Supporting Information

Gold-catalyzed Reactions of Propargylic Esters with Vinylazide for the Synthesis of *Z*- or *E*-Configured Buta-1,3-dien-2-yl esters

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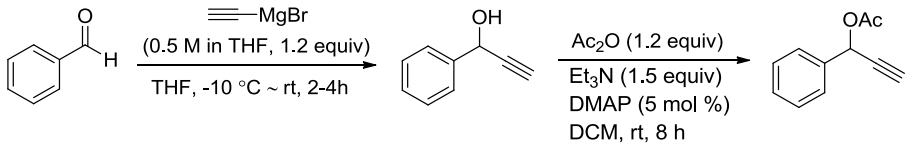
Content:

(1) General procedure:

Unless otherwise noted, all the reaction for the preparation of the substrates were performed in oven-dried glassware under nitrogen atmosphere with freshly distilled solvents. The catalytic reactions were performed in wet solvent. DCM was distilled from CaH_2 under nitrogen from Na metal under nitrogen. All other commercial reagents were used without further purification, unless otherwise indicated. ^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker 400 MHz, Varian 500 MHz and 600 MHz Spectrometers using chloroform-d as the internal standards. All the vinylazides (2a-2d) and 2*H*-azirine (6a) were prepared according to literature procedures [S1].

(1.1) Synthesis of propargylic ester compounds (1a-p)



To a solution of benzaldehyde (2.00 g, 11.86 mmol) in 30 mL anhydrous THF, was added ethynylmagnesium bromide (0.50 M Solution in THF 40 mL, 22.26 mmol) at -10 ℃ and the resulting solution was stirred at -10 ℃ for 15 min and warmed to room temperature and stirred for 2 h after completion of reaction, the resulting solution was quenched with aqueous NH_4Cl solution (50 mL). The THF was evaporated and the residue was diluted with water (100 mL) and extracted with ether (100 mL ×2) and dried over anhydrous $MgSO_4$. After the solvent was evaporated, the crude product was purified by column chromatography (hexane/ethyl acetate = 4/1) to give 1-phenylprop-2-yn-1-ol as a colorless oil (1.12 g, 71 % yield).

To a solution of 1-phenylprop-2-yn-1-ol (1.1 g, 8.33 mmol) and DMAP (51 mg, 0.41 mmol) in 20 mL anhydrous DCM, was added triethylamine (0.91 mL, 12.50 mmol) and the resulting solution was stirred at 0 ℃ for 5 min and slowly added Acetic anhydride (0.94 mL, mmol) and the reaction mixture was stirred at room

temperature for 8 h. After completion of reaction, the resulting solution was quenched with aqueous $NaHCO_3$ solution (30 mL) .The reaction mixture was extracted with DCM (30 mL ×3) and dried over anhydrous $MgSO_4$. After the solvent was evaporated, the crude product was purified by column chromatography (hexane/ethyl acetate = 4/1) to give 1-phenylprop-2-yn-1-yl acetate **(1a)** as a colorless oil (1.09 g, 76% yield). All the propargylic ester compound are prepared using same method, compounds 1a, 1b, 1c and 1i was prepared according to the reference[S2].

References:

[S1] For compounds **2a-d and 6a**: (a) S. K. Pawar, R. L. Sahani, R. -S. Liu, *J. Am. Chem. Eur. J*. 2015, **21**, DOI: 10.1002/Chem.201500694; (b) X. Zhu, Y. F. Wang, F. L. Zhang, S. Chiba, *Chem. Asian J*. 2014, **9**, 2458; (c)L. Xiang, Y. Niu, X. Pang and R. Yan *Chem. commun*. 2015, **51**, 6598; (d) F. W. Fowler, A. Hassner, L. A. Levy, *J. Am. Chem. Soc.*, 1967, **89** (9), 2077.

[S2] For propargyl ester Compounds **1a, 1b, 1c and 1i**: (a) V. V. Pagar, A. M. Jadhav, R. -S. Liu, *J. Am. Chem. Soc*. 2011, **133**, 20728; (b) Sebastien j.-C. Albrecht and P. W. Davies , *Chem. commun*. 2008, **238**; (c) C. V. L. Bray, S. Derien, and P. H. Dixneuf, *Angew. Chem. Int. Ed.*, 2009, **48**, 1439; (d) C. H. M. Amjis, V. L. Carrillo and A. M. Echavarren, *Org. Lett.* 2007, **9**, 4021; (e) A. Furstner and P. W. Davies , *Tetrahedron*., 2008, **65**, 6320.

(2) Standard procedures for catalytic operations:

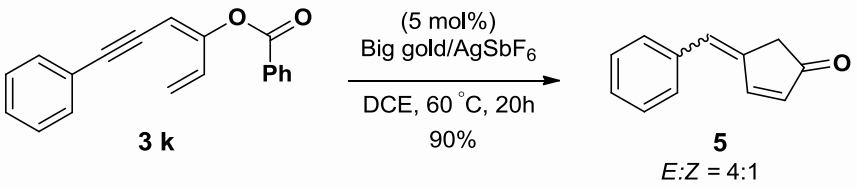
(i) Standard procedure for gold catalyzed synthesis of buta-1,3-dien-2-yl esters.

A 20 mL sample vial was charged with Chloro[(1,1′-biphenyl-2-yl)-di-tert-butylphosphine]gold(I) (0.0152 g, 0.0287 mmol) and Silver hexafluoro-antimonate (0.0098 g, 0.0287 mmol) and to this mixture was added compound **1a** (0.05 g, 0.287 mmol) together with compound **2a** (0.0083 g, 0.574 mmol) dissolved in DCE (dichloroethane), The resulting mixture was heated at 80 ^{o}C for 26 h and after the complete consumption of starting material reaction mixture was cooled to room temperature and the reaction mixture were filterd from small silica bed and dried over

$MgSO_4$ and then purified by coloum chromatography to get pure compound **3a** as a colorless oil (36.3 mg, 67%).

(ii) Standard procedure for gold catalyzed synthesis of compound (5).

A 20 mL sample vial was charged with Chloro[(1,1′-biphenyl-2-yl)-di-tert-butylphosphine]gold(I) (0.0043 g, 0.0082 mmol) and Silver hexafluoro-antimonate (0.0028 g, 0.0082 mmol) and to this mixture was added compound **3k** (0.045 g, 0.164 mmol) dissolved in DCE (dichloroethane), The resulting mixture was heated at 60 ^{o}C for 20 h and after the complete consumption of starting material reaction mixture was cooled to room temperature and the reaction mixture were filterd from small silica bed and dried over $MgSO_4$ and then purified by coloum chromatography to get pure compound **5** as a pale yellow solid (25.2 mg, 90%).

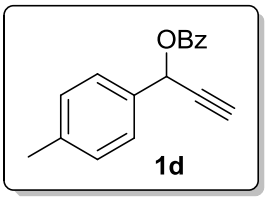


3 k **5**

E:Z = 4:1

(3) Spectral data for compounds :

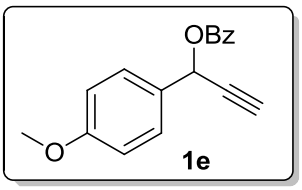
Spectral data for 1-(p-tolyl)prop-2-yn-1-yl benzoate (1d)



1d

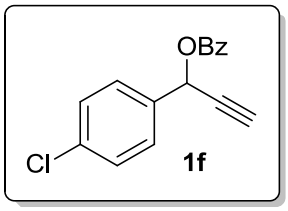
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07 (d, *J* = 7.6 Hz, 2 H), 7.56 ~ 7.51 (m, 3 H), 7.43 ~ 7.40 (m, 2 H), 7.21 (d, *J* = 8.0 Hz, 2 H), 6.67 (d, *J* = 2.2 Hz, 1 H), 2.68 (d, *J* = 2.2 Hz, 1 H), 2.36 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.3, 139.0, 133.6, 133.2, 129.8, 129.5, 129.3, 128.3, 127.6, 80.3, 75.4, 65.6, 21.1; HRMS calcd. For $C_{17}H_{14}O_2$: 250.0994; Found: 250.0993.

Spectral data for 1-(4-methoxyphenyl)prop-2-yn-1-yl benzoate (1e)



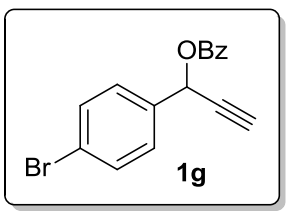
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05 ~ 8.03 (m, 2 H), 7.55 ~ 7.53 (m, 3 H), 7.42 ~ 7.39 (m, 2 H), 6.91 ~ 6.90 (m, 2 H), 6.64 (d, *J* = 2.2 Hz, 1 H), 3.80 (s, 3 H), 2.66 (d, *J* = 2.2 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.4, 160.2, 133.2, 129.8, 129.7, 129.2, 128.7, 128.3, 114.06, 80.4, 75.3, 65.5, 55.3; HRMS calcd. for $C_{17}H_{14}O_3$: 266.0943; Found: 266.0948.

Spectral data for 1-(4-chlorophenyl)prop-2-yn-1-yl benzoate (1f)



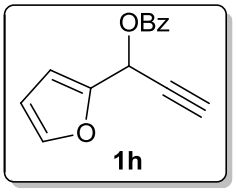
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.05 ~ 8.02 (m, 2 H), 7.57 ~ 7.49 (m, 5 H), 7.43 ~ 7.41 (m, 2 H), 6.63 (d, *J* = 2.1 Hz, 1 H), 2.69 (d, *J* = 2.1 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.2, 135.5, 133.4, 131.8, 129.8, 129.4, 129.3, 128.4, 123.2, 79.7, 75.9, 65.1; HRMS calcd. for $C_{16}H_{11}ClO_2$: 270.0448; Found: 270.0449.

Spectral data for 1-(4-bromophenyl)prop-2-yn-1-yl benzoate (1g)



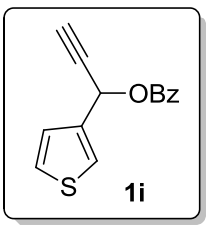
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.06 ~ 8.04 (m, 2 H), 7.56 ~ 7.54 (m, 3 H), 7.43 ~ 7.41 (m, 2 H), 7.38 ~ 7.35 (m, 2 H), 6.65 (d, *J* = 2.2 Hz, 1 H), 2.69 (d, *J* = 2.3 Hz, 1 H); ^{13}CNMR (150 MHz, $CDCl_3$): δ 165.1, 135.0, 133.4, 129.8, 129.3, 129.0, 128.9, 128.4, 79.7, 75.9, 65.0; HRMS calcd. for $C_{16}H_{11}BrO_2$: 313.9942; Found: 313.9945.

Spectral data for 1-(furan-2-yl)prop-2-yn-1-yl benzoate (1h)



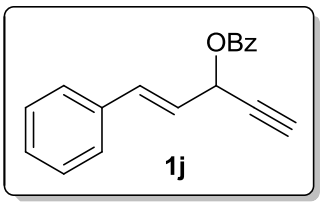
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.08 ~ 8.04 (m, 2 H), 7.55 ~ 7.53 (m, 1 H), 7.44 ~ 7.40 (m, 3 H), 6.74 (d, *J* = 2.3 Hz, 1 H), 6.63 ~ 6.62 (m, 1 H), 6.38 (d, *J* = 1.8, 3.3 Hz, 1 H), 2.64 (d, *J* = 2.3 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 148.8, 143.7, 133.3, 129.9, 129.2, 128.3, 110.6, 110.5, 77.7, 74.8, 58.7; HRMS calcd. for $C_{14}H_{10}O_3$: 226.0630; Found: 226.0630.

Spectral data for 1-(thiophen-3-yl)prop-2-yn-1-yl benzoate (1i)



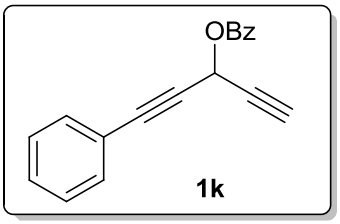
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.07~ 8.06 (m, 2 H), 7.56 ~ 7.54 (m, 2 H), 7.44 ~ 7.41 (m, 2 H), 7.33 (dd, *J* = 3.0, 5.0 Hz, 1 H), 7.26 (dd, *J* = 1.3, 4.2 Hz, 1 H), 6.74 (d, *J* = 2.3 Hz, 1 H), 2.67 (d, *J* = 2.3 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.2, 137.2, 133.3, 129.8, 129.4, 128.3, 126.7, 126.5, 124.8, 79.9, 74.8, 61.3; HRMS calcd. for $C_{14}H_{10}O_2S$: 242.0402; Found: 242.0400.

Spectral data for (E)-1-phenylpent-1-en-4-yn-3-yl benzoate (1j)



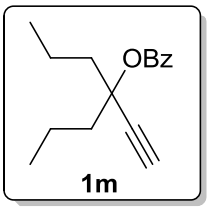
Pale yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.09 ~ 8.07 (m, 2 H), 7.56 ~ 7.54 (m, 1 H), 7.45 ~ 7.42 (m, 4 H), 7.33 ~ 7.31(m, 2 H), 7.28 ~ 7.27(m, 1 H), 6.96 (d, *J* = 15.6 Hz, 1 H), 6.34 (dd, *J* = 6.4, 15.6 Hz, 1 H), 6.30 ~ 6.29 (m, 1 H), 2.67 (d, *J* = 2.2 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.3, 135.5, 134.9, 133.3, 129.8, 129.6, 128.6, 128.5, 128.4, 126.9, 123.4, 79.3, 75.5, 64.5; HRMS calcd. for $C_{18}H_{14}O_2$: 262.0994; Found: 262.1002.

Spectral data for 1-phenylpenta-1,4-diyn-3-yl benzoate (1k)



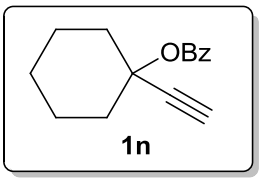
Colorless viscous Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.12 ~ 8.10 (m, 2 H), 7.59 ~ 7.56 (m, 1 H), 7.49 ~ 7.44 (m, 4 H), 7.34 ~ 7.29 (m, 3 H), 6.53 (d, *J* = 2.3 Hz, 1 H), 2.64 (d, *J* = 2.3 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.7, 133.5, 132.0, 130.0, 129.1, 129.0, 128.4, 128.2, 121.4, 85.5, 82.2, 76.7, 73.8, 53.9; HRMS calcd. for $C_{18}H_{12}O_2$: 260.0837; Found: 260.0834.

Spectral data for 4-ethynylheptan-4-yl benzoate (1m)



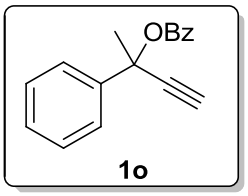
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.99 ~ 7.98 (m, 2 H), 7.53 ~ 7.51 (m, 1 H), 7.50 ~ 7.39 (m, 2 H), 2.59 (s, 1 H), 2.15 ~ 2.10 (m, 2 H), 2.00 ~ 1.95 (m, 2 H), 1.63 ~ 1.49 (m, 4 H), 0.97 ~ 0.94 (m, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.6, 132.7, 130.9, 129.5, 128.2, 83.3, 79.0, 74.1, 40.6, 17.3, 14.0; HRMS calcd. For $C_{16}H_{20}O_2$: 244.1463; Found: 244.1464.

Spectral data for 1-ethynylcyclohexyl benzoate (1n)



Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.02 ~ 8.01 (m, 2 H), 7.53 ~ 7.51 (m, 1 H), 7.42 ~ 7.39 (m, 2 H), 2.63 (s, 1 H), 2.21 ~ 2.19 (m, 2 H), 2.08 ~ 2.07 (m, 2 H), 1.69 ~ 1.65 (m, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.5, 132.7, 130.8, 129.5, 128.2, 83.6, 75.4, 74.2, 36.9, 25.0, 22.3; HRMS calcd. For $C_{15}H_{16}O_2$: 228.1150; Found: 228.1141.

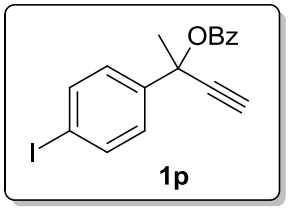
Spectral data for 2-phenylbut-3-yn-2-yl benzoate (1o)



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.06 ~ 8.05 (m, 2 H), 7.66 ~ 7.64 (m, 2 H), 7.55 ~ 7.54 (m, 1 H), 7.44 ~ 7.42 (m, 2 H), 7.38 ~ 7.36 (m, 2 H), 7.36 ~ 7.35 (m, 1

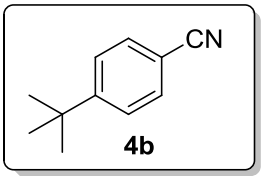
H), 2.86 (s, 1 H), 2.04 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 142.1, 133.0, 130.4, 129.6, 128.4, 128.3, 127.9, 124.7, 82.8, 75.9, 75.8, 32.1; HRMS calcd. For $C_{17}H_{14}O_2$: 250.0994; Found: 250.0995.

Spectral data for 2-(4-iodophenyl)but-3-yn-2-yl benzoate (1p)



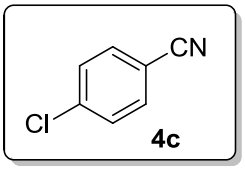
Off white solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.04 ~ 8.02 (m, 2 H), 7.69 ~ 7.67 (m, 2 H), 7.57 ~ 7.54 (m, 1 H), 7.44 ~ 7.41 (m, 2 H), 7.40 ~ 7.38 (m, 2 H), 2.86 (s, 1 H), 2.00 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.1, 141.9, 137.5, 133.1, 130.1, 129.6, 128.3, 126.8, 93.7, 82.2, 76.1, 75.4, 32.0; HRMS calcd. For $C_{17}H_{13}IO_2$: 375.9960; Found: 375.9959.

Spectral data for 4-(tert-butyl)benzonitrile (4b)



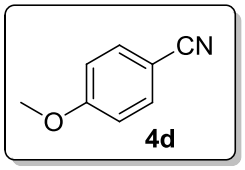
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 (d, *J* = 8.7 Hz, 2 H), 7.46 (d, *J* = 8.7 Hz, 2 H), 1.26 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 156.3, 131.6, 125.9, 118.8, 109.0, 34.9, 30.6; HRMS calcd. For $C_{11}H_{13}N$: 159.1048; Found: 159.1047.

Spectral data for 4-chlorobenzonitrile (4c)



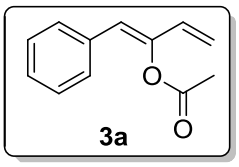
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (d, *J* = 8.7 Hz, 2 H), 7.45 (d, *J* = 8.8 Hz, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 139.5, 133.3, 129.6, 117.9, 110.7; HRMS calcd. For C_7H_4ClN: 137.0032; Found: 137.0029

Spectral data for 4-chlorobenzonitrile (4d)



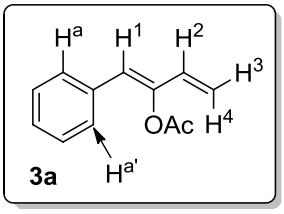
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 (d, *J* = 9.0 Hz, 2 H), 6.92 (d, *J* = 8.9 Hz, 2 H), 3.83 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.8, 133.9, 119.1, 114.7, 103.9, 55.4; HRMS calcd. For C_8H_7NO: 133.0528; Found: 133.0530

Spectral data for (Z)-1-phenylbuta-1,3-dien-2-yl acetate (3a)



Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.42 ~ 7.40 (m, 2 H), 7.31 ~ 7.29 (m, 2 H), 7.24 ~ 7.22 (m, 1 H), 6.38 (dd, *J* = 10.8 Hz, 17.2 Hz, 1 H), 6.21 (s, 1 H), 5.25 (d, *J* = 16.8 Hz, 1 H), 5.19 (d, *J* = 10.8 Hz, 1 H), 2.26 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 167.9, 145.9, 134.0, 132.1, 128.6, 128.5, 127.8, 120.8, 114.3, 20.8; HRMS calcd. for $C_{12}H_{12}O_2$: 188.0837; Found: 188.0838.

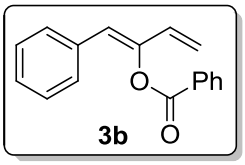
^{1}H NOE Data of compound (3a)



Irradiation	Intensity Increases
H^1	H^2 (d 6.38, 5.25%), $H^{a,a'}$ (d 7.42 ~ 7.40, 4.84%)
H^2	H^1 (d 6.21, 3.40%), H^3 (d 5.19, 2.96%), H^4 (d 5.25, 0.46%)
H^3	H^4 (d 5.25, 2.40%), H^2 (d 6.38, 3.72%)
H^4	H^3 (d 5.19, 6.80%)

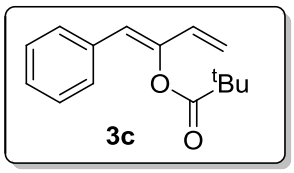
(H^a and $H^{a'}$ are aromatic protons)

Spectral data for (Z)-1-phenylbuta-1,3-dien-2-yl benzoate (3b)



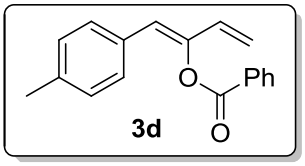
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.21 ~ 8.20 (m, 2 H), 7.64 ~ 7.63 (m, 1 H), 7.52 ~ 7.50 (m, 2 H), 7.45 ~ 7.43 (m, 2 H), 7.24 ~ 7.23 (m, 2 H), 7.21 ~ 7.20 (m, 1 H), 6.47 (dd, *J* = 10.8 Hz, 17.1 Hz, 1 H), 6.34 (s, 1 H), 5.29 (d, *J* = 17.0 Hz, 1 H), 5.19 (d, *J* = 10.9 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.6, 145.9, 133.8, 133.7, 132.1, 130.2, 129.1, 128.8, 128.7, 128.5, 127.8, 121.2, 114.5; HRMS calcd. for $C_{17}H_{14}O_2$: 250.0994; Found: 250.0995.

Spectral data for (Z)-1-phenylbuta-1,3-dien-2-yl pivalate (3c)



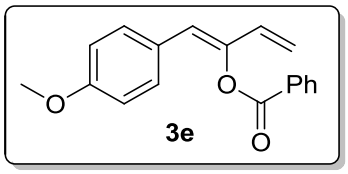
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.40 ~ 7.38 (m, 2 H), 7.29 ~ 7.27 (m, 2 H), 7.22 ~ 7.20 (m, 1 H), 6.37 (dd, *J* = 10.9 Hz, 17.2 Hz, 1 H), 6.25 (s, 1 H), 5.22 (d, *J* = 17.2 Hz, 1 H), 5.15 (d, *J* = 10.9 Hz, 1 H), 1.31 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 175.2, 146.0, 133.9, 132.4, 128.8, 128.2, 127.7, 121.1, 113.9, 39.1, 27.3; HRMS calcd. for $C_{15}H_{18}O_2$: 230.1307; Found: 230.1309.

Spectral data for (Z)-1-(p-tolyl)buta-1,3-dien-2-yl benzoate (3d)



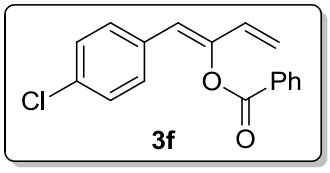
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 ~ 8.21 (m, 2 H), 7.66 ~ 7.63 (m, 1 H), 7.53 ~ 7.51 (m, 2 H), 7.35 (d, *J* = 8.2 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2 H), 6.47 (dd, *J* = 10.8 Hz, 17.1 Hz, 1 H), 6.31 (s, 1 H), 5.26 (d, *J* = 17.1 Hz, 1 H), 5.17 (d, *J* = 10.8 Hz, 1 H) 2.26 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.6, 145.2, 137.8, 133.6, 132.1, 131.0, 130.1, 129.2, 129.1, 128.7, 128.6, 121.1, 113.9, 21.1; HRMS calcd. for $C_{18}H_{16}O_2$: 264.1150; Found: 264.1149.

Spectral data for (Z)-1-(4-methoxyphenyl)buta-1,3-dien-2-yl benzoate (3e)



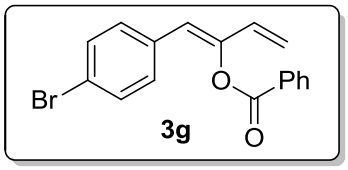
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.23 ~ 8.21 (m, 2 H), 7.64 ~ 7.63 (m, 1 H), 7.53 ~ 7.50 (m, 2 H), 7.40 ~ 7.38 (m, 2 H), 6.75 (d, *J* = 8.9 Hz, 2 H), 6.46 (dd, *J* = 10.8 Hz, 17.1 Hz, 1 H), 6.27 (s, 1 H), 5.22 (d, *J* = 17.1 Hz, 1 H), 5.13 (d, *J* = 10.8 Hz, 1 H), 3.72 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.7, 159.1, 144.4, 133.6, 132.1, 130.2, 130.1, 129.1, 128.7, 126.5, 120.8, 114.0, 113.3, 55.1; HRMS calcd. for $C_{18}H_{16}O_3$: 280.1099; Found: 280.1103.

Spectral data for (Z)-1-(4-chlorophenyl)buta-1,3-dien-2-yl benzoate (3f)



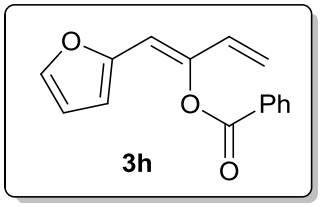
Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.20 ~ 8.18 (m, 2 H), 7.65 ~ 7.64 (m, 1 H), 7.53 ~ 7.50 (m, 2 H), 7.37 ~ 7.36 (m, 2 H), 7.19 ~ 7.18 (m, 2 H), 6.45 (dd, *J* = 10.9 Hz, 17.1 Hz, 1 H), 6.28 (s, 1 H), 5.30 (d, *J* = 17.1 Hz, 1 H), 5.21 (d, *J* = 10.8 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.5, 146.3, 133.8, 133.5, 132.4, 131.9, 130.1, 129.9, 128.9, 128.8, 119.9, 115.0; HRMS calcd. for $C_{17}H_{13}ClO_2$: 284.0604; Found: 284.0599.

Spectral data for (Z)-1-(4-bromophenyl)buta-1,3-dien-2-yl benzoate (3g)



Off white solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.19 (d, *J* = 8.0 Hz, 2 H), 7.67 ~ 7.64 (m, 1 H), 7.53 ~ 7.51 (m, 2 H), 7.35 ~ 7.24 (m, 4 H), 6.46 (dd, *J* = 10.8 Hz, 17.1 Hz, 1 H), 6.27 (s, 1 H), 5.32 (d, *J* = 17.1 Hz, 1 H), 5.22 (d, *J* = 10.8 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.5, 146.4, 133.9, 132.8, 131.9, 131.7, 130.1, 128.8, 121.7, 120.0, 115.1; HRMS calcd. for $C_{17}H_{13}BrO_2$: 328.0099; Found: 328.0092.

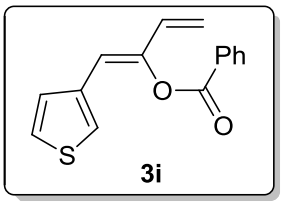
Spectral data for (Z)-1-(furan-2-yl)buta-1,3-dien-2-yl benzoate (3h)



Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.24 ~ 8.22 (m, 2 H), 7.66 ~ 7.63 (m, 1 H), 7.53 ~ 7.51 (m, 2 H), 7.26 (d, *J* = 1.8 Hz, 1 H), 6.43 (dd, *J* = 10.8 Hz, 17.1 Hz, 1 H), 6.37 (d, *J* = 3.4 Hz, 1 H), 6.30 (dd, *J* = 1.8 Hz, 3.4 Hz, 1 H), 6.28 (s, 1 H), 5.30 (d, *J* = 17.1 Hz, 1H), 5.18 (d, *J* = 10.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.8,

149.4, 144.0, 142.6, 133.6, 131.2, 130.2, 129.2, 128.7, 114.7, 111.8, 111.0, 110.0; HRMS calcd. for $C_{15}H_{12}O_3$: 240.0786; Found: 240.0781.

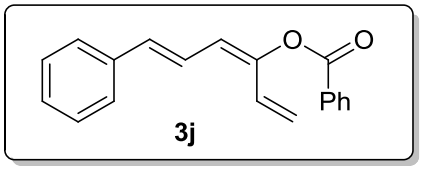
Spectral data for (Z)-1-(thiophen-3-yl)buta-1,3-dien-2-yl benzoate (3i)



3i

Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.25 ~ 8.23 (m, 2 H), 7.66 ~ 7.65 (m, 1 H), 7.54 ~ 7.52 (m, 2 H), 7.33 ~ 7.32 (m, 1 H), 7.18 ~ 7.15 (m, 2 H), 6.45 (dd, *J* = 10.9 Hz, 17.1 Hz, 1 H), 6.39 (s, 1 H), 5.26 (d, *J* = 17.1 Hz, 1 H), 5.17 (d, *J* = 10.8 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.7, 144.9, 134.8, 133.8, 131.6, 130.2, 129.0, 128.8, 127.6, 125.6, 124.8, 115.6, 114.2; HRMS calcd. for $C_{15}H_{12}O_2S$: 256.0558; Found: 256.0556.

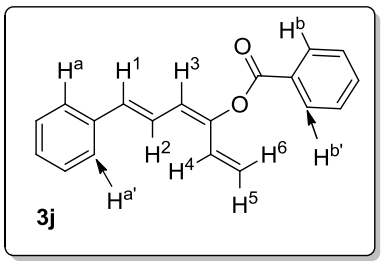
Spectral data for (3E,5E)-6-phenylhexa-1,3,5-trien-3-yl benzoate (3j)



3j

Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.16 (d, *J* = 7.6 Hz, 2 H), 7.63 ~ 7.60 (m, 1 H), 7.50 ~ 7.47 (m, 2 H), 7.42 ~ 7.41 (m, 2 H), 7.33 ~ 7.30 (m, 2 H), 7.23 ~ 7.22 (m, 1 H), 7.09 (dd, *J* = 11.5 Hz, 15.4 Hz, 1 H), 6.91 (dd, *J* = 1.8 Hz, 3.4 Hz, 1 H), 6.61 (d, *J* = 15.4 Hz, 1 H), 6.18 (d, *J* = 11.5 Hz, 1 H), 5.36 (d, *J* = 17.0 Hz, 1 H), 5.25 (d, *J* = 11.0 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.9, 146.3, 137.0, 134.7, 133.5, 130.1, 129.3, 128.7, 128.6, 127.9, 126.5, 126.3, 122.4, 121.6, 115.4; HRMS calcd. for $C_{19}H_{16}O_2$: 276.1150; Found: 276.1153.

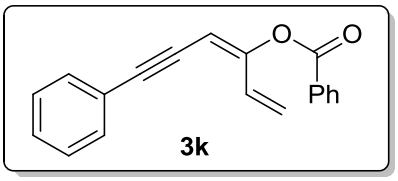
^{1}H NOE Data of compound (3j)



Irradiation	Intensity Increases
H^1	H^3 (d 6.18, 7.99%), $H^{a,a'}$ (d 7.42 ~ 7.41, 6.87%)
H^2	$H^{a,a'}$(d 6.21, 6.40%), H^4 (d 6.91, 4.76%), H^3 (d 6.18, 0.49%)
H^3	H^1 (d 6.61, 8.33%)
H^4	H^2 (d 7.09, 8.56%), H^5 (d 5.25, 4.26%)
H^5	H^6 (d 5.36, 15.97%), H^4 (d 6.91, 4.78%)
H^6	H^5 (d 5.25, 10.74%), $H^{b,b'}$(d 8.16, 1%)

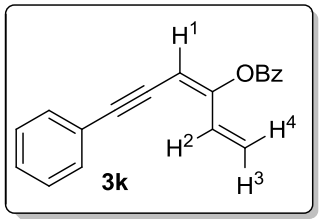
(H^a, $H^{a'}$ and H^b, $H^{b'}$are aromatic protons)

Spectral data for (E)-6-phenylhexa-1,3-dien-5-yn-3-yl benzoate (3k)



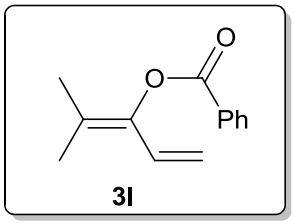
Colorless viscous Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 ~ 8.15 (m, 2 H), 7.64 ~ 7.62 (m, 1 H), 7.51 ~ 7.46 (m, 4 H), 7.34 ~ 7.31 (m, 3 H), 7.02 (dd, *J* = 11.0 Hz, 17.3 Hz, 1 H), 5.76 (s, 1 H), 5.51 ~ 5.48 (m, 1 H), 5.37 ~ 5.35 (m, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 155.3, 133.7, 131.3, 130.1, 128.9, 128.6, 128.4, 128.3, 128.2, 123.0, 117.5, 102.7, 97.5, 83.6; HRMS calcd. for $C_{19}H_{14}O_2$: 274.0994; Found: 274.0998.

^{1}H NOE Data of compound (3k)



Irradiation	Intensity Increases
H^1	no effect
H^2	H^3 (d 5.37 ~ 5.35, 3.61%), H^4 (d 5.51 ~ 5.48, 1.81%)
H^3	H^4 (d 5.51 ~ 5.48, 23.65%), H^2 (d 7.02, 6.31%)
H^4	H^3 (d 5.37 ~ 5.35, 21.68%)

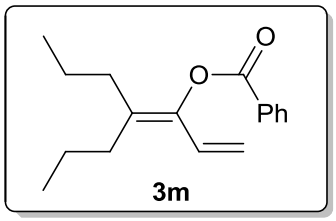
Spectral data for 4-methylpenta-1,3-dien-3-yl benzoate (3l)



3l

Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 ~ 8.16 (m, 2 H), 7.61 ~ 7.58 (m, 1 H), 7.49 ~ 7.46 (m, 2 H), 6.67 (dd, *J* = 11.0 Hz, 17.0 Hz, 1 H), 5.00 (d, *J* = 17.2 Hz, 1 H), 5.02 (d, *J* = 11.0 Hz, 1 H), 1.91 (s, 3 H), 1.69 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.4, 140.7, 133.3, 130.0, 129.4, 128.5, 127.2, 124.8, 112.1, 18.6; HRMS calcd. for $C_{13}H_{14}O_2$: 202.0994; Found: 202.0995.

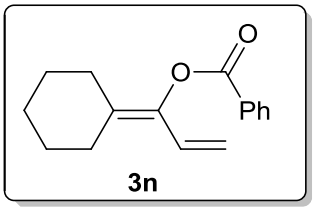
Spectral data for 4-propylhepta-1,3-dien-3-yl benzoate (3m)



3m

Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.16 ~ 8.15 (m, 2 H), 7.60 ~ 7.62 (m, 1 H), 7.49 ~ 7.46 (m, 2 H), 6.66 (dd, *J* = 11.0 Hz, 16.9 Hz, 1 H), 5.07 (d, *J* = 16.9 Hz, 1 H), 5.01 (d, *J* = 11.1 Hz, 1 H), 2.22 (t, *J* = 7.6 Hz, 2 H), 2.00 (t, *J* = 7.7 Hz, 2 H), 1.54 ~ 1.51 (m, 2 H), 1.43 ~ 1.41 (m, 2 H), 0.96 (t, *J* = 7.3 Hz, 3 H), 0.83 (t, *J* = 7.3 Hz, 3 H) ; ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.6, 141.6, 133.2, 132.9, 129.9, 128.5, 127.4, 112.3, 32.4, 32.3, 31.5, 22.0, 20.9, 14.2, 13.9; HRMS calcd. for $C_{17}H_{22}O_2$: 258.1620; Found: 258.1617.

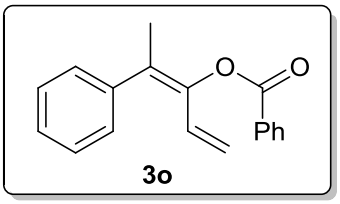
Spectral data for 1-cyclohexylideneallyl benzoate (3n)



3n

Pale yellow Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.17 ~ 8.16 (m, 2 H), 7.60 ~ 7.58 (m, 1 H), 7.48 ~ 7.46 (m, 2 H), 6.71 (dd, *J* = 11.0 Hz, 17.0 Hz, 1 H), 5.13 (d, *J* = 16.9 Hz, 1 H), 5.02 (d, *J* = 11.0 Hz, 1 H), 2.38 (t, *J* = 6.0 Hz, 2 H), 2.13 (t, *J* = 6.0 Hz, 2 H), 1.65 ~ 1.62 (m, 2 H), 1.56 ~ 1.53 (m, 4 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.5, 138.0, 133.2, 132.4, 130.0, 129.5, 128.5, 126.8, 112.4, 29.0, 28.5, 27.5, 26.9, 26.3; HRMS calcd. for $C_{16}H_{18}O_2$: 242.1307; Found: 242.1304.

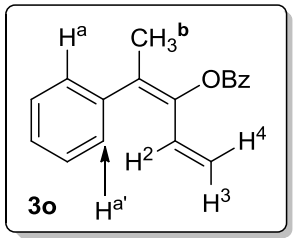
Spectral data for (E)-4-phenylpenta-1,3-dien-3-yl benzoate (3o)



3o

Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.24 ~ 8.22 (m, 2 H), 7.64 ~ 7.62 (m, 1 H), 7.53 ~ 7.50 (m, 2 H), 7.38 ~ 7.30 (m, 5 H), 6.42 (dd, *J* = 11.0 Hz, 17.1 Hz, 1 H), 5.18 (d, *J* = 17.1 Hz, 1 H), 4.98 (d, *J* = 11.0 Hz, 1 H), 2.03 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.1, 142.9, 139.8, 133.5, 130.0, 129.8, 129.3, 129.0, 128.8, 128.6, 128.2, 127.4, 113.1, 18.9; HRMS calcd. for $C_{18}H_{16}O_2$: 264.1150; Found: 264.1147.

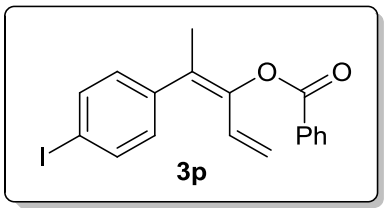
^{1}H NOE Data of compound (3o)



Irradiation	Intensity Increases
$CH_3{}^b$	$H^{a,a'}$ (d 7.38 ~ 7.30, 0.49%)
H^2	H^3 (d 4.98, 1.75%), $H^{a,a'}$ (d 7.38 ~ 7.30, 1.03%)
H^3	H^4 (d 5.18, 9.67%), H^2 (d 6.42, 2.12%)
H^4	H^3 (d 4.98, 9.67%)

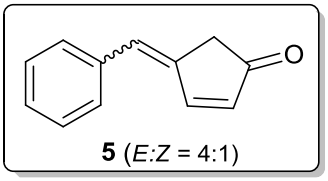
(H^a and $H^{a'}$ are aromatic protons)

Spectral data for (E)-4-(4-iodophenyl)penta-1,3-dien-3-yl benzoate (3p)



Colorless Oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 8.21 ~ 8.20 (m, 2 H), 7.70 (d, *J* = 8.3 Hz, 2 H), 7.64 ~ 7.62 (m, 1 H), 7.52 ~ 7.49 (m, 2 H), 7.07 (d, *J* = 8.3 Hz, 2 H), 6.37 (dd, *J* = 11.0 Hz, 17.1 Hz, 1 H), 5.20 (d, *J* = 17.1 Hz, 1 H), 5.01 (d, *J* = 11.0 Hz, 1 H), 1.98 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.0, 143.1, 139.4, 137.4, 133.5, 130.7, 130.0, 129.1, 128.6, 113.9, 93.1, 18.7; HRMS calcd. for $C_{18}H_{15}IO_2$: 390.0117; Found: 390.0110.

Spectral data for 4-benzylidenecyclopent-2-enone (5)



Pale yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) for trans(*E*) major isomer: δ 7.86 (d, *J* = 5.4 Hz, 1 H), 7.41 ~ 7.38 (m, 2 H), 7.37 ~ 7.35 (m, 2 H), 7.28 ~ 7.27 (m, 1 H), 6.65 (s, 1 H), 6.28 (d, *J* = 5.4 Hz, 1 H), 3.24 (d, *J* = 1.5 Hz, 2 H); ^{13}C NMR (150 MHz,

$CDCl_3$): δ 206.2, 162.2, 155.4, 136.0, 132.5, 129.2, 129.1, 128.8, 128.3, 39.2; HRMS calcd. for $C_{12}H_{10}O$: 170.0732; Found: 170.0732.

Pale yellow solid; ^{1}H NMR (600 MHz, $CDCl_3$) for Cis(*Z*) minor isomer: δ 8.21 (d, *J* = 5.6 Hz, 1 H), 7.30 ~ 7.29 (m, 1 H), 6.69 (s, 1 H), 6.39 (d, *J* = 5.6 Hz, 1 H), 3.11 (d, *J* = 0.5 Hz, 2 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 206.2,137.5, 136.3, 128.6, 128.1, 127.9, 40.6; HRMS calcd. for $C_{12}H_{10}O$: 170.0732; Found: 170.0732.

(4) DFT calculation data of compounds 3j, 3k and 3o:

Computational Details

The geometry optimizations were carried out using density functional theory (DFT) at B3LYP/6-31G* level, implemented in Gaussian09 program. The effect of the solvent (DCE) was taken into account using the polarizable continuum model (PCM). The normal vibrations within the harmonic approximation were used to confirmed the nature of stationary points (minima). All relative energies are corrected with zero-point vibrational energies (ZPVE).

Table S1: DCE solvent

Compounds	Isomer	Relative energy	K_{298} (*E*/*Z*)
3j	*E*	0	0.06
	Z	-1.65	
3k	*E*	0	0.37
	Z	-0.59	
3o	*E*	0	8.23
	Z	1.25	

(5) X-ray crystallographic structure and data for compound (3e)

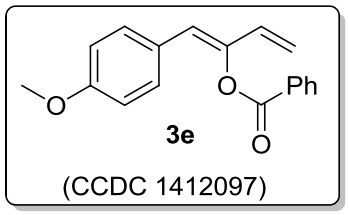


Table 1. Crystal data and structure refinement for mo_150443LT_0m.

Identification code	mo_150443LT_0m	
Empirical formula	C18 H16 O3	
Formula weight	280.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.9279(6) Å	a= 90°.
	b = 7.9230(3) Å	b= 98.2320(10)°.
	c = 14.2519(6) Å	g = 90°.

Volume	1444.75(11) Å ^{3}
Z	4
Density (calculated)	1.289 Mg/m^3
Absorption coefficient	0.087 mm^{-1}
F(000)	592
Crystal size	0.25 x 0.20 x 0.20 mm^3
Theta range for data collection	1.592 to 26.387°.
Index ranges	-16<=h<=16, -9<=k<=6, -17<=l<=7
Reflections collected	10840
Independent reflections	2947 [R(int) = 0.0249]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8807
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2947 / 0 / 191
Goodness-of-fit on F^2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0375, wR2 = 0.0891
R indices (all data)	R1 = 0.0458, wR2 = 0.0948
Extinction coefficient	n/a
Largest diff. peak and hole	0.431 and -0.190 e.Å $^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å ^{2}x 10^3) for mo_150443LT_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)

O(1)	9642(1)	-559(1)	6333(1)	22(1)
O(2)	6865(1)	706(1)	9780(1)	20(1)
O(3)	7880(1)	2892(1)	10353(1)	24(1)
C(1)	10705(1)	-913(2)	6225(1)	27(1)
C(2)	9374(1)	-724(2)	7223(1)	19(1)
C(3)	8353(1)	-224(2)	7317(1)	20(1)
C(4)	7997(1)	-350(2)	8184(1)	20(1)
C(5)	8643(1)	-985(2)	8986(1)	18(1)
C(6)	8338(1)	-1158(2)	9932(1)	20(1)
C(7)	7581(1)	-392(2)	10322(1)	19(1)
C(8)	7098(1)	2379(2)	9879(1)	18(1)
C(9)	6276(1)	3461(2)	9344(1)	18(1)
C(10)	5384(1)	2807(2)	8811(1)	22(1)
C(11)	4635(1)	3877(2)	8350(1)	25(1)
C(12)	4770(1)	5601(2)	8422(1)	26(1)
C(13)	6416(1)	5212(2)	9416(1)	23(1)
C(14)	5655(1)	6280(2)	8951(1)	26(1)
C(15)	7413(1)	-612(2)	11301(1)	22(1)
C(16)	6683(1)	166(2)	11709(1)	27(1)
C(17)	10024(1)	-1355(2)	8002(1)	21(1)
C(18)	9653(1)	-1488(2)	8865(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for mo_150443LT_0m.

