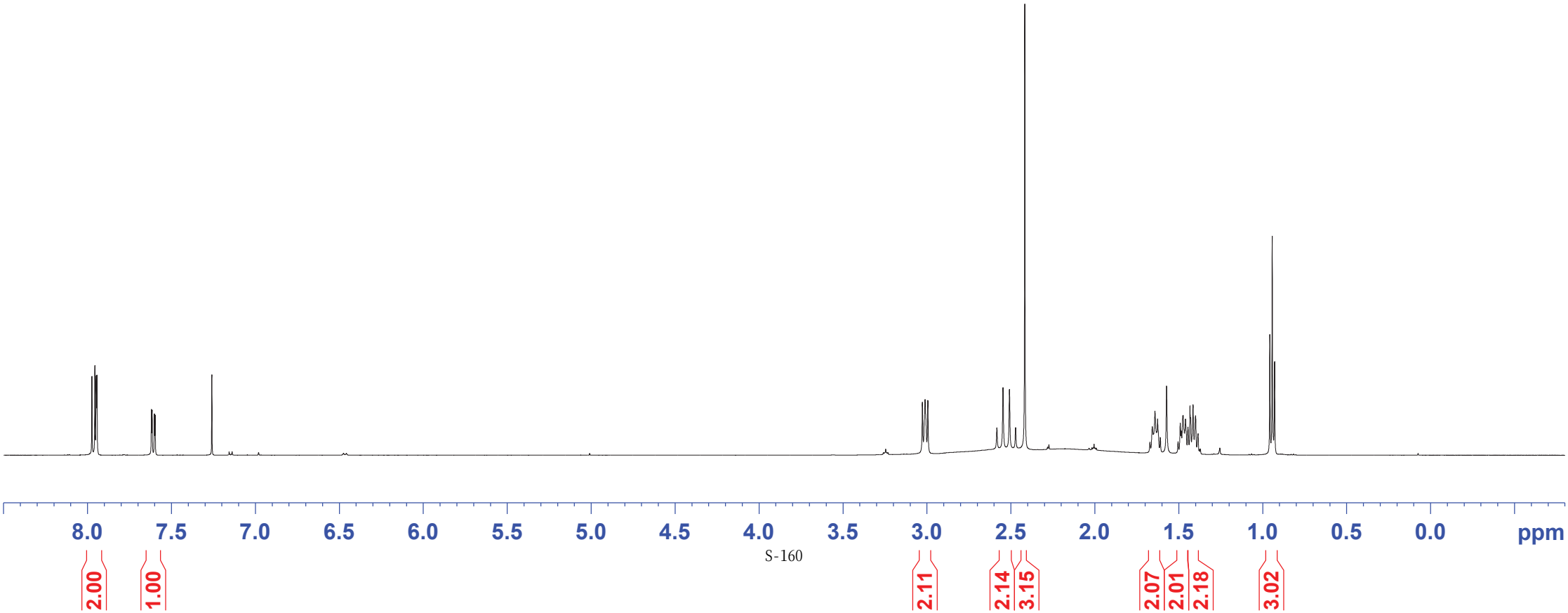


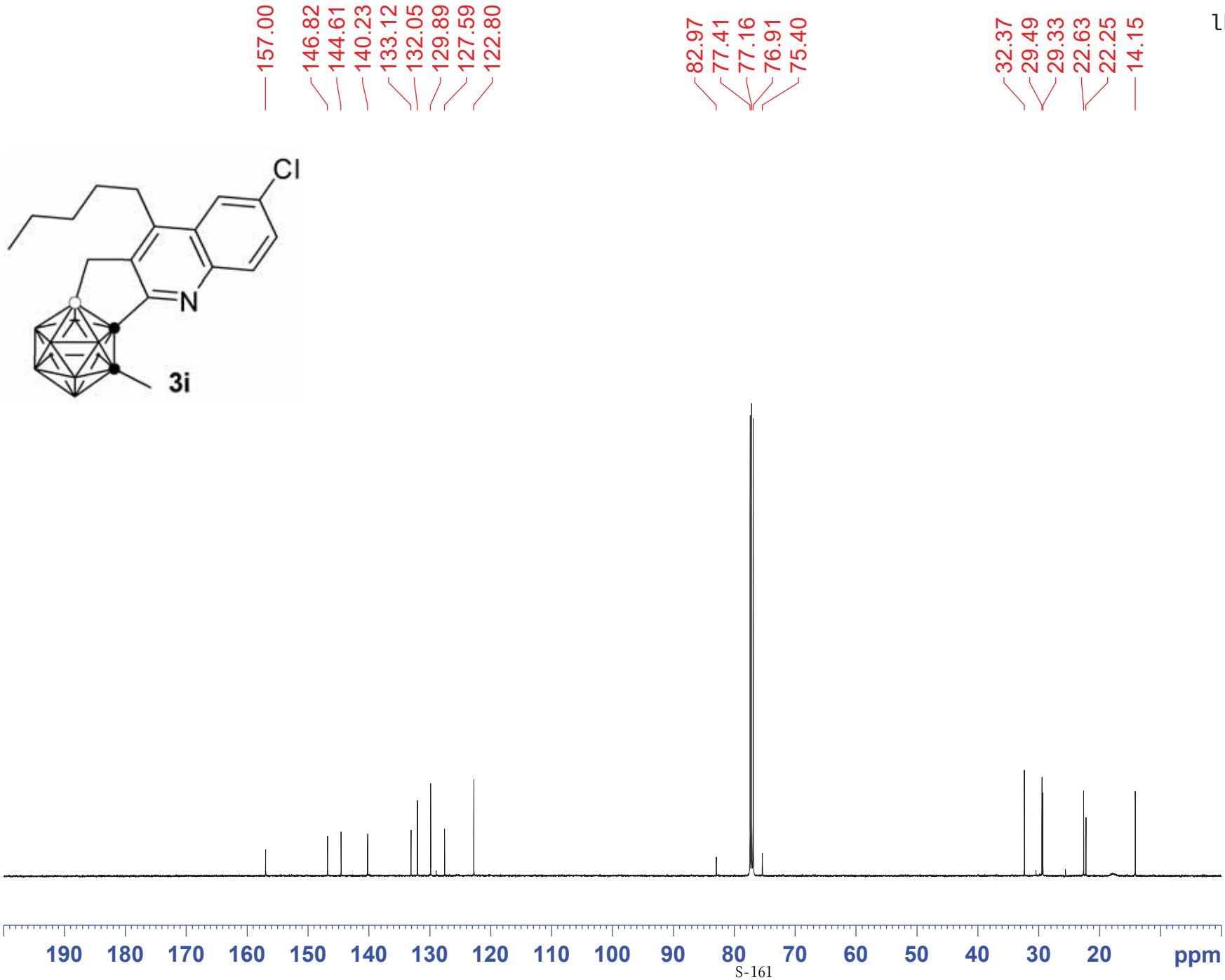
7.974 7.957 7.949 7.944 7.620 7.615 7.602 7.598 7.260

3.027 3.011 2.995 2.584 2.547 2.509 2.472 2.418 1.672 1.658 1.642 1.632 1.626 1.610 1.573 1.505 1.491 1.485 1.474 1.460 1.446 1.434 1.430 1.415 1.400 1.385 0.958 0.944 0.929



3i

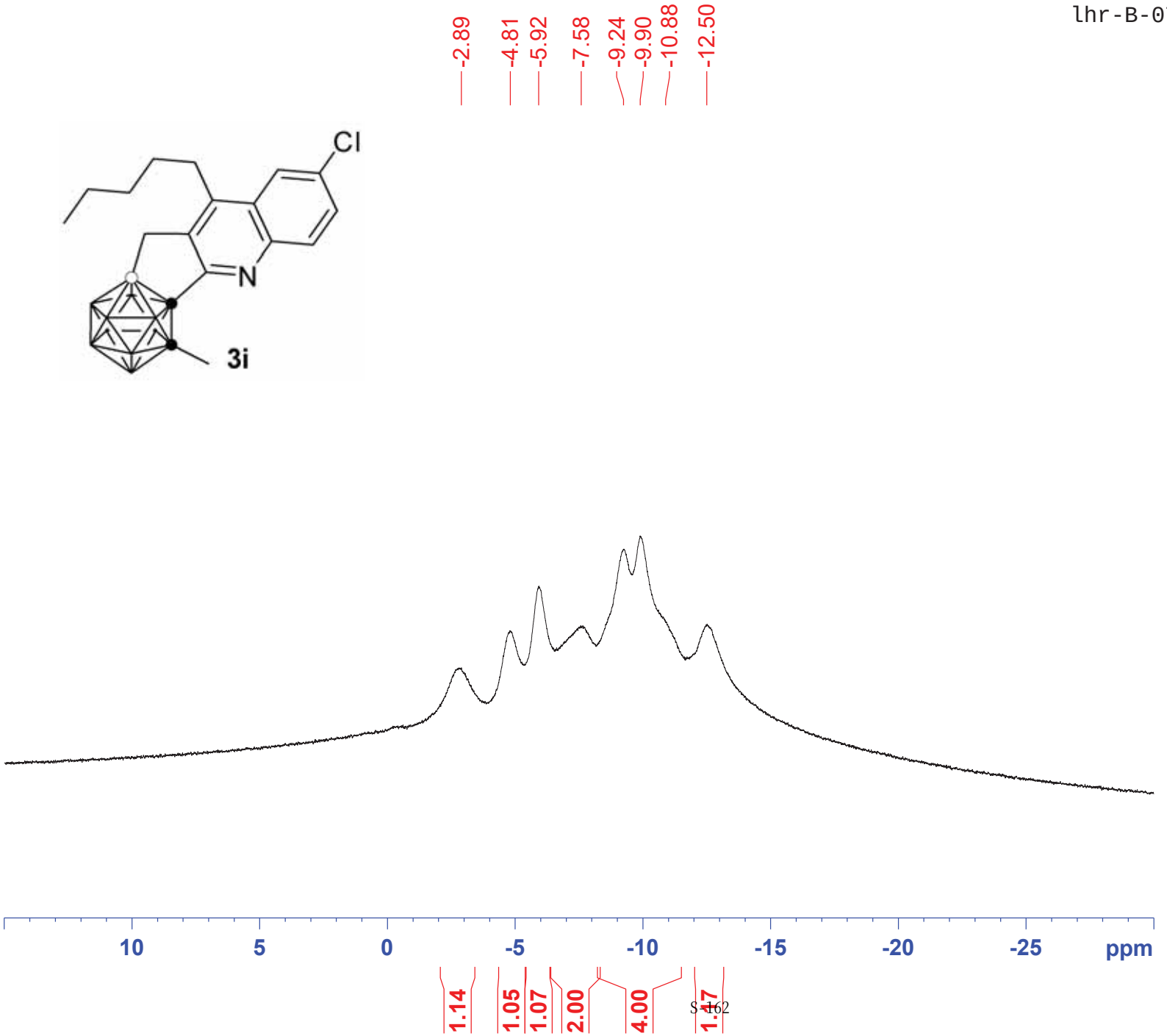




lhr-C-0754

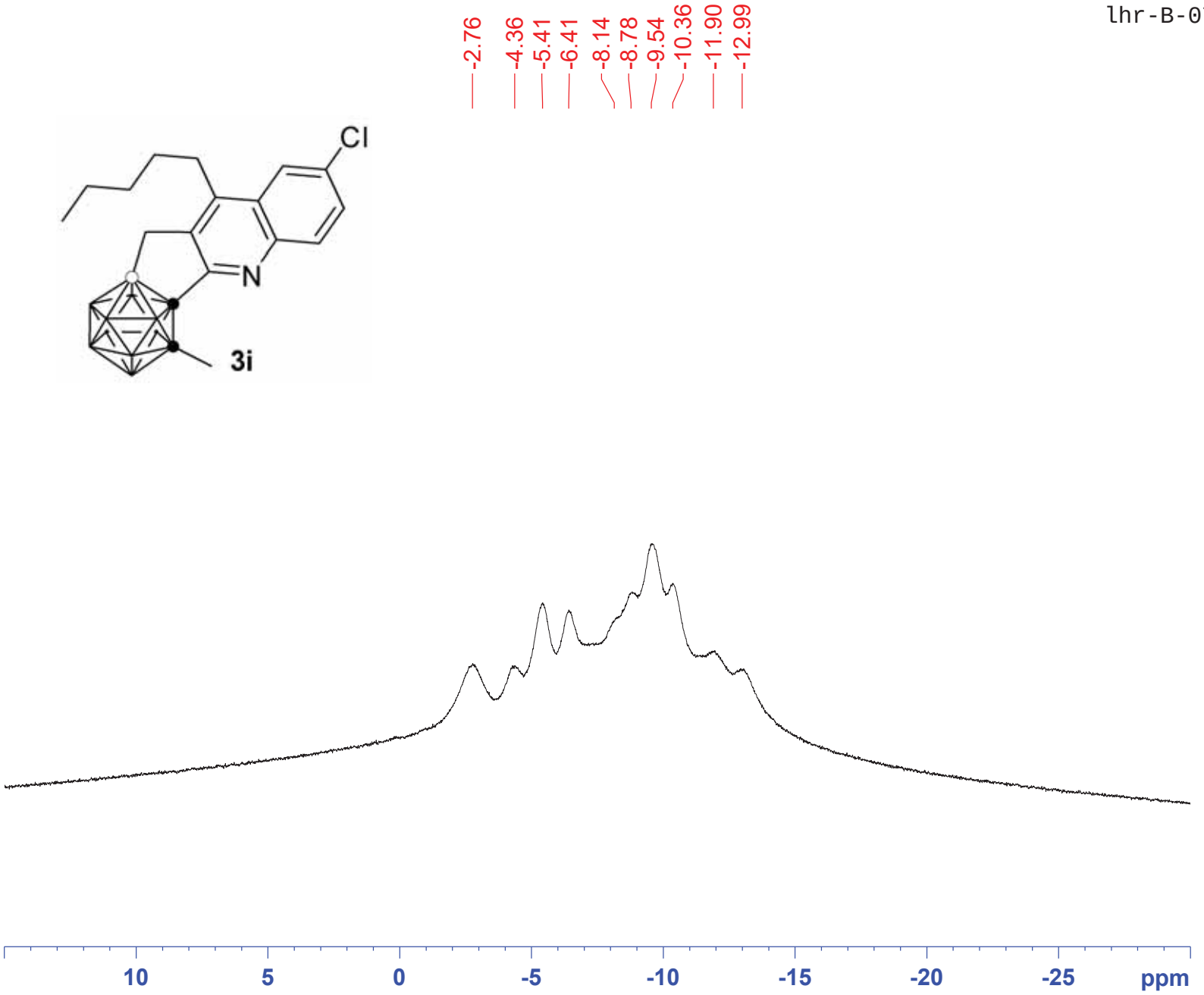
```
Current Data Parameters
NAME          lhr-C-0754
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170908
Time               9.56 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577721 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-0754-cascdcl3

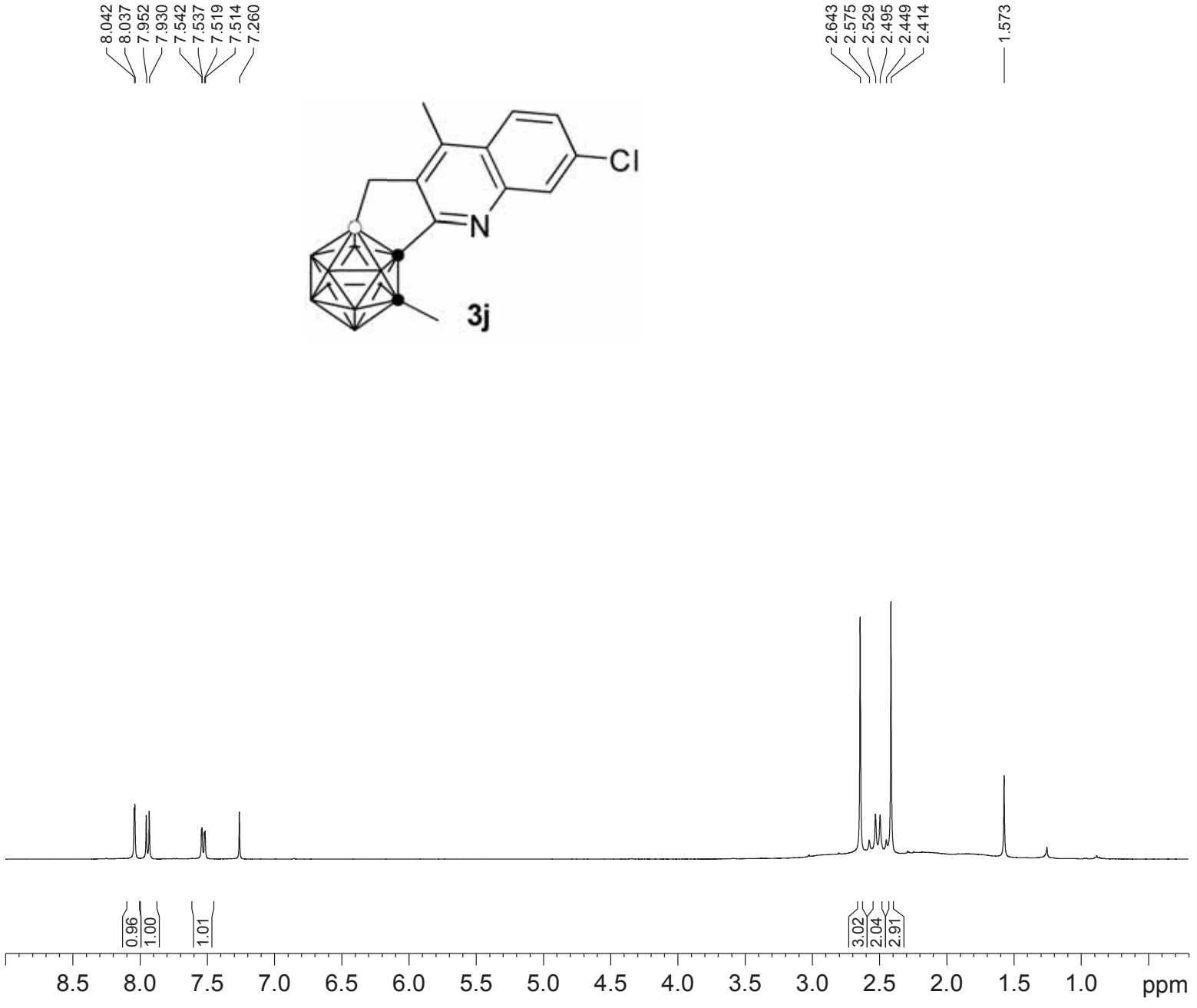



```
Current Data Parameters
NAME      lhr-B-0754-cascdcl3
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_            20170828
Time                18.58 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     24
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ              1.3762560 sec
RG                 163.99
DW                 21.000 usec
DE                 18.00 usec
TE                 298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1         160.4599621 MHz
NUC1                11B
P1                 10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                  32768
SF           160.4615719 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-0754-cascdcl3(C)




```
Current Data Parameters
NAME      lhr-B-0754-cascdcl3(C)
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20170828
Time                  19.00 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        24
DS                         4
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                   186.15
DW                   20.800 usec
DE                   18.00 usec
TE                   298.0 K
D1             1.00000000 sec
TD0                        1
SFO1            160.4615792 MHz
NUC1                    11B
P1                   10.00 usec
PLW1           50.00000000 W

F2 - Processing parameters
SI                     16384
SF              160.4615792 MHz
WDW                       EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

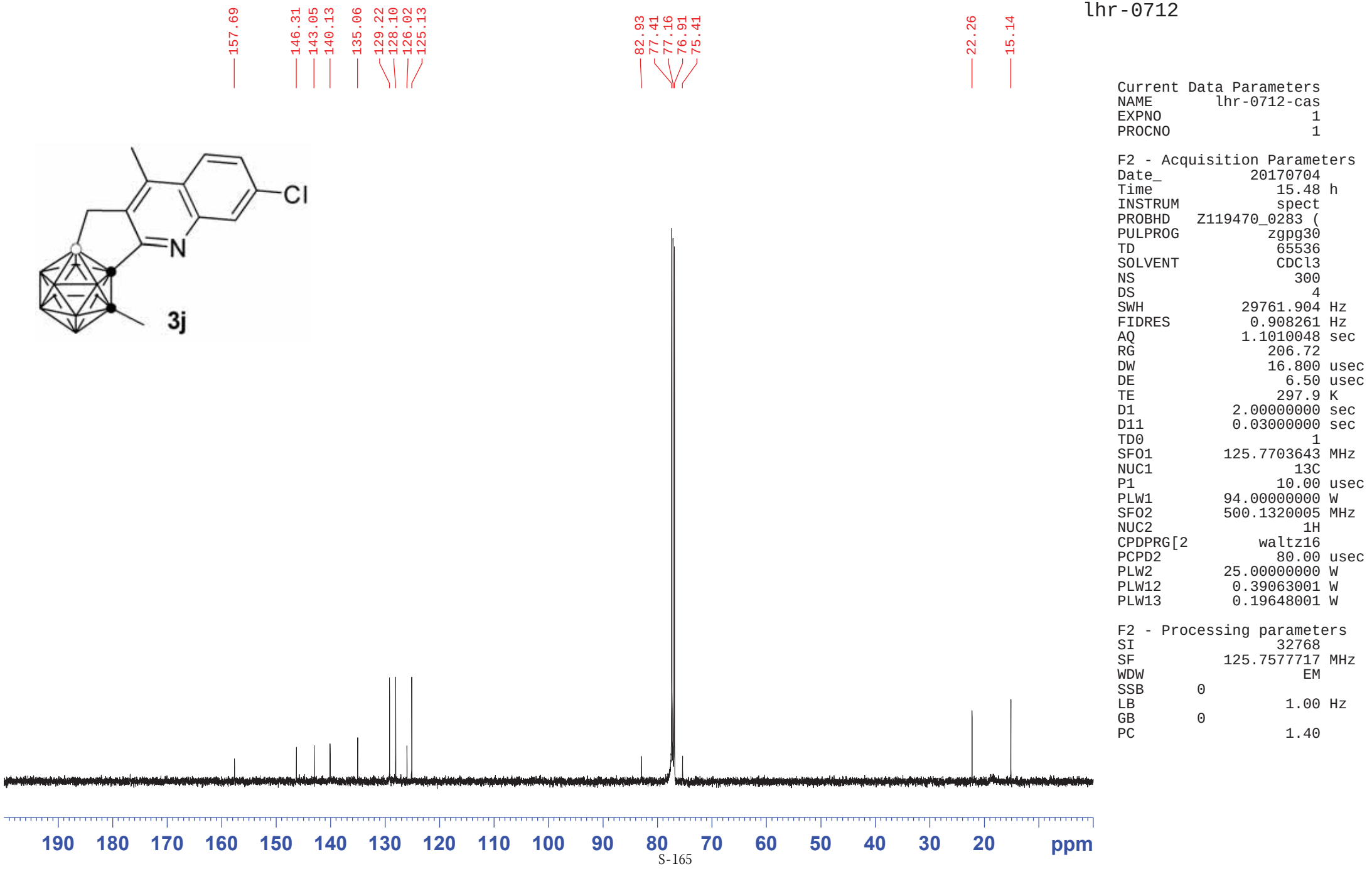


lhr-H-0712-3cl-casc

Current Data Parameters
NAME lhr-H-0712-3cl-casc
EXPNO 1
PROCNO 1

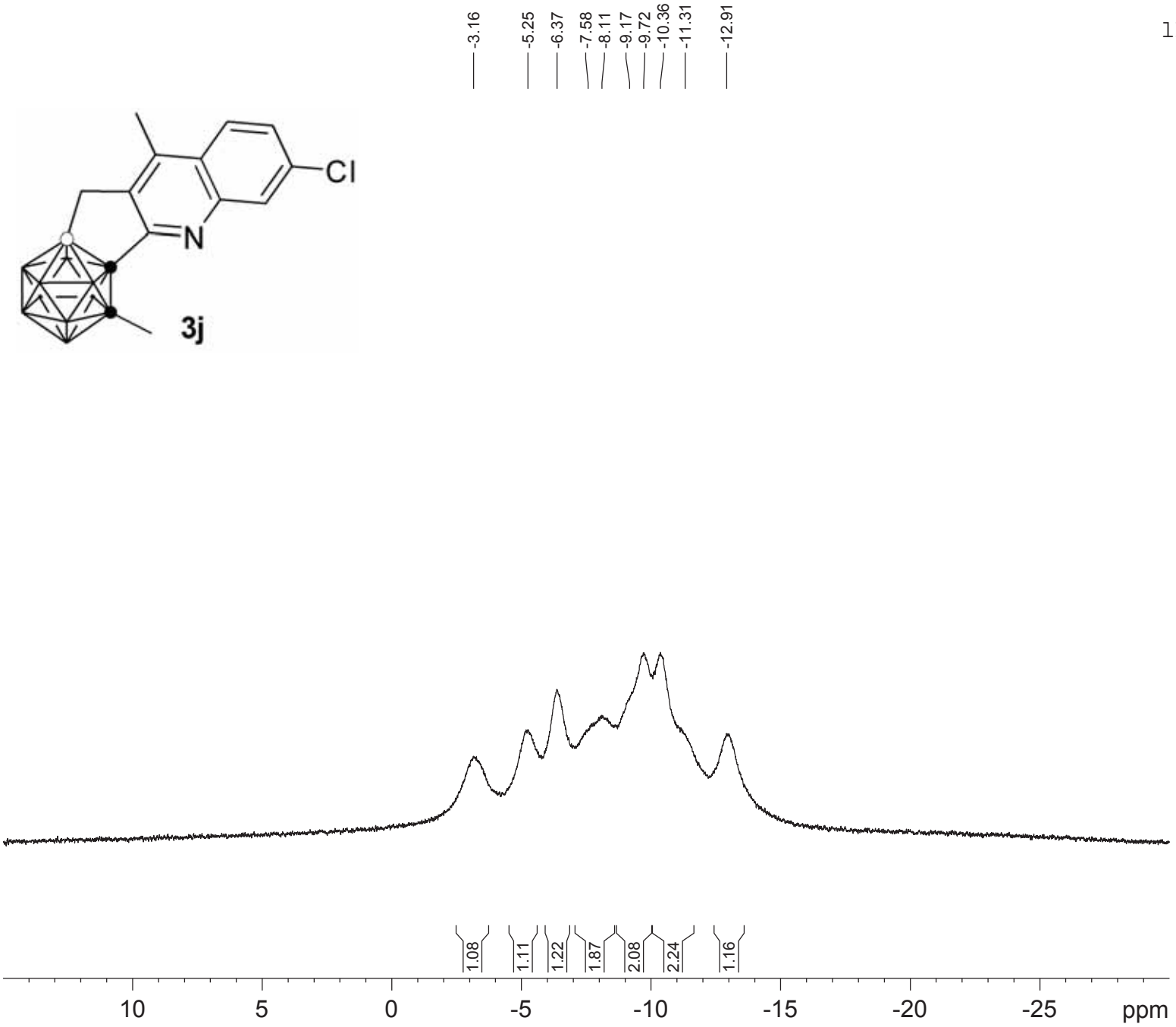
F2 - Acquisition Parameters
Date_ 20170704
Time 10.22 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300111 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



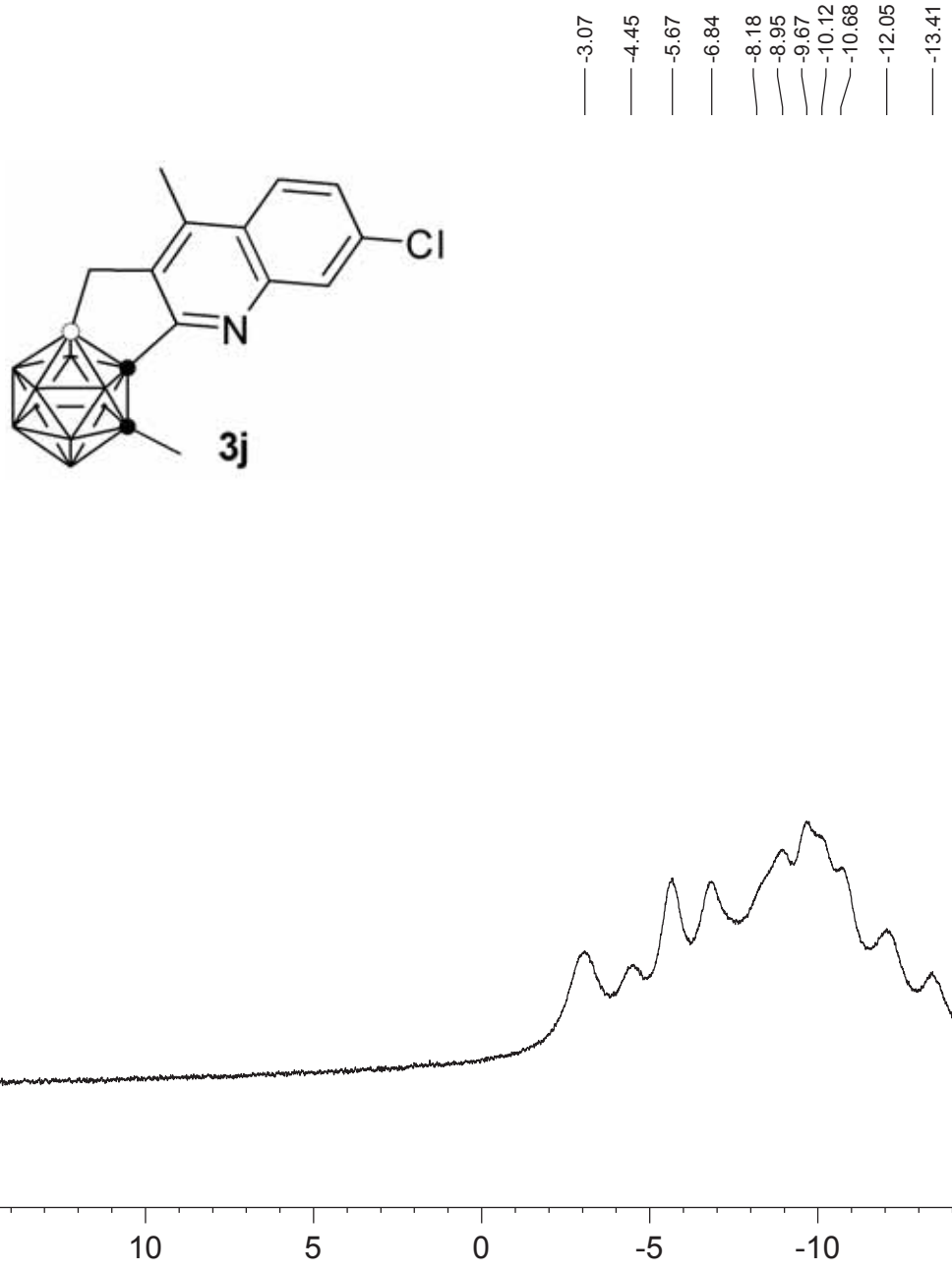
lhr-0712

```
Current Data Parameters
NAME        lhr-0712-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170704
Time              15.48 h
INSTRUM             spect
PROBHD    Z119470_0283 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                  300
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE                6.50 usec
TE               297.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        94.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        25.00000000 W
PLW12        0.39063001 W
PLW13        0.19648001 W

F2 - Processing parameters
SI                32768
SF          125.7577717 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



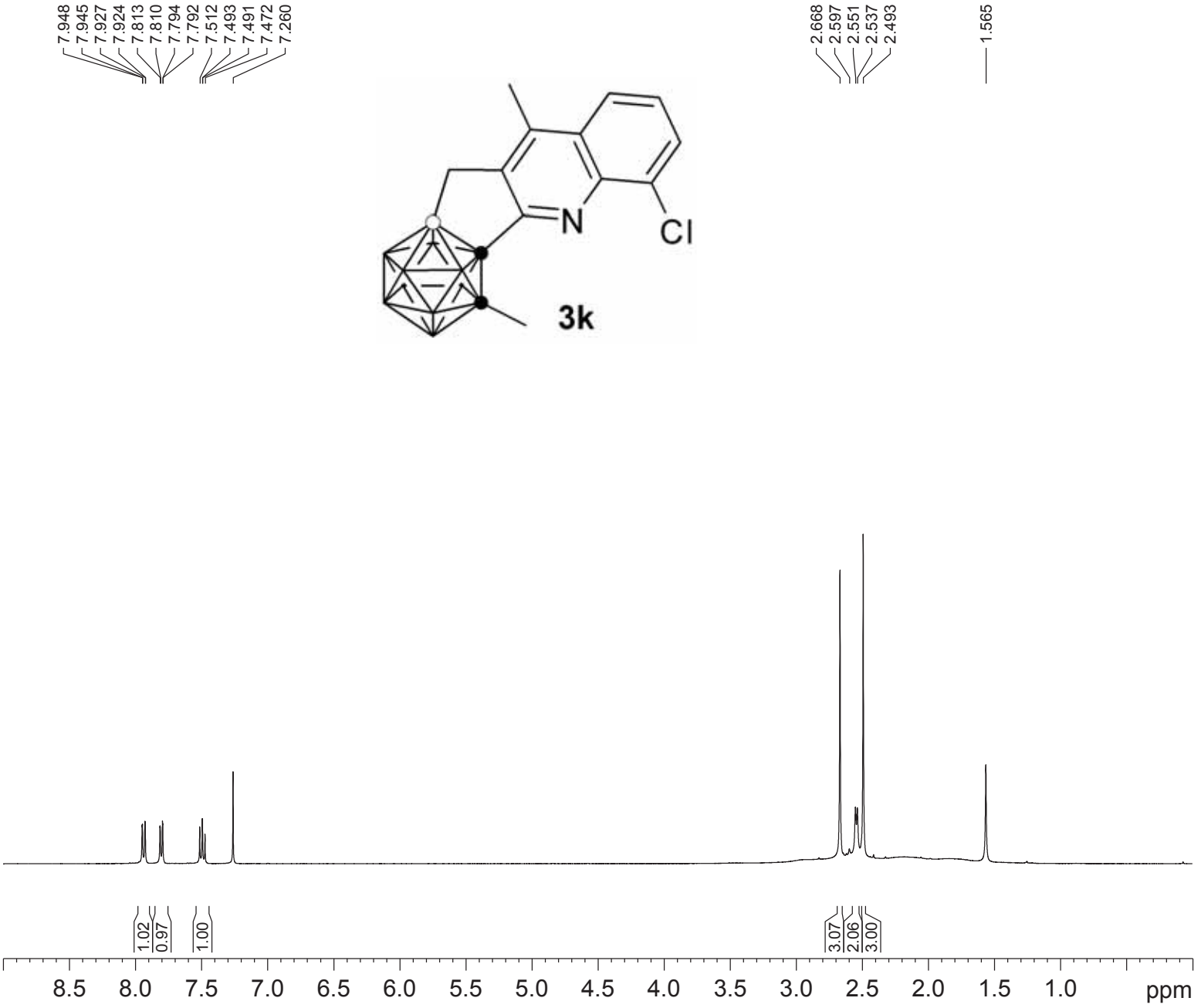
lhr-B-0712-3cl-cascdcl3

```
Current Data Parameters
NAME      lhr-B-0712-3cl-cascdcl3
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_               20170704
Time                   10.04 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       287
DW                    20.800 usec
DE                     6.50 usec
TE                    297.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                       32768
SF               128.4097615 MHz
WDW                         EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



lhr-B-0712-3cl-cascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0712-3cl-cascdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170704
Time              10.07 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    287
DW                20.800 usec
DE                 6.50 usec
TE                296.6 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

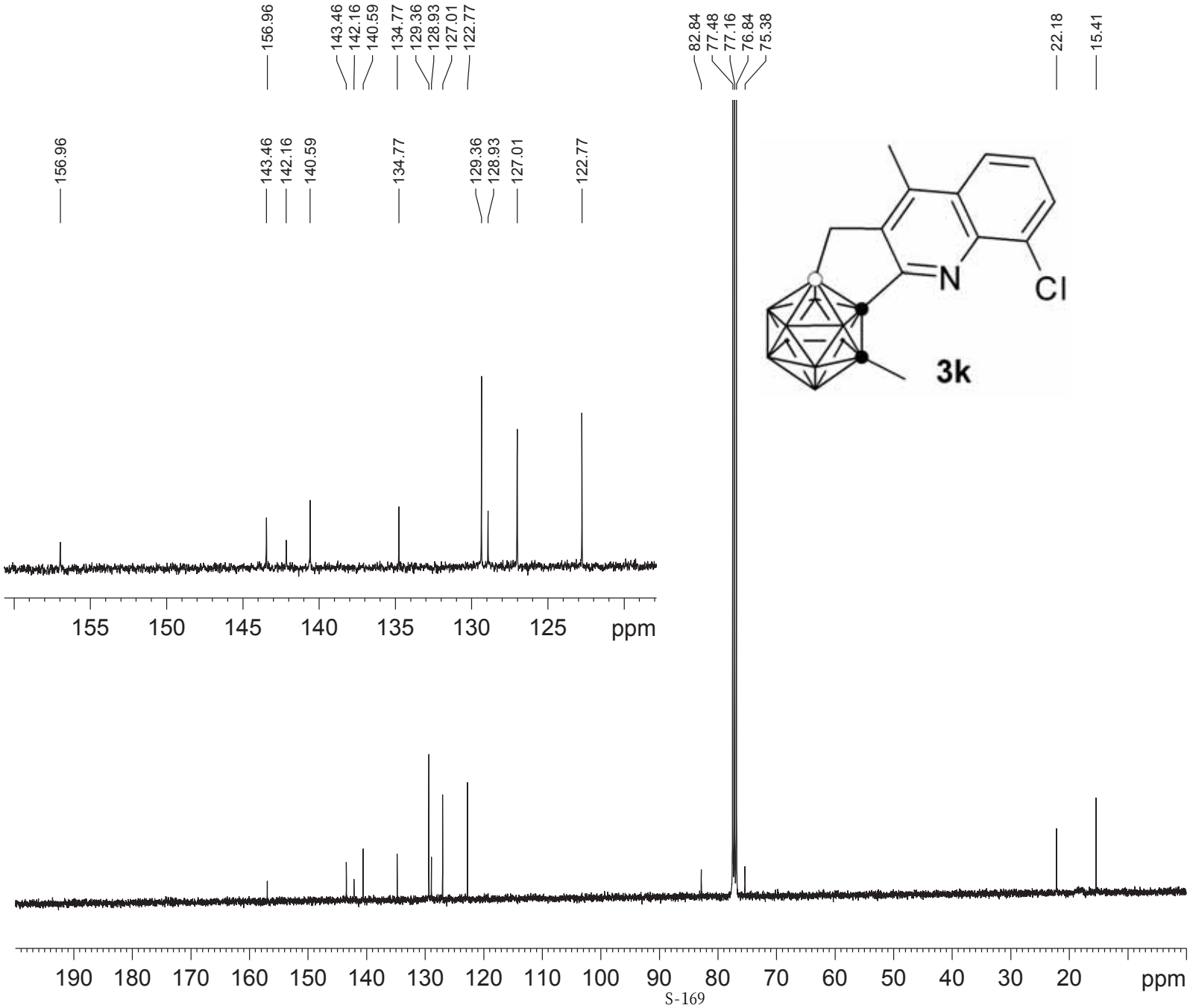


lhr-H-0713-2cl-ccca

Current Data Parameters
NAME lhr-H-0713-2cl-cccasc
EXPNO 1
PROCNO 1

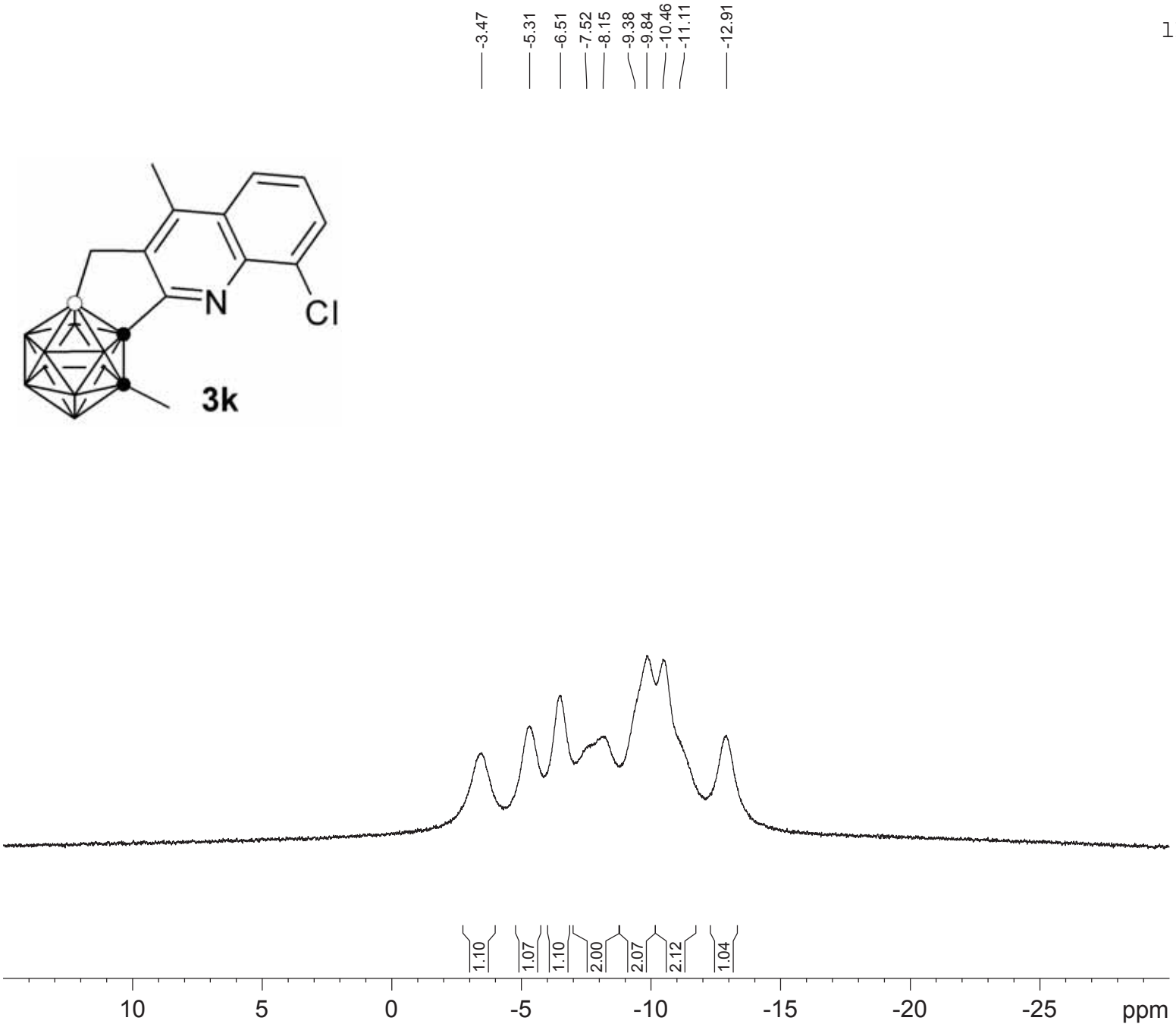
F2 - Acquisition Parameters
Date_ 20170713
Time 15.09 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300107 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



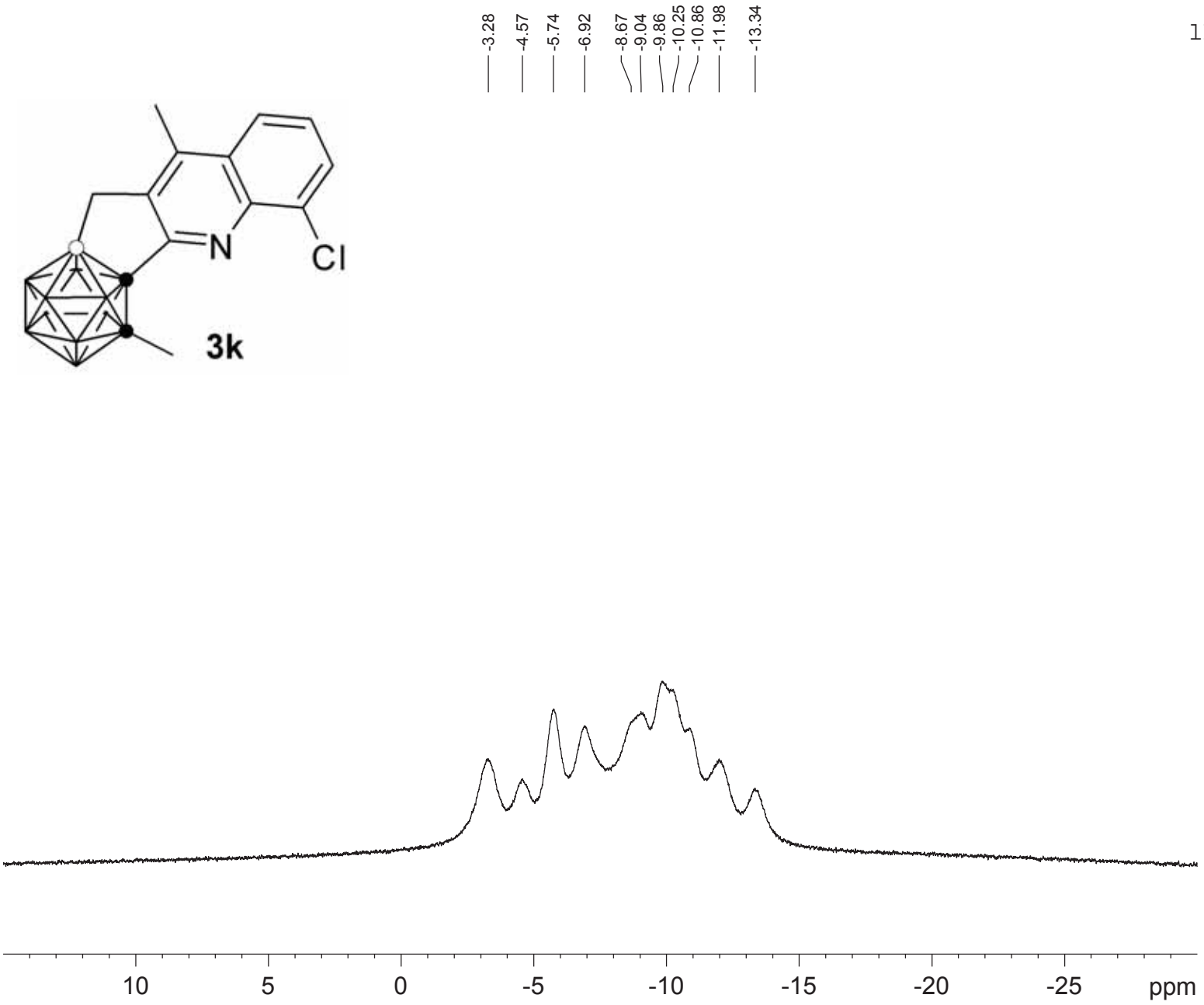
lhr-C-0713-2cl-ccc

```
Current Data Parameters
NAME      lhr-C-0713-2cl-cccascdcl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170713
Time              15.13 h
INSTRUM            spect
PROBHD    Z108618_0257 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1300
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW                12.267 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        100.6479773 MHz
NUC1               13C
P1                 9.50 usec
PLW1        55.34000015 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W
PLW13        0.13796000 W

F2 - Processing parameters
SI                32768
SF          100.6379003 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



