

## Supporting Information

### Anti-inflammatory Cembranoids from a Formosa Soft Coral *Sarcophyton cherbonnieri*

Chia-Chi Peng <sup>1,†</sup>, Chiung-Yao Huang <sup>1,†</sup>, Atallah F. Ahmed <sup>2,3</sup>, Tsong-Long Hwang <sup>4,5,6</sup> and Jyh-Horng Sheu <sup>1,7,8,\*</sup>

<sup>1</sup> Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan; m045020008@student.nsysu.edu.tw (C.-C.P.), huangcy@mail.nsysu.edu.tw (C.-Y.H.)

<sup>2</sup> Department of Pharmacognosy, College of Pharmacy, King Saud University, Riyadh 11451, Saudi Arabia; afahmed@ksu.edu.sa (A.F.A.)

<sup>3</sup> Department of Pharmacognosy, Faculty of Pharmacy, Mansoura University, Mansoura 35516, Egypt

<sup>4</sup> Graduate Institute of Natural Products, College of Medicine, Chang Gung University, Taoyuan 333, Taiwan; htl@mail.cgu.edu.tw

<sup>5</sup> Research Center for Industry of Human Ecology and Graduate Institute of Health Industry Technology, Chang Gung University of Science and Technology, Taoyuan 333, Taiwan

<sup>6</sup> Department of Anesthesiology, Chang Gung Memorial Hospital, Taoyuan 333, Taiwan

<sup>7</sup> Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan

<sup>8</sup> Department of Medical Research, China Medical University Hospital, China Medical University, Taichung 404, Taiwan

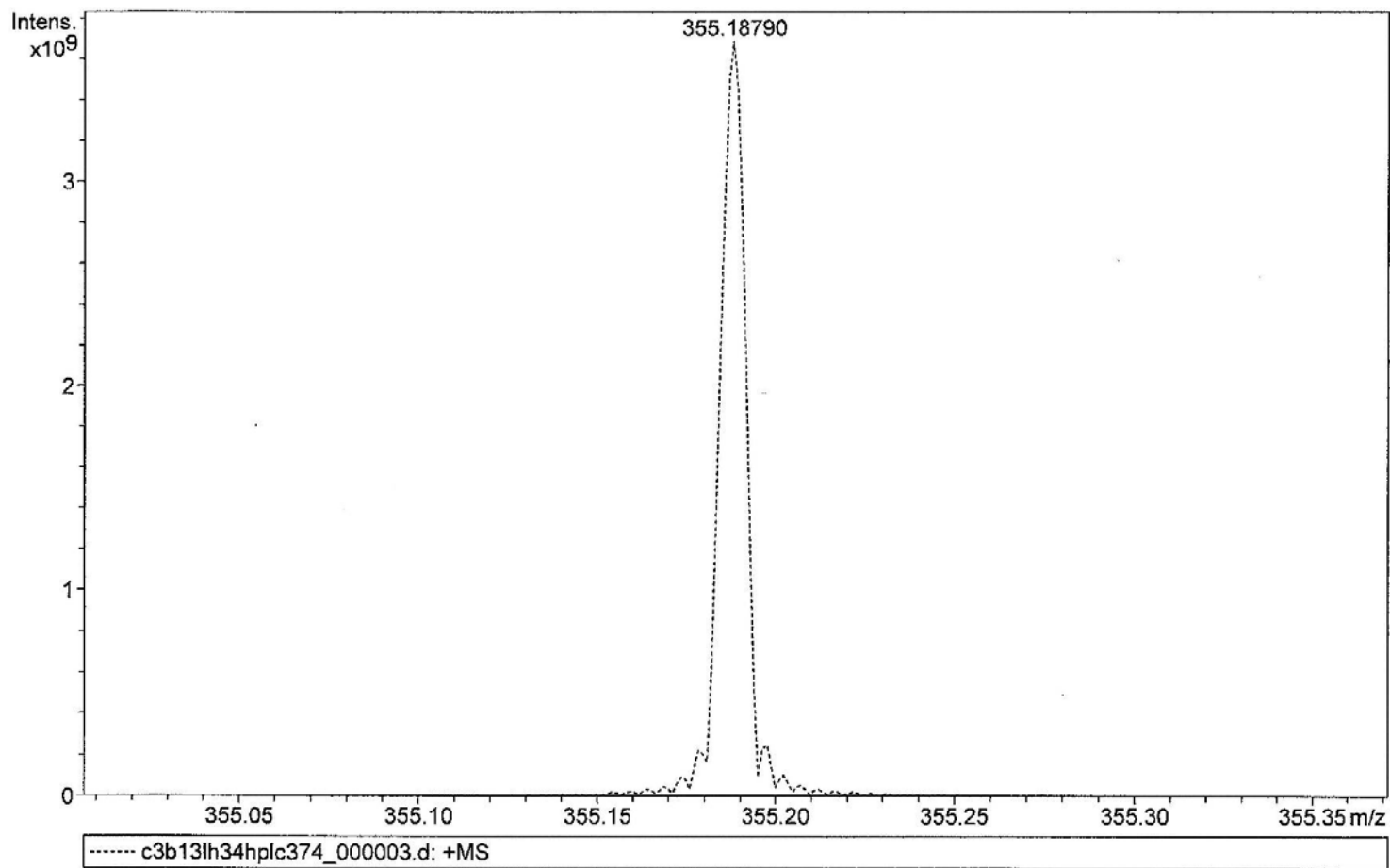
\* Correspondence: sheu@mail.nsysu.edu.tw; Tel.: +886-7-525-2000 (ext. 5030); Fax: +886-7-525-5020.

<sup>†</sup> These authors contributed equally to this work

## Table of Contents

Figure S1. HREIMS spectrum of <b>1</b>	S4
Figure S2. <sup>1</sup> H NMR spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S5
Figure S3. <sup>13</sup> C NMR spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S6
Figure S4. HSQC spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S7
Figure S5. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S8
Figure S6. HMBC spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S9
Figure S7. NOESY spectrum of <b>1</b> in C <sub>6</sub> D <sub>6</sub>	S10
Figure S8. HREIMS spectrum of <b>2</b>	S11
Figure S9. <sup>1</sup> H NMR spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S12
Figure S10. <sup>13</sup> C NMR spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S13
Figure S11. HSQC spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S14
Figure S12. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S15
Figure S13. HMBC spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S16
Figure S14. NOESY spectrum of <b>2</b> in C <sub>6</sub> D <sub>6</sub>	S17
Figure S15. HREIMS spectrum of <b>3</b>	S18
Figure S16. <sup>1</sup> H NMR spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S19
Figure S17. <sup>13</sup> C NMR spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S20
Figure S18. HSQC spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S21
Figure S19. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S22
Figure S20. HMBC spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S23
Figure S21. NOESY spectrum of <b>3</b> in C <sub>6</sub> D <sub>6</sub>	S24
Figure S22. HREIMS spectrum of <b>4</b>	S25
Figure S23. <sup>1</sup> H NMR spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S26
Figure S24. <sup>13</sup> C NMR spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S27
Figure S25. HSQC spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S28
Figure S26. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S29
Figure S27. HMBC spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S30
Figure S28. NOESY spectrum of <b>4</b> in C <sub>6</sub> D <sub>6</sub>	S31
Figure S29. HREIMS spectrum of <b>5</b>	S32
Figure S30. <sup>1</sup> H NMR spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S33
Figure S31. <sup>13</sup> C NMR spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S34
Figure S32. HSQC spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S35
Figure S33. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S36
Figure S34. HMBC spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S37
Figure S35. NOESY spectrum of <b>5</b> in C <sub>6</sub> D <sub>6</sub>	S38

Figure S36. HREIMS spectrum of <b>6</b>	S39
Figure S37. <sup>1</sup> H NMR spectrum of <b>6</b> in CDCl <sub>3</sub>	S40
Figure S38. <sup>13</sup> C NMR spectrum of <b>6</b> in CDCl <sub>3</sub>	S41
Figure S39. HSQC spectrum of <b>6</b> in CDCl <sub>3</sub>	S42
Figure S40. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>6</b> in CDCl <sub>3</sub>	S43
Figure S41. HMBC spectrum of <b>6</b> in CDCl <sub>3</sub>	S44
Figure S42. NOESY spectrum of <b>6</b> in CDCl <sub>3</sub>	S45
Figure S43. HREIMS spectrum of <b>7</b>	S46
Figure S44. <sup>1</sup> H NMR spectrum of <b>7</b> in CDCl <sub>3</sub>	S47
Figure S45. <sup>13</sup> C NMR spectrum of <b>7</b> in CDCl <sub>3</sub>	S48
Figure S46. HSQC spectrum of <b>7</b> in CDCl <sub>3</sub>	S49
Figure S47. <sup>1</sup> H- <sup>1</sup> H COSY spectrum of <b>7</b> in CDCl <sub>3</sub>	S50
Figure S48. HMBC spectrum of <b>7</b> in CDCl <sub>3</sub>	S51
Figure S49. NOESY spectrum of <b>7</b> in CDCl <sub>3</sub>	S52



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
355.18790	1	C <sub>20</sub> H <sub>28</sub> NaO <sub>4</sub>	100.00	355.18798	0.08	0.23	4.6	6.5	even	ok

Figure S1. HRESIMS spectrum of 1

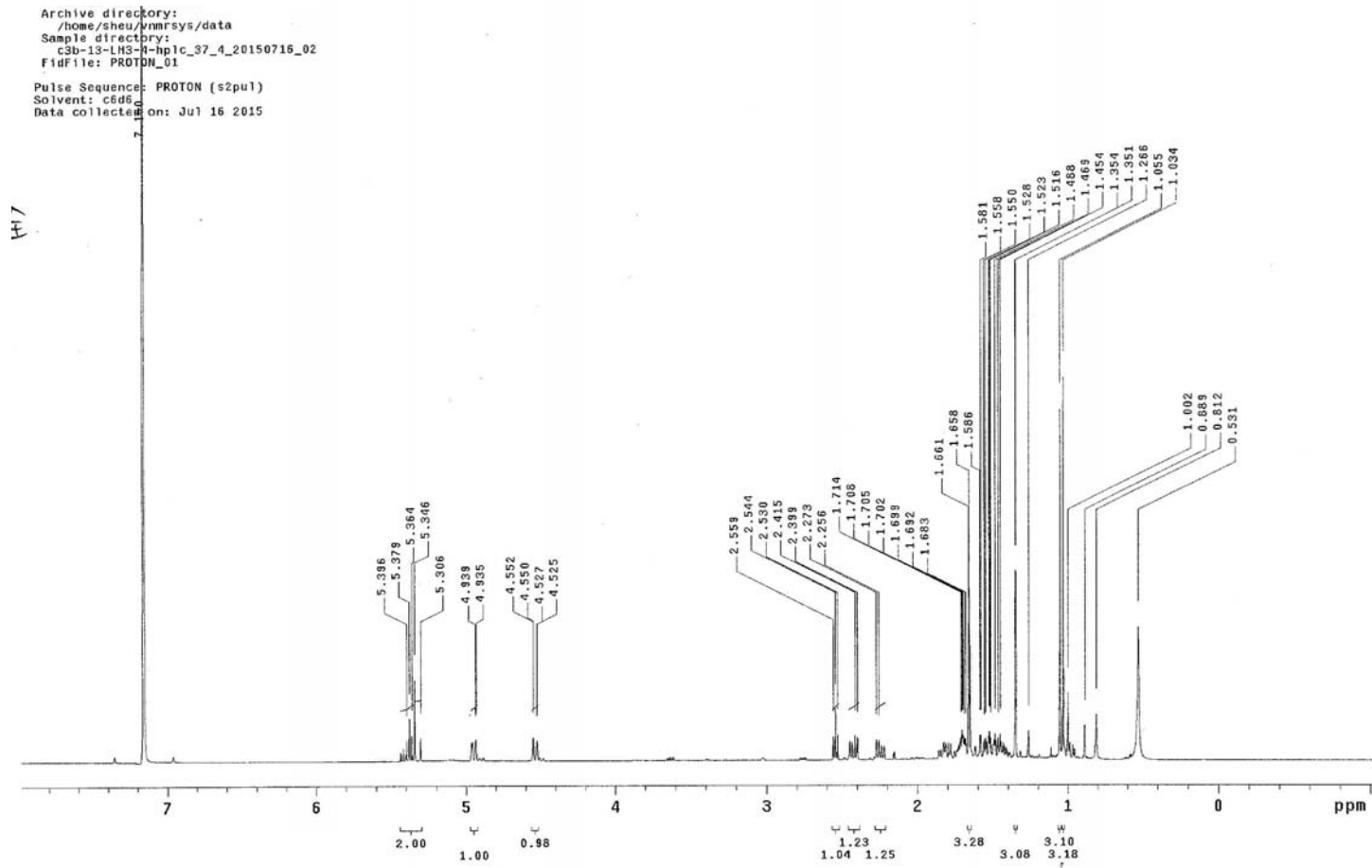


Figure S2.  $^1\text{H}$  NMR spectrum of **1** in  $\text{C}_6\text{D}_6$

c3b-13-LH3-4-hplc 37.4  
Sample Name:  
c3b-13-LH3-4-hplc\_37\_4  
Data Collected on:  
Varian-NMR-vnmrs400  
Archive directory:  
/home/shou/vnmrsys/data  
Sample directory:  
c3b-13-LH3-4-hplc\_37\_4\_20150716\_02  
FidFile: CARBON\_01  
Pulse Sequence: CARBON (s2pul)  
Solvent: c6d6  
Data collected on: Jul 17 2015

