Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

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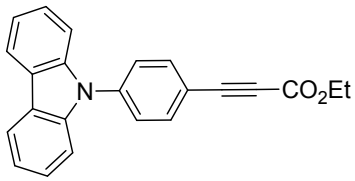
General Procedures.

All reactions were carried out in oven-dried glassware under an atmosphere of dry N_2 with the rigid exclusion of air and moisture using standard Schlenk techniques or in a glovebox. All organic solvents were freshly distilled from sodium benzophenone ketyl immediately prior to use. Compounds **5**,[1] **6**,[2] ethyl 4-tolylpropiolate,[3] ethyl 3-tolylpropiolate,[4] ethyl 4-*tert*-butylphenyl propiolate,[5] ethyl (4-methoxyphenyl)propiolate,[3] ethyl 4-dimethyl aminophenylpropiolate,[6] ethyl 4-fluorophenylpropiolate,[4] ethyl 4-chlorophenylpropiolate,[4] ethyl 4-bromophenylpropiolate,[7] ethyl 3-([1,1'-biphenyl]-4-yl)propiolate,[8] ethyl 3-(naphthalen-2-yl)propiolate,[8] ethyl 3-(6-methoxy-2-naphthalenyl)propiolate,[9] ethyl 2-furylpropiolate,[10] ethyl 3-furylpropiolate,[11] ethyl 2-thienylpropiolate,[12] ethyl 3-thienylpropiolate,[3] and ethyl 2-pyridinylpropiolate,[3] were prepared according to literature procedures. All other chemicals were purchased from either Aldrich or Acros Chemical Co. and used as received unless otherwise specified. ^{1}H, ^{13}C, and ^{11}B NMR spectra were recorded on a Bruker DPX 400 spectrometer at 400 MHz, 100 MHz and 128 MHz, respectively. All signals were reported in δ unit 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) for boron chemical shifts. Mass spectra were collected on an Agilent GC/MS 5975C system, or a MALDI Micro MX mass spectrometer, or an API QSTAR XL System.

Experimental Section.

Preparation of ethyl 3-[4-(*N*-carbazolyl)phenyl]propiolate (2t). To a diethyl ether solution (20 mL) of *N*-(4-ethynylphenyl)carbazole (500 mg, 1.87mmol) was added *n*-BuLi (0.75 mL, 2.5M in *n*-hexane, 1.87 mmol) at -78 °C and stirred for 0.5 h. Ethyl chloroformate (0.27 mL, 2.84 mmol) was then added at -78 °C. The reaction mixture was allowed to warm to room temperature and stirred overnight. After water (20 mL) was added to reaction mixture, the aqueous layer was extracted with ether (15 × 3 mL). The combined organic layer was then dried over anhydrous Na_2SO_4. After filtration and removal of solvent in vacuo, the residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/diethyl ether (8/1 in v/v) as eluent to give **2t** (420 mg, 66%, 1.24 mmol).

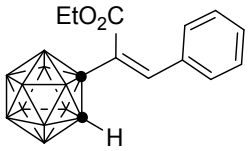


2t

2t: light yellow crystals. ^{1}H NMR (C_6D_6, 400 MHz) δ 8.00 (m, 2H) (aromatic *H*), 7.24 (m, 6H) (aromatic *H*), 7.15 (m, 2H) (aromatic *H*), 6.85 (m, 2H) (aromatic *H*), 4.00 (q, J = 7.1 Hz, 2H) (OC*H*$_2$CH$_3$), 0.95 (t, J = 7.1 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz): δ 153.93 (*C*OOEt), 140.57, 139.85, 134.65, 126.81, 126.46, 124.26, 120.94, 120.74, 118.32, 110.06 (aromatic *C*), 85.20, 82.41 (acetylenic *C*), 62.01 (O*C*H$_2$CH$_3$), 13.99 (OCH$_2$*C*H$_3$). HRMS: *m/z* calcd for $C_{23}H_{17}NO_2$ $[M]^+$: 339.1259. Found: 339.1259.

Preparation of 1-Alkenyl-*o*-Carboranes (3). A Representative Procedure. *o*-Carborane (**1**, 29 mg, 0.20 mmol), alkyne (**2**, 0.40 mmol) and tris(4-methoxy

phenyl)phosphine (7 mg, 0.02 mmol) were mixed in dioxane (0.6 mL). The resulting mixture was heated at 110 °C for 72 h. Then the reaction solution was concentrated to dryness in vacuo. The residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/dichloromethane (20/1 in v/v) as eluent to give 1-alkenyl-*o*-carboranes (**3**).



3a

3a: Colorless crystals. Yield: 82%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.34 (m, 3H) (phenyl *H*), 7.23 (m, 2H) (phenyl *H*), 7.19 (s, 1H) (olefinic *H*), 4.23 (s, 1H) (cage *H*), 4.14 (q, J = 6.4 Hz, 2H) (OCH_2CH_3), 1.11 (t, J = 6.8 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.5 (*C*OOEt), 139.1, 133.7, 129.7, 128.8, 128.3, 127.7 (phenyl & olefinic *C*), 72.9 (cage *C*-C), 62.5 (OCH_2CH_3), 59.4 (cage *C*-H), 13.7 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.4 (1B), -7.6 (2B), -9.2 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{13}H_{21}{}^{11}B_8{}^{10}B_2O_2$ $[M - H]^+$: 317.2545. Found: 317.2552.

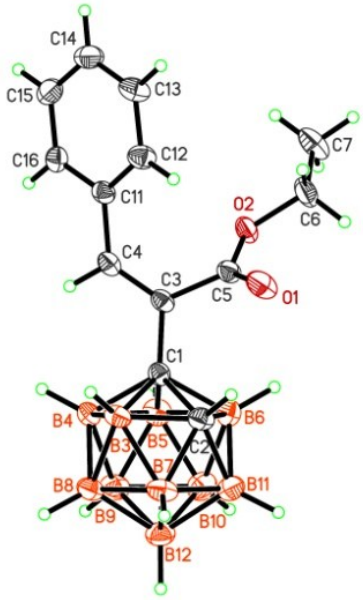


Figure S1. Molecular structure of **3a**

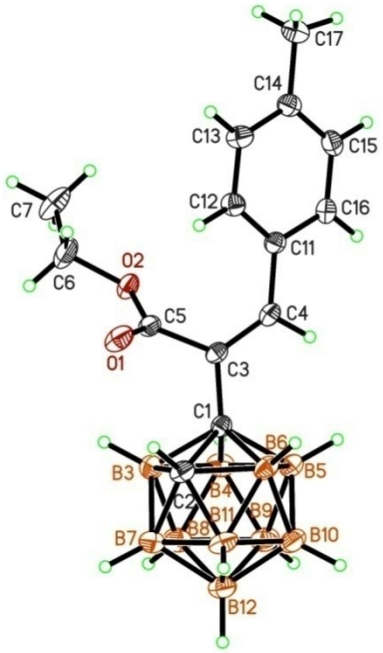
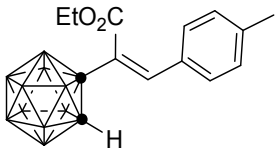
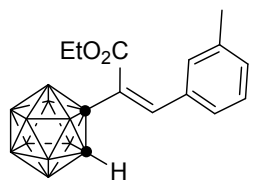


Figure S2. Molecular structure of **3b**



3b

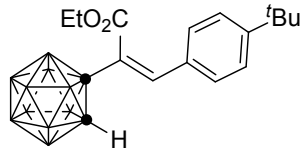
3b: Colorless crystals. Yield: 85%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.14 (m, 5H) (phenyl & olefinic *H*), 4.21 (s, 1H) (cage *H*), 4.18 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 2.34 (s, 3H) ($C_6H_4CH_3$), 1.16 (t, J = 6.8 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.8 (*C*OOEt), 140.2, 139.1, 130.7, 129.5, 128.4, 126.6 (phenyl & olefinic *C*), 73.3 (cage *C*-C), 62.5 (OCH_2CH_3), 59.6 (cage *C*-H), 21.6 ($C_6H_4CH_3$), 13.8 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.5 (1B), -7.8 (2B), -9.3 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{14}H_{23}{}^{11}B_8{}^{10}B_2O_2$ $[M - H]^+$: 331.2701. Found: 331.2695.



3c

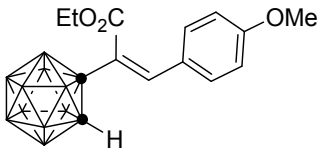
3c: White solid. Yield: 89%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ

7.25 – 7.03 (m, 5H) (phenyl & olefinic *H*), 4.24 (s, 1H) (cage *H*), 4.16 (q, *J* = 7.2 Hz, 2H) (OC*H*$_2$CH$_3$), 2.34 (s, 3H) (C$_6$H$_4$C*H*$_3$), 1.13 (t, *J* = 7.2 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz): *δ* 166.7 (*C*OOEt), 139.3, 138.5, 133.6, 130.6, 129.1, 128.7, 127.4, 125.4 (phenyl & olefinic *C*), 73.1 (cage *C*-C), 62.5 (O*C*H$_2$CH$_3$), 59.5 (cage *C*-H), 21.5 (C$_6$H$_4$*C*H$_3$), 13.7 (OCH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR (CDCl$_3$, 128 MHz): *δ* -0.8 (1B), -2.4 (1B), -7.7 (2B), -9.3 (2B), -10.1 (2B), -11.4 (2B). HRMS: *m/z* calcd for C$_{14}$H$_{23}$^{11}B$_8$^{10}B$_2$O$_2$ [M – H]$^+$: 331.2701. Found: 331.2703.



3d

3d: White solid. Yield: 83%. ^{1}H NMR (CDCl$_3$, 400 MHz): *δ* 7.37 – 7.16 (m, 4H) (phenyl *H*), 7.14 (s, 1H) (olefinic *H*), 4.21 (s, 1H) (cage *H*), 4.19 (q, *J* = 6.8 Hz, 2H) (OC*H*$_2$CH$_3$), 1.31 (s, 9H) (C(C*H*$_3$)$_3$), 1.15 (t, *J* = 7.2 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz): *δ* 166.8 (*C*OOEt), 153.4, 139.0, 130.7, 128.3, 126.8, 125.8 (phenyl & olefinic *C*), 73.3 (cage *C*-C), 62.5 (O*C*H$_2$CH$_3$), 59.6 (cage *C*-H), 35.0 (*C*(CH$_3$)$_3$), 31.3 (C(*C*H$_3$)$_3$), 13.8 (OCH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR (CDCl$_3$, 128 MHz): *δ* -0.8 (1B), -2.5 (1B), -7.8 (2B), -9.3 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for C$_{17}$H$_{30}$^{11}B$_8$^{10}B$_2$O$_2$ [M]$^+$: 374.3249. Found: 374.3236.



3e

3e: Colorless oil. Yield: 83%. ^{1}H NMR (CDCl$_3$, 400 MHz): *δ* 7.18 (d, *J* = 8.0 Hz, 2H) (phenyl *H*), 7.08 (s, 1H) (olefinic *H*), 6.85 (d, *J* = 8.0 Hz, 2H) (phenyl *H*), 4.22 – 4.17 (m, 3H) (OC*H*$_2$CH$_3$ & cage *H*), 3.82 (s, 3H) (OC*H*$_3$), 1.19 (t, *J* = 7.2 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR (CDCl$_3$, 100 MHz): *δ* 167.0 (*C*OOEt), 160.9, 138.6, 130.3, 126.0,

125.3, 114.3 (phenyl & olefinic *C*), 73.5 (cage *C*-C), 62.5 (OCH_2CH_3), 59.7 (cage *C*-H), 55.6 (OCH_3), 13.9 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.6 (1B), -7.8 (2B), -9.3 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{14}H_{23}{}^{11}B_8{}^{10}B_2O_3$ $[M - H]^+$: 347.2650. Found: 347.2648.

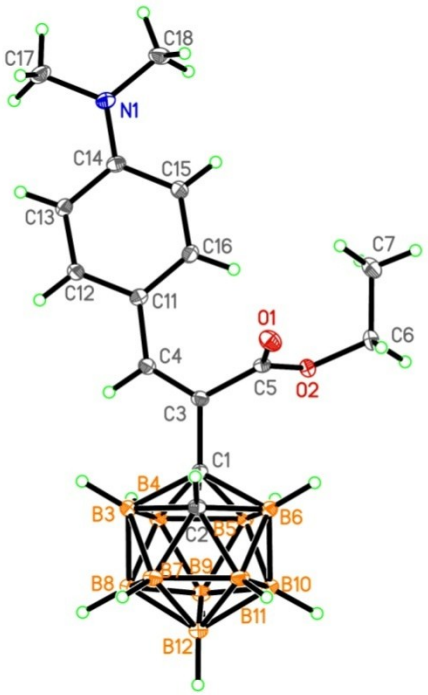
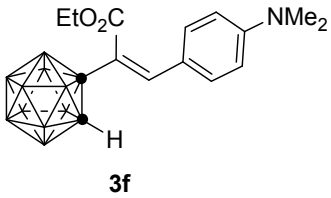


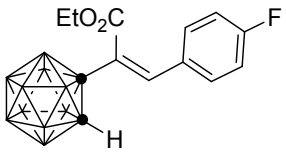
Figure S3. Molecular structure of **3f**



3f

3f: Light yellow crystals. Yield: 70%. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.12 (d, J = 8.8 Hz, 2H) (phenyl *H*), 6.98 (s, 1H) (olefinic *H*), 6.60 (d, J = 9.2 Hz, 2H) (phenyl *H*), 4.24 (q, J = 6.8 Hz, 2H) (OCH_2CH_3), 4.17 (s, 1H) (cage *H*), 3.00 (s, 6H) (NCH_3), 1.25 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 167.7 (*C*OOEt), 151.4, 139.3, 130.4, 121.6, 120.7, 111.7 (phenyl & olefinic *C*), 74.6 (cage *C*-C), 62.3 (OCH_2CH_3), 60.1 (cage *C*-H), 40.3 (NCH_3), 14.0 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$,

128 MHz): δ -0.8 (1B), -2.9 (1B), -8.0 (2B), -9.2 (2B), -9.9 (2B), -11.5 (2B). HRMS: *m/z* calcd for $C_{15}H_{27}{}^{11}B_8{}^{10}B_2NO_2$ $[M]^+$: 361.3045. Found: 361.3040.



3g

3g: White solid. Yield: 32%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.24 – 7.21 (m, 2H) (phenyl *H*), 7.13 (s, 1H) (olefinic *H*), 7.06 – 7.01 (m, 2H) (phenyl *H*), 4.21 (s, 1H) (cage *H*), 4.15 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 1.14 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 166.5 (*C*OOEt), 164.7, 162.2, 137.9, 130.5, 130.4, 129.9, 129.8, 127.8, 116.1, 115.9 (phenyl & olefinic *C*), 72.8 (cage *C*-C), 62.7 (OCH_2CH_3), 59.5 (cage *C*-H), 13.8 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.4 (1B), -7.7 (2B), -9.3 (2B), -10.1 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{13}H_{20}{}^{11}B_8{}^{10}B_2FO_2$ $[M - H]^+$: 335.2451. Found: 335.2435.

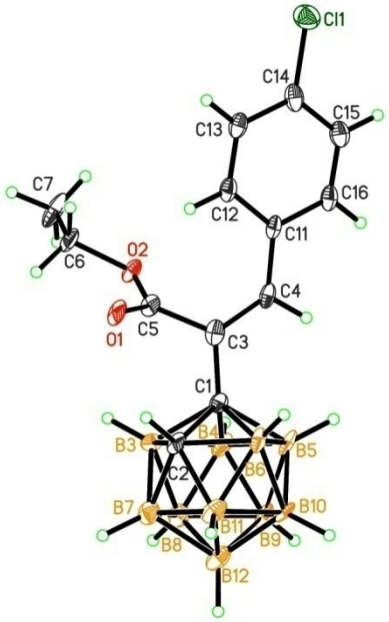
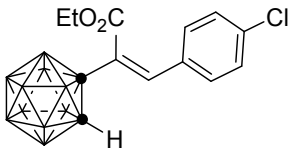


Figure S4. Molecular structure of **3h**



3h

3h: Colorless crystals. Yield: 40%. ^{1}H NMR ($CDCl_3$, 400

MHz): δ 7.34 – 7.15 (m, 4H) (phenyl *H*), 7.12 (s, 1H) (olefinic *H*), 4.21 (s, 1H) (cage *H*), 4.15 (q, J = 7.2 Hz, 2H) (OCH_2CH$_3$), 1.14 (t, J = 7.2 Hz, 3H) (OCH$_2$CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.3 (*C*OOEt), 137.7, 135.8, 132.2, 129.7, 129.1, 128.5 (phenyl & olefinic *C*), 72.7 (cage *C*-C), 62.7 (O*C*H$_2$CH$_3$), 59.5 (cage *C*-H), 13.8 (OCH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.3 (1B), -7.7 (2B), -9.3 (2B), -10.1 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{13}H_{20}{}^{11}B_9{}^{10}BClO_2$ [M – H]$^+$: 352.2119. Found: 352.2128.

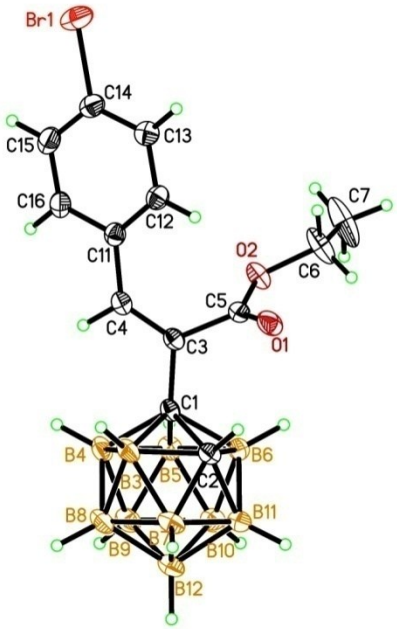
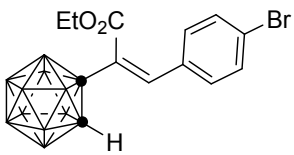


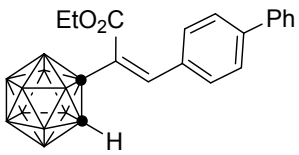
Figure S5. Molecular structure of **3i**



3i

3i: Colorless crystals. Yield: 46%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.49 – 7.10 (m, 4H) (phenyl *H*), 7.09 (s, 1H) (olefinic *H*), 4.20 (s, 1H) (cage *H*), 4.15 (q, J = 7.2 Hz, 2H) (OCH_2CH$_3$), 1.14 (t, J = 7.2 Hz, 3H) (OCH$_2$CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.3 (*C*OOEt), 137.8, 132.6, 132.1, 129.9, 128.6, 124.1 (phenyl & olefinic *C*), 72.7

(cage *C*-C), 62.8 (O*C*$H_2$$CH_3$), 59.5 (cage *C*-H), 13.8 (OCH_2*C*H_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.2 (1B), -7.6 (2B), -9.3 (2B), -10.1 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{13}H_{21}{}^{11}B_9{}^{10}BBrO_2$ $[M]^+$: 397.1692. Found: 397.1686.



3j

3j: Colorless crystals. Yield: 72%. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.60 – 7.30 (m, 9H) (aromatic *H*), 7.20 (s, 1H) (olefinic *H*), 4.23 (s, 1H) (cage *H*), 4.19 (q, *J* = 7.2 Hz, 2H) (OC*H*$_2$$CH_3$), 1.16 (t, *J* = 7.2 Hz, 3H) (OCH_2C*H*$_3$). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 166.7 (*C*OOEt), 142.6, 140.1, 138.7, 132.5, 129.1, 129.0, 128.2, 127.5, 127.4, 127.2 (aromatic & olefinic *C*), 73.1 (cage *C*-C), 62.6 (O*C*$H_2$$CH_3$), 59.6 (cage *C*-H), 13.8 (OCH_2*C*H_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.3 (1B), -7.7 (2B), -9.3 (2B), -9.9 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{19}H_{26}{}^{11}B_8{}^{10}B_2O_2$ $[M]^+$: 394.2936. Found: 394.2940.

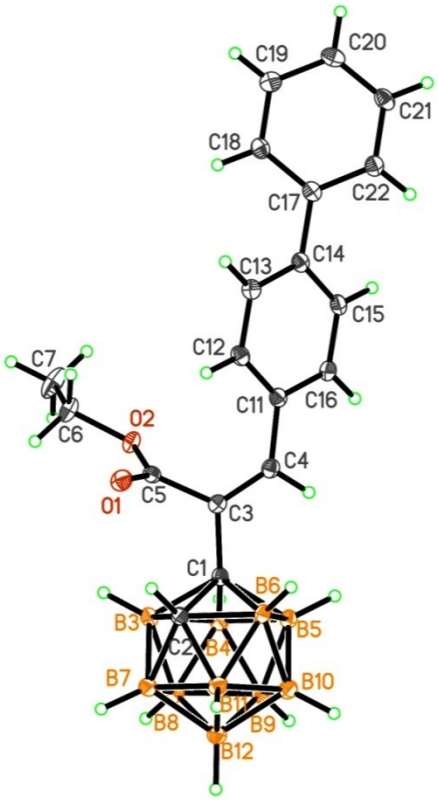
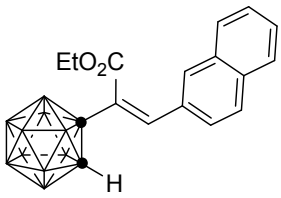


Figure S6. Molecular structure of **3j**



3k

3k: Colorless crystals. Yield: 90%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.81 – 7.29 (m, 8H) (aromatic & olefinic *H*), 4.27 (s, 1H) (cage *H*), 4.16 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 1.08 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.8 (*C*OOEt), 139.2, 133.7, 133.2, 131.1, 129.0, 128.6, 127.9, 127.8, 127.5, 127.1, 125.0 (aromatic & olefinic *C*), 73.1 (cage *C*-C), 62.6 (OCH_2CH_3), 59.6 (cage *C*-H), 13.8 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.3 (1B), -7.6 (2B), -9.2 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{17}H_{24}{}^{11}B_8{}^{10}B_2O_2$ $[M]^+$: 368.2779. Found: 368.2761.

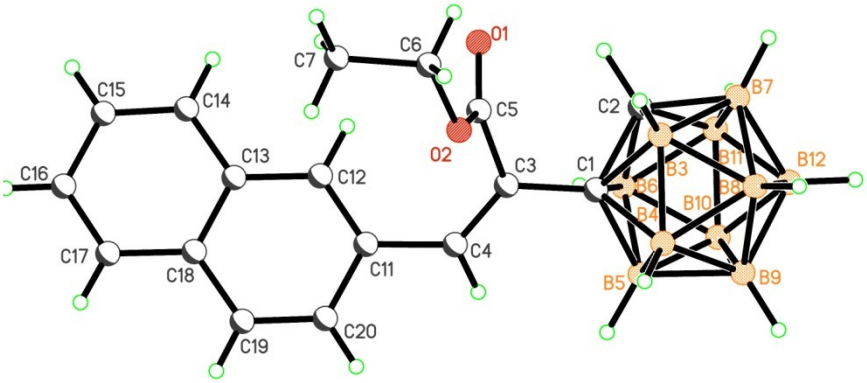
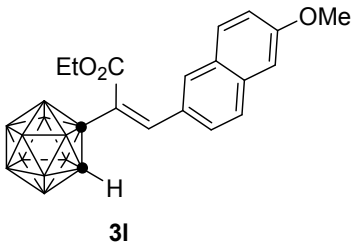


Figure S7. Molecular structure of **3k**



3l

3l: Colorless crystals. Yield: 86%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.71 – 7.11 (m, 7H) (aromatic & olefinic *H*), 4.27 (s, 1H) (cage *H*), 4.19 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 3.93 (s, 3H) (OCH_3), 1.11 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 167.0 (*C*OOEt), 159.0, 139.3, 135.1, 130.1, 129.0, 128.8, 128.5, 127.3, 126.7, 125.6, 119.9, 105.9 (aromatic & olefinic *C*), 73.4 (cage *C*-C), 62.5 (OCH_2CH_3), 59.7 (cage *C*-H), 55.6 (OCH_3), 13.8 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.4 (1B), -7.7 (2B), -9.3 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{18}H_{26}{}^{11}B_8{}^{10}B_2O_3$ $[M]^+$: 398.2885. Found: 398.2878.

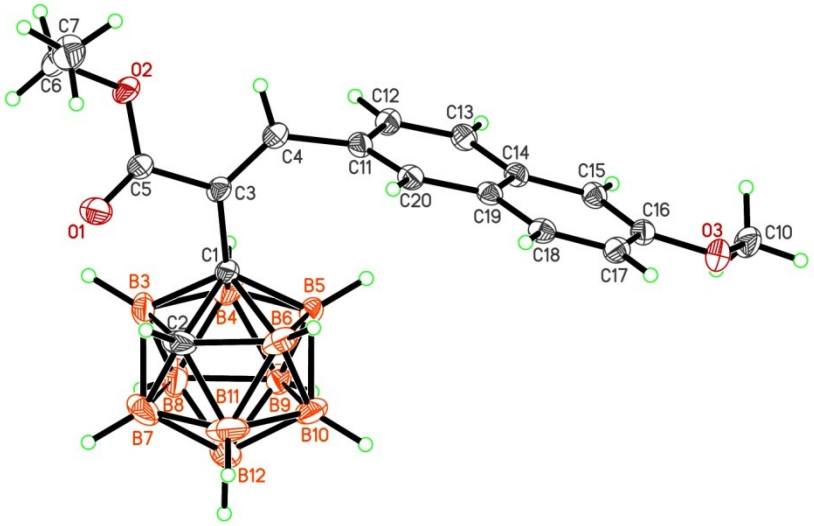


Figure S8. Molecular structure of **3l**

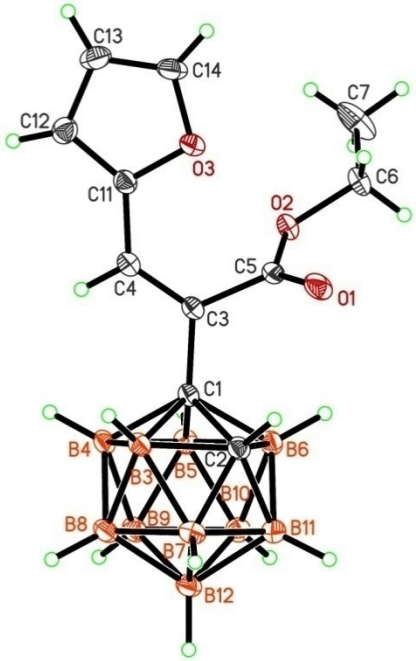
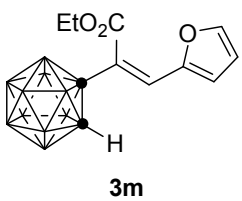


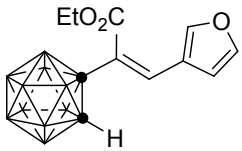
Figure S9. Molecular structure of **3m**



3m

3m: Colorless crystals. Yield: 74%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.41 – 6.44 (m, 4H) (aromatic & olefinic *H*), 4.34 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.07 (s, 1H) (cage *H*), 1.35 (t, J = 7.2 Hz,

3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 166.4 (*C*OOEt), 148.6, 145.1, 124.6, 123.5, 115.8, 112.4 (aromatic & olefinic *C*), 73.2 (cage *C*-C), 62.6 (OCH_2CH_3), 59.9 (cage *C*-H), 14.2 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.5 (1B), -2.5 (1B), -7.9 (2B), -9.4 (2B), -10.0 (2B), -11.3 (2B). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{11}B_8{}^{10}B_2O_3$ $[M - H]^+$: 307.2337. Found: 307.2349.



3n

3n: White solid. Yield: 80%. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.59 – 6.29 (m, 4H) (aromatic & olefinic *H*), 4.30 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.08 (s, 1H) (cage *H*), 1.33 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 166.5 (*C*OOEt), 145.0, 144.4, 128.7, 125.5, 120.0, 108.5 (aromatic & olefinic *C*), 73.3 (cage *C*-C), 62.7 (OCH_2CH_3), 59.9 (cage *C*-H), 14.0 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.5 (1B), -2.5 (1B), -7.9 (2B), -9.4 (2B), -10.1 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{11}H_{20}{}^{11}B_8{}^{10}B_2O_3$ $[M]^+$: 308.2416. Found: 308.2402.

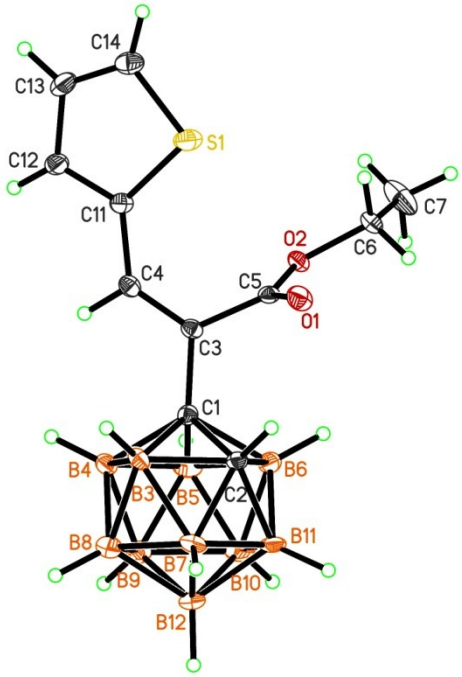
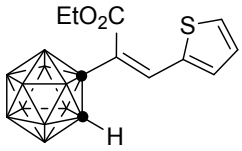


Figure S10. Molecular structure of **3o**



3o

3o: Colorless crystals. Yield: 36%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.43 – 7.03 (m, 4H) (aromatic & olefinic *H*), 4.35 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.13 (s, 1H) (cage *H*), 1.36 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.2 (*C*OOEt), 135.9, 132.7, 131.3, 130.0, 127.7, 123.9 (aromatic & olefinic *C*), 73.5 (cage *C*-C), 63.0 (OCH_2CH_3), 60.0 (cage *C*-H), 14.0 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.5 (1B), -2.5 (1B), -7.9 (2B), -9.4 (2B), -10.0 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{11}H_{20}{}^{11}B_8{}^{10}B_2O_2S$ $[M]^+$: 324.2187. Found: 324.2181.

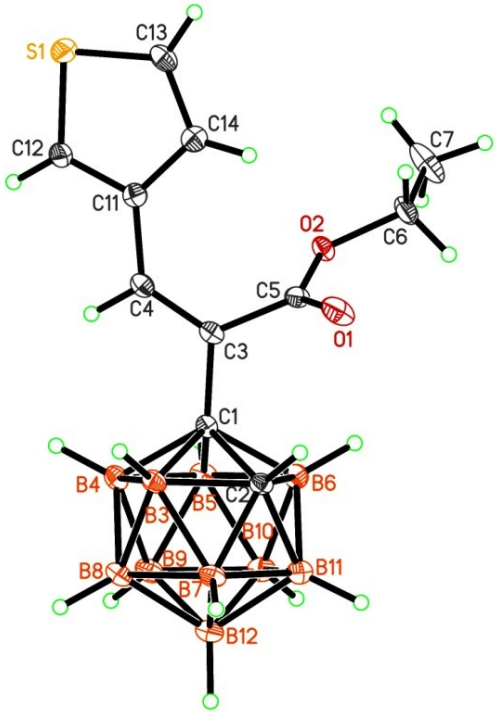
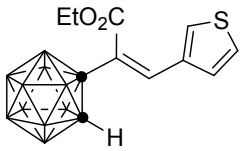
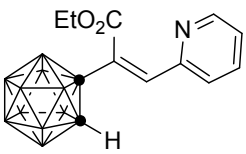


Figure S11. Molecular structure of **3p**



3p

3p: Colorless crystals. Yield: 97%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.37 – 6.97 (m, 4H) (aromatic & olefinic *H*), 4.26 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.11 (s, 1H) (cage *H*), 1.27 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.8 (*C*OOEt), 134.7, 132.3, 128.1, 126.9, 126.6, 126.0 (aromatic & olefinic *C*), 73.2 (cage *C*-C), 62.7 (OCH_2CH_3), 59.9 (cage *C*-H), 14.0 (OCH_2CH_3). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.6 (1B), -2.5 (1B), -7.8 (2B), -9.4 (2B), -10.0 (2B), -11.3 (2B). HRMS: *m/z* calcd for $C_{11}H_{20}{}^{11}B_8{}^{10}B_2O_2S$ $[M]^+$: 324.2187. Found: 324.2176.



3q

3q: Colorless crystals. Yield: 88%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.51 – 7.21 (m, 4H) (aromatic *H*), 7.00 (s, 1H) (olefinic *H*), 4.30 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.13 (s, 1H) (cage *H*), 1.28

(t, J = 7.2 Hz, 3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 166.6 (*C*OOEt), 151.2, 149.5, 137.0, 135.7, 130.5, 125.3, 124.2 (aromatic & olefinic *C*), 72.7 (cage *C*-C), 62.3 (OCH_2CH_3), 59.4 (cage *C*-H), 14.0 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -0.7 (1B), -2.3 (1B), -7.7 (2B), -9.4 (2B), -9.9 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{12}H_{20}{}^{11}B_8{}^{10}B_2NO_2$ $[M - H]^+$: 318.2497. Found: 318.2505.

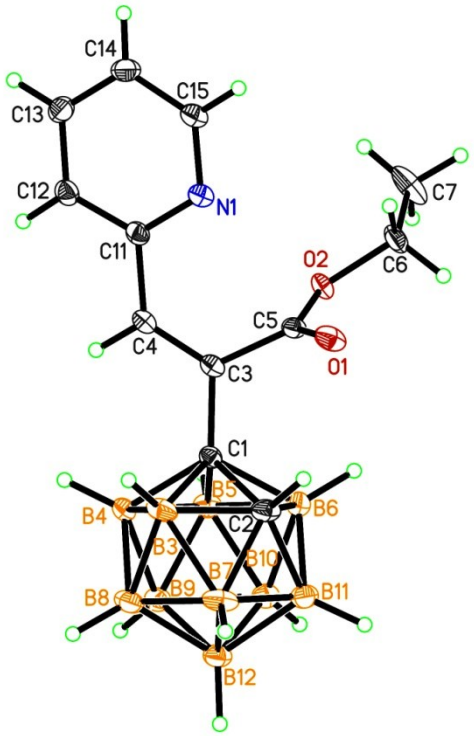
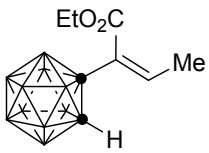


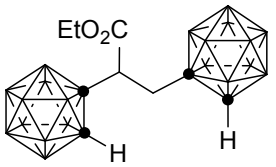
Figure S12. Molecular structure of **3q**



3r

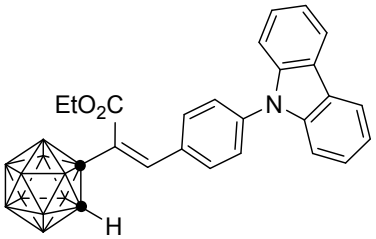
3r: Colorless oil. Yield: 87%. ^1H NMR ($CDCl_3$, 400 MHz): δ 6.44 (q, J = 7.2 Hz, 1H) (olefinic *H*), 4.27 (q, J = 7.2 Hz, 2H) (OCH_2CH_3), 4.25 (s, 1H) (cage *H*), 1.81 (d, J = 7.2 Hz, 3H) (=CHCH_3), 1.25 (t, J = 7.2 Hz, 3H) (OCH_2CH_3). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz): δ 165.8 (*C*OOEt), 138.8, 129.0 (olefinic *C*), 72.8 (cage *C*-C), 62.2 (OCH_2CH_3), 59.4 (cage *C*-H), 16.2 (=$CHCH_3$), 14.0 (OCH_2CH_3). $^{11}B\{^1H\}$ NMR ($CDCl_3$, 128 MHz): δ -1.1 (1B), -2.7 (1B), -7.9 (2B), -9.3 (2B), -10.2 (2B), -11.6 (2B). HRMS: *m/z* calcd for

$C_8H_{19}{}^{11}B_8{}^{10}B_2O_2$ [M – H]$^+$: 255.2388. Found: 255.2388.



3s

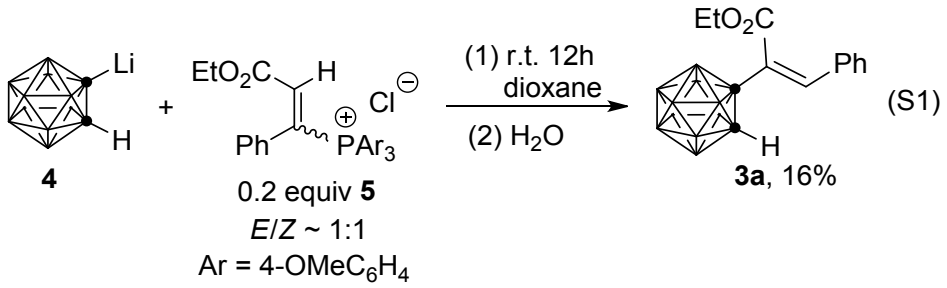
3s: White solid. Yield: 10%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 4.28 (m, 2H) (OC*H*$_2$CH$_3$), 3.93 (s, 1H) (cage *H*), 3.63 (s, 1H) (cage *H*), 3.33 (d, J = 11.6 Hz, 1H) (CHC*H*$_2$), 2.97 (t, J = 12.0 Hz, 1H) (C*H*CH$_2$), 2.68 (d, J = 15.2 Hz, 1H) (CHC*H*$_2$), 1.37 (t, J = 7.2 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 168.7 (*C*OOEt), 72.2, 72.0 (cage *C*-C), 63.6 (O*C*H$_2$CH$_3$), 61.9, 59.7 (cage *C*-H), 50.9 (*C*HCH$_2$), 40.1 (CH*C*H$_2$), 14.1 (OCH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.2 (2B), -2.1 (1B), -3.3 (1B), -7.8 (4B), -9.5 (2B), -10.1 (2B), -11.3 (8B). HRMS: *m/z* calcd for $C_9H_{29}{}^{11}B_{16}{}^{10}B_4O_2$ [M – H]$^+$: 385.4174. Found: 385.4185.



3t

3t: Light yellow solid. Yield: 33%. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.15 – 7.28 (m, 13H) (aromatic & olefinic *H*), 4.27 (s, 1H) (cage *H*), 4.25 (q, J = 7.2 Hz, 2H) (OC*H*$_2$CH$_3$), 1.22 (t, J = 7.2 Hz, 3H) (OCH$_2$C*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 166.5 (*C*OOEt), 140.5, 139.1, 138.0, 132.4, 130.1, 128.4, 127.0, 126.3, 123.8, 120.7, 120.6, 109.7 (aromatic & olefinic *C*), 72.9 (cage *C*-C), 62.8 (O*C*H$_2$CH$_3$), 59.5 (cage *C*-H), 13.9 (OCH$_2$*C*H$_3$). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.7 (1B), -2.1 (1B), -7.6 (2B), -9.3 (2B), -9.9 (2B), -11.3 (2B). HRMS: *m/z* calcd for $C_{25}H_{29}{}^{11}B_9{}^{10}BNO_2$ [M]$^+$: 484.3165. Found: 484.3156.

Mechanistic study.



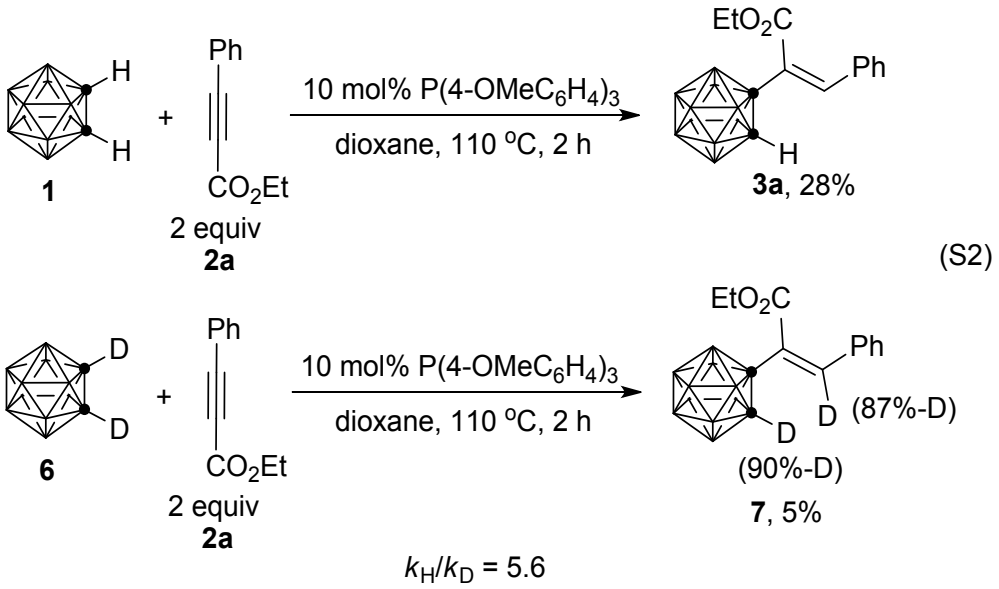
Reaction of 1-Li-1,2-$C_2B_{10}H_{11}$ (4) with Vinylphosphonium Salt (5). To a dioxane solution (10 mL) of *o*-carborane (72 mg, 0.50 mmol) was added ^{n}BuLi (0.2 mL, 2.5 M in hexane, 0.50 mmol) at 0 °C. After stirring for 1 h at room temperature, a solution of vinylphosphonium salt (**5**)[1] (57 mg, 0.10 mmol) in dioxane (10 mL) was added dropwise to the reaction suspension at room temperature. The yellow suspension was stirred overnight. After water (10 mL) was added to reaction mixture, the aqueous layer was extracted with ethyl acetate (10 × 3 mL). The combined organic layer was then dried over anhydrous Na_2SO_4. After filtration and removal of solvent in vacuo, the residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/dichloromethane (20/1 in v/v) as eluent to give **3a** (26 mg, 16%, 0.08 mmol). See eq S1.

Kinetic Isotope Effect Experiments.

Reaction of *o*-Carborane (1) with Ethyl Phenylpropiolate (2a). *o*-Carborane (29 mg, 0.20 mmol), ethyl phenylpropiolate (70 mg, 0.40 mmol) and tris(4-methoxy phenyl)phosphine (7 mg, 0.02 mmol) were mixed in dioxane (0.6 mL). The resulting mixture was heated at 100 °C for 2 h. GC-MS yield: 28%. See eq S2.

Reaction of 1,2-D_2-1,2-$C_2B_{10}H_{10}$ (6) with Ethyl Phenylpropiolate (2a). 1,2-D_2-

1,2-$C_2B_{10}H_{10}$[2] (29 mg, 0.20 mmol), ethyl phenylpropiolate (70 mg, 0.40 mmol) and tris(4-methoxy phenyl)phosphine (7 mg, 0.02 mmol) were mixed in dioxane (0.6 mL). The resulting mixture was heated at 110 °C for 2 h. GC-MS yield: 5%. See eq S2.



Calculations based on the GC-MS showed a k_H/k_D value of 5.6 (eq S2). Moreover, product **7** was obtained with 87% deuterium incorporation by flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/dichloromethane (20/1 in v/v) as eluent. See eq S2 and Figures S13 and S14.

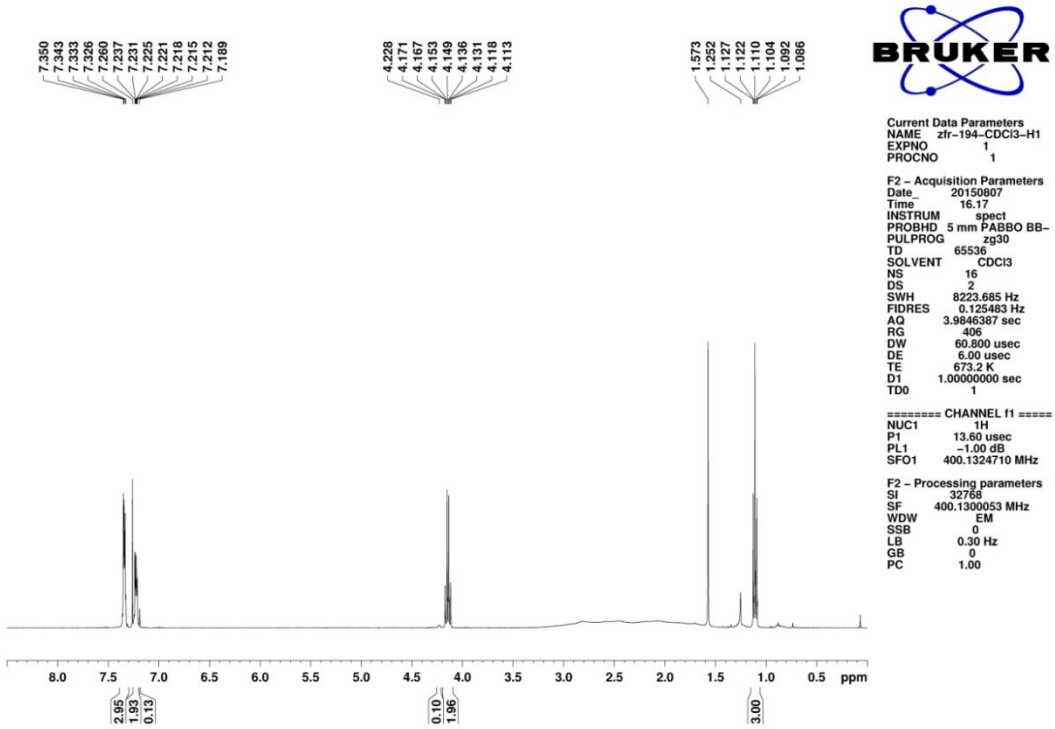


Figure S13. [1]H NMR spectrum of **7**

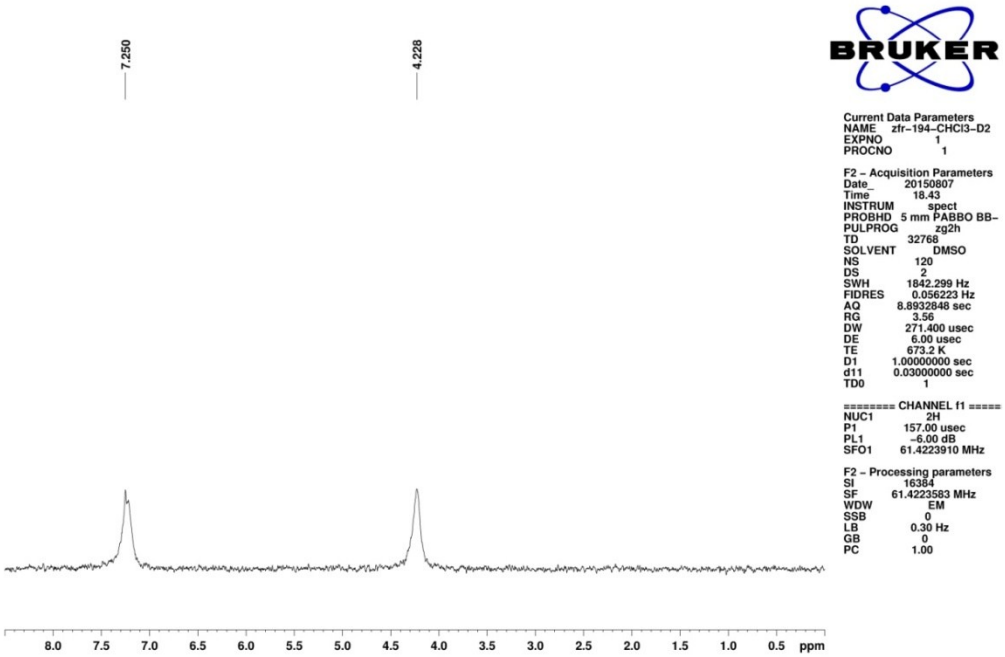
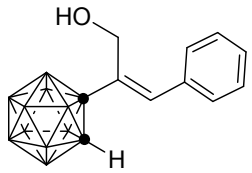


Figure S14. [2]H NMR spectrum of **7**

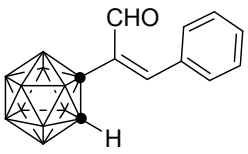
Preparation of 8: To a solution of **3a** (64 mg, 0.20 mmol) in dry dichloromethane (5 mL) at – 78 °C was added DIBAL-H (0.4 mL of 1.0 M in *n*-hexane, 0.40 mmol) dropwise. The resulting mixture was further stirred at this temperature for another 2 h and then quenched by addition of potassium sodium tartrate solution (5 mL, 1.0 M in H_2O). The organic layer was separated from the aqueous layer which was further extracted with dichloromethane (10 x 3 mL). The combined organic layer was dried with anhydrous Na_2SO_4. After filtration and removal of solvent in vacuo, the residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/ethyl acetate (10/1 in v/v) as eluent to give **8** (32 mg, 58%, 0.12 mmol).



8

8: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.30 (m, 3H) (phenyl *H*), 7.19 (m, 2H) (phenyl *H*), 7.07 (s, 1H) (olefinic *H*), 4.23 (s, 2H) (C*H*$_2$OH), 4.19 (s, 1H) (cage *H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 137.7, 133.7, 131.6, 127.7, 127.6, 127.5 (phenyl & olefinic *C*), 59.1 (*C*H$_2$OH), 58.3 (cage *C*-H), cage *C*-C atom was not observed. ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -1.3 (1B), -2.7 (1B), -7.7 (2B), -9.0 (2B), -10.2 (2B), -11.6 (2B). HRMS: *m/z* calcd for $C_{11}H_{20}{}^{11}B_8{}^{10}B_2O$ $[M]^+$: 276.2517. Found: 276.2522.

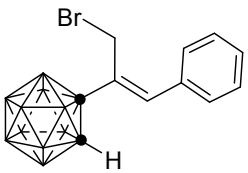
Preparation of 9: To a solution of **8** (55 mg, 0.20 mmol) in dry dichloromethane (5 mL) at room temperature was added activated MnO_2 (348 mg, 4.0 mmol) in one portion. The resulting mixture was further stirred at this temperature for 48 h. After filtration through celite and removal of solvent in vacuo, the residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane/ethyl acetate (15/1 in v/v) as eluent to give **9** (46 mg, 83%, 0.17 mmol).



9

9: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 9.59 (s, 1H) (C*H*O), 8.25 (s, 1H) (olefinic *H*), 7.47 (m, 3H) (phenyl *H*), 7.29 (m, 2H) (phenyl *H*), 5.49 (s, 1H) (cage *H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 189.7 (*C*HO), 155.0, 131.9, 131.8, 131.3, 130.7, 129.1 (phenyl & olefinic *C*), 72.4 (cage *C*-C), 57.5 (cage *C*-H). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -2.3 (2B), -7.2 (2B), -8.4 (2B), -10.6 (2B), -11.8 (2B). HRMS: *m/z* calcd for $C_{11}H_{18}{}^{11}B_8{}^{10}B_2O$ $[M]^+$: 274.2361. Found: 274.2363.

Preparation of 10: To a solution of **8** (55 mg, 0.20 mmol) and tetrabromomethane (133mg, 0.40 mmol) in dry dichloromethane (2 mL) at 0 ^{o}C was added triphenylphosphine (157 mg, 0.60 mmol) in one portion. The resulting mixture was allowed to warm to room temperature gradually. A mixture of *n*-hexane/diethyl ether (10 mL, 20/1 in v/v) was added. After filtration through celite and removal of solvents in vacuo, the residue was subjected to flash column chromatography on silica gel (230−400 mesh) using *n*-hexane as eluent to give **10** (54 mg, 80%, 0.16 mmol).



10

10: White solid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.42 (m, 5H) (phenyl *H*), 7.18 (s, 1H) (olefinic *H*), 4.16 (br, 3H) (CH_2Br & cage *H*). ^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ 141.0, 134.5, 129.6, 129.4, 129.1, 128.9 (phenyl & olefinic *C*), 77.4 (cage *C*-C), 59.8 (cage *C*-H), 30.7 (*C*H_2Br). ^{11}B{^{1}H} NMR ($CDCl_3$, 128 MHz): δ -0.8 (1B), -2.4 (1B), -7.9 (2B), -8.9 (2B), -10.4 (2B), -11.4 (2B). HRMS: *m/z* calcd for $C_{11}H_{19}{}^{11}B_8{}^{10}B_2Br$ $[M]^+$: 338.1673. Found: 338.1689.