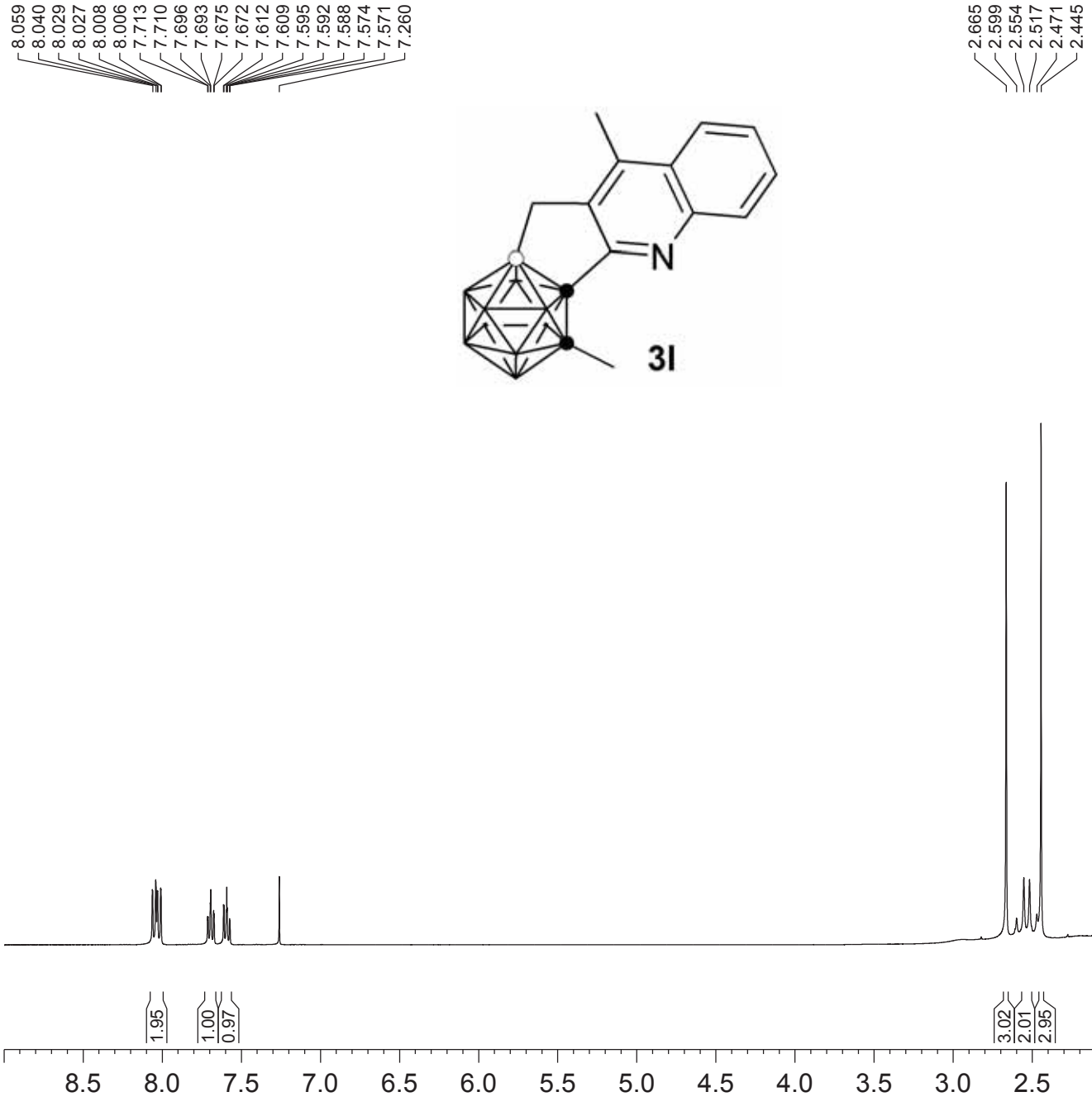
lhr-B-0713-2cl-cccascdcl3

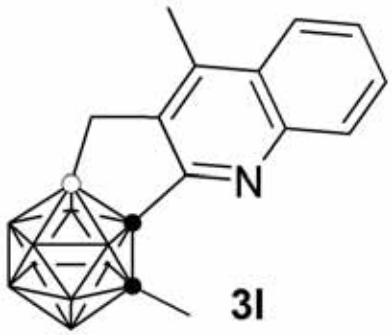
```
Current Data Parameters
NAME      lhr-B-0713-2cl-cccascdcl3
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170713
Time                16.26 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                    406
DW                 20.800 usec
DE                  6.50 usec
TE                 295.7 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                  7.50 usec
PLW1           55.09999847 W
SFO2          400.2316009 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           13.56000042 W
PLW12           0.27428001 W

F2 - Processing parameters
SI                  32768
SF            128.4097615 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



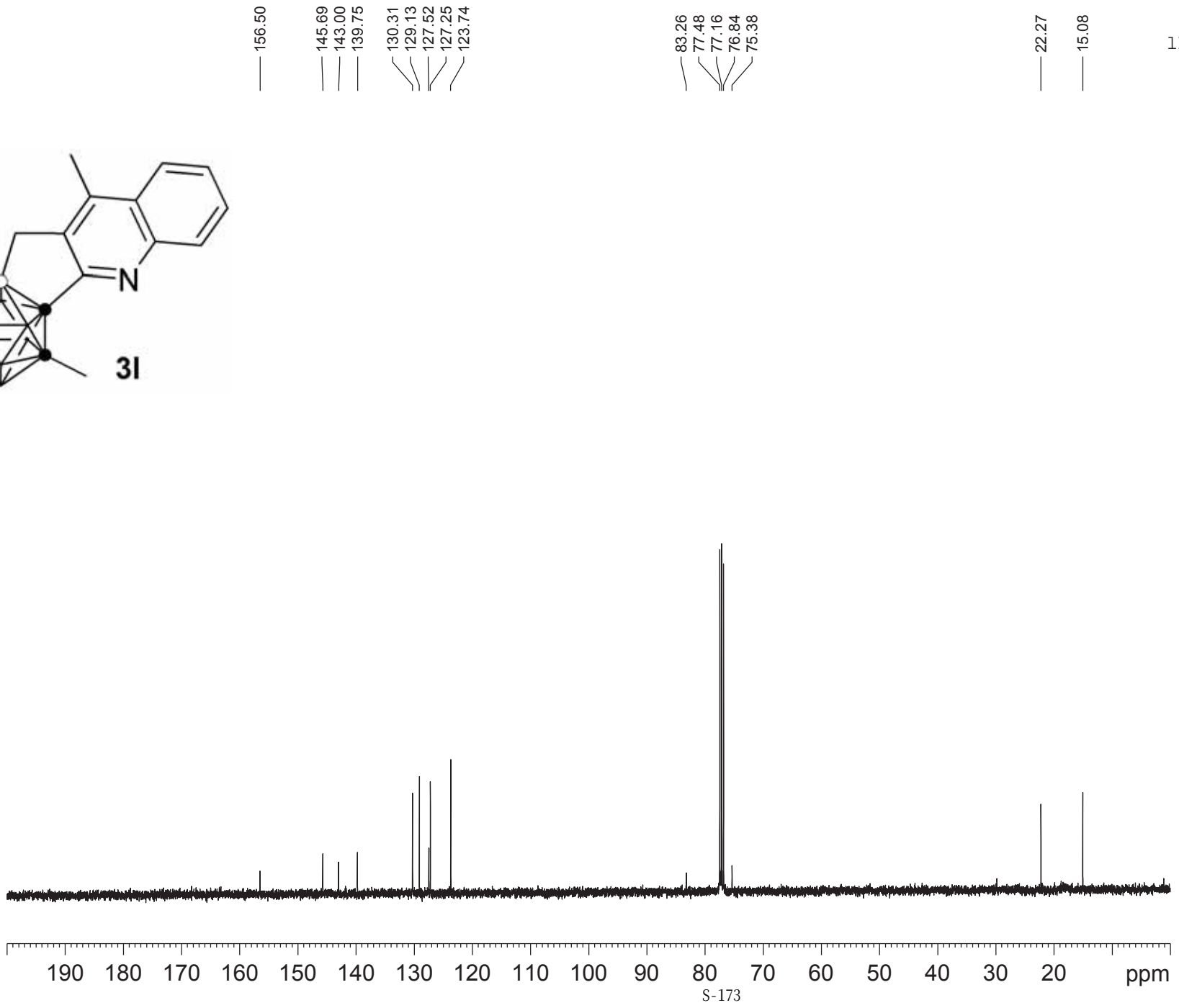
lhr-B-0713-2cl-cccascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0713-2cl-cccascdcl3(C)
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170713
Time              16.29 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD               65536
SOLVENT          CDCl3
NS                  24
DS                   2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 362
DW                20.800 usec
DE                 6.50 usec
TE                295.4 K
D1            2.00000000 sec
TD0                  1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


8.059
8.040
8.029
8.027
8.008
8.006
7.713
7.710
7.696
7.693
7.675
7.672
7.612
7.609
7.595
7.592
7.588
7.574
7.571
7.260
2.665
2.599
2.554
2.517
2.471
2.445
lhr-H-cas-0367-CDCl3
N
3l
Current Data Parameters
NAME lhr-H-cas-0367-CDCl3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160509
Time 9.56 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 20
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.95
1.00
0.97
3.02
2.01
2.95
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm

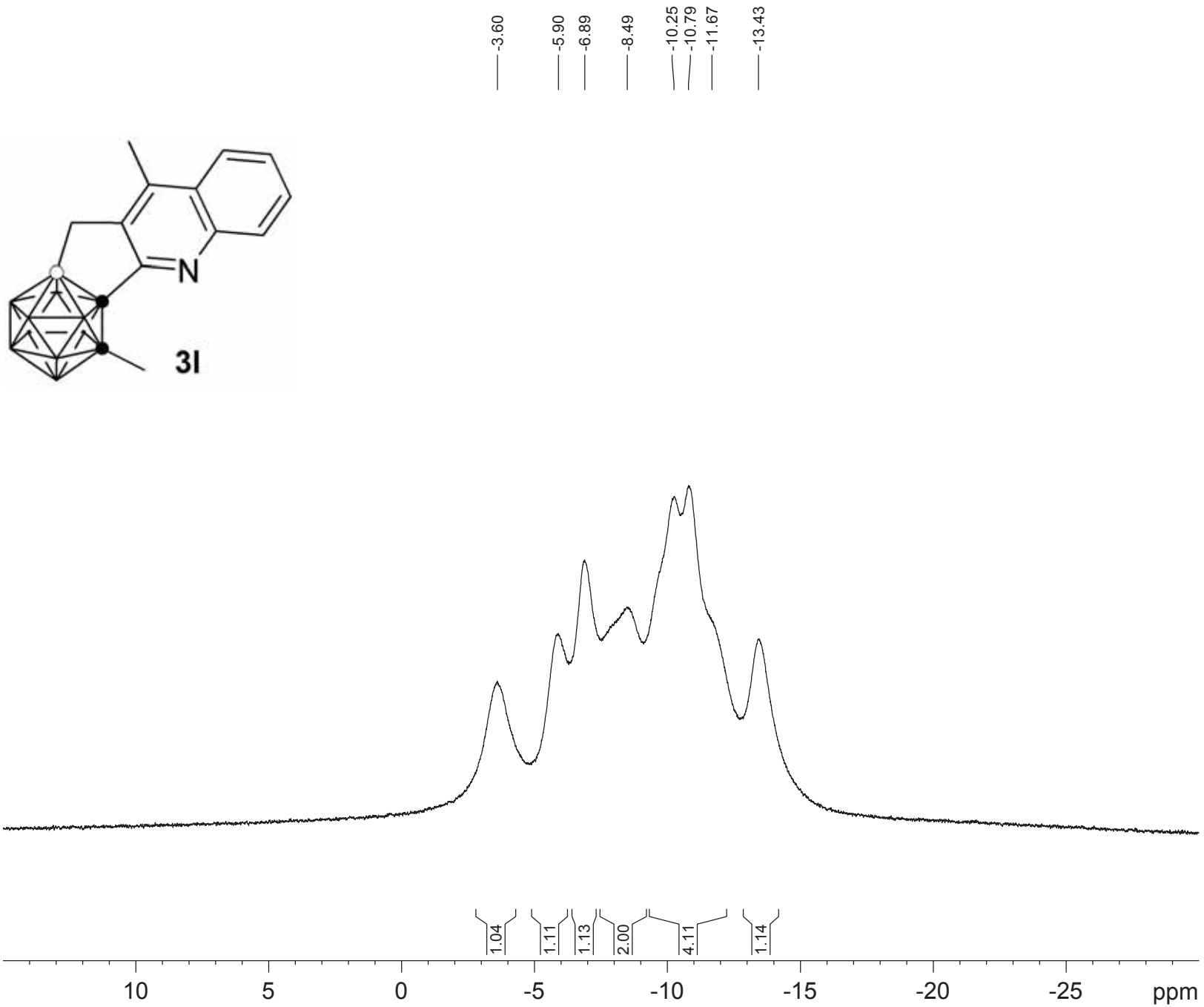


3l



lhr-C-cas-0367-CDCl3

```
Current Data Parameters
NAME      lhr-C-cas-0367-CDCl3
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20160509
Time                 10.02 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG            zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     100
DS                       4
SWH              29761.904 Hz
FIDRES            0.454131 Hz
AQ                1.1010048 sec
RG                    90.5
DW                  16.800 usec
DE                   6.50 usec
TE                  295.3 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1           100.6479773 MHz
NUC1                   13C
P1                    9.50 usec
PLW1           55.34000015 W
SFO2           400.2316009 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           13.56000042 W
PLW12           0.27428001 W
PLW13           0.13796000 W

F2 - Processing parameters
SI                   32768
SF             100.6379019 MHz
WDW                    EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

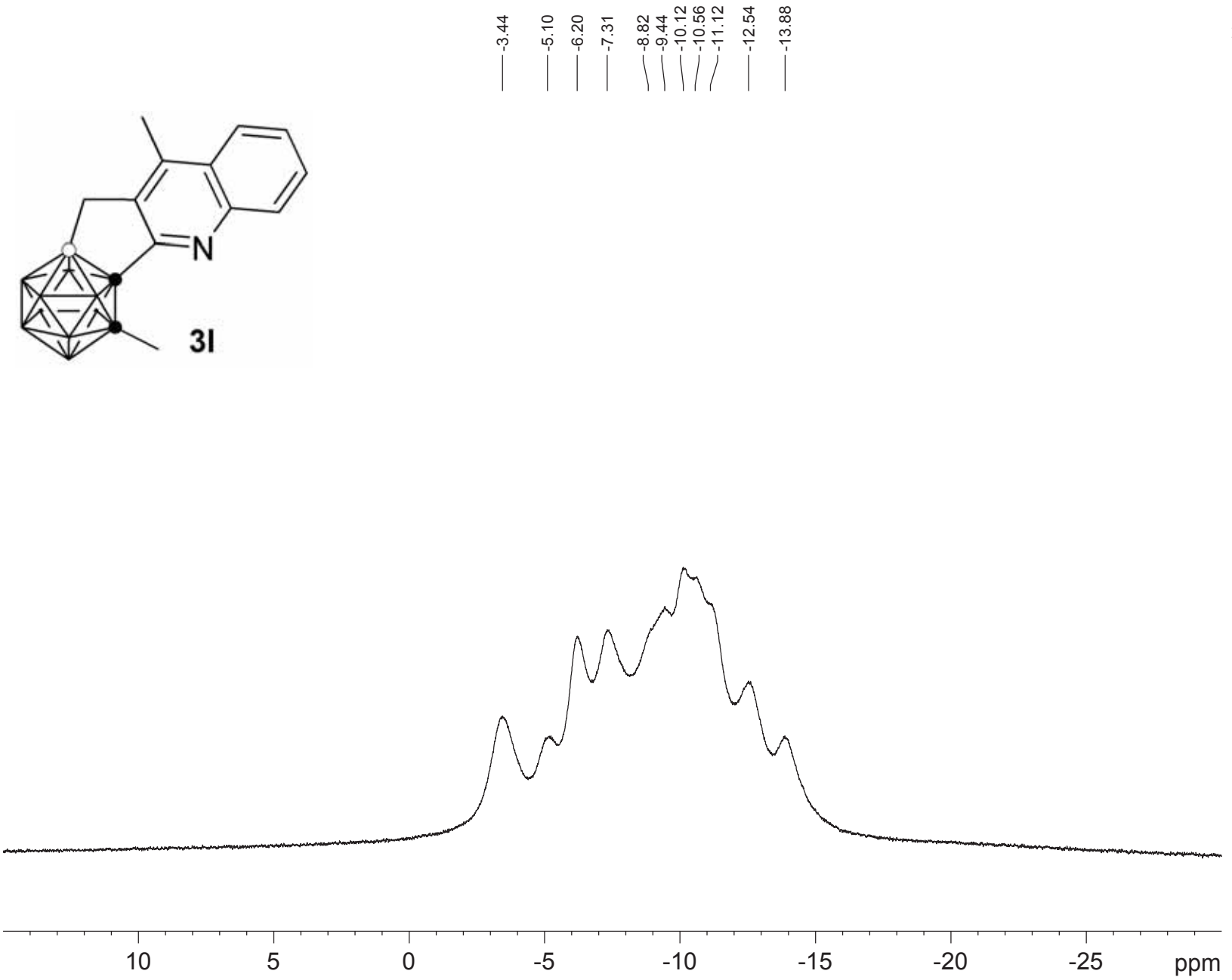


lhr-B-cas-0367-CDCl3

Current Data Parameters
NAME lhr-B-cas-0367-CDCl3
EXPNO 1
PROCNO 1

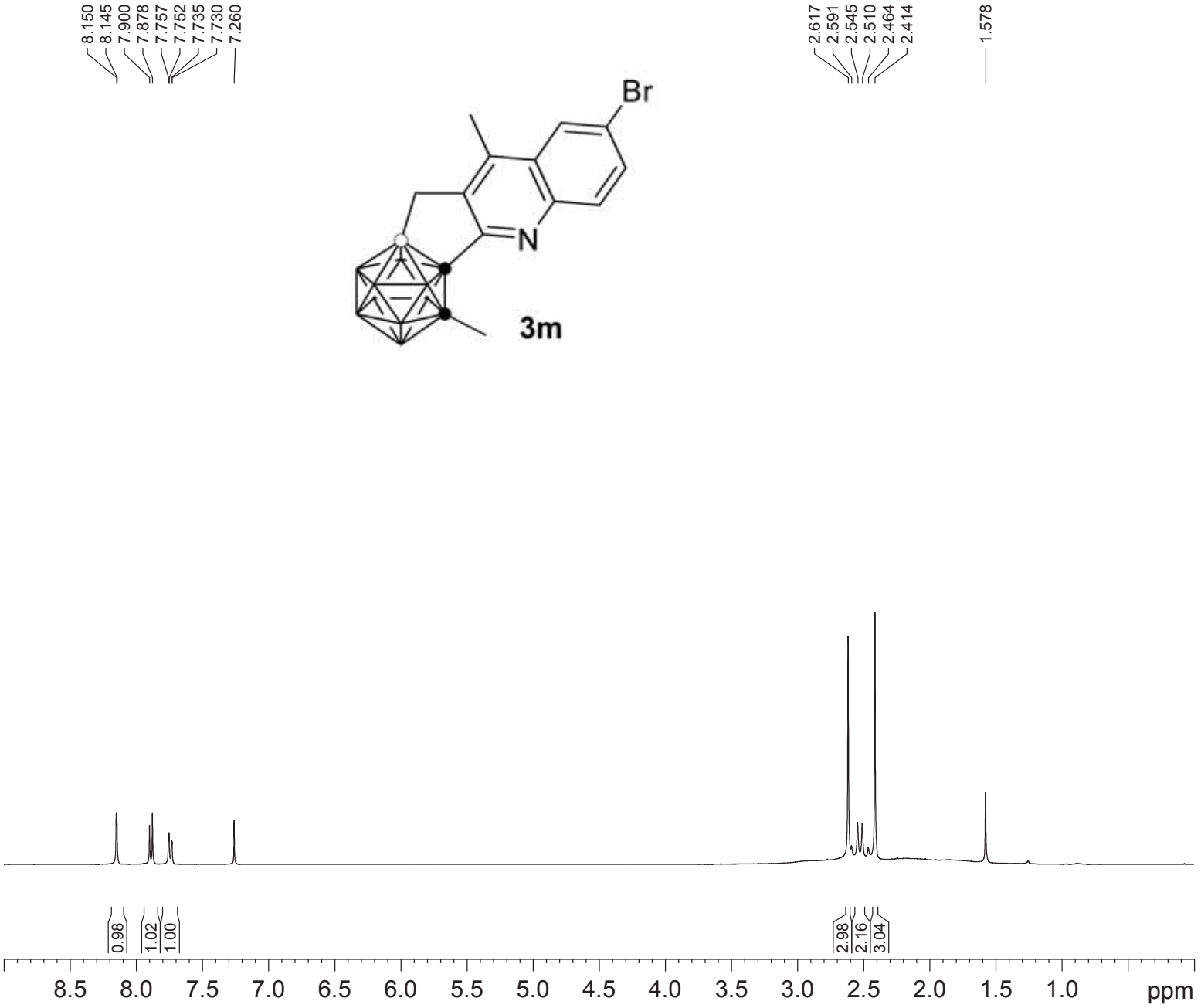
F2 - Acquisition Parameters
Date_ 20160509
Time 9.45 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgdc
TD 65536
SOLVENT THF
NS 22
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 287
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 128.4096890 MHz
NUC1 11B
P1 7.50 usec
PLW1 55.09999847 W
SFO2 400.2316009 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 13.56000042 W
PLW12 0.27428001 W

F2 - Processing parameters
SI 32768
SF 128.4097615 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



lhr-B-cas-0367-CDCl3(C)

```
Current Data Parameters
NAME      lhr-B-cas-0367-CDCl3(C)
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20160509
Time                    9.46 h
INSTRUM                 spect
PROBHD    Z108618_0257 (
PULPROG                   zg
TD                     65536
SOLVENT                  THF
NS                        20
DS                         2
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                 1.3631488 sec
RG                       287
DW                    20.800 usec
DE                     6.50 usec
TE                     295.6 K
D1                2.00000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1             55.09999847 W

F2 - Processing parameters
SI                     32768
SF               128.4097430 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```

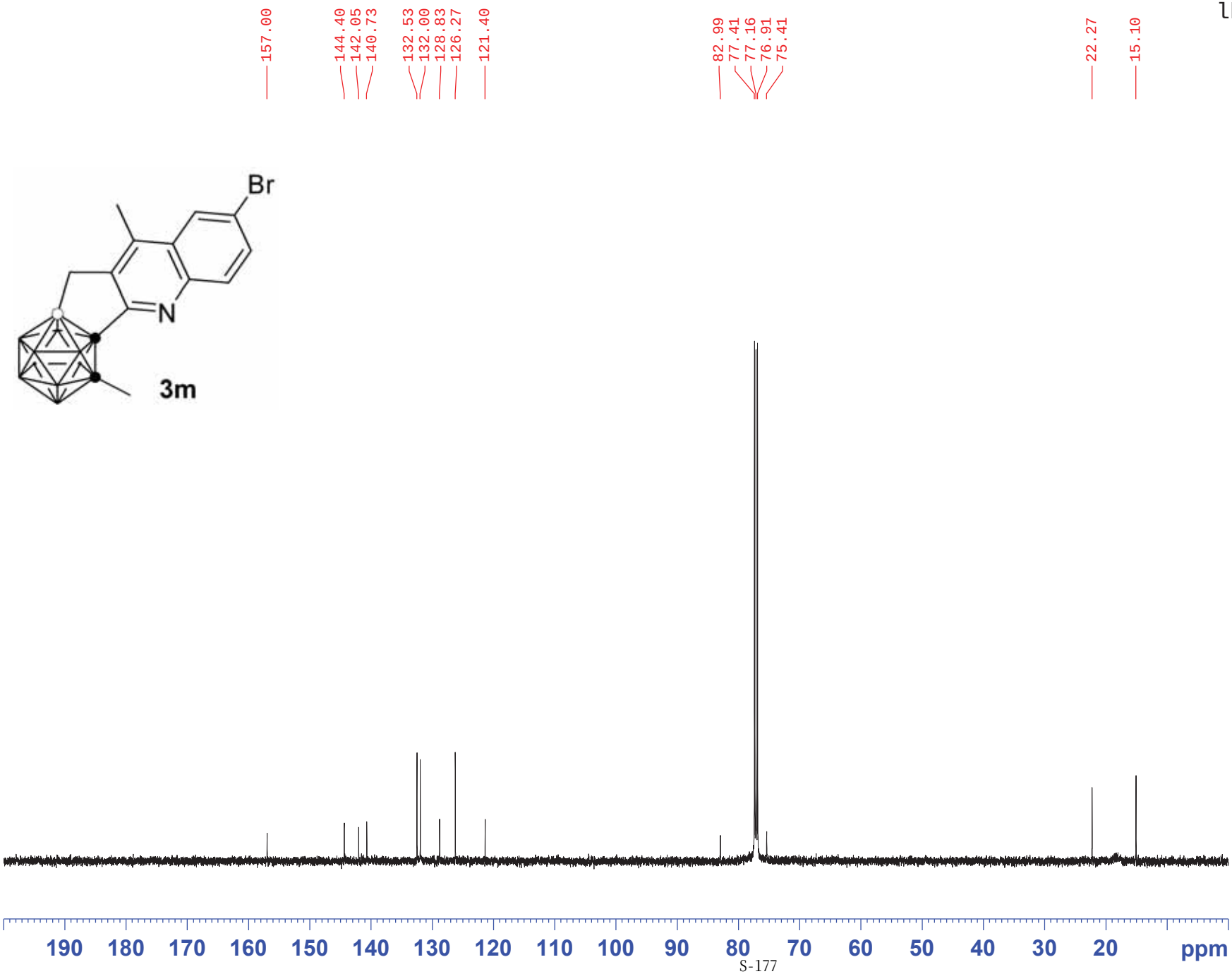


lhr-H-0715-4brcascd

Current Data Parameters
NAME lhr-H-0715-4brcasc
EXPNO 1
PROCNO 1

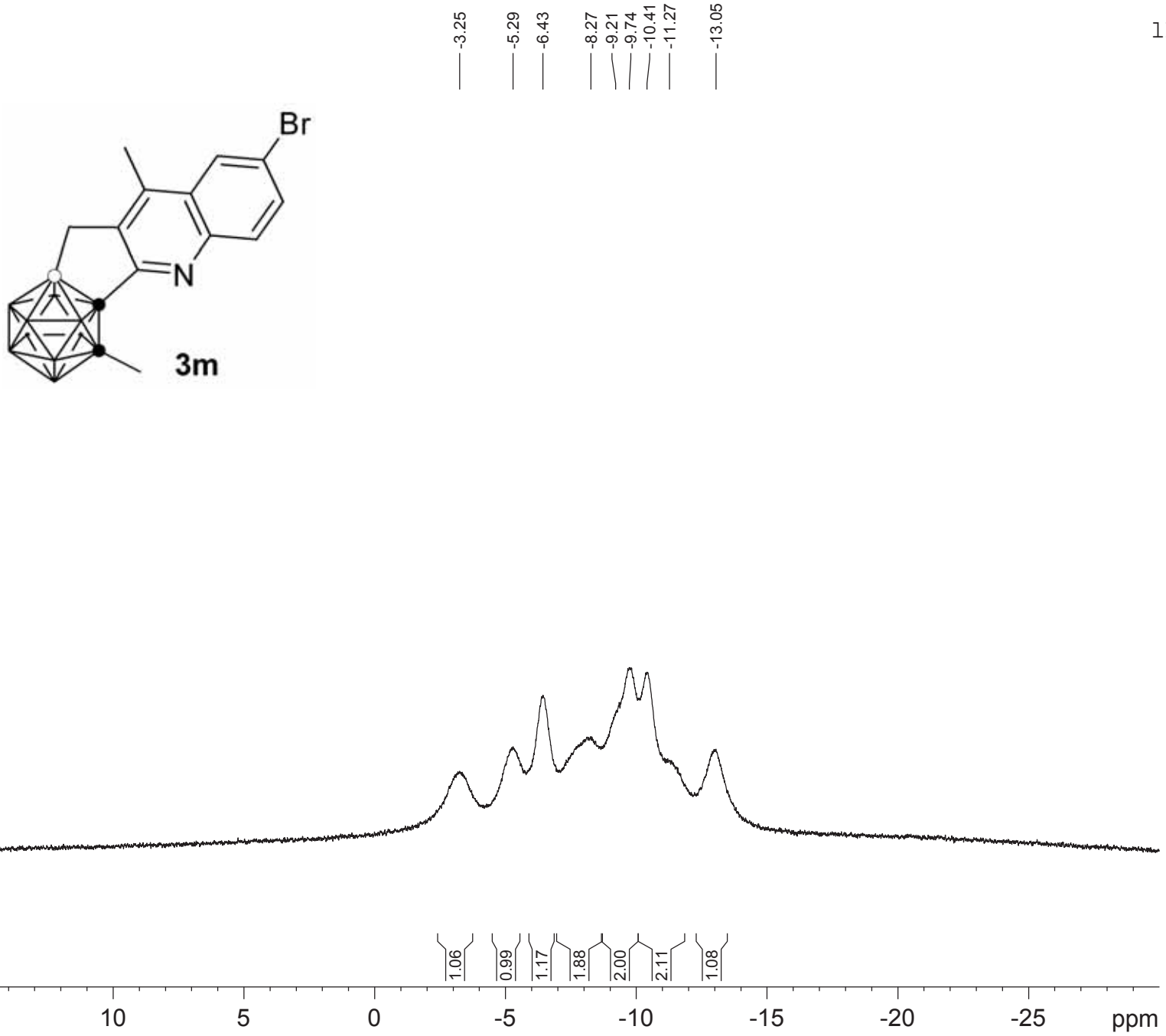
F2 - Acquisition Parameters
Date_ 20170705
Time 16.51 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300109 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



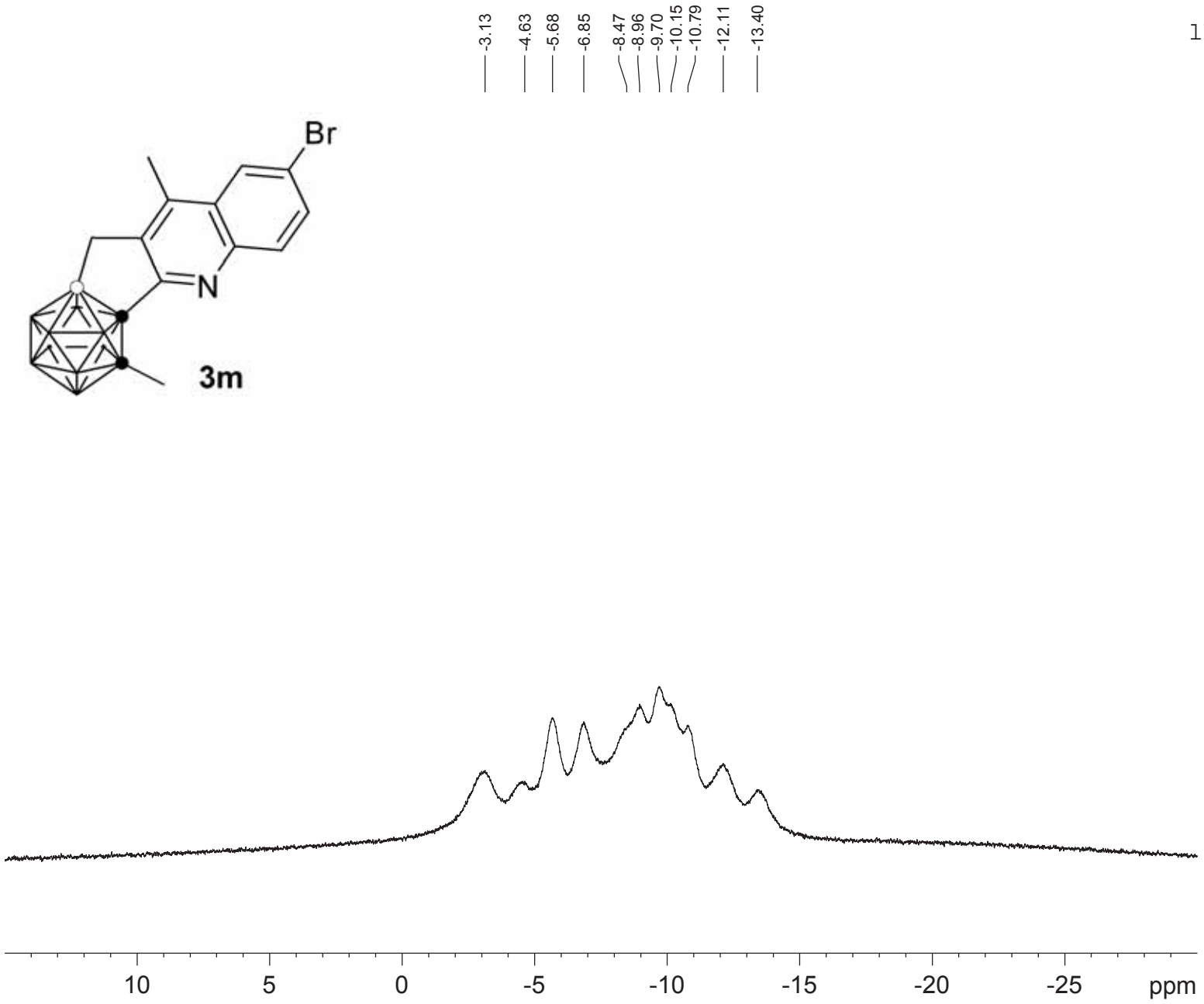
lhr-0715-4brcascdcl3

```
Current Data Parameters
NAME      lhr-0715-4brcascdcl3
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
Date_              20170705
Time                 19.54 h
INSTRUM                spect
PROBHD   Z119470_0283 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     400
DS                       4
SWH              29761.904 Hz
FIDRES            0.908261 Hz
AQ               1.1010048 sec
RG                  206.72
DW                  16.800 usec
DE                   6.50 usec
TE                  299.0 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1
SFO1           125.7703643 MHz
NUC1                   13C
P1                  10.00 usec
PLW1           94.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2               80.00 usec
PLW2           25.00000000 W
PLW12           0.39063001 W
PLW13           0.19648001 W

F2 - Processing parameters
SI                   32768
SF             125.7577717 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```



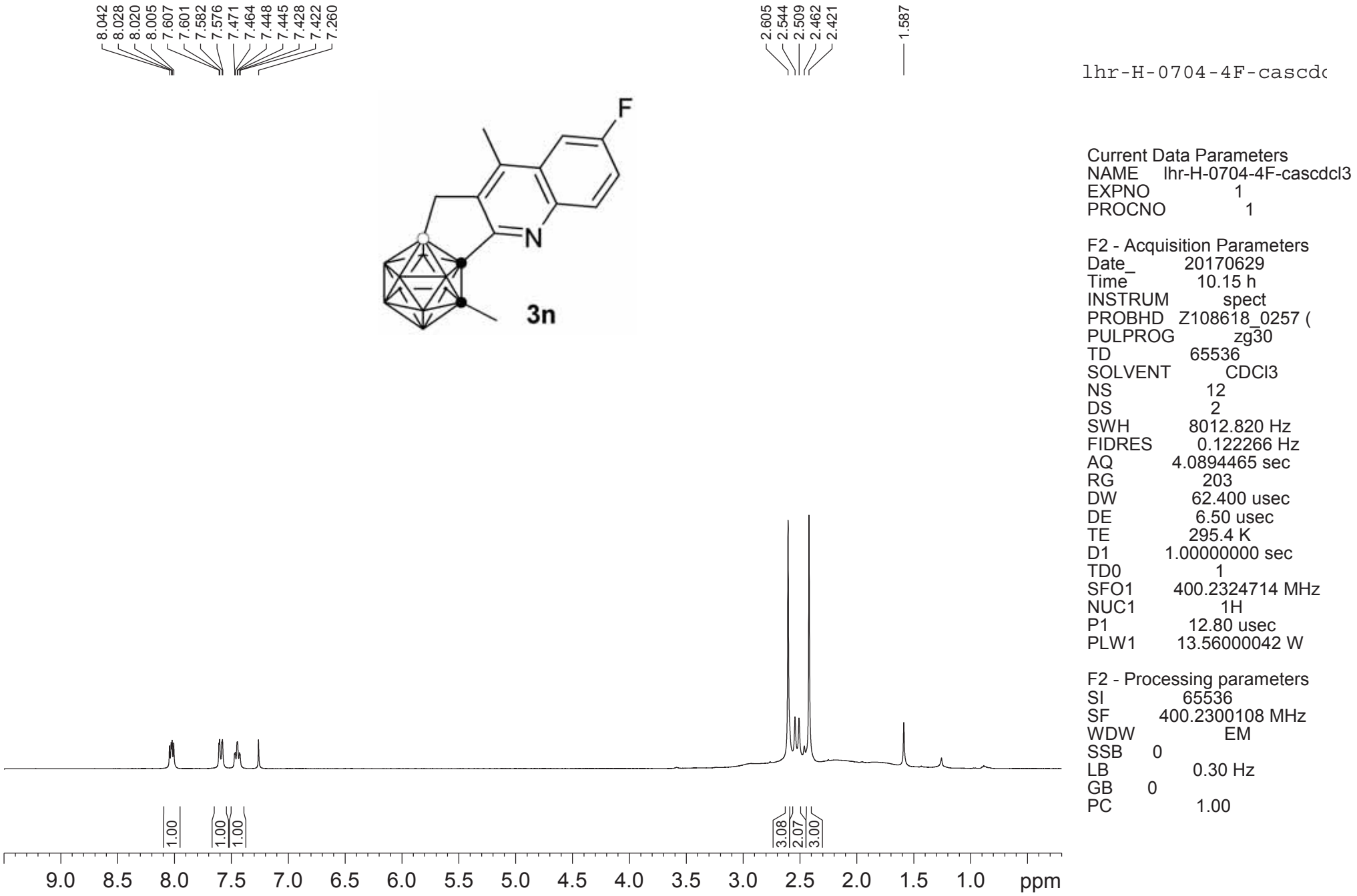
lhr-B-0715-4brcascdcl3

```
Current Data Parameters
NAME      lhr-B-0715-4brcascdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20170705
Time                   16.54 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                        24
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                 1.3631488 sec
RG                       512
DW                    20.800 usec
DE                     6.50 usec
TE                    295.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                     32768
SF               128.4097615 MHz
WDW                       EM
SSB       0
LB                     1.00 Hz
GB        0
PC                     1.40
```



lhr-B-0715-4brcascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0715-4brcascdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170705
Time                16.57 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      32
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     512
DW                  20.800 usec
DE                   6.50 usec
TE                  295.3 K
D1             2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                   32768
SF            128.4097430 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

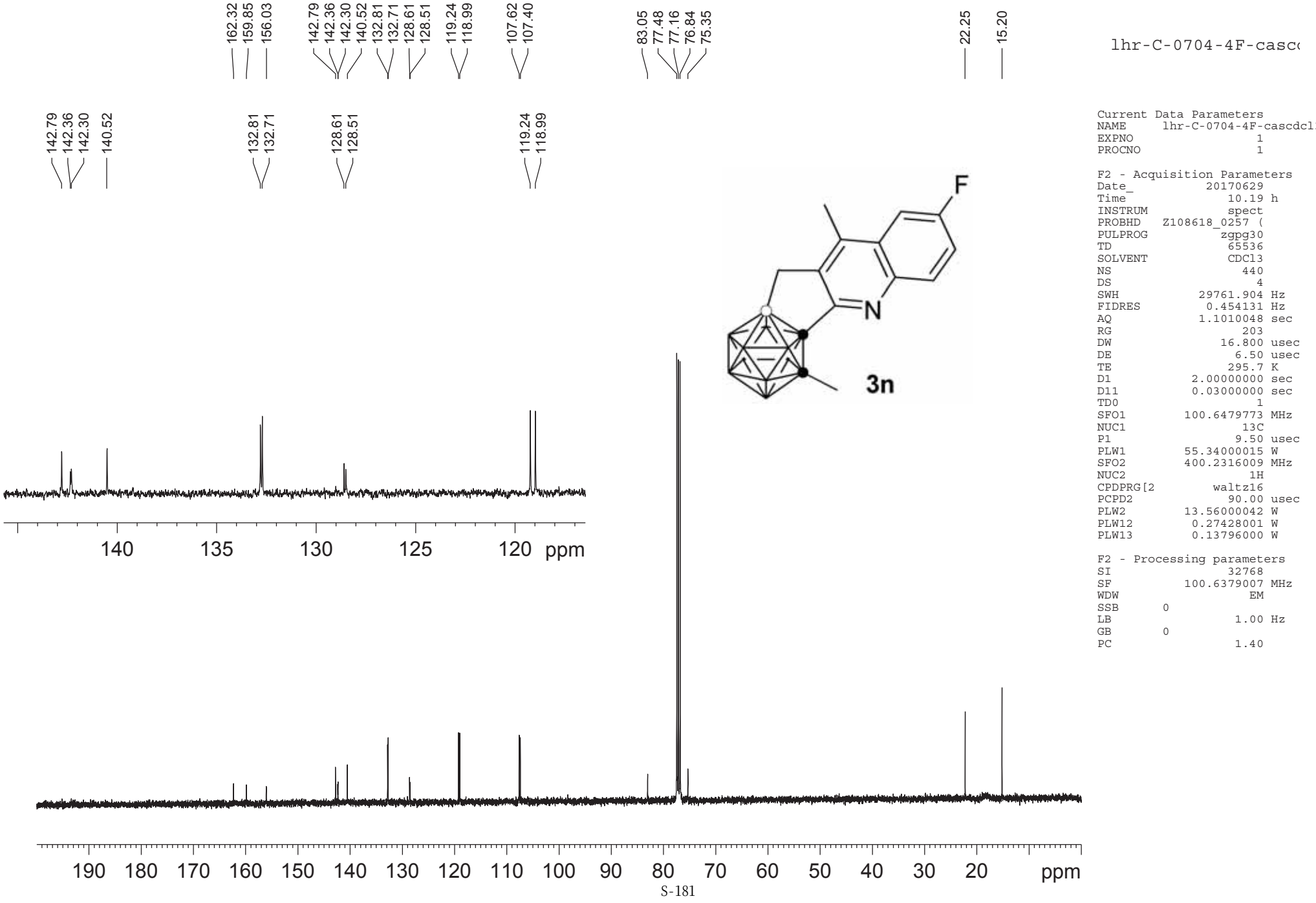


lhr-H-0704-4F-cascdc

Current Data Parameters
NAME lhr-H-0704-4F-cascdcl3
EXPNO 1
PROCNO 1

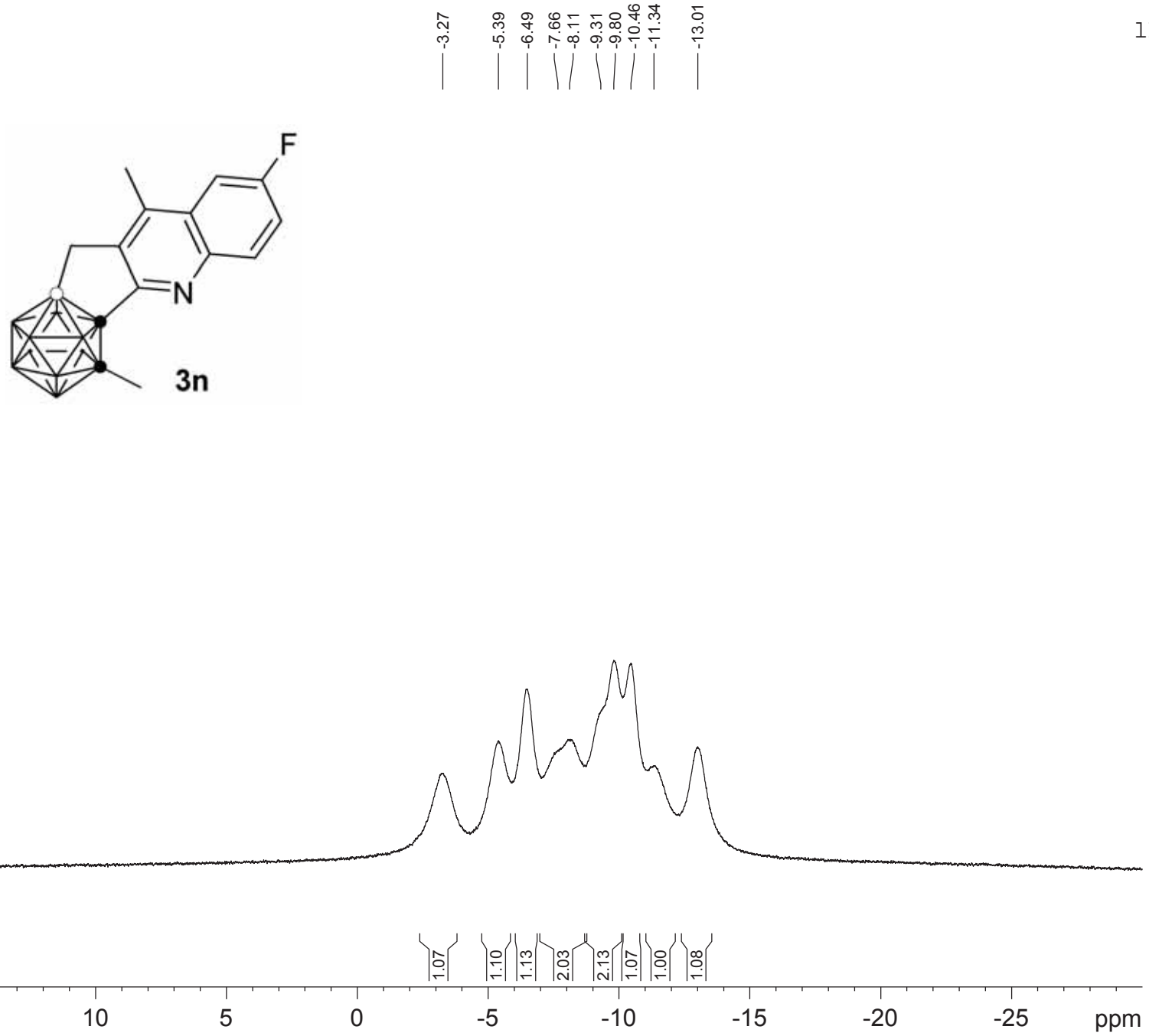
F2 - Acquisition Parameters
Date_ 20170629
Time 10.15 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



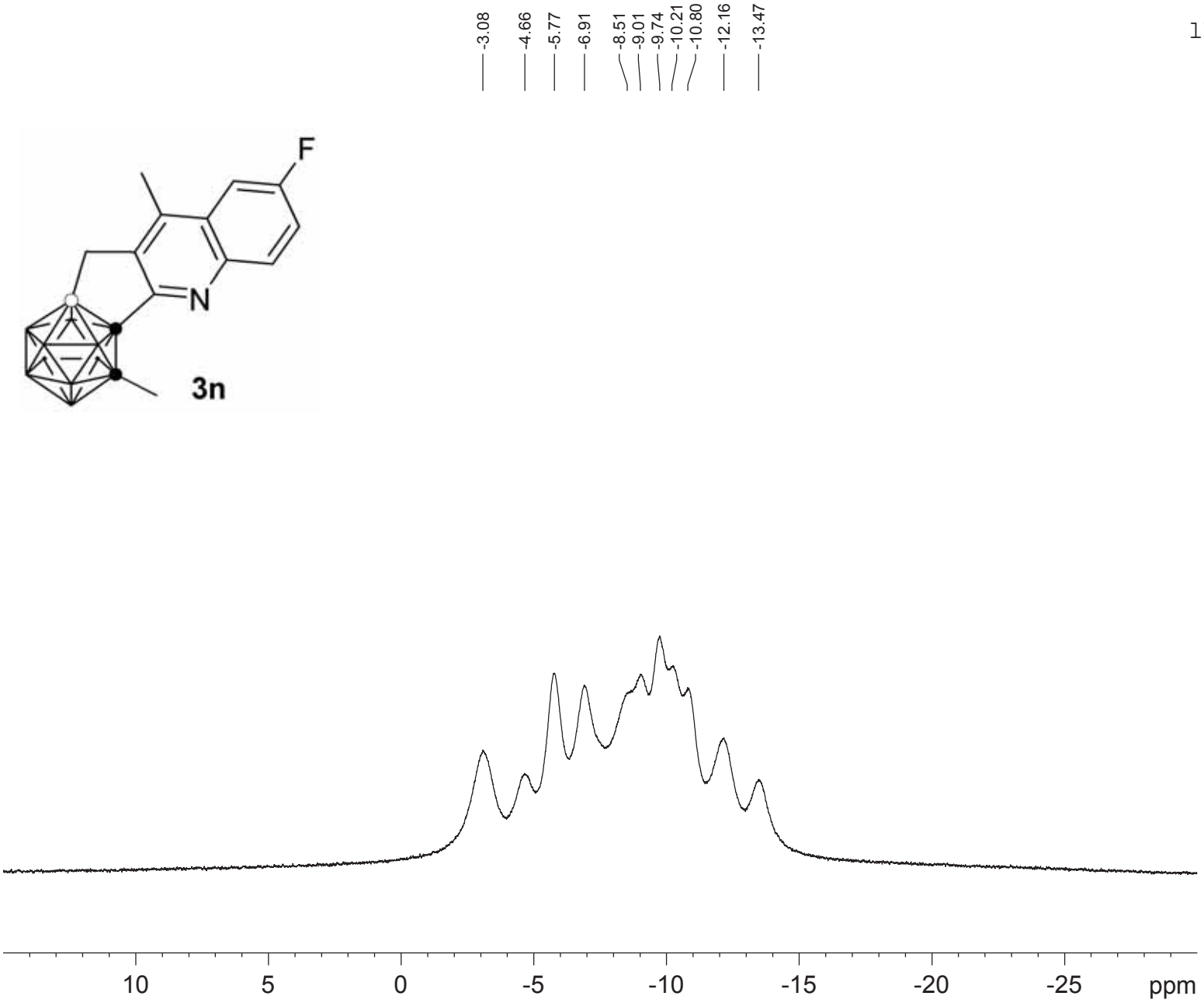
lhr-C-0704-4F-casc

```
Current Data Parameters
NAME      lhr-C-0704-4F-cascdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_               20170629
Time                   10.19 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                      440
DS                        4
SWH                29761.904 Hz
FIDRES             0.454131 Hz
AQ                 1.1010048 sec
RG                      203
DW                   16.800 usec
DE                    6.50 usec
TE                   295.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1
SFO1             100.6479773 MHz
NUC1                    13C
P1                    9.50 usec
PLW1             55.34000015 W
SFO2             400.2316009 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2             13.56000042 W
PLW12             0.27428001 W
PLW13             0.13796000 W

F2 - Processing parameters
SI                      32768
SF               100.6379007 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```



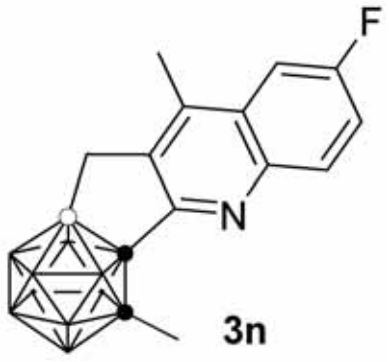
lhr-B-0704-4F-cascdcl3

```
Current Data Parameters
NAME      lhr-B-0704-4F-cascdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20170629
Time                      10.43 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                    zgdc
TD                        65536
SOLVENT                   CDCl3
NS                           12
DS                            4
SWH                   24038.461 Hz
FIDRES                 0.366798 Hz
AQ                    1.3631488 sec
RG                          287
DW                       20.800 usec
DE                        6.50 usec
TE                       295.9 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                           1
SFO1                128.4096890 MHz
NUC1                         11B
P1                        7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                    90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

F2 - Processing parameters
SI                        32768
SF                  128.4097615 MHz
WDW                          EM
SSB               0
LB                        1.00 Hz
GB                0
PC                        1.40
```



lhr-B-0704-4F-cascdcl3(C)

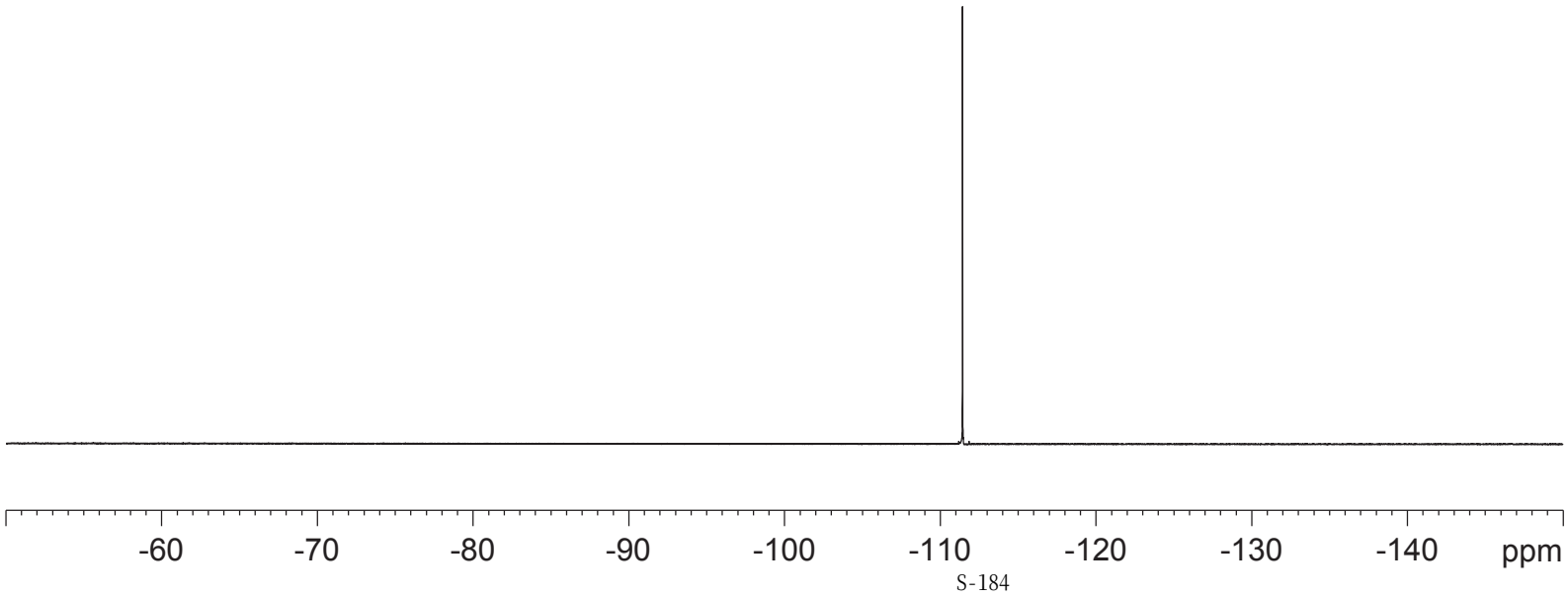
```
Current Data Parameters
NAME      lhr-B-0704-4F-cascdcl3(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170629
Time              10.45 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  287
DW               20.800 usec
DE                6.50 usec
TE               295.7 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

