Supporting Information

Gold-catalyzed Formal [4π+2π]-Cycloadditions of *tert*-Butyl Propiolates with Aldehydes and Ketones

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Contents:

(1) Natural products containing 1,3-dioxin-6-one cores (Figure S1):

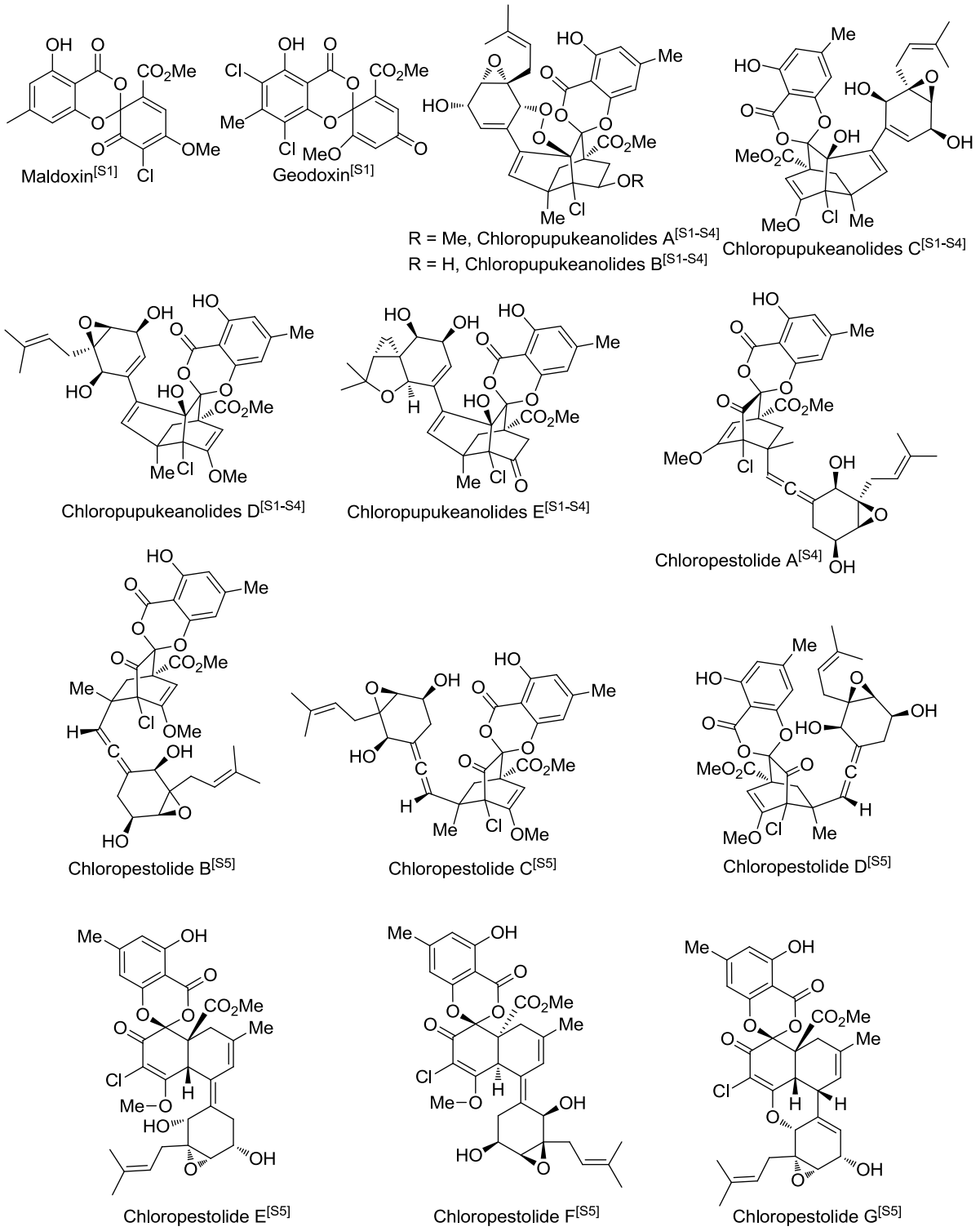


Figure S1: Representataive natural products containing 1,3-dioxin-4-one skeleton

[S1] M. O. Adeboya, R. L. Edwards, T. Lassøe, D. J. Maitland, L. Shields and A. J. S. Whalley, *J. Chem. Soc., Perkin Trans., 1* 1996, 1419–1425.

[S2] L. Liu, T. Bruhn, L. Guo, D. C. Gotz, R. Brun, A. Stich, Y.Che and G. Bringmann, *Chem. Eur. J.*, 2011, **17**, 2604–2613.

[S3] L. Liu, S. B. Niu, X. H. Lu, X. L. Chen, H. Zhang, L. D. Guo and Y. S. Che, *Chem. Commun.*, 2010, **46**, 460–462.

[S4] X.-L. Yang, J.-Z. Zhang and D.-Q. Luo, *Nat. Prod. Rep.*, 2012, **29**, 622-641.

[S5] L. Liu, Y. Li, L. Li, Y. Cao, L. Guo, G. Liu and Y. Che, *J. Org. Chem.*, 2013, **8**, 2992−3000;

[S6] a) Y. Yasuhara, T. Nishimura and T. Hayashi, *Chem. Commun.*, 2010, **46**, 2130-2132; b) D. H. Wadsworth, S. M. Geer and M. R. Detty, *J. Org. Chem.*, 1987, **52**, 3662-3668; c) S. Vercruysse, L. Cornelissen, F. Nahra, L. Collard and O. Riant, *Chem. Eur. J.*, 2014, **20,** 1834-1838; d) H. Gao and J. Zhang, *Chem. Eur. J.*, 2012, **18**, 2777–2782.

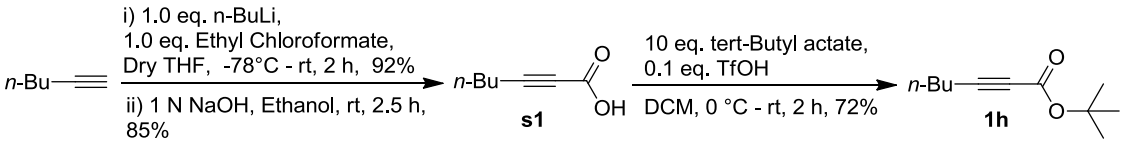
(2) Representative Synthetic procedures:

(a) General procedure:

Unless otherwise noted, all reactions were carried out under a nitrogen atmosphere in oven-dried glassware using standard syringe, cannula and septa apparatus. Tetrahydrofuran and hexanes were dried with sodium, benzophenone and distilled before use. Dichloromethane and DCE were dried over CaH_2 and distilled before use. Methanol and triethylamine (Et_3N) were stored over 4Å molecular sieves prior to use. Reagents were purchased from commercial sources and used without purification, unless otherwise stated. Reactions were magnetically stirred and monitored by thin layer chromatography carried out on 0.25 mm E. Merck silica gel plate (60f- 254) using UV light as visualizing agents and ethanolic solution of phosphomolybdic acid, and heat as deveoling agents. ^{1}H NMR and ^{13}C

NMR spectra were recorded on a Bruker 400, Varian 500 MHz and a Bruker 600 MHz spectrometers using chloroform-*d* ($CDCl_3$) as the internal standard.

(b) Preparation of *tert*-butyl 3-phenylpropiolate (1h). [S6]



To a solution of 1-hexyne (1.0 g, 12.19 mmol) in dry THF (25 mL) at -78 ˚C was added *n*-BuLi (4.95 mL, 2.5 M in hexanes, 12.19 mmol), and reaction mixture was stirred for 30 min at -78 ˚C. Ethyl chloroformate (1.16 mL, 12.19 mmol) was then added, and the reaction mixture was warmed room temperature for additional stirring for 1.5 h. The reaction was quenched with ice cold water (100 mL) and extracted with Et_2O (3 x 100 mL). The organic layers were then combined and washed with brine (100 mL), and then dried over $MgSO_4$. The resulting organic layer was concentrated under reduced pressure, and the crude product was purified by flash chromatography on silica column (Hexanes/Ethyl acetate as a mobile phase) to afford 1.72g of ethyl hept-2-ynoate (**1a**) (92% yield, 11.21 mmol) as a colorless oil.

To a solution of ethyl hept-2-ynoate (1.0 g, 6.49 mmol) in 45 mL of ethanol was added slowly with stirring an aqueous sodium hydroxide solution (25 mL, 1 N). After 2.5 h, the reaction mixture was diluted with water (50 mL) and was washed with dichloromethane (2 X 25 mL). The aqueous phase was acidified with 20% HCl solution and was extracted with dichloromethane (3 X 50 mL). The combined extracts were dried over $MgSO_4$ and concentrated under reduced pressure to give 686 mg of hept-2-ynoic acid (85% yield, 5.44 mmol).

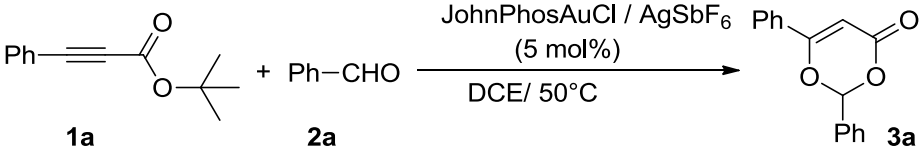
To a solution of hept-2-ynoic acid (1.0 g, 7.93 mmol) in 75 ml of DCM at 0 ℃ was added *tert*-butyl acetate (10.6 ml, 79.36 mmol) and TfOH (0.070 ml, 0.79 mmol) dropwise; the resulting solution was warmed room temperature with stirring for 2 hours before saturated $NaHCO_3$ was slowly introduced. The aqueous layer was extracted with DCM

(3x100 ml); the combined extracts were washed with saturated NaCl, then dried over $MgSO_4$, filtered, and concentrated under reduced pressure to give crude product. The crude product was purified by column chromatography on silica using ethyl acetate/hexanes = 1/10 as a mobile phase to give *tert*-butyl hept-2-ynoate (**1h)** (1.04 g, 2.63 mmol, 72%) as a colourless oil.

Other *tert*-butyl 3-propiolates **(1a – 1k)** were prepared by using the same procedure as that of *tert*-butyl hept-2-ynoate **(1h)**.

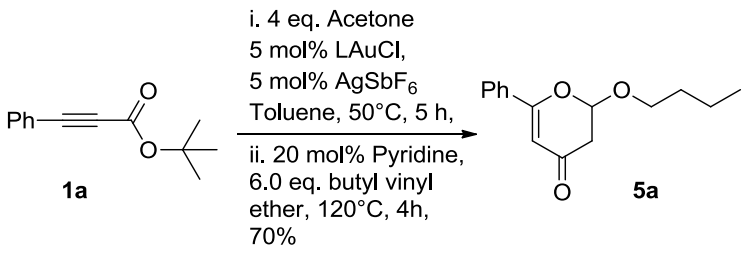
(c) Typical procedure for standard catalytic operations:

(i) Typical procedure for the synthesis of 2,6-diphenyl-4*H*-1,3-dioxin-4-one (3a).



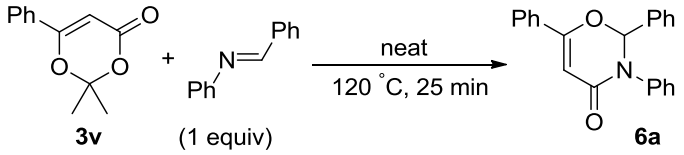
A two-neck flask was charged with chloro[(1,1′-biphenyl-2-yl)di-*tert*-butylphosphine] AuCl (13.1 mg, 0.0247 mmol) and silver hexafluoride (8.5 mg, 0.0247 mmol), and to this mixture was added dry DCE (1.0 mL). The resulting mixture was stirred at room temperature for 10 min. To this mixture was added a dry DCE solution (2 mL) of *tert*-butyl 3-phenylpropiolate (**1a)** (100 mg, 0.495 mmol) and benzaldehyde (209 mg, 1.98 mmol) dropwise. After stirring at 50 ℃ for 3.5 h, the reaction mixture was filtered over a short celite bed, concentrated, and eluted through a silica column to give the desired 2,6-diphenyl-4*H*-1,3-dioxin-4-one (**3a**) (108 mg, 0.396 mmol, 87 %) as white solid.

(ii) Typical procedure for the synthesis of 2-butoxy-6-phenyl-2*H*-pyran-4(3*H*)-one (5a).



A sealed tube was charged with chloro[(1,1′-biphenyl-2-yl)di-*tert*-butylphosphine] AuCl (13.1 mg, 0.0247 mmol) and silver hexafluoride (8.5 mg, 0.0247 mmol), and to this mixture was added dry toluene (1.0 mL); the resulting mixture was stirred at room temperature for 10 min. To this mixture was added a dry toluene solution (4 mL) of *tert*-butyl 3-phenylpropiolate (**1a)** (100 mg, 0.495 mmol) and acetone (114 mg, 1.98 mmol) dropwise. After stirring at 50 ℃ for 5 hour, the reaction mixture was added pyridine (7.8 mg, 0.99 mmol) and *n*-butyl vinyl ether (247 mg, 2.47 mmol) followed by stirring at 120 ℃ for 4 h. After completion of reaction, the resulting mixture was filtered over a short celite bed, concentrated, and eluted through a silica column to give the desired 2-butoxy-6-phenyl-2*H*-pyran-4(3*H*)-one (**5a**) (85 mg, 0.346 mmol, 70 %) as white solid.

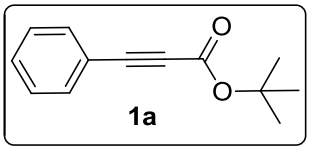
(iii) Typical procedure for the synthesis of 2,3,6-triphenyl-2H-1,3-oxazin-4(3*H*)-one (6a):



A mixture of 2,2-dimethyl-6-phenyl-4*H*-1,3-dioxin-4-one (**3v**) (100 mg, 0.490 mmol) and (*E*)-N-benzylideneaniline (88.7 mg, 0.490 mmol) was heated at 120 ℃ without any solvent for 25 min. The white solid obtained was recrystallized from a mixture of ether-hexane (1:1) to afford desired product 2,3,6-triphenyl-2*H*-1,3-oxazin-4(3*H*)-one **(6a)** (104 mg, 0.524 mmol, 65 %) as white crystals.

(4) Spectral data:

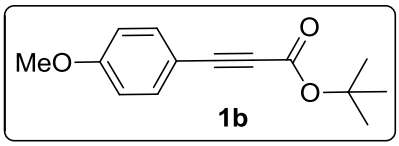
Spectral data for *tert*-butyl 3-phenylpropiolate (1a).



Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.55 ~ 7.53 (m, 2 H), 7.41 ~ 7.38 (m, 1 H), 7.34 ~ 7.31 (m, 2 H), 1.52 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.1, 132.8, 130.3,

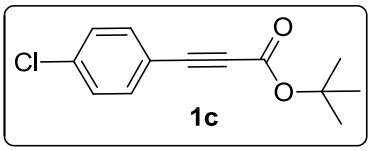
128.5, 120.0, 83.8, 83.4, 82.0, 28.0; HRMS calcd. for $C_{13}H_{14}O_2$: 202.0994; found: 202.0984.

Spectral data for *tert*-butyl 3-(4-methoxyphenyl)propiolate (1b).



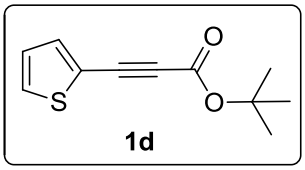
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (d, *J* = 8.8 Hz, 2 H), 6.84 (d, *J* = 8.8 Hz, 2 H), 3.80 (s, 3 H), 1.52 (s, 9 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 153.3, 134.6, 114.1, 111.6, 84.5, 83.1, 81.3, 55.2, 28.0; HRMS calcd. for $C_{14}H_{16}O_3$: 232.1099; found: 232.1096.

Spectral data for *tert*-butyl 3-(4-chlorophenyl)propiolate (1c).



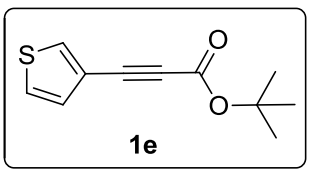
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.4 Hz, 2 H), 7.31 (d, *J* = 8.4 Hz, 2 H), 1.51 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.9, 136.6, 134.0, 128.9, 118.5, 83.7, 82.8, 82.4, 28.0; HRMS calcd. for $C_{13}H_{13}ClO_2$: 236.0604; found: 236.0601.

Spectral data for *tert*-butyl 3-(thiophen-2-yl)propiolate (1d).



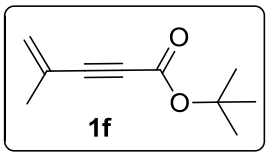
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.67 (dd, *J* = 3.0, 1.2 Hz, 1 H), 7.26 (d, *J* = 5.1, 3.0 Hz, 1 H), 7.17 (d, *J* = 5.1, 1.2 Hz, 1 H), 1.50 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.1, 133.1, 130.1, 125.9, 119.1, 83.4, 81.9, 79.2, 28.0; HRMS calcd. for $C_{11}H_{12}O_2S$: 208.0558; found: 208.0559.

Spectral data for *tert*-butyl 3-(thiophen-3-yl)propiolate (1e).



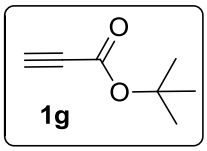
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.39 ~ 7.37 (m, 2 H), 6.99 ~ 6.96 (m, 1 H), 1.49 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.9, 136.0, 130.6, 127.3, 119.6, 86.0, 83.5, 77.6, 27.9; HRMS calcd. for $C_{11}H_{12}O_2S$: 208.0558; found: 208.0550.

Spectral data for *tert*-butyl 4-methylpent-4-en-2-ynoate (1f).



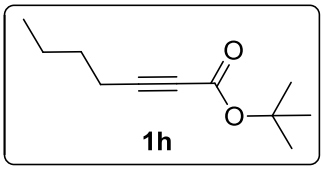
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.53 ~ 5.52 (m, 1 H), 5.44 ~ 5.43 (m, 1 H), 1.89 (m, 3 H), 1.47 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.0, 126.9, 124.5, 84.7, 83.3, 80.8, 28.0, 22.4; HRMS calcd. for $C_{10}H_{14}O_2$: 166.0994; found: 166.0996.

Spectral data for *tert*-butyl propiolate (1g).



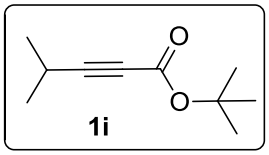
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.74 (s, 1 H), 1.45 (s, 9 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 151.6, 84.0, 75.9, 72.2, 27.8; HRMS calcd. for $C_7H_{10}O_2$: 126.0681; found: 126.0681.

Spectral data for *tert*-butyl hept-2-ynoate (1h).



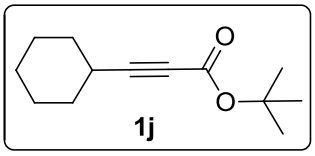
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.27 (t, J = 7.2, 2 H), 1.54 ~ 1.49 (m, 2 H), 1.46 (s, 9 H), 1.43 ~ 1.35 (m, 2 H), 0.88 (t, J = 7.3 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.0, 87.0, 82.8, 74.4, 29.6, 28.0, 21.9, 18.3, 13.4; HRMS calcd. for $C_{11}H_{18}O_2$: 182.1307; found: 182.1306.

Spectral data for *tert*-butyl 4-methylpent-2-ynoate (1i).



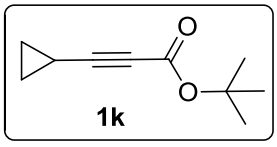
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.66 ~ 2.59 (m, 1 H), 1.46 (s, 9 H), 1.19 (d, *J* = 6.6 Hz, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.1, 91.5, 82.8, 73.7, 28.0, 21.8, 20.4; HRMS calcd. for $C_{10}H_{16}O_2$: 168.1150; found: 168.1155.

Spectral data for *tert*-butyl 3-cyclohexylpropiolate (1j).



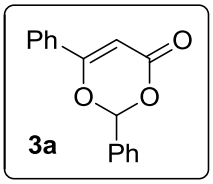
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 2.43 ~ 2.39 (m, 1 H), 1.78 ~ 1.75 (m, 2 H), 1.66 ~ 1.64 (m, 2 H), 1.46 ~ 1.40 (m, 12 H), 1.27 ~ 1.22 (m, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 153.1, 90.2, 82.6, 74.3, 31.4, 28.7, 27.9, 25.5, 24.6; HRMS calcd. for $C_{13}H_{20}O_2$: 208.1463; found: 208.1463.

Spectral data for *tert*-butyl 3-cyclopropylpropiolate (1k).



Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 1.40 (s, 9 H), 1.29 ~ 1.25 (m, 1 H), 0.83 ~ 0.80 (m, 4 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 152.7, 90.3, 82.6, 69.7, 27.9, 8.8, -0.81; HRMS calcd. for $C_{10}H_{14}O_2$: 166.0994; found: 166.1000.

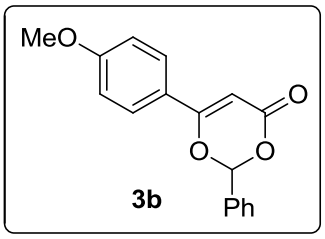
Spectral data for 2,6-diphenyl-4*H*-1,3-dioxin-4-one (3a).



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75 ~ 7.73 (m, 2 H), 7.67 ~ 7.65 (m, 2 H), 7.53 ~ 7.43 (m, 6 H), 6.55 (s, 1 H), 6.06 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.1, 162.9,

133.7, 132.5, 130.4, 130.1, 128.9, 128.6, 126.6, 126.5, 100.3, 93.2; HRMS calcd. for $C_{16}H_{12}O_3$: 252.0786; found: 252.0786.

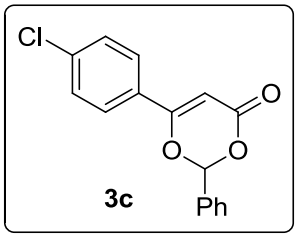
Spectral data for 6-(4-methoxyphenyl)-2-phenyl-4*H*-1,3-dioxin-4-one (3b).



3b

White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.69 ~ 7.64 (m, 4 H), 7.48 ~ 7.45 (m, 3 H), 6.93 (d, *J* = 9.0 Hz, 2 H), 6.52 (s, 1 H), 5.94 (s, 1 H), 3.84 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.1, 163.3, 163.1, 133.8, 130.3, 128.6, 128.5, 126.7, 122.3, 114.3, 100.0, 91.2, 55.5; HRMS calcd. for $C_{17}H_{14}O_4$: 282.0892; found: 282.0887.

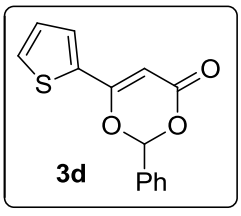
Spectral data for 6-(4-chlorophenyl)-2-phenyl-4*H*-1,3-dioxin-4-one (3c).



3c

White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.67 ~ 7.63 (m, 4 H), 7.49 ~ 7.46 (m, 3 H), 7.41 (d, *J* = 8.4 Hz, 2 H), 6.54 (s, 1 H), 6.03 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 167.0, 162.6, 138.8, 133.5, 130.5, 129.2, 128.7, 128.5, 127.8, 126.7, 100.4, 93.5; HRMS calcd. for $C_{16}H_{11}ClO_3$: 286.0397; found: 286.0392.

Spectral data for 2-phenyl-6-(thiophen-2-yl)-4H-1,3-dioxin-4-one (3d).

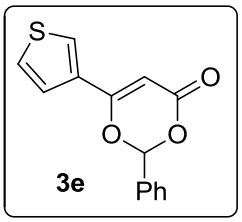


3d

White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.62 ~ 7.61 (m, 2 H), 7.56 (dd, *J* = 3.9, 0.9 Hz, 1

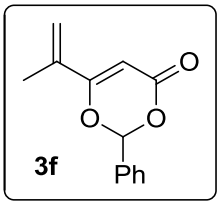
H), 7.54 (dd, *J* = 5.1, 0.9 Hz, 1 H), 7.45 ~ 7.43 (m, 3 H), 7.09 (dd, *J* = 5.1, 3.9 Hz, 1 H), 6.52 (s, 1 H), 5.87 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.1, 162.5, 133.4, 133.3, 131.4, 130.3, 129.8, 128.5, 128.4, 126.5, 100.0, 91.6; HRMS calcd. for $C_{14}H_{10}O_3S$: 258.0351; found: 258.0352.

Spectral data for 2-phenyl-6-(thiophen-3-yl)-4*H*-1,3-dioxin-4-one (3e).



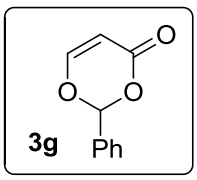
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.84 (dd, *J* = 3.0, 1.2 Hz, 1 H), 7.63 ~ 7.62 (m, 2 H), 7.47 ~ 7.44 (m, 3 H), 7.37 (dd, *J* = 4.8, 3.0 Hz, 1 H), 7.32 (dd, *J* = 4.8, 1.2 Hz, 1 H), 6.51 (s, 1 H), 5.87 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 163.8, 163.0, 133.6, 132.6, 130.3, 128.5, 128.5, 127.4, 126.5, 124.9, 100.0, 92.7; HRMS calcd. for $C_{14}H_{10}O_3S$: 258.0351; found: 258.0351.

Spectral data for 2-phenyl-6-(prop-1-en-2-yl)-4*H*-1,3-dioxin-4-one (3f).



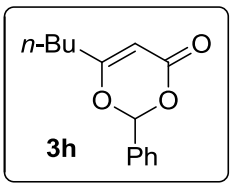
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.59 ~ 7.57 (m, 2 H), 7.44 ~ 7.43 (m, 3 H), 6.39 (s, 1 H), 5.89 (s, 1 H), 5.61 (s, 1 H), 5.43 (s, 1 H), 1.95 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 167.6, 162.9, 134.4, 133.7, 130.3, 128.5, 126.5, 122.1, 99.9, 94.9, 18.1; HRMS calcd. for $C_{13}H_{12}O_3$: 216.0786; found: 216.0791.

Spectral data for 2-phenyl-4*H*-1,3-dioxin-4-one (3g).



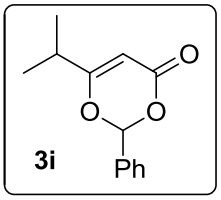
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 ~ 7.55 (m, 2 H), 7.45 ~ 7.42 (m, 4 H), 6.41 (s, 1 H), 5.60 (d, *J* = 5.4 Hz, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.2, 160.6, 133.3, 130.5, 128.6, 126.5, 100.5, 100.1; HRMS calcd. for $C_{10}H_8O_3$: 176.0473; found: 176.474.

Spectral data for 6-butyl-2-phenyl-4*H*-1,3-dioxin-4-one (3h).



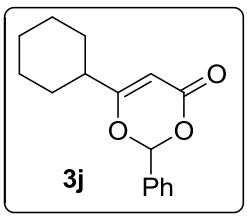
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.53 ~ 7.51 (m, 2 H), 7.40 ~ 7.37 (m, 3 H), 6.30 (s, 1 H), 5.36 (s, 1 H), 2.30 ~ 2.27 (m, 2 H), 1.54 ~ 1.49 (m, 2 H), 1.35 ~ 1.28 (m, 2 H), 0.87 (t, *J* = 7.5 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 175.3, 162.1, 133.5, 130.0, 128.3, 126.3, 99.6, 95.3, 32.6, 27.6, 21.8, 13.4; HRMS calcd. for $C_{14}H_{16}O_3$: 232.1099; found: 232.1091.

Spectral data for 6-isopropyl-2-phenyl-4*H*-1,3-dioxin-4-one (3i).



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.55 ~ 7.52 (m, 2 H), 7.41 ~ 7.38 (m, 3 H), 6.30 (s, 1 H), 5.38 (s, 1 H), 2.55 ~ 2.50 (m, 1 H), 1.16 ~ 1.13 (m, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 179.7, 162.4, 133.6, 130.1, 128.4, 126.3, 99.7, 93.4, 32.1, 19.1, 19.0; HRMS calcd. for $C_{13}H_{14}O_3$: 218.0943; found: 218.0942.

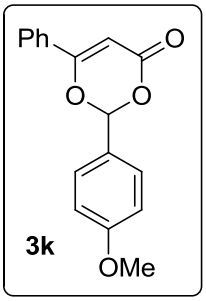
Spectral data for 6-cyclohexyl-2-phenyl-4*H*-1,3-dioxin-4-one (3j).



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.56 ~ 7.55 (m, 2 H), 7.44 ~ 7.43 (m, 3 H), 6.30

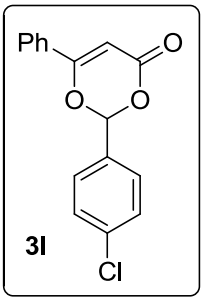
(s, 1 H), 5.38 (d, *J* = 0.6 Hz, 1 H), 2.26 ~ 2.22 (m, 1 H), 1.93 ~ 1.88 (m, 2 H), 1.80 ~ 1.78 (m, 2 H), 1.70 ~ 1.67 (m, 1 H), 1.34 ~ 1.17 (m, 5 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 179.0, 162.8, 133.8, 130.3, 128.6, 126.5, 99.9, 93.8, 41.7, 29.7, 29.5, 25.6, 25.5 (one carbon merged with others); HRMS calcd. for $C_{16}H_{18}O_3$: 258.1256; found: 258.1258.

Spectral data for 2-(4-methoxyphenyl)-6-phenyl-4*H*-1,3-dioxin-4-one (3k).



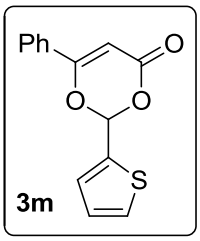
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.72 (d, *J* = 8.1 Hz, 2 H), 7.57 (d, *J* = 8.4 Hz, 2 H), 7.52 ~ 7.49 (m, 1 H), 7.42 (t, *J* = 7.8 Hz, 2 H), 6.97 (d, *J* = 8.4 Hz, 2 H), 6.48 (s, 1 H), 6.03 (s, 1 H), 3.82 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.2, 163.2, 161.1, 132.4, 130.0, 128.8, 128.2, 126.5, 125.9, 113.9, 100.3, 93.0, 55.3; HRMS calcd. for $C_{17}H_{14}O_4$: 282.0892; found: 282.0886.

Spectral data for 2-(4-chlorophenyl)-6-phenyl-4*H*-1,3-dioxin-4-one (3l).



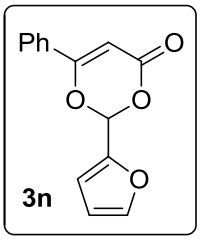
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.4 Hz, 2 H), 7.58 (d, *J* = 8.4 Hz, 2 H), 7.52 ~ 7.49 (m, 1 H), 7.44 ~ 7.41 (m, 4 H), 6.50 (s, 1 H), 6.03 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 168.0, 162.4, 136.3, 132.5, 132.1, 129.7, 128.8, 128.0, 126.5, 99.4, 93.1 (one carbon merged with others); HRMS calcd. for $C_{16}H_{11}ClO_3$: 286.0397; found: 286.0399.

Spectral data for 6-phenyl-2-(thiophen-2-yl)-4*H*-1,3-dioxin-4-one (3m).



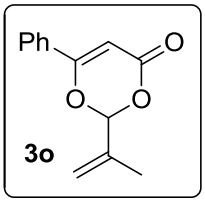
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.72 (d, *J* = 7.8 Hz, 2 H), 7.52 (t, *J* = 7.4 Hz, 1 H), 7.46 ~ 7.43 (m, 3 H), 7.39 (d, *J* = 3.6 Hz, 1 H), 7.09 ~ 7.06 (m, 1 H), 6.78 (s, 1 H), 6.03 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.8, 162.2, 135.9, 132.5, 129.8, 128.8, 127.9, 127.8, 126.8, 126.6, 97.0, 93.2; HRMS calcd. for $C_{14}H_{10}O_3S$: 258.0351; found: 258.0355.

Spectral data for 2-(furan-2-yl)-6-phenyl-4*H*-1,3-dioxin-4-one (3n).



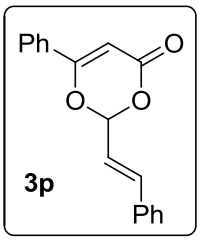
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.0 Hz, 2 H), 7.49 ~ 7.46 (m, 2 H), 7.40 (t, *J* = 7.6 Hz, 2 H), 6.72 (d, *J* = 3.2 Hz, 1 H), 6.56 (s, 1 H), 6.44 ~ 6.43 (m, 1 H), 5.98 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 167.7, 161.9, 146.3, 144.0, 132.4, 129.7, 128.7, 126.5, 110.9, 110.5, 94.1, 93.0; HRMS calcd. for $C_{14}H_{10}O_4$: 242.0579; found: 242.0576.

Spectral data for 6-phenyl-2-(prop-1-en-2-yl)-4*H*-1,3-dioxin-4-one (3o).



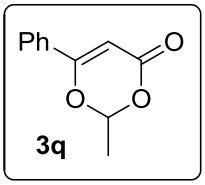
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 7.8 Hz, 2 H), 7.51 (t, *J* = 7.4 Hz, 1 H), 7.44 (t, *J* = 7.6 Hz, 2 H), 5.95 (s, 1 H), 5.89 (s, 1 H), 5.43 (s, 1 H), 5.28 (s, 1 H), 1.95 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 163.0, 137.9, 132.4, 130.1, 128.9, 126.5, 118.2, 101.8, 92.9, 16.5; HRMS calcd. for $C_{13}H_{12}O_3$: 216.0786; found: 216.0785.

Spectral data for (*E*)-6-phenyl-2-styryl-4*H*-1,3-dioxin-4-one (3p).



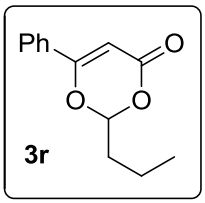
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.74 (d, *J* = 8.6 Hz, 2 H), 7.54 ~ 7.43 (m, 5 H), 7.39 ~ 7.30 (m, 3 H), 7.05 (d, *J* = 16.4 Hz, 1 H), 6.44 (dd, *J* = 16.4, 5.6 Hz, 1 H), 6.18 (d, *J* = 5.6 Hz, 1 H), 6.00 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 162.8, 137.0, 134.7, 132.4, 130.1, 129.1, 128.8, 128.7, 127.1, 126.5, 120.4, 100.0, 93.1; HRMS calcd. for $C_{18}H_{14}O_3$: 278.0943; found: 278.0913.

Spectral data for 2-methyl-6-phenyl-4*H*-1,3-dioxin-4-one (3q).



White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 ~ 7.66 (m, 2 H), 7.51 ~ 7.47 (m, 1 H), 7.43 ~ 7.39 (m, 2 H), 5.90 (s, 1 H), 5.73 (q, *J* = 5.2 Hz, 1 H), 1.75 (d, *J* = 5.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.2, 163.3, 132.3, 130.0, 128.8, 126.4, 98.6, 92.7, 19.4; HRMS calcd. for $C_{11}H_{10}O_3$: 190.0630; found: 190.0633.

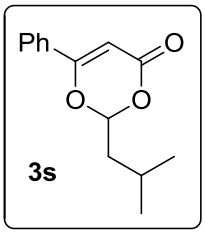
Spectral data for 6-phenyl-2-propyl-4*H*-1,3-dioxin-4-one (3r).



White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 ~ 7.65 (m, 2 H), 7.50 ~ 7.46 (m, 1 H), 7.43 ~ 7.39 (m, 2 H), 5.89 (s, 1 H), 5.59 (t, *J* = 5.2 Hz, 1 H), 2.09 ~ 1.96 (m, 2 H), 1.69 ~ 1.56 (m, 2 H), 1.01 (t, *J* = 7.4 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.1, 163.4, 132.2, 130.1, 128.7, 126.3, 101.1, 92.7, 34.9, 16.4, 13.6; HRMS calcd. for $C_{13}H_{14}O_3$: 218.0943; found:

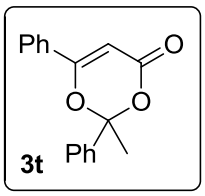
218.0946.

Spectral data for 2-isobutyl-6-phenyl-4*H*-1,3-dioxin-4-one (3s).



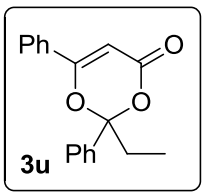
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 8.0 Hz, 2 H), 7.52 ~ 7.49 (m, 1 H), 7.44 (t, *J* = 7.4 Hz, 2 H), 5.92 (s, 1 H), 5.65 (t, *J* = 5.6 Hz, 1 H), 2.14 ~ 2.02 (m, 1 H), 2.01 ~ 1.89 (m, 2 H), 1.04 ~ 1.02 (m, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 163.5, 132.3, 130.2, 128.9, 126.4, 100.6, 92.9, 41.6, 23.5, 22.7, 22.6; HRMS calcd. for $C_{14}H_{16}O_3$: 232.1099; found: 232.1098.

Spectral data for 2-methyl-2,6-diphenyl-4*H*-1,3-dioxin-4-one (3t).



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75 (d, *J* = 7.2 Hz, 2 H), 7.51 ~ 7.48 (m, 3 H), 7.43 (t, *J* = 7.5 Hz, 2 H), 7.30 ~ 7.29 (m, 3 H), 5.80 (s, 1 H), 1.99 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.0, 162.0, 139.9, 132.1, 130.5, 129.0, 128.8, 128.5, 126.1, 124.7, 106.7, 93.3, 29.4; HRMS calcd. for $C_{17}H_{14}O_3$: 266.0943; found: 266.0944.

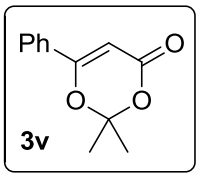
Spectral data for 2-ethyl-2,6-diphenyl-4*H*-1,3-dioxin-4-one (3u).



White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 ~ 7.74 (m, 2 H), 7.51 ~ 7.43 (m, 5 H), 7.31 ~ 7.28 (m, 3 H), 5.78 (s, 1 H), 2.28 ~ 2.17 (m, 2 H), 1.05 (t, *J* = 7.5 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 165.1, 162.2, 139.0, 132.1, 130.7, 129.0, 128.8, 128.4, 126.2, 125.3, 108.6,

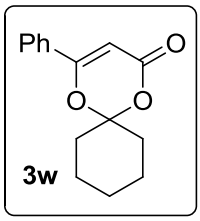
93.4, 35.3, 7.3; HRMS calcd. for $C_{18}H_{16}O_3$: 280.1099; found: 280.1099.

Spectral data for 2,2-dimethyl-6-phenyl-4*H*-1,3-dioxin-4-one (3v).



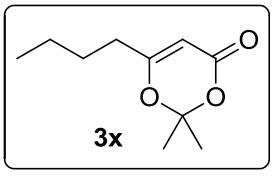
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.61 ~ 7.60 (m, 2 H), 7.44 ~ 7.41 (m, 1 H), 7.37 ~ 7.35 (m, 2 H), 5.81 (s, 1 H), 1.72 (s, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.7, 161.5, 131.8, 130.7, 128.5, 126.0, 106.3, 90.9, 24.7; HRMS calcd. for $C_{12}H_{12}O_3$: 204.0786; found: 204.0787.

Spectral data for 4-phenyl-1,5-dioxaspiro[5.5]undec-3-en-2-one (3w).



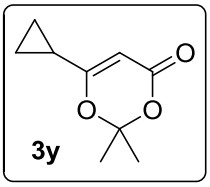
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.64 ~ 7.62 (m, 2 H), 7.44 ~ 7.41 (m, 1 H), 7.38 ~ 7.35 (m, 2 H), 5.80 (s, 1 H), 2.13 ~ 2.10 (m, 2 H), 1.93 ~ 1.89 (m, 2 H), 1.69 ~ 1.50 (m, 5 H), 1.42 ~ 1.36 (m, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 164.2, 161.5, 131.8, 130.8, 128.6, 126.0, 106.9, 91.1, 33.4, 24.4, 21.2; HRMS calcd. for $C_{15}H_{16}O_3$: 244.1099; found: 244.1097.

Spectral data for 6-butyl-2,2-dimethyl-4*H*-1,3-dioxin-4-one (3x).



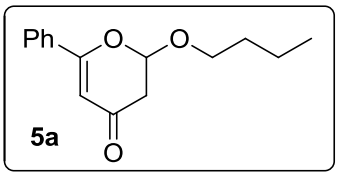
Colorless oil; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.18 (m, 1 H), 2.17 (t, *J* = 7.8 Hz, 2 H), 1.63 (s, 6 H), 1.50 ~ 1.45 (m, 2 H), 1.35 ~ 1.29 (m, 2 H), 0.88 (t, *J* = 7.2 Hz, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 172.1, 161.4, 106.1, 93.0, 33.2, 27.7, 24.9, 22.0, 13.6; HRMS calcd. for $C_{10}H_{16}O_3$: 184.1099; found: 184.1100.

Spectral data for 6-cyclopropyl-2,2-dimethyl-4*H*-1,3-dioxin-4-one (3y).



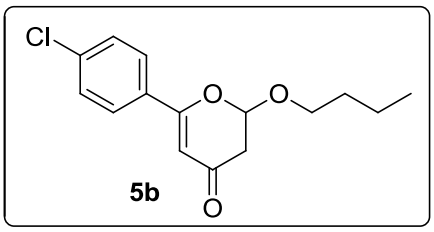
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.28 (s, 1 H), 1.61 (s, 6 H), 1.58 ~ 1.52 (m, 1 H), 0.94 ~ 0.87 (m, 4 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 172.3, 161.0, 106.0, 91.0, 24.6, 13.7, 7.0; HRMS calcd. for $C_9H_{12}O_3$: 168.0786; found: 168.0788.

Spectral data for 2-butoxy-6-phenyl-2*H*-pyran-4(3*H*)-one (5a).



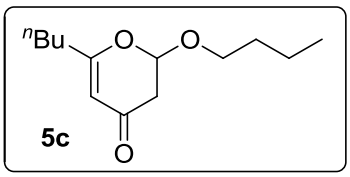
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.71 (d, *J* = 8.0 Hz, 2 H), 7.46 ~7.36 (m, 3 H), 6.02 (s, 1 H), 5.55 ~ 5.53 (m, 1 H), 3.94 ~ 3.88 (m, 1 H), 3.67 ~ 3.62 (m, 1 H), 2.82 ~ 2.66 (m, 2 H), 1.59 ~ 1.52 (m, 2 H), 1.37 ~ 1.28 (m, 2 H), 0.85 (t, *J* = 7.4 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.4, 166.3, 132.6, 131.5, 128.6, 126.2,, 102.4, 101.8, 69.5, 42.0, 31.3, 19.0, 13.6; HRMS calcd. for $C_{15}H_{18}O_3$: 246.1256; found: 246.1259.

Spectral data for 2-butoxy-6-(4-chlorophenyl)-2*H*-pyran-4(3*H*)-one (5b).



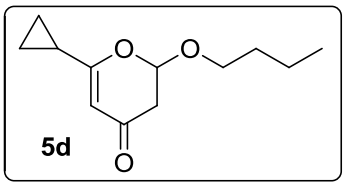
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.62 (d, *J* = 8.4 Hz, 2 H), 7.34 (d, *J* = 8.4 Hz, 2 H), 5.96 (s, 1 H), 5.54 ~ 5.52 (m, 1 H), 3.89 ~ 3.83 (m, 1 H), 3.65 ~ 3.59 (m, 1 H), 2.81 ~ 2.63 (m, 2 H), 1.56 ~ 1.49 (m, 2 H), 1.34 ~ 1.25 (m, 2 H), 0.82 (t, *J* = 7.4 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 191.1, 164.9, 137.5, 131.1, 128.8, 127.4, 102.5, 101.9, 69.5, 41.9, 31.3, 19.0, 13.6; HRMS calcd. for $C_{15}H_{17}ClO_3$: 280.0866; found: 280.0865.

Spectral data for 2-butoxy-6-butyl-2*H*-pyran-4(3*H*)-one (5c).



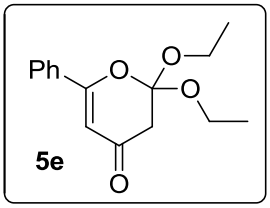
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.32 ~ 5.30 (m, 2 H), 3.81 ~ 3.77 (m, 1 H), 3.54 ~ 3.51 (m, 1 H), 2.65 (dd, *J* = 16.5, 3.9 Hz, 1 H), 2.54 (dd, *J* = 16.5, 6.0 Hz, 1 H), 2.22 ~ 2.19 (m, 2 H), 1.54 ~ 1.50 (m, 4 H), 1.34 ~ 1.30 (m, 4 H), 0.89 ~ 0.86 (m, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 191.3, 174.0, 104.5, 101.5, 69.4, 41.7, 34.5, 31.4, 28.4, 22.0, 19.1, 13.7, 13.6; HRMS calcd. for $C_{13}H_{22}O_3$: 226.1569; found: 226.1568.

Spectral data for 2-butoxy-6-cyclopropyl-2*H*-pyran-4(3*H*)-one (5d).



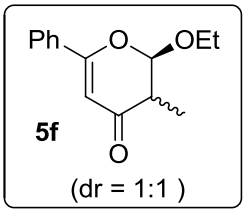
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.42 (s, 1 H), 5.25 ~ 5.23 (m, 1 H), 3.74 ~ 3.68 (m, 1 H), 3.50 ~ 3.45 (m, 1 H), 2.64 ~ 2.48 (m, 2 H), 1.57 ~ 1.46 (m, 3 H), 1.35 ~ 1.25 (m, 2 H), 0.94 ~ 0.92 (m, 2 H), 0.87 ~ 0.83 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 190.2, 174.5, 103.1, 101.7, 69.3, 41.8, 31.3, 19.0, 15.0, 13.6, 7.9; HRMS calcd. for $C_{12}H_{18}O_3$: 210.1256; found: 210.1252.

Spectral data for 2,2-diethoxy-6-phenyl-2*H*-pyran-4(3*H*)-one (5e).



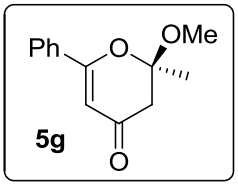
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.76 ~ 7.74 (m, 2 H), 7.47 ~ 7.39 (m, 3 H), 6.04 (s, 1 H), 3.82 ~ 3.77 (m, 2 H), 3.70 ~ 3.63 (m, 2 H), 2.89 (s, 2 H), 1.21 ~ 1.17 (m, 6 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.4, 166.2, 132.2, 131.6, 128.7, 126.3, 116.4, 102.0, 58.7, 43.7, 15.0; HRMS calcd. for $C_{15}H_{18}O_4$: 262.1205; found: 262.1204.

Spectral data for 2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one (5f).



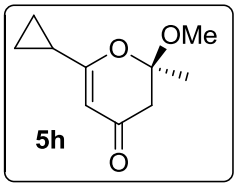
Colorless liquid; ^{1}H NMR for **cis**-2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one **(5f)** (600 MHz, $CDCl_3$): δ 7.74 ~ 7.71 (m, 2 H), 7.47 ~ 7.39 (m, 3 H), 6.00 (s, 1 H), 5.46 (d, *J* = 3.6 Hz, 1 H), 3.96 ~ 3.91 (m, 1 H), 3.72 ~ 3.66 (m, 1 H), 2.83 ~ 2.79 (m, 1 H), 1.28 ~ 1.18 (m, 6 H); ^{13}C NMR for **cis**-2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one **(5f)** (150 MHz, $CDCl_3$): δ 195.5, 165.9, 132.9, 131.5, 128.7, 126.3, 106.5, 101.8, 65.6, 45.2, 15.0, 11.3; ^{1}H NMR for **trans**-2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one **(5f')** (600 MHz, $CDCl_3$): δ 7.74 ~ 7.71 (m, 2 H), 7.47 ~ 7.39 (m, 3 H), 6.00 (s, 1 H), 5.16 (d, *J* = 7.2 Hz, 1 H), 4.07 ~ 4.02 (m, 1 H), 3.77 ~ 3.72 (m, 1 H), 2.64 ~ 2.59 (m, 1 H), 1.27 ~ 1.18 (m, 6 H); ^{13}C NMR for **trans** -2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one **(5f')** (150 MHz, $CDCl_3$): δ 194.9, 165.4, 132.6, 131.3, 128.6, 126.2, 104.4, 101.4, 65.5, 44.4, 14.9, 8.9; HRMS calcd. for $C_{14}H_{16}O_3$: 232.1099; found: 232.1098.

Spectral data for 2-methoxy-2-methyl-6-phenyl-2*H*-pyran-4(3*H*)-one (5g).



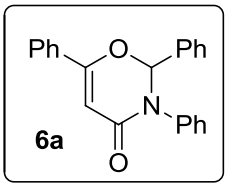
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.75 ~ 7.74 (m, 2 H), 7.47 ~ 7.39 (m, 3 H), 6.04 (s, 1 H), 3.33 (s, 3 H), 2.75 (s, 1 H), 2.74 (s, 1 H), 1.69 (s, 3 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 192.4, 165.6, 132.7, 131.4, 128.7, 126.2, 105.0, 102.0, 50.2, 46.8, 22.3; HRMS calcd. for $C_{13}H_{14}O_3$: 218.0943; found: 218.0941.

Spectral data for 6-cyclopropyl-2-methoxy-2-methyl-2*H*-pyran-4(3*H*)-one (5h).



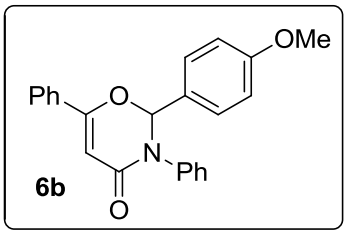
Colorless liquid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 5.43 (s, 1 H), 3.24 (s, 3 H), 2.61 ~ 2.53 (m, 2 H), 1.57 ~ 1.53 (m, 1 H), 1.49 (s, 3 H), 0.99 ~ 0.84 (m, 4 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 191.1, 173.8, 104.7, 102.3, 49.9, 46.4, 22.2, 14.9, 8.2, 7.6; HRMS calcd. for $C_{10}H_{14}O_3$: 182.0943; found: 182.0935.

Spectral data for 2,3,6-triphenyl-2*H*-1,3-oxazin-4(3*H*)-one (6a).



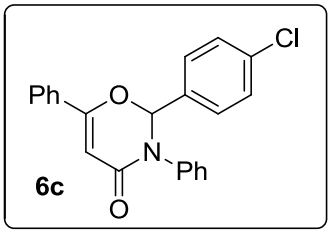
White solid; ^{1}H NMR (600 MHz, $CDCl_3$): δ 7.69 (d, *J* = 8.1 Hz, 2 H), 7.57 (d, *J* = 7.5 Hz, 2 H), 7.45 ~ 7.30 (m, 10 H), 7.20 (t, *J* = 7.2 Hz, 1 H), 6.83 (s, 1 H), 6.04 (s, 1 H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 162.9, 161.3, 139.6, 136.4, 131.6, 131.3, 129.4, 129.0, 128.6, 128.5, 127.1, 126.3, 126.2, 124.9, 98.9, 90.0; HRMS calcd. for $C_{22}H_{17}NO_2$: 327.1259; found: 327.1262.

Spectral data for 2-(4-methoxyphenyl)-3,6-diphenyl-2*H*-1,3-oxazin-4(3*H*)-one (6b).



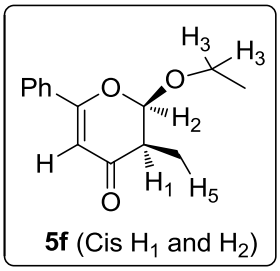
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.67 (d, *J* = 7.2 Hz, 2 H), 7.48 ~ 7.17 (m, 10 H), 6.86 (d, *J* = 8.8 Hz, 2 H), 6.77 (s, 1 H), 6.03 (s, 1 H), 3.75 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.1, 161.2, 160.4, 139.5, 131.7, 131.3, 129.0, 128.6, 128.5, 128.3, 126.3, 126.2, 125.0, 113.9, 98.7, 89.9, 55.2; HRMS calcd. for $C_{23}H_{19}NO_3$: 357.1365; found: 357.1363.

Spectral data for 2-(4-chlorophenyl)-3,6-diphenyl-2*H*-1,3-oxazin-4(3*H*)-one (6c).



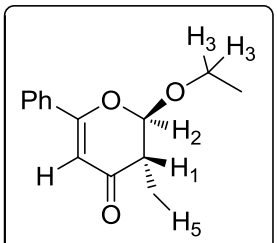
White solid; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 ~ 7.65 (m, 2 H), 7.50 ~ 7.19 (m, 12 H), 6.78 (s, 1 H), 6.03 (s, 1 H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 162.7, 161.3, 139.4, 135.5, 135.0, 131.5, 131.4, 129.1, 128.9, 128.7, 128.5, 126.4, 126.3, 125.0, 98.8, 89.4; HRMS calcd. for $C_{22}H_{16}ClNO_2$: 361.0870; found: 361.0869.

(4) NOE of 2-ethoxy-3-methyl-6-phenyl-2H-pyran-4(3*H*)-one (5f).



5f (Cis H_1 and H_2)

Sr. no.	Irradiation	Intensity increase % (Key peaks)
1)	H_1 (δ 2.83 ~ 2.79)	H_2 (δ 5.46, 1.44%), H_5 (δ ~1.19, 2.43%)
2)	H_2 (δ 5.46)	H_1 (δ 2.83 ~ 2.79, 1.57%), H_3 (δ 3.92, 3.69 0.45% and 1.26%)



5f' (trans H_1 and H_2)

Sr. no.	Irradiation	Intensity increase % (Key peaks)
1)	H_1 (δ 2.63 ~ 2.60)	H_2 (δ 5.16, 0.70%), H_5 (δ ~1.26, 2.23%)
2)	H_2 (δ 5.16)	H_1 (δ 2.63 ~ 2.60, 0.80%), H_3 (δ 4.04, 3.75 0.55% and 1.23%), H_5 (δ ~1.26, 1.30%)

(7) X-Ray crystallographic structure and data for compound (3a):

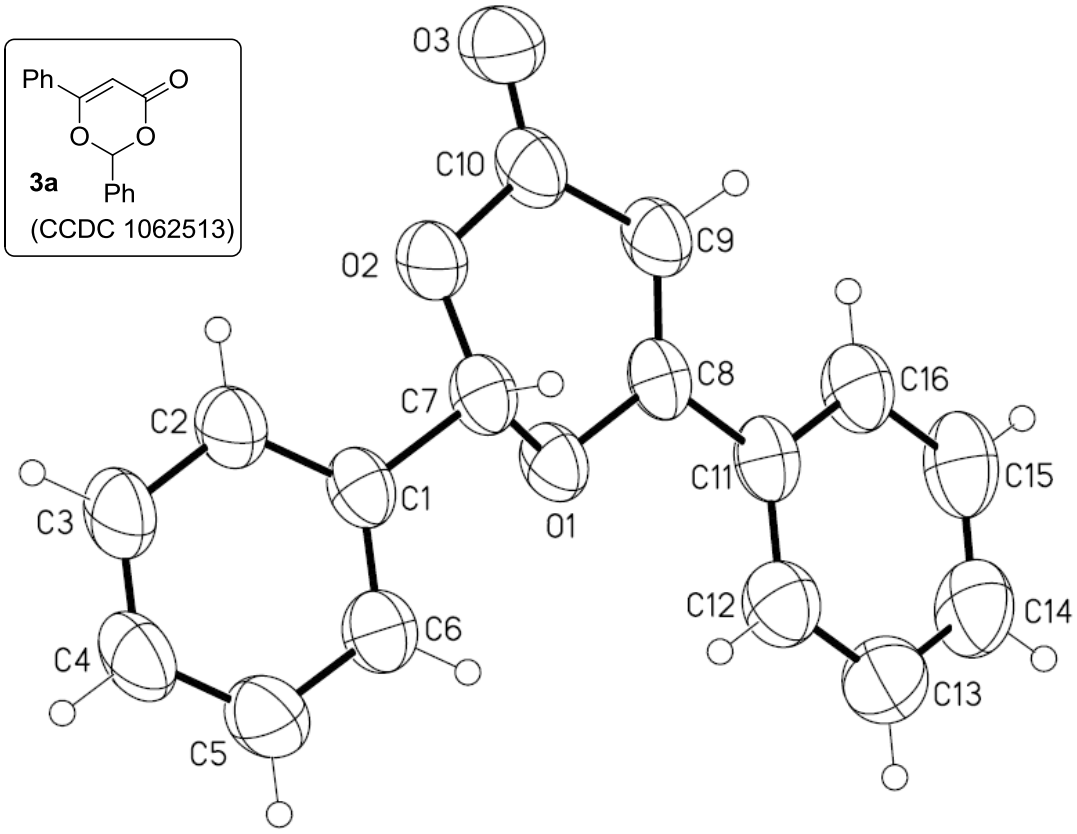


Table 1. Crystal data and structure refinement for 141246_0m.

Identification code	141246_0m	
Empirical formula	C16 H12 O3	
Formula weight	252.26	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 6.0914(7) Å	α= 90°.
	b = 8.5177(11) Å	β= 90.598(7)°.
	c = 23.947(3) Å	γ = 90°.
Volume	1242.4(3) Å ^{3}	
Z	4	
Density (calculated)	1.349 Mg/m^3	
Absorption coefficient	0.093 mm^{-1}	
F(000)	528	

Crystal size	0.30 x 0.05 x 0.05 mm^3
Theta range for data collection	0.850 to 26.424°.
Index ranges	-7<=h<=7, -10<=k<=10, -29<=l<=29
Reflections collected	8860
Independent reflections	2531 [R(int) = 0.0528]
Completeness to theta = 25.242°	99.6 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.7225
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2531 / 0 / 174
Goodness-of-fit on F^2	1.388
Final R indices [I>2sigma(I)]	R1 = 0.1269, wR2 = 0.3426
R indices (all data)	R1 = 0.1690, wR2 = 0.3920
Extinction coefficient	0.27(5)
Largest diff. peak and hole	0.866 and -1.044 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 141246_0m. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	4946(8)	6899(5)	3242(2)	49(1)
C(2)	6341(10)	6736(6)	2793(2)	62(1)
C(3)	5650(11)	5880(7)	2330(2)	71(2)
C(4)	3641(10)	5194(7)	2310(2)	68(2)
C(5)	2253(10)	5353(7)	2758(2)	72(2)
C(6)	2902(9)	6213(7)	3224(2)	60(1)
C(7)	5653(8)	7843(5)	3747(2)	48(1)
C(8)	5804(8)	7754(5)	4710(2)	48(1)
C(9)	7512(8)	8750(6)	4687(2)	53(1)
C(10)	8836(9)	8857(6)	4185(2)	54(1)
C(11)	4600(8)	7309(6)	5217(2)	50(1)
C(12)	2561(9)	6618(7)	5180(2)	63(1)
C(13)	1380(11)	6245(8)	5650(2)	75(2)
C(14)	2294(12)	6548(7)	6168(2)	75(2)
C(15)	4333(12)	7224(7)	6216(2)	72(2)
C(16)	5517(10)	7601(7)	5748(2)	60(1)
O(1)	5066(6)	7014(4)	4240(1)	51(1)

O(2)	7928(6)	8103(4)	3728(1)	57(1)
O(3)	10624(6)	9401(5)	4147(1)	71(1)

Table 3. Bond lengths [Å] and angles [°] for 141246_0m.

