

## Supporting Information

### **Gold-catalyzed [4+3] and [4+4]-Annulation Reactions of Propiolate Derivatives with Epoxides and Oxetanes to Construct 1,4-Dioxepane and 1,5-Dioxocane Cores**

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#### **Contents:**

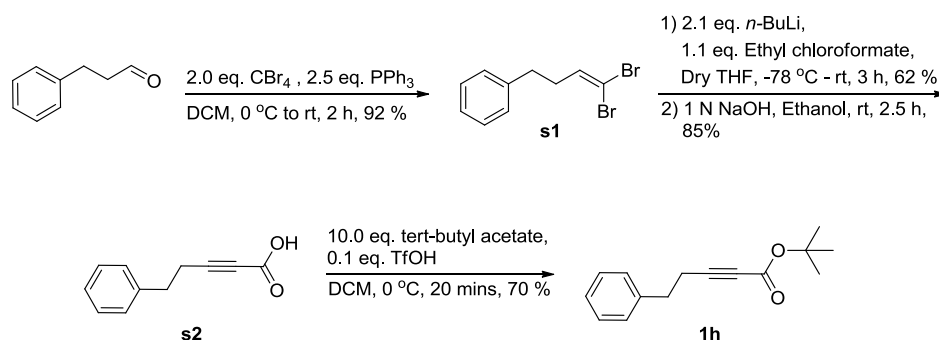
(1) Representative synthetic procedures -----	2
(2) References-----	5
(3) Spectral data for key compounds ( <b>1c</b> , <b>1h</b> , <b>1a'</b> , <b>2c-2d</b> , <b>3a-3p</b> , <b>5a-5m</b> and <b>7</b> ) -----	6
(4) X-ray crystallographic structure and data for compound <b>3d</b> and <b>3o</b> -----	20
(5) <sup>1</sup> H and <sup>13</sup> C spectra of key compounds ( <b>1c</b> , <b>1h</b> , <b>1a'</b> , <b>2c-cd</b> , <b>3a-3p</b> , <b>5a-5m</b> and <b>7</b> )-----	38

## (1) Representative synthetic procedures:

### (a) General procedure:

Unless otherwise noted, all reactions were carried out under nitrogen atmosphere in oven-dried glassware using standard syringe, cannula and septa apparatus. Tetrahydrofuran and hexane were dried with sodium, benzophenone and distilled before use. Dichloromethane and DCE were dried over  $\text{CaH}_2$  and distilled. Methanol and triethylamine ( $\text{Et}_3\text{N}$ ) were stored over  $4\text{\AA}$  molecular sieves prior to use. Reagents were purchased from commercial sources and used without purification, unless otherwise stated.  $^1\text{H}$  NMR and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker 400, Varian 500 MHz and a Bruker 600 MHz spectrometers using chloroform-d ( $\text{CDCl}_3$ ) as the internal standard. Compounds **2a** (Aldrich), **2b** (Alfa Aesar), **2e** (Alfa Aesar) were bought commercially and used as it is. Digold complex  $[(\text{IPrAu})_2\text{OH}]\text{SbF}_6$  is prepared according known literature procedure.<sup>[S8]</sup>

### (b) Preparation of tert-butyl 5-phenylpent-2-ynoate (**1h**).<sup>[S1] [S2]</sup>



To a dichloromethane ( $\text{DCM}$ , 150 mL) solution of carbon tetrabromide (14.83 g, 44.71 mmol) was added a  $\text{DCM}$  solution (10 mL) of triphenylphosphine (14.66 g, 55.89 mmol) at  $0\text{ }^\circ\text{C}$  over 10 min; the cooling was then removed before the mixture was stirred at room temperature for 30 min before a  $\text{DCM}$  solution (10 mL) of 3-phenylpropanal (3.00 g, 22.35 mmol) was slowly added. The resulting mixture was stirred for 2 h at room temperature before treatment with  $\text{H}_2\text{O}$  (100 mL) to partition the organic layer. The resulting mixture was extracted with  $\text{DCM}$  (3 x 20 mL); the combined organic layer was washed with brine, dried over  $\text{MgSO}_4$ , and concentrated under reduced pressure. To this residue was added 100 mL of diethyl ether, and the resulting suspension is filtered to remove triphenylphosphine oxide. The ethereal filtrate is concentrated in vacuo, and chromatographed through a silica gel column (ether/hexane = 1:10) to afford (4,4-dibromobut-3-en-1-yl)benzene (5.96 g, 20.6 mmol, 92 %).

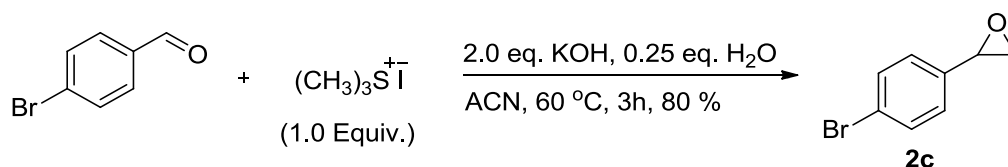
To a dry THF solution (100 mL) of (4,4-dibromobut-3-en-1-yl)benzene (5.00 g, 17.24 mmol) was added *n*-BuLi (14.50 mL, 2.5 M in hexane, 36.21 mmol) slowly at  $-78\text{ }^\circ\text{C}$ ; the resulting solution was stirred for 30 min before a dry THF solution (10 mL) of ethyl chloroformate (2.06 g, 18.97 mmol) was added at  $-78\text{ }^\circ\text{C}$ . The resulting mixture was stirred at  $-78\text{ }^\circ\text{C}$  for 30 min, and warmed to room temperature before stirring for 2 h. To this solution was added a saturated aqueous

NH<sub>4</sub>Cl (100 mL), and the aqueous layer was separated and extracted with (3 x 20 mL) of ether. The organic layer is washed with brine (50 mL), dried over MgSO<sub>4</sub>, and concentrated under reduced pressure. The residue was eluted through a silica column (EA/Hexane = 1:20) to afford ethyl 5-phenylpent-2-ynoate (2.18 g, 10.8 mmol, 62 %) as colorless liquid.

To an ethanol solution (20 mL) of ethyl 5-phenylpent-2-ynoate (2.0 g, 9.89 mmol) was added slowly an aqueous NaOH solution (50 mL, 1 N). The mixture was stirred for 2.5 h before treatment with water (100 mL); the organic layer was extracted with DCM. The aqueous phase was acidified with 20% HCl solution until pH = 3.0 and the organic layer was extracted with dichloromethane. The combined extracts were dried over MgSO<sub>4</sub>, and concentrated under reduced pressure to give 5-phenylpent-2-ynoic acid (1.46 g, 8.4 mmol, 85 %).

To a DCM solution (75 mL) of 5-phenylpent-2-ynoic acid (1.46 g, 8.38 mmol) at 0 °C was added *tert*-butyl acetate (11.3 mL, 83.81 mmol) and TfOH (0.070 mL, 0.84 mmol) dropwise. The resulting solution was stirred for 20 min and carefully washed with a saturated NaHCO<sub>3</sub> solution. The aqueous layer was extracted with DCM (3x100 mL) and the combined extracts were washed with a saturated NaCl solution, dried over MgSO<sub>4</sub>, filtered, and concentrated under reduced pressure to give crude product. The purification was conducted by a silica column using (EA/hexane = 1:20) as a mobile phase to give *tert*-butyl 5-phenylpent-2-ynoate (**1h**) (1.35 g, 5.7 mmol, 70 %) as colorless oil.

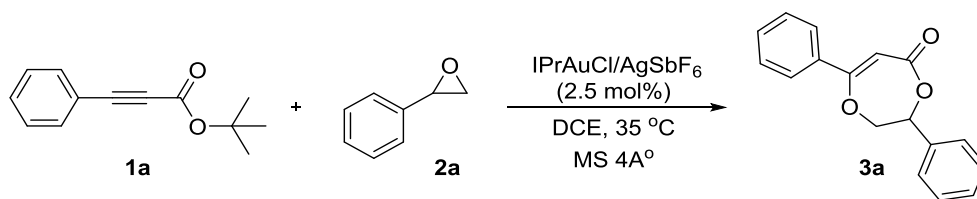
**(c) Preparation of 2-(4-bromophenyl)oxirane (2c).**<sup>[S4]</sup>



To an acetonitrile solution (50 mL) of 4-bromobenzaldehyde (2.0 g, 10.80 mmol) was added potassium hydroxide (1.21 g, 21.62 mmol) and water (0.05 mL, 2.7 mmol). To this solution was added trimethylsulfonium iodide (2.21 g, 10.80 mmol); the mixture was heated to reflux at 60 °C for 3 h. The reaction mixture was treated with water (100 mL), and extracted with diethyl ether. The extracts were washed with water, dried over MgSO<sub>4</sub>, and concentrated to give crude product. The purification was conducted on a silica column with (EA/hexane = 1: 10) to give 2-(4-bromophenyl)oxirane (**2c**) (1.72 g, 8.6 mmol, 80 %) as a colorless oil.

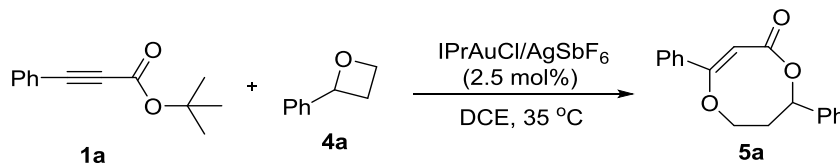
**(d) Typical procedure for standard catalytic operations:**

**(i) Typical procedure for the synthesis of 3,7-diphenyl-2*H*-1,4-dioxepin-5(3*H*)-one (3a).**



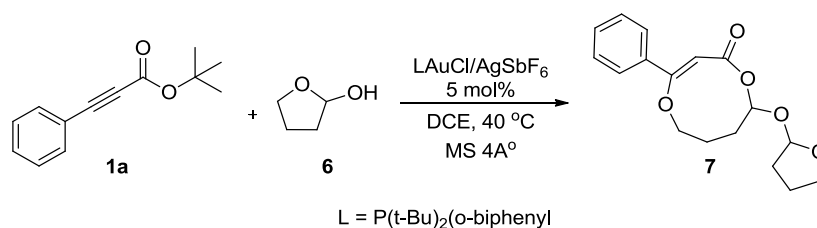
A two-neck flask was charged with IPrAuCl (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene, 7.68 mg, 0.0124 mmol), silver hexafluoride (4.24 mg, 0.0124 mmol) and MS 4A; to this mixture was added dry DCE (1.0 mL). The resulting solution was stirred at room temperature for 10 min before it was added a dry DCE solution (2 mL) of tert-butyl 3-phenylpropiolate (**1a**) (100 mg, 0.495 mmol) and freshly prepared 2-phenyloxirane (**2a**) (178 mg, 1.48 mmol) slowly. After stirring at 35 °C for 6 h, the resulting solution was filtered over a short celite bed, concentrated, and eluted through a silica column (EA/hexane = 1 : 10) to give the desired 3,7-diphenyl-2*H*-1,4-dioxepin-5(3*H*)-one (**3a**) (95 mg, 0.356 mmol, 72 %) as colorless liquid.

**(ii) Typical procedure for the synthesis of (Z)-4,8-diphenyl-7,8-dihydro-1,5-dioxocin-2(6*H*)-one (**5a**).**



A two-neck flask was charged with IPrAuCl (7.68 mg, 0.0124 mmol) and silver hexafluoride (4.24 mg, 0.0124 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 freshly prepared 2-phenyloxetane (**4a**) (199 mg, 1.48 mmol) dropwise. After stirring at 35 °C for 6 h, the reaction mixture was filtered over a short celite bed, concentrated, and eluted through a silica column (EA/hexane = 1.5 : 10) to give the desired (Z)-4,8-diphenyl-7,8-dihydro-1,5-dioxocin-2(6*H*)-one (**5a**) (93 mg, 0.331 mmol, 67 %) as white solid.

**(iii) Typical Procedure for the synthesis of (Z)-4-phenyl-9-((tetrahydrofuran-2-yl)oxy)-6,7,8,9-tetrahydro-2*H*-1,5-dioxonin-2-one (**7**).**



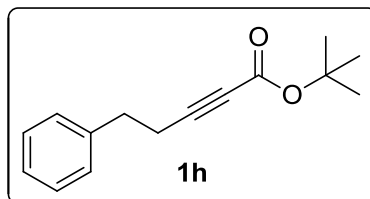
A two-neck flask was charged with P(t-Bu)<sub>2</sub>(o-biphenyl)AuCl (13.1 mg, 0.0248 mmol) and silver hexafluoride (8.5 mg, 0.0247 mmol), and to this mixture was added dry DCE (1.0 mL). The resulting mixture was stirred at room temperature for 10 min. To this mixture was added a dry DCE solution (2 mL) of *tert*-butyl 3-phenylpropiolate (**1a**) (100 mg, 0.495 mmol) and freshly prepared tetrahydrofuran-2-ol (131 mg, 1.48 mmol) slowly. After stirring at 40 °C for 8 h, the reaction mixture was filtered over a short celite bed, concentrated, and eluted through a silica column (EA/hexane = 1.5 : 10) to give the desired (*Z*)-4-phenyl-9-((tetrahydrofuran-2-yl)oxy)-6,7,8,9-tetrahydro-2*H*-1,5-dioxonin-2-one (**7**) (113 mg, 0.372 mmol, 75 %) as colorless oil.

## (2) References:

- S1. a) R. B. Dateer, K. Pati, R.-S. Liu, *Chem. Comm.* 2012, **48**, 7200-7202; b) Ohashi, Masao et al, *European Journal of Medicinal Chemistry* 2015, **90**, 53-67; c) S. Vercruyssen, L. Cornelissen, F. Nahra, L. Collard and O. Riant, *Chem. Eur. J.*, 2014, **20**, 1834-1838.
- S2. Compound **1a-1b**, **1d-1g**, **1i-1j**: Somnath Narayan Karad, Wei-Kang Chung and Rai-Shung Liu\*, *Chem. Commun.*, 2015, **51**, 13004-13007.
- S3. Somnath Narayan Karad, Wei-Kang Chung and Rai-Shung Liu *Chem. Sci.*, 2015, **6**, 5964-5968.
- S4. E. Borredon, F. Clavellinas, M. Delmas, A. Gaset, J. V. Sinisterra *J. Org. Chem.*, 1990, **55**, 501-504.
- S5. Compound **6**: K. Kojima, M. Kimura, S. Uedab, Y. Tamarub *Tetrahedron* 2006, **62**, 7512-7520.
- S6. a) Compound **2f**: Fringuelli, F.; Germani, R.; Pizzo, F.; Savelli, G. *Tetrahedron Lett.*, 1989, **30**, 1427-1428. b) Compound racemic **2g**: i) Stradi, R.; Pocar, D.; Cassio, C. *J. Chem. Soc., Perkin Trans. 1*, 1974, 2671-2672. ii) Singaram, B.; Goralski, C.; Rangaishenvi, M.; Brown, H. *J. Am. Chem. Soc.*, 1989, **111**, 384-386. iii) Sello, G.; Orsini, F.; Bernasconi, S.; Gennaro, P. *Tetrahedron: asymmetry*, 2006, **17**, 372-376; c) Compound **2h** was prepared from commercially available trans-beta-methylstyrene (available from Aldrich) by using the procedure by Sello, G.; Orsini, F.; Bernasconi, S.; Gennaro, P. *Tetrahedron: asymmetry*, 2006, **17**, 372-376.
- S7. a) Compound **4a-4e**: F. Bertolini, S. Crotti, V. D. Bussolo, M. Pienschi, *J. Org. Chem.* 2008, **73**, 8998-9007; K. Okuma, Y. Tanaka, H. Ohta, *J. Org. Chem.* 1983, **48**, 5133-5134.
- S8. Ruben S. Ramon,<sup>[a]</sup> Sylvain Gaillard,<sup>[a]</sup> Albert Poater,<sup>[b, c]</sup> Luigi Cavallo,<sup>[b]</sup> Alexandra M. Z. Slawin,<sup>[a]</sup> and Steven P. Nolan\*<sup>[a]</sup> *Chem. Eur. J.* 2011, **17**, 1238 - 1246.

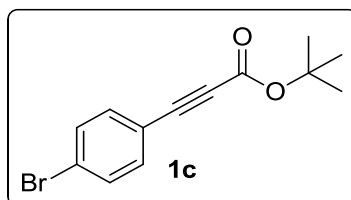
### (3) Spectral data:

#### Spectral data for *tert*-butyl 5-phenylpent-2-ynoate (**1h**).



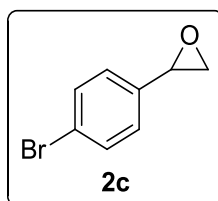
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.30 ~ 7.28 (m, 2H), 7.23 ~ 7.19 (m, 3H), 2.87 (t,  $J = 7.7$  Hz, 2H), 2.57 (t,  $J = 7.4$  Hz, 2H), 1.48 (s, 9H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  152.7, 139.7, 128.5, 128.3, 126.5, 85.8, 82.9, 74.9, 33.9, 27.9, 20.8; ESI-MS calcd for  $\text{C}_{15}\text{H}_{18}\text{O}_2$ : 230.1307; found 230.1309.

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



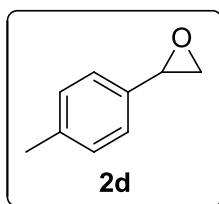
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.47 (d,  $J = 8.4$  Hz, 2H), 7.39 (d,  $J = 8.4$  Hz, 2H), 1.51 (s, 9H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  152.8, 134.1, 131.9, 124.9, 118.9, 83.7, 82.9, 82.5, 28.0; ESI-MS calcd for  $\text{C}_{13}\text{H}_{13}\text{BrO}_2$ : 280.0099; found 280.0098.

#### Spectral data for 2-(4-bromophenyl)oxirane (**2c**).



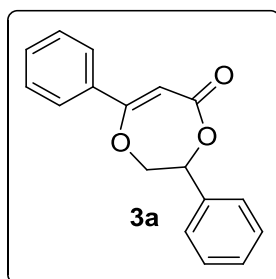
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.45 (d,  $J = 8.4$  Hz, 2H), 7.13 (d,  $J = 8.4$  Hz, 2H), 3.80 (dd,  $J = 4.2, 2.4$  Hz, 1H), 3.12 (dd,  $J = 5.4, 3.6$  Hz, 1H), 2.72 (dd,  $J = 5.4, 2.4$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  136.7, 131.6, 127.1, 121.9, 51.8, 51.2; ESI-MS calcd for  $\text{C}_8\text{H}_7\text{BrO}$ : 197.9680; found 197.9679.

#### Spectral data for 2-(*p*-tolyl)oxirane (**2d**).



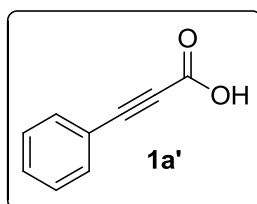
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ): 7.17 ~ 7.13 (m, 4H), 3.82 (dd,  $J = 4.0, 2.7$  Hz, 1H), 3.11 (dd,  $J = 5.5, 4.1$  Hz, 1H), 2.78 (dd,  $J = 5.5, 2.6$  Hz, 1H), 2.33 (s, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  137.9, 134.5, 129.2, 125.5, 52.3, 51.0, 21.1; ESI-MS calcd for  $\text{C}_9\text{H}_{10}\text{O}$ : 134.0732; found 134.0733.

**Spectral data for 3,7-diphenyl-2H-1,4-dioxepin-5(3H)-one (3a).**



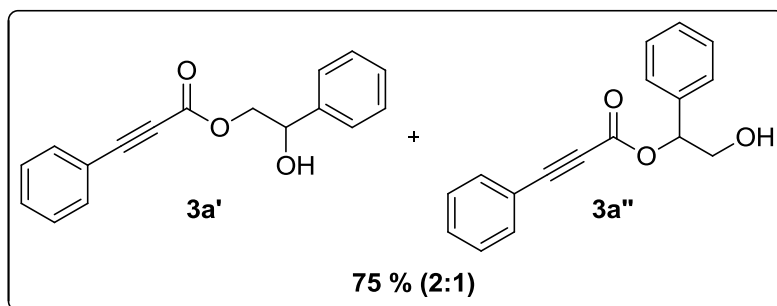
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.67 (t,  $J = 7.8$  Hz, 2H), 7.47 ~ 7.34 (m, 8H), 5.89 (s, 1H), 5.59 (d,  $J = 6.0$  Hz, 1H), 4.76 (d,  $J = 13.2$  Hz, 1H), 4.69 (dd,  $J = 13.2, 5.4$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  166.1, 162.8, 135.7, 134.2, 131.1, 128.9, 128.8, 128.6, 126.8, 125.9, 94.0, 78.3, 77.2; ESI-MS calcd for  $\text{C}_{17}\text{H}_{14}\text{O}_3$ : 266.0943; found 266.0943.

**Spectral data for 3-phenylpropionic acid (1a').**



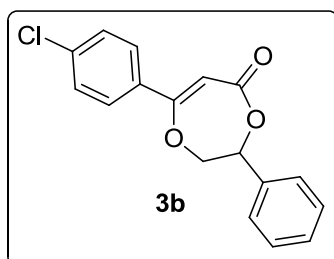
White Solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  10.95 (s, 1H), 7.61 ~ 7.59 (m, 2H), 7.48 ~ 7.45 (m, 1H), 7.39 ~ 7.37 (m, 2H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  158.8, 133.3, 131.2, 128.6, 119.0, 89.2, 80.0; ESI-MS calcd for  $\text{C}_9\text{H}_6\text{O}_2$ : 146.0368; found 146.0372.

**Spectral data for 2-hydroxy-2-phenylethyl 3-phenylpropiolate (3a') and 2-hydroxy-1-phenylethyl 3-phenylpropiolate (3a'')**



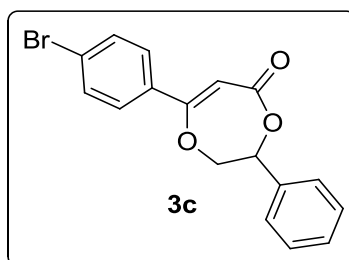
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.59 ~ 7.57 (m, 3H), 7.46 ~ 7.43 (m, 1H), 7.42 ~ 7.40 (m, 2H), 7.39 ~ 7.35 (m, 7H), 7.34 ~ 7.31 (m, 2H), 5.95 (dd,  $J = 7.9, 3.9$  Hz, 1H), 5.04 (dd,  $J = 8.8, 3.1$  Hz, 1H), 4.41 (dd,  $J = 11.6, 3.1$  Hz, 1H), 4.29 (dd,  $J = 11.5, 8.8$  Hz, 1H), 3.97 (dd,  $J = 12.3, 7.9$  Hz, 1H), 3.86 (dd,  $J = 12.3, 3.9$  Hz, 1H), 2.6 (s, 1H), 1.7 (s, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  153.9, 153.4, 139.2, 136.2, 133.03, 133.01, 130.8, 130.7, 128.8, 128.7, 128.6, 128.5, 128.47, 128.42, 126.7, 126.1, 119.4, 87.3, 87.2, 80.4, 80.2, 78.6, 72.1, 70.5, 65.6; ESI-MS calcd for  $\text{C}_{17}\text{H}_{14}\text{O}_3$ : 266.0943; found 266.0944.

**Spectral data for 7-(4-chlorophenyl)-3-phenyl-2H-1,4-dioxepin-5(3H)-one (3b).**



White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.61 (d,  $J = 8.8$  Hz, 2H), 7.44 ~ 7.37 (m, 7H), 5.86 (s, 1H),  $\delta$  5.59 (d,  $J = 5.9$  Hz, 1H), 4.75 (dd,  $J = 13.5, 0.7$  Hz, 1H), 4.69 (dd,  $J = 13.4, 6.0$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.9, 161.6, 137.4, 135.6, 132.6, 129.0, 128.9, 128.1, 125.9, 94.3, 78.3, 77.3 (one CH merging); ESI-MS calcd for  $\text{C}_{17}\text{H}_{13}\text{ClO}_3$ : 300.0553; found 300.0552.

**Spectral data 7-(4-bromophenyl)-3-phenyl-2H-1,4-dioxepin-5(3H)-one (3c).**

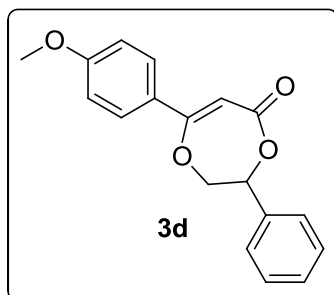


White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.53 (d,  $J = 4.7$  Hz, 4H), 7.44 ~ 7.39 (m, 4H), 7.36 (d,  $J = 7.1$  Hz, 1H), 5.86 (s, 1H), 5.58 (d,  $J = 5.9$  Hz, 1H), 4.75 (d,  $J = 13.5$  Hz, 1H), 4.69 (dd,  $J = 13.4,$



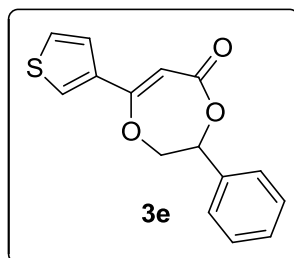
6.0 Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.9, 161.6, 135.6, 133.1, 131.9, 129.0, 128.9, 128.3, 125.9, 125.7, 94.3, 78.3, 77.3; ESI-MS calcd for  $\text{C}_{17}\text{H}_{13}\text{BrO}_3$ : 344.0048; found 344.0049.

**Spectral data for 7-(4-methoxyphenyl)-3-phenyl-2H-1,4-dioxepin-5(3H)-one (3d).**



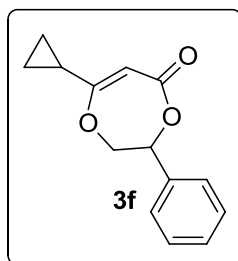
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.64 ~ 7.62 (m, 2H), 7.43 (d,  $J$  = 7.3 Hz, 2H), 7.40 ~ 7.38 (m, 2H), 7.35 (d,  $J$  = 7.1 Hz, 1H), 6.91 ~ 6.89 (m, 2H), 5.82 (s, 1H), 5.55 (d,  $J$  = 5.9 Hz, 1H), 4.73 (d,  $J$  = 13.4 Hz, 1H), 4.66 (dd,  $J$  = 13.4, 6.0 Hz, 1H), 3.83 (s, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  166.3, 162.8, 162.0, 135.9, 128.9, 128.7, 128.5, 126.3, 125.9, 113.9, 92.4, 78.3, 77.1, 55.4; ESI-MS calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_4$ : 296.1049; found 296.1050.

**Spectral data for 3-phenyl-7-(thiophen-3-yl)-2H-1,4-dioxepin-5(3H)-one (3e).**



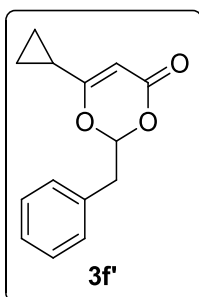
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.73 (dd,  $J$  = 3.1, 1.3 Hz, 1H), 7.44 ~ 7.38 (m, 4H), 7.37 ~ 7.33 (m, 2H), 7.29 (dd,  $J$  = 5.2, 1.3 Hz, 1H), 5.86 (s, 1H), 5.57 (d,  $J$  = 5.9 Hz, 1H), 4.71 (dd,  $J$  = 13.4, 0.6 Hz, 1H), 4.65 (dd,  $J$  = 13.4, 5.9 Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  166.4, 158.3, 136.2, 135.7, 128.9, 128.8, 126.9, 126.7, 125.9, 125.6, 93.4, 78.3, 77.1; ESI-MS calcd for  $\text{C}_{15}\text{H}_{12}\text{O}_3\text{S}$ : 272.0507; found 272.0506.

**Spectral data for 7-cyclopropyl-3-phenyl-2H-1,4-dioxepin-5(3H)-one (3f).**



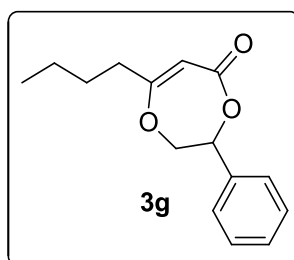
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.37 ~ 7.31 (m, 5H), 5.40 (d,  $J = 5.8$  Hz, 1H), 5.30 (s, 1H), 4.48 (dd,  $J = 13.4, 0.6$  Hz, 1H), 4.42 (dd,  $J = 13.4, 5.9$  Hz, 1H), 1.56 ~ 1.51 (m, 1H), 0.95 ~ 0.93 (m, 1H), 0.83 ~ 0.78 (m, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.5, 165.6, 135.8, 128.8, 128.7, 125.9, 92.4, 77.9, 76.6, 16.1, 7.9, 7.1; ESI-MS calcd for  $\text{C}_{14}\text{H}_{14}\text{O}_3$ : 230.0943; found 230.0944.

**Spectral data for 2-benzyl-6-cyclopropyl-4H-1,3-dioxin-4-one (3f').**



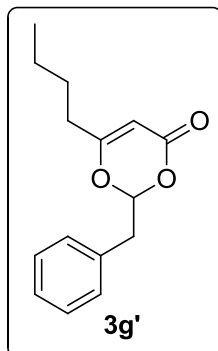
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.32 ~ 7.29 (m, 2H), 7.27 ~ 7.23 (m, 3H), 5.48 (t,  $J = 5.4$  Hz, 1H), 5.32 (s, 1H), 3.19 (d,  $J = 5.4$  Hz, 2H), 1.57 ~ 1.53 (m, 1H), 1.08 ~ 1.04 (m, 1H), 0.92 ~ 0.87 (m, 2H), 0.71 ~ 0.67 (m, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  175.9, 162.3, 133.6, 129.9, 128.5, 127.3, 100.7, 93.3, 39.6, 13.4, 9.0, 6.8; ESI-MS calcd for  $\text{C}_{14}\text{H}_{14}\text{O}_3$ : 230.0943; found 230.0943.

**Spectral data for 7-butyl-3-phenyl-2H-1,4-dioxepin-5(3H)-one (3g).**



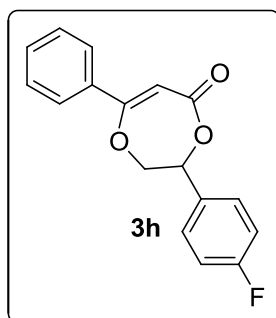
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.38 ~ 7.33 (m, 5H), 5.43 (d,  $J = 5.8$  Hz, 1H), 5.21 (s, 1H), 4.53 (d,  $J = 13.5$  Hz, 1H), 4.48 (dd,  $J = 13.5, 5.8$  Hz, 1H), 2.23 ~ 2.19 (m, 2H), 1.54 ~ 1.48 (m, 2H), 1.33 ~ 1.24 (m, 2H), 0.89 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.5, 166.2, 135.8, 128.8, 128.7, 125.9, 94.4, 78.0, 76.6, 36.0, 29.4, 21.9, 13.7; ESI-MS calcd for  $\text{C}_{15}\text{H}_{18}\text{O}_3$ : 246.1256; found 246.1256.

**Spectral data for 2-benzyl-6-butyl-4H-1,3-dioxin-4-one (3g').**



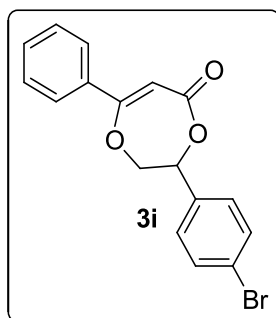
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.32 ~ 7.24 (m, 5H), 5.56 (t,  $J = 5.2$  Hz, 1H), 5.25 (s, 1H), 3.23 (d,  $J = 5.1$  Hz, 2H), 2.26 ~ 2.21 (m, 2H), 1.50 ~ 1.42 (m, 2H), 1.32 ~ 1.26 (m, 2H), 0.87 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  175.5, 162.5, 133.6, 129.9, 128.5, 127.2, 100.8, 95.3, 39.7, 32.7, 27.8, 21.9, 13.6; ESI-MS calcd for  $\text{C}_{15}\text{H}_{18}\text{O}_3$ : 246.1256; found 246.1258.

**Spectral data for 3-(4-fluorophenyl)-7-phenyl-2H-1,4-dioxepin-5(3H)-one (3h).**



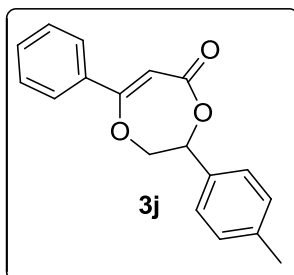
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 ~ 7.66 (m, 2H), 7.48 ~ 7.44 (m, 1H), 7.43 ~ 7.39 (m, 4H), 7.11 ~ 7.08 (m, 2H), 5.89 (s, 1H), 5.58 (d,  $J = 6.0$  Hz, 1H), 4.73 (dd,  $J = 13.2, 0.6$  Hz, 1H), 4.68 (dd,  $J = 13.2, 6.0$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.9, 163.7, 162.5 (d,  $J_{\text{CF}} = 126.0$  Hz), 134.1, 131.6, 131.2, 128.6, 127.9 (d,  $J_{\text{CF}} = 7.5$  Hz), 126.8, 116.0 (d,  $J_{\text{CF}} = 21.0$  Hz), 93.9, 77.7, 77.1; ESI-MS calcd for  $\text{C}_{17}\text{H}_{13}\text{FO}_3$ : 284.0849; found 284.0848.

**Spectral data for 3-(4-bromophenyl)-7-phenyl-2H-1,4-dioxepin-5(3H)-one (3i).**



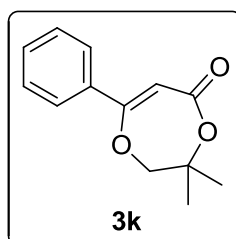
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.67 ~ 7.65 (m, 2H), 7.54 ~ 7.52 (m, 2H), 7.47 ~ 7.45 (m, 1H), 7.41 ~ 7.38 (m, 2H), 7.33 ~ 7.31 (m, 2H), 5.88 (s, 1H), 5.55 (d,  $J = 5.8$  Hz, 1H), 4.71 (dd,  $J = 13.4, 0.6$  Hz, 1H), 4.66 (dd,  $J = 13.5, 5.9$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.8, 162.9, 134.7, 133.9, 132.1, 131.2, 128.6, 127.7, 126.8, 122.9, 93.9, 77.6, 76.8; ESI-MS calcd for  $\text{C}_{17}\text{H}_{13}\text{BrO}_3$ : 344.0048; found 344.0046.

**Spectral data for 7-phenyl-3-(*p*-tolyl)-2H-1,4-dioxepin-5(3H)-one (3j).**



Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.68 ~ 7.67 (m, 2H), 7.44 (t,  $J = 7.5$  Hz, 1H), 7.40 (t,  $J = 6.4$  Hz, 2H), 7.31 (d,  $J = 8.1$  Hz, 2H), 7.20 (d,  $J = 7.9$  Hz, 2H), 5.89 (s, 1H), 5.55 (d,  $J = 5.9$  Hz, 1H), 4.74 (dd,  $J = 13.4, 0.7$  Hz, 1H), 4.68 (dd,  $J = 13.4, 6.0$  Hz, 1H), 2.35 (s, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  166.3, 162.8, 138.7, 134.2, 132.8, 131.1, 129.6, 128.6, 126.8, 125.9, 94.0, 78.3, 77.3, 21.1; ESI-MS calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_3$ : 280.1099; found 280.1098.

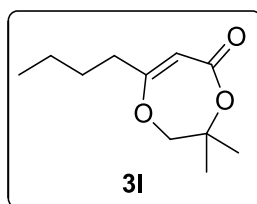
**Spectral data for 3,3-dimethyl-7-phenyl-2H-1,4-dioxepin-5(3H)-one (3k).**



White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.67 ~ 7.66 (m, 2H), 7.46 ~ 7.43 (m, 1H), 7.40 ~ 7.37 (m, 2H), 5.84 (s, 1H), 4.39 (s, 2H), 1.46 (s, 6H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.7, 163.2, 133.9, 131.0, 128.6, 126.8, 95.2, 78.2, 78.1( $\text{CH}_2$ ), 23.9; ESI-MS calcd for  $\text{C}_{13}\text{H}_{14}\text{O}_3$ : 218.0943; found

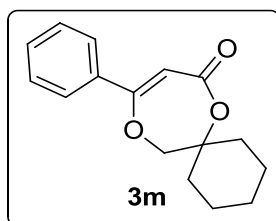
218.0942.

**Spectral data for 7-butyl-3,3-dimethyl-2*H*-1,4-dioxepin-5(3*H*)-one (3l).**



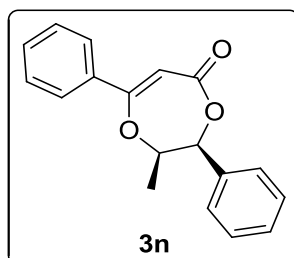
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  5.17 (s, 1H), 4.15 (s, 2H), 2.18 (t,  $J = 7.4$  Hz, 2H), 1.54 ~ 1.51 (m, 2H), 1.39 (s, 6H), 1.35 ~ 1.31 (m, 2H), 0.90 (t,  $J = 7.4$  Hz, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.9, 165.7, 95.8, 77.8, 77.7, 35.7, 29.3, 23.8, 22.1, 13.7; ESI-MS calcd for  $\text{C}_{11}\text{H}_{18}\text{O}_3$ : 198.1256; found 198.1257.

**Spectral data for 10-phenyl-7,11-dioxaspiro[5.6]dodec-9-en-8-one (3m).**



White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.66 ~ 7.65 (m, 2H), 7.43 (t,  $J = 6.2$  Hz, 1H), 7.40 ~ 7.37 (m, 2H), 5.82 (s, 1H), 4.43 (s, 2H), 1.91 ~ 1.87 (m, 2H), 1.79 ~ 1.74 (m, 2H), 1.62 ~ 1.57 (m, 3H), 1.54 ~ 1.50 (m, 2H), 1.42 ~ 1.40 (m, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  165.8, 163.3, 134.1, 130.9, 128.6, 126.8, 95.2, 79.3, 77.2, 32.1, 25.2, 21.6; ESI-MS calcd for  $\text{C}_{16}\text{H}_{18}\text{O}_3$ : 258.1256; found 258.1255.

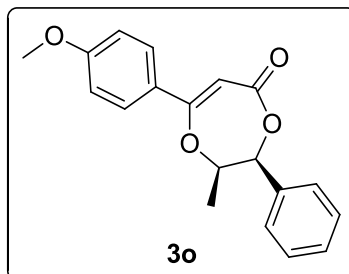
**Spectral data for (2*R*,3*S*)-2-methyl-3,7-diphenyl-2*H*-1,4-dioxepin-5(3*H*)-one (3n).**



Colorless oil;  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 ~ 7.67 (m, 2H), 7.47 ~ 7.44 (m, 3H), 7.42 ~ 7.31 (m, 5H), 5.84 (s, 1H), 5.72 (s, 1H), 4.93 (q,  $J = 6.8$  Hz, 1H), 1.43 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (100MHz,  $\text{CDCl}_3$ ):  $\delta$  166.6, 160.7, 135.9, 135.0, 130.9, 128.7, 128.6, 128.5, 126.8, 126.1, 93.3, 82.4,

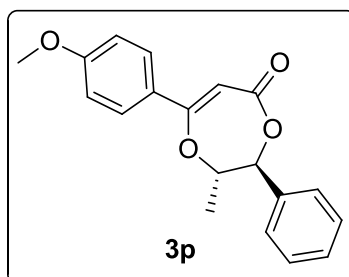
79.2, 10.7; EI-MS calcd for C<sub>18</sub>H<sub>16</sub>O<sub>3</sub>: 280.1099; found 280.1099.

**Spectral data for (2*R*,3*S*)-7-(4-methoxyphenyl)-2-methyl-3-phenyl-2*H*-1,4-dioxepin-5(3*H*)-one (3o).**



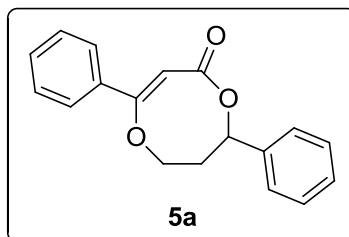
White solid; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.65 ~ 7.62 (m, 2H), 7.46 ~ 7.45 (m, 2H), 7.39 ~ 7.37 (m, 2H), 7.34 ~ 7.31 (m, 1H), 6.91 ~ 6.89 (m, 2H), 5.78 (s, 1H), 5.68 (s, 1H), 4.91 (q, *J* = 7.2 Hz, 1H), 3.83 (s, 3H), 1.42 (d, *J* = 7.2 Hz, 3H); <sup>13</sup>C NMR (150MHz, CDCl<sub>3</sub>): δ 166.8, 161.9, 160.6, 136.0, 128.7, 128.5, 128.4, 127.1, 126.1, 113.9, 91.8, 82.2, 79.2, 55.4, 10.7; EI-MS calcd for C<sub>19</sub>H<sub>18</sub>O<sub>4</sub>: 310.1205; found 310.1195.

**Spectral data for (2*S*,3*S*)-7-(4-methoxyphenyl)-2-methyl-3-phenyl-2*H*-1,4-dioxepin-5(3*H*)-one (3p).**



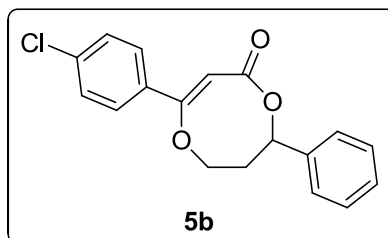
Colorless oil; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ 7.64 (d, *J* = 8.9 Hz, 2H), 7.40 ~ 7.30 (m, 5H), 6.90 (d, *J* = 8.8 Hz, 2H), 5.80 (s, 1H), 5.28 (d, *J* = 4.8 Hz, 1H), 4.81 ~ 4.75 (m, 1H), 3.84 (s, 3H), 1.13 (d, *J* = 6.7 Hz, 3H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>): δ 166.9, 162.2, 161.9, 136.4, 128.9, 128.7, 128.5, 127.2, 126.7, 113.9, 91.8, 82.9, 82.5, 55.4, 19.1; EI-MS calcd for C<sub>19</sub>H<sub>18</sub>O<sub>4</sub>: 310.1205; found 310.1211.

**Spectral data for (*Z*)-4,8-diphenyl-7,8-dihydro-1,5-dioxocin-2(6*H*)-one (5a).<sup>[S3]</sup>**



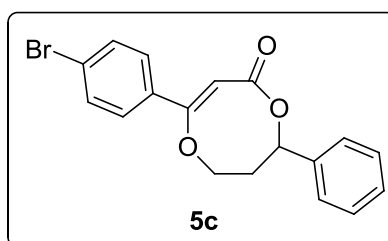
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 ~ 7.67 (m, 2H), 7.44 ~ 7.32 (m, 8H), 5.67 (dd,  $J = 10.5, 2.7$  Hz, 1H), 5.56 (s, 1H), 4.61 ~ 4.58 (m, 1H), 4.48 (td,  $J = 12.6, 2.4$  Hz, 1H), 2.48 ~ 2.43 (m, 1H), 2.22 ~ 2.17 (m, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  167.8, 163.7, 138.6, 135.0, 130.6, 128.6, 128.5, 128.3, 126.7, 125.9, 89.7, 76.7, 67.3, 37.9; ESI-MS calcd for  $\text{C}_{18}\text{H}_{16}\text{O}_3$ : 280.1099; found 280.1100.

**Spectral data for (Z)-4-(4-chlorophenyl)-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5b).**



White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.60 (d,  $J = 8.6$  Hz, 2H), 7.41 (d,  $J = 7.4$  Hz, 2H), 7.38 ~ 7.35 (m, 4H), 7.32 (t,  $J = 7.2$  Hz, 1H), 5.64 (dd,  $J = 12.2, 2.4$  Hz, 1H), 5.53 (s, 1H), 4.59 (dd,  $J = 12.6, 5.1$  Hz, 1H), 4.47 (td,  $J = 12.6, 2.0$  Hz, 1H), 2.48 ~ 2.43 (m, 1H), 2.19 (t,  $J = 12.8$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  167.5, 162.4, 138.6, 136.8, 133.5, 128.8, 128.7, 128.4, 128.0, 125.9, 90.1, 76.8, 67.4, 37.9; ESI-MS calcd for  $\text{C}_{18}\text{H}_{15}\text{ClO}_3$ : 314.0710; found 314.0707.

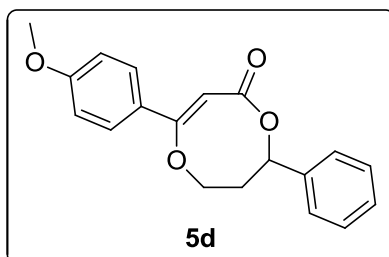
**Spectral data for (Z)-4-(4-bromophenyl)-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5c).**



White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.55 ~ 7.52 (m, 4H), 7.41 (d,  $J = 7.5$  Hz, 2H), 7.36 (t,  $J = 7.2$  Hz, 2H), 7.33 ~ 7.31 (m, 1H), 5.63 (dd,  $J = 12.2, 2.5$  Hz, 1H), 5.53 (s, 1H), 4.59 (dd,  $J = 12.7, 5.4$  Hz, 1H), 4.47 (td,  $J = 12.6, 2.1$  Hz, 1H), 2.46 ~ 2.43 (m, 1H), 2.19 (t,  $J = 12.5$  Hz, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  167.4, 162.4, 138.5, 133.9, 131.7, 128.7, 128.4, 128.2, 125.9, 125.1,

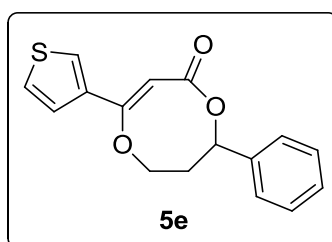
90.1, 76.8, 67.4, 37.9; ESI-MS calcd for C<sub>18</sub>H<sub>15</sub>BrO<sub>3</sub>: 358.0205; found 358.0202.

**Spectral data for (Z)-4-(4-methoxyphenyl)-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5d).**



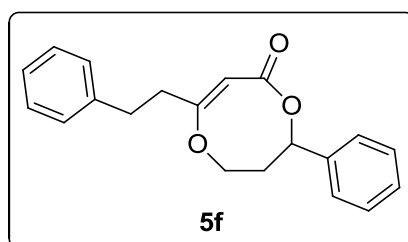
White solid; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.63 ~ 7.62 (m, 2H), 7.42 (t, *J* = 8.9 Hz, 2H), 7.37 ~ 7.35 (m, 2H), 7.32 ~ 7.31 (m, 1H), 6.92 ~ 6.89 (m, 2H), 5.64 (dd, *J* = 12.2, 2.6 Hz, 1H), 5.48 (s, 1H), 4.56 (dd, *J* = 12.6, 4.7 Hz, 1H), 4.47 (td, *J* = 12.3, 2.3 Hz, 1H), 3.84 (s, 3H), 2.45 ~ 2.42 (m, 1H), 2.20 ~ 2.15 (m, 1H); <sup>13</sup>C NMR (150MHz, CDCl<sub>3</sub>): δ 168.0, 163.9, 161.7, 138.9, 128.7, 128.4, 128.3, 127.4, 126.0, 113.9, 88.3, 76.6, 67.3, 55.4, 37.9; ESI-MS calcd for C<sub>19</sub>H<sub>18</sub>O<sub>4</sub>: 310.1205; found 310.1204.

**Spectral data for (Z)-8-phenyl-4-(thiophen-3-yl)-7,8-dihydro-1,5-dioxocin-2(6H)-one (5e).**



White solid; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>): δ 7.70 (d, *J* = 3.1 Hz, 1H), 7.41 (d, *J* = 7.4 Hz, 2H), 7.37 ~ 7.35 (m, 2H), 7.32 ~ 7.31 (m, 2H), 7.27 ~ 7.26 (m, 1H), 5.64 (dd, *J* = 12.3, 2.6 Hz, 1H), 5.55 (s, 1H), 4.55 (dd, *J* = 12.7, 5.3 Hz, 1H), 4.45 (td, *J* = 12.6, 2.3 Hz, 1H), 2.45 ~ 2.42 (m, 1H), 2.20 ~ 2.15 (m, 1H); <sup>13</sup>C NMR (150MHz, CDCl<sub>3</sub>): δ 167.8, 159.2, 138.8, 137.2, 128.7, 128.4, 126.5, 126.0, 125.9, 125.6, 89.3, 76.8, 67.1, 37.9; ESI-MS calcd for C<sub>16</sub>H<sub>14</sub>O<sub>3</sub>S: 286.0664; found 286.0665.

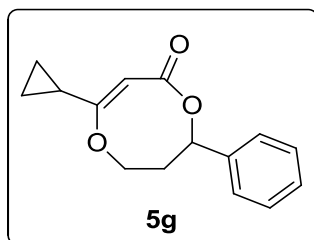
**Spectral data for (Z)-4-phenethyl-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5f).**





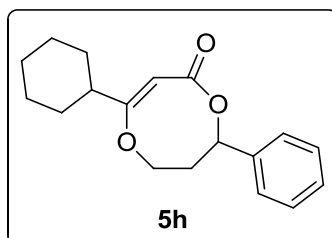
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.35 ~ 7.29 (m, 7H), 7.21 (t,  $J = 8.0$  Hz, 3H), 5.33 (dd,  $J = 12.3, 2.8$  Hz, 1H), 4.86 (s, 1H), 4.36 ~ 4.33 (m, 1H), 4.22 (td,  $J = 12.6, 2.2$  Hz, 1H), 2.93 ~ 2.87 (m, 2H), 2.56 ~ 2.52 (m, 2H), 2.29 ~ 2.27 (m, 1H), 2.08 ~ 2.04 (m, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  167.8, 166.7, 140.3, 138.8, 128.6, 128.4, 128.3, 126.4, 126.0, 90.4, 76.7, 66.6, 38.4, 37.8, 33.4; ESI-MS calcd for  $\text{C}_{20}\text{H}_{20}\text{O}_3$ : 308.1412; found 308.1414.

**Spectral data for (Z)-4-cyclopropyl-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5g).**



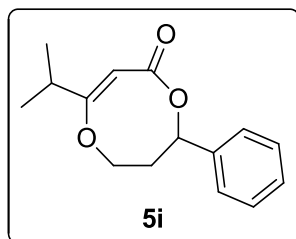
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.40 ~ 7.39 (m, 2H), 7.37 ~ 7.34 (m, 2H), 7.31 (t,  $J = 7.1$  Hz, 3H), 5.51 (dd,  $J = 12.3, 2.7$  Hz, 1H), 4.99 (s, 1H), 4.28 (dd,  $J = 5.6, 1.0$  Hz, 1H), 4.23 (td,  $J = 12.4, 2.2$  Hz, 1H), 2.31 ~ 2.28 (m, 1H), 2.10 ~ 2.05 (m, 1H), 1.56 ~ 1.49 (m, 1H), 0.96 ~ 0.93 (m, 1H) 0.80 ~ 0.77 (m, 1H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.7, 167.6, 138.9, 128.6, 128.3, 126.0, 87.9, 76.5, 66.9, 37.7, 16.5, 7.4, 6.5; ESI-MS calcd for  $\text{C}_{15}\text{H}_{16}\text{O}_3$ : 244.1099; found 244.1101.

**Spectral data for (Z)-4-cyclohexyl-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5h).**



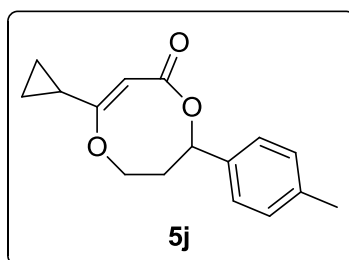
White solid;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.39 ~ 7.29 (m, 5H), 5.50 (dd,  $J = 12.3, 2.7$  Hz, 1H), 4.86 (s, 1H), 4.33 (dd,  $J = 5.4, 1.1$  Hz, 1H), 4.22 (td,  $J = 12.6, 2.2$  Hz, 1H), 2.33 ~ 2.30 (m, 1H), 2.10 ~ 2.05 (m, 2H), 1.86 ~ 1.77 (m, 4H), 1.69 ~ 1.67 (m, 1H) 1.35 ~ 1.18 (m, 5H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  172.7, 168.6, 138.9, 128.6, 128.3, 125.9, 87.6, 76.7, 66.5, 45.5, 37.9, 31.4, 31.0, 26.2, 25.9, 25.8; ESI-MS calcd for  $\text{C}_{18}\text{H}_{22}\text{O}_3$ : 286.1569; found 286.1568.