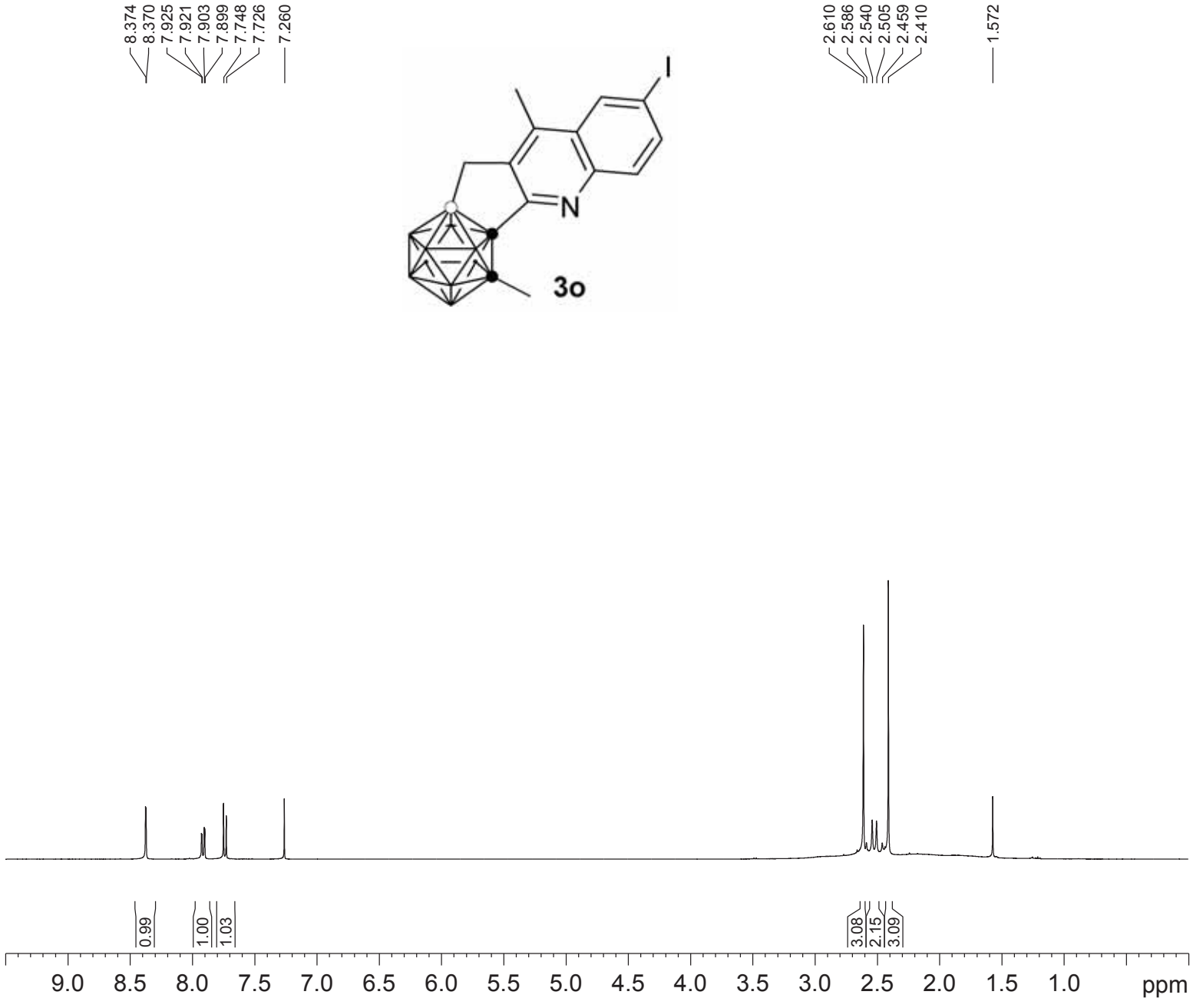


-111.43

lhr-F-0704-4F-cascdcl3

```
Current Data Parameters
NAME      lhr-F-0704-4F-cascdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170629
Time              10.47 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG       zgfhigqn.2
TD                131072
SOLVENT             CDCl3
NS                     11
DS                      4
SWH            89285.711 Hz
FIDRES          0.681196 Hz
AQ              0.7340032 sec
RG                    645
DW                5.600 usec
DE                6.50 usec
TE                295.7 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                    1
SFO1         376.5548010 MHz
NUC1                 19F
P1                14.70 usec
PLW1         18.36000061 W
SFO2         400.2316009 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 65536
SF           376.5924602 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



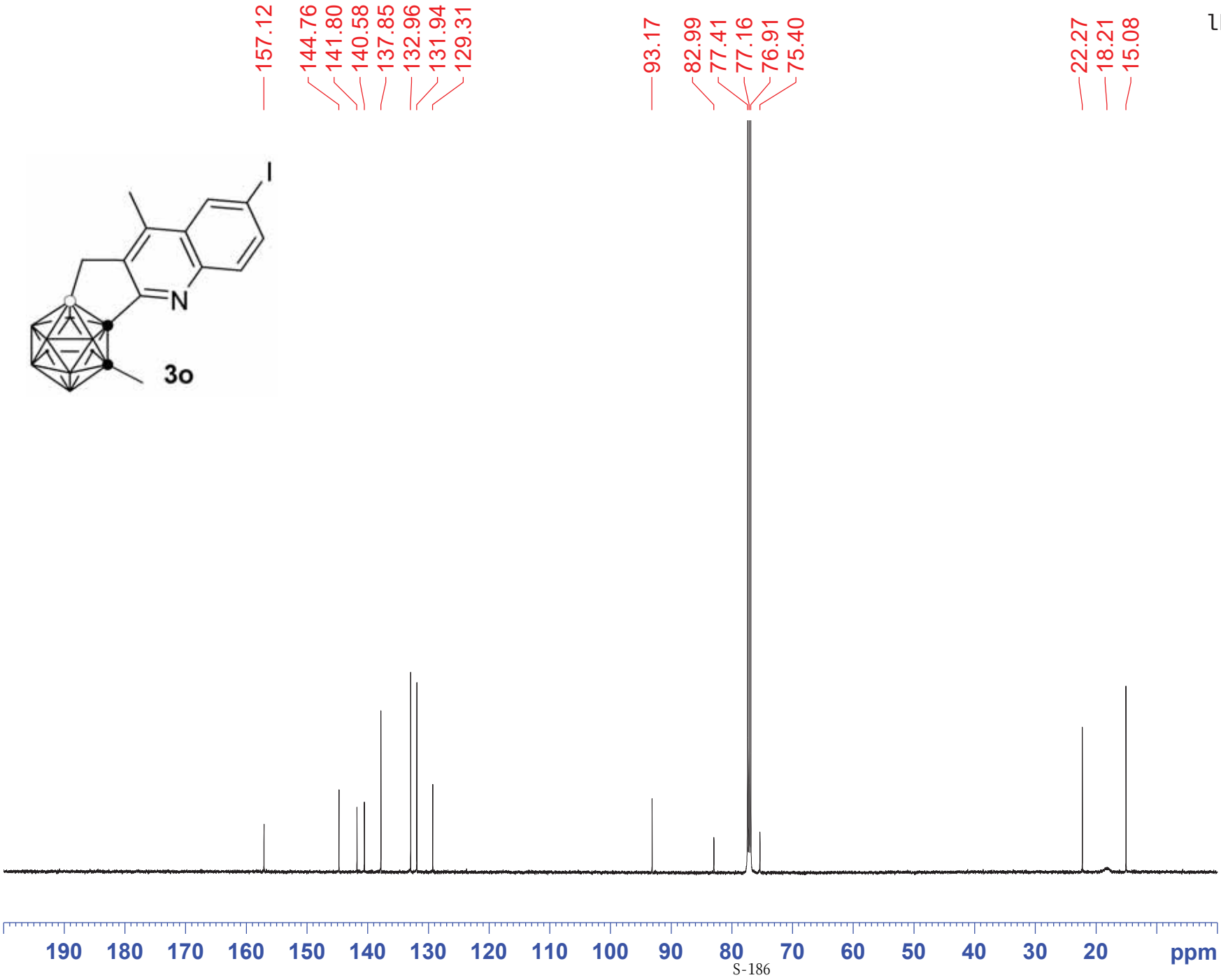


lhr-H-0739-i-cascdc

Current Data Parameters
NAME lhr-H-0739-i-cascd
EXPNO 1
PROCNO 1

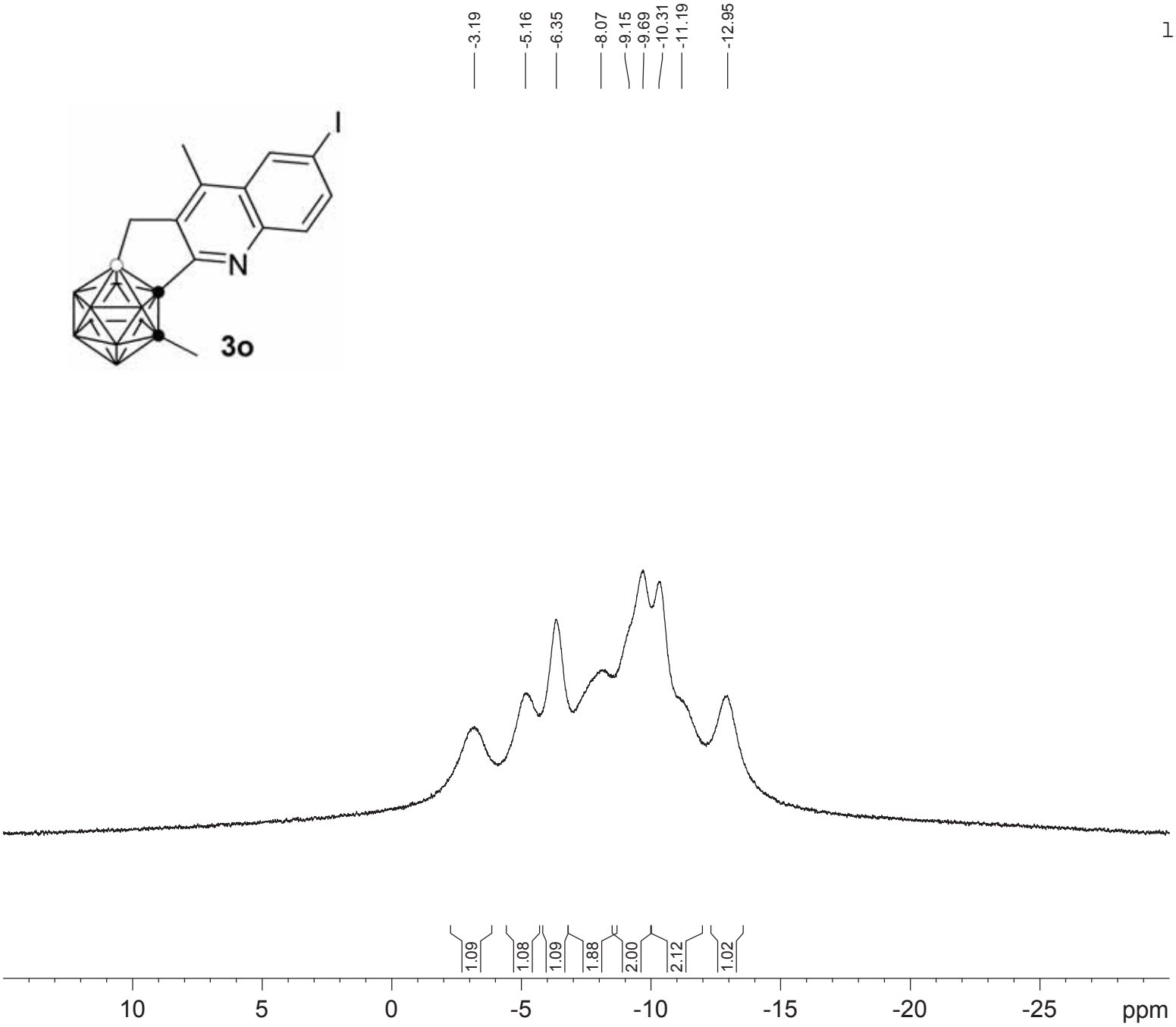
F2 - Acquisition Parameters
Date_ 20170810
Time 20.14 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MH
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300100 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



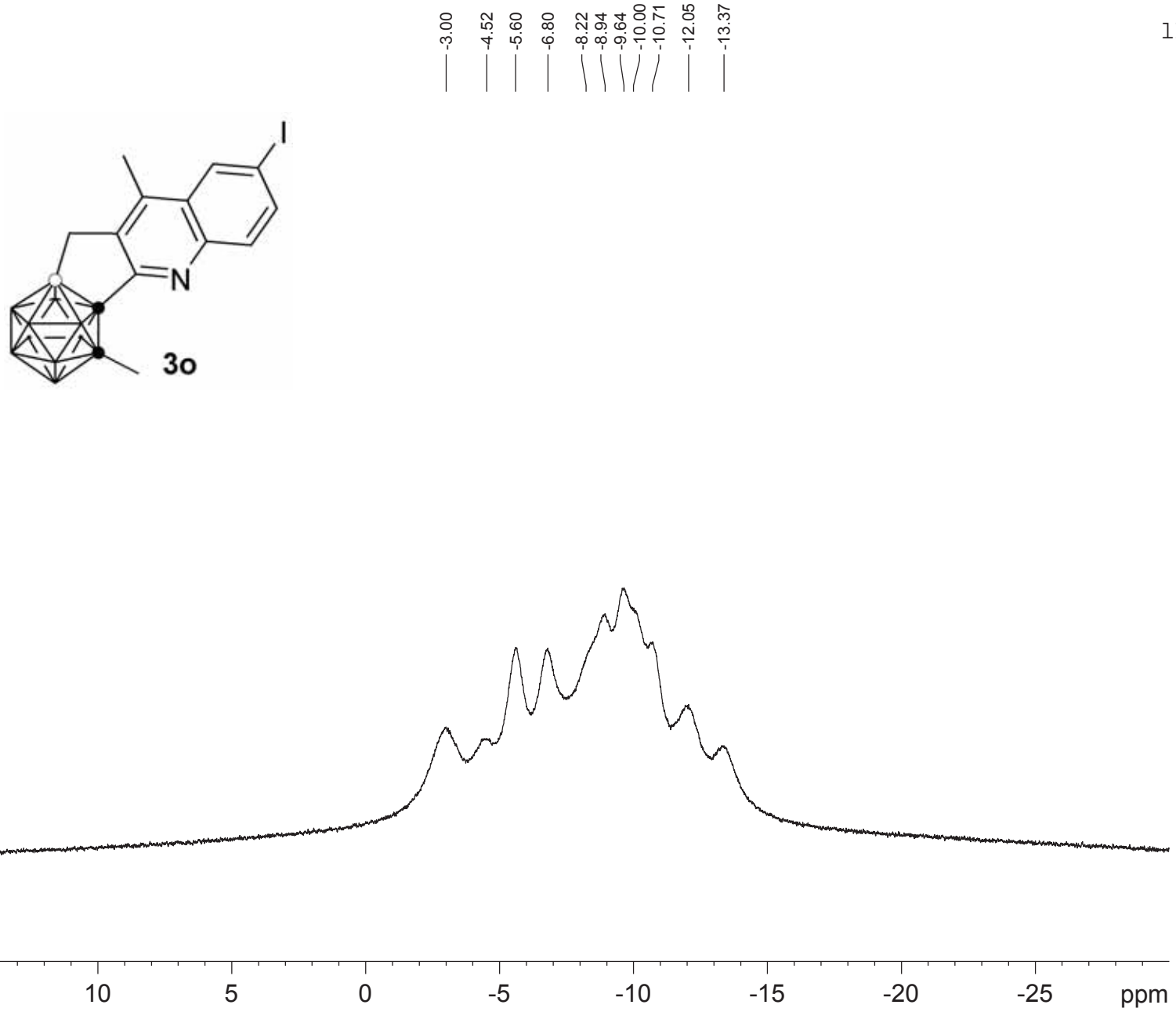
lhr-C-0739-Icas

```
Current Data Parameters
NAME      lhr-C-0739-Icas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170811
Time              10.06 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  683
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577725 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



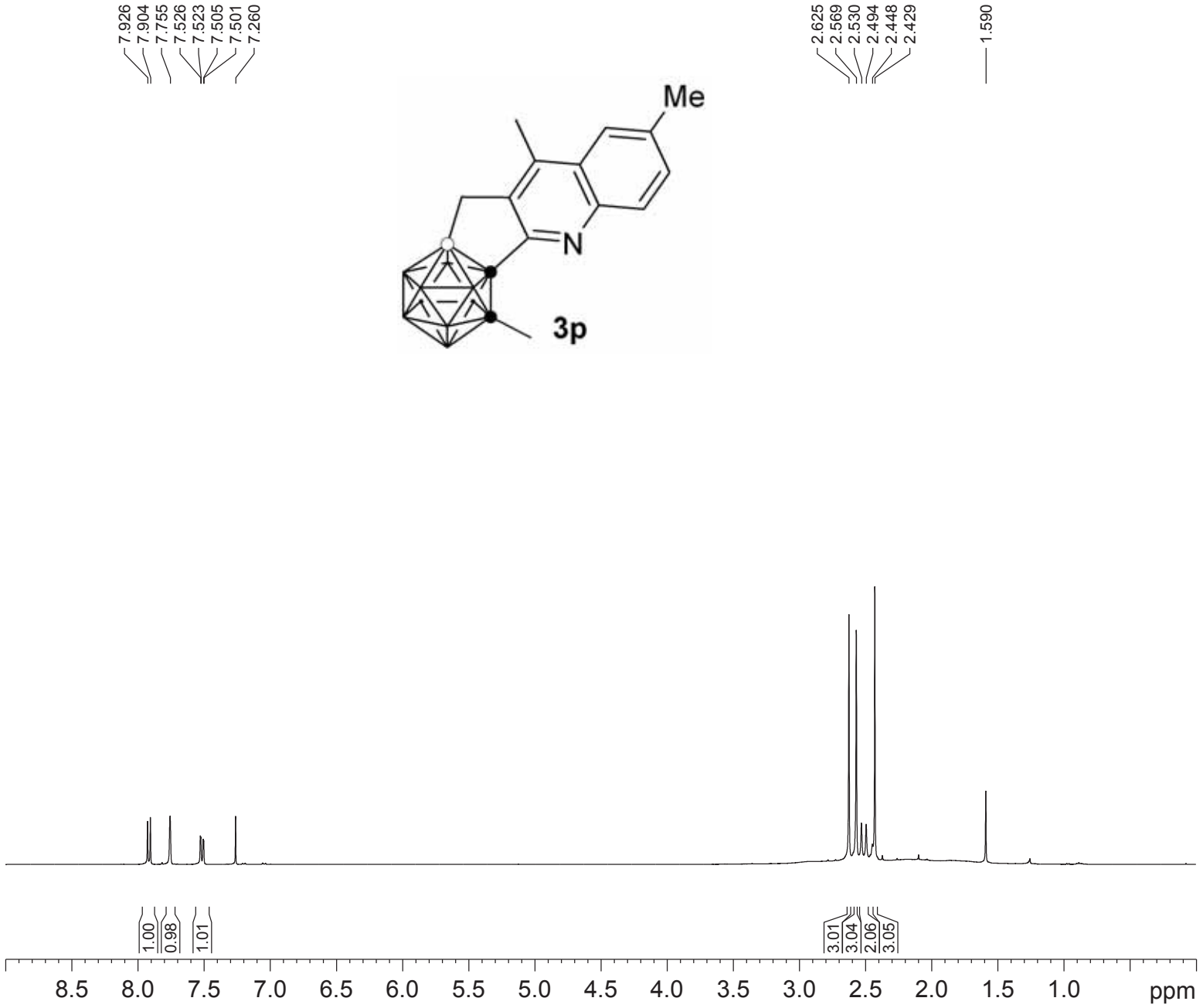
lhr-B-0739-i-cascdcl3

```
Current Data Parameters
NAME      lhr-B-0739-i-cascdcl3
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_              20170811
Time                   18.39 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                        28
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                       322
DW                    20.800 usec
DE                     6.50 usec
TE                     295.7 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                       32768
SF               128.4097615 MHz
WDW                         EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



lhr-B-0739-i-cascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0739-i-cascdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170811
Time              18.42 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG                 zg
TD                  65536
SOLVENT             CDCl3
NS                     28
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    322
DW                20.800 usec
DE                 6.50 usec
TE                295.3 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

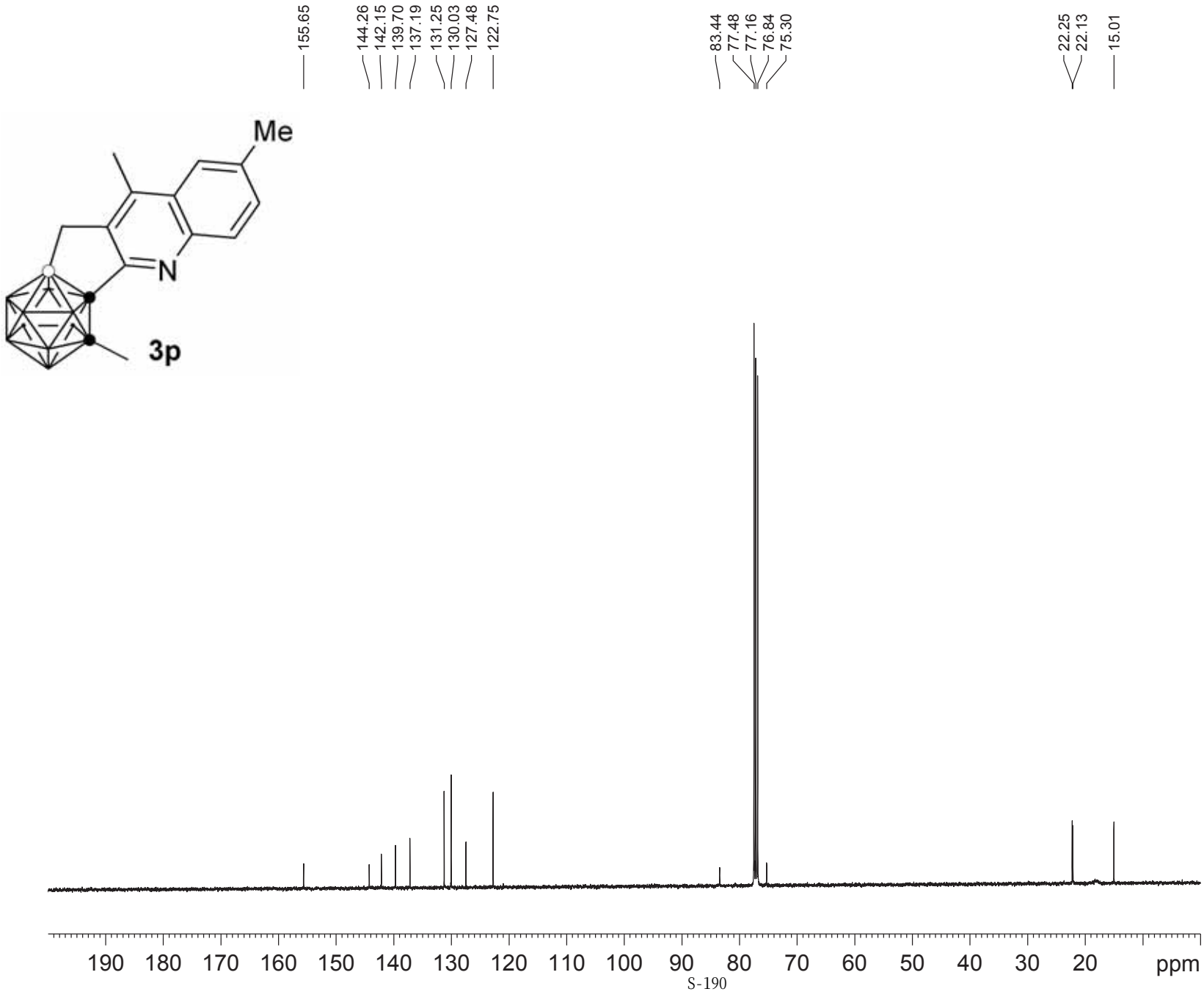


lhr-H-0732-ch3cascd

Current Data Parameters
NAME lhr-H-0732-ch3casc
EXPNO 1
PROCNO 1

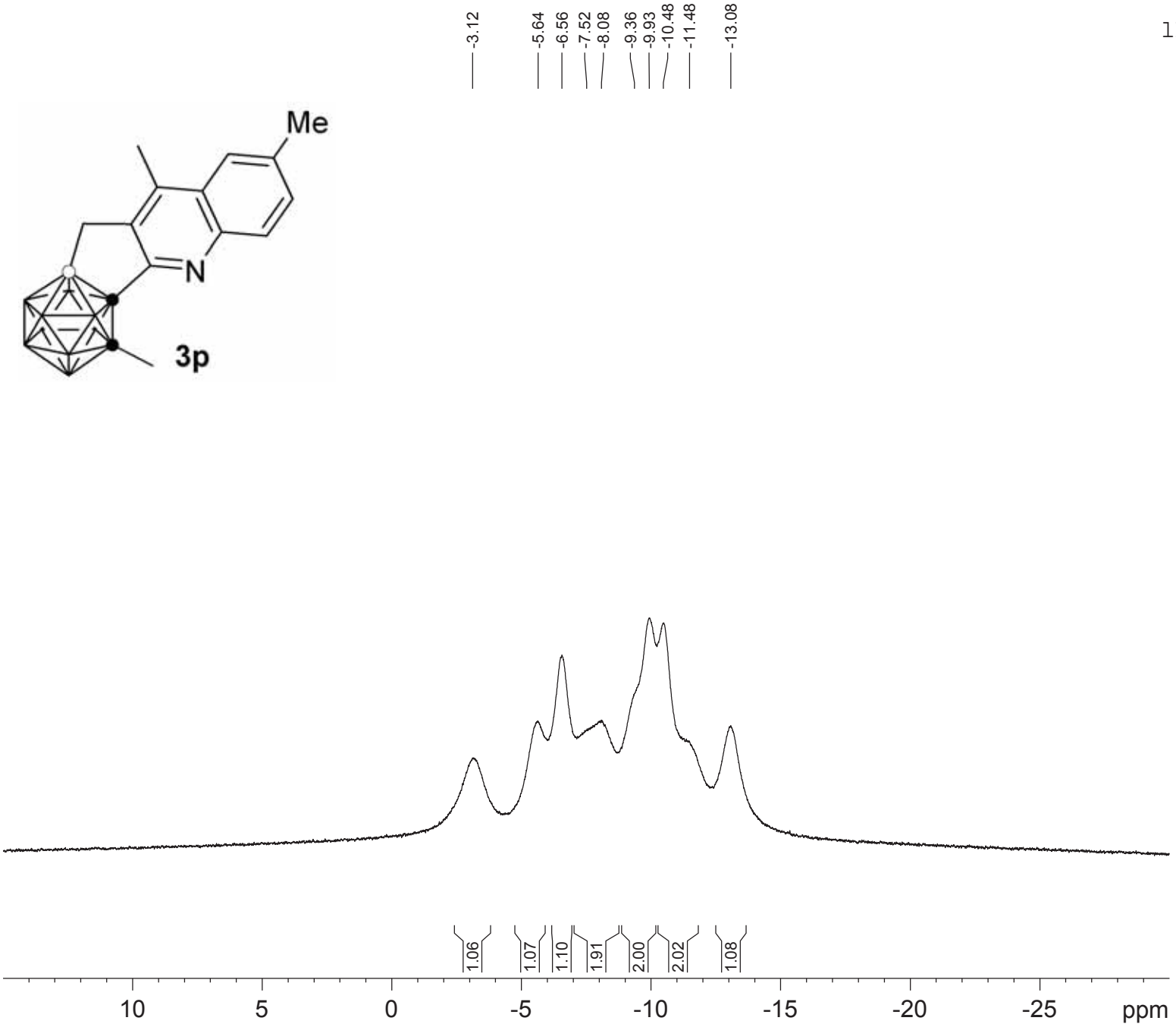
F2 - Acquisition Parameters
Date_ 20170729
Time 18.36 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



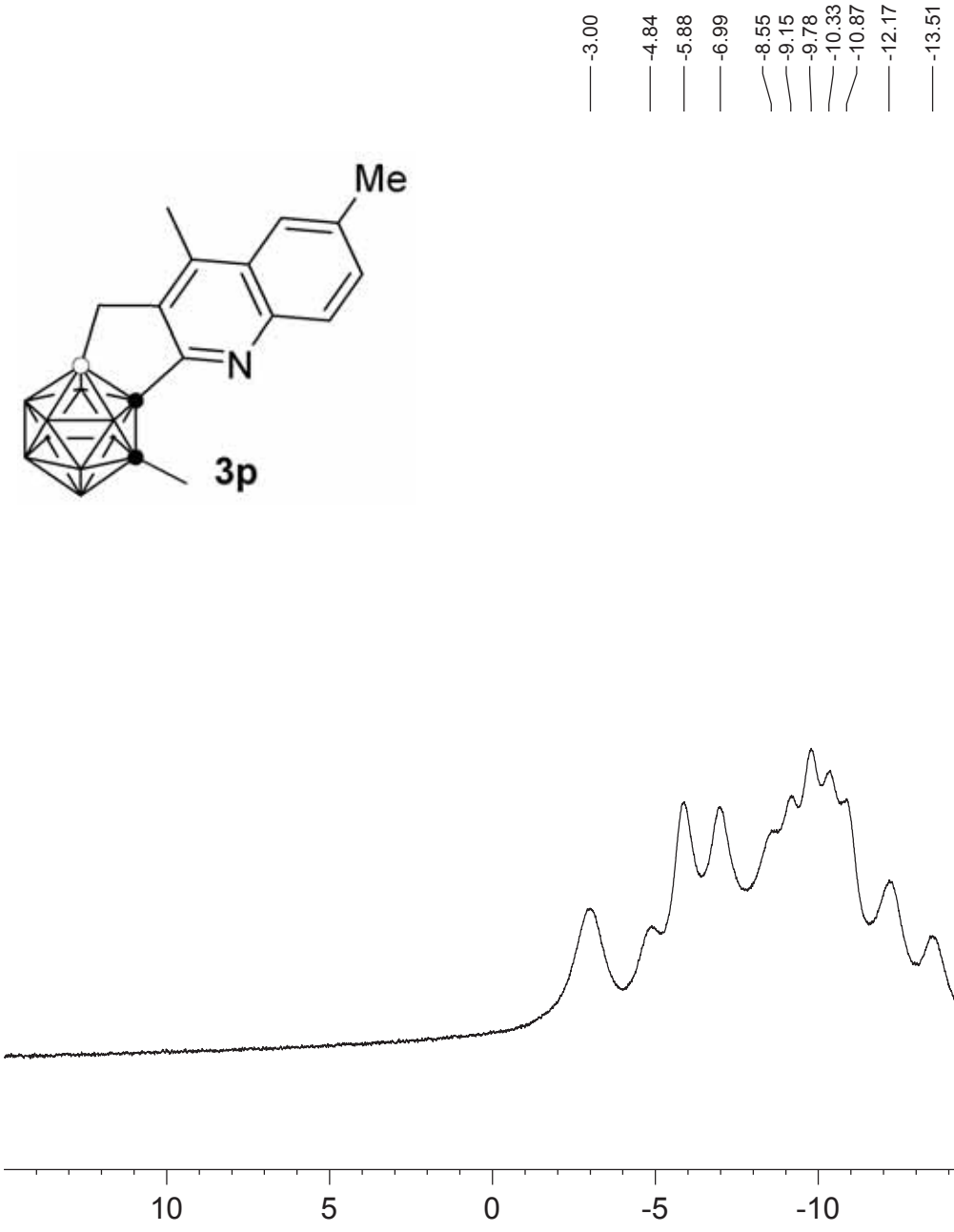
lhr-C-0732-ch3casc

```
Current Data Parameters
NAME      lhr-C-0732-ch3cascdcl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170729
Time              18.41 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1412
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW                12.267 usec
DE                 6.50 usec
TE                295.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                 32768
SF           100.6379006 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



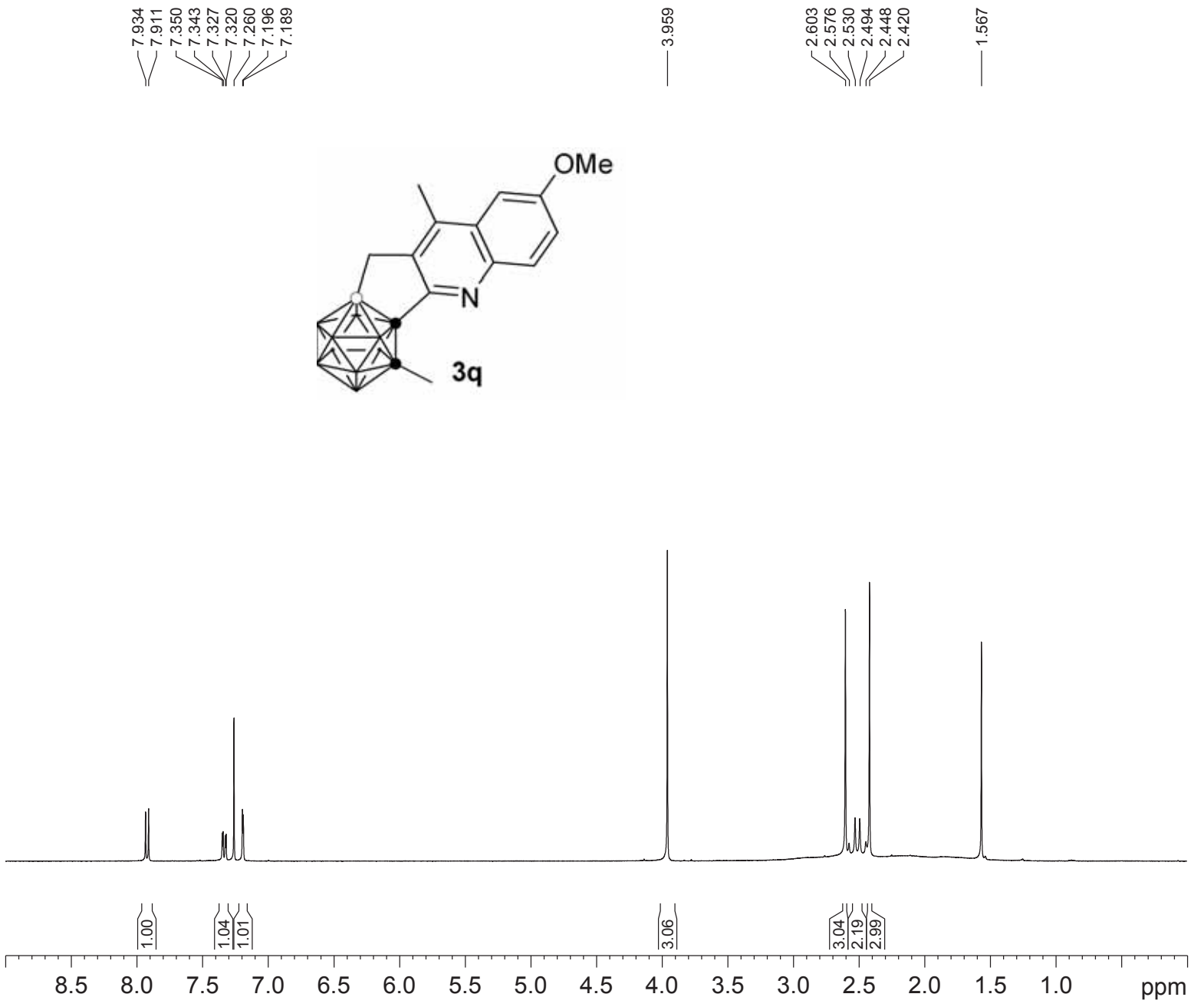
lhr-B-0732-ch3cascdcl3

```
Current Data Parameters
NAME      lhr-B-0732-ch3cascdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170729
Time              19.50 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    24
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



lhr-B-0732-ch3cascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0732-ch3cascdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170729
Time                19.53 h
INSTRUM             spect
PROBHD    Z108618_0257 (
PULPROG                 zg
TD                   65536
SOLVENT              CDCl3
NS                      35
DS                       2
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ              1.3631488 sec
RG                     362
DW                  20.800 usec
DE                   6.50 usec
TE                  294.8 K
D1             2.00000000 sec
TD0                     1
SFO1          128.4096890 MHz
NUC1                  11B
P1                   7.50 usec
PLW1          55.09999847 W

F2 - Processing parameters
SI                   32768
SF            128.4097430 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

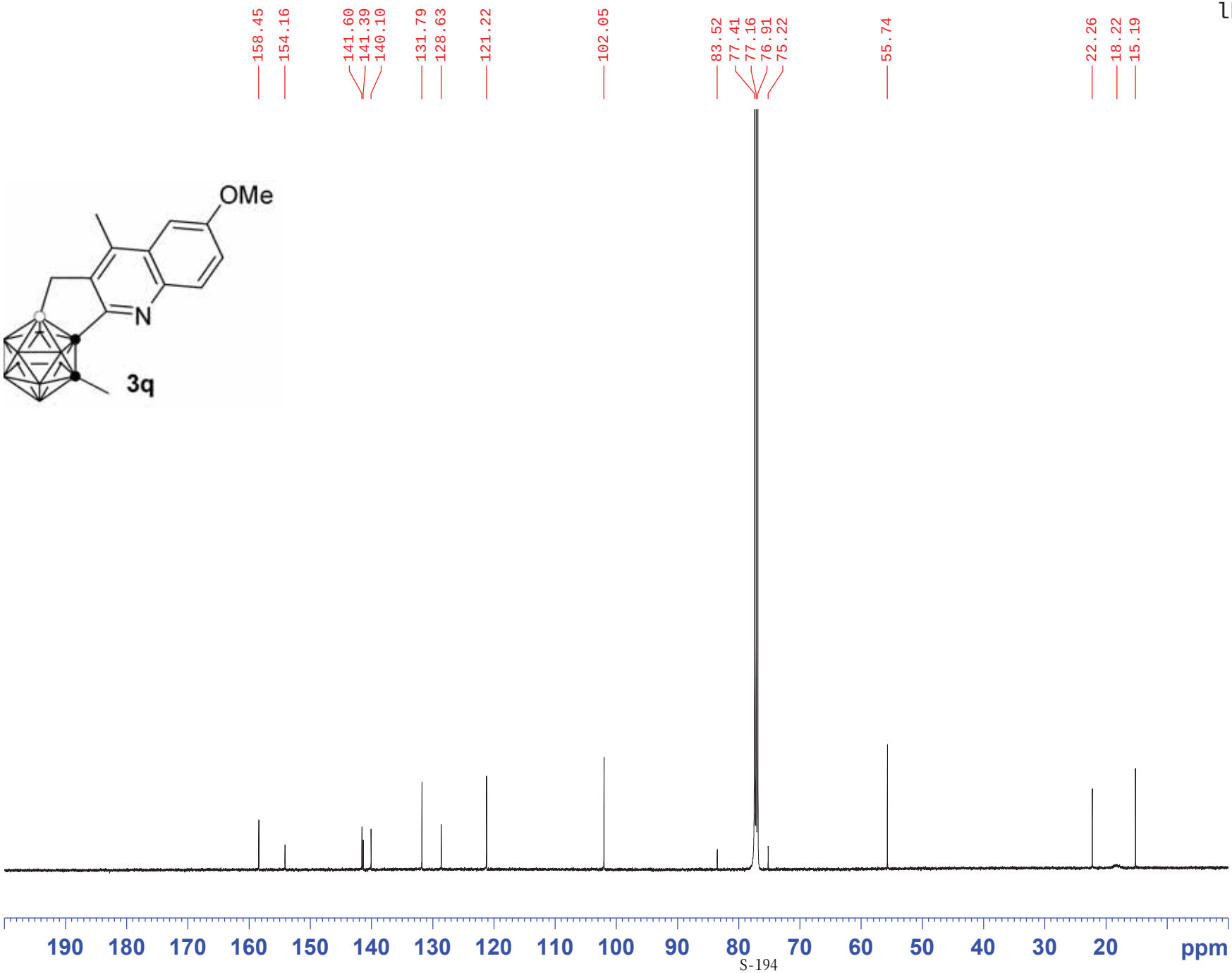


lhr-H-0722-3-ome-ca

Current Data Parameters
NAME lhr-H-0722-3-ome-casc
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170812
Time 10.30 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 11
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

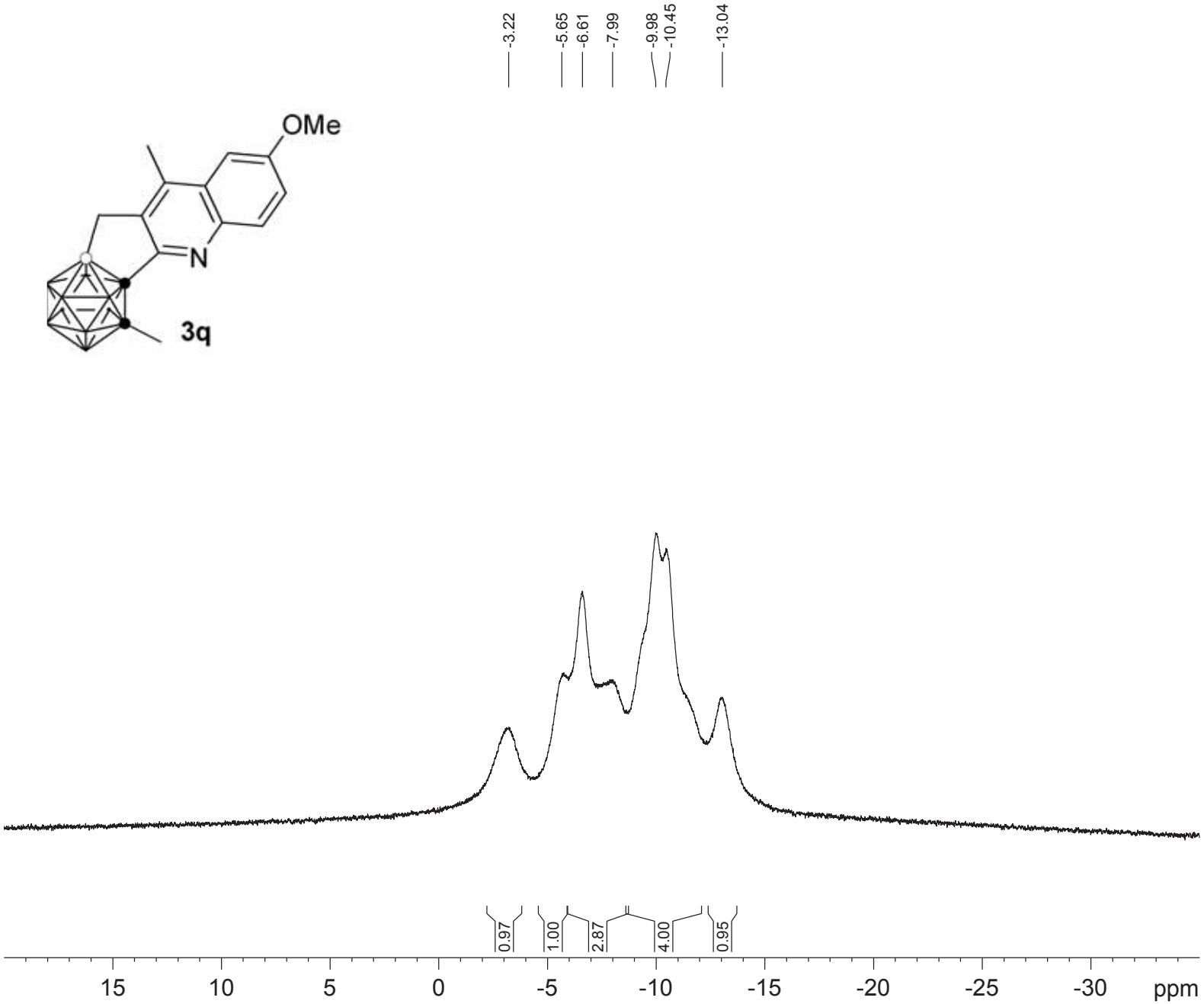


lhr-0722-3-C

Current Data Parameters
NAME lhr-0722-3-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170812
Time 12.23 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2100
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 206.72
DW 16.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 61.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W
PLW13 0.16976000 W

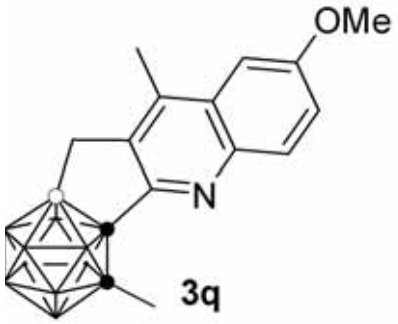
F2 - Processing parameters
SI 32768
SF 125.7577716 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



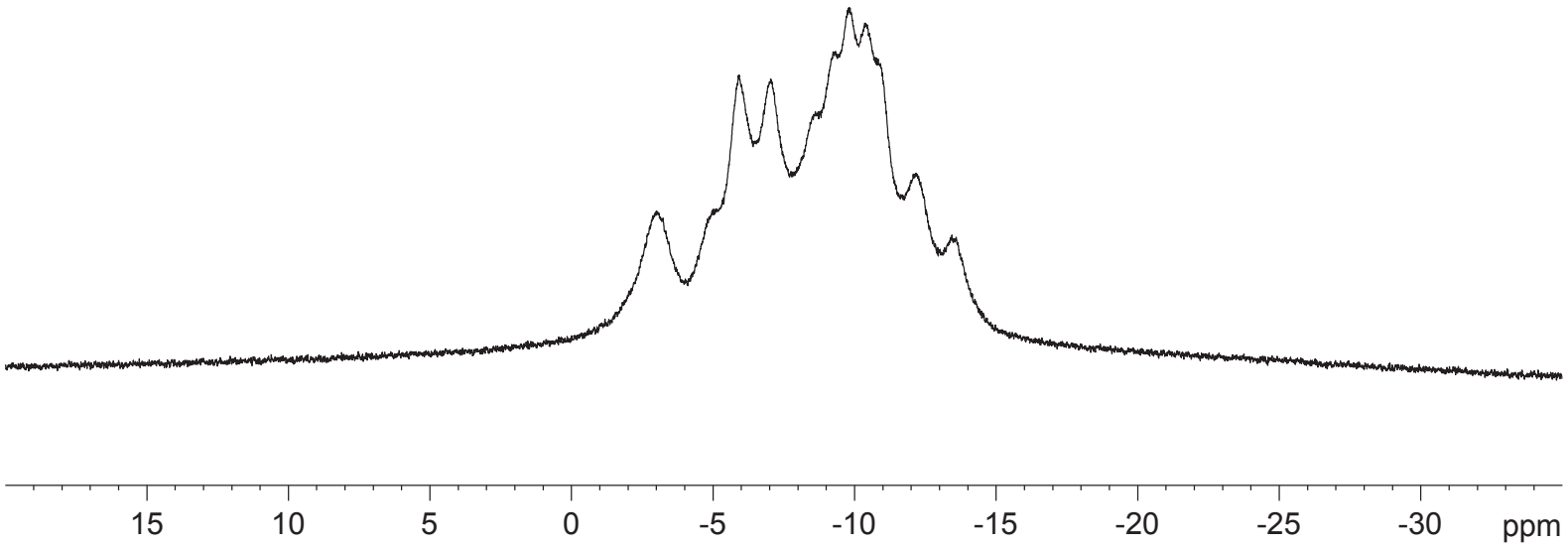
lhr-B-cas-0396-OMe-CDCl3

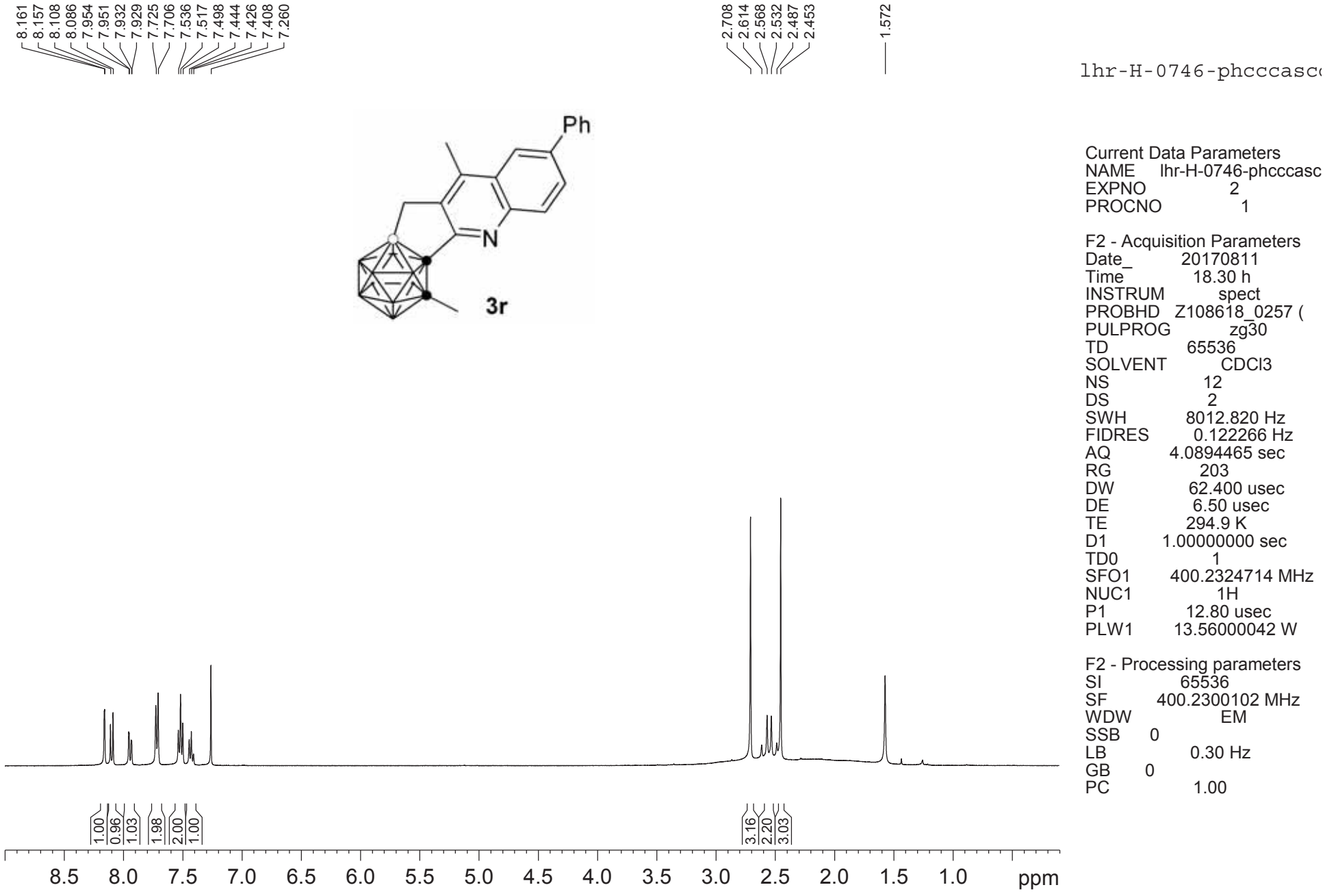
```
Current Data Parameters
NAME      lhr-B-cas-0396-OMe-CDCl
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20160622
Time              14.45 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG           zgdc
TD               65536
SOLVENT          CDCl3
NS                  12
DS                   4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                 287
DW               20.800 usec
DE                6.50 usec
TE               295.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1         55.09999847 W
SFO2        400.2316009 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                32768
SF          128.4097615 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-cas-0396-OMe-CDCl3(C)




```
Current Data Parameters
NAME      lhr-B-cas-0396-OMe-CDCl3(C
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_           20160622
Time              14.46 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   15
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  406
DW               20.800 usec
DE                6.50 usec
TE               294.7 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



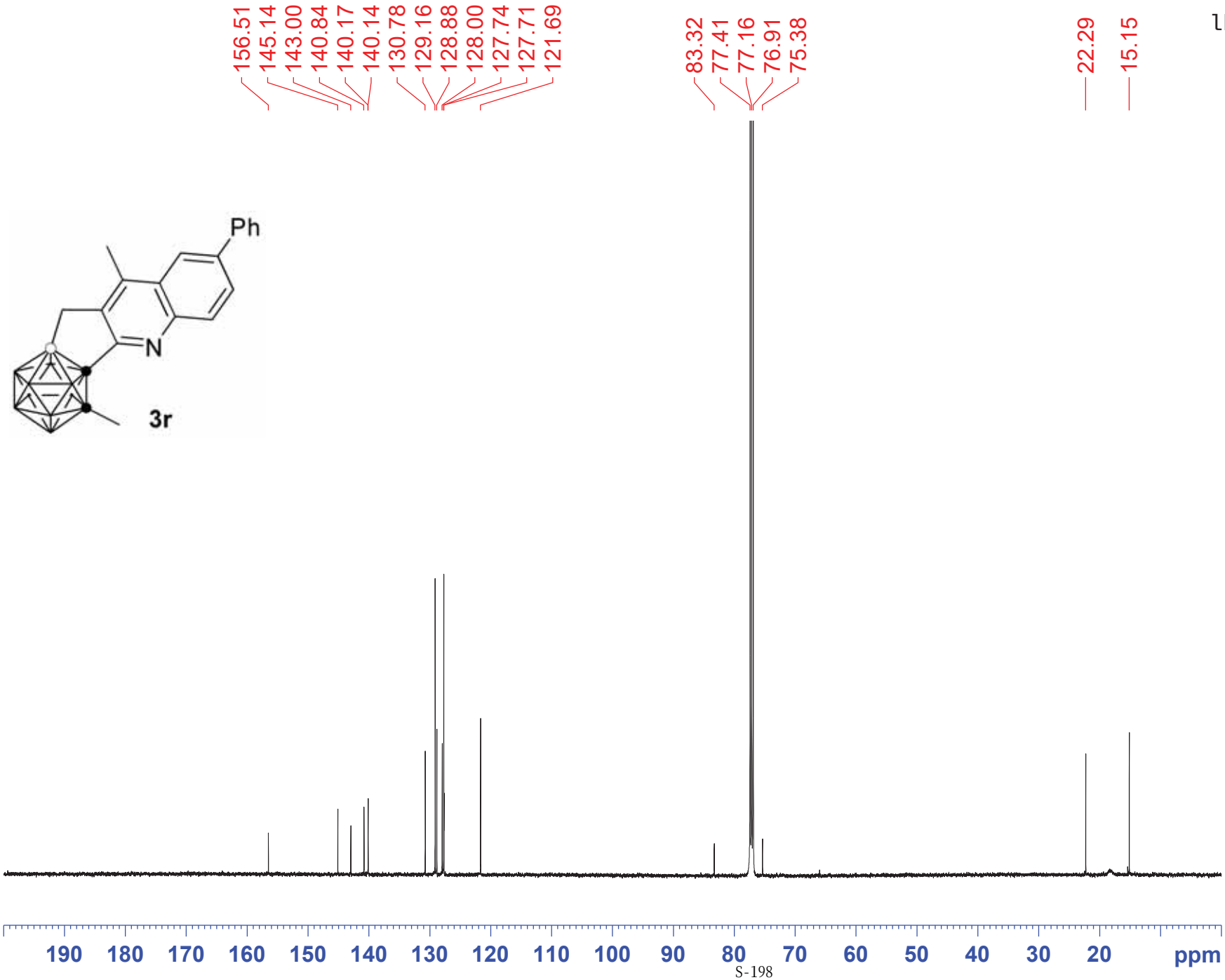


lhr-H-0746-phcccasc

Current Data Parameters
NAME lhr-H-0746-phcccasc
EXPNO 2
PROCNO 1

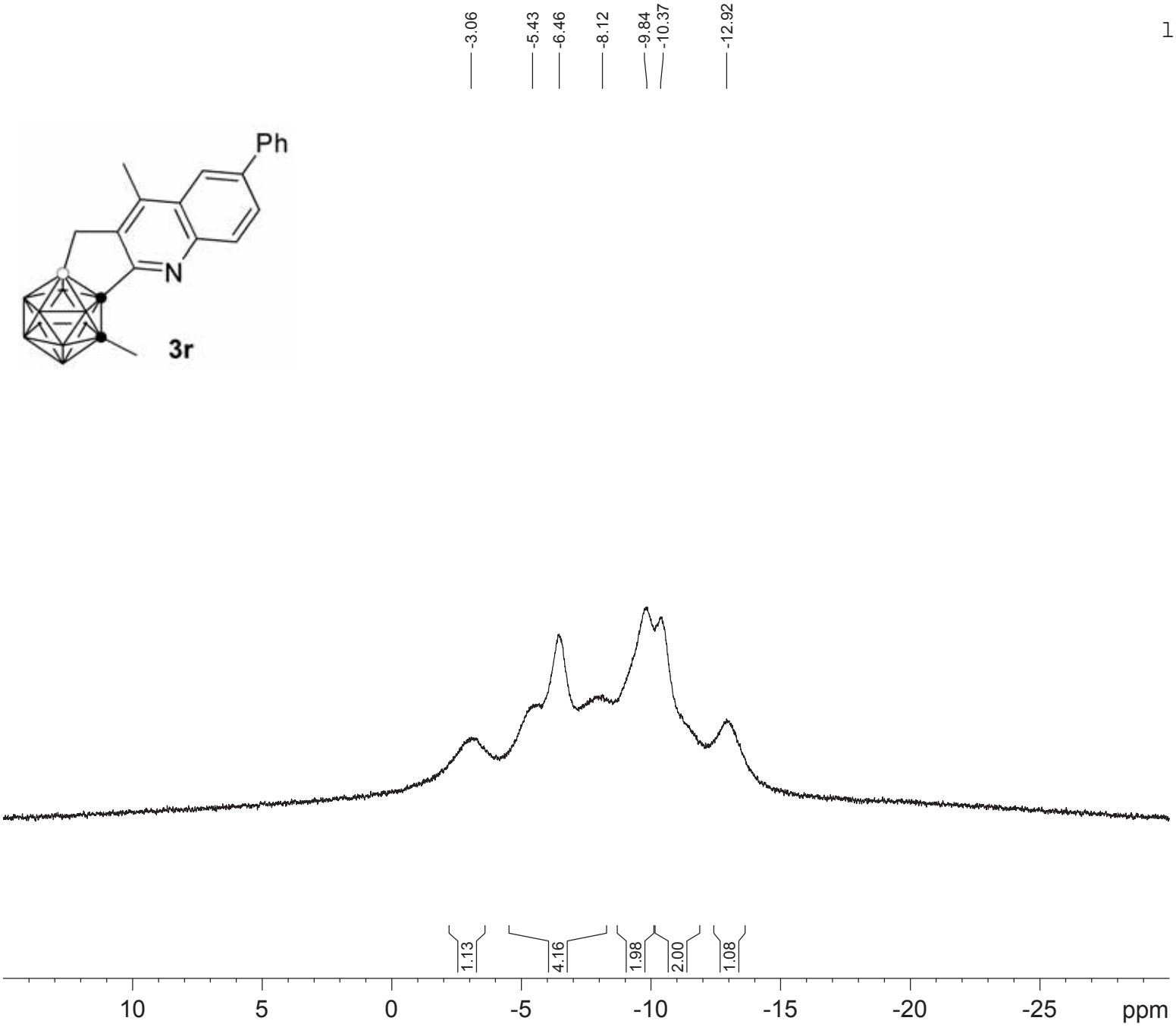
F2 - Acquisition Parameters
Date_ 20170811
Time 18.30 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



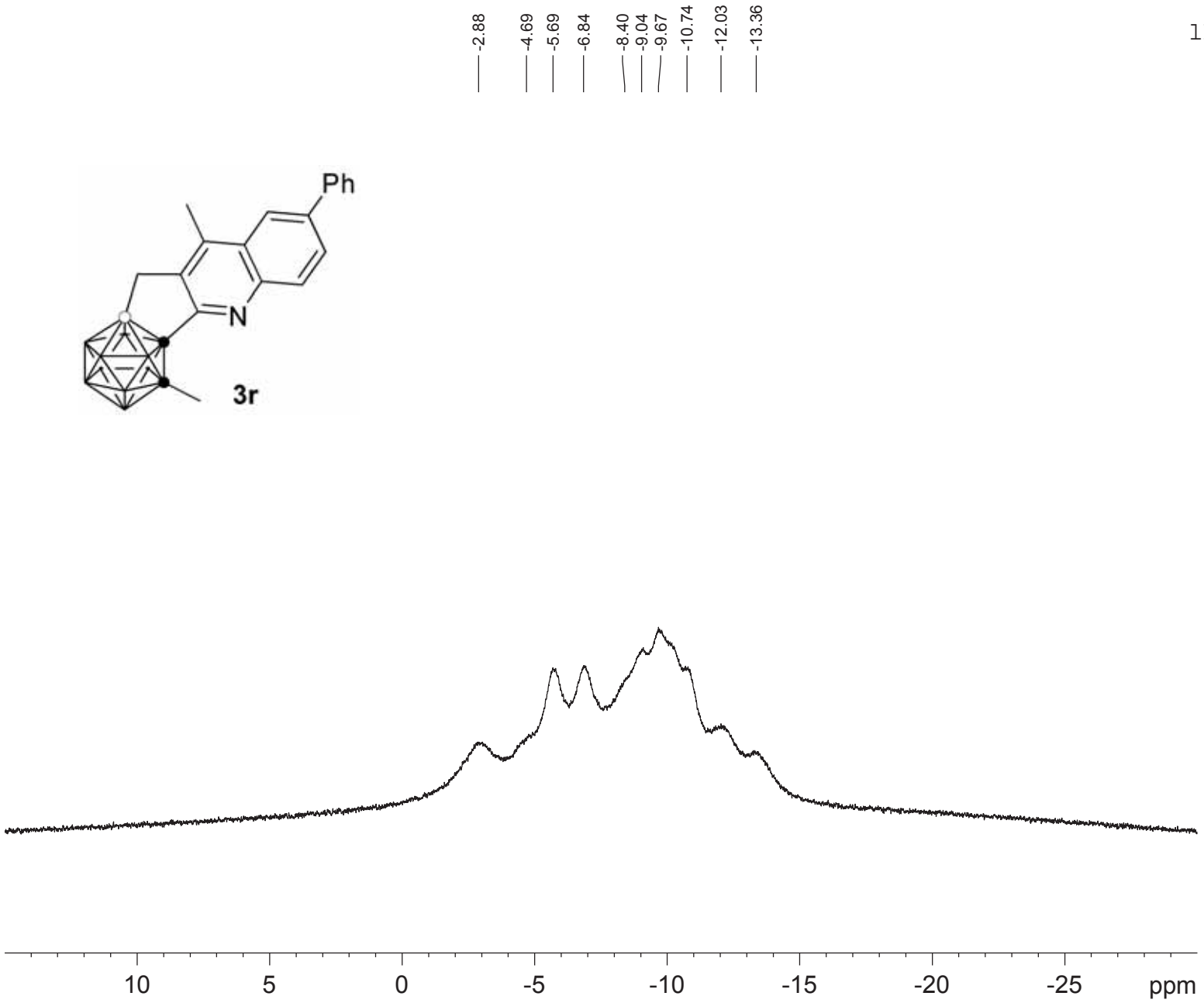
lhr-C-0746