O(1)-C(2)	1.3676(15)
O(1)-C(1)	1.4323(16)

O(2)-C(8)	1.3616(16)
O(2)-C(7)	1.4170(16)
O(3)-C(8)	1.2032(16)
C(1)-H(1)	0.9800
C(1)-H(11)	0.9800
C(1)-H(10)	0.9800
C(2)-C(17)	1.3865(19)
C(2)-C(3)	1.4029(18)
C(3)-C(4)	1.3820(18)
C(3)-H(9)	0.9500
C(4)-C(5)	1.4082(18)
C(4)-H(14)	0.9500
C(5)-C(18)	1.3993(18)
C(5)-C(6)	1.4638(18)
C(6)-C(7)	1.3372(19)
C(6)-H(15)	0.9500
C(7)-C(15)	1.4532(18)
C(8)-C(9)	1.4882(18)
C(9)-C(10)	1.3868(19)
C(9)-C(13)	1.4010(19)
C(10)-C(11)	1.380(2)
C(10)-H(3)	0.9500
C(11)-C(12)	1.379(2)
C(11)-H(16)	0.9500
C(12)-C(14)	1.386(2)

C(12)-H(2)	0.9500
C(13)-C(14)	1.392(2)
C(13)-H(4)	0.9500
C(14)-H(5)	0.9500
C(15)-C(16)	1.330(2)
C(15)-H(8)	0.9500
C(16)-H(6)	0.9500
C(16)-H(7)	0.9500
C(17)-C(18)	1.3874(19)
C(17)-H(13)	0.9500
C(18)-H(12)	0.9500
C(2)-O(1)-C(1)	117.16(10)
C(8)-O(2)-C(7)	115.06(10)
O(1)-C(1)-H(1)	109.5
O(1)-C(1)-H(11)	109.5
H(1)-C(1)-H(11)	109.5
O(1)-C(1)-H(10)	109.5
H(1)-C(1)-H(10)	109.5
H(11)-C(1)-H(10)	109.5
O(1)-C(2)-C(17)	124.82(12)
O(1)-C(2)-C(3)	115.44(12)
C(17)-C(2)-C(3)	119.74(12)
C(4)-C(3)-C(2)	120.22(12)
C(4)-C(3)-H(9)	119.9
C(2)-C(3)-H(9)	119.9

C(3)-C(4)-C(5)	121.14(12)
C(3)-C(4)-H(14)	119.4
C(5)-C(4)-H(14)	119.4
C(18)-C(5)-C(4)	117.17(12)
C(18)-C(5)-C(6)	117.79(12)
C(4)-C(5)-C(6)	125.04(12)
C(7)-C(6)-C(5)	130.50(13)
C(7)-C(6)-H(15)	114.8
C(5)-C(6)-H(15)	114.8
C(6)-C(7)-O(2)	120.79(12)
C(6)-C(7)-C(15)	124.32(12)
O(2)-C(7)-C(15)	114.89(11)
O(3)-C(8)-O(2)	122.86(12)
O(3)-C(8)-C(9)	125.03(12)
O(2)-C(8)-C(9)	112.11(11)
C(10)-C(9)-C(13)	119.96(13)
C(10)-C(9)-C(8)	122.80(12)
C(13)-C(9)-C(8)	117.22(12)
C(11)-C(10)-C(9)	120.15(13)
C(11)-C(10)-H(3)	119.9
C(9)-C(10)-H(3)	119.9
C(12)-C(11)-C(10)	120.05(14)
C(12)-C(11)-H(16)	120.0
C(10)-C(11)-H(16)	120.0
C(11)-C(12)-C(14)	120.67(13)

C(11)-C(12)-H(2)	119.7
C(14)-C(12)-H(2)	119.7
C(14)-C(13)-C(9)	119.42(13)
C(14)-C(13)-H(4)	120.3
C(9)-C(13)-H(4)	120.3
C(12)-C(14)-C(13)	119.75(13)
C(12)-C(14)-H(5)	120.1
C(13)-C(14)-H(5)	120.1
C(16)-C(15)-C(7)	125.35(13)
C(16)-C(15)-H(8)	117.3
C(7)-C(15)-H(8)	117.3
C(15)-C(16)-H(6)	120.0
C(15)-C(16)-H(7)	120.0
H(6)-C(16)-H(7)	120.0
C(2)-C(17)-C(18)	119.35(12)
C(2)-C(17)-H(13)	120.3
C(18)-C(17)-H(13)	120.3
C(17)-C(18)-C(5)	122.37(12)
C(17)-C(18)-H(12)	118.8
C(5)-C(18)-H(12)	118.8

Symmetry transformations used to generate equivalent atoms:

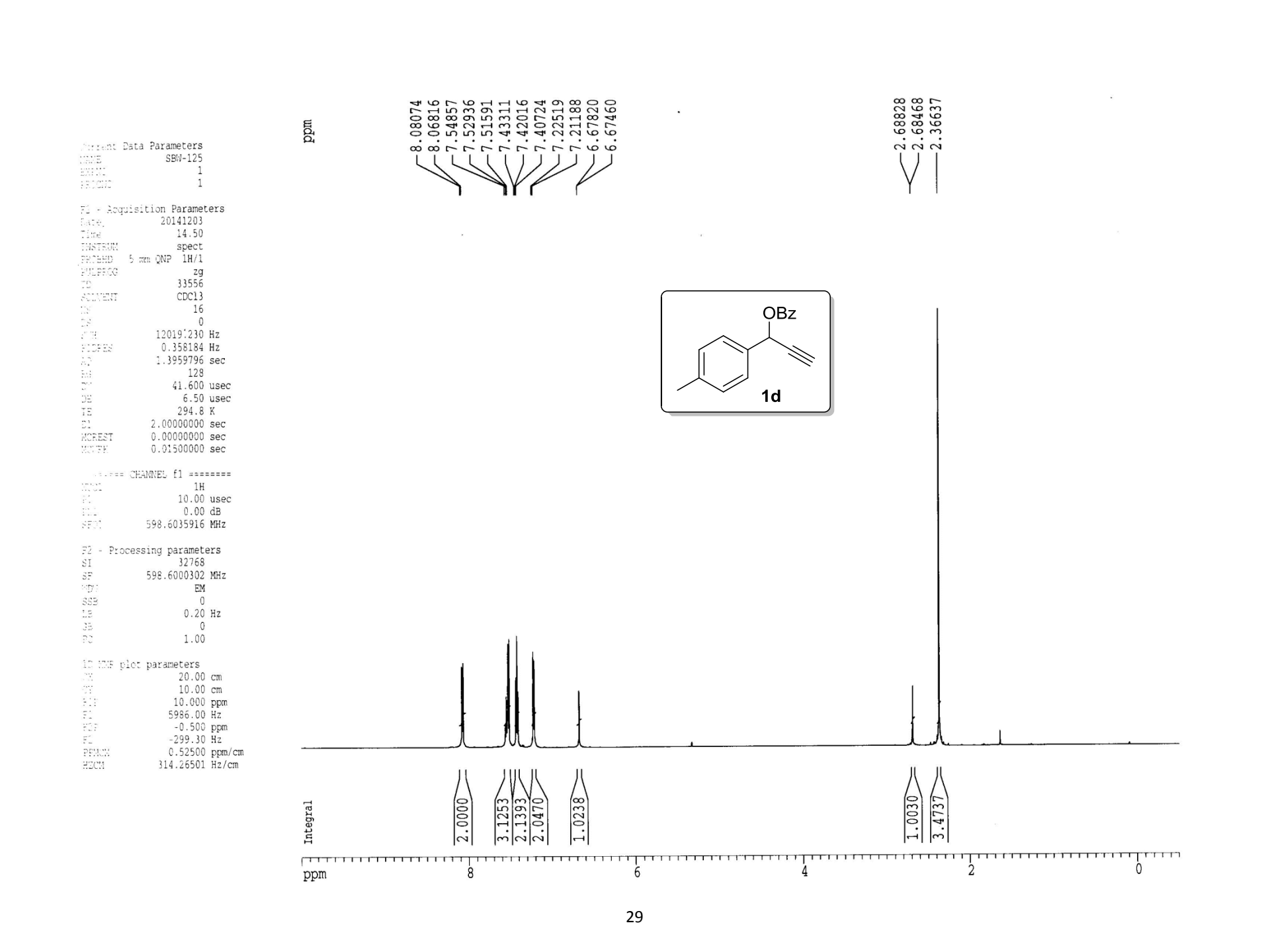
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for mo_150443LT_0m. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	22(1)	26(1)	20(1)	-2(1)	3(1)	3(1)
O(2)	21(1)	17(1)	23(1)	1(1)	1(1)	1(1)
O(3)	22(1)	23(1)	27(1)	1(1)	-1(1)	-4(1)
C(1)	24(1)	33(1)	25(1)	-2(1)	7(1)	7(1)
C(2)	22(1)	14(1)	20(1)	-4(1)	2(1)	-2(1)
C(3)	19(1)	20(1)	21(1)	-2(1)	-3(1)	1(1)
C(4)	16(1)	19(1)	23(1)	-2(1)	1(1)	1(1)
C(5)	19(1)	14(1)	22(1)	-1(1)	0(1)	-1(1)
C(6)	20(1)	16(1)	22(1)	2(1)	-1(1)	0(1)
C(7)	18(1)	16(1)	22(1)	2(1)	-1(1)	0(1)
C(8)	20(1)	20(1)	17(1)	-1(1)	6(1)	-3(1)
C(9)	21(1)	20(1)	14(1)	1(1)	6(1)	2(1)
C(10)	24(1)	20(1)	21(1)	-1(1)	4(1)	-1(1)
C(11)	23(1)	28(1)	24(1)	0(1)	2(1)	2(1)
C(12)	28(1)	28(1)	21(1)	3(1)	4(1)	10(1)
C(13)	28(1)	23(1)	19(1)	-2(1)	4(1)	-3(1)
C(14)	38(1)	16(1)	26(1)	0(1)	10(1)	3(1)
C(15)	23(1)	20(1)	24(1)	3(1)	2(1)	-2(1)
C(16)	31(1)	26(1)	27(1)	4(1)	9(1)	-1(1)
C(17)	17(1)	19(1)	27(1)	-2(1)	2(1)	3(1)
C(18)	20(1)	18(1)	23(1)	2(1)	-2(1)	3(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10 ^{3}) for mo_150443LT_0m.

	x	y	z	U(eq)
H(1)	11173	-196	6657	41
H(11)	10811	-682	5570	41
H(10)	10859	-2102	6373	41
H(9)	7904	202	6784	24
H(14)	7305	-2	8240	24
H(15)	8743	-1942	10334	23
H(3)	5289	1620	8763	26
H(16)	4027	3425	7984	30
H(2)	4251	6331	8105	31
H(4)	7026	5667	9779	28
H(5)	5741	7469	8997	31
H(8)	7861	-1373	11680	27
H(6)	6218	938	11355	33
H(7)	6625	-49	12355	33
H(13)	10717	-1694	7945	25
H(12)	10100	-1936	9393	25

(5) ^{1}H, ^{13}C NMR and NOE spectra of key compounds: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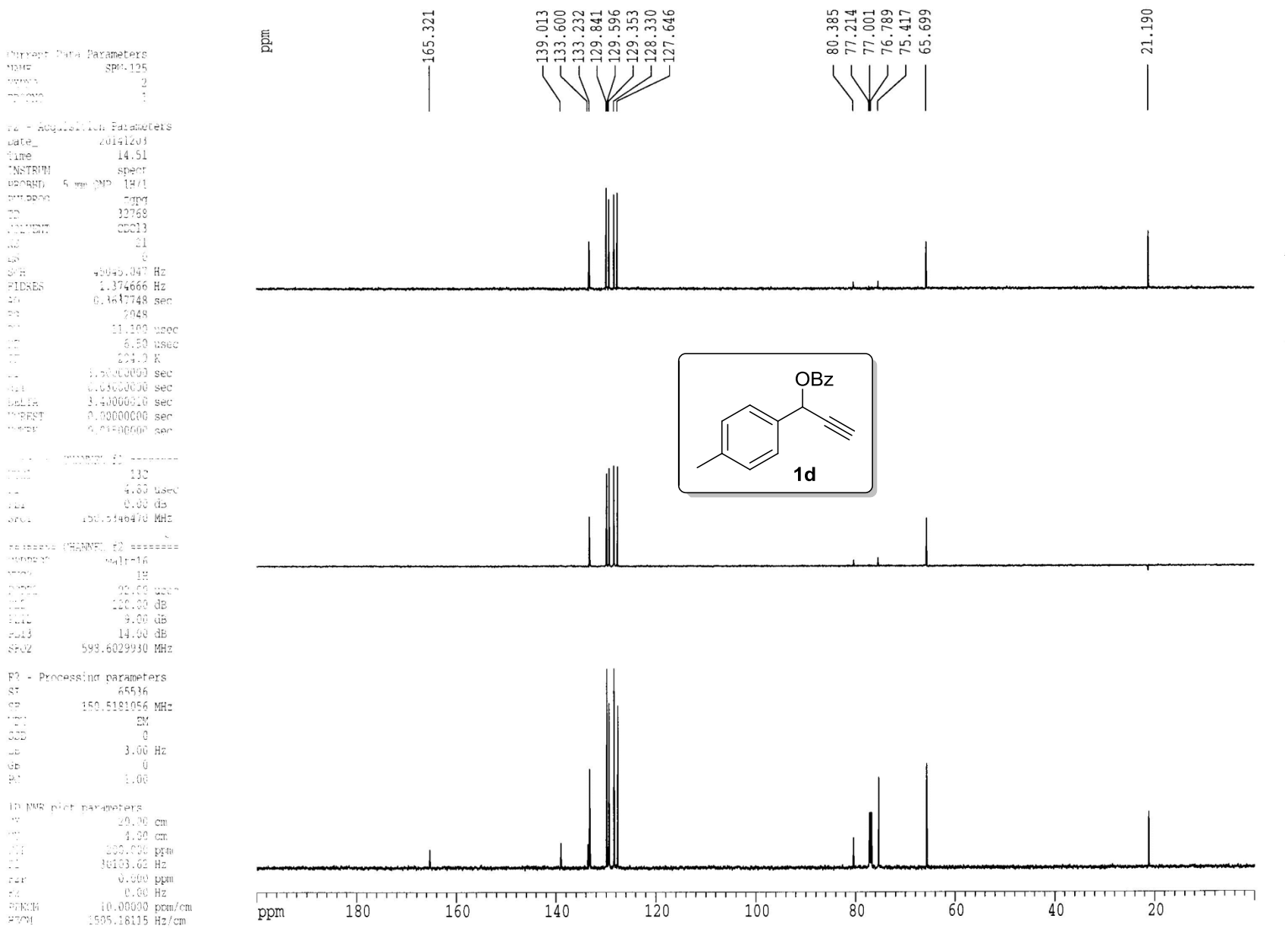
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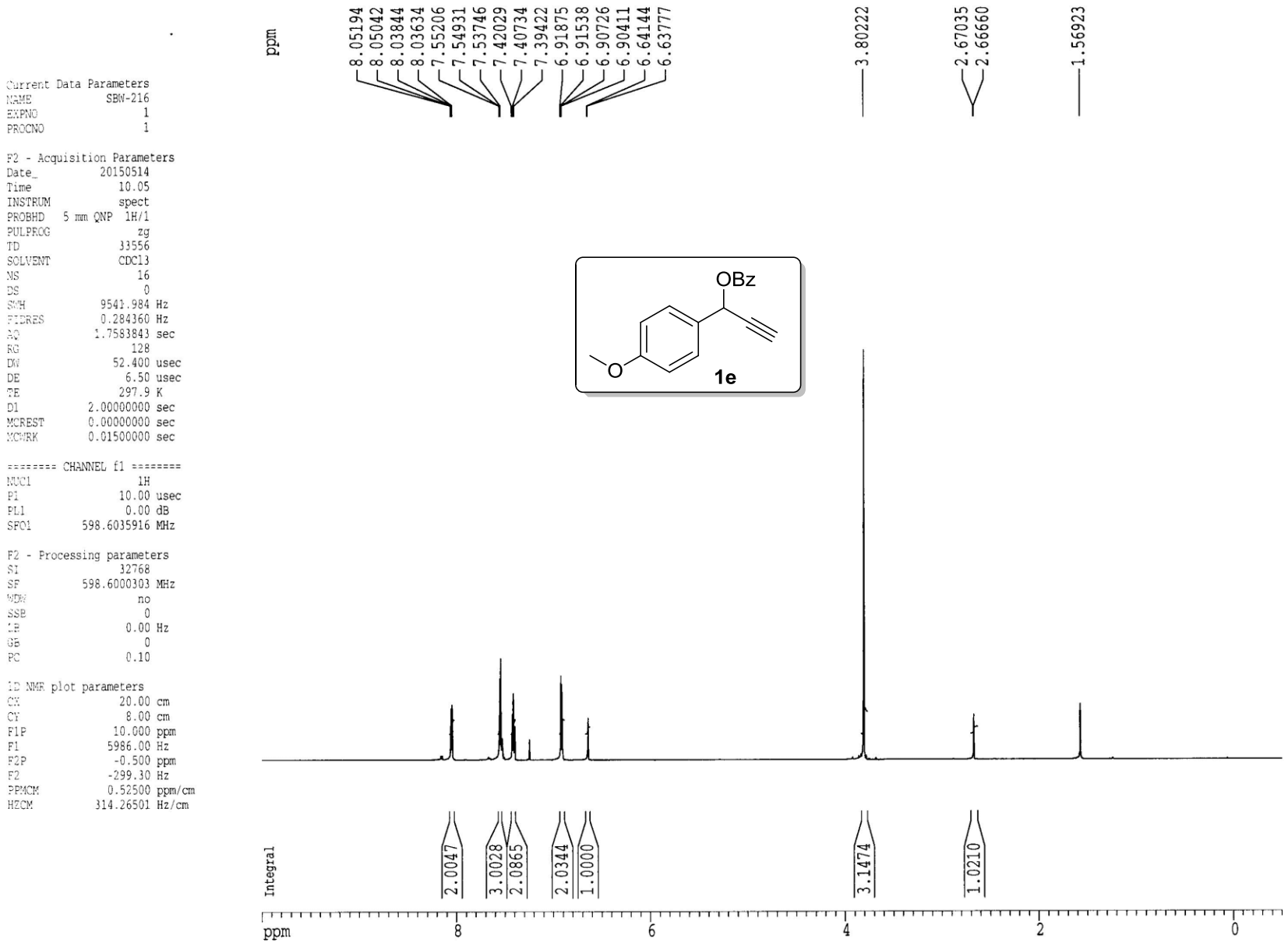
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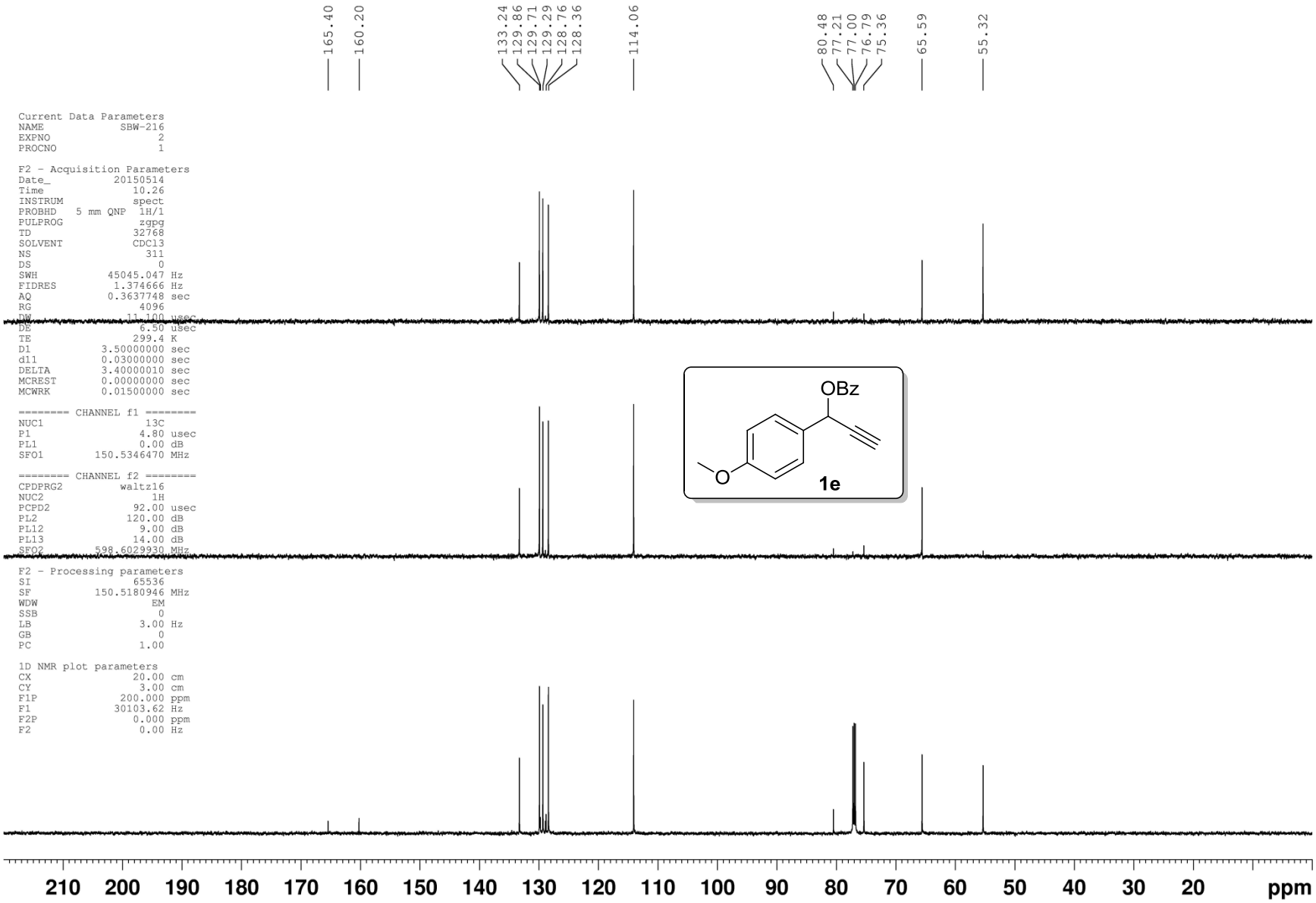
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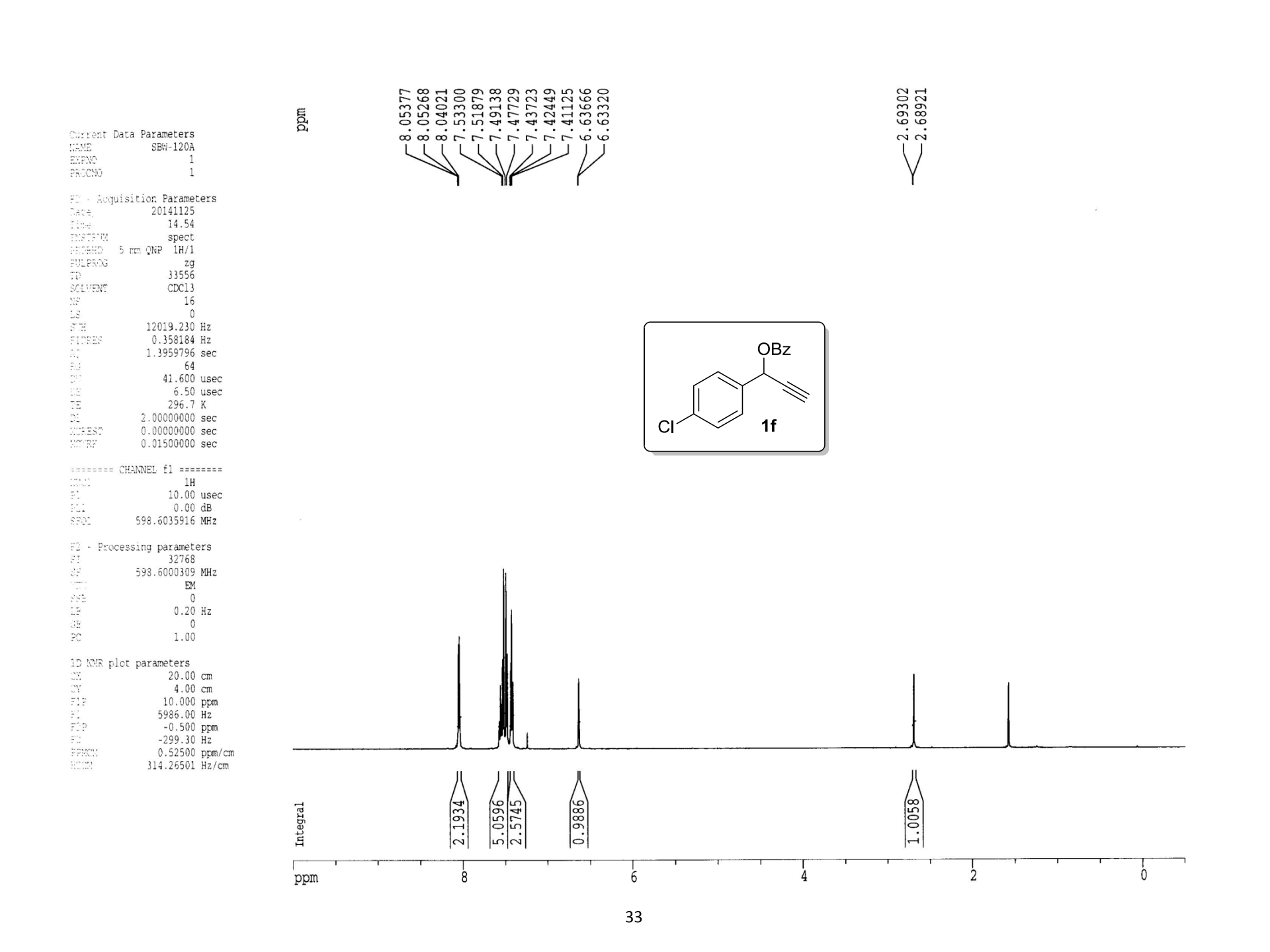
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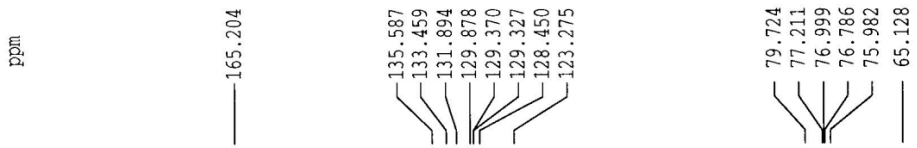
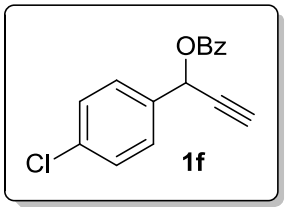
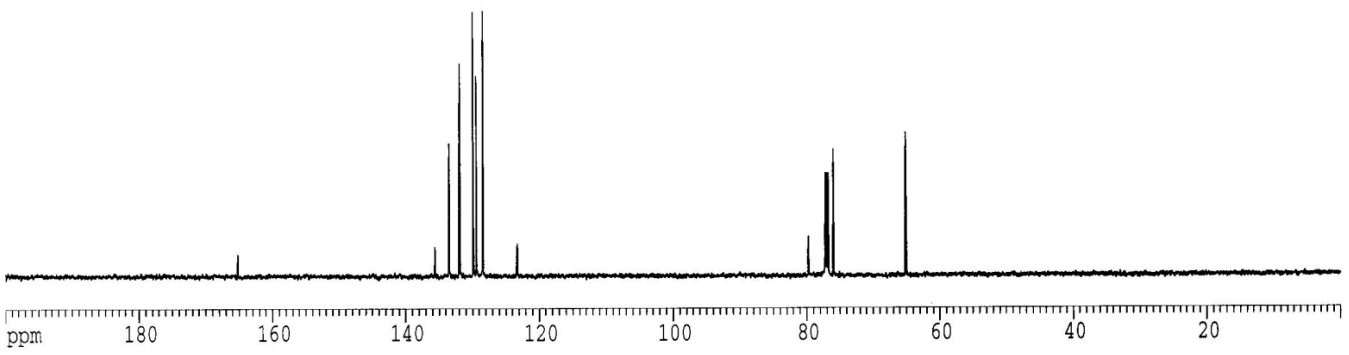
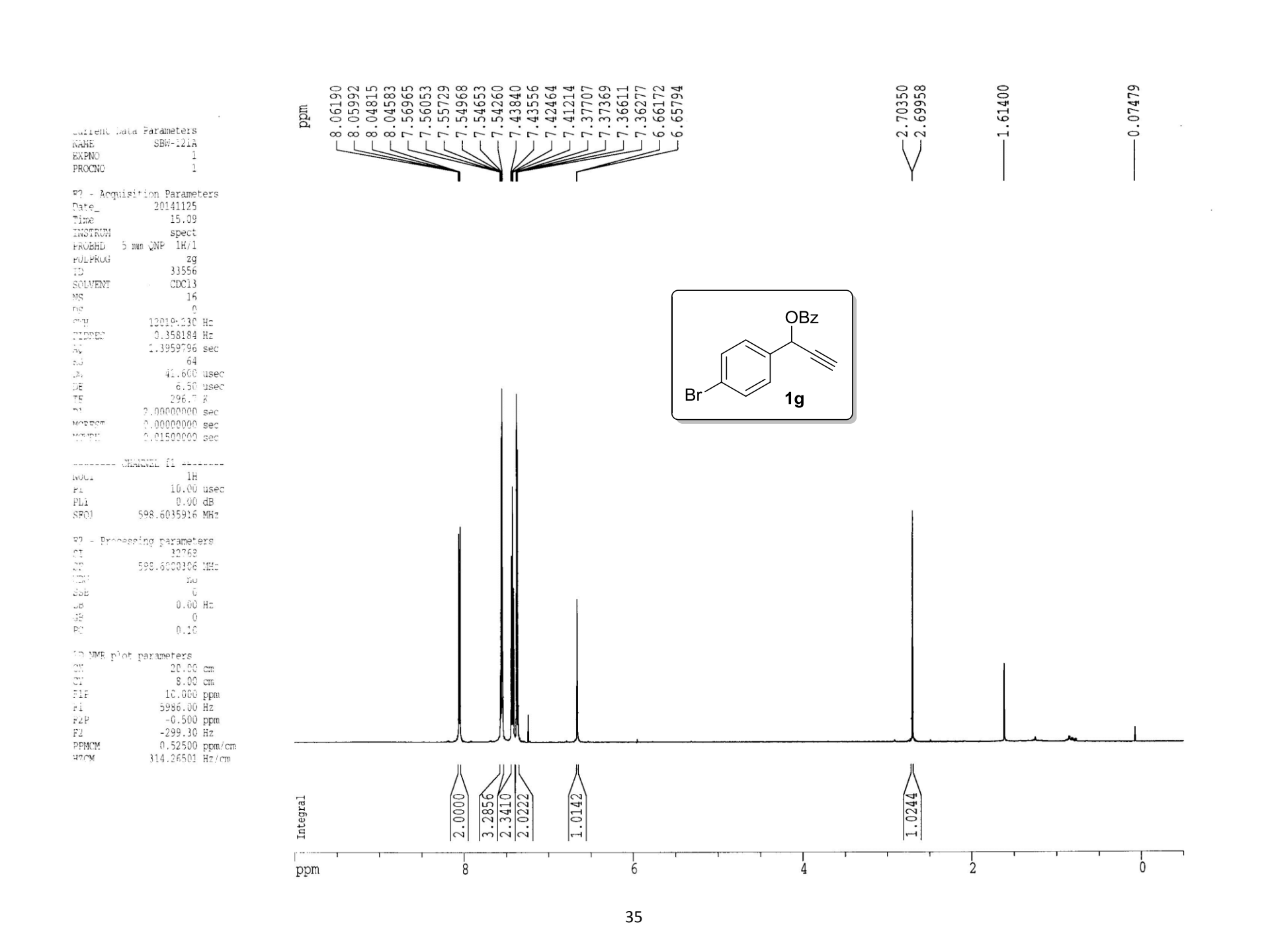
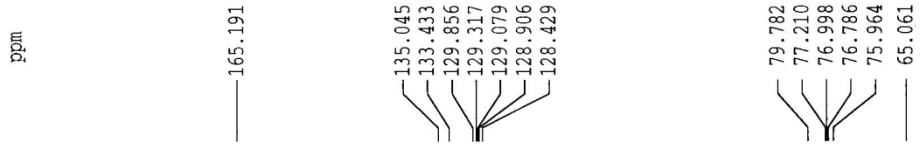


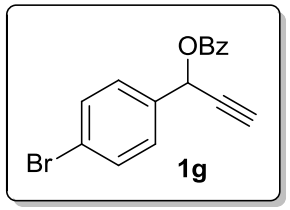


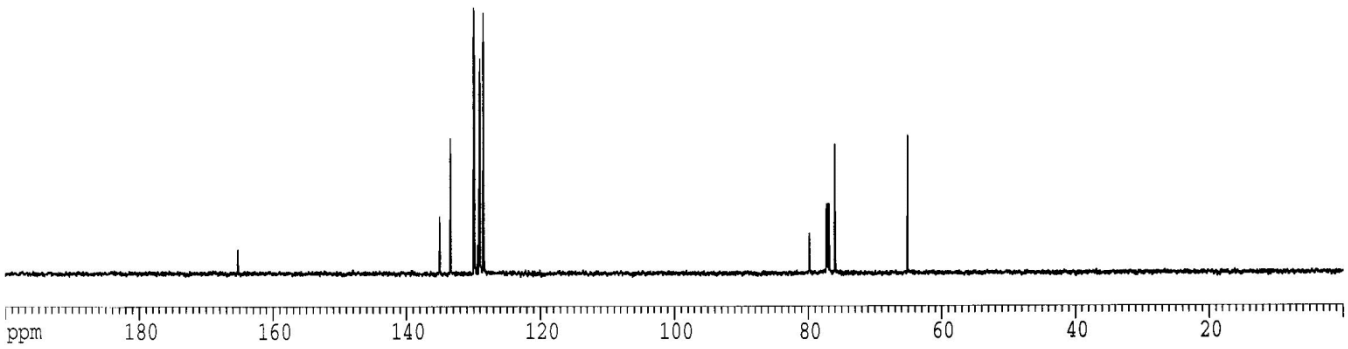



Current Data Parameters
NAME SBW-121A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141125
Time 15.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
CHANNEL f1
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000306 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.10
1D NMR plot parameters
WC 20.00 cm
WC 8.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.06190
8.05992
8.04815
8.04583
7.56965
7.56053
7.55729
7.54968
7.54653
7.54260
7.43840
7.43556
7.42464
7.41214
7.37707
7.37369
7.36611
7.36277
6.66172
6.65794
2.70350
2.69958
1.61400
0.07479
OBz
Br
1g
Integral
2.0000
3.2856
2.3410
2.0222
1.0142
1.0244
ppm
8
6
4
2
0

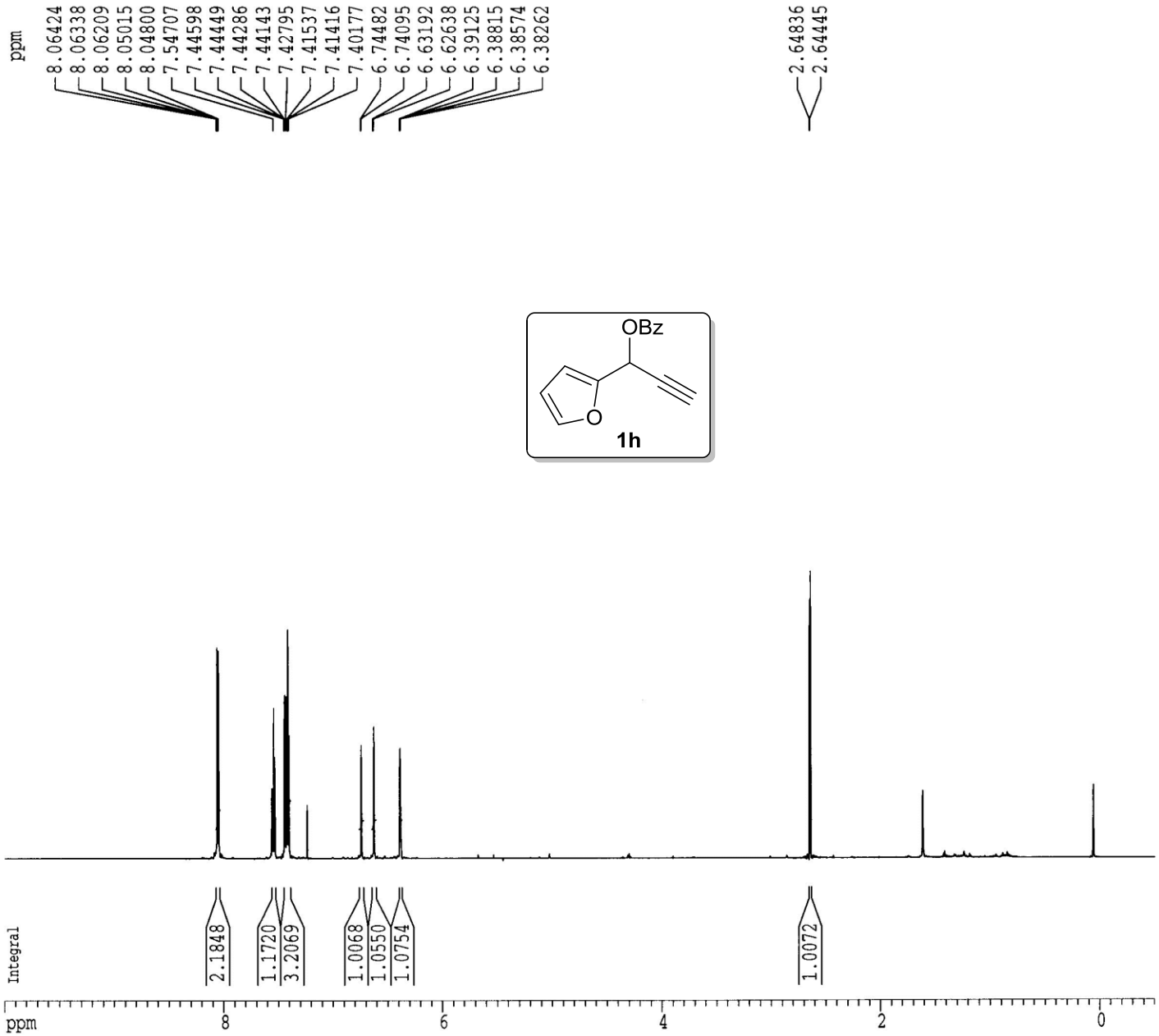
```
Current Data Parameters
NAME            SBW-121A
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141125
Time                15.10
INSTRUM              spect
PROBHD   5 mm QNP  1H/1
PULPROG              zgpg
TD                  32768
SOLVENT             CDCl3
NS                    100
DS                      0
SWH             45045.047 Hz
FIDRES              1.374666 Hz
AQ              0.3637748 sec
RG                    2048
DW                 11.100 usec
DE                  6.50 usec
TE                296.8 K
D1              1.50000000 sec
D11             0.03000000 sec
DELTA           2.40000010 sec
TDREST          0.00000000 sec
TDRXR           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   4.80 usec
PL1                  0.00 dB
SFO1          150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2               92.00 usec
PL2                120.00 dB
PL12                9.00 dB
PL13               14.00 dB
SFO2          599.6029930 MHz

F2 - Processing parameters
SI                  65536
SF            150.5181014 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   0.50

1D NMR plot parameters
CX                  20.00 cm
CY                   4.00 cm
F1P               200.000 ppm
F1                30103.62 Hz
F2P                 0.000 ppm
F2                  0.00 Hz
PPMCM            13.00000 ppm/cm
HZCM          1505.18091 Hz/cm
```

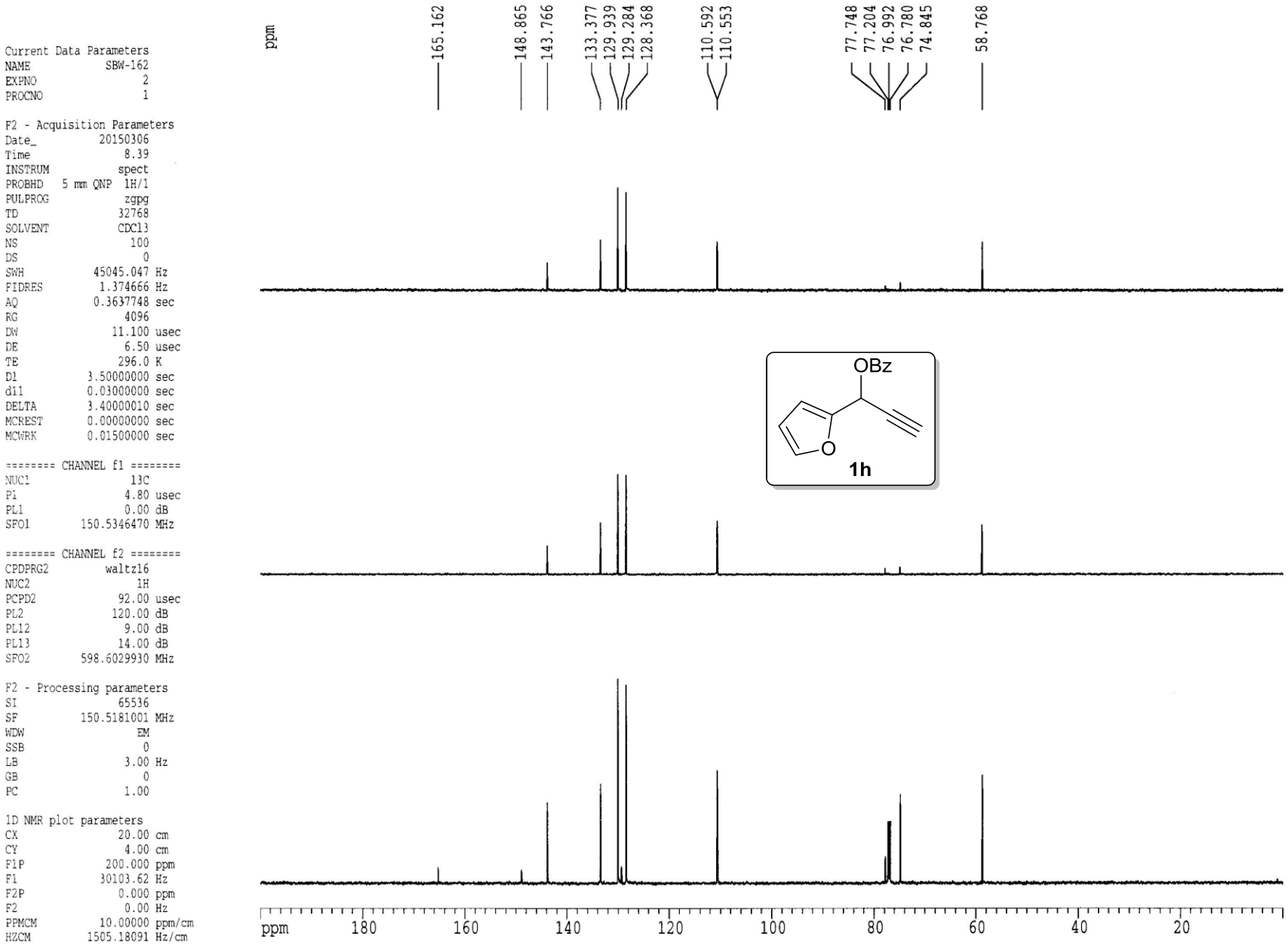


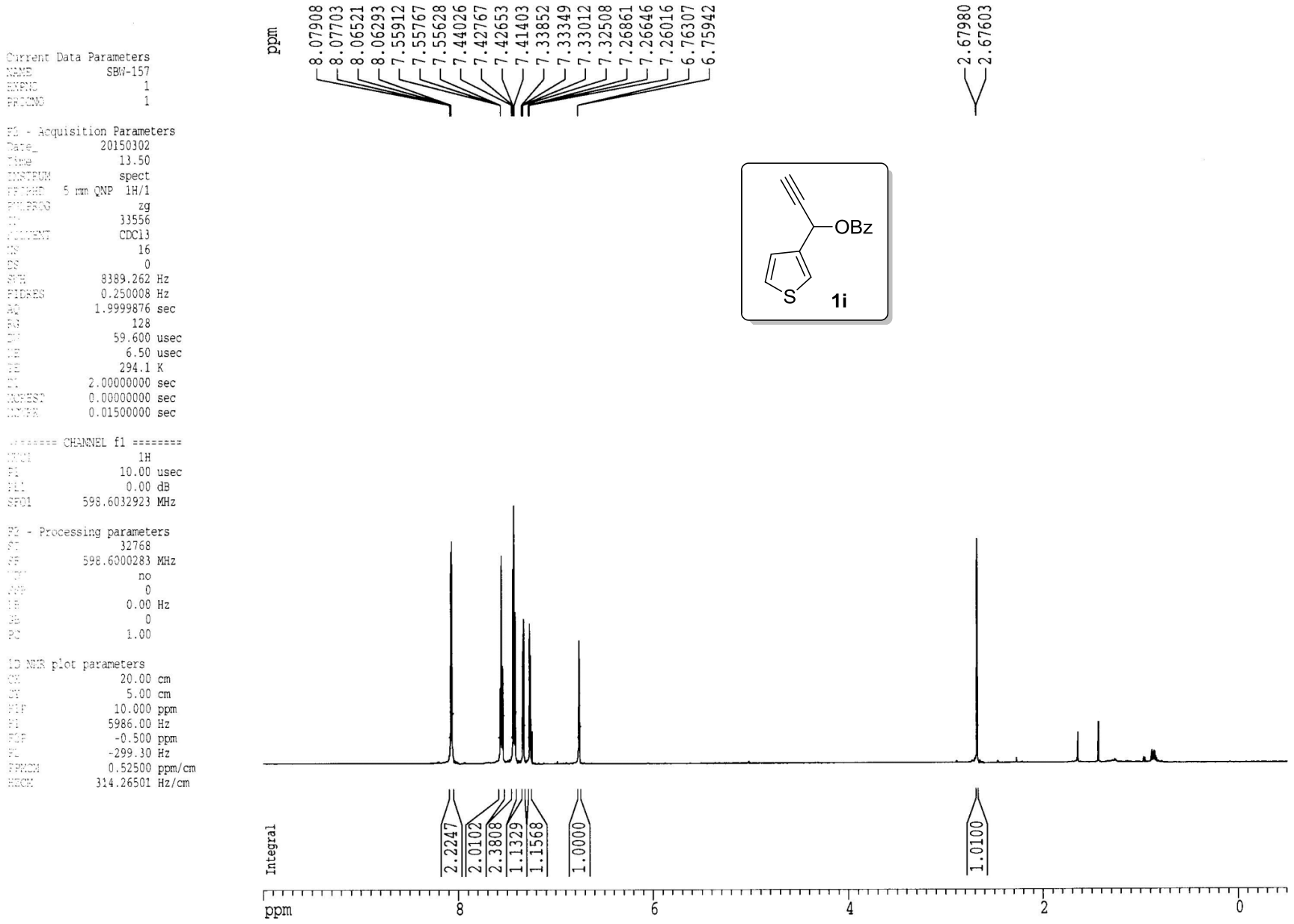




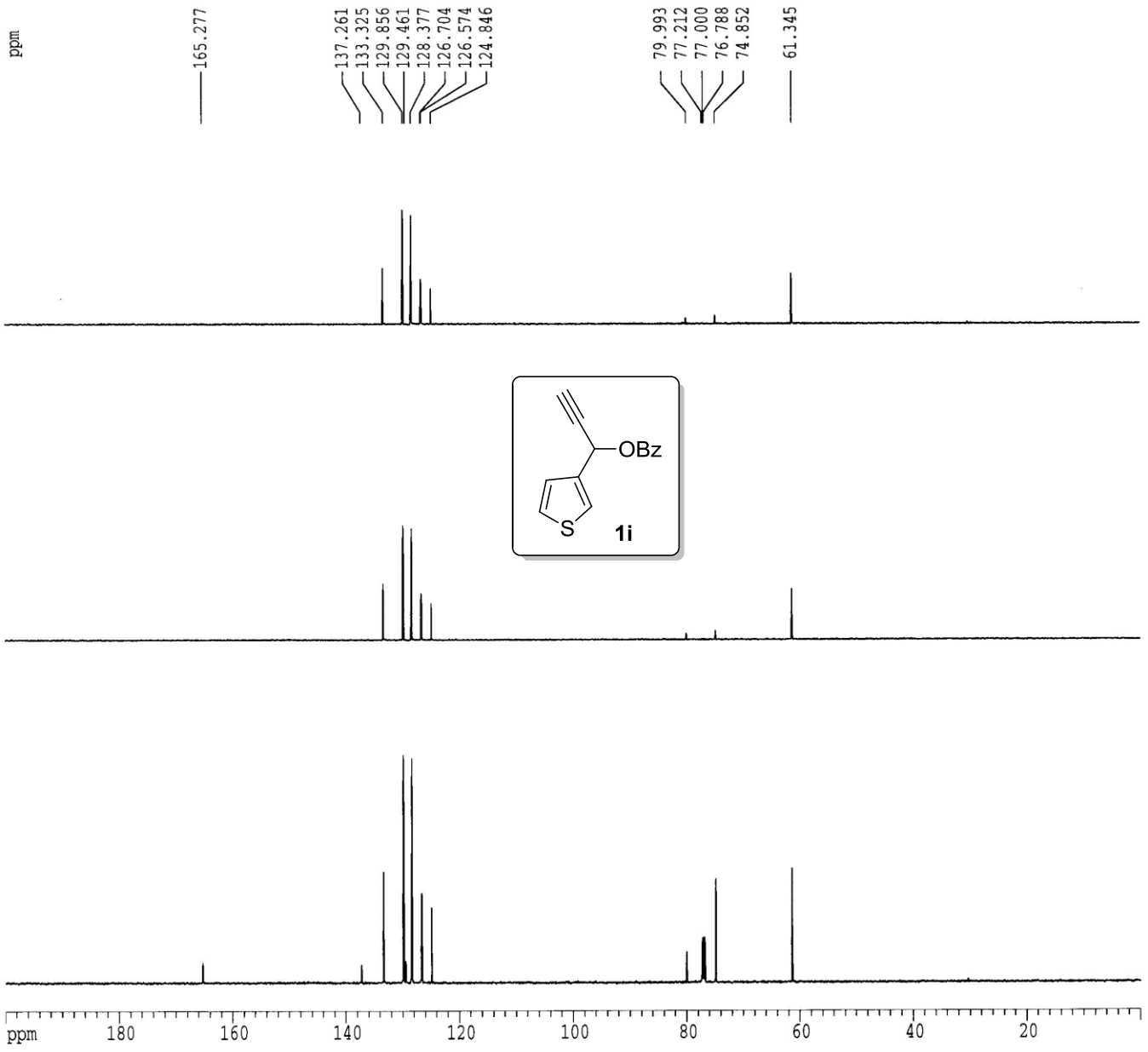
```
Current Data Parameters
NAME            SBW-162
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20150306
Time              8.33
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG             zg
TD                33556
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8389.262 Hz
FIDRES         0.250008 Hz
AQ           1.9999876 sec
RG                 128
DW              59.600 usec
DE               6.50 usec
TE              294.6 K
D1           2.00000000 sec
D11RELAY     0.00000000 sec
D11PW        0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                10.00 usec
PL1                0.00 dB
SFO1       598.6032923 MHz

F2 - Processing parameters
SI                 32768
SF         598.6000301 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  5.00 cm
F1P               10.000 ppm
F1                5986.00 Hz
F2P                -0.500 ppm
F2                -299.30 Hz
PPMCM             0.52500 ppm/cm
HZCM            314.26501 Hz/cm
```



