Electronic Supplementary Material (ESI) for Chemical Communications

Stereoselective Synthesis of Aminoindanols via An Efficient Cascade aza-Michael-aldol Reaction

Supplementary Information

Hui Qian, Wanxiang Zhao, Herman H-Y. Sung,
Ian D. Williams and Jianwei Sun*

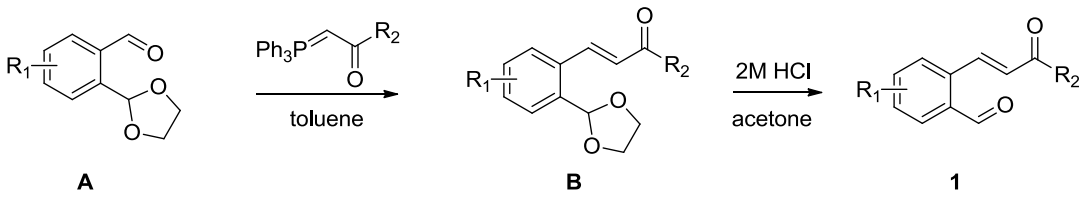
Department of Chemistry, the Hong Kong University of Science and Technology
Clear Water Bay, Kowloon, Hong Kong SAR, China

I. General Information

All air or moisture sensitive reactions were conducted in oven-dried glassware under nitrogen atmosphere using dry solvents. Flash column chromatography was performed over silica gel (230-400 mesh) purchased from Qindao Puke Co., China. Anhydrous dichloromethane and toluene were purified by distillation over calcium hydride. Anhydrous tetrahydrofuran was freshly distilled from sodium-benzophenone. ^{1}H and ^{13}C NMR spectra were collected on a Bruker AV 400 MHz NMR spectrometer using residue solvent peaks as an internal standard. Mass spectra were collected on an Agilent GC/MS 5975C system, or a MALDI Micro MX mass spectrometer, or an API QSTAR XL System. IR spectra were recorded on Bruker TENSOR 27 spectrometer and are reported in terms of frequency of absorption (cm^{-1}).

II. Synthesis of the Enone Substrates

General Procedure A: Preparation of Enone Substrates

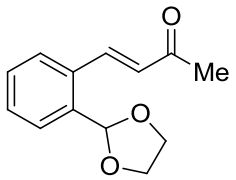


The enone substrates were prepared employing a modified literature procedure.[1] A 20-mL vial was charged with a solution of **A** (3.0 mmol, 1 equiv.) and the phosphorane (6.0 mmol, 2 equiv.) in toluene (6.0 mL, 0.5 M). The vial was sealed and heated in an oil bath at 150°C for 12 h. After cooling to room temperature, the solvent was removed in vacuo and the remaining thick oil was purified by flash column chromatography to afford **B**. To a solution of **B** (1.0 mmol, 1 equiv.) in acetone (6 mL) was added aqueous HCl (2 mL, 2M). The reaction mixture was

1. Eduardo S.-L., J. M. Holmes, C. L. Daschner, M. Gravel, *Org*, *Lett*., 2010, **12**, 5772.

allowed to stir at room temperature for 2 h before it was extracted with Et_2O (3 × 10 mL). The organic layers were combined, dried with anhydrous $MgSO_4$, and concentrated under reduced pressure. The residue was purified by flash column chromatography to give enone **1**.

Compounds **1a**, **1b**, **1g, 1h, 1i,** and **1j** are known compounds and their characterizations match the literature reports.[1,2]



B1

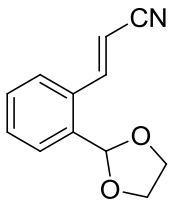
(*E*)-4-(2-(1,3-Dioxolan-2-yl)phenyl)but-3-en-2-one (B1) was prepared from 2-(1,3-dioxolan-2-yl)benzaldehyde (0.53 g, 3.0 mmol) and 1-(triphenyl phosphoranylidene)propan-2-one (318 mg, 6.0 mmol) according to the General Procedure A in 46% yield (301 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, J = 16.0 Hz, 1H), 7.62 – 7.61 (m, 2H), 7.43 – 7.36 (m, 2H), 6.64 (d, J = 16.0 Hz, 1H), 6.03 (s, 1H), 4.19 – 4.06 (m, 4H), 2.38 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 198.3, 140.4, 136.2, 133.7, 130.0, 129.4, 129.0, 127.0, 102.0, 65.4, 27.6 (two carbons).

IR (thin film) 2961, 1668, 1609, 1261 cm^{-1}.

HRMS (CI+) Calcd for $C_{13}H_{15}O_3$ (M^++H): 219.1021, Found: 219.1021.



B2

2. (a) Z. L. Sun, Ying Cheng, *Org. Biomol. Chem.*, 2012, **10**, 4088. (b) E. E. Maciver, P. C. Knipe, M. D. Smith, *Chem. Sci.*, 2012, **3**, 537. (c) W. Xia, Y. Shao, W. Cui, C. Yang, *Chem. Commun.*, 2011, **47**, 11098.

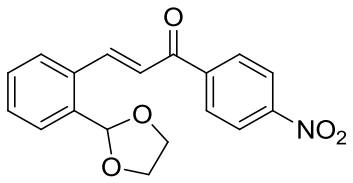
(*E*)-3-(2-(1,3-Dioxolan-2-yl)phenyl)acrylonitrile (B2) was prepared from 2-(1,3-dioxolan-2-yl)benzaldehydes (535 mg, 3.0 mmol) and 2-(triphenylphosphoranylidene)acetonitrile (1.81 g, 6.0 mmol) according to the General Procedure A in 42% yield (254 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 16.4 Hz, 1H), 7.64 – 7.61 (m, 1H), 7.52 – 7.49 (m, 1H), 7.47 – 7.38 (m, 2H), 5.92 (s, 1H), 5.83 (d, J = 16.4 Hz, 1H), 4.18 – 4.06 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 148.2, 135.7, 132.7, 130.6, 129.5, 127.1, 126.3, 118.1, 101.8, 98.2, 65.3.

IR (thin film) 2217, 1612, 1115, 1074 cm^{-1}.

HRMS (CI+) Calcd for $C_{12}H_{12}NO_2$ (M^++H): 202.0868, Found: 202.0868.



B3

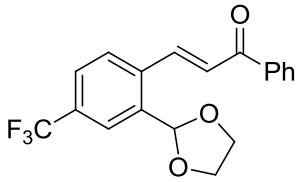
(*E*)-3-(2-(1,3-Dioxolan-2-yl)phenyl)-1-(4-nitrophenyl)prop-2-en-1-one (B3) was prepared from 2-(1,3-dioxolan-2-yl)benzaldehydes (535 mg, 3.0 mmol) and 1-(4-nitrophenyl)-2-(triphenylphosphoranylidene)ethanone (3.40 g, 8.0 mmol) according to the General Procedure A in 85% yield (277.3 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 – 8.29 (m, 3H), 8.15 – 8.12 (m, 2H), 7.75 – 7.73 (m, 1H), 7.66 – 7.64 (m, 1H), 7.48 – 7.42 (m, 2H), 7.39 (d, J = 15.6 Hz, 1H), 6.03 (s, 1H), 4.18 – 4.05 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 150.0, 143.9, 142.9, 136.8, 133.6, 130.5, 129.5 (two carbons), 127.2, 127.0, 123.8, 123.4, 102.0, 65.4.

IR (thin film) 1662, 1600, 1524, 1335 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{16}NO_5$ (M^++H): 326.1028, Found: 326.1028.



B4

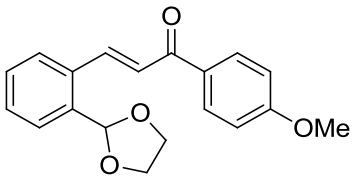
(*E*)-3-(2-(1,3-Dioxolan-2-yl)-4-(trifluoromethyl)phenyl)-1-phenylprop-2-en-1-one (B4) was prepared from 2-(1,3-dioxolan-2-yl)-4-(trifluoromethyl)-benzaldehyde (739 mg, 3.0 mmol) and 1-phenyl-2-(triphenyl-phosphoranylidene)ethanone (2.28 g, 6.0 mmol) according to the General Procedure A in 81% yield (283 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23 (d, J = 15.6 Hz, 1H), 8.04 – 8.02 (m, 2H), 7.94 (s, 1H), 7.82 (d, J = 8.4 Hz, 1H), 8.67 (d, J = 8.0 Hz, 1H), 7.63 – 7.60 (m, 1H), 7.54 – 7.49 (m, 3H), 6.08 (s, 1H) , 4.22 – 4.08 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 140.0, 137.7, 137.6, 137.4, 133.1, 131.3 (q, J = 32.7 Hz), 128.8, 128.6, 128.5, 127.5, 125.9 (q, J = 2.4 Hz), 125.1 (q, J = 270.9 Hz), 123.9 (q, J = 3.6 Hz), 110.9, 65.5.

IR (thin film) 2892, 1672, 1609, 1328 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{16}F_3O_3$ (M^++H): 349.1052, Found: 349.1052.



B5

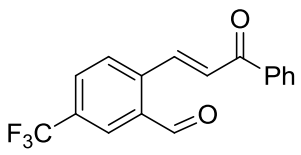
(*E*)-3-(2-(1,3-Dioxolan-2-yl)phenyl)-1-(4-methoxyphenyl)prop-2-en-1-one (B5) was prepared from 2-(1,3-dioxolan-2-yl)benzaldehydes (267 mg, 1.5 mmol) and 1-(4-nitrophenyl)-2-(triphenylphosphoranylidene)ethanone (1.23 g, 3.0 mmol) according to the General Procedure A in 76% yield (248 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (d, J = 15.6 Hz, 1H), 8.06 – 8.04 (m, 2H), 7.74 – 7.72 (m, 1H), 7.66 – 7.64 (m, 1H), 7.47 (d, J = 15.6 Hz, 1H), 7.43 – 7.41 (m, 2H), 6.99 – 6.97 (m, 2H), 6.07 (s, 1H), 4.21 – 4.06 (m, 4H), 3.89 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 188.5, 163.4, 140.9, 136.4, 134.4, 130.9, 130.8, 129.7, 129.3, 127.0, 126.9, 124.2, 113.8, 101.9, 65.4, 55.4.

IR (thin film) 2959, 1657, 1601, 1261 cm^{-1}.

HRMS (CI+) Calcd for $C_{19}H_{19}O_4$ (M^++H): 311.1283, Found: 311.1286.



1c

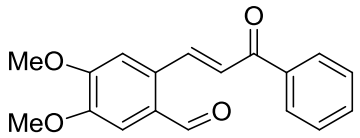
(*E*)-2-(3-Oxo-3-phenylprop-1-en-1-yl)-5-(trifluoromethyl)benzaldehydes (1c) was prepared from **B4** (349 mg, 1.0 mmol) according to the General Procedure A in 92% yield (281 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.4 (s, 1H), 8.52 (d, J = 15.6 Hz, 1H), 8.12 (s, 1H), 8.18 – 8.03 (m, 2H), 7.91 – 7.85 (m, 2H), 7.65 – 7.61 (m, 1H), 7.56 – 7.52 (m, 2H), 7.44 (d, J = 15.6 Hz, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 190.1, 189.6, 140.5, 139.2, 137.1, 134.2, 133.2, 131.8 (q, J = 33.3 Hz), 130.1 (q, J= 3.4 Hz), 128.8, 128.8, 128.7, 128.6, 128.4 (q, J = 3.8 Hz), 124.5 (q, J = 270.7 Hz).

IR (thin film) 1699, 1329, 1172, 1128 cm^{-1}.

HRMS (CI+) Calcd for $C_{17}H_{12}F_3O_2$ (M^++H): 305.0789, Found: 305.0789.



1d

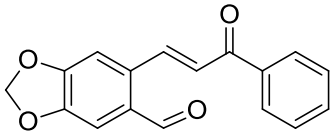
(*E*)-4,5-Dimethoxy-2-(3-oxo-3-phenylprop-1-en-1-yl)benzaldehyde (1d) was prepared from (*E*)-3-(2-(1,3-dioxolan-2-yl)-4,5-dimethoxyphenyl)-1-phenylprop-2-en-1-one (340 mg, 1.0 mmol) according to the General Procedure A in 81% yield (276 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.37 (s, 1H), 8.52 (d, J = 15.2 Hz, 1H), 8.04 – 8.02 (m, 2H), 7.64 – 7.60 (m, 1H), 7.55 – 7.51 (m, 2H), 7.45 (s, 1H), 7.34 (d, J = 15.6 Hz, 1H), 7.16 (s, 1H), 4.04 (s, 3H), 4.00 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 189.2, 153.6, 150.7, 139.8, 137.8, 133.0, 132.2, 128.7, 128.6, 128.3, 126.1, 111.2, 109.2, 56.3, 56.2.

IR (thin film) 1665, 1580, 1286, 1212 cm^{-1}.

HRMS (CI+) Calcd for $C_{18}H_{17}O_4$ (M^++H): 297.1127, Found: 297.1130.



1e

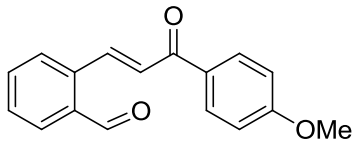
(*E*)-6-(3-Oxo-3-phenylprop-1-en-1-yl)benzo[d][1,3]dioxole-5-carbaldehyde (1e) was prepared from (*E*)-3-(6-(1,3-dioxolan-2-yl)benzo[d][1,3]dioxol-5-yl)-1-phenylprop-2-en-1-one (324 mg, 1.0 mmol) according to the General Procedure A in 73% yield (205 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.31 (s, 1H), 8.51 (d, J = 16.0 Hz, 1H), 8.03 – 8.01 (m, 2H), 7.63 – 7.59 (m, 1H), 7.54 – 7.50 (m, 2H), 7.39 (s, 1H), 7.35 (d, J = 15.2 Hz, 1H), 7.19 (s, 1H), 6.13 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 188.7, 152.6, 149.7, 139.5, 137.7, 134.4, 133.1, 130.2, 128.7, 128.6, 126.1, 109.0, 106.8, 102.5.

IR (thin film) 1661, 1613, 1481, 1271 cm^{-1}.

HRMS (CI+) Calcd for $C_{17}H_{13}O_4$ (M^++H): 281.0814, Found: 281.0816.



1f

(*E*)-2-(3-(4-Methoxyphenyl)-3-oxoprop-1-en-1-yl)benzaldehyde (1f) was prepared from **B5** (311 mg, 1.0 mmol) according to the General Procedure A in 87% yield (231 mg).

^{1}H NMR (400 MHz, $CDCl_3$) δ 10.35 (s, 1H), 8.52 (d, J = 16.0 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.91 – 7.89 (m, 1H), 7.74 – 7.72 (m, 1H), 7.66 – 7.62 (m, 1H), 7.58 – 7.54 (m, 1H), 7.37 (d, J = 15.6 Hz, 1H), 6.99 – 6.97 (m, 2H), 3.88 (s, 3H).

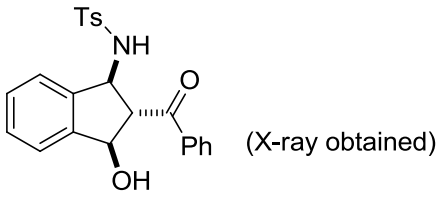
^{13}C NMR (100 MHz, $CDCl_3$) δ 191.6, 188.6, 163.6, 140.1, 137.6, 134.2, 133.9, 131.8, 131.1, 131.0, 129.8, 128.1, 127.3, 113.9, 55.5.

IR (thin film) 2891, 1658, 1606, 1261 cm^{-1}.

HRMS (CI-) Calcd for $C_{17}H_{14}O_3$ (M^+): 266.0943, Found: 266.0944.

III. Stereoselective aza-Michael/Aldol Reaction (Tables 2 and 3, Eqs. 1-3)

General Procedure B. An oven-dried 10-mL vial was charged with enone **1** (0.3 mmol, 1 equiv.) and **2** (0.45 mmol, 1.5 equiv.) in anhydrous MeCN (3 mL). The mixture was cooled to 0 °C and then DBU (9.0 μL, 0.6 mmol, 0.2 equiv.) was added. The reaction was stirred at 0 °C and monitored by TLC. Upon completion, the reaction mixture was concentrated under reduced pressure and the residue was purified by flash column chromatography to give the desired 3-amino-1-indanol product.



3a

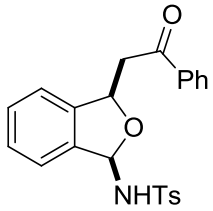
***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-methylbenzene-sulfonamide (3a, Table 2, entry 1)** was prepared from **1a** (71 mg) and $TsNH_2$ according to the General Procedure B in 92% yield (108 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.91 (d, J = 7.2 Hz, 2H), 7.90 – 7.58 (m, 3H), 7.51 – 7.47 (m, 2H), 7.37 – 7.32 (m, 4H), 7.06 (d, J = 8.0 Hz, 2H), 5.26 (d, J = 6.4 Hz, 1H), 5.20 (d, J = 6.4 Hz, 1H), 5.02 (d, J = 6.4 Hz, 1H), 4.16 – 4.13 (m, 1H), 2.21 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 200.1, 144.0, 143.7, 141.9, 139.7, 138.0, 134.1, 130.4, 129.8, 129.6, 129.5, 129.2, 127.7, 125.4, 125.1, 78.6, 65.2, 59.5, 21.4.

IR (thin film) 3452, 3267, 1169, 1155 cm^{-1}.

HRMS (CI+) Calcd for $C_{23}H_{20}NO_3S$ (M^+-OH): 390.1164, Found: 390.1172.



4a

4-Methyl-*N*-(3-(2-oxo-2-phenylethyl)-1,3-dihydroisobenzofuran-1-yl)benzene-sulfonamide (4a) was obtained as a byproduct from **1a** and $TsNH_2$ (Table 1).

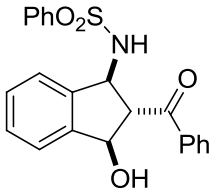
^{1}H NMR (400 MHz, acetone-d_6) δ 8.02 – 8.00 (m, 2H), 7.82 (d, J = 8.0 Hz, 2H), 7.67

– 7.63 (m, 1H), 7.56 – 7.52 (m, 2H), 7.41 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.32 (m, 3H), 7.29 – 7.25 (m, 1H), 7.20 (d, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 5.58 (d, *J* = 7.2 Hz, 1H), 5.36 – 5.34 (m, 1H), 3.98 – 3.93 (m, 1H), 3.70 – 3.63 (m, 1H), 2.06 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 198.8, 144.7, 141.3, 139.7, 137.8, 137.2, 134.3, 130.7, 130.2, 129.6, 129.1, 129.0, 128.2, 125.1, 123.6, 88.2, 60.8, 47.7, 21.4.

IR (thin film) 3450, 1678, 1597, 1164 cm^{-1}.

HRMS (CI-) Calcd for $C_{23}H_{21}NO_4S$ (M^+): 407.1191, Found: 407.1196.



3b

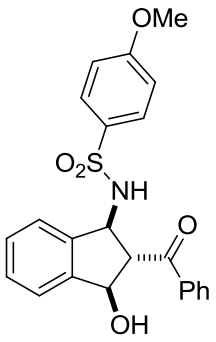
***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)benzenesulfonamide (3b, Table 2, entry 2)** was prepared from **1a** (71 mg) and benzenesulfonamide according to the General Procedure B in 88% yield (104 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.97 – 7.94 (m, 2H), 7.77 – 7.75 (m, 2H), 7.65 – 7.56 (m, 2H), 7.51 – 7.47 (m, 2H), 7.38 – 7.32 (m, 6H), 5.29 – 5.25 (m, 2H), 5.07 (d, *J* = 6.0 Hz, 1H), 4.24 – 4.21 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 200.2, 143.8, 142.4, 141.5, 138.0, 134.0, 133.0, 129.7, 129.6, 129.4, 129.1, 127.4, 125.1, 124.9, 78.3, 65.3, 59.3.

IR (thin film) 3477, 3268, 1670, 1158 cm^{-1}.

HRMS (CI) Calcd for $C_{22}H_{19}NO_4S$ (M^+): 393.1035, Found: 393.1034.



3c

***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-methoxybenzene-sulfonamide (3c, Table 2, entry 3)** was prepared from **1a** (71 mg) and $NosNH_2$

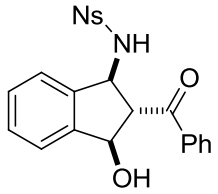
according to the General Procedure B in 84% yield (106 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.94 – 7.92 (m, 2H), 7.65 – 7.61 (m, 3H), 7.50 – 7.46 (m, 2H), 7.37 – 7.33 (m, 4H), 6.76 (d, J = 8.8 Hz, 2H), 5.26 – 5.23 (m, 2H), 5.04 (d, J = 6.4 Hz, 1H), 4.19 – 4.15 (m, 1H), 3.73 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 198.1, 161.3, 141.8, 139.7, 135.9, 132.0, 131.9, 127.6, 127.5, 127.4, 127.1, 123.2, 123.0, 112.7, 76.5, 63.1, 57.3, 53.7.

IR (thin film) 3453, 3365, 1628, 1595 cm^{-1}.

HRMS (CI) Calcd for $C_{23}H_{21}NO_5S$ (M^+): 423.1140, Found: 423.1142.



3d

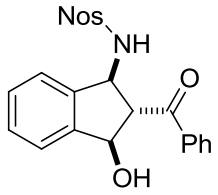
***N*-(2-benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-2-nitrobenzene-sulfonamide (3d, Table 2, entry 4)** was prepared from **1a** (71 mg) and $NsNH_2$ according to the General Procedure B in 72% yield (95 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.01 – 7.99 (m, 1H), 7.95 – 7.93 (m, 2H), 7.71 – 7.67 (m, 3H), 7.61 – 7.57 (m, 1H), 7.46 – 7.31 (m, 6H), 5.38 (d, J = 7.2 Hz, 1H), 5.34 (brs, 1H), 5.14 (d, J = 6.0 Hz, 1H), 4.84 – 4.45 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 200.4, 148.5, 143.9, 141.0, 137.8, 134.8, 134.6, 134.2, 133.5, 131.5, 129.6, 129.5, 129.2, 125.5, 125.0, 124.8, 78.1, 64.8, 60.1.

IR (thin film) 3318, 3096, 1538, 1165 cm^{-1}.

HRMS (CI-) Calcd for $C_{22}H_{18}N_2O_6S$ (M^+): 438.0886, Found: 438.0881.



3e

***N*-(2-benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-nitrobenzene-sulfonamide (3e, Table 2, entry 5)** was prepared from **1a** (71 mg) and $NosNH_2$ according to the General Procedure B in 89% yield (117 mg).

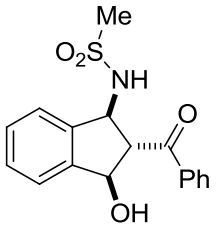
^{1}H NMR (400 MHz, acetone-d_6) δ 8.11 – 8.09 (m, 2H), 7.99 – 7.97 (m, 2H), 7.90 –

7.88 (m, 2H), 7.62 – 7.58 (m, 1H), 7.46 – 7.42 (m, 6H), 5.37 (d, *J* = 7.6 Hz, 1H), 5.09 (d, *J* = 6.8 Hz, 1H), 4.25 – 4.21 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 200.6, 151.0, 148.5, 144.4, 141.6, 138.0, 134.9, 130.2, 130.1, 130.0, 129.7, 129.5, 125.6, 125.5, 78.9, 65.5, 60.1.

IR (thin film) 3410, 3106, 1705, 1529 cm^{-1}.

HRMS (CI) Calcd for $C_{22}H_{18}N_2O_6S$ (M^+): 438.0886, Found: 438.0889.



3f

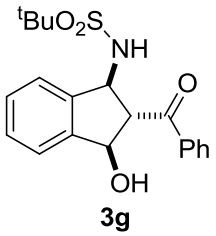
***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)methanesulfonamide (3f, Table 2, entry 6)** was prepared from **1a** (71 mg) and $MsNH_2$ according to the General Procedure B in 82% yield (81 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.22 – 8.20 (m, 2H), 7.71 – 7.67 (m, 1H), 7.60 – 7.56 (m, 2H), 7.53 – 7.52 (m, 1H), 7.41 – 7.37 (m, 3H), 6.79 (d, *J* = 8.8 Hz, 1H), 5.34 – 5.29 (m, 2H), 5.20 – 5.17 (m, 1H), 4.39 (dd, J_1 = 8.0 Hz, J_2 = 7.6 Hz, 1H), 2.87 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 201.3, 143.8, 141.9, 138.7, 134.3, 130.0, 129.5, 129.4, 129.4, 125.2, 124.8, 77.5, 66.1, 59.0, 41.5.

IR (thin film) 3336, 3141, 1664, 1110 cm^{-1}.

HRMS (CI-) Calcd for $C_{17}H_{17}NO_4S$ (M^+): 331.0878, Found: 331.0874.



3g

***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-2-methylpropane-2-sulfonamide (3g, Table 2, entry 7)** was prepared from **1a** (71 mg) and 2-methylpropane-2-sulfonamide according to the General Procedure B in 84% yield (94 mg).

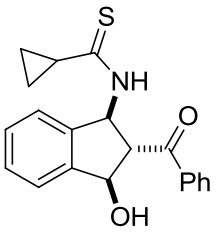
^{1}H NMR (400 MHz, acetone-d_6) δ 8.22 – 8.20 (m, 2H), 7.69 – 7.67 (m, 1H), 7.62 – 7.57 (m, 3H), 7.40 – 7.39 (m, 3H), 7.33 (d, *J* = 10.0 Hz, 1H), 5.25 – 5.21 (m, 3H), 4.44

(dd, J_1 = 8.0 Hz, J_2 = 6.8 Hz, 1H), 1.22 (s, 9H).

^{13}C NMR (100 MHz, acetone-d_6) δ 201.4, 144.0, 142.6, 138.9, 134.3, 129.7, 129.5, 129.3, 129.2, 125.4, 124.7, 77.8, 65.4, 61.4, 59.8, 24.4.

IR (thin film) 3436, 3278, 1674, 1125 cm^{-1}.

HRMS (CI) Calcd for $C_{20}H_{23}NO_4S$ (M^+): 373.1348, Found: 373.1340.



(X-ray obtained)

3h

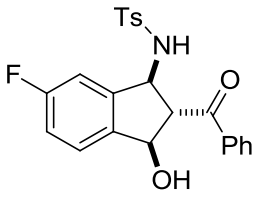
***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)cyclopropanecarbothioamide (3h, Table 2, entry 8)** was prepared from **1a** (71 mg) and cyclopropanecarbothioamide according to the General Procedure B in 86% yield (87 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 9.66 (d, J = 5.6 Hz, 1H), 8.13 – 8.11 (m, 2H), 7.67 – 7.63 (m, 1H), 7.56 – 7.52 (m, 2H), 7.46 – 7.44 (m, 1H), 7.42 – 7.30 (m, 3H), 6.52 – 6.48 (m, 1H), 5.38 – 5.35 (m, 1H), 5.27 (d, J = 6.4 Hz, 1H), 4.38 – 4.35 (m, 1H), 2.14 – 2.10 (m, 1H), 1.02 – 0.99 (m, 1H), 0.89 – 0.84 (m, 1H), 0.82 – 0.80 (m, 2H).

^{13}C NMR (100 MHz, acetone-d_6) δ 208.5, 200.0, 145.0, 141.3, 138.3, 134.0, 130.0, 129.5, 129.4, 129.3, 125.4, 125.1, 77.7, 64.2, 61.4, 23.8, 12.0, 11.9.

IR (thin film) 3408, 3350, 1665, 1448 cm^{-1}.

HRMS (CI) Calcd for $C_{20}H_{20}NO_2S$ (M^++H): 338.1215, Found: 338.1211.



3i

***N*-(2-Benzoyl-6-fluoro-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-methylbenzenesulfonamide (3i, Table 3, entry 1)** was prepared from **1b** (76 mg) and $TsNH_2$ according to the General Procedure B in 87% yield (111 mg).

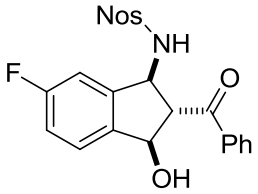
^{1}H NMR (400 MHz, acetone-d_6) δ 7.92 – 7.90 (m, 2H), 7.66 – 7.64 (m, 1H), 7.62 – 7.59 (m, 2H), 7.51 – 7.47 (m, 2H), 7.40 – 7.37 (m, 1H), 7.28 (bs, 1H), 7.18 – 7.15 (m,

1H), 7.13 – 7.07 (m, 2H), 7.03 – 7.00 (m, 1H), 5.25 (d, *J* = 6.8 Hz, 1H), 5.01 (d, *J* = 6.4 Hz, 1H), 4.24 – 4.20 (m, 1H), 2.22 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.5, 164.1 (d, *J* = 240 Hz), 144.2 (d, *J* = 8.2Hz), 143.6, 139.6 (d, *J* = 2.3 Hz), 139.2, 137.6, 134.0, 130.2, 129.6, 129.0, 127.4, 126.7 (d, *J* = 8.9 Hz), 116.6 (d, *J* = 23.1 Hz), 111.5 (d, *J* = 23.0 Hz), 77.5, 65.1, 58.8 (d, *J* = 1.9 Hz), 21.2.

IR (thin film) 3452, 3267, 1704, 1157 cm^{-1}.

HRMS (CI-) Calcd for $C_{23}H_{20}FNO_4S$ (M^+): 425.1097, Found: 425.1093.



3j

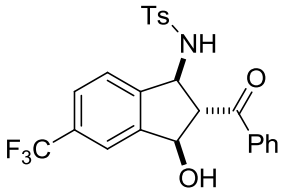
***N*-(2-Benzoyl-6-fluoro-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-nitrobenzene-sulfonamide (3j, Table 3, entry 2)** was prepared from **1b** (76 mg) and $NsNH_2$ according to the General Procedure B in 80% yield (109 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.06 (d, *J* = 8.0 Hz, 2H), 7.94 (d, *J* = 8.8 Hz, 2H), 7.85 – 7.83 (m, 2H), 7.45 – 7.37 (m, 4H), 7.16 – 7.13 (m, 2H), 5.30 (d, *J* = 8.0 Hz, 1H), 5.02 (d, *J* = 6.8 Hz, 1H), 4.26 – 4.22 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.6, 164.2 (d, *J* = 250 Hz), 150.4, 147.6, 143.5 (d, *J* = 8.0 Hz), 139.5 (d, *J* = 2.2 Hz), 137.1, 134.3, 129.5, 129.2, 129.0, 124.9, 116.8 (d, *J* = 23.1 Hz), 111.4 (d, *J* = 23.0 Hz), 77.5, 65.0, 58.9 (d, *J* = 1.9 Hz).

IR (thin film) 3488, 3268, 1530, 1349 cm^{-1}.

HRMS (CI) Calcd for $C_{22}H_{17}FN_2O_6S$ (M^+): 456.0791, Found: 456.0794.



3k

***N*-(2-Benzoyl-3-hydroxy-5-(trifluoromethyl)-2,3-dihydro-1H-inden-1-yl)-4-methylbenzenesulfonamide (3k, Table 3, entry 3)** was prepared from **1c** (91 mg) and $TsNH_2$ according to the General Procedure B in 93% yield (132 mg).

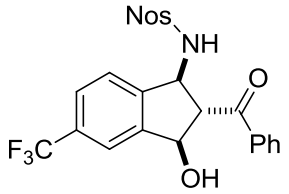
^{1}H NMR (400 MHz, acetone-d_6) δ 7.91 (d, *J* = 7.6 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 1H),

7.68 – 7.63 (m, 2H), 7.59 – 7.56 (m, 3H), 7.51 – 7.47 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 5.44 (d, *J* = 6.8 Hz, 1H), 5.34 – 5.29 (m, 1H), 5.16 – 5.12 (m, 1H), 4.30 – 4.26 (m, 1H), 2.22 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.6, 146.3, 145.1, 143.8, 139.4, 137.8, 134.2, 131.3 (d, *J* = 31.5 Hz), 130.4, 129.7, 129.2, 127.9 (q, *J* = 118.6 Hz), 127.6, 126.6 (d, *J* = 3.6 Hz), 126.3, 122.0 (d, *J* = 4.0 Hz), 77.8, 65.1, 59.2, 21.4.

IR (thin film) 3264, 2916, 1669, 1331 cm^{-1}.

HRMS (CI) Calcd for $C_{24}H_{20}F_3NO_4S$ (M^+): 475.1065, Found: 475.1065.



3l

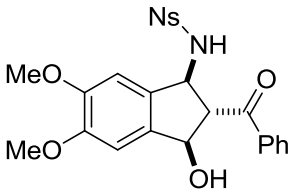
***N*-(2-Benzoyl-3-hydroxy-5-(trifluoromethyl)-2,3-dihydro-1H-inden-1-yl)-4-nitrobenzenesulfonamide (3l, Table 3, entry 4)** was prepared from **1c** (91 mg) and $NosNH_2$ according to the General Procedure B in 82% yield (124 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.08 – 8.06 (m, 2H), 7.96 – 7.93 (m, 2H), 7.86 – 7.83 (m, 2H), 7.78 (d, *J* = 7.6 Hz, 1H), 7.69 – 7.65 (m, 2H), 7.59 – 7.58 (m, 1H), 7.43 – 7.39 (m, 2H), 5.55 (brs, 1H), 5.39 (d, *J* = 8.0 Hz, 1H), 5.15 (d, *J* = 6.8 Hz, 1H), 4.33 – 4.29 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.5, 150.5, 147.7, 145.6, 145.0, 137.2, 134.5, 131.5 (q, *J* = 31.6 Hz), 129.6, 129.2, 129.0, 126.6 (d, *J* = 3.7 Hz), 126.1, 125.1, 121.9 (d, *J* = 3.9 Hz), 77.6, 64.9, 59.2.

IR (thin film) 3452, 3270, 1674, 1532 cm^{-1}.

HRMS (CI-) Calcd for $C_{23}H_{17}F_3N_2O_6S$ (M^+): 506.0759, Found: 506.0758.



3m

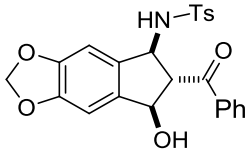
***N*-(2-Benzoyl-3-hydroxy-5,6-dimethoxy-2,3-dihydro-1H-inden-1-yl)-2-nitrobenzenesulfonamide (3m, Table 3, entry 5)** was prepared from **1d** (89 mg) and $NsNH_2$ according to the General Procedure B in 84% yield (125 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.03 – 8.01 (m, 1H), 7.98 – 7.96 (m, 2H), 7.76 – 7.74 (m, 1H), 7.72 – 7.68 (m, 2H), 7.63 – 7.59 (m, 1H), 7.49 – 7.45 (m, 2H), 6.91 (s, 1H), 6.69 (s, 1H), 5.31 (d, J = 6.4 Hz, 1H), 5.05 – 5.00 (m, 2H), 4.39 – 4.36 (m, 1H), 3.80 (s, 3H), 3.70 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 200.3, 151.8, 151.7, 137.8, 135.9, 135.0, 134.7, 134.3, 133.7, 132.8, 131.8, 129.7, 129.4, 125.7, 107.9, 107.4, 78.5, 65.4, 60.2, 56.3, 56.2.

IR (thin film) 3491, 3305, 1706, 1539 cm^{-1}.

HRMS (CI-) Calcd for $C_{24}H_{22}N_2O_8S$ (M^+): 498.1097, Found: 498.1095.



3n

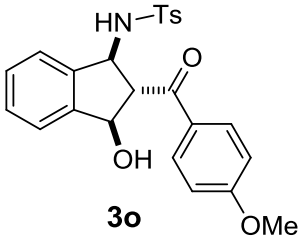
***N*-(6-Benzoyl-7-hydroxy-6,7-dihydro-5H-indeno[5,6-d][1,3]dioxol-5-yl)-4-methylbenzenesulfonamide (3n, Table 3, entry 6)** was prepared from **1e** (84 mg) and $TsNH_2$ according to the General Procedure B in 86% yield (114 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.91 – 7.89 (m, 2H), 7.65 – 7.62 (m, 1H), 7.62 – 7.58 (m, 2H), 7.50 – 7.46 (m, 2H), 7.07 (d, J = 8.0 Hz, 2H), 6.76 (s, 1H), 6.69 (s, 1H), 6.04 (s, 1H), 6.00 (s, 1H), 5.13 (bs, 2H), 4.88 (d, J = 5.6 Hz, 1H), 4.11 – 4.08 (m, 1H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.7, 149.7, 143.6, 139.4, 137.7, 137.3, 135.0, 134.0, 130.3, 130.0, 129.1, 127.6, 104.8, 104.7, 102.5, 78.1, 65.3, 59.0, 21.3.

IR (thin film) 3275, 2896, 1672, 1476 cm^{-1}.

HRMS (CI) Calcd for $C_{24}H_{21}NO_6S$ (M^+): 451.1090, Found: 451.1097.



3o

***N*-(3-Hydroxy-2-(4-methoxybenzoyl)-2,3-dihydro-1H-inden-1-yl)-4-methylbenzenesulfonamide (3o, Table 3, entry 7)** was prepared from **1e** (80 mg) and $TsNH_2$ according to the General Procedure B in 89% yield (117 mg).

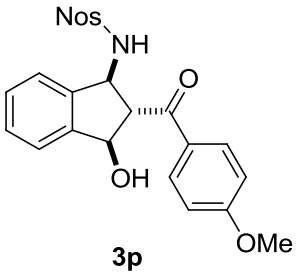
^{1}H NMR (400 MHz, acetone-d_6) δ 7.86 (d, J = 9.2 Hz, 2H), 7.57 (d, J = 8.4 Hz, 2H),

7.35 (m, 4H), 7.14 (d, *J* = 8.4 Hz, 1H), 7.06 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.8 Hz, 2H), 5.26 – 5.22 (m, 1H), 5.16 (d, *J* = 6.4 Hz, 1H), 5.02 – 4.99 (m, 1H), 4.09 – 4.07 (m, 1H), 3.93 (s, 3H), 2.22 (s, 3H).

^{13}C NMR (100 MHz, acetone-*d*$_6$) δ 196.8, 163.2, 142.5, 142.0, 140.4, 138.2, 130.6, 129.6, 128.7, 128.0, 127.9, 126.1, 123.8, 123.5, 112.7, 77.0, 63.3, 57.9, 54.5, 19.8.

IR (thin film) 3470, 3270, 1663, 1153 cm^{-1}.

HRMS (CI) Calcd for $C_{24}H_{23}NO_5S$ (M^+): 437.1297, Found: 437.1296.



3p

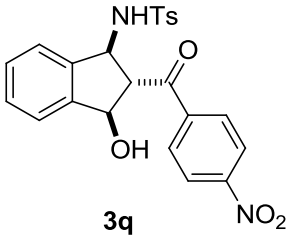
***N*-(3-Hydroxy-2-(4-methoxybenzoyl)-2,3-dihydro-1H-inden-1-yl)-4-nitrobenzenesulfonamide (3p, Table 3, entry 8)** was prepared from **1f** (80 mg) and $NsNH_2$ according to the General Procedure B in 80% yield (112 mg).

^{1}H NMR (400 MHz, acetone-*d*$_6$) δ 8.05 – 8.03 (m, 2H), 8.03 – 7.92 (m, 2H), 7.91 – 7.77 (m, 2H), 7.44 – 7.34 (m, 4H), 6.92 – 6.86 (m, 2H), 5.27 (d, *J* = 7.6 Hz, 1H), 5.24 (bs, 1H), 5.01 (d, *J* = 6.4 Hz, 1H), 4.11 – 4.07 (m, 1H), 3.88 (s, 3H).

^{13}C NMR (100 MHz, acetone-*d*$_6$) δ 198.4, 165.0, 150.3, 148.1, 144.0, 141.2, 132.0, 131.2, 129.7, 129.6, 129.0, 125.1, 125.0, 124.9, 114.2, 78.4, 64.6, 59.7, 56.0.

IR (thin film) 3238, 1656, 1348, 1164 cm^{-1}.

HRMS (CI) Calcd for $C_{23}H_{20}N_2O_7S$ (M^+): 468.0991, Found: 468.0989.



3q

***N*-(3-Hydroxy-2-(4-nitrobenzoyl)-2,3-dihydro-1H-inden-1-yl)-4-methylbenzenesulfonamide (3q, Table 3, entry 9)** was prepared from **1f** (84 mg) and $TsNH_2$ according to the General Procedure B in 90% yield (112 mg).

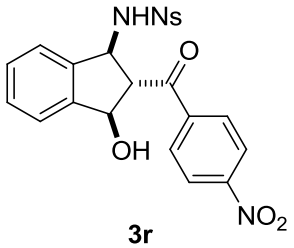
^{1}H NMR (400 MHz, Acetone-*d6*) δ 8.32 (d, *J* = 8.4 Hz, 2H), 8.14 (d, *J* = 8.4 Hz, 2H), 7.62 (d, *J* = 8.0 Hz, 2H), 7.40 – 7.34 (m, 5H), 7.12 (d, *J* = 8.4 Hz, 2H), 5.36 (brs, 1H),

5.27 – 5.23 (m, 1H), 5.11 (d, *J* = 6.4 Hz, 1H), 4.24 – 4.20 (m, 1H), 2.20 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 197.7, 149.9, 142.3, 142.0, 140.8, 139.6, 138.0, 129.4, 128.9, 128.2, 126.2, 123.7, 123.5, 122.8, 77.0, 64.4, 57.9, 19.8.

IR (thin film) 3482, 3302, 1674, 1159 cm^{-1}.

HRMS (CI) Calcd for $C_{23}H_{20}N_2O_6S$ (M^+): 452.1042, Found: 452.1041.



3r

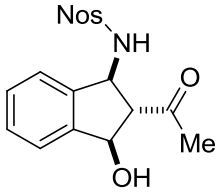
***N*-(3-Hydroxy-2-(4-nitrobenzoyl)-2,3-dihydro-1H-inden-1-yl)-2-nitrobenzene-sulfonamide (3r, Table 3, entry 10)** was prepared from **1f** (84 mg) and $NsNH_2$ according to the General Procedure B in 76% yield (110 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.31 – 8.29 (m, 2H), 8.19 – 8.17 (m, 2H), 8.05 – 8.02 (m, 1H), 7.76 – 7.75 (m, 3H), 7.41 – 7.36 (m, 3H), 7.32 (d, *J* = 5.6 Hz, 1H), 5.41 – 5.32 (m, 2H), 5.19 (d, *J* = 6.4 Hz, 1H), 4.53 – 4.50 (m, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 199.7, 151.5, 143.7, 142.2, 140.7, 135.0, 134.5, 133.6, 131.7, 130.9, 129.8, 129.7, 125.6, 125.0, 124.9, 124.4, 78.0, 65.6, 60.6.

IR (thin film) 3349, 1602, 1347, 1165 cm^{-1}.

HRMS (CI) Calcd for $C_{22}H_{17}N_3O_8S$ (M^+): 483.0736, Found: 483.0732.



3s

***N*-(2-Acetyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-4-nitrobenzenesulfonamide (3s, Table 3, entry 11)** was prepared from **1h** (52 mg) and $TsNH_2$ according to the General Procedure B in 84% yield (95 mg).

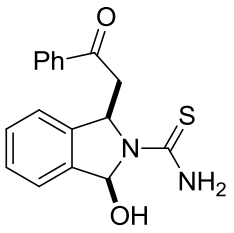
^{1}H NMR (400 MHz, acetone-d_6) δ 8.47 (d, *J* = 8.8 Hz, 2H), 8.19 (d, *J* = 8.8 Hz, 2H), 7.35 – 7.29 (m, 3H), 7.21 (d, *J* = 6.8 Hz, 1H), 5.05 (d, *J* = 8.0 Hz, 1H), 4.99 (d, *J* = 6.0 Hz, 1H), 3.35 – 3.31 (m, 1H), 2.14 (s, 3H).

^{13}C NMR (100 MHz, acetone-d_6) δ 207.2, 151.0, 148.4, 143.8, 140.7, 129.5, 129.4,

125.3, 125.0, 124.9, 76.5, 70.8, 57.5, 31.0.

IR (thin film) 3410, 1705, 1529, 1349 cm^{-1}.

HRMS (CI) Calcd for $C_{17}H_{16}N_2O_6S$ (M^+): 376.0729, Found: 376.0724.



5a

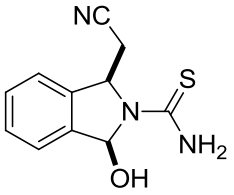
1-Hydroxy-3-(2-oxo-2-phenylethyl)isoindoline-2-carbothioamide (5a, Equation 1) was prepared from **1a** (71 mg) and thiourea according to the General Procedure B in 84% yield (79 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.04 – 8.00 (m, 1H), 7.64 – 7.62 (m, 2H), 7.56 – 7.54 (m, 1H), 7.44 – 7.41 (m, 3H), 7.40 – 7.33 (m, 2H), 6.87 (s, 1H), 5.83 (s, 1H), 5.36 – 5.33 (m, 1H), 5.25 (d, J = 3.2 Hz, 1H), 2.73 – 2.69 (m, 1H), 1.70 (t, J = 12.8 Hz, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 177.8, 145.0, 140.0, 138.5, 130.2, 129.0, 128.9, 126.3, 125.0, 122.9, 88.0, 82.1, 57.4, 42.2.

IR (thin film) 3381, 1706, 1470, 759 cm^{-1}.

HRMS (CI) Calcd for $C_{17}H_{16}N_2O_2S$ (M^+): 312.0932, Found:312.0937.



5b

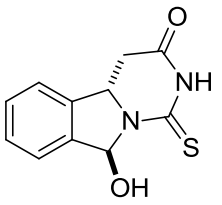
1-(Cyanomethyl)-3-hydroxyisoindoline-2-carbothioamide (5b, Equation 2) was prepared from **1i** (47 mg) and thiourea according to the General Procedure B in 90% yield (63 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 7.49 – 7.37 (m, 5H), 6.70 (s, 1H), 6.23 (brs, 1H), 5.05 (dd, J_1 = 14.0 Hz, J_2 = 4.0 Hz, 1H), 3.17 (dd, J_1 = 15.2 Hz, J_2 = 4.4 Hz, 1H), 2.33 (t, J = 14.4 Hz, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 162.8, 139.0, 138.4, 129.3, 128.6, 124.2, 122.4, 86.0, 56.9, 30.4.

IR (thin film) 3408, 3350, 1658, 1464 cm^{-1}.

HRMS (CI) Calcd for $C_{11}H_{11}N_3OS$ (M^+): 233.0623, Found: 233.0617.



(X-ray obtained)

5c

9-Hydroxy-1-thioxo-1,2,4,4a-tetrahydropyrimido[6,1-a]isoindol-3(9H)-one (5c, Equation 3) was prepared from **1j** (71 mg) and thiourea according to the General Procedure B in 91% yield (64 mg).

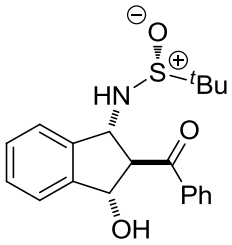
^{1}H NMR (400 MHz, acetone-d_6) δ 10.07 (brs, 1H), 7.59 – 7.57 (m, 1H), 7.52 – 7.48 (m, 3H), 6.78 (s, 1H), 5.49 – 5.43 (m, 1H), 3.26 (dd, J_1 = 16.0 Hz, J_2 = 4.4 Hz, 1H), 2.80 (s, 1H), 2.69 (dd, J_1 = 16.0 Hz, J_2 = 13.6 Hz, 1H).

^{13}C NMR (100 MHz, acetone-d_6) δ 177.1, 165.4, 137.6, 136.9, 129.2, 128.2, 123.8, 121.7, 86.0, 58.1, 34.5.