C(1)-C(6)	1.375(7)
C(1)-C(2)	1.384(7)
C(1)-C(7)	1.511(6)
C(2)-C(3)	1.389(7)
C(2)-H(2)	0.9300
C(3)-C(4)	1.357(8)
C(3)-H(3)	0.9300
C(4)-C(5)	1.379(9)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(7)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-O(2)	1.404(6)
C(7)-O(1)	1.423(5)
C(7)-H(7)	0.9800
C(8)-C(9)	1.344(7)
C(8)-O(1)	1.364(5)
C(8)-C(11)	1.473(7)
C(9)-C(10)	1.458(7)
C(9)-H(9)	0.9300
C(10)-O(3)	1.188(6)
C(10)-O(2)	1.380(5)
C(11)-C(12)	1.377(8)
C(11)-C(16)	1.407(7)
C(12)-C(13)	1.380(8)
C(12)-H(12)	0.9300
C(13)-C(14)	1.379(8)
C(13)-H(13)	0.9300
C(14)-C(15)	1.373(10)
C(14)-H(14)	0.9300
C(15)-C(16)	1.377(8)

C(15)-H(15)	0.9300
C(16)-H(16)	0.9300

C(6)-C(1)-C(2)	119.7(4)
C(6)-C(1)-C(7)	120.2(4)
C(2)-C(1)-C(7)	120.2(4)
C(1)-C(2)-C(3)	119.3(5)
C(1)-C(2)-H(2)	120.3
C(3)-C(2)-H(2)	120.3
C(4)-C(3)-C(2)	121.3(5)
C(4)-C(3)-H(3)	119.3
C(2)-C(3)-H(3)	119.3
C(3)-C(4)-C(5)	119.4(5)
C(3)-C(4)-H(4)	120.3
C(5)-C(4)-H(4)	120.3
C(4)-C(5)-C(6)	120.3(5)
C(4)-C(5)-H(5)	119.8
C(6)-C(5)-H(5)	119.8
C(1)-C(6)-C(5)	120.0(5)
C(1)-C(6)-H(6)	120.0
C(5)-C(6)-H(6)	120.0
O(2)-C(7)-O(1)	111.3(4)
O(2)-C(7)-C(1)	109.3(4)
O(1)-C(7)-C(1)	109.1(4)
O(2)-C(7)-H(7)	109.1
O(1)-C(7)-H(7)	109.1
C(1)-C(7)-H(7)	109.1
C(9)-C(8)-O(1)	120.4(4)
C(9)-C(8)-C(11)	126.0(4)
O(1)-C(8)-C(11)	113.5(4)
C(8)-C(9)-C(10)	120.5(4)
C(8)-C(9)-H(9)	119.7
C(10)-C(9)-H(9)	119.7
O(3)-C(10)-O(2)	118.7(4)
O(3)-C(10)-C(9)	127.1(4)
O(2)-C(10)-C(9)	113.9(4)
C(12)-C(11)-C(16)	118.9(5)
C(12)-C(11)-C(8)	120.9(4)

C(16)-C(11)-C(8)	120.2(5)
C(11)-C(12)-C(13)	121.6(5)
C(11)-C(12)-H(12)	119.2
C(13)-C(12)-H(12)	119.2
C(14)-C(13)-C(12)	118.8(6)
C(14)-C(13)-H(13)	120.6
C(12)-C(13)-H(13)	120.6
C(15)-C(14)-C(13)	120.7(5)
C(15)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	120.7(5)
C(14)-C(15)-H(15)	119.6
C(16)-C(15)-H(15)	119.6
C(15)-C(16)-C(11)	119.3(6)
C(15)-C(16)-H(16)	120.4
C(11)-C(16)-H(16)	120.4
C(8)-O(1)-C(7)	111.8(3)
C(10)-O(2)-C(7)	115.8(4)

Symmetry transformations used to generate equivalent atoms:

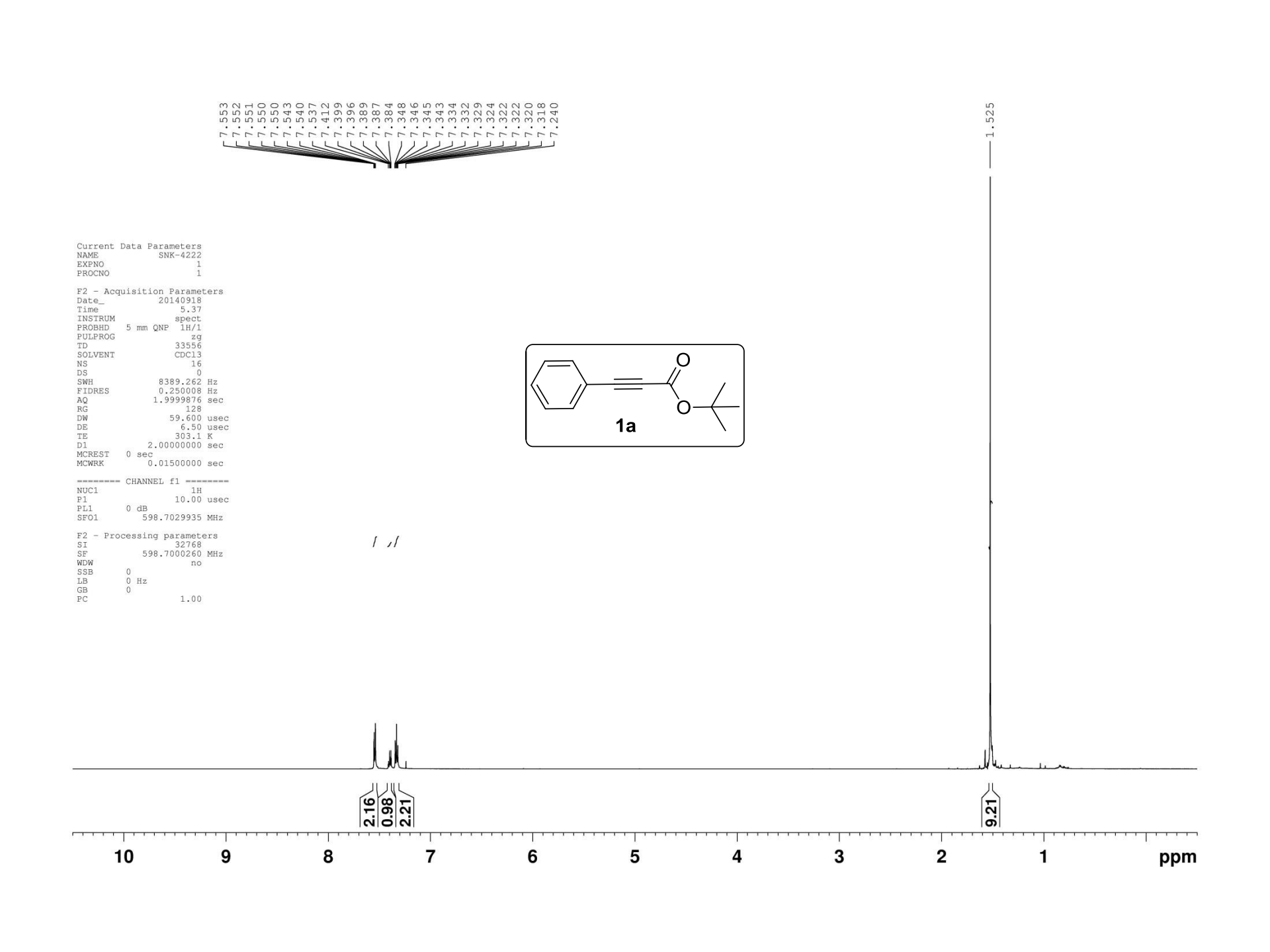
Table 4. Anisotropic displacement parameters ($Å^2 x 10^3$) for 141246_0m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

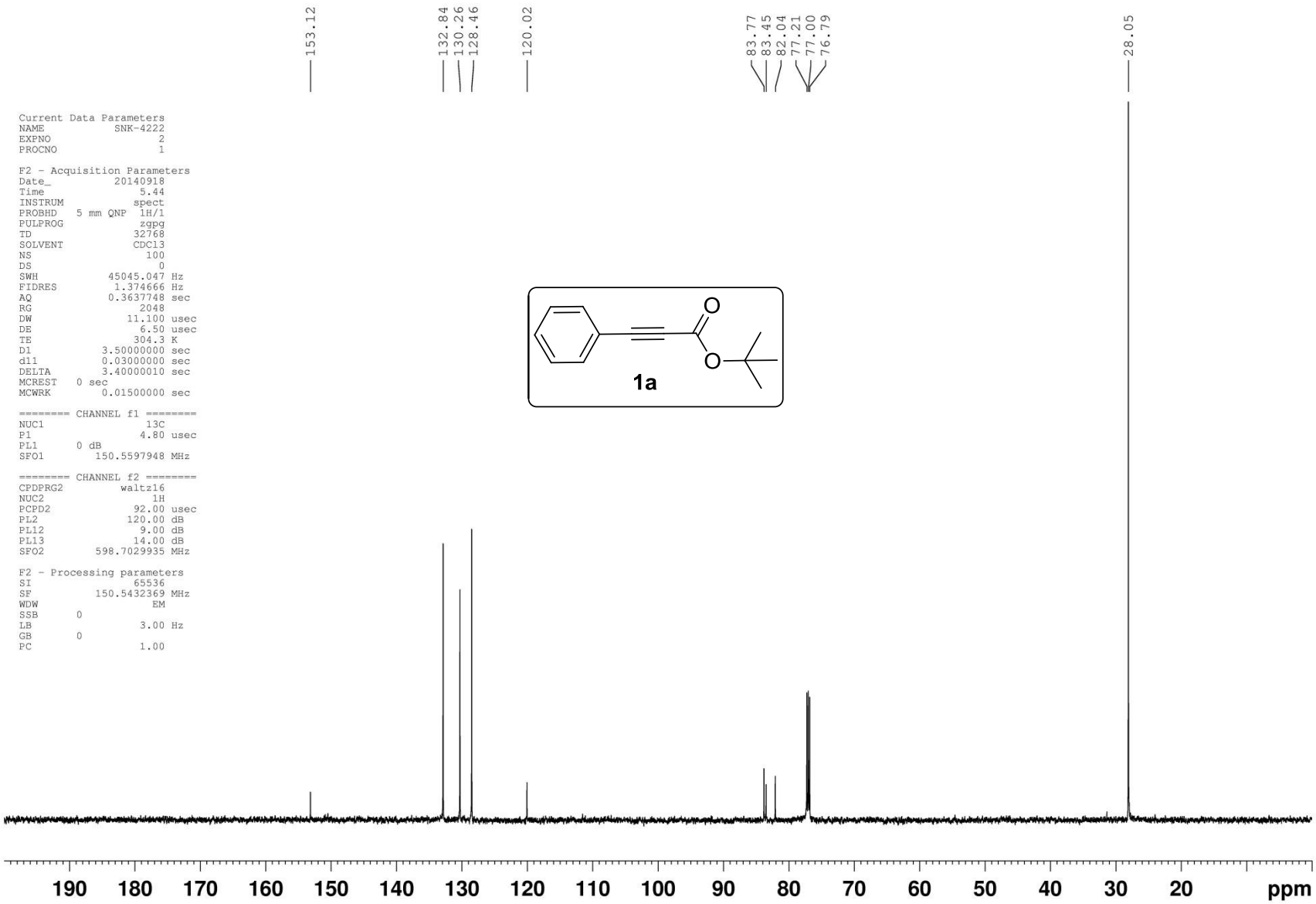
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	65(3)	47(2)	34(2)	0(2)	-4(2)	1(2)
C(2)	71(3)	68(3)	46(3)	-8(2)	6(2)	-10(3)
C(3)	93(4)	81(4)	41(3)	-12(3)	11(3)	-13(3)
C(4)	92(4)	69(3)	43(3)	-11(2)	-5(3)	-12(3)
C(5)	75(4)	84(4)	59(3)	-10(3)	-5(3)	-15(3)
C(6)	64(3)	72(3)	45(3)	-7(2)	-1(2)	-5(3)
C(7)	62(3)	47(2)	37(2)	-1(2)	-2(2)	3(2)
C(8)	62(3)	47(2)	35(2)	-4(2)	-2(2)	6(2)
C(9)	65(3)	58(3)	37(2)	-5(2)	-1(2)	-6(2)
C(10)	68(3)	60(3)	35(2)	-5(2)	-6(2)	-5(2)
C(11)	64(3)	48(3)	38(2)	-1(2)	-2(2)	10(2)

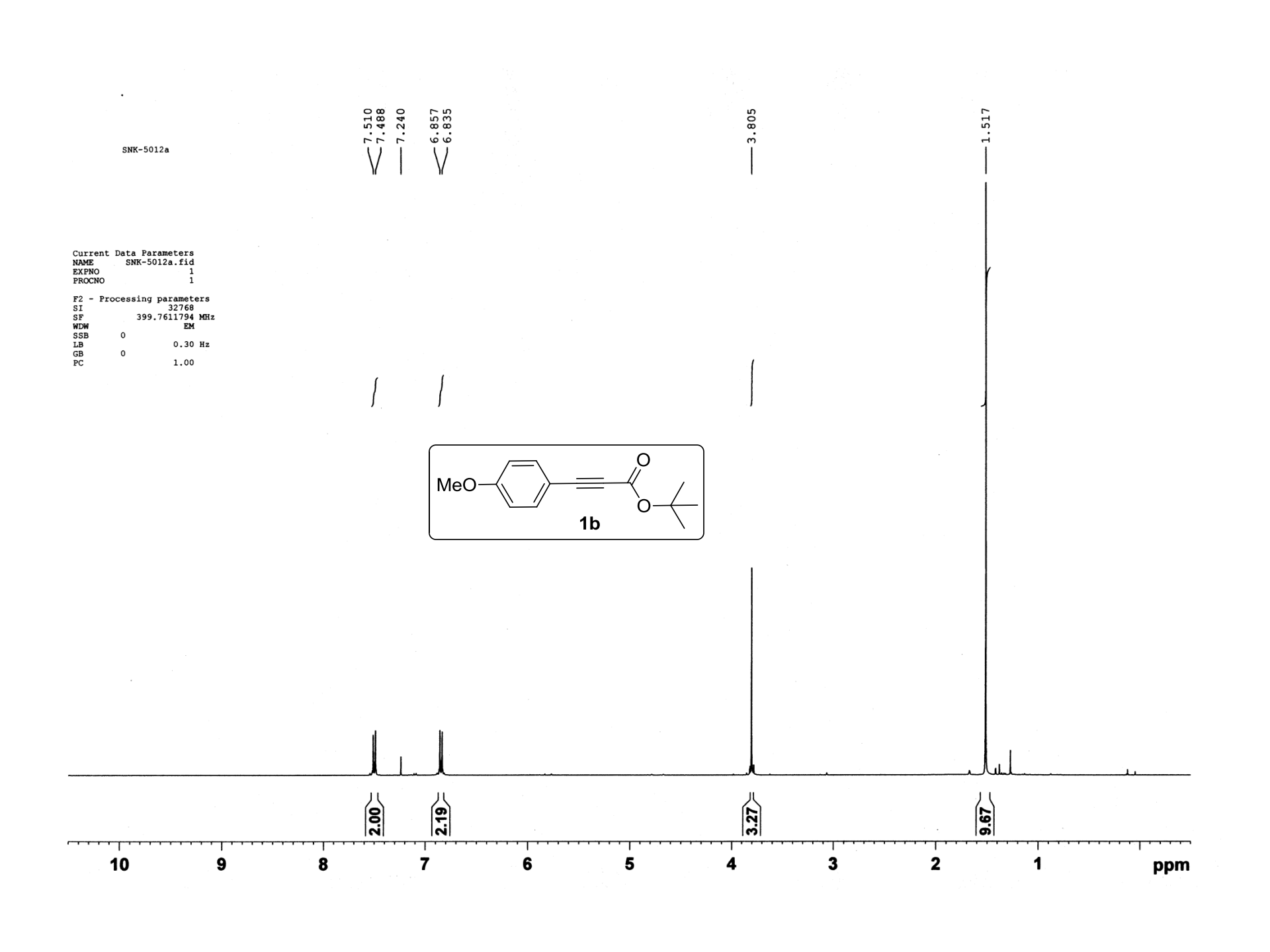
C(12)	72(4)	66(3)	51(3)	-2(2)	0(2)	-1(3)
C(13)	83(4)	72(4)	71(4)	0(3)	14(3)	-12(3)
C(14)	101(5)	74(4)	49(3)	9(3)	20(3)	-4(4)
C(15)	100(5)	78(4)	38(3)	1(2)	3(3)	10(3)
C(16)	76(3)	67(3)	37(2)	-3(2)	0(2)	3(3)
O(1)	67(2)	51(2)	34(2)	-2(1)	-1(1)	-5(2)
O(2)	66(2)	69(2)	35(2)	-7(1)	2(1)	-10(2)
O(3)	72(3)	90(3)	50(2)	-5(2)	1(2)	-26(2)

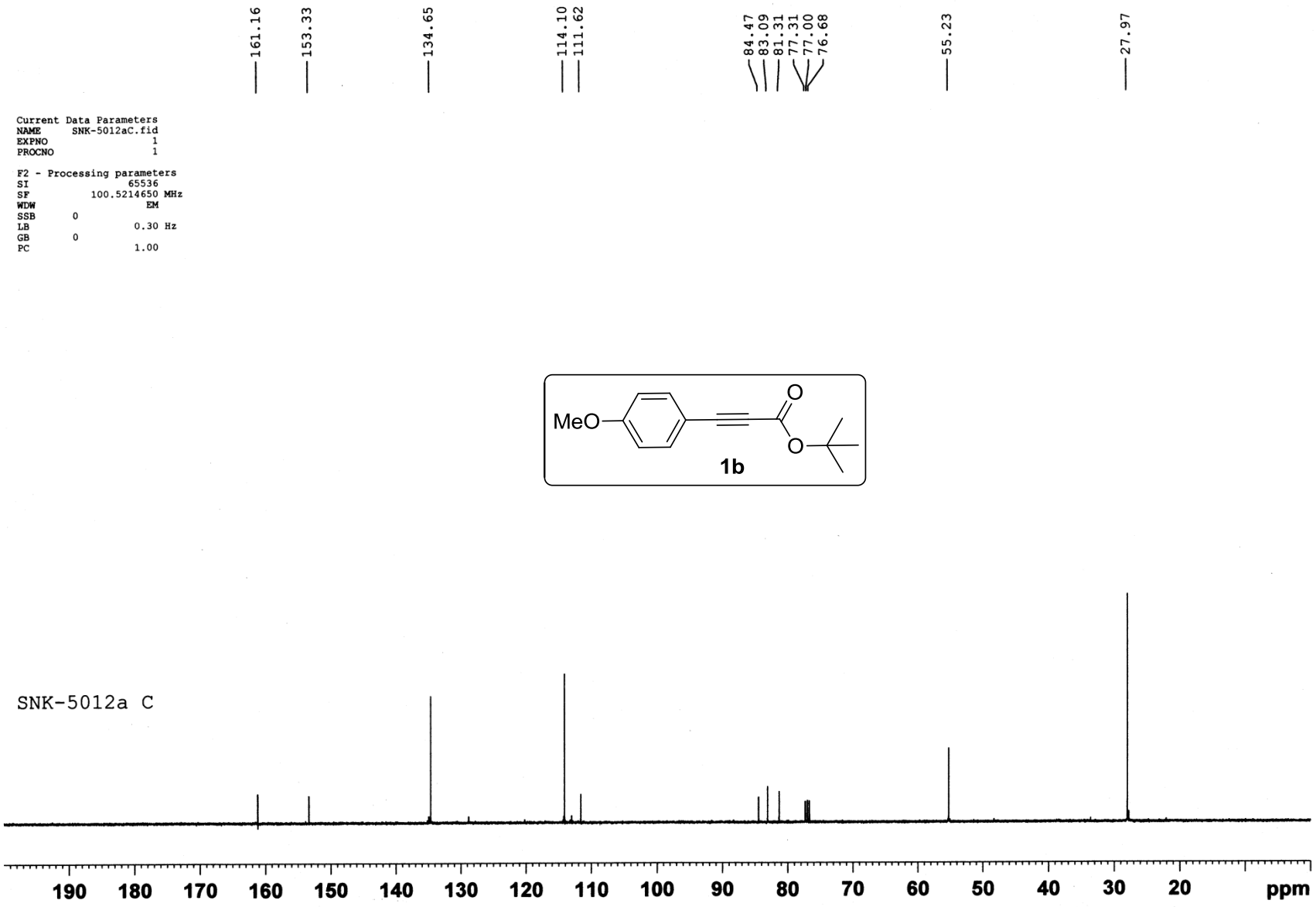
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å ^{2}x 10^{-3}) for 141246_0m.

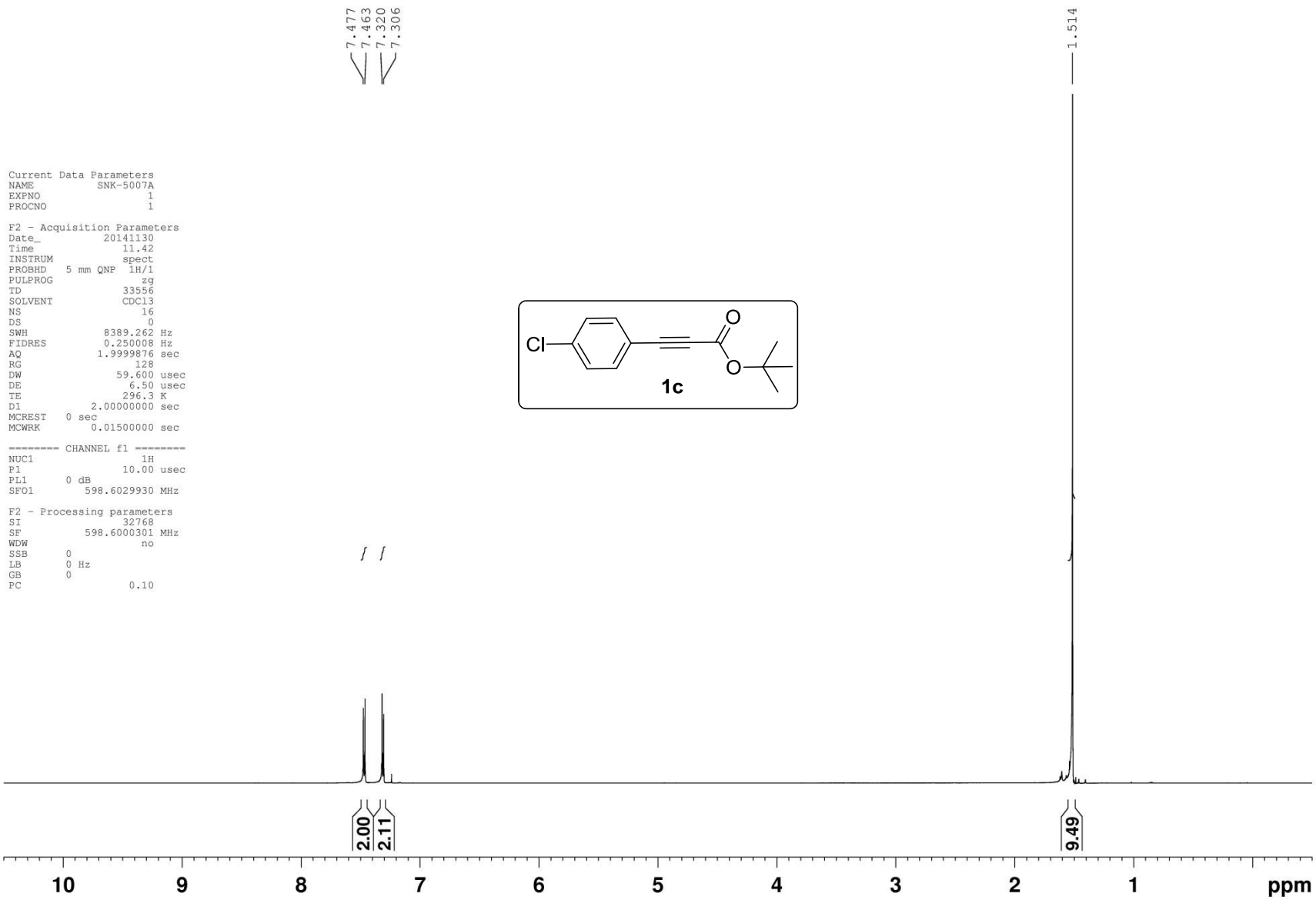
	x	y	z	U(eq)
H(2)	7726	7195	2802	74
H(3)	6584	5774	2028	86
H(4)	3203	4622	1998	81
H(5)	876	4882	2748	87
H(6)	1955	6325	3523	73
H(7)	4893	8857	3741	58
H(9)	7852	9377	4994	64
H(12)	1965	6397	4829	76
H(13)	-8	5798	5618	90
H(14)	1521	6292	6489	90
H(15)	4922	7429	6569	86
H(16)	6908	8043	5783	72

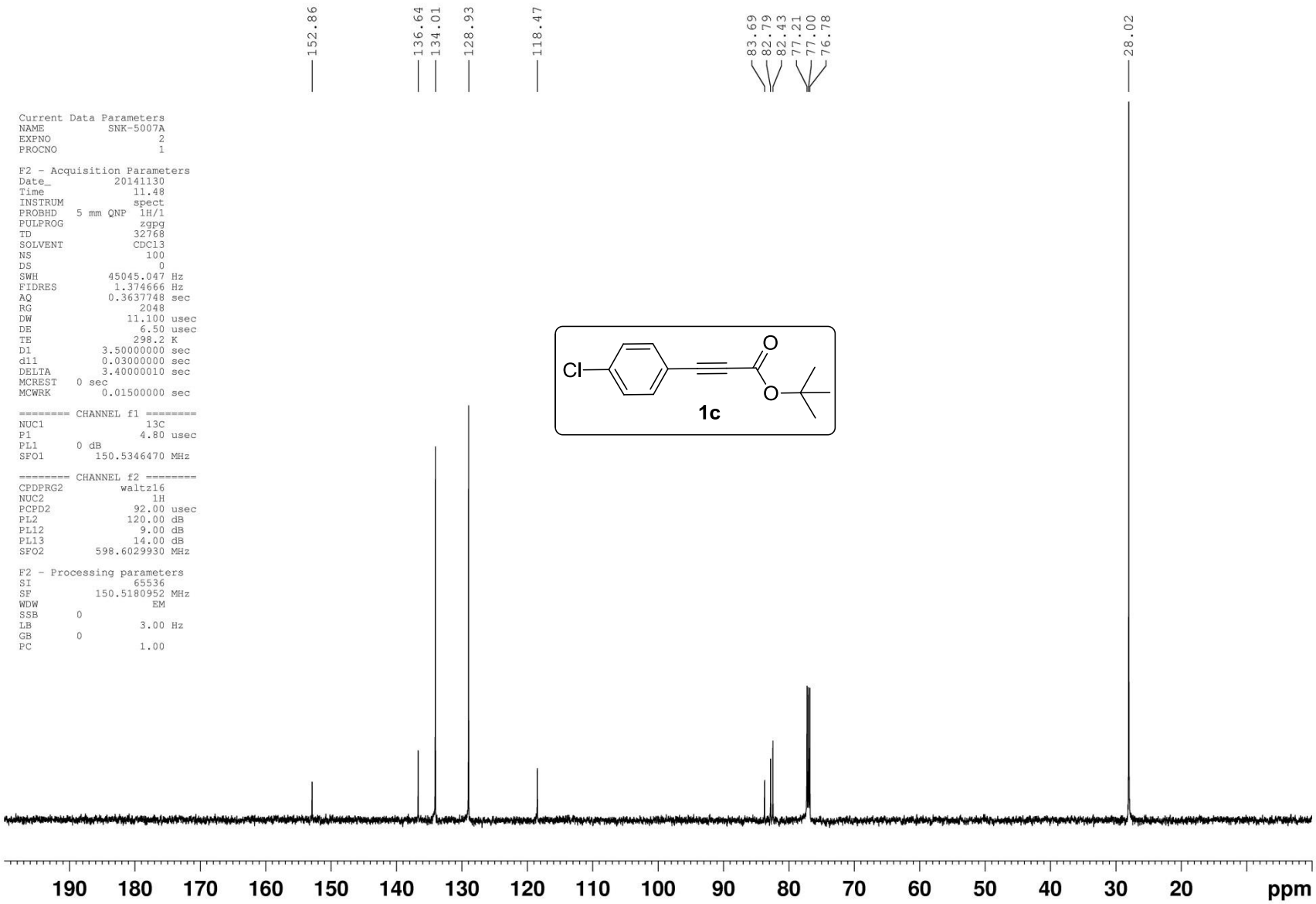

7.553
7.552
7.551
7.550
7.550
7.543
7.540
7.537
7.412
7.399
7.396
7.389
7.387
7.384
7.348
7.346
7.345
7.343
7.334
7.332
7.329
7.324
7.322
7.322
7.320
7.318
7.240
1.525
Current Data Parameters
NAME SNK-4222
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140918
Time 5.37
INSTRUM spect
PROBHD 5 mm 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 303.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.7029935 MHz
F2 - Processing parameters
SI 32768
SF 598.7000260 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
1a
2.16
0.98
2.21
9.21
10
9
8
7
6
5
4
3
2
1
ppm

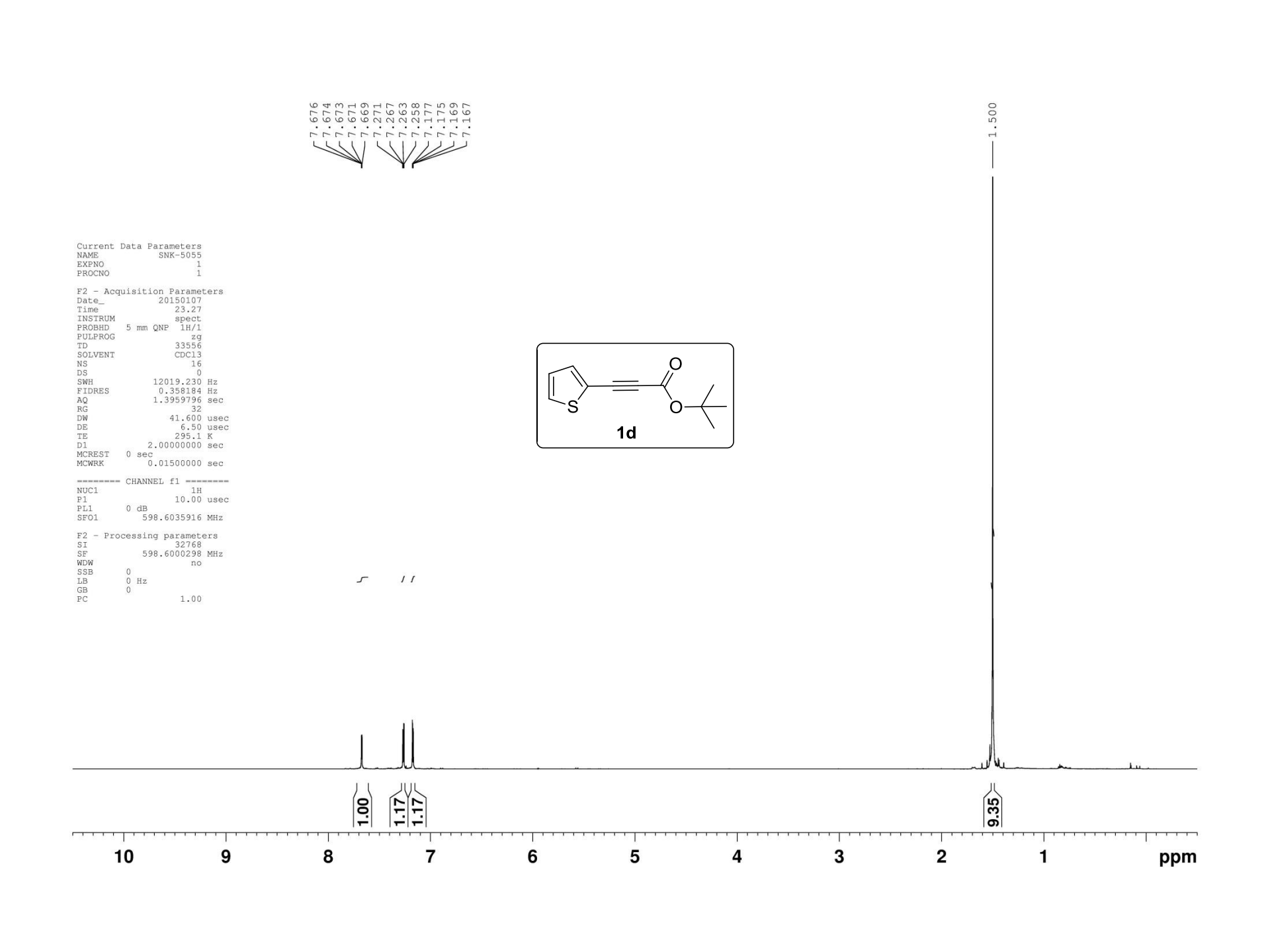

153.12
132.84
130.26
128.46
120.02
83.77
83.45
82.04
77.21
77.00
76.79
28.05
Current Data Parameters
NAME SNK-4222
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20140918
Time 5.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 304.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 dB
SFO1 150.5597948 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 92.00 usec
PL2 120.00 dB
PL12 9.00 dB
PL13 14.00 dB
SFO2 598.7029935 MHz
F2 - Processing parameters
SI 65536
SF 150.5432369 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

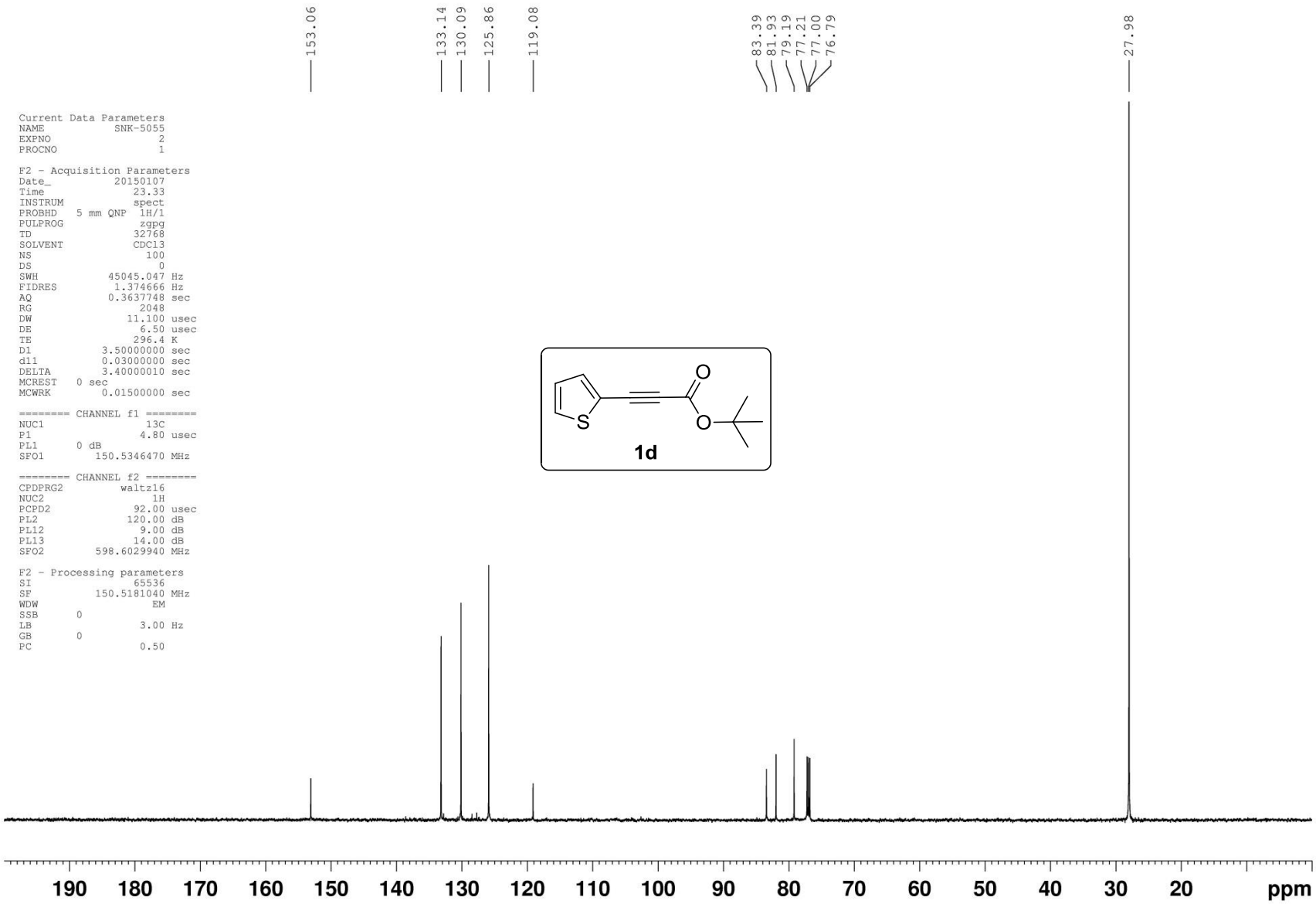

SNK-5012a
7.510
7.488
7.240
6.857
6.835
3.805
1.517
Current Data Parameters
NAME SNK-5012a.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611794 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
O
O
1b
2.00
2.19
3.27
9.67
10
9
8
7
6
5
4
3
2
1
ppm

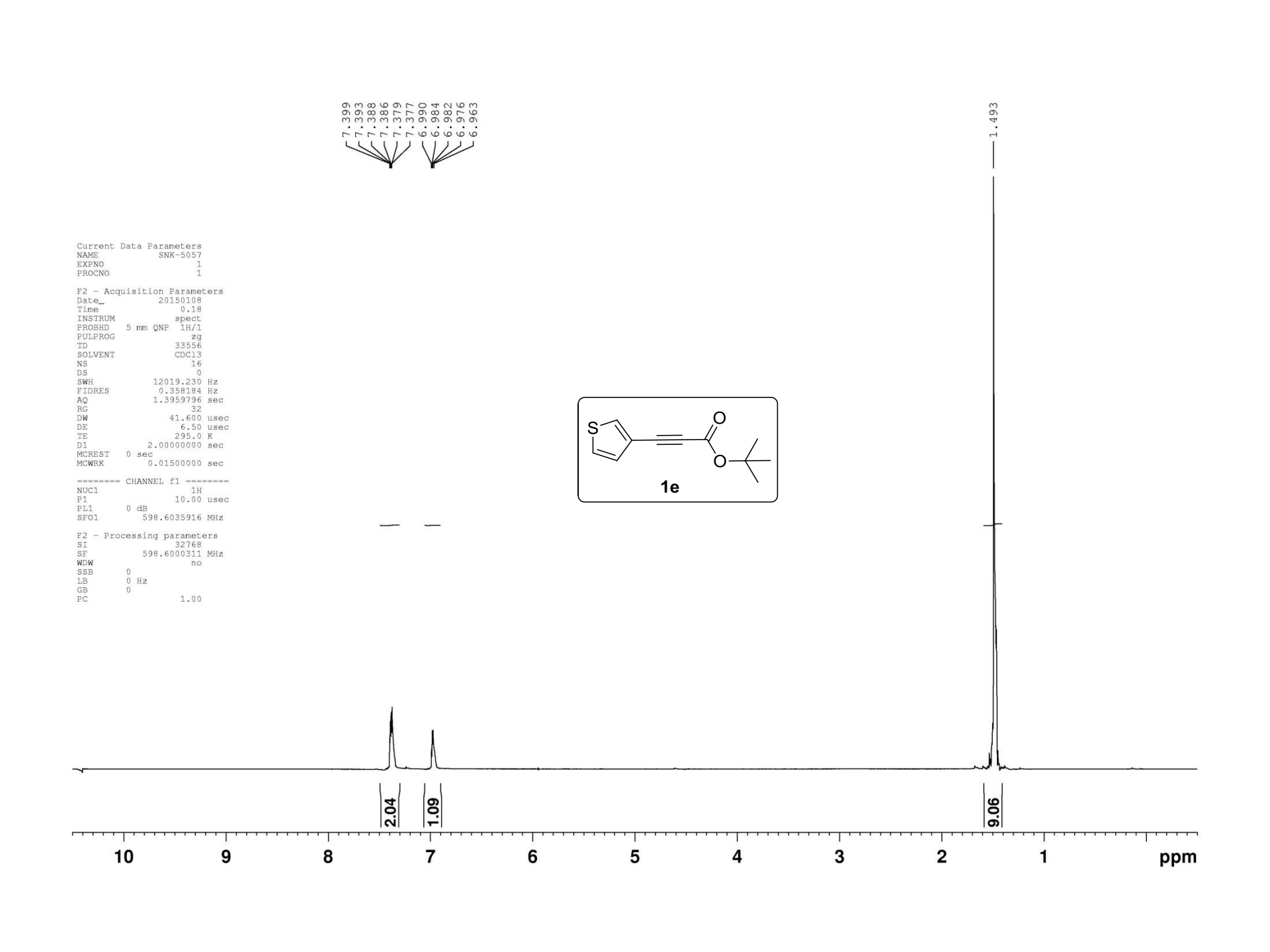

161.16
153.33
134.65
114.10
111.62
84.47
83.09
81.31
77.31
77.00
76.68
55.23
27.97
Current Data Parameters
NAME SNK-5012aC.fid
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214650 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
O
O
1b
SNK-5012a C
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

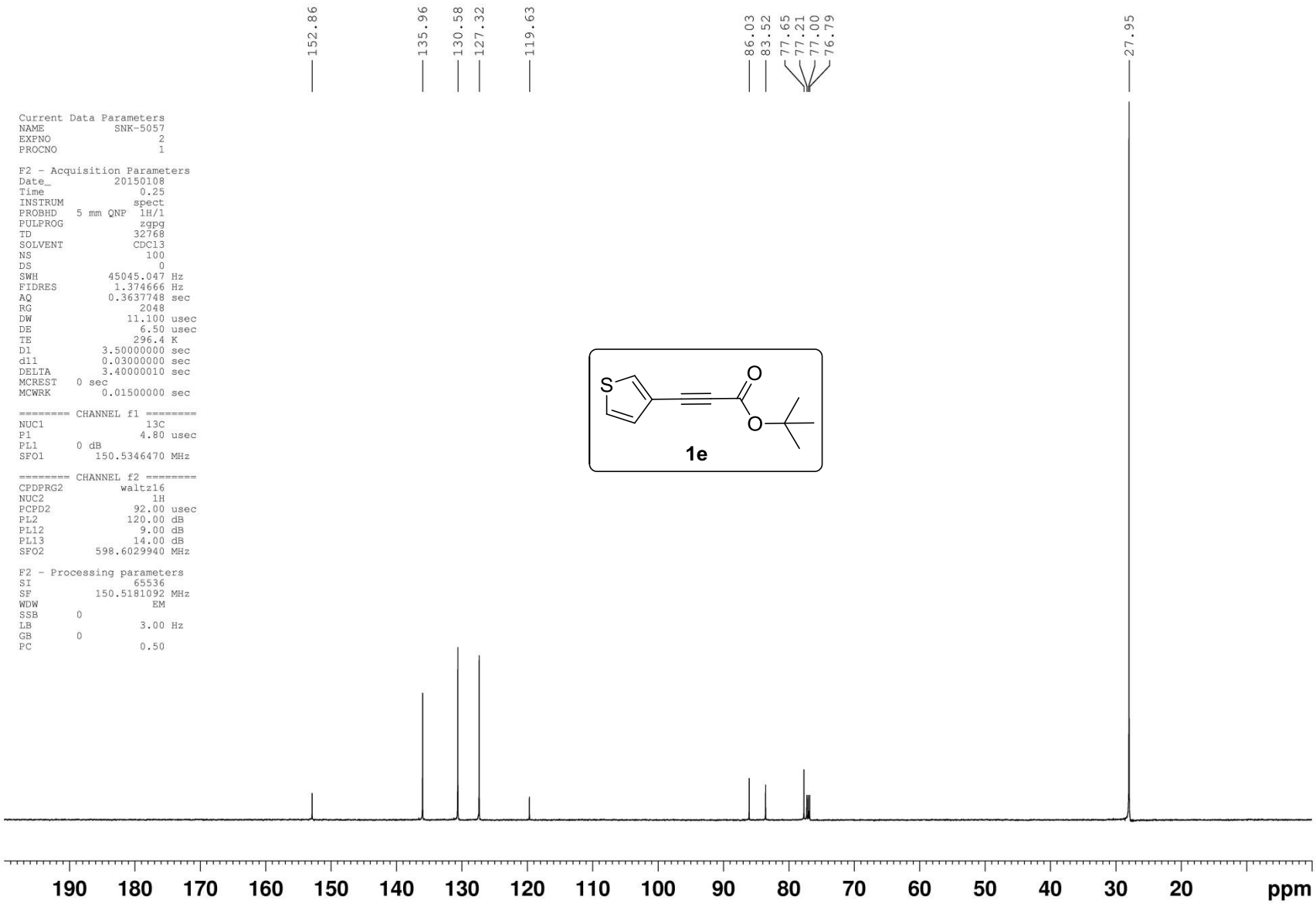

7.477
7.463
7.320
7.306
1.514
Current Data Parameters
NAME SNK-5007A
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141130
Time 11.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 296.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
Cl
O
O
1c
2.00
2.11
9.49
10
9
8
7
6
5
4
3
2
1
ppm

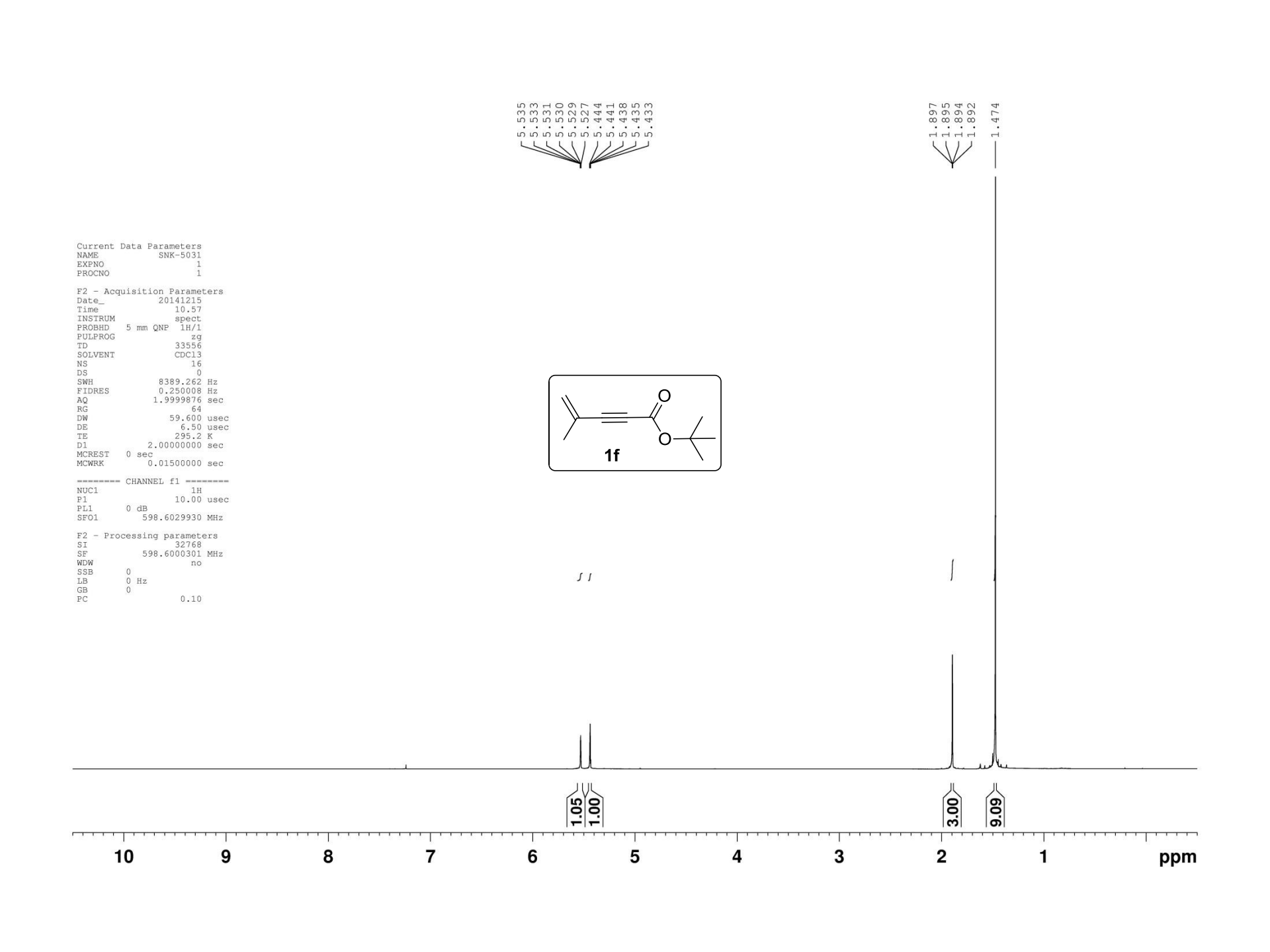

152.86
136.64
134.01
128.93
118.47
83.69
82.79
82.43
77.21
77.00
76.78
28.02
Current Data Parameters
NAME SNK-5007A
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141130
Time 11.48
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 298.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
Cl
O
O
1c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

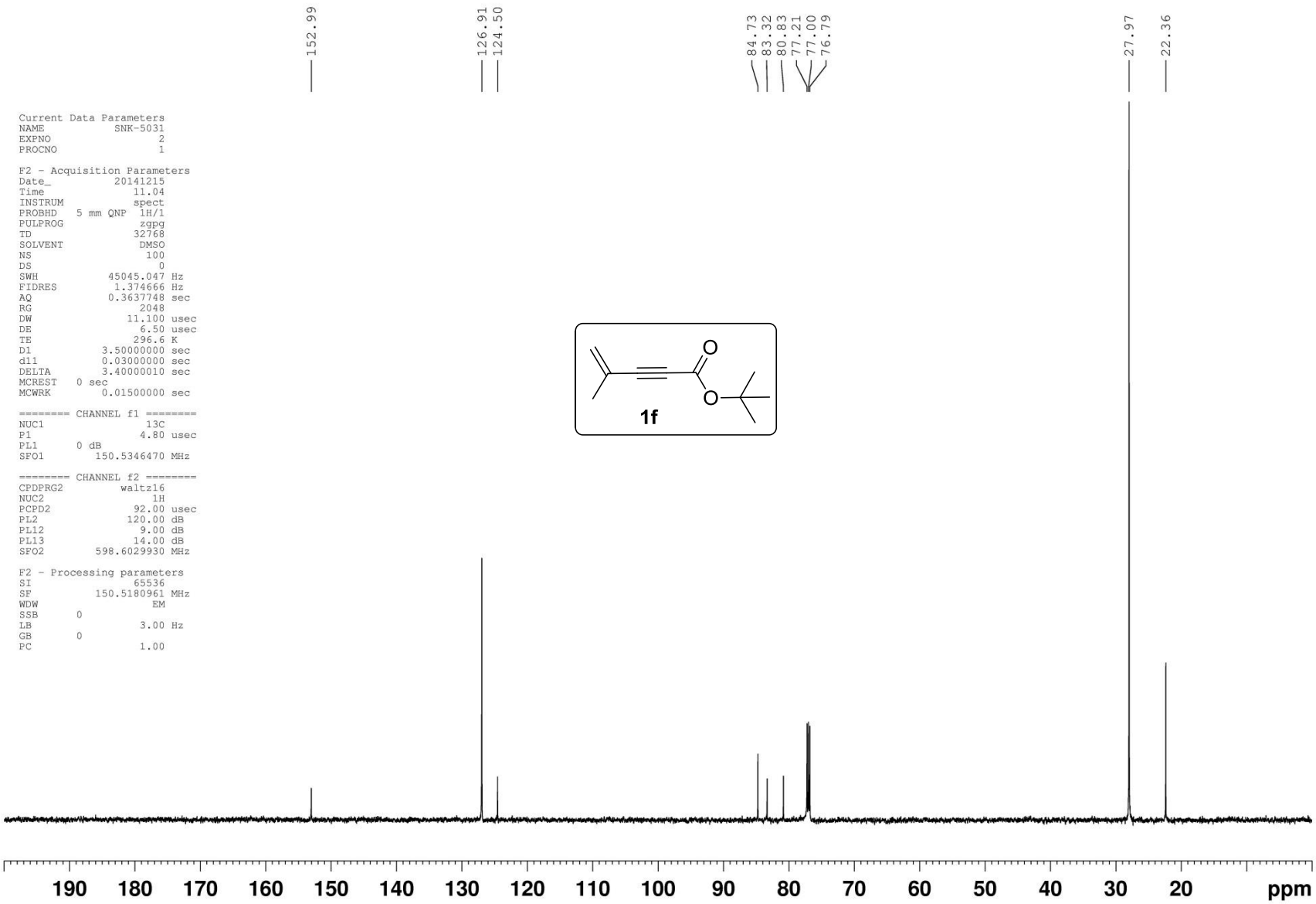

7.676
7.674
7.673
7.671
7.669
7.271
7.267
7.263
7.258
7.177
7.175
7.169
7.167
1.500
Current Data Parameters
NAME SNK-5055
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 23.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 32
DW 41.600 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
S
O
1d
1.00
1.17
1.17
9.35
10
9
8
7
6
5
4
3
2
1
ppm

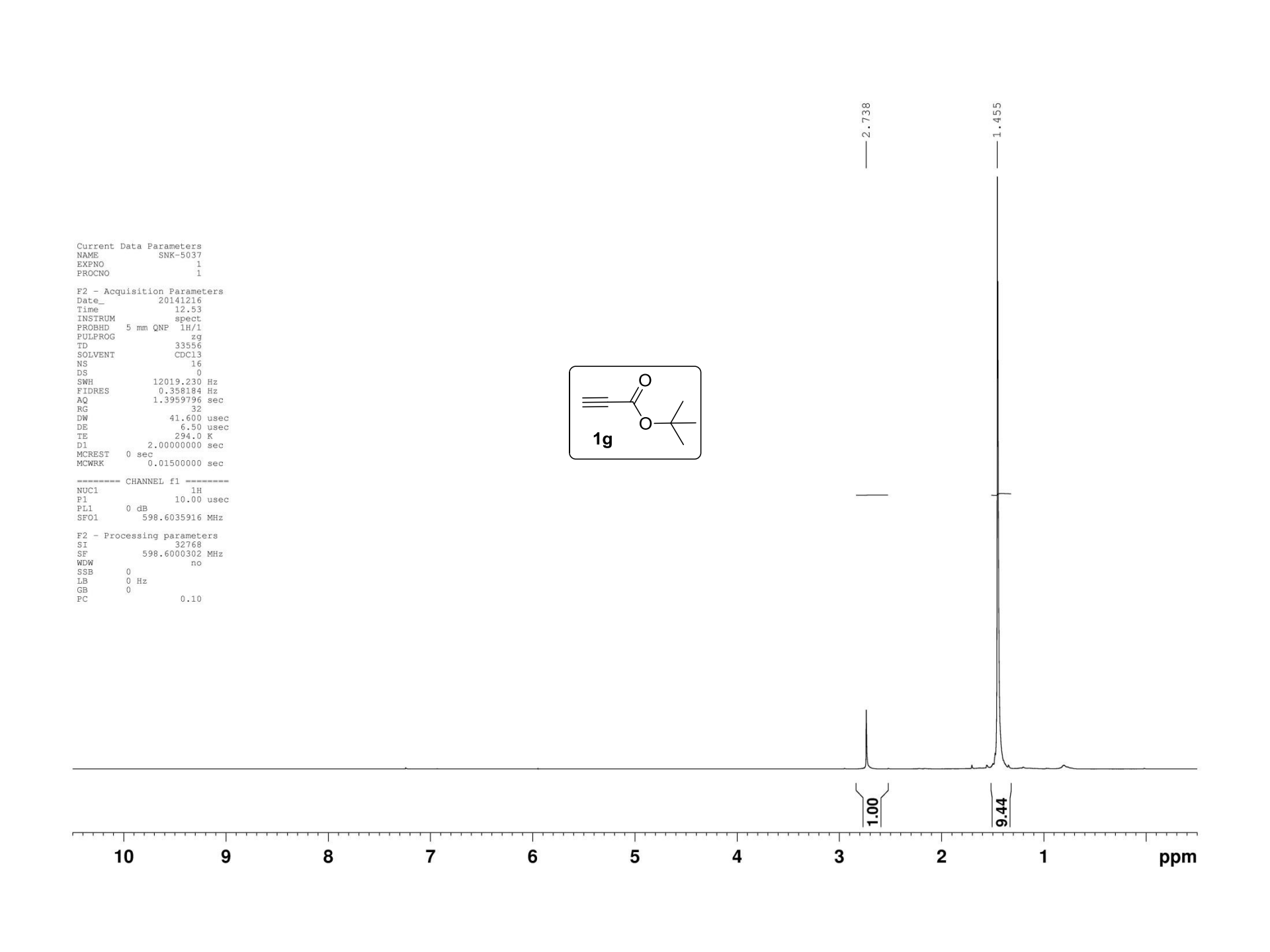

153.06
133.14
130.09
125.86
119.08
83.39
81.93
79.19
77.21
77.00
76.79
27.98
Current Data Parameters
NAME SNK-5055
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 23.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181040 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
O
S
O
1d
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