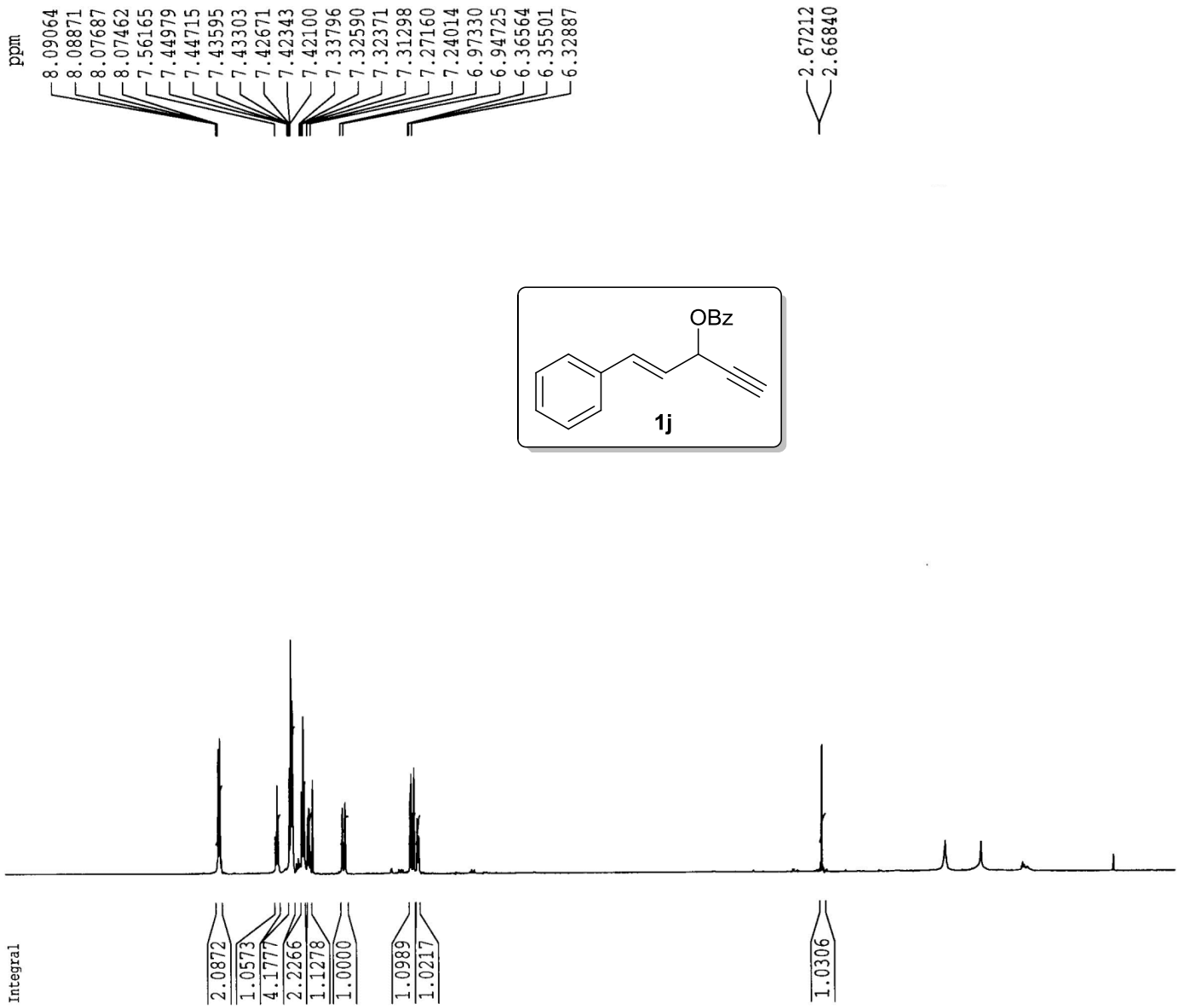

Current Data Parameters
NAME SBW-162
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150306
Time 8.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5181001 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
165.162
148.865
143.766
133.377
129.939
129.284
128.368
110.592
110.553
77.748
77.204
76.992
76.780
74.845
58.768
OBz
O
1h
ppm
180
160
140
120
100
80
60
40
20

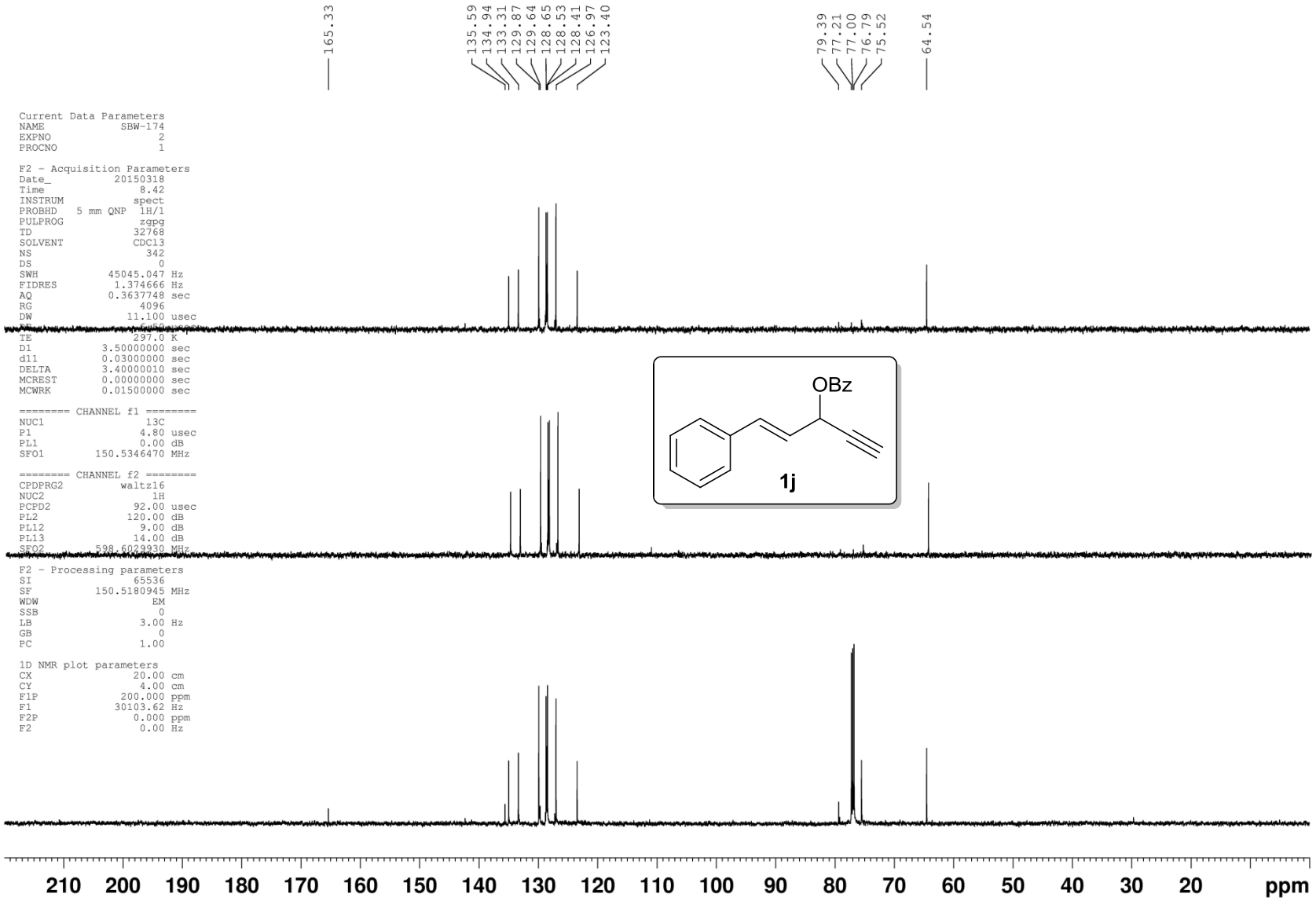

Current Data Parameters
NAME SBW-157
EXPNO 1
PROCNO 1
F1 - Acquisition Parameters
Date_ 20150302
Time 13.50
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
D13 0.00001500 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SF01 598.6032923 MHz
F2 - Processing parameters
SI 32768
SF 598.6000283 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.07908
8.07703
8.06521
8.06293
7.55912
7.55767
7.55628
7.44026
7.42767
7.42653
7.41403
7.33852
7.33349
7.33012
7.32508
7.26861
7.26646
7.26016
6.76307
6.75942
2.67980
2.67603
OBz
S
1i
Integral
2.2247
2.0102
2.3808
1.1329
1.1568
1.0000
1.0100
ppm
8
6
4
2
0

```
Current Data Parameters
NAME                  SBW-157
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150302
Time                  13.55
INSTRUM               spect
PROBHD   5 mm QNP  1H/1
PULPROG                zgpg
TD                    32768
SOLVENT               CDCl3
NS                      100
DS                        0
SWH               45045.047 Hz
FIDRES             1.374666 Hz
AQ                 0.3637748 sec
RG                     4096
DW                   11.100 usec
DE                    6.50 usec
TE                   295.4 K
D1                3.50000000 sec
d11               0.03000000 sec
DELTA             3.40000010 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                      4.80 usec
PL1                     0.00 dB
SFO1            150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                92.00 usec
PL2                 120.00 dB
PL12                  9.00 dB
PL13                 14.00 dB
SFO2            598.6029930 MHz

F2 - Processing parameters
SI                      65536
SF              150.5181042 MHz
WDW                        EM
SSB                         0
LB                       3.00 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                       4.00 cm
F1P                    200.000 ppm
F1                   30103.62 Hz
F2P                      0.000 ppm
F2                       0.00 Hz
PPMCM                10.00000 ppm/cm
HZCM              1505.18091 Hz/cm
```

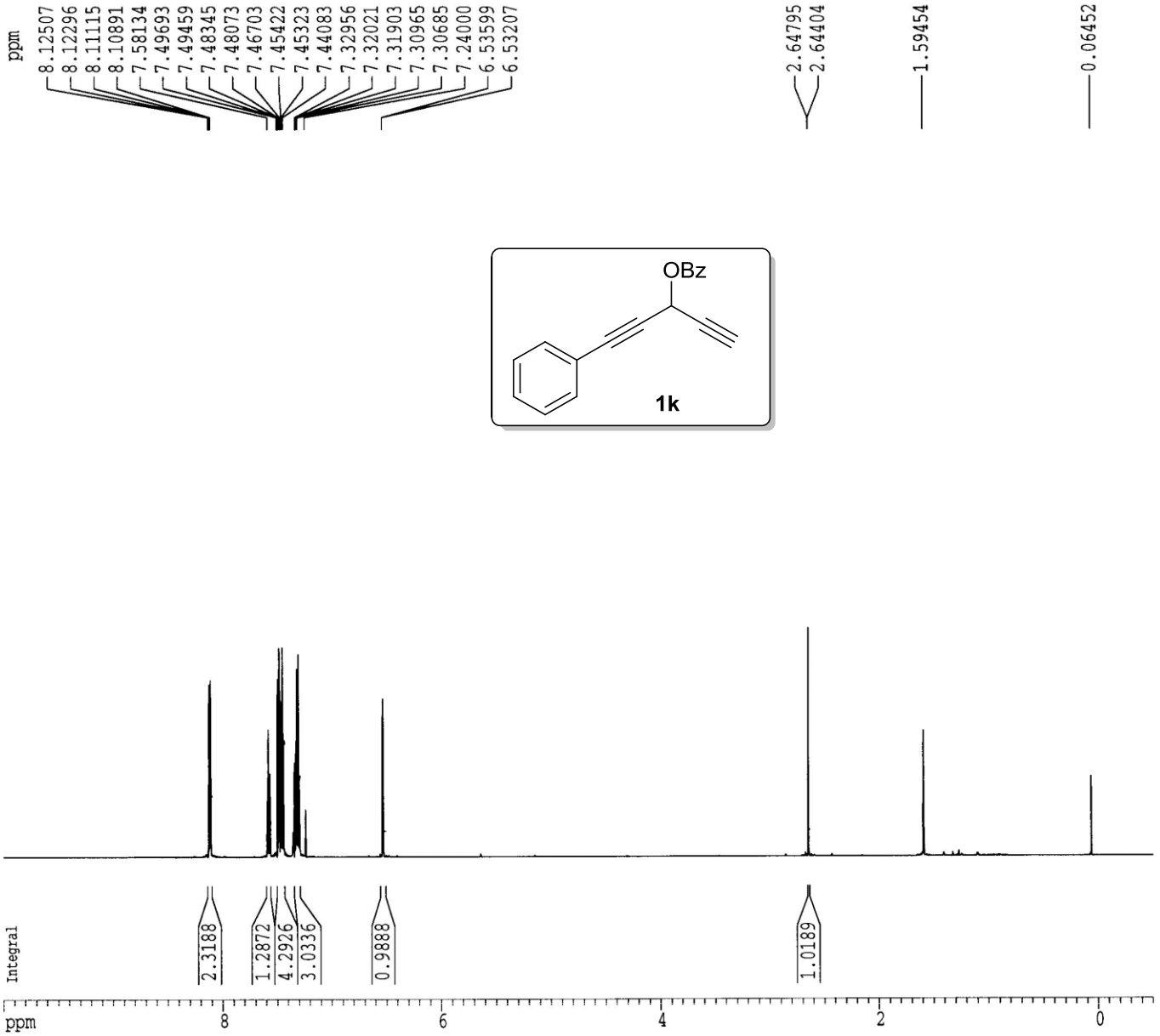


```
Current Data Parameters
NAME                  SBW-174
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_               20150318
Time                    8.32
INSTRUM                spect
PROBHD   5 mm QNP  1H/1
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                12019.230 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                       512
DW                    41.600 usec
DE                     6.50 usec
TE                    295.3 K
D1                1.50000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     10.00 usec
PL1                     0.00 dB
SFO1              598.6035916 MHz

F2 - Processing parameters
SI                     32768
SF                598.6000306 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                      4.00 cm
F1P                   10.000 ppm
F1                   5986.00 Hz
F2P                   -0.500 ppm
F2                   -299.30 Hz
PPMCM                0.52500 ppm/cm
HZCM                314.26501 Hz/cm
```




165.33
135.59
134.94
133.31
129.87
129.64
128.65
128.53
128.41
126.97
123.40
79.39
77.21
77.00
76.79
75.52
64.54
Current Data Parameters
NAME SBW-174
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150318
Time 8.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 342
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
TE 297.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180945 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
OBz
1j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

```
Current Data Parameters
NAME                  SBW-208
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150417
Time                   12.35
INSTRUM                spect
PROBHD   5 mm QNP  1H/1
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                8389.262 Hz
FIDRES                0.256020 Hz
AQ                 1.9530228 sec
RG                       128
DW                    59.600 usec
DE                     6.50 usec
TE                    296.7 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                      10.00 usec
PL1                      0.00 dB
SFO1               598.6029930 MHz

F2 - Processing parameters
SI                         32768
SF                 598.6000301 MHz
WDW                           no
SSB                            0
LB                          0.00 Hz
GB                             0
PC                          1.00

1D NMR plot parameters
CX                         20.00 cm
CY                          4.00 cm
F1P                       10.000 ppm
F1                       5986.00 Hz
F2P                       -0.500 ppm
F2                       -299.30 Hz
PPMCM                    0.52500 ppm/cm
HZCM                   314.26501 Hz/cm
```



Current Data Parameters
NAME SBW-208
EXPNO 2
PROCNO 1

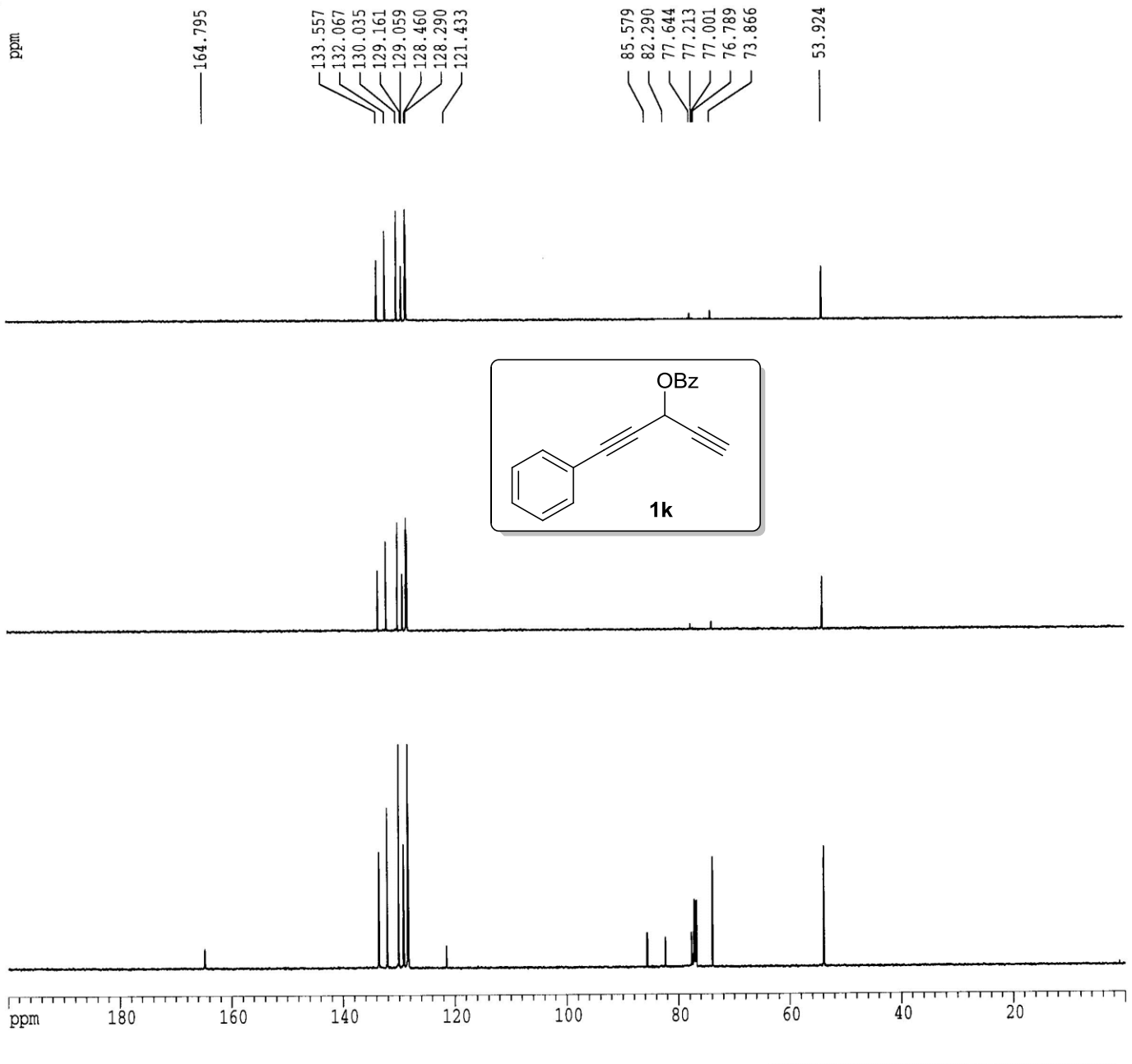
F2 - Acquisition Parameters
Date_ 20150417
Time 12.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

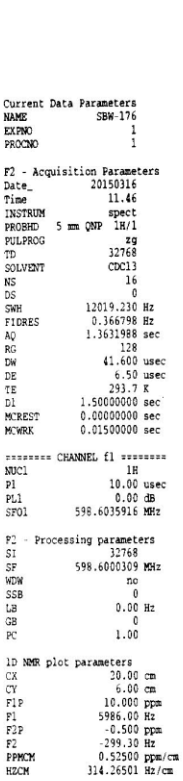
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

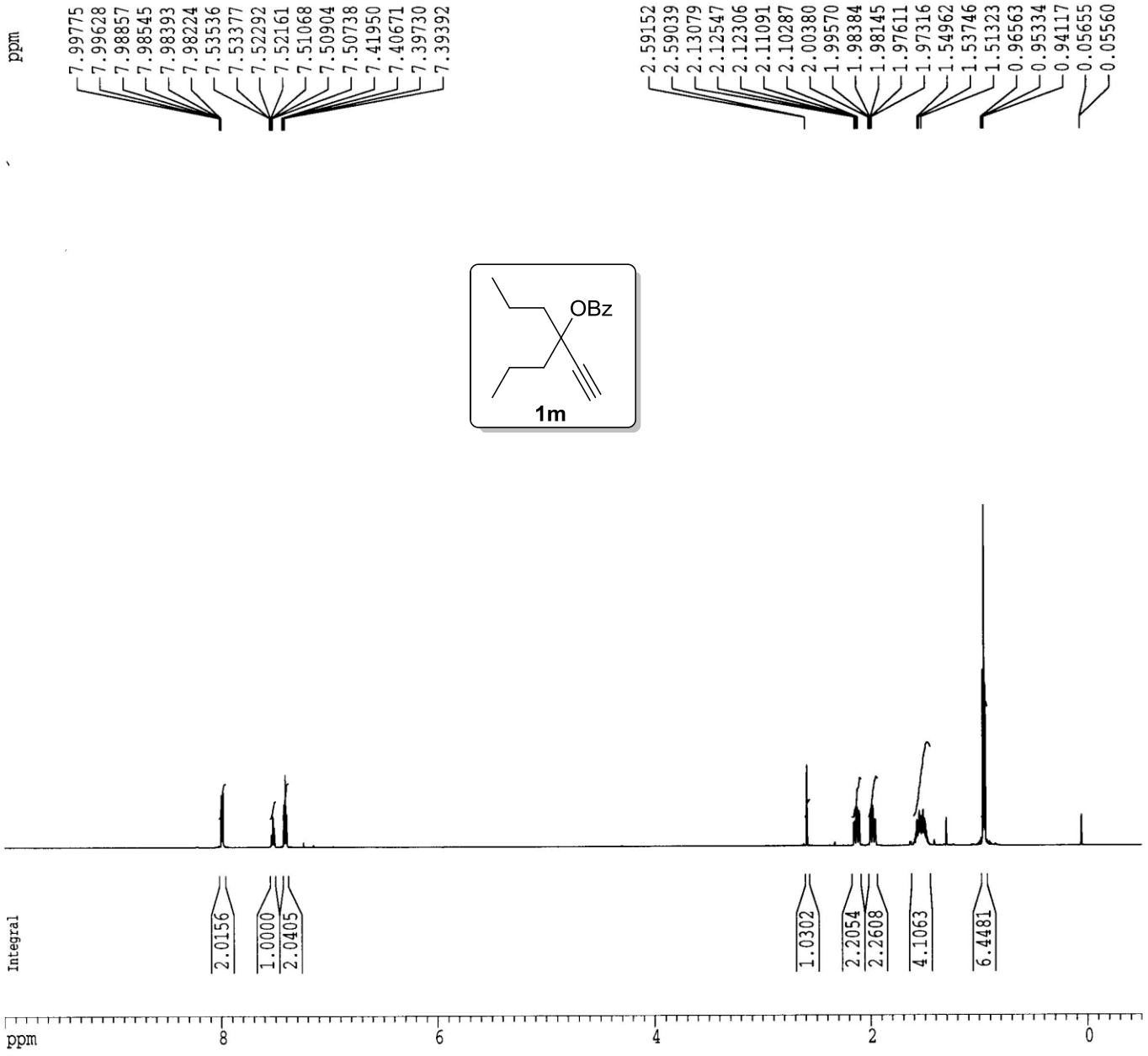
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

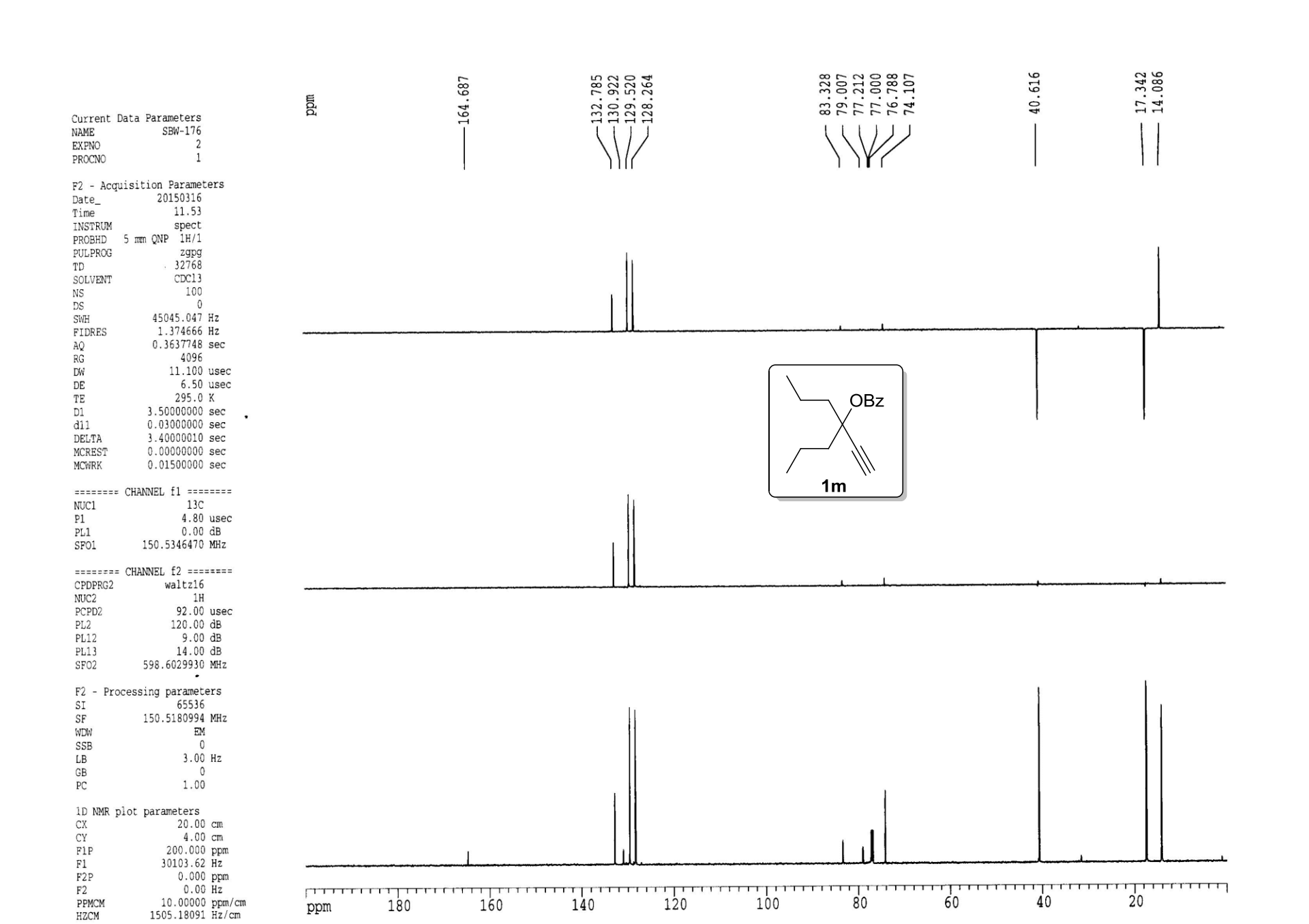
F2 - Processing parameters
SI 65536
SF 150.5180980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm

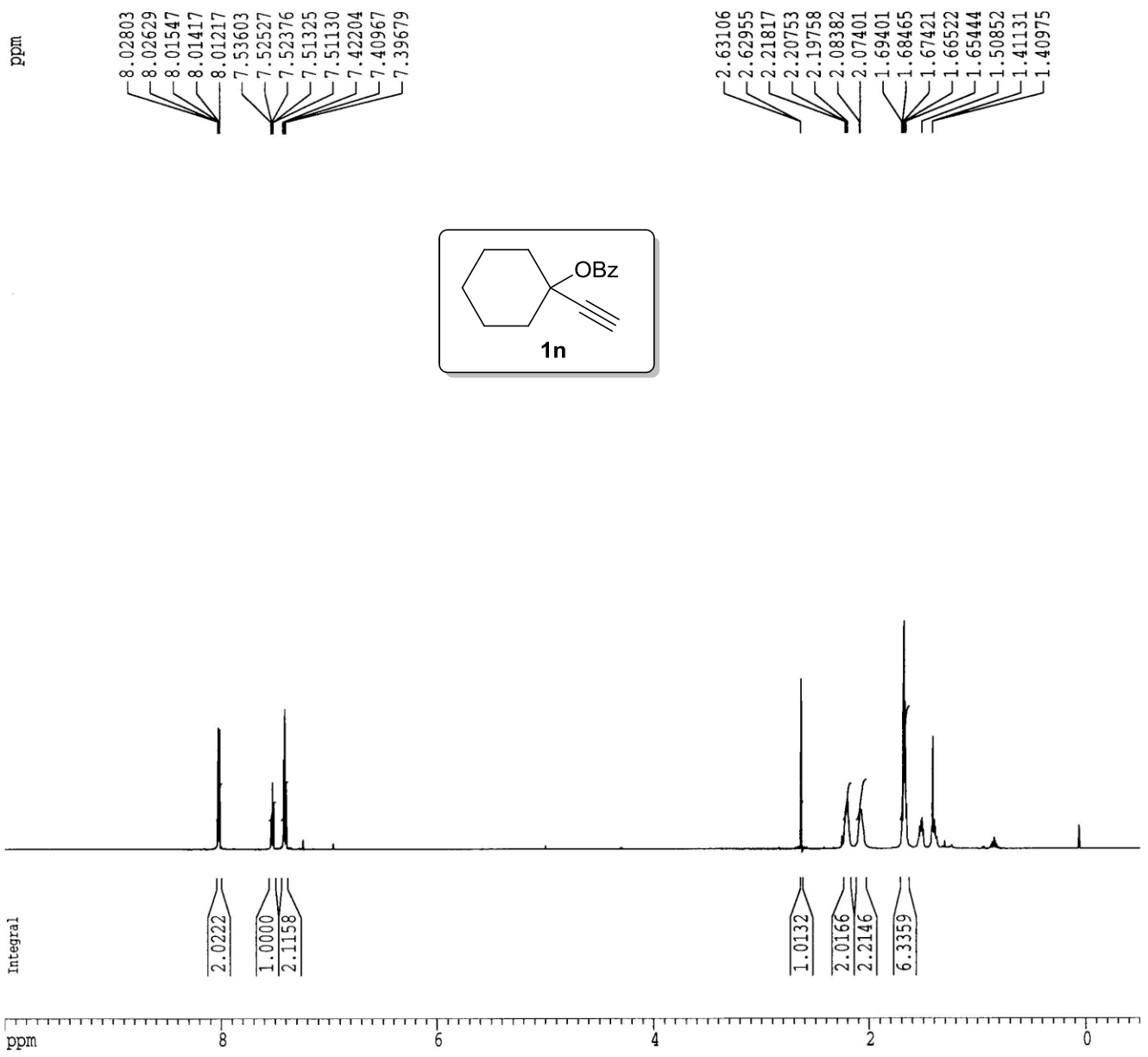


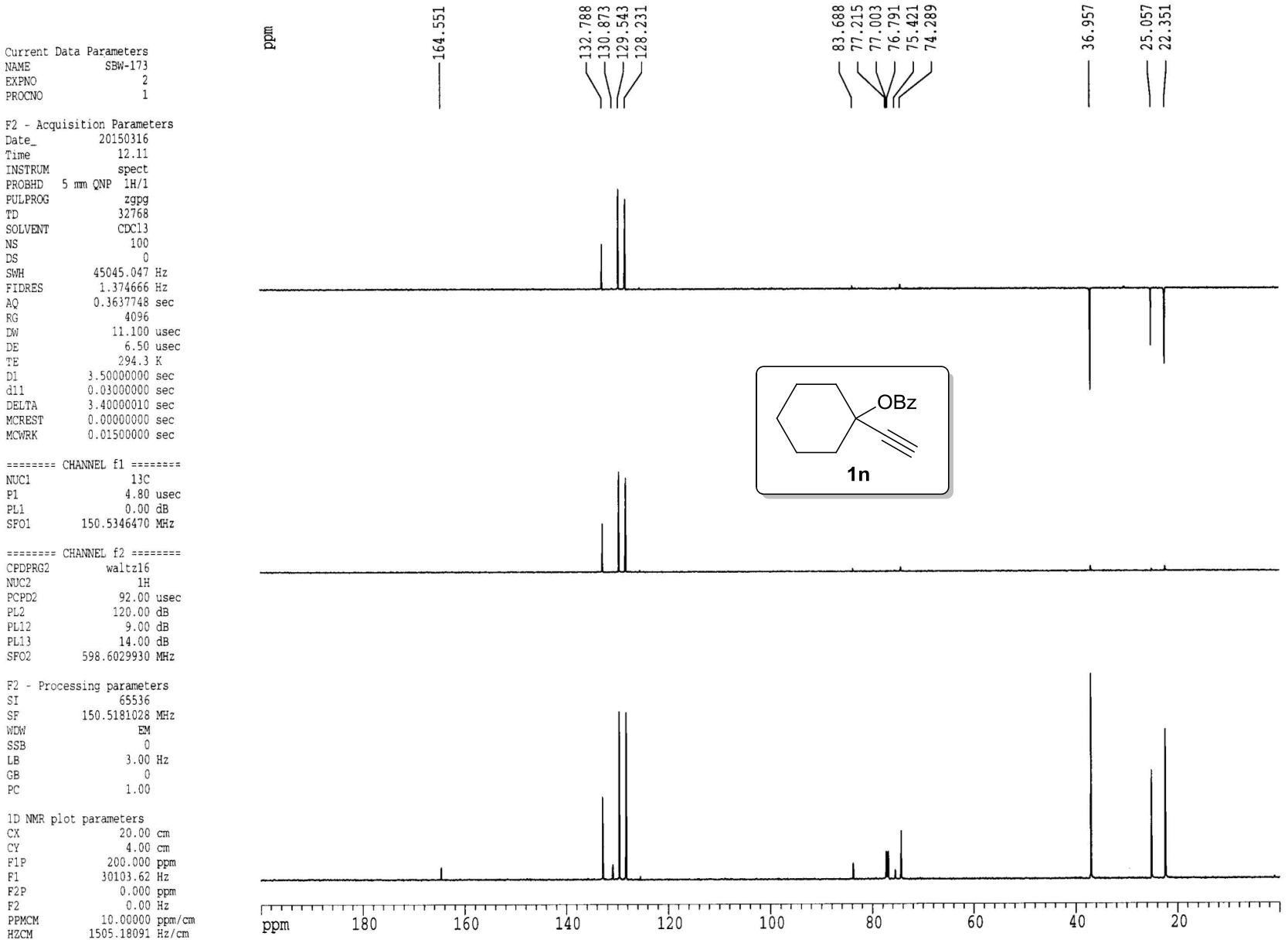

Current Data Parameters
NAME SBW-176
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150316
Time 11.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 293.7 K
D1 1.50000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000309 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm


ppm
7.99775
7.99628
7.98857
7.98545
7.98393
7.98224
7.53536
7.53377
7.52292
7.52161
7.51068
7.50904
7.50738
7.41950
7.40671
7.39730
7.39392
2.59152
2.59039
2.13079
2.12547
2.12306
2.11091
2.10287
2.00380
1.99570
1.98384
1.98145
1.97611
1.97316
1.54962
1.53746
1.51323
0.96563
0.95334
0.94117
0.05655
0.05560
OBz
1m
Integral
2.0156
1.0000
2.0405
1.0302
2.2054
2.2608
4.1063
6.4481
ppm
8
6
4
2
0


Current Data Parameters
NAME SBW-176
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150316
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180994 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
164.687
132.785
130.922
129.520
128.264
83.328
79.007
77.212
77.000
76.788
74.107
40.616
17.342
14.086
OBz
1m
ppm
180
160
140
120
100
80
60
40
20

```
Current Data Parameters
NAME              SBW-173
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150316
Time                12.11
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             12019.230 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                     128
DW                 41.600 usec
DE                  6.50 usec
TE                 294.0 K
D1              1.50000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
PL1                  0.00 dB
SFO1          598.6035916 MHz

F2 - Processing parameters
SI                  32768
SF            598.6000302 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   4.00 cm
F1P                10.000 ppm
F1                 5986.00 Hz
F2P                -0.500 ppm
F2                 -299.30 Hz
PPMCM              0.52500 ppm/cm
HZCM             314.26501 Hz/cm
```





Current Data Parameters
NAME SBW-173
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150316
Time 12.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 294.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

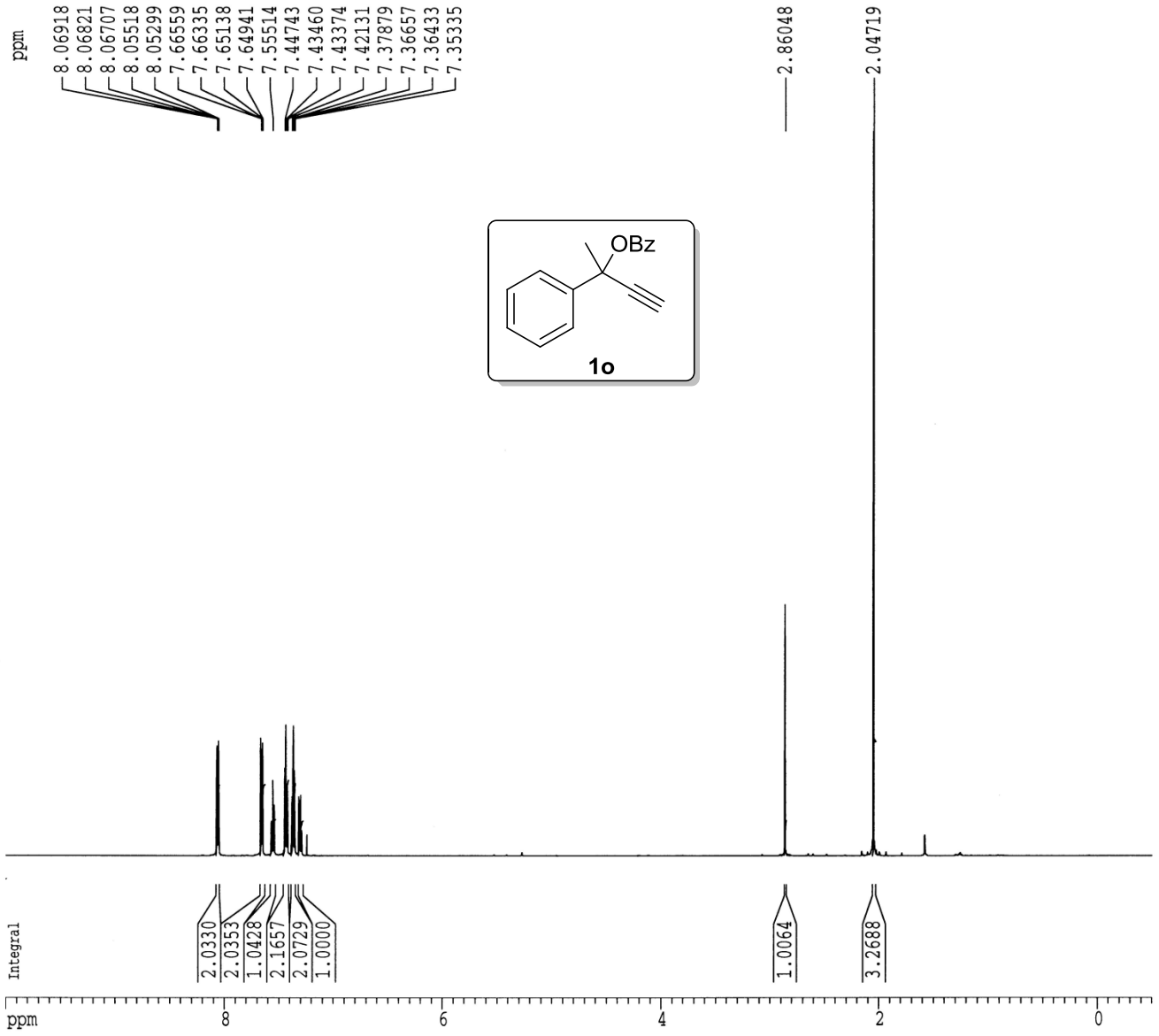
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

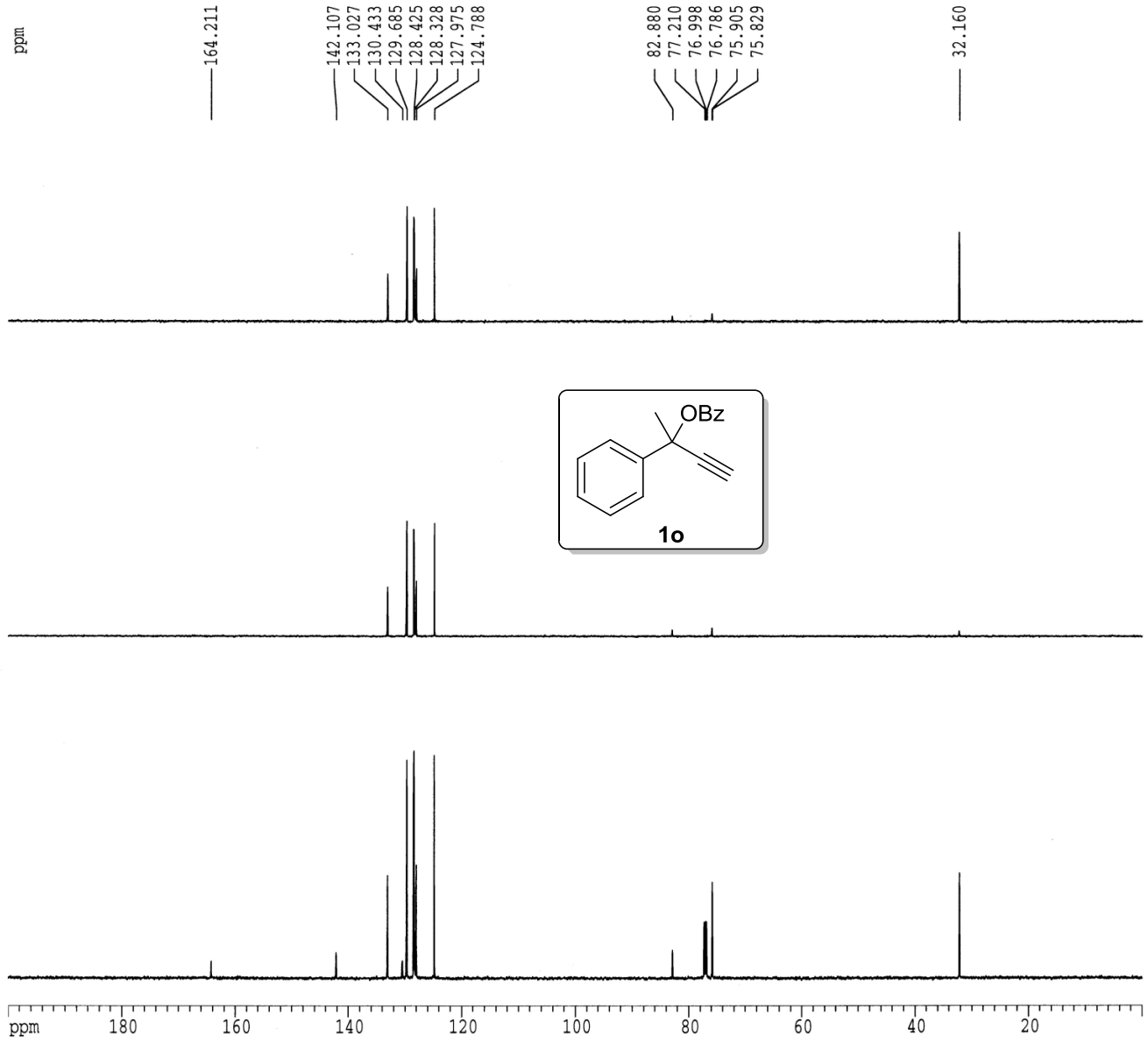
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

F2 - Processing parameters
SI 65536
SF 150.5181028 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm

```
Current Data Parameters
NAME                  SBW-198
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150414
Time                    8.59
INSTRUM                spect
PROBHD    5 mm QNP  1H/1
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                 8389.262 Hz
FIDRES              0.256020 Hz
AQ                  1.9530228 sec
RG                       128
DW                    59.600 usec
DE                     6.50 usec
TE                    294.4 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                     10.00 usec
PL1                     0.00 dB
SFO1            598.6029930 MHz

F2 - Processing parameters
SI                     32768
SF                598.6000299 MHz
WDW                       no
SSB                        0
LB                      0.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                     15.00 cm
F1P                   10.000 ppm
F1                   5986.00 Hz
F2P                   -0.500 ppm
F2                   -299.30 Hz
PPMCM                0.52500 ppm/cm
HZCM               314.26501 Hz/cm
```





Current Data Parameters
NAME SBW-198
EXPNO 2
PROCNO 1

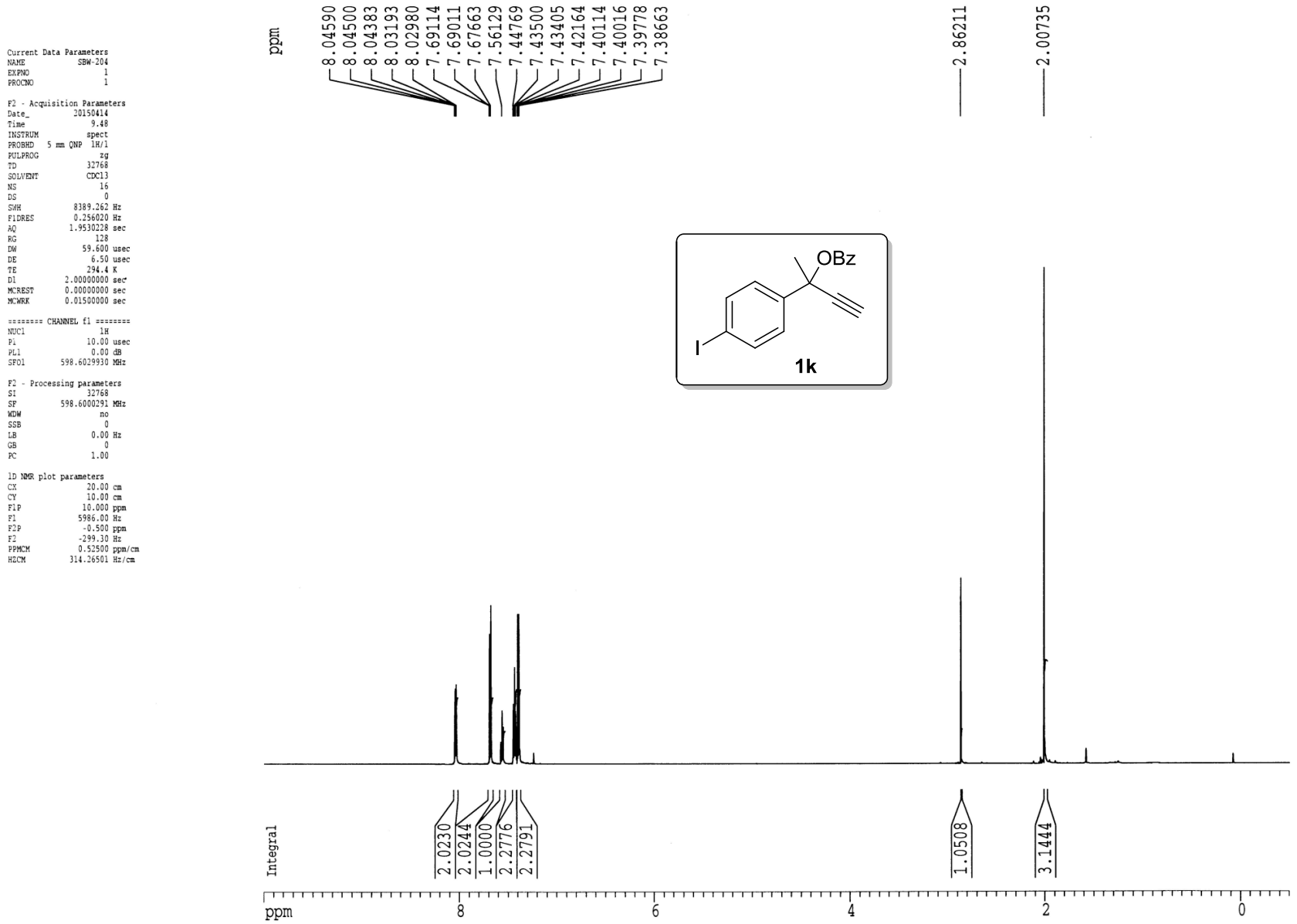
F2 - Acquisition Parameters
Date_ 20150414
Time 9.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