X-ray Structure Determination. All data were collected with an Oxford

Diffraction Gemini™ S Ultra X-ray Diffractometer with monochromatized Cu-Kα radiation (λ = 1.54178 Å) at 173 K or 100 K. Diffraction data were collected and processed using the CrysAlisPro software (version 1.171.35.19). Empirical absorption corrections were performed using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm in the CrysAlisPro software suite. Structure solution and refinement for all compounds were performed using the Olex2 software package[13] (which embedded SHELXTL).[14] All the structures were solved by direct methods, expanded by difference Fourier syntheses and refined by full matrix least-squares on F^2. All non-hydrogen atoms were refined anisotropically with a riding model for the hydrogen atoms except noted separately.

CCDC 1432244−1432255 (**3a, 3b, 3f, 3h−3m and 3o−3q**) contains 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.

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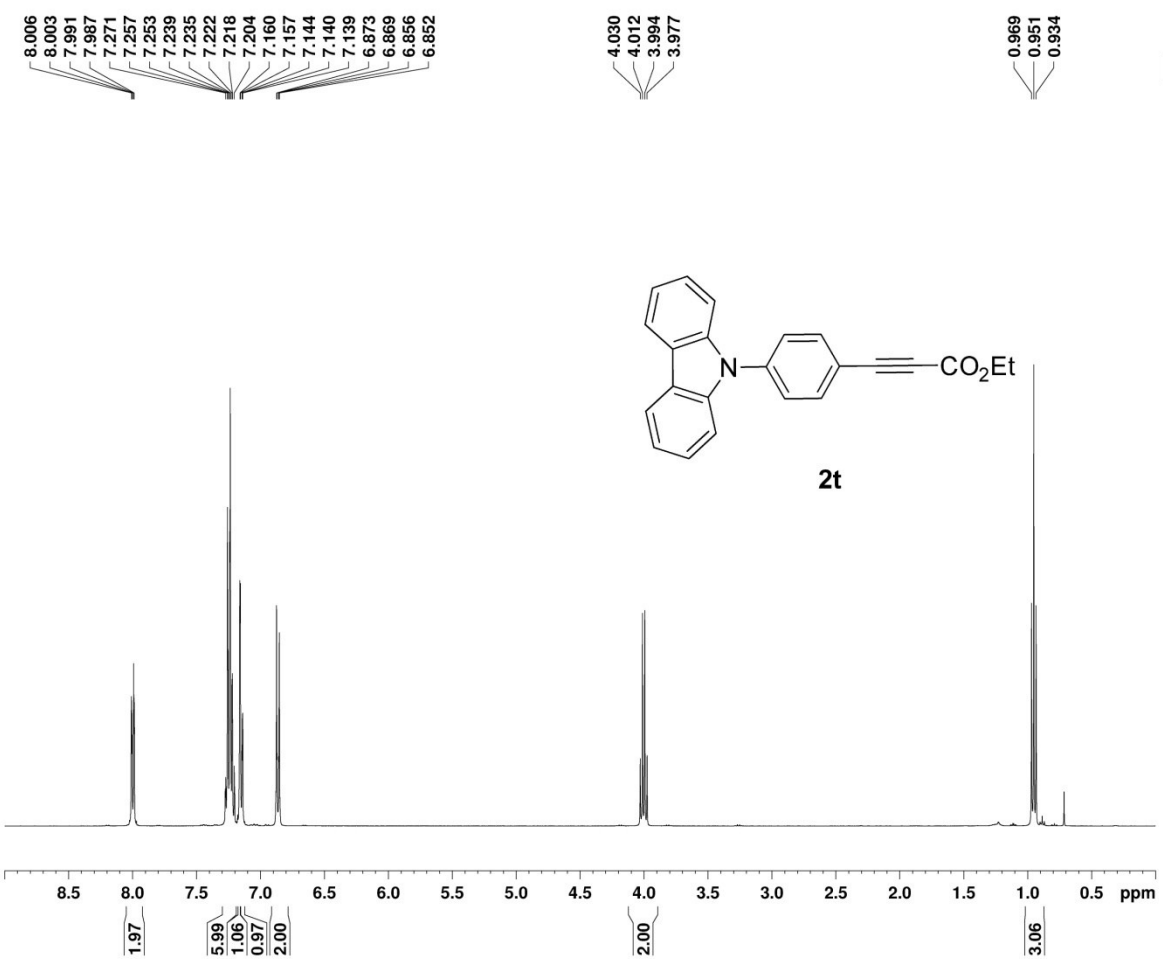

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PROCNO 1

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FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
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DE 6.00 usec
TE 294.3 K
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TD0 1

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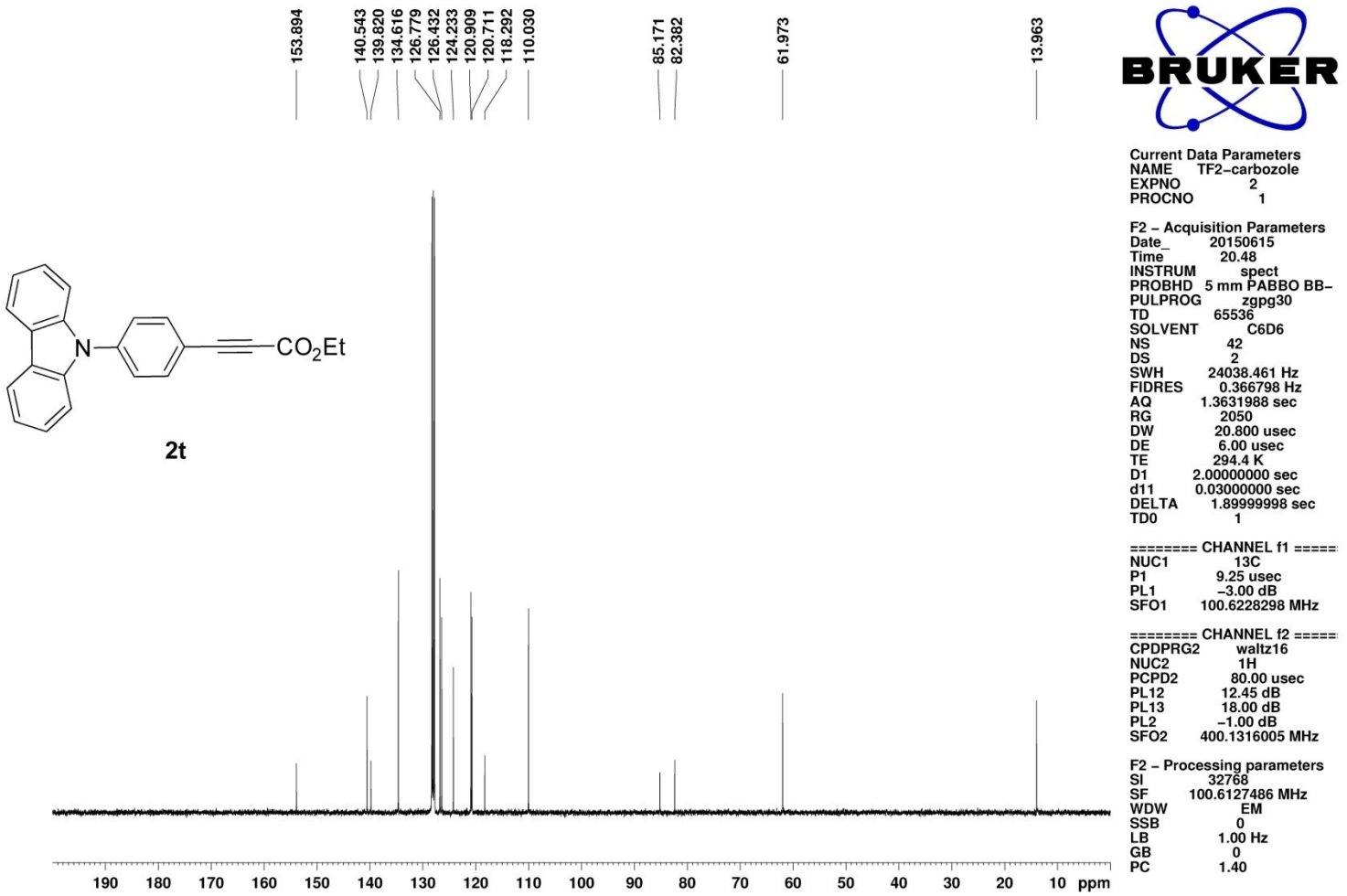
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61.973
13.963
N
CO2Et
2t
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EXPNO 2
PROCNO 1
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SOLVENT C6D6
NS 42
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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PL1 –3.00 dB
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PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 –1.00 dB
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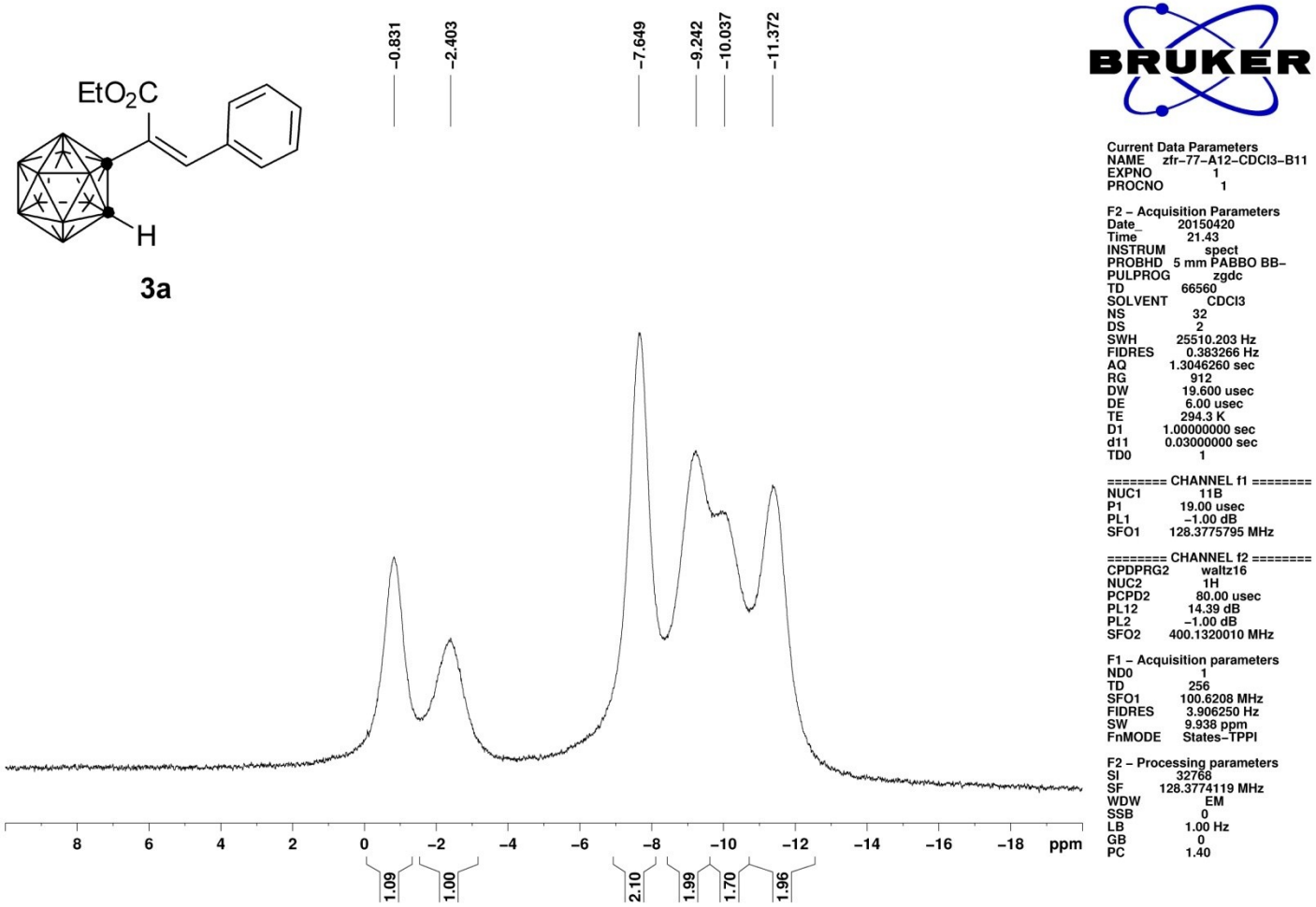

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FIDRES 0.383266 Hz
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RG 912
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

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PL1 −1.00 dB
SFO1 128.3775795 MHz

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NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

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FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

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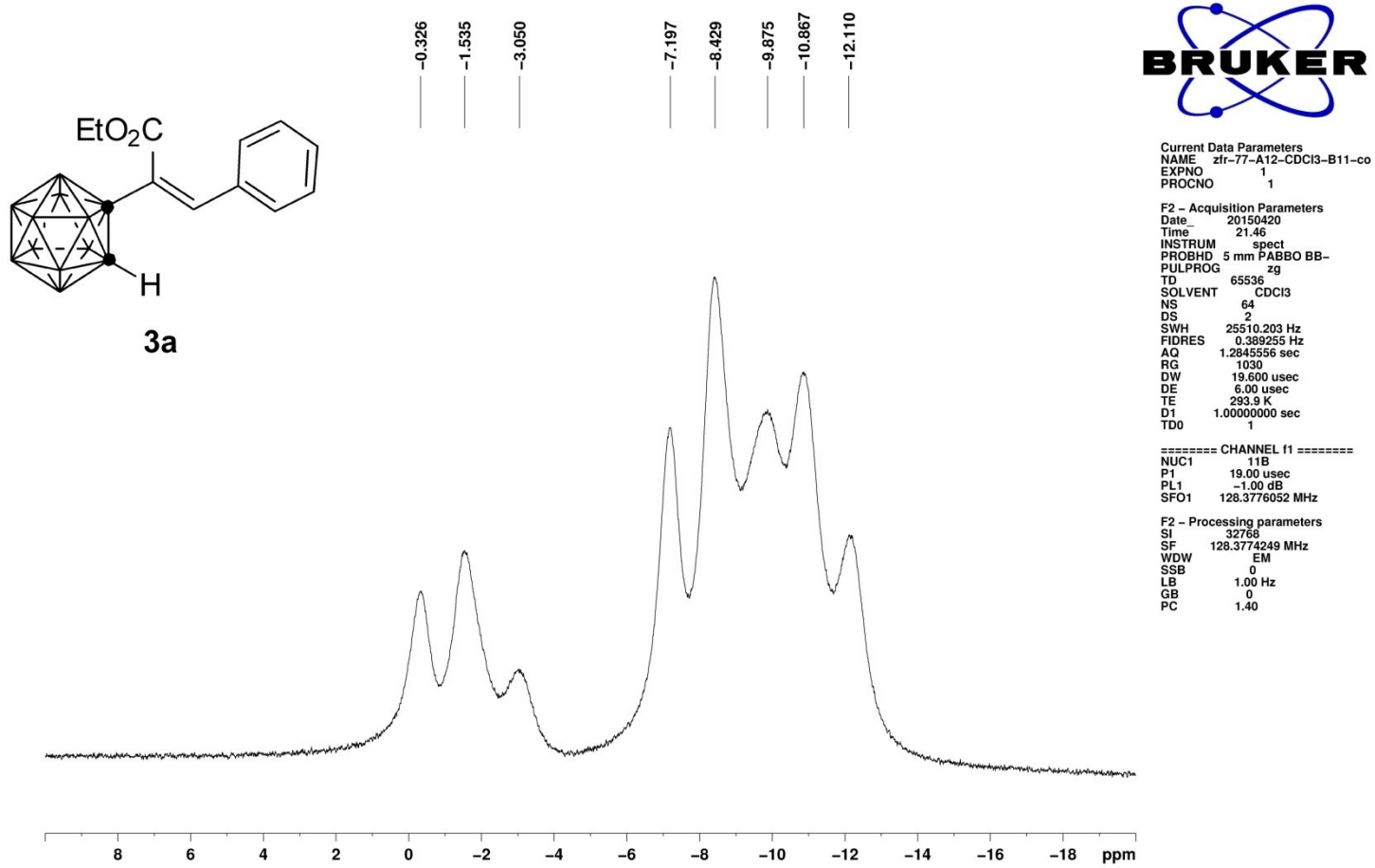
GB 0
PC 1.40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H
3a
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
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EXPNO 1
PROCNO 1
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FIDRES 0.389255 Hz
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DE 6.00 usec
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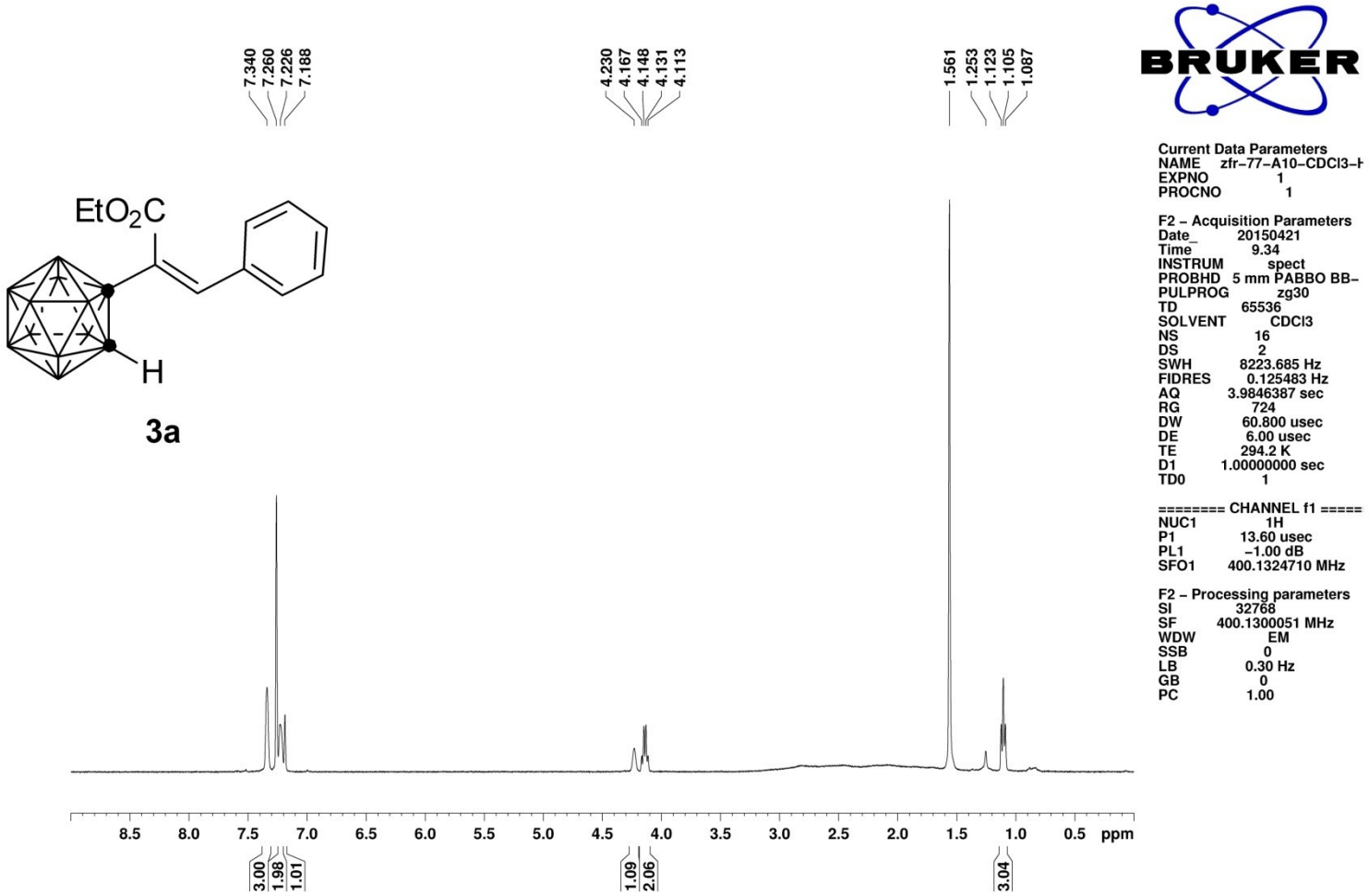
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EtO2C
H
3a
8.5
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7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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1.0
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ppm
3.00
1.98
1.01
1.09
2.06
3.04
BRUKER
Current Data Parameters
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PULPROG zg30
TD 65536
SOLVENT CDCl3
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DS 2
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FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 724
DW 60.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
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P1 13.60 usec
PL1 -1.00 dB
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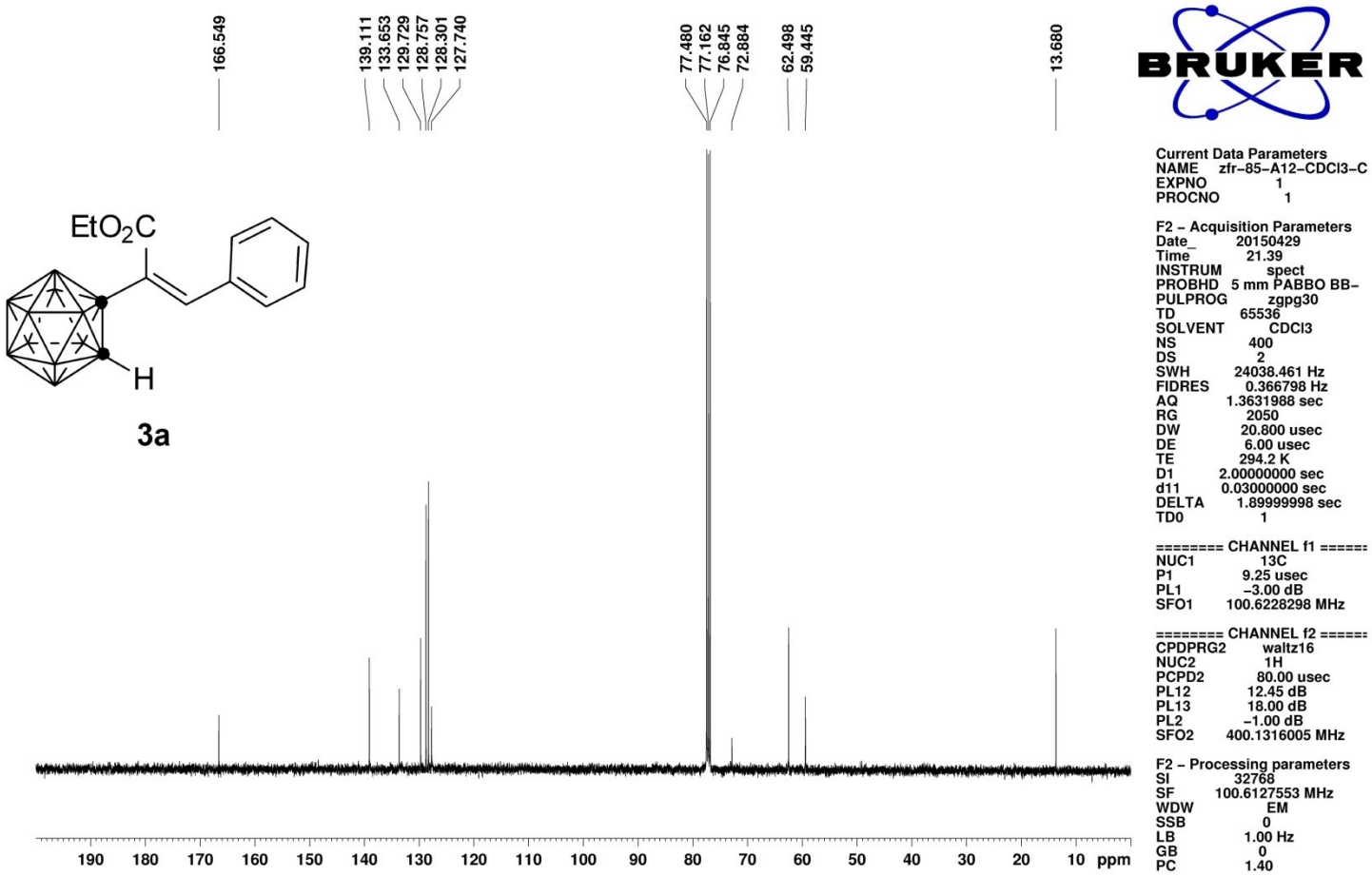
PC 1.00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13.680
EtO2C
H
3a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
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Time 21.39
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PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
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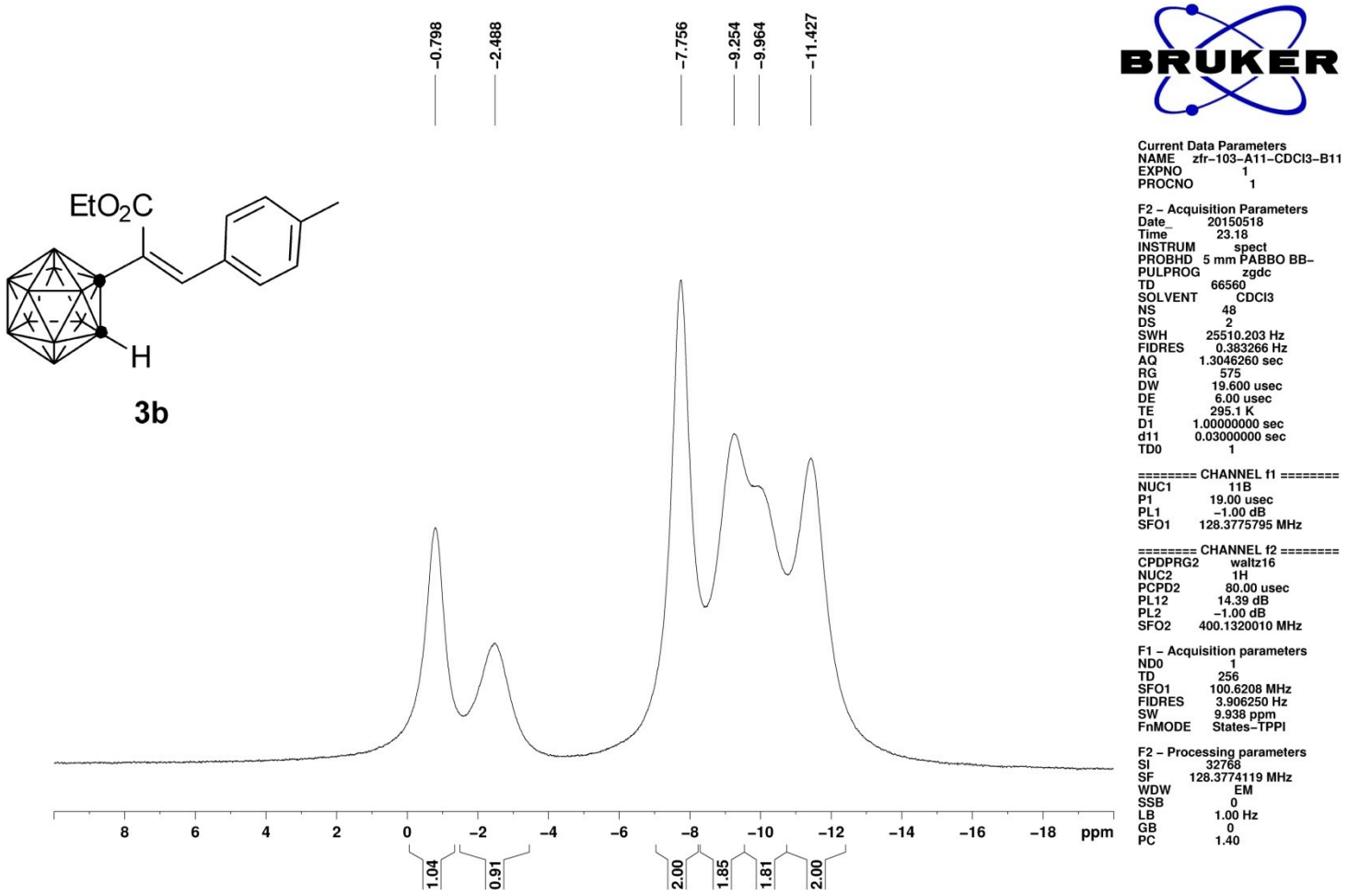

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TD 66560
SOLVENT CDCl3
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FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
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DE 6.00 usec
TE 295.1 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

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P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
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FIDRES 3.906250 Hz
SW 9.938 ppm
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F2 − Processing parameters
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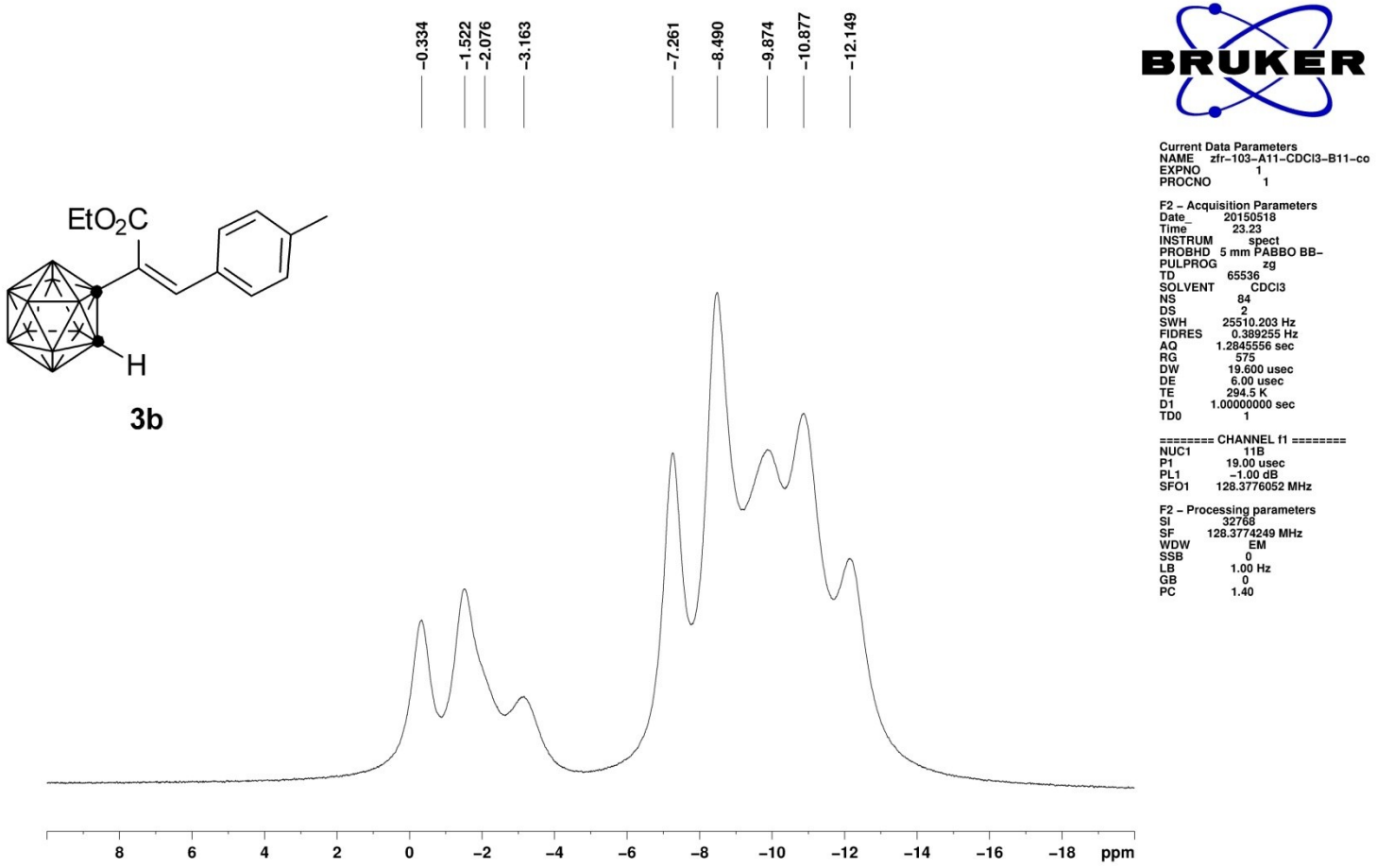
PC 1.40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EtO2C
H
3b
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
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EXPNO 1
PROCNO 1
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Time 23.23
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PULPROG zg
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SOLVENT CDCl3
NS 84
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
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RG 575
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DE 6.00 usec
TE 294.5 K
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TD0 1
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PL1 −1.00 dB
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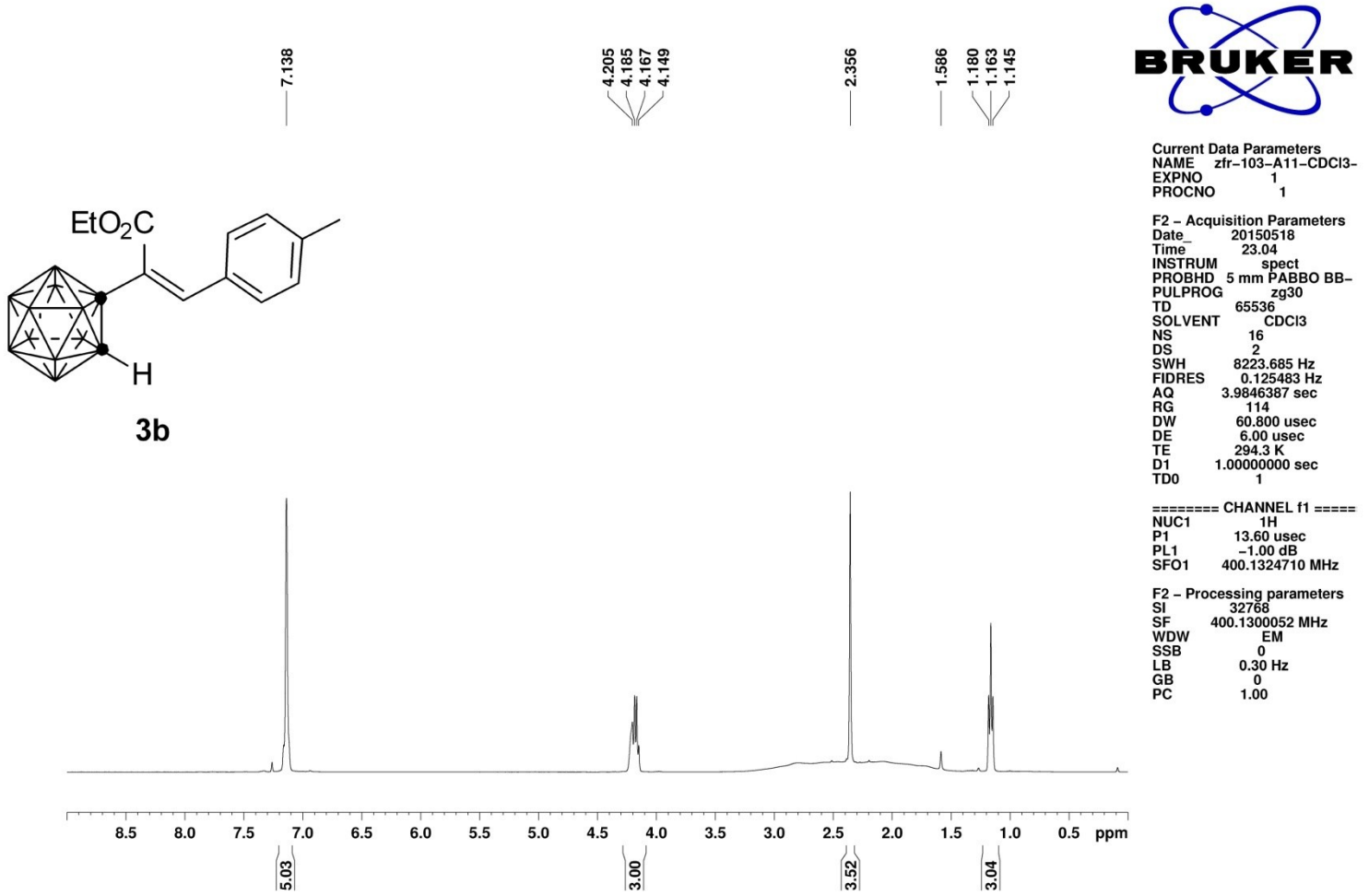

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PROCNO 1

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FIDRES 0.125483 Hz
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DW 60.800 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1

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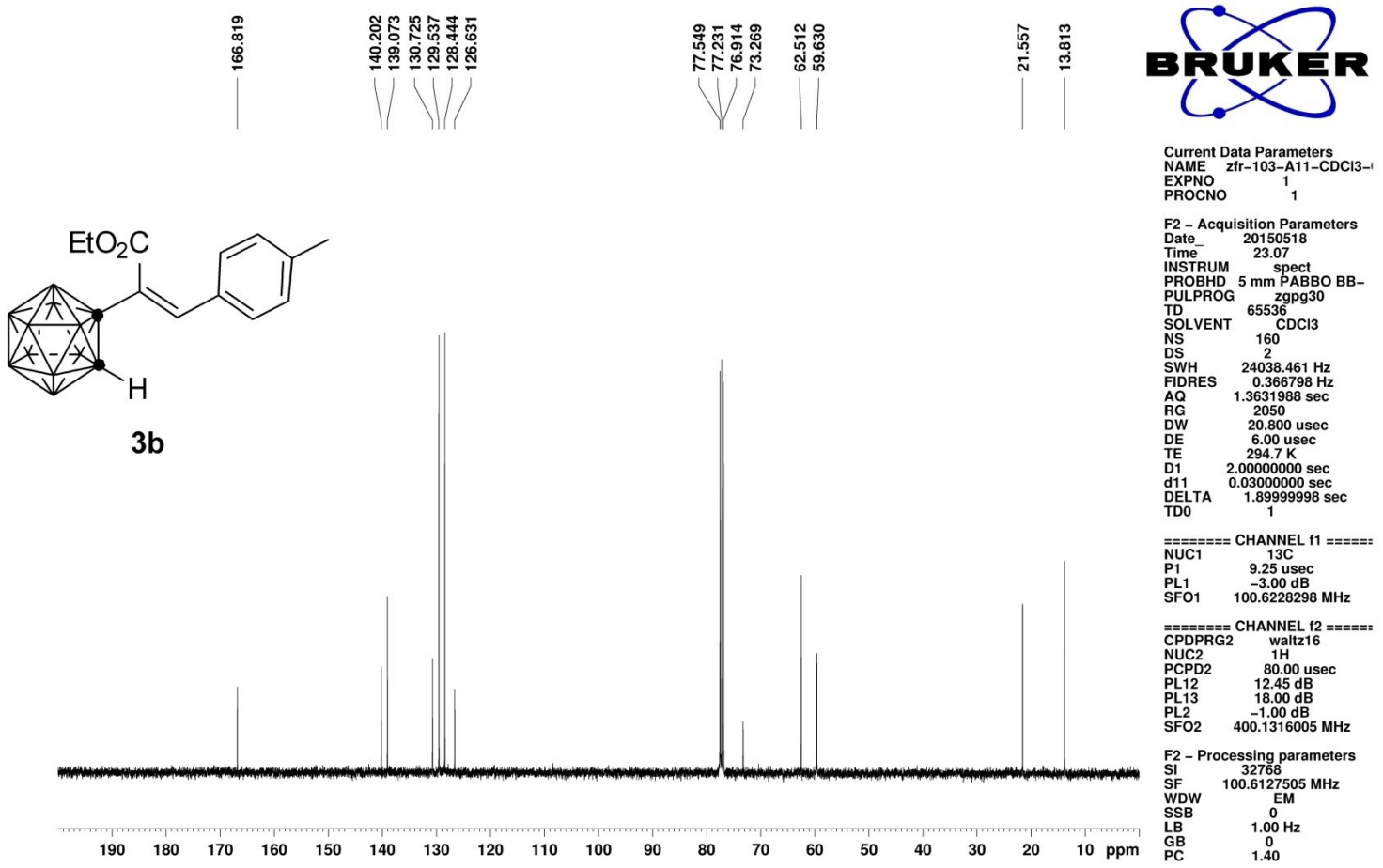
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62.512
59.630
21.557
13.813
EtO2C
H
3b
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
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PROCNO 1
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SOLVENT CDCl3
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DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
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RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
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PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
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NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
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F2 - Processing parameters
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WDW EM
SSB 0
LB 1.00 Hz
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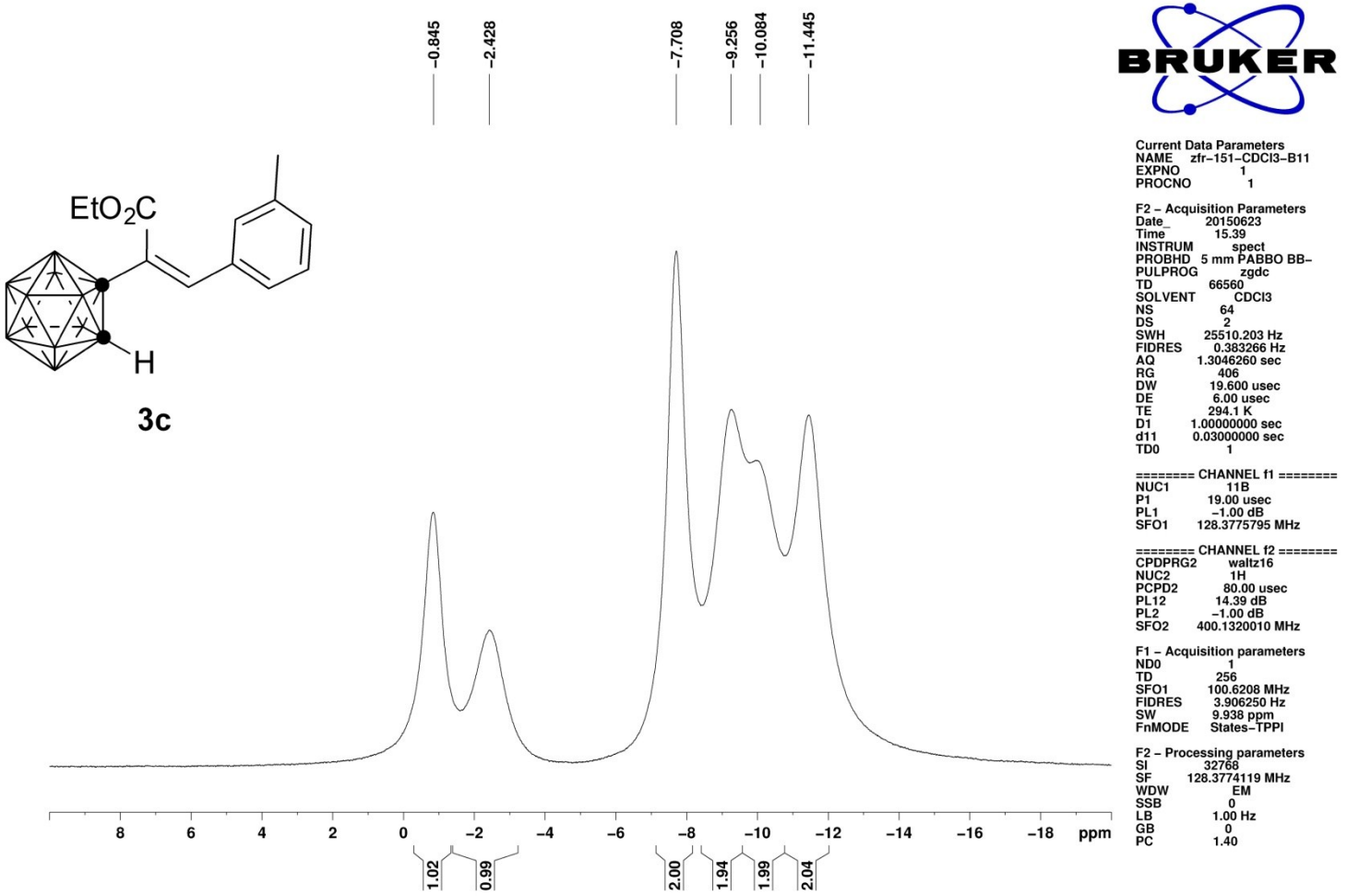
PC 1.40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EtO2C
H
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6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.02
0.99
2.00
1.94
1.99
2.04
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RG 406
DW 19.600 usec
DE 6.00 usec
TE 294.1 K
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======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
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TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
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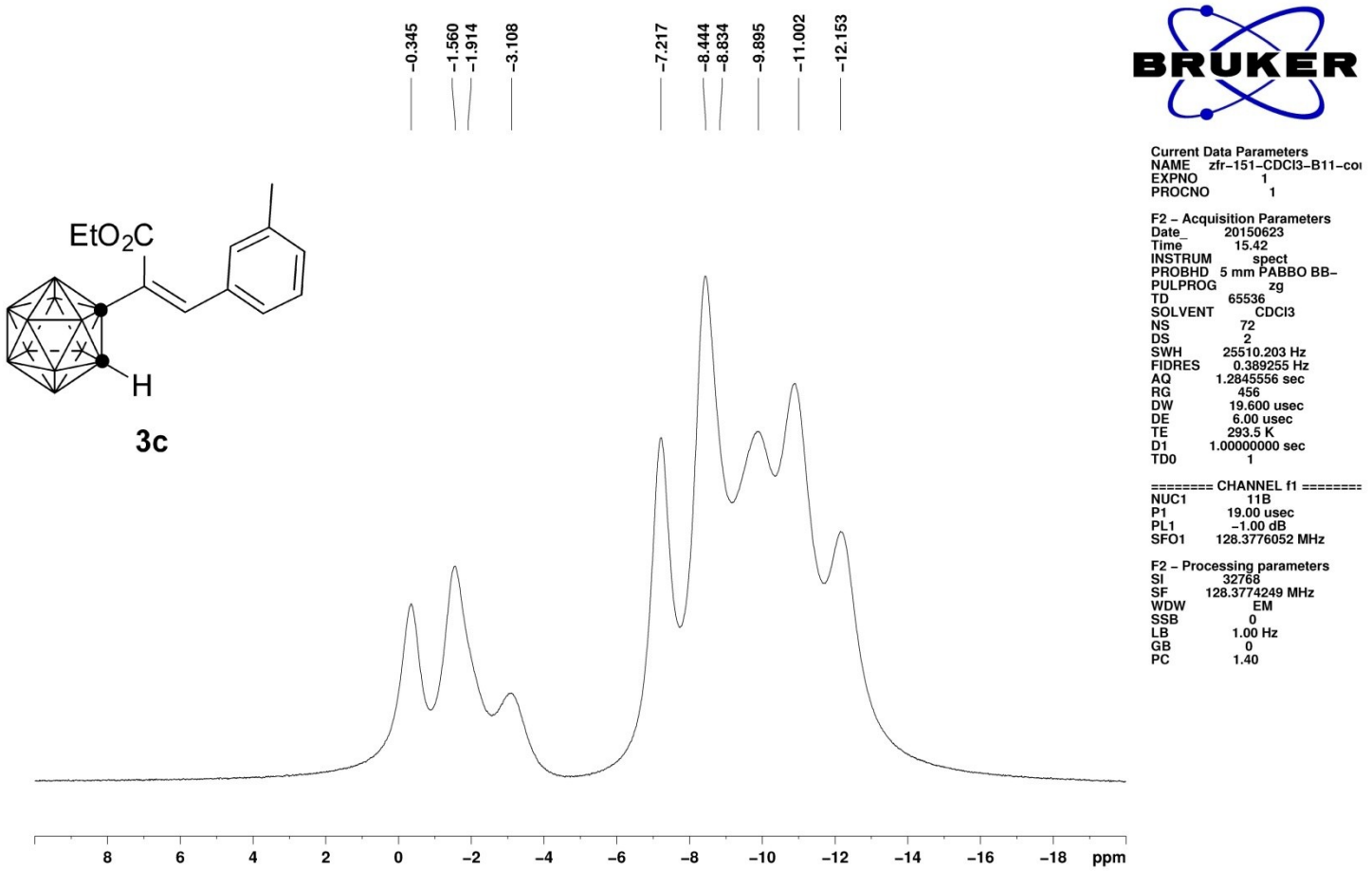
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EtO2C
H
3c
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
ppm
BRUKER
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PROCNO 1
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FIDRES 0.389255 Hz
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RG 456
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DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
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NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
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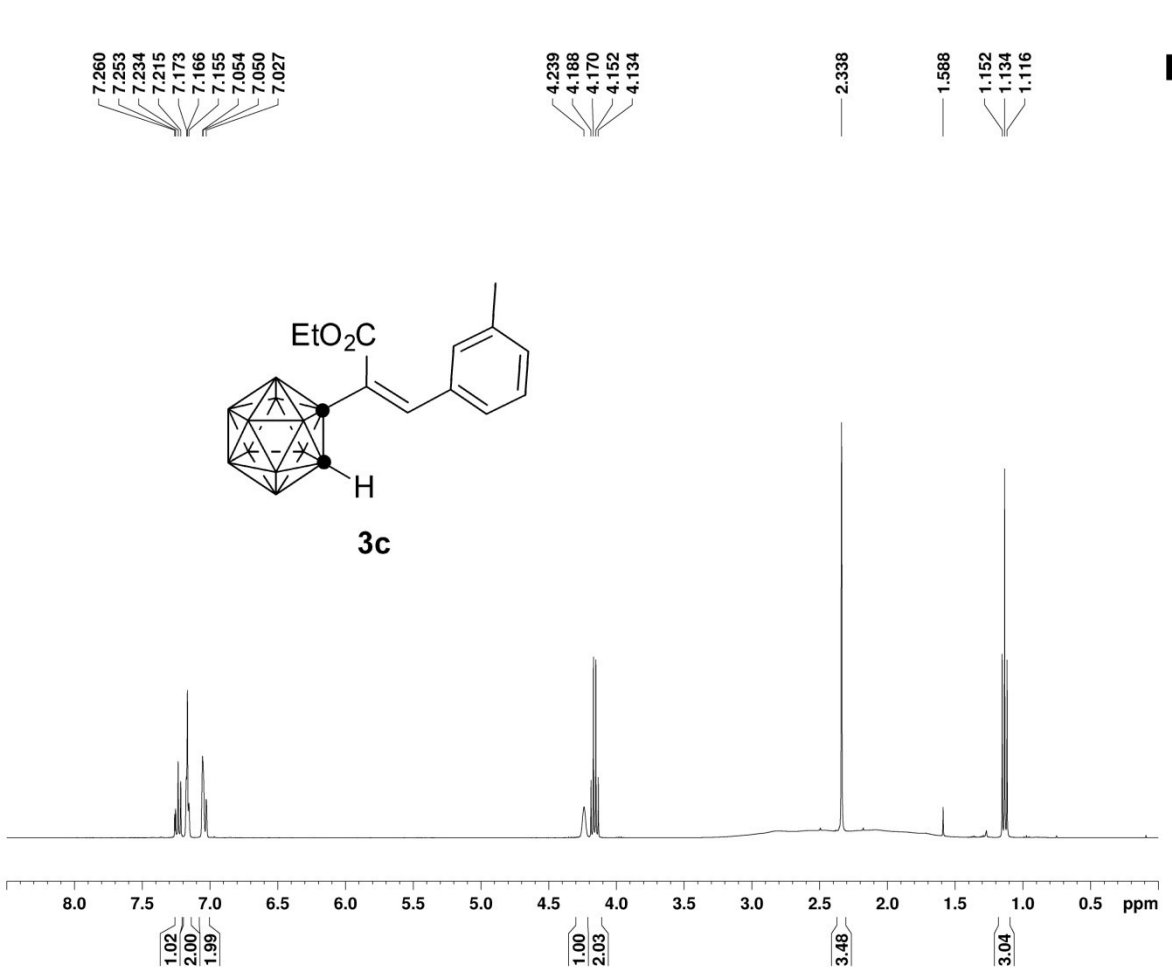
PC 1.40