IR (thin film) 3414, 3238, 1709, 1511 cm^{-1}.

HRMS (CI) Calcd for $C_{11}H_{10}N_2O_2S$ (M^+): 234.0463, Found: 234.0465.

IV. Synthesis of Enantioenriched 3-Amino-1-indanol Derivatives (Scheme 2)



(X-ray obtained)

3t

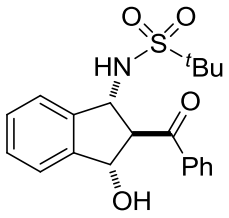
***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-2-methylpropane-2-sulfinamide (3t)** was prepared from **1a** (71 mg) and (*R*)-*tert*-butanesulfinamide according to the General Procedure B in 81% yield (87 mg).

^{1}H NMR (400 MHz, acetone-d_6) δ 8.20 – 8.18 (m, 2H), 7.71 – 7.64 (m, 2H), 7.58 – 7.54 (m, 2H), 7.41 – 7.36 (m, 3H), 5.30 (d, J = 6.8 Hz, 1H), 5.24 – 5.19 (m, 2H), 5.09 – 5.05 (m, 1H), 4.45 – 4.42 (m, 1H), 1.07 (s, 9H).

^{13}C NMR (100 MHz, acetone-d_6) δ 201.5, 144.4, 142.5, 139.0, 134.2, 129.8, 129.5, 129.2, 129.1, 126.0, 124.7, 77.3, 66.5, 64.8, 56.2, 23.0.

IR (thin film) 3297, 2959, 1705, 1039 cm^{-1}.

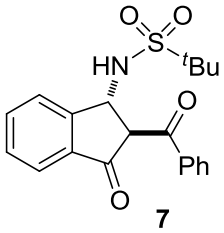
HRMS (CI) Calcd for $C_{20}H_{23}NO_3S$ (M^+): 357.1399, Found: 357.1394.



6

***N*-(2-Benzoyl-3-hydroxy-2,3-dihydro-1H-inden-1-yl)-2-methylpropane-2-sulfonamide (6).** To a solution of **3t** (107 mg, 0.3 mmol) in DCM (12 mL) was added mCPBA (85%, 91 mg, 0.45 mmol). The reaction mixture was stirred at room temperature for 1h and quenched with 5 mL saturated aqueous Na_2SO_3 at 0℃. The mixture was stirred for 5 min at the same temperature. The reaction mixture was extracted with DCM and washed with saturated aqueous $NaHCO_3$. The combined organic layers were washed with brine, dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by flash column chromatography to afford sulfonamide **6** in 84% yield (94 mg).

The characterization data are in agreement with those of compound **3g**.
$[\alpha]_D^{1}$: +130.1 (*c* = 5.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 30.0% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 17.8 min (major), 13.0 min (minor).

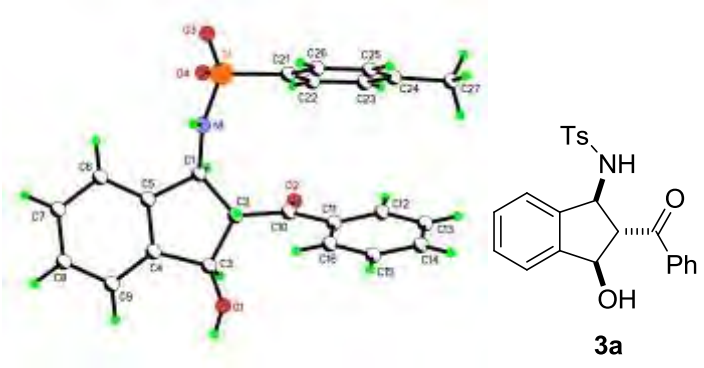


7

***N*-(2-Benzoyl-3-oxo-2,3-dihydro-1H-inden-1-yl)-2-methylpropane-2-sulfonamide** (**7**). To a solution of **6** (37 mg, 0.1 mmol) in DCM (1 mL) was added MnO_2 (435 mg, 5.0 mmol, 50 equiv). The reaction mixture was stirred at room temperature for 3h and filtered through a pad of celite and the filtrate was concentrated under reduced pressure. Purification of the residue by column chromatography recovered starting material (8.7 mg) and afforded the pure product **7** (24 mg, 83% yield based on the recovered starting material).
^{1}H NMR (400 MHz, acetone-d_6) δ 8.16 (d, *J* = 7.2 Hz, 2H), 8.12 (d, *J* = 8.0 Hz, 1H), 7.99 – 7.86 (m, 1H), 7.74 – 7.69 (m, 2H), 7.64 – 7.60 (m, 3H), 6.58 (d, *J* = 10 Hz, 1H), 5.77 – 5.74 (m, 1H), 5.14 (d, *J* = 3.2 Hz, 1H), 1.37 (s, 9H).
^{13}C NMR (100 MHz, acetone-d_6) δ 198.1, 195.2, 154.9, 138.0, 137.0, 136.0, 134.6, 130.7, 130.5, 129.7, 127.6, 124.4, 66.2, 60.3, 57.7, 24.6.
IR (thin film) 3553, 3279, 1719, 1674 cm^{-1}.
HRMS (CI) Calcd for $C_{20}H_{21}NO_4S$ (M^+): 371.1191, Found: 371.1188.
$[\alpha]_D^{2}$: +50.7 (*c* = 5.0, $CHCl_3$). HPLC analysis of the product: Daicel CHIRALPAK AD-H column; 20.0% *i*-PrOH in hexanes; 1.0 mL/min; retention times: 13.1 min (major), 26.3 min (minor).

V. Structure and Stereochemistry Determination (X-Ray)

The crystal structures of **3a**, **3h**, **5c** and **3t** have been deposited at the Cambridge Crystallographic Data Centre and allocated deposition numbers are CCDC 902390 (**3a**), CCDC 902391 (**3h**), CCDC 904189 (**5c**) and CCDC 902392 (**3t**).



3a

Table 1. Crystal data and structure refinement for qian1MoLT.

Identification code	qian1molt	
Empirical formula	C23 H21 N O4 S	
Formula weight	407.47	
Temperature	173.00(14) K	
Wavelength	0.7107 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 17.9255(5) Å	α= 90 °.
	b = 9.5117(2) Å	β= 102.966(3) °.
	c = 24.5699(8) Å	γ = 90 °.
Volume	4082.41(19) $Å^3$	
Z	8	
Density (calculated)	1.326 Mg/m^3	
Absorption coefficient	0.188 mm^{-1}	
F(000)	1712	
Crystal size	0.35 x 0.28 x 0.24 mm^3	
Theta range for data collection	3.34 to 26.99 °.	
Index ranges	-22<=h<=22, -12<=k<=12, -31<=l<=19	
Reflections collected	11559	
Independent reflections	4353 [R(int) = 0.0327]	

Completeness to theta = 25.00 °	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.97783
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4353 / 0 / 264
Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0480, wR2 = 0.1015
R indices (all data)	R1 = 0.0588, wR2 = 0.1079
Largest diff. peak and hole	0.287 and -0.332 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for qian1MoLT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1517(1)	4367(1)	3125(1)	25(1)
O(3)	2350(1)	10615(1)	2987(1)	27(1)
O(4)	1938(1)	7826(1)	4101(1)	31(1)
O(2)	759(1)	4484(1)	3215(1)	35(1)
O(1)	1703(1)	3223(1)	2793(1)	32(1)
N(1)	1710(1)	5750(2)	2815(1)	26(1)
C(1)	1461(1)	7149(2)	2932(1)	21(1)
C(2)	2114(1)	8177(2)	3185(1)	20(1)
C(3)	1760(1)	9639(2)	3023(1)	22(1)
C(4)	1194(1)	9357(2)	2479(1)	24(1)
C(5)	1035(1)	7932(2)	2421(1)	23(1)
C(6)	524(1)	7421(2)	1954(1)	31(1)
C(7)	172(1)	8381(2)	1550(1)	37(1)
C(8)	326(1)	9802(2)	1612(1)	39(1)
C(9)	838(1)	10314(2)	2079(1)	33(1)
C(10)	2401(1)	8024(2)	3813(1)	22(1)
C(11)	3234(1)	8155(2)	4072(1)	23(1)
C(12)	3485(1)	7824(2)	4636(1)	33(1)
C(13)	4245(1)	7977(2)	4897(1)	42(1)
C(14)	4766(1)	8462(2)	4603(1)	40(1)
C(15)	4525(1)	8779(3)	4044(1)	44(1)
C(16)	3761(1)	8626(2)	3779(1)	35(1)
C(21)	2147(1)	4255(2)	3787(1)	28(1)
C(22)	1881(1)	4505(2)	4266(1)	38(1)
C(23)	2382(1)	4437(2)	4781(1)	45(1)
C(24)	3150(1)	4147(2)	4831(1)	44(1)
C(25)	3406(1)	3896(3)	4350(1)	50(1)
C(26)	2908(1)	3947(2)	3829(1)	42(1)
C(27)	3698(2)	4153(3)	5395(1)	64(1)

Table 3. Bond lengths [Å] and angles [°] for qian1MoLT.

S(1)-O(2)	1.4290(13)
S(1)-O(1)	1.4433(13)
S(1)-N(1)	1.5978(15)
S(1)-C(21)	1.7640(19)
O(3)-C(3)	1.425(2)
O(4)-C(10)	1.2196(19)
N(1)-C(1)	1.453(2)
C(1)-C(2)	1.544(2)
C(1)-C(5)	1.512(2)
C(2)-C(3)	1.544(2)
C(2)-C(10)	1.521(2)
C(3)-C(4)	1.509(2)
C(4)-C(5)	1.386(2)
C(4)-C(9)	1.385(2)
C(5)-C(6)	1.385(2)
C(6)-C(7)	1.392(3)
C(7)-C(8)	1.382(3)
C(8)-C(9)	1.387(3)
C(10)-C(11)	1.490(2)
C(11)-C(12)	1.392(2)
C(11)-C(16)	1.385(2)
C(12)-C(13)	1.378(3)
C(13)-C(14)	1.380(3)
C(14)-C(15)	1.378(3)
C(15)-C(16)	1.385(3)
C(21)-C(22)	1.385(3)
C(21)-C(26)	1.376(3)
C(22)-C(23)	1.378(3)
C(23)-C(24)	1.382(3)
C(24)-C(25)	1.379(3)
C(24)-C(27)	1.509(3)
C(25)-C(26)	1.387(3)
O(2)-S(1)-O(1)	119.71(8)

O(2)-S(1)-N(1)	109.02(8)
O(2)-S(1)-C(21)	107.22(8)
O(1)-S(1)-N(1)	104.41(8)
O(1)-S(1)-C(21)	107.06(8)
N(1)-S(1)-C(21)	109.10(8)
C(1)-N(1)-S(1)	123.34(12)
N(1)-C(1)-C(2)	114.84(14)
N(1)-C(1)-C(5)	113.95(14)
C(5)-C(1)-C(2)	102.59(13)
C(3)-C(2)-C(1)	103.66(13)
C(10)-C(2)-C(1)	113.66(13)
C(10)-C(2)-C(3)	111.97(13)
O(3)-C(3)-C(2)	109.58(13)
O(3)-C(3)-C(4)	114.92(14)
C(4)-C(3)-C(2)	102.94(13)
C(5)-C(4)-C(3)	110.31(15)
C(9)-C(4)-C(3)	128.49(16)
C(9)-C(4)-C(5)	121.17(17)
C(4)-C(5)-C(1)	109.98(14)
C(6)-C(5)-C(1)	129.20(17)
C(6)-C(5)-C(4)	120.75(17)
C(5)-C(6)-C(7)	118.09(18)
C(8)-C(7)-C(6)	121.02(18)
C(7)-C(8)-C(9)	120.89(18)
C(4)-C(9)-C(8)	118.07(19)
O(4)-C(10)-C(2)	118.87(15)
O(4)-C(10)-C(11)	120.79(15)
C(11)-C(10)-C(2)	120.31(14)
C(12)-C(11)-C(10)	118.39(15)
C(16)-C(11)-C(10)	122.65(15)
C(16)-C(11)-C(12)	118.93(16)
C(13)-C(12)-C(11)	120.30(18)
C(12)-C(13)-C(14)	120.40(18)
C(15)-C(14)-C(13)	119.79(18)
C(14)-C(15)-C(16)	120.06(19)
C(15)-C(16)-C(11)	120.52(18)

C(22)-C(21)-S(1)	120.10(15)
C(26)-C(21)-S(1)	120.06(14)
C(26)-C(21)-C(22)	119.82(18)
C(23)-C(22)-C(21)	119.5(2)
C(22)-C(23)-C(24)	121.5(2)
C(23)-C(24)-C(27)	120.8(2)
C(25)-C(24)-C(23)	118.27(19)
C(25)-C(24)-C(27)	121.0(2)
C(24)-C(25)-C(26)	121.0(2)
C(21)-C(26)-C(25)	119.84(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for qian1MoLT. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	30(1)	17(1)	28(1)	1(1)	7(1)	-1(1)
O(3)	32(1)	17(1)	33(1)	0(1)	8(1)	-2(1)
O(4)	31(1)	40(1)	23(1)	2(1)	10(1)	-2(1)
O(2)	31(1)	32(1)	45(1)	6(1)	13(1)	-4(1)
O(1)	46(1)	18(1)	32(1)	-3(1)	6(1)	1(1)
N(1)	36(1)	18(1)	29(1)	-1(1)	16(1)	1(1)
C(1)	24(1)	19(1)	22(1)	-1(1)	7(1)	1(1)
C(2)	22(1)	19(1)	20(1)	1(1)	6(1)	1(1)
C(3)	25(1)	18(1)	23(1)	1(1)	6(1)	1(1)
C(4)	25(1)	25(1)	22(1)	1(1)	6(1)	2(1)
C(5)	23(1)	26(1)	21(1)	-1(1)	7(1)	0(1)
C(6)	29(1)	34(1)	28(1)	-4(1)	6(1)	-7(1)
C(7)	29(1)	54(1)	24(1)	-1(1)	-1(1)	-7(1)
C(8)	36(1)	46(1)	31(1)	12(1)	-1(1)	6(1)
C(9)	36(1)	29(1)	32(1)	5(1)	3(1)	4(1)
C(10)	28(1)	17(1)	20(1)	1(1)	7(1)	2(1)
C(11)	27(1)	21(1)	22(1)	1(1)	4(1)	2(1)
C(12)	36(1)	38(1)	24(1)	4(1)	7(1)	1(1)
C(13)	42(1)	53(1)	25(1)	5(1)	-4(1)	4(1)
C(14)	28(1)	50(1)	38(1)	-4(1)	-3(1)	1(1)
C(15)	30(1)	61(2)	42(1)	7(1)	8(1)	-6(1)
C(16)	31(1)	48(1)	26(1)	6(1)	4(1)	-3(1)
C(21)	37(1)	20(1)	27(1)	1(1)	9(1)	1(1)
C(22)	46(1)	38(1)	34(1)	-1(1)	16(1)	6(1)
C(23)	67(2)	42(1)	28(1)	-1(1)	14(1)	11(1)
C(24)	64(2)	30(1)	31(1)	-3(1)	-2(1)	14(1)
C(25)	43(1)	64(2)	39(1)	-7(1)	0(1)	16(1)
C(26)	38(1)	56(1)	32(1)	-4(1)	9(1)	9(1)
C(27)	87(2)	57(2)	37(1)	-11(1)	-10(1)	27(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for qian1MoLT.

	x	y	z	U(eq)
H(3)	2177	11437	2978	40
H(1)	1982	5661	2559	32
H(1A)	1116	7059	3199	26
H(2)	2550	8029	2999	24
H(3A)	1481	9963	3310	26
H(6)	416	6445	1912	37
H(7)	-180	8053	1226	44
H(8)	79	10438	1330	47
H(9)	940	11292	2124	39
H(12)	3130	7492	4841	39
H(13)	4413	7749	5281	50
H(14)	5289	8576	4786	48
H(15)	4883	9103	3840	53
H(16)	3598	8845	3393	42
H(22)	1357	4723	4240	46
H(23)	2195	4591	5108	54
H(25)	3930	3684	4377	60
H(26)	3092	3770	3502	50
H(27A)	3706	5091	5562	96
H(27B)	4213	3912	5351	96
H(27C)	3531	3462	5638	96

Table 6. Hydrogen bonds for qian1MoLT [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(3)-H(3)...O(1)#1	0.84	1.91	2.7336(17)	167.8
N(1)-H(1)...O(3)#2	0.88	1.99	2.8671(18)	174.7

Symmetry transformations used to generate equivalent atoms:

#1 x, y+1, z

#2 -x+1/2, y-1/2, -z+1/2

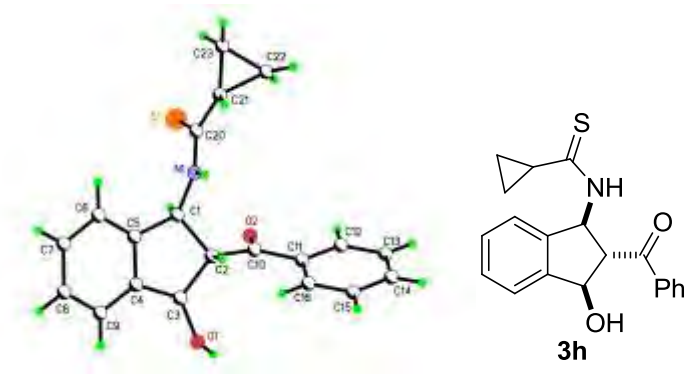


Table 1. Crystal data and structure refinement for qian4CuLT.

Identification code	qian4cult	
Empirical formula	C20 H19 N O2 S	
Formula weight	337.42	
Temperature	173.00(14) K	
Wavelength	1.5418 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.2087(2) Å	α= 90 °.
	b = 10.6761(4) Å	β= 90 °.
	c = 31.3923(11) Å	γ = 90 °.
Volume	1745.68(11) $Å^3$	
Z	4	
Density (calculated)	1.284 Mg/m^3	
Absorption coefficient	1.733 mm^{-1}	
F(000)	712	
Crystal size	0.30 x 0.28 x 0.25 mm^3	
Theta range for data collection	4.37 to 67.50 °.	
Index ranges	-6<=h<=6, -8<=k<=12, -35<=l<=37	
Reflections collected	6109	
Independent reflections	2795 [R(int) = 0.0292]	
Completeness to theta = 66.50 °	97.15 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.60637	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2795 / 0 / 216	
Goodness-of-fit on F^2	1.002	

Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.0922
R indices (all data)	R1 = 0.0412, wR2 = 0.0930
Absolute structure parameter	0.01(2)
Largest diff. peak and hole	0.233 and -0.218 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for qian4CuLT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	1233(2)	5699(1)	3043(1)	53(1)
O(1)	3079(3)	2906(2)	4901(1)	40(1)
O(2)	-1000(3)	2949(2)	3821(1)	49(1)
N(1)	4723(4)	4354(2)	3460(1)	34(1)
C(1)	3516(4)	4545(2)	3871(1)	32(1)
C(2)	5067(5)	5294(2)	4188(1)	31(1)
C(3)	4471(4)	4872(2)	4598(1)	31(1)
C(4)	2601(4)	3807(2)	4576(1)	31(1)
C(5)	3103(4)	3317(2)	4120(1)	32(1)
C(6)	6898(5)	6207(2)	4121(1)	34(1)
C(7)	8114(5)	6719(3)	4473(1)	37(1)
C(8)	7495(5)	6327(2)	4883(1)	38(1)
C(9)	5666(5)	5408(2)	4950(1)	35(1)
C(10)	1037(5)	2488(2)	3932(1)	34(1)
C(11)	1523(4)	1118(2)	3880(1)	33(1)
C(12)	-164(5)	415(3)	3631(1)	41(1)
C(13)	226(6)	-848(3)	3571(1)	47(1)
C(14)	2309(6)	-1428(3)	3760(1)	47(1)
C(15)	3985(6)	-755(3)	4010(1)	43(1)
C(16)	3600(5)	516(3)	4067(1)	39(1)
C(20)	3811(5)	4787(3)	3091(1)	40(1)
C(21)	5307(6)	4347(4)	2716(1)	57(1)
C(22A)	4016(15)	4018(8)	2318(2)	53(2)
C(22)	3707(15)	3526(7)	2375(2)	50(2)
C(23)	4855(14)	4779(8)	2288(2)	47(2)
C(23A)	5349(15)	5246(8)	2306(2)	58(2)

Table 3. Bond lengths [Å] and angles [°] for qian4CuLT.

S(1)-C(20)	1.665(3)
O(1)-C(4)	1.424(3)
O(2)-C(10)	1.221(3)
N(1)-C(1)	1.451(3)
N(1)-C(20)	1.334(3)
C(1)-C(2)	1.509(3)
C(1)-C(5)	1.542(3)
C(2)-C(3)	1.399(3)
C(2)-C(6)	1.380(4)
C(3)-C(4)	1.499(3)
C(3)-C(9)	1.391(3)
C(4)-C(5)	1.547(3)
C(5)-C(10)	1.513(3)
C(6)-C(7)	1.386(4)
C(7)-C(8)	1.391(4)
C(8)-C(9)	1.384(4)
C(10)-C(11)	1.493(4)
C(11)-C(12)	1.394(4)
C(11)-C(16)	1.389(3)
C(12)-C(13)	1.376(4)
C(13)-C(14)	1.382(4)
C(14)-C(15)	1.377(4)
C(15)-C(16)	1.384(4)
C(20)-C(21)	1.488(4)
C(21)-C(22A)	1.462(7)
C(21)-C(22)	1.616(7)
C(21)-C(23)	1.440(7)
C(21)-C(23A)	1.604(8)
C(22A)-C(23A)	1.484(11)
C(22)-C(23)	1.490(10)
C(20)-N(1)-C(1)	124.8(2)
N(1)-C(1)-C(2)	115.4(2)
N(1)-C(1)-C(5)	113.1(2)

C(2)-C(1)-C(5)	101.02(17)
C(3)-C(2)-C(1)	108.5(2)
C(6)-C(2)-C(1)	130.1(2)
C(6)-C(2)-C(3)	121.4(2)
C(2)-C(3)-C(4)	110.3(2)
C(9)-C(3)-C(2)	119.9(2)
C(9)-C(3)-C(4)	129.7(2)
O(1)-C(4)-C(3)	111.50(18)
O(1)-C(4)-C(5)	113.9(2)
C(3)-C(4)-C(5)	100.88(18)
C(1)-C(5)-C(4)	101.82(19)
C(10)-C(5)-C(1)	113.50(19)
C(10)-C(5)-C(4)	116.05(19)
C(2)-C(6)-C(7)	118.3(2)
C(6)-C(7)-C(8)	120.9(2)
C(9)-C(8)-C(7)	120.8(2)
C(8)-C(9)-C(3)	118.7(2)
O(2)-C(10)-C(5)	119.6(2)
O(2)-C(10)-C(11)	120.7(2)
C(11)-C(10)-C(5)	119.7(2)
C(12)-C(11)-C(10)	118.8(2)
C(16)-C(11)-C(10)	122.6(2)
C(16)-C(11)-C(12)	118.6(3)
C(13)-C(12)-C(11)	120.7(3)
C(12)-C(13)-C(14)	119.8(3)
C(15)-C(14)-C(13)	120.5(3)
C(14)-C(15)-C(16)	119.6(3)
C(15)-C(16)-C(11)	120.8(3)
N(1)-C(20)-S(1)	124.55(19)
N(1)-C(20)-C(21)	113.0(2)
C(21)-C(20)-S(1)	122.4(2)
C(20)-C(21)-C(22)	115.2(3)
C(20)-C(21)-C(23A)	116.9(4)
C(22A)-C(21)-C(20)	120.7(4)
C(22A)-C(21)-C(22)	20.9(3)
C(22A)-C(21)-C(23A)	57.7(4)

C(23)-C(21)-C(20)	123.5(4)
C(23)-C(21)-C(22A)	37.3(3)
C(23)-C(21)-C(22)	58.0(4)
C(23)-C(21)-C(23A)	20.4(4)
C(23A)-C(21)-C(22)	78.5(4)
C(21)-C(22A)-C(23A)	66.0(5)
C(23)-C(22)-C(21)	55.0(4)
C(21)-C(23)-C(22)	66.9(4)
C(22A)-C(23A)-C(21)	56.3(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for qian4CuLT. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	46(1)	76(1)	37(1)	5(1)	-5(1)	19(1)
O(1)	31(1)	47(1)	44(1)	18(1)	-2(1)	-4(1)
O(2)	25(1)	50(1)	71(1)	2(1)	-9(1)	7(1)
N(1)	24(1)	46(1)	32(1)	-3(1)	2(1)	6(1)
C(1)	26(1)	38(1)	31(1)	5(1)	1(1)	4(1)
C(2)	28(1)	33(1)	30(1)	2(1)	2(1)	7(1)
C(3)	25(1)	32(1)	35(1)	3(1)	3(1)	7(1)
C(4)	25(1)	35(1)	32(1)	8(1)	1(1)	5(1)
C(5)	23(1)	33(1)	39(1)	3(1)	-1(1)	3(1)
C(6)	37(1)	30(1)	34(1)	6(1)	5(1)	5(1)
C(7)	38(1)	32(1)	43(1)	2(1)	3(1)	1(1)
C(8)	41(1)	34(1)	40(1)	-5(1)	-2(1)	2(1)
C(9)	36(1)	41(1)	29(1)	1(1)	2(1)	4(1)
C(10)	24(1)	44(1)	34(1)	2(1)	-1(1)	2(1)
C(11)	27(1)	41(1)	31(1)	2(1)	4(1)	-1(1)
C(12)	34(1)	51(2)	38(1)	5(1)	-2(1)	-4(1)
C(13)	54(2)	45(2)	41(1)	-4(1)	0(1)	-12(2)
C(14)	56(2)	39(2)	46(2)	0(1)	16(1)	-4(1)
C(15)	40(1)	39(1)	50(2)	6(1)	5(1)	4(1)
C(16)	33(1)	42(2)	40(1)	4(1)	-1(1)	-1(1)
C(20)	32(1)	54(2)	33(1)	-2(1)	-3(1)	-3(1)
C(21)	45(2)	95(3)	32(1)	-11(2)	2(1)	7(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for qian4CuLT.

	x	y	z	U(eq)
H(1)	1709	2529	4960	61
H(1A)	6160	3922	3453	41
H(1B)	1819	4964	3828	38
H(4)	804	4130	4600	37
H(5)	4755	2839	4121	38
H(6)	7314	6478	3841	40
H(7)	9387	7345	4434	45
H(8)	8340	6695	5120	46
H(9)	5235	5148	5230	43
H(12)	-1597	812	3501	49
H(13)	-933	-1319	3401	56
H(14)	2585	-2298	3716	56
H(15)	5398	-1161	4142	52
H(16)	4771	983	4236	46
H(21A)	6935	3887	2779	69
H(21)	7089	4049	2778	69
H(22A)	2116	4031	2318	64
H(22B)	4773	3330	2148	64
H(22C)	4544	2779	2249	60
H(22D)	1821	3468	2409	60
H(23A)	6352	4805	2094	56
H(23B)	3651	5489	2252	56
H(23C)	4289	6015	2313	70
H(23D)	6965	5309	2142	70

Table 6. Torsion angles [°] for qian4CuLT.

S(1)-C(20)-C(21)-C(22A)	-36.8(6)
S(1)-C(20)-C(21)-C(22)	-59.7(5)
S(1)-C(20)-C(21)-C(23)	7.4(6)
S(1)-C(20)-C(21)-C(23A)	29.8(5)
O(1)-C(4)-C(5)-C(1)	-158.09(18)
O(1)-C(4)-C(5)-C(10)	78.1(3)
O(2)-C(10)-C(11)-C(12)	11.9(4)
O(2)-C(10)-C(11)-C(16)	-168.5(2)
N(1)-C(1)-C(2)-C(3)	-149.0(2)
N(1)-C(1)-C(2)-C(6)	27.8(4)
N(1)-C(1)-C(5)-C(4)	163.79(18)
N(1)-C(1)-C(5)-C(10)	-70.7(3)
N(1)-C(20)-C(21)-C(22A)	141.9(5)
N(1)-C(20)-C(21)-C(22)	119.1(4)
N(1)-C(20)-C(21)-C(23)	-173.9(5)
N(1)-C(20)-C(21)-C(23A)	-151.4(4)
C(1)-N(1)-C(20)-S(1)	4.2(4)
C(1)-N(1)-C(20)-C(21)	-174.5(3)
C(1)-C(2)-C(3)-C(4)	2.1(3)
C(1)-C(2)-C(3)-C(9)	179.5(2)
C(1)-C(2)-C(6)-C(7)	-177.6(2)
C(1)-C(5)-C(10)-O(2)	-45.0(3)
C(1)-C(5)-C(10)-C(11)	134.2(2)
C(2)-C(1)-C(5)-C(4)	39.9(2)
C(2)-C(1)-C(5)-C(10)	165.35(19)
C(2)-C(3)-C(4)-O(1)	144.5(2)
C(2)-C(3)-C(4)-C(5)	23.3(2)
C(2)-C(3)-C(9)-C(8)	-2.1(3)
C(2)-C(6)-C(7)-C(8)	-0.4(4)
C(3)-C(2)-C(6)-C(7)	-1.1(4)
C(3)-C(4)-C(5)-C(1)	-38.5(2)
C(3)-C(4)-C(5)-C(10)	-162.3(2)
C(4)-C(3)-C(9)-C(8)	174.8(2)
C(4)-C(5)-C(10)-O(2)	72.5(3)

C(4)-C(5)-C(10)-C(11)	-108.3(2)
C(5)-C(1)-C(2)-C(3)	-26.7(2)
C(5)-C(1)-C(2)-C(6)	150.2(2)
C(5)-C(10)-C(11)-C(12)	-167.3(2)
C(5)-C(10)-C(11)-C(16)	12.3(3)
C(6)-C(2)-C(3)-C(4)	-175.1(2)
C(6)-C(2)-C(3)-C(9)	2.4(3)
C(6)-C(7)-C(8)-C(9)	0.6(4)
C(7)-C(8)-C(9)-C(3)	0.6(4)
C(9)-C(3)-C(4)-O(1)	-32.6(3)
C(9)-C(3)-C(4)-C(5)	-153.8(2)
C(10)-C(11)-C(12)-C(13)	179.4(2)
C(10)-C(11)-C(16)-C(15)	-179.9(2)
C(11)-C(12)-C(13)-C(14)	0.0(4)
C(12)-C(11)-C(16)-C(15)	-0.3(4)
C(12)-C(13)-C(14)-C(15)	0.6(4)
C(13)-C(14)-C(15)-C(16)	-1.0(4)
C(14)-C(15)-C(16)-C(11)	0.9(4)
C(16)-C(11)-C(12)-C(13)	-0.2(4)
C(20)-N(1)-C(1)-C(2)	-116.8(3)
C(20)-N(1)-C(1)-C(5)	127.6(3)
C(20)-C(21)-C(22A)-C(23A)	104.3(5)
C(20)-C(21)-C(22)-C(23)	115.2(5)
C(20)-C(21)-C(23)-C(22)	-100.9(5)
C(20)-C(21)-C(23A)-C(22A)	-110.9(5)
C(22A)-C(21)-C(22)-C(23)	4.5(12)
C(22A)-C(21)-C(23)-C(22)	-2.7(7)
C(22)-C(21)-C(22A)-C(23A)	-175.5(15)
C(22)-C(21)-C(23A)-C(22A)	1.6(5)
C(23)-C(21)-C(22A)-C(23A)	-1.9(7)
C(23)-C(21)-C(23A)-C(22A)	3.2(12)
C(23A)-C(21)-C(22)-C(23)	0.7(5)
C(23A)-C(21)-C(23)-C(22)	-178.2(14)

Symmetry transformations used to generate equivalent atoms:

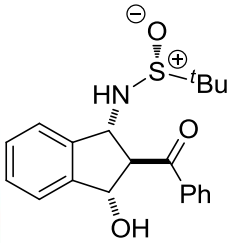
Table 7. Hydrogen bonds for qian4CuLT [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(1)#1	0.84	2.00	2.8142(13)	164.7
N(1)-H(1A)...O(2)#2	0.88	2.14	2.915(3)	145.9

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2, -y+1/2, -z+1

#2 x+1, y, z



3t

Table 1. Crystal data and structure refinement for qian5CuLT.

Identification code	qian5cult	
Empirical formula	C20 H23 N O3 S	
Formula weight	357.45	
Temperature	173.00(14) K	
Wavelength	1.5418 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 5.687 Å	α= 90 °.
	b = 10.66360(10) Å	β= 90 °.
	c = 29.8209(2) Å	γ = 90 °.
Volume	1808.42(2) $Å^3$	
Z	4	
Density (calculated)	1.313 Mg/m^3	
Absorption coefficient	1.740 mm^{-1}	
F(000)	760	
Crystal size	0.25 x 0.22 x 0.10 mm^3	
Theta range for data collection	4.40 to 66.93 °.	
Index ranges	-6<=h<=6, -12<=k<=11, -35<=l<=32	
Reflections collected	9437	
Independent reflections	3171 [R(int) = 0.0206]	
Completeness to theta = 66.50 °	99.09 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.86309	
Refinement method	Full-matrix least-squares on F^2	

Data / restraints / parameters	3171 / 0 / 229
Goodness-of-fit on F^2	1.006
Final R indices [I>2sigma(I)]	R1 = 0.0254, wR2 = 0.0682
R indices (all data)	R1 = 0.0255, wR2 = 0.0682
Absolute structure parameter	0.001(12)
Largest diff. peak and hole	0.185 and -0.187 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for qian5CuLT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	2367(1)	6246(1)	1843(1)	28(1)
O(1)	2867(2)	2766(1)	144(1)	32(1)
O(2)	-2184(2)	3872(1)	1073(1)	39(1)
O(3)	3732(3)	7422(1)	1779(1)	43(1)
N(1)	3241(2)	5110(1)	1498(1)	25(1)
C(1)	2309(2)	5140(1)	1040(1)	23(1)
C(2)	3981(2)	5654(1)	690(1)	24(1)
C(3)	3923(2)	4925(1)	305(1)	23(1)
C(4)	2104(2)	3902(1)	351(1)	24(1)
C(5)	1870(2)	3793(1)	870(1)	22(1)
C(6)	5557(3)	6637(1)	732(1)	29(1)
C(7)	7096(3)	6876(1)	380(1)	33(1)
C(8)	7046(2)	6143(1)	-5(1)	31(1)
C(9)	5439(3)	5160(1)	-48(1)	27(1)
C(10)	-438(2)	3225(1)	1022(1)	24(1)
C(11)	-575(2)	1845(1)	1099(1)	23(1)
C(12)	1260(2)	1184(1)	1298(1)	26(1)
C(13)	1010(3)	-91(1)	1390(1)	32(1)
C(14)	-1040(3)	-708(1)	1274(1)	34(1)
C(15)	-2863(3)	-61(1)	1067(1)	33(1)
C(16)	-2643(2)	1212(1)	983(1)	27(1)
C(21)	3500(3)	5552(1)	2368(1)	29(1)
C(22)	6175(3)	5456(2)	2343(1)	41(1)
C(23)	2768(3)	6501(2)	2729(1)	40(1)
C(24)	2350(3)	4286(1)	2448(1)	37(1)

Table 3. Bond lengths [Å] and angles [°] for qian5CuLT.

S(1)-O(3)	1.4872(12)
S(1)-N(1)	1.6649(11)
S(1)-C(21)	1.8479(14)
O(1)-C(4)	1.4269(16)
O(2)-C(10)	1.2182(17)
N(1)-C(1)	1.4679(16)
C(1)-C(2)	1.5132(18)
C(1)-C(5)	1.5435(16)
C(2)-C(3)	1.3889(18)
C(2)-C(6)	1.3847(19)
C(3)-C(4)	1.5092(17)
C(3)-C(9)	1.3821(19)
C(4)-C(5)	1.5590(16)
C(5)-C(10)	1.5146(17)
C(6)-C(7)	1.389(2)
C(7)-C(8)	1.389(2)
C(8)-C(9)	1.396(2)
C(10)-C(11)	1.4916(18)
C(11)-C(12)	1.3930(19)
C(11)-C(16)	1.3990(19)
C(12)-C(13)	1.394(2)
C(13)-C(14)	1.383(2)
C(14)-C(15)	1.389(2)
C(15)-C(16)	1.3862(19)
C(21)-C(22)	1.526(2)
C(21)-C(23)	1.535(2)
C(21)-C(24)	1.519(2)

O(3)-S(1)-N(1)	112.21(6)
O(3)-S(1)-C(21)	105.34(7)
N(1)-S(1)-C(21)	97.35(6)
C(1)-N(1)-S(1)	116.87(8)
N(1)-C(1)-C(2)	114.98(11)
N(1)-C(1)-C(5)	110.08(10)

C(2)-C(1)-C(5)	102.32(10)
C(3)-C(2)-C(1)	110.61(11)
C(6)-C(2)-C(1)	128.30(12)
C(6)-C(2)-C(3)	120.88(12)
C(2)-C(3)-C(4)	110.24(11)
C(9)-C(3)-C(2)	120.86(12)
C(9)-C(3)-C(4)	128.87(12)
O(1)-C(4)-C(3)	111.47(11)
O(1)-C(4)-C(5)	113.10(10)
C(3)-C(4)-C(5)	101.70(10)
C(1)-C(5)-C(4)	104.01(10)
C(10)-C(5)-C(1)	114.45(11)
C(10)-C(5)-C(4)	113.66(10)
C(2)-C(6)-C(7)	118.63(13)
C(6)-C(7)-C(8)	120.54(13)
C(7)-C(8)-C(9)	120.72(13)
C(3)-C(9)-C(8)	118.36(12)
O(2)-C(10)-C(5)	121.18(11)
O(2)-C(10)-C(11)	119.77(12)
C(11)-C(10)-C(5)	119.03(11)
C(12)-C(11)-C(10)	121.73(12)
C(12)-C(11)-C(16)	119.41(12)
C(16)-C(11)-C(10)	118.81(12)
C(11)-C(12)-C(13)	120.06(14)
C(14)-C(13)-C(12)	120.06(14)
C(13)-C(14)-C(15)	120.24(13)
C(16)-C(15)-C(14)	119.98(14)
C(15)-C(16)-C(11)	120.22(13)
C(22)-C(21)-S(1)	109.44(10)
C(22)-C(21)-C(23)	110.42(13)
C(23)-C(21)-S(1)	103.60(10)
C(24)-C(21)-S(1)	109.81(10)
C(24)-C(21)-C(22)	112.19(13)
C(24)-C(21)-C(23)	111.04(12)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for qian5CuLT. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	31(1)	26(1)	26(1)	-3(1)	-3(1)	7(1)
O(1)	36(1)	24(1)	35(1)	-8(1)	4(1)	-5(1)
O(2)	24(1)	29(1)	64(1)	4(1)	5(1)	4(1)
O(3)	68(1)	24(1)	37(1)	-1(1)	-2(1)	-1(1)
N(1)	23(1)	25(1)	26(1)	-2(1)	-1(1)	5(1)
C(1)	23(1)	19(1)	26(1)	0(1)	-3(1)	1(1)
C(2)	25(1)	19(1)	28(1)	3(1)	-4(1)	4(1)
C(3)	25(1)	19(1)	26(1)	4(1)	-4(1)	2(1)
C(4)	24(1)	22(1)	26(1)	-2(1)	-2(1)	0(1)
C(5)	20(1)	19(1)	26(1)	1(1)	-2(1)	1(1)
C(6)	34(1)	20(1)	33(1)	2(1)	-2(1)	-3(1)
C(7)	32(1)	24(1)	44(1)	5(1)	-1(1)	-6(1)
C(8)	31(1)	29(1)	35(1)	10(1)	3(1)	-1(1)
C(9)	30(1)	26(1)	26(1)	4(1)	-2(1)	1(1)
C(10)	21(1)	24(1)	28(1)	0(1)	-1(1)	2(1)
C(11)	24(1)	26(1)	20(1)	0(1)	5(1)	-1(1)
C(12)	24(1)	26(1)	29(1)	2(1)	2(1)	-1(1)
C(13)	35(1)	27(1)	33(1)	6(1)	3(1)	4(1)
C(14)	42(1)	22(1)	38(1)	1(1)	8(1)	-3(1)
C(15)	31(1)	30(1)	38(1)	-6(1)	5(1)	-9(1)
C(16)	23(1)	30(1)	28(1)	-2(1)	2(1)	1(1)
C(21)	26(1)	35(1)	25(1)	1(1)	-1(1)	2(1)
C(22)	27(1)	62(1)	34(1)	1(1)	-5(1)	2(1)
C(23)	46(1)	44(1)	29(1)	-7(1)	3(1)	-4(1)
C(24)	37(1)	35(1)	38(1)	5(1)	1(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for qian5CuLT.

	x	y	z	U(eq)
H(1)	1672	2401	33	38
H(1A)	4732	5216	1470	30
H(1B)	804	5626	1033	27
H(4)	579	4181	217	29
H(5)	3175	3248	982	26
H(6)	5586	7138	995	35
H(7)	8191	7545	403	40
H(8)	8118	6312	-242	38
H(9)	5388	4666	-313	33
H(12)	2683	1602	1372	32
H(13)	2249	-537	1532	38
H(14)	-1203	-1578	1335	41
H(15)	-4260	-490	984	39
H(16)	-3901	1657	846	32
H(22A)	6613	4776	2139	62
H(22B)	6807	5282	2642	62
H(22C)	6822	6249	2232	62
H(23A)	3535	7307	2670	60
H(23B)	3245	6191	3025	60
H(23C)	1058	6610	2722	60
H(24A)	637	4387	2455	55
H(24B)	2886	3945	2736	55
H(24C)	2784	3709	2206	55

Table 6. Torsion angles [°] for qian5CuLT.

S(1)-N(1)-C(1)-C(2)	101.30(11)
S(1)-N(1)-C(1)-C(5)	-143.81(9)
O(1)-C(4)-C(5)-C(1)	151.98(10)
O(1)-C(4)-C(5)-C(10)	-82.92(13)
O(2)-C(10)-C(11)-C(12)	-142.10(14)
O(2)-C(10)-C(11)-C(16)	35.23(19)
O(3)-S(1)-N(1)-C(1)	-81.58(11)
O(3)-S(1)-C(21)-C(22)	-52.13(12)
O(3)-S(1)-C(21)-C(23)	65.65(11)
O(3)-S(1)-C(21)-C(24)	-175.69(10)
N(1)-S(1)-C(21)-C(22)	63.37(12)
N(1)-S(1)-C(21)-C(23)	-178.85(10)
N(1)-S(1)-C(21)-C(24)	-60.18(11)
N(1)-C(1)-C(2)-C(3)	136.93(11)
N(1)-C(1)-C(2)-C(6)	-37.80(18)
N(1)-C(1)-C(5)-C(4)	-153.26(10)
N(1)-C(1)-C(5)-C(10)	82.14(13)
C(1)-C(2)-C(3)-C(4)	3.28(14)
C(1)-C(2)-C(3)-C(9)	-175.10(12)
C(1)-C(2)-C(6)-C(7)	173.80(13)
C(1)-C(5)-C(10)-O(2)	33.46(17)
C(1)-C(5)-C(10)-C(11)	-148.13(12)
C(2)-C(1)-C(5)-C(4)	-30.57(12)
C(2)-C(1)-C(5)-C(10)	-155.17(10)
C(2)-C(3)-C(4)-O(1)	-143.26(11)
C(2)-C(3)-C(4)-C(5)	-22.46(13)
C(2)-C(3)-C(9)-C(8)	0.59(19)
C(2)-C(6)-C(7)-C(8)	0.1(2)
C(3)-C(2)-C(6)-C(7)	-0.5(2)
C(3)-C(4)-C(5)-C(1)	32.33(12)
C(3)-C(4)-C(5)-C(10)	157.43(10)
C(4)-C(3)-C(9)-C(8)	-177.45(12)
C(4)-C(5)-C(10)-O(2)	-85.85(16)
C(4)-C(5)-C(10)-C(11)	92.56(13)

C(5)-C(1)-C(2)-C(3)	17.62(13)
C(5)-C(1)-C(2)-C(6)	-157.11(13)
C(5)-C(10)-C(11)-C(12)	39.47(18)
C(5)-C(10)-C(11)-C(16)	-143.20(12)
C(6)-C(2)-C(3)-C(4)	178.46(12)
C(6)-C(2)-C(3)-C(9)	0.08(19)
C(6)-C(7)-C(8)-C(9)	0.5(2)
C(7)-C(8)-C(9)-C(3)	-0.9(2)
C(9)-C(3)-C(4)-O(1)	34.95(18)
C(9)-C(3)-C(4)-C(5)	155.75(13)
C(10)-C(11)-C(12)-C(13)	176.00(12)
C(10)-C(11)-C(16)-C(15)	-177.29(12)
C(11)-C(12)-C(13)-C(14)	1.4(2)
C(12)-C(11)-C(16)-C(15)	0.10(19)
C(12)-C(13)-C(14)-C(15)	-0.3(2)
C(13)-C(14)-C(15)-C(16)	-0.9(2)
C(14)-C(15)-C(16)-C(11)	1.0(2)
C(16)-C(11)-C(12)-C(13)	-1.31(19)
C(21)-S(1)-N(1)-C(1)	168.49(10)

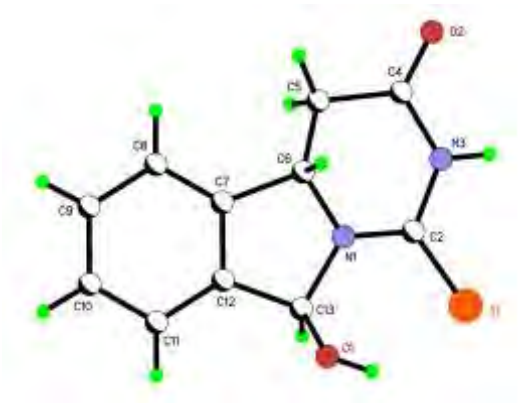
Symmetry transformations used to generate equivalent atoms:

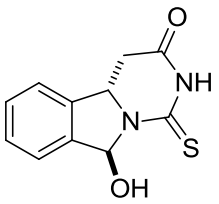
Table 7. Hydrogen bonds for qian5CuLT [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1)...O(1)#1	0.85	2.23	3.0232(6)	154.4
N(1)-H(1A)...O(2)#2	0.86	2.56	3.1818(15)	130.5

Symmetry transformations used to generate equivalent atoms:

#1 x-1/2, -y+1/2, -z #2 x+1, y, z





5c

Table 1. Crystal data and structure refinement for qian6CuLT.