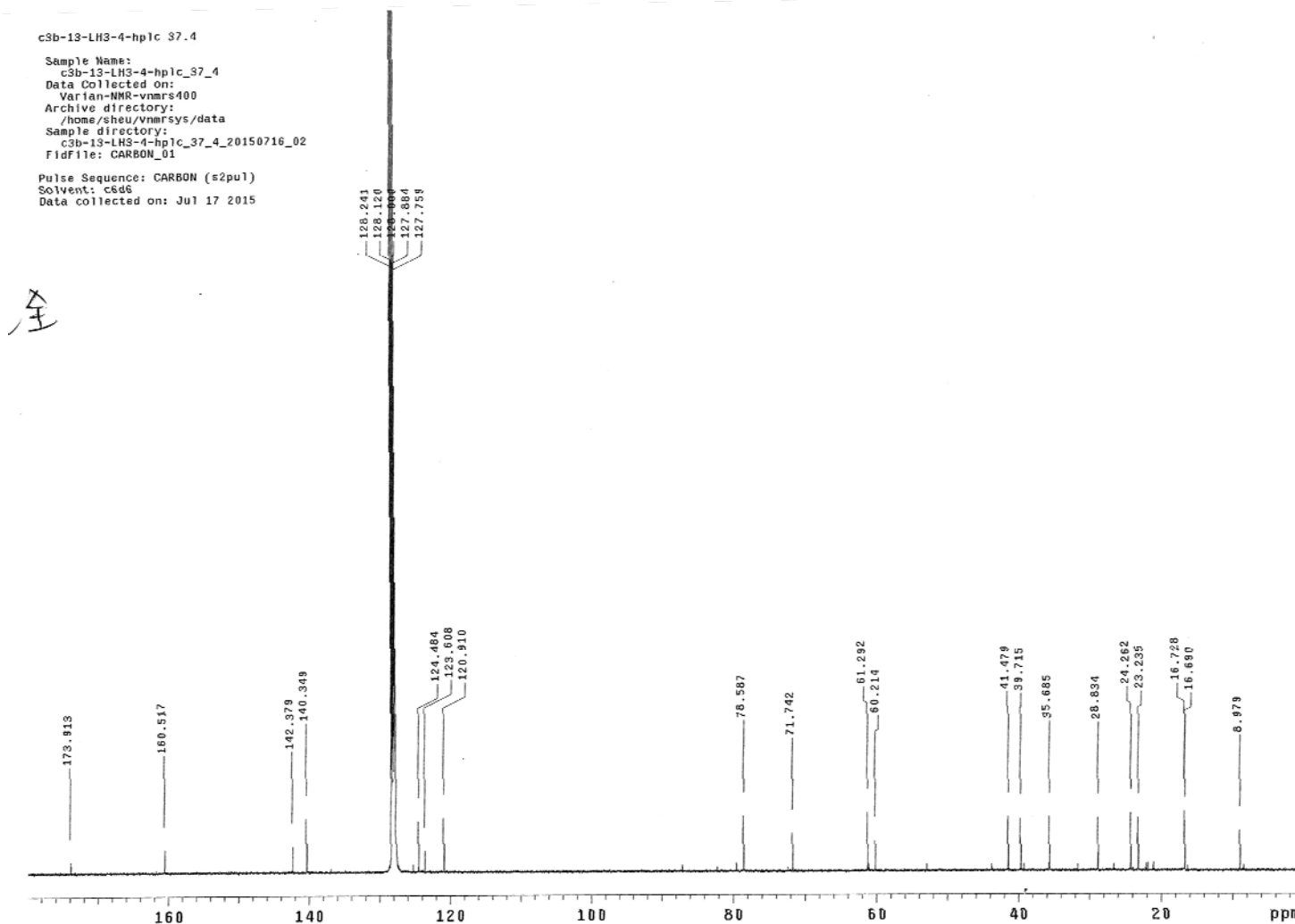


Figure S3.  $^{13}\text{C}$  NMR spectrum of 1 in  $\text{C}_6\text{D}_6$   
S6

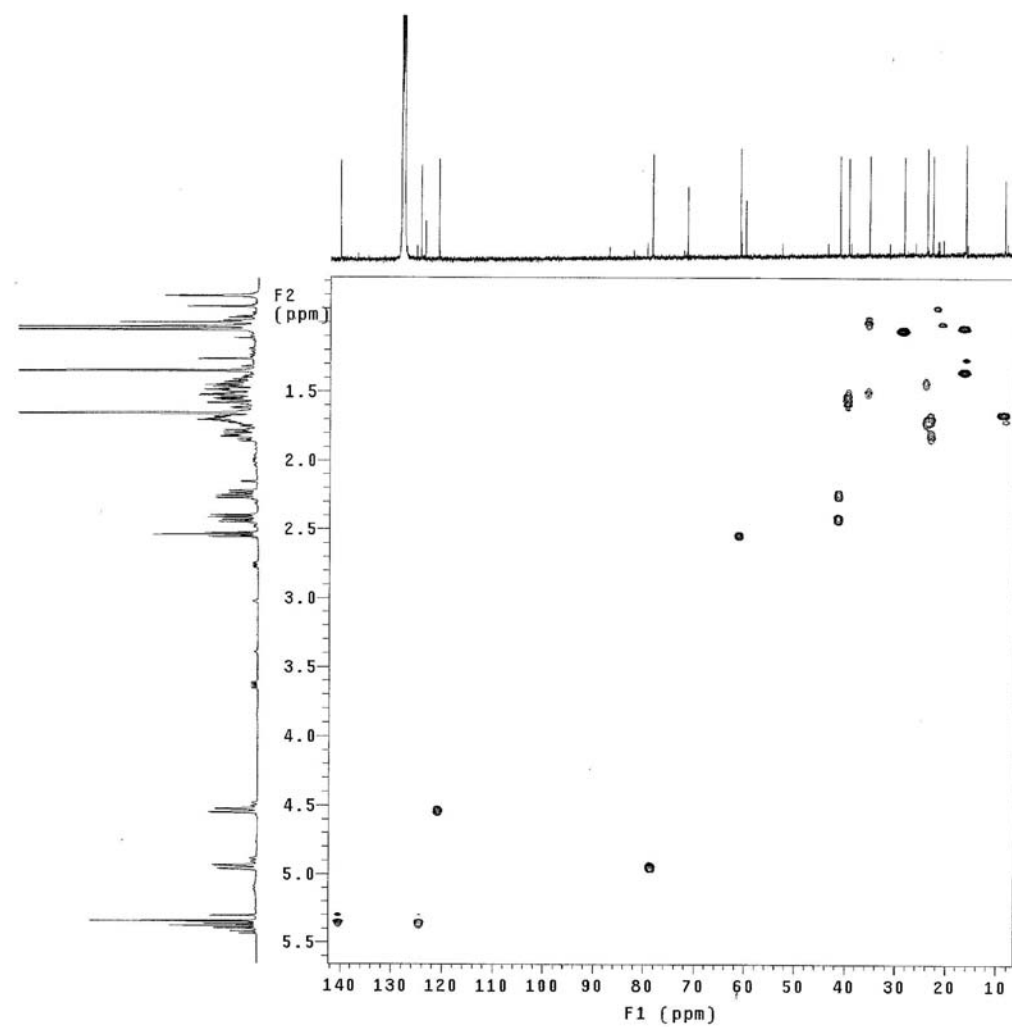


Figure S4. HSQC spectrum of 1 in  $\text{C}_6\text{D}_6$

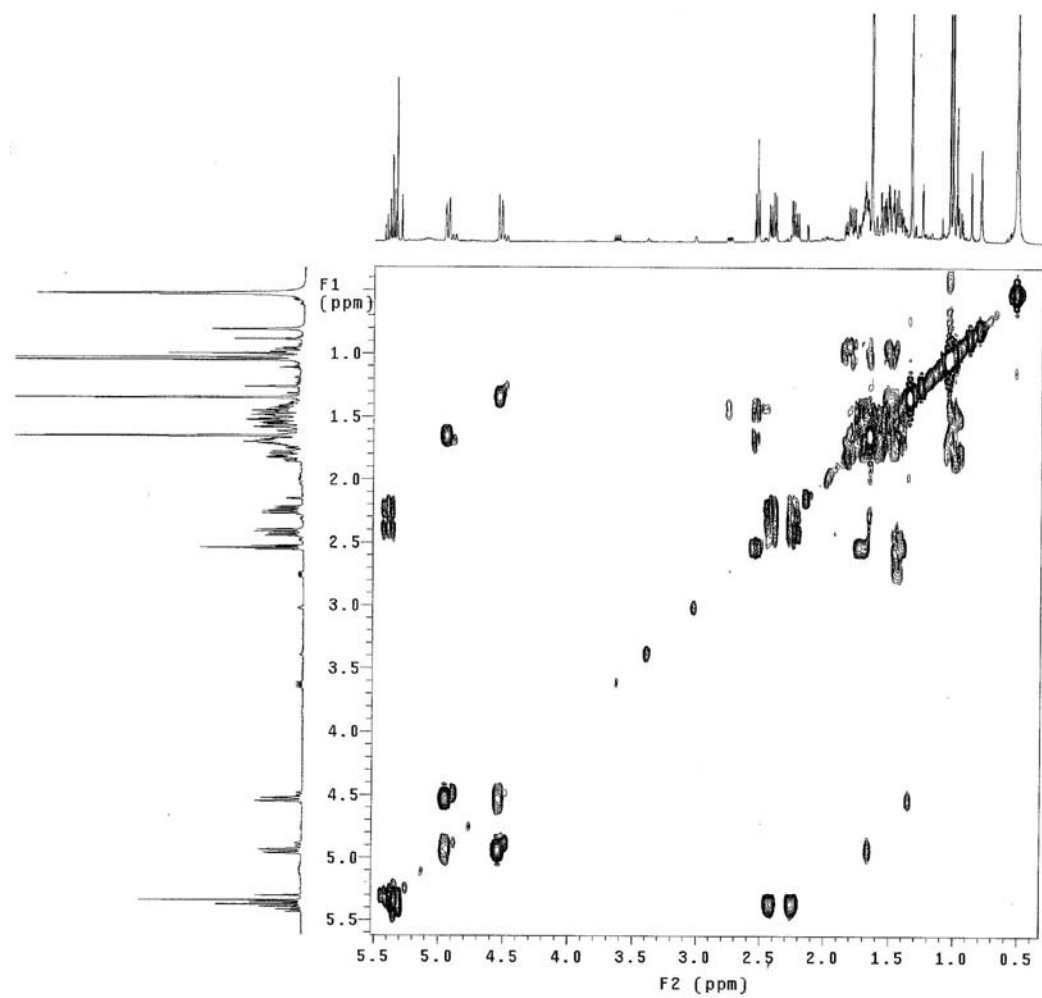


Figure S5.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **1** in  $\text{C}_6\text{D}_6$