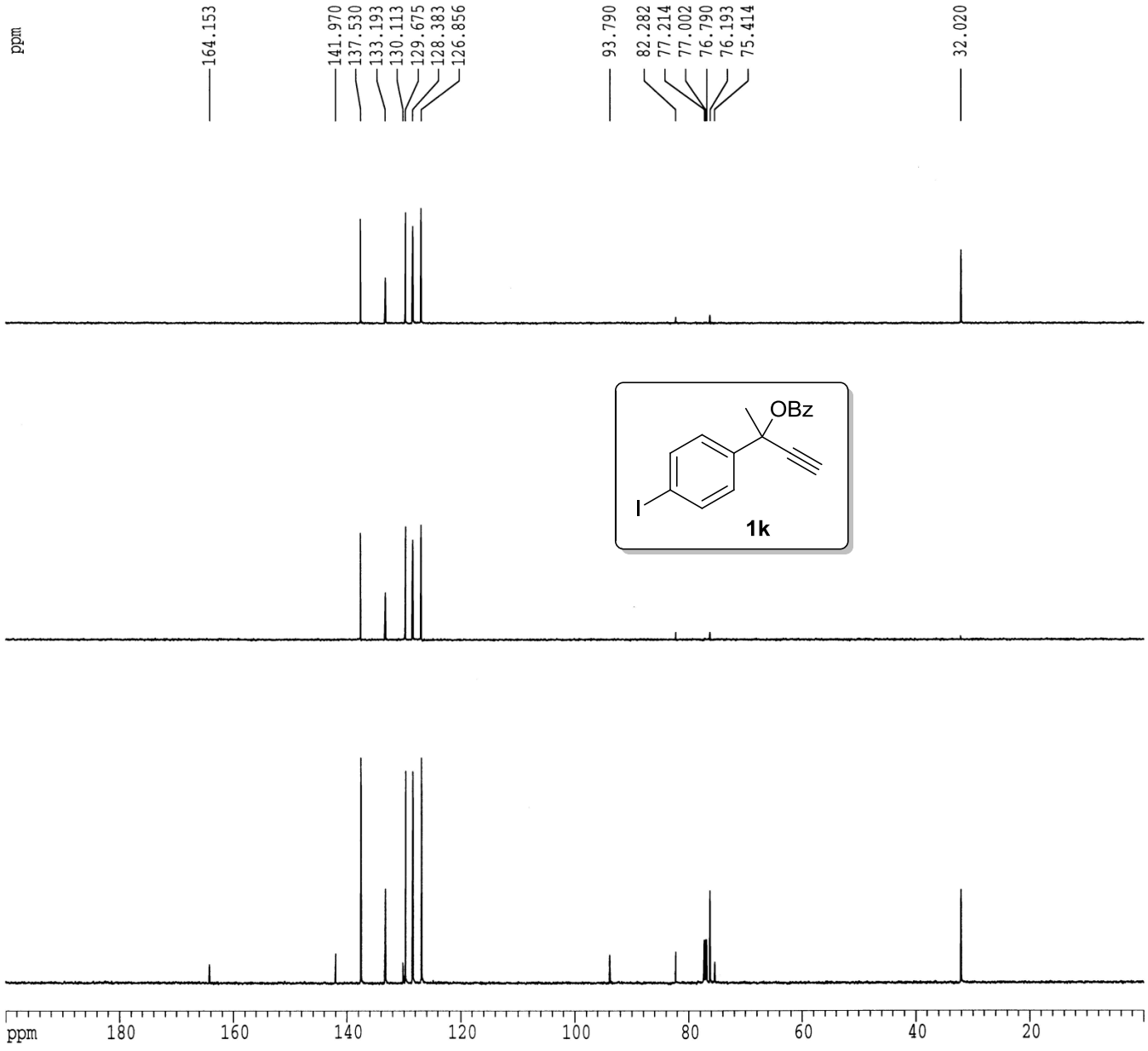
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

F2 - Processing parameters
SI 65536
SF 150.5181014 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm


Current Data Parameters
NAME SBW-204
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150414
Time 9.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 294.4 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000291 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.04590
8.04500
8.04383
8.03193
8.02980
7.69114
7.69011
7.67663
7.56129
7.44769
7.43500
7.43405
7.42164
7.40114
7.40016
7.39778
7.38663
2.86211
2.00735
OBz
I
1k
Integral
2.0230
2.0244
1.0000
2.2776
2.2791
1.0508
3.1444
ppm
8
6
4
2
0



Current Data Parameters
NAME SBW-204
EXPNO 2
PROCNO 1

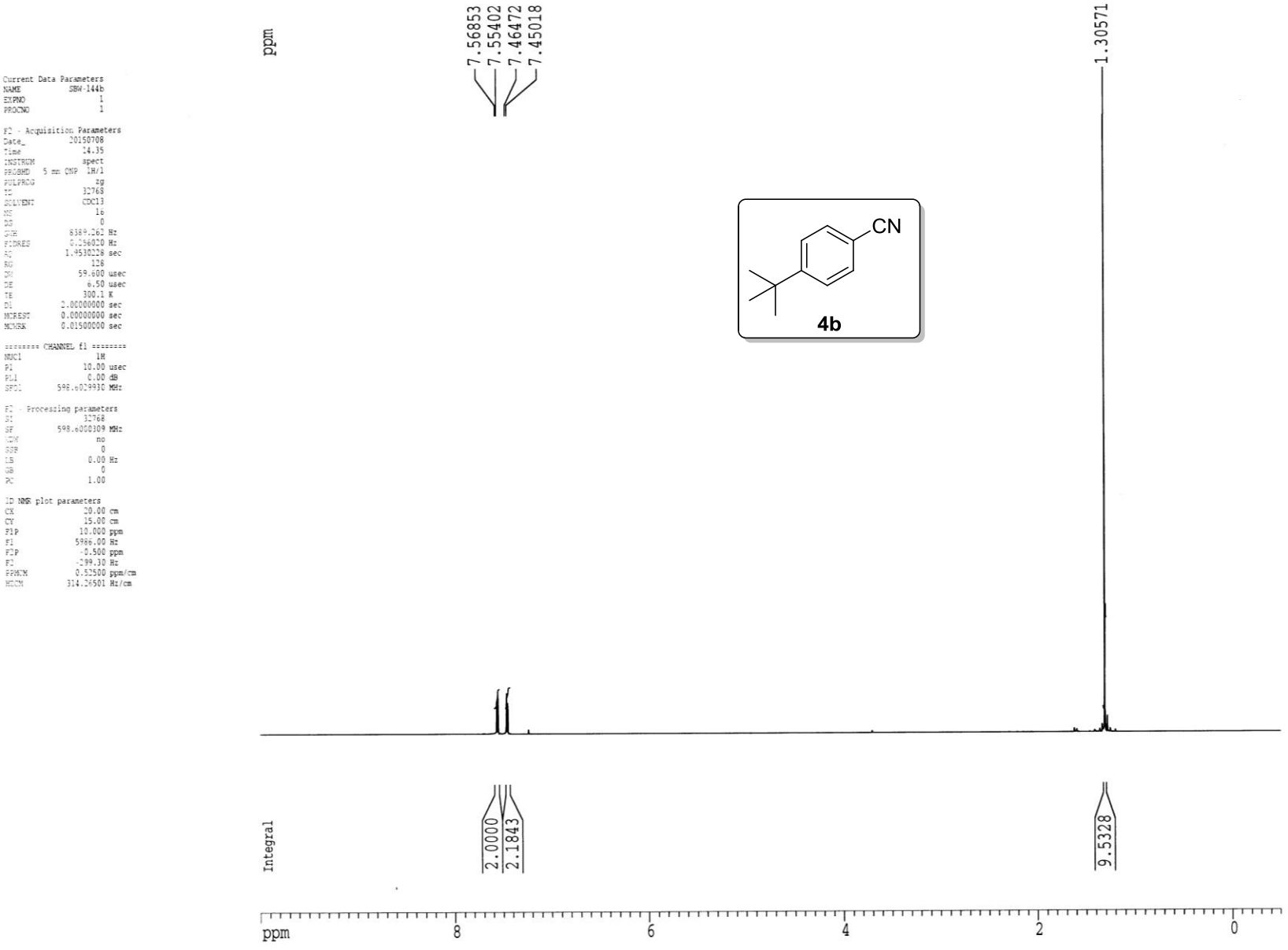
F2 - Acquisition Parameters
Date_ 20150414
Time 9.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

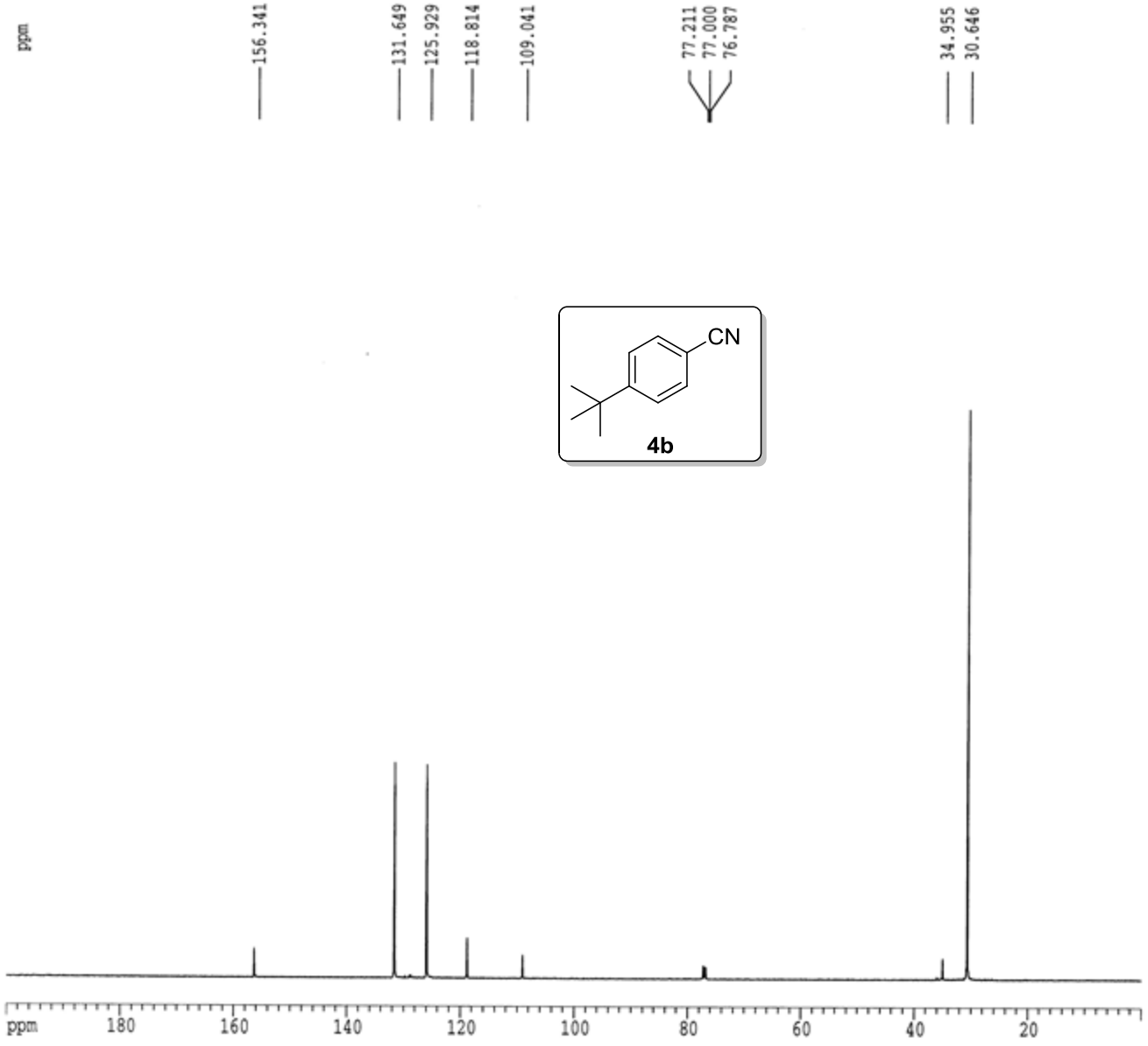
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

F2 - Processing parameters
SI 65536
SF 150.5181028 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

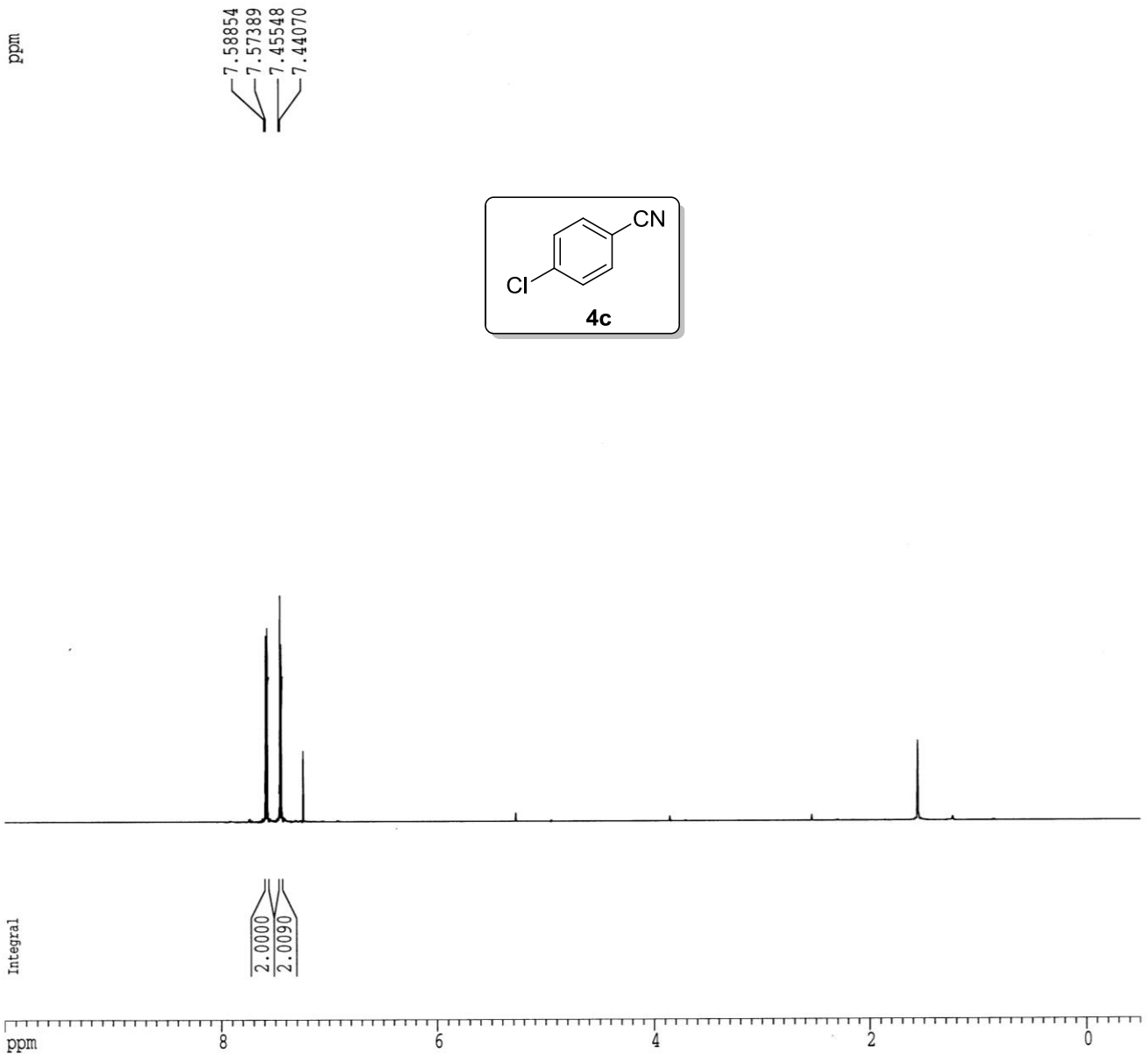
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm

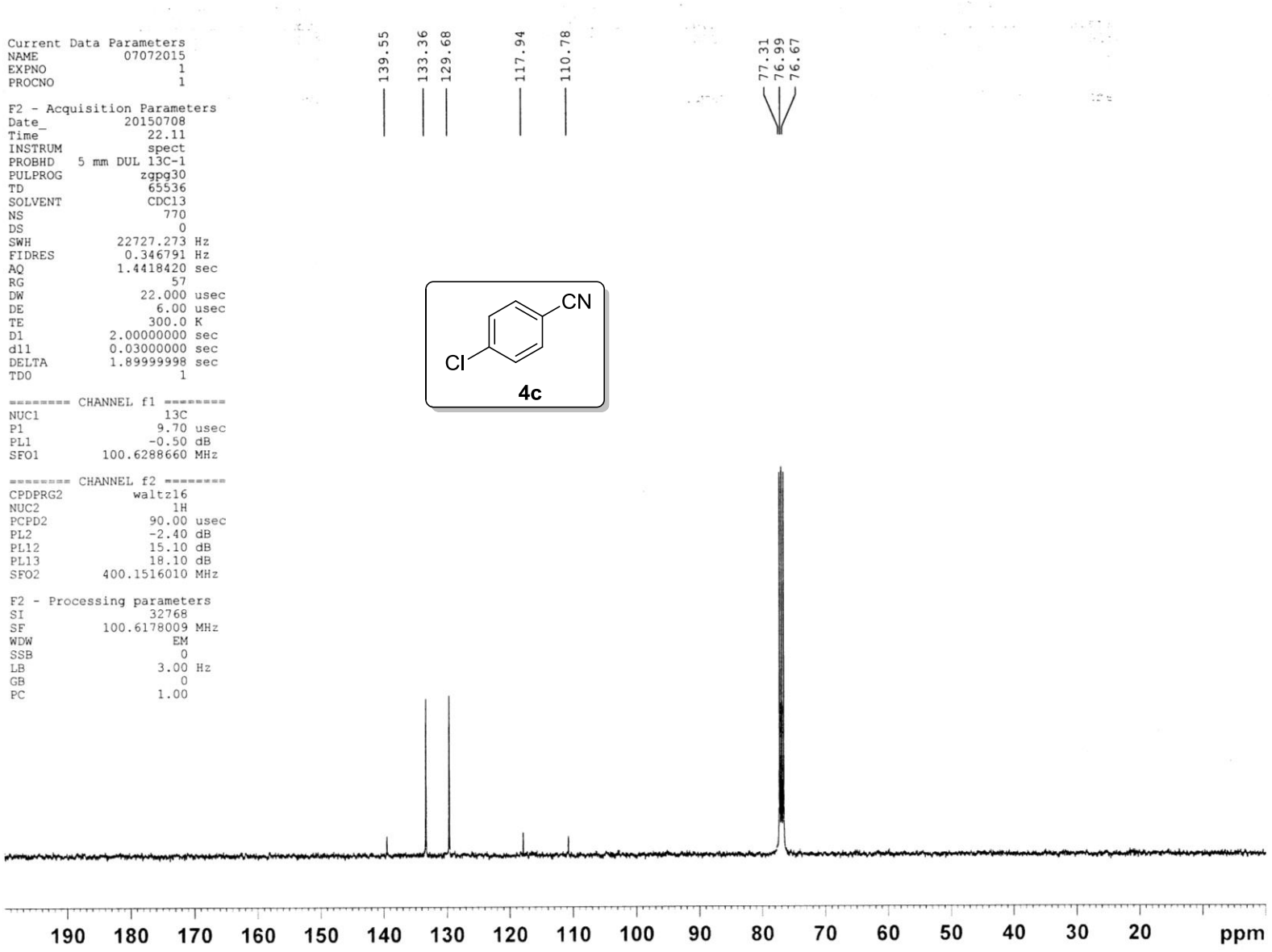

Current Data Parameters
NAME SBW-144b
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150708
Time 14.35
INSTRUM spect
PROBHD 5 mm CNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000309 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
7.56853
7.55402
7.46472
7.45018
1.30571
CN
4b
Integral
2.0000
2.1843
9.5328
ppm
8
6
4
2
0

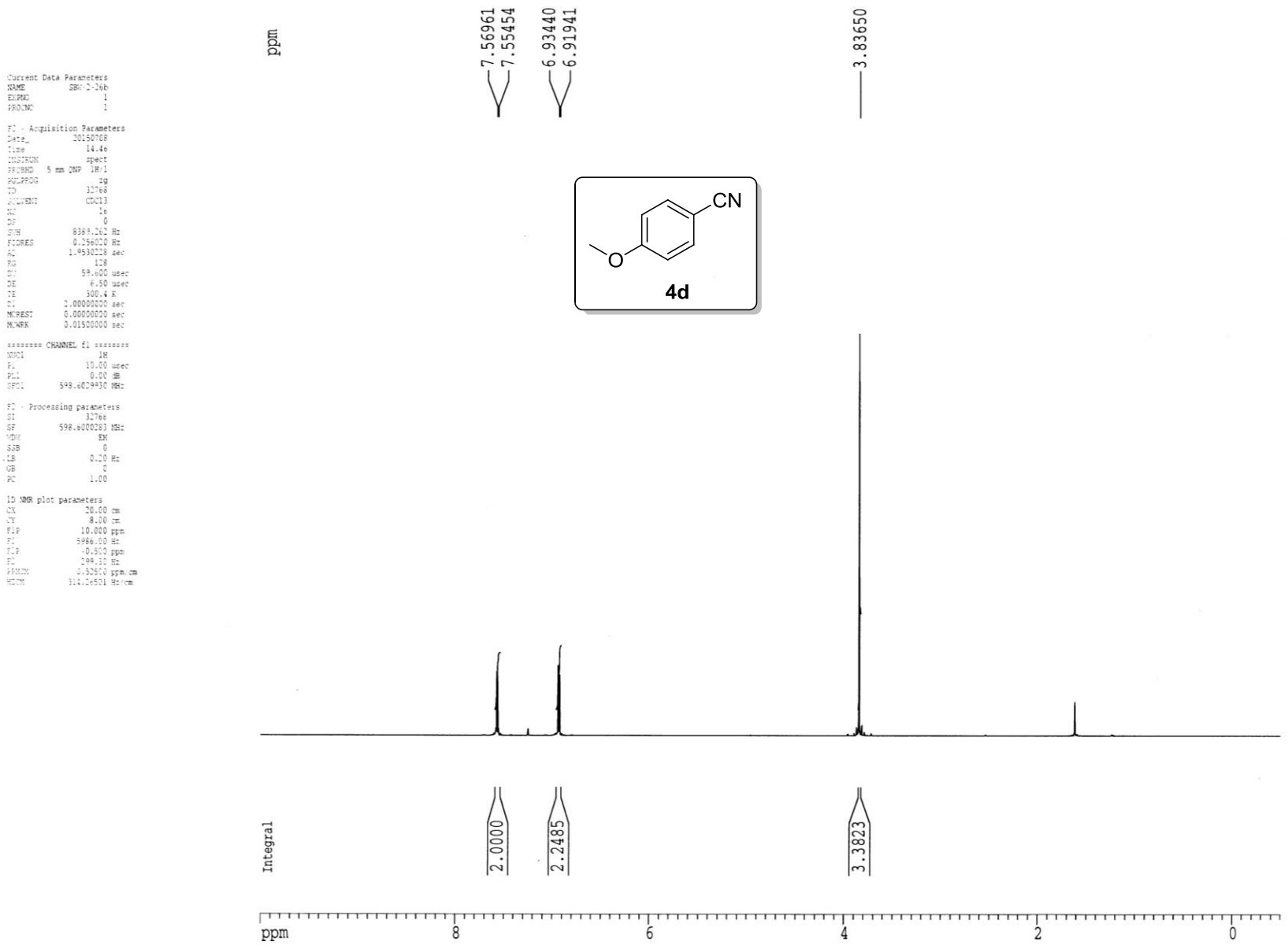
```
Current Data Parameters
NAME                  SBM-145
EXPNO                       2
PROCNO                      1

F2 - Acquisition Parameters
Date_              20150203
Time                  14.58
INSTRUM                spect
PROBHD    5 mm QNP  1H/1
PULPROG                zgpg
TD                    32768
SOLVENT               CDCl3
NS                       73
DS                        0
SWH               45045.047 Hz
FIDRES             1.374666 Hz
AQ                0.3637748 sec
RG                     2048
DW                   11.100 usec
DE                    6.50 usec
TE                   295.0 K
D1              3.50000000 sec
d11             0.03000000 sec
DELTA           3.40000010 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                     4.80 usec
PL1                    0.00 dB
SFO1            150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                92.00 usec
PL2                 120.00 dB
PL12                 9.00 dB
PL13                14.00 dB
SFO2            598.6029940 MHz

F2 - Processing parameters
SI                     65536
SP              150.5181317 MHz
WDW                       EM
SSB                        0
LB                      5.00 Hz
GB                         0
PC                      0.50

1D NMR plot parameters
CX                     20.00 cm
CY                     10.00 cm
F1P                   200.000 ppm
F1                  30103.62 Hz
F2P                    0.000 ppm
F2                     0.00 Hz
PPMCM                10.00000 ppm/cm
HZCM              1505.18127 Hz/cm
```



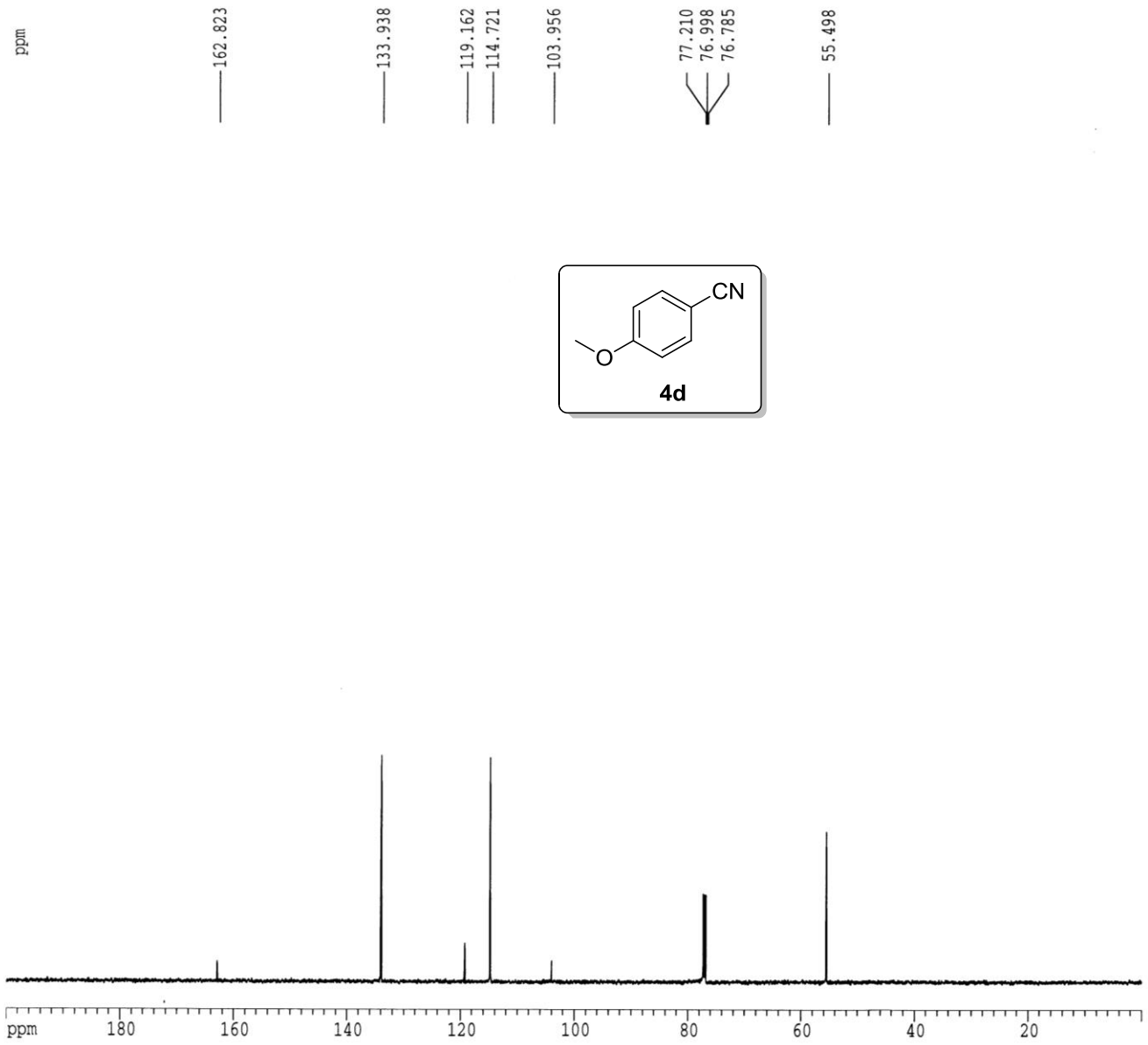
```
Current Data Parameters
NAME                  SBW-2-27
EXPNO                        1
PROCNO       .               1

F2 - Acquisition Parameters
Date_              20150708
Time                   20.04
INSTRUM                spect
PROBHD   5 mm QNP  1H/1
PULPROG                   zg
TD                     32768
SOLVENT                CDCl3
NS                        16
DS                         0
SWH                8389.262 Hz
FIDRES                0.256020 Hz
AQ                 1.9530228 sec
RG                       128
DW                    59.600 usec
DE                     6.50 usec
TE                    300.7 K
D1                 2.00000000 sec
MCREST             0.00000000 sec
MCWRK              0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
PL1                    0.00 dB
SFO1            598.6029930 MHz

F2 - Processing parameters
SI                     32768
SF              598.6000306 MHz
WDW                       no
SSB                        0
LB                     0.00 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                    20.00 cm
CY                     4.00 cm
F1P                  10.000 ppm
F1                  5986.00 Hz
F2P                  -0.500 ppm
F2                  -299.30 Hz
PPMCM                0.52500 ppm/cm
HZCM               314.26501 Hz/cm
```

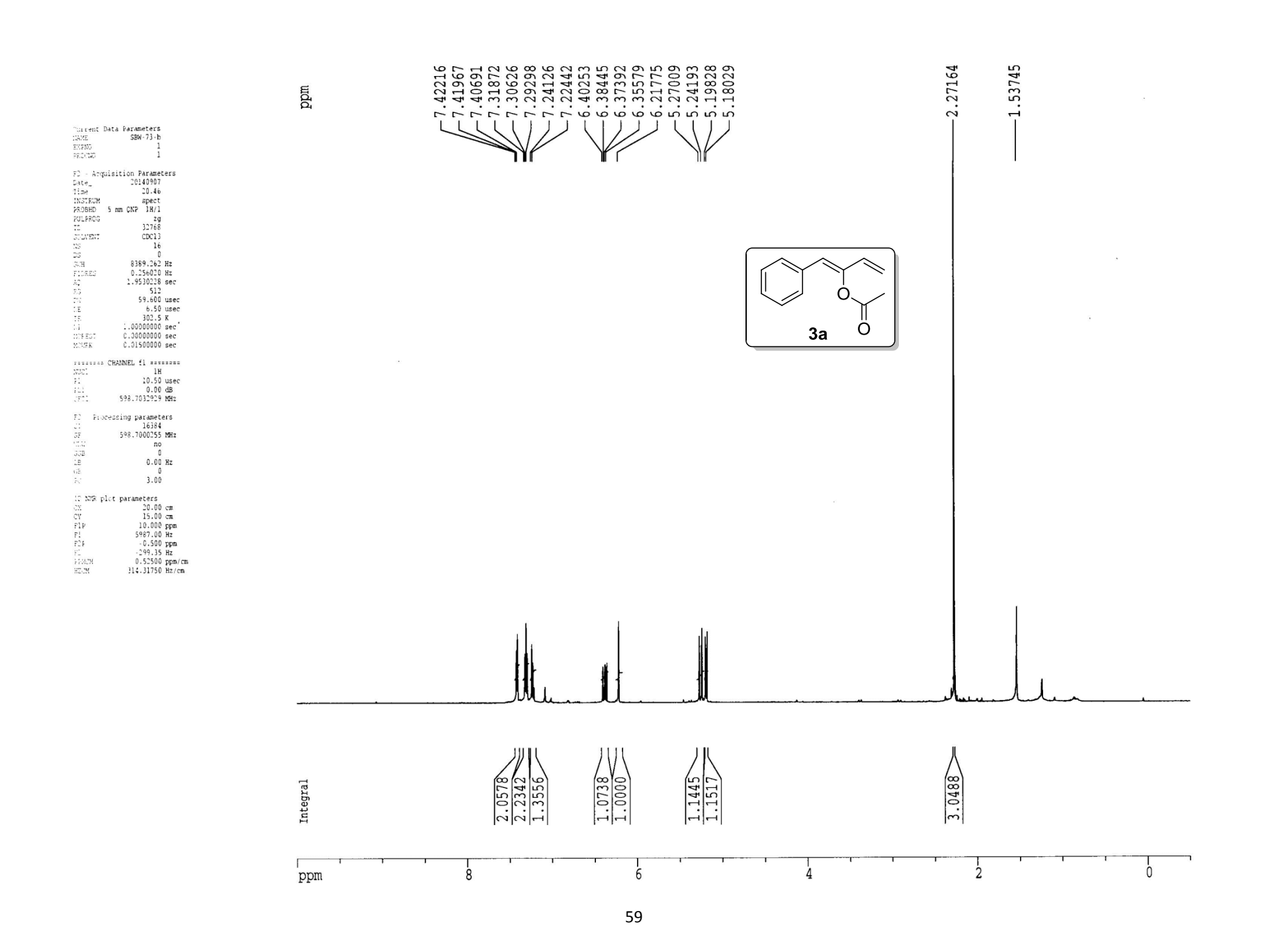


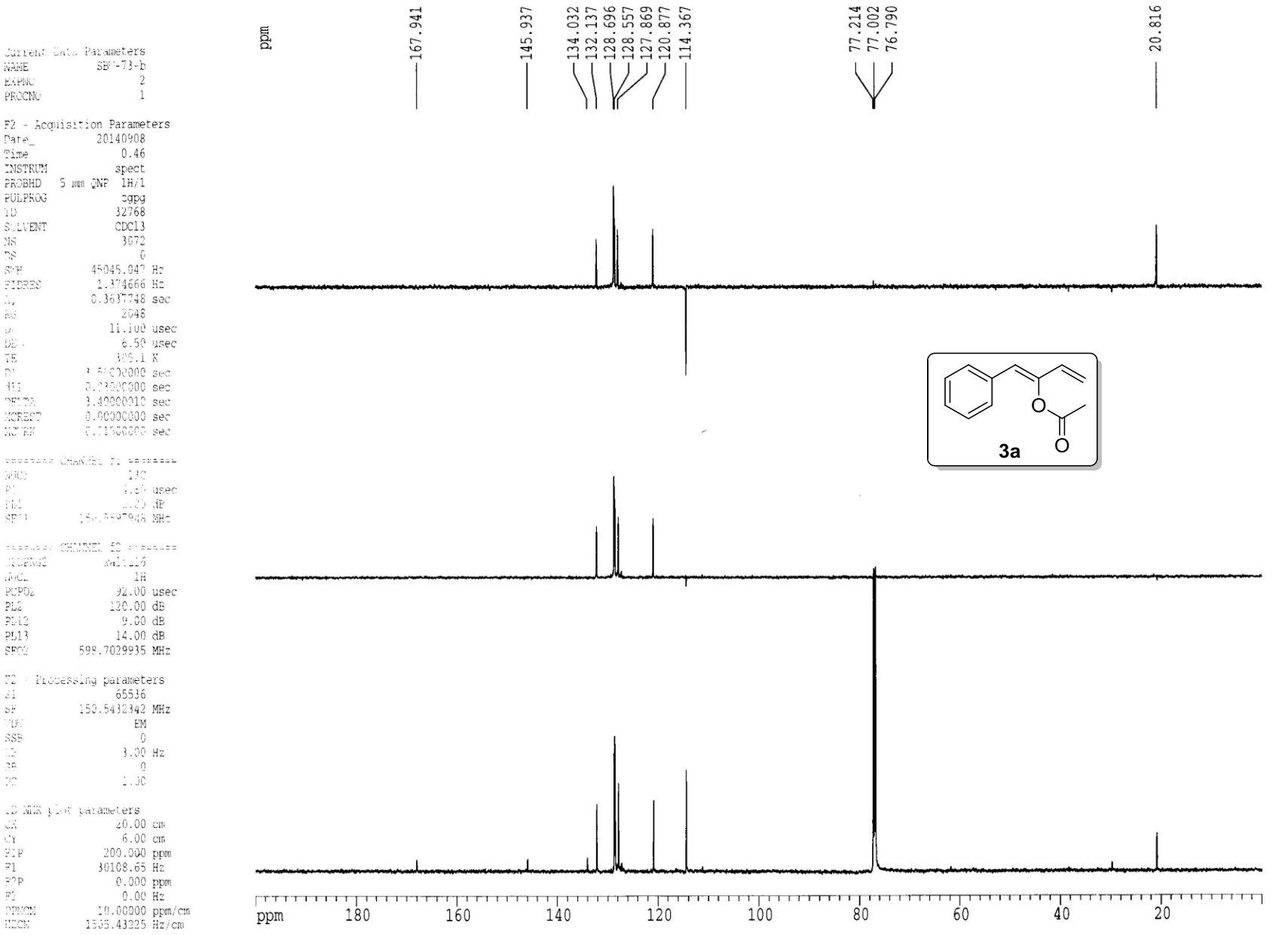

Current Data Parameters
NAME 07072015
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150708
Time 22.11
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 770
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178009 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
139.55
133.36
129.68
117.94
110.78
77.31
76.99
76.67
CN
Cl
4c
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

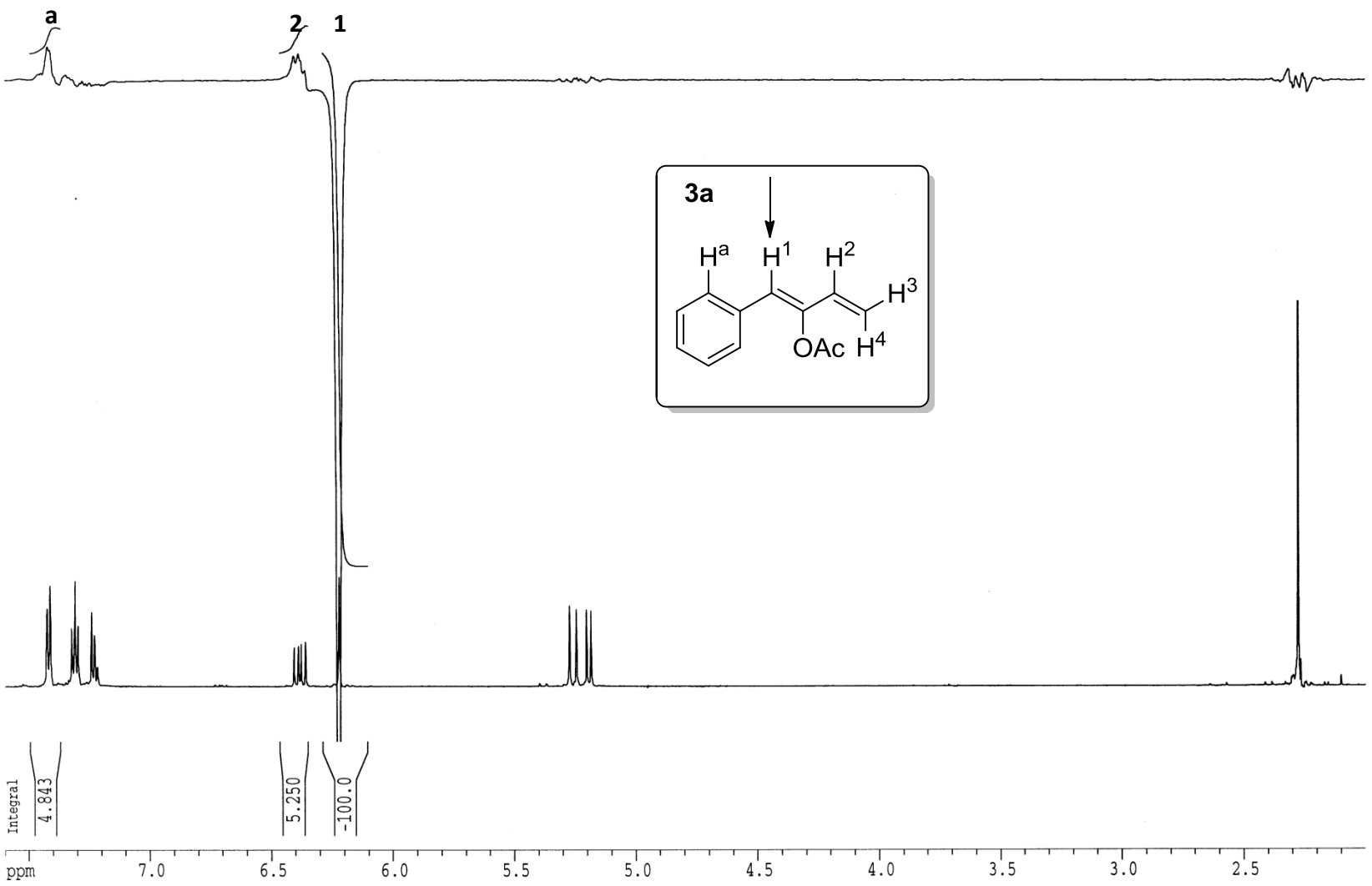

Current Data Parameters
NAME SBW-2-26b
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150708
Time 14.4e
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 1e
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000283 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.10 Hz
PPMCM 0.52670 ppm/cm
HZCM 315.2e501 Hz/cm
ppm
7.56961
7.55454
6.93440
6.91941
3.83650
CN
O
4d
Integral
2.0000
2.2485
3.3823
ppm
8
6
4
2
0

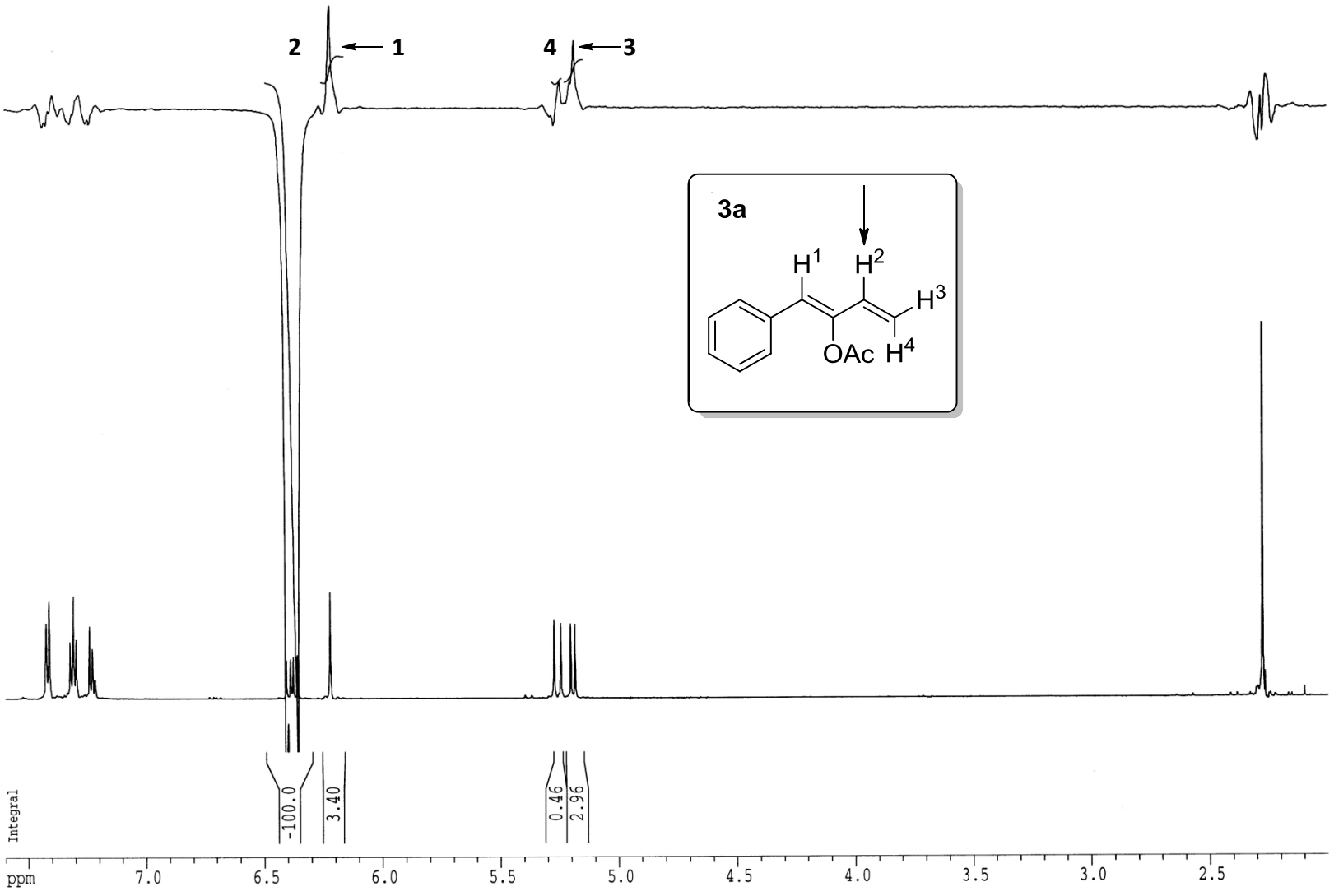
```
Current Data Parameters
NAME          SBY-2-26b
EXPNO                 2
PROCNO                1

F1 - Acquisition Parameters
Date_          20150708
Time              14.55
INSTRUM           spect
PROBHD   5 mm QNP 1H/1
PULPROG           zgpg
TD                65536
SOLVENT           CDCl3
NS                  126
DS                    0
SWH           45045.047 Hz
FIDRES        1.374666 Hz
AQ            0.3637748 sec
RG                 2048
DW               11.100 usec
DE                6.50 usec
TE               301.3 K
D1           3.50000000 sec
D11          0.03000000 sec
DELTA        3.40000010 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1               13C
P1                4.80 usec
PL1               0.00 dB
SFO1        150.5331418 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2            92.00 usec
PL2             120.00 dB
PL12              9.00 dB
PL13             14.00 dB
SFO2        598.6029930 MHz

F2 - Processing parameters
SI                65536
SF          150.5180981 MHz
WDW                EM
SSB                0
LB                3.00 Hz
GB                 0
PC                1.00

1D NMR plot parameters
CX               20.00 cm
CY                4.00 cm
F1P             200.000 ppm
F1             30103.62 Hz
F2P               0.000 ppm
F2                0.00 Hz
PPMCM         10.00000 ppm/cm
HZCM        1505.18091 Hz/cm
```