```
Current Data Parameters
NAME                  lhr-C-0746
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20170810
Time                       11.29 h
INSTRUM                    spect
PROBHD    Z149001_0010 (
PULPROG                   zgpg30
TD                         65536
SOLVENT                    CDCl3
NS                          1024
DS                             4
SWH                    29761.904 Hz
FIDRES                  0.908261 Hz
AQ                     1.1010048 sec
RG                        206.72
DW                        16.800 usec
DE                        18.00 usec
TE                        298.0 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                            1
SFO1                125.7703643 MHz
NUC1                        13C
P1                        10.00 usec
PLW1                61.00000000 W
SFO2                500.1320005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                     80.00 usec
PLW2                15.00000000 W
PLW12                 0.33750001 W
PLW13                 0.16976000 W

F2 - Processing parameters
SI                         32768
SF                  125.7577722 MHz
WDW                           EM
SSB                0
LB                         1.00 Hz
GB                 0
PC                         1.40
```



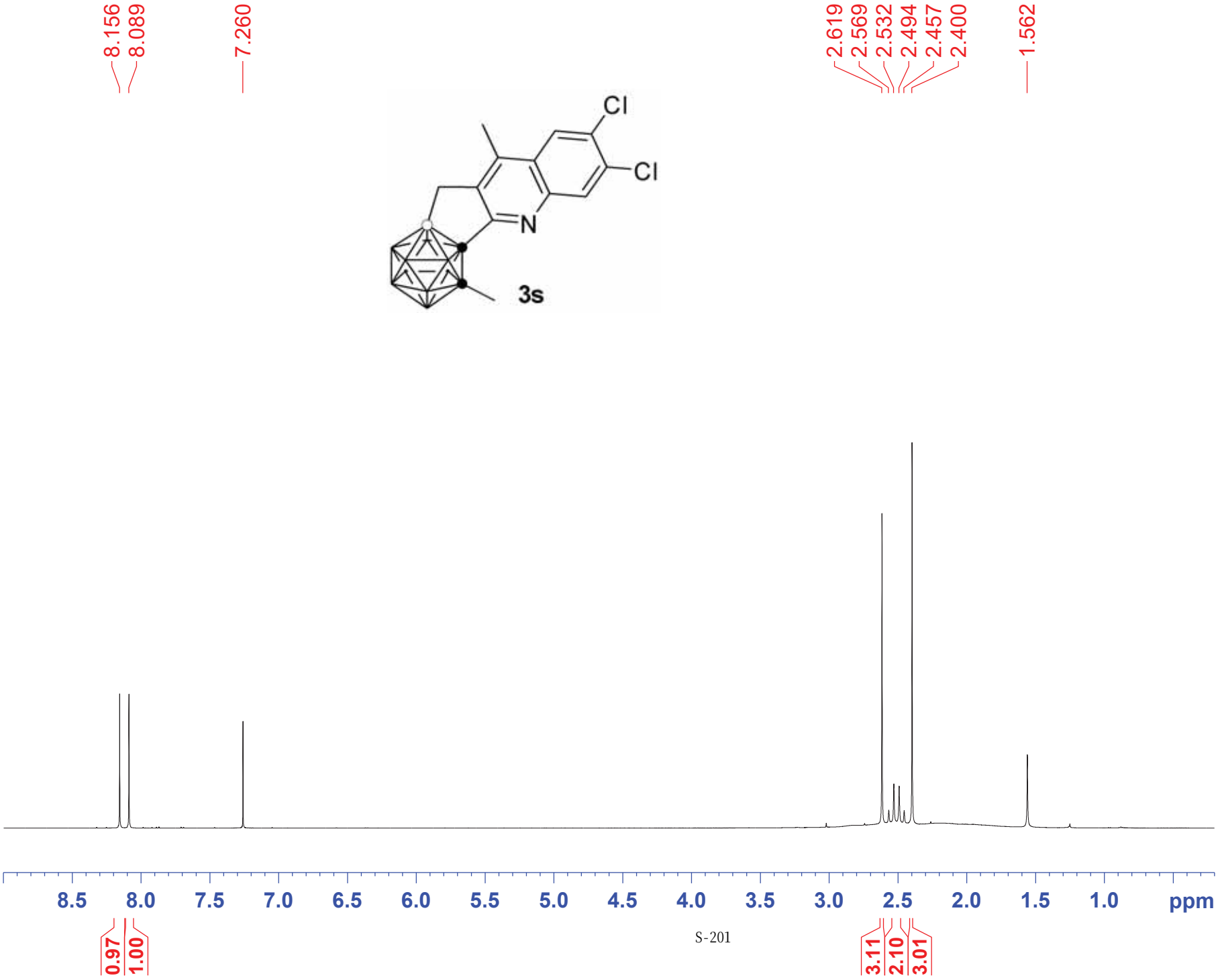
lhr-B-0746-phcccascdcl3

```
Current Data Parameters
NAME      lhr-B-0746-phcccascdcl3
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_              20170811
Time                   18.34 h
INSTRUM                spect
PROBHD    Z108618_0257 (
PULPROG                 zgdc
TD                     65536
SOLVENT                CDCl3
NS                        36
DS                         4
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                       322
DW                    20.800 usec
DE                     6.50 usec
TE                    295.6 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             128.4096890 MHz
NUC1                     11B
P1                     7.50 usec
PLW1              55.09999847 W
SFO2             400.2316009 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              13.56000042 W
PLW12              0.27428001 W

F2 - Processing parameters
SI                       32768
SF               128.4097615 MHz
WDW                         EM
SSB       0
LB                      1.00 Hz
GB        0
PC                      1.40
```



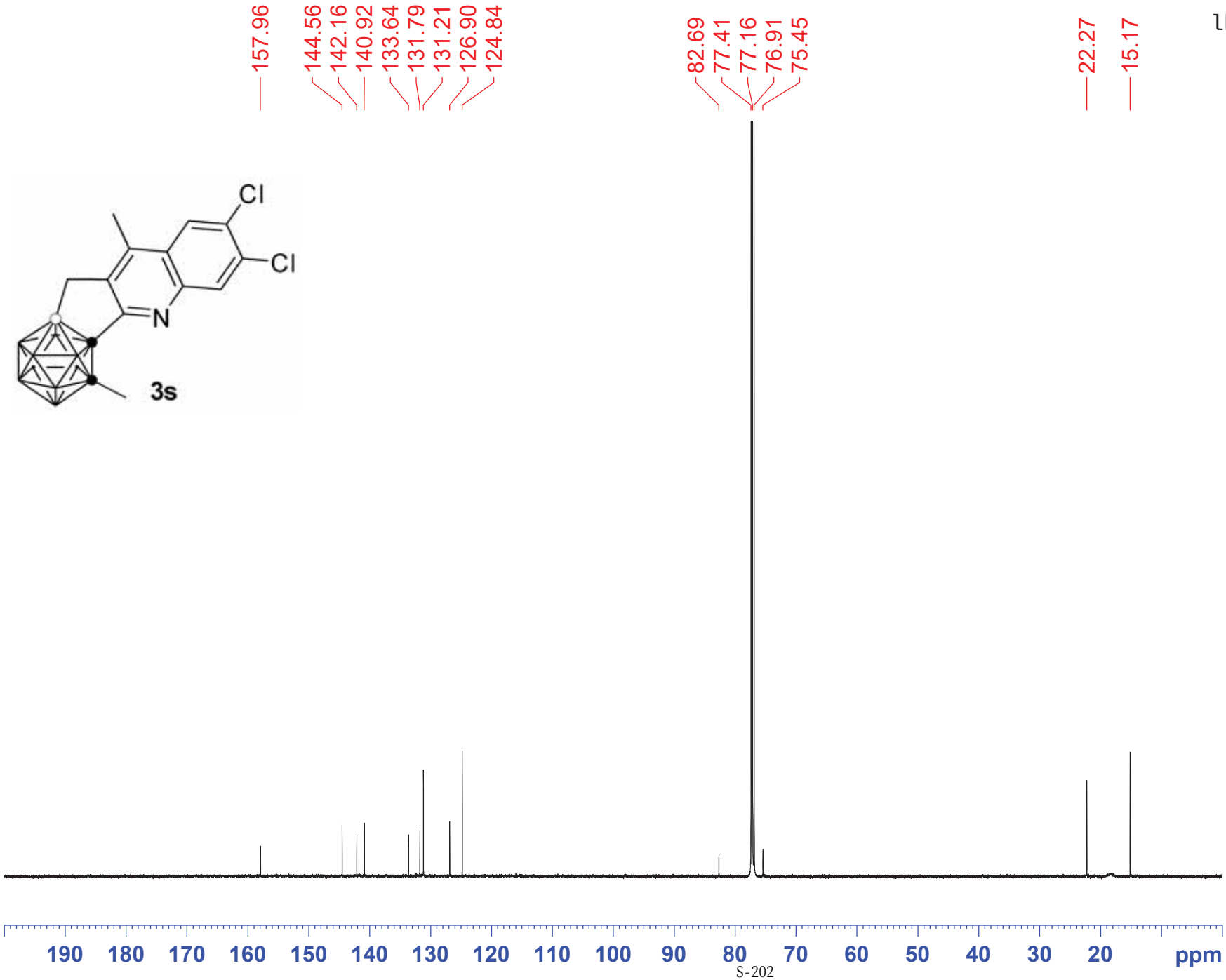
lhr-B-0746-phcccascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0746-phcccascdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170811
Time              18.37 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     47
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    322
DW                20.800 usec
DE                 6.50 usec
TE                295.2 K
D1            2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                 11B
P1                  7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



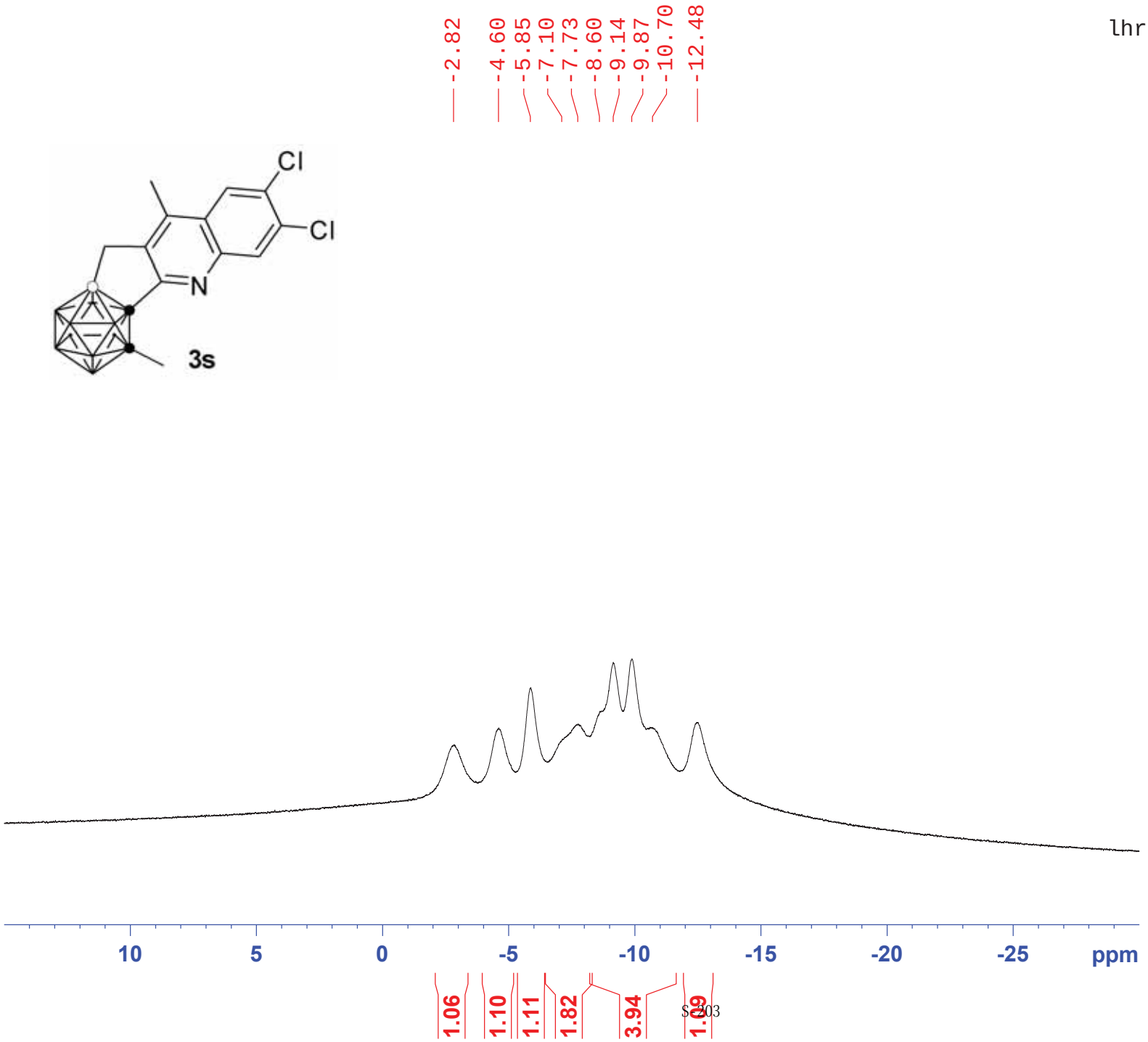
lhr-H-0764-cas

```
Current Data Parameters
NAME      lhr-H-0754-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20170922
Time                9.29
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH             10000.000
FIDRES          0.305176
AQ              3.2767999
RG                 30.85
DW                50.000
DE                10.00
TE                298.0
D1             1.00000000
TD0                    1
SFO1          500.1330883
NUC1                  1H
P1                 12.00
PLW1          15.00000000

F2 - Processing paramete
SI                 65536
SF          500.1300124
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```



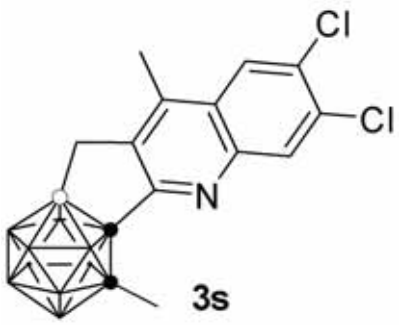
lhr-C-0754-cas

```
Current Data Parameters
NAME      lhr-C-0754-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170922
Time               9.55 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  450
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577718 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



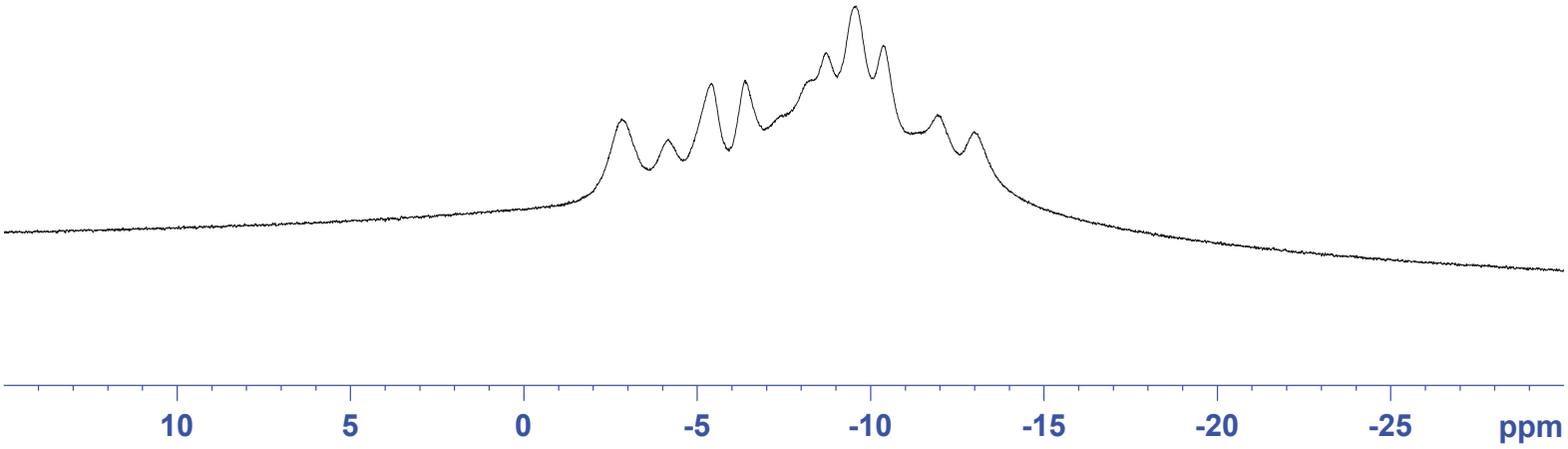
lhr-B-0754-cas

```
Current Data Parameters
NAME      lhr-B-0754-cas
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170922
Time                9.58 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    20
DS                     4
SWH            23809.523 Hz
FIDRES          0.726609 Hz
AQ             1.3762560 sec
RG                186.15
DW                21.000 usec
DE                18.00 usec
TE                298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         160.4599621 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                 32768
SF          160.4615719 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

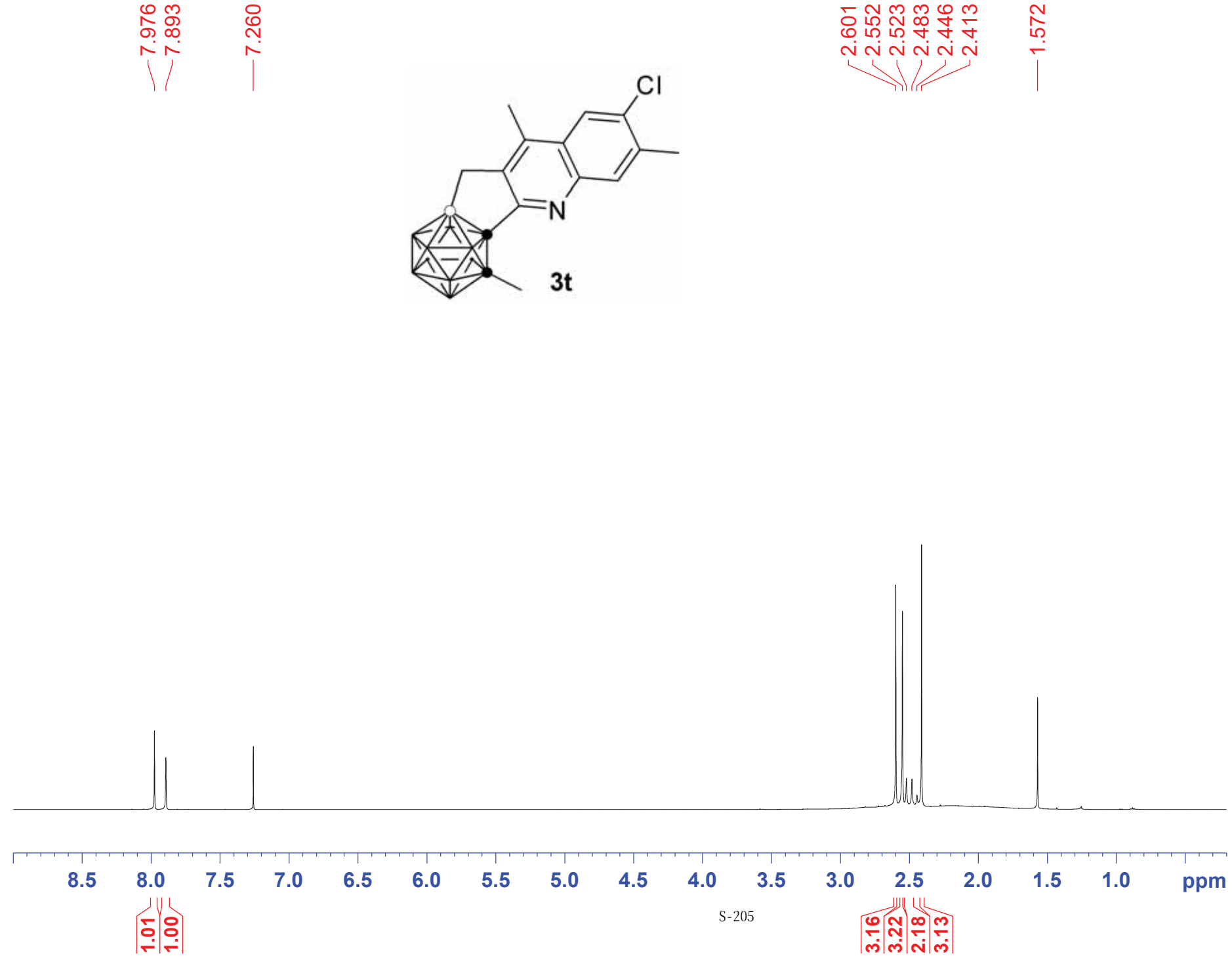


-2.82
-4.11
-5.40
-6.38
-7.39
-8.16
-8.69
-9.57
-10.36
-11.33
-11.92
-12.98

lhr-B-0754-cas(c)

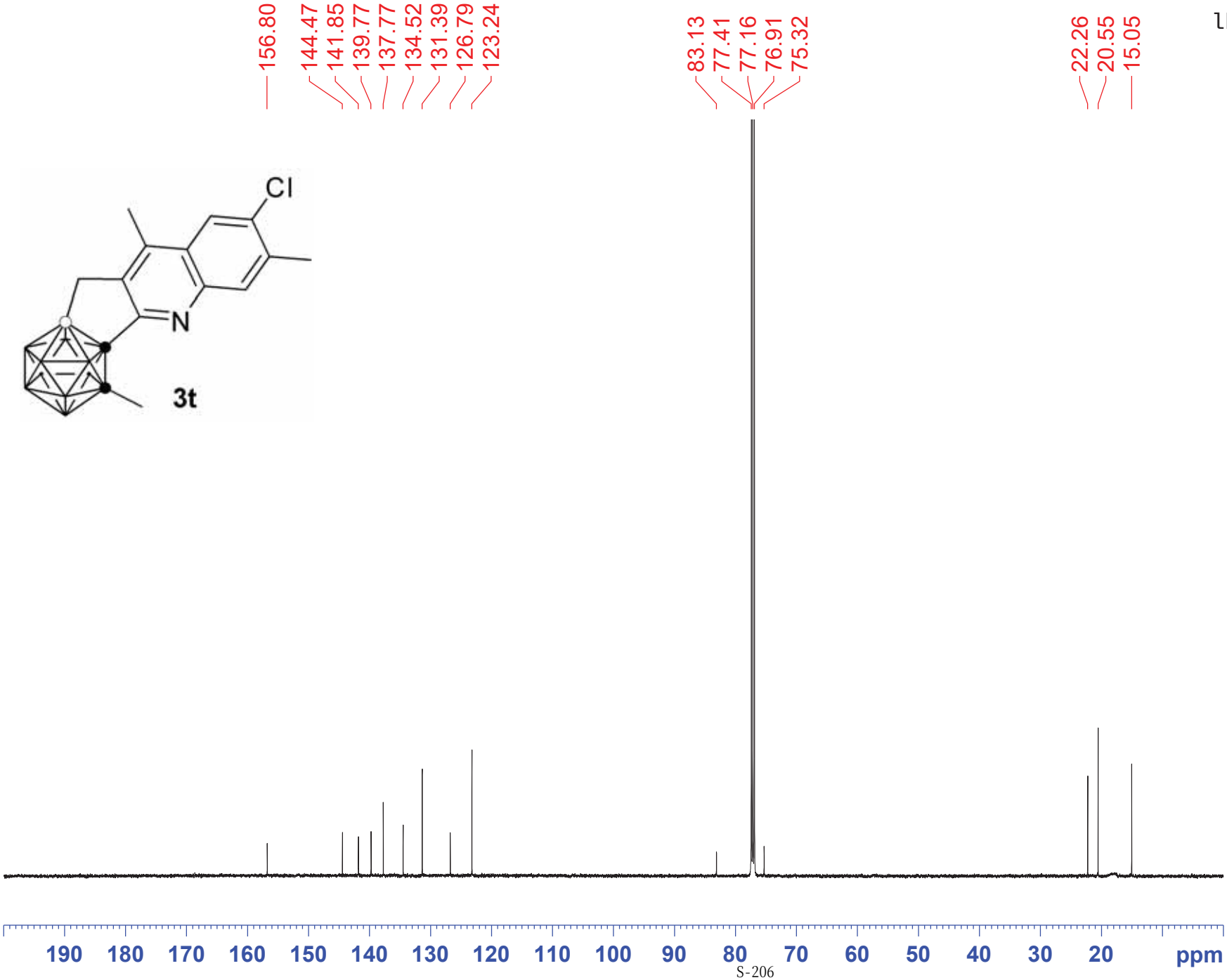



```
Current Data Parameters
NAME      lhr-B-0754-cas(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170922
Time                 9.59 h
INSTRUM              spect
PROBHD   Z149001_0010 (
PULPROG                 zg
TD                   32768
SOLVENT              CDCl3
NS                      20
DS                       4
SWH              24038.461 Hz
FIDRES            1.467191 Hz
AQ               0.6815744 sec
RG                  186.15
DW                  20.800 usec
DE                  18.00 usec
TE                  298.0 K
D1              1.00000000 sec
TD0                      1
SFO1           160.4615792 MHz
NUC1                   11B
P1                  10.00 usec
PLW1           50.00000000 W

F2 - Processing parameters
SI                   16384
SF             160.4615792 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



lhr-H-0783-cas

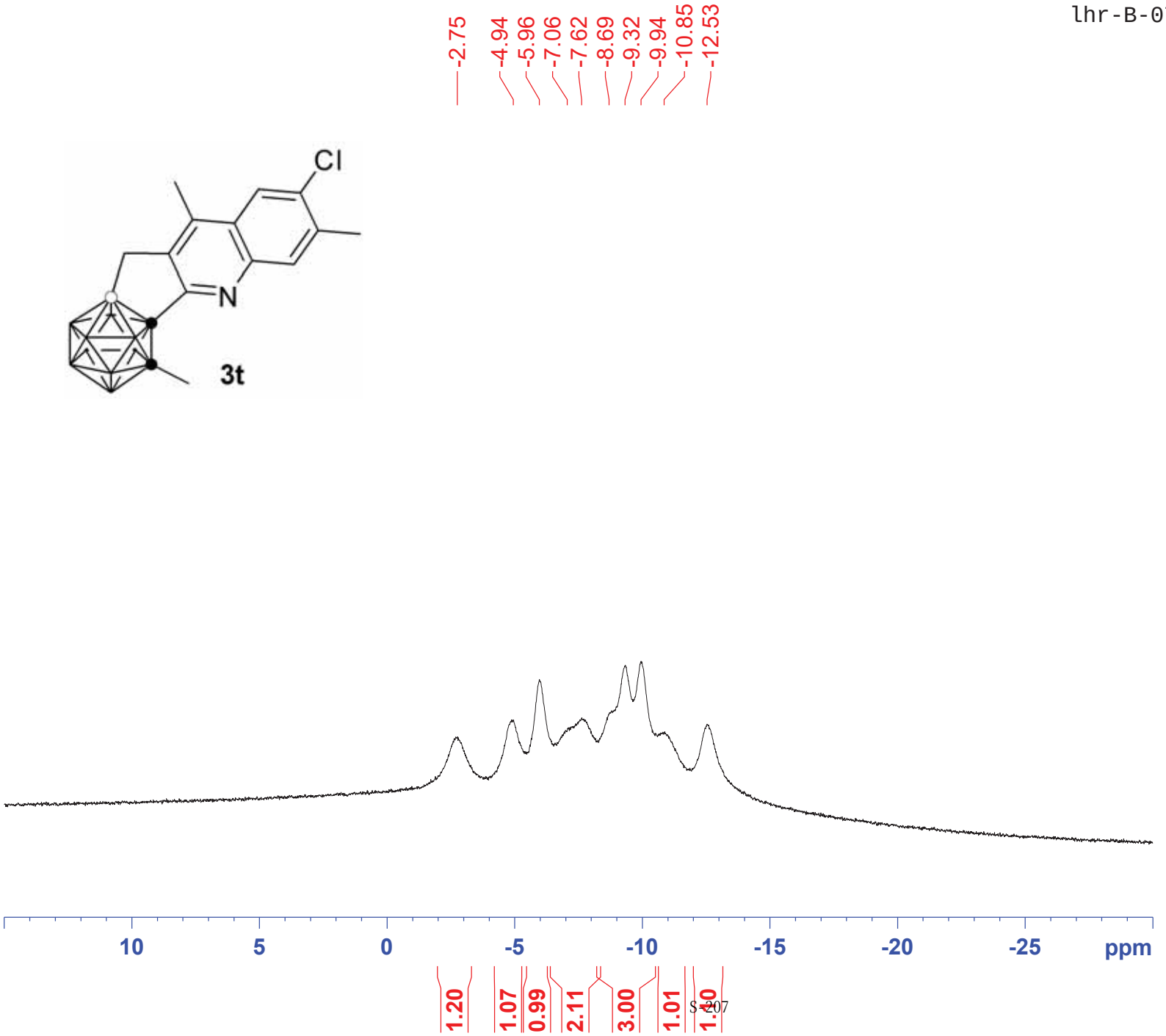
```
Current Data Parameters
NAME      lhr-H-0783-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20171021
Time               10.22
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 30.85
DW                 50.000
DE                 10.00
TE                298.0
D1            1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1         15.00000000

F2 - Processing paramete
SI                 65536
SF         500.1300125
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```



lhr-C-0783-cas

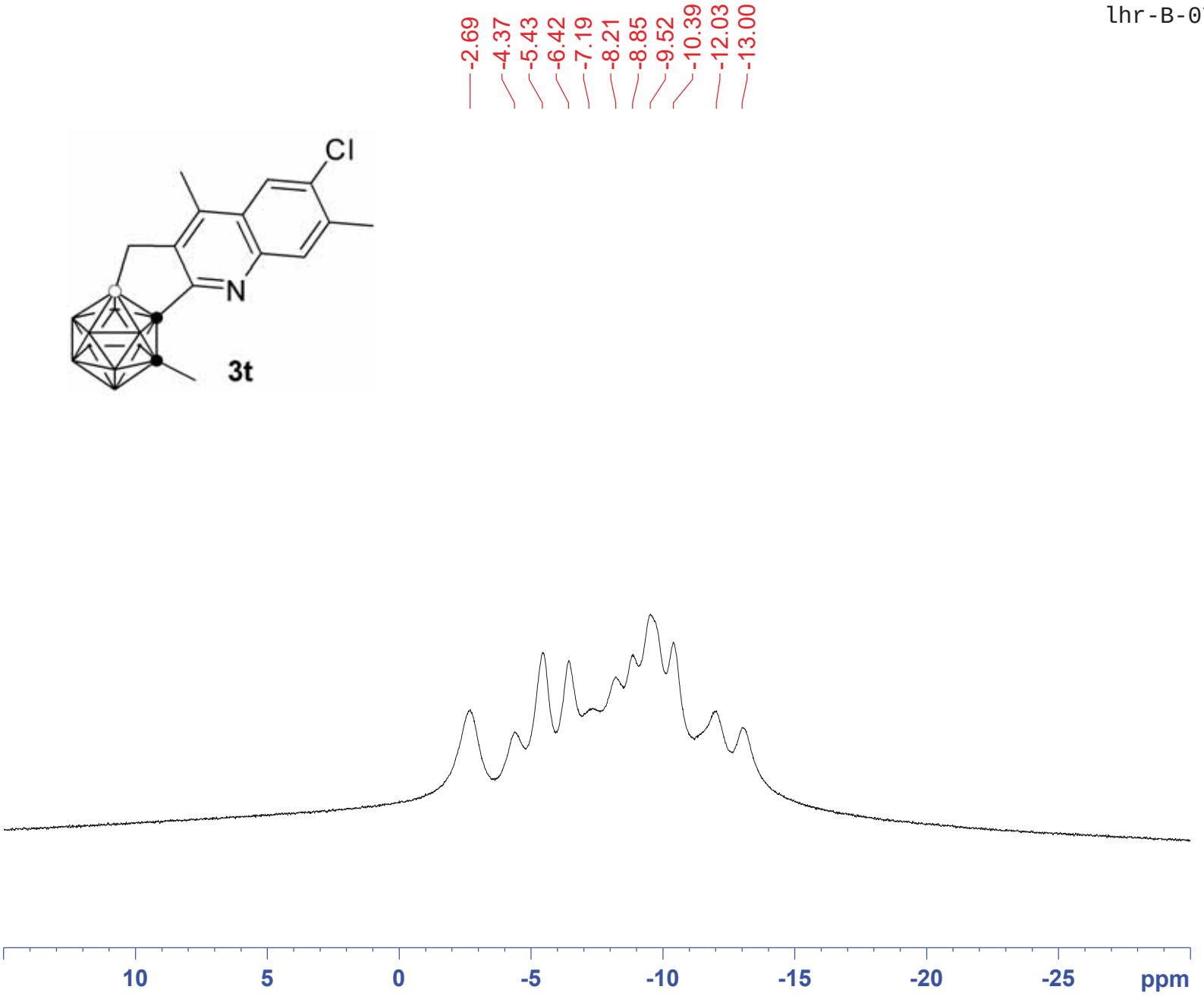
```
Current Data Parameters
NAME      lhr-C-0783-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171021
Time              10.41 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  360
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577721 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-0783-cas

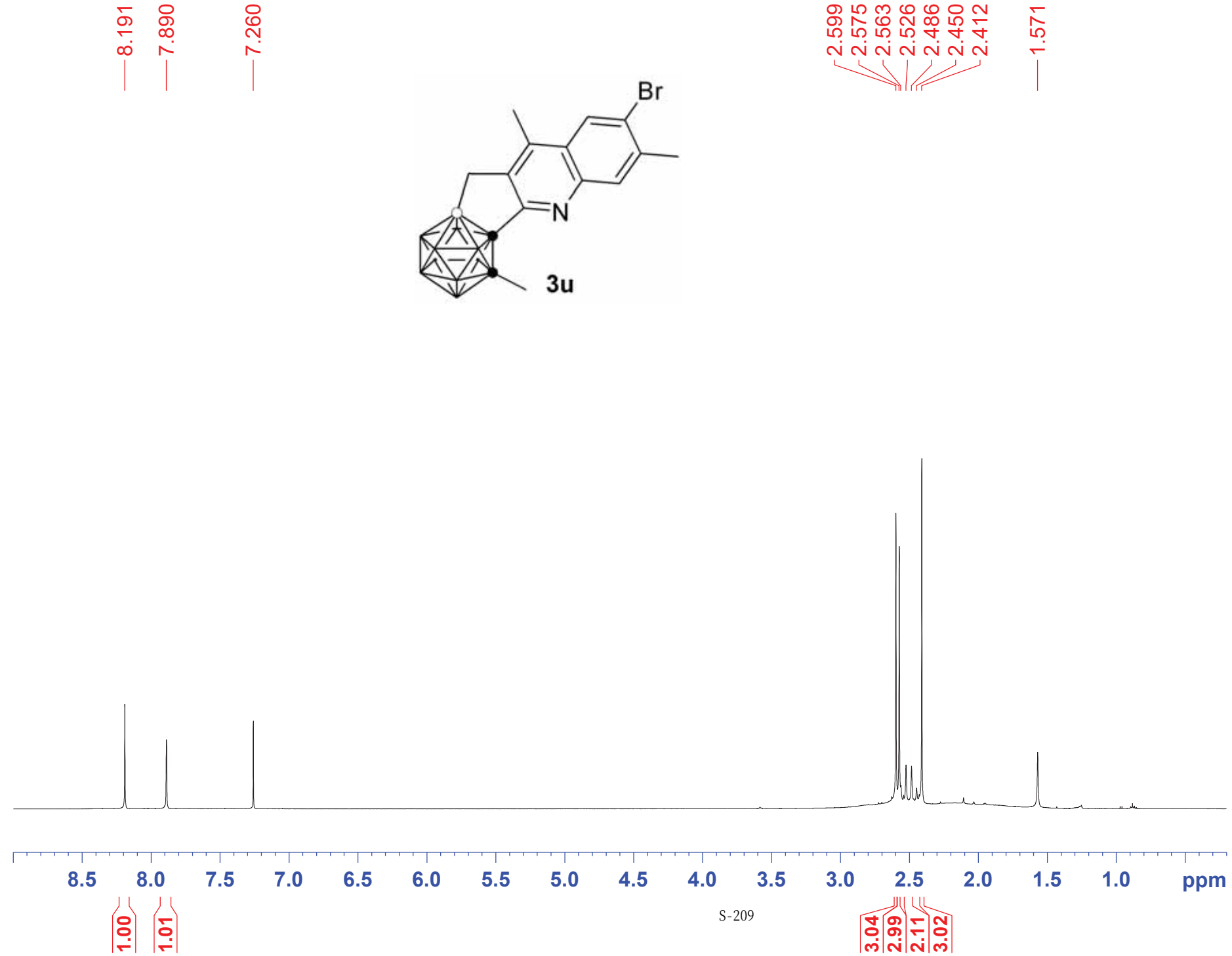



```
Current Data Parameters
NAME      lhr-B-0783-cas
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20171021
Time             10.43 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                  20
DS                   4
SWH          24038.461 Hz
FIDRES        1.467191 Hz
AQ           0.6815744 sec
RG              206.72
DW              20.800 usec
DE              18.00 usec
TE              298.0 K
D1          1.00000000 sec
D11         0.03000000 sec
TD0                  1
SFO1       160.4615790 MHz
NUC1              11B
P1              10.00 usec
PLW1       50.00000000 W
SFO2       500.1320005 MHz
NUC2              1H
CPDPRG[2       waltz16
PCPD2           80.00 usec
PLW2       15.00000000 W
PLW12       0.33750001 W
PLW13       0.16976000 W