Identification code	qian6cult	
Empirical formula	C11 H10 N2 O2 S	
Formula weight	234.27	
Temperature	173.00(14) K	
Wavelength	1.5418 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 14.0959(6) Å	α= 90 °.
	b = 7.5933(3) Å	β= 104.158(4) °.
	c = 20.2857(8) Å	γ = 90 °.
Volume	2105.31(15) $Å^3$	
Z	8	
Density (calculated)	1.478 Mg/m^3	
Absorption coefficient	2.629 mm^{-1}	
F(000)	976	
Crystal size	0.35 x 0.28 x 0.25 mm^3	
Theta range for data collection	10.04 to 66.98 °.	
Index ranges	-16<=h<=16, -9<=k<=8, -24<=l<=22	
Reflections collected	7985	
Independent reflections	3575 [R(int) = 0.0247]	
Completeness to theta = 66.50 °	95.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.45580	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3575 / 0 / 291	

Goodness-of-fit on F^2	1.005
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1546
R indices (all data)	R1 = 0.0616, wR2 = 0.1573
Largest diff. peak and hole	0.579 and -0.393 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for qian6CuLT. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
S(1)	9305(1)	1751(1)	5662(1)	45(1)
O(1)	8960(2)	1115(3)	3997(1)	48(1)
O(2)	5927(2)	800(3)	5781(1)	51(1)
N(1)	7754(2)	1799(3)	4607(1)	39(1)
C(2)	8118(2)	1574(4)	5273(1)	38(1)
N(3)	7447(2)	1161(3)	5639(1)	42(1)
C(4)	6442(2)	1220(4)	5413(1)	42(1)
C(5)	6058(2)	1883(4)	4696(1)	43(1)
C(6)	6734(2)	1370(4)	4259(1)	41(1)
C(7)	6644(2)	2318(4)	3590(1)	41(1)
C(8)	5809(2)	2579(5)	3075(2)	50(1)
C(9)	5916(3)	3394(5)	2480(2)	58(1)
C(10)	6823(3)	3916(5)	2413(2)	62(1)
C(11)	7662(3)	3664(5)	2932(2)	55(1)
C(12)	7545(2)	2844(4)	3524(1)	41(1)
C(13)	8344(2)	2425(4)	4148(1)	39(1)
S(1A)	3241(1)	3837(1)	2327(1)	47(1)
O(1A)	3872(2)	5239(3)	3896(1)	56(1)
O(2A)	-248(2)	3056(4)	2093(1)	72(1)
N(1A)	2348(2)	3878(3)	3336(1)	42(1)
C(2A)	2270(2)	3821(4)	2665(1)	41(1)
N(3A)	1340(2)	3756(3)	2264(1)	42(1)
C(4A)	503(3)	3267(5)	2478(2)	53(1)
C(5A)	672(2)	2933(5)	3230(2)	55(1)
C(6A)	1485(2)	4084(4)	3612(2)	47(1)
C(7A)	1918(3)	3633(4)	4360(1)	47(1)
C(8A)	1438(3)	3432(5)	4880(2)	53(1)
C(9A)	2016(3)	3175(4)	5536(2)	52(1)
C(10A)	3018(3)	3168(4)	5669(2)	56(1)
C(11A)	3498(3)	3312(4)	5145(2)	50(1)
C(12A)	2916(2)	3534(4)	4487(1)	44(1)

C(13A)	3280(2)	3719(4)	3852(1)	43(1)

Table 3. Bond lengths [Å] and angles [°] for qian6CuLT.

S(1)-C(2)	1.672(3)
O(1)-C(13)	1.403(3)
O(2)-C(4)	1.205(4)
N(1)-C(2)	1.334(3)
N(1)-C(6)	1.475(4)
N(1)-C(13)	1.470(4)
C(2)-N(3)	1.374(4)
N(3)-C(4)	1.379(4)
C(4)-C(5)	1.508(4)
C(5)-C(6)	1.504(4)
C(6)-C(7)	1.514(4)
C(7)-C(8)	1.383(4)
C(7)-C(12)	1.368(4)
C(8)-C(9)	1.398(5)
C(9)-C(10)	1.376(6)
C(10)-C(11)	1.392(5)
C(11)-C(12)	1.398(4)
C(12)-C(13)	1.508(4)
S(1A)-C(2A)	1.675(3)
O(1A)-C(13A)	1.414(4)
O(2A)-C(4A)	1.163(4)
N(1A)-C(2A)	1.339(4)
N(1A)-C(6A)	1.467(4)
N(1A)-C(13A)	1.470(4)
C(2A)-N(3A)	1.364(4)
N(3A)-C(4A)	1.403(4)
C(4A)-C(5A)	1.507(4)
C(5A)-C(6A)	1.498(5)
C(6A)-C(7A)	1.529(4)
C(7A)-C(8A)	1.394(5)
C(7A)-C(12A)	1.370(5)
C(8A)-C(9A)	1.393(5)
C(9A)-C(10A)	1.371(5)
C(10A)-C(11A)	1.396(5)

C(11A)-C(12A)	1.395(4)
C(12A)-C(13A)	1.506(4)

C(2)-N(1)-C(6)	123.1(2)
C(2)-N(1)-C(13)	123.1(2)
C(13)-N(1)-C(6)	113.8(2)
N(1)-C(2)-S(1)	124.1(2)
N(1)-C(2)-N(3)	115.5(3)
N(3)-C(2)-S(1)	120.33(19)
C(2)-N(3)-C(4)	126.9(2)
O(2)-C(4)-N(3)	120.7(3)
O(2)-C(4)-C(5)	123.9(3)
N(3)-C(4)-C(5)	115.4(2)
C(6)-C(5)-C(4)	110.6(2)
N(1)-C(6)-C(5)	110.1(2)
N(1)-C(6)-C(7)	100.5(2)
C(5)-C(6)-C(7)	118.6(2)
C(8)-C(7)-C(6)	127.9(3)
C(12)-C(7)-C(6)	110.4(2)
C(12)-C(7)-C(8)	121.6(3)
C(7)-C(8)-C(9)	117.6(3)
C(10)-C(9)-C(8)	120.8(3)
C(9)-C(10)-C(11)	121.6(3)
C(10)-C(11)-C(12)	117.1(3)
C(7)-C(12)-C(11)	121.4(3)
C(7)-C(12)-C(13)	112.2(2)
C(11)-C(12)-C(13)	126.5(3)
O(1)-C(13)-N(1)	112.7(2)
O(1)-C(13)-C(12)	110.0(2)
N(1)-C(13)-C(12)	100.2(2)
C(2A)-N(1A)-C(6A)	121.5(2)
C(2A)-N(1A)-C(13A)	123.9(2)
C(6A)-N(1A)-C(13A)	114.7(2)
N(1A)-C(2A)-S(1A)	122.9(2)
N(1A)-C(2A)-N(3A)	115.8(3)
N(3A)-C(2A)-S(1A)	121.2(2)

C(2A)-N(3A)-C(4A)	125.7(2)
O(2A)-C(4A)-N(3A)	121.7(3)
O(2A)-C(4A)-C(5A)	123.3(3)
N(3A)-C(4A)-C(5A)	114.9(3)
C(6A)-C(5A)-C(4A)	109.7(3)
N(1A)-C(6A)-C(5A)	109.9(3)
N(1A)-C(6A)-C(7A)	100.8(2)
C(5A)-C(6A)-C(7A)	116.9(3)
C(8A)-C(7A)-C(6A)	128.7(3)
C(12A)-C(7A)-C(6A)	110.0(3)
C(12A)-C(7A)-C(8A)	121.2(3)
C(9A)-C(8A)-C(7A)	117.3(3)
C(10A)-C(9A)-C(8A)	121.5(3)
C(9A)-C(10A)-C(11A)	121.2(3)
C(12A)-C(11A)-C(10A)	117.1(3)
C(7A)-C(12A)-C(11A)	121.6(3)
C(7A)-C(12A)-C(13A)	112.5(3)
C(11A)-C(12A)-C(13A)	125.9(3)
O(1A)-C(13A)-N(1A)	112.9(2)
O(1A)-C(13A)-C(12A)	109.9(2)
N(1A)-C(13A)-C(12A)	100.7(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for qian6CuLT. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(1)	43(1)	63(1)	26(1)	-3(1)	2(1)	10(1)
O(1)	49(1)	64(1)	30(1)	-1(1)	6(1)	17(1)
O(2)	48(1)	66(1)	39(1)	-12(1)	13(1)	-15(1)
N(1)	40(1)	51(1)	25(1)	2(1)	5(1)	5(1)
C(2)	49(2)	40(1)	25(1)	0(1)	8(1)	7(1)
N(3)	53(1)	52(1)	21(1)	4(1)	6(1)	5(1)
C(4)	55(2)	41(2)	29(1)	-3(1)	8(1)	-9(1)
C(5)	41(2)	54(2)	33(1)	2(1)	7(1)	-5(1)
C(6)	46(2)	45(2)	30(1)	1(1)	6(1)	2(1)
C(7)	50(2)	45(2)	26(1)	1(1)	8(1)	8(1)
C(8)	47(2)	67(2)	34(1)	0(1)	3(1)	6(1)
C(9)	60(2)	77(2)	31(1)	7(1)	-3(1)	15(2)
C(10)	71(2)	81(2)	30(1)	18(2)	9(1)	14(2)
C(11)	57(2)	71(2)	38(2)	11(1)	12(1)	4(2)
C(12)	46(2)	47(2)	26(1)	-1(1)	4(1)	10(1)
C(13)	44(1)	50(2)	25(1)	0(1)	8(1)	5(1)
S(1A)	45(1)	65(1)	33(1)	1(1)	11(1)	-3(1)
O(1A)	60(1)	62(1)	42(1)	-2(1)	7(1)	-13(1)
O(2A)	40(1)	127(2)	47(1)	-9(1)	11(1)	-23(1)
N(1A)	42(1)	54(1)	30(1)	2(1)	7(1)	-1(1)
C(2A)	55(2)	38(1)	30(1)	-1(1)	7(1)	0(1)
N(3A)	51(1)	50(1)	23(1)	0(1)	6(1)	1(1)
C(4A)	58(2)	67(2)	34(2)	2(1)	15(1)	0(2)
C(5A)	46(2)	85(2)	34(2)	0(2)	11(1)	-3(2)
C(6A)	47(2)	54(2)	41(2)	5(1)	14(1)	7(1)
C(7A)	66(2)	45(2)	29(1)	-7(1)	7(1)	6(1)
C(8A)	58(2)	61(2)	41(2)	-9(1)	15(1)	0(2)
C(9A)	81(2)	46(2)	31(1)	1(1)	21(2)	2(2)
C(10A)	85(3)	46(2)	29(1)	-2(1)	-2(1)	9(2)
C(11A)	61(2)	48(2)	37(2)	-3(1)	4(1)	2(1)
C(12A)	61(2)	38(1)	31(1)	-3(1)	10(1)	-1(1)

C(13A)	45(2)	48(2)	32(1)	-1(1)	3(1)	1(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for qian6CuLT.

	x	y	z	U(eq)
H(1)	9439	972	4332	72
H(3)	7684	824	6062	51
H(5A)	5400	1383	4503	52
H(5B)	5997	3181	4701	52
H(6)	6680	73	4172	49
H(8)	5185	2216	3124	60
H(9)	5356	3591	2117	70
H(10)	6877	4461	2002	74
H(11)	8287	4034	2887	66
H(13)	8722	3505	4332	47
H(1A)	4089	5314	3547	83
H(3A)	1258	4045	1834	50
H(5AA)	66	3187	3377	66
H(5AB)	844	1680	3329	66
H(6A)	1268	5342	3572	56
H(8A)	744	3468	4791	64
H(9A)	1709	3002	5899	62
H(10A)	3391	3062	6125	67
H(11A)	4191	3262	5233	60
H(13A)	3645	2643	3772	51

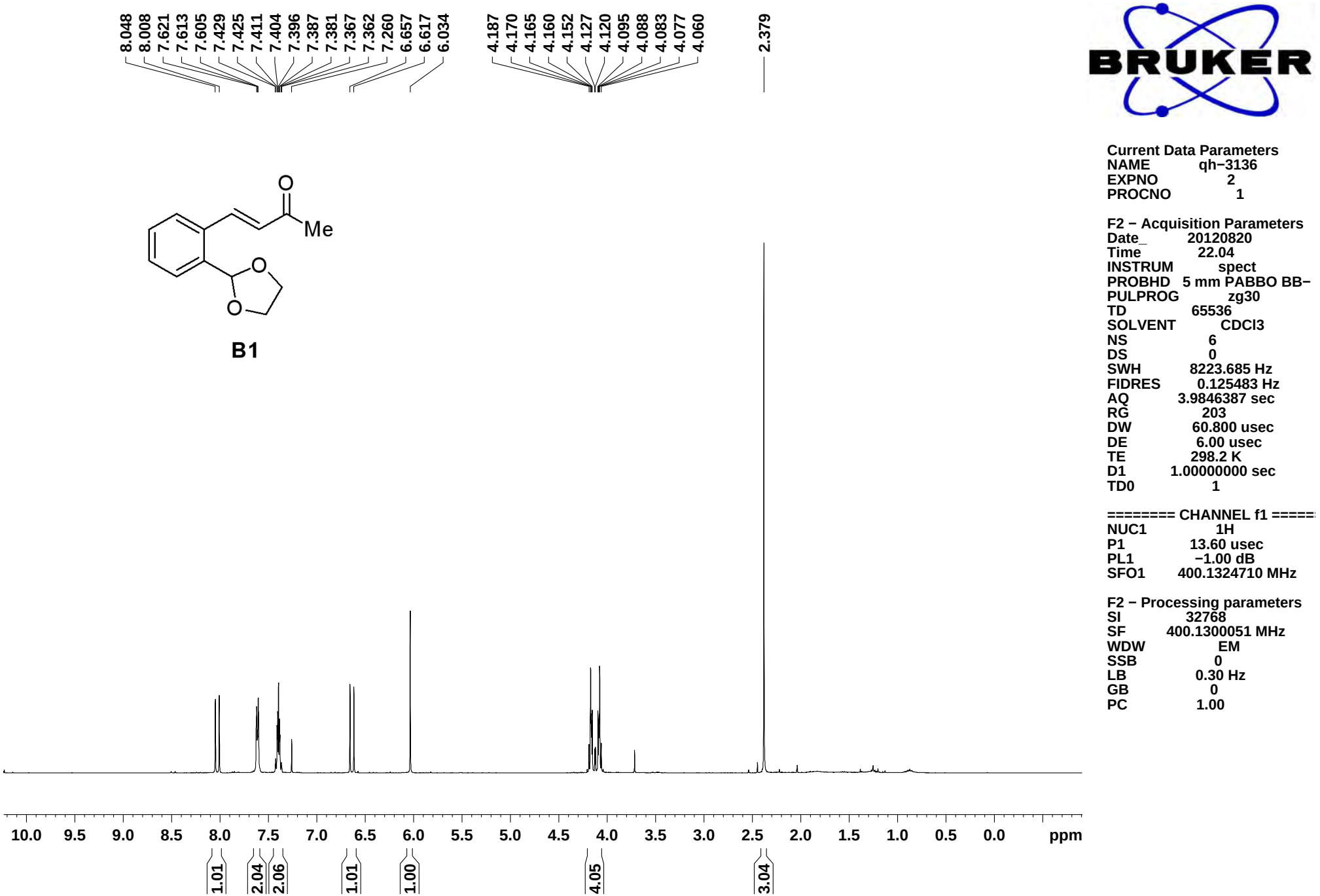
Table 6. Torsion angles [°] for qian6CuLT.

S(1)-C(2)-N(3)-C(4)	169.8(2)
O(2)-C(4)-C(5)-C(6)	-149.0(3)
N(1)-C(2)-N(3)-C(4)	-10.6(4)
N(1)-C(6)-C(7)-C(8)	-171.5(3)
N(1)-C(6)-C(7)-C(12)	12.1(3)
C(2)-N(1)-C(6)-C(5)	39.2(4)
C(2)-N(1)-C(6)-C(7)	165.2(2)
C(2)-N(1)-C(13)-O(1)	76.1(3)
C(2)-N(1)-C(13)-C(12)	-167.0(3)
C(2)-N(3)-C(4)-O(2)	179.0(3)
C(2)-N(3)-C(4)-C(5)	-2.7(4)
N(3)-C(4)-C(5)-C(6)	32.8(3)
C(4)-C(5)-C(6)-N(1)	-48.1(3)
C(4)-C(5)-C(6)-C(7)	-163.0(3)
C(5)-C(6)-C(7)-C(8)	-51.5(4)
C(5)-C(6)-C(7)-C(12)	132.1(3)
C(6)-N(1)-C(2)-S(1)	170.2(2)
C(6)-N(1)-C(2)-N(3)	-9.4(4)
C(6)-N(1)-C(13)-O(1)	-101.4(3)
C(6)-N(1)-C(13)-C(12)	15.5(3)
C(6)-C(7)-C(8)-C(9)	-175.7(3)
C(6)-C(7)-C(12)-C(11)	176.4(3)
C(6)-C(7)-C(12)-C(13)	-3.4(3)
C(7)-C(8)-C(9)-C(10)	0.0(5)
C(7)-C(12)-C(13)-O(1)	111.9(3)
C(7)-C(12)-C(13)-N(1)	-7.0(3)
C(8)-C(7)-C(12)-C(11)	-0.2(5)
C(8)-C(7)-C(12)-C(13)	180.0(3)
C(8)-C(9)-C(10)-C(11)	-0.4(6)
C(9)-C(10)-C(11)-C(12)	0.5(6)
C(10)-C(11)-C(12)-C(7)	-0.2(5)
C(10)-C(11)-C(12)-C(13)	179.6(3)
C(11)-C(12)-C(13)-O(1)	-67.9(4)
C(11)-C(12)-C(13)-N(1)	173.3(3)

C(12)-C(7)-C(8)-C(9)	0.4(5)
C(13)-N(1)-C(2)-S(1)	-7.0(4)
C(13)-N(1)-C(2)-N(3)	173.4(2)
C(13)-N(1)-C(6)-C(5)	-143.3(2)
C(13)-N(1)-C(6)-C(7)	-17.3(3)
S(1A)-C(2A)-N(3A)-C(4A)	161.8(3)
O(2A)-C(4A)-C(5A)-C(6A)	-152.6(4)
N(1A)-C(2A)-N(3A)-C(4A)	-18.5(4)
N(1A)-C(6A)-C(7A)-C(8A)	-173.4(3)
N(1A)-C(6A)-C(7A)-C(12A)	10.3(3)
C(2A)-N(1A)-C(6A)-C(5A)	43.1(4)
C(2A)-N(1A)-C(6A)-C(7A)	167.1(3)
C(2A)-N(1A)-C(13A)-O(1A)	72.9(3)
C(2A)-N(1A)-C(13A)-C(12A)	-170.0(3)
C(2A)-N(3A)-C(4A)-O(2A)	-171.4(3)
C(2A)-N(3A)-C(4A)-C(5A)	4.9(5)
N(3A)-C(4A)-C(5A)-C(6A)	31.2(4)
C(4A)-C(5A)-C(6A)-N(1A)	-52.2(4)
C(4A)-C(5A)-C(6A)-C(7A)	-166.2(3)
C(5A)-C(6A)-C(7A)-C(8A)	-54.3(5)
C(5A)-C(6A)-C(7A)-C(12A)	129.4(3)
C(6A)-N(1A)-C(2A)-S(1A)	172.3(2)
C(6A)-N(1A)-C(2A)-N(3A)	-7.5(4)
C(6A)-N(1A)-C(13A)-O(1A)	-108.0(3)
C(6A)-N(1A)-C(13A)-C(12A)	9.2(3)
C(6A)-C(7A)-C(8A)-C(9A)	-174.2(3)
C(6A)-C(7A)-C(12A)-C(11A)	173.6(3)
C(6A)-C(7A)-C(12A)-C(13A)	-5.5(4)
C(7A)-C(8A)-C(9A)-C(10A)	1.7(5)
C(7A)-C(12A)-C(13A)-O(1A)	117.5(3)
C(7A)-C(12A)-C(13A)-N(1A)	-1.8(3)
C(8A)-C(7A)-C(12A)-C(11A)	-3.1(5)
C(8A)-C(7A)-C(12A)-C(13A)	177.8(3)
C(8A)-C(9A)-C(10A)-C(11A)	-3.9(5)
C(9A)-C(10A)-C(11A)-C(12A)	2.5(5)
C(10A)-C(11A)-C(12A)-C(7A)	1.0(4)

C(10A)-C(11A)-C(12A)-C(13A)	179.9(3)
C(11A)-C(12A)-C(13A)-O(1A)	-61.6(4)
C(11A)-C(12A)-C(13A)-N(1A)	179.1(3)
C(12A)-C(7A)-C(8A)-C(9A)	1.7(5)
C(13A)-N(1A)-C(2A)-S(1A)	-8.6(4)
C(13A)-N(1A)-C(2A)-N(3A)	171.6(2)
C(13A)-N(1A)-C(6A)-C(5A)	-136.1(3)
C(13A)-N(1A)-C(6A)-C(7A)	-12.1(3)

Symmetry transformations used to generate equivalent atoms:



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NAME qh−3136
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120820
Time 22.04
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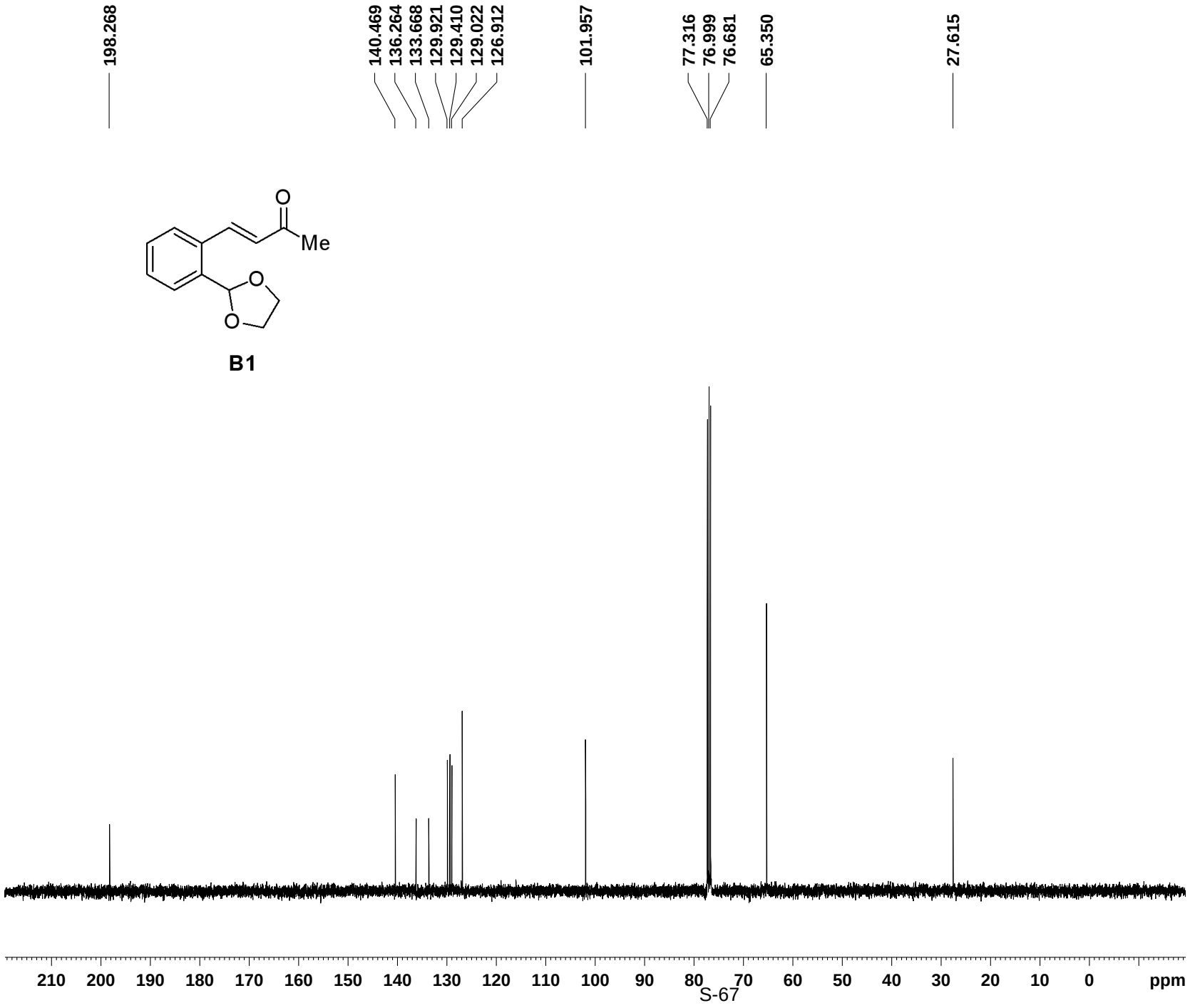
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

======== 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



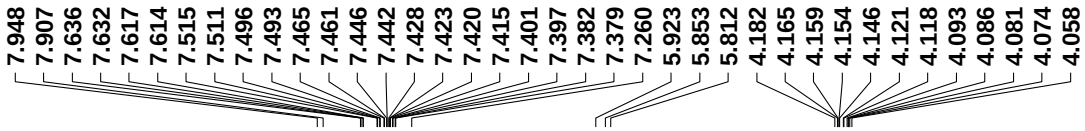
Current Data Parameters
NAME qh−3136
EXPNO 3
PROCNO 1

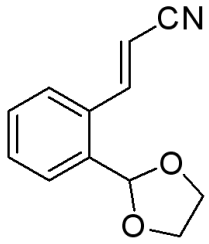
F2 − Acquisition Parameters
Date_ 20120820
Time 22.06
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 1440
DW 20.800 usec
DE 6.00 usec
TE 298.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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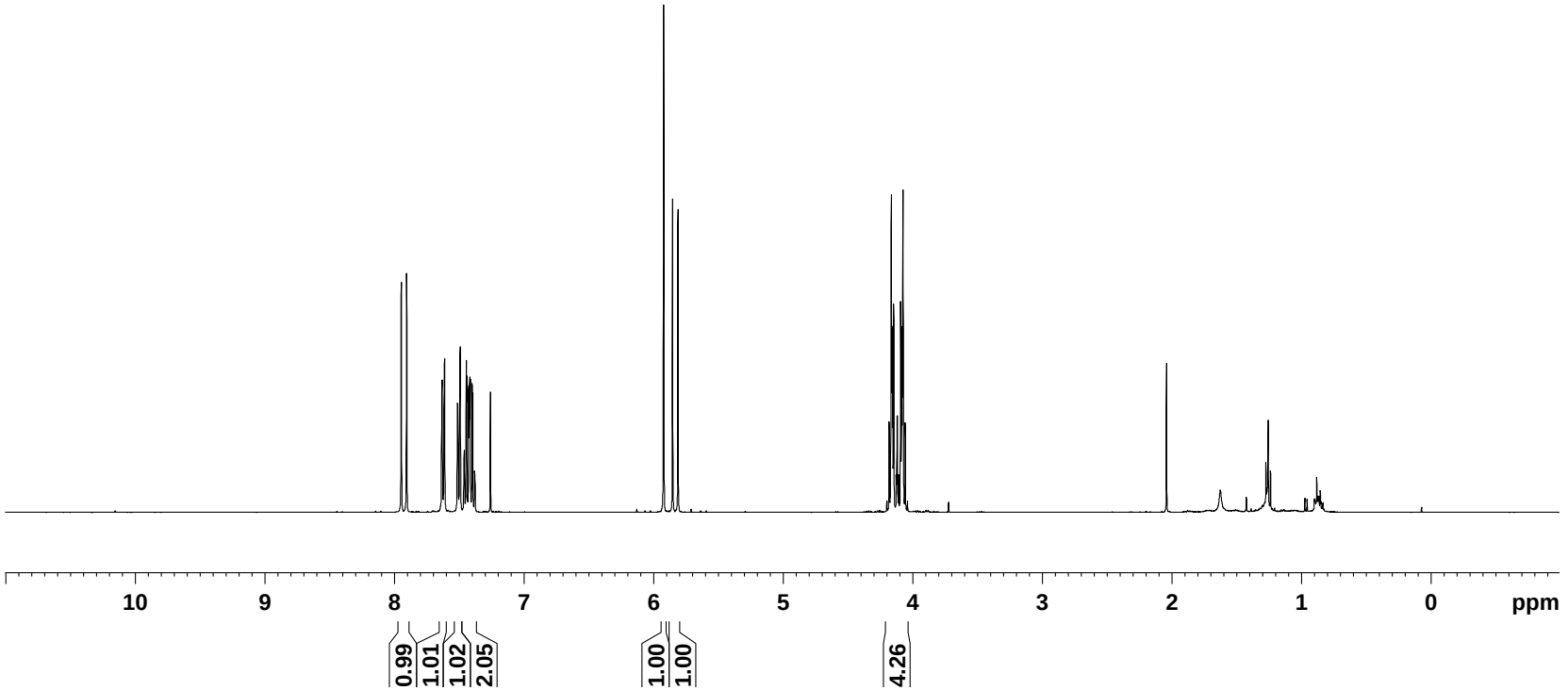
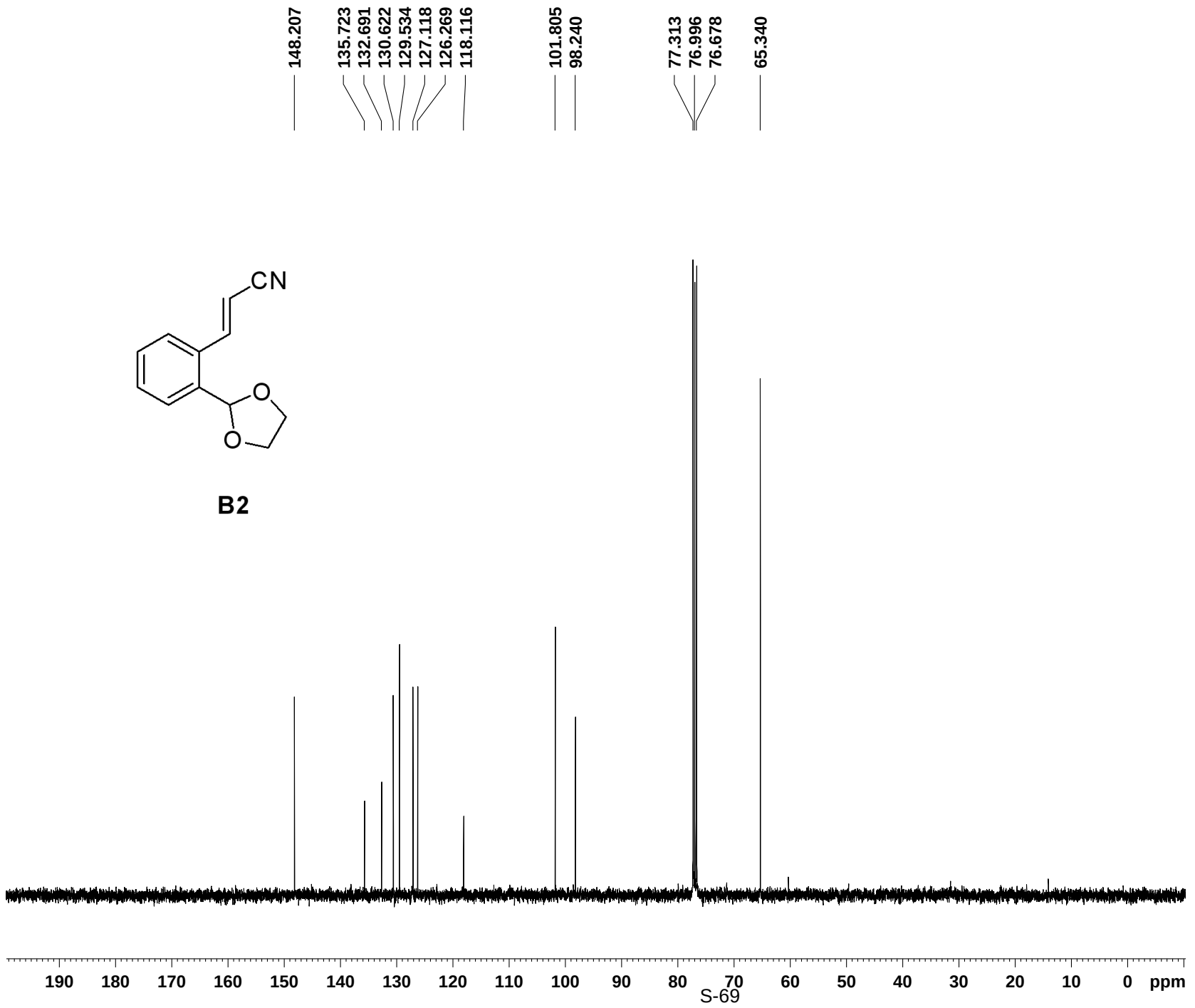


Current Data Parameters
NAME qh−3140
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120821
Time 19.33
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 297.1 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 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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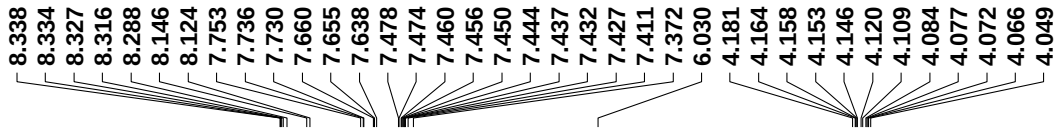
Current Data Parameters
NAME qh−3140
EXPNO 4
PROCNO 1

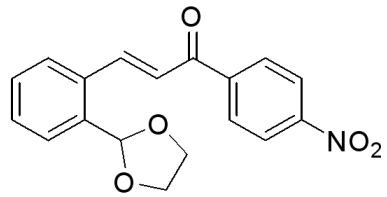
F2 − Acquisition Parameters
Date_ 20120821
Time 19.53
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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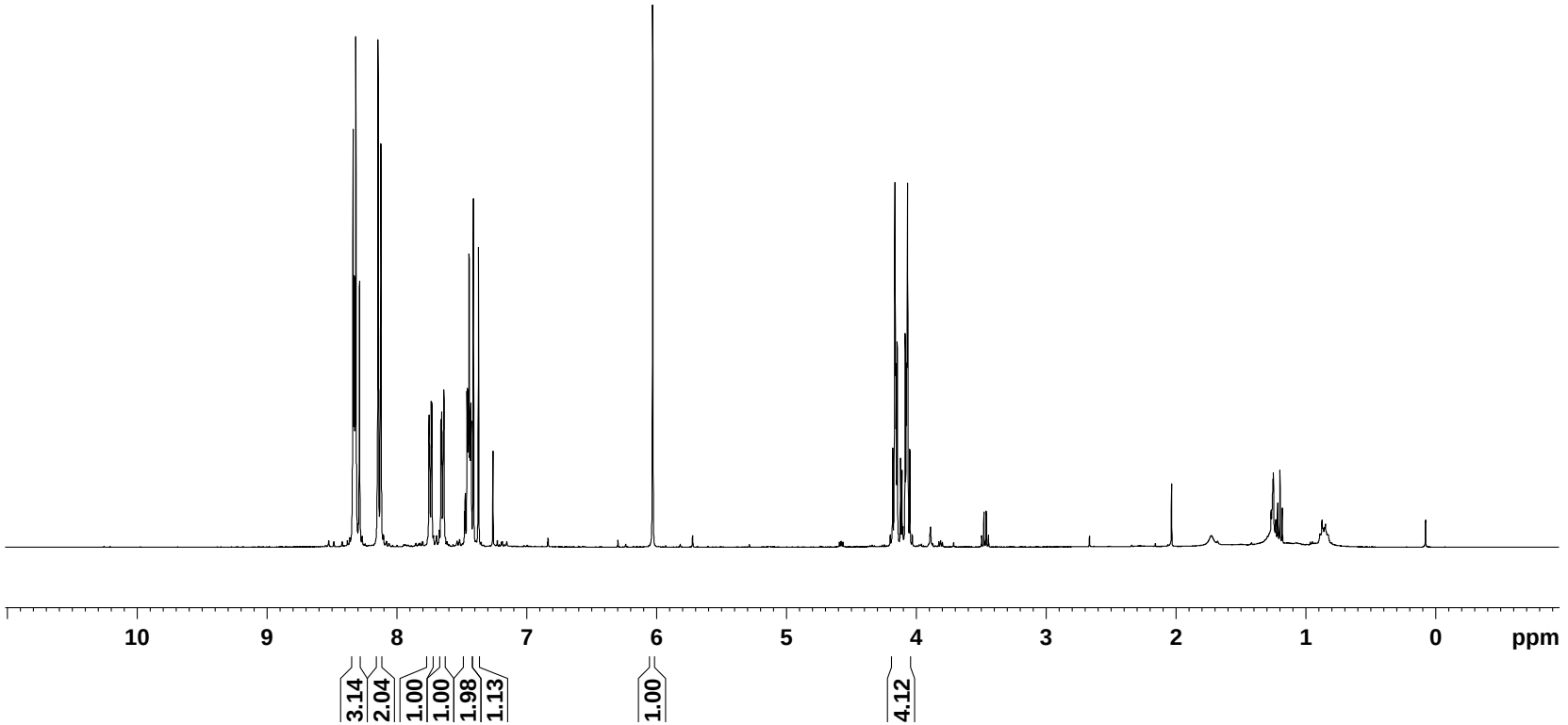
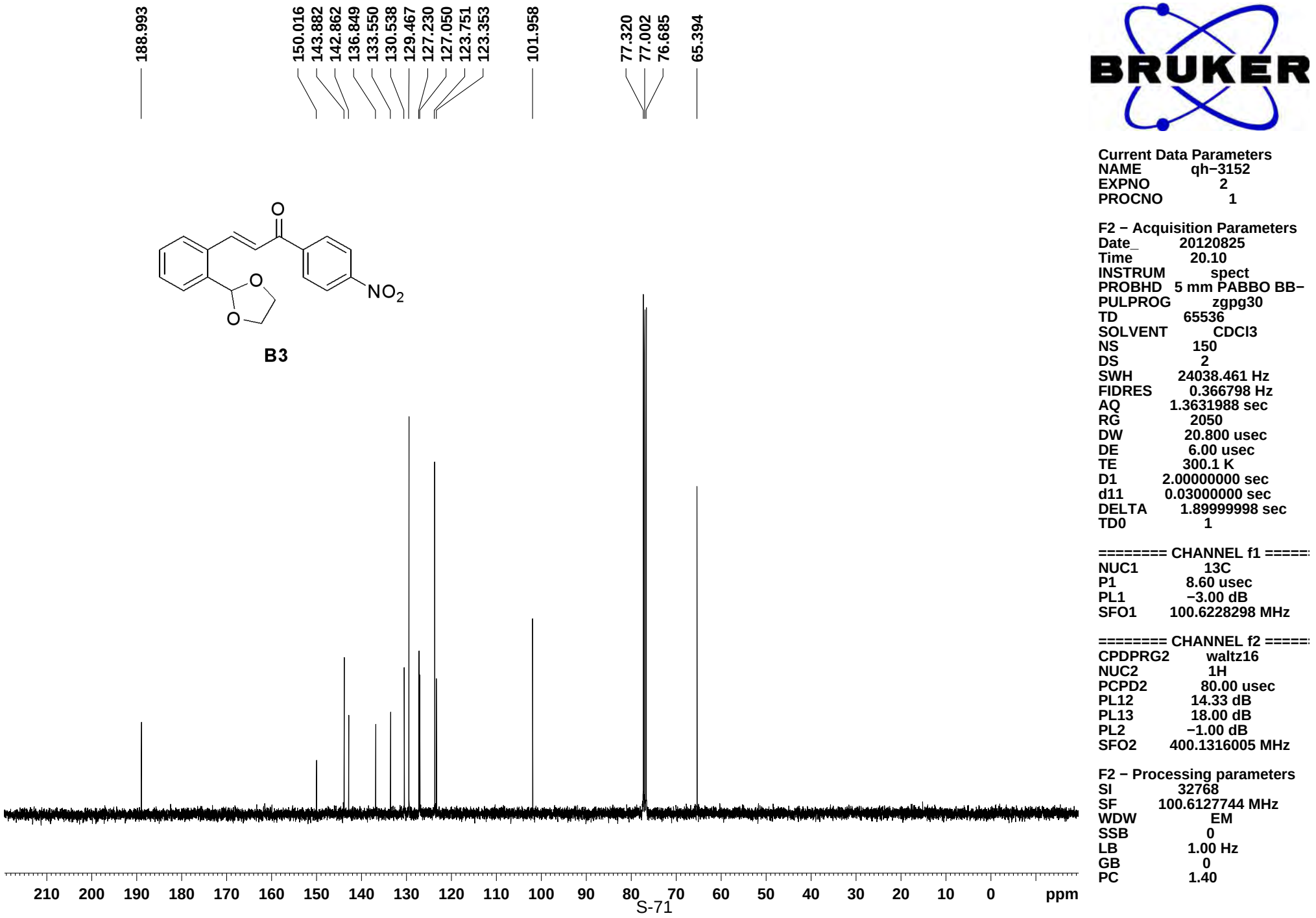


Current Data Parameters
NAME qh−3152
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120825
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 299.5 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 400.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



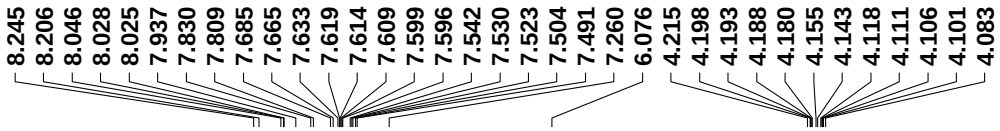
Current Data Parameters
NAME qh−3152
EXPNO 2
PROCNO 1

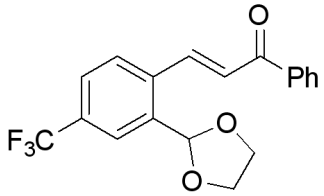
F2 − Acquisition Parameters
Date_ 20120825
Time 20.10
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 150
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





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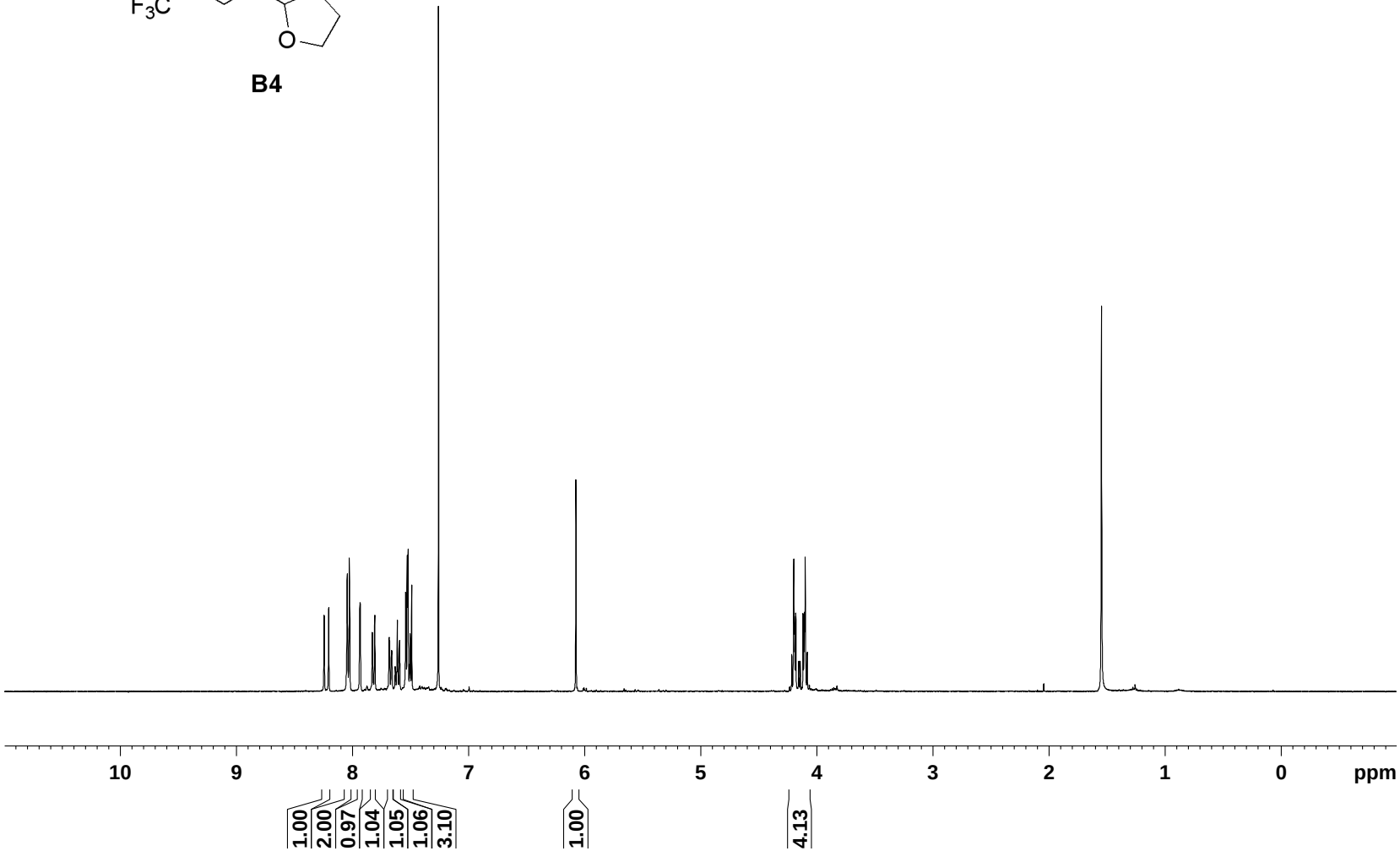
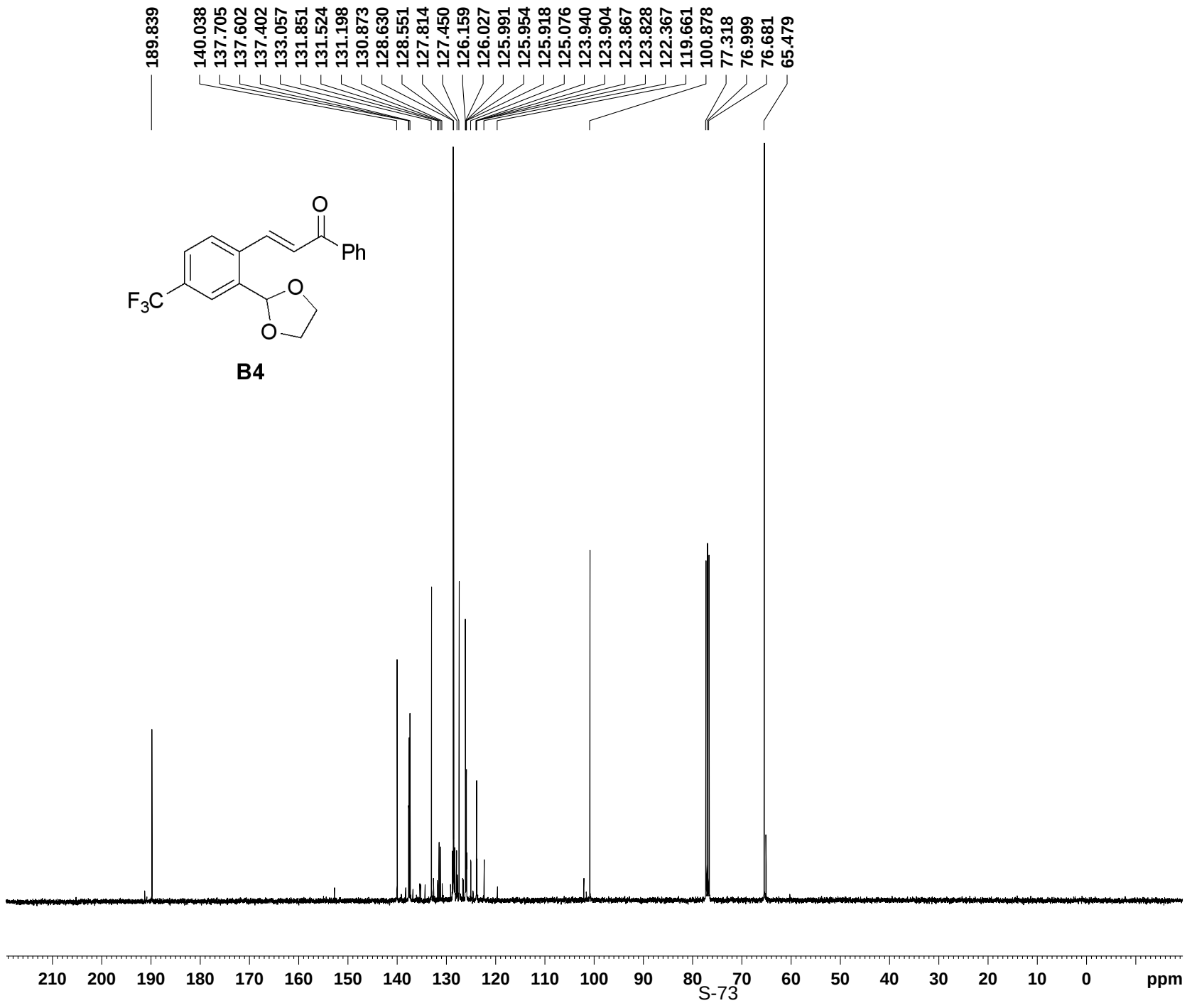