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SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
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P1 13.60 usec
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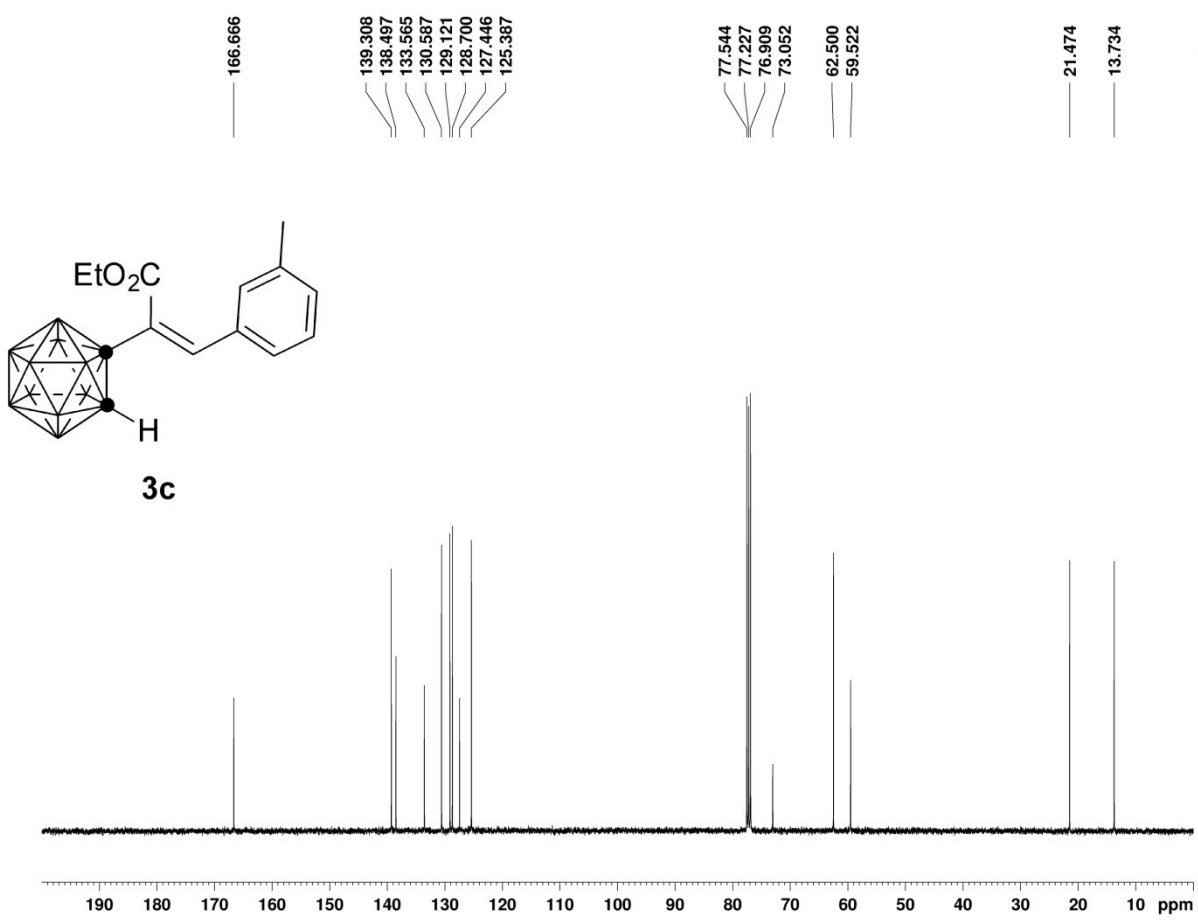


BRUKER

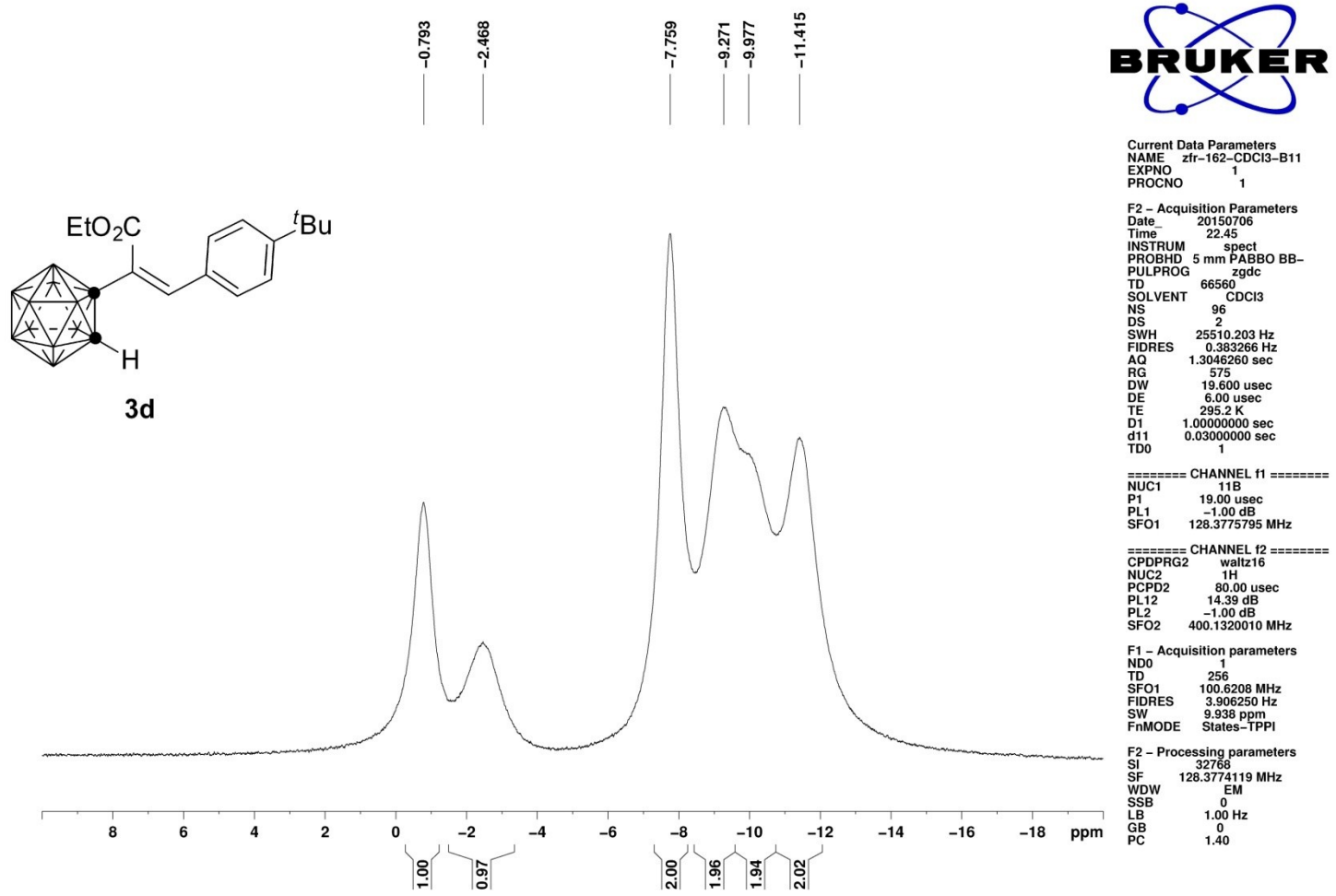
Current Data Parameters
NAME zfr-151-CDCl3-C13
EXPNO 1
PROCNO 1

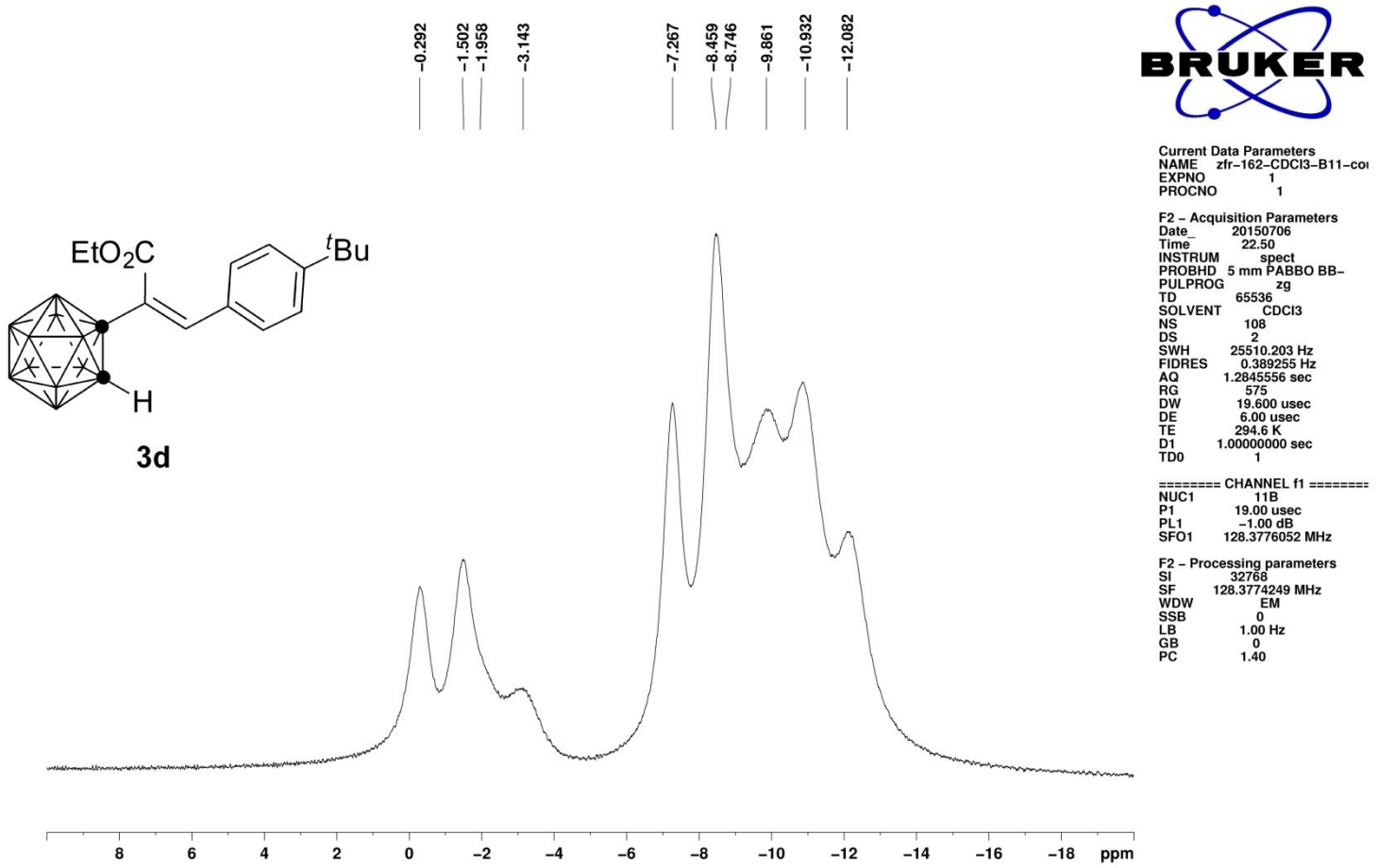
F2 - Acquisition Parameters
Date_ 20150623
Time 15.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

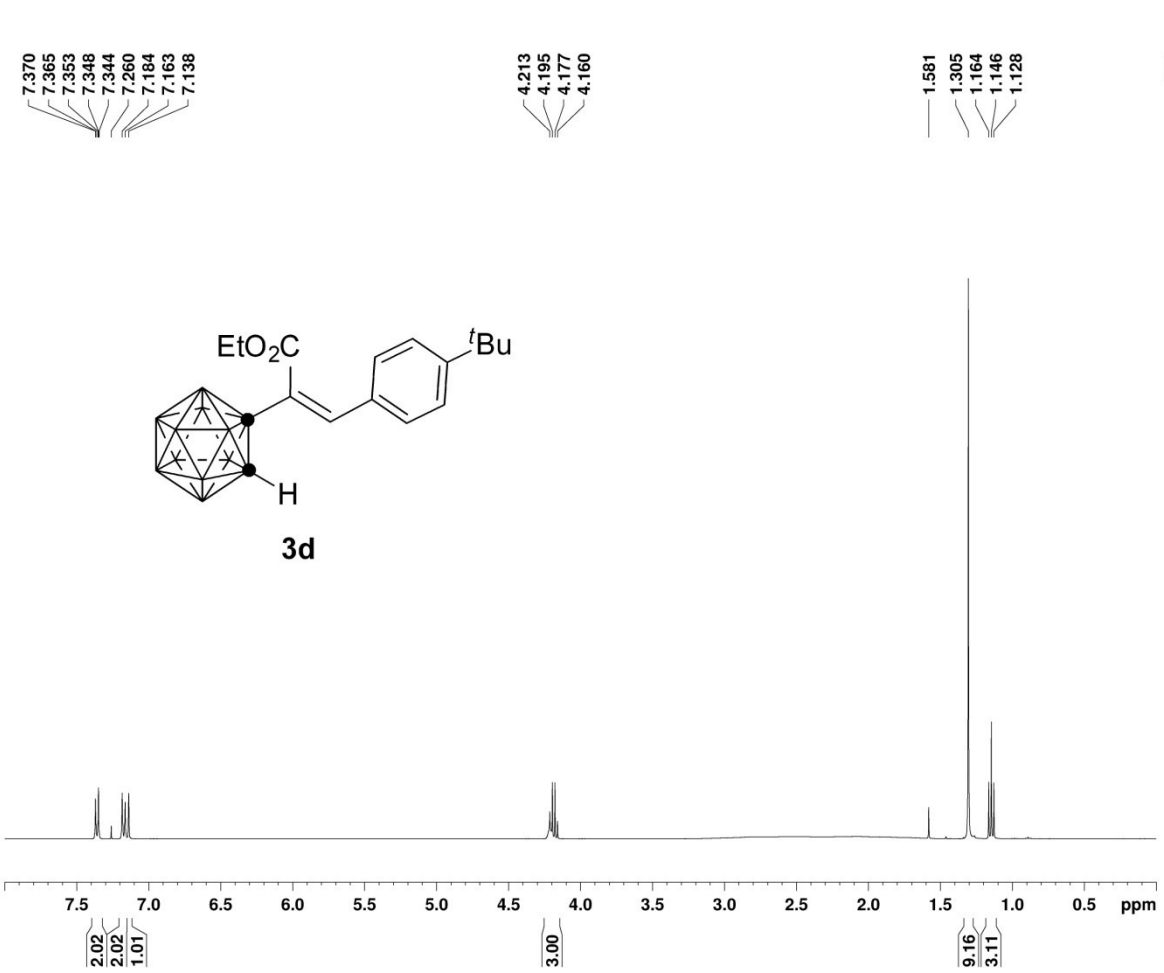
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127519 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.793
−2.468
−7.759
−9.271
−9.977
−11.415
EtO2C
tBu
H
3d
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.00
0.97
2.00
1.96
1.94
2.02
BRUKER
Current Data Parameters
NAME zfr−162−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150706
Time 22.45
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-0.292
-1.502
-1.958
-3.143
-7.267
-8.459
-8.746
-9.861
-10.932
-12.082
EtO2C
tBu
H
3d
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
NAME zfr-162-CDCl3-B11-co
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150706
Time 22.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 108
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

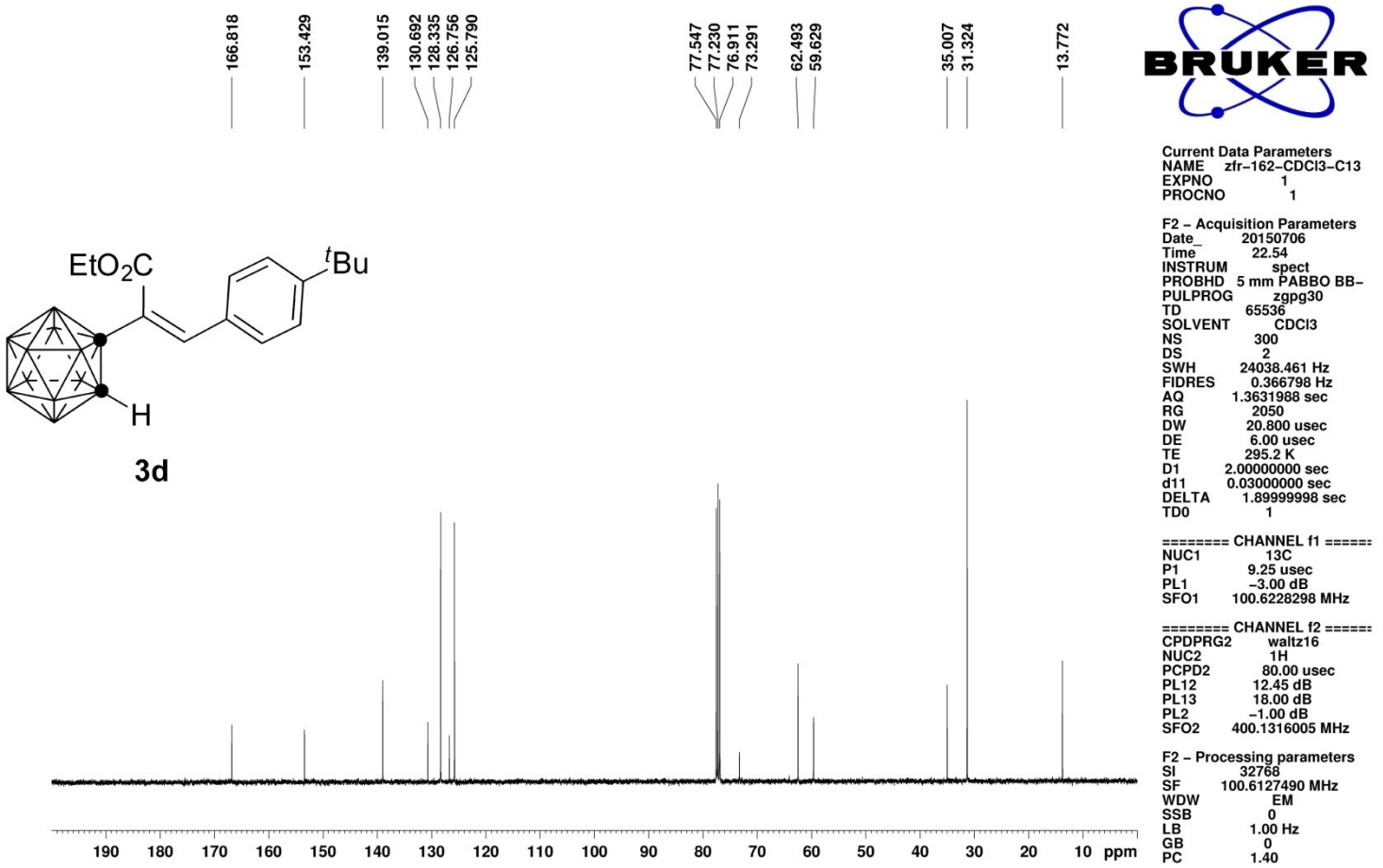


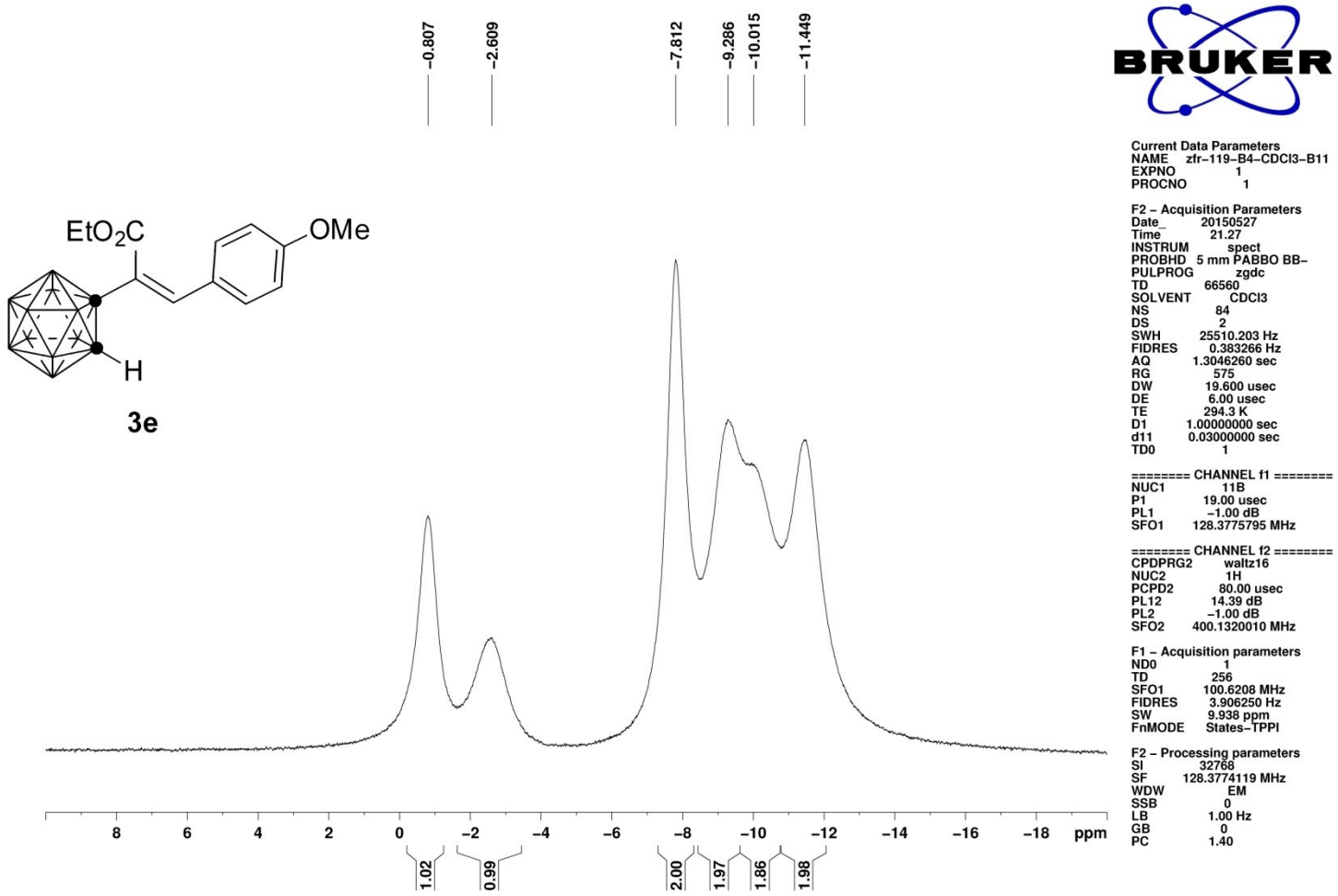
Current Data Parameters
NAME zfr-162-CDCl3-H1
EXPNO 1
PROCNO 1

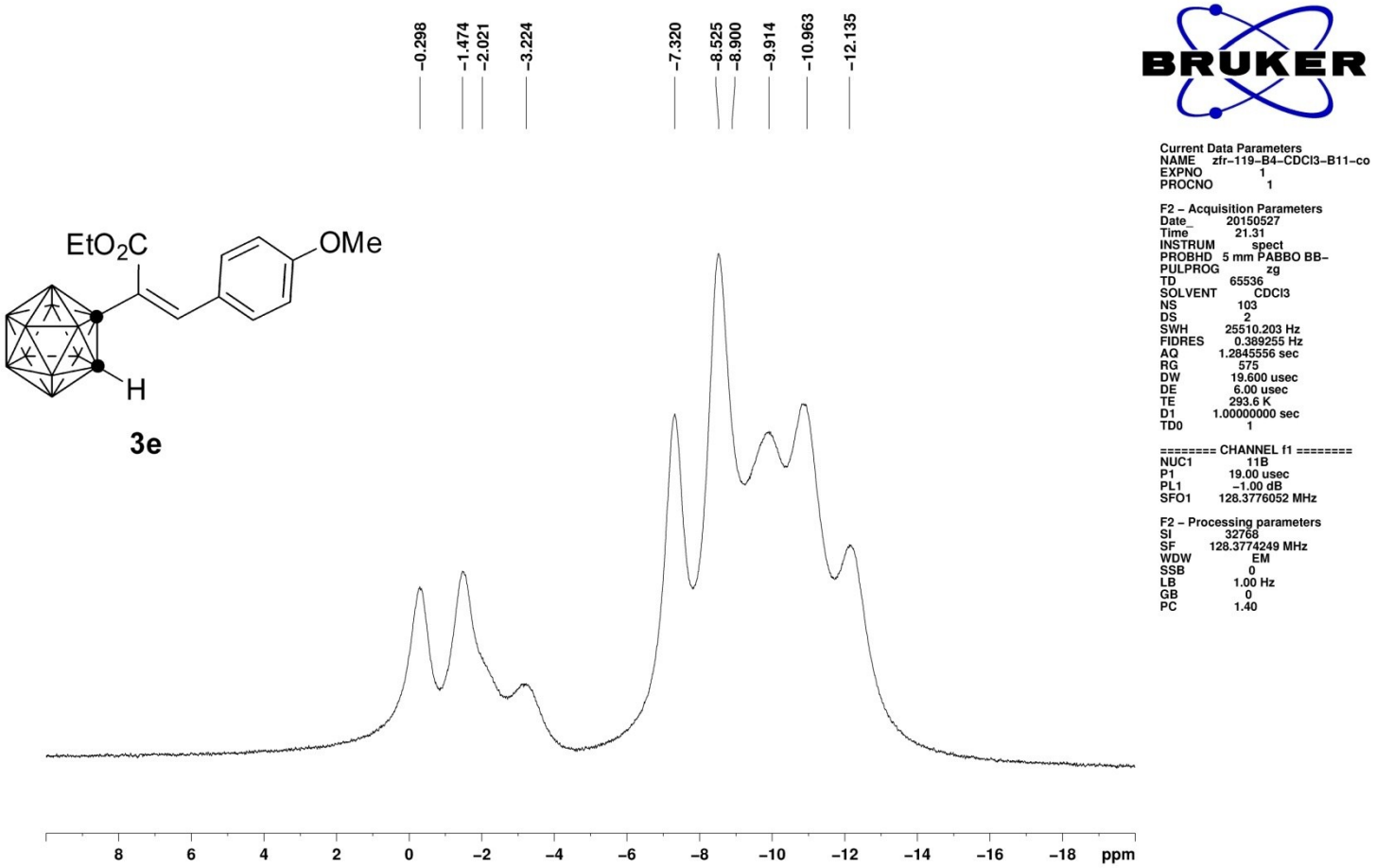
F2 - Acquisition Parameters
Date_ 20150706
Time 22.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.818
153.429
139.015
130.692
128.335
126.756
125.790
77.547
77.230
76.911
73.291
62.493
59.629
35.007
31.324
13.772
EtO2C
tBu
H
3d
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME zfr-162-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150706
Time 22.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.807
−2.609
−7.812
−9.286
−10.015
−11.449
EtO2C
OMe
H
3e
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.02
0.99
2.00
1.97
1.86
1.98
BRUKER
Current Data Parameters
NAME zfr−119−B4−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150527
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 84
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



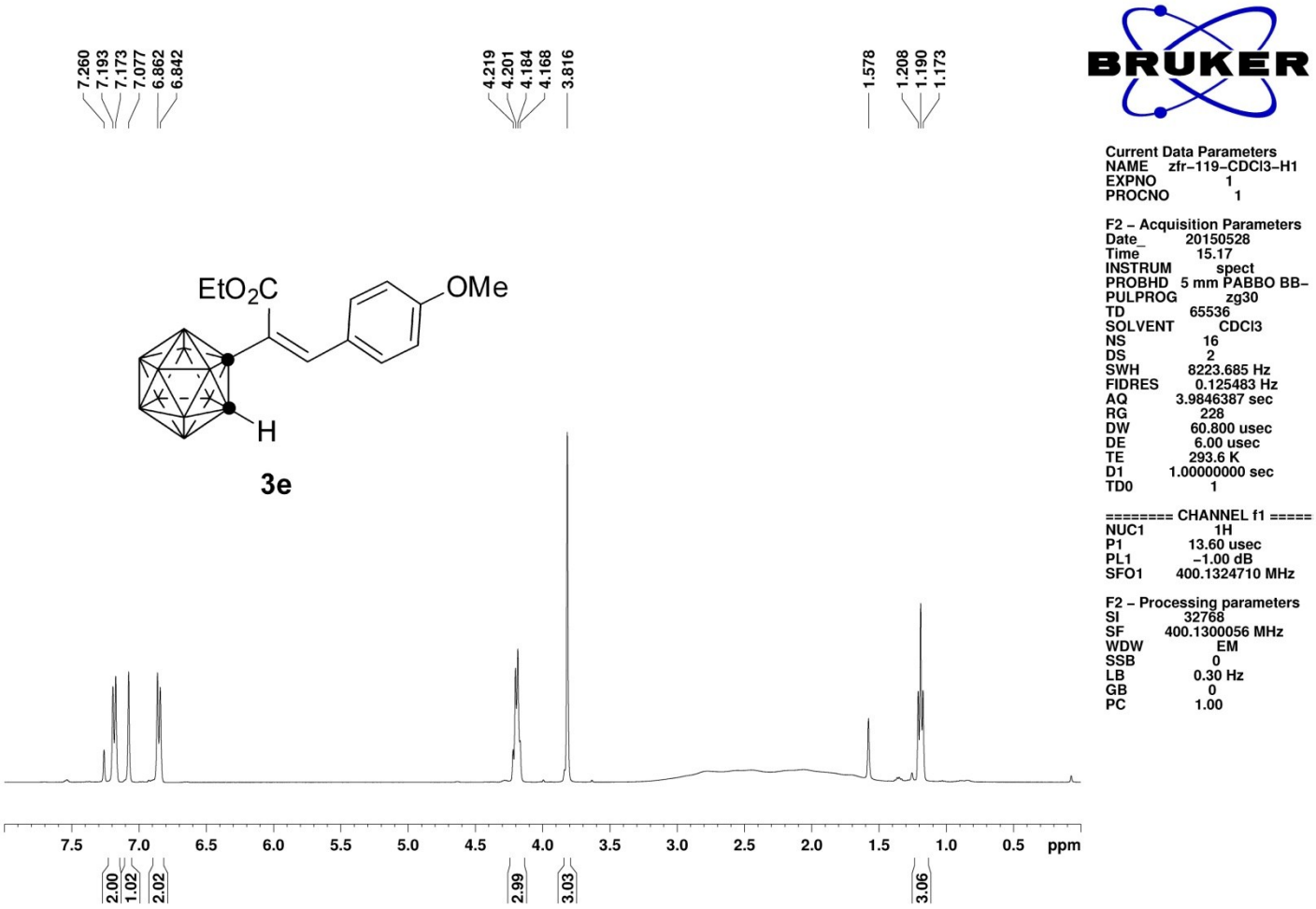
BRUKER

Current Data Parameters
NAME zfr-119-B4-CDCl3-B11-co
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150527
Time 21.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 103
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz

F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



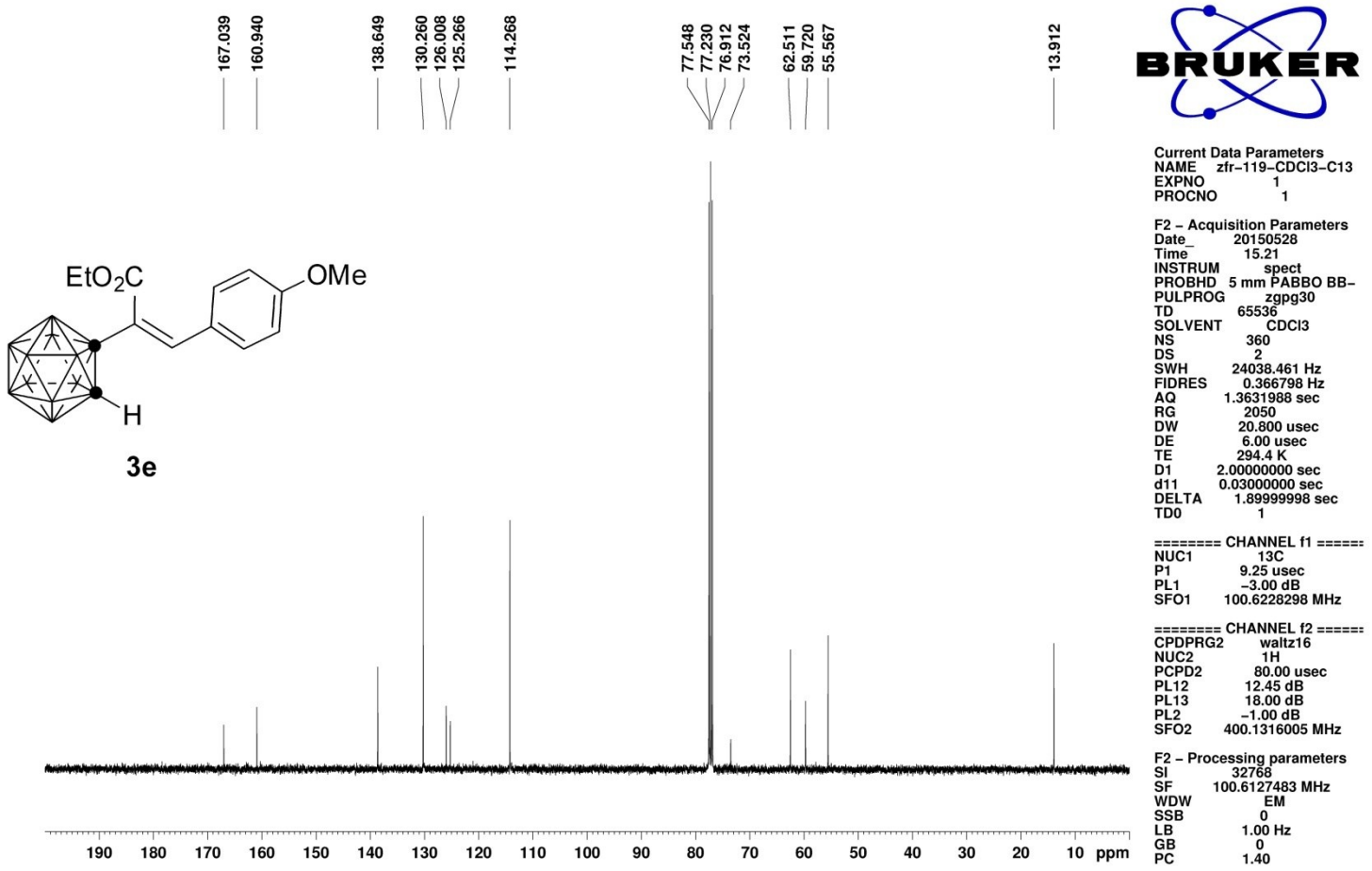
BRUKER

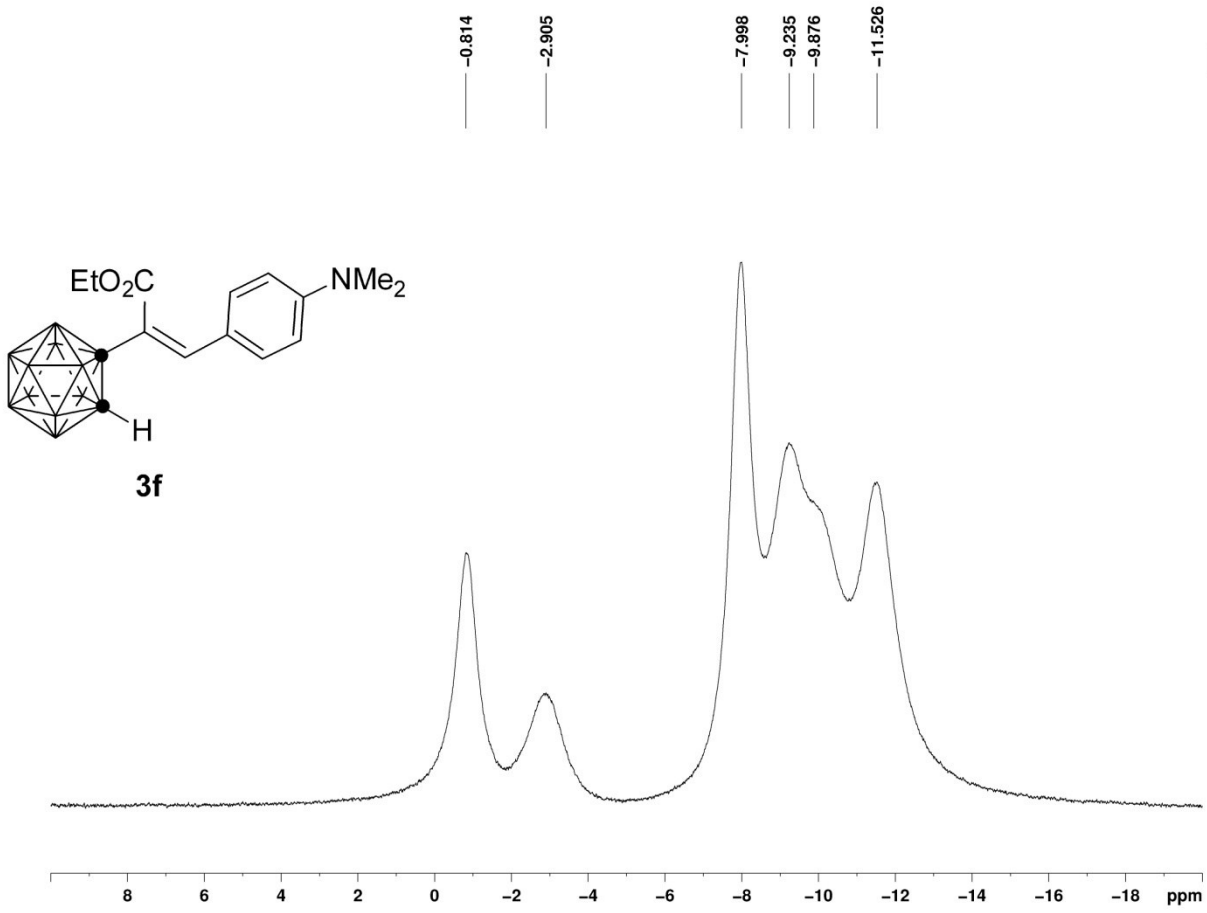
Current Data Parameters
NAME zfr-119-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150528
Time 15.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300056 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


167.039
160.940
138.649
130.260
126.008
125.266
114.268
77.548
77.230
76.912
73.524
62.511
59.720
55.567
13.912
EtO2C
OMe
H
3e
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME zfr-119-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150528
Time 15.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 360
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127483 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME zfr−175−CDCl3−B11
EXPNO 1
PROCNO 1

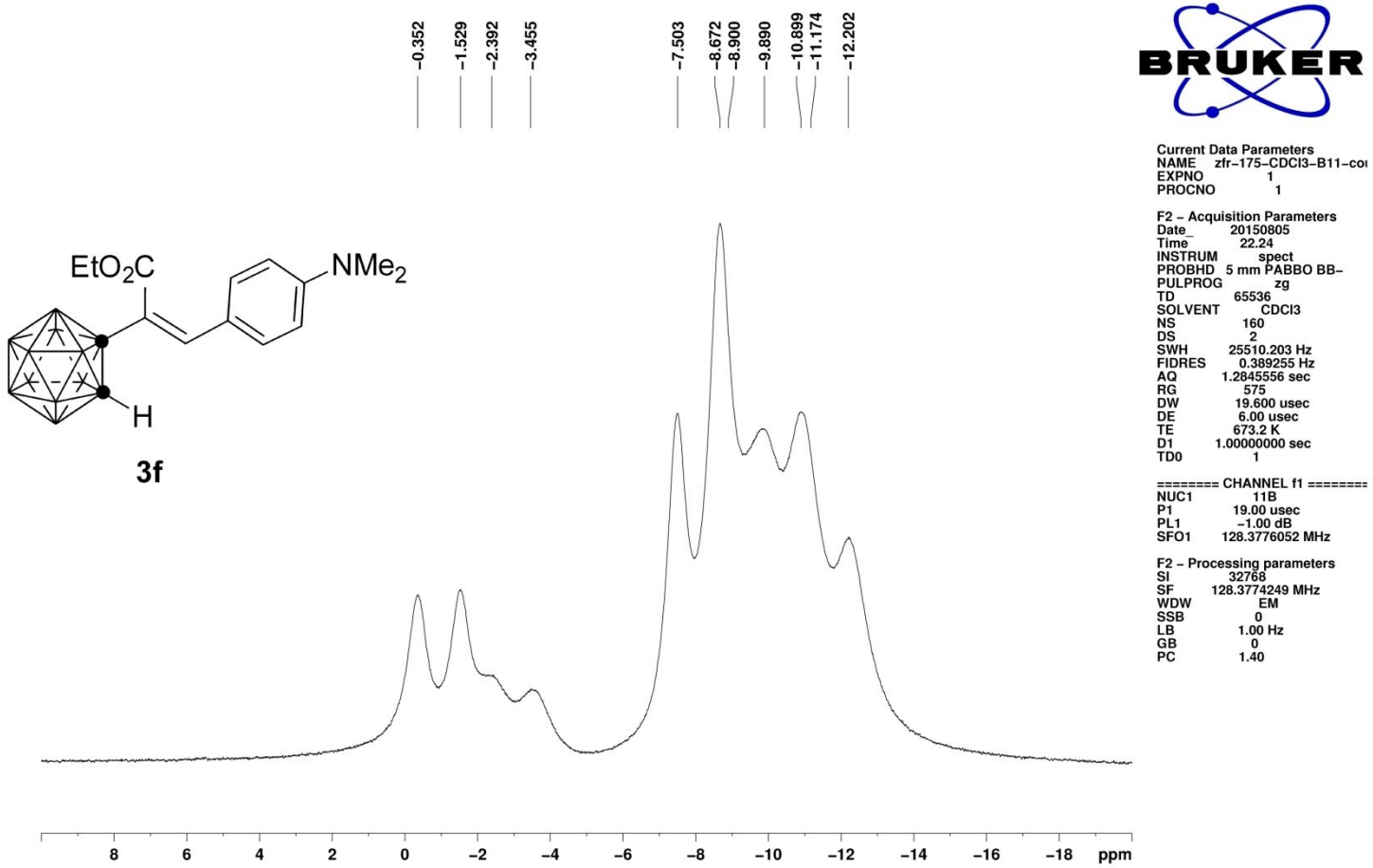
F2 − Acquisition Parameters
Date_ 20150805
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 72
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

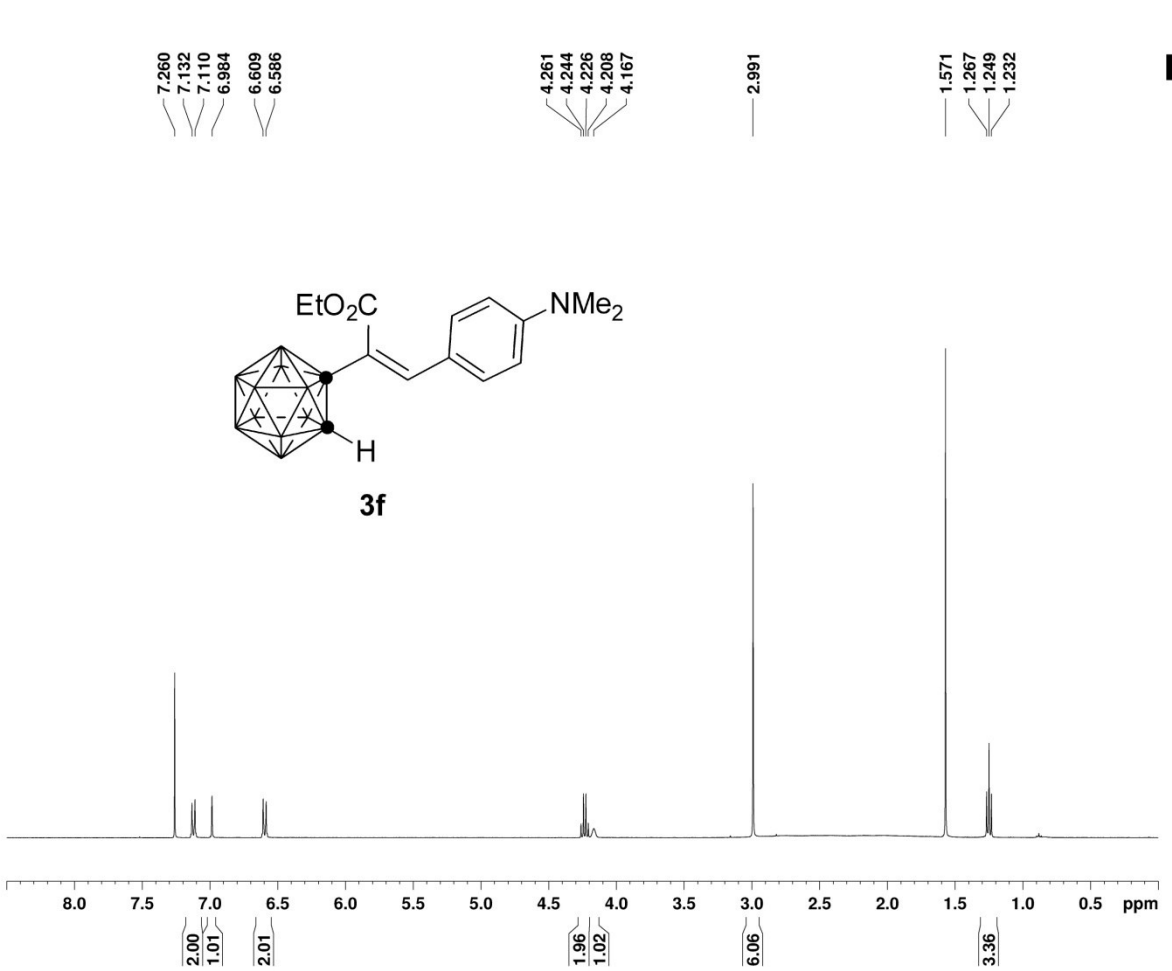
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.352
−1.529
−2.392
−3.455
−7.503
−8.672
−8.900
−9.890
−10.899
−11.174
−12.202
EtO2C
NMe2
H
3f
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
Current Data Parameters
NAME zfr−175−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150805
Time_ 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 673.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

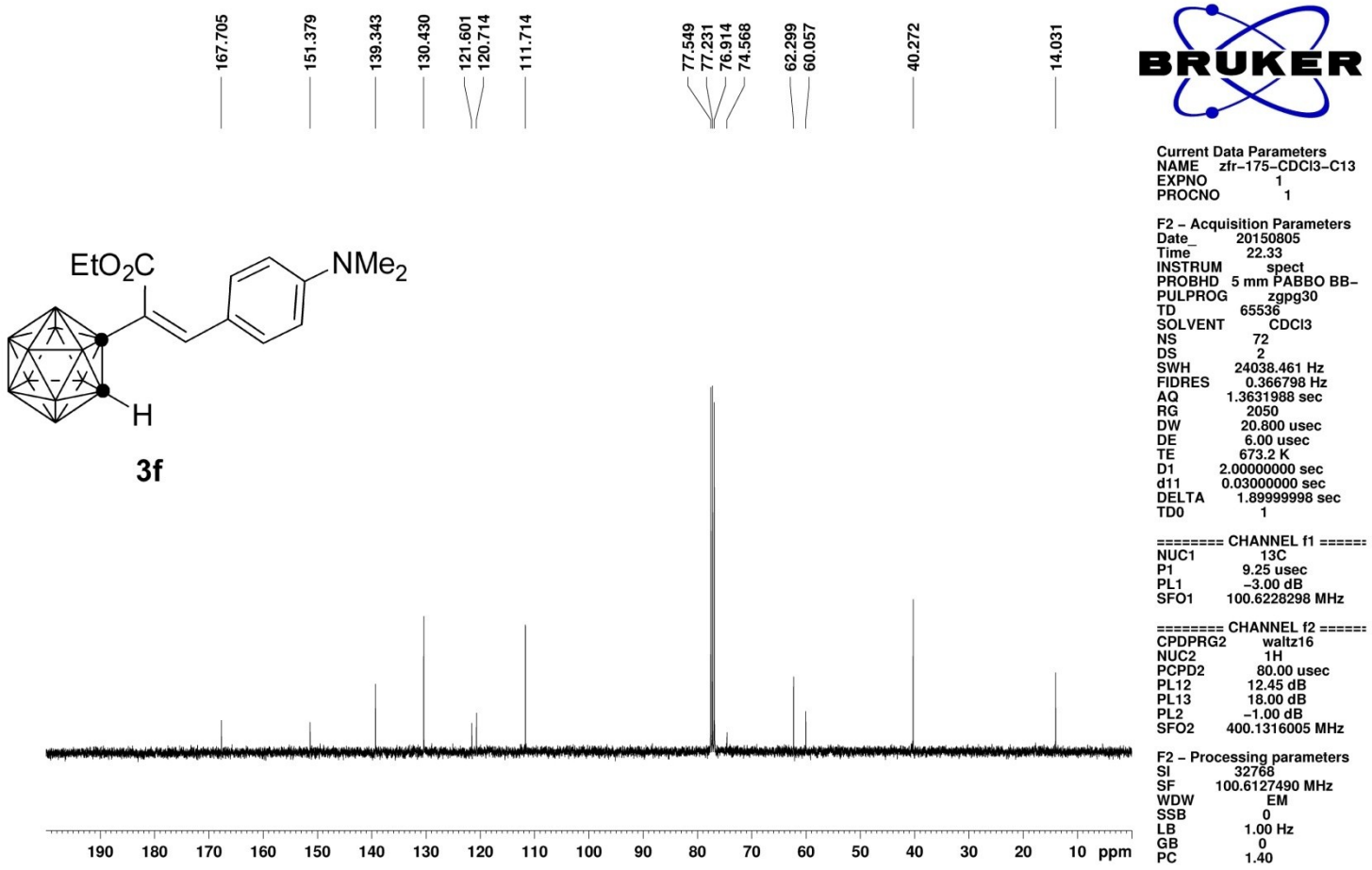


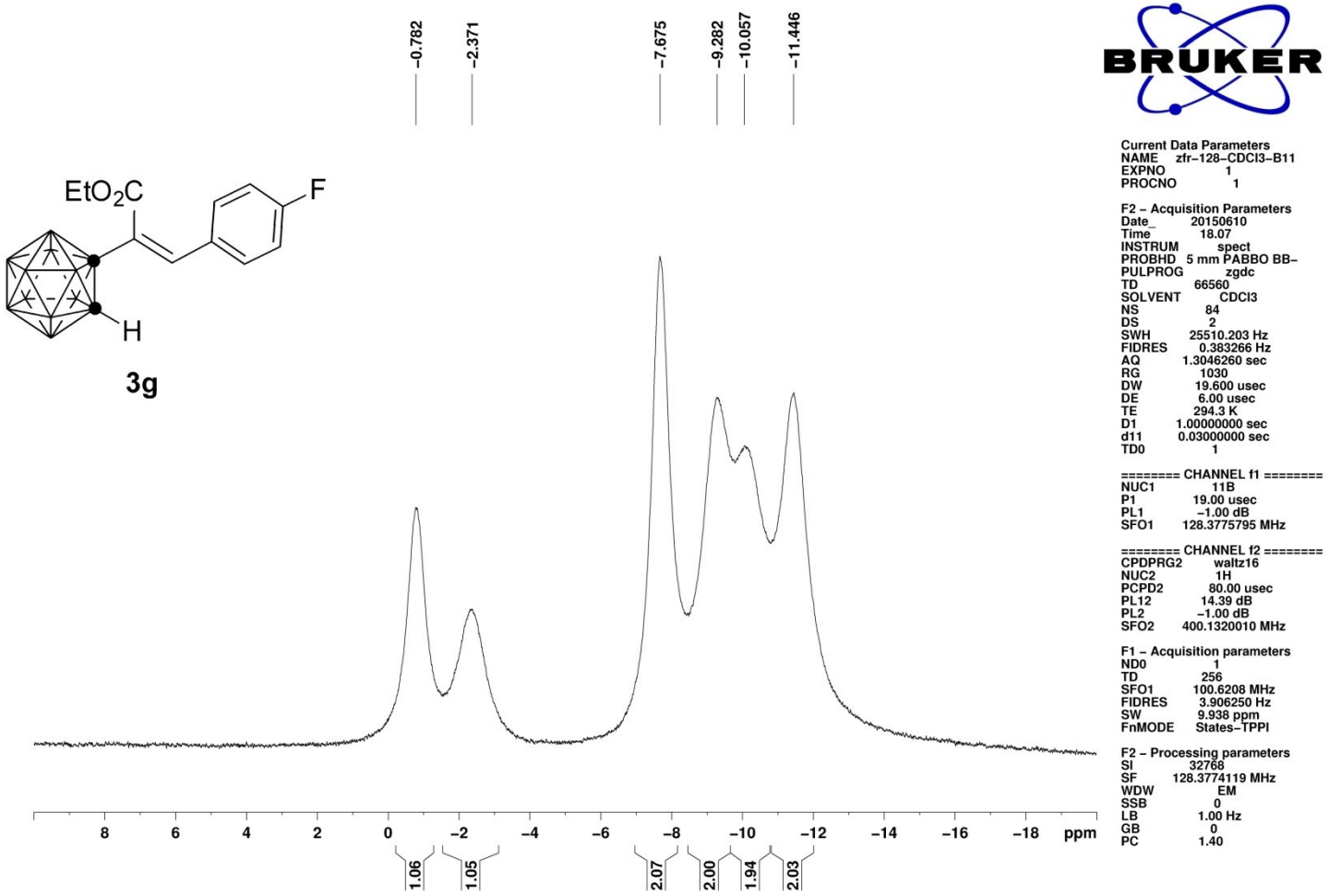
Current Data Parameters
NAME zfr-192-CDCl3-H1
EXPNO 2
PROCNO 1