**Spectral data for (Z)-4-isopropyl-8-phenyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5i).**



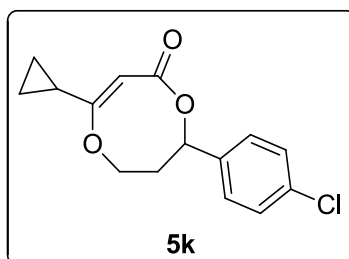
Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.40 ~ 7.38 (m, 2H), 7.37 ~ 7.34 (m, 2H), 7.32 ~ 7.29 (m, 1H), 5.51 (dd,  $J = 12.3, 2.7$  Hz, 1H), 4.89 (s, 1H), 4.38 ~ 4.35 (m, 1H), 4.23 (td,  $J = 12.6, 2.3$  Hz, 1H), 2.44 ~ 2.40 (m, 1H), 2.35 ~ 2.32 (m, 1H), 2.11 ~ 2.06 (m, 1H), 1.16 (d,  $J = 6.9$  Hz, 3H) 1.13 (d,  $J = 6.8$  Hz, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  173.3, 168.5, 138.8, 128.6, 128.3, 125.9, 87.4, 76.7, 66.6, 37.9, 35.6, 20.9, 20.6; ESI-MS calcd for  $\text{C}_{15}\text{H}_{18}\text{O}_3$ : 246.1256; found 246.1257.

**Spectral data for (Z)-4-cyclopropyl-8-(*p*-tolyl)-7,8-dihydro-1,5-dioxocin-2(6H)-one (5j).**



Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.45 (d,  $J = 8.1$  Hz, 2H), 7.33 ((d,  $J = 8.1$  Hz, 2H), 5.65 (dd,  $J = 12.3, 2.6$  Hz, 1H), 5.16 (s, 1H), 4.45 (dd,  $J = 12.6, 5.4$  Hz, 1H), 4.38 (td,  $J = 12.5, 2.3$  Hz, 1H), 2.49 (s, 3H) 2.47 ~ 2.41 (m, 1H), 2.25 ~ 2.21 (m, 1H), 1.69 ~ 1.65 (m, 1H), 1.13 ~ 1.09 (m, 1H) 0.96 ~ 0.94 (m, 3H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.5, 167.7, 138.0, 135.9, 129.2, 125.9, 87.9, 76.5, 66.9, 37.7, 21.1, 16.4, 7.3, 6.4; ESI-MS calcd for  $\text{C}_{16}\text{H}_{18}\text{O}_3$ : 258.1256; found 258.1256.

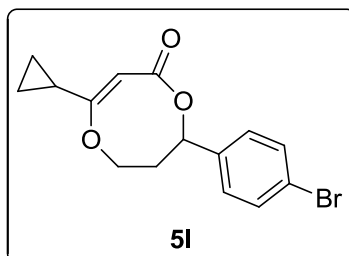
**Spectral data for (Z)-8-(4-chlorophenyl)-4-cyclopropyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5k).**



Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.34 ~ 7.31 (m, 4H), 5.48 (dd,  $J = 12.3, 2.6$  Hz, 1H), 4.99 (s, 1H), 4.29 (dd,  $J = 12.7, 5.4$  Hz, 1H), 4.21 (td,  $J = 12.5, 1.8$  Hz, 1H), 2.29 ~ 2.25 (m, 1H), 2.01 (t,  $J = 13.2$  Hz, 1H), 1.51 ~ 1.49 (m, 1H), 0.95 ~ 0.93 (m, 1H) 0.79 ~ 0.76 (m, 3H);  $^{13}\text{C}$  NMR

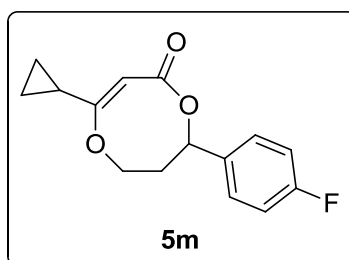
(150MHz, CDCl<sub>3</sub>):  $\delta$  168.8, 167.3, 137.5, 134.1, 128.8, 127.4, 87.8, 75.8, 66.8, 37.7, 16.5, 7.4, 6.5; ESI-MS calcd for C<sub>15</sub>H<sub>15</sub>ClO<sub>3</sub>: 278.0710; found 278.0710.

**Spectral data for (Z)-8-(4-bromophenyl)-4-cyclopropyl-7,8-dihydro-1,5-dioxocin-2(6H)-one (5l).**



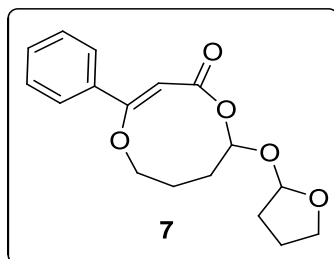
White solid; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.48 (d, *J* = 6.6 Hz, 2H), 7.28 ~ 7.27 (m, 2H), 5.47 (dd, *J* = 12.3, 2.7 Hz, 1H), 4.99 (s, 1H), 4.29 ~ 4.27 (m, 1H), 4.21 (td, *J* = 12.5, 2.3 Hz, 1H), 2.28 ~ 2.25 (m, 1H), 2.03 ~ 1.98 (m, 1H), 1.51 ~ 1.49 (m, 1H), 0.95 ~ 0.93 (m, 1H) 0.79 ~ 0.76 (m, 3H); <sup>13</sup>C NMR (150MHz, CDCl<sub>3</sub>):  $\delta$  168.8, 167.2, 138.0, 131.8, 127.7, 122.2, 87.8, 75.8, 66.8, 37.7, 16.5, 7.4, 6.5; ESI-MS calcd for C<sub>15</sub>H<sub>15</sub>BrO<sub>3</sub>: 322.0205; found 322.0202.

**Spectral data for (Z)-4-cyclopropyl-8-(4-fluorophenyl)-7,8-dihydro-1,5-dioxocin-2(6H)-one (5m).**



Colorless oil; <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>):  $\delta$  7.37 ~ 7.35 (m, 2H), 7.03 ~ 7.00 (m, 2H), 5.48 (dd, *J* = 12.3, 2.6 Hz, 1H), 4.99 (s, 1H), 4.29 ~ 4.26 (m, 1H), 4.20 (td, *J* = 12.5, 2.3 Hz, 1H), 2.27 ~ 2.23 (m, 1H), 2.05 ~ 2.00 (m, 1H), 1.52 ~ 1.47 (m, 1H), 0.95 ~ 0.92 (m, 1H) 0.79 ~ 0.75 (m, 3H); <sup>13</sup>C NMR (150MHz, CDCl<sub>3</sub>):  $\delta$  168.8, 167.3, 162.5 (d, *J*<sub>CF</sub> = 246.0 Hz), 134.8, 127.9 (d, *J*<sub>CF</sub> = 8.1 Hz), 115.5 (d, *J*<sub>CF</sub> = 21.5 Hz), 87.8, 75.9, 66.8, 37.7, 16.4, 7.4, 6.5; ESI-MS calcd for C<sub>15</sub>H<sub>15</sub>FO<sub>3</sub>: 262.1005; found 262.1005.

**Spectral data for (Z)-4-phenyl-9-((tetrahydrofuran-2-yl)oxy)-6,7,8,9-tetrahydro-2H-1,5-dioxonin-2-one (7)**



Colorless oil;  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J = 7.6$  Hz, 2H), 7.51 (t,  $J = 7.3$  Hz, 1H), 7.44 (t,  $J = 7.9$  Hz, 2H), 5.92 (s, 1H), 4.68 ~ 4.66 (m, 1H), 5.11 (dd,  $J = 3.3, 1.8$  Hz, 1H), 3.88 ~ 3.84 (m, 2H), 3.76 ~ 3.73 (m, 1H), 3.49 ~ 3.47 (m, 1H), 2.16 ~ 2.13 (m, 2H), 1.93 ~ 1.83 (m, 6H);  $^{13}\text{C}$  NMR (150MHz,  $\text{CDCl}_3$ ):  $\delta$  168.3, 163.4, 132.4, 130.3, 128.9, 126.5, 103.8, 101.2, 92.9, 66.9, 66.2, 32.4, 30.3, 30.2, 23.5; ESI-MS calcd for  $\text{C}_{17}\text{H}_{20}\text{NaO}_5^+$ : 327.1203; found 327.1309.

**(4) (a) X-ray Crystallographic structure and data of compound (3d).**

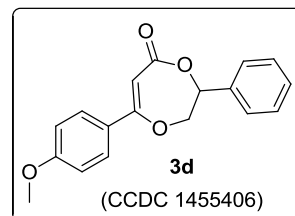
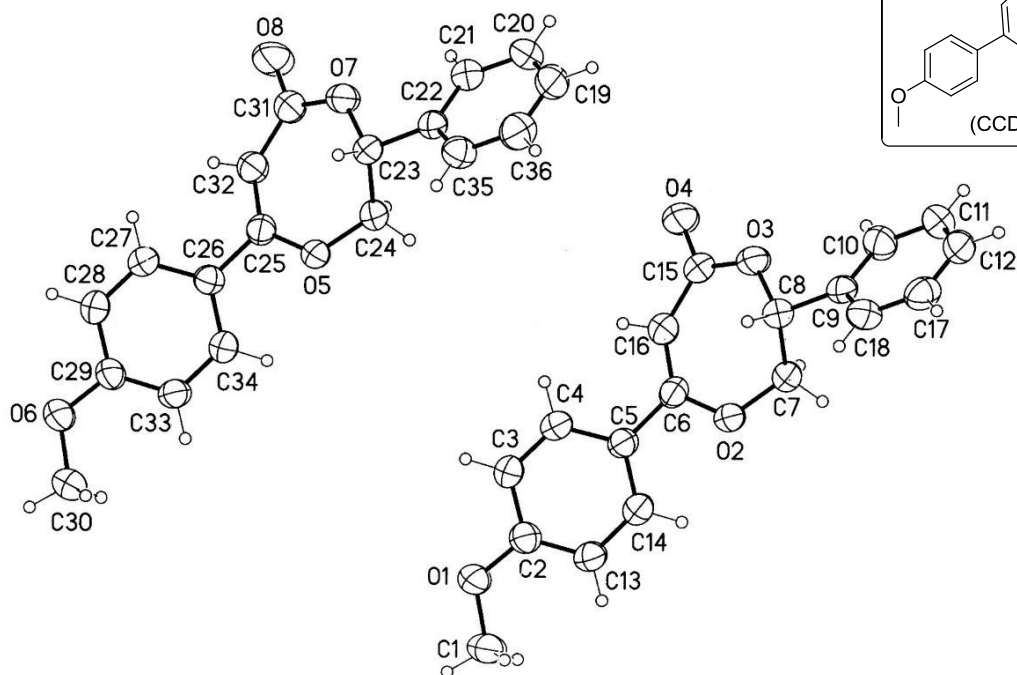


Table 1. Crystal data and structure refinement for 151129\_0M.

Identification code	151129_0m	
Empirical formula	C <sub>36</sub> H <sub>32</sub> O <sub>8</sub>	
Formula weight	592.61	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 11.8910(9) Å	α = 90°.
	b = 16.2219(12) Å	β = 93.262(4)°.
	c = 15.2941(11) Å	γ = 90°.
Volume	2945.4(4) Å <sup>3</sup>	
Z	4	
Density (calculated)	1.336 Mg/m <sup>3</sup>	
Absorption coefficient	0.094 mm <sup>-1</sup>	
F(000)	1248	
Crystal size	0.20 x 0.15 x 0.15 mm <sup>3</sup>	
Theta range for data collection	1.715 to 26.387°.	
Index ranges	-14 ≤ h ≤ 14, -20 ≤ k ≤ 20, -19 ≤ l ≤ 15	
Reflections collected	25025	
Independent reflections	6020 [R(int) = 0.0534]	
Completeness to theta = 25.242°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9485 and 0.8722	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	6020 / 0 / 399	
Goodness-of-fit on F <sup>2</sup>	0.990	
Final R indices [I > 2σ(I)]	R1 = 0.0489, wR2 = 0.1296	
R indices (all data)	R1 = 0.0986, wR2 = 0.1720	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.177 and -0.202 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement parameters (Å<sup>2</sup> x 10<sup>3</sup>) for 151129\_0M. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	x	y	z	U(eq)
O(1)	7137(1)	4049(1)	8676(1)	60(1)

O(2)	8799(1)	378(1)	9022(1)	52(1)
O(3)	7430(1)	-1313(1)	8692(1)	57(1)
O(4)	5673(1)	-1030(1)	8869(1)	74(1)
O(5)	3812(1)	1774(1)	3922(1)	49(1)
O(6)	2145(1)	5443(1)	3522(1)	65(1)
O(7)	2423(1)	86(1)	3733(1)	57(1)
O(8)	693(1)	376(1)	3973(1)	84(1)
C(1)	8014(2)	4608(1)	8943(2)	67(1)
C(2)	7355(2)	3228(1)	8744(1)	45(1)
C(3)	6536(2)	2713(1)	8353(1)	50(1)
C(4)	6666(2)	1878(1)	8391(1)	47(1)
C(5)	7610(2)	1516(1)	8826(1)	41(1)
C(6)	7719(2)	616(1)	8888(1)	41(1)
C(7)	9026(2)	-469(1)	9233(1)	48(1)
C(8)	8559(2)	-1070(1)	8552(1)	43(1)
C(9)	9246(2)	-1856(1)	8556(1)	41(1)
C(10)	8942(2)	-2545(1)	9018(1)	51(1)
C(11)	9586(2)	-3256(1)	9007(2)	57(1)
C(12)	10535(2)	-3281(1)	8539(2)	57(1)
C(13)	8302(2)	2890(1)	9163(1)	50(1)
C(14)	8419(2)	2044(1)	9203(1)	50(1)
C(15)	6611(2)	-755(1)	8808(1)	50(1)
C(16)	6808(2)	123(1)	8829(1)	48(1)
C(17)	10852(2)	-2598(1)	8086(2)	56(1)
C(18)	10210(2)	-1887(1)	8091(1)	49(1)
C(19)	5492(2)	-1924(2)	3652(2)	63(1)
C(20)	4492(2)	-1894(1)	4046(2)	60(1)
C(21)	3852(2)	-1182(1)	4027(1)	50(1)
C(22)	4221(2)	-487(1)	3602(1)	40(1)
C(23)	3559(2)	308(1)	3563(1)	42(1)
C(24)	4044(2)	944(1)	4195(1)	46(1)
C(25)	2729(2)	2016(1)	3838(1)	40(1)
C(26)	2622(2)	2919(1)	3740(1)	40(1)
C(27)	1652(2)	3270(1)	3341(1)	48(1)
C(28)	1525(2)	4105(1)	3272(1)	50(1)
C(29)	2374(2)	4626(1)	3600(1)	46(1)
C(30)	3016(2)	6018(1)	3752(2)	64(1)
C(31)	1621(2)	650(1)	3867(2)	51(1)

C(32)	1813(2)	1526(1)	3854(1)	46(1)
C(33)	3356(2)	4296(1)	3976(1)	46(1)
C(34)	3474(2)	3449(1)	4047(1)	45(1)
C(35)	5237(2)	-525(1)	3205(1)	49(1)
C(36)	5868(2)	-1237(2)	3232(2)	59(1)

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Table 3. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for 151129\_0M.

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O(1)-C(2)	1.359(2)
O(1)-C(1)	1.424(2)
O(2)-C(6)	1.345(2)
O(2)-C(7)	1.433(2)
O(3)-C(15)	1.349(2)
O(3)-C(8)	1.428(2)
O(4)-C(15)	1.210(2)
O(5)-C(25)	1.345(2)
O(5)-C(24)	1.432(2)
O(6)-C(29)	1.358(2)
O(6)-C(30)	1.422(2)
O(7)-C(31)	1.345(3)
O(7)-C(23)	1.436(2)
O(8)-C(31)	1.210(2)
C(1)-H(3)	0.9600
C(1)-H(1)	0.9600
C(1)-H(16)	0.9600
C(2)-C(13)	1.377(3)
C(2)-C(3)	1.393(3)
C(3)-C(4)	1.363(3)
C(3)-H(12)	0.9300
C(4)-C(5)	1.401(3)
C(4)-H(13)	0.9300
C(5)-C(14)	1.388(3)
C(5)-C(6)	1.469(3)
C(6)-C(16)	1.346(3)
C(7)-C(8)	1.508(3)
C(7)-H(10)	0.9700
C(7)-H(11)	0.9700

C(8)-C(9)	1.514(3)
C(8)-H(9)	0.9800
C(9)-C(10)	1.382(3)
C(9)-C(18)	1.384(3)
C(10)-C(11)	1.386(3)
C(10)-H(8)	0.9300
C(11)-C(12)	1.370(3)
C(11)-H(7)	0.9300
C(12)-C(17)	1.372(3)
C(12)-H(2)	0.9300
C(13)-C(14)	1.381(3)
C(13)-H(15)	0.9300
C(14)-H(14)	0.9300
C(15)-C(16)	1.443(3)
C(16)-H(4)	0.9300
C(17)-C(18)	1.382(3)
C(17)-H(5)	0.9300
C(18)-H(6)	0.9300
C(19)-C(20)	1.365(3)
C(19)-C(36)	1.373(3)
C(19)-H(17)	0.9300
C(20)-C(21)	1.383(3)
C(20)-H(32)	0.9300
C(21)-C(22)	1.384(3)
C(21)-H(31)	0.9300
C(22)-C(35)	1.385(3)
C(22)-C(23)	1.510(3)
C(23)-C(24)	1.506(3)
C(23)-H(28)	0.9800
C(24)-H(20)	0.9700
C(24)-H(19)	0.9700
C(25)-C(32)	1.349(3)
C(25)-C(26)	1.478(3)
C(26)-C(34)	1.390(3)
C(26)-C(27)	1.395(3)
C(27)-C(28)	1.367(3)
C(27)-H(26)	0.9300
C(28)-C(29)	1.388(3)



C(28)-H(25)	0.9300
C(29)-C(33)	1.379(3)
C(30)-H(18)	0.9600
C(30)-H(21)	0.9600
C(30)-H(22)	0.9600
C(31)-C(32)	1.441(3)
C(32)-H(27)	0.9300
C(33)-C(34)	1.386(3)
C(33)-H(24)	0.9300
C(34)-H(23)	0.9300
C(35)-C(36)	1.376(3)
C(35)-H(30)	0.9300
C(36)-H(29)	0.9300

C(2)-O(1)-C(1)	117.91(17)
C(6)-O(2)-C(7)	118.44(16)
C(15)-O(3)-C(8)	121.79(16)
C(25)-O(5)-C(24)	117.99(16)
C(29)-O(6)-C(30)	118.65(17)
C(31)-O(7)-C(23)	122.70(16)
O(1)-C(1)-H(3)	109.5
O(1)-C(1)-H(1)	109.5
H(3)-C(1)-H(1)	109.5
O(1)-C(1)-H(16)	109.5
H(3)-C(1)-H(16)	109.5
H(1)-C(1)-H(16)	109.5
O(1)-C(2)-C(13)	124.98(19)
O(1)-C(2)-C(3)	115.44(18)
C(13)-C(2)-C(3)	119.59(19)
C(4)-C(3)-C(2)	120.24(19)
C(4)-C(3)-H(12)	119.9
C(2)-C(3)-H(12)	119.9
C(3)-C(4)-C(5)	121.46(19)
C(3)-C(4)-H(13)	119.3
C(5)-C(4)-H(13)	119.3
C(14)-C(5)-C(4)	117.16(18)
C(14)-C(5)-C(6)	121.97(18)
C(4)-C(5)-C(6)	120.87(17)

O(2)-C(6)-C(16)	126.61(19)
O(2)-C(6)-C(5)	112.11(17)
C(16)-C(6)-C(5)	121.26(18)
O(2)-C(7)-C(8)	114.01(16)
O(2)-C(7)-H(10)	108.7
C(8)-C(7)-H(10)	108.7
O(2)-C(7)-H(11)	108.7
C(8)-C(7)-H(11)	108.7
H(10)-C(7)-H(11)	107.6
O(3)-C(8)-C(7)	112.78(18)
O(3)-C(8)-C(9)	106.15(16)
C(7)-C(8)-C(9)	111.36(16)
O(3)-C(8)-H(9)	108.8
C(7)-C(8)-H(9)	108.8
C(9)-C(8)-H(9)	108.8
C(10)-C(9)-C(18)	118.7(2)
C(10)-C(9)-C(8)	121.8(2)
C(18)-C(9)-C(8)	119.44(19)
C(9)-C(10)-C(11)	120.5(2)
C(9)-C(10)-H(8)	119.8
C(11)-C(10)-H(8)	119.8
C(12)-C(11)-C(10)	120.2(2)
C(12)-C(11)-H(7)	119.9
C(10)-C(11)-H(7)	119.9
C(11)-C(12)-C(17)	119.9(2)
C(11)-C(12)-H(2)	120.1
C(17)-C(12)-H(2)	120.1
C(2)-C(13)-C(14)	119.61(19)
C(2)-C(13)-H(15)	120.2
C(14)-C(13)-H(15)	120.2
C(13)-C(14)-C(5)	121.93(19)
C(13)-C(14)-H(14)	119.0
C(5)-C(14)-H(14)	119.0
O(4)-C(15)-O(3)	115.9(2)
O(4)-C(15)-C(16)	120.8(2)
O(3)-C(15)-C(16)	123.2(2)
C(6)-C(16)-C(15)	135.8(2)
C(6)-C(16)-H(4)	112.1

C(15)-C(16)-H(4)	112.1
C(12)-C(17)-C(18)	120.2(2)
C(12)-C(17)-H(5)	119.9
C(18)-C(17)-H(5)	119.9
C(17)-C(18)-C(9)	120.5(2)
C(17)-C(18)-H(6)	119.7
C(9)-C(18)-H(6)	119.7
C(20)-C(19)-C(36)	119.5(2)
C(20)-C(19)-H(17)	120.2
C(36)-C(19)-H(17)	120.2
C(19)-C(20)-C(21)	120.8(2)
C(19)-C(20)-H(32)	119.6
C(21)-C(20)-H(32)	119.6
C(20)-C(21)-C(22)	120.1(2)
C(20)-C(21)-H(31)	119.9
C(22)-C(21)-H(31)	119.9
C(21)-C(22)-C(35)	118.54(19)
C(21)-C(22)-C(23)	122.4(2)
C(35)-C(22)-C(23)	119.05(19)
O(7)-C(23)-C(24)	112.66(18)
O(7)-C(23)-C(22)	105.82(16)
C(24)-C(23)-C(22)	112.37(16)
O(7)-C(23)-H(28)	108.6
C(24)-C(23)-H(28)	108.6
C(22)-C(23)-H(28)	108.6
O(5)-C(24)-C(23)	113.43(16)
O(5)-C(24)-H(20)	108.9
C(23)-C(24)-H(20)	108.9
O(5)-C(24)-H(19)	108.9
C(23)-C(24)-H(19)	108.9
H(20)-C(24)-H(19)	107.7
O(5)-C(25)-C(32)	126.64(18)
O(5)-C(25)-C(26)	112.03(17)
C(32)-C(25)-C(26)	121.32(18)
C(34)-C(26)-C(27)	117.64(18)
C(34)-C(26)-C(25)	121.44(17)
C(27)-C(26)-C(25)	120.92(17)
C(28)-C(27)-C(26)	121.55(19)

C(28)-C(27)-H(26)	119.2
C(26)-C(27)-H(26)	119.2
C(27)-C(28)-C(29)	120.03(19)
C(27)-C(28)-H(25)	120.0
C(29)-C(28)-H(25)	120.0
O(6)-C(29)-C(33)	125.12(19)
O(6)-C(29)-C(28)	115.13(18)
C(33)-C(29)-C(28)	119.75(18)
O(6)-C(30)-H(18)	109.5
O(6)-C(30)-H(21)	109.5
H(18)-C(30)-H(21)	109.5
O(6)-C(30)-H(22)	109.5
H(18)-C(30)-H(22)	109.5
H(21)-C(30)-H(22)	109.5
O(8)-C(31)-O(7)	115.5(2)
O(8)-C(31)-C(32)	120.7(2)
O(7)-C(31)-C(32)	123.7(2)
C(25)-C(32)-C(31)	135.2(2)
C(25)-C(32)-H(27)	112.4
C(31)-C(32)-H(27)	112.4
C(29)-C(33)-C(34)	119.78(19)
C(29)-C(33)-H(24)	120.1
C(34)-C(33)-H(24)	120.1
C(33)-C(34)-C(26)	121.21(19)
C(33)-C(34)-H(23)	119.4
C(26)-C(34)-H(23)	119.4
C(36)-C(35)-C(22)	120.7(2)
C(36)-C(35)-H(30)	119.6
C(22)-C(35)-H(30)	119.6
C(19)-C(36)-C(35)	120.3(2)
C(19)-C(36)-H(29)	119.9
C(35)-C(36)-H(29)	119.9

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Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for 151129\_0M. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

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	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
O(1)	46(1)	39(1)	93(1)	-7(1)	-6(1)	1(1)
O(2)	38(1)	38(1)	78(1)	-6(1)	-9(1)	-2(1)
O(3)	38(1)	43(1)	88(1)	-6(1)	-4(1)	-4(1)
O(4)	37(1)	54(1)	131(2)	7(1)	-5(1)	-9(1)
O(5)	36(1)	35(1)	74(1)	-1(1)	-7(1)	0(1)
O(6)	46(1)	37(1)	110(1)	-1(1)	-9(1)	4(1)
O(7)	39(1)	39(1)	94(1)	-8(1)	-1(1)	-1(1)
O(8)	39(1)	56(1)	159(2)	9(1)	14(1)	-9(1)
C(1)	57(2)	43(1)	101(2)	-9(1)	0(1)	-10(1)
C(2)	41(1)	41(1)	53(1)	-6(1)	4(1)	3(1)
C(3)	39(1)	45(1)	65(2)	0(1)	-6(1)	4(1)
C(4)	39(1)	45(1)	55(1)	-4(1)	-6(1)	-4(1)
C(5)	37(1)	42(1)	43(1)	-2(1)	0(1)	-1(1)
C(6)	36(1)	45(1)	42(1)	-2(1)	-3(1)	2(1)
C(7)	45(1)	40(1)	57(1)	-3(1)	-10(1)	2(1)
C(8)	41(1)	41(1)	47(1)	-1(1)	-1(1)	-4(1)
C(9)	40(1)	39(1)	44(1)	-6(1)	-3(1)	-3(1)
C(10)	51(2)	50(1)	53(1)	7(1)	6(1)	-2(1)
C(11)	60(2)	43(1)	67(2)	10(1)	-6(1)	-3(1)
C(12)	55(2)	44(1)	70(2)	-9(1)	-11(1)	6(1)
C(13)	44(1)	45(1)	60(2)	-9(1)	-8(1)	-2(1)
C(14)	42(1)	47(1)	58(1)	-3(1)	-9(1)	2(1)
C(15)	38(1)	46(1)	65(2)	3(1)	-8(1)	-4(1)
C(16)	39(1)	44(1)	60(2)	3(1)	-1(1)	0(1)
C(17)	41(1)	58(2)	69(2)	-15(1)	4(1)	1(1)
C(18)	49(1)	44(1)	55(1)	1(1)	6(1)	-8(1)
C(19)	62(2)	42(1)	82(2)	-17(1)	-14(1)	12(1)
C(20)	67(2)	37(1)	75(2)	5(1)	-13(1)	-7(1)
C(21)	45(1)	46(1)	58(2)	2(1)	-1(1)	-4(1)
C(22)	38(1)	37(1)	43(1)	-4(1)	-2(1)	0(1)
C(23)	36(1)	39(1)	49(1)	-1(1)	-2(1)	0(1)
C(24)	44(1)	36(1)	57(1)	-2(1)	-9(1)	3(1)
C(25)	39(1)	40(1)	40(1)	-1(1)	0(1)	3(1)
C(26)	41(1)	38(1)	42(1)	-1(1)	3(1)	-1(1)
C(27)	41(1)	42(1)	59(1)	-4(1)	-7(1)	-2(1)
C(28)	39(1)	45(1)	66(2)	1(1)	-5(1)	6(1)

C(29)	40(1)	36(1)	62(1)	0(1)	3(1)	4(1)
C(30)	58(2)	40(1)	92(2)	3(1)	-6(1)	-5(1)
C(31)	41(1)	45(1)	67(2)	4(1)	2(1)	0(1)
C(32)	38(1)	42(1)	57(1)	2(1)	6(1)	1(1)
C(33)	38(1)	42(1)	56(1)	-6(1)	1(1)	-4(1)
C(34)	38(1)	43(1)	54(1)	0(1)	-2(1)	3(1)
C(35)	49(1)	45(1)	54(1)	-4(1)	8(1)	-2(1)
C(36)	51(2)	59(2)	68(2)	-16(1)	6(1)	9(1)

Table 5. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for 151129\_0M.

	x	y	z	U(eq)
H(3)	8216	4530	9554	101
H(1)	7758	5164	8847	101
H(16)	8659	4508	8608	101
H(12)	5899	2938	8065	60
H(13)	6115	1542	8122	56
H(10)	8709	-595	9787	57
H(11)	9835	-545	9307	57
H(9)	8578	-812	7973	52
H(8)	8300	-2532	9338	62
H(7)	9374	-3718	9318	69
H(2)	10963	-3761	8529	68
H(15)	8859	3230	9417	60
H(14)	9058	1821	9491	59
H(4)	6140	422	8792	57
H(5)	11501	-2612	7774	67
H(6)	10428	-1427	7780	59
H(17)	5917	-2405	3667	75
H(32)	4238	-2359	4331	72
H(31)	3173	-1170	4299	60
H(28)	3567	530	2968	50
H(20)	3739	856	4762	55
H(19)	4853	869	4263	55

H(26)	1078	2928	3117	57
H(25)	869	4325	3006	60
H(18)	3255	5949	4357	96
H(21)	2738	6568	3658	96
H(22)	3642	5924	3395	96
H(27)	1147	1827	3859	55
H(24)	3936	4642	4182	55
H(23)	4136	3230	4304	54
H(30)	5496	-64	2916	59
H(29)	6551	-1252	2966	71

**(b) X-ray Crystallographic structure and data of compound (3o).**

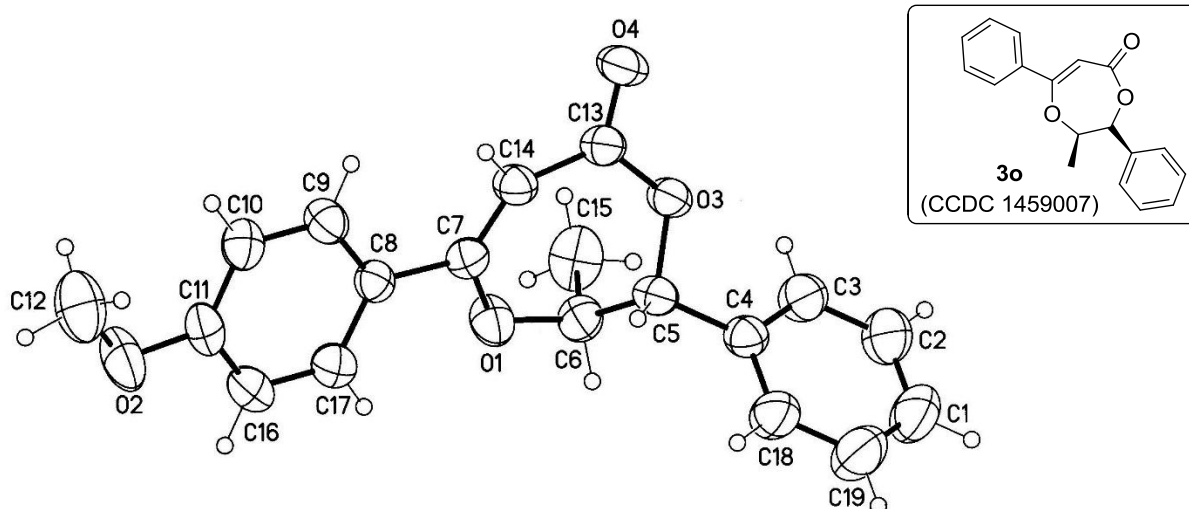


Table 7. Crystal data and structure refinement for MO\_160219\_0M.

Identification code	mo_160219_0m	
Empirical formula	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	
Formula weight	310.33	
Temperature	302(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2 <sub>1</sub> /n	
Unit cell dimensions	a = 5.7294(5) Å	α = 90°.
	b = 16.4971(16) Å	β = 96.391(2)°.
	c = 16.9275(16) Å	γ = 90°.
Volume	1590.0(3) Å <sup>3</sup>	

Z	4
Density (calculated)	1.296 Mg/m <sup>3</sup>
Absorption coefficient	0.090 mm <sup>-1</sup>
F(000)	656
Crystal size	0.15 x 0.12 x 0.10 mm <sup>3</sup>
Theta range for data collection	1.729 to 26.406°.
Index ranges	-7<=h<=4, -20<=k<=20, -21<=l<=20
Reflections collected	13264
Independent reflections	3257 [R(int) = 0.0492]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.8614
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3257 / 0 / 210
Goodness-of-fit on F <sup>2</sup>	1.009
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1007
R indices (all data)	R1 = 0.0982, wR2 = 0.1197
Extinction coefficient	n/a
Largest diff. peak and hole	0.119 and -0.157 e.Å <sup>-3</sup>

Table 8. Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for MO\_160219\_0M.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{ij}$  tensor.

	x	y	z	U(eq)
O(1)	4797(2)	747(1)	3092(1)	52(1)
O(2)	8925(3)	-2701(1)	3702(1)	73(1)
O(3)	1514(2)	1881(1)	4012(1)	46(1)
O(4)	-955(2)	1086(1)	4520(1)	59(1)
C(1)	5062(5)	4545(2)	3741(2)	76(1)
C(2)	2929(4)	4251(1)	3426(2)	66(1)
C(3)	2508(4)	3430(1)	3427(1)	54(1)
C(4)	4224(3)	2892(1)	3743(1)	44(1)
C(5)	3821(3)	1992(1)	3767(1)	41(1)
C(6)	4030(4)	1574(1)	2978(1)	47(1)
C(7)	3994(3)	265(1)	3646(1)	39(1)
C(8)	5205(3)	-532(1)	3654(1)	38(1)
C(9)	4475(3)	-1192(1)	4073(1)	46(1)



C(10)	5657(4)	-1919(1)	4101(1)	48(1)
C(11)	7614(4)	-2007(1)	3704(1)	49(1)
C(12)	8475(5)	-3322(2)	4234(2)	84(1)
C(13)	882(3)	1130(1)	4230(1)	42(1)
C(14)	2355(3)	432(1)	4132(1)	42(1)
C(15)	1870(4)	1599(2)	2385(1)	69(1)
C(16)	8341(4)	-1368(1)	3271(1)	57(1)
C(17)	7160(3)	-644(1)	3247(1)	50(1)
C(18)	6377(4)	3200(1)	4052(1)	61(1)
C(19)	6782(4)	4022(2)	4053(2)	79(1)

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Table 9. Bond lengths [ $\text{\AA}$ ] and angles [ $^\circ$ ] for MO\_160219\_0M.

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O(1)-C(7)	1.348(2)
O(1)-C(6)	1.439(2)
O(2)-C(11)	1.371(2)
O(2)-C(12)	1.407(3)
O(3)-C(13)	1.354(2)
O(3)-C(5)	1.441(2)
O(4)-C(13)	1.212(2)
C(1)-C(2)	1.367(3)
C(1)-C(19)	1.370(3)
C(1)-H(1)	0.9300
C(2)-C(3)	1.375(3)
C(2)-H(18)	0.9300
C(3)-C(4)	1.387(3)
C(3)-H(17)	0.9300
C(4)-C(18)	1.381(3)
C(4)-C(5)	1.505(3)
C(5)-C(6)	1.518(3)
C(5)-H(14)	0.9800
C(6)-C(15)	1.505(3)
C(6)-H(3)	0.9800
C(7)-C(14)	1.344(2)
C(7)-C(8)	1.486(3)
C(8)-C(9)	1.388(3)
C(8)-C(17)	1.391(3)

C(9)-C(10)	1.377(3)
C(9)-H(12)	0.9300
C(10)-C(11)	1.377(3)
C(10)-H(11)	0.9300
C(11)-C(16)	1.374(3)
C(12)-H(7)	0.9600
C(12)-H(8)	0.9600
C(12)-H(2)	0.9600
C(13)-C(14)	1.448(3)
C(14)-H(13)	0.9300
C(15)-H(5)	0.9600
C(15)-H(4)	0.9600
C(15)-H(6)	0.9600
C(16)-C(17)	1.372(3)
C(16)-H(10)	0.9300
C(17)-H(9)	0.9300
C(18)-C(19)	1.377(3)
C(18)-H(16)	0.9300
C(19)-H(15)	0.9300

C(7)-O(1)-C(6)	121.97(15)
C(11)-O(2)-C(12)	117.86(19)
C(13)-O(3)-C(5)	118.42(14)
C(2)-C(1)-C(19)	120.0(2)
C(2)-C(1)-H(1)	120.0
C(19)-C(1)-H(1)	120.0
C(1)-C(2)-C(3)	119.9(2)
C(1)-C(2)-H(18)	120.0
C(3)-C(2)-H(18)	120.0
C(2)-C(3)-C(4)	120.9(2)
C(2)-C(3)-H(17)	119.5
C(4)-C(3)-H(17)	119.5
C(18)-C(4)-C(3)	118.4(2)
C(18)-C(4)-C(5)	119.01(18)
C(3)-C(4)-C(5)	122.56(18)
O(3)-C(5)-C(4)	106.29(14)
O(3)-C(5)-C(6)	111.17(15)
C(4)-C(5)-C(6)	113.39(16)

O(3)-C(5)-H(14)	108.6
C(4)-C(5)-H(14)	108.6
C(6)-C(5)-H(14)	108.6
O(1)-C(6)-C(15)	109.38(17)
O(1)-C(6)-C(5)	111.41(16)
C(15)-C(6)-C(5)	115.71(17)
O(1)-C(6)-H(3)	106.6
C(15)-C(6)-H(3)	106.6
C(5)-C(6)-H(3)	106.6
C(14)-C(7)-O(1)	128.30(18)
C(14)-C(7)-C(8)	122.22(17)
O(1)-C(7)-C(8)	109.49(15)
C(9)-C(8)-C(17)	117.05(18)
C(9)-C(8)-C(7)	122.09(17)
C(17)-C(8)-C(7)	120.85(18)
C(10)-C(9)-C(8)	121.72(18)
C(10)-C(9)-H(12)	119.1
C(8)-C(9)-H(12)	119.1
C(11)-C(10)-C(9)	119.9(2)
C(11)-C(10)-H(11)	120.1
C(9)-C(10)-H(11)	120.1
O(2)-C(11)-C(16)	116.13(19)
O(2)-C(11)-C(10)	124.4(2)
C(16)-C(11)-C(10)	119.47(19)
O(2)-C(12)-H(7)	109.5
O(2)-C(12)-H(8)	109.5
H(7)-C(12)-H(8)	109.5
O(2)-C(12)-H(2)	109.5
H(7)-C(12)-H(2)	109.5
H(8)-C(12)-H(2)	109.5
O(4)-C(13)-O(3)	115.85(17)
O(4)-C(13)-C(14)	122.86(18)
O(3)-C(13)-C(14)	121.28(16)
C(7)-C(14)-C(13)	133.62(19)
C(7)-C(14)-H(13)	113.2
C(13)-C(14)-H(13)	113.2
C(6)-C(15)-H(5)	109.5
C(6)-C(15)-H(4)	109.5

H(5)-C(15)-H(4)	109.5
C(6)-C(15)-H(6)	109.5
H(5)-C(15)-H(6)	109.5
H(4)-C(15)-H(6)	109.5
C(17)-C(16)-C(11)	120.4(2)
C(17)-C(16)-H(10)	119.8
C(11)-C(16)-H(10)	119.8
C(16)-C(17)-C(8)	121.5(2)
C(16)-C(17)-H(9)	119.3
C(8)-C(17)-H(9)	119.3
C(19)-C(18)-C(4)	120.4(2)
C(19)-C(18)-H(16)	119.8
C(4)-C(18)-H(16)	119.8
C(1)-C(19)-C(18)	120.4(2)
C(1)-C(19)-H(15)	119.8
C(18)-C(19)-H(15)	119.8

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Symmetry transformations used to generate equivalent atoms:

Table 10. Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for MO\_160219\_0M. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{23}$	$U^{13}$	$U^{12}$
O(1)	69(1)	45(1)	46(1)	7(1)	23(1)	8(1)
O(2)	89(1)	55(1)	79(1)	0(1)	23(1)	29(1)
O(3)	37(1)	42(1)	60(1)	10(1)	14(1)	5(1)
O(4)	43(1)	56(1)	81(1)	10(1)	26(1)	5(1)
C(1)	78(2)	44(1)	106(2)	6(1)	7(2)	-7(1)
C(2)	67(2)	46(1)	84(2)	14(1)	5(1)	10(1)
C(3)	47(1)	48(1)	67(2)	9(1)	1(1)	3(1)
C(4)	41(1)	43(1)	48(1)	6(1)	9(1)	1(1)
C(5)	35(1)	45(1)	44(1)	7(1)	8(1)	3(1)
C(6)	54(1)	41(1)	46(1)	8(1)	11(1)	1(1)
C(7)	38(1)	40(1)	40(1)	2(1)	4(1)	-2(1)
C(8)	38(1)	40(1)	36(1)	-5(1)	3(1)	0(1)
C(9)	47(1)	47(1)	45(1)	1(1)	12(1)	6(1)
C(10)	60(1)	41(1)	43(1)	0(1)	7(1)	3(1)

C(11)	55(1)	45(1)	47(1)	-10(1)	3(1)	12(1)
C(12)	103(2)	58(2)	90(2)	8(2)	6(2)	30(2)
C(13)	36(1)	45(1)	46(1)	5(1)	6(1)	1(1)
C(14)	39(1)	41(1)	48(1)	7(1)	11(1)	2(1)
C(15)	86(2)	63(2)	54(2)	4(1)	-9(1)	5(1)
C(16)	51(1)	56(1)	66(2)	-5(1)	23(1)	6(1)
C(17)	49(1)	48(1)	57(2)	0(1)	15(1)	0(1)
C(18)	46(1)	50(1)	85(2)	5(1)	-1(1)	-1(1)
C(19)	61(2)	57(2)	115(2)	4(2)	-6(2)	-11(1)

Table 11. Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for MO\_160219\_0M.

	x	y	z	U(eq)
H(1)	5346	5101	3744	92
H(18)	1764	4605	3212	79
H(17)	1052	3234	3213	65
H(14)	4978	1754	4171	49
H(3)	5269	1858	2734	56
H(12)	3151	-1140	4341	55
H(11)	5135	-2351	4387	58
H(7)	8629	-3112	4767	126
H(8)	9580	-3755	4200	126
H(2)	6909	-3524	4100	126
H(13)	2116	10	4478	51
H(5)	2189	1335	1904	104
H(4)	1438	2153	2273	104
H(6)	604	1326	2601	104
H(10)	9641	-1428	2992	68
H(9)	7678	-217	2952	61
H(16)	7559	2849	4260	73
H(15)	8232	4225	4267	94

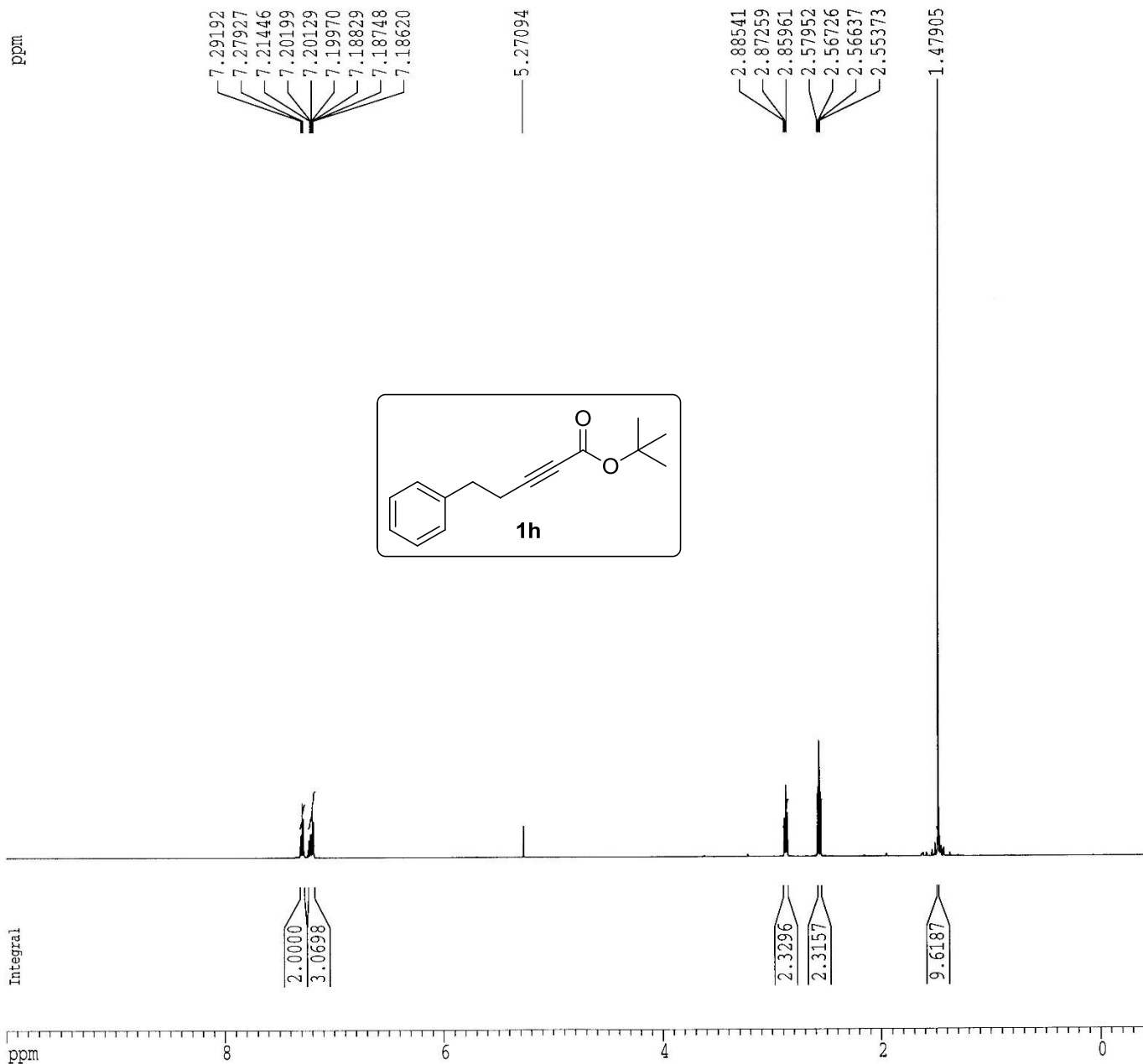
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NAME RFS-2-240  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150409  
Time 13:51  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 9341.984 Hz  
FIDRES 0.291198 Hz  
AQ 1.7170933 sec  
RG 32  
CW 52.400 usec  
DE 6.50 usec  
TE 295.2 K  
D1 2.0000000 sec  
MCKBSC 0.0300000 sec  
MCKBKC 0.0150000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 0.00 dB  
SFO1 500.6035916 MHz

F2 - Processing parameters  
SI 32768  
SF 500.6000000 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 20.00 cm  
PLP 10.000 ppm  
P1 5006.00 Hz  
P2 -0.500 ppm  
P3 -299.10 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 314.26501 Hz/cm



Current Data Parameters  
 NAME RKS-2-240  
 EXPNO 2  
 PROCNO 1

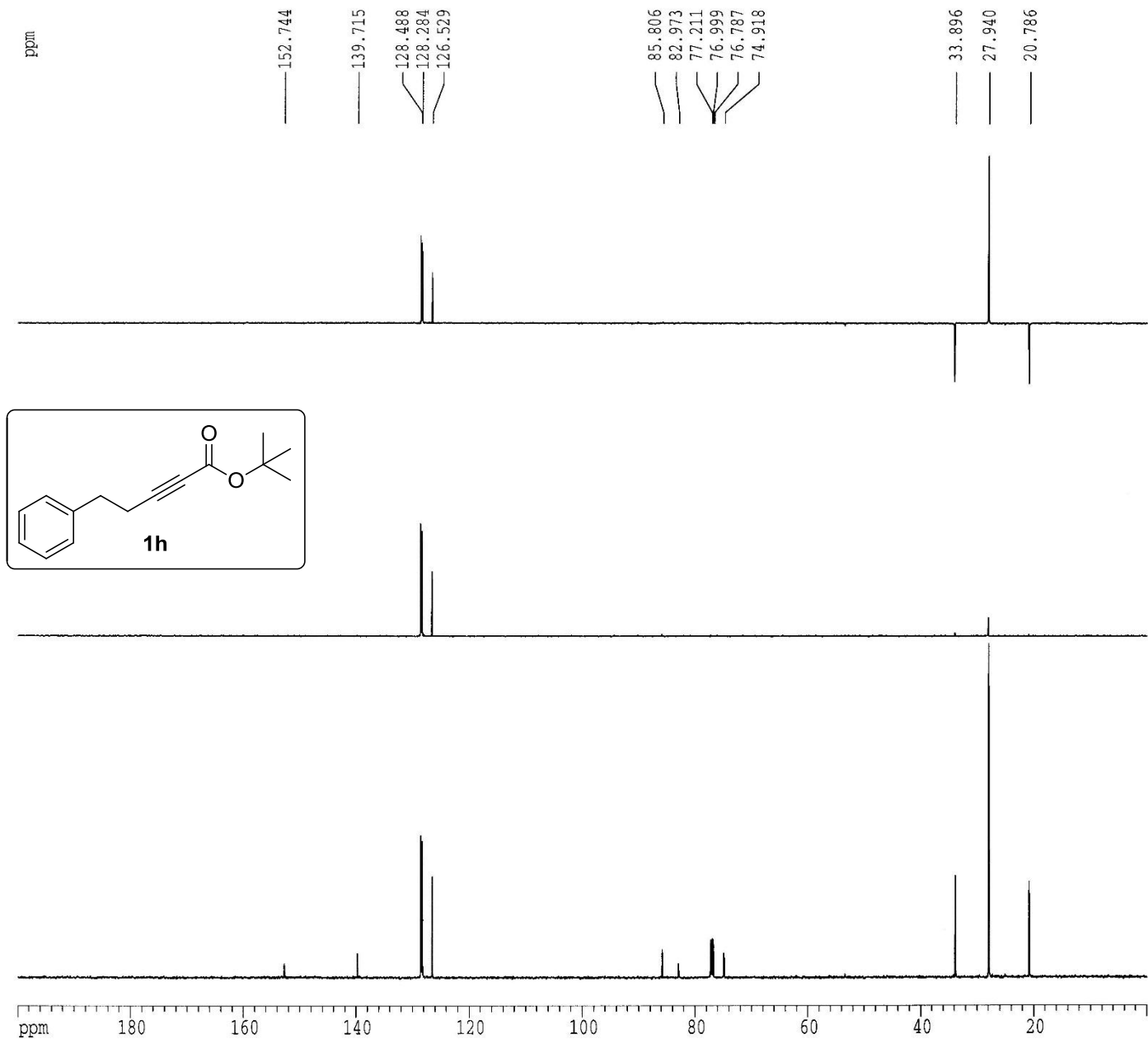
F2 - Acquisition Parameters  
 Date\_ 20150409  
 Time 13.54  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 100  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 296.2 K  
 DI 3.50000000 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 wa1tz16  
 NUC2 1H  
 FCPD2 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  
 WDM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 6.00 cm  
 FLP 200.000 ppm  
 F1 30103.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME          SNK-5029
EXPNO         1
PROCNO        1