Current Data Parameters
NAME qh−3141
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120823
Time 16.08
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 645
DW 60.800 usec
DE 6.00 usec
TE 297.0 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 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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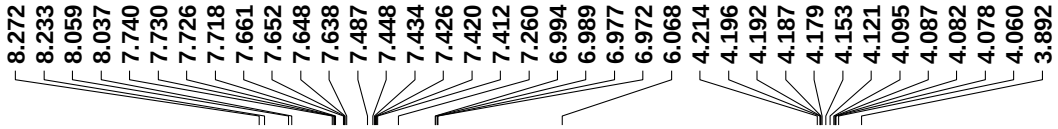
Current Data Parameters
NAME qh−3141
EXPNO 5
PROCNO 1

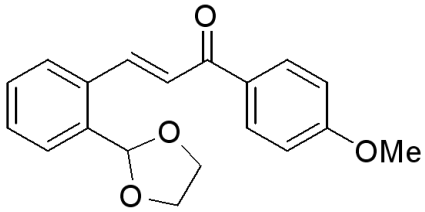
F2 − Acquisition Parameters
Date_ 20120823
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 912
DW 20.800 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127780 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





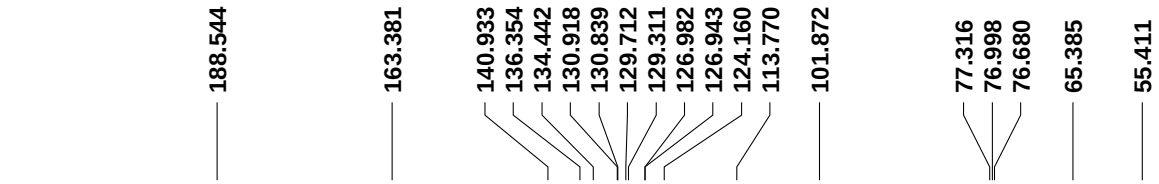
B5

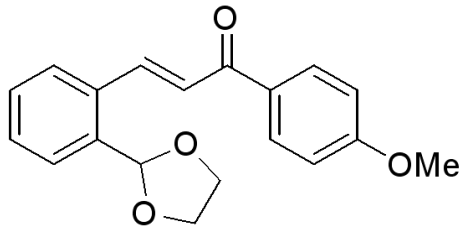
Current Data Parameters
NAME qh−3165
EXPNO 5
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120830
Time 17.23
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 297.1 K
D1 1.00000000 sec
TD0 1

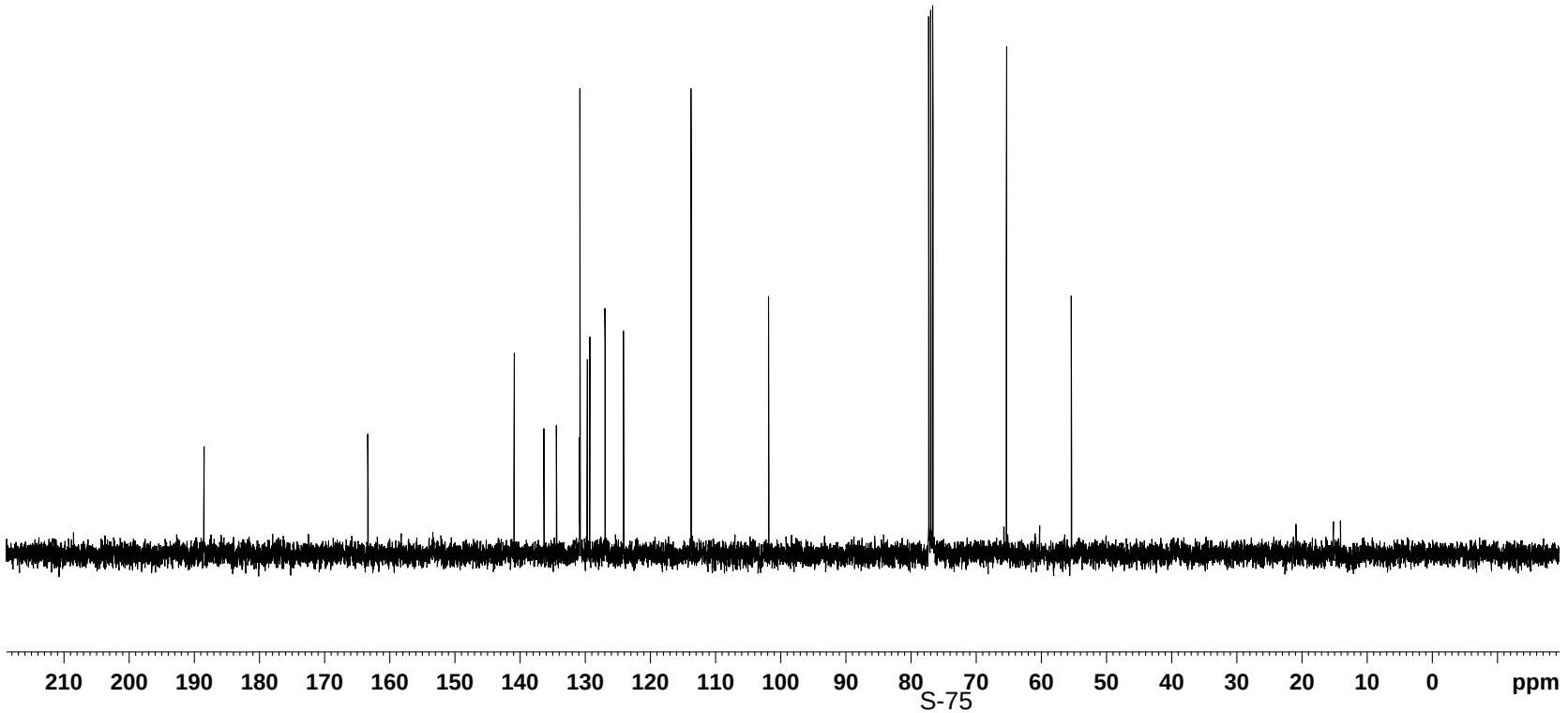
======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 −1.00 dB
SFO1 400.1324710 MHz

F2 − Processing parameters
SI 32768
SF 400.1300049 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





B5



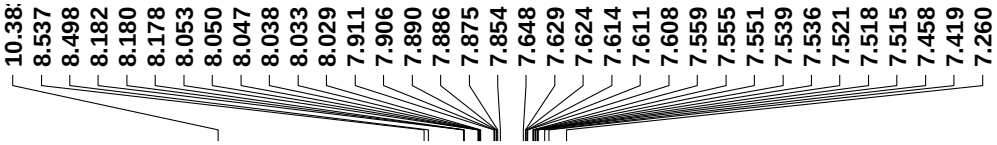
Current Data Parameters
NAME qh−3165
EXPNO 4
PROCNO 1

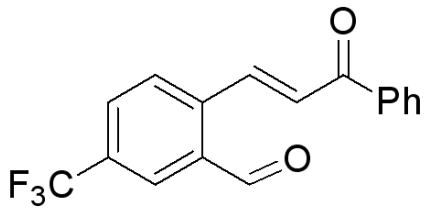
F2 − Acquisition Parameters
Date_ 20120830
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 57
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

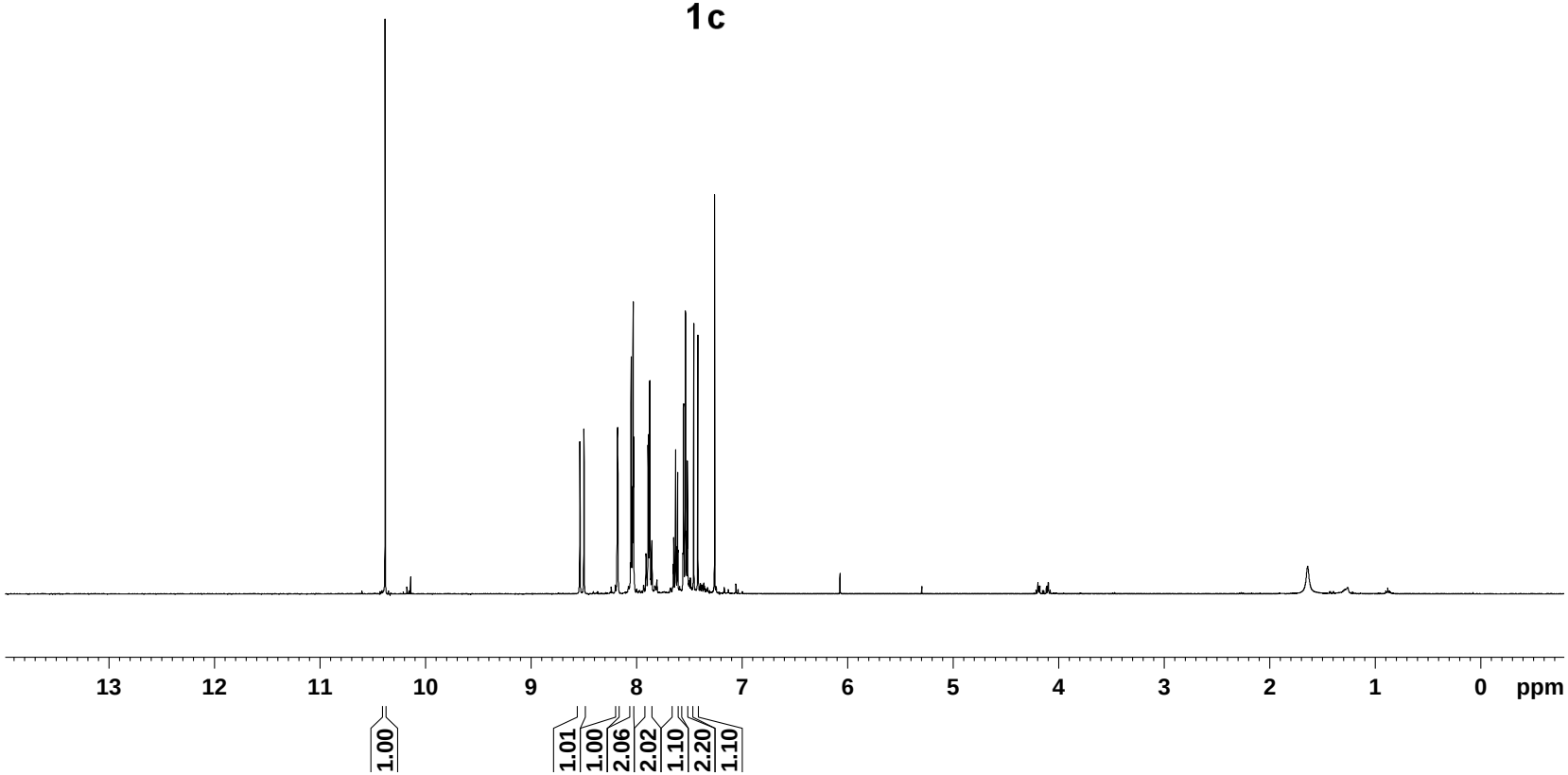
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127765 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





1c

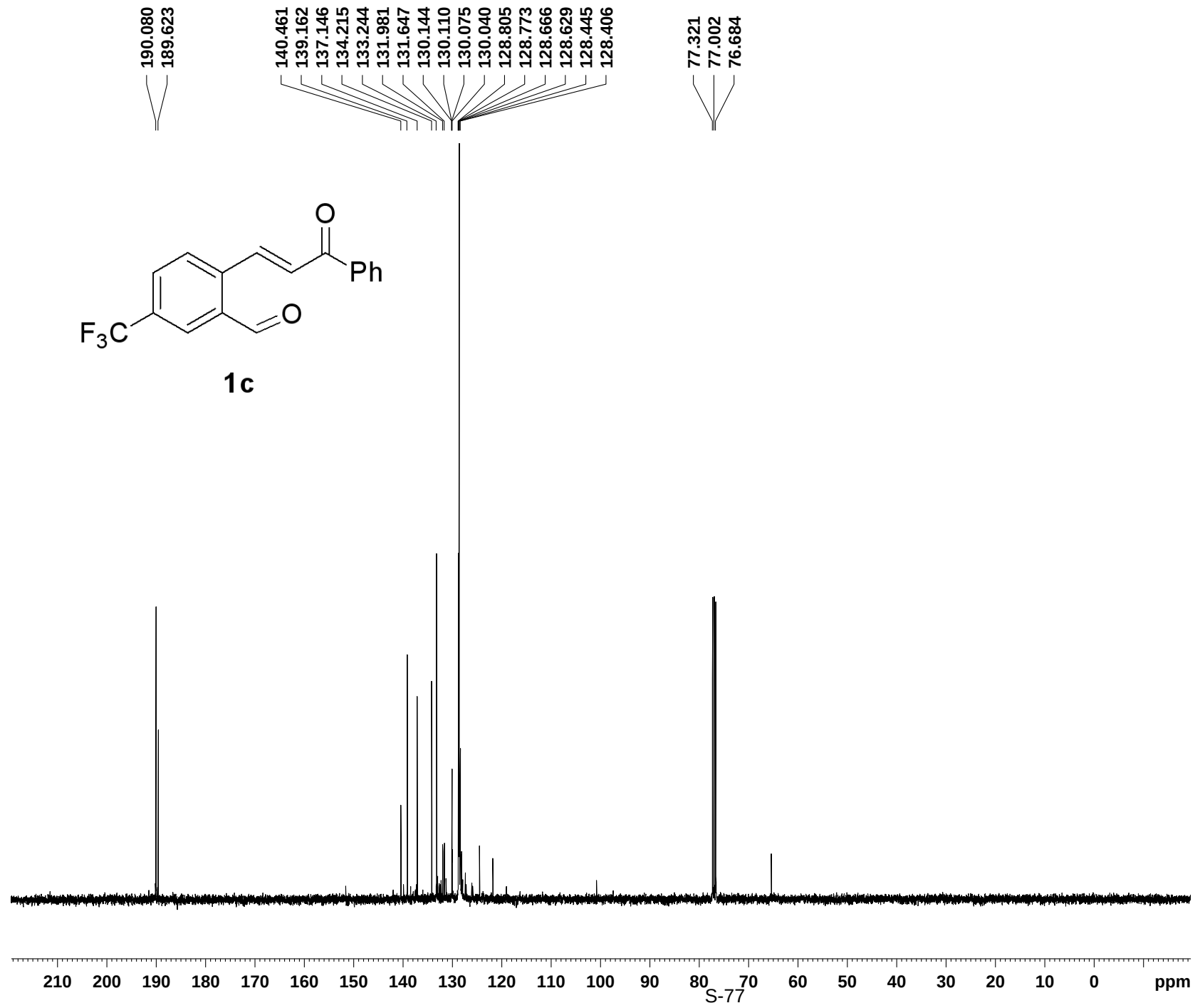


Current Data Parameters
NAME qh−3163
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120830
Time 18.44
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 297.1 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 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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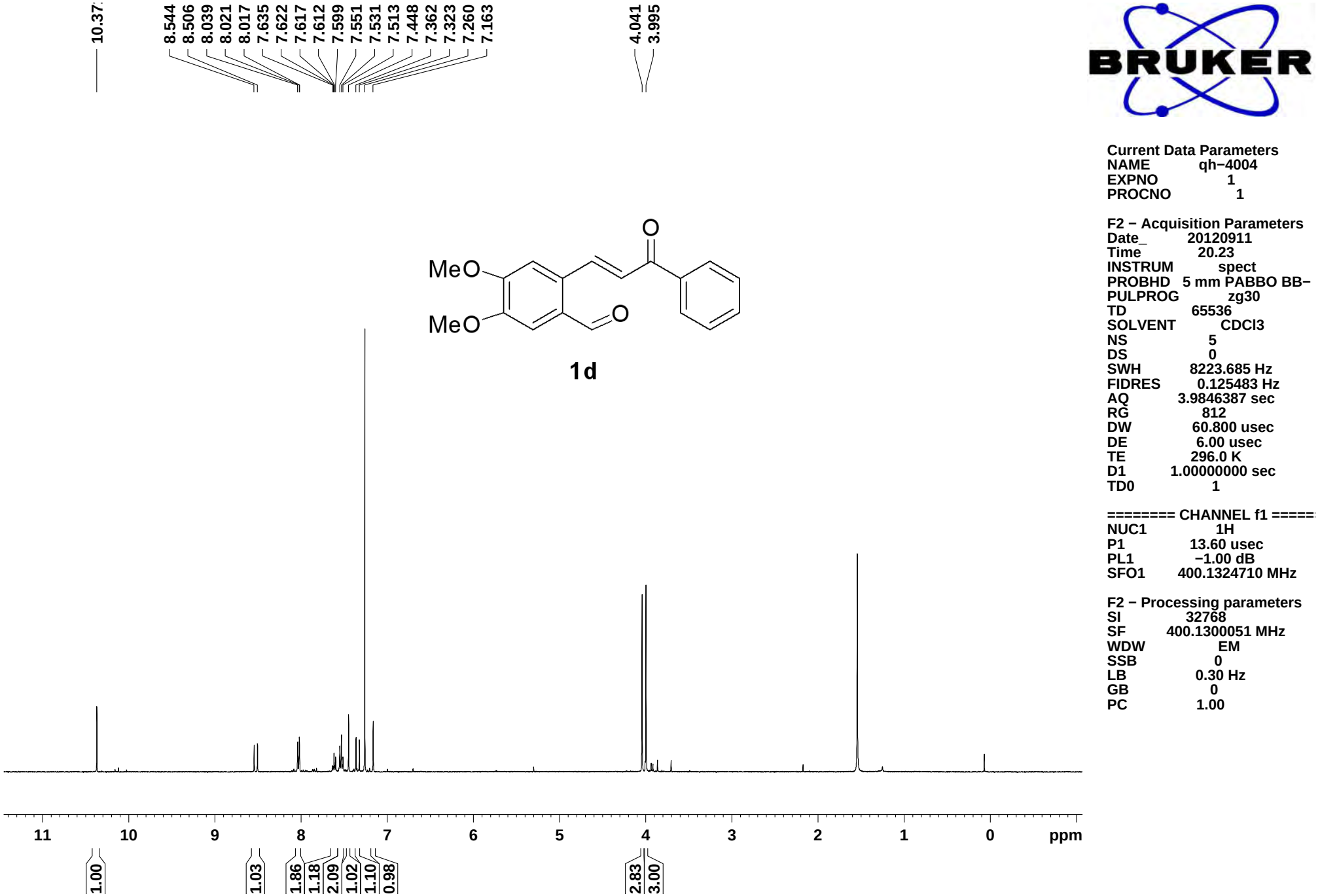
Current Data Parameters
NAME qh−3163
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120830
Time 18.59
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 80
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 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127802 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

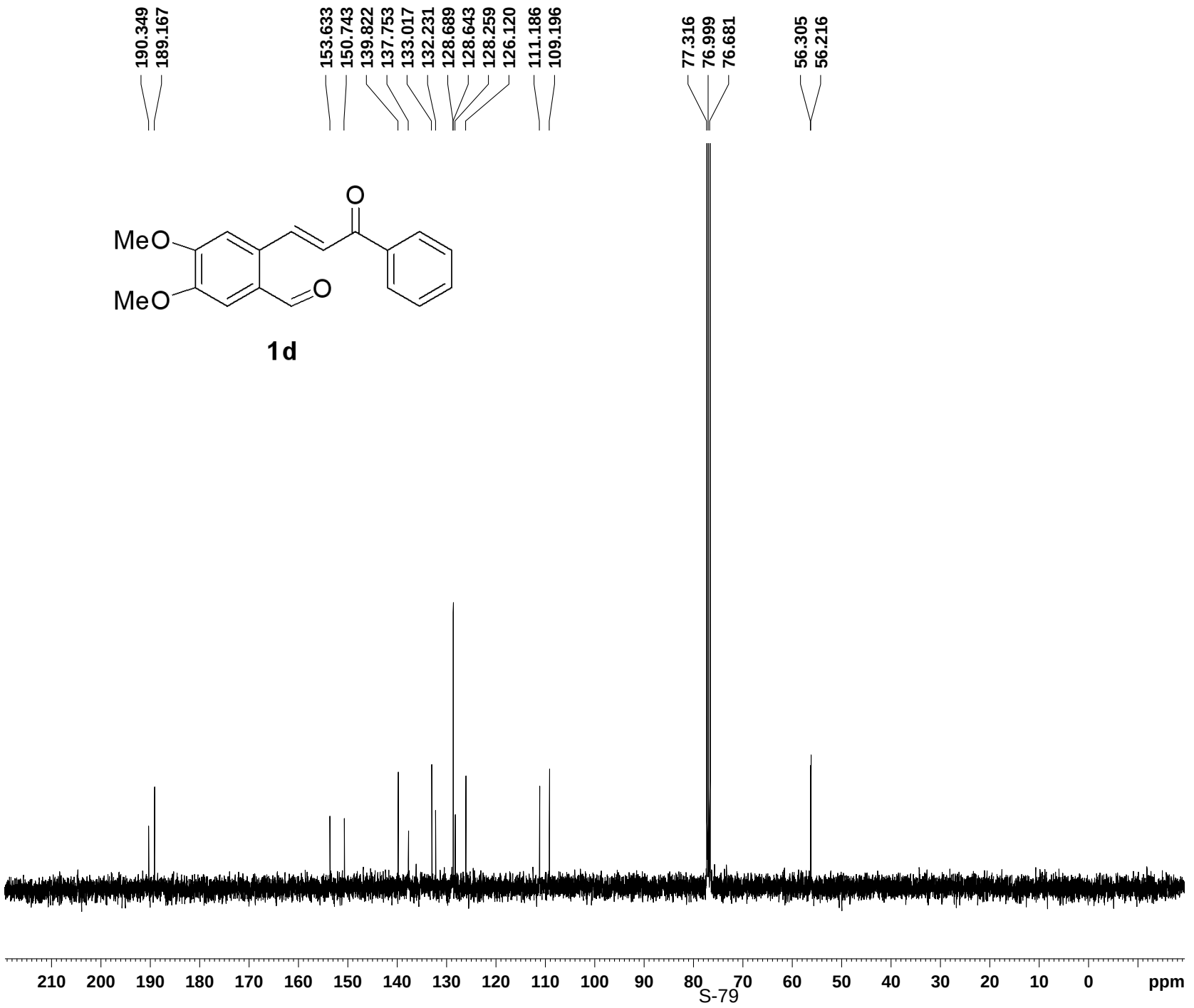


Current Data Parameters
NAME qh−4004
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120911
Time 20.23
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 812
DW 60.800 usec
DE 6.00 usec
TE 296.0 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 400.1300051 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



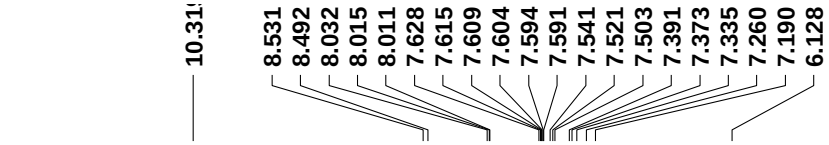
Current Data Parameters
NAME qh−4004
EXPNO 4
PROCNO 1

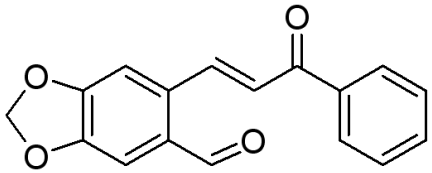
F2 − Acquisition Parameters
Date_ 20120925
Time 16.54
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

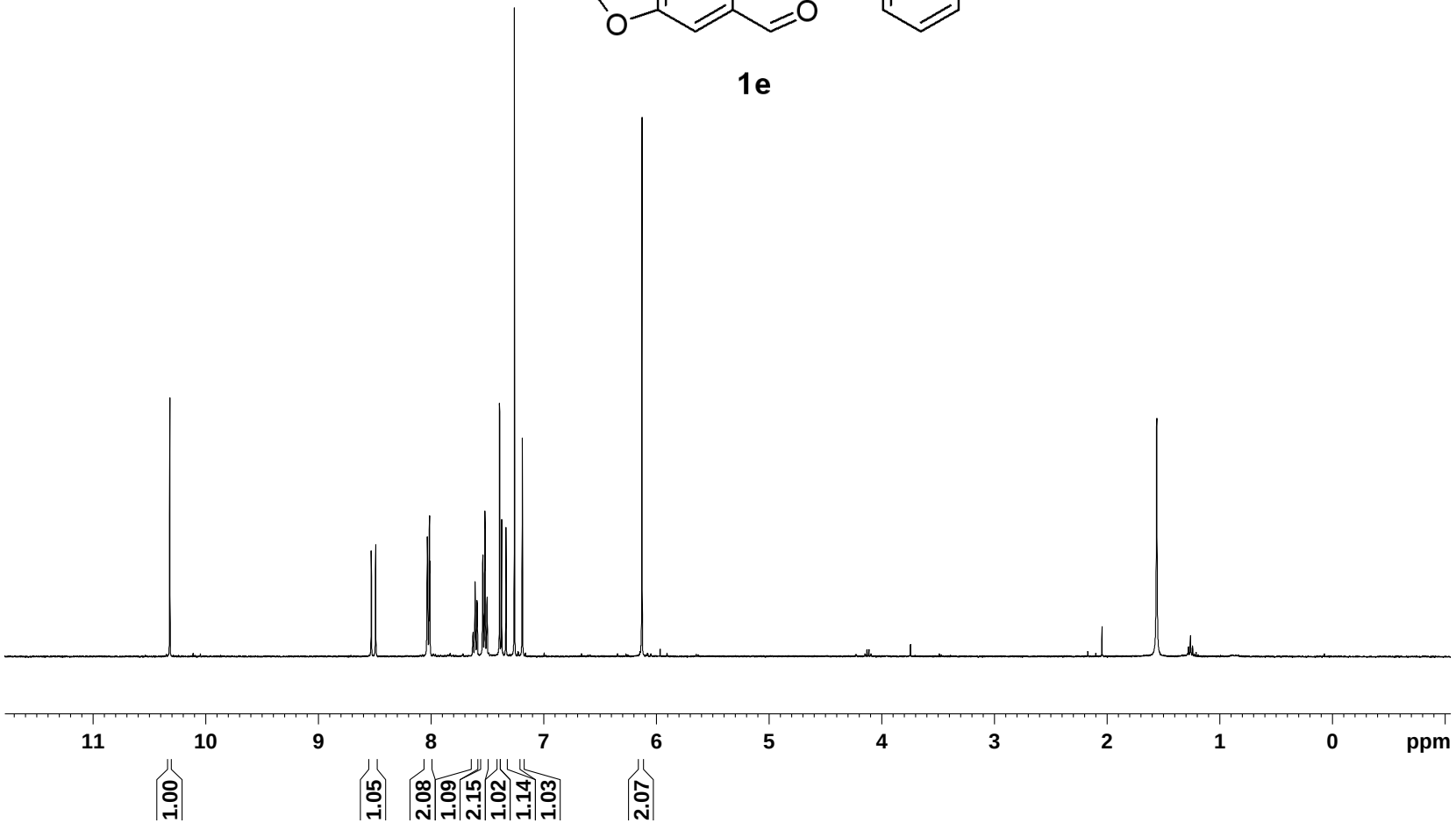
======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





1e

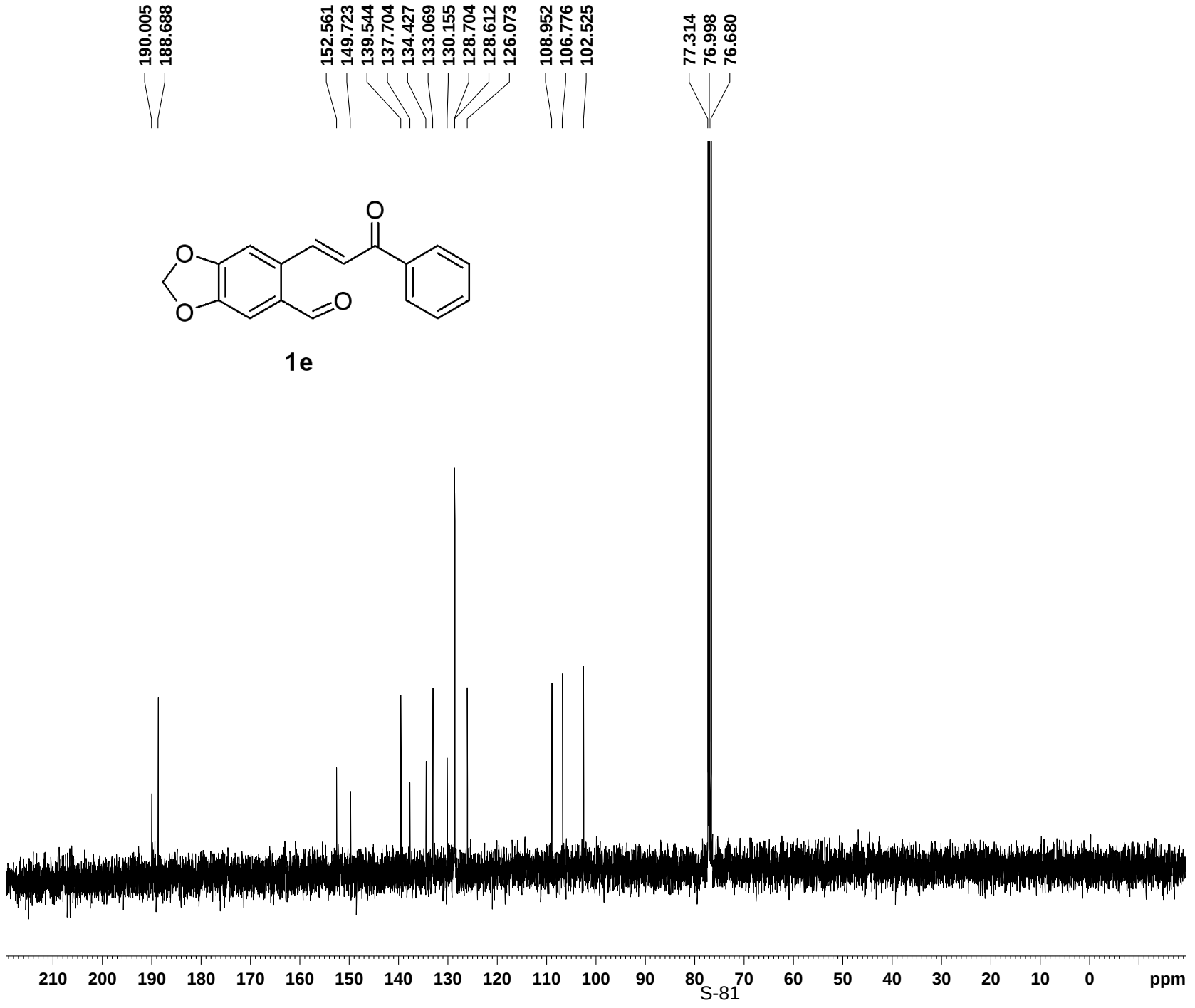


Current Data Parameters
NAME qh−4003−crude
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120910
Time 23.32
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 812
DW 60.800 usec
DE 6.00 usec
TE 298.6 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



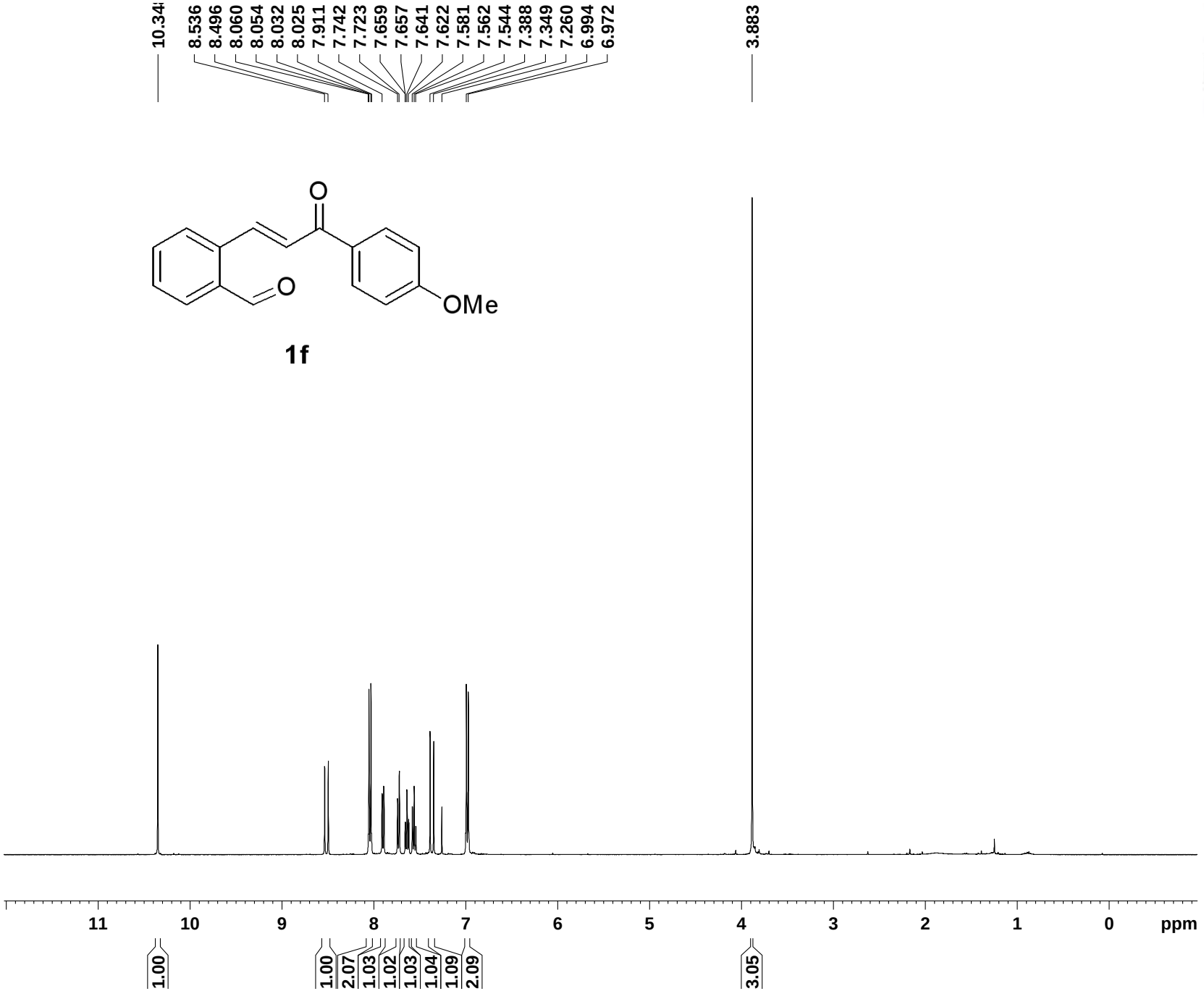
Current Data Parameters
NAME qh−4003
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120925
Time 16.43
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 299.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127707 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

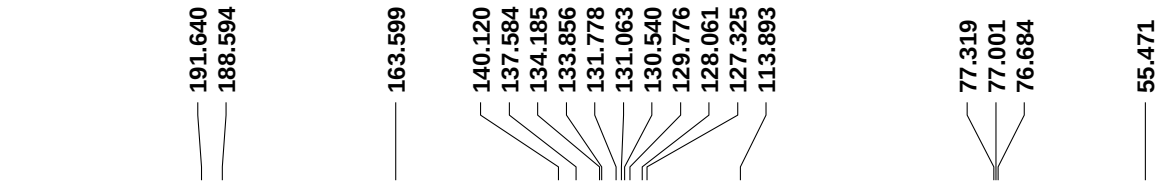


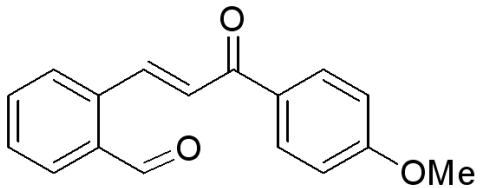
Current Data Parameters
NAME qh−3168
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120831
Time 1.12
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 3
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1

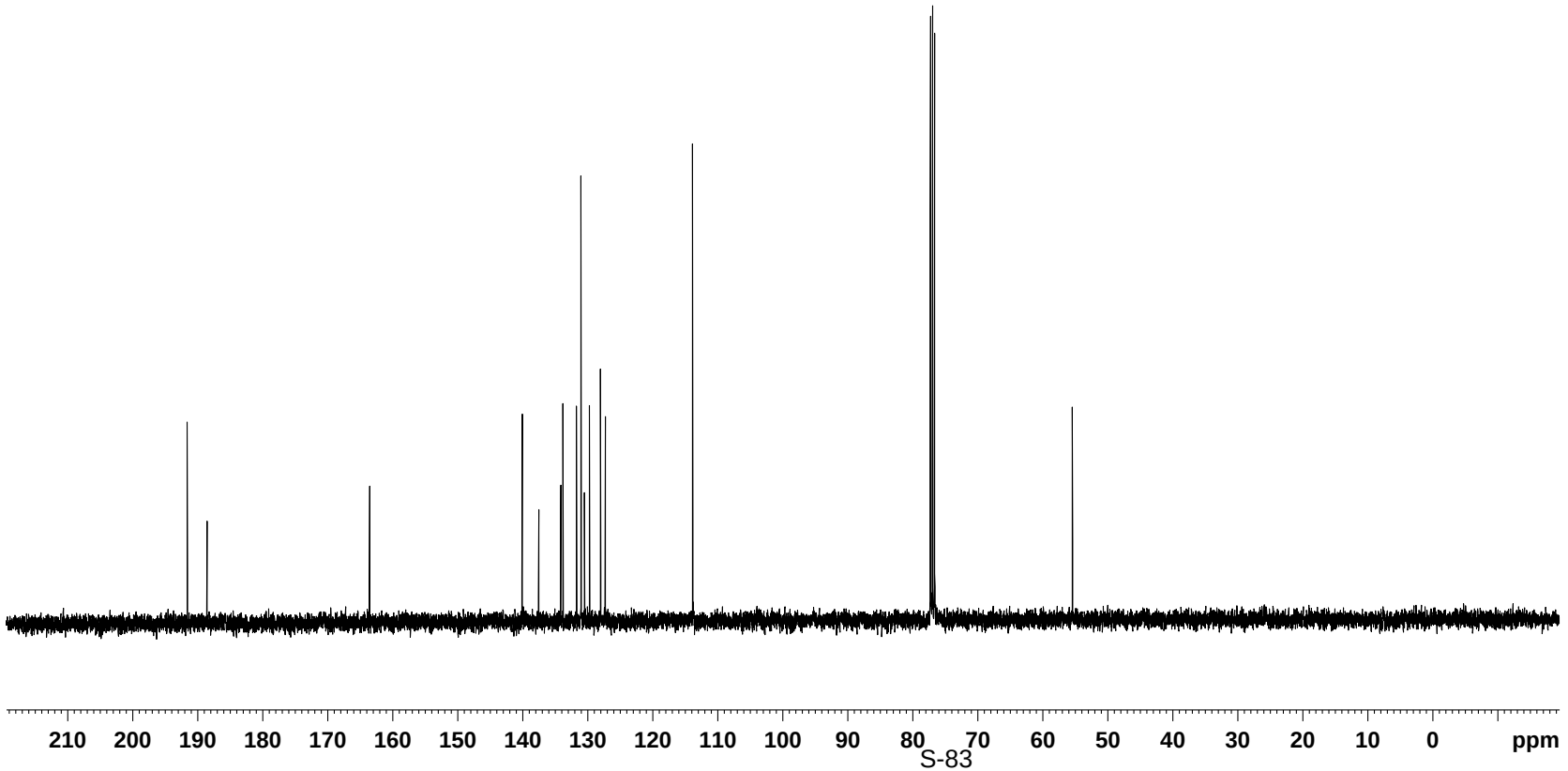
======== CHANNEL f1 =====
NUC1 1H
P1 13.60 usec
PL1 −1.00 dB
SFO1 400.1324710 MHz

F2 − Processing parameters
SI 32768
SF 400.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00





1f



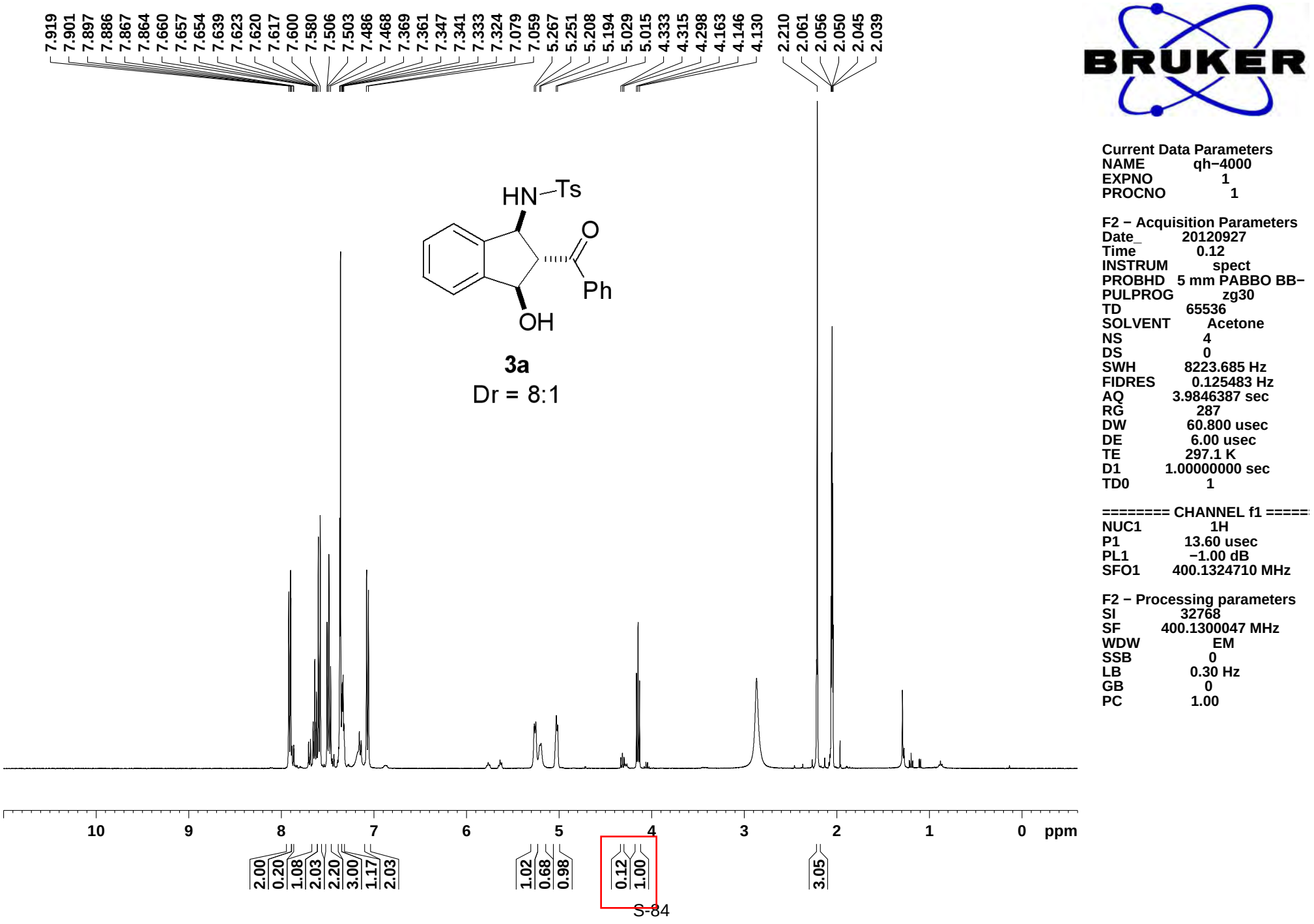
Current Data Parameters
NAME qh−3168
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120831
Time 1.14
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
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 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

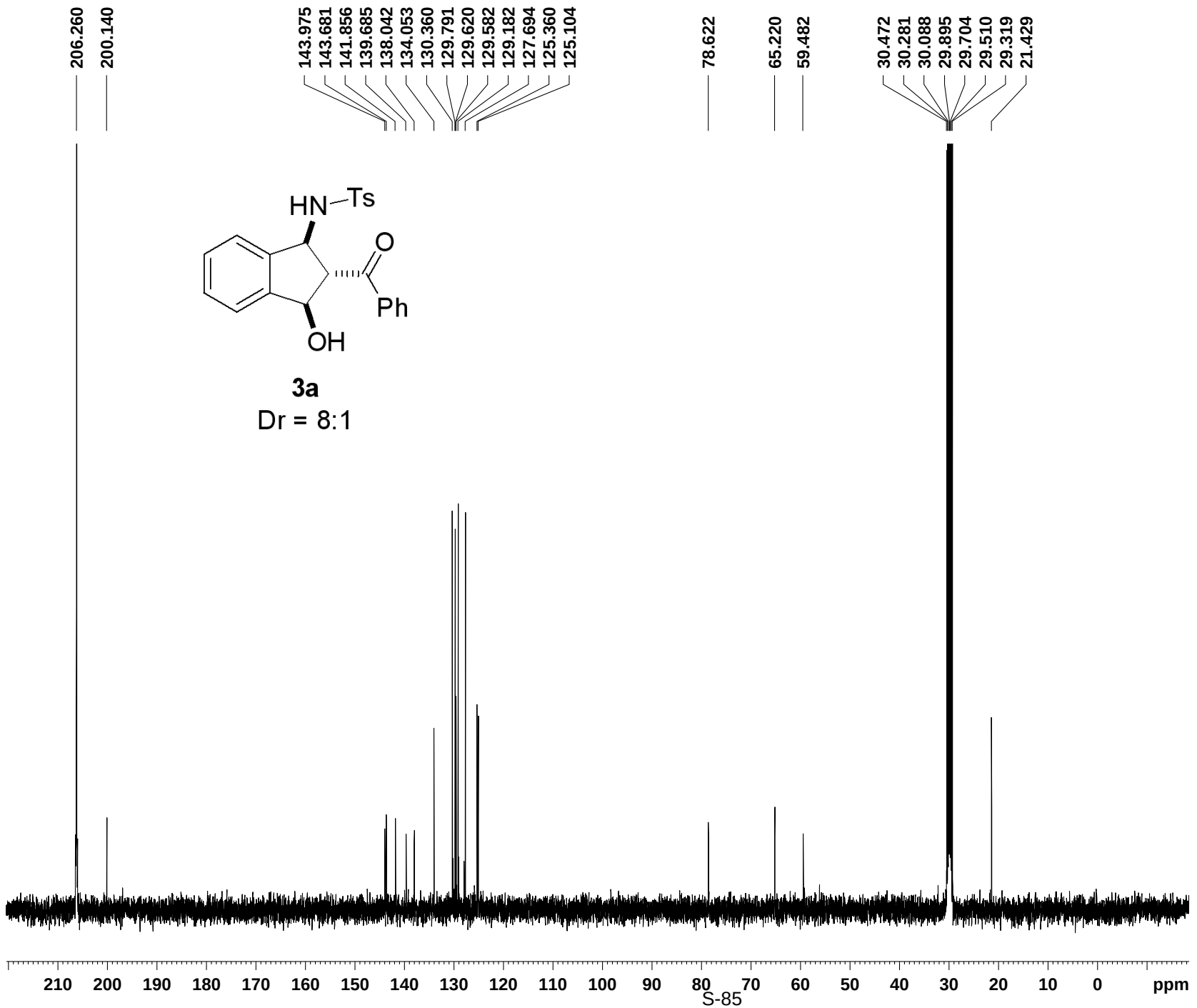


Current Data Parameters
NAME qh−4000
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 0.12
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 297.1 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



