

## Supporting information for journal *Marine drugs*

# Isolation, Structure-activity Relationship of Subergorgic Acid and Synthesis of Its Derivatives as Antifouling Agent

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## Table of contents

<b>Figure S1.</b> Key NOE correlations of <b>4</b> .	Page 3	<b>Figure S43.</b> <sup>13</sup> C NMR (100 MHz, CDCl <sub>3</sub> ) of compound <b>19</b>	45
<b>Figure S2.</b> <sup>1</sup> H NMR (400 MHz, CDCl <sub>3</sub> ) of compound <b>SA</b>	4	<b>Figure S44.</b> <sup>1</sup> H NMR (400 MHz, CDCl <sub>3</sub> ) of compound <b>20</b>	46
<b>Figure S3.</b> <sup>13</sup> C NMR (100 MHz, CDCl <sub>3</sub> ) of compound <b>SA</b>	5	<b>Figure S45.</b> <sup>13</sup> C NMR (100 MHz, CDCl <sub>3</sub> ) of compound <b>20</b>	47
<b>Figure S4.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>1</b>	6	<b>Figure S46.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>21</b>	48
<b>Figure S5.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>1</b>	7	<b>Figure S47.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>21</b>	49
<b>Figure S6.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>2</b>	8	<b>Figure S48.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>22</b>	50
<b>Figure S7.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>2</b>	9	<b>Figure S49.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>22</b>	51
<b>Figure S8.</b> <sup>1</sup> H NMR (400 MHz, CDCl <sub>3</sub> ) of compound <b>3</b>	10	<b>Figure S50.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>23</b>	52
<b>Figure S9.</b> <sup>13</sup> C NMR (100 MHz, CDCl <sub>3</sub> ) of compound <b>3</b>	11	<b>Figure S51.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>23</b>	53
<b>Figure S10.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>4</b>	12	<b>Figure S52.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>24</b>	54
<b>Figure S11.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>4</b>	13	<b>Figure S53.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>24</b>	55
<b>Figure S12.</b> HSQC spectrum of compound <b>4</b>	14	<b>Figure S54.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>25</b>	56
<b>Figure S13.</b> NOESY spectrum of compound <b>4</b>	15	<b>Figure S55.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>25</b>	57
<b>Figure S14.</b> <sup>1</sup> H NMR (400 MHz, CDCl <sub>3</sub> ) of compound <b>5</b>	16	<b>Figure S56.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>26</b>	58
<b>Figure S15.</b> <sup>13</sup> C NMR (100 MHz, CDCl <sub>3</sub> ) of compound <b>5</b>	17	<b>Figure S57.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>26</b>	59
<b>Figure S16.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>6</b>	18	<b>Figure S58.</b> HRMS of compound <b>4</b>	60
<b>Figure S17.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>6</b>	19	<b>Figure S59.</b> HRMS of compound <b>5</b>	61
<b>Figure S18.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>7</b>	20	<b>Figure S60.</b> HRMS of compound <b>8</b>	62
<b>Figure S19.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>7</b>	21	<b>Figure S61.</b> HRMS of compound <b>10</b>	63
<b>Figure S20.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>8</b>	22	<b>Figure S62.</b> HRMS of compound <b>11</b>	64
<b>Figure S21.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>8</b>	23	<b>Figure S63.</b> HRMS of compound <b>13</b>	65
<b>Figure S22.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>9</b>	24	<b>Figure S64.</b> HRMS of compound <b>14</b>	66
<b>Figure S23.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>9</b>	25	<b>Figure S65.</b> HRMS of compound <b>1</b>	67
<b>Figure S24.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>10</b>	26	<b>Figure S66.</b> HRMS of compound <b>2</b>	68
<b>Figure S25.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>10</b>	27	<b>Figure S67.</b> HRMS of compound <b>3</b>	69
<b>Figure S26.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>11</b>	28	<b>Figure S68.</b> HRMS of compound <b>6</b>	70
<b>Figure S27.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>11</b>	29	<b>Figure S69.</b> HRMS of compound <b>7</b>	71
<b>Figure S28.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>12</b>	30	<b>Figure S70.</b> HRMS of compound <b>9</b>	72
<b>Figure S29.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>12</b>	31	<b>Figure S71.</b> HRMS of compound <b>12</b>	73
<b>Figure S30.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>13</b>	32	<b>Figure S72.</b> HRMS of compound <b>15</b>	74
<b>Figure S31.</b> <sup>13</sup> C NMR (75 MHz, CDCl <sub>3</sub> ) of compound <b>13</b>	33	<b>Figure S73.</b> HRMS of compound <b>16</b>	75
<b>Figure S32.</b> <sup>1</sup> H NMR (300 MHz, CDCl <sub>3</sub> ) of compound <b>14</b>	34	<b>Figure S74.</b> HRMS of compound <b>17</b>	76

<b>Figure S33.</b> $^{13}\text{C}$ NMR (75 MHz, $\text{CDCl}_3$ ) of compound <b>14</b>	35	<b>Figure S75.</b> HRMS of compound <b>18</b>	77
<b>Figure S34.</b> $^1\text{H}$ NMR (300 MHz, $\text{CDCl}_3$ ) of compound <b>15</b>	36	<b>Figure S76.</b> HRMS of compound <b>19</b>	78
<b>Figure S35.</b> $^{13}\text{C}$ NMR (75 MHz, $\text{CDCl}_3$ ) of compound <b>15</b>	37	<b>Figure S77.</b> HRMS of compound <b>20</b>	79
<b>Figure S36.</b> $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ) of compound <b>16</b>	38	<b>Figure S78.</b> HRMS of compound <b>21</b>	80
<b>Figure S37.</b> $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ ) of compound <b>16</b>	39	<b>Figure S79.</b> HRMS of compound <b>22</b>	81
<b>Figure S38.</b> $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ) of compound <b>17</b> .	40	<b>Figure S80.</b> HRMS of compound <b>23</b>	82
<b>Figure S39.</b> $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ ) of compound <b>17</b>	41	<b>Figure S81.</b> HRMS of compound <b>24</b>	83
<b>Figure S40.</b> $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ) of compound <b>18</b>	42	<b>Figure S82.</b> HRMS of compound <b>25</b>	84
<b>Figure S41.</b> $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ ) of compound <b>18</b>	43	<b>Figure S83.</b> HRMS of compound <b>26</b>	85
<b>Figure S42.</b> $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ ) of compound <b>19</b>	44		

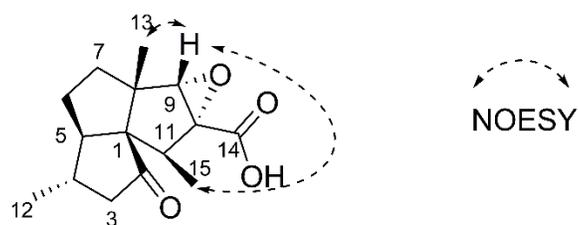


Figure S1. Key NOE correlations of **4**.

Figure S2. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound SA

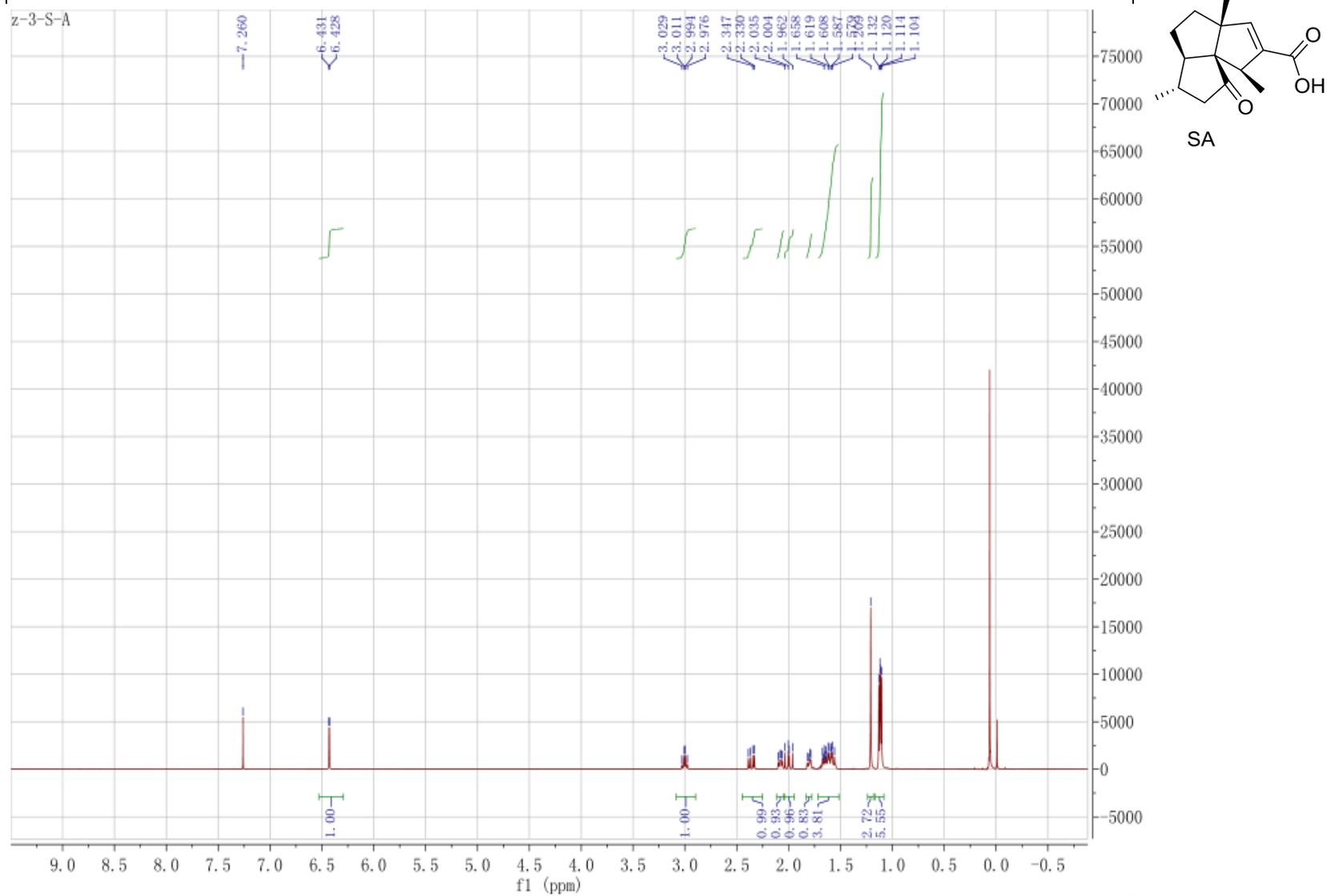
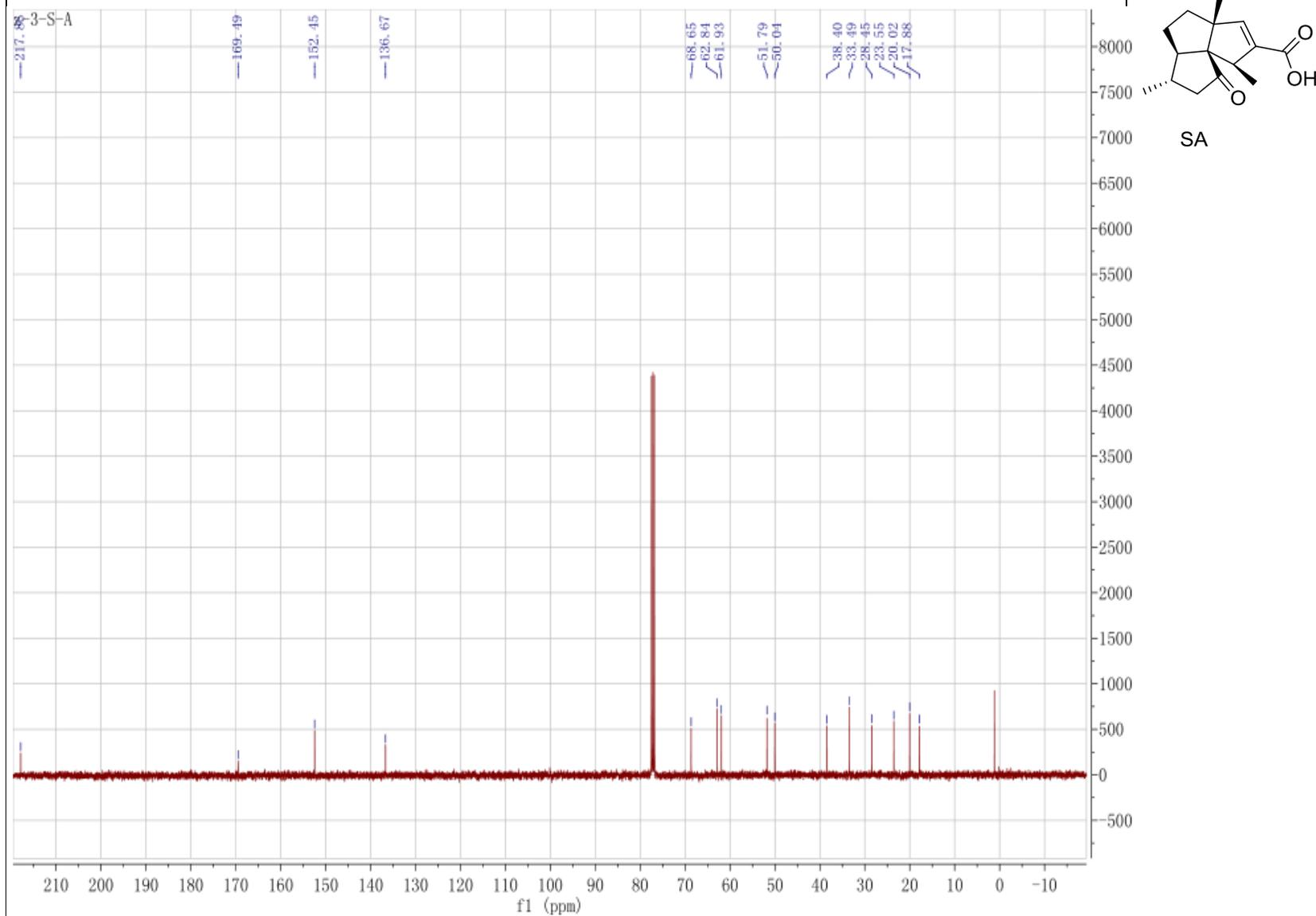


Figure S3. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound SA



**Figure S4.**  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound **1**

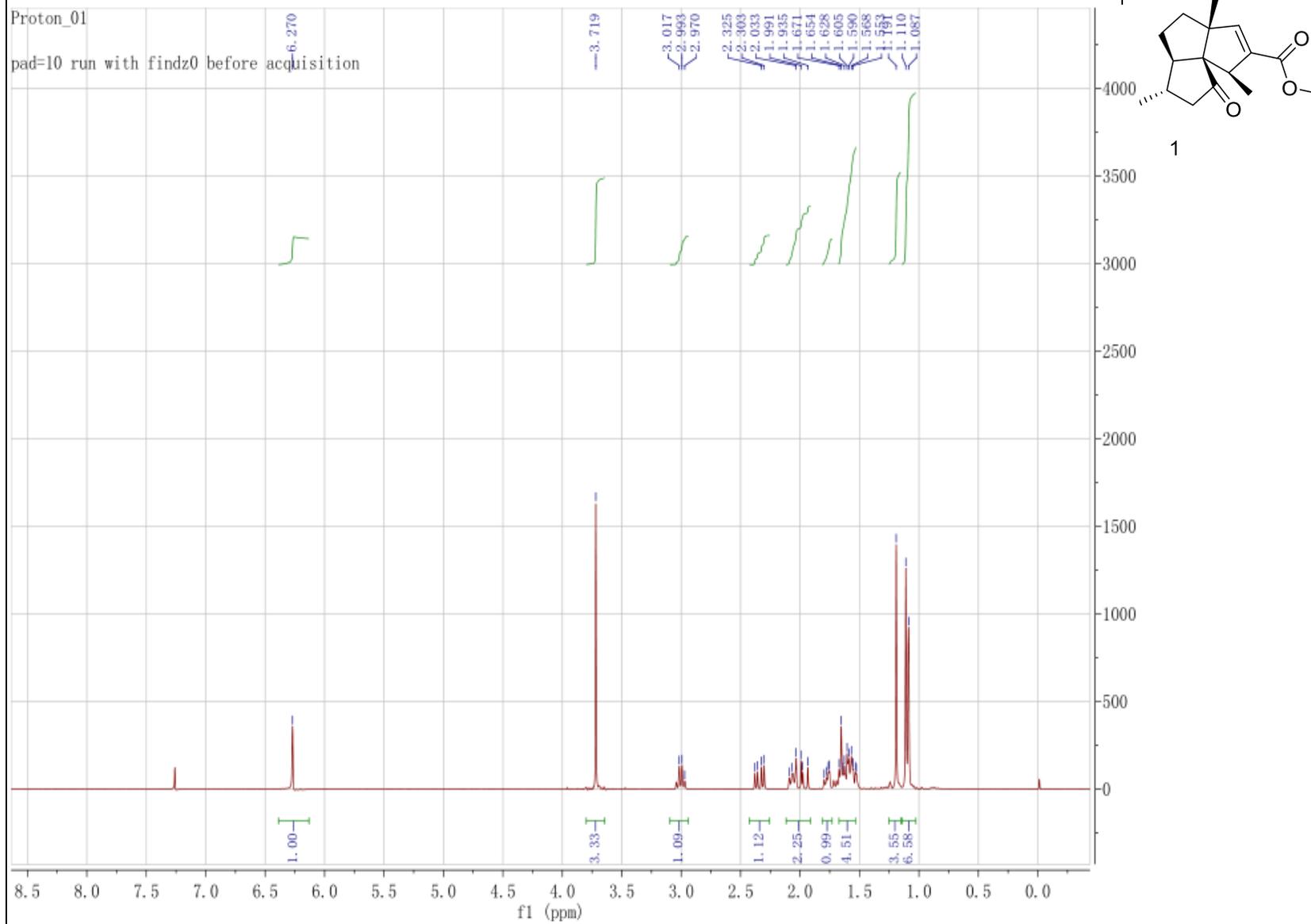


Figure S5.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **1**

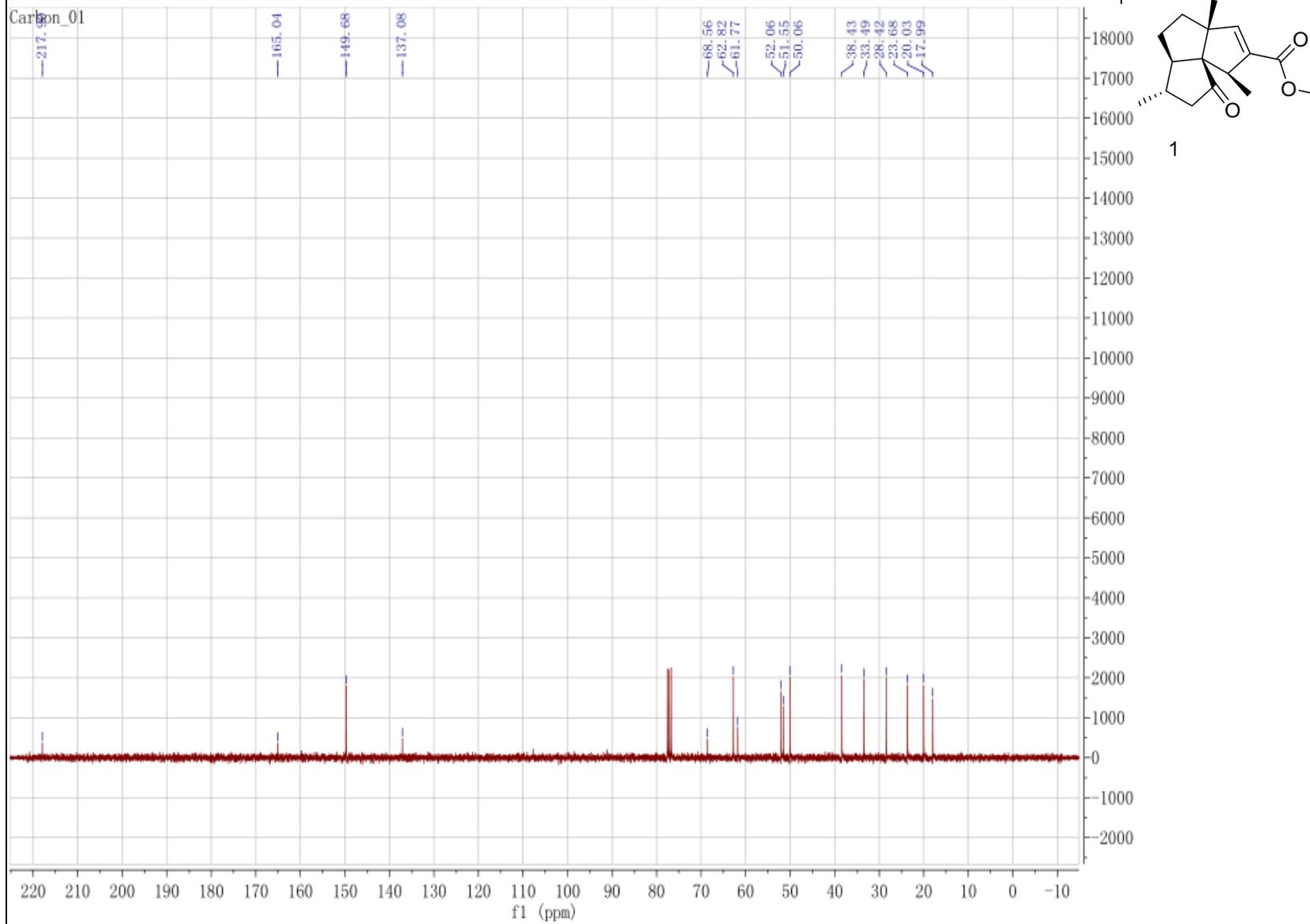


Figure S6. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 2

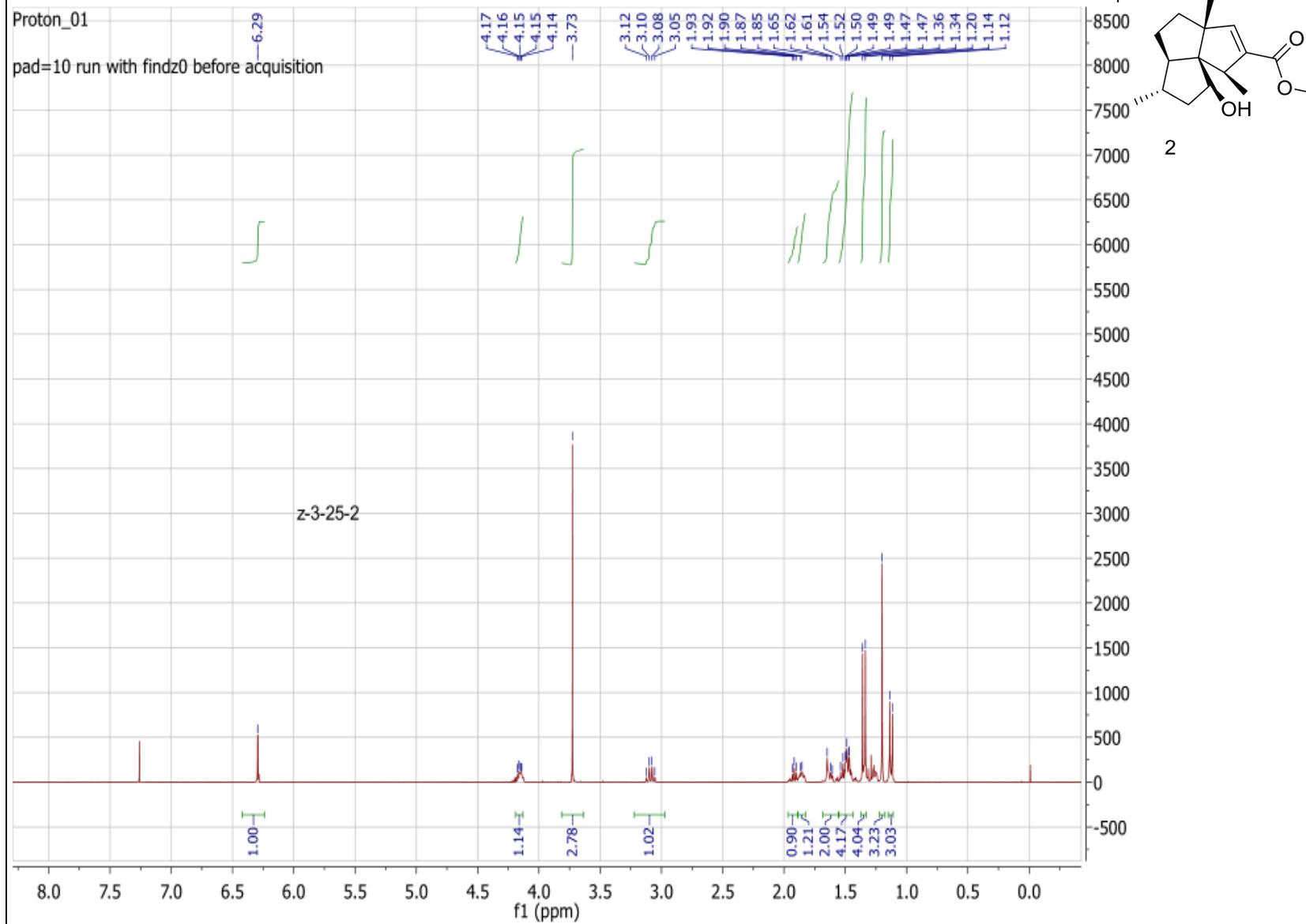


Figure S7.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 2

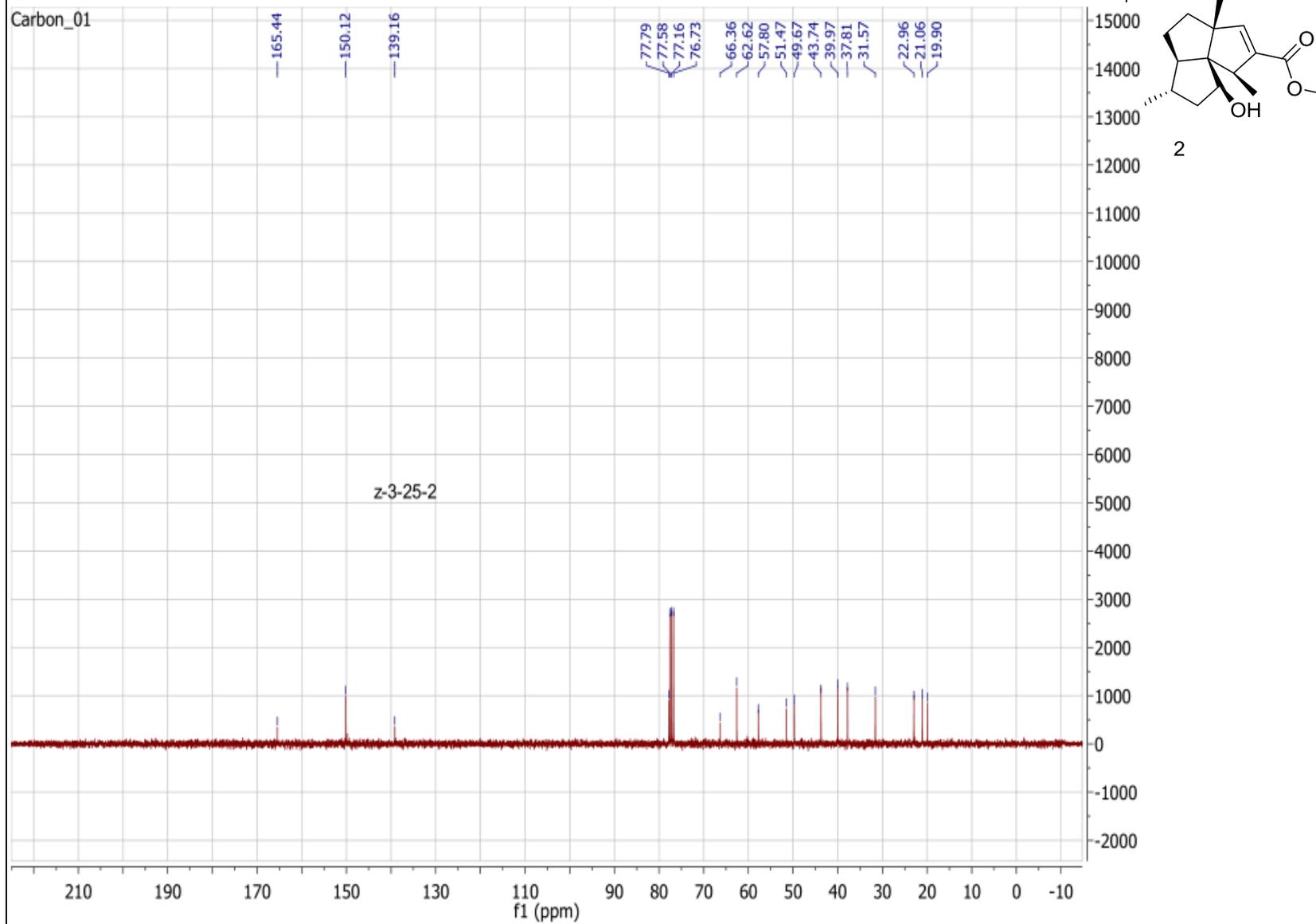


Figure S8. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound **3**

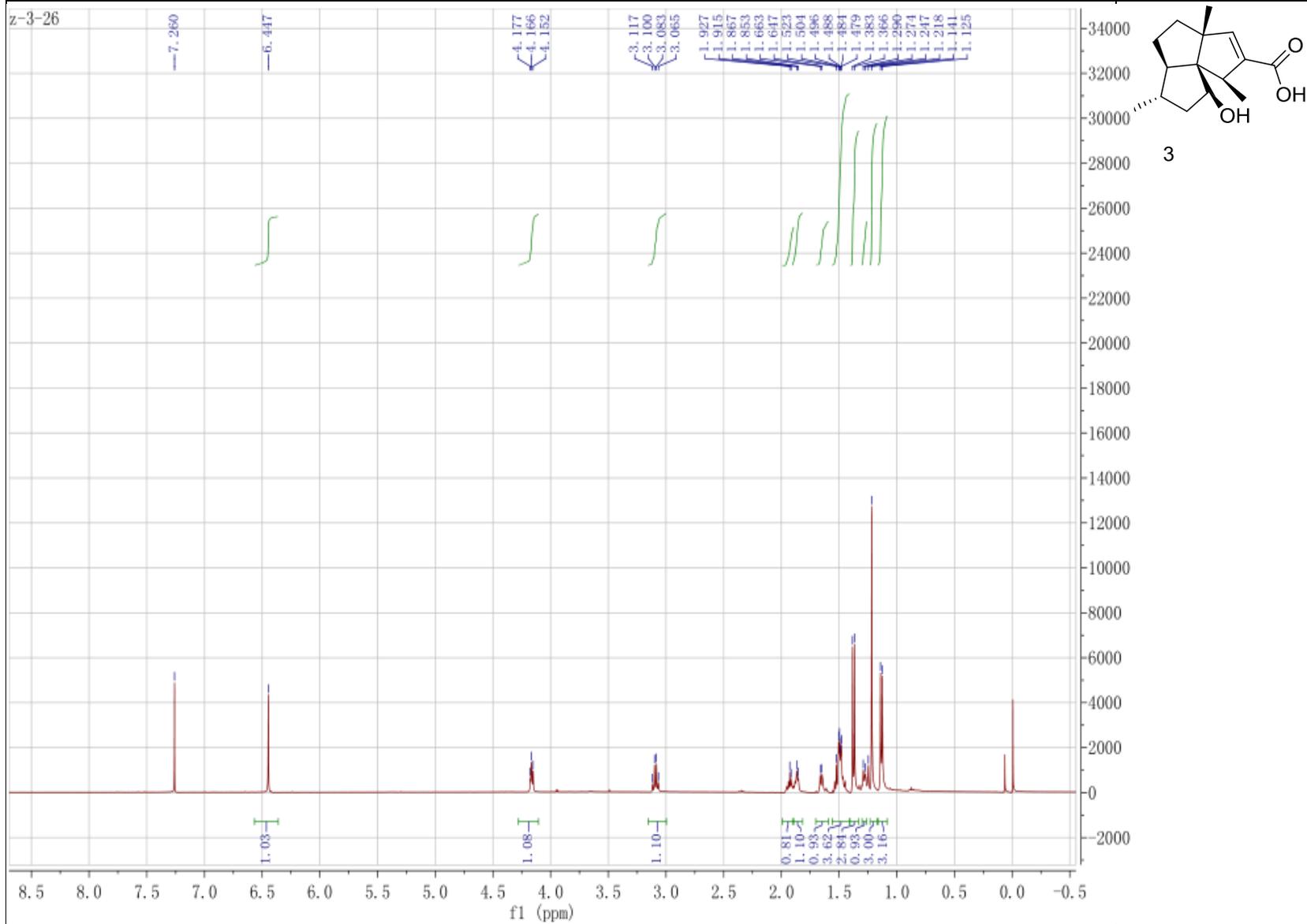


Figure S9.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **3**

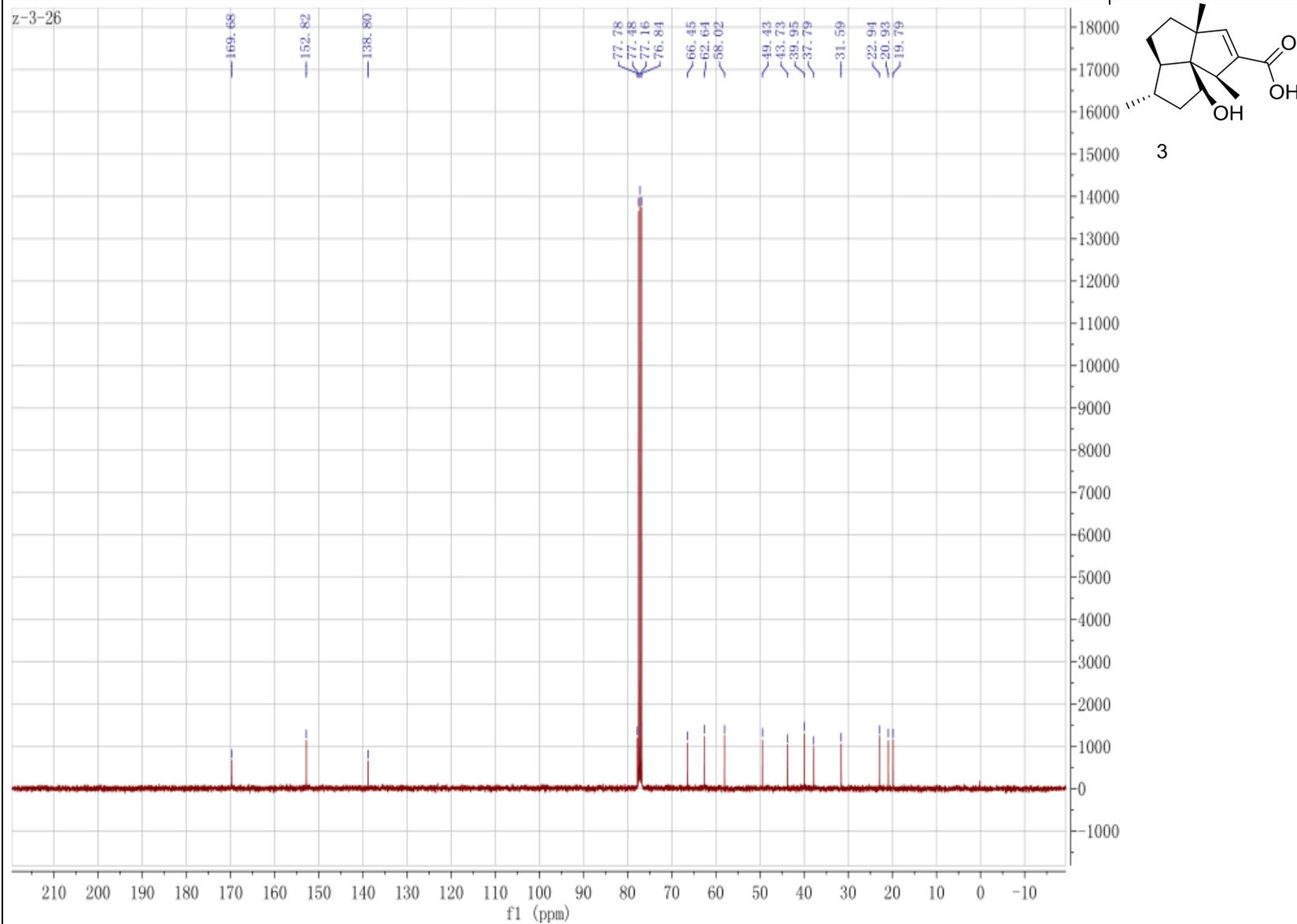
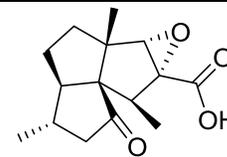
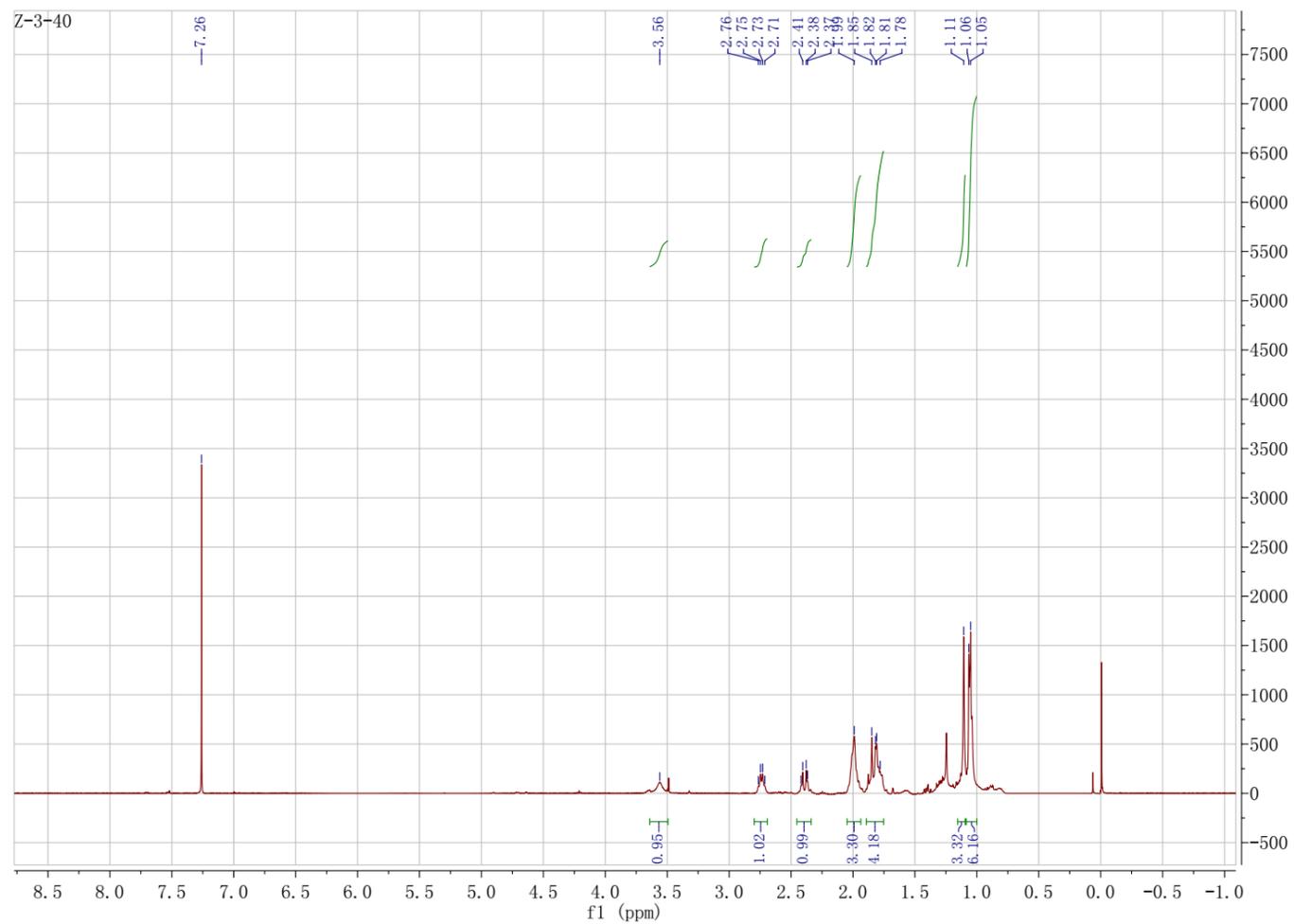