F2 - Acquisition Parameters
Date_         20141214
Time          18.26
INSTRUM       spect
PROBHD        5 mm QNP 1H/1
PULPROG       zg
TD            33556
SOLVENT       CDCl3
NS            1
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            295.1 K
D1            2.0000000 sec
MCREST        0.0000000 sec
MCWRK         0.0150000 sec

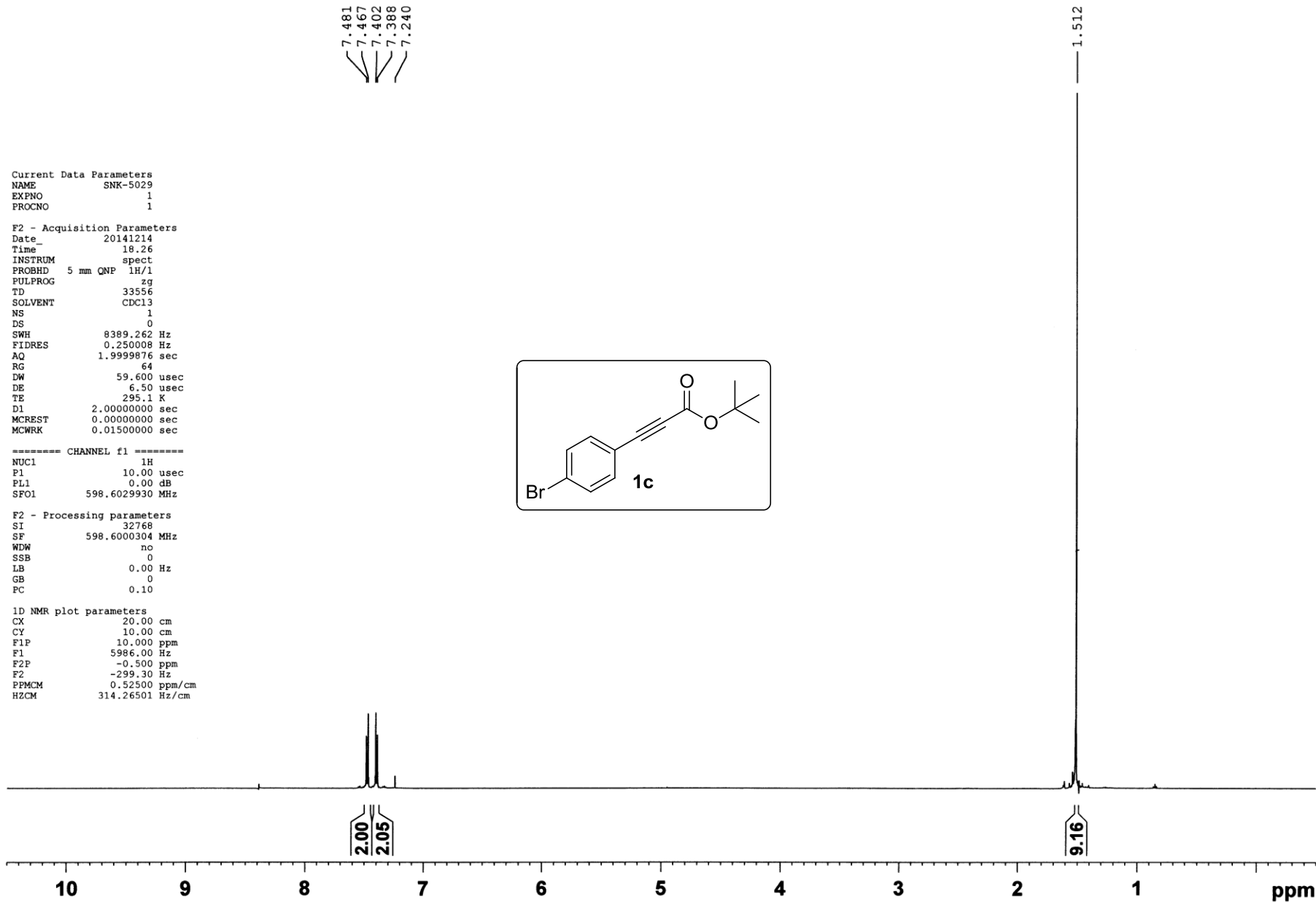
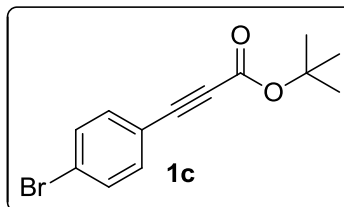
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NUC1           1H
P1             10.00 usec
PL1            0.00 dB
SFO1           598.6029930 MHz

F2 - Processing parameters
SI             32768
SF            598.6000304 MHz
WDW            no
SSB            0
LB             0.00 Hz
GB             0
PC             0.10

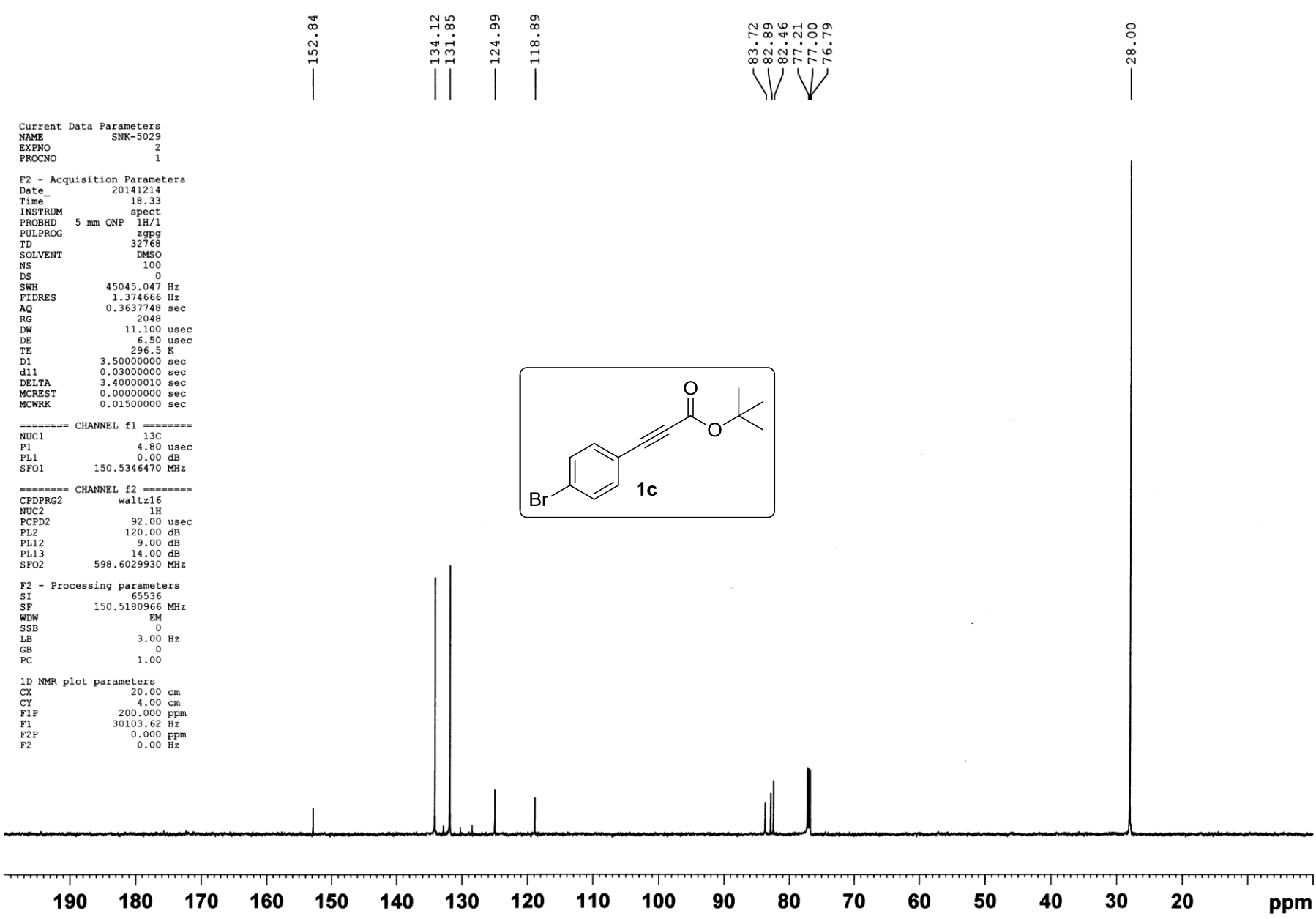
1D NMR plot parameters
CX             20.00 cm
CY             10.00 cm
F1P            10.000 ppm
F1             5986.00 Hz
F2P            -0.500 ppm
F2             -299.30 Hz
PPMCM          0.52500 ppm/cm
HZCM           314.26501 Hz/cm

```

7.481  
7.467  
7.402  
7.388  
7.240







```

Current Data Parameters
NAME      SNK-5029
EXPNO    2
PROCNO    1

F2 - Acquisition Parameters
Date_     20141214
Time      18.33
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         296.5 K
D1         3.5000000 sec
d11        0.03000000 sec
DELTA     3.40000010 sec
MCREST    0.00000000 sec
MCWRK     0.01500000 sec

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

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

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

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

```

— 152.84  
 — 134.12  
 — 131.85  
 — 124.99  
 — 118.89  
 83.72  
 82.89  
 82.46  
 77.21  
 77.00  
 76.79  
 — 28.00



7.454  
7.440  
7.240  
7.135  
7.121

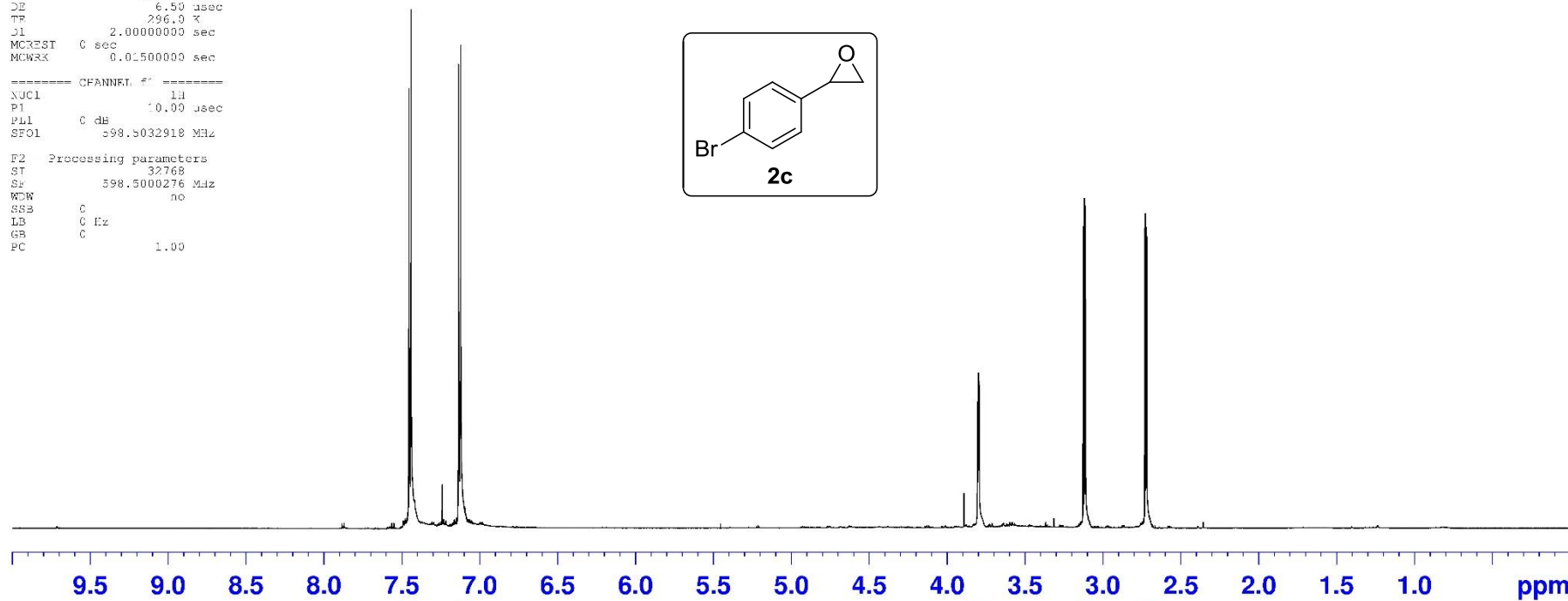
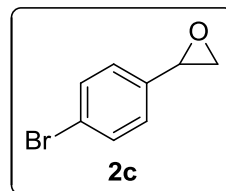
3.805  
3.801  
3.798  
3.794  
3.127  
3.121  
3.118  
3.112  
2.732  
2.728  
2.723  
2.718

Current Data Parameters  
NAME RS 2 81 1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160304  
Time 1.59  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8889.262 Hz  
FIDRES 0.256020 Hz  
AQ 1.9530228 sec  
RG 128  
DW 59.600 usec  
DE 6.50 usec  
TE 296.3 K  
SI 2.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 10.00 usec  
PL1 0 dB  
SFO1 598.5032918 MHz

F2 Processing parameters  
SI 32768  
SF 598.5000276 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

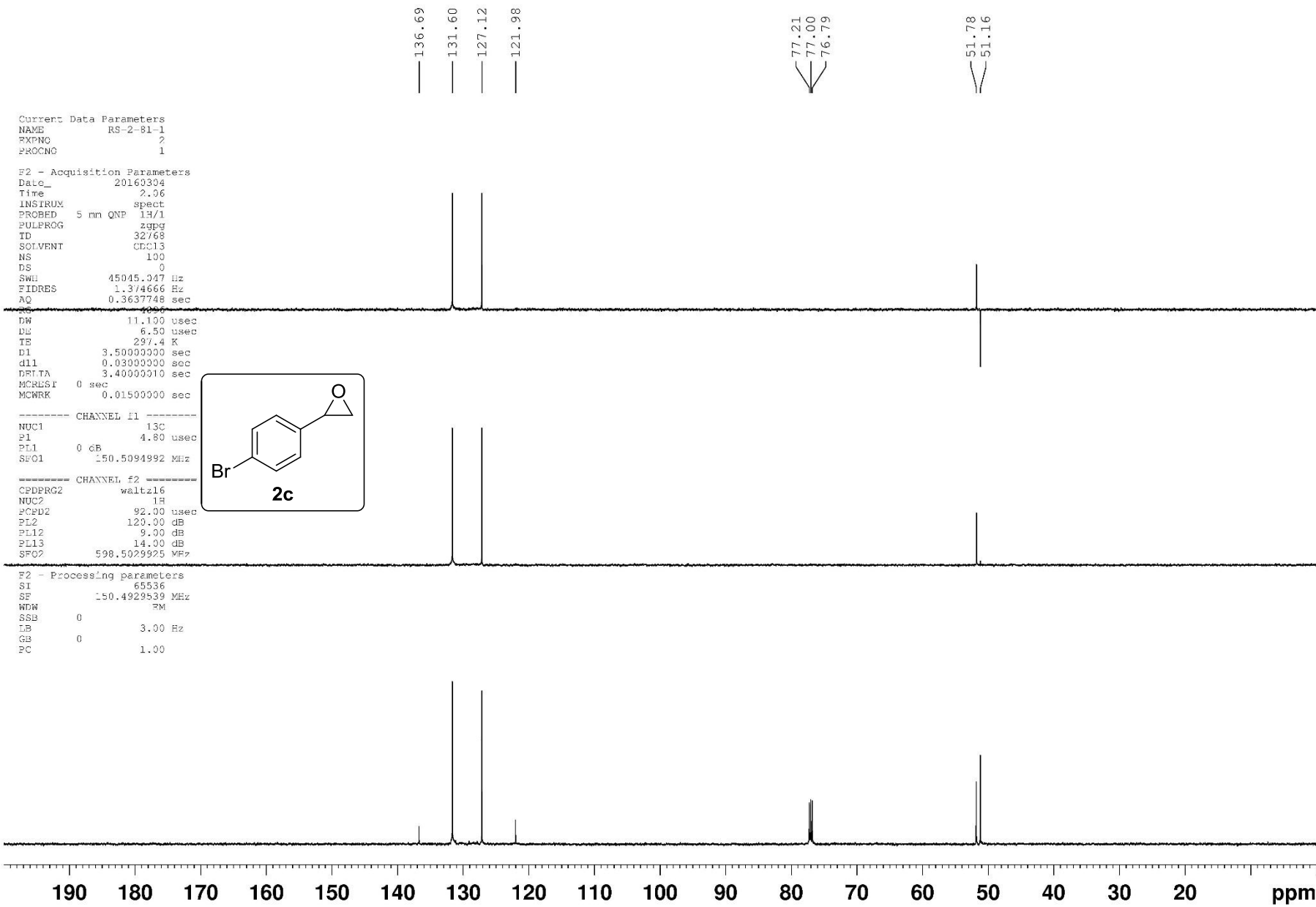


2.04  
2.04

1.01

1.26

1.30







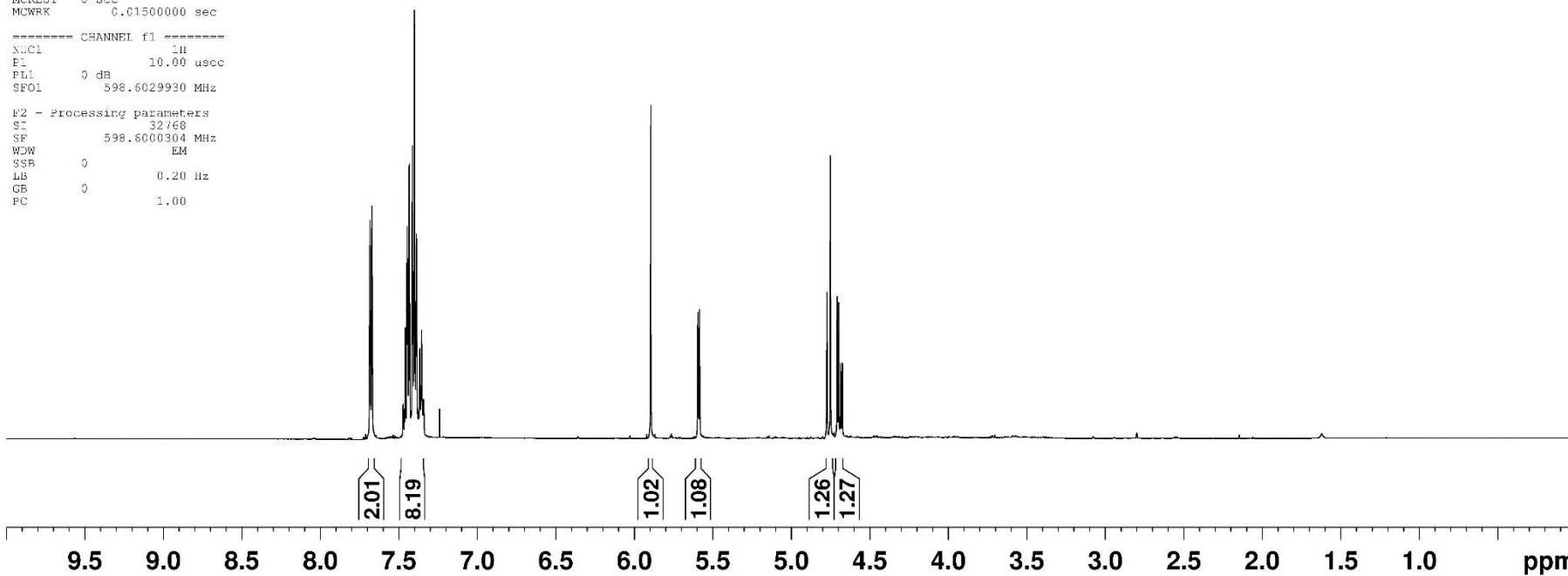
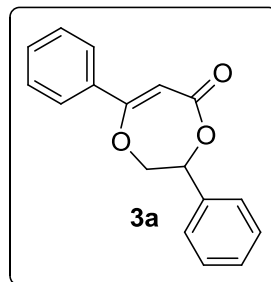
7.683  
7.670  
7.668  
7.471  
7.470  
7.458  
7.454  
7.445  
7.432  
7.414  
7.401  
7.389  
7.368  
7.366  
7.355  
7.350  
7.344  
7.342  
7.241  
7.240

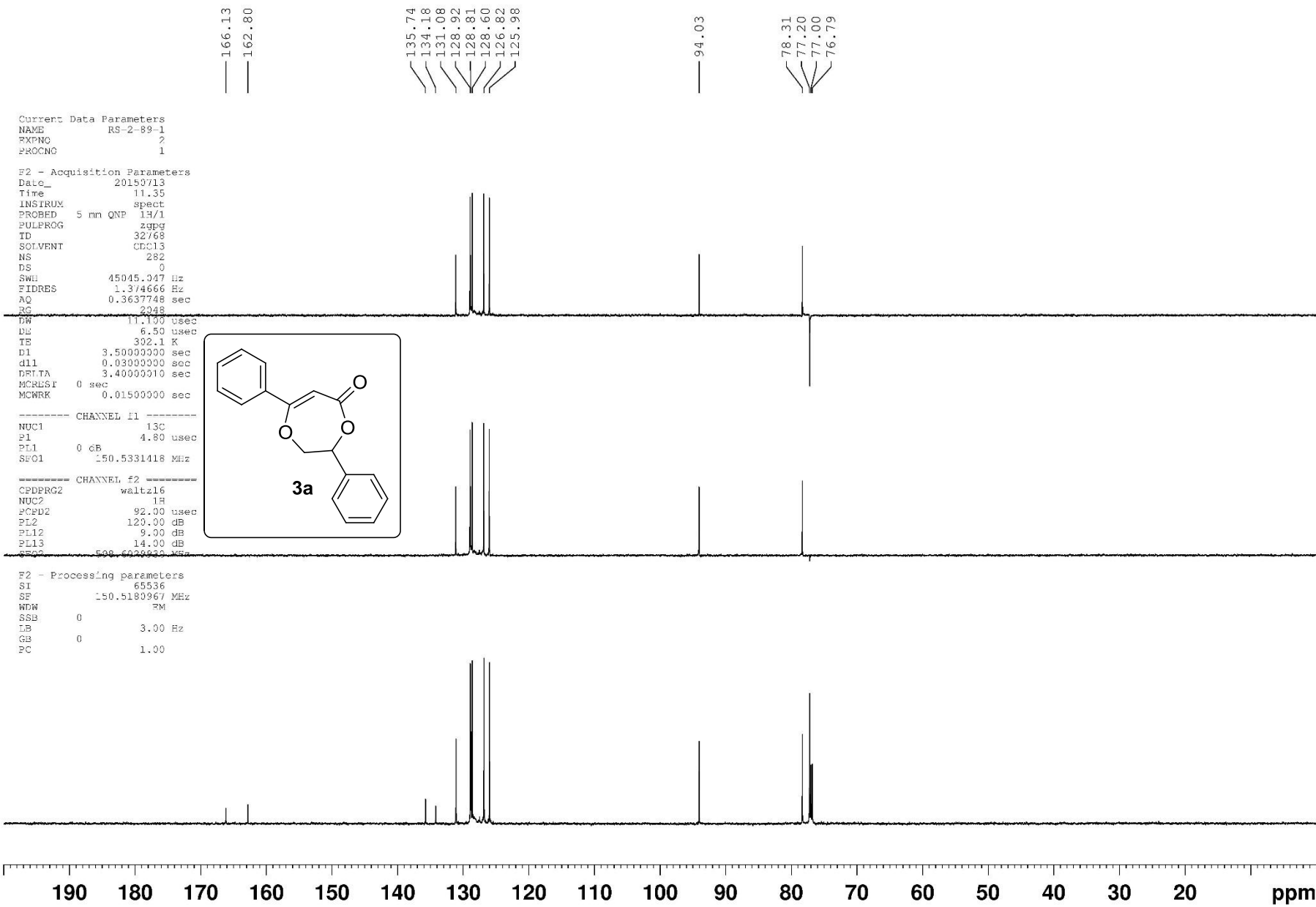
5.895  
5.595  
5.585

4.773  
4.751  
4.707  
4.698  
4.685  
4.675

Current Data Parameters  
NAME RS-2-89-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20150713  
Time 11.32  
INSTRUM spect  
PROBHD 5 mm QNP 1H/  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8889.262 Hz  
FIDRES 0.256020 Hz  
AQ 1.9530228 sec  
RG 128  
RW 59.600 usec  
DE 6.50 usec  
TE 301.6 K  
D1 2.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec





Current Data Parameters  
 NAME RS-2-89-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150713  
 Time 11.35  
 INSTRUM spect  
 PROBED 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 282  
 DS 0  
 SWH 45045.347 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2248  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 302.1 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000000 sec  
 MCHRESF 0 sec  
 MCWRR 0.0150000 sec

----- CHANNEL f1 -----  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0 dB  
 SFO1 150.5331418 MHz

----- CHANNEL f2 -----  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 500.6229950 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.5180967 MHz  
 WDW FM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

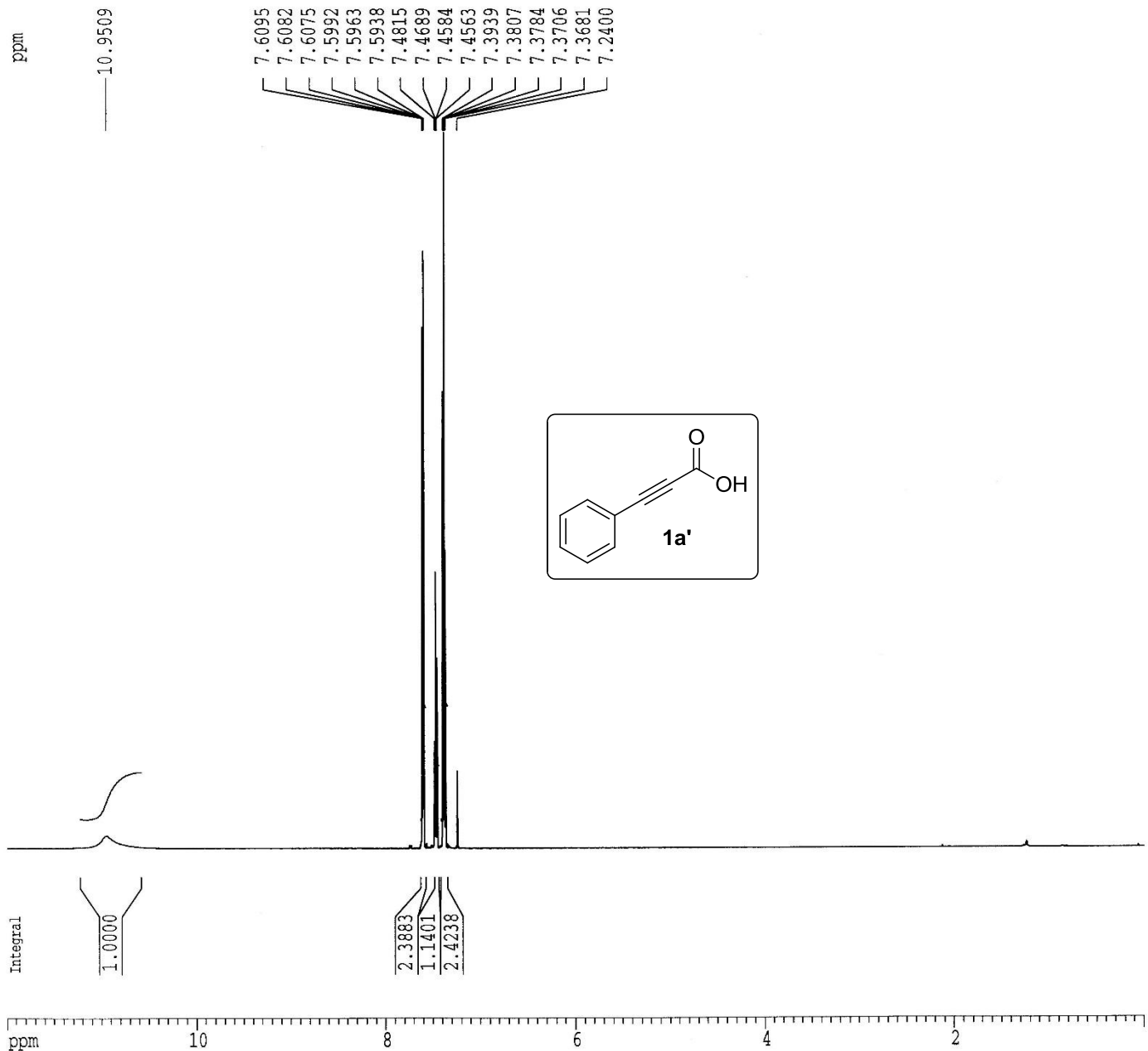
Current Data Parameters  
NAME RS-2-137-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20160429  
Time 12.48  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 9541.984 Hz  
FIDRES 0.291198 Hz  
AQ 1.7170932 sec  
RG 512  
DW 52.400 usec  
DE 6.50 usec  
TE 296.0 K  
D1 1.50000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

==== CHANNEL f1 =====  
NUC1 1H  
P1 8.50 usec  
PL1 3.00 dB  
SFO1 598.5035910 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000275 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 12.50 cm  
F1P 12.000 ppm  
F1 7182.00 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCK 0.60000 ppm/cm  
HZCM 359.10001 Hz/cm





Current Data Parameters  
NAME RS-2-137-1  
EXPNO 2  
PROCNO 1

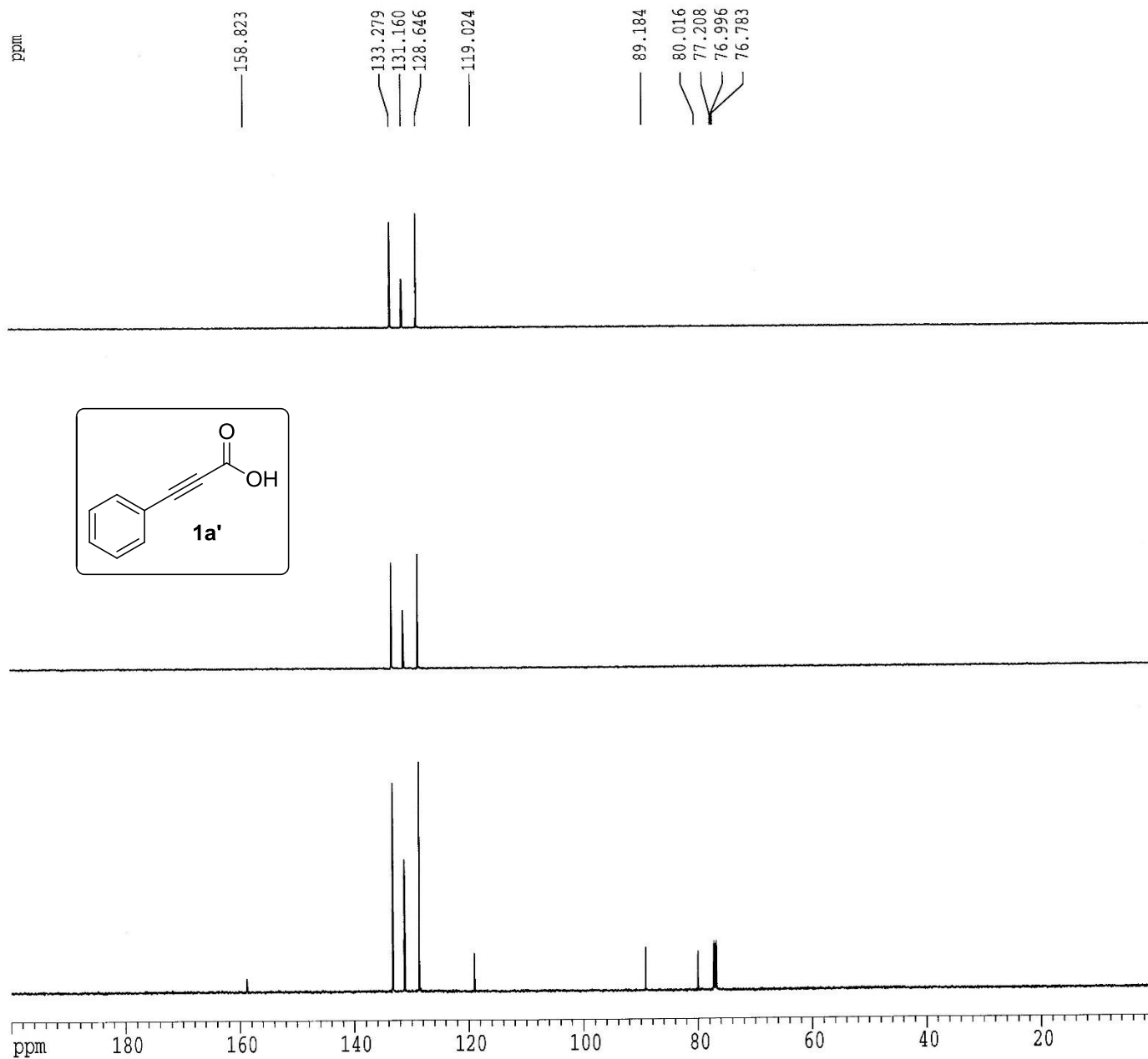
F2 - Acquisition Parameters  
Date\_ 20160429  
Time 12.33  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zgpg  
TD 32768  
SOLVENT CDCl3  
NS 100  
DS 0  
SWE 45045.047 Hz  
FIDRES 1.374666 Hz  
AQ 0.3637748 sec  
RG 4096  
DW 11.100 usec  
DE 6.50 usec  
TE 295.8 K  
D1 3.50000000 sec  
d11 0.03000000 sec  
DELTA 3.40000010 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 13C  
P1 4.80 usec  
PL1 0.00 dB  
SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 92.00 usec  
PL2 120.00 dB  
PL12 9.00 dB  
PL13 14.00 dB  
SFO2 598.5029925 MHz

F2 - Processing parameters  
SI 32768  
SF 150.4929529 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 4.00 cm  
F1P 200.000 ppm  
F1 30098.59 Hz  
F2P 0.000 ppm  
F2 0.00 Hz  
PPMCM 10.00000 ppm/cm  
HZCM 1504.92944 Hz/cm



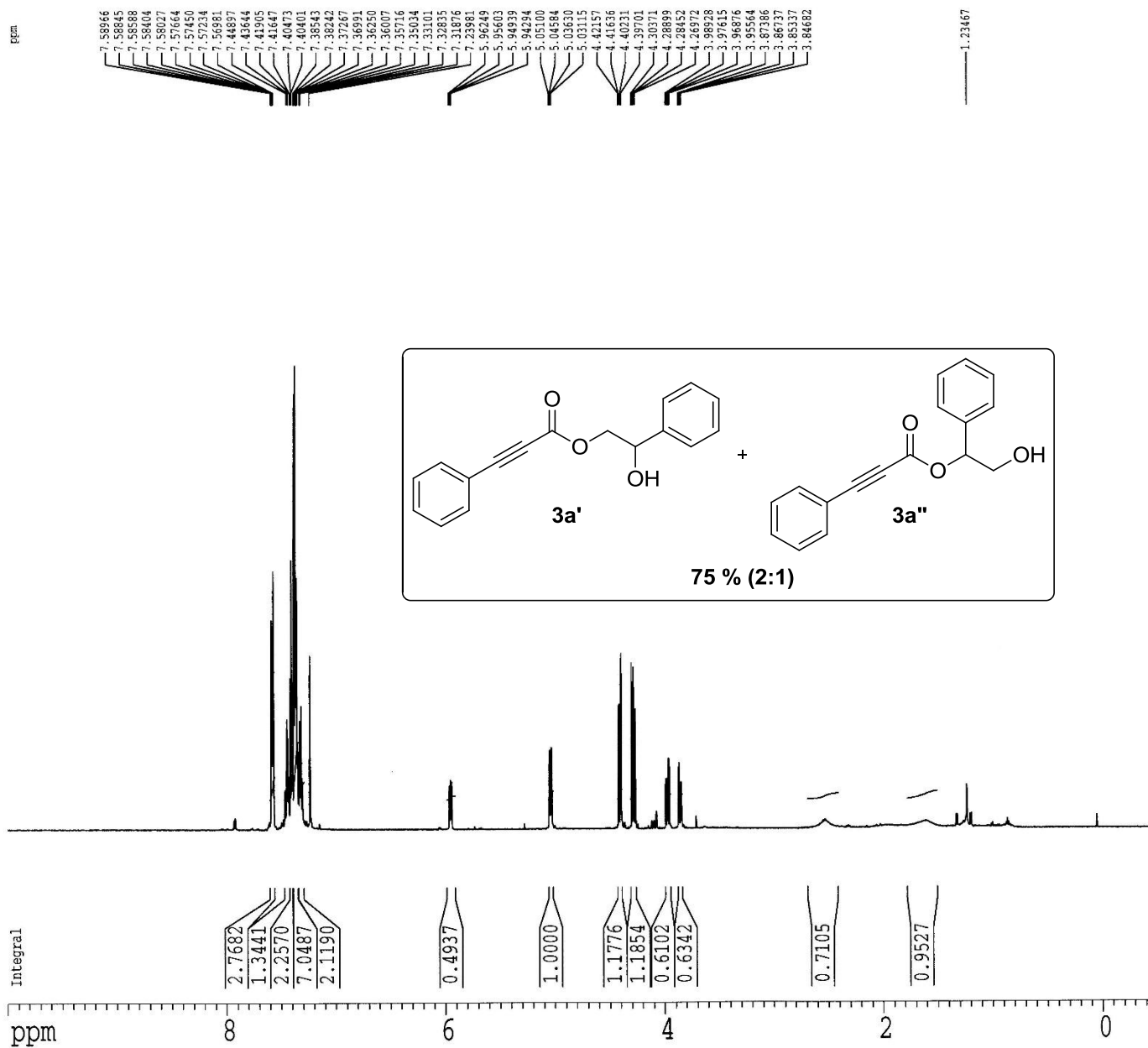
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 NAME RS-2-197-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160415  
 Time 9.24  
 INSTRUM spect  
 PROBEID 5 mm GNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 9541.984 Hz  
 FIDRES 0.291198 Hz  
 AQ 1.7170932 sec  
 RG 128  
 DW 52.400 usec  
 DE 6.50 usec  
 TE 295.0 K  
 U1 2.00000000 sec  
 MCREST 0.00000000 sec  
 MCWEX 0.01500000 sec

==== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SFO1 598.5029925 MHz

F2 - Processing parameters  
 SI 32768  
 SF 598.5000277 MHz  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 FC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 10.000 ppm  
 F1 5985.00 Hz  
 F2P -0.500 ppm  
 F2 -399.25 Hz  
 PPMCM 0.52500 ppm/cm  
 HZCM 314.21249 Hz/cm



Current Data Parameters  
 NAME RS-2-197-1  
 EXPNO 2  
 PROCNO 1

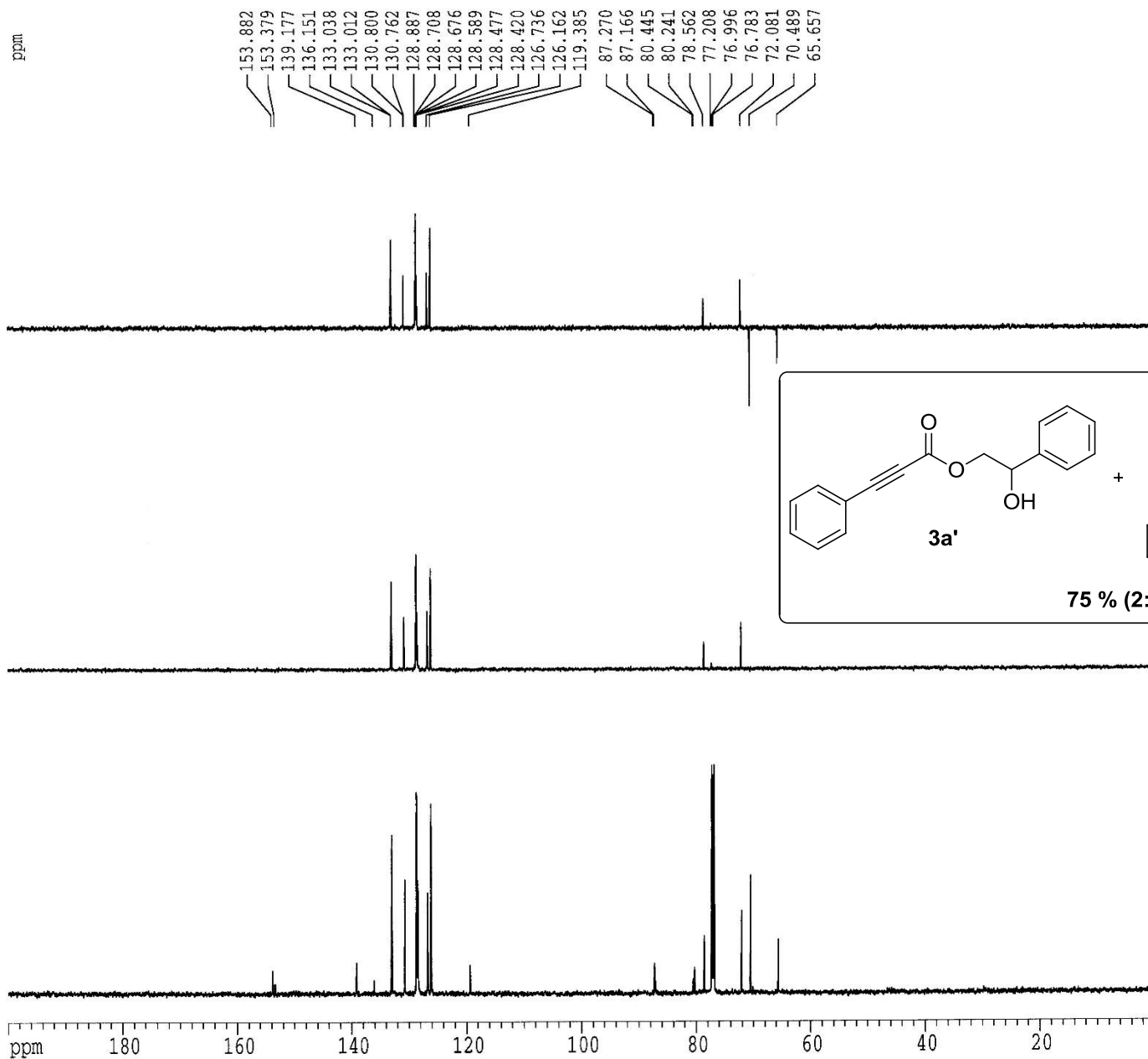
F2 - Acquisition Parameters  
 Date\_ 20160415  
 Time 8.41  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 400  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 295.2 K  
 D1 3.50000000 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  
 SFC1 150.5094992 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 32768  
 SF 150.4929529 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 30098.59 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1504.92944 Hz/cm



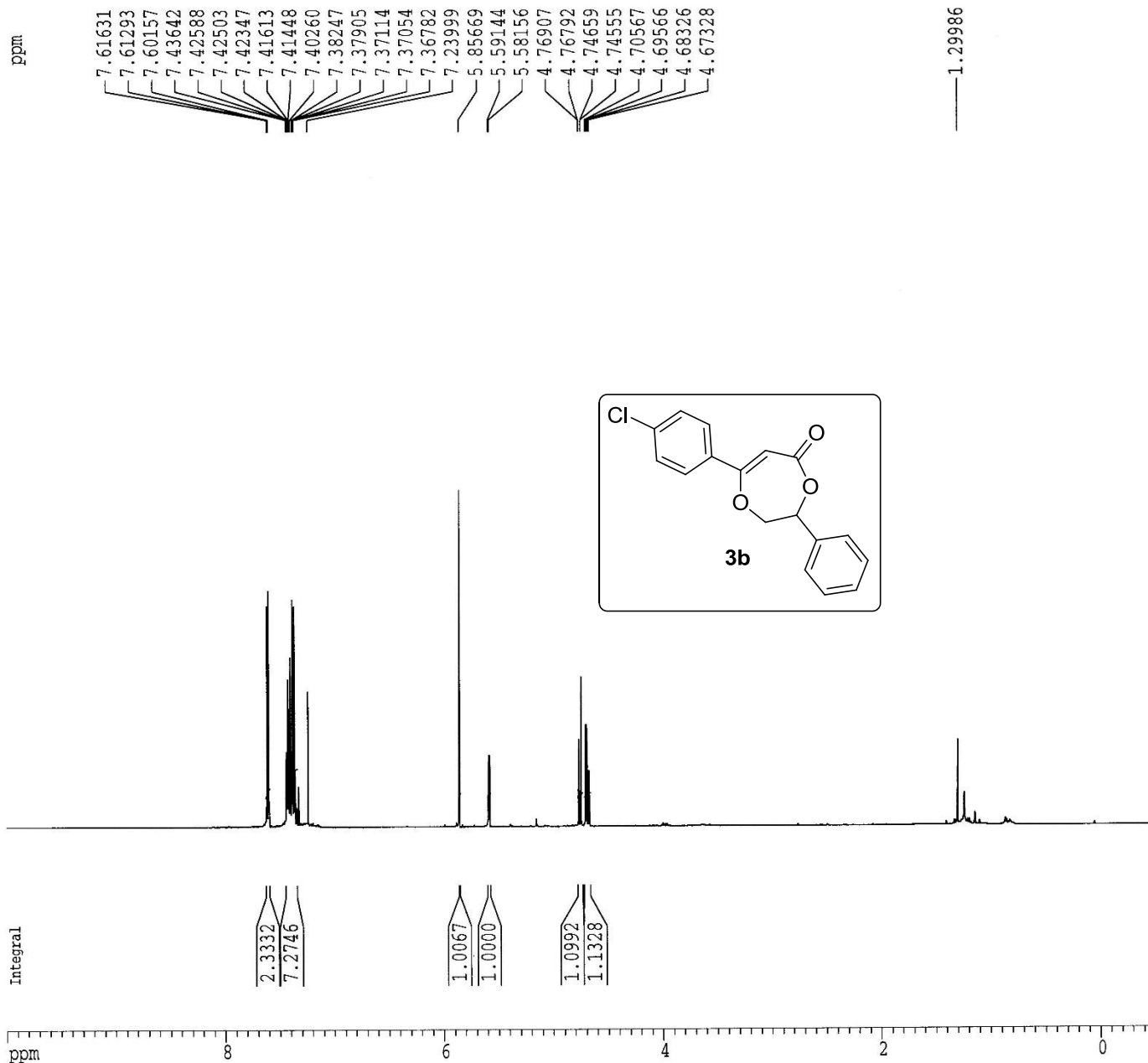
Experiment Data Parameters  
 NAME RS-2-92-1  
 OPER 1  
 PROC 1

15 - Acquisition Parameters  
 DATE\_ 20150817  
 TIME 16.11  
 INSTRUM spect  
 PROBR1 5 cm QNP 1H/1  
 PULPROG zg  
 PC 32768  
 PROGRAM CDCL3  
 CH 16  
 F2 0  
 SFO 3389.262 Hz  
 P1P2 0.256020 Hz  
 AQ 1.4530228 sec  
 R1 512  
 SFO 59.600 usec  
 CP 6.50 usec  
 TE 302.0 K  
 D1 2.0000000 sec  
 D11 0.0000000 sec  
 D12 0.0000000 sec  
 D13 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 CH1 1H  
 PC 8.90 usec  
 P1 0.00 dB  
 SFO 596.6029930 MHz

17 - Processing parameters  
 SI 32768  
 SF 596.6000001 MHz  
 GM no  
 GB 0  
 TE 0.00 Hz  
 AS 0  
 PC 1.00

19 - 1D plot parameters  
 SI 20.00 cm  
 SF 6.00 cm  
 F1 10.000 ppm  
 F2 996.00 Hz  
 F3 0.500 ppm  
 F4 209.10 Hz  
 F5 0.52500 ppm/cm  
 F6 314.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-92-1  
 PULSE 2  
 PROCNO 1

F2 - Acquisition Parameters

DATE\_ 20150827  
 Time 16.16  
 INSTRUM spect  
 PULSEPRG 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TO 32768  
 SOLVENT CDCl3  
 NS 374  
 DS 0  
 SFO 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 LG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 302.9 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MDPRST 0.00000000 sec  
 MDPRK 0.01500000 sec

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

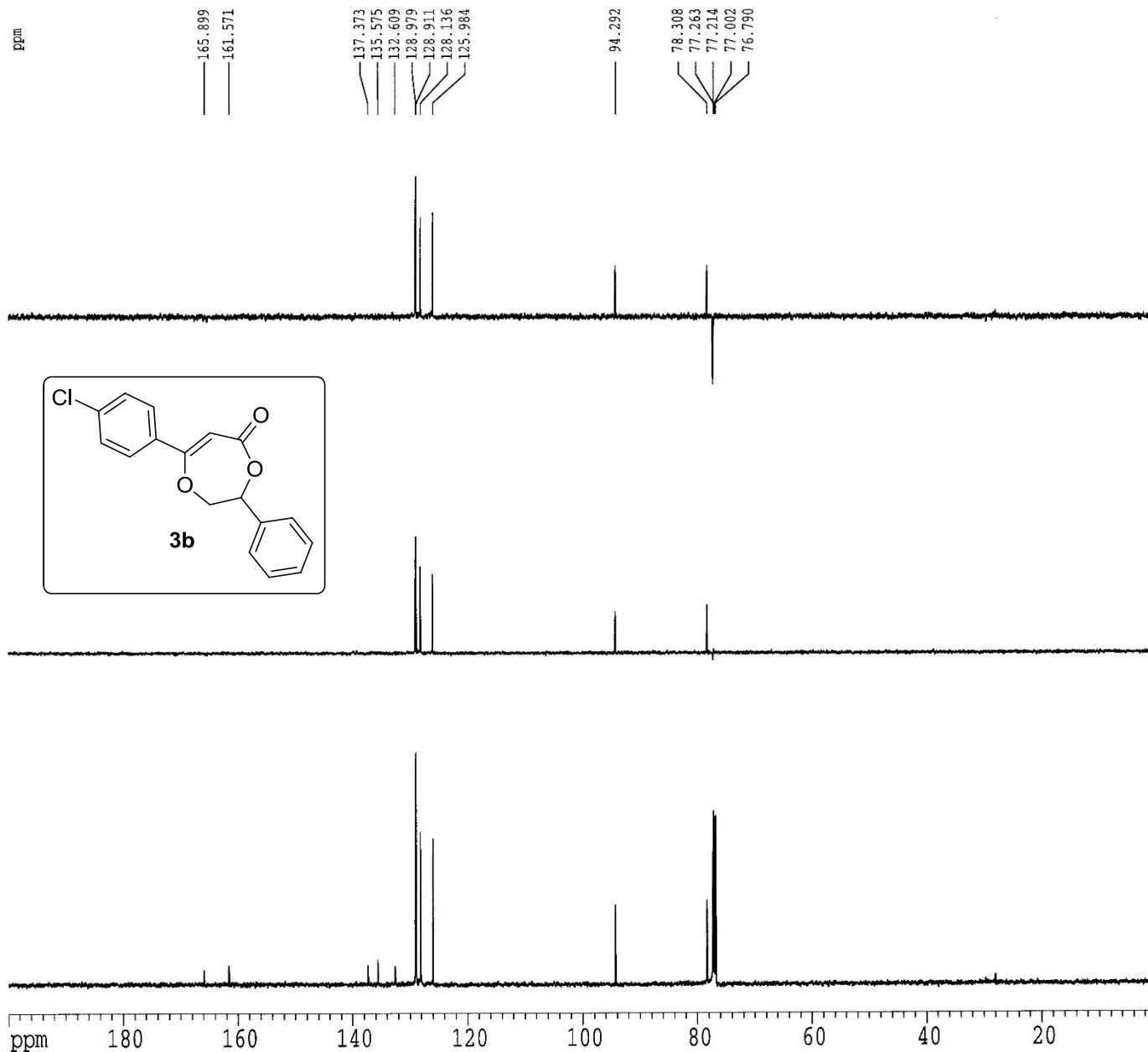
===== CHANNEL f2 =====  
 PULPROG waltz16  
 NAME 1H  
 PULSEPRG 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.6029930 MHz

F2 - Processing parameters

SF 65536  
 CF 150.5180925 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  
 FIP 200.000 ppm  
 F1 30103.62 Hz  
 F2 0.000 ppm  
 F2 0.00 Hz  
 FREQCM 10.00000 ppm/cm  
 RECM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      R02-01-2
EXPNO    1
PROCNO   1

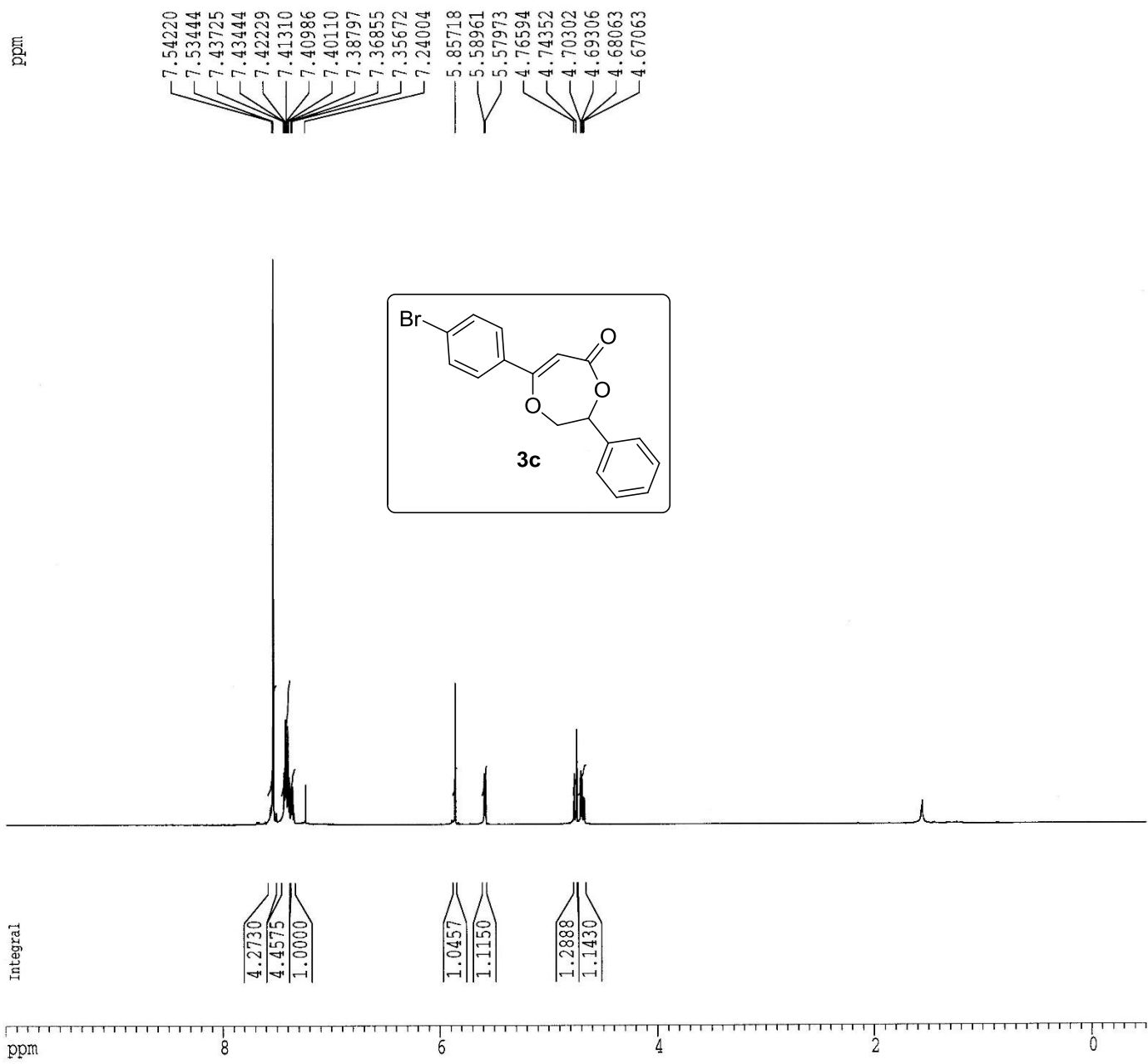
F2 Acquisition Parameters
Date_    20150806
Time     18.48
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD        32768
SOLVENT  CDCl3
NS        16
DS        4
SWH       1329.262 Hz
FIDRES    0.256020 Hz
AQ        1.9530228 sec
RG         512
SFO       50.000 MHz
SF         500.600000 MHz
AQ         0.50 usec
TE        300.2 K
DELTA     1.00000000 sec
WIDEPK    0.03000000 sec
SMPR      0.01500000 sec

***** CHANNEL f1 *****
NUC1      1H
P1         12.00 usec
PL1        0.00 dB
SFO1      500.600000 MHz

F2 - Processing parameters
SI         32768
SF         500.600000 MHz
WDW        EM
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

1D 1H F2 plot parameters
CY         20.00 cm
CY         10.00 cm
FIDP       10.000 ppm
FI         5066.00 Hz
FPC        0.000 ppm
F         -299.10 Hz
FHMW       0.62500 ppm/cm
FHMN       314.26501 Hz/cm