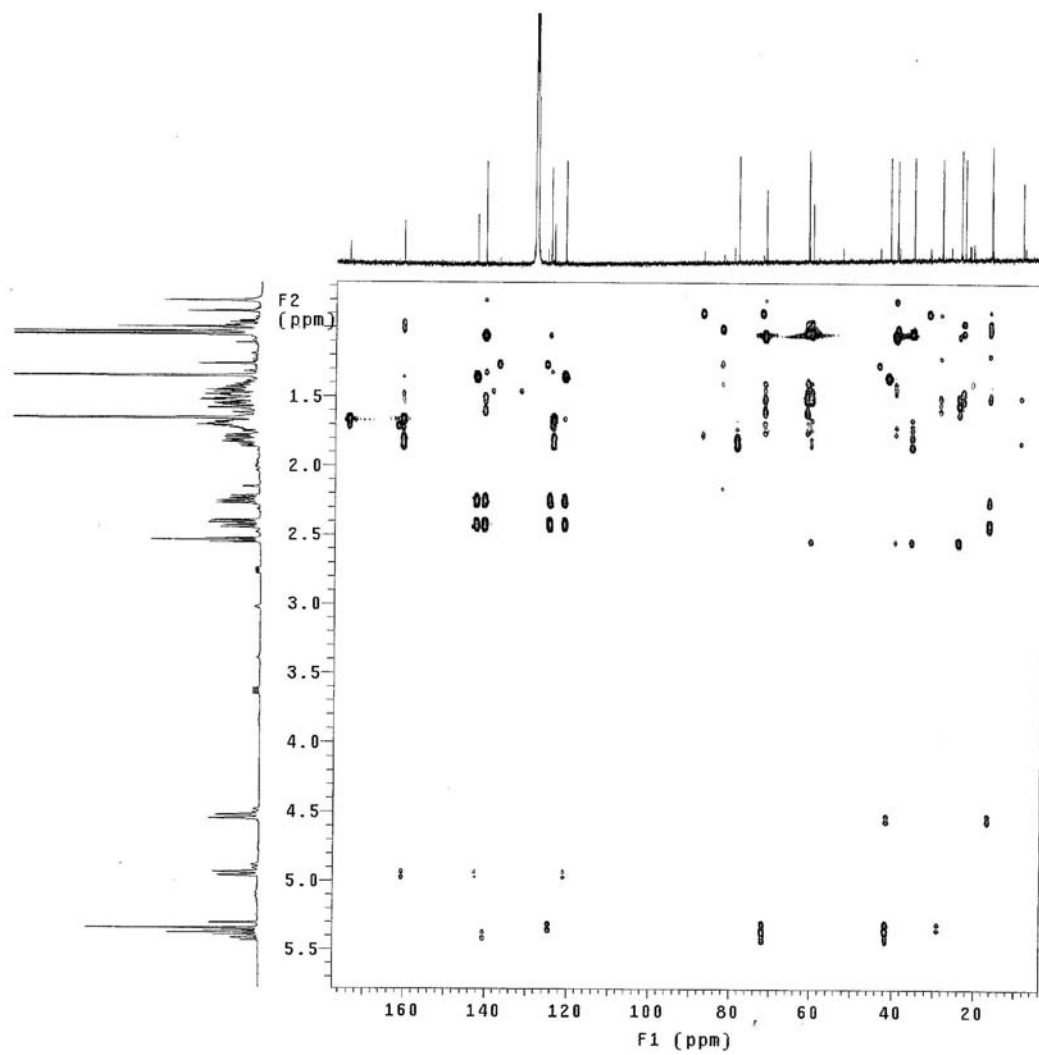


Figure S6. HMBC spectrum of 1 in  $C_6D_6$

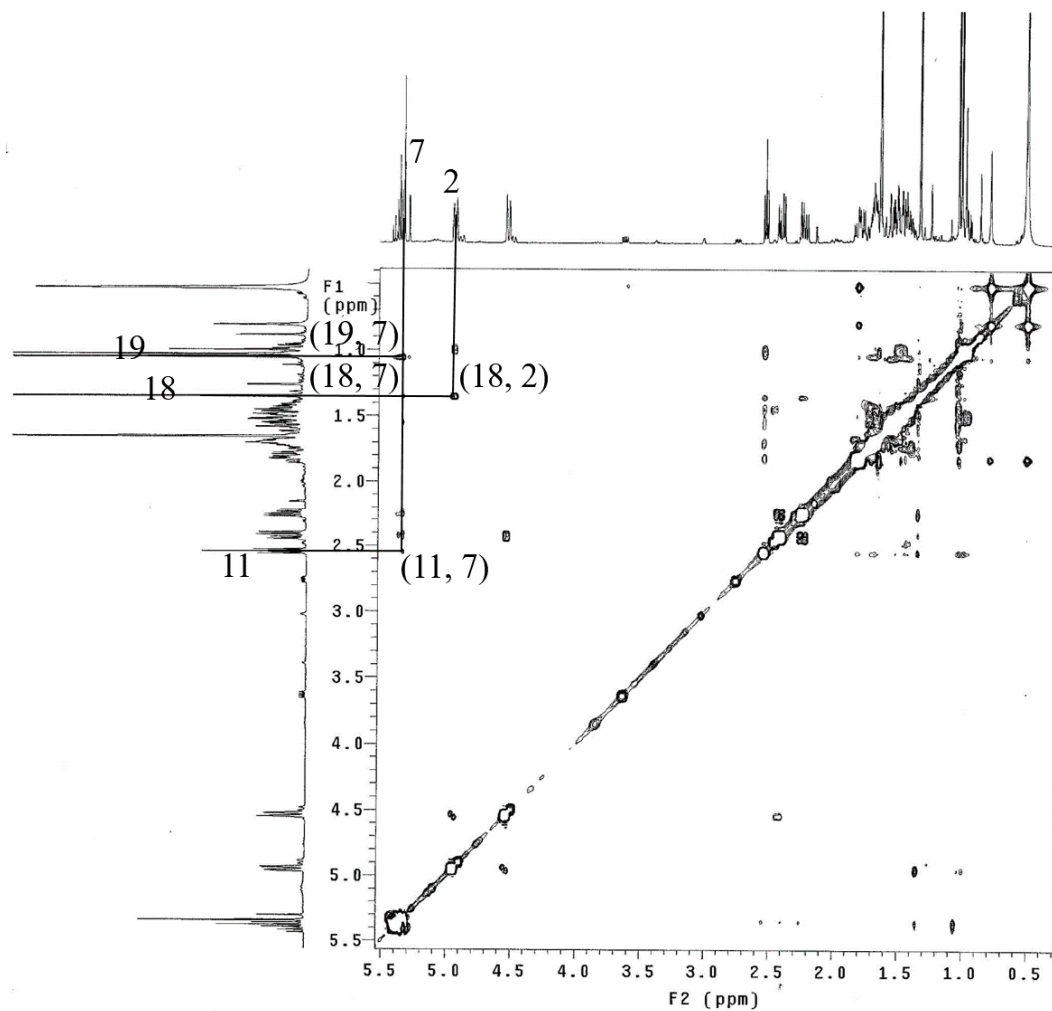
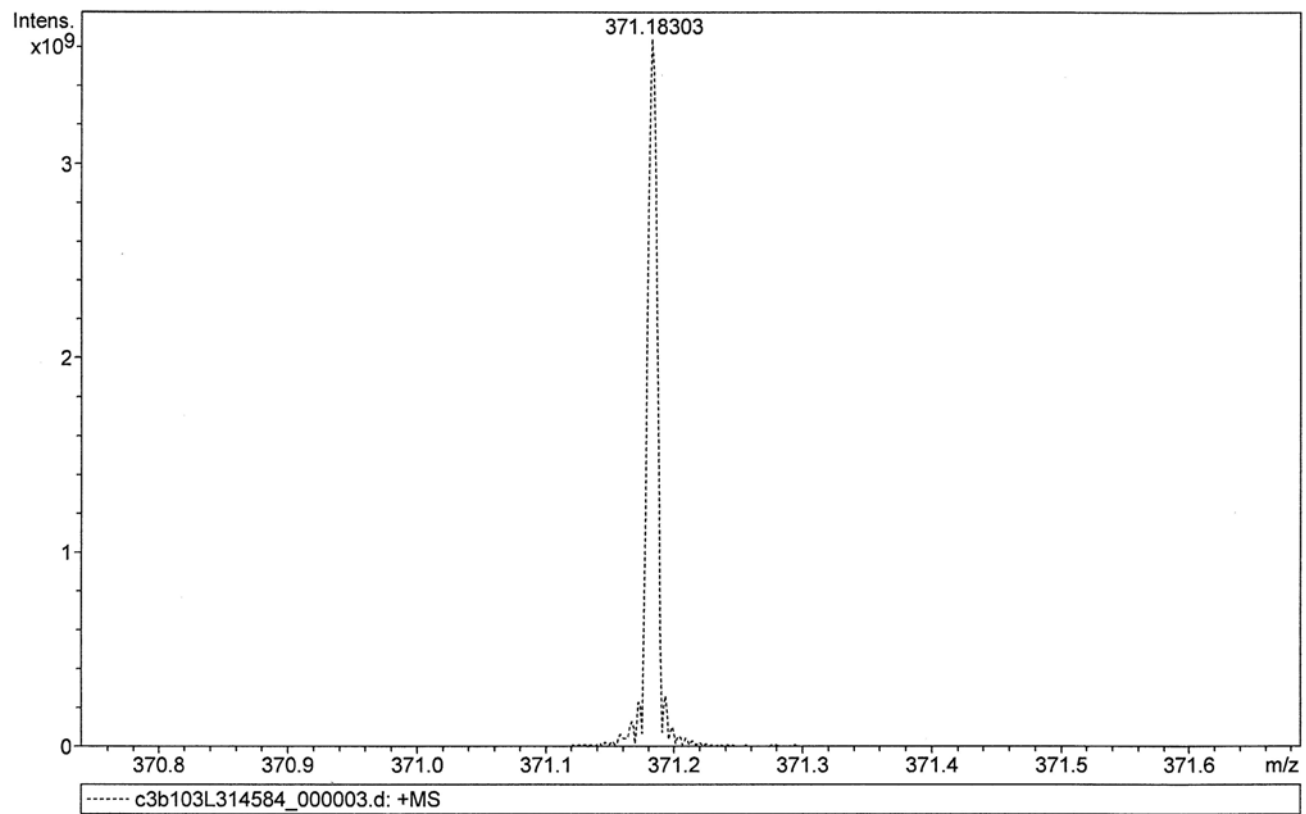


Figure S7. NOESY spectrum of 1 in  $C_6D_6$



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
371.18303	1	C <sub>20</sub> H <sub>28</sub> NaO <sub>5</sub>	100.00	371.18290	-0.14	-0.37	6.9	6.5	even	ok

**Figure S8.** HRESIMS spectrum of **2**

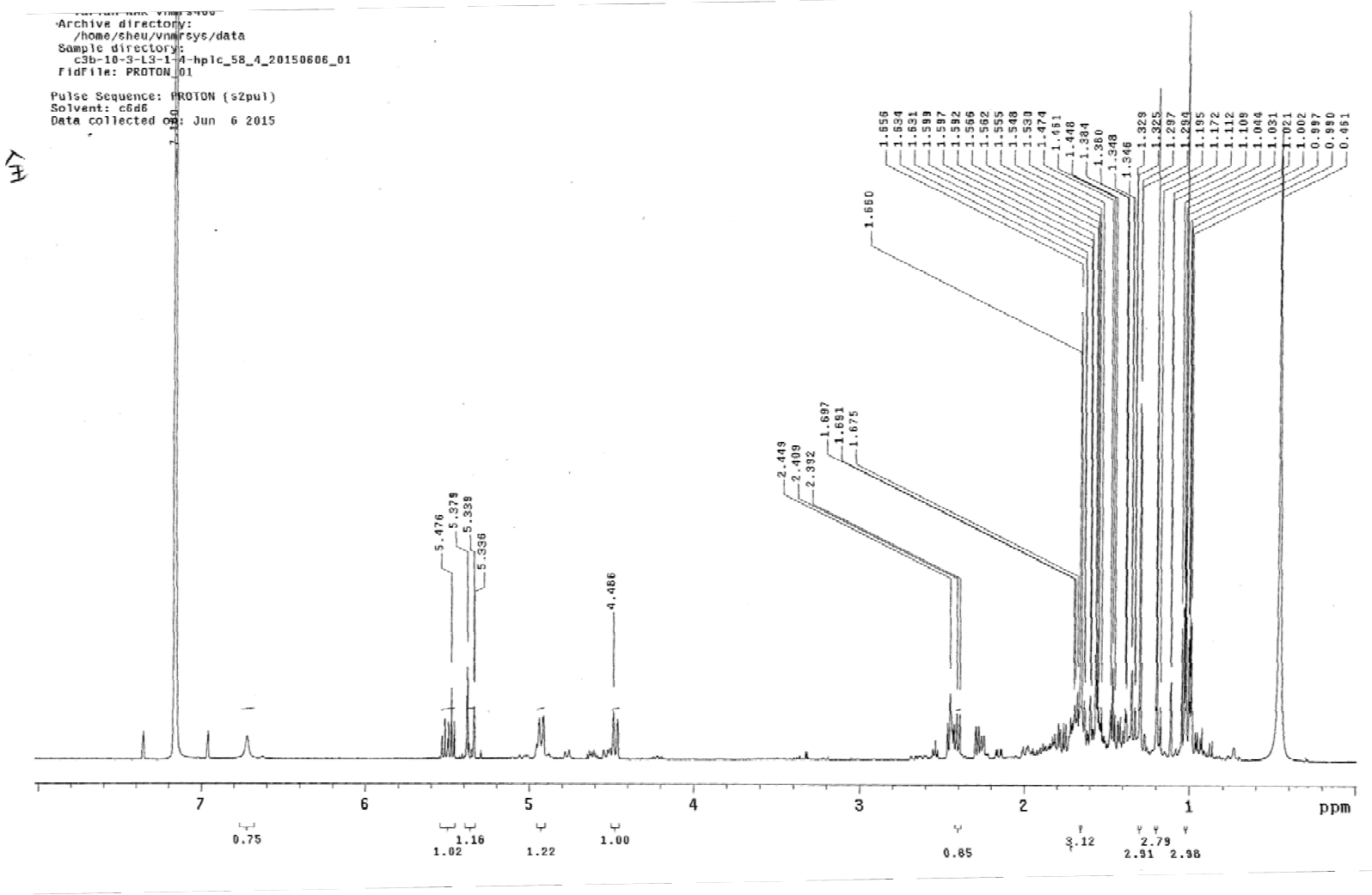


Figure S9. <sup>1</sup>H NMR spectrum of 2 in C<sub>6</sub>D<sub>6</sub>  
S12

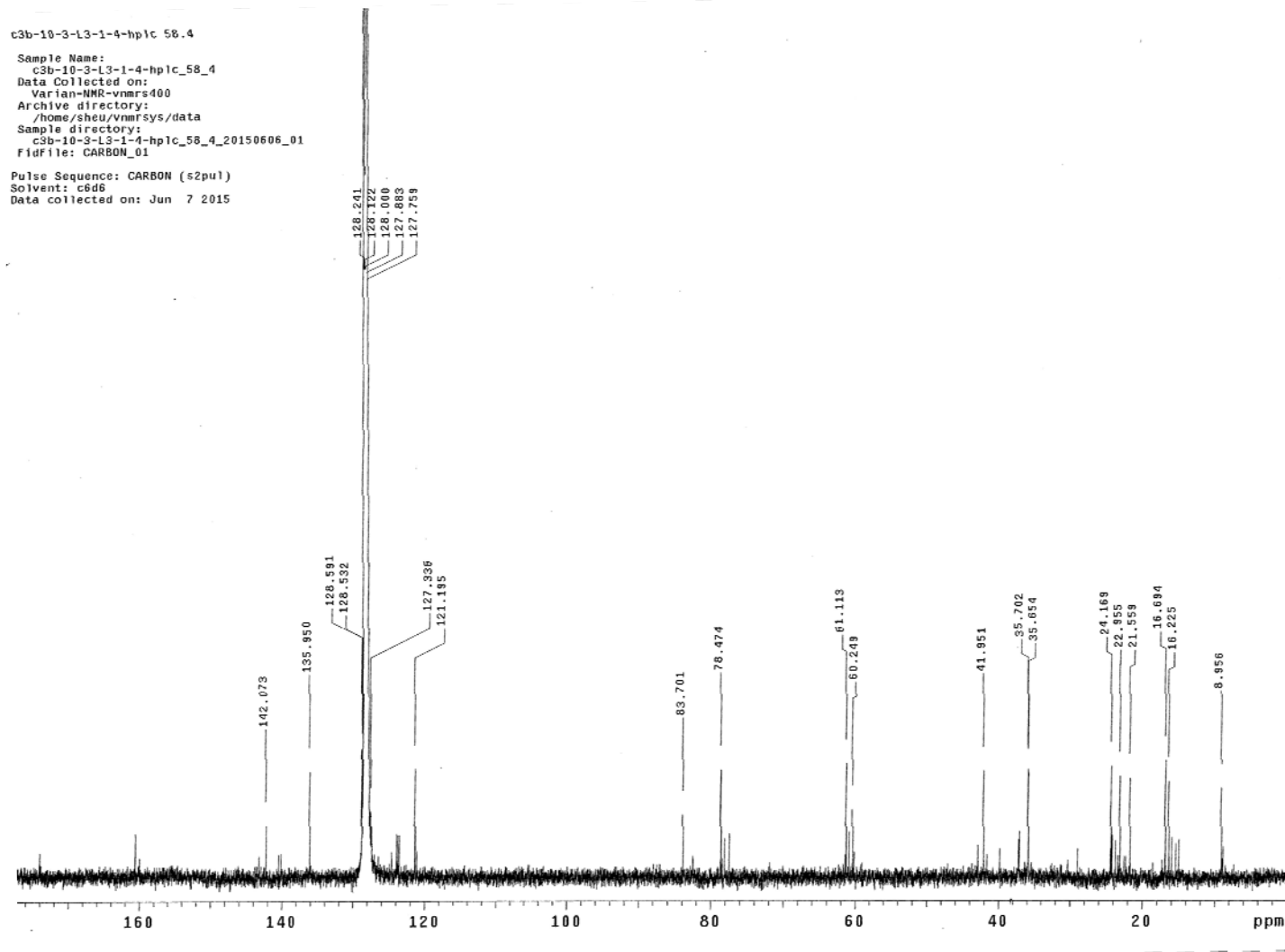


Figure S10.  $^{13}\text{C}$  NMR spectrum of **2** in  $\text{C}_6\text{D}_6$   
S13

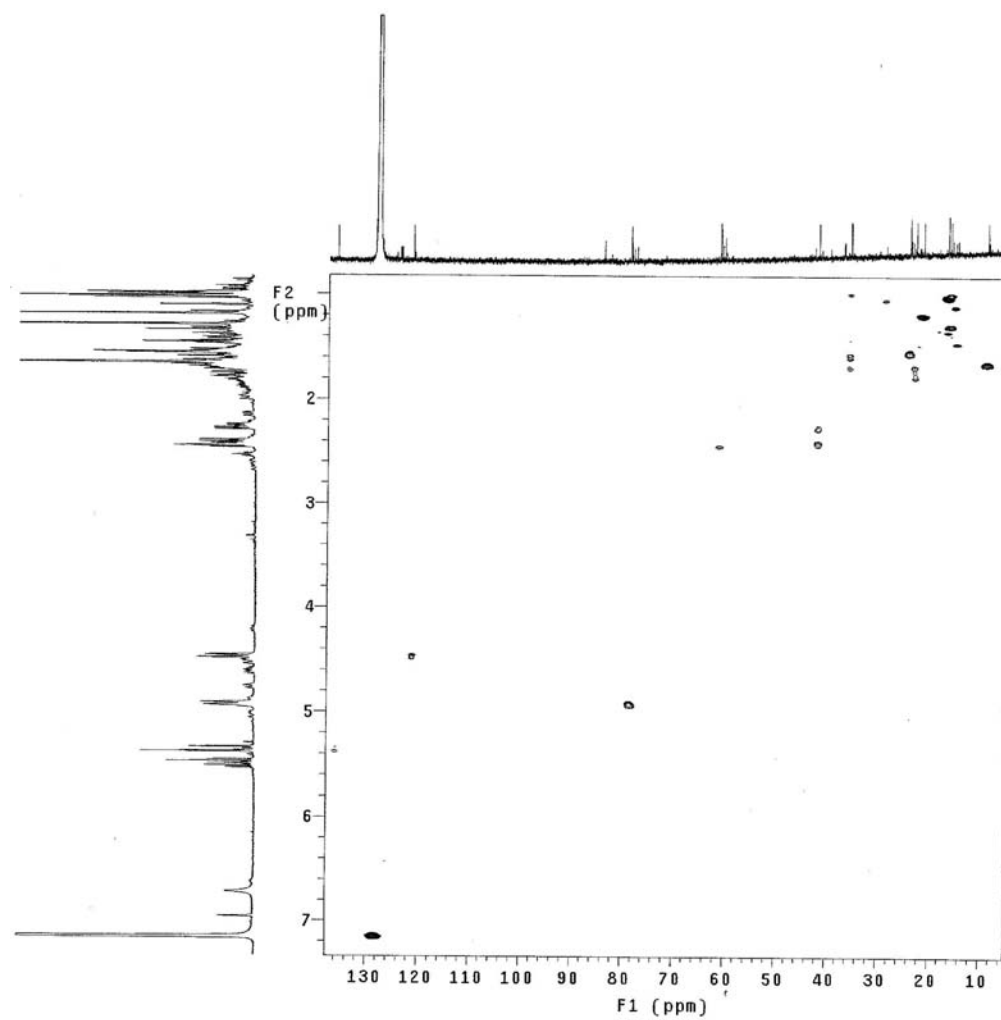


Figure S11. HSQC spectrum of **2** in  $\text{C}_6\text{D}_6$

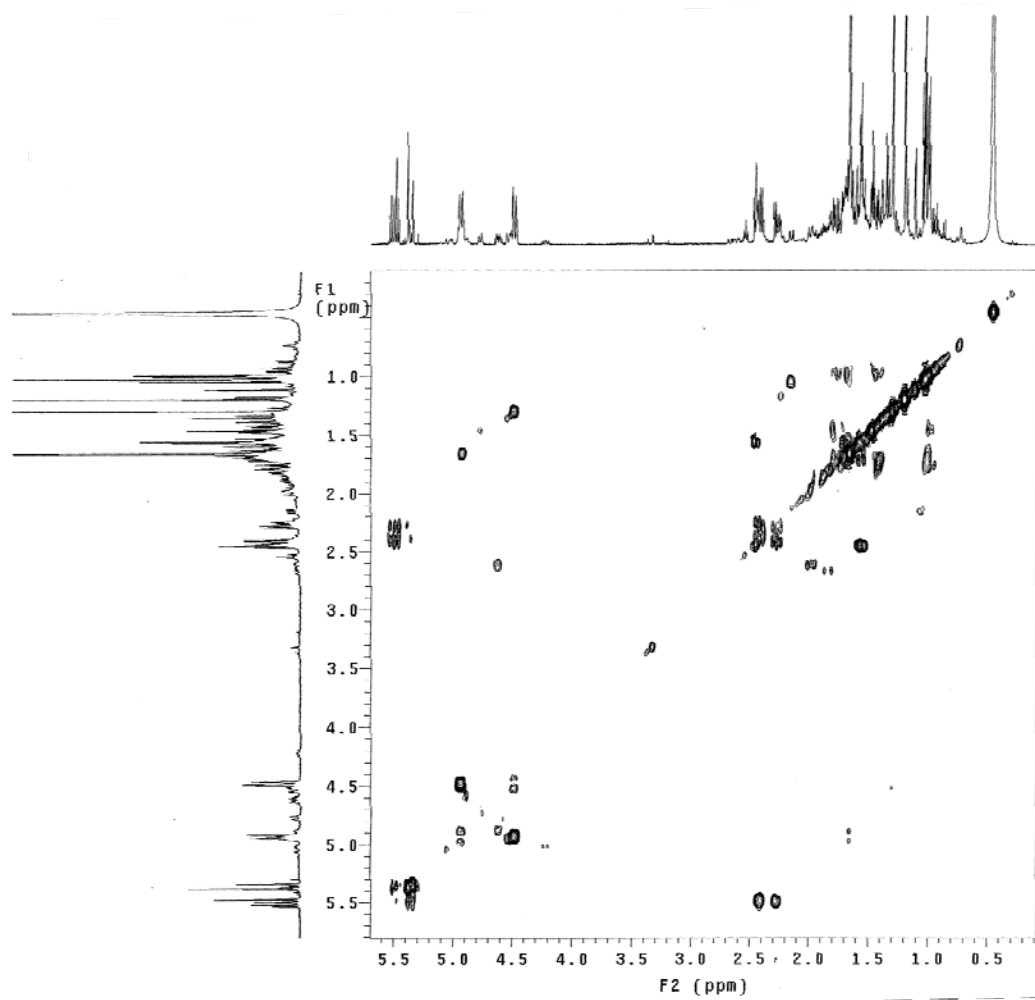


Figure S12.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **2** in  $\text{C}_6\text{D}_6$

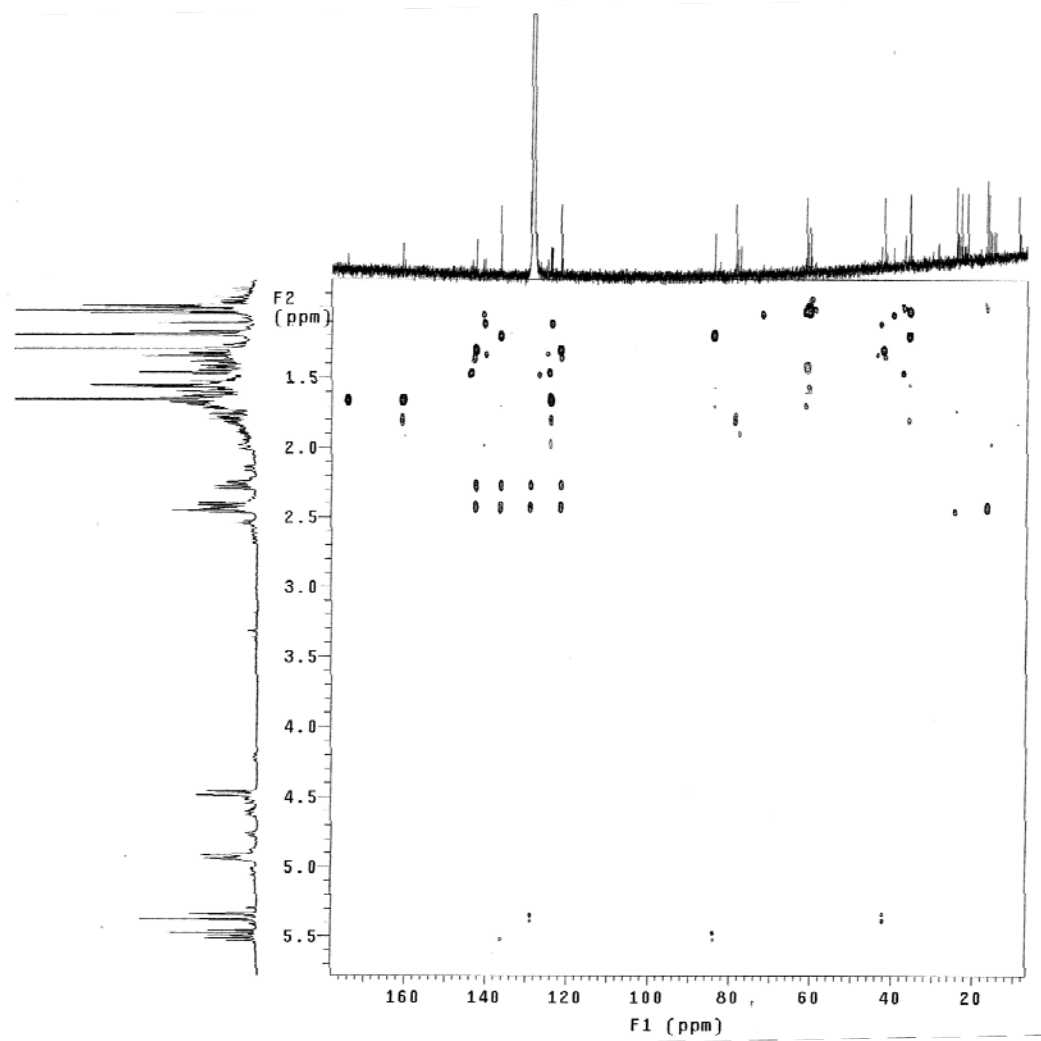


Figure S13. HMBC spectrum of 2 in  $C_6D_6$



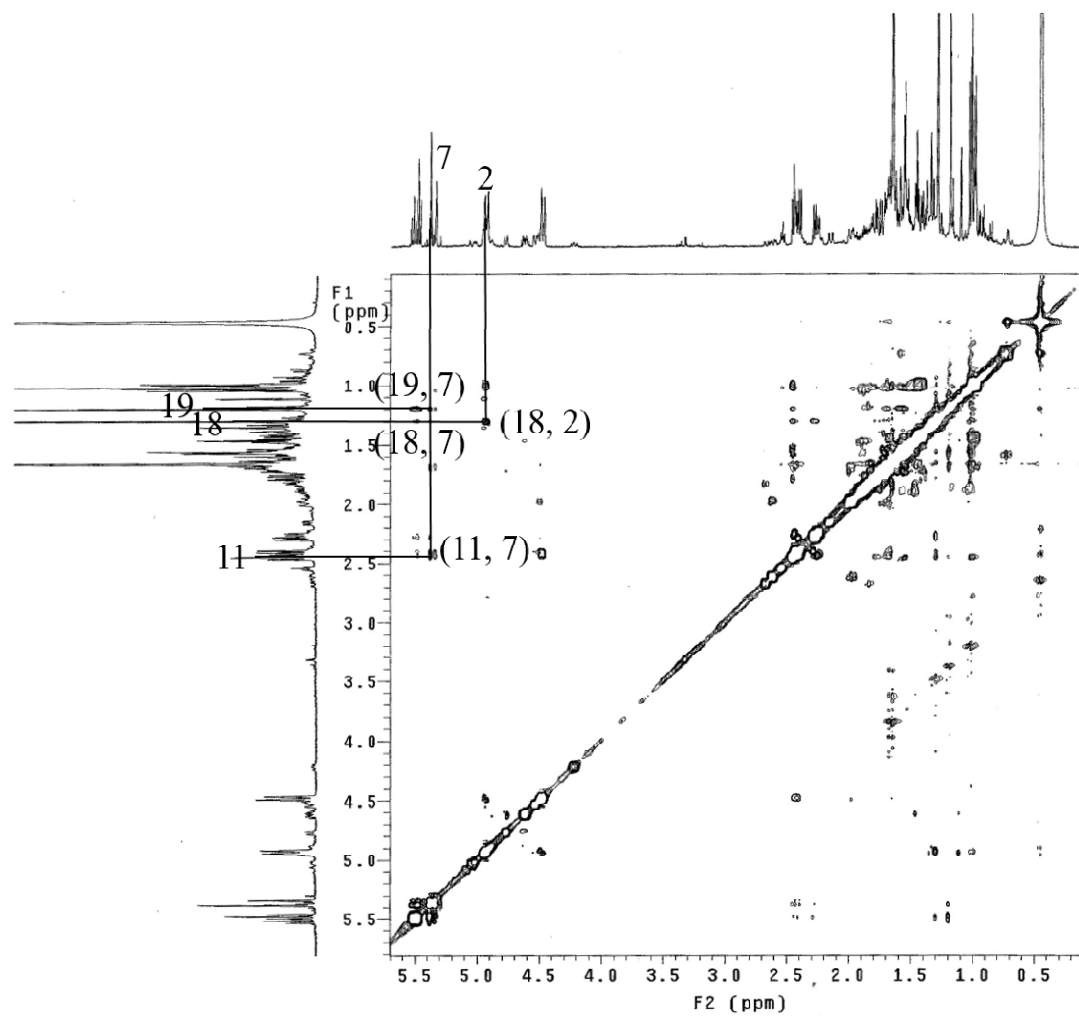
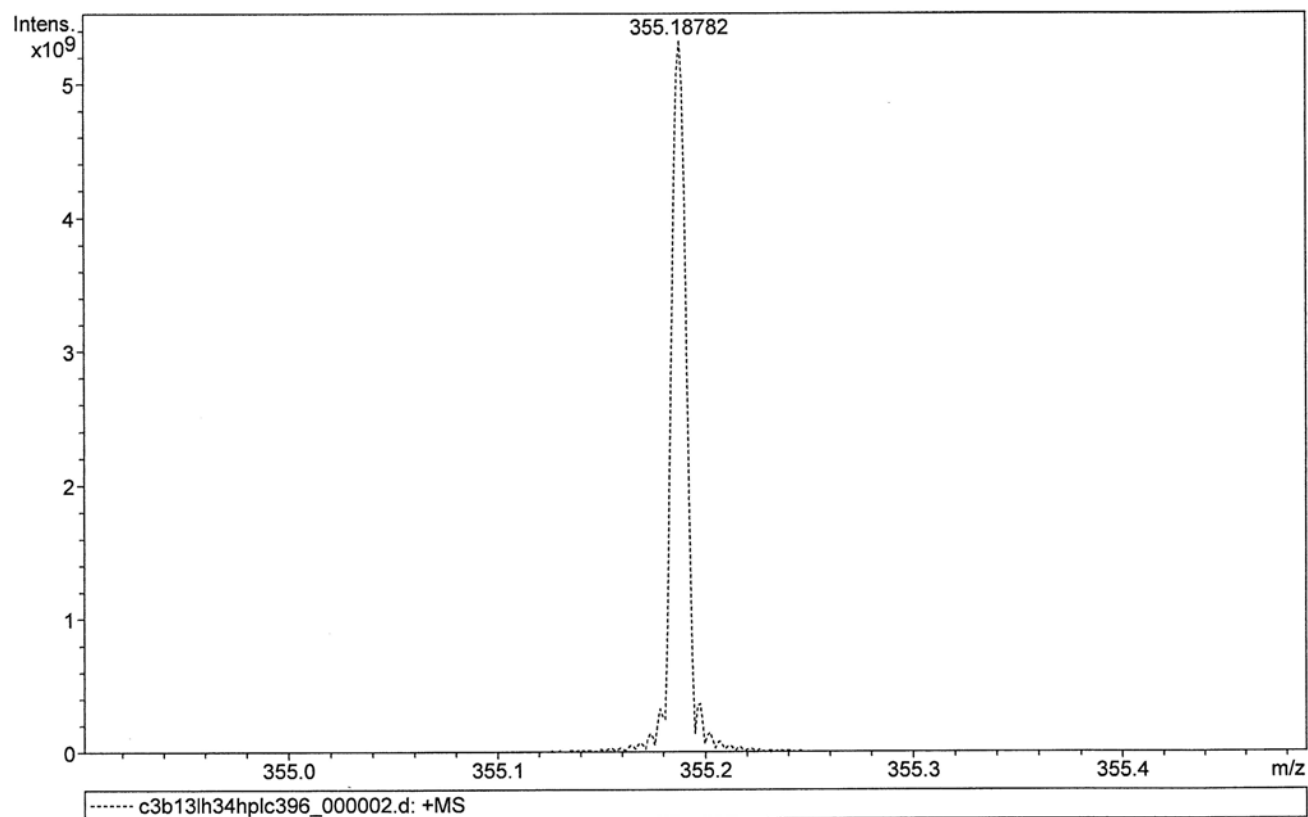


Figure S14. NOESY spectrum of 2 in  $C_6D_6$



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup>	Conf	N-Rule
355.18782	1	C <sub>20</sub> H <sub>28</sub> NaO <sub>4</sub>	100.00	355.18798	0.16	0.45	14.0	6.5	even		ok

**Figure S15.** HRESIMS spectrum of **3**

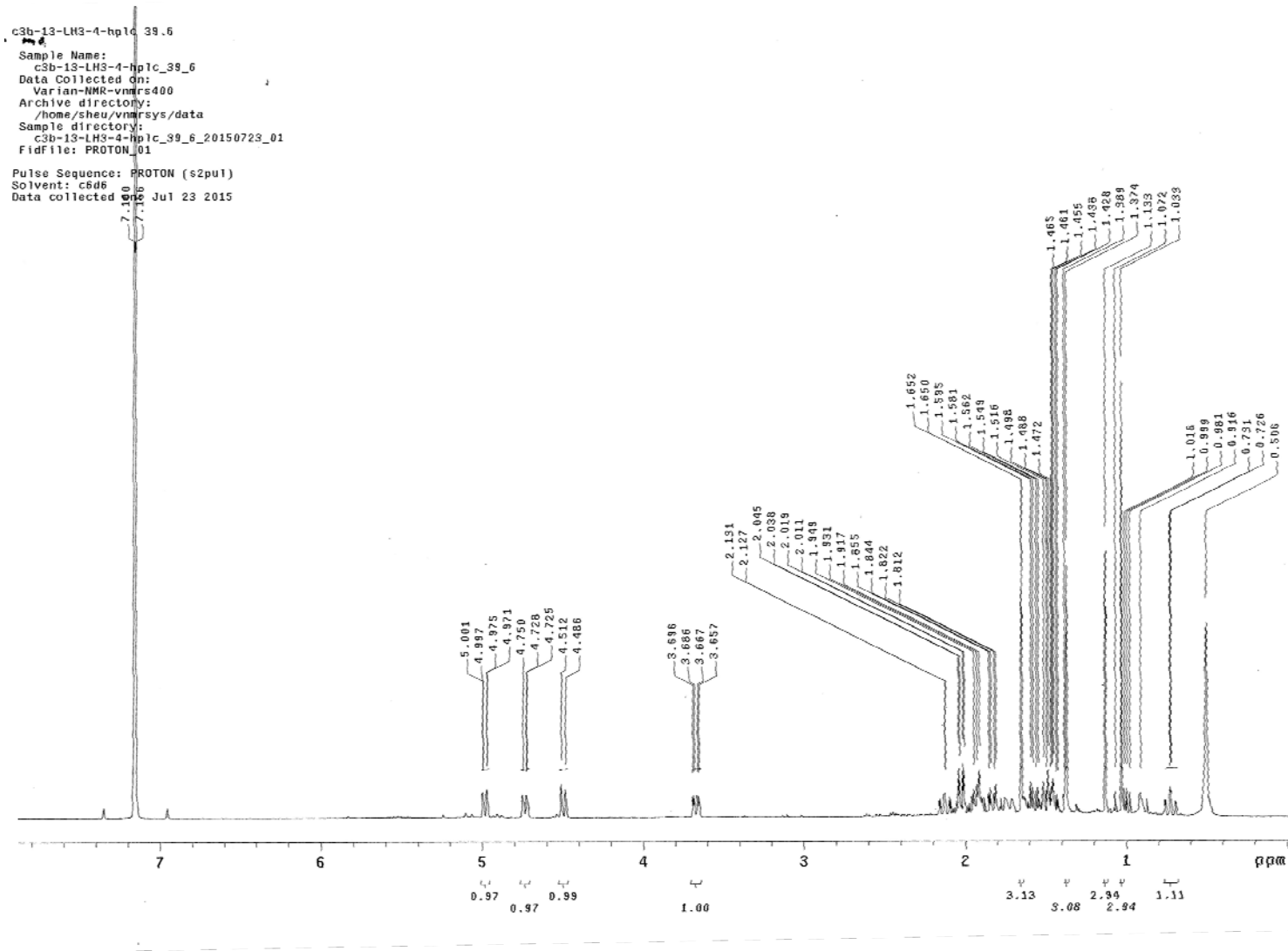


Figure S16.  $^1\text{H}$  NMR spectrum of **3** in  $\text{C}_6\text{D}_6$   
 S19

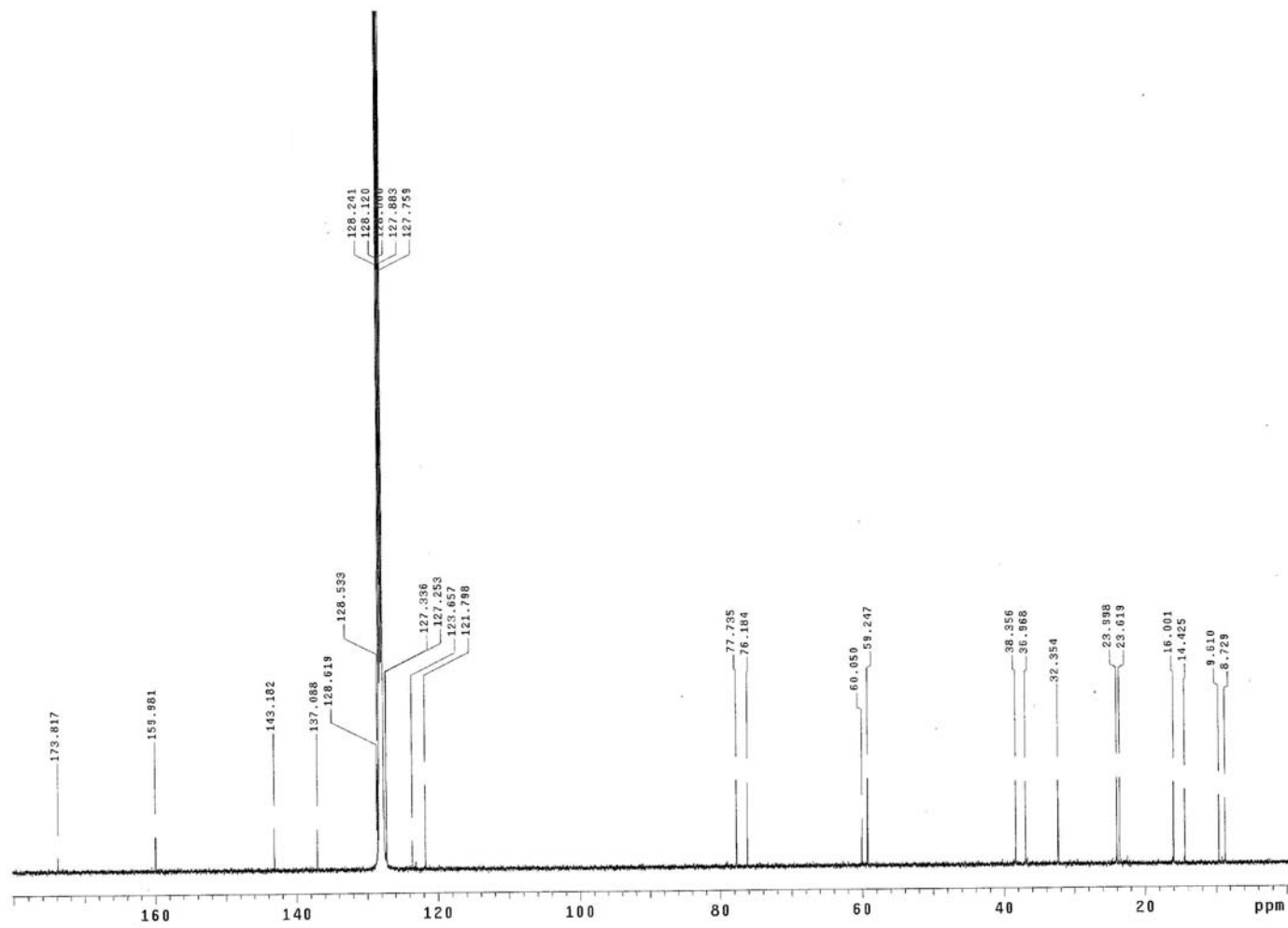


Figure S17.  $^{13}\text{C}$  NMR spectrum of 3 in  $\text{C}_6\text{D}_6$

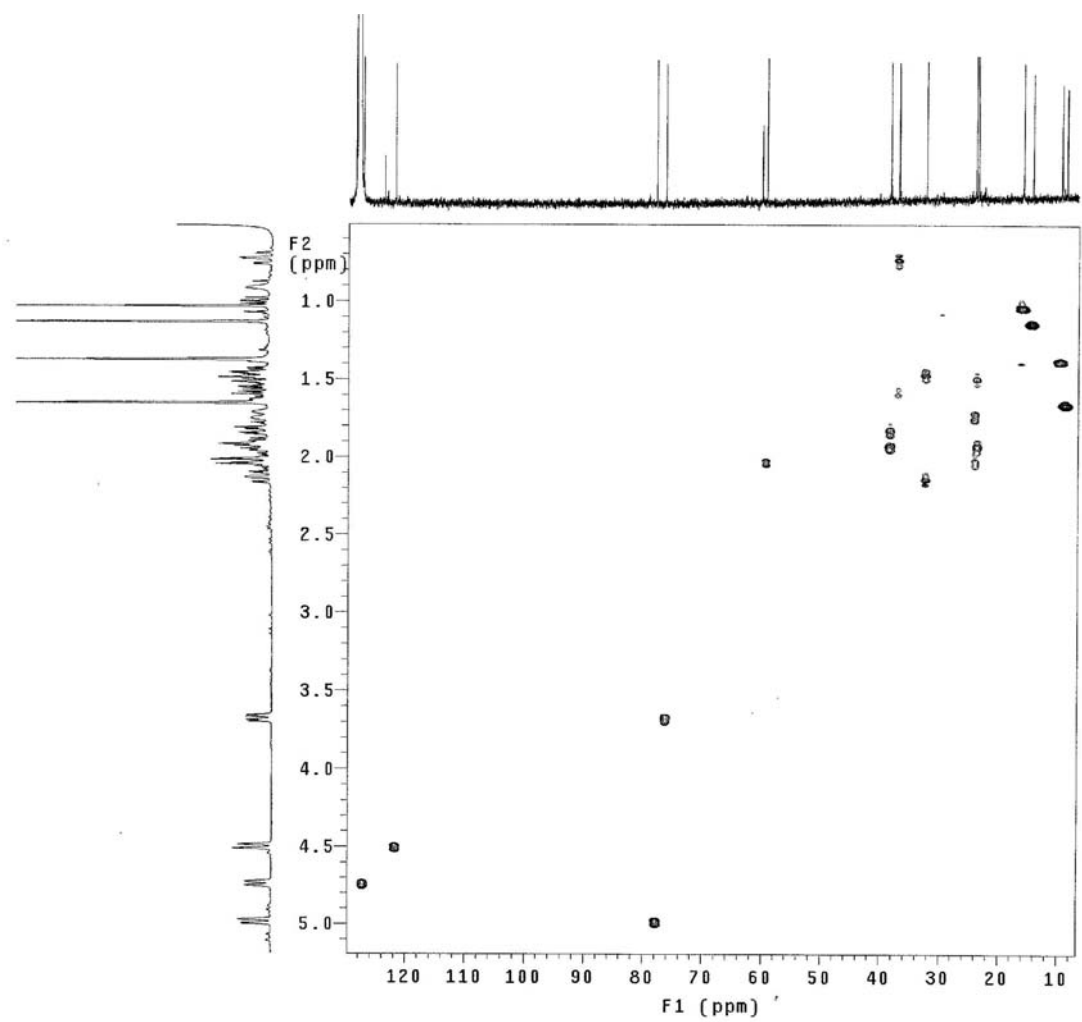


Figure S18. HSQC spectrum of 3 in  $C_6D_6$

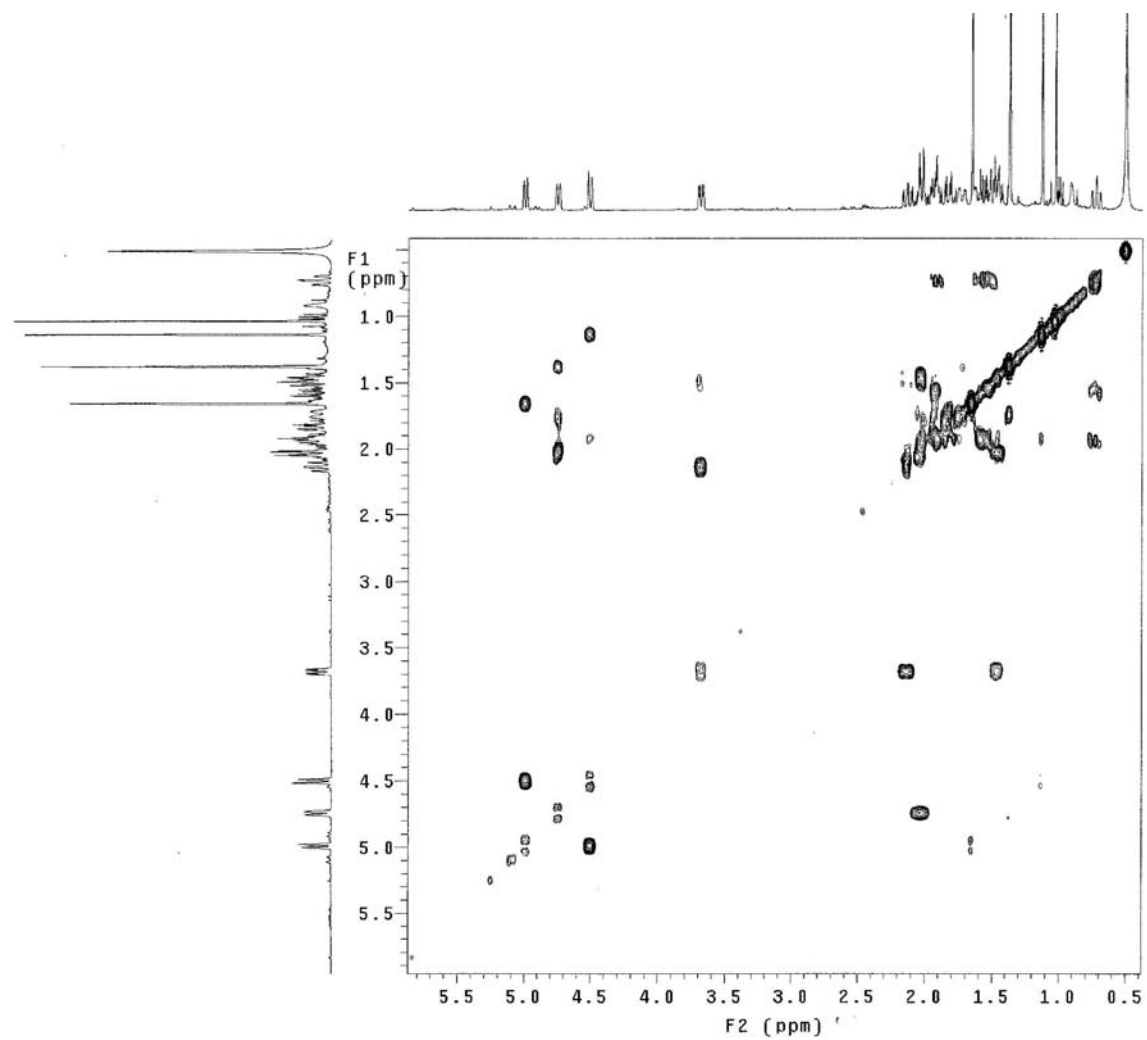


Figure S19.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **3** in  $\text{C}_6\text{D}_6$

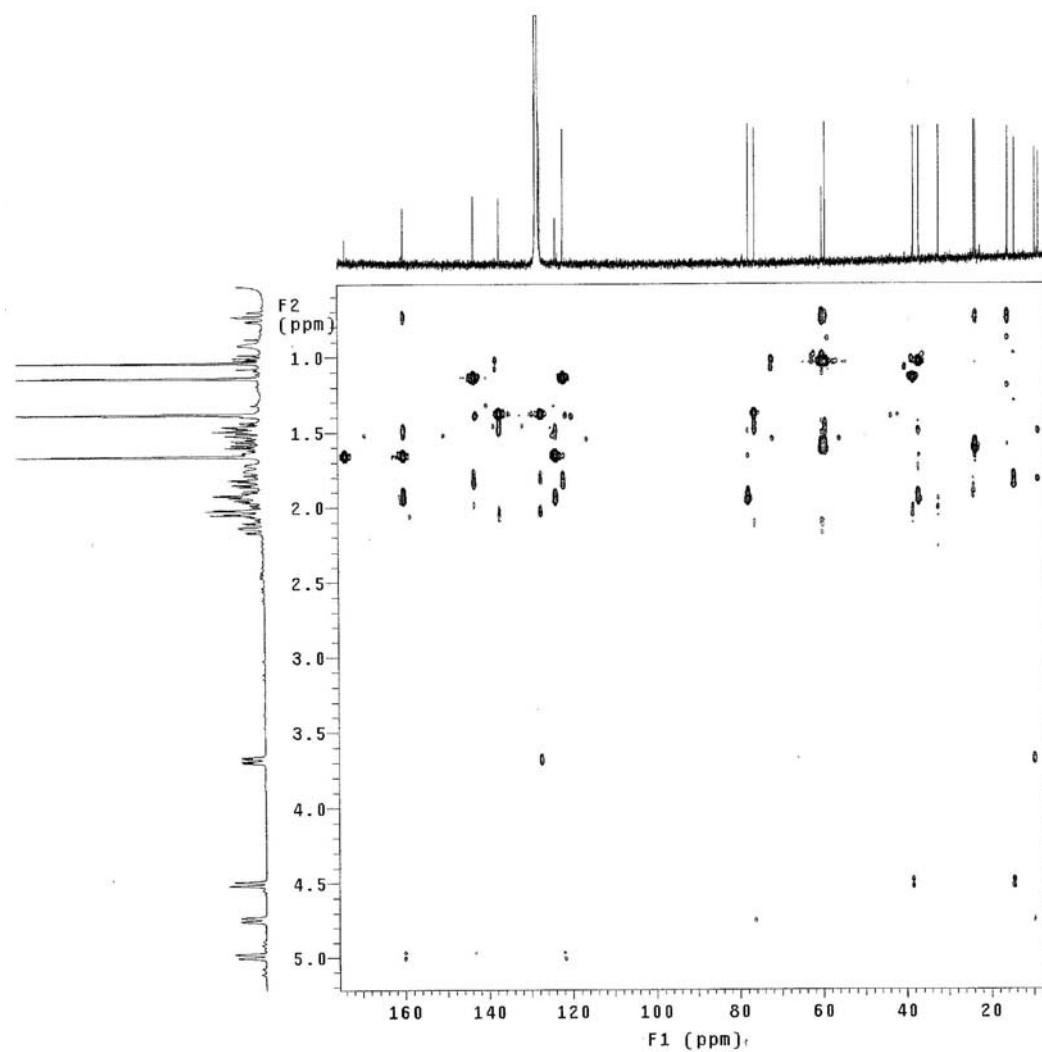


Figure S20. HMBC spectrum of 3 in  $C_6D_6$

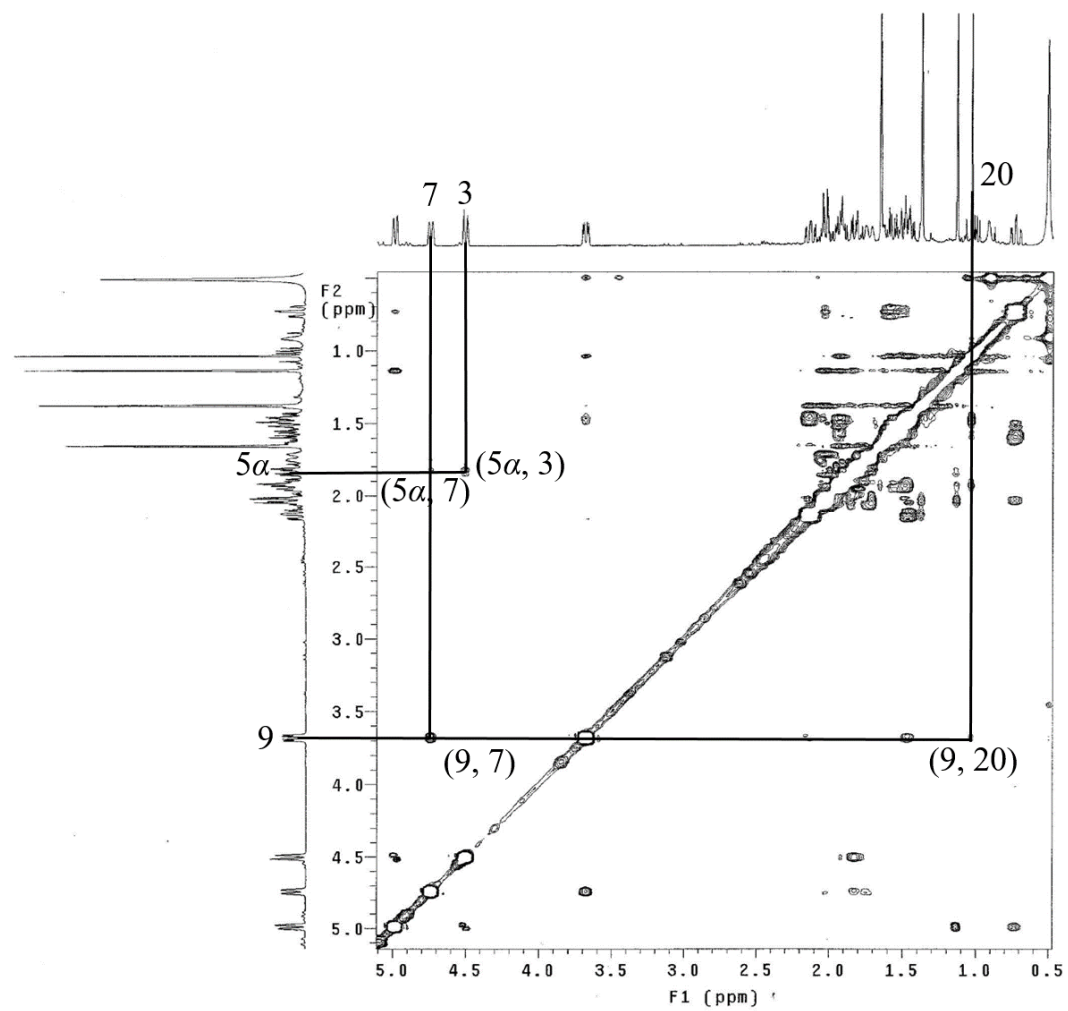


Figure S21. NOESY spectrum of 3 in  $C_6D_6$



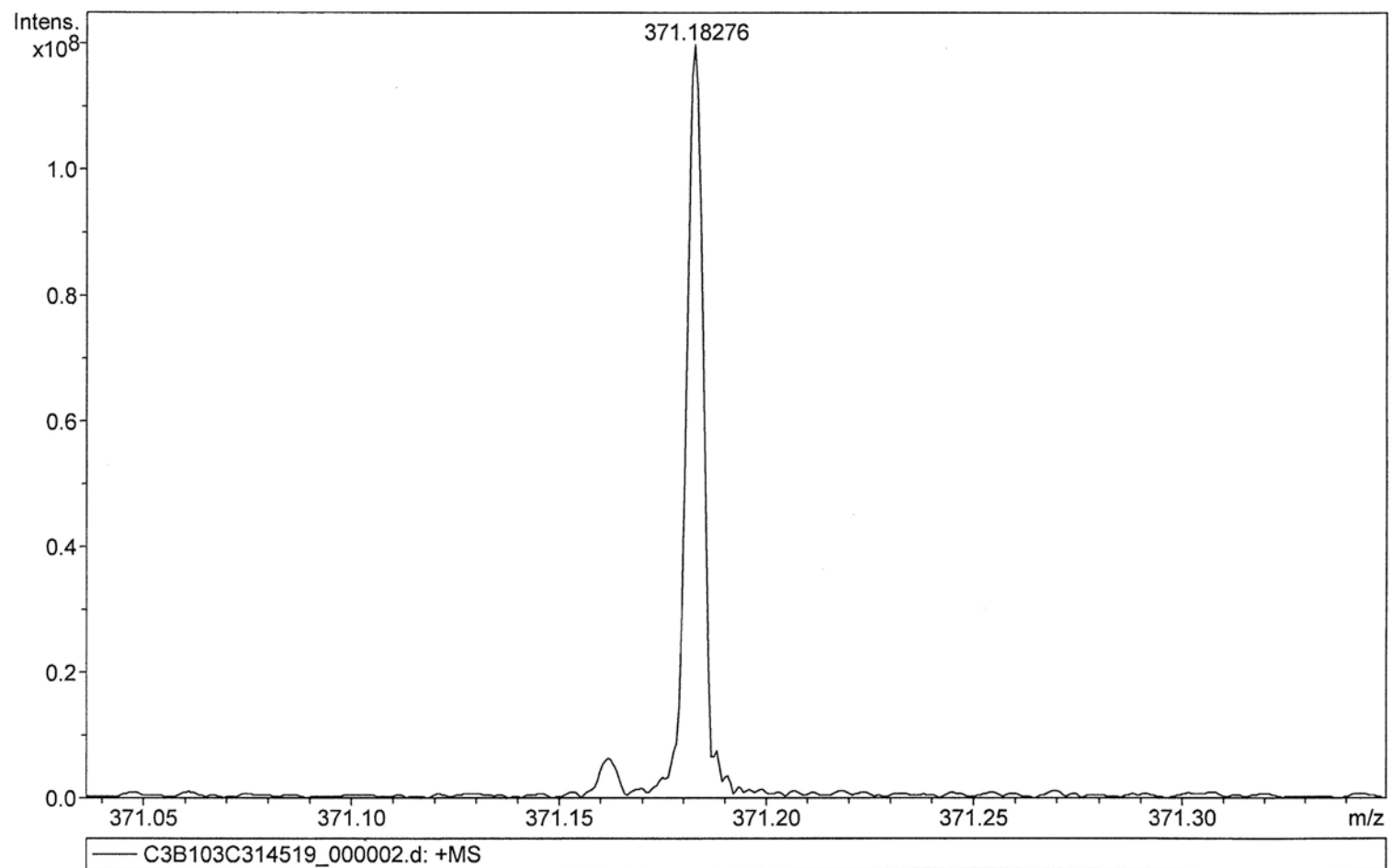
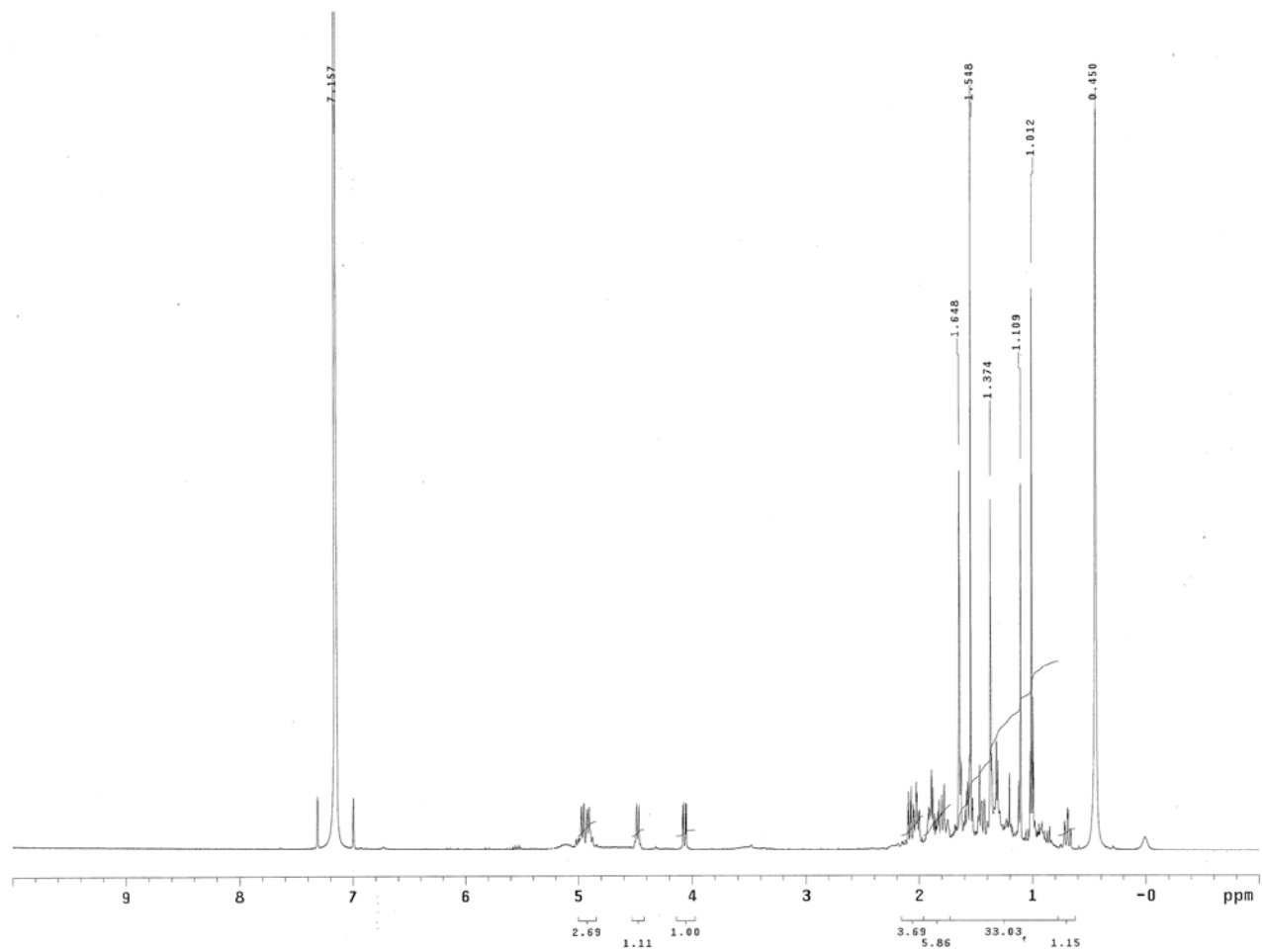