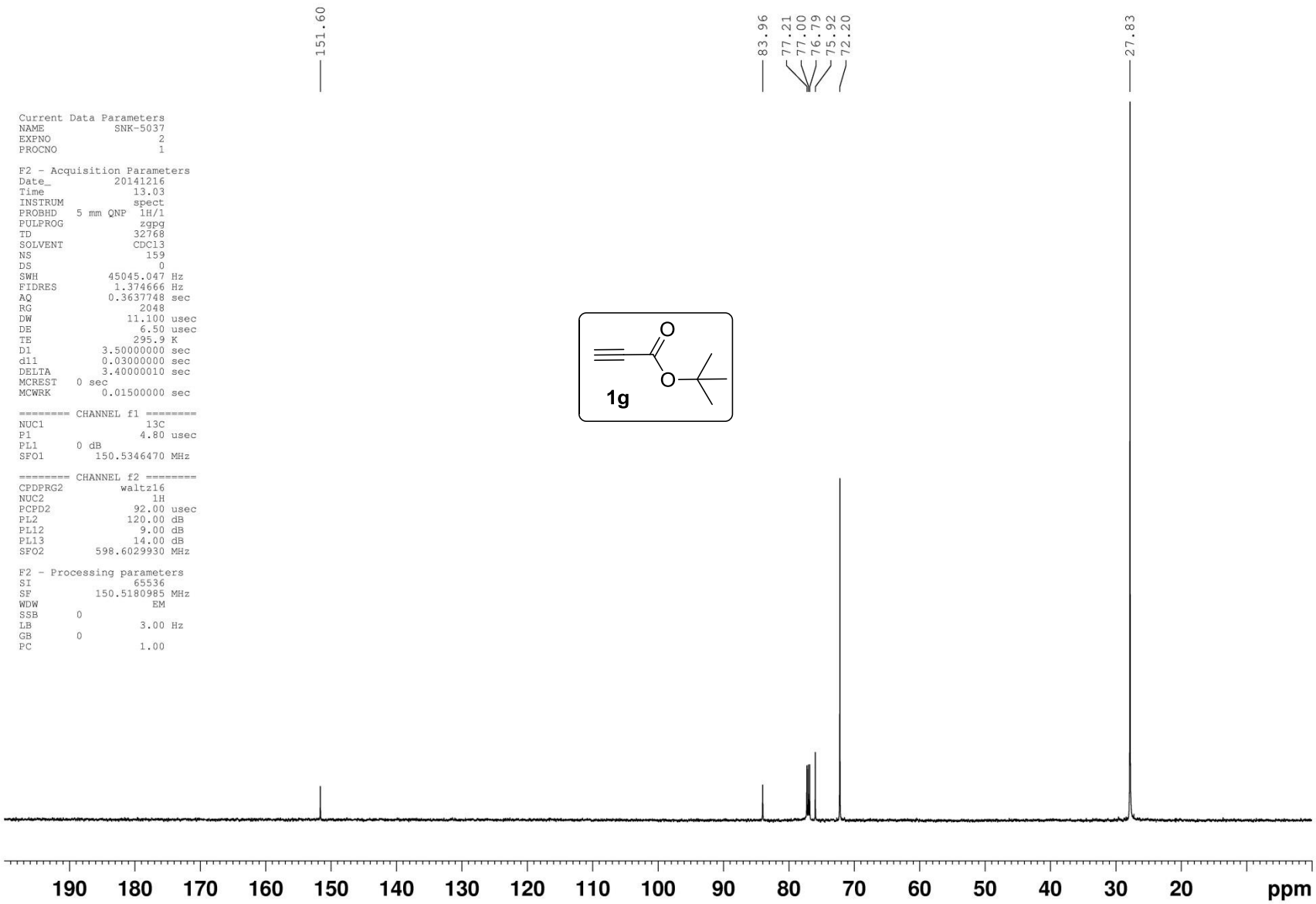

7.399
7.393
7.388
7.386
7.379
7.377
6.990
6.984
6.982
6.976
6.963
1.493
Current Data Parameters
NAME SNK-5057
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150108
Time 0.18
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 32
DW 41.600 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000311 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
S
O
O
1e
2.04
1.09
9.06
10
9
8
7
6
5
4
3
2
1
ppm

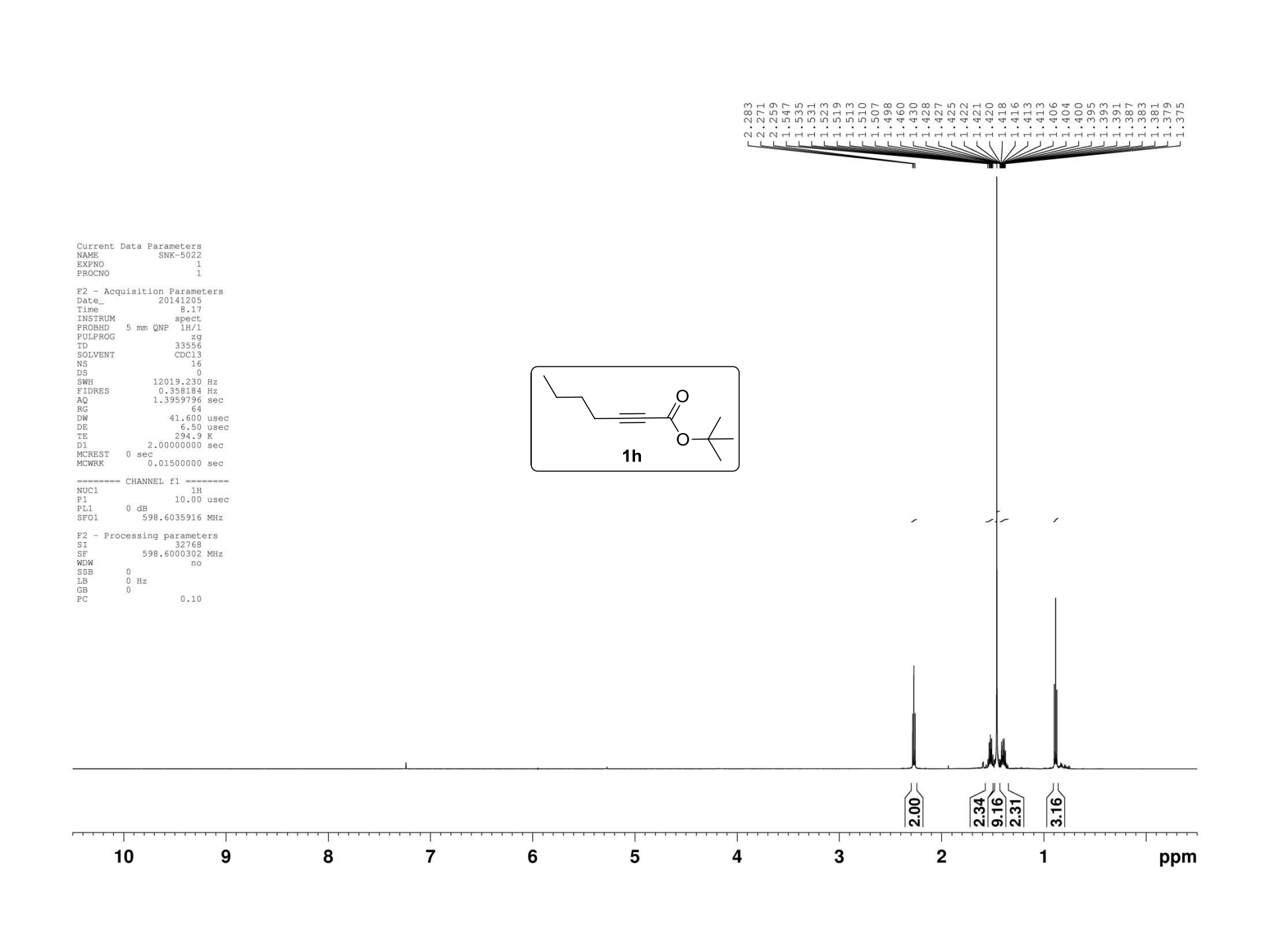

152.86
135.96
130.58
127.32
119.63
86.03
83.52
77.65
77.21
77.00
76.79
27.95
Current Data Parameters
NAME SNK-5057
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150108
Time 0.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181092 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
S
O
O
1e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

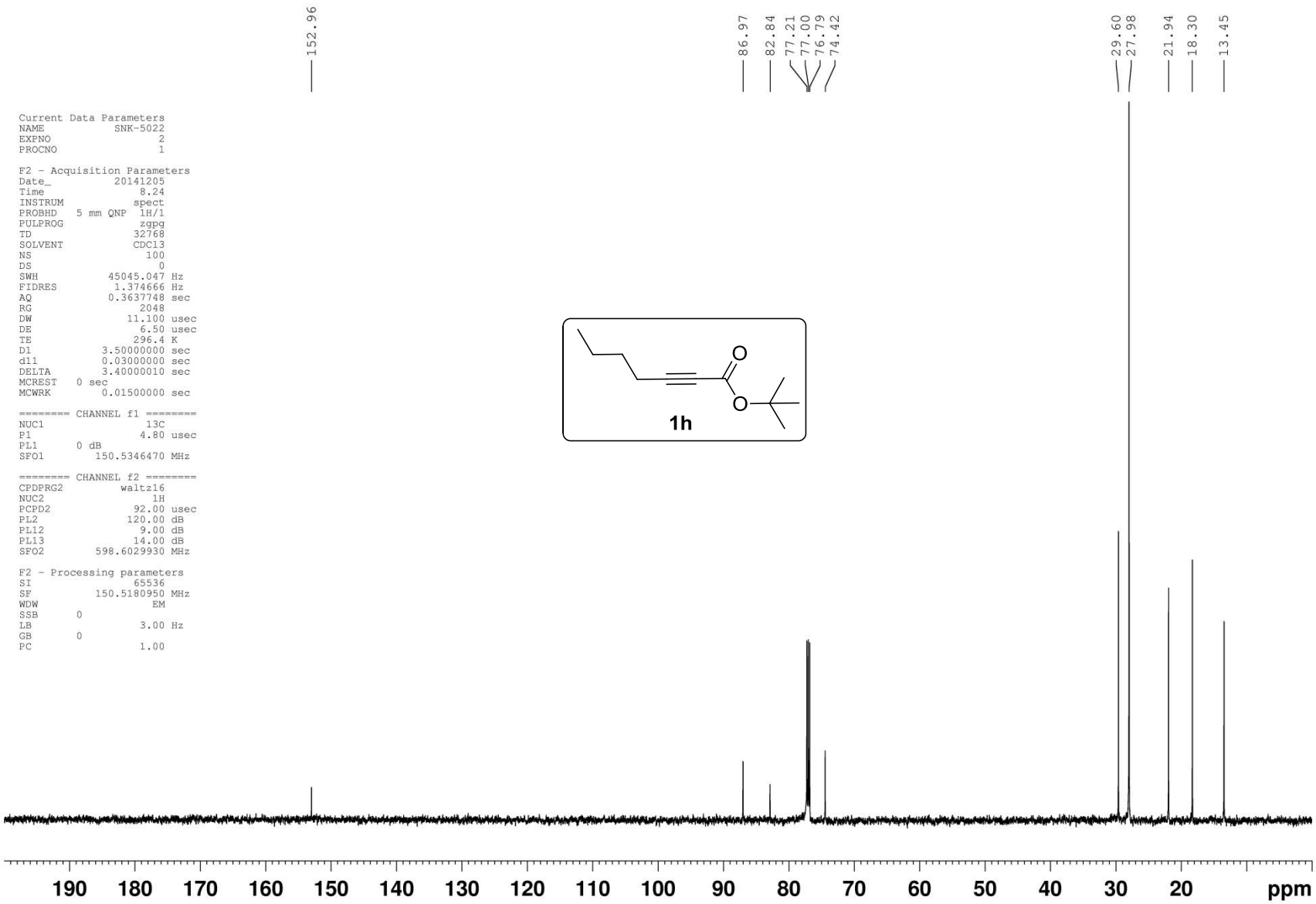

5.535
5.533
5.531
5.530
5.529
5.527
5.444
5.441
5.438
5.435
5.433
1.897
1.895
1.894
1.892
1.474
Current Data Parameters
NAME SNK-5031
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141215
Time 10.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 64
DW 59.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
O
O
1f
1.05
1.00
3.00
9.09
10
9
8
7
6
5
4
3
2
1
ppm

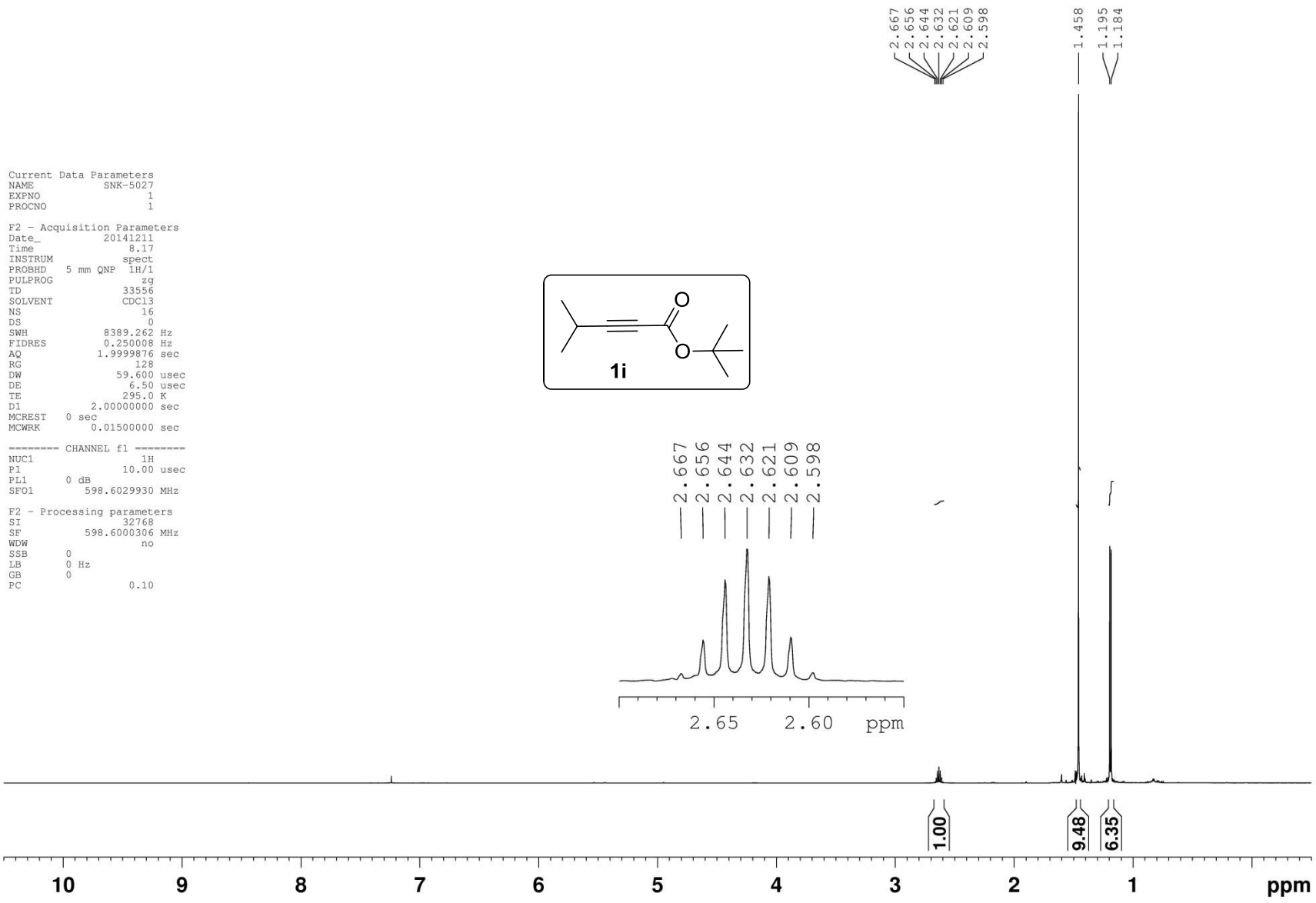

152.99
126.91
124.50
84.73
83.32
80.83
77.21
77.00
76.79
27.97
22.36
Current Data Parameters
NAME SNK-5031
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141215
Time 11.04
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180961 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1f
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

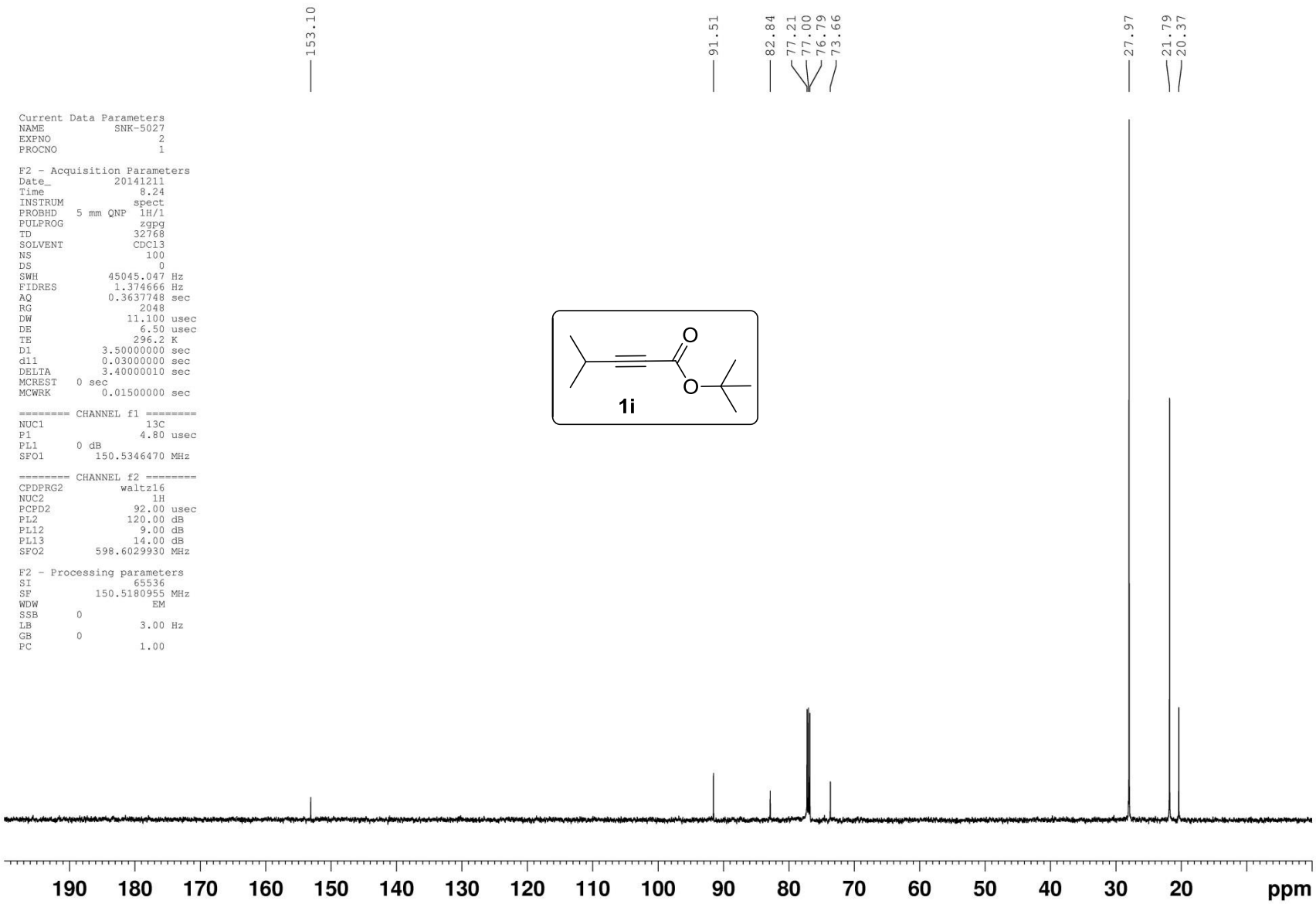

Current Data Parameters
NAME SNK-5037
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141216
Time 12.53
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 32
DW 41.600 usec
DE 6.50 usec
TE 294.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000302 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
1g
2.738
1.455
1.00
9.44
10
9
8
7
6
5
4
3
2
1
ppm

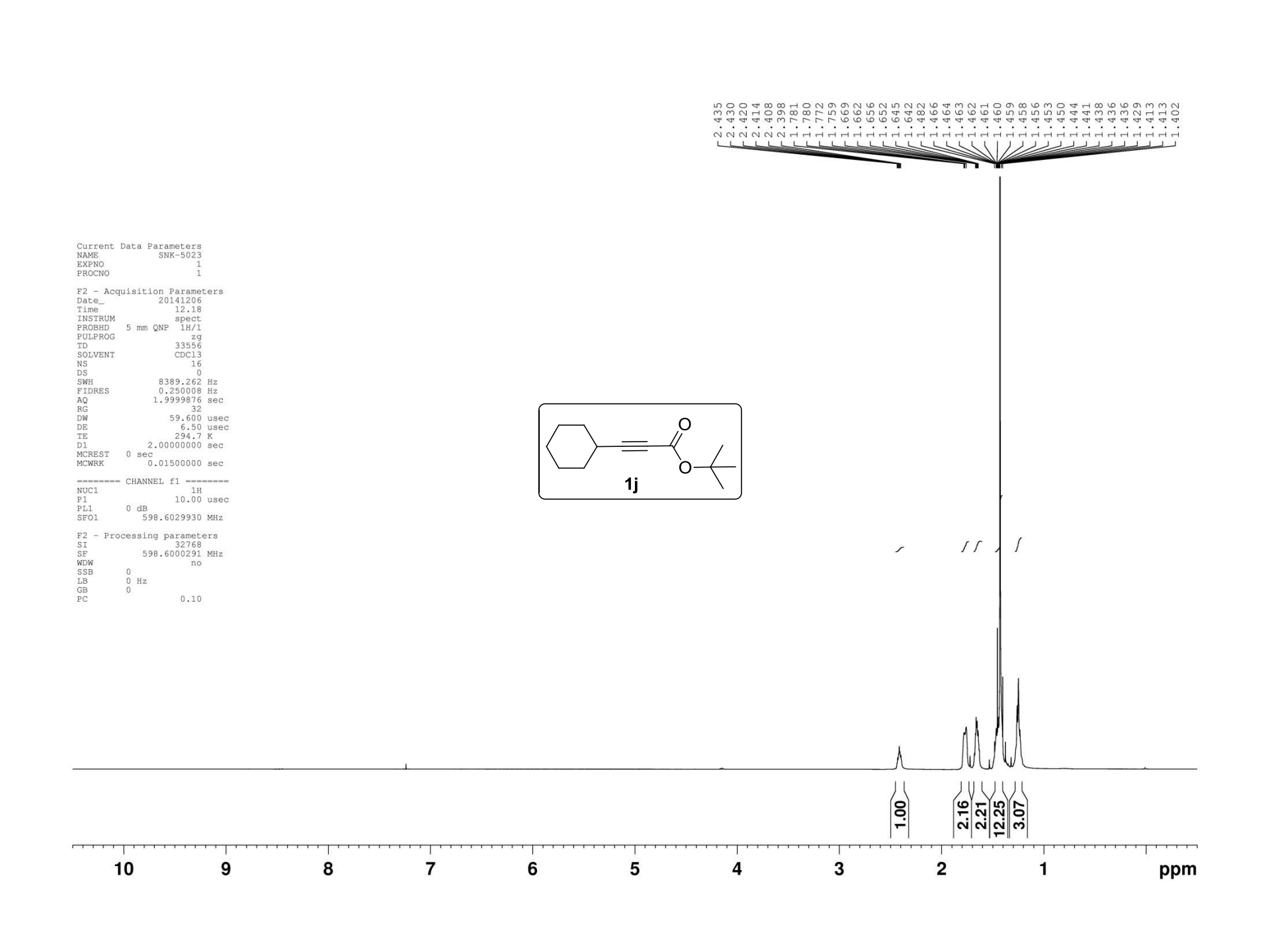

151.60
83.96
77.21
77.00
76.79
75.92
72.20
27.83
Current Data Parameters
NAME SNK-5037
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141216
Time 13.03
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 159
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180985 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

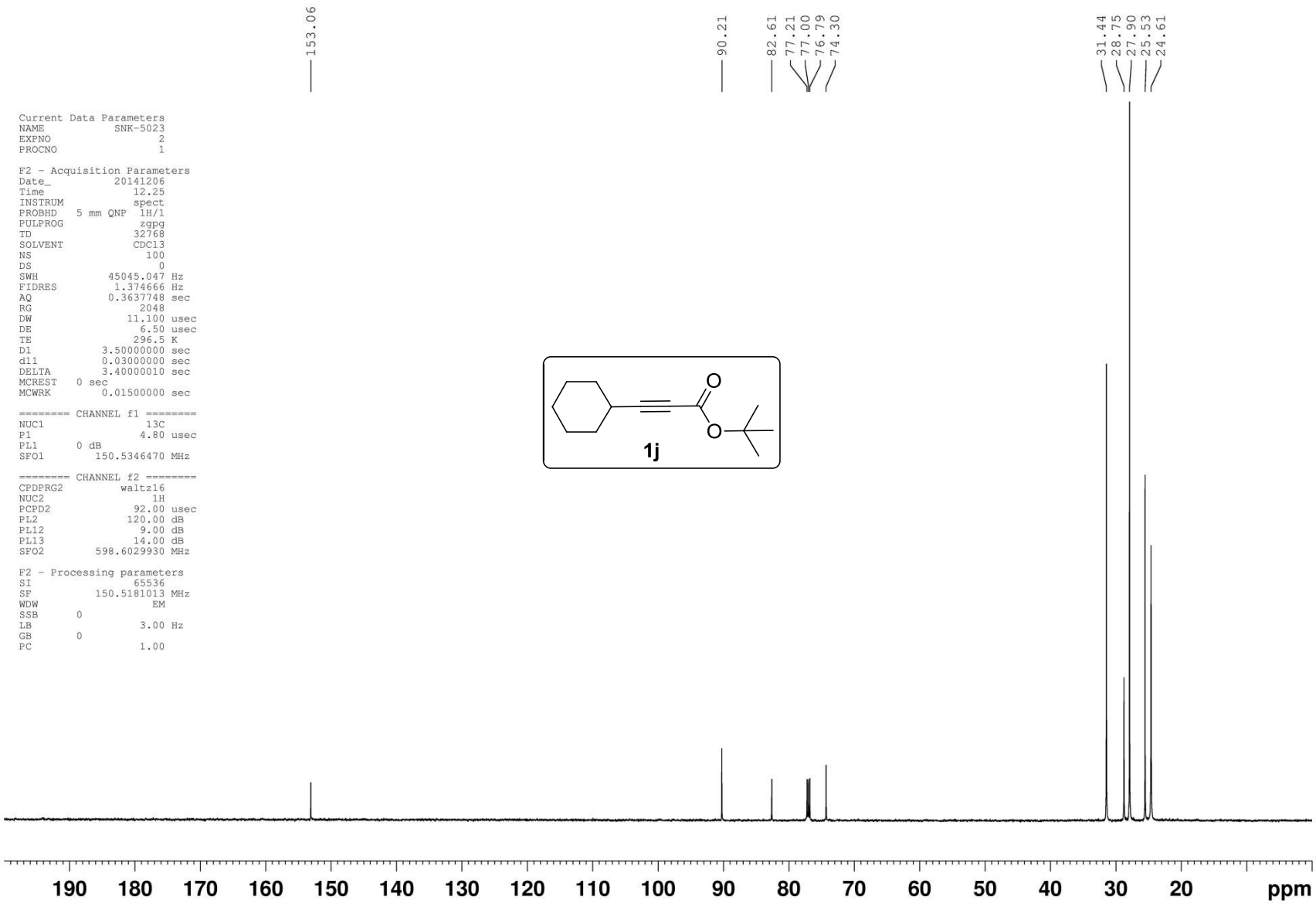

Current Data Parameters
NAME SNK-5022
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141205
Time 8.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000302 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
2.283
2.271
2.259
1.547
1.535
1.531
1.523
1.519
1.513
1.510
1.507
1.498
1.460
1.430
1.428
1.427
1.425
1.422
1.421
1.420
1.418
1.416
1.413
1.413
1.406
1.404
1.400
1.395
1.393
1.391
1.387
1.383
1.381
1.379
1.375
O
O
1h
2.00
2.34
9.16
2.31
3.16
10
9
8
7
6
5
4
3
2
1
ppm

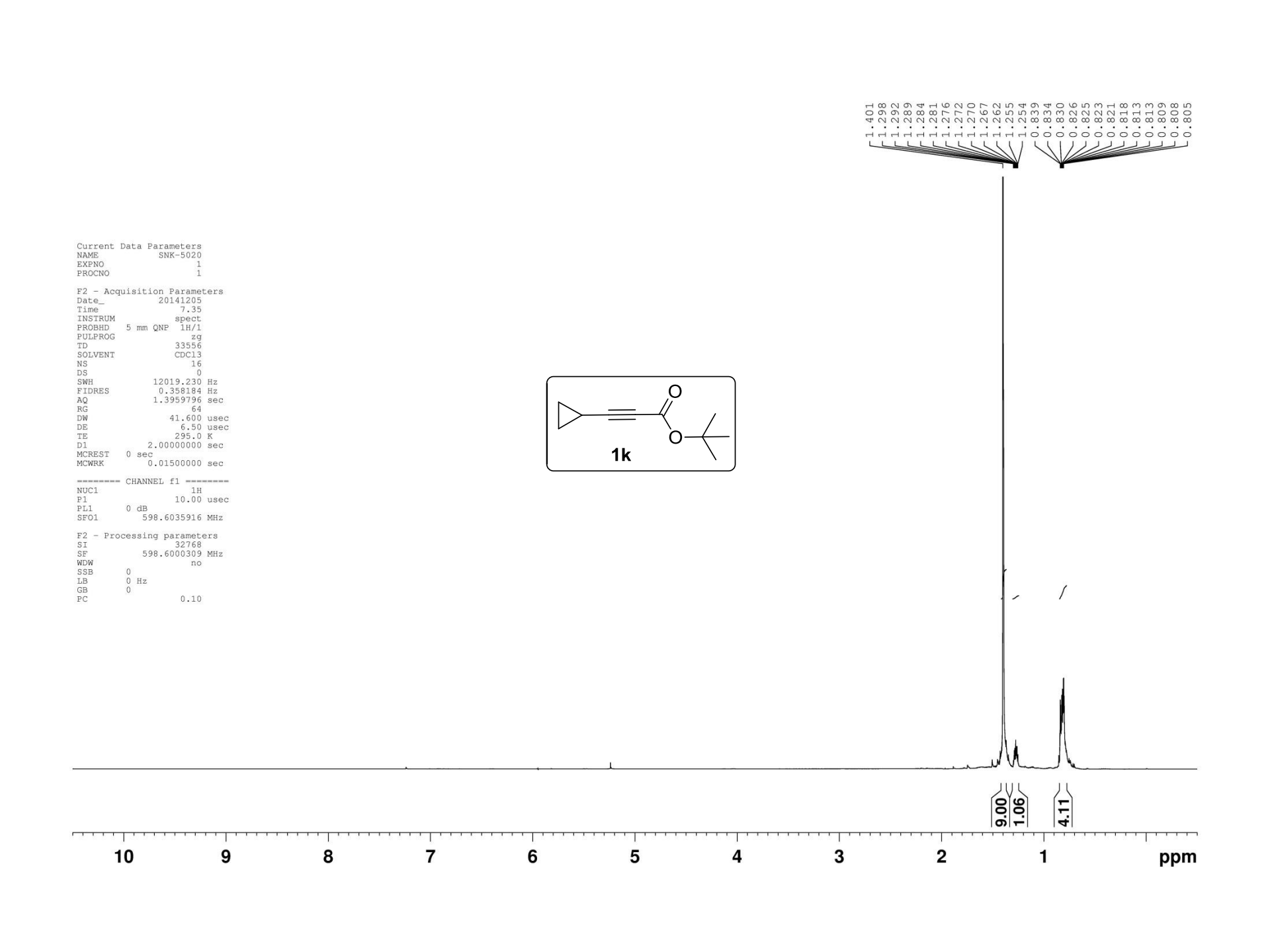

152.96
86.97
82.84
77.21
77.00
76.79
74.42
29.60
27.98
21.94
18.30
13.45
Current Data Parameters
NAME SNK-5022
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141205
Time 8.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180950 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

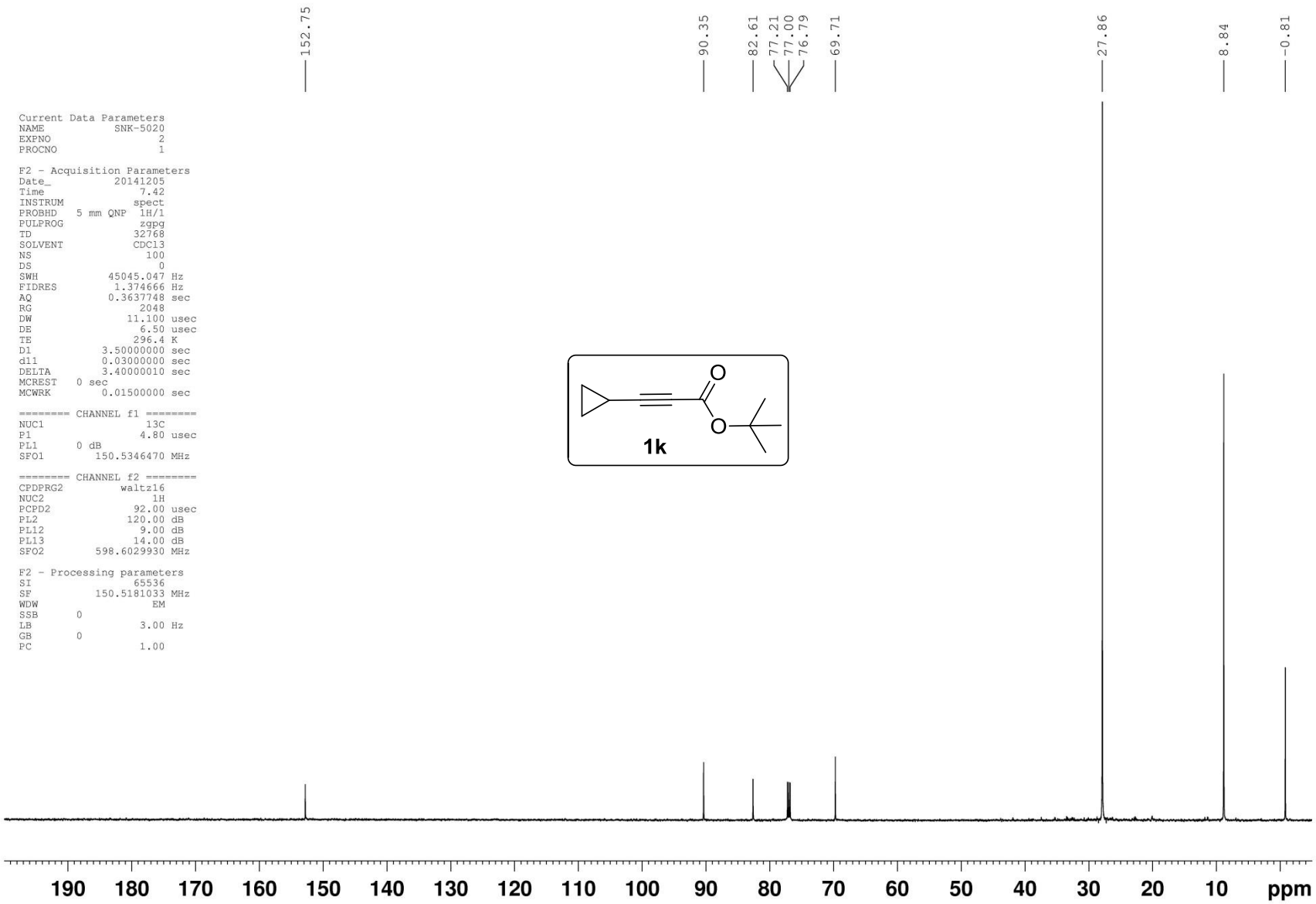

Current Data Parameters
NAME SNK-5027
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141211
Time 8.17
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 128
DW 59.600 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000306 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
2.667
2.656
2.644
2.632
2.621
2.609
2.598
1.458
1.195
1.184
1i
2.65
2.60
ppm
1.00
9.48
6.35
10
9
8
7
6
5
4
3
2
1
ppm

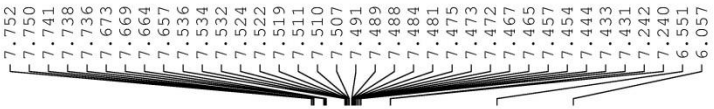

153.10
91.51
82.84
77.21
77.00
76.79
73.66
27.97
21.79
20.37
Current Data Parameters
NAME SNK-5027
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141211
Time 8.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180955 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1i
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


Current Data Parameters
NAME SNK-5023
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141206
Time 12.18
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 32
DW 59.600 usec
DE 6.50 usec
TE 294.7 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000291 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
2.435
2.430
2.420
2.414
2.408
2.398
1.781
1.780
1.772
1.759
1.669
1.662
1.656
1.652
1.645
1.642
1.482
1.466
1.464
1.463
1.462
1.461
1.460
1.459
1.458
1.456
1.453
1.450
1.444
1.441
1.438
1.436
1.436
1.429
1.413
1.413
1.402
O
O
1j
1.00
2.16
2.21
12.25
3.07
10
9
8
7
6
5
4
3
2
1
ppm

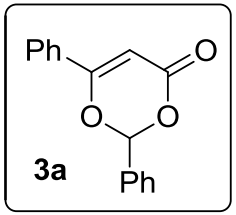

153.06
90.21
82.61
77.21
77.00
76.79
74.30
31.44
28.75
27.90
25.53
24.61
Current Data Parameters
NAME SNK-5023
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141206
Time 12.25
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 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
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181013 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1j
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

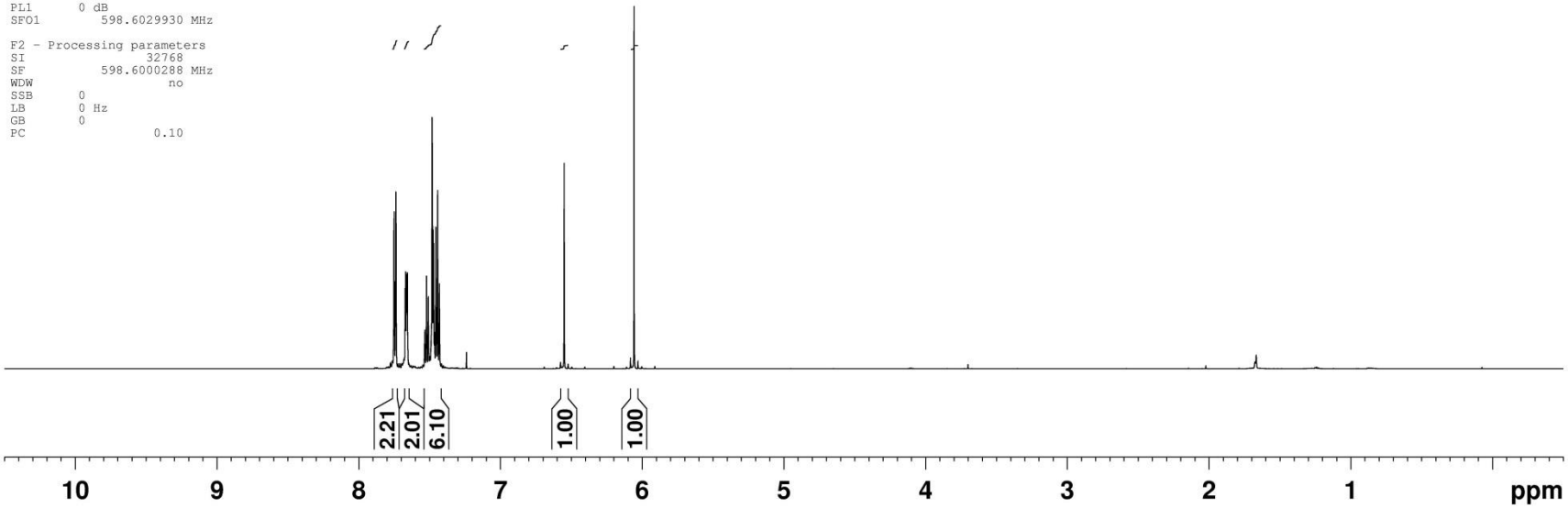

Current Data Parameters
NAME SNK-5020
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141205
Time 7.35
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000309 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
1k
1.401
1.298
1.292
1.289
1.284
1.281
1.276
1.272
1.270
1.267
1.262
1.255
1.254
0.839
0.834
0.830
0.826
0.825
0.823
0.821
0.818
0.813
0.809
0.808
0.805
9.00
1.06
4.11
10
9
8
7
6
5
4
3
2
1
ppm

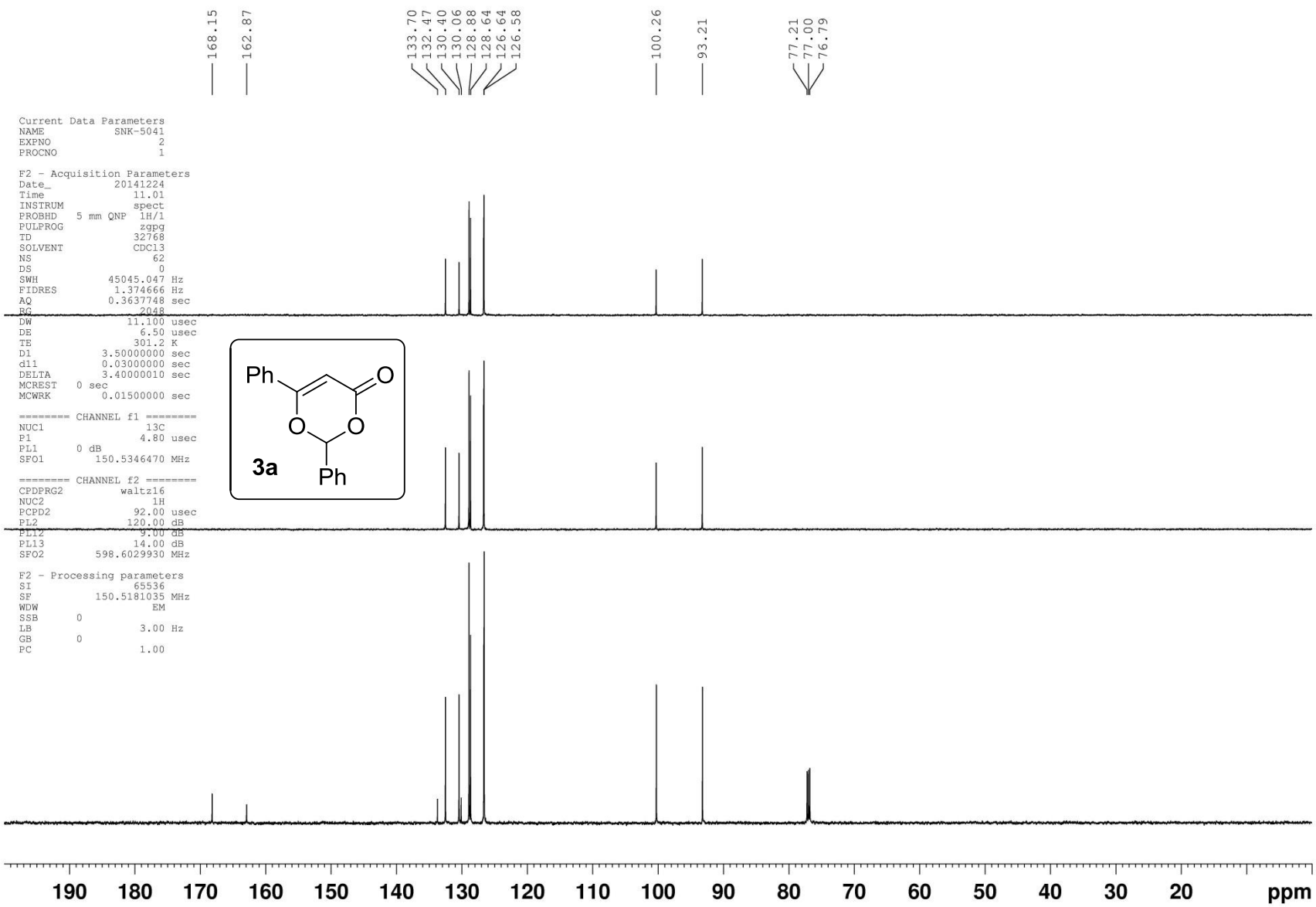

152.75
90.35
82.61
77.21
77.00
76.79
69.71
27.86
8.84
-0.81
Current Data Parameters
NAME SNK-5020
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141205
Time 7.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181033 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O
1k
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

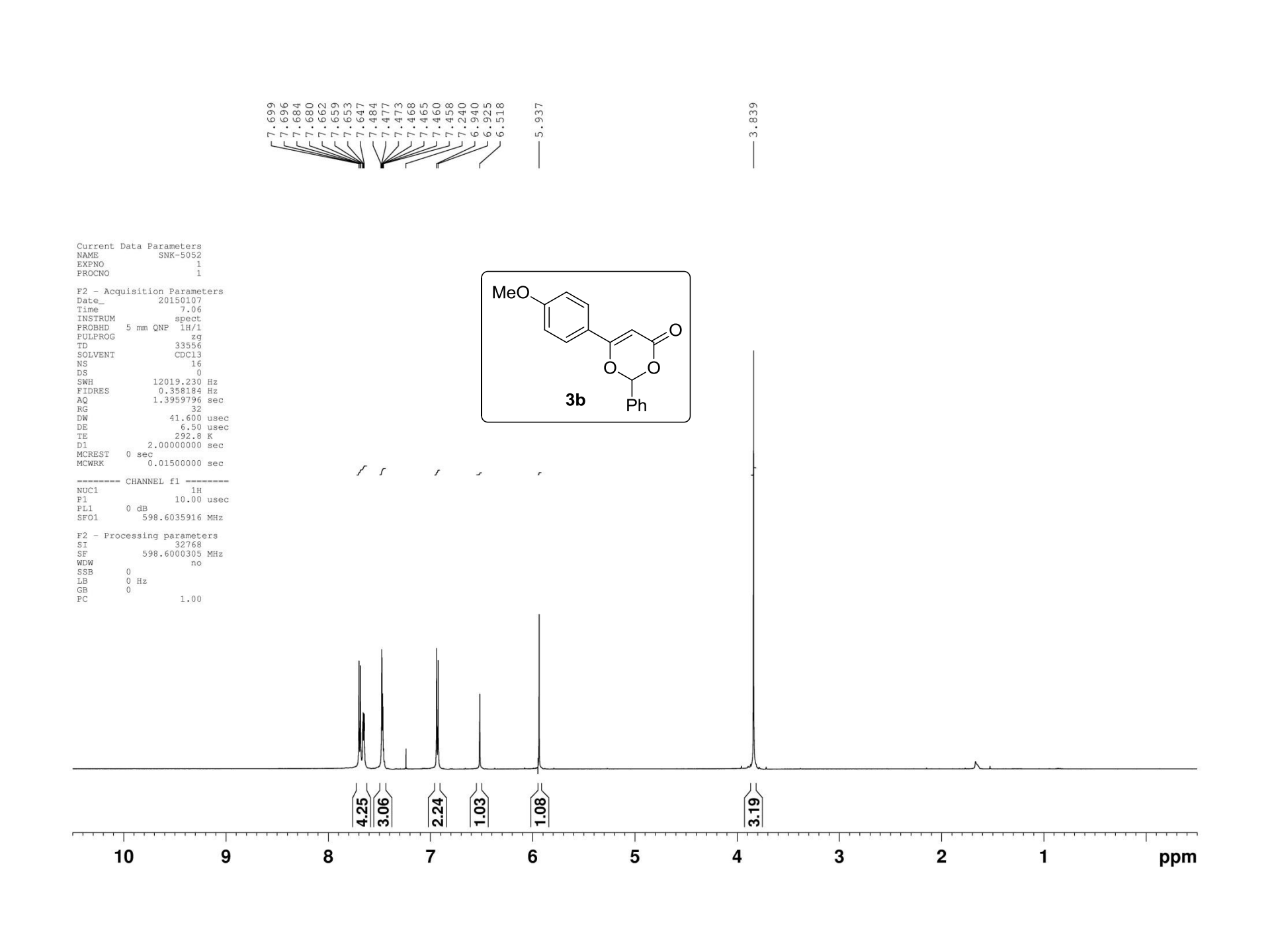


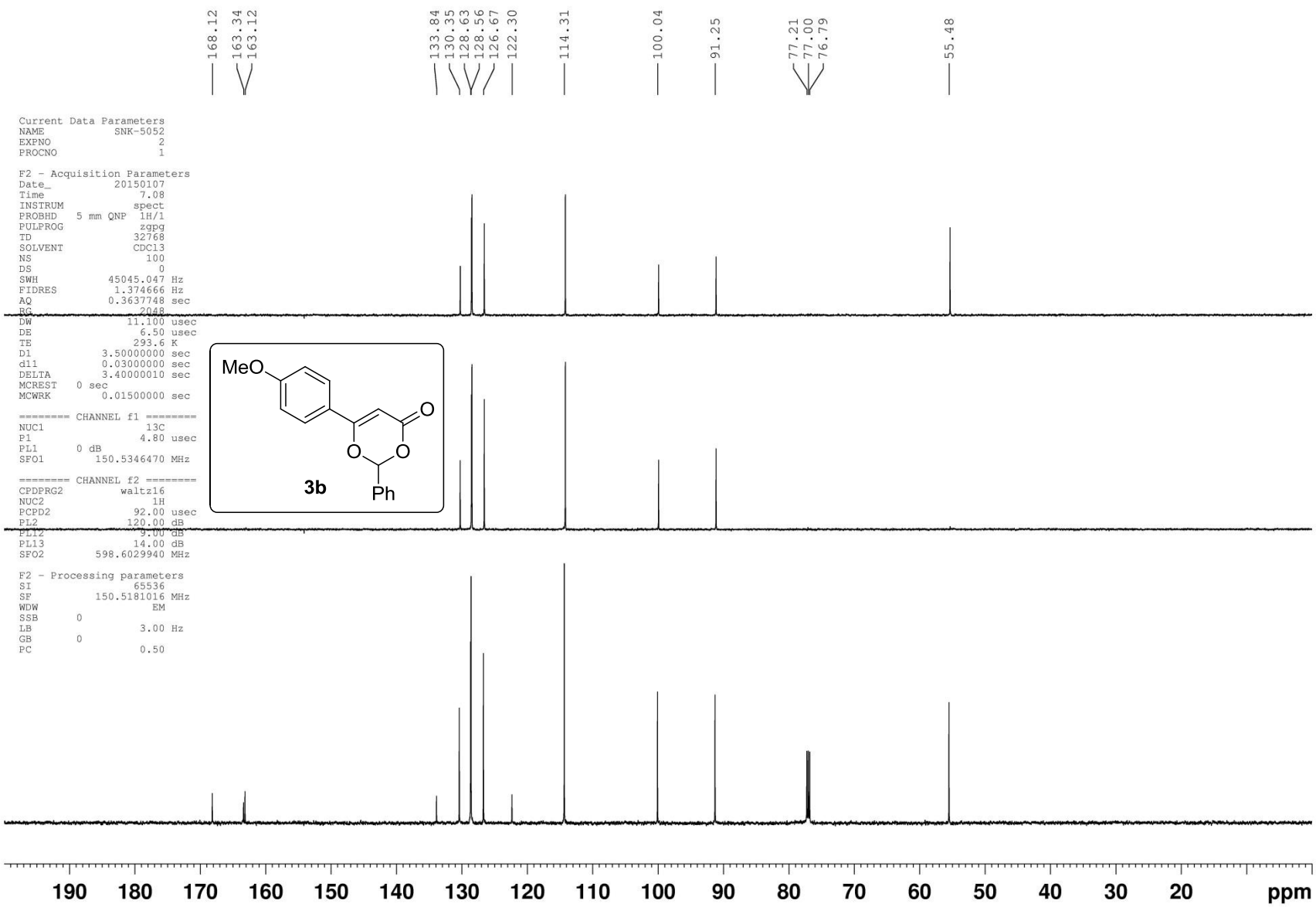

```
Current Data Parameters
NAME             SNK-5041
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20141224
Time               10.58
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                300.9 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1       0 dB
SFO1         598.6029930 MHz

F2 - Processing parameters
SI                 32768
SF           598.6000288 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                  0.10
```

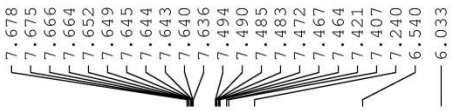




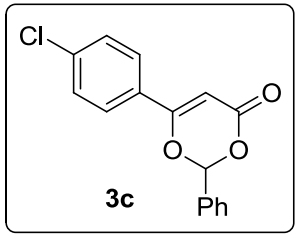

168.15
162.87
133.70
132.47
130.40
130.06
128.88
128.64
126.64
126.58
100.26
93.21
77.21
77.00
76.79
Current Data Parameters
NAME SNK-5041
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141224
Time 11.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 62
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 301.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181035 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
Ph
3a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

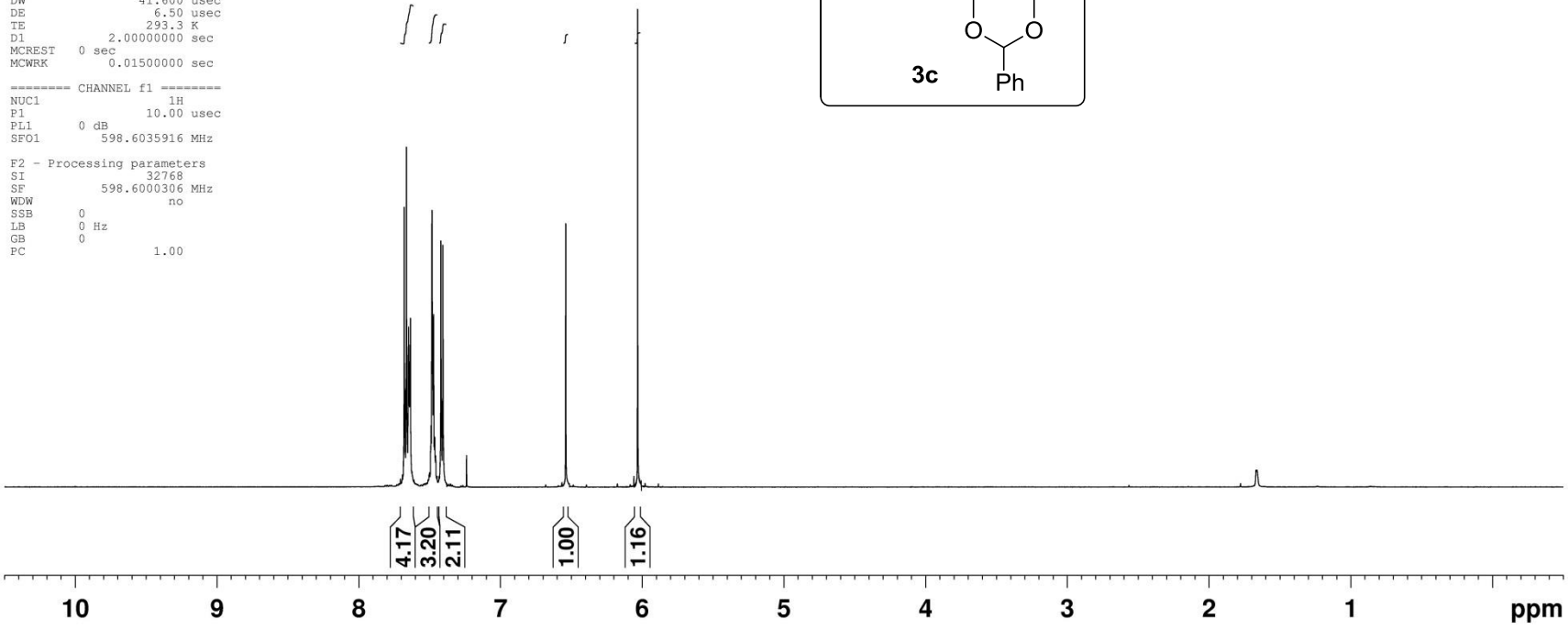

7.699
7.696
7.684
7.680
7.662
7.659
7.653
7.647
7.484
7.477
7.473
7.468
7.465
7.460
7.458
7.240
6.940
6.925
6.518
5.937
3.839
Current Data Parameters
NAME SNK-5052
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 7.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 32
DW 41.600 usec
DE 6.50 usec
TE 292.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000305 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
MeO
O
O
O
3b
Ph
4.25
3.06
2.24
1.03
1.08
3.19
10
9
8
7
6
5
4
3
2
1
ppm

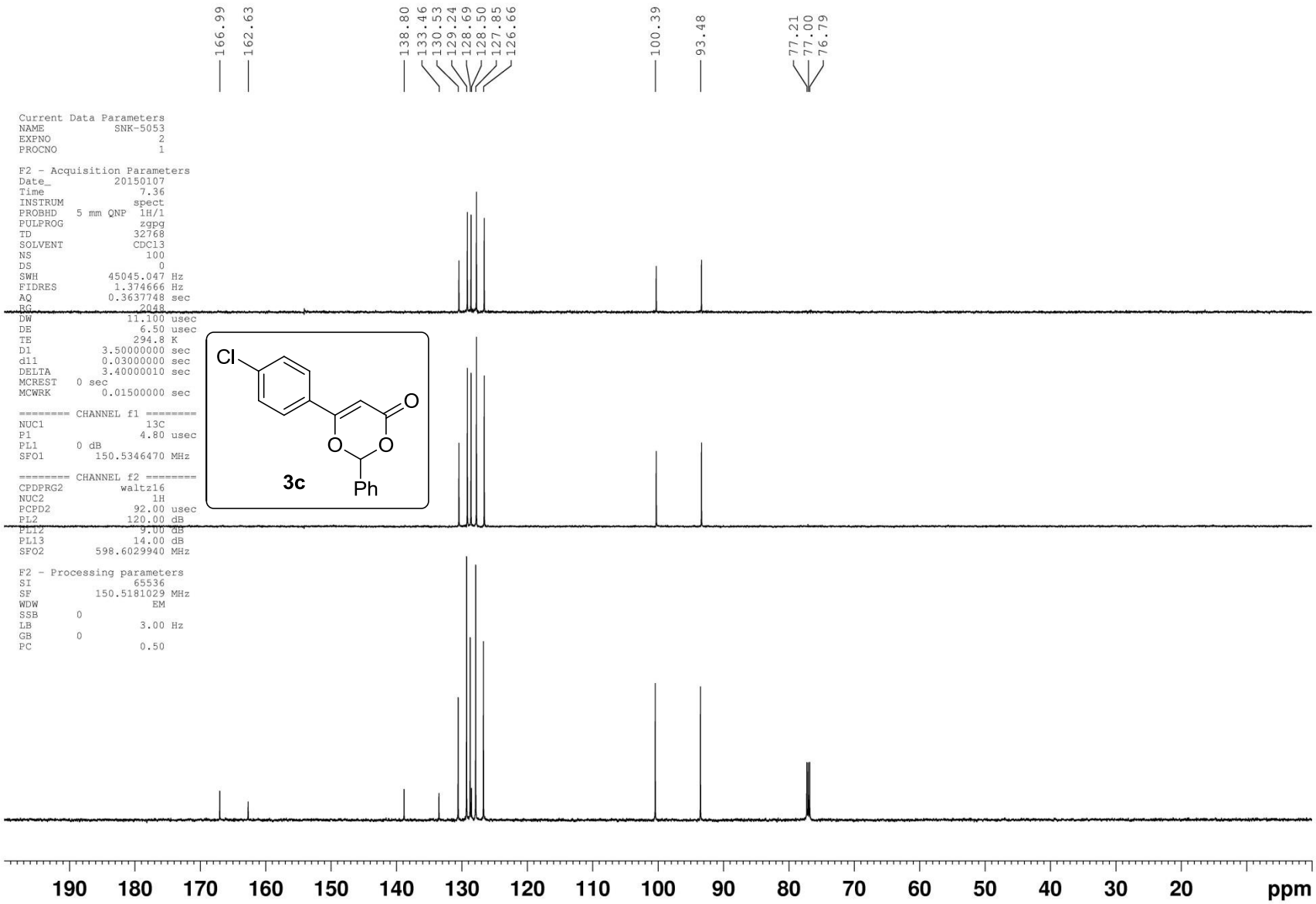

168.12
163.34
163.12
133.84
130.35
128.63
128.56
126.67
122.30
114.31
100.04
91.25
77.21
77.00
76.79
55.48
Current Data Parameters
NAME SNK-5052
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 7.08
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 293.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181016 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
MeO
O
O
O
Ph
3b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