F2 - Processing parameters
SI               16384
SF         160.4615792 MHz
WDW                EM
SSB      0
LB              1.00 Hz
GB       0
PC              1.40
```

lhr-B-0783-cas(c)

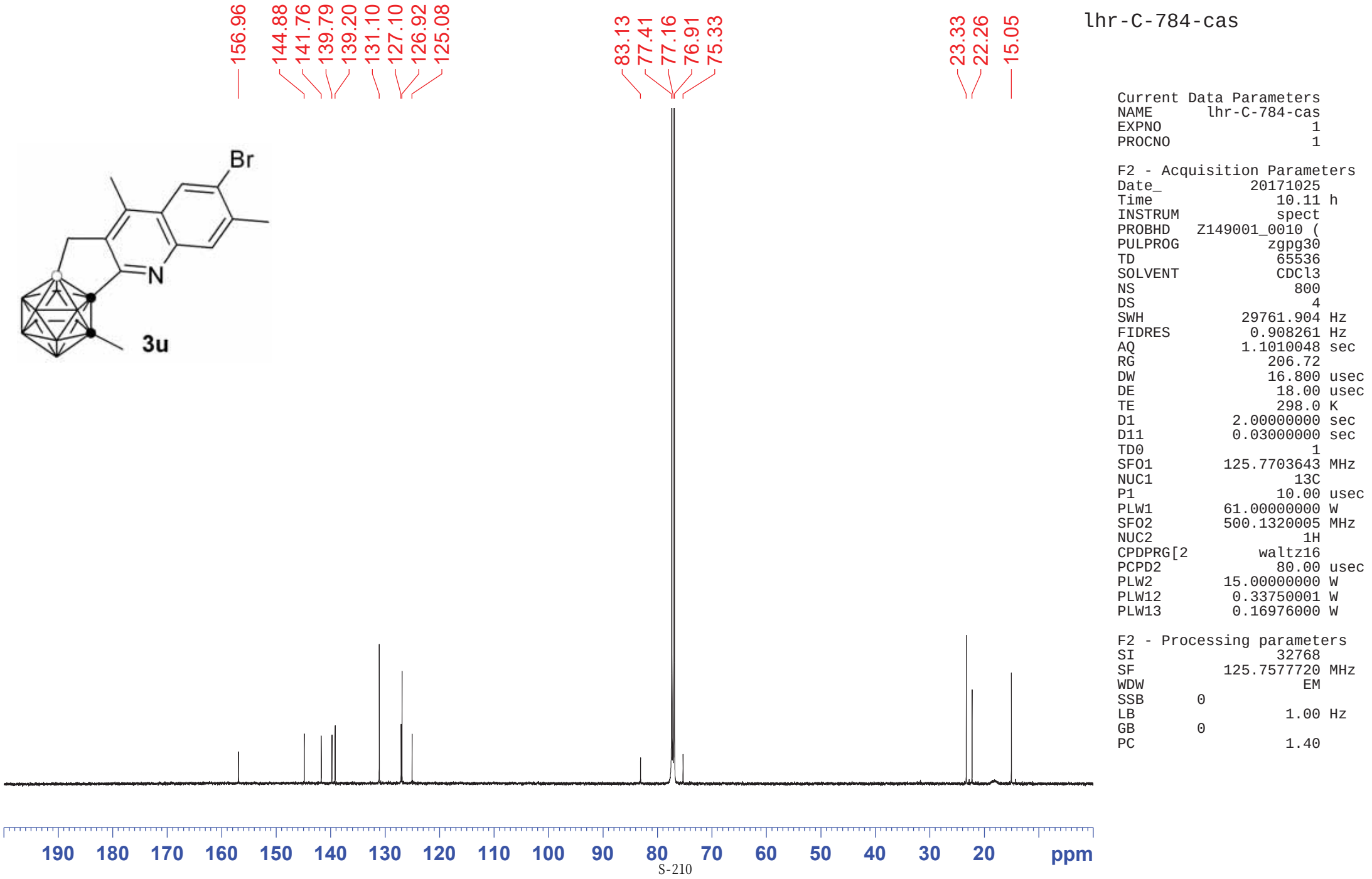



```
Current Data Parameters
NAME      lhr-B-0783-cas(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171021
Time                10.44 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                 186.15
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1            1.00000000 sec
TD0                     1
SFO1          160.4615792 MHz
NUC1                  11B
P1                 10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                  16384
SF            160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



lhr-H-784-cas

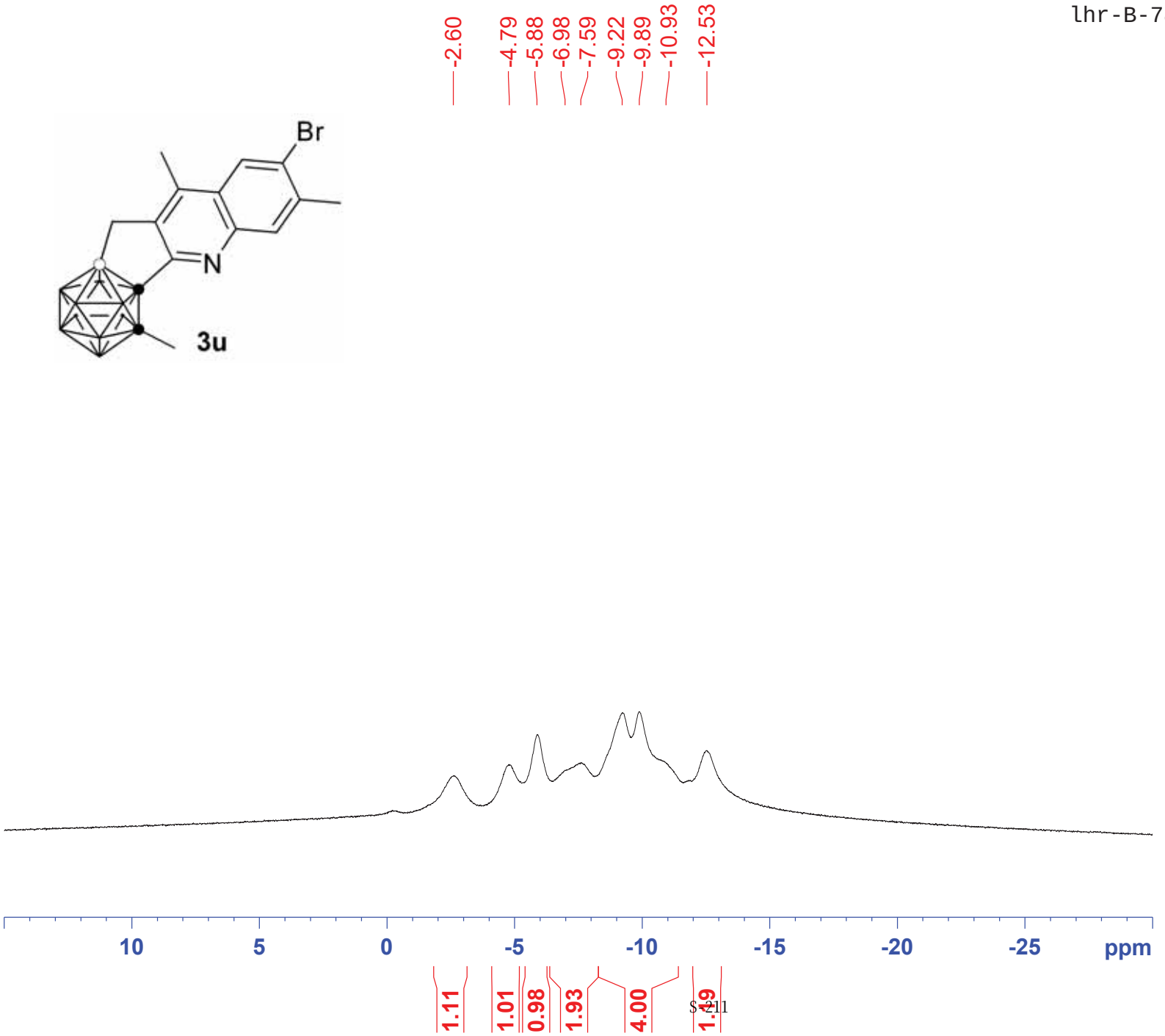
```
Current Data Parameters
NAME      lhr-H-784-cas
EXPNO                 1
PROCNO                1

F2 - Acquisition Paramet
Date_          20171025
Time               9.26
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000
FIDRES         0.305176
AQ             3.2767999
RG                30.85
DW                50.000
DE                10.00
TE                298.0
D1           1.00000000
TD0                   1
SFO1        500.1330883
NUC1               1H
P1                12.00
PLW1         15.00000000

F2 - Processing paramete
SI                65536
SF         500.1300127
WDW                EM
SSB       0
LB                0.30
GB        0
PC                1.00
```



lhr-C-784-cas

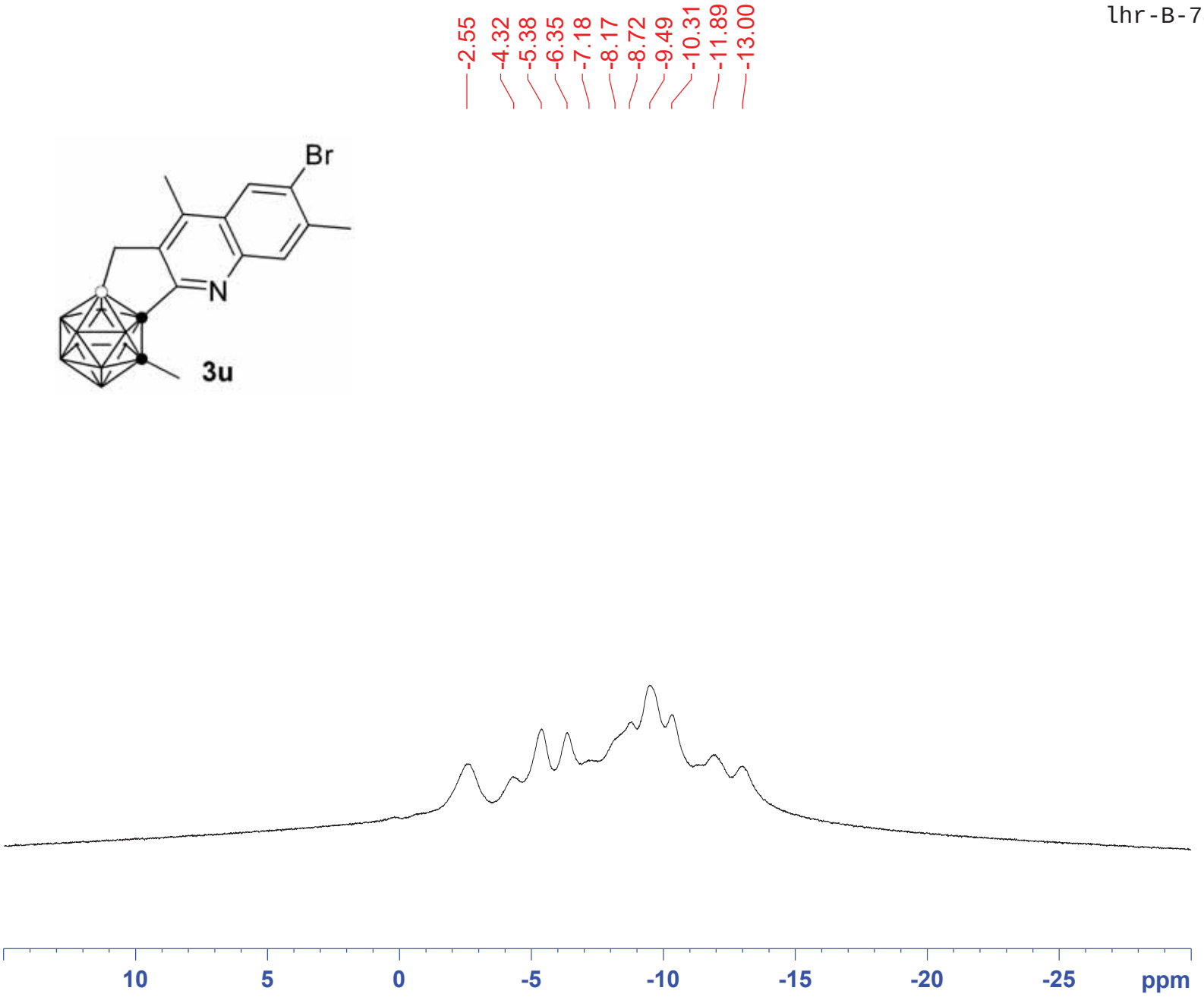
```
Current Data Parameters
NAME      lhr-C-784-cas
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20171025
Time              10.11 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  800
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577720 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

lhr-B-784-cas

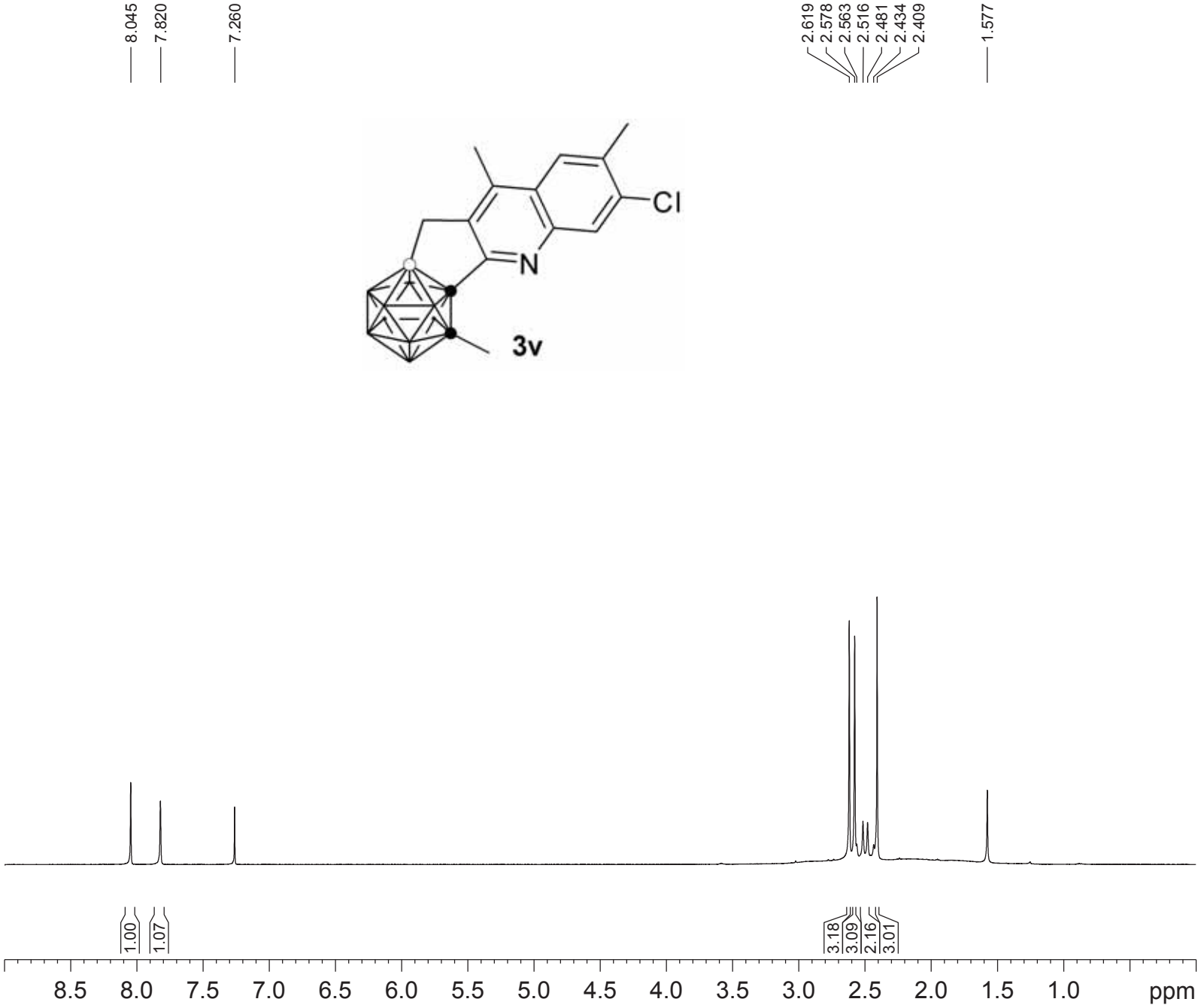



```
Current Data Parameters
NAME       lhr-B-784-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171025
Time               9.21 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG            zgig
TD                32768
SOLVENT            None
NS                   20
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               186.15
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        160.4615790 MHz
NUC1               11B
P1               10.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W

F2 - Processing parameters
SI                16384
SF          160.4615792 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

lhr-B-784-cas(c)




```
Current Data Parameters
NAME      lhr-B-784-cas(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171025
Time                9.22 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG               zg
TD                 32768
SOLVENT             None
NS                    20
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                186.15
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        160.4615792 MHz
NUC1                11B
P1                10.00 usec
PLW1        50.00000000 W

F2 - Processing parameters
SI                 16384
SF          160.4615792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

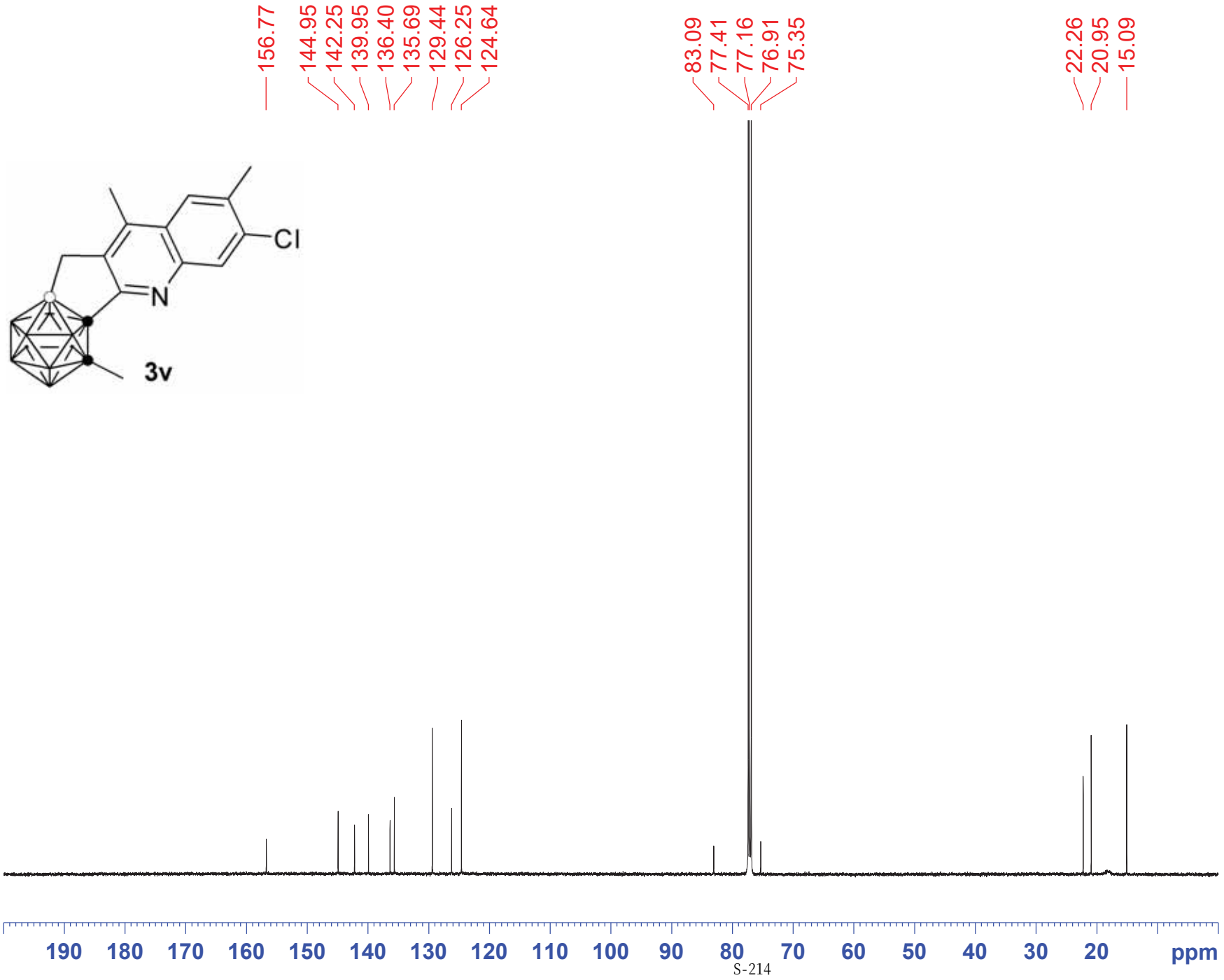


lhr-H-0795-cccascdcl

Current Data Parameters
NAME lhr-H-0795-cccascdcl3
EXPNO 1
PROCNO 1

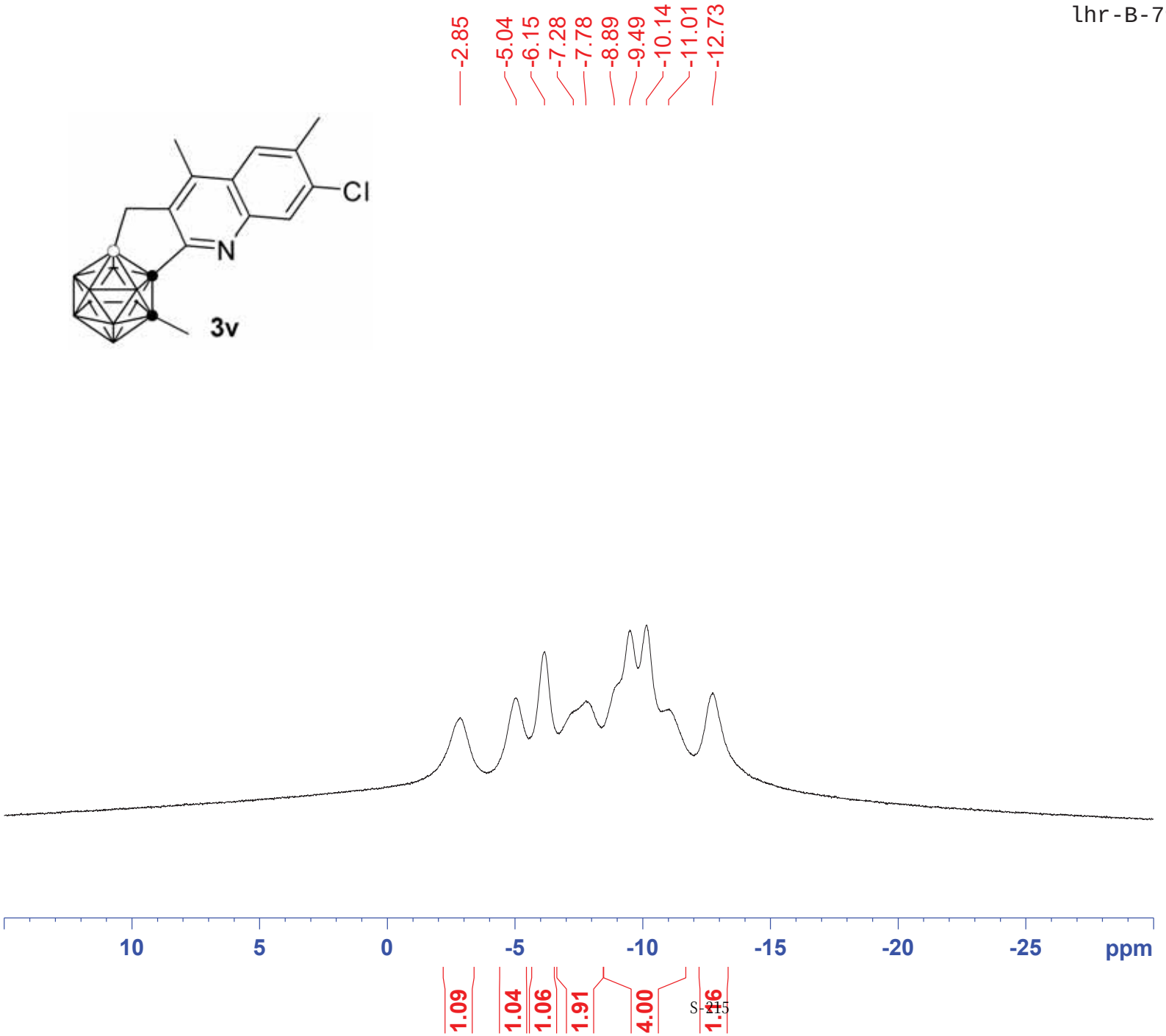
F2 - Acquisition Parameters
Date_ 20171026
Time 21.32 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300104 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



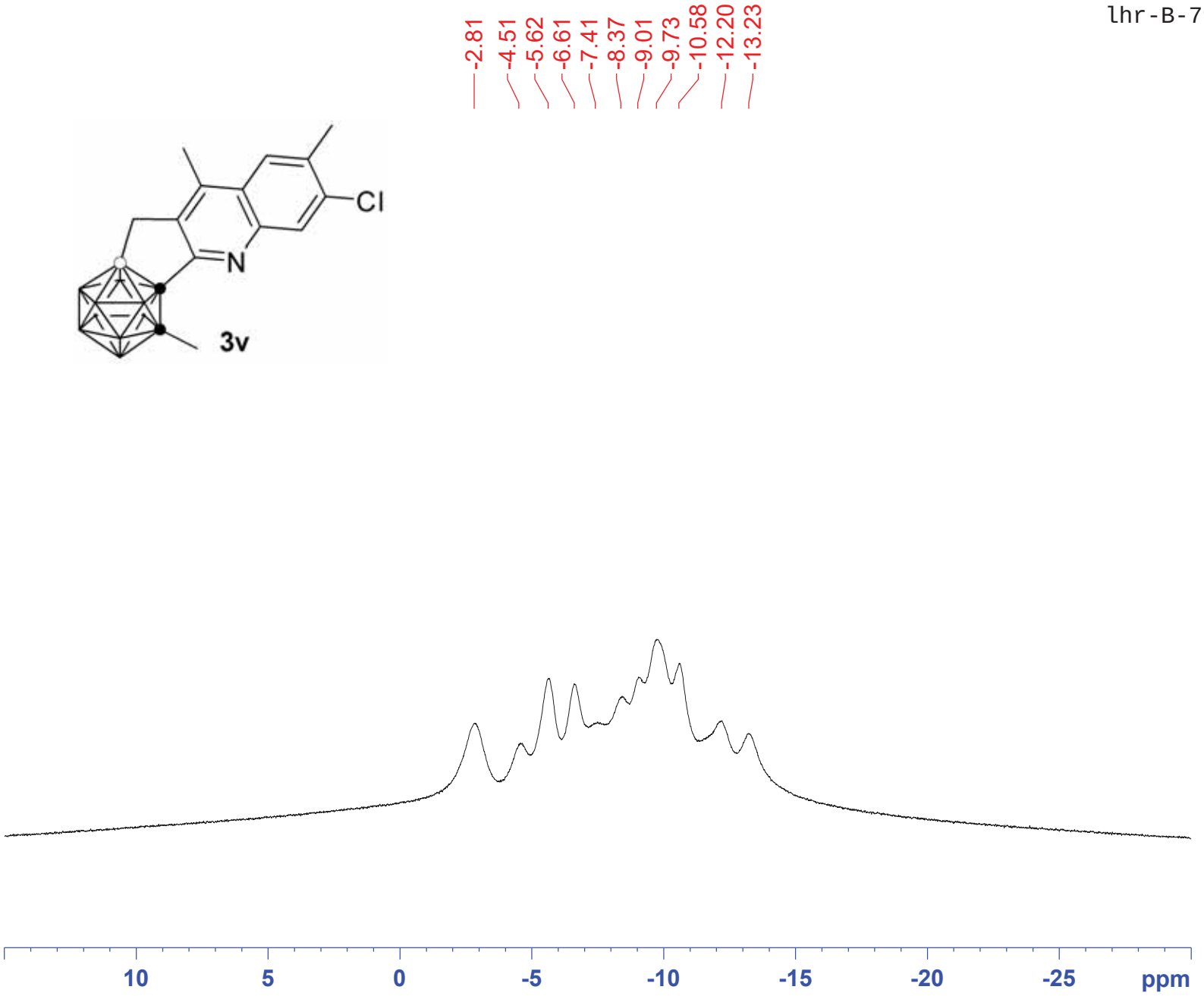

```
Current Data Parameters
NAME                  lhr-795
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_                20171027
Time                    2.26 h
INSTRUM                 spect
PROBHD    Z149001_0010 (
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        600
DS                          4
SWH                 29761.904 Hz
FIDRES                0.908261 Hz
AQ                  1.1010048 sec
RG                     206.72
DW                     16.800 usec
DE                     18.00 usec
TE                     298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1
SFO1              125.7703643 MHz
NUC1                      13C
P1                     10.00 usec
PLW1              61.00000000 W
SFO2              500.1320005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  80.00 usec
PLW2              15.00000000 W
PLW12              0.33750001 W
PLW13              0.16976000 W

F2 - Processing parameters
SI                        32768
SF                125.7577721 MHz
WDW                          EM
SSB           0
LB                      1.00 Hz
GB            0
PC                      1.40
```

lhr-B-795-cas

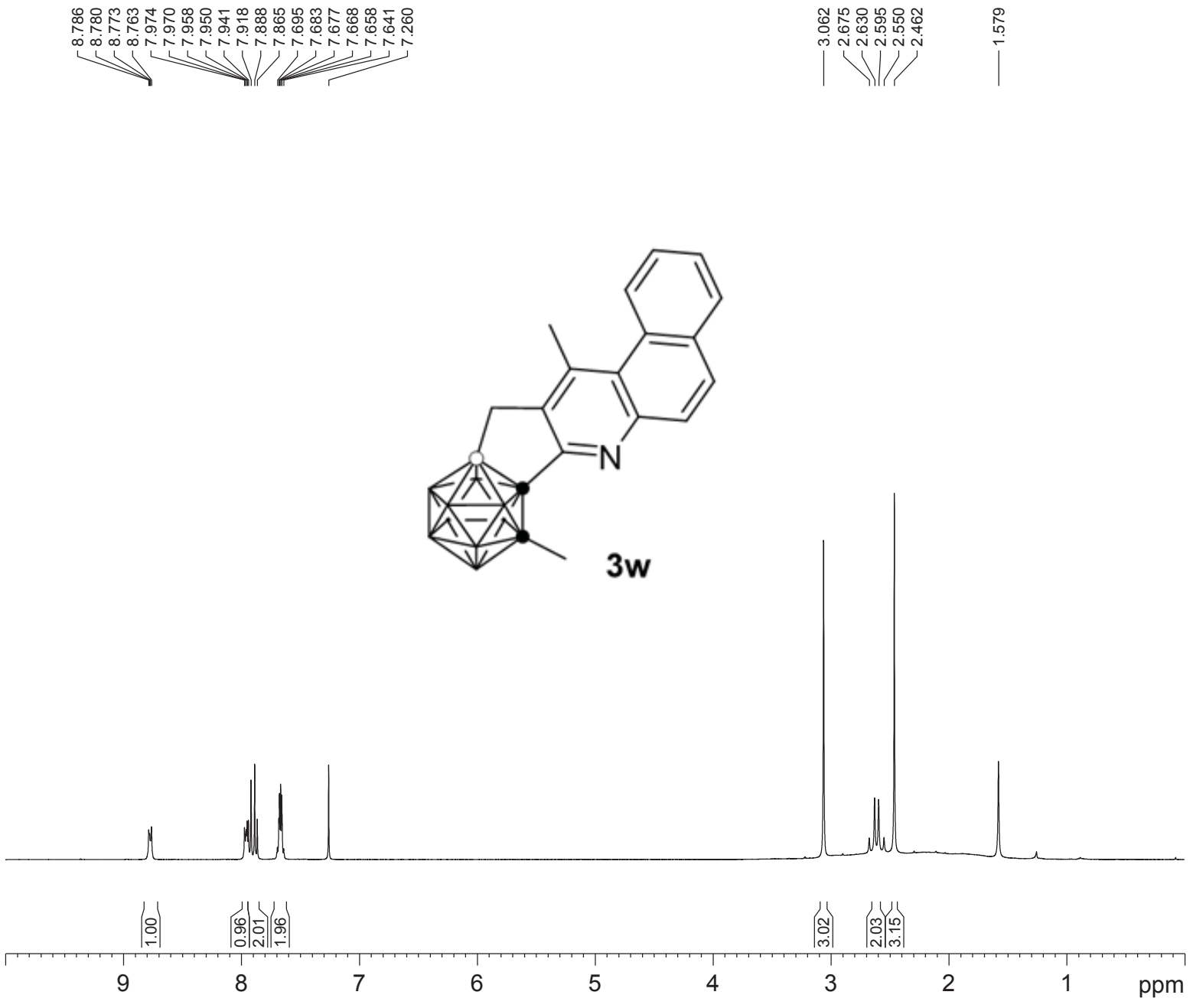



```
Current Data Parameters
NAME       lhr-B-795-cas
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171027
Time               9.18 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG            zgig
TD                32768
SOLVENT            None
NS                   20
DS                    4
SWH           24038.461 Hz
FIDRES         1.467191 Hz
AQ            0.6815744 sec
RG               186.15
DW               20.800 usec
DE               18.00 usec
TE               298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        160.4615790 MHz
NUC1               11B
P1               10.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W

F2 - Processing parameters
SI                16384
SF          160.4615792 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

lhr-B-795-cas(c)




```
Current Data Parameters
NAME      lhr-B-795-cas(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171027
Time                 9.19 h
INSTRUM              spect
PROBHD   Z149001_0010 (
PULPROG                 zg
TD                   32768
SOLVENT               None
NS                      20
DS                       4
SWH              24038.461 Hz
FIDRES            1.467191 Hz
AQ               0.6815744 sec
RG                  186.15
DW                  20.800 usec
DE                  18.00 usec
TE                  298.0 K
D1             1.00000000 sec
TD0                      1
SFO1          160.4615792 MHz
NUC1                  11B
P1                  10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                   16384
SF            160.4615792 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

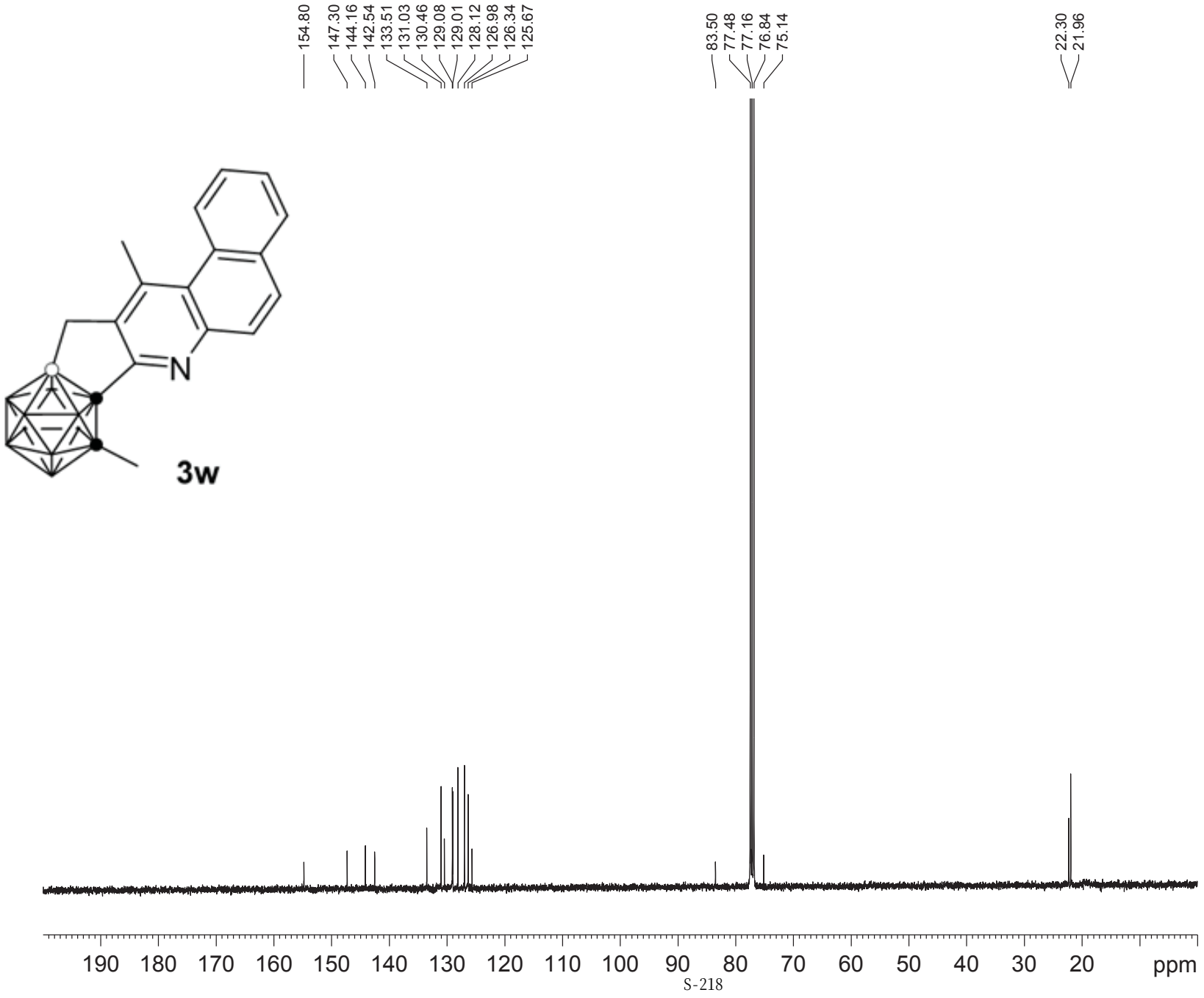


lhr-H-0735-napcascd

Current Data Parameters
NAME lhr-H-0735-napcasc
EXPNO 1
PROCNO 1

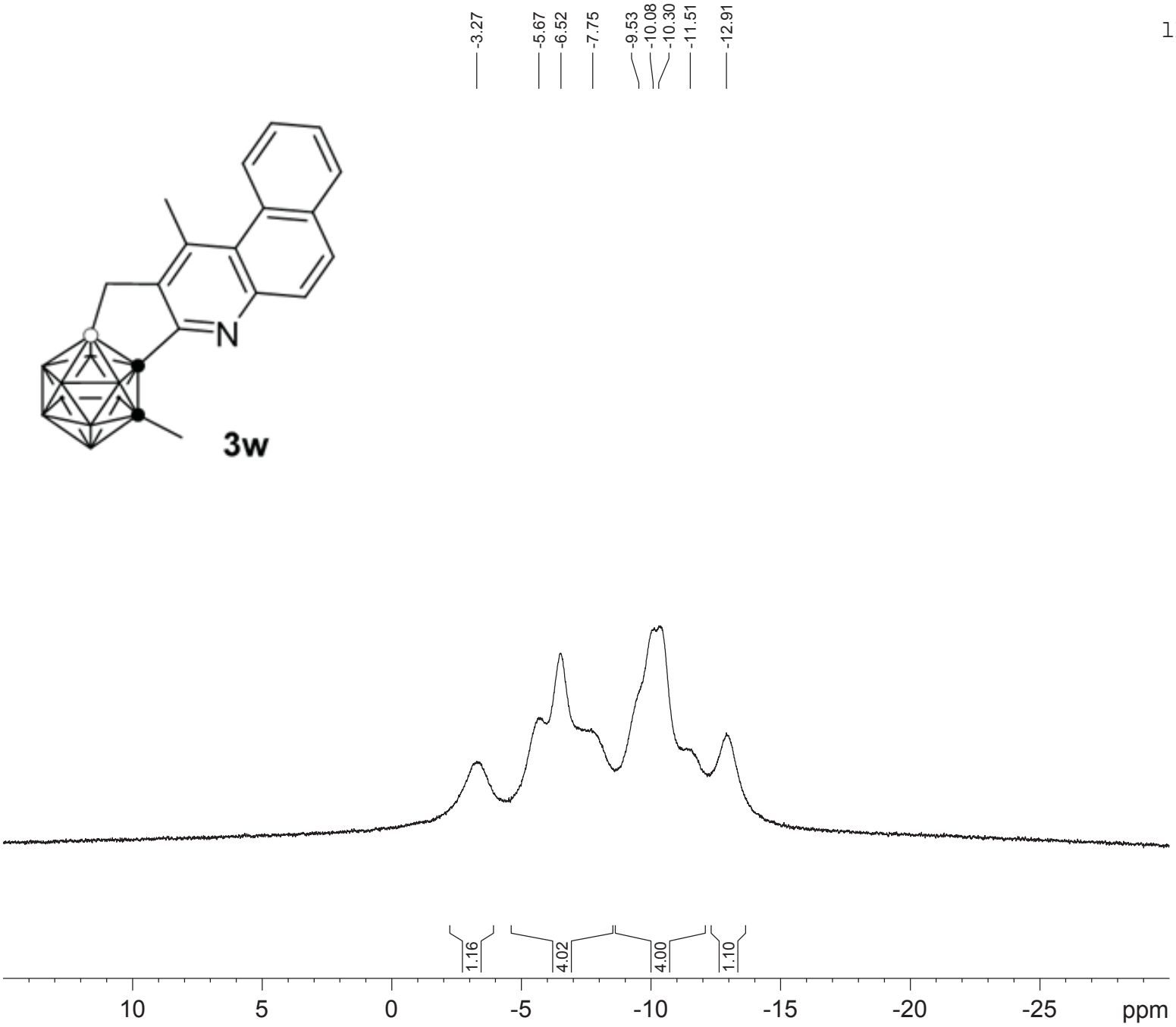
F2 - Acquisition Parameters
Date_ 20170724
Time 21.21 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300106 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



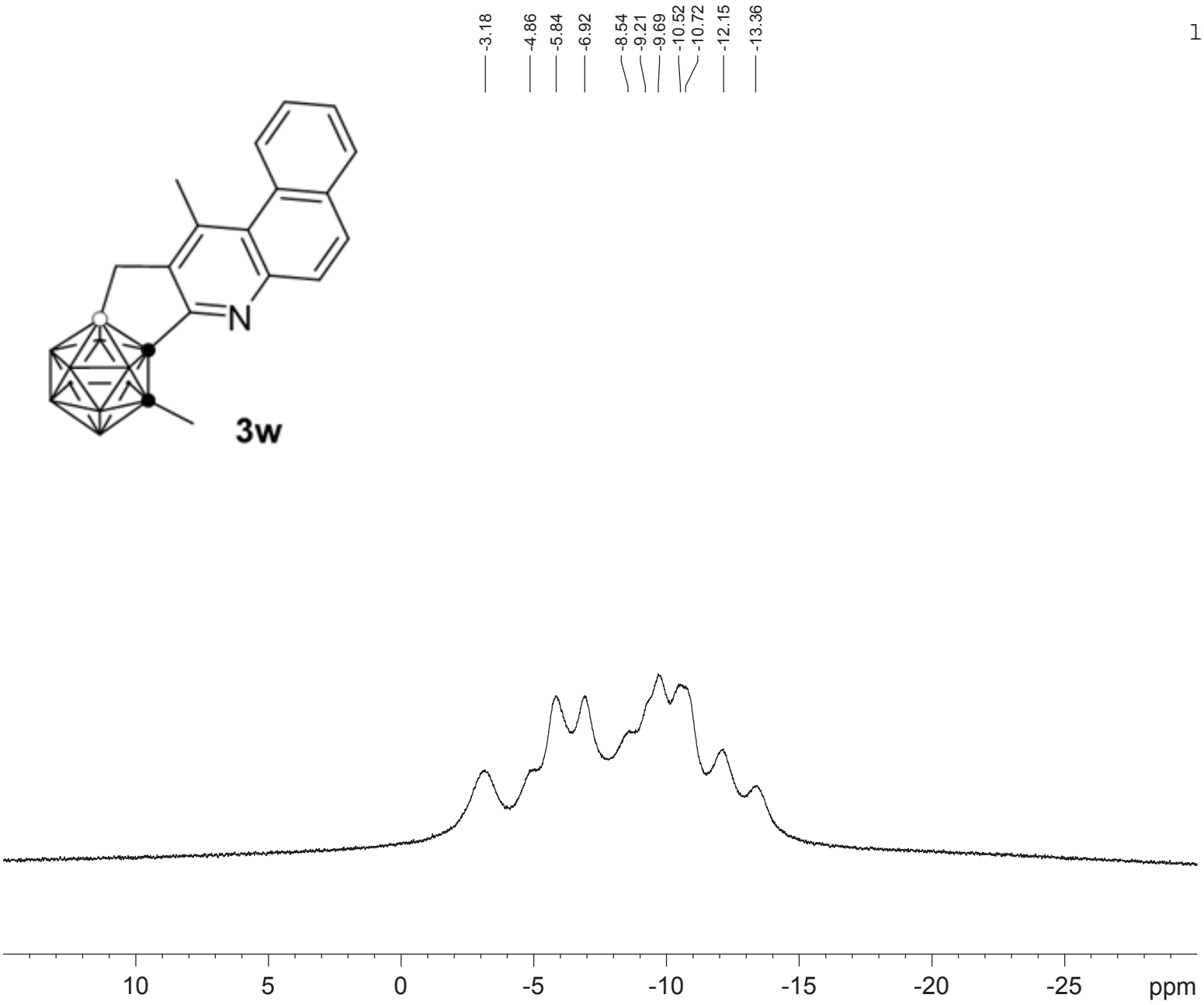
lhr-C-0735-napcasc

```
Current Data Parameters
NAME      lhr-C-0735-napcascdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170725
Time                8.37 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1000
DS                    4
SWH           40760.871 Hz
FIDRES         0.621962 Hz
AQ             0.8039083 sec
RG                  203
DW                12.267 usec
DE                 6.50 usec
TE                295.3 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1         100.6479773 MHz
NUC1                13C
P1                 9.50 usec
PLW1         55.34000015 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W
PLW13         0.13796000 W

F2 - Processing parameters
SI                 32768
SF           100.6379005 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



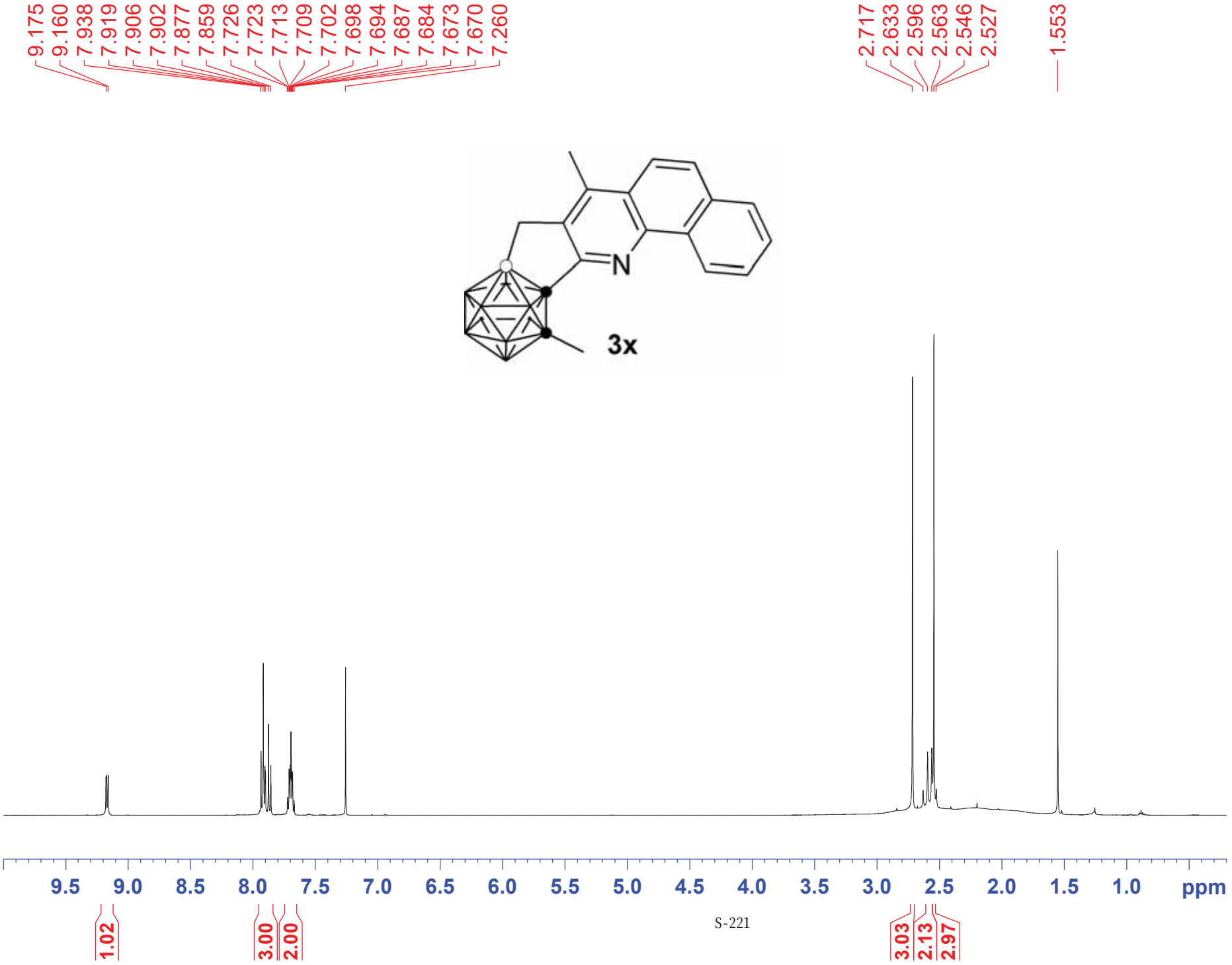
lhr-B-0735-napcascdcl3

```
Current Data Parameters
NAME      lhr-B-0735-napcascdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20170724
Time                       21.25 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                     zgdc
TD                         65536
SOLVENT                    CDCl3
NS                            28
DS                             4
SWH                    24038.461 Hz
FIDRES                   0.366798 Hz
AQ                     1.3631488 sec
RG                           322
DW                        20.800 usec
DE                         6.50 usec
TE                        295.7 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                            1
SFO1                 128.4096890 MHz
NUC1                         11B
P1                         7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

F2 - Processing parameters
SI                         32768
SF                   128.4097615 MHz
WDW                           EM
SSB               0
LB                         1.00 Hz
GB                0
PC                         1.40
```