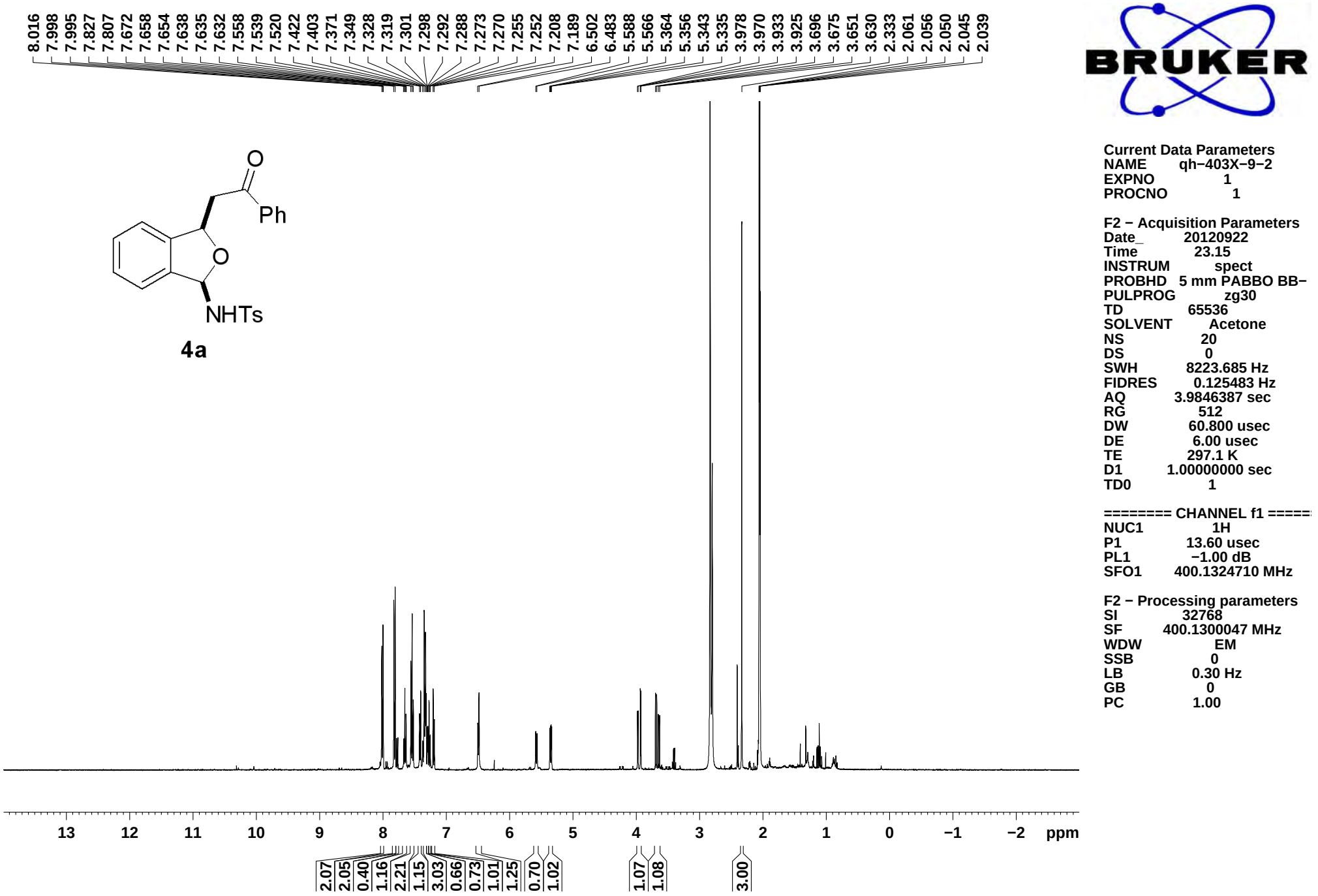
Current Data Parameters
NAME qh−4000
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 0.17
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 273
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 297.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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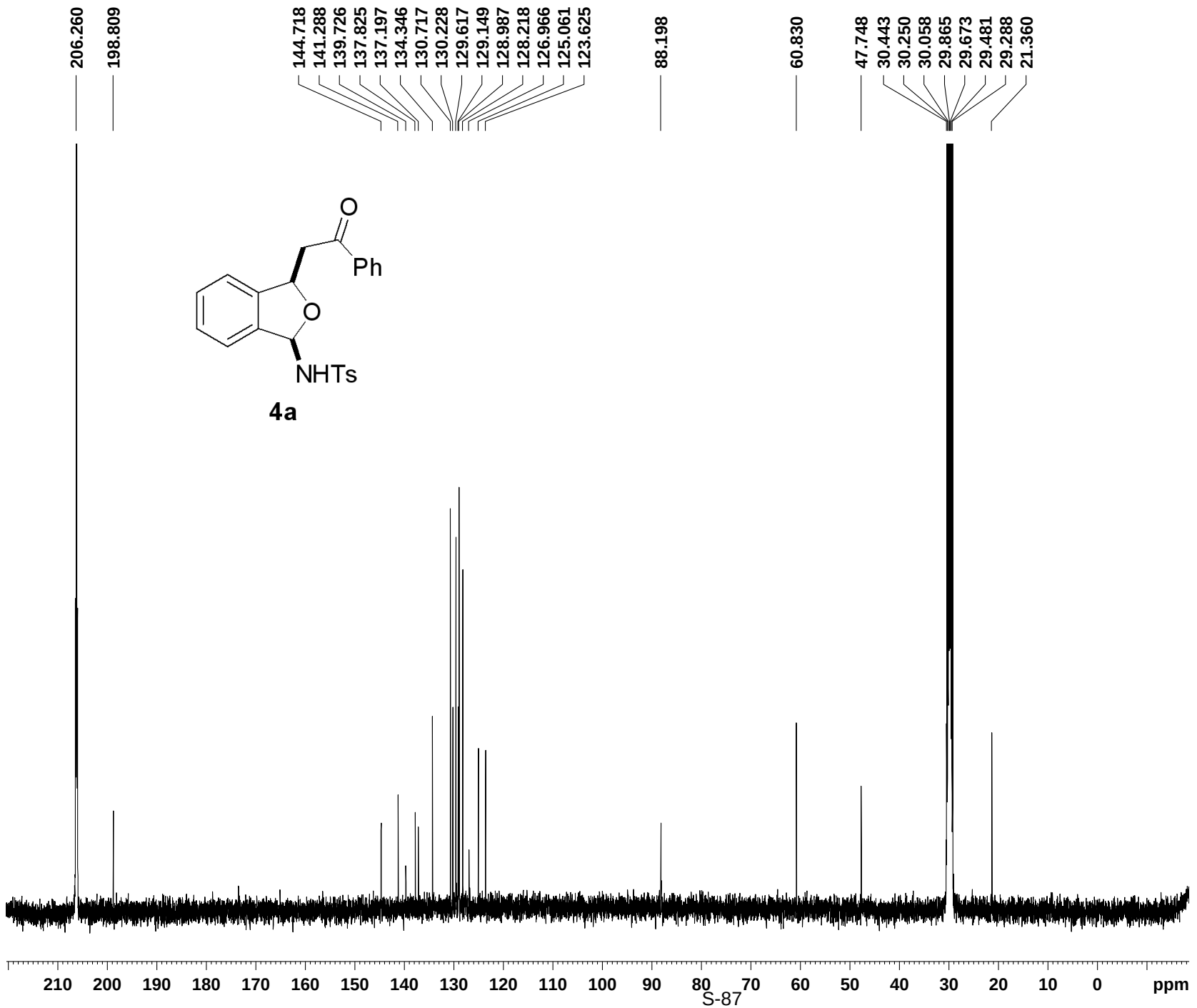
Current Data Parameters
NAME qh−403X−9−2
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120922
Time 23.15
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 20
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 297.1 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



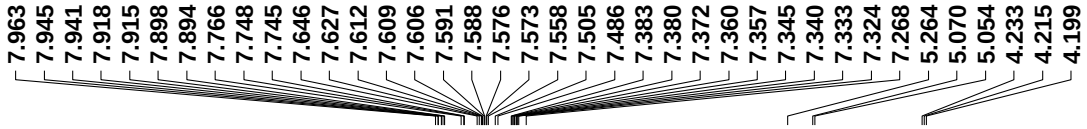
Current Data Parameters
NAME qh−403X−9−2
EXPNO 5
PROCNO 1

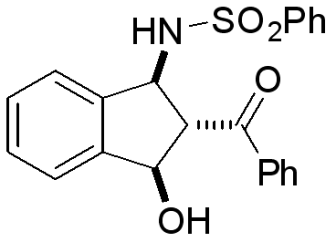
F2 − Acquisition Parameters
Date_ 20120927
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 9
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 90.5
DW 20.800 usec
DE 6.00 usec
TE 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

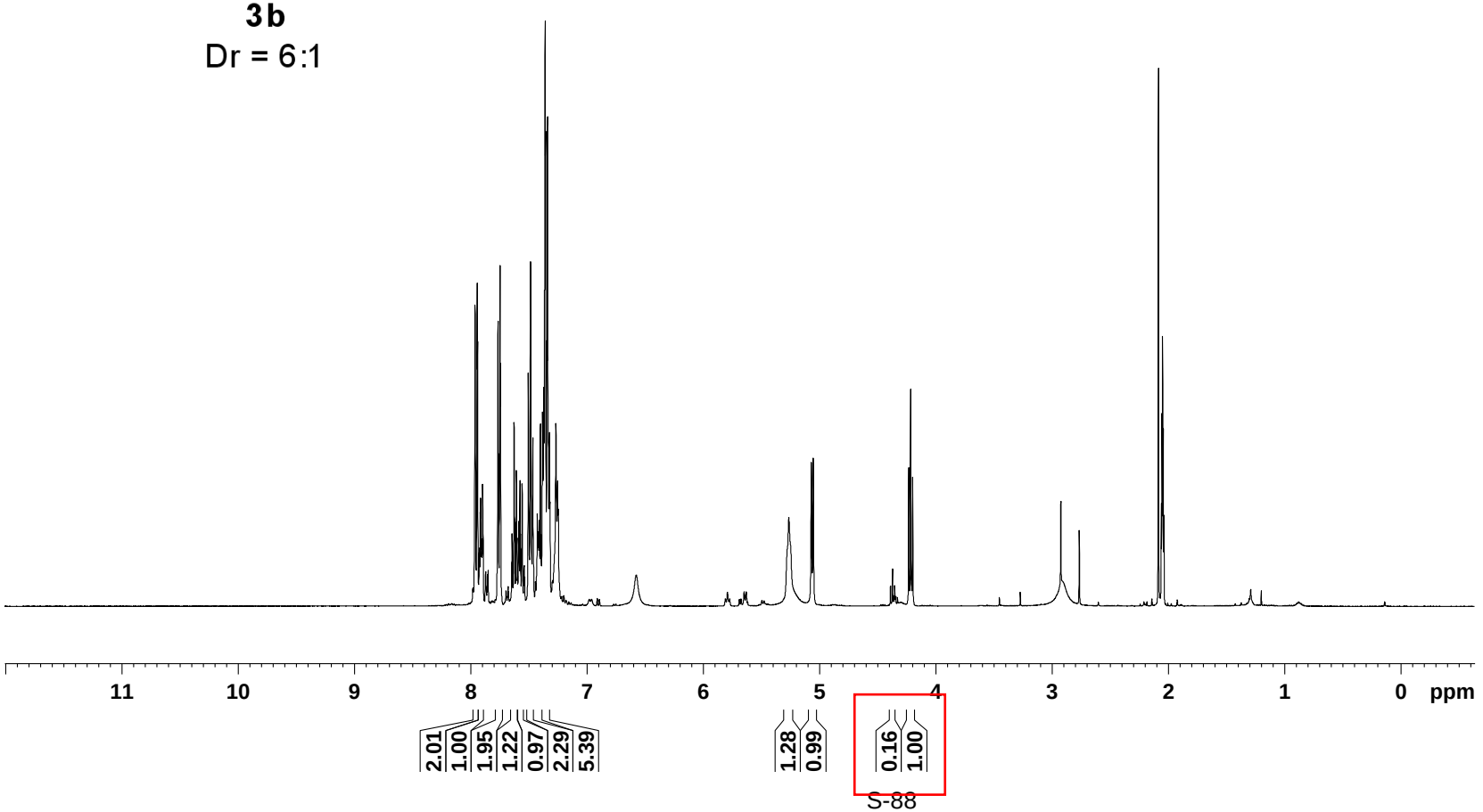
F2 − Processing parameters
SI 32768
SF 100.6126752 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3b

Dr = 6:1

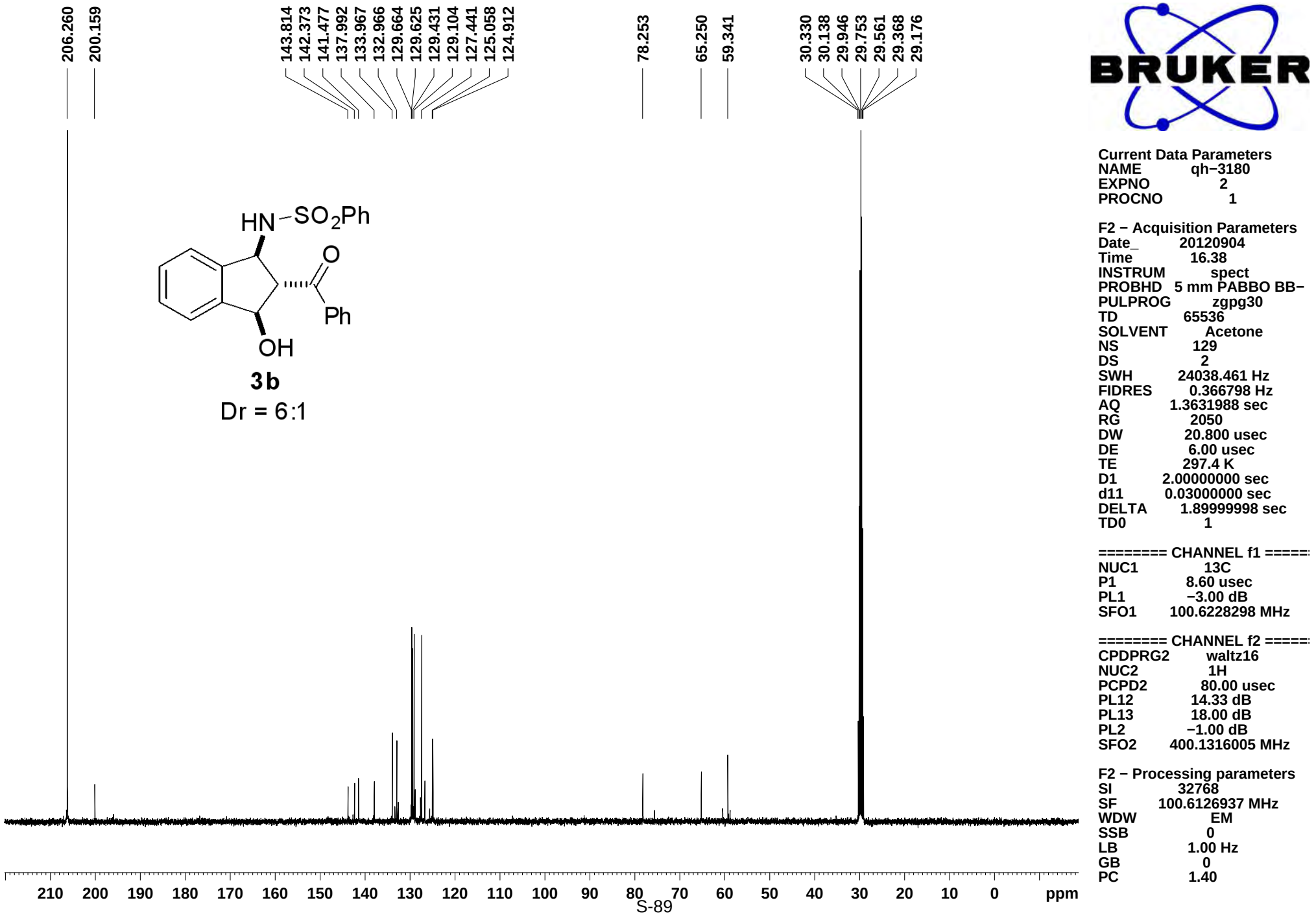


Current Data Parameters
NAME qh−3180
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20121021
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 10
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 296.7 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 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

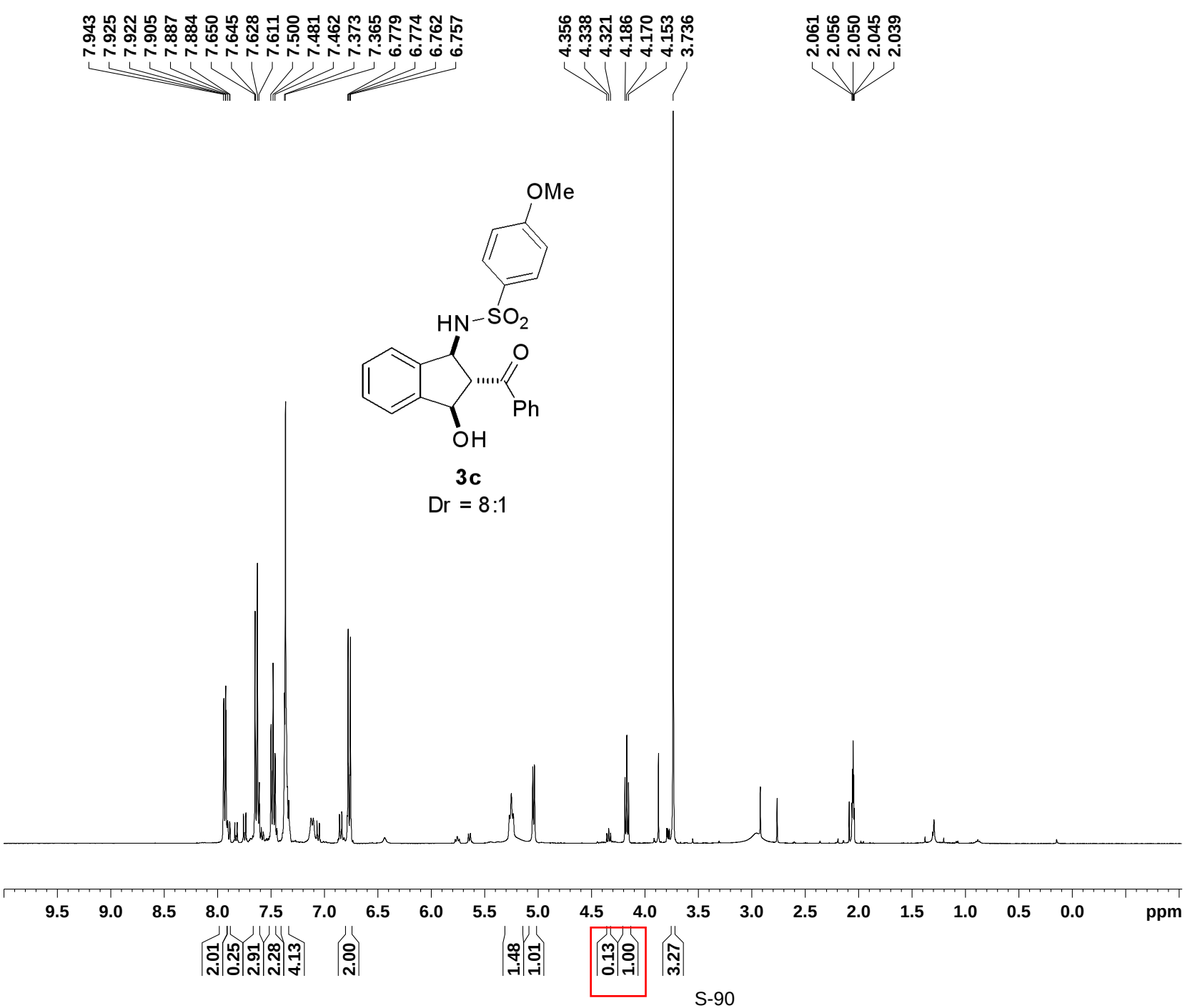
Current Data Parameters
NAME qh−3180
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120904
Time 16.38
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 129
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 297.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126937 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



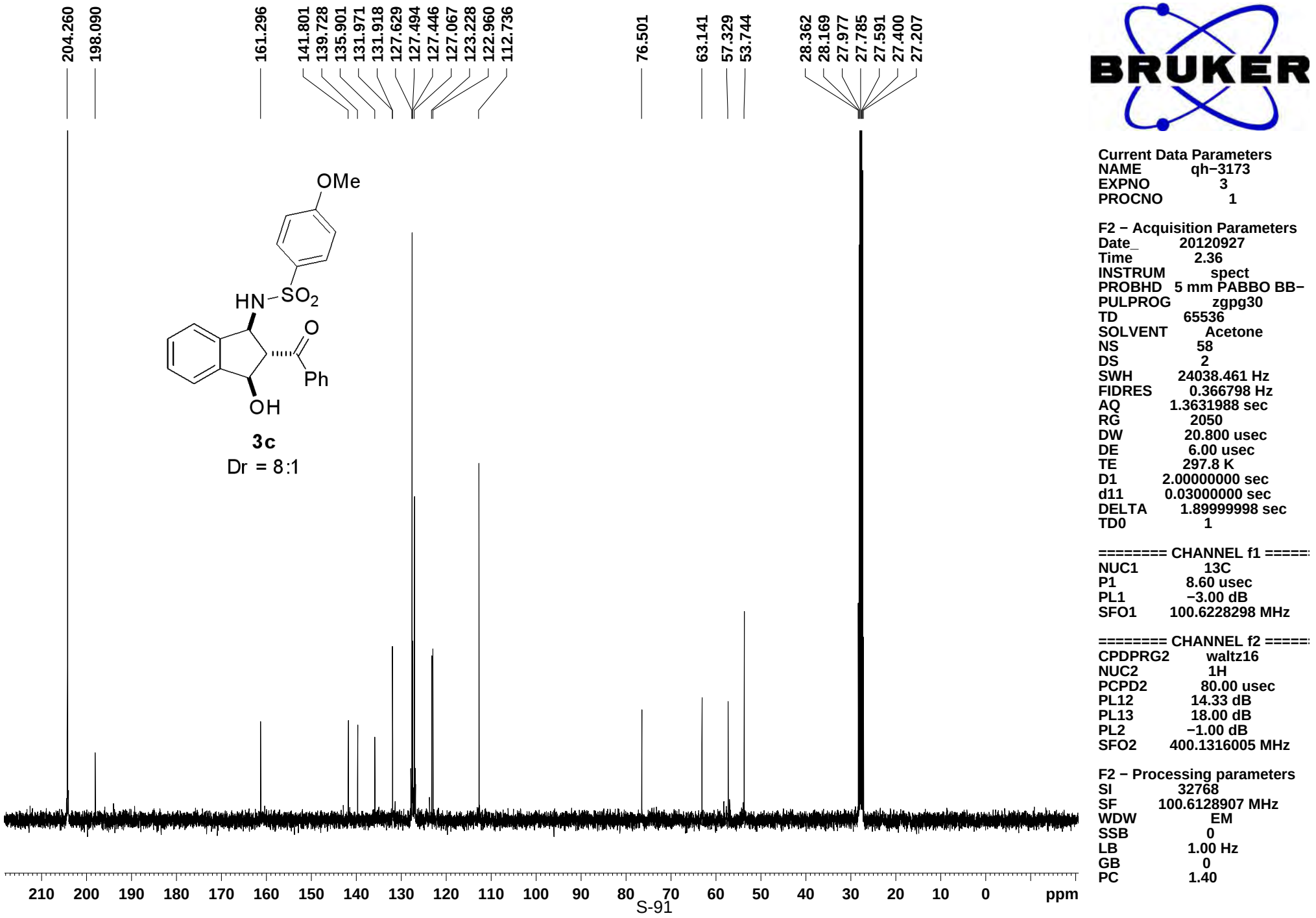
BRUKER

Current Data Parameters
NAME qh−3173
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 2.32
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 4
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 297.2 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

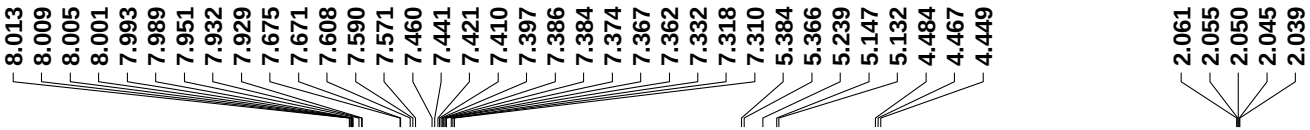
Current Data Parameters
NAME qh−3173
EXPNO 3
PROCNO 1

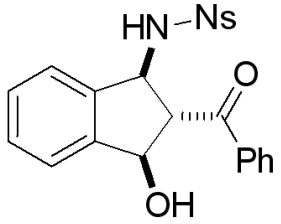
F2 − Acquisition Parameters
Date_ 20120927
Time 2.36
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 58
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

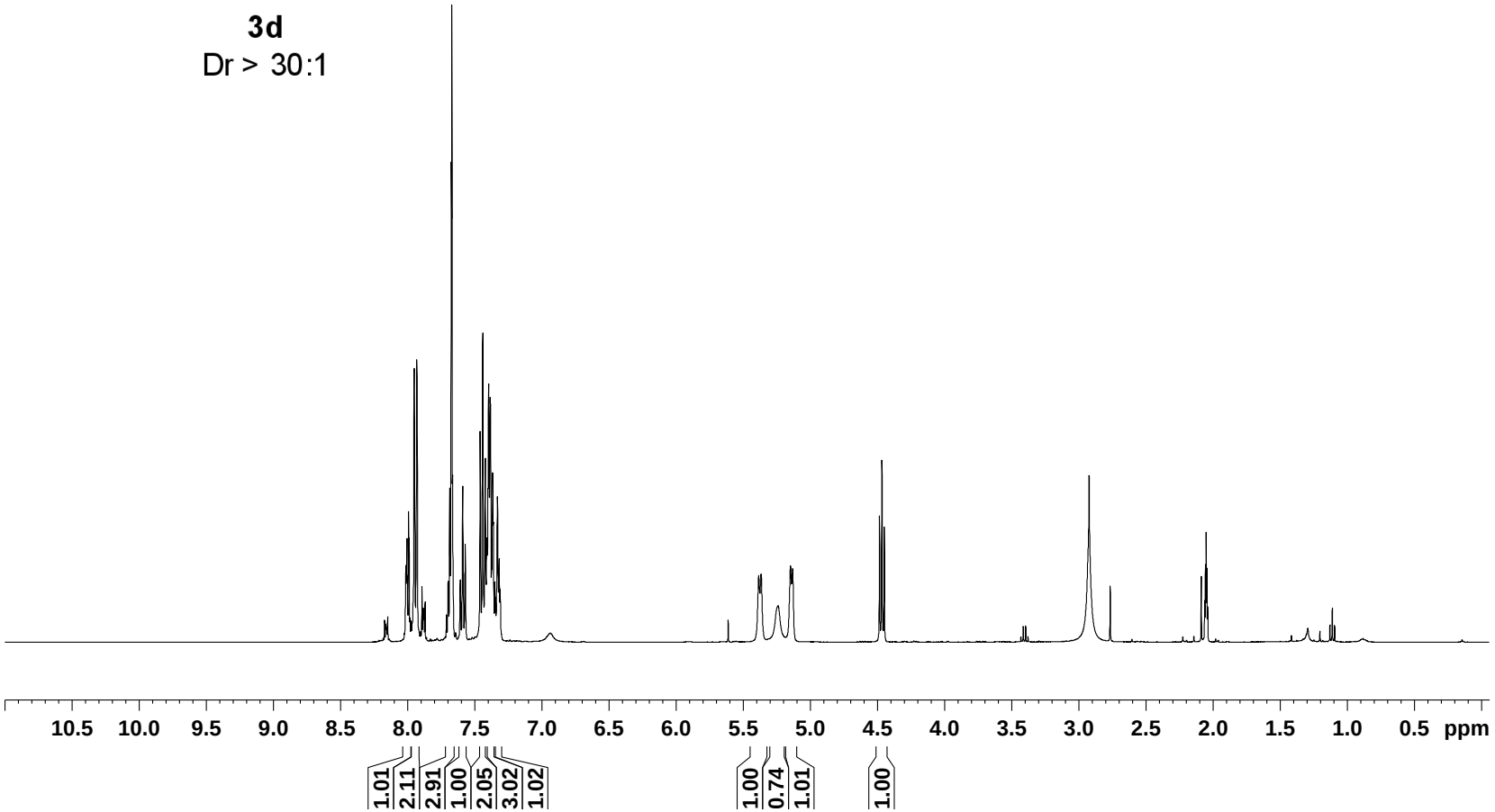
F2 − Processing parameters
SI 32768
SF 100.6128907 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3d

Dr > 30:1

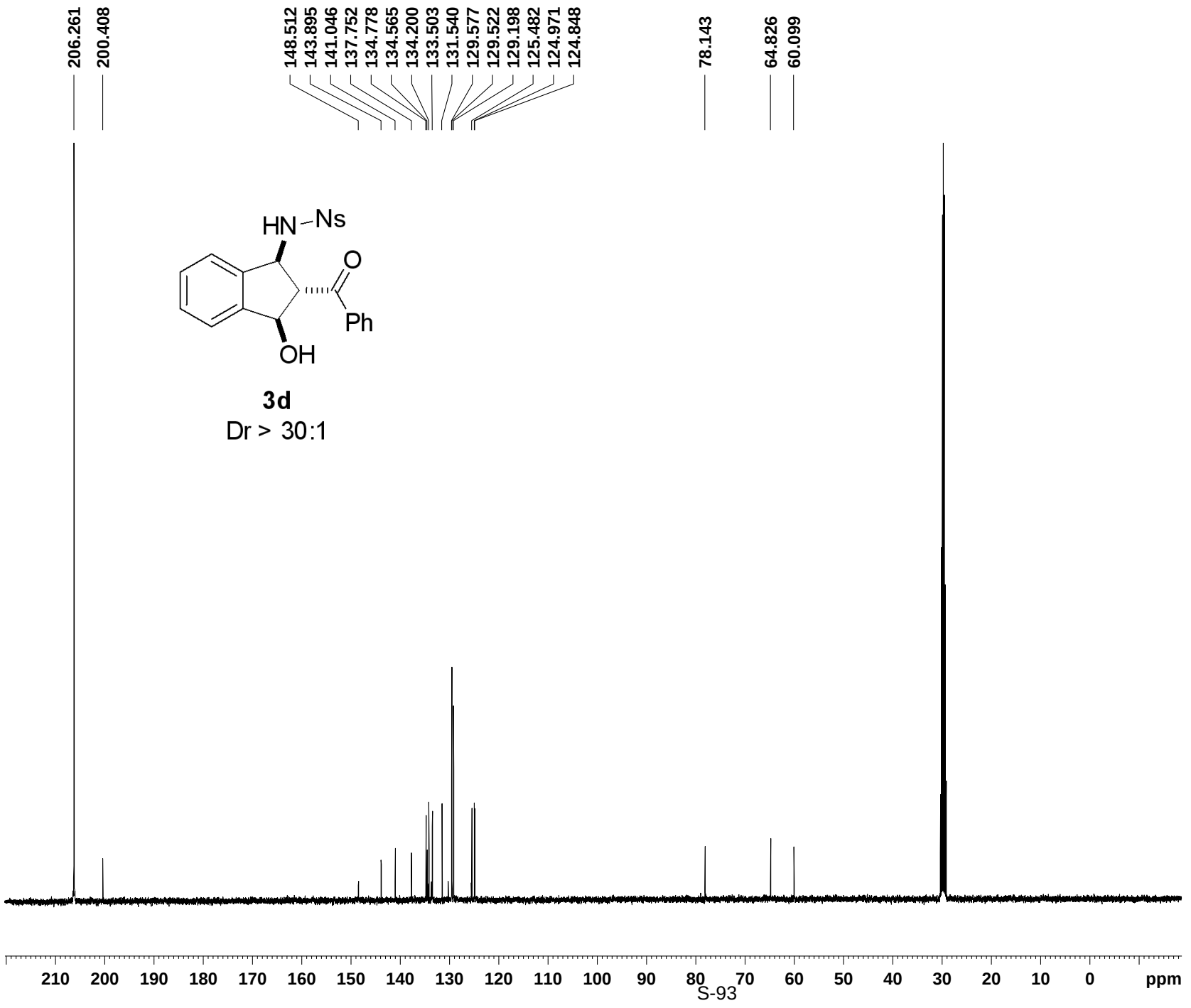


Current Data Parameters
NAME qh−3179
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120909
Time 22.54
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
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 299.9 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



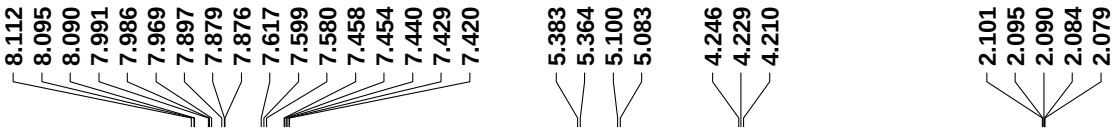
Current Data Parameters
NAME qh−3179
EXPNO 3
PROCNO 1

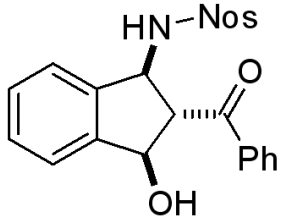
F2 − Acquisition Parameters
Date_ 20120909
Time 23.04
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2000
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 300.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

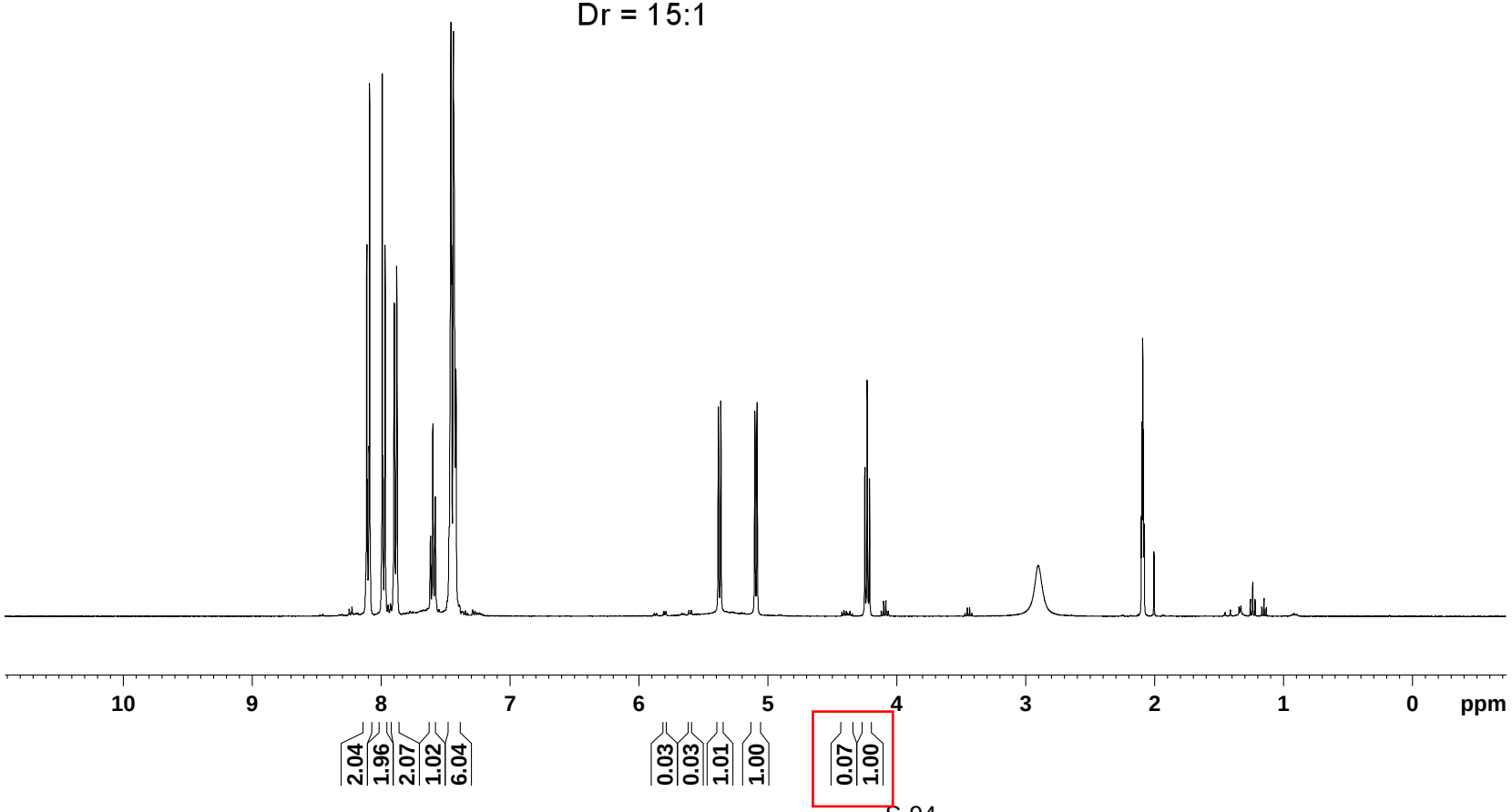
F2 − Processing parameters
SI 32768
SF 100.6126885 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3e

Dr = 15:1

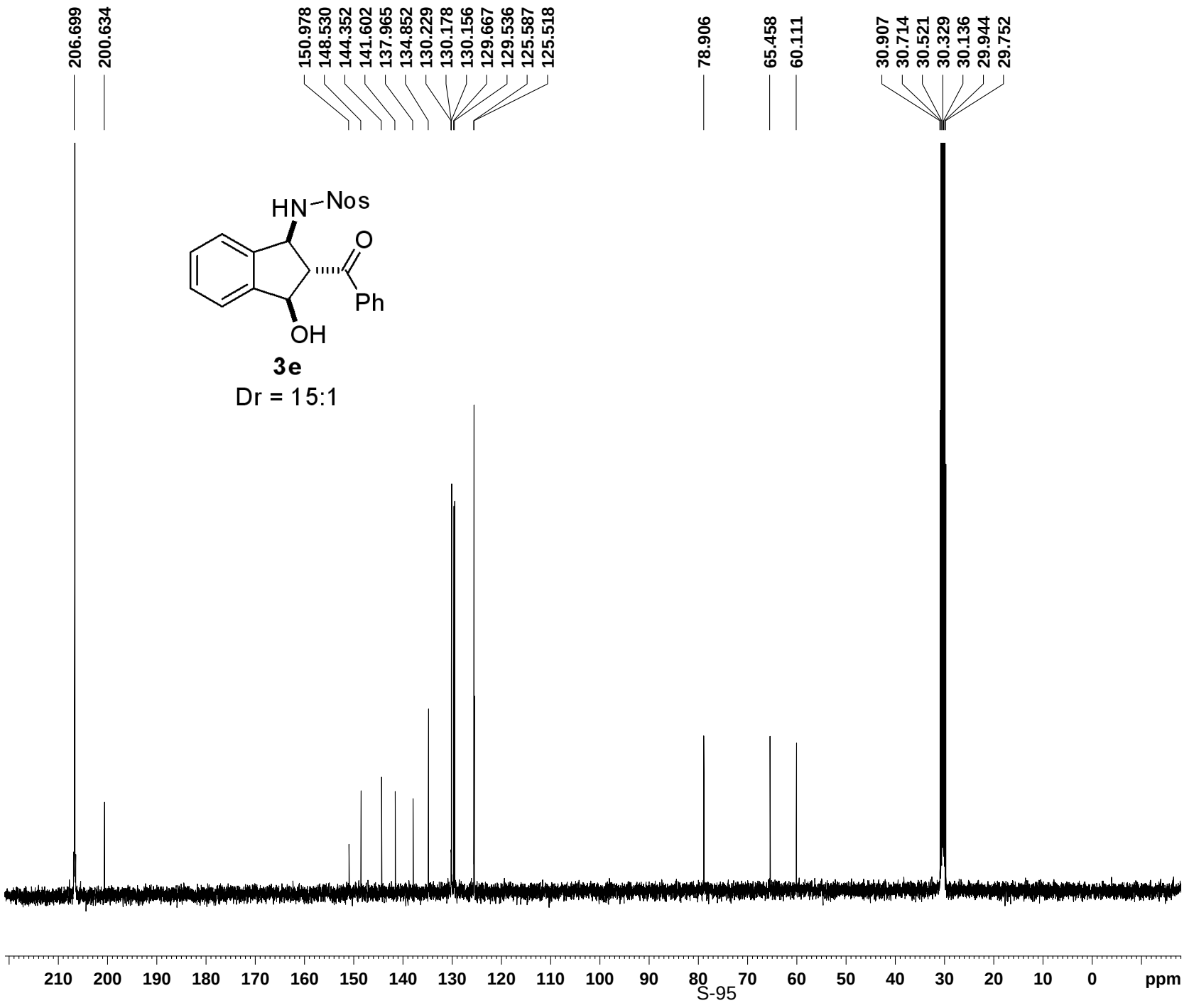


Current Data Parameters
NAME qh−3194
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120908
Time 19.47
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 7
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 298.8 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 400.1299887 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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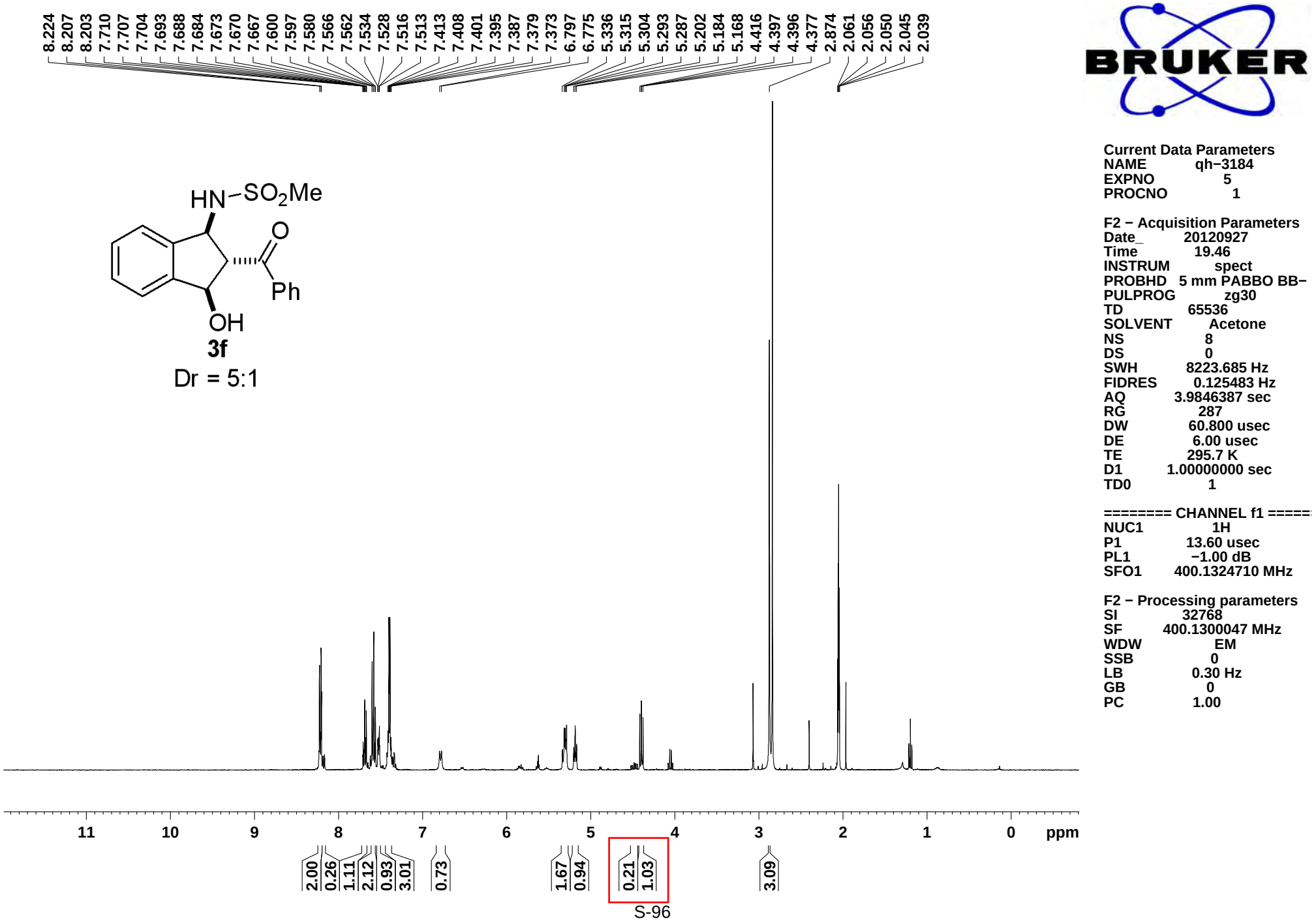
Current Data Parameters
NAME qh−3194
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120908
Time 19.49
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
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 299.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126296 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

