

## Supporting Information

# Ring-opening reactions of donor-acceptor cyclopropanes with cyclic ketals and thiol ketals

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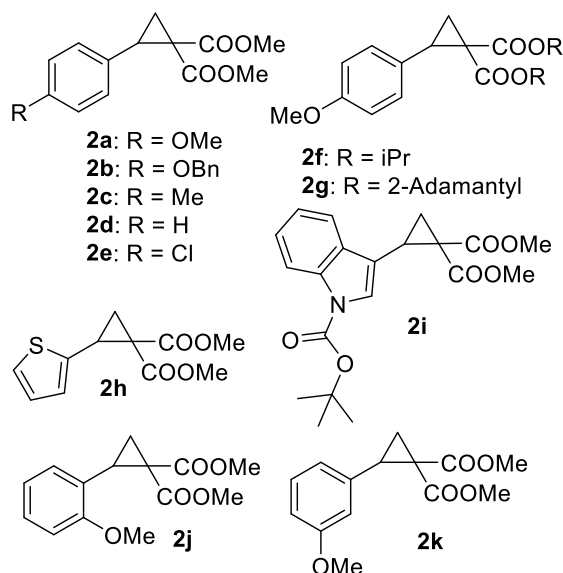
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## 1. General

$^1\text{H}$  NMR and  $^{13}\text{C}$  NMR were recorded on a Bruker-400 MHz spectrometer. Proton chemical shifts are reported in ppm downfield from tetramethylsilane or from the residual solvent as internal standard in  $\text{CDCl}_3$  ( $\delta$  7.26 ppm) and in  $(\text{CD}_3)_2\text{SO}$  (2.50 ppm). Carbon chemical shifts were internally referenced to the deuterated solvent signals in  $\text{CDCl}_3$  ( $\delta$  77.0 ppm) and in  $(\text{CD}_3)_2\text{SO}$  (39.5 ppm). High-resolution mass spectra were recorded on a Thermo Scientific LTQ Orbitrap ESI ion trap mass spectrometer. Reagents obtained from commercial sources are used without further purification and all solvents were purified and dried according to standard methods prior to use, unless stated otherwise.

## 2. D-A cyclopropanes **2** used in this study

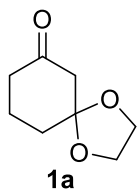


Donor-acceptor (D-A) cyclopropanes **2** used in this study were all prepared according to literature procedures from the corresponding aromatic aldehydes through a sequence of Knoevenagel condensation followed by a Corey-Chaykovsky cyclopropanation.<sup>[1],[2]</sup> **2a**,<sup>[3]</sup> **2b**,<sup>[4]</sup> **2c-2e**,<sup>[3]</sup> **2f**,<sup>[5]</sup> **2g**,<sup>[2]</sup> **2h**,<sup>[6]</sup> **2i**<sup>[1]</sup>, **2j**<sup>[4]</sup> are all known compounds and the characterization data all corresponded to the reported values.

## 3. Procedures for the preparation of 1,3-cyclohexanedione derived cyclic ketals **1**

To a mixture of 1,3-cyclohexanedione (1.12 g, 10.0 mmol) and glycol (11.0 mmol) in toluene (150 mL), TsOH (34.4 mg, 0.2 mmol) was added. The reaction mixture was heated to reflux for 24 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 ) to provide cyclic ketals **1**.

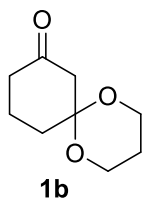
### 1,4-Dioxaspiro[4.5]decan-7-one (**1a**)



Flash chromatography (petroleum ether : ethyl acetate = 4:1); 687.2 mg (44%).

Colorless oil.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.79-1.88 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.29 (t,  $J$  = 5.6 Hz, 2H,  $\text{CH}_2$ ), 2.55 (s, 2H,  $\text{CH}_2$ ), 3.88-3.96 (m, 4H,  $\text{OCH}_2 \times 2$ ) ppm;  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 20.0, 34.1, 40.1, 51.6, 64.6, 109.9, 207.5 ppm. HRMS (ESI): calcd. for  $\text{C}_8\text{H}_{13}\text{O}_3$  ( $[\text{M} + \text{H}]^+$ ) 157.0859, found 157.0857.

#### 1,5-Dioxaspiro[5.5]undecan-8-one (1b)



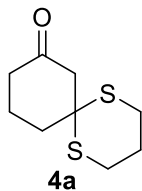
Flash chromatography (petroleum ether : ethyl acetate = 4:1); 663.8 mg (39%).

White solid. mp 97-99 °C.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.65-1.74 (m, 2H,  $\text{CH}_2$ ), 1.76-1.83 (m, 2H,  $\text{CH}_2$ ), 2.05 (t,  $J$  = 5.9 Hz, 2H,  $\text{CH}_2$ ), 2.30 (t,  $J$  = 6.7 Hz, 2H,  $\text{CH}_2$ ), 2.74 (s, 2H,  $\text{CH}_2$ ), 3.82-3.92 (m, 4H,  $\text{OCH}_2 \times 2$ ) ppm;  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 19.3, 25.0, 32.2, 40.0, 49.0, 59.6, 99.7, 207.7 ppm. HRMS (ESI): calcd. for  $\text{C}_9\text{H}_{15}\text{O}_3$  ( $[\text{M} + \text{H}]^+$ ) 171.1016, found 171.1020.

#### 4. Procedures for the preparation of 1,3-cyclohexanedione derived cyclic thiol ketals **4**

To a mixture of 1,3-cyclohexanedione (1.12 g, 10.0 mmol) and dithiols (11.0 mmol) in  $\text{CH}_2\text{Cl}_2$  (100 mL), boron trifluoride diethyl ether complex (141.9 mg, 1.0 mmol) was added at room temperature. The reaction mixture was stirred at the same temperature for 24 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petroleum ether : ethyl acetate = 4:1) to provide cyclic thiol ketals **4**.

#### 1,5-Dithiaspiro[5.5]undecan-8-one (4a)

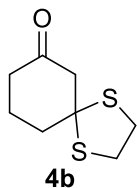


Flash chromatography (petroleum ether : ethyl acetate = 4:1); 1.66 g (82%).

White solid. mp 115-117 °C.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.87-2.09 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.21-2.24 (m, 2H,  $\text{CH}_2$ ), 2.33 (t,  $J$  = 6.6 Hz, 2H,  $\text{CH}_2$ ), 2.76-2.82 (m, 2H,  $\text{SCH}_2$ ), 2.85-2.92 (m,

2H, SCH<sub>2</sub>), 2.90 (s, 2H, CH<sub>2</sub>) ppm; HRMS (ESI): calcd. for C<sub>8</sub>H<sub>13</sub>OS<sub>2</sub> ([M + H]<sup>+</sup>) 203.0559, found 203.0555.

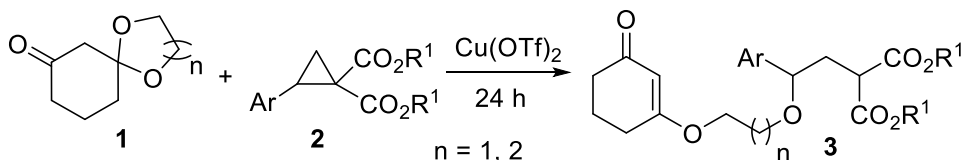
### 1,4-Dithiaspiro[4.5]decan-7-one (4b)



Flash chromatography (petroleum ether : ethyl acetate = 4:1); 1.30 g (69%).

White solid. mp 85-87 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.93-2.00 (m, 2H, CH<sub>2</sub>), 2.24-2.30 (m, 4H, CH<sub>2</sub>×2), 2.87 (s, 2H, CH<sub>2</sub>), 3.27-3.33 (m, 4H, SCH<sub>2</sub>×2) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 24.9, 39.3, 39.9, 40.6, 57.6, 68.1, 206.8 ppm. HRMS (ESI): calcd. for C<sub>8</sub>H<sub>13</sub>OS<sub>2</sub> ([M + H]<sup>+</sup>) 189.0402, found 189.0405.

### 5. Procedures for the reactions of 1 and 2 to afford 3.



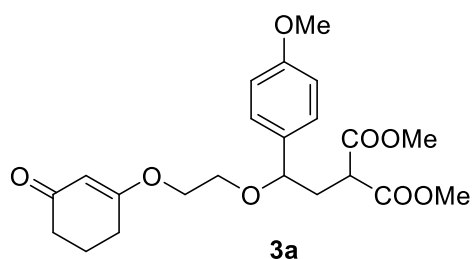
**General procedures for the reactions of 1 and 2 to afford 3 (A).** To a mixture of **1** (0.18 mmol) and D-A cyclopropanes **2** (0.15 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (1.0 mL), Cu(OTf)<sub>2</sub> (5.4 mg, 0.015 mmol) was added. The mixture was stirred at room temperature (25 °C) for 24 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **3**.

**General procedures for the reactions of 1 and 2 to afford 3 (B).** To a mixture of **1** (0.18 mmol), D-A cyclopropanes **2** (0.15 mmol), 4 Å MS (100 mg), and Cu(OTf)<sub>2</sub> (5.4 mg, 0.015 mmol), 1,2-dichloroethane (1.0 mL) was added under N<sub>2</sub> atmosphere. The mixture was stirred 45 °C for 24 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **3**.

**General procedures for the reactions of 1 and 2 to afford 3 (C).** To a mixture of **1** (0.18 mmol), D-A cyclopropanes **2** (0.15 mmol), 4 Å MS (100 mg), and Cu(OTf)<sub>2</sub> (5.4 mg, 0.015 mmol), CH<sub>2</sub>Cl<sub>2</sub> (1.0 mL) was added under N<sub>2</sub> atmosphere. The mixture was stirred at room temperature (25 °C) for 24 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **3**.

**Procedure for a 5 mmol-scale reaction to synthesize 3a.** To a mixture of 1,3-cyclohexanedione derived cyclic ketal **1a** (937.1 mg, 6.0 mmol) and D-A cyclopropanes **2a** (1.32 g, 5.0 mmol) in CH<sub>2</sub>Cl<sub>2</sub> (20.0 mL), Cu(OTf)<sub>2</sub> (180.0 mg, 0.5 mmol) was added. The mixture was stirred at room temperature (25 °C) for 24 h. Then, the mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (20.0 mL), and washed with saturated NaHCO<sub>3</sub>. The aqueous phase was extracted with CH<sub>2</sub>Cl<sub>2</sub> (20 mL x 3). The organic layers were combined, washed with brine, dried over Na<sub>2</sub>SO<sub>4</sub>, and concentrated. The residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **3a** (1.93 g, 92%).

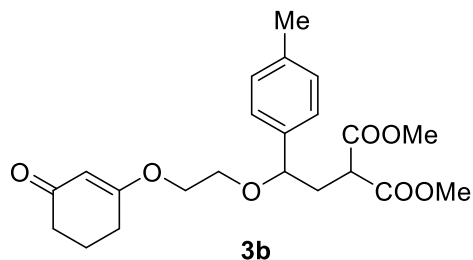
**Dimethyl 2-(2-(4-methoxyphenyl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3a)**



Synthesized by the general procedure **A**; 58.6 mg (93%).

Colorless gum. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.93-2.00 (m, 2H, CH<sub>2</sub>), 2.18-2.36 (m, 4H, CH<sub>2</sub>×2), 2.59 (t, *J* = 6.7 Hz, 2H, CH<sub>2</sub>), 3.46-3.51 (m, 1H, OCH<sub>2</sub>×1/2), 3.53-3.58 (m, 1H, OCH<sub>2</sub>×1/2), 3.61 (dd, *J* = 6.3 Hz, 8.1 Hz, 1H, CH), 3.70 (s, 3H, CH<sub>3</sub>), 3.72 (s, 3H, CH<sub>3</sub>), 3.79 (s, 3H, CH<sub>3</sub>), 3.87 (t, *J* = 4.56 Hz, 2H, OCH<sub>2</sub>), 4.28 (dd, *J* = 4.3 Hz, 9.2 Hz, 1H, OCH), 5.28 (s, 1H, CH), 6.87 (d, *J* = 8.7 Hz, 2H, ArH), 7.2 (d, *J* = 8.6 Hz, 2H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.1, 28.9, 36.6, 37.1, 48.6, 52.5, 55.2, 66.1, 67.5, 79.6, 102.7, 113.9, 127.7, 132.6, 159.4, 169.6, 169.7, 177.9, 199.8 ppm. HRMS (ESI): calcd. for C<sub>22</sub>H<sub>29</sub>O<sub>8</sub> ([M + H]<sup>+</sup>) 421.1857, found 421.1854.

**Dimethyl 2-(2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)-2-(p-tolyl)ethyl)malonate (3b)**



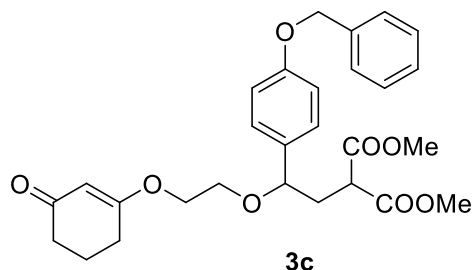
Synthesized by the general procedure **A**; 54.0 mg (89%).

Colorless gum. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.97 (quintet, *J* = 6.5 Hz, 2H, CH<sub>2</sub>), 2.22-2.35 (m, 6H, CH<sub>2</sub>×3), 2.33 (s, 3H, CH<sub>3</sub>), 2.42 (t, *J* = 6.3 Hz, 2H, CH<sub>2</sub>), 3.48-3.52 (m, 1H, CH<sub>2</sub>×1/2), 3.55-3.59 (m, 1H, CH<sub>2</sub>×1/2), 3.63 (dd, *J* = 6.2 Hz, 8.3 Hz, 1H, CH), 3.70 (s, 3H, CH<sub>3</sub>), 3.72 (s,

3H, CH<sub>3</sub>), 3.87 (t, *J* = 4.5 Hz, 2H, CH<sub>2</sub>), 4.30 (dd, *J* = 4.3 Hz, 9.3 Hz, 1H, CH), 5.28 (s, 1H, CH), 7.13-7.19 (m, 4H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.06, 21.11, 28.8, 36.7, 37.1, 48.6, 52.46, 52.48, 66.2, 67.5, 79.9, 102.7, 126.4, 129.2, 137.6, 137.7, 169.6, 169.7, 177.8, 199.6 ppm. HRMS (ESI): calcd. for C<sub>22</sub>H<sub>29</sub>O<sub>7</sub> ([M + H]<sup>+</sup>) 405.1908, found 405.1913.

### Dimethyl

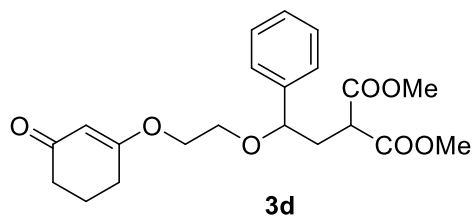
#### 2-(2-(4-(benzyloxy)phenyl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3c)



Synthesized by the general procedure A; 67.1 mg (90%).

White Solid. mp 114-116 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.97 (quintet, *J* = 6.4 Hz, 2H, CH<sub>2</sub>), 2.19-2.26 (m, 1H, CH<sub>2</sub>×1/2), 2.29-2.37 (m, 3H, CH<sub>2</sub> + CH<sub>2</sub>×1/2), 2.42 (t, *J* = 6.2 Hz, 2H, CH<sub>2</sub>), 3.47-3.52 (m, 1H, CH<sub>2</sub>×1/2), 3.55-3.60 (m, 1H, CH<sub>2</sub>×1/2), 3.63 (dd, *J* = 6.2 Hz, 8.3 Hz, 1H, CH), 2.96 (s, 3H, CH<sub>3</sub>), 3.73 (s, 3H, CH<sub>3</sub>), 3.88 (t, *J* = 4.6 Hz, 2H, CH<sub>2</sub>), 4.29 (dd, *J* = 4.3 Hz, 9.2 Hz, 1H, CH), 5.05 (s, 2H, OCH<sub>2</sub>), 5.29 (s, 1H, CH), 6.94-6.97 (m, 2H, ArH), 7.20-7.24 (m, 2H, ArH), 7.30-7.44 (m, 5H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.1, 28.9, 36.7, 37.1, 48.6, 52.5, 66.1, 67.5, 70.0, 79.6, 102.8, 114.8, 127.4, 127.7, 128.0, 128.5, 132.9, 136.8, 158.6, 169.6, 169.7, 177.7, 199.7 ppm. HRMS (ESI): calcd. for C<sub>28</sub>H<sub>33</sub>O<sub>8</sub> ([M + H]<sup>+</sup>) 497.2170, found 497.2166.

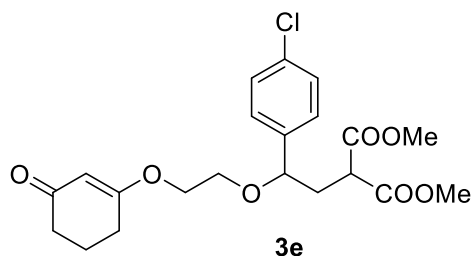
#### Dimethyl 2-(2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)-2-phenylethyl)malonate (3d)



Synthesized by the general procedure B; 45.1 mg (77%).

Colorless gum. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.9 (quintet, *J* = 6.4 Hz, 2H, CH<sub>2</sub>), 2.22-2.36 (m, 4H, CH<sub>2</sub>×2), 2.43 (t, *J* = 6.3 Hz, 2H, CH<sub>2</sub>), 3.49-3.55 (m, 1H, CH<sub>2</sub>×1/2), 3.58-3.63 (m, 1H, CH<sub>2</sub>×1/2), 3.66 (dd, *J* = 6.1 Hz, 8.4 Hz, 1H, CH), 3.71 (s, 3H, CH<sub>3</sub>), 3.74 (s, 3H, CH<sub>3</sub>), 3.89 (t, *J* = 4.5 Hz, 2H, CH<sub>2</sub>), 4.35 (dd, *J* = 4.4 Hz, 9.1 Hz, 1H, CH), 5.30 (s, 1H, CH), 7.26-7.37 (s, 5H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.1, 28.9, 36.7, 37.2, 48.6, 52.52, 52.54, 66.4, 67.5, 80.1, 102.8, 126.4, 128.1, 128.6, 140.8, 169.6, 169.7, 177.7, 199.7 ppm. HRMS (ESI): calcd. for C<sub>21</sub>H<sub>27</sub>O<sub>7</sub> ([M + H]<sup>+</sup>) 391.1751, found 391.1754.

**Dimethyl 2-(2-(4-chlorophenyl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3e)**

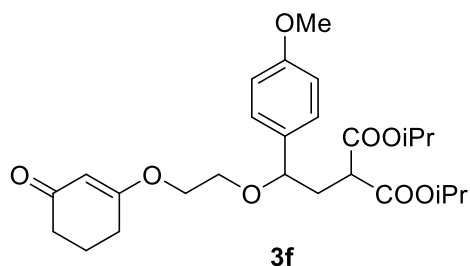


Synthesized by the general procedure **B**; 40.7 mg (64%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.98 (quintet,  $J$  = 6.5 Hz, 2H,  $\text{CH}_2$ ), 2.19-2.31 (m, 2H,  $\text{CH}_2$ ), 2.34 (t,  $J$  = 6.6 Hz, 2H,  $\text{CH}_2$ ), 2.43 (t,  $J$  = 6.3 Hz, 2H,  $\text{CH}_2$ ), 3.49-3.54 (m, 1H,  $\text{CH}_2 \times 1/2$ ), 3.56-3.61 (m, 1H,  $\text{CH}_2 \times 1/2$ ), 3.64 (dd,  $J$  = 6.1 Hz, 8.2 Hz, 1H, CH), 3.71 (s, 3H,  $\text{CH}_3$ ), 3.74 (s, 3H,  $\text{CH}_3$ ), 3.85-3.93 (m, 2H,  $\text{CH}_2$ ), 4.34 (dd,  $J$  = 4.6 Hz, 8.9 Hz, 1H, CH), 5.30 (s, 1H, CH), 7.24-7.27 (m, 2H, ArH), 7.31-7.35 (m, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.2, 28.9, 36.7, 37.1, 48.5, 52.6, 66.6, 67.4, 79.5, 102.8, 127.8, 128.8, 133.8, 139.4, 169.5, 169.6, 177.6, 199.6 ppm. HRMS (ESI): calcd. for  $\text{C}_{21}\text{H}_{26}\text{ClO}_7$  ( $[\text{M} + \text{H}]^+$ ) 425.1362, found 425.1364.

**Diisopropyl**

**2-(2-(4-methoxyphenyl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3f)**

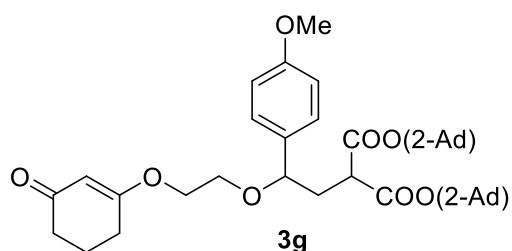


Synthesized by the general procedure **A**; 64.3 mg (90%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.17 (dd,  $J$  = 6.2 Hz, 9.4 Hz, 12H,  $\text{CH}_3 \times 4$ ), 1.90 (quintet,  $J$  = 6.4 Hz, 2H,  $\text{CH}_2$ ), 2.08-2.15 (m, 1H,  $\text{CH}_2 \times 1/2$ ), 2.20-2.27 (m, 3H,  $\text{CH}_2 + \text{CH}_2 \times 1/2$ ), 2.37 (t,  $J$  = 6.2 Hz, 2H,  $\text{CH}_2$ ), 3.42-3.55 (m, 3H,  $\text{CH}_2 + \text{CH}$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 3.82-3.85 (m, 2H,  $\text{CH}_2$ ), 4.23 (dd,  $J$  = 4.5 Hz, 9.2 Hz, 1H, CH), 4.97 (heptet,  $J$  = 6.2 Hz, 2H,  $\text{CH} \times 2$ ), 5.23 (s, 1H, CH), 6.81 (d,  $J$  = 8.7 Hz, 2H, ArH), 7.16 (d,  $J$  = 8.6 Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 20.9, 21.3, 21.35, 21.40, 21.5, 36.5, 36.8, 49.1, 55.0, 66.0, 67.4, 68.53, 68.54, 79.5, 102.5, 113.7, 127.5, 132.7, 159.2, 168.5, 168.6, 177.6, 199.4 ppm. HRMS (ESI): calcd. for  $\text{C}_{26}\text{H}_{37}\text{O}_8$  ( $[\text{M} + \text{H}]^+$ ) 477.2483, found 477.2487.

**Di(adamantan-2-yl)**

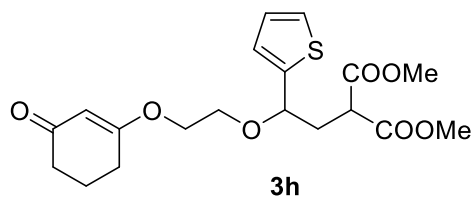
**2-(2-(4-methoxyphenyl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3g)**



Synthesized by the general procedure A; 82.2 mg (83%).

White Solid. mp 136-138 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.52-1.55 (m, 4H, HAd), 1.71-1.86 (m, 16H, HAd), 1.95-1.98 (m, 10H, HAd), 2.31-2.34 (m, 4H, CH<sub>2</sub>×2), 2.42 (t, *J* = 6.2 Hz, 2H, CH<sub>2</sub>), 3.52-3.64 (m, 3H, CH<sub>2</sub> + CH), 3.80 (s, 3H, CH<sub>3</sub>), 3.86-3.90 (m, 2H, CH<sub>2</sub>), 4.29 (dd, *J* = 4.6 Hz, 9.1 Hz, 1H, CH), 4.96 (d, *J* = 10.0 Hz, 2H, HAd), 5.28 (s, 1H, CH), 6.88 (d, *J* = 8.6 Hz, 2H, ArH), 7.22 (d, *J* = 8.6 Hz, 2H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.1, 26.8, 27.1, 28.9, 31.6, 31.78, 31.81, 31.9, 36.18, 36.21, 36.7, 37.18, 37.20, 49.8, 55.2, 66.2, 67.6, 78.06, 78.07, 79.9, 102.7, 113.9, 127.7, 132.9, 159.3, 168.6, 168.7, 177.8, 199.7 ppm. HRMS (ESI): calcd. for C<sub>40</sub>H<sub>53</sub>O<sub>8</sub> ([M + H]<sup>+</sup>) 661.3735, found 661.3738.

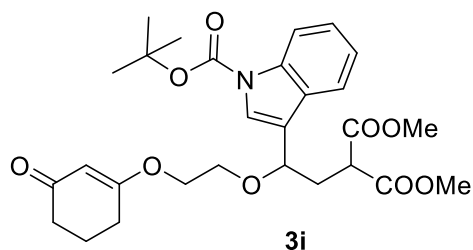
**Dimethyl 2-(2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)-2-(thiophen-2-yl)ethyl)malonate (3h)**



Synthesized by the general procedure A; 54.1 mg (91%).

Pale yellow gum. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.94-1.99 (quintet, *J* = 6.5 Hz, 2H, CH<sub>2</sub>), 2.30-2.49 (m, 6H, CH<sub>2</sub>×3), 3.55-3.69 (m, 3H, CH<sub>2</sub> + CH), 3.71 (s, 3H, CH<sub>3</sub>), 3.72 (s, 3H, CH<sub>3</sub>), 3.88 (t, *J* = 4.6 Hz, 2H, CH<sub>2</sub>), 4.64 (dd, *J* = 4.6 Hz, 9.2 Hz, 1H, CH), 5.28 (s, 1H, CH), 6.94-6.98 (m, 2H, ArH), 7.27 (s, 1H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 21.1, 28.8, 36.7, 37.2, 48.4, 52.55, 52.57, 66.2, 67.4, 75.6, 102.8, 125.5, 125.6, 126.5, 144.3, 169.4, 169.5, 177.7, 199.6 ppm. HRMS (ESI): calcd. for C<sub>19</sub>H<sub>25</sub>O<sub>7</sub>S ([M + H]<sup>+</sup>) 397.1316, found 397.1319.

**Dimethyl 2-(2-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)-2-(2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethyl)malonate (3i)**

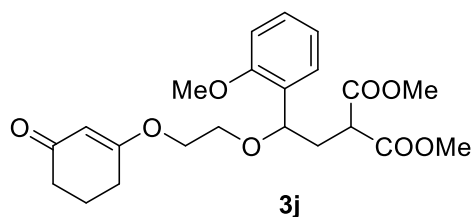




Synthesized by the general procedure A; 64.3mg (81%).

Pale yellow amorphous solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.67 (s, 9H,  $\text{CH}_3 \times 3$ ), 1.91-1.98 (m, 2H,  $\text{CH}_2$ ), 2.30-2.39 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.40-2.62 (m, 2H,  $\text{CH}_2$ ), 3.56-3.70 (m, 3H,  $\text{CH}_2 + \text{CH}$ ), 3.71 (s, 3H,  $\text{CH}_3$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 3.88-3.91 (m, 2H,  $\text{CH}_2$ ), 4.66 (dd,  $J$  = 4.3 Hz, 9.5 Hz, 1H, CH), 5.27 (s, 1H, CH), 7.20-7.26 (m, 1H, ArH), 7.30-7.34 (m, 1H, ArH), 7.53 (s, 1H, ArH), 7.70 (d,  $J$  = 7.8 Hz, 1H, ArH), 8.11 (d,  $J$  = 7.7 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.1, 28.1, 28.8, 35.1, 36.6, 48.5, 52.52, 52.54, 66.1, 67.5, 73.9, 83.9, 102.7, 115.3, 119.8, 120.1, 122.6, 123.7, 124.7, 128.2, 135.8, 149.4, 169.6, 169.7, 177.8, 199.7 ppm. HRMS (ESI): calcd. for  $\text{C}_{28}\text{H}_{36}\text{NO}_9$  ( $[\text{M} + \text{H}]^+$ ) 530.2385, found 530.2382.

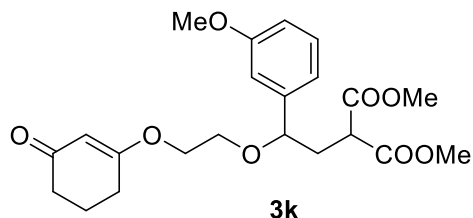
**Dimethyl 2-(2-(2-methoxyphenyl)-2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethylmalonate (3j)**



Synthesized by the general procedure C; 45.4 mg (72%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.96 (quintet,  $J$  = 6.4 Hz, 2H,  $\text{CH}_2$ ), 2.25-2.34 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.43 (t,  $J$  = 6.2 Hz, 2H,  $\text{CH}_2$ ), 3.55-3.57 (m, 1H, CH), 3.61-3.65 (m, 2H,  $\text{CH}_2$ ), 3.68 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 3.80 (s, 3H,  $\text{CH}_3$ ), 3.88-3.92 (m, 2H,  $\text{CH}_2$ ), 4.80 (dd,  $J$  = 4.7 Hz, 8.1 Hz, 1H, CH), 5.29 (s, 1H, CH), 6.84 (d,  $J$  = 8.2 Hz, 1H, ArH), 6.96 (t,  $J$  = 7.5 Hz, 1H, ArH), 7.24 (m, 1H, ArH), 7.37 (dd,  $J$  = 1.2 Hz, 7.5 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.1, 28.9, 35.5, 36.7, 48.7, 52.38, 52.43, 55.2, 66.6, 67.5, 73.8, 102.7, 110.2, 120.7, 126.4, 128.7, 128.8, 156.6, 169.7, 169.8, 177.8, 199.7 ppm. HRMS (ESI): calcd. for  $\text{C}_{22}\text{H}_{29}\text{O}_8$  ( $[\text{M} + \text{H}]^+$ ) 421.1857, found 421.1855.

**Dimethyl 2-(2-(3-methoxyphenyl)-2-((3-oxocyclohex-1-en-1-yl)oxy)ethoxy)ethylmalonate (3k)**

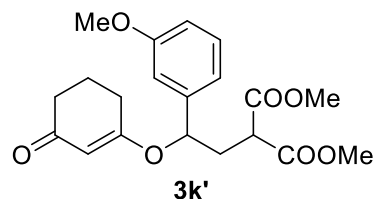


Synthesized by the general procedure C; 46.6 mg (74%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.98 (quintet,  $J$  = 6.5 Hz, 2H,  $\text{CH}_2$ ), 2.22-2.35 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.43 (t,  $J$  = 6.3 Hz, 2H,  $\text{CH}_2$ ), 3.50-3.55 (m, 1H, CH), 3.60-3.68 (m, 2H,  $\text{CH}_2$ ), 3.71 (s, 3H,  $\text{CH}_3$ ), 3.74 (s, 3H,  $\text{CH}_3$ ), 3.81 (s, 3H,  $\text{CH}_3$ ), 3.89-3.91 (m, 2H,  $\text{CH}_2$ ), 4.32 (dd,  $J$  = 4.5

Hz, 9.0 Hz, 1H, CH), 5.30 (s, 1H, CH), 6.81-6.84 (m, 3H, ArH), 7.24-7.28 (m, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 21.2, 28.9, 36.7, 37.1, 48.6, 52.5, 52.6, 55.2, 66.5, 67.5, 80.0, 102.8, 111.8, 113.4, 118.8, 129.7, 142.5, 159.9, 169.6, 169.7, 177.8, 199.7$  ppm. HRMS (ESI): calcd. for  $\text{C}_{22}\text{H}_{29}\text{O}_8$  ( $[\text{M} + \text{H}]^+$ ) 421.1857, found 421.1853.

**Dimethyl 2-(2-(3-methoxyphenyl)-2-((3-oxocyclohex-1-en-1-yl)oxy)ethyl)malonate (3k')**

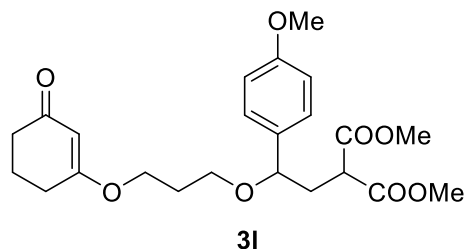


Synthesized by the general procedure A; 49.7 mg (88%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 1.92\text{-}1.96$  (m, 2H,  $\text{CH}_2$ ), 2.25 (m, 2H,  $\text{CH}_2$ ), 2.37-2.53 (m, 4H,  $\text{CH}_2 \times 2$ ), 3.52 (dd,  $J = 6.5$  Hz, 8.0 Hz, 1H, CH), 3.73 (s, 3H,  $\text{CH}_3$ ), 3.74 (s, 3H,  $\text{CH}_3$ ), 3.79 (s, 3H,  $\text{CH}_3$ ), 5.05 (dd,  $J = 4.7$  Hz, 8.6 Hz, 1H, CH), 5.17 (s, 1H, CH), 6.75 (t,  $J = 1.8$  Hz, 1H, ArH), 6.81 (dd,  $J = 4.6$  Hz, 8.0 Hz, 2H, ArH), 7.23-7.27 (m, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 21.0, 28.9, 36.5, 36.7, 48.3, 52.7, 52.8, 55.2, 78.0, 105.2, 111.3, 113.5, 117.8, 130.1, 140.3, 160.0, 169.0, 169.1, 175.9, 199.5$  ppm. HRMS (ESI): calcd. for  $\text{C}_{20}\text{H}_{25}\text{O}_7$  ( $[\text{M} + \text{H}]^+$ ) 377.1595, found 377.1598.

**Dimethyl**

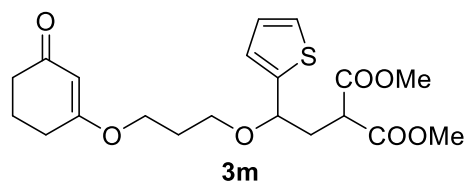
**2-(2-(4-methoxyphenyl)-2-(3-((3-oxocyclohex-1-en-1-yl)oxy)propoxy)ethyl)malonate (3l)**



Synthesized by the general procedure A; 60.6 mg (93%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 1.87\text{-}1.97$  (m, 4H,  $\text{CH}_2 + \text{CH}_2$ ), 2.18-2.36 (m, 6H,  $\text{CH}_2 \times 3$ ), 3.26-3.41 (m, 2H,  $\text{OCH}_2$ ), 3.58 (dd,  $J = 6.3$  Hz, 8.3 Hz, 1H, CH), 3.70 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 3.79 (s, 3H,  $\text{CH}_3$ ), 3.86 (td,  $J = 1.2$  Hz, 6.2 Hz, 2H,  $\text{OCH}_2$ ), 4.18 (dd,  $J = 4.4$  Hz, 9.2 Hz, 1H, CH), 5.33 (s, 1H, CH), 6.85 (d,  $J = 8.7$  Hz, 2H, ArH), 7.16 (d,  $J = 8.7$  Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 21.1, 28.77, 28.78, 36.7, 37.1, 48.7, 52.5, 55.2, 64.5, 65.3, 79.2, 102.7, 113.9, 127.6, 133.1, 159.3, 169.6, 169.7, 177.9, 199.8$  ppm. HRMS (ESI): calcd. for  $\text{C}_{23}\text{H}_{31}\text{O}_8$  ( $[\text{M} + \text{H}]^+$ ) 435.2013, found 435.2009.

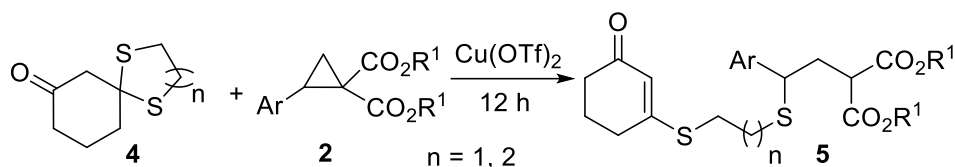
**Dimethyl 2-(2-(3-((3-oxocyclohex-1-en-1-yl)oxy)propoxy)-2-(thiophen-2-yl)ethyl)malonate (3m)**



Synthesized by the general procedure **A**; 56.6 mg (92%).

Colorless gum.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.88-1.96 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.25-2.45 (m, 6H,  $\text{CH}_2 \times 3$ ), 3.33-3.38 (m, 1H,  $\text{OCH}_2 \times 1/2$ ), 3.43-3.49 (m, 1H,  $\text{OCH}_2 \times 1/2$ ), 3.58 (dd,  $J$  = 6.5 Hz, 8.1 Hz, 1H, CH), 3.70 (s, 3H,  $\text{CH}_3$ ), 3.71 (s, 3H,  $\text{CH}_3$ ), 3.81-3.90 (m, 2H,  $\text{OCH}_2$ ), 4.52 (dd,  $J$  = 4.7 Hz, 9.1 Hz, 1H, CH), 5.32 (s, 1H, CH), 6.92-6.94 (m, 2H, ArH), 7.23-7.25 (m, 1H, ArH) ppm;  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.1, 28.7, 28.8, 36.6, 37.2, 48.4, 52.5, 64.6, 65.2, 75.2, 102.7, 125.2, 125.3, 126.4, 144.8, 169.4, 169.5, 177.8, 199.7 ppm. HRMS (ESI): calcd. for  $\text{C}_{20}\text{H}_{27}\text{O}_7\text{S}$  ( $[\text{M} + \text{H}]^+$ ) 411.1472, found 411.1478.

## 6. Procedures for the reactions of **4** and **2** to afford **5**.



**General procedures for the reactions of **4** and **2** to afford **5** (D).** To a mixture of **4** (0.18 mmol) and D-A cyclopropanes **2** (0.15 mmol) in  $\text{CH}_2\text{Cl}_2$  (1.0 mL),  $\text{Cu}(\text{OTf})_2$  (5.4 mg, 0.015 mmol) was added. The mixture was stirred at room temperature (25 °C) for 12 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **5**.

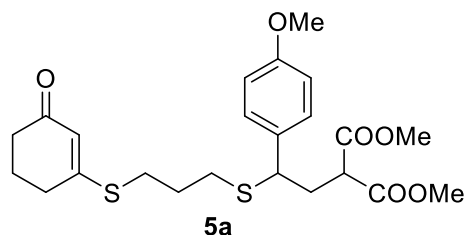
**General procedures for the reactions of **4** and **2** to afford **5** (E).** To a mixture of **4** (0.18 mmol) and D-A cyclopropanes **2** (0.15 mmol) in 1,2-dichloroethane (1.0 mL),  $\text{Cu}(\text{OTf})_2$  (5.4 mg, 0.015 mmol) was added. The mixture was stirred at 45 °C for 12 h. Then, the solvent was removed in vacuo and the residue was purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **5**.

**Procedure for a 5 mmol-scale reaction to synthesize **5a**.** To a mixture of 1,3-cyclohexanedione derived cyclic thiol ketal **4a** (1.21 g, 6.0 mmol) and D-A cyclopropanes **2a** (1.32 g, 5.0 mmol) in  $\text{CH}_2\text{Cl}_2$  (20.0 mL),  $\text{Cu}(\text{OTf})_2$  (180.0 mg, 0.5 mmol) was added. The mixture was stirred at room temperature (25 °C) for 12 h. Then, the mixture was diluted with  $\text{CH}_2\text{Cl}_2$  (20.0 mL), and washed with saturated  $\text{NaHCO}_3$ . The aqueous phase was extracted with  $\text{CH}_2\text{Cl}_2$  (20 mL x 3). The organic layers were combined, washed with brine, dried over  $\text{Na}_2\text{SO}_4$ , and concentrated. The residue was

purified by silica gel flash chromatography (petrol ether : ethyl acetate = 4:1 to 2:1) to provide product **5a** (2.12 g, 91%).

### Dimethyl

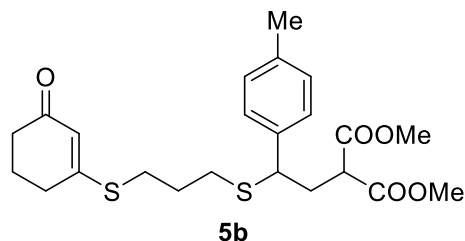
#### 2-(2-(4-methoxyphenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (**5a**)



Synthesized by the general procedure **D**; 66.5 mg (95%).

Colorless gum.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.73-1.81 (m, 2H,  $\text{CH}_2$ ), 1.96-2.04 (m, 2H,  $\text{CH}_2$ ), 2.30-2.49 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.70-2.86 (m, 2H,  $\text{CH}_2$ ), 3.39 (dd,  $J$  = 6.5 Hz, 8.2 Hz, 1H, CH), 3.65 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 3.73-3.77 (m, 1H, CH), 3.78 (s, 3H,  $\text{CH}_3$ ), 5.78 (s, 1H, CH), 6.84 (d,  $J$  = 8.7 Hz, 2H, ArH), 7.18 (d,  $J$  = 8.7 Hz, 2H, ArH) ppm;  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.8, 27.2, 29.4, 29.8, 30.8, 35.1, 37.2, 46.7, 49.6, 52.56, 52.57, 55.2, 114.0, 119.4, 128.8, 132.5, 158.9, 165.1, 169.20, 169.24, 195.5 ppm. HRMS (ESI): calcd. for  $\text{C}_{23}\text{H}_{31}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 467.1557, found 467.1560.

#### Dimethyl 2-(2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)-2-(p-tolyl)ethyl)malonate (**5b**)

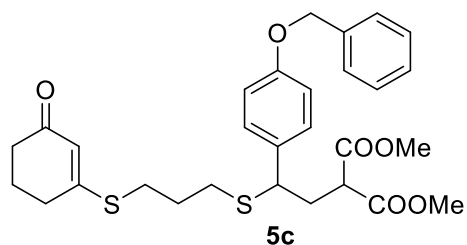


Synthesized by the general procedure **D**; 58.1 mg (86%).

Colorless gum.  $^1\text{H NMR}$  (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.77 (quintet,  $J$  = 7.1 Hz, 2H,  $\text{CH}_2$ ), 1.96-2.02 (m, 2H,  $\text{CH}_2$ ), 2.31 (s, 3H,  $\text{CH}_3$ ), 2.35-2.49 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.70-2.83 (m, 2H,  $\text{CH}_2$ ), 3.39 (dd,  $J$  = 6.5 Hz, 8.2 Hz, 1H, CH), 3.65 (s, 3H,  $\text{CH}_3$ ), 3.71 (s, 3H,  $\text{CH}_3$ ), 3.73 (dd,  $J$  = 6.8 Hz, 8.8 Hz, 1H, CH), 5.78 (s, 1H, CH), 7.10-7.15 (m, 4H, ArH) ppm;  $^{13}\text{C NMR}$  (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.0, 22.8, 27.1, 29.4, 29.8, 30.8, 35.0, 37.2, 47.0, 49.6, 52.5, 52.6, 119.4, 127.6, 129.4, 137.3, 137.6, 165.2, 169.20, 169.24, 195.6 ppm. HRMS (ESI): calcd. for  $\text{C}_{23}\text{H}_{31}\text{O}_5\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 451.1607, found 451.1603.

### Dimethyl

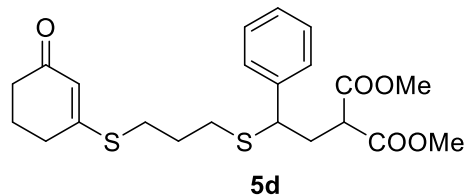
#### 2-(2-(4-(benzyloxy)phenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (**5c**)



Synthesized by the general procedure **D**; 72.5 mg (89%).