```



Current Data Parameters  
 NAME RS-2-91-2  
 EXPNO 2  
 PROCNO 1

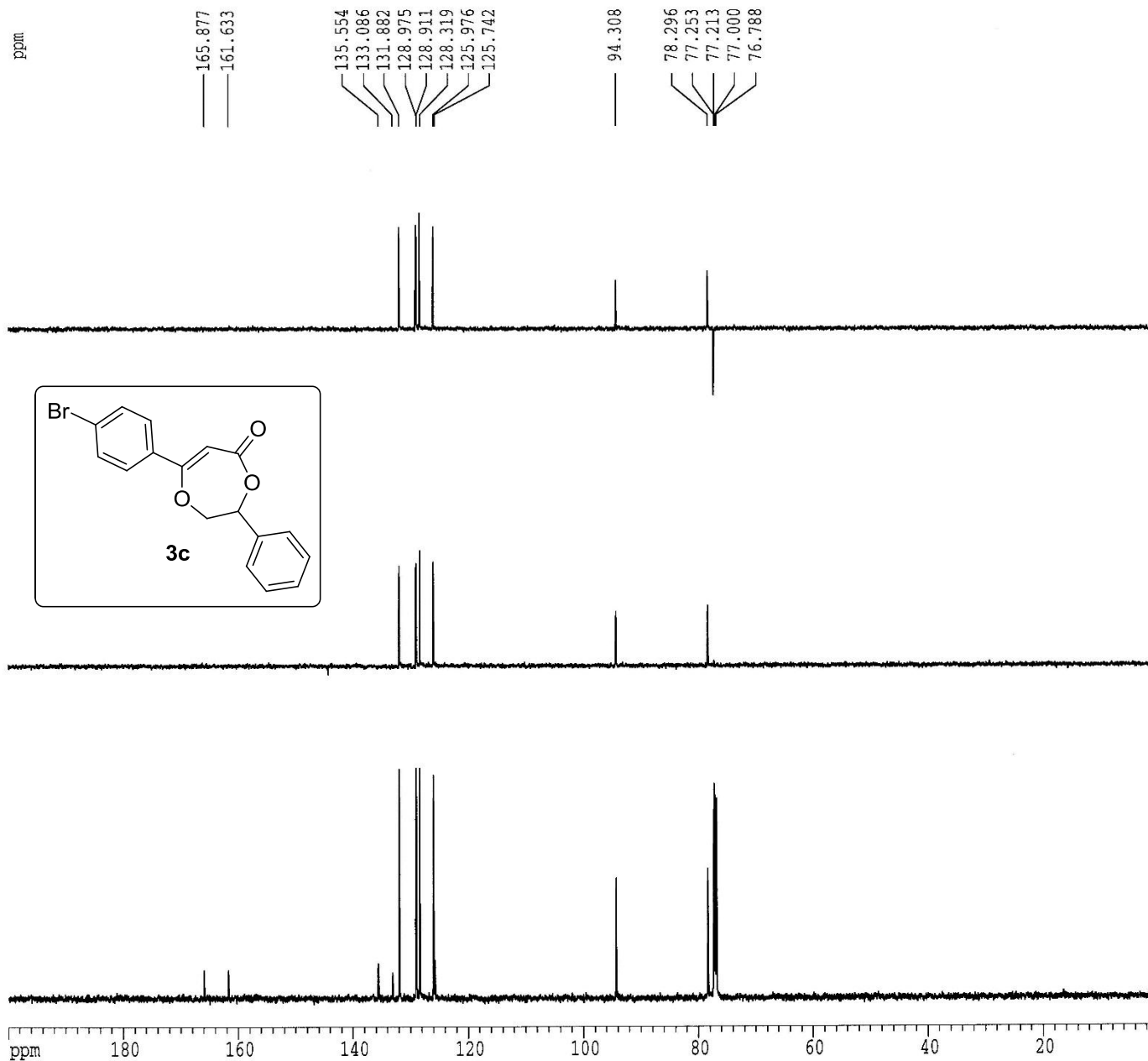
F2 - Acquisition Parameters  
 Date\_ 20150806  
 Time 15.49  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 265  
 DS 0  
 SWS 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RB 2048  
 DR 11.100 usec  
 DE 6.50 usec  
 TE 303.0 K  
 DE 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.40000010 sec  
 NOFREQ 0.0000000 sec  
 NOVER 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.5311418 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.6229930 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.5180933 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  
 FIP 230.000 ppm  
 F1 30103.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 FFXM 10.30000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

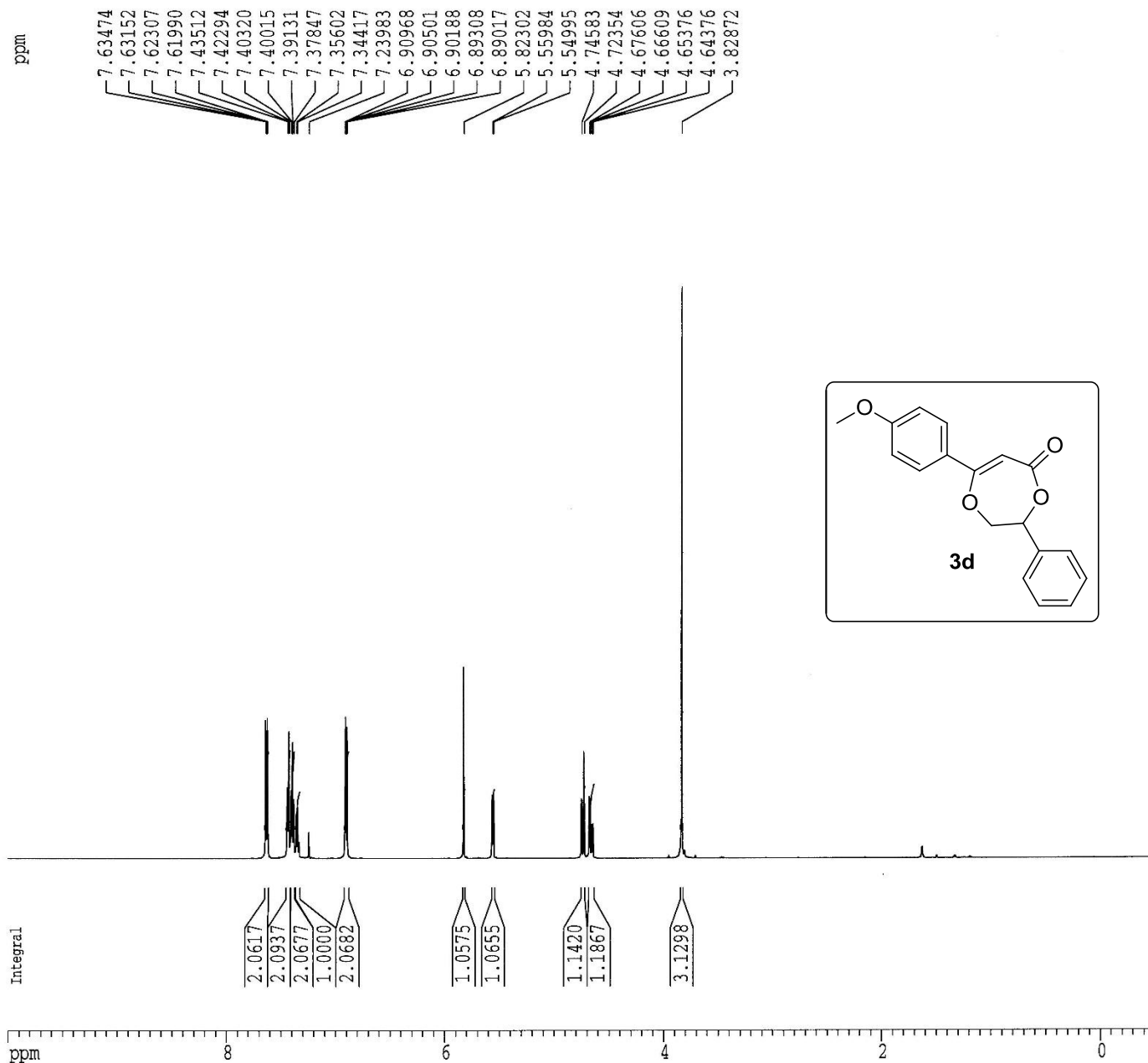
Current Data Parameters
NAME      RS 2-102-1
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150730
Time     16:46
INSTRUM  spect
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       6
DS       4
SWH      9541.984 Hz
FIDRES   0.2911498 Hz
AQ       1.7170932 sec
RG       512
DD       52.400 usec
DE       6.50 usec
TE       301.0 K
NUC1     13C
NUC2     13C
NUC3     13C
NUC4     13C
===== CHANNEL f1 =====
NUC1     13C
P1       10.00 usec
PL1     -6.00 dB
SFO1    500.603516 MHz

F2 - Processing parameters
SI       32768
SF       998.600000 MHz
WDW      none
SSB      0
LB       0.00 Hz
GB       0
PC       2.00

F2 - NMR plot parameters
CX       20.00 cm
CY       10.00 cm
FIDRES   10.000 ppm
SI       32768
SF       998.600000 MHz
WDW      none
SSB      0
LB       0.00 Hz
GB       0
PC       2.00
=====

```





Current Data Parameters  
 NAME RS-2-102-1  
 EXFNO 2  
 PROCNO 1

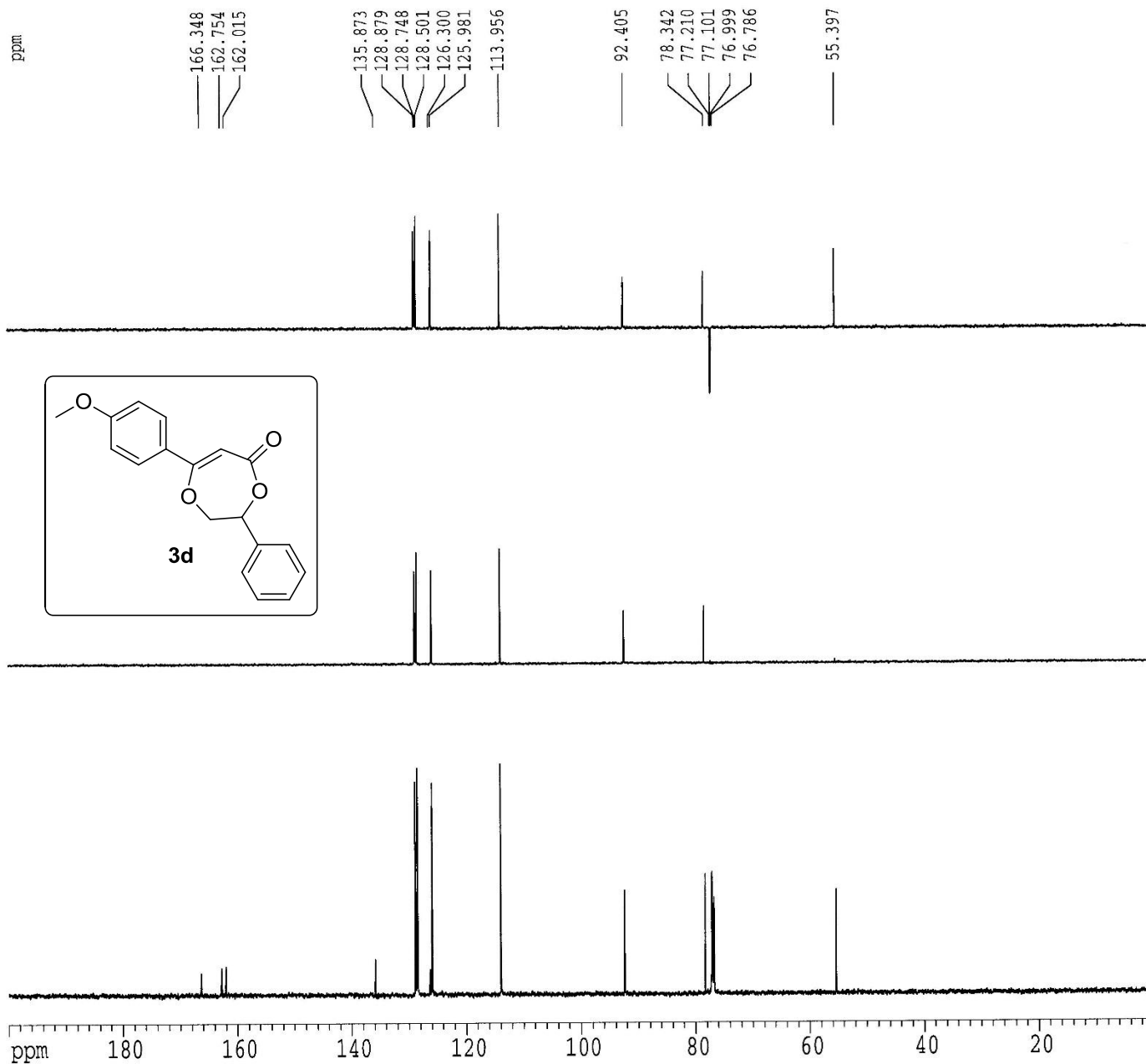
F2 - Acquisition Parameters  
 Date\_ 20150730  
 Time 16.53  
 INSTRUM spect  
 PROBRD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 F2 - Acquisition Parameters  
 SOLVENT CDCl3  
 NS 100  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 SFO1 150.5346470 MHz  
 SF02 598.6029930 MHz  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 302.1 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 ACQRES 0.00000000 sec  
 NS2 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  
 P2 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  
 GDV 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 30193.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 FWHM 10.00000 ppm/cm  
 HZCM 1505.19091 Hz/cm



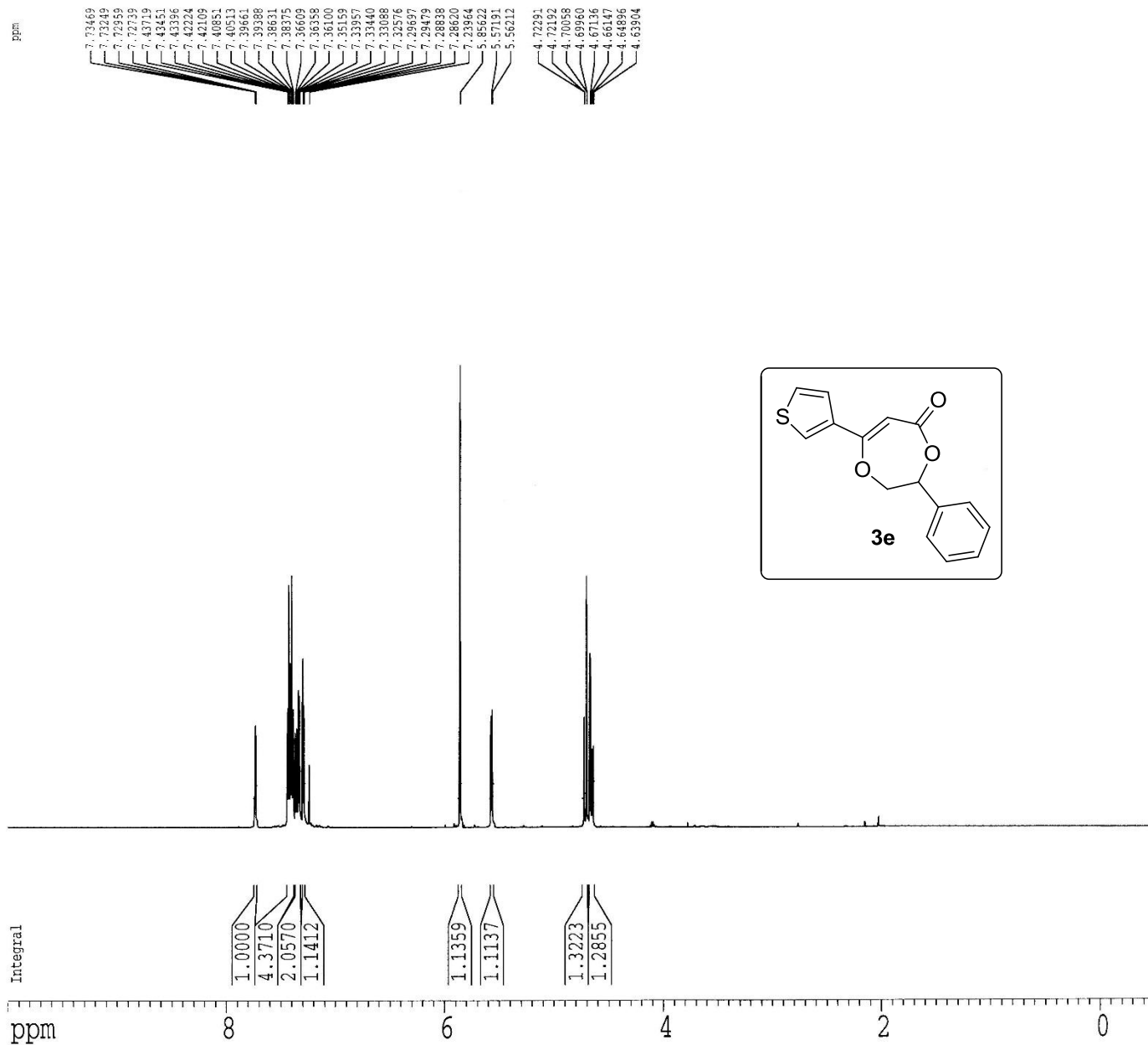
Current Data Parameters  
 NAME RG-2-168-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20160219  
 Time 9.22  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8389.262 Hz  
 FIDRES 0.256020 Hz  
 AQ 1.9530228 sec  
 RG 512  
 DW 59.600 usec  
 DE 6.50 usec  
 FE 294.8 K  
 DI 2.0000000 sec  
 MEFFET 0.0000000 sec  
 MEKXK 0.01300000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PC1 0.00 dB  
 SFO1 500.132499 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.132499 MHz  
 WCW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 FC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 FIP 10.000 ppm  
 FI 5985.00 Hz  
 F2P -0.500 ppm  
 F2 -299.25 Hz  
 PPMCM 0.52500 ppm/cm  
 HZCM 314.21249 Hz/cm



Current Data Parameters  
 NAME RS-2-168-1  
 EXPNO 2  
 PROCNO 1

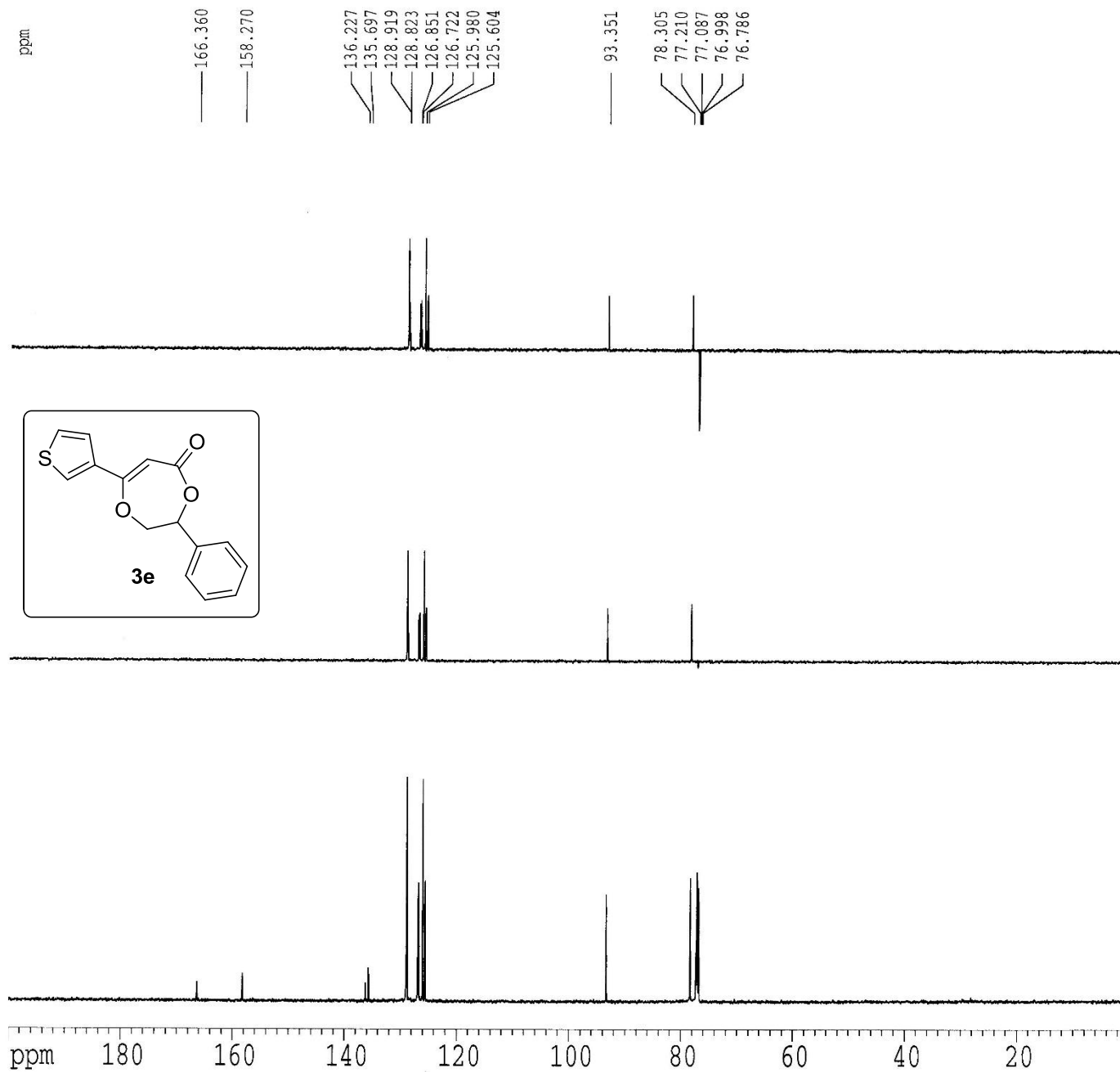
F2 - Acquisition Parameters  
 Date\_ 20160219  
 Time 8.28  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 365  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 295.6 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MCWRR 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4929522 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 30098.59 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCK 10.00000 ppm/cm  
 HZCM 1504.92944 Hz/cm



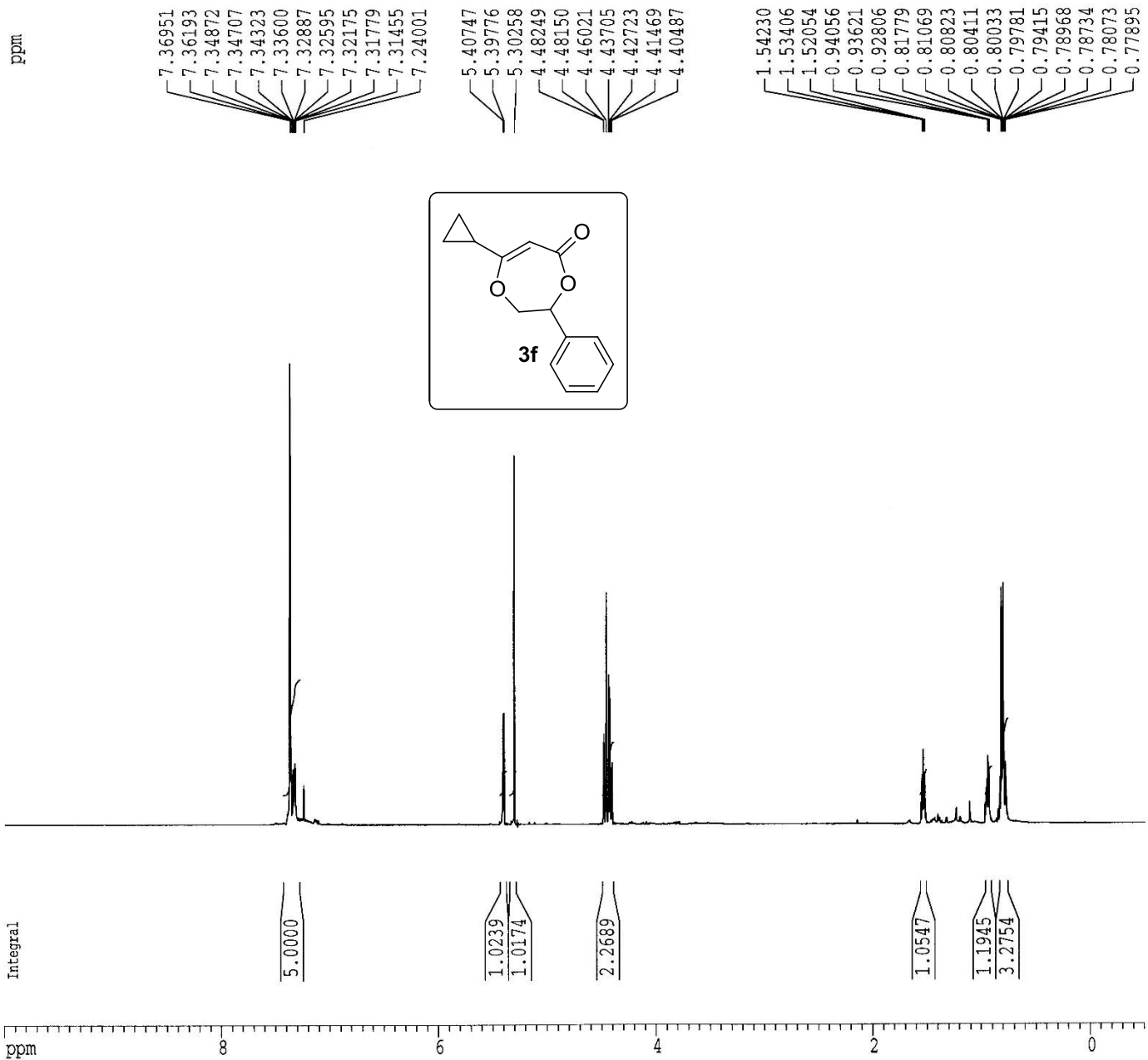
Correct Data Parameters  
 NAME 86-0-90-2  
 EXPNO 1  
 PROCNO 1

F2 Acquisition Parameters  
 Date\_ 20150716  
 Time 16.36  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SFO 8369.262 Hz  
 FIDRES 0.1256000 Hz  
 AQ 1.9530228 sec  
 RG 128  
 DR 59.600 usec  
 DE 6.50 usec  
 TE 300.4 K  
 D1 2.0000000 sec  
 MTRFRST 0.0000000 sec  
 MTRFR 0.0100000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.00 usec  
 PA1 0.00 dB  
 SFO1 500.000000 MHz

F2 Processing parameters  
 SI 32768  
 SF 500.000000 MHz  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1F 10.000 ppm  
 F1 5060.00 Hz  
 F1F -0.500 ppm  
 F2 -99.30 Hz  
 PPMCM 0.52500 ppm/cm  
 HSCM 314.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-90-2  
 EXPNO 2  
 PROCNO 1

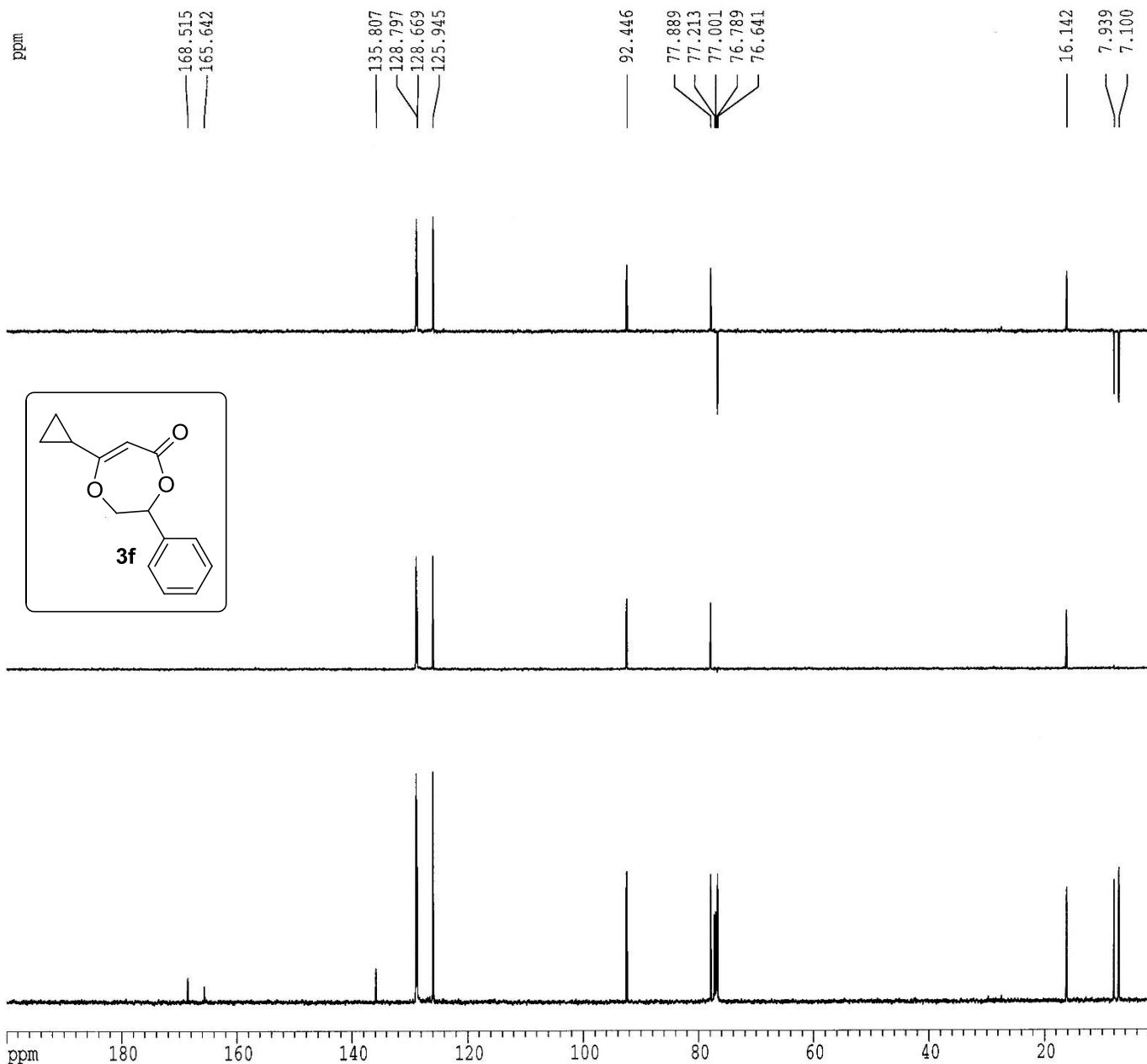
F2 - Acquisition Parameters  
 Date\_ 20150716  
 Time 16.43  
 INSTRUM spect  
 PROBD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 100  
 DS 0  
 SMC 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 301.8 K  
 DE 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MOWRK 0.0150000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180981 MHz  
 MDW 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  
 SFOCM 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      RS-2-90-1
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150730
Time     10.04
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      9541.984 Hz
FIDRES   0.291198 Hz
AQ       1.7170932 sec
RG       512
AW       52.400 usec
DE       6.50 usec
TE       300.2 K
D1       1.5000000 sec
MCREST   0 sec
MCWRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PL1      6.00 dB
SFO1     598.6035916 MHz

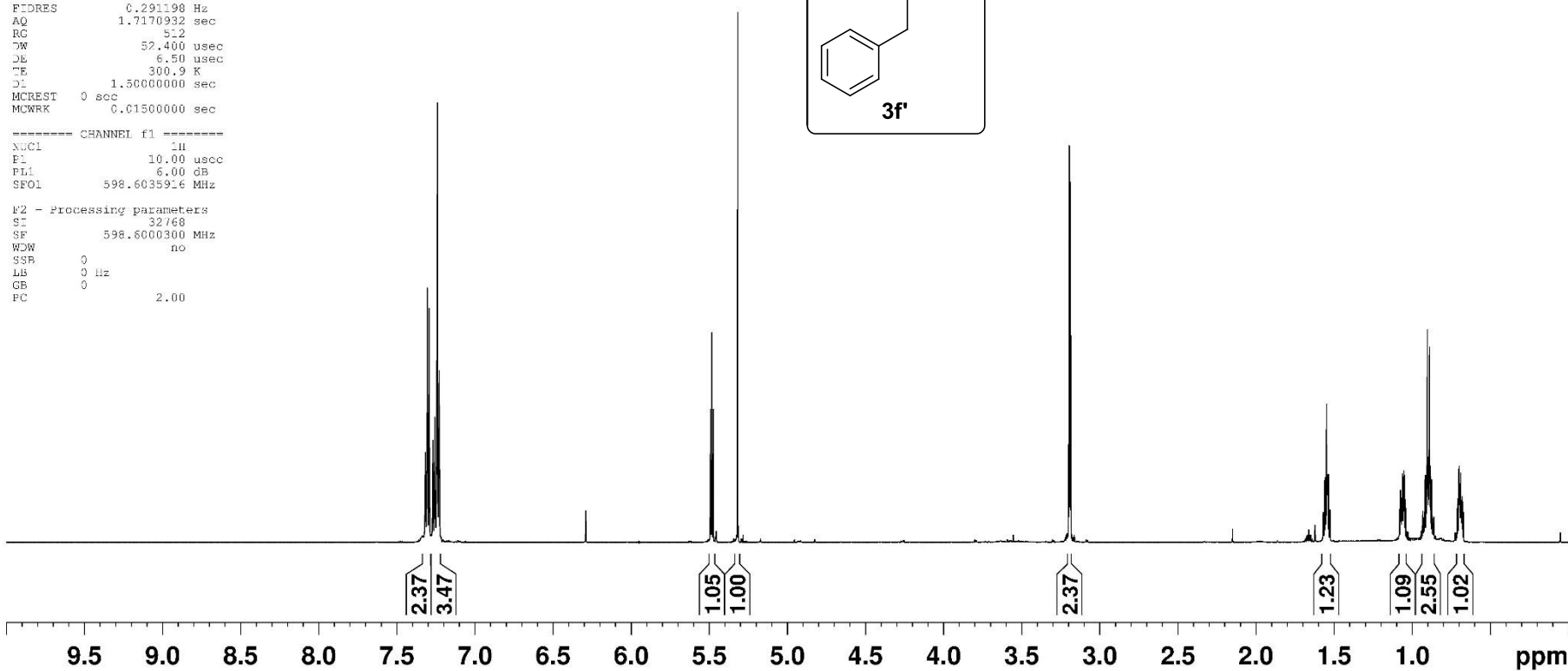
F2 - Processing parameters
SI       32768
SF       598.6000300 MHz
WDW      no
SSB      0
LB       0 Hz
GB       0
PC       2.00

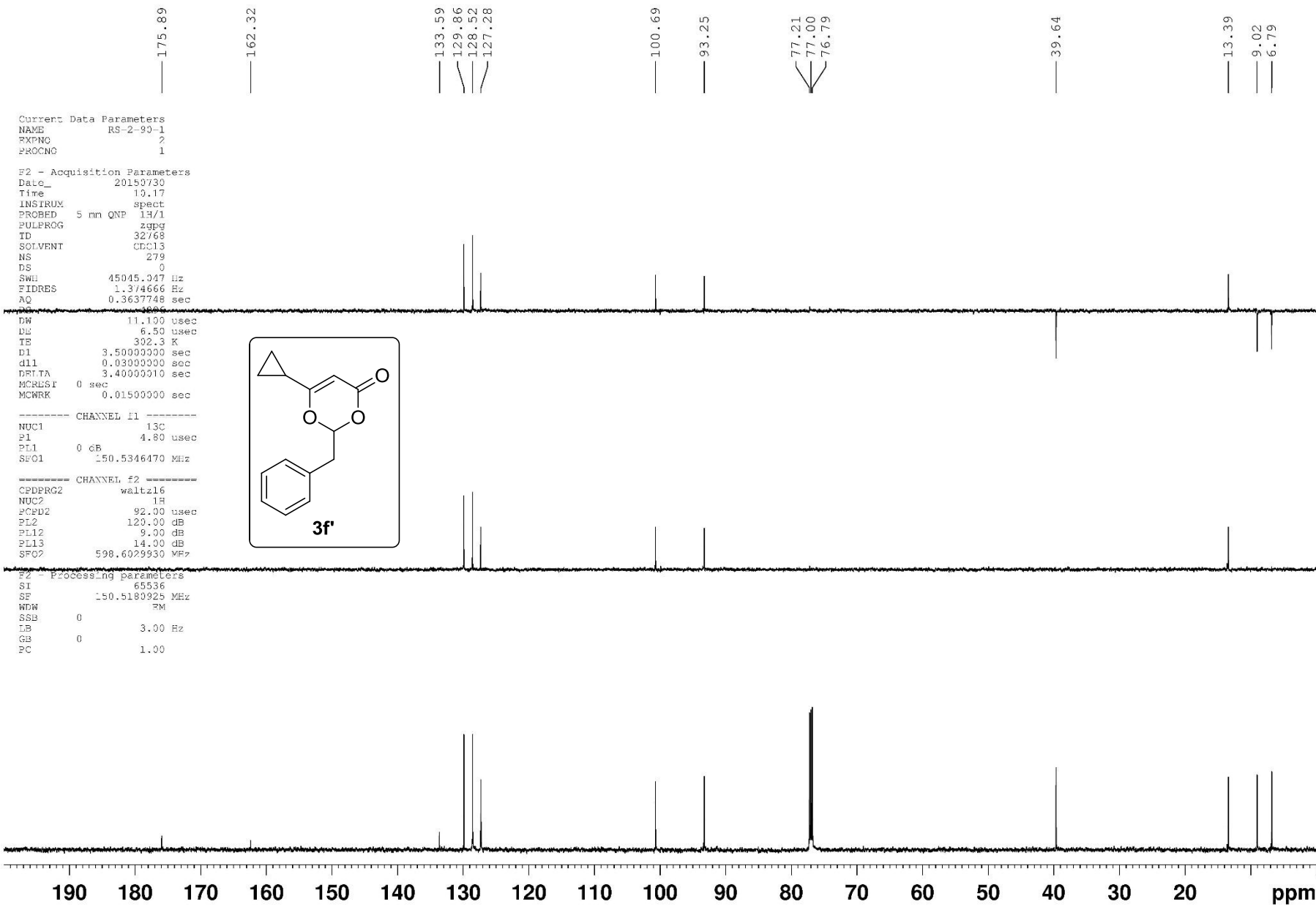
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7.315  
7.306  
7.303  
7.293  
7.269  
7.267  
7.261  
7.257  
7.253  
7.240  
7.229

5.492  
5.483  
5.474  
5.318

3.196  
3.187  
1.570  
1.562  
1.556  
1.554  
1.548  
1.542  
1.540  
1.534  
1.526  
1.080  
1.074  
1.072  
1.070  
1.066  
1.063  
1.061  
1.058  
1.055  
1.053  
1.050  
1.045  
1.042  
0.917  
0.910  
0.906  
0.902  
0.899





```

Current Data Parameters
NAME      SS-2-96-2
EXPNO    1
PROCNO   1

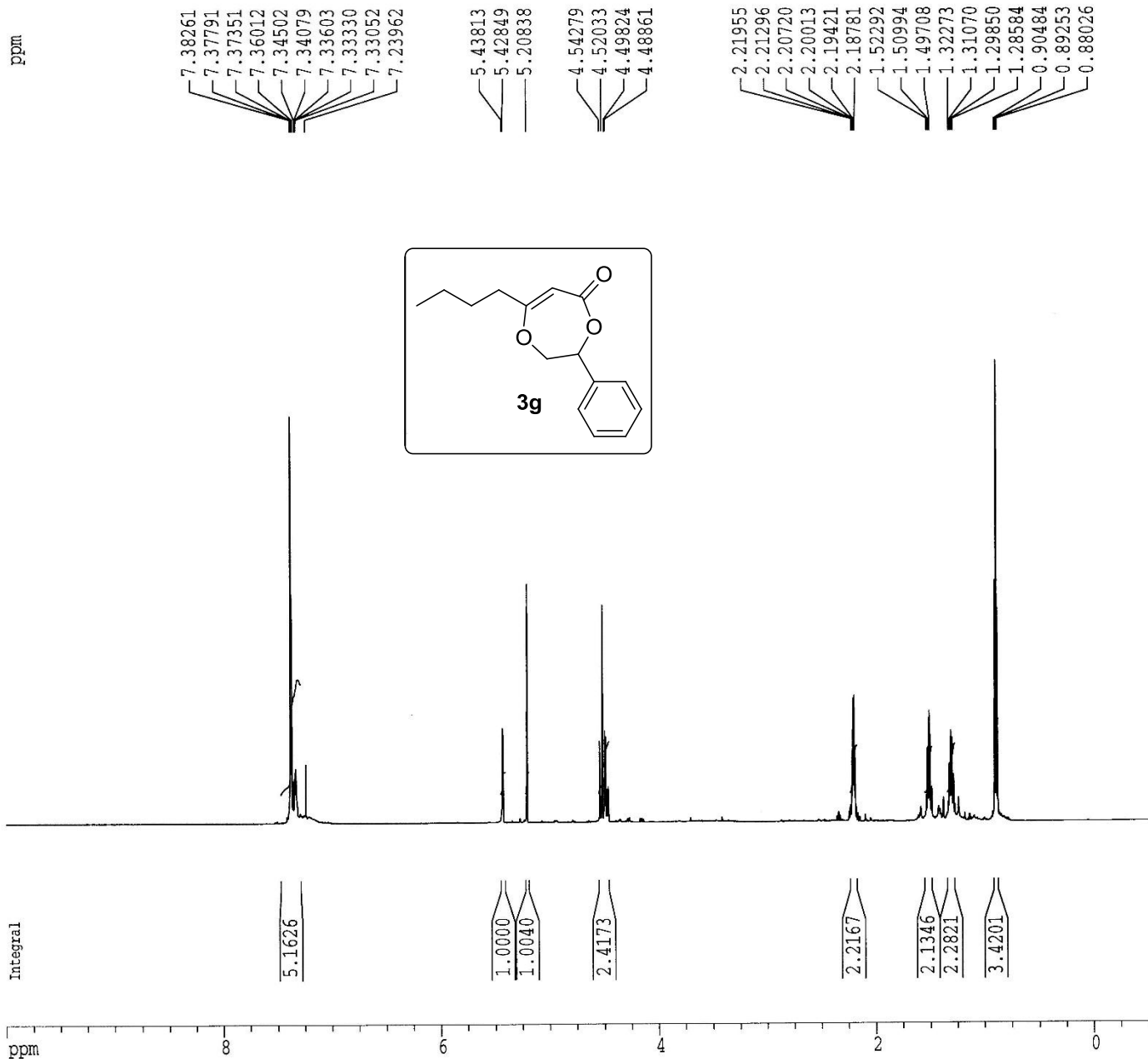
F2 - Acquisition Parameters
Date_    20150731
Time     18.21
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
PC      32768
AQ      1.8
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.256620 Hz
AQ       1.9330028 sec
RG        128
DQ       59.600 usec
DE        6.50 usec
TE       301.4 K
SI        1.00000000 sec
MKRES1   0.00000000 sec
MKRES2   0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PL1       0.00 dB
SFO1     500.136450 MHz

F1 - Processing parameters
SI        32768
SF        500.136450 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00