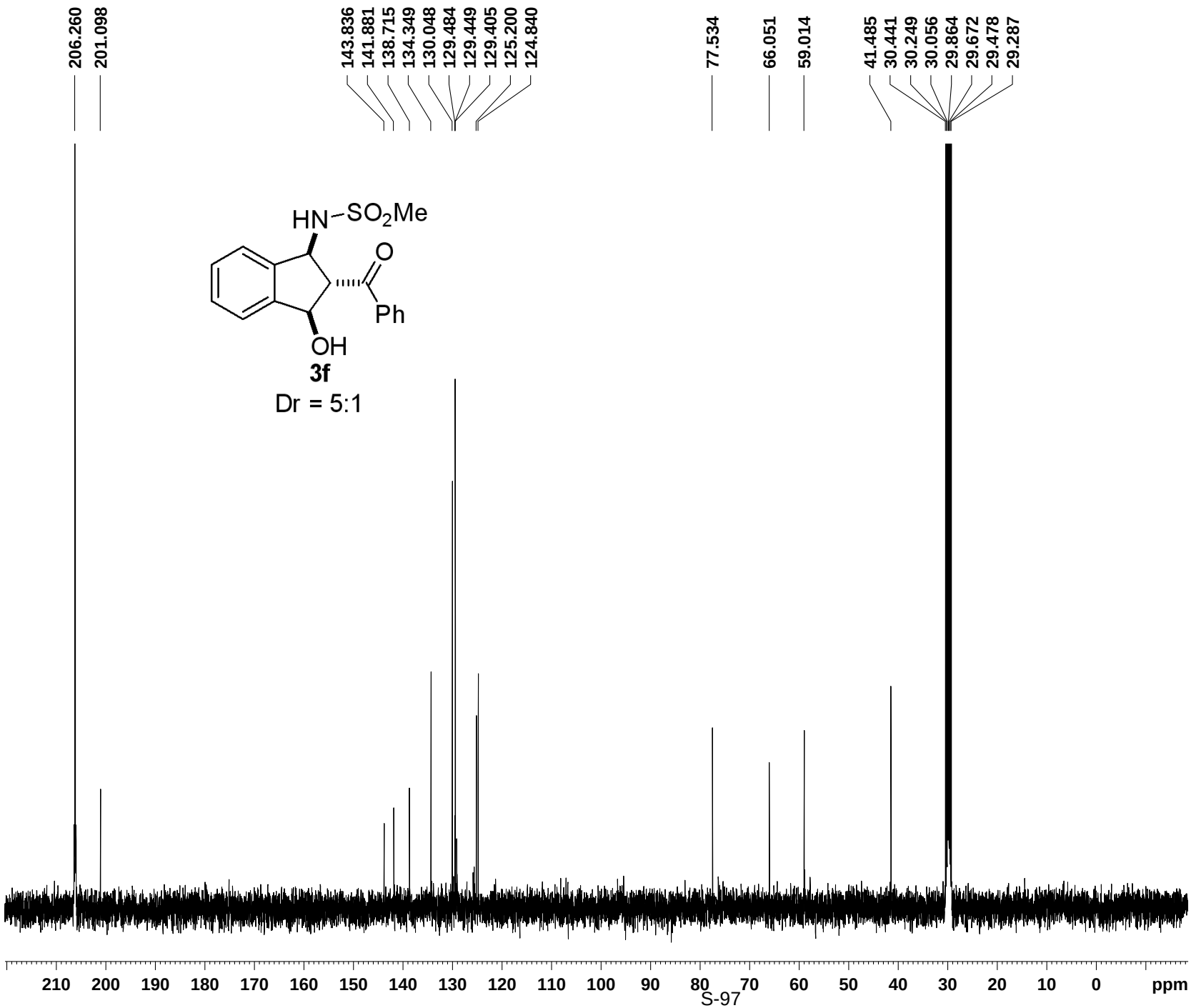


Current Data Parameters
NAME qh−3184
EXPNO 5
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 19.46
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 295.7 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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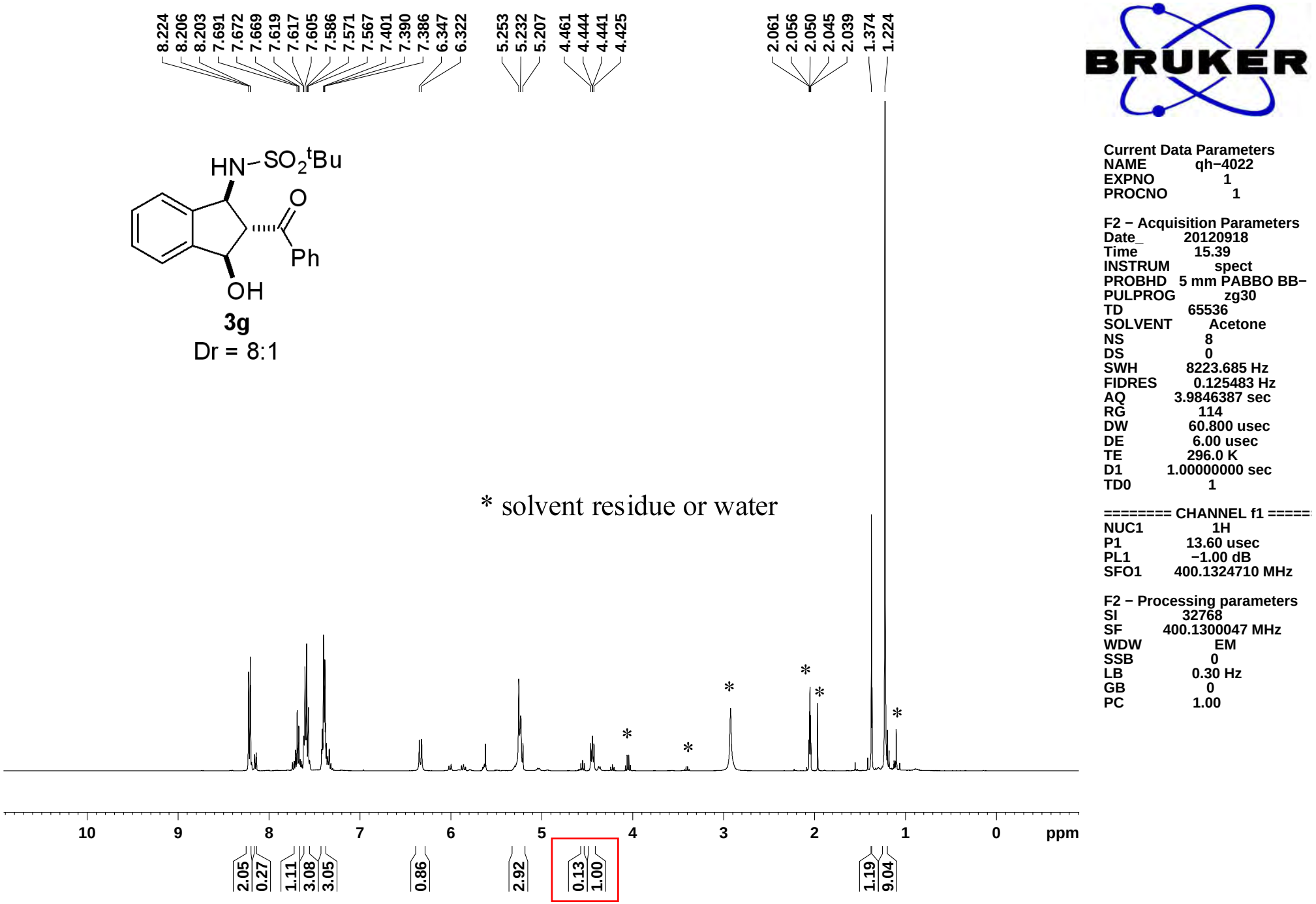
Current Data Parameters
NAME qh−3184
EXPNO 6
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 19.56
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
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 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126773 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

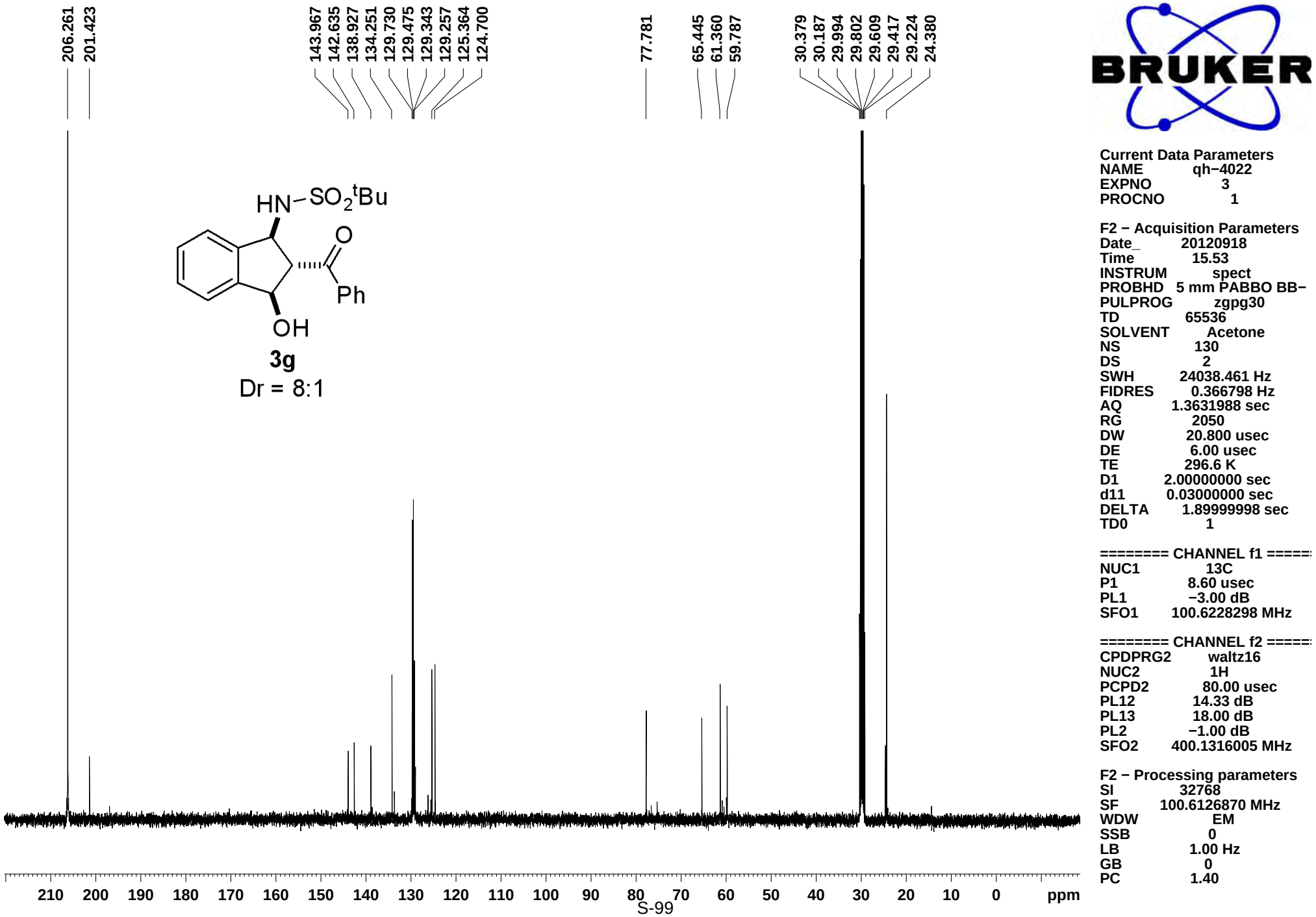


Current Data Parameters
NAME qh−4022
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120918
Time 15.39
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 296.0 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



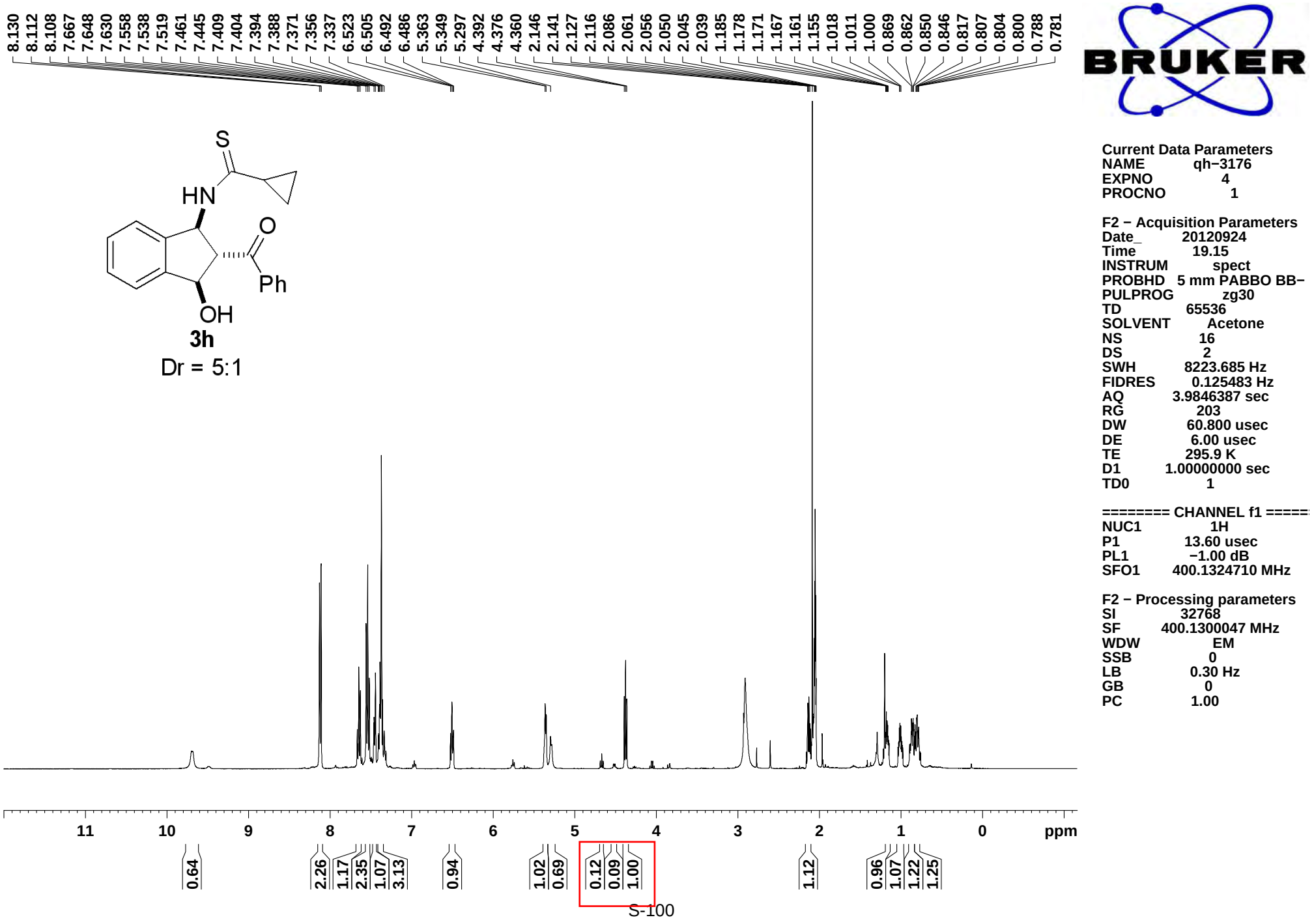
Current Data Parameters
NAME qh−4022
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120918
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 130
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 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126870 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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Current Data Parameters

NAME	qh−3176
EXPNO	4
PROCNO	1

F2 − Acquisition Parameters

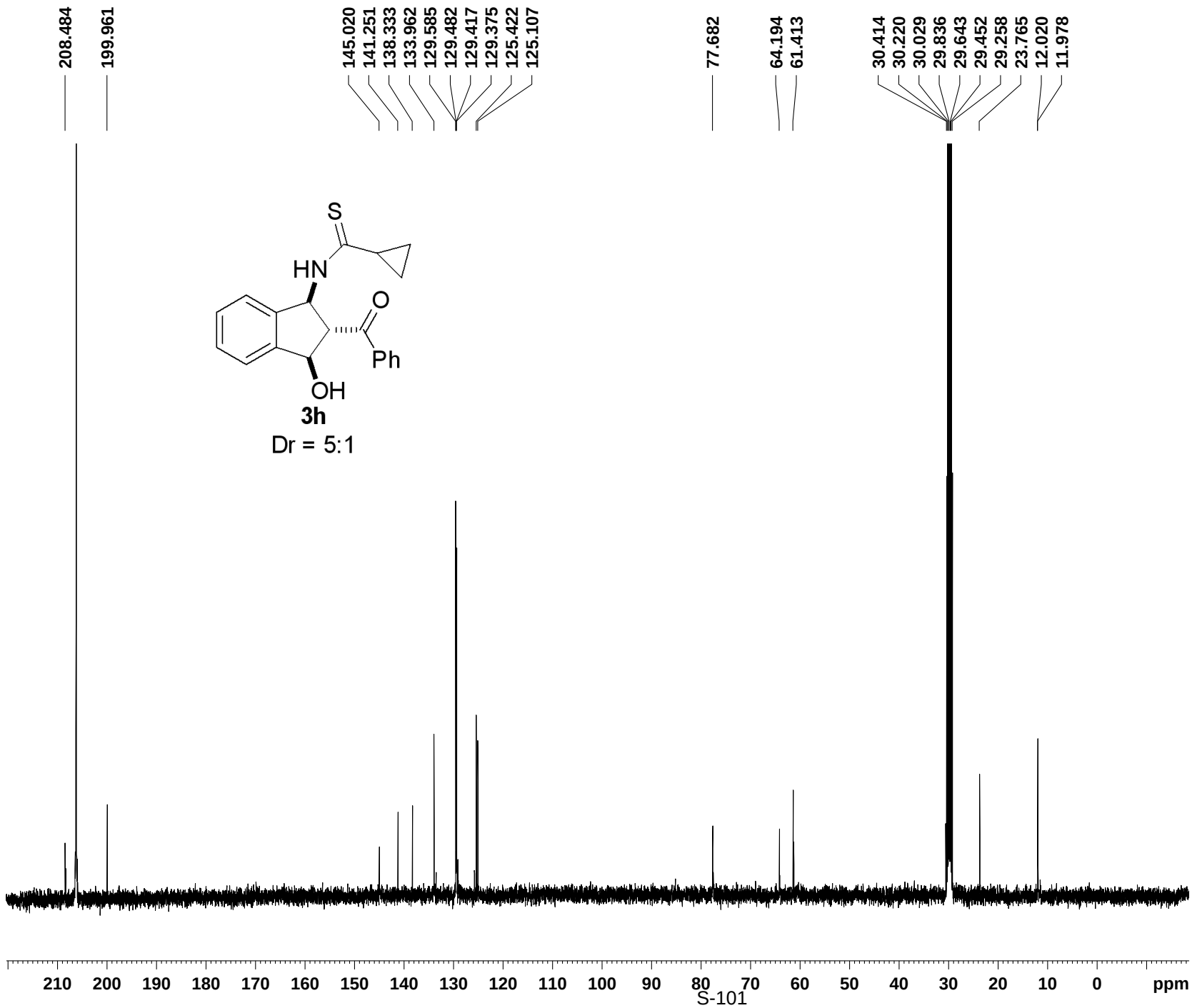
Date_	20120924
Time	19.15
INSTRUM	spect
PROBHD	5 mm PABBO BB−
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	203
DW	60.800 usec
DE	6.00 usec
TE	295.9 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 =====

NUC1	1H
P1	13.60 usec
PL1	−1.00 dB
SFO1	400.1324710 MHz

F2 − Processing parameters

SI	32768
SF	400.1300047 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



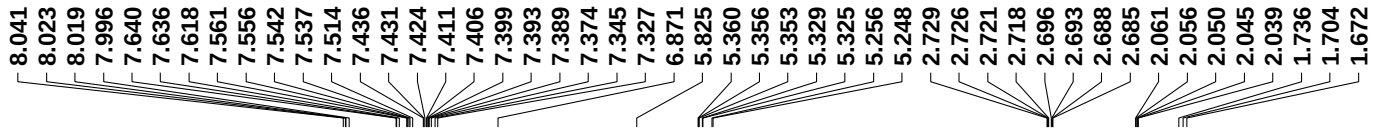
Current Data Parameters
NAME qh−3176
EXPNO 1
PROCNO 1

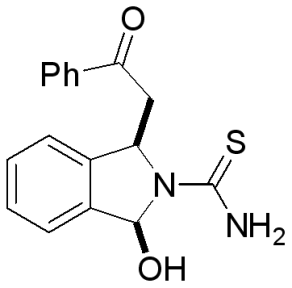
F2 − Acquisition Parameters
Date_ 20120924
Time 18.56
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 300
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

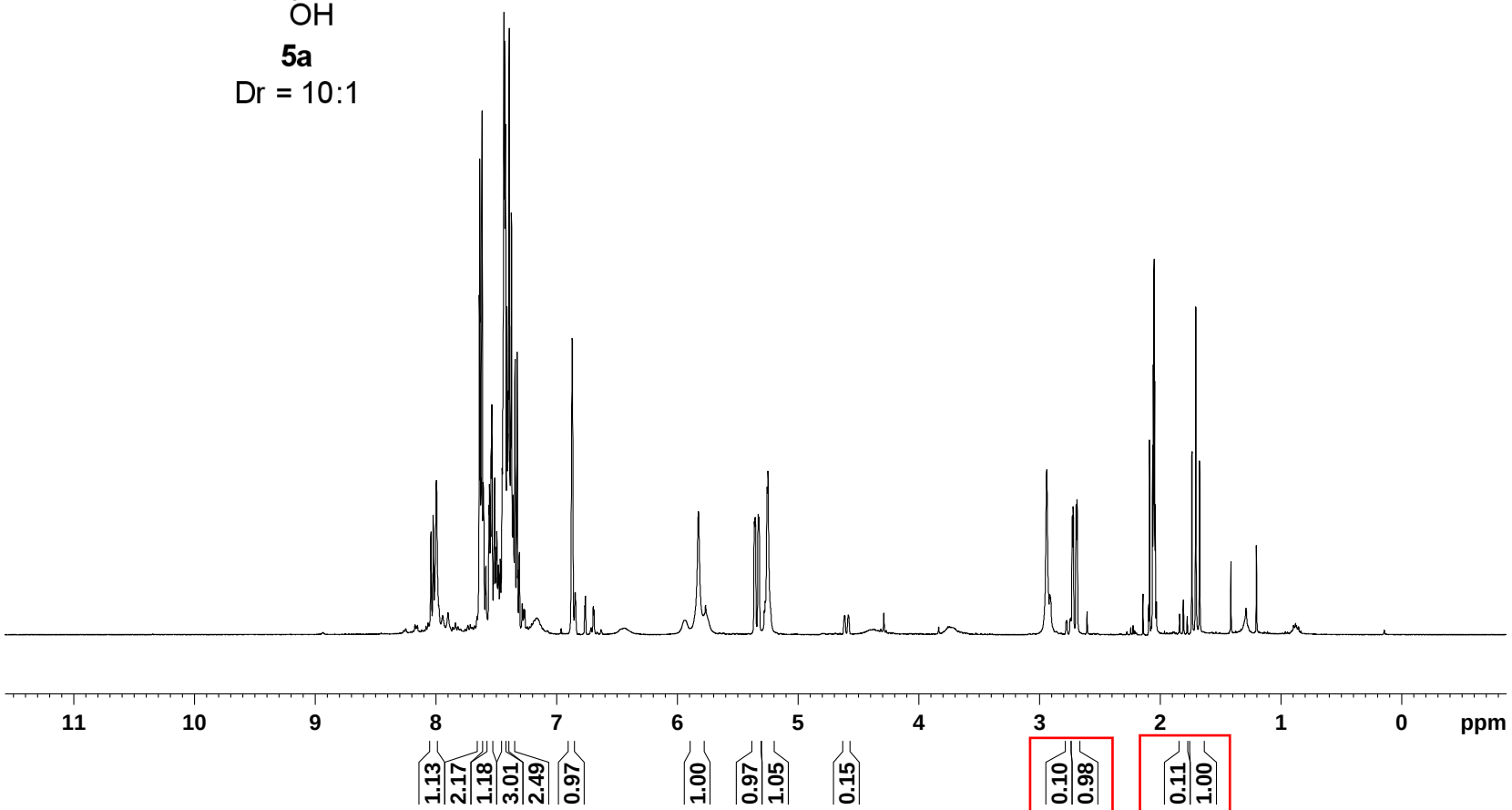
F2 − Processing parameters
SI 32768
SF 100.6126820 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





5a

Dr = 10:1

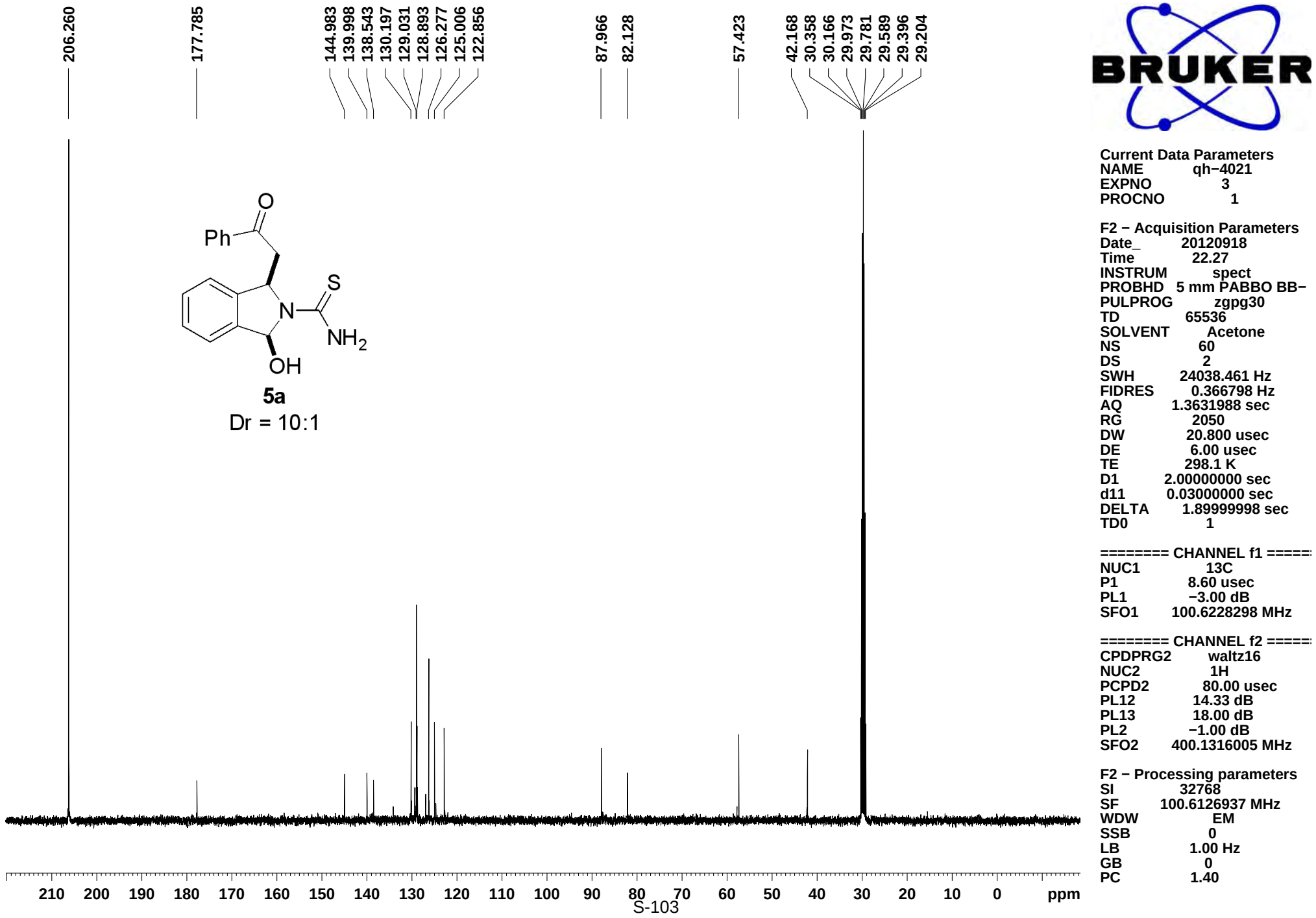


Current Data Parameters
NAME qh−4021
EXPNO 5
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120919
Time 21.15
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 295.9 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



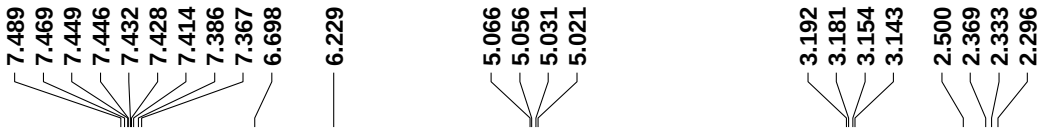
Current Data Parameters
NAME qh−4021
EXPNO 3
PROCNO 1

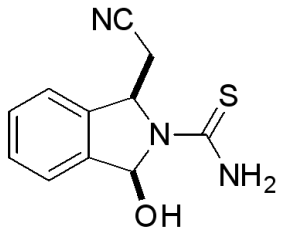
F2 − Acquisition Parameters
Date_ 20120918
Time 22.27
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 60
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

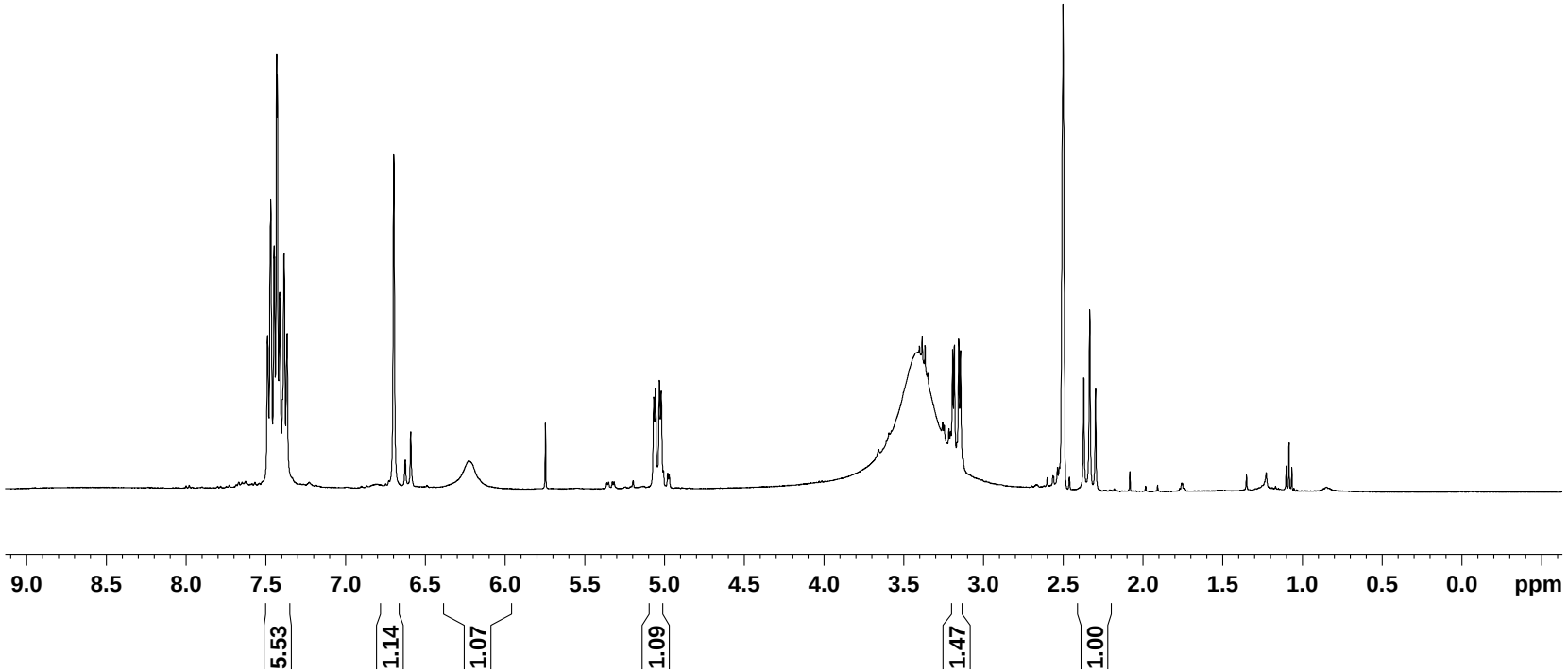
F2 − Processing parameters
SI 32768
SF 100.6126937 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





5b

Dr > 20:1

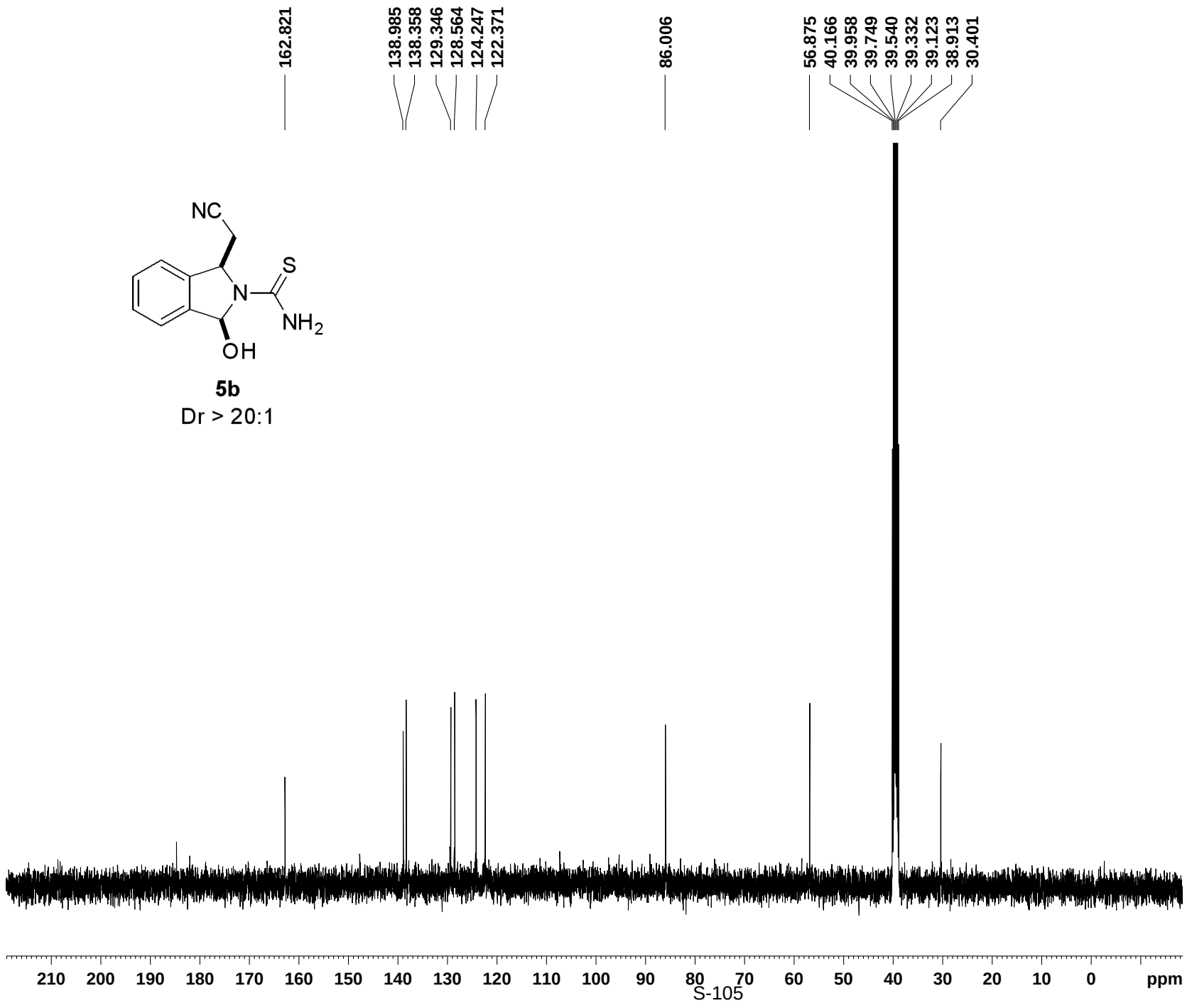


Current Data Parameters
NAME qh−4013
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120914
Time 20.43
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 9
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 295.9 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 400.1299968 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

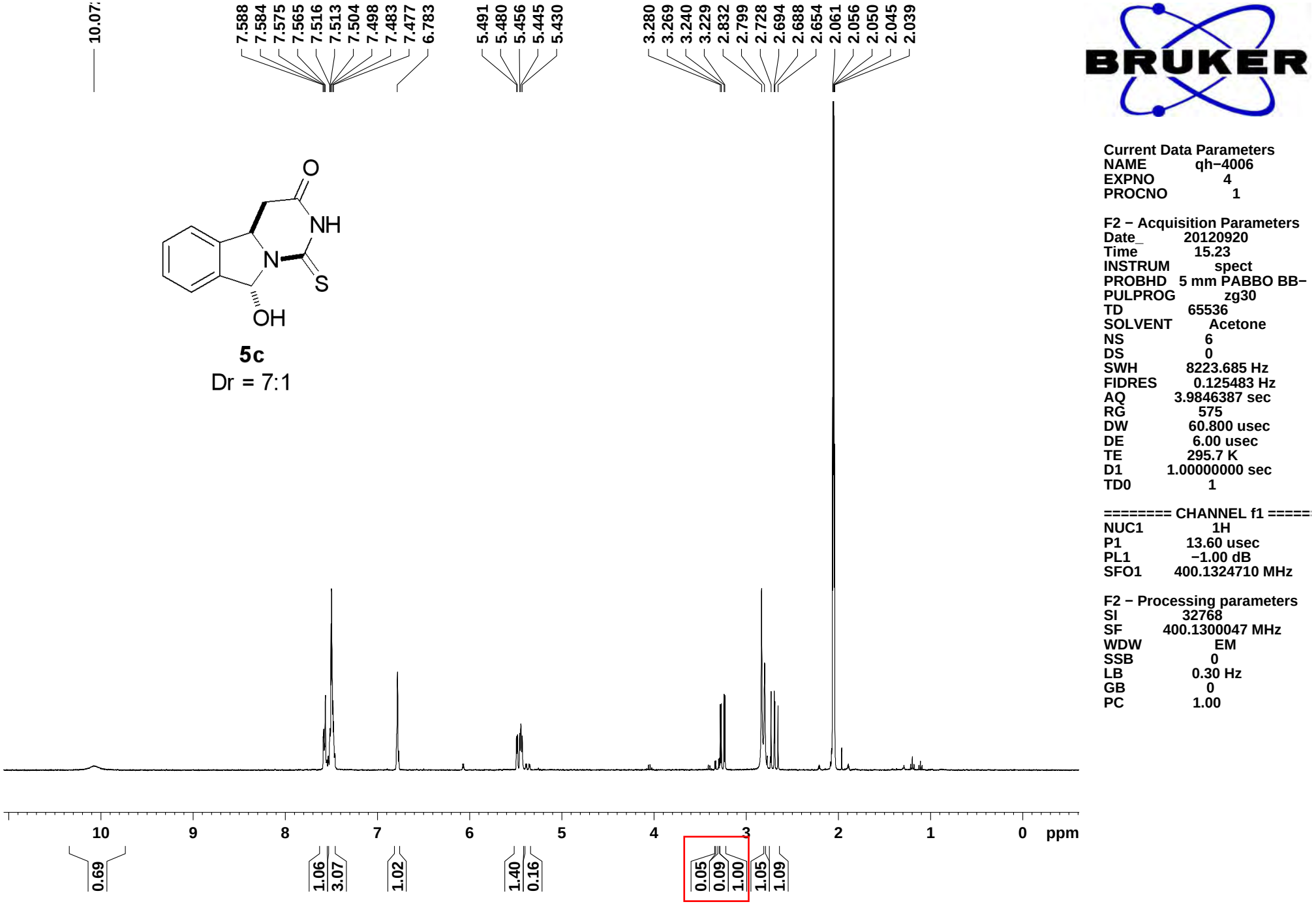
Current Data Parameters
NAME qh−4013
EXPNO 5
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120914
Time 20.49
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 259
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 296.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6128072 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

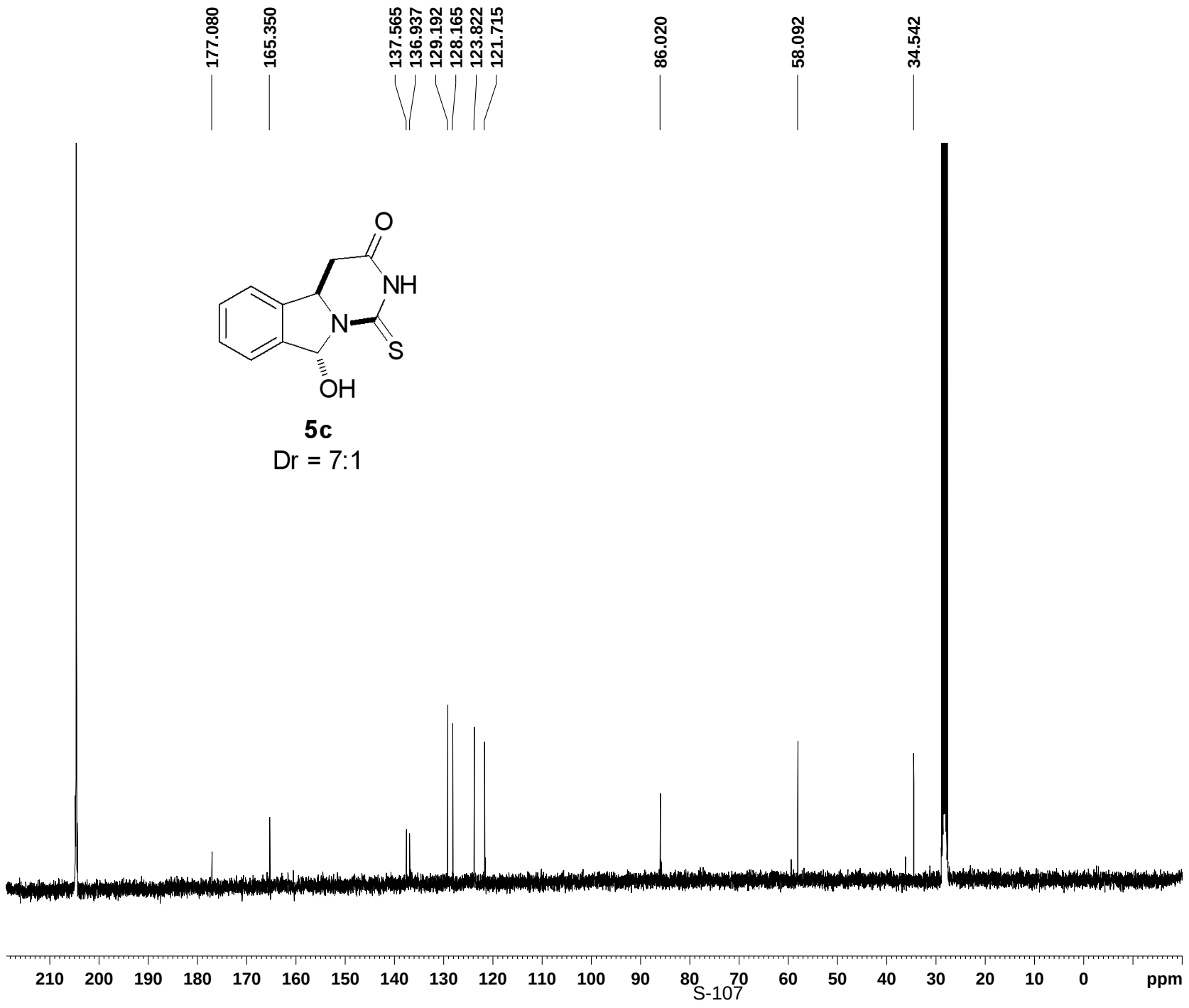


Current Data Parameters
NAME qh−4006
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120920
Time 15.23
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 575
DW 60.800 usec
DE 6.00 usec
TE 295.7 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

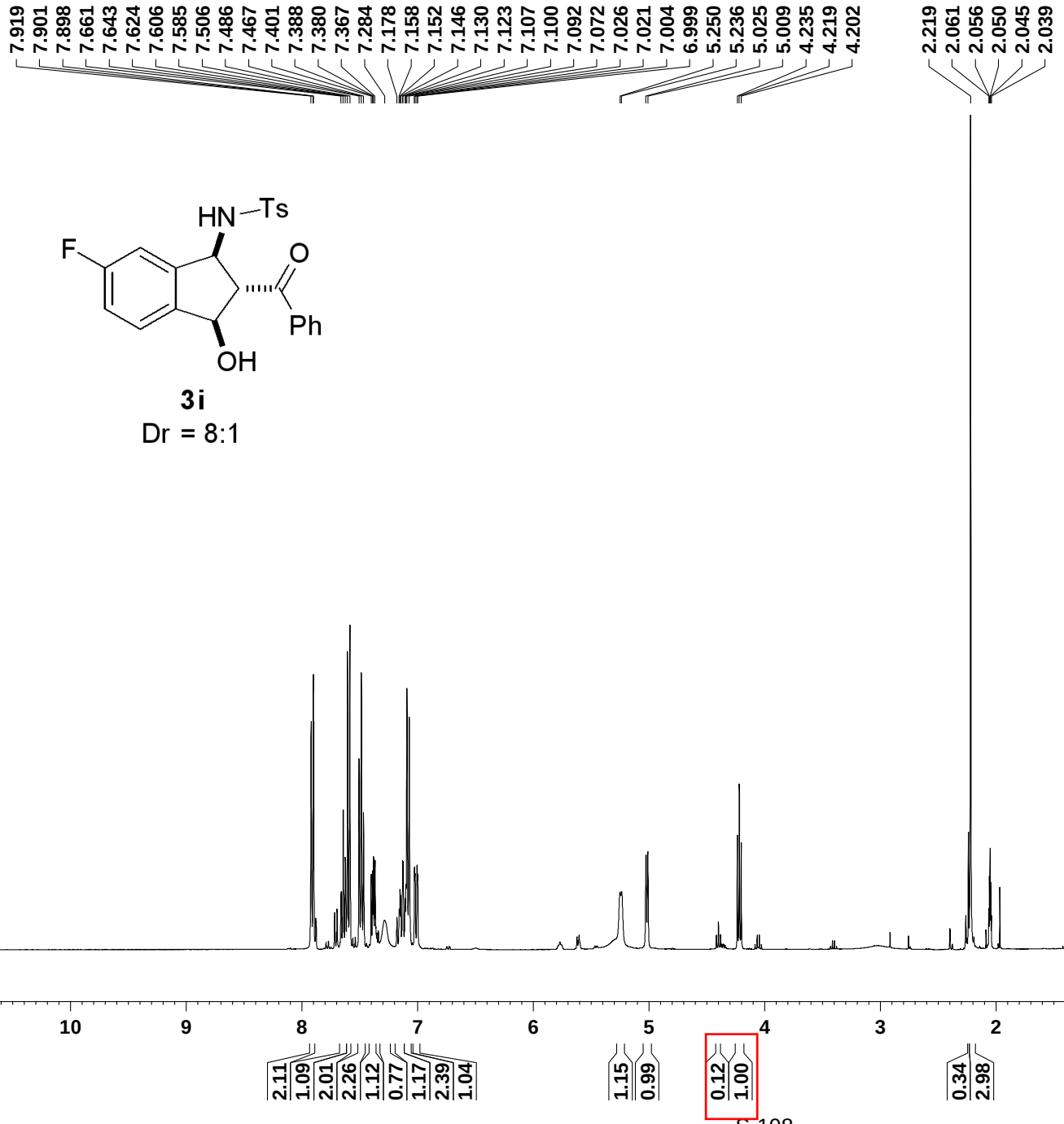
Current Data Parameters
NAME qh−4002−4
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120911
Time 1.12
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1335
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 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6128330 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