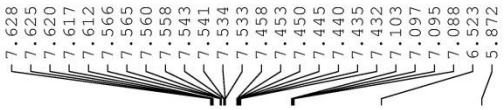



```
Current Data Parameters
NAME             SNK-5053
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150107
Time                7.30
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                     32
DW                41.600 usec
DE                 6.50 usec
TE                293.3 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1       0 dB
SFO1          598.6035916 MHz

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

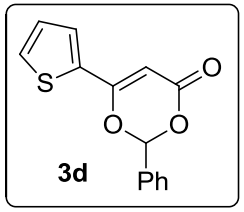


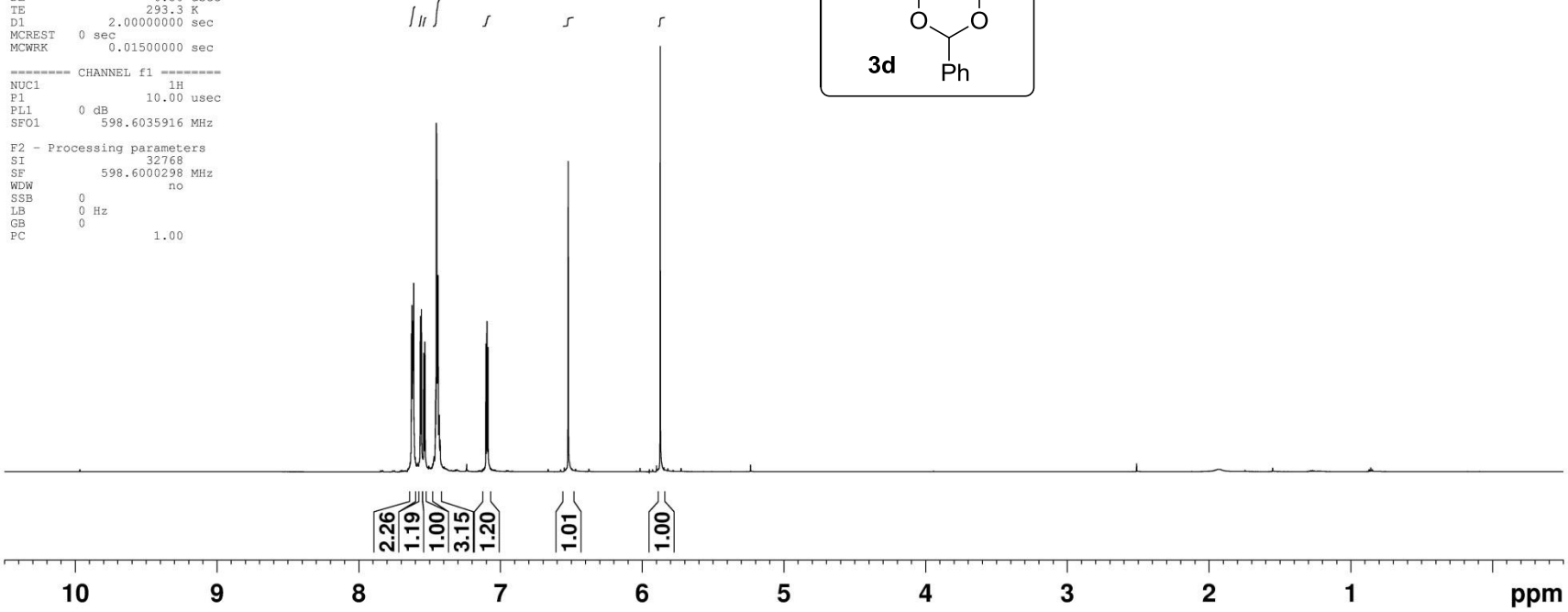


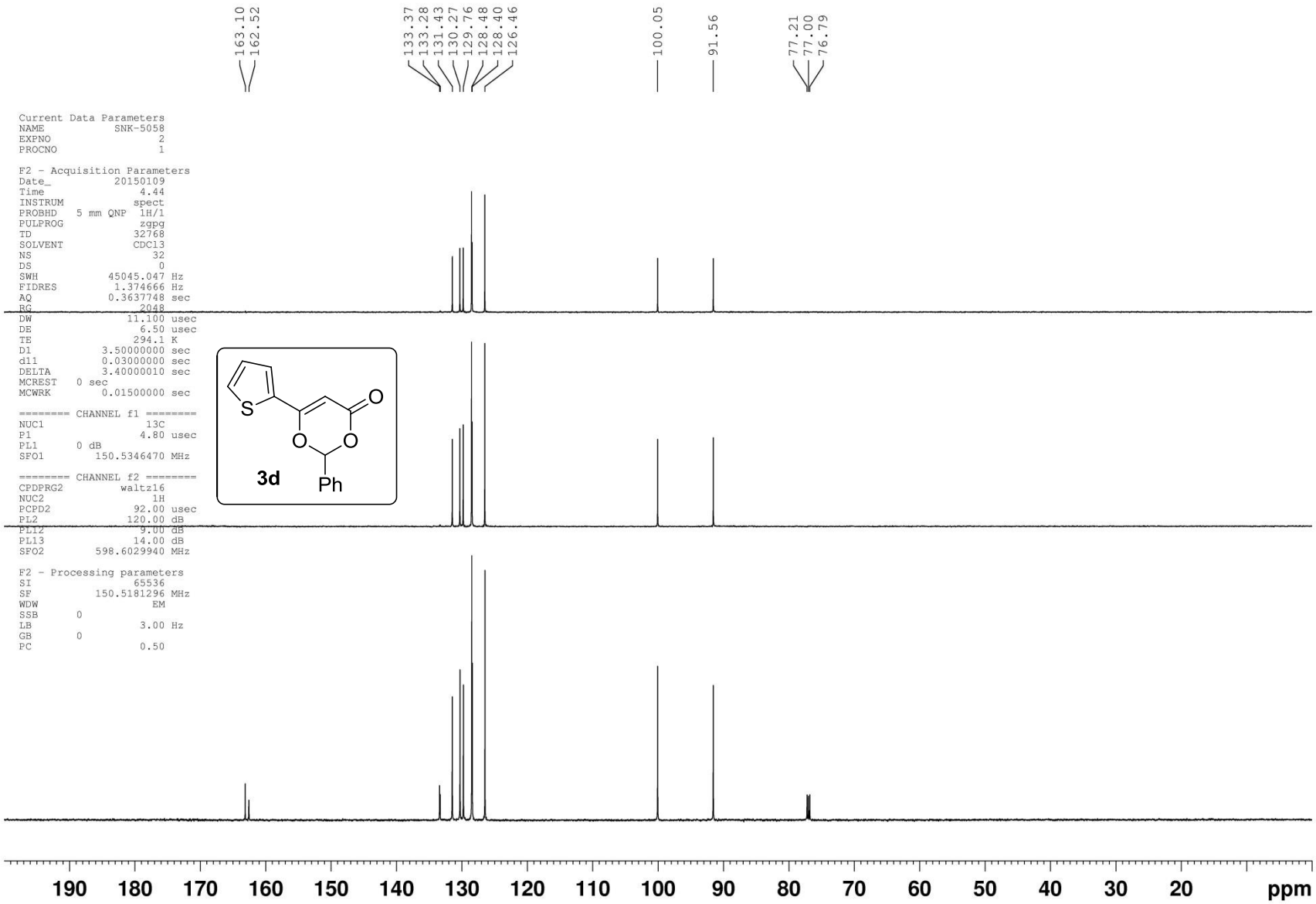

166.99
162.63
138.80
133.46
130.53
129.24
128.69
128.50
127.85
126.66
100.39
93.48
77.21
77.00
76.79
Current Data Parameters
NAME SNK-5053
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 7.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 294.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181029 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Cl
O
O
O
Ph
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

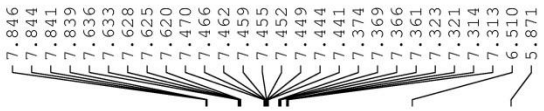



```
Current Data Parameters
NAME             SNK-5058
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150109
Time                4.43
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                 293.3 K
D1              2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1        0 dB
SFO1          598.6035916 MHz

F2 - Processing parameters
SI                  32768
SF            598.6000298 MHz
WDW                    no
SSB        0
LB         0 Hz
GB         0
PC                  1.00
```

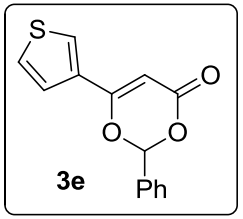


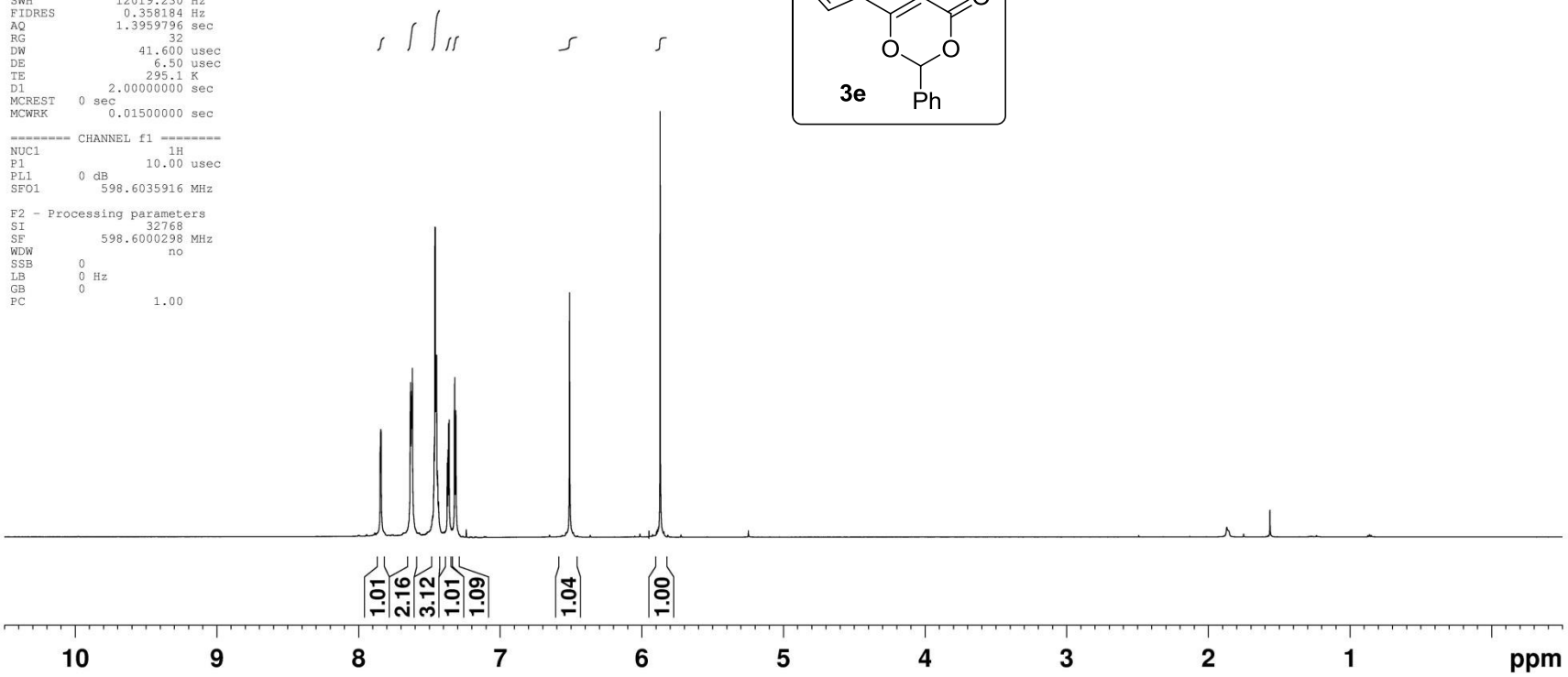


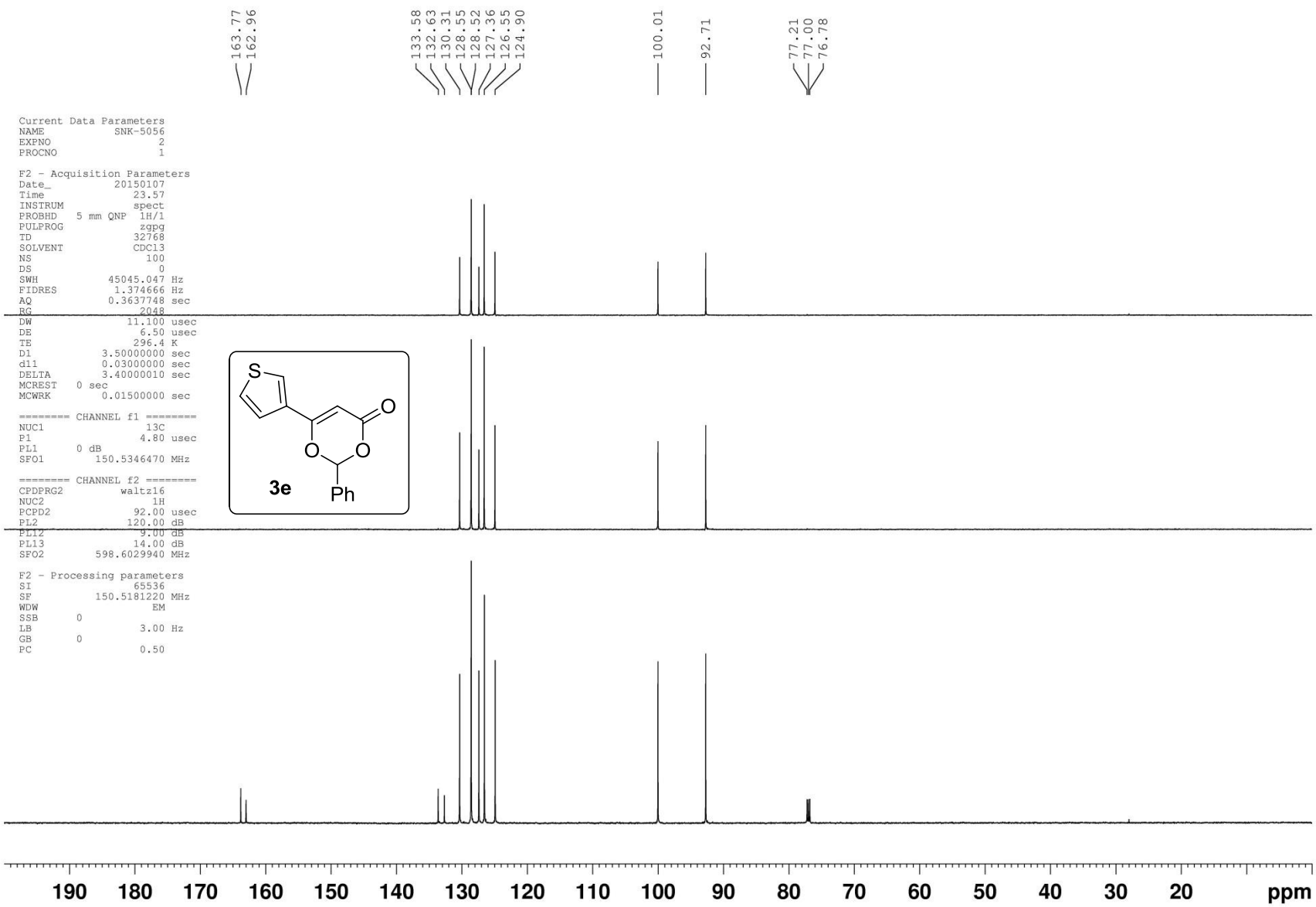

163.10
162.52
133.37
133.28
131.43
130.27
129.76
128.48
128.40
126.46
100.05
91.56
77.21
77.00
76.79
Current Data Parameters
NAME SNK-5058
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150109
Time 4.44
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 294.1 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181296 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
S
O
O
O
3d
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

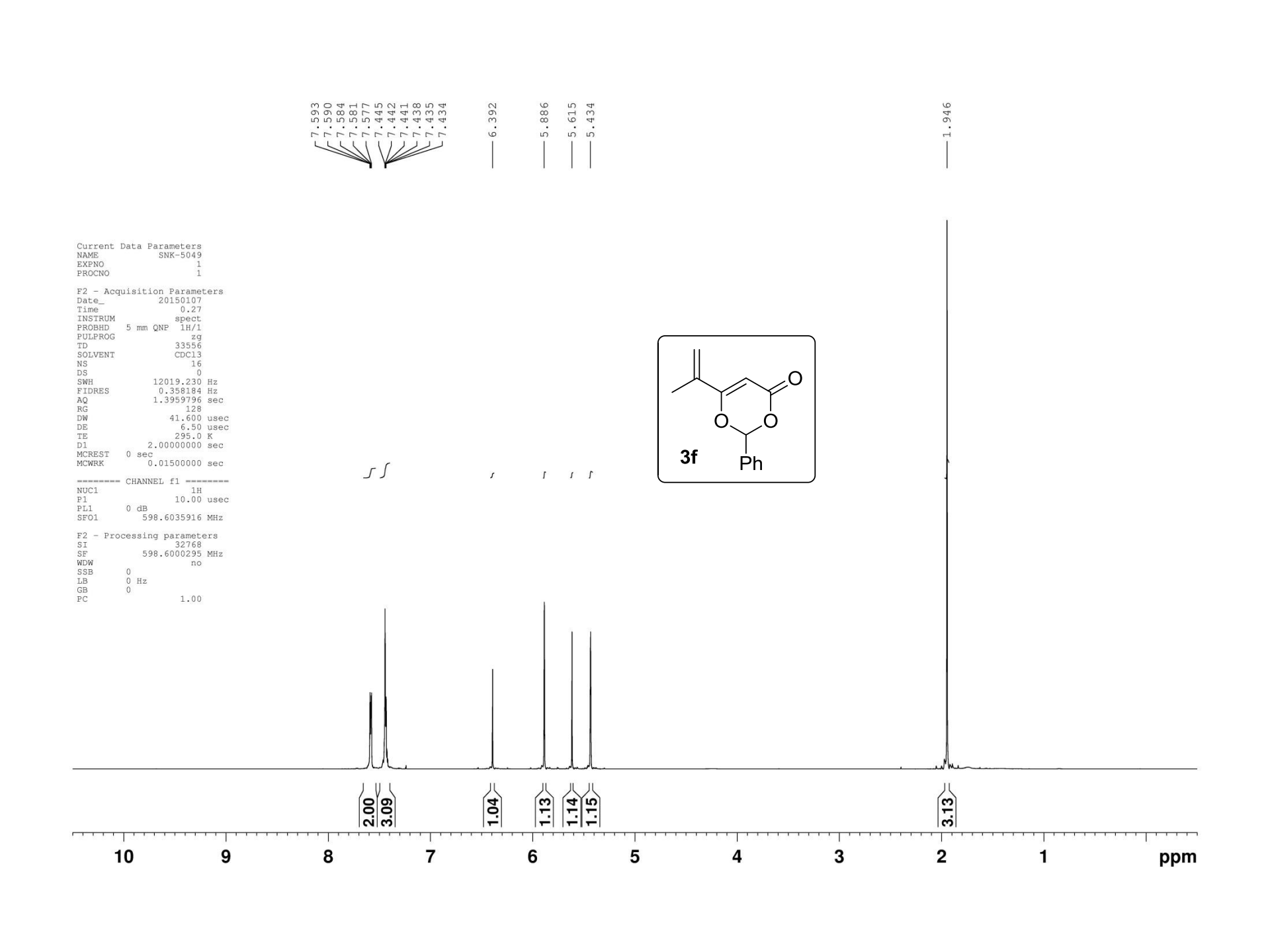


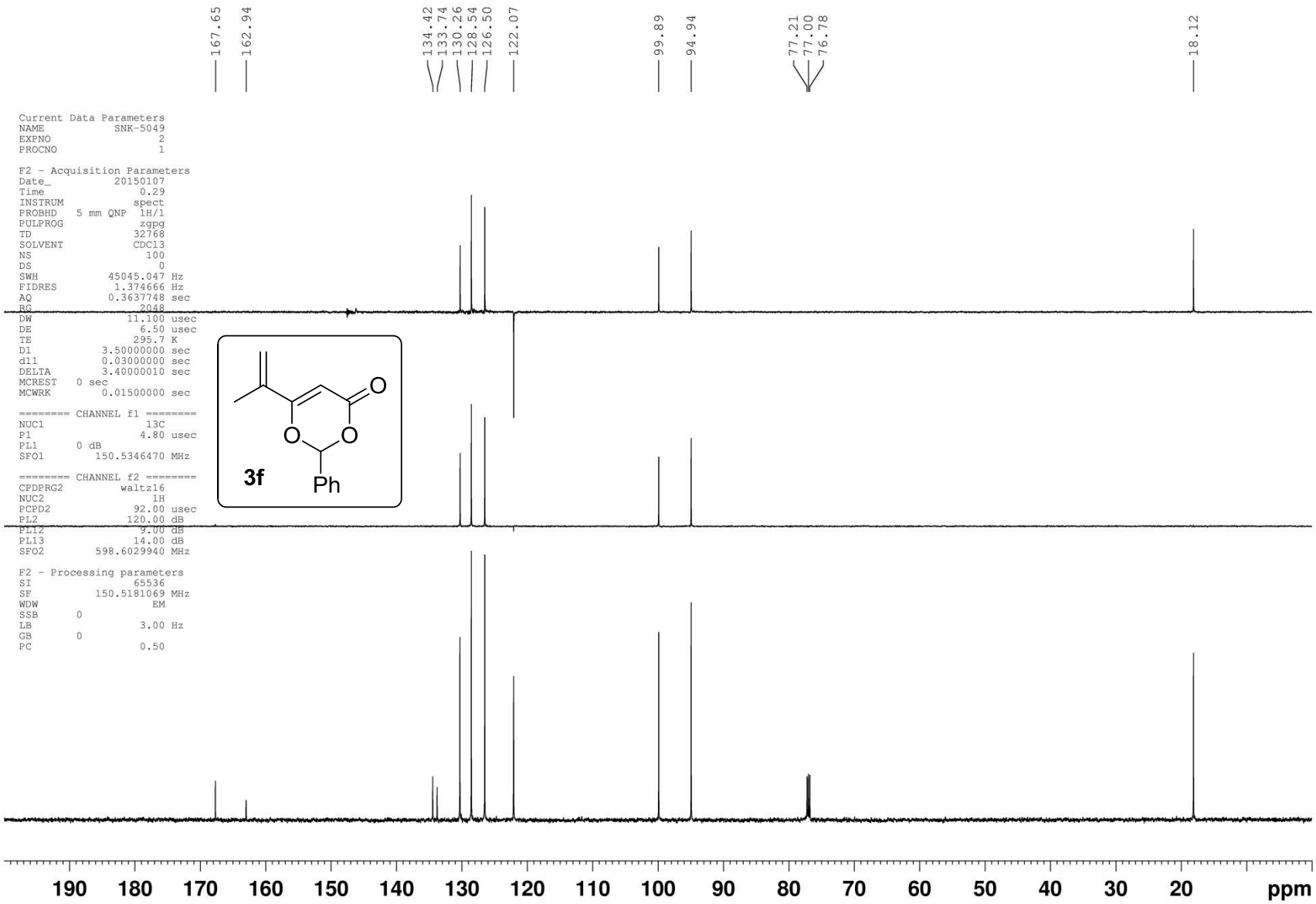

```
Current Data Parameters
NAME             SNK-5056
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150107
Time               23.50
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                   32
DW               41.600 usec
DE                6.50 usec
TE                295.1 K
D1            2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1       0 dB
SFO1         598.6035916 MHz

F2 - Processing parameters
SI                32768
SF           598.6000298 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

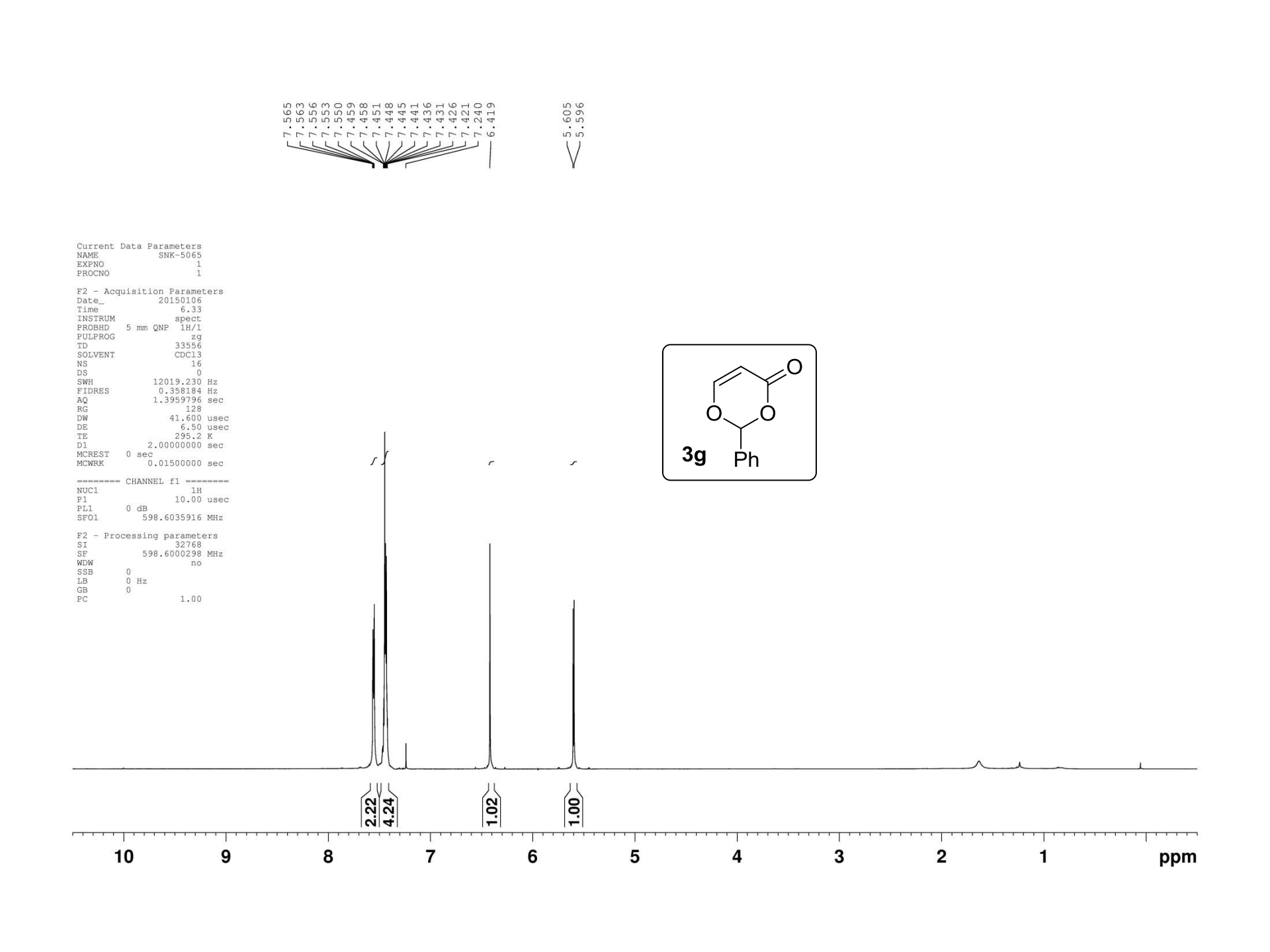


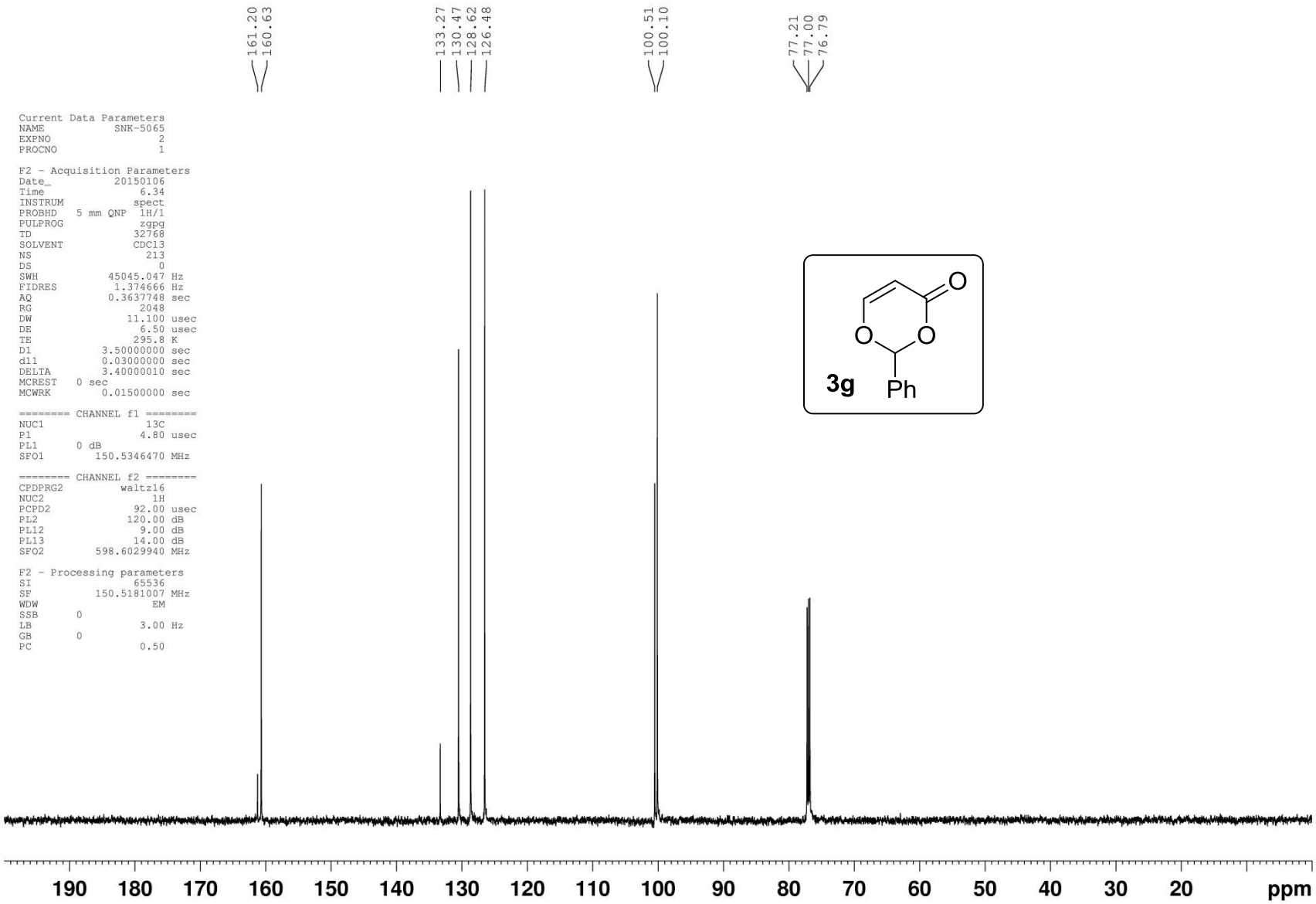


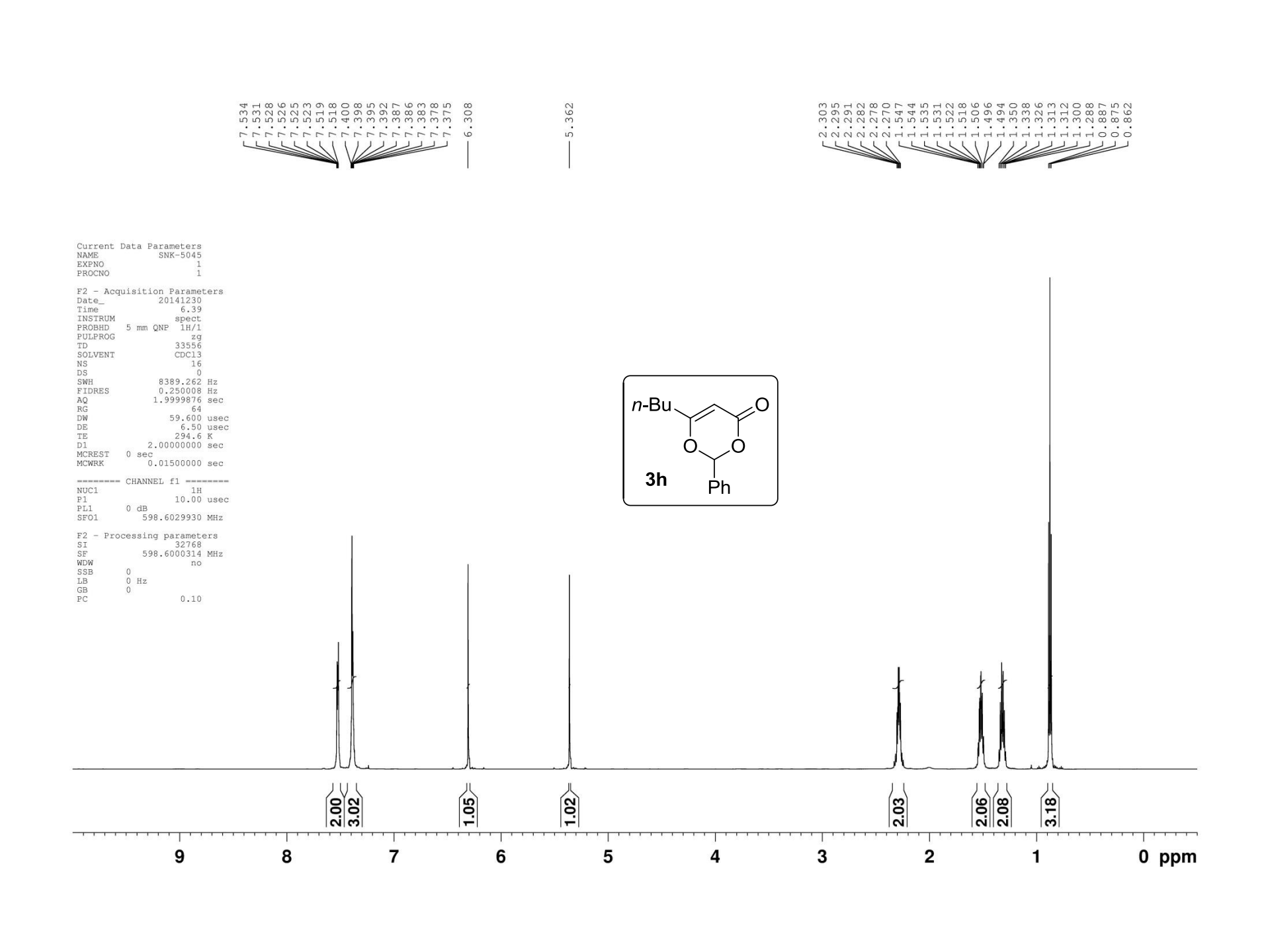

163.77
162.96
133.58
132.63
130.31
128.55
128.52
127.36
126.55
124.90
100.01
92.71
77.21
77.00
76.78
Current Data Parameters
NAME SNK-5056
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 23.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181220 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
S
O
O
O
Ph
3e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

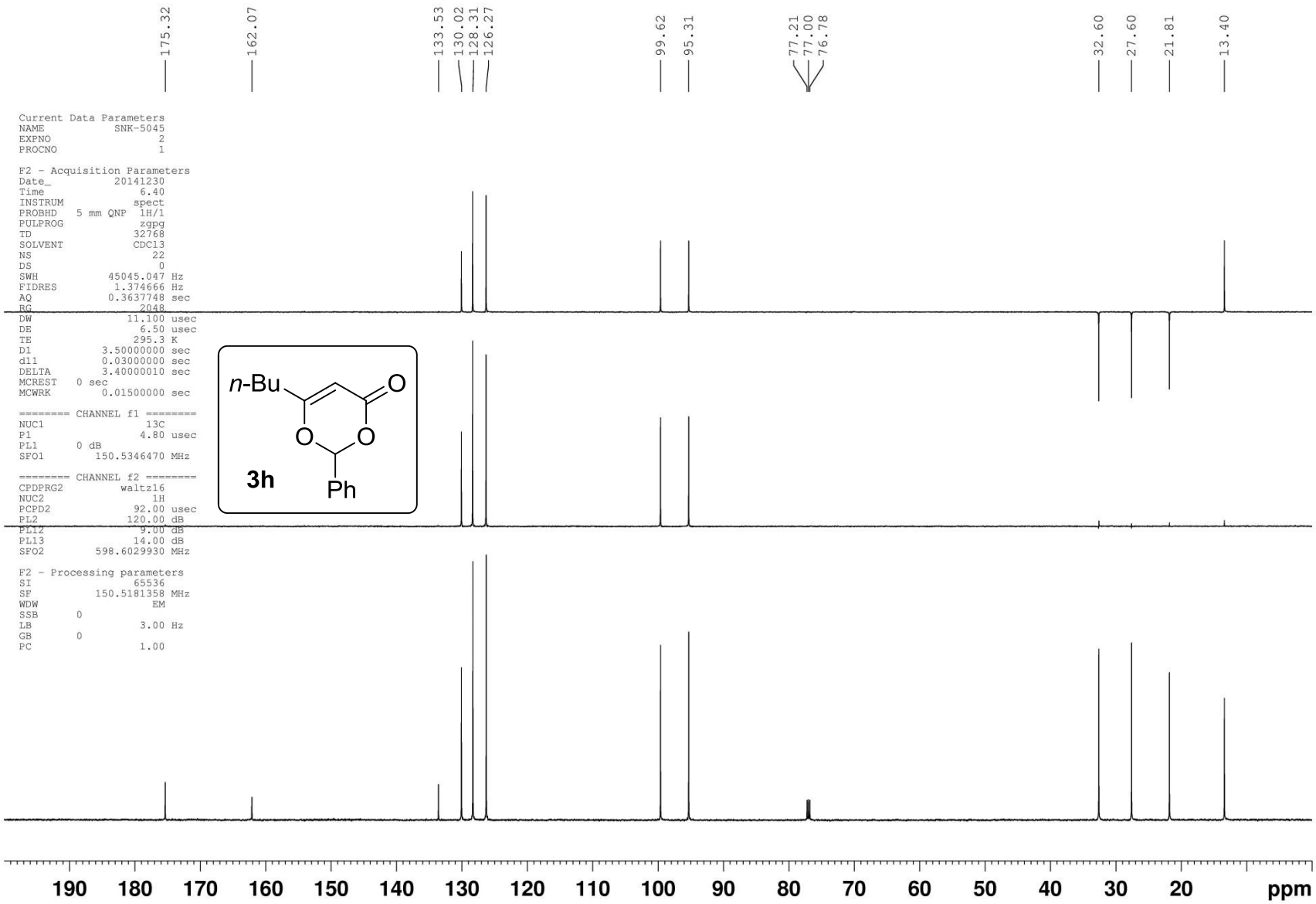

7.593
7.590
7.584
7.581
7.577
7.445
7.442
7.441
7.438
7.435
7.434
6.392
5.886
5.615
5.434
1.946
Current Data Parameters
NAME SNK-5049
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 0.27
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
O
3f
Ph
2.00
3.09
1.04
1.13
1.14
1.15
3.13
10
9
8
7
6
5
4
3
2
1
ppm

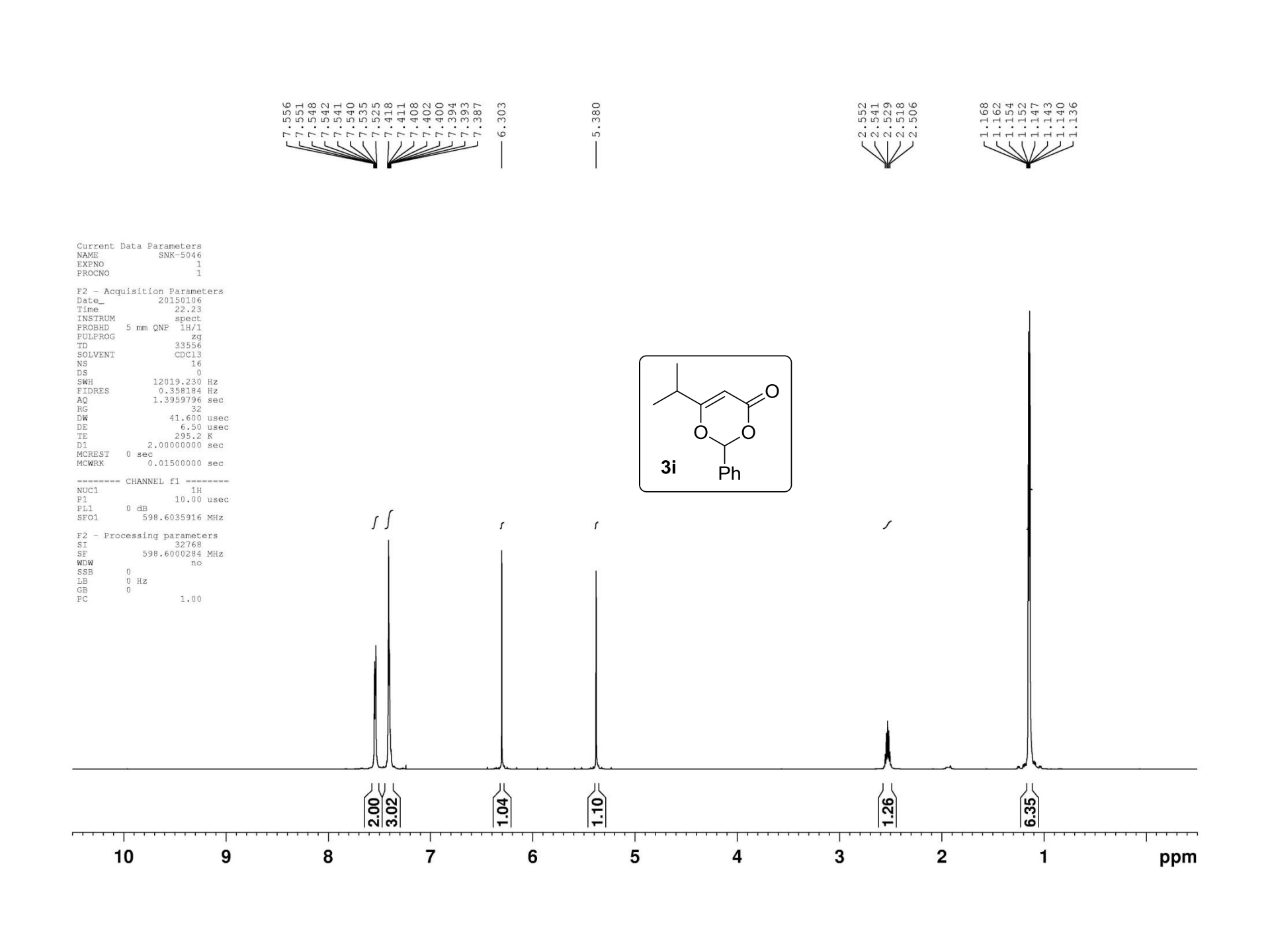

167.65
162.94
134.42
133.74
130.26
128.54
126.50
122.07
99.89
94.94
77.21
77.00
76.78
18.12
Current Data Parameters
NAME SNK-5049
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150107
Time 0.29
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.7 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181069 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
O
O
O
3f
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

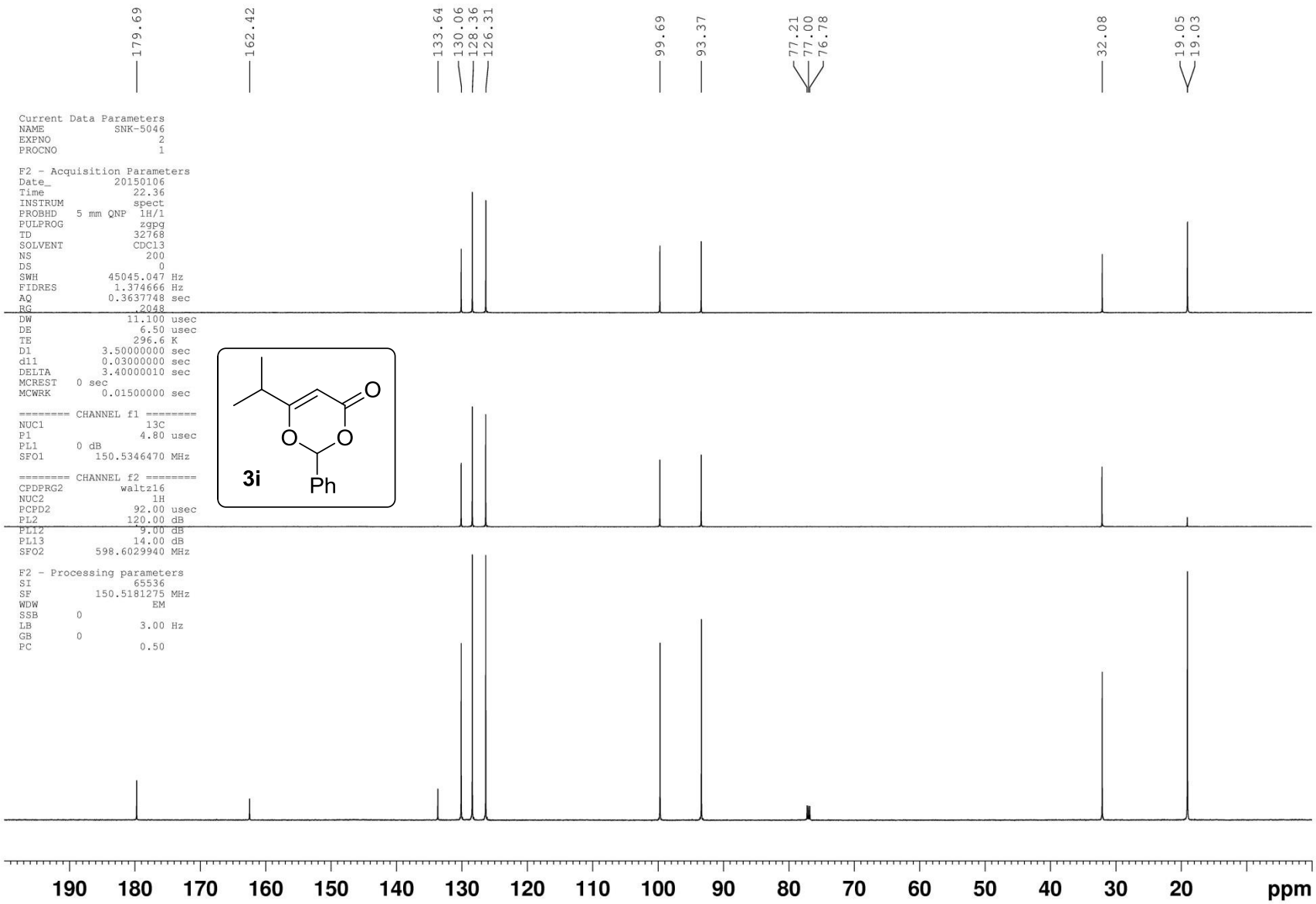

7.565
7.563
7.556
7.553
7.550
7.459
7.458
7.451
7.448
7.445
7.441
7.436
7.431
7.426
7.421
7.240
6.419
5.605
5.596
Current Data Parameters
NAME SNK-5065
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 6.33
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 128
DW 41.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
O
3g
Ph
2.22
4.24
1.02
1.00
10
9
8
7
6
5
4
3
2
1
ppm

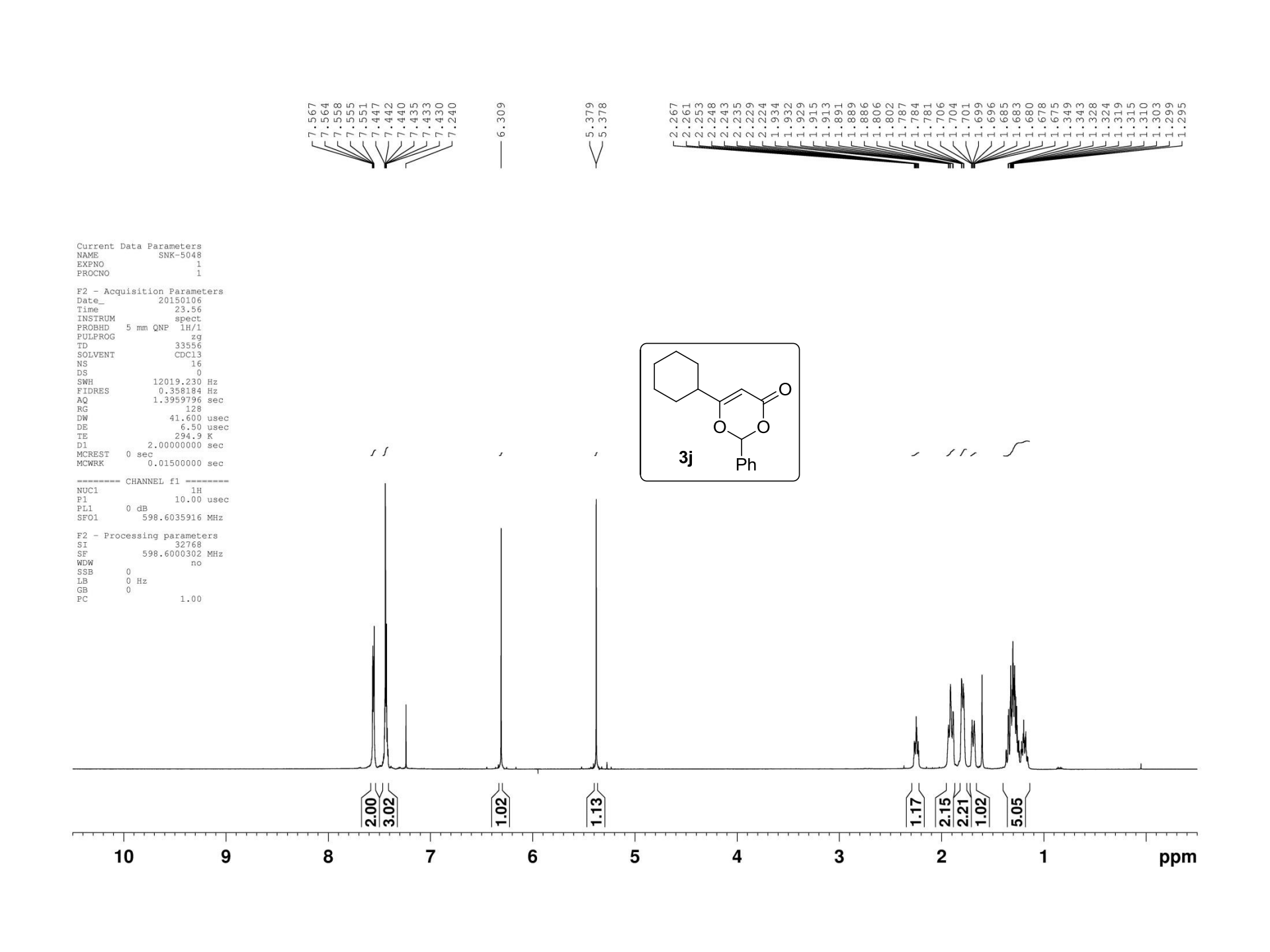

161.20
160.63
133.27
130.47
128.62
126.48
100.51
100.10
77.21
77.00
76.79
Current Data Parameters
NAME SNK-5065
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 6.34
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 213
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.8 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181007 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
O
O
O
3g
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

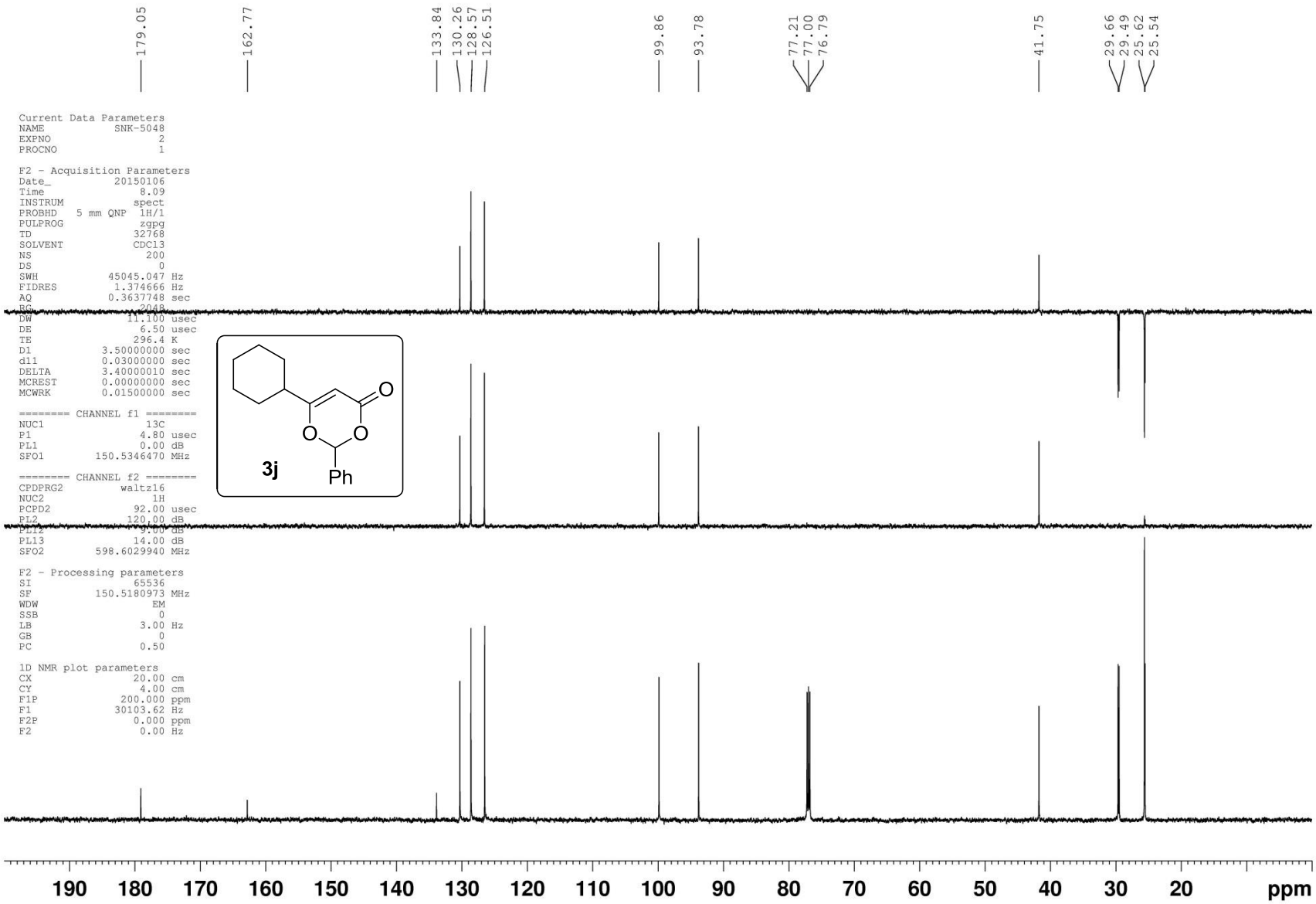

7.534
7.531
7.528
7.526
7.525
7.523
7.519
7.518
7.400
7.398
7.395
7.392
7.387
7.386
7.383
7.378
7.375
6.308
5.362
2.303
2.295
2.291
2.282
2.278
2.270
1.547
1.544
1.535
1.531
1.522
1.518
1.506
1.496
1.494
1.350
1.338
1.326
1.313
1.312
1.300
1.288
0.887
0.875
0.862
Current Data Parameters
NAME SNK-5045
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 6.39
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 64
DW 59.600 usec
DE 6.50 usec
TE 294.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000314 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
n-Bu
O
O
O
3h
Ph
2.00
3.02
1.05
1.02
2.03
2.06
2.08
3.18
9
8
7
6
5
4
3
2
1
0 ppm