ID MS: plot parameters
CX        10.00 cm
CY         8.00 cm
FIDP      10.000 ppm
F1        500.136450 Hz
FIDP      -0.500 ppm
F0        299.30 Hz
FPMAX     0.52500 ppm/cm
FIDCM     314.26501 Hz/cm

```





Current Data Parameters  
 NAME RS-2-96-2  
 EXPNO 2  
 PROCNO 1

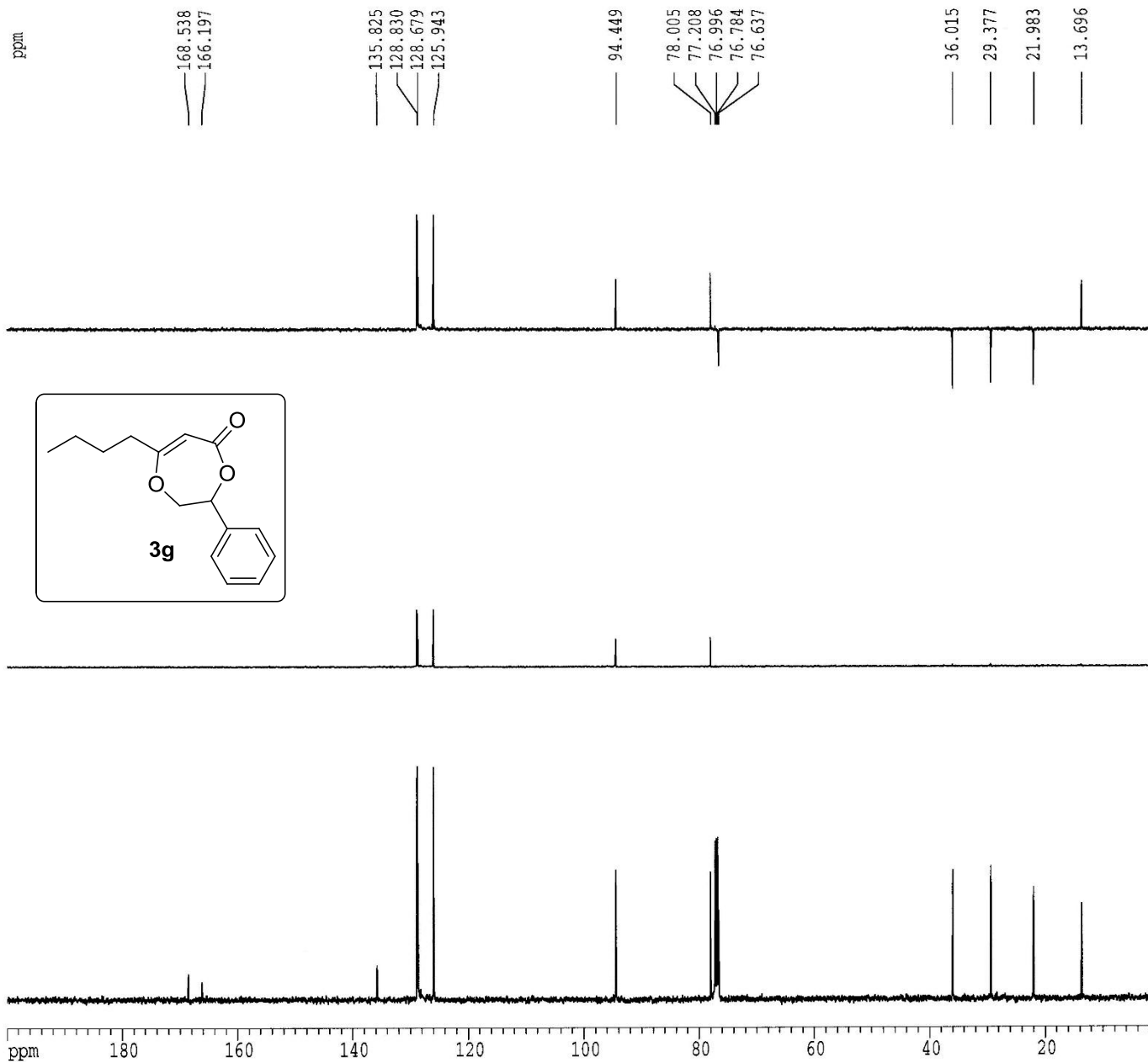
F2 - Acquisition Parameters  
 Date\_ 20150723  
 Time 18.25  
 INSTRUM spect  
 PROBO 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 200  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DN 11.100 usec  
 DE 6.50 usec  
 TE 302.7 K  
 FI 3.50000000 sec  
 SII 0.03000000 sec  
 USHA 3.40000010 sec  
 HOREST 0.00000000 sec  
 HONEK 0.01500000 sec

----- CHANNEL f1 -----  
 NUCL1 13C  
 FI 4.80 usec  
 FM 0.00 dB  
 SFO1 150.5346470 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCL2 1H  
 PCPD1 92.00 usec  
 PL1 120.00 dB  
 PL2 9.00 dB  
 PL12 14.00 dB  
 SFO2 598.6029930 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.5180939 MHz  
 UCM EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 4.00 cm  
 FIP 200.000 ppm  
 F1 30103.62 Hz  
 PCP 0.000 ppm  
 F2 0.00 Hz  
 PRNCH 10.00000 ppm/cm  
 HZCH 1505.18091 Hz/cm





7.336  
7.321  
7.309  
7.297  
7.286  
7.274  
7.257  
7.245  
7.239

5.566  
5.558  
5.549  
5.255

3.239  
3.231  
2.282  
2.269  
2.256  
2.244  
2.233  
2.221  
2.208  
2.196  
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1.499  
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1.476  
1.464  
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1.284  
1.271  
1.259  
1.240  
0.881  
0.869

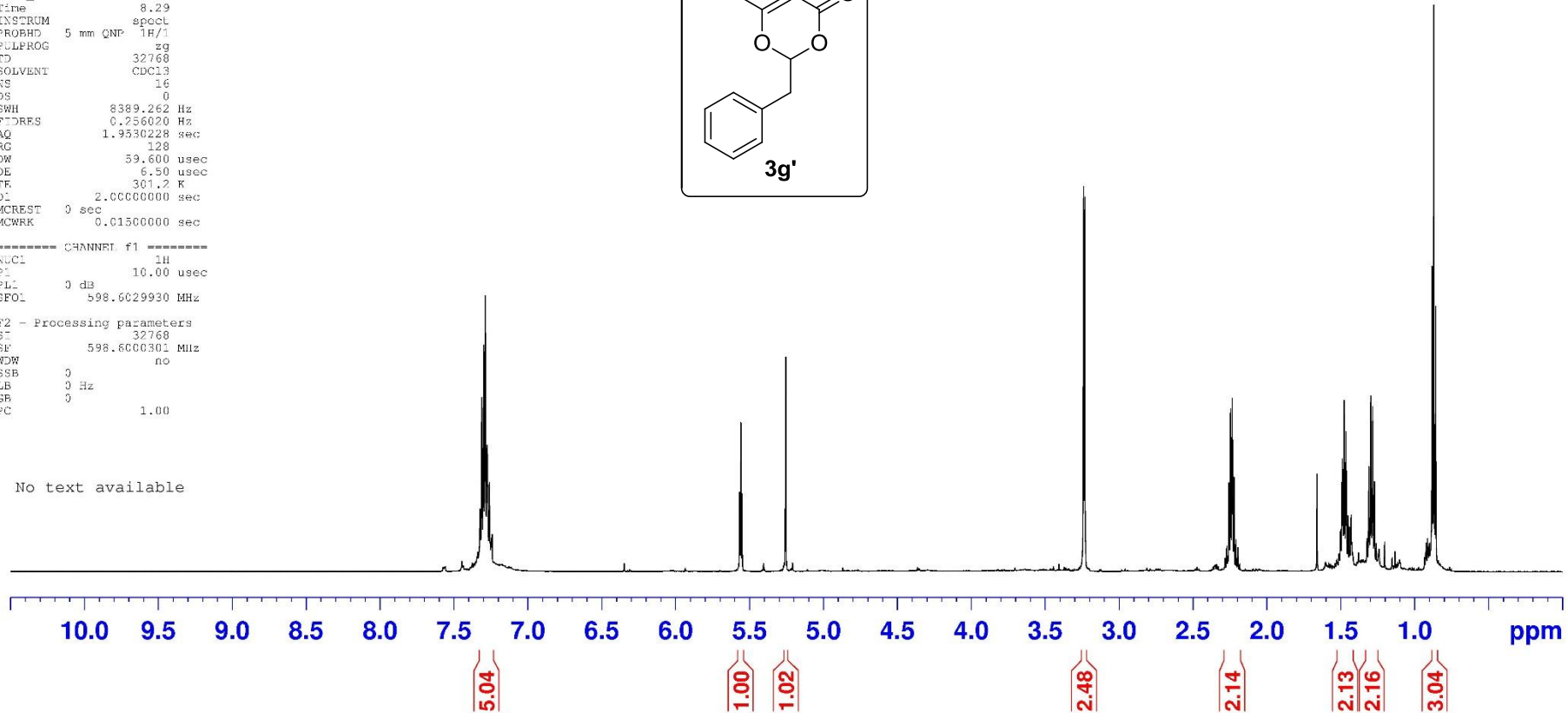
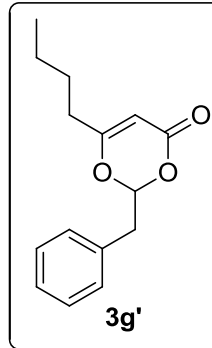
Current Data Parameters  
NAME RS-2-96-1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20130724  
Time 8.29  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT CDCl3  
NS 16  
DS 0  
SWH 8389.262 Hz  
FIDRES 0.256020 Hz  
AQ 1.9530228 sec  
RG 128  
DW 59.600 usec  
DE 6.50 usec  
TE 301.2 K  
D1 2.0000000 sec  
MCREST 0 sec  
MCWRK 0.01500000 sec

----- CHANNEL f1 -----  
NUC1 1H  
P1 10.00 usec  
PL1 0 dB  
SPOL 598.6029930 MHz

F2 - Processing parameters  
SI 32768  
SF 598.600301 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

No text available



Current Data Parameters  
 NAME R8-2-96-1  
 EXPNO 2  
 PROCNO 1

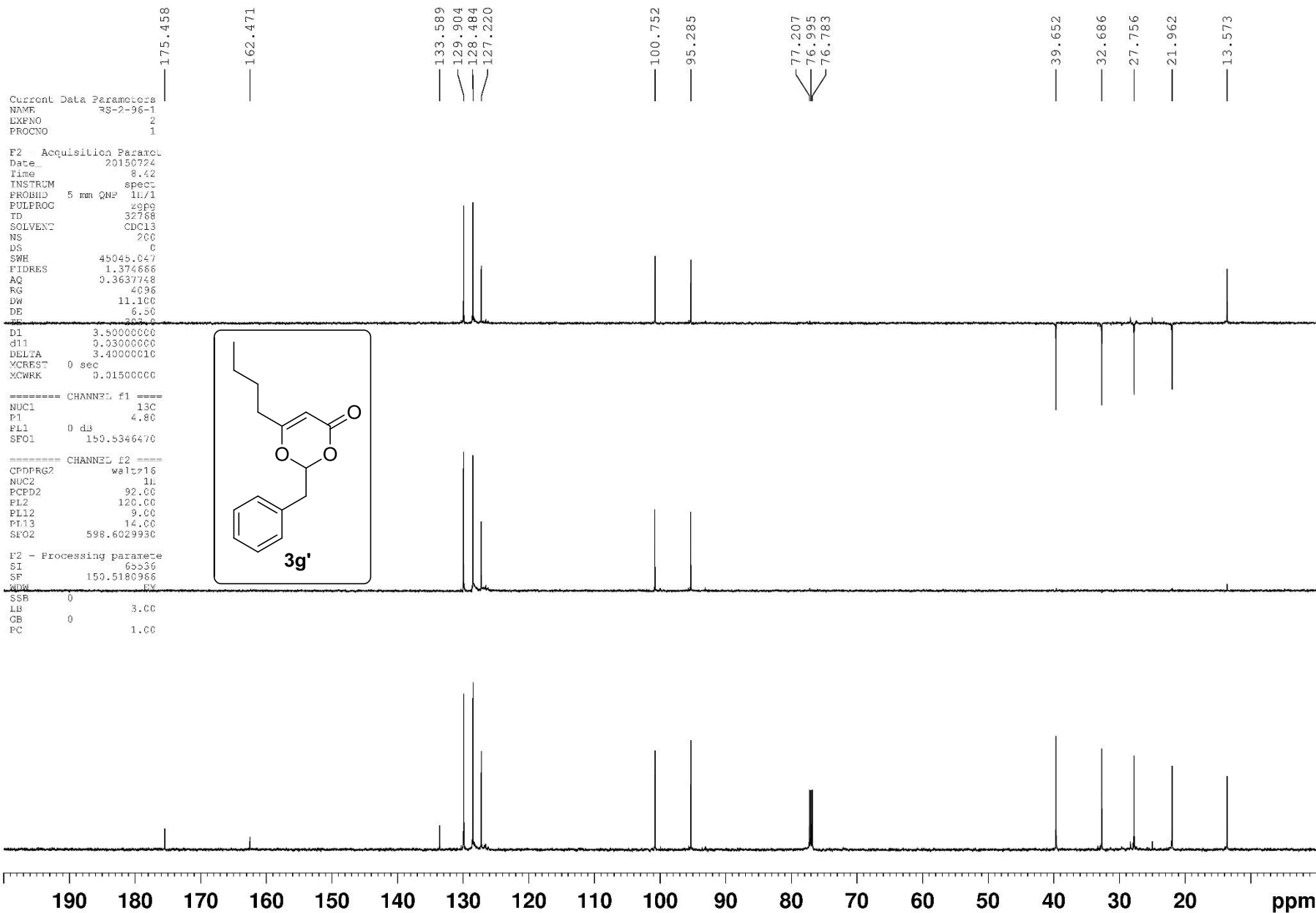
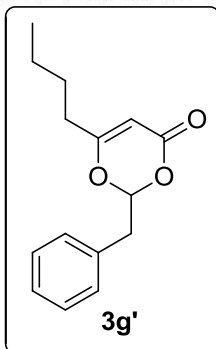
F2 - Acquisition Parameters  
 Date\_ 20150724  
 Time 8.42  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg30  
 TD 32768  
 SOLVENT CDCl3  
 NS 200  
 DS c  
 SWH 45045.047  
 FIDRES 1.374666  
 AQ 0.3637748  
 RG 4096  
 DW 11.100  
 DE 6.50  
~~TE~~

D1 3.5000000  
 d11 0.0300000  
 DELTA 3.4000000  
 XCFST 0 sec  
 XCFWK 0.0150000

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80  
 PL1 0 dB  
 SFO1 150.5346470

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180966  
 GDW BY  
 SSB 0  
 LB 3.00  
 GB 0  
 PC 1.00



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7.660  
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4.661

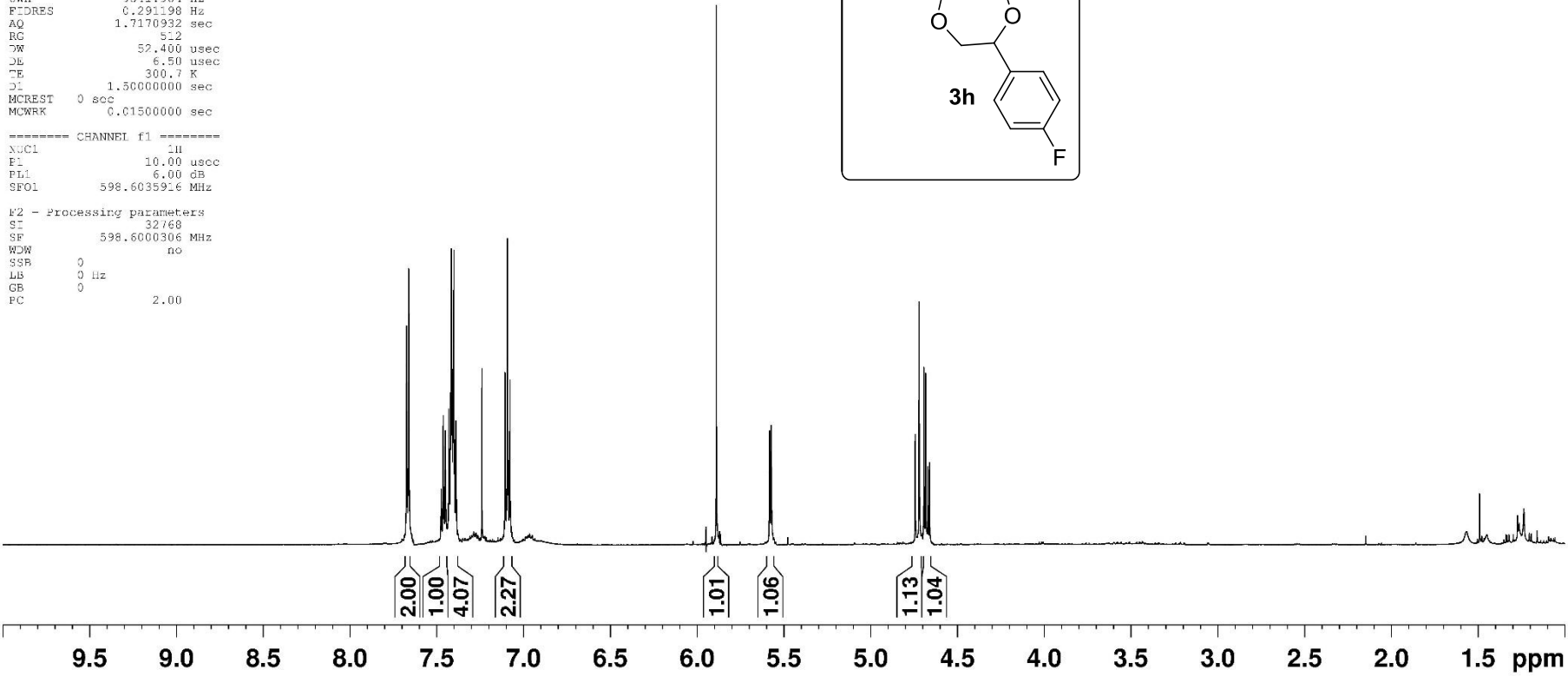
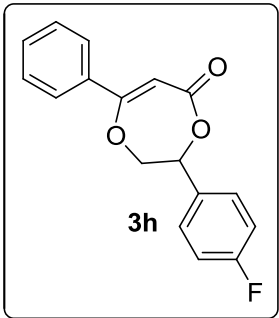
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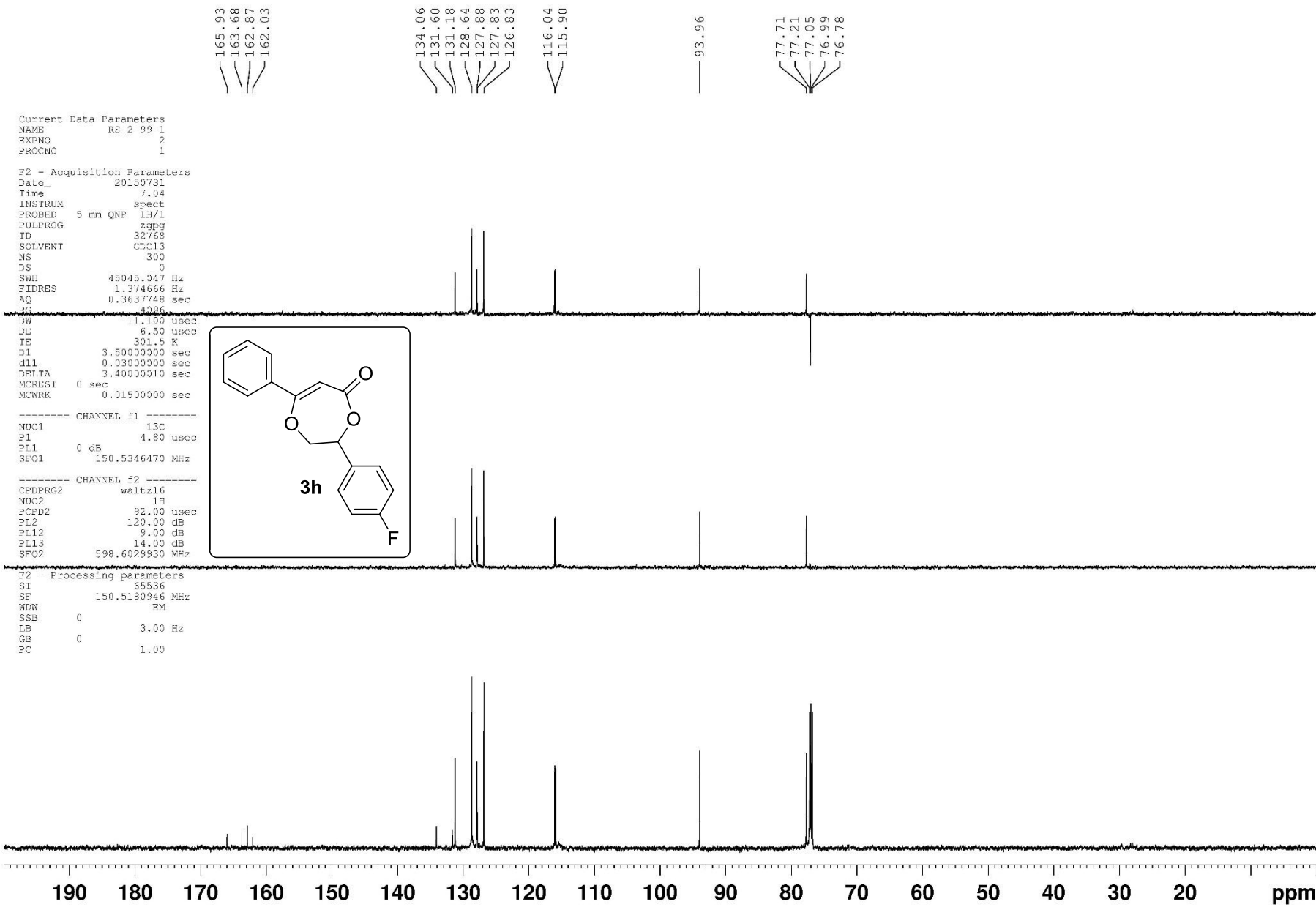
Current Data Parameters
NAME      RS-2-99-1
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150731
Time     7.02
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zgpg30
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      9541.984 Hz
FIDRES   0.291198 Hz
AQ       1.7170932 sec
RG       512
AW       52.400 usec
DE       6.50 usec
TE       300.7 K
D1       1.50000000 sec
MCREST   0 sec
MCWRK    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PL1       6.00 dB
SFO1     598.6035916 MHz

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





```

Current Data Parameters
NAME      RS-2-99-1
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20150731
Time     7.04
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         4086
-----
DW        11.100 usec
DE         6.50 usec
TE        301.5 K
D1         3.5000000 sec
d11        0.0300000 sec
DELTA     3.4000000 sec
MCRESF1   0 sec
MCWRR     0.0150000 sec
-----
CHANNEL f1
NUC1       13C
P1         4.80 usec
PL1        0 dB
SFO1      150.5346470 MHz
-----
CHANNEL f2
CPDPRG2   waltz16
NUC2       13C
PCPD2     92.00 usec
PL2       120.00 dB
PL12      9.00 dB
PL13      14.00 dB
SFO2     598.6029930 MHz
-----
F2 - Processing parameters
SI         65536
SF        150.5180946 MHz
WDW        RM
SSB        0
LB         3.00 Hz
GB         0
PC         1.00

```

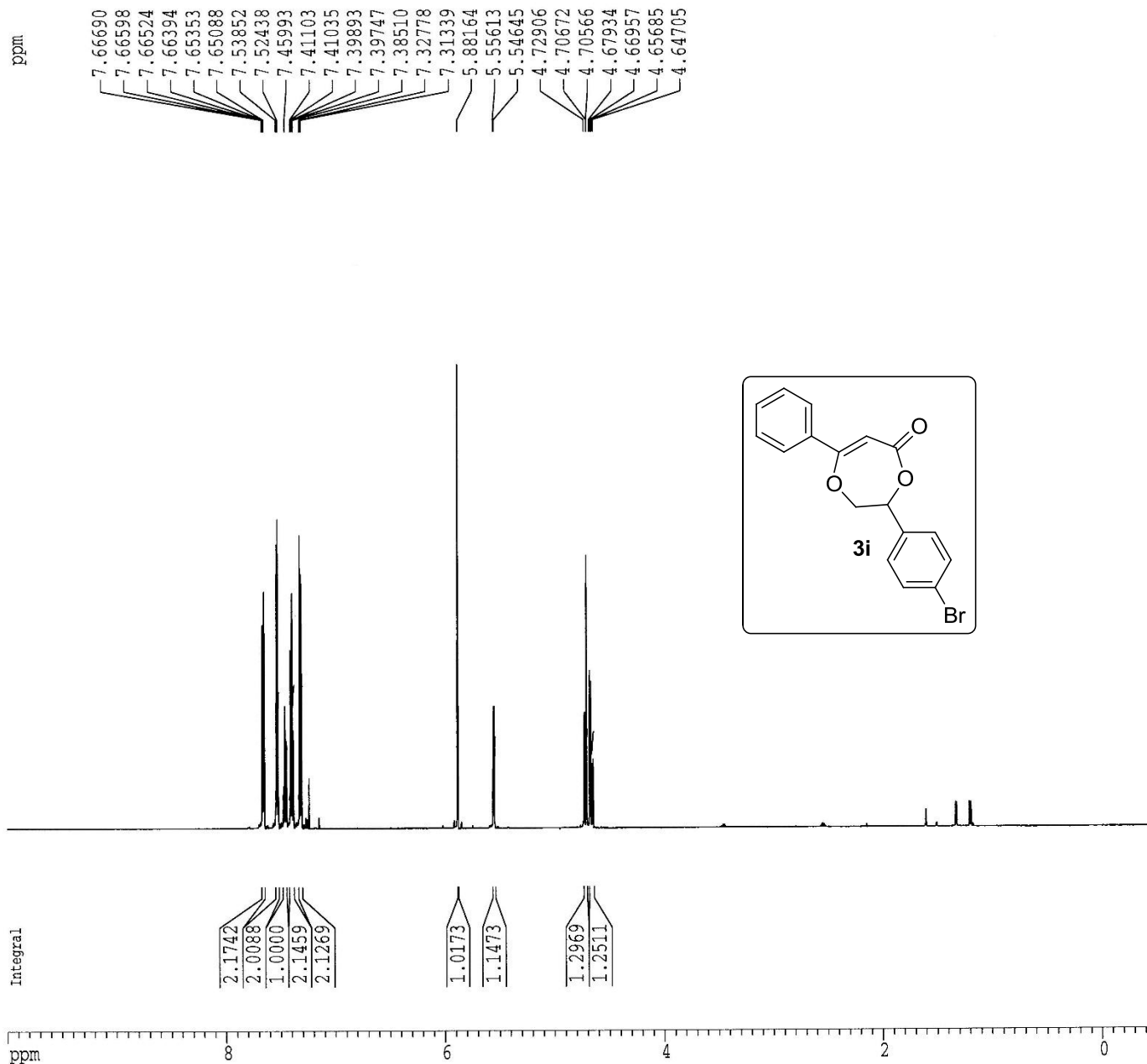
Current Data Parameters  
 NAME RS-2-88-1  
 EXPNO 1  
 PROCNO 1

TD Acquisition Parameters  
 Date\_ 20150729  
 Time 14.46  
 INSTRUM spect  
 PROBE 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 FWH 3189.262 Hz  
 FREQ0 0.126020 Hz  
 AQ 1.9510238 sec  
 RG 128  
 DD 59.600 usec  
 DE 6.50 usec  
 TE 301.2 K  
 D1 1.0000000 sec  
 MWDW 0.0000000 sec  
 MONK 0.0150000 sec

===== CHANNEL f1 =====  
 NUQC 1H  
 P1 10.00 usec  
 PL1 3.00 dB  
 SFO1 500.1314910 MHz

TD Processing parameters  
 SI 32768  
 SF 500.1314910 MHz  
 TD 16  
 GB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

RG MRF plot parameters  
 CR 20.00 cm  
 CY 8.00 cm  
 FIP 10.000 ppm  
 FI 5966.00 Hz  
 FT -0.500 ppm  
 RT -294.30 Hz  
 HXMC 0.52500 ppm/cm  
 HZMC 34.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-98-1  
 EXPNO 2  
 PROCNO 1

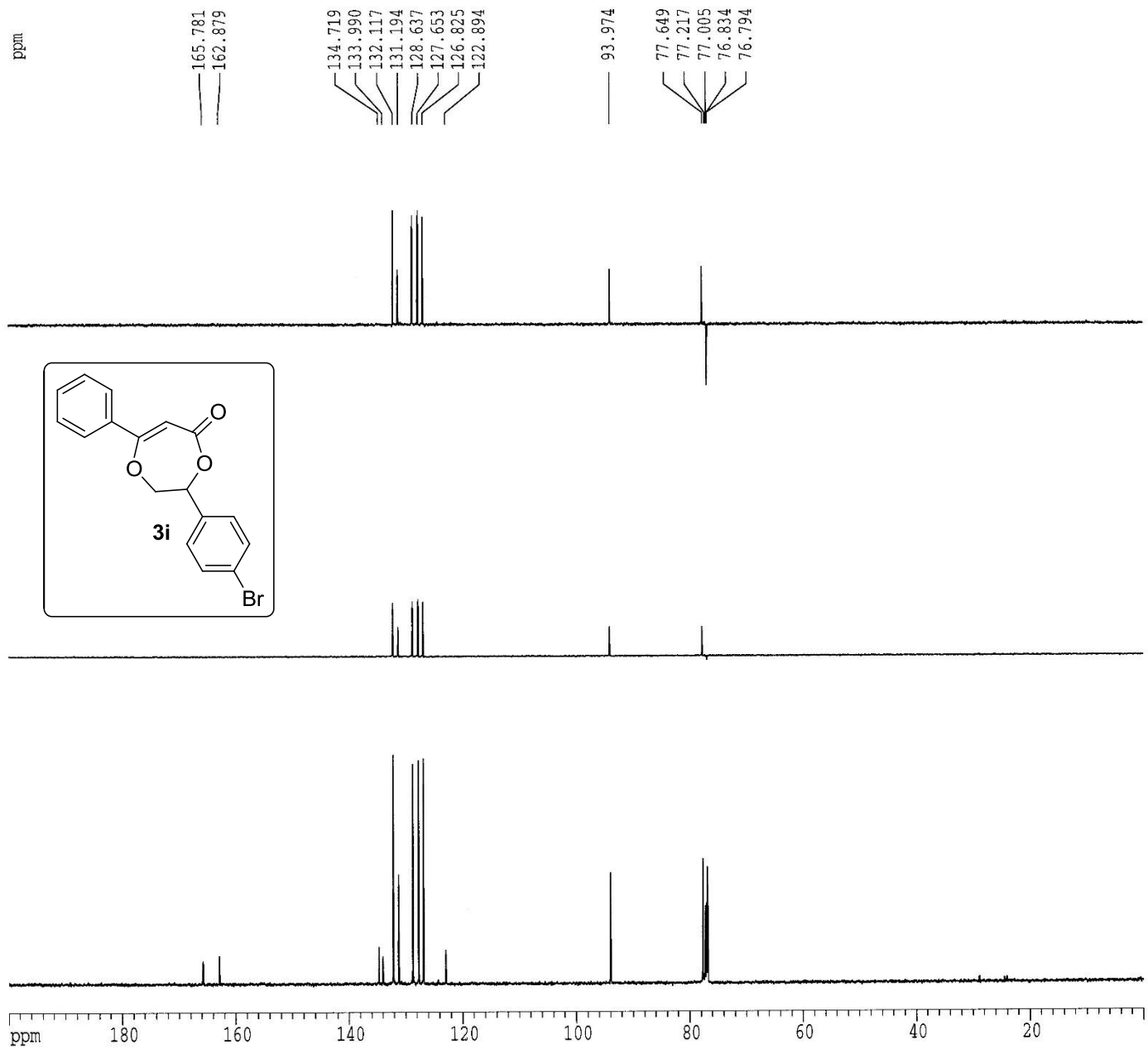
F2 - Acquisition Parameters  
 Date\_ 20150727  
 Time 14.47  
 INSTRUM spect  
 PROBRD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 221  
 DS 0  
 SFR 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DM 12.100 usec  
 DE 6.50 usec  
 TE 301.6 K  
 DL 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCOBK 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 150.5180959 MHz  
 MD 4 EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

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



```

Current Data Parameters
NAME      RS-3-101-1
EXPNO    1
PROCNO   1

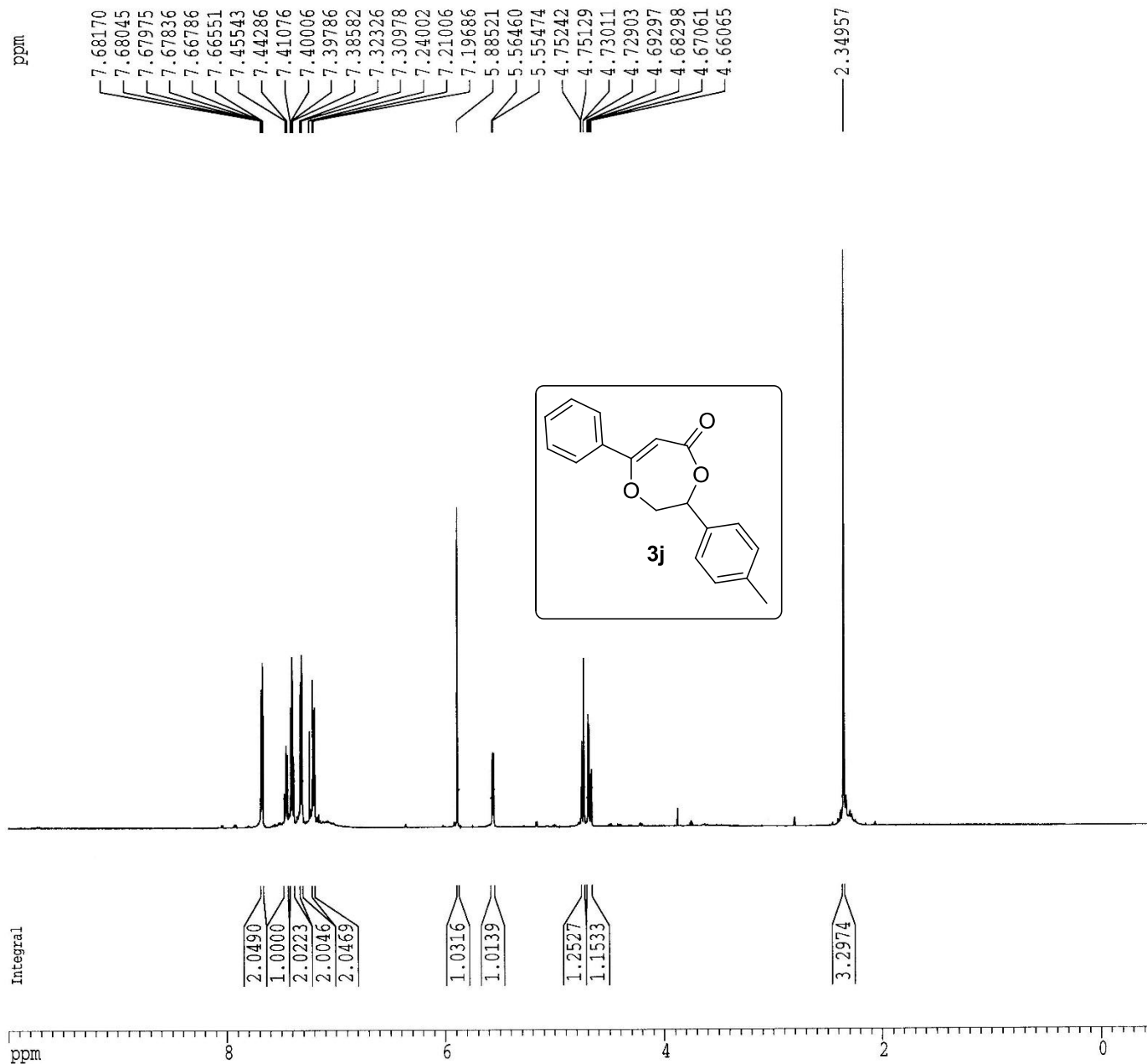
F2 Acquisition Parameters
Date_    20150327
Time     15.16
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        4
SWH       8189.262 Hz
FIDRES    0.256000 Hz
AQ         1.4930228 sec
RG         312
DQ         54.600 usec
DE         6.50 usec
TE        302.0 K
SI         2.0000000 sec
RG2       0.2000000 sec
RG3       0.2000000 sec
RG4       0.2000000 sec
RG5       0.2000000 sec

===== CHANNEL f1 =====
NUC1      1H
P1         8.90 usec
PC1        0.00 dB
SFO1      500.6029930 MHz

F2 - Processing parameters
SI         32768
SF         500.6002999 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

F2 MNE plot parameters
AQ         20.00 cm
AV         10.00 cm
PIF        10.000 ppm
PI         5966.00 Hz
PF         -0.500 ppm
PT         -244.30 Hz
RG2        0.52500 ppm/cm
RG3        314.26501 Hz/cm

```





Current Data Parameters  
 NAME RS-2-101-1  
 EXPNO 2  
 PROCNO 1

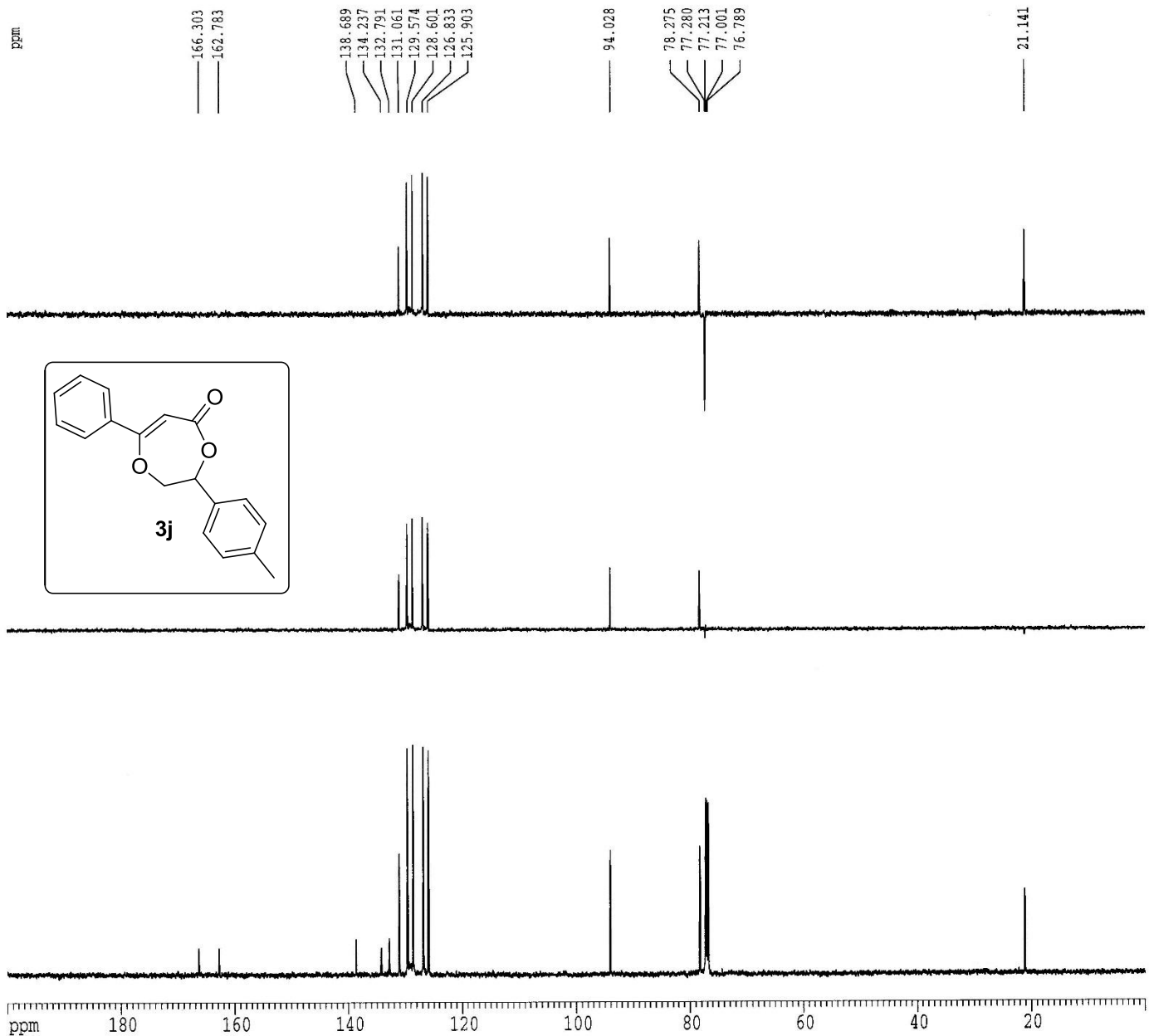
F2 - Acquisition Parameters  
 Date\_ 20150827  
 Time 15.17  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 402  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 302.3 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 ACQRES 0.00000000 sec  
 AQRN 0.01500000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180946 MHz  
 GDV EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 0.50

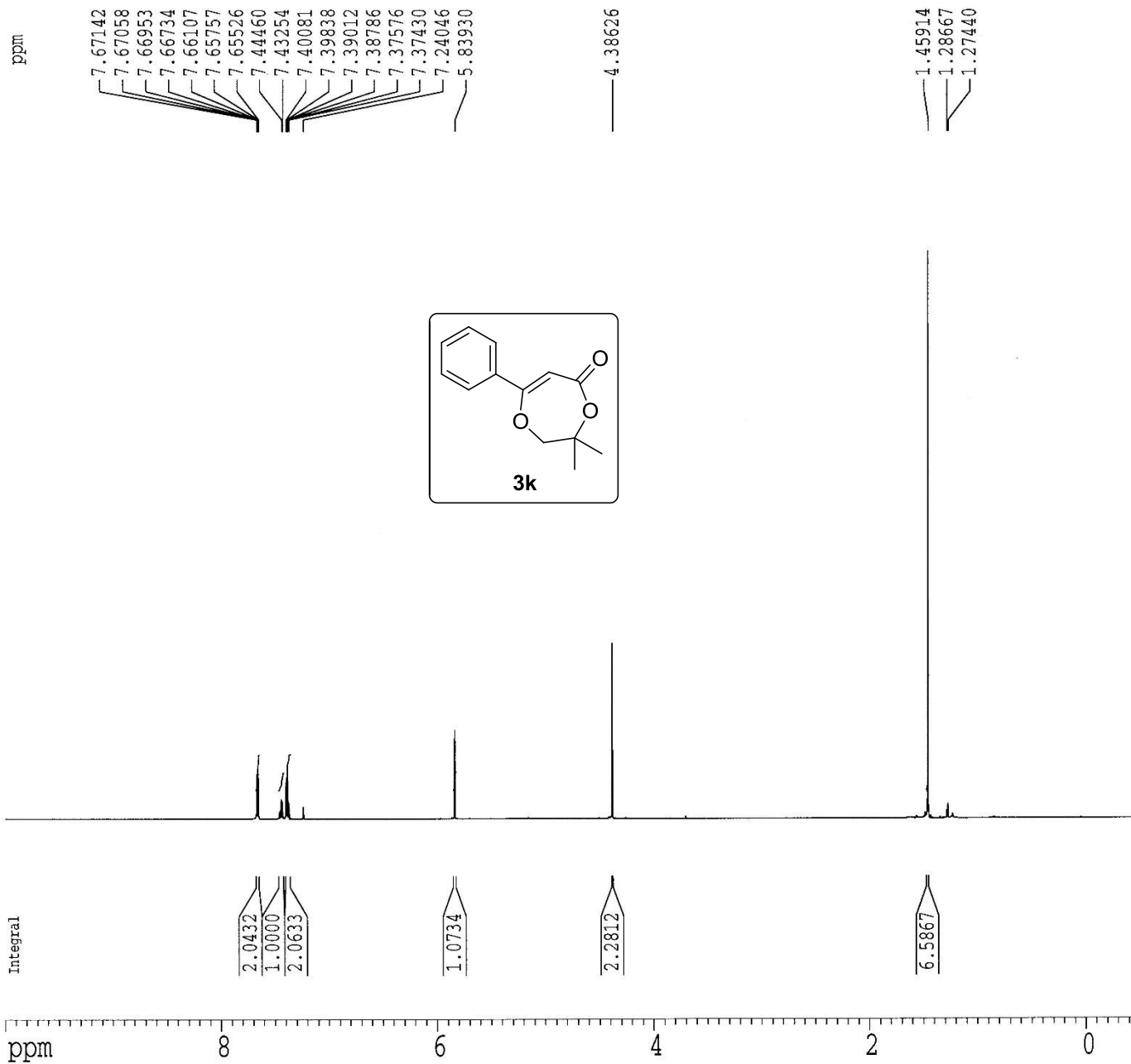
1D NMR plot parameters  
 CX 20.00 cm  
 CY 4.00 cm  
 F1P 200.000 ppm  
 F1 30103.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PRMCM 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      SF-0-9412
PROBHD    :
PULPROG   :
PC         Application Parameters
Date_     20150803
Time      13:28
INSTRUM    spect
PROBHD     5 mm QNP 1H/1
PULPROG    zgpg30
PC         32768
SOLVENT    CDCl3
NS         64
DS         4
SWH         131.400 MHz
AQ         0.56000 sec
RG         655
AQ         0.56000 sec
DE         6.50 usec
TE         301.2 K
AQ         1.0000000 sec
SFO1       500.136098 MHz
===== CHANNEL f1 =====
NUC1       13C
P1         10.00 usec
PL1        0.00 dB
SFO2       101.626120 MHz
===== Processing parameters =====
SI         32768
SF         500.136098 MHz
WDW         EM
SSB         0
LB         0.300 Hz
GB         0
PC         1.00
===== 13C NMR plot parameters =====
AQ         10.00 usec
PL         0.00 dB
SFO1       101.626120 MHz
SFO2       500.136098 MHz
WDW         EM
SSB         0
LB         0.300 Hz
GB         0
PC         1.00
===== 13C NMR plot parameters =====
AQ         10.00 usec
PL         0.00 dB
SFO1       101.626120 MHz
SFO2       500.136098 MHz
WDW         EM
SSB         0
LB         0.300 Hz
GB         0
PC         1.00

```



Current Data Parameters  
 NAME RS-2-94-2  
 EXPNO 2  
 PROCNO 1

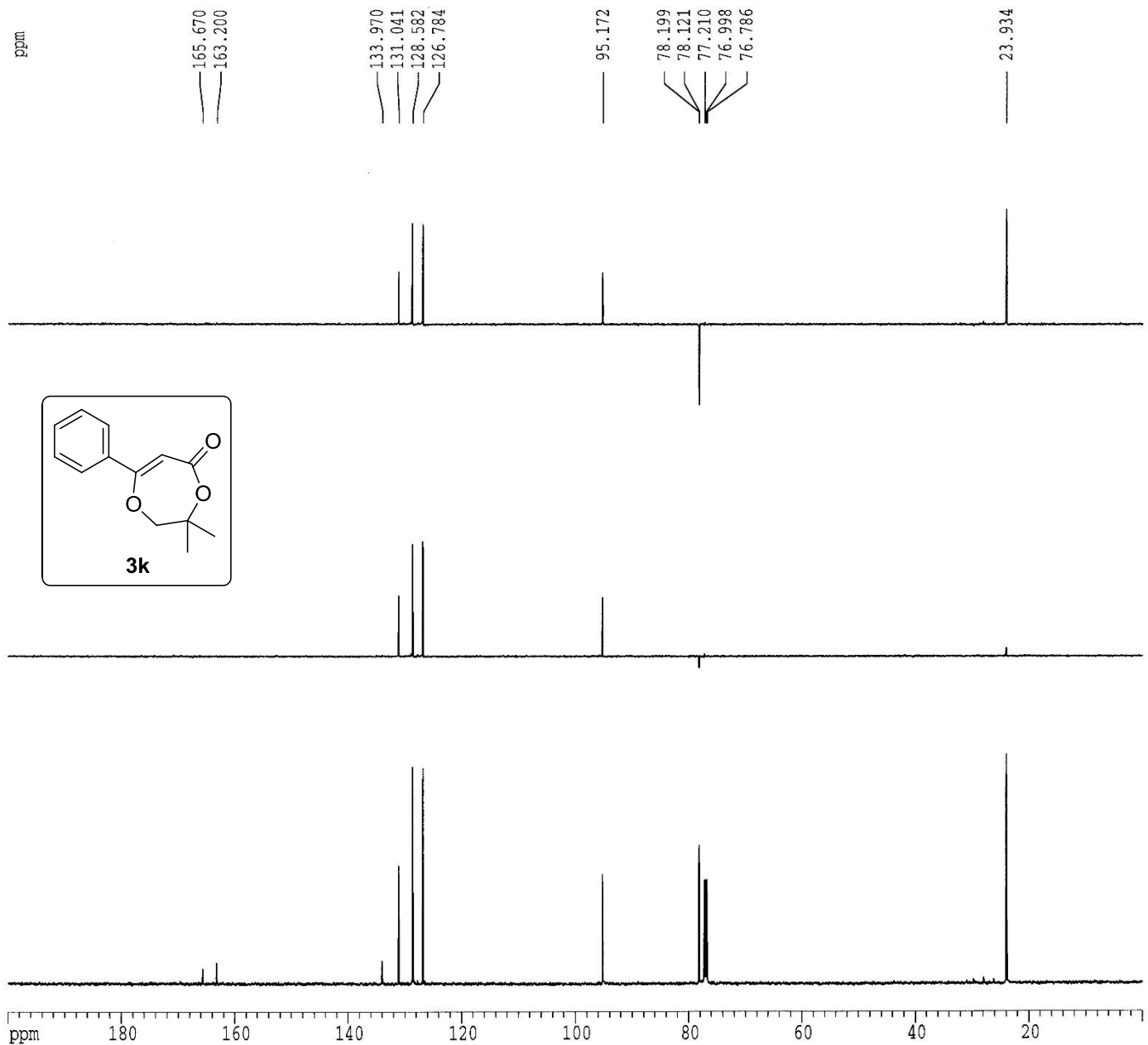
F2 - Acquisition Parameters  
 Date\_ 20150903  
 Time 12.47  
 INSTRUM spect  
 PROBRF 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 300  
 DS 0  
 SFR 45048.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 302.6 K  
 SI 3.50000000 sec  
 SII 0.03000000 sec  
 SIII 3.40000010 sec  
 SIV 0.00000000 sec  
 SVI 0.01500000 sec

===== CHANNEL f1 =====  
 NUCL1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.5346470 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUCL2 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 150.5180959 MHz  
 FINE EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 EC 1.00

1D NMR plot parameters  
 CH 20.00 cm  
 CY 4.00 cm  
 FID 200.000 ppm  
 FI 30103.62 Hz  
 FFP 0.000 ppm  
 FZ 0.00 Hz  
 FWHM 10.0000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      RS-2 106-2
EXPNO    1
PROCNO   1

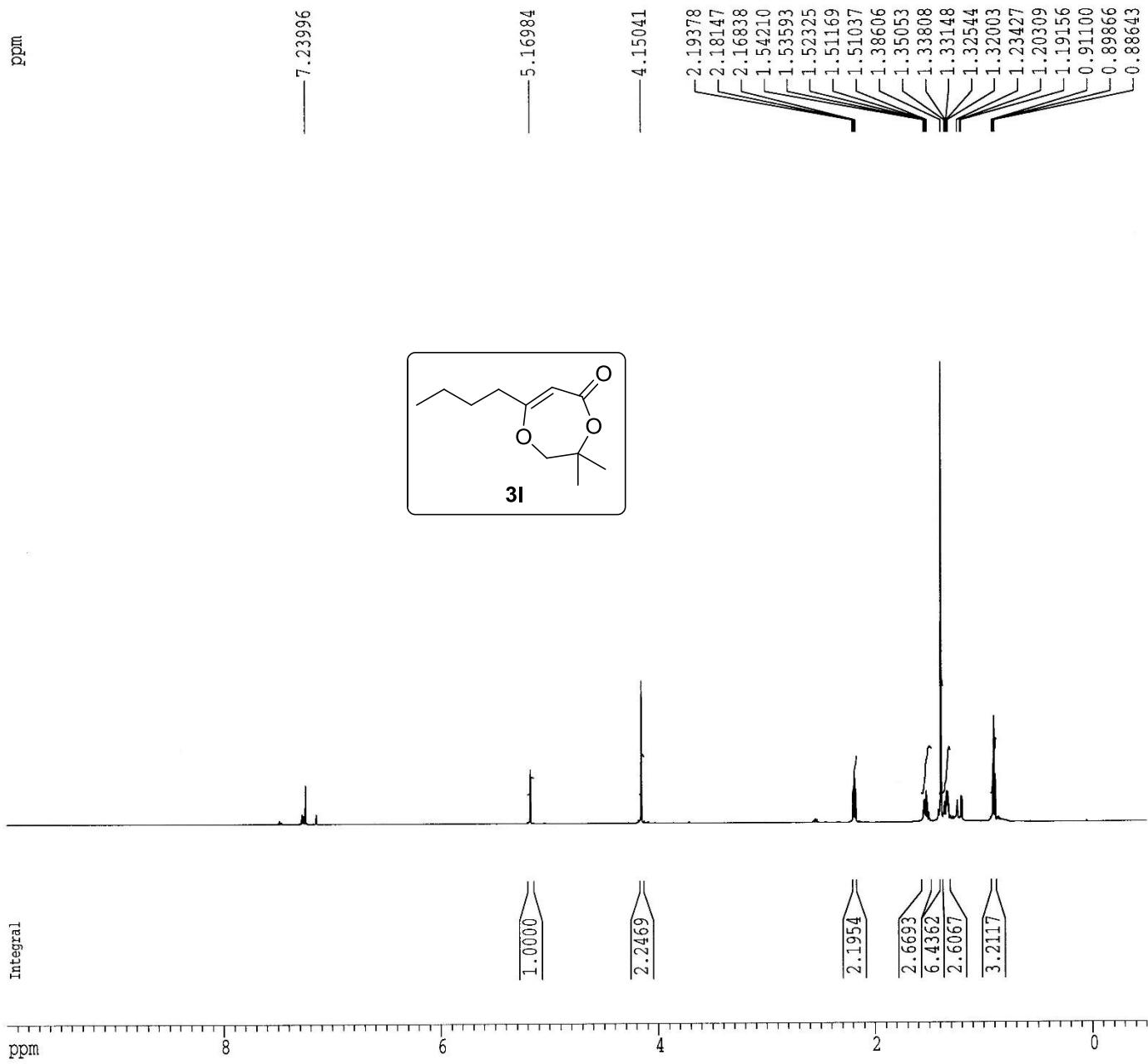
F2 Acquisition Parameters
LNAME     2050826
FILE      17.28
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zgpg30
TD         32768
SOLVENT   CDCl3
NS         32
DS         4
SWH        8389.262 Hz
FIDRES    0.256020 Hz
AQ         1.4530228 sec
RG         512
DC         29.600 usec
DE         0.50 usec
TE         301.2 K
AQ         1.4530228 sec
NUC1       13C
NUC2       13C
MWDW      0.0000000 sec
MURMR     0.0150000 sec