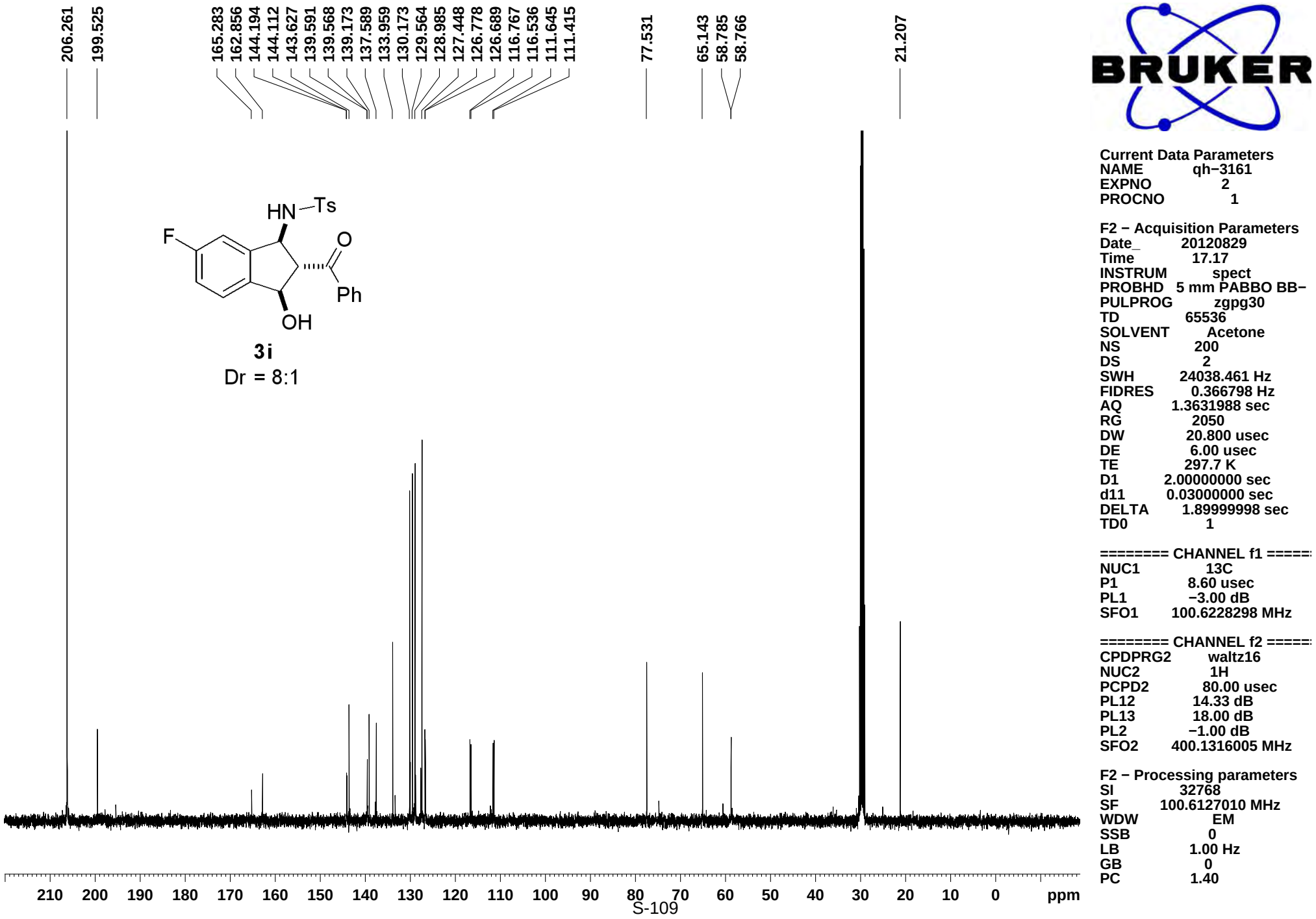


Current Data Parameters
NAME qh−3161
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120918
Time 22.33
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 64
DW 60.800 usec
DE 6.00 usec
TE 297.8 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

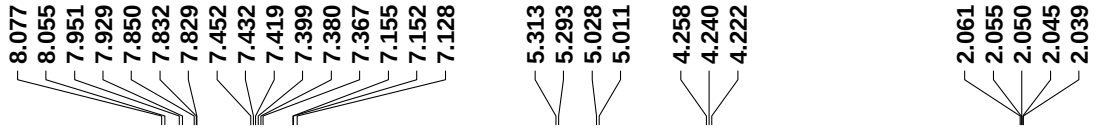
Current Data Parameters
NAME qh−3161
EXPNO 2
PROCNO 1

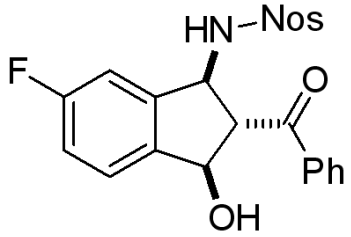
F2 − Acquisition Parameters
Date_ 20120829
Time 17.17
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 297.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

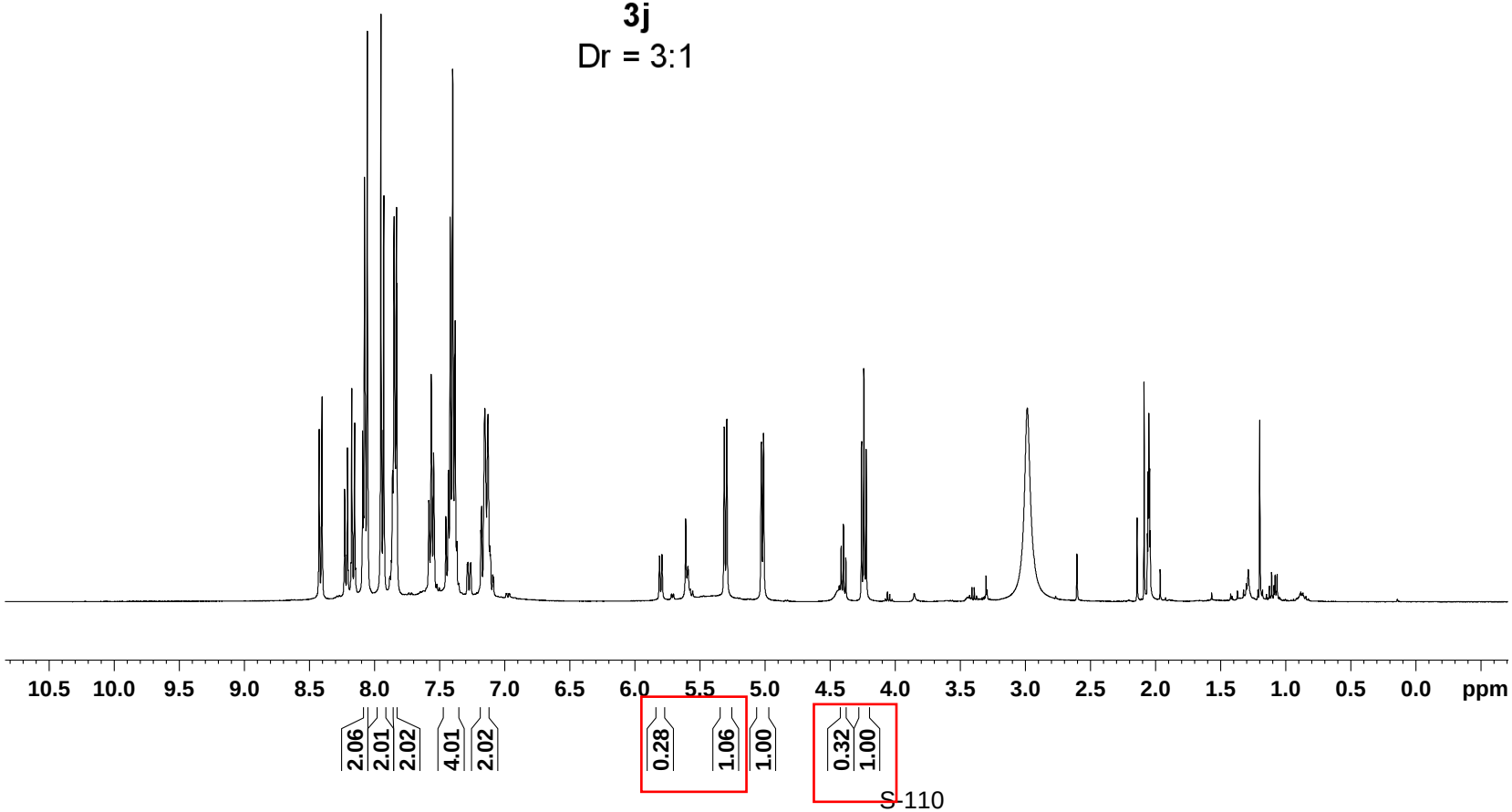
F2 − Processing parameters
SI 32768
SF 100.6127010 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3j

Dr = 3:1

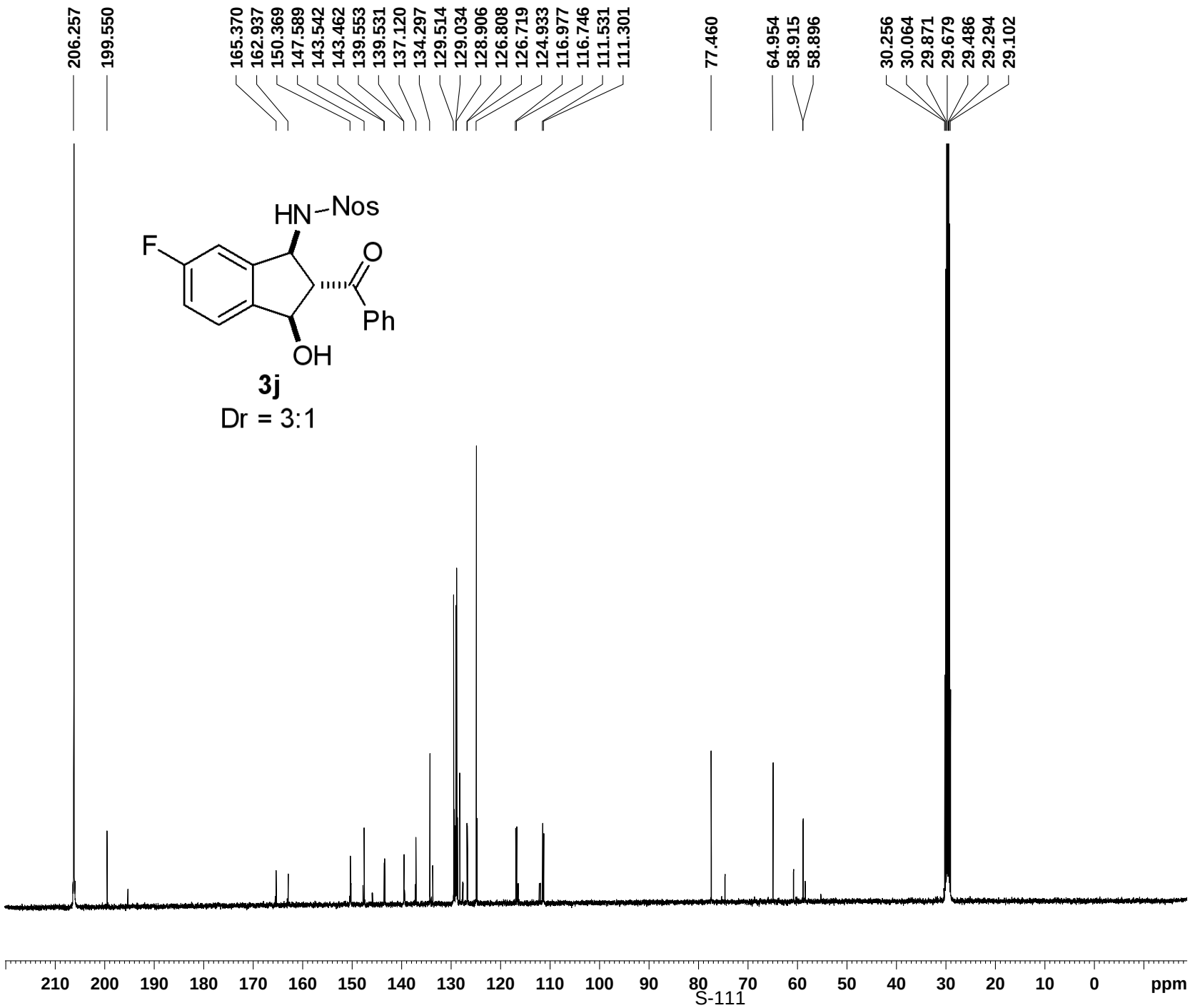



```
Current Data Parameters
NAME          qh−3196
EXPNO            1
PROCNO           1

F2 − Acquisition Parameters
Date_        20120909
Time           18.20
INSTRUM         spect
PROBHD  5 mm PABBO BB−
PULPROG         zg30
TD            65536
SOLVENT       Acetone
NS                8
DS                0
SWH          8223.685 Hz
FIDRES       0.125483 Hz
AQ           3.9846387 sec
RG              181
DW           60.800 usec
DE            6.00 usec
TE           299.0 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        400.1300047 MHz
WDW              EM
SSB               0
LB            0.30 Hz
GB                0
PC            1.00
```



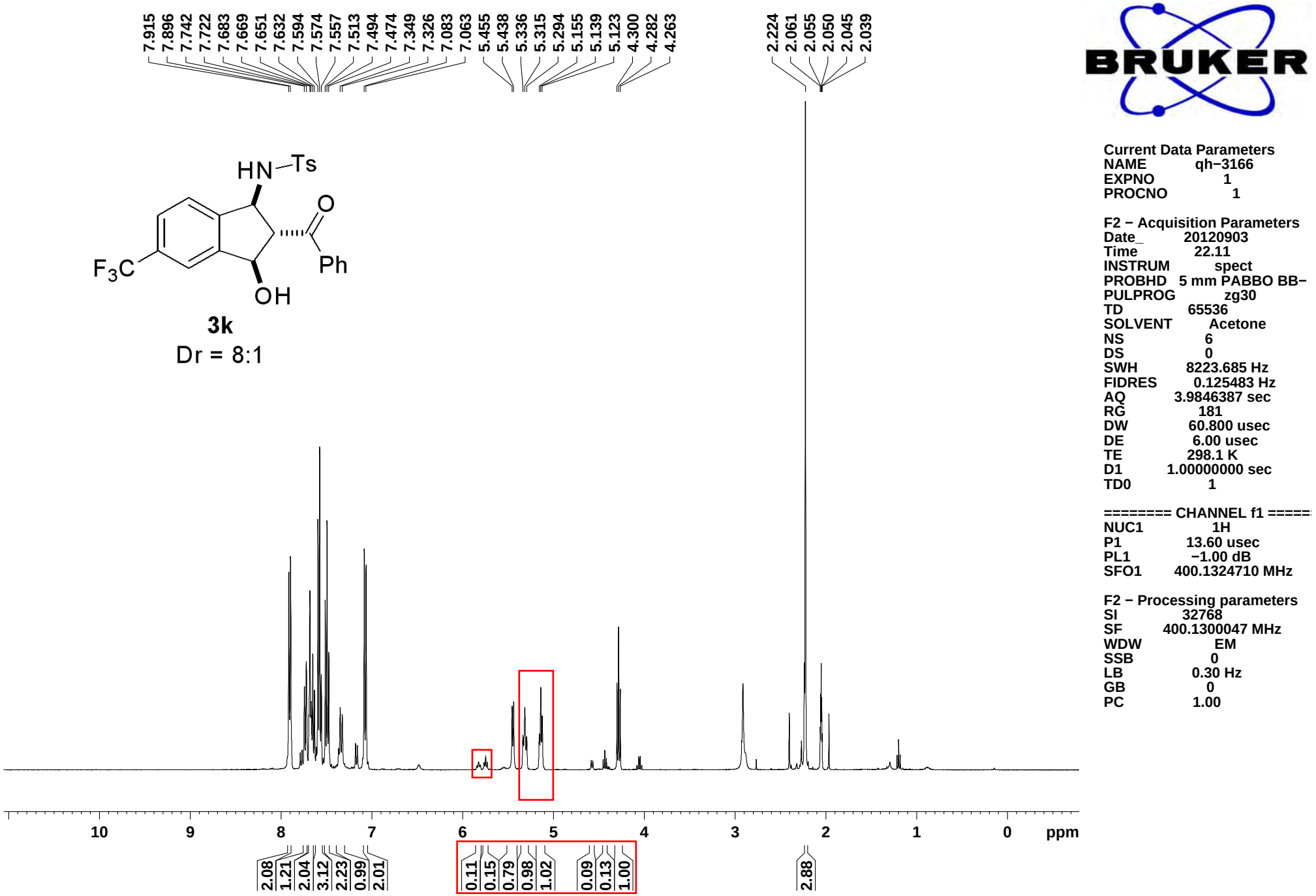
Current Data Parameters
NAME qh−3196
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120909
Time 18.33
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1264
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 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126980 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

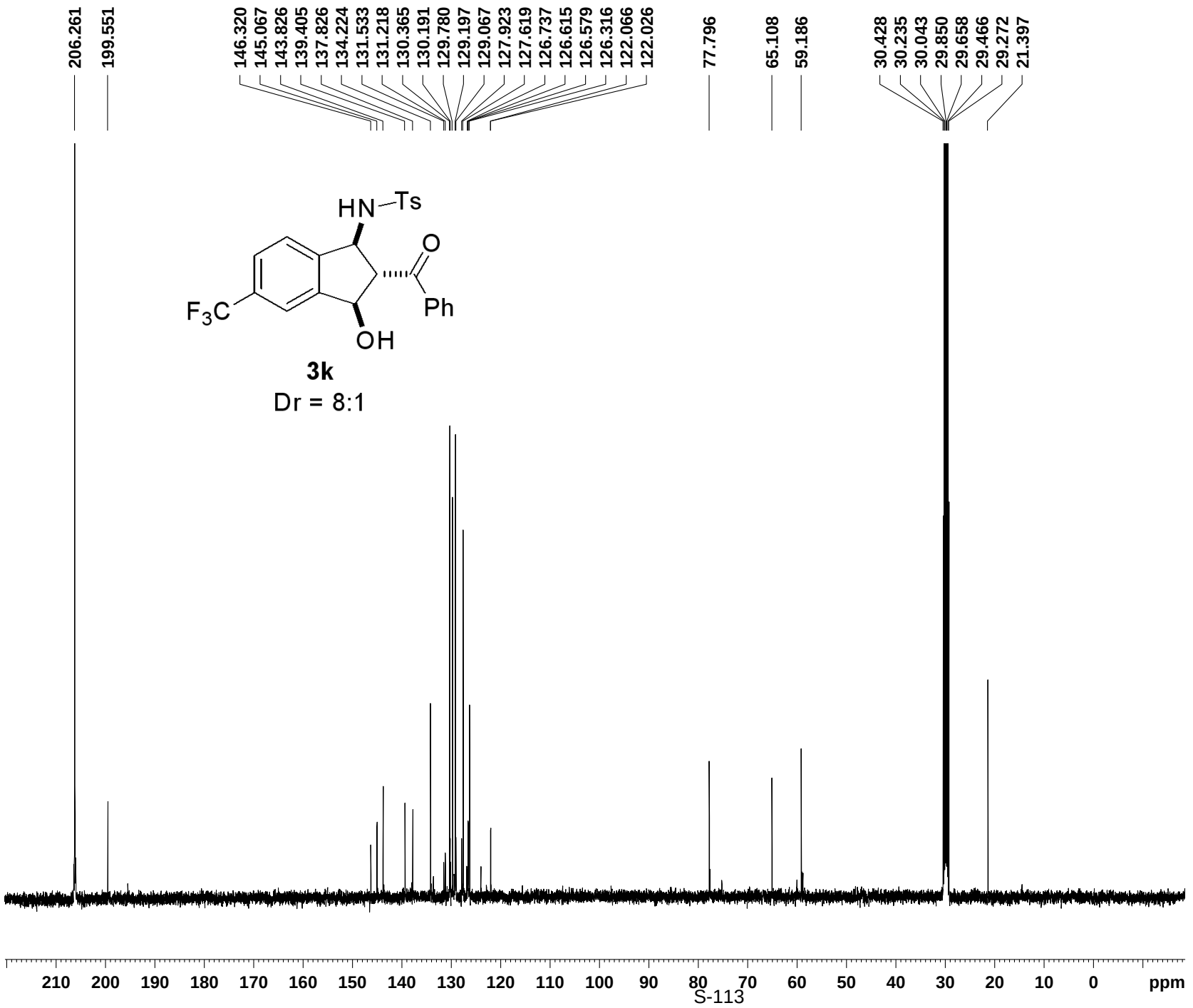


Current Data Parameters
NAME qh−3166
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120903
Time 22.11
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 298.1 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



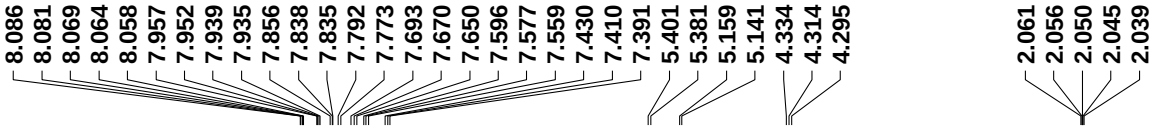
Current Data Parameters
NAME qh−3166
EXPNO 2
PROCNO 1

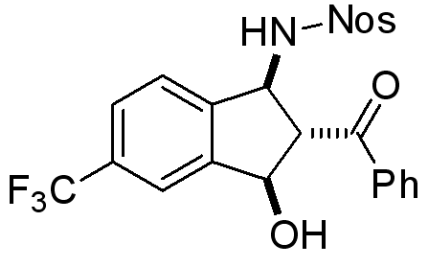
F2 − Acquisition Parameters
Date_ 20120903
Time 22.13
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

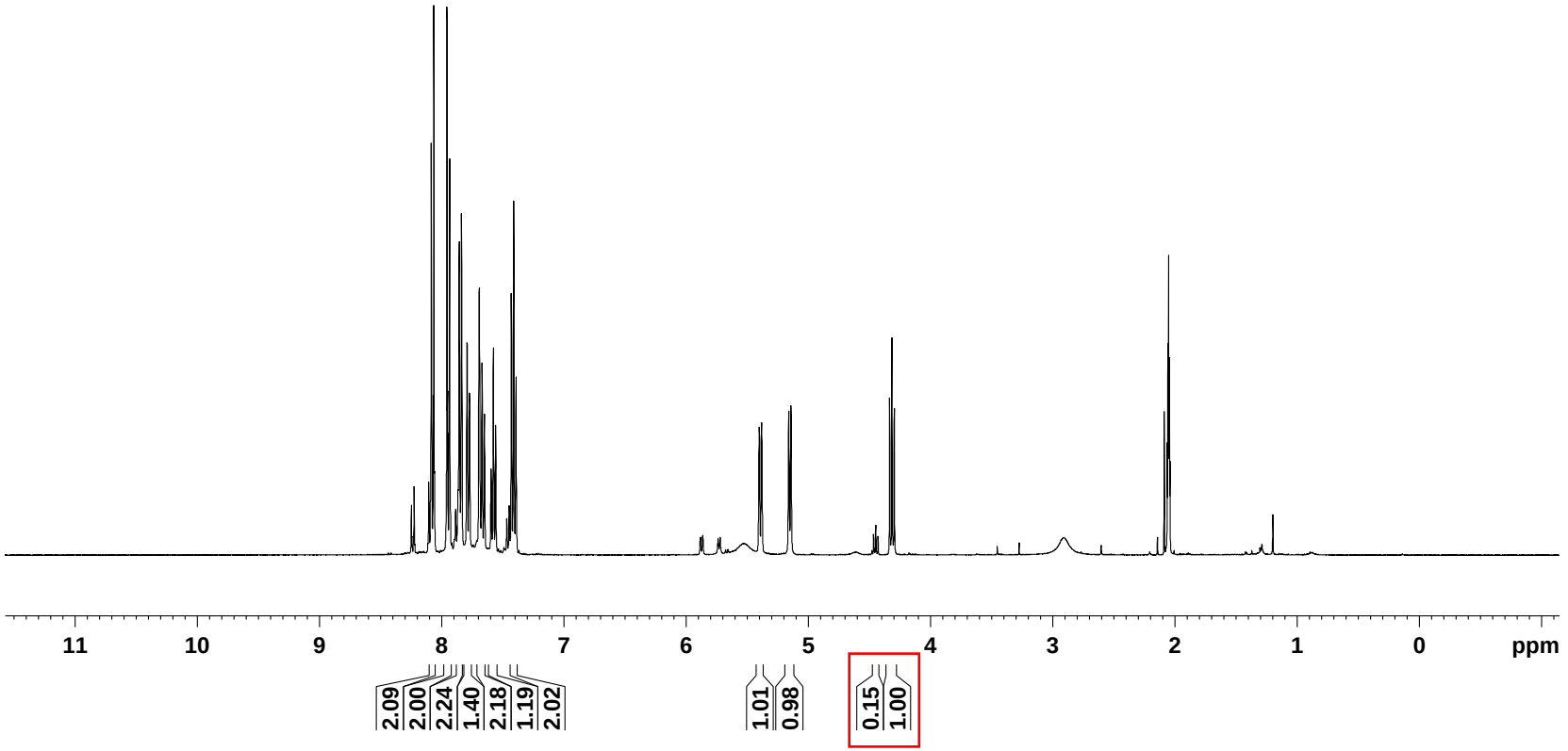
F2 − Processing parameters
SI 32768
SF 100.6126790 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3l

Dr = 7:1

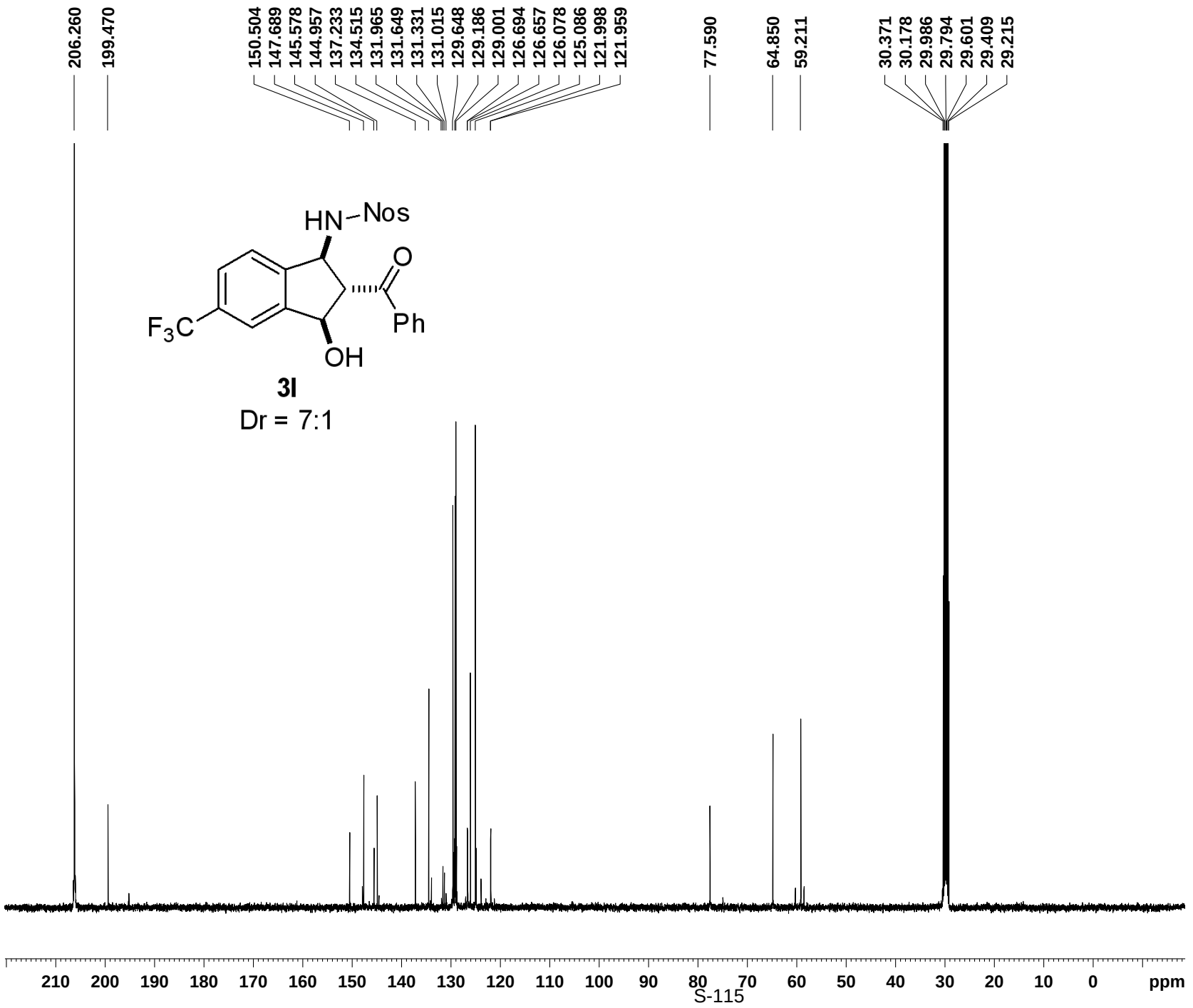


Current Data Parameters
NAME qh−3198−1
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20121021
Time 16.00
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 5
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 296.7 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



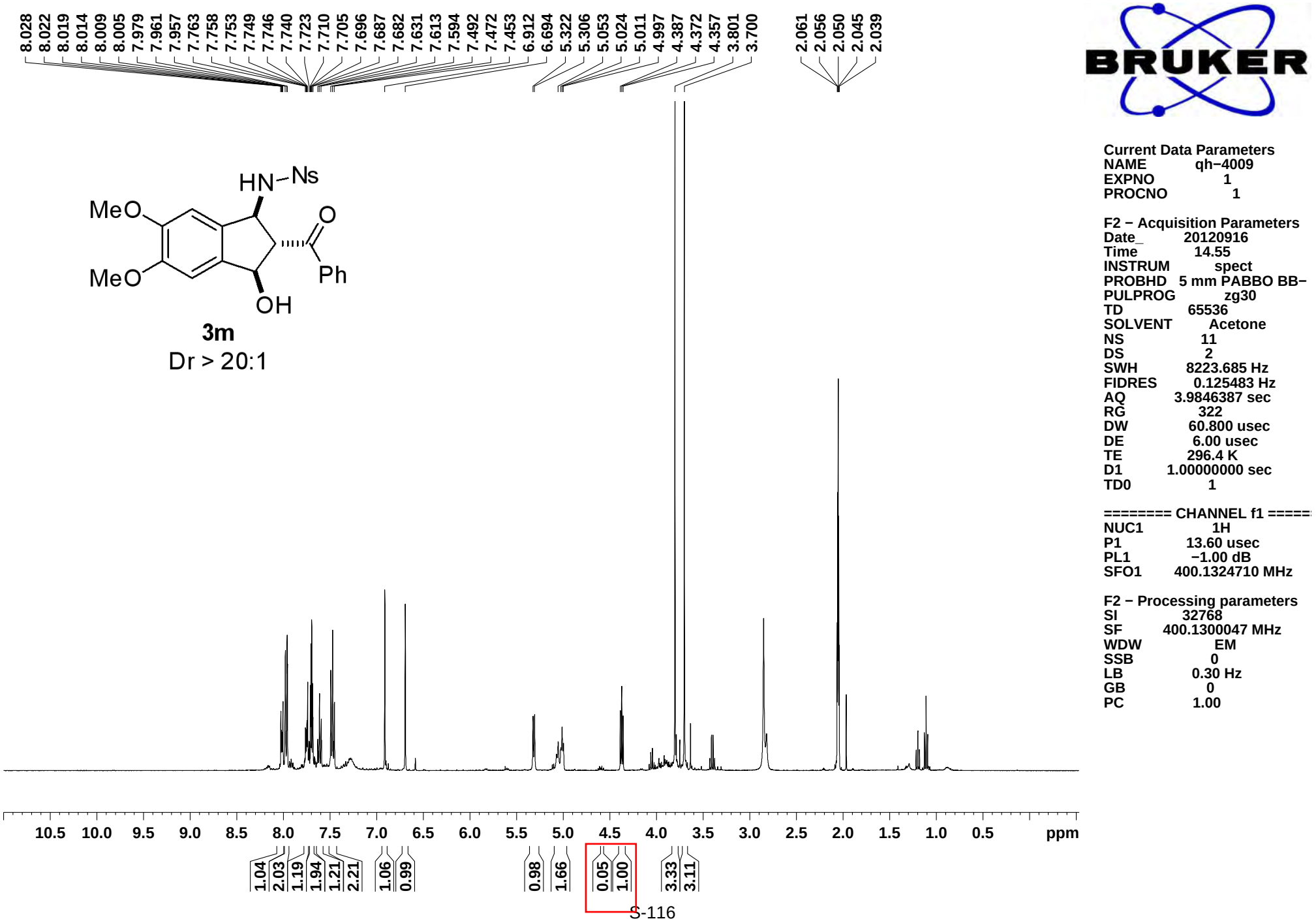
Current Data Parameters
NAME qh−3198−1
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120927
Time 12.03
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 920
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 90.5
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126856 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



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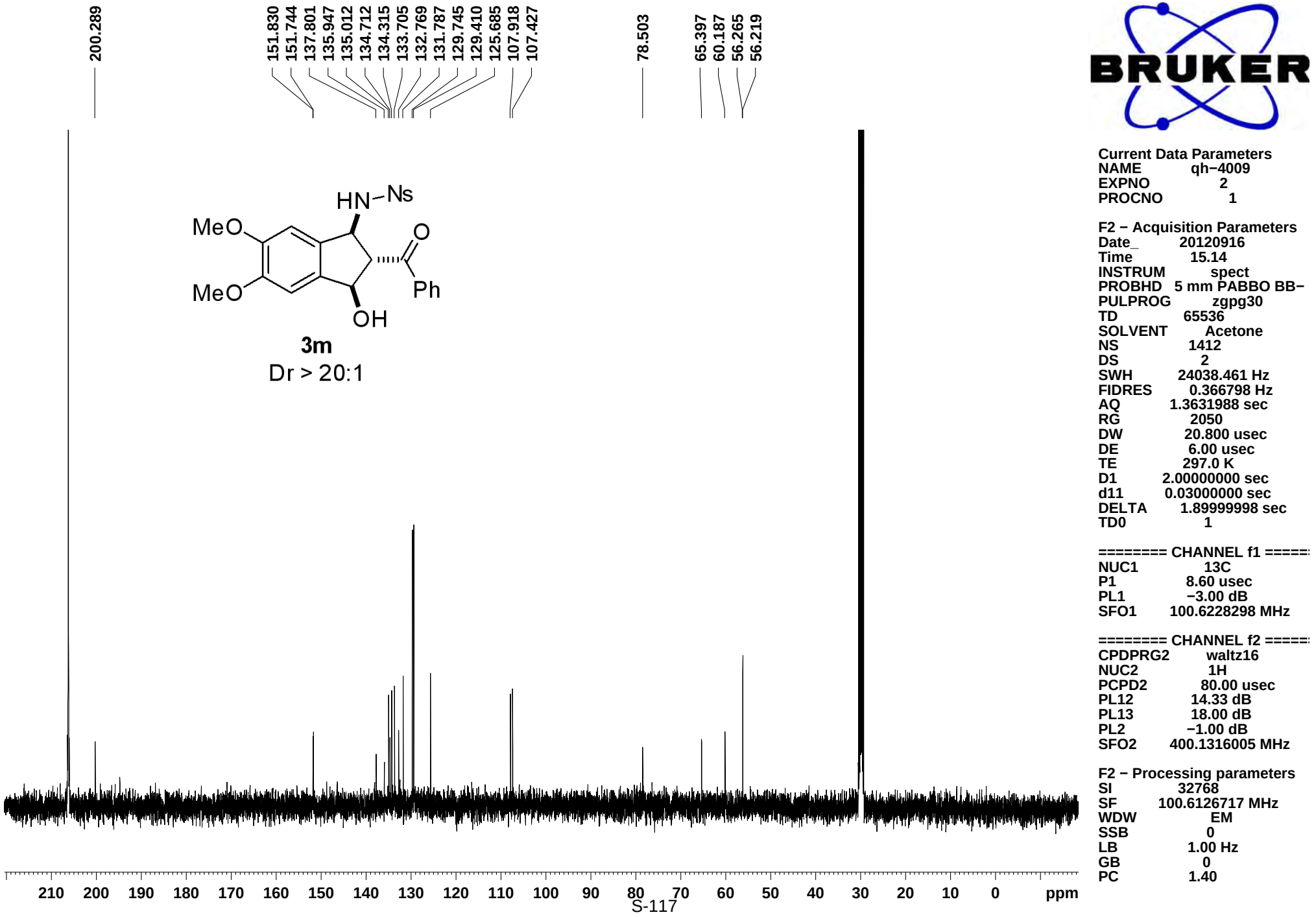
Current Data Parameters
NAME qh−4009
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120916
Time 14.55
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 11
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 322
DW 60.800 usec
DE 6.00 usec
TE 296.4 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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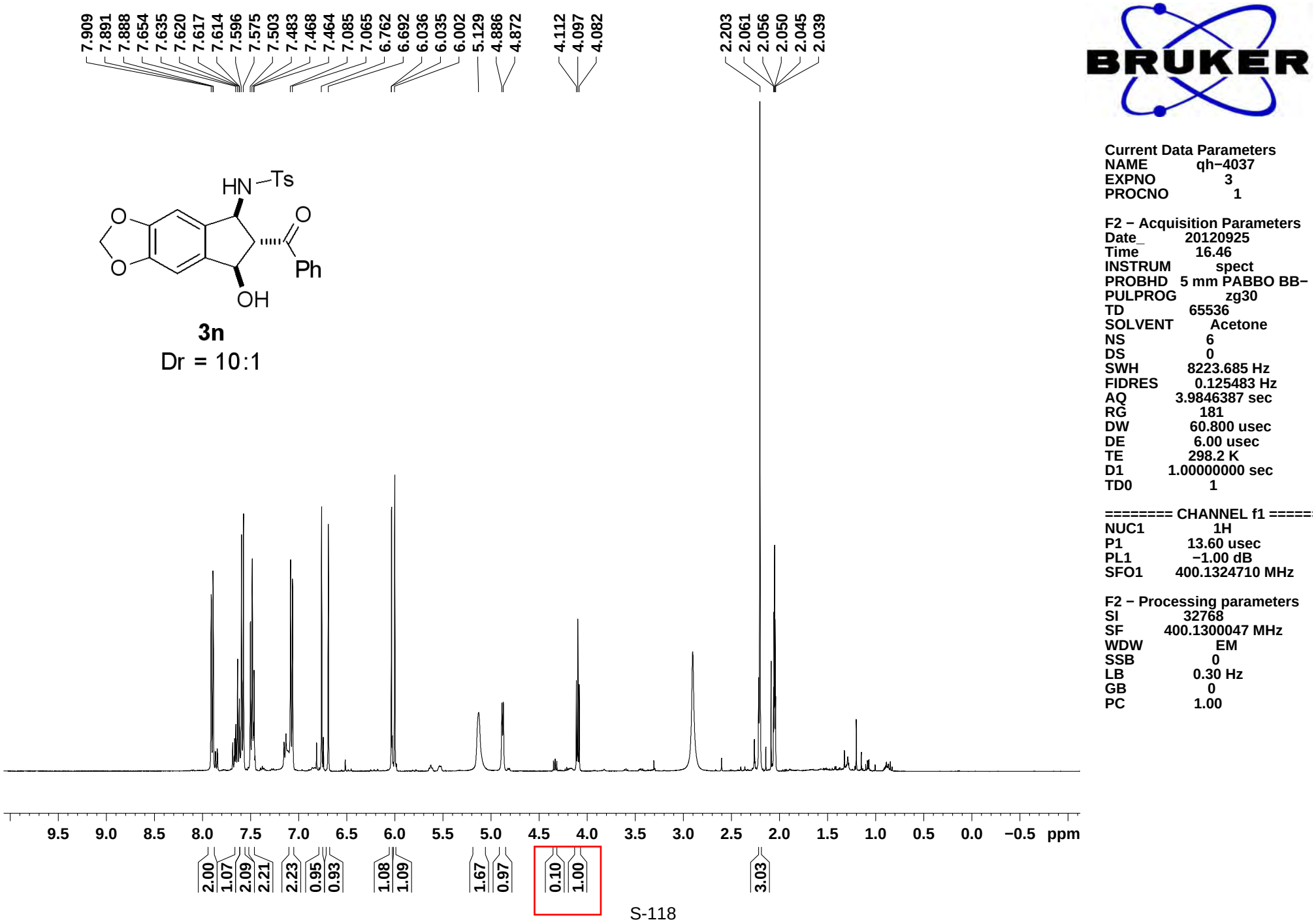
Current Data Parameters
NAME qh−4009
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120916
Time 15.14
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1412
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 297.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 =====
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

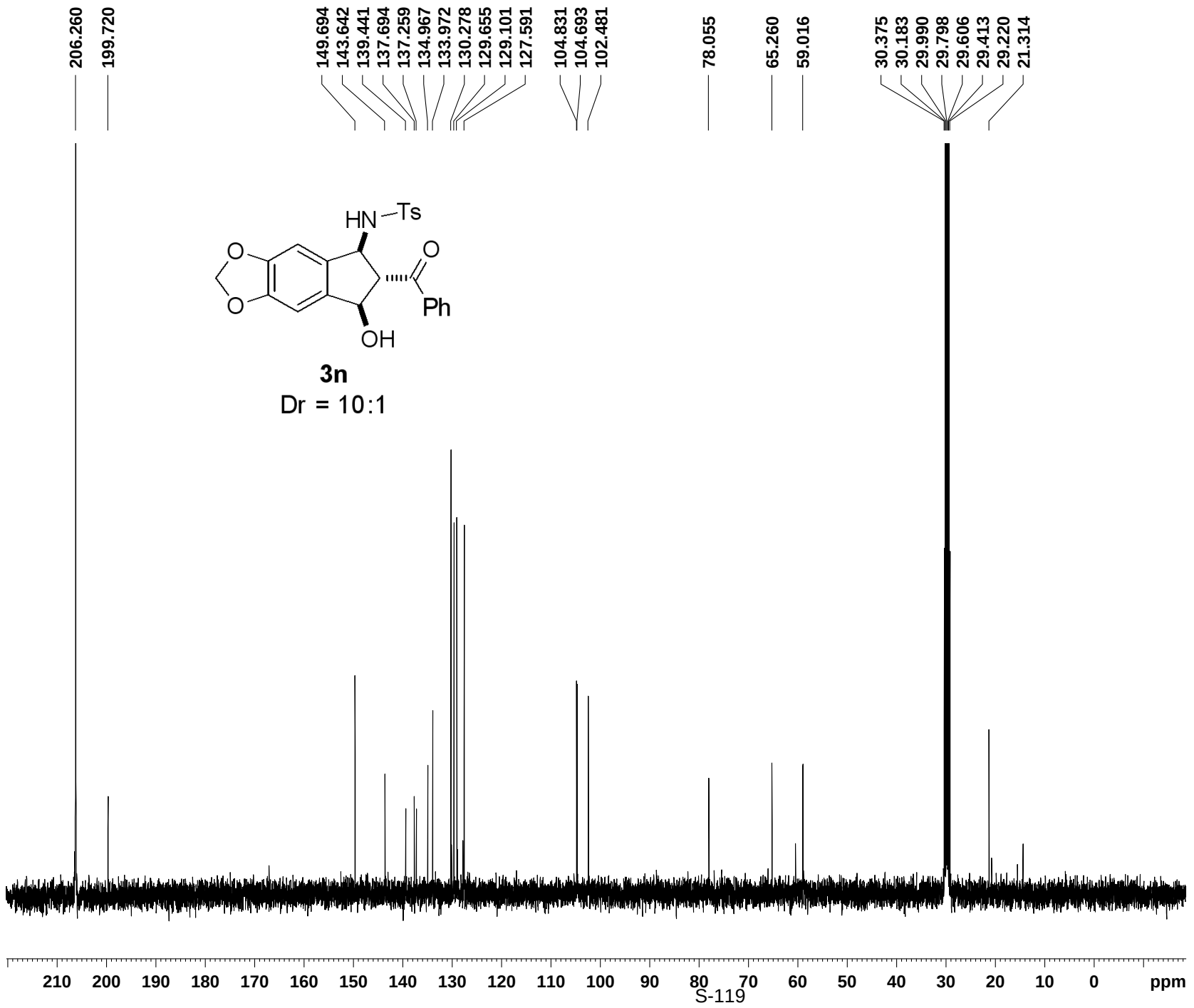


Current Data Parameters
NAME qh−4037
EXPNO 3
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120925
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 298.2 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



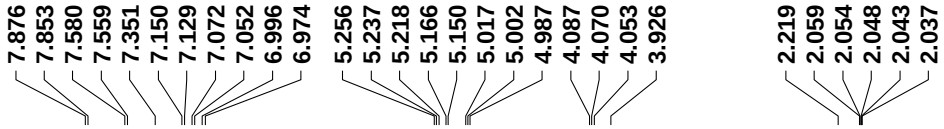
Current Data Parameters
NAME qh−4037
EXPNO 2
PROCNO 1

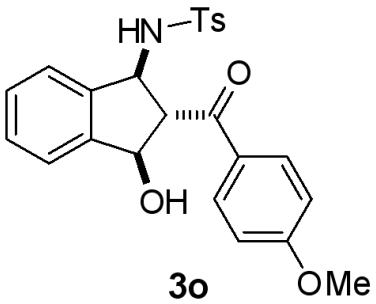
F2 − Acquisition Parameters
Date_ 20120924
Time 22.17
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 82
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126863 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3o

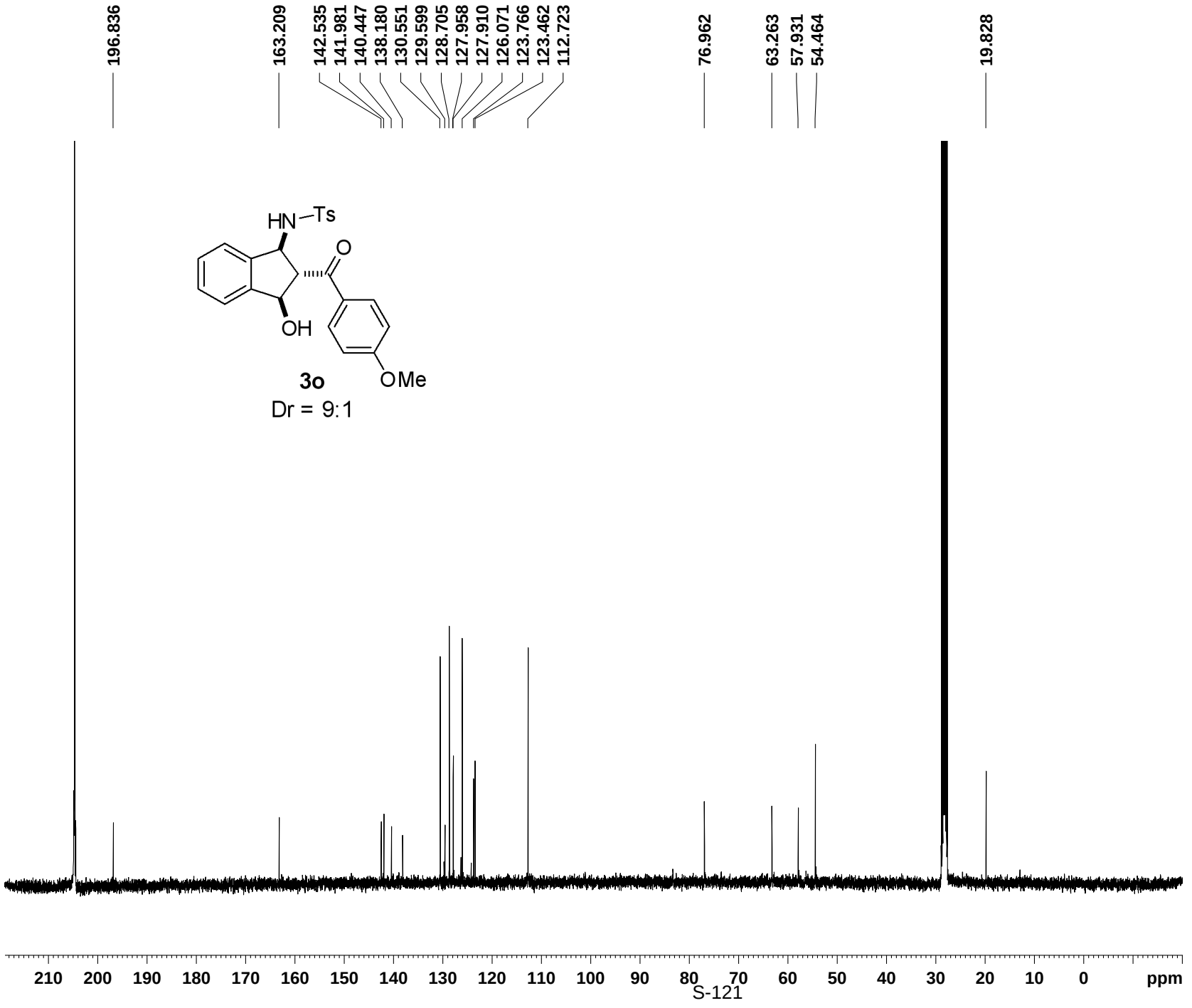
Dr = 9:1

Current Data Parameters
NAME qh−3169
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120902
Time 14.09
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 14
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 297.3 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 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