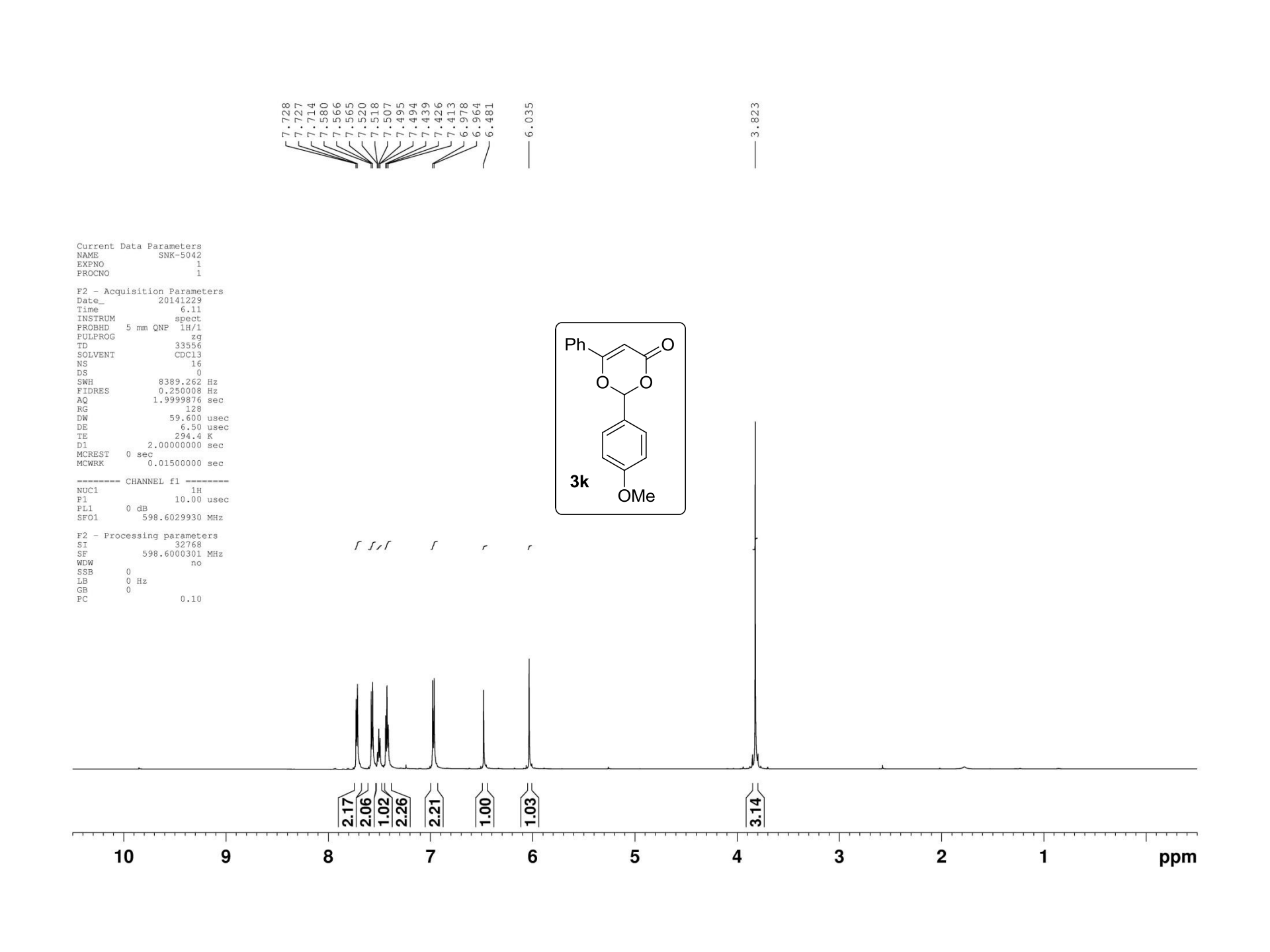

175.32
162.07
133.53
130.02
128.31
126.27
99.62
95.31
77.21
77.00
76.78
32.60
27.60
21.81
13.40
Current Data Parameters
NAME SNK-5045
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 6.40
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 295.3 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181358 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
n-Bu
O
O
O
Ph
3h
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

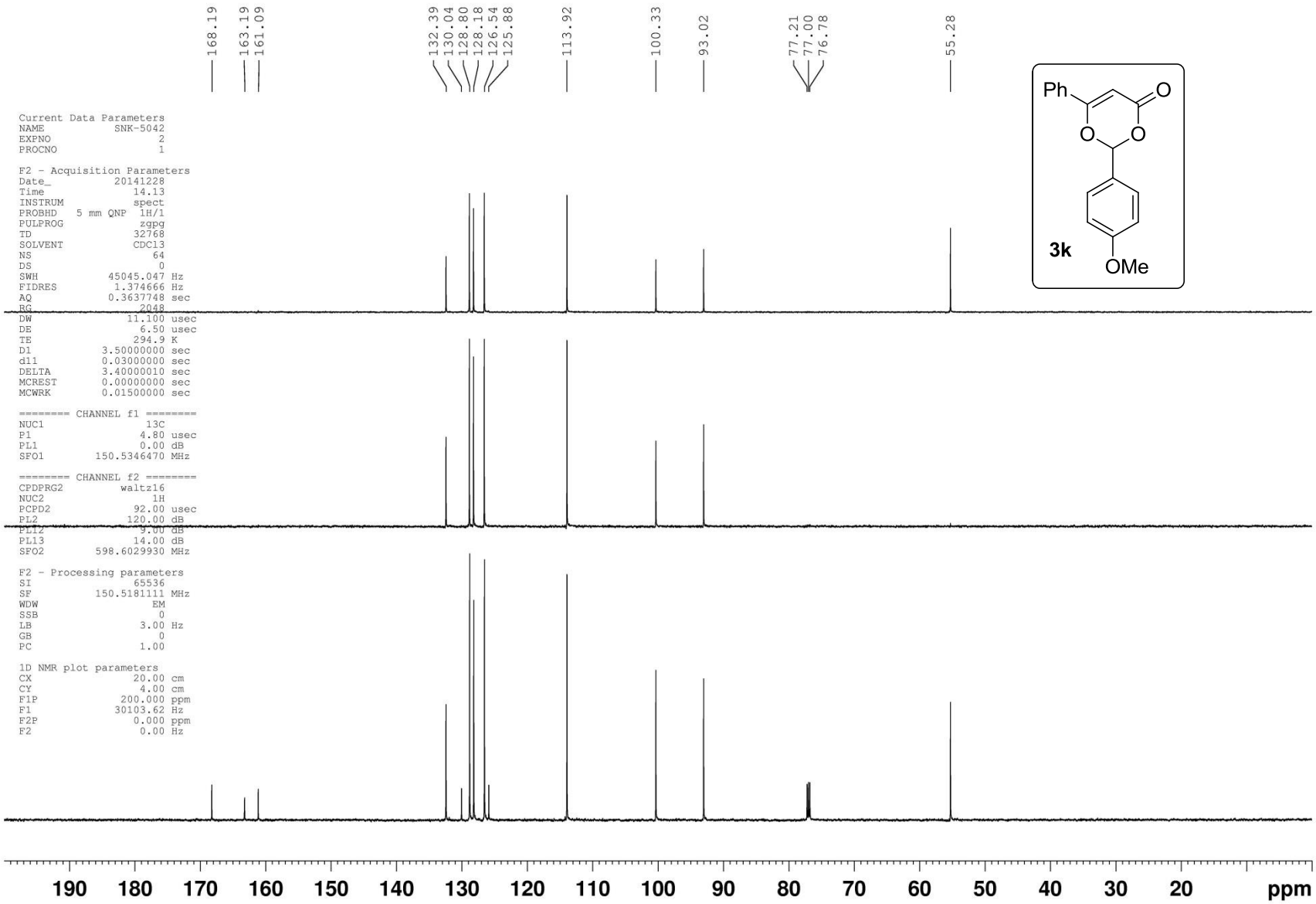

7.556
7.551
7.548
7.542
7.541
7.540
7.535
7.525
7.418
7.411
7.408
7.402
7.400
7.394
7.393
7.387
6.303
5.380
2.552
2.541
2.529
2.518
2.506
1.168
1.162
1.154
1.152
1.147
1.143
1.140
1.136
Current Data Parameters
NAME SNK-5046
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 22.23
INSTRUM 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 32
DW 41.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000284 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
O
3i
Ph
2.00
3.02
1.04
1.10
1.26
6.35
10
9
8
7
6
5
4
3
2
1
ppm

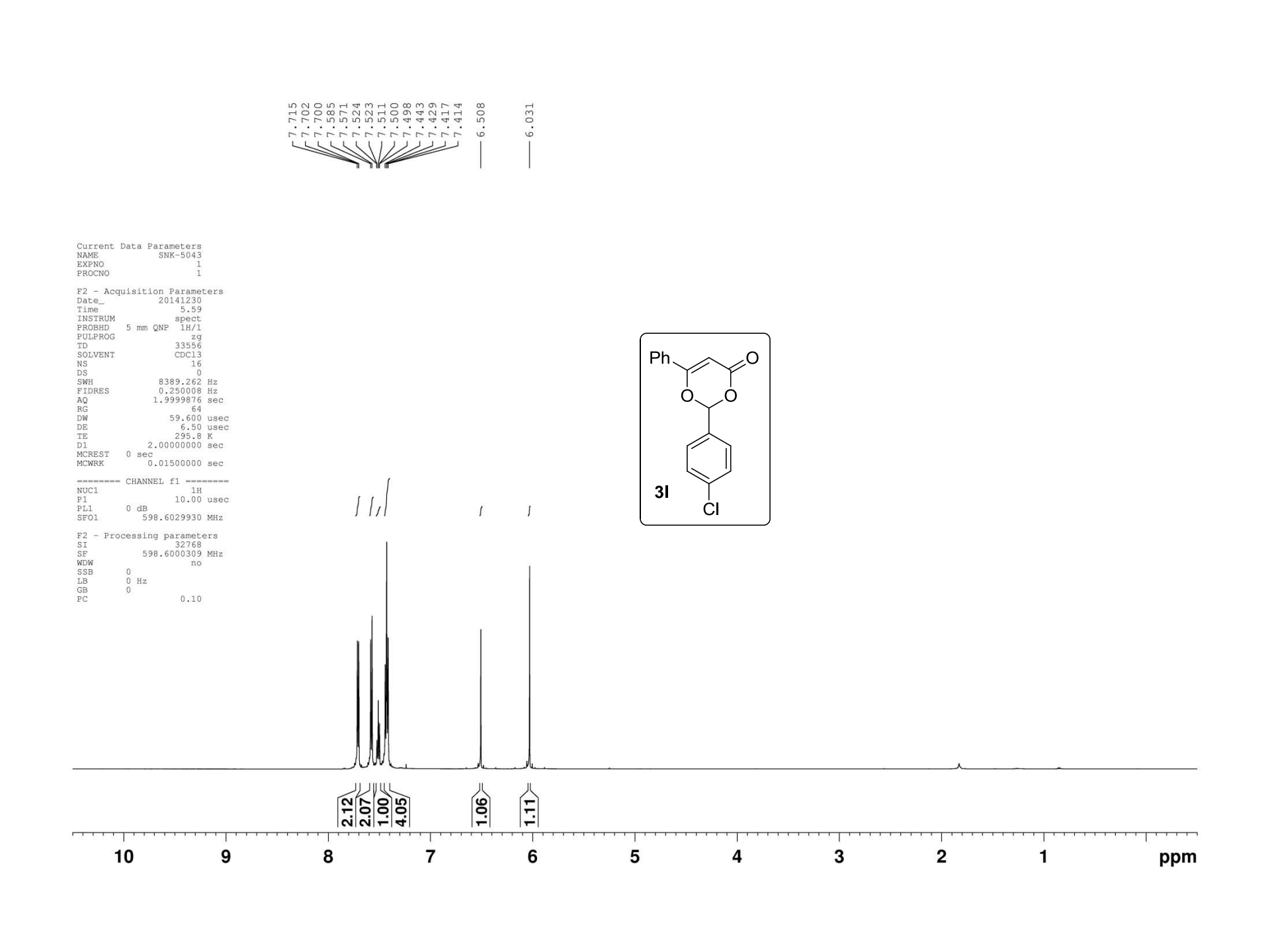

179.69
162.42
133.64
130.06
128.36
126.31
99.69
93.37
77.21
77.00
76.78
32.08
19.05
19.03
Current Data Parameters
NAME SNK-5046
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 22.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG .2048
DW 11.100 usec
DE 6.50 usec
TE 296.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181275 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
O
O
O
3i
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

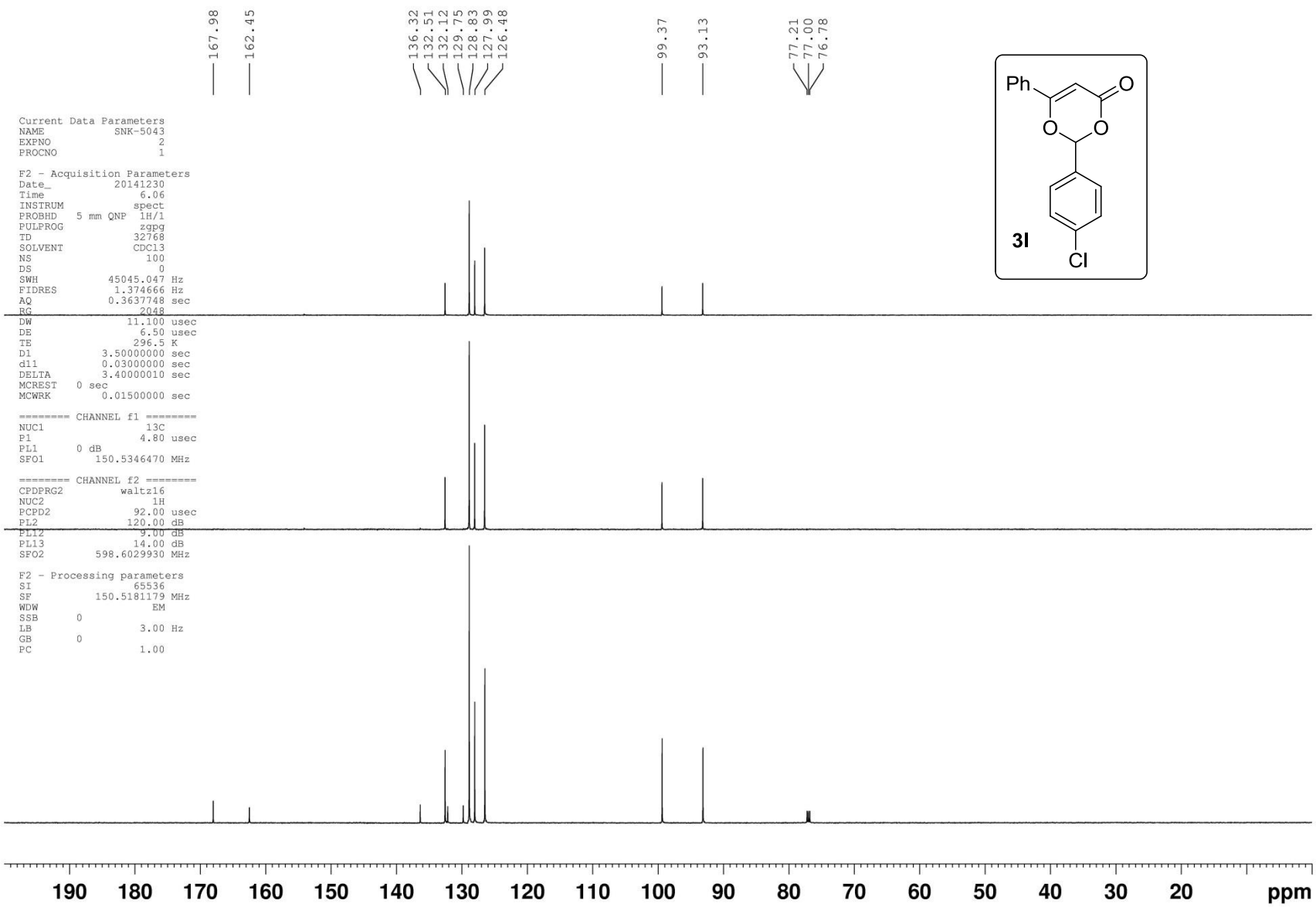

7.567
7.564
7.558
7.555
7.551
7.447
7.442
7.440
7.435
7.433
7.430
7.240
6.309
5.379
5.378
2.267
2.261
2.253
2.248
2.243
2.235
2.229
2.224
1.934
1.932
1.929
1.915
1.913
1.891
1.889
1.886
1.806
1.802
1.787
1.784
1.781
1.706
1.704
1.701
1.699
1.696
1.685
1.683
1.680
1.678
1.675
1.349
1.343
1.328
1.324
1.319
1.315
1.310
1.303
1.299
1.295
Current Data Parameters
NAME SNK-5048
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 23.56
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 128
DW 41.600 usec
DE 6.50 usec
TE 294.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000302 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O
O
3j
Ph
2.00
3.02
1.02
1.13
1.17
2.15
2.21
1.02
5.05
10
9
8
7
6
5
4
3
2
1
ppm

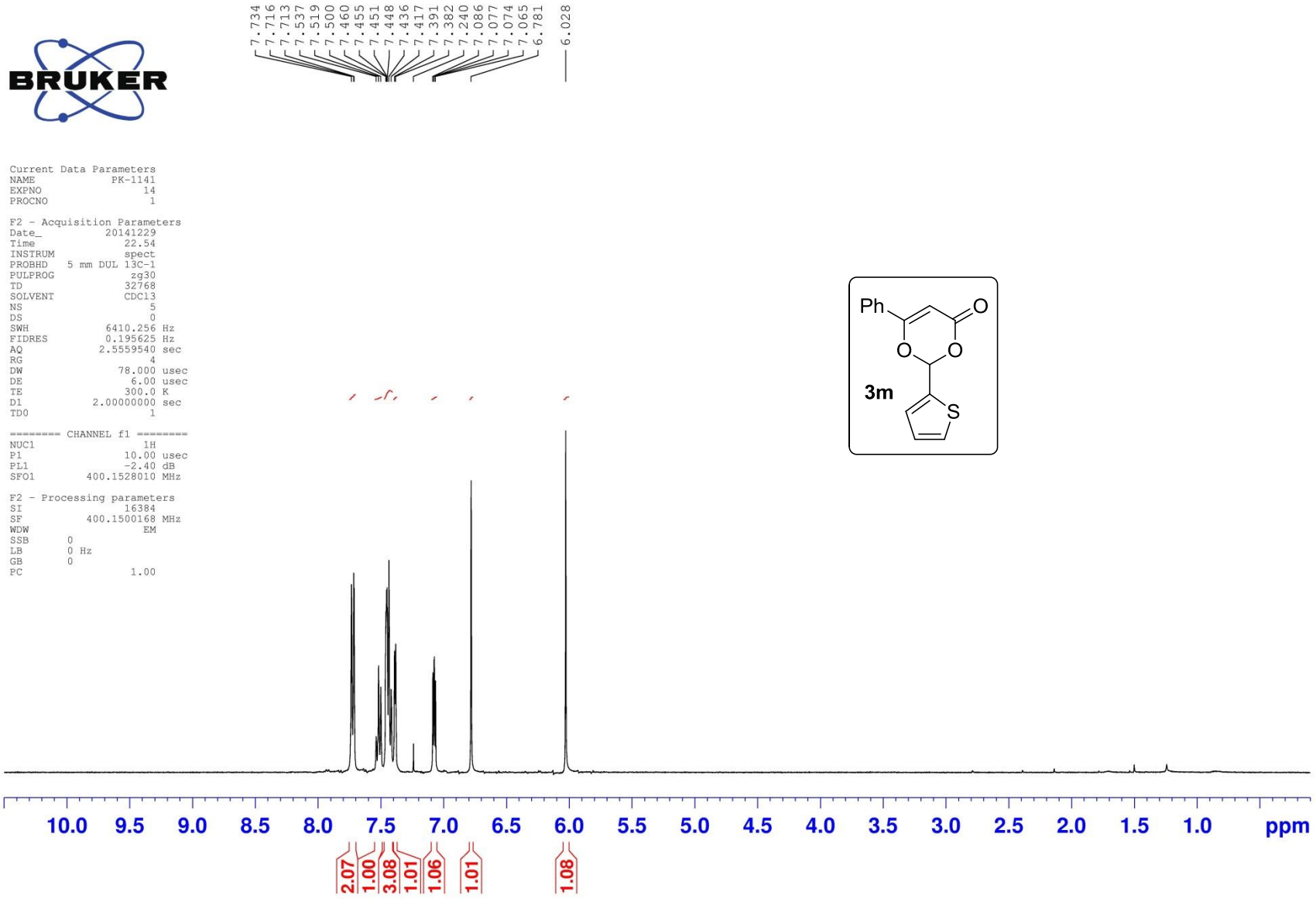

179.05
162.77
133.84
130.26
128.57
126.51
99.86
93.78
77.21
77.00
76.79
41.75
29.66
29.49
25.62
25.54
Current Data Parameters
NAME SNK-5048
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150106
Time 8.09
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 200
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.4 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 19.00 dB
PL13 14.00 dB
SFO2 598.6029940 MHz
F2 - Processing parameters
SI 65536
SF 150.5180973 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
O
O
O
3j
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

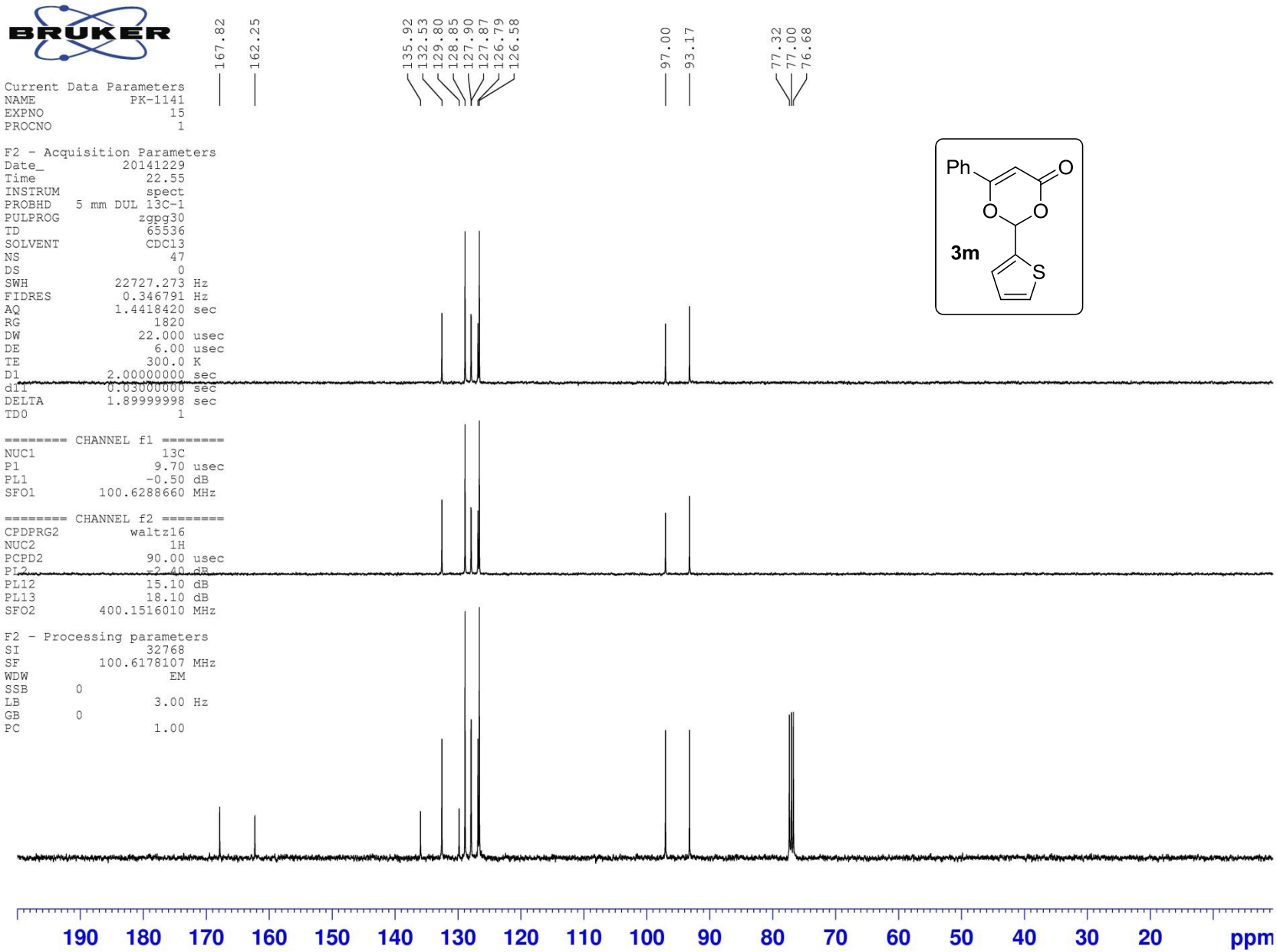

7.728
7.727
7.714
7.580
7.566
7.565
7.520
7.518
7.507
7.495
7.494
7.439
7.426
7.413
6.978
6.964
6.481
6.035
3.823
Current Data Parameters
NAME SNK-5042
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 6.11
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
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 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000301 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
Ph
O
O
O
3k
OMe
2.17
2.06
1.02
2.26
2.21
1.00
1.03
3.14
10
9
8
7
6
5
4
3
2
1
ppm

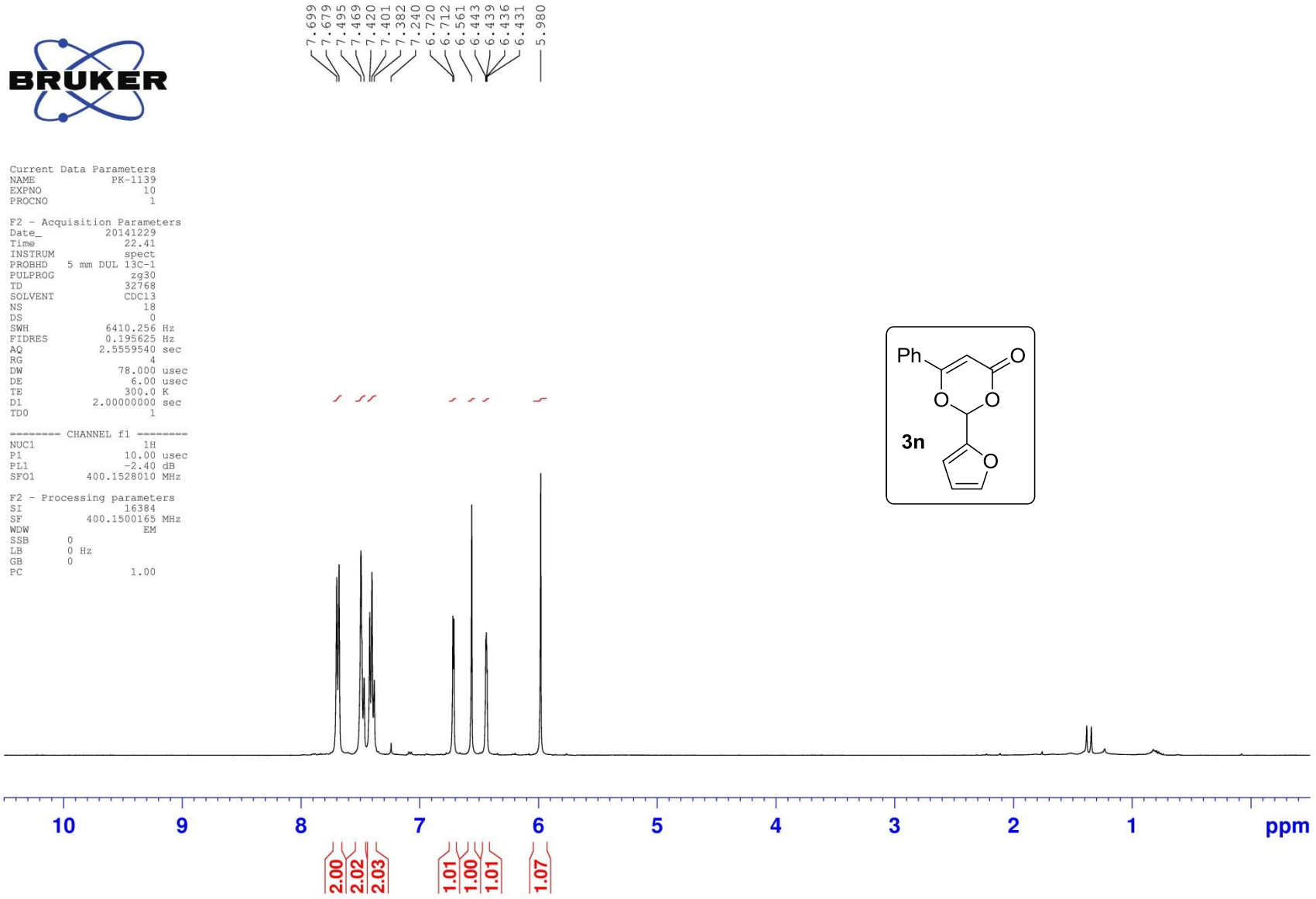

168.19
163.19
161.09
132.39
130.04
128.80
128.18
126.54
125.88
113.92
100.33
93.02
77.21
77.00
76.78
55.28
Ph
O
O
O
3k
OMe
Current Data Parameters
NAME SNK-5042
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141228
Time 14.13
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 64
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 294.9 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 150.5181111 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
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

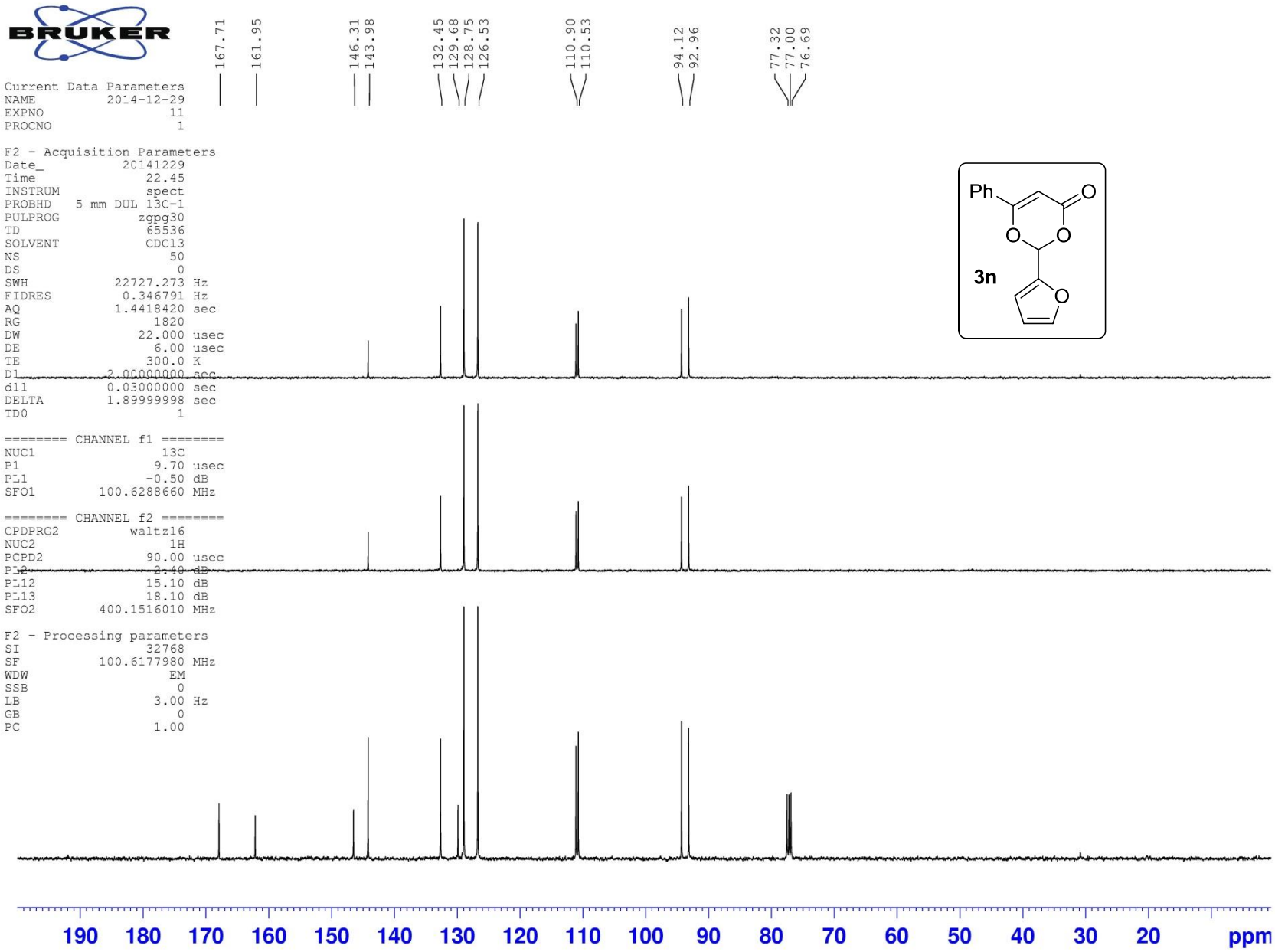

7.715
7.702
7.700
7.585
7.571
7.524
7.523
7.511
7.500
7.498
7.443
7.429
7.417
7.414
6.508
6.031
Current Data Parameters
NAME SNK-5043
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 5.59
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 8389.262 Hz
FIDRES 0.250008 Hz
AQ 1.9999876 sec
RG 64
DW 59.600 usec
DE 6.50 usec
TE 295.8 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000309 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 0.10
Ph
O
O
O
3l
Cl
2.12
2.07
1.00
4.05
1.06
1.11
10
9
8
7
6
5
4
3
2
1
ppm

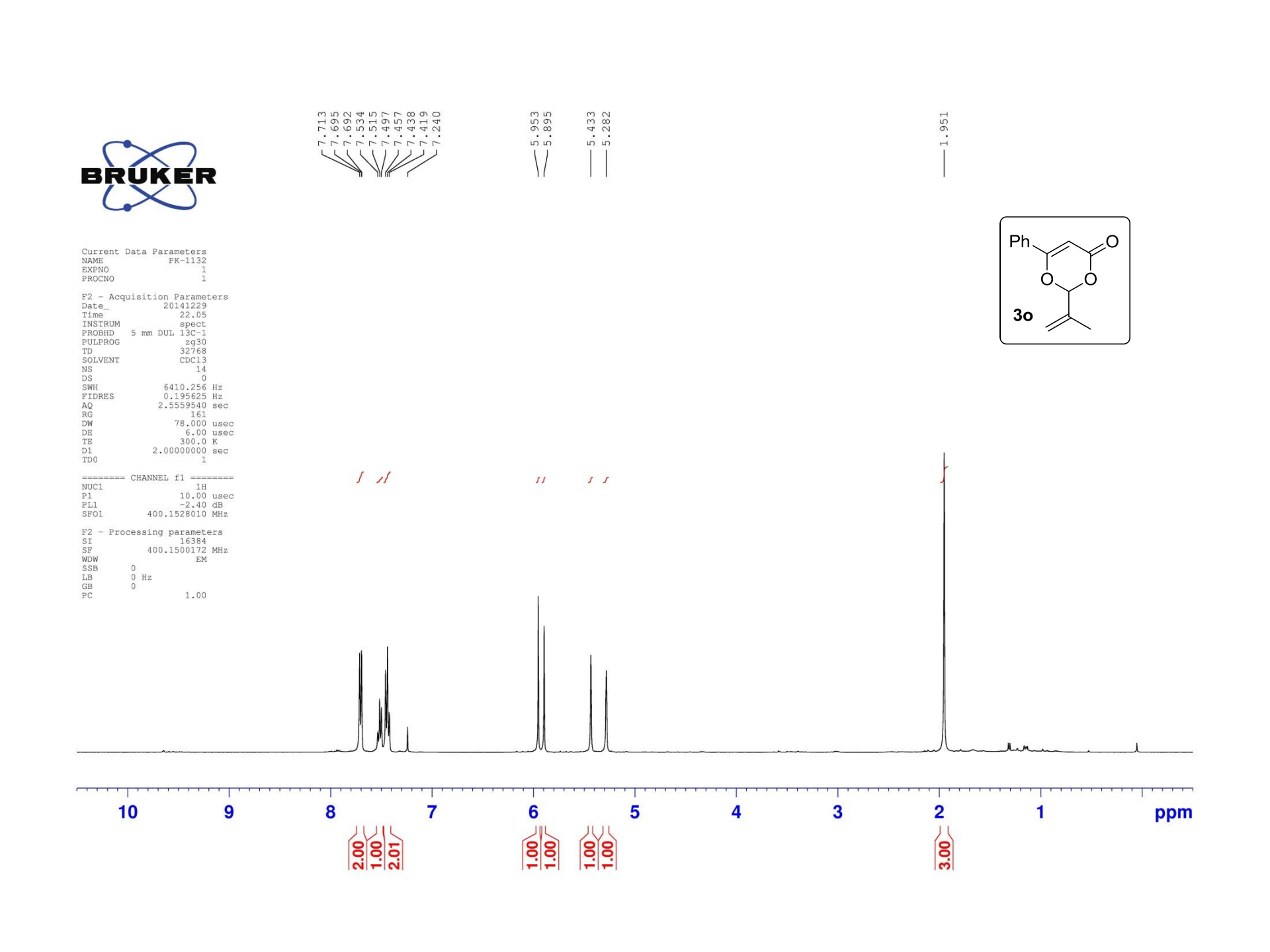

167.98
162.45
136.32
132.51
132.12
129.75
128.83
127.99
126.48
99.37
93.13
77.21
77.00
76.78
Ph
O
O
O
3l
Cl
Current Data Parameters
NAME SNK-5043
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141230
Time 6.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181179 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.734
7.716
7.713
7.537
7.519
7.500
7.460
7.455
7.451
7.448
7.436
7.417
7.391
7.382
7.240
7.086
7.077
7.074
7.065
6.781
6.028
Current Data Parameters
NAME PK-1141
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.54
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 5
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3m
S
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
2.07
1.00
3.08
1.01
1.06
1.01
1.08


167.82
162.25
135.92
132.53
129.80
128.85
127.90
127.87
126.79
126.58
97.00
93.17
77.32
77.00
76.68
Current Data Parameters
NAME PK-1141
EXPNO 15
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 47
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 1820
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 100.6178107 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
3m
S
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.699
7.679
7.495
7.469
7.420
7.401
7.382
7.240
6.720
6.712
6.561
6.443
6.439
6.436
6.431
5.980
Current Data Parameters
NAME PK-1139
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.41
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 18
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
O
3n
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.02
2.03
1.01
1.00
1.01
1.07


167.71
161.95
146.31
143.98
132.45
129.68
128.75
126.53
110.90
110.53
94.12
92.96
77.32
77.00
76.69
Current Data Parameters
NAME 2014-12-29
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.45
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 50
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 1820
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 100.6177980 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
O
3n
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.713
7.695
7.692
7.534
7.515
7.497
7.457
7.438
7.419
7.240
5.953
5.895
5.433
5.282
1.951
Current Data Parameters
NAME PK-1132
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.05
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 14
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 161
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3o
10
9
8
7
6
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4
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2
1
ppm
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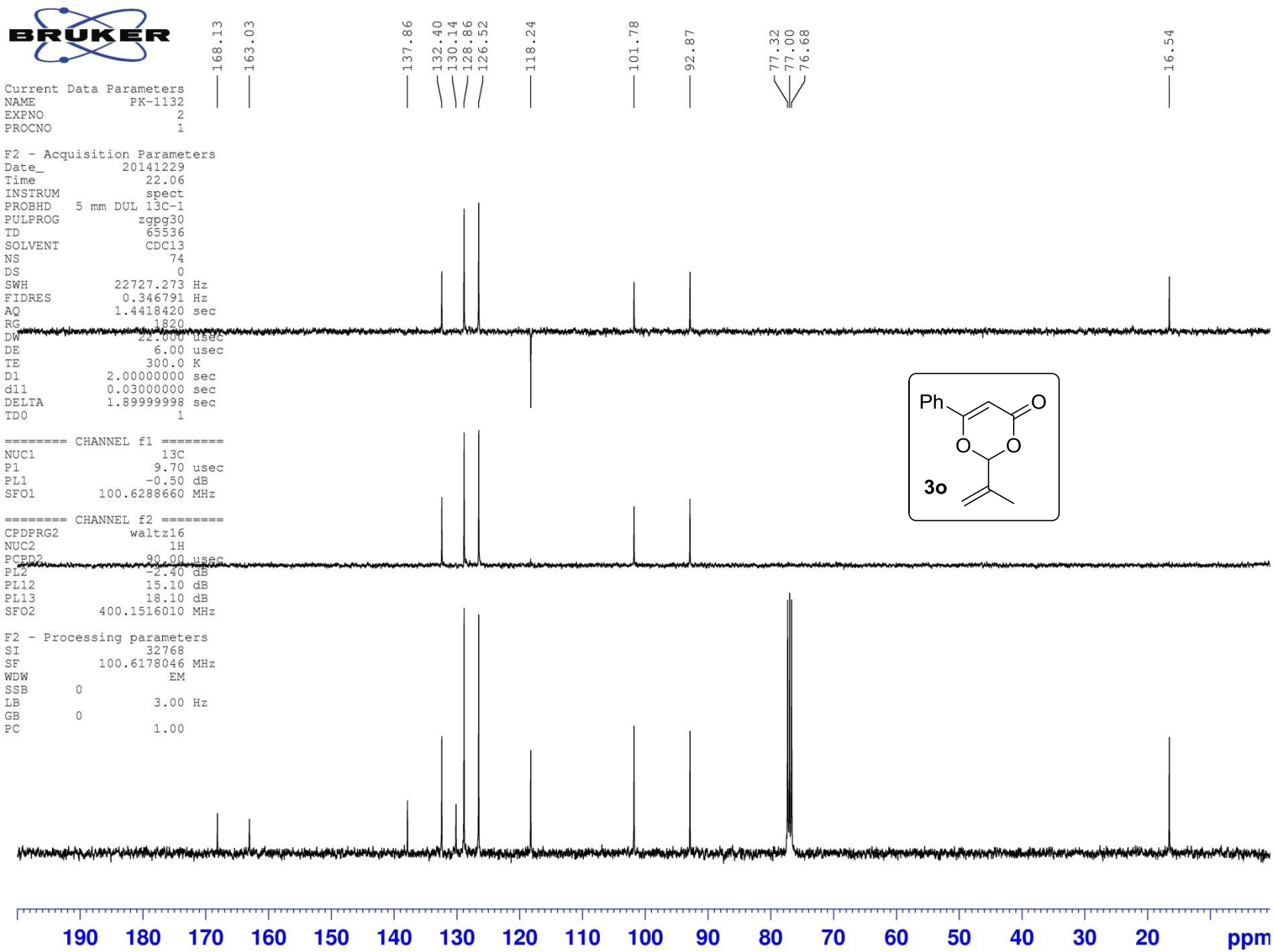
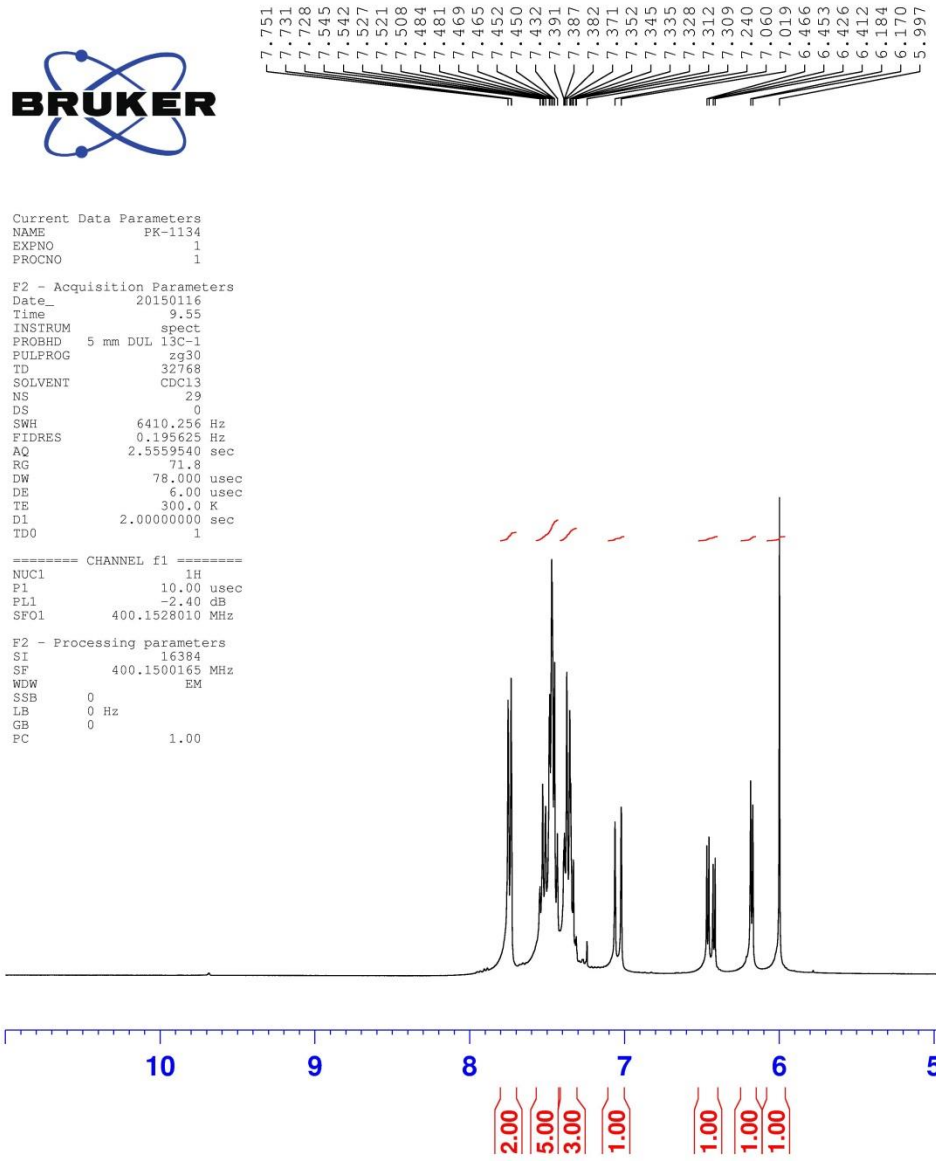
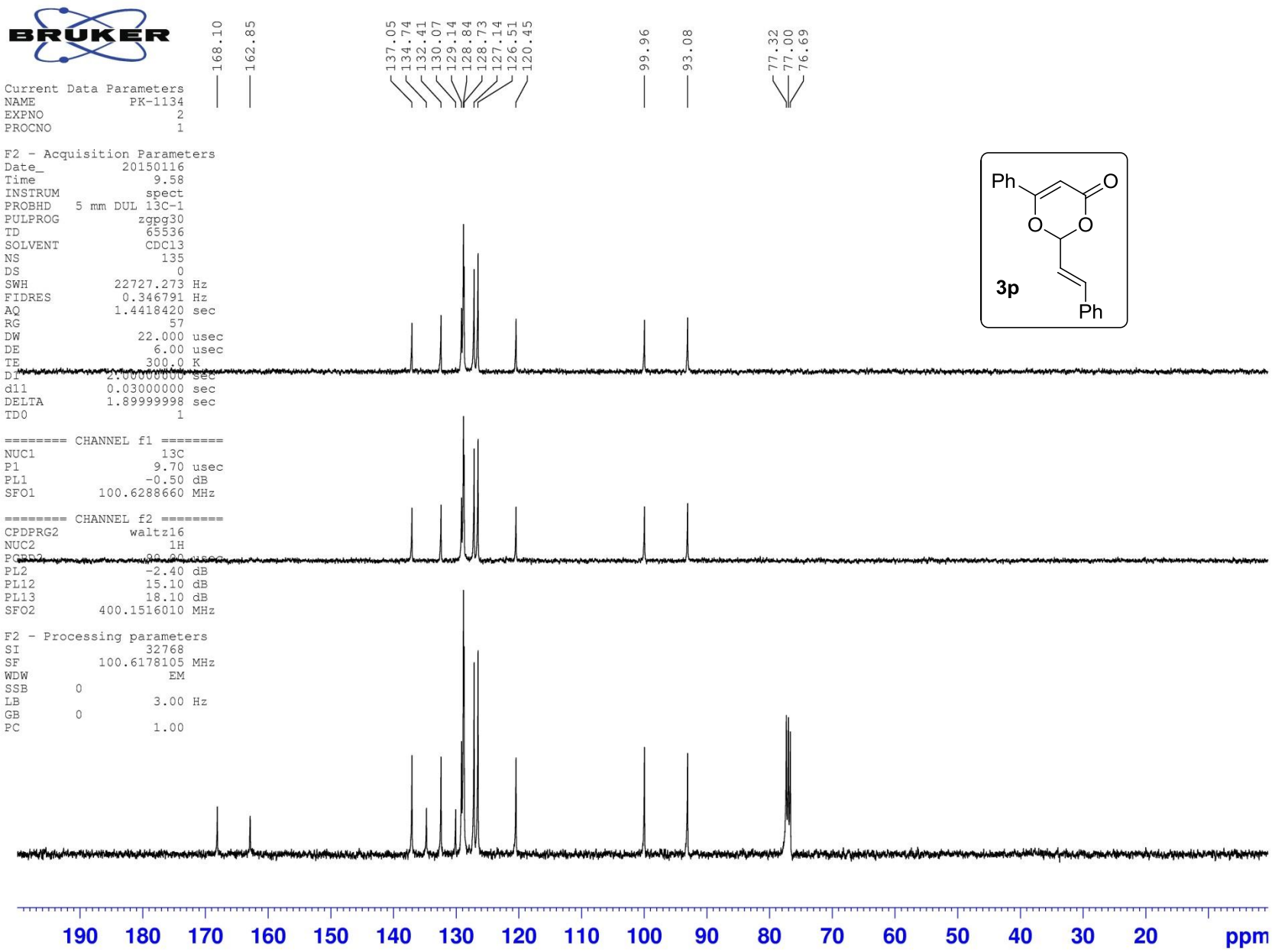
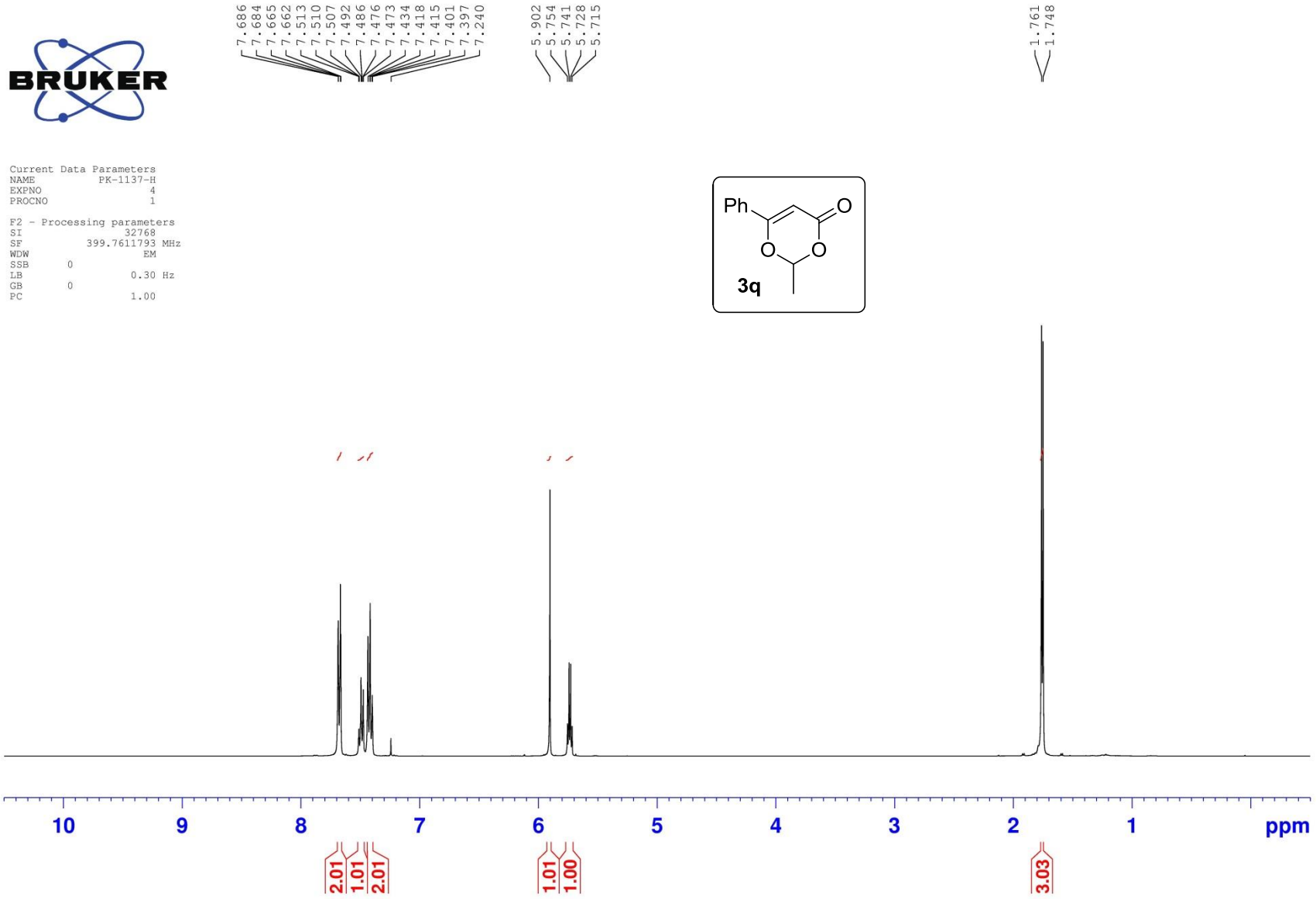
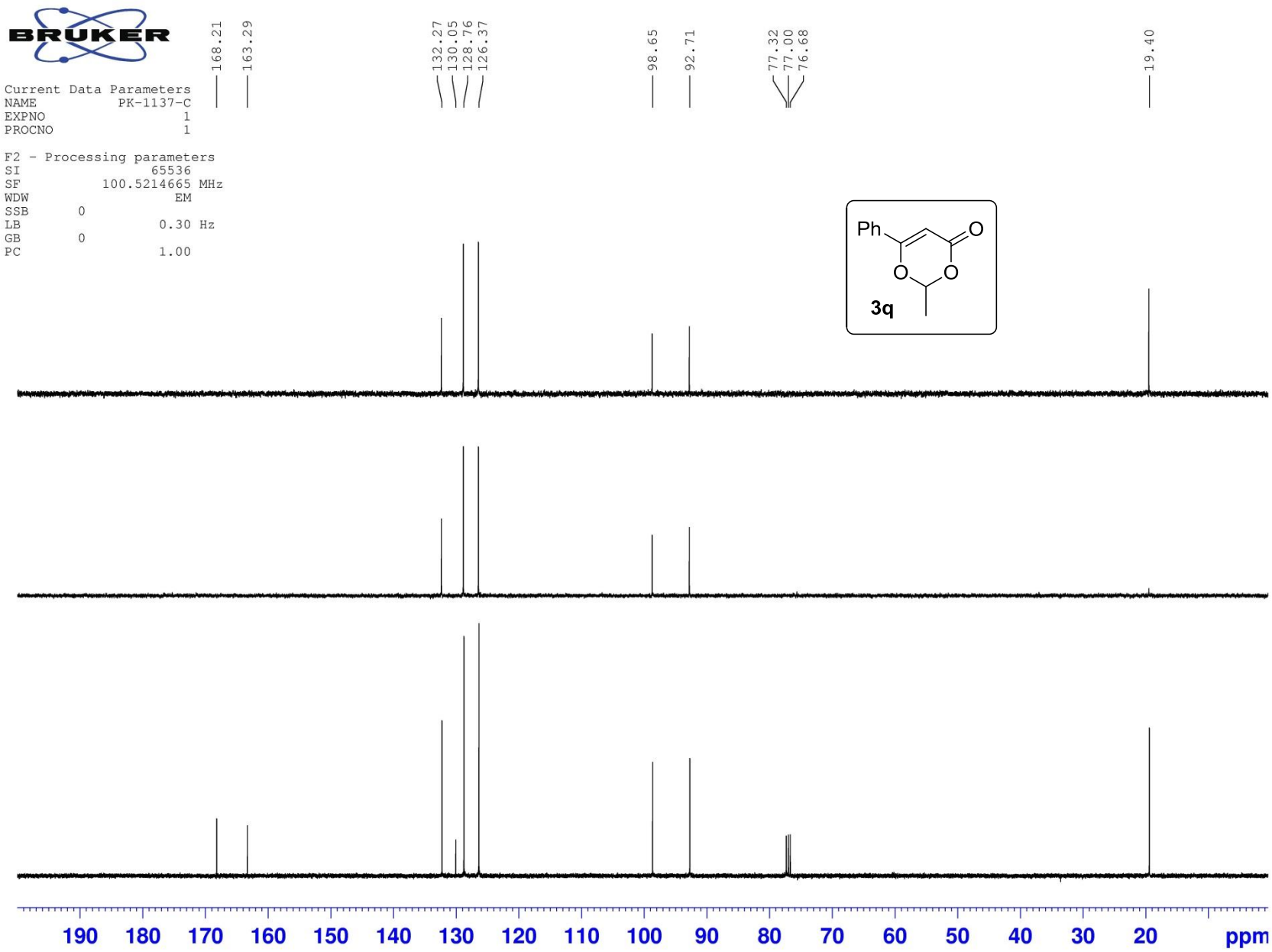
1.00
2.01
1.00
1.00
1.00
1.00
3.00

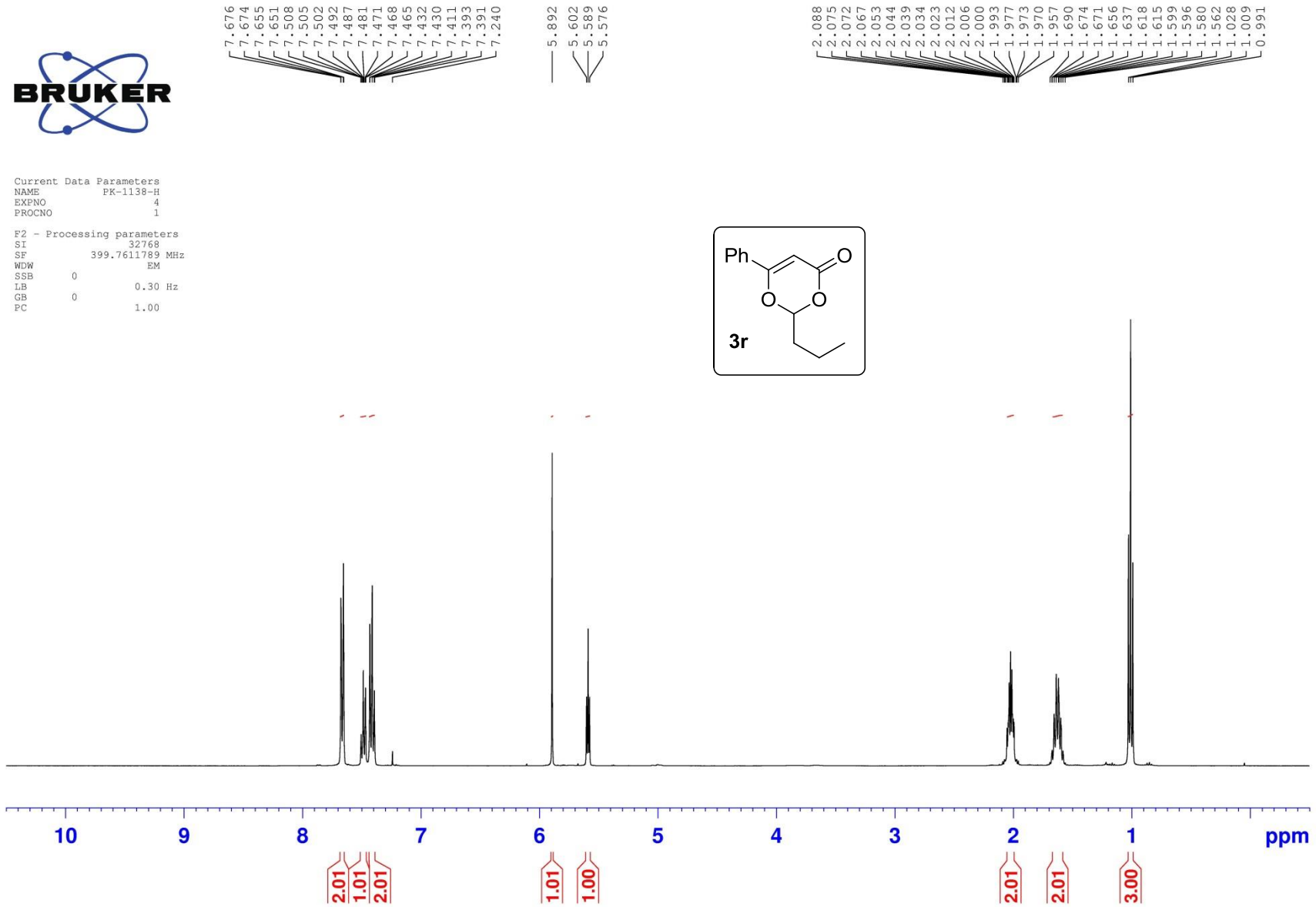

168.13
163.03
137.86
132.40
130.14
128.86
126.52
118.24
101.78
92.87
77.32
77.00
76.68
16.54
Current Data Parameters
NAME PK-1132
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20141229
Time 22.06
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 74
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 1820
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 100.6178046 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
3o
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