Figure S10. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 4



4

Figure S11.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 4

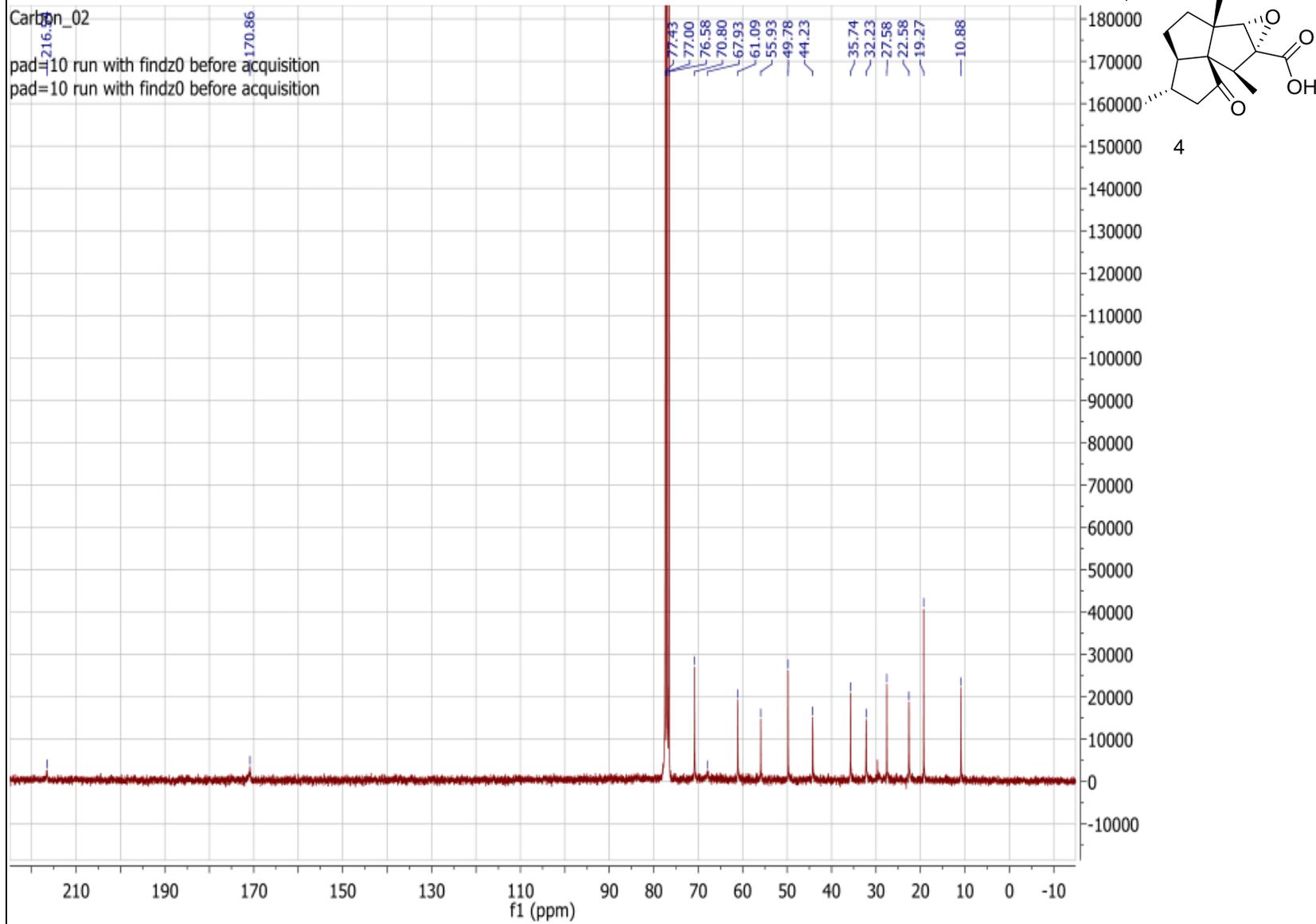


Figure S12. HSQC spectrum of compound 4

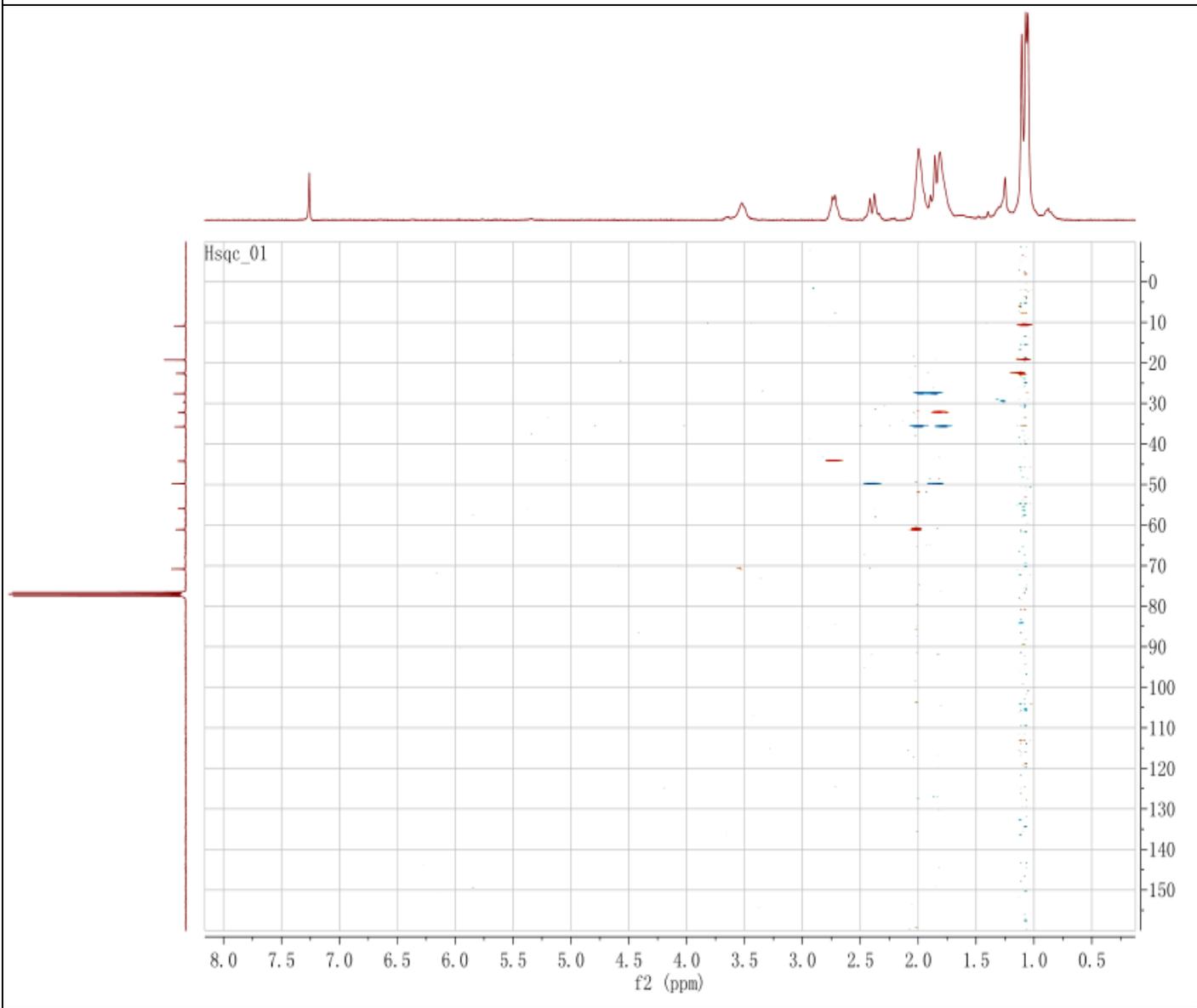
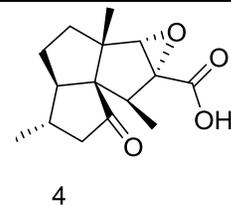


Figure S13. NOESY spectrum of compound 4

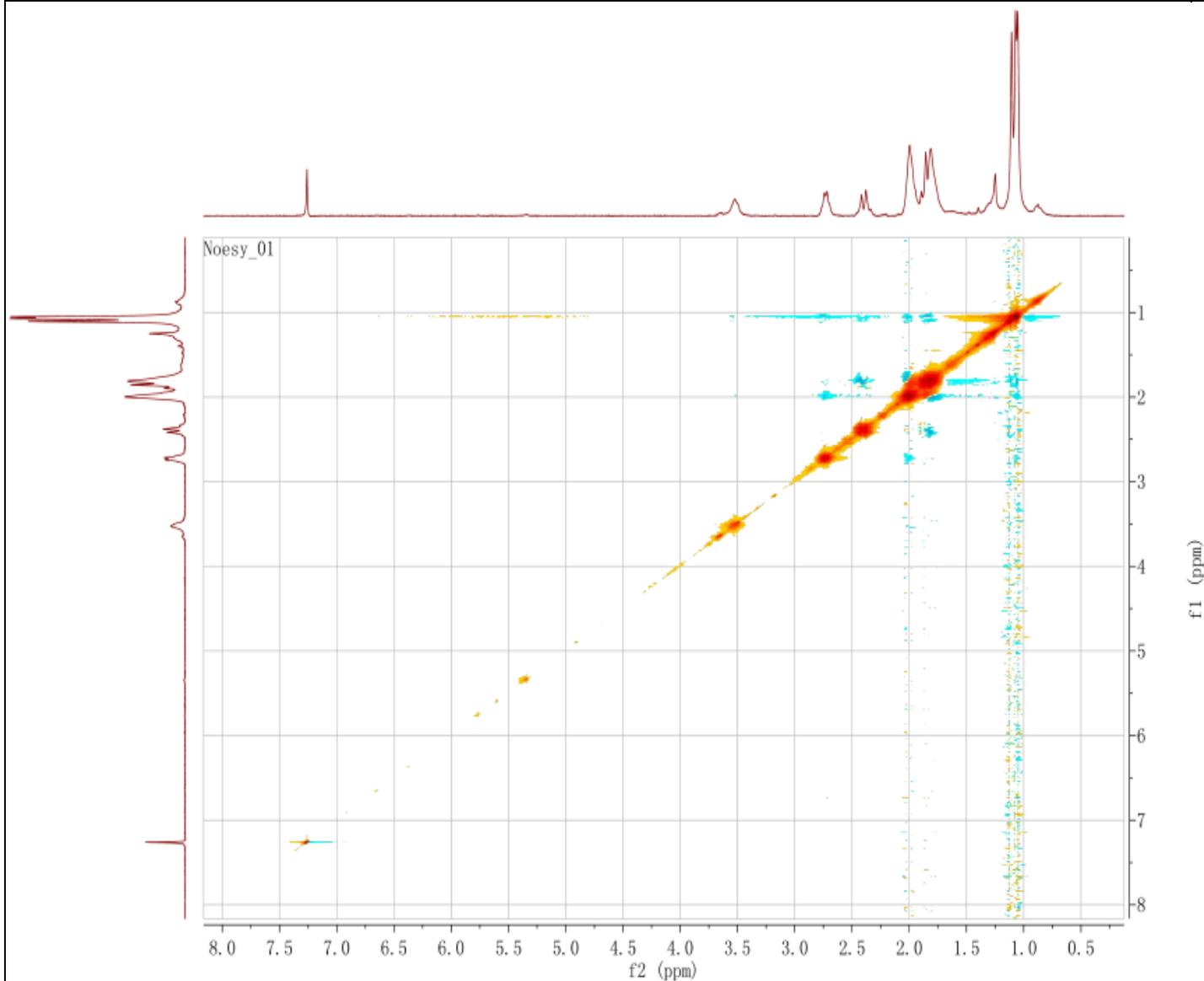
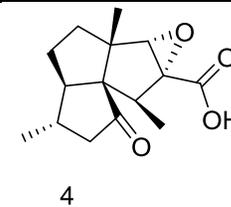