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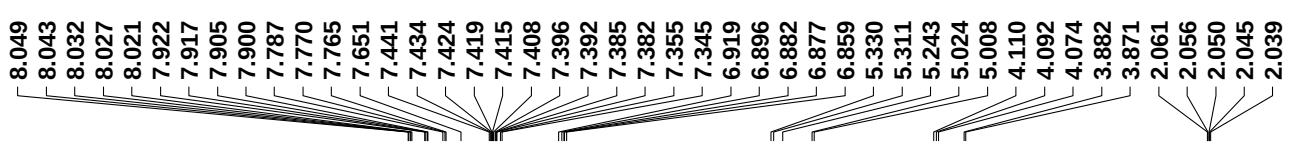
Current Data Parameters
NAME qh−3169
EXPNO 2
PROCNO 1

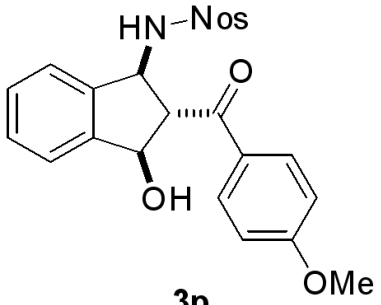
F2 − Acquisition Parameters
Date_ 20120902
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2000
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

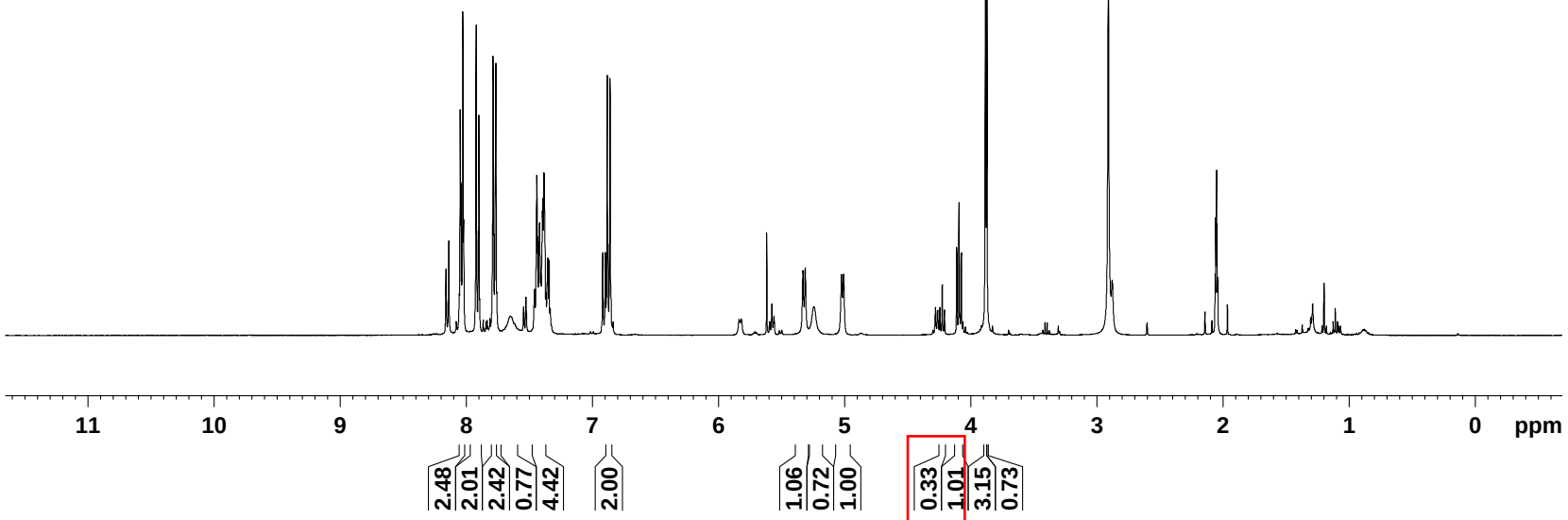
F2 − Processing parameters
SI 32768
SF 100.6128330 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3p

Dr = 3:1



Current Data Parameters

NAME	qh−3197
EXPNO	1
PROCNO	1

F2 − Acquisition Parameters

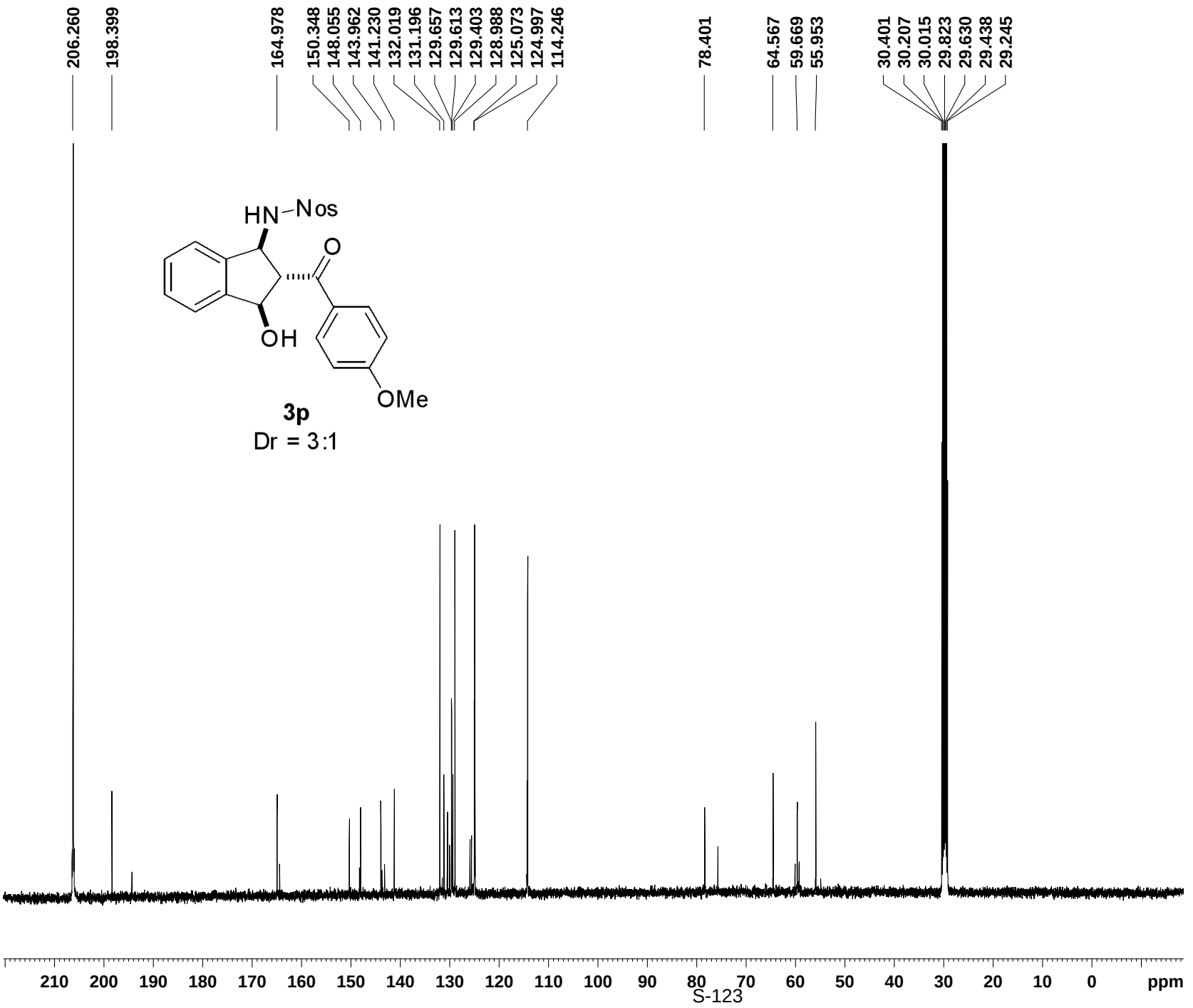
Date_	20120909
Time	17.11
INSTRUM	spect
PROBHD	5 mm PABBO BB−
PULPROG	zg30
TD	65536
SOLVENT	Acetone
NS	14
DS	0
SWH	8223.685 Hz
FIDRES	0.125483 Hz
AQ	3.9846387 sec
RG	181
DW	60.800 usec
DE	6.00 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1

======== CHANNEL f1 =====

NUC1	1H
P1	13.60 usec
PL1	−1.00 dB
SFO1	400.1324710 MHz

F2 − Processing parameters

SI	32768
SF	400.1300047 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



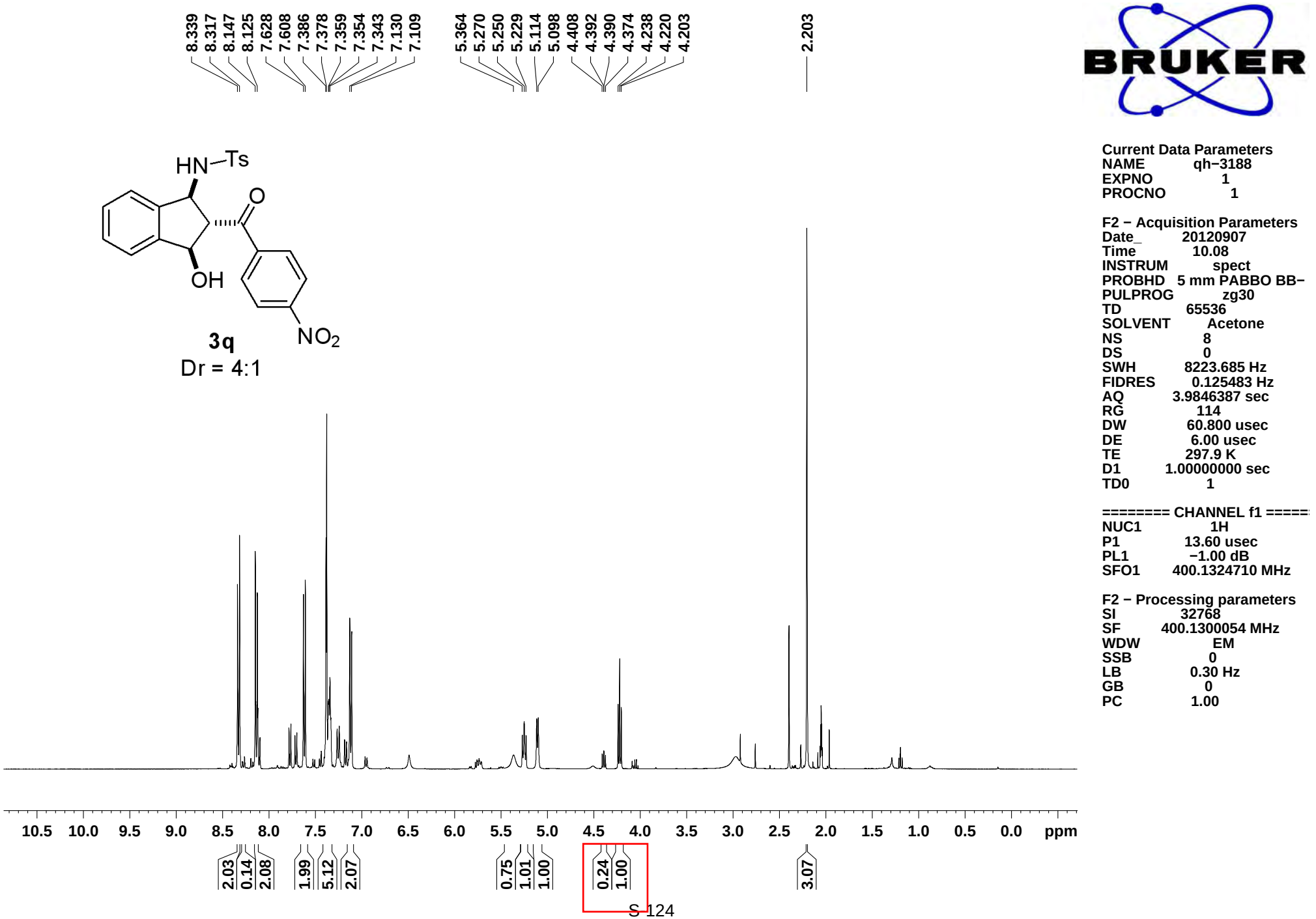
Current Data Parameters
NAME qh−3197
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120909
Time 17.21
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 1032
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 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126819 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



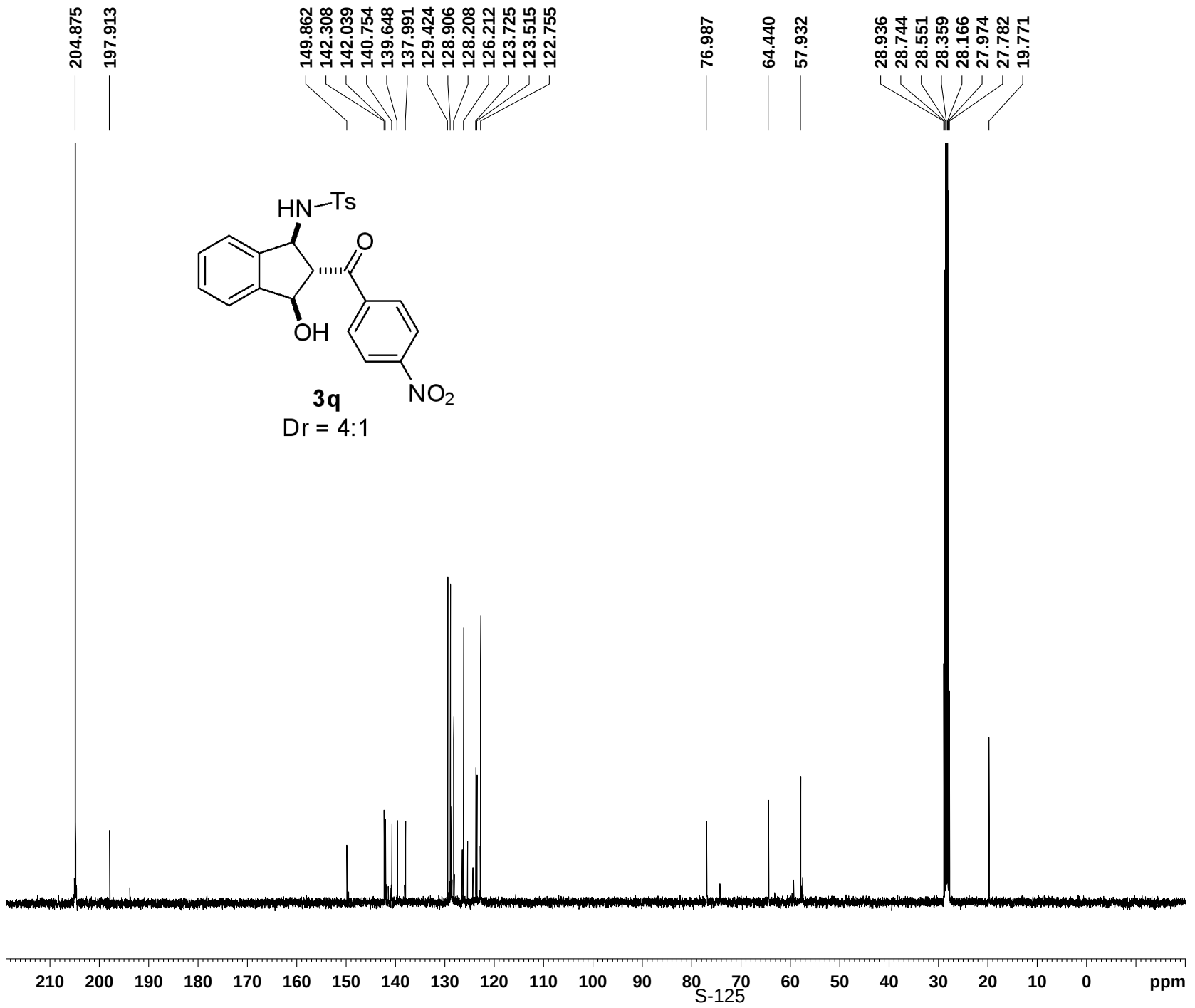
BRUKER

Current Data Parameters
NAME qh−3188
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120907
Time 10.08
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 297.9 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 400.1300054 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



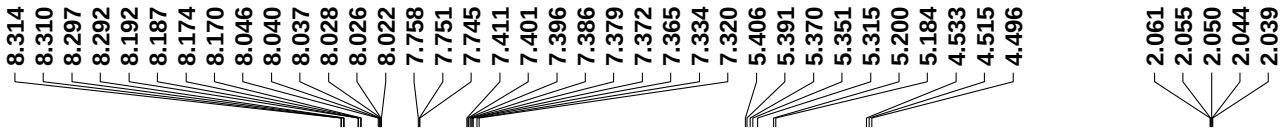
Current Data Parameters
NAME qh−3188
EXPNO 2
PROCNO 1

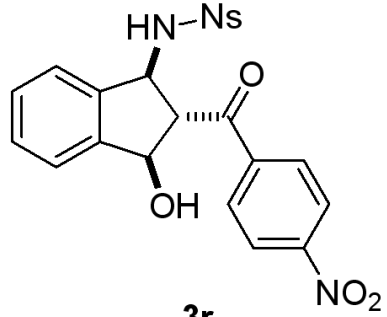
F2 − Acquisition Parameters
Date_ 20120907
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 400
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 298.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

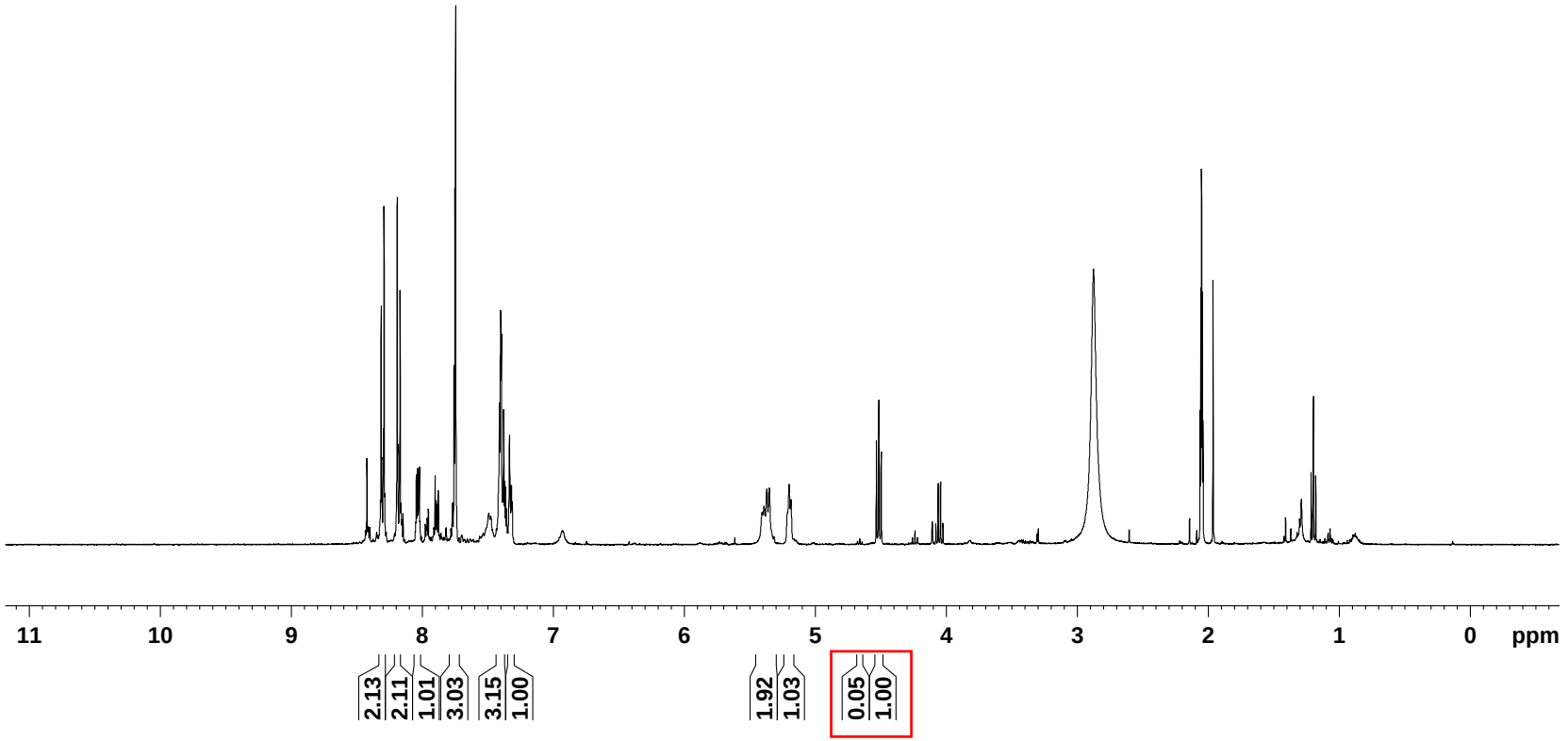
F2 − Processing parameters
SI 32768
SF 100.6128330 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3r

Dr > 20:1



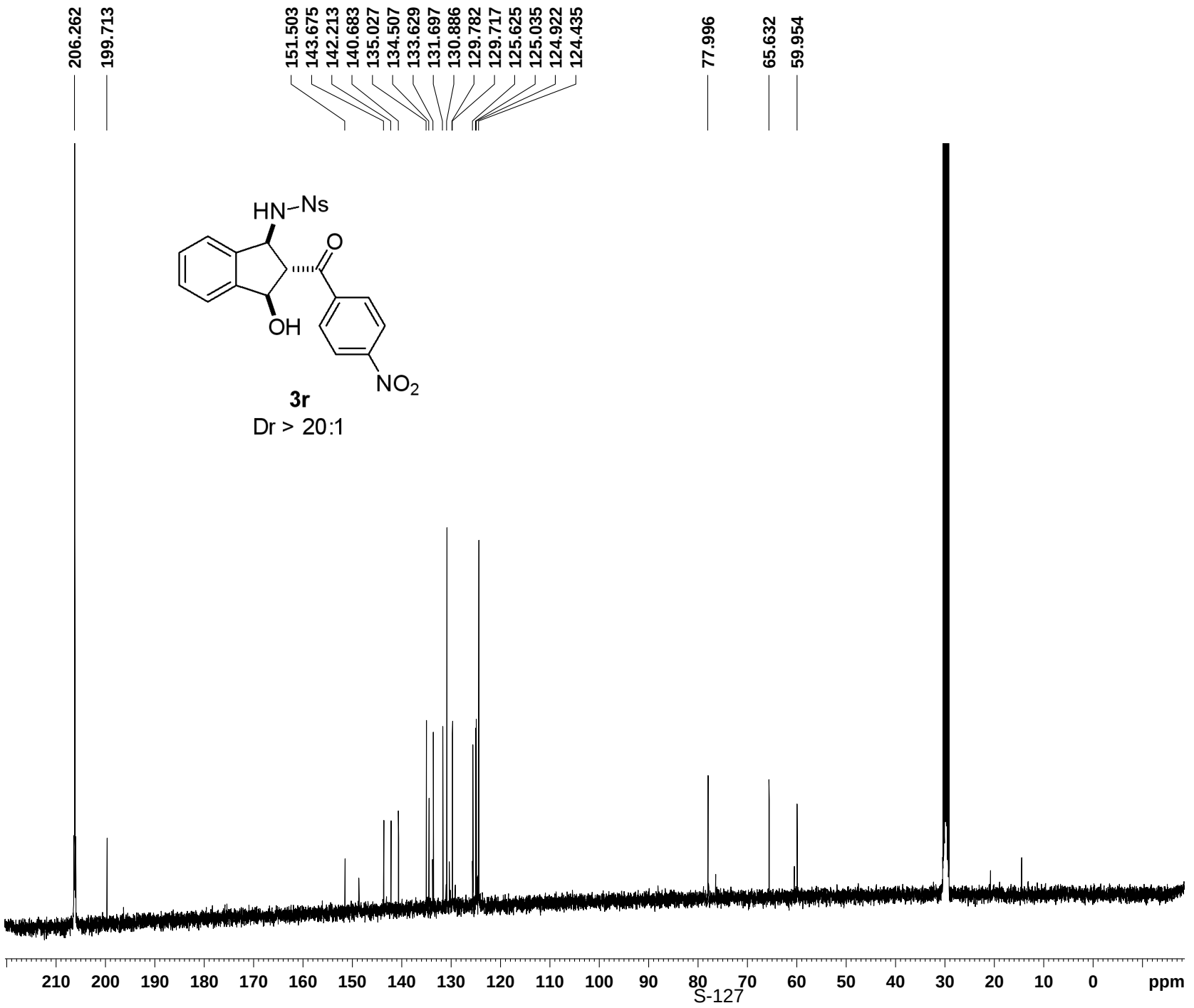
BRUKER

Current Data Parameters
NAME qh−3191
EXPNO 4
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120909
Time 19.51
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 6
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 300.0 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



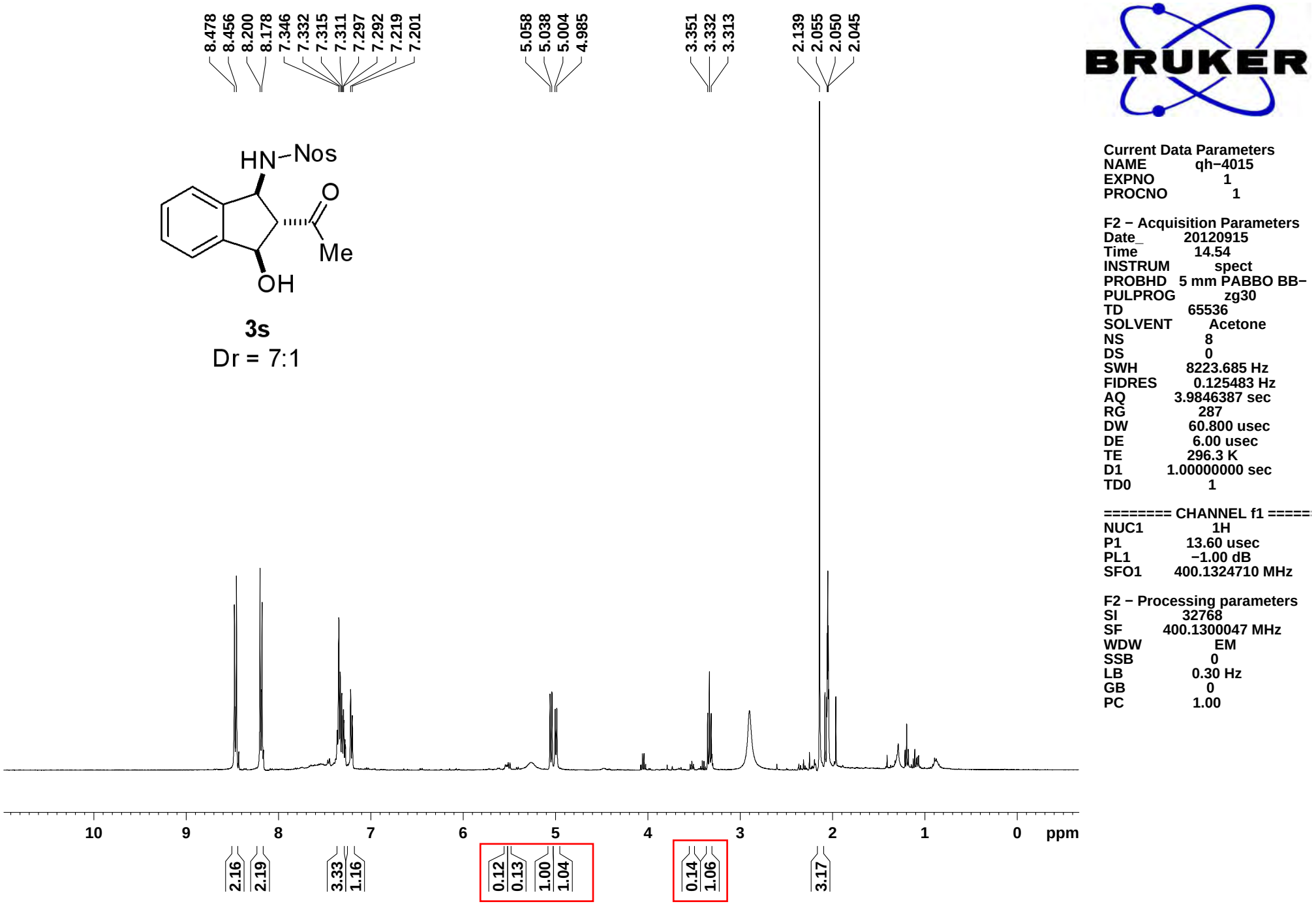
Current Data Parameters
NAME qh−3191
EXPNO 5
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120909
Time 19.53
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 3000
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 300.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126790 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

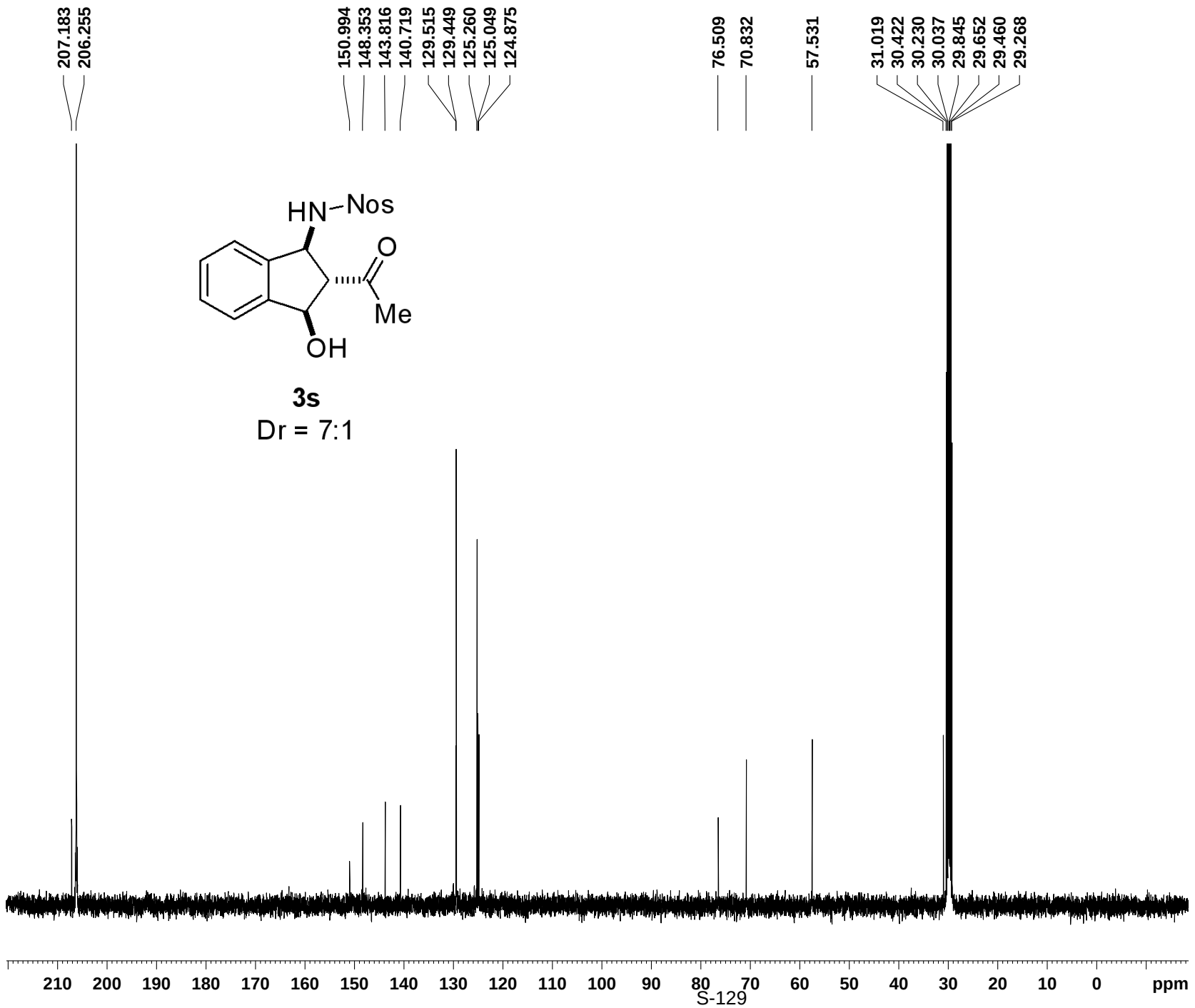


Current Data Parameters
NAME qh−4015
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120915
Time 14.54
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 8
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 296.3 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



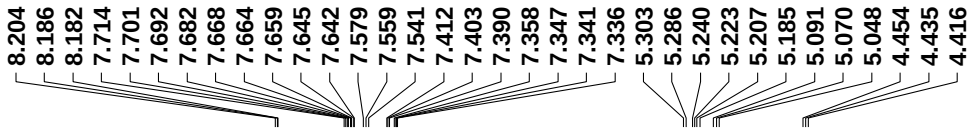
Current Data Parameters
NAME qh−4015
EXPNO 2
PROCNO 1

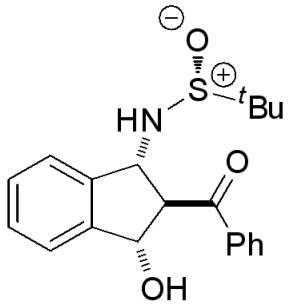
F2 − Acquisition Parameters
Date_ 20120915
Time 15.03
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 404
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 2050
DW 20.800 usec
DE 6.00 usec
TE 296.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

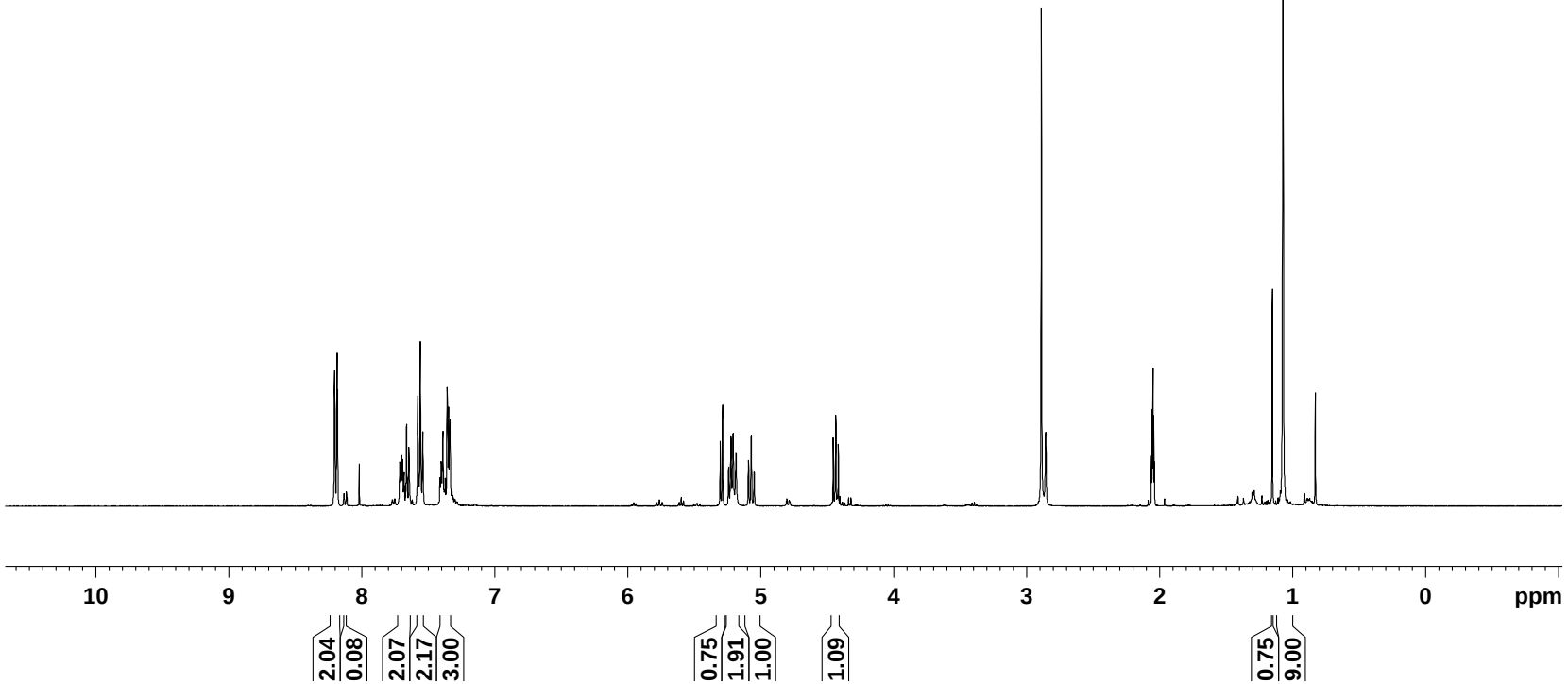
F2 − Processing parameters
SI 32768
SF 100.6126798 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





3t

Dr > 20:1

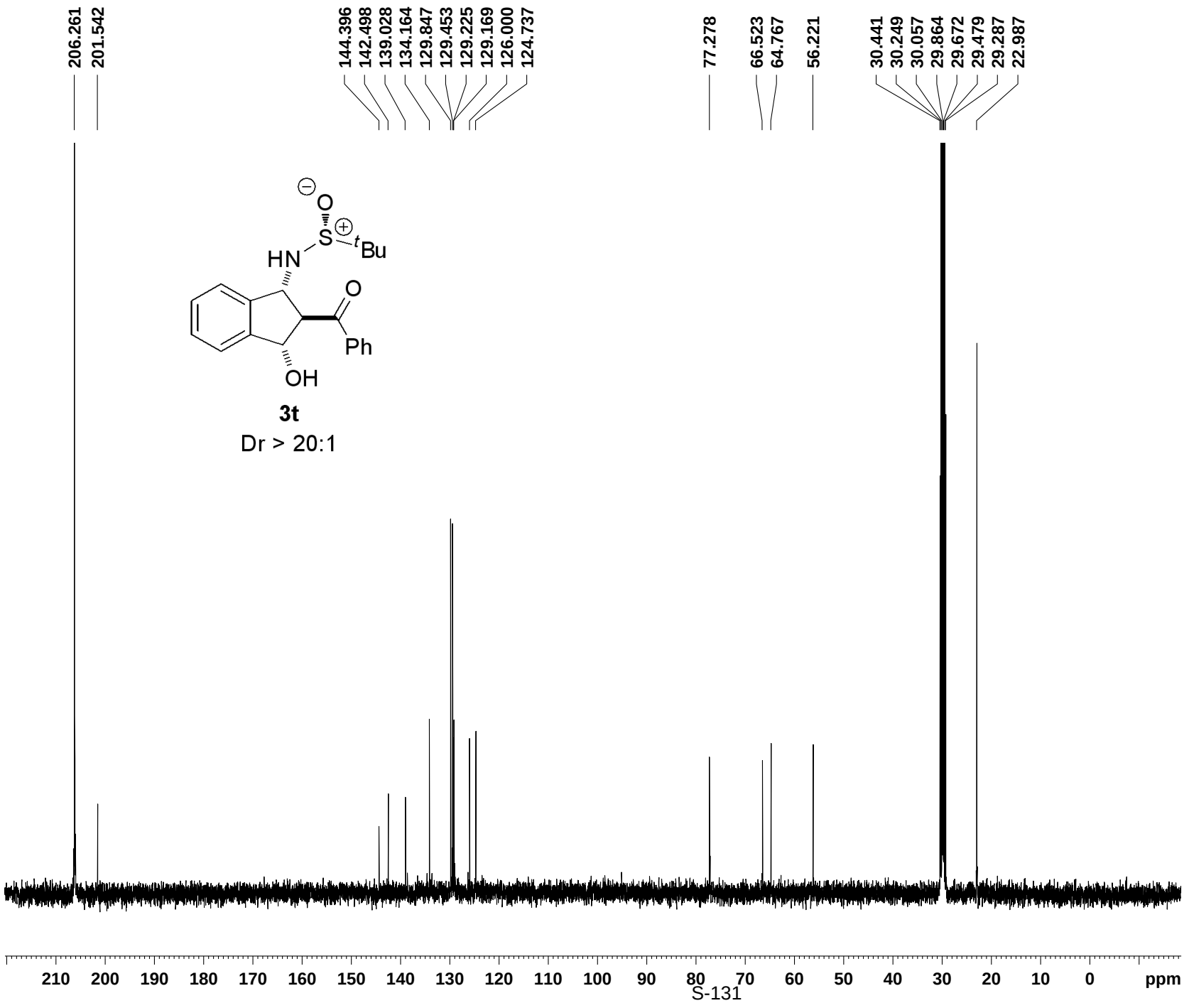



```
Current Data Parameters
NAME          qh−4011
EXPNO            1
PROCNO           1

F2 − Acquisition Parameters
Date_        20120915
Time            13.39
INSTRUM         spect
PROBHD  5 mm PABBO BB−
PULPROG         zg30
TD             65536
SOLVENT       Acetone
NS                7
DS                0
SWH          8223.685 Hz
FIDRES       0.125483 Hz
AQ           3.9846387 sec
RG              203
DW           60.800 usec
DE            6.00 usec
TE            296.6 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         400.1300054 MHz
WDW              EM
SSB               0
LB            0.30 Hz
GB                0
PC             1.00
```



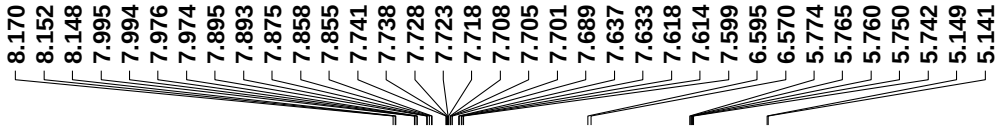
Current Data Parameters
NAME qh−4011
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120915
Time 13.46
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 200
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 297.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

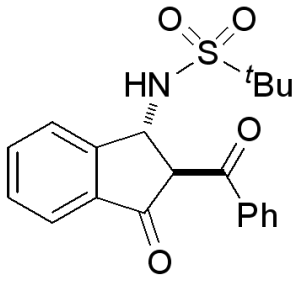
======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126782 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Characterizations of compound **6** are same as those for compound **3g**



7

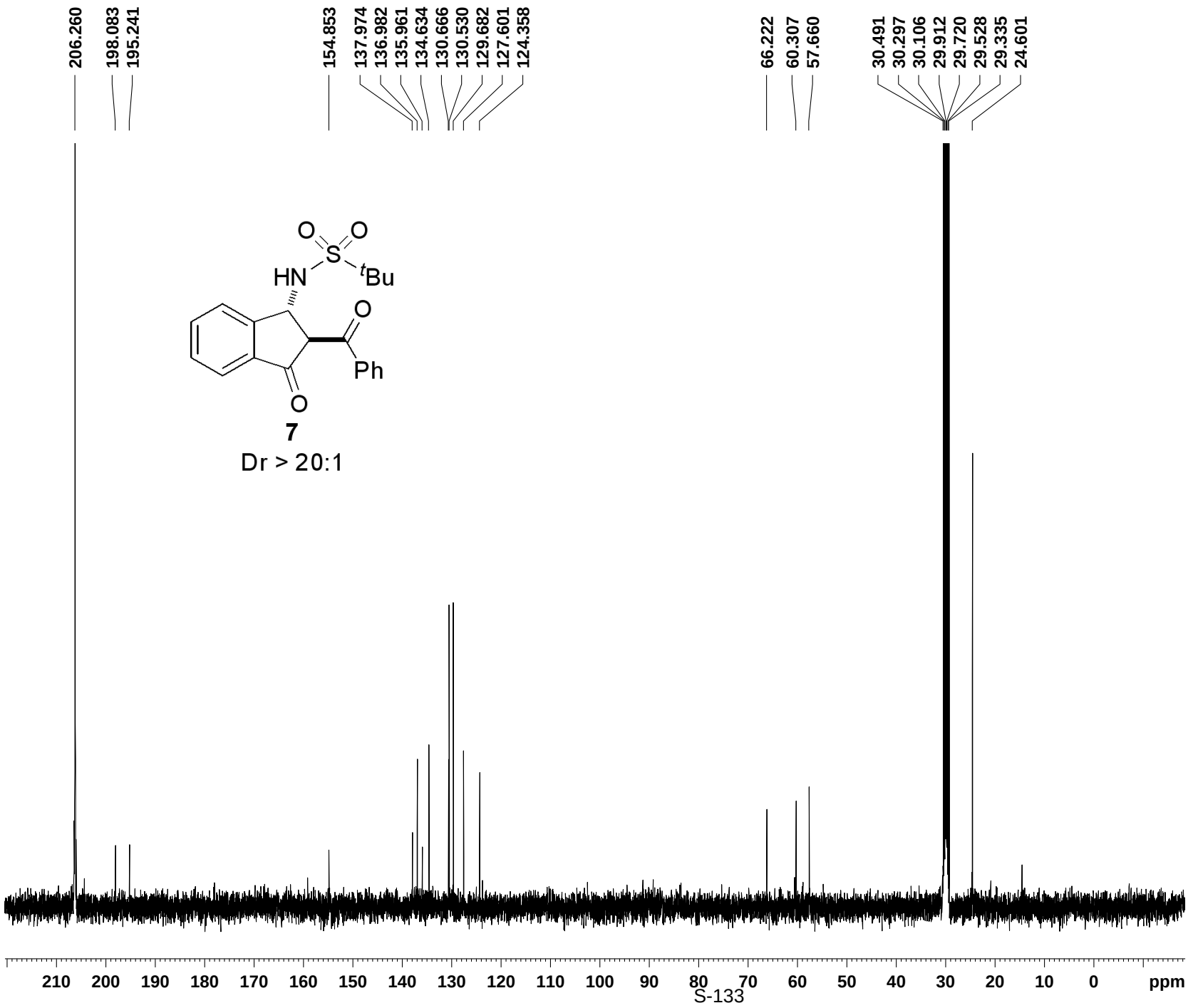
Dr > 20:1

Current Data Parameters
NAME qh−4042
EXPNO 1
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120926
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zg30
TD 65536
SOLVENT Acetone
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 456
DW 60.800 usec
DE 6.00 usec
TE 295.8 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 400.1300047 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



Current Data Parameters
NAME qh−4044
EXPNO 2
PROCNO 1

F2 − Acquisition Parameters
Date_ 20120926
Time 23.57
INSTRUM spect
PROBHD 5 mm PABBO BB−
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 260
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 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ======
NUC1 13C
P1 8.60 usec
PL1 −3.00 dB
SFO1 100.6228298 MHz

======== CHANNEL f2 ======
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL12 14.33 dB
PL13 18.00 dB
PL2 −1.00 dB
SFO2 400.1316005 MHz

F2 − Processing parameters
SI 32768
SF 100.6126712 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40