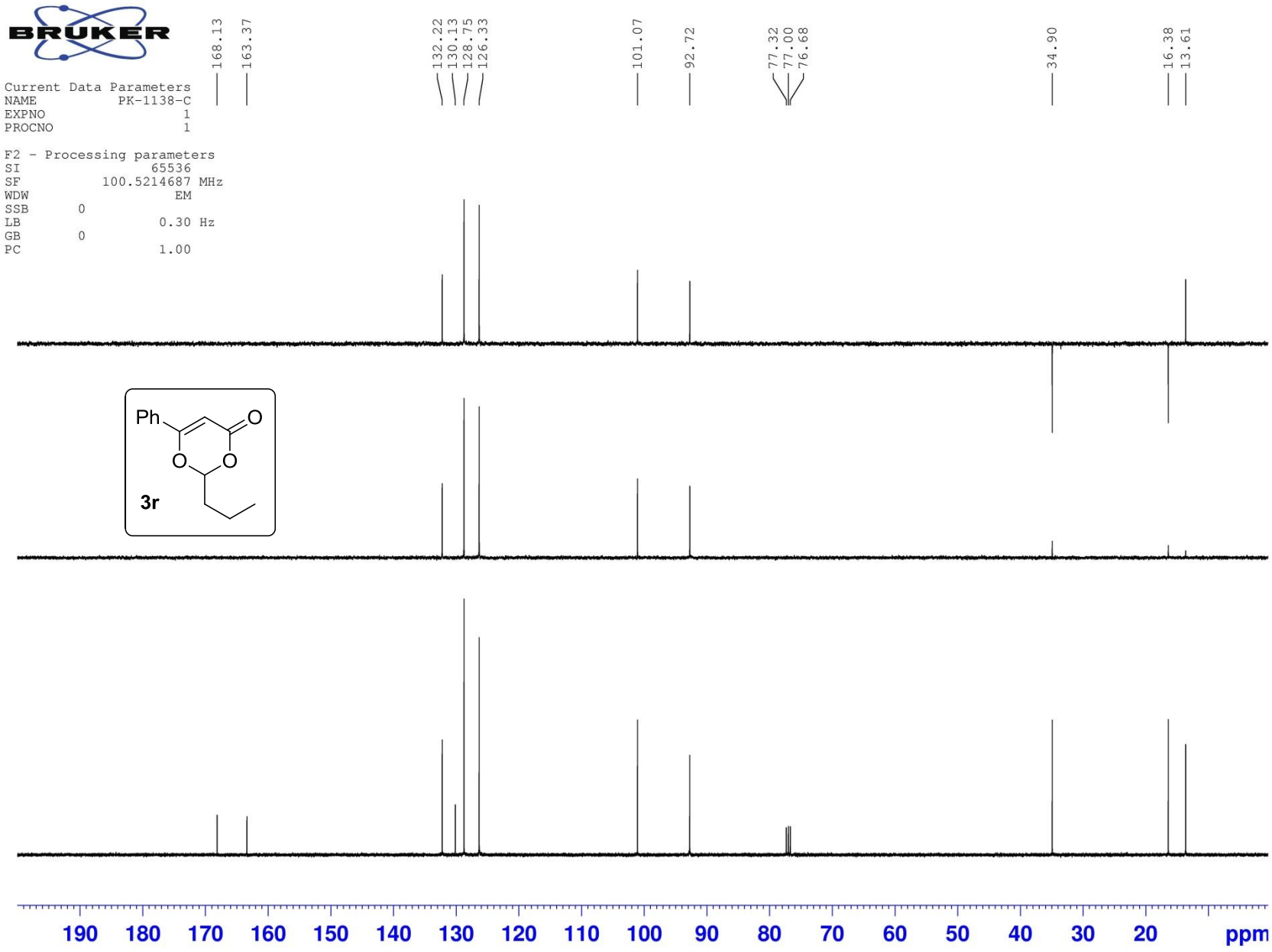

7.751
7.731
7.728
7.545
7.542
7.527
7.521
7.508
7.484
7.481
7.469
7.465
7.452
7.450
7.432
7.391
7.387
7.382
7.371
7.352
7.345
7.335
7.328
7.312
7.309
7.240
7.060
7.019
6.466
6.453
6.426
6.412
6.184
6.170
5.997
Current Data Parameters
NAME PK-1134
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150116
Time 9.55
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 29
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 71.8
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500165 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3p
Ph
10
9
8
7
6
5
4
3
2
1
ppm
2.00
5.00
3.00
1.00
1.00
1.00
1.00


168.10
162.85
137.05
134.74
132.41
130.07
129.14
128.84
128.73
127.14
126.51
120.45
99.96
93.08
77.32
77.00
76.69
Current Data Parameters
NAME PK-1134
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150116
Time 9.58
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 135
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 99.20 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
F2 - Processing parameters
SI 32768
SF 100.6178105 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
3p
Ph
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.686
7.684
7.665
7.662
7.513
7.510
7.507
7.492
7.486
7.476
7.473
7.434
7.418
7.415
7.401
7.397
7.240
5.902
5.754
5.741
5.728
5.715
1.761
1.748
Current Data Parameters
NAME PK-1137-H
EXPNO 4
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611793 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
O
O
3q
10
9
8
7
6
5
4
3
2
1
ppm
2.01
1.01
2.01
1.01
1.00
3.03


168.21
163.29
132.27
130.05
128.76
126.37
98.65
92.71
77.32
77.00
76.68
19.40
Current Data Parameters
NAME PK-1137-C
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214665 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
O
O
3q
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm


7.676
7.674
7.655
7.651
7.508
7.505
7.502
7.492
7.487
7.481
7.471
7.468
7.465
7.432
7.430
7.411
7.393
7.391
7.240
5.892
5.602
5.589
5.576
2.088
2.075
2.072
2.067
2.053
2.044
2.039
2.034
2.023
2.012
2.006
2.000
1.993
1.977
1.973
1.970
1.957
1.690
1.674
1.671
1.656
1.637
1.618
1.615
1.599
1.596
1.580
1.562
1.028
1.009
0.991
Current Data Parameters
NAME PK-1138-H
EXPNO 4
PROCNO 1
F2 - Processing parameters
SI 32768
SF 399.7611789 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
O
O
3r
10
9
8
7
6
5
4
3
2
1
ppm
2.01
1.01
2.01
1.01
1.00
2.01
2.01
3.00


168.13
163.37
132.22
130.13
128.75
126.33
101.07
92.72
77.32
77.00
76.68
34.90
16.38
13.61
Current Data Parameters
NAME PK-1138-C
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214687 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
O
O
3r
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

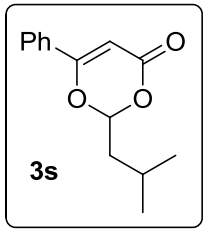
7.693
7.675
7.671
7.529
7.516
7.511
7.506
7.493
7.455
7.435
7.418
7.240

5.923
5.666
5.652
5.638

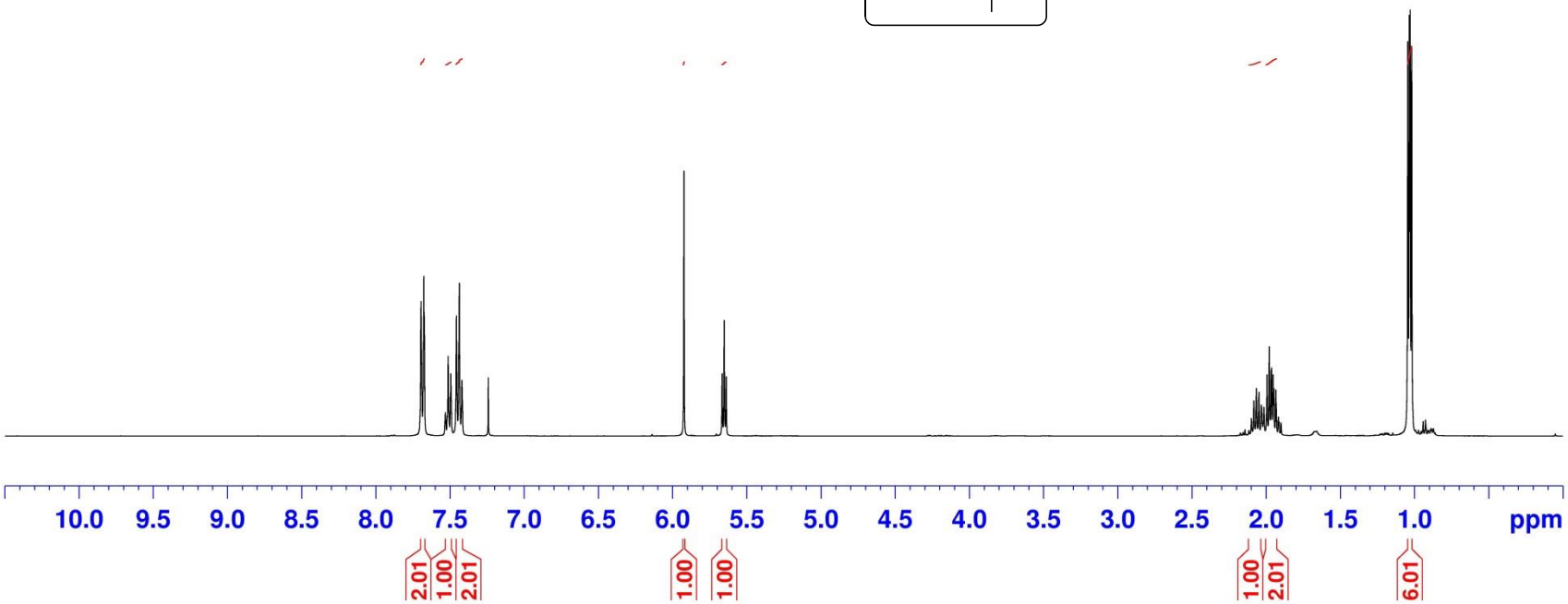
2.142
2.115
2.098
2.081
2.064
2.048
2.031
2.029
2.014
1.993
1.978
1.963
1.952
1.947
1.934
1.917
1.912
1.898
1.044
1.034
1.028
1.018

Current Data Parameters
NAME PK-1140-H
EXPNO 1
PROCNO 1

F2 - Processing parameters
SI 32768
SF 399.7611791 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

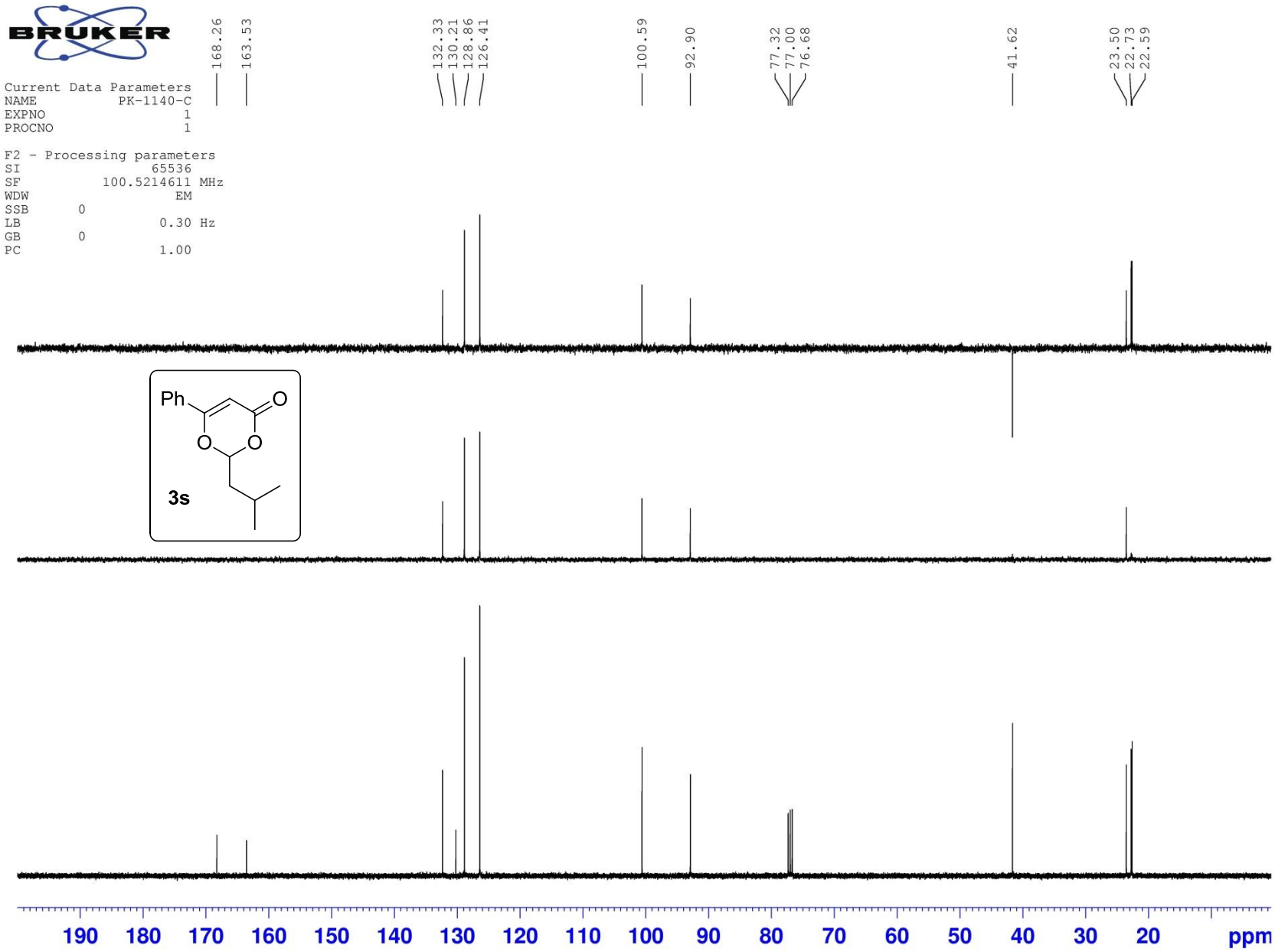


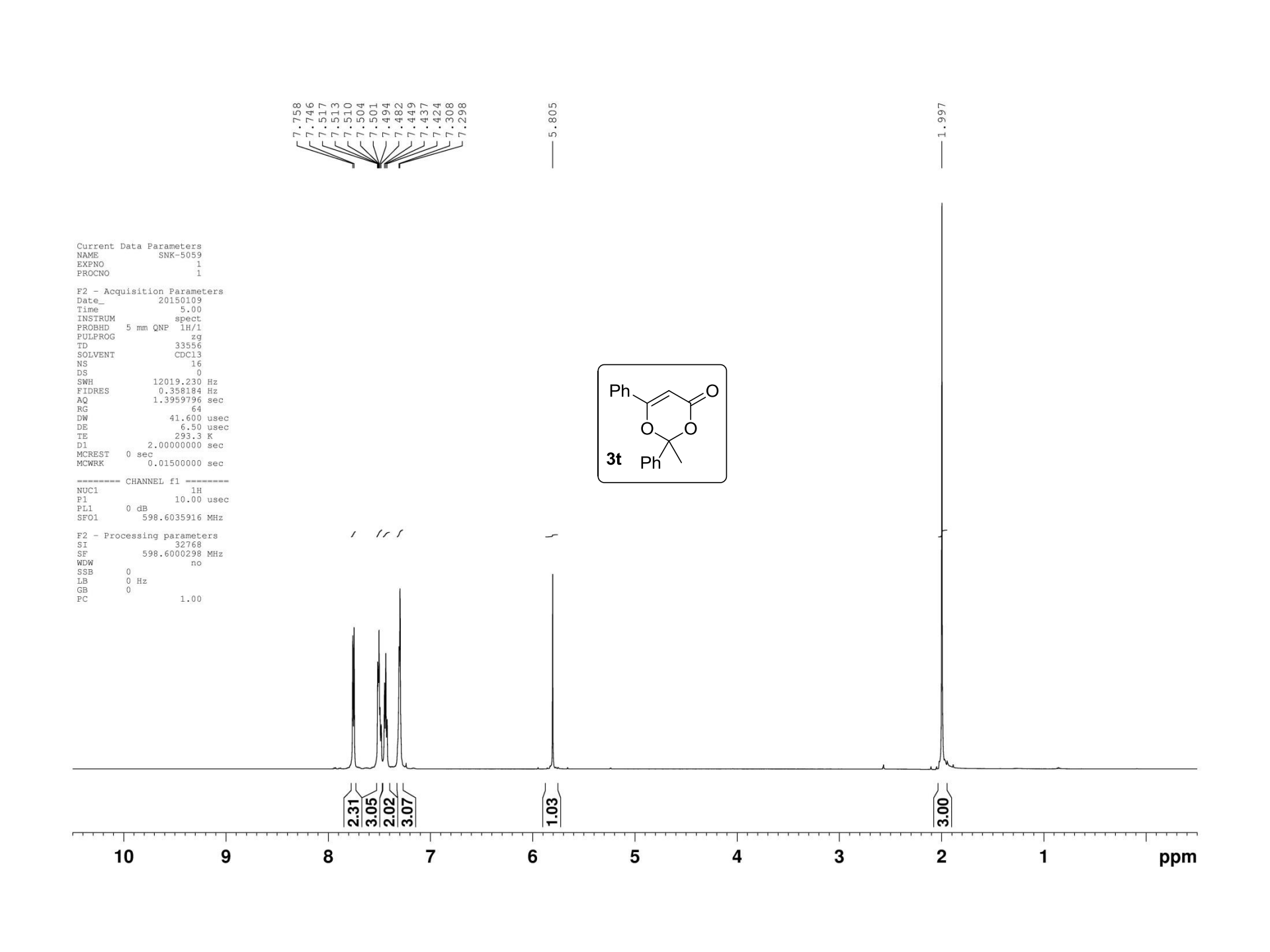
3s

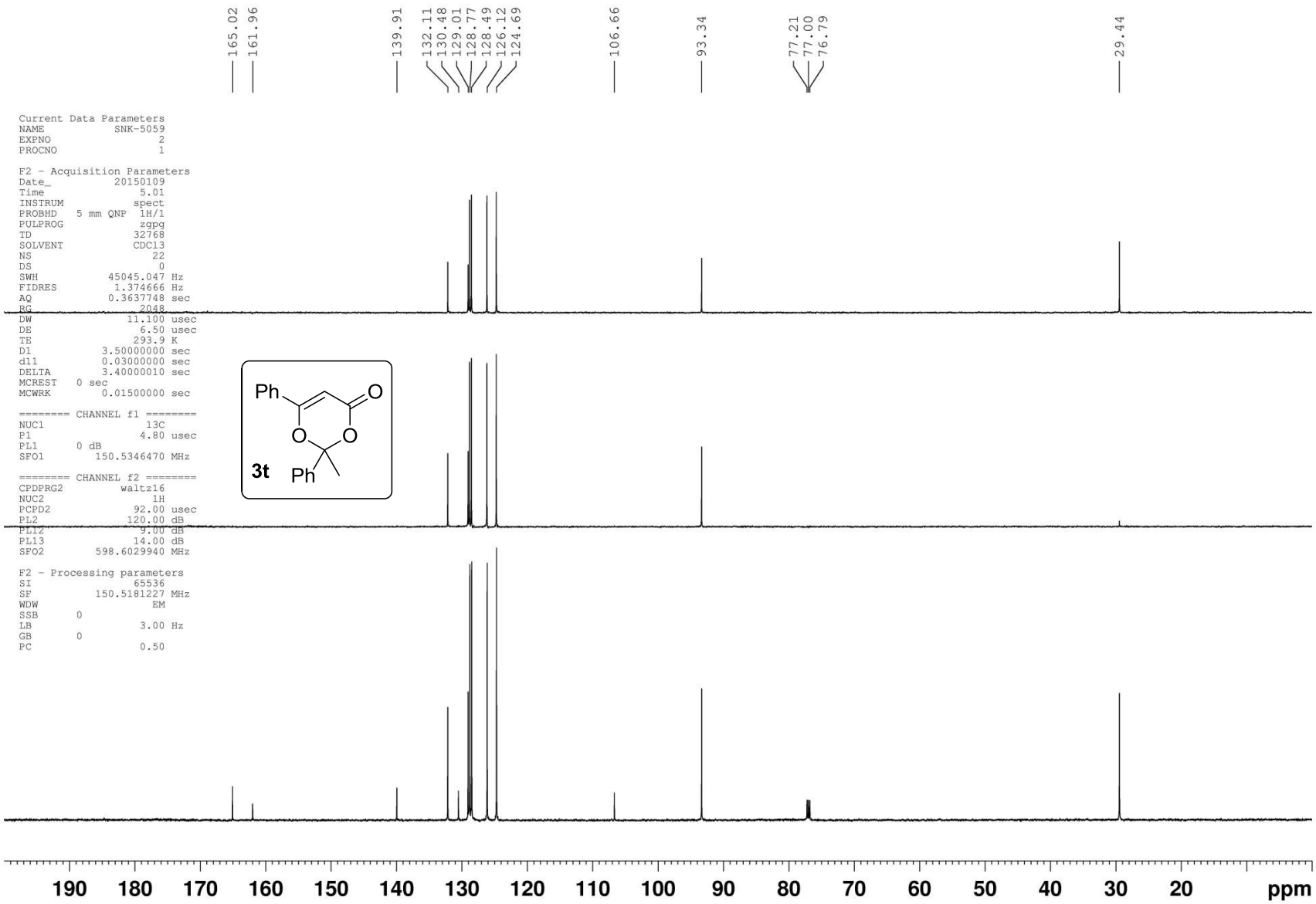


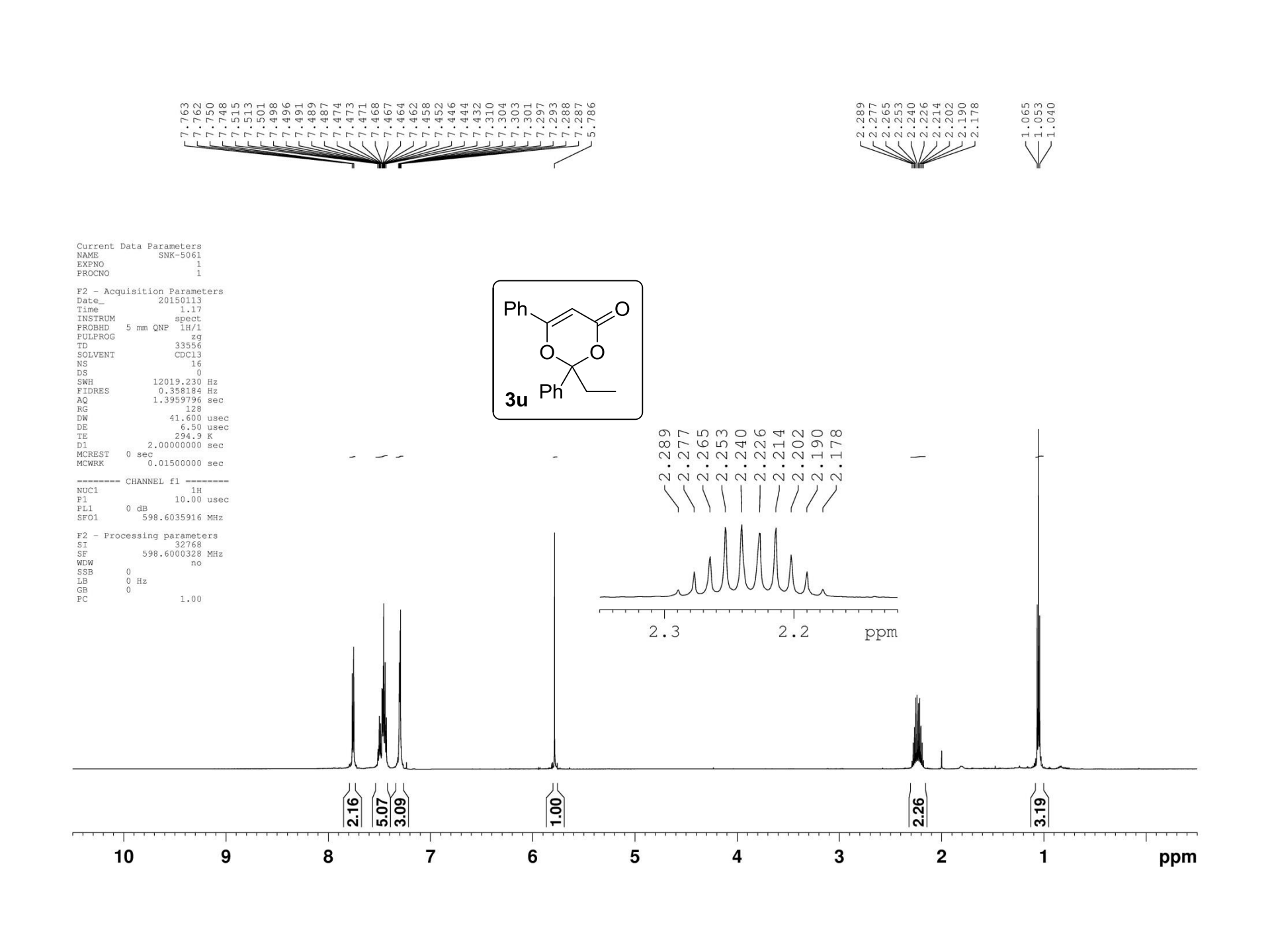
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

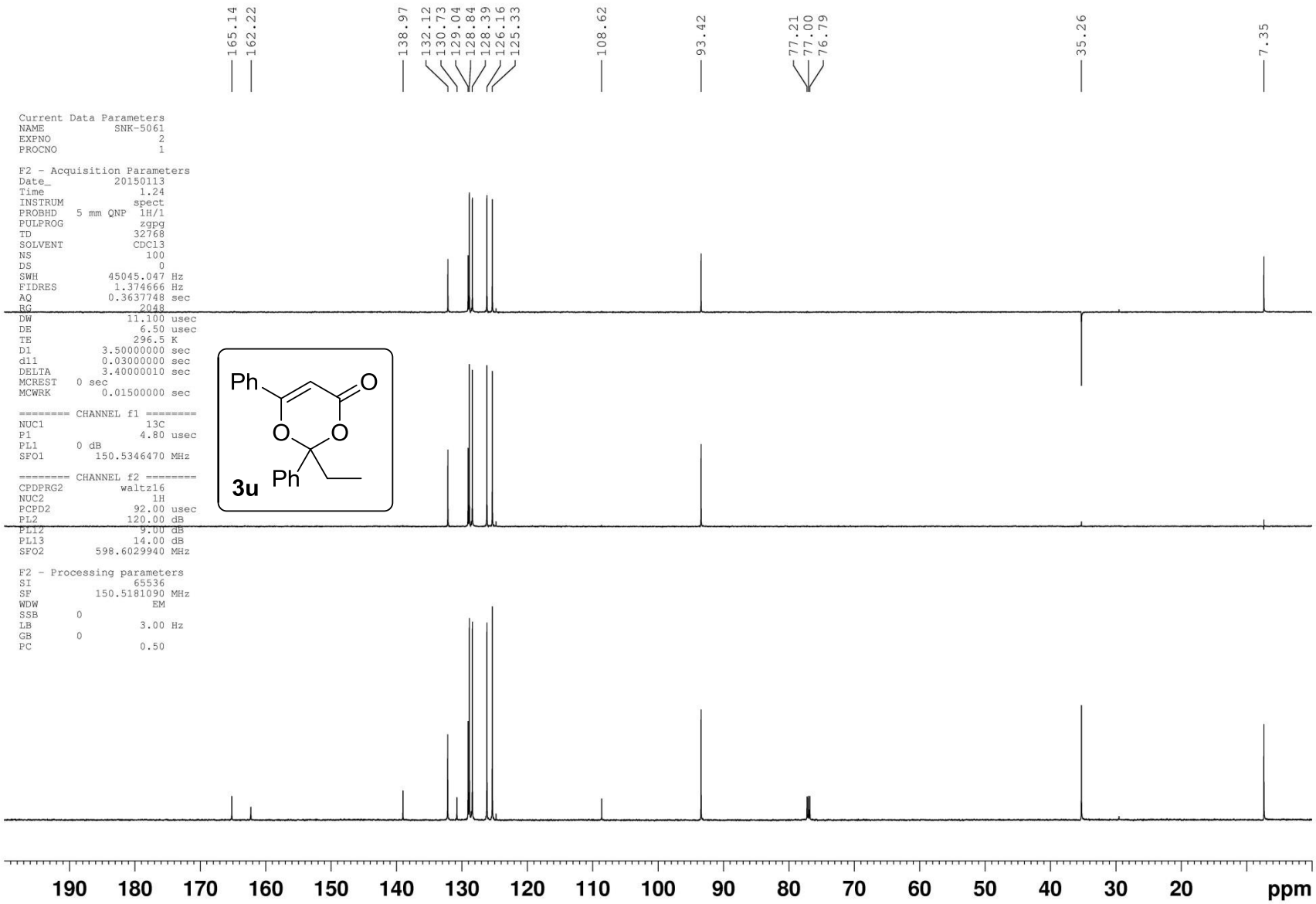
2.01 1.00 2.01 1.00 1.00 1.00 2.01 6.01

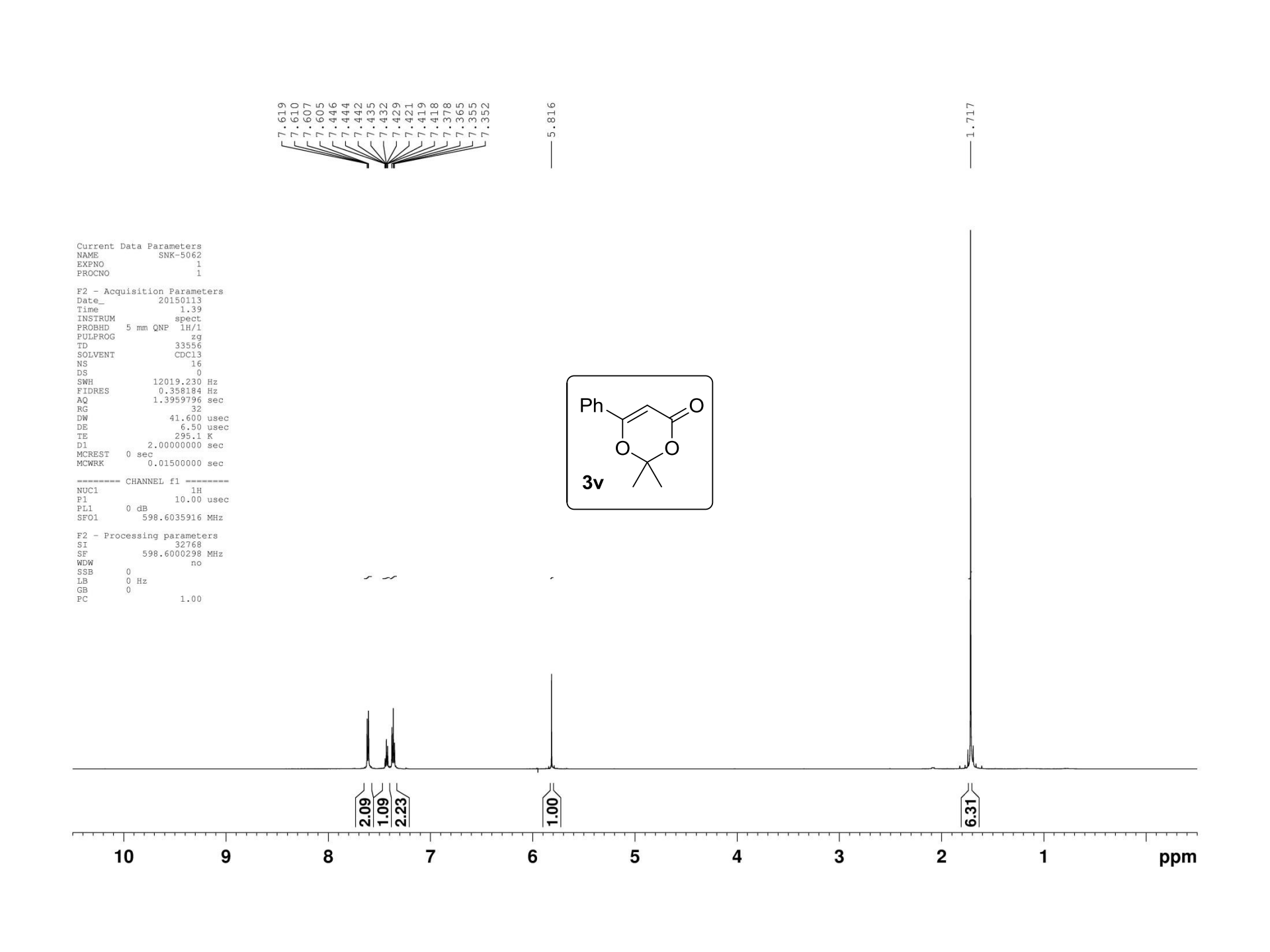

168.26
163.53
132.33
130.21
128.86
126.41
100.59
92.90
77.32
77.00
76.68
41.62
23.50
22.73
22.59
Current Data Parameters
NAME PK-1140-C
EXPNO 1
PROCNO 1
F2 - Processing parameters
SI 65536
SF 100.5214611 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Ph
O
O
O
3s
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

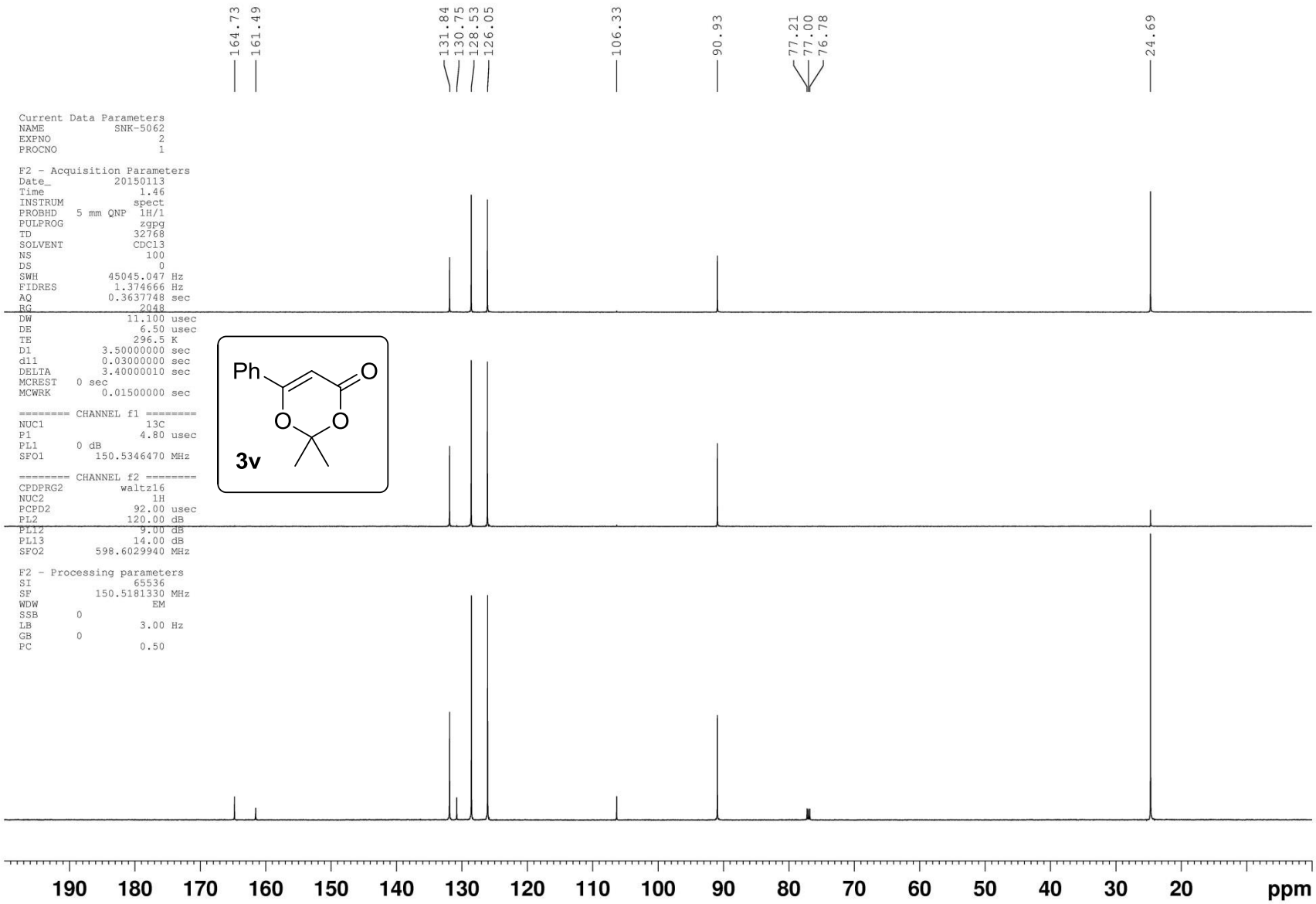

7.758
7.746
7.517
7.513
7.510
7.504
7.501
7.494
7.482
7.449
7.437
7.424
7.308
7.298
5.805
1.997
Current Data Parameters
NAME SNK-5059
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150109
Time 5.00
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 33556
SOLVENT CDCl3
NS 16
DS 0
SWH 12019.230 Hz
FIDRES 0.358184 Hz
AQ 1.3959796 sec
RG 64
DW 41.600 usec
DE 6.50 usec
TE 293.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3t
Ph
2.31
3.05
2.02
3.07
1.03
3.00
10
9
8
7
6
5
4
3
2
1
ppm

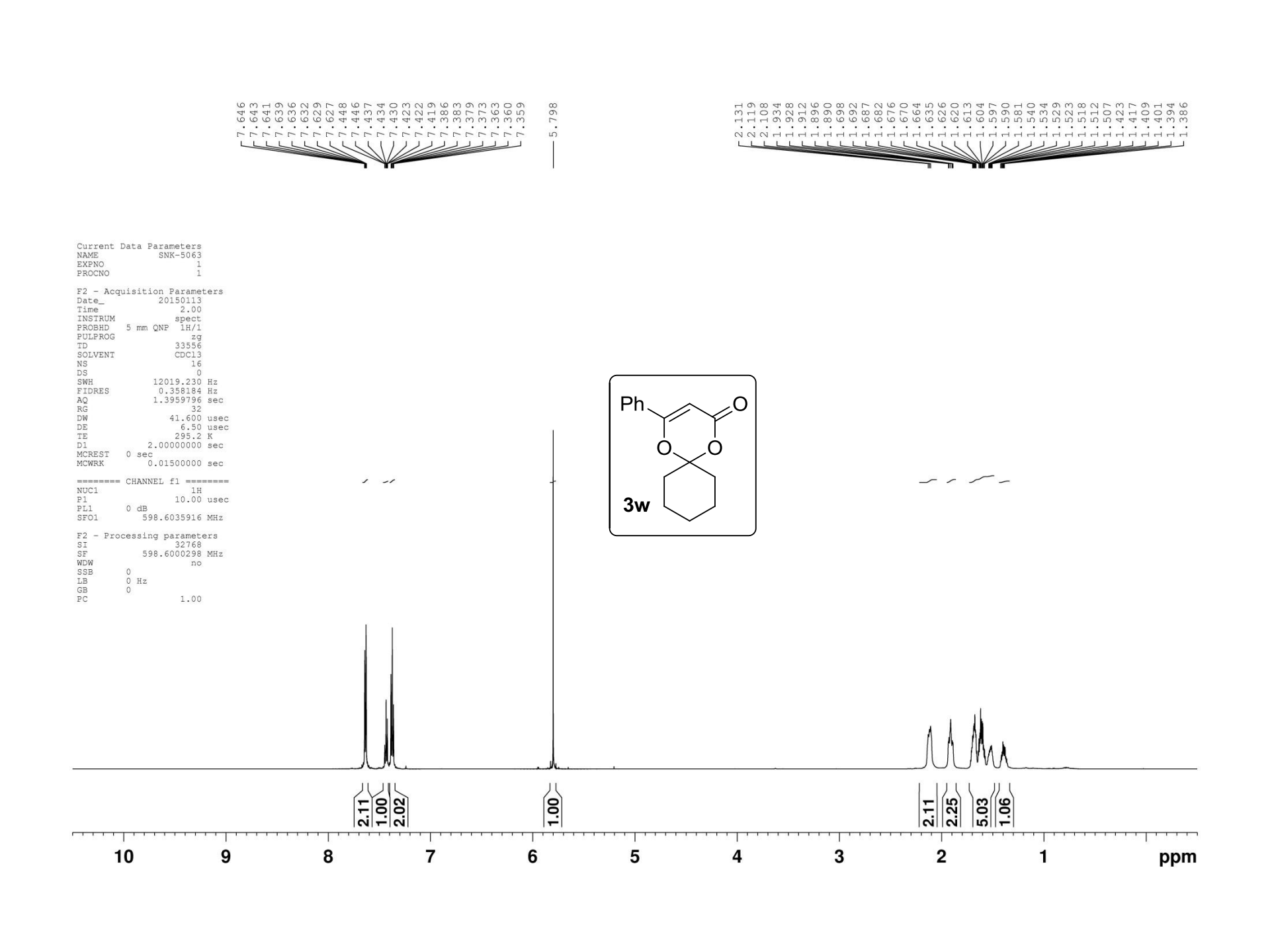

165.02
161.96
139.91
132.11
130.48
129.01
128.77
128.49
126.12
124.69
106.66
93.34
77.21
77.00
76.79
29.44
Current Data Parameters
NAME SNK-5059
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150109
Time 5.01
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 22
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 293.9 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181227 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ph
O
O
O
Ph
3t
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

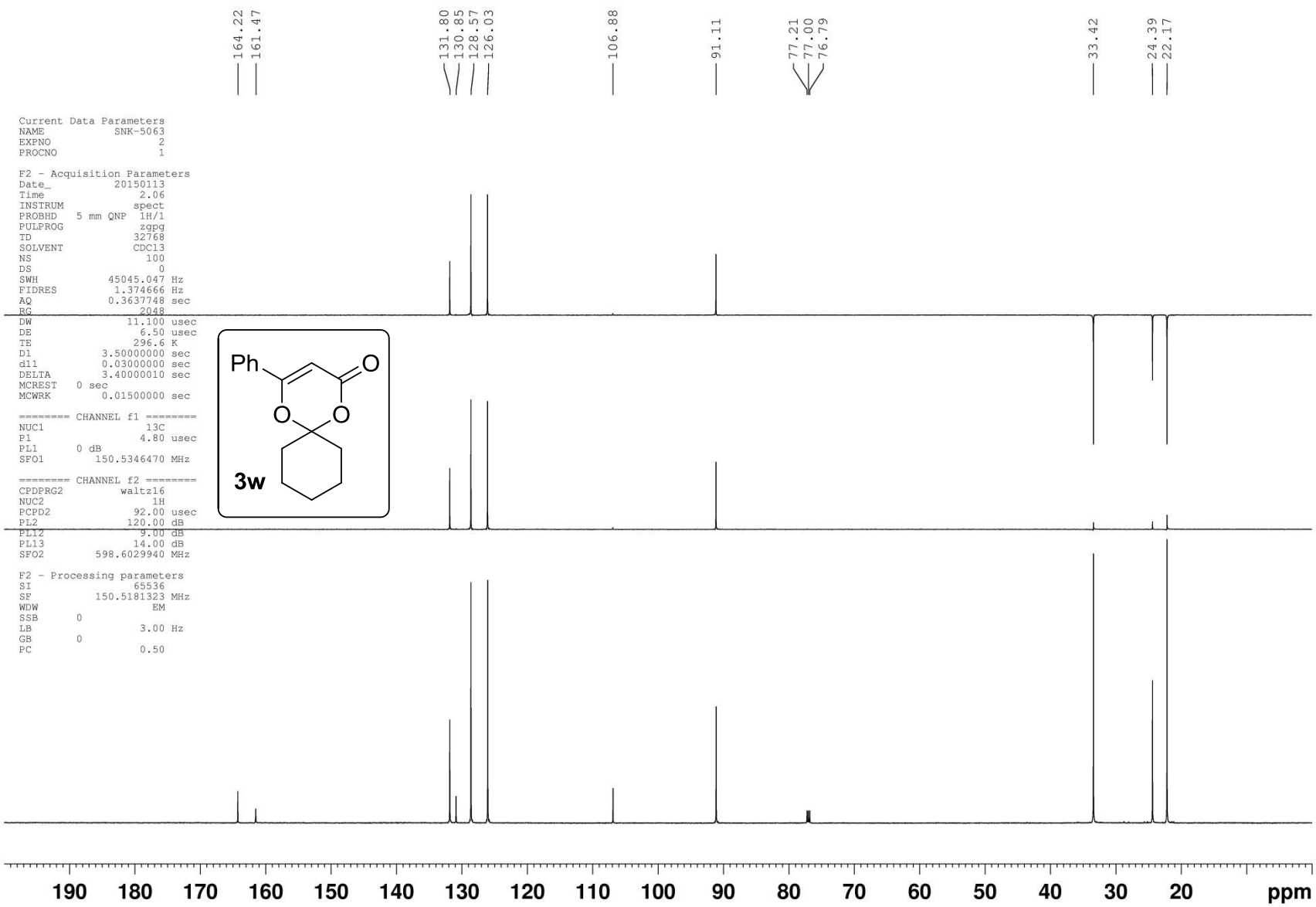

7.763
7.762
7.750
7.748
7.515
7.513
7.501
7.498
7.496
7.491
7.489
7.487
7.474
7.473
7.471
7.468
7.467
7.464
7.462
7.458
7.452
7.446
7.444
7.432
7.310
7.304
7.303
7.301
7.297
7.293
7.288
7.287
5.786
2.289
2.277
2.265
2.253
2.240
2.226
2.214
2.202
2.190
2.178
1.065
1.053
1.040
Current Data Parameters
NAME SNK-5061
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 1.17
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 294.9 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000328 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
Ph
3u
2.3
2.2
ppm
2.16
5.07
3.09
1.00
2.26
3.19
10
9
8
7
6
5
4
3
2
1
ppm

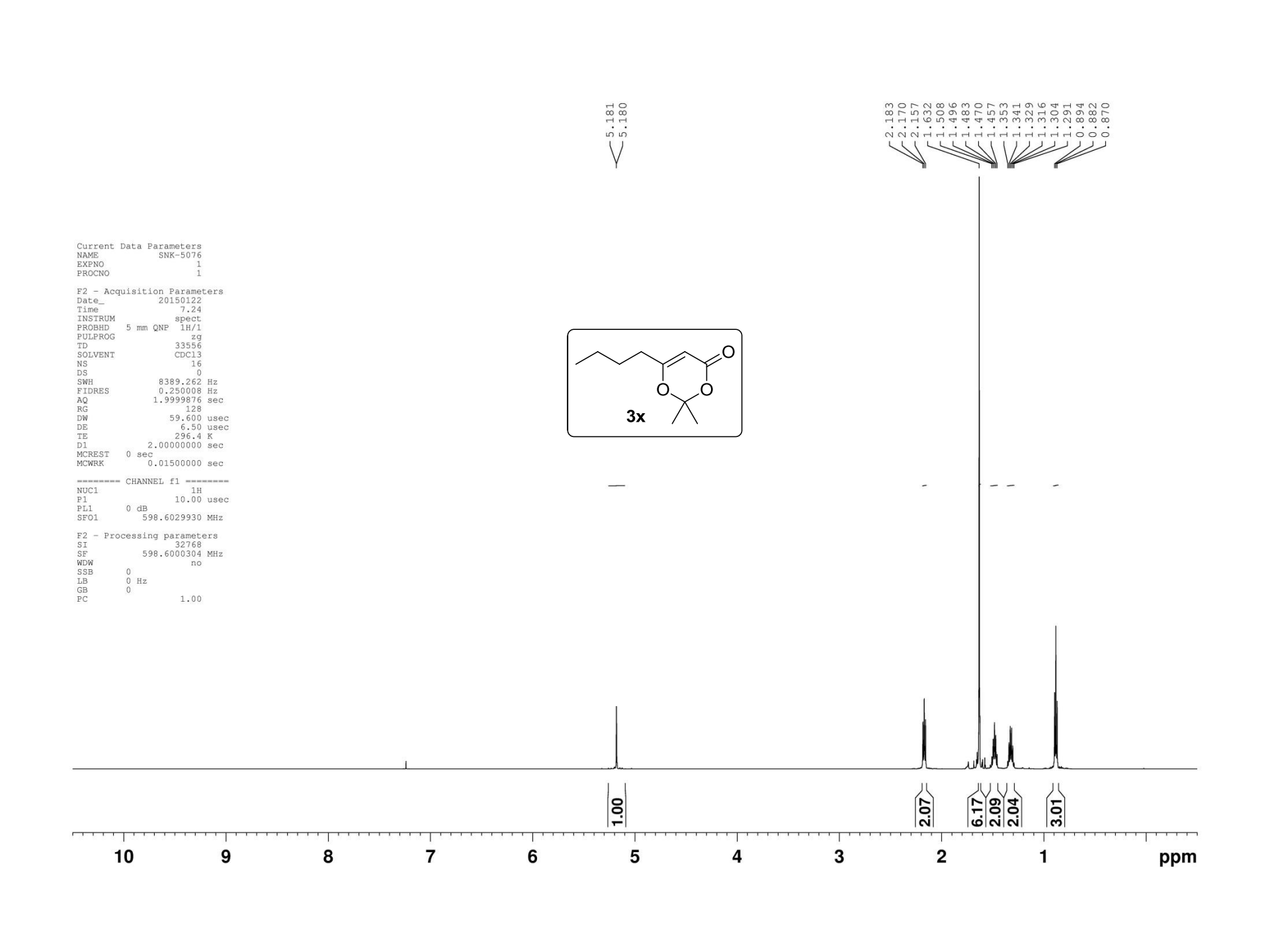

165.14
162.22
138.97
132.12
130.73
129.04
128.84
128.39
126.16
125.33
108.62
93.42
77.21
77.00
76.79
35.26
7.35
Current Data Parameters
NAME SNK-5061
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 1.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181090 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ph
O
O
O
Ph
3u
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.619
7.610
7.607
7.605
7.446
7.444
7.442
7.435
7.432
7.429
7.421
7.419
7.418
7.378
7.365
7.355
7.352
5.816
1.717
Current Data Parameters
NAME SNK-5062
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 1.39
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 32
DW 41.600 usec
DE 6.50 usec
TE 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3v
2.09
1.09
2.23
1.00
6.31
10
9
8
7
6
5
4
3
2
1
ppm

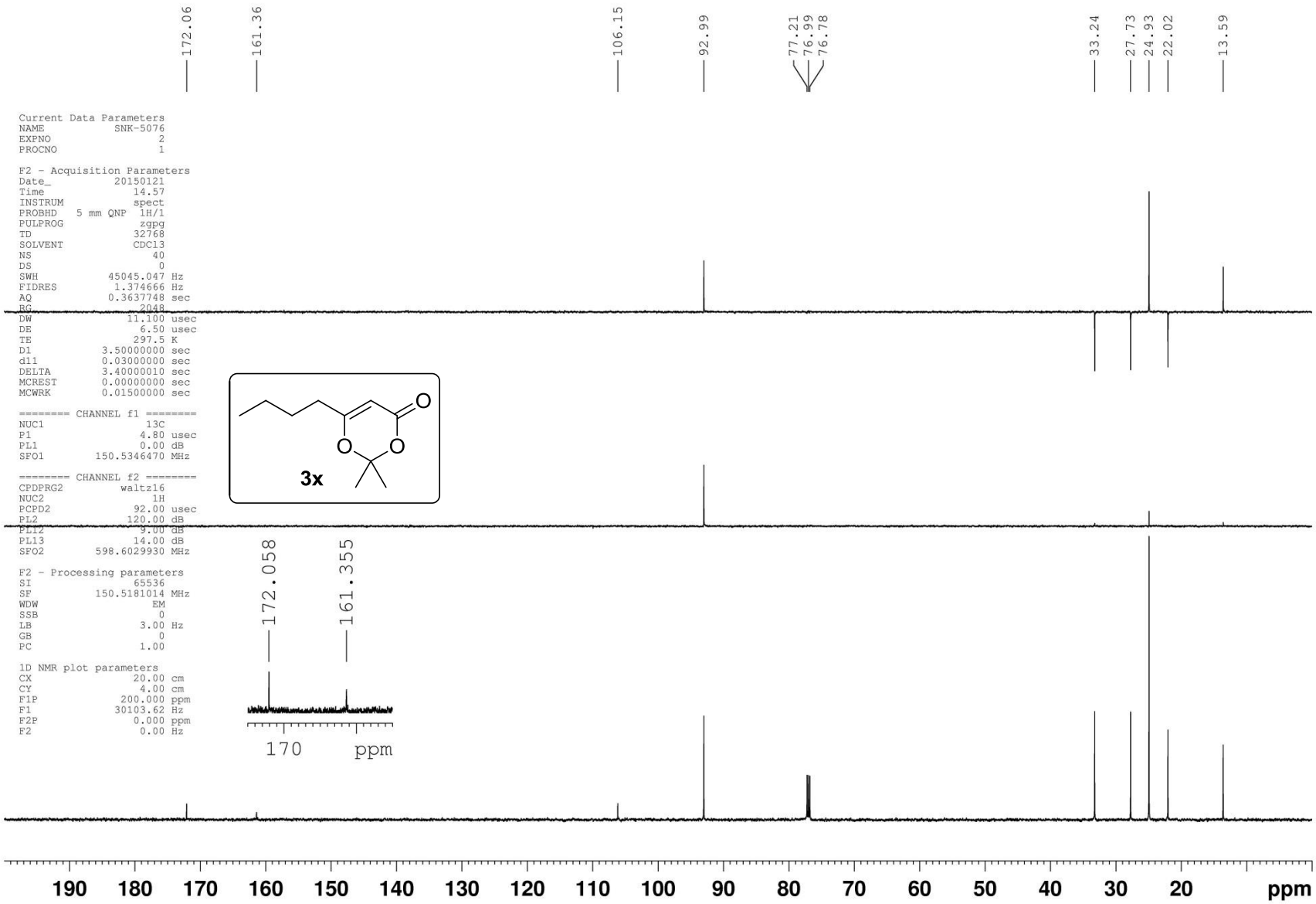

164.73
161.49
131.84
130.75
128.53
126.05
106.33
90.93
77.21
77.00
76.78
24.69
Current Data Parameters
NAME SNK-5062
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 1.46
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181330 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ph
O
O
O
3v
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

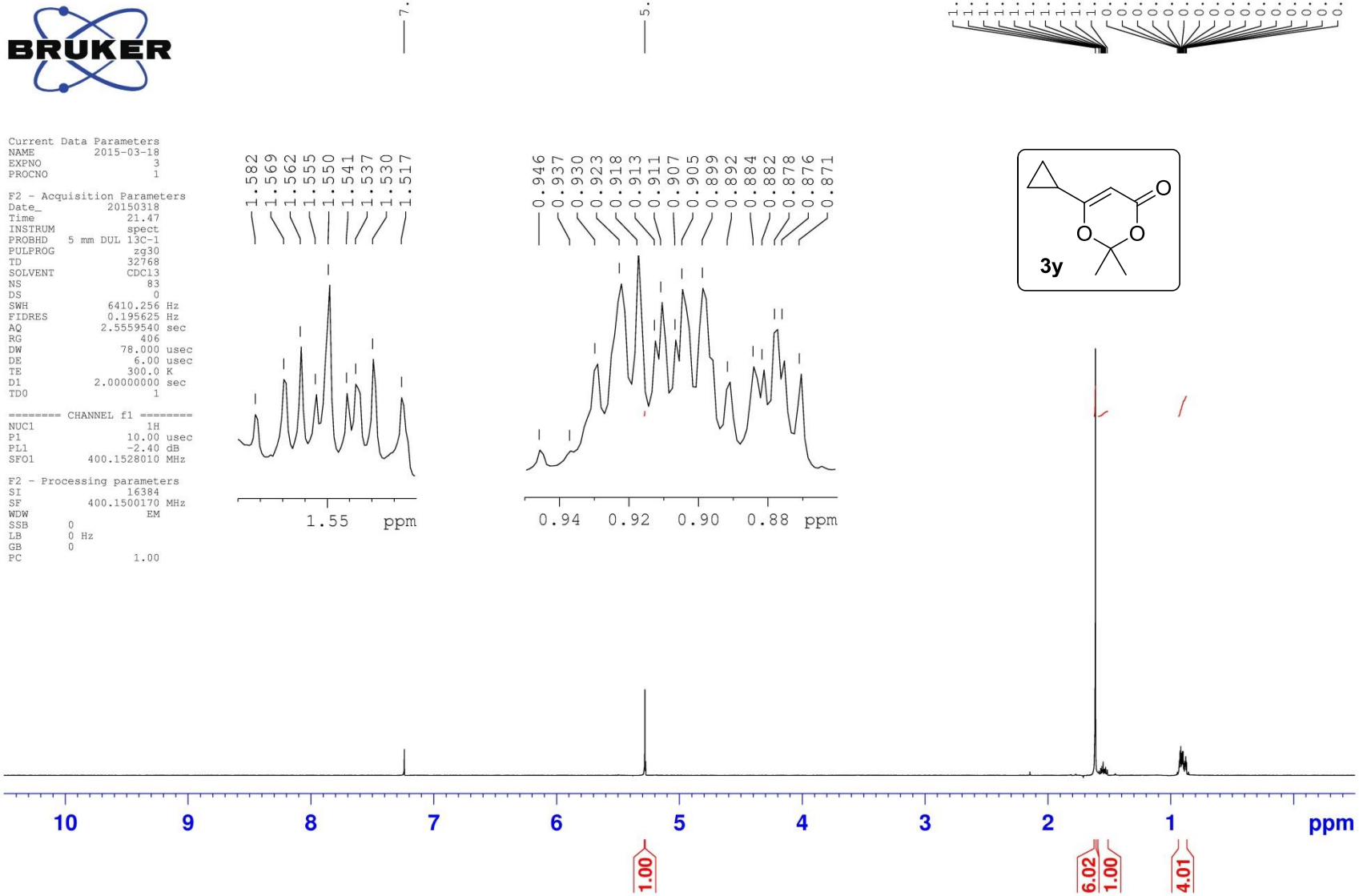

7.646
7.643
7.641
7.639
7.636
7.632
7.629
7.627
7.448
7.446
7.437
7.434
7.430
7.423
7.422
7.419
7.386
7.383
7.379
7.373
7.363
7.360
7.359
5.798
2.131
2.119
2.108
1.934
1.928
1.912
1.896
1.890
1.698
1.692
1.687
1.682
1.676
1.670
1.664
1.635
1.626
1.620
1.613
1.604
1.597
1.590
1.581
1.540
1.534
1.529
1.523
1.518
1.512
1.507
1.423
1.417
1.409
1.401
1.394
1.386
Current Data Parameters
NAME SNK-5063
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 2.00
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 32
DW 41.600 usec
DE 6.50 usec
TE 295.2 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000298 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
O
O
3w
2.11
1.00
2.02
1.00
2.11
2.25
5.03
1.06
10
9
8
7
6
5
4
3
2
1
ppm