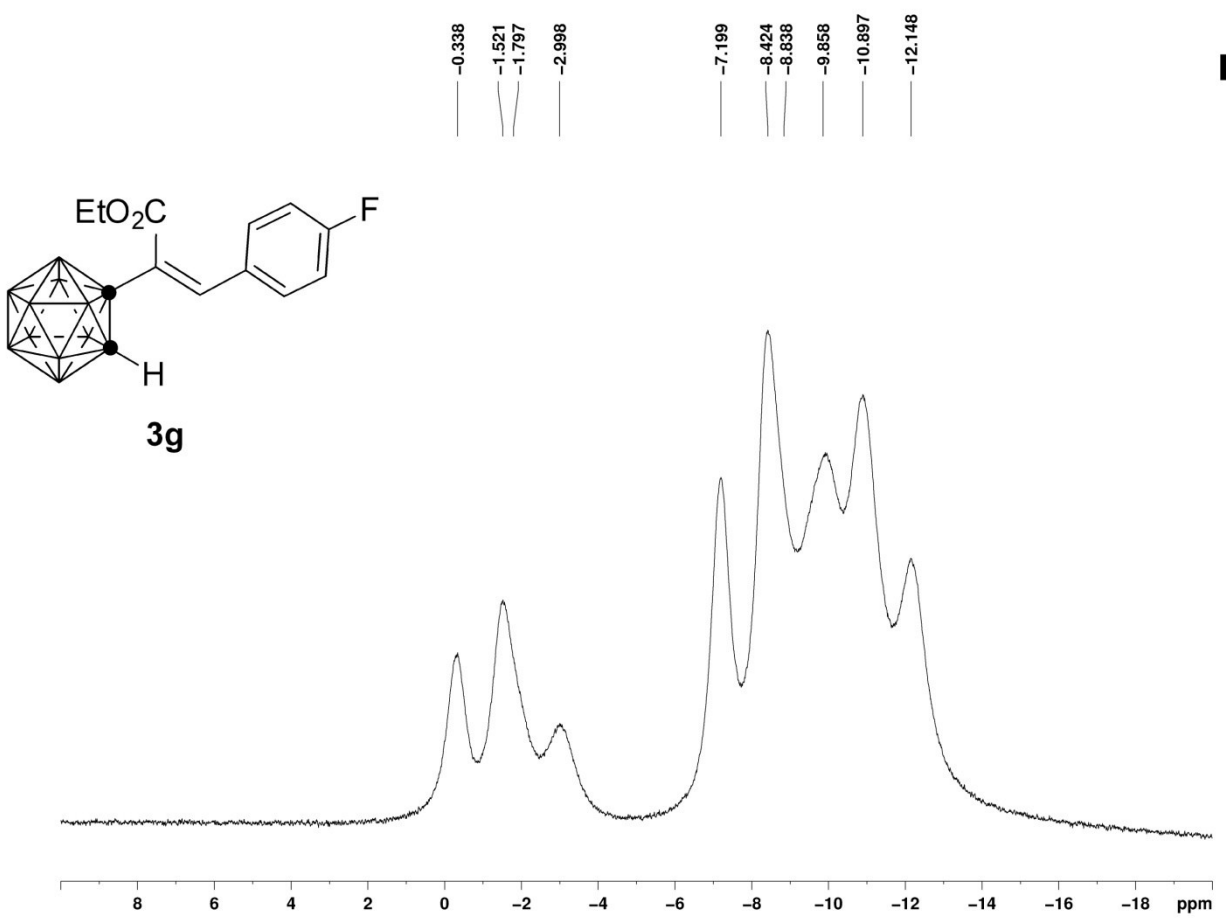
F2 – Acquisition Parameters
Date_ 20150818
Time 12.11
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 575
DW 60.800 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 – Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


167.705
151.379
139.343
130.430
121.601
120.714
111.714
77.549
77.231
76.914
74.568
62.299
60.057
40.272
14.031
EtO2C
NMe2
H
3f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-175-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150805
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 72
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 673.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.782
−2.371
−7.675
−9.282
−10.057
−11.446
EtO2C
F
H
3g
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.06
1.05
2.07
2.00
1.94
2.03
BRUKER
Current Data Parameters
NAME zfr−128−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150610
Time 18.07
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 84
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 1030
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



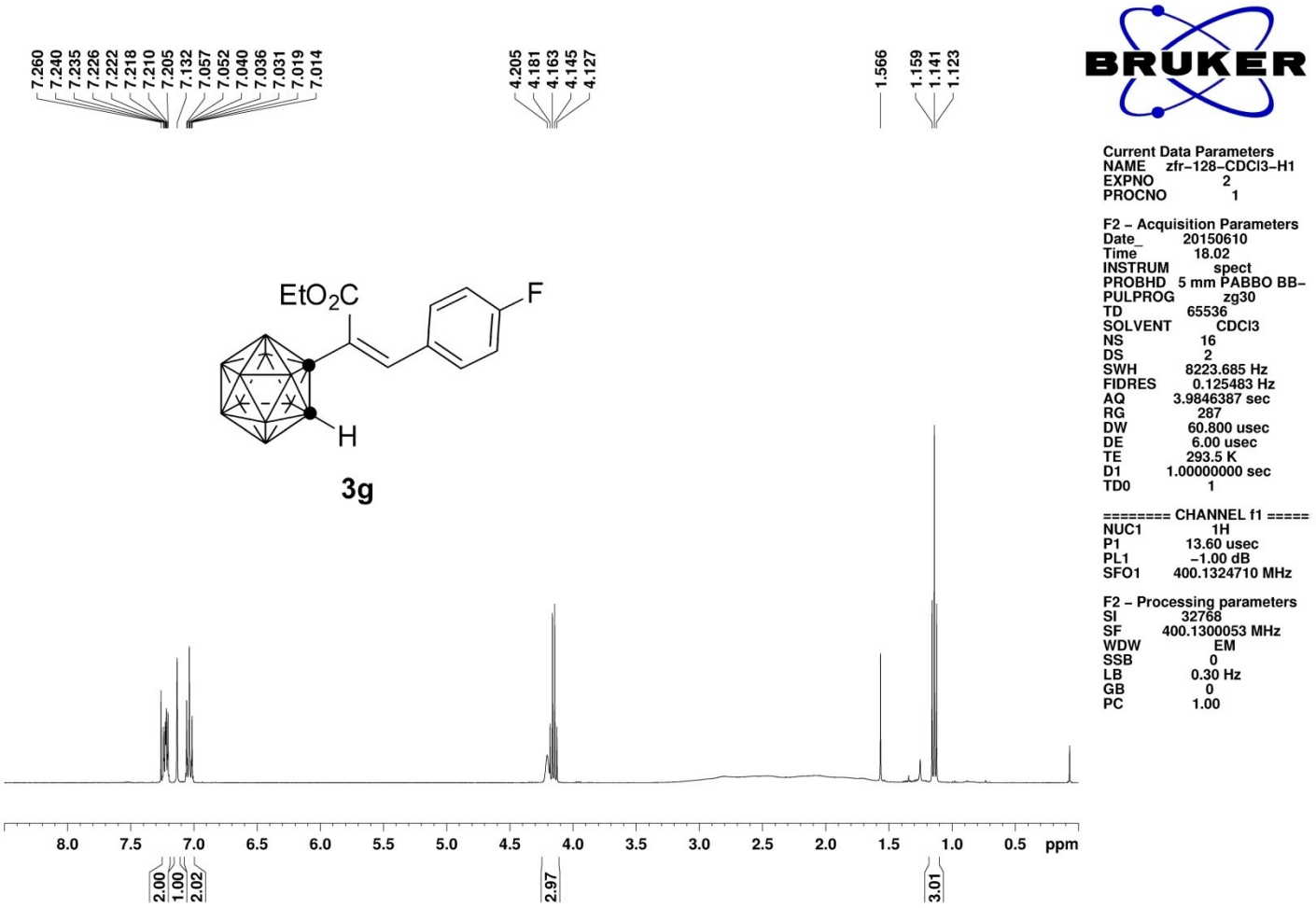
BRUKER

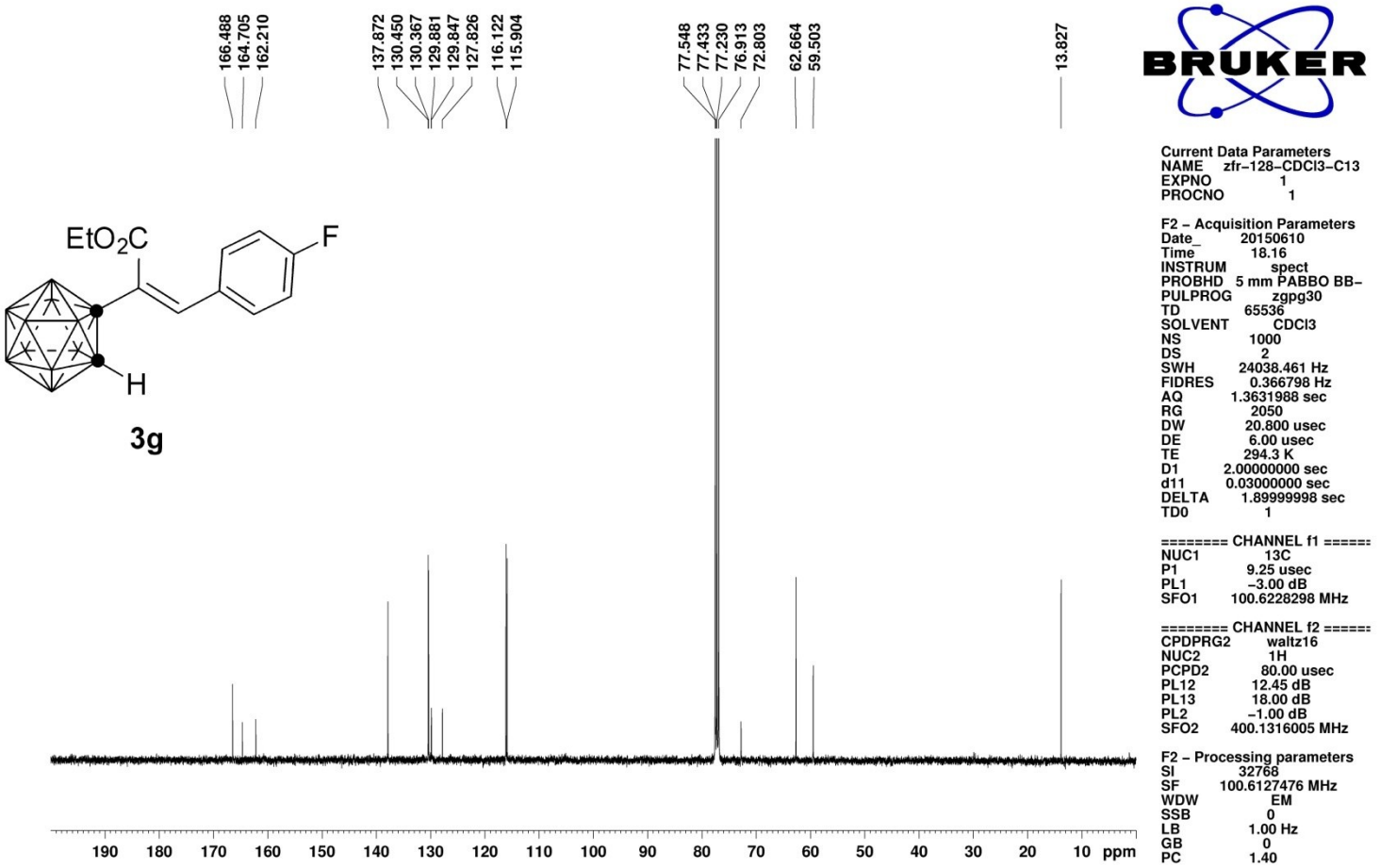
Current Data Parameters
NAME zfr−128−CDCl3−B11−co
EXPNO 1
PROCNO 1

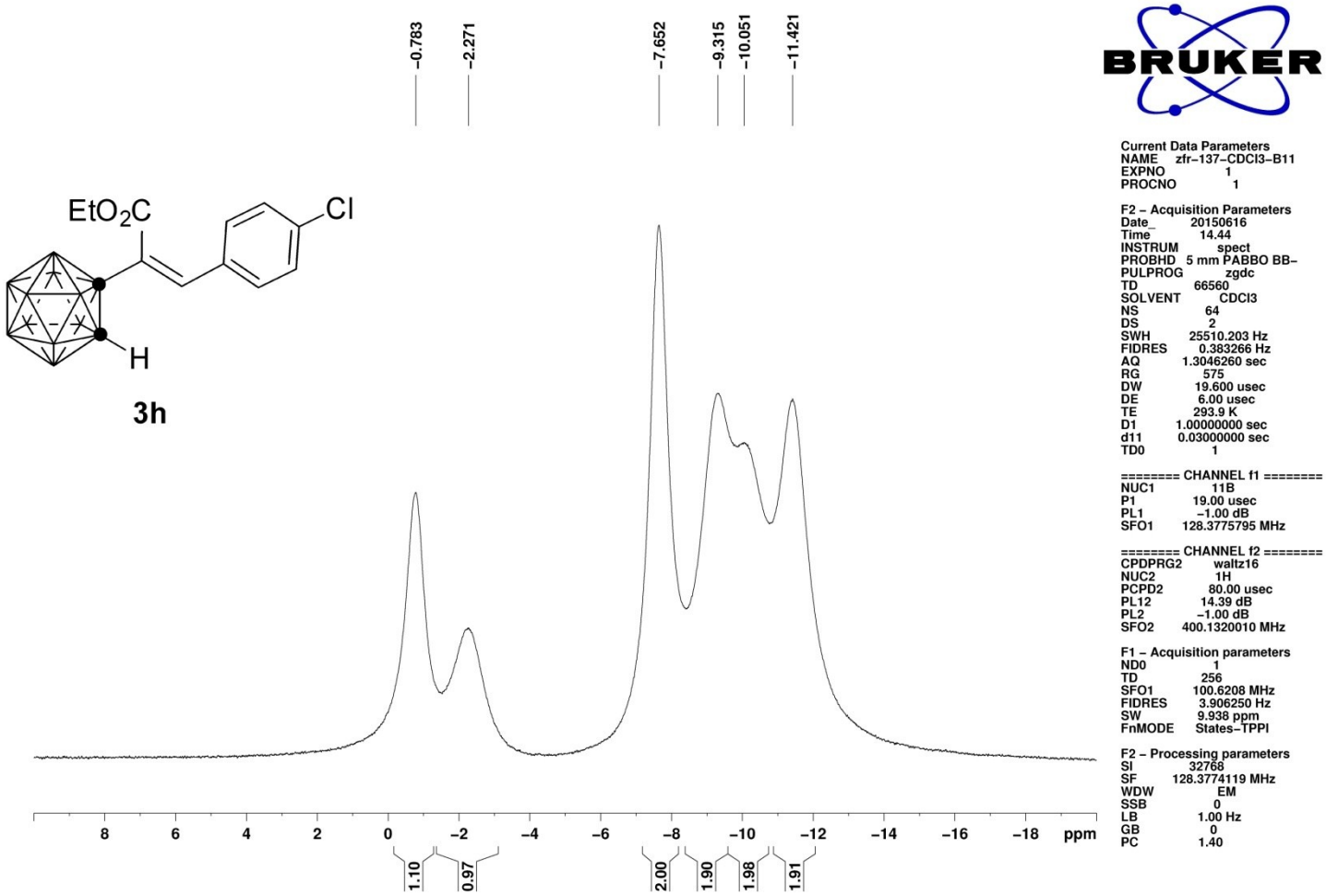
F2 − Acquisition Parameters
Date_ 20150610
Time 18.10
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.260
7.240
7.235
7.226
7.222
7.218
7.210
7.205
7.132
7.057
7.052
7.040
7.036
7.031
7.019
7.014
4.205
4.181
4.163
4.145
4.127
1.566
1.159
1.141
1.123
EtO2C
F
H
3g
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
ppm
2.00
1.00
2.02
2.97
3.01
Current Data Parameters
NAME zfr-128-CDCl3-H1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150610
Time 18.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.488
164.705
162.210
137.872
130.450
130.367
129.881
129.847
127.826
116.122
115.904
77.548
77.433
77.230
76.913
72.803
62.664
59.503
13.827
EtO2C
F
H
3g
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
Current Data Parameters
NAME zfr-128-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150610
Time 18.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1000
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127476 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME zfr−137−CDCl3−B11
EXPNO 1
PROCNO 1

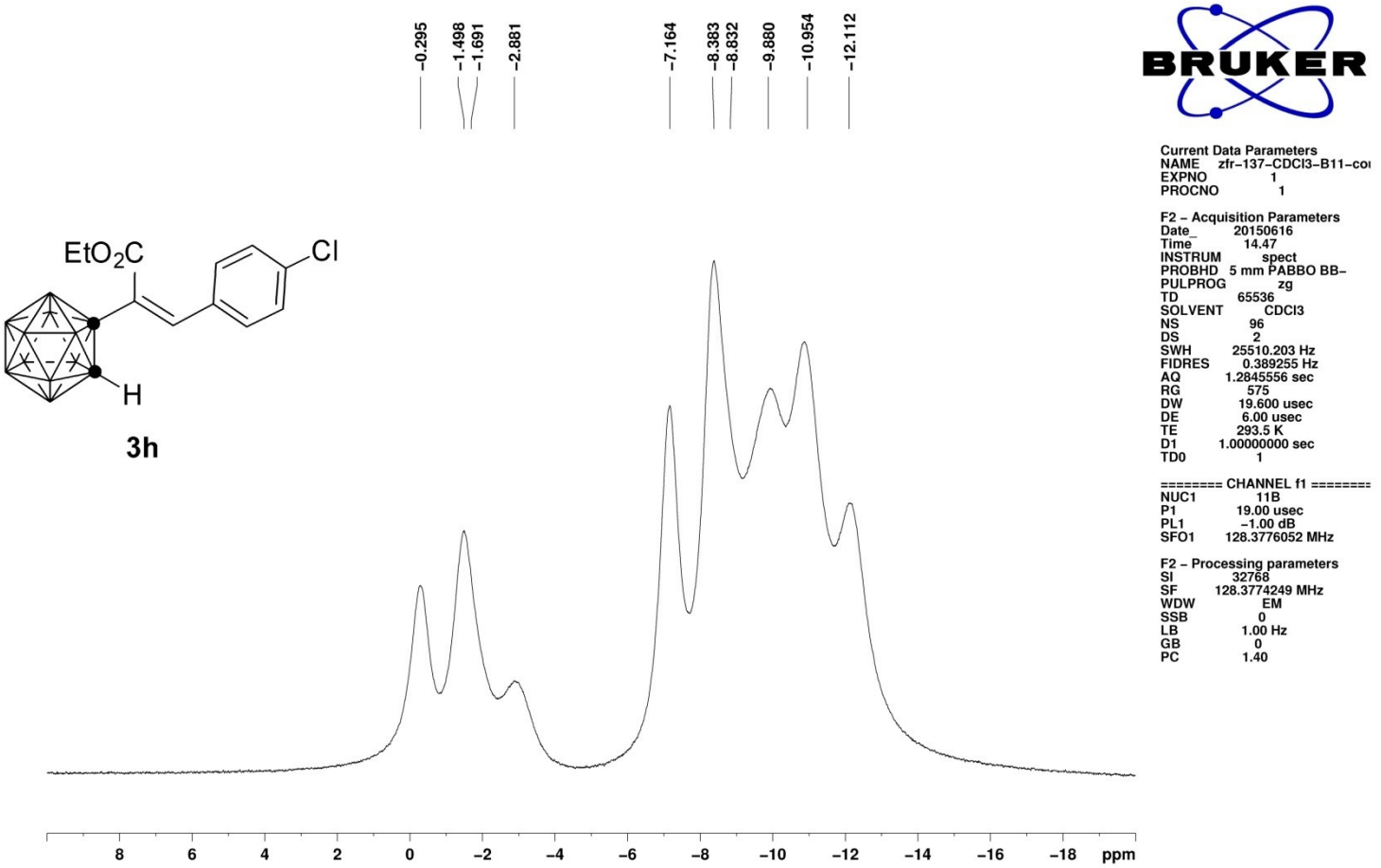
F2 − Acquisition Parameters
Date_ 20150616
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

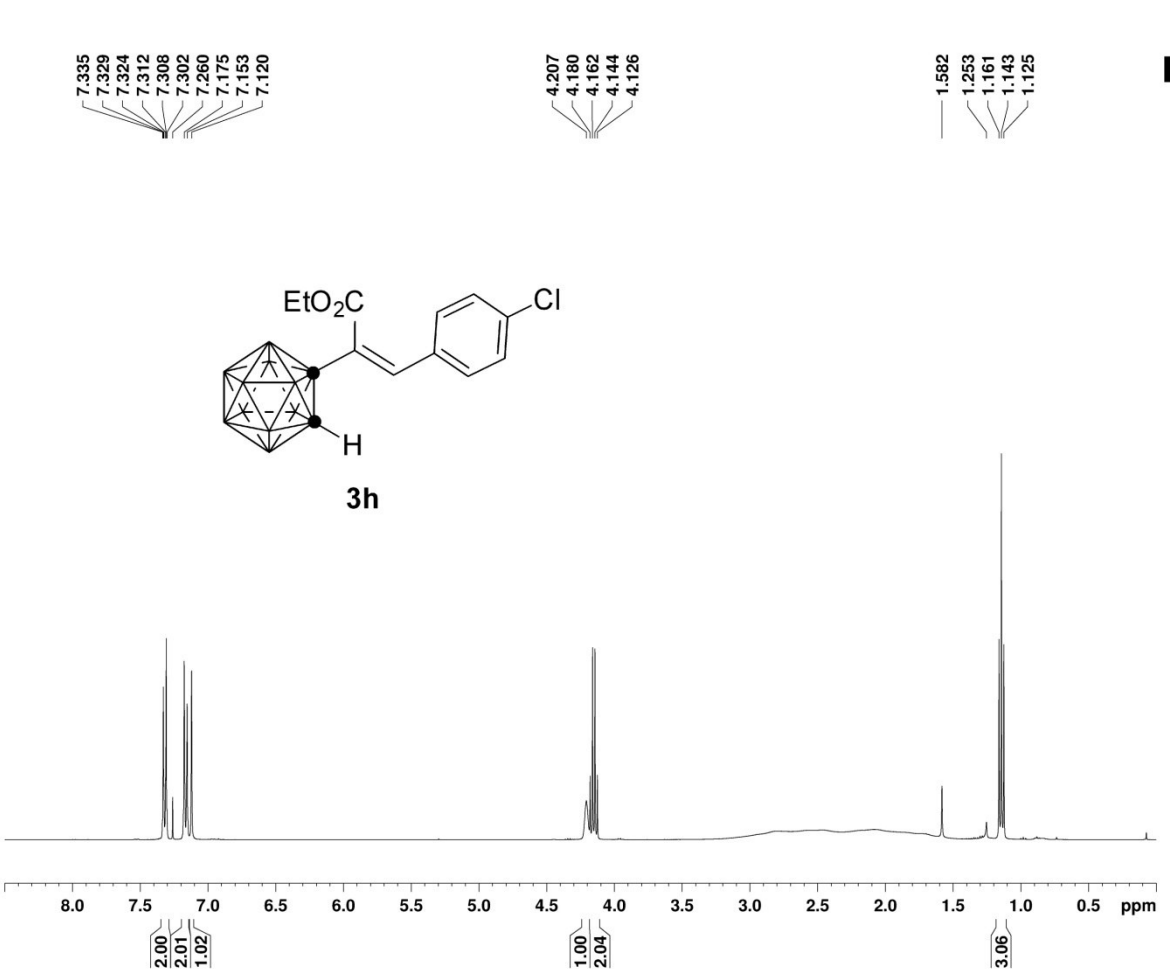
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-0.295
-1.498
-1.691
-2.881
-7.164
-8.383
-8.832
-9.880
-10.954
-12.112
EtO2C
Cl
H
3h
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
ppm
BRUKER
Current Data Parameters
NAME zfr-137-CDCl3-B11-co
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150616
Time 14.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



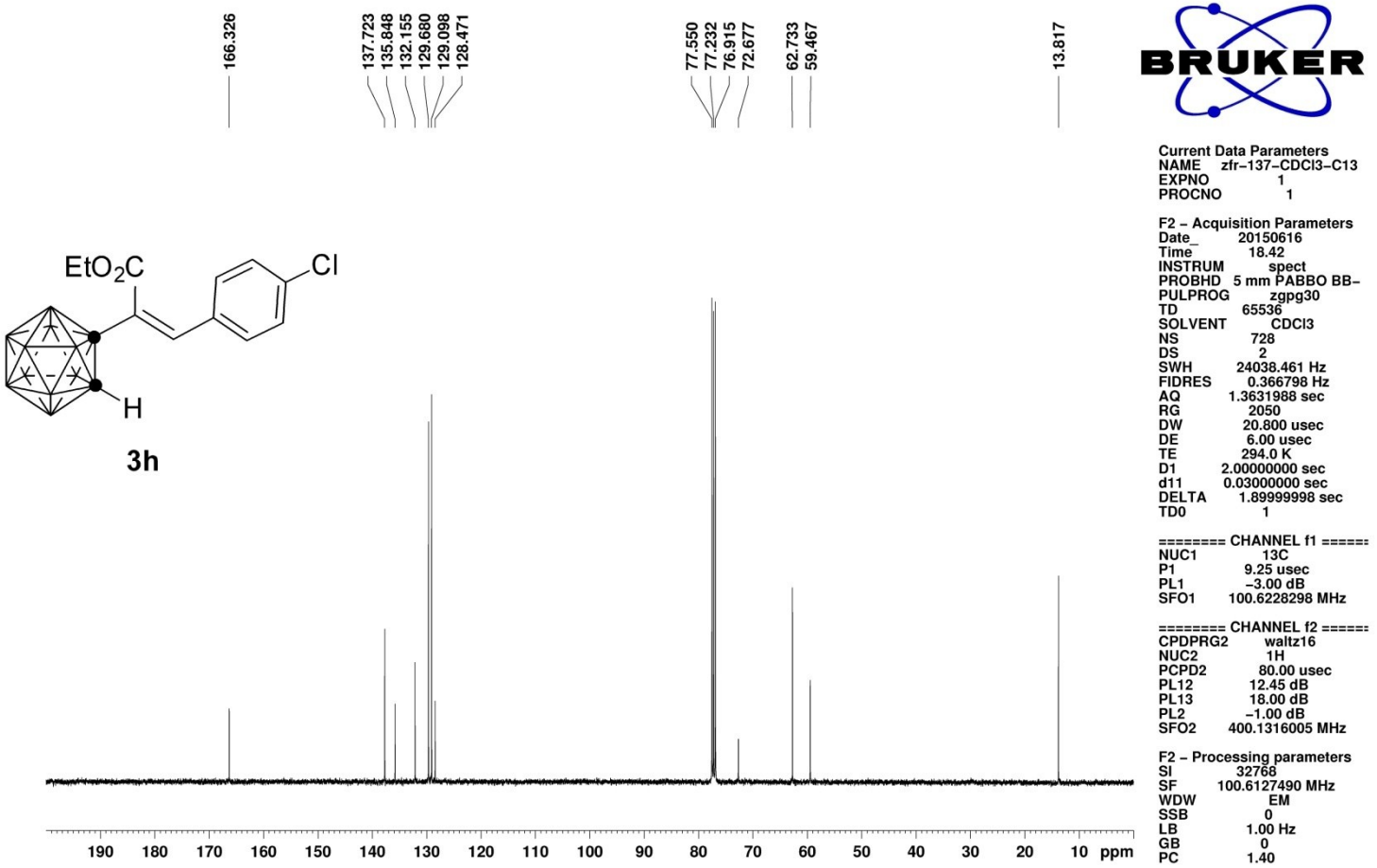
BRUKER

Current Data Parameters
NAME zfr-137-CDCl3-H1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150616
Time 18.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

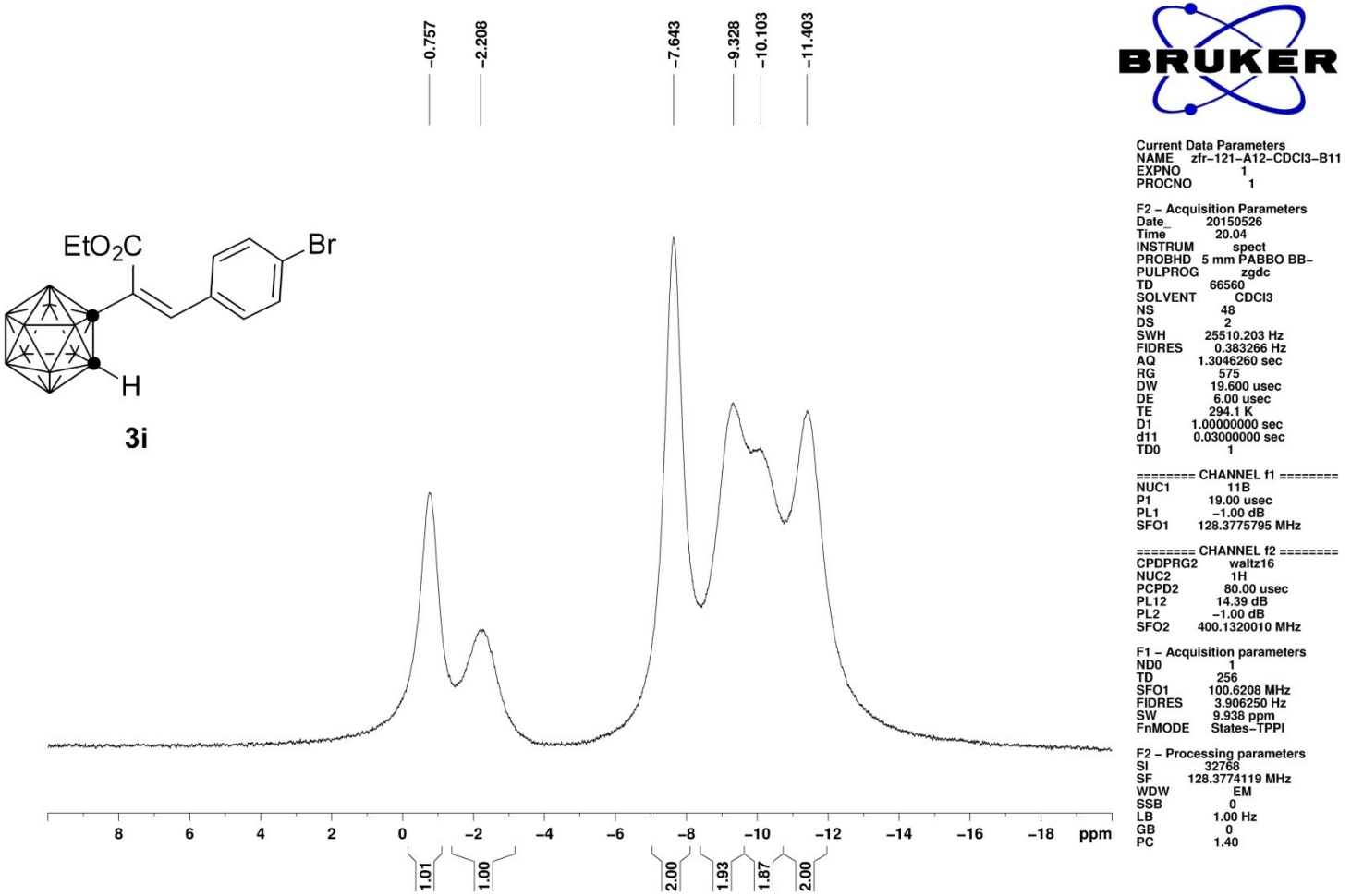
Current Data Parameters
NAME zfr-137-CDCl3-C13
EXPNO 1
PROCNO 1

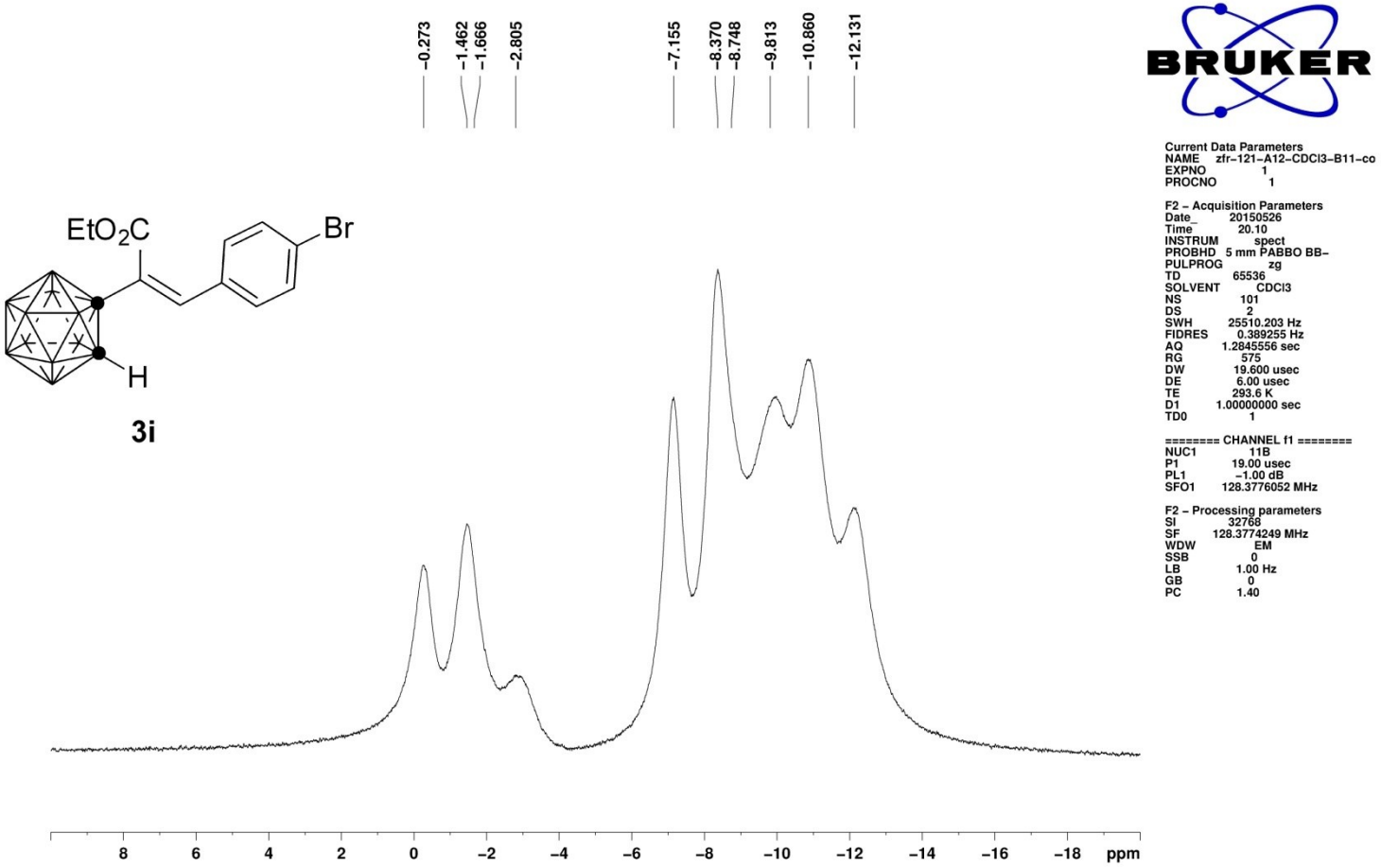
F2 - Acquisition Parameters
Date_ 20150616
Time 18.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 728
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

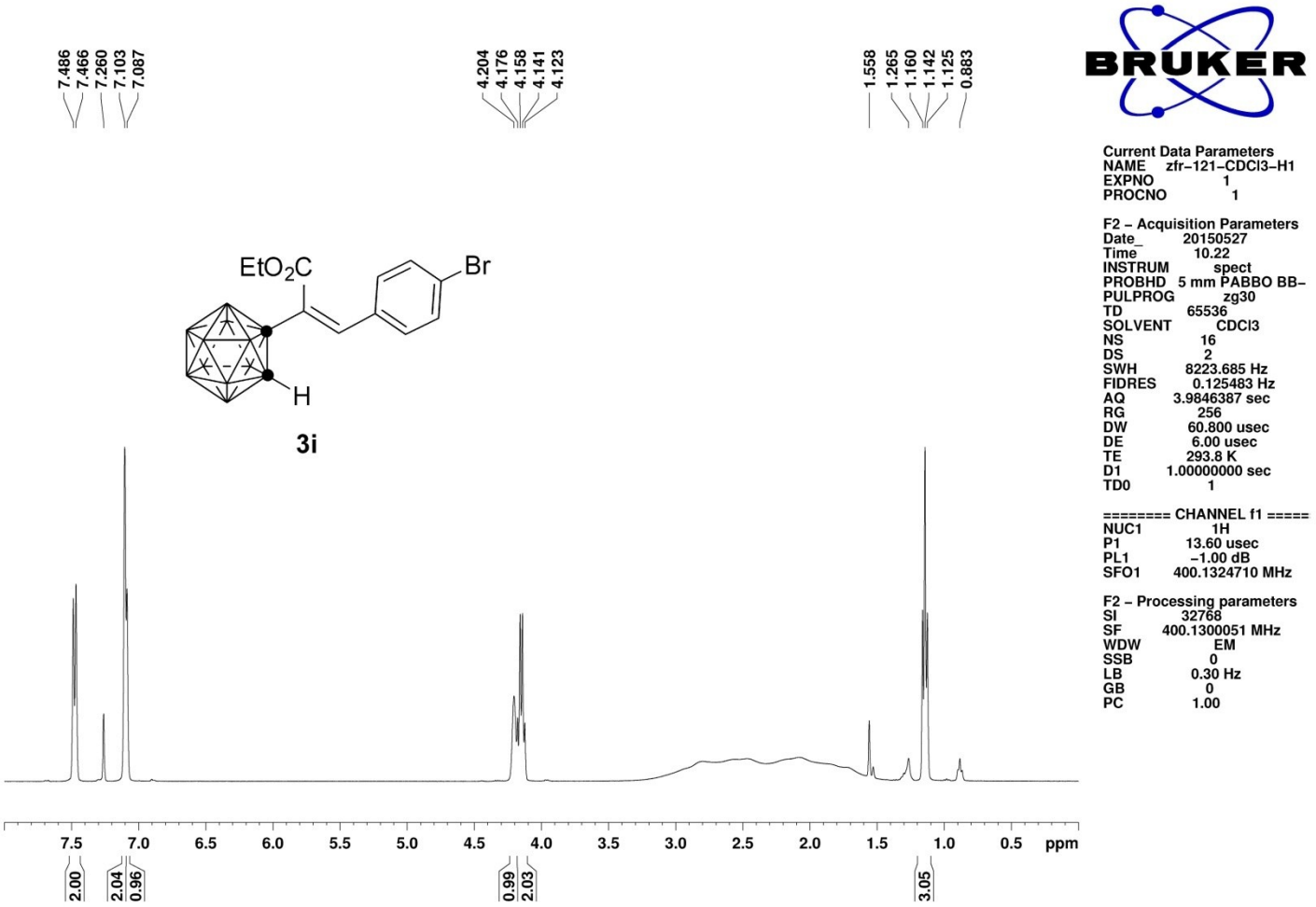
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.757
−2.208
−7.643
−9.328
−10.103
−11.403
EtO2C
Br
H
3i
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.01
1.00
2.00
1.93
1.87
2.00
BRUKER
Current Data Parameters
NAME zfr−121−A12−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date 20150526
Time 20.04
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 48
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.273
−1.462
−1.666
−2.805
−7.155
−8.370
−8.748
−9.813
−10.860
−12.131
EtO2C
Br
H
3i
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
NAME zfr−121−A12−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150526
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 101
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

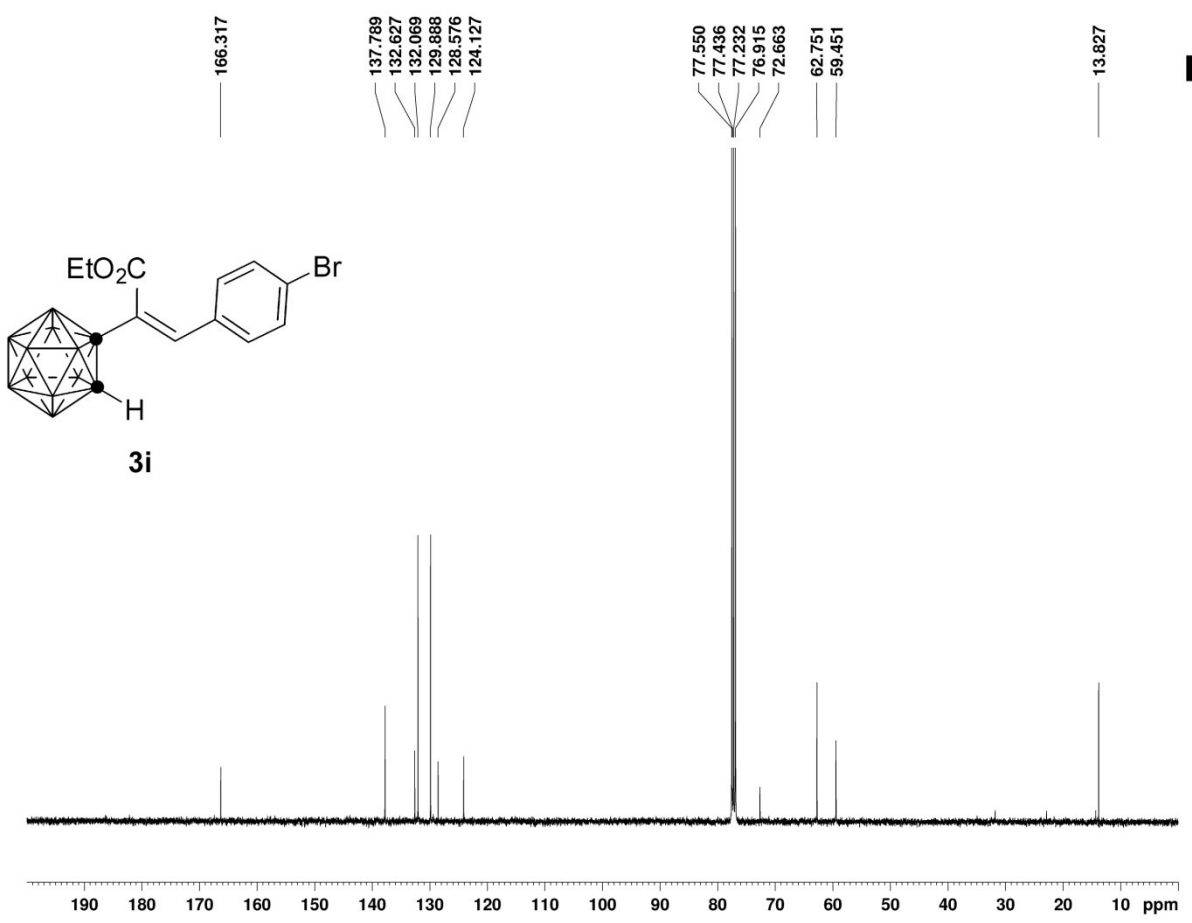


Current Data Parameters
NAME zfr-121-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150527
Time 10.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

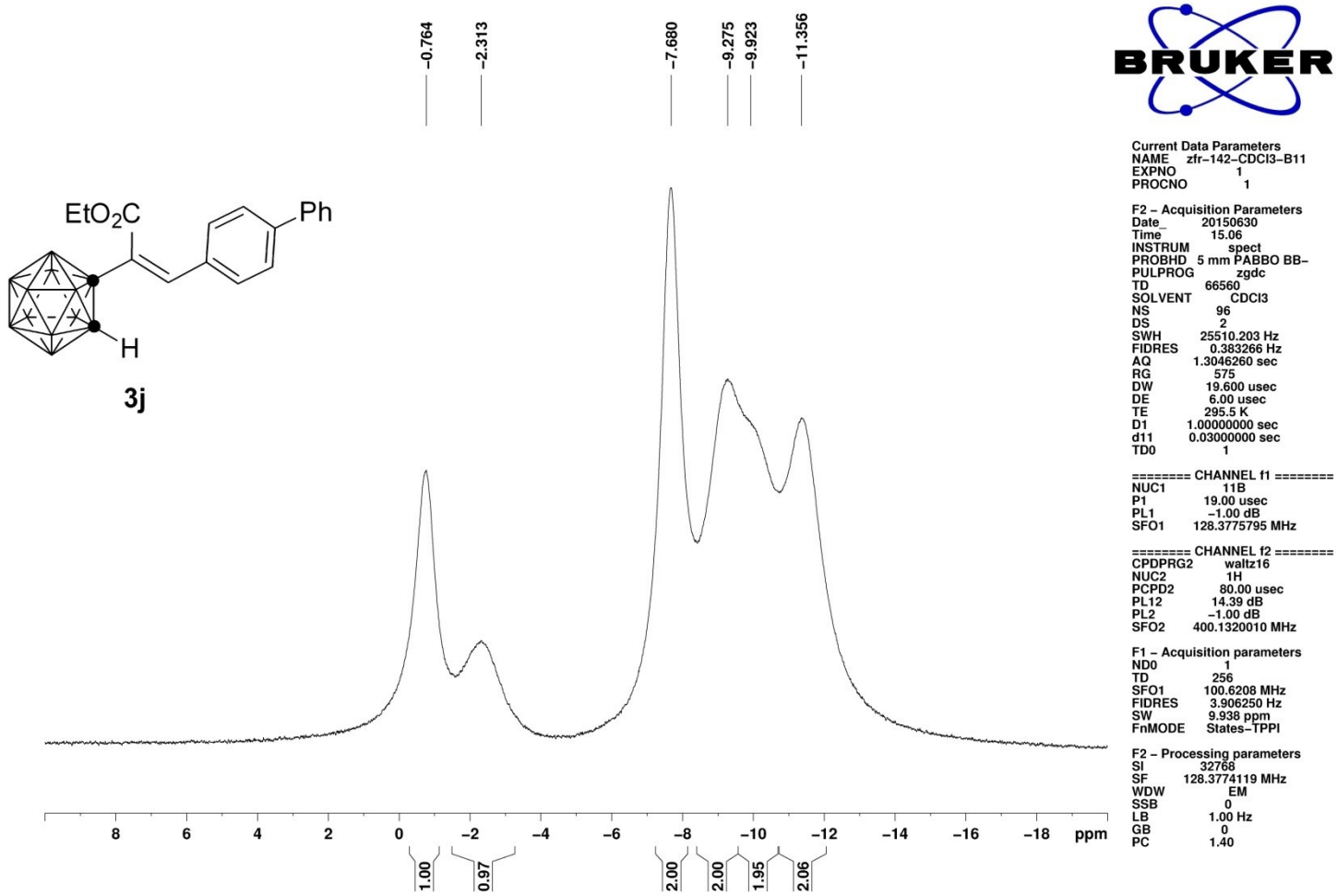
Current Data Parameters
NAME zfr-121-CDCl3-C13
EXPNO 1
PROCNO 1

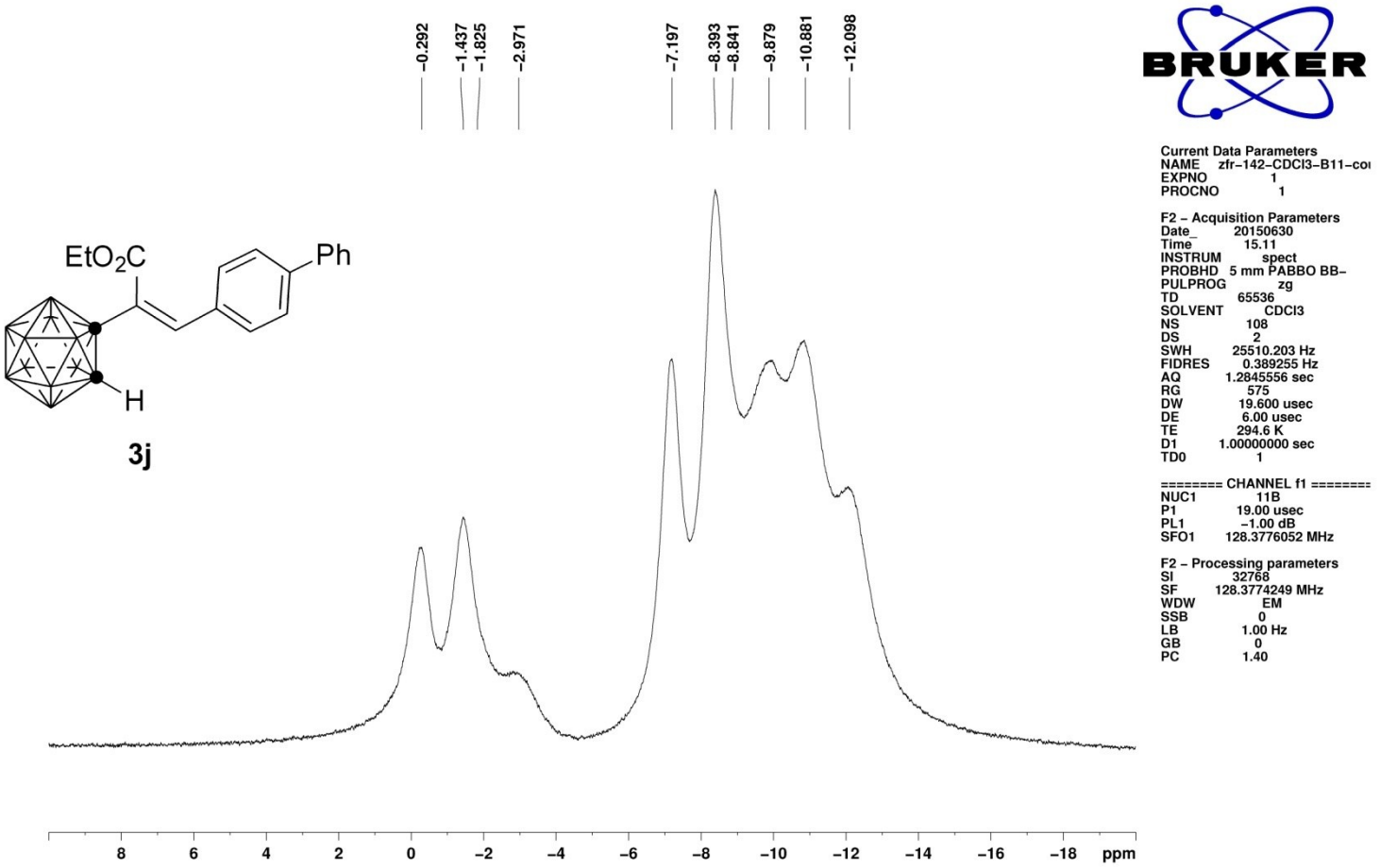
F2 - Acquisition Parameters
Date_ 20150527
Time 10.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 747
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