Figure S14. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 5

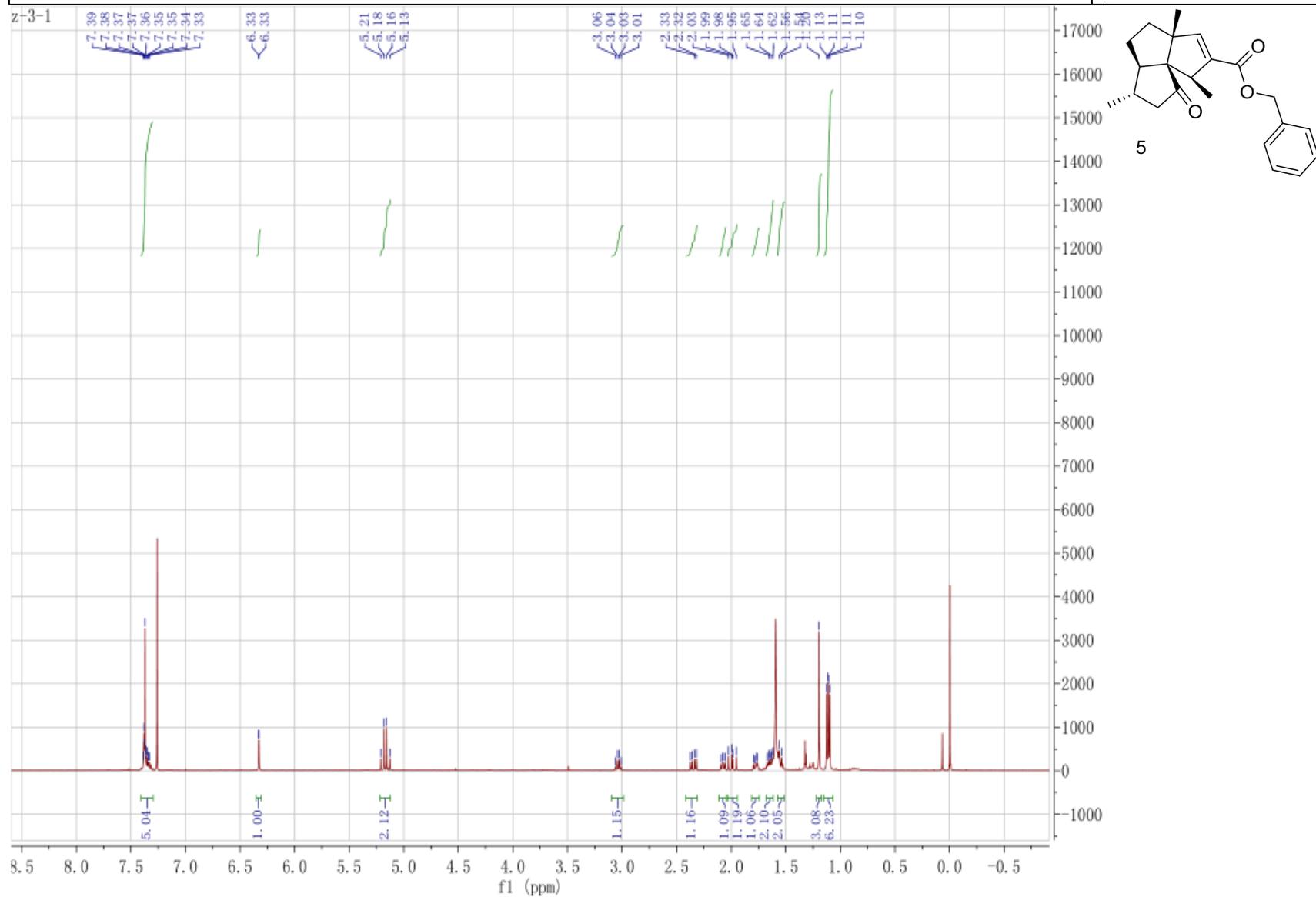


Figure S15.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **5**

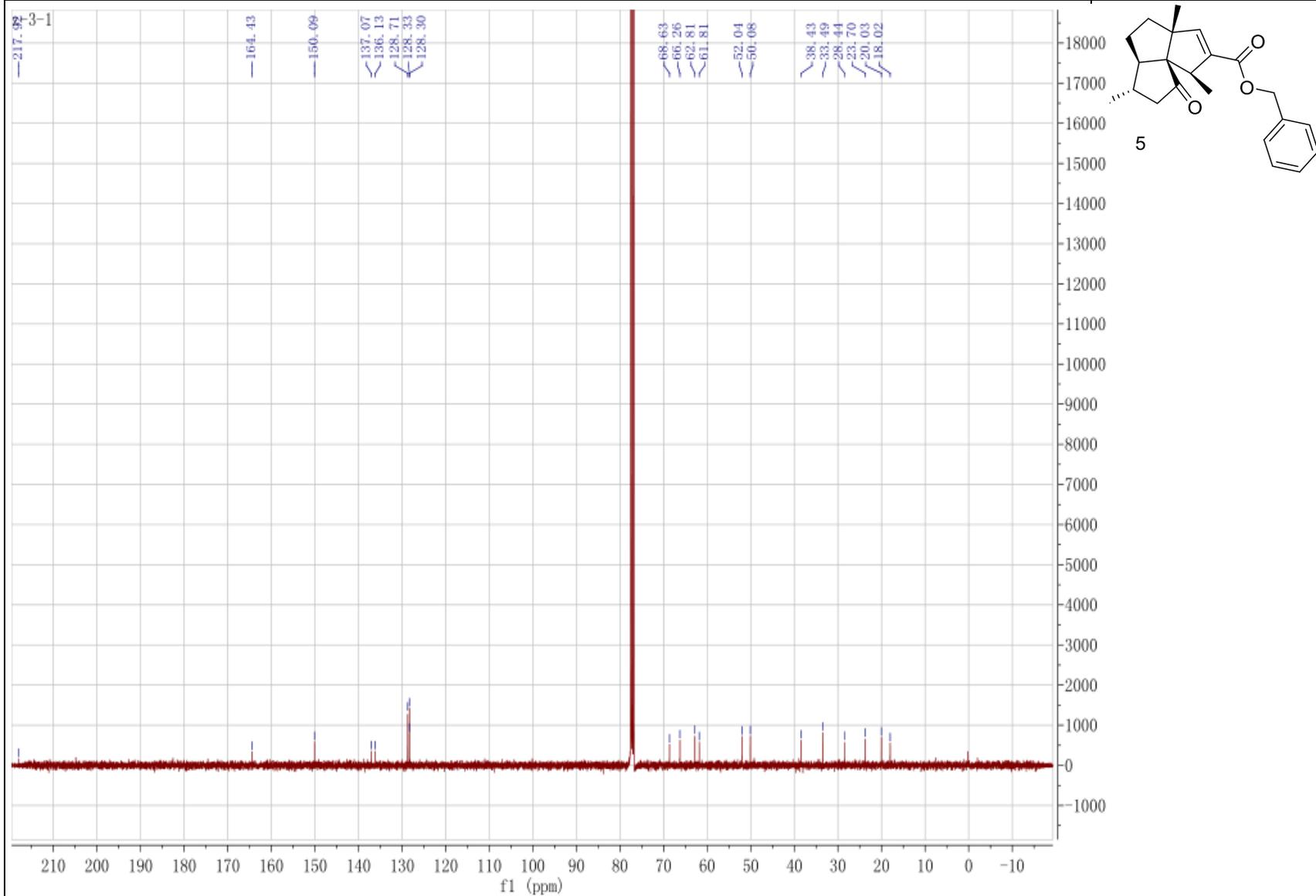


Figure S16. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 6

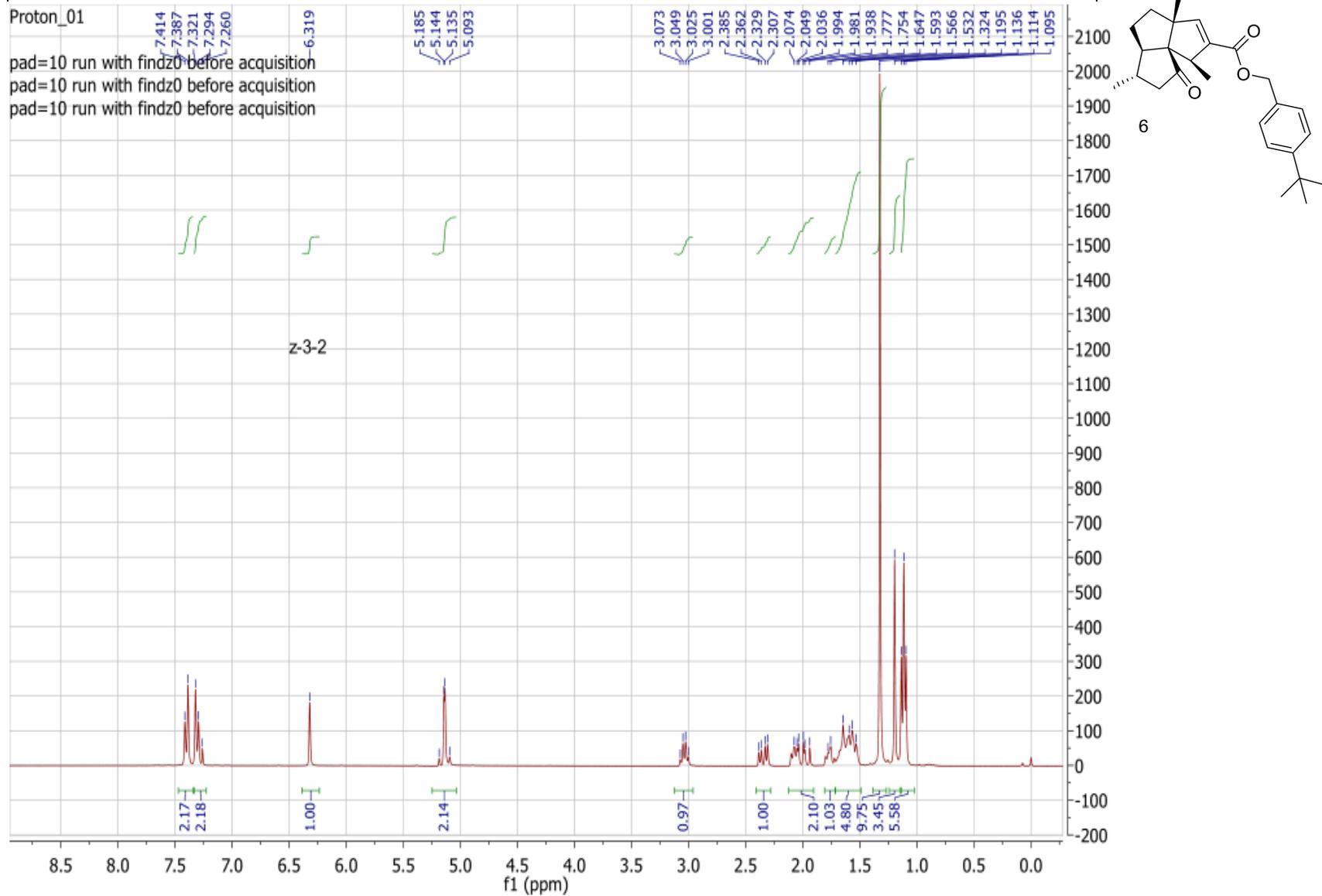


Figure S17. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 6

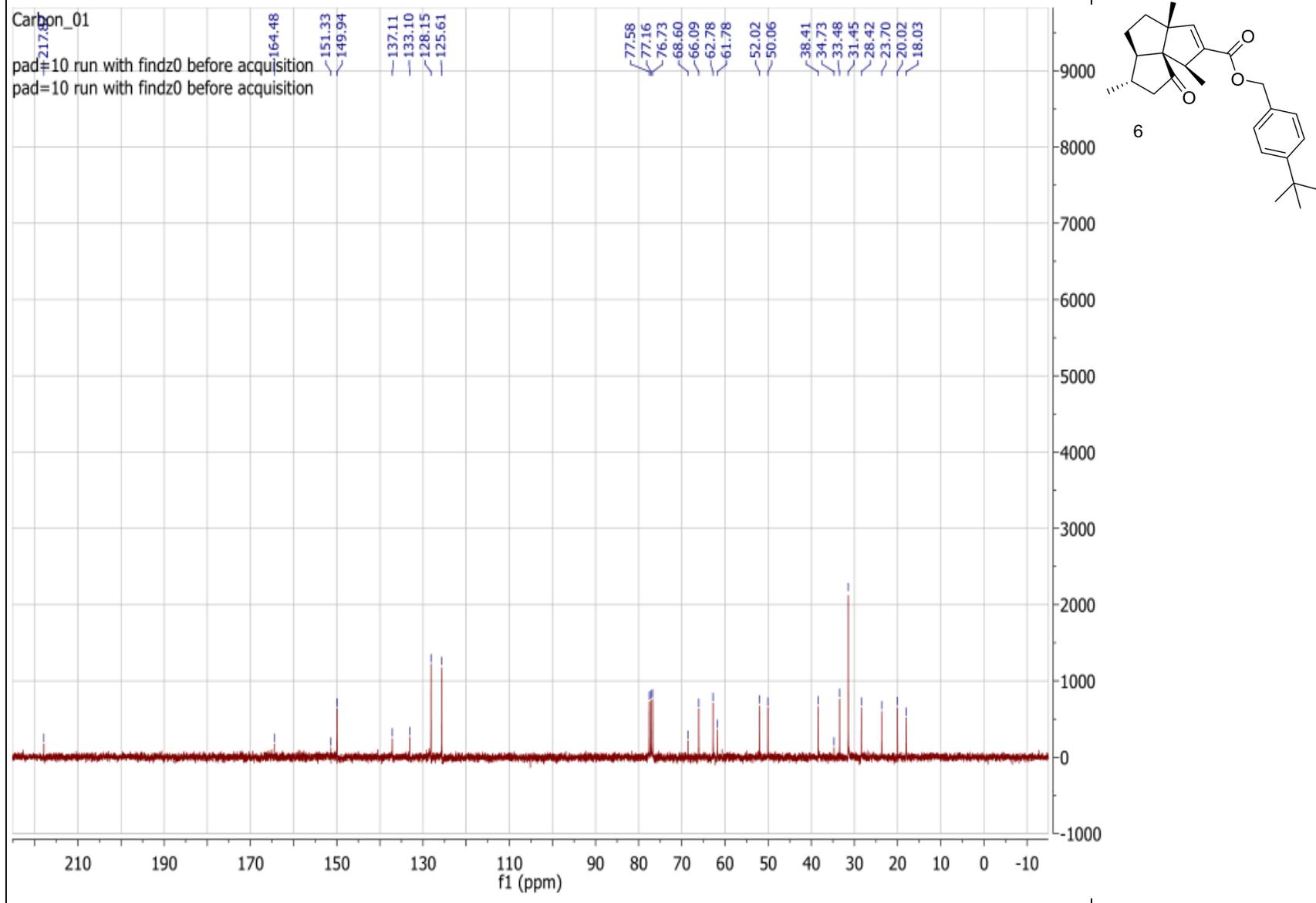


Figure S18. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 7

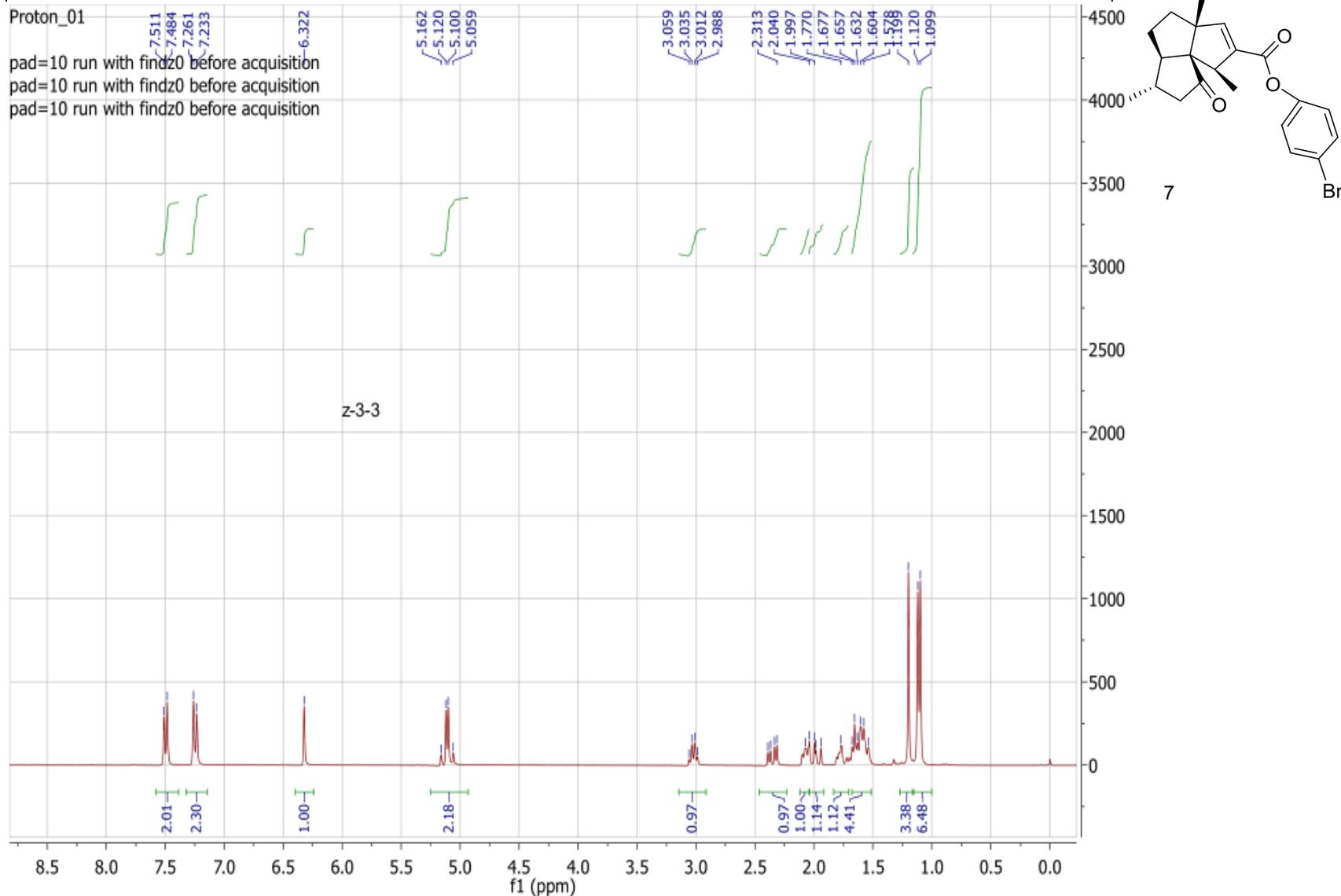


Figure S19. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 7

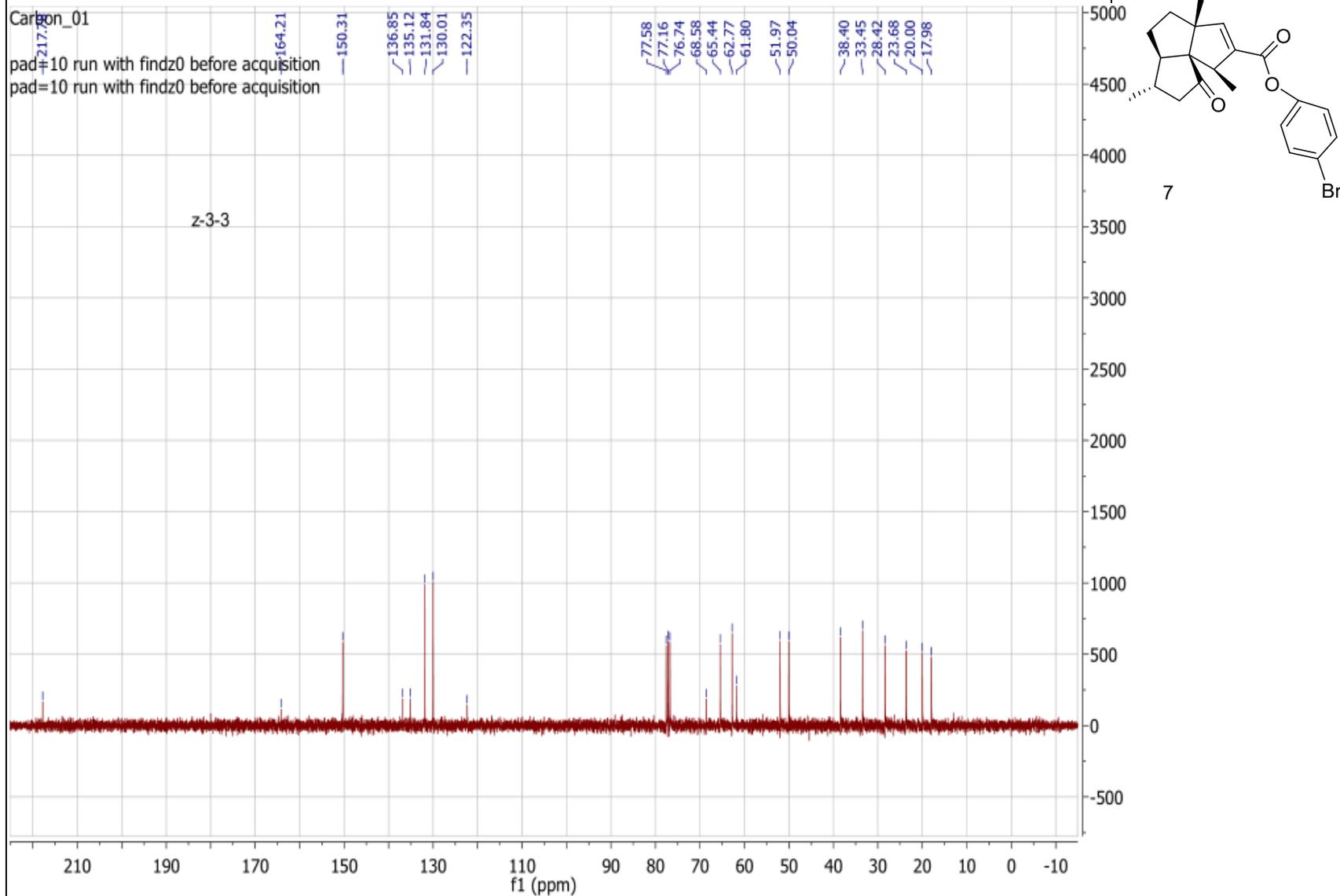


Figure S20. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 8

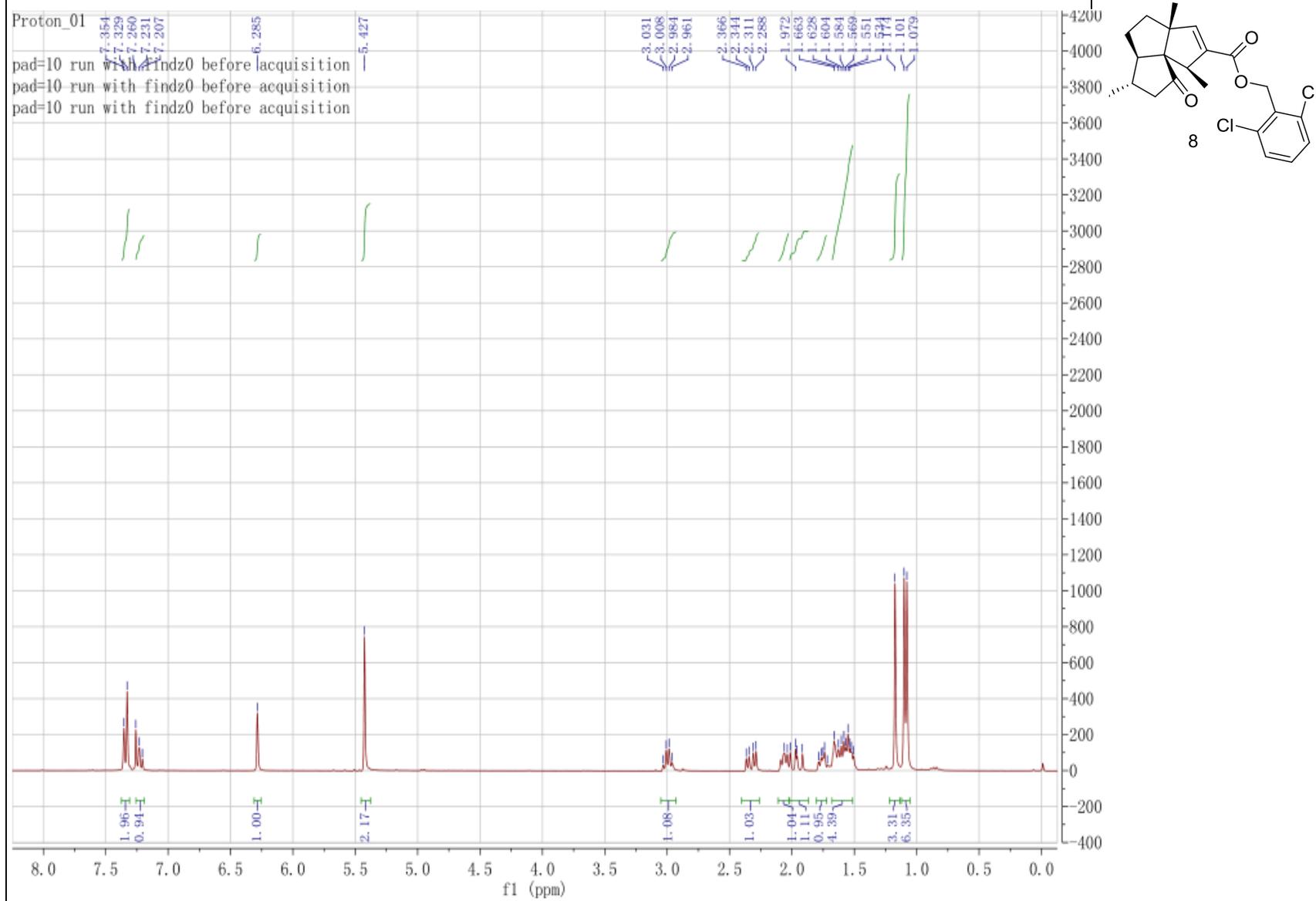


Figure S21.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **8**

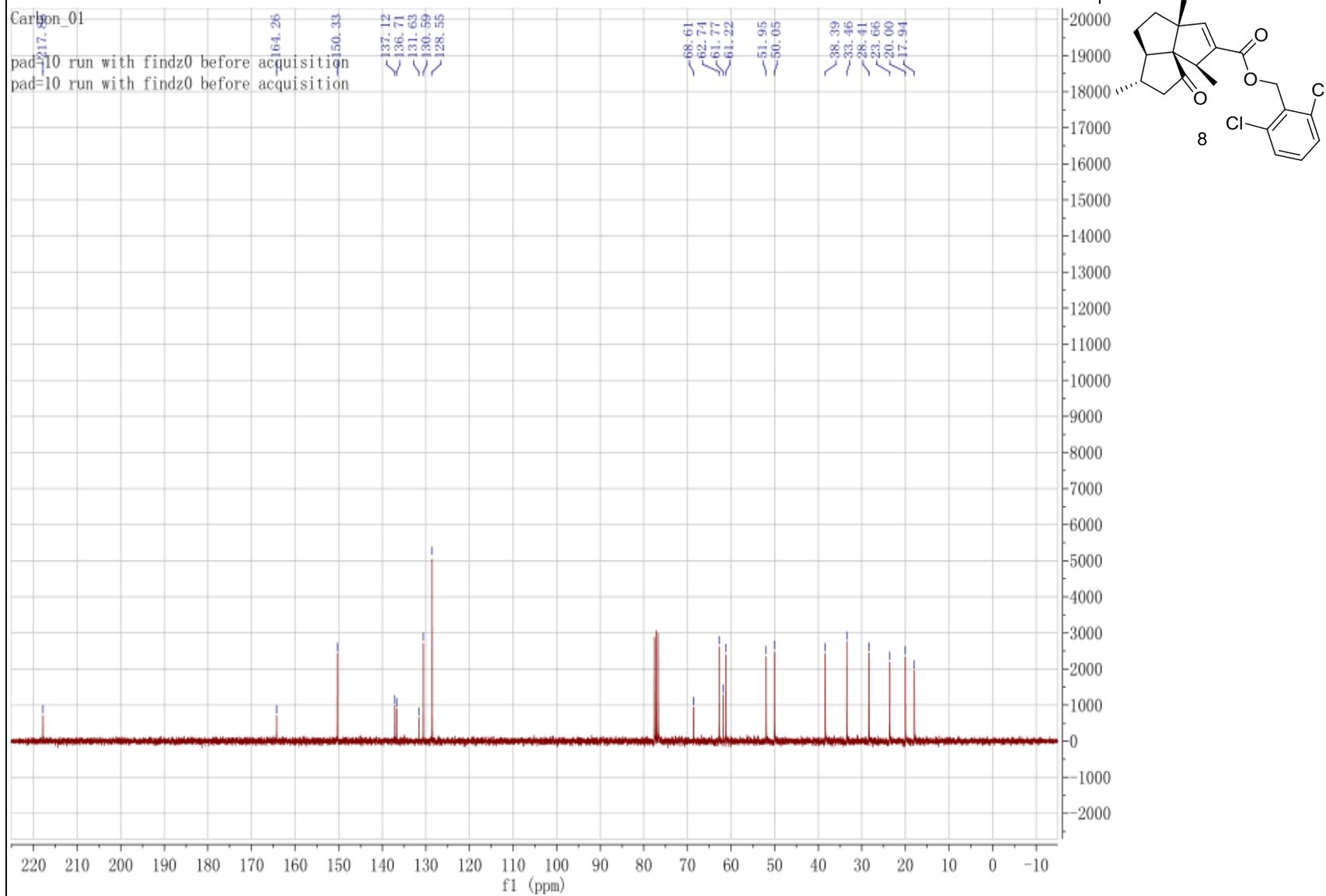


Figure S22. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 9

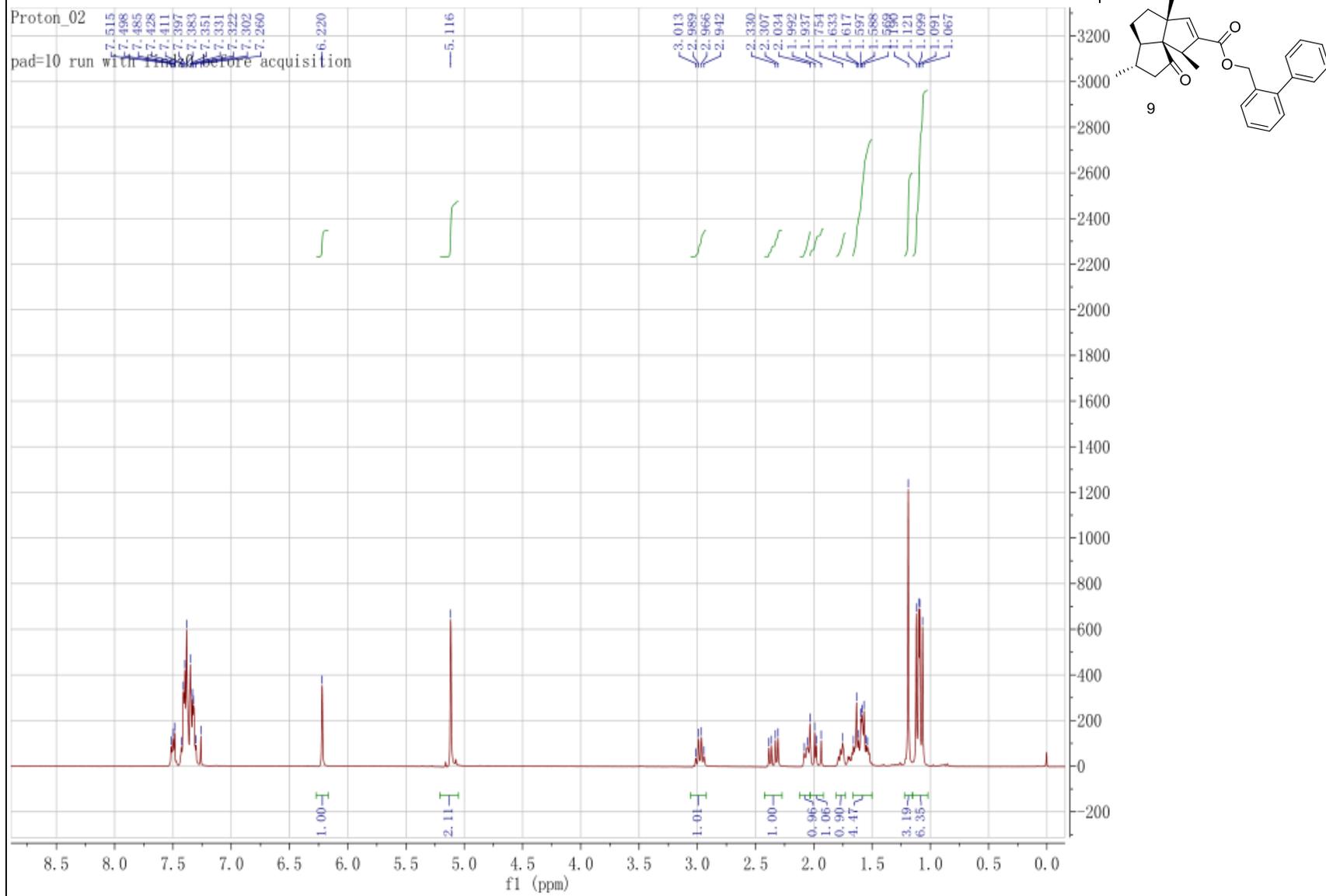


Figure S23. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound **9**

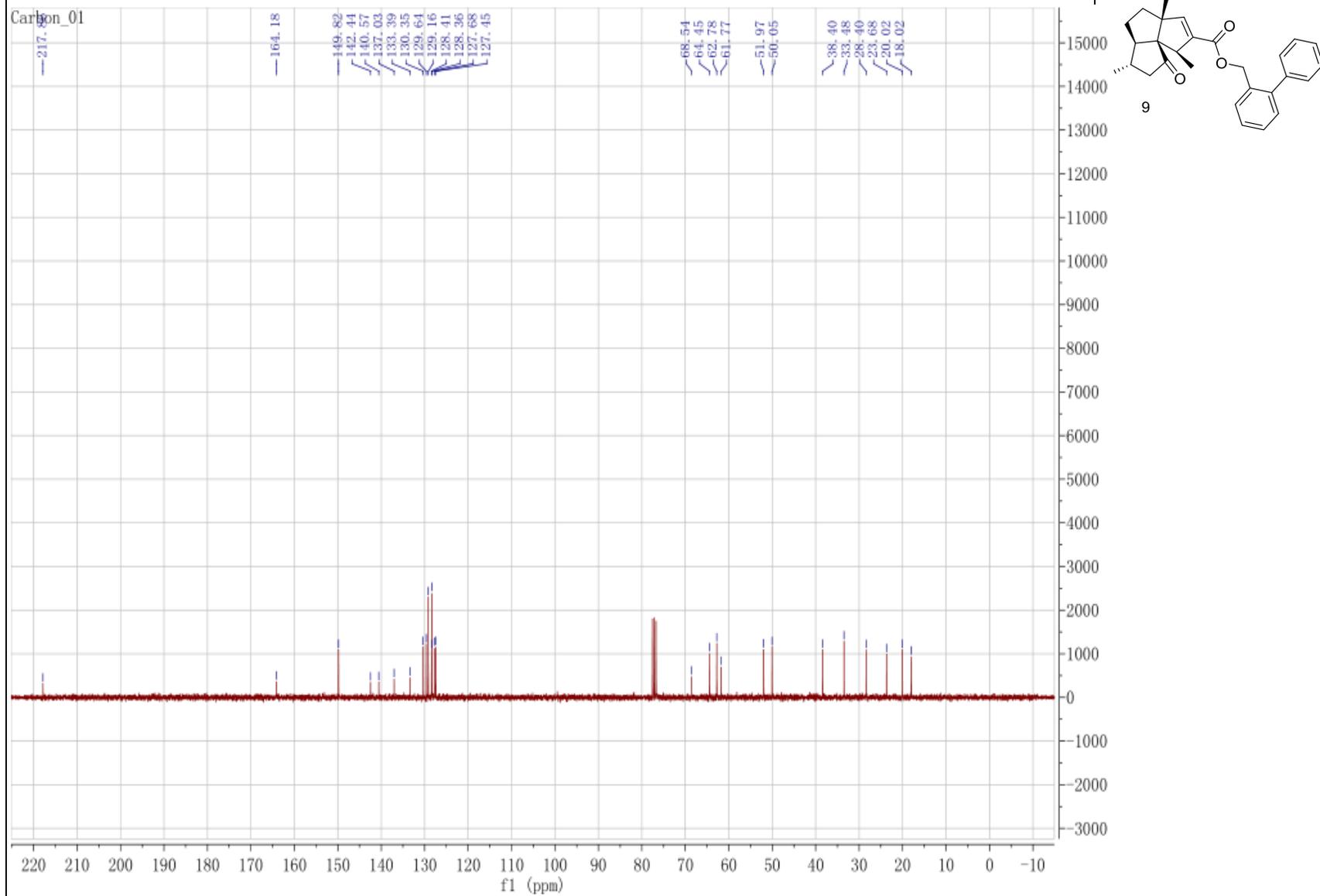


Figure S24. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 10

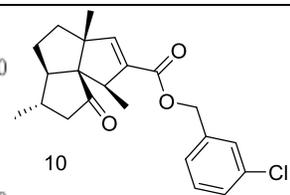


Figure S25.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **10**

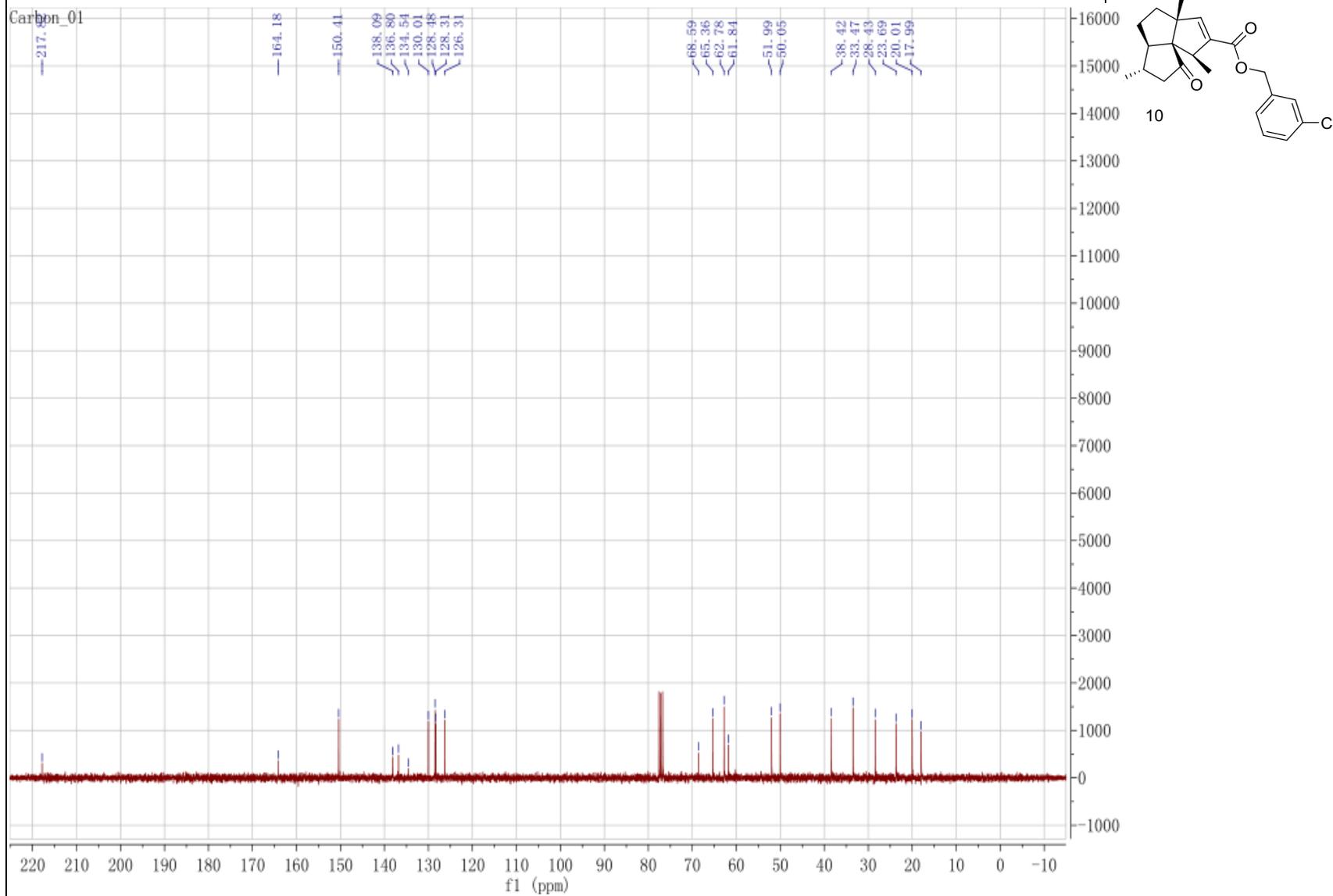


Figure S26. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 11

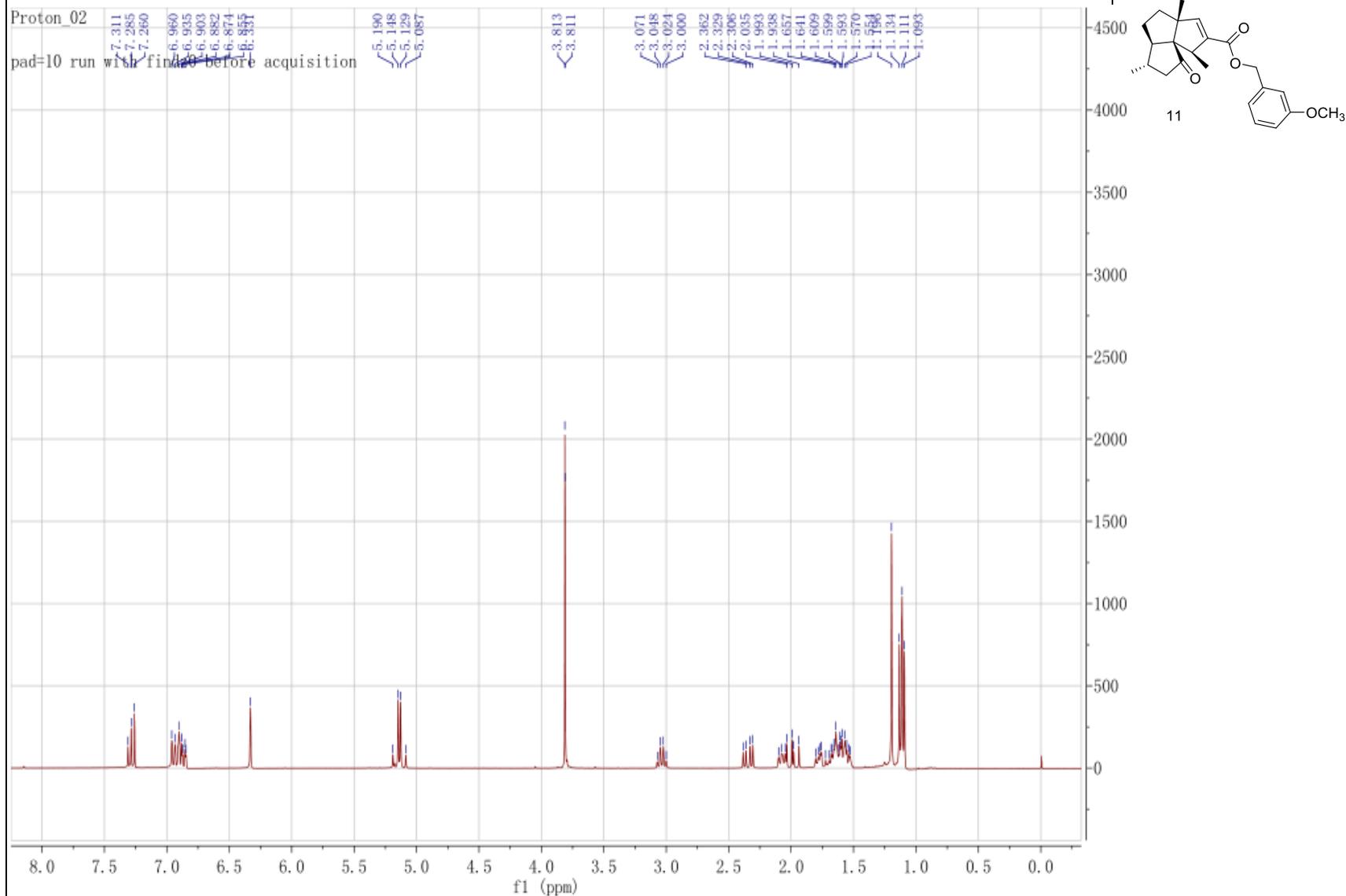
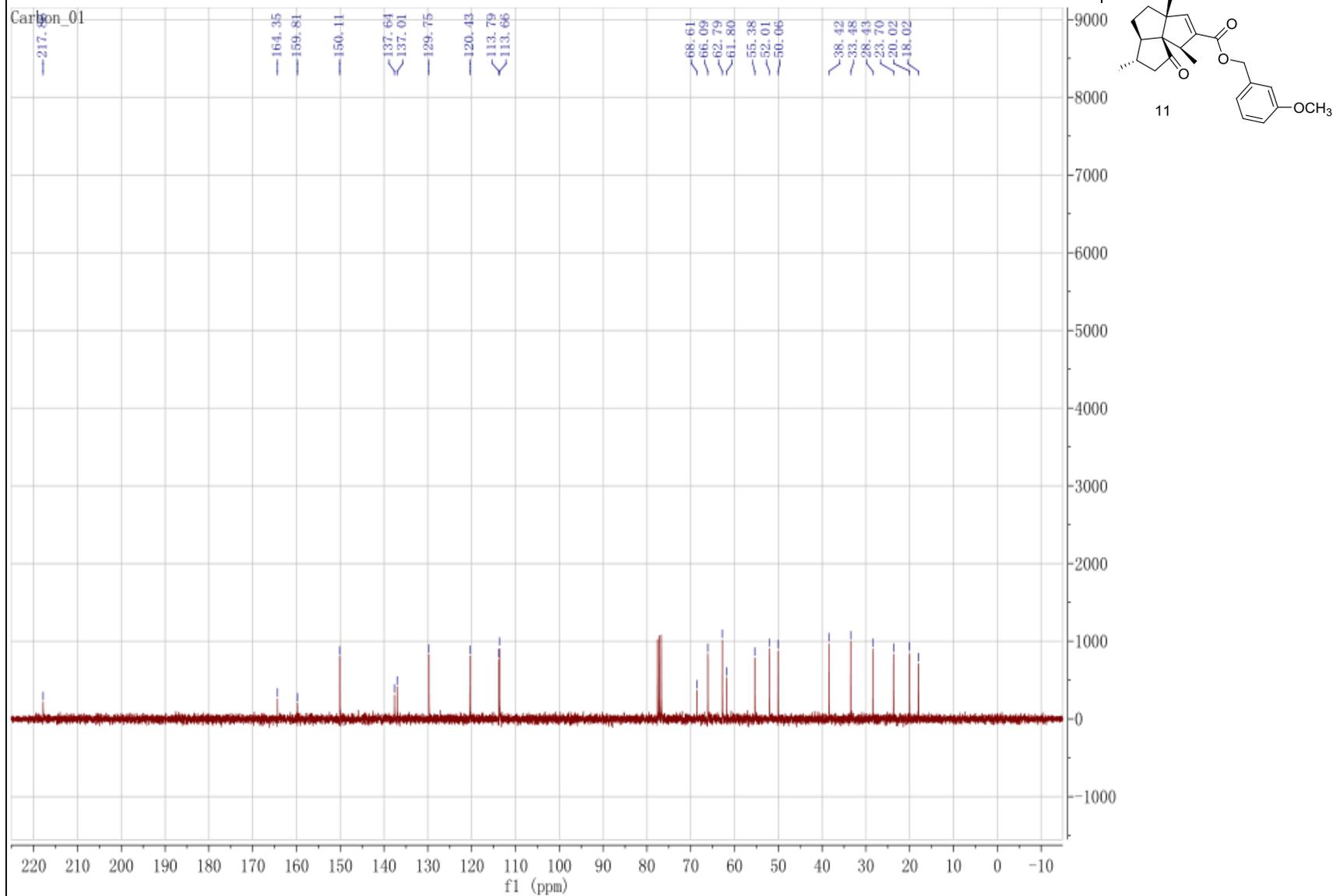