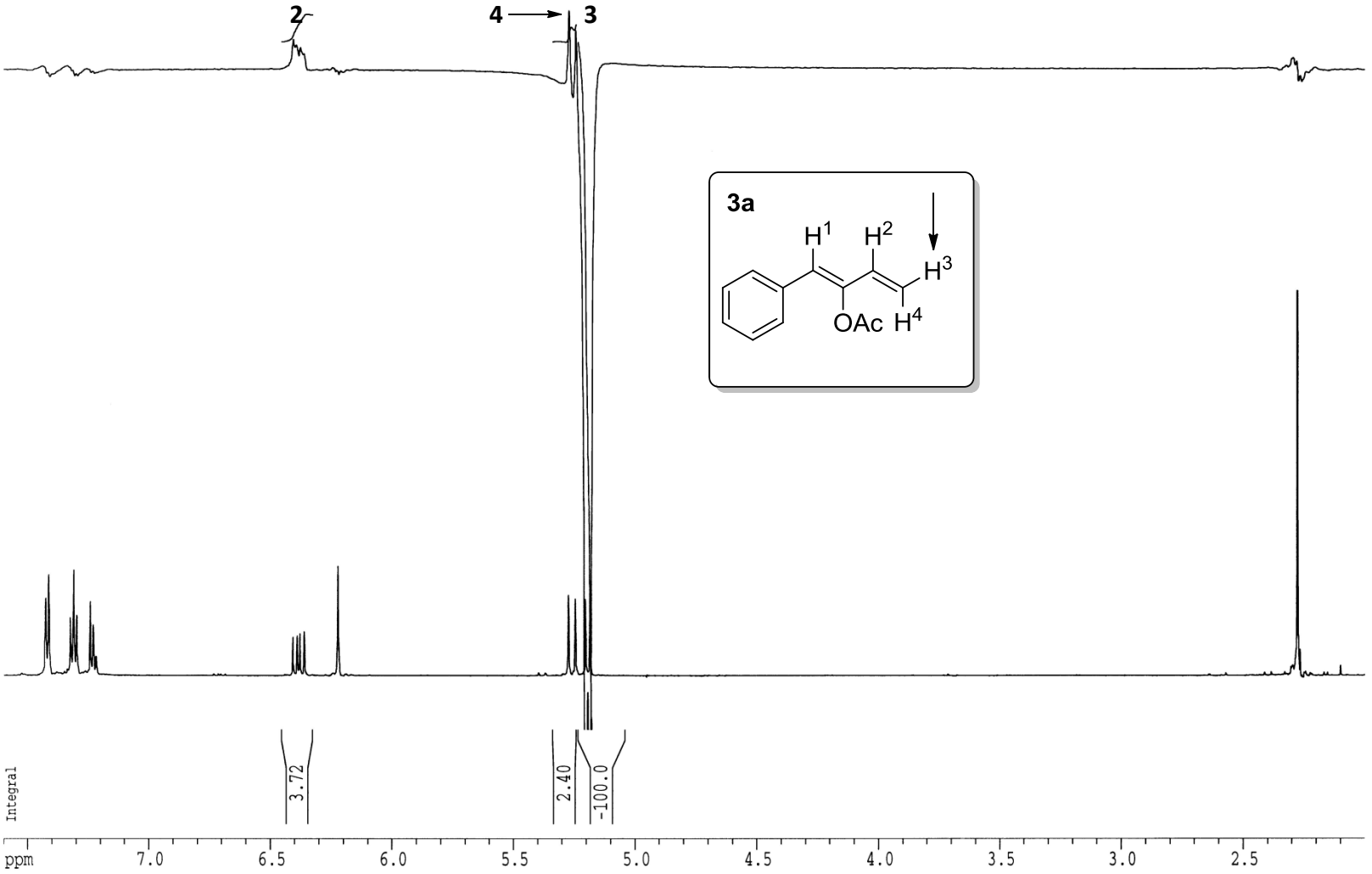


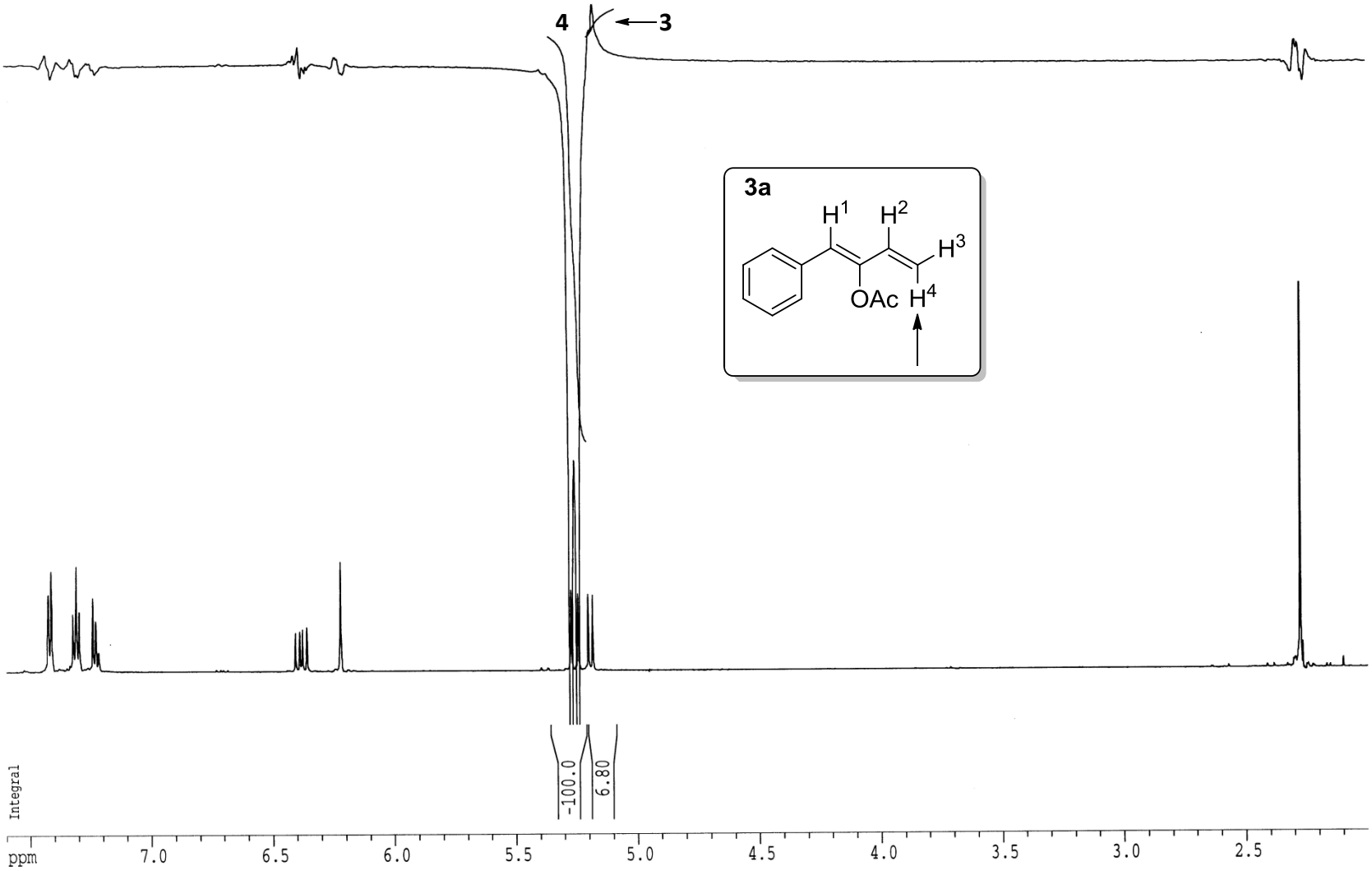

Current Data Parameters
NAME SBW-73-b
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140907
Time 20.46
INSTRUM spect
PROBHD 5 mm CNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 512
DW 59.600 usec
DE 6.50 usec
TE 302.5 K
D1 1.00000000 sec
D11 0.00000000 sec
D12 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.50 usec
PL1 0.00 dB
SFO1 598.7032929 MHz
F2 - Processing parameters
SI 16384
SF 598.7000355 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 3.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 10.000 ppm
F1 5987.00 Hz
F2P -0.500 ppm
F2 -299.35 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.31750 Hz/cm
ppm
7.42216
7.41967
7.40691
7.31872
7.30626
7.29298
7.24126
7.22442
6.40253
6.38445
6.37392
6.35579
6.21775
5.27009
5.24193
5.19828
5.18029
2.27164
1.53745
3a
Integral
2.0578
2.2342
1.3556
1.0738
1.0000
1.1445
1.1517
3.0488
ppm
8
6
4
2
0

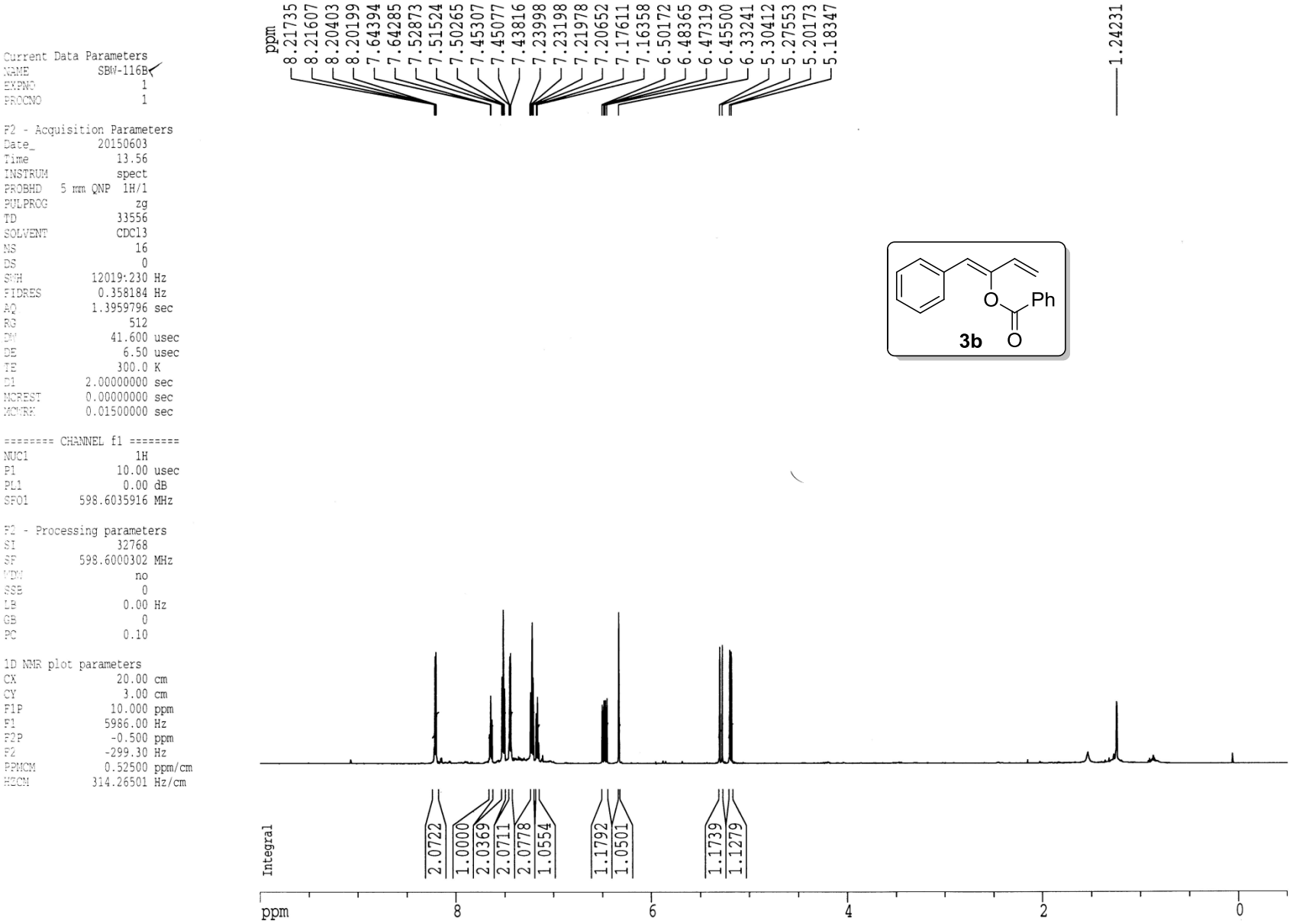

Current Data Parameters
NAME SB-73-b
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140908
Time 0.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 3072
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 305.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 6.25 usec
PL1 0.00 dB
SFO1 150.5447946 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 599.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432342 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 30108.65 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.43225 Hz/cm
ppm
167.941
145.937
134.032
132.137
128.696
128.557
127.869
120.877
114.367
77.214
77.002
76.790
20.816
3a
O
O
ppm
180
160
140
120
100
80
60
40
20

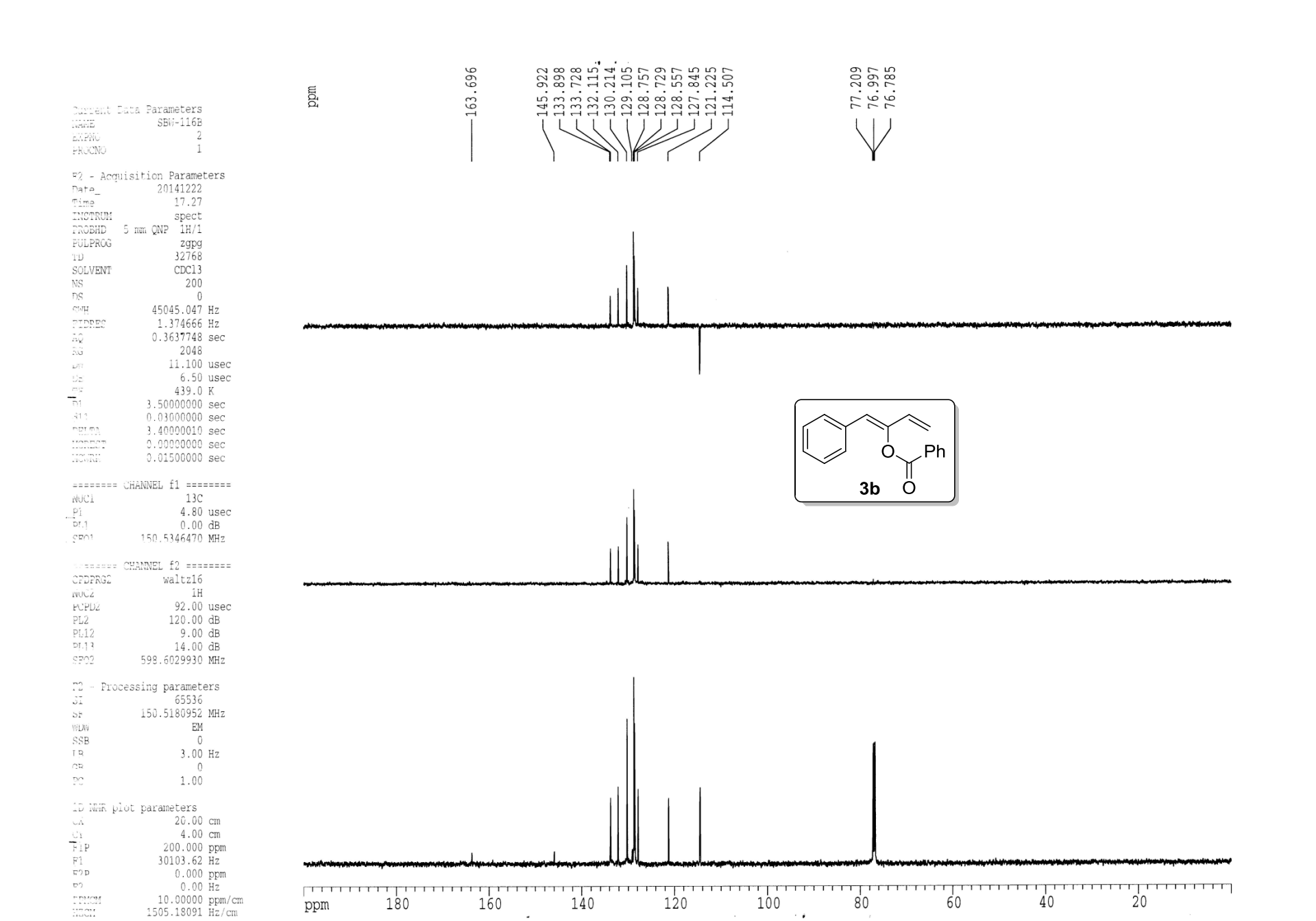

a
2
1
3a
H^a
H^1
H^2
H^3
OAc
H^4
Integral
4.843
5.250
-100.0
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

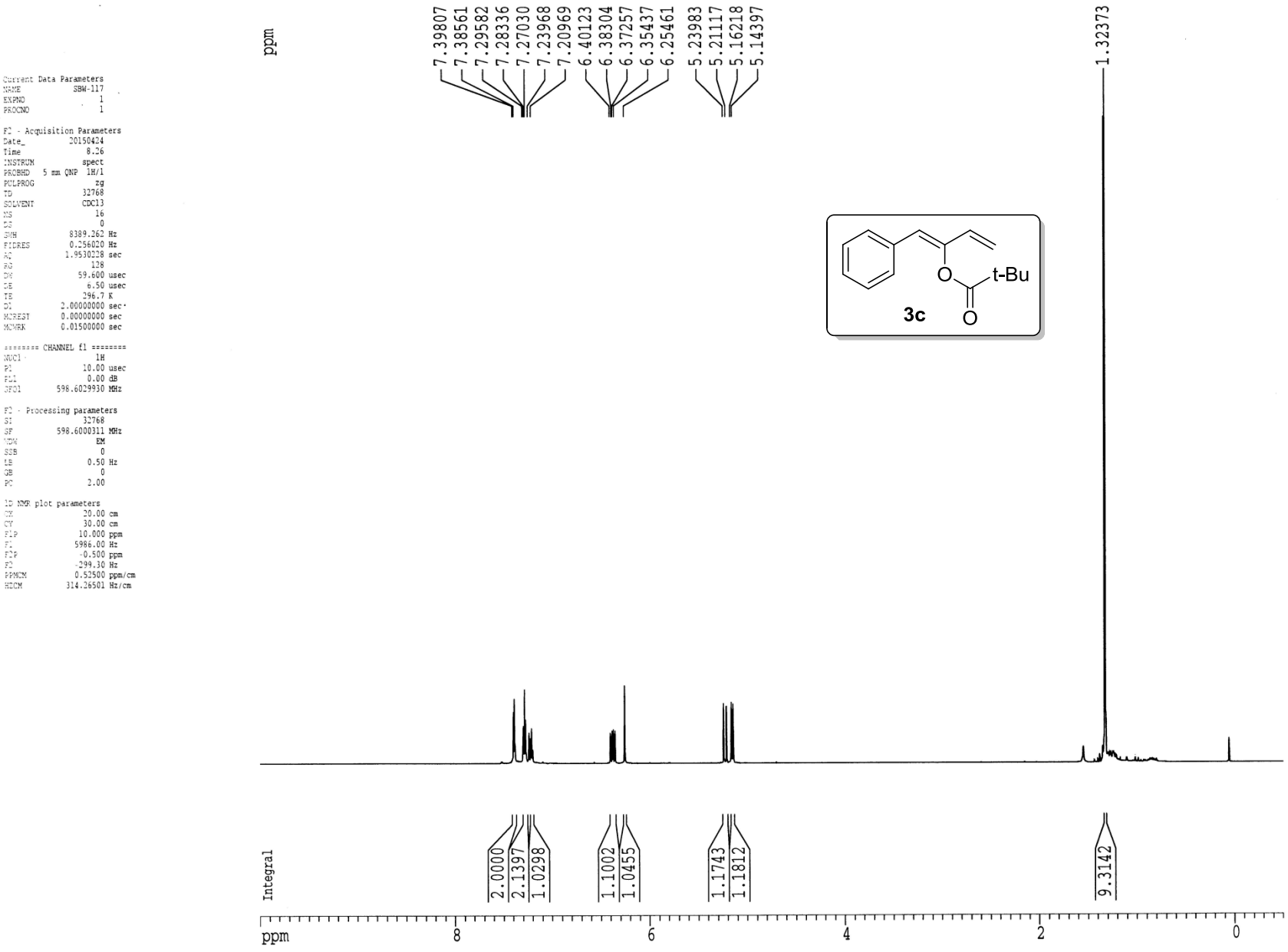

2
1
4
3
3a
H1
H2
H3
OAc
H4
Integral
-100.0
3.40
0.46
2.96
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

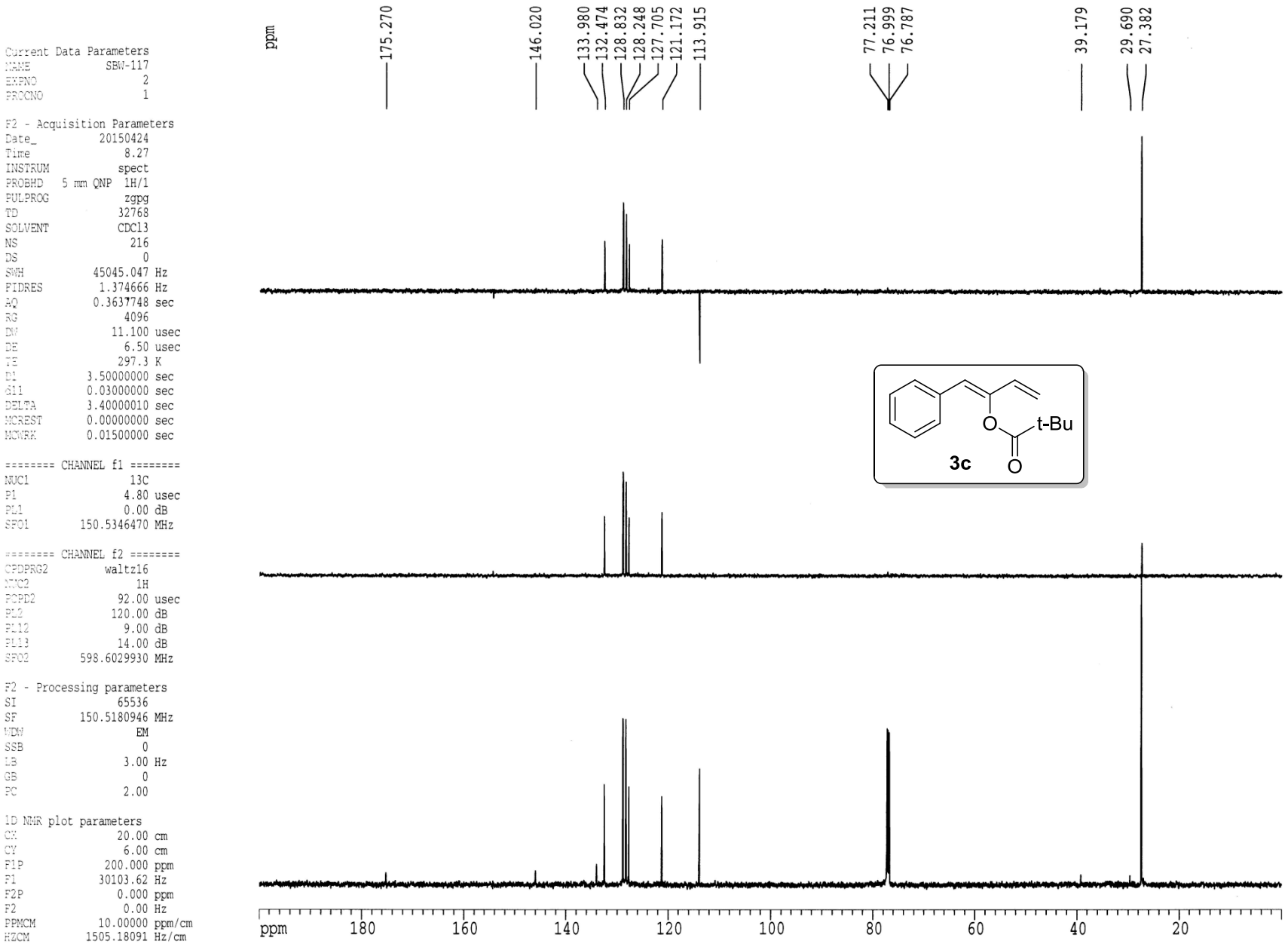

2
4
3
3a
H1
H2
H3
OAc
H4
Integral
3.72
2.40
-100.0
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

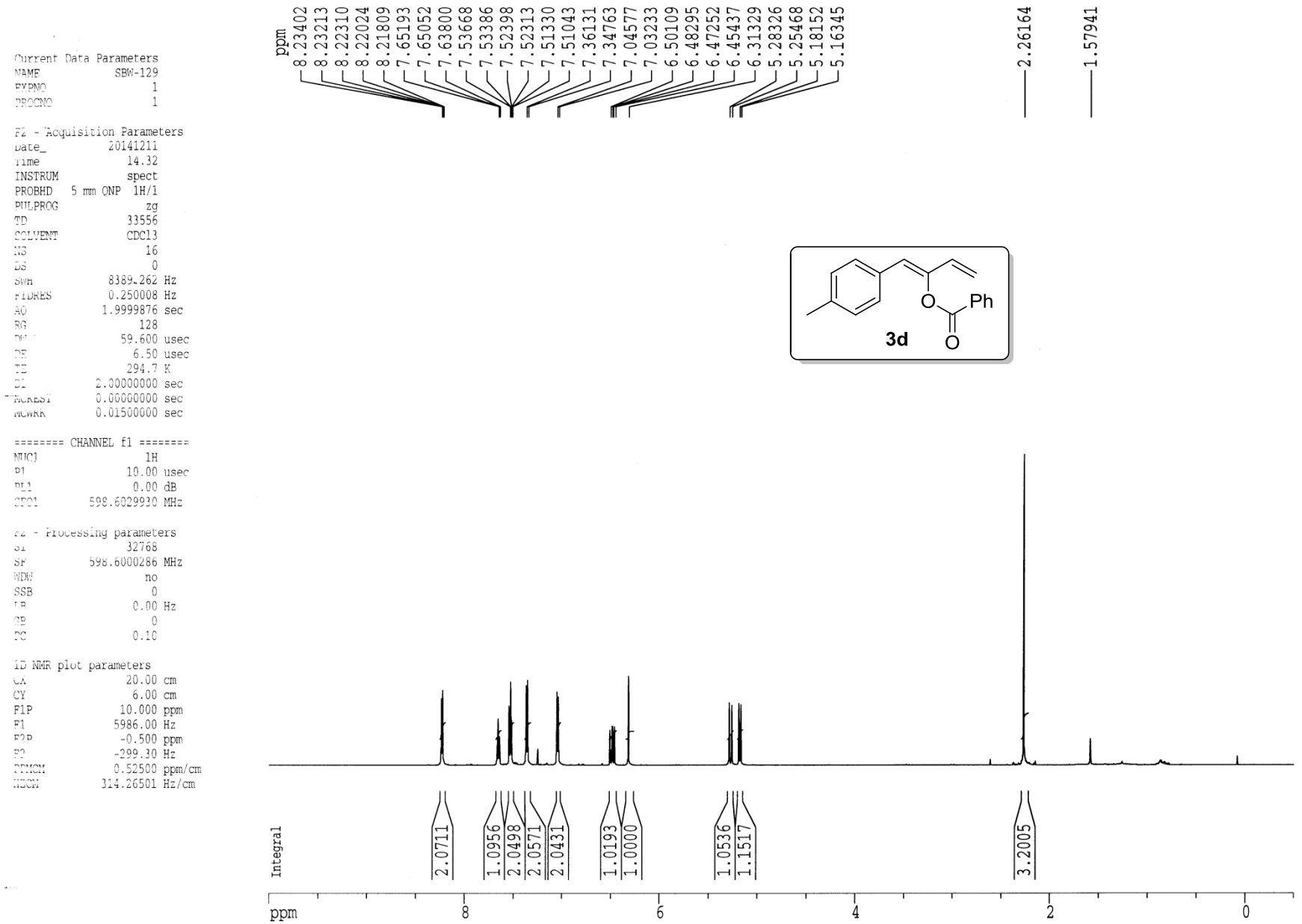

4
3
3a
H1
H2
H3
OAc
H4
Integral
-100.0
6.80
ppm
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5

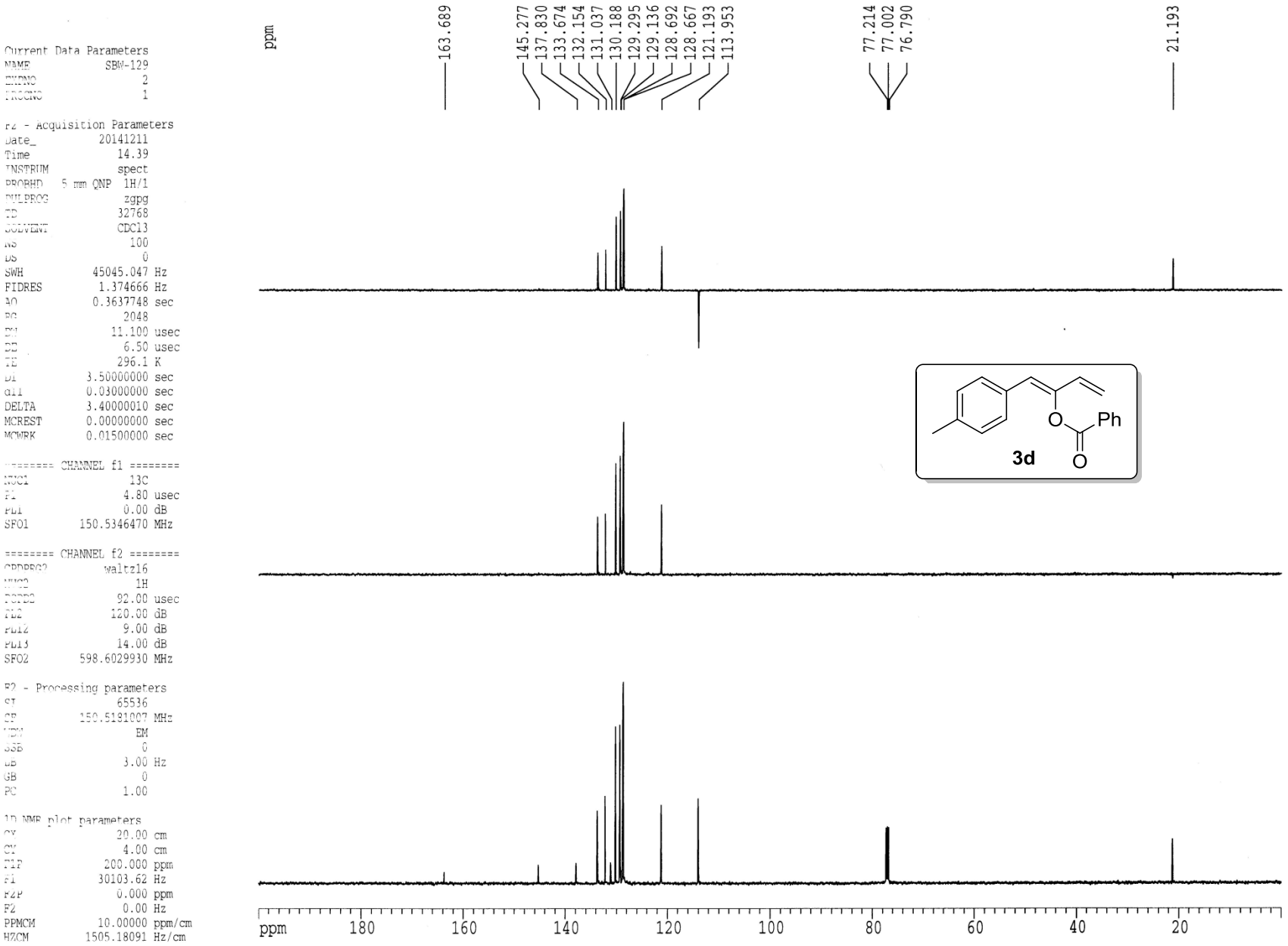

Current Data Parameters
NAME SBW-116B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150603
Time 13.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000302 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.10
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.21735
8.21607
8.20403
8.20199
7.64394
7.64285
7.52873
7.51524
7.50265
7.45307
7.45077
7.43816
7.23998
7.23198
7.21978
7.20652
7.17611
7.16358
6.50172
6.48365
6.47319
6.45500
6.33241
5.30412
5.27553
5.20173
5.18347
1.24231
O
Ph
O
3b
Integral
2.0722
1.0000
2.0369
2.0711
2.0778
1.0554
1.1792
1.0501
1.1739
1.1279
ppm
8
6
4
2
0


Current Data Parameters
NAME SBW-116B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141222
Time 17.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 439.0 K
D1 3.50000000 sec
D12 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180952 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
163.696
145.922
133.898
133.728
132.115
130.214
129.105
128.757
128.729
128.557
127.845
121.225
114.507
77.209
76.997
76.785
O
Ph
O
3b
ppm
180
160
140
120
100
80
60
40
20

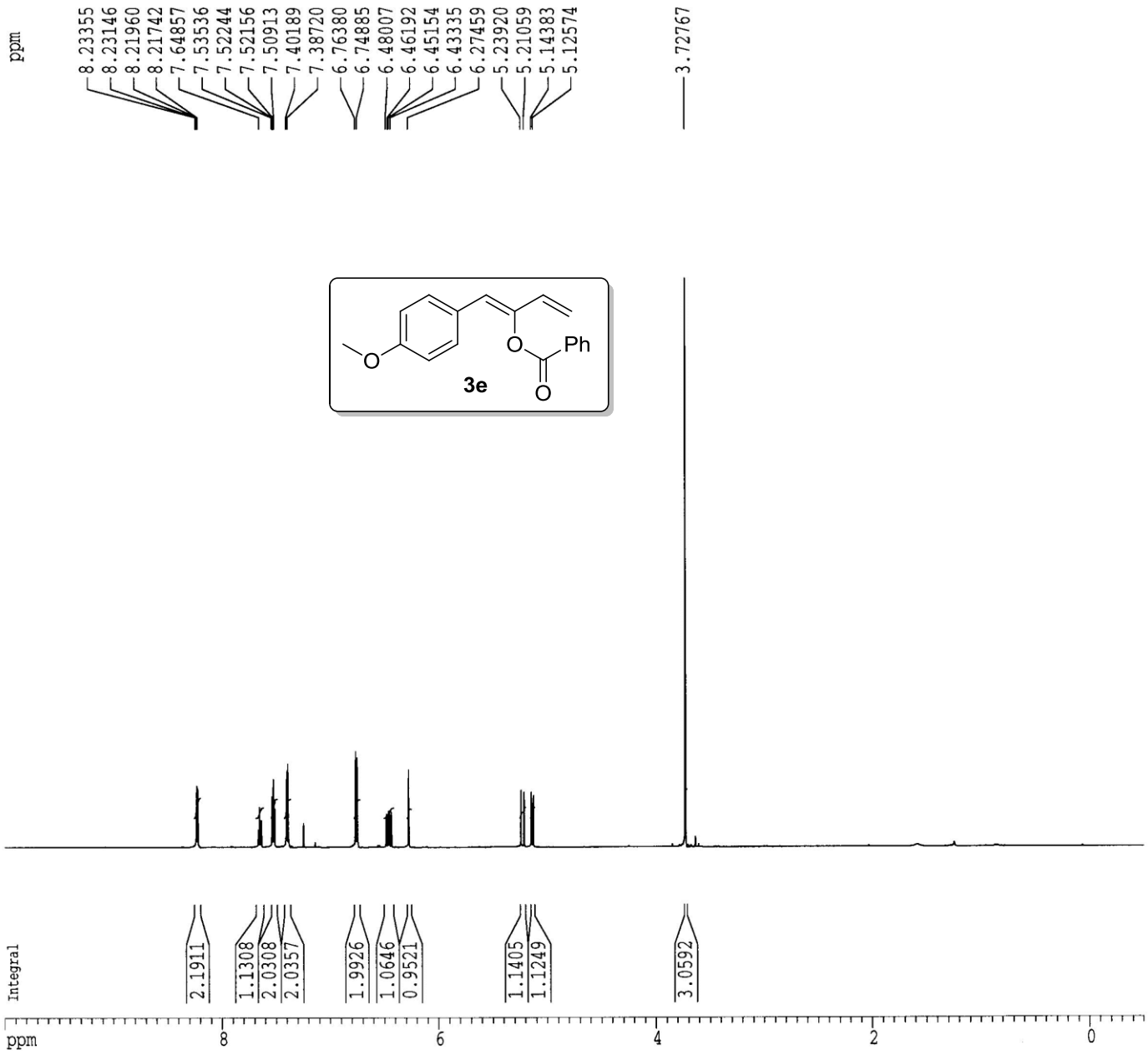

Current Data Parameters
NAME SBW-117
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150424
Time 8.26
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000311 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 20.00 cm
CY 30.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
7.39807
7.38561
7.29582
7.28336
7.27030
7.23968
7.20969
6.40123
6.38304
6.37257
6.35437
6.25461
5.23983
5.21117
5.16218
5.14397
1.32373
O
t-Bu
O
3c
Integral
2.0000
2.1397
1.0298
1.1002
1.0455
1.1743
1.1812
9.3142
ppm
8
6
4
2
0

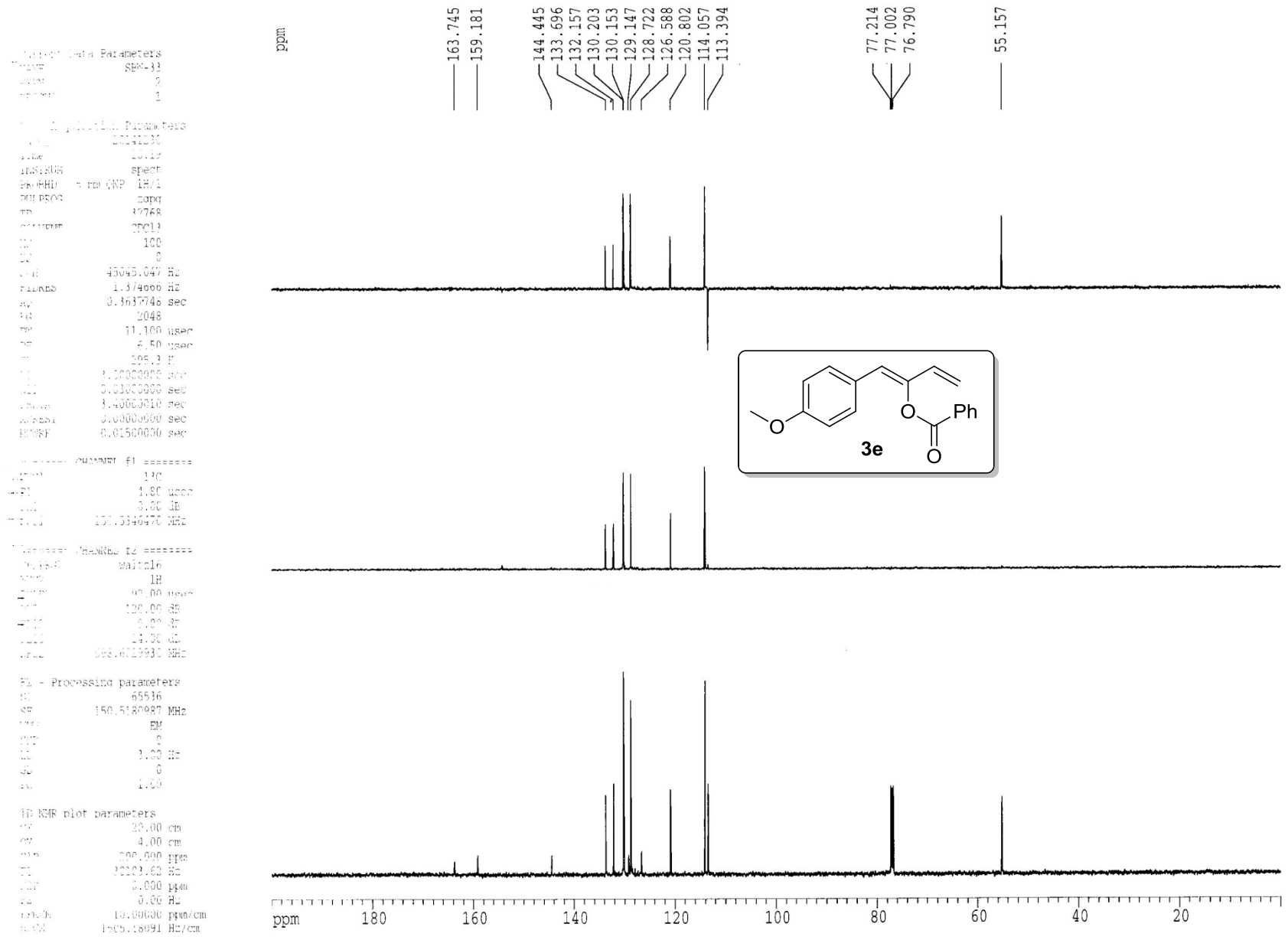

Current Data Parameters
NAME SBW-117
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150424
Time 8.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 216
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.3 K
D1 3.50000000 sec
D11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180946 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
175.270
146.020
133.980
132.474
128.832
128.248
127.705
121.172
113.915
77.211
76.999
76.787
39.179
29.690
27.382
O
t-Bu
O
3c
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME SBW-129
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141211
Time 14.32
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
TMCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000286 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 0.10
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.23402
8.23213
8.22310
8.22024
8.21809
7.65193
7.65052
7.63800
7.53668
7.53386
7.52398
7.52313
7.51330
7.51043
7.36131
7.34763
7.04577
7.03233
6.50109
6.48295
6.47252
6.45437
6.31329
5.28326
5.25468
5.18152
5.16345
2.26164
1.57941
O
Ph
O
3d
Integral
2.0711
1.0956
2.0498
2.0571
2.0431
1.0193
1.0000
1.0536
1.1517
3.2005
ppm
8
6
4
2
0

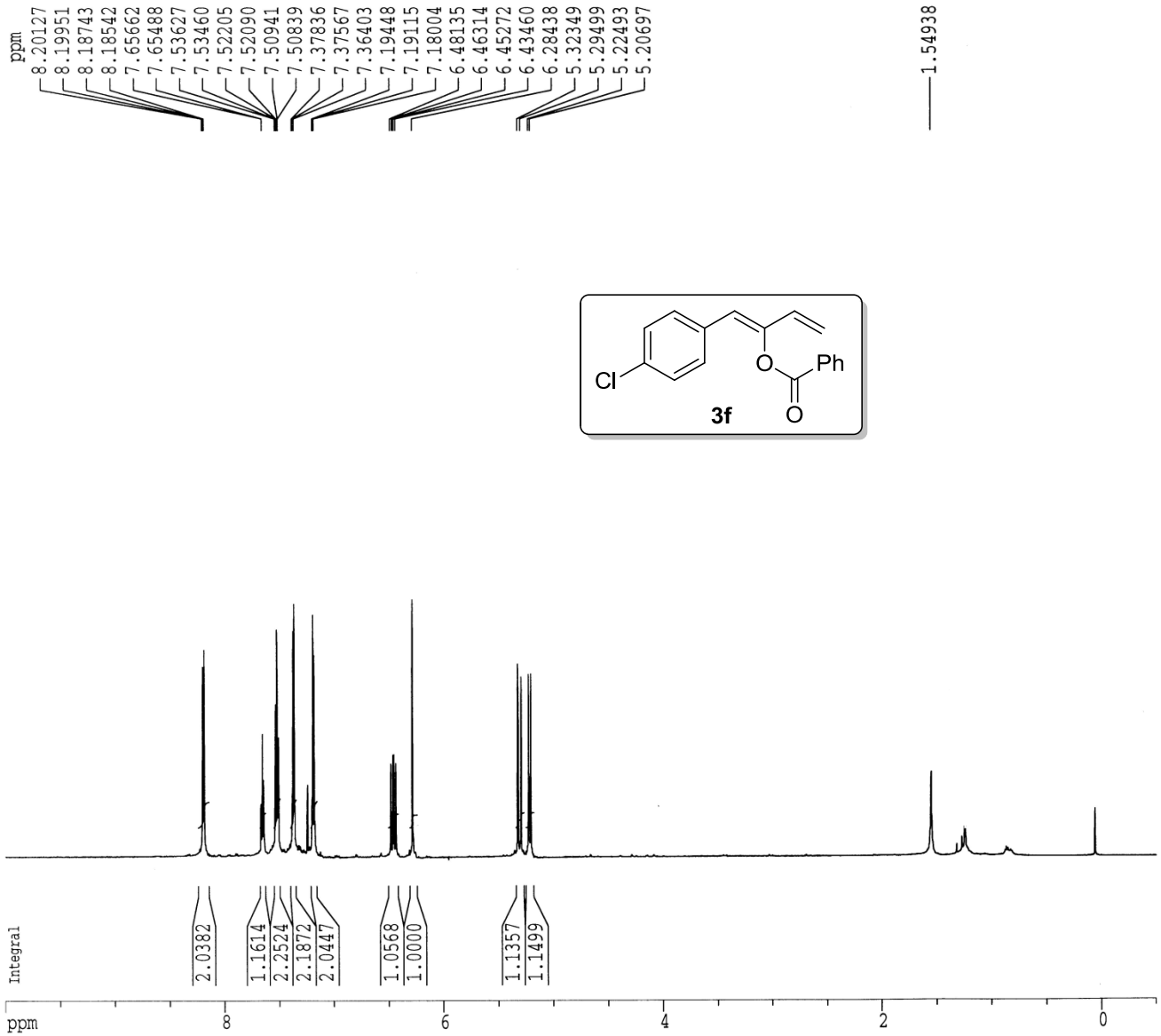

Current Data Parameters
NAME SBW-129
EXPNO 2
PROCNO 1
f2 - Acquisition Parameters
Date_ 20141211
Time 14.39
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5181007 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
163.689
145.277
137.830
133.674
132.154
131.037
130.188
129.295
129.136
128.692
128.667
121.193
113.953
77.214
77.002
76.790
21.193
O
Ph
O
3d
ppm
180
160
140
120
100
80
60
40
20

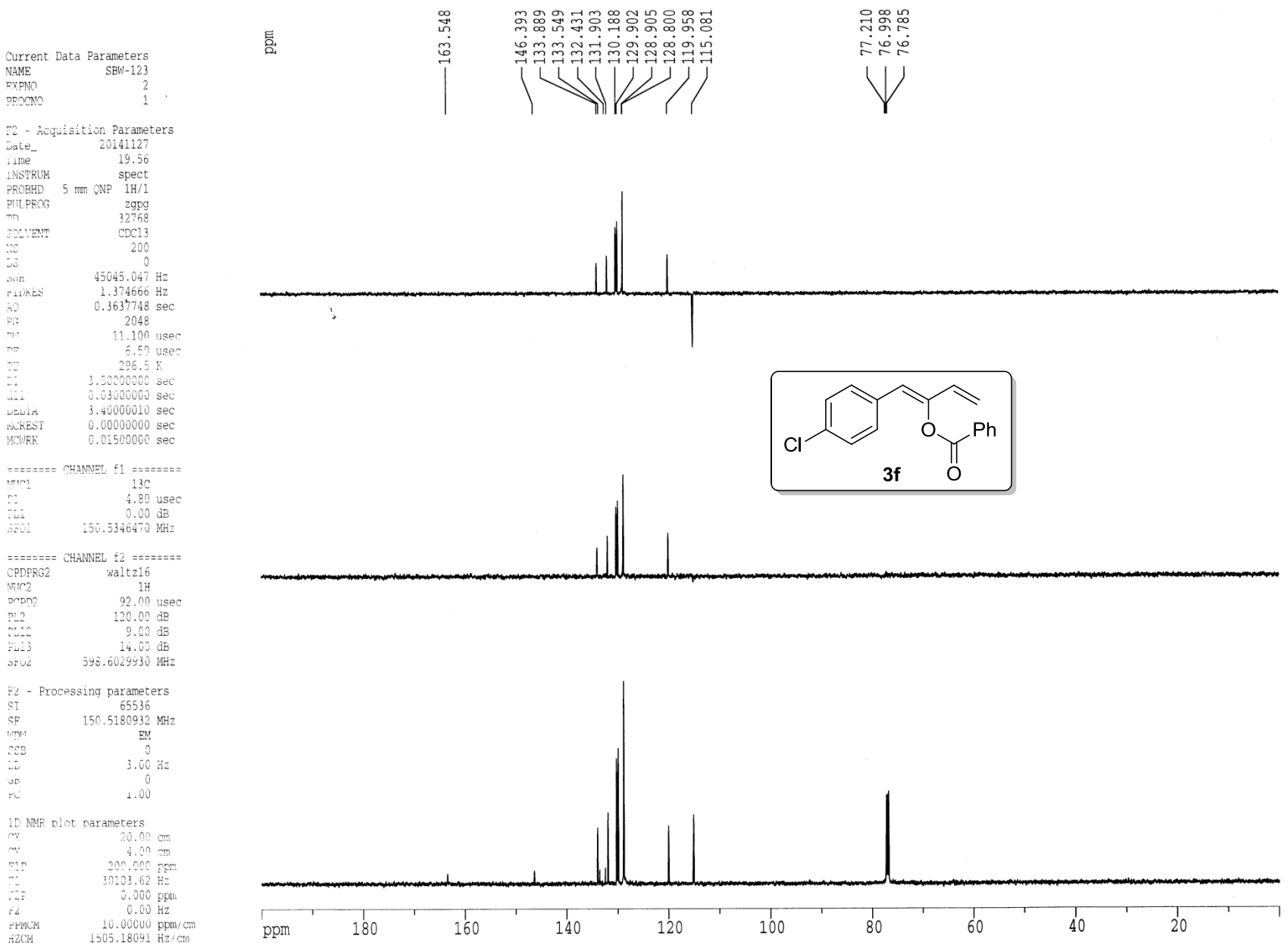
```
Current Data Parameters
NAME              SBW-33
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20141230
Time              10.13
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG              zg
TD                33556
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            8389.262 Hz
FIDRES         0.250008 Hz
AQ             1.9999876 sec
RG                  512
DW                59.600 usec
DE                 6.50 usec
TE                293.8 K
D1           2.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                1H
P1                10.00 usec
PL1                0.00 dB
SFO1        598.6029930 MHz

F2 - Processing parameters
SI                 32768
SF          598.6000306 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  2.00

1D NMR plot parameters
CX                 20.00 cm
CY                 10.00 cm
F1P               10.000 ppm
F1                5986.00 Hz
F2P                -0.500 ppm
F2                -299.30 Hz
PPMCM             0.52500 ppm/cm
HZCM            314.26501 Hz/cm
```