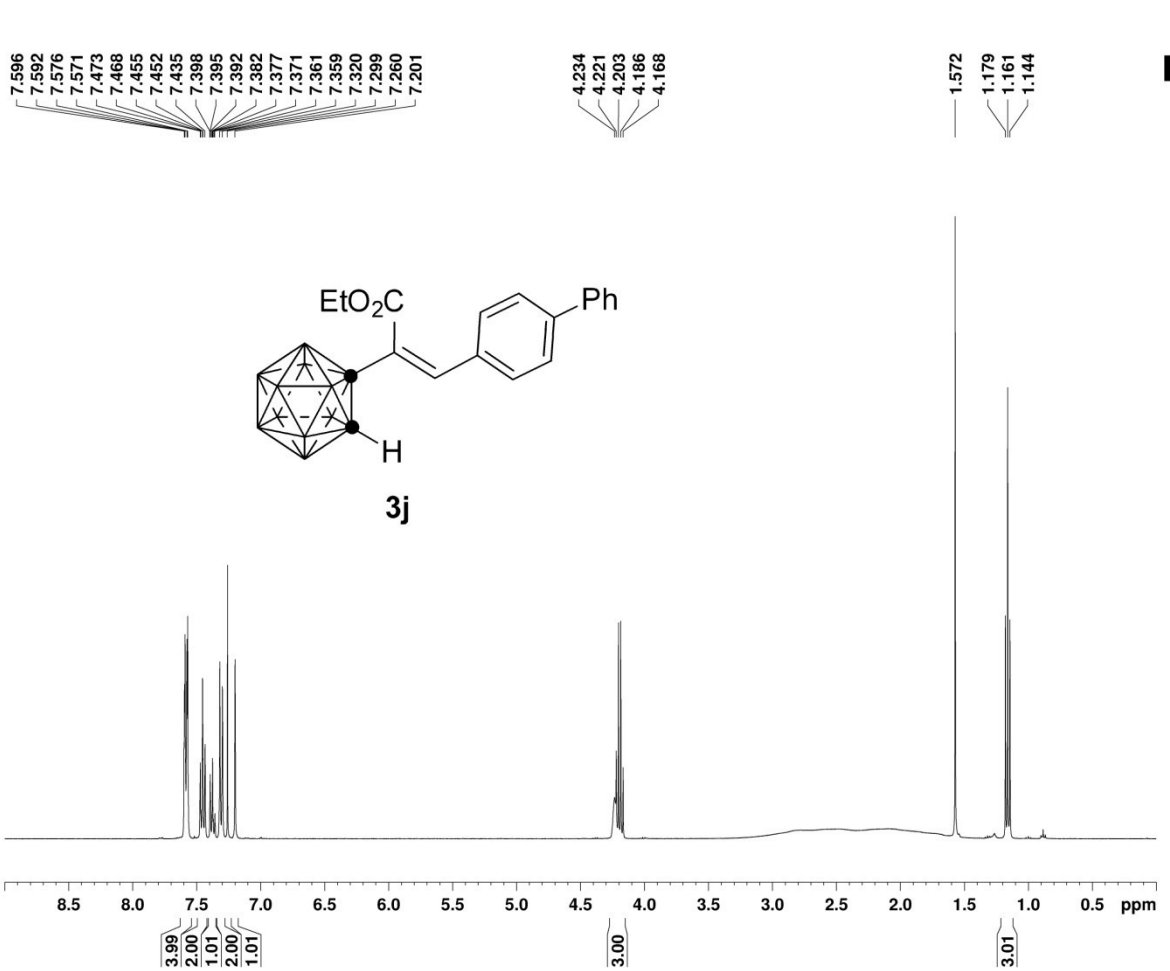
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127476 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.764
−2.313
−7.680
−9.275
−9.923
−11.356
EtO2C
Ph
H
3j
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.00
0.97
2.00
2.00
1.95
2.06
BRUKER
Current Data Parameters
NAME zfr−142−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150630
Time 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.292
−1.437
−1.825
−2.971
−7.197
−8.393
−8.841
−9.879
−10.881
−12.098
EtO2C
Ph
H
3j
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
NAME zfr−142−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150630
Time 15.11
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 108
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



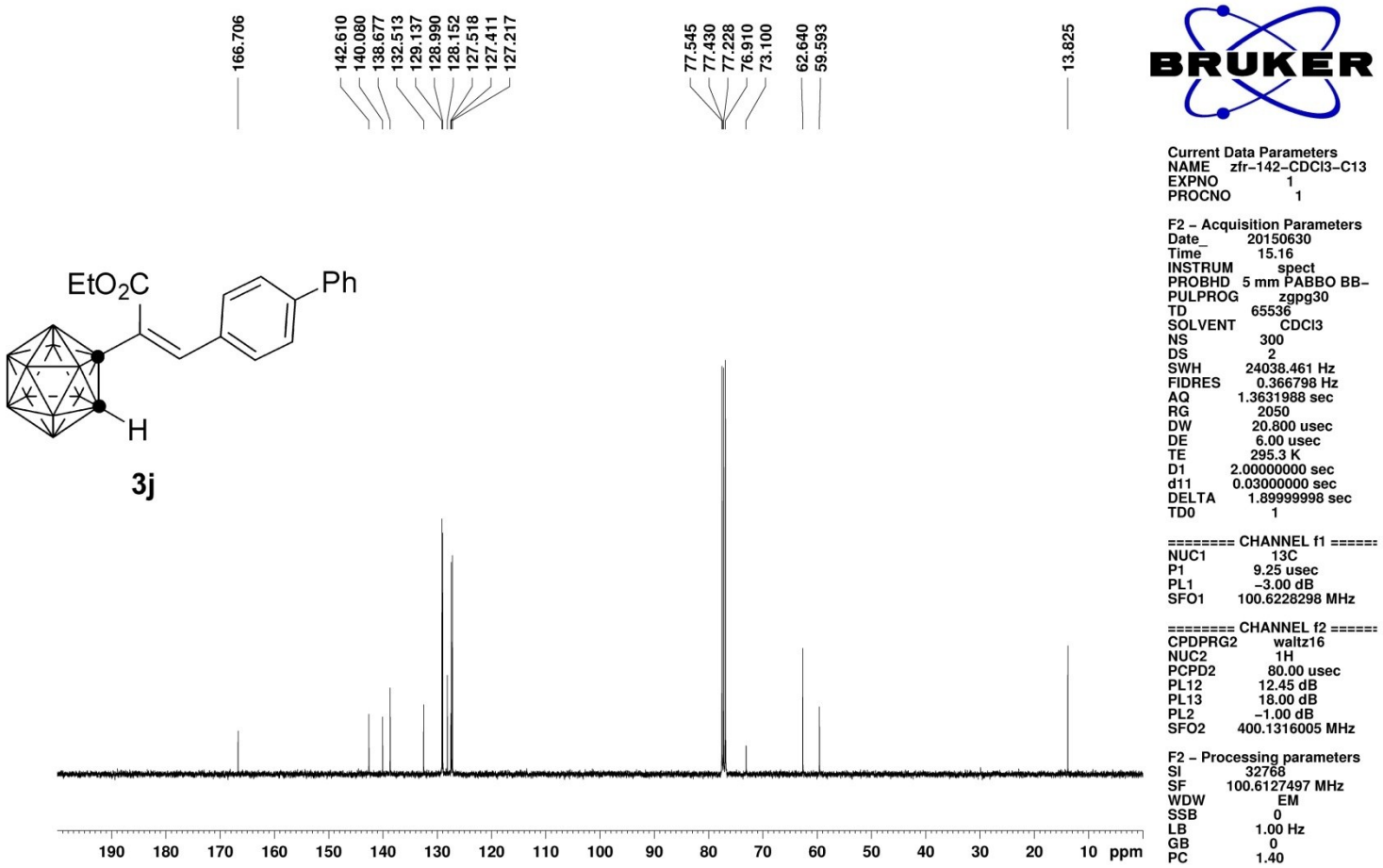
BRUKER

Current Data Parameters
NAME zfr-142-CDCl3-H1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150630
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

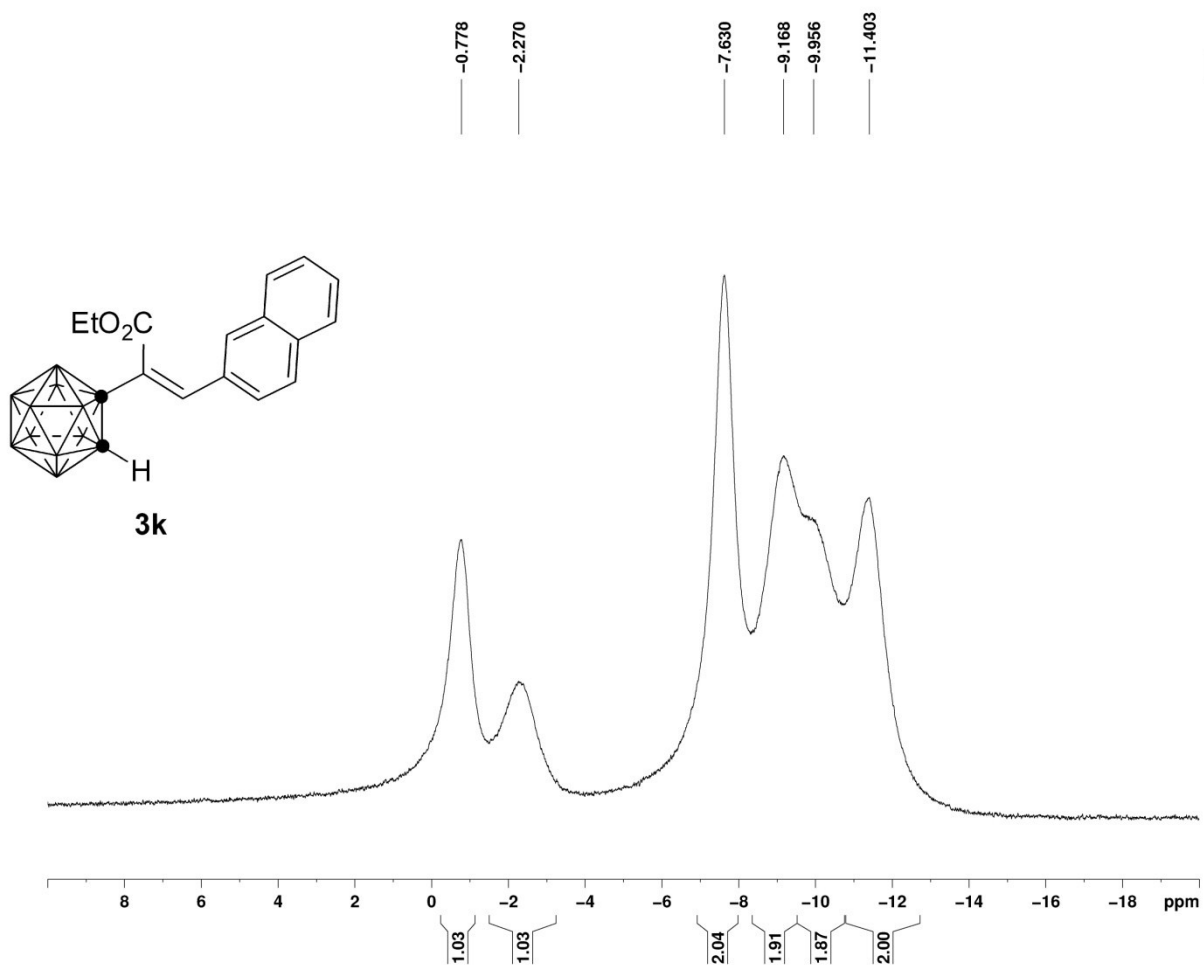
Current Data Parameters
NAME zfr-142-CDCl3-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150630
Time 15.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127497 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−83−B2−CDCl3−B11
EXPNO 1
PROCNO 1

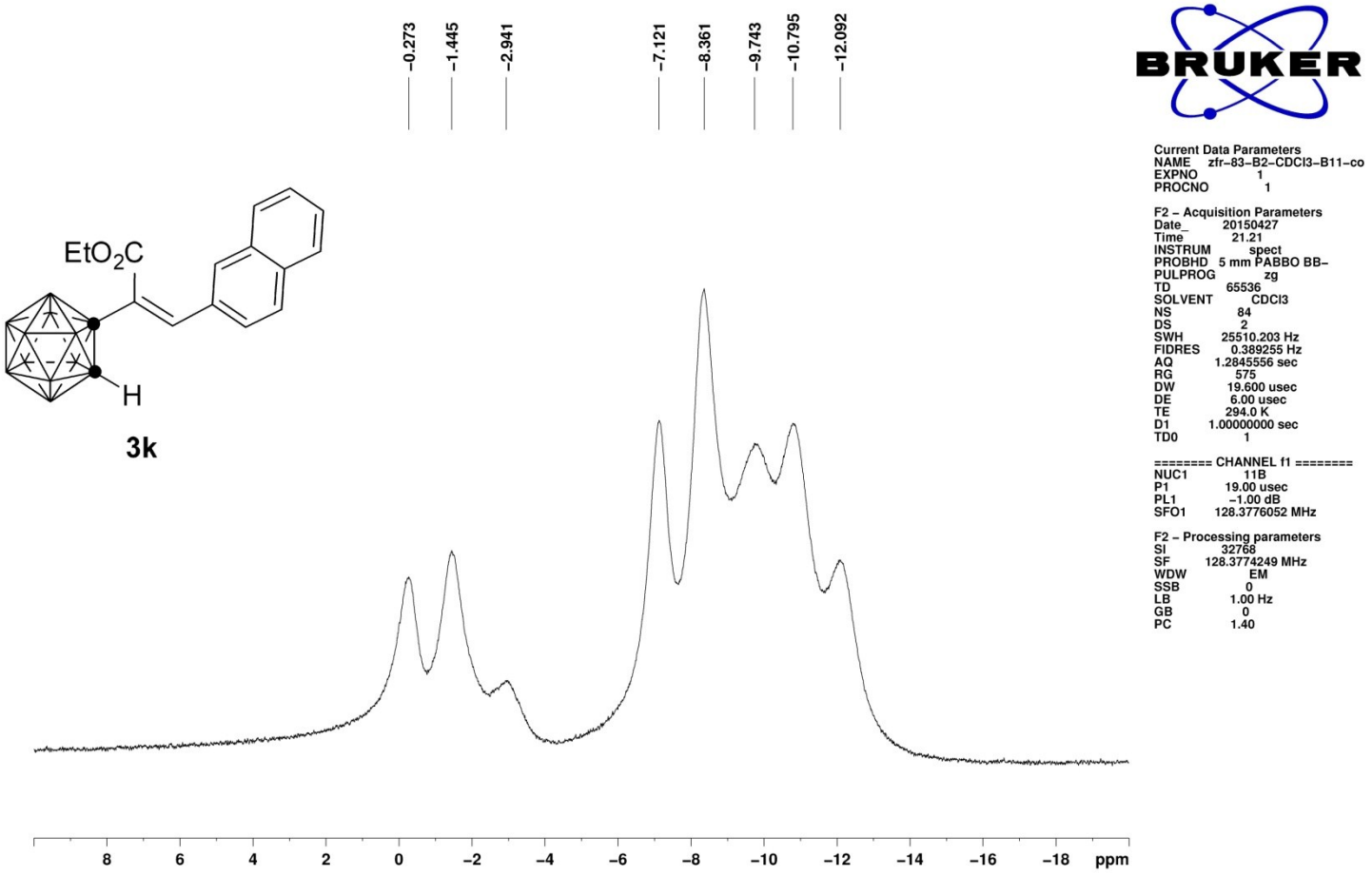
F2 − Acquisition Parameters
Date 20150427
Time 21.16
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

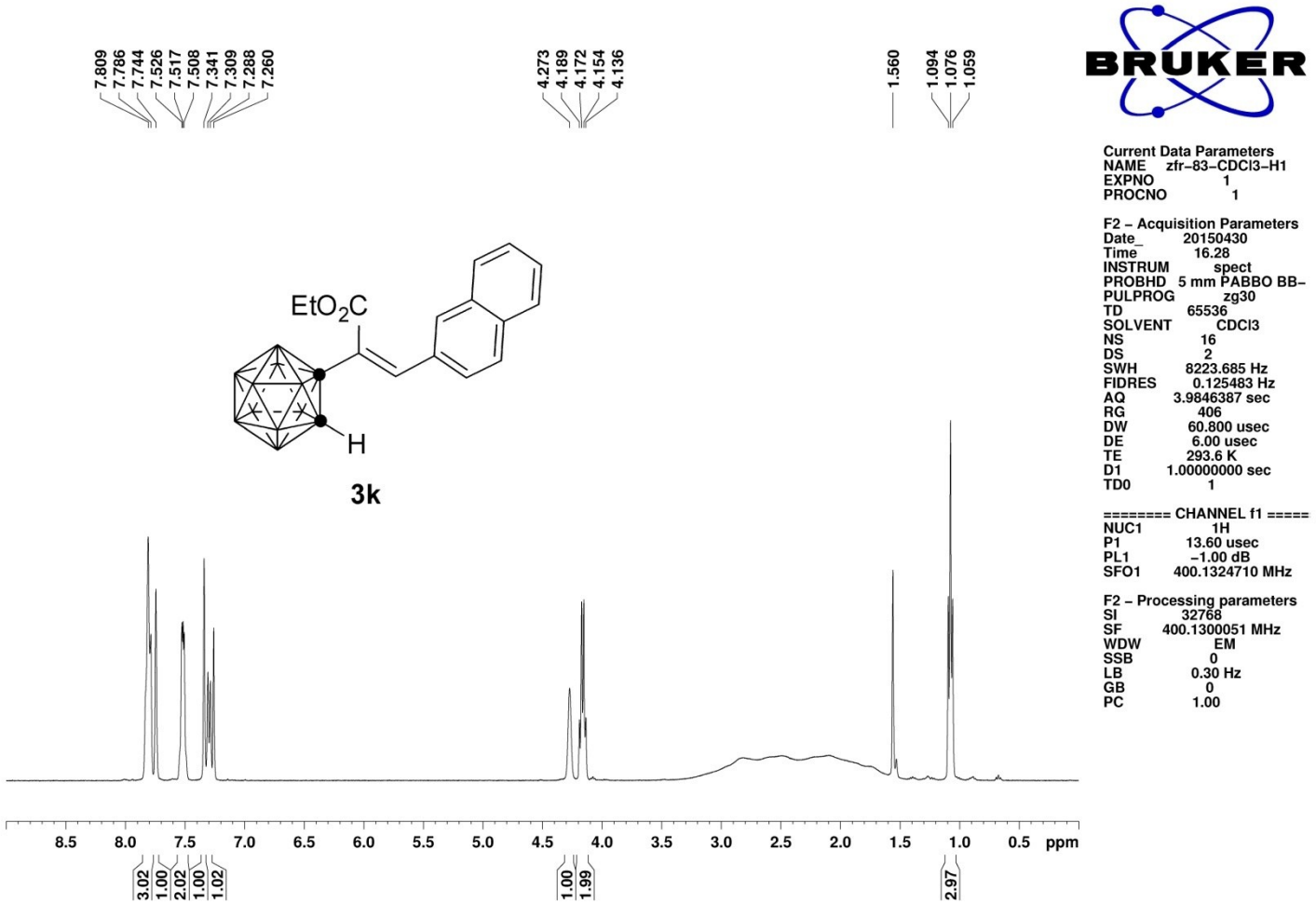
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.273
−1.445
−2.941
−7.121
−8.361
−9.743
−10.795
−12.092
EtO2C
H
3k
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
NAME zfr−83−B2−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150427
Time 21.21
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 84
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



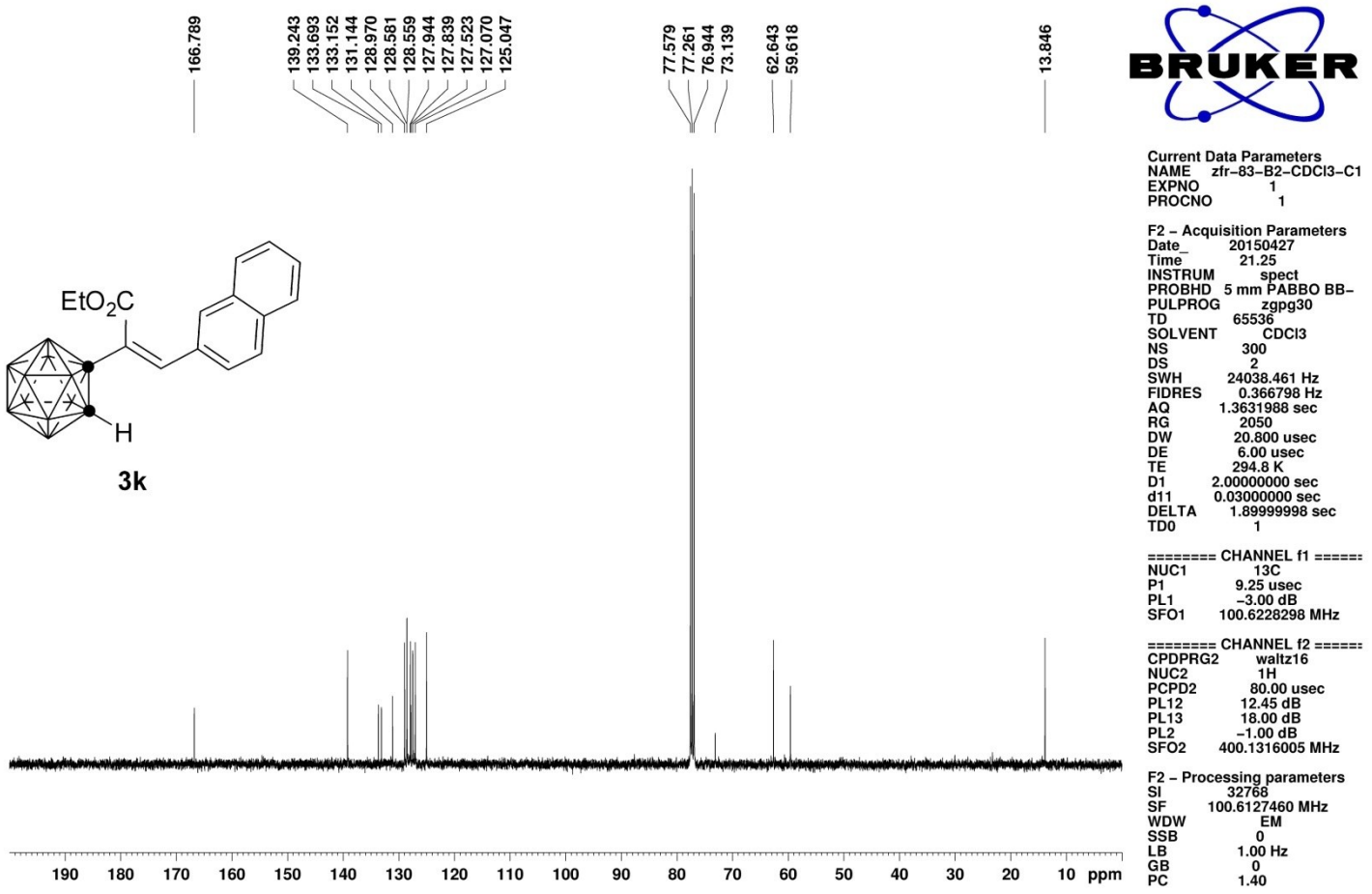
BRUKER

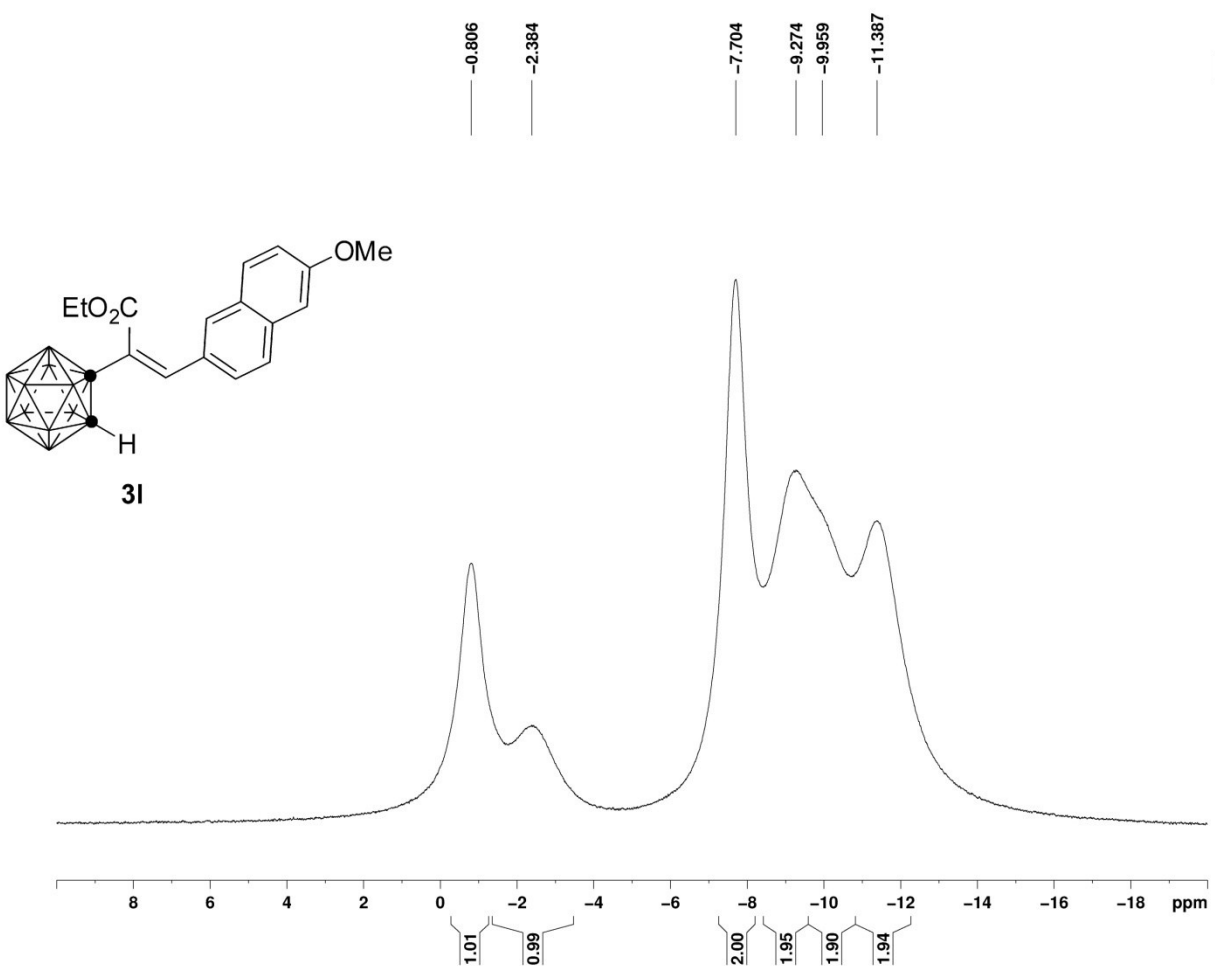
Current Data Parameters
NAME zfr-83-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150430
Time 16.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.789
139.243
133.693
133.152
131.144
128.970
128.581
128.559
127.944
127.839
127.523
127.070
125.047
77.579
77.261
76.944
73.139
62.643
59.618
13.846
EtO2C
H
3k
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-83-B2-CDCl3-C1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150427
Time 21.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 300
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127460 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−140−CDCl3−B11
EXPNO 2
PROCNO 1

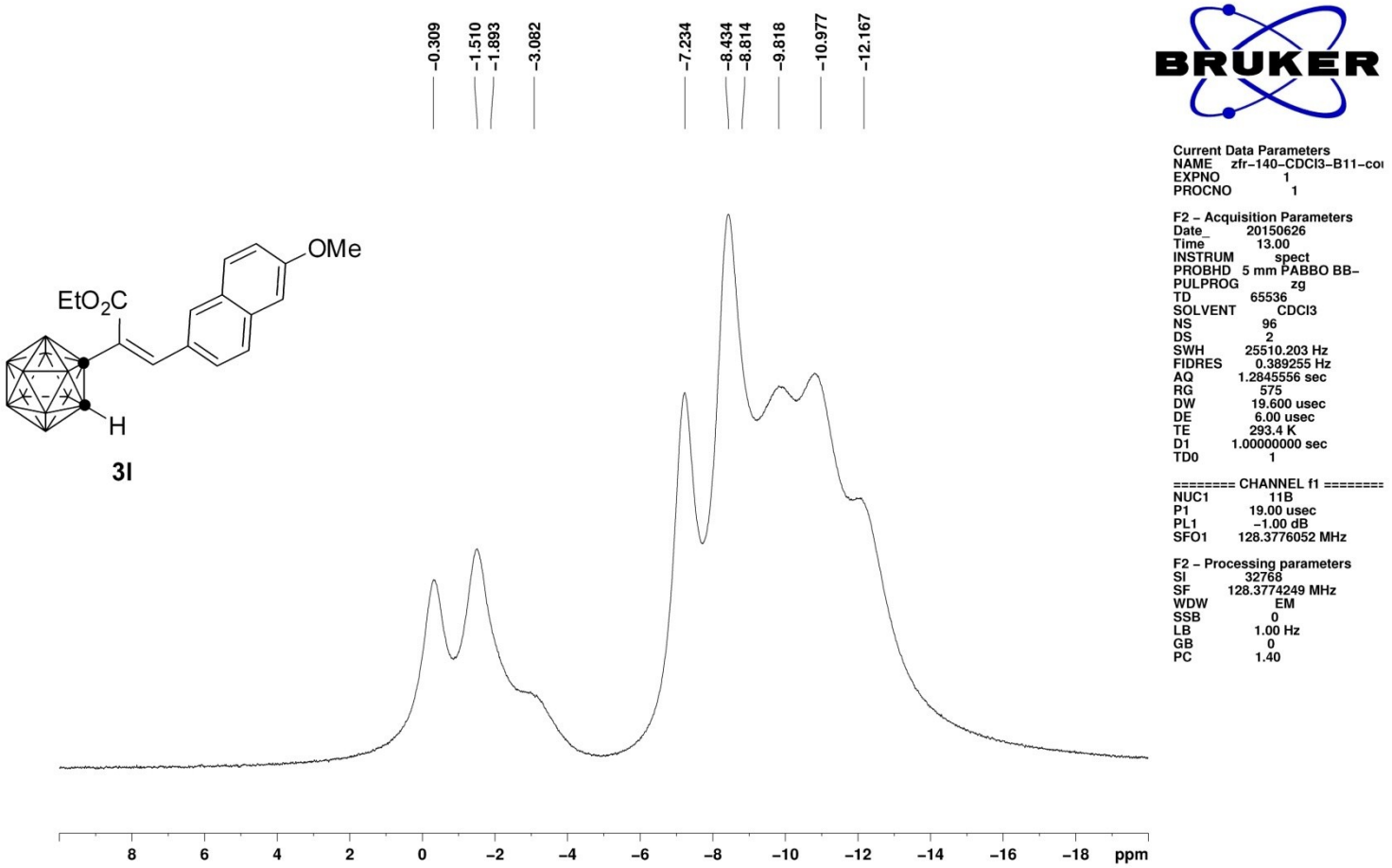
F2 − Acquisition Parameters
Date_ 20150626
Time 12.55
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

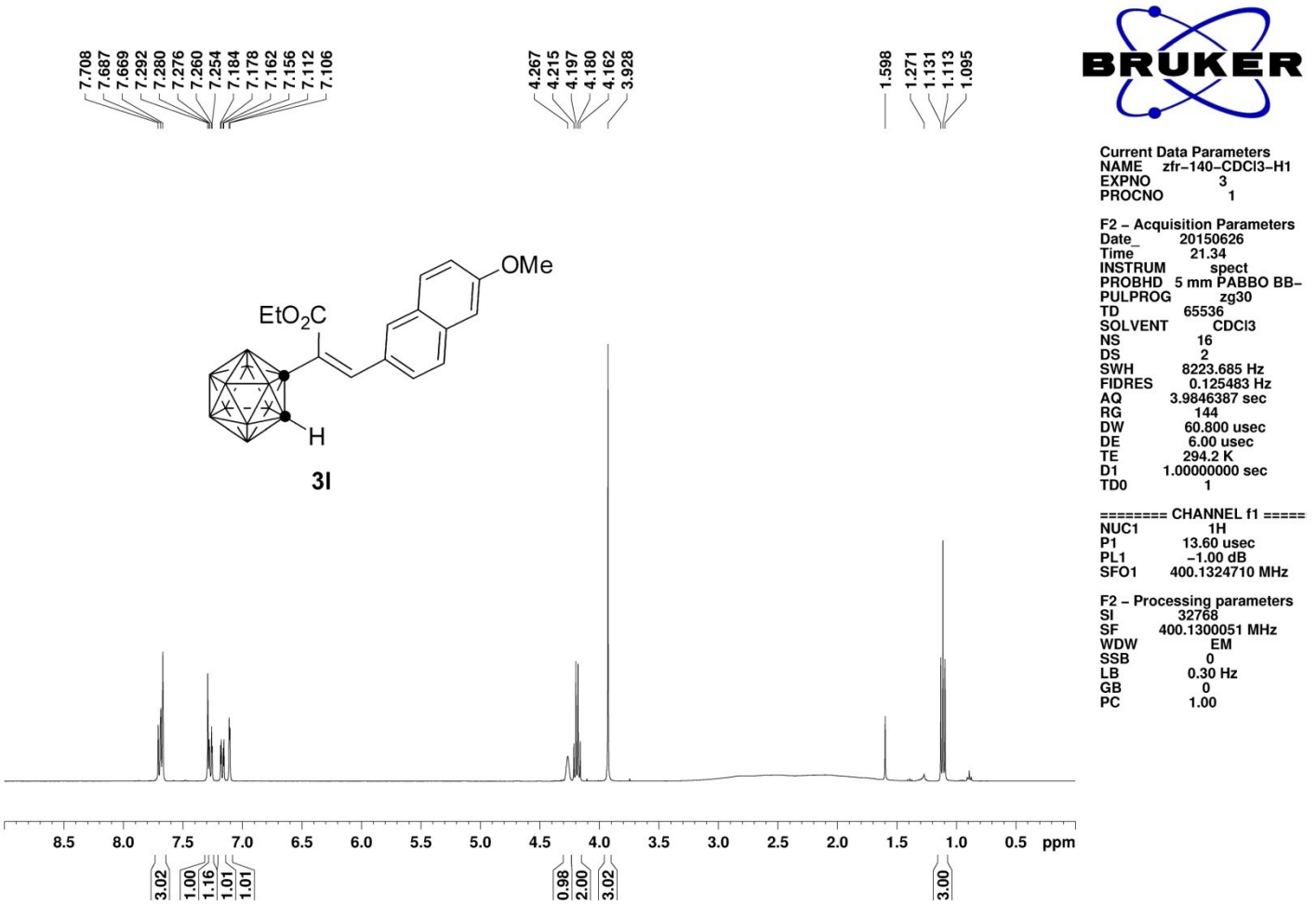
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-0.309
-1.510
-1.893
-3.082
-7.234
-8.434
-8.814
-9.818
-10.977
-12.167
OMe
EtO2C
H
3l
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
ppm
BRUKER
Current Data Parameters
NAME zfr-140-CDCl3-B11-co
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150626
Time 13.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

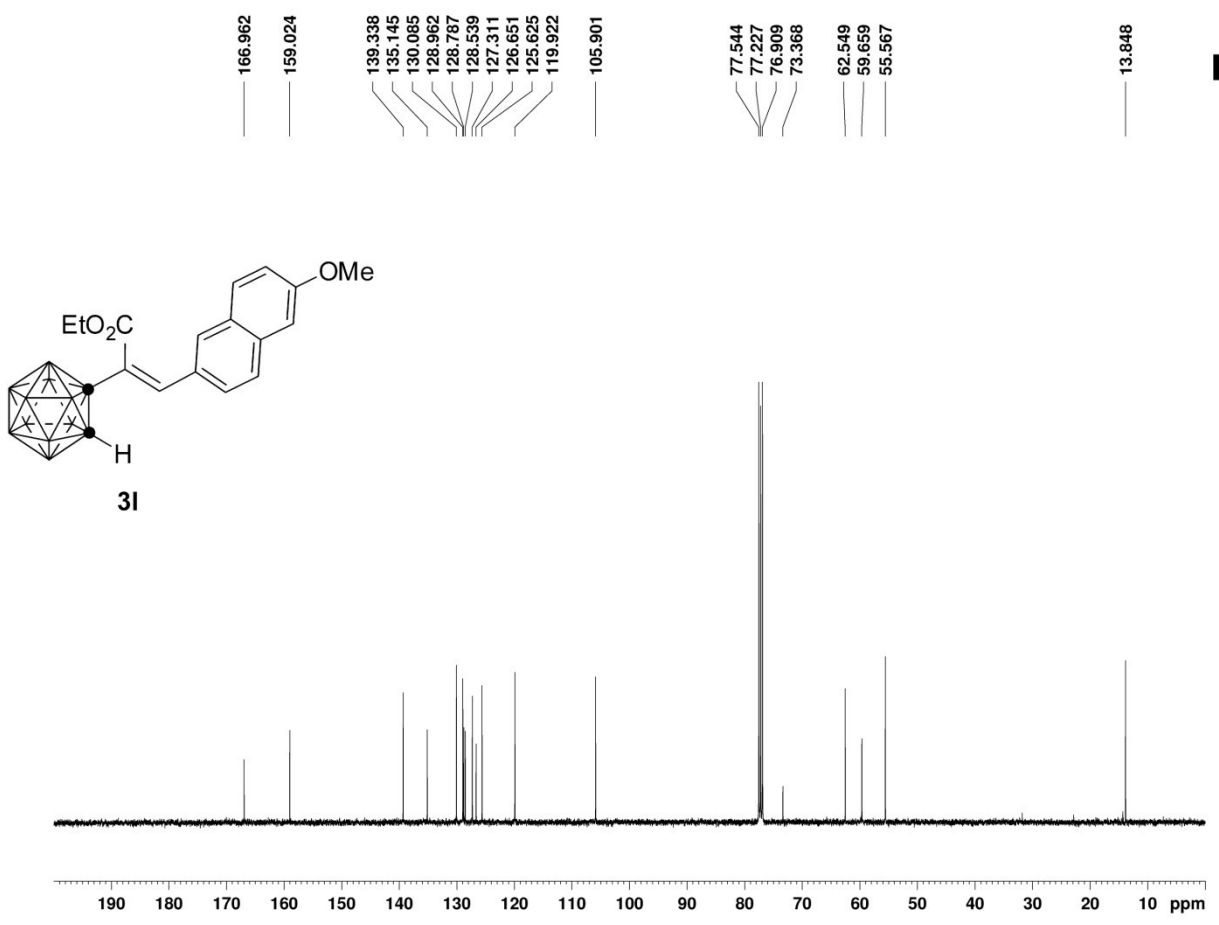


Current Data Parameters
NAME zfr-140-CDCl3-H1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150626
Time 21.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

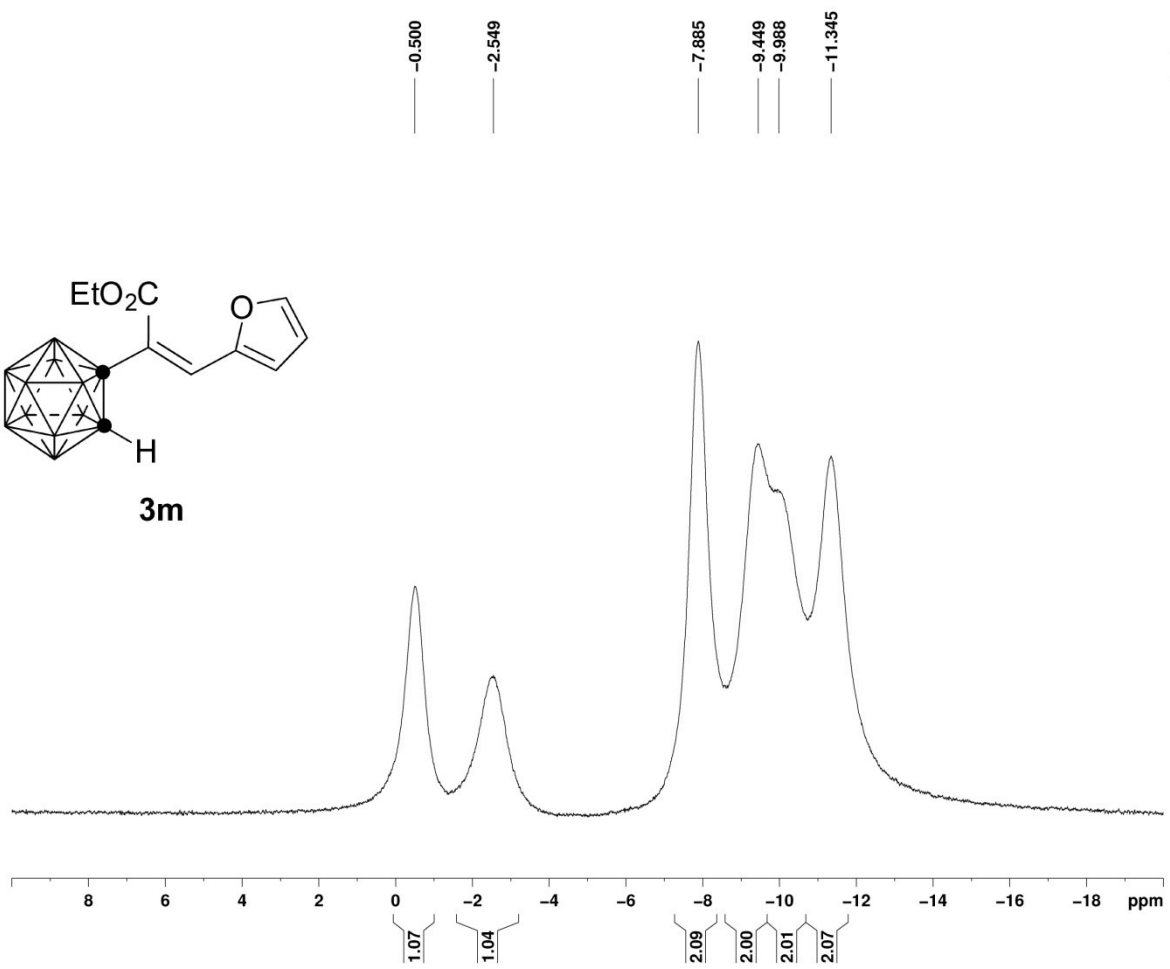
Current Data Parameters
NAME zfr-140-CDCl3-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150626
Time 21.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 463
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127504 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−136−CDCl3−B11
EXPNO 1
PROCNO 1

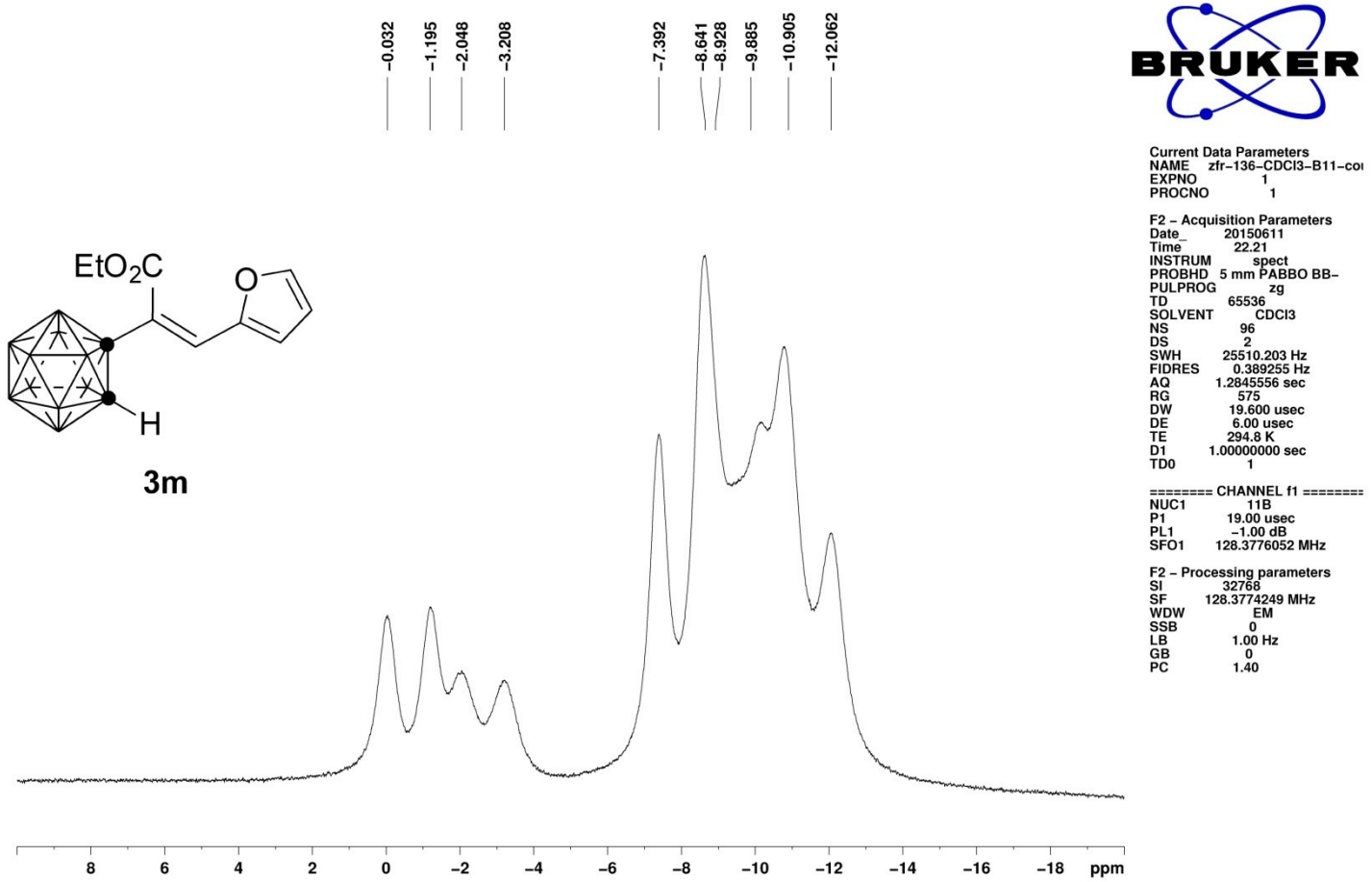
F2 − Acquisition Parameters
Date_ 20150611
Time 22.19
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



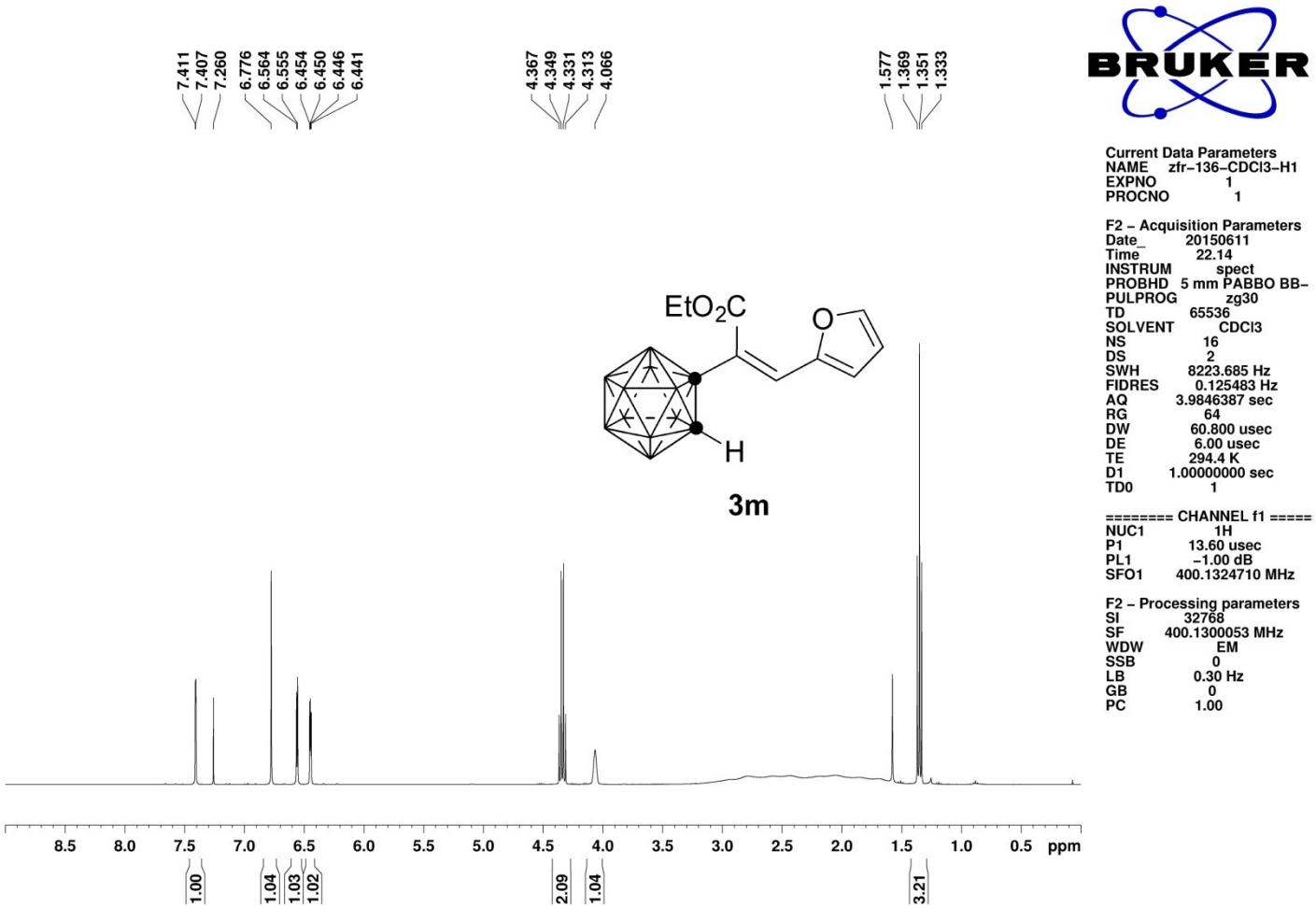
BRUKER

Current Data Parameters
NAME zfr−136−CDCl3−B11−co
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20150611
Time 22.21
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 96
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