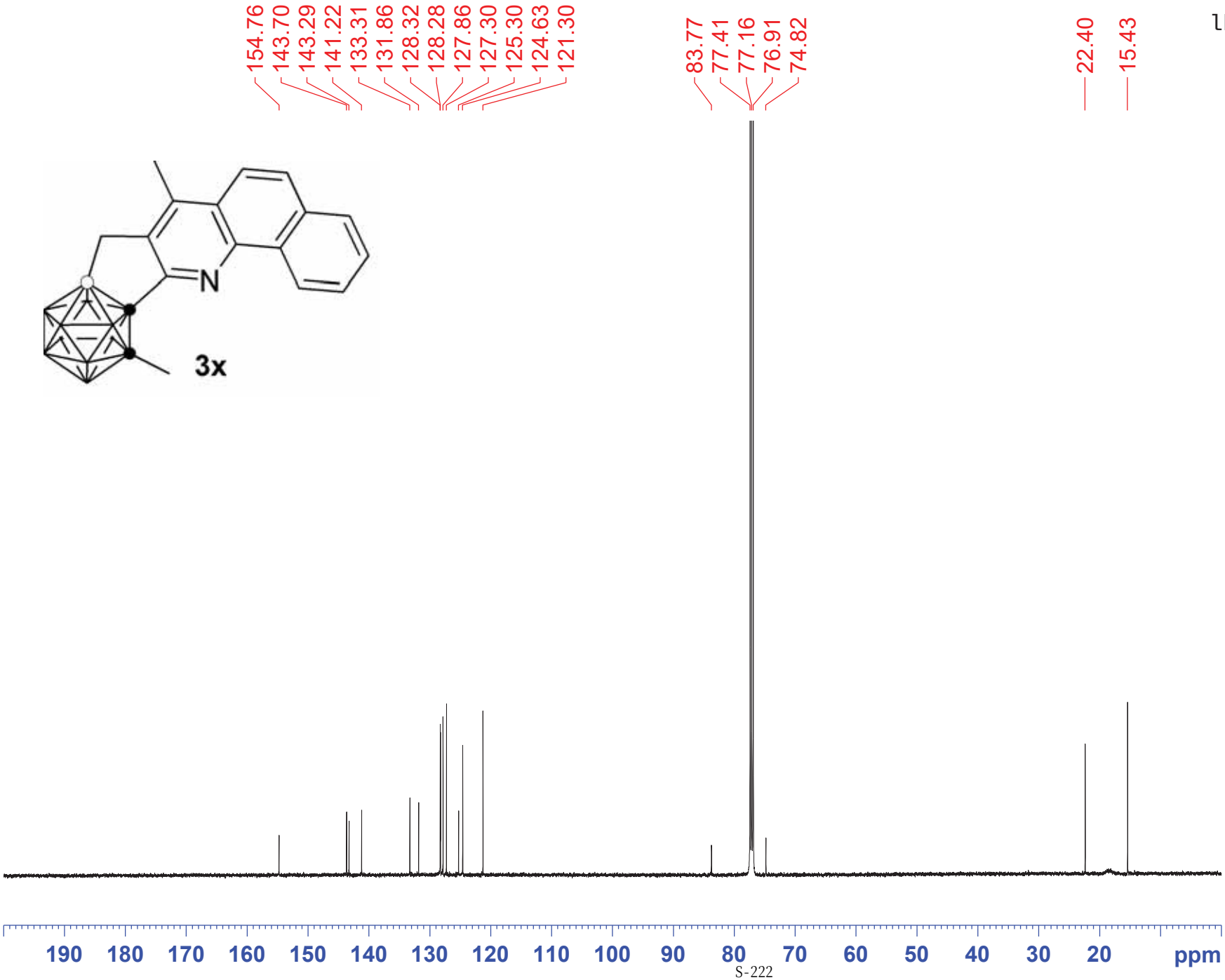
lhr-B-0735-napcascdcl3(C)

```
Current Data Parameters
NAME      lhr-B-0735-napcascdcl3(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170724
Time              21.27 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   36
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  362
DW               20.800 usec
DE                6.50 usec
TE               295.3 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-H-0748-cas1np

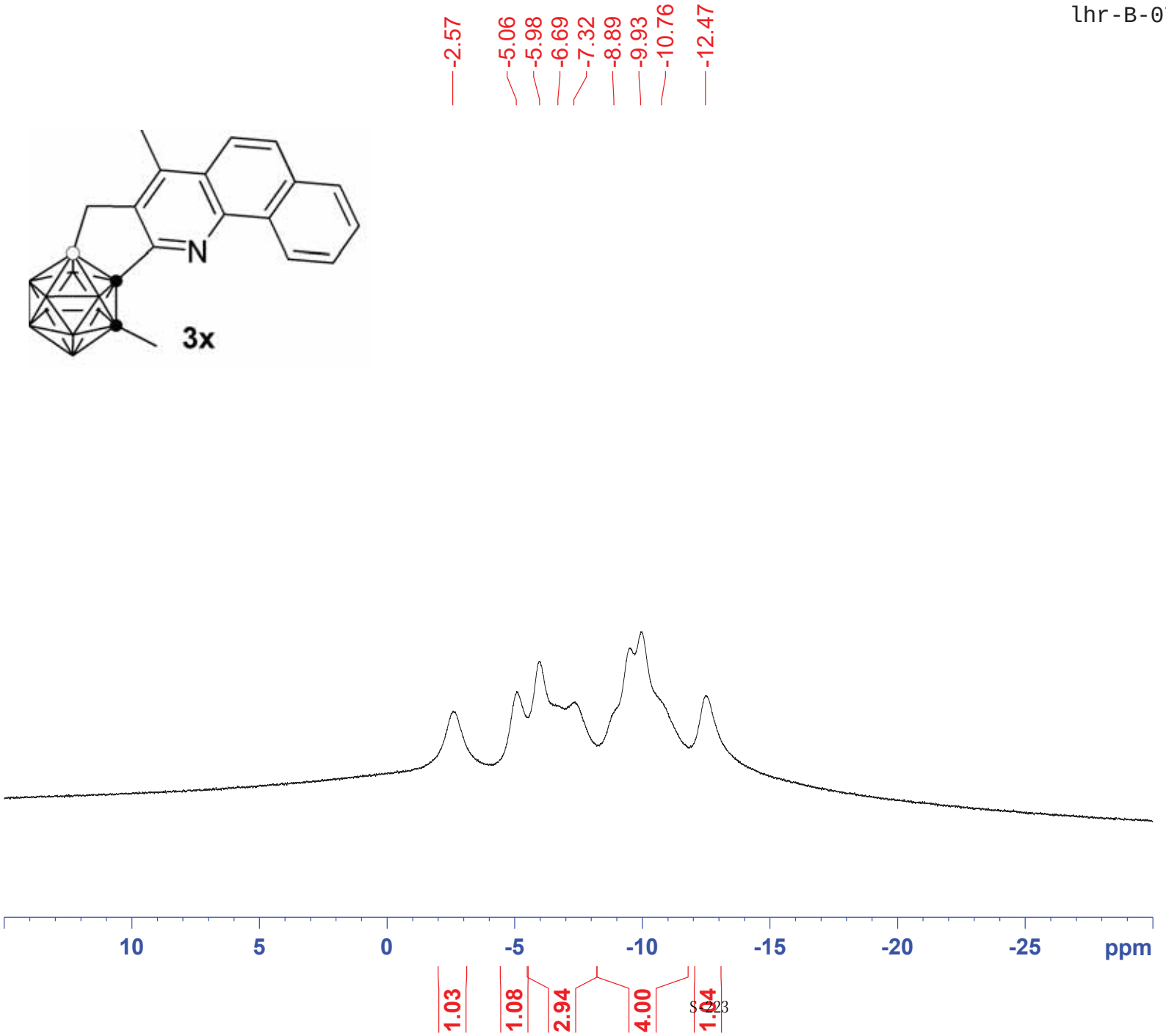
```
Current Data Parameters
NAME      lhr-H-0748-cas1
EXPNO                   1
PROCNO                  1

F2 - Acquisition Paramet
Date_            20170817
Time                10.38
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             10000.000
FIDRES          0.305176
AQ              3.2767999
RG                 30.85
DW                 50.000
DE                 10.00
TE                298.0
D1             1.00000000
TD0                    1
SFO1          500.1330883
NUC1                  1H
P1                 12.00
PLW1          15.00000000

F2 - Processing paramete
SI                 65536
SF          500.1300126
WDW                   EM
SSB       0
LB                 0.30
GB        0
PC                 1.00
```



lhr-C-0748-cas1np

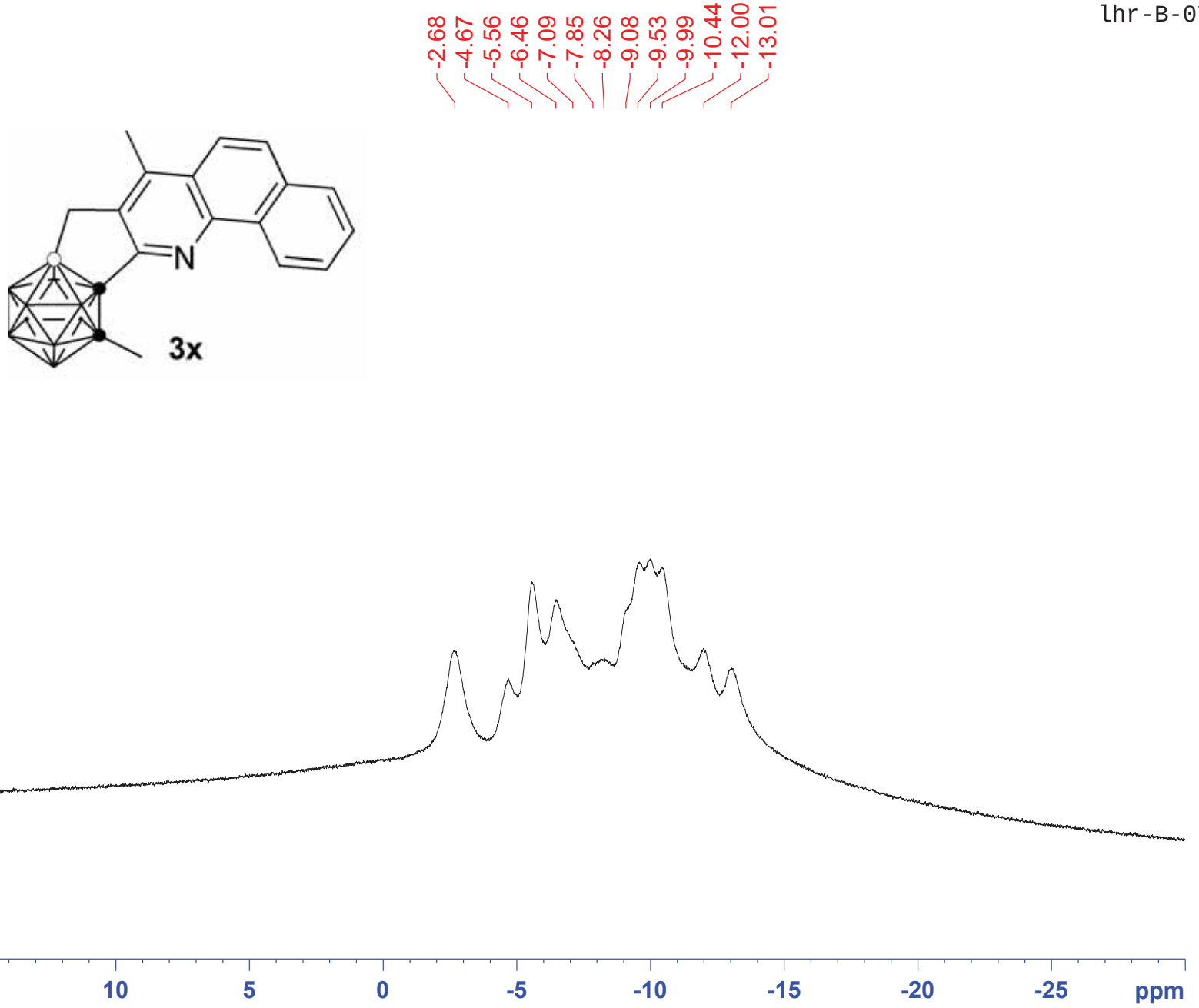
```
Current Data Parameters
NAME      lhr-C-0748-cas1np
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170817
Time                11.26 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    900
DS                      4
SWH             29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                 206.72
DW                 16.800 usec
DE                 18.00 usec
TE                 298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         125.7703643 MHz
NUC1                13C
P1                 10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W
PLW13         0.16976000 W

F2 - Processing parameters
SI                  32768
SF           125.7577722 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-0748-cas1np

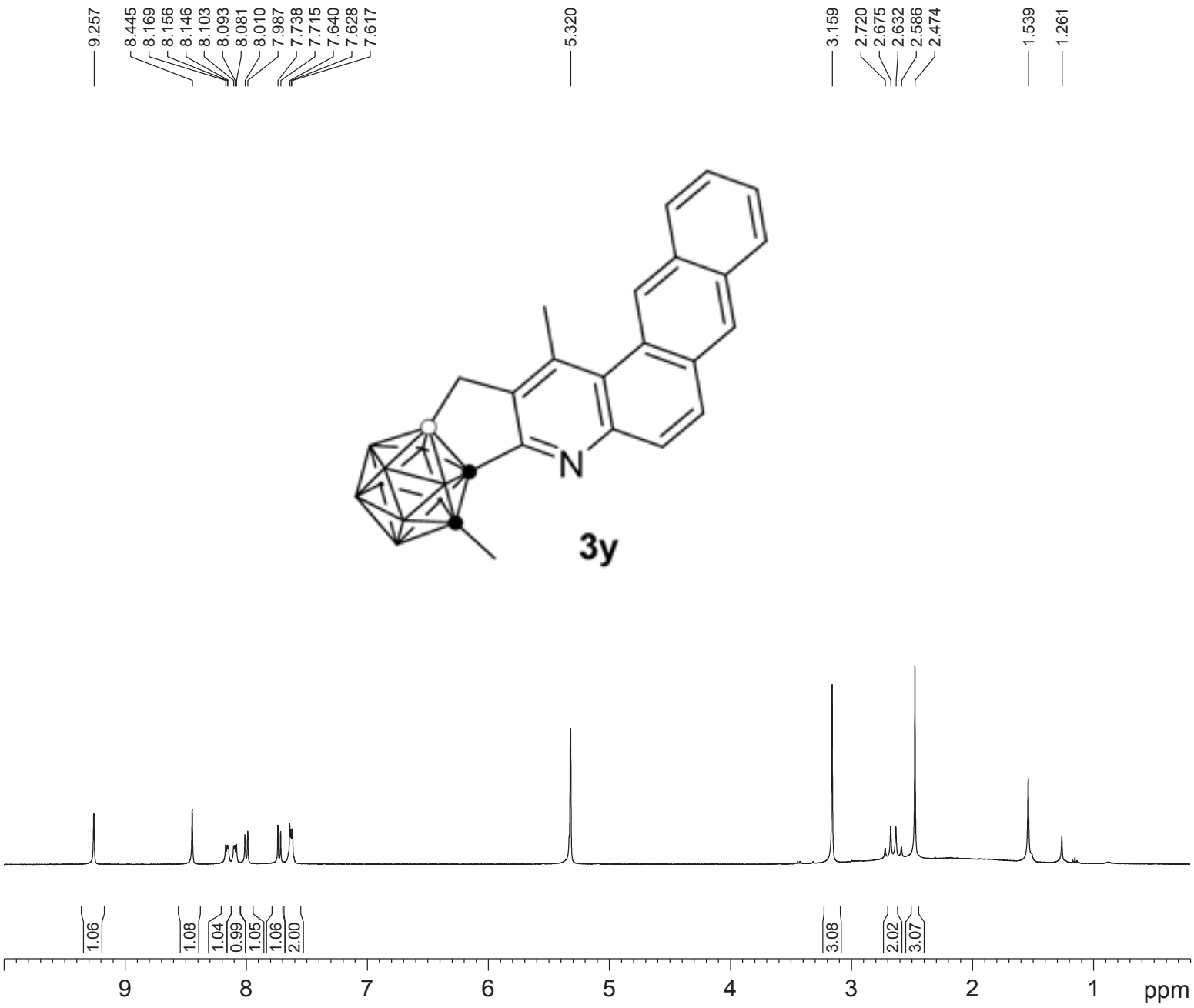


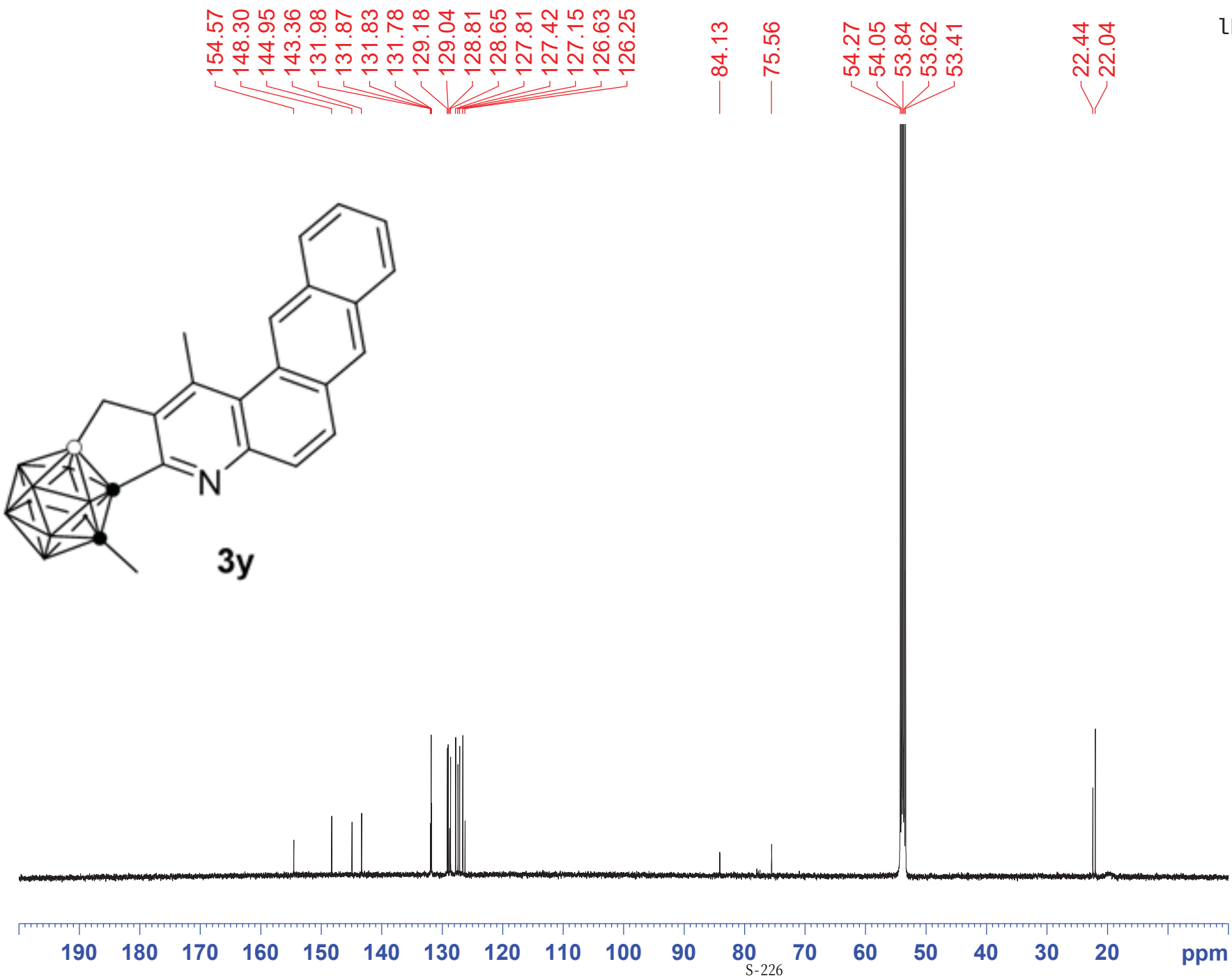

```
Current Data Parameters
NAME      lhr-B-0748-cas1np
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20170817
Time                11.30 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG              zgdc
TD                  65536
SOLVENT             CDCl3
NS                     18
DS                      4
SWH             23809.523 Hz
FIDRES           0.726609 Hz
AQ               1.3762560 sec
RG                 163.99
DW                21.000 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1         160.4599621 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W

F2 - Processing parameters
SI                  32768
SF           160.4615719 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

lhr-B-0748-cas1np(c)



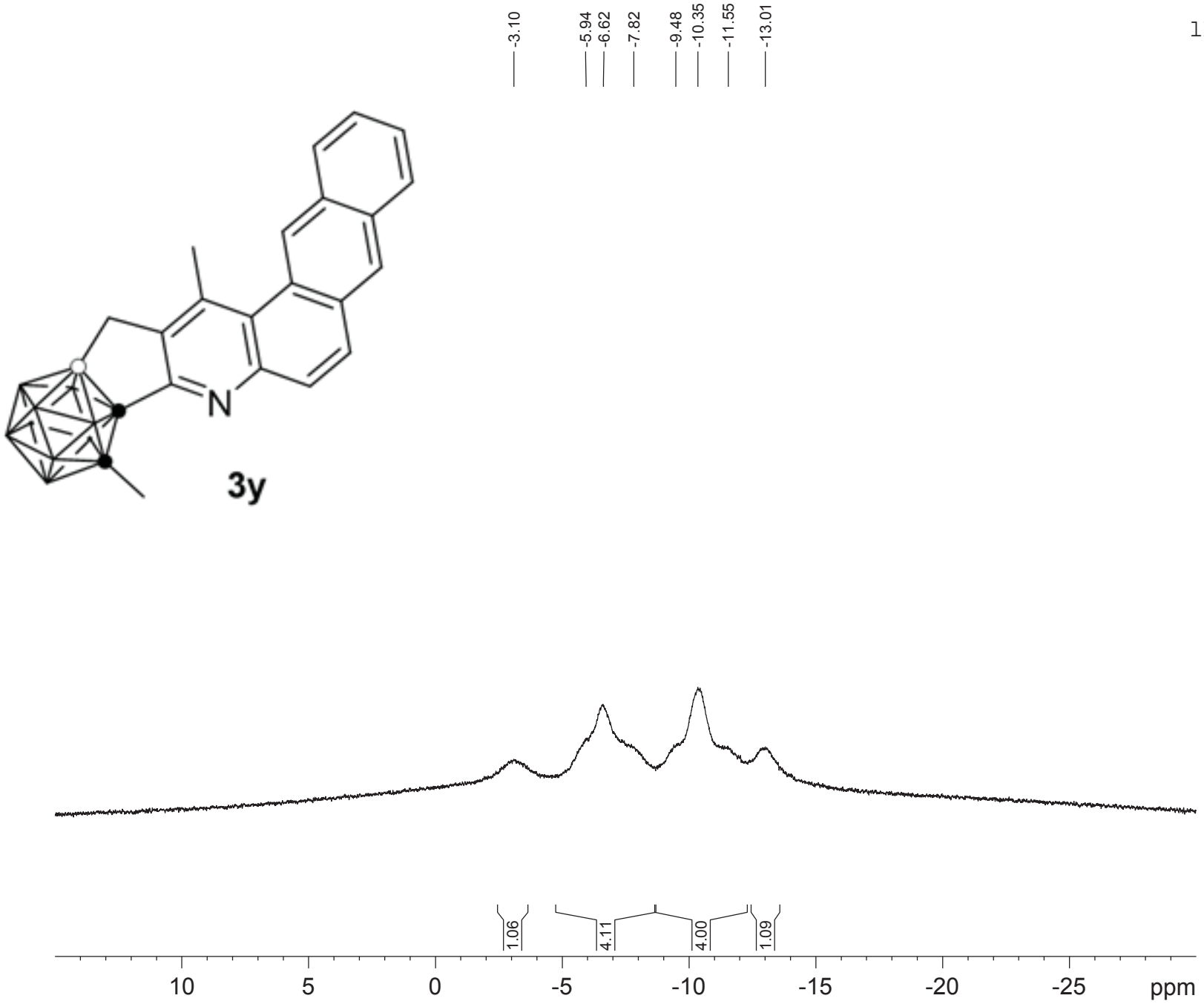

```
Current Data Parameters
NAME      lhr-B-0748-cas1np(c)
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20170817
Time                  11.31 h
INSTRUM               spect
PROBHD    Z149001_0010 (
PULPROG                   zg
TD                     32768
SOLVENT               CDCl3
NS                       20
DS                        4
SWH               24038.461 Hz
FIDRES             1.467191 Hz
AQ                0.6815744 sec
RG                   186.15
DW                   20.800 usec
DE                   18.00 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1
SFO1            160.4615792 MHz
NUC1                    11B
P1                   10.00 usec
PLW1           50.00000000 W

F2 - Processing parameters
SI                     16384
SF              160.4615792 MHz
WDW                      EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```


9.257
8.445
8.169
8.156
8.146
8.103
8.093
8.081
8.010
7.987
7.738
7.715
7.640
7.628
7.617
5.320
3.159
2.720
2.675
2.632
2.586
2.474
1.539
1.261
lhr-H-0756-cascdcl3
N
3y
Current Data Parameters
NAME lhr-H-0756-cascdcl3-cd
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170906
Time 9.39 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
F2 - Processing parameters
SI 65536
SF 400.2300158 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.06
1.08
1.04
0.99
1.05
1.06
2.00
3.08
2.02
3.07
9
8
7
6
5
4
3
2
1
ppm



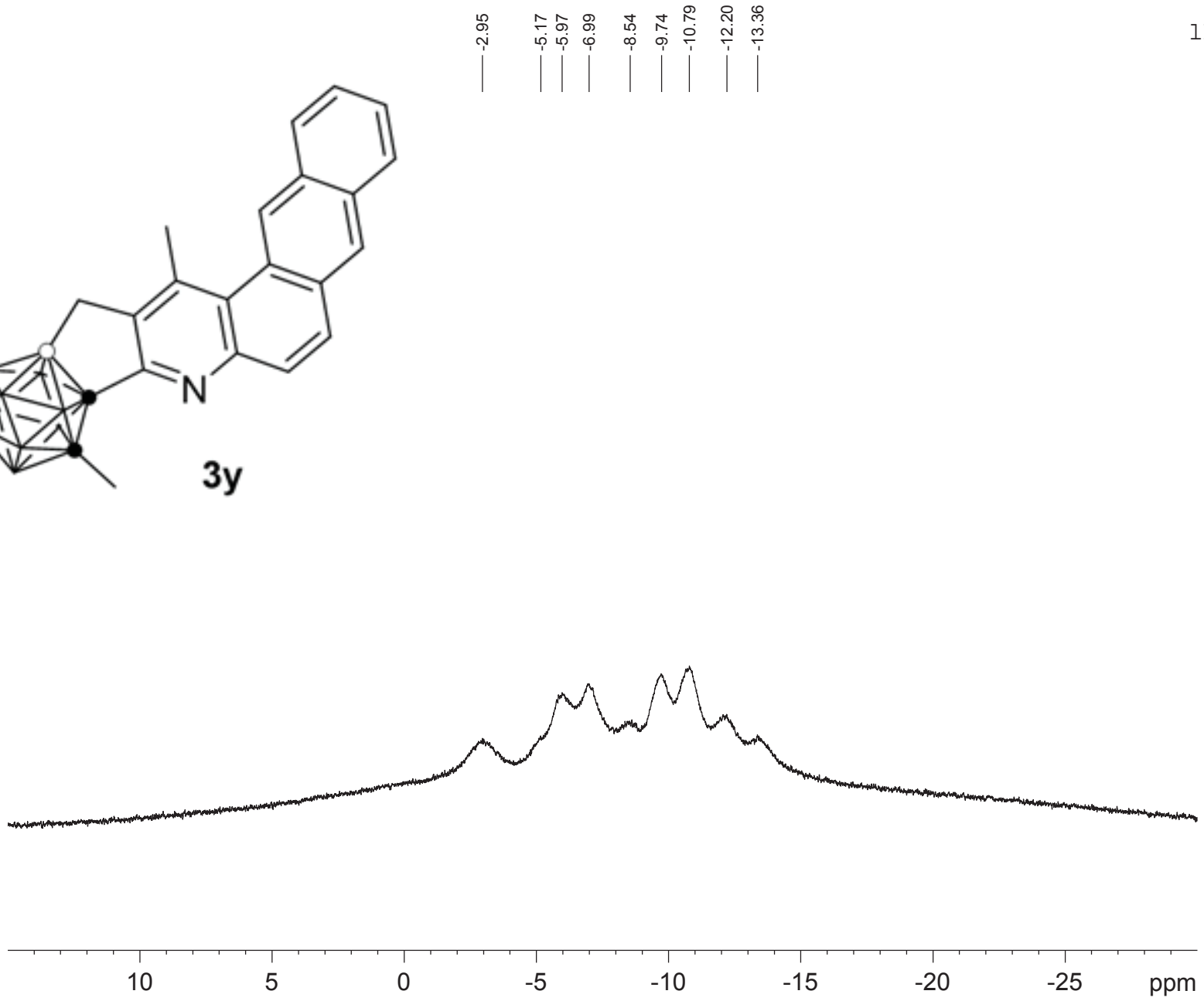
lhr-0756-re-c

```
Current Data Parameters
NAME      lhr-0756-re-c
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170916
Time              11.19 h
INSTRUM           spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2235
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7579786 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



lhr-B-0756-cascdcl3-cd2cl2

```
Current Data Parameters
NAME      lhr-B-0756-cascdcl3-cd2cl2
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20170830
Time              17.05 h
INSTRUM             spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    40
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                   575
DW                20.800 usec
DE                 6.50 usec
TE                295.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1         55.09999847 W
SFO2         400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.56000042 W
PLW12         0.27428001 W

F2 - Processing parameters
SI                 32768
SF           128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

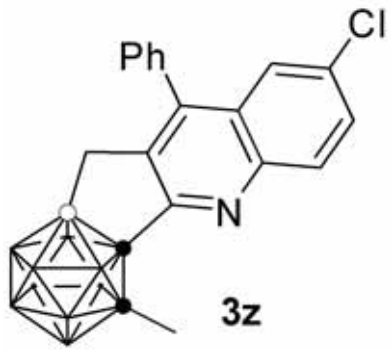


lhr-B-0756-cascdcl3-cd2cl2(C)

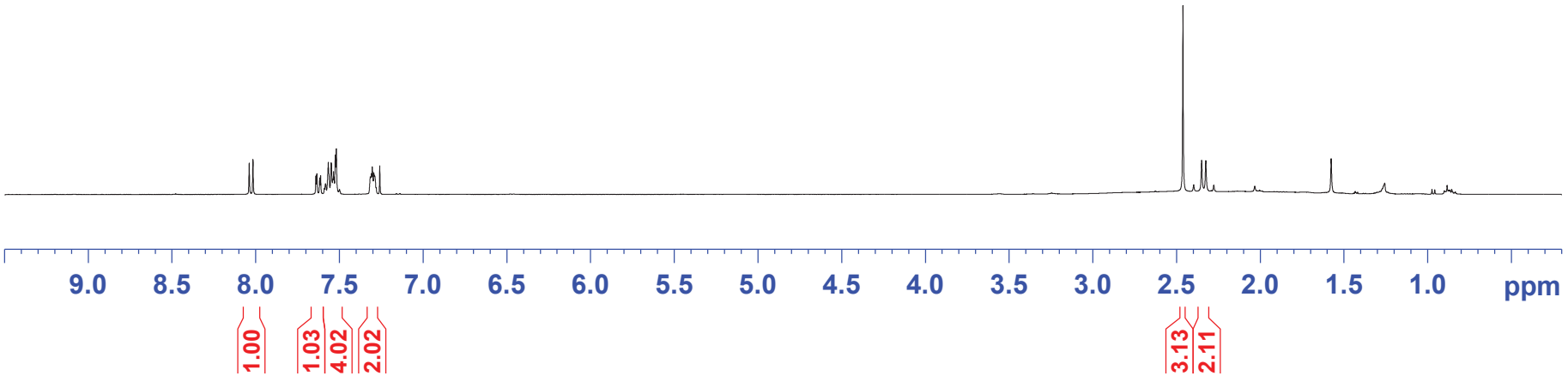
```
Current Data Parameters
NAME      lhr-B-0756-cascdcl3-cd2cl2(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170830
Time              17.09 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG                zg
TD                  65536
SOLVENT             CDCl3
NS                     52
DS                      2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                    575
DW                20.800 usec
DE                 6.50 usec
TE                295.5 K
D1           2.00000000 sec
TD0                     1
SFO1         128.4096890 MHz
NUC1                  11B
P1                 7.50 usec
PLW1         55.09999847 W

F2 - Processing parameters
SI                  32768
SF           128.4097430 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

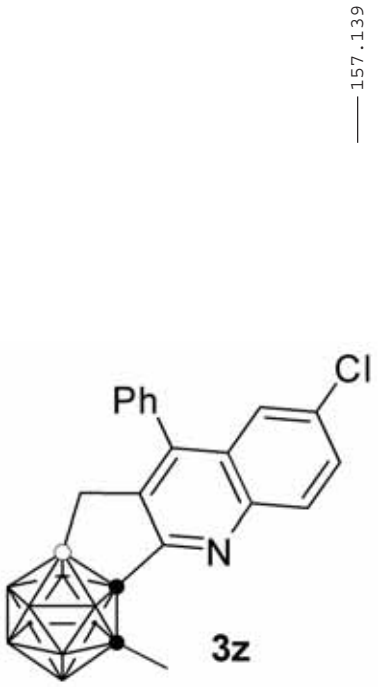
8.040 8.018 7.636 7.613 7.591 7.584 7.567 7.550 7.540 7.536 7.533 7.526 7.520 7.500 7.317 7.310 7.305 7.296 7.293 7.290 7.260

2.465 2.401 2.353 2.328 2.280 1.579




```
Current Data Parameters
NAME      lhr-H-0889-1-cas-cdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180602
Time              15.42 h
INSTRUM             spect
PROBHD   Z824601_0021 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    19
DS                     2
SWH             8012.820 Hz
FIDRES          0.244532 Hz
AQ              4.0894465 sec
RG                   161
DW                62.400 usec
DE                 6.50 usec
TE                297.3 K
D1             1.00000000 sec
TD0                    1
SFO1         400.1324708 MHz
NUC1                1H
P1                15.00 usec
PLW1           8.31000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300098 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





157.139
146.837
144.635
140.494
135.436
133.376
131.422
130.272
129.122
129.080
128.819
127.894
124.911
82.826
77.477
77.160
76.842
75.444
22.317

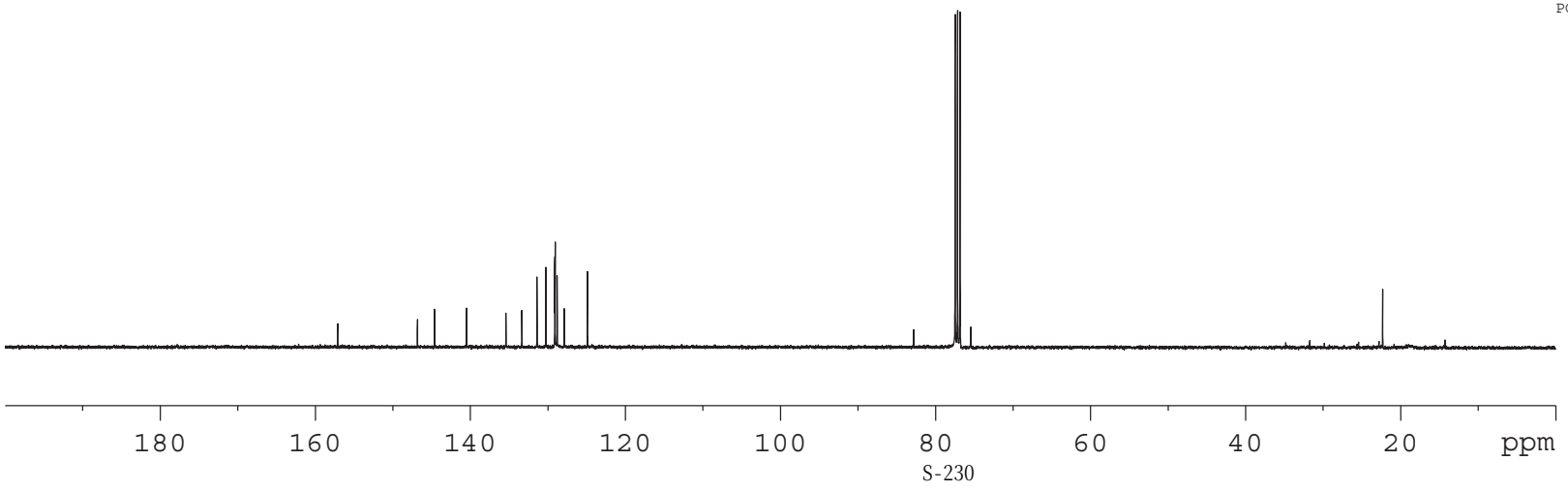
lhr-C-0889-1-cas-cdcl3

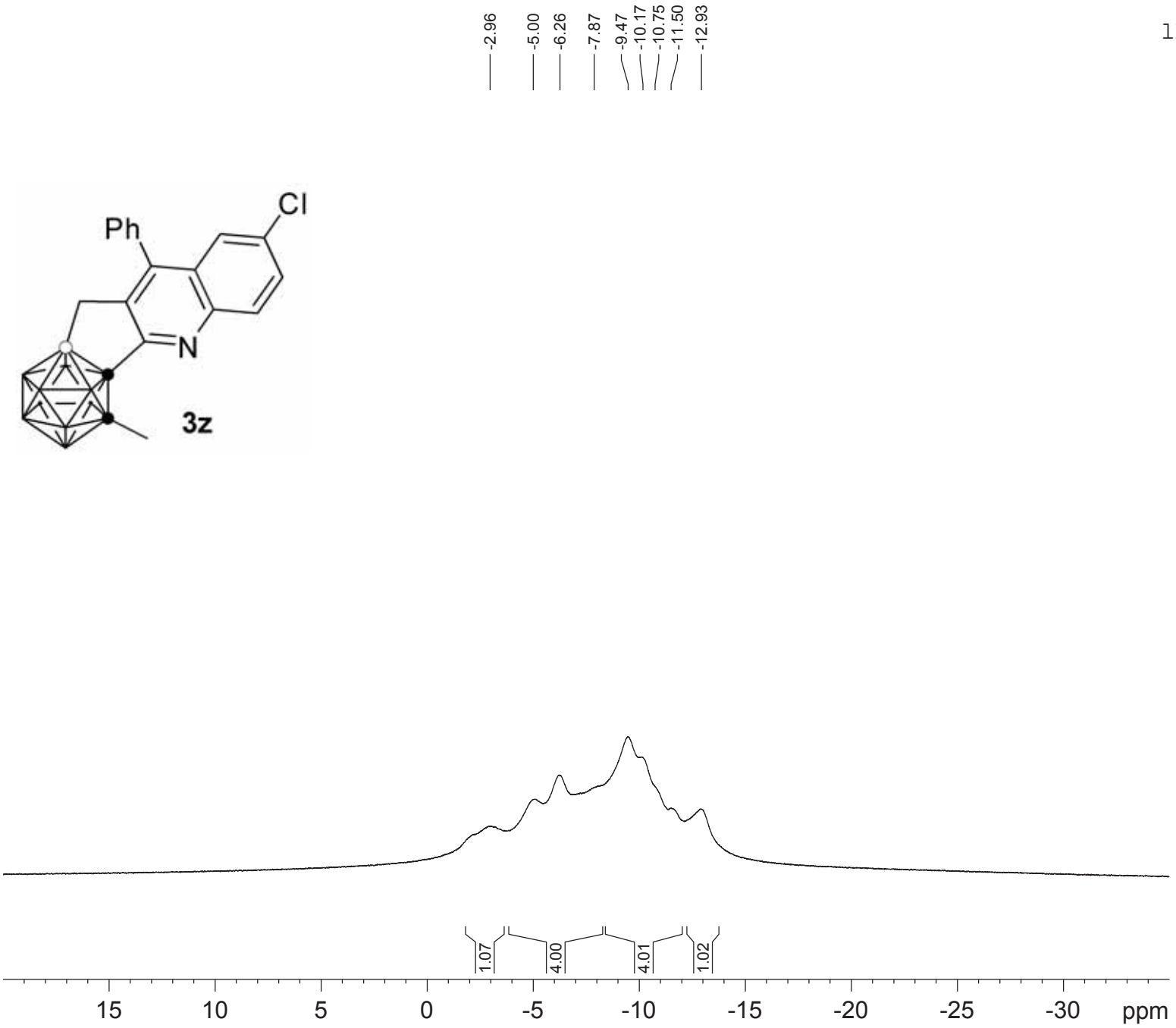
Bruker Advance III 400

Current Data Parameters
NAME lhr-C-0889-1-cas-cdcl3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180602
Time 17.07 h
INSTRUM spect
PROBHD Z824601_0021 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1330
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6228298 MHz
NUC1 13C
P1 9.50 usec
PLW1 41.25000000 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 8.31000042 W
PLW12 0.23083000 W
PLW13 0.11611000 W

F2 - Processing parameters
SI 32768
SF 100.6127551 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

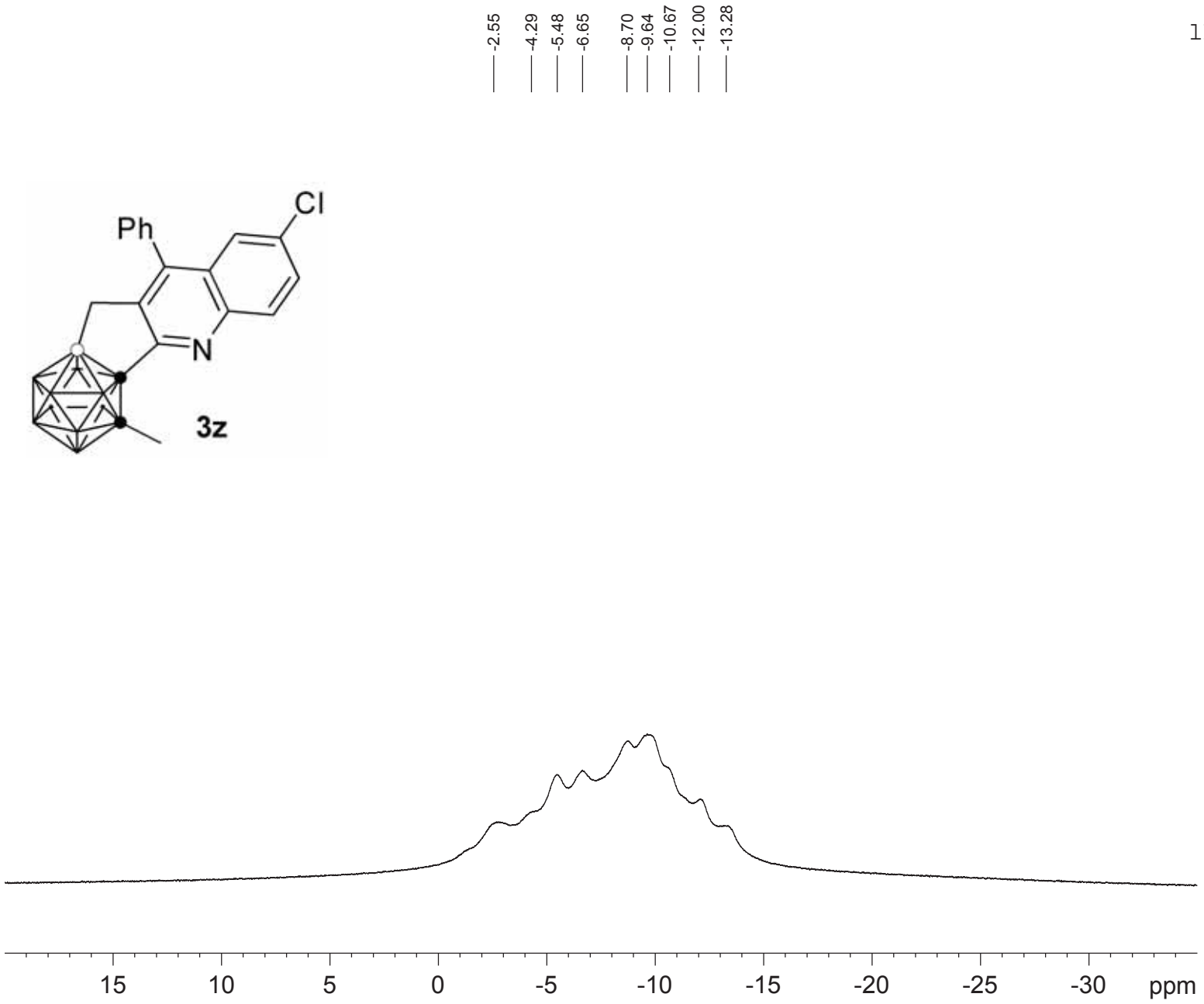




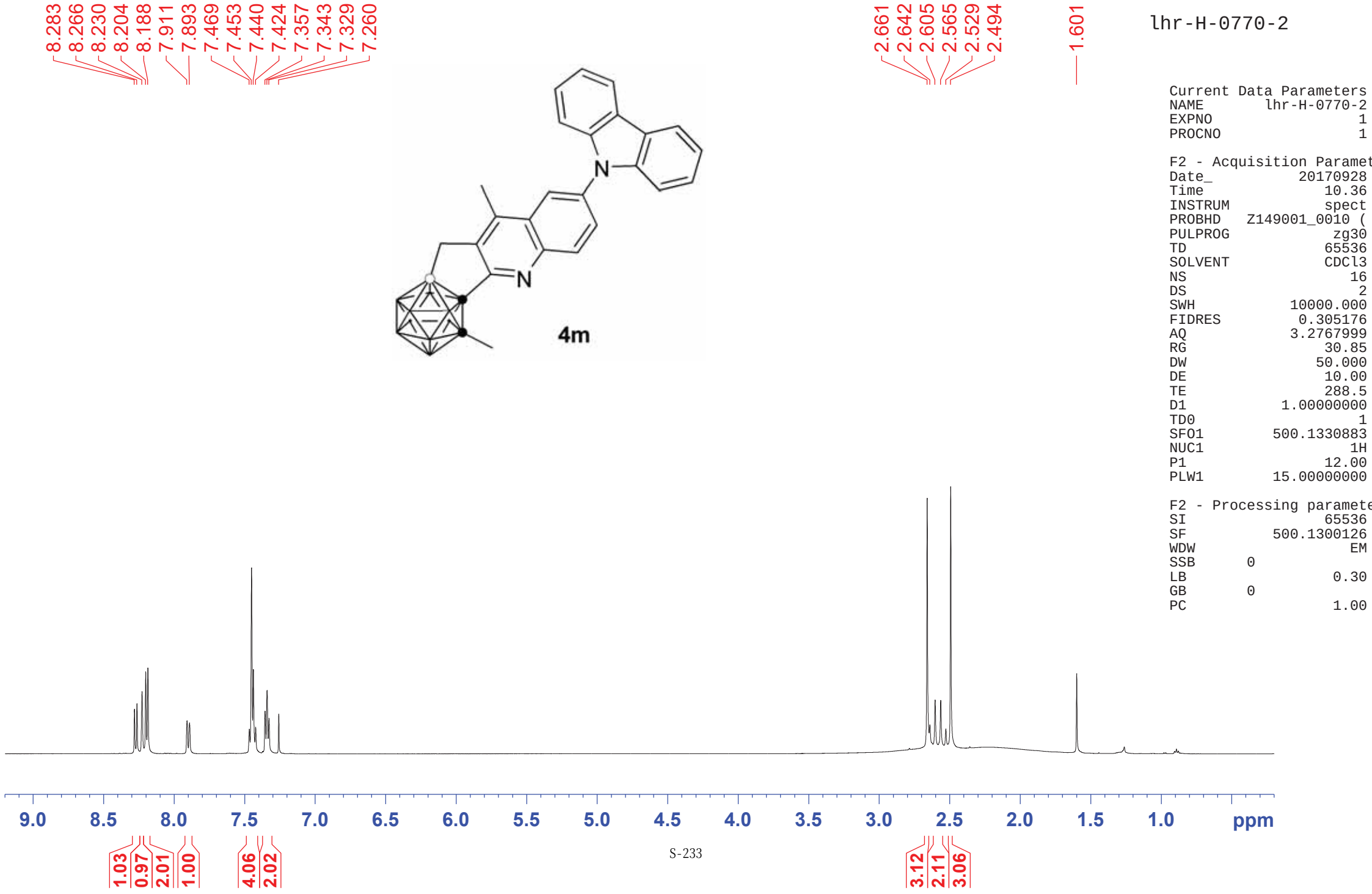
lhr-B-0889-1-cas-cdcl3

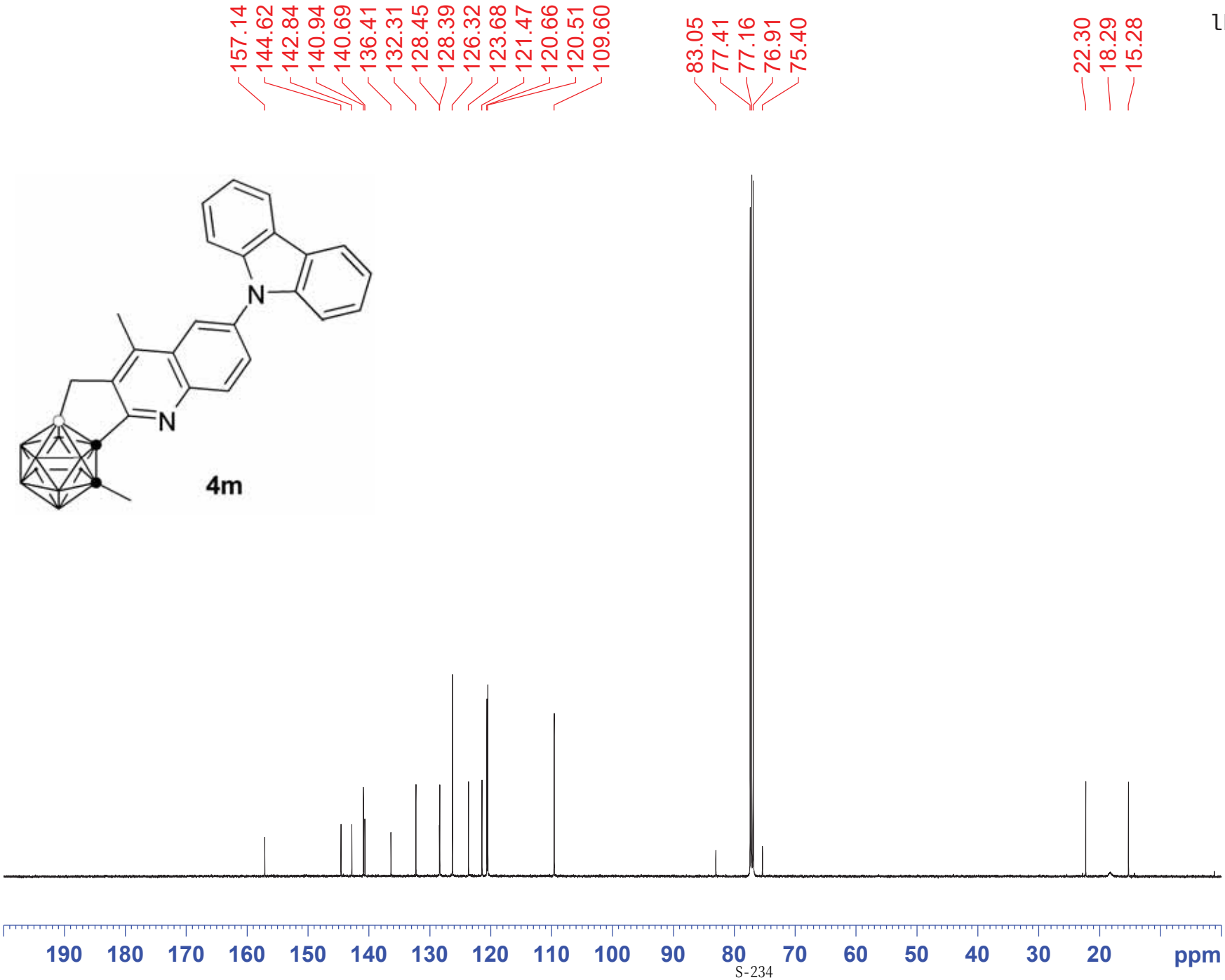
```
Current Data Parameters
NAME      lhr-B-0889-1-cas-cdcl3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180603
Time              16.26 h
INSTRUM            spect
PROBHD   Z108618_0257 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    68
DS                     4
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                   322
DW                20.800 usec
DE                 6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W
SFO2        400.2316009 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2        13.56000042 W
PLW12        0.27428001 W

F2 - Processing parameters
SI                 32768
SF          128.4097615 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

lhr-B-0889-1-cas-cdcl3(C)