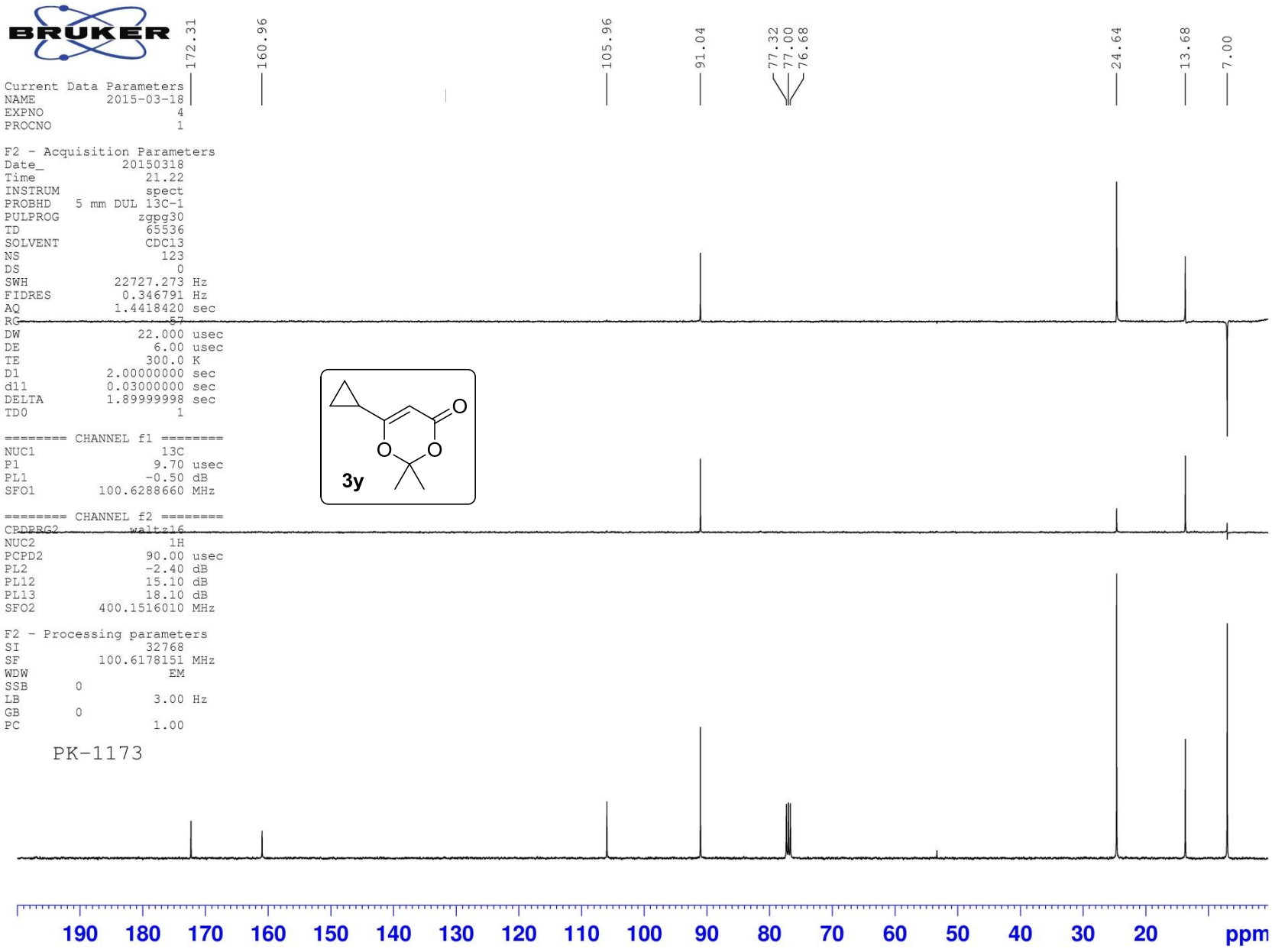

164.22
161.47
131.80
130.85
128.57
126.03
106.88
91.11
77.21
77.00
76.79
33.42
24.39
22.17
Current Data Parameters
NAME SNK-5063
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150113
Time 2.06
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 296.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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
SF 150.5181323 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.50
Ph
O
O
O
3w
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

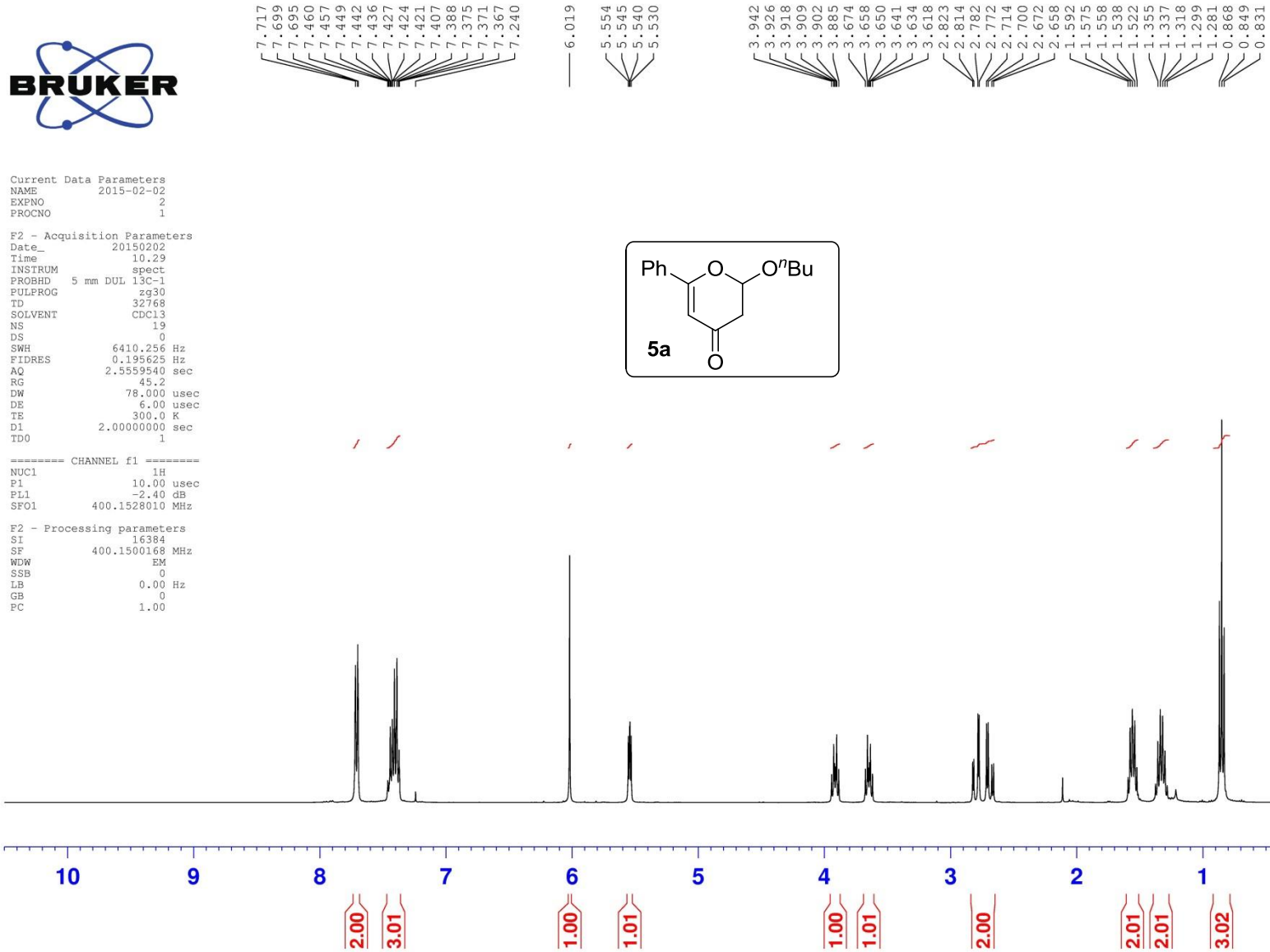


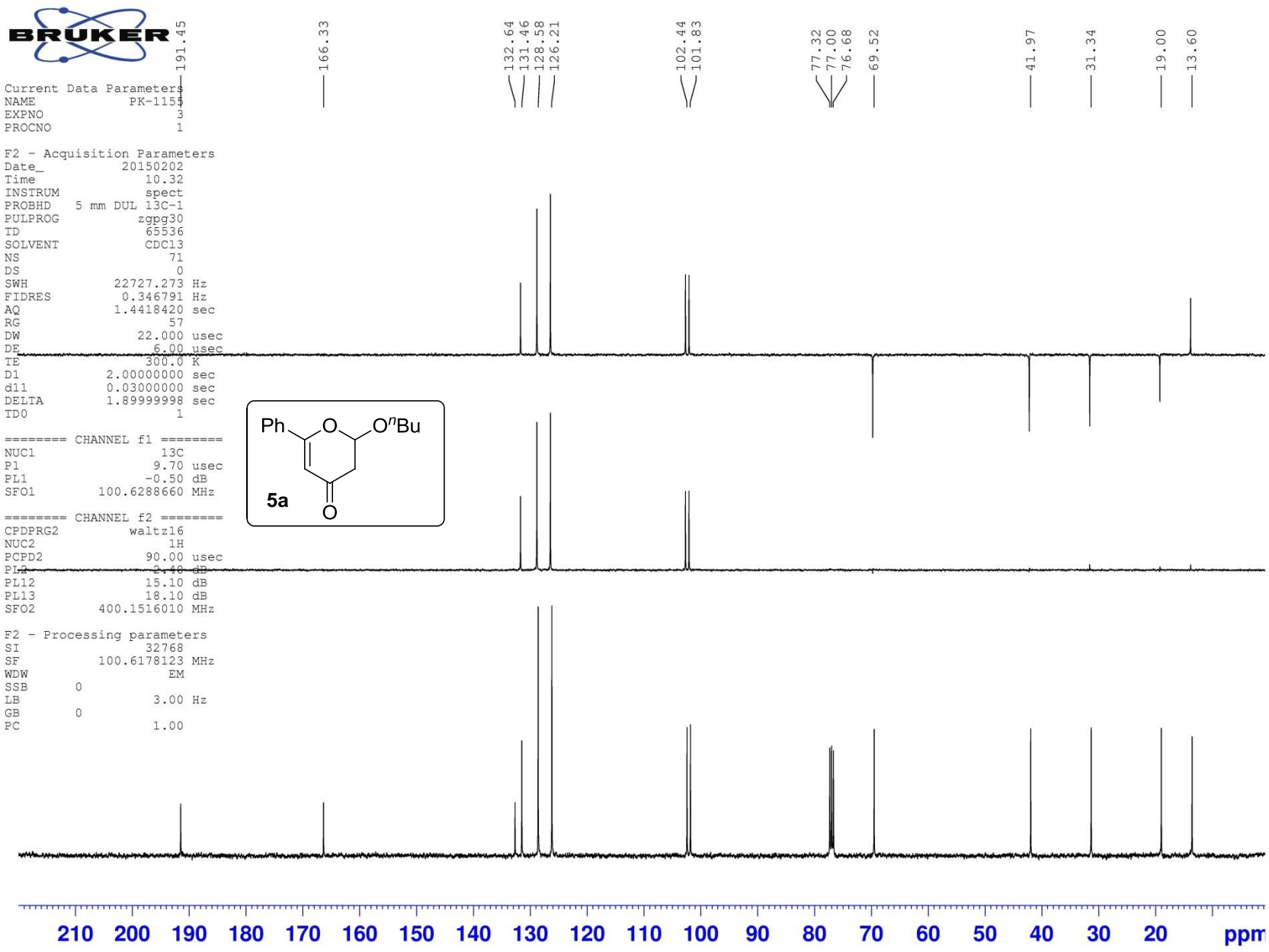

```
Current Data Parameters
NAME            SNK-5076
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150122
Time                7.24
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               296.4 K
D1            2.00000000 sec
MCREST    0 sec
MCWRK         0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1       0 dB
SFO1        598.6029930 MHz

F2 - Processing parameters
SI                32768
SF          598.6000304 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

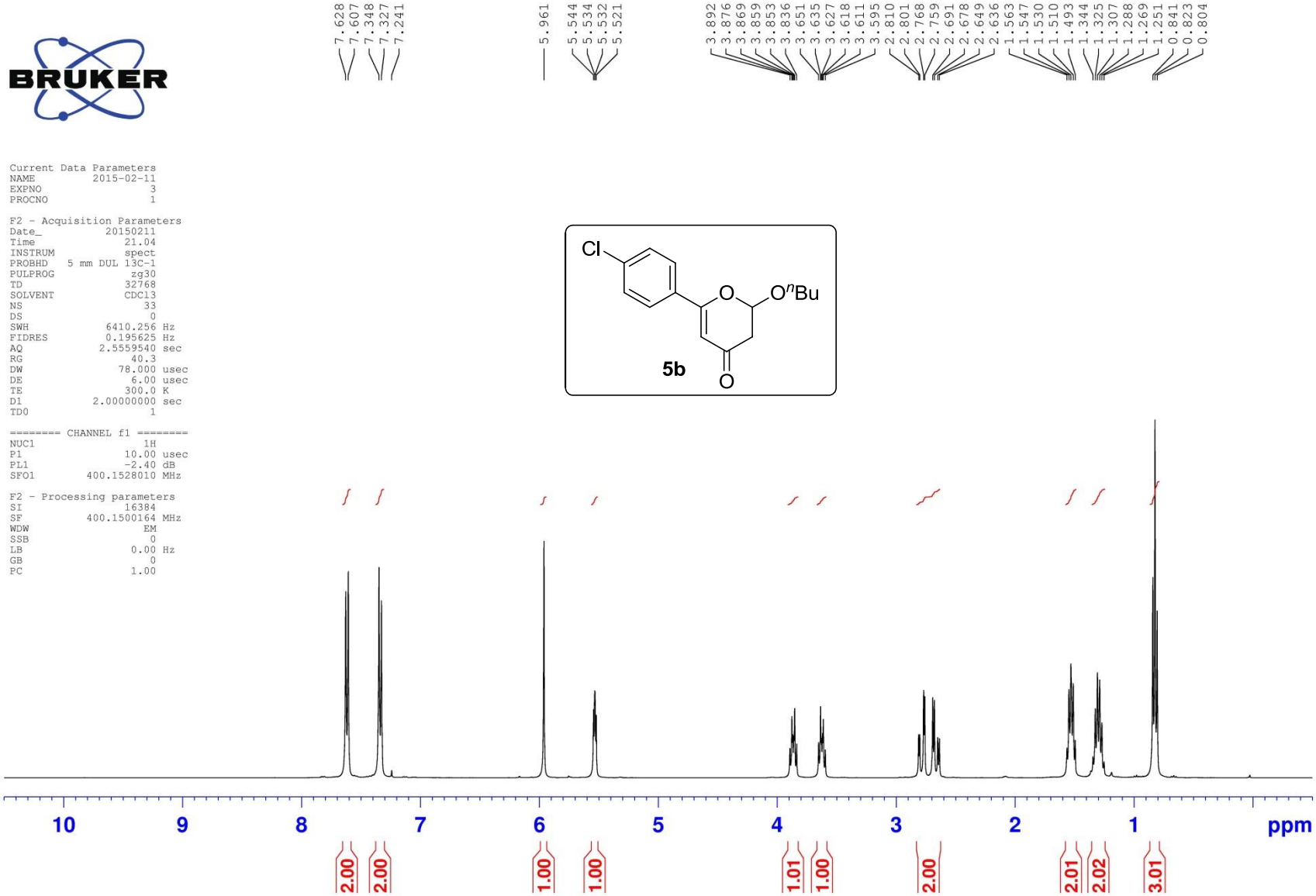

172.06
161.36
106.15
92.99
77.21
76.99
76.78
33.24
27.73
24.93
22.02
13.59
Current Data Parameters
NAME SNK-5076
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150121
Time 14.57
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 40
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 297.5 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 150.5181014 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
O
O
O
3x
172.058
161.355
170
ppm
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

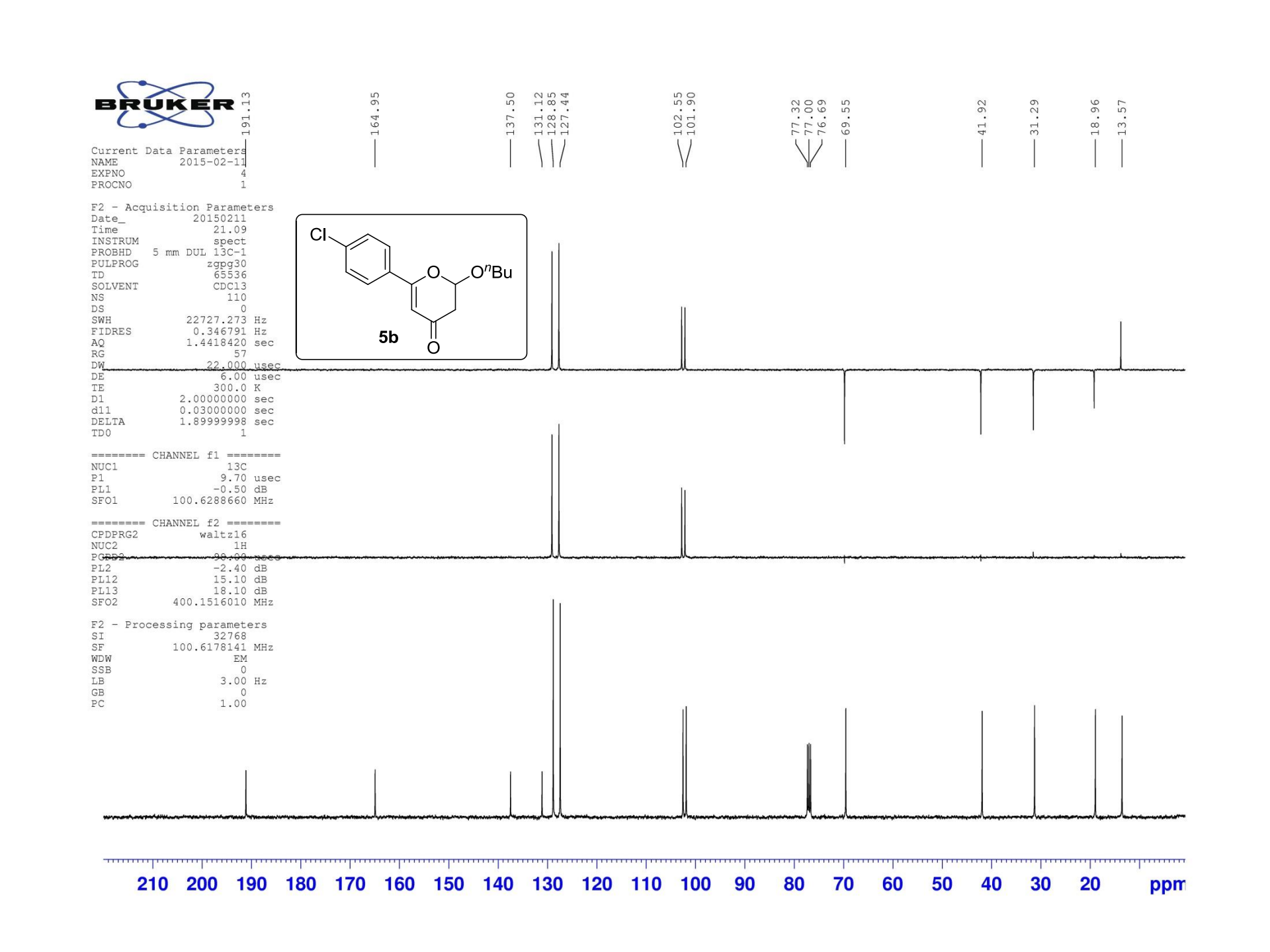

7.240
5.282
1.613
1.582
1.569
1.562
1.555
1.550
1.541
1.537
1.530
1.517
0.946
0.937
0.930
0.923
0.918
0.913
0.911
0.907
0.905
0.899
0.892
0.884
0.882
0.878
0.876
0.871
Current Data Parameters
NAME 2015-03-18
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150318
Time 21.47
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 83
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 406
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
1.582
1.569
1.562
1.555
1.550
1.541
1.537
1.530
1.517
1.55 ppm
0.946
0.937
0.930
0.923
0.918
0.913
0.911
0.907
0.905
0.899
0.892
0.884
0.882
0.878
0.876
0.871
0.94 0.92 0.90 0.88 ppm
O
O
O
3y
10 9 8 7 6 5 4 3 2 1 ppm
1.00
6.02
1.00
4.01

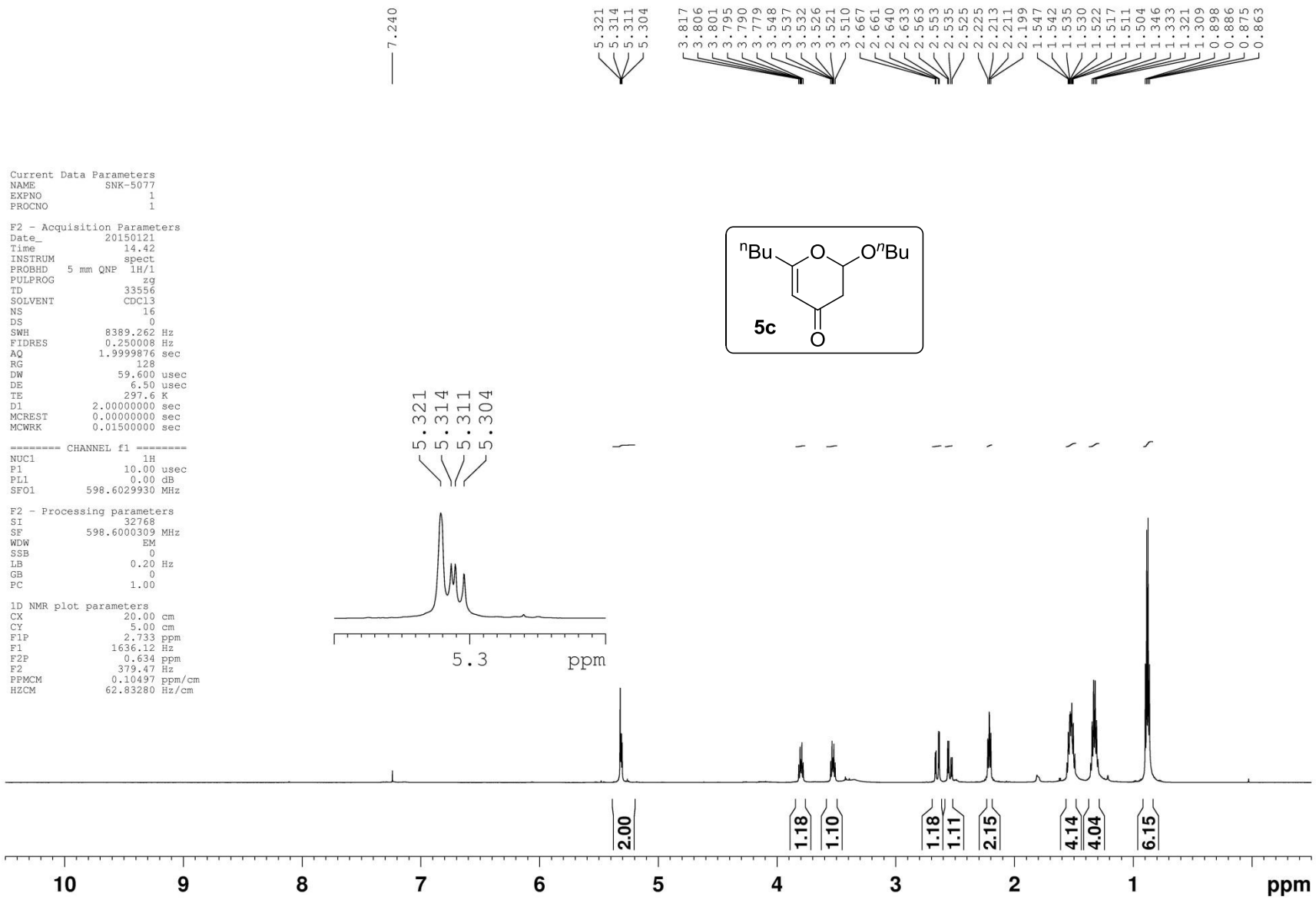

172.31
160.96
105.96
91.04
77.32
77.00
76.68
24.64
13.68
7.00
Current Data Parameters
NAME 2015-03-18
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150318
Time 21.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 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 100.6178151 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
3y
PK-1173
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

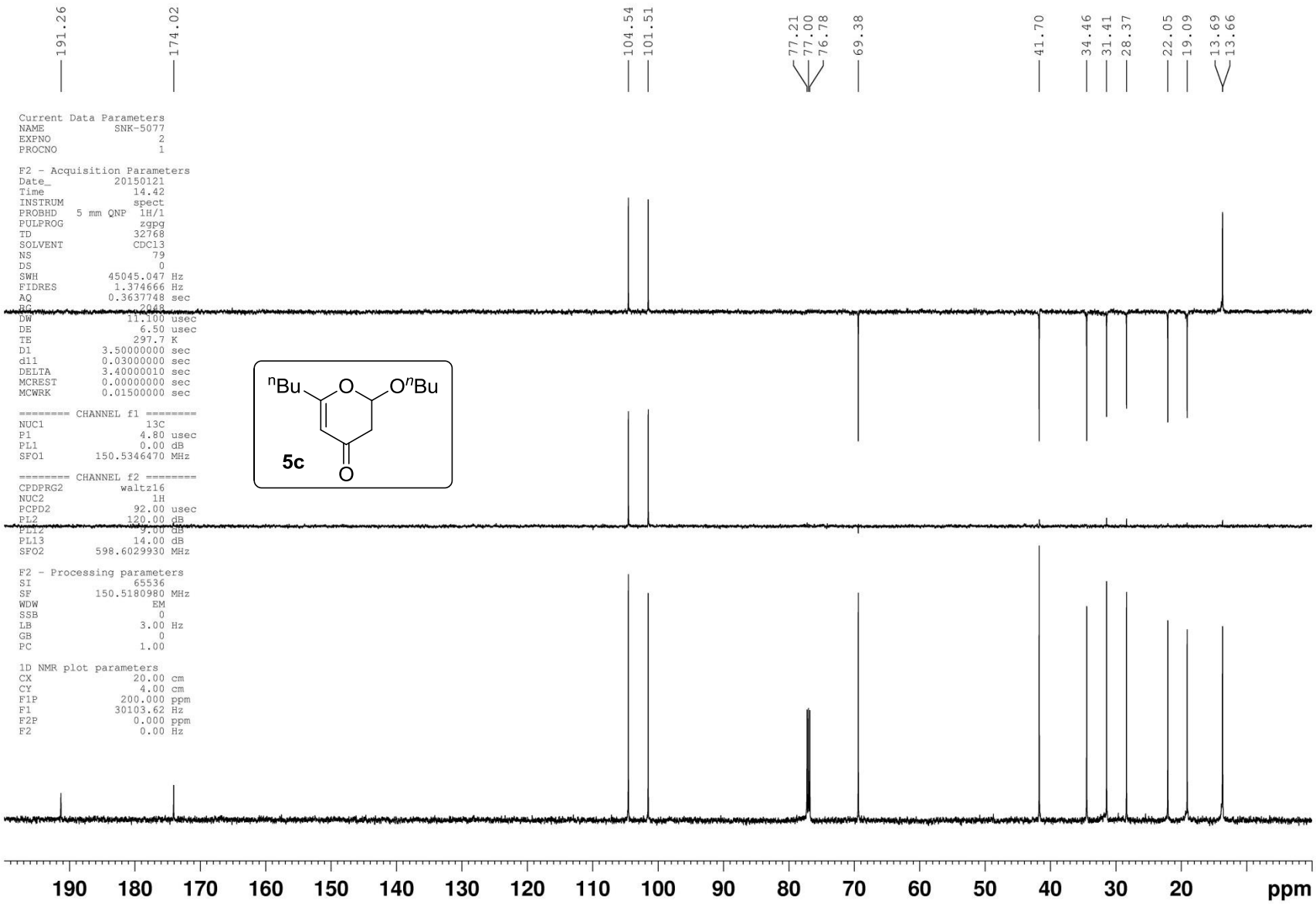

7.717
7.699
7.695
7.460
7.457
7.449
7.442
7.436
7.427
7.424
7.421
7.407
7.388
7.375
7.371
7.367
7.240
6.019
5.554
5.545
5.540
5.530
3.942
3.926
3.918
3.909
3.902
3.885
3.674
3.658
3.650
3.641
3.634
3.618
2.823
2.814
2.782
2.772
2.714
2.700
2.672
2.658
1.592
1.575
1.558
1.538
1.522
1.355
1.337
1.318
1.299
1.281
0.868
0.849
0.831
Current Data Parameters
NAME 2015-02-02
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150202
Time 10.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 19
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 45.2
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500168 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Ph
O
O^{n}Bu
5a
O
10
9
8
7
6
5
4
3
2
1
ppm
2.00
3.01
1.00
1.01
1.00
1.01
2.00
2.01
2.01
3.02

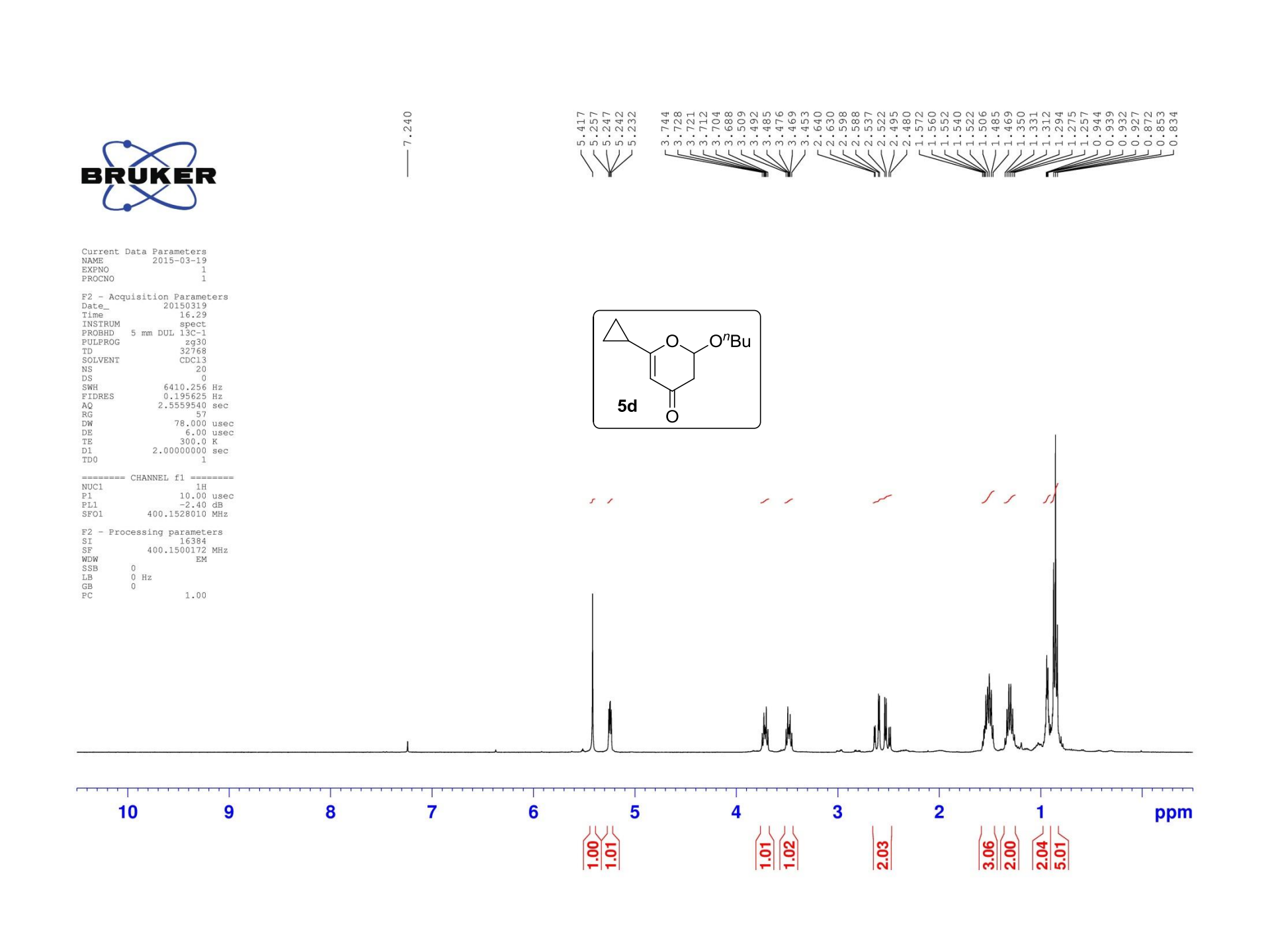

191.45
166.33
132.64
131.46
128.58
126.21
102.44
101.83
77.32
77.00
76.68
69.52
41.97
31.34
19.00
13.60
Current Data Parameters
NAME PK-1155
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150202
Time 10.32
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 71
DS 0
SWH 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 100.6178123 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O^{n}Bu
O
5a
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

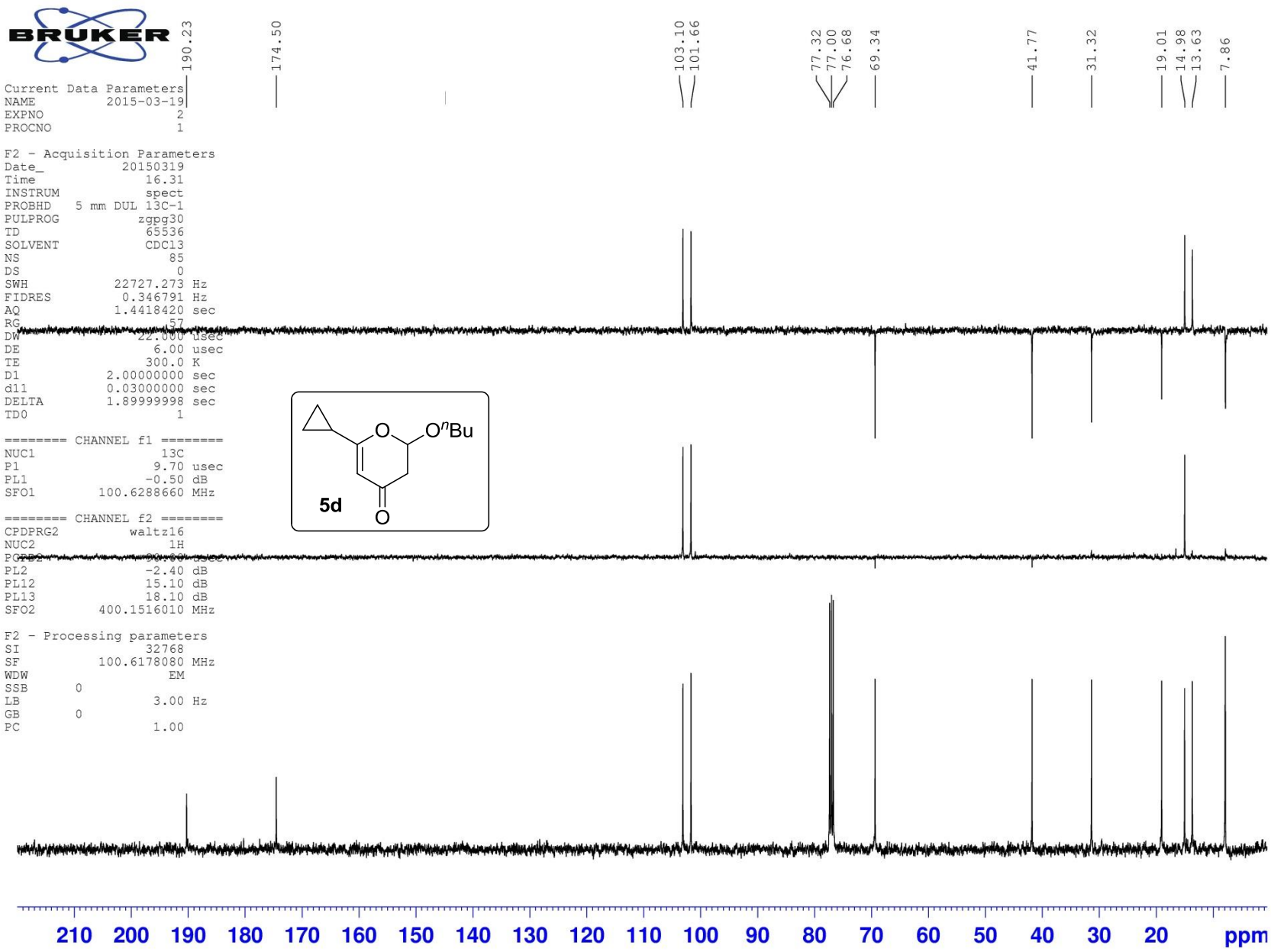

7.628
7.607
7.348
7.327
7.241
5.961
5.544
5.534
5.532
5.521
3.892
3.876
3.869
3.859
3.853
3.836
3.651
3.635
3.627
3.618
3.611
3.595
2.810
2.801
2.768
2.759
2.691
2.678
2.649
2.636
1.563
1.547
1.530
1.510
1.493
1.344
1.325
1.307
1.288
1.269
1.251
0.841
0.823
0.804
Current Data Parameters
NAME 2015-02-11
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150211
Time 21.04
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 33
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 40.3
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500164 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
Cl
O
O^{n}Bu
O
5b
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.00
1.00
1.00
1.01
1.00
2.00
2.01
2.02
3.01


191.13
164.95
137.50
131.12
128.85
127.44
102.55
101.90
77.32
77.00
76.69
69.55
41.92
31.29
18.96
13.57
Current Data Parameters
NAME 2015-02-11
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150211
Time 21.09
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 110
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 100.6178141 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Cl
O
O
nBu
5b
O
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

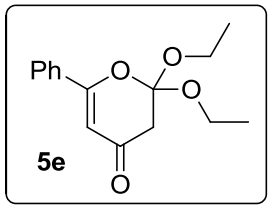

7.240
5.321
5.314
5.311
5.304
3.817
3.806
3.801
3.795
3.790
3.779
3.548
3.537
3.532
3.526
3.521
3.510
2.667
2.661
2.640
2.633
2.563
2.553
2.535
2.525
2.225
2.213
2.211
2.199
1.547
1.542
1.535
1.530
1.522
1.517
1.511
1.504
1.346
1.333
1.321
1.309
0.898
0.886
0.875
0.863
Current Data Parameters
NAME SNK-5077
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150121
Time 14.42
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 297.6 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 598.6029930 MHz
F2 - Processing parameters
SI 32768
SF 598.6000309 MHz
WDW EM
SSB 0
LB 0.20 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 5.00 cm
F1P 2.733 ppm
F1 1636.12 Hz
F2P 0.634 ppm
F2 379.47 Hz
PPMCM 0.10497 ppm/cm
HZCM 62.83280 Hz/cm
nBu
O
OnBu
5c
O
5.321
5.314
5.311
5.304
5.3
ppm
2.00
1.18
1.10
1.18
1.11
2.15
4.14
4.04
6.15
10
9
8
7
6
5
4
3
2
1
ppm

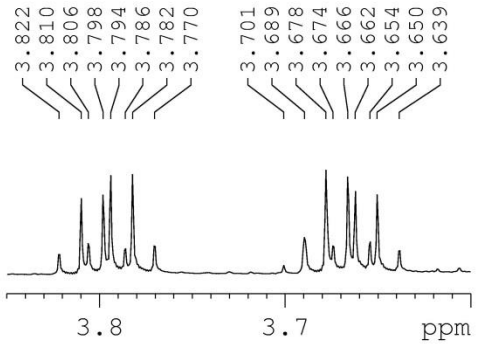

191.26
174.02
104.54
101.51
77.21
77.00
76.78
69.38
41.70
34.46
31.41
28.37
22.05
19.09
13.69
13.66
Current Data Parameters
NAME SNK-5077
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150121
Time 14.42
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 79
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 2048
DW 11.100 usec
DE 6.50 usec
TE 297.7 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 150.5180980 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
nBu
O
OnBu
5c
O
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

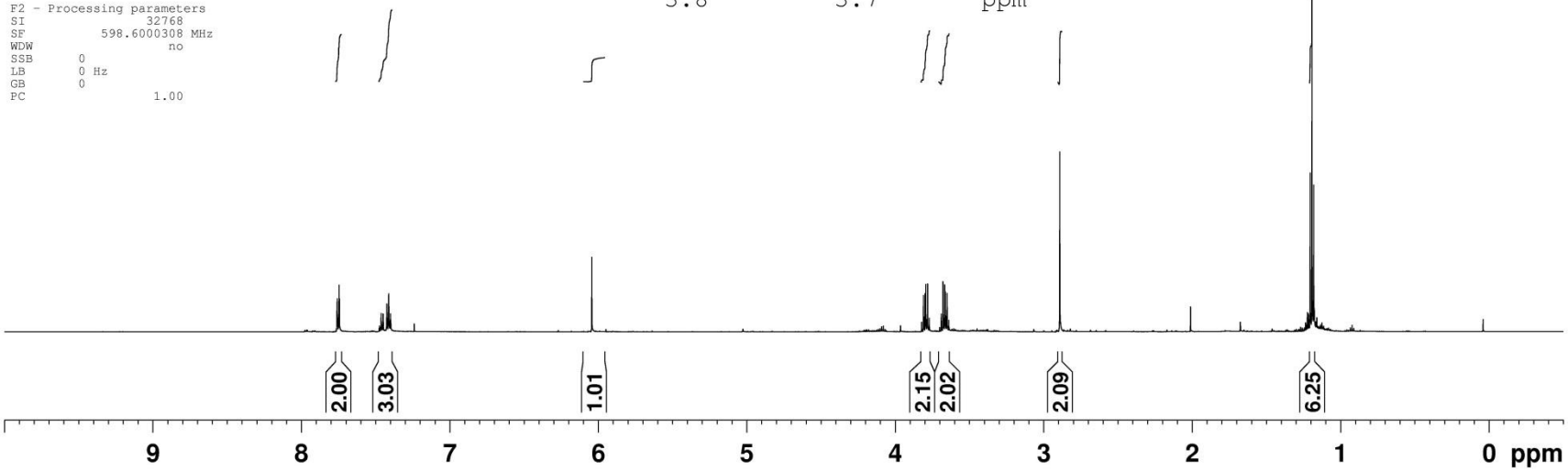

7.240
5.417
5.257
5.247
5.242
5.232
3.744
3.728
3.721
3.712
3.704
3.688
3.509
3.492
3.485
3.476
3.469
3.453
2.640
2.630
2.598
2.588
2.537
2.522
2.495
2.480
1.572
1.560
1.552
1.540
1.522
1.506
1.485
1.469
1.350
1.331
1.312
1.294
1.275
1.257
0.944
0.939
0.932
0.927
0.872
0.853
0.834
Current Data Parameters
NAME 2015-03-19
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150319
Time 16.29
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 20
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 57
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500172 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00
O
O^{n}Bu
5d
O
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.01
1.02
2.03
3.06
2.00
2.04
5.01

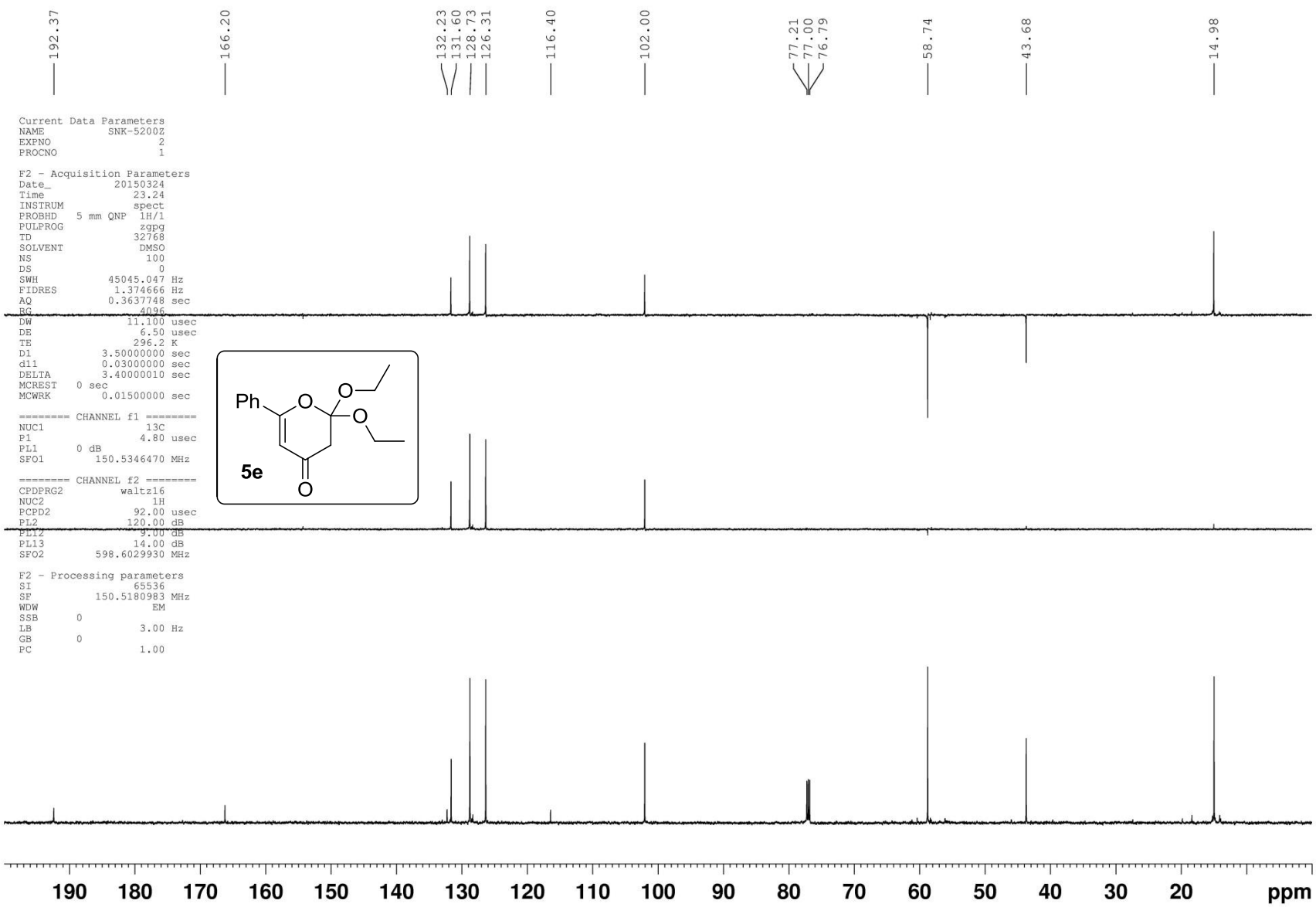

190.23
174.50
103.10
101.66
77.32
77.00
76.68
69.34
41.77
31.32
19.01
14.98
13.63
7.86
Current Data Parameters
NAME 2015-03-19
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150319
Time 16.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 85
DS 0
SWH 22727.273 Hz
FIDRES 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 100.6178080 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
O
O^{n}Bu
O
5d
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

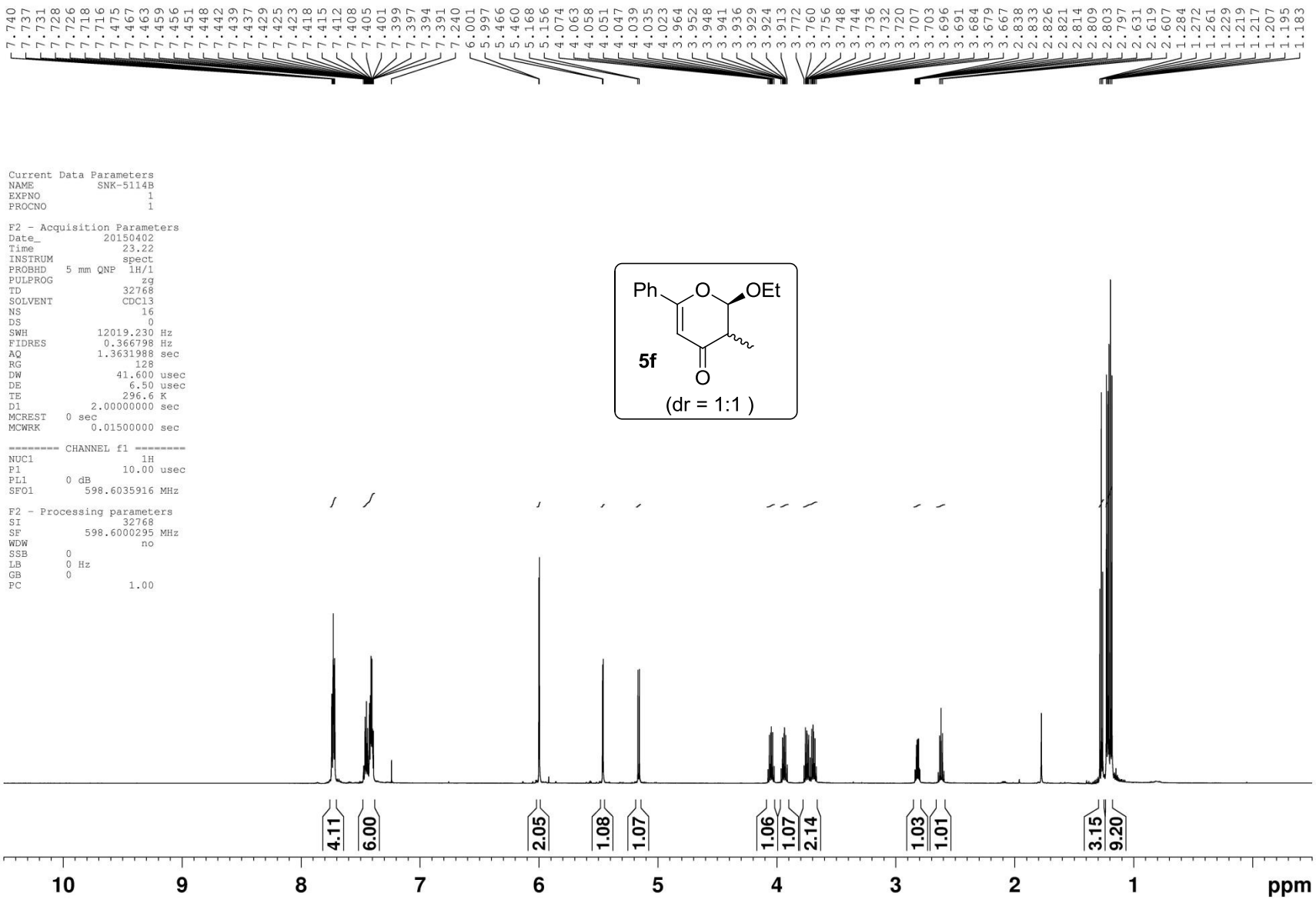

```
Current Data Parameters
NAME            SNK-5200Z
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150324
Time               23.17
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                294.6 K
D1             2.00000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1       0 dB
SFO1         598.6035916 MHz

F2 - Processing parameters
SI                32768
SF           598.6000308 MHz
WDW                  no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