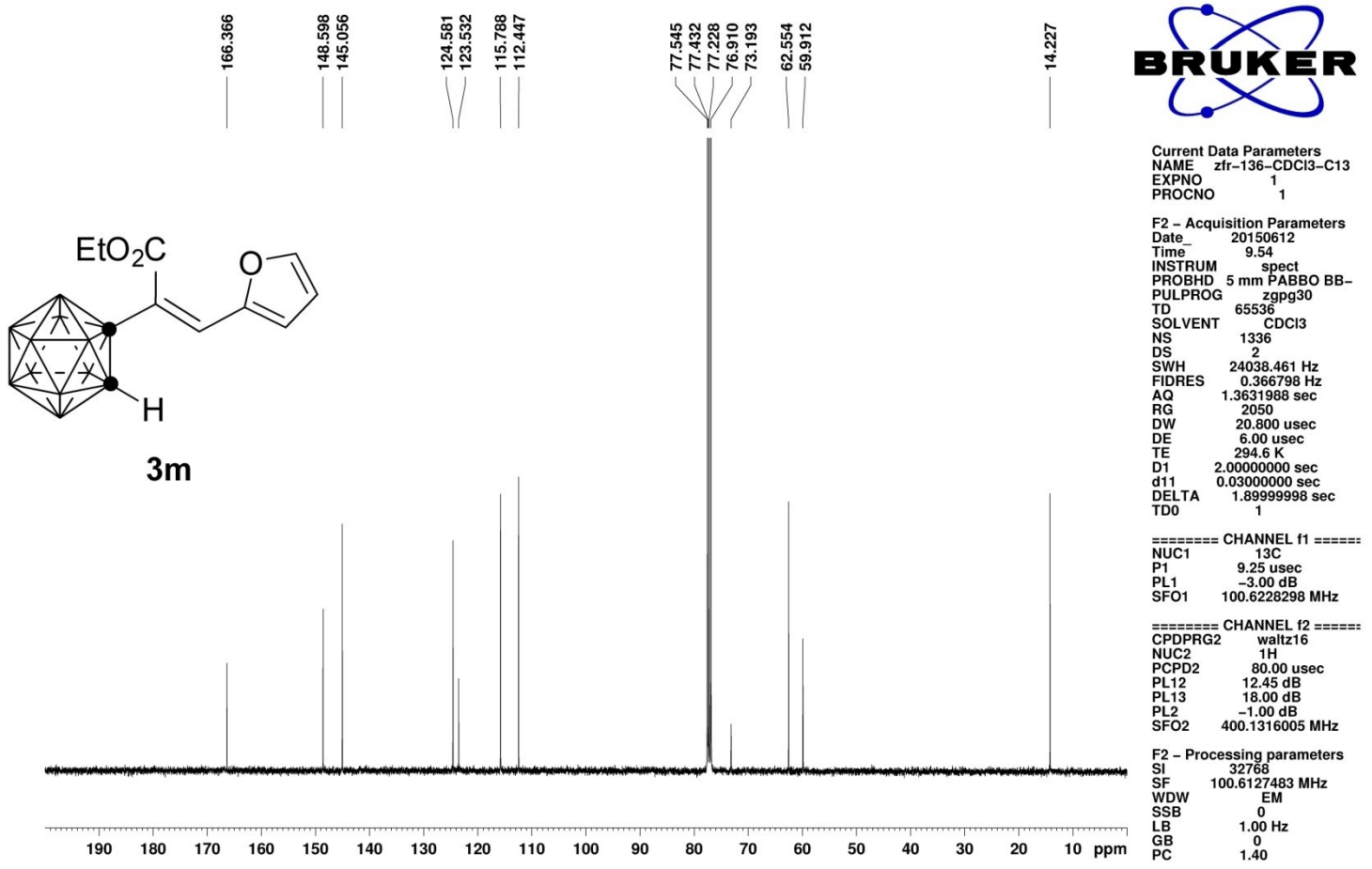


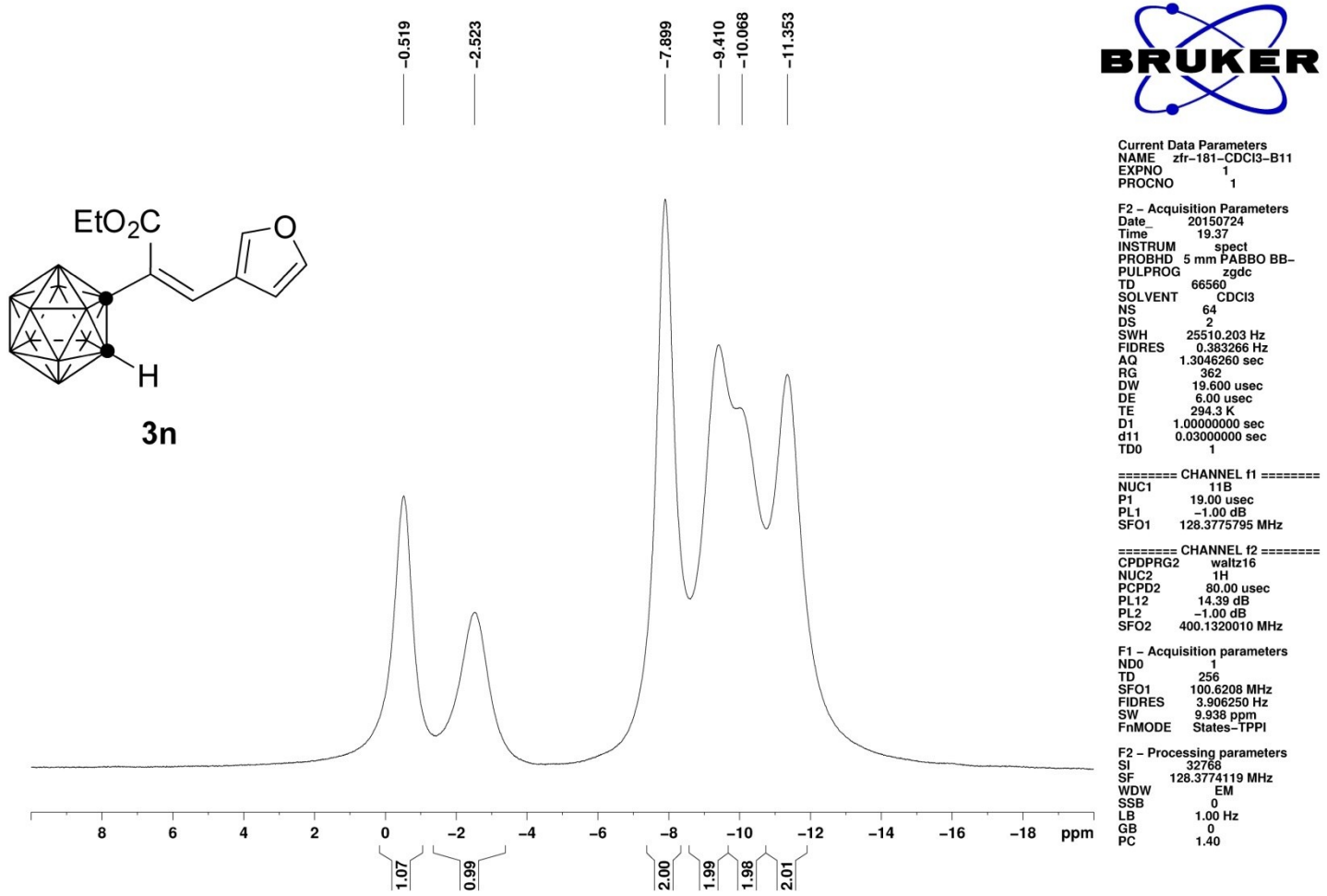
Current Data Parameters
NAME zfr-136-CDCl3-H1
EXPNO 1
PROCNO 1

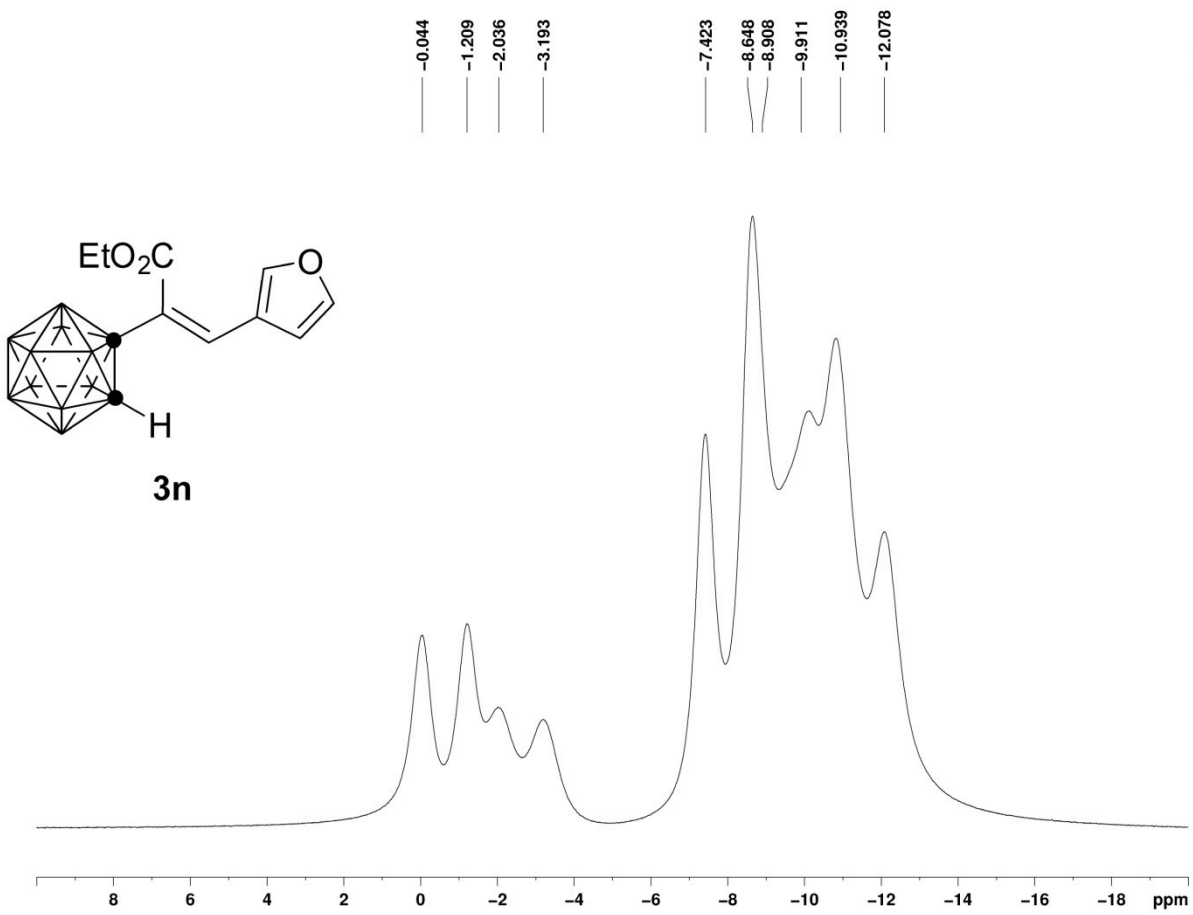
F2 - Acquisition Parameters
Date_ 20150611
Time 22.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.366
148.598
145.056
124.581
123.532
115.788
112.447
77.545
77.432
77.228
76.910
73.193
62.554
59.912
14.227
EtO2C
O
H
3m
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-136-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150612
Time 9.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1336
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127483 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.519
−2.523
−7.899
−9.410
−10.068
−11.353
EtO2C
O
H
3n
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.07
0.99
2.00
1.99
1.98
2.01
BRUKER
Current Data Parameters
NAME zfr−181−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150724
Time 19.37
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 362
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



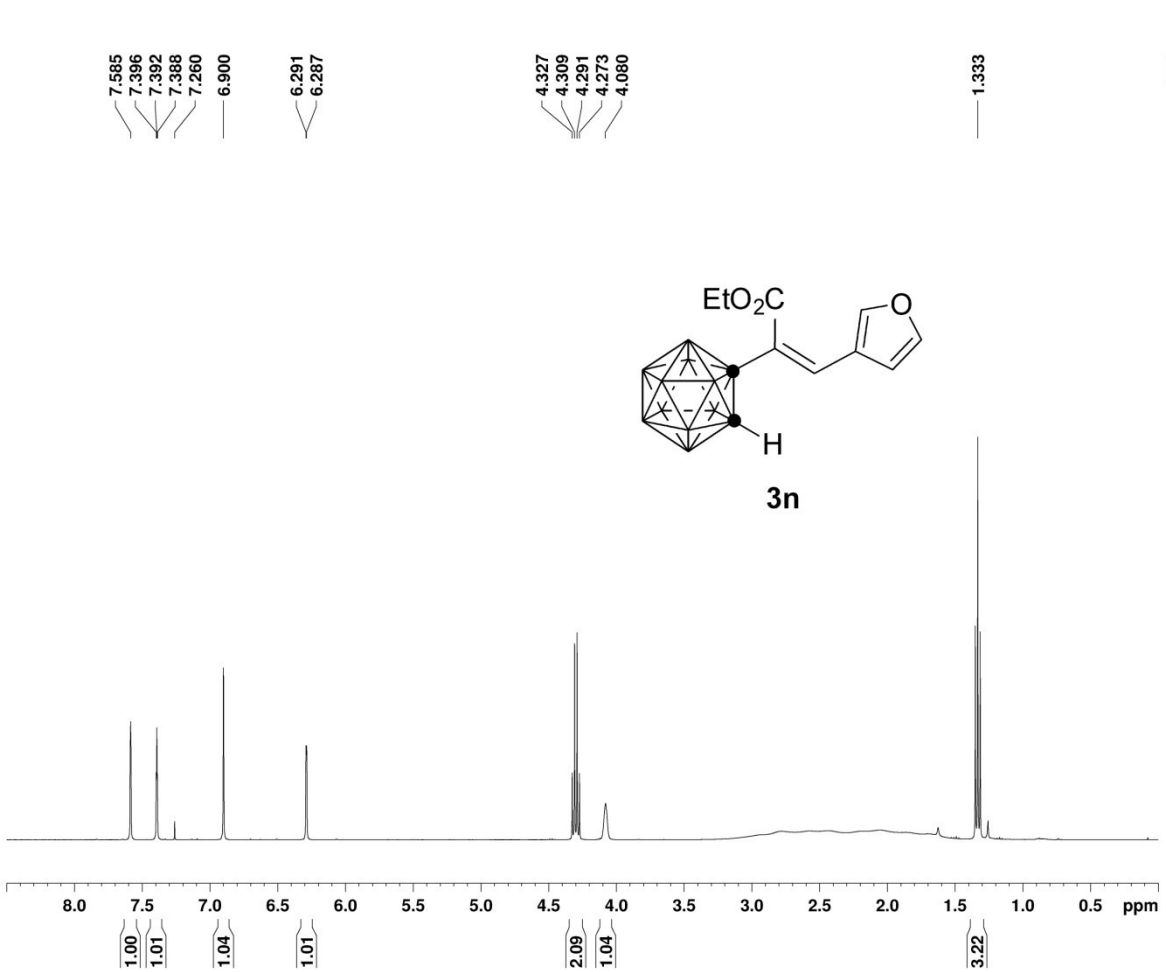
BRUKER

Current Data Parameters
NAME zfr−181−CDCl3−B11−co
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20150724
Time 19.44
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 164
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 362
DW 19.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

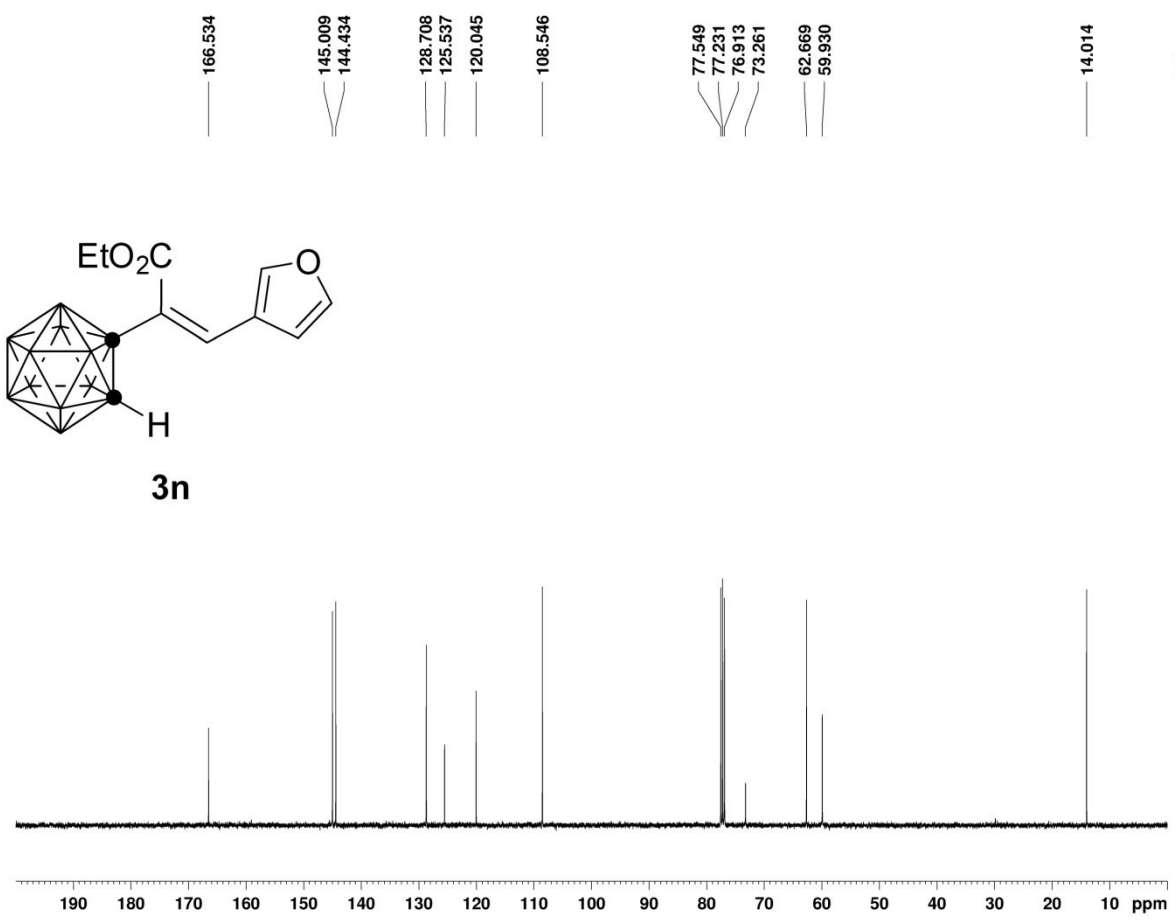


Current Data Parameters
NAME zfr-181-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150724
Time 19.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

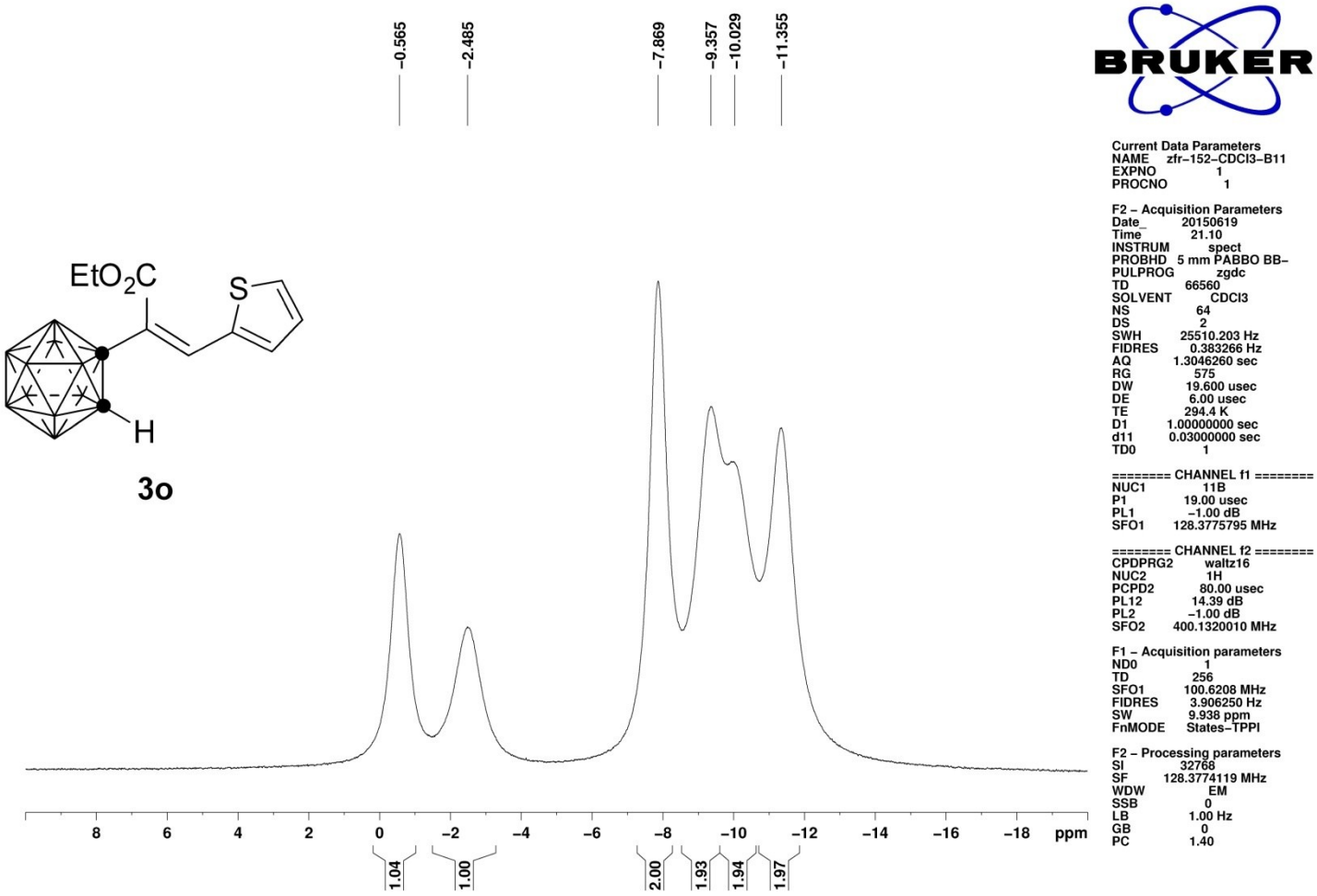
Current Data Parameters
NAME zfr-181-CDCl3-C13
EXPNO 1
PROCNO 1

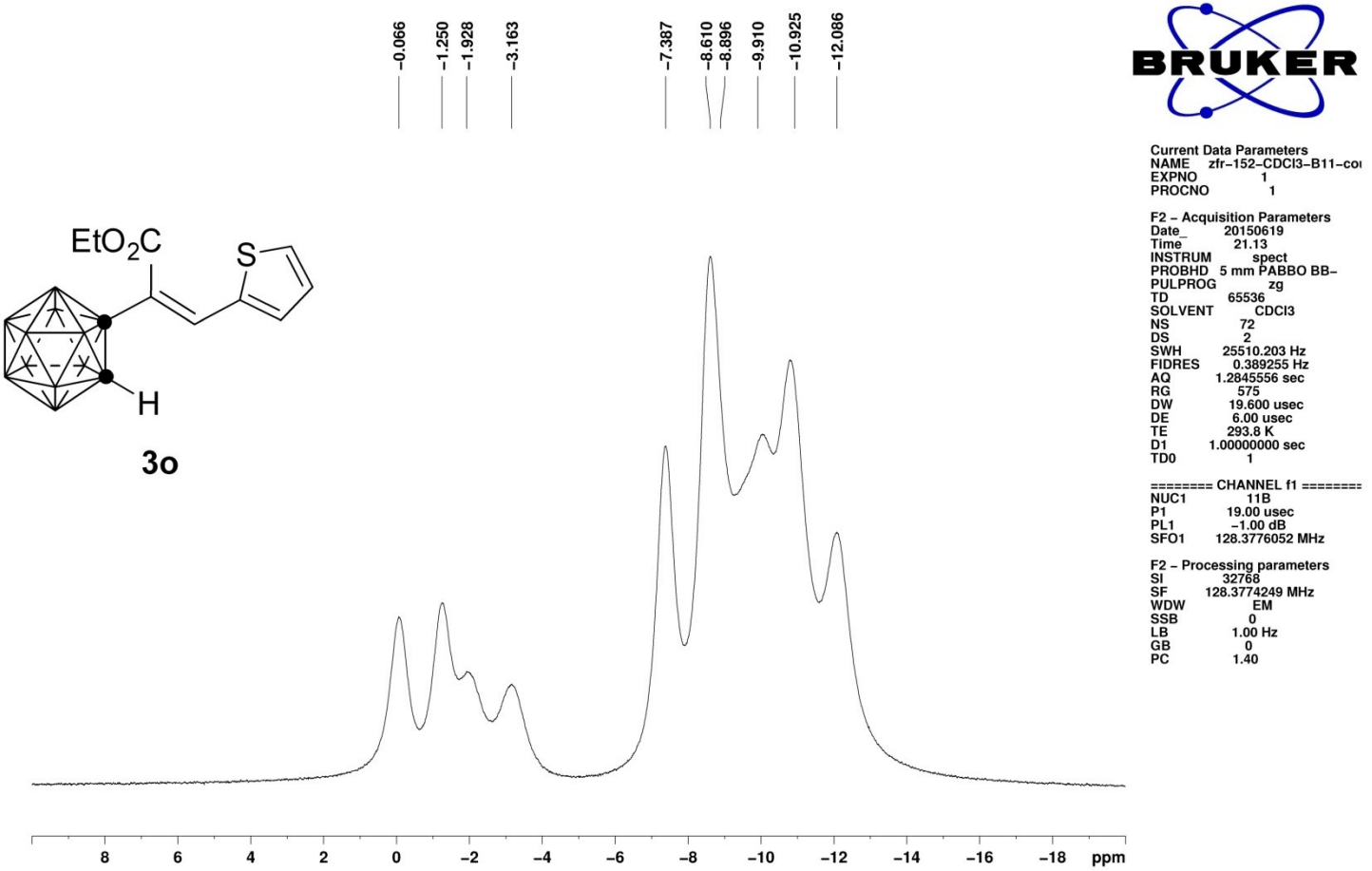
F2 - Acquisition Parameters
Date_ 20150724
Time 19.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

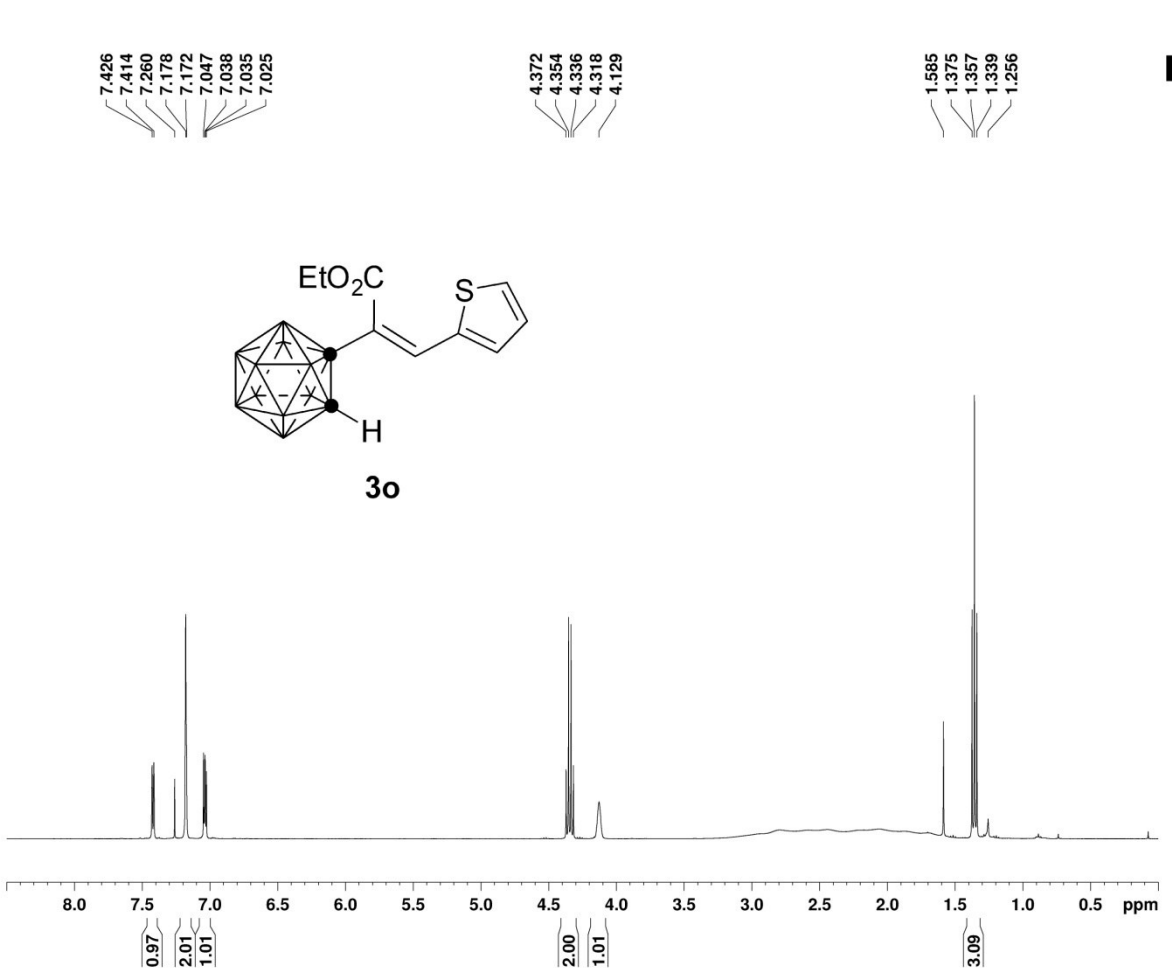
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127520 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.565
−2.485
−7.869
−9.357
−10.029
−11.355
EtO2C
S
H
3o
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.04
1.00
2.00
1.93
1.94
1.97
BRUKER
Current Data Parameters
NAME zfr−152−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150619
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.066
−1.250
−1.928
−3.163
−7.387
−8.610
−8.896
−9.910
−10.925
−12.086
EtO2C
S
H
3o
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
Current Data Parameters
NAME zfr−152−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150619
Time 21.13
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 72
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



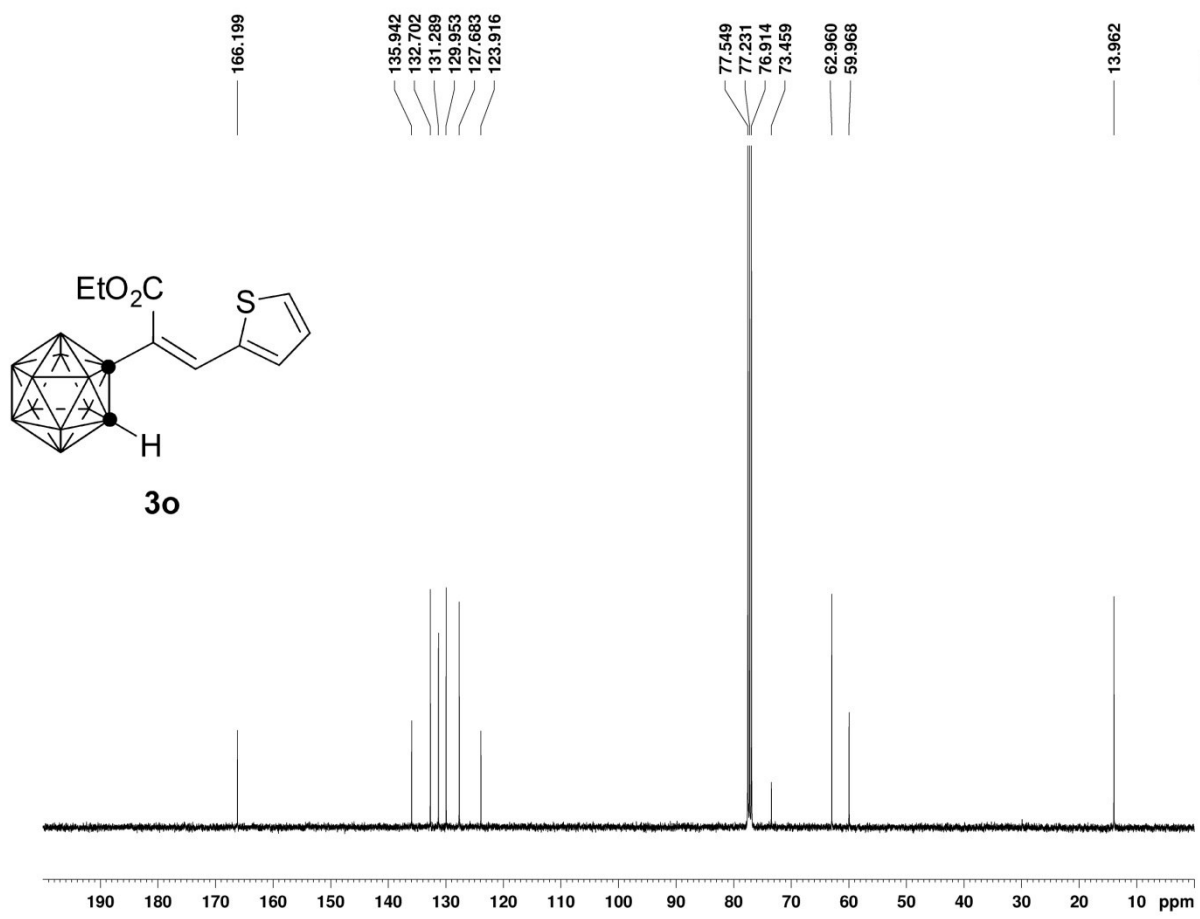
BRUKER

Current Data Parameters
NAME zfr-152-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150619
Time 21.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

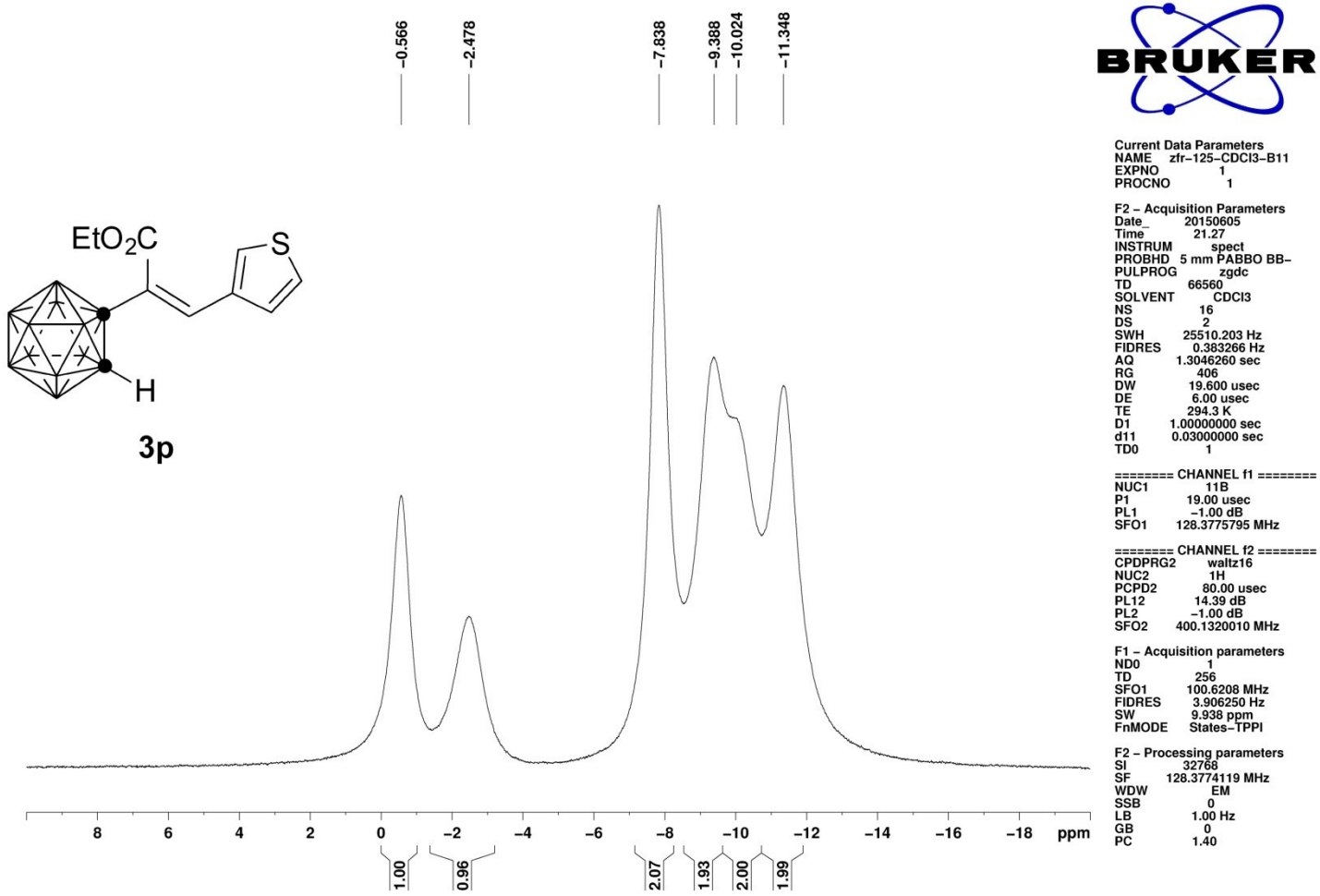
Current Data Parameters
NAME zfr-152-CDCl3-C13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150619
Time 21.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 800
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127490 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−125−CDCl3−B11
EXPNO 1
PROCNO 1

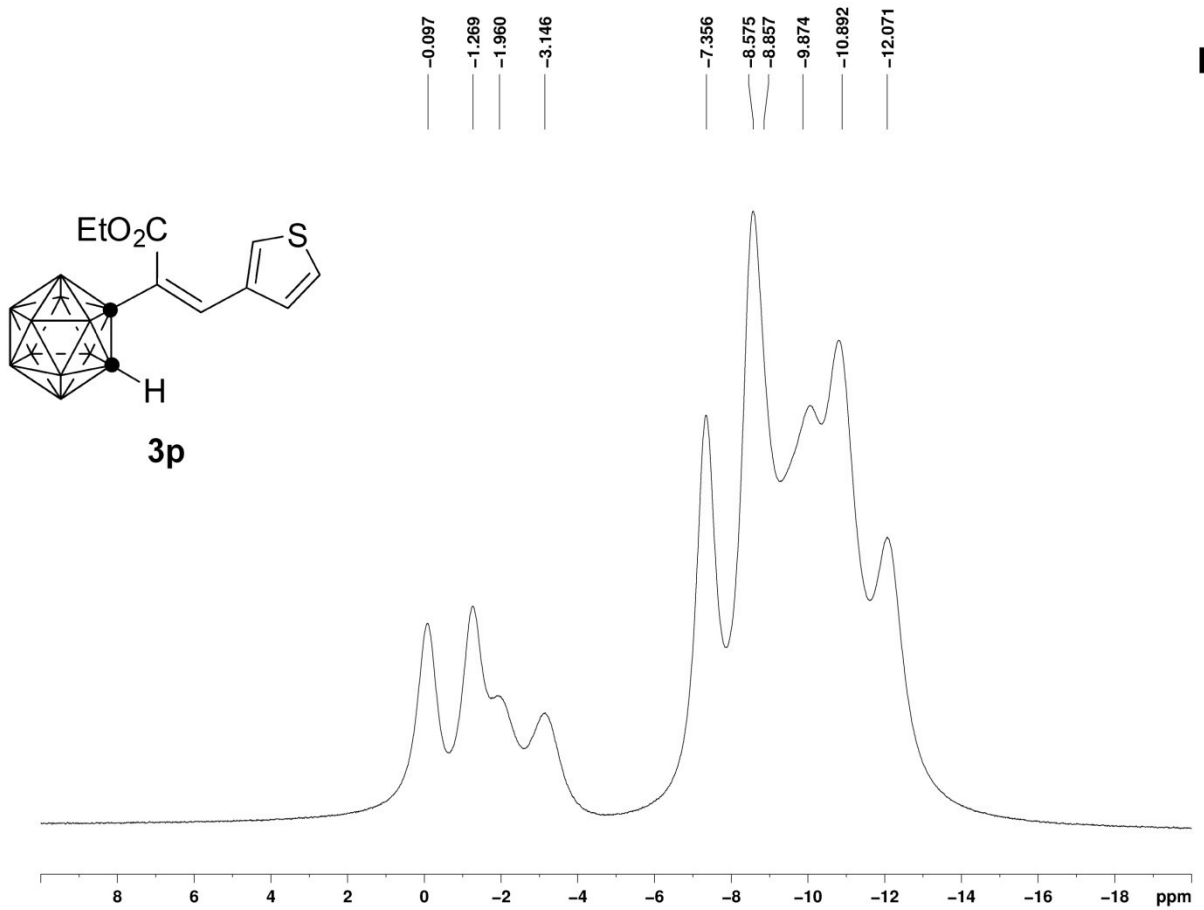
F2 − Acquisition Parameters
Date_ 20150605
Time 21.27
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 16
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 406
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



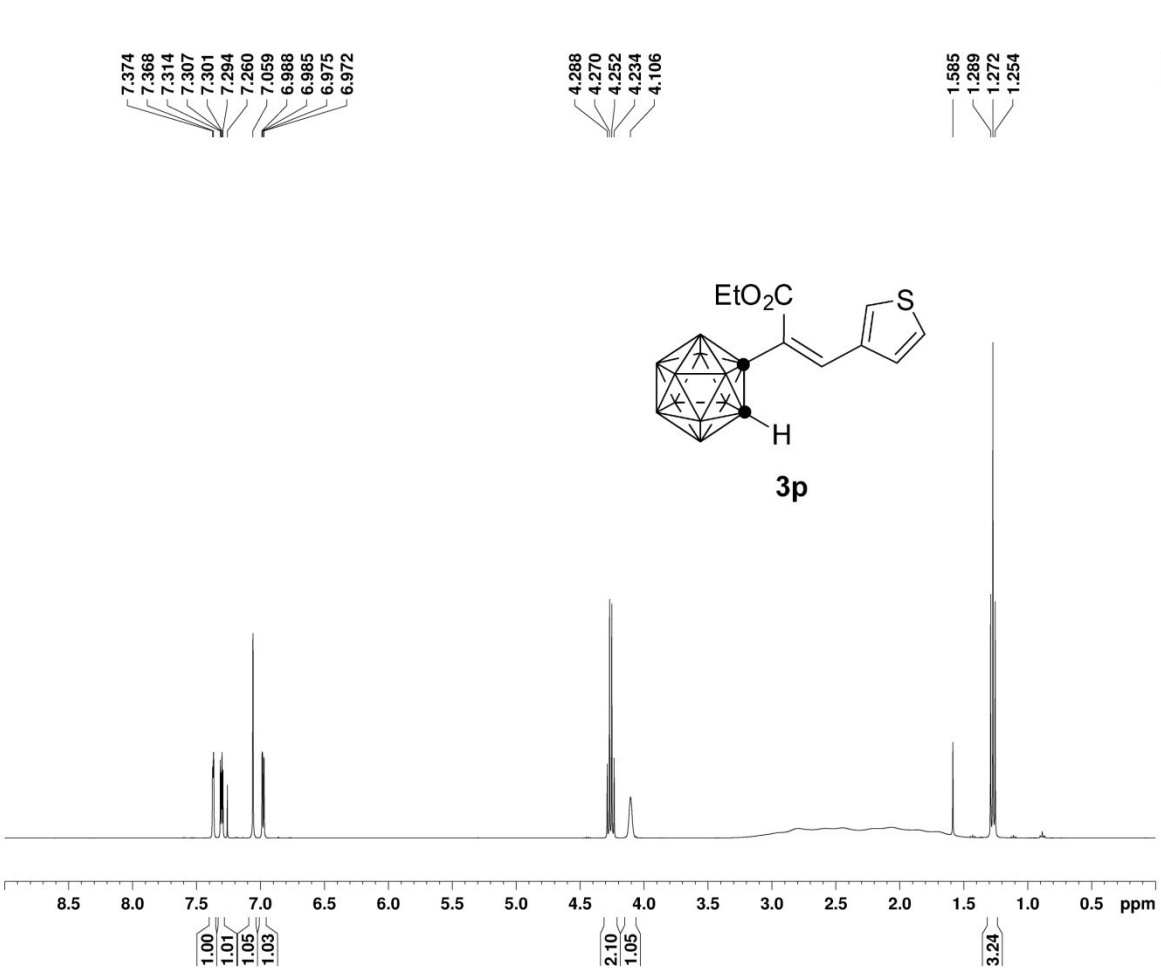
BRUKER

Current Data Parameters
NAME zfr−125−CDCl3−B11−co
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20150605
Time 21.30
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 65
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 362
DW 19.600 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

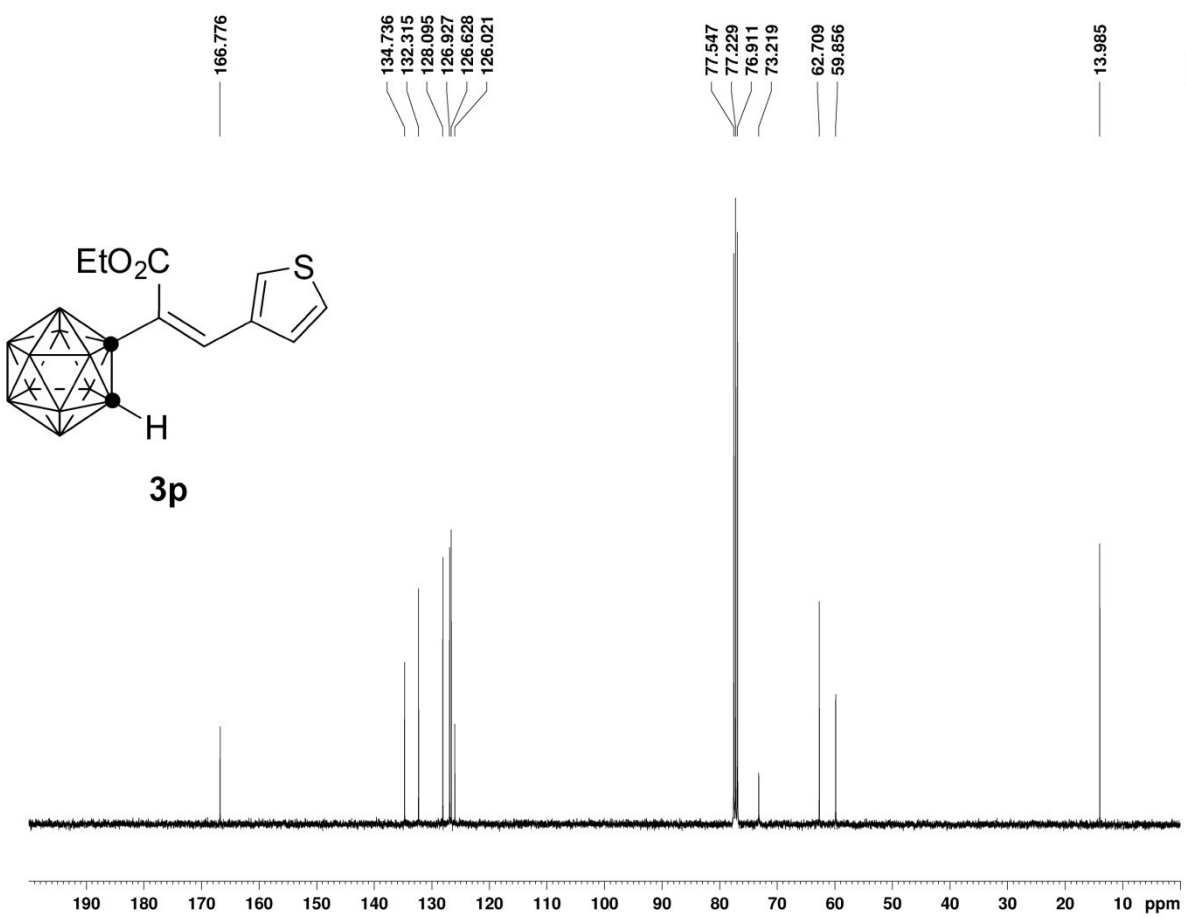


Current Data Parameters
NAME zfr-125-CDCl3-H1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150608
Time 18.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

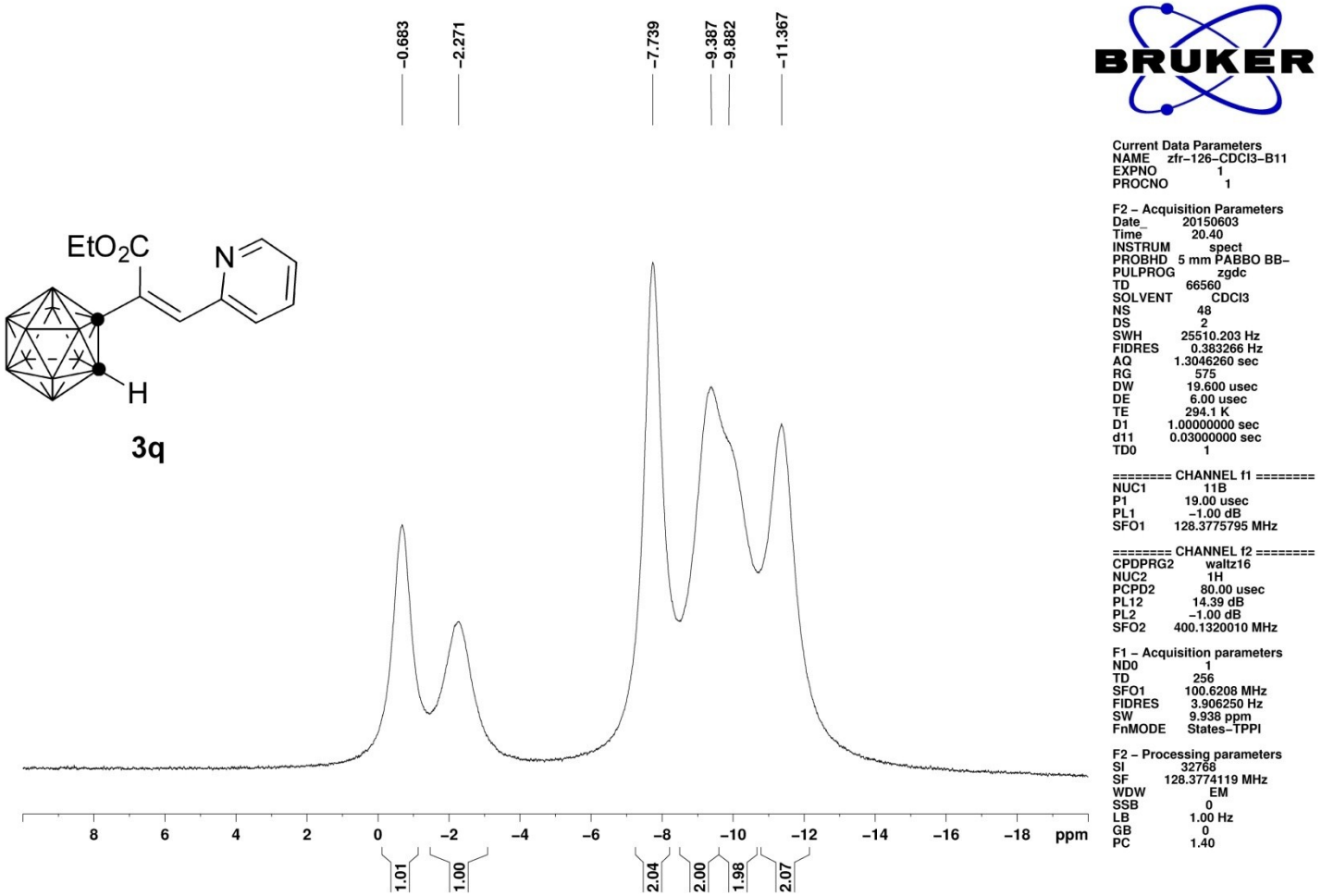
Current Data Parameters
NAME zfr-125-CDCl3-C13
EXPNO 2
PROCNO 1

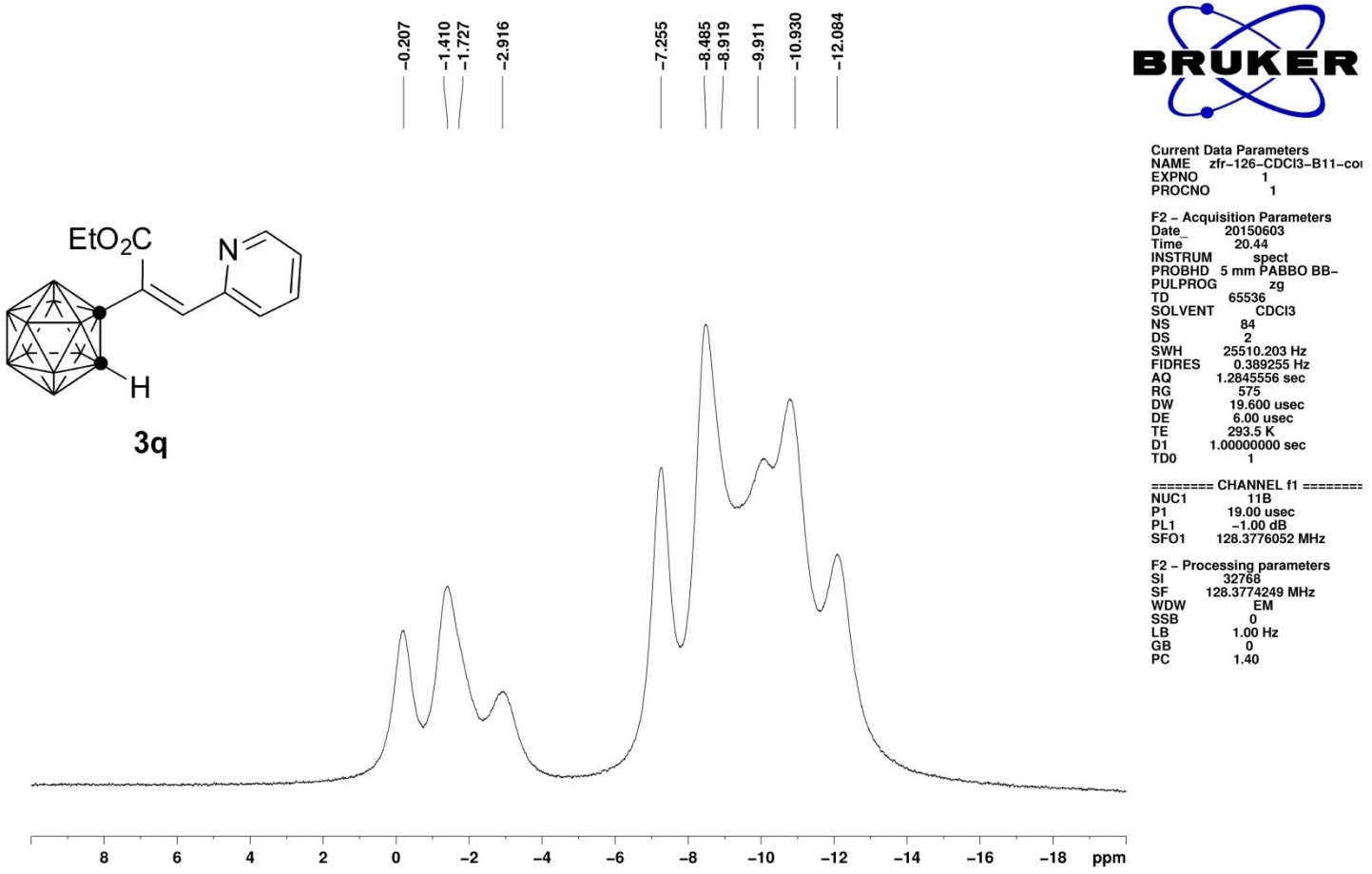
F2 - Acquisition Parameters
Date_ 20150608
Time 18.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127498 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.683
−2.271
−7.739
−9.387
−9.882
−11.367
EtO2C
N
H
3q
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.01
1.00
2.04
2.00
1.98
2.07
BRUKER
Current Data Parameters
NAME zfr−126−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150603
Time 20.40
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 48
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