Pale yellow Solid. mp 123-125 °C. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.76 (quintet, *J* = 7.1 Hz, 2H, CH<sub>2</sub>), 1.97 (quintet, *J* = 6.3 Hz, 2H, CH<sub>2</sub>), 2.30-2.48 (m, 8H, CH<sub>2</sub>×4), 2.70-2.82 (m, 2H, CH<sub>2</sub>), 3.40 (dd, *J* = 6.6 Hz, 8.1 Hz, 1H, CH), 3.63 (s, 3H, CH<sub>3</sub>), 3.70 (s, 3H, CH<sub>3</sub>), 3.74 (dd, *J* = 6.8 Hz, 8.8 Hz, 1H, CH), 5.02 (s, 2H, CH<sub>2</sub>), 5.78 (s, 1H, CH), 6.91 (d, *J* = 8.7 Hz, 2H, ArH), 7.18 (d, *J* = 8.7 Hz, 2H, ArH), 7.26-7.41 (m, 5H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 22.6, 27.0, 29.2, 29.6, 30.6, 34.9, 37.0, 46.6, 49.4, 52.3, 52.4, 69.7, 114.8, 119.2, 127.2, 127.7, 128.3, 128.6, 132.7, 136.6, 158.0, 164.9, 168.95, 169.00, 195.2 ppm. HRMS (ESI): calcd. for C<sub>29</sub>H<sub>35</sub>O<sub>6</sub>S<sub>2</sub> ([M + H]<sup>+</sup>) 543.1870, found 543.1877.

**Dimethyl 2-(2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)-2-phenylethyl)malonate (5d)**

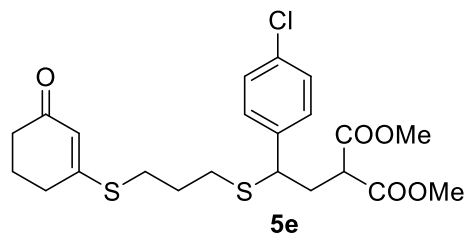


Synthesized by the general procedure **E**; 51.7 mg (79%).

Colorless gum. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 1.73-1.84 (m, 2H, CH<sub>2</sub>), 1.97-2.05 (m, 2H, CH<sub>2</sub>), 2.35-2.51 (m, 8H, CH<sub>2</sub>×4), 2.62-2.83 (m, 2H, CH<sub>2</sub>), 3.42 (t, *J* = 7.2 Hz, 1H, CH), 3.66 (s, 3H, CH<sub>3</sub>), 3.72 (s, 3H, CH<sub>3</sub>), 3.77 (t, *J* = 7.8 Hz, 1H, CH), 5.78 (s, 1H, CH), 7.22-7.33 (m, 5H, ArH) ppm; <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 22.9, 27.1, 29.4, 29.9, 30.9, 35.0, 37.3, 47.4, 49.6, 52.60, 52.62, 119.5, 127.67, 127.73, 128.7, 140.8, 165.1, 169.2, 169.3, 195.6 ppm. HRMS (ESI): calcd. for C<sub>22</sub>H<sub>29</sub>O<sub>5</sub>S<sub>2</sub> ([M + H]<sup>+</sup>) 437.1451, found 437.1445.

**Dimethyl**

**2-(2-(4-chlorophenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5e)**

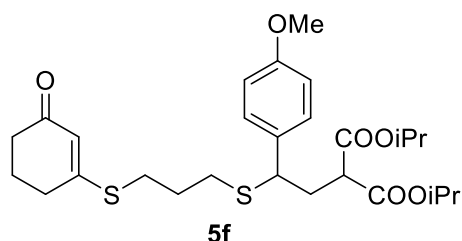


Synthesized by the general procedure **E**; 44.5 mg (63%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.78 (quintet,  $J$  = 7.1 Hz, 2H,  $\text{CH}_2$ ), 2.01 (quintet,  $J$  = 6.2 Hz, 2H,  $\text{CH}_2$ ), 2.32-2.48 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.75-2.90 (m, 2H,  $\text{CH}_2$ ), 3.40 (t,  $J$  = 7.3 Hz, 1H, CH), 3.67 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 3.76 (t,  $J$  = 7.8 Hz, 1H, CH), 5.78 (s, 1H, CH), 7.21-7.26 (m, 2H, ArH), 7.28 (d,  $J$  = 8.6 Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.9, 27.1, 29.4, 29.9, 30.9, 35.0, 37.3, 46.8, 49.5, 52.65, 52.68, 119.5, 128.9, 129.1, 133.3, 139.5, 165.0, 165.1, 169.06, 169.11, 195.6 ppm. HRMS (ESI): calcd. for  $\text{C}_{22}\text{H}_{28}\text{ClO}_5\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 471.1061, found 471.1067.

## Diisopropyl

### 2-(2-(4-methoxyphenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5f)

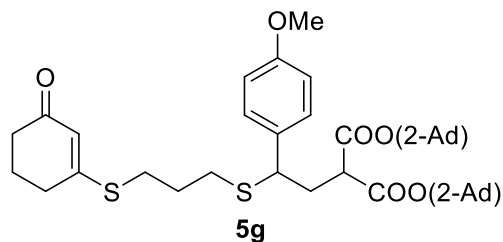


Synthesized by the general procedure **D**; 72.1 mg (92%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.18-1.24 (m, 12H,  $\text{CH}_3 \times 4$ ), 1.78 (quintet,  $J$  = 7.1 Hz, 2H,  $\text{CH}_2$ ), 2.00 (quintet,  $J$  = 6.3 Hz, 2H,  $\text{CH}_2$ ), 2.25-2.46 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.74-2.84 (m, 2H,  $\text{CH}_2$ ), 3.25 (dd,  $J$  = 6.3 Hz, 8.6 Hz, 1H, CH), 3.75 (dd,  $J$  = 6.8 Hz, 9.1 Hz, 1H, CH), 3.78 (s, 3H,  $\text{CH}_3$ ), 4.96 (hep,  $J$  = 6.2 Hz, 1H, CH), 5.04 (hep,  $J$  = 6.3 Hz, 1H, CH), 5.78 (m, 1H, CH), 6.84 (d,  $J$  = 8.7 Hz, 2H, ArH), 7.18 (d,  $J$  = 8.7 Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 21.46, 21.51, 21.53, 21.60, 22.9, 27.2, 29.4, 29.9, 30.8, 35.0, 37.3, 46.7, 50.3, 55.2, 68.9, 69.0, 114.0, 119.5, 128.8, 132.8, 158.9, 165.2, 168.37, 168.42, 195.5 ppm. HRMS (ESI): calcd. for  $\text{C}_{27}\text{H}_{39}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 523.2183, found 523.2188.

## Di(adamantan-2-yl)

### 2-(2-(4-methoxyphenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5g)



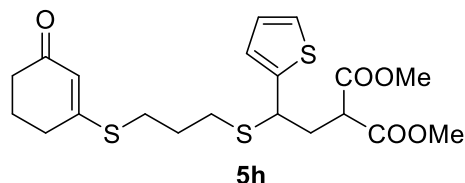
Synthesized by the general procedure **D**; 90.1 mg (85%).

Pale yellow Solid. mp 148-150  $^\circ\text{C}$ .  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.48-1.55 (m, 4H, HAd), 1.70-1.83 (m, 16H, HAd), 1.89-2.03 (m, 10H, HAd), 2.32-2.52 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.70-2.83 (m, 2H,  $\text{CH}_2$ ), 3.38 (dd,  $J$  = 6.2 Hz, 8.6 Hz, 1H, CH), 3.77 (dd,  $J$  = 6.5 Hz, 9.0 Hz, 1H, CH), 3.79 (s, 3H,  $\text{CH}_3$ ), 4.90 (s, 1H, HAd), 4.98 (s, 1H, HAd), 5.78 (s, 1H, CH), 6.84 (d,  $J$  = 8.7 Hz, 2H, ArH),

7.19 (d,  $J = 8.7$  Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 22.8, 26.71, 26.73, 26.9, 27.0, 27.1, 29.3, 29.8, 30.7, 31.50, 31.52, 31.6, 31.65, 31.74, 35.3, 36.0, 36.06, 36.11, 37.06, 37.08, 37.2, 46.7, 50.6, 55.1, 78.05, 78.12, 113.9, 119.3, 128.7, 132.6, 158.8, 165.0, 168.1, 168.2, 195.3$  ppm. HRMS (ESI): calcd. for  $\text{C}_{41}\text{H}_{55}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 707.3435, found 707.3443.

### Dimethyl

#### 2-(2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)-2-(thiophen-2-yl)ethyl)malonate (5h)

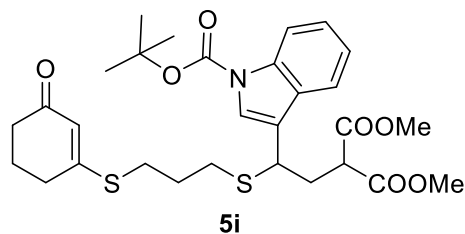


Synthesized by the general procedure **D**; 59.1 mg (89%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 1.79$ -1.86 (m, 2H,  $\text{CH}_2$ ), 1.97-2.05 (m, 2H,  $\text{CH}_2$ ), 2.37-2.54 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.78-2.83 (m, 2H,  $\text{CH}_2$ ), 3.53 (dd,  $J = 6.8$  Hz, 8.0 Hz, 1H, CH), 3.69 (s, 3H,  $\text{CH}_3$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 4.12 (dd,  $J = 7.2$  Hz, 8.2 Hz, 1H, CH), 5.80 (s, 1H, CH), 6.89-6.90 (m, 2H, ArH), 7.22-7.24 (m, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 22.8, 27.1, 29.4, 29.9, 30.8, 35.9, 37.3, 42.6, 49.5, 52.7, 119.5, 125.2, 125.7, 126.5, 145.4, 165.1, 169.08, 169.14, 195.6$  ppm. HRMS (ESI): calcd. for  $\text{C}_{20}\text{H}_{27}\text{O}_5\text{S}_3$  ( $[\text{M} + \text{H}]^+$ ) 443.1015, found 443.1018.

### Dimethyl

#### 2-(2-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5i)

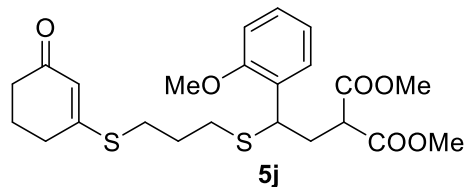


Synthesized by the general procedure **D**; 70.8 mg (82%).

Yellow amorphous solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta = 1.68$  (s, 9H,  $\text{CH}_3 \times 3$ ), 1.81 (quintet,  $J = 7.1$  Hz, 2H,  $\text{CH}_2$ ), 1.99 (quintet,  $J = 6.3$  Hz, 2H,  $\text{CH}_2$ ), 2.36-2.39 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.46-2.64 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.77 (td,  $J = 1.7$  Hz, 7.0 Hz, 2H,  $\text{CH}_2$ ), 3.64 (t,  $J = 7.2$  Hz, 1H, CH), 3.68 (s, 3H,  $\text{CH}_3$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 4.06 (t,  $J = 7.7$  Hz, 1H, CH), 5.76 (s, 1H, CH), 7.22-7.26 (m, 1H, ArH), 7.32 (td,  $J = 1.2$  Hz, 7.3 Hz, 1H, ArH), 7.50 (s, 1H, ArH), 7.72 (d,  $J = 7.7$  Hz, 1H, ArH), 8.11 (d,  $J = 7.7$  Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta = 22.8, 27.1, 28.2, 29.4, 30.8, 33.6, 37.2, 39.4, 49.7, 52.6, 84.0, 115.4, 119.5, 119.6, 120.0, 122.6, 123.7, 124.8, 128.4, 135.8, 149.5, 165.1, 169.2, 169.4, 195.6$  ppm. HRMS (ESI): calcd. for  $\text{C}_{29}\text{H}_{38}\text{NO}_7\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 576.2084, found 576.2089.

### Dimethyl

#### 2-(2-(2-methoxyphenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5j)

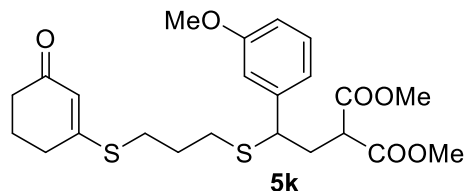


Synthesized by the general procedure **D**; 52.5 mg (76%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.83 (quintet,  $J$  = 7.1 Hz, 2H,  $\text{CH}_2$ ), 2.00 (quintet,  $J$  = 6.2 Hz, 2H,  $\text{CH}_2$ ), 2.31-2.42 (m, 5H,  $\text{CH}_2 \times 2.5$ ), 2.46-2.56 (m, 3H,  $\text{CH}_2 \times 1.5$ ), 2.77-2.84 (m, 2H,  $\text{CH}_2$ ), 3.38 (dd,  $J$  = 6.3 Hz, 8.4 Hz, 1H, CH), 3.64 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 3.79 (s, 3H,  $\text{CH}_3$ ), 4.35 (dd,  $J$  = 6.6 Hz, 8.9 Hz, 1H, CH), 5.80 (s, 1H, CH), 6.84 (d,  $J$  = 8.2 Hz, 1H, ArH), 6.94 (t,  $J$  = 7.4 Hz, 1H, ArH), 7.21 (td,  $J$  = 1.7 Hz, 7.8 Hz, 1H, ArH), 7.36 (dd,  $J$  = 1.6 Hz, 7.6 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.7, 27.1, 29.3, 29.9, 30.7, 34.5, 37.1, 39.1, 49.6, 52.31, 52.34, 55.3, 110.4, 119.3, 120.8, 127.9, 128.3, 128.7, 156.6, 165.2, 169.1, 169.2, 195.3 ppm. HRMS (ESI): calcd. for  $\text{C}_{23}\text{H}_{31}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 467.1557, found 467.1558.

### Dimethyl

#### 2-(2-(3-methoxyphenyl)-2-((3-((3-oxocyclohex-1-en-1-yl)thio)propyl)thio)ethyl)malonate (5k)



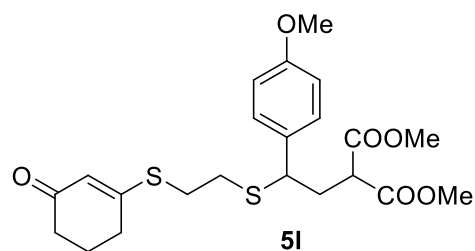
Synthesized by the general procedure **D**; 52.5 mg (75%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.79 (quintet,  $J$  = 7.1 Hz, 2H,  $\text{CH}_2$ ), 1.97-2.03 (m, 2H,  $\text{CH}_2$ ), 2.33-2.50 (m, 8H,  $\text{CH}_2 \times 4$ ), 2.71-2.85 (m, 2H,  $\text{CH}_2$ ), 3.42 (dd,  $J$  = 6.6 Hz, 8.1 Hz, 1H, CH), 3.67 (s, 3H,  $\text{CH}_3$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 3.75 (dd,  $J$  = 7.08 Hz, 8.5 Hz, 1H, CH), 3.80 (s, 3H,  $\text{CH}_3$ ), 5.79 (s, 1H, CH), 6.77-6.80 (m, 1H, ArH), 6.82-6.85 (m, 2H, ArH), 7.23 (t,  $J$  = 7.8 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.9, 27.1, 29.4, 29.9, 30.9, 35.0, 37.3, 47.4, 49.6, 52.6, 55.2, 113.1, 113.2, 119.5, 120.1, 129.7, 142.4, 159.8, 165.2, 169.2, 169.3, 195.6 ppm. HRMS (ESI): calcd. for  $\text{C}_{23}\text{H}_{31}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 467.1557, found 467.1560.

### Dimethyl

#### 2-(2-(4-methoxyphenyl)-2-((2-((3-oxocyclohex-1-en-1-yl)thio)ethyl)thio)ethyl)malonate (5l)



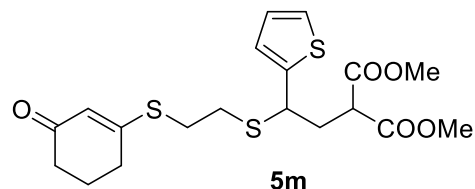


Synthesized by the general procedure **D**; 61.7 mg (91%).

Colorless gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.96 (quintet,  $J$  = 6.4 Hz, 2H,  $\text{CH}_2$ ), 2.28-2.37 (m, 5H,  $\text{CH}_2 \times 2.5$ ), 2.39-2.47 (m, 1H,  $\text{CH}_2 \times 1/2$ ), 2.54 (t,  $J$  = 7.7 Hz, 2H,  $\text{CH}_2$ ), 2.73-2.82 (m, 2H,  $\text{CH}_2$ ), 3.35 (dd,  $J$  = 6.4 Hz, 8.2 Hz, 1H, CH), 3.63 (s, 3H,  $\text{CH}_3$ ), 3.70 (s, 3H,  $\text{CH}_3$ ), 3.76 (s, 3H,  $\text{CH}_3$ ), 3.80 (dd,  $J$  = 6.6 Hz, 9.0 Hz, 1H, CH), 5.69 (s, 1H, CH), 6.83 (d,  $J$  = 8.7 Hz, 2H, ArH), 7.18 (d,  $J$  = 8.7 Hz, 2H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.6, 29.0, 30.5, 30.6, 35.0, 37.1, 46.9, 49.4, 52.4, 52.5, 55.1, 114.0, 119.3, 128.7, 132.1, 158.9, 164.2, 168.95, 169.00, 195.2 ppm. HRMS (ESI): calcd. for  $\text{C}_{22}\text{H}_{29}\text{O}_6\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 453.1400, found 453.1398.

### Dimethyl

#### 2-(2-((2-((3-oxocyclohex-1-en-1-yl)thio)ethyl)thio)-2-(thiophen-2-yl)ethyl)malonate (5m)

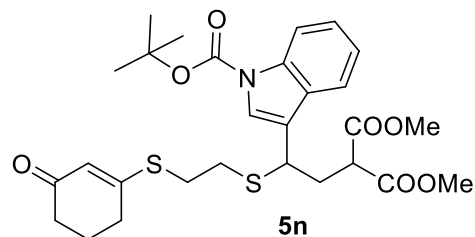


Synthesized by the general procedure **D**; 57.9 mg (90%).

Pale yellow gum.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.96-2.01 (m, 2H,  $\text{CH}_2$ ), 2.34-2.49 (m, 6H,  $\text{CH}_2 \times 3$ ), 2.65 (m, 2H,  $\text{CH}_2$ ), 2.83-2.87 (m, 2H,  $\text{CH}_2$ ), 3.48-3.51 (m, 1H, CH), 3.68 (s, 3H,  $\text{CH}_3$ ), 3.72 (s, 3H,  $\text{CH}_3$ ), 4.17-4.21 (m, 1H, CH), 5.73 (s, 1H, CH), 6.88-6.93 (s, 2H, ArH), 7.23 (dd,  $J$  = 1.08, 5.0 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.6, 29.1, 30.4, 30.6, 35.8, 37.0, 42.7, 49.2, 52.5, 119.3, 125.3, 125.9, 126.4, 144.9, 164.1, 168.8, 168.9, 195.2 ppm. HRMS (ESI): calcd. for  $\text{C}_{19}\text{H}_{25}\text{O}_5\text{S}_3$  ( $[\text{M} + \text{H}]^+$ ) 429.0859, found 429.0862.

### Dimethyl

#### 2-(2-(1-(tert-butoxycarbonyl)-1H-indol-3-yl)-2-((2-((3-oxocyclohex-1-en-1-yl)thio)ethyl)thio)ethyl)malonate (5n)



Synthesized by the general procedure **D**; 68.2 mg (81%).

Yellow amorphous solid.  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 1.68 (s, 9H,  $\text{CH}_3 \times 3$ ), 1.98 (quintet,  $J$  = 6.4 Hz, 2H,  $\text{CH}_2$ ), 2.34-2.38 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.50-2.72 (m, 4H,  $\text{CH}_2 \times 2$ ), 2.83-2.93 (m, 2H,  $\text{CH}_2$ ), 3.62 (t,  $J$  = 7.4 Hz, 1H, CH), 3.68 (s, 3H,  $\text{CH}_3$ ), 3.73 (s, 3H,  $\text{CH}_3$ ), 4.14 (t,  $J$  = 7.7 Hz, 1H, CH), 5.73 (s, 1H, CH), 7.22-7.26 (m, 1H, ArH), 7.30-7.34 (m, 1H, ArH), 7.51 (s, 1H, ArH), 7.73 (d,  $J$  = 7.6 Hz, 1H, ArH), 8.11 (d,  $J$  = 7.8 Hz, 1H, ArH) ppm;  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta$  = 22.7, 28.1, 28.8, 30.70, 30.72, 33.6, 37.2, 39.8, 49.6, 52.65, 52.68, 84.1, 115.4, 119.3, 119.5, 120.0, 122.6, 123.9, 124.9, 128.3, 135.8, 149.4, 164.3, 169.2, 169.3, 195.4 ppm. HRMS (ESI): calcd. for  $\text{C}_{28}\text{H}_{36}\text{NO}_7\text{S}_2$  ( $[\text{M} + \text{H}]^+$ ) 562.1928, found 562.1933.

## 7. Stability test of **1a** and **4a** in the presence of $\text{Cu}(\text{OTf})_2$

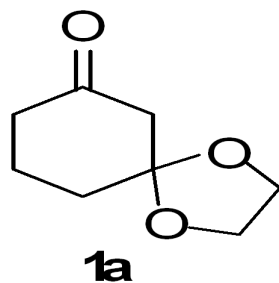
To a mixture of 1,3-cyclohexanedione derived cyclic ketal **1a** (93.7 mg, 0.6 mmol) in  $\text{CDCl}_3$  (2.0 mL),  $\text{Cu}(\text{OTf})_2$  (21.6 mg, 0.06 mmol) was added. The mixture was stirred at room temperature (25 °C) and monitored by TLC and crude  $^1\text{H}$  NMR. No corresponding ring-opening product was detected up to three days while partial decomposition of **1a** was observed after 12 h.

To a mixture of 1,3-cyclohexanedione derived cyclic thiol ketal **4a** (121.4 mg, 0.6 mmol) in  $\text{CDCl}_3$  (2.0 mL),  $\text{Cu}(\text{OTf})_2$  (21.6 mg, 0.06 mmol) was added. The mixture was stirred at room temperature (25 °C) and monitored by TLC and crude  $^1\text{H}$  NMR. No corresponding ring-opening product was detected up to three days while partial decomposition of **4a** was observed after 12 h.

These information suggested that the proposed O- or S- nucleophiles are kinetically unstable under the reaction conditions, and in the presence of Lewis acid, they reacted quickly with D-A cyclopropanes.

## 8. References

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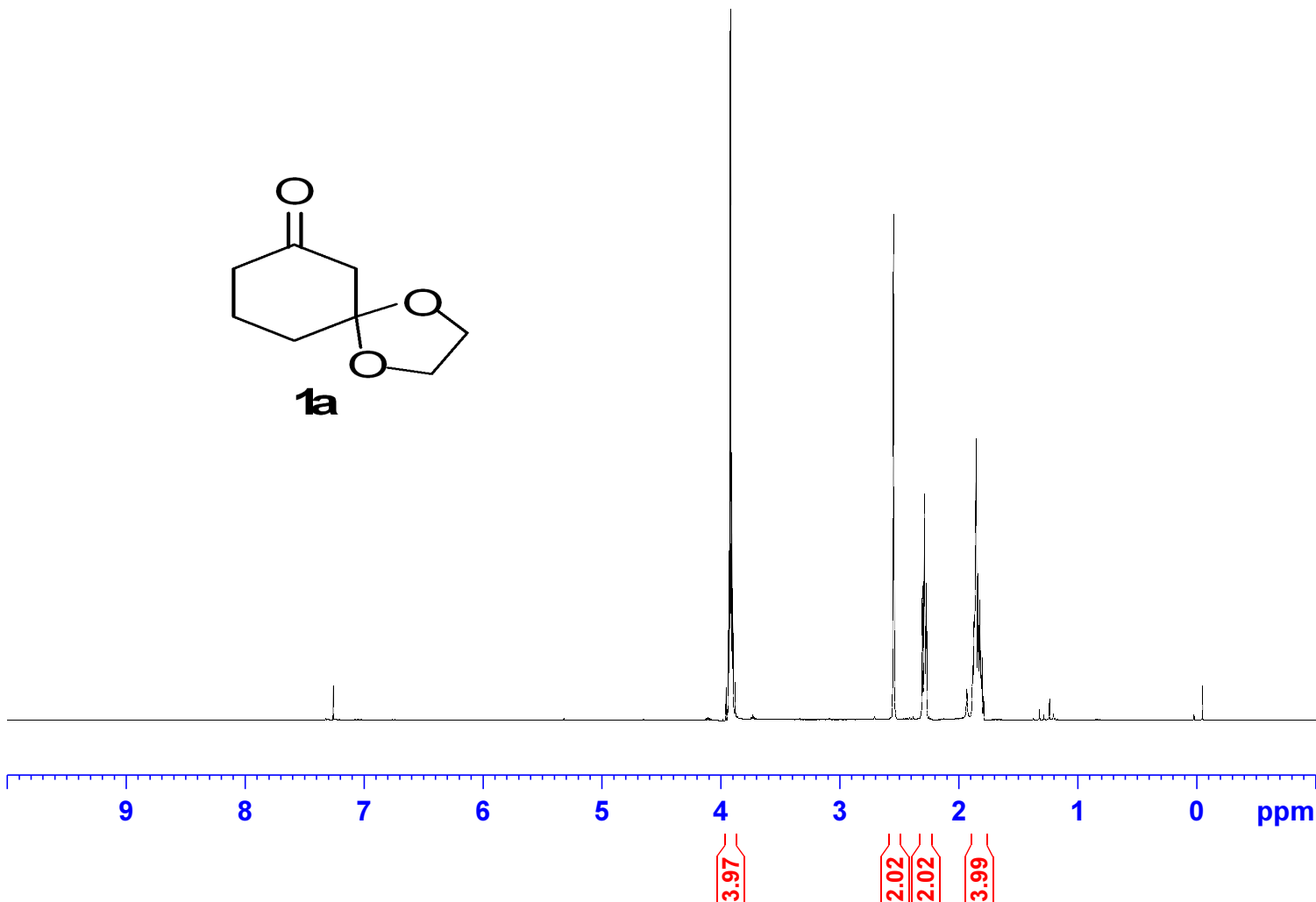
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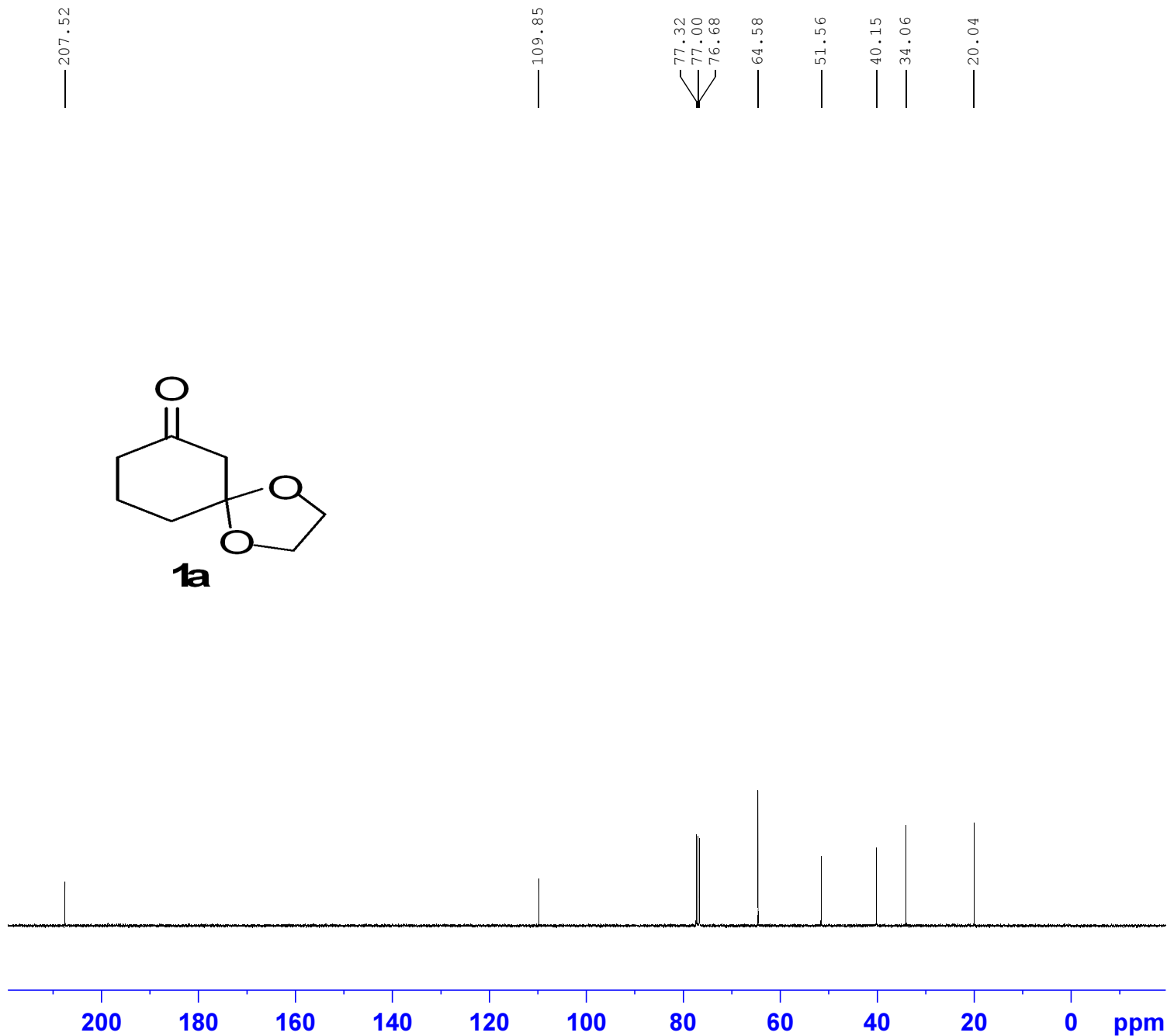
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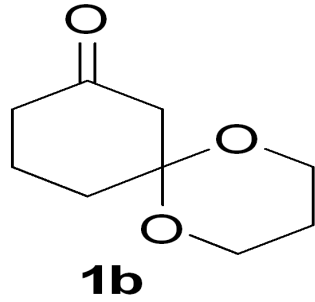
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 EXPNO 2019122402  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191224  
 Time 18.45  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 47  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 292.2 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

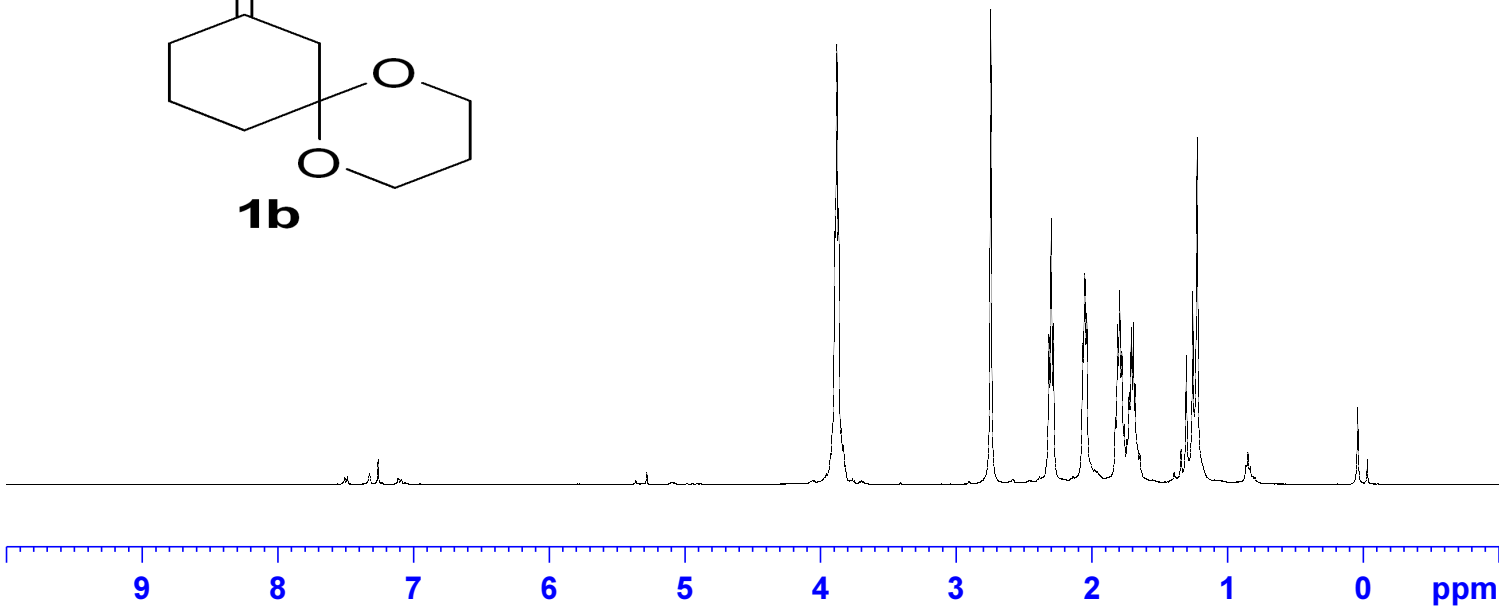
==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228403 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



— 7.260

3.925  
3.896  
3.890  
3.878  
3.867  
3.847  
3.832  
3.816  
2.744  
2.315  
2.299  
2.282  
2.066  
2.052  
2.036  
1.826  
1.809  
1.794  
1.778  
1.761  
1.739  
1.723  
1.708  
1.694  
1.680  
1.667  
1.660



```

Current Data Parameters
NAME          zjc-93
EXPNO        2019122401
PROCNO       1

F2 - Acquisition Parameters
Date_        20191224
Time_        17.12
INSTRUM      spect
PROBHD       5 mm PABBO BB-
PULPROG      zg30
TD           65536
SOLVENT      CDC13
NS           16
DS           2
SWH          8223.685 Hz
FIDRES       0.125483 Hz
AQ           3.9845889 sec
RG           57
DW           60.800 usec
DE           6.50 usec
TE           291.5 K
D1           1.00000000 sec
TD0          1

===== CHANNEL f1 =====
NUC1         1H
P1           14.80 usec
PL1          -1.00 dB
PL1W         10.90985775 W
SF01         400.1724712 MHz

F2 - Processing parameters
SI           32768
SF           400.1700146 MHz
WDW          no
SSB          0
LB           0 Hz
GB           0
PC           1.00
  
```

— 207.74

— 99.66

77.31  
77.00  
76.68

— 59.63

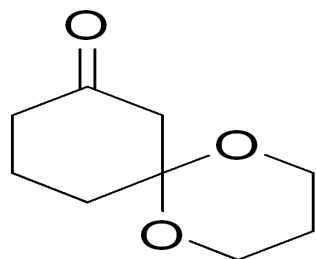
— 48.99

— 40.43

— 32.22

— 25.03

— 19.27



**1b**



Current Data Parameters  
NAME zjc-93  
EXPNO 2019122402  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 20191224  
Time 18.49  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDC13  
NS 73  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 292.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

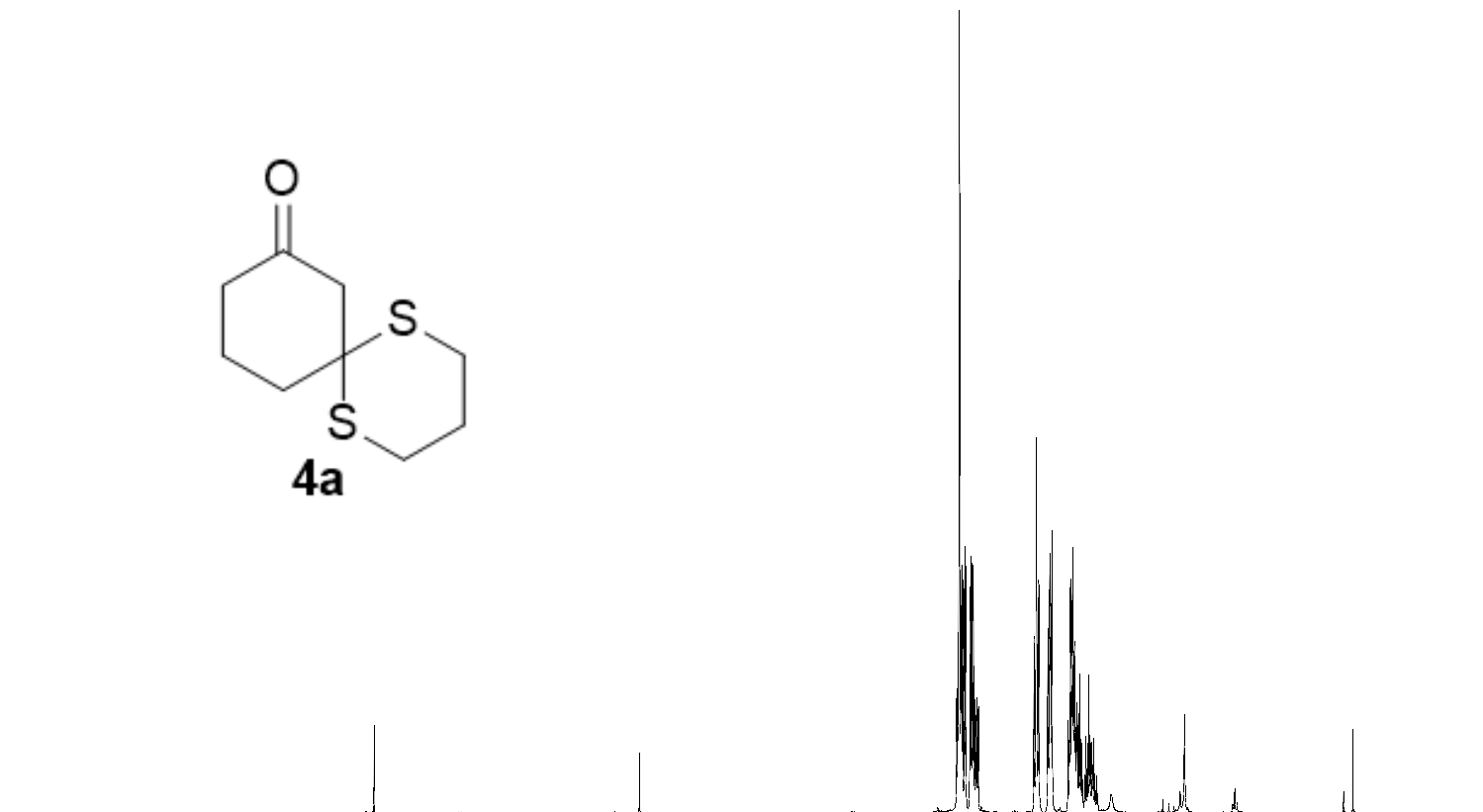
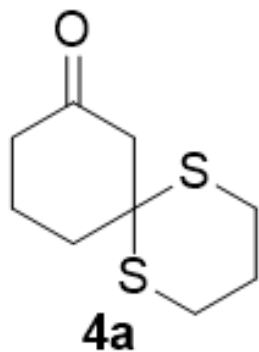
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.90 usec  
PL1 -1.10 dB  
PL1W 40.29647064 W  
SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -1.00 dB  
PL12 14.68 dB  
PL13 17.68 dB  
PL2W 10.90985775 W  
PL12W 0.29499799 W  
PL13W 0.14784923 W  
SFO2 400.1716007 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6228374 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.40

200 180 160 140 120 100 80 60 40 20 0 ppm

7.260  
 2.919  
 2.912  
 2.900  
 2.888  
 2.883  
 2.875  
 2.860  
 2.852  
 2.821  
 2.813  
 2.803  
 2.795  
 2.785  
 2.776  
 2.767  
 2.759  
 2.343  
 2.342  
 2.326  
 2.310  
 2.240  
 2.226  
 2.219  
 2.209  
 2.089  
 2.088  
 2.080  
 2.072  
 2.064  
 2.055  
 2.046  
 2.041  
 2.039  
 2.030  
 2.022  
 2.012  
 2.004  
 1.996  
 1.957  
 1.934  
 1.926  
 1.911  
 1.900



3.98  
 2.00  
 2.00  
 1.98  
 2.00  
 4.08

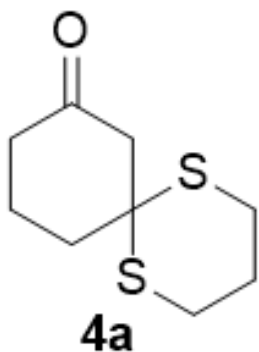
Current Data Parameters  
 NAME yl-43  
 EXPNO 2019122401  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20191224  
 Time\_ 17.23  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.125483 Hz  
 AQ 3.9845889 sec  
 RG 90.5  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 291.5 K  
 D1 1.00000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 1H  
 P1 14.80 usec  
 PL1 -1.00 dB  
 PL1W 10.90985775 W  
 SFO1 400.1724712 MHz

F2 - Processing parameters  
 SI 32768  
 SF 400.1700156 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00

— 206.17



77.32  
77.00  
76.68

52.54  
50.66

40.20  
36.42

25.98  
24.95  
21.16

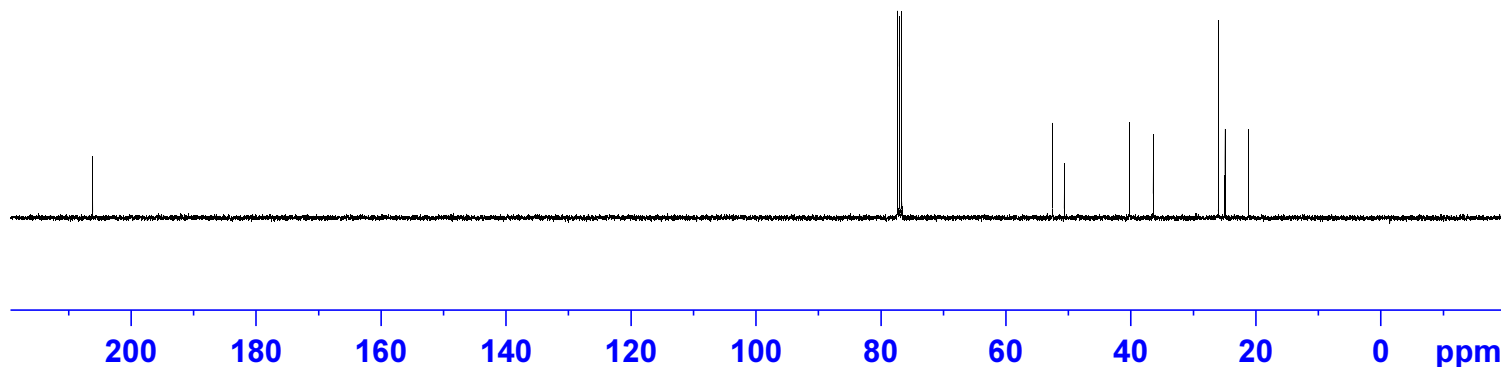
Current Data Parameters  
NAME yl-43  
EXPNO 2019122402  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20191224  
Time\_ 19.02  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 64  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 292.0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1

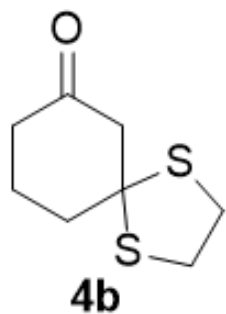
==== CHANNEL f1 =====  
NUC1 13C  
P1 9.90 usec  
PL1 -1.10 dB  
PL1W 40.29647064 W  
SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -1.00 dB  
PL12 14.68 dB  
PL13 17.68 dB  
PL2W 10.90985775 W  
PL12W 0.29499799 W  
PL13W 0.14784923 W  
SFO2 400.1716007 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6228396 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40





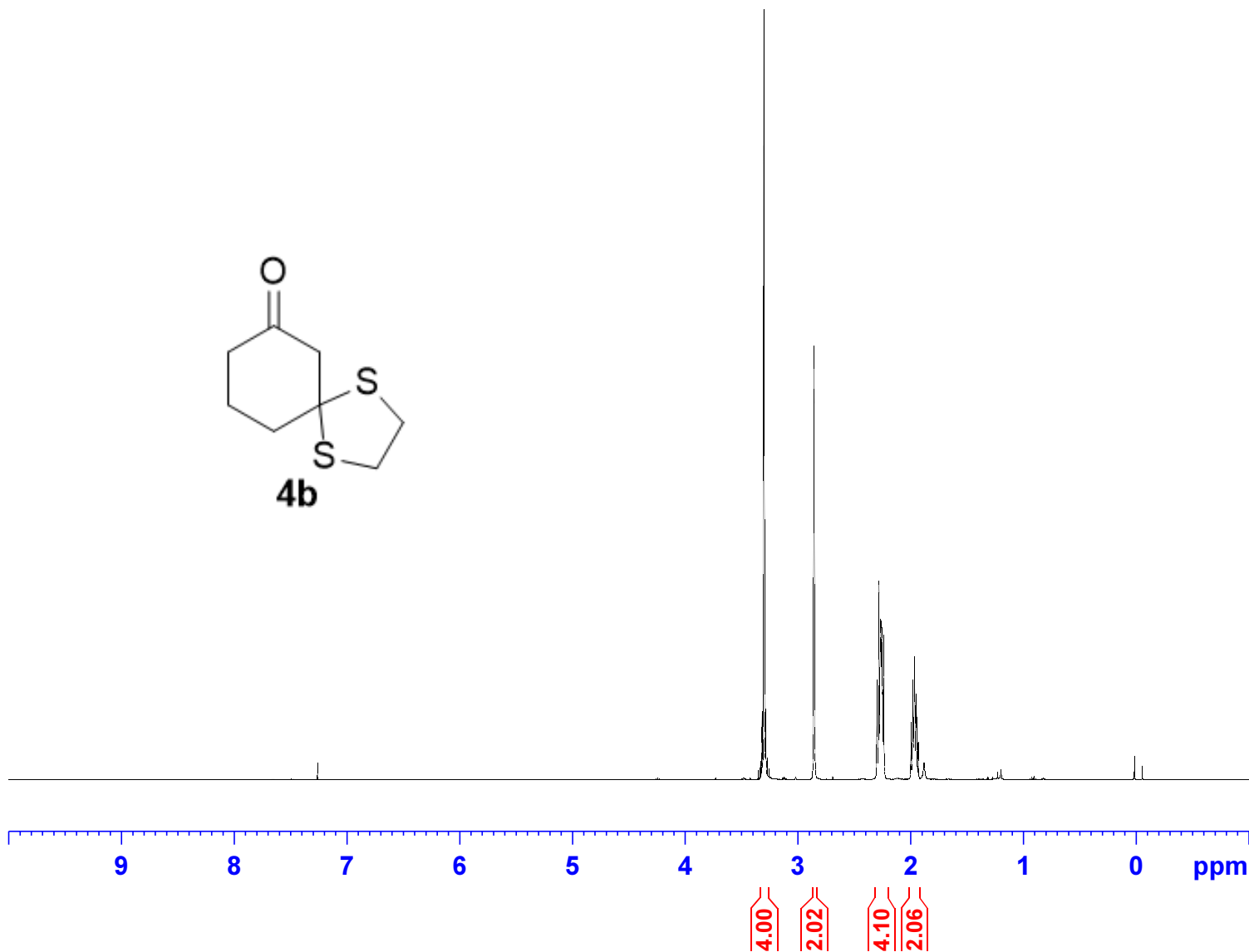


3.332  
3.317  
3.302  
3.299  
3.285  
3.270  
2.857  
2.298  
2.297  
2.281  
2.266  
2.262  
2.254  
2.249  
2.239  
1.996  
1.987  
1.981  
1.979  
1.971  
1.967  
1.963  
1.953  
1.948  
1.943  
1.933

Current Data Parameters  
NAME zjc-41 new  
EXPNO 2020070601  
PROCNO 1

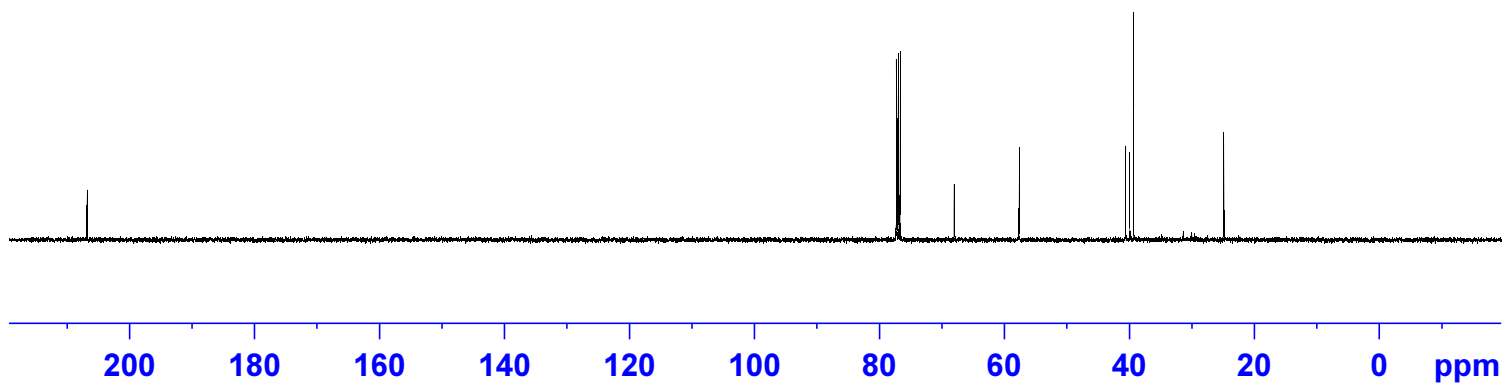
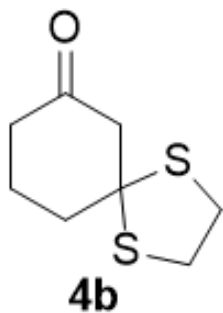
F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.32 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 45.2  
DW 60.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 206.80

77.31  
76.99  
76.68  
68.06  
57.63  
40.57  
39.94  
39.30  
24.86



Current Data Parameters  
NAME zjc-41  
EXPNO 2019122402  
PROCNO 1

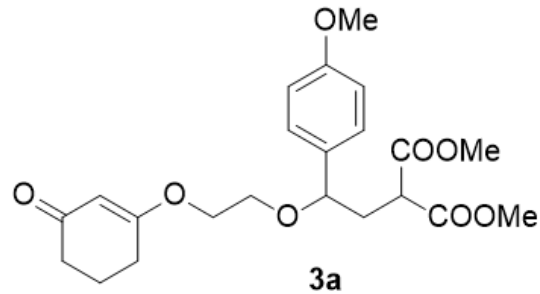
F2 - Acquisition Parameters  
Date\_ 20191224  
Time\_ 18.57  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 56  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 2050  
DW 20.800 usec  
DE 6.50 usec  
TE 292.1 K  
D1 2.0000000 sec  
D11 0.03000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 13C  
P1 9.90 usec  
PL1 -1.10 dB  
PL1W 40.29647064 W  
SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
CPDPRG[2] waltz16  
NUC2 1H  
PCPD2 90.00 usec  
PL2 -1.00 dB  
PL12 14.68 dB  
PL13 17.68 dB  
PL2W 10.90985775 W  
PL12W 0.29499799 W  
PL13W 0.14784923 W  
SFO2 400.1716007 MHz

F2 - Processing parameters  
SI 32768  
SF 100.6228410 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

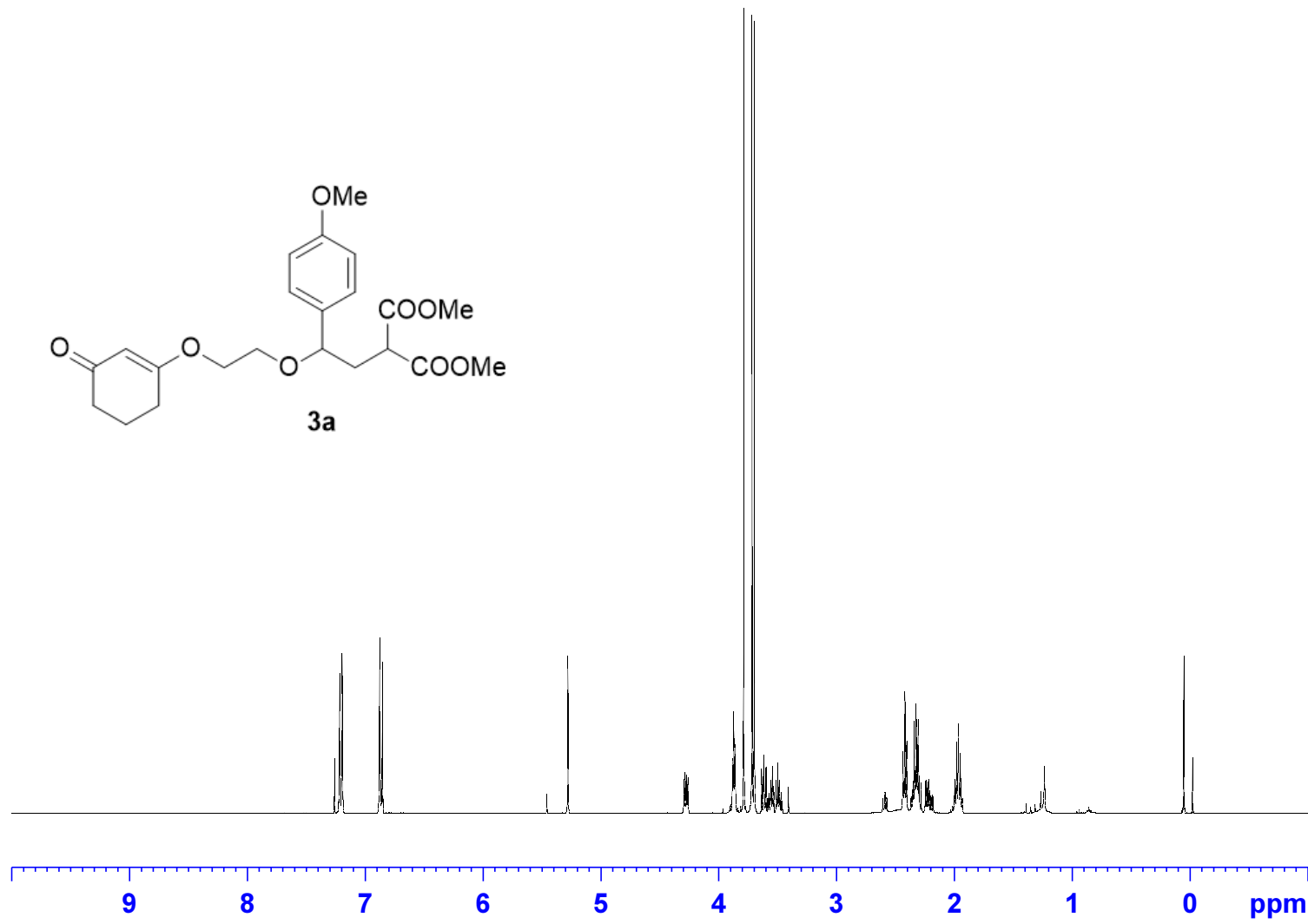
7.260  
7.217  
7.195  
6.877  
6.855  
5.280  
4.295  
4.284  
4.272  
4.261  
3.883  
3.871  
3.859  
3.788  
3.718  
3.697  
3.635  
3.619  
3.614  
3.599  
3.556  
3.545  
3.511  
3.499  
3.487  
2.435  
2.420  
2.404  
2.350  
2.340  
2.333  
2.325  
2.321  
2.307  
2.297  
2.281  
2.246  
2.235  
2.226  
2.214  
1.997  
1.981  
1.965  
1.948



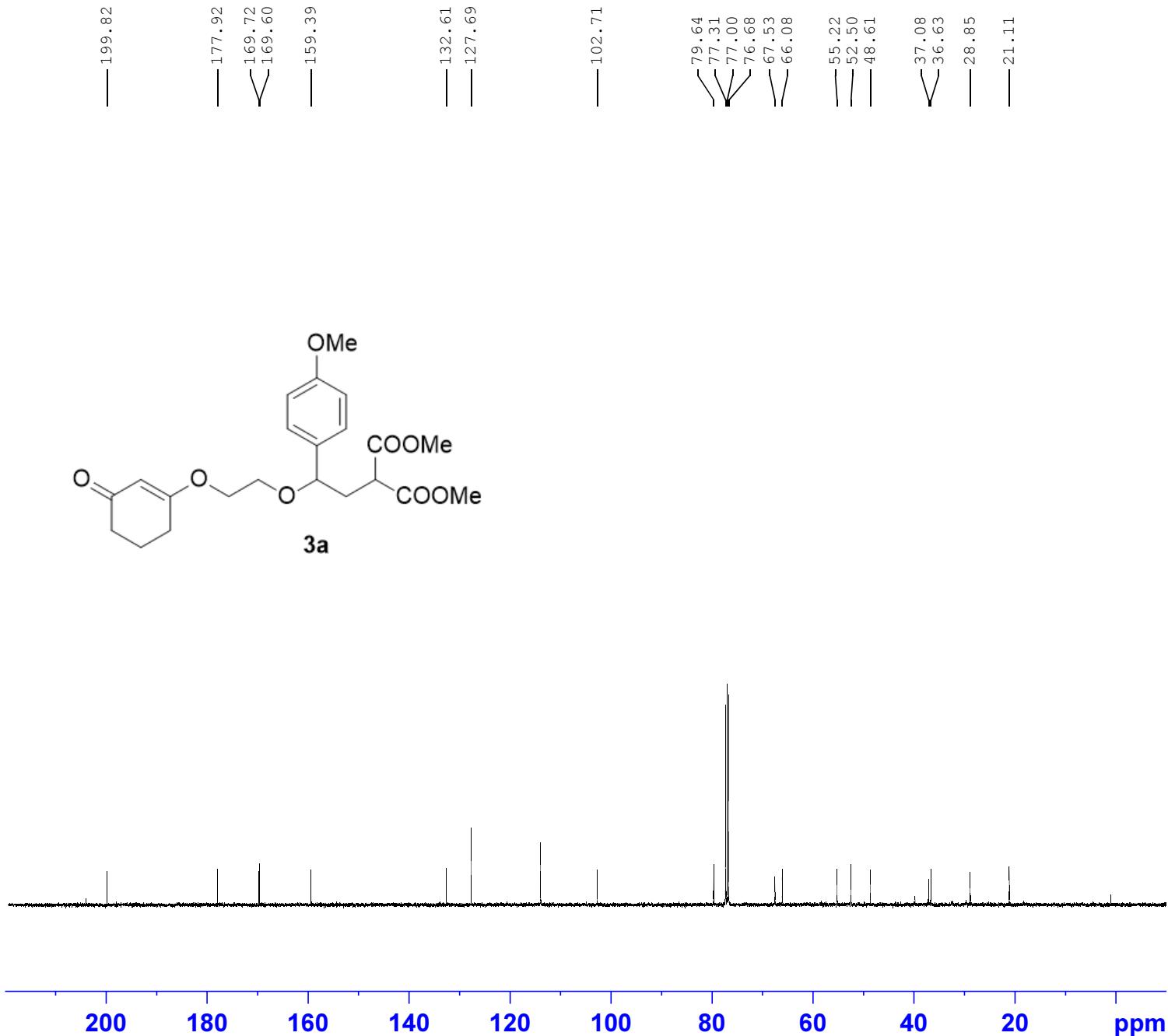
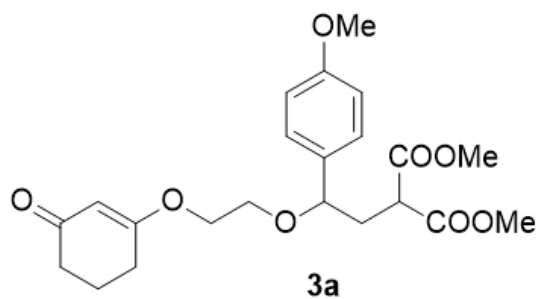
Current Data Parameters  
NAME zjc-4 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time 1.12 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



2.00  
2.01  
1.00  
1.03  
2.10  
3.01  
3.01  
2.99  
1.02  
1.02  
1.02  
2.19  
3.13  
1.09  
2.36

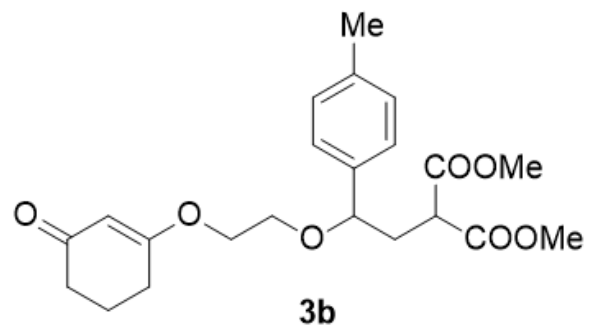


Current Data Parameters  
 NAME zjc-4 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 3.13 h  
 INSTRUM spect  
 PROBHD z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 138  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228337 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

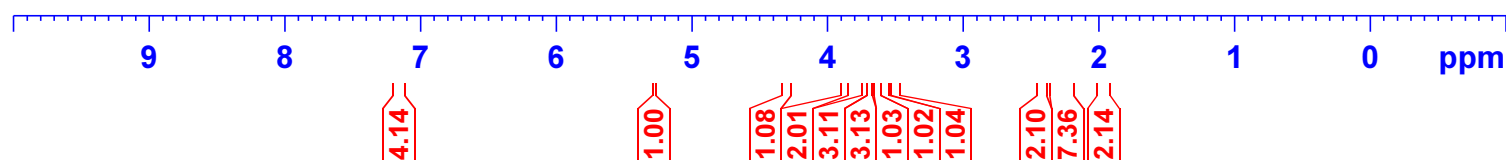
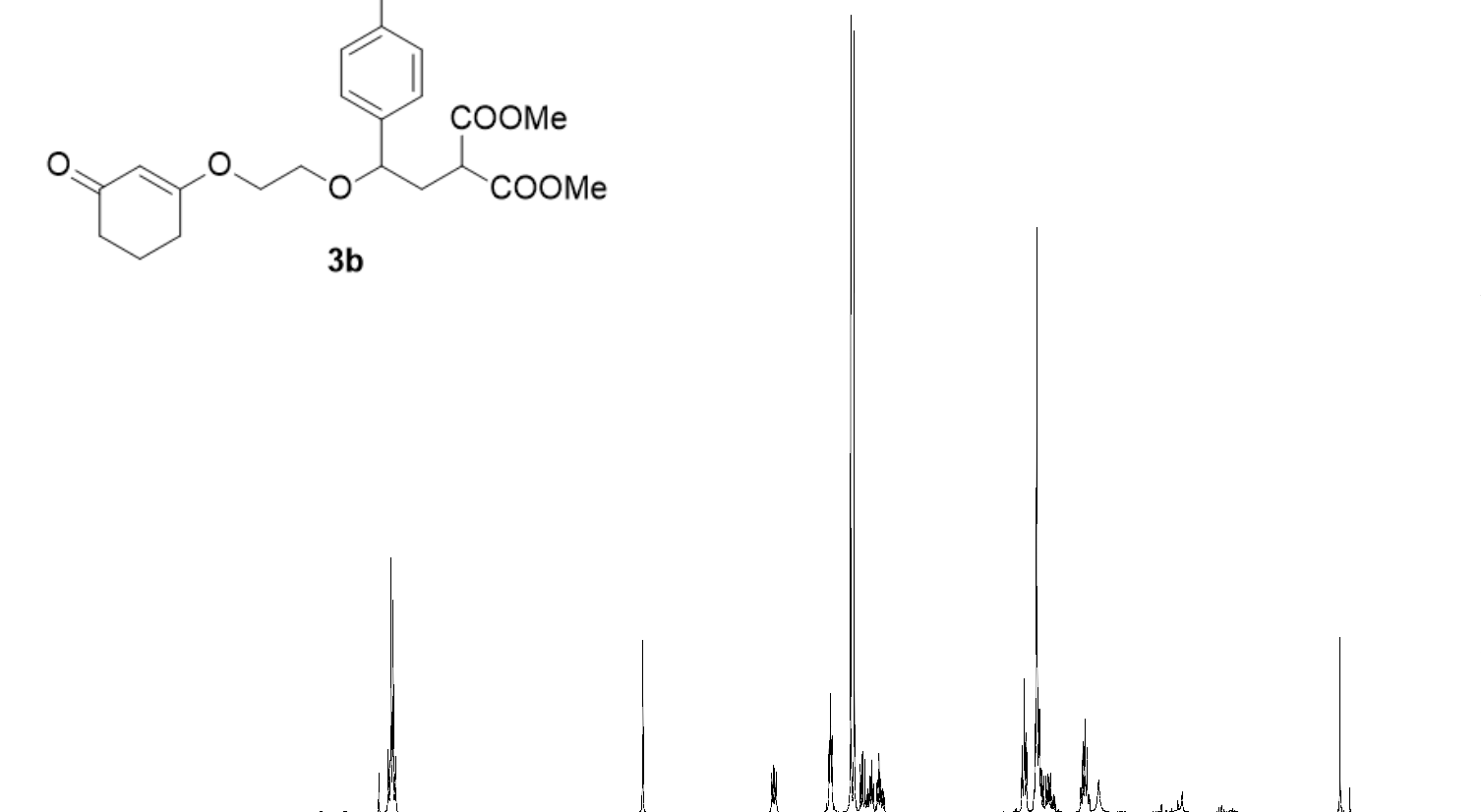
7.259  
7.189  
7.174  
7.154  
7.134  
5.281  
4.315  
4.304  
4.292  
4.281  
3.886  
3.874  
3.862  
3.722  
3.696  
3.651  
3.636  
3.631  
3.615  
3.575  
3.564  
3.552  
3.522  
3.510  
3.499  
2.437  
2.422  
2.406  
2.341  
2.327  
2.315  
2.308  
2.300  
2.292  
2.276  
2.259  
2.248  
2.238  
2.227  
2.223  
1.999  
1.983  
1.966  
1.950

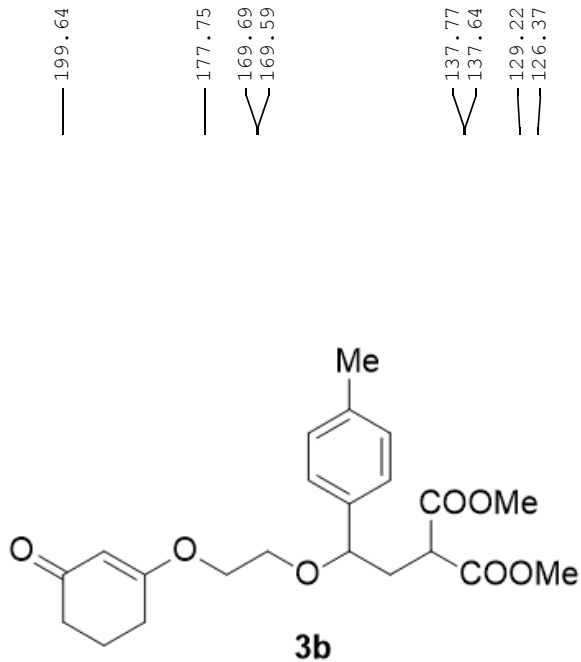


Current Data Parameters  
NAME yl-12 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200706  
Time\_ 23.58 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



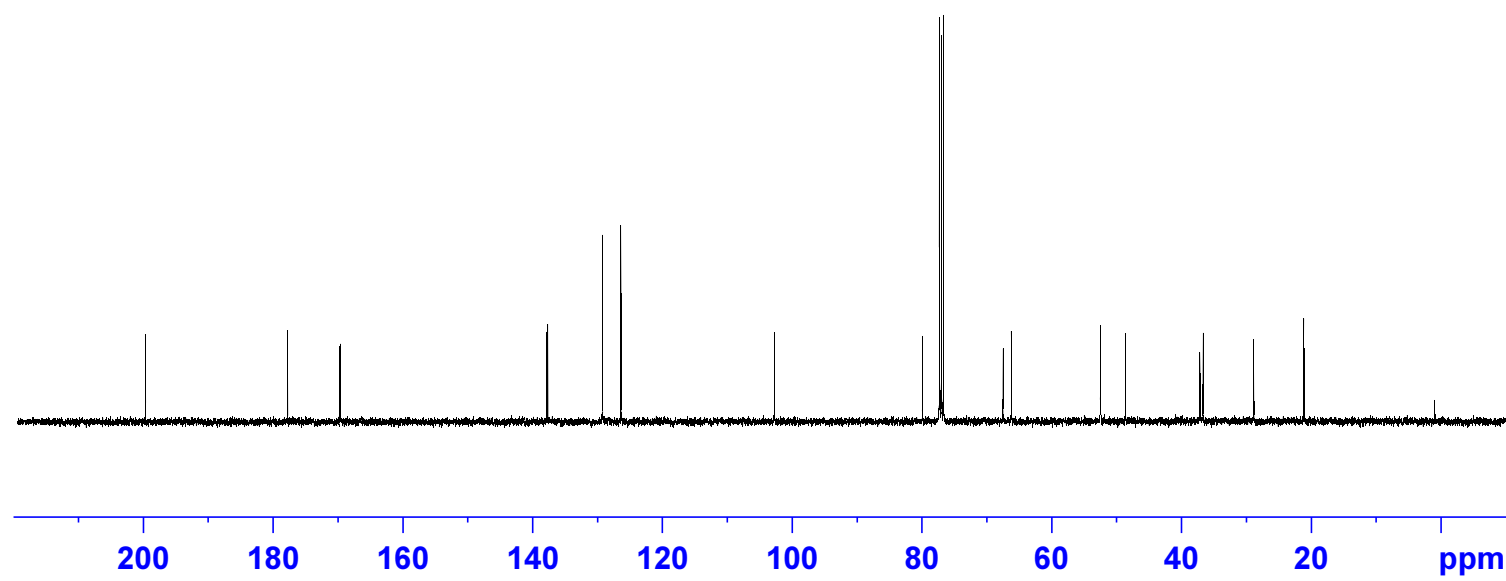


— 199.64  
 — 177.75  
 — 169.69  
 — 169.59  
 — 137.77  
 — 137.64  
 — 129.22  
 — 126.37  
 — 102.73  
 — 79.91  
 — 77.31  
 — 76.99  
 — 76.67  
 — 67.49  
 — 66.23  
 — 52.48  
 — 52.46  
 — 48.59  
 — 37.12  
 — 36.66  
 — 28.84  
 — 21.11  
 — 21.06

Current Data Parameters  
 NAME yl-12 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time 2.10 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 153  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.0000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

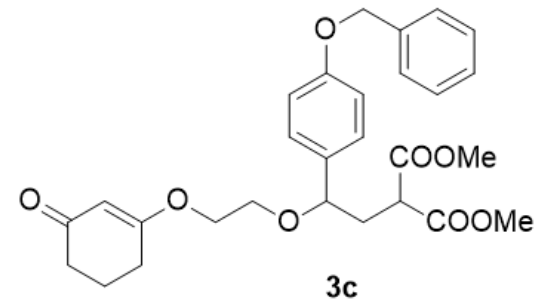
F2 - Processing parameters  
 SI 32768  
 SF 100.6228344 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



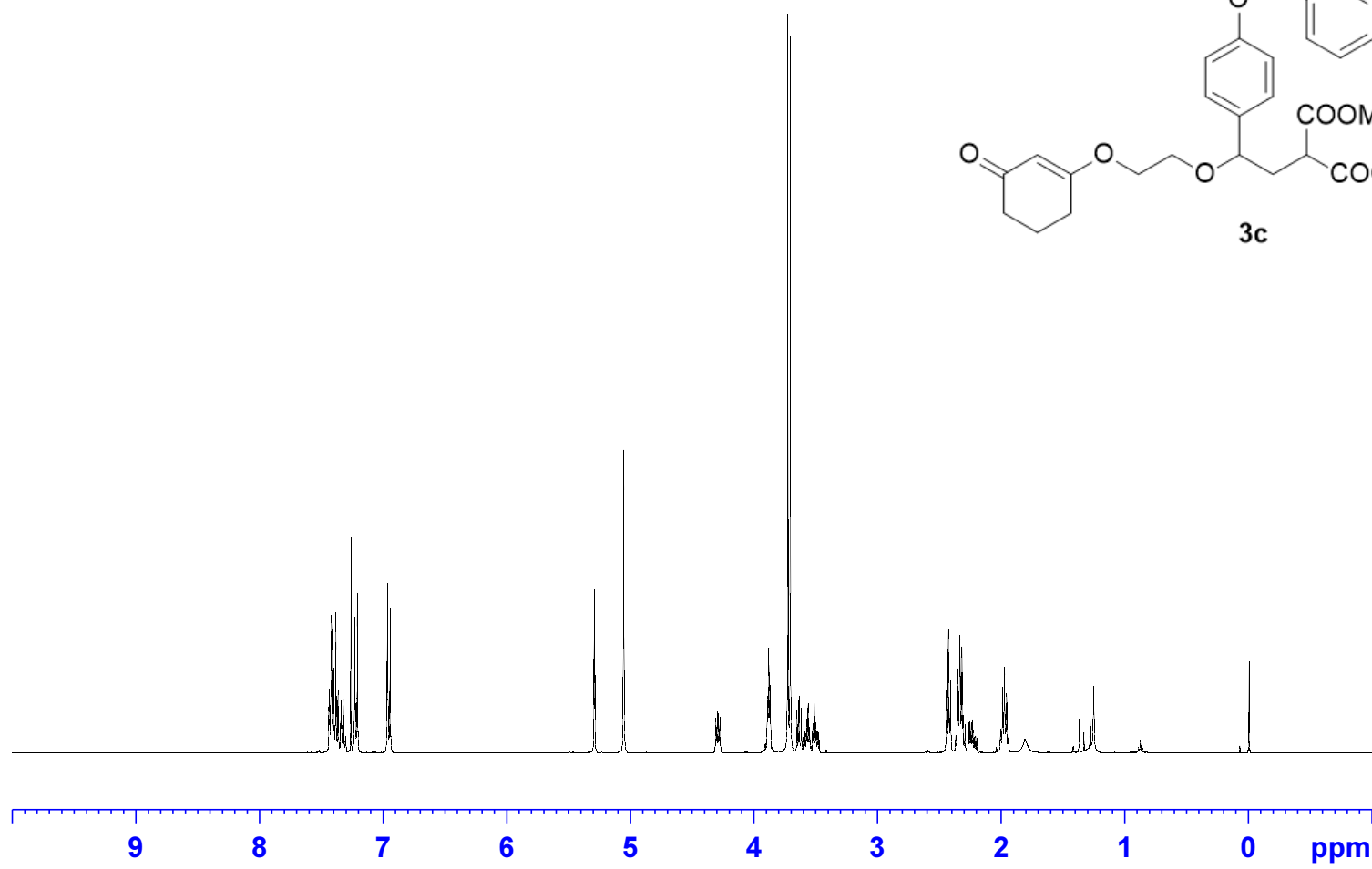
7.439  
7.435  
7.418  
7.402  
7.399  
7.382  
7.378  
7.363  
7.339  
7.321  
7.260  
7.230  
7.225  
7.208  
6.964  
6.959  
6.947  
6.943  
5.291  
5.053  
4.297  
4.285  
3.890  
3.879  
3.867  
3.725  
3.704  
3.652  
3.636  
3.631  
3.615  
3.560  
3.510  
2.440  
2.424  
2.409  
2.349  
2.343  
2.334  
2.331  
2.316  
1.987  
1.971  
1.955

Current Data Parameters  
NAME: yl-13  
2019051701  
O 1

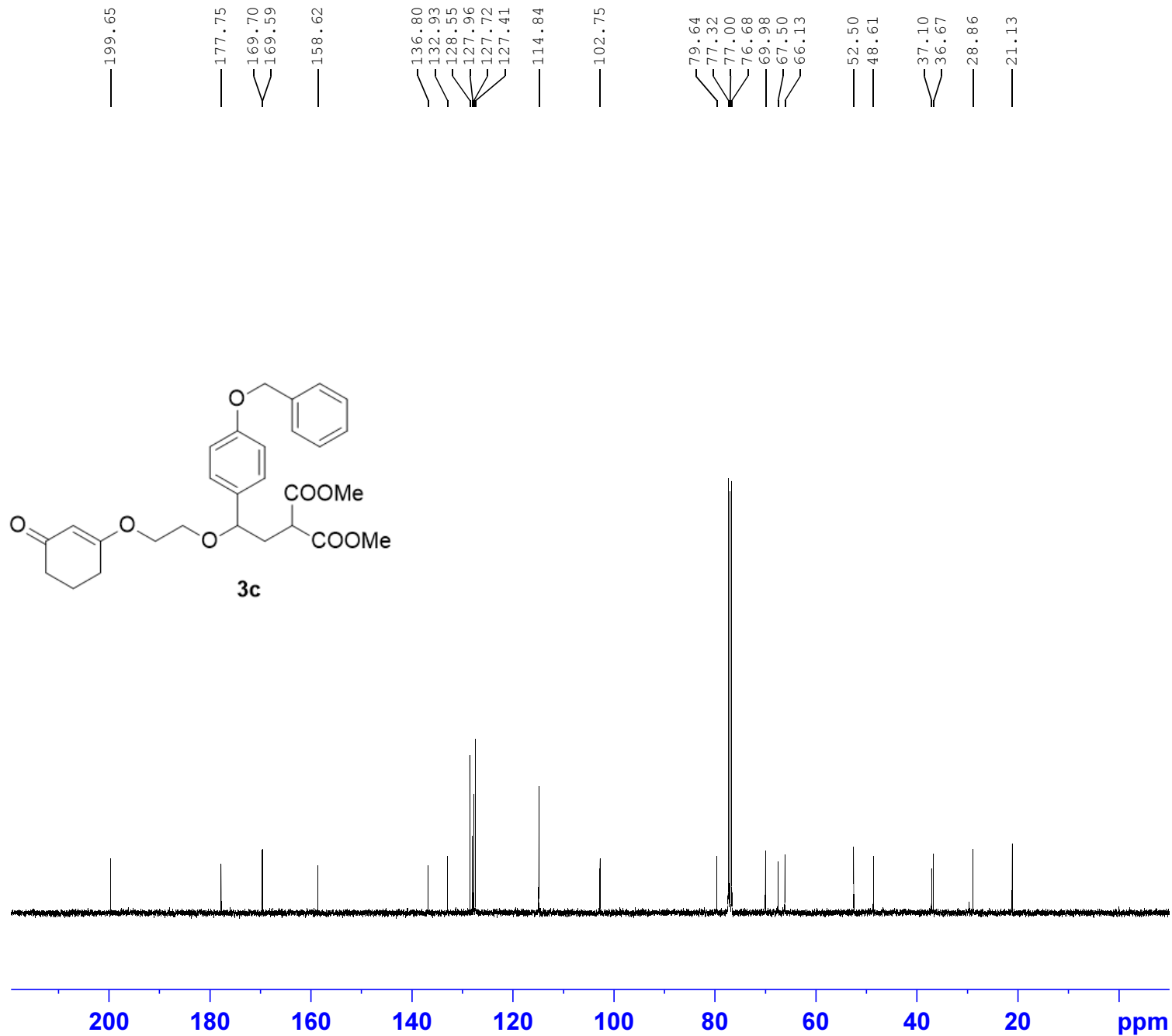
Acquisition Parameters  
20190517  
16.06  
UM spect  
D 5 mm PABBO BB-  
OG zg30  
65536  
NT CDC13  
16  
2  
8223.685 Hz  
0.125483 Hz  
3.9845889 sec  
28.5  
60.800 usec  
6.50 usec  
296.2 K  
--  
D1 1.00000000 sec  
TD0 1



==== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz  
  
F2 - Processing parameters  
SI 32768  
SF 400.1700158 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



4.92  
1.95  
1.93  
  
1.16  
1.95  
  
1.00  
2.02  
2.88  
2.96  
0.97  
1.00  
0.98  
  
1.99  
2.94  
1.04  
2.05



Current Data Parameters  
 NAME yl-13  
 EXPNO 2019051702  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190517  
 Time\_ 16.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 192  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

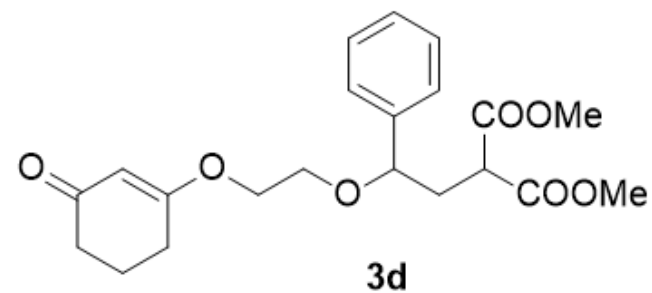
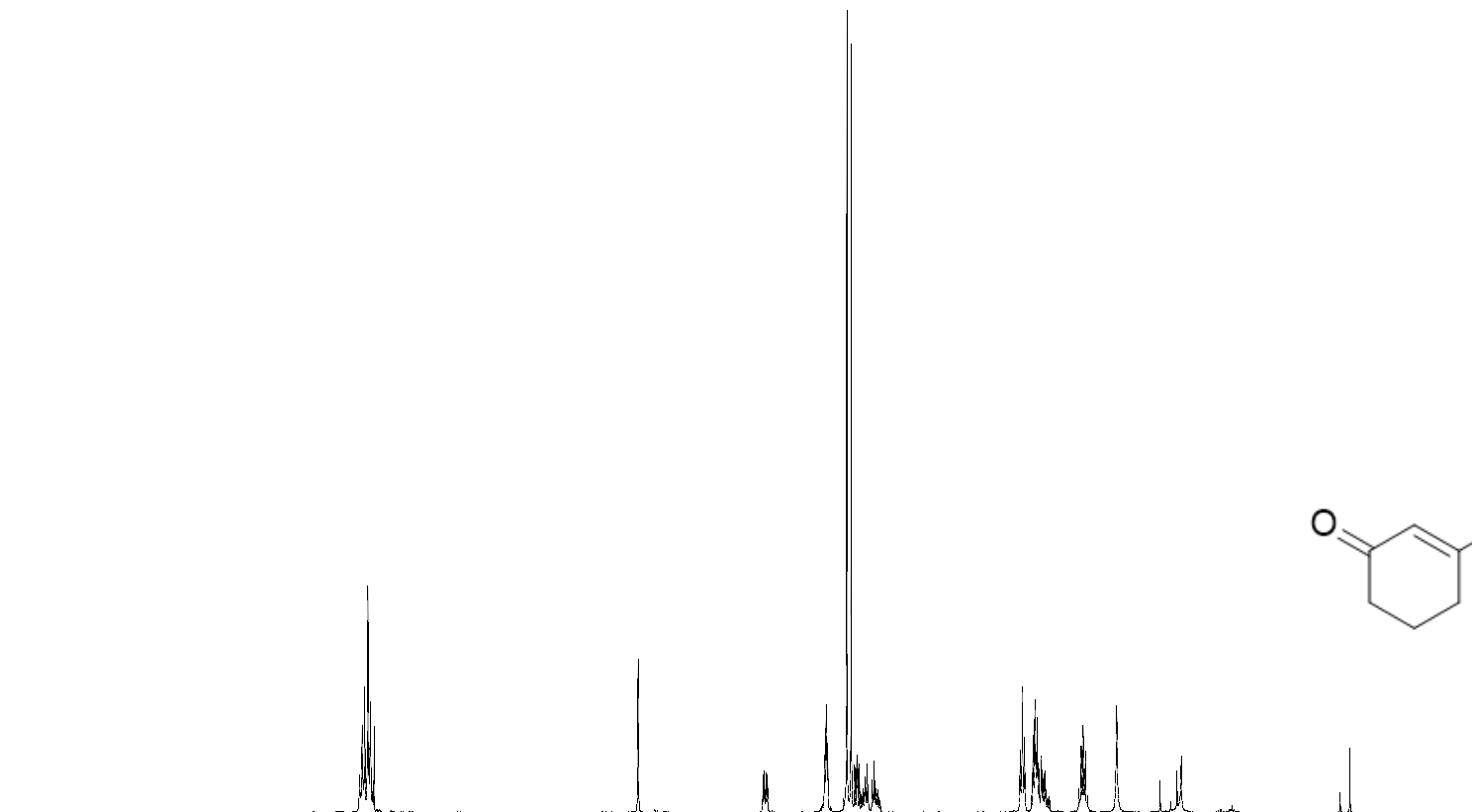
F2 - Processing parameters  
 SI 32768  
 SF 100.6228359 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



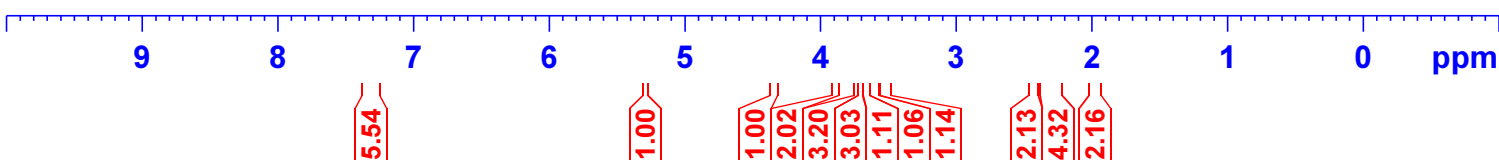
7.368  
7.349  
7.347  
7.332  
7.306  
7.300  
7.293  
7.289  
7.260  
5.292  
4.363  
4.352  
4.340  
4.329  
3.903  
3.892  
3.880  
3.738  
3.705  
3.679  
3.664  
3.658  
3.643  
3.601  
3.590  
3.536  
2.445  
2.429  
2.414  
2.351  
2.335  
2.327  
2.318  
2.312  
2.304  
2.290  
2.280  
2.270  
2.259  
1.992  
1.976  
1.960  
1.280  
1.245

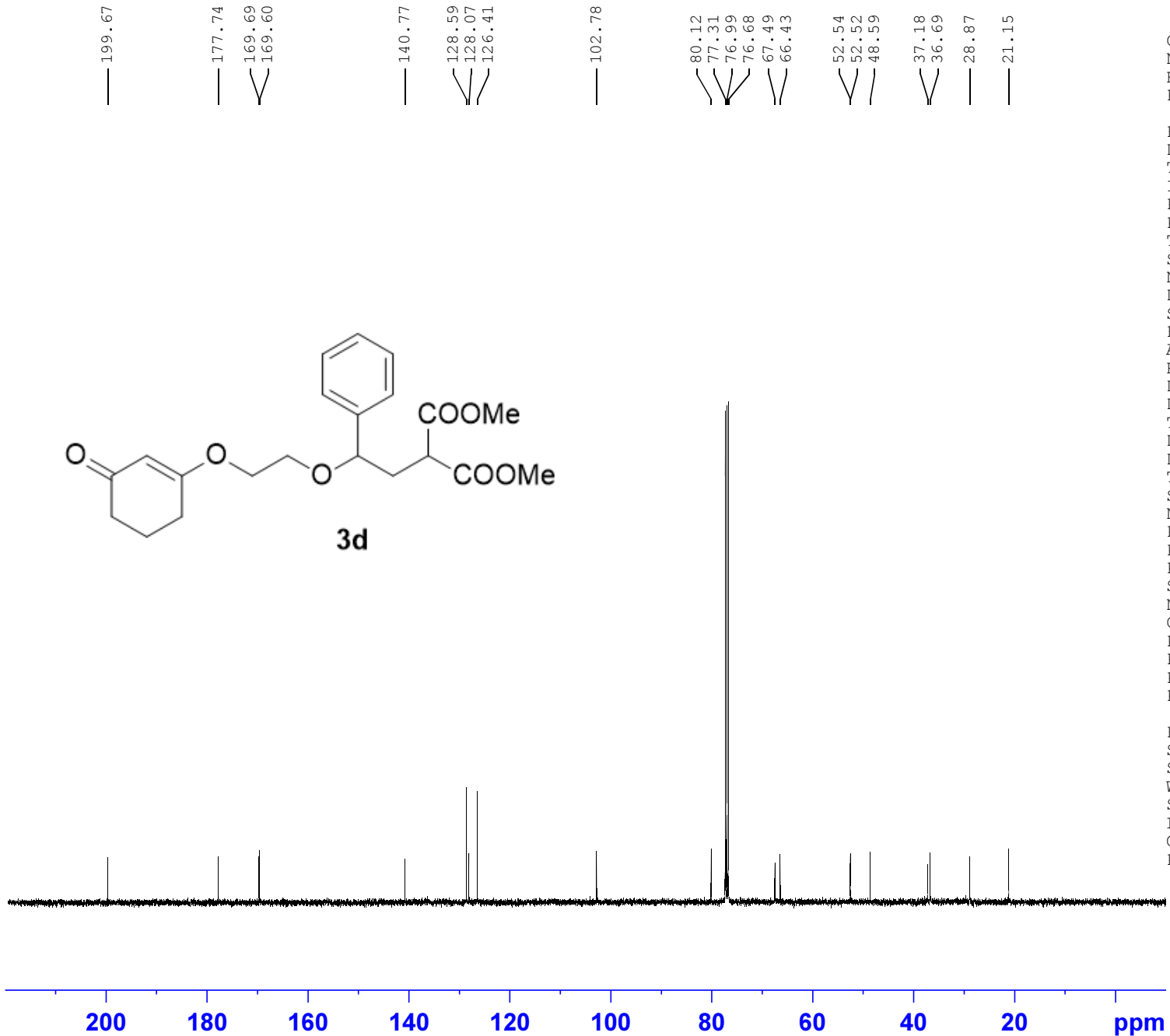
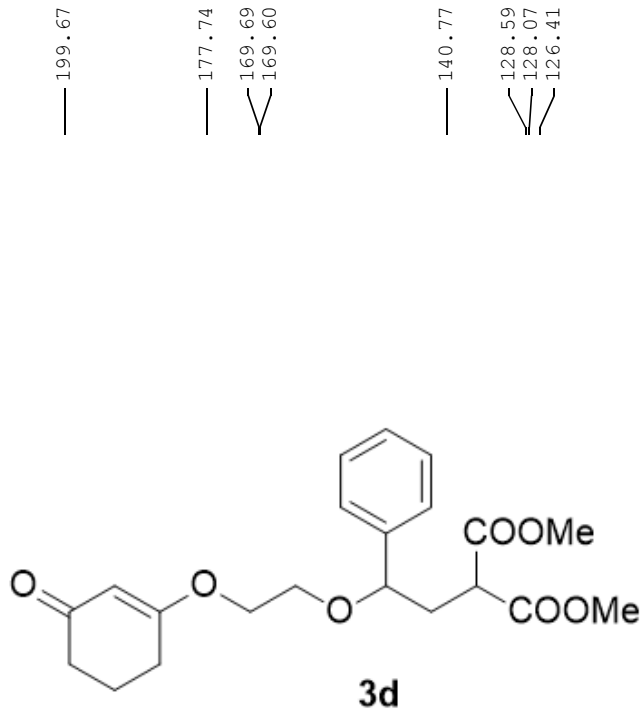
Current Data Parameters  
 NAME zjc-52 new rep  
 EXPNO 2020070902  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200710  
 Time\_ 0.57 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 0.0845880 sec



FC 1.00



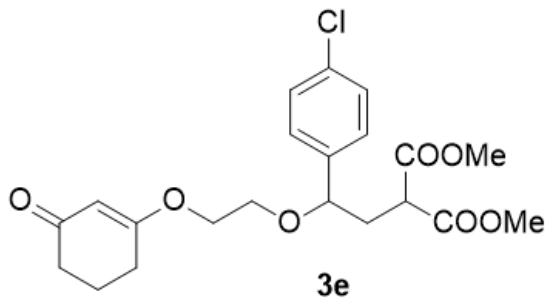


Current Data Parameters  
 NAME zjc-52 new rep  
 EXPNO 2020070903  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200710  
 Time\_ 2.00 h  
 INSTRUM spect  
 PROBHD z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 307  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.0000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228315 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

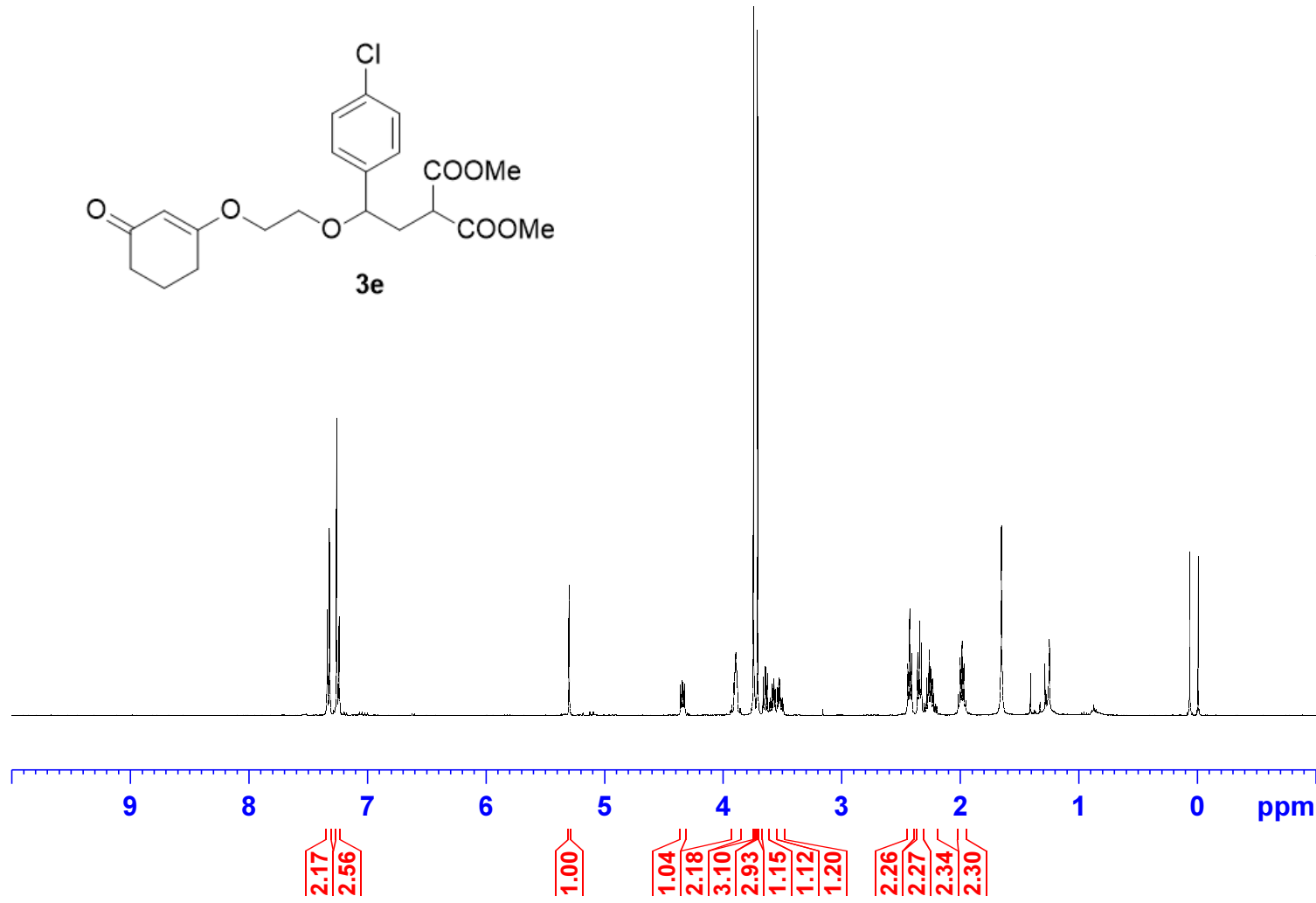
7.341  
7.336  
7.325  
7.320  
7.314  
7.265  
7.255  
7.243  
7.239  
5.298  
4.347  
4.336  
3.908  
3.898  
3.893  
3.888  
3.885  
3.879  
3.743  
3.710  
3.662  
3.647  
3.641  
3.626  
3.573  
3.531  
3.529  
3.519  
2.441  
2.425  
2.410  
2.359  
2.344  
2.326  
2.284  
2.269  
2.262  
2.249  
2.247  
2.240  
2.229  
2.000  
1.984  
1.968



Current Data Parameters  
NAME zjc-53 new rep  
EXPNO 2020070901  
PROCNO 1

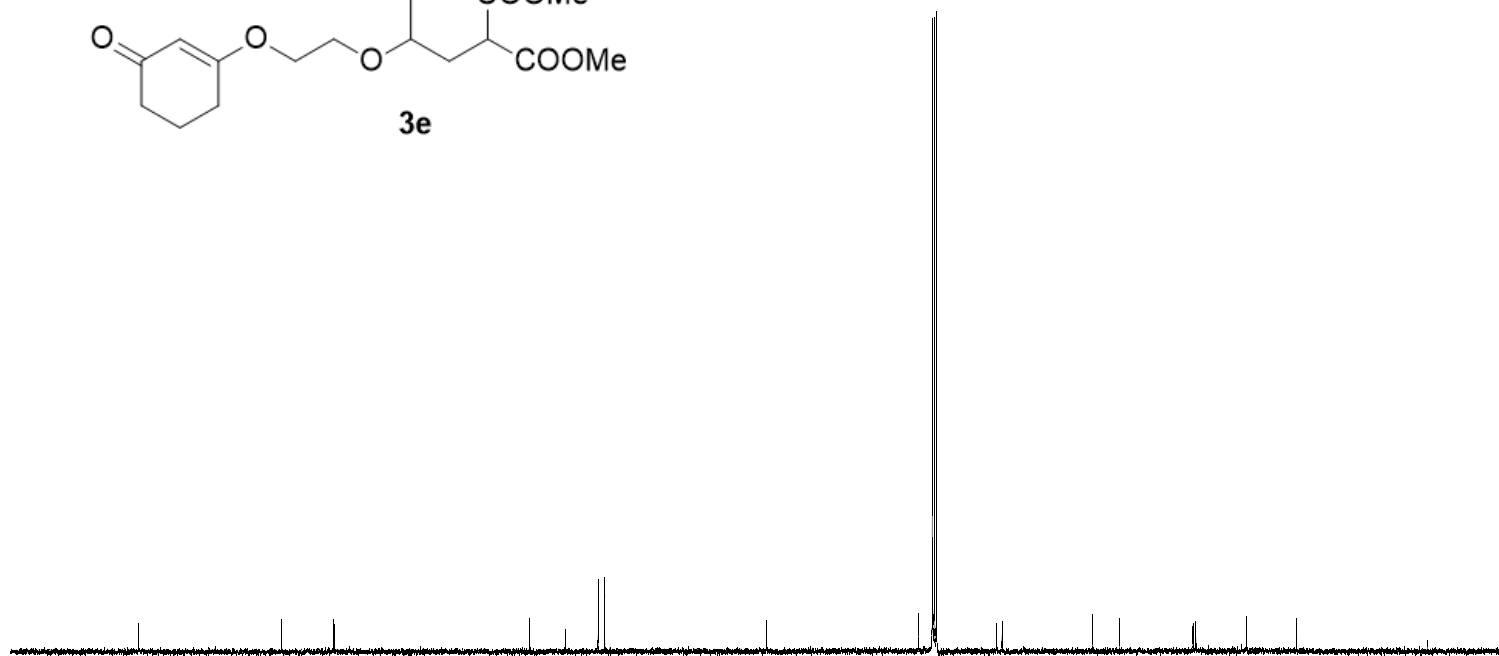
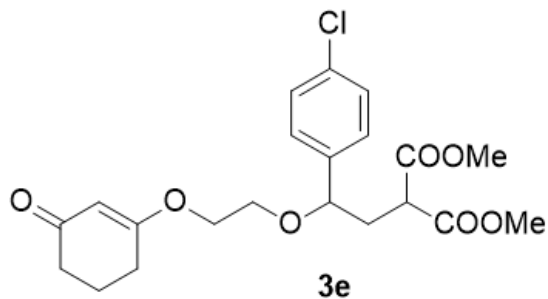
F2 - Acquisition Parameters  
Date\_ 20200710  
Time\_ 1.01 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 203  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 199.64  
 — 177.62  
 — 169.58  
 — 169.51  
 — 139.37  
 — 133.82  
 — 128.82  
 — 127.80  
 — 102.85

79.47  
 77.31  
 76.99  
 76.68  
 67.42  
 66.57  
 — 52.61  
 — 48.45  
 37.13  
 36.70  
 — 28.87  
 — 21.16



Current Data Parameters  
 NAME zjc-53 new rep  
 EXPNO 2020070903  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200710  
 Time\_ 2.35 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 522  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228300 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

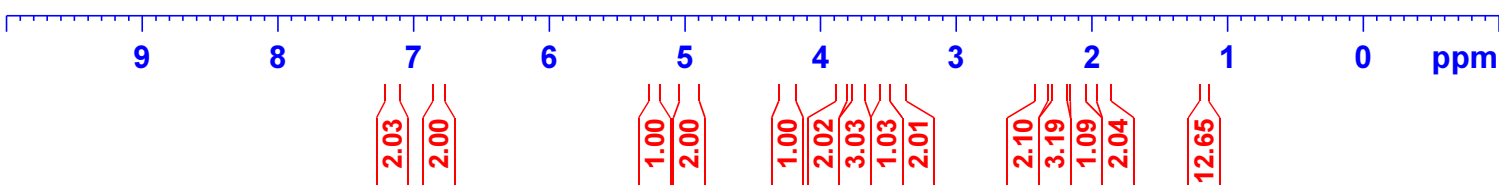
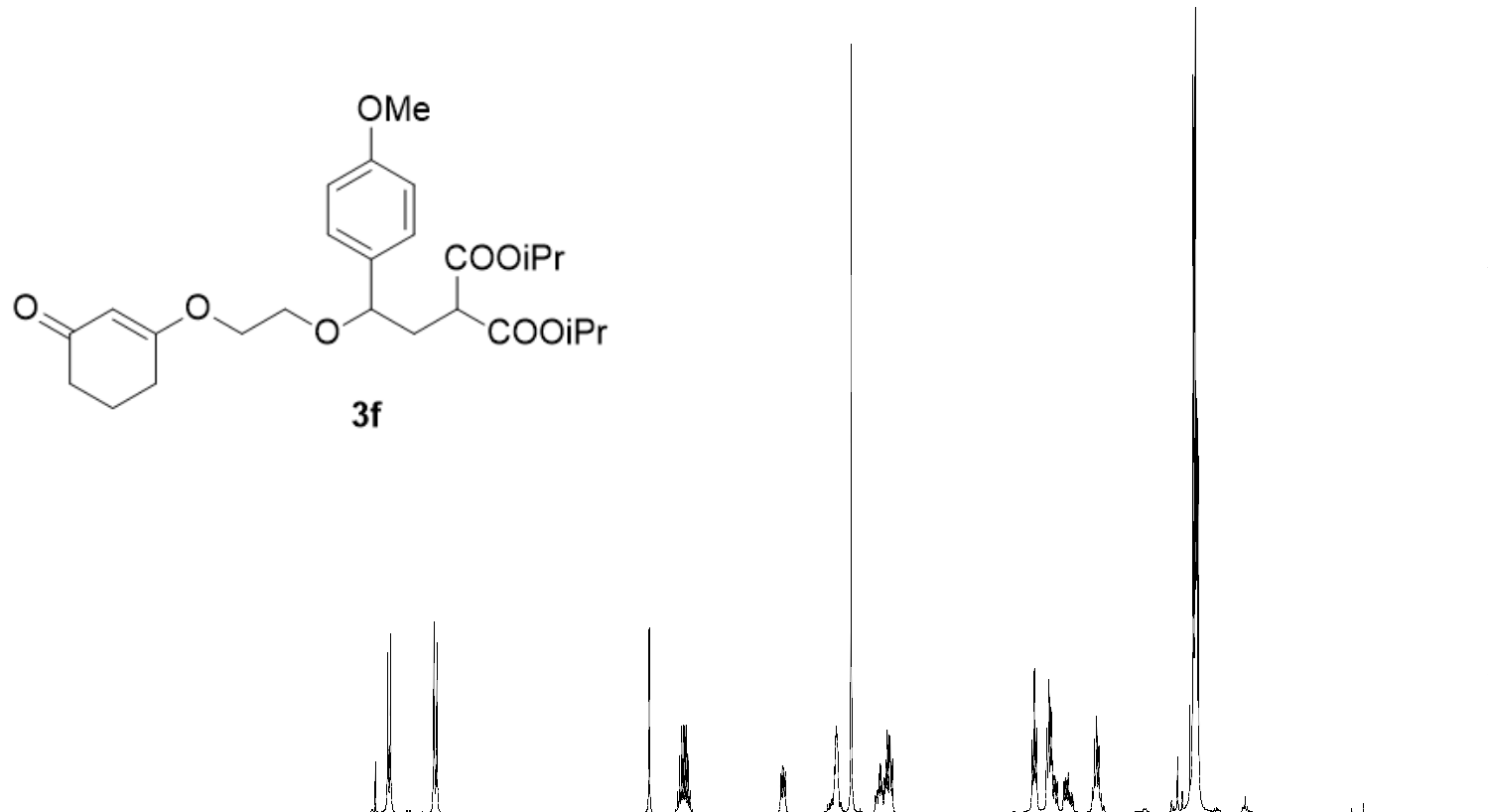
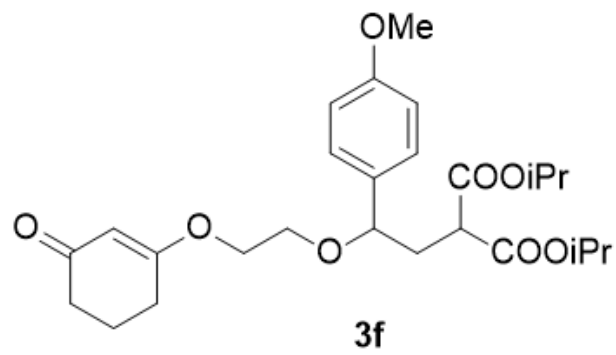
7.260  
7.169  
7.148  
6.826  
6.804  
5.227  
5.000  
4.985  
4.970  
4.955  
4.939  
4.250  
4.239  
4.227  
4.216  
3.851  
3.842  
3.837  
3.831  
3.822  
3.727  
3.509  
3.506  
3.468  
3.458  
3.443  
3.437  
3.421  
2.382  
2.367  
2.351  
2.275  
2.259  
2.247  
2.242  
2.235  
2.116  
1.920  
1.904  
1.888  
1.188  
1.172  
1.164  
1.148

Current Data Parameters  
NAME yl--15  
EXPNO 2019052001  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190521  
Time\_ 0.13  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 64  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz

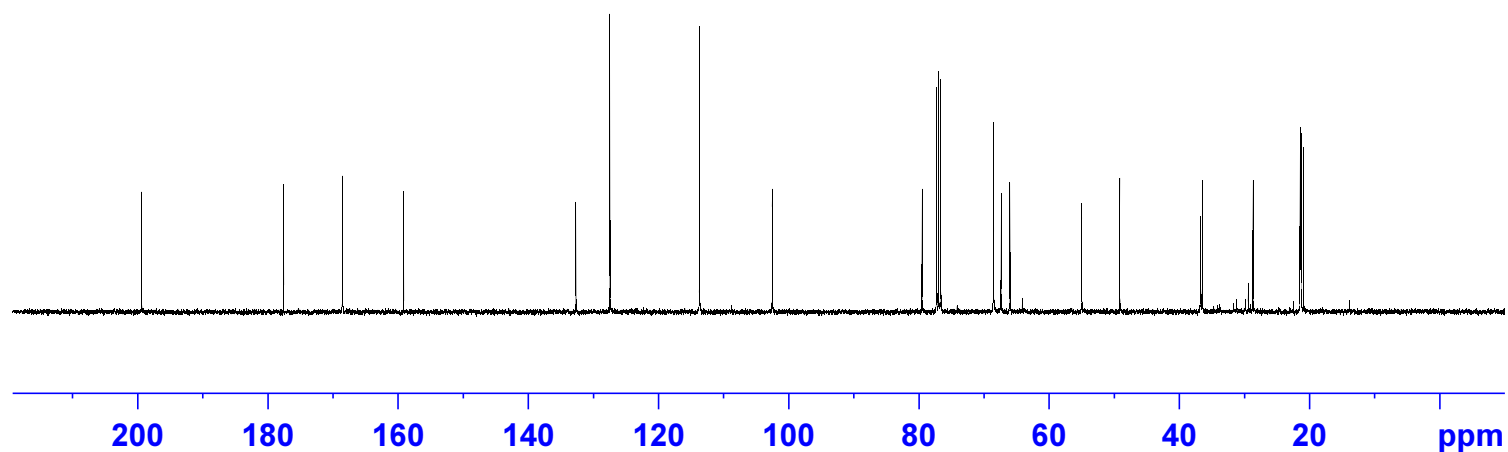
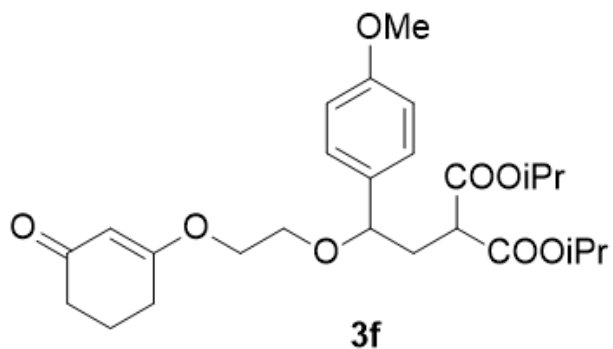
F2 - Processing parameters  
SI 32768  
SF 400.1700147 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



199.40  
 177.59  
 168.60  
 168.53  
 159.16  
 132.71  
 127.49  
 113.72  
 102.54

79.53  
 77.31  
 77.00  
 76.68  
 68.55  
 68.53  
 67.37  
 66.02  
 55.00  
 49.14

36.76  
 36.48  
 28.69  
 21.46  
 21.40  
 21.35  
 21.30  
 20.94



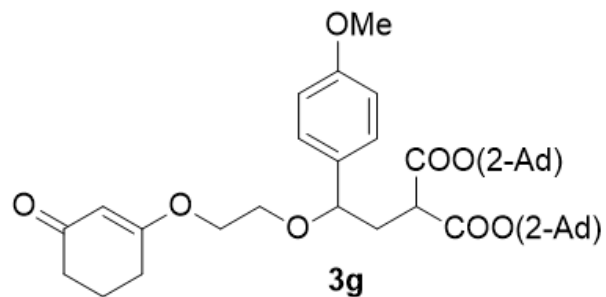
Current Data Parameters  
 NAME yl-15  
 EXPNO 2019052002  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190521  
 Time\_ 0.51  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 105  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228484 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.228  
7.207  
6.887  
6.866  
5.277  
4.975  
4.950  
4.312  
4.300  
4.289  
4.277  
3.895  
3.886  
3.882  
3.878  
3.873  
3.864  
3.796  
3.638  
3.622  
3.617  
3.601  
3.555  
3.521  
2.438  
2.423  
2.407  
2.338  
2.323  
2.305  
1.977  
1.962  
1.946  
1.855  
1.848  
1.826  
1.806

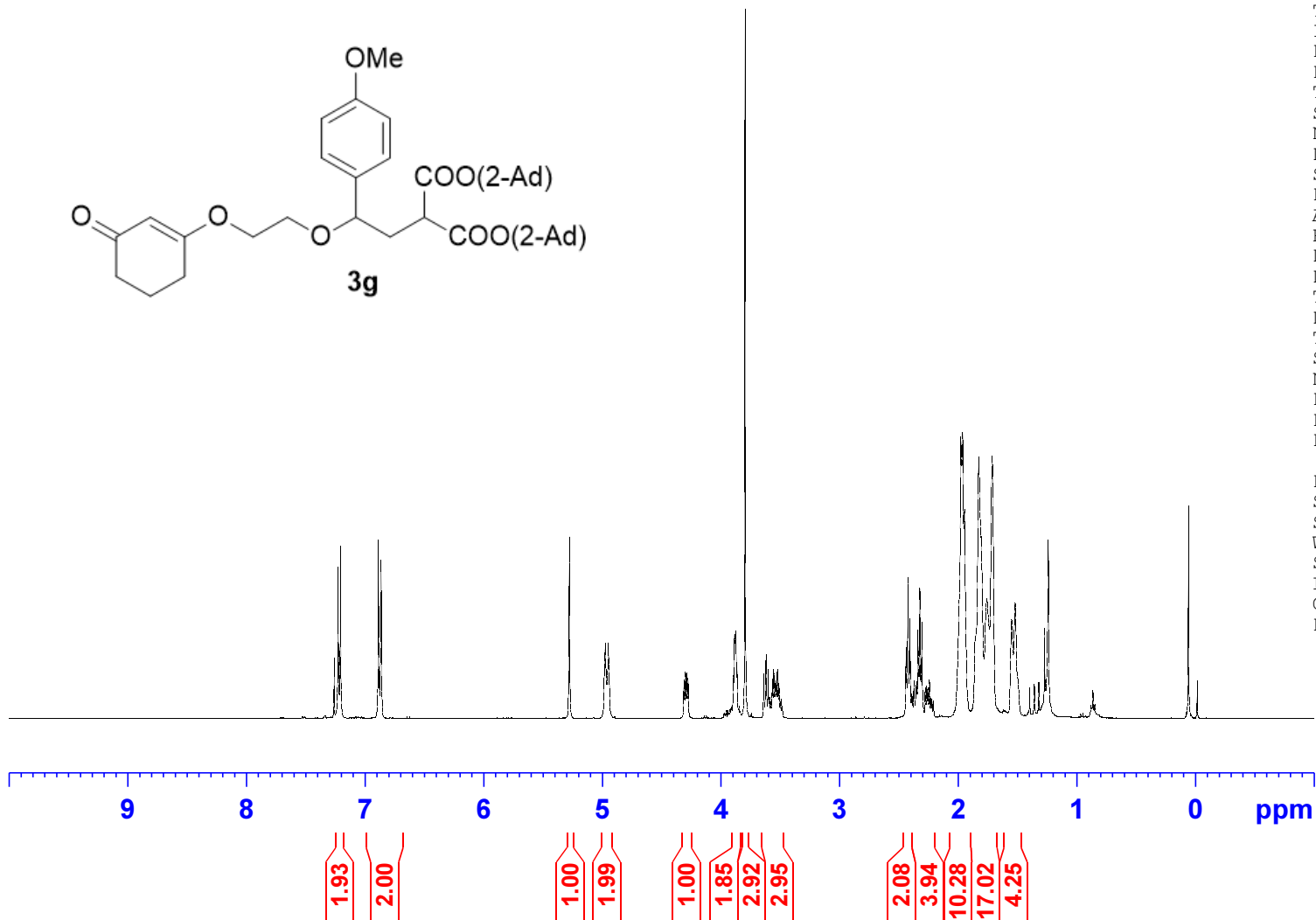
Current Data Parameters  
NAME yl-18 rep  
EXPNO 2020070201  
PROCNO 1

F2 - Acquisition Parameters

Date\_ 20200702  
Time\_ 23.49 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 101  
DW 60.800 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

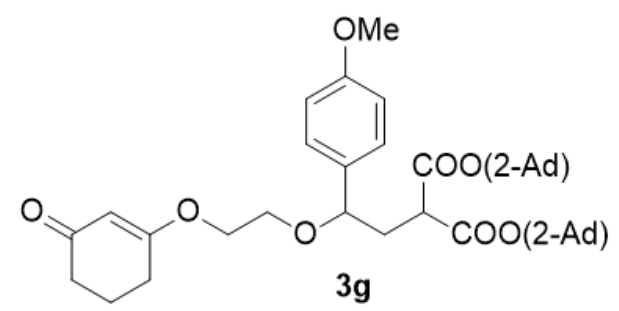
F2 - Processing parameters

SI 32768  
SF 400.1700087 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 199.66  
 — 177.78  
 — 168.67  
 — 168.64  
 — 159.36  
 — 132.90  
 — 127.74  
 — 113.94  
 — 102.74

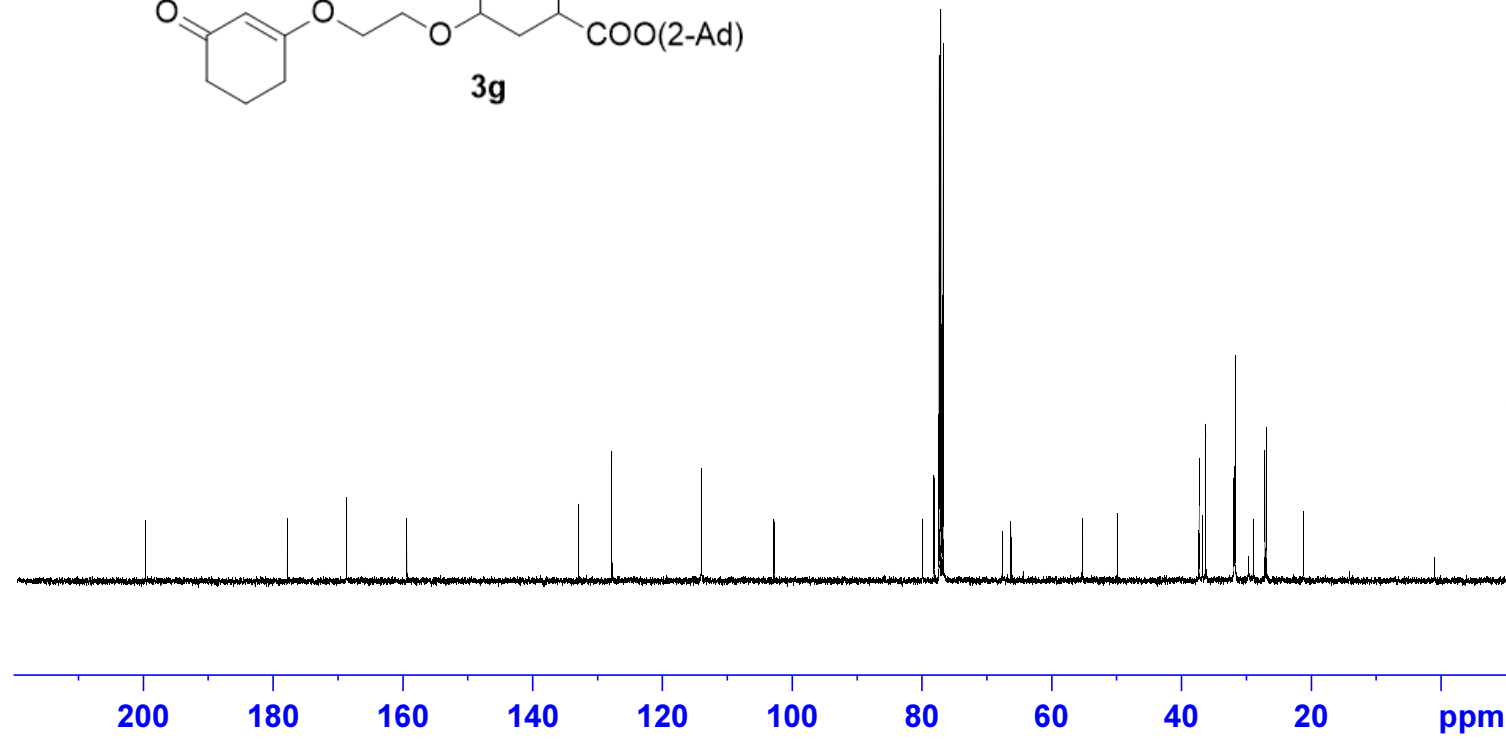
79.86  
 78.07  
 78.06  
 77.31  
 77.00  
 76.68  
 67.57  
 66.23  
 55.22  
 49.85  
 37.20  
 37.18  
 36.68  
 36.22  
 36.18  
 31.86  
 31.81  
 31.78  
 31.67  
 29.62  
 28.88  
 27.07  
 26.83  
 21.13



Current Data Parameters  
 NAME yl-18 rep  
 EXPNO 2020070202  
 PROCNO 1

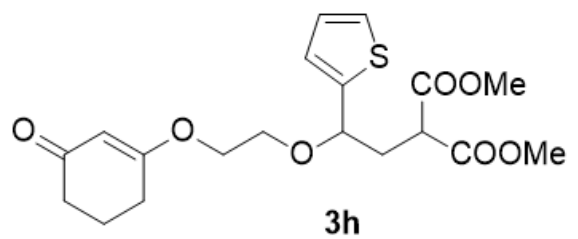
F2 - Acquisition Parameters  
 Date\_ 20200703  
 Time\_ 1.08 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 310  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228330 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40





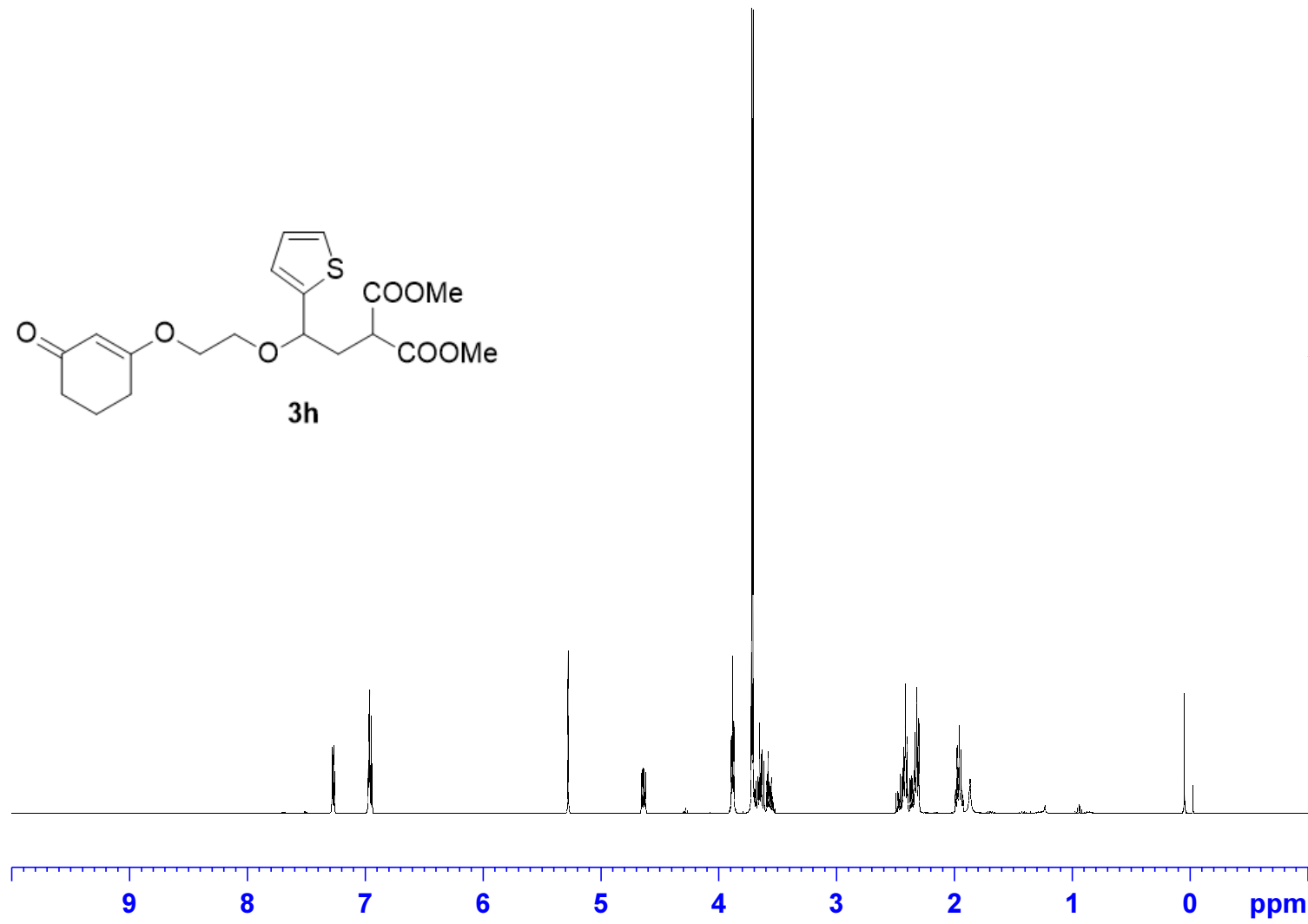
7.282  
7.279  
7.270  
7.266  
7.260  
6.974  
6.969  
6.966  
6.961  
6.952  
6.948  
6.940  
5.278  
4.656  
4.644  
4.633  
4.621  
3.893  
3.882  
3.870  
3.721  
3.709  
3.665  
3.653  
3.636  
3.631  
3.616  
3.581  
2.458  
2.435  
2.430  
2.419  
2.415  
2.399  
2.362  
2.342  
2.338  
2.334  
2.318  
2.306  
2.301  
1.975  
1.959  
1.942



Current Data Parameters  
NAME yl-10 new  
EXPNO 2020070602  
PROCNO 1

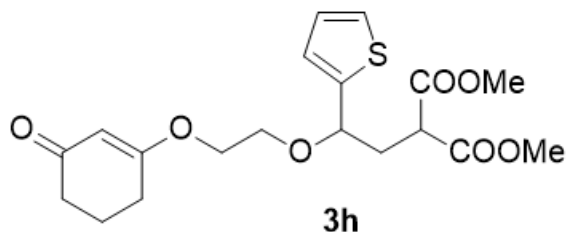
F2 - Acquisition Parameters  
Date\_ 20200706  
Time\_ 23.54 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



1.08  
2.01  
1.00  
1.01  
2.02  
2.98  
3.04  
3.19  
3.06  
3.12  
2.07

199.64  
 177.71  
 169.48  
 169.38  
 144.25  
 126.55  
 125.60  
 125.50  
 102.76  
 77.31  
 77.00  
 76.68  
 75.64  
 67.38  
 66.19  
 52.57  
 52.55  
 48.42  
 37.17  
 36.65  
 28.82  
 21.10



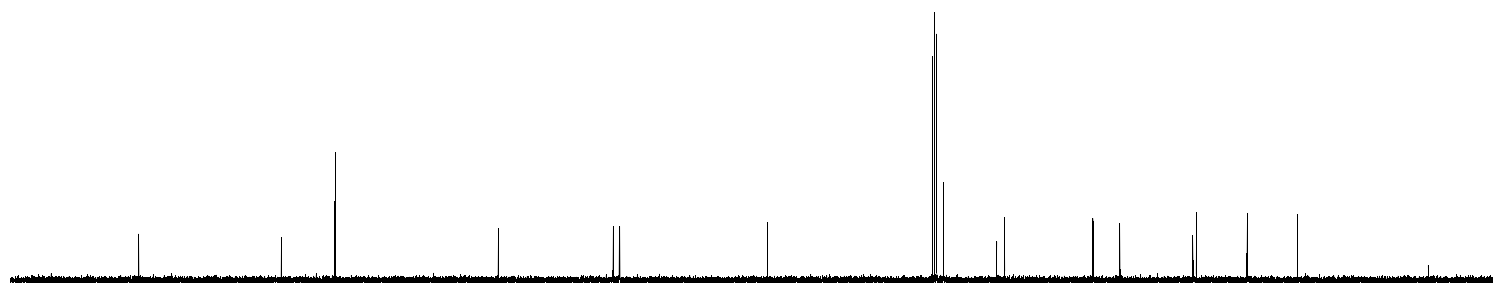
Current Data Parameters  
 NAME yl-10 new  
 EXPNO 2020070603  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20200707  
 Time 1.59 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 159  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

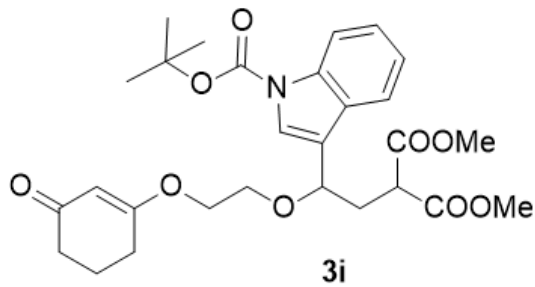
F2 - Processing parameters

SI 32768  
 SF 100.6228344 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40



200 180 160 140 120 100 80 60 40 20 ppm

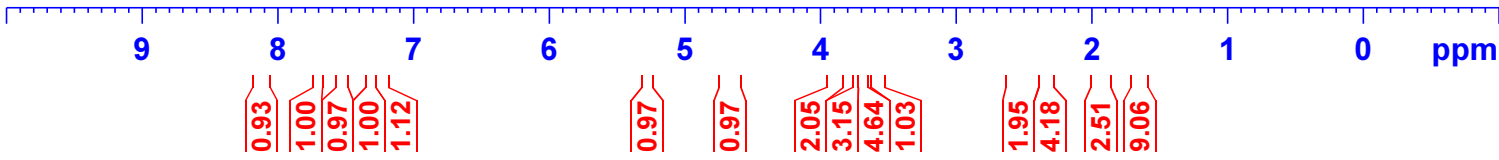
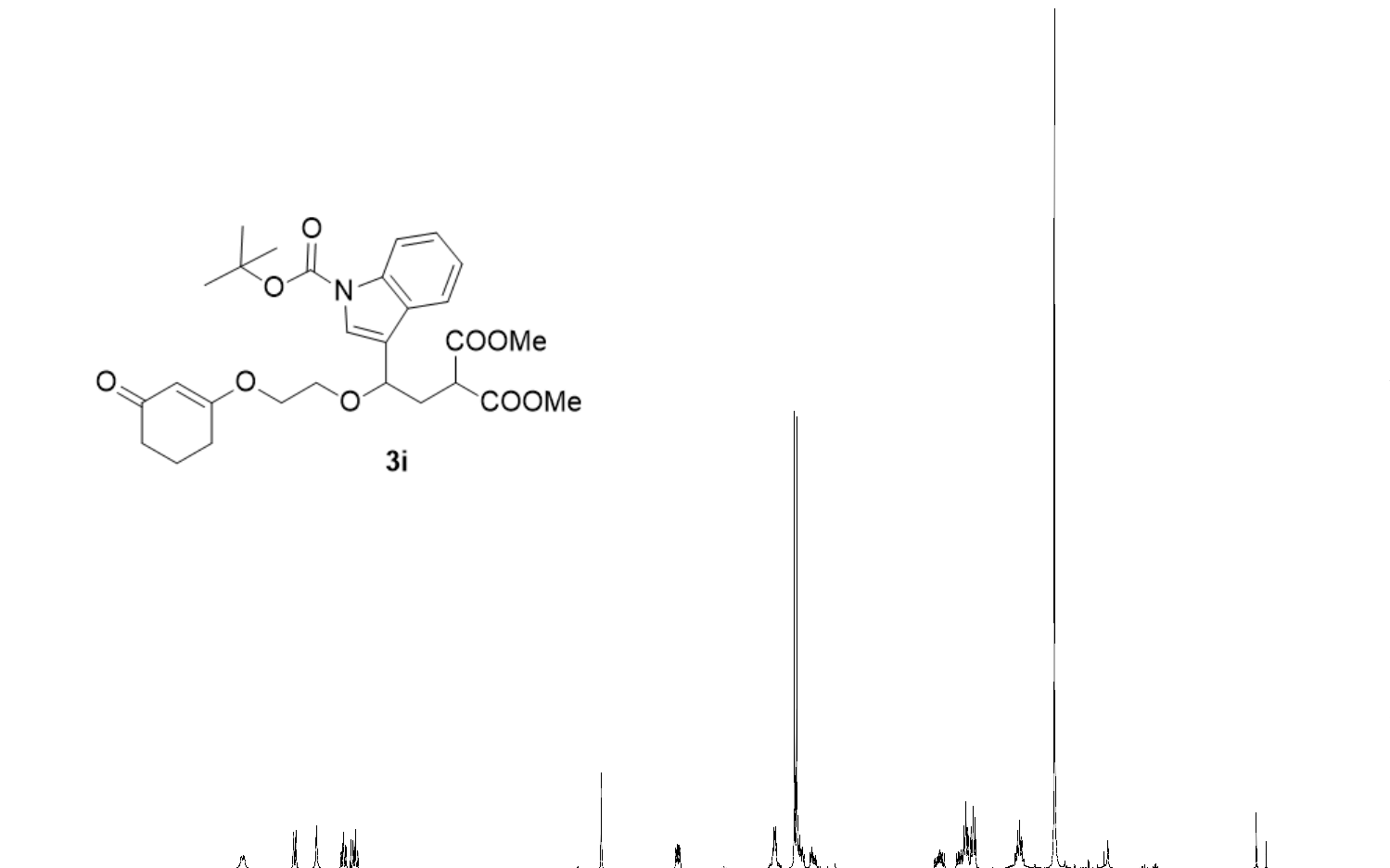
7.715  
7.695  
7.532  
7.319  
7.317  
7.299  
7.296  
7.260  
7.243  
7.240  
7.223  
7.205  
5.268  
4.675  
4.664  
4.651  
4.640  
3.905  
3.897  
3.891  
3.889  
3.883  
3.875  
3.733  
3.715  
3.707  
3.699  
3.691  
3.680  
3.671  
3.598  
3.594  
2.581  
2.410  
2.385  
2.370  
2.354  
2.328  
2.313  
2.295  
1.959  
1.943  
1.926  
1.665



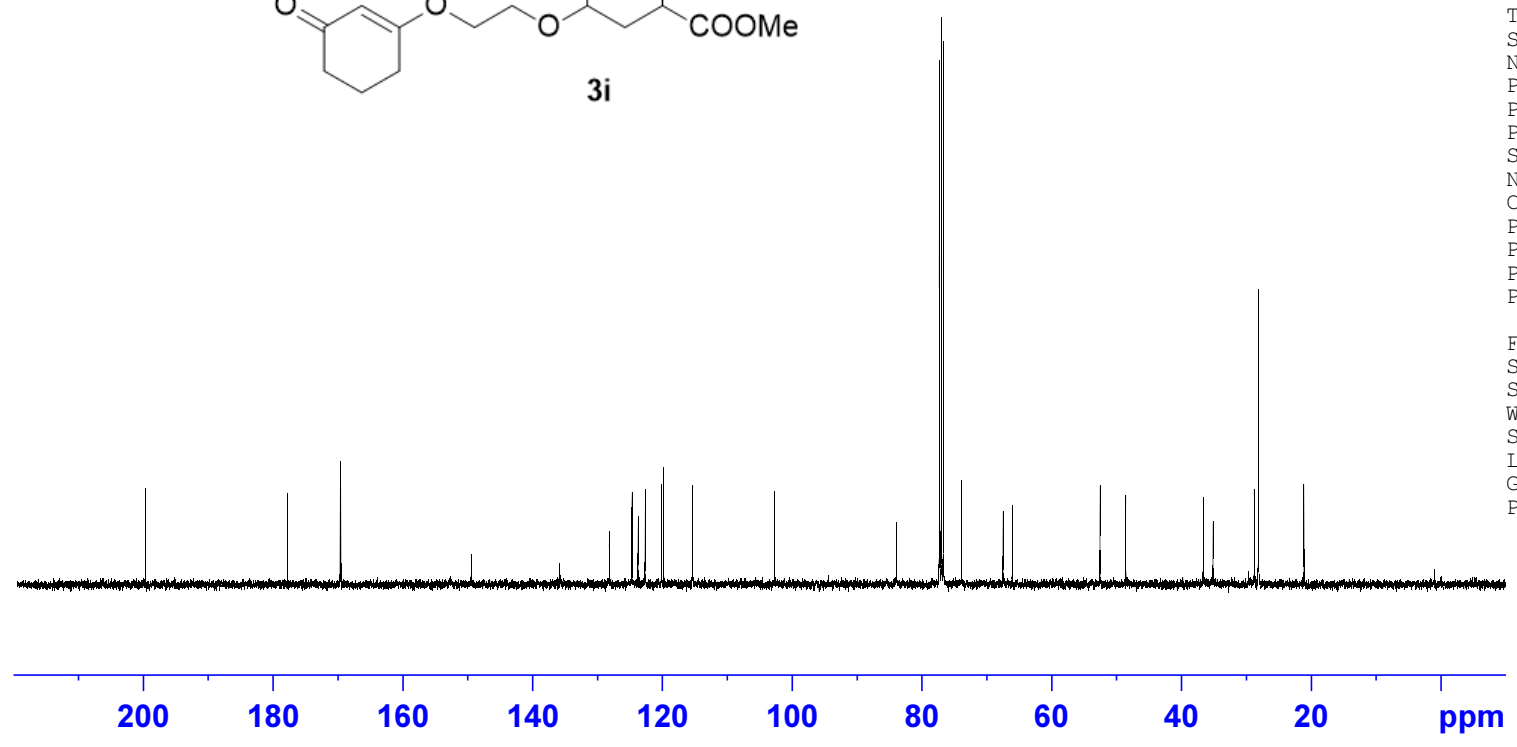
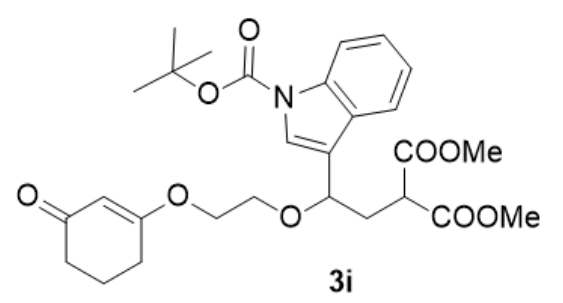
Current Data Parameters  
 NAME yl-32 new  
 EXPNO 2020070604  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 0.46 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 3.9845889 sec  
 RG 114  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 297.0 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1724712 MHz  
 NUC1 1H  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 15.00000000 W

F2 - Processing parameters  
 SI 32768  
 SF 400.1700089 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00



— 199.69  
 — 177.79  
 169.67  
 169.55  
 — 149.48  
 135.83  
 128.19  
 124.68  
 123.73  
 122.65  
 120.10  
 119.78  
 115.31  
 — 102.69  
 83.92  
 77.31  
 77.00  
 76.68  
 73.88  
 67.49  
 66.07  
 52.54  
 52.52  
 48.54  
 36.63  
 35.11  
 28.78  
 28.12  
 — 21.09

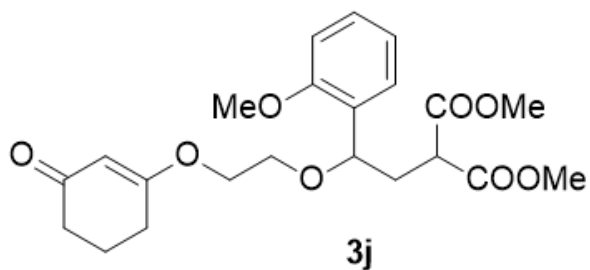


Current Data Parameters  
 NAME yl-32 new  
 EXPNO 2020070601  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 0.41 h  
 INSTRUM spect  
 PROBHD z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.9 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.0000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228344 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

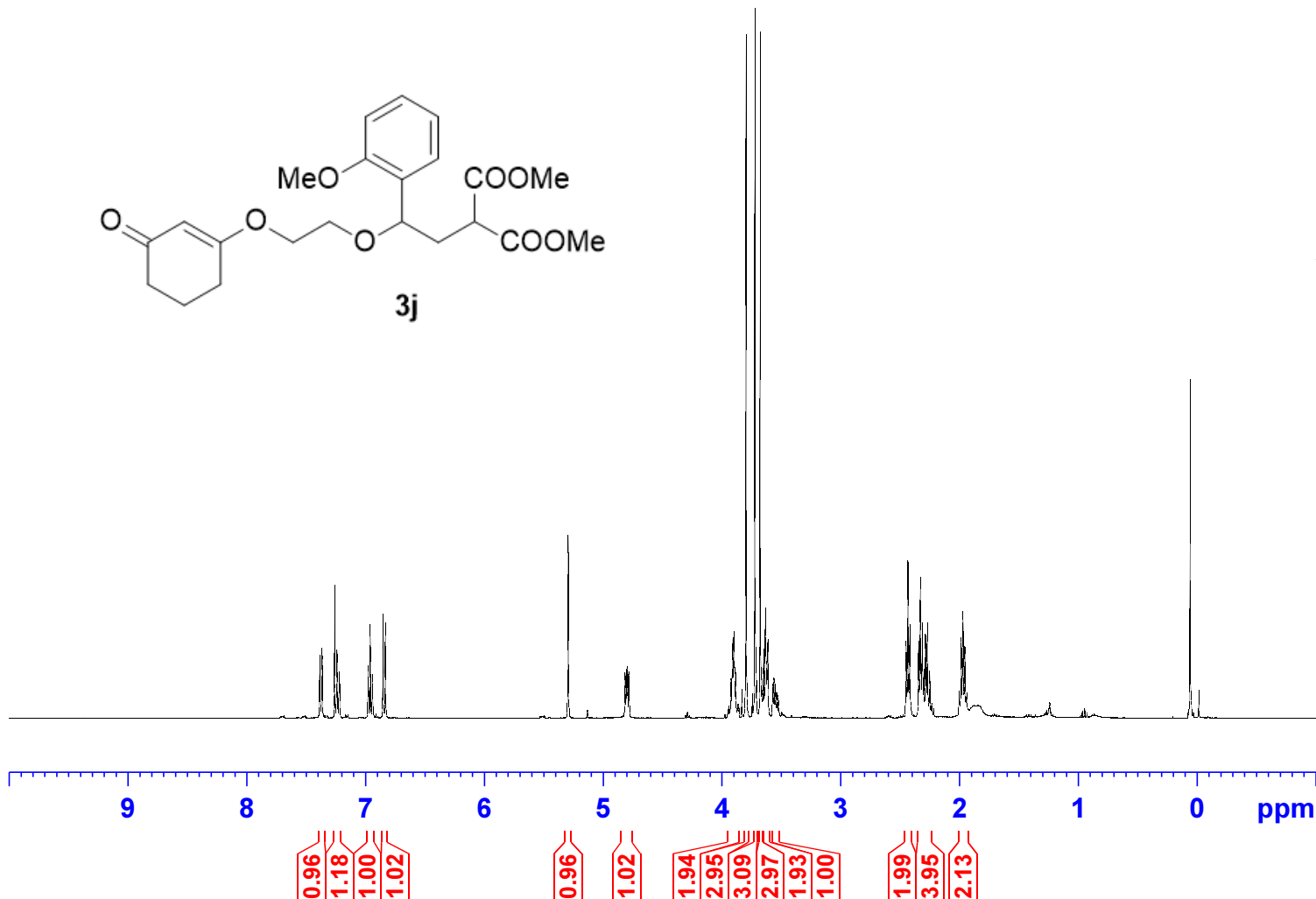
7.385  
7.382  
7.366  
7.363  
7.260  
7.242  
7.240  
7.221  
6.978  
6.960  
6.853  
6.832  
5.294  
4.814  
4.802  
4.794  
4.782  
3.913  
3.907  
3.898  
3.893  
3.884  
3.796  
3.721  
3.675  
3.648  
3.632  
3.619  
3.612  
2.449  
2.433  
2.417  
2.344  
2.328  
2.311  
2.298  
2.287  
2.279  
2.269  
2.267  
2.251  
1.986  
1.969  
1.954



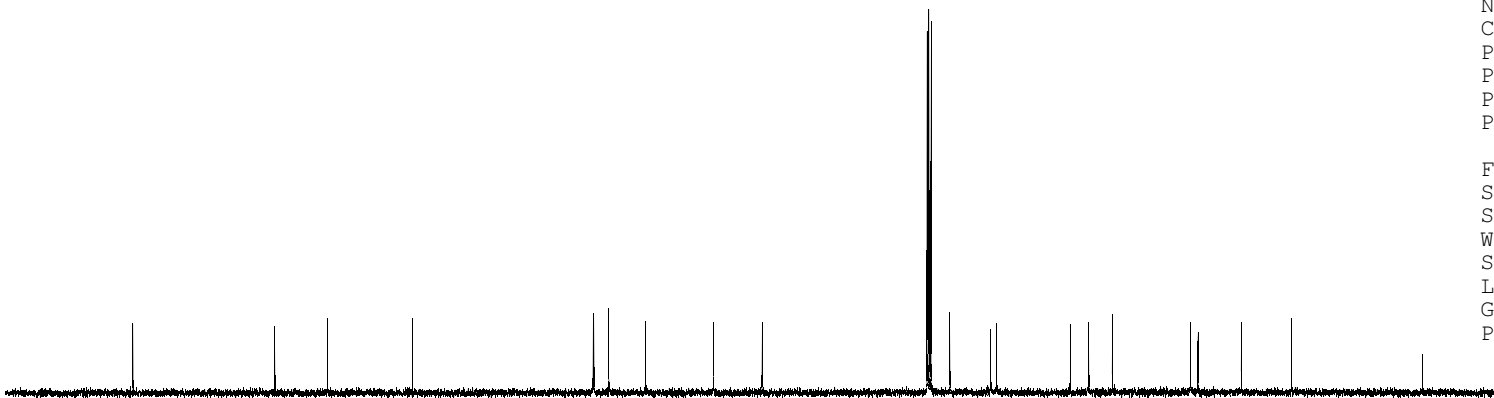
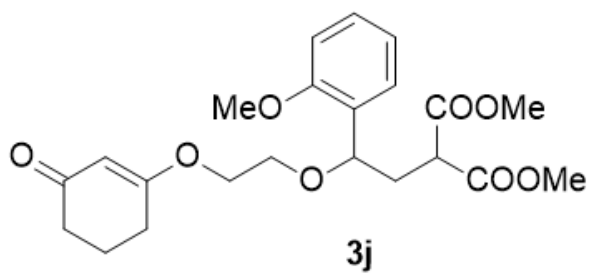
Current Data Parameters  
NAME yl-57 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 0.51 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 199.71  
 — 177.84  
 169.76  
 169.73  
 — 156.64  
 128.78  
 128.66  
 126.35  
 120.68  
 — 110.21  
 — 102.73  
 77.31  
 77.00  
 76.68  
 73.79  
 67.50  
 66.58  
 55.23  
 52.43  
 52.38  
 48.75  
 36.68  
 35.54  
 28.86  
 — 21.14



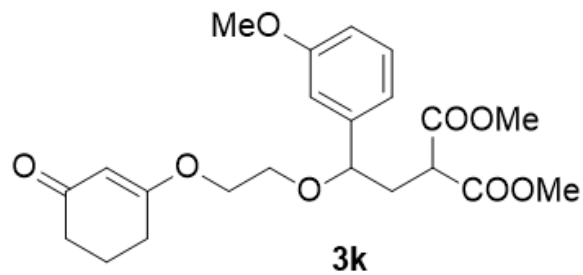
Current Data Parameters  
 NAME yl-57 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 2.45 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228330 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

200 180 160 140 120 100 80 60 40 20 ppm

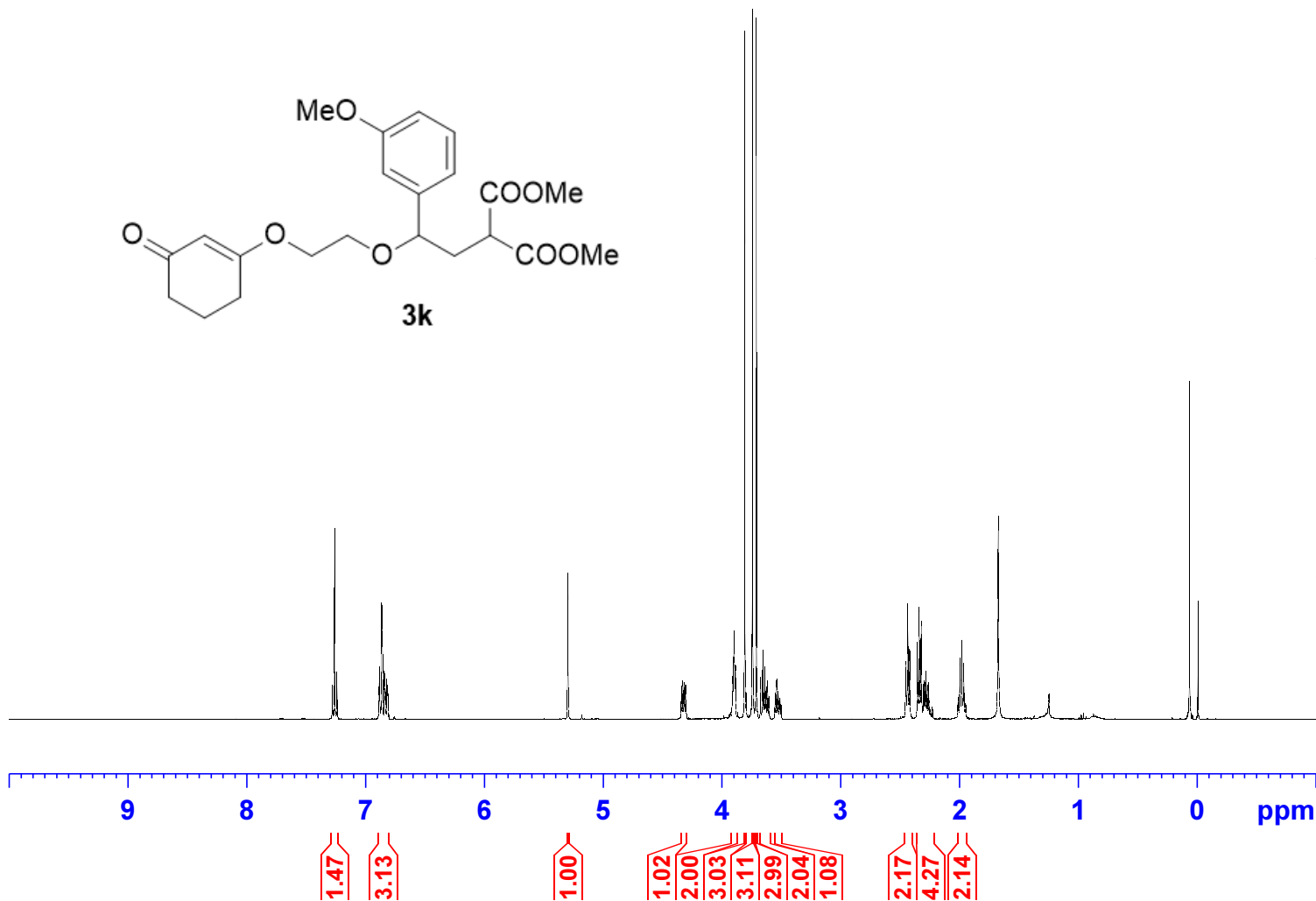
7.280  
7.260  
7.241  
6.883  
6.864  
6.841  
6.840  
6.821  
6.818  
5.296  
4.340  
4.329  
4.317  
4.306  
3.910  
3.908  
3.898  
3.887  
3.807  
3.742  
3.711  
3.675  
3.659  
3.654  
3.639  
3.626  
3.616  
3.539  
2.451  
2.435  
2.419  
2.354  
2.339  
2.321  
2.304  
2.297  
2.290  
2.281  
2.279  
2.269  
2.258  
1.995  
1.979  
1.963



Current Data Parameters  
NAME zjc-47 new  
EXPNO 2020070601  
PROCNO 1

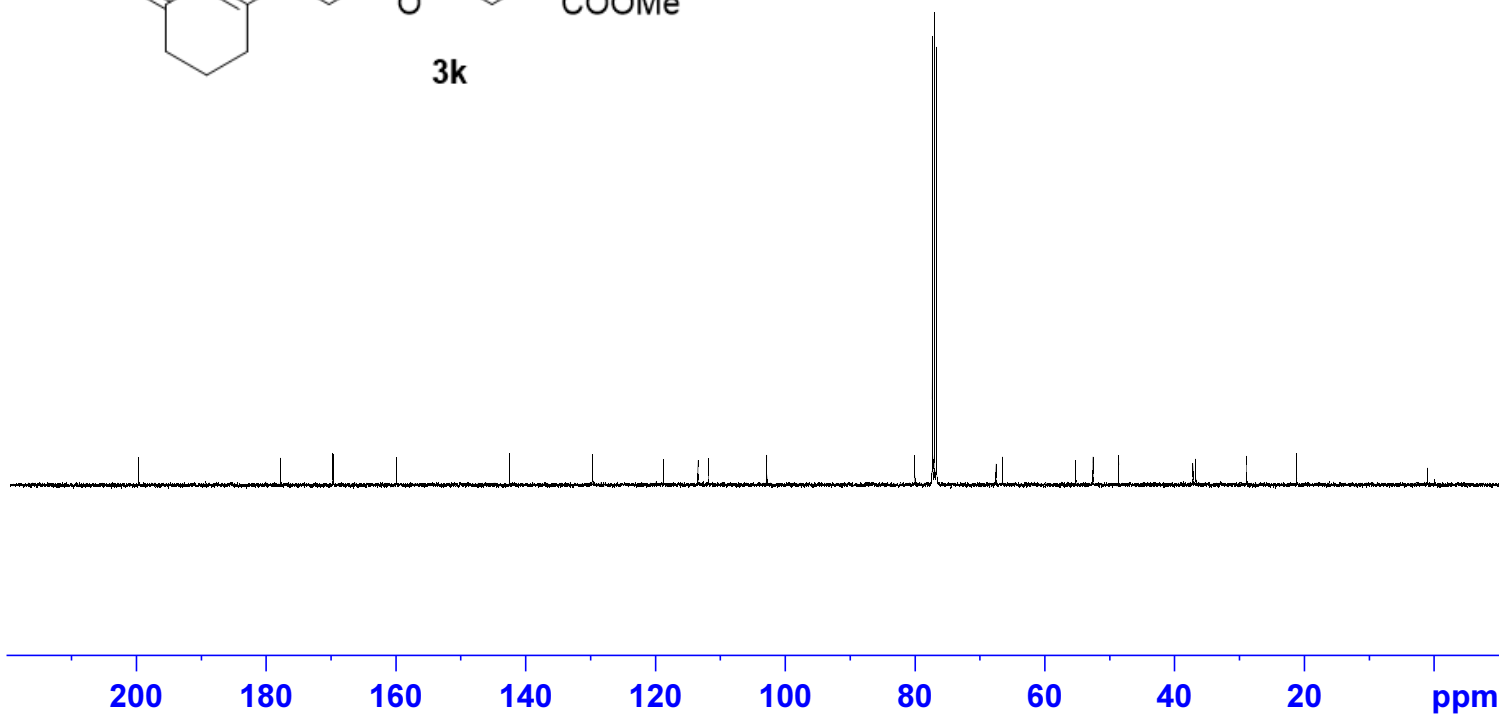
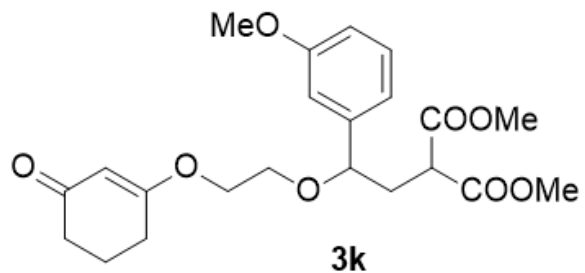
F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.08 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 297.0 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 199.68  
 — 177.75  
 — 169.70  
 — 169.61  
 — 159.90  
 — 142.51  
 — 129.66  
 — 118.79  
 — 113.44  
 — 111.82  
 — 102.81

— 80.02  
 — 77.31  
 — 77.00  
 — 76.68  
 — 67.52  
 — 66.48  
 — 55.22  
 — 52.56  
 — 52.54  
 — 48.58  
 — 37.14  
 — 36.71  
 — 28.88  
 — 21.17  
 — 0.99



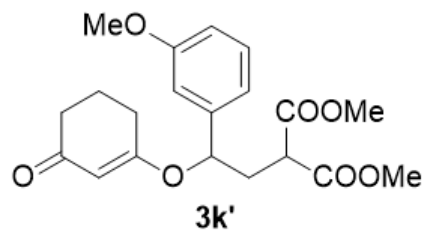
Current Data Parameters  
 NAME zjc-47 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 5.11 h  
 INSTRUM spect  
 PROBHD z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.0000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228300 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



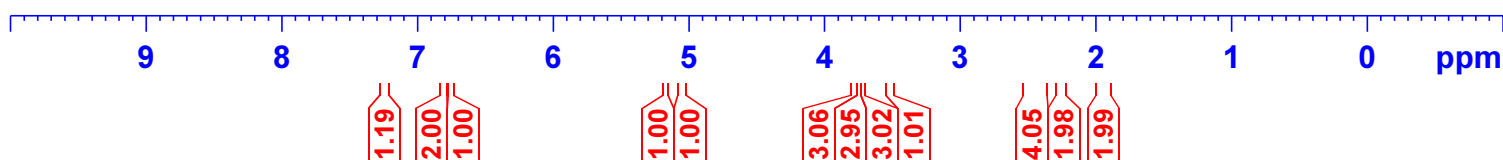
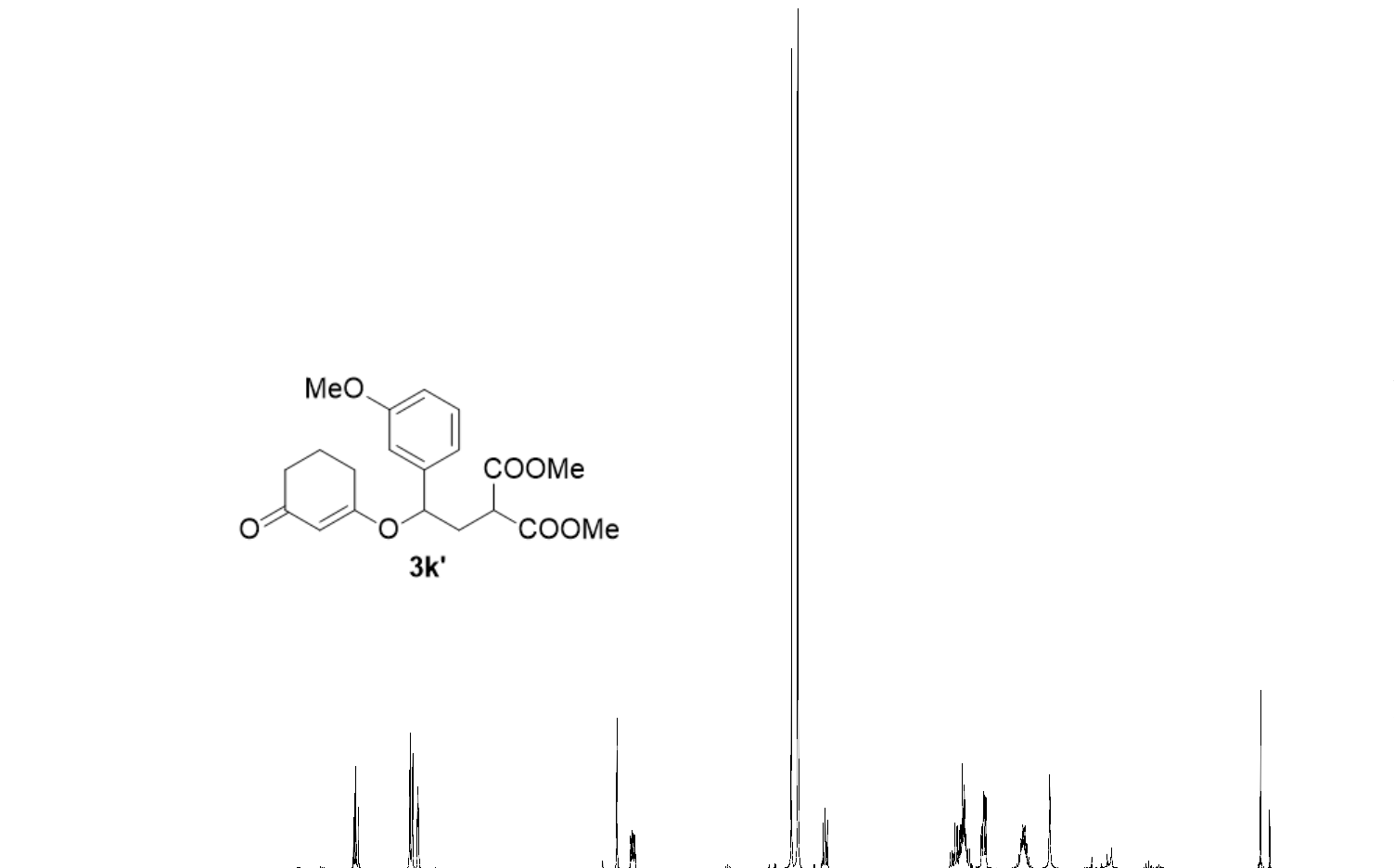
7.268  
7.260  
7.248  
7.229  
6.823  
6.818  
6.803  
6.798  
6.759  
6.755  
6.749  
5.173  
5.064  
5.053  
5.043  
5.031  
3.788  
3.738  
3.733  
3.537  
3.521  
3.517  
3.501  
2.490  
2.474  
2.469  
2.453  
2.443  
2.440  
2.428  
2.419  
2.413  
2.408  
2.403  
2.398  
2.277  
2.273  
2.261  
2.256  
2.242  
1.962  
1.948  
1.941  
1.932



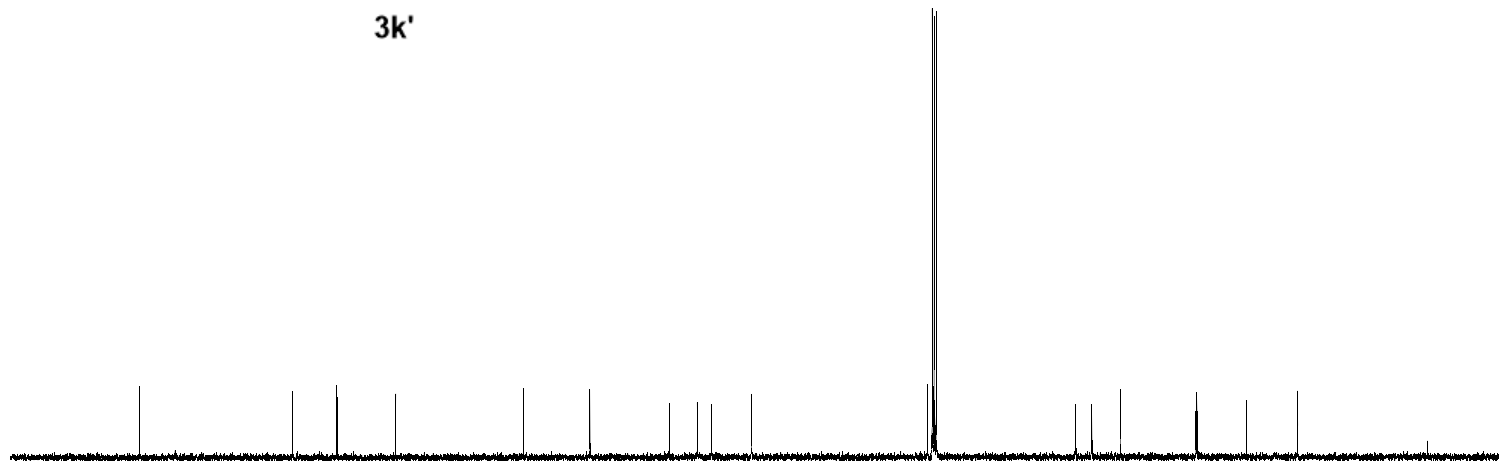
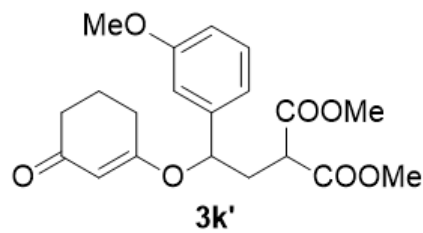
Current Data Parameters  
NAME yl-14 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 0.02 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.3 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 199.51  
 — 175.89  
 — 169.14  
 — 169.04  
 — 159.98  
 — 140.29  
 — 130.07  
 — 117.84  
 — 113.54  
 — 111.33  
 — 105.17  
 — 78.05  
 — 77.32  
 — 77.00  
 — 76.68  
 — 55.21  
 — 52.76  
 — 52.71  
 — 48.28  
 — 36.67  
 — 36.52  
 — 28.87  
 — 20.99

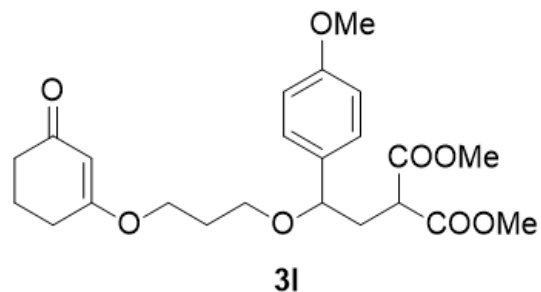


Current Data Parameters  
 NAME yl-14 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 2.25 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG \_zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228315 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

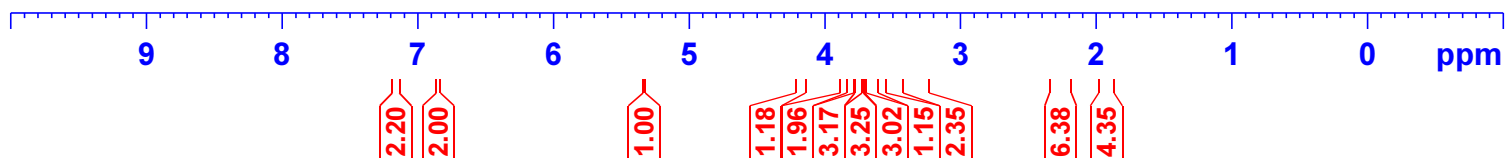
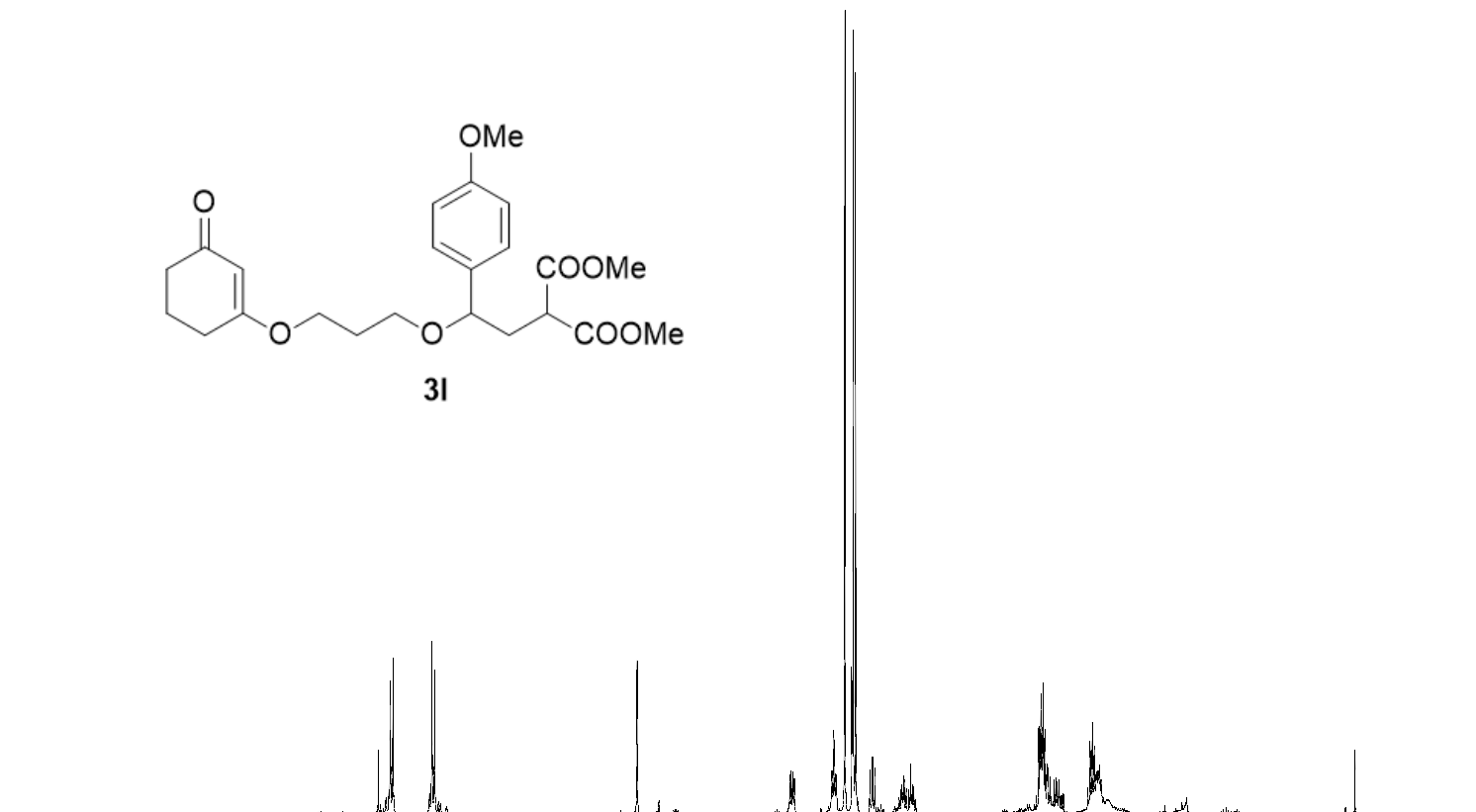
7.172  
7.151  
6.861  
6.840  
5.332  
4.194  
4.183  
4.171  
4.160  
3.882  
3.879  
3.867  
3.863  
3.851  
3.847  
3.785  
3.722  
3.704  
3.596  
3.580  
3.575  
3.560  
3.343  
3.293  
2.339  
2.323  
2.306  
2.295  
2.291  
2.280  
2.273  
2.257  
2.211  
2.190  
1.957  
1.940  
1.924  
1.910  
1.903  
1.897  
1.895  
1.888  
1.880  
1.873



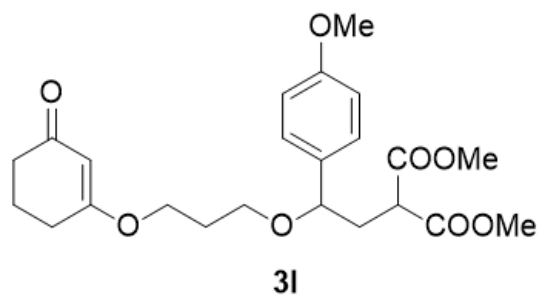
Current Data Parameters  
NAME zjc-84 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.36 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



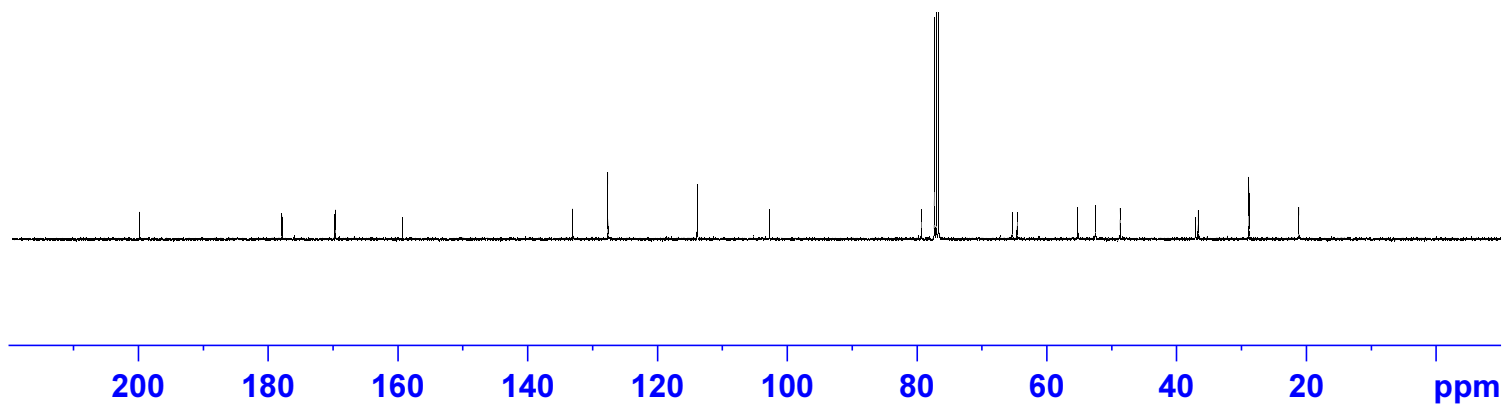
— 199.79  
 — 177.87  
 — 169.74  
 — 169.65  
 — 159.27  
 — 133.11  
 — 127.63  
 — 113.85  
 — 102.71  
 — 79.32  
 — 77.31  
 — 76.99  
 — 76.68  
 — 65.32  
 — 64.54  
 — 55.21  
 — 52.47  
 — 48.69  
 — 37.06  
 — 36.67  
 — 28.85  
 — 21.12



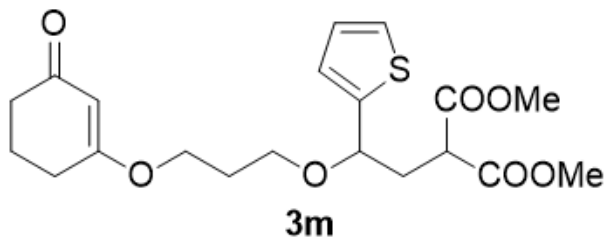
Current Data Parameters  
 NAME zjc-84 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 4.26 h  
 INSTRUM spect  
 PROBHD z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228329 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



7.260  
7.249  
7.244  
7.239  
7.233  
6.929  
6.924  
6.919  
5.318  
4.541  
4.529  
4.518  
4.507  
3.870  
3.861  
3.855  
3.845  
3.829  
3.714  
3.703  
3.601  
3.584  
3.581  
3.564  
3.451  
3.365  
3.342  
2.411  
2.395  
2.389  
2.337  
2.324  
2.308  
2.292  
2.279  
1.961  
1.945  
1.929  
1.913  
1.905  
1.897  
1.890  
1.883  
1.875

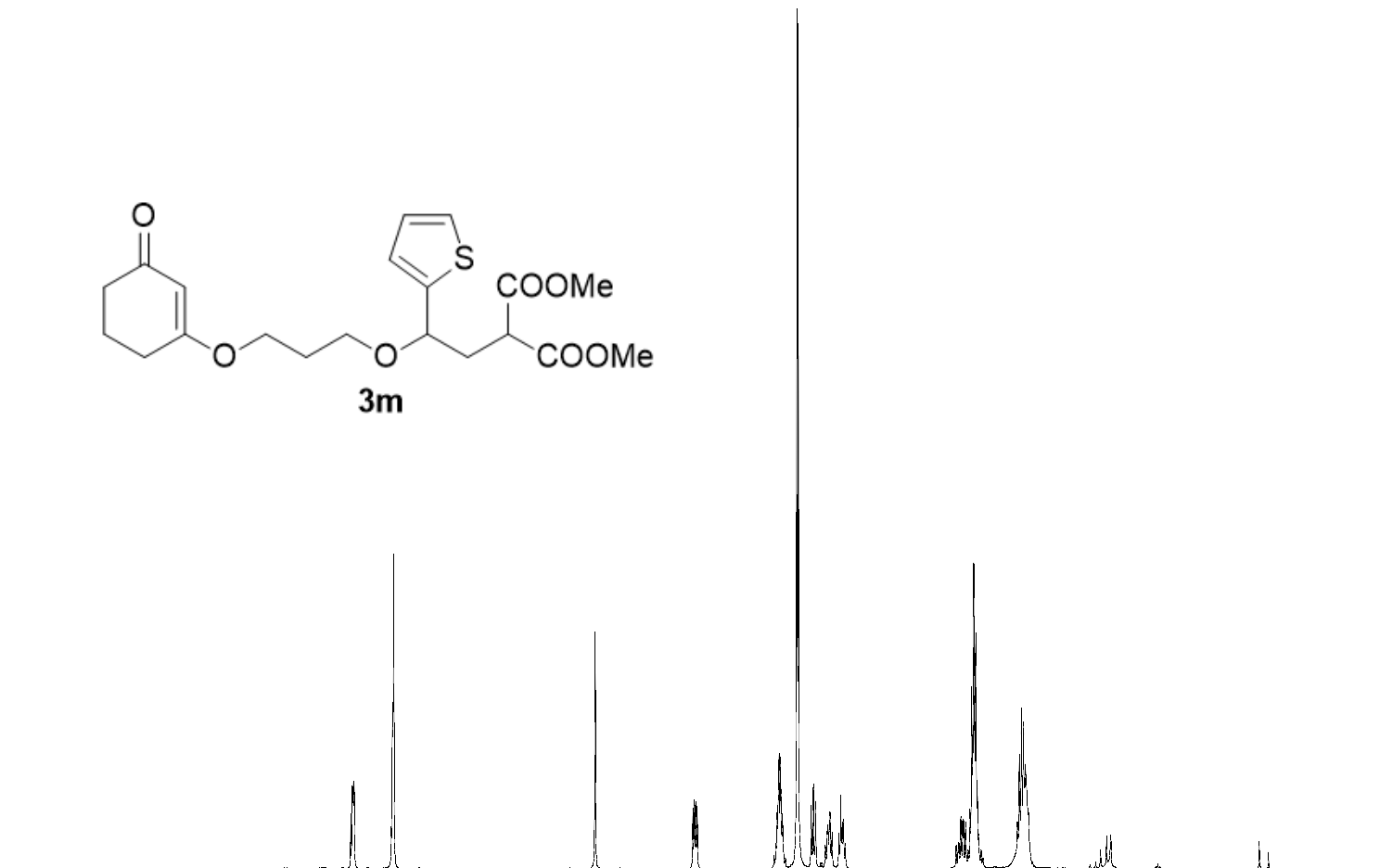


Current Data Parameters  
NAME zjc-85 rep  
EXPNO 2019122401  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20191224  
Time\_ 16.50  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 57  
DW 60.800 usec  
DE 6.50 usec  
TE 291.6 K  
D1 1.00000000 sec  
TD0 1

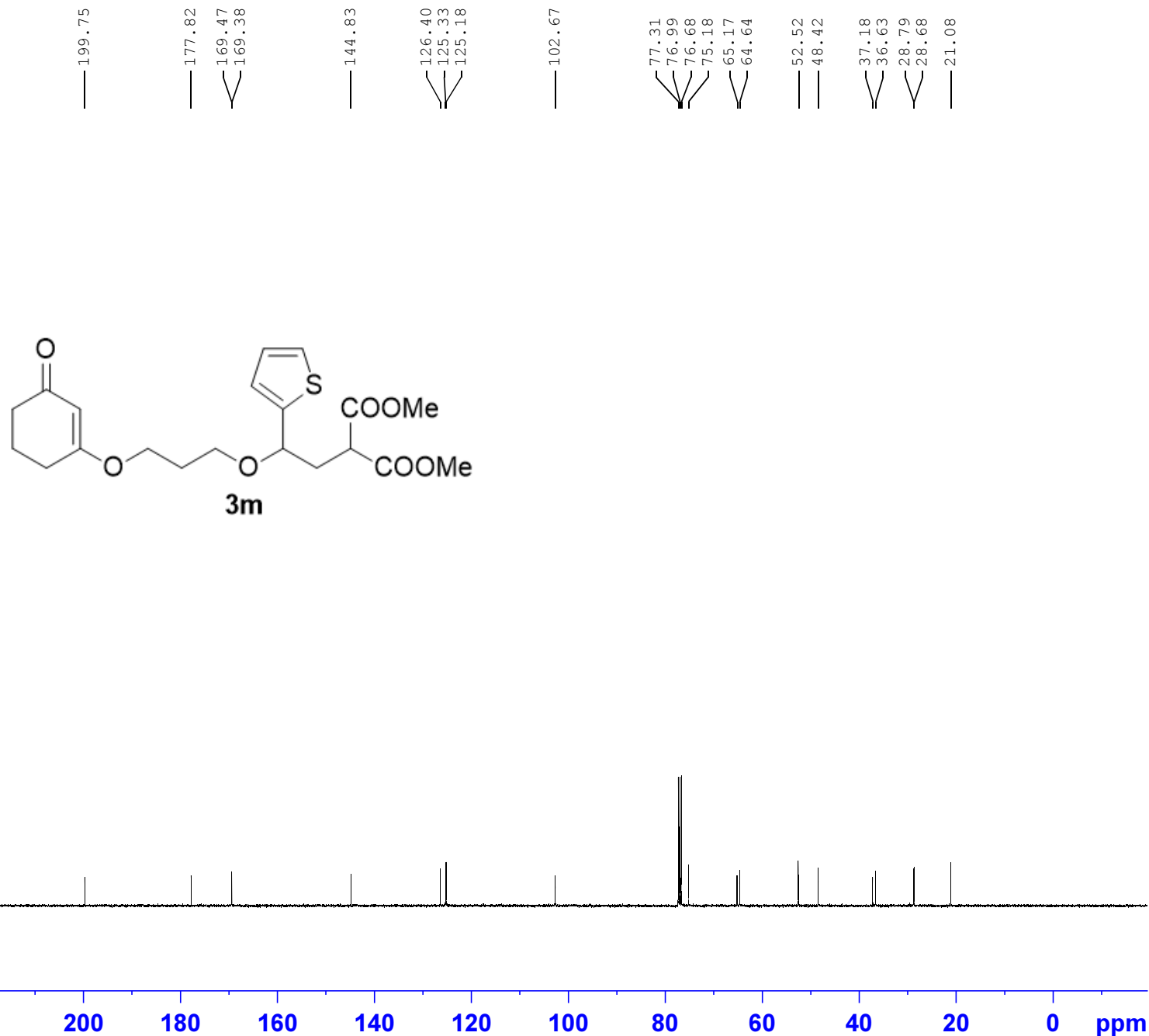
==== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1700152 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

0.97  
2.00  
1.02  
1.02  
2.09  
3.04  
2.95  
1.04  
1.04  
1.03  
6.25  
4.54



Current Data Parameters  
 NAME zjc-85 rep  
 EXPNO 2019122402  
 PROCNO 1

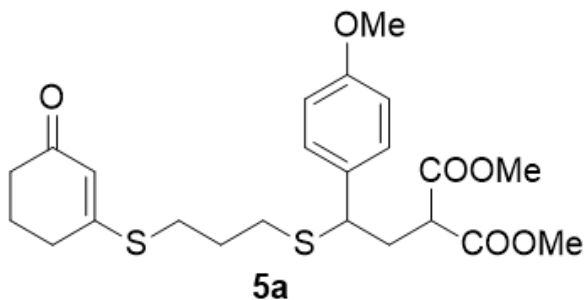
F2 - Acquisition Parameters  
 Date\_ 20191224  
 Time\_ 18.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 112  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 292.1 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228410 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

7.260  
7.186  
7.165  
6.848  
6.826  
5.780  
3.780  
3.772  
3.771  
3.769  
3.756  
3.740  
3.734  
3.715  
3.650  
3.403  
3.387  
3.383  
3.367  
2.795  
2.777  
2.759  
2.742  
2.451  
2.434  
2.431  
2.414  
2.397  
2.382  
2.377  
2.365  
2.359  
2.350  
2.336  
2.333  
2.026  
2.010  
1.995  
1.979  
1.801  
1.794  
1.784  
1.766  
1.748

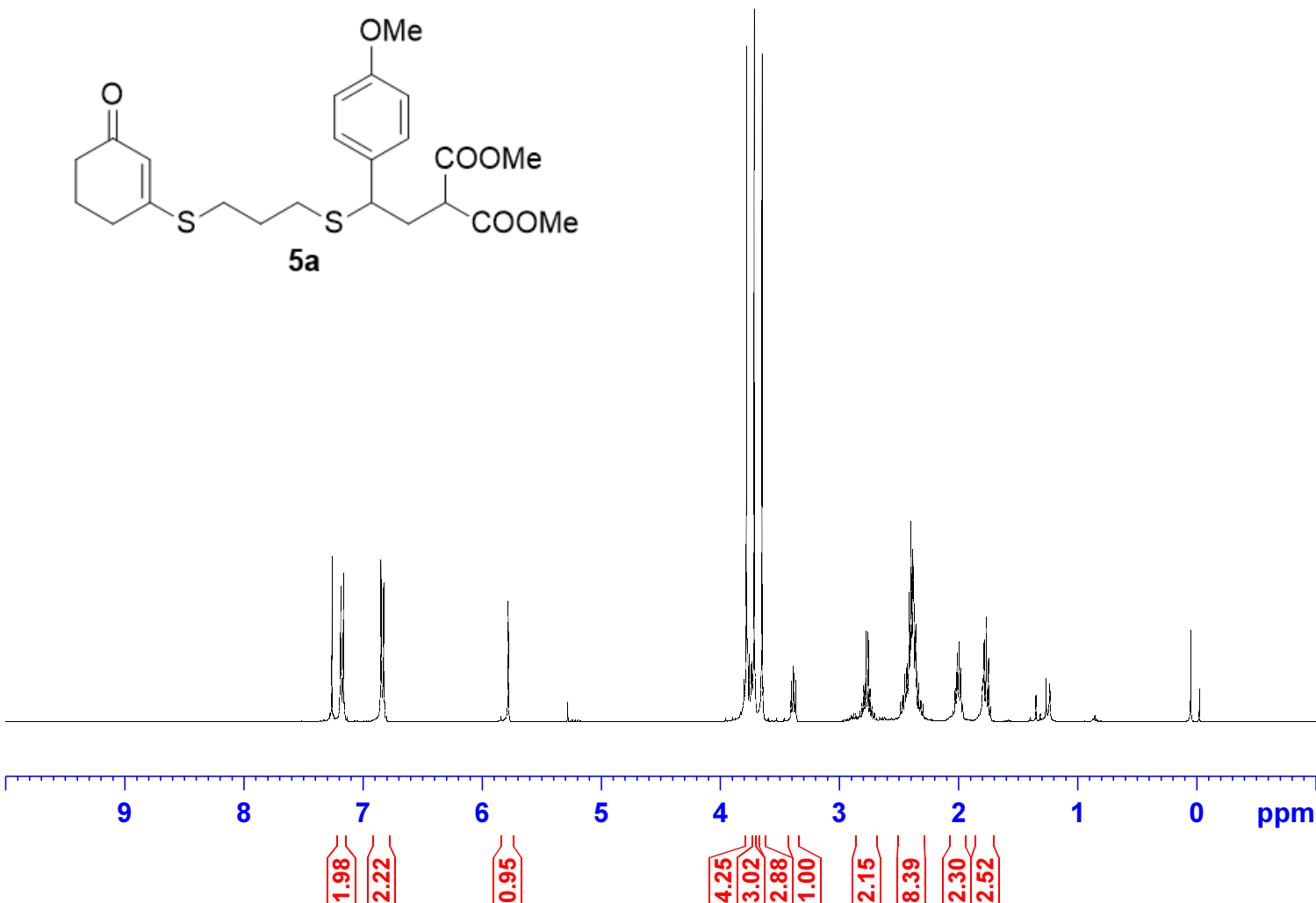


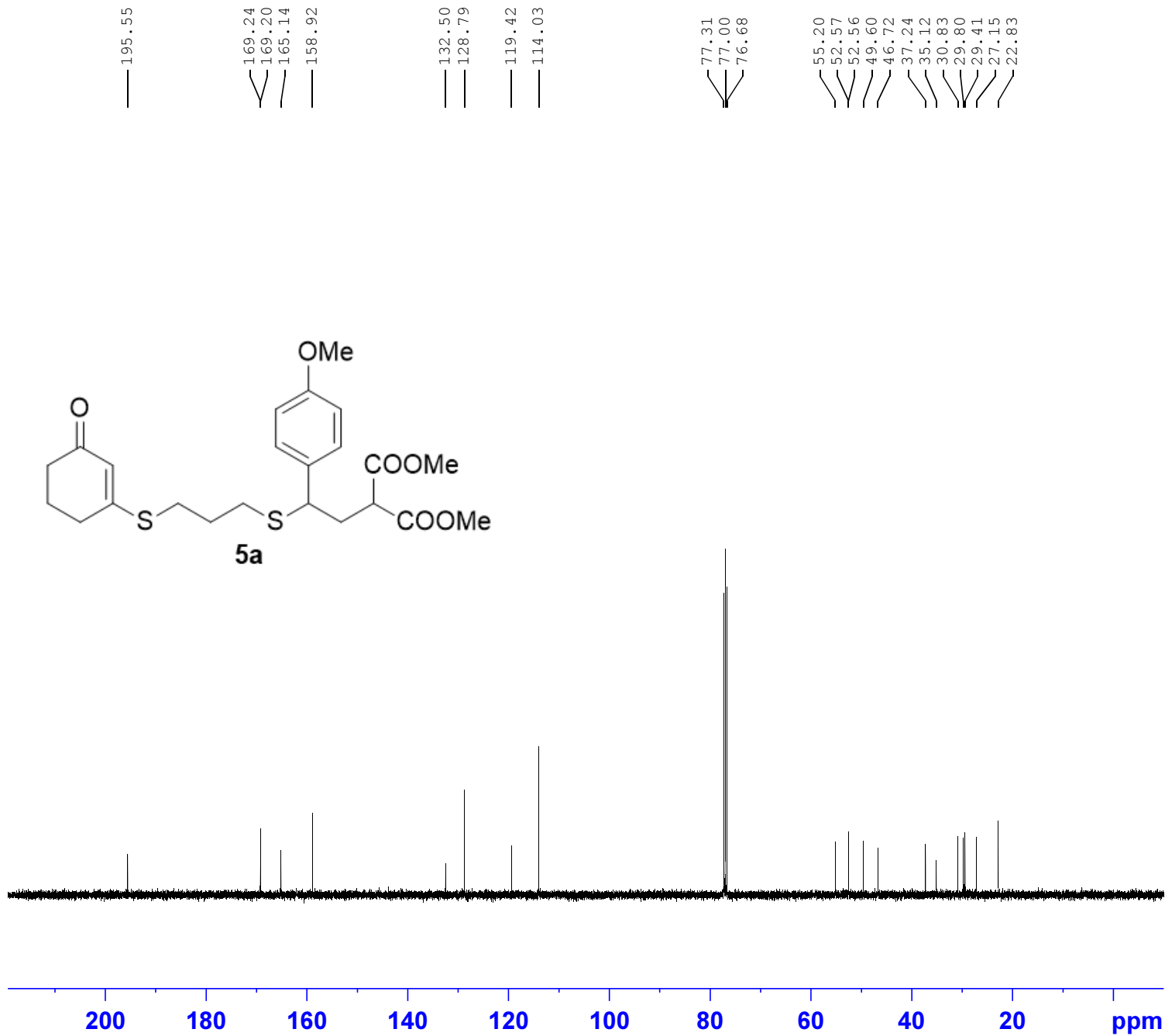
Current Data Parameters  
NAME zjc-12  
EXPNO 2019050801  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190510  
Time\_ 23.48  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 71.8  
DW 60.800 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.00000000 sec  
TD0 1

==== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1700156 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME zjc-12  
 EXPNO 2019051002  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190511  
 Time 1.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 264  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

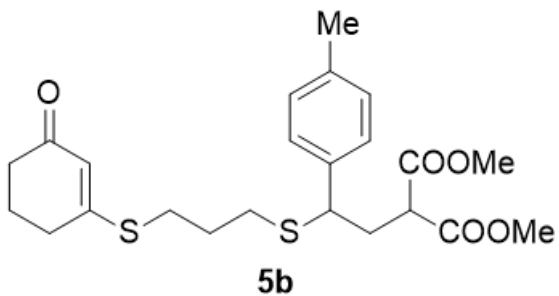
==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228374 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40



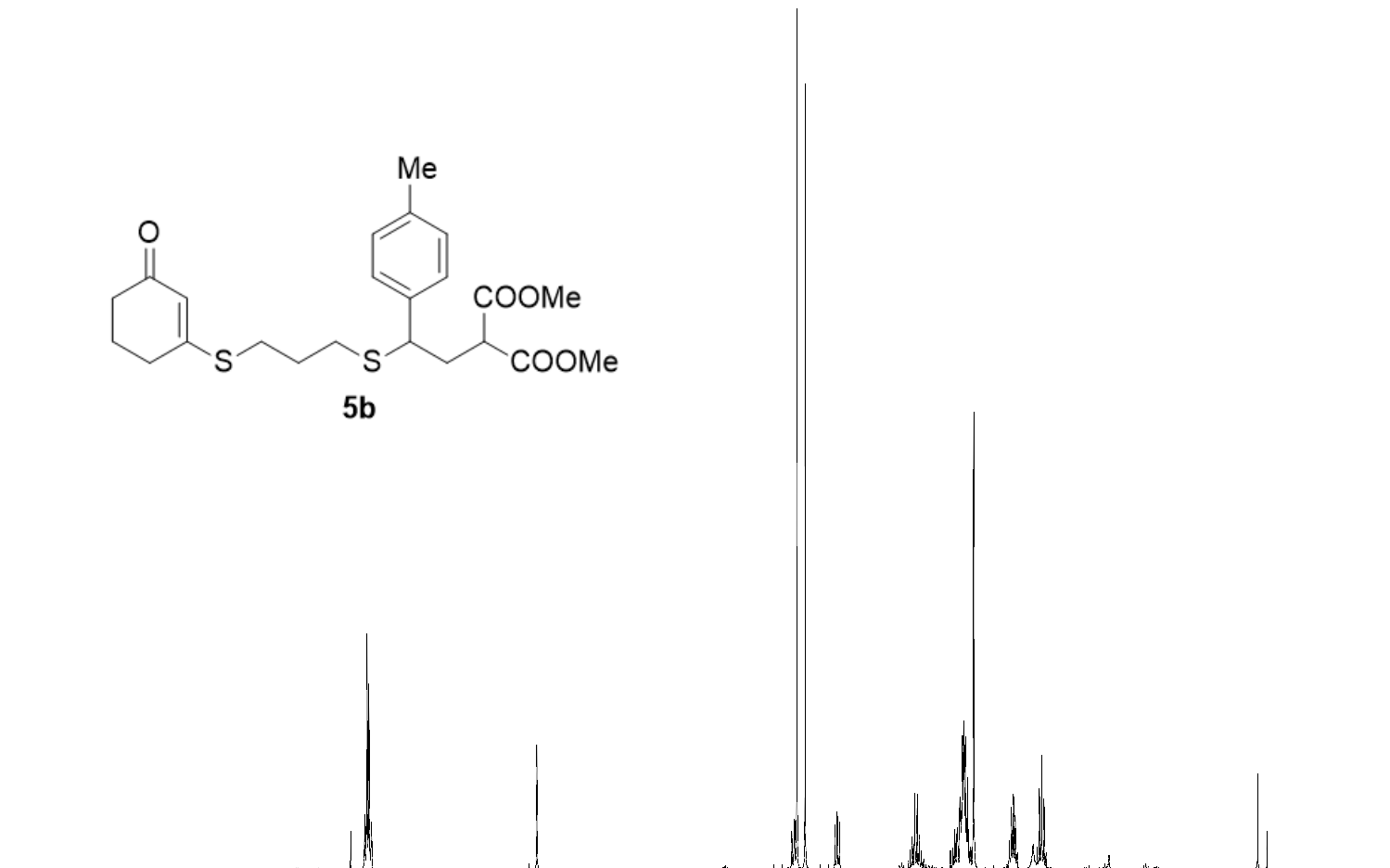
7.150  
7.145  
7.135  
7.129  
7.116  
7.095  
5.780  
3.752  
3.735  
3.731  
3.713  
3.647  
3.411  
3.395  
3.391  
3.374  
2.796  
2.777  
2.757  
2.739  
2.456  
2.439  
2.436  
2.419  
2.412  
2.405  
2.400  
2.397  
2.388  
2.383  
2.375  
2.371  
2.365  
2.357  
2.352  
2.349  
2.307  
2.024  
2.008  
1.992  
1.976  
1.785  
1.767  
1.749



Current Data Parameters  
NAME zjc-29 new  
EXPNO 2020070601  
PROCNO 1

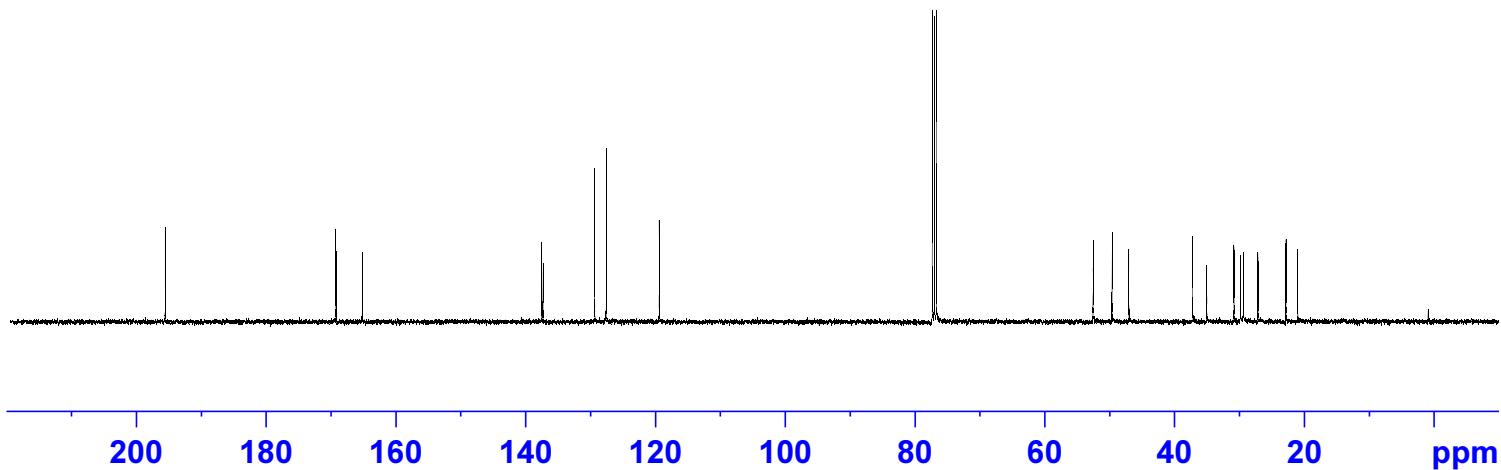
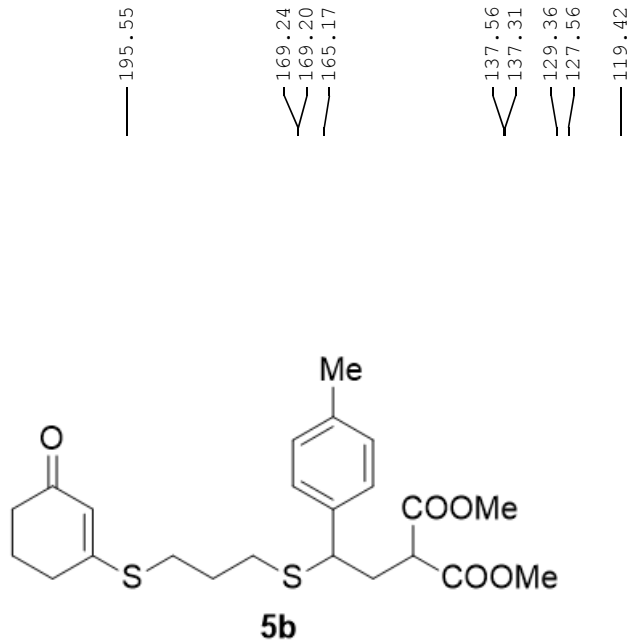
F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 0.06 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.4 K  
D1 1.00000000 sec  
TDO 1  
SFO1 400.1724712 MHz  
NUC1 1H  
PO 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

4.34  
1.00  
4.32  
3.27  
1.09  
2.20  
8.80  
3.31  
2.25  
2.17

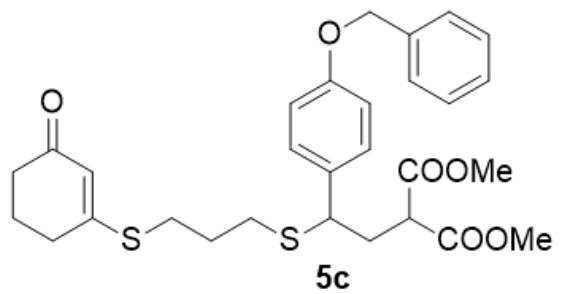


Current Data Parameters  
 NAME zjc-29 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 4.07 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.0000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.0000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228361 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

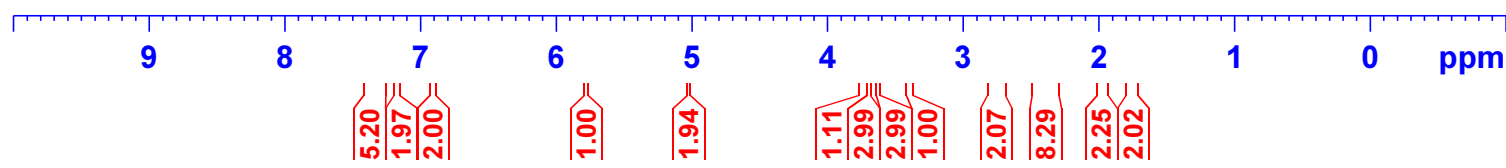
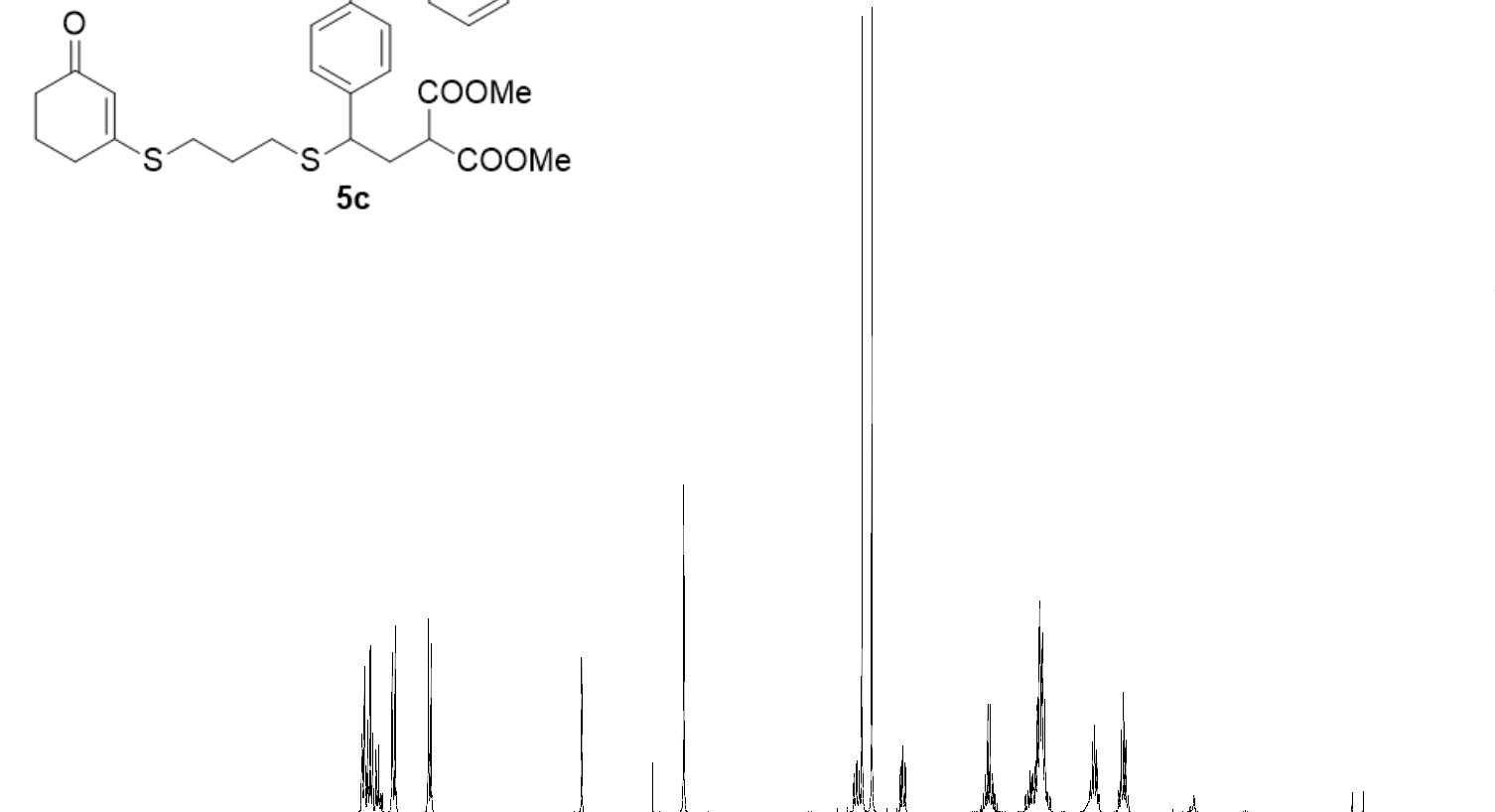
7.414  
7.410  
7.393  
7.371  
7.368  
7.350  
7.346  
7.335  
7.331  
7.306  
7.288  
7.186  
7.165  
6.920  
6.898  
5.779  
5.022  
3.741  
3.736  
3.719  
3.698  
3.625  
3.414  
3.397  
3.393  
3.377  
2.765  
2.746  
2.449  
2.409  
2.397  
2.392  
2.380  
2.375  
2.364  
2.359  
2.346  
2.342  
1.987  
1.971  
1.955  
1.774  
1.756  
1.739

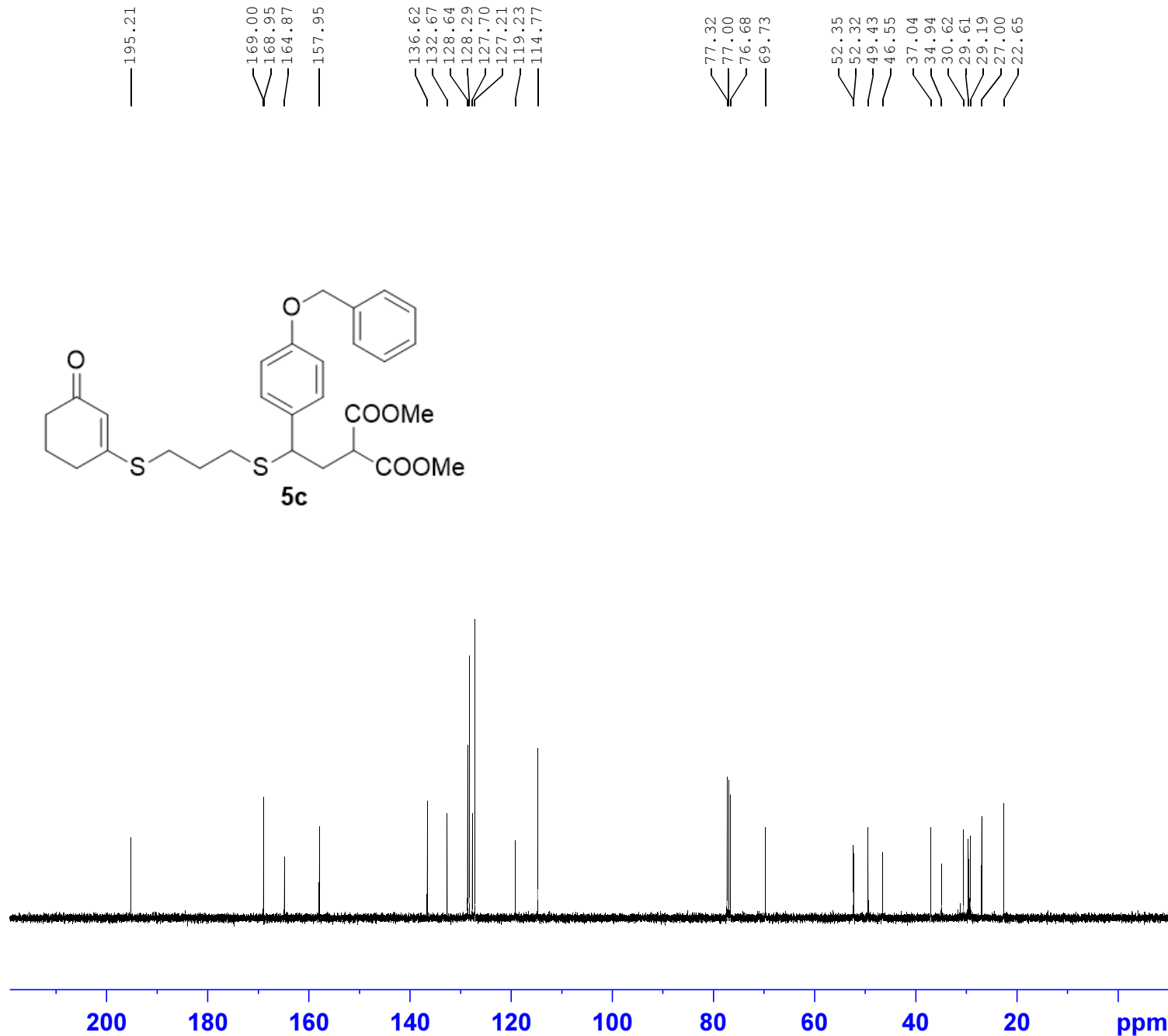
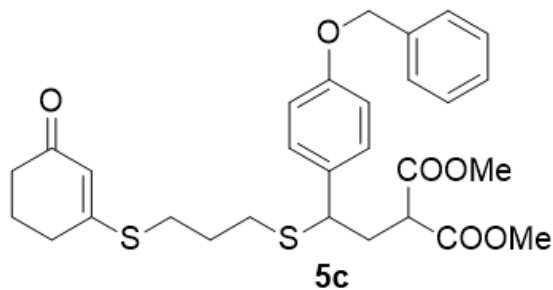


Current Data Parameters  
NAME zjc-31 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.23 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700084 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME zjc-31  
 EXPNO 2019060302  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190604  
 Time 3.18  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 66  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

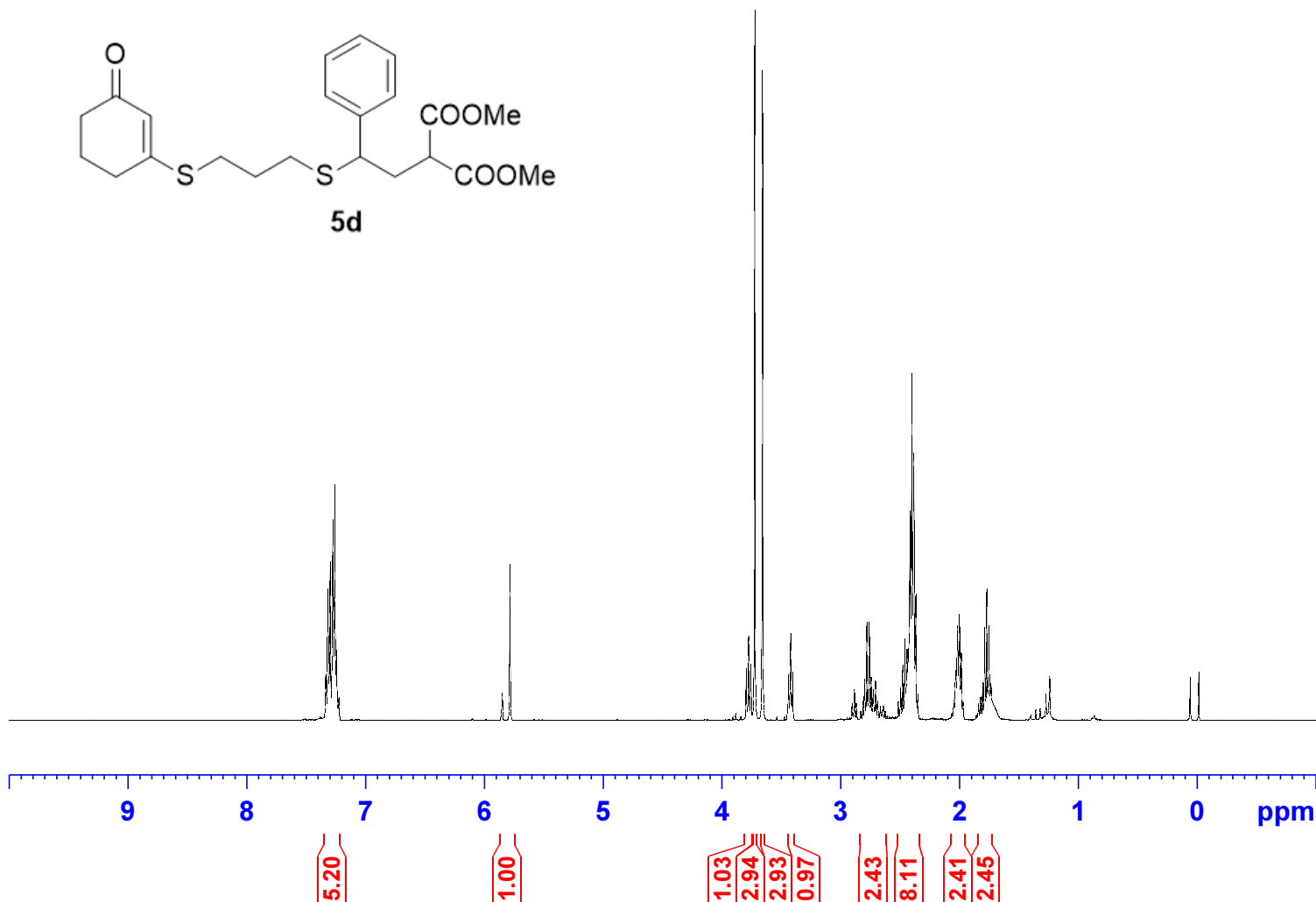
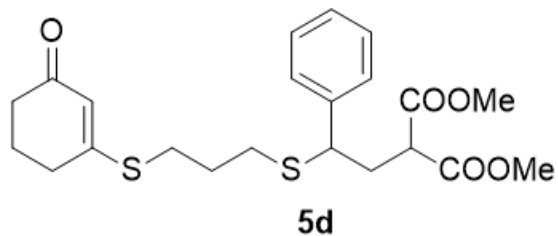
F2 - Processing parameters  
 SI 32768  
 SF 100.6228564 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40

7.336  
7.334  
7.318  
7.315  
7.298  
7.274  
7.260  
7.244  
5.784  
3.794  
3.775  
3.755  
3.724  
3.722  
3.659  
3.657  
3.439  
3.421  
3.402  
2.798  
2.780  
2.761  
2.742  
2.726  
2.707  
2.494  
2.476  
2.459  
2.439  
2.431  
2.423  
2.416  
2.400  
2.385  
2.367  
2.031  
2.017  
2.001  
1.985  
1.804  
1.787  
1.769  
1.752  
1.734

Current Data Parameters  
NAME zjc-18 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.16 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700090 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 195.59

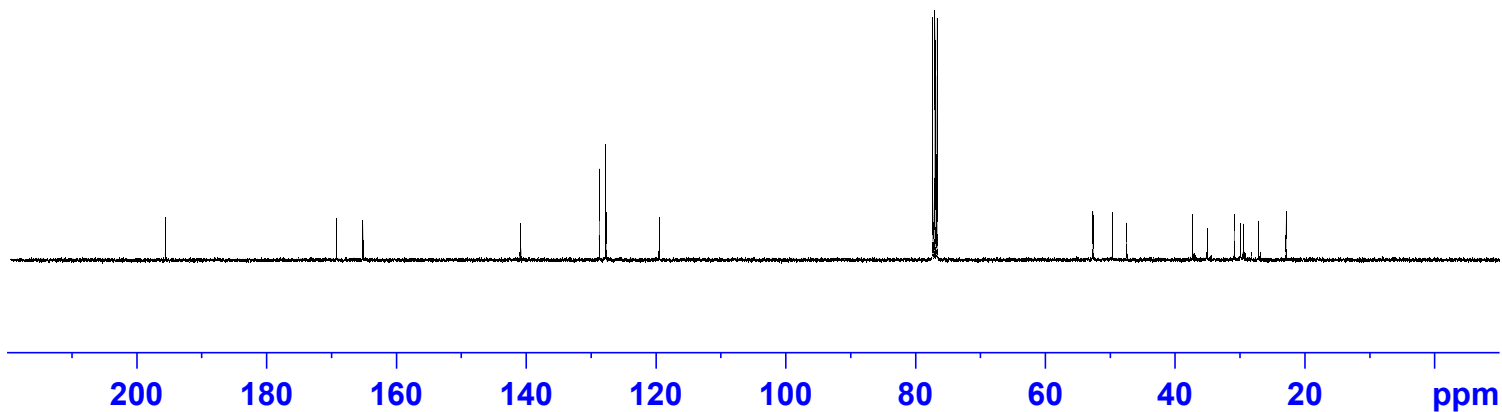
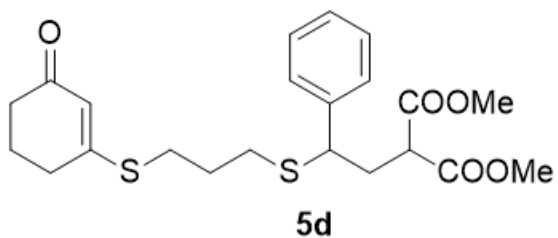
169.25  
169.19  
165.15

— 140.79

128.73  
127.73  
127.67  
— 119.47

77.31  
77.00  
76.68

52.62  
52.60  
49.64  
47.43  
37.26  
35.01  
30.85  
29.89  
29.41  
27.14  
22.86



Current Data Parameters  
 NAME zjc-18 new  
 EXPNO 2020070602  
 PROCNO 1

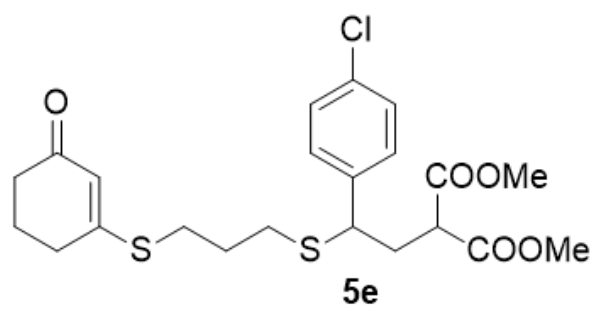
F2 - Acquisition Parameters

Date\_ 20200707  
 Time\_ 4.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 360  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters

SI 32768  
 SF 100.6228330 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

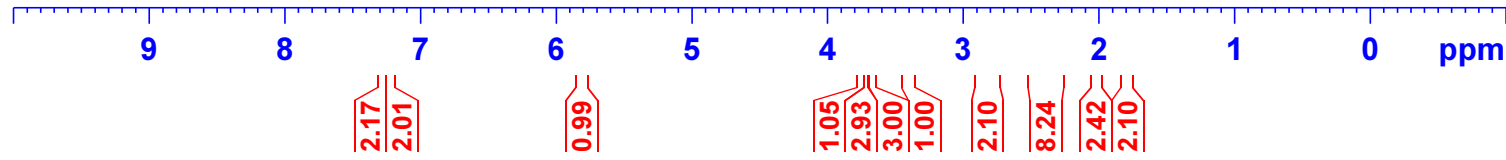
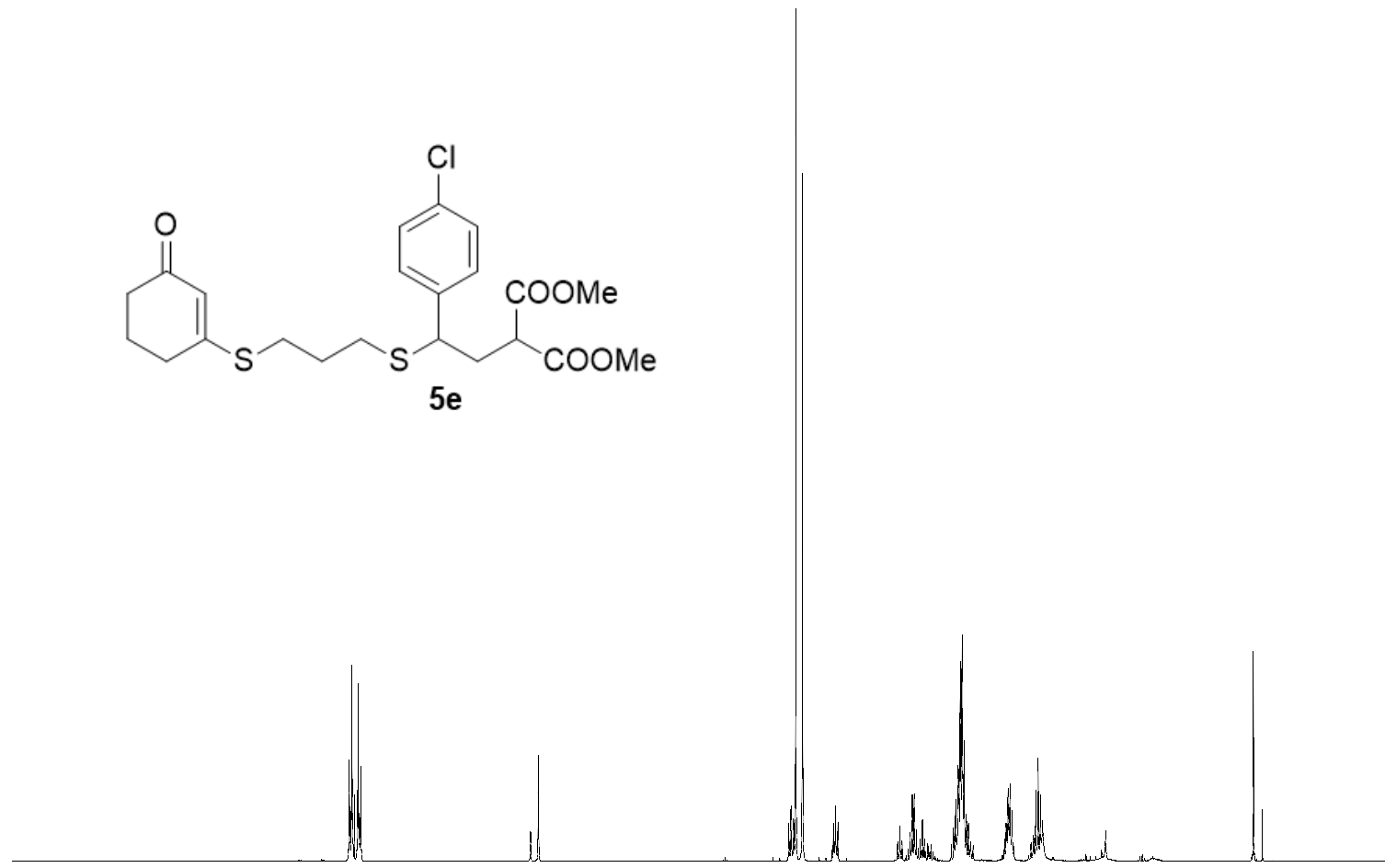
7.301  
7.279  
7.260  
7.235  
7.229  
7.223  
7.213  
7.207  
5.784  
3.777  
3.757  
3.739  
3.721  
3.668  
3.420  
3.403  
3.401  
3.383  
2.887  
2.787  
2.772  
2.754  
2.456  
2.439  
2.438  
2.420  
2.416  
2.403  
2.398  
2.388  
2.381  
2.370  
2.356  
2.353  
2.336  
2.035  
2.019  
2.004  
1.988  
1.818  
1.796  
1.778  
1.760  
1.743



Current Data Parameters  
NAME zjc-39 new rep  
EXPNO 2020070903  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200710  
Time\_ 1.05 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 203  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



— 195.58  
 — 169.11  
 — 169.06  
 — 165.05  
 — 165.04  
 — 139.49  
 — 133.31  
 — 129.10  
 — 128.90  
 — 119.46

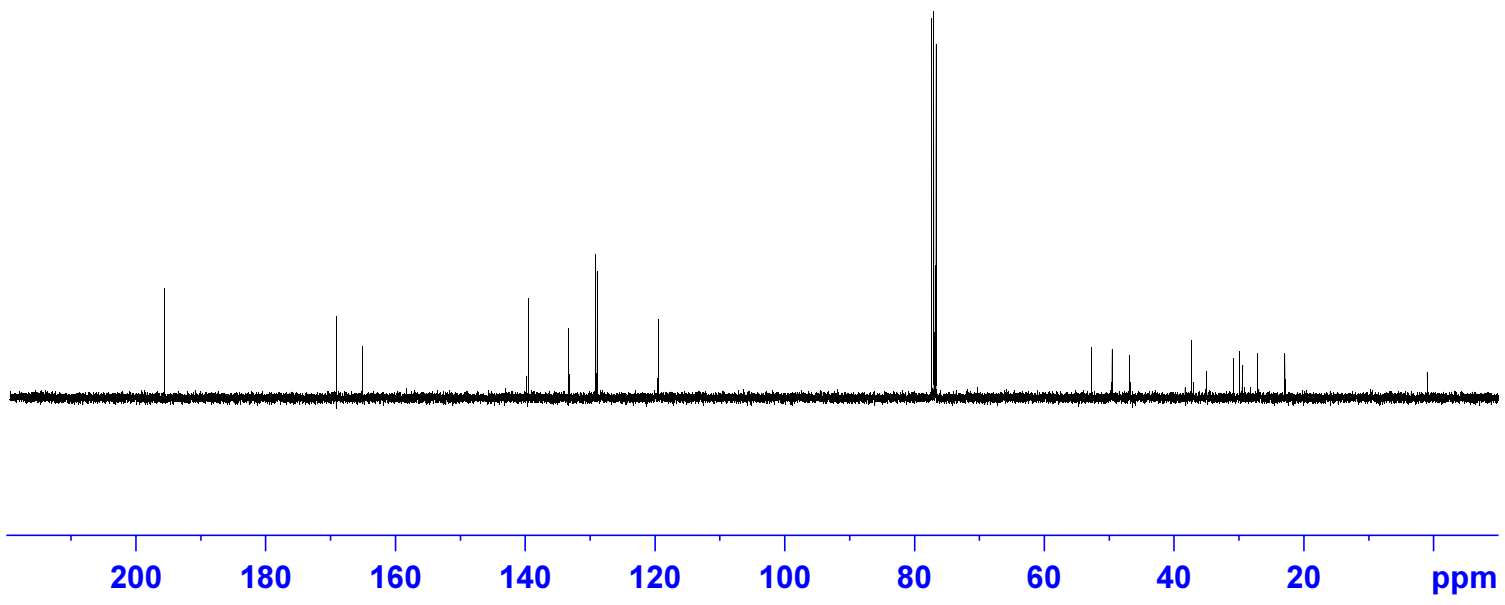
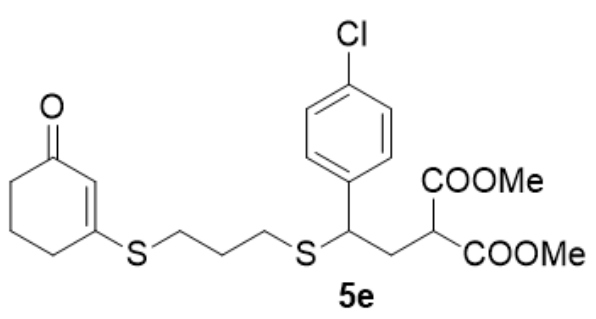
77.32  
 77.00  
 76.68

52.68  
 52.65  
 49.53  
 46.80  
 37.26  
 34.98  
 30.85  
 29.86  
 29.36  
 27.11  
 22.86

Current Data Parameters  
 NAME zjc-39 new rep  
 EXPNO 2020070904  
 PROCNO 1

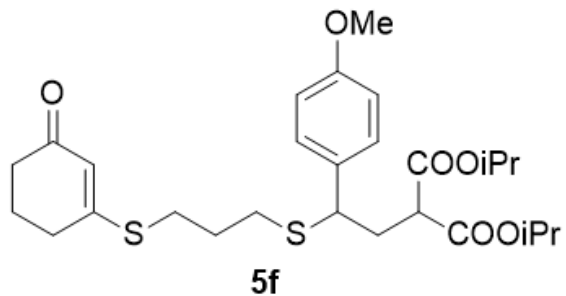
F2 - Acquisition Parameters  
 Date\_ 20200710  
 Time 2.50 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228330 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.40





7.260  
7.193  
7.171  
6.850  
6.828  
5.782  
5.059  
5.043  
5.027  
4.978  
4.962  
4.947  
3.784  
3.770  
3.753  
3.747  
3.730  
3.267  
3.251  
3.246  
3.230  
2.785  
2.770  
2.752  
2.426  
2.421  
2.412  
2.409  
2.399  
2.394  
2.383  
2.378  
2.361  
2.011  
1.996  
1.980  
1.794  
1.776  
1.759  
1.239  
1.224  
1.209  
1.193  
1.178

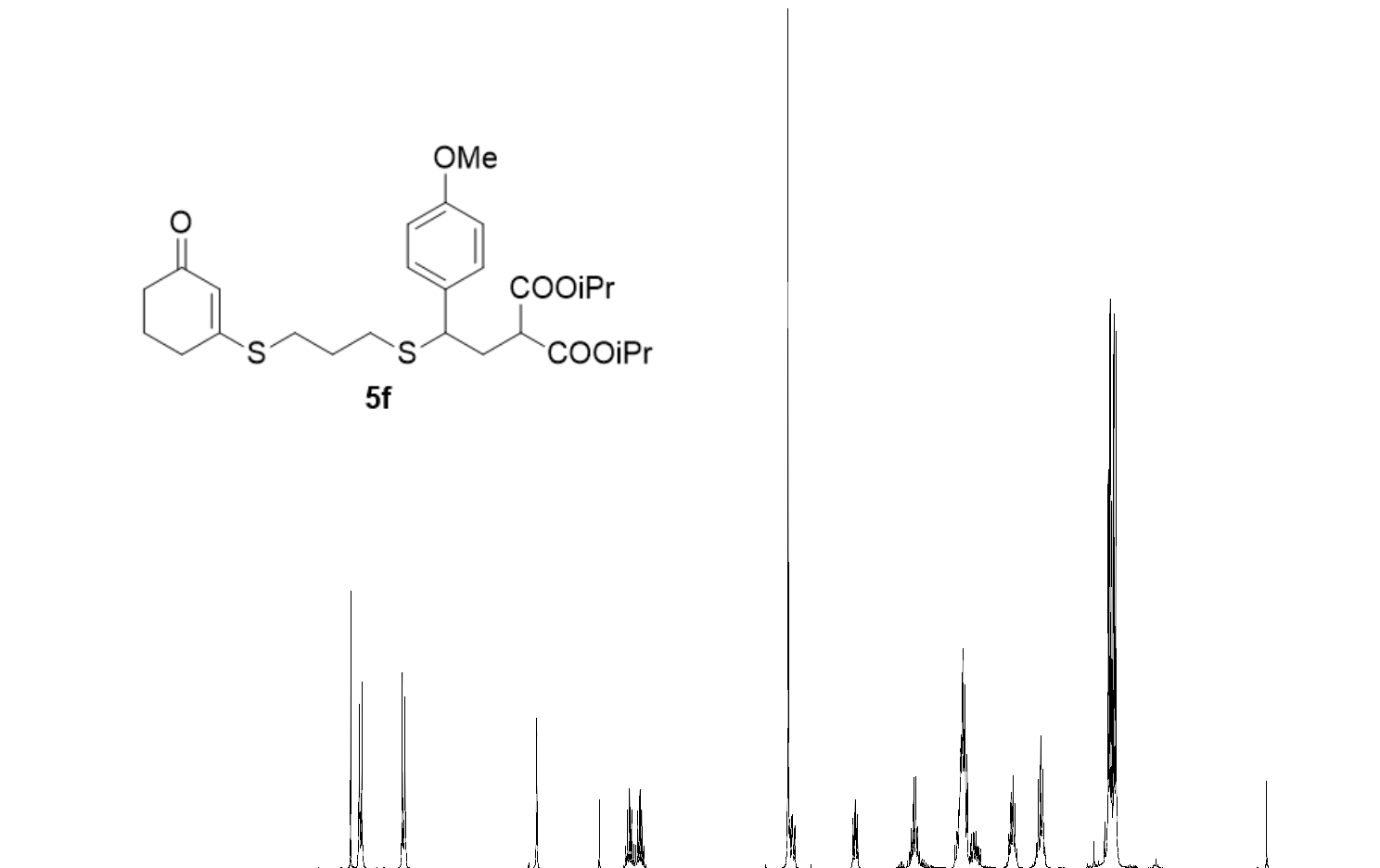


Current Data Parameters  
NAME yl--16  
EXPNO 2019052001  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190521  
Time\_ 0.17  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 64  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1

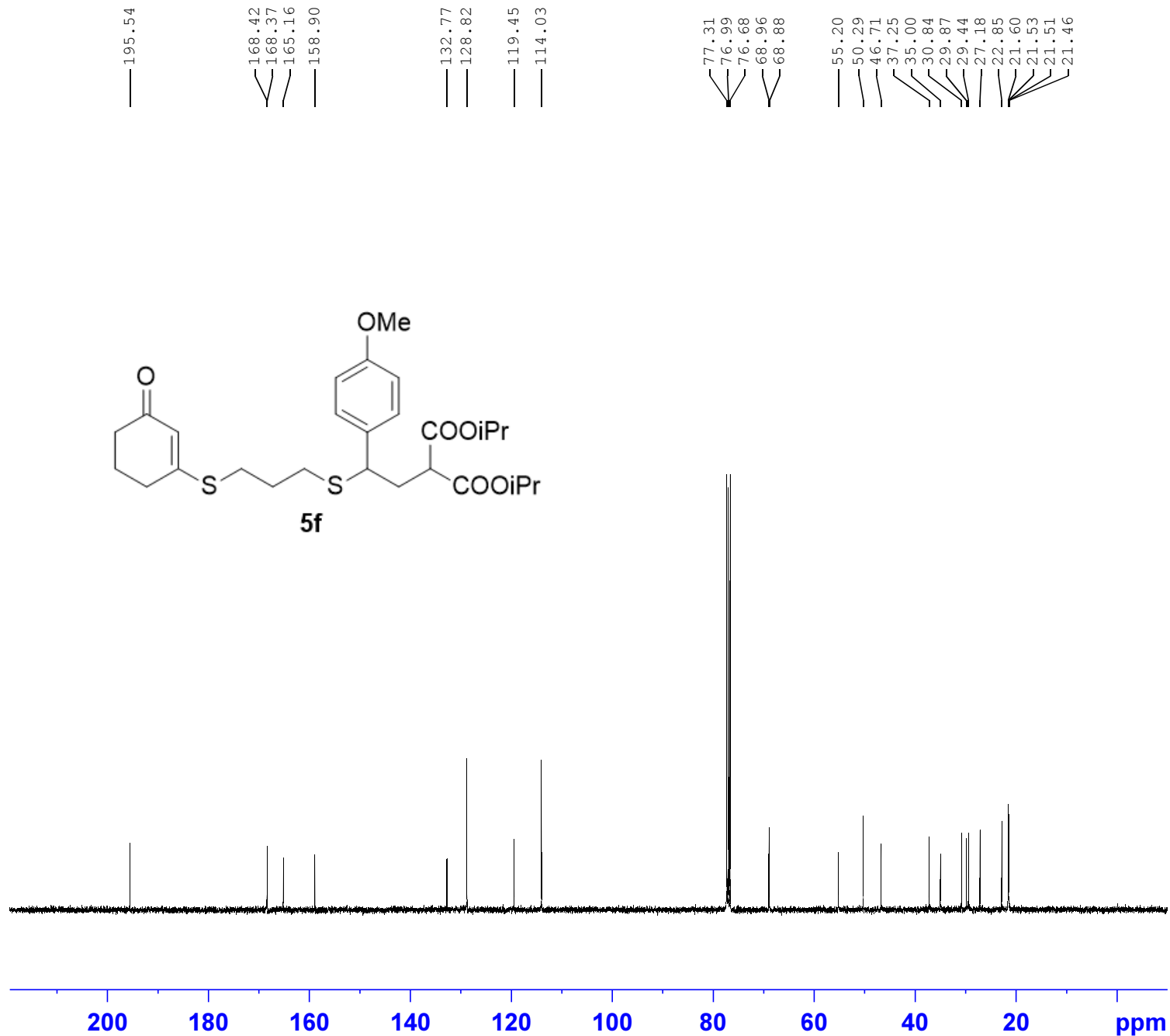
===== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1700153 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



9 8 7 6 5 4 3 2 1 0 ppm

1.99  
2.00  
0.95  
0.97  
0.99  
2.81  
1.18  
0.98  
1.89  
7.00  
1.13  
2.16  
2.49  
12.46



Current Data Parameters  
 NAME yl--16  
 EXPNO 2019052002  
 PROCNO 1

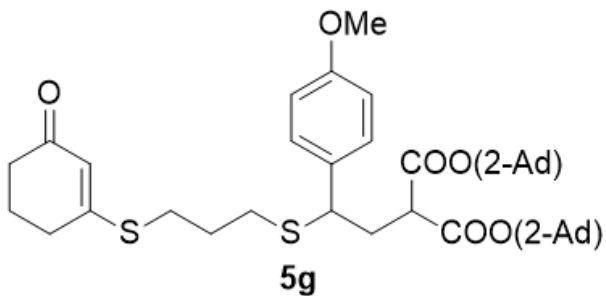
F2 - Acquisition Parameters  
 Date\_ 20190521  
 Time\_ 1.01  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 269  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228359 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

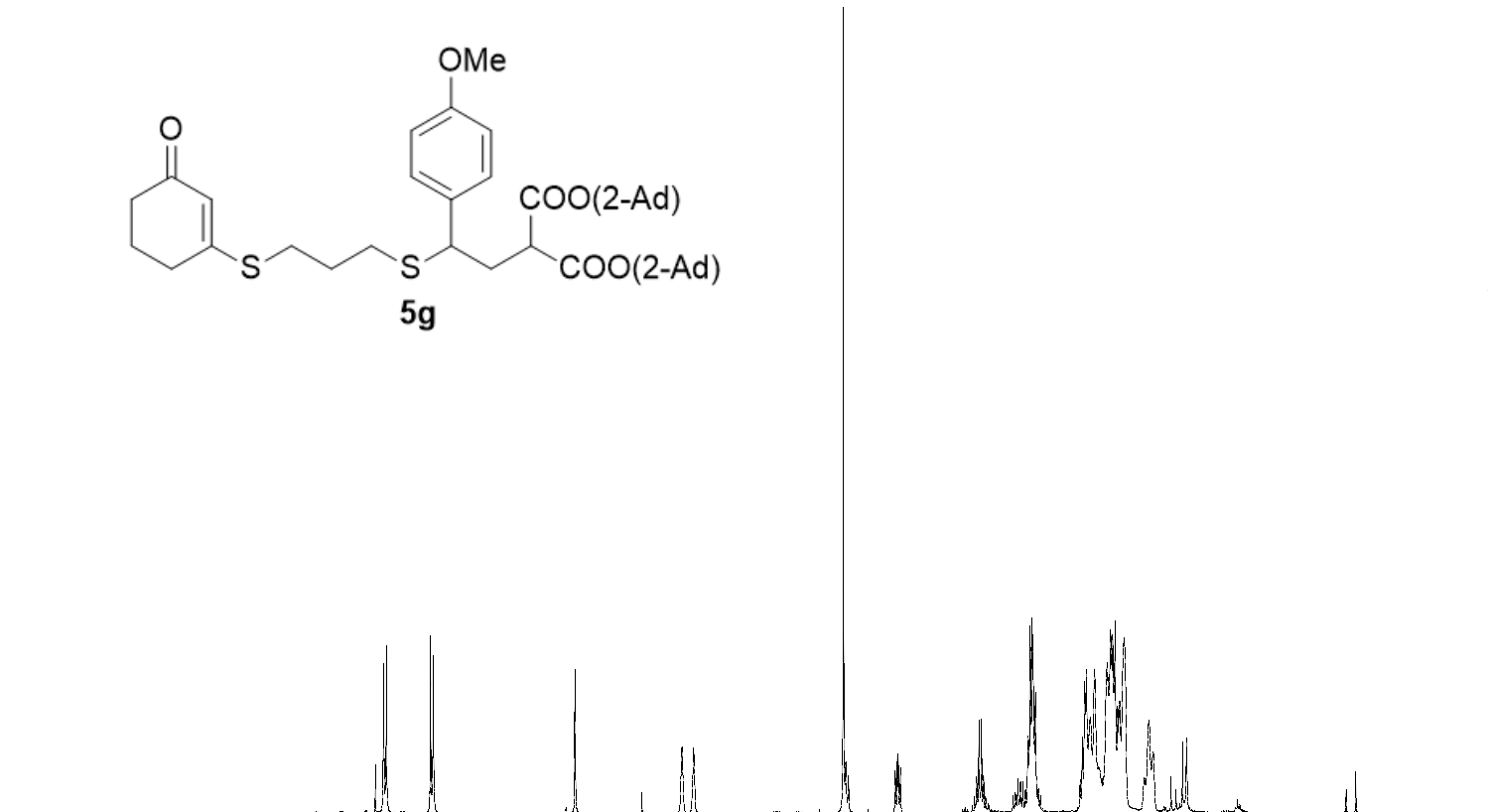
7.199  
7.178  
6.851  
6.829  
5.777  
4.983  
4.898  
3.785  
3.770  
3.763  
3.747  
3.399  
3.383  
3.377  
3.362  
2.795  
2.778  
2.760  
2.743  
2.413  
2.399  
2.394  
2.384  
2.377  
2.367  
2.359  
2.010  
1.994  
1.979  
1.962  
1.952  
1.920  
1.890  
1.827  
1.819  
1.802  
1.785  
1.767  
1.749  
1.733  
1.701  
1.549  
1.516  
1.484



Current Data Parameters  
NAME zjc-22 rep  
EXPNO 2020070201  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200702  
Time\_ 23.54 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 45.2  
DW 60.800 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

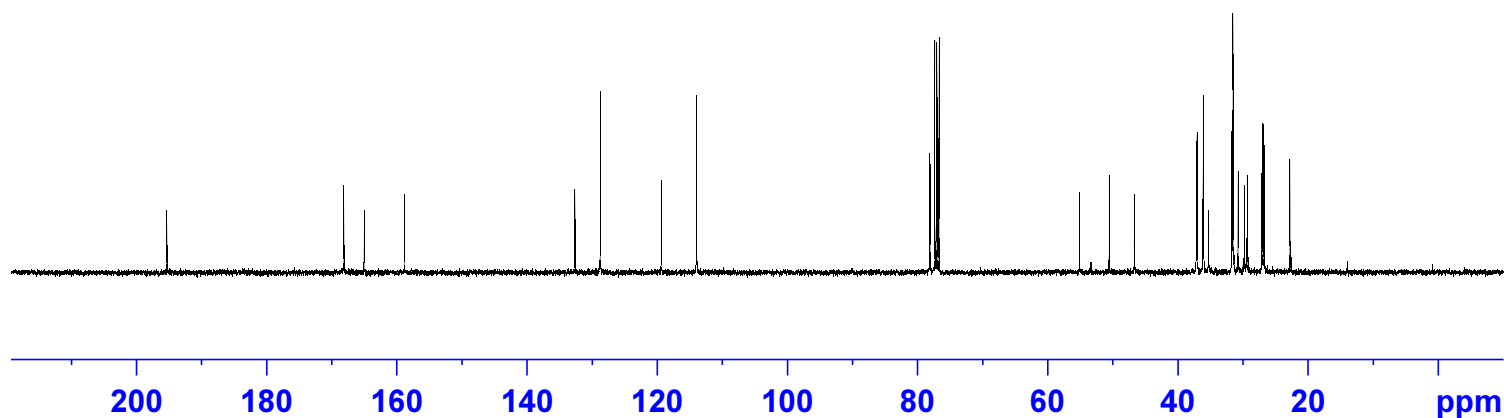
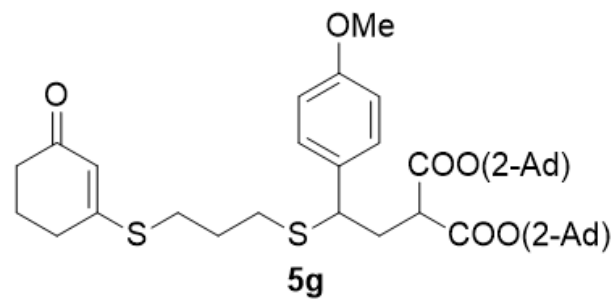


9 8 7 6 5 4 3 2 1 0 ppm

2.06  
2.06  
1.00  
1.04  
1.04  
4.22  
1.00  
2.11  
8.03  
10.73  
19.05  
4.34

— 195.33  
 — 168.19  
 — 168.13  
 — 165.00  
 — 158.80  
 — 132.62  
 — 128.72  
 — 119.33  
 — 113.94

78.12  
 78.05  
 77.32  
 77.00  
 76.68  
 55.09  
 50.55  
 46.68  
 37.15  
 37.08  
 37.06  
 36.11  
 36.06  
 36.03  
 35.25  
 31.74  
 31.65  
 31.60  
 31.52  
 31.50  
 30.74  
 29.77  
 29.34  
 27.10  
 26.95  
 26.92  
 26.73  
 26.71  
 22.77



Current Data Parameters  
 NAME zjc-22  
 EXPNO 2019052202  
 PROCNO 1

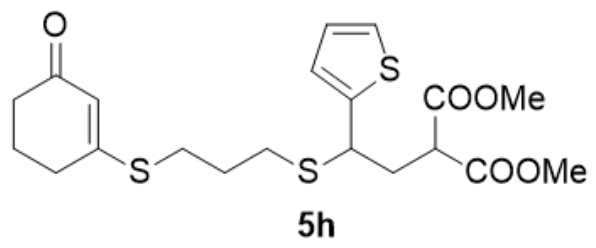
F2 - Acquisition Parameters  
 Date\_ 20190523  
 Time\_ 0.46  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 151  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228447 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

7.260  
7.239  
7.233  
7.230  
7.228  
7.224  
6.904  
6.899  
6.898  
6.893  
5.794  
4.117  
4.114  
3.732  
3.695  
3.544  
3.527  
3.524  
3.507  
2.809  
2.796  
2.523  
2.515  
2.506  
2.498  
2.488  
2.485  
2.480  
2.467  
2.441  
2.437  
2.423  
2.421  
2.409  
2.401  
2.398  
2.383  
2.365  
2.017  
2.002  
1.986  
1.828  
1.810  
1.793

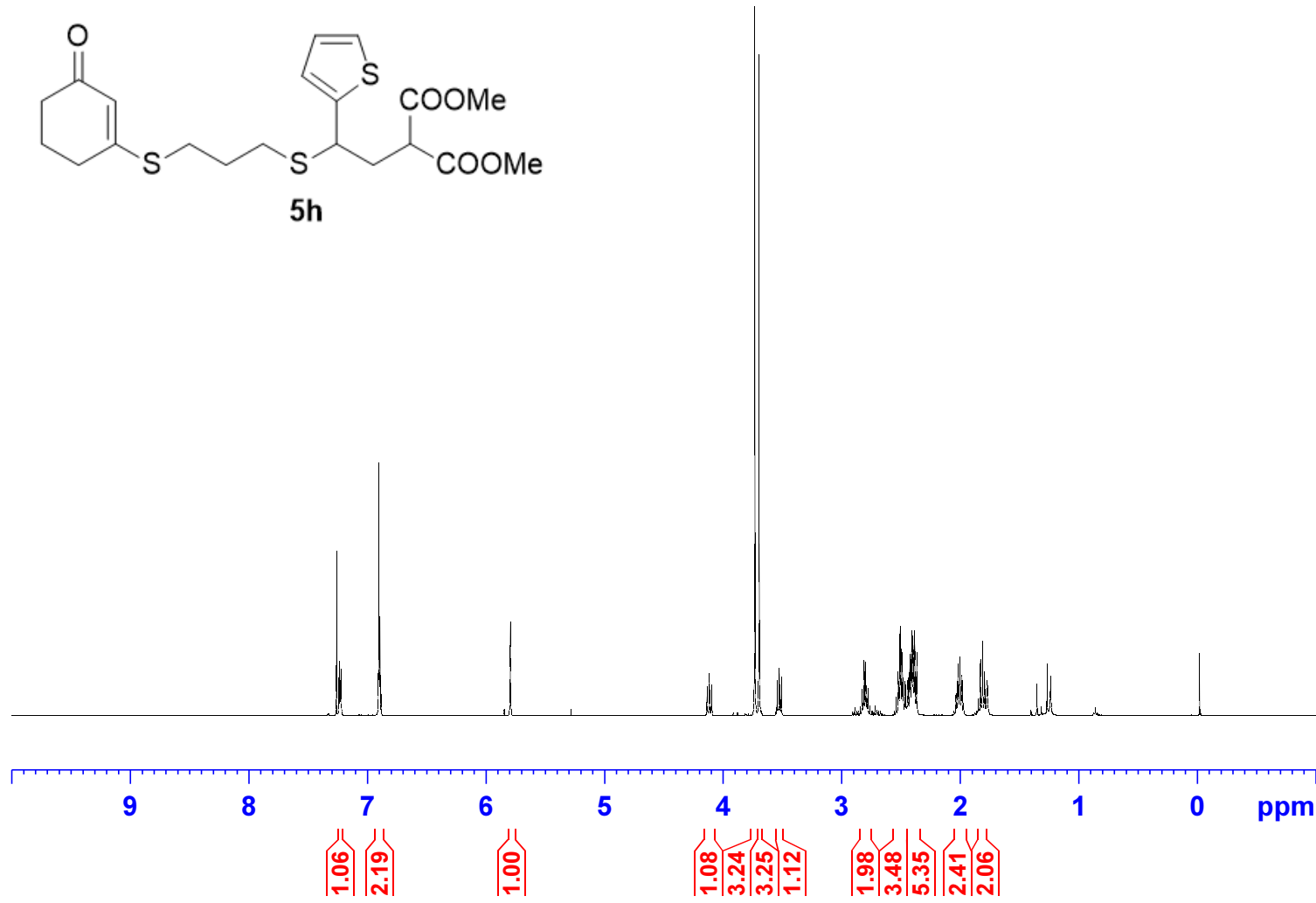


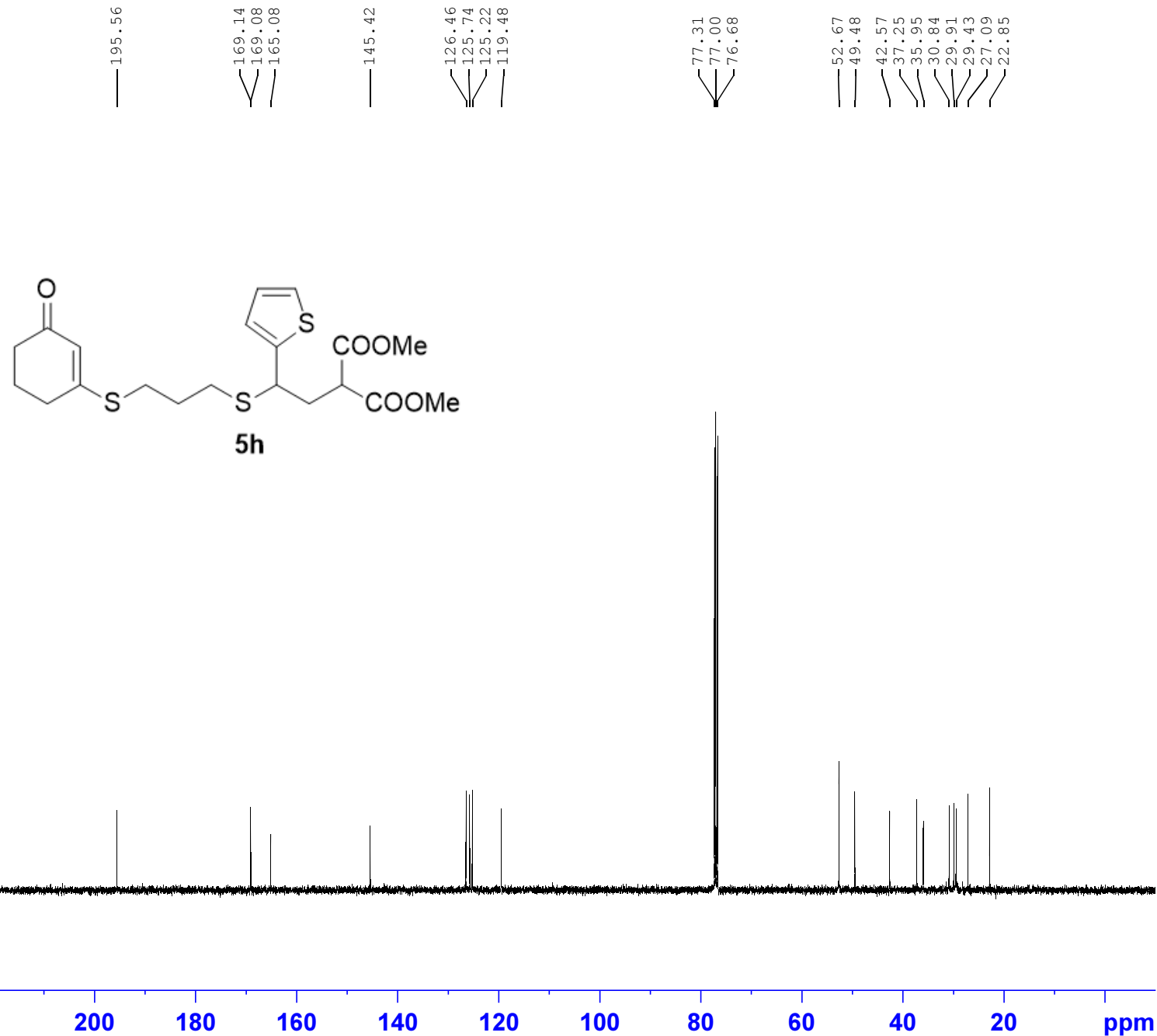
Current Data Parameters  
NAME zjc-19  
EXPNO 2019051701  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20190517  
Time\_ 15.46  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zg30  
TD 65536  
SOLVENT CDC13  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.125483 Hz  
AQ 3.9845889 sec  
RG 287  
DW 60.800 usec  
DE 6.50 usec  
TE 296.3 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
NUC1 1H  
P1 14.80 usec  
PL1 -1.00 dB  
PL1W 10.90985775 W  
SFO1 400.1724712 MHz

F2 - Processing parameters  
SI 32768  
SF 400.1700156 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





Current Data Parameters  
 NAME zjc-19  
 EXPNO 2019051702  
 PROCNO 1

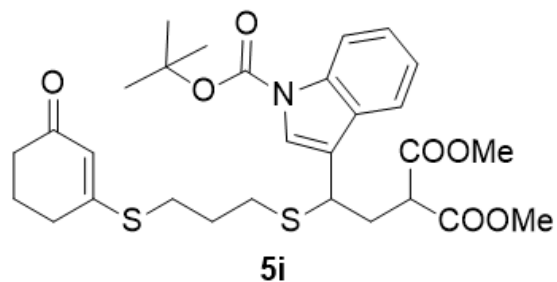
F2 - Acquisition Parameters  
 Date\_ 20190517  
 Time\_ 16.19  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 169  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228366 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

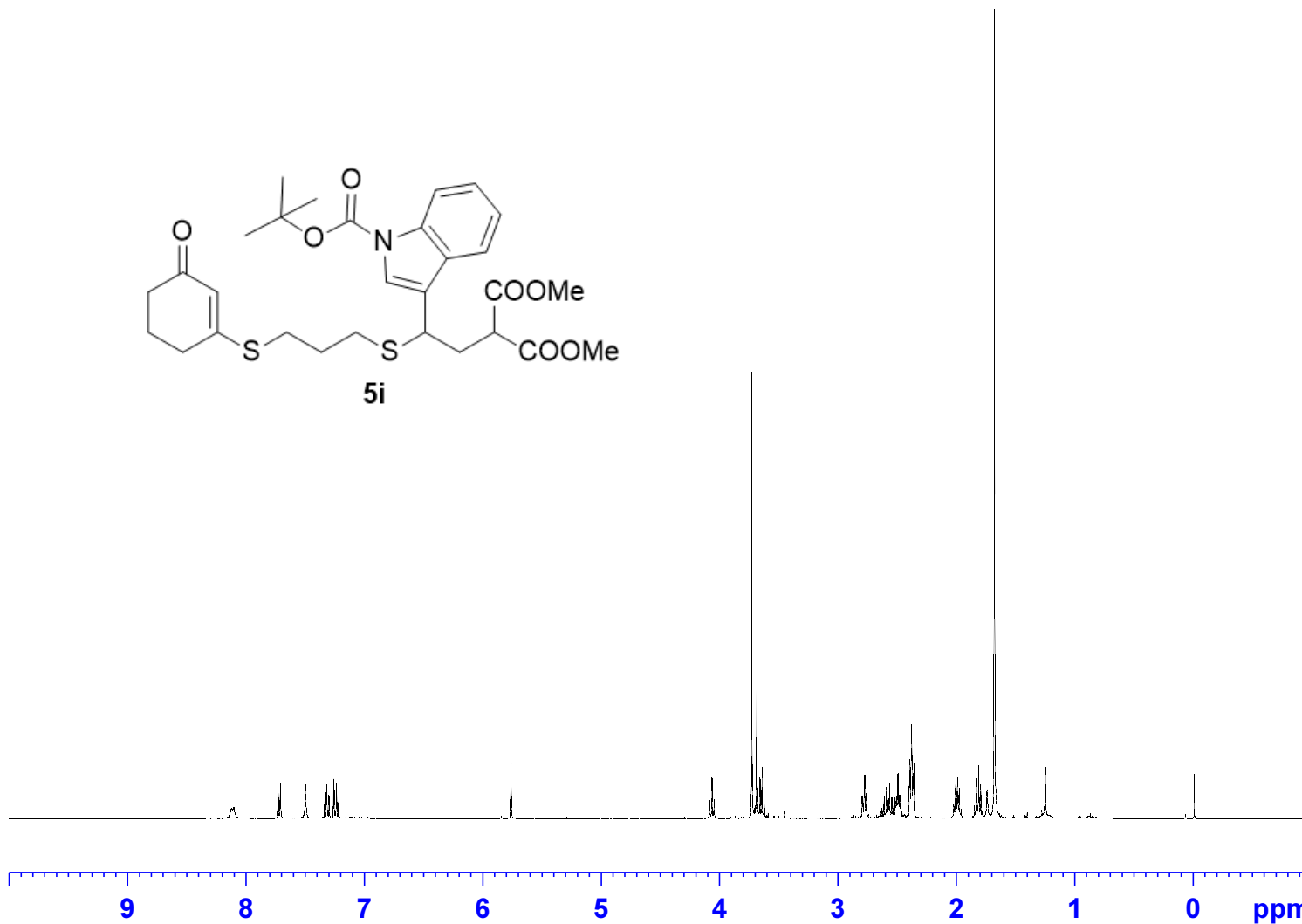
7.728  
7.709  
7.497  
7.320  
7.317  
7.299  
7.296  
7.260  
7.256  
7.253  
7.235  
5.761  
4.064  
3.726  
3.684  
3.658  
3.640  
3.622  
2.795  
2.790  
2.777  
2.772  
2.759  
2.755  
2.608  
2.590  
2.563  
2.544  
2.505  
2.497  
2.488  
2.480  
2.471  
2.391  
2.376  
2.363  
2.358  
2.005  
1.990  
1.974  
1.828  
1.810  
1.793  
1.677



Current Data Parameters  
NAME zjc-25 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.20 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 114  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

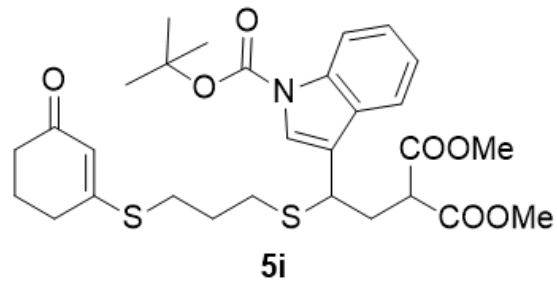


0.95  
1.10  
1.02  
1.14  
1.31  
1.00  
1.09  
3.05  
3.00  
1.33  
1.96  
4.19  
4.16  
2.29  
2.25  
9.40

195.56  
 169.37  
 169.24  
 165.11  
 149.48  
 135.80  
 128.45  
 124.80  
 123.68  
 122.57  
 119.97  
 119.63  
 119.46  
 115.36

83.98  
 77.31  
 76.99  
 76.68

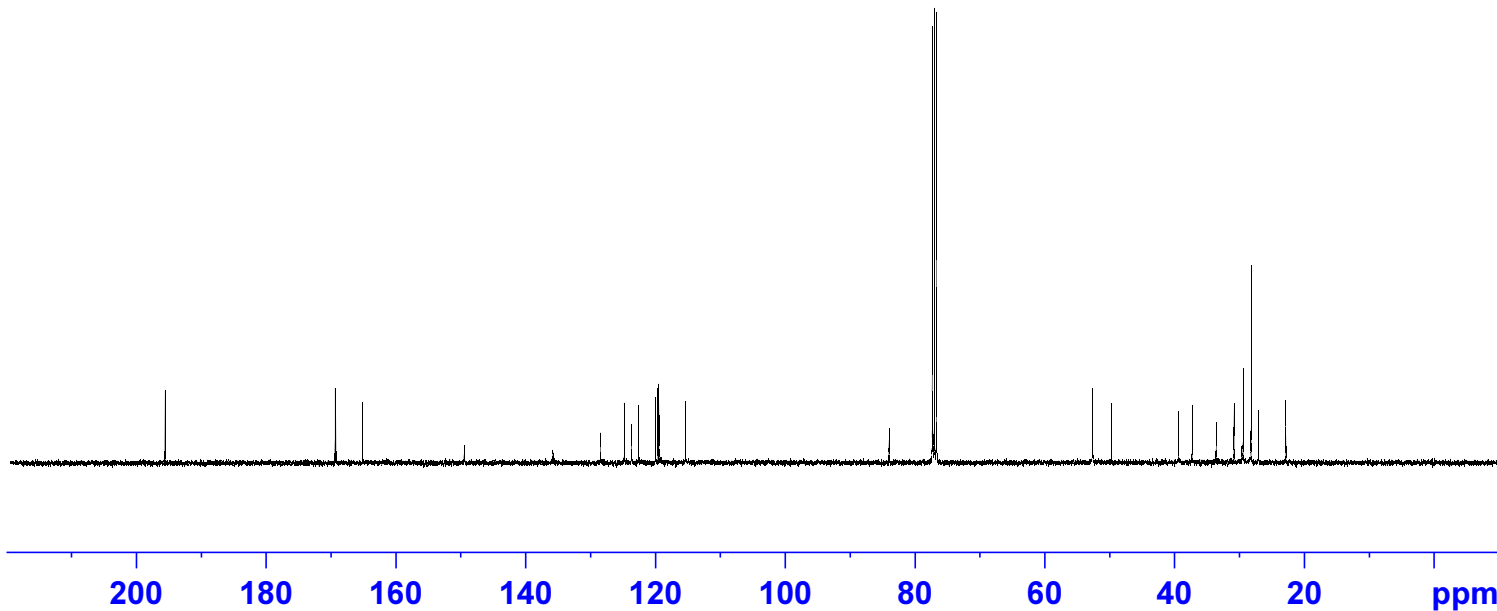
52.63  
 49.66  
 39.38  
 37.24  
 33.55  
 30.81  
 29.40  
 28.16  
 27.06  
 22.84



Current Data Parameters  
 NAME zjc-25 new  
 EXPNO 2020070602  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200707  
 Time\_ 3.53 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 365  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6228337 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



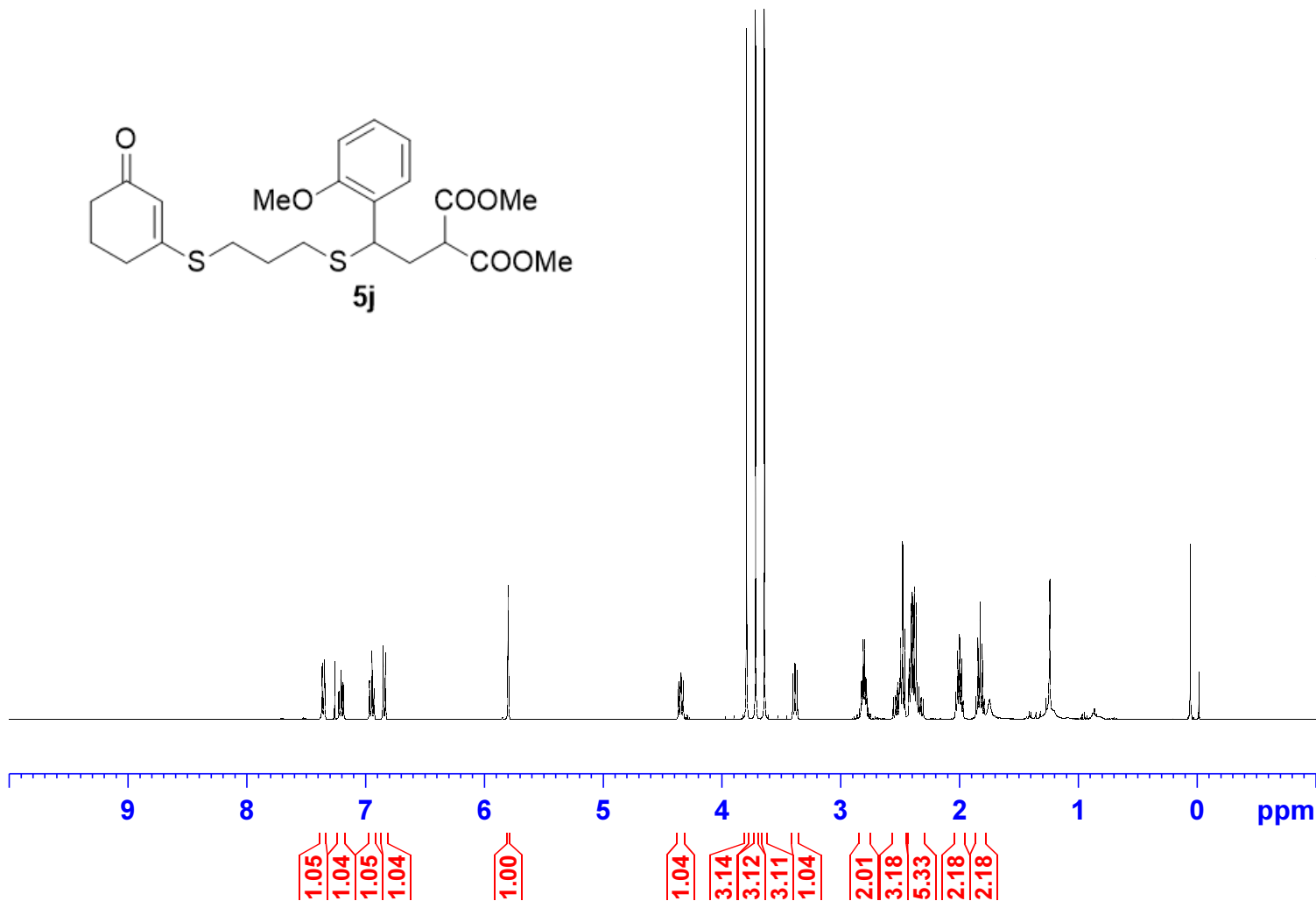
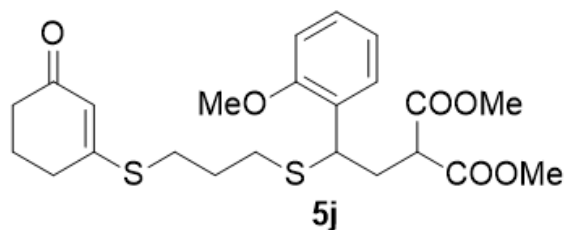


7.368  
7.364  
7.349  
7.345  
7.208  
7.206  
7.204  
6.966  
6.948  
6.853  
6.832  
5.799  
4.348  
4.342  
4.326  
3.793  
3.717  
3.642  
3.402  
3.387  
3.381  
3.366  
2.828  
2.818  
2.810  
2.800  
2.791  
2.782  
2.501  
2.496  
2.484  
2.478  
2.461  
2.424  
2.408  
2.396  
2.380  
2.363  
2.015  
1.999  
1.983  
1.844  
1.826  
1.808

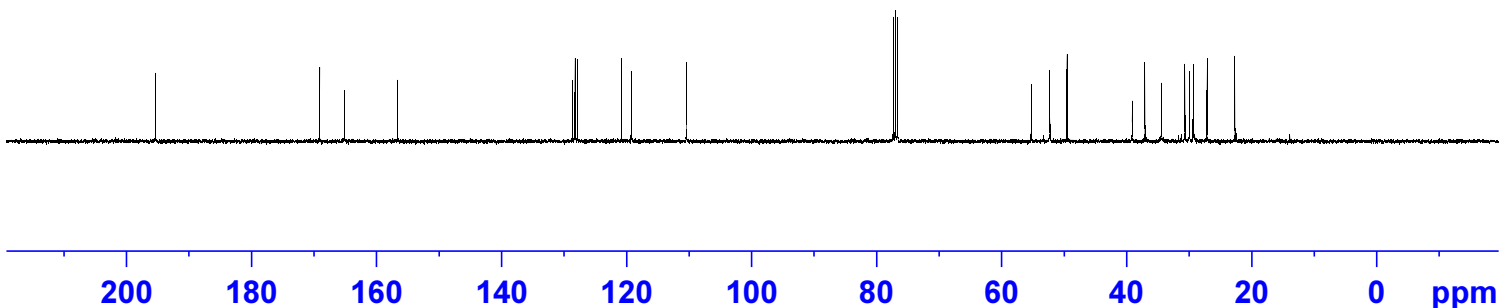
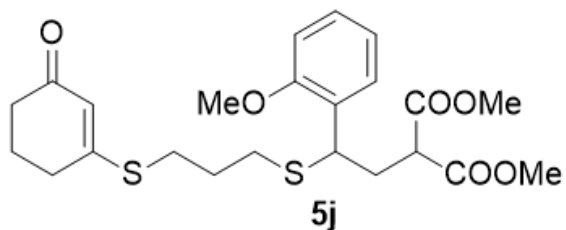
Current Data Parameters  
NAME zjc-34 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 1.28 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.9 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



195.34  
 169.16  
 169.07  
 165.16  
 156.63  
 128.70  
 128.27  
 127.85  
 120.85  
 119.27  
 110.43  
 77.31  
 77.00  
 76.68  
 55.26  
 52.34  
 52.31  
 49.56  
 39.10  
 37.10  
 34.47  
 30.69  
 29.95  
 29.29  
 27.13  
 22.71



Current Data Parameters  
 NAME zjc-34  
 EXPNO 2019061903  
 PROCNO 1

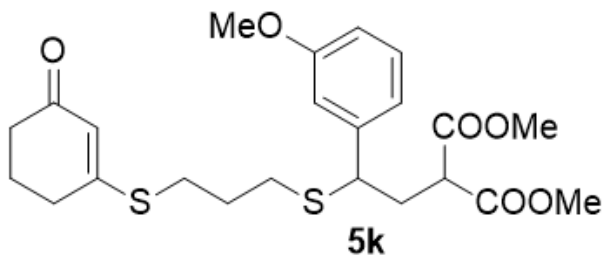
F2 - Acquisition Parameters  
 Date\_ 20190620  
 Time\_ 4.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 64  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

==== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228491 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

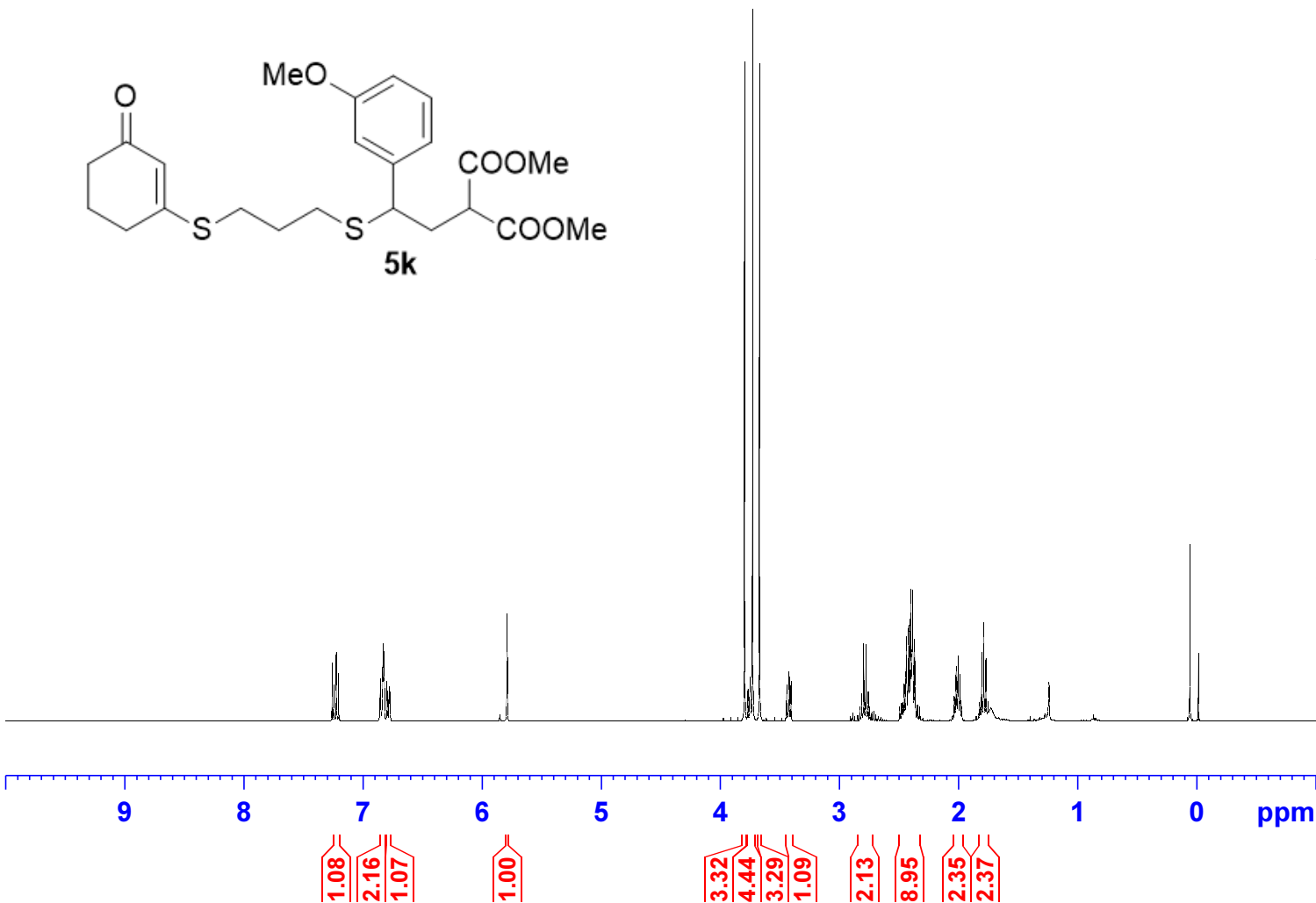
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7.225  
7.206  
6.853  
6.831  
6.824  
6.821  
6.801  
6.800  
6.795  
6.781  
6.779  
5.791  
3.796  
3.768  
3.750  
3.747  
3.729  
3.671  
3.442  
3.425  
3.422  
3.405  
2.795  
2.777  
2.759  
2.460  
2.454  
2.442  
2.437  
2.421  
2.417  
2.406  
2.401  
2.389  
2.385  
2.368  
2.363  
2.019  
2.003  
1.987  
1.805  
1.787  
1.770



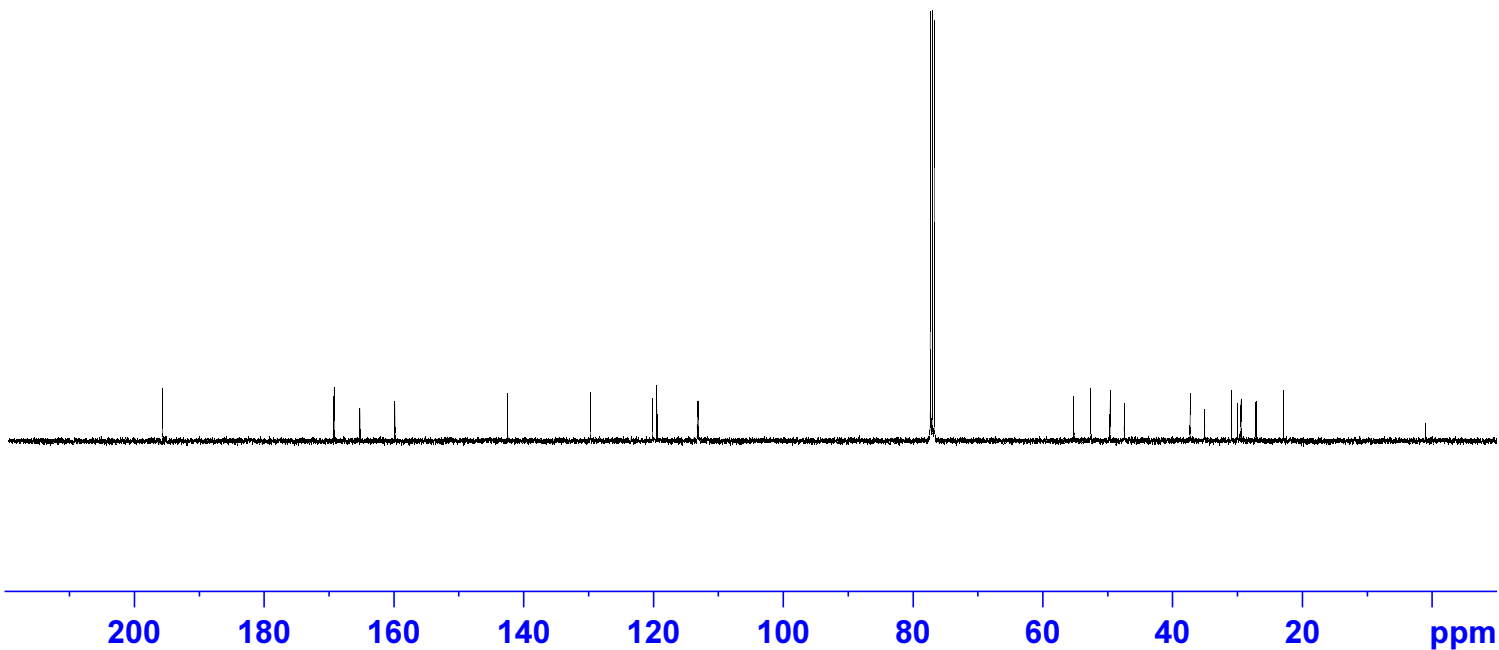
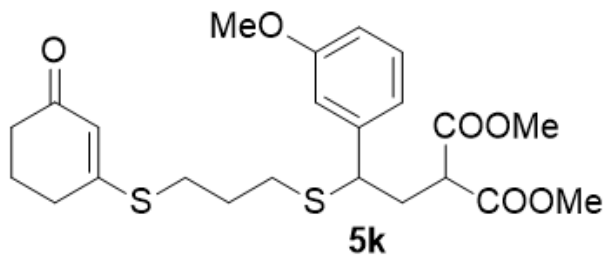
Current Data Parameters  
NAME zjc-30 new  
EXPNO 2020070601  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200707  
Time\_ 0.10 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 161  
DW 60.800 usec  
DE 6.50 usec  
TE 296.5 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700090 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



195.63  
 169.27  
 169.21  
 165.21  
 159.83  
 142.43  
 129.71  
 120.13  
 119.47  
 113.24  
 113.07  
 77.32  
 77.00  
 76.68  
 55.21  
 52.62  
 49.61  
 47.44  
 37.26  
 35.03  
 30.86  
 29.95  
 29.43  
 27.12  
 22.87



Current Data Parameters  
 NAME zjc-30 new  
 EXPNO 2020070602  
 PROCNO 1

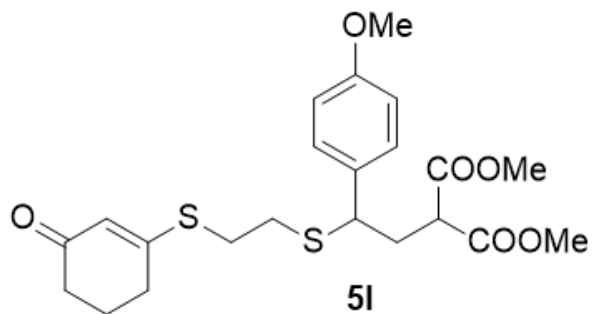
F2 - Acquisition Parameters

Date\_ 20200707  
 Time\_ 0.26 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 200  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters

SI 32768  
 SF 100.6228323 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

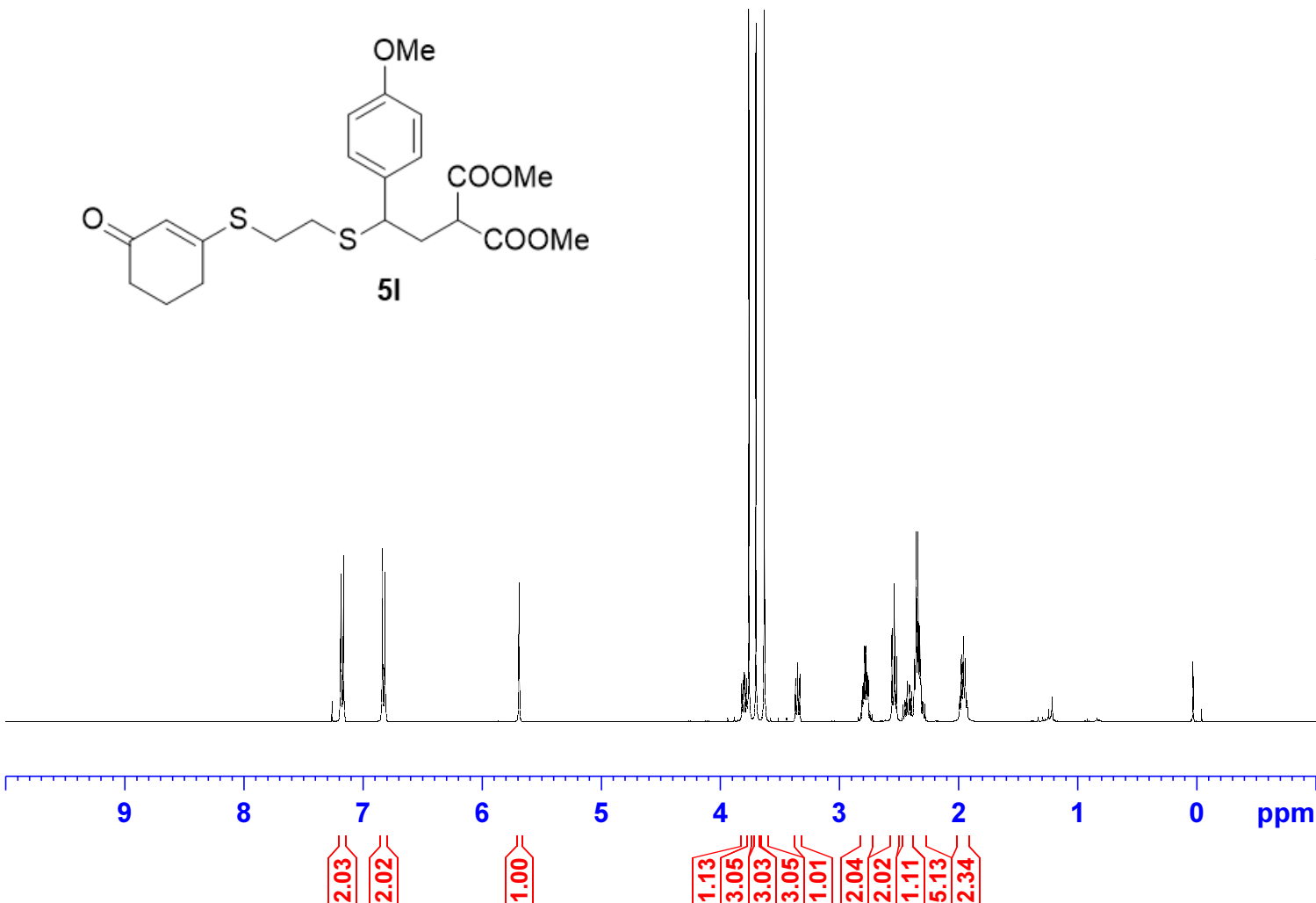
7.186  
7.164  
6.837  
6.815  
5.689  
3.820  
3.803  
3.797  
3.781  
3.760  
3.700  
3.630  
3.369  
3.353  
3.348  
3.332  
2.806  
2.796  
2.787  
2.776  
2.767  
2.759  
2.558  
2.539  
2.520  
2.467  
2.450  
2.431  
2.415  
2.411  
2.394  
2.370  
2.355  
2.341  
2.331  
2.324  
2.315  
2.303  
2.296  
1.990  
1.974  
1.959  
1.943  
1.927



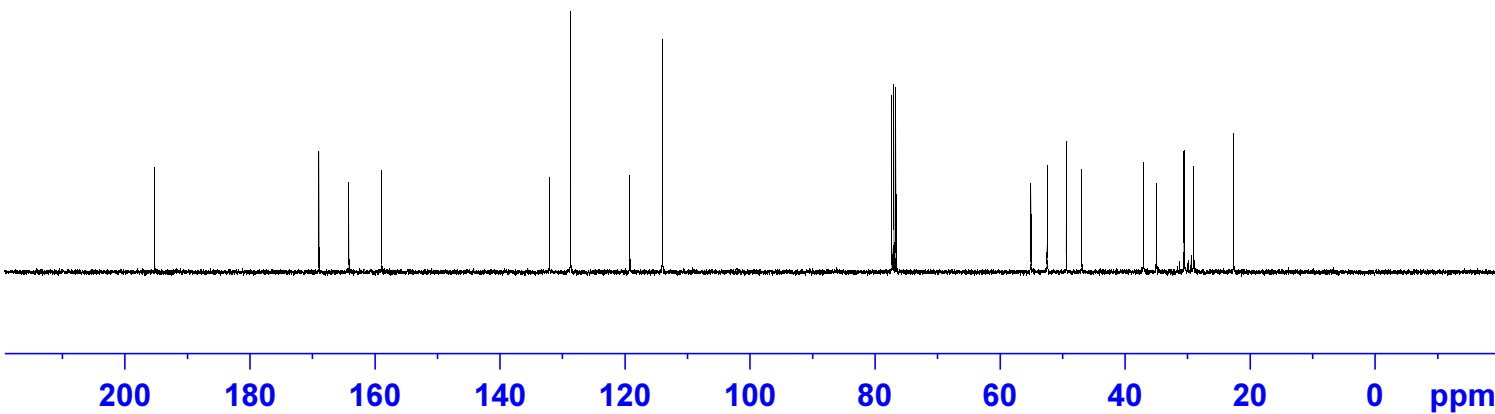
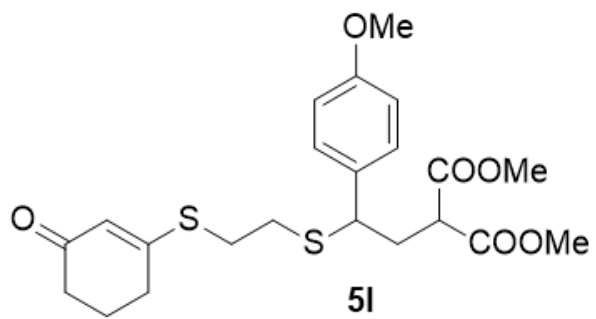
Current Data Parameters  
NAME yl-48 rep  
EXPNO 2020070201  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200703  
Time\_ 0.03 h  
INSTRUM spect  
PROBHD z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 45.2  
DW 60.800 usec  
DE 6.50 usec  
TE 296.7 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700087 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00



195.24  
 169.00  
 168.95  
 164.20  
 158.93  
 132.06  
 128.70  
 119.26  
 114.03  
 77.31  
 77.00  
 76.68  
 55.06  
 52.46  
 52.43  
 49.40  
 46.95  
 37.06  
 34.99  
 30.60  
 30.52  
 29.02  
 22.64



Current Data Parameters  
 NAME y1-48  
 EXPNO 2019061902  
 PROCNO 1

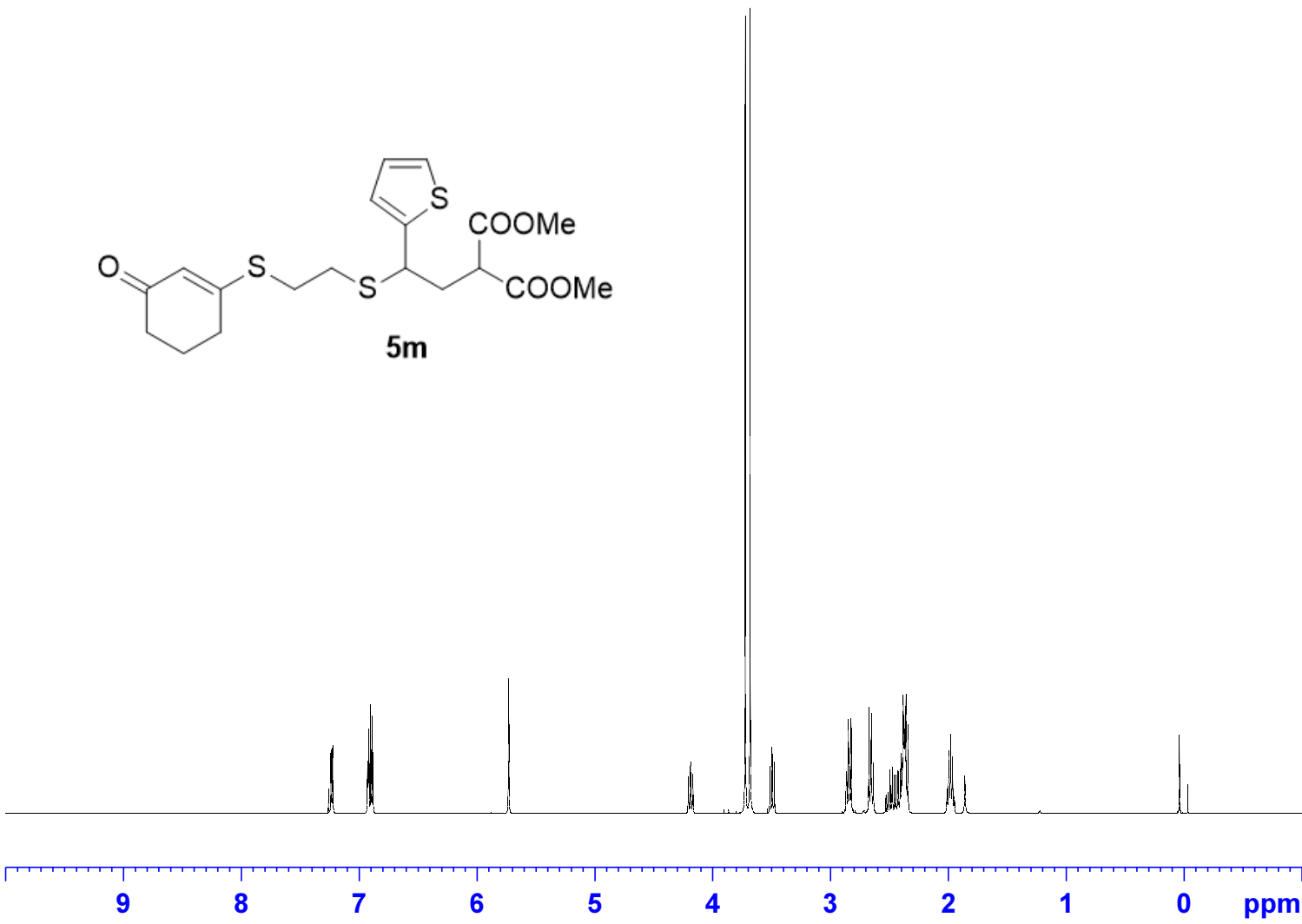
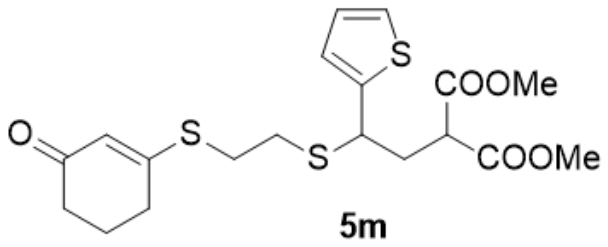
F2 - Acquisition Parameters  
 Date\_ 20190620  
 Time 5.37  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 96  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228484 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

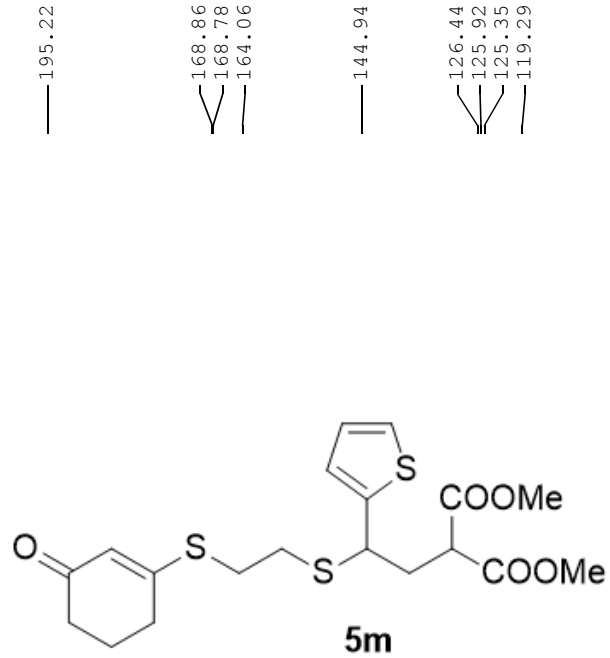
7.240  
7.237  
7.227  
7.224  
6.929  
6.927  
6.926  
6.920  
6.918  
6.902  
6.893  
6.890  
6.881  
5.731  
4.188  
4.185  
3.723  
3.682  
3.513  
3.496  
3.493  
3.476  
2.847  
2.843  
2.840  
2.825  
2.673  
2.652  
2.635  
2.494  
2.476  
2.474  
2.428  
2.407  
2.397  
2.388  
2.382  
2.375  
2.368  
2.360  
2.342  
1.995  
1.980  
1.963



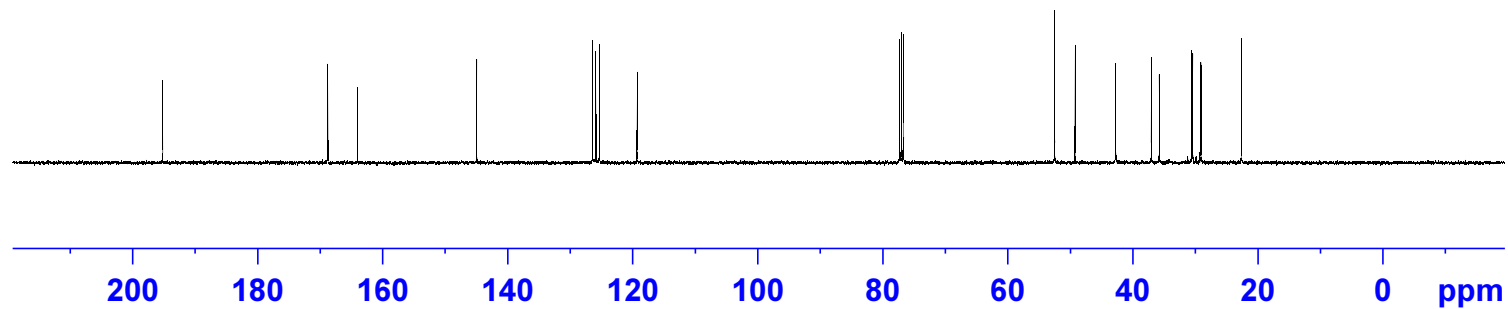
Current Data Parameters  
 NAME yl-60 rep  
 EXPNO 2020070201  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200702  
 Time\_ 23.41 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDC13  
 NS 16  
 DS 2  
 SWH 8223.685 Hz  
 FIDRES 0.250967 Hz  
 AQ 3.9845889 sec  
 RG 90.5  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 296.5 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 400.1724712 MHz  
 NUC1 1H  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 15.00000000 W

F2 - Processing parameters  
 SI 32768  
 SF 400.1700089 MHz  
 WDW no  
 SSB 0  
 LB 0 Hz  
 GB 0  
 PC 1.00



195.22  
 168.86  
 168.78  
 164.06  
 144.94  
 126.44  
 125.92  
 125.35  
 119.29  
 77.31  
 76.99  
 76.68  
 52.52  
 49.25  
 42.75  
 37.05  
 35.80  
 30.58  
 30.40  
 29.08  
 22.63



Current Data Parameters  
 NAME yl-60  
 EXPNO 2019061902  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20190620  
 Time 5.28  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 134  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

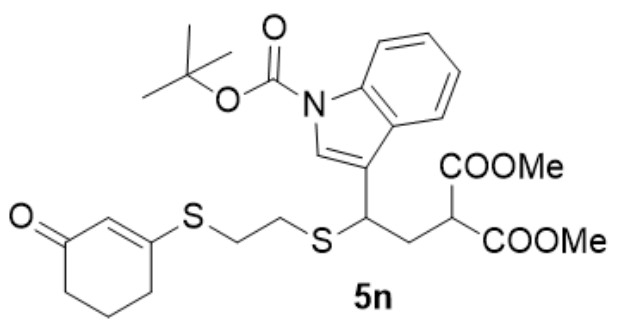
===== CHANNEL f1 =====  
 NUC1 13C  
 P1 9.90 usec  
 PL1 -1.10 dB  
 PL1W 40.29647064 W  
 SFO1 100.6328888 MHz

===== CHANNEL f2 =====  
 CPDPRG[2] waltz16  
 NUC2 1H  
 PCPD2 90.00 usec  
 PL2 -1.00 dB  
 PL12 14.68 dB  
 PL13 17.68 dB  
 PL2W 10.90985775 W  
 PL12W 0.29499799 W  
 PL13W 0.14784923 W  
 SFO2 400.1716007 MHz

F2 - Processing parameters  
 SI 32768  
 SF 100.6228506 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



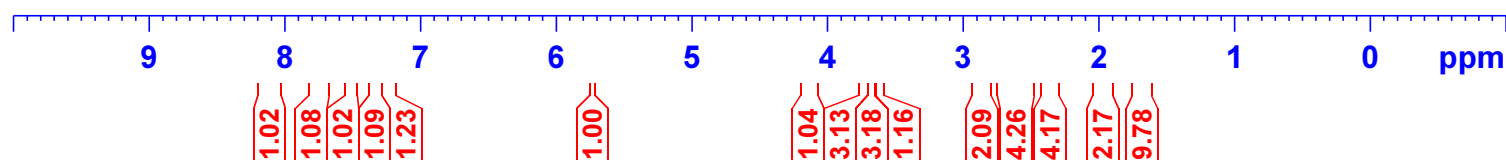
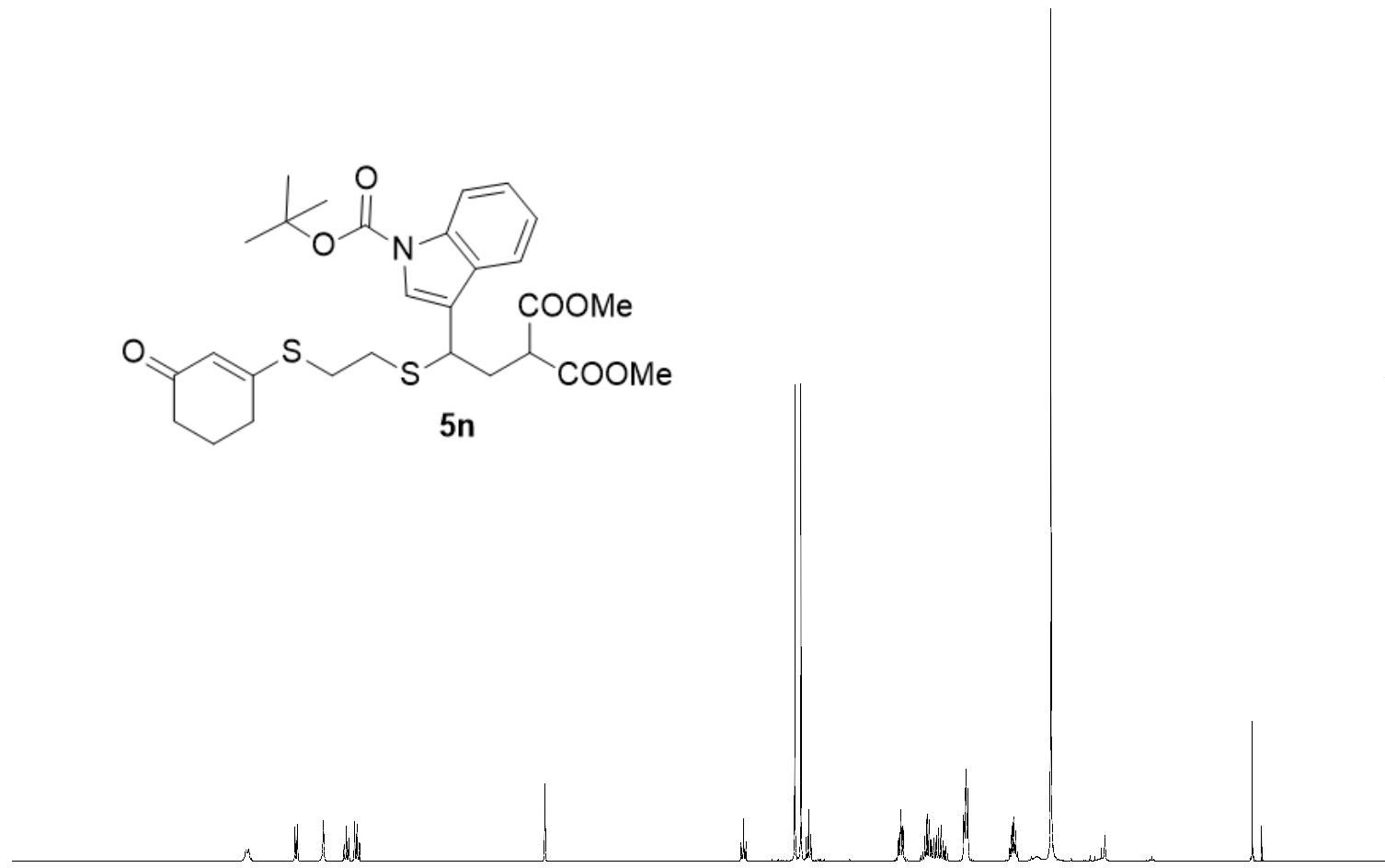
7.735  
7.716  
7.715  
7.509  
7.324  
7.322  
7.304  
7.301  
7.260  
7.258  
7.255  
7.238  
7.235  
5.732  
4.140  
4.120  
3.728  
3.680  
3.636  
3.618  
3.600  
2.902  
2.896  
2.884  
2.863  
2.686  
2.671  
2.668  
2.654  
2.650  
2.633  
2.612  
2.594  
2.576  
2.557  
2.538  
2.376  
2.369  
2.357  
2.342  
1.990  
1.974  
1.958  
1.675

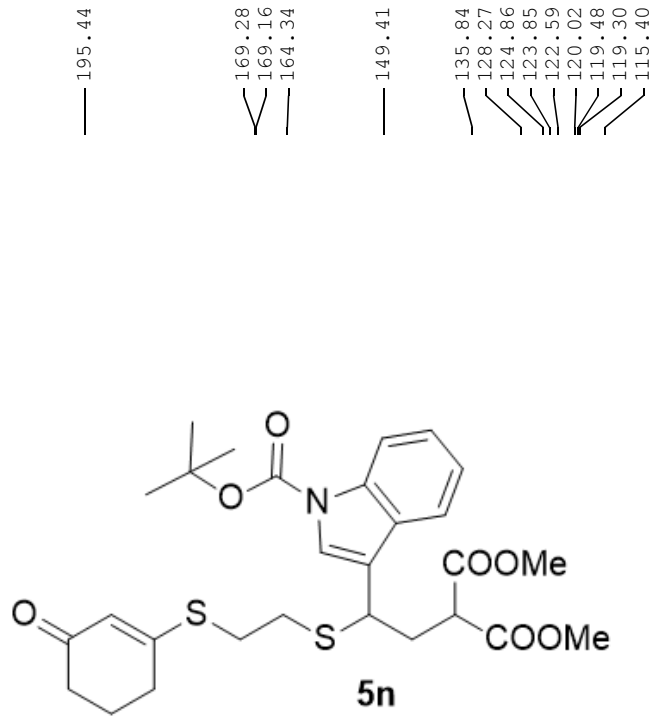


Current Data Parameters  
NAME yl-49 new  
EXPNO 2020070201  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200702  
Time\_ 23.58 h  
INSTRUM spect  
PROBHD Z108618\_0256 (  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8223.685 Hz  
FIDRES 0.250967 Hz  
AQ 3.9845889 sec  
RG 101  
DW 60.800 usec  
DE 6.50 usec  
TE 296.6 K  
D1 1.00000000 sec  
TD0 1  
SFO1 400.1724712 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 15.00000000 W

F2 - Processing parameters  
SI 32768  
SF 400.1700089 MHz  
WDW no  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00





195.44  
 169.28  
 169.16  
 164.34  
 149.41  
 135.84  
 128.27  
 124.86  
 123.85  
 122.59  
 120.02  
 119.48  
 119.30  
 115.40  
 84.07  
 77.32  
 77.00  
 76.68  
 52.68  
 52.65  
 49.59  
 39.80  
 37.18  
 33.61  
 30.72  
 30.70  
 28.83  
 28.14  
 22.77

Current Data Parameters  
 NAME yl-49 new  
 EXPNO 2020070202  
 PROCNO 1

F2 - Acquisition Parameters

Date\_ 20200703  
 Time\_ 0.33 h  
 INSTRUM spect  
 PROBHD Z108618\_0256 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDC13  
 NS 308  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.733596 Hz  
 AQ 1.3631488 sec  
 RG 2050  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 100.6328888 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 50.00000000 W  
 SFO2 400.1716007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 90.00 usec  
 PLW2 15.00000000 W  
 PLW12 0.18519001 W  
 PLW13 0.09314700 W

F2 - Processing parameters

SI 32768  
 SF 100.6228345 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