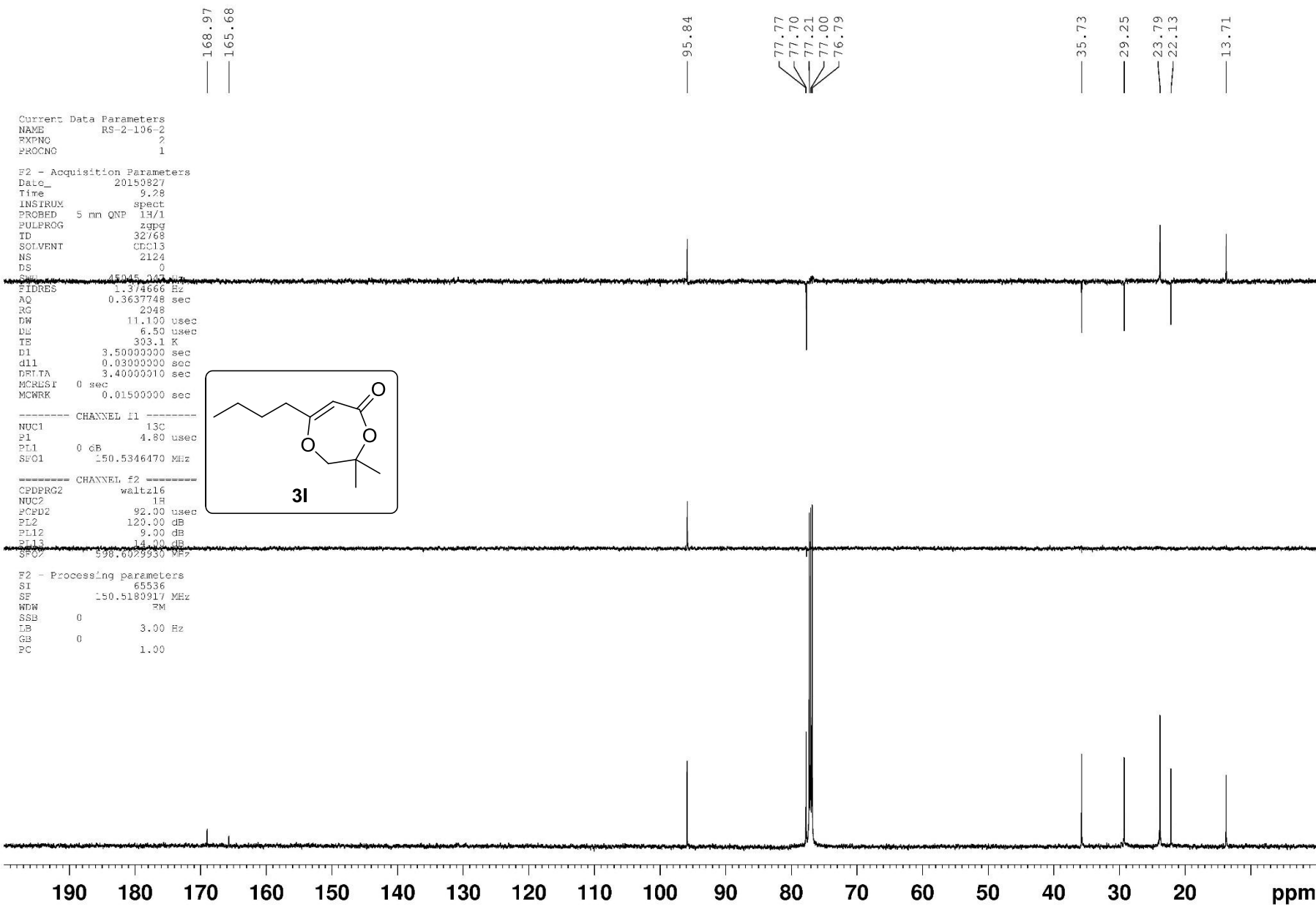
***** CHANNEL f1 *****
NUC1       13C
P1         10.00 usec
PL1        0.00 dB
PL2        192.0019388 Hz

F1 Processing parameters
SI         32768
SF         598.600296 MHz
WDW        no
SSB         0
LB         0.00 Hz
GB         0
PC         1.00

1D MMR plot parameters
CW         20.00 cm
CY         8.00 cm
P1P        10.000 ppm
F1         598.600 Hz
F2         0.500 ppm
P2         -299.30 Hz
RFMHZ     0.52600 ppm/cm
HWDW      314.26501 Hz/cm

```





Current Data Parameters  
 NAME RS-2-106-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150827  
 Time 9.28  
 INSTRUM spect  
 PROBED 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CEC13  
 NS 2124  
 DS 0  
 SWH 45045.000 MHz

FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 303.1 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCHRES1 0 sec  
 MCWRR 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 150.5180917 MHz  
 WDW FM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME RS-2-105-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20150823  
 Time 19.14  
 INSTRUM spect  
 PROBRD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 467  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 303.9 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 ACQRES 0.0000000 sec  
 MCHRX 0.0150000 sec

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

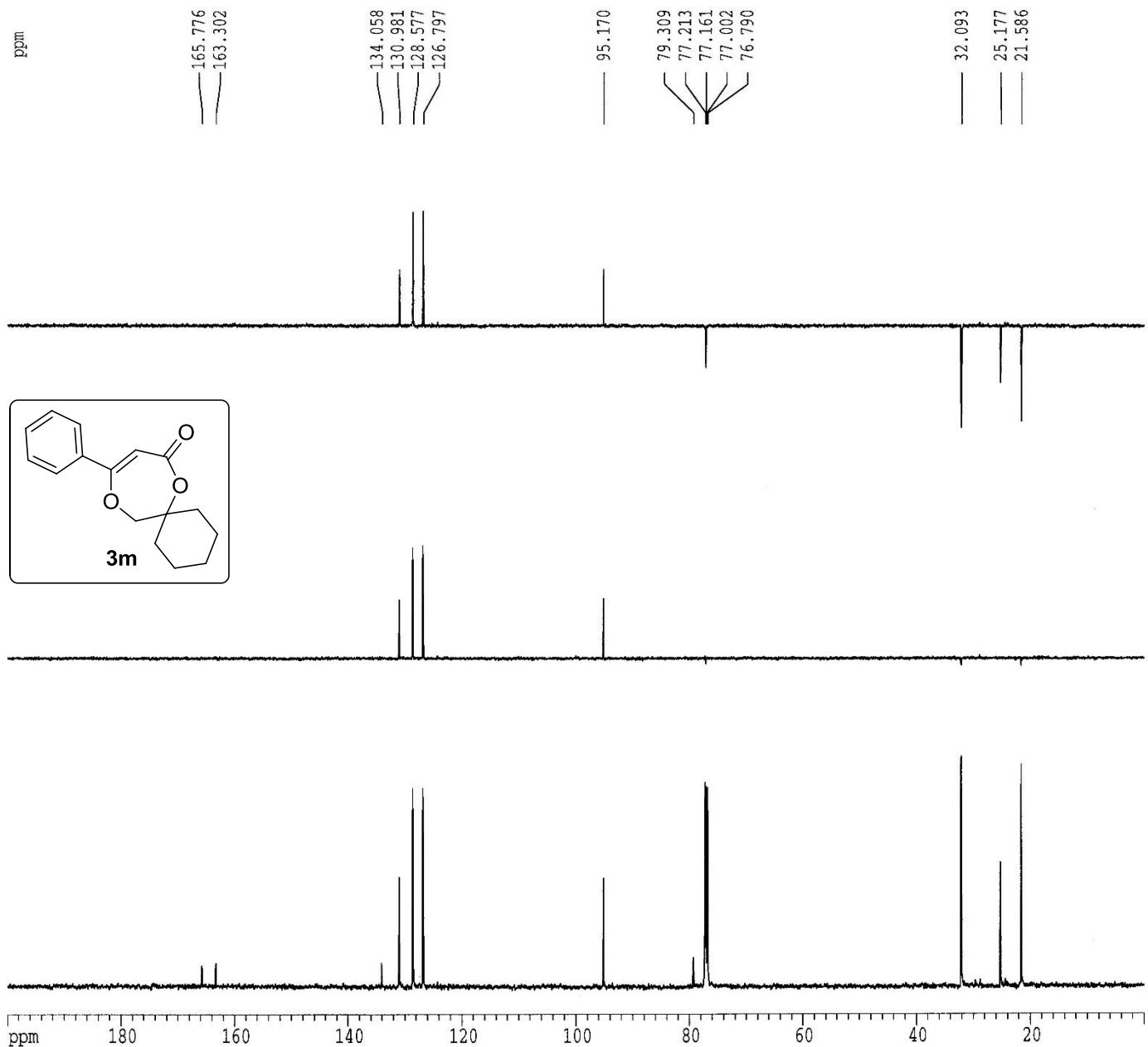
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.6029930 MHz

F2 - Processing parameters

SI 65536  
 SF 150.5180926 MHz  
 WDW EM  
 SSB 0  
 LB 5.00 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  
 PRGCM 10.90000 ppm/cm  
 HZCM 1505.18091 Hz/cm



7.692  
7.679  
7.674  
7.670  
7.473  
7.456  
7.442  
7.439  
7.420  
7.414  
7.410  
7.405  
7.400  
7.392  
7.388  
7.383  
7.377  
7.373  
7.353  
7.350  
7.338  
7.332  
7.325  
7.314  
7.240  
5.843  
5.715  
4.956  
4.939  
4.922  
4.905

1.441  
1.424

Current Data Parameters

NAME 20151121  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

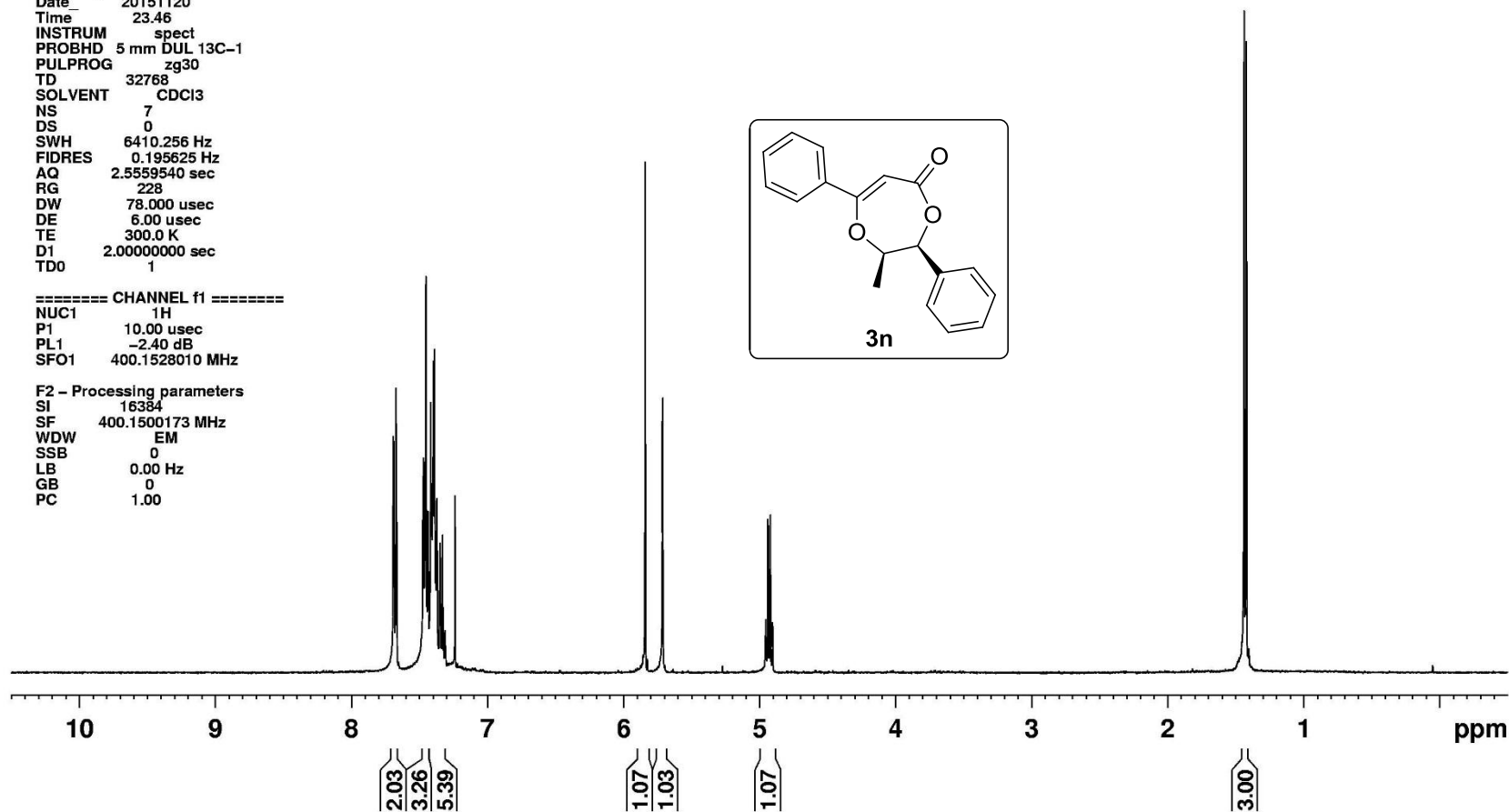
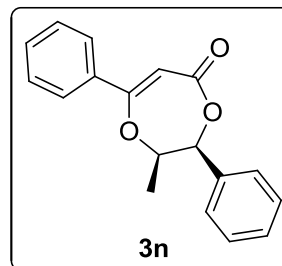
Date 20151120  
Time 23.46  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 7  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 228  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.00000000 sec  
TD0 1

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

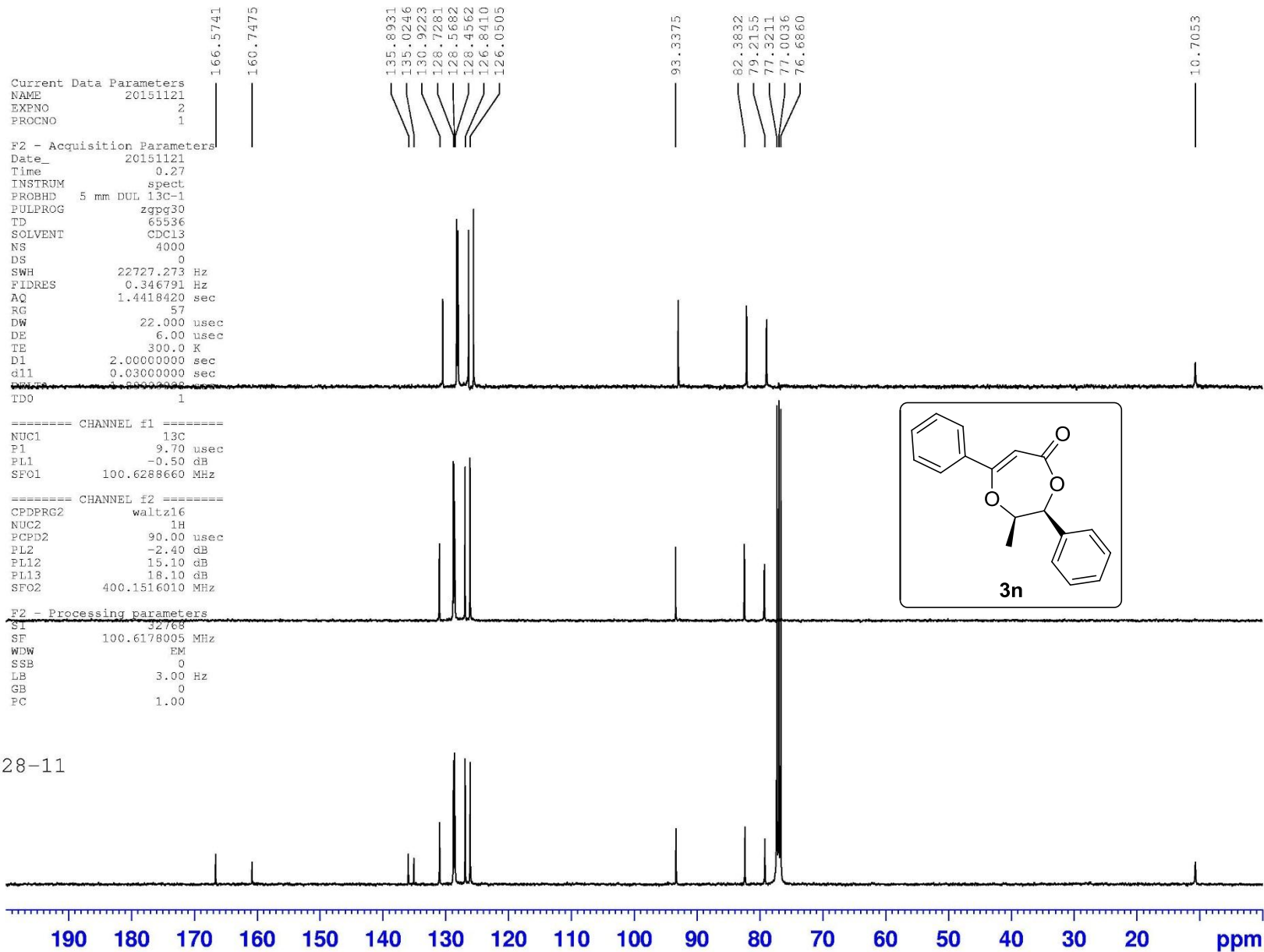
NUC1 1H  
P1 10.00 usec  
PL1 -2.40 dB  
SFO1 400.1528010 MHz

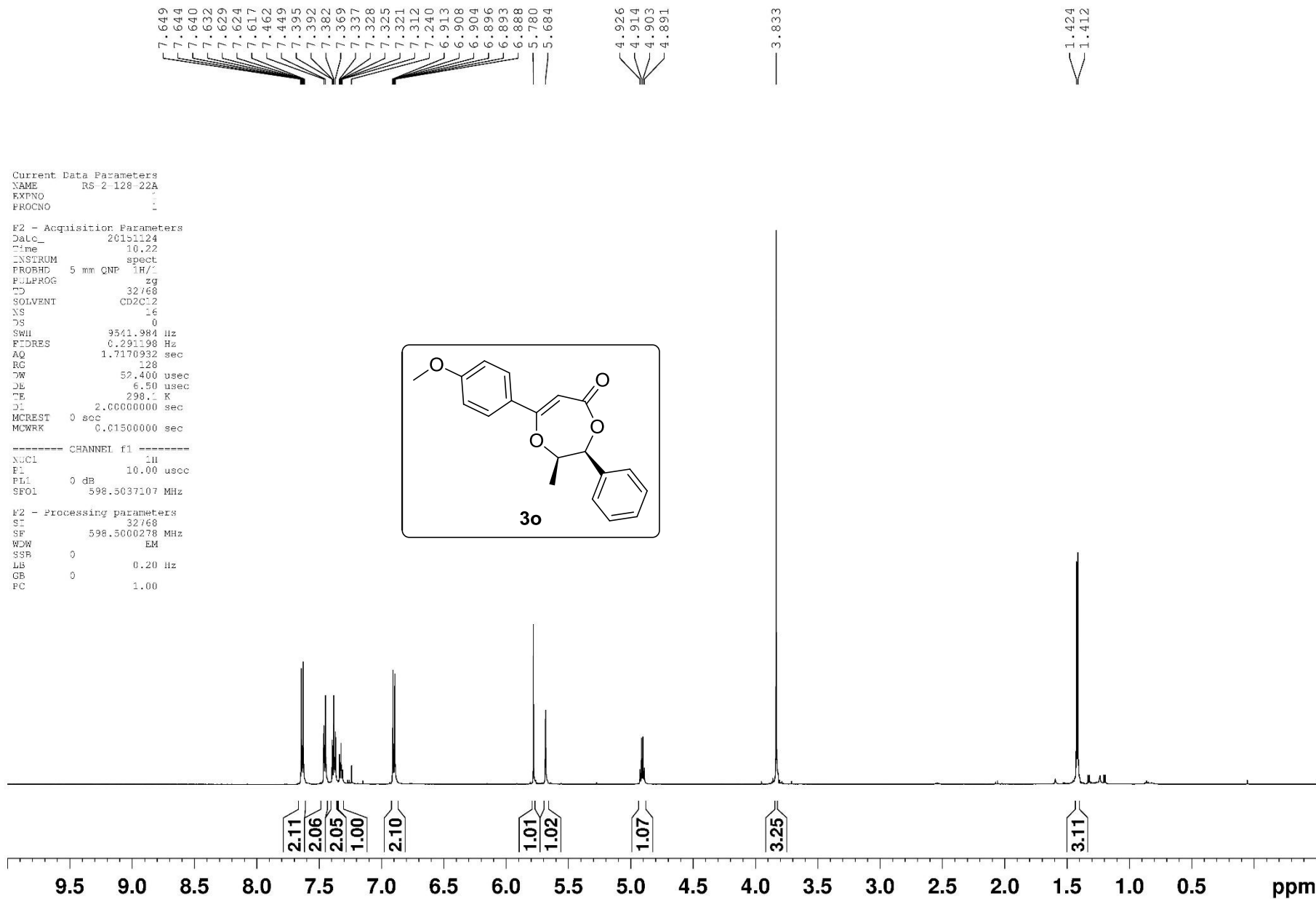
F2 - Processing parameters

SI 16384  
SF 400.1500173 MHz  
WDW EM  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00









Current Data Parameters  
 NAME RS-2-128-22A  
 EXPAO 2  
 PROCNO 1

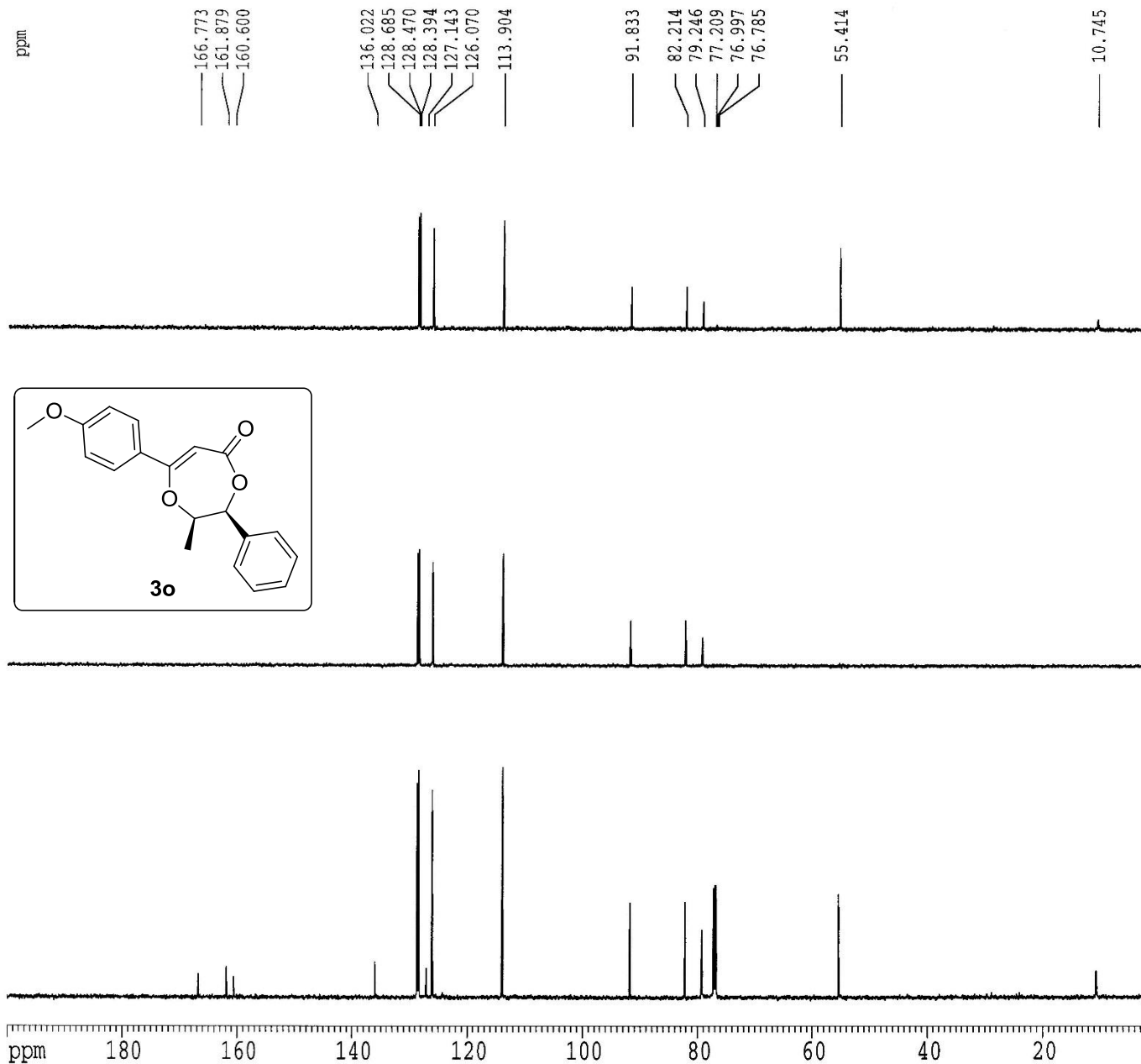
F2 - Acquisition Parameters  
 Date\_ 20151123  
 Time 18.22  
 INSTRUM spect  
 PROBAD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 293  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCHKA 0.01500000 sec

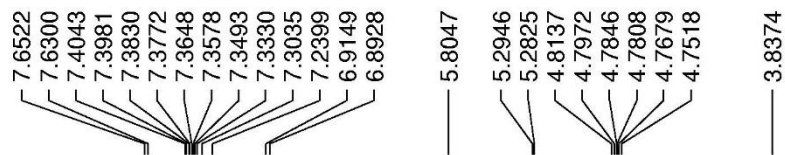
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.5094992 MHz

===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 FCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4929501 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  
 FLP 200.000 ppm  
 F1 30098.59 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.00000 ppm/cm  
 HZCM 1504.92944 Hz/cm





Current Data Parameters

NAME 20160217  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters

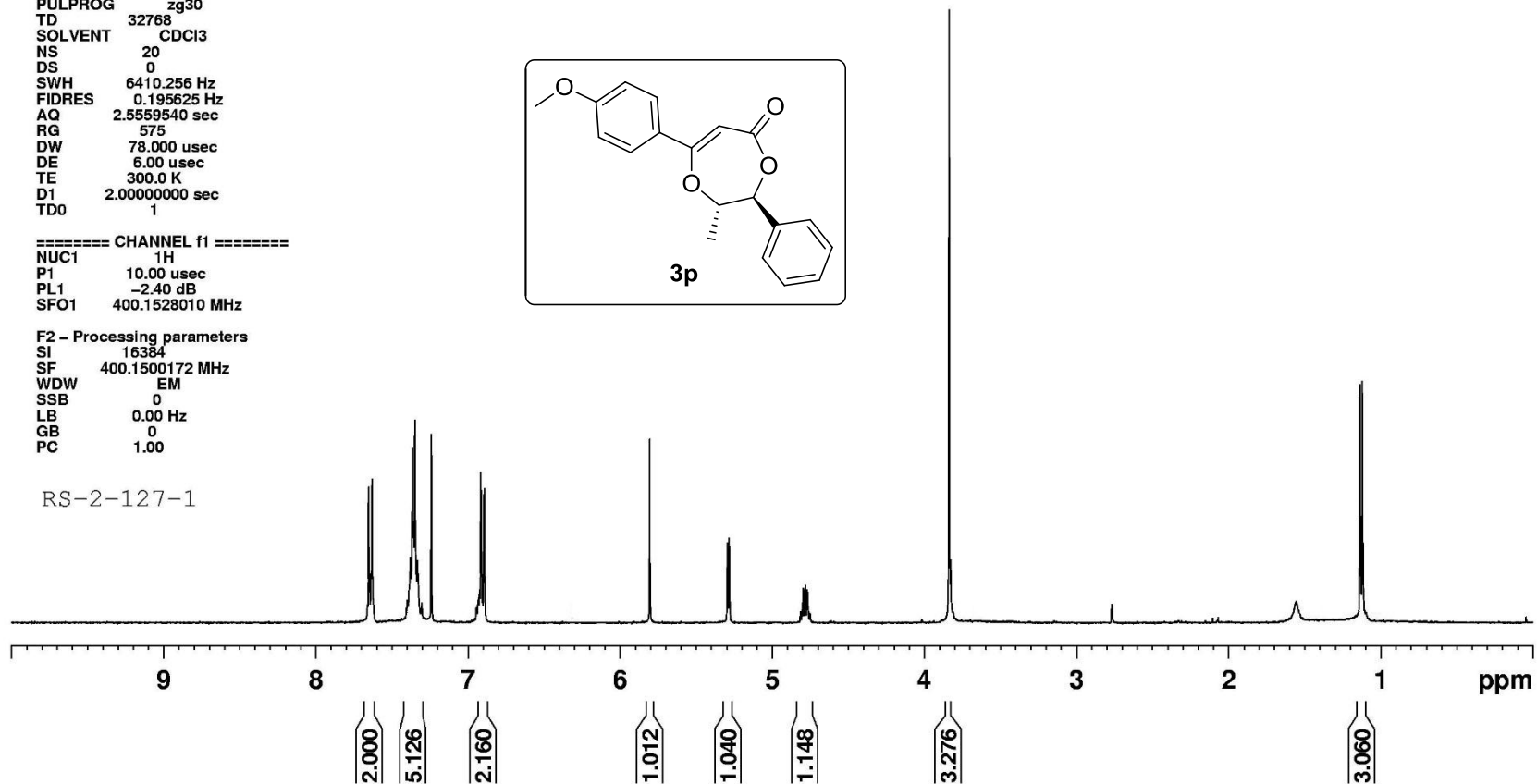
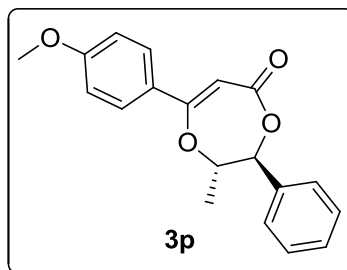
Date 20160217  
Time 16.49  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zg30  
TD 32768  
SOLVENT CDCl3  
NS 20  
DS 0  
SWH 6410.256 Hz  
FIDRES 0.195625 Hz  
AQ 2.5559540 sec  
RG 575  
DW 78.000 usec  
DE 6.00 usec  
TE 300.0 K  
D1 2.0000000 sec  
TD0 1

===== 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 0.00 Hz  
GB 0  
PC 1.00





166.903  
162.171  
161.957

136.361  
128.855  
128.714  
128.530  
127.231  
126.650

113.934

91.826

82.898  
82.517  
77.317  
77.000  
76.683

55.429

19.127

Current Data Parameters  
NAME 20160216  
EXPNO 2  
PROCNO 1

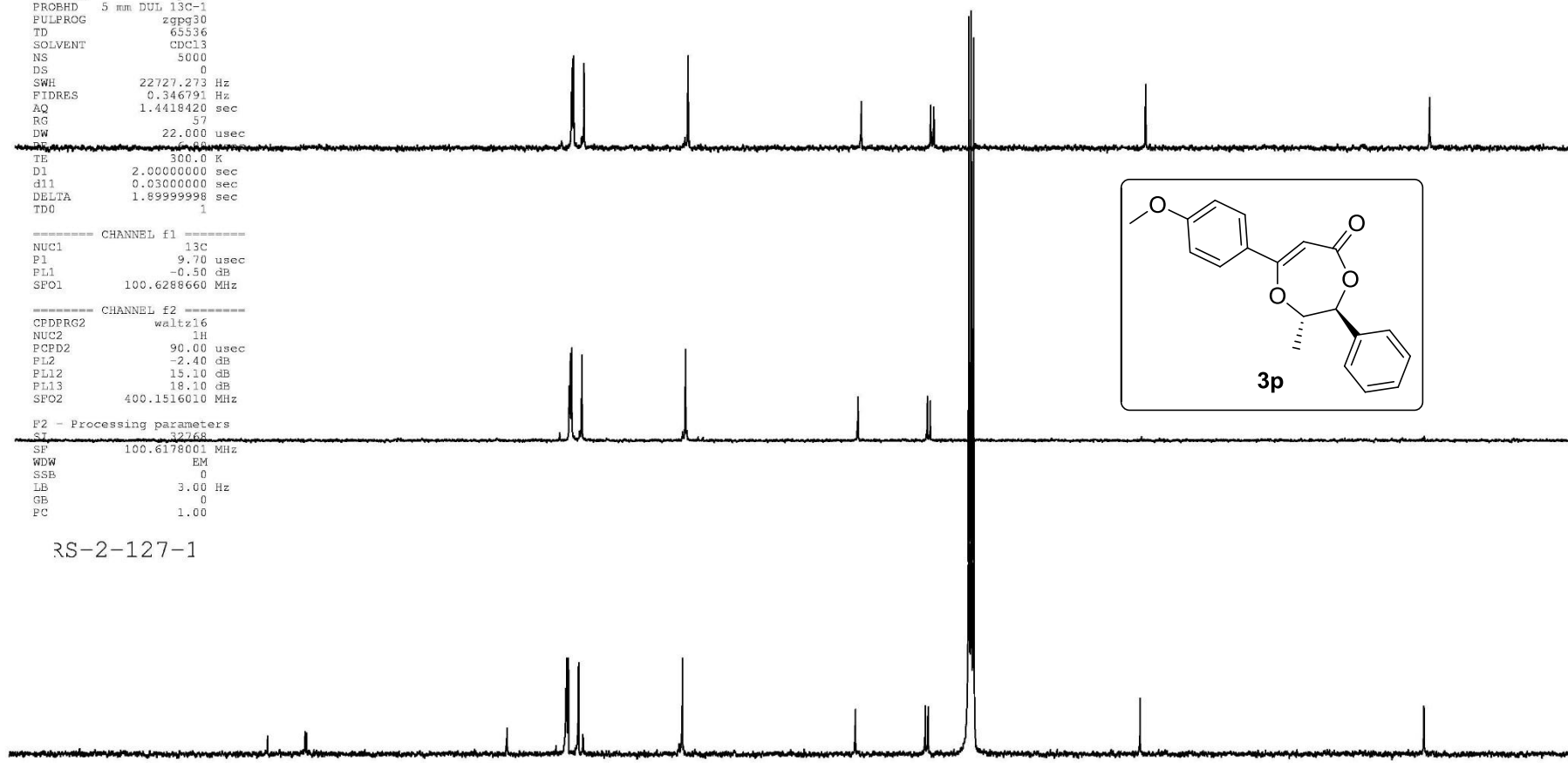
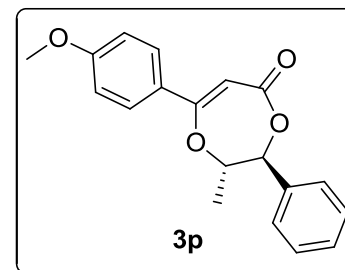
F2 - Acquisition Parameters  
Date\_ 20160216  
Time 0.11  
INSTRUM spect  
PROBHD 5 mm DUL 13C-1  
PULPROG zgpg30  
TD 65536  
SOLVENT cdcl3  
NS 5000  
DS 0  
SWH 22727.273 Hz  
FIDRES 0.346791 Hz  
AQ 1.4418420 sec  
RG 57  
DW 22.000 usec  
DE 0.0000000 sec  
TE 300.0 K  
D1 2.00000000 sec  
d11 0.03000000 sec  
DELTA 1.89999998 sec  
TDG 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 100.6178001 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.00

RS-2-127-1



190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

```

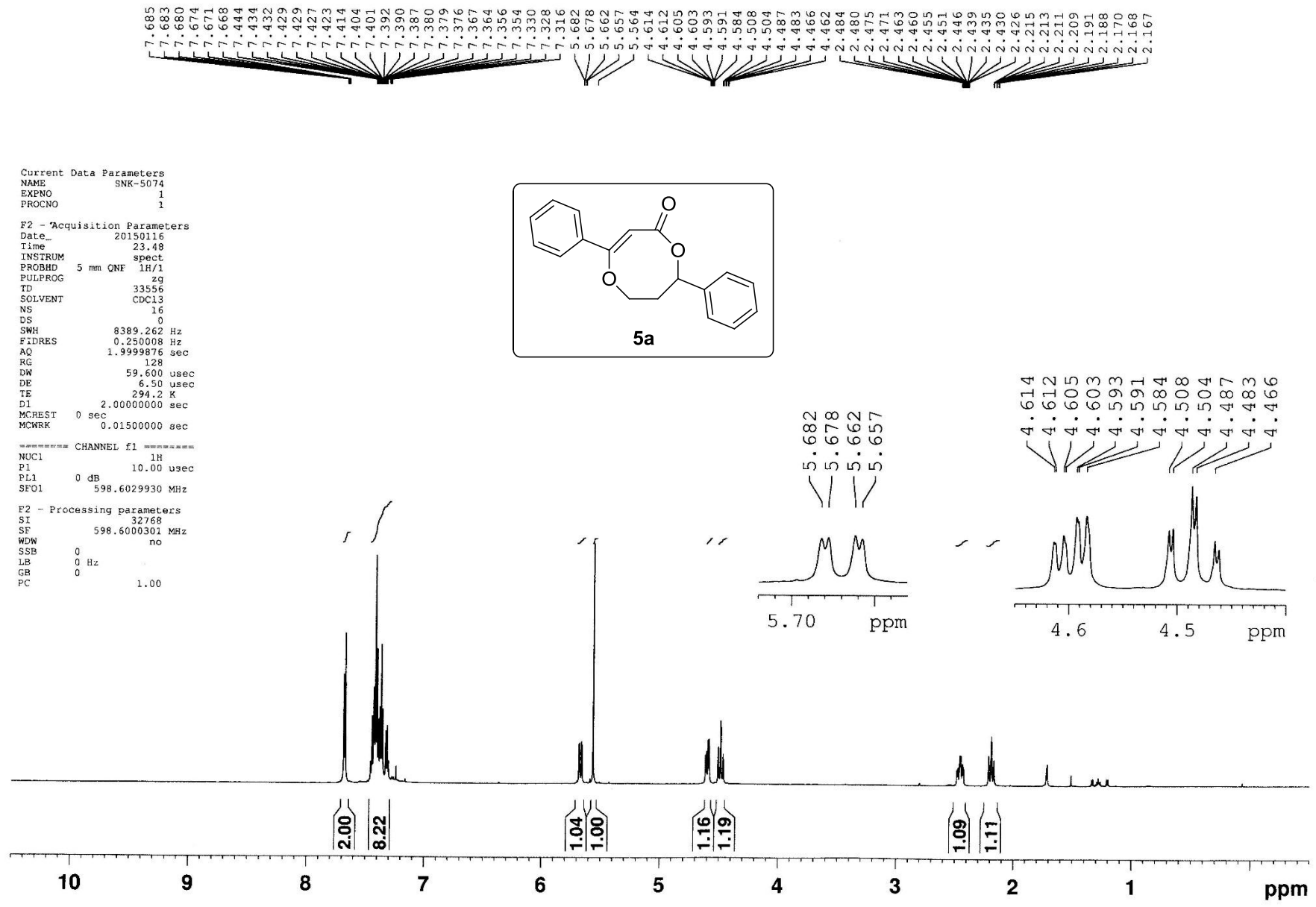
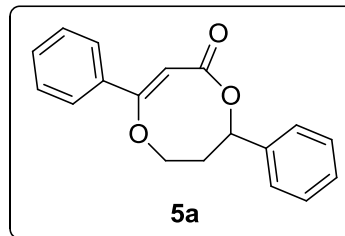
Current Data Parameters
NAME          SNK-5074
EXPNO         1
PROCNO        1

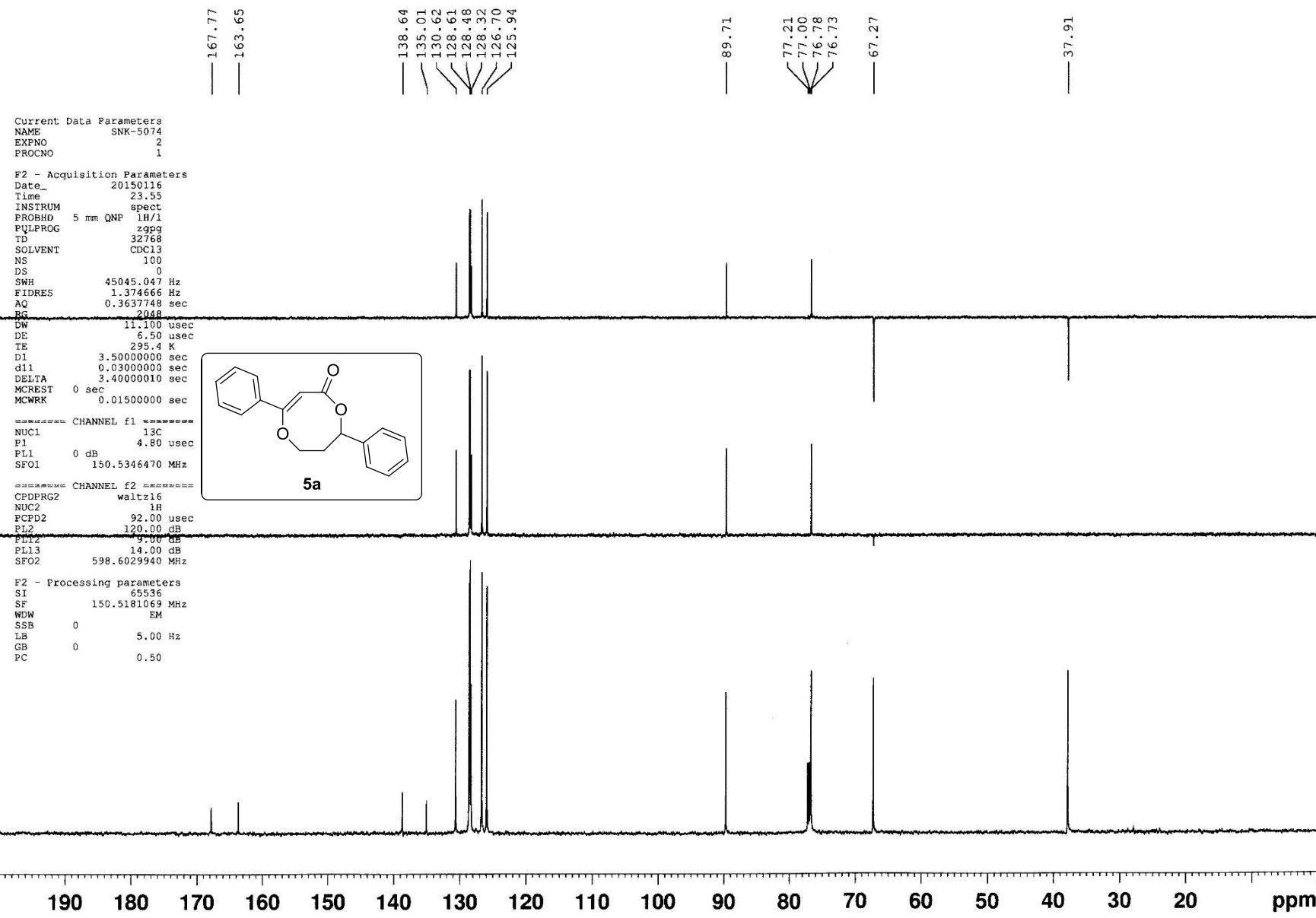
F2 - Acquisition Parameters
Date_         20150116
Time          23.48
INSTRUM       spect
PROBHD        5 mm QNP 1H/1
PULPROG       zg
TD            33556
SOLVENT       CDC13
NS            16
DS            0
SWH           8389.262 Hz
FIDRES        0.250008 Hz
AQ            1.9999876 sec
RG            128
DW            59.600 usec
DE            6.50 usec
TE            294.2 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            1.00

```





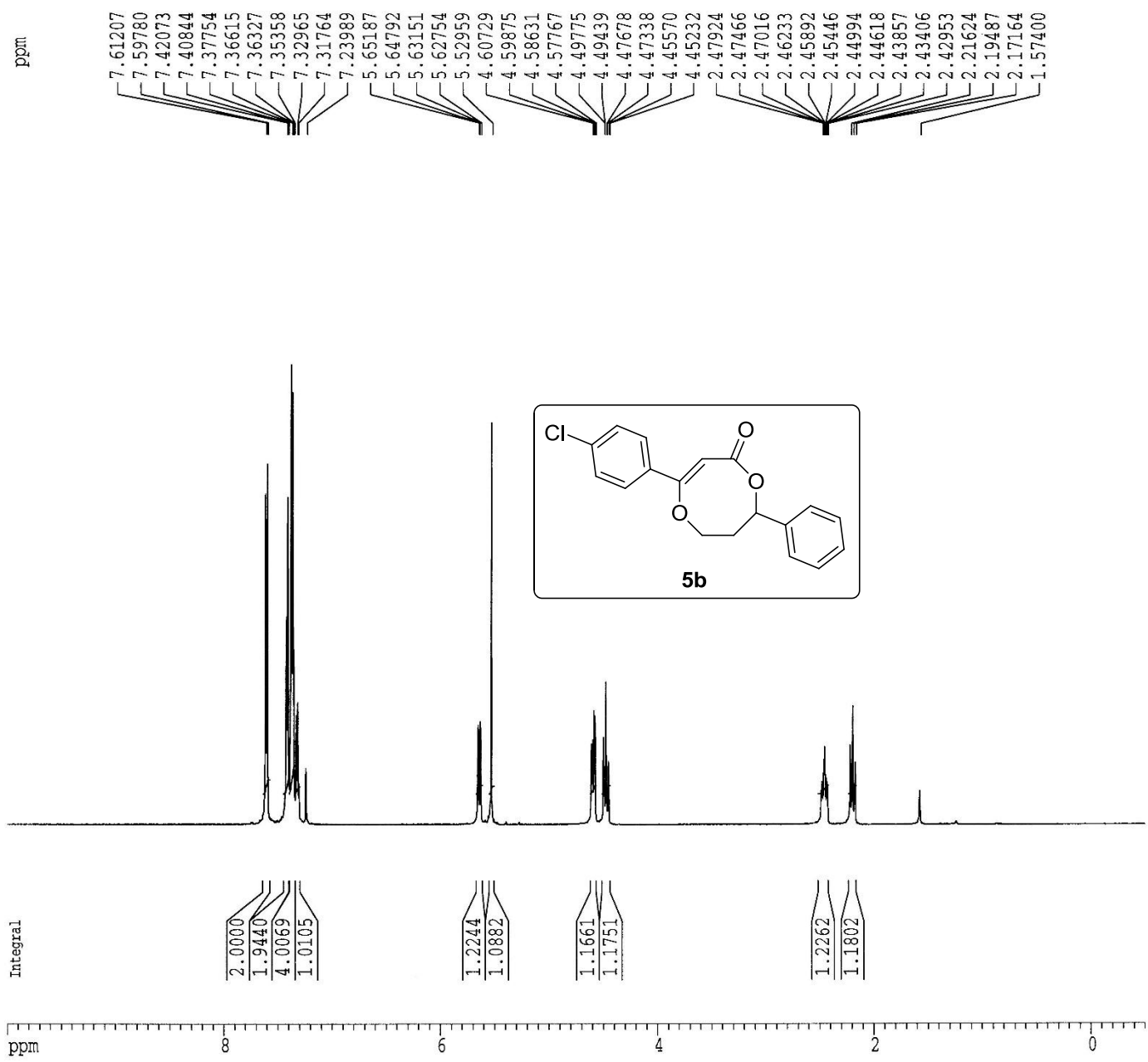
Current Data Parameters  
 NAME RS-2-42-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150507  
 Time 10.37  
 INSTRUM spect  
 PROBEHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8382.229 Hz  
 FIDRES 0.255805 Hz  
 AQ 1.9546613 sec  
 RG 128  
 DM 59.650 usec  
 DE 85.21 usec  
 TE 297.3 K  
 D1 2.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SFC1 598.6029930 MHz

F2 - Processing parameters  
 SI 32768  
 SF 598.600305 MHz  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 10.000 ppm  
 F1 5986.00 Hz  
 F2P -0.500 ppm  
 F2 -299.30 Hz  
 PRGCM 0.52500 ppm/cm  
 HZCM 314.26501 Hz/cm





Current Data Parameters  
 NAME RS-2-42-1  
 EXPNO 2  
 PROCNO 1

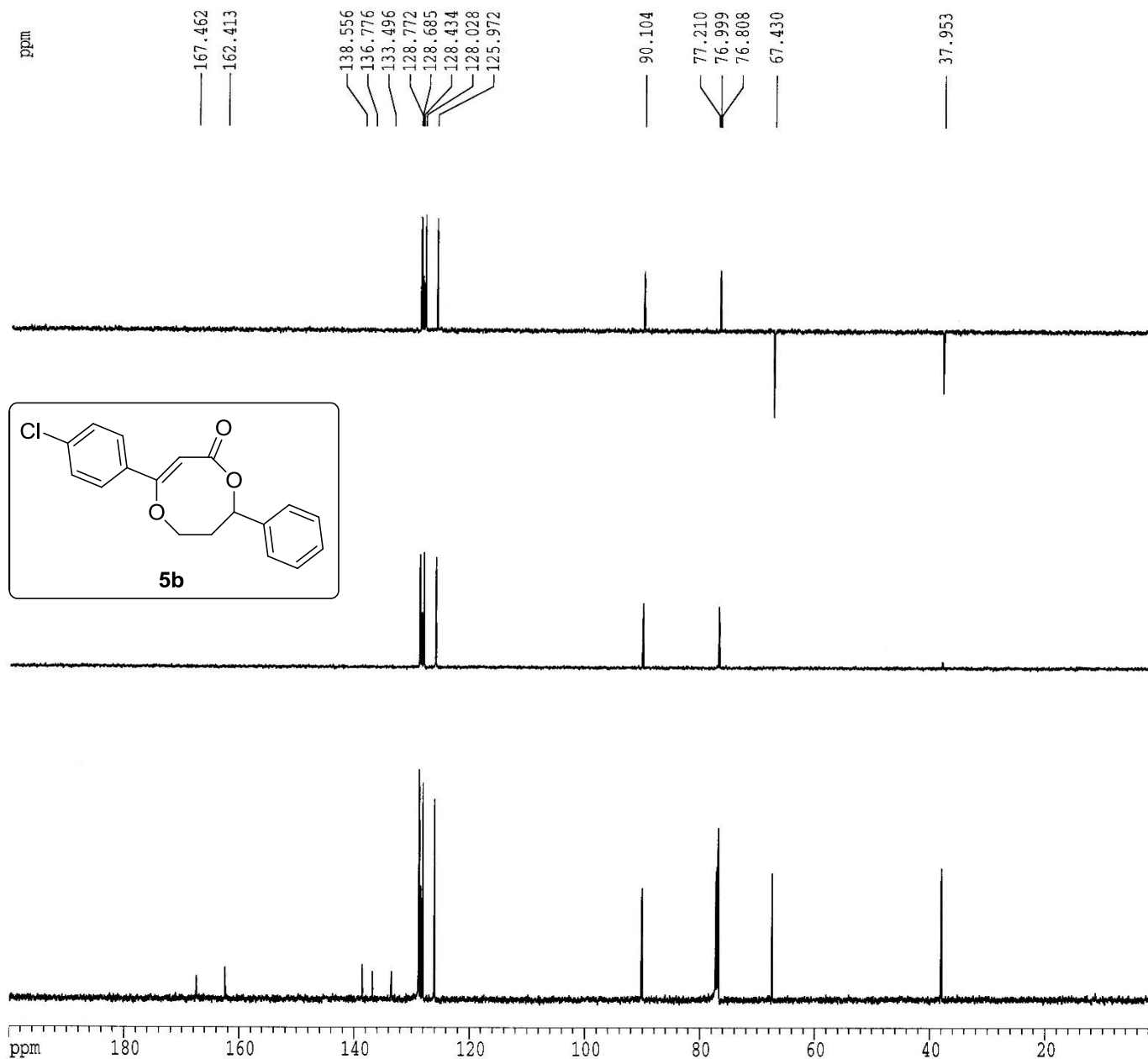
F2 - Acquisition Parameters  
 Date\_ 20150507  
 Time 10.39  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT DMSO  
 NS 100  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCWRR 0.01500000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180966 MHz  
 WDM 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  
 PPMCK 10.03000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      RS-2-37-1
EXPNO    1
PROCNO   1

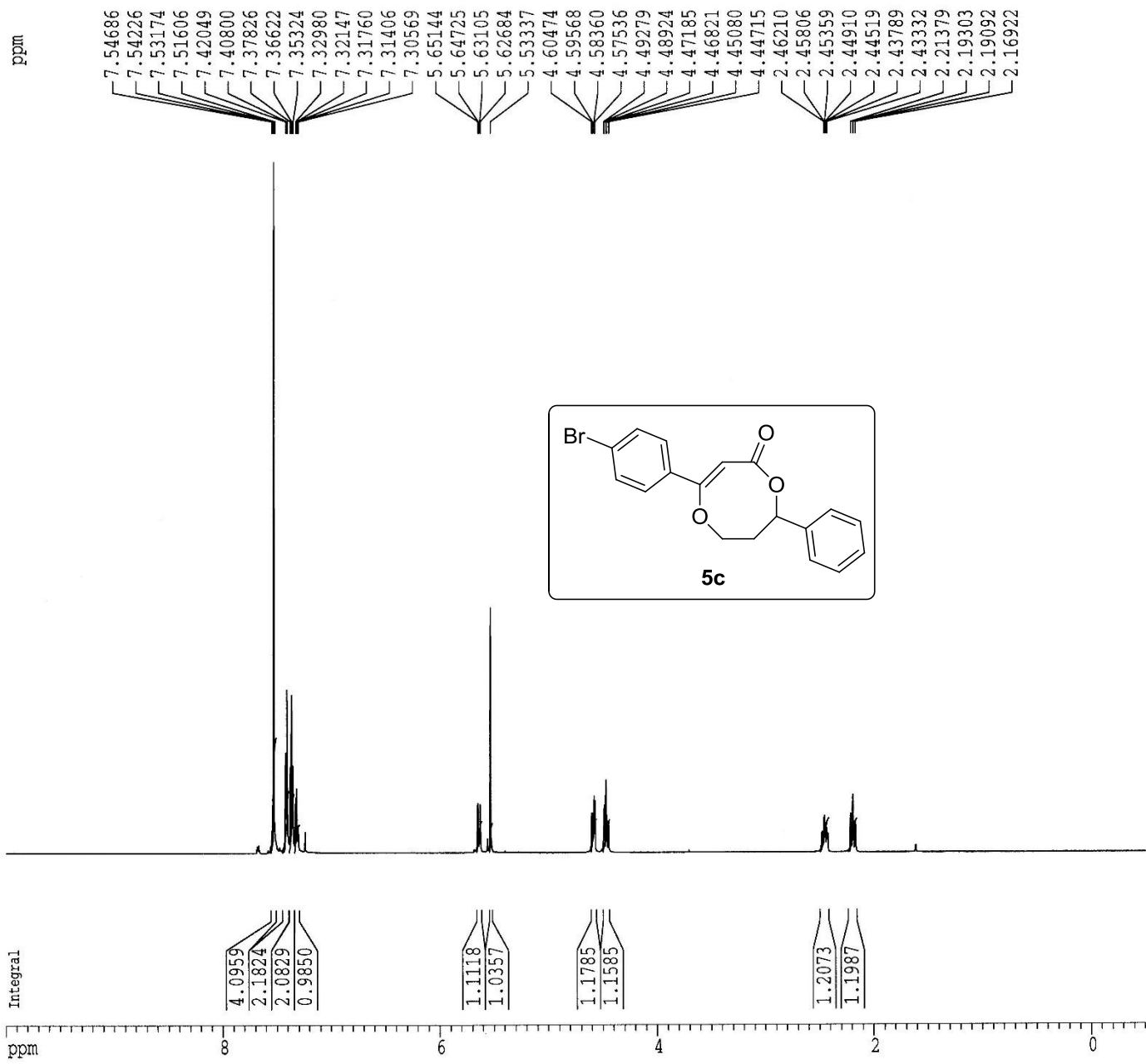
F2 - Acquisition Parameters
Date_    20150430
Time     15.54
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD       32768
SOLVENT  CDCl3
NS       16
DS       0
SWH      8389.262 Hz
FIDRES   0.256020 Hz
AQ       1.9530228 sec
RG       128
CW       59.680 usec
DE       6.50 usec
TE       297.9 K
D1       2.0000000 sec
NORESC   0.0000000 sec
RG/RK    0.0150000 sec

===== CHANNEL f1 =====
NUC1     1H
P1       10.00 usec
PL1      0.00 dB
SFO1     500.6029930 MHz

F2 - Processing parameters
S1       32768
SF       500.6000296 MHz
WDW      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.00

1D NMR plot parameters
CX       20.00 cm
CY       15.00 cm
F1P      10.000 ppm
F1       500.600 Hz
F2P      -0.500 ppm
F2       -299.30 Hz
PPMCM    0.52500 ppm/cm
HDCM     334.26501 Hz/cm

```



Current Data Parameters  
 NAME RS-2-37-1  
 EXPNO 2  
 PROCNO 1

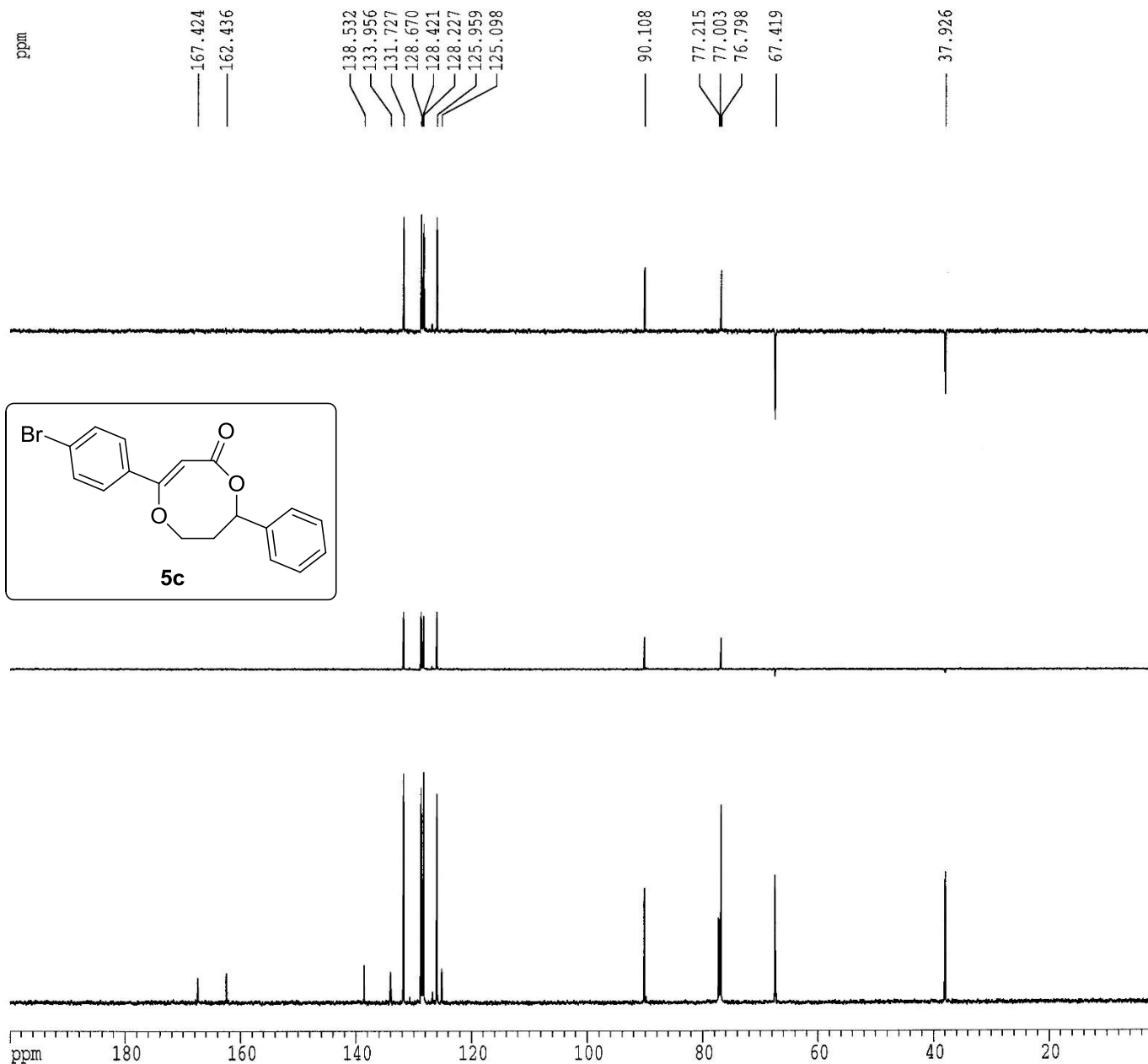
F2 - Acquisition Parameters  
 Date\_ 20150430  
 Time 16.01  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT CDC13  
 NS 100  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCWPK 0.01500000 sec

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

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

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

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



Current Data Parameters  
 NAME RS-2-36-2  
 EXPNO 1  
 PROCNO 1

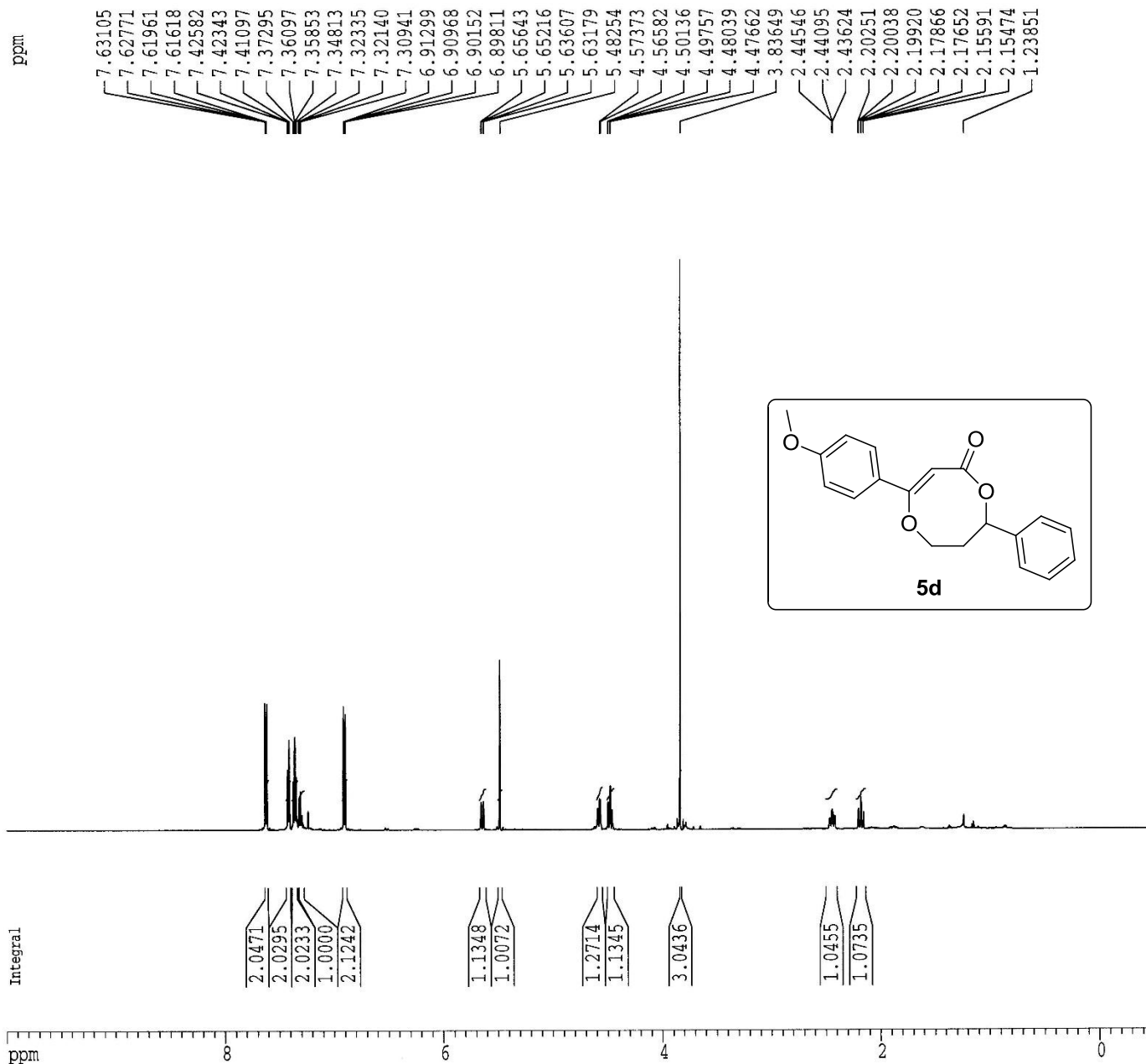
F2 - Acquisition Parameters

Date\_ 20150507  
 Time 9.38  
 INSTRUM spect  
 PROSHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8382.229 Hz  
 FIDRES 0.255805 Hz  
 AQ 1.9546613 sec  
 RG 128  
 DH 59.650 usec  
 DE 85.21 usec  
 TE 296.9 K  
 D1 2.0000000 sec  
 MCREST 0.0000000 sec  
 MCNRK 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SF01 598.6029930 MHz

F2 - Processing parameters  
 SI 32768  
 SF 598.6000295 MHz  
 WDN no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

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



Current Data Parameters  
 NAME RS-2-36-2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

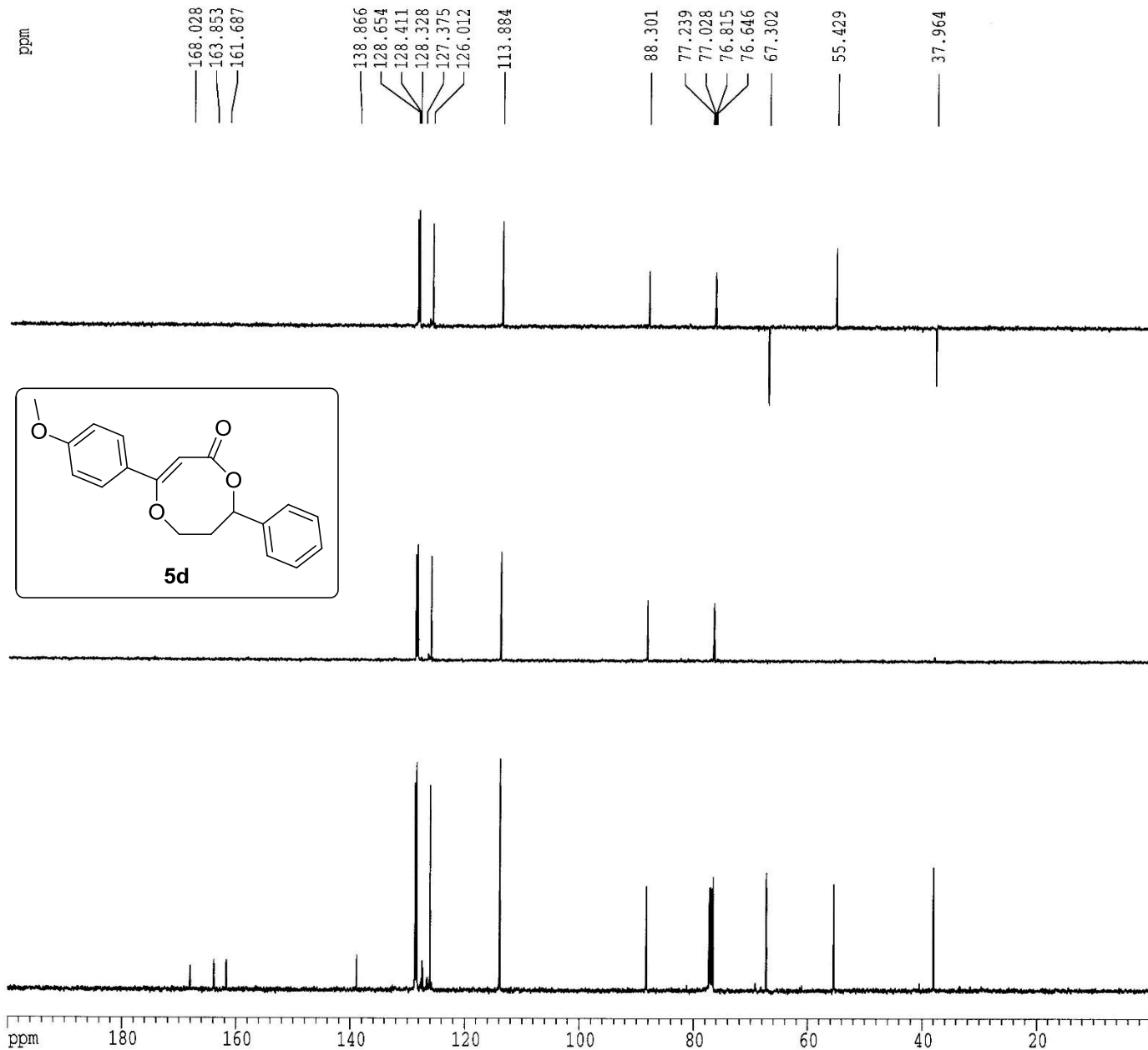
Date\_ 20150507  
 Time 9.41  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT DMSO  
 NS 154  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180932 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

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



```

Current Data Parameters
NAME      RS-2-74-1
EXPNO    1
PROCNO   1

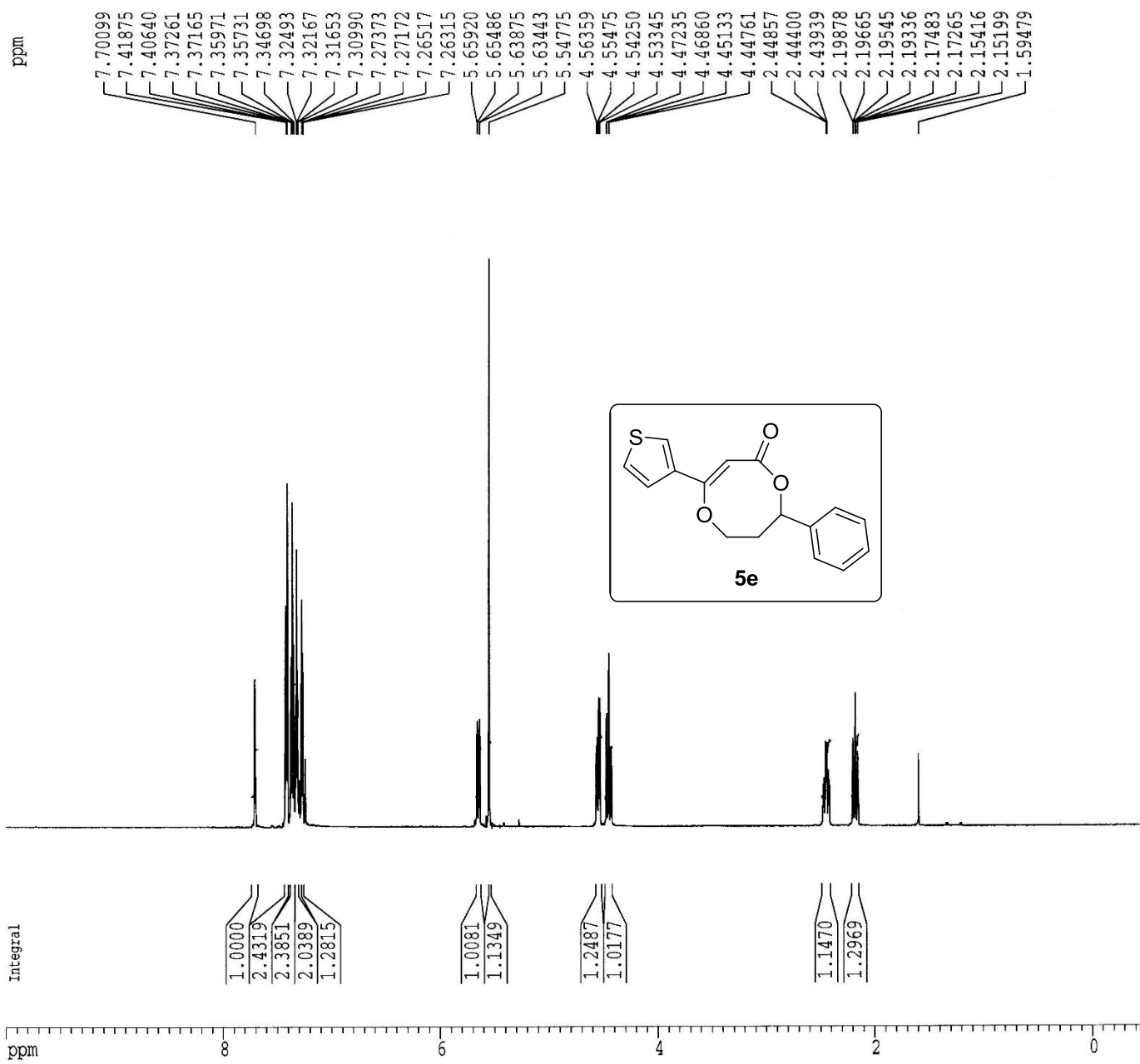
F2 - Acquisition Parameters
Date_    20150612
Time     10.42
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       8189.262 Hz
FIDRES    0.256020 Hz
AQ        1.9530228 sec
RG         128
CW        59.680 usec
DE         6.50 usec
TE        300.6 K
SI        1.5000000 sec
SF        0.0000000 sec
MORPH    0.0000000 sec
MORPH    0.01500000 sec

===== CHANNEL f1 =====
NUC1      1H
P1        10.00 usec
PL1       0.00 dB
SFO1     500.1363913 MHz

F2 - Processing parameters
SI        32768
SF        500.1363913 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
CY        10.00 cm
F1P       10.000 ppm
F1        500.1363913 MHz
F2P       -0.500 ppm
F2        -299.10 Hz
FPCX      0.52500 ppm/cm
FDCX      314.26501 Hz/cm

```



Current Data Parameters  
 NAME RS-2-74-1  
 EXPNO 2  
 PROCNO 1

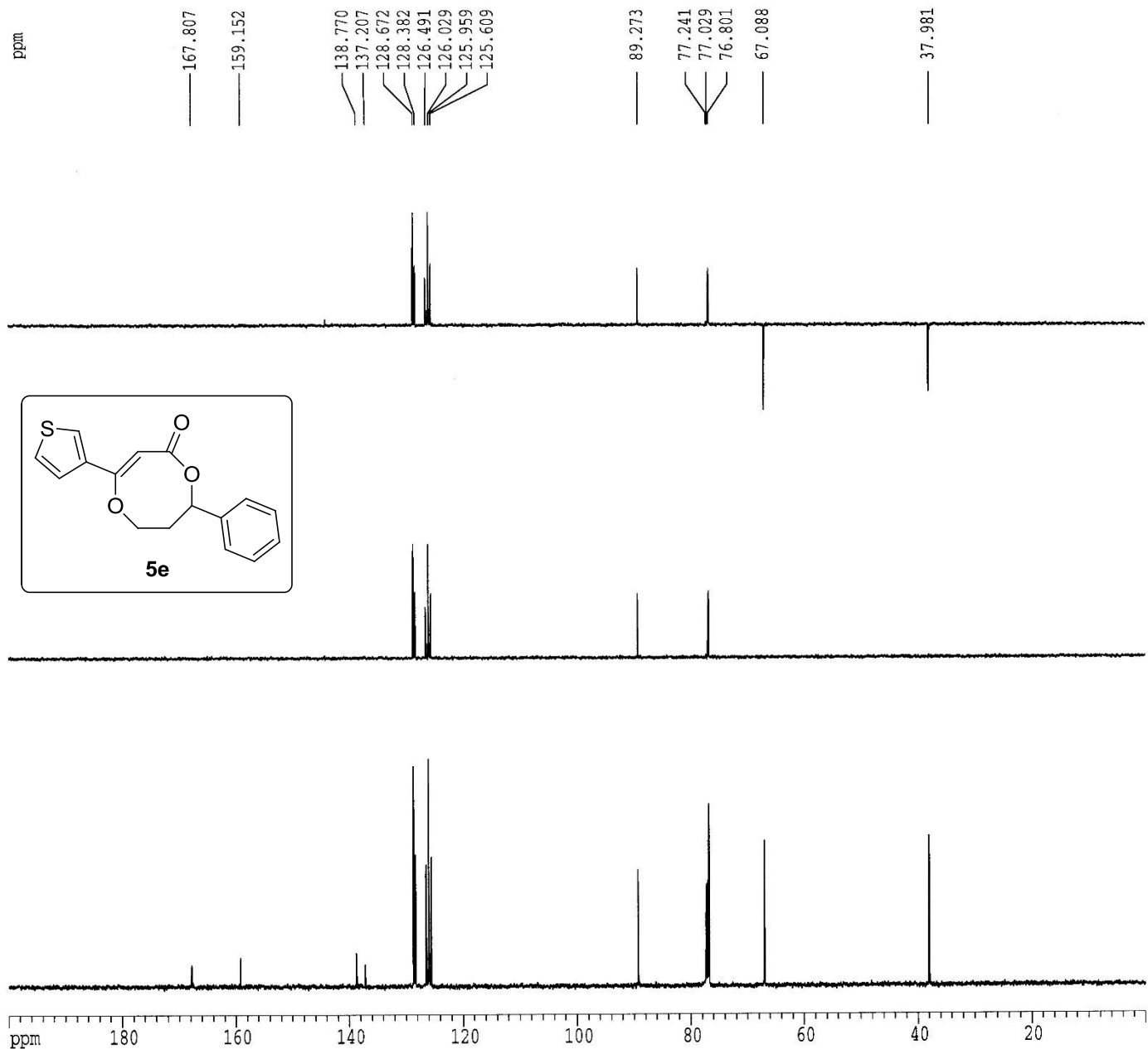
F2 - Acquisition Parameters  
 Date\_ 20150612  
 Time 10.46  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 150  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 BW 11.100 usec  
 DE 6.50 usec  
 TE 301.8 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCKEPT 0.0000000 sec  
 MCKERR 0.0150000 sec

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PM1 0.00 dB  
 SFO1 150.5331418 MHz

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180926 MHz  
 WDH 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 30133.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.30000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      SS-2-73-1
EXPNO    1
PROCNO   1

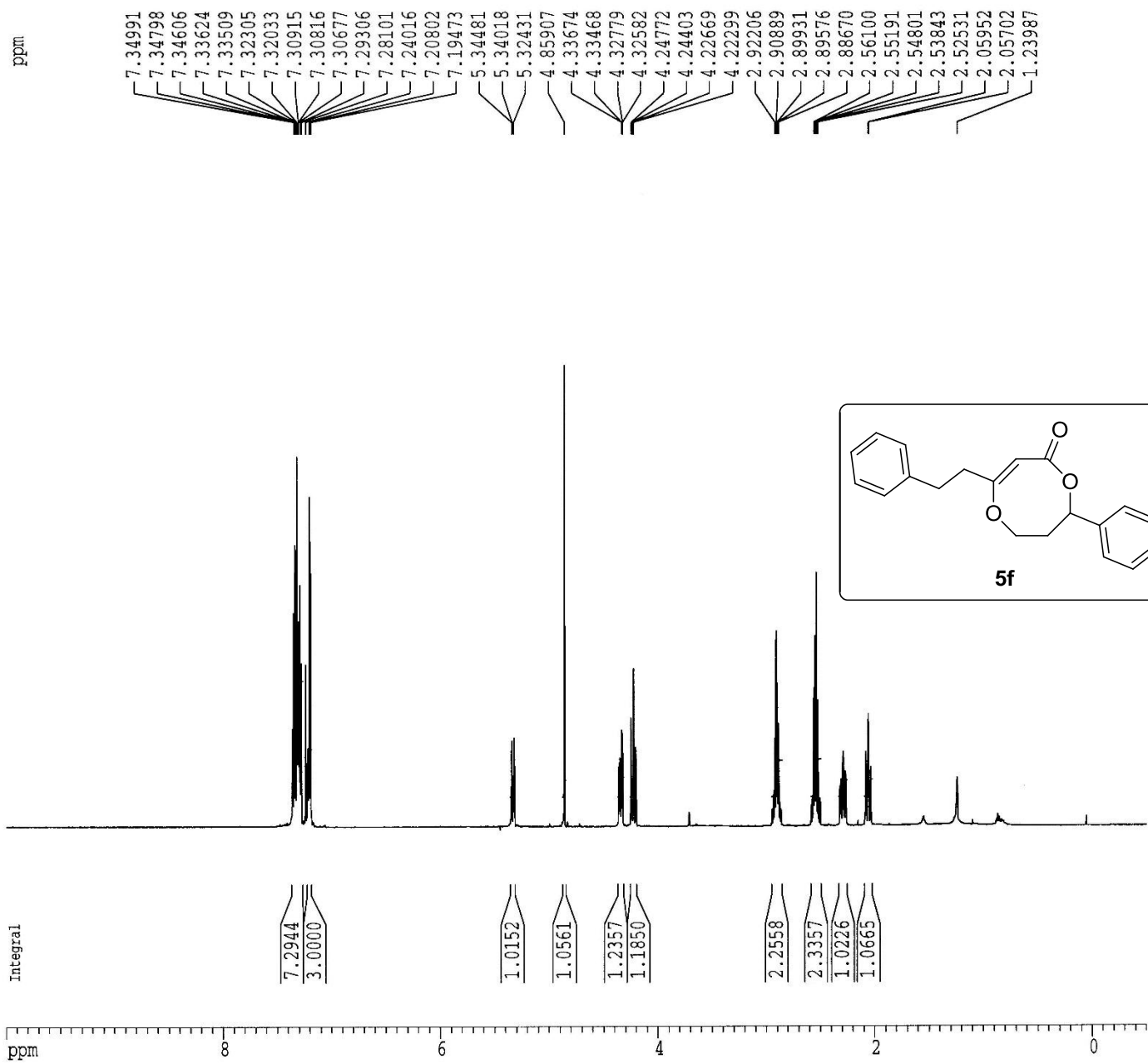
F2 - Acquisition Parameters
Date_    20150612
Time     11:27
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SFO      8389.262 Hz
FIDRES   0.256020 Hz
AQ        1.9530228 sec
RG         512
CW        59.600 usec
DE        6.50 usec
TE        300.6 K
DQ        1.5000000 sec
MCKEY    0.0000000 sec
MCHNK    0.0150000 sec

***** CHANNEL f1 *****
NUC1      1H
P1        10.00 usec
PL1       0.00 dB
SFO1     508.6032913 MHz

F2 - Processing parameters
SI        32768
SF        508.600306 MHz
RG        EM
SGB       0
LRF       0.20 Hz
GB        0
FI        1.00

1D NMR plot parameters
CY        20.00 cm
TY        8.00 cm
F1P       10.000 ppm
F1        5086.00 Hz
F2P       0.500 ppm
F2        -999.30 Hz
PFMHK    0.52500 ppm/cm
HOCK     314.26501 Hz/cm

```





Current Data Parameters  
 NAME RS-2-73-1  
 EXPNO 2  
 PROCNO 1

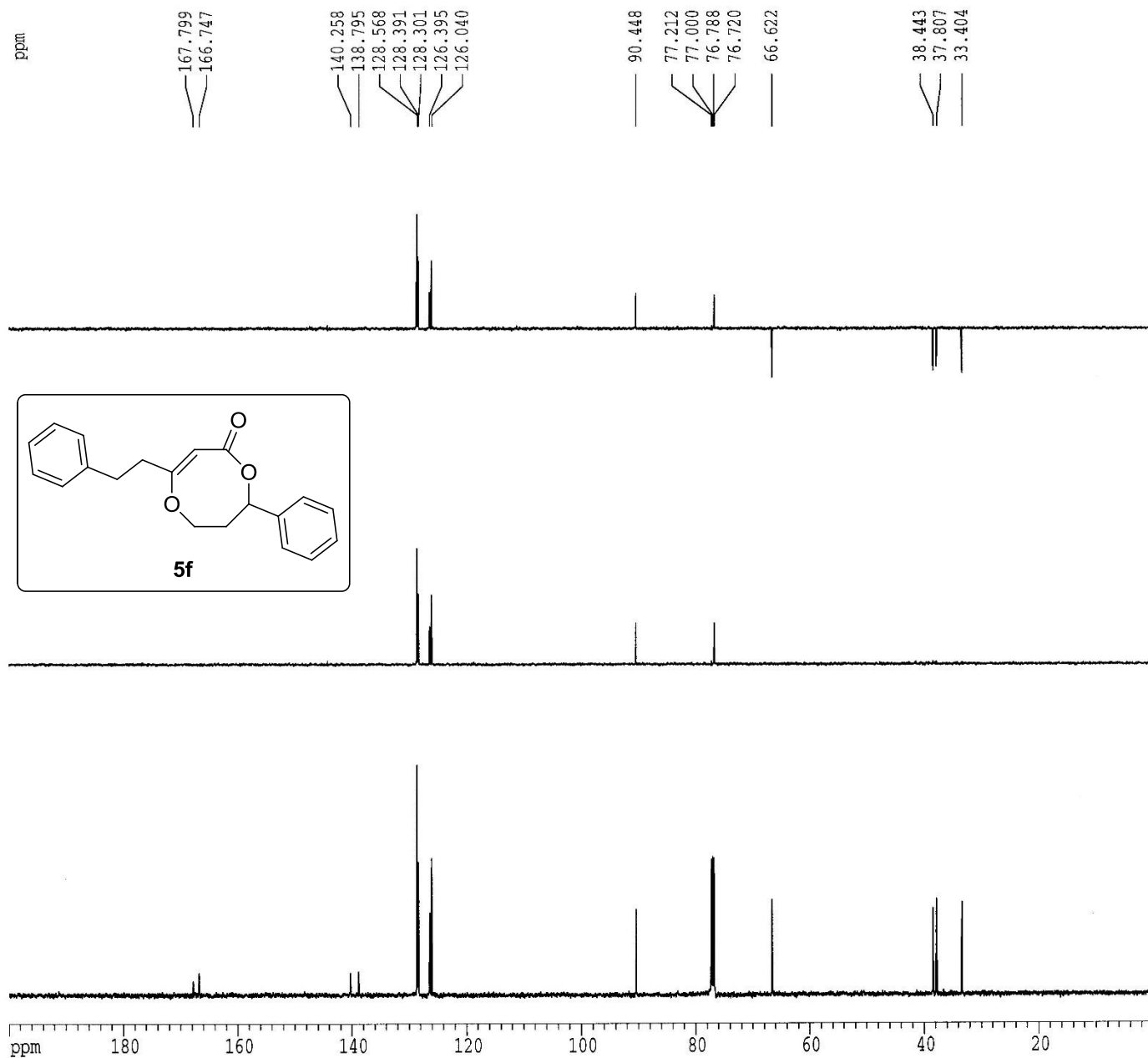
F2 - Acquisition Parameters  
 Date\_ 20150612  
 Time 11.30  
 INSTRUM spect  
 PROCPRD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 255  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 EQ 2048  
 EM 11.100 usec  
 DE 6.50 usec  
 TE 301.7 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCHPR 0.01500000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180933 MHz  
 MD 0  
 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  
 FWHM 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current Data Parameters
NAME      RS-2-27-1
EXPNO    1
PROCNO   1

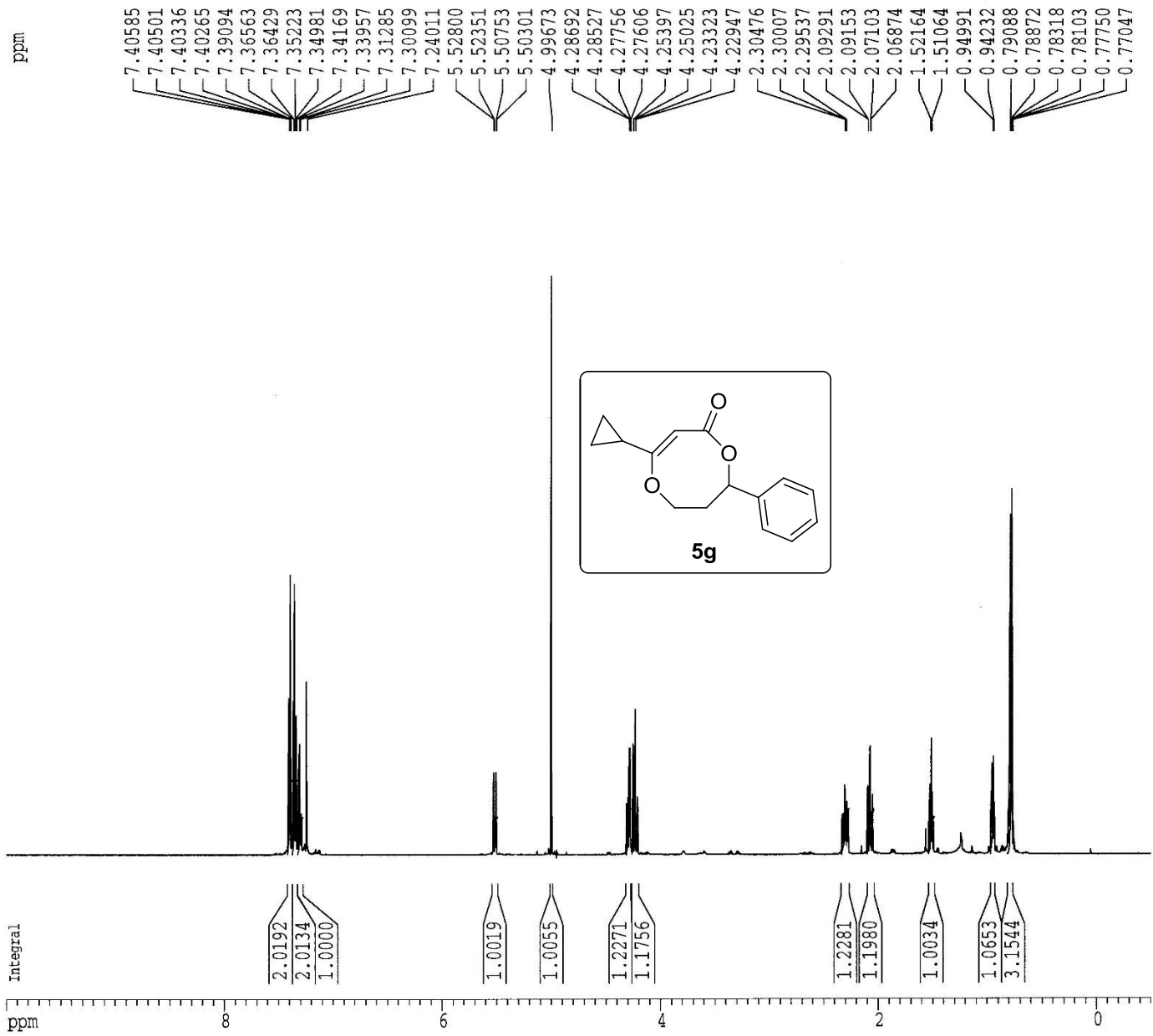
F2 - Acquisition Parameters
Date_    20150423
Time     16.54
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        0
SWH       8389.362 Hz
FIDRES   0.256020 Hz
AQ        1.9530228 sec
RG        512
DW        59.600 usec
DE        6.50 usec
TE        298.1 K
D1        2.00000000 sec
NUC1      13C
NUC2      13C
MURST    0.00000000 sec
MURKX    0.01500000 sec

===== CHANNEL f1 =====
NUC1      13C
P1        10.00 usec
PL1       0.00 dB
SFO1     598.5029930 MHz

F2 - Processing parameters
SI        32768
SP        598.600304 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
CY        10.00 cm
FIP       10.000 ppm
F1        5986.00 Hz
F2        -0.500 ppm
F3        -299.30 Hz
PPMCK    0.52500 ppm/cm
HZCM     314.26501 Hz/cm

```



Current Data Parameters  
 NAME RS-2-27-1  
 EXPNO 2  
 PROCNO 1

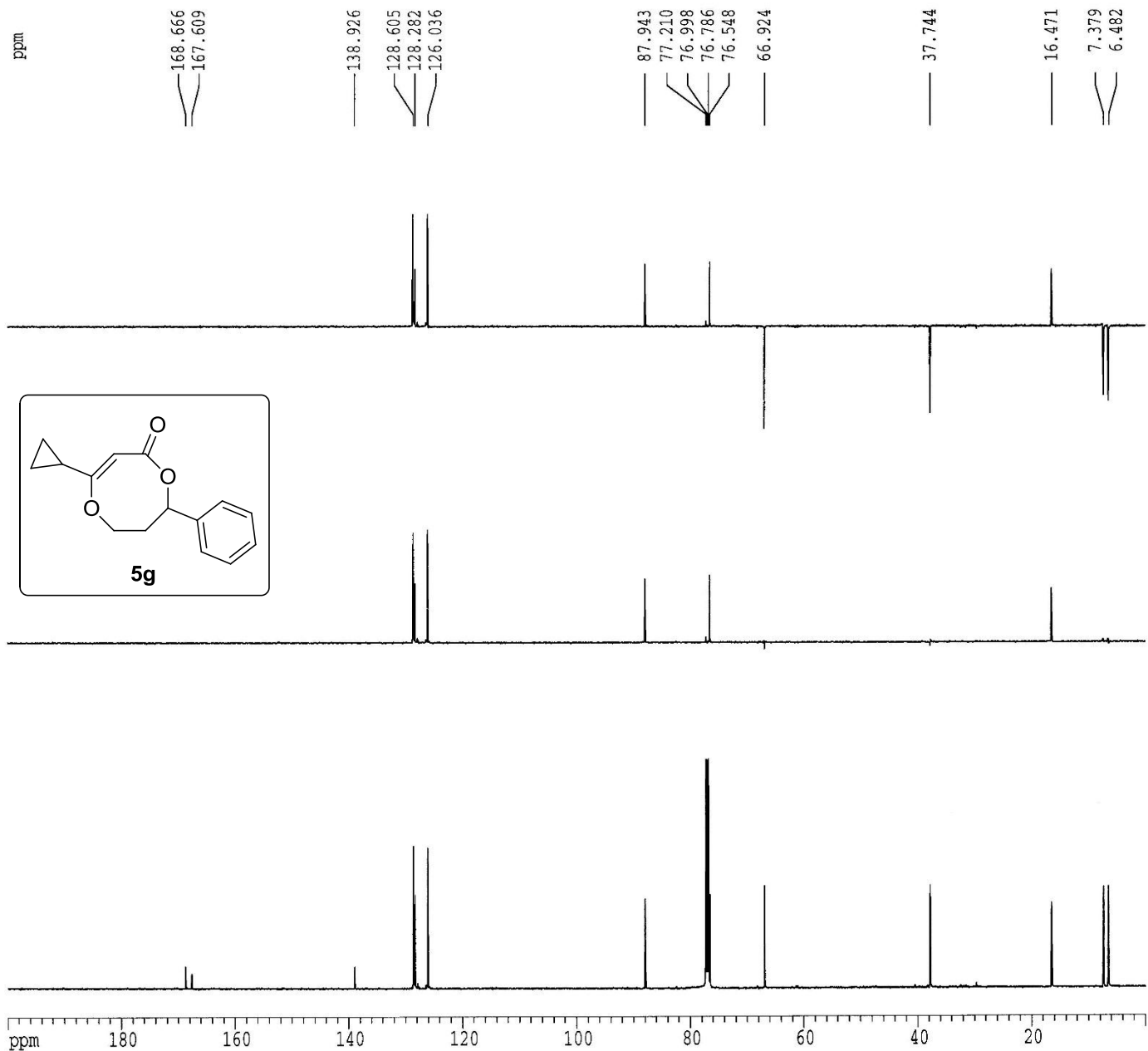
F2 - Acquisition Parameters  
 Date\_ 20150422  
 Time 16.56  
 INSTRUM spect  
 PRGBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 6144  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 MCREST 0.0000000 sec  
 MCNRK 0.0150000 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  
 SFC2 598.6029930 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.5180945 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

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



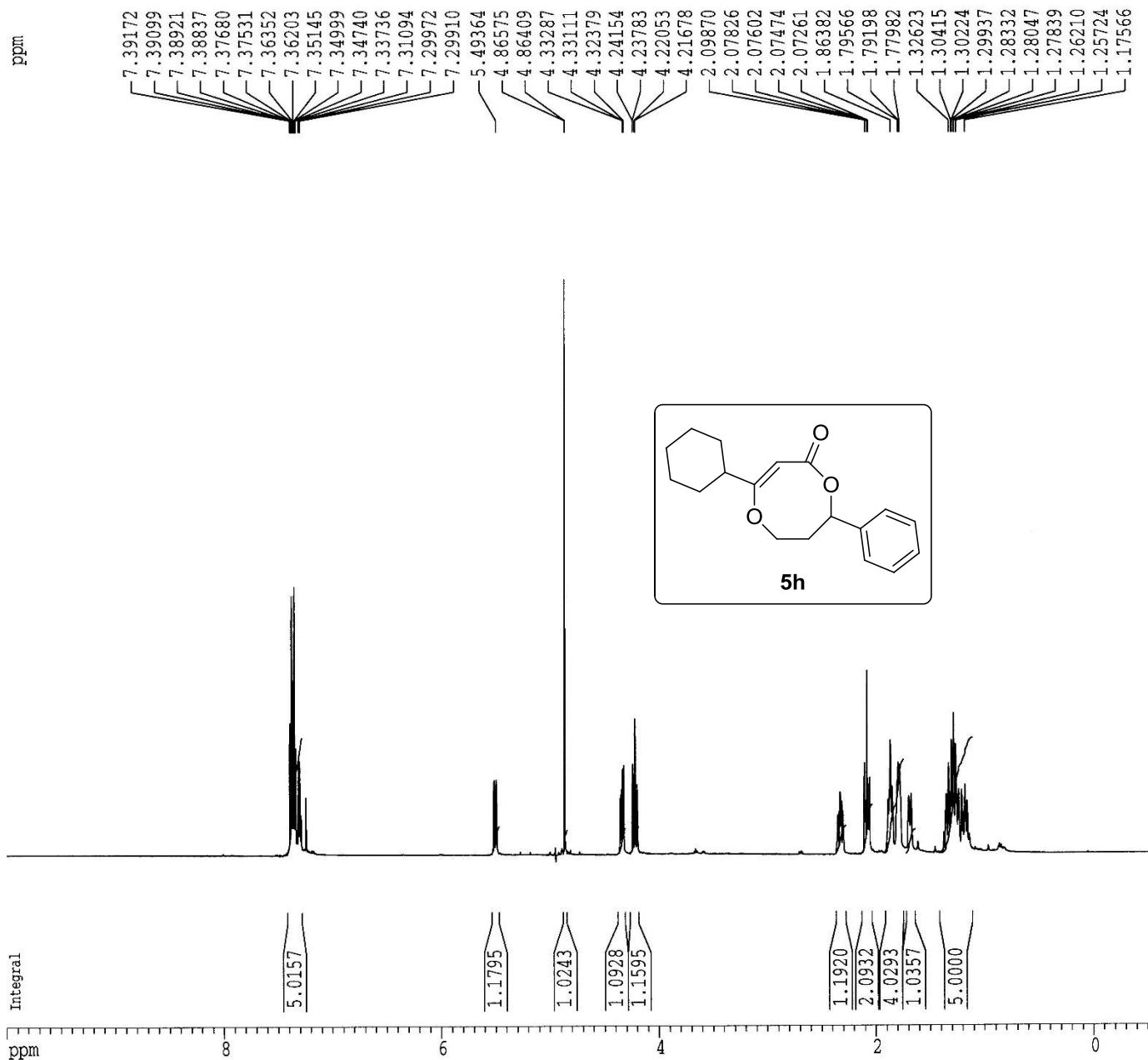
Current Data Parameters  
 NAME RS-2-32-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150424  
 Time 10.35  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8389.262 Hz  
 FIDRES 0.256020 Hz  
 AQ 1.9530228 sec  
 RG 128  
 BW 59.600 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 2.00000000 sec  
 MCREST 0.00000000 sec  
 MCWFK 0.01500000 sec

===== CHANNEL f1 =====  
 NUCL1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SFO1 500.6029930 MHz

F2 - Processing parameters  
 SI 32768  
 SF 500.6000306 MHz  
 WDW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 10.00 cm  
 F1P 10.000 ppm  
 F2 5986.00 Hz  
 F2P 0.500 ppm  
 F2 -299.30 Hz  
 FPKCM 0.52500 ppm/cm  
 HSCM 314.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-32-1  
 EXPNO 2  
 PROCNO 1

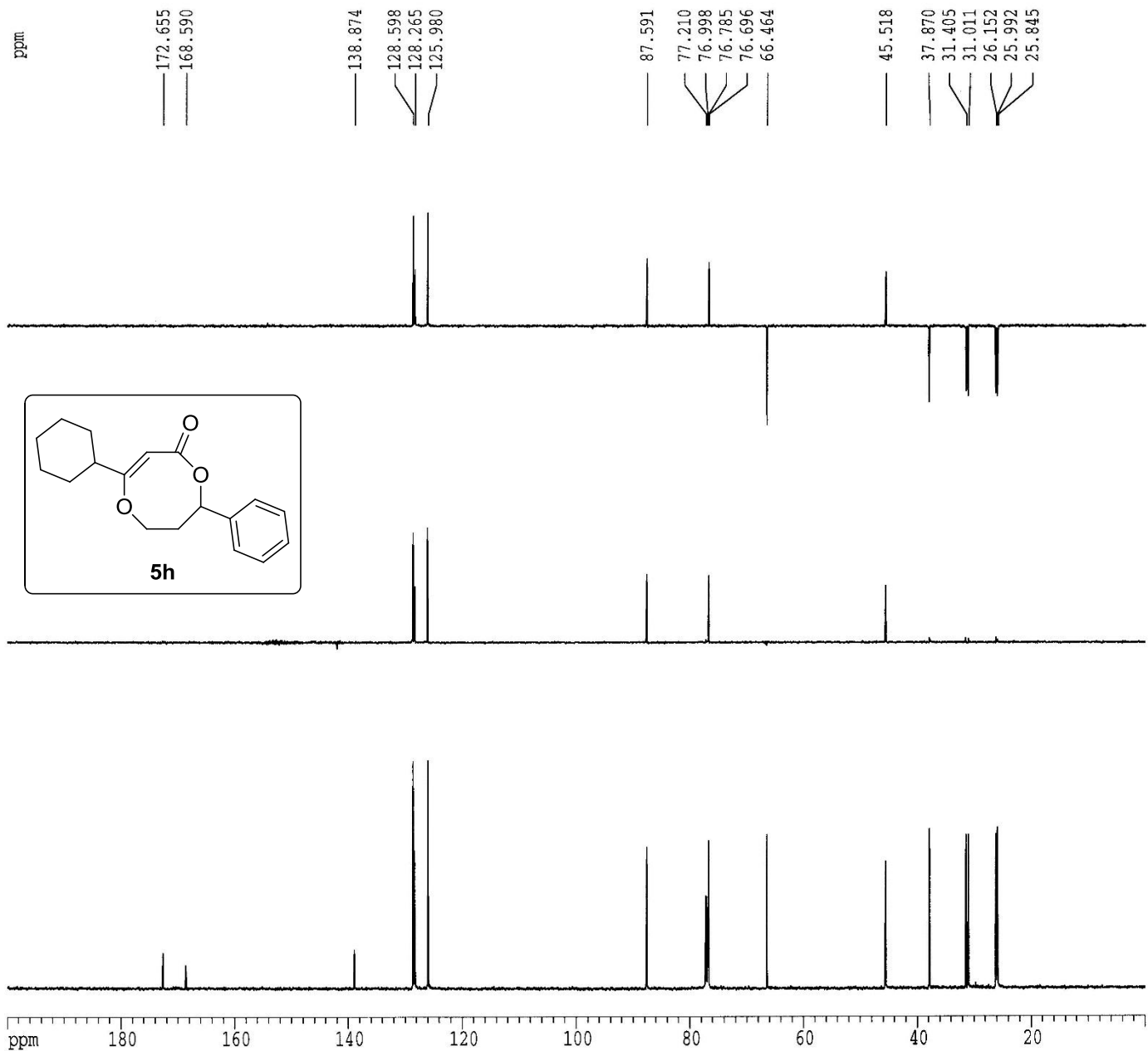
F2 - Acquisition Parameters  
 Date\_ 20150424  
 Time 10.37  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 558  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 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  
 SFG2 598.6029930 MHz

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

1D NMR plot parameters  
 CX 20.00 cm  
 CY 4.00 cm  
 F1P 200.000 ppm  
 F1 30103.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCM 10.30000 ppm/cm  
 HZCM 1505.18091 Hz/cm



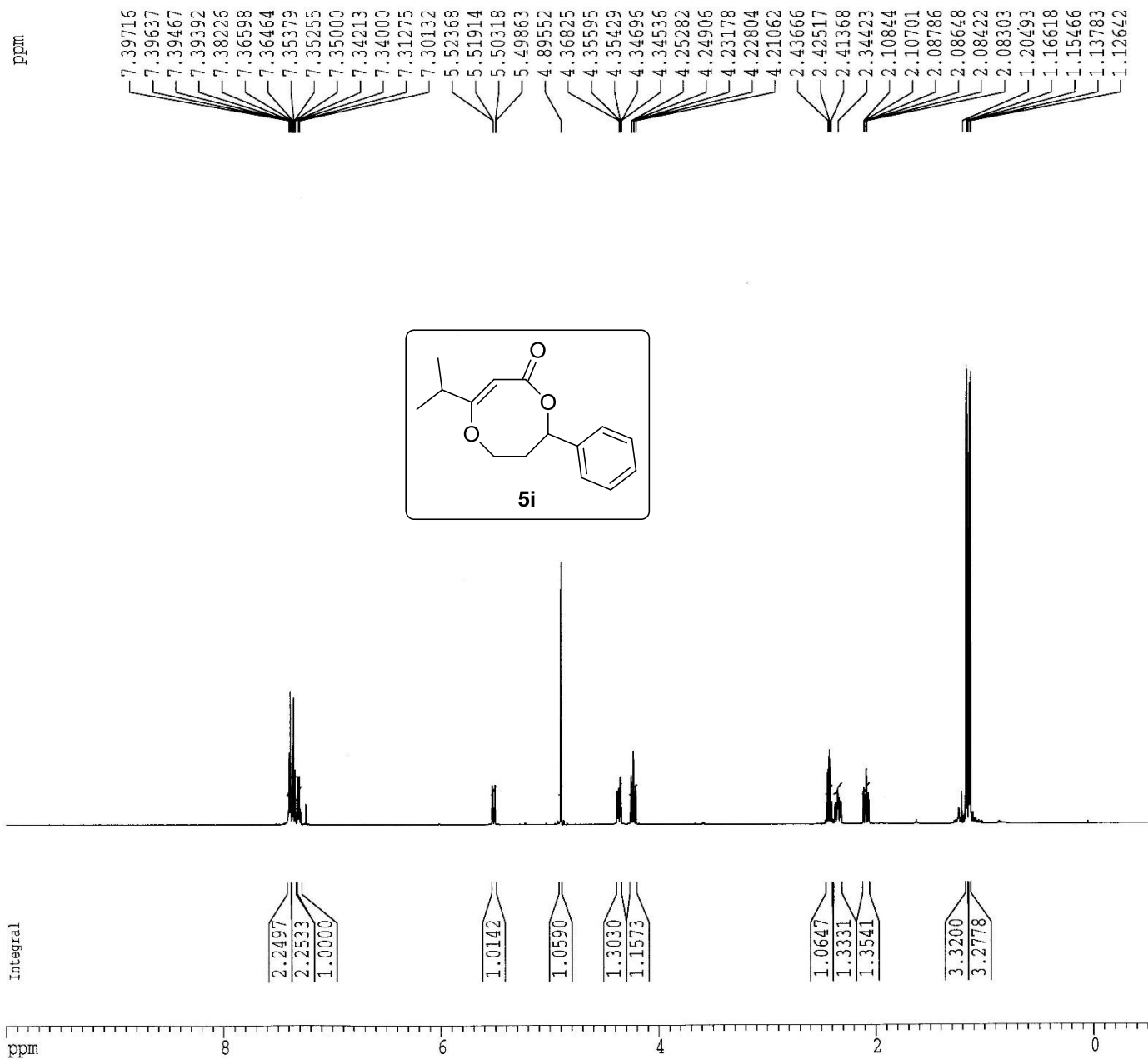
Current Data Parameters  
 NAME RS-2-40-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150507  
 Time 10.14  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG .zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 8382.229 Hz  
 FIDRES 0.255805 Hz  
 AQ 1.9546613 sec  
 RG 128  
 DW 59.650 usec  
 DE 85.21 usec  
 TE 297.2 K  
 D1 2.0000000 sec  
 MCREST 0.0000000 sec  
 MCWRK 0.0150000 sec

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

F2 - Processing parameters  
 SI 32768  
 SF 598.600303 MHz  
 WDM no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 8.00 cm  
 F1P 10.000 ppm  
 F1 5986.00 Hz  
 F2P -0.500 ppm  
 F2 -299.30 Hz  
 PPKCM 0.52500 ppm/cm  
 HZCM 314.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-40-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20150507  
 Time 10.16  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT DMSO  
 NS 102  
 DS 0  
 SSBH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DW 11.100 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 3.50000000 sec  
 c11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCGRK 0.01500000 sec

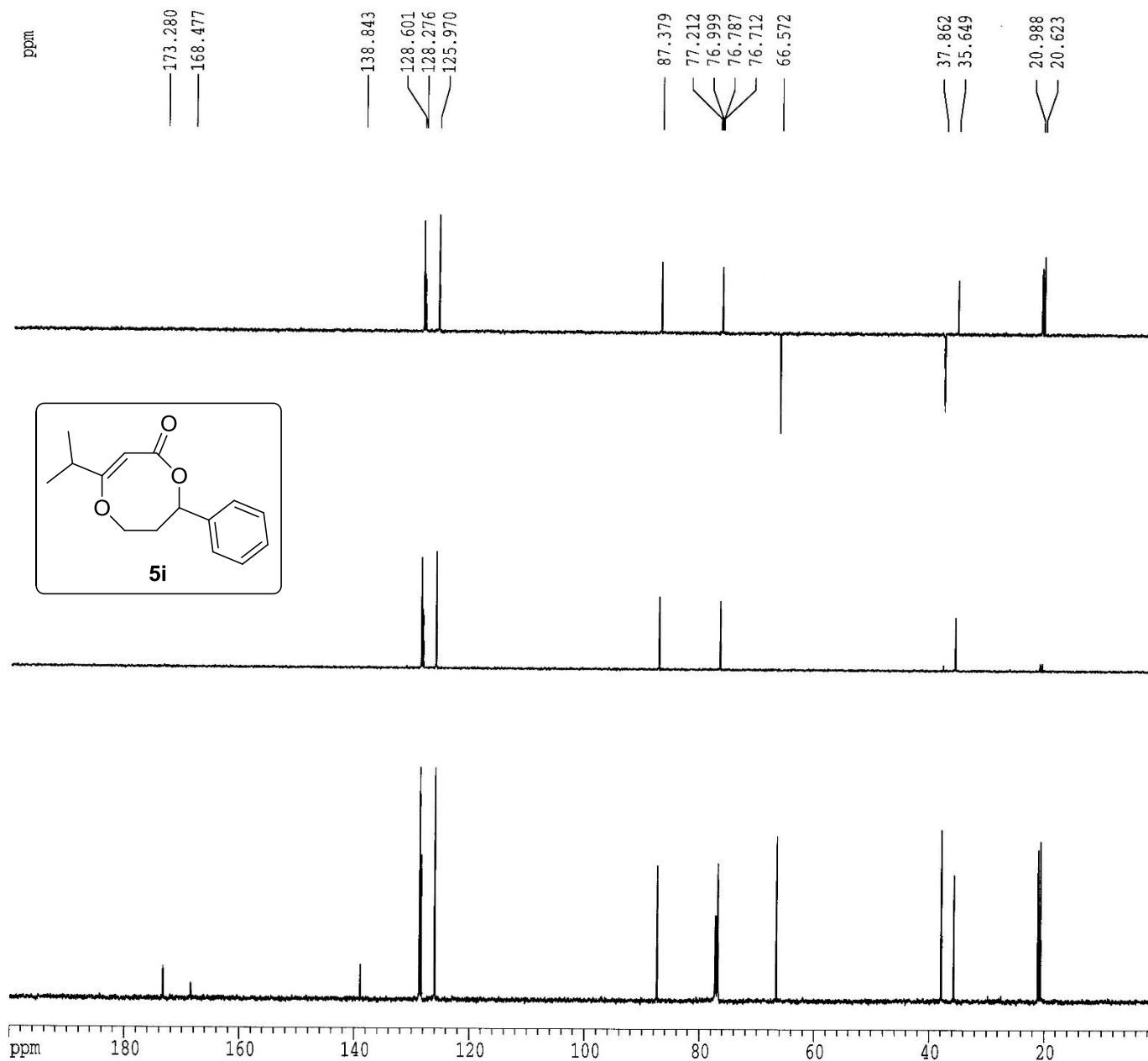
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 4.80 usec  
 PL1 0.00 dB  
 SFO1 150.5346470 MHz

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

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

1D NMR plot parameters

CX 20.00 cm  
 CY 4.00 cm  
 F1P 200.000 ppm  
 F1 30103.62 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPMCK 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

Current: Data Parameters
NAME      RS-2-59-1
EXPNO    1
PROCNO    1

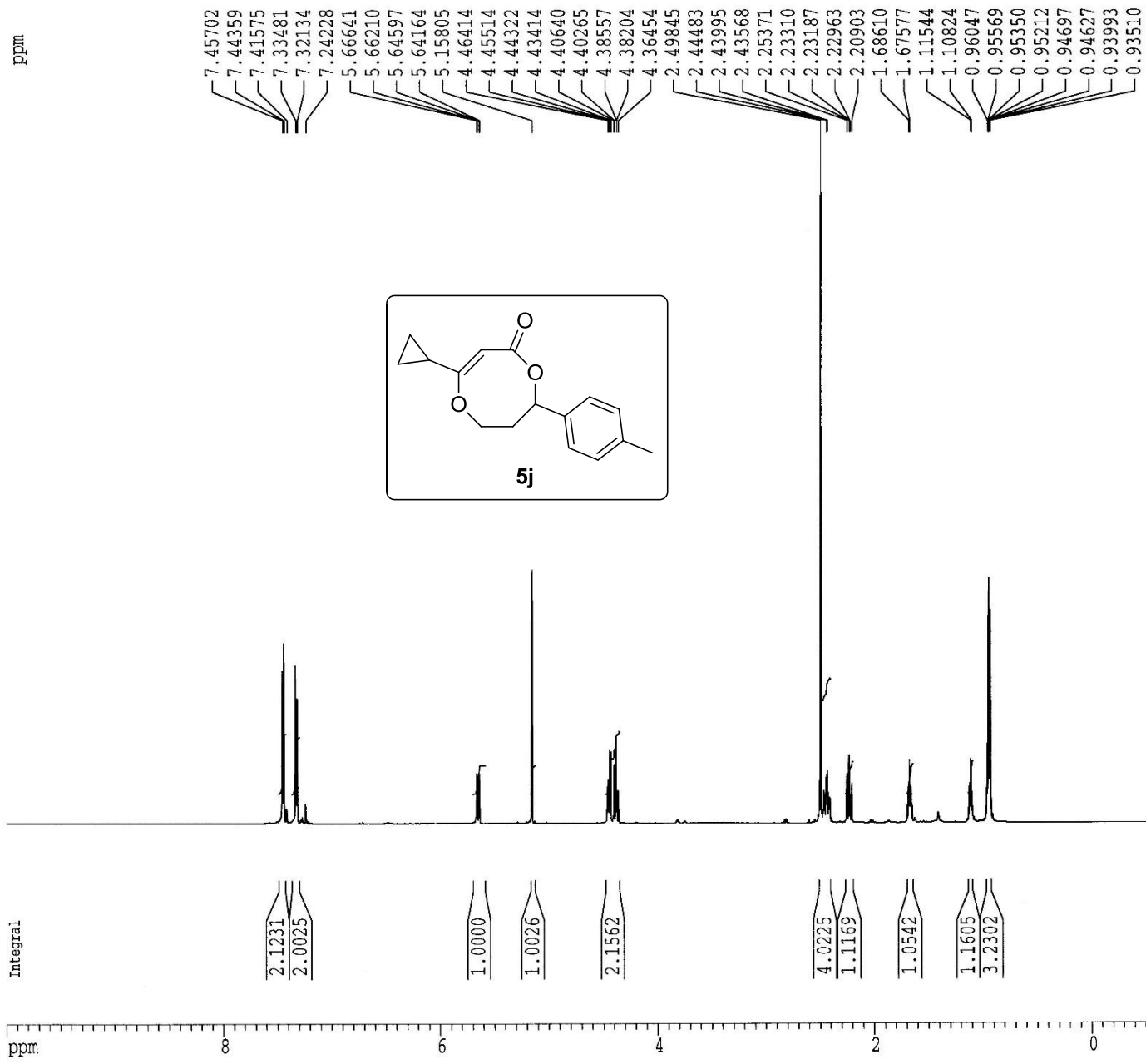
F2 - Acquisition Parameters
Date_     20150526
Time      14.18
INSTRUM   spect
PROBHD    5 mm QNP 1H/1
PULPROG   zg
TD         32768
SOLVENT   CDCl3
NS         16
DS         0
SWH        9541.984 Hz
FIDRES     0.291198 Hz
AQ         1.7170932 sec
RG         256
SW         51.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.50000000 sec
MCKRES2    0.00000000 sec
MUMSK      0.01500000 sec

***** CHANNEL f1 *****
NUC1       1H
P1         10.00 usec
PL1        0.00 dB
SFO1       500.6035916 MHz

F2 - Processing parameters
SI         32768
SF         500.6035916 MHz
WDW        no
SSB        0
LB         0.00 Hz
GB         0
PC         1.00

1D NMR plot parameters
CX         20.00 cm
CY         12.00 cm
F1P        10.000 ppm
F2P        5986.00 Hz
F3P        -0.500 ppm
F2         -299.30 Hz
PPHMM      0.52500 ppm/cm
HDCM       324.26495 Hz/cm

```





Current Data Parameters  
 NAME RS-2-59-1  
 EXPNO 2  
 PROCNO 1

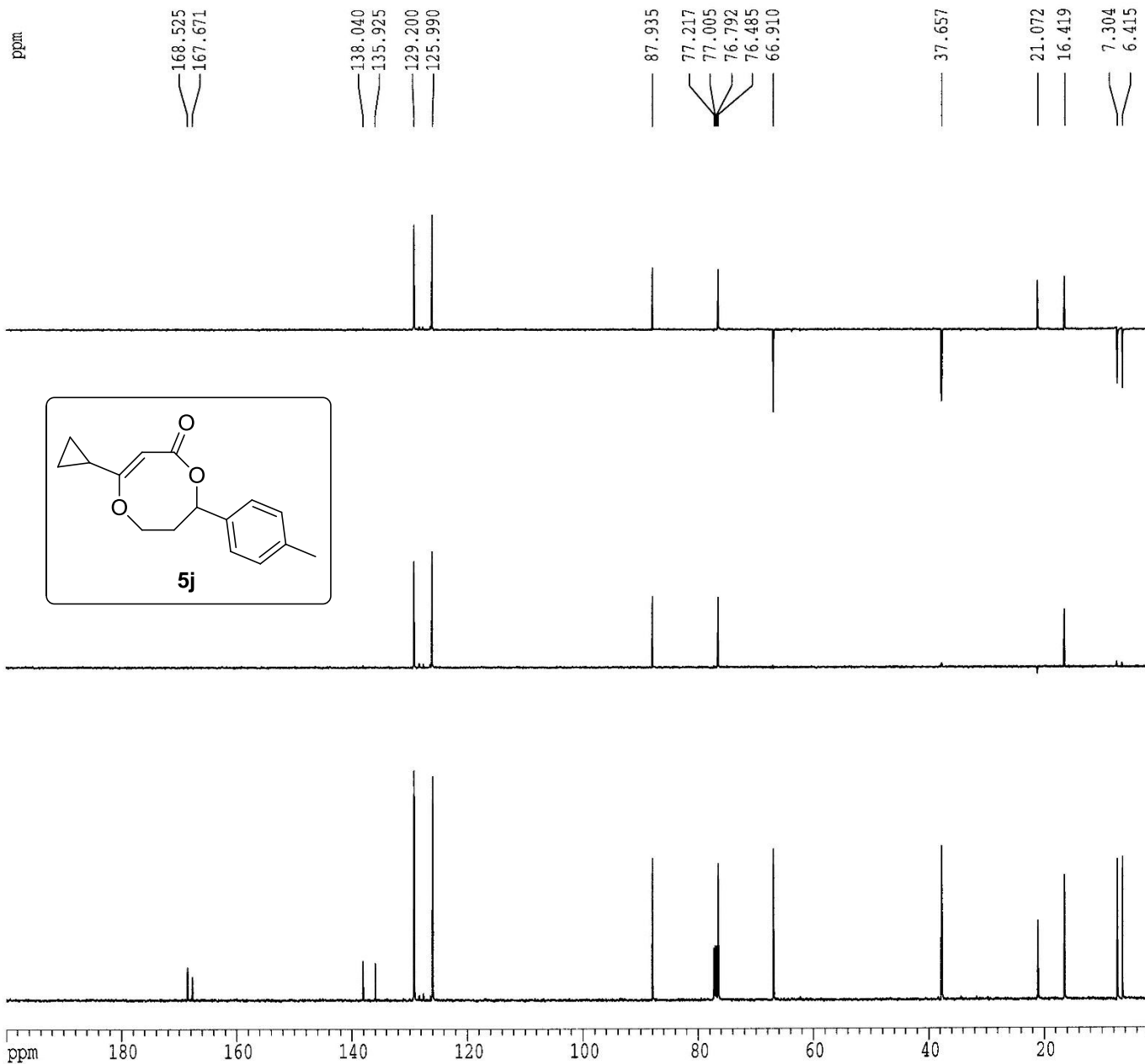
F2 - Acquisition Parameters  
 Date\_ 20150526  
 Time 14.30  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 200  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 EN 11.100 usec  
 DE 6.50 usec  
 TE 299.7 K  
 D1 3.5000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCGRK 0.01500000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5181001 MHz  
 MDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

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



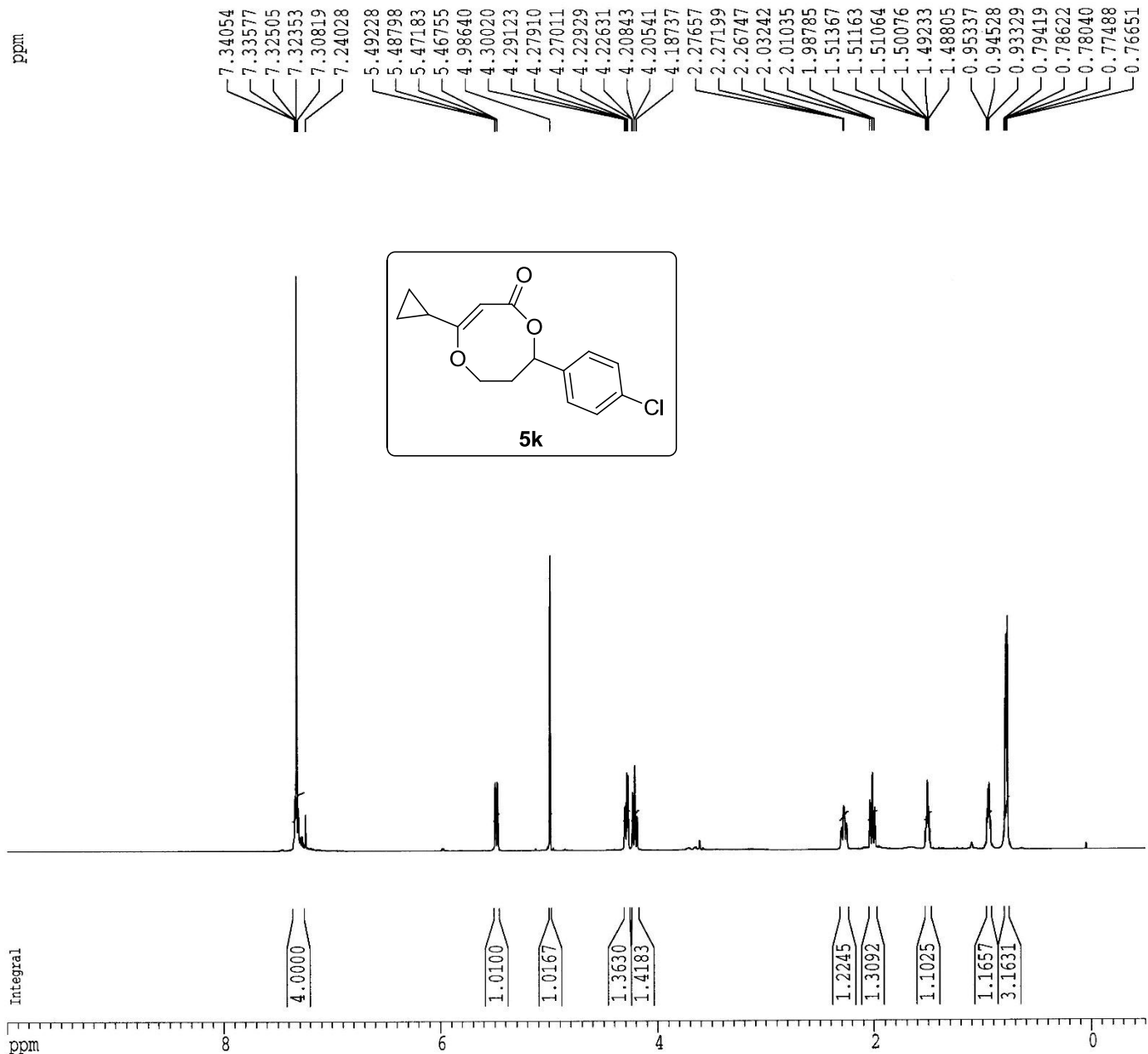
Current Data Parameters  
 NAME RS-2-51-1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20150515  
 Time 11.38  
 INSTRUM spect  
 PROCPRD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 33556  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SWH 9541.984 Hz  
 FIDRES 0.284360 Hz  
 AQ 1.7583843 sec  
 RG 512  
 TH 52.400 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 2.0000000 sec  
 MCREST 0.0000000 sec  
 MCKSK 0.0150000 sec

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SFG1 598.6035916 MHz

F2 - Processing parameters  
 SI 32768  
 SF 598.600303 MHz  
 WDM no  
 SSE 0  
 LB 0.00 Hz  
 GB 0  
 PC 0.10

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



Current Data Parameters  
 NAME RS-2-51-1  
 EXPNO 2  
 PROCNO 1

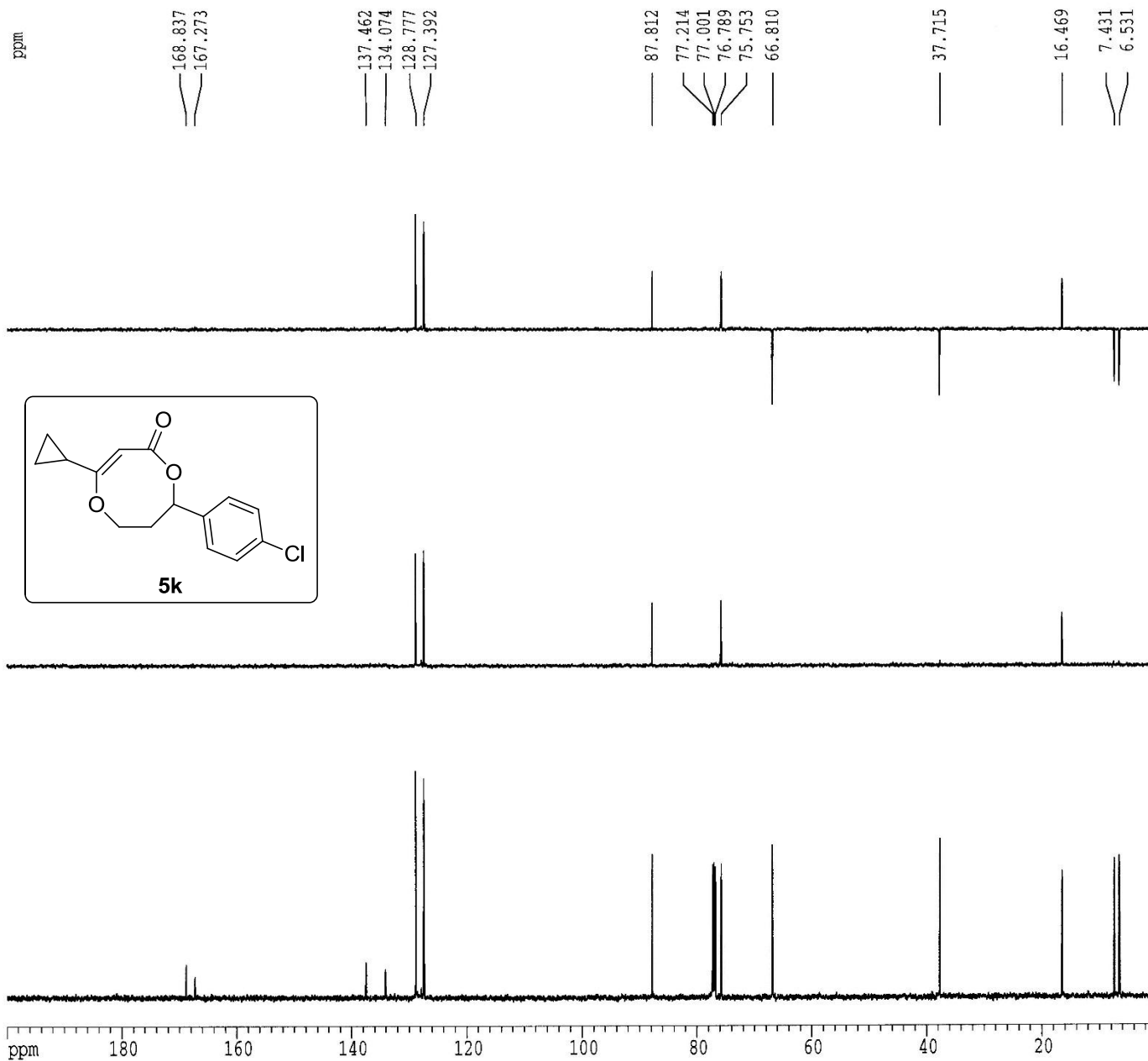
F2 - Acquisition Parameters  
 Date\_ 20150515  
 Time 11.43  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT CDCl3  
 NS 104  
 DS 0  
 SWE 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 299.8 K  
 D1 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MCREST 0.00000000 sec  
 MCREK 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  
 FCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.6029930 MHz

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

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



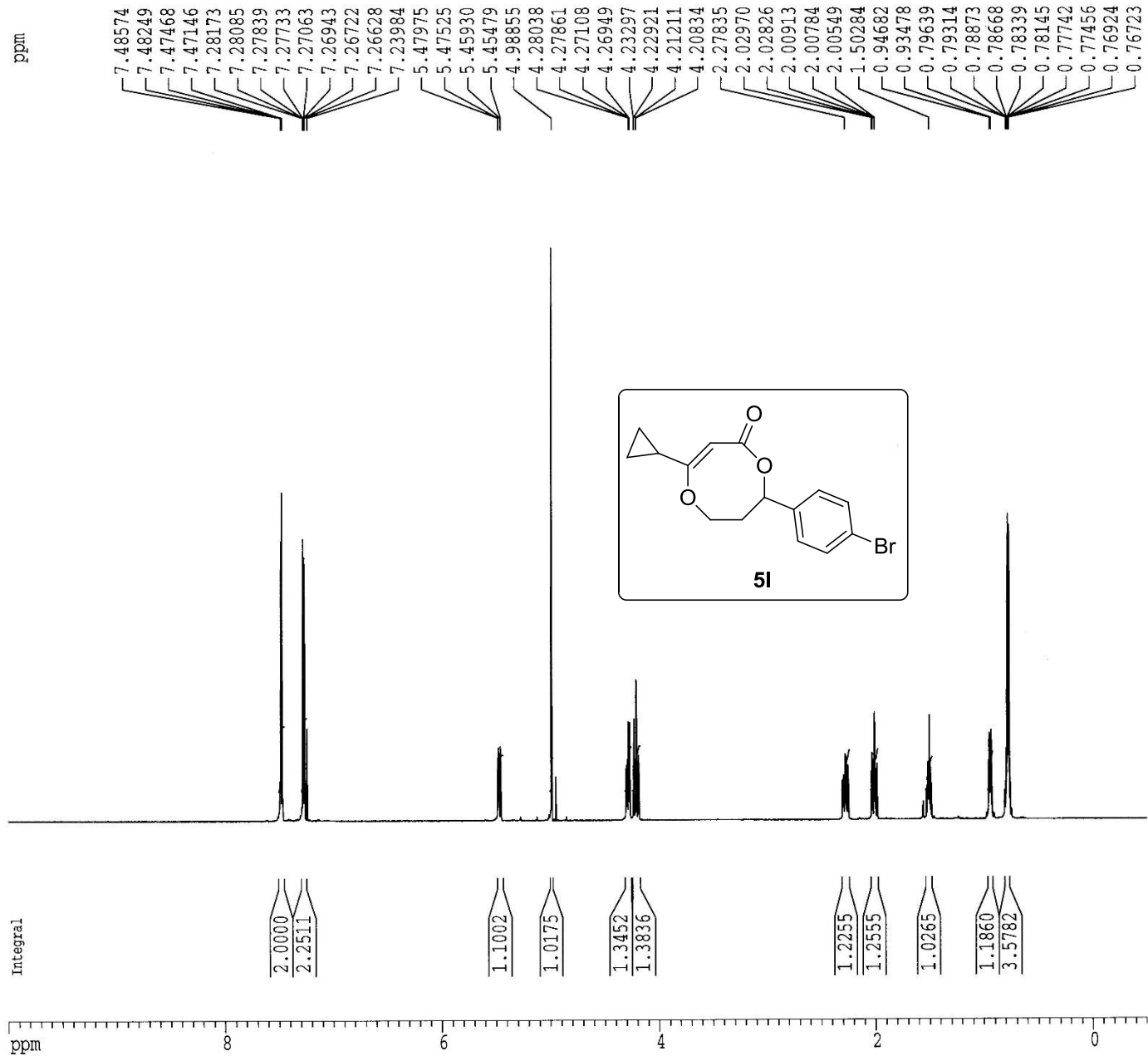
Current Data Parameters  
 NAME RS-2-77-1  
 EXPNO 1  
 PROCNO 1

F1 - Acquisition Parameters  
 Date\_ 20150616  
 Time 7.55  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zg  
 TD 32768  
 SOLVENT CDCl3  
 NS 16  
 DS 0  
 SSB 8389.262 Hz  
 FIDRES 0.256020 Hz  
 AQ 1.9530228 sec  
 RG 512  
 DW 59.600 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 1.50000000 sec  
 MERESE 0.03000000 sec  
 MZGWA 0.01500000 sec

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 10.00 usec  
 PL1 0.00 dB  
 SFO1 500.6029930 MHz

F1 - Processing parameters  
 SI 32768  
 SF 500.600304 MHz  
 GCW no  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters  
 CX 20.00 cm  
 CY 10.00 cm  
 FLP 10.000 ppm  
 F1 5986.00 Hz  
 FCP -0.500 ppm  
 FQ -299.30 Hz  
 FPMW 0.62500 ppm/cm  
 HZCM 314.26501 Hz/cm



Current Data Parameters  
 NAME RS-2-77-1  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20150616  
 Time 7.56  
 INSTRUM spect  
 PROBRG 5 mm QNP 1H/1  
 PULPROG zgpgg  
 TD 32768  
 SOLVENT CDCl3  
 NS 409  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.1637748 sec  
 RG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 300.4 K  
 D1 3.5000000 sec  
 d11 0.0300000 sec  
 DELTA 3.4000010 sec  
 ACQRES 0.0000000 sec  
 NS2 0.0150000 sec

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

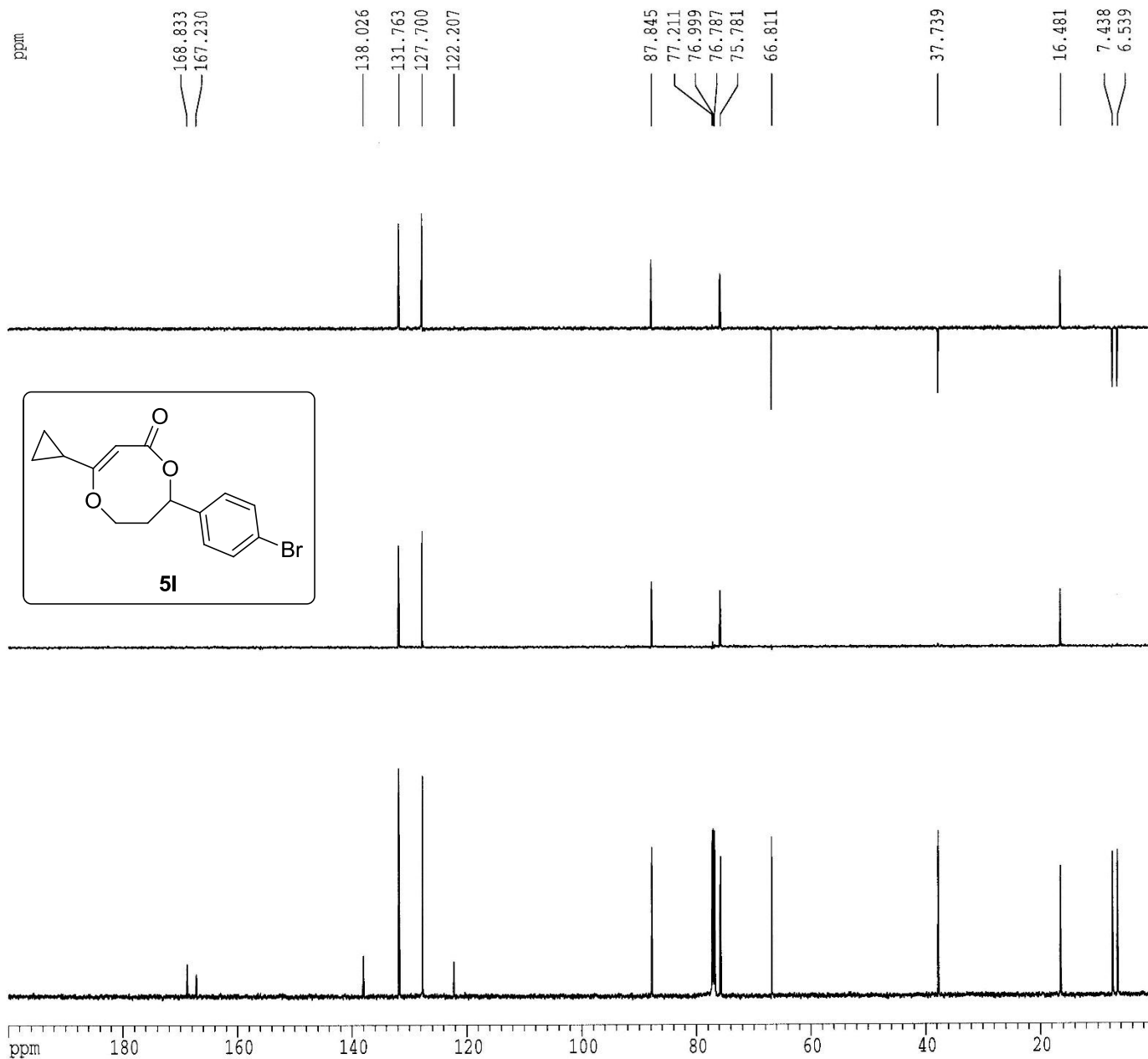
===== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 P2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.6029930 MHz

F2 - Processing parameters

SI 65536  
 SF 150.5180926 MHz  
 WDW EM  
 SSB 0  
 LB 3.00 Hz  
 GB 0  
 PC 1.00

1D NMR plot parameters

CA 20.00 cm  
 CY 4.00 cm  
 F1F 200.000 ppm  
 F1 30103.62 Hz  
 F2 0.000 ppm  
 F2 0.00 Hz  
 FWHM 10.00000 ppm/cm  
 HZCM 1505.18091 Hz/cm



```

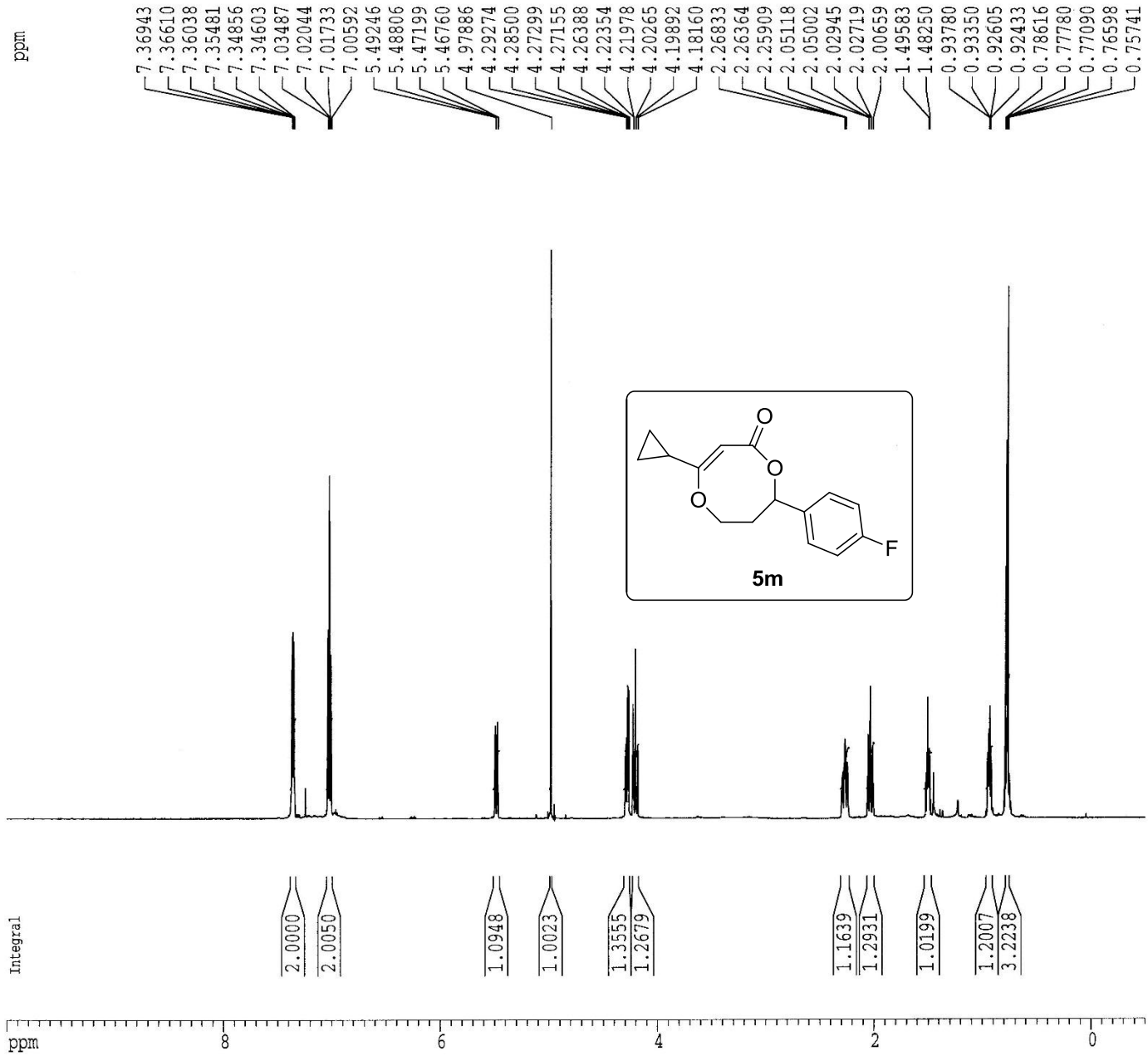
Current Data Parameters
NAME      RS-2-75-1
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20150616
Time     19.32
INSTRUM  spect
PROBHD   5 mm QNP 1H/1
PULPROG  zg
TD        32768
SOLVENT  CDCl3
NS        16
DS        4
SWH       8399.262 Hz
FIDRES    0.256020 Hz
AQ        1.9510228 sec
RG        128
DA        59.600 usec
DE        6.50 usec
TE        300.8 K
D1        1.5000000 sec
d11       0.0000000 sec
d12       0.0000000 sec
d13       0.0150000 sec
***** CHANNEL f1 *****
NUC1      1H
P1        10.00 usec
PC1       0.00 dB
SFO1      500.13629930 MHz

F2 - Processing parameters
SI        32768
SF        500.13629930 MHz
WDW       no
SSB       0
LB        0.00 Hz
GB        0
PC        1.00

1D NMR plot parameters
CX        20.00 cm
CY        10.00 cm
PIP       10.000 ppm
F1        506.000 Hz
F2P       -0.500 ppm
F2        -199.10 Hz
PPMCH    0.62500 ppm/cm
HZCM     314.26501 Hz/cm

```



Current Data Parameters  
 NAME RS-2-75-1  
 EXPNO 2  
 PROCNO 1

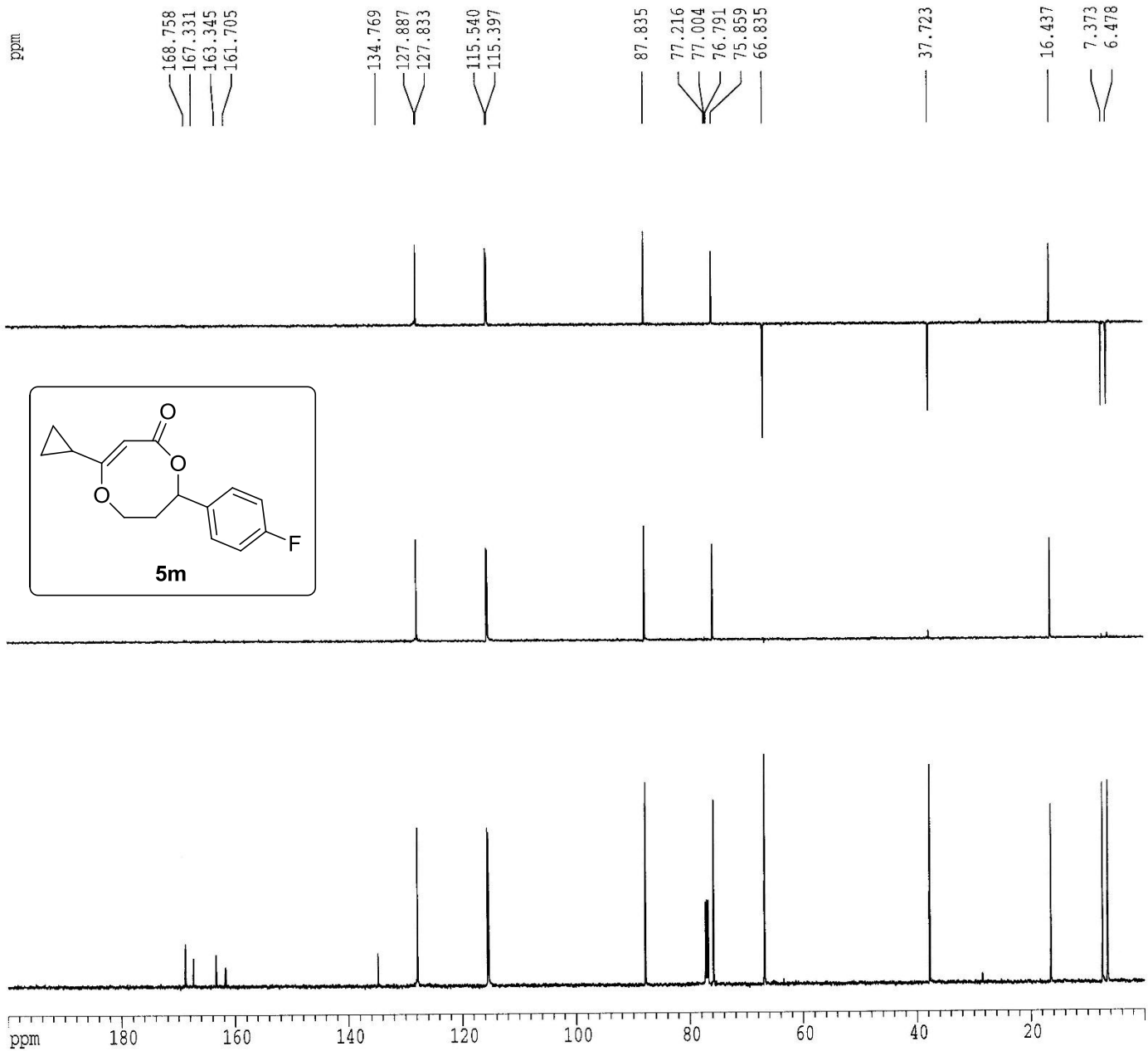
F2 - Acquisition Parameters  
 Date\_ 20150616  
 Time 9.54  
 INSTRUM spect  
 PROBRD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 157  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 2048  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 301.2 K  
 DL 3.50000000 sec  
 d11 0.03000000 sec  
 DELTA 3.40000010 sec  
 MORGST 0.00000000 sec  
 MORGX 0.01500000 sec

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

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

F2 - Processing parameters  
 SI 65536  
 SF 150.5180974 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 203.000 ppm  
 F1 30133.62 Hz  
 F2F 0.000 ppm  
 F2 0.00 Hz  
 PPKCM 10.00000 ppm/cm  
 HSCM 1505.18091 Hz/cm



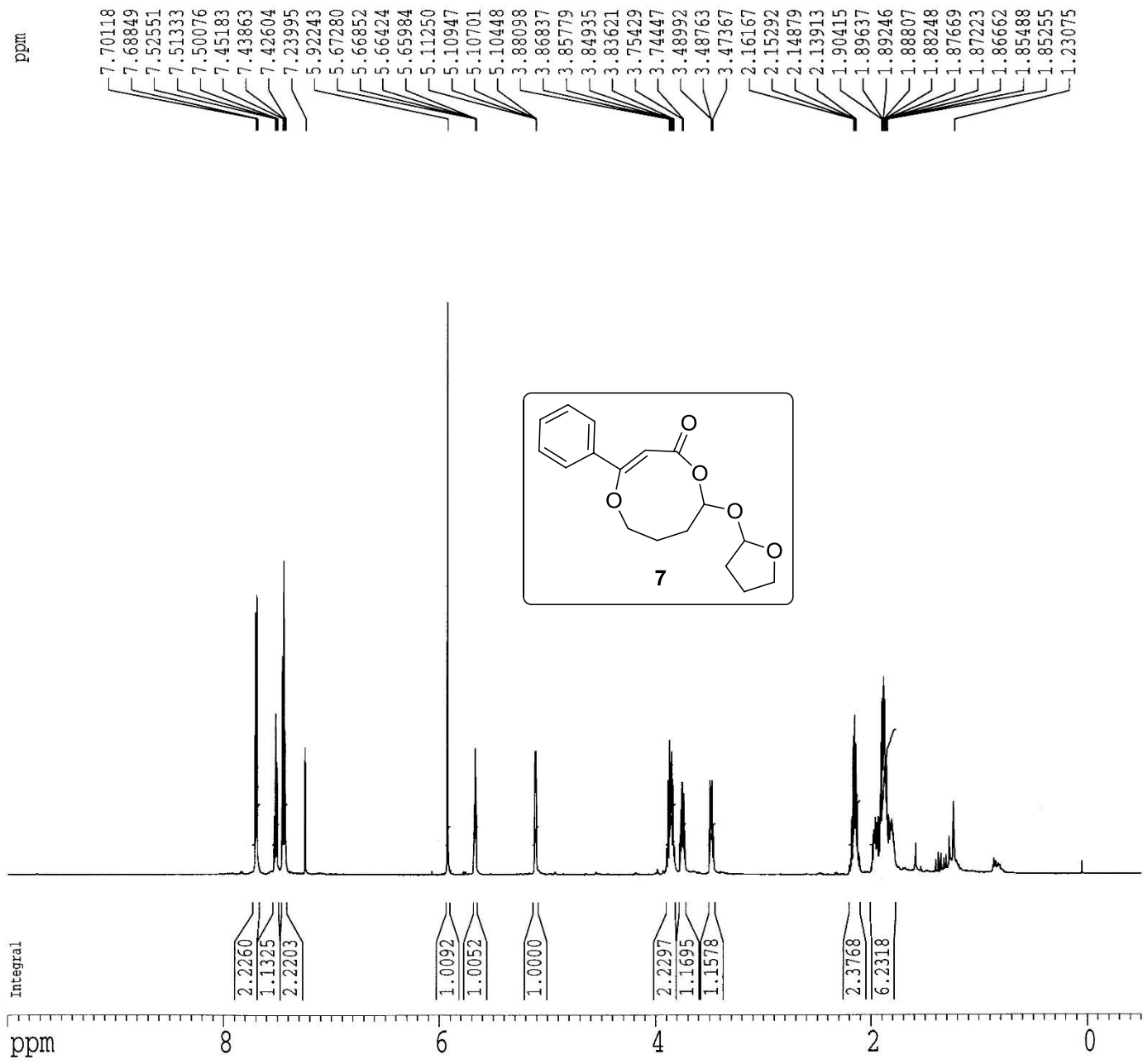
Current Data Parameters  
NAME RS-3-117-4  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20151102  
Time 12.27  
INSTRUM spect  
PROBHD 5 mm QNP 1H/1  
PULPROG zg  
TD 32768  
SOLVENT cdc13  
NS 16  
DS 0  
SWH 9541.984 Hz  
FIDRES 0.291198 Hz  
AQ 1.7170932 sec  
RG 512  
DW 51.400 usec  
DE 6.50 usec  
TE 297.8 K  
D1 2.00000000 sec  
MCREST 0.00000000 sec  
MCWRK 0.01500000 sec

===== CHANNEL f1 =====  
NUC1 1H  
FL1 12.30 usec  
PL1 3.00 dB  
SFO1 598.5028148 MHz

F2 - Processing parameters  
SI 32768  
SF 598.5000383 MHz  
WDW no  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.00

1D NMR plot parameters  
CX 20.00 cm  
CY 10.00 cm  
F1P 10.000 ppm  
F1 5985.00 Hz  
F2P -0.500 ppm  
F2 -299.25 Hz  
PPMCM 0.52500 ppm/cm  
HZCM 314.21249 Hz/cm





Current Data Parameters  
 NAME RS-2-117-4  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20151102  
 Time 12.43  
 INSTRUM spect  
 PROBHD 5 mm QNP 1H/1  
 PULPROG zgpg  
 TD 32768  
 SOLVENT CDCl3  
 NS 262  
 DS 0  
 SWH 45045.047 Hz  
 FIDRES 1.374666 Hz  
 AQ 0.3637748 sec  
 RG 4096  
 DM 11.100 usec  
 DE 6.50 usec  
 TE 299.0 K  
 DL 3.50000000 sec  
 GI1 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 150.5094992 MHz

==== CHANNEL f2 =====  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 92.00 usec  
 PL2 120.00 dB  
 PL12 9.00 dB  
 PL13 14.00 dB  
 SFO2 598.5029925 MHz

F2 - Processing parameters  
 SI 65536  
 SF 150.4929487 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 30098.59 Hz  
 F2P 0.000 ppm  
 F2 0.00 Hz  
 PPRCM 10.00000 ppm/cm  
 HZCH 1504.92944 Hz/cm