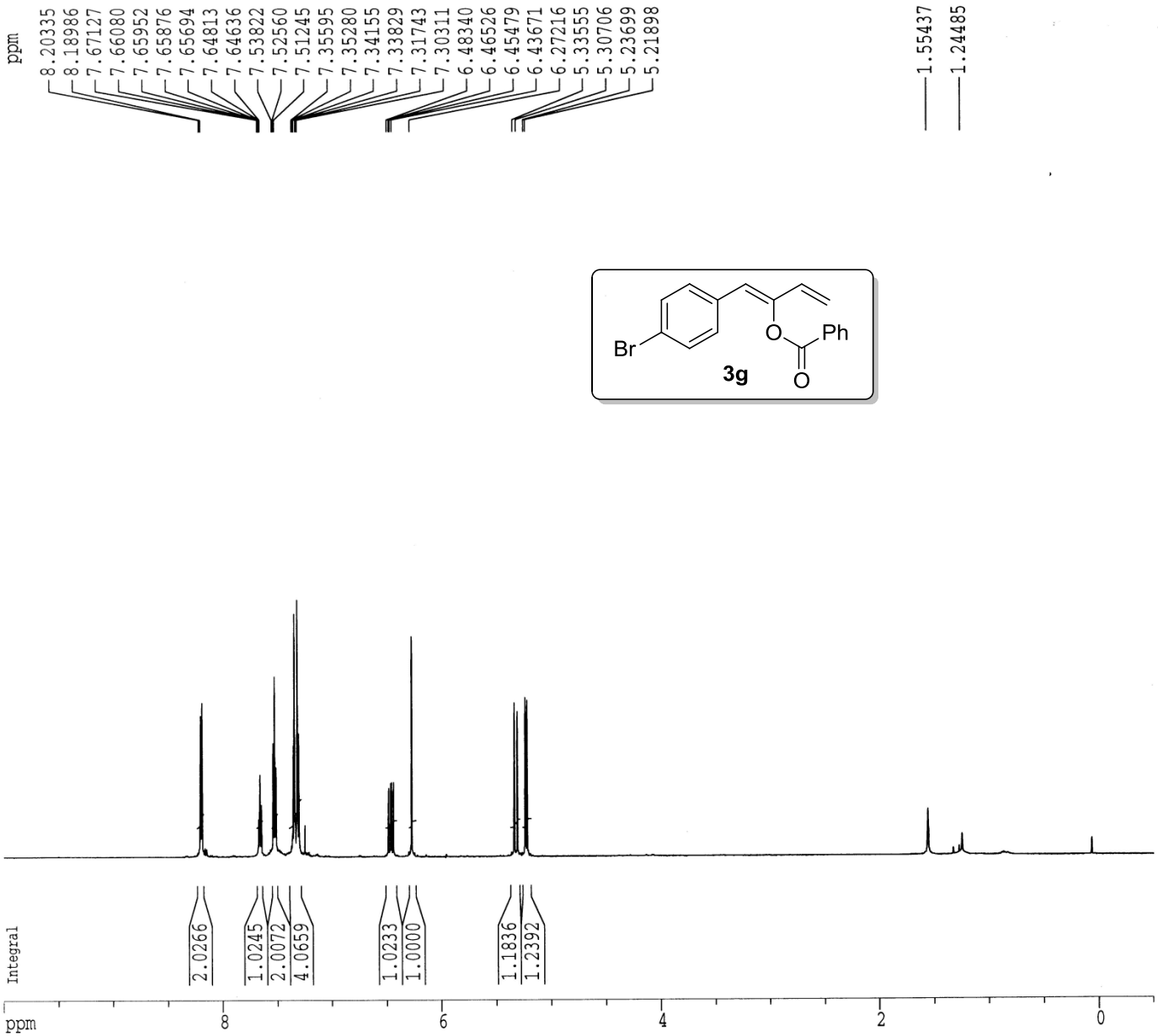

ppm
163.745
159.181
144.445
133.696
132.157
130.203
130.153
129.147
128.722
126.588
120.802
114.057
113.394
77.214
77.002
76.790
55.157
O
O
Ph
O
3e
ppm
180
160
140
120
100
80
60
40
20

```
Current Data Parameters
NAME                  SBW-123
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141127
Time                  19.53
INSTRUM               spect
PROBHD   5 mm QNP  1H/1
PULPROG                   zg
TD                     33556
SOLVENT                CDCl3
NS                        16
DS                         0
SWH               12019.230 Hz
FIDRES             0.358184 Hz
AQ                 1.3959796 sec
RG                       128
DW                  41.600 usec
DE                   6.50 usec
TE                   295.5 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
PL1                    0.00 dB
SFO1            598.6035916 MHz

F2 - Processing parameters
SI                        32768
SF               598.6000295 MHz
WDW                          EM
SSB                           0
LB                     0.20 Hz
GB                            0
PC                     0.10

1D NMR plot parameters
WX                    20.00 cm
WY                     4.50 cm
F1P                  10.000 ppm
F1                  5986.00 Hz
F2P                  -0.500 ppm
F2                  -299.30 Hz
PPMCM                0.52500 ppm/cm
HZCM               314.26501 Hz/cm
```



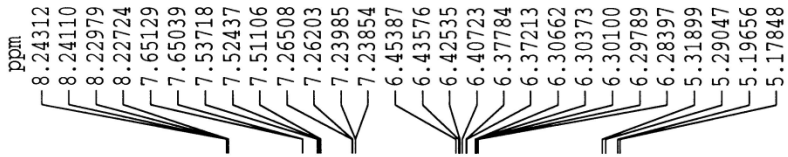

Current Data Parameters
NAME SBW-123
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141127
Time 19.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
D11 0.03000000 sec
DELTA 3.40000010 sec
RCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180932 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
163.548
146.393
133.889
133.549
132.431
131.903
130.188
129.902
128.905
128.800
119.958
115.081
77.210
76.998
76.785
Cl
O
Ph
O
3f
ppm
180
160
140
120
100
80
60
40
20

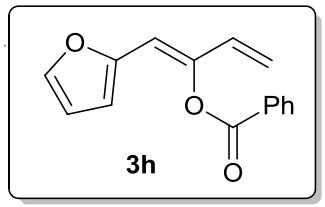
```
Current Data Parameters
NAME                  SBW-122
EXPNO                       1
PROCNO                      1

F2 - Acquisition Parameters
Date_              20141127
Time                  19.04
INSTRUM               spect
PROBHD   5 mm QNP  1H/1
PULPROG                   zg
TD                     33556
SOLVENT                CDCl3
NS                        16
DS                         0
SWH               12019.230 Hz
FIDRES             0.358184 Hz
AQ                 1.3959796 sec
RG                       128
DW                    41.600 usec
DE                     6.50 usec
TE                    295.6 K
D1                2.00000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.00 usec
PL1                     0.00 dB
SFO1             598.6035916 MHz

F2 - Processing parameters
SI                        32768
SF               598.6000265 MHz
WDW                          no
SSB                           0
LB                         0.00 Hz
GB                            0
PC                         0.10

1D NMR plot parameters
CX                        20.00 cm
CY                         4.50 cm
F1P                      10.000 ppm
F1                     5986.00 Hz
F2P                      -0.500 ppm
F2                     -299.30 Hz
PPMCM                  0.52500 ppm/cm
HZCM                 314.26501 Hz/cm
```

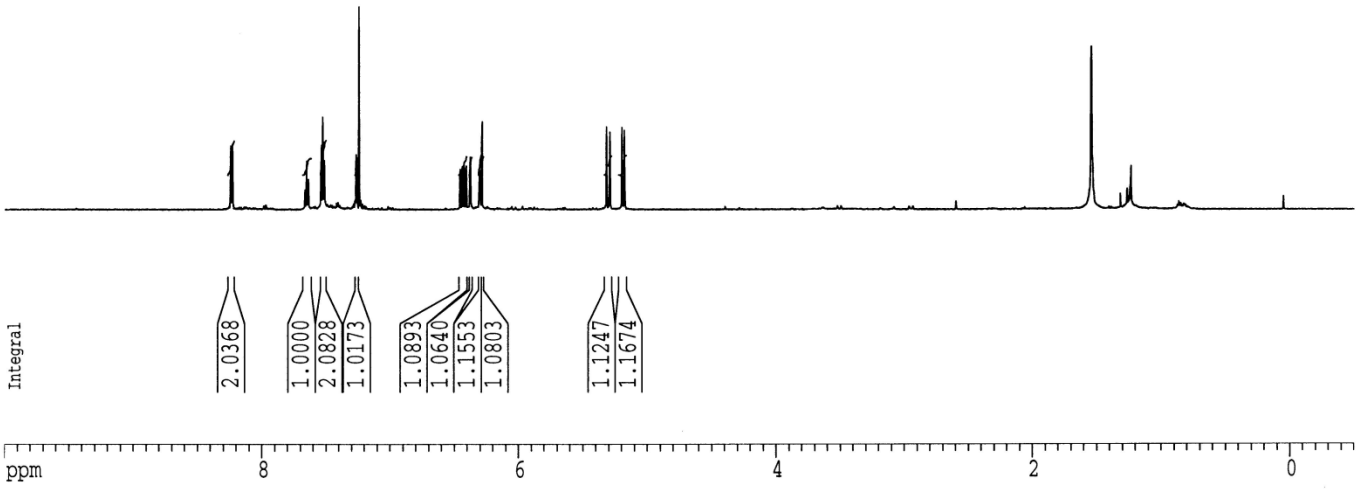


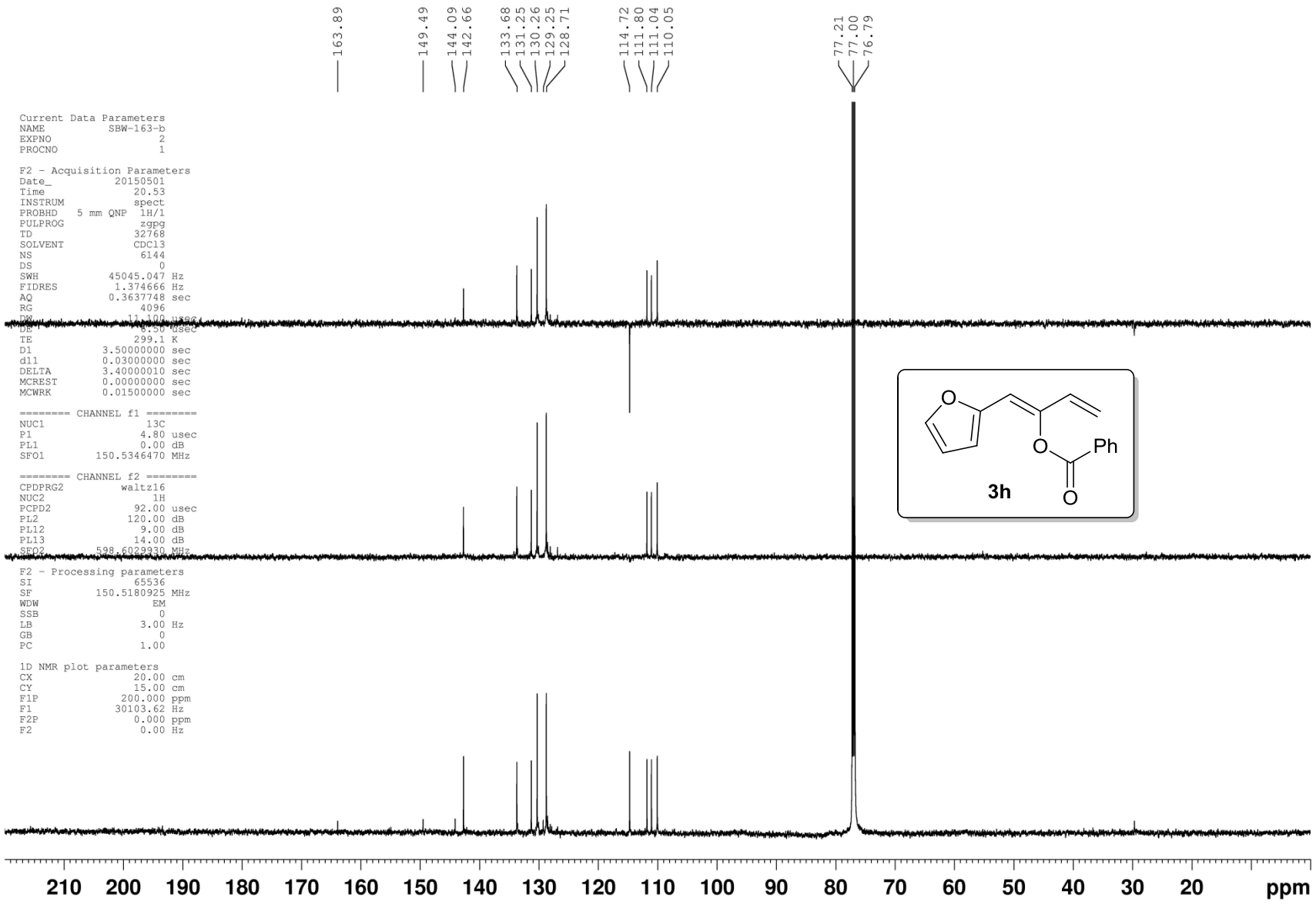
Current Data Parameters
NAME SBM-122
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141127
Time 18.43
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.9 K
D1 3.50000000 sec
D11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5330932 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
163.513
146.499
133.903
132.869
131.915
131.748
130.177
128.814
121.795
120.013
115.174
77.216
77.004
76.792
Br
O
Ph
O
3g
ppm
180
160
140
120
100
80
60
40
20

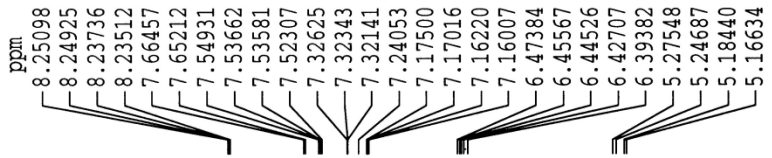
```
Current Data Parameters
NAME          SBW-163-b
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20150430
Time              13.13
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG             zg
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH           10775.862 Hz
FIDRES         0.328853 Hz
AQ            1.5204852 sec
RG                  512
DW               46.400 usec
DE               66.29 usec
TE               297.6 K
D1           1.00000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1                0.00 dB
SFO1        598.6029321 MHz

F2 - Processing parameters
SI                32768
SF          598.6000307 MHz
WDW                  no
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00

1D NMR plot parameters
CX                20.00 cm
CY                 3.00 cm
F1P               10.000 ppm
F1              5986.00 Hz
F2P               -0.500 ppm
F2              -299.30 Hz
PPMCM           0.52500 ppm/cm
HZCM          314.26501 Hz/cm
```



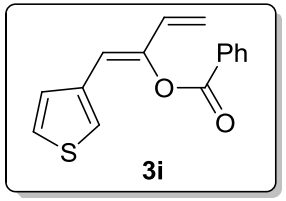




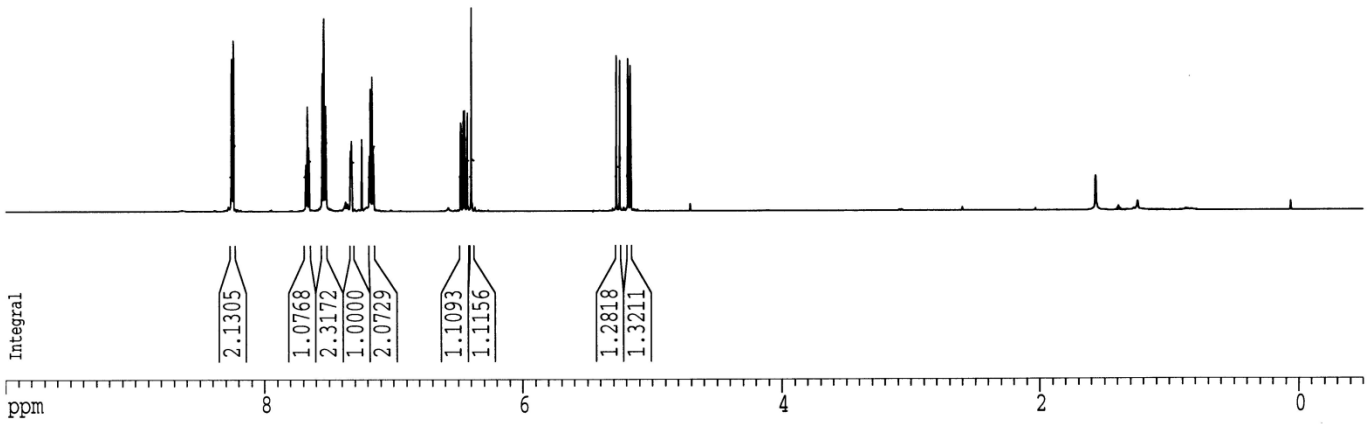

163.89
149.49
144.09
142.66
133.68
131.25
130.26
129.25
128.71
114.72
111.80
111.04
110.05
77.21
77.00
76.79
Current Data Parameters
NAME SBW-163-b
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150501
Time 20.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 6144
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
F2 - Processing parameters
SI 65536
SF 150.5180925 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 15.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
O
O
Ph
O
3h
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm




```
Current Data Parameters
NAME              SBW-158
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150306
Time                9.00
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG               zg
TD                 33556
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             8389.262 Hz
FIDRES          0.250008 Hz
AQ             1.9999876 sec
RG                   128
DW                59.600 usec
DE                 6.50 usec
TE                294.4 K
D1            2.00000000 sec
MCREST        0.00000000 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1                 0.00 dB
SFO1         598.6032923 MHz

F2 - Processing parameters
SI                 32768
SF           598.6000299 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  3.00 cm
F1P               10.000 ppm
F1                5986.00 Hz
F2P                -0.500 ppm
F2                -299.30 Hz
PPMCM             0.52500 ppm/cm
HZCM            314.26501 Hz/cm
```



3i



Current Data Parameters
NAME SBW-158
EXPNO 2
PROCNO 1

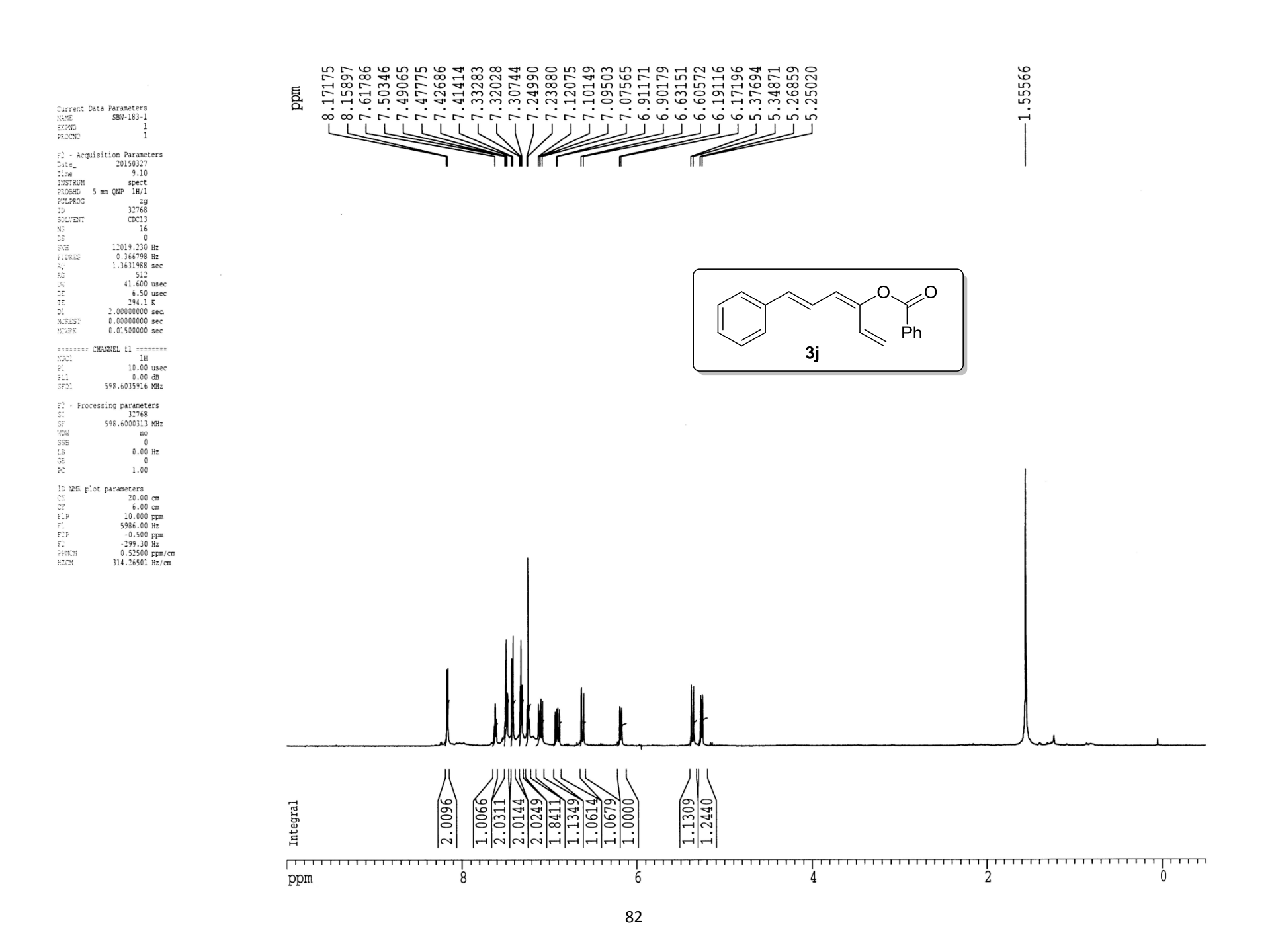
F2 - Acquisition Parameters
Date_ 20150306
Time 9.05
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 400
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

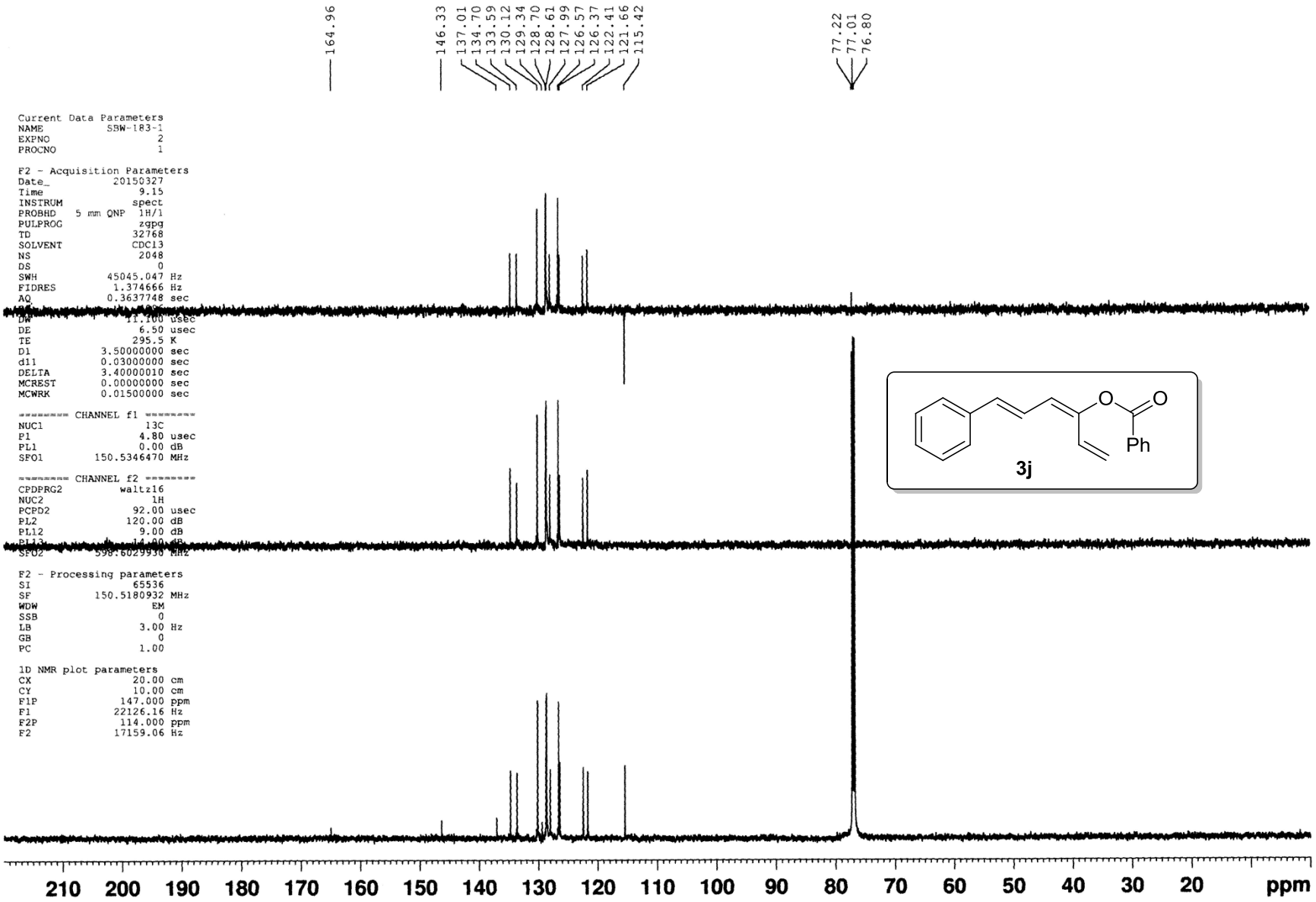
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

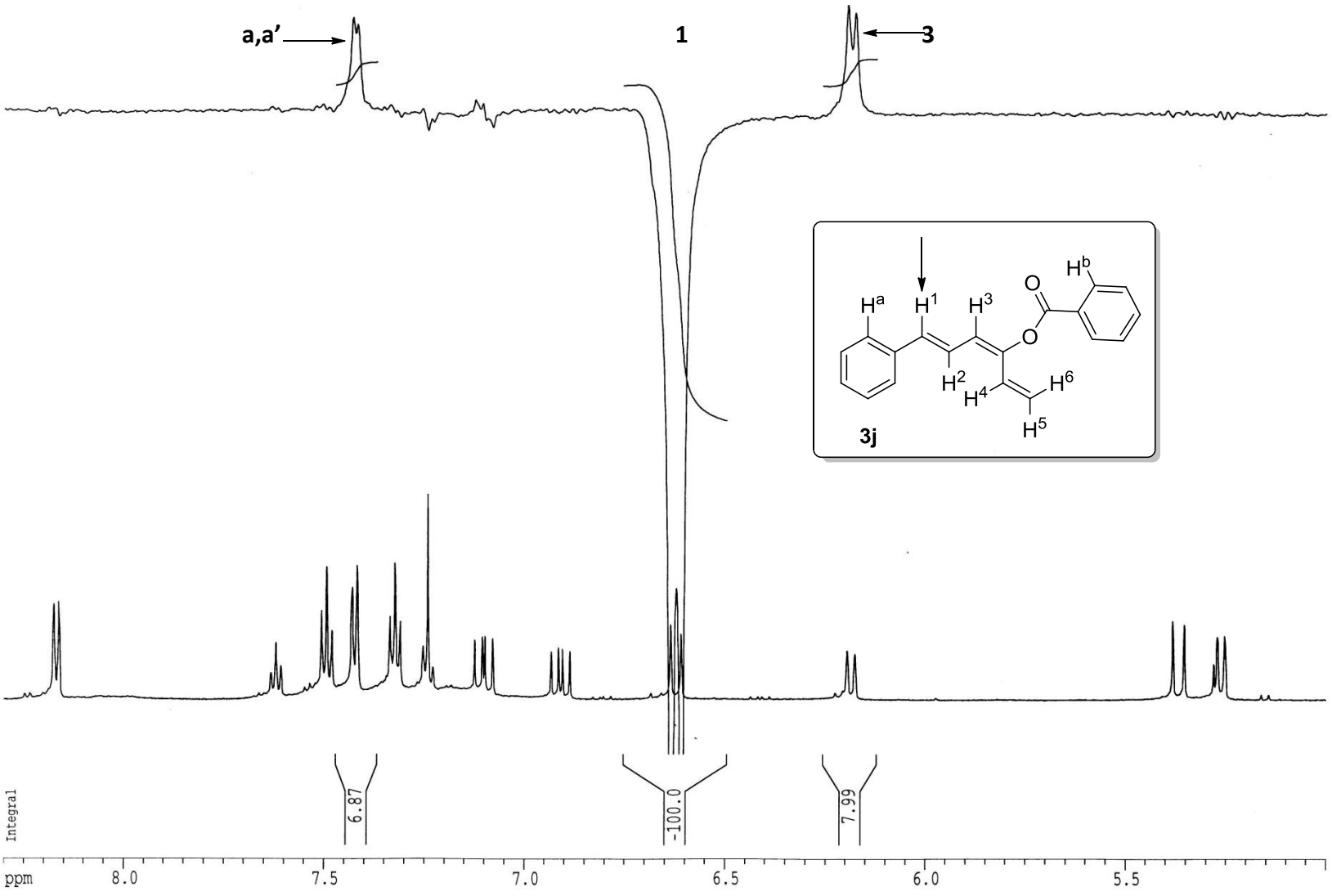
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

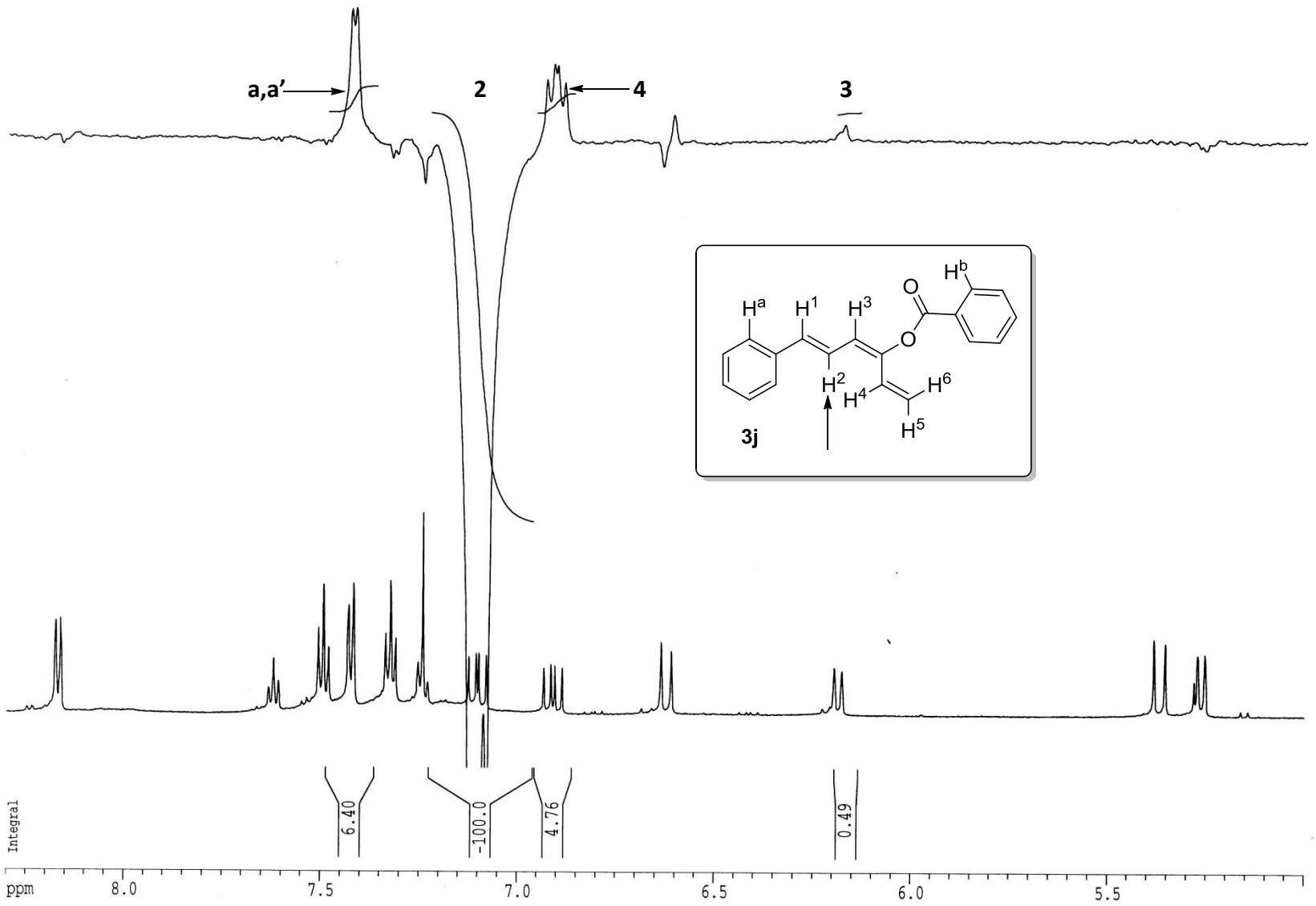
F2 - Processing parameters
SI 65536
SF 150.5180973 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

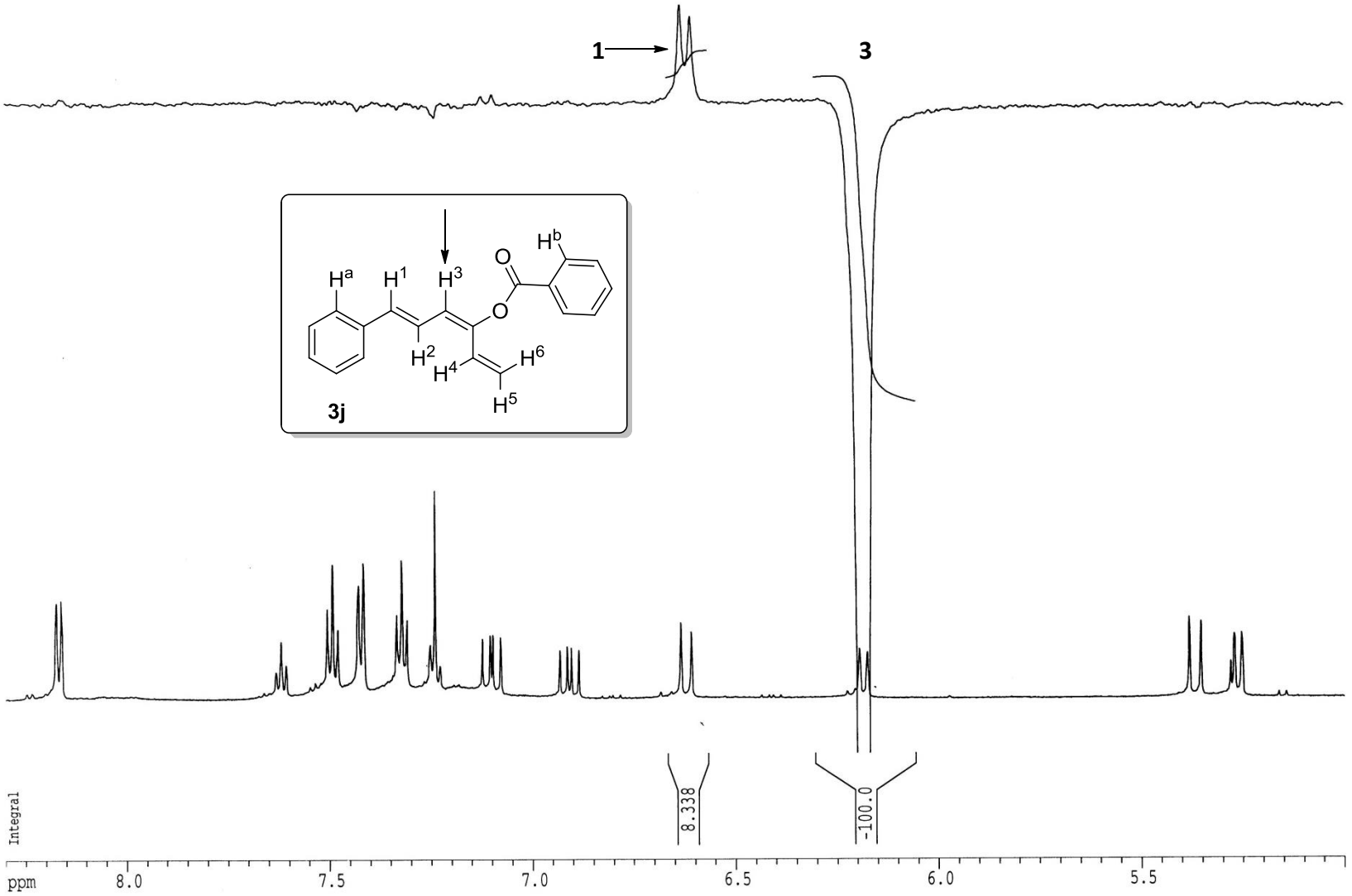
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm

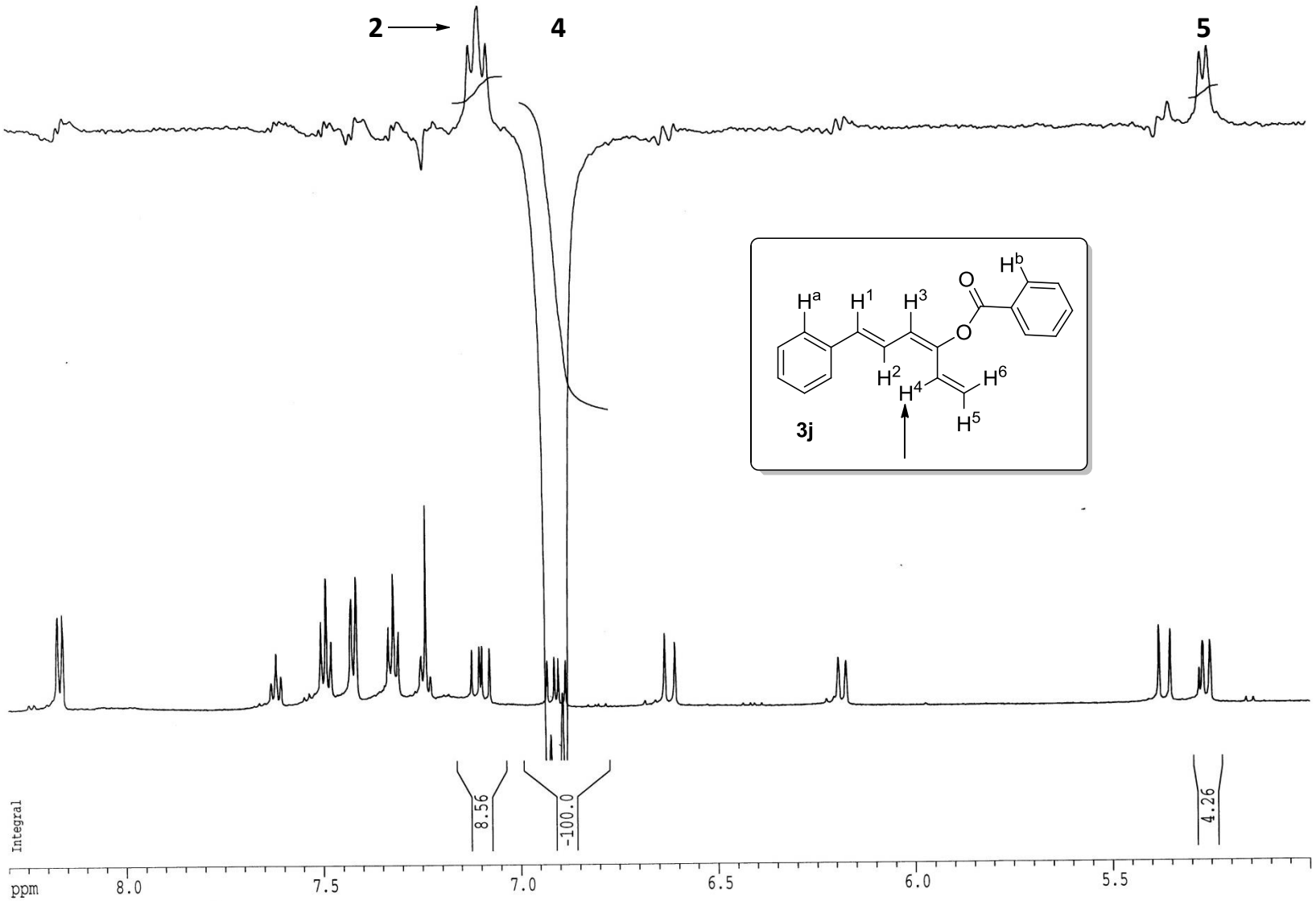

Current Data Parameters
NAME SBW-183-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150327
Time 9.10
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000313 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.17175
8.15897
7.61786
7.50346
7.49065
7.47775
7.42686
7.41414
7.33283
7.32028
7.30744
7.24990
7.23880
7.12075
7.10149
7.09503
7.07565
6.91171
6.90179
6.63151
6.60572
6.19116
6.17196
5.37694
5.34871
5.26859
5.25020
1.55566
O
O
Ph
3j
Integral
2.0096
1.0066
2.0311
2.0144
2.0249
1.8411
1.1349
1.0614
1.0679
1.0000
1.1309
1.2440
ppm
8
6
4
2
0

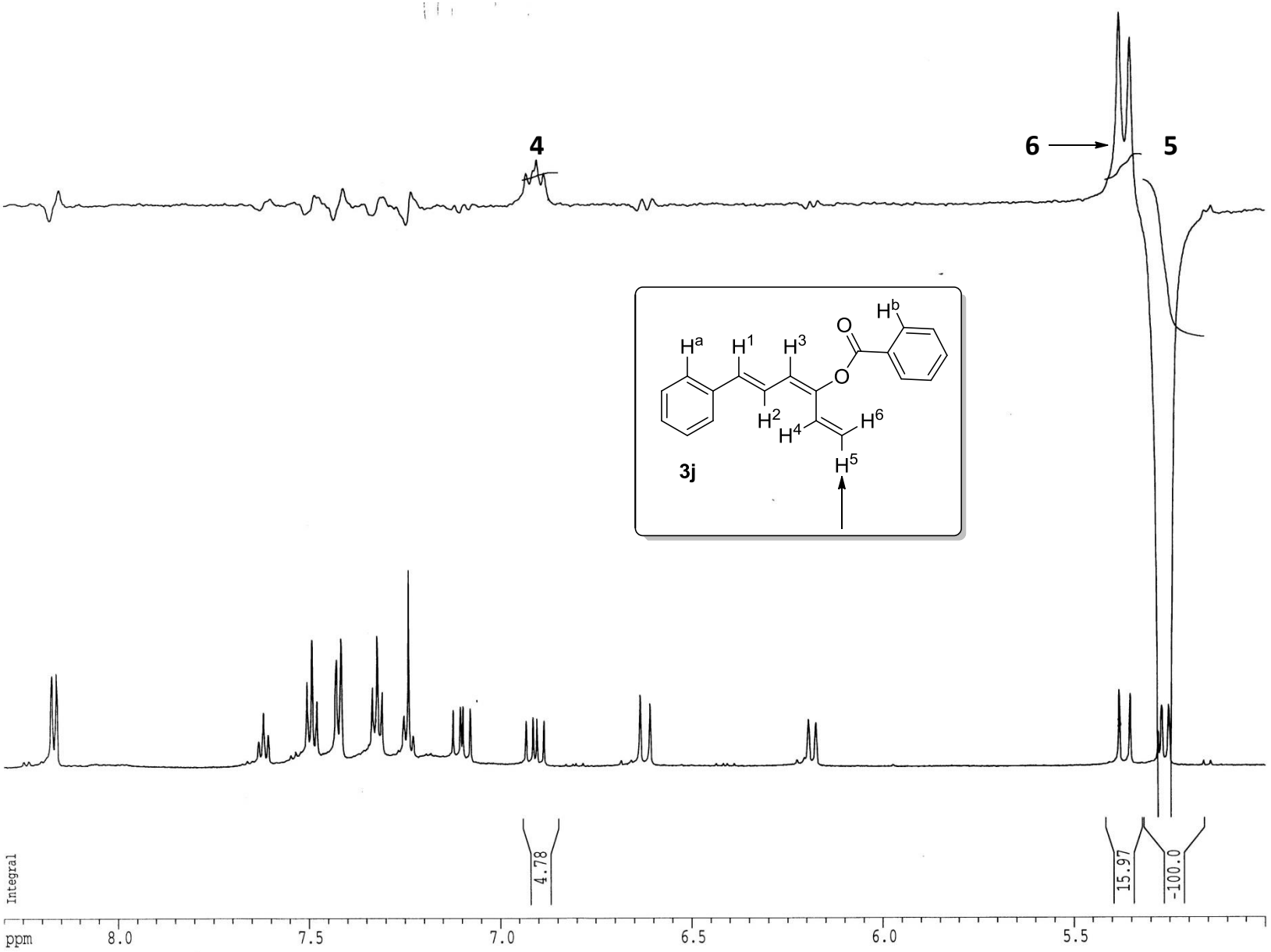

164.96
146.33
137.01
134.70
133.59
130.12
129.34
128.70
128.61
127.99
126.57
126.37
122.41
121.66
115.42
77.22
77.01
76.80
Current Data Parameters
NAME SBW-183-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150327
Time 9.15
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
DW 11.100 usec
DE 6.50 usec
TE 295.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
SFO2 600.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180932 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 147.000 ppm
F1 22126.16 Hz
F2P 114.000 ppm
F2 17159.06 Hz
O
O
Ph
3j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

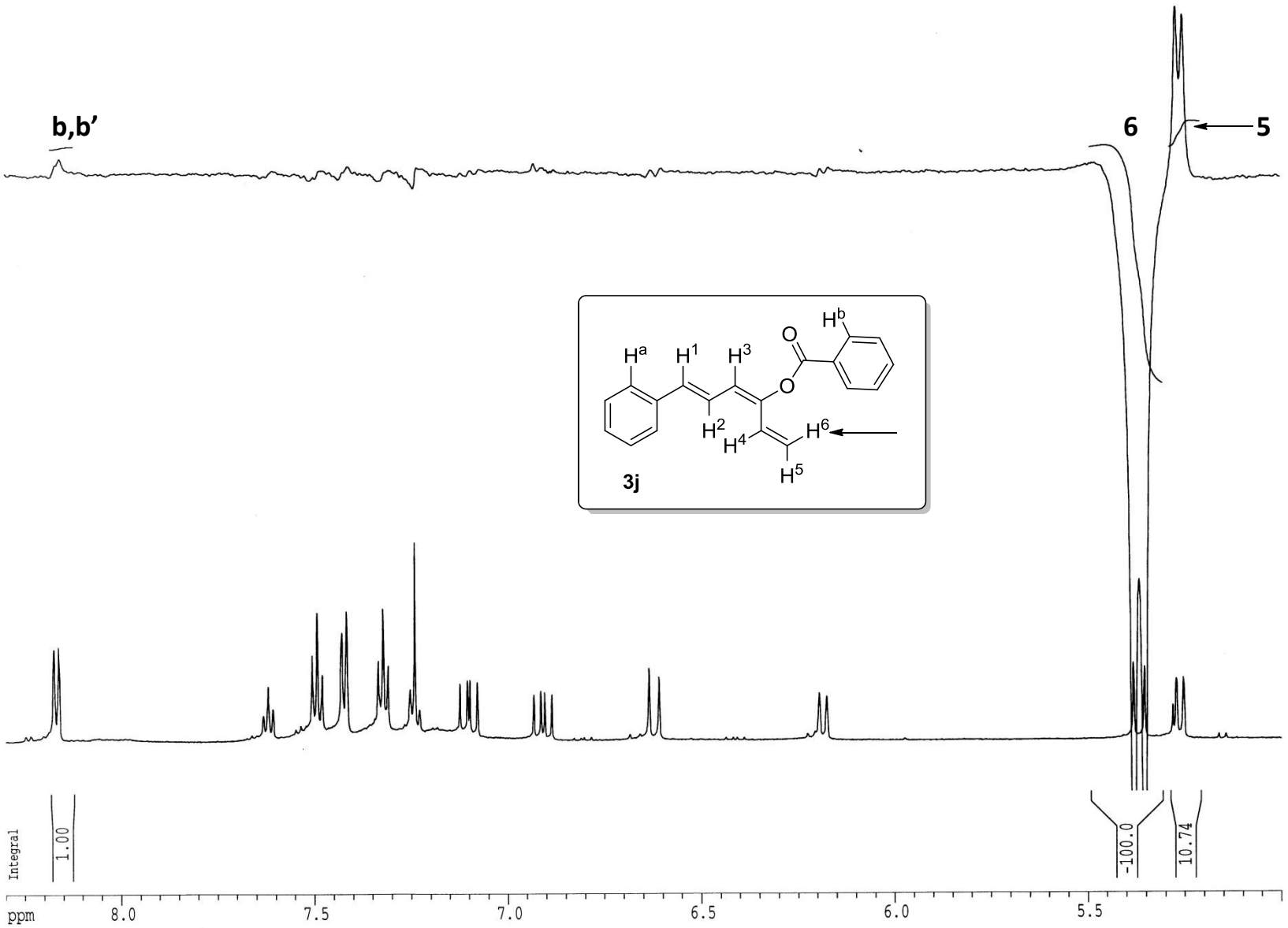

a,a'
1
3
Ha
H1
H3
Hb
O
O
H2
H4
H6
H5
3j
Integral
6.87
-100.0
7.99
ppm
8.0
7.5
7.0
6.5
6.0
5.5

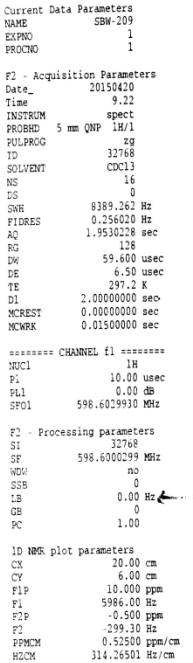

a,a'
2
4
3
Ha
H1
H3
Hb
O
O
H2
H4
H6
H5
3j
Integral
6.40
-100.0
4.76
0.49
ppm
8.0
7.5
7.0
6.5
6.0
5.5

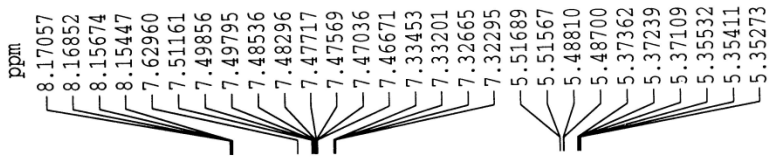

1
3
Ha
H1
H3
Hb
O
O
H2
H4
H6
H5
3j
Integral
8.338
-100.0
ppm
8.0
7.5
7.0
6.5
6.0
5.5

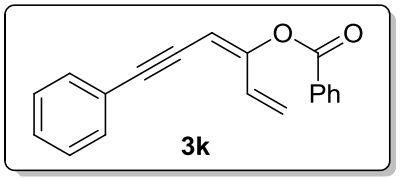

2
4
5
Ha
H1
H3
O
Hb
O
H2
H4
H6
H5
3j
Integral
8.56
-100.0
4.26
ppm
8.0
7.5
7.0
6.5
6.0
5.5

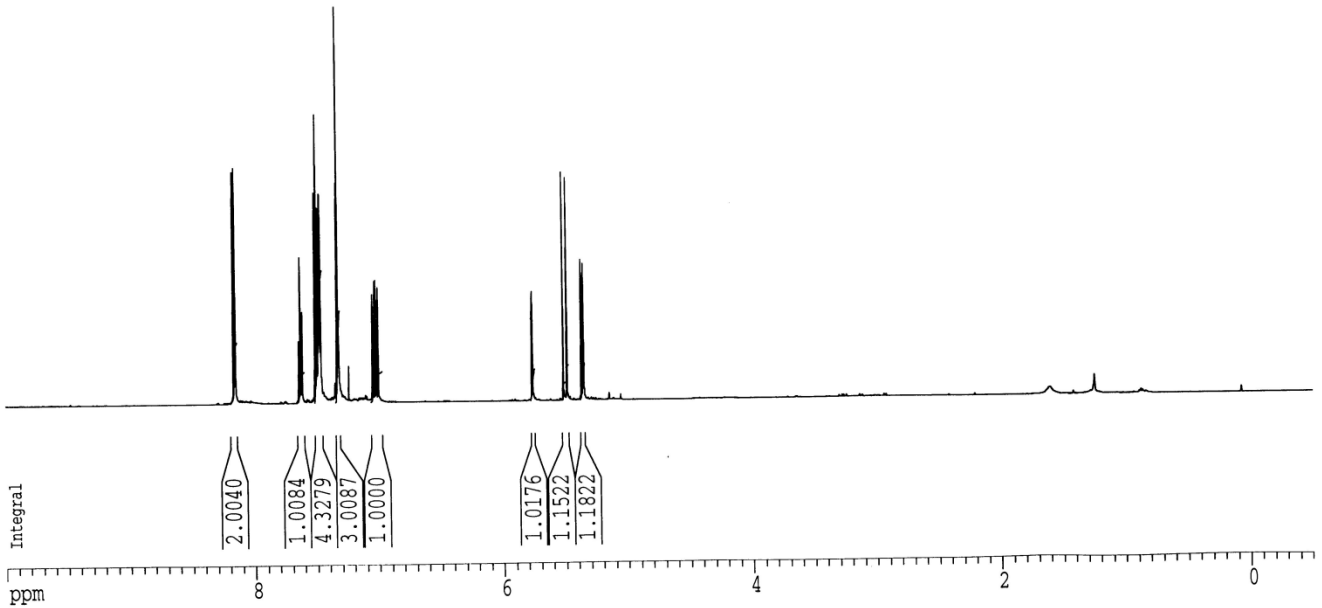

4
6
5
Ha
H1
H3
O
Hb
O
H2
H4
H6
H5
3j
Integral
4.78
15.97
-100.0
ppm
8.0
7.5
7.0
6.5
6.0
5.5


b,b'
6
5
Ha
H1
H3
O
Hb
O
H2
H4
H6
H5
3j
Integral
1.00
-100.0
10.74
ppm
8.0
7.5
7.0
6.5
6.0
5.5

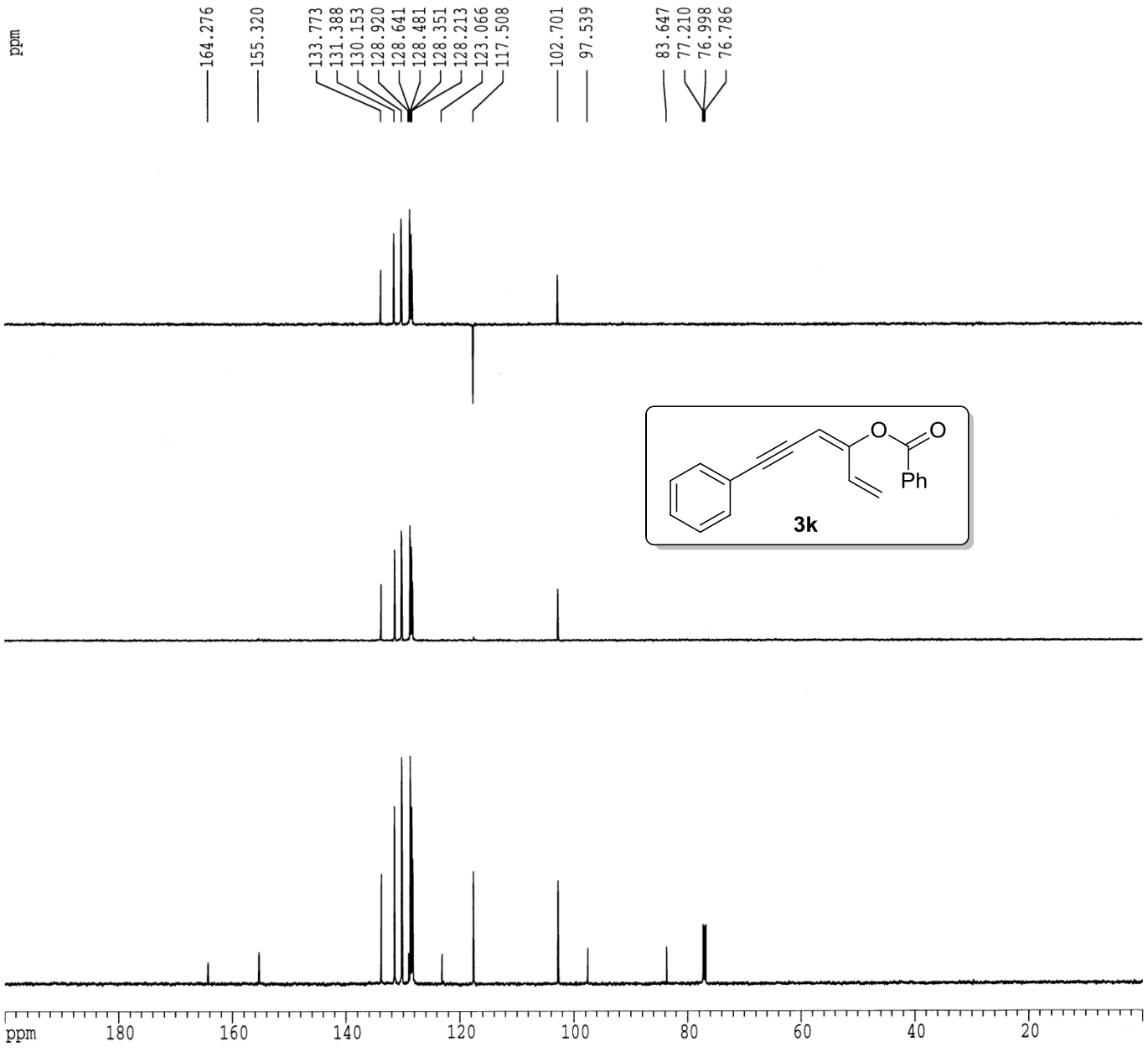

Current Data Parameters
NAME SBW-209
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150420
Time 9.22
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 297.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000299 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm

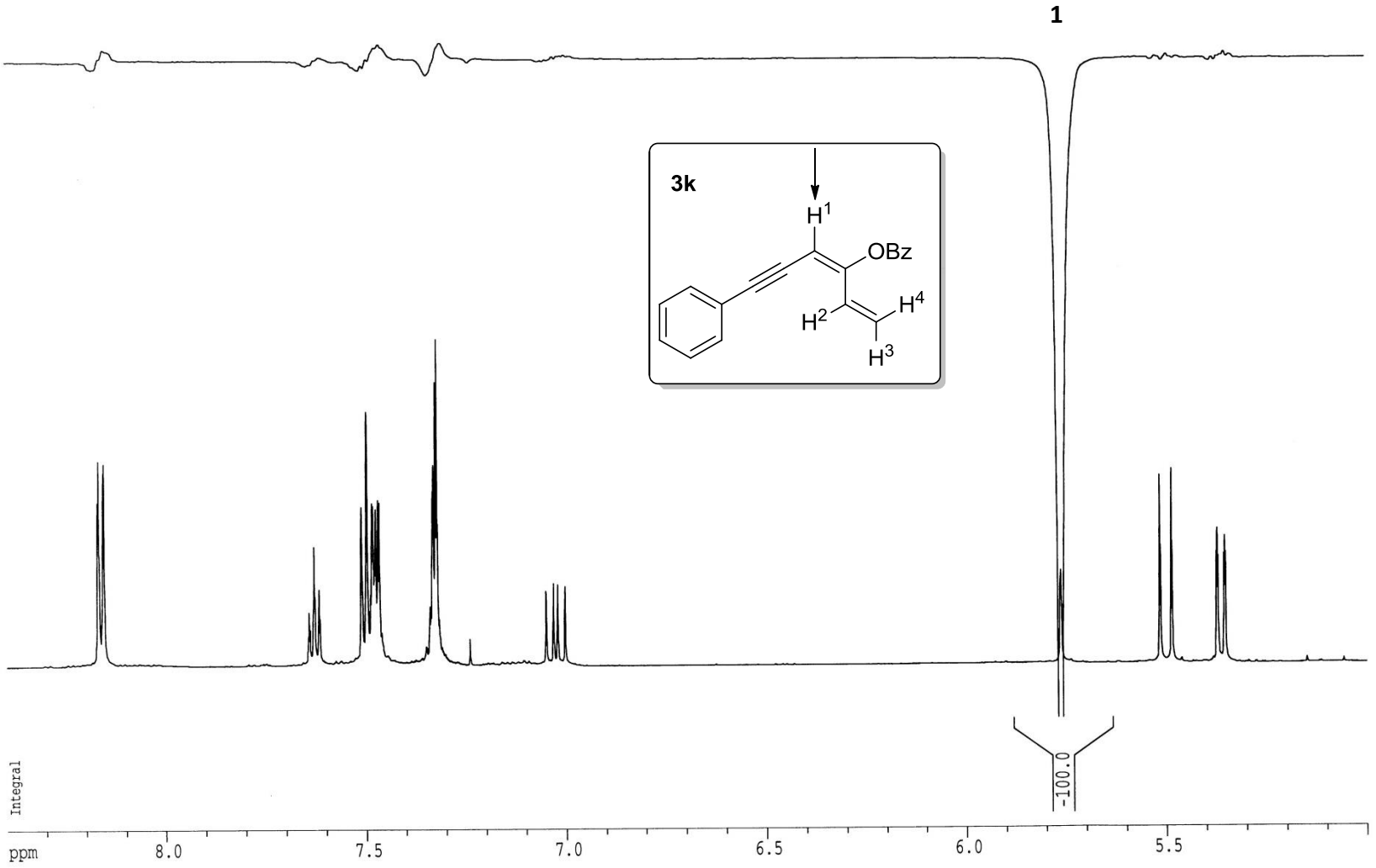

ppm
8.17057
8.16852
8.15674
8.15447
7.62960
7.51161
7.49856
7.49795
7.48536
7.48296
7.47717
7.47569
7.47036
7.46671
7.33453
7.33201
7.32665
7.32295
5.51689
5.51567
5.48810
5.48700
5.37362
5.37239
5.37109
5.35532
5.35411
5.35273

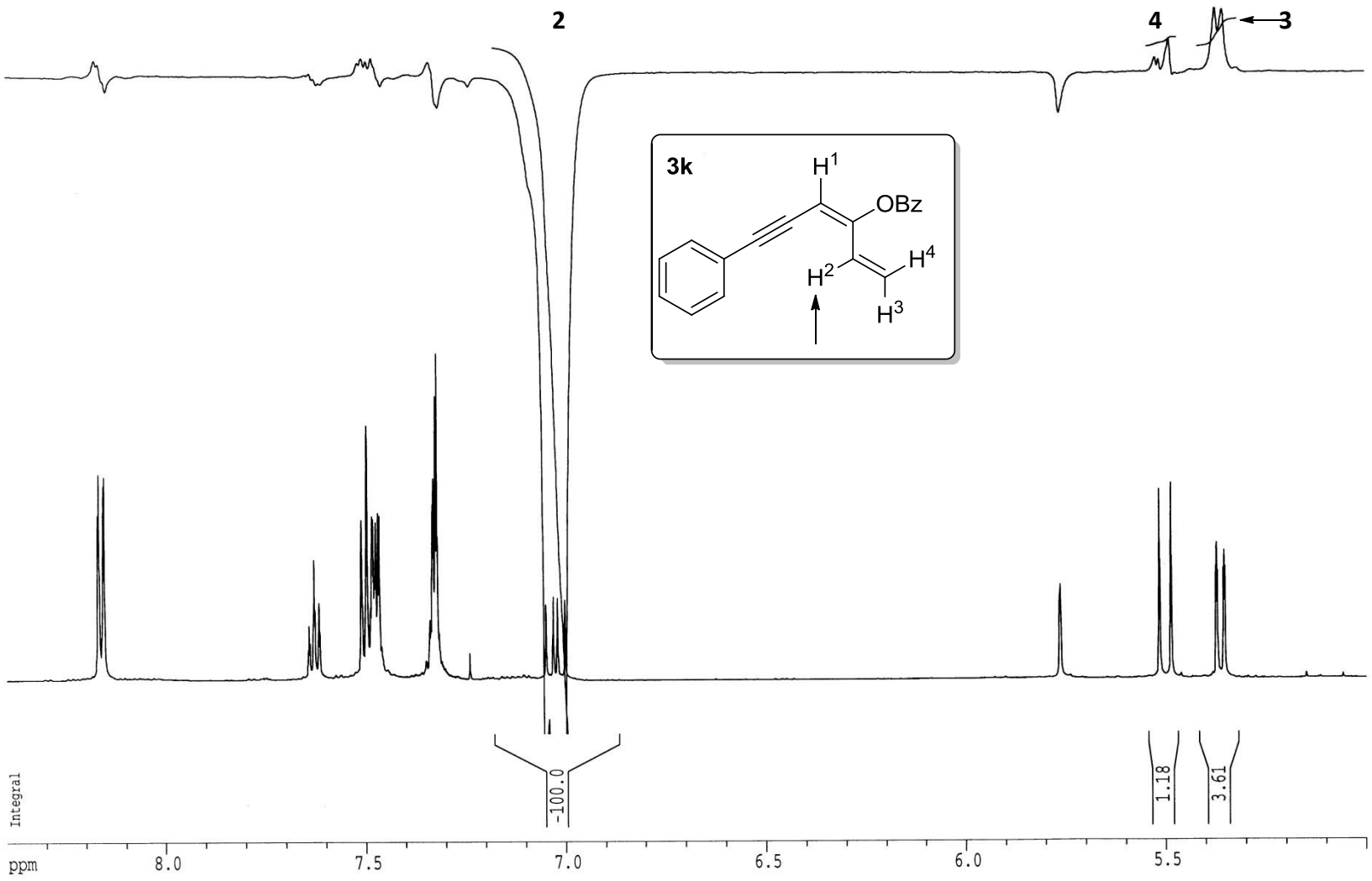

O
O
Ph
3k

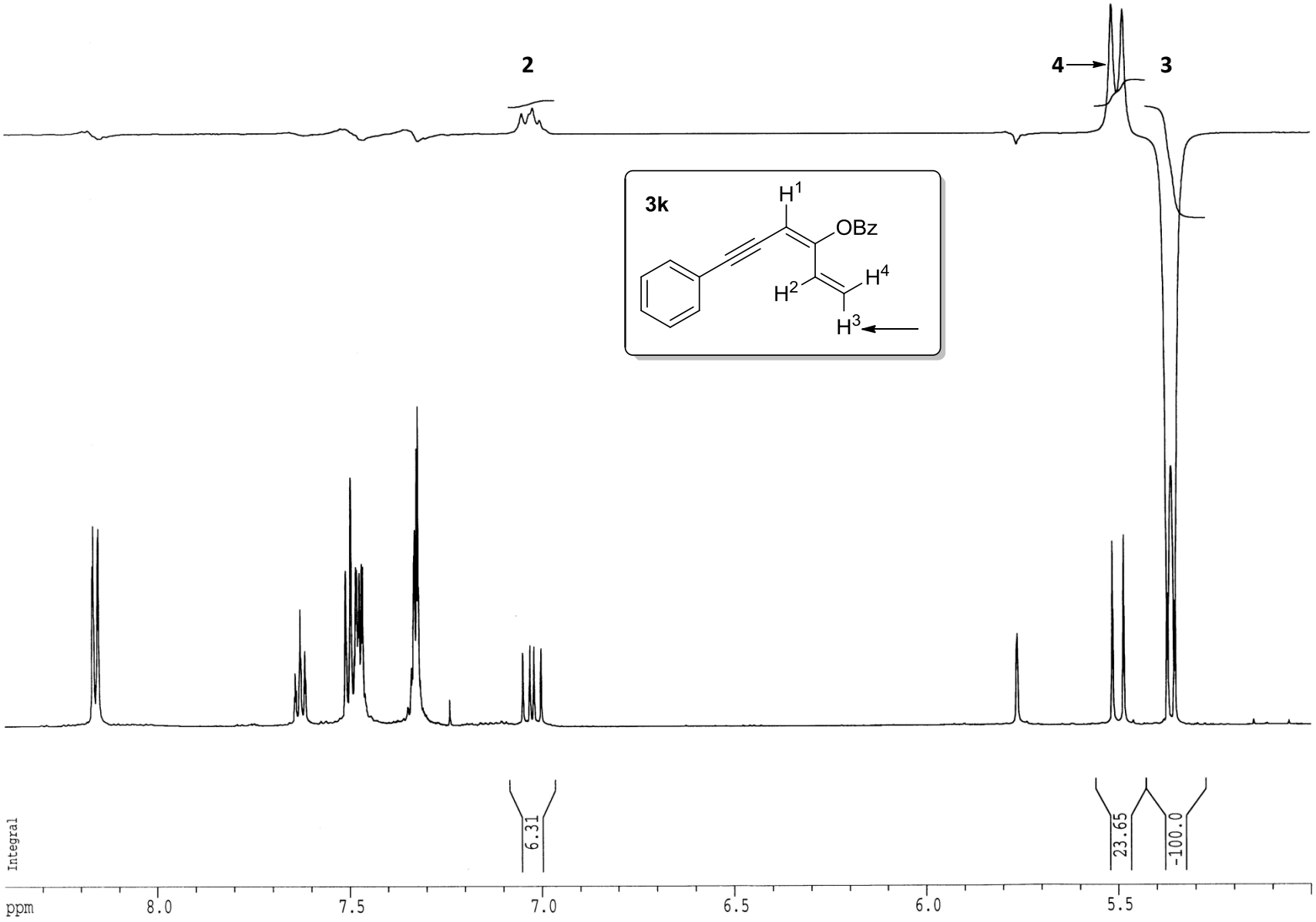

Integral
2.0040
1.0084
4.3279
3.0087
1.0000
1.0176
1.1522
1.1822
ppm
8
6
4
2
0

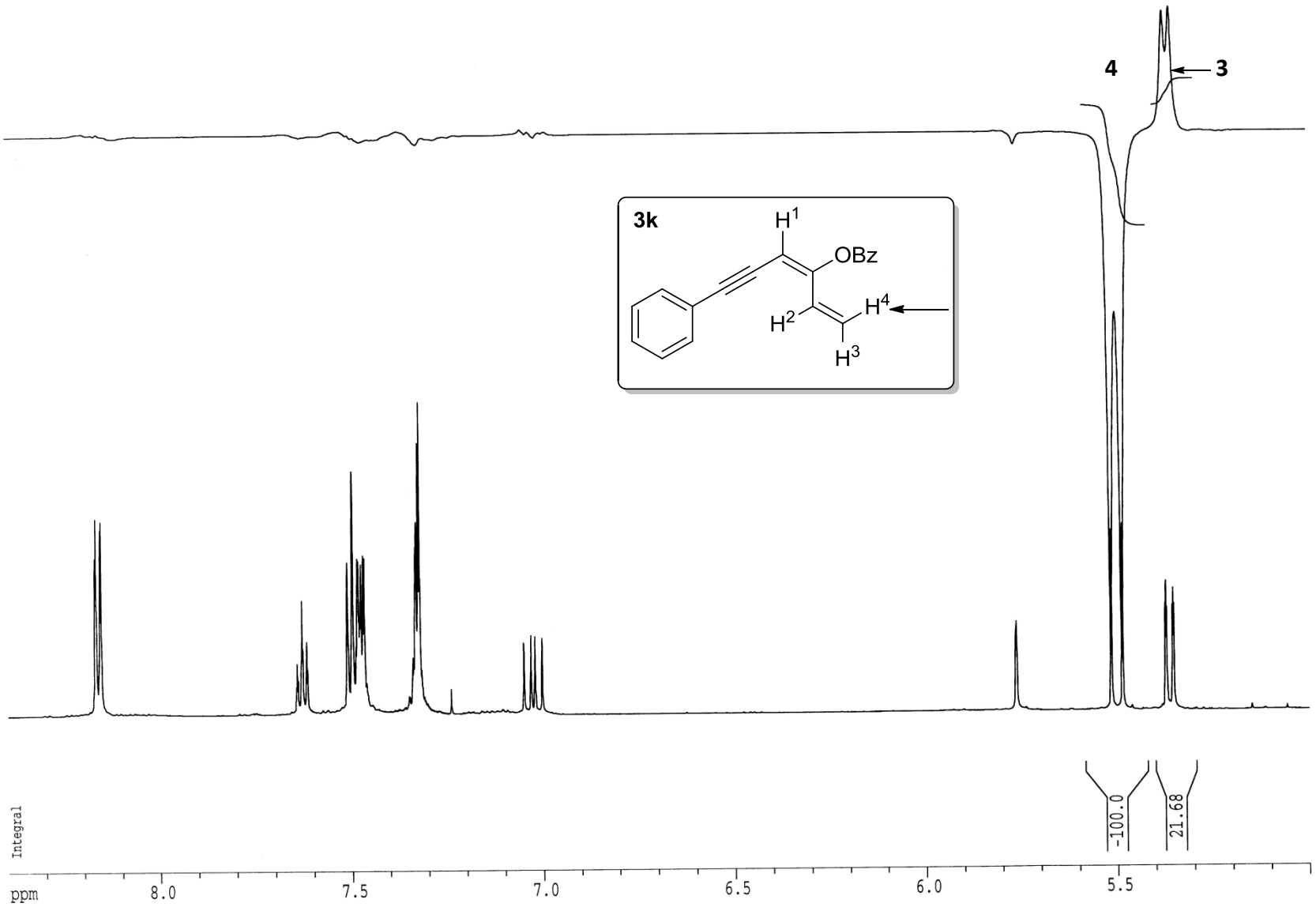
```
Current Data Parameters
NAME            SBW-209
EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20150420
Time               9.25
INSTRUM           spect
PROBHD   5 mm QNP  1H/1
PULPROG           zgpg
TD               32768
SOLVENT           CDCl3
NS                  100
DS                    0
SWH           45045.047 Hz
FIDRES         1.374666 Hz
AQ            0.3637748 sec
RG                 4096
DW               11.100 usec
DE                6.50 usec
TE               298.1 K
D1           3.50000000 sec
d11          0.03000000 sec
DELTA        3.40000010 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 4.80 usec
PL1                0.00 dB
SFO1        150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             92.00 usec
PL2              120.00 dB
PL12               9.00 dB
PL13              14.00 dB
SFO2        598.6029930 MHz

F2 - Processing parameters
SI                 65536
SF          150.5180994 MHz
WDW                   EM
SSB                    0
LB                  3.00 Hz
GB                     0
PC                  1.00

1D NMR plot parameters
CX                 20.00 cm
CY                  4.00 cm
F1P              200.000 ppm
F1              30103.62 Hz
F2P              0.000 ppm
F2                0.00 Hz
PPMCM          10.00000 ppm/cm
HZCM         1505.18091 Hz/cm
```



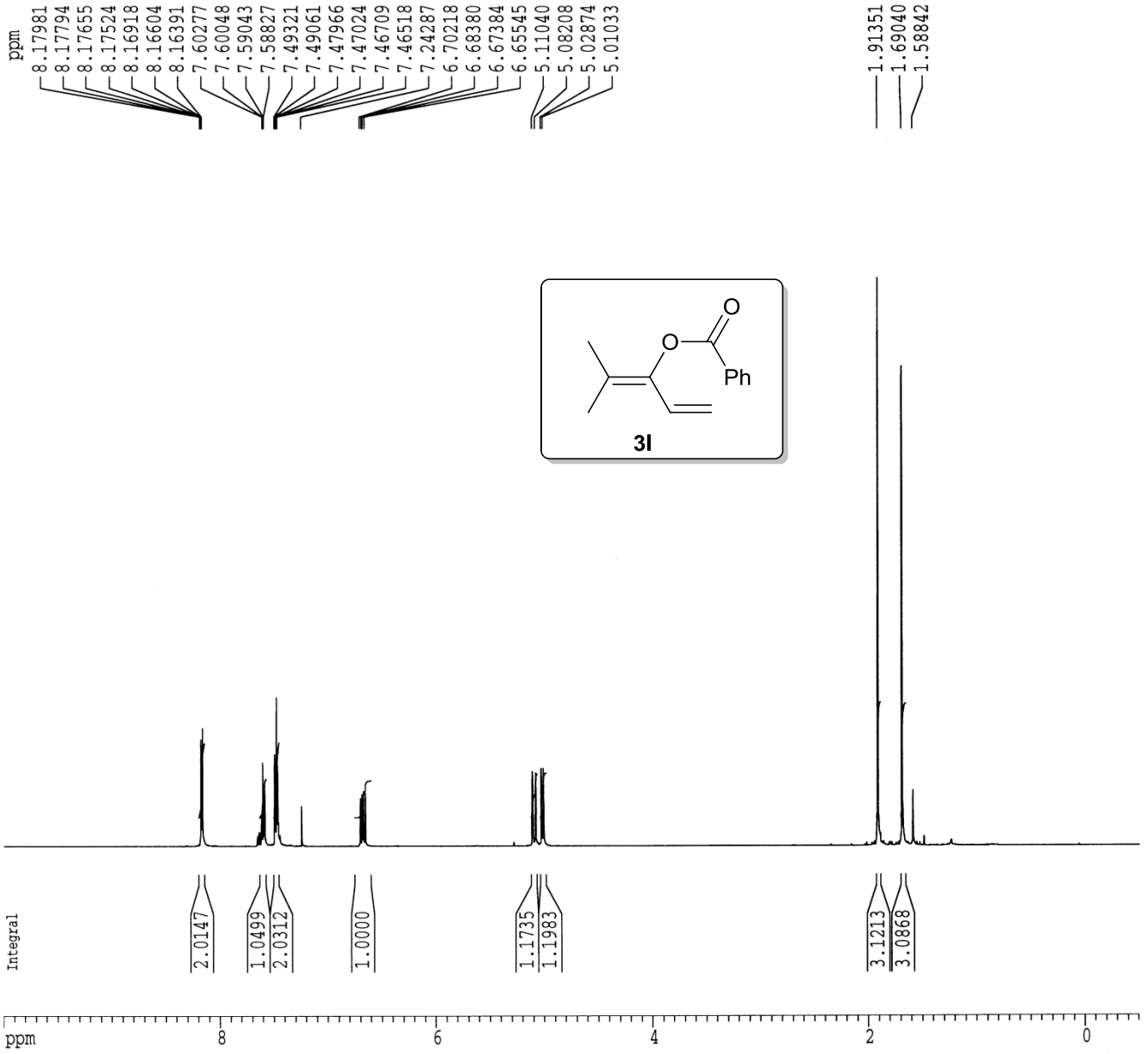

1
3k
H1
OBz
H2
H4
H3
Integral
-100.0
ppm
8.0
7.5
7.0
6.5
6.0
5.5

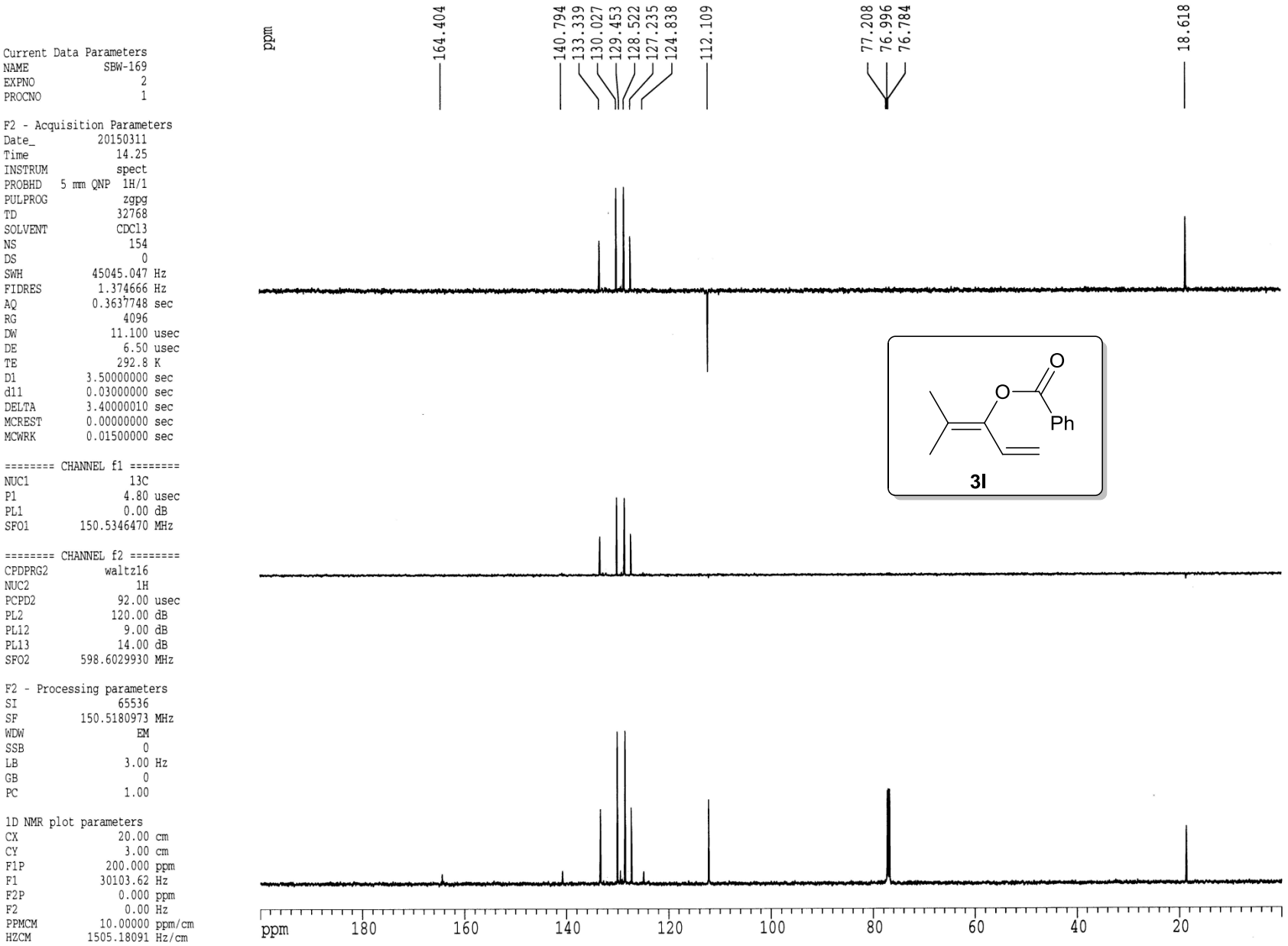

2
4
3
3k
H1
OBz
H4
H2
H3
Integral
-100.0
1.18
3.61
ppm
8.0
7.5
7.0
6.5
6.0
5.5

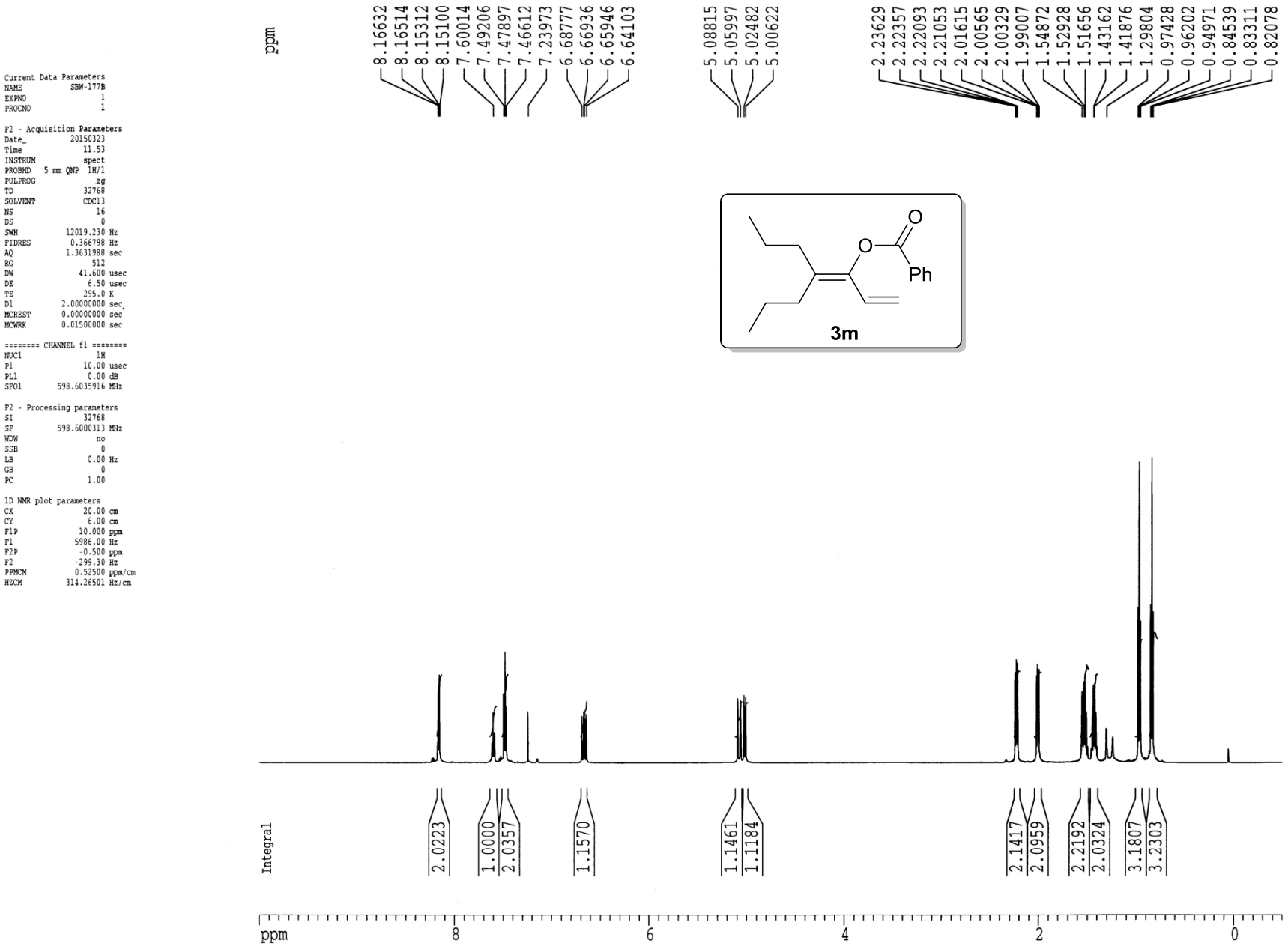

2
4
3
3k
H1
OBz
H2
H4
H3
Integral
6.31
23.65
-100.0
ppm
8.0
7.5
7.0
6.5
6.0
5.5

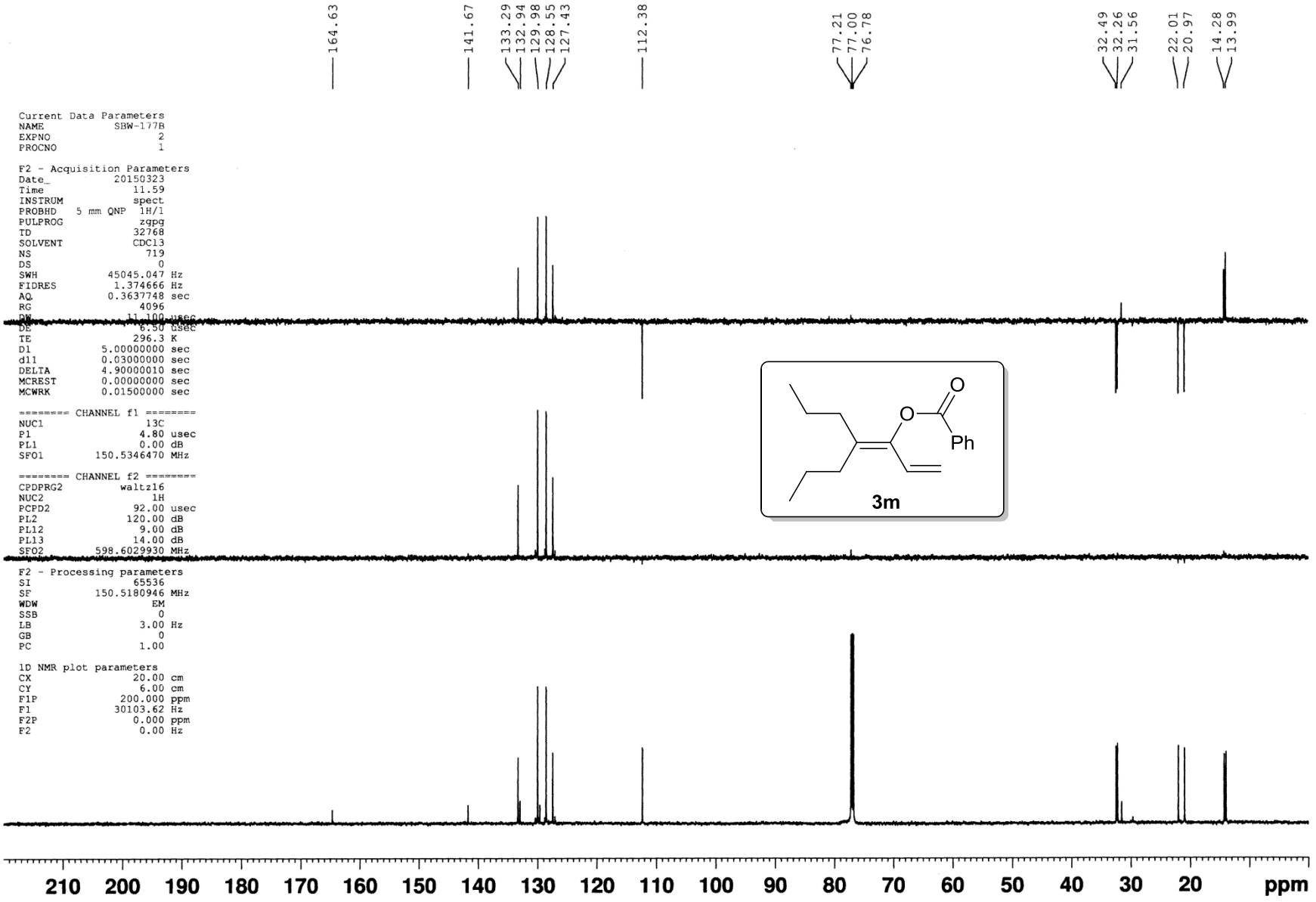

4
3
3k
H1
OBz
H2
H4
H3
Integral
-100.0
21.68
ppm
8.0
7.5
7.0
6.5
6.0
5.5

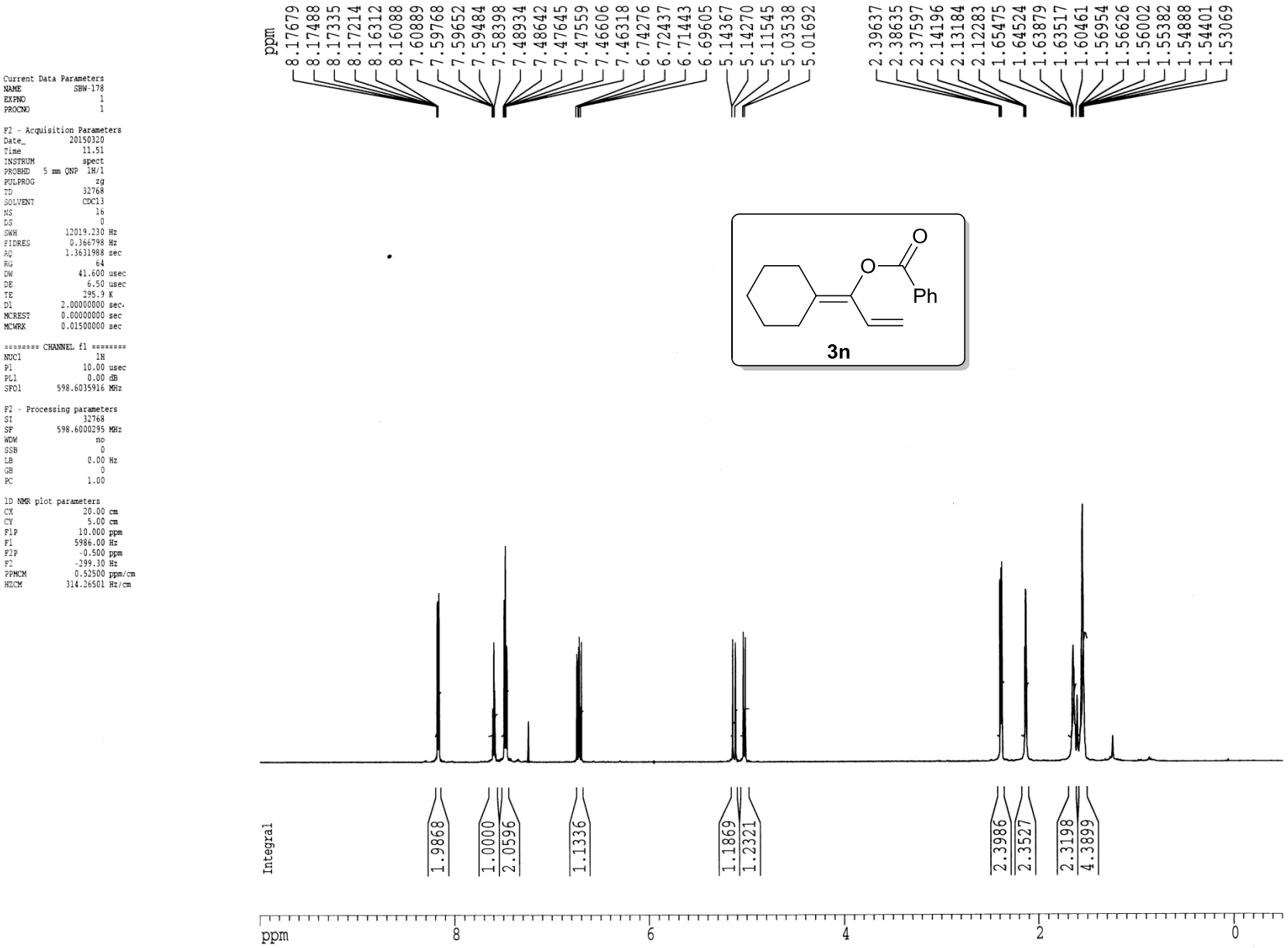
```
Current Data Parameters
NAME              SBW-169
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20150311
Time                14.24
INSTRUM             spect
PROBHD   5 mm QNP  1H/1
PULPROG                zg
TD                  32768
SOLVENT             CDCl3
NS                     16
DS                      0
SWH             12019.230 Hz
FIDRES              0.366798 Hz
AQ                1.3631988 sec
RG                     512
DW                  41.600 usec
DE                   6.50 usec
TE                  292.5 K
D1              1.50000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
PL1                  0.00 dB
SFO1          598.6035916 MHz

F2 - Processing parameters
SI                  32768
SF            598.6000291 MHz
WDW                    EM
SSB                     0
LB                   0.10 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                  10.00 cm
F1P                10.000 ppm
F1                 5986.00 Hz
F2P                -0.500 ppm
F2                 -299.30 Hz
PPMCM              0.52500 ppm/cm
HZCM             314.26501 Hz/cm
```