Figure S27. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound **11**



**Figure S28.**  $^1\text{H}$  NMR (300 MHz,  $\text{CDCl}_3$ ) of compound **12**

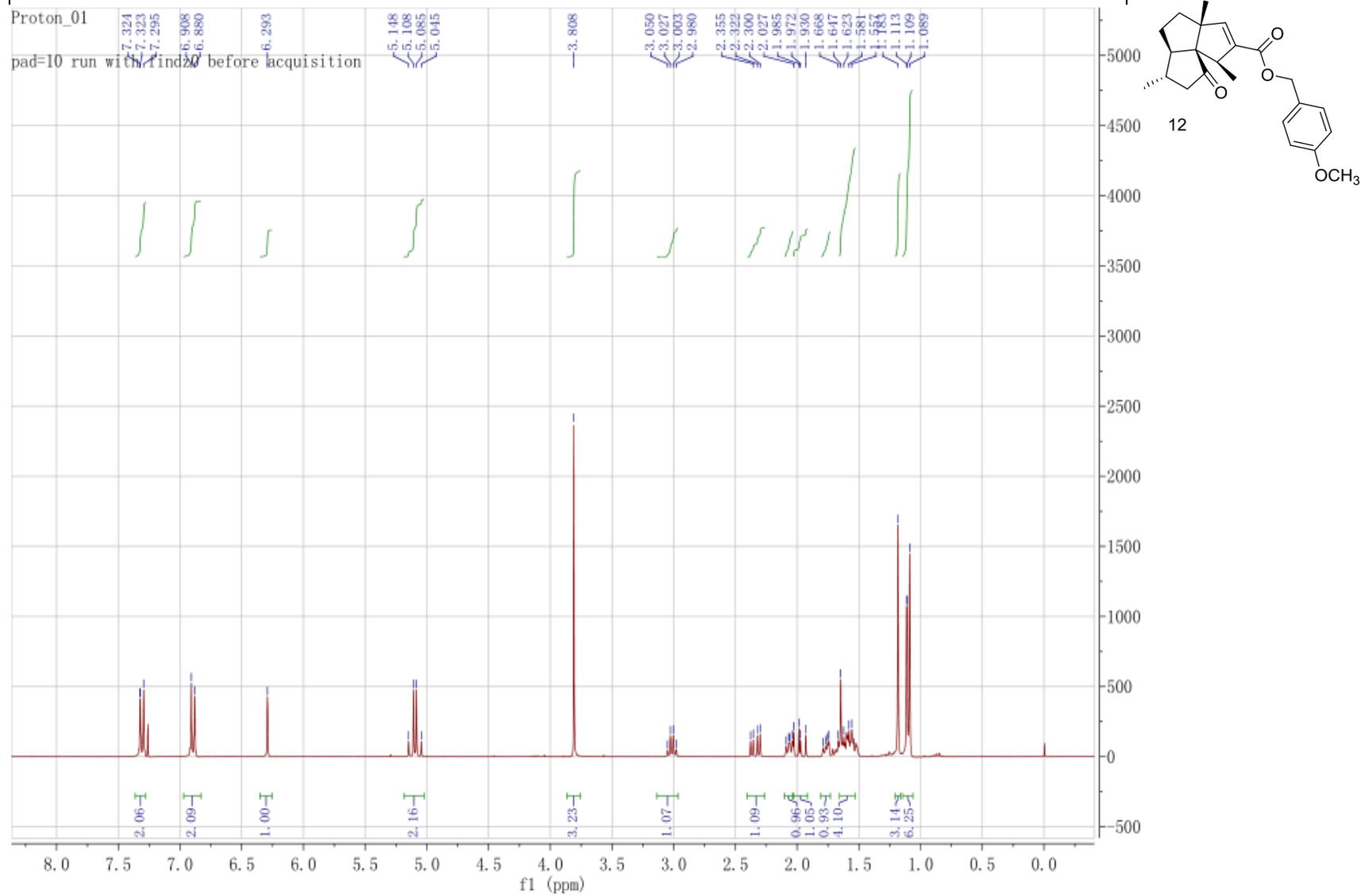


Figure S29. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 12

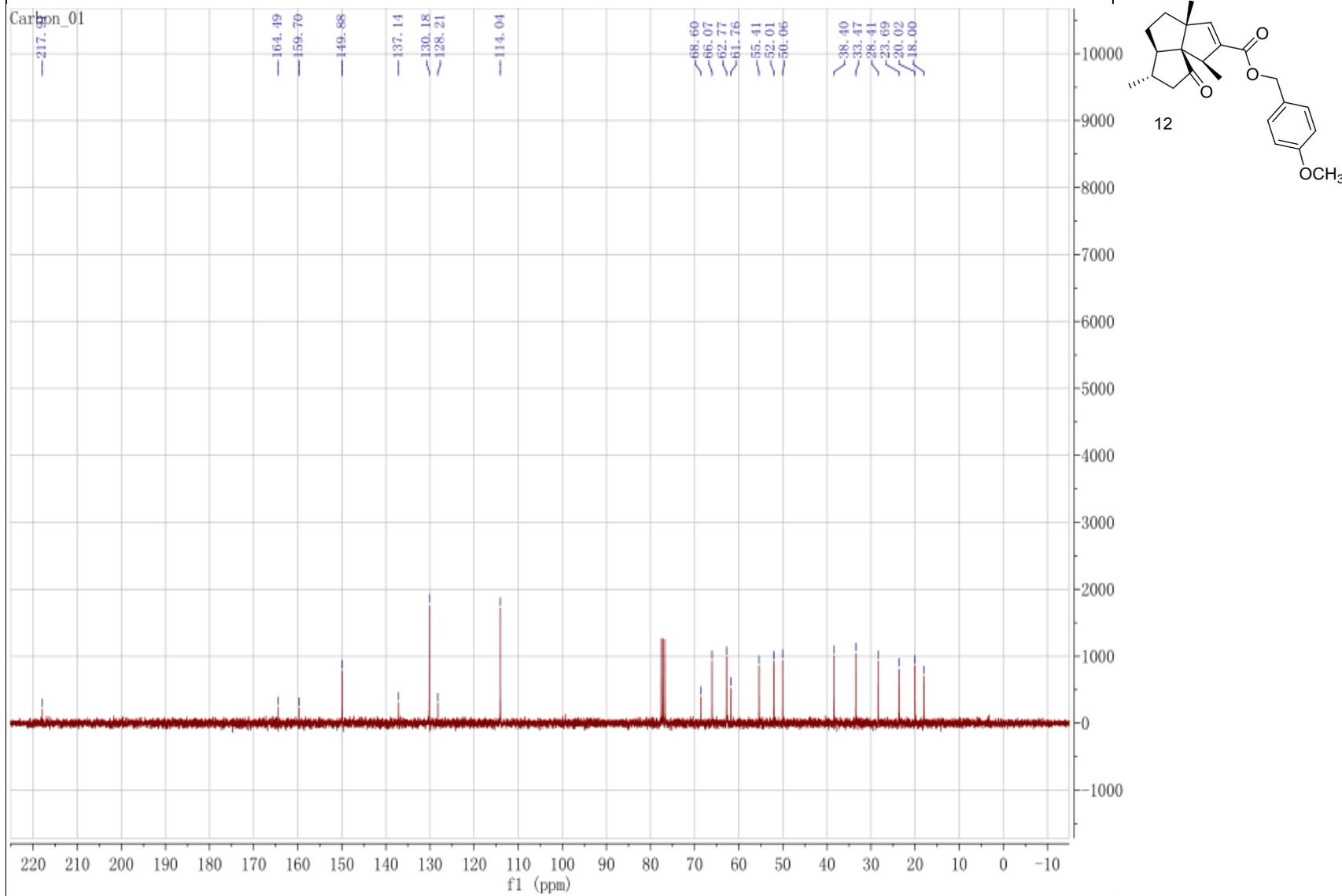


Figure S30. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 13

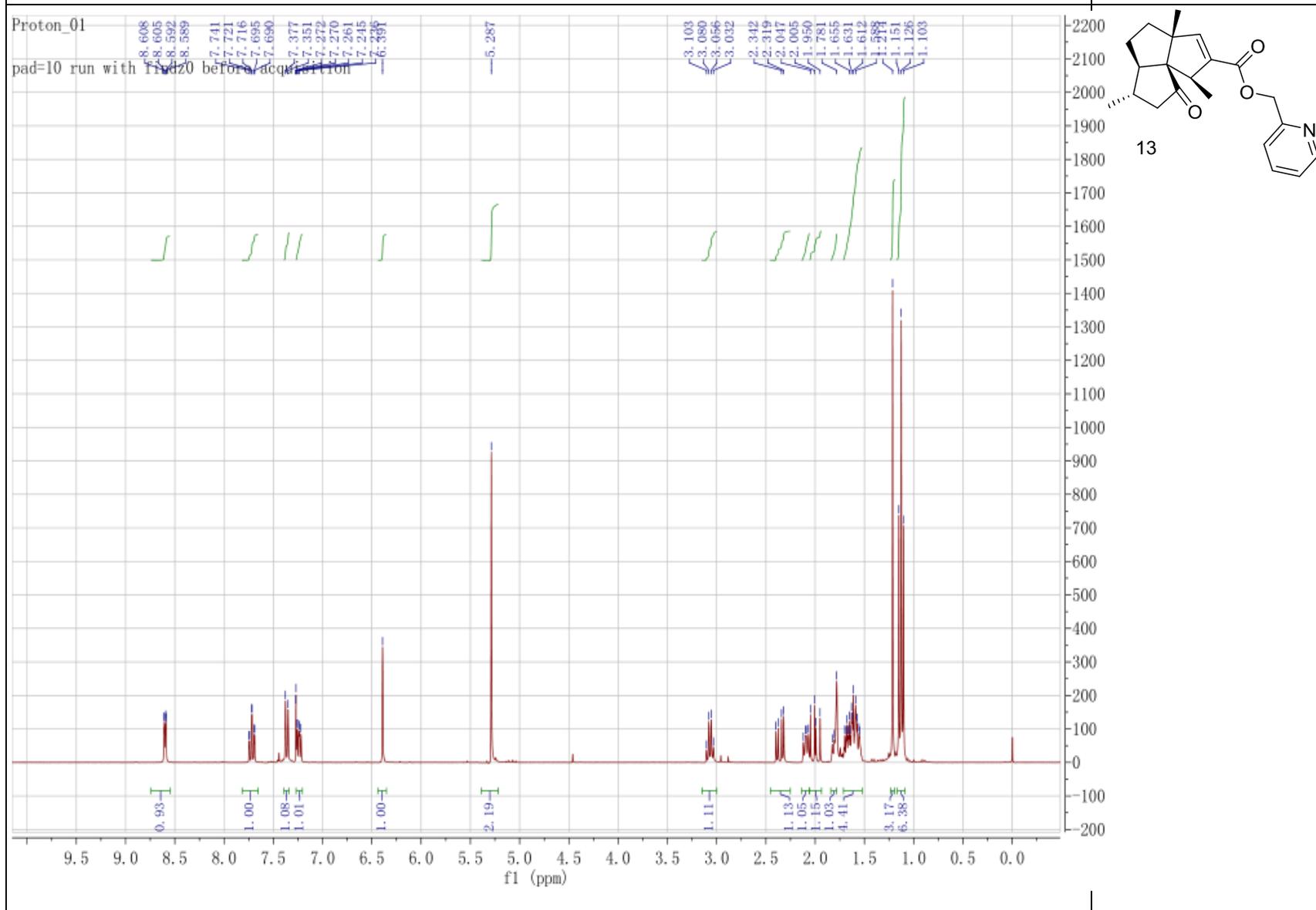


Figure S31.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound **13**

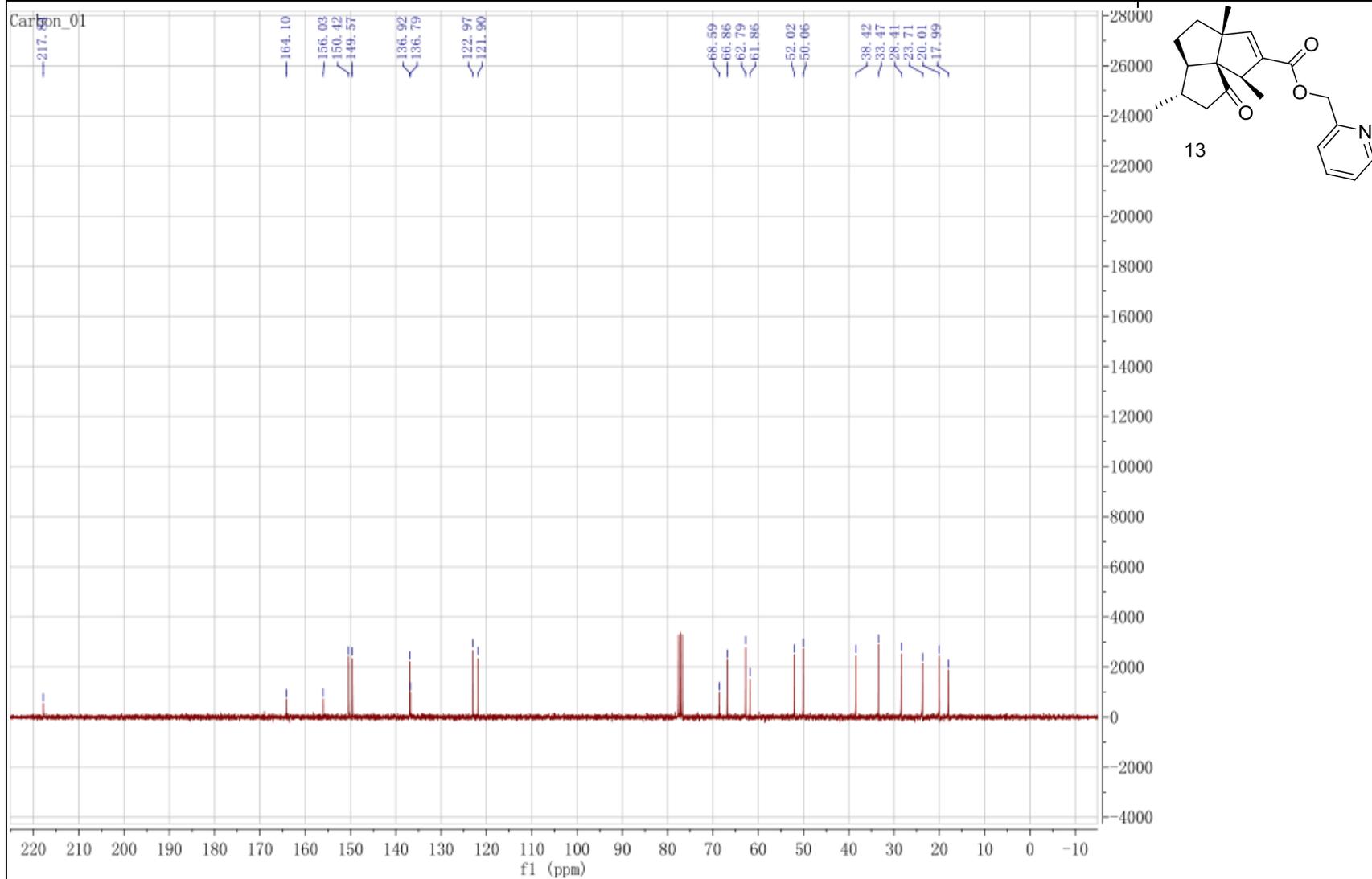


Figure S32. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 14

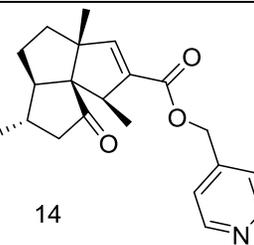
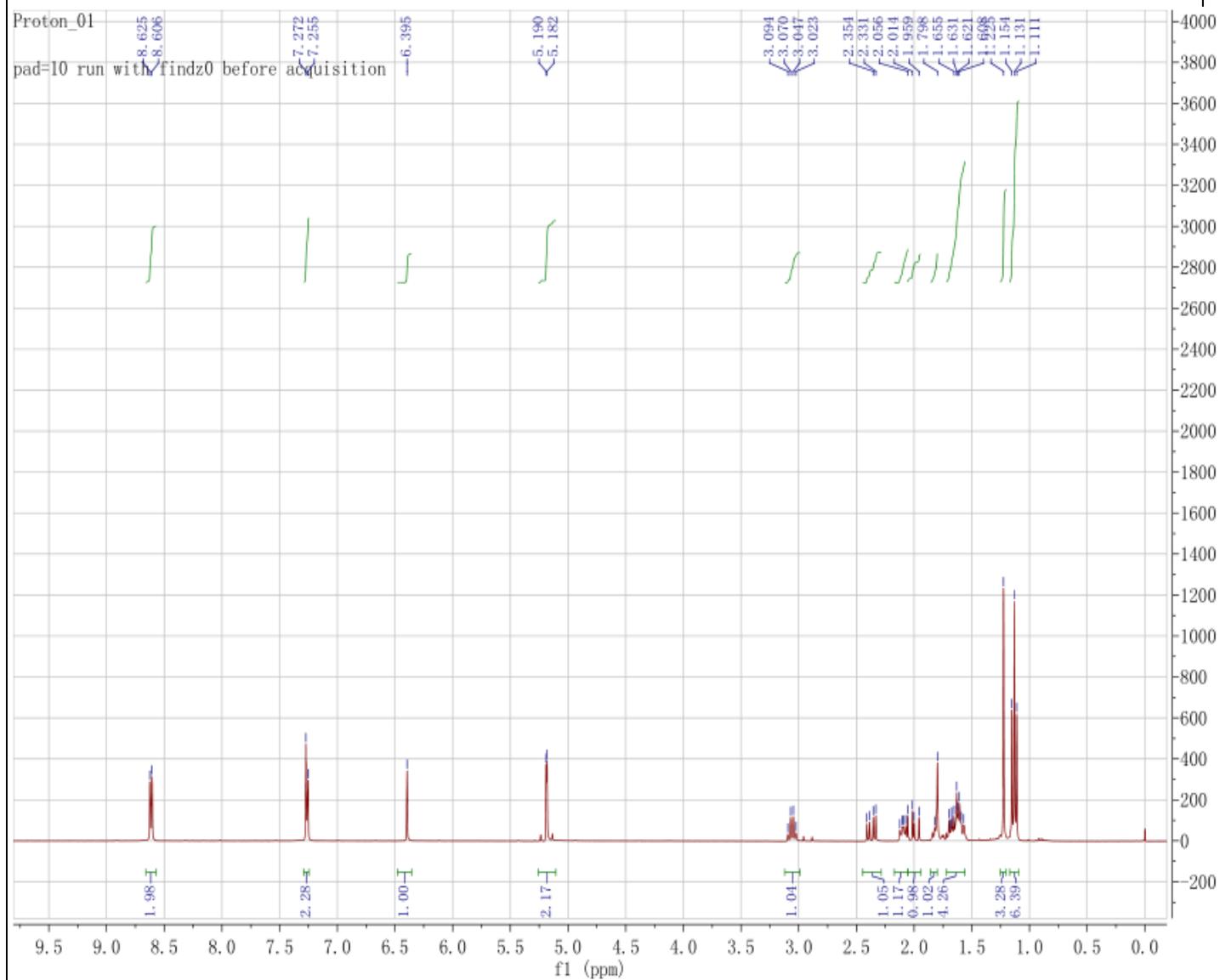