```
Current Data Parameters
NAME      lhr-B-0889-1-cas-cdcl3(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180603
Time              16.32 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG              zg
TD                65536
SOLVENT           CDCl3
NS                   51
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  322
DW                20.800 usec
DE                 6.50 usec
TE                294.4 K
D1           2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1                11B
P1                 7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```


8.283
8.266
8.230
8.204
8.188
7.911
7.893
7.469
7.453
7.440
7.424
7.357
7.343
7.329
7.260
2.661
2.642
2.605
2.565
2.529
2.494
1.601
N
N
4m
lhr-H-0770-2
Current Data Parameters
NAME lhr-H-0770-2
EXPNO 1
PROCNO 1
F2 - Acquisition Paramet
Date_ 20170928
Time 10.36
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 3.2767999
RG 30.85
DW 50.000
DE 10.00
TE 288.5
D1 1.00000000
TD0 1
SFO1 500.1330883
NUC1 1H
P1 12.00
PLW1 15.00000000
F2 - Processing paramete
SI 65536
SF 500.1300126
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.03
0.97
2.01
1.00
4.06
2.02
3.12
2.11
3.06

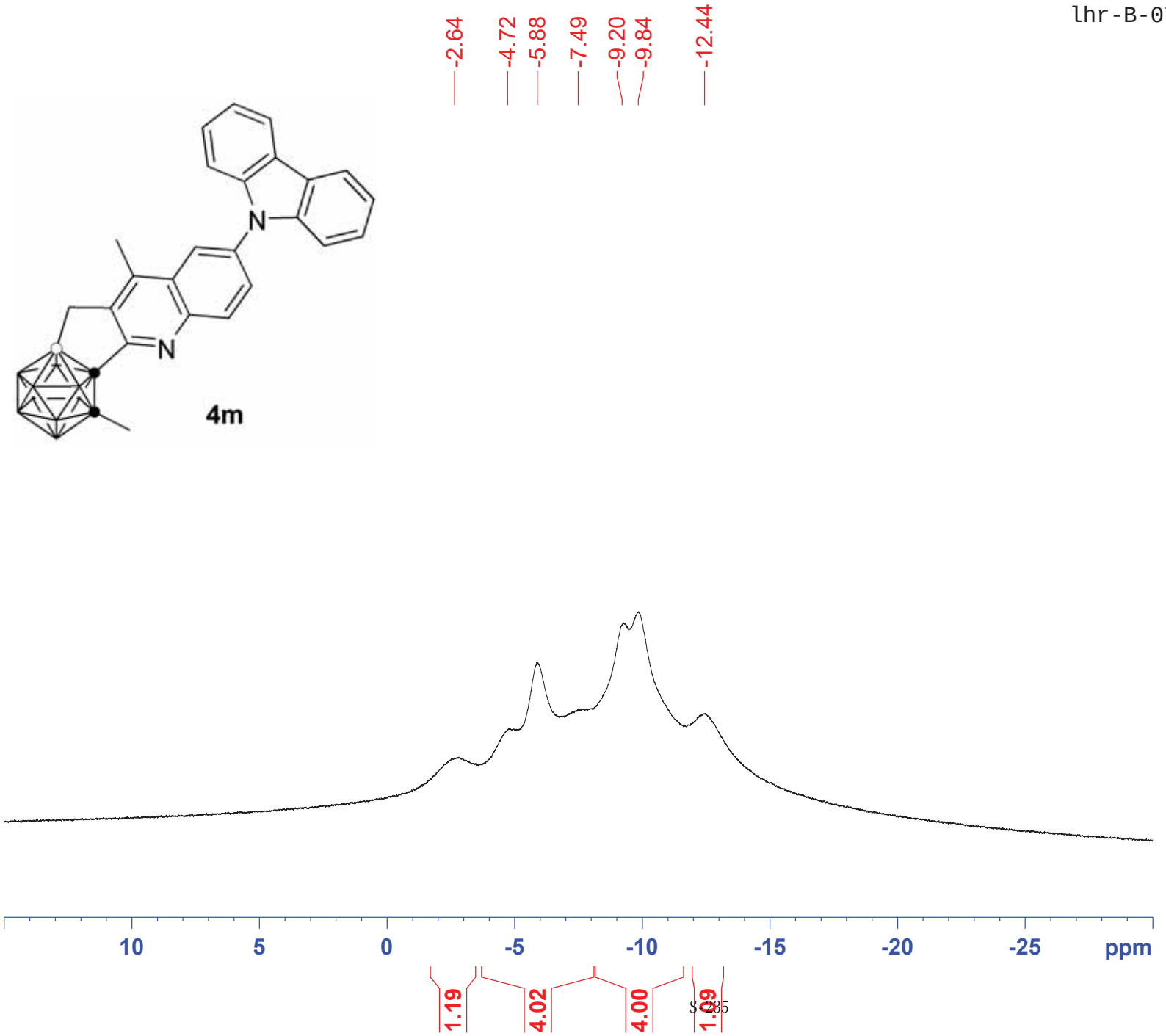


lhr-C-0770-2

```
Current Data Parameters
NAME        lhr-C-0770-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170928
Time              10.56 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  360
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               288.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577776 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

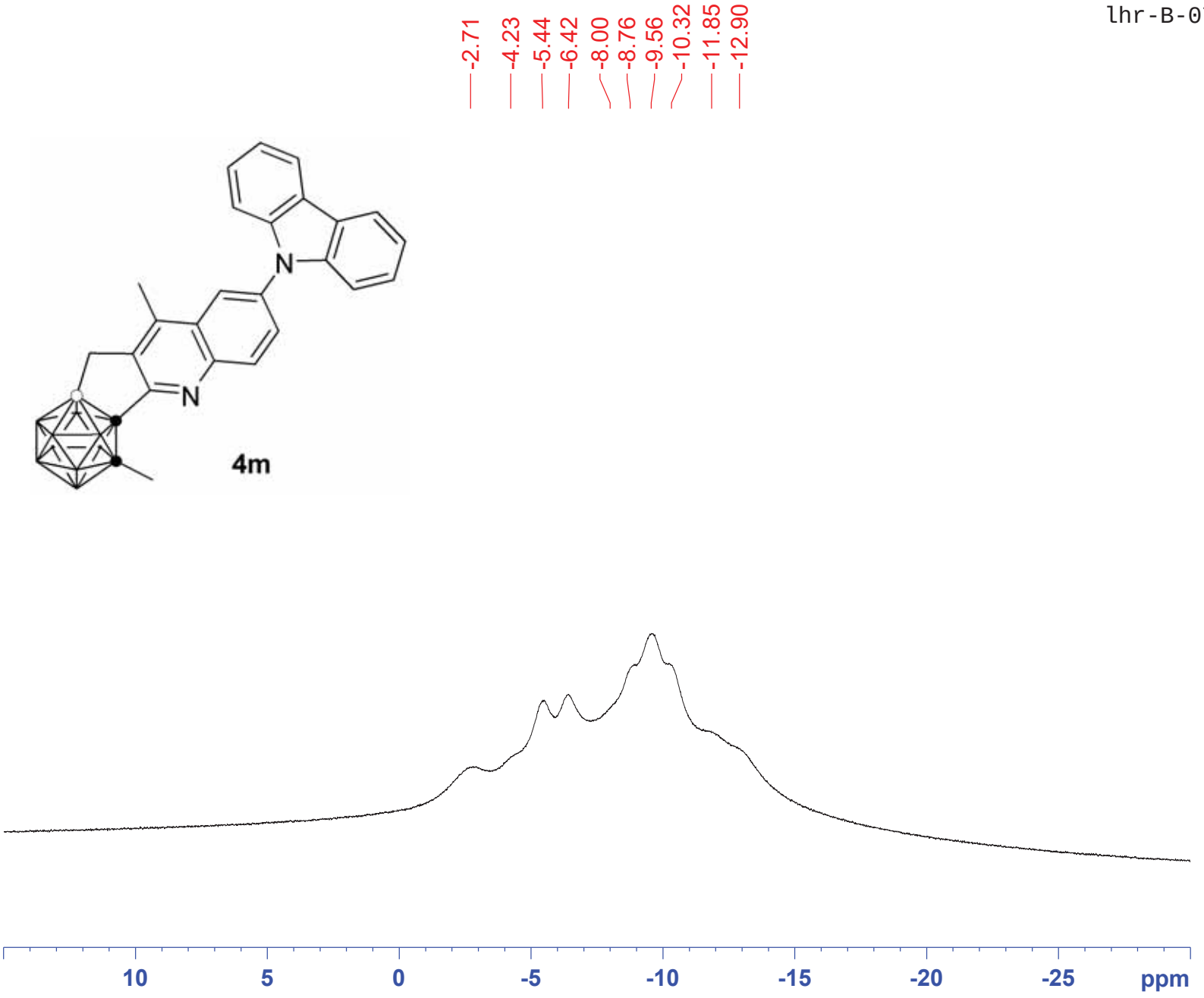
lhr-B-0770-2

4m

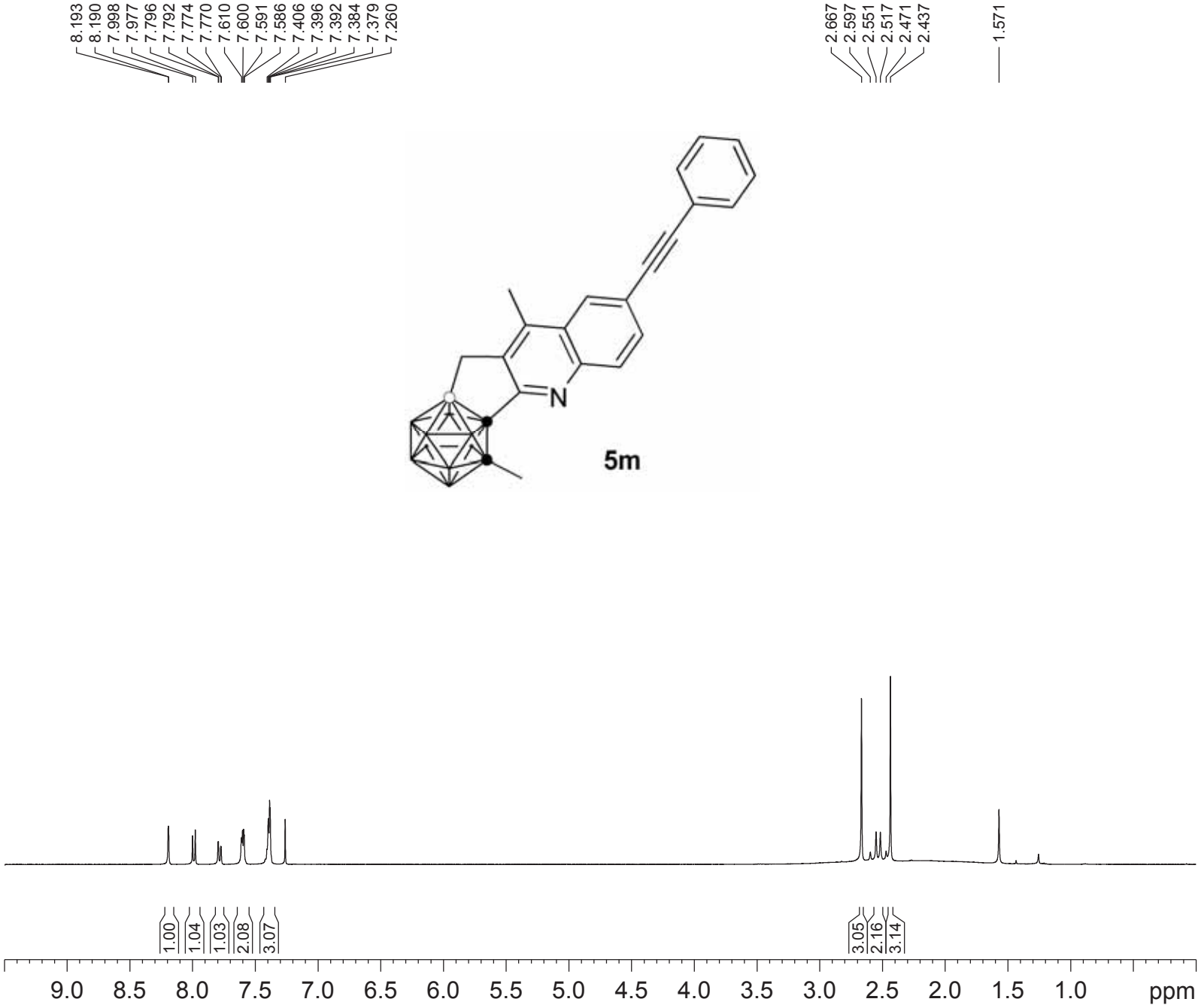



```
Current Data Parameters
NAME        lhr-B-0770-2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170928
Time              10.59 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    20
DS                     4
SWH           23809.523 Hz
FIDRES         0.726609 Hz
AQ            1.3762560 sec
RG               163.99
DW               21.000 usec
DE               18.00 usec
TE               288.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        160.4599621 MHz
NUC1               11B
P1               10.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W

F2 - Processing parameters
SI                 32768
SF          160.4615719 MHz
WDW                EM
SSB      0
LB               1.00 Hz
GB       0
PC               1.40
```

lhr-B-0770-2(c)




```
Current Data Parameters
NAME      lhr-B-0770-2(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170928
Time               11.00 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    20
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                186.15
DW                20.800 usec
DE                18.00 usec
TE                288.5 K
D1           1.00000000 sec
TD0                    1
SFO1        160.4615792 MHz
NUC1                11B
P1                10.00 usec
PLW1        50.00000000 W

F2 - Processing parameters
SI                 16384
SF          160.4615792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

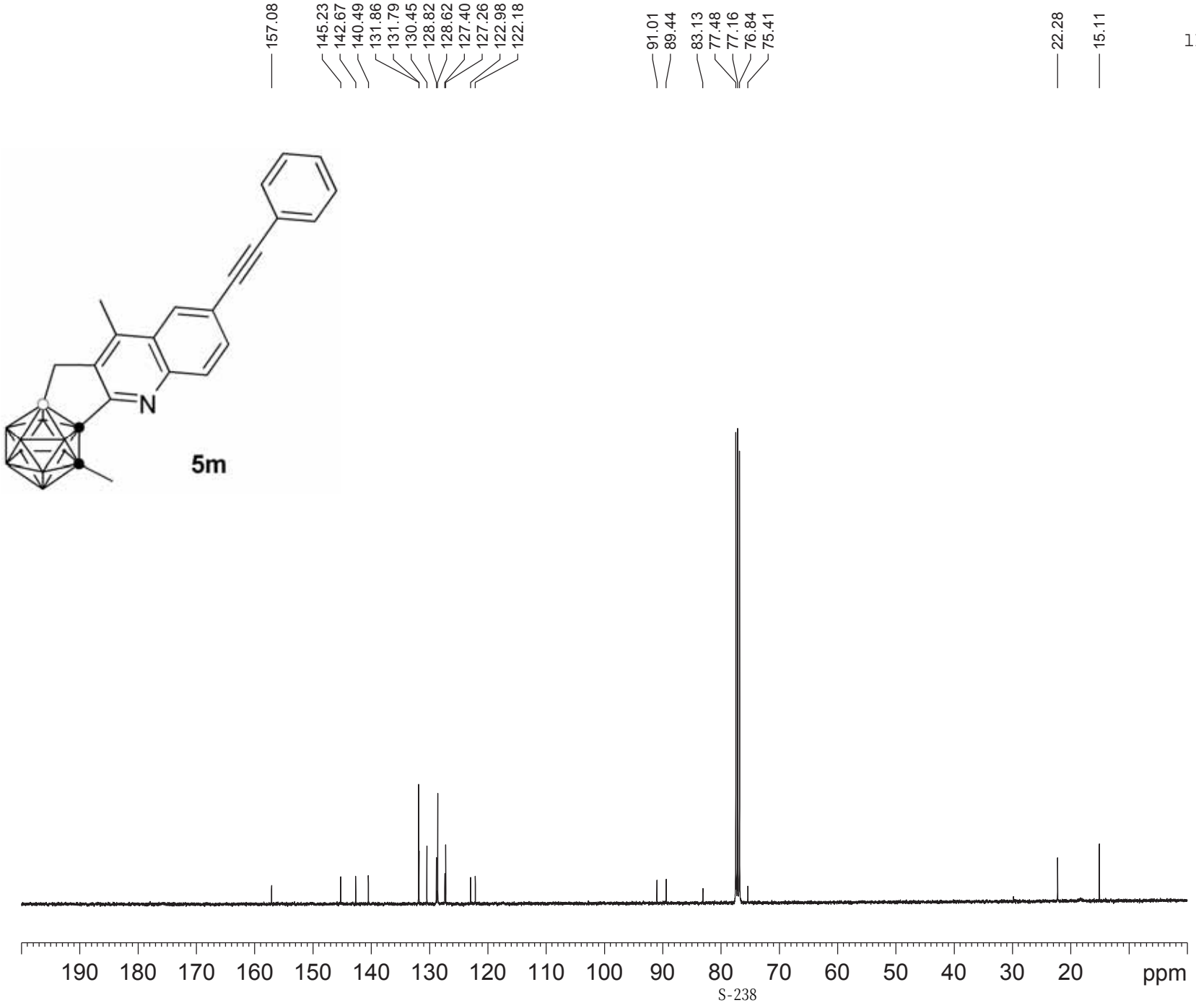


lhr-H-0770-3-cdcl3

Current Data Parameters
NAME lhr-H-0770-3-cdcl3
EXPNO 1
PROCNO 1

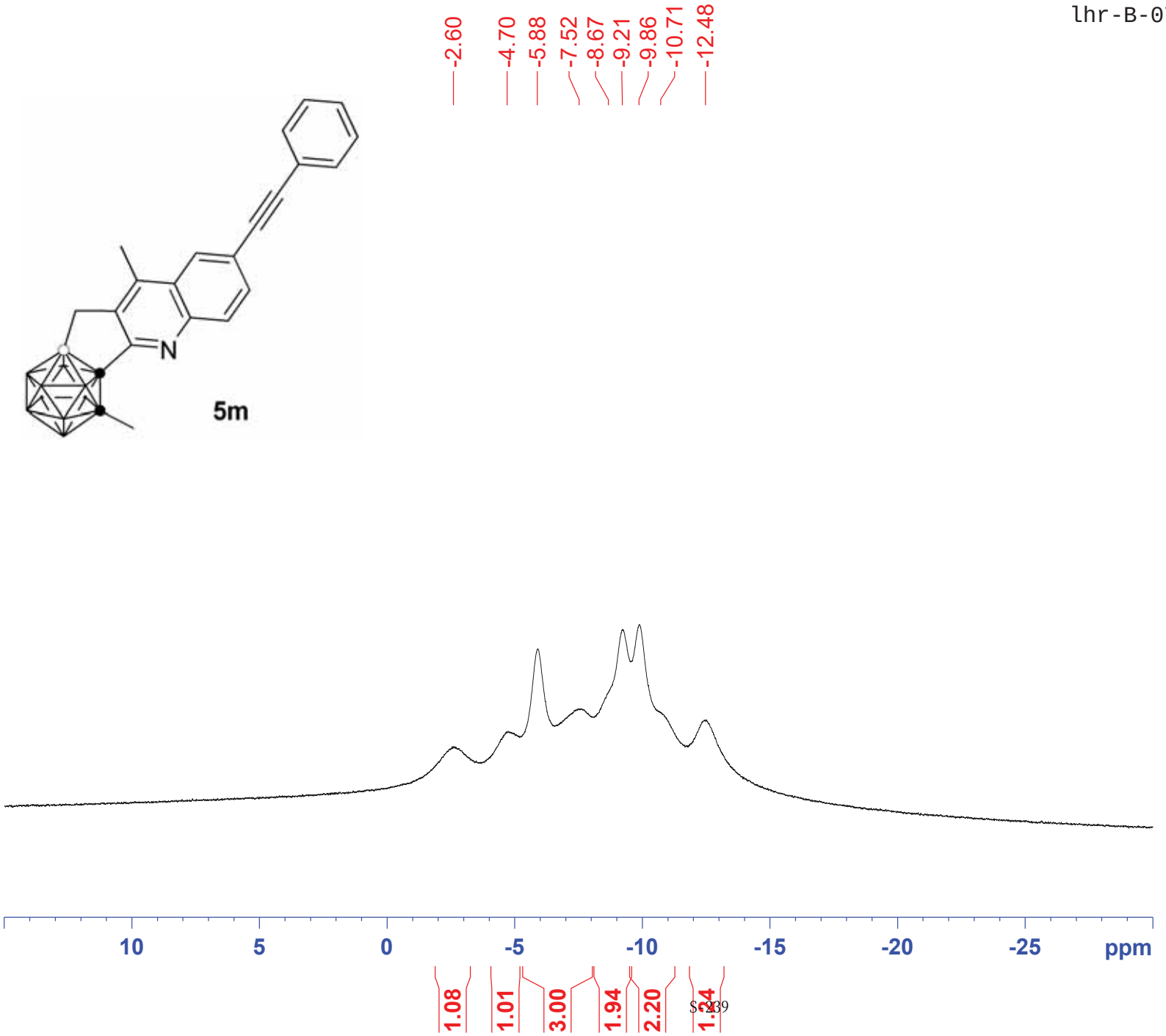
F2 - Acquisition Parameters
Date_ 20170930
Time 19.10 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 203
DW 62.400 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

F2 - Processing parameters
SI 65536
SF 400.2300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



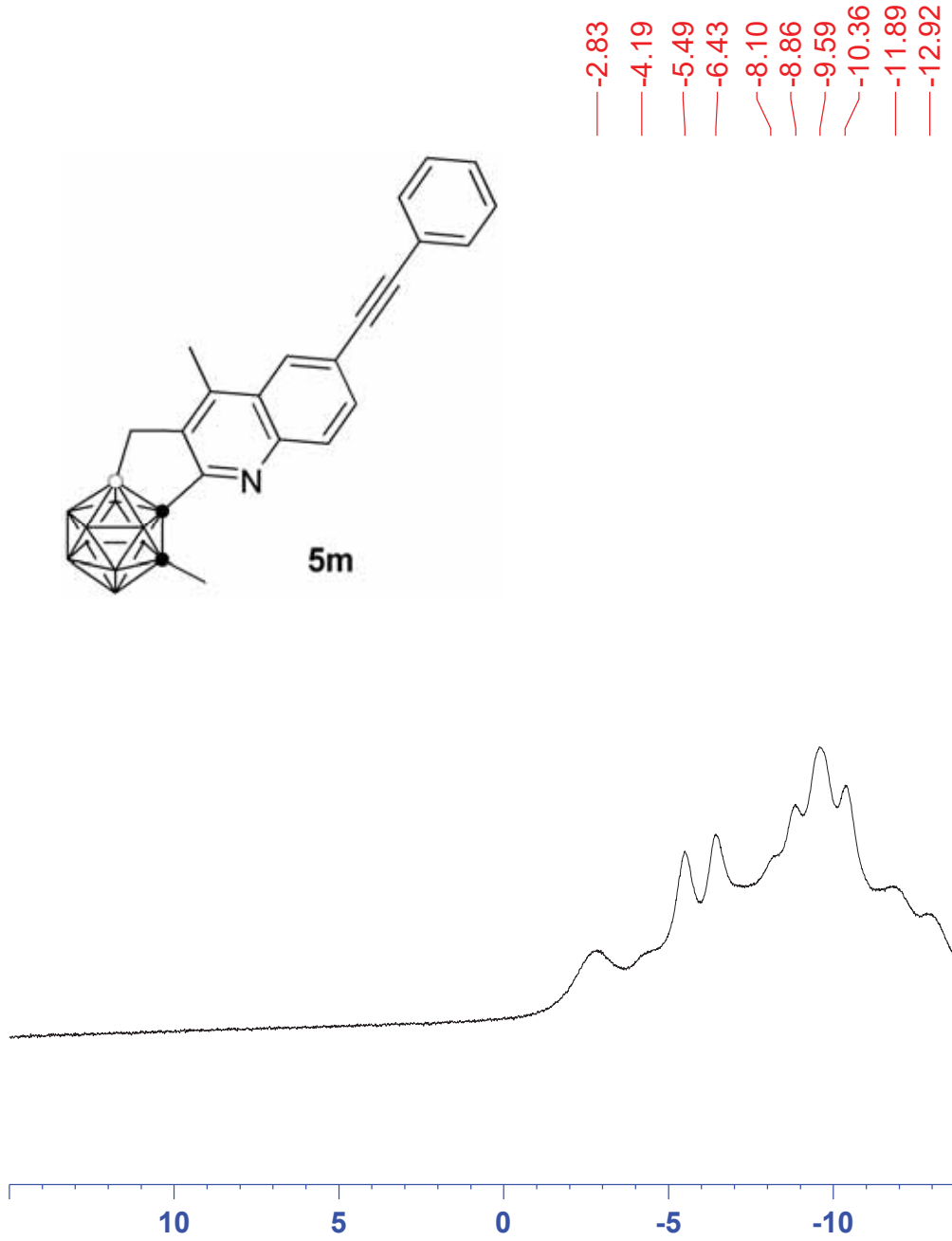

```
Current Data Parameters
NAME      lhr-C-0770-3-cdcl3
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170930
Time                 19.13 h
INSTRUM              spect
PROBHD    Z108618_0257 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   1467
DS                      4
SWH             29761.904 Hz
FIDRES           0.454131 Hz
AQ               1.1010048 sec
RG                    203
DW                 16.800 usec
DE                  6.50 usec
TE                 295.5 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1
SFO1           100.6479773 MHz
NUC1                  13C
P1                  9.50 usec
PLW1           55.34000015 W
SFO2           400.2316009 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2           13.56000042 W
PLW12           0.27428001 W
PLW13           0.13796000 W

F2 - Processing parameters
SI                   32768
SF             100.6379009 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

lhr-B-0770-3

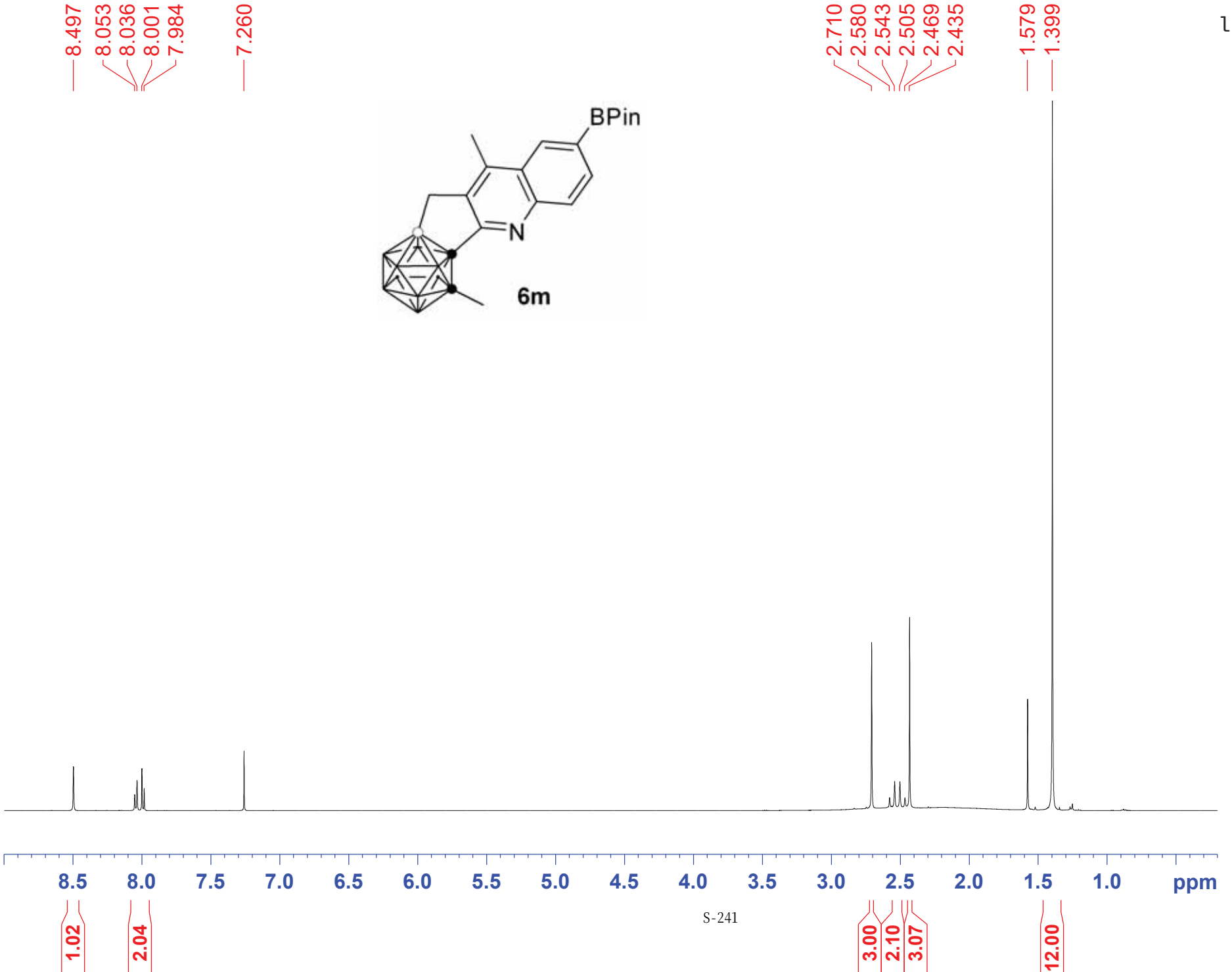



```
Current Data Parameters
NAME        lhr-B-0770-3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170930
Time              10.35 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG             zgdc
TD                 65536
SOLVENT            CDCl3
NS                    20
DS                     4
SWH           24038.461 Hz
FIDRES         0.733596 Hz
AQ            1.3631488 sec
RG               163.99
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        160.4599621 MHz
NUC1                11B
P1                10.00 usec
PLW1        50.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W

F2 - Processing parameters
SI                 32768
SF          160.4615719 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

lhr-B-0770-3(c)

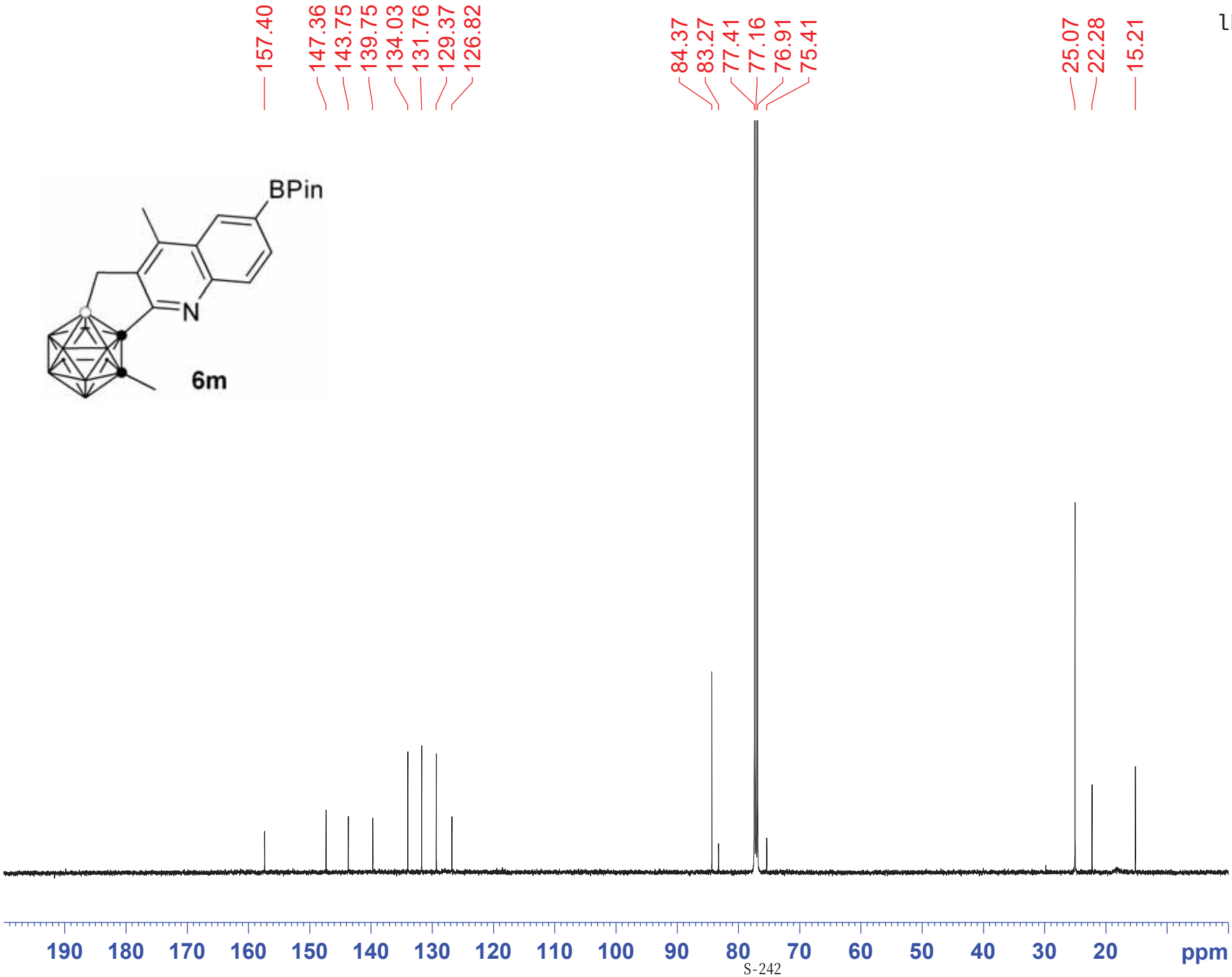



```
Current Data Parameters
NAME      lhr-B-0770-3(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170930
Time                10.36 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                 186.15
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                     1
SFO1          160.4615792 MHz
NUC1                  11B
P1                 10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                  16384
SF            160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



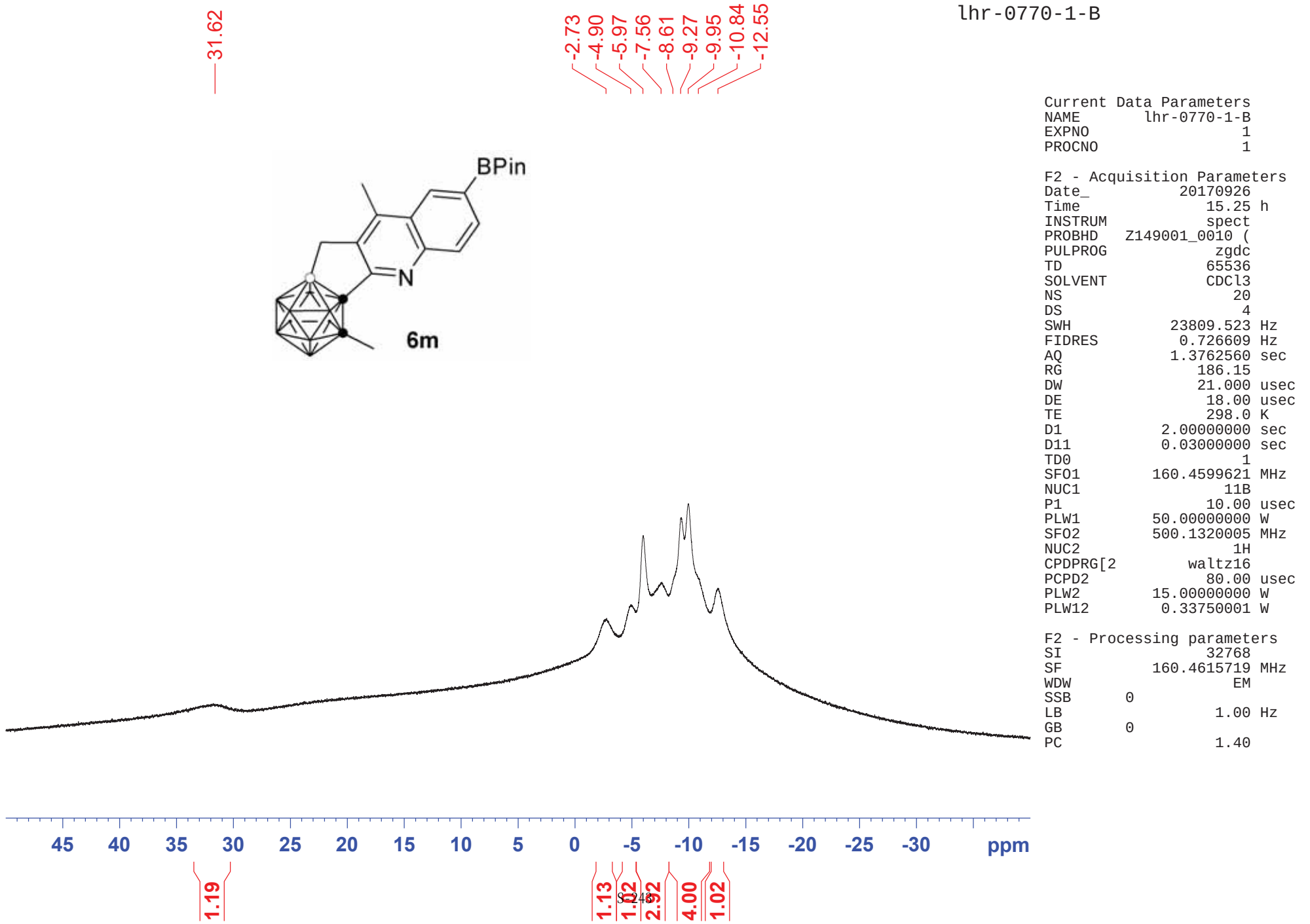
lhr-0770-1-H

```
Current Data Parameters
NAME        lhr-0770-1-H
EXPNO                  1
PROCNO                 1

F2 - Acquisition Paramet
Date_           20170926
Time               15.01
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    12
DS                     2
SWH            10000.000
FIDRES          0.305176
AQ             3.2767999
RG                 56.83
DW                50.000
DE                10.00
TE                298.0
D1           1.00000000
TD0                    1
SFO1         500.1330883
NUC1                1H
P1                 12.00
PLW1         15.00000000

F2 - Processing paramete
SI                 65536
SF          500.1300125
WDW                   EM
SSB       0
LB                  0.30
GB        0
PC                  1.00
```



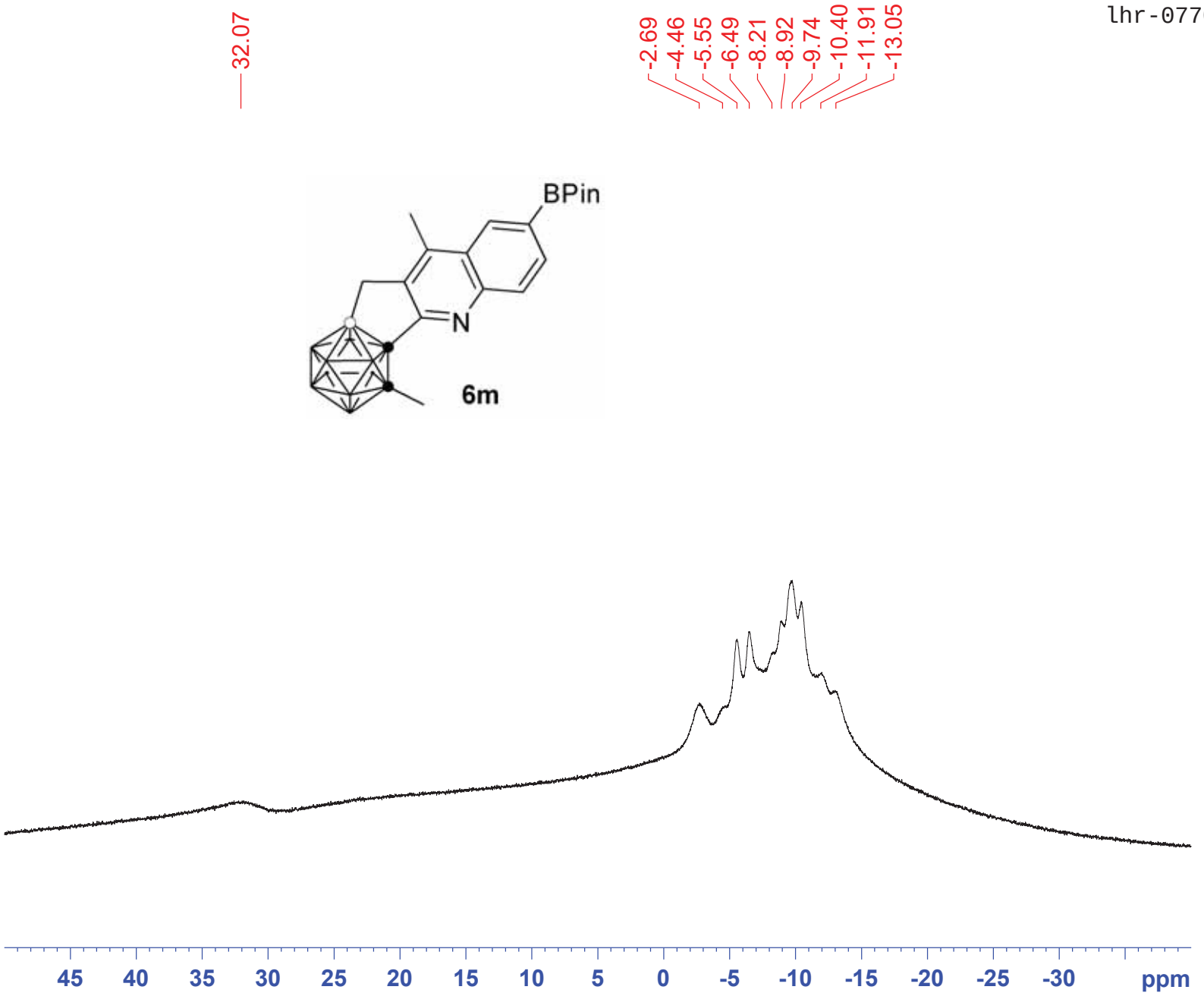
lhr-0770-1-C

```
Current Data Parameters
NAME        lhr-0770-1-C
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170926
Time              15.22 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  400
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577717 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



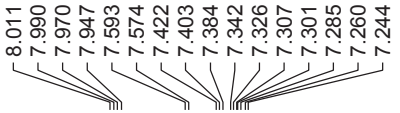
lhr-0770-1-B

```
Current Data Parameters
NAME                 lhr-0770-1-B
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20170926
Time                        15.25 h
INSTRUM                      spect
PROBHD          Z149001_0010 (
PULPROG                      zgdc
TD                          65536
SOLVENT                     CDCl3
NS                             20
DS                              4
SWH                     23809.523 Hz
FIDRES                   0.726609 Hz
AQ                       1.3762560 sec
RG                          186.15
DW                          21.000 usec
DE                          18.00 usec
TE                          298.0 K
D1                       2.00000000 sec
D11                      0.03000000 sec
TD0                             1
SFO1                160.4599621 MHz
NUC1                         11B
P1                          10.00 usec
PLW1                50.00000000 W
SFO2                500.1320005 MHz
NUC2                         1H
CPDPRG[2                 waltz16
PCPD2                       80.00 usec
PLW2                15.00000000 W
PLW12                0.33750001 W

F2 - Processing parameters
SI                           32768
SF                  160.4615719 MHz
WDW                             EM
SSB                 0
LB                          1.00 Hz
GB                  0
PC                          1.40
```