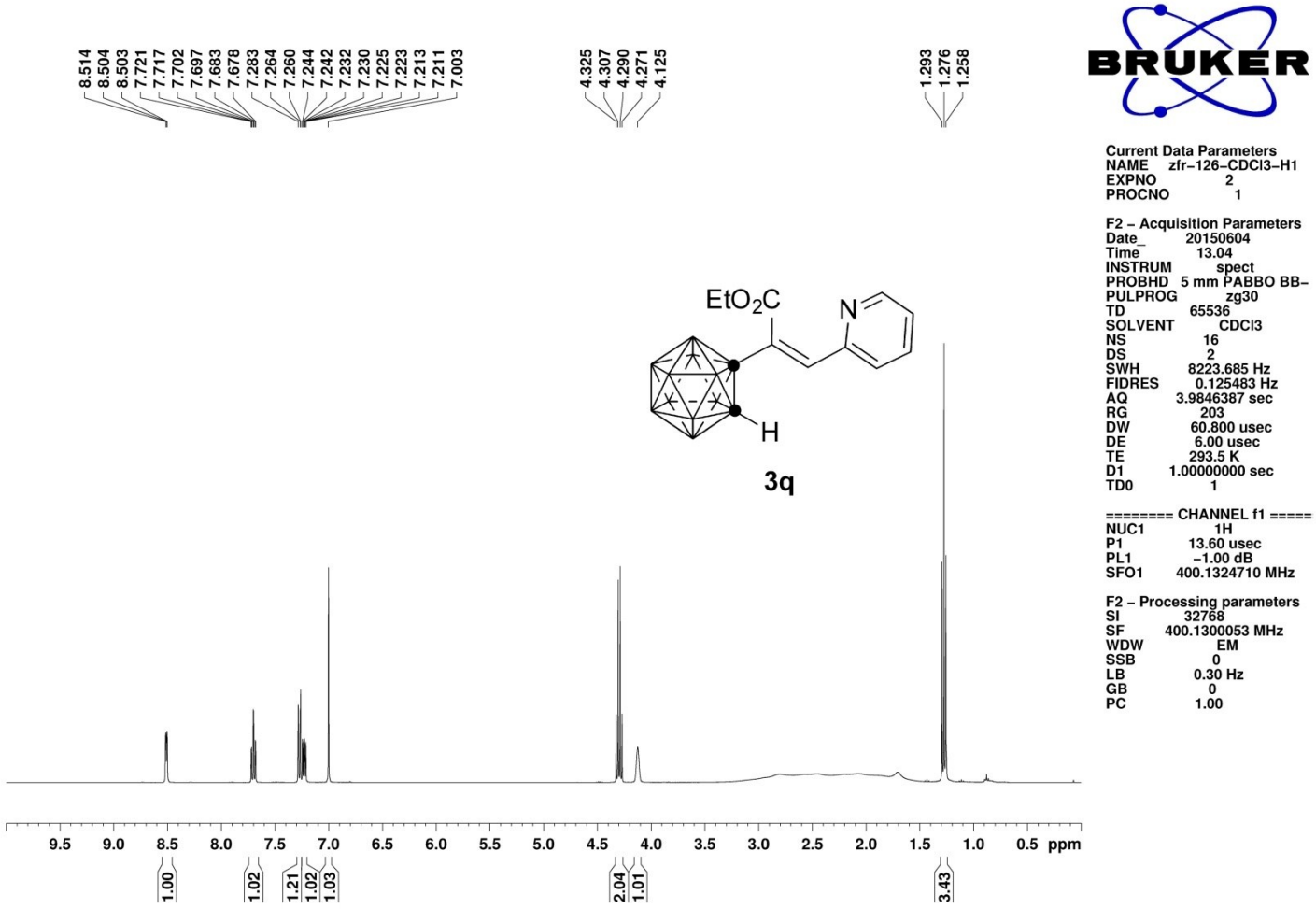
BRUKER

Current Data Parameters
NAME zfr−126−CDCl3−B11−co
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20150603
Time_ 20.44
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 84
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

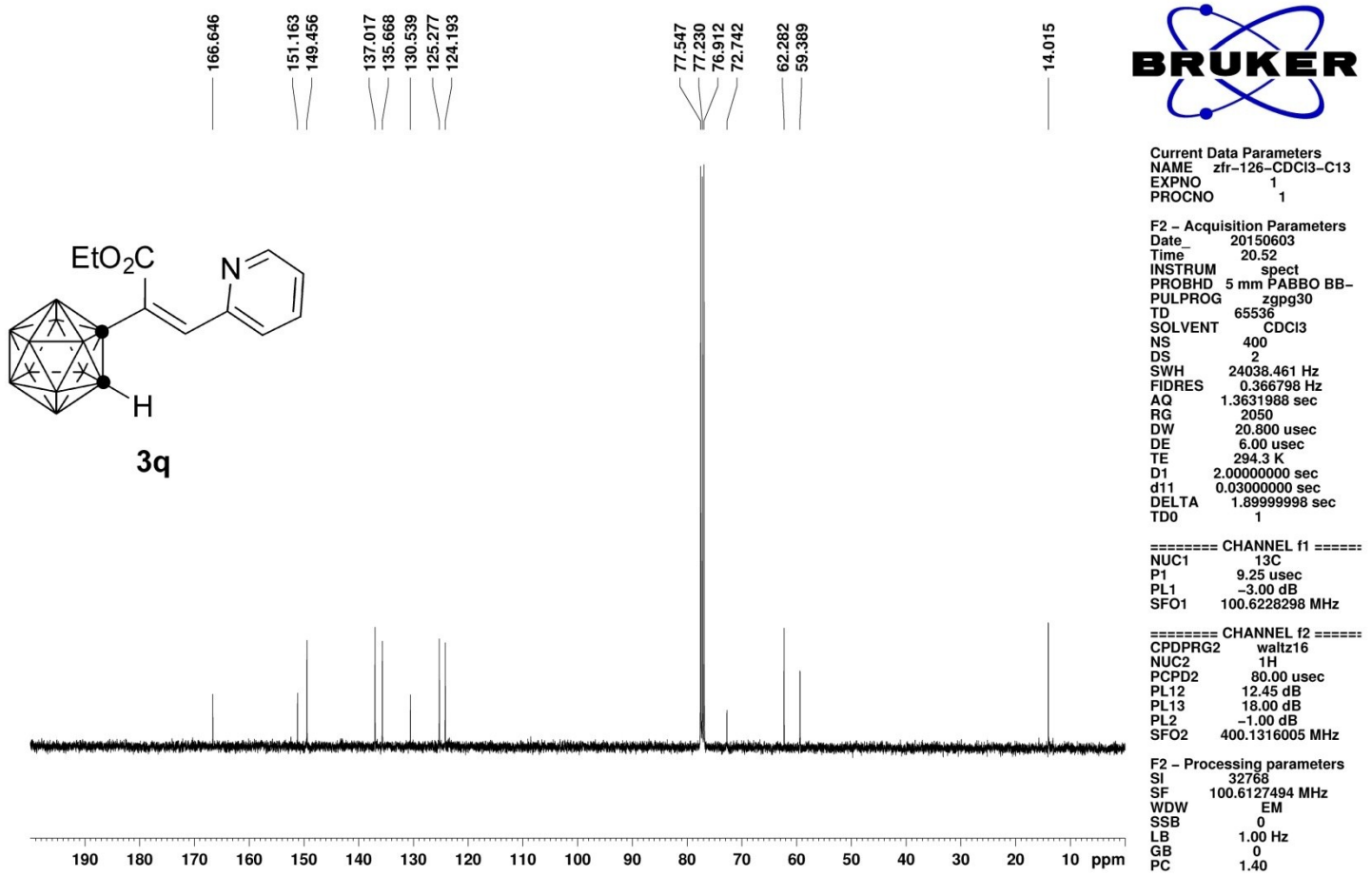


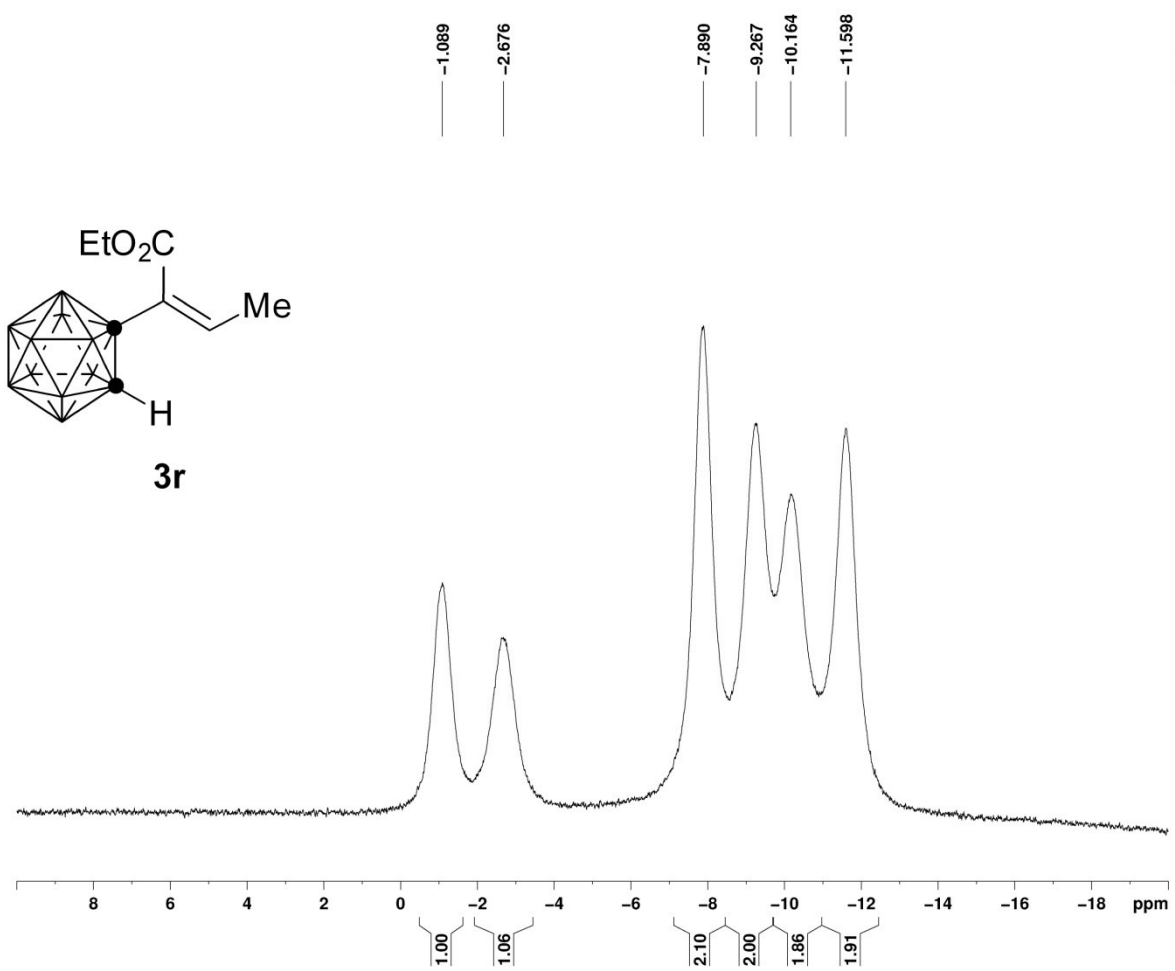
Current Data Parameters
NAME zfr-126-CDCl3-H1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150604
Time 13.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


166.646
151.163
149.456
137.017
135.668
130.539
125.277
124.193
77.547
77.230
76.912
72.742
62.282
59.389
14.015
EtO2C
N
H
3q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-126-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150603
Time 20.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127494 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−91−A12−CDCl3−B11
EXPNO 1
PROCNO 1

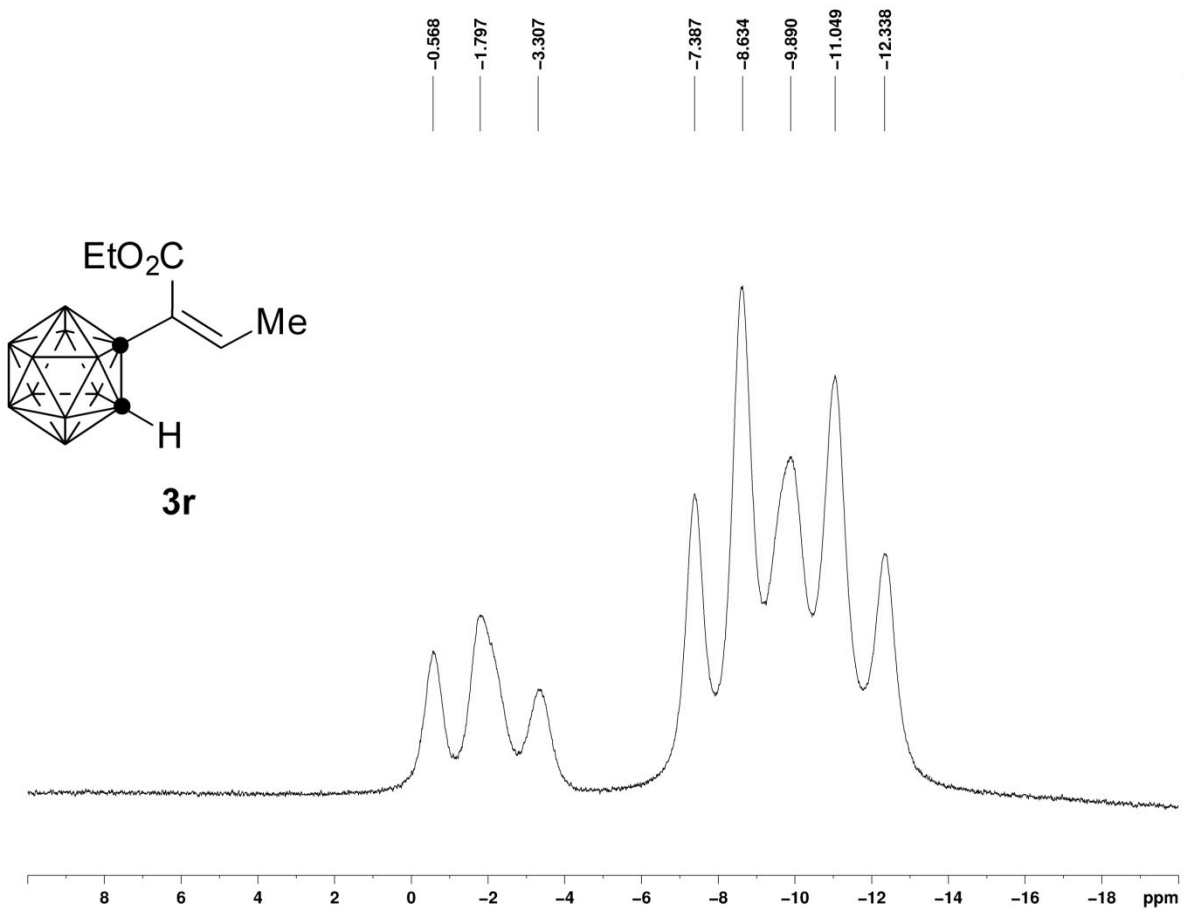
F2 − Acquisition Parameters
Date_ 20150504
Time 21.10
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 72
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 1150
DW 19.600 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

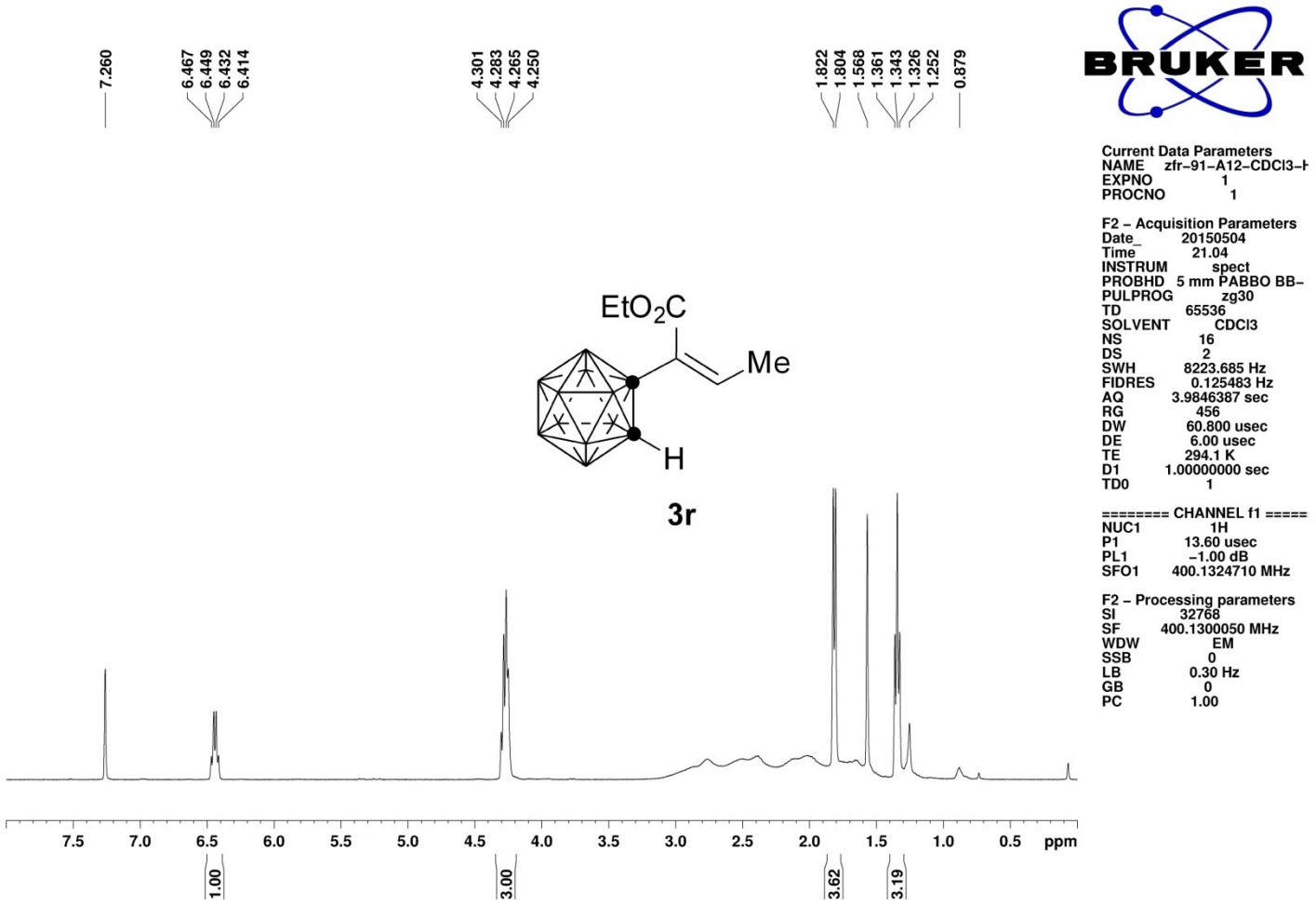


Current Data Parameters
NAME zfr−91−A12−CDCl3−B11−co
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20150504
Time 21.15
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 1150
DW 19.600 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



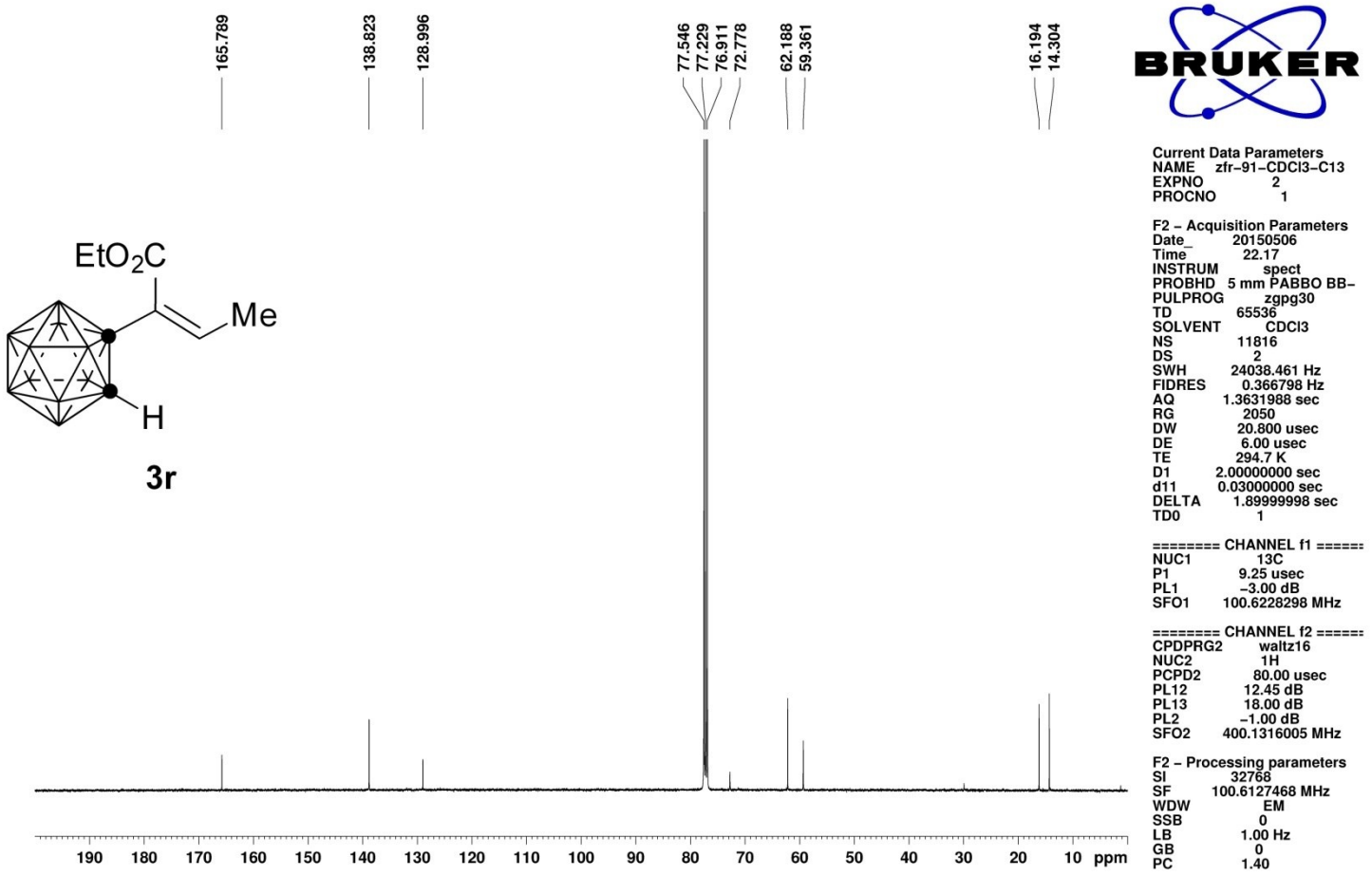
BRUKER

Current Data Parameters
NAME zfr-91-A12-CDCl3-H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150504
Time 21.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300050 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

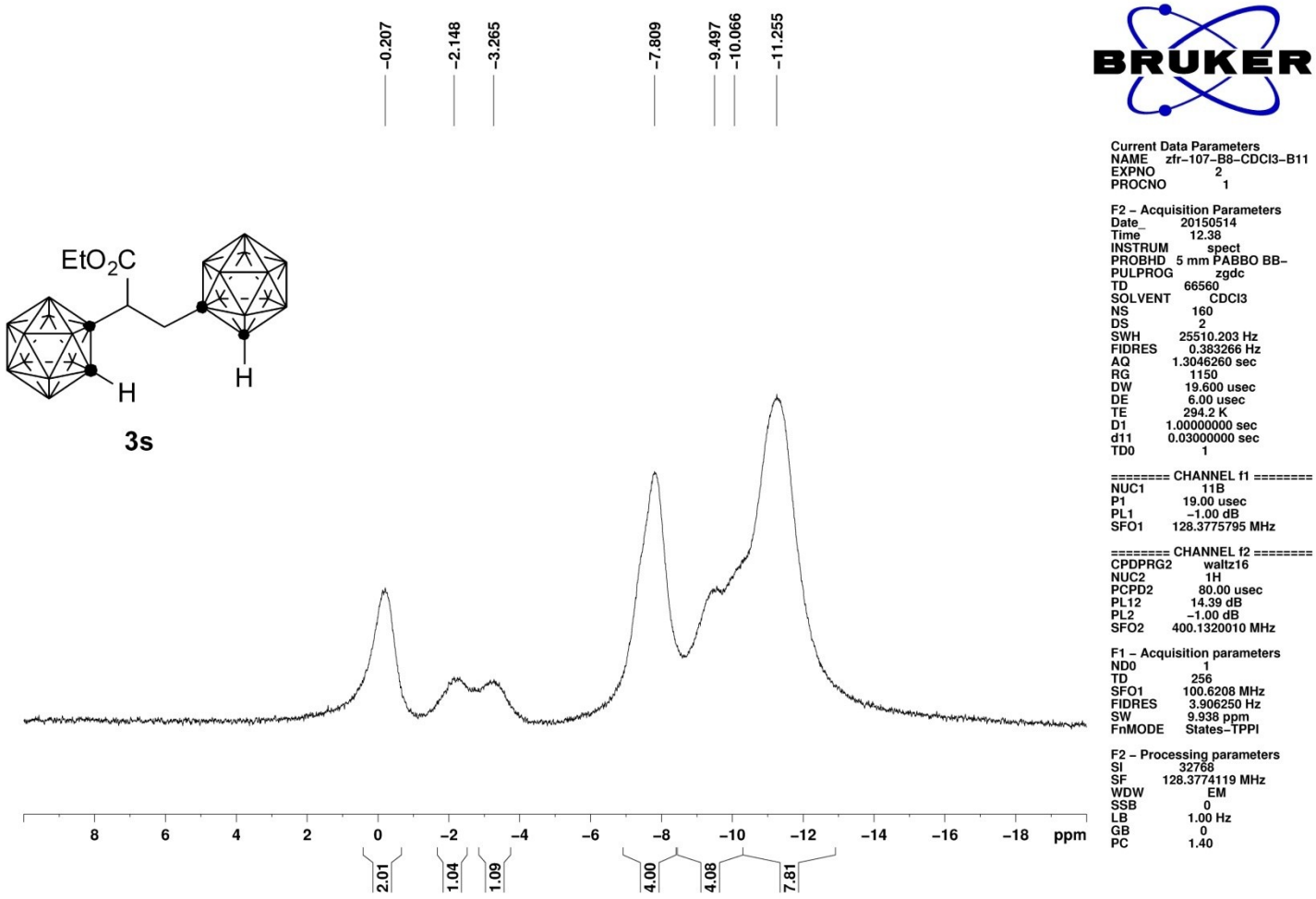
Current Data Parameters
NAME zfr-91-CDCl3-C13
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150506
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 11816
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127468 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−107−B8−CDCl3−B11
EXPNO 2
PROCNO 1

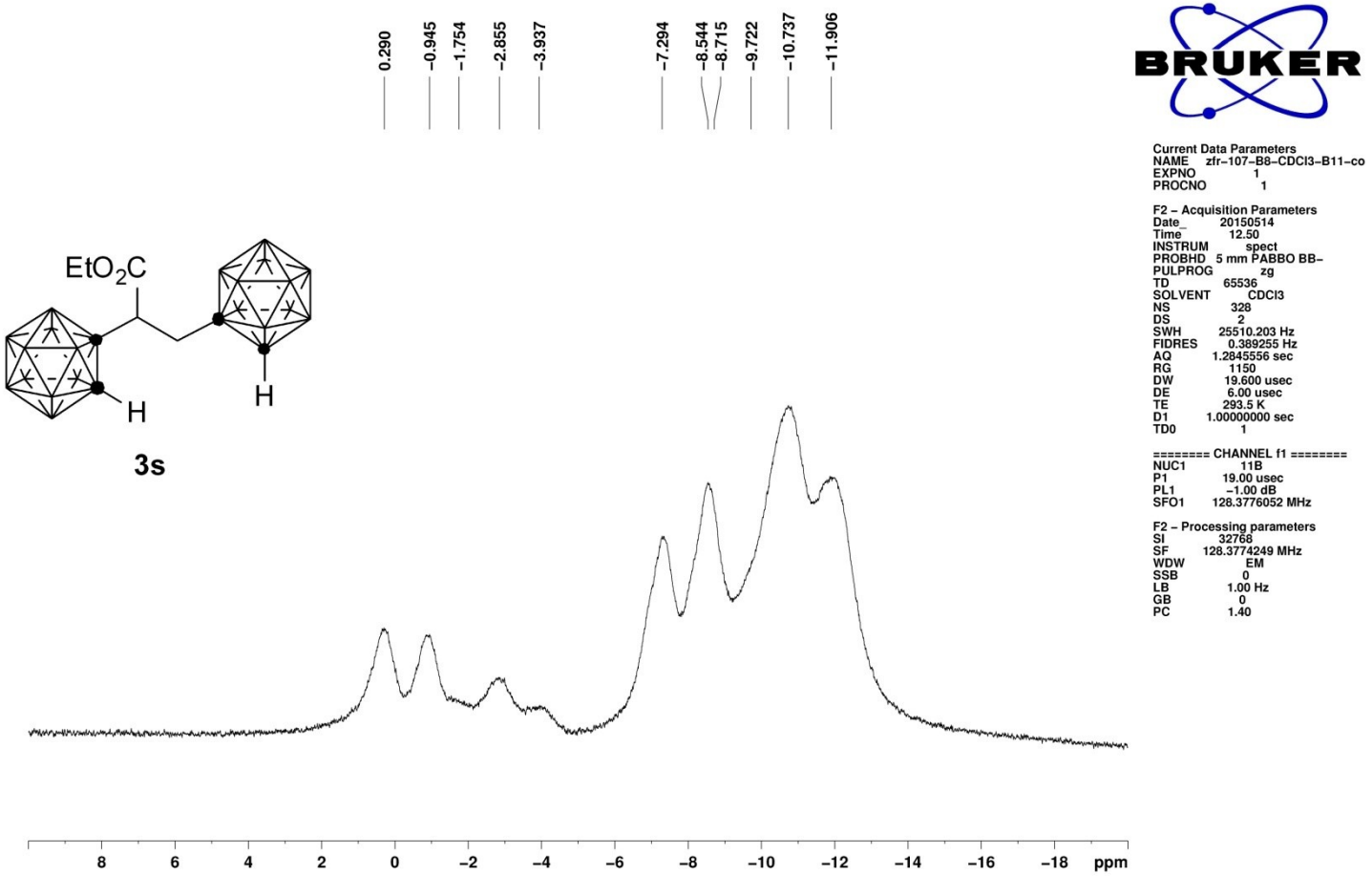
F2 − Acquisition Parameters
Date_ 20150514
Time 12.38
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 1150
DW 19.600 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

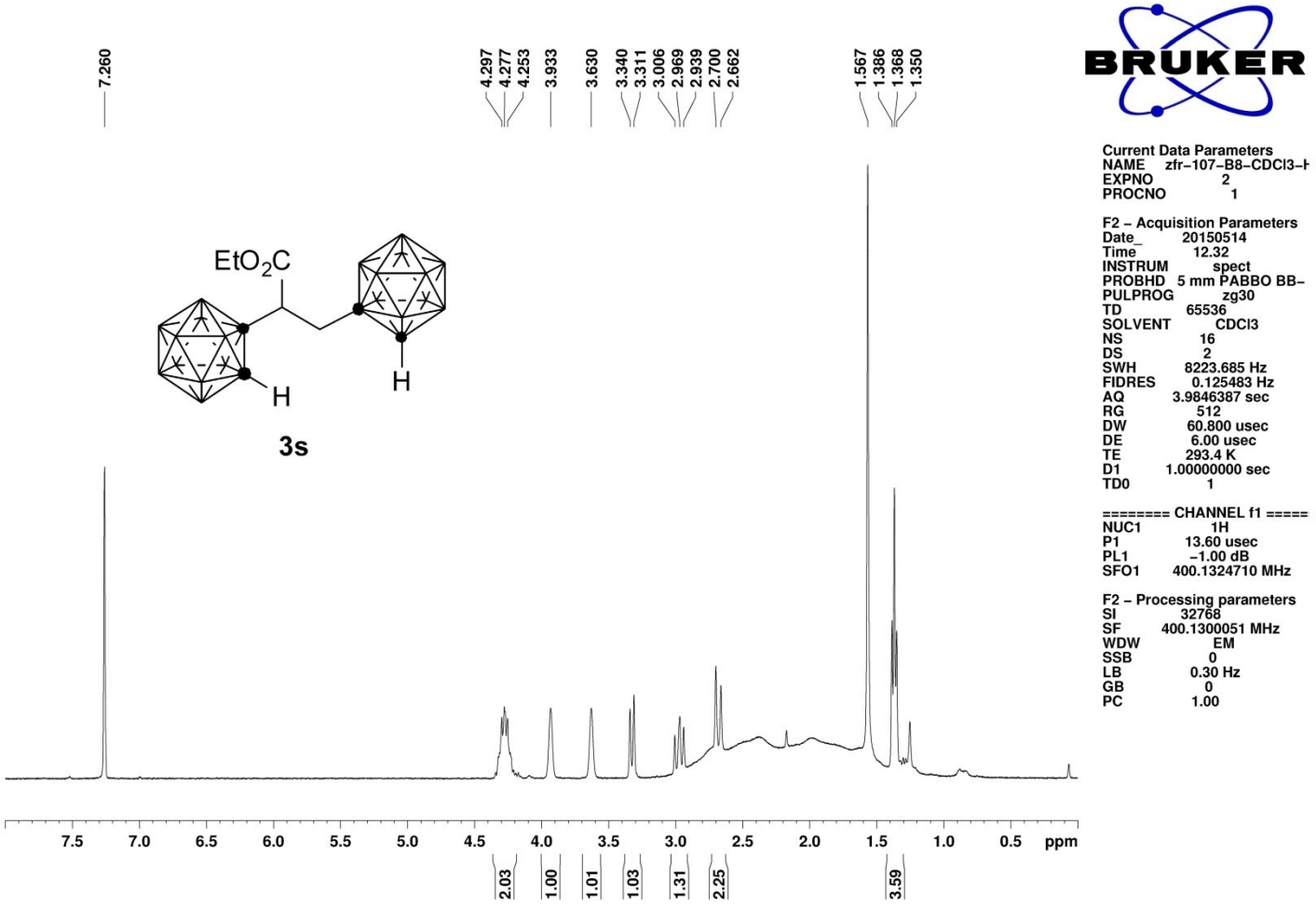
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

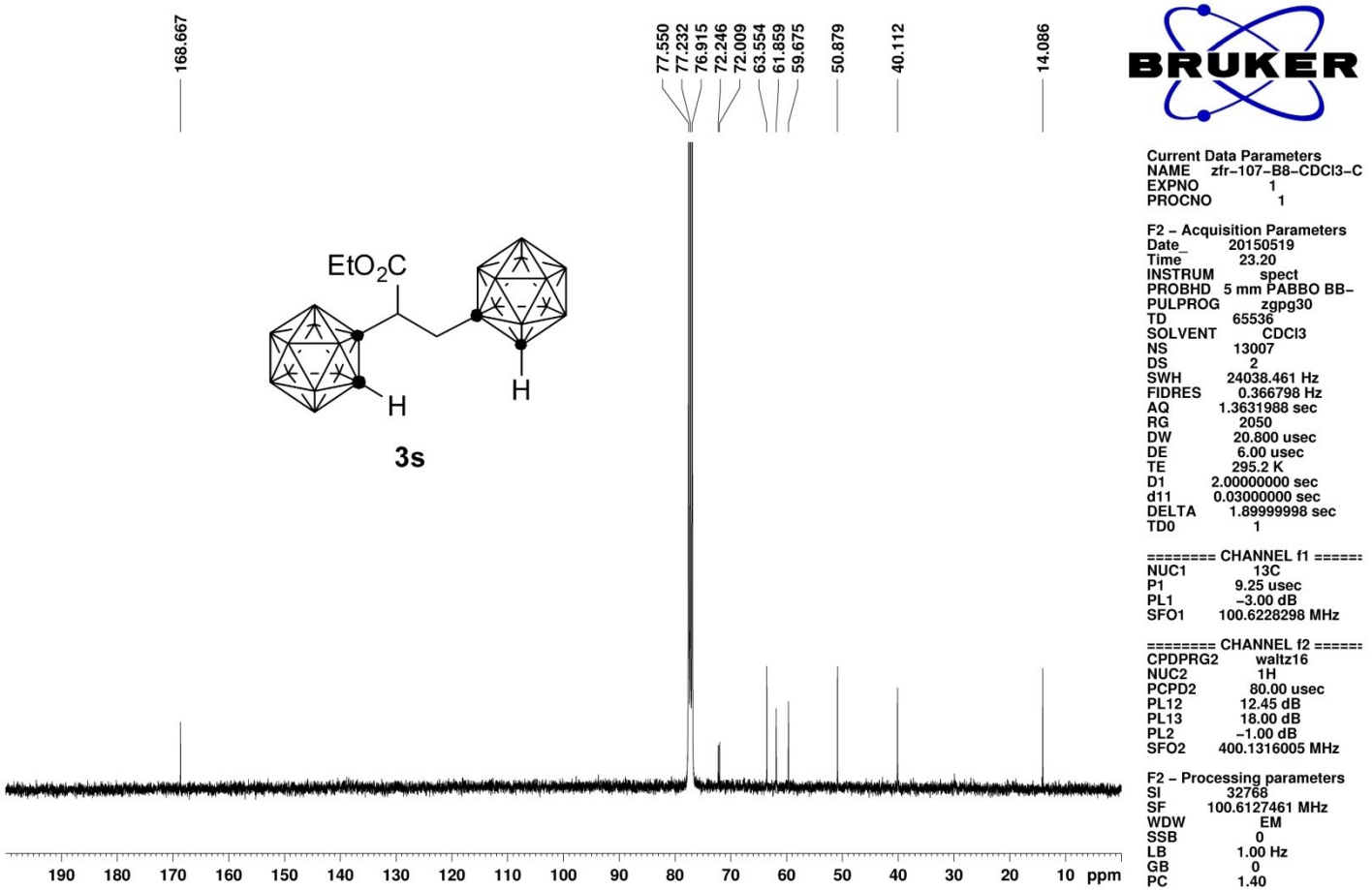
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

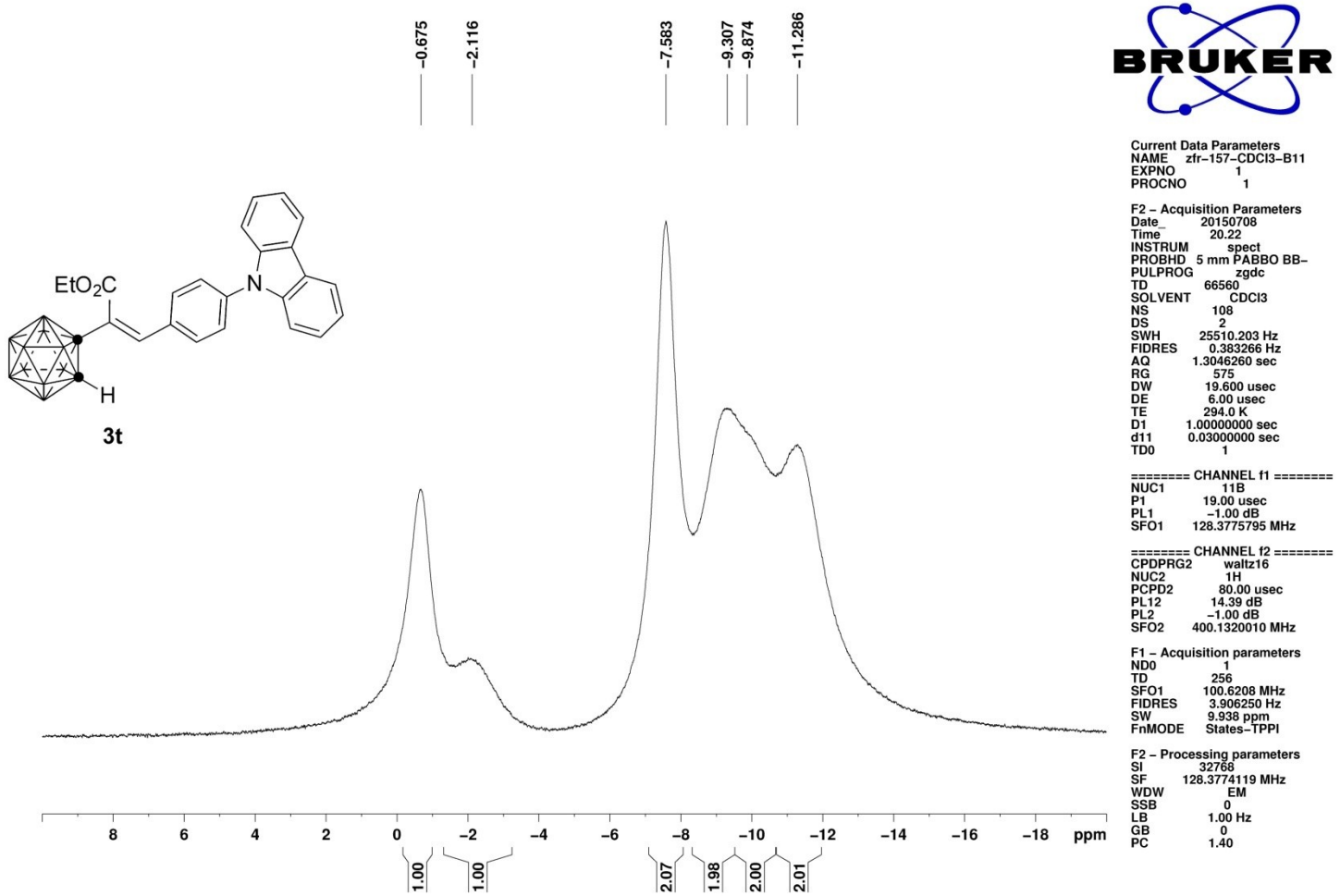
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


0.290
-0.945
-1.754
-2.855
-3.937
-7.294
-8.544
-8.715
-9.722
-10.737
-11.906
EtO2C
H
H
3s
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
ppm
BRUKER
Current Data Parameters
NAME zfr-107-B8-CDCl3-B11-co
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150514
Time 12.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 328
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 1150
DW 19.600 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


7.260
4.297
4.277
4.253
3.933
3.630
3.340
3.311
3.006
2.969
2.939
2.700
2.662
1.567
1.386
1.368
1.350
EtO2C
H
H
3s
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
ppm
2.03
1.00
1.01
1.03
1.31
2.25
3.59
BRUKER
Current Data Parameters
NAME zfr-107-B8-CDCl3-H
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150514
Time 12.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


168.667
77.550
77.232
76.915
72.246
72.009
63.554
61.859
59.675
50.879
40.112
14.086
EtO2C
H
H
3s
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-107-B8-CDCl3-C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150519
Time 23.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 13007
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127461 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



BRUKER

Current Data Parameters
NAME zfr−157−CDCl3−B11
EXPNO 1
PROCNO 1

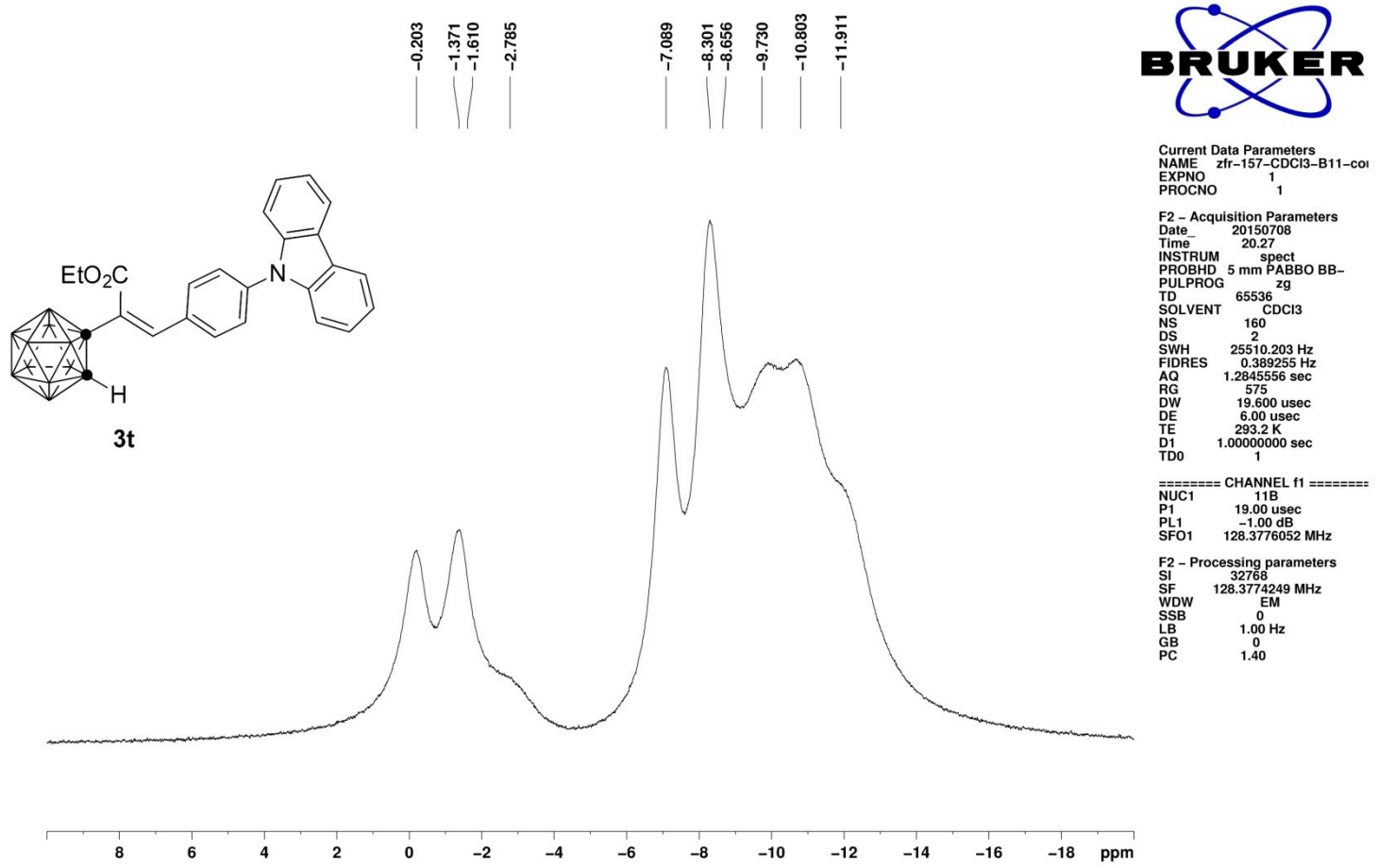
F2 − Acquisition Parameters
Date_ 20150708
Time 20.22
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 108
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.0 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

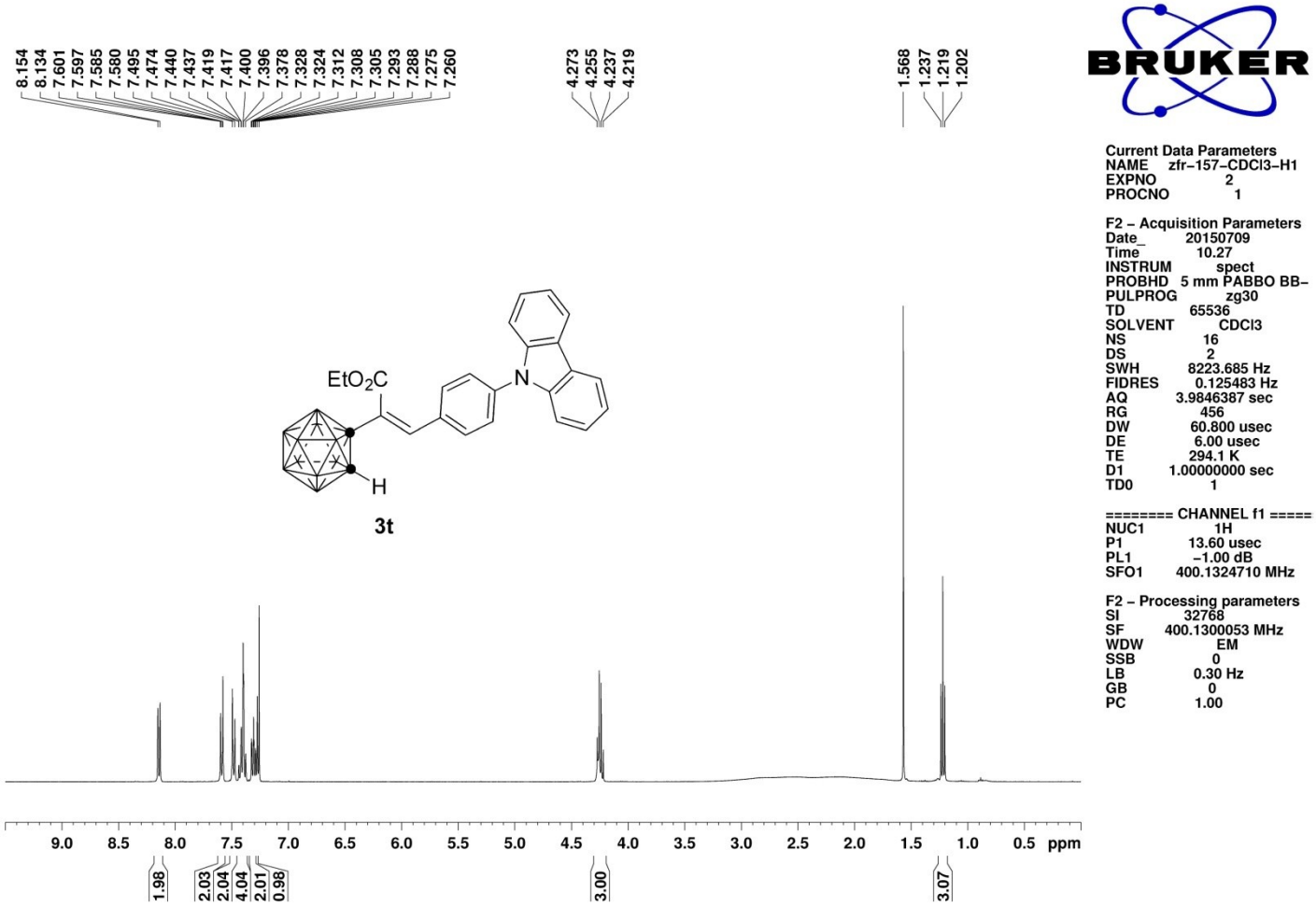
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz

F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI

F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.203
−1.371
−1.610
−2.785
−7.089
−8.301
−8.656
−9.730
−10.803
−11.911
EtO2C
N
H
3t
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
BRUKER
Current Data Parameters
NAME zfr−157−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20150708
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



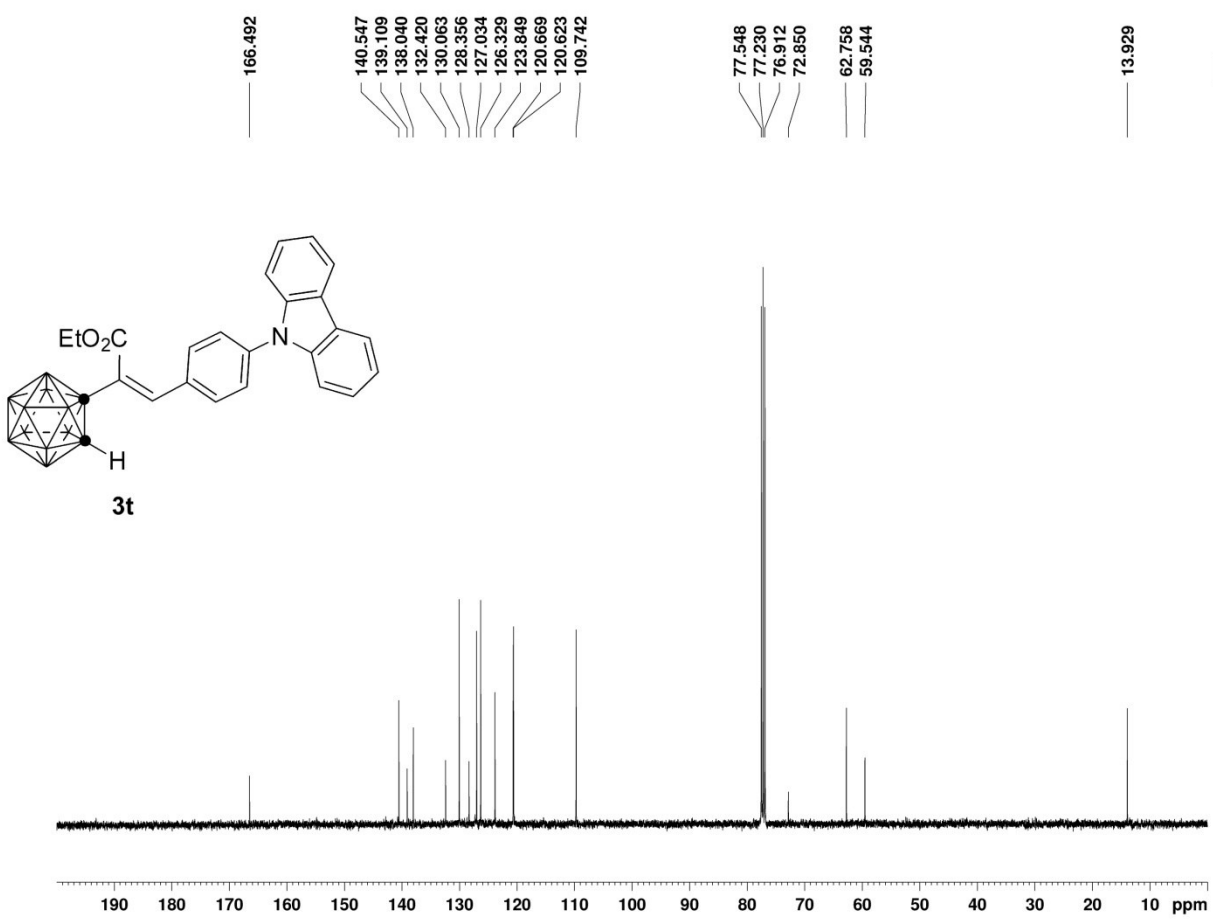
BRUKER

Current Data Parameters
NAME zfr-157-CDCl3-H1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150709
Time 10.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

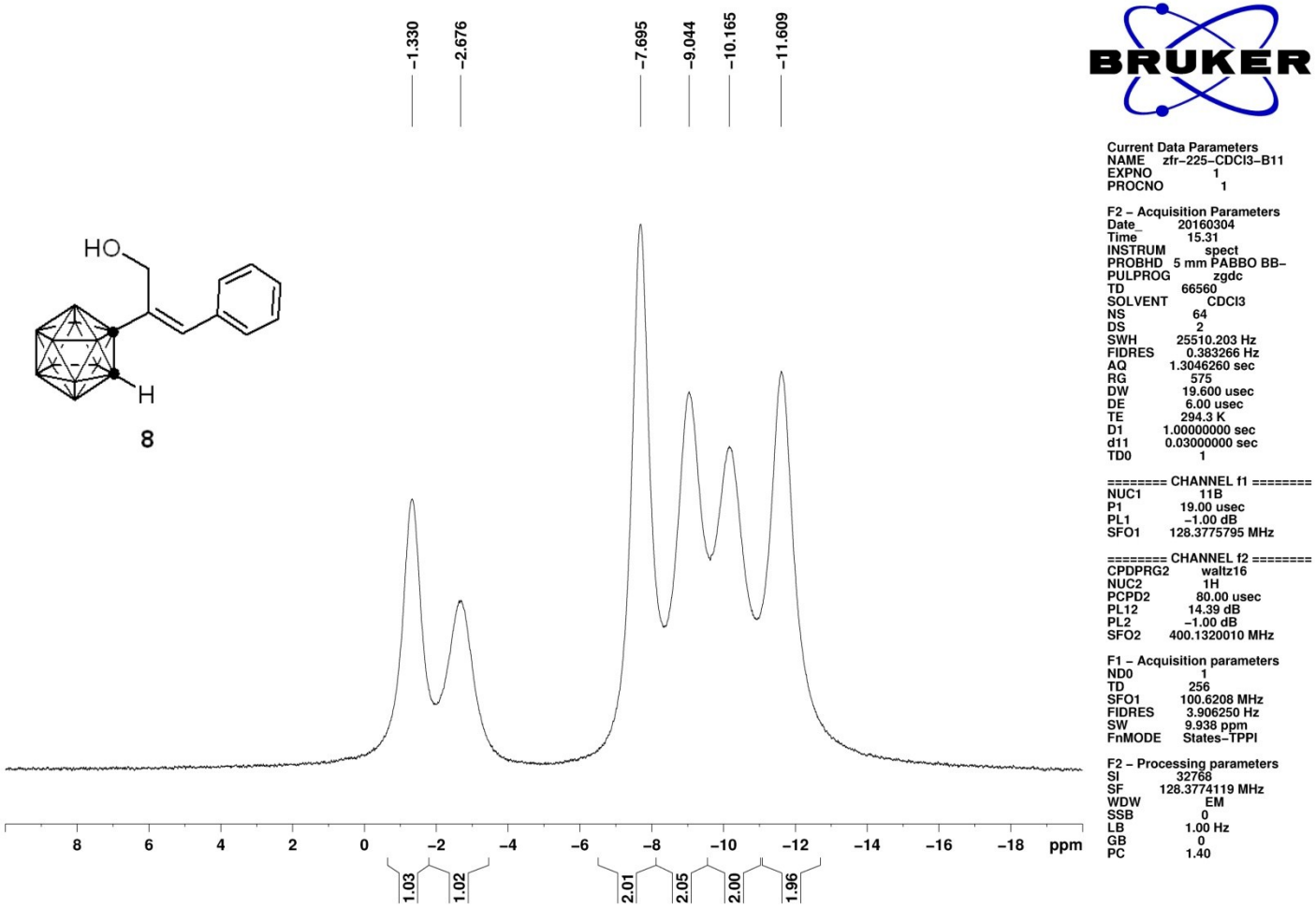
Current Data Parameters
NAME zfr-157-CDCl3-C13
EXPNO 1
PROCNO 1

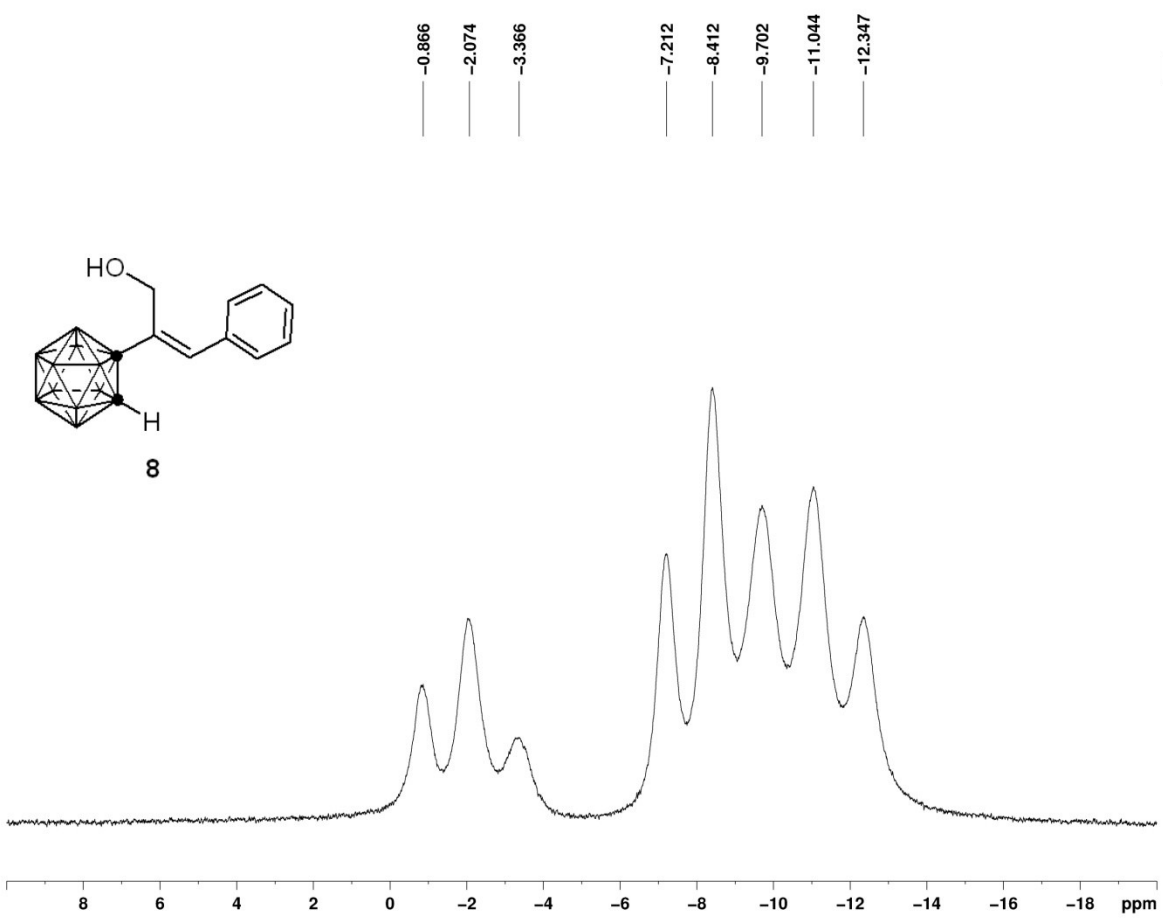
F2 - Acquisition Parameters
Date_ 20150708
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 333
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 293.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127512 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−1.330
−2.676
−7.695
−9.044
−10.165
−11.609
HO
H
8
8 6 4 2 0 −2 −4 −6 −8 −10 −12 −14 −16 −18 ppm
1.03
1.02
2.01
2.05
2.00
1.96
BRUKER
Current Data Parameters
NAME zfr−225−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date 20160304
Time 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 294.3 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

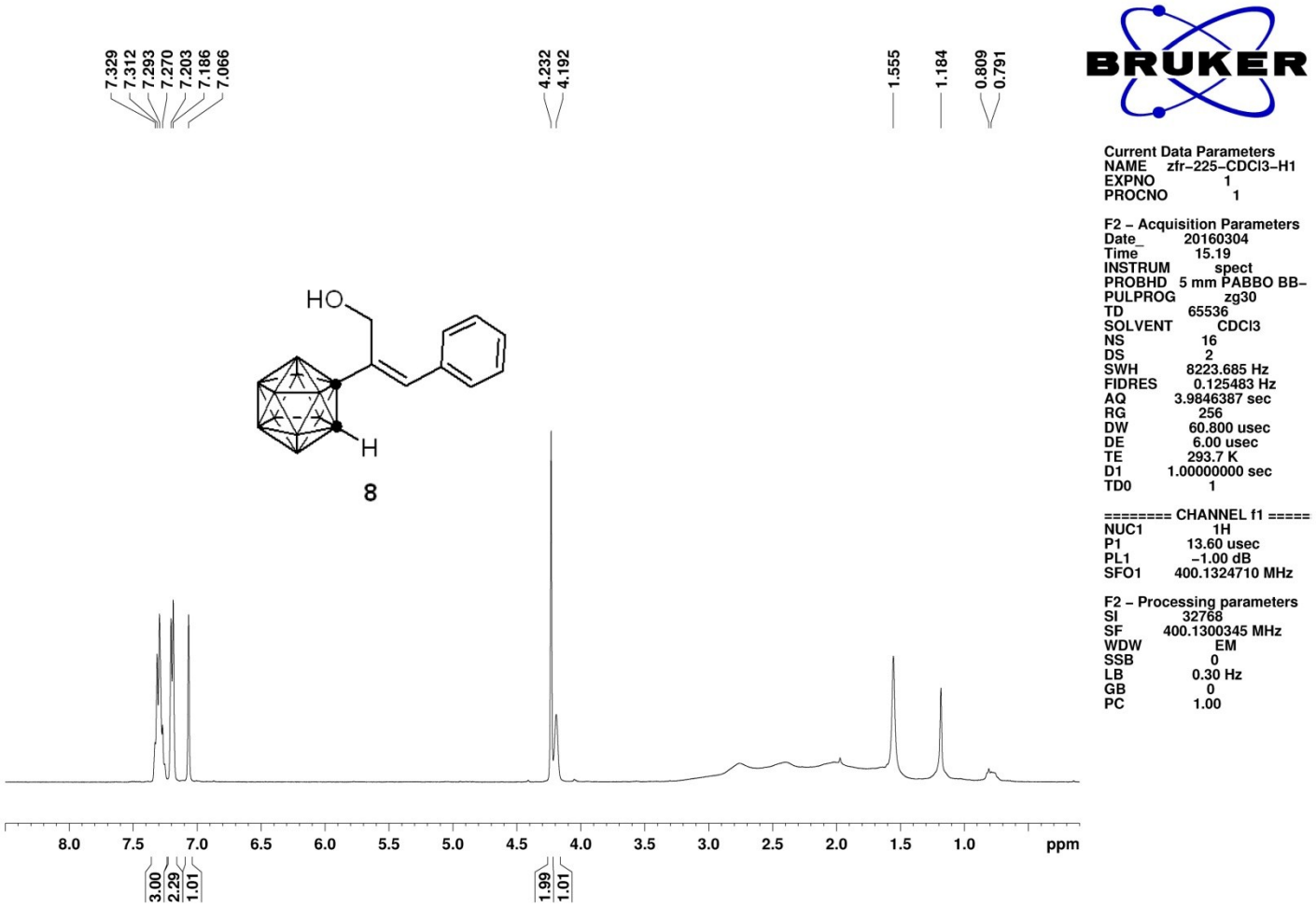


Current Data Parameters
NAME TF−zfr−225
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20160304
Time 19.47
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 25
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 575
DW 19.600 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz

F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



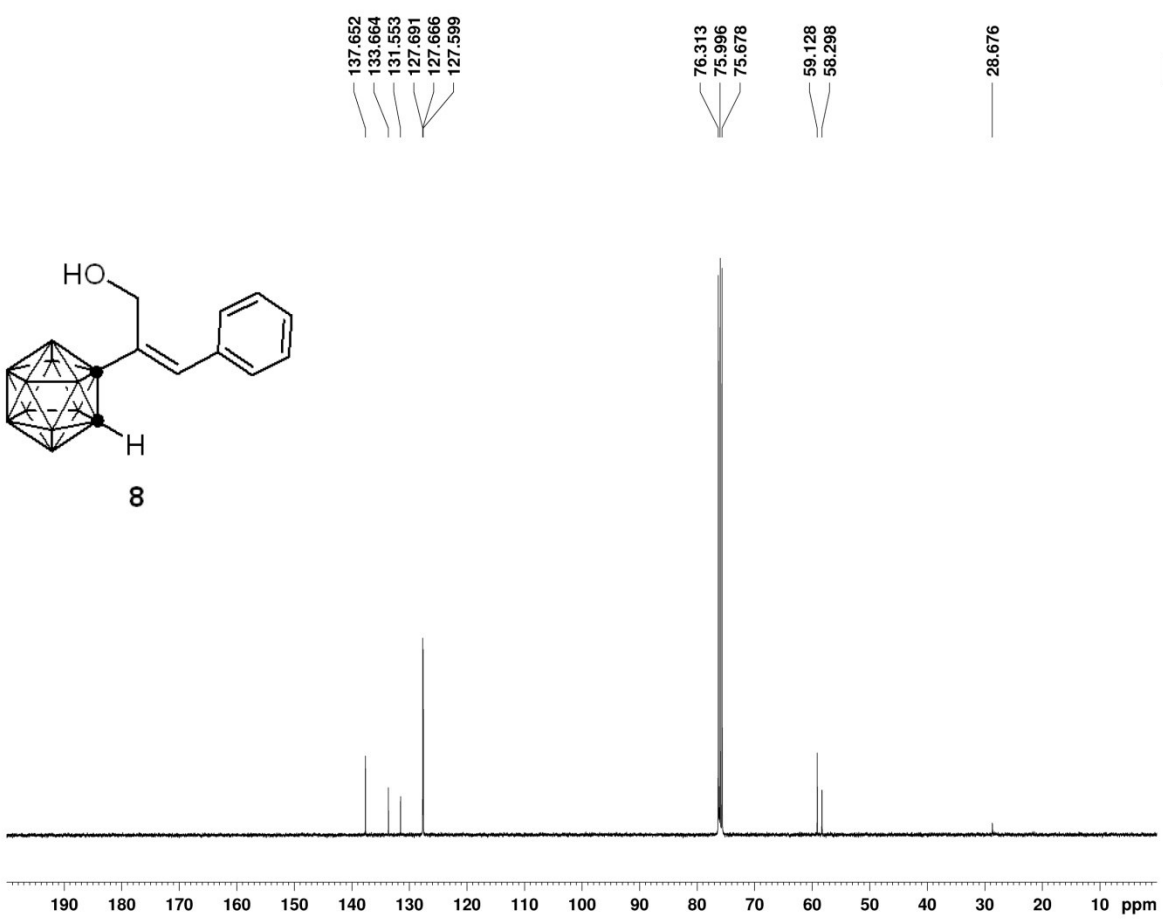
BRUKER

Current Data Parameters
NAME zfr-225-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160304
Time 15.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 293.7 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300345 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

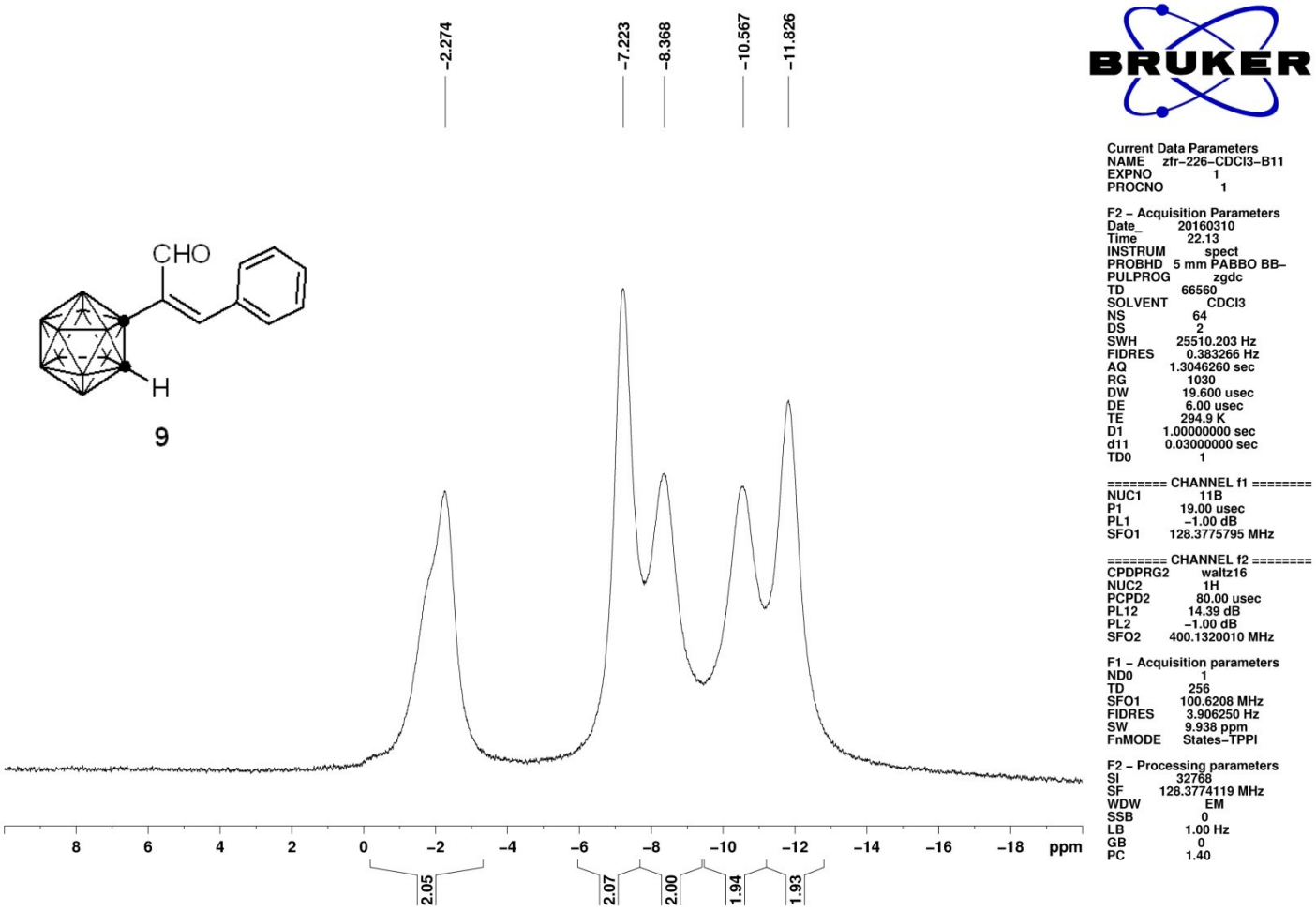
Current Data Parameters
NAME TF-zfr-225
EXPNO 1
PROCNO 1

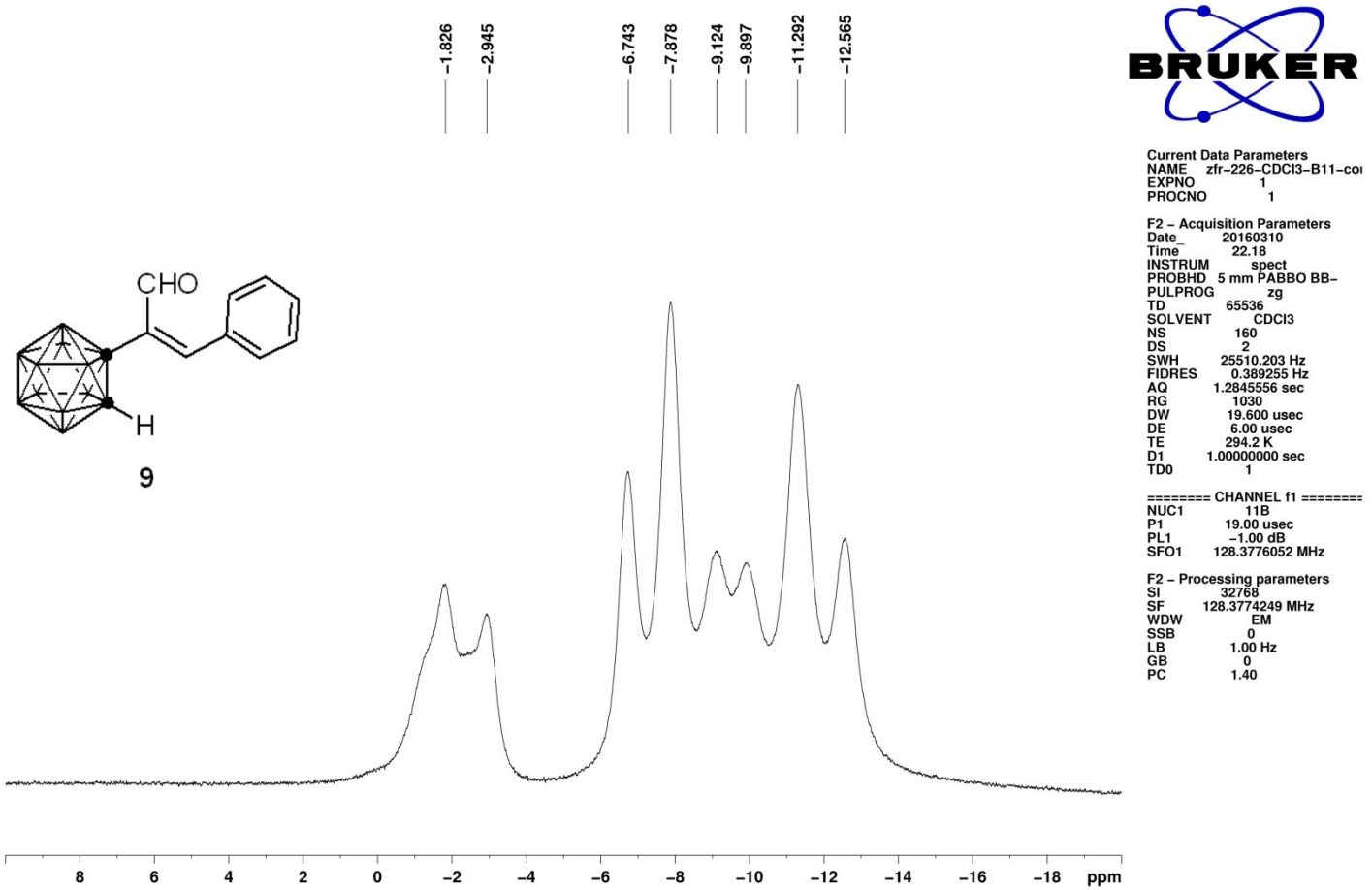
F2 - Acquisition Parameters
Date_ 20160304
Time 19.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2409
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 294.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

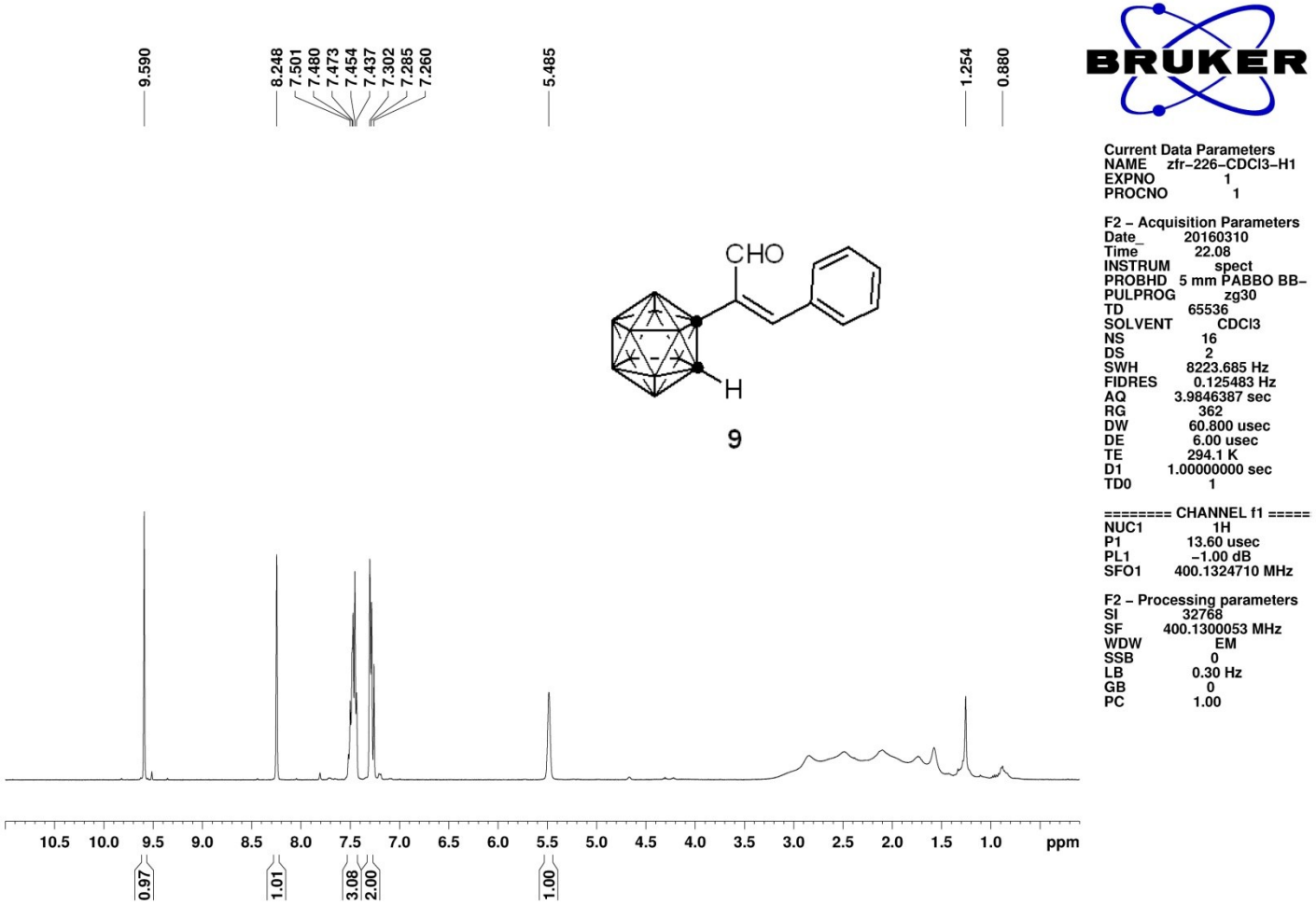
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128723 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−2.274
−7.223
−8.368
−10.567
−11.826
CHO
H
9
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
2.05
2.07
2.00
1.94
1.93
BRUKER
Current Data Parameters
NAME zfr−226−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20160310
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 64
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 1030
DW 19.600 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-1.826
-2.945
-6.743
-7.878
-9.124
-9.897
-11.292
-12.565
CHO
H
9
8
6
4
2
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
ppm
Current Data Parameters
NAME zfr-226-CDCl3-B11-co
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160310
Time 22.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 1030
DW 19.600 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 -1.00 dB
SFO1 128.3776052 MHz
F2 - Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



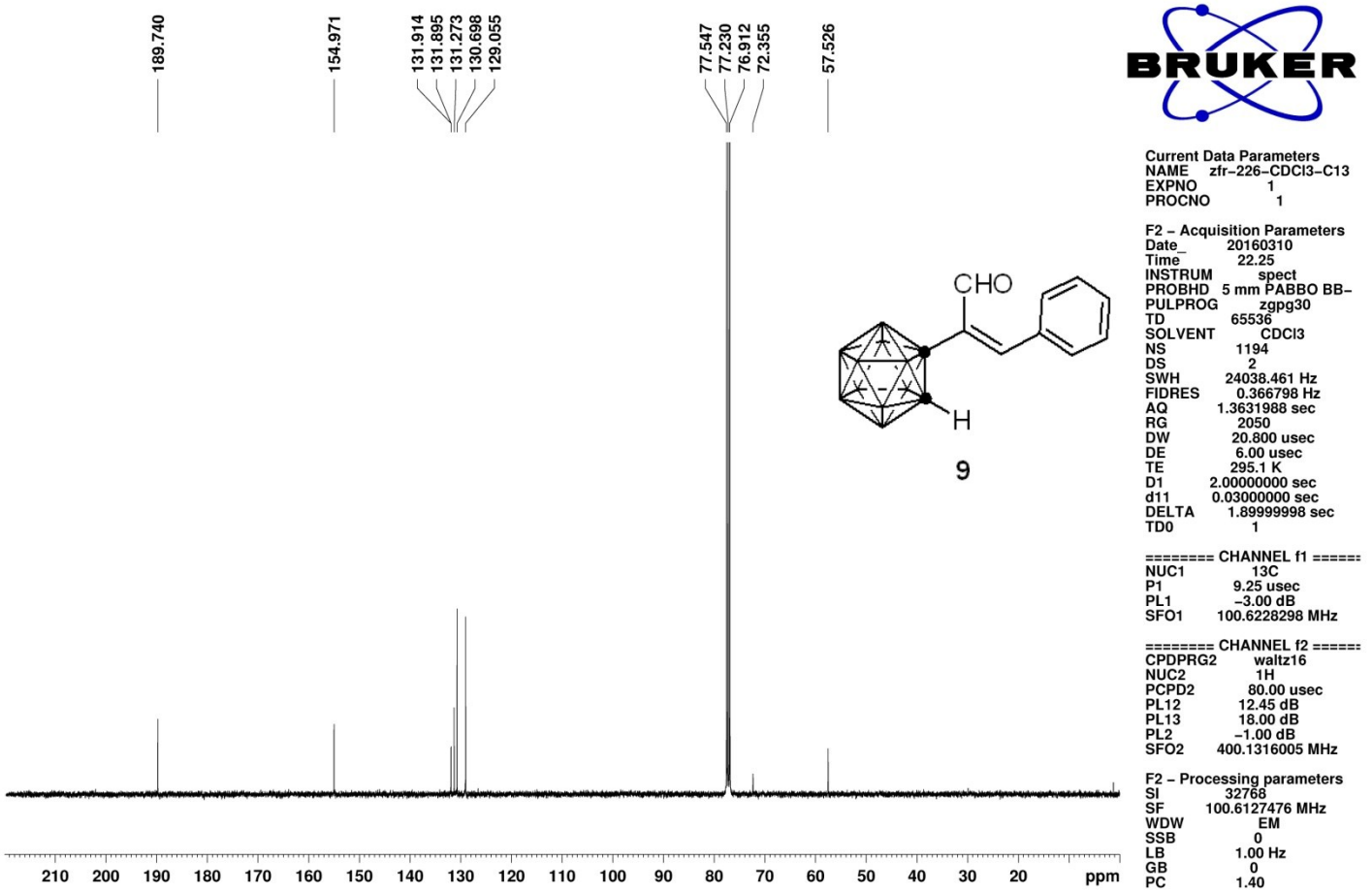
BRUKER

Current Data Parameters
NAME zfr-226-CDCl3-H1
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160310
Time 22.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 362
DW 60.800 usec
DE 6.00 usec
TE 294.1 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

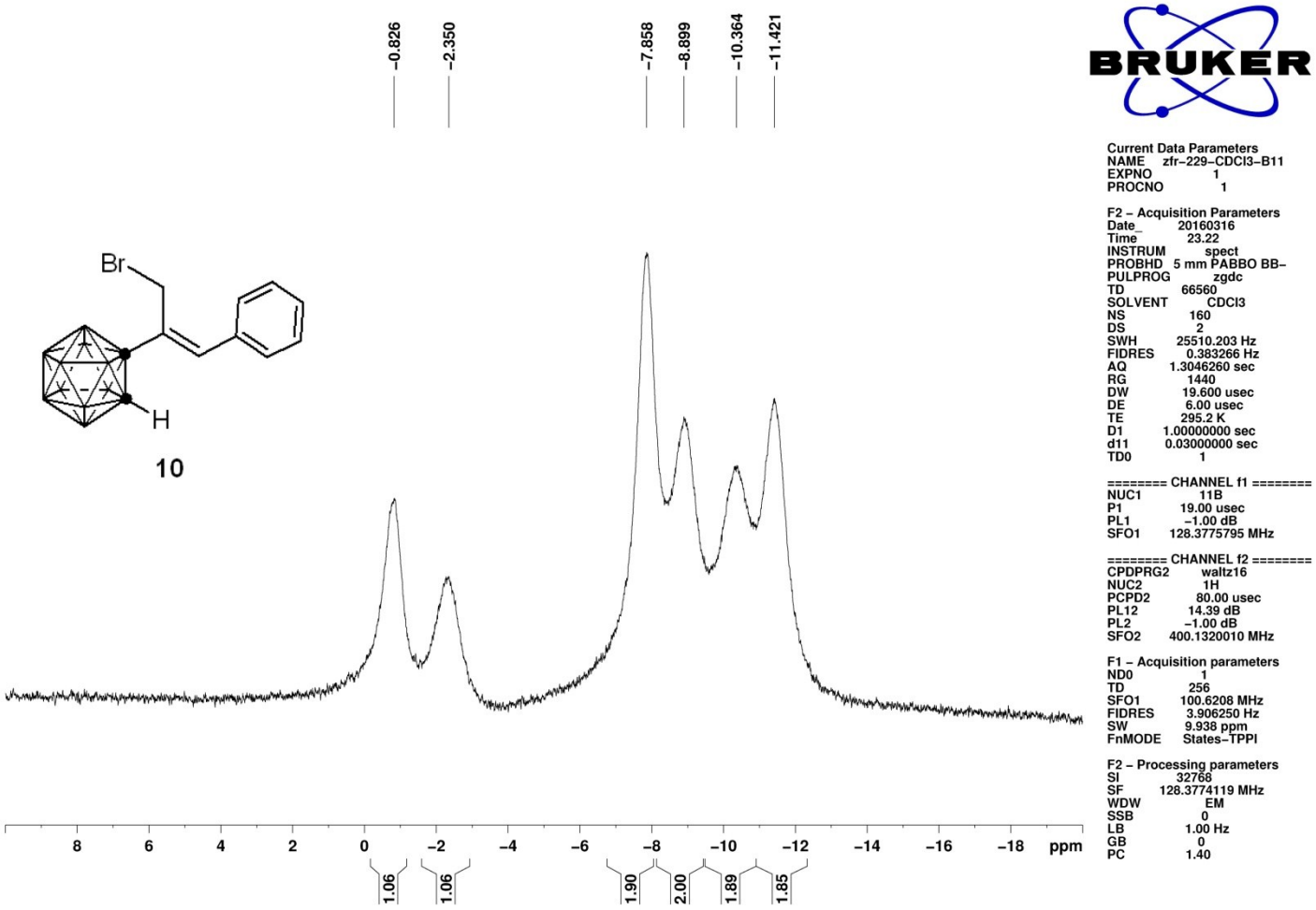
Current Data Parameters
NAME zfr-226-CDCl3-C13
EXPNO 1
PROCNO 1

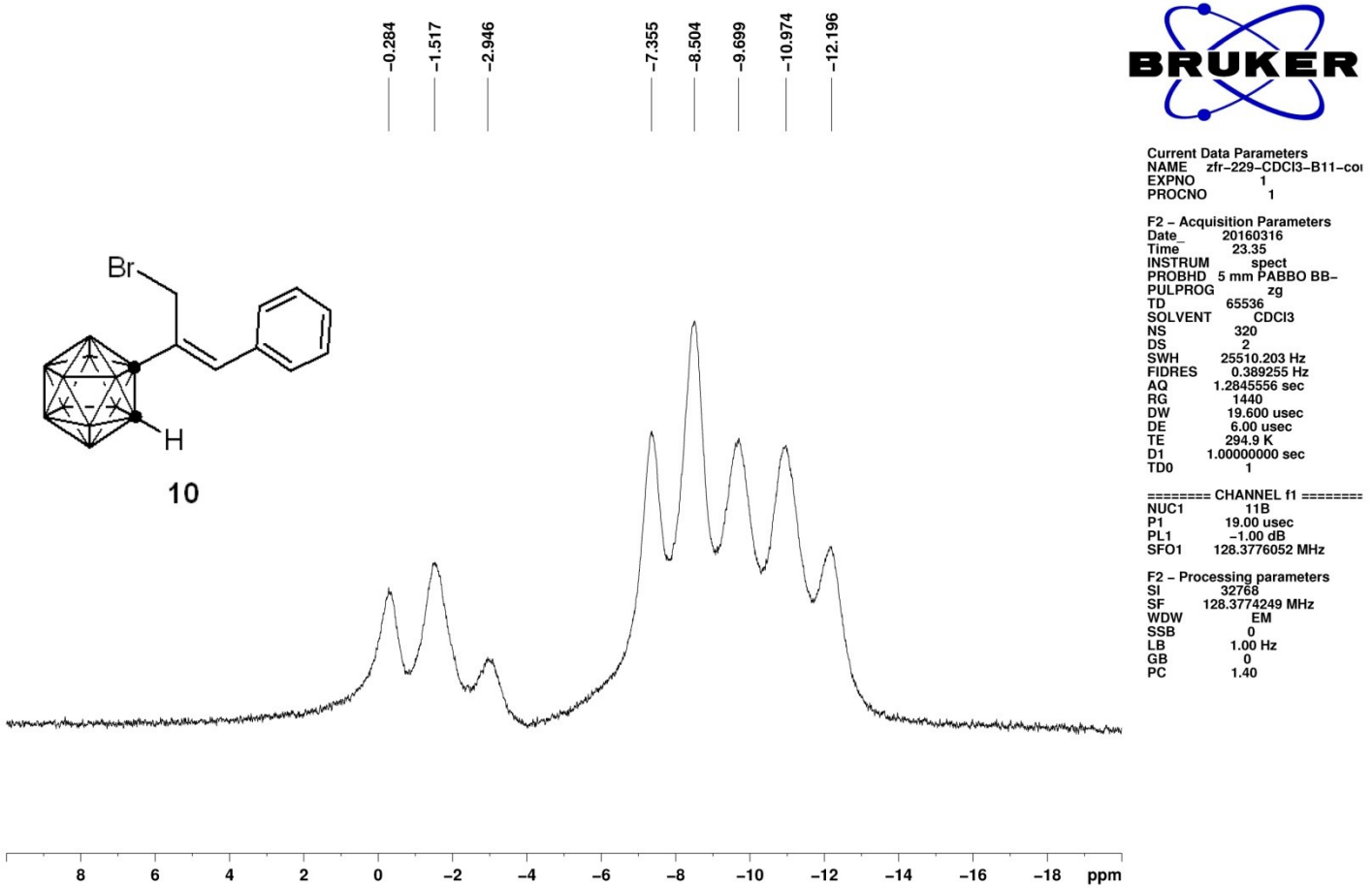
F2 - Acquisition Parameters
Date_ 20160310
Time 22.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1194
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 295.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

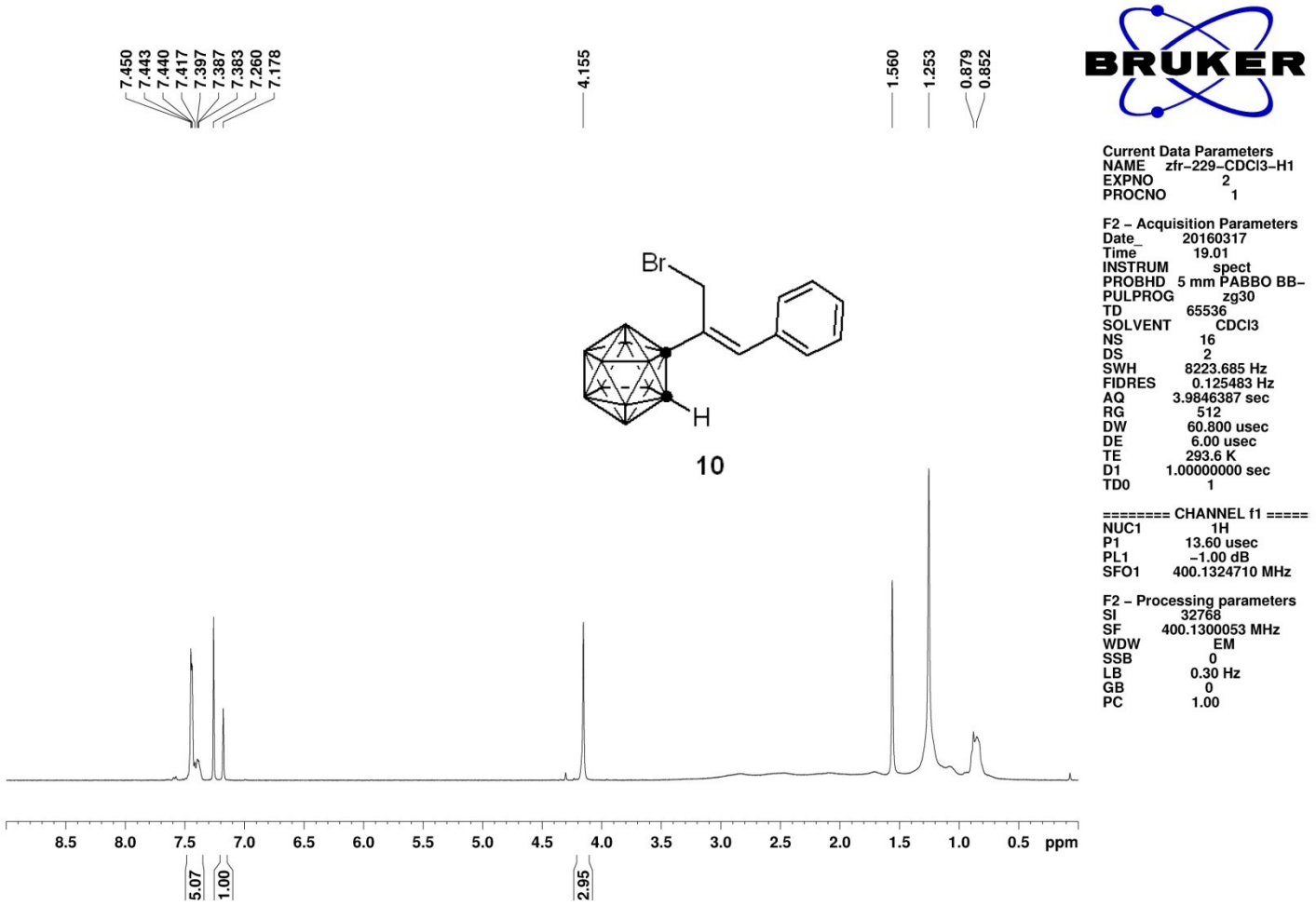
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127476 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


−0.826
−2.350
−7.858
−8.899
−10.364
−11.421
Br
H
10
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
1.06
1.06
1.90
2.00
1.89
1.85
BRUKER
Current Data Parameters
NAME zfr−229−CDCl3−B11
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20160316
Time 23.22
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgdc
TD 66560
SOLVENT CDCl3
NS 160
DS 2
SWH 25510.203 Hz
FIDRES 0.383266 Hz
AQ 1.3046260 sec
RG 1440
DW 19.600 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3775795 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.39 dB
PL2 −1.00 dB
SFO2 400.1320010 MHz
F1 − Acquisition parameters
ND0 1
TD 256
SFO1 100.6208 MHz
FIDRES 3.906250 Hz
SW 9.938 ppm
FnMODE States−TPPI
F2 − Processing parameters
SI 32768
SF 128.3774119 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


-0.284
-1.517
-2.946
-7.355
-8.504
-9.699
-10.974
-12.196
Br
H
10
8
6
4
2
0
−2
−4
−6
−8
−10
−12
−14
−16
−18
ppm
Current Data Parameters
NAME zfr−229−CDCl3−B11−co
EXPNO 1
PROCNO 1
F2 − Acquisition Parameters
Date_ 20160316
Time 23.35
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg
TD 65536
SOLVENT CDCl3
NS 320
DS 2
SWH 25510.203 Hz
FIDRES 0.389255 Hz
AQ 1.2845556 sec
RG 1440
DW 19.600 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 11B
P1 19.00 usec
PL1 −1.00 dB
SFO1 128.3776052 MHz
F2 − Processing parameters
SI 32768
SF 128.3774249 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



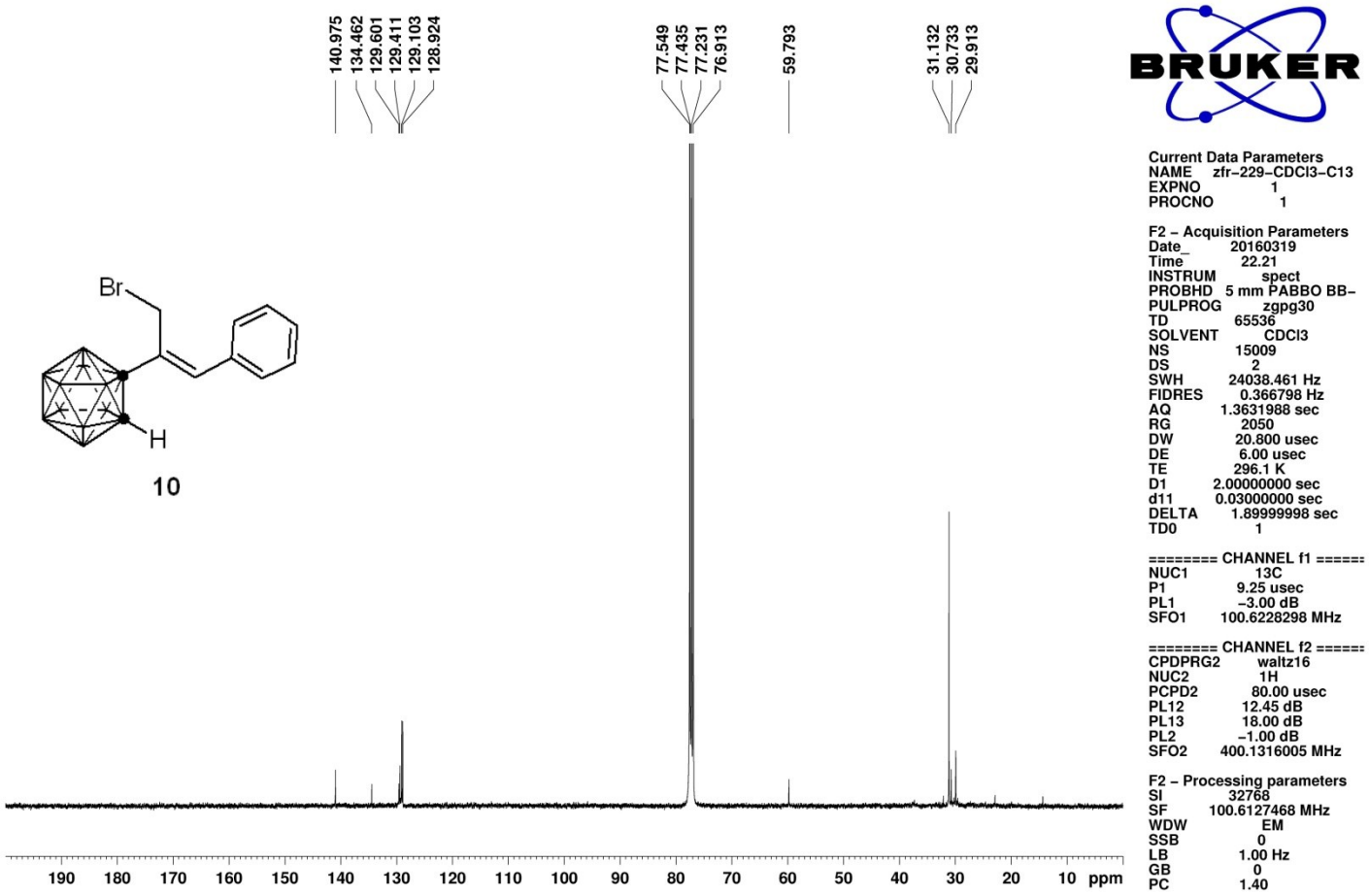
BRUKER

Current Data Parameters
NAME zfr-229-CDCl3-H1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160317
Time 19.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 293.6 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300053 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00


140.975
134.462
129.601
129.411
129.103
128.924
77.549
77.435
77.231
76.913
59.793
31.132
30.733
29.913
Br
H
10
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
BRUKER
Current Data Parameters
NAME zfr-229-CDCl3-C13
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160319
Time 22.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 15009
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ======
NUC1 13C
P1 9.25 usec
PL1 -3.00 dB
SFO1 100.6228298 MHz
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 12.45 dB
PL13 18.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127468 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40