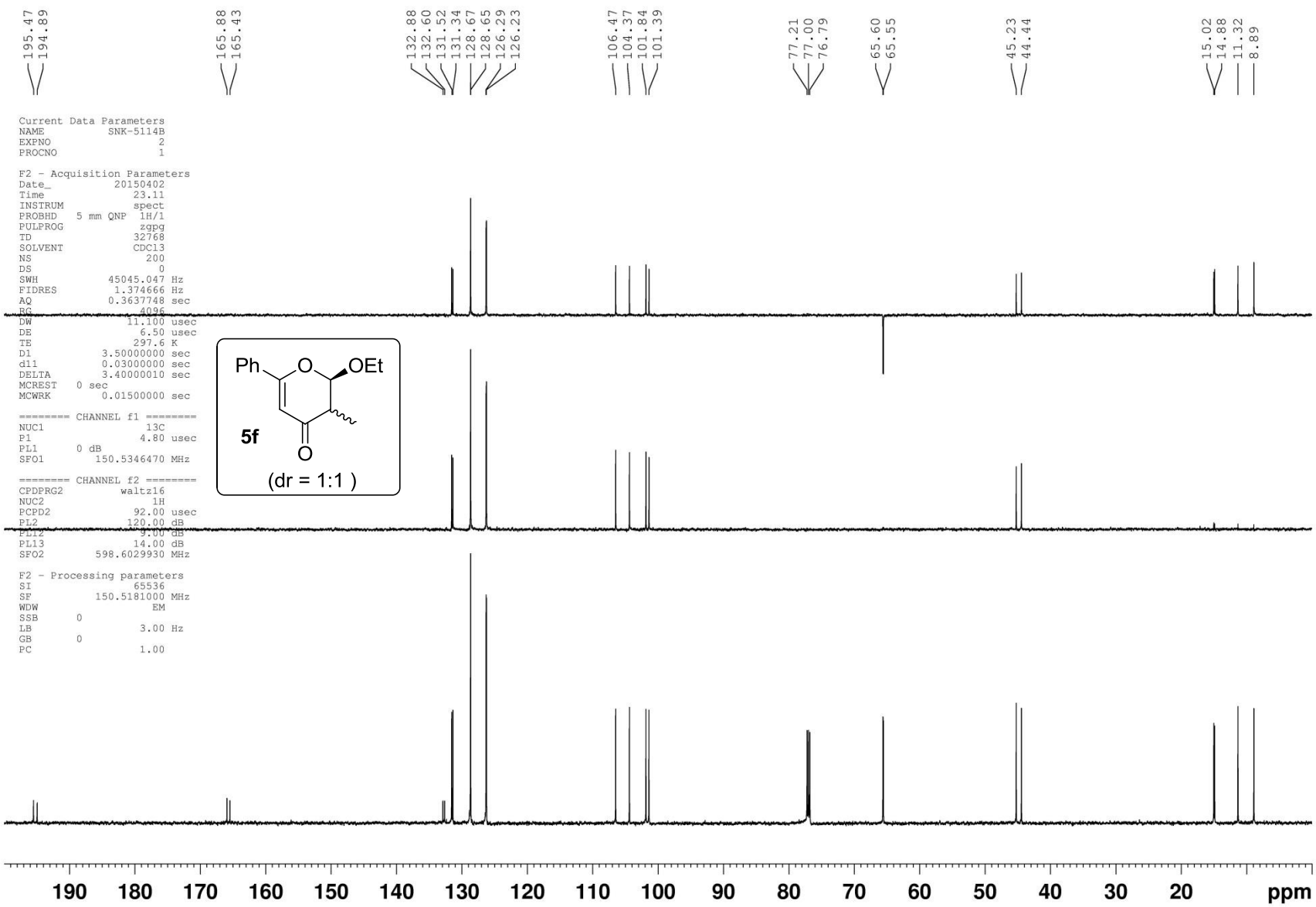


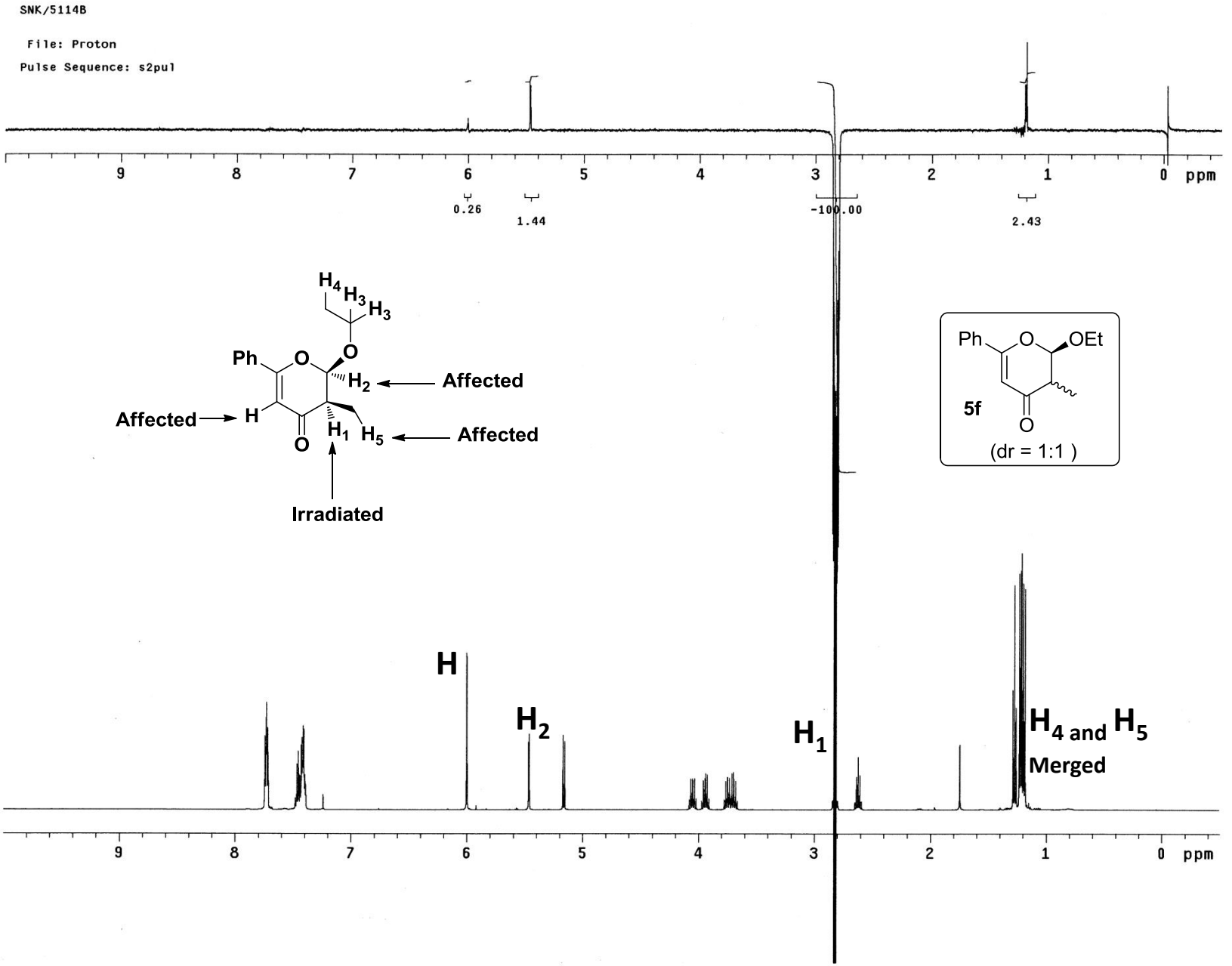


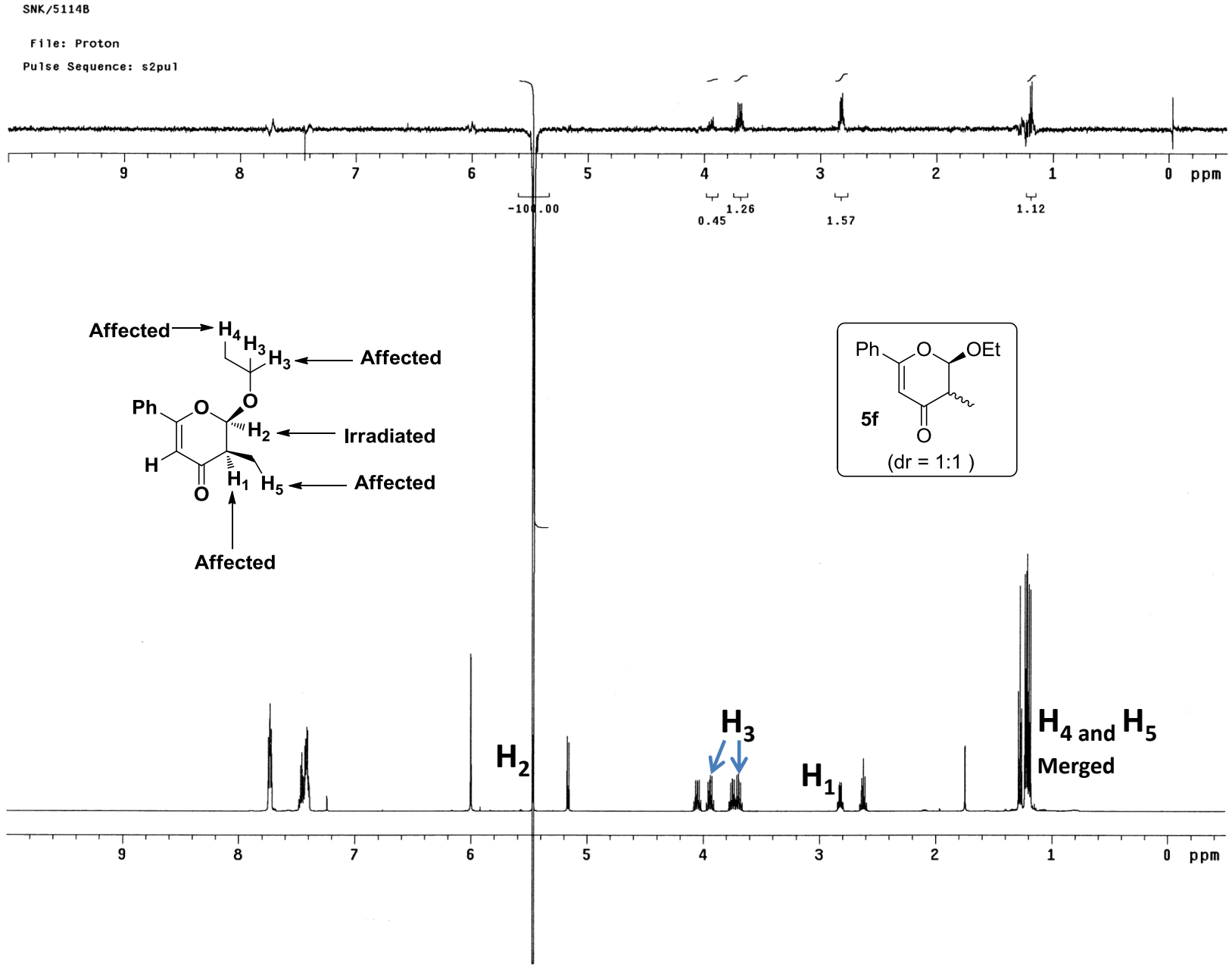


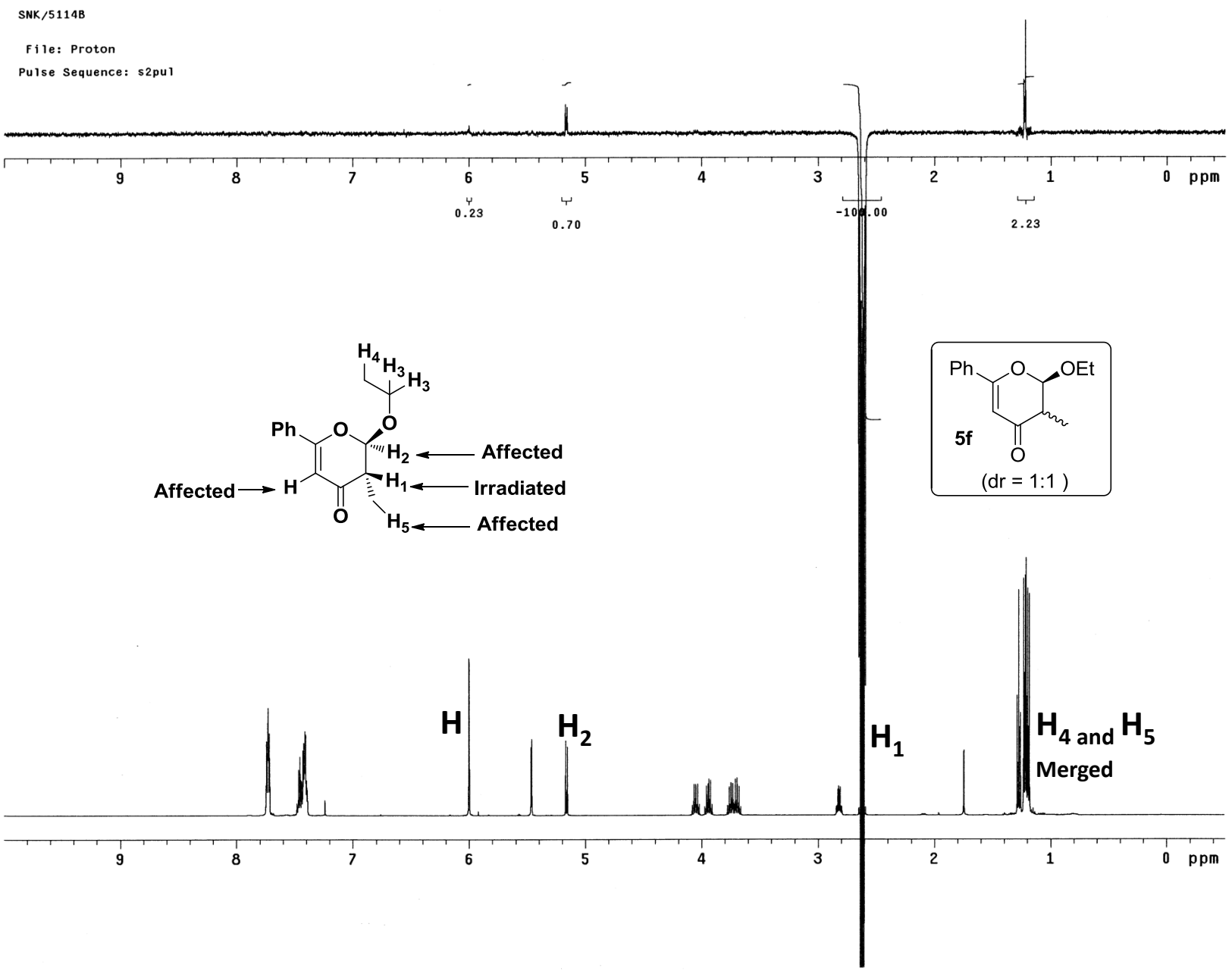

192.37
166.20
132.23
131.60
128.73
126.31
116.40
102.00
77.21
77.00
76.79
58.74
43.68
14.98
Current Data Parameters
NAME SNK-5200Z
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150324
Time 23.24
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180983 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
O
O
O
5e
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

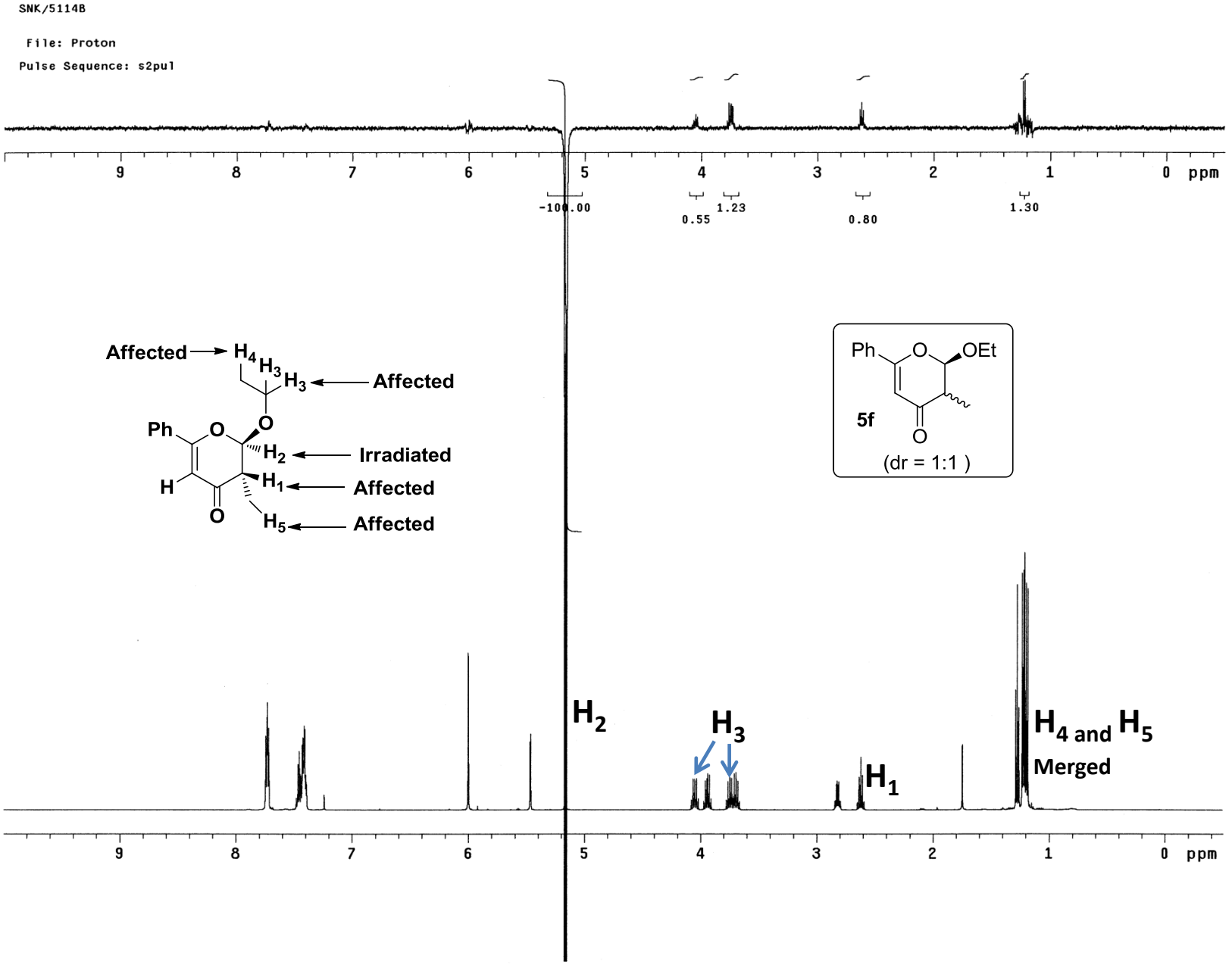

7.740 7.737 7.731 7.728 7.726 7.718 7.716 7.475 7.467 7.463 7.459 7.456 7.451 7.448 7.442 7.439 7.437 7.429 7.425 7.423 7.418 7.415 7.412 7.408 7.405 7.401 7.399 7.397 7.394 7.391 7.240 6.001 5.997 5.466 5.460 5.168 5.156 4.074 4.063 4.058 4.051 4.047 4.039 4.035 4.023 3.964 3.952 3.948 3.941 3.936 3.929 3.924 3.913 3.772 3.760 3.756 3.748 3.744 3.736 3.732 3.720 3.707 3.703 3.696 3.691 3.684 3.679 3.667 2.838 2.833 2.826 2.821 2.814 2.809 2.803 2.797 2.631 2.619 2.607 1.284 1.272 1.261 1.229 1.219 1.217 1.207 1.195 1.183
Current Data Parameters
NAME SNK-5114B
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150402
Time 23.22
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 296.6 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000295 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
OEt
5f
O
(dr = 1:1)
4.11
6.00
2.05
1.08
1.07
1.06
1.07
2.14
1.03
1.01
3.15
9.20
10
9
8
7
6
5
4
3
2
1
ppm

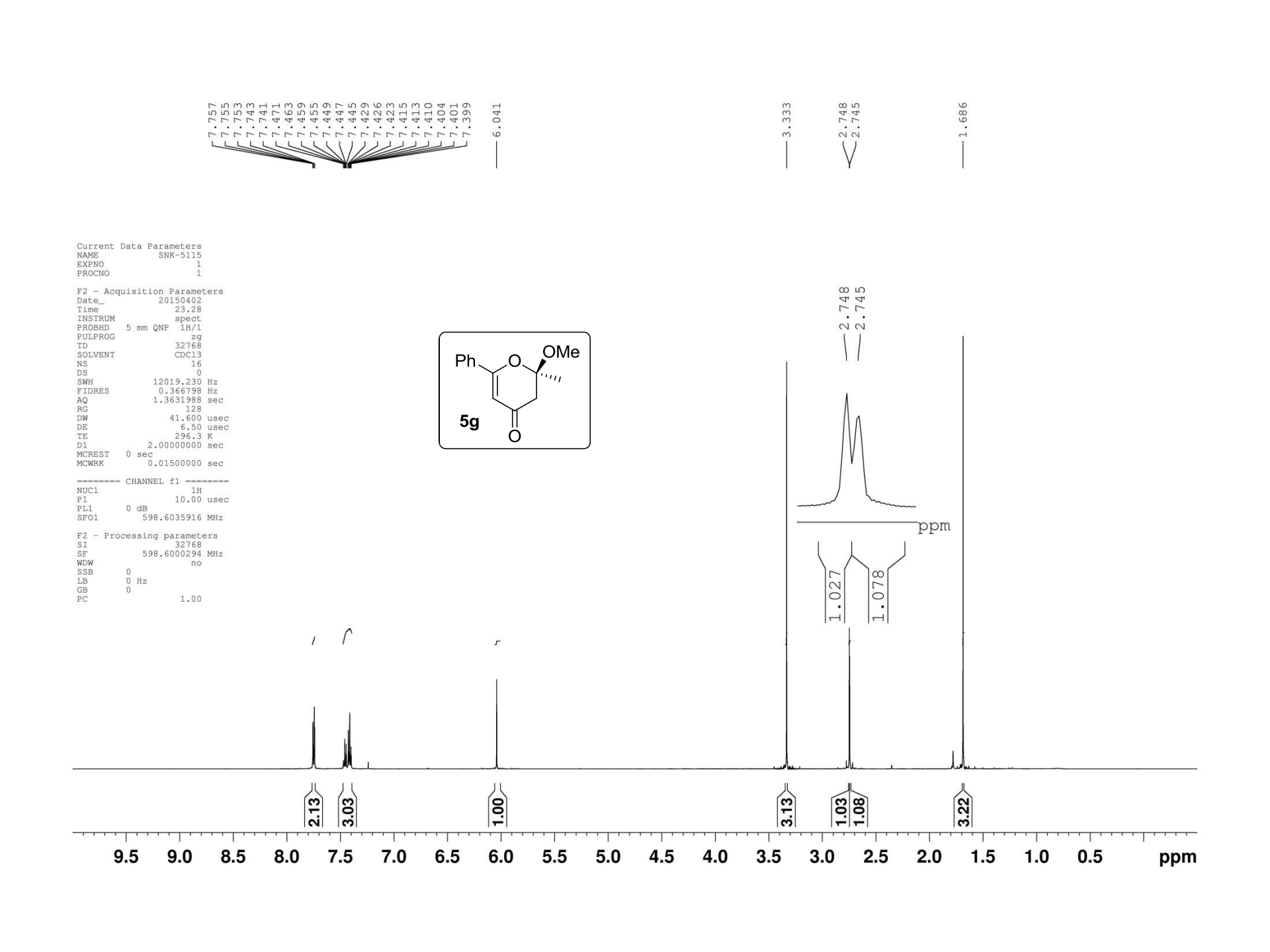

195.47
194.89
165.88
165.43
132.88
132.60
131.52
131.34
128.67
128.65
126.29
126.23
106.47
104.37
101.84
101.39
77.21
77.00
76.79
65.60
65.55
45.23
44.44
15.02
14.88
11.32
8.89
Current Data Parameters
NAME SNK-5114B
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150402
Time 23.11
INSTRUM spect
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 4096
DW 11.100 usec
DE 6.50 usec
TE 297.6 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
OEt
5f
O
(dr = 1:1)
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

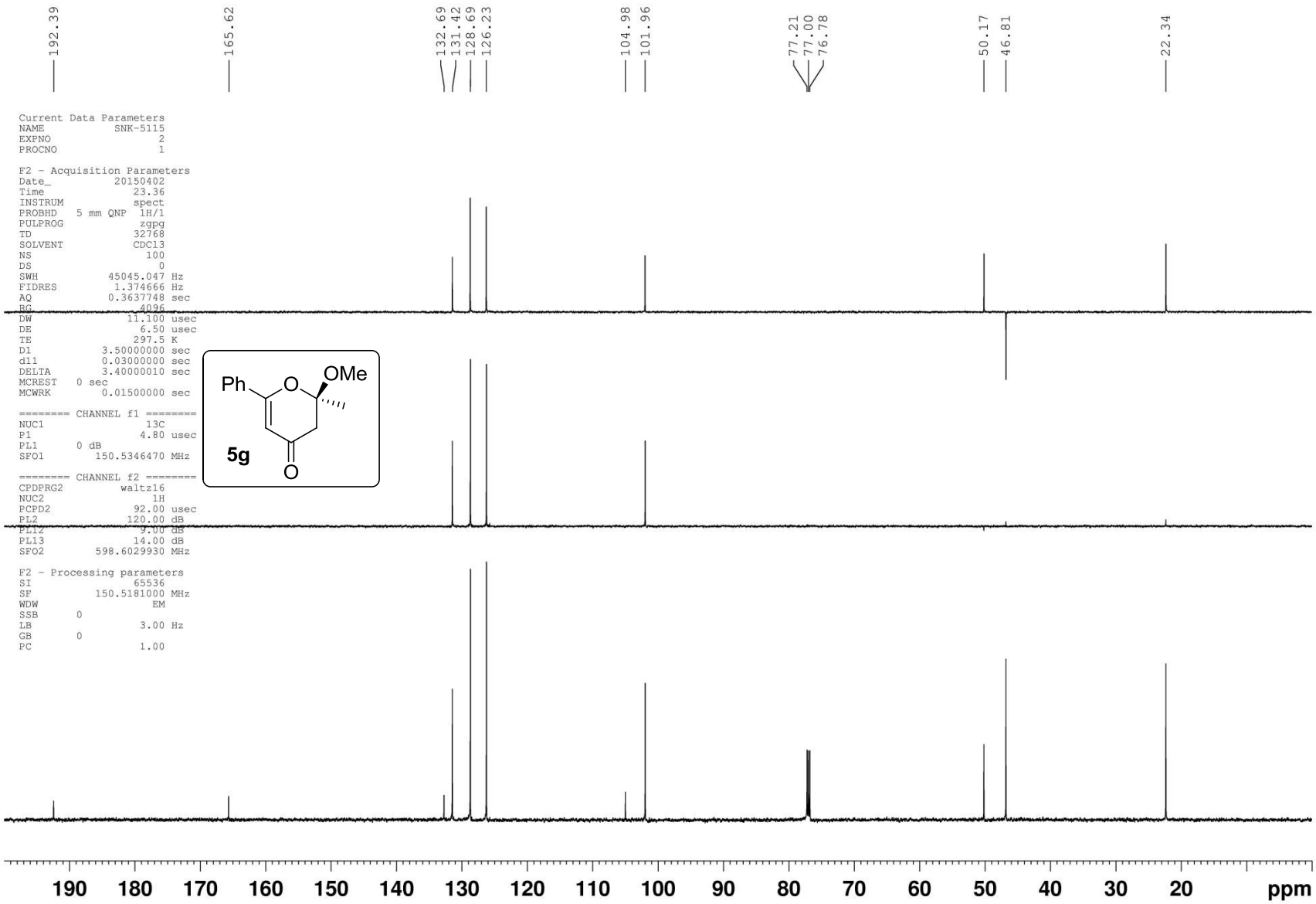

SNK/5114B
File: Proton
Pulse Sequence: s2pul
9 8 7 6 5 4 3 2 1 0 ppm
0.26
1.44
-100.00
2.43
H4 H3 H3
O
Ph
O
H2
Affected
Affected
H
H1 H5
Affected
O
Irradiated
Ph
O
OEt
5f
O
(dr = 1:1)
H
H2
H1
H4 and H5
Merged
9 8 7 6 5 4 3 2 1 0 ppm

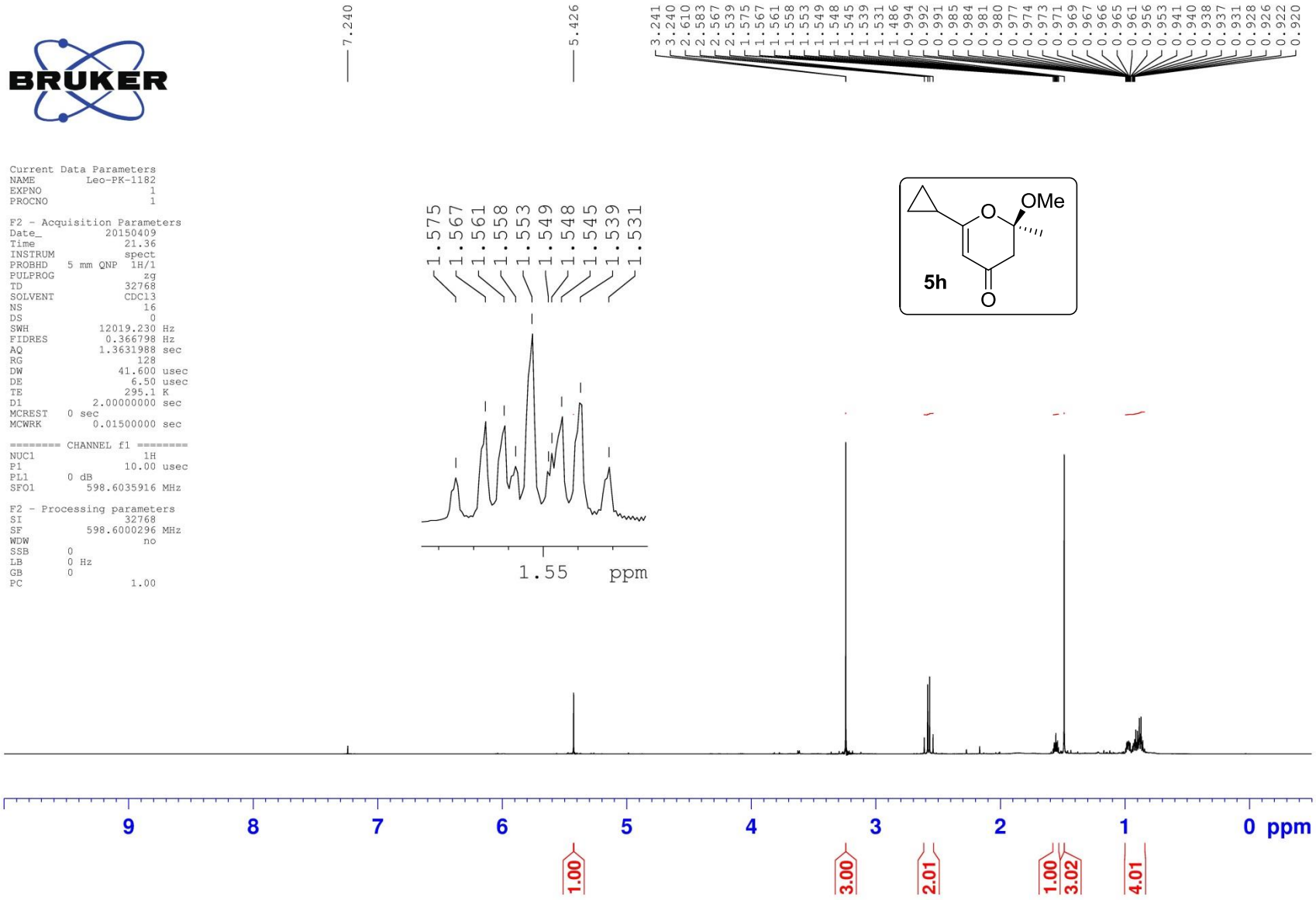

SNK/5114B
File: Proton
Pulse Sequence: s2pul
9 8 7 6 5 4 3 2 1 0 ppm
-100.00
0.45
1.26
1.57
1.12
Affected
H4
H3
H3
Affected
Ph
O
O
H2
Irradiated
H
O
H1
H5
Affected
Affected
Ph
O
OEt
5f
O
(dr = 1:1)
H2
H3
H1
H4 and H5
Merged
9 8 7 6 5 4 3 2 1 0 ppm

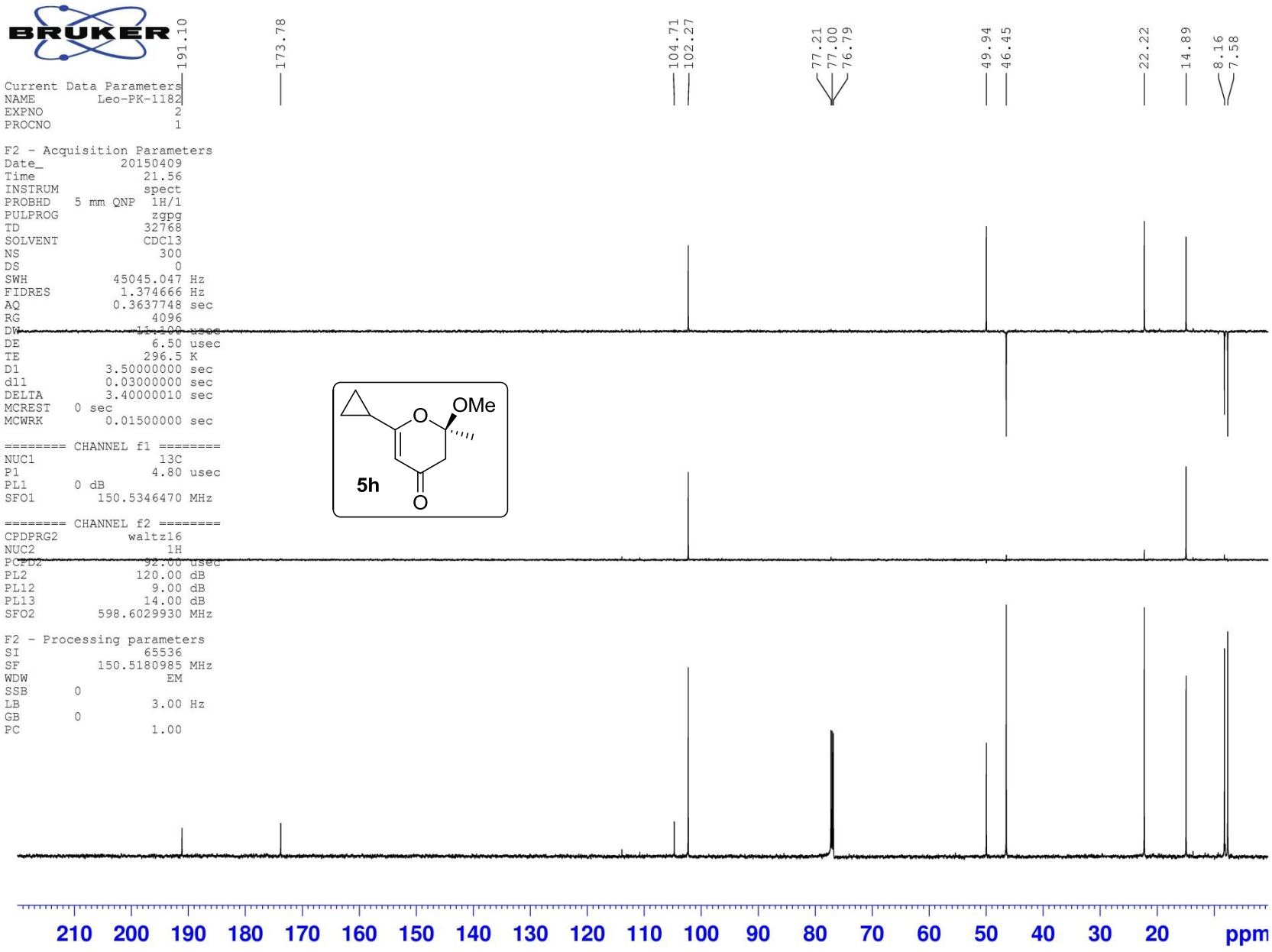

SNK/5114B
File: Proton
Pulse Sequence: s2pul
9 8 7 6 5 4 3 2 1 0 ppm
0.23
0.70
-100.00
2.23
Ph
O
OEt
5f
O
(dr = 1:1)
H4 H3 H3
O
Ph
O
H2
Affected
Affected
H
H1
Irradiated
O
H5
Affected
H
H2
H1
H4 and H5
Merged
9 8 7 6 5 4 3 2 1 0 ppm

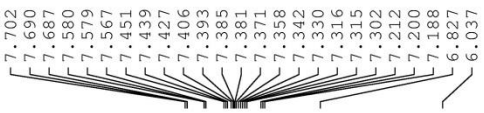

SNK/5114B
File: Proton
Pulse Sequence: s2pul
9 8 7 6 5 4 3 2 1 0 ppm
-100.00
0.55
1.23
0.80
1.30
Affected
H4
H3
H3
Affected
Ph
O
O
H2
Irradiated
H
H1
Affected
O
H5
Affected
Ph
O
OEt
5f
O
(dr = 1:1)
H2
H3
H1
H4 and H5
Merged
9 8 7 6 5 4 3 2 1 0 ppm


7.757
7.755
7.753
7.743
7.741
7.471
7.463
7.459
7.455
7.449
7.447
7.445
7.429
7.426
7.423
7.415
7.413
7.410
7.404
7.401
7.399
6.041
3.333
2.748
2.745
1.686
Current Data Parameters
NAME SNK-5115
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150402
Time 23.28
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 296.3 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000294 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
Ph
O
OMe
O
5g
2.748
2.745
ppm
1.027
1.078
2.13
3.03
1.00
3.13
1.03
1.08
3.22
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm

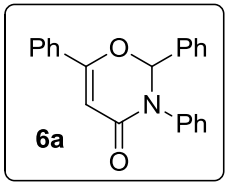

192.39
165.62
132.69
131.42
128.69
126.23
104.98
101.96
77.21
77.00
76.78
50.17
46.81
22.34
Current Data Parameters
NAME SNK-5115
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150402
Time 23.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 100
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 297.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181000 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
OMe
O
5g
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm


7.240
5.426
3.241
3.240
2.610
2.583
2.567
2.539
1.575
1.567
1.561
1.558
1.553
1.549
1.548
1.545
1.539
1.531
1.486
0.994
0.992
0.991
0.985
0.984
0.981
0.980
0.977
0.974
0.973
0.971
0.969
0.967
0.966
0.965
0.961
0.956
0.953
0.941
0.940
0.938
0.937
0.931
0.928
0.926
0.922
0.920
Current Data Parameters
NAME Leo-PK-1182
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150409
Time 21.36
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zg
TD 32768
SOLVENT CDC13
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 295.1 K
D1 2.00000000 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 0 dB
SFO1 598.6035916 MHz
F2 - Processing parameters
SI 32768
SF 598.6000296 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00
1.575
1.567
1.561
1.558
1.553
1.549
1.548
1.545
1.539
1.531
1.55 ppm
OMe
O
5h
O
9
8
7
6
5
4
3
2
1
0 ppm
1.00
3.00
2.01
1.00
3.02
4.01

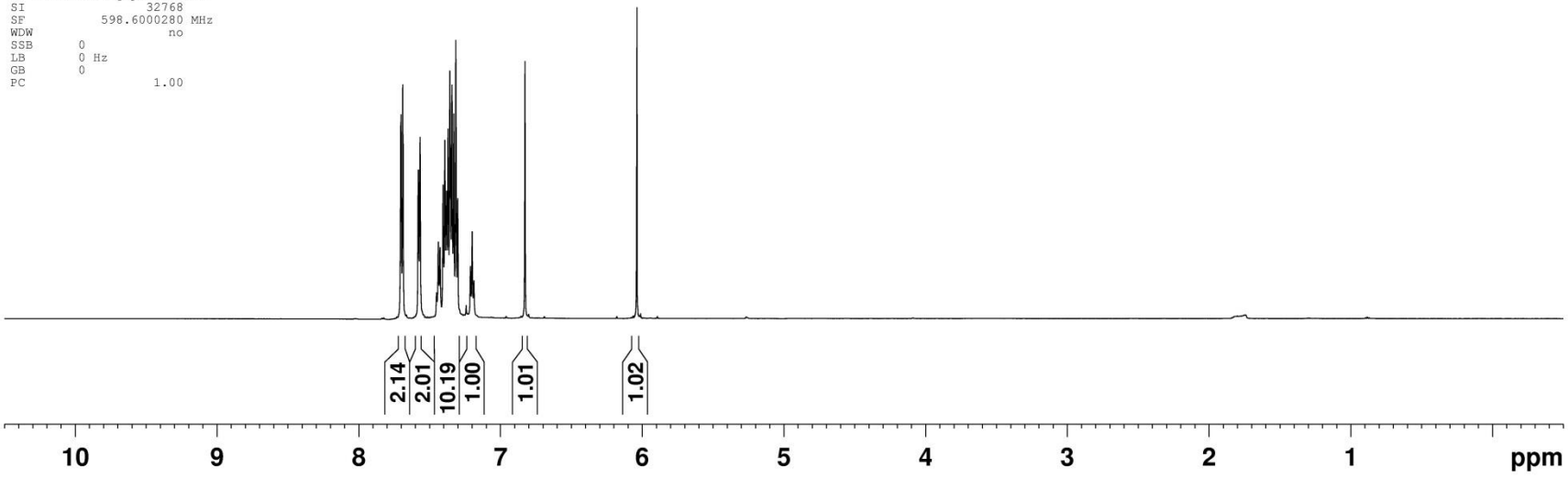

191.10
173.78
104.71
102.27
77.21
77.00
76.79
49.94
46.45
22.22
14.89
8.16
7.58
Current Data Parameters
NAME Leo-PK-1182
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150409
Time 21.56
INSTRUM spect
PROBHD 5 mm QNP 1H/1
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 300
DS 0
SWH 45045.047 Hz
FIDRES 1.374666 Hz
AQ 0.3637748 sec
RG 4096
DW 11.100 usec
DE 6.50 usec
TE 296.5 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5180985 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
O
O
5h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

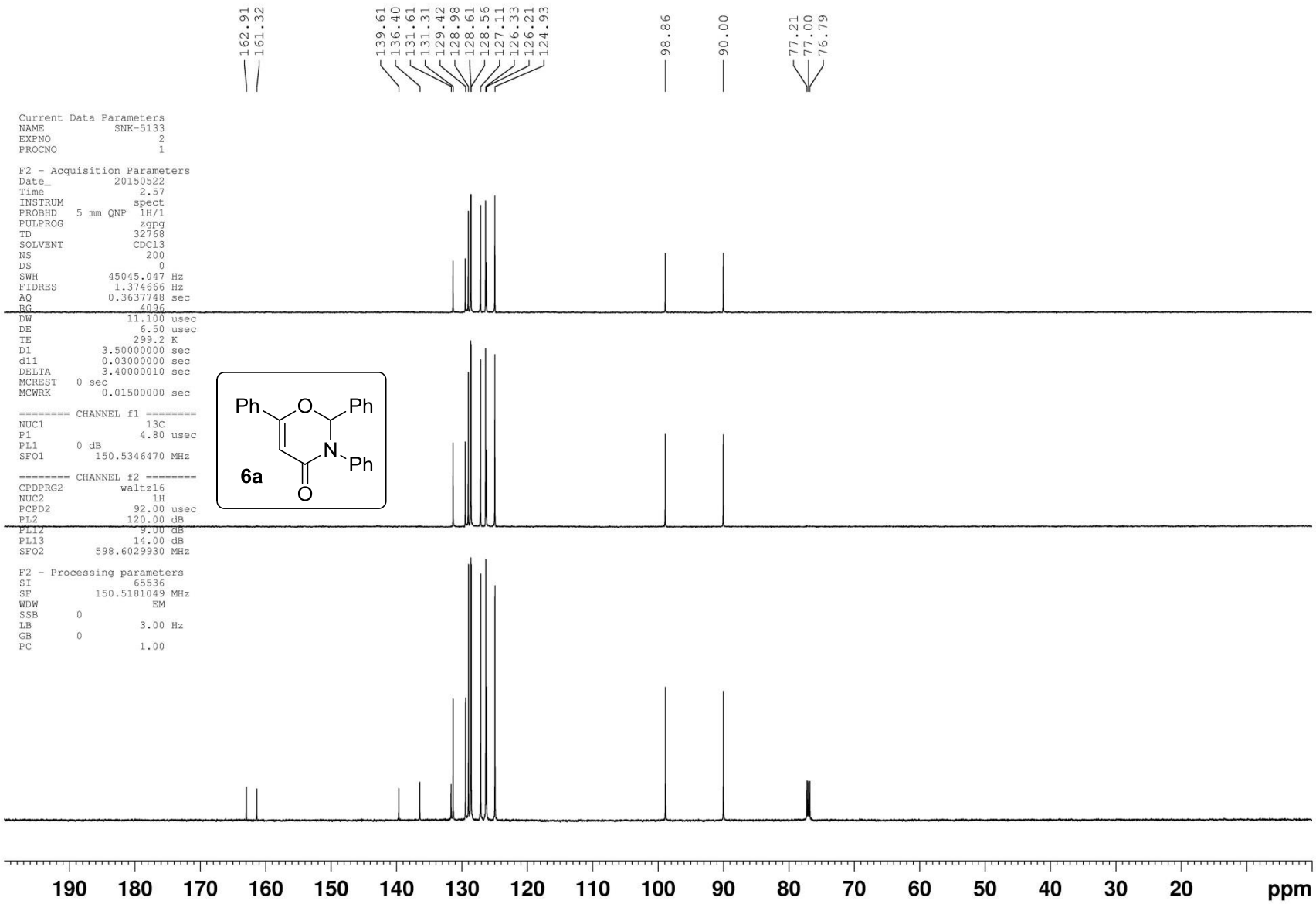


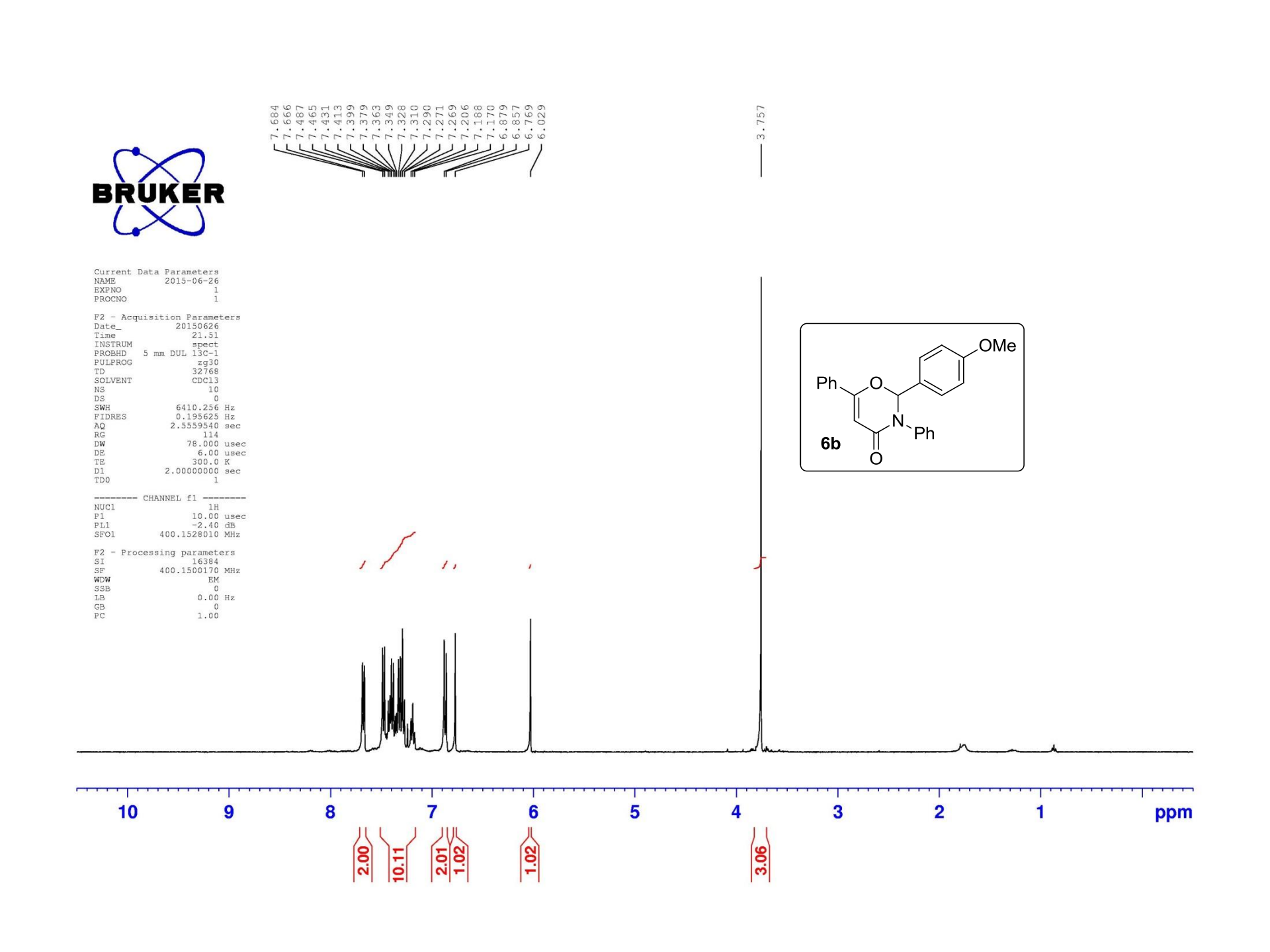

```
Current Data Parameters
NAME             SNK-5133
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20150522
Time                3.51
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                   128
DW                41.600 usec
DE                 6.50 usec
TE                297.7 K
D1             1.50000000 sec
MCREST    0 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1       0 dB
SFO1         598.6029930 MHz

F2 - Processing parameters
SI                 32768
SF           598.6000280 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

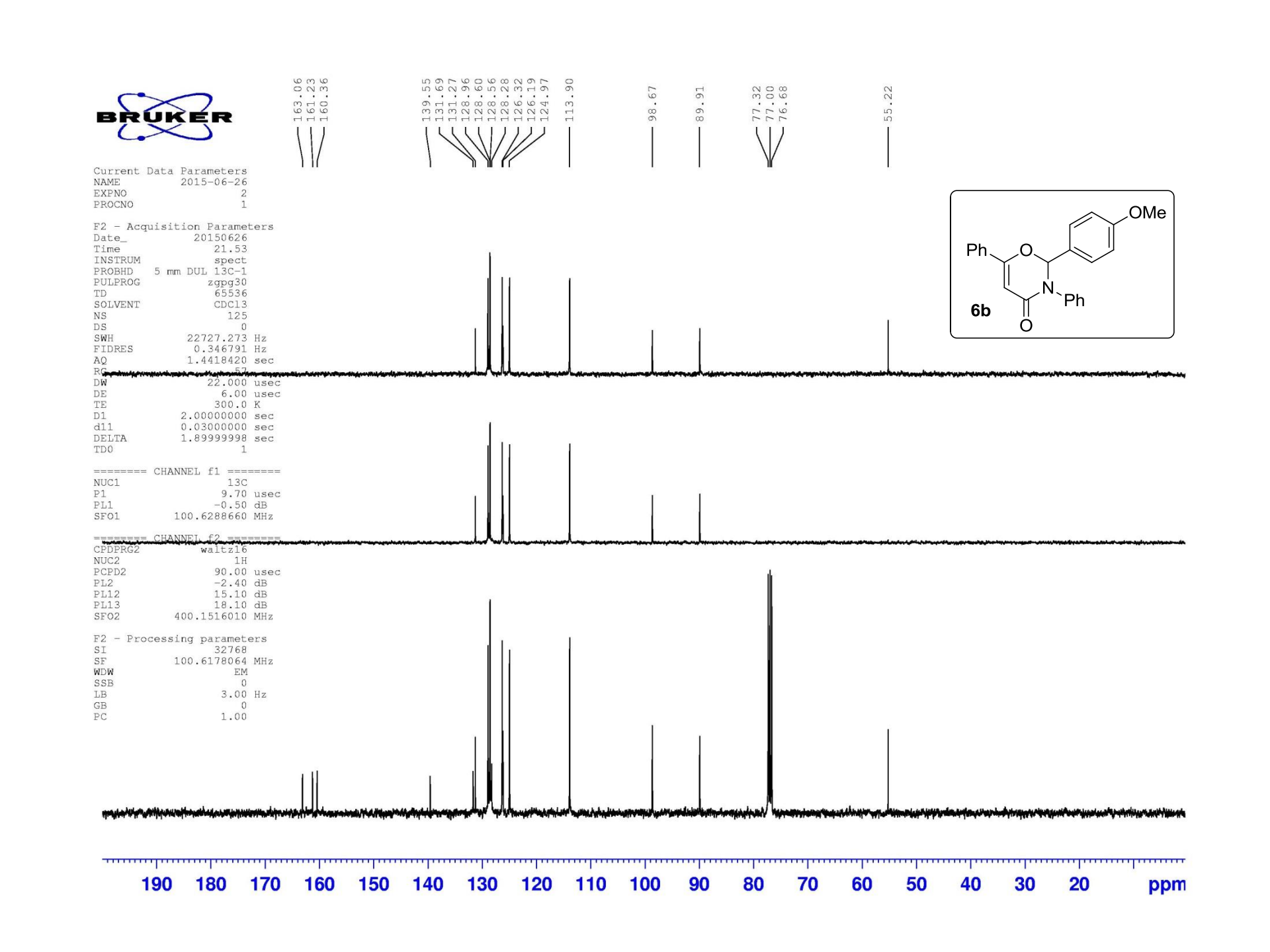


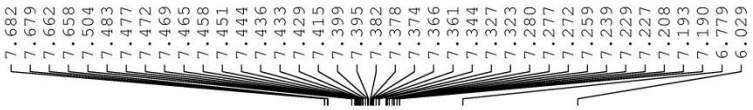
6a




162.91
161.32
139.61
136.40
131.61
131.31
129.42
128.98
128.61
128.56
127.11
126.33
126.21
124.93
98.86
90.00
77.21
77.00
76.79
Current Data Parameters
NAME SNK-5133
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150522
Time 2.57
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 4096
DW 11.100 usec
DE 6.50 usec
TE 299.2 K
D1 3.50000000 sec
d11 0.03000000 sec
DELTA 3.40000010 sec
MCREST 0 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.80 usec
PL1 0 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 150.5181049 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
Ph
N
Ph
O
6a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

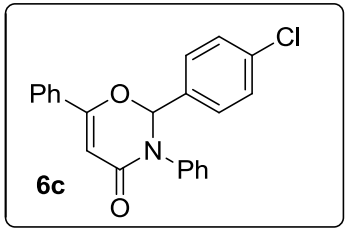

7.684
7.666
7.487
7.465
7.431
7.413
7.399
7.379
7.363
7.349
7.328
7.310
7.290
7.271
7.269
7.206
7.188
7.170
6.879
6.857
6.769
6.029
3.757
BRUKER
Current Data Parameters
NAME 2015-06-26
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150626
Time 21.51
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 10
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 114
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
F2 - Processing parameters
SI 16384
SF 400.1500170 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
OMe
Ph
O
N
Ph
6b
O
10
9
8
7
6
5
4
3
2
1
ppm
2.00
10.11
2.01
1.02
1.02
3.06


BRUKER
163.06
161.23
160.36
139.55
131.69
131.27
128.96
128.60
128.56
128.28
126.32
126.19
124.97
113.90
98.67
89.91
77.32
77.00
76.68
55.22
Current Data Parameters
NAME 2015-06-26
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150626
Time 21.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 125
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
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 100.6178064 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
OMe
Ph
O
N
Ph
6b
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

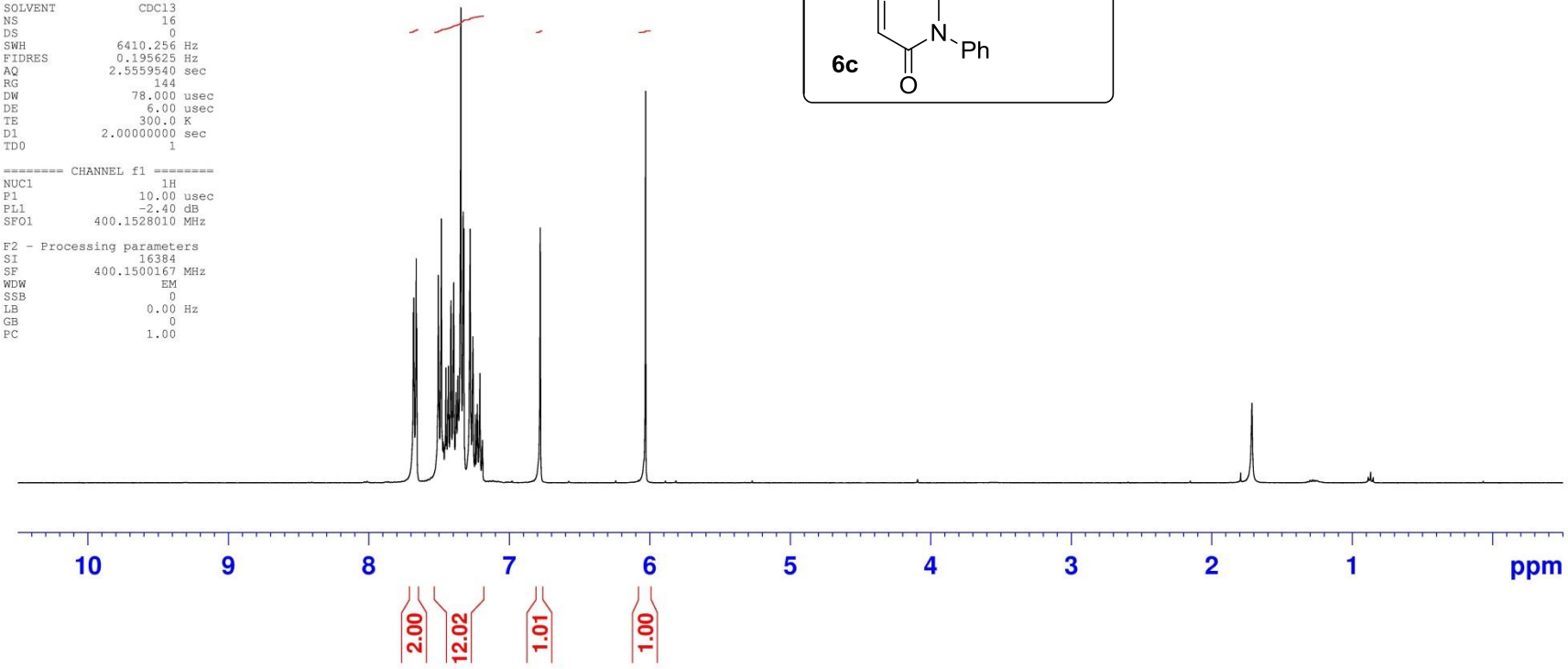


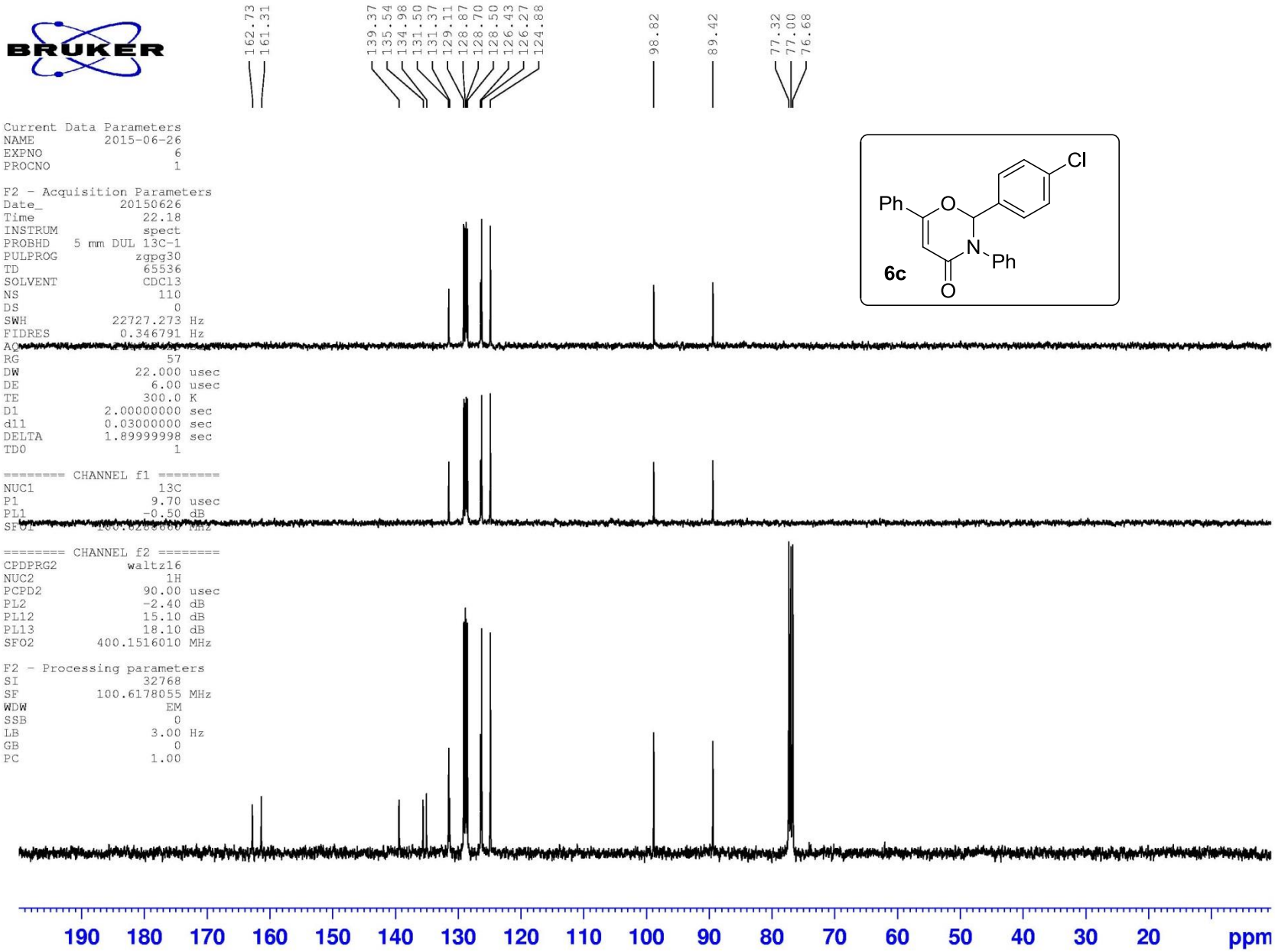
BRUKER

```
Current Data Parameters
NAME          2015-06-26
EXPNO                  5
PROCNO                 1

F2 - Acquisition Parameters
Date_          20150626
Time              22.16
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            6410.256 Hz
FIDRES            0.195625 Hz
AQ             2.5559540 sec
RG                  144
DW                78.000 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1        400.1528010 MHz

F2 - Processing parameters
SI                 16384
SF          400.1500167 MHz
WDW                   EM
SSB                   0
LB                 0.00 Hz
GB                    0
PC                 1.00
```



6c




162.73
161.31
139.37
135.54
134.98
131.50
131.37
129.11
128.87
128.70
128.50
126.43
126.27
124.88
98.82
89.42
77.32
77.00
76.68
Current Data Parameters
NAME 2015-06-26
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150626
Time 22.18
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 110
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
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
======== 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 100.6178055 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
Ph
O
Cl
N
Ph
O
6c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm