

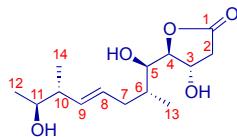
## An expedient total synthesis of mupirocin H.

N. Hari krishna, Y. Sridhar, A. Krishnam Raju, P. Srihari\*

### Contents:

1. $^1\text{H}$ and $^{13}\text{C}$ NMR data of mupirocin H (comparative tables)	S2
2. $^1\text{H}$ and $^{13}\text{C}$ NMR spectra of new compounds	S3- S17
3. References	S18

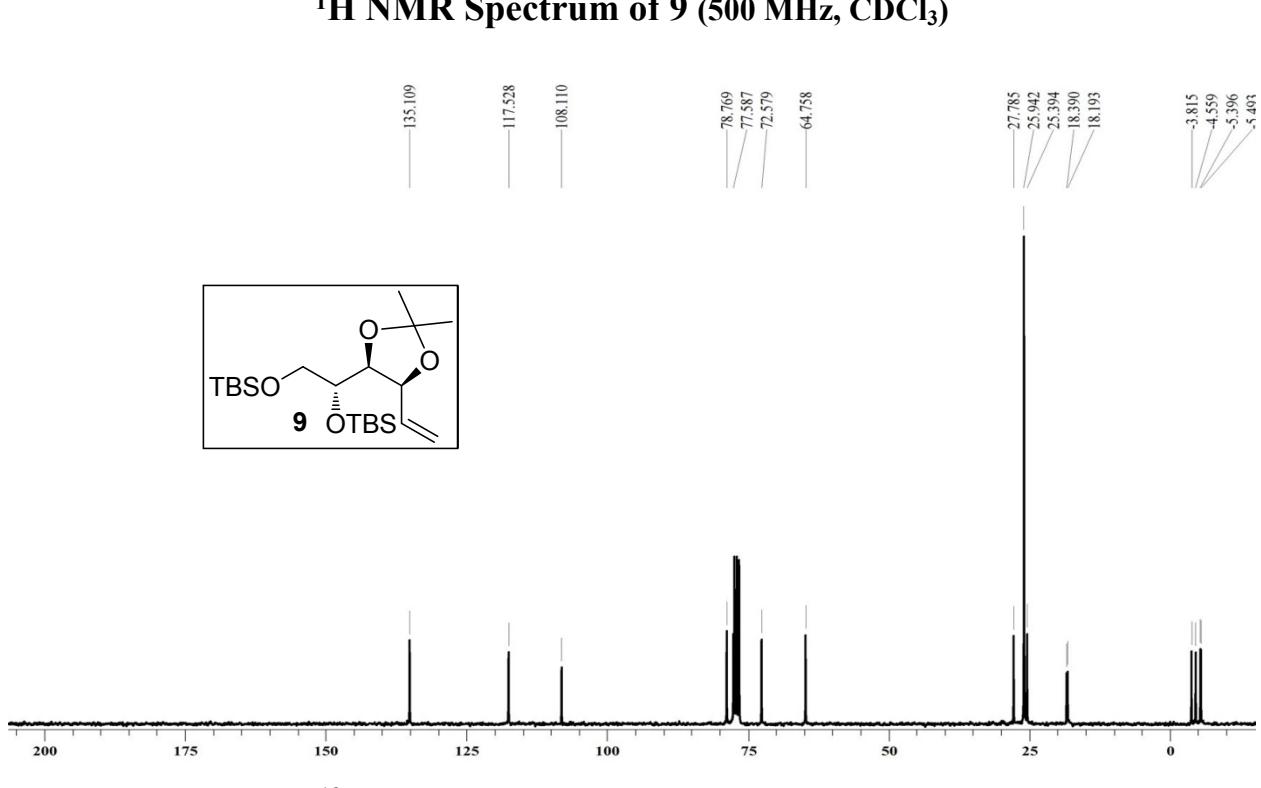
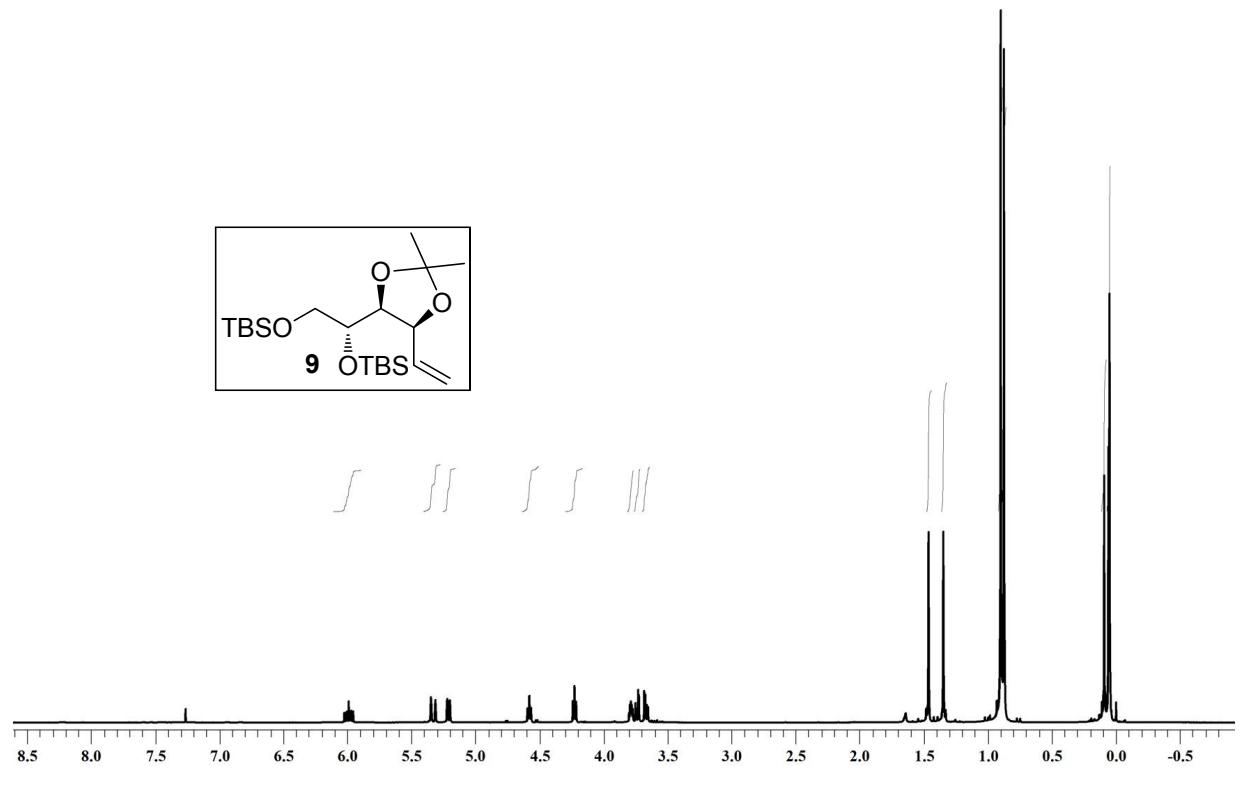
<sup>1</sup>H NMR spectral comparative table :

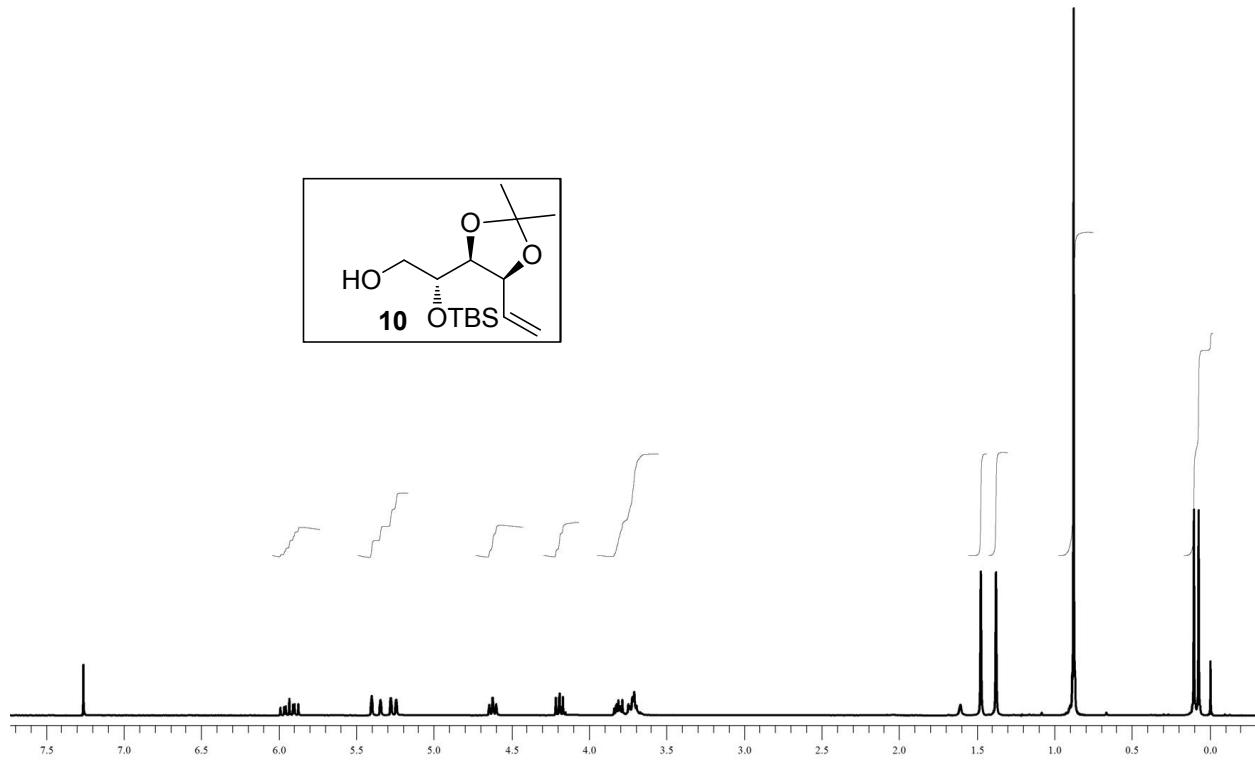


Position	Our data (500 MHz, CDCl <sub>3</sub> )	Chakraborty's <sup>1</sup> synthesis data (300 MHz, CDCl <sub>3</sub> )	Changgui's <sup>2</sup> synthesis data (400 MHz, CDCl <sub>3</sub> )	Simpson's <sup>3</sup> isolation data
<b>2</b>	2.52 (dd, <i>J</i> = 18.2, 4.4 Hz, 1H) 2.93 (dd, <i>J</i> = 18.2, 7.5 Hz, 1H)	2.50 (dd, <i>J</i> = 18.1, 3.8 Hz, 1H) 2.93 (dd, <i>J</i> = 18.1, 7.6 Hz, 1H)	2.52 (dd, <i>J</i> = 18.4, 3.6 Hz, 1H) 2.93 (dd, <i>J</i> = 18.4, 7.6 Hz, 1H)	a: 2.54 (dd, <i>J</i> = 18.3, 4.4 Hz, 1H) b: 2.94 (dd, <i>J</i> = 18.3, 7.6 Hz, 1H)
<b>3</b>	4.62-4.56 (m, 1H)	4.58 (m, 1H)	4.60 - 4.57 (m, 1H)	4.61 (ddd, <i>J</i> = 7.6, 4.4, 3.2 Hz, 1H)
<b>4</b>	4.42 (dd, <i>J</i> = 5.6, 3.2 Hz, 1H)	4.44 (dd, <i>J</i> = 5.3, 3.0 Hz, 1H)	4.44 (dd, <i>J</i> = 5.2, 2.8 Hz, 1H)	4.44 (dd, <i>J</i> = 5.8, 3.2 Hz, 1H)
<b>5</b>	3.60-3.56 (m, 1H)	3.57 (dd, <i>J</i> = 6.8, 6.0 Hz, 1H)	3.57 (dd, <i>J</i> = 6.4, 6.0 Hz, 1H)	3.60 (dd, <i>J</i> = 6.6, 5.8 Hz, 1H)
<b>6</b>	1.94-1.84 (m, 1H)	1.89 (m, 1H)	1.93 - 1.86 (m, 2H)	1.92 (dqdd, <i>J</i> = 7.1, 6.8, 6.6, 6.6 Hz, 1H)
<b>7</b>	2.30-2.20 (m, 2H)	2.36-2.21 (m, 2H)	2.29 - 2.19 (m, 2H)	a: 2.27 (m, 1H) b: 2.25 (m, 1H)
<b>8</b>	5.61 (ddd, <i>J</i> = 15.0, 8.2, 6.3 Hz, 1H)	5.59 (ddd, <i>J</i> = 15.1, 8.3, 6.8 Hz, 1H)	5.60 (ddd, <i>J</i> = 14.8, 8.0, 6.8 Hz, 1H)	5.63 (ddd, <i>J</i> = 15.4, 8.6, 6.1 Hz, 1H)
<b>9</b>	5.39 (dd, <i>J</i> = 15.4, 8.7 Hz, 1H)	5.37 (dd, <i>J</i> = 15.1, 8.3 Hz, 1H)	5.38 (dd, <i>J</i> = 15.2, 8.8 Hz, 1H)	5.40 (dd, <i>J</i> = 15.4, 8.6 Hz, 1H)
<b>10</b>	2.10-2.02 (m, 1H)	2.06 (m, 1H)	2.11 - 2.02 (m, 1H)	2.07 (ddq, <i>J</i> = 8.6, 7.3, 6.8 Hz, 1H)
<b>11</b>	3.54-3.48 (m, 1H)	3.49 (m, 1H)	3.52 - 3.48 (m, 1H)	3.53 (dq, <i>J</i> = 7.3, 6.4 Hz, 1H)
<b>12</b>	1.18 (d, <i>J</i> = 6.1 Hz, 3H)	1.18 (d, <i>J</i> = 6.8 Hz, 3H)	1.18 (d, <i>J</i> = 6.4 Hz, 3H)	1.20 (d, <i>J</i> = 6.4 Hz, 3H)
<b>13</b>	1.05 (d, <i>J</i> = 7.0 Hz, 3H)	1.04 (d, <i>J</i> = 6.8 Hz, 3H)	1.04 (d, <i>J</i> = 7.2 Hz, 3H)	1.05 (d, <i>J</i> = 6.8 Hz, 3H)
<b>14</b>	0.98 (d, <i>J</i> = 6.9 Hz, 3H)	0.98 (d, <i>J</i> = 6.8 Hz, 3H)	0.98 (d, <i>J</i> = 6.8 Hz, 3H)	1.00 (d, <i>J</i> = 6.8 Hz, 3H)

<sup>13</sup>C NMR spectral comparative table:

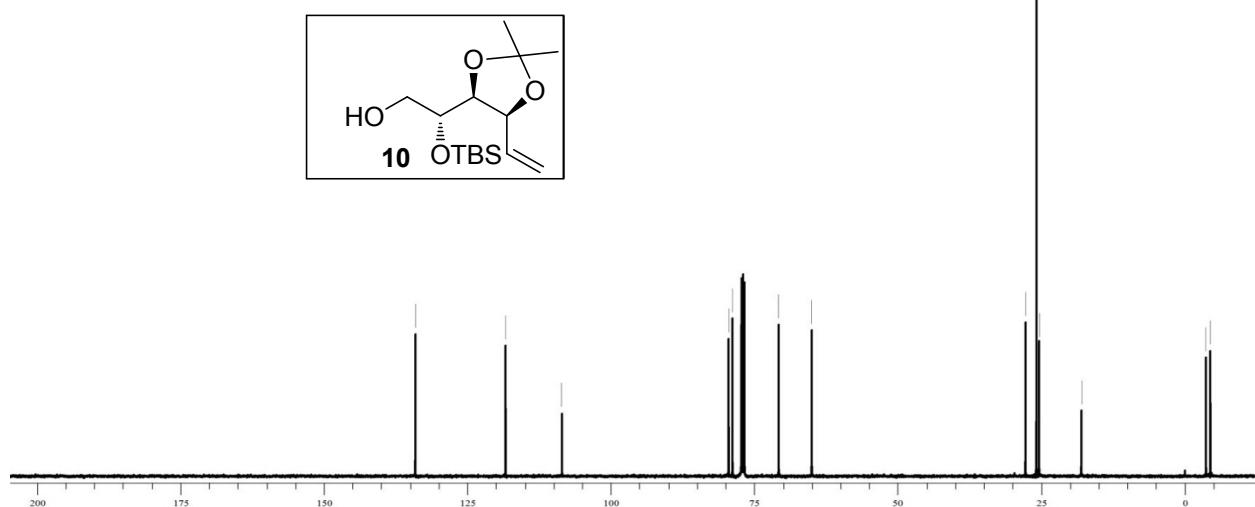
Position	Our data (75 MHz, CDCl <sub>3</sub> )	Chakraborty's <sup>1</sup> synthesis data (75 MHz, CDCl <sub>3</sub> )	Changgui's <sup>2</sup> synthesis data (100 MHz, CDCl <sub>3</sub> )	Simpson's <sup>3</sup> isolation data
<b>1</b>	175.8	176.2	176.5	175.8
<b>2</b>	38.2	38.3	38.4	38.1
<b>3</b>	68.4	68.4	68.3	68.6
<b>4</b>	87.6	88.0	88.2	87.5
<b>5</b>	75.1	75.1	75.0	75.6
<b>6</b>	35.2	35.3	35.4	35.3
<b>7</b>	34.5	34.6	34.8	34.6
<b>8</b>	129.5	129.6	129.5	129.7
<b>9</b>	134.7	134.7	134.7	134.8
<b>10</b>	45.2	45.3	45.2	45.3
<b>11</b>	71.5	71.6	71.6	71.5
<b>12</b>	20.5	20.6	20.6	20.6
<b>13</b>	16.8	17.0	17.0	16.9
<b>14</b>	15.9	16.0	16.0	16.0



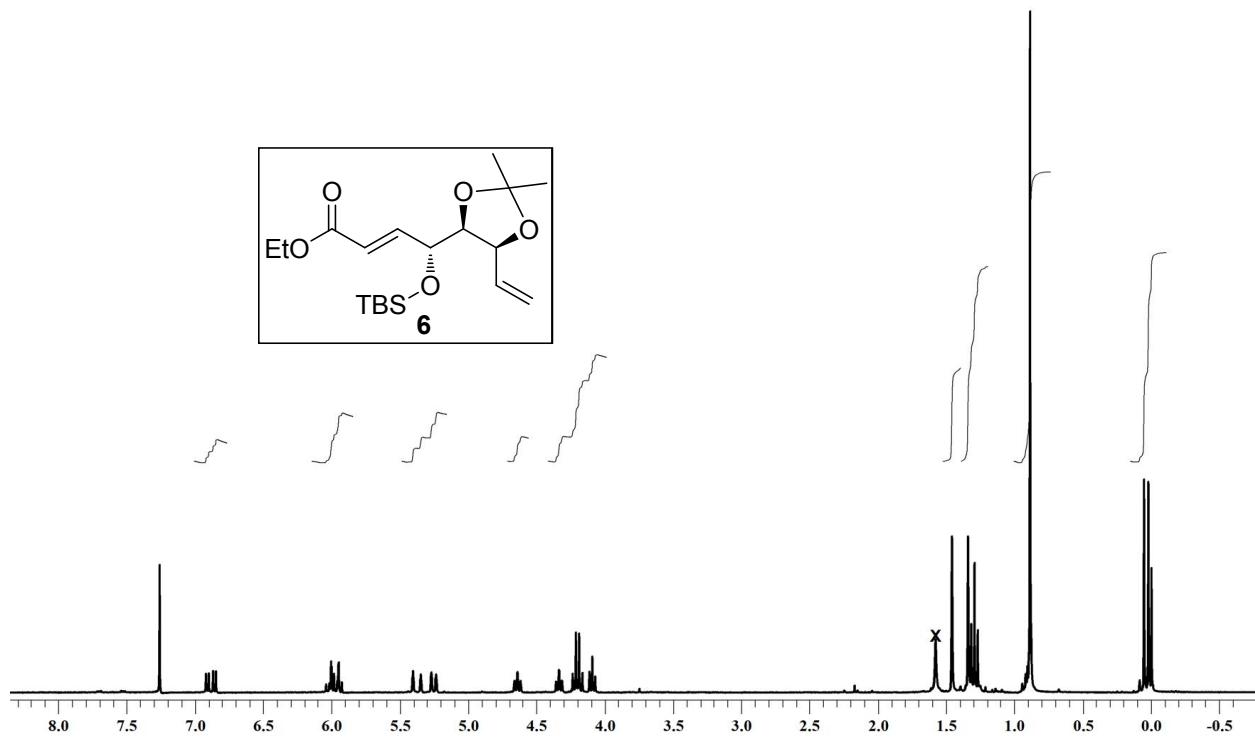


**<sup>1</sup>H NMR Spectrum of 10 (300 MHz, CDCl<sub>3</sub>)**

134.083	118.362	108.523	79.486	78.823	70.771	65.007	27.766	25.853	25.395	18.030	-3.692	-4.449
---------	---------	---------	--------	--------	--------	--------	--------	--------	--------	--------	--------	--------

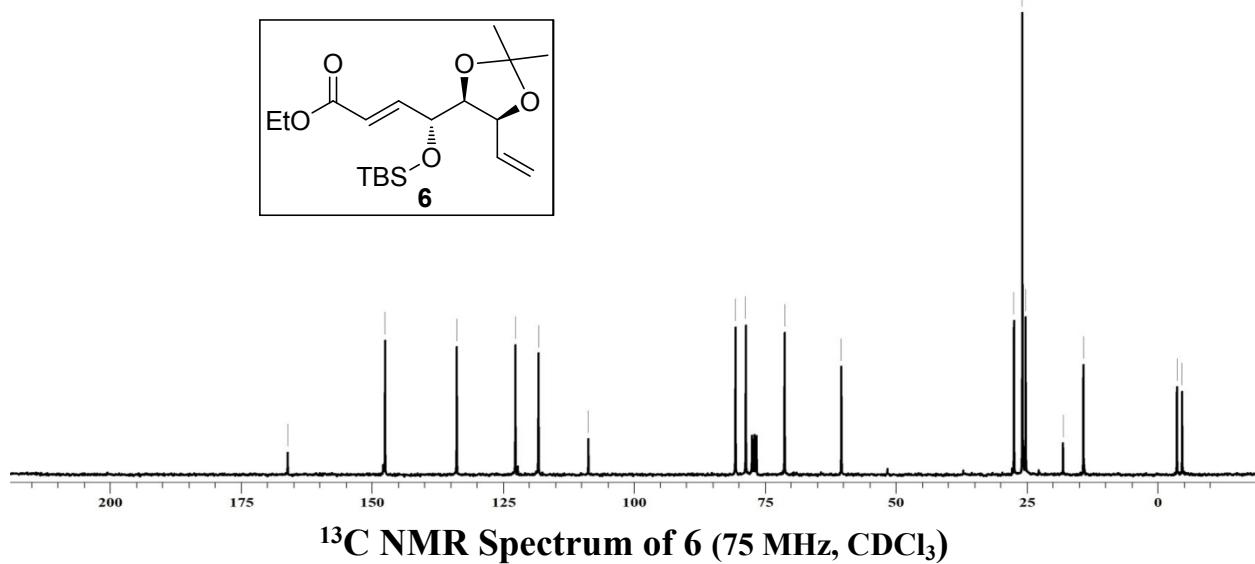


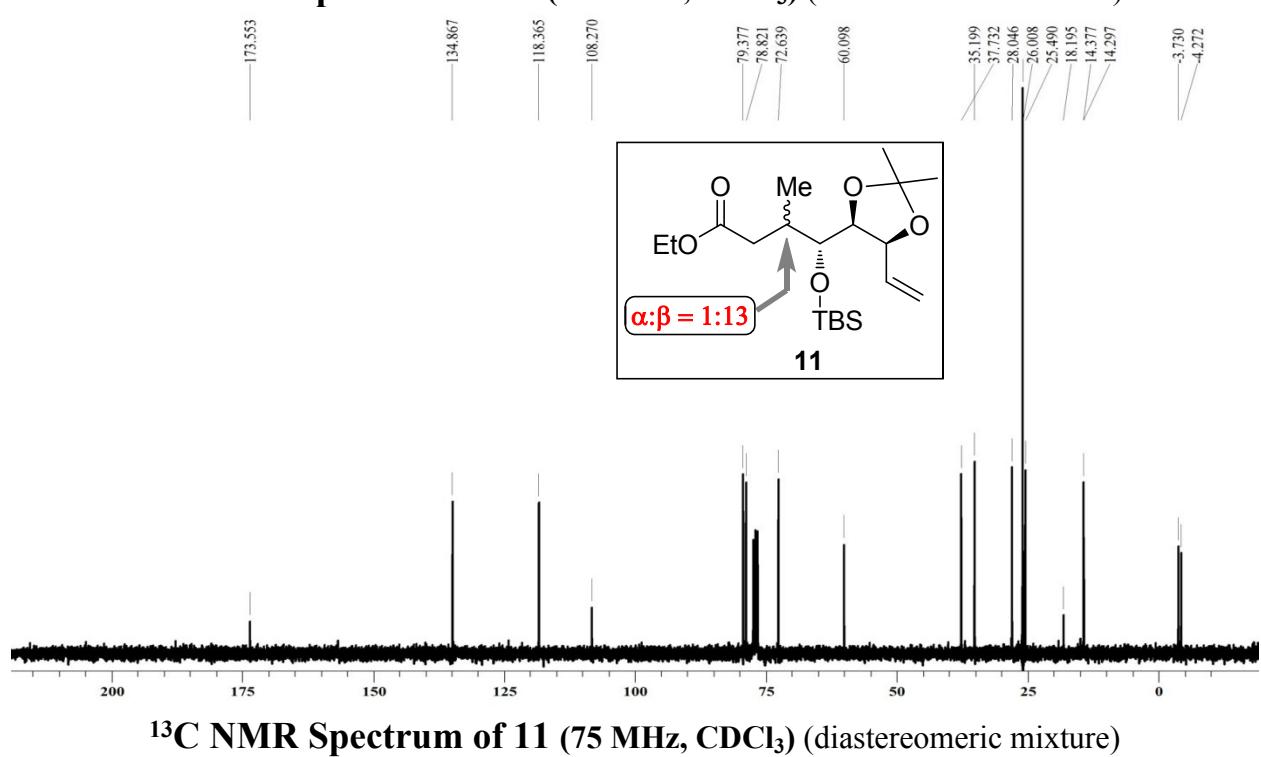
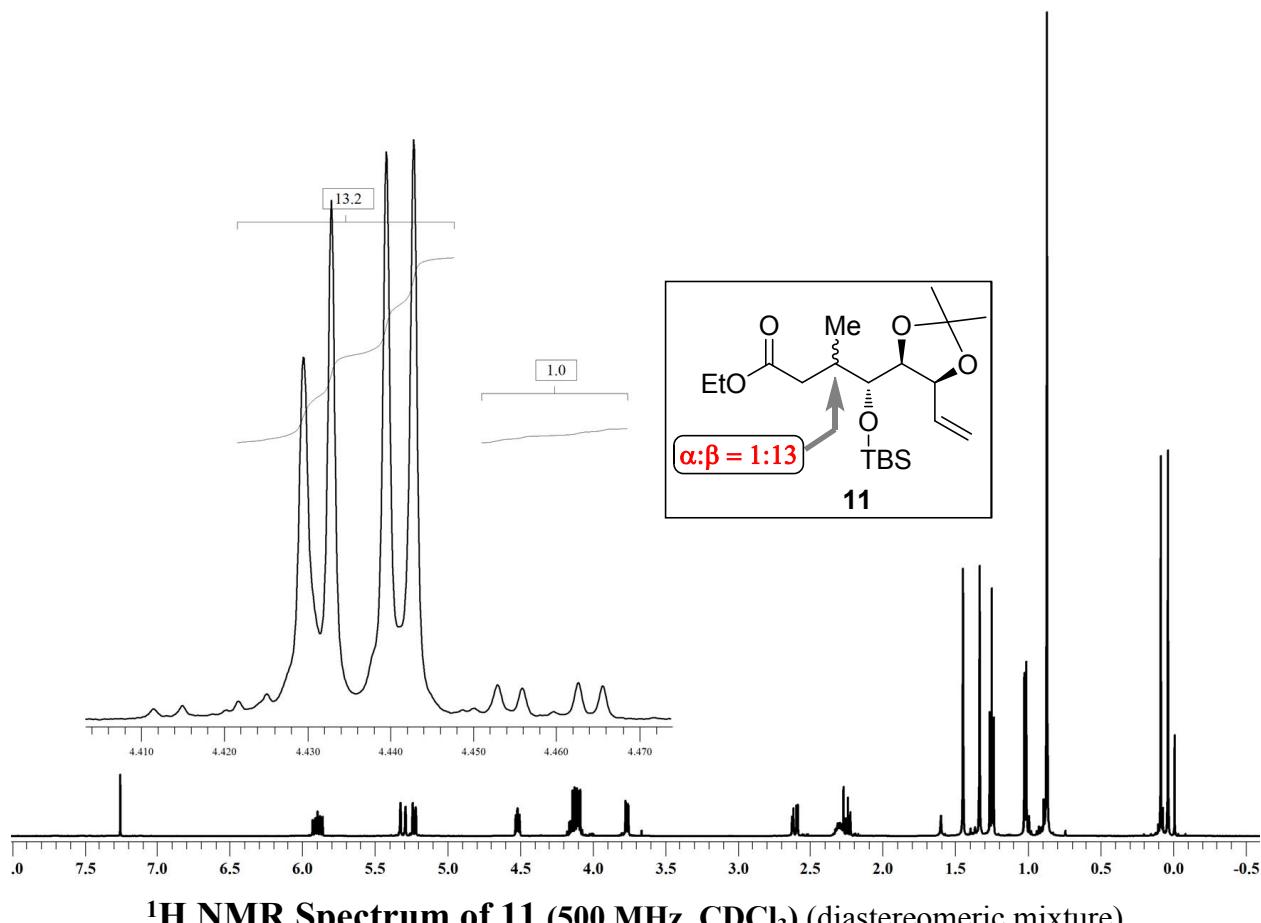
**<sup>13</sup>C NMR Spectrum of 10 (125 MHz, CDCl<sub>3</sub>)**

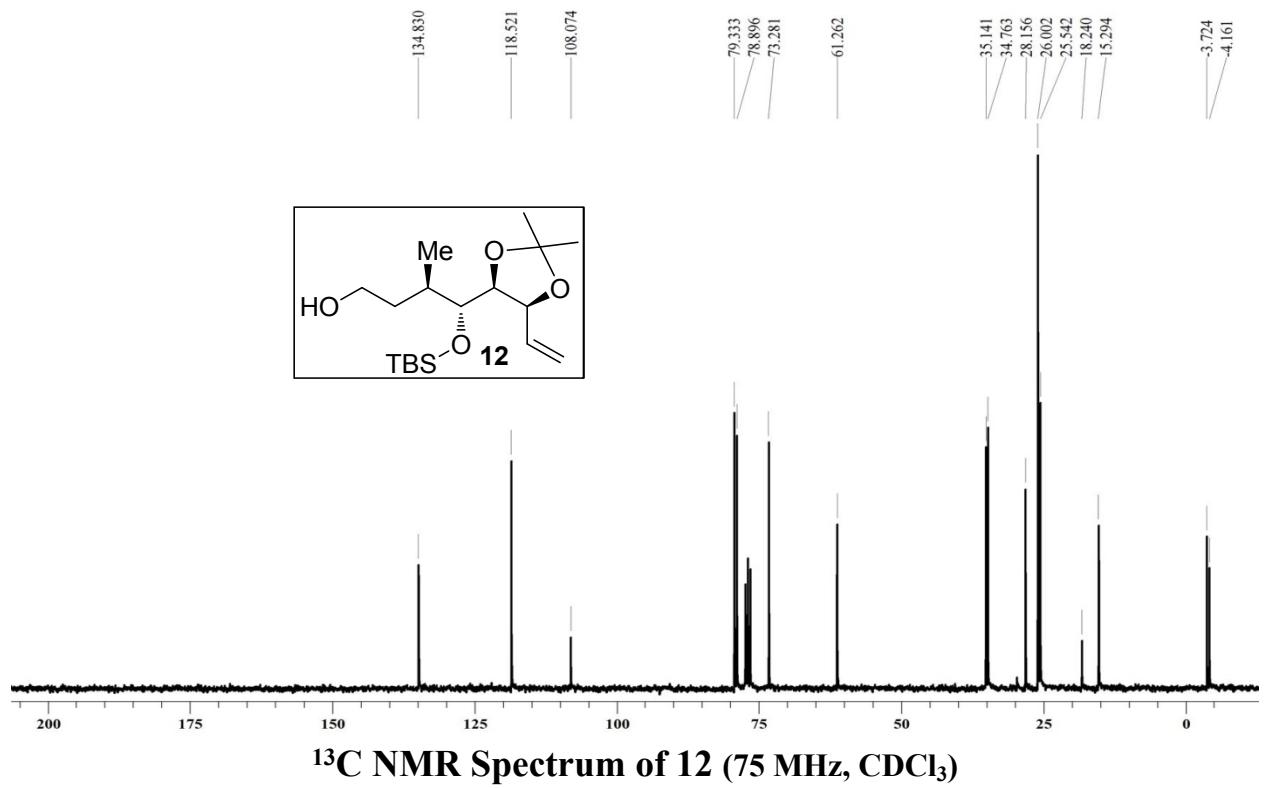
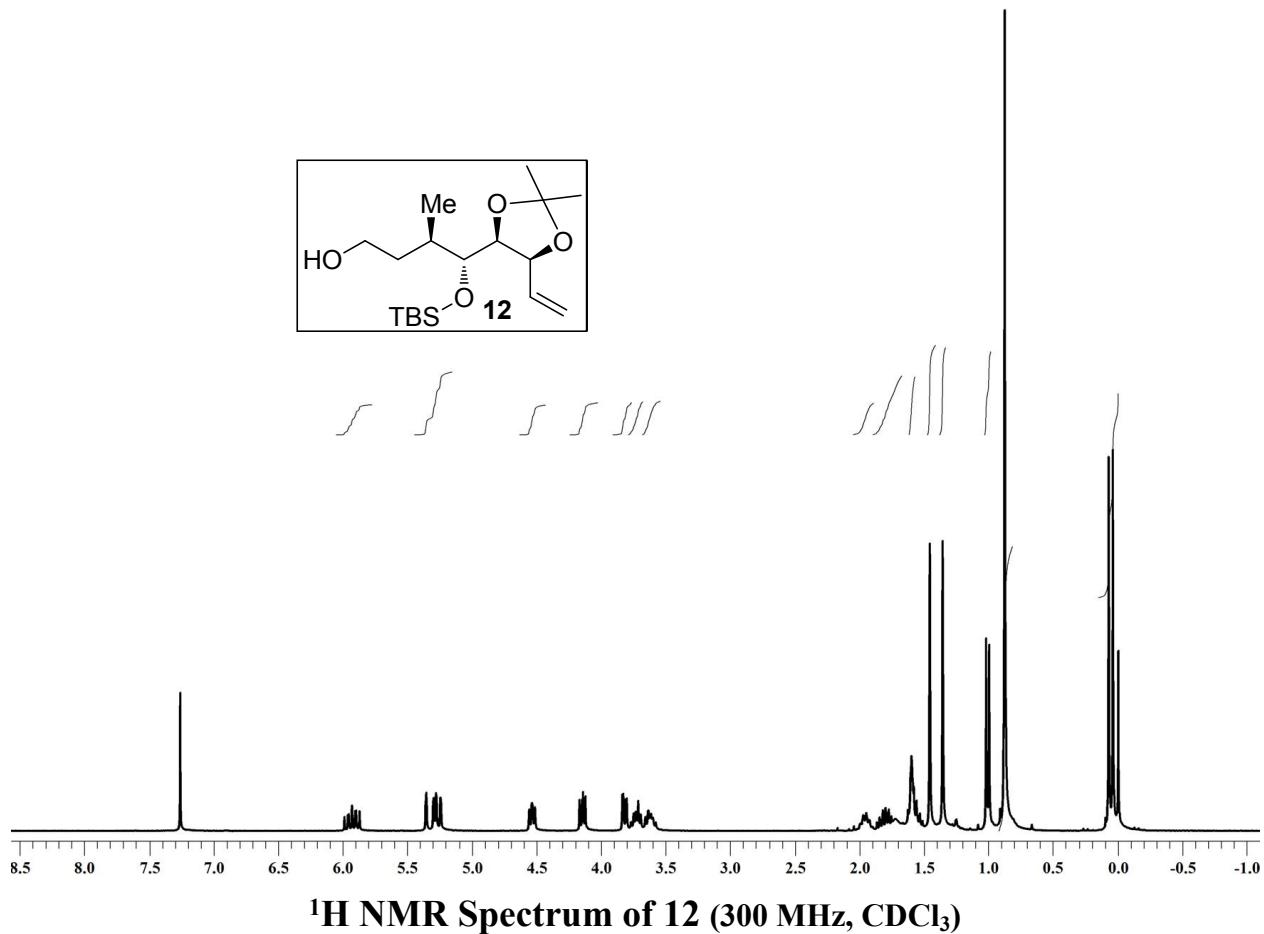


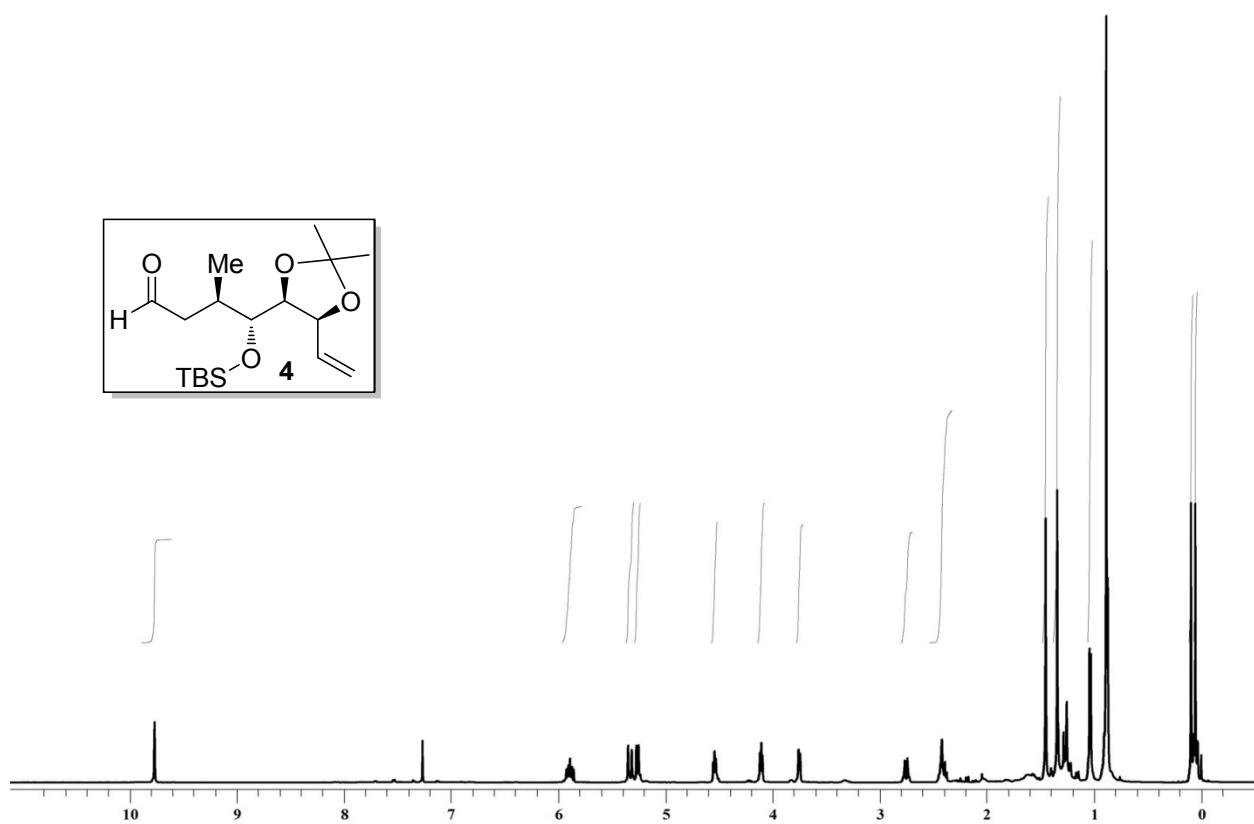
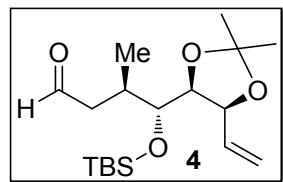
**<sup>1</sup>H NMR Spectrum of 6 (300 MHz, CDCl<sub>3</sub>)**

166.090	147.502	133.815	122.617	118.215	108.684	80.590	78.620	71.215	60.372	27.415	25.816	25.198	18.054	-3.695
---------	---------	---------	---------	---------	---------	--------	--------	--------	--------	--------	--------	--------	--------	--------

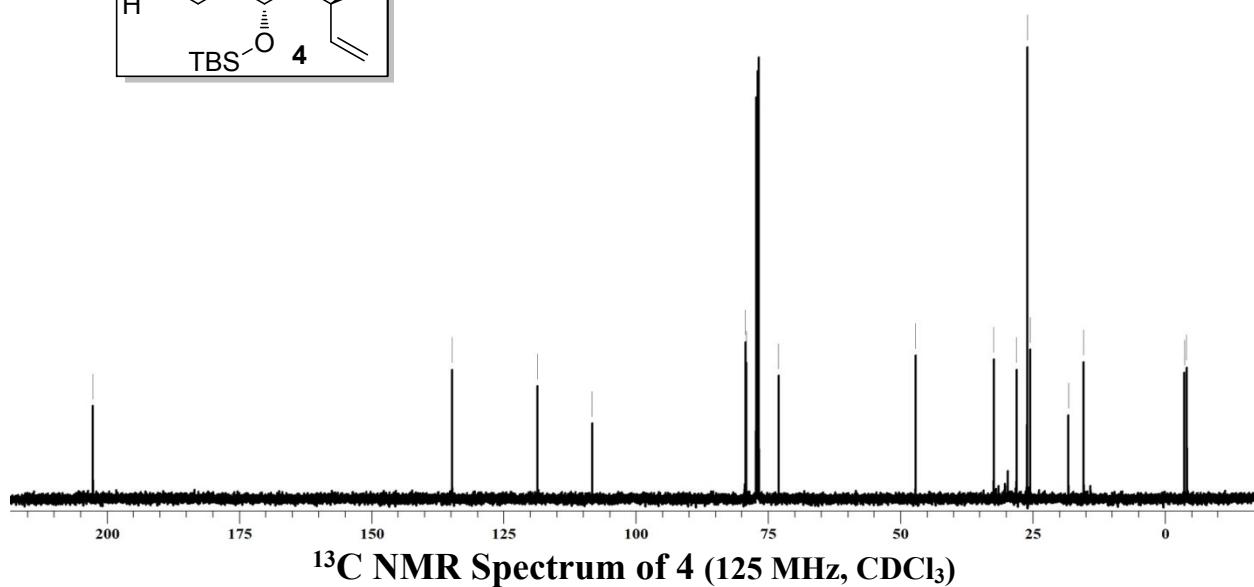
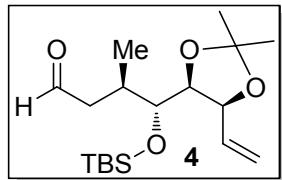


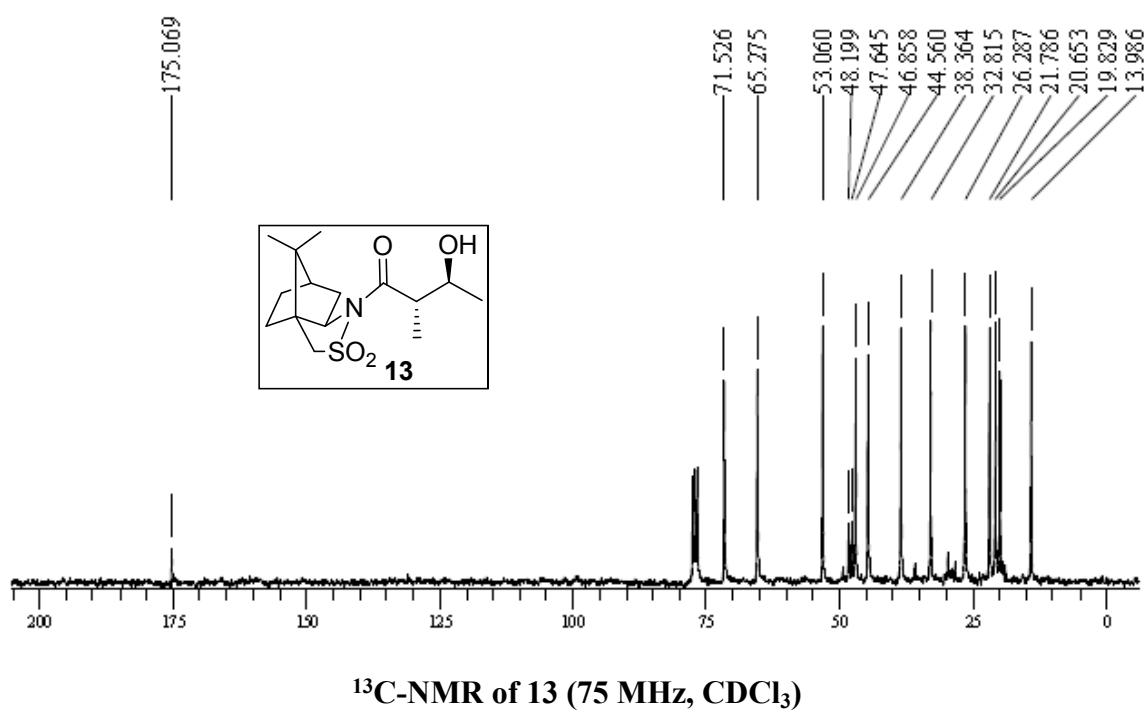
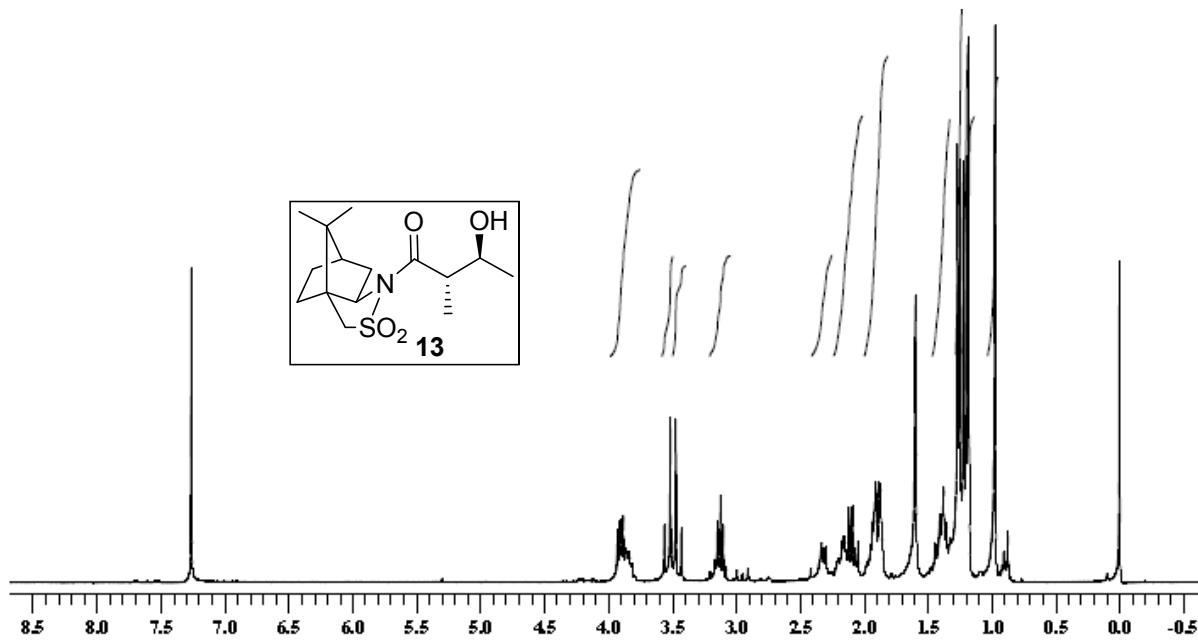


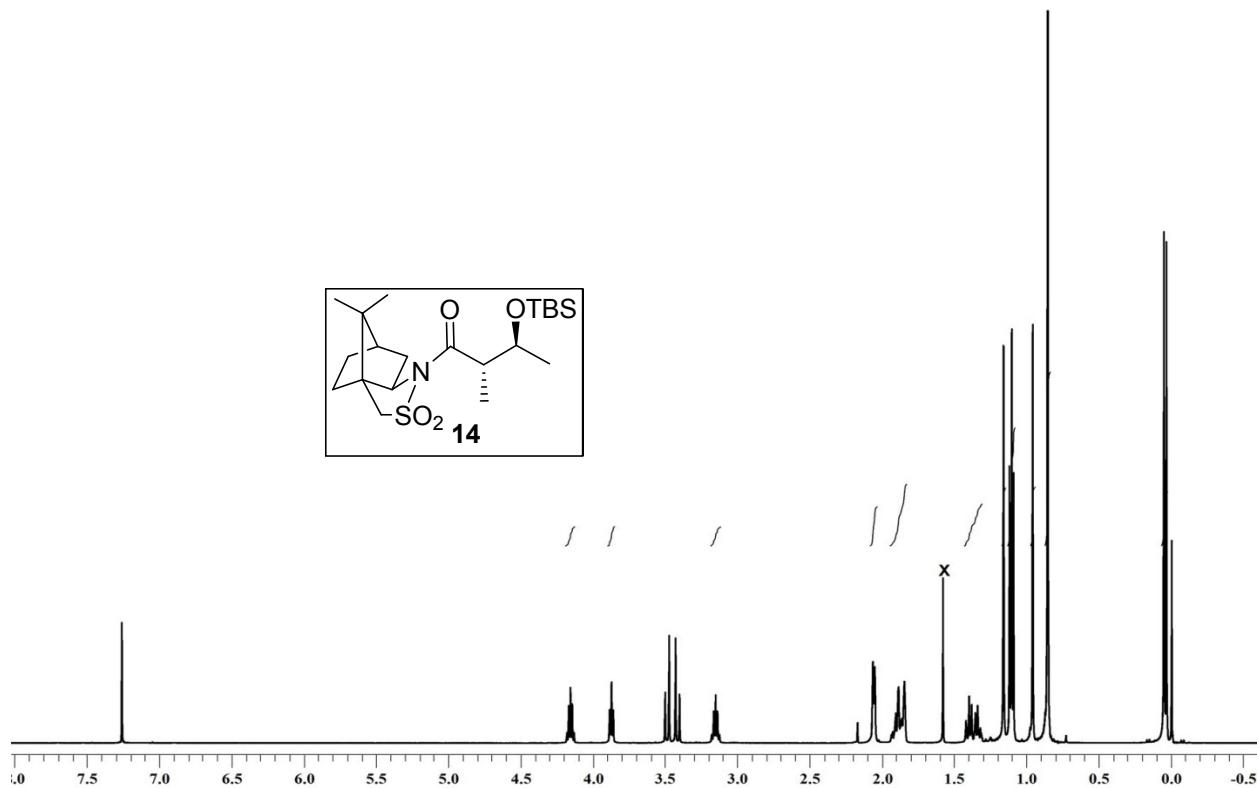




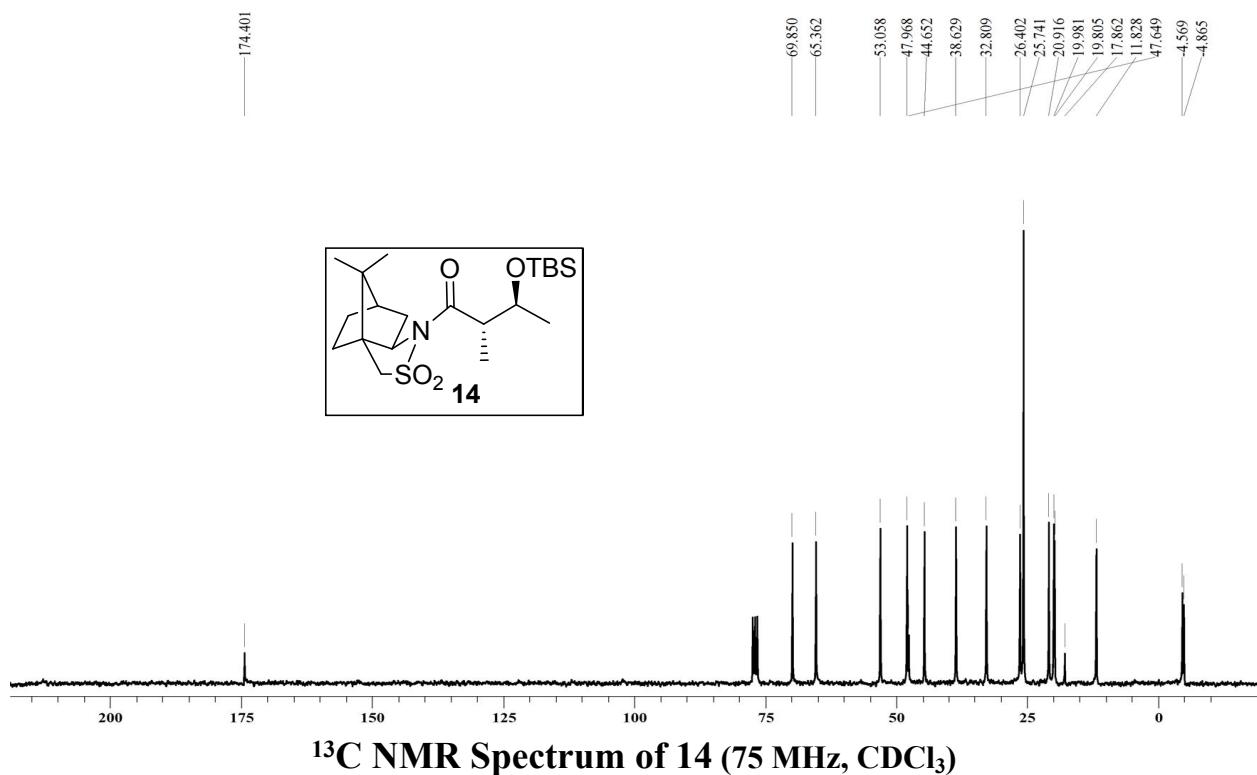
Peak labels (ppm): 202.644, 134.713, 118.603, 108.253, 79.232, 79.146, 72.977, 47.119, 32.328, 28.024, 25.995, 25.418, 18.219, 15.323, -3.713, -4.189



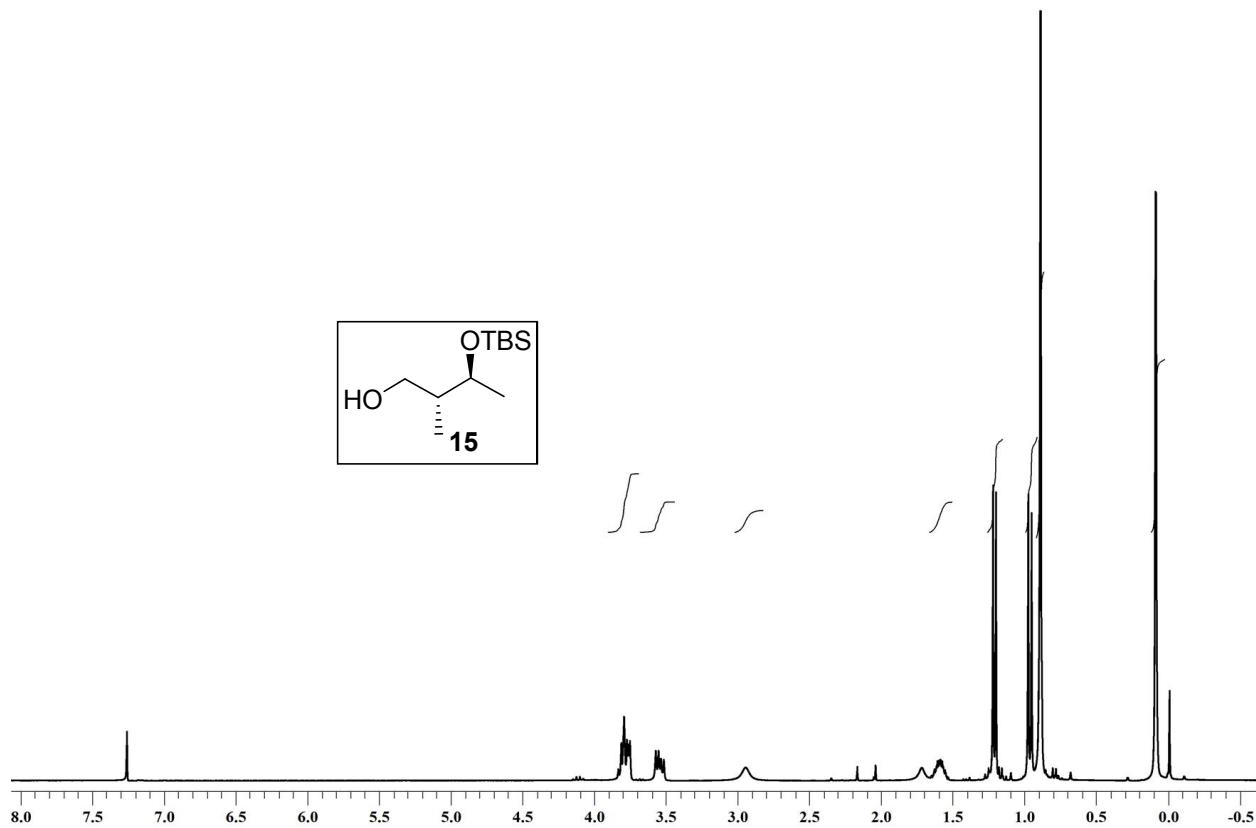




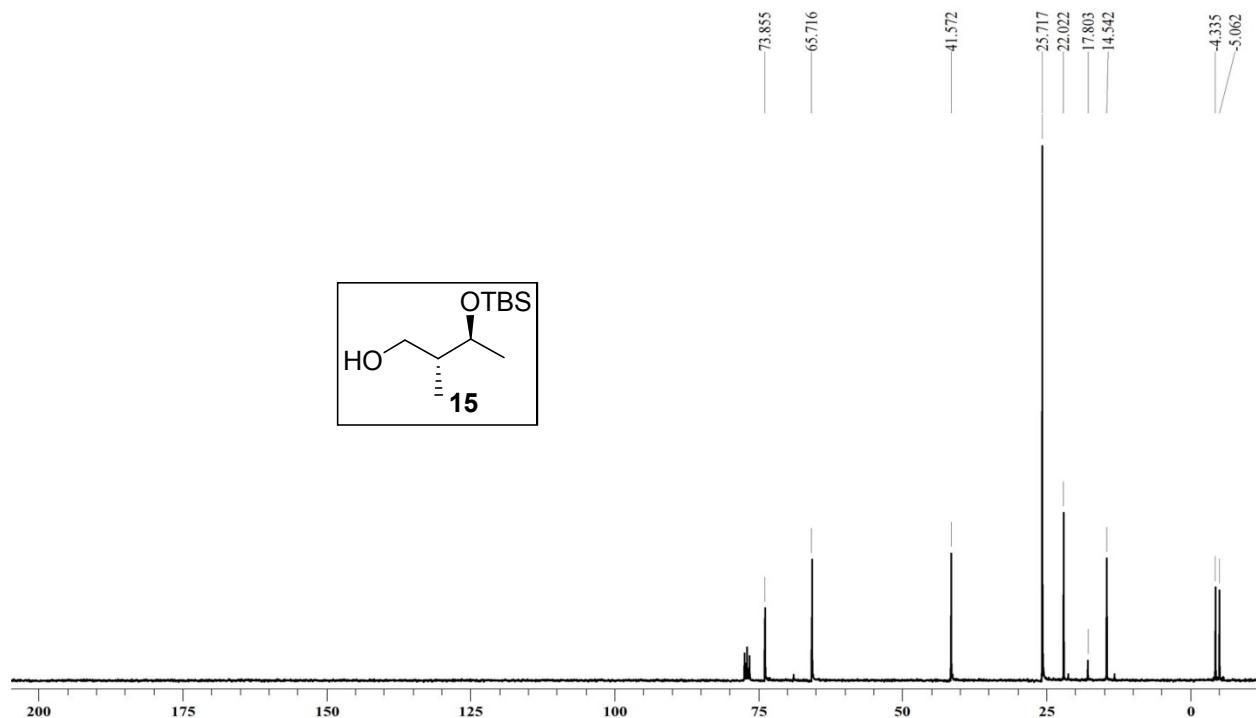
**<sup>1</sup>H NMR Spectrum of 14 (500 MHz, CDCl<sub>3</sub>)**



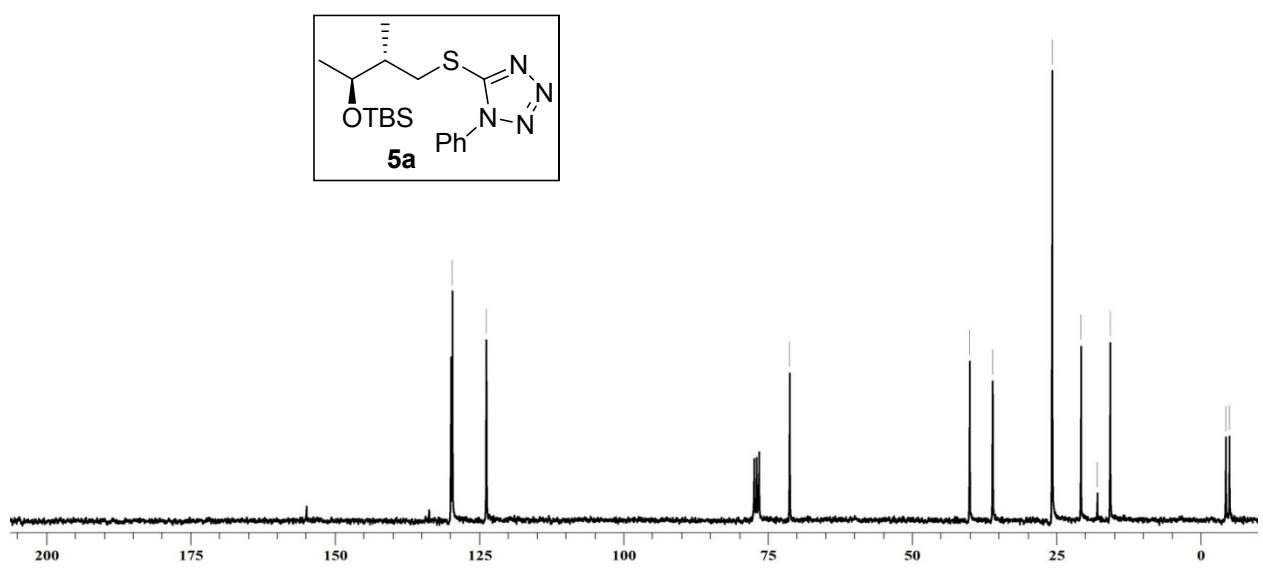
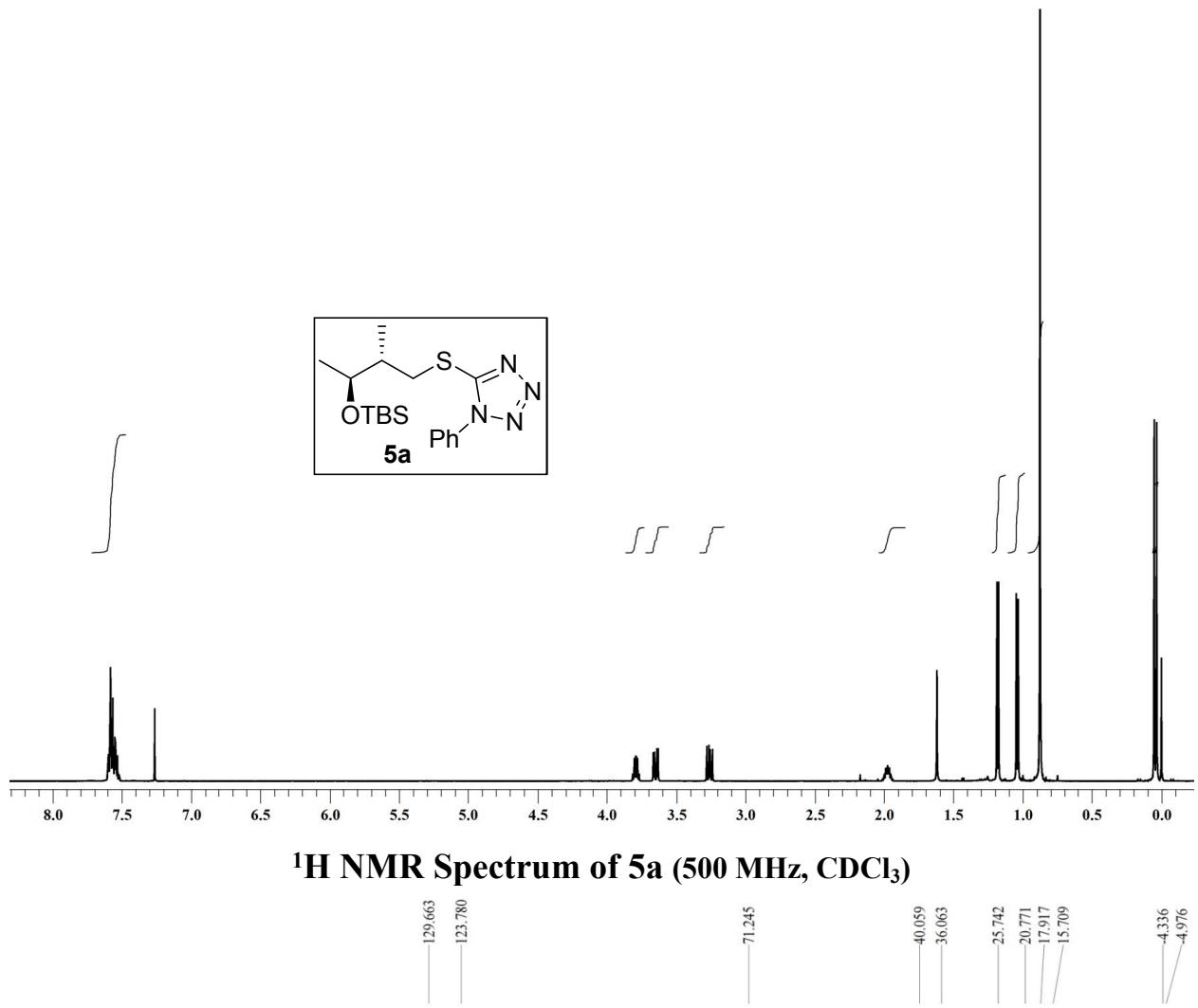
**<sup>13</sup>C NMR Spectrum of 14 (75 MHz, CDCl<sub>3</sub>)**

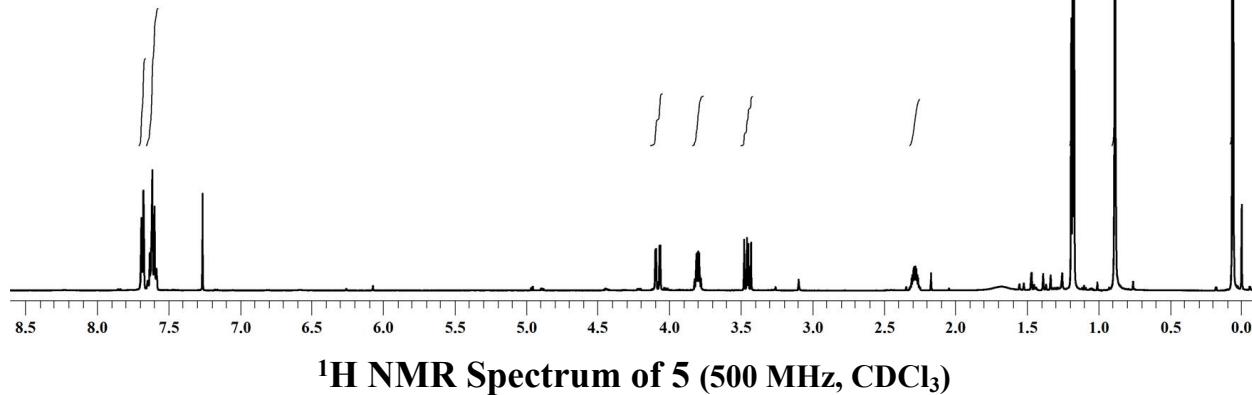
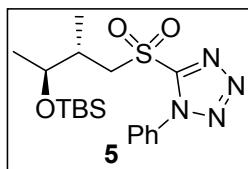


**$^1\text{H}$  NMR Spectrum of **15** (300 MHz,  $\text{CDCl}_3$ )**

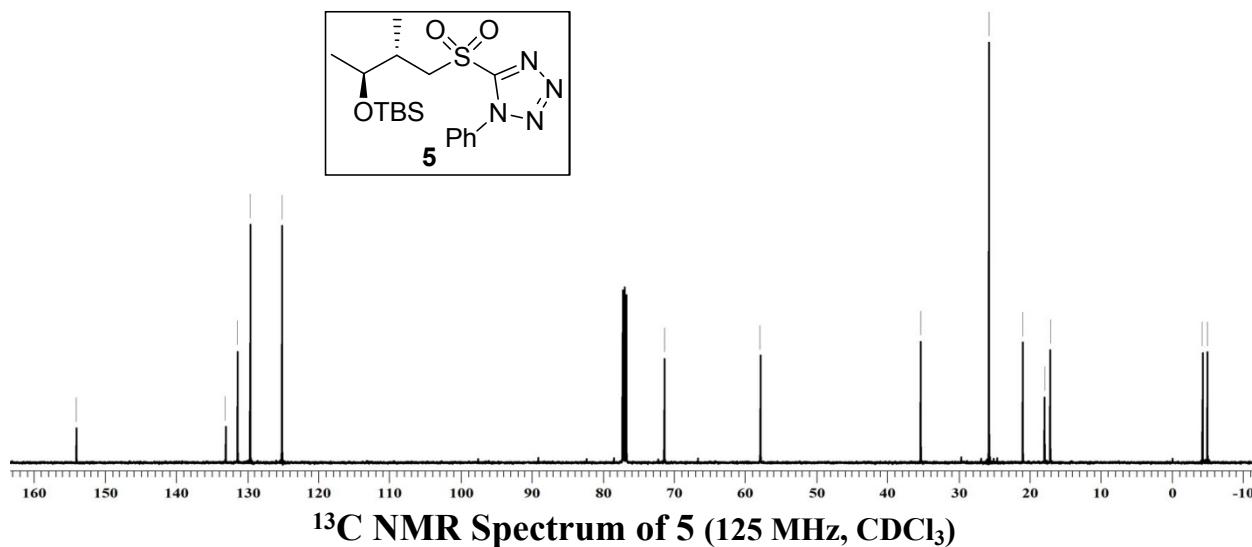
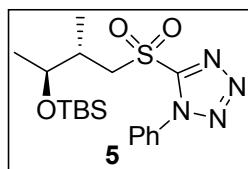


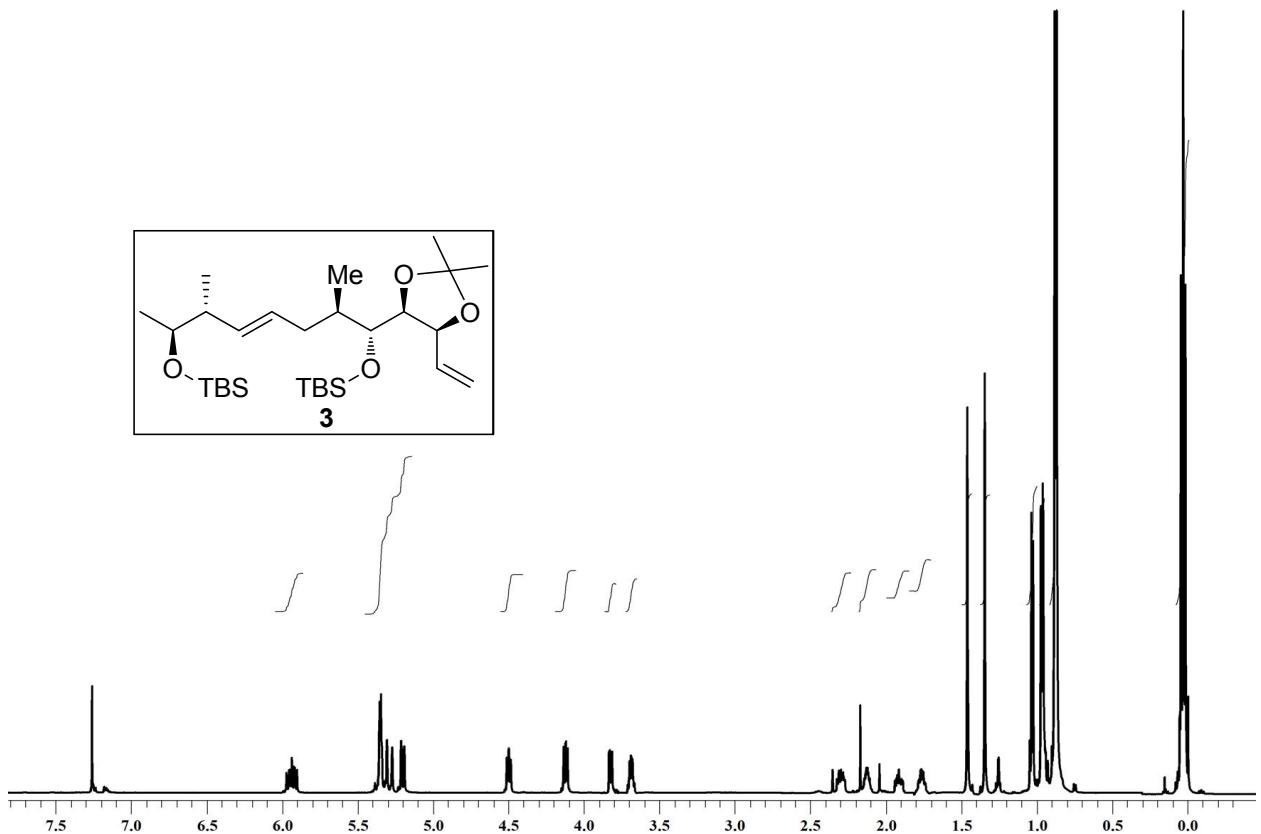
**$^{13}\text{C}$  NMR Spectrum of **15** (75 MHz,  $\text{CDCl}_3$ )**



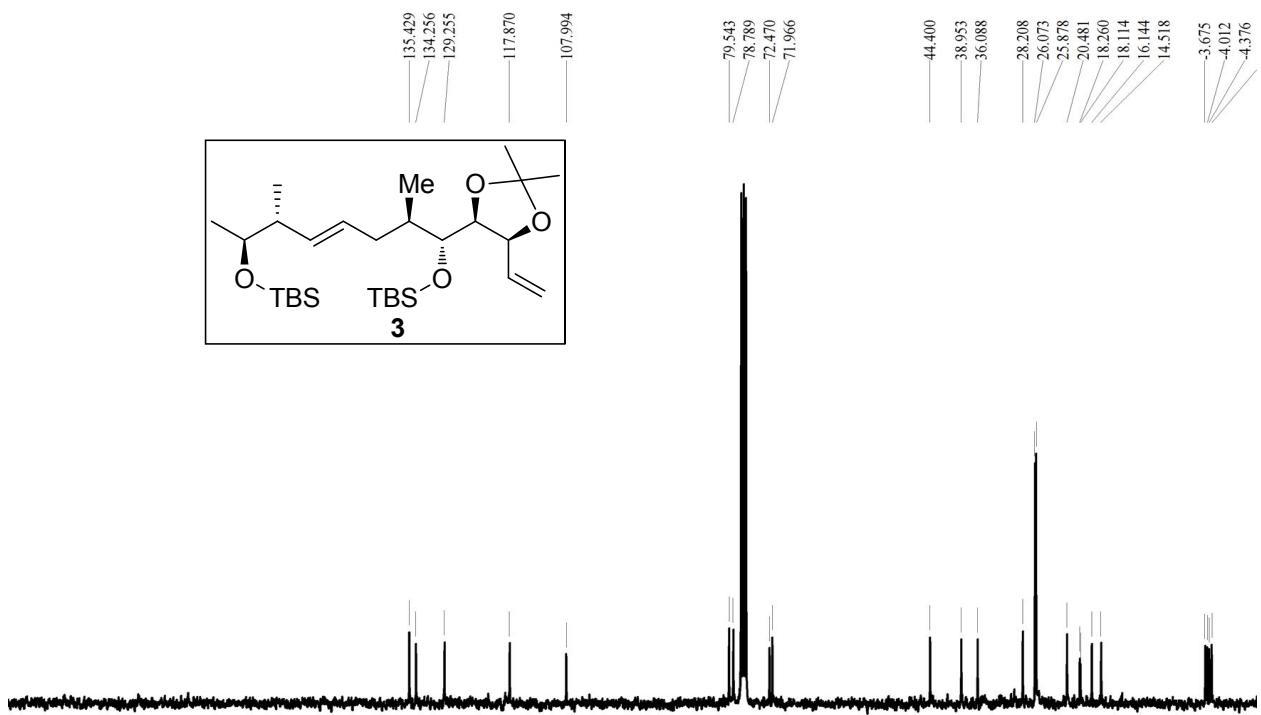


154.045  
133.060  
131.384  
129.616  
125.145  
71.380  
57.878  
35.347  
25.751  
20.999  
17.929  
17.142  
-4.290  
-4.955

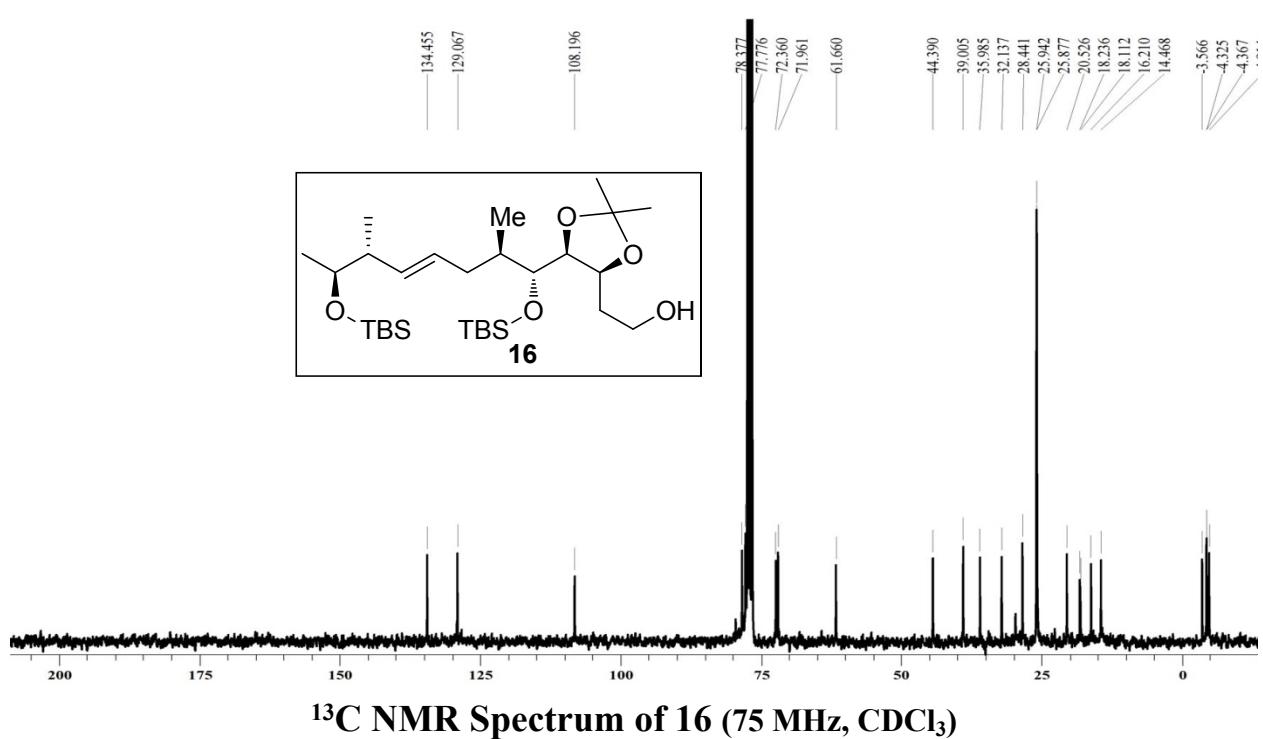
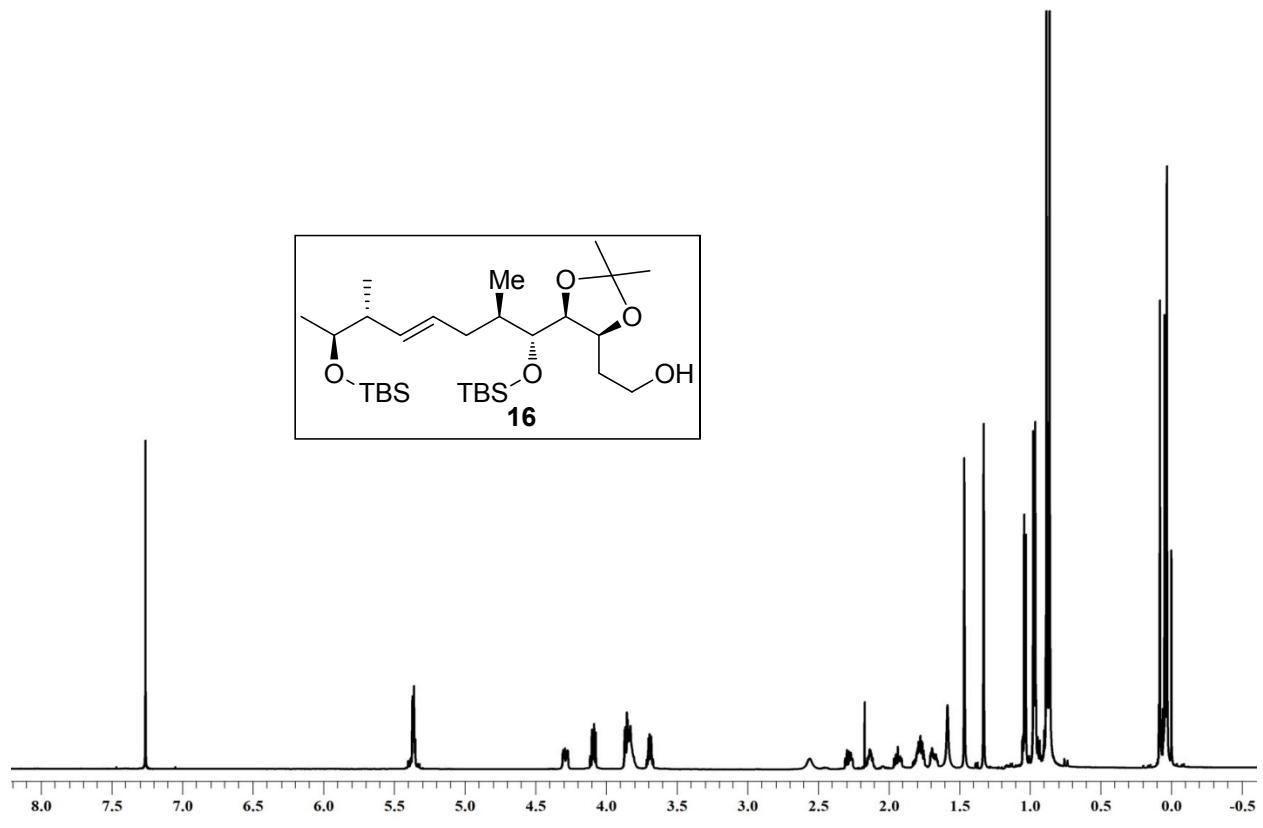


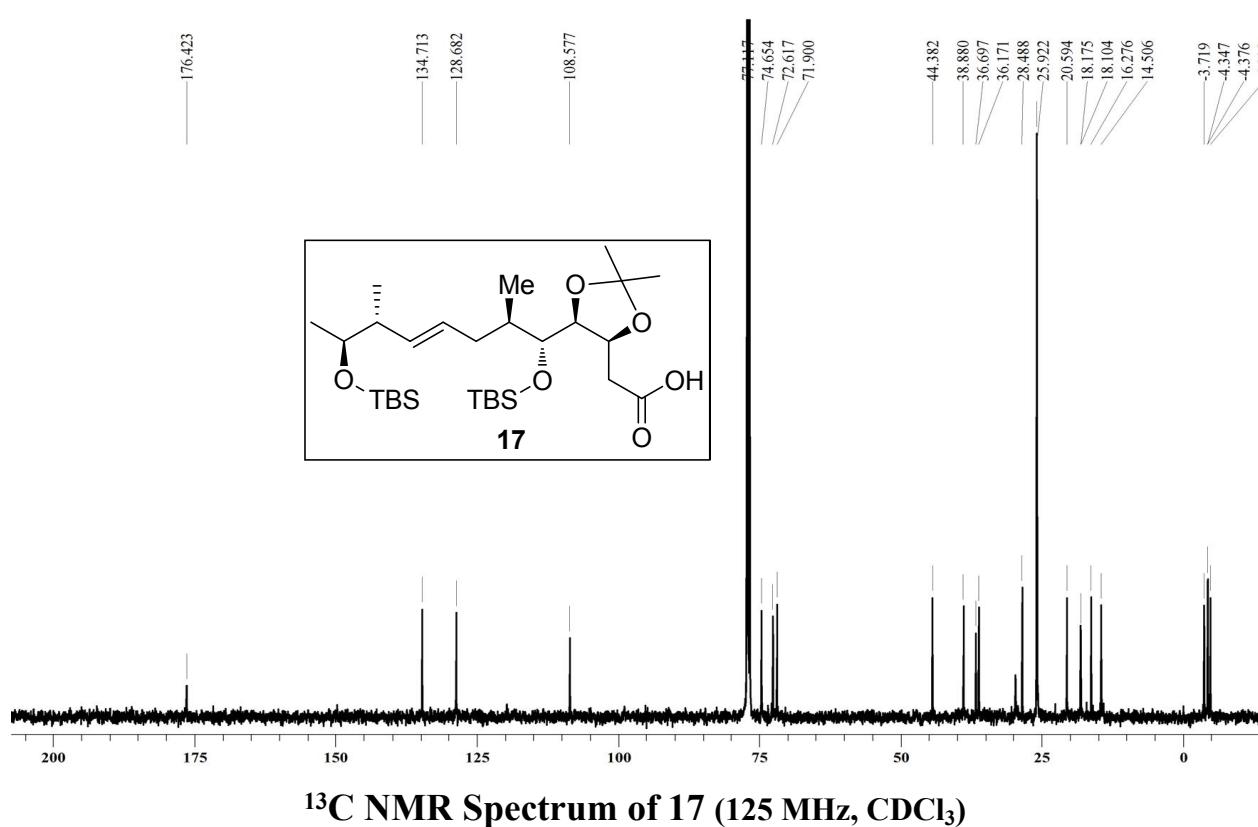
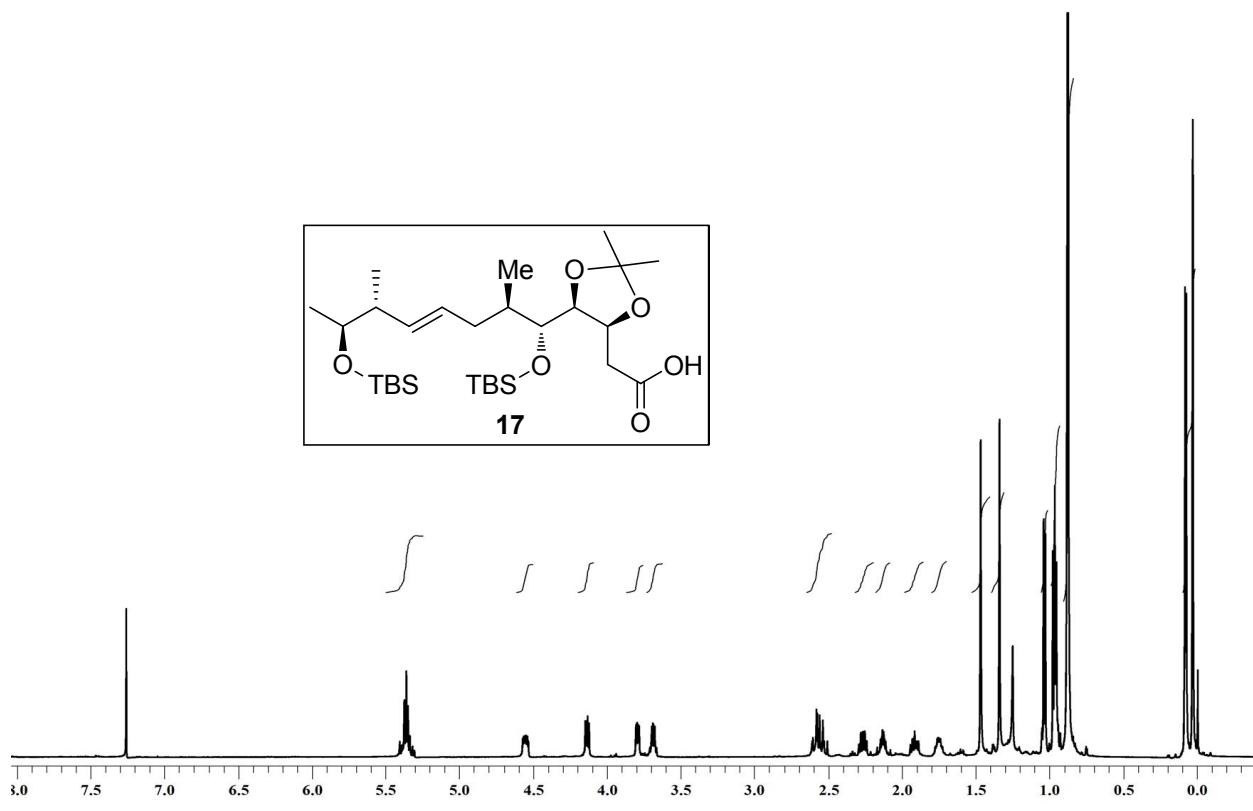


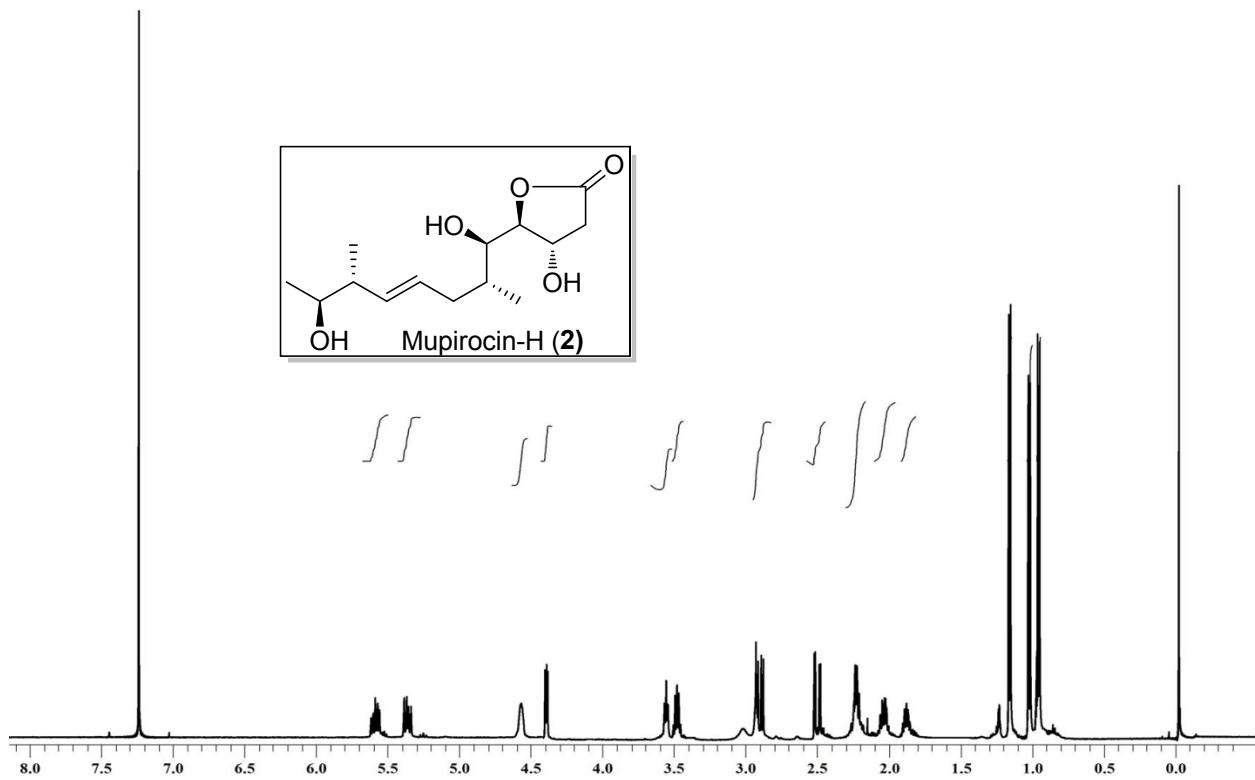
**<sup>1</sup>H NMR Spectrum of 3 (500 MHz, CDCl<sub>3</sub>)**



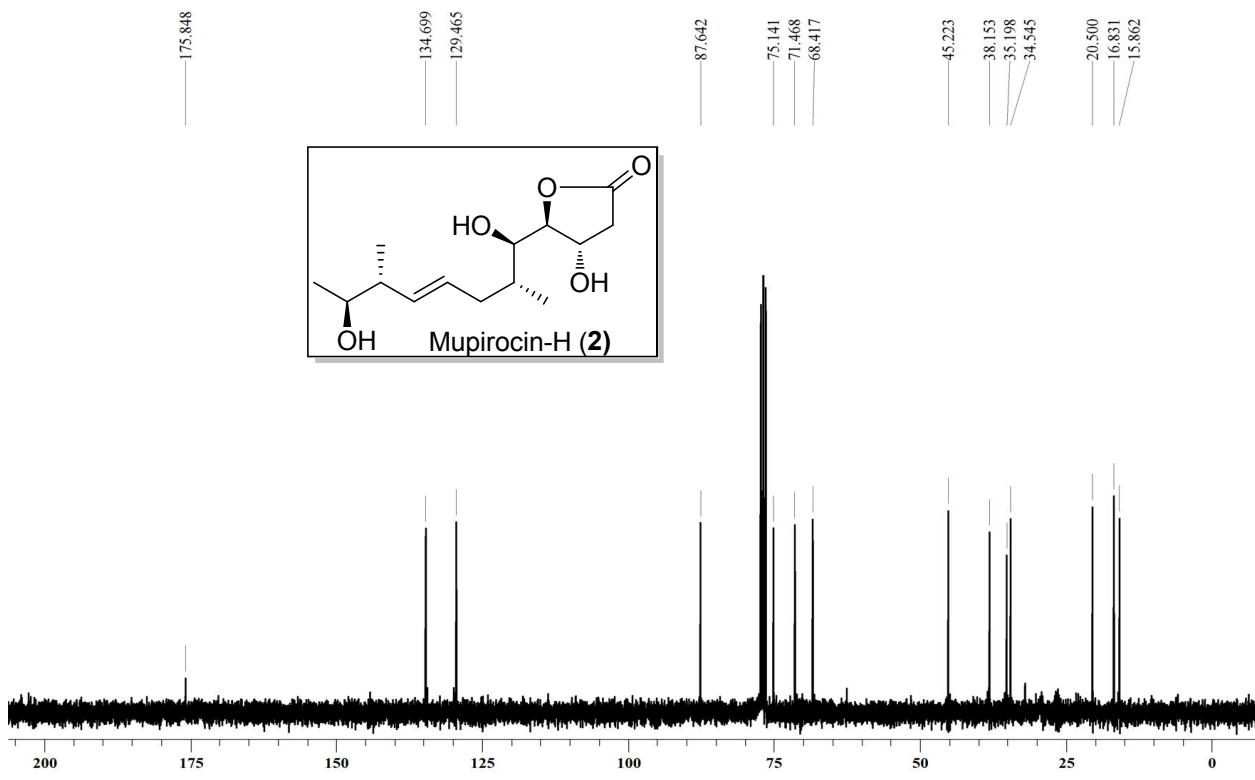
**<sup>13</sup>C NMR Spectrum of 3 (75 MHz, CDCl<sub>3</sub>)**







### **<sup>1</sup>H NMR Spectrum of 2 (500 MHz, CDCl<sub>3</sub>)**



### **<sup>13</sup>C NMR Spectrum of 2 (75 MHz, CDCl<sub>3</sub>)**

**References:**

1. Udwant, S.; Chakraborty, T. K. *J. Org. Chem.* **2011**, *76*, 6331-6337.
2. Zhao, C.; Yuan, Z.; Zhang, Y.; Ma, B.; Li, H.; Tang, S.; Xie X.; X. She. *Org. Chem. Front.* **2014**, *1*, 105-108.
3. Wu, J.; Cooper, S. M.; Cox, R. J.; Crosby, J.; Crump, M. P.; Hothersall, J.; Simpson, T. J.; Thomas, C. M.; Willis, C. L. *Chem. Commun.* **2007**, 2040-2042