Figure S33.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 14

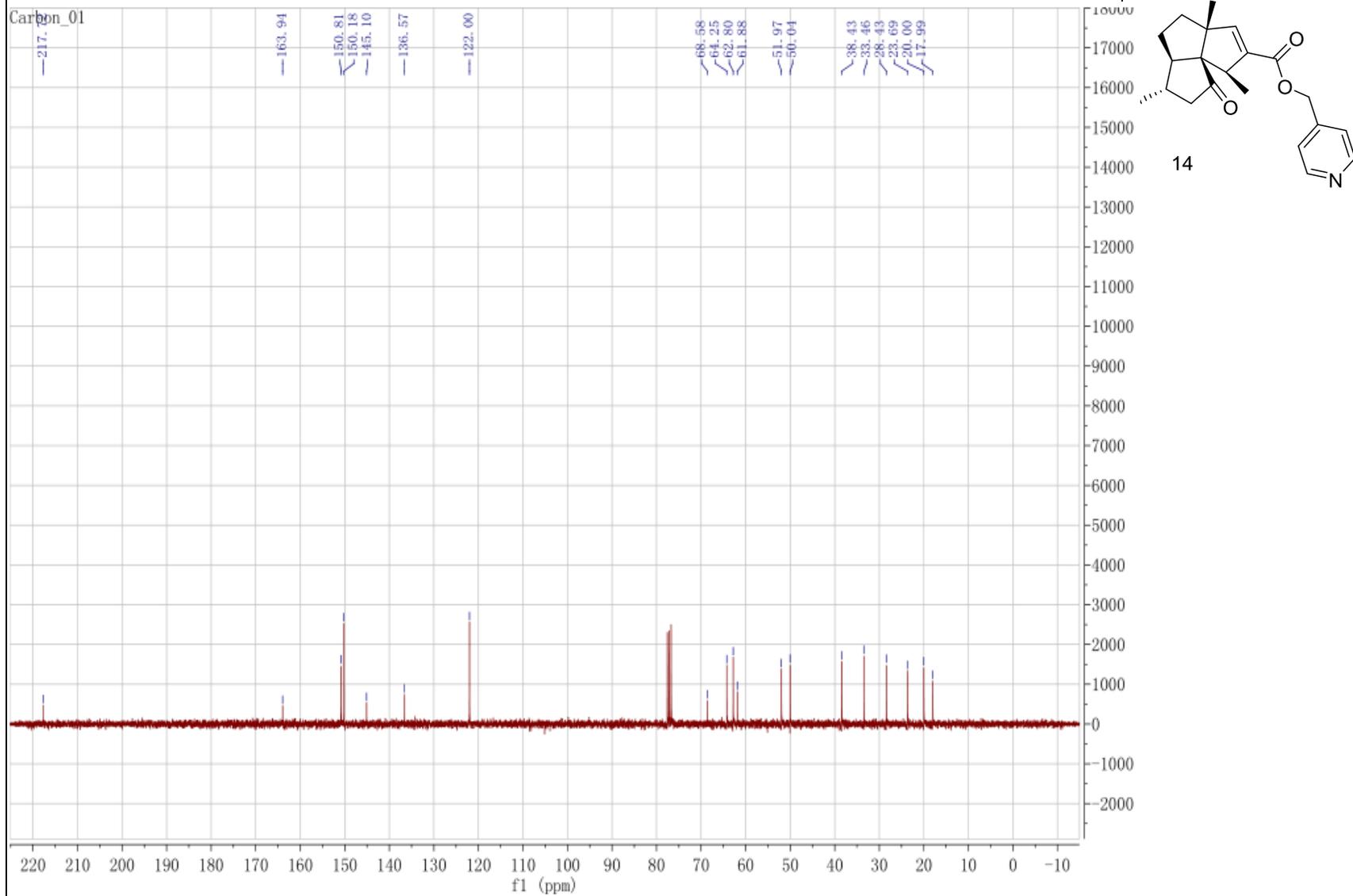


Figure S34. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 15

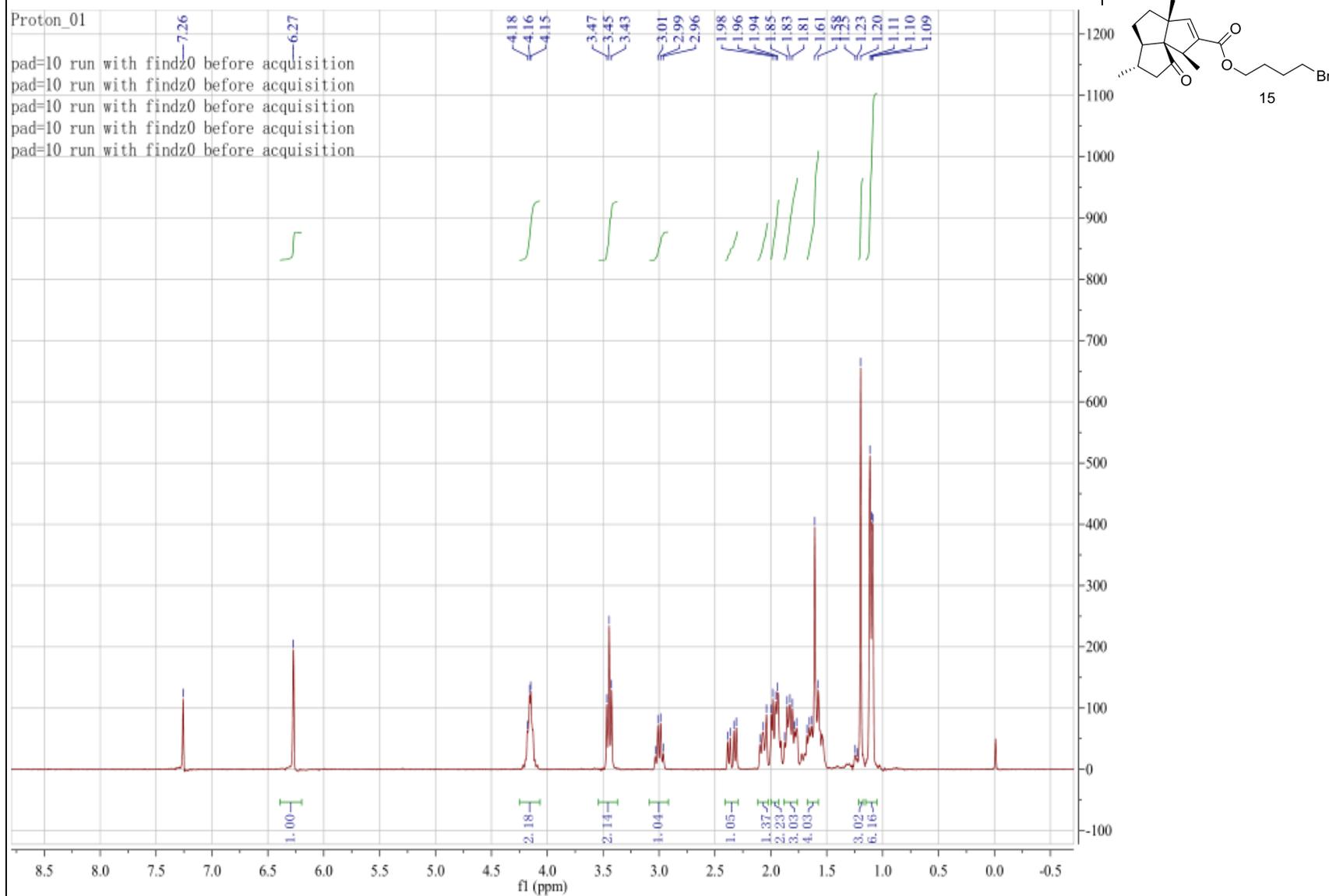


Figure S35. <sup>13</sup>C NMR (75 MHz, CDCl<sub>3</sub>) of compound 15

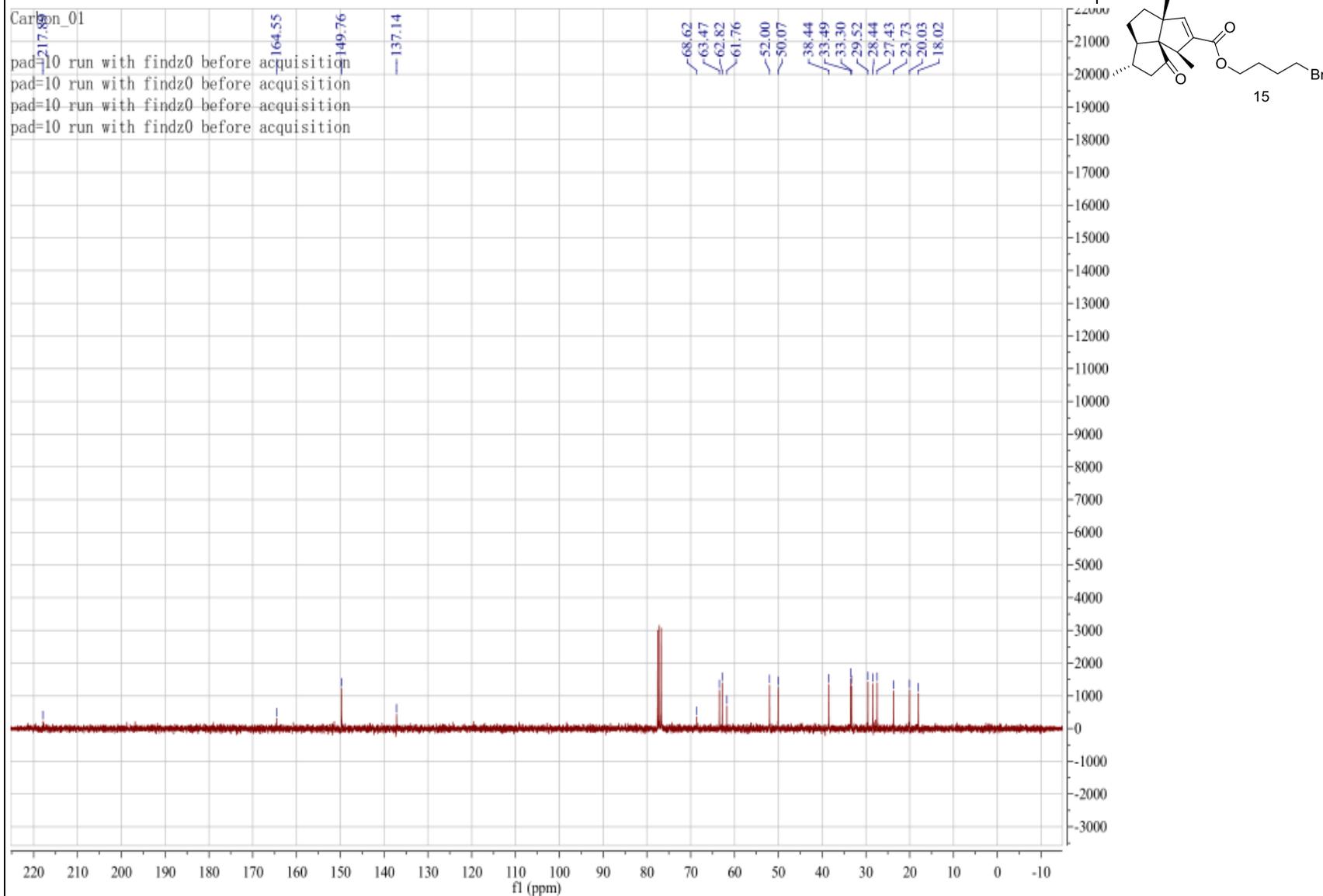


Figure S36. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 16

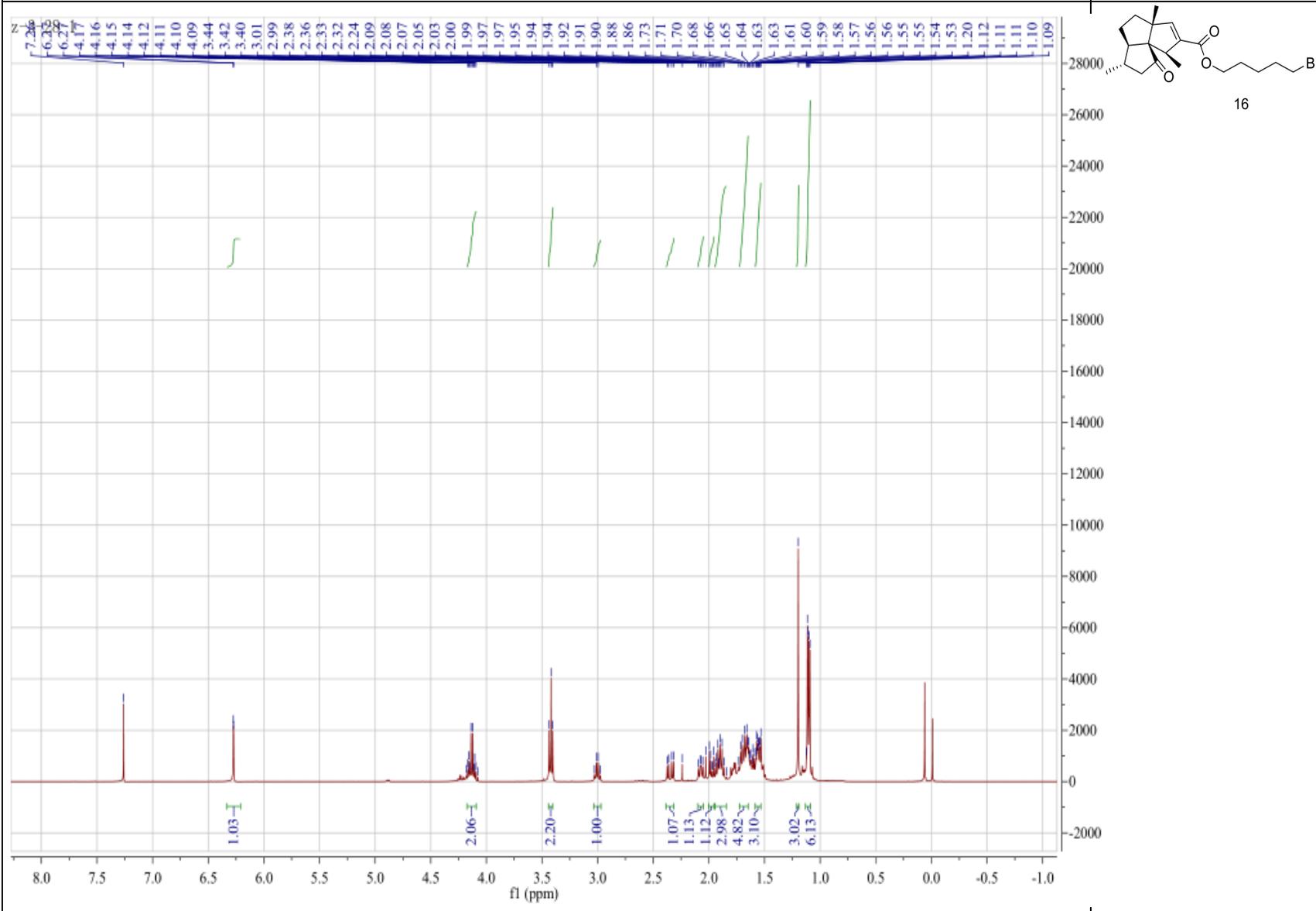


Figure S37.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound 16

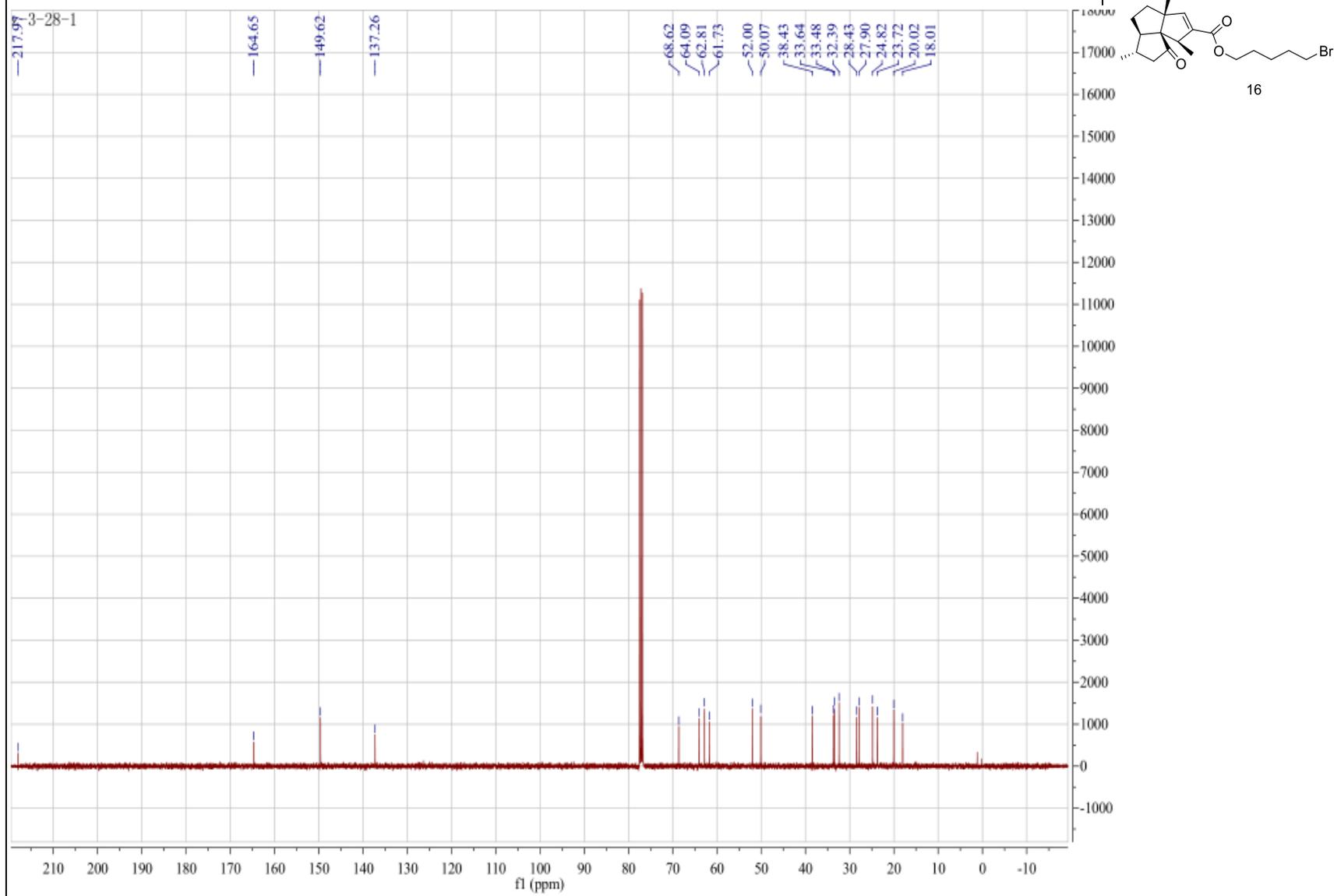


Figure S38. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 17

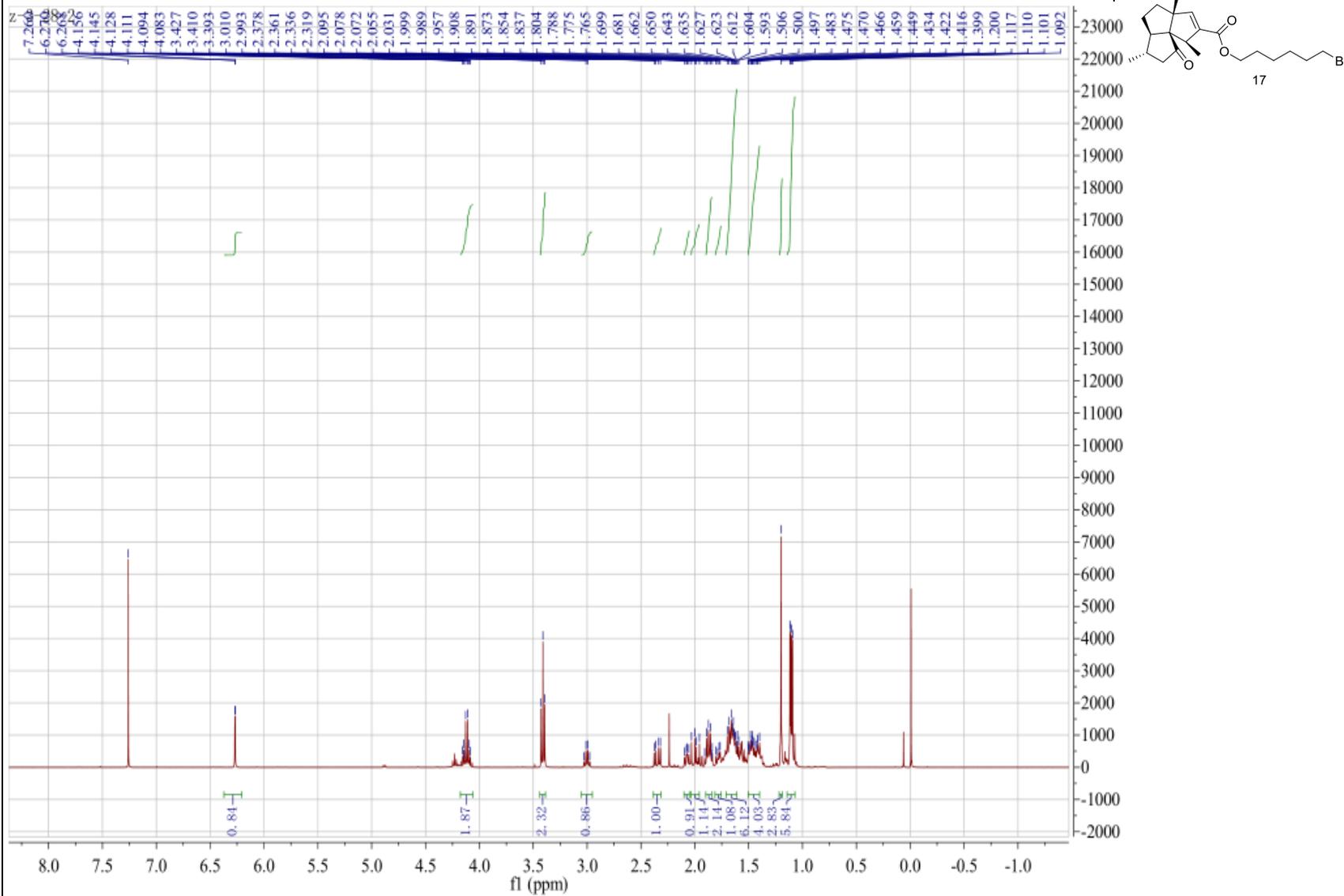


Figure S39.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound 17

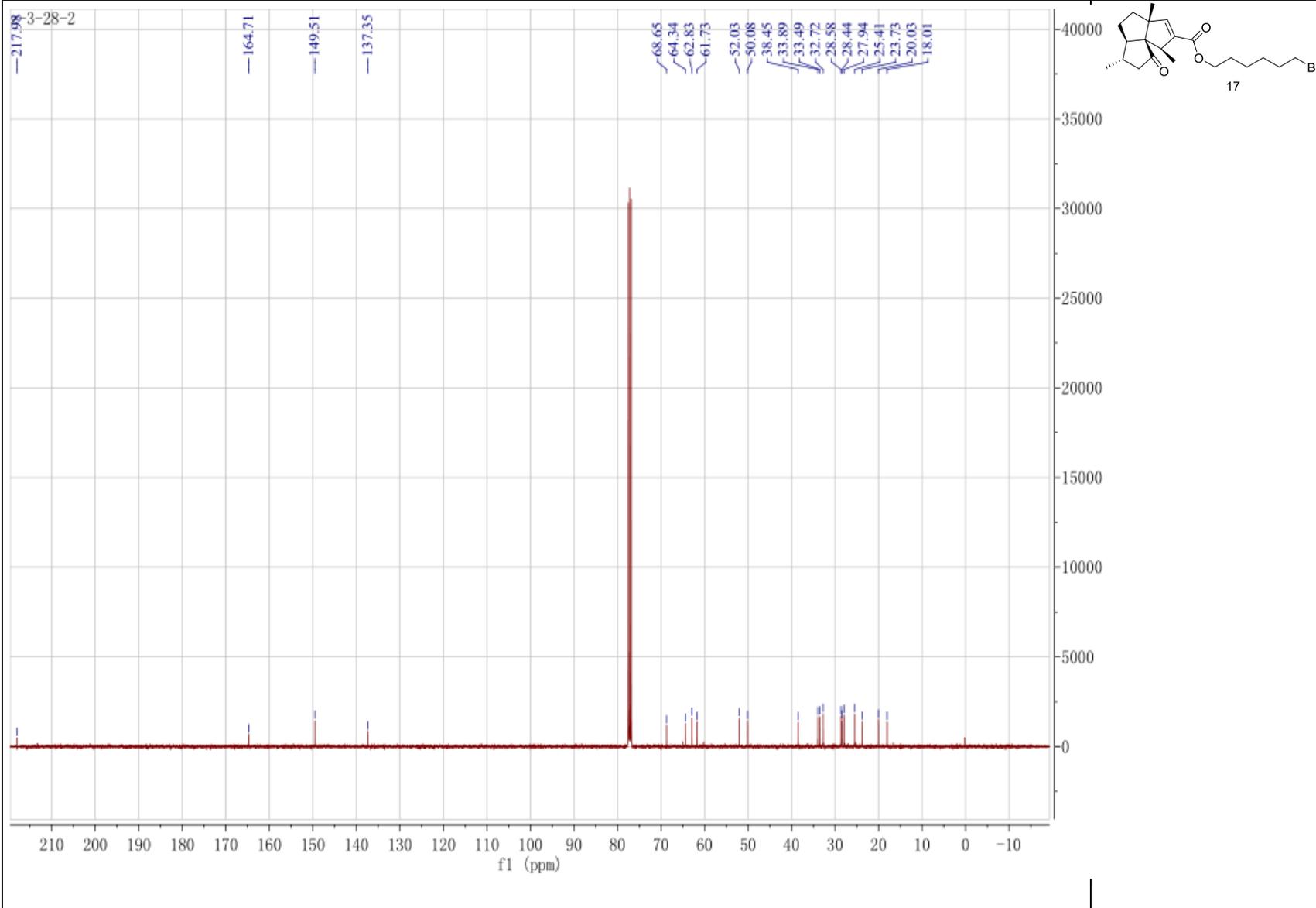


Figure S40. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 18

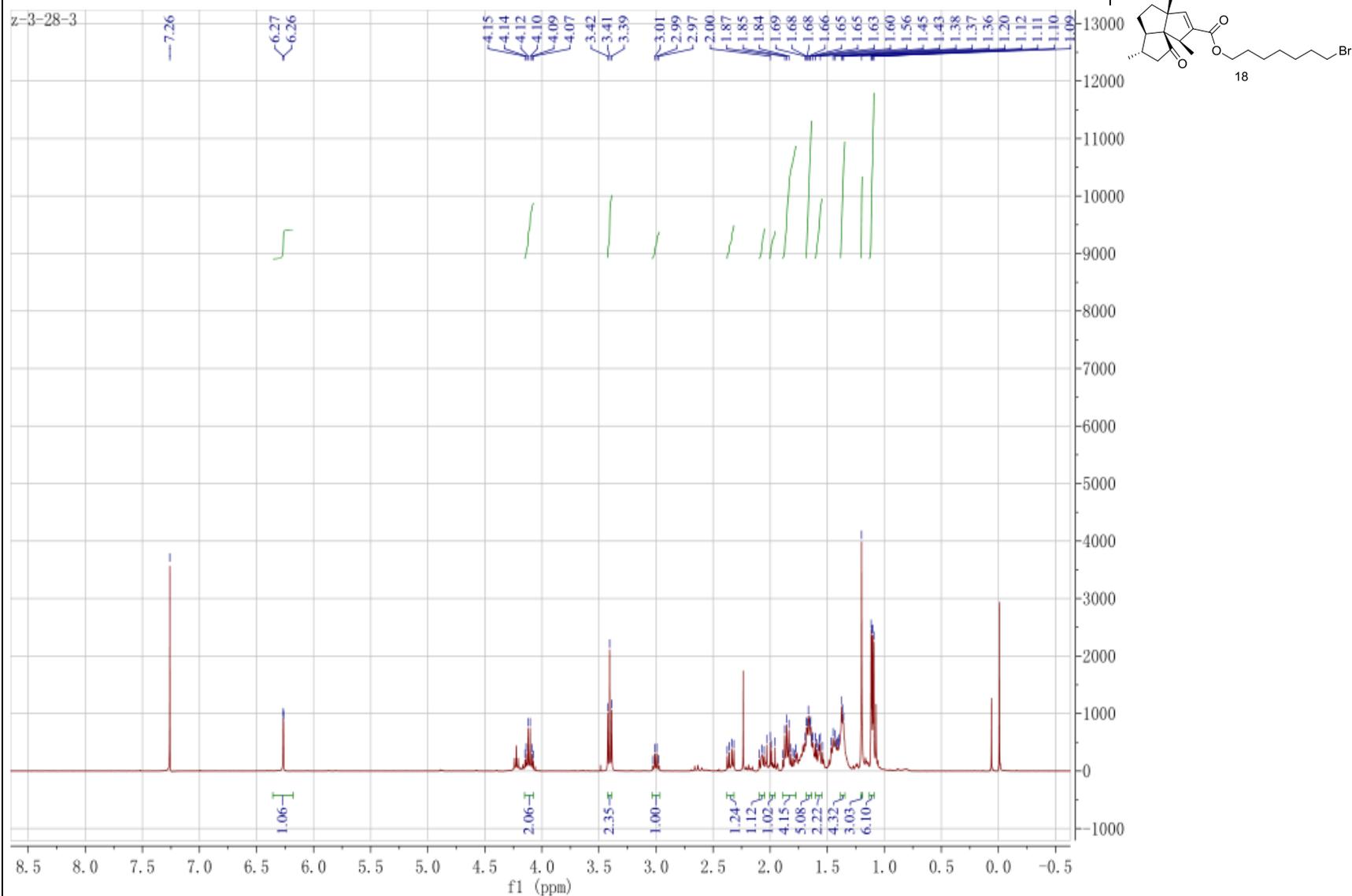


Figure S41.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **18**

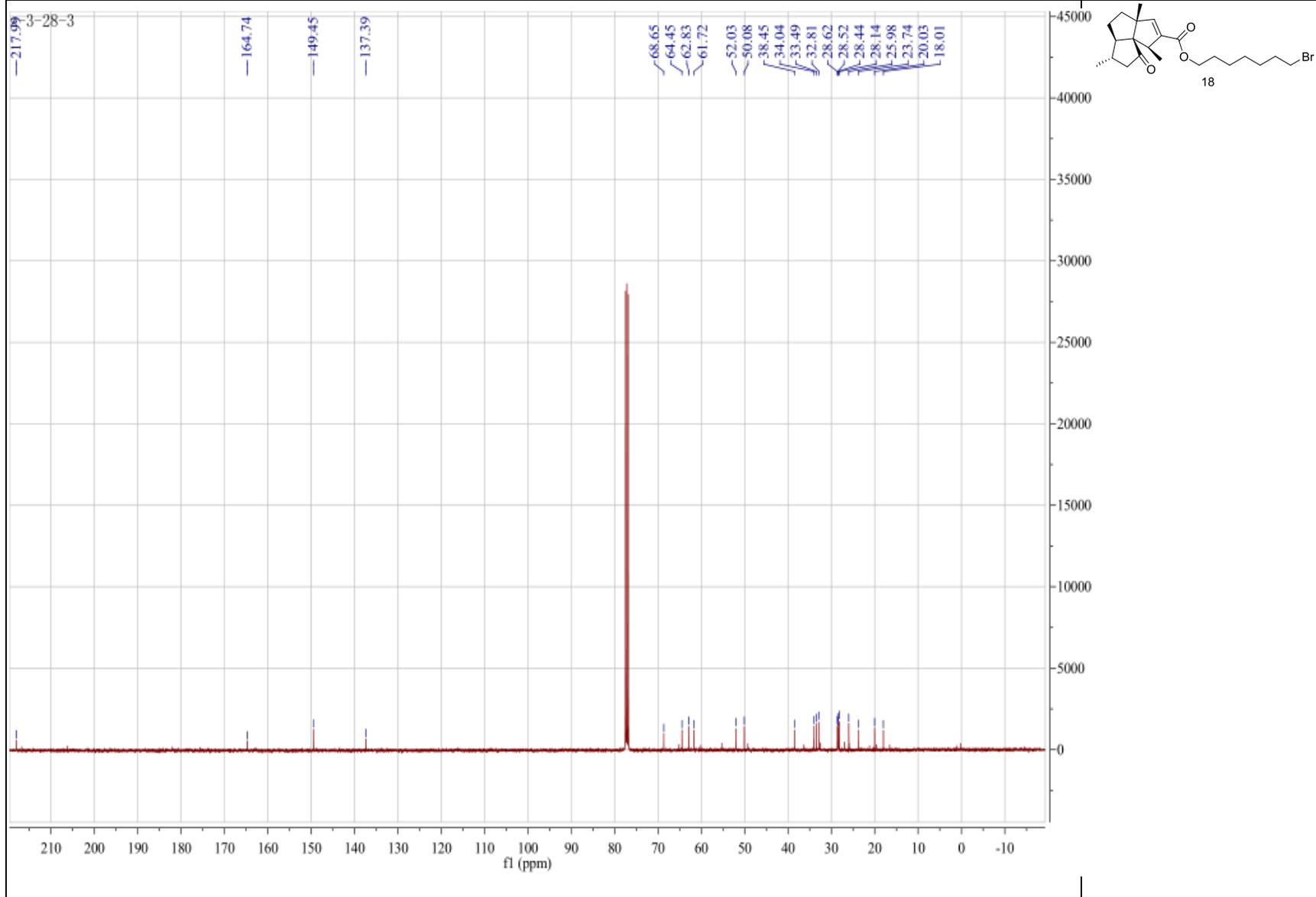


Figure S42. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 19

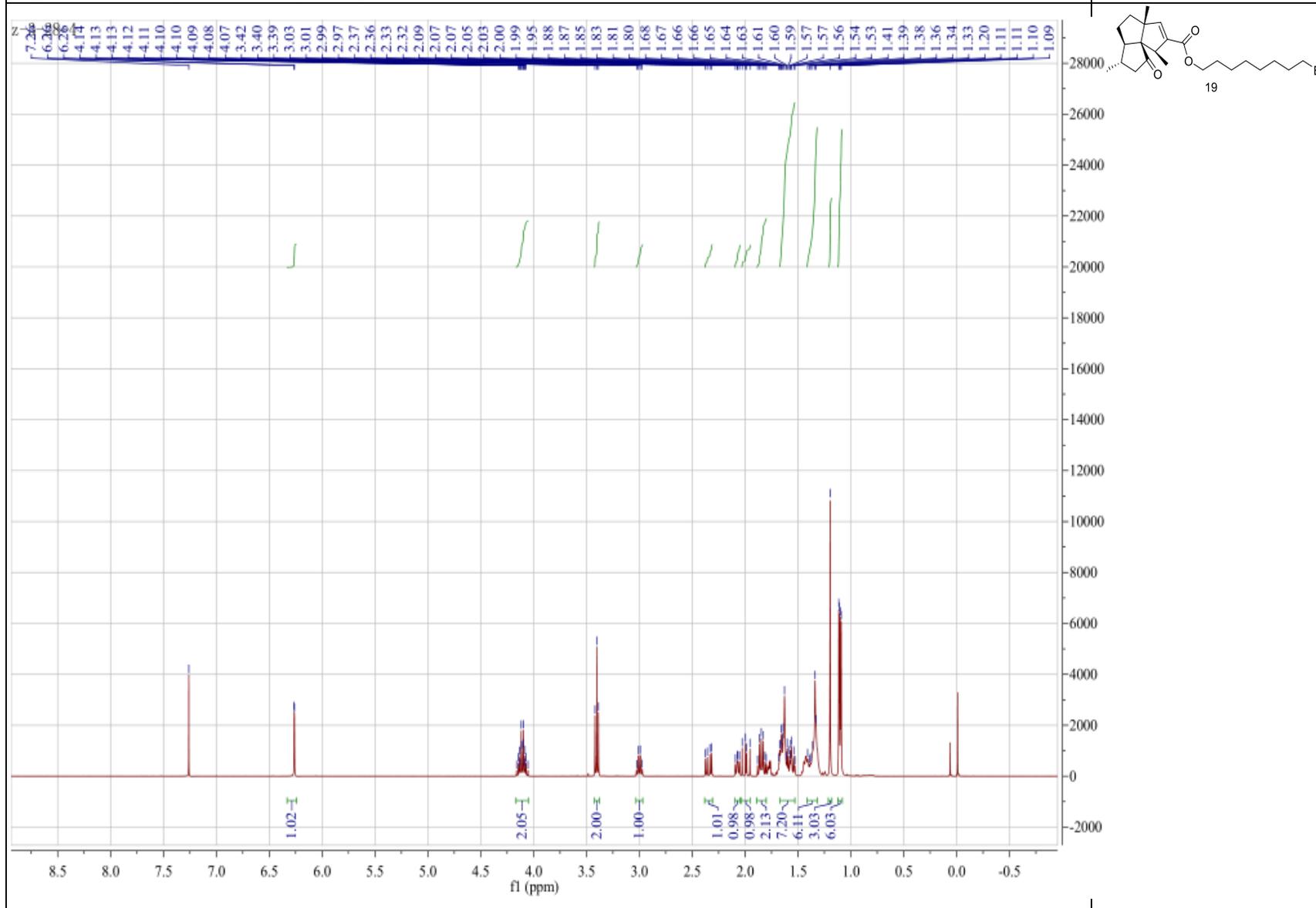


Figure S43.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **19**

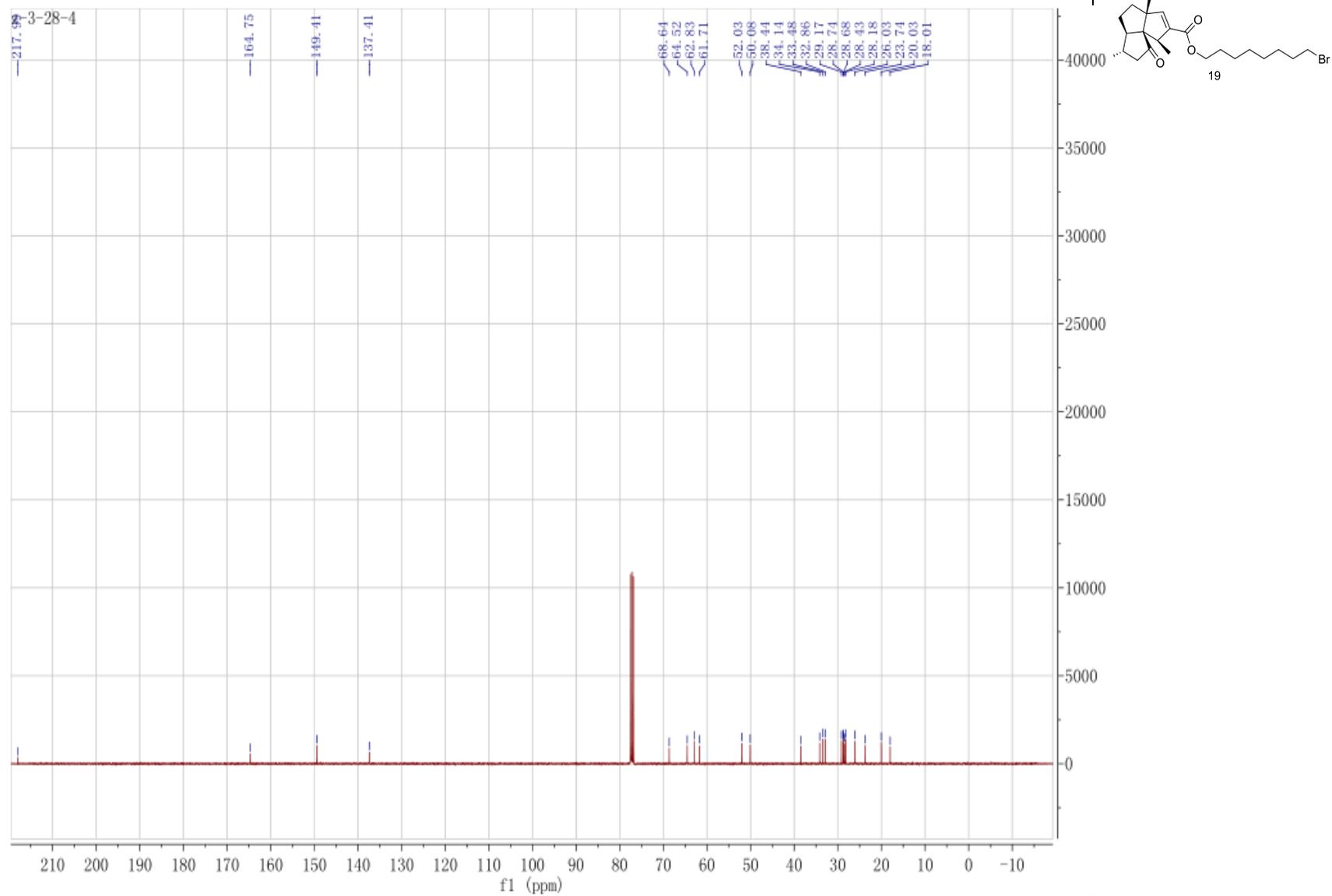


Figure S44. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) of compound 20

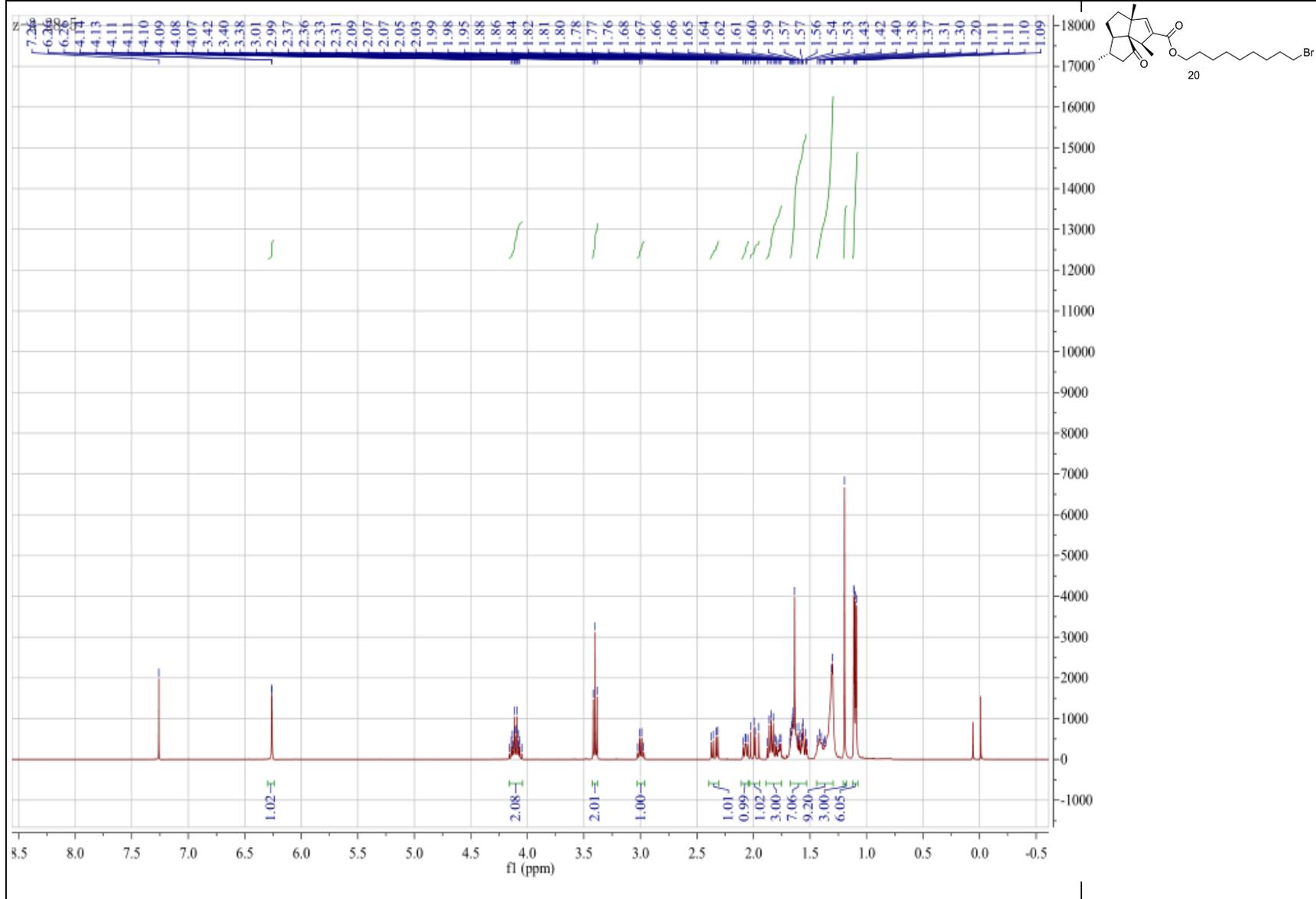


Figure S45.  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ) of compound **20**

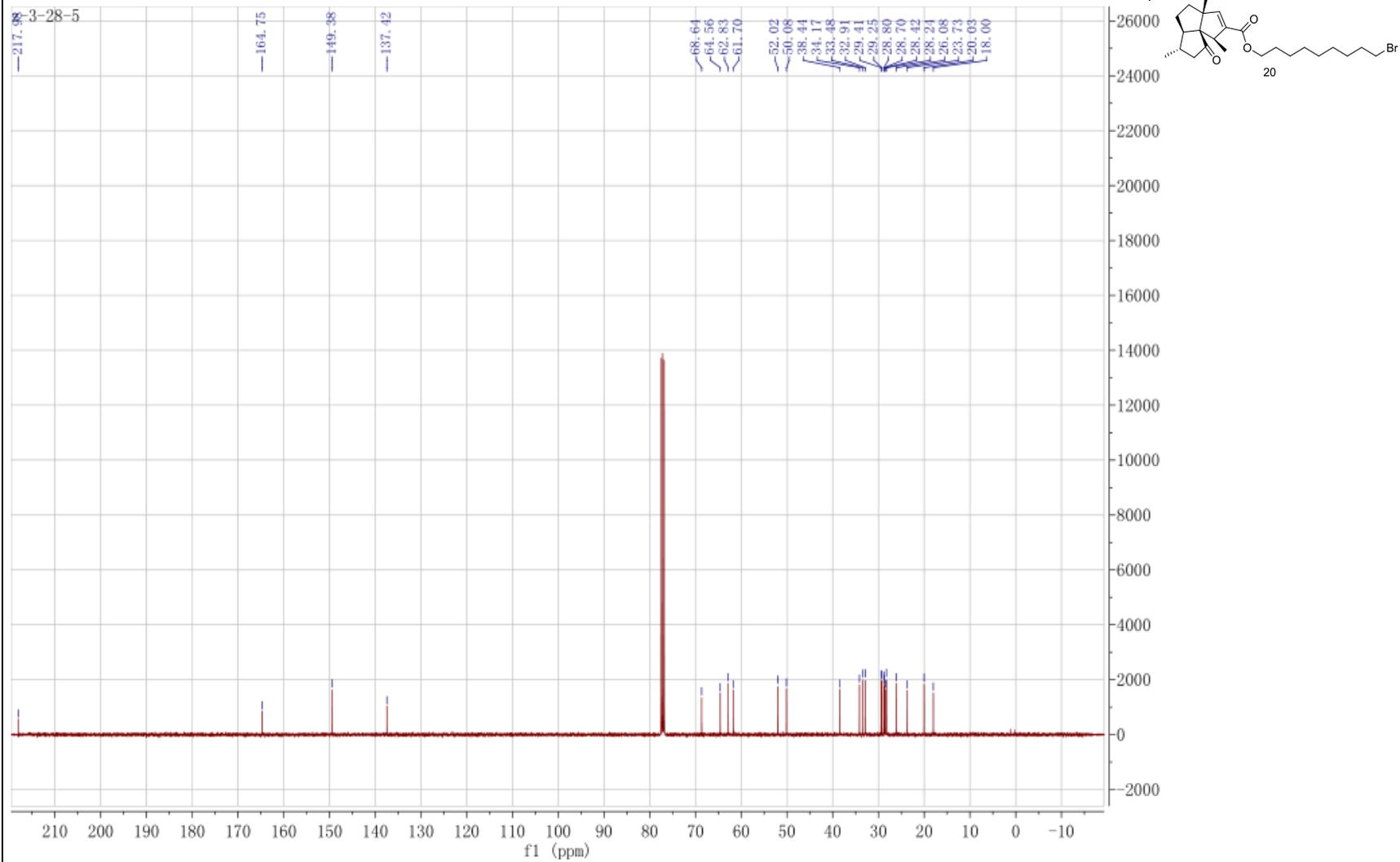


Figure S46. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 21

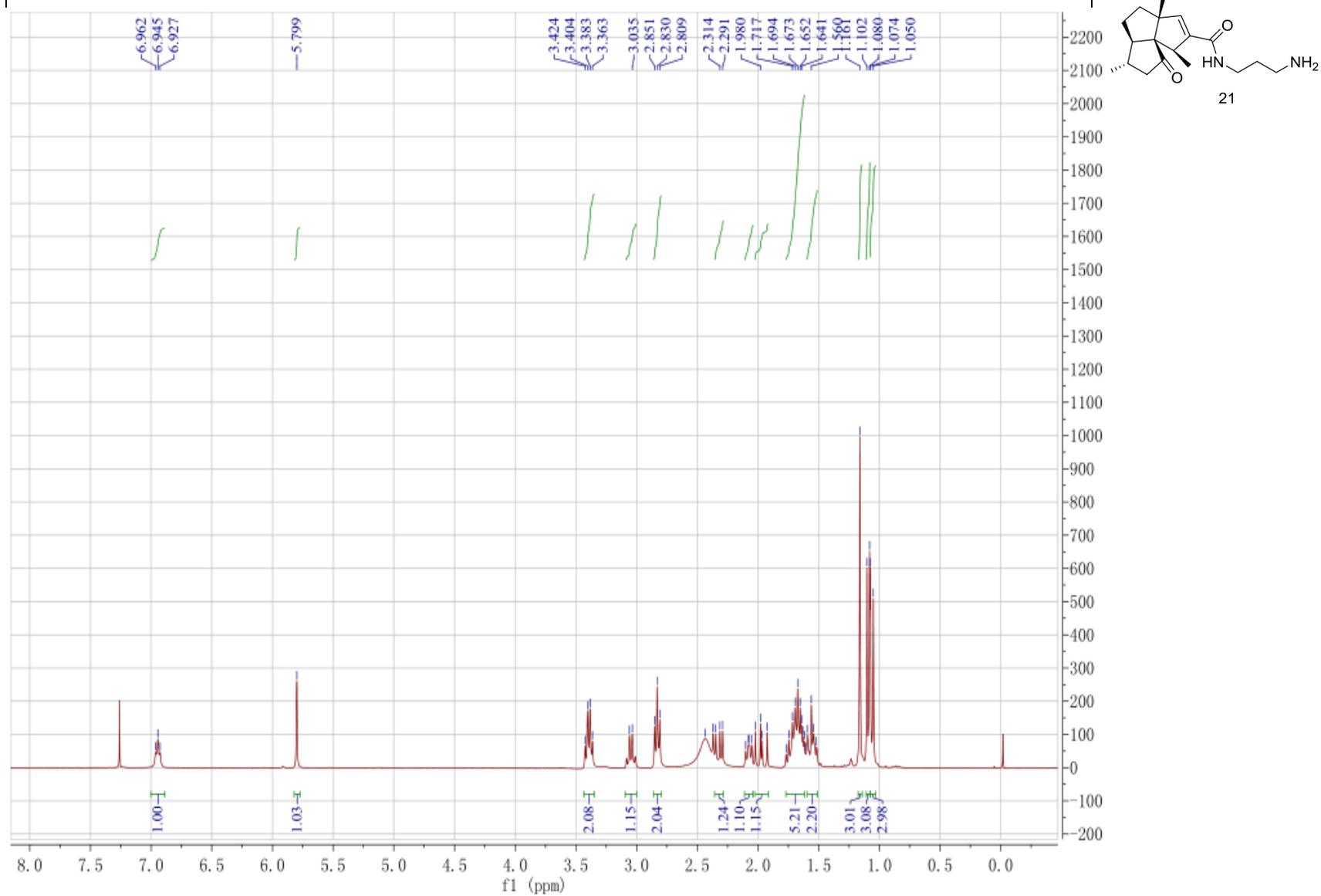


Figure S47.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 21

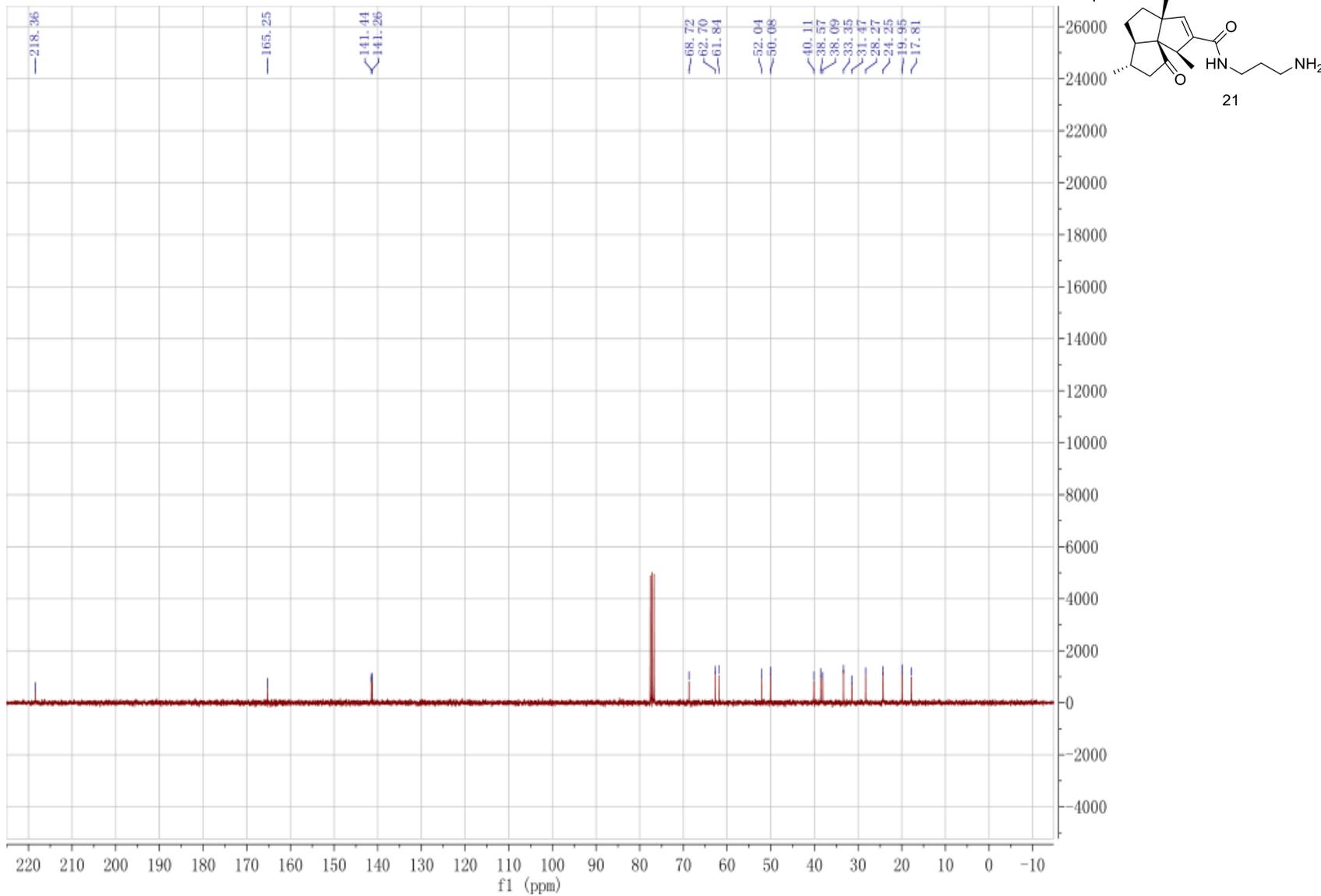


Figure S48. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 22

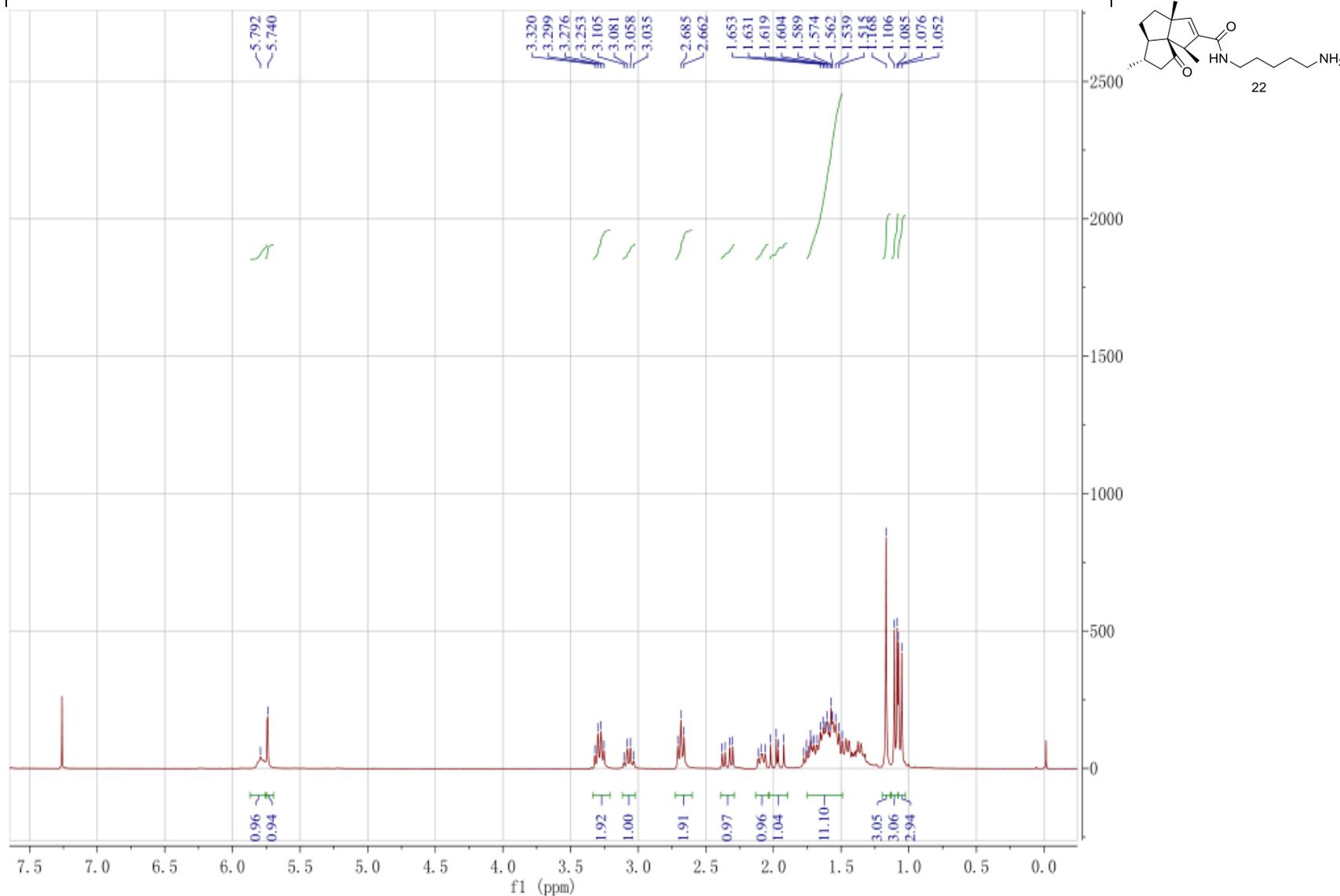


Figure S49.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 22

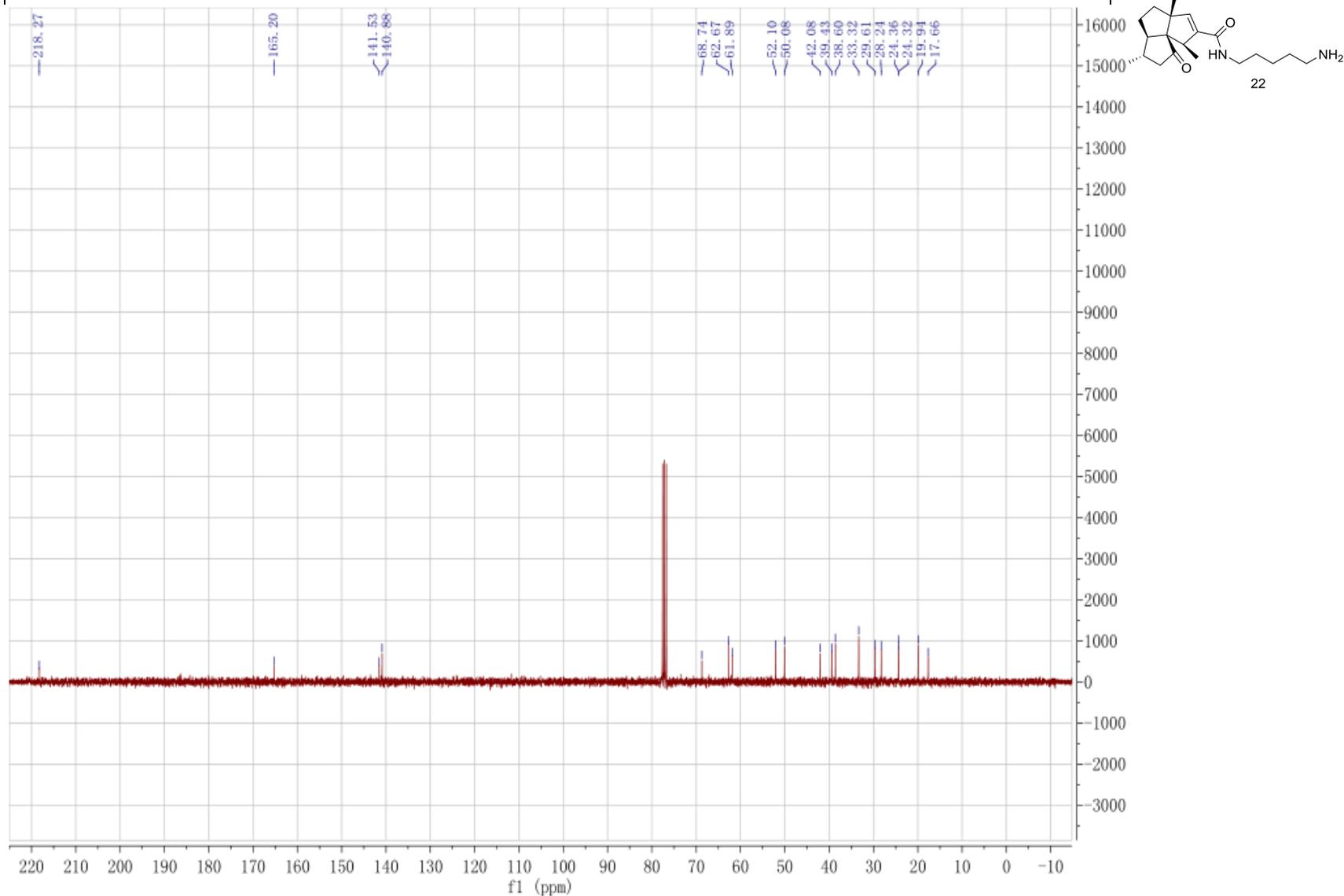


Figure S50. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 23

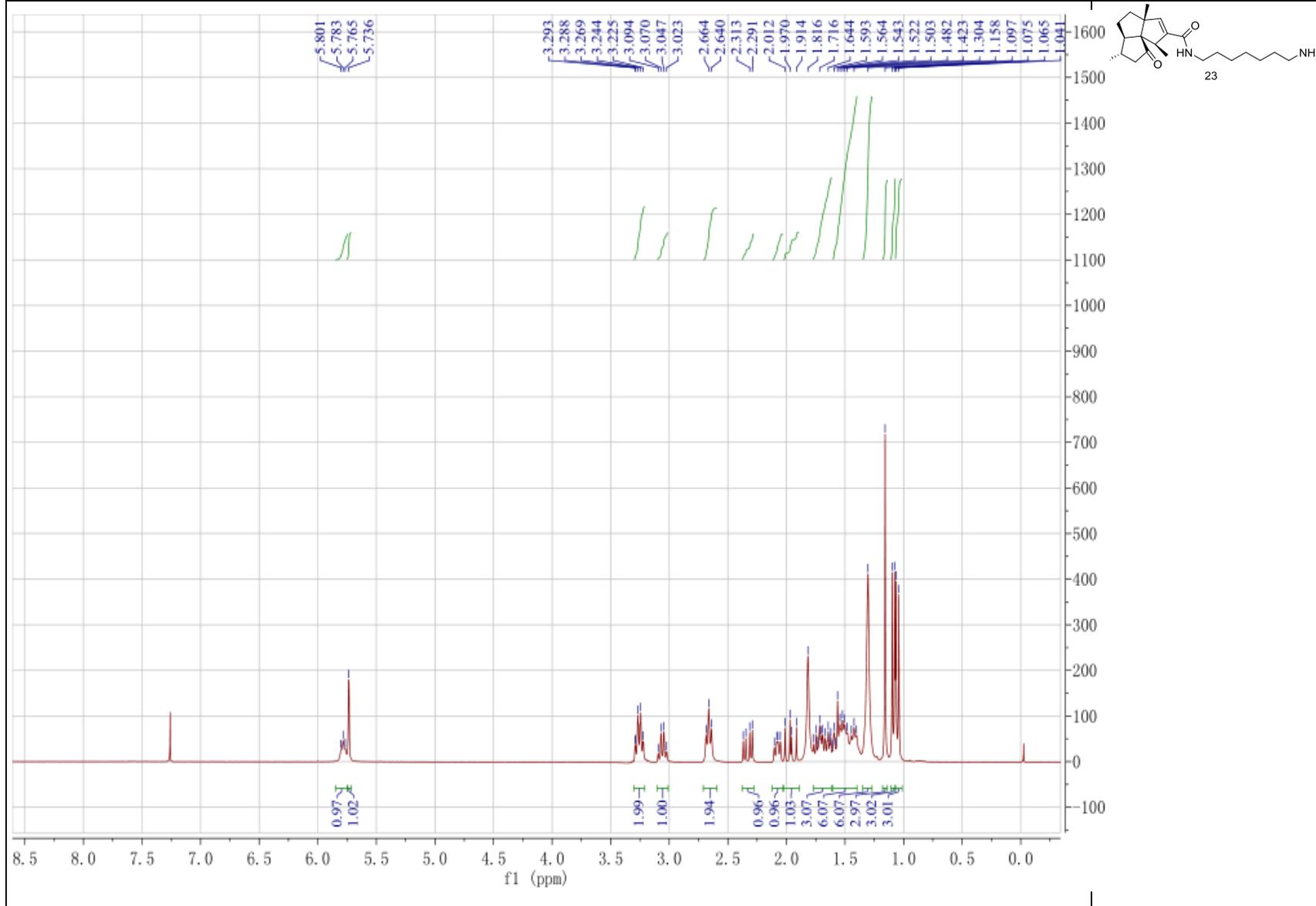


Figure S51.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 23

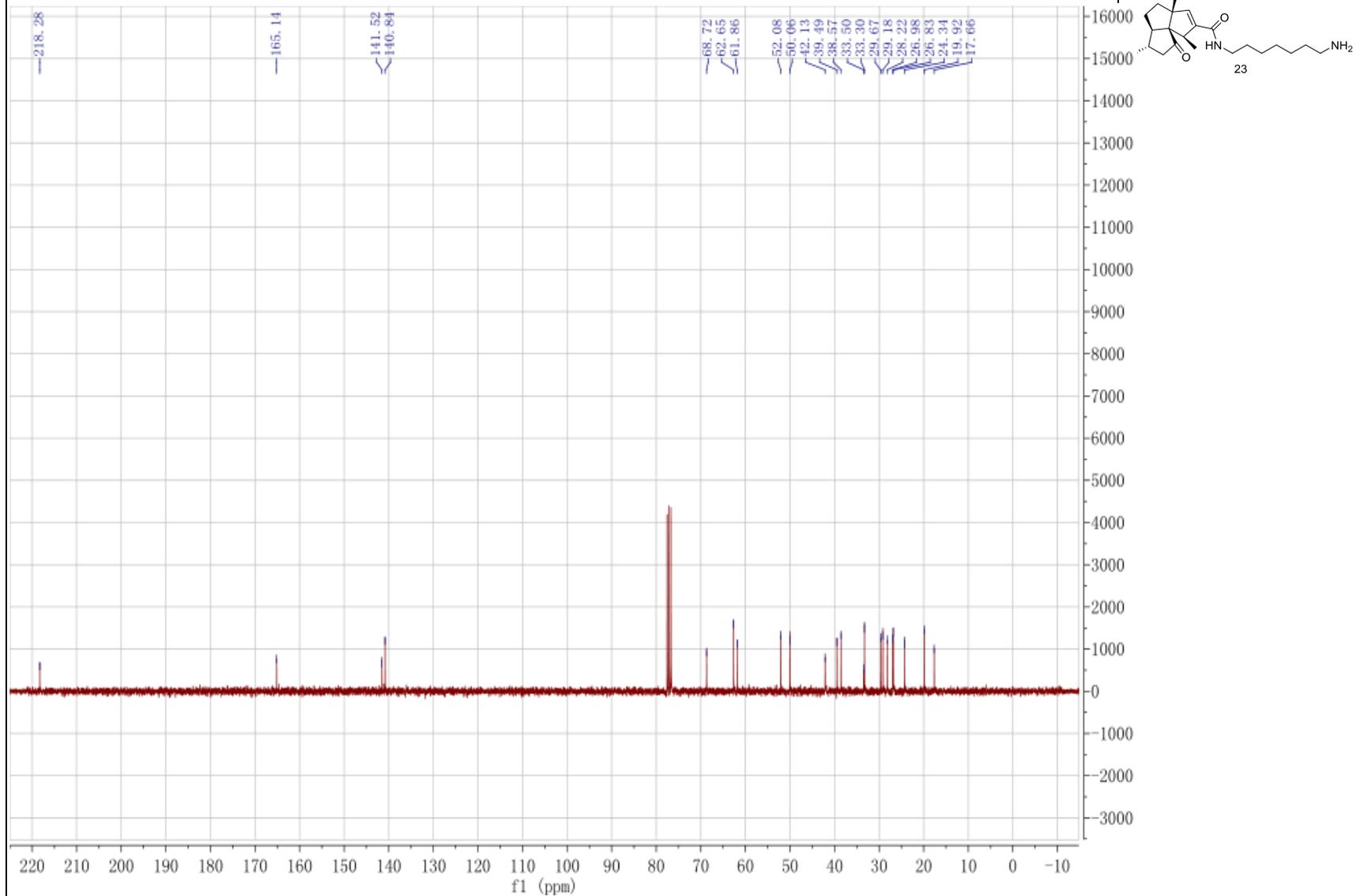


Figure S52. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 24

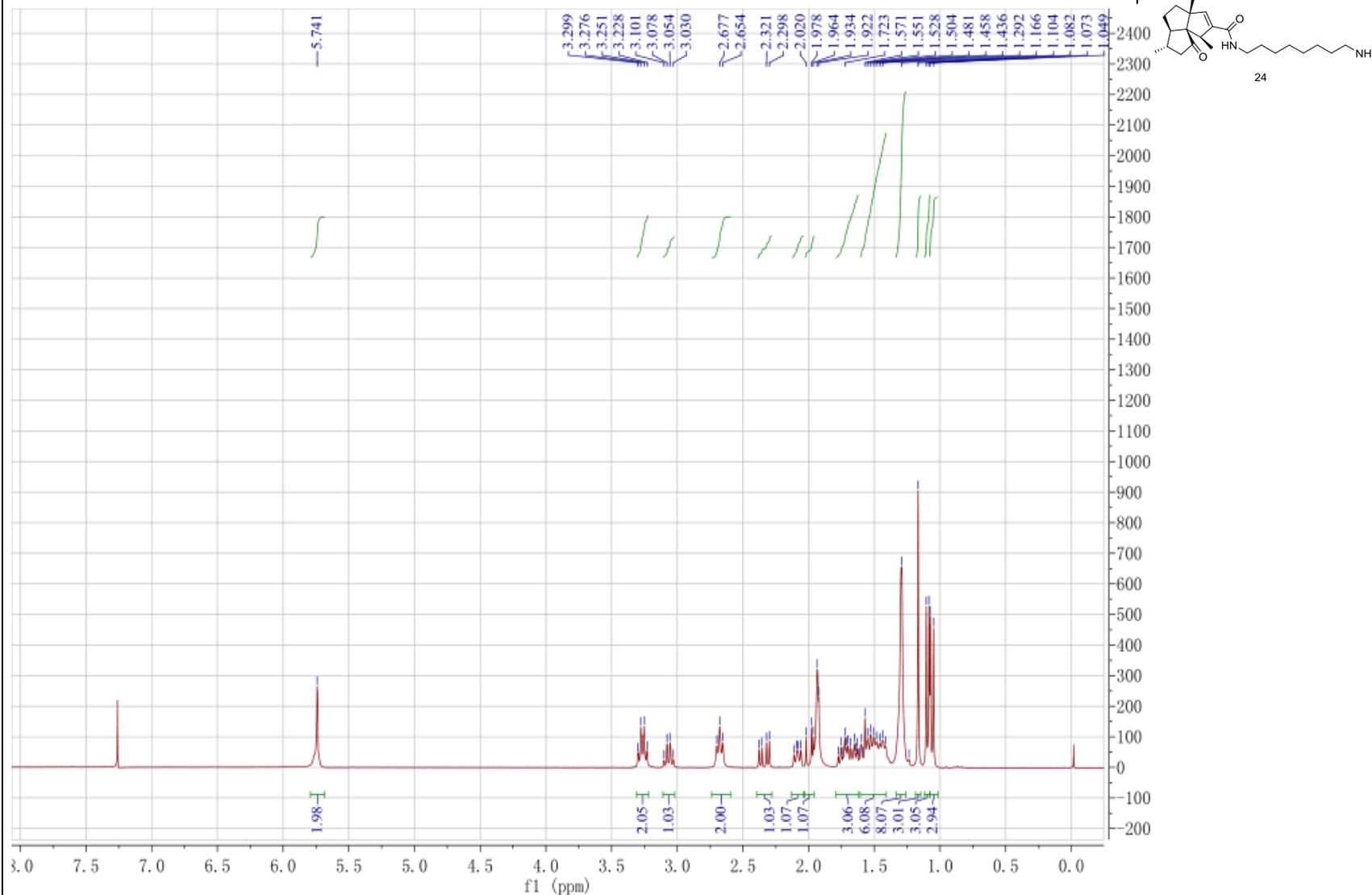


Figure S53.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 24

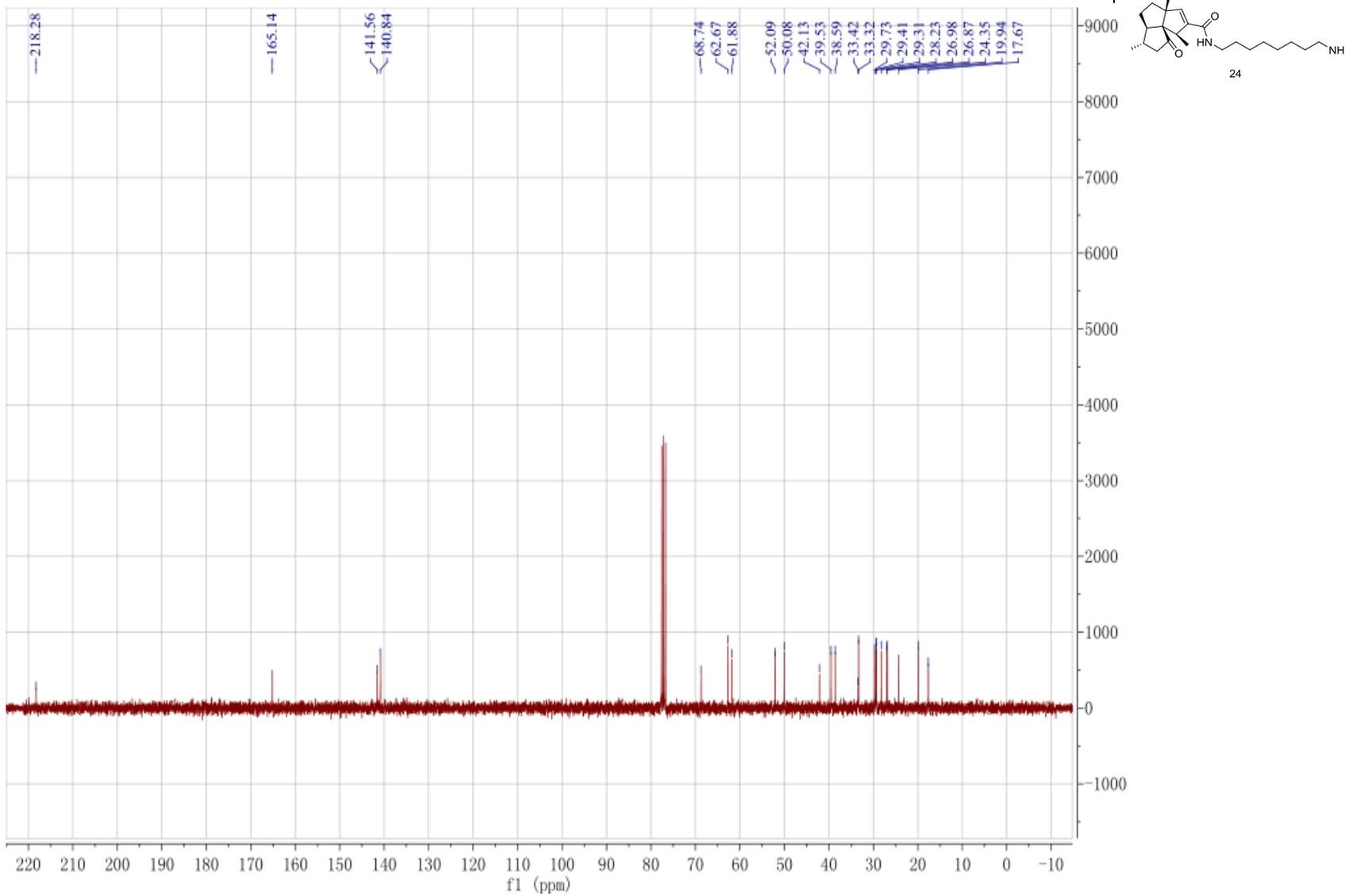


Figure S54. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 25

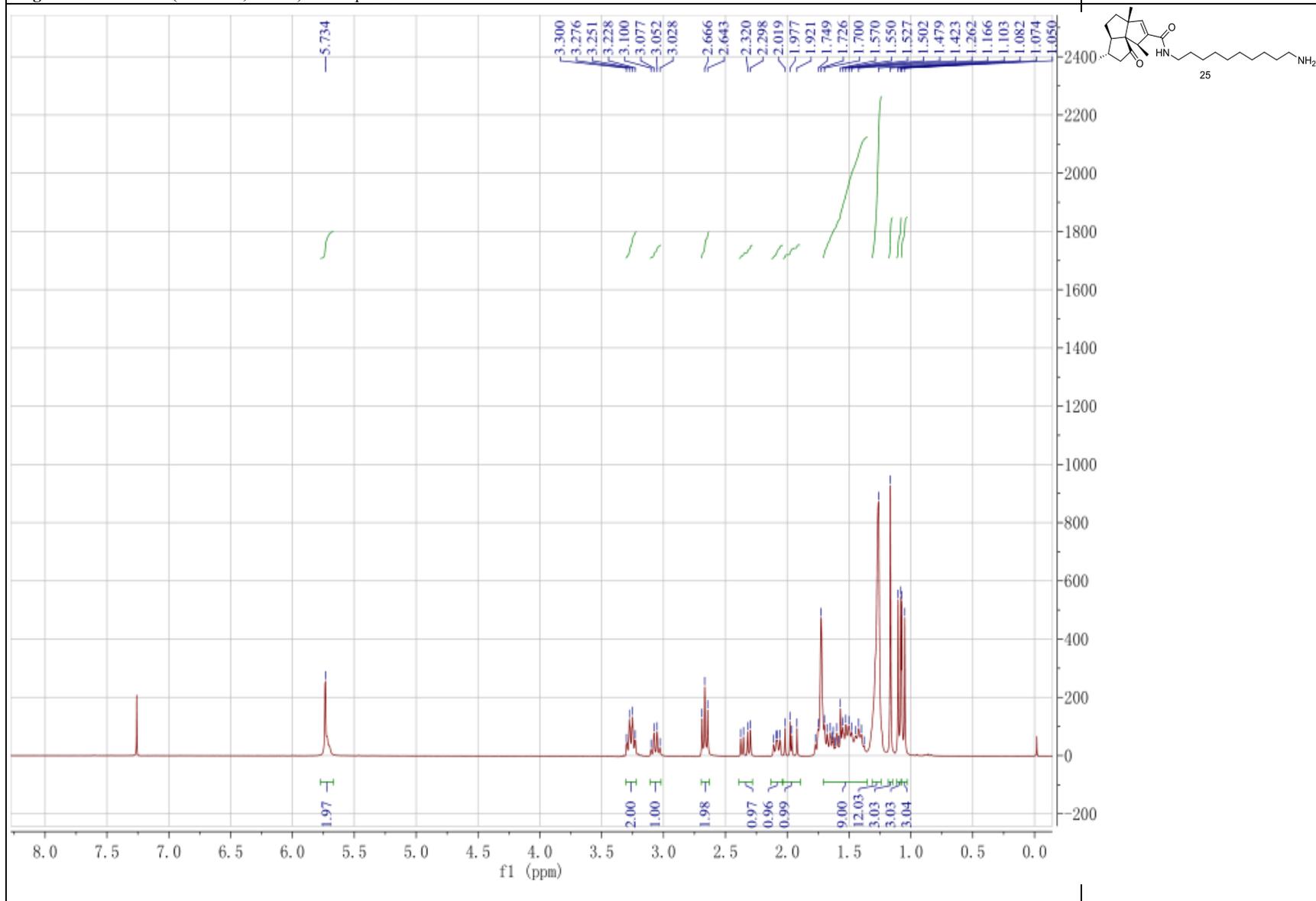


Figure S55.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 25

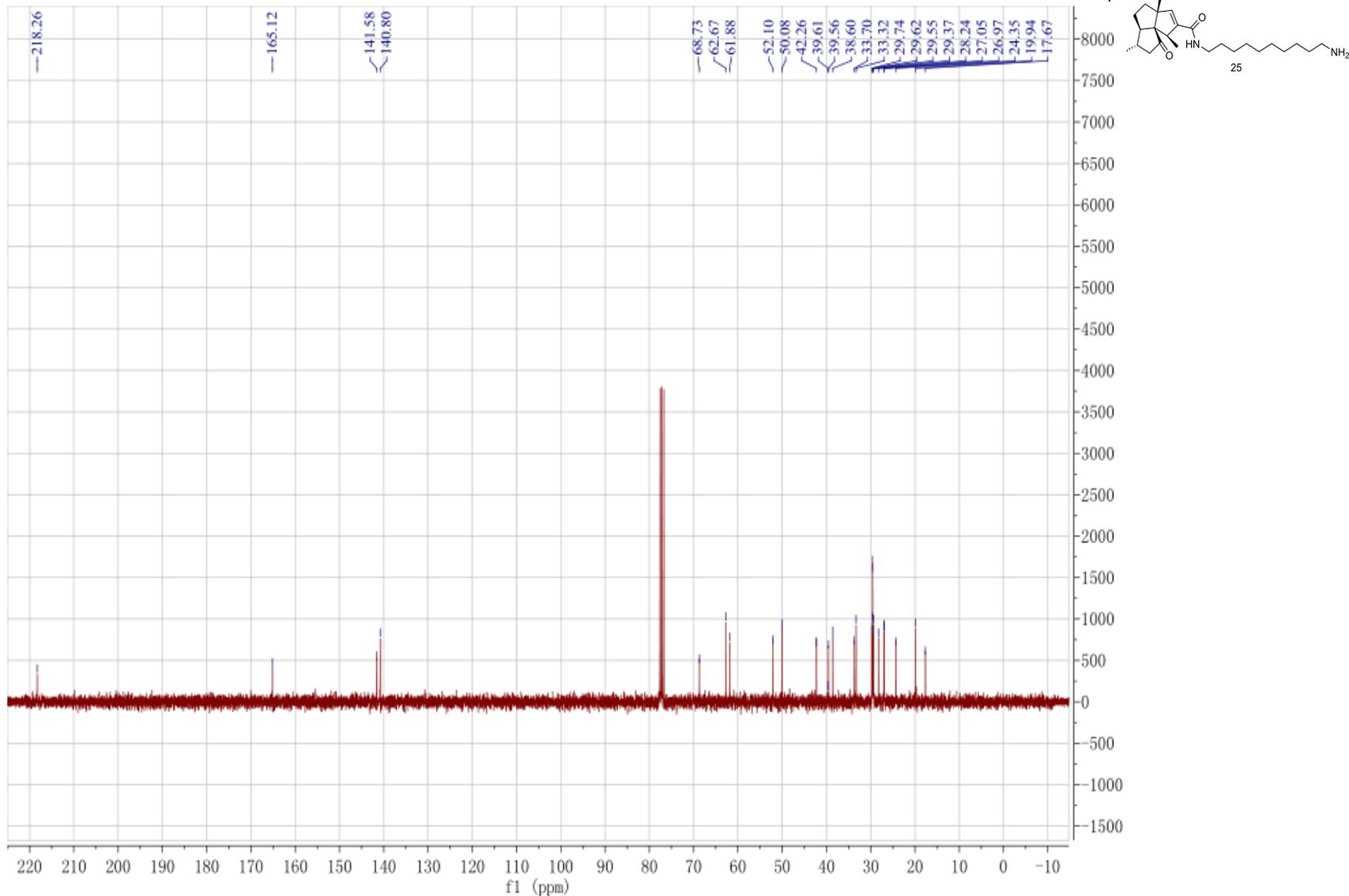


Figure S56. <sup>1</sup>H NMR (300 MHz, CDCl<sub>3</sub>) of compound 26

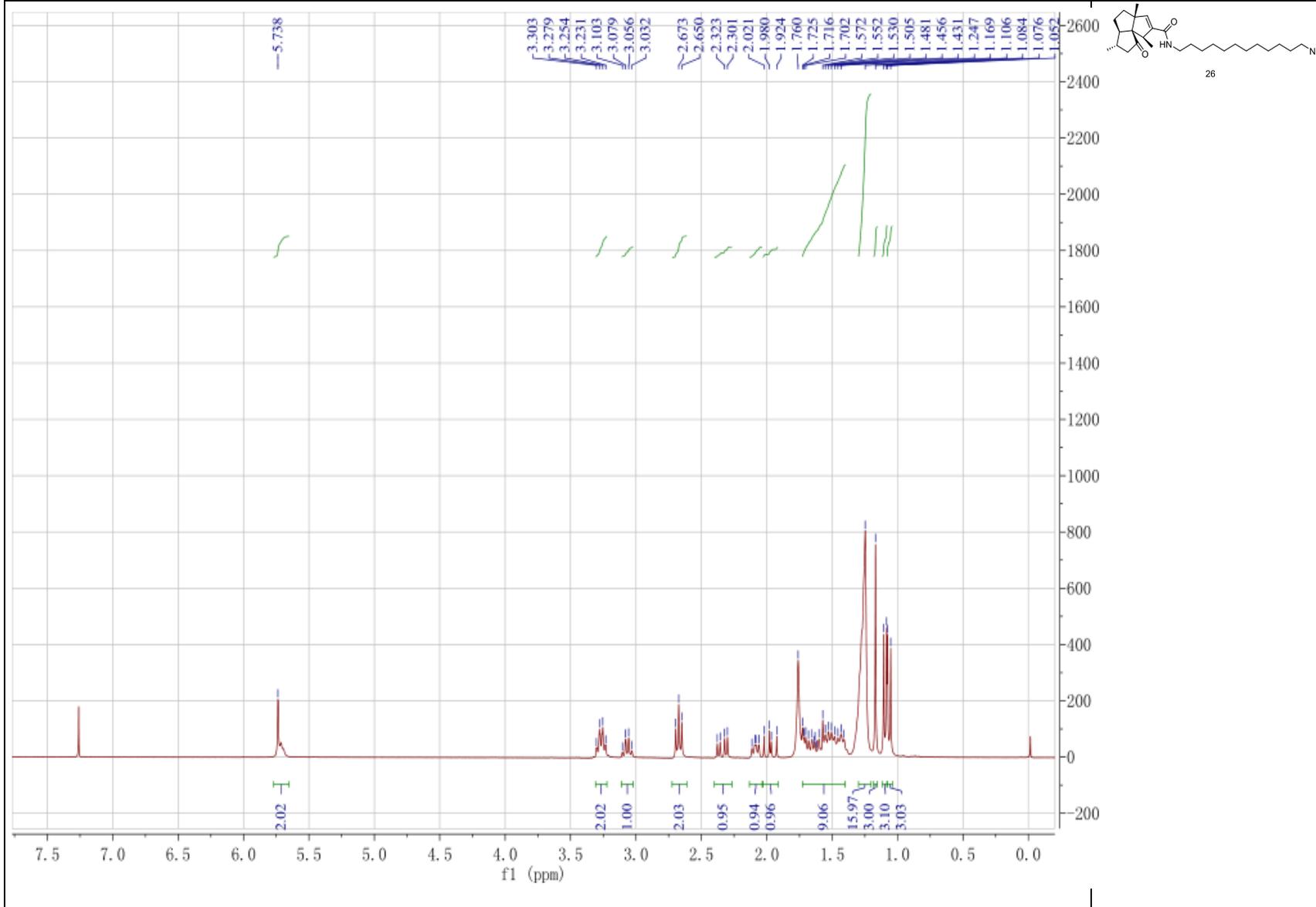


Figure S57.  $^{13}\text{C}$  NMR (75 MHz,  $\text{CDCl}_3$ ) of compound 26

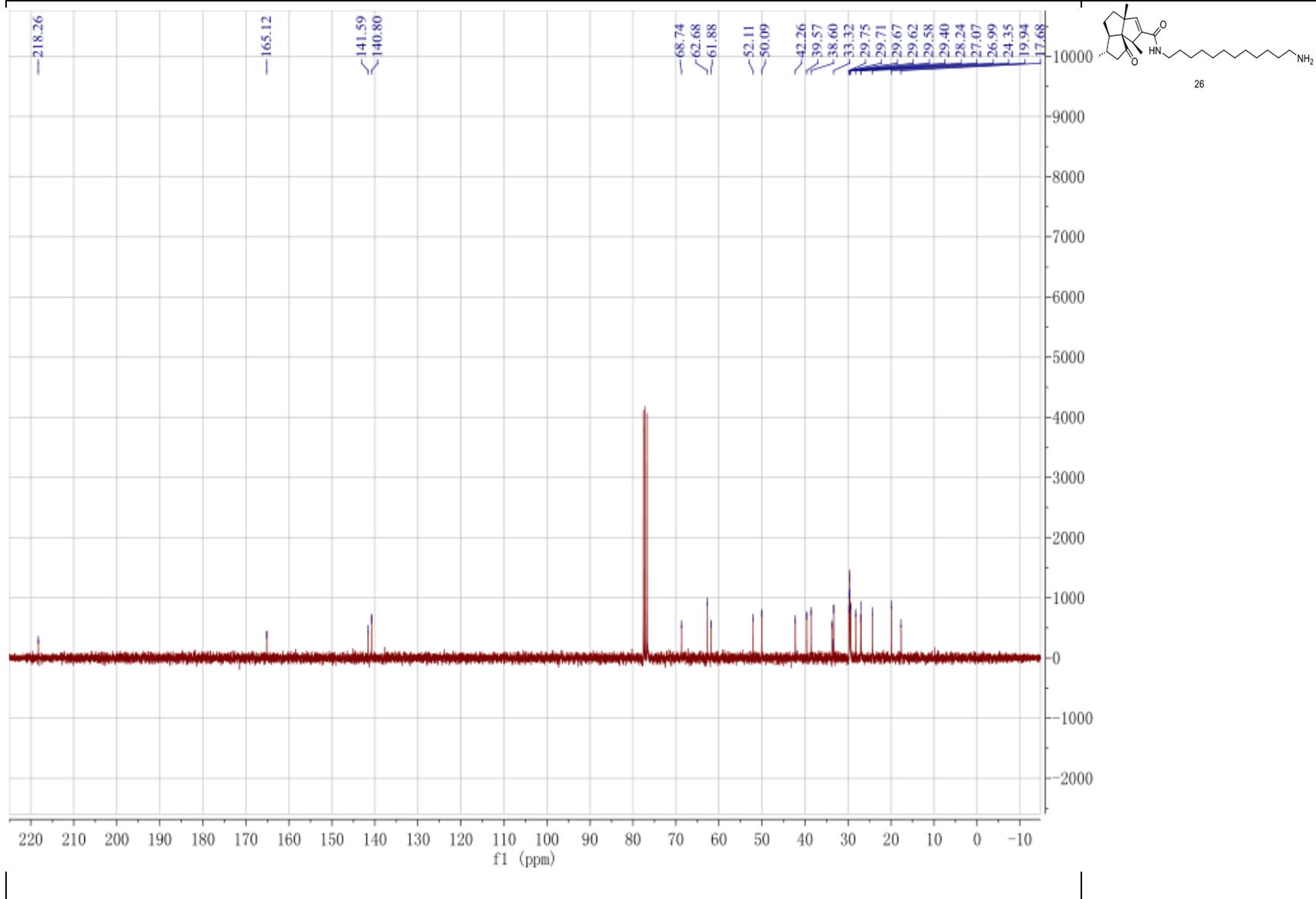


Figure S58. HRMS of compound 4

zi-10, MW=264, NH3; neg. ion  
br140806\_10 184 (3.087) Cm (187:189-1:74)

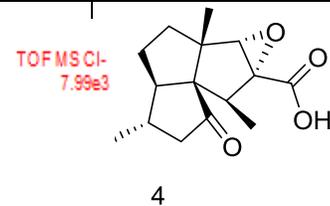
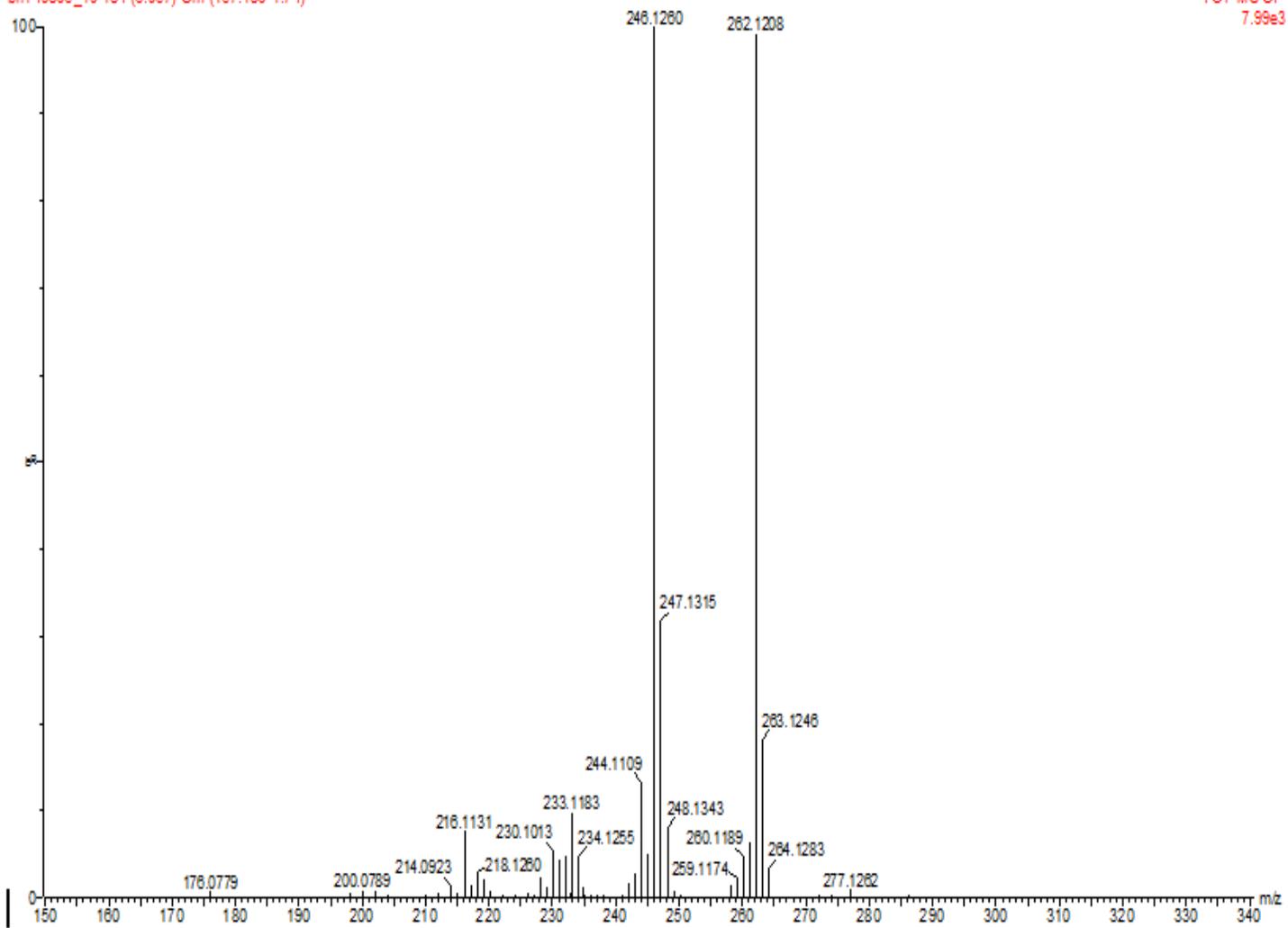


Figure S59. HRMS of compound 5

z<sup>-</sup> 5, MW=338, NH3; neg. ion  
br140808\_5.89 (1.484) Cm (89.92-1.64)

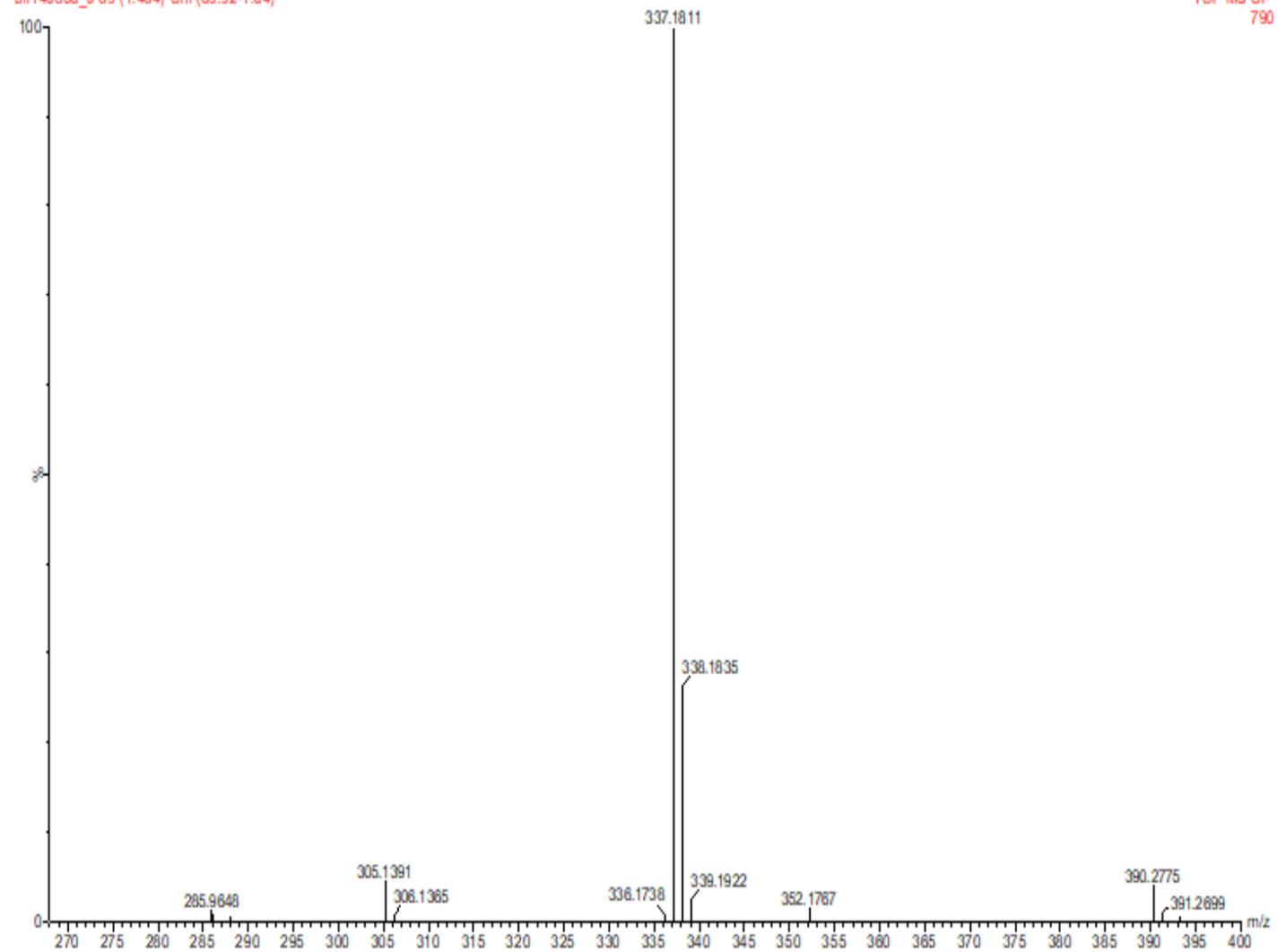


Figure S60. HRMS of compound 8

zj-6, MW=406, NH3; neg. ion  
bn140806\_8 148 (2.467) Cm (145:160-1:105)

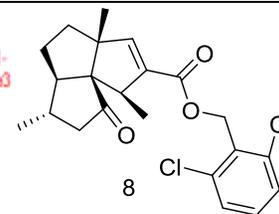
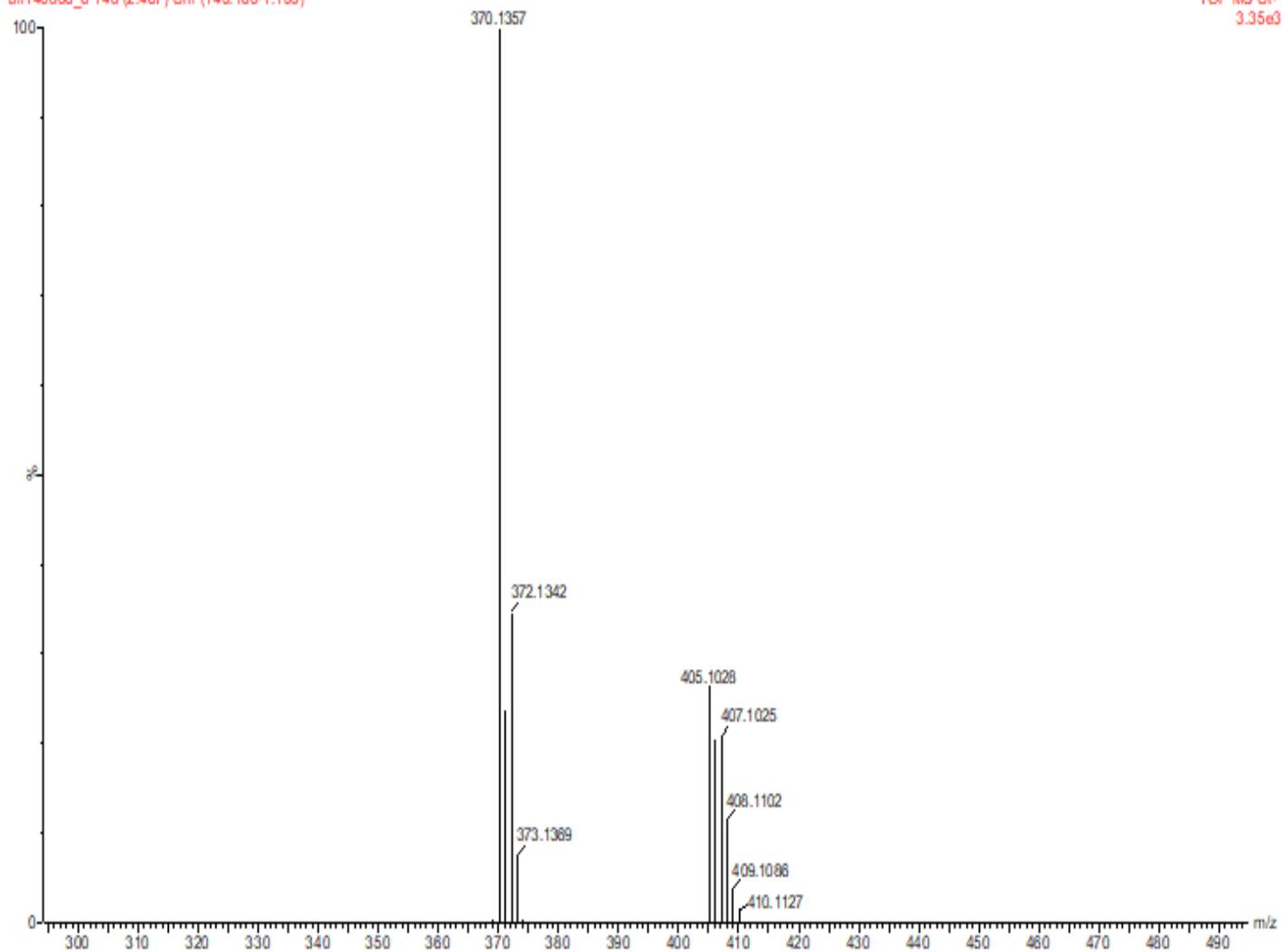


Figure S61. HRMS of compound 10

zj-9, MW=372, NH3; neg. ion  
bri140808\_9 90 (1.500) Cm (90.96-1.67)

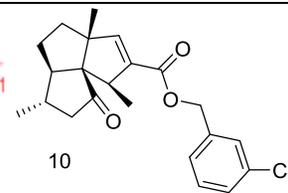
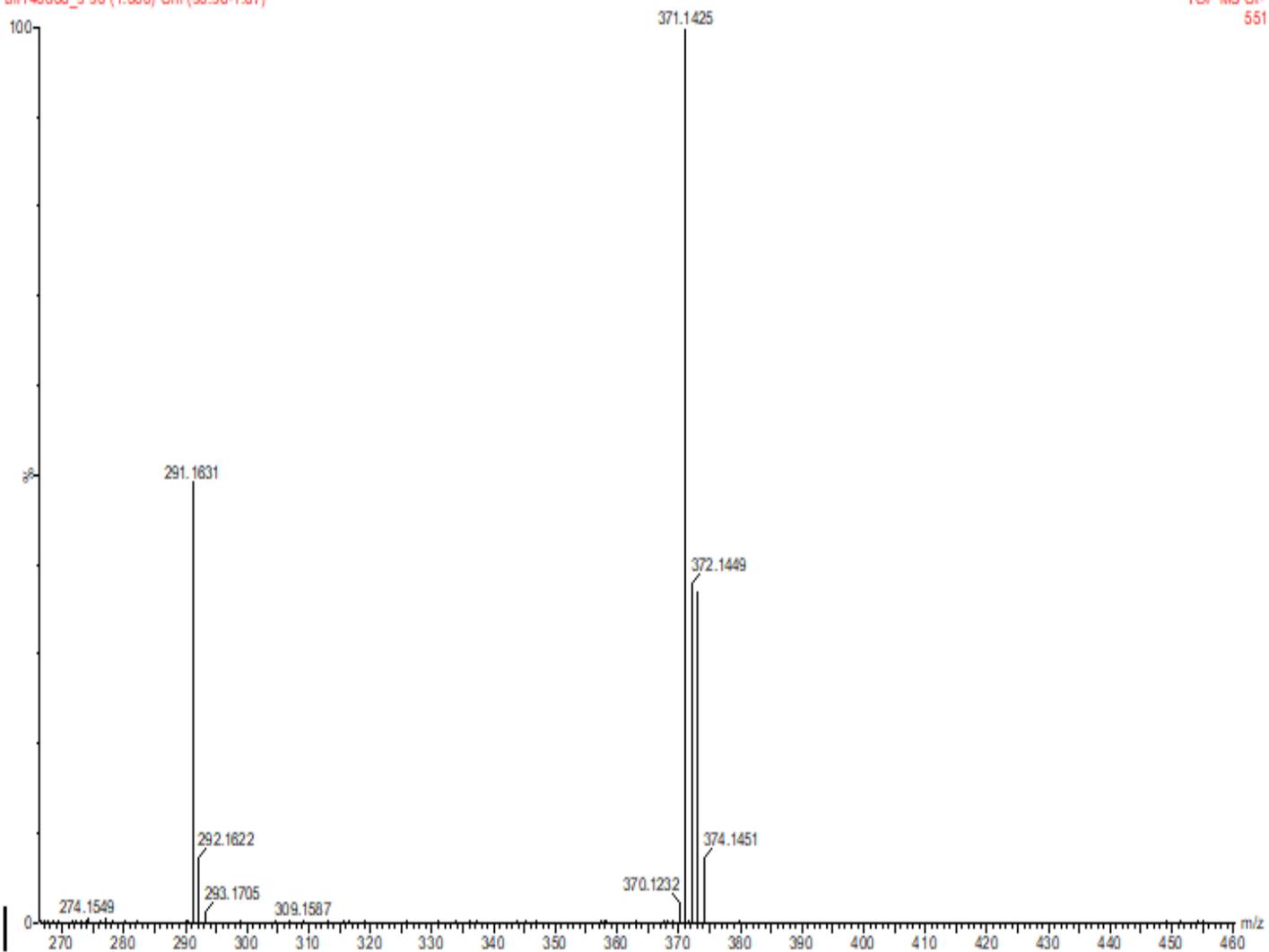


Figure S62. HRMS of compound 11

z: 7, MW=368, NH3; neg. ion

bn140808\_7 121 (2.017) Cm (118:122-1:105)

TOF MS Cl-  
1.97e4

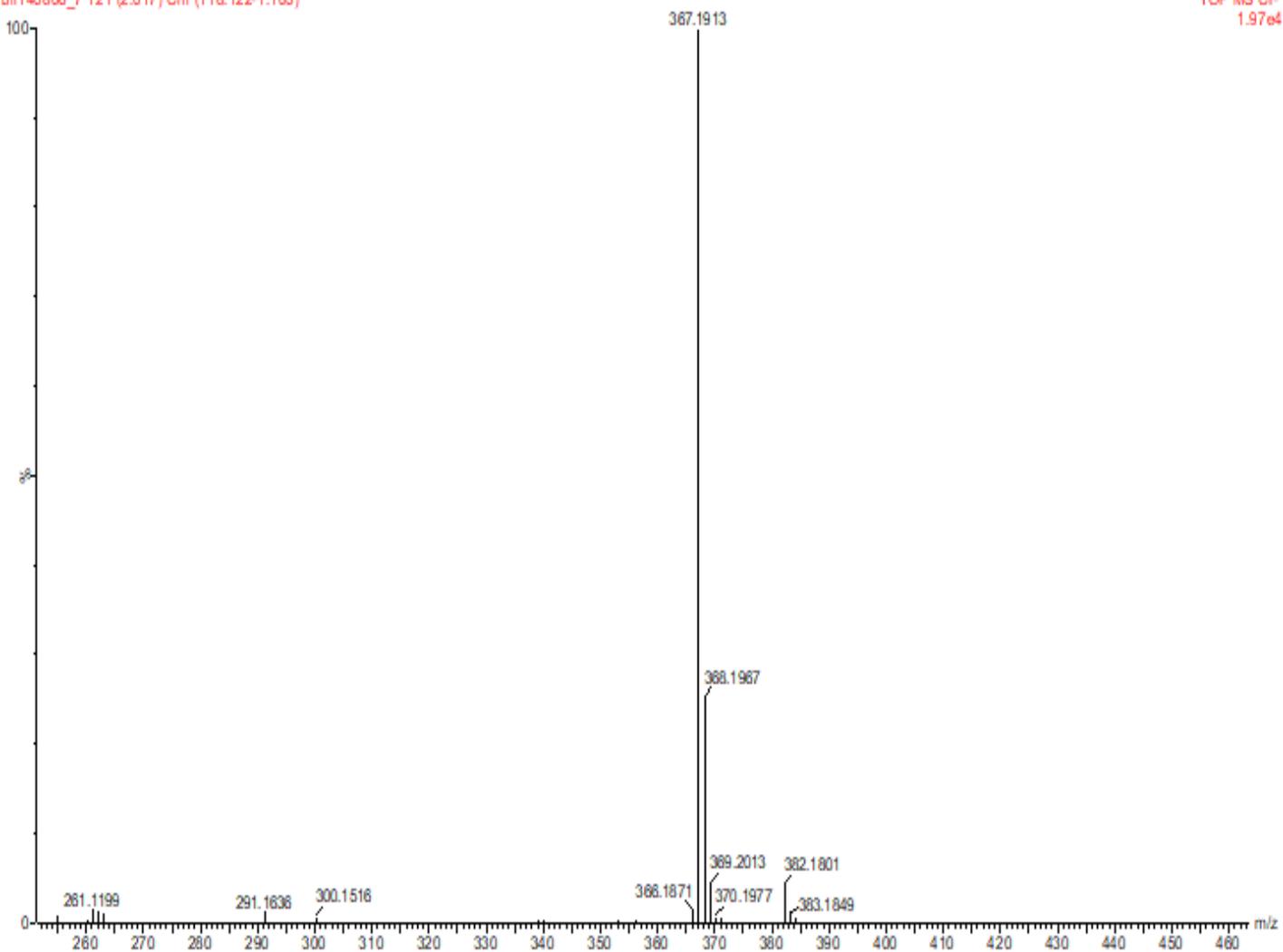
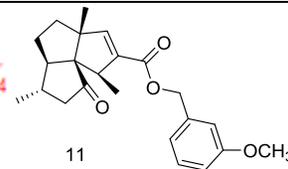


Figure S63. HRMS of compound 13

z]-4, MW=339, NH3; neg. ion

br140806\_4 251 (4.184) Cm (248:257-1:193)

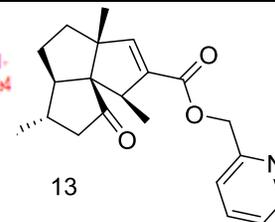
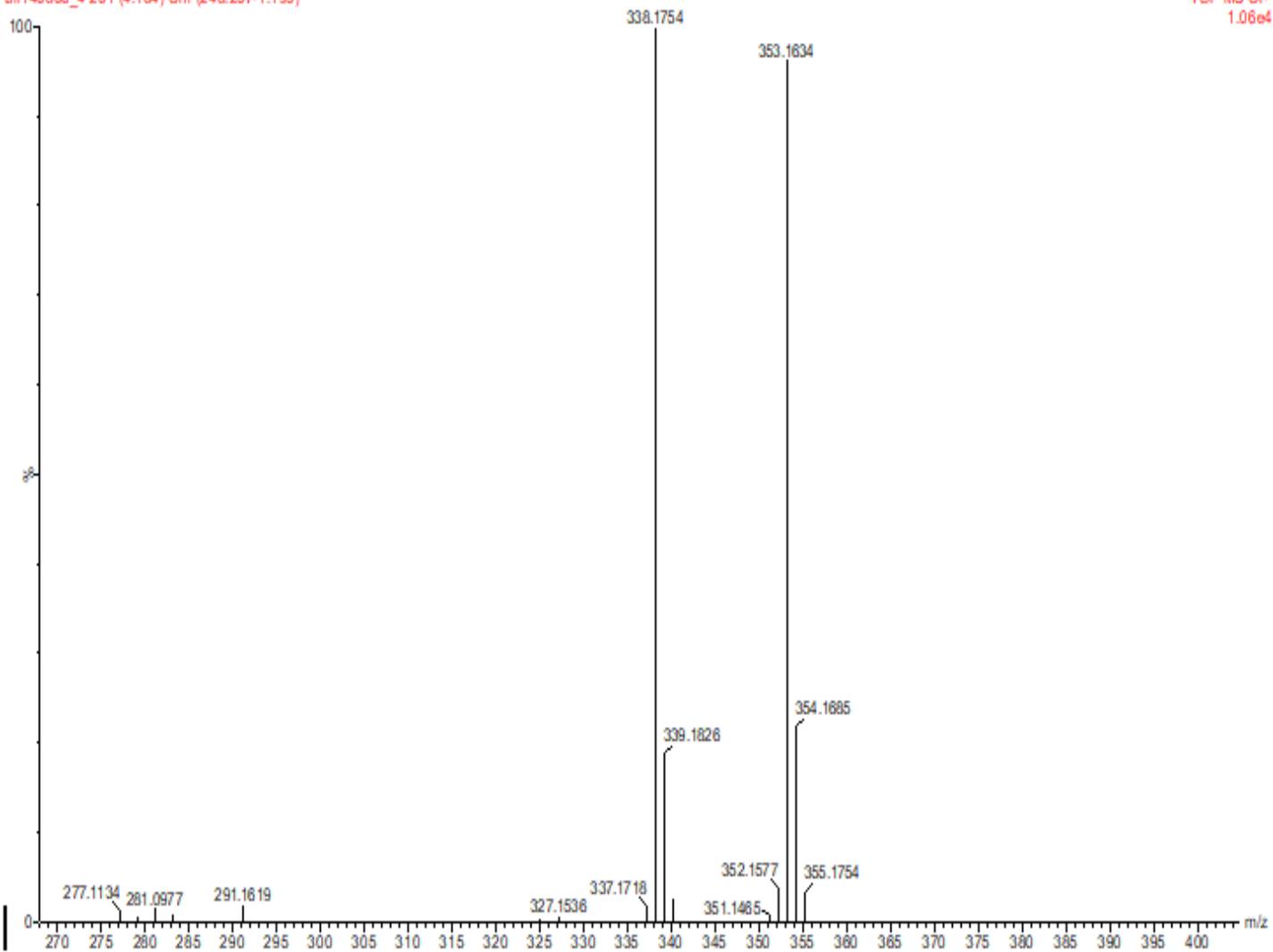
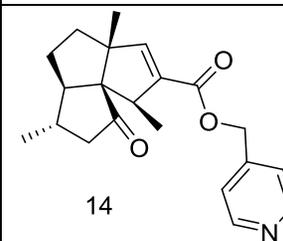
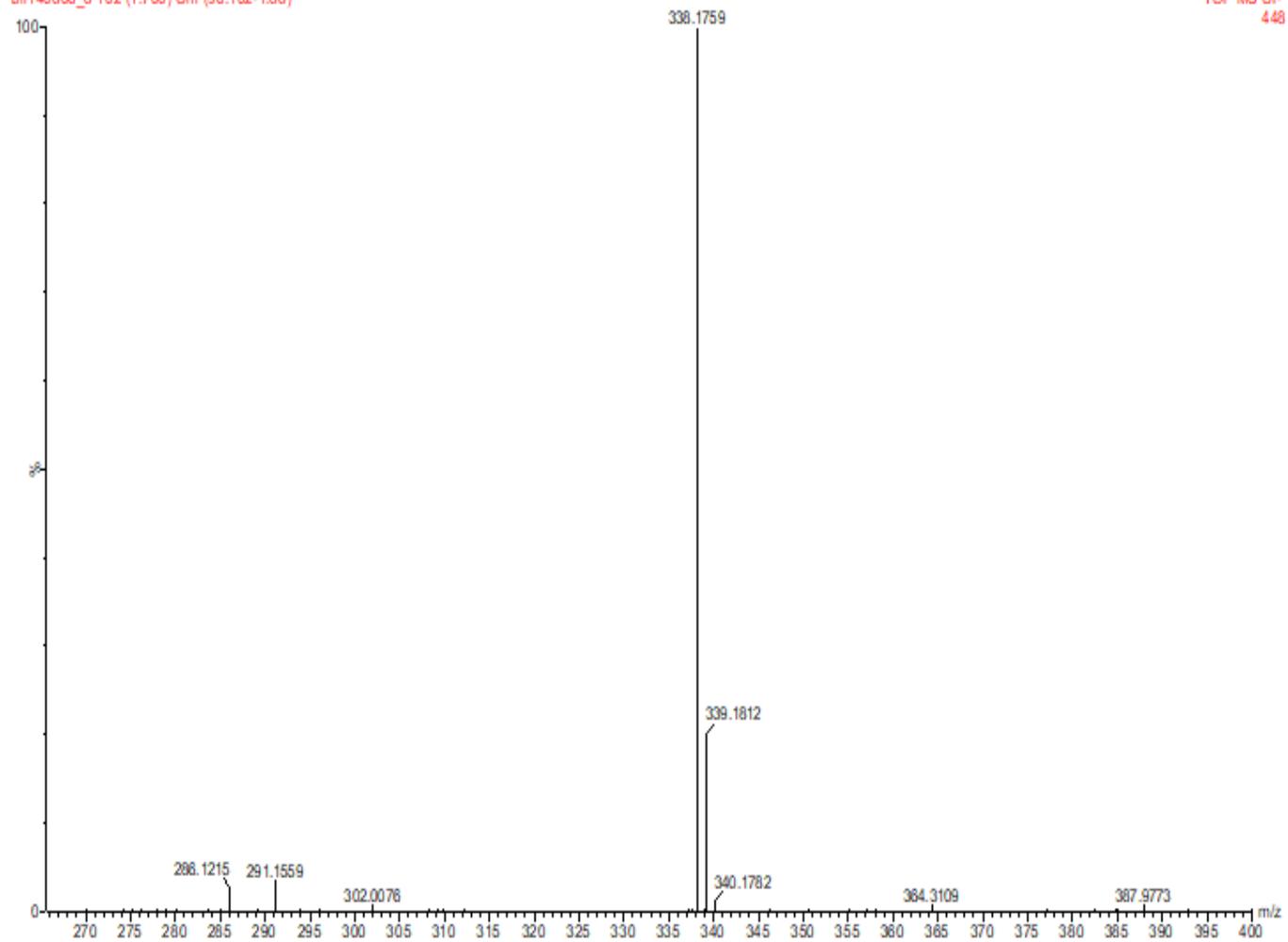
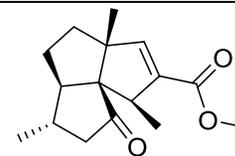


Figure S64. HRMS of compound 14

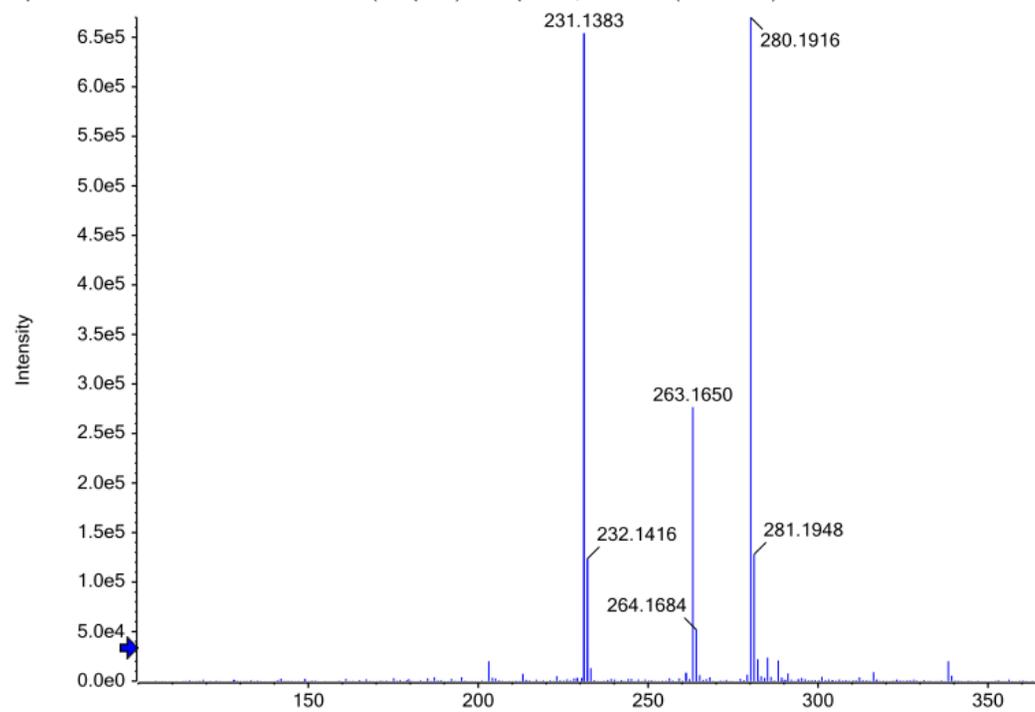
z1-8, MW=339, NH3; neg. ion  
bin140806\_8 102 (1.700) Cm (98:102-1.88)



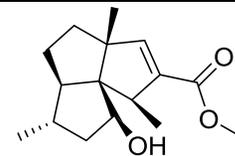
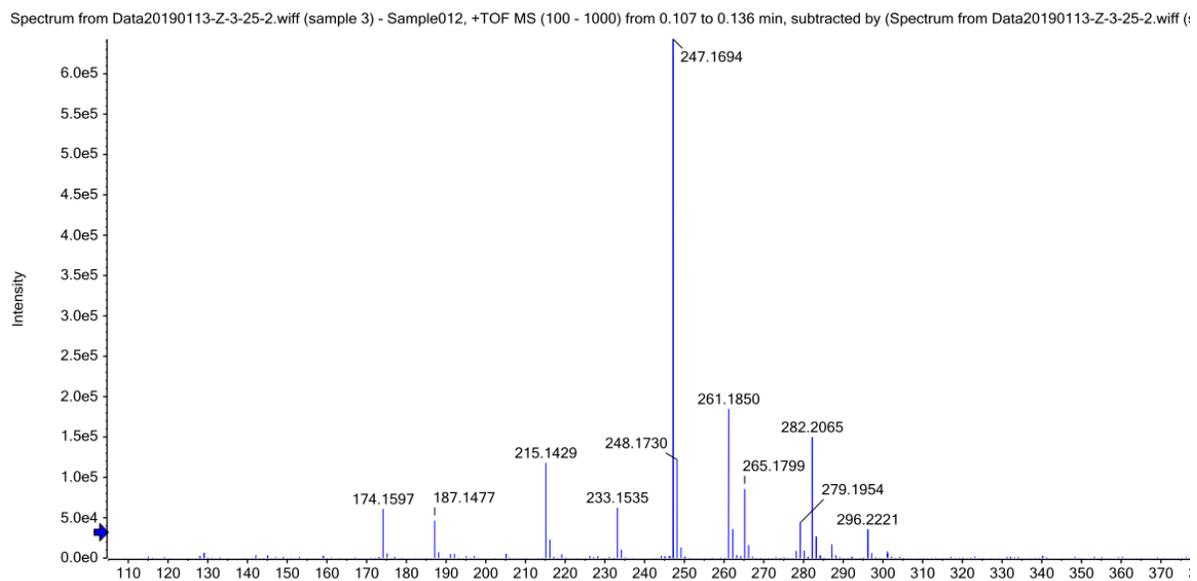
**Figure S65.** HRMS of compound **1**



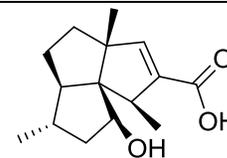
Spectrum from Data20190113-Z-3-15.wiff (sample 1) - Sample020, +TOF MS (100 - 1000) from 0.100 to 0.150 min



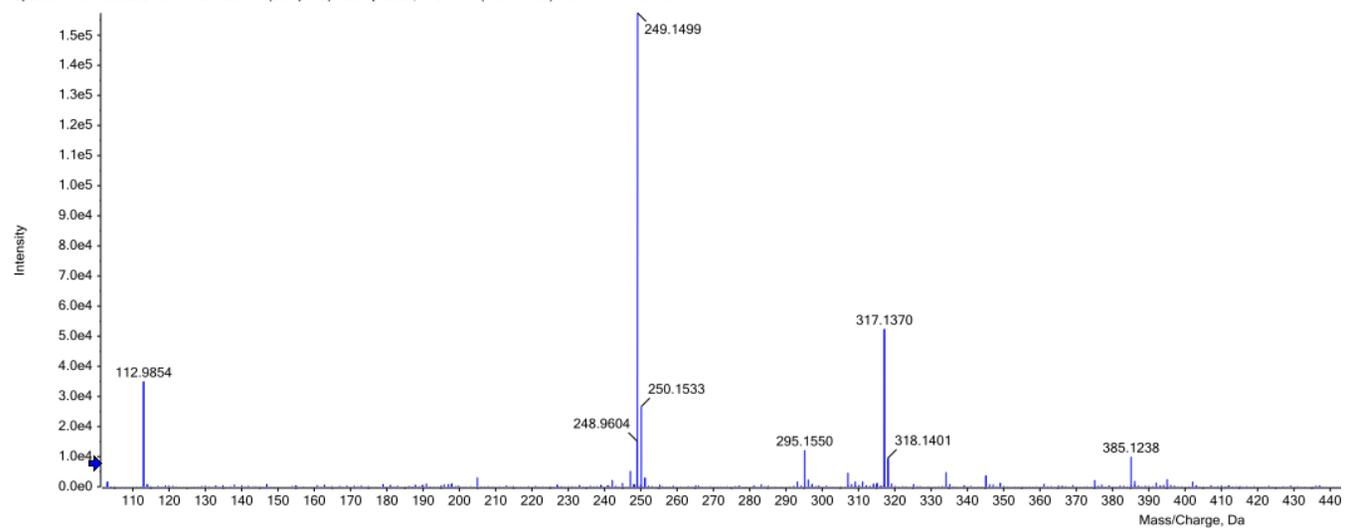
**Figure S66.** HRMS of compound **2**



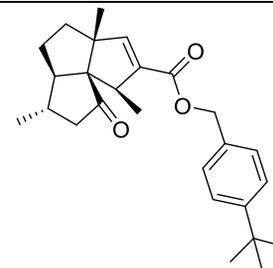
**Figure S67.** HRMS of compound **3**



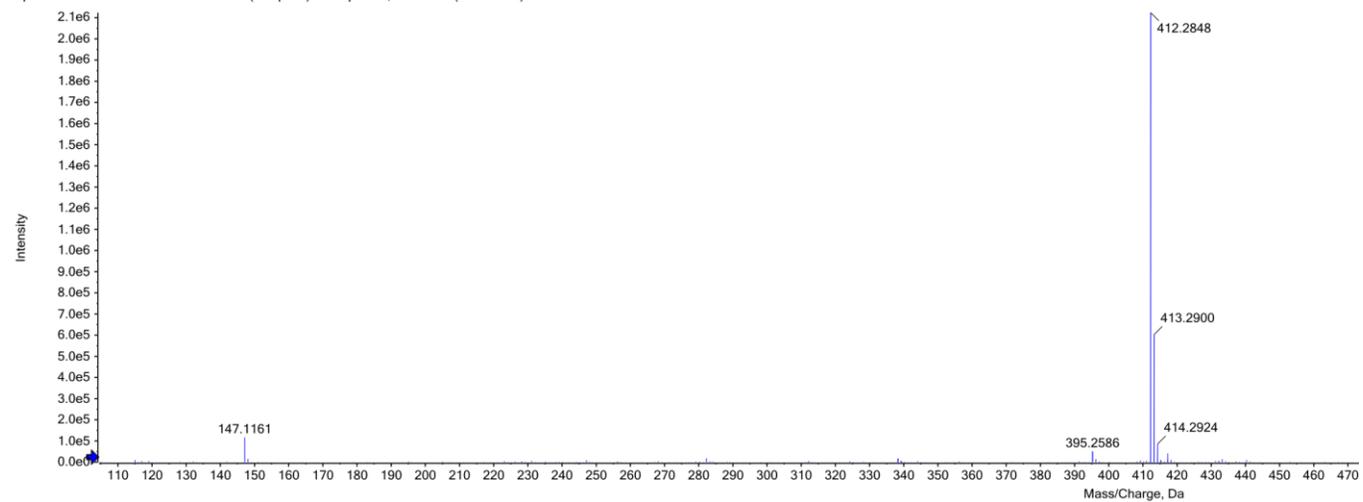
Spectrum from Data20190113-Z-3-26.wiff (sample 2) - Sample002, -TOF MS (100 - 1000) from 0.114 to 0.150 min



**Figure S68.** HRMS of compound **6**

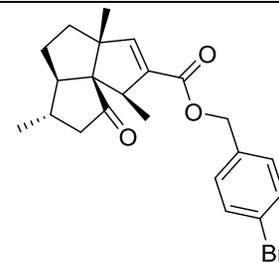
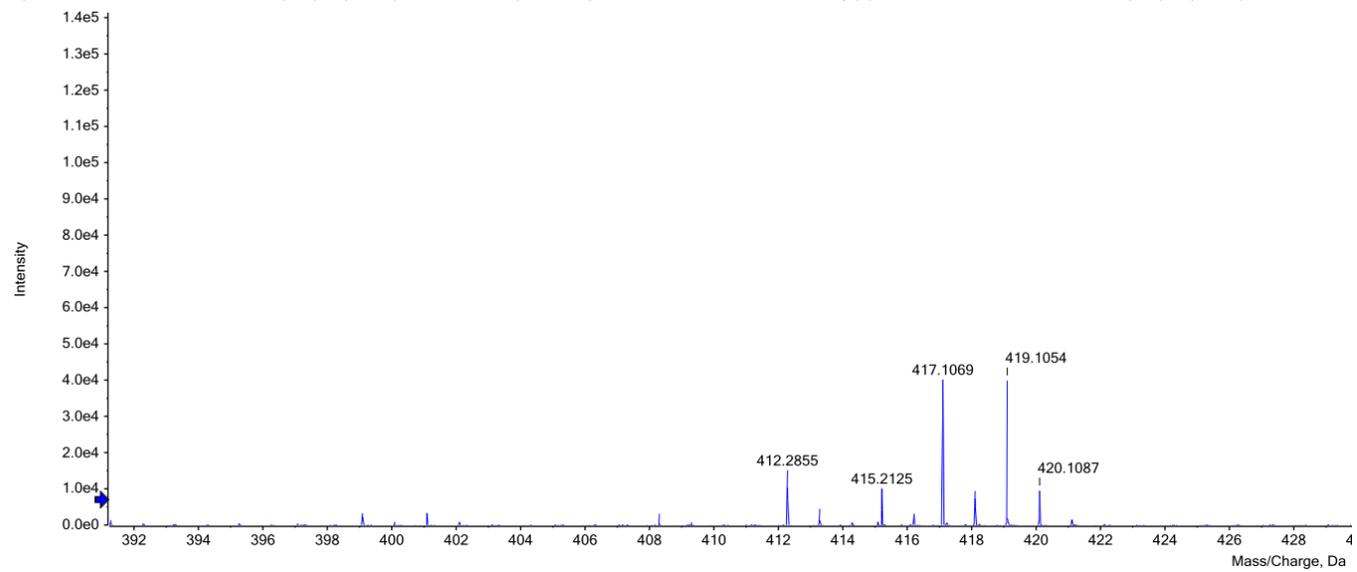


Spectrum from Data20190113-Z-3-2.wiff (sample 1) - Sample013, +TOF MS (100 - 1000) from 0.100 to 0.164 min



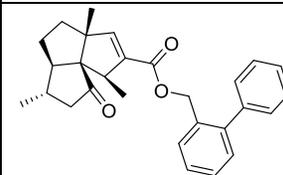
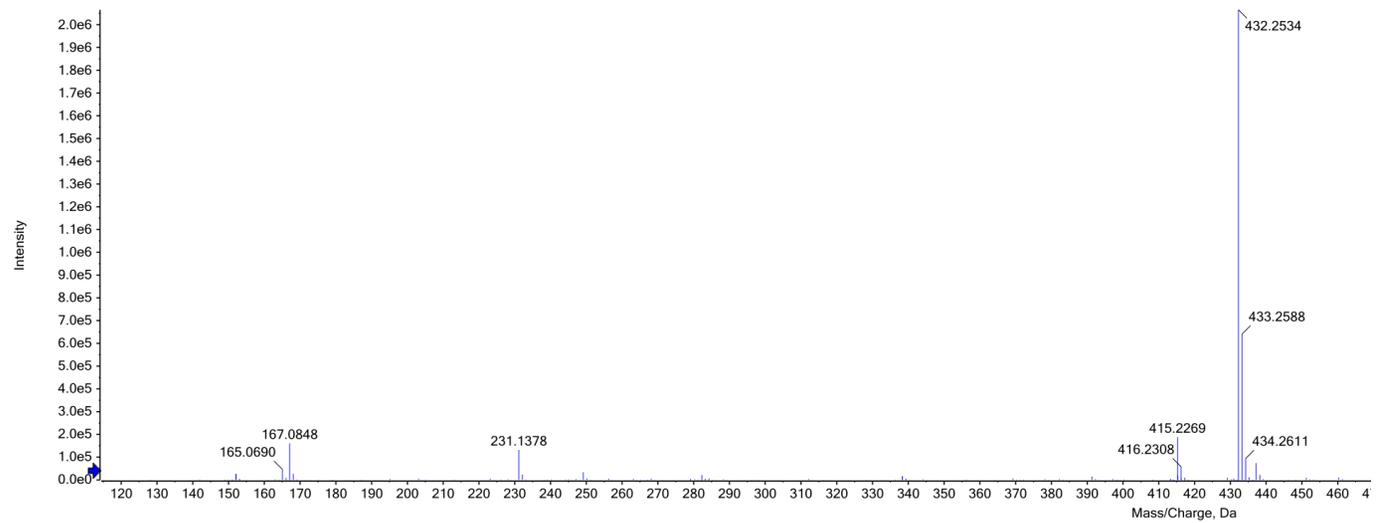
**Figure S69.** HRMS of compound 7

Spectrum from Data20190113-Z-3-3.wiff (sample 1) - Sample014, +TOF MS (100 - 1000) from 0.100 to 0.165 min, subtracted by (Spectrum from Data20190113-Z-3-3.wiff (sample 1) - Sample014, +TOF MS

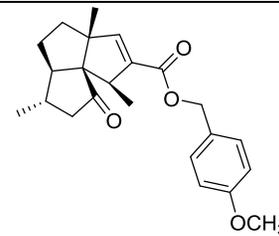


**Figure S70. HRMS of compound 9**

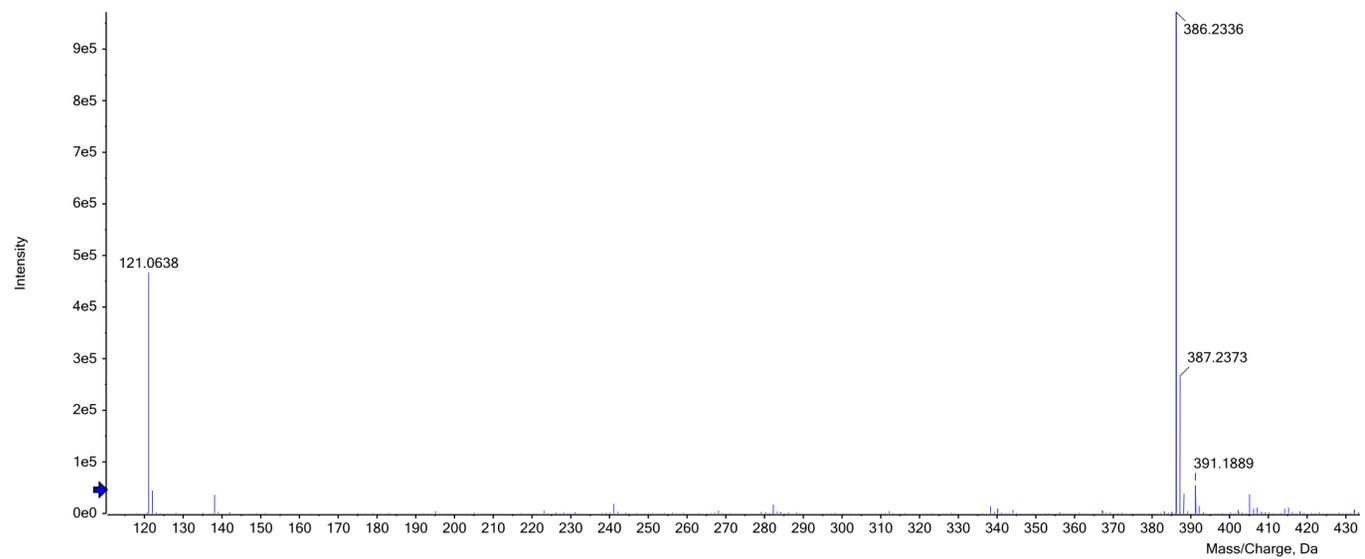
Spectrum from Data20190113-Z-3-7.wiff (sample 1) - Sample016, +TOF MS (100 - 1000) from 0.100 to 0.157 min



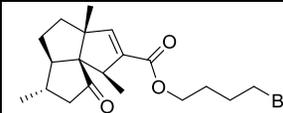
**Figure S71.** HRMS of compound **12**



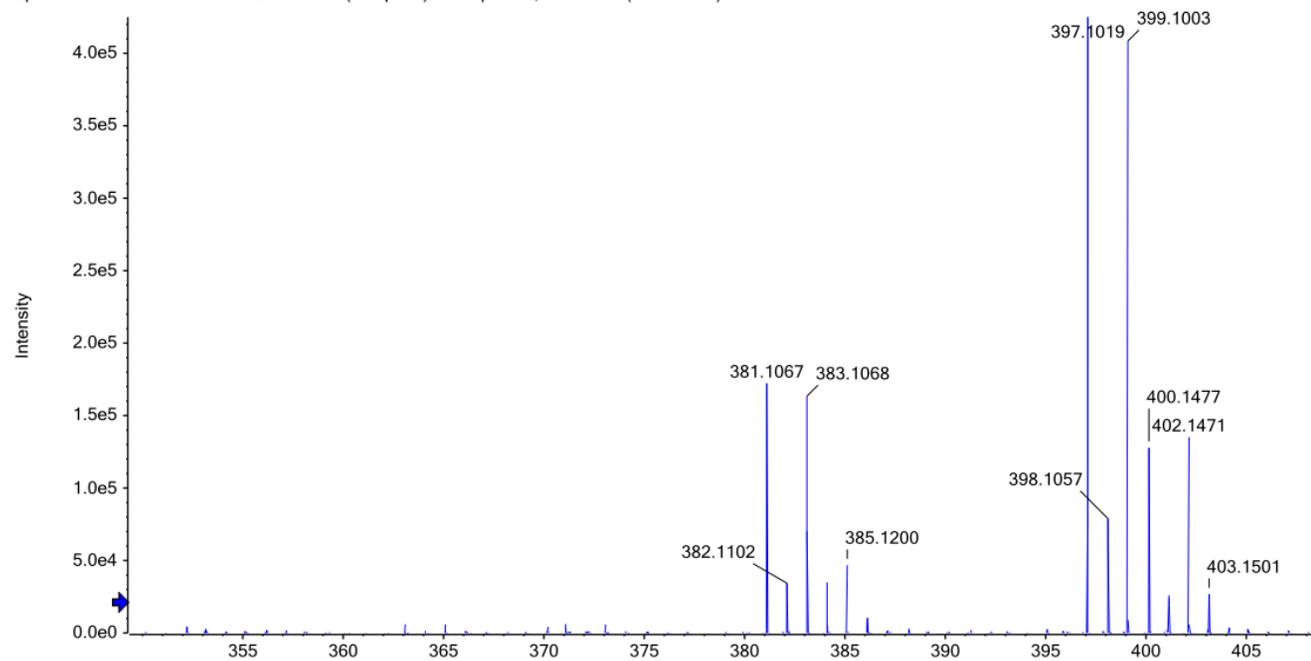
Spectrum from Data20190113-Z-3-13.wiff (sample 1) - Sample015, +TOF MS (100 - 1000) from 0.093 to 0.164 min



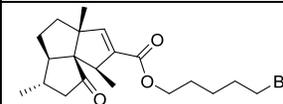
**Figure S72.** HRMS of compound **15**



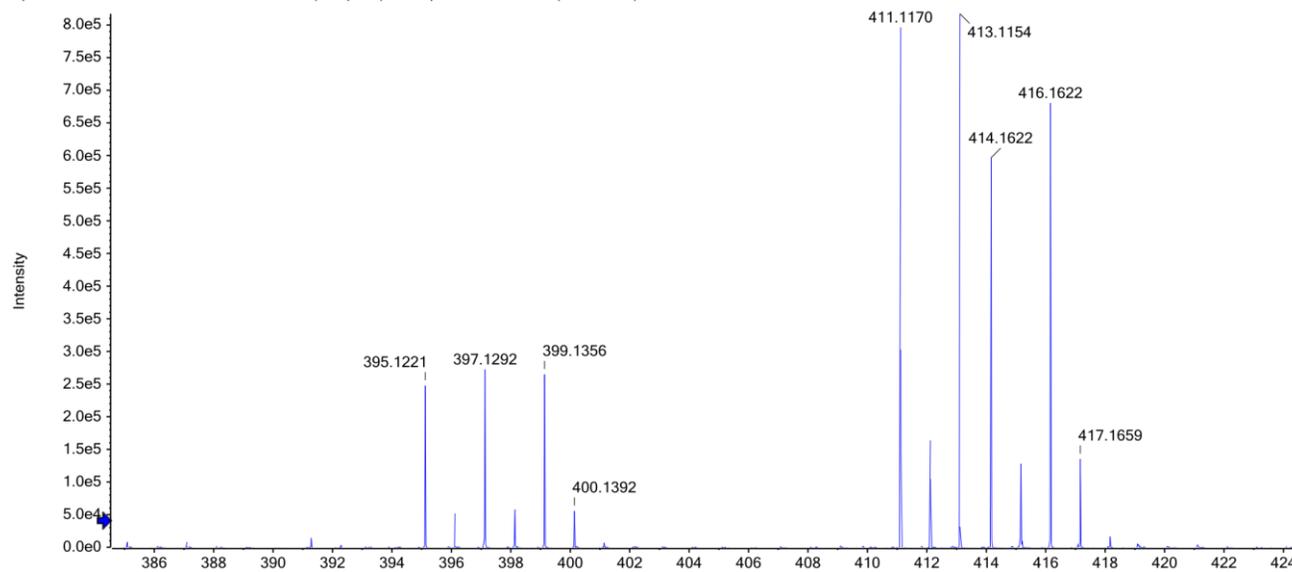
Spectrum from Data20190113-Z-3-17.wiff (sample 1) - Sample019, +TOF MS (100 - 1000) from 0.107 to 0.150 min



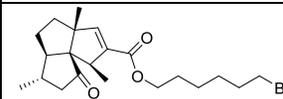
**Figure S73.** HRMS of compound **16**



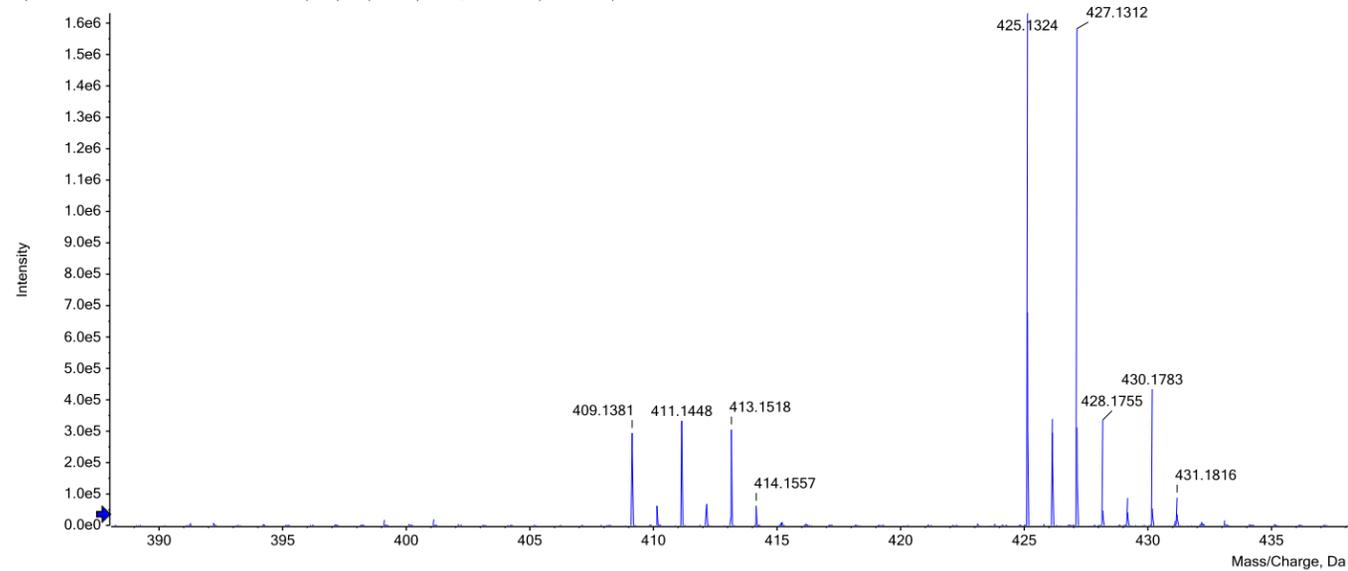
Spectrum from Data20190113-Z-3-28-1.wiff (sample 1) - Sample006, +TOF MS (100 - 1000) from 0.107 to 0.157 min



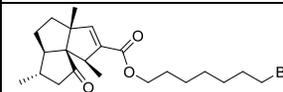
**Figure S74.** HRMS of compound **17**



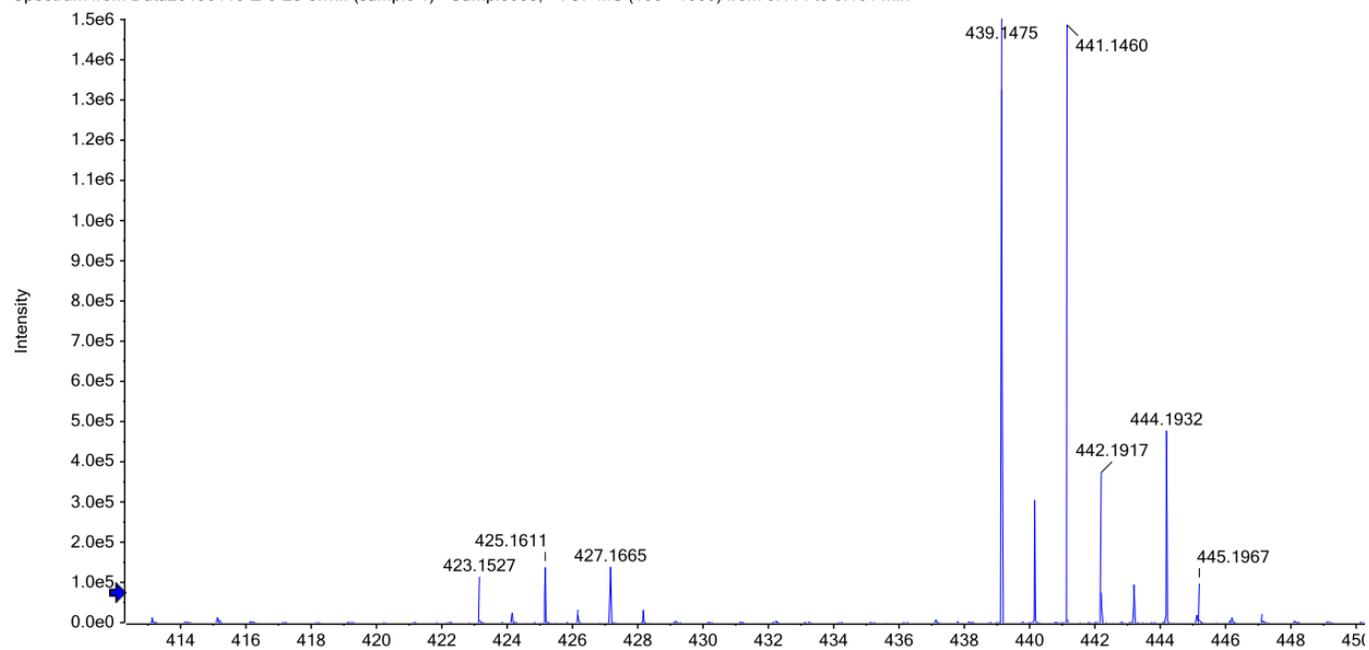
Spectrum from Data20190113-Z-3-28-2.wiff (sample 1) - Sample010, +TOF MS (100 - 1000) from 0.107 to 0.150 min



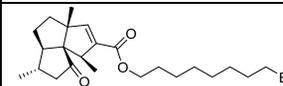
**Figure S75. HRMS of compound 18**



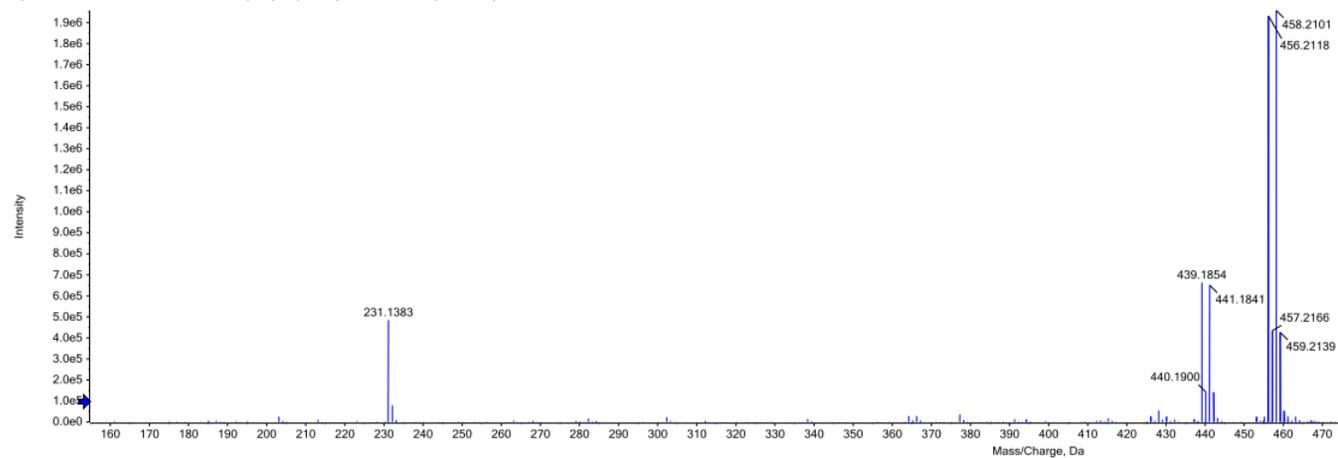
Spectrum from Data20190113-Z-3-28-3.wiff (sample 1) - Sample003, +TOF MS (100 - 1000) from 0.114 to 0.164 min



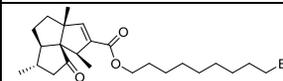
**Figure S76.** HRMS of compound **19**



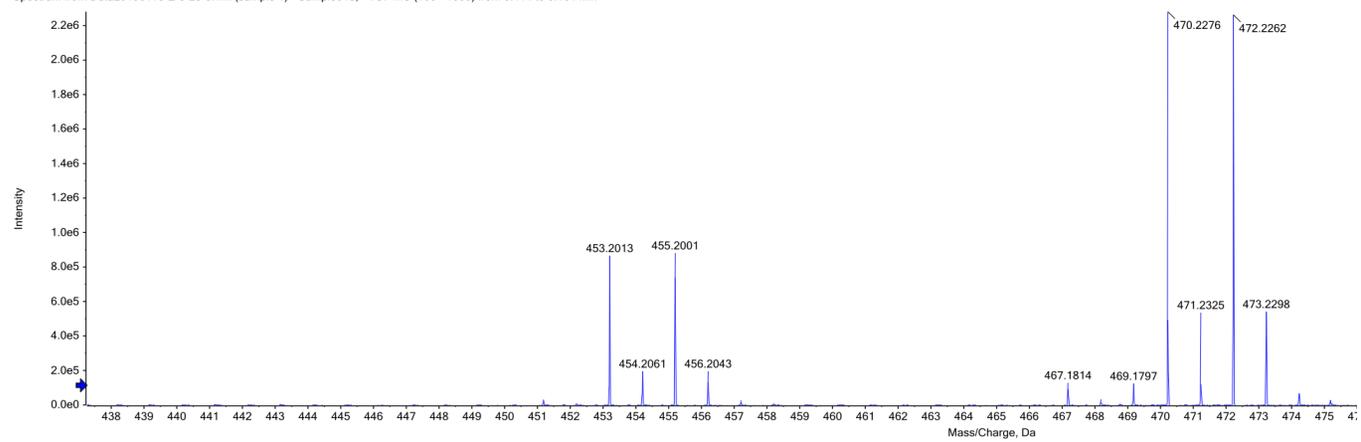
Spectrum from Data20190113-Z-3-28-4.wiff (sample 1) - Sample011, +TOF MS (100 - 1000) from 0.100 to 0.172 min



**Figure S77.** HRMS of compound **20**

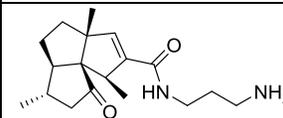
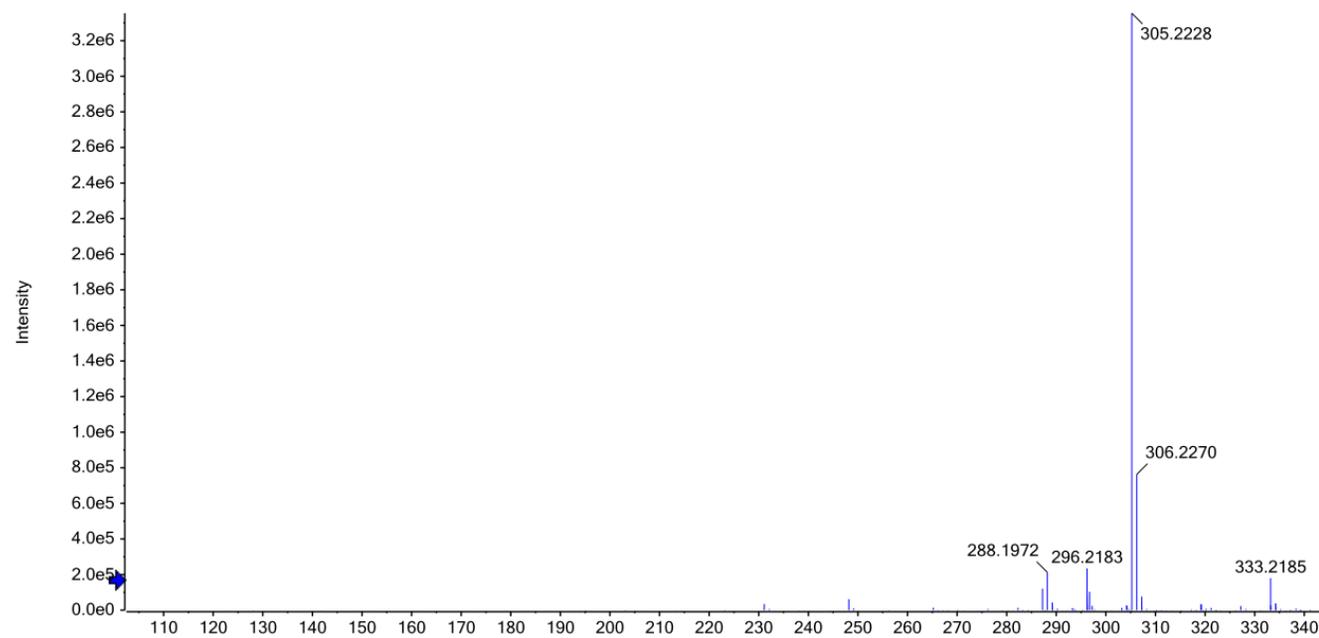


Spectrum from Data20190113-Z-3-28-5.wiff (sample 1) - Sample018, +TOF MS (100 - 1000) from 0.114 to 0.164 min



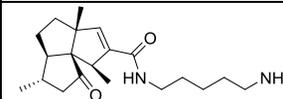
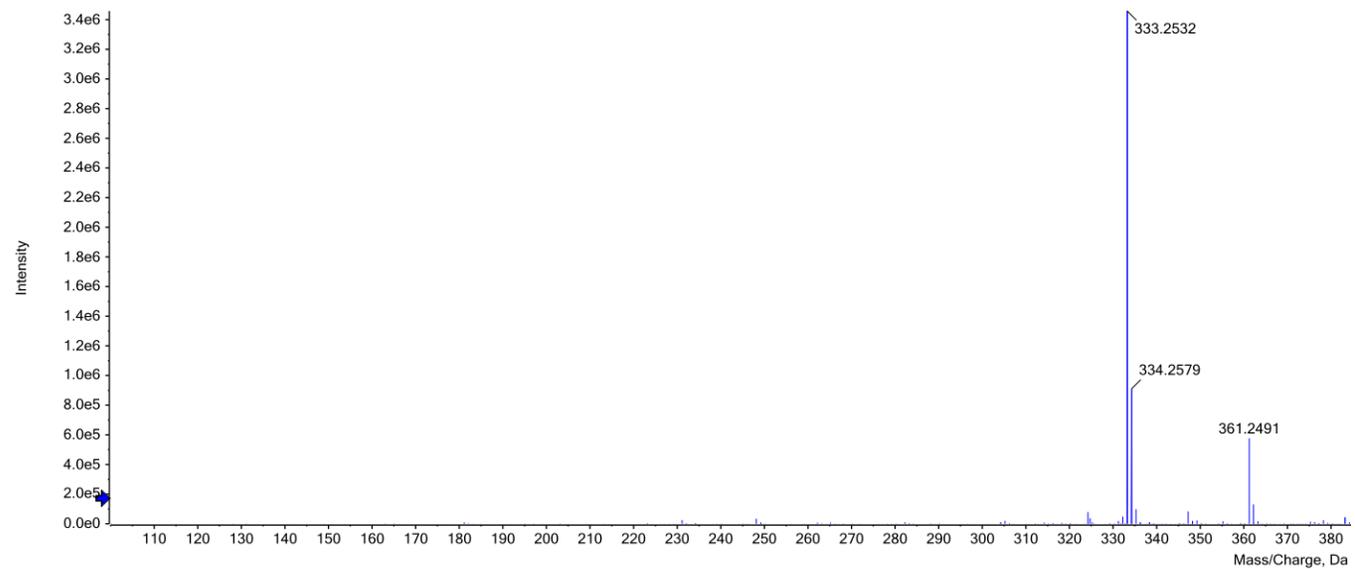
**Figure S78.** HRMS of compound **21**

Spectrum from Data20190113-Z-3-21-1.wiff (sample 1) - Sample017, +TOF MS (100 - 1000) from 0.114 to 0.164 min

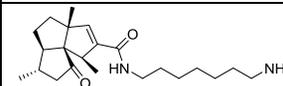


**Figure S79.** HRMS of compound **22**

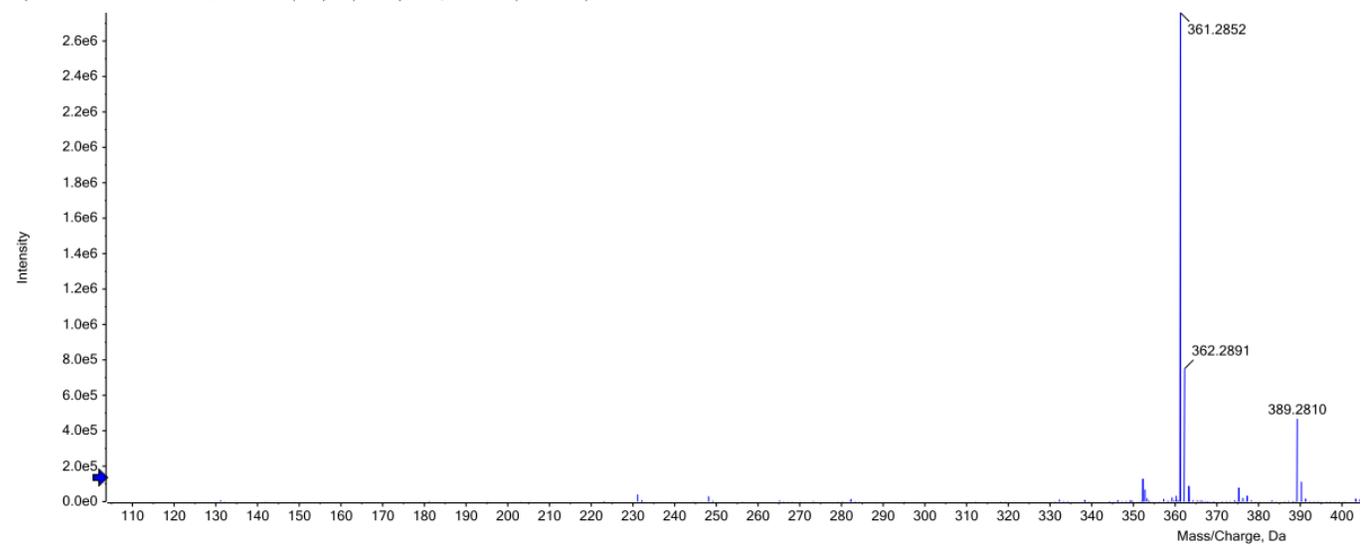
Spectrum from Data20190113-Z-3-21-2.wiff (sample 1) - Sample004, +TOF MS (100 - 1000) from 0.107 to 0.150 min



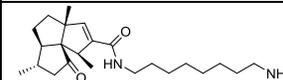
**Figure S80.** HRMS of compound **23**



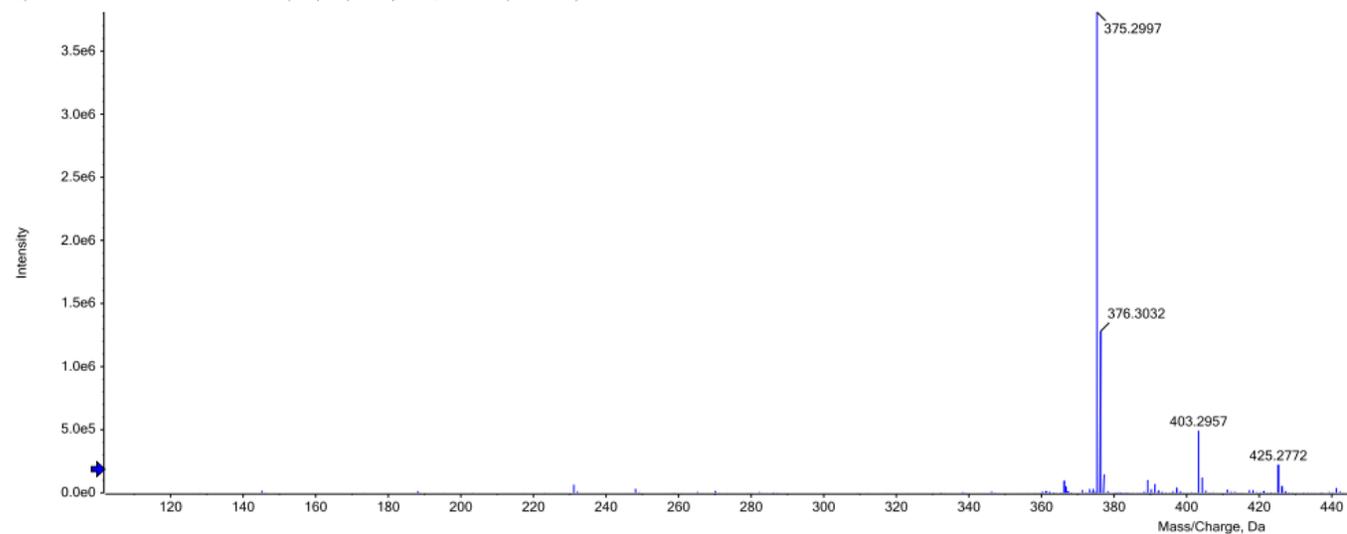
Spectrum from Data20190113-Z-3-21-3.wiff (sample 1) - Sample009, +TOF MS (100 - 1000) from 0.093 to 0.172 min



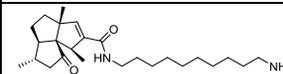
**Figure S81.** HRMS of compound **24**



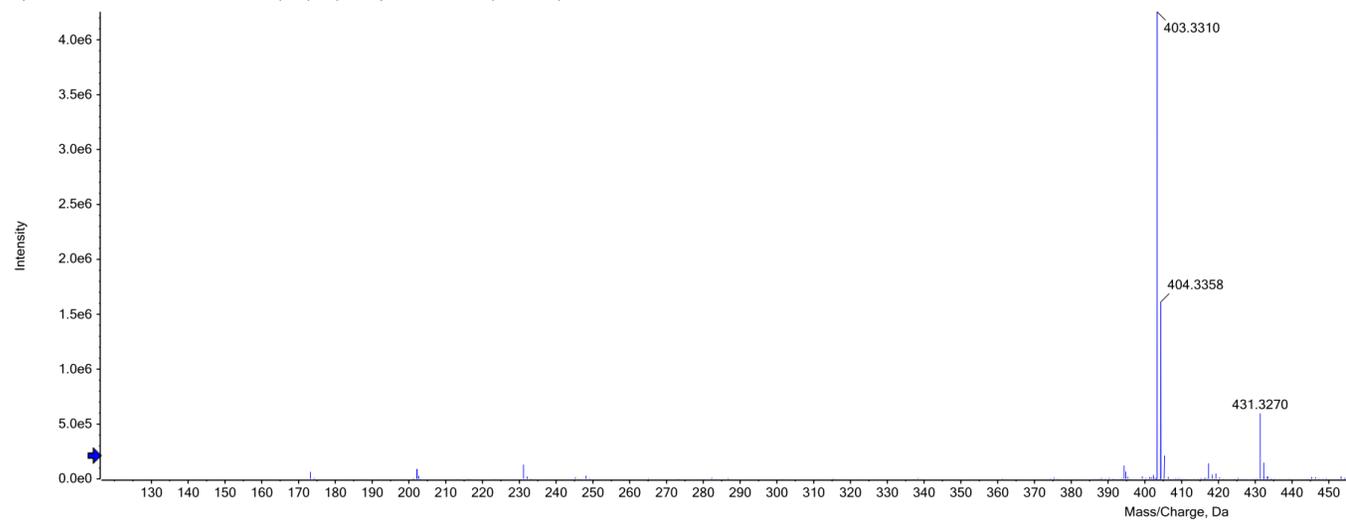
Spectrum from Data20190113-Z-3-21-4.wiff (sample 1) - Sample007, +TOF MS (100 - 1000) from 0.100 to 0.172 min



**Figure S82.** HRMS of compound **25**



Spectrum from Data20190113-Z-3-21-5.wiff (sample 1) - Sample008, +TOF MS (100 - 1000) from 0.107 to 0.164 min



**Figure S83.** HRMS of compound **26**