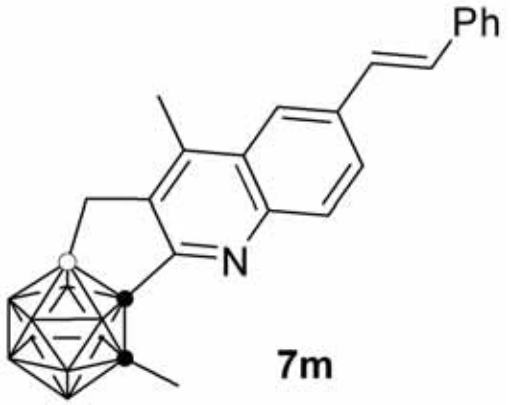


lhr-0770-1-B(c)

```
Current Data Parameters
NAME      lhr-0770-1-B(c)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20170926
Time               15.26 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    20
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                186.15
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         160.4615792 MHz
NUC1                11B
P1                10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                 16384
SF           160.4615792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



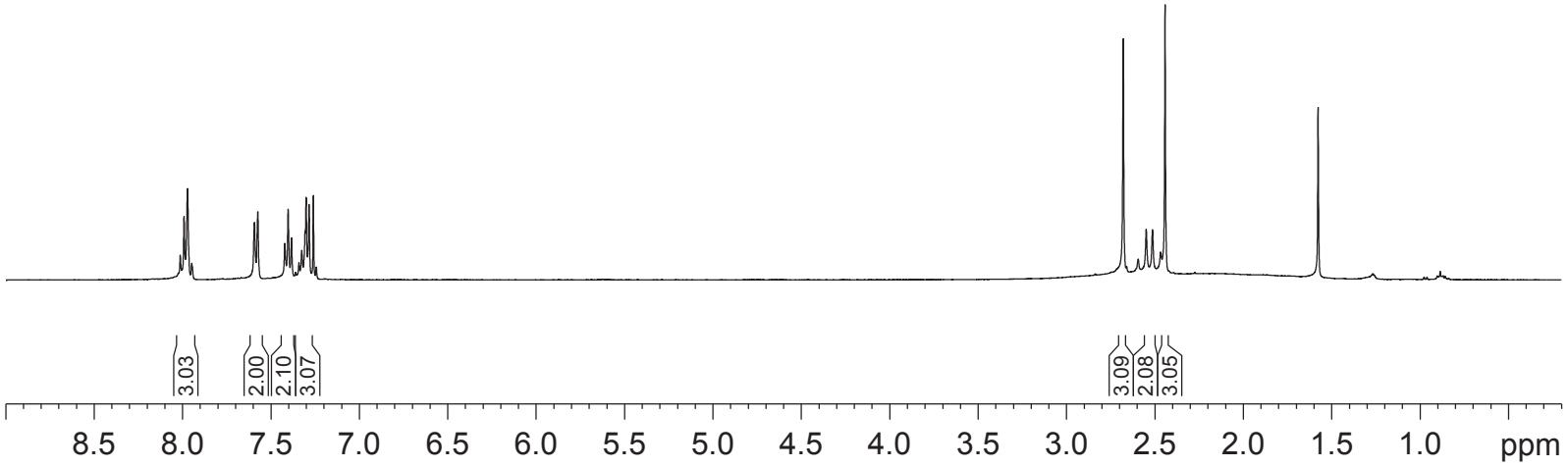
lhr-H-0770-10-cc-cdc

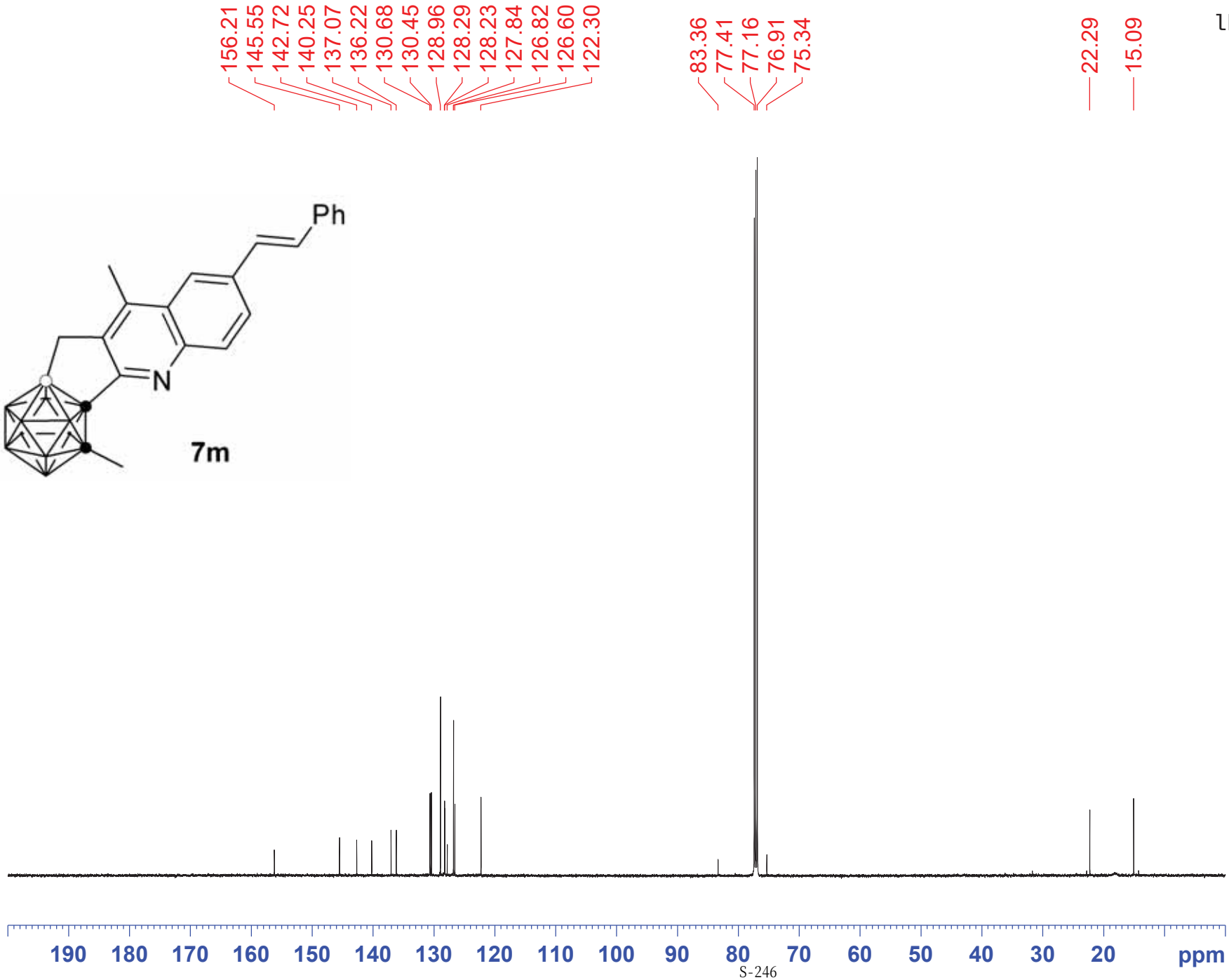


Current Data Parameters
NAME lhr-H-0770-10-cc-cdcl3
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171009
Time 14.25 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W

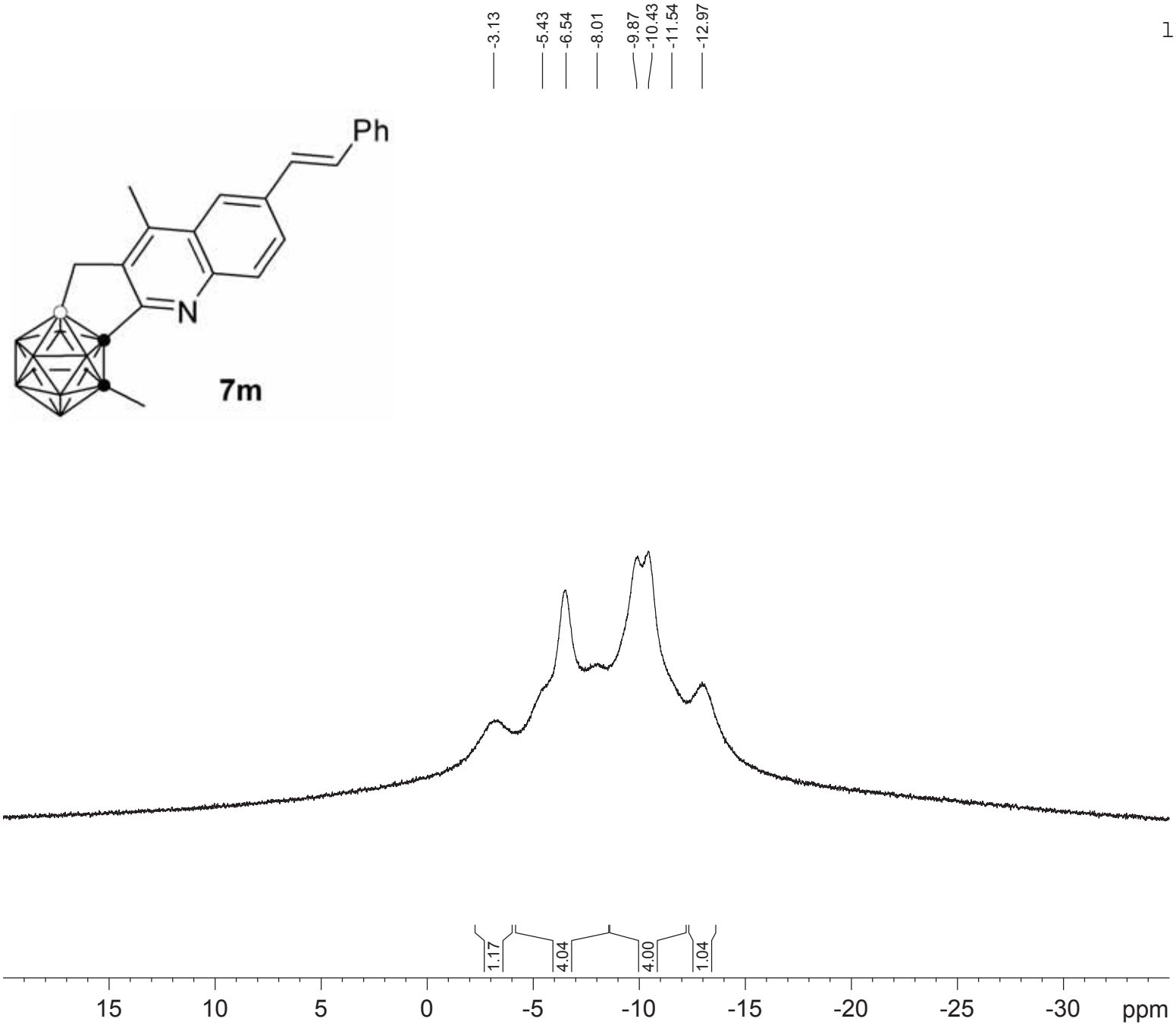
F2 - Processing parameters
SI 65536
SF 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





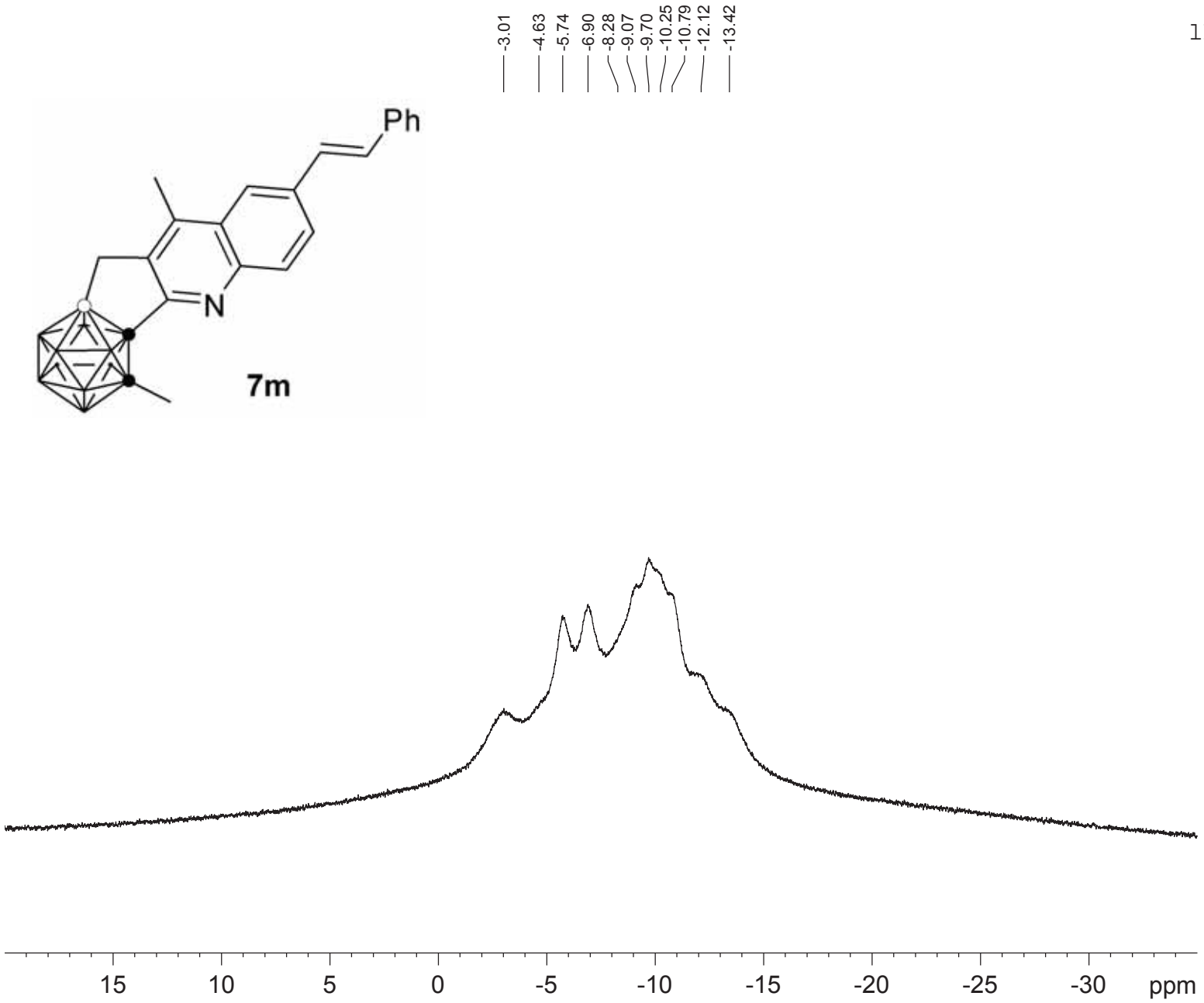
lhr-C-0770-10

```
Current Data Parameters
NAME       lhr-C-0770-10
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171009
Time              19.17 h
INSTRUM             spect
PROBHD    Z149001_0010 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   396
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                206.72
DW                16.800 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                 10.00 usec
PLW1         61.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         15.00000000 W
PLW12         0.33750001 W
PLW13         0.16976000 W

F2 - Processing parameters
SI                 32768
SF           125.7577723 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



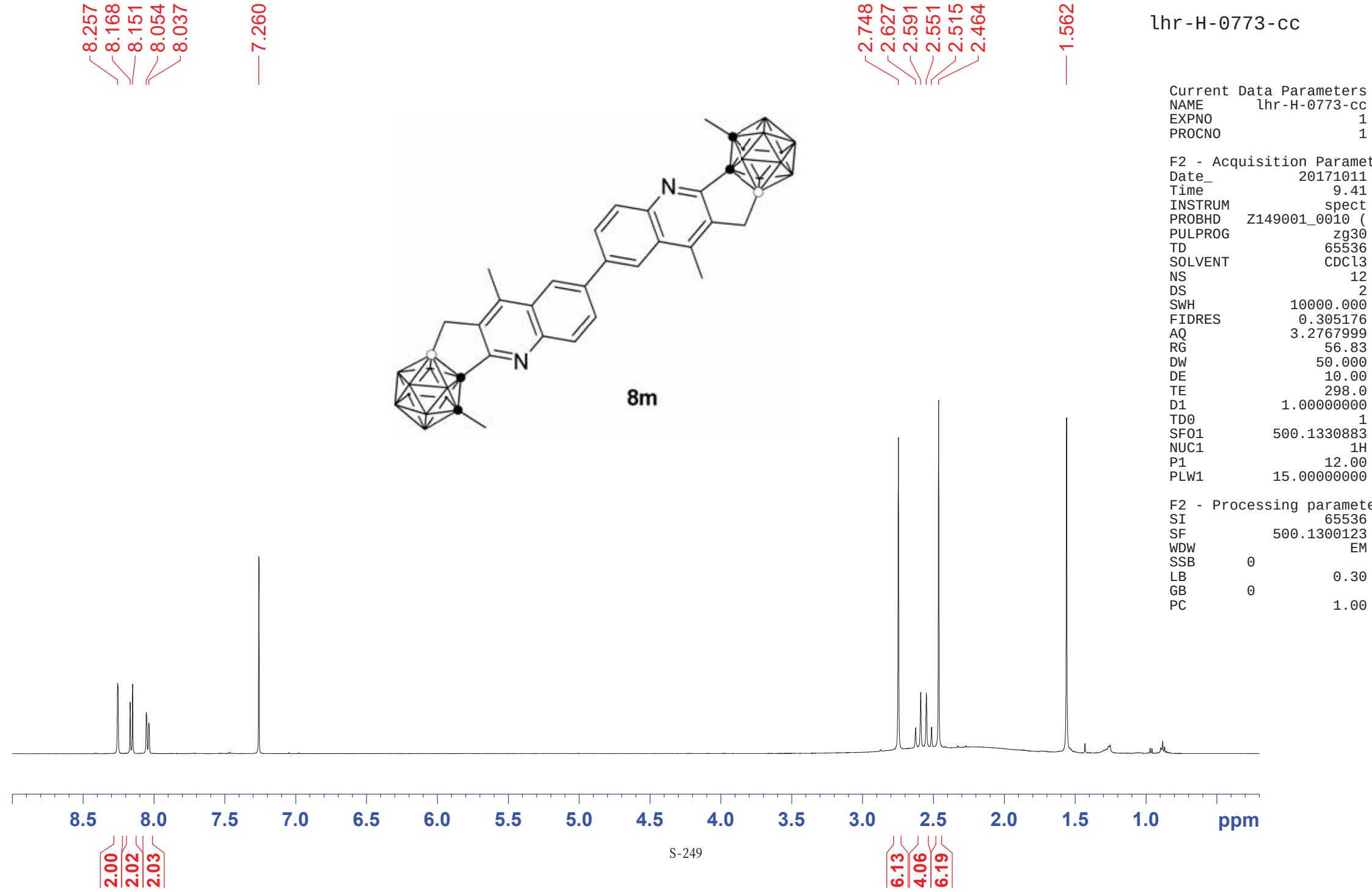
lhr-B-0770-10-cc-cdcl3

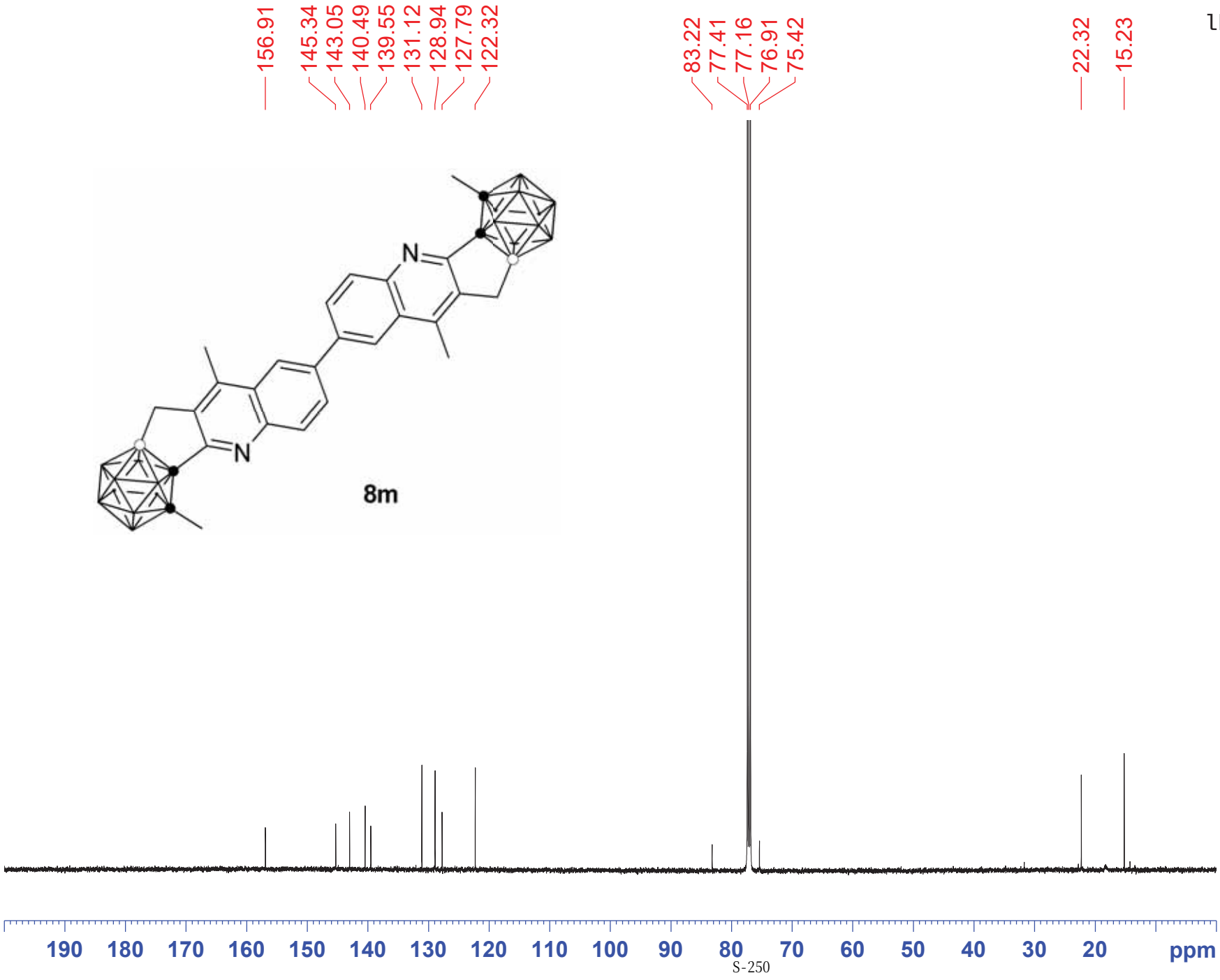
```
Current Data Parameters
NAME      lhr-B-0770-10-cc-cdcl3
EXPNO                          1
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20171009
Time                       14.29 h
INSTRUM                    spect
PROBHD    Z108618_0257 (
PULPROG                     zgdc
TD                         65536
SOLVENT                    CDCl3
NS                            52
DS                             4
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3631488 sec
RG                           456
DW                        20.800 usec
DE                         6.50 usec
TE                        295.3 K
D1                   2.00000000 sec
D11                  0.03000000 sec
TD0                            1
SFO1                128.4096890 MHz
NUC1                         11B
P1                         7.50 usec
PLW1                55.09999847 W
SFO2                400.2316009 MHz
NUC2                         1H
CPDPRG[2                waltz16
PCPD2                     90.00 usec
PLW2                13.56000042 W
PLW12                0.27428001 W

F2 - Processing parameters
SI                         32768
SF                  128.4097615 MHz
WDW                           EM
SSB       0
LB                         1.00 Hz
GB        0
PC                         1.40
```



lhr-B-0770-10-cc-cdcl3(C)

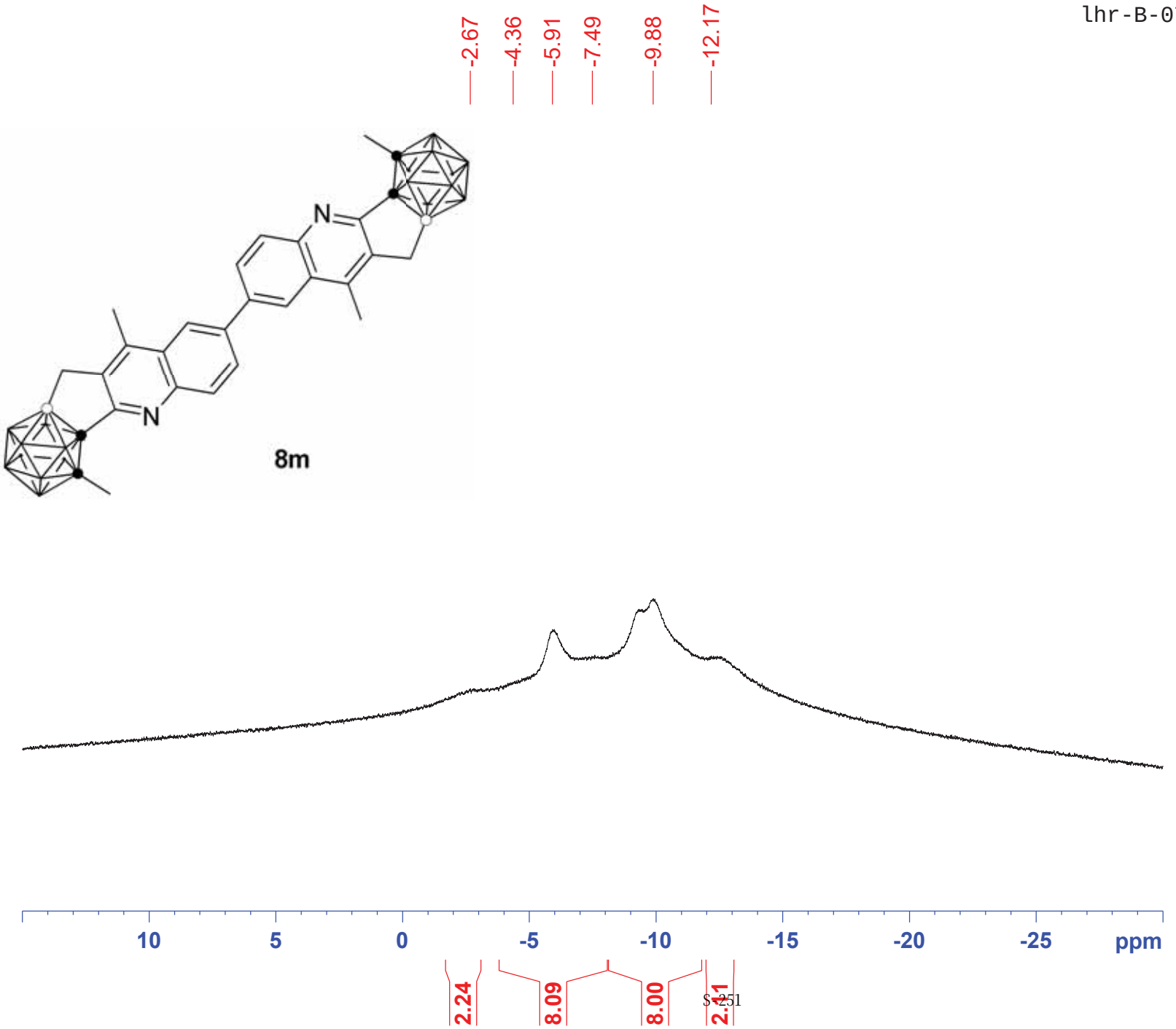
```
Current Data Parameters
NAME      lhr-B-0770-10-cc-cdcl3(C)
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171009
Time              14.34 h
INSTRUM           spect
PROBHD   Z108618_0257 (
PULPROG             zg
TD                65536
SOLVENT           CDCl3
NS                   60
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  456
DW               20.800 usec
DE                6.50 usec
TE               294.9 K
D1            2.00000000 sec
TD0                   1
SFO1        128.4096890 MHz
NUC1               11B
P1                7.50 usec
PLW1        55.09999847 W

F2 - Processing parameters
SI                32768
SF          128.4097430 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```


8.257
8.168
8.151
8.054
8.037
7.260
2.748
2.627
2.591
2.551
2.515
2.464
1.562
lhr-H-0773-cc
Current Data Parameters
NAME lhr-H-0773-cc
EXPNO 1
PROCNO 1
F2 - Acquisition Paramet
Date_ 20171011
Time 9.41
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 12
DS 2
SWH 10000.000
FIDRES 0.305176
AQ 3.2767999
RG 56.83
DW 50.000
DE 10.00
TE 298.0
D1 1.00000000
TD0 1
SFO1 500.1330883
NUC1 1H
P1 12.00
PLW1 15.00000000
F2 - Processing paramete
SI 65536
SF 500.1300123
WDW EM
SSB 0
LB 0.30
GB 0
PC 1.00
N
N
8m
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.00
2.02
2.03
6.13
4.06
6.19



lhr-C-0773-cc

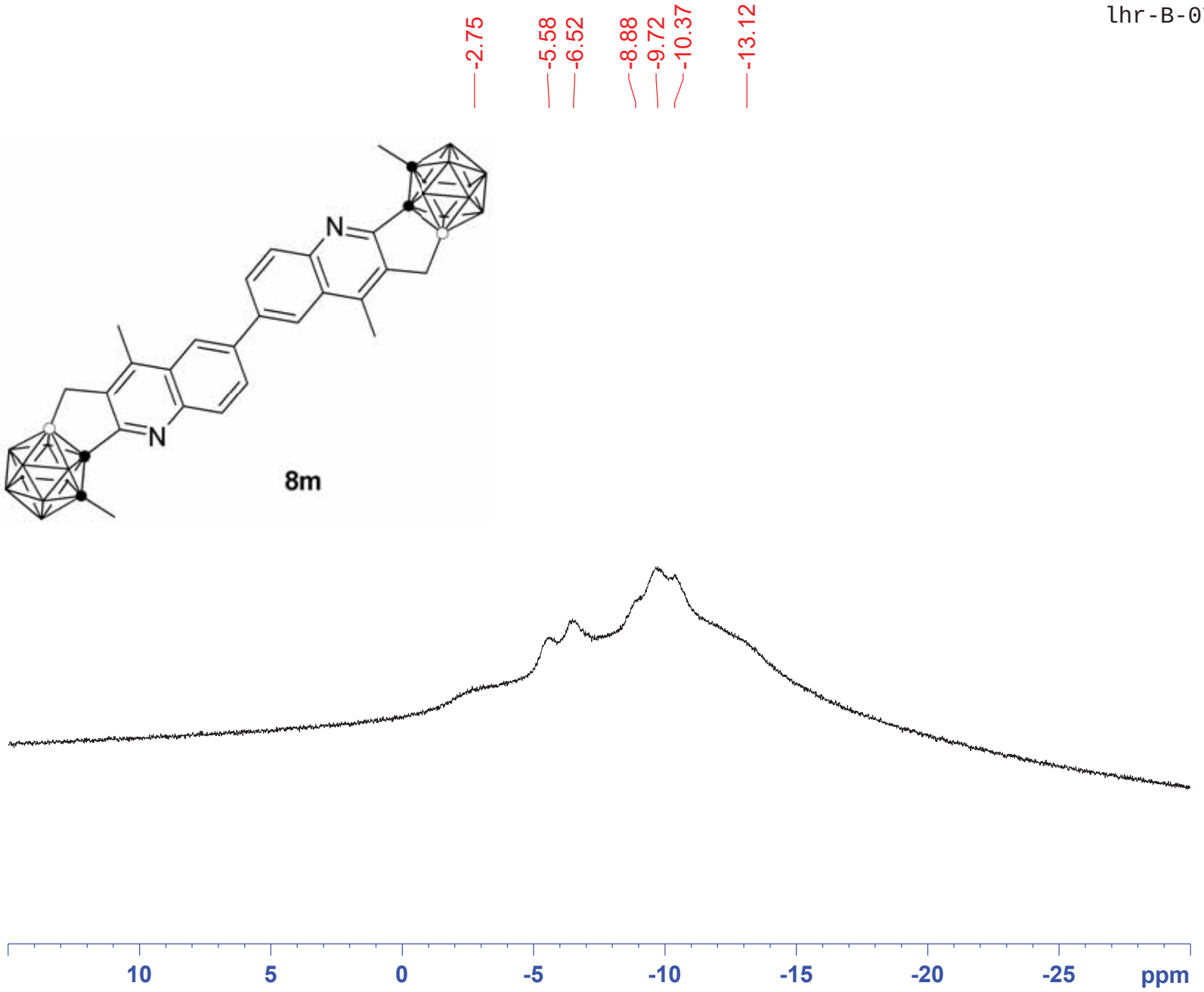
```
Current Data Parameters
NAME      lhr-C-0773-cc
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20171011
Time              10.24 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  781
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ            1.1010048 sec
RG               206.72
DW               16.800 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        61.00000000 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            80.00 usec
PLW2        15.00000000 W
PLW12        0.33750001 W
PLW13        0.16976000 W

F2 - Processing parameters
SI                32768
SF          125.7577714 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



Current Data Parameters
NAME lhr-B-0773-cc
EXPNO 1
PROCNO 1

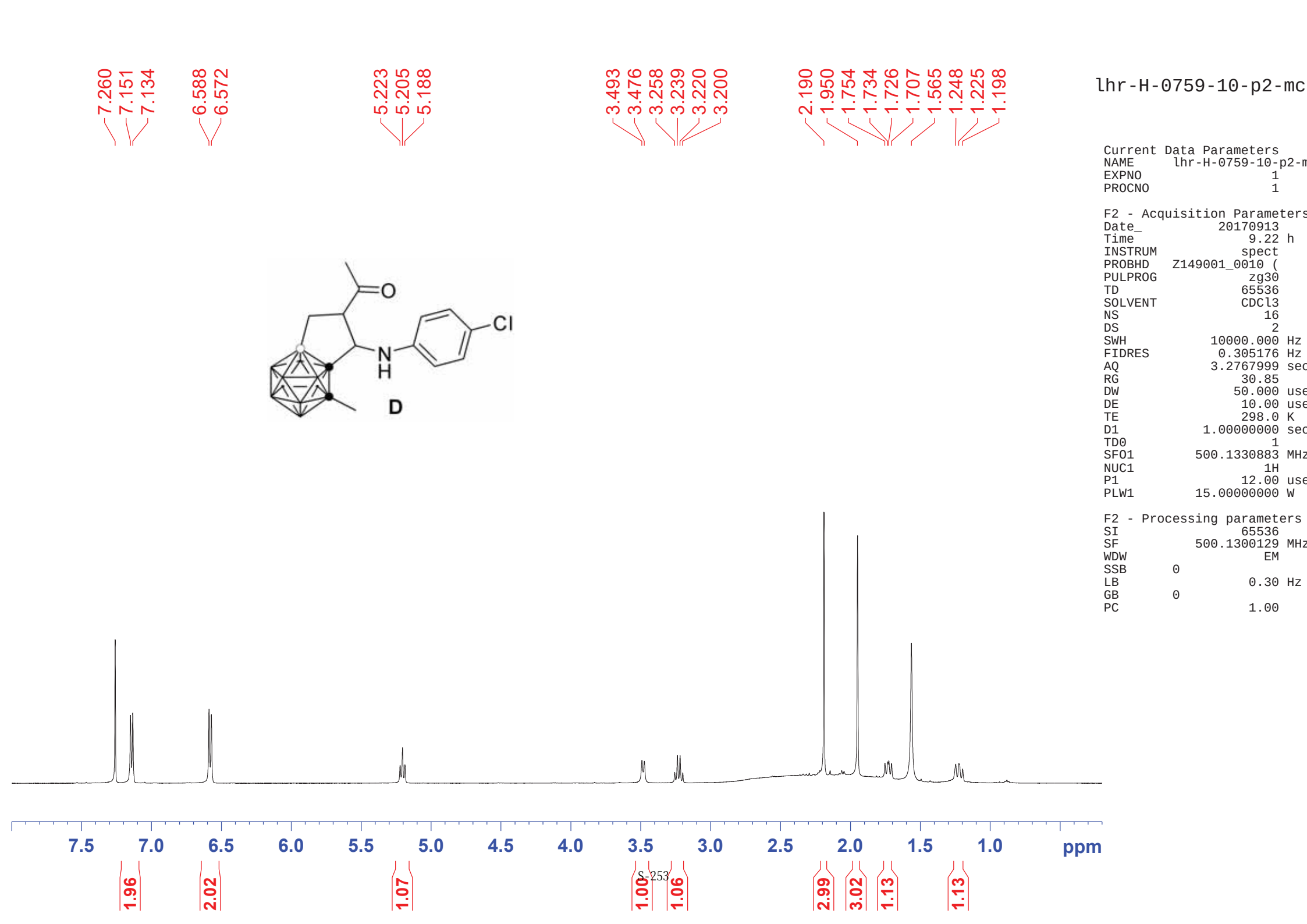
F2 - Acquisition Parameters
Date_ 20171011
Time 10.27 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 20
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 186.15
DW 20.800 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 160.4599621 MHz
NUC1 11B
P1 10.00 usec
PLW1 50.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W

F2 - Processing parameters
SI 32768
SF 160.4615719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



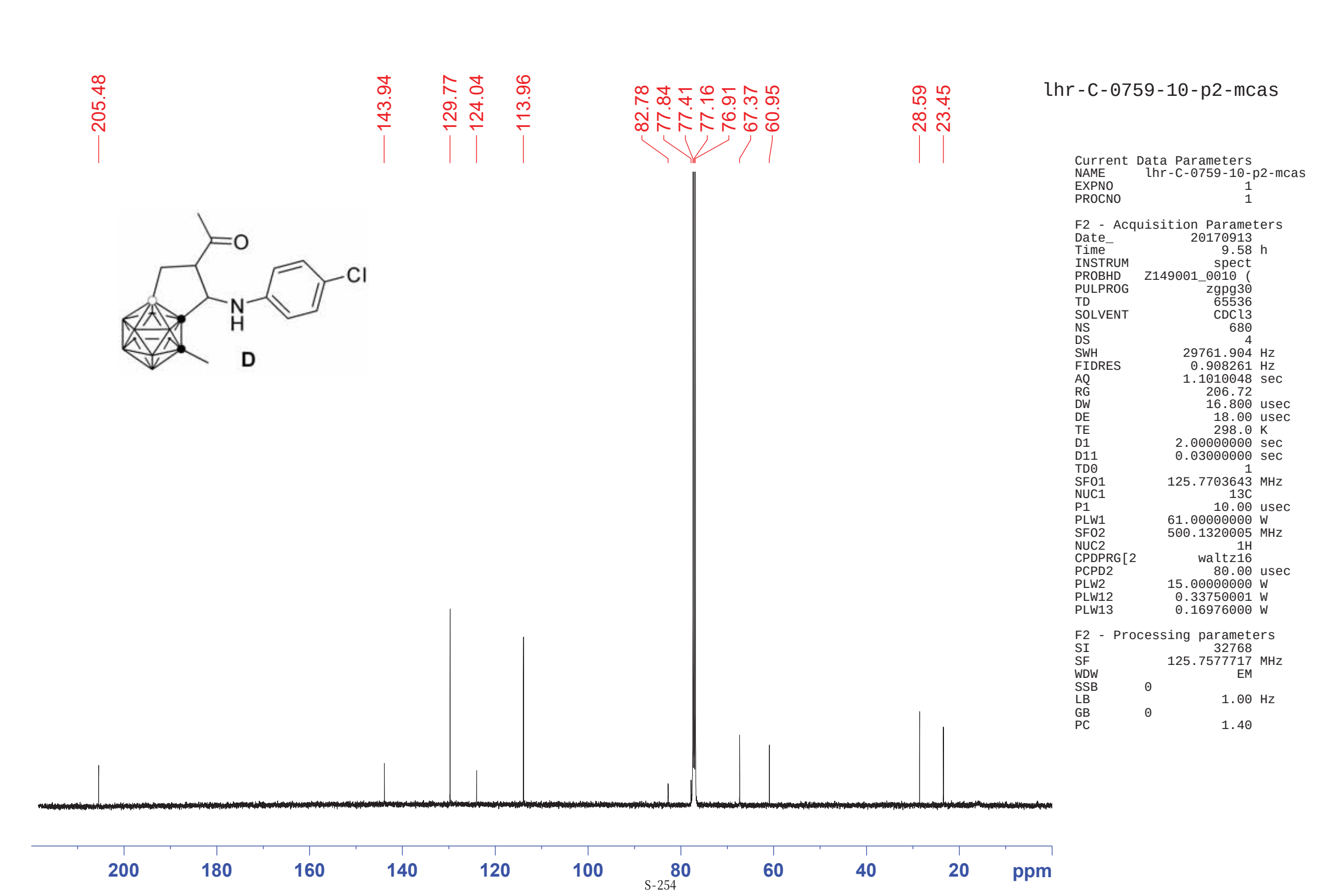
lhr-B-0773-cc(c)

```
Current Data Parameters
NAME      lhr-B-0773-cc(c)
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_             20171011
Time                10.28 h
INSTRUM             spect
PROBHD   Z149001_0010 (
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     20
DS                      4
SWH             24038.461 Hz
FIDRES           1.467191 Hz
AQ              0.6815744 sec
RG                 206.72
DW                 20.800 usec
DE                 18.00 usec
TE                 298.0 K
D1              1.00000000 sec
TD0                     1
SFO1          160.4615792 MHz
NUC1                  11B
P1                 10.00 usec
PLW1          50.00000000 W

F2 - Processing parameters
SI                  16384
SF            160.4615792 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```



lhr-H-0759-10-p2-mc

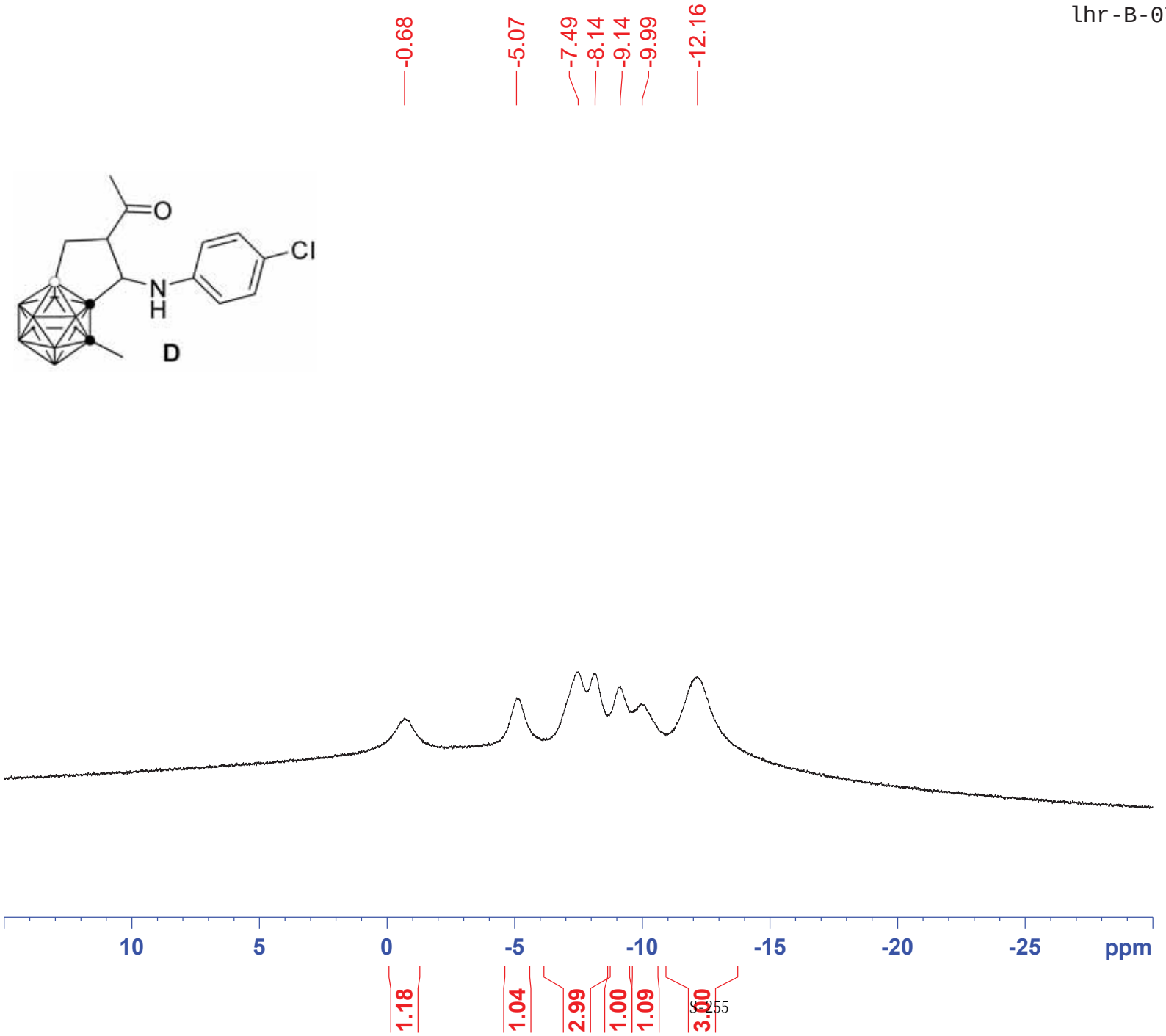
```
Current Data Parameters
NAME      lhr-H-0759-10-p2-m
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_           20170913
Time                9.22 h
INSTRUM            spect
PROBHD    Z149001_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES         0.305176 Hz
AQ             3.2767999 sec
RG                 30.85
DW                50.000 use
DE                10.00 use
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         500.1330883 MHz
NUC1                  1H
P1                 12.00 use
PLW1        15.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300129 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



lhr-C-0759-10-p2-mcas

```
Current Data Parameters
NAME      lhr-C-0759-10-p2-mcas
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20170913
Time                    9.58 h
INSTRUM                spect
PROBHD    Z149001_0010 (
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       680
DS                         4
SWH                29761.904 Hz
FIDRES             0.908261 Hz
AQ                 1.1010048 sec
RG                    206.72
DW                    16.800 usec
DE                    18.00 usec
TE                    298.0 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1             125.7703643 MHz
NUC1                     13C
P1                    10.00 usec
PLW1              61.00000000 W
SFO2              500.1320005 MHz
NUC2                     1H
CPDPRG[2              waltz16
PCPD2                 80.00 usec
PLW2              15.00000000 W
PLW12              0.33750001 W
PLW13              0.16976000 W

F2 - Processing parameters
SI                       32768
SF                125.7577717 MHz
WDW                         EM
SSB           0
LB                     1.00 Hz
GB            0
PC                     1.40
```

lhr-B-0759-10-p2-mcas

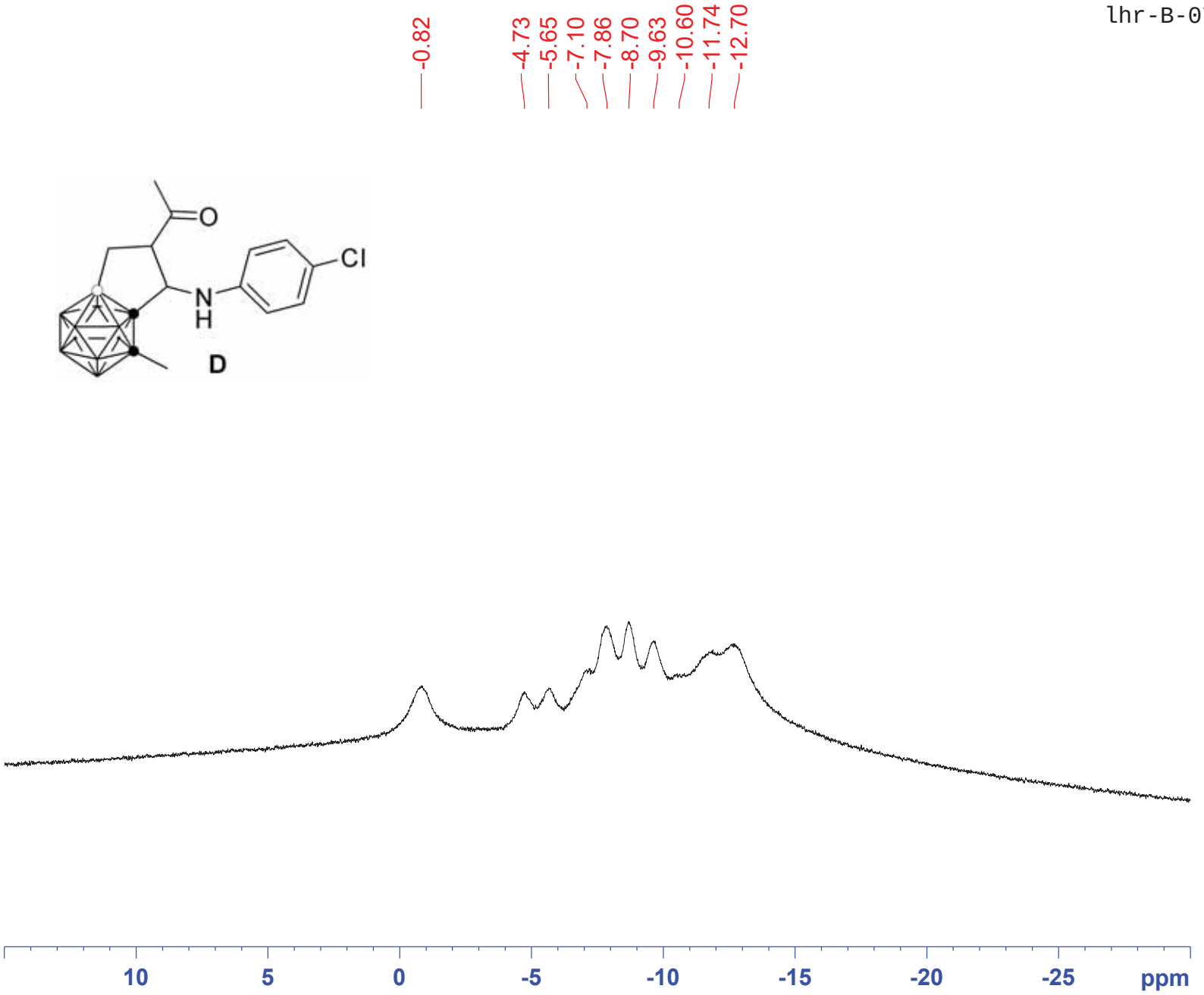


Current Data Parameters
NAME lhr-B-0759-10-p2-mcas
EXPNO 1
PROCNO 1

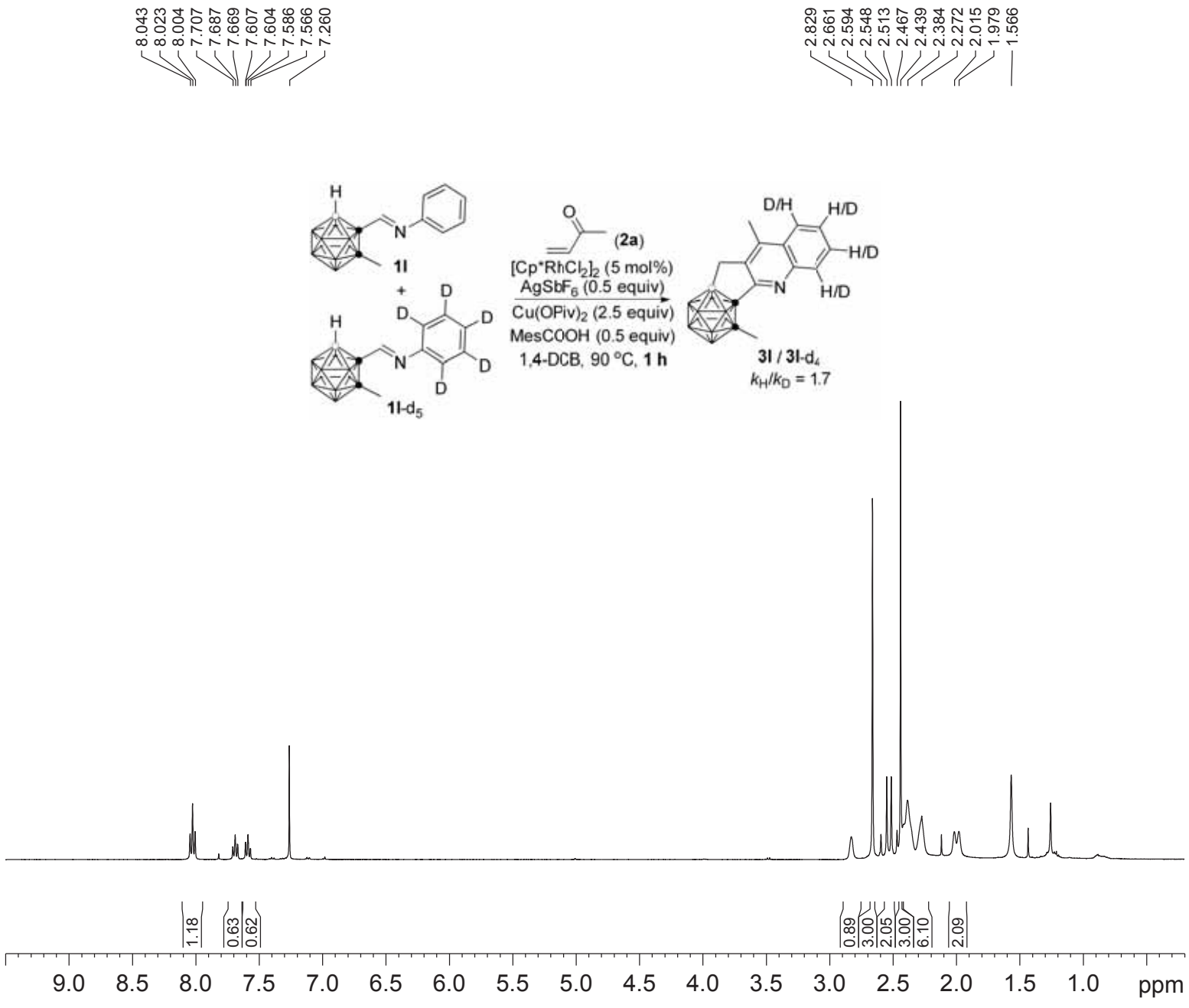
F2 - Acquisition Parameters
Date_ 20170913
Time 10.02 h
INSTRUM spect
PROBHD Z149001_0010 (
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 20
DS 4
SWH 23809.523 Hz
FIDRES 0.726609 Hz
AQ 1.3762560 sec
RG 186.15
DW 21.000 usec
DE 18.00 usec
TE 298.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 160.4599621 MHz
NUC1 11B
P1 10.00 usec
PLW1 50.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 15.00000000 W
PLW12 0.33750001 W

F2 - Processing parameters
SI 32768
SF 160.4615719 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

lhr-B-0759-10-p2-mcas(C)




```
Current Data Parameters
NAME      lhr-B-0759-10-p2-mcas(C)
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170913
Time              10.03 h
INSTRUM            spect
PROBHD   Z149001_0010 (
PULPROG               zg
TD                 32768
SOLVENT            CDCl3
NS                    20
DS                     4
SWH            24038.461 Hz
FIDRES          1.467191 Hz
AQ             0.6815744 sec
RG                186.15
DW                20.800 usec
DE                18.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         160.4615792 MHz
NUC1                 11B
P1                10.00 usec
PLW1         50.00000000 W

F2 - Processing parameters
SI                 16384
SF           160.4615792 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



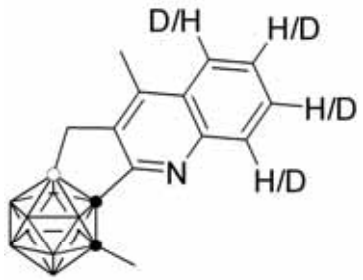
lhr-H-decoB-d5cc-co

Current Data Parameters
NAME lhr-H-decoB-d5cc-com-product-
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20171117
Time 19.34 h
INSTRUM spect
PROBHD Z108618_0257 (
PULPROG zgig
TD 65536
SOLVENT CDCl3
NS 13
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 400.2324714 MHz
NUC1 1H
P1 12.80 usec
PLW1 13.56000042 W
SFO2 128.4068641 MHz
NUC2 11B
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 55.09999847 W
PLW12 0.48427999 W

F2 - Processing parameters
SI 32768
SF 400.2300103 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

8.109
7.762
5.319



3l / 3l-d_4

```
Current Data Parameters
NAME      lhr-2H-casd5-chloroform
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180529
Time               16.30 h
INSTRUM            spect
PROBHD    Z824601_0021 (
PULPROG            zg2h
TD                 4096
SOLVENT            CDCl3
NS                 18190
DS                    0
SWH             6142.506 Hz
FIDRES          2.999271 Hz
AQ              0.3334144 sec
RG                  0.5
DW                81.400 usec
DE                 6.50 usec
TE                296.8 K
D1             0.05000000 sec
D11            0.03000000 sec
TD0                   1
SFO1           61.4226981 MHz
NUC1                  2H
P1                300.00 usec
PLW1           3.00000000 W

F2 - Processing parameters
SI                 4096
SF             61.4223898 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.00
```