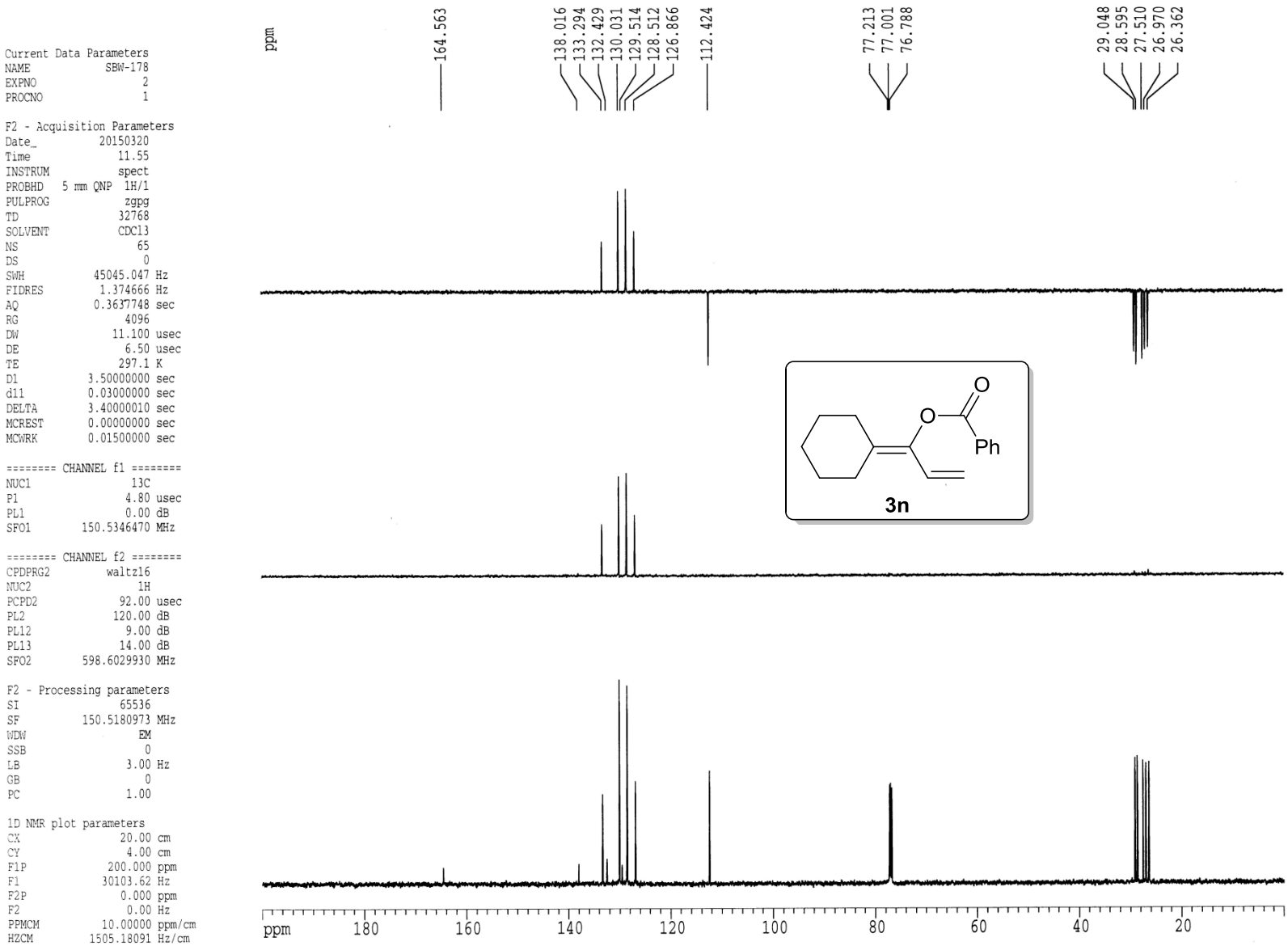


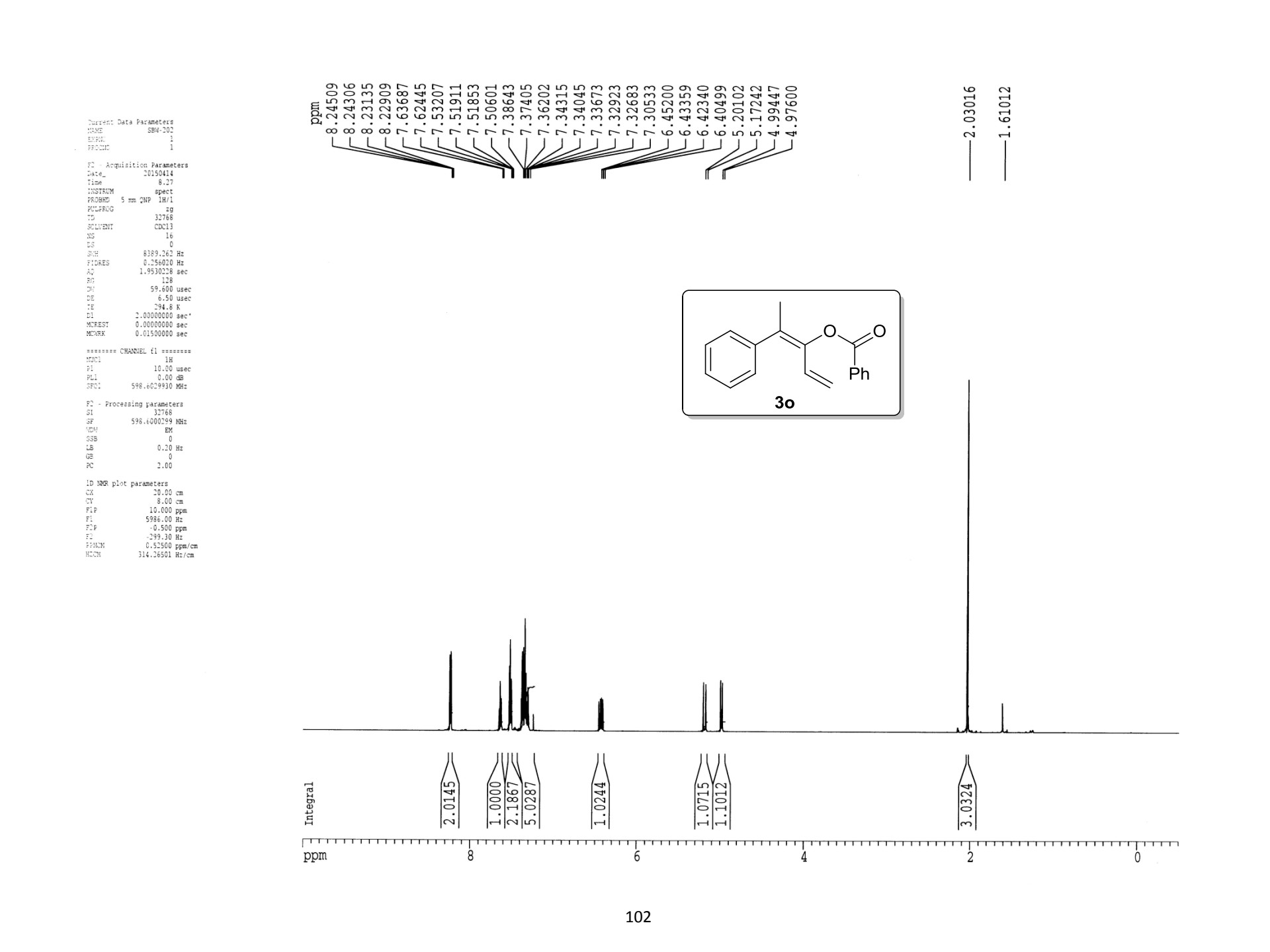

Current Data Parameters
NAME SBW-169
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150311
Time 14.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 154
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 292.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180973 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 3.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
164.404
140.794
133.339
130.027
129.453
128.522
127.235
124.838
112.109
77.208
76.996
76.784
18.618
O
O
Ph
3l
ppm
180
160
140
120
100
80
60
40
20

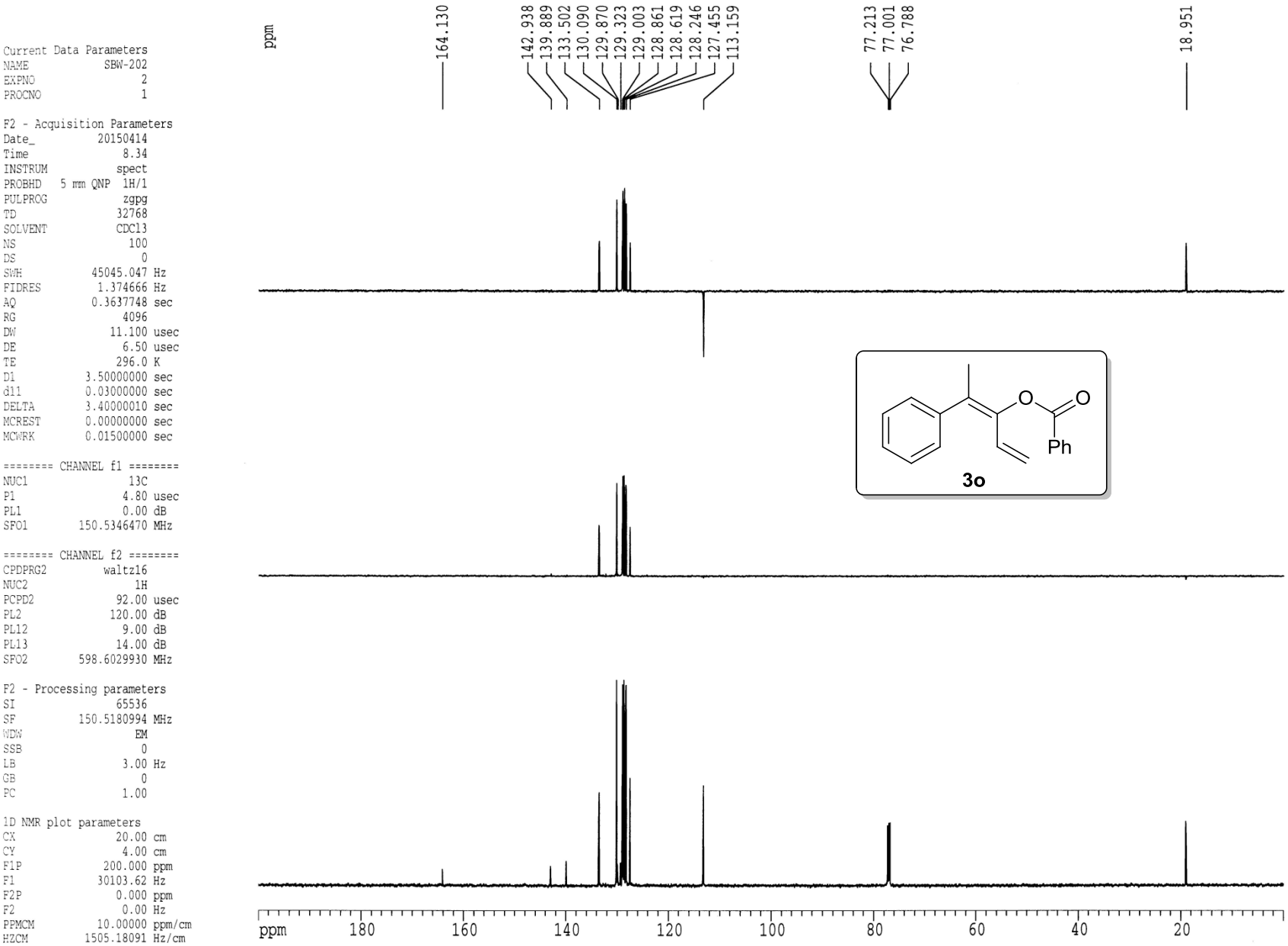

Current Data Parameters
NAME SBW-177B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150323
Time 11.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000313 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.16632
8.16514
8.15312
8.15100
7.60014
7.49206
7.47897
7.46612
7.23973
6.68777
6.66936
6.65946
6.64103
5.08815
5.05997
5.02482
5.00622
2.23629
2.22357
2.22093
2.21053
2.01615
2.00565
2.00329
1.99007
1.54872
1.52928
1.51656
1.43162
1.41876
1.29804
0.97428
0.96202
0.94971
0.84539
0.83311
0.82078
O
O
Ph
3m
Integral
2.0223
1.0000
2.0357
1.1570
1.1461
1.1184
2.1417
2.0959
2.2192
2.0324
3.1807
3.2303
ppm
8
6
4
2
0

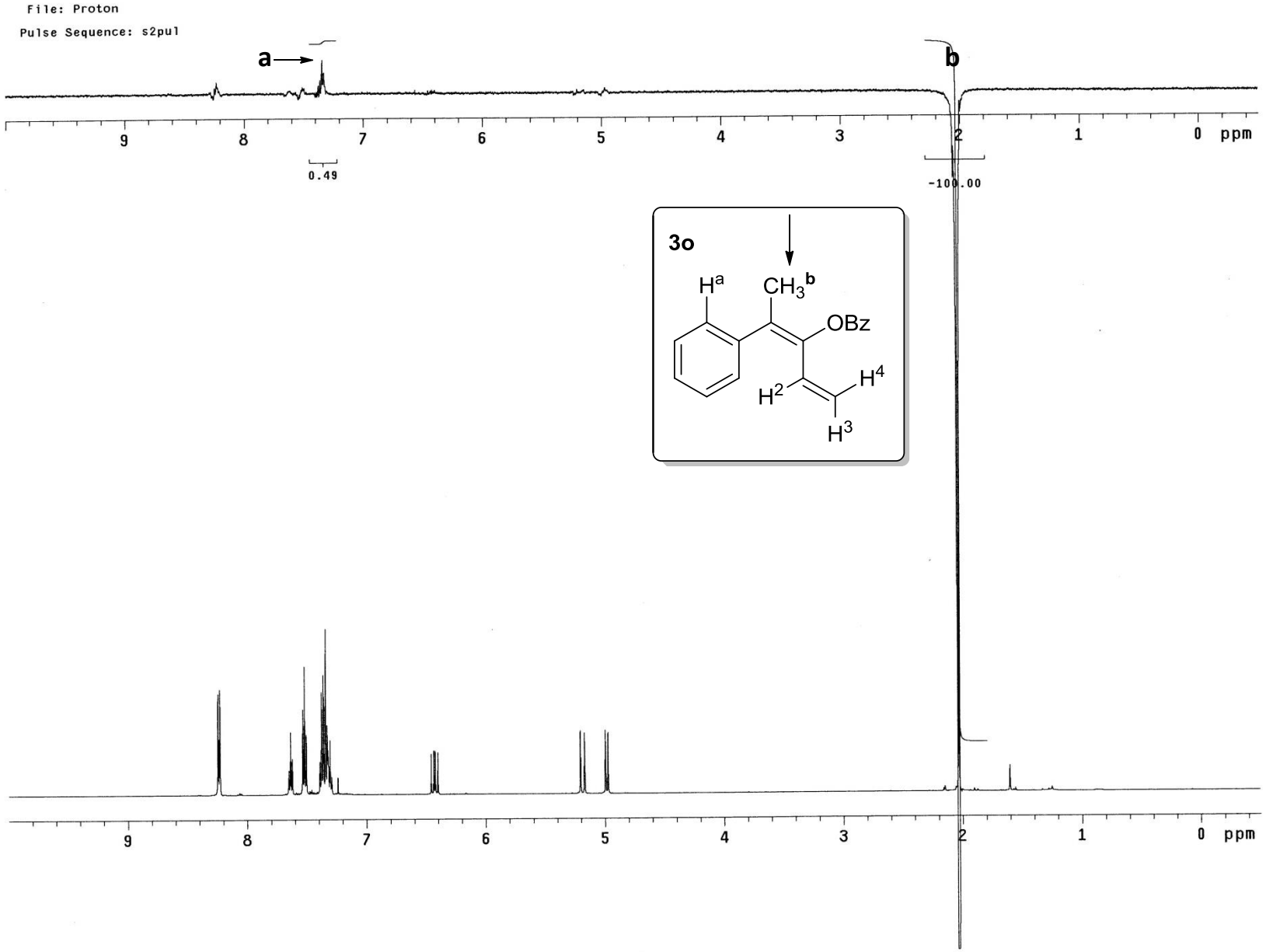

164.63
141.67
133.29
132.94
129.98
128.55
127.43
112.38
77.21
77.00
76.78
32.49
32.26
31.56
22.01
20.97
14.28
13.99
Current Data Parameters
NAME SBW-177B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150323
Time 11.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 719
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.3 K
D1 5.00000000 sec
d11 0.03000000 sec
DELTA 4.90000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180946 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
O
O
Ph
3m
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

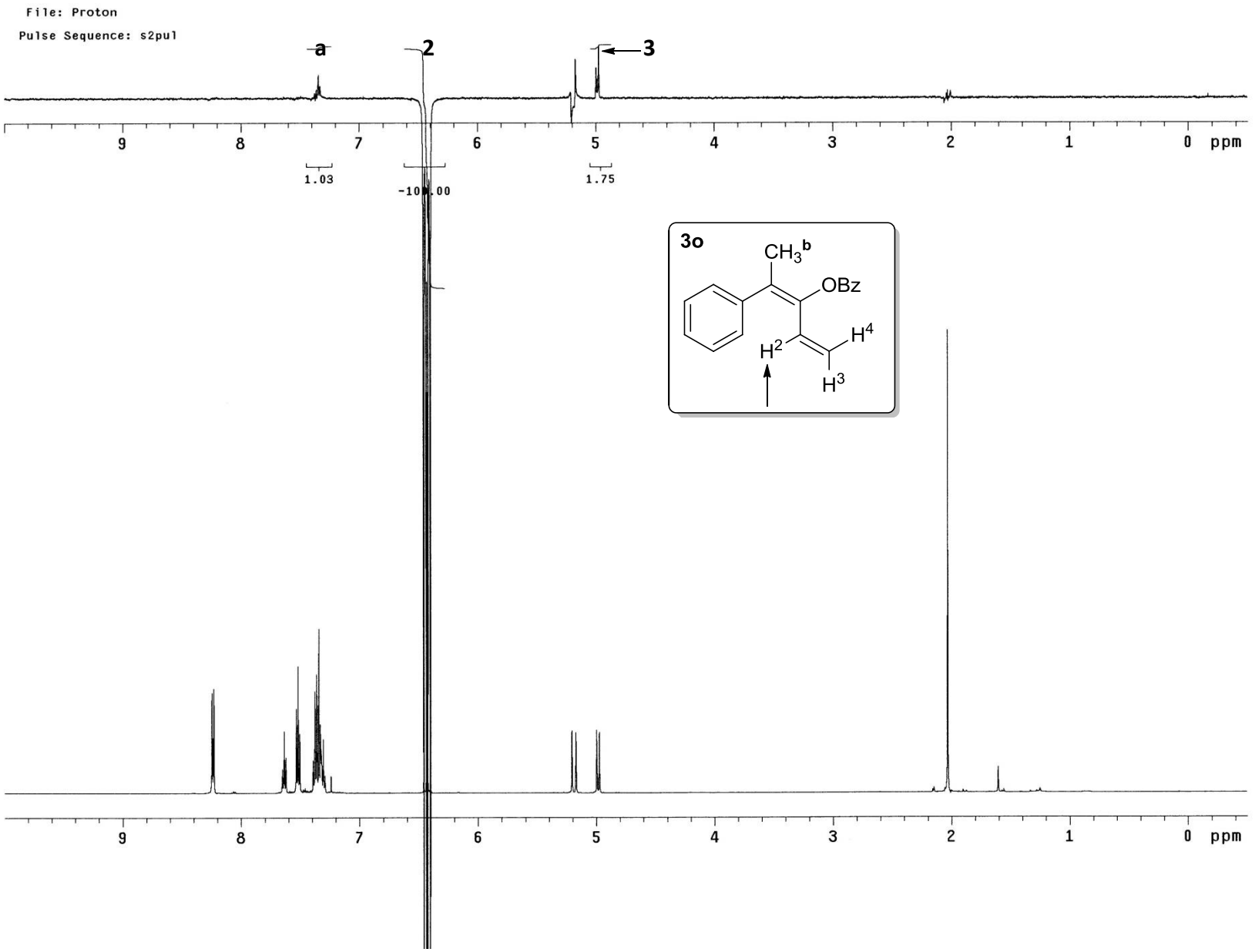

Current Data Parameters
NAME SBW-178
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150320
Time 11.51
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 295.9 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000295 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.17679
8.17488
8.17335
8.17214
8.16312
8.16088
7.60889
7.59768
7.59652
7.59484
7.58398
7.48934
7.48642
7.47645
7.47559
7.46606
7.46318
6.74276
6.72437
6.71443
6.69605
5.14367
5.14270
5.11545
5.03538
5.01692
2.39637
2.38635
2.37597
2.14196
2.13184
2.12283
1.65475
1.64524
1.63879
1.63517
1.60461
1.56954
1.56626
1.56002
1.55382
1.54888
1.54401
1.53069
O
O
Ph
3n
Integral
1.9868
1.0000
2.0596
1.1336
1.1869
1.2321
2.3986
2.3527
2.3198
4.3899
ppm
8
6
4
2
0

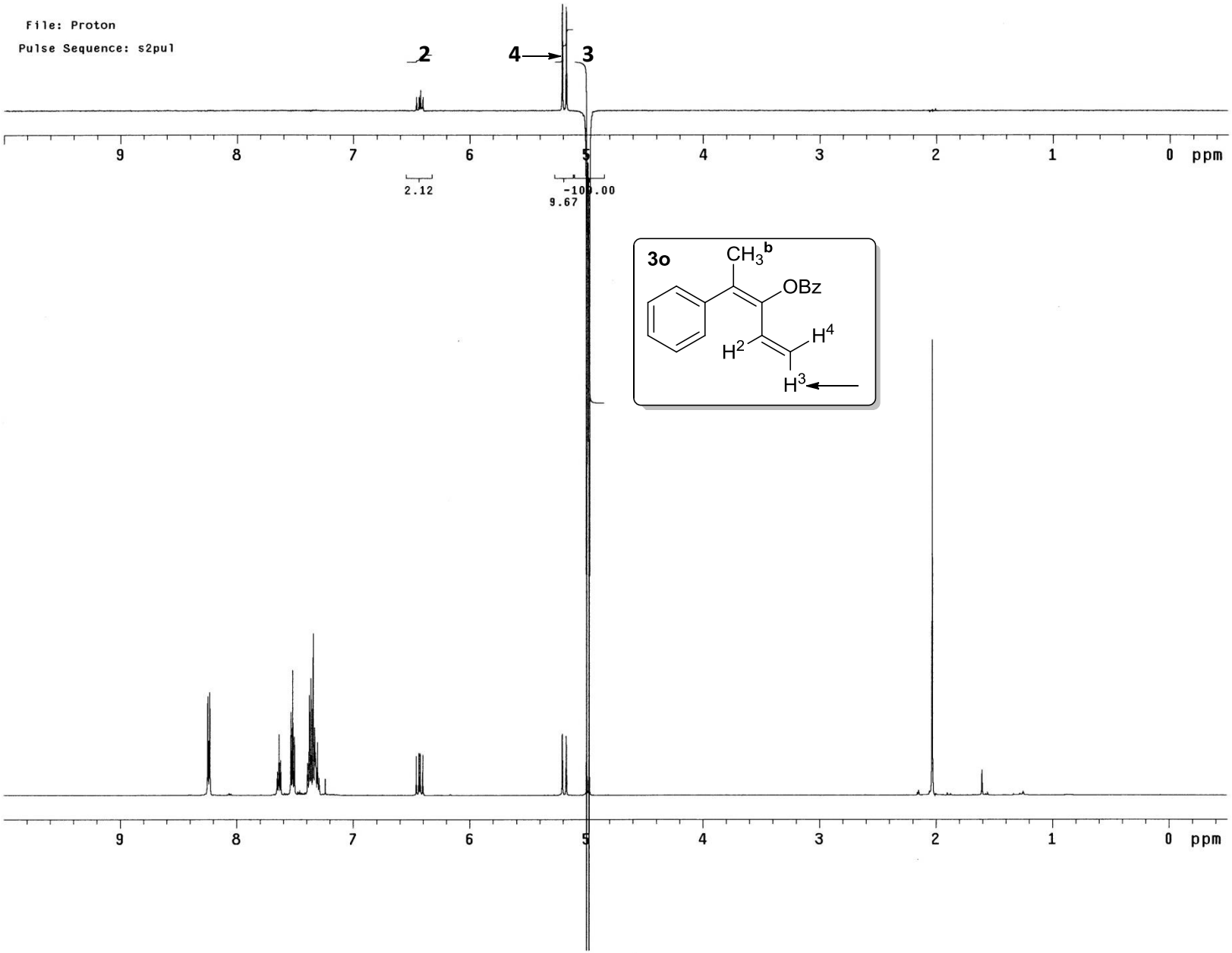

Current Data Parameters
NAME SBW-178
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150320
Time 11.55
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 65
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180973 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
164.563
138.016
133.294
132.429
130.031
129.514
128.512
126.866
112.424
77.213
77.001
76.788
29.048
28.595
27.510
26.970
26.362
O
O
Ph
3n
ppm
180
160
140
120
100
80
60
40
20

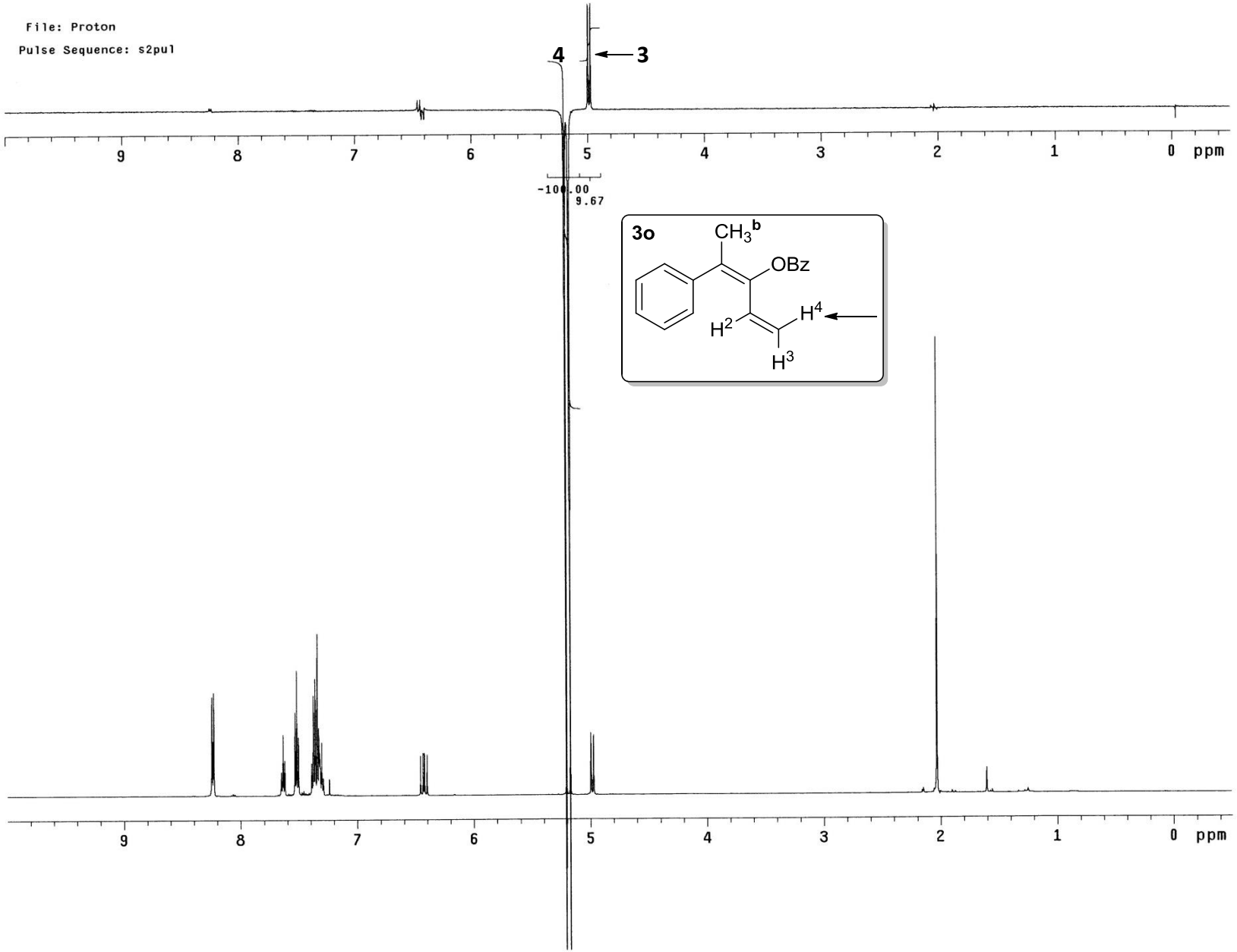

Current Data Parameters
NAME SB4-202
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150414
Time 8.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 294.8 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000299 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 2.00
1D NMR plot parameters
CX 20.00 cm
CY 8.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.24509
8.24306
8.23135
8.22909
7.63687
7.62445
7.53207
7.51911
7.51853
7.50601
7.38643
7.37405
7.36202
7.34315
7.34045
7.33673
7.32923
7.32683
7.30533
6.45200
6.43359
6.42340
6.40499
5.20102
5.17242
4.99447
4.97600
2.03016
1.61012
O
O
Ph
3o
Integral
2.0145
1.0000
2.1867
5.0287
1.0244
1.0715
1.1012
3.0324
ppm
8
6
4
2
0

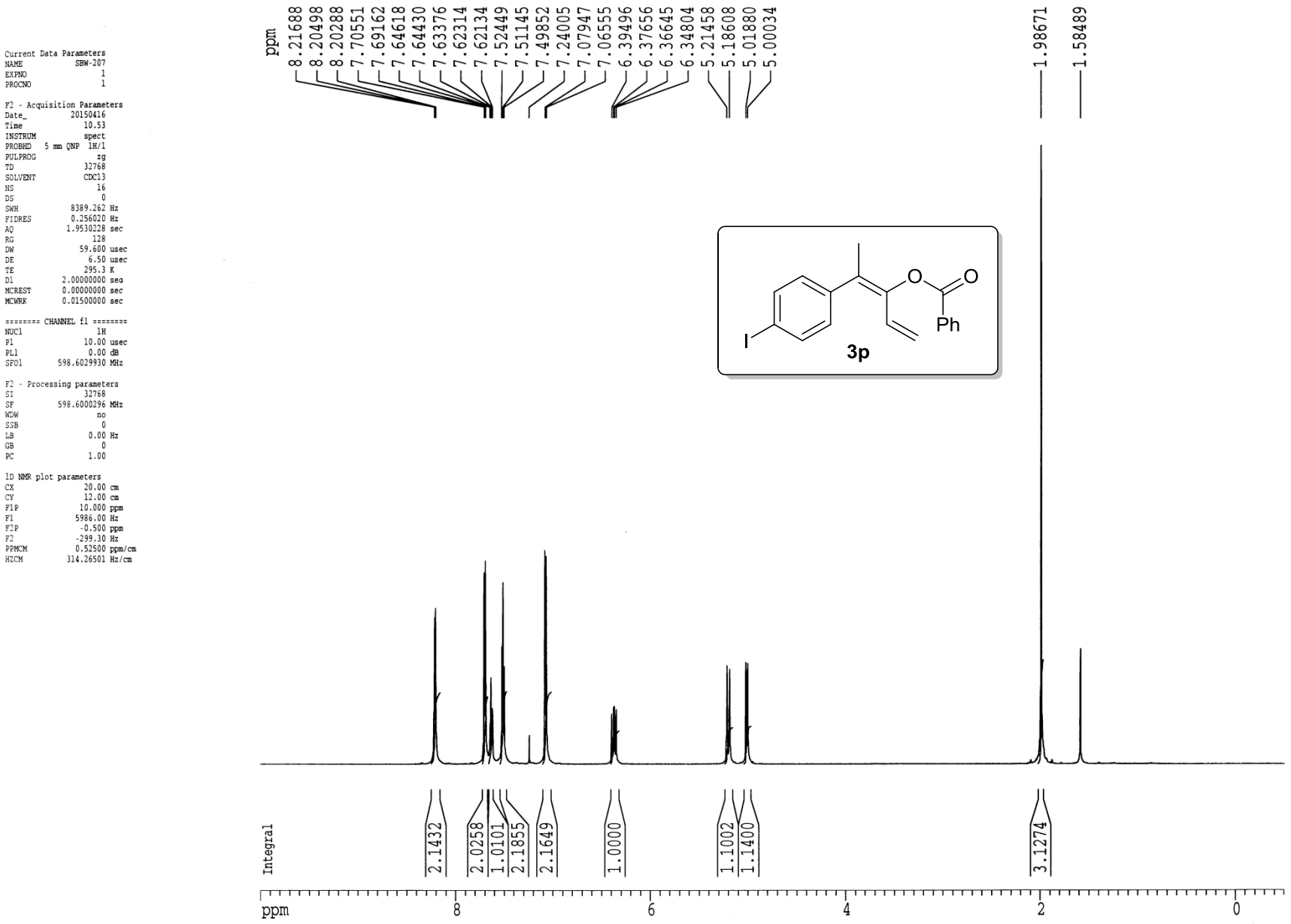

Current Data Parameters
NAME SBW-202
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150414
Time 8.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180994 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
164.130
142.938
139.889
133.502
130.090
129.870
129.323
129.003
128.861
128.619
128.246
127.455
113.159
77.213
77.001
76.788
18.951
O
O
Ph
3o
ppm
180
160
140
120
100
80
60
40
20

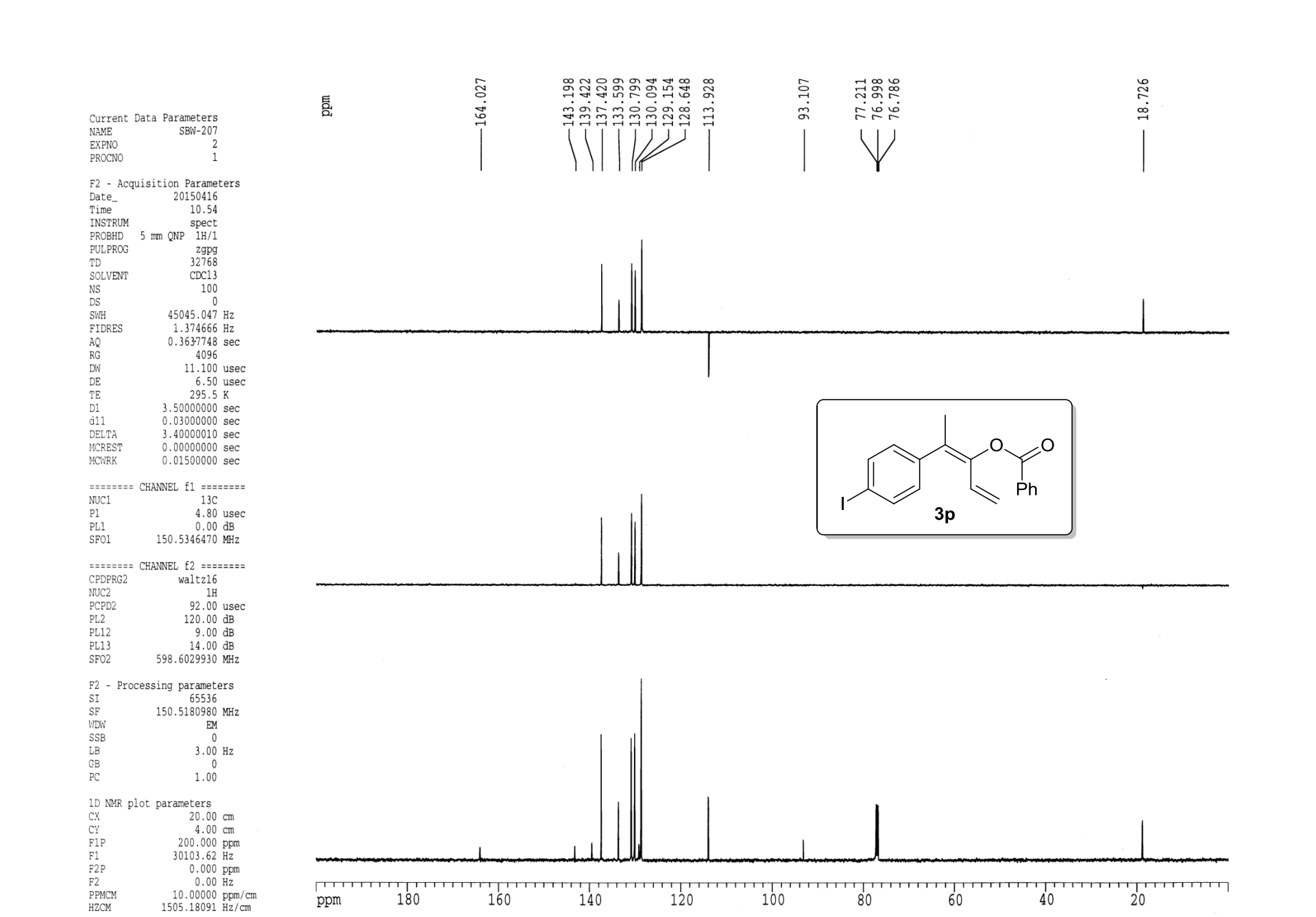

File: Proton
Pulse Sequence: s2pul
a
b
0.49
-100.00
9
8
7
6
5
4
3
2
1
0 ppm
3o
Ha
CH3b
OBz
H2
H4
H3

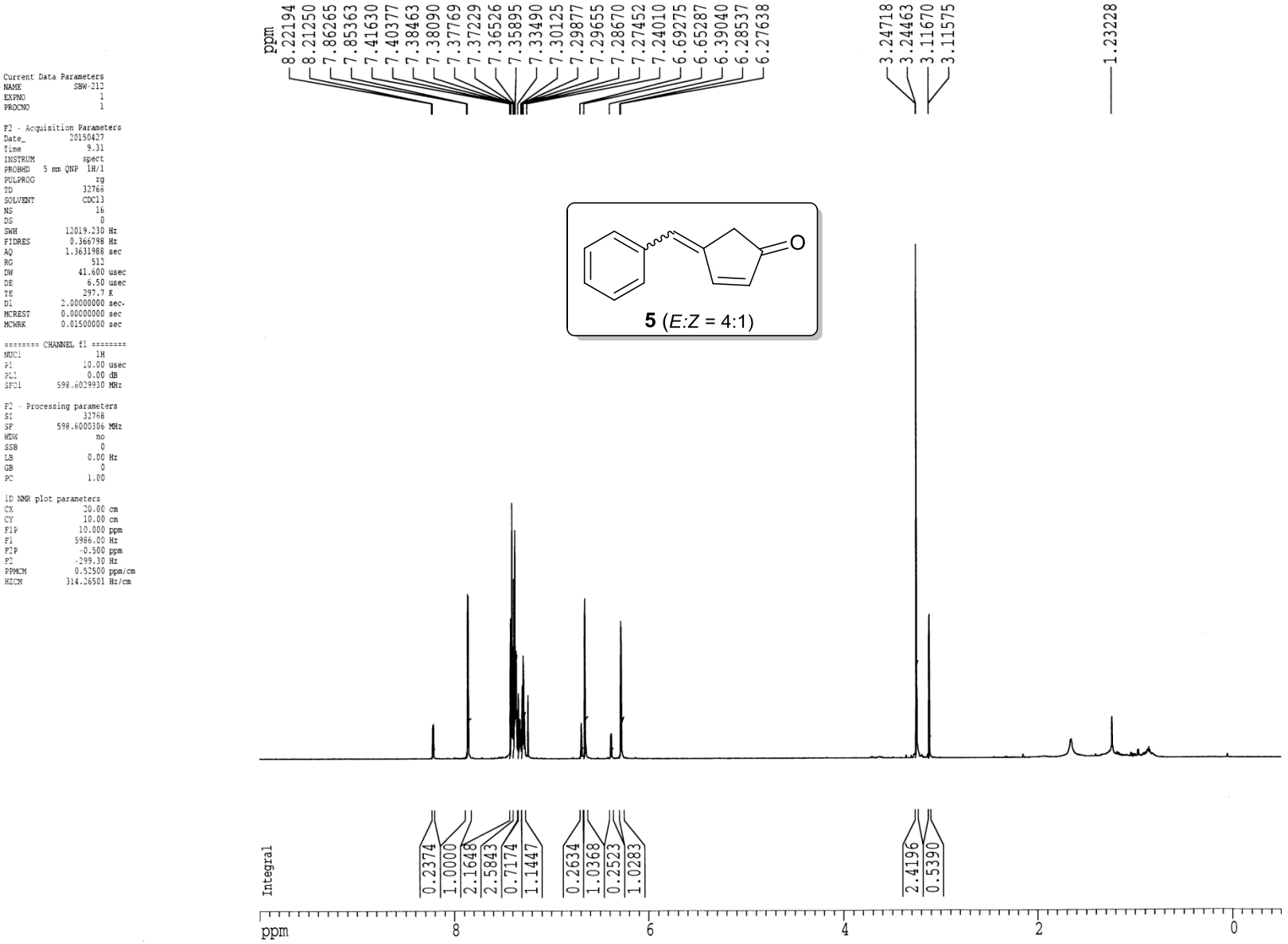

File: Proton
Pulse Sequence: s2pul
a
2
3
1.03
-10.00
1.75
9
8
7
6
5
4
3
2
1
0
ppm
3o
CH3b
OBz
H4
H2
H3

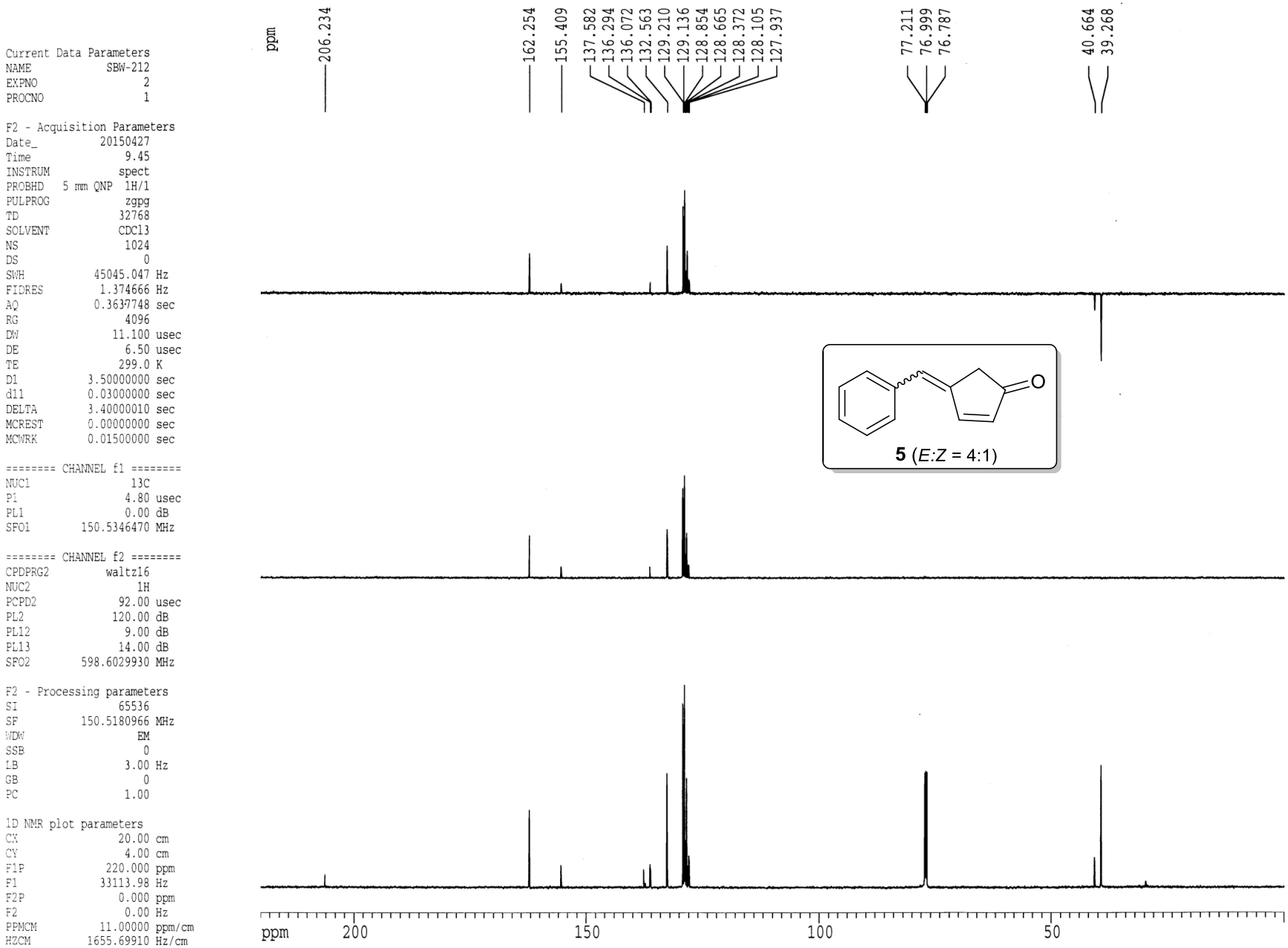

File: Proton
Pulse Sequence: s2pul
2
4
3
2.12
9.67
-100.00
3o
CH3b
OBz
H4
H2
H3
9
8
7
6
5
4
3
2
1
0 ppm


File: Proton
Pulse Sequence: s2pul
4
3
9 8 7 6 5 4 3 2 1 0 ppm
-100.00
9.67
3o
CH3b
OBz
H2
H4
H3
9 8 7 6 5 4 3 2 1 0 ppm


Current Data Parameters
NAME SBW-207
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 10.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.256020 Hz
AQ 1.9530228 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 295.3 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000296 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.21688
8.20498
8.20288
7.70551
7.69162
7.64618
7.64430
7.63376
7.62314
7.62134
7.52449
7.51145
7.49852
7.24005
7.07947
7.06555
6.39496
6.37656
6.36645
6.34804
5.21458
5.18608
5.01880
5.00034
1.98671
1.58489
O
O
Ph
I
3p
Integral
2.1432
2.0258
1.0101
2.1855
2.1649
1.0000
1.1002
1.1400
3.1274
ppm
8
6
4
2
0


Current Data Parameters
NAME SBW-207
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150416
Time 10.54
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 295.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz
F2 - Processing parameters
SI 65536
SF 150.5180980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 200.000 ppm
F1 30103.62 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 10.00000 ppm/cm
HZCM 1505.18091 Hz/cm
ppm
164.027
143.198
139.422
137.420
133.599
130.799
130.094
129.154
128.648
113.928
93.107
77.211
76.998
76.786
18.726
I
O
O
Ph
3p
ppm
180
160
140
120
100
80
60
40
20


Current Data Parameters
NAME SBW-212
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150427
Time 9.31
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 512
DW 41.600 usec
DE 6.50 usec
TE 297.7 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0.00 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000306 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.00 cm
F1P 10.000 ppm
F1 5986.00 Hz
F2P -0.500 ppm
F2 -299.30 Hz
PPMCM 0.52500 ppm/cm
HZCM 314.26501 Hz/cm
ppm
8.22194
8.21250
7.86265
7.85363
7.41630
7.40377
7.38463
7.38090
7.37769
7.37229
7.36526
7.35895
7.33490
7.30125
7.29877
7.29655
7.28670
7.27452
7.24010
6.69275
6.65287
6.39040
6.28537
6.27638
3.24718
3.24463
3.11670
3.11575
1.23228
O
5 (E:Z = 4:1)
Integral
0.2374
1.0000
2.1648
2.5843
0.7174
1.1447
0.2634
1.0368
0.2523
1.0283
2.4196
0.5390
ppm
8
6
4
2
0



Current Data Parameters
NAME SBW-212
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150427
Time 9.45
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 1024
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 299.0 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0.00 dB
SFO1 150.5346470 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.6029930 MHz

F2 - Processing parameters
SI 65536
SF 150.5180966 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 220.000 ppm
F1 33113.98 Hz
F2P 0.000 ppm
F2 0.00 Hz
PPMCM 11.00000 ppm/cm
HZCM 1655.69910 Hz/cm