Figure S22. HREIMS spectrum of 4



**Figure S23.**  $^1\text{H}$  NMR spectrum of **4** in  $\text{C}_6\text{D}_6$

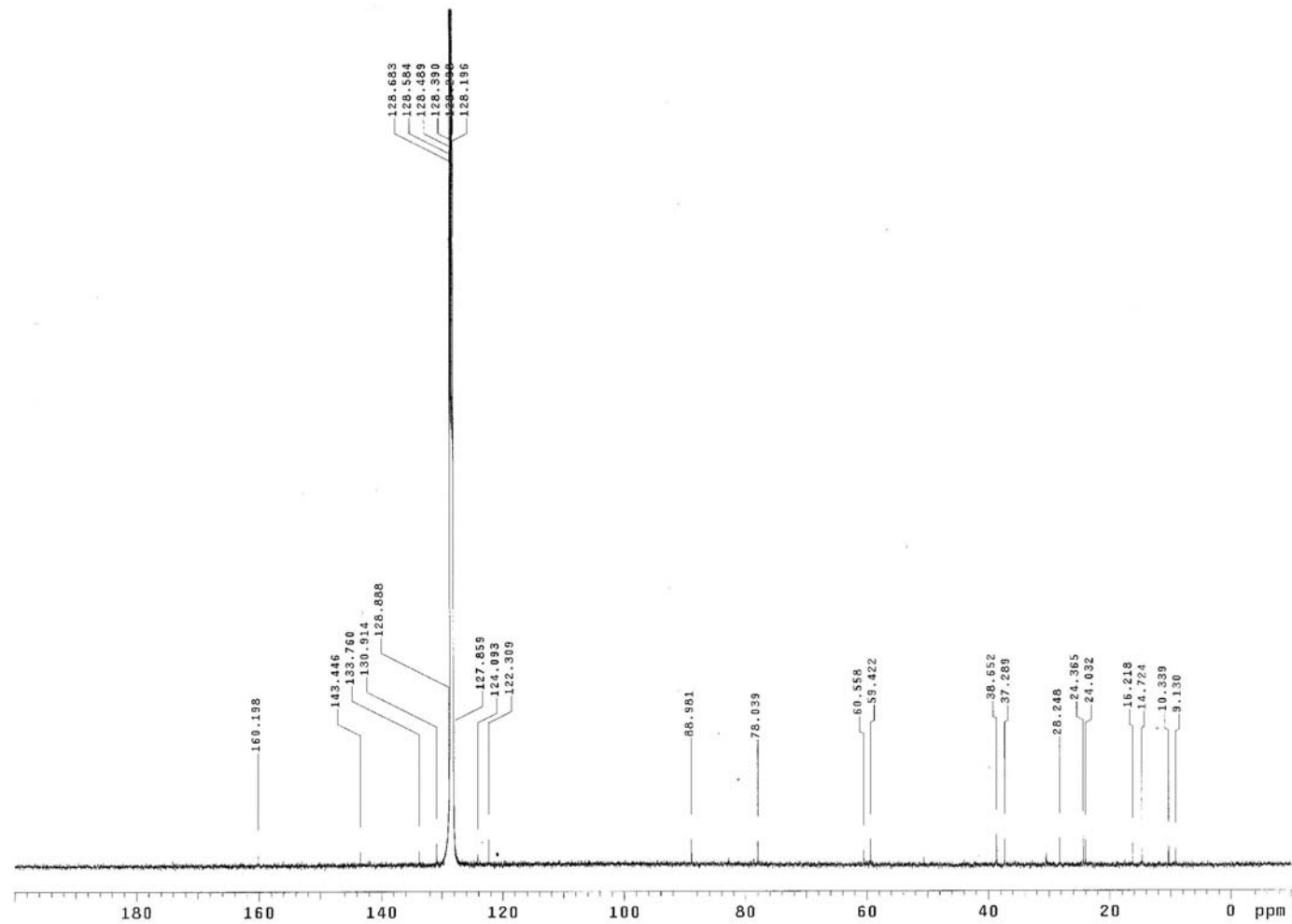


Figure S24.  $^{13}\text{C}$  NMR spectrum of **4** in  $\text{C}_6\text{D}_6$

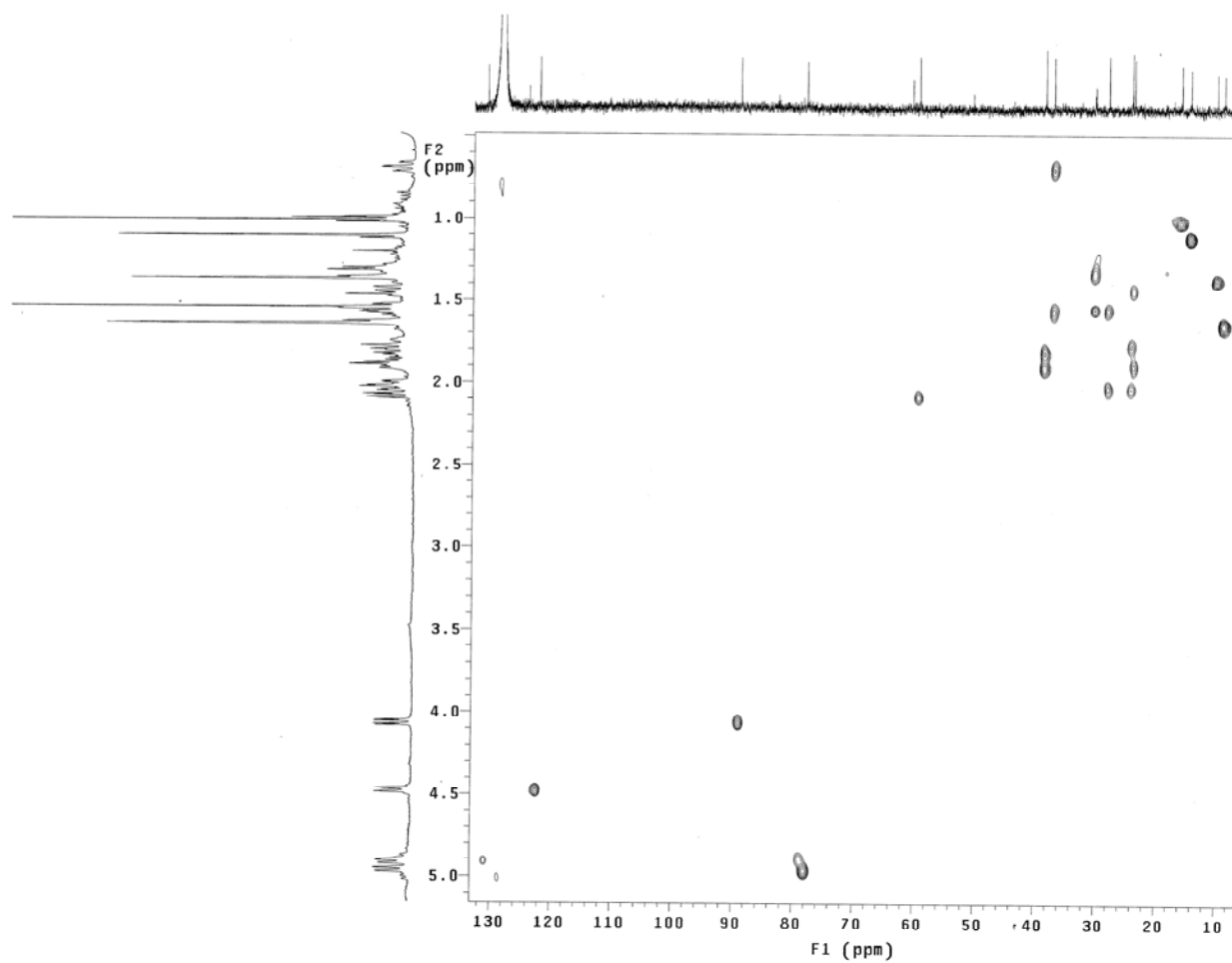


Figure S25. HSQC spectrum of **4** in  $\text{C}_6\text{D}_6$

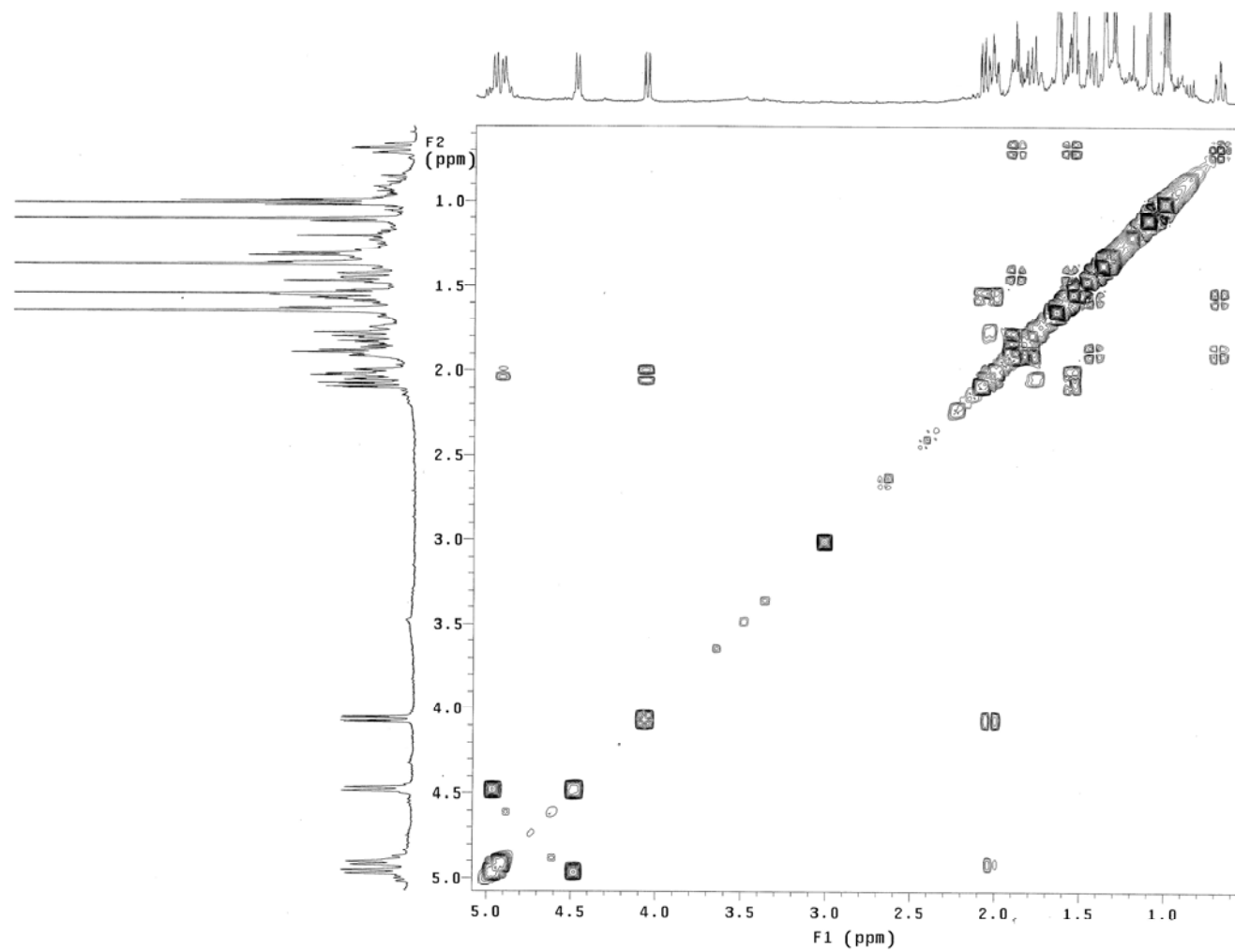


Figure S26.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **4** in  $\text{C}_6\text{D}_6$

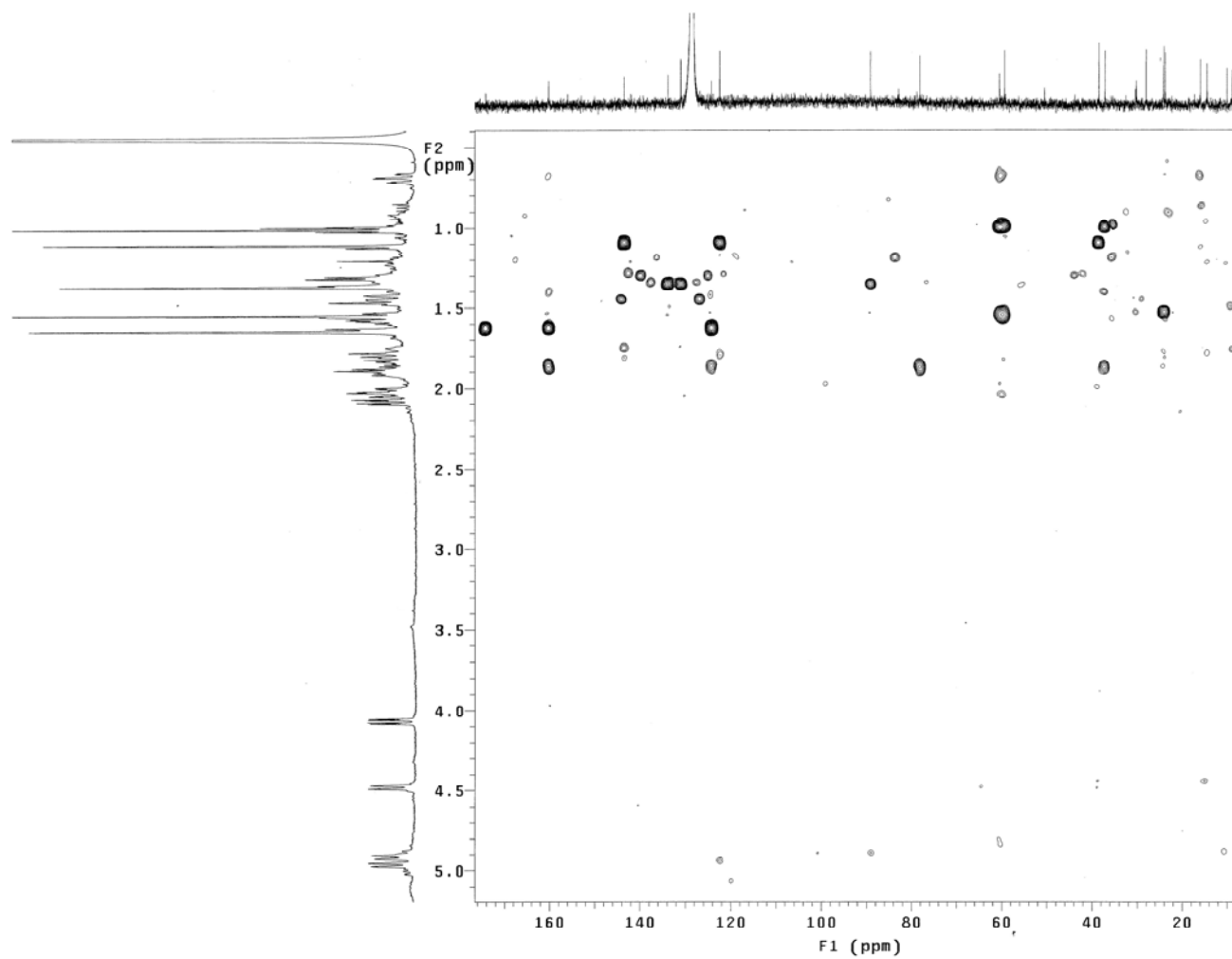


Figure S27. HMBC spectrum of **4** in C<sub>6</sub>D<sub>6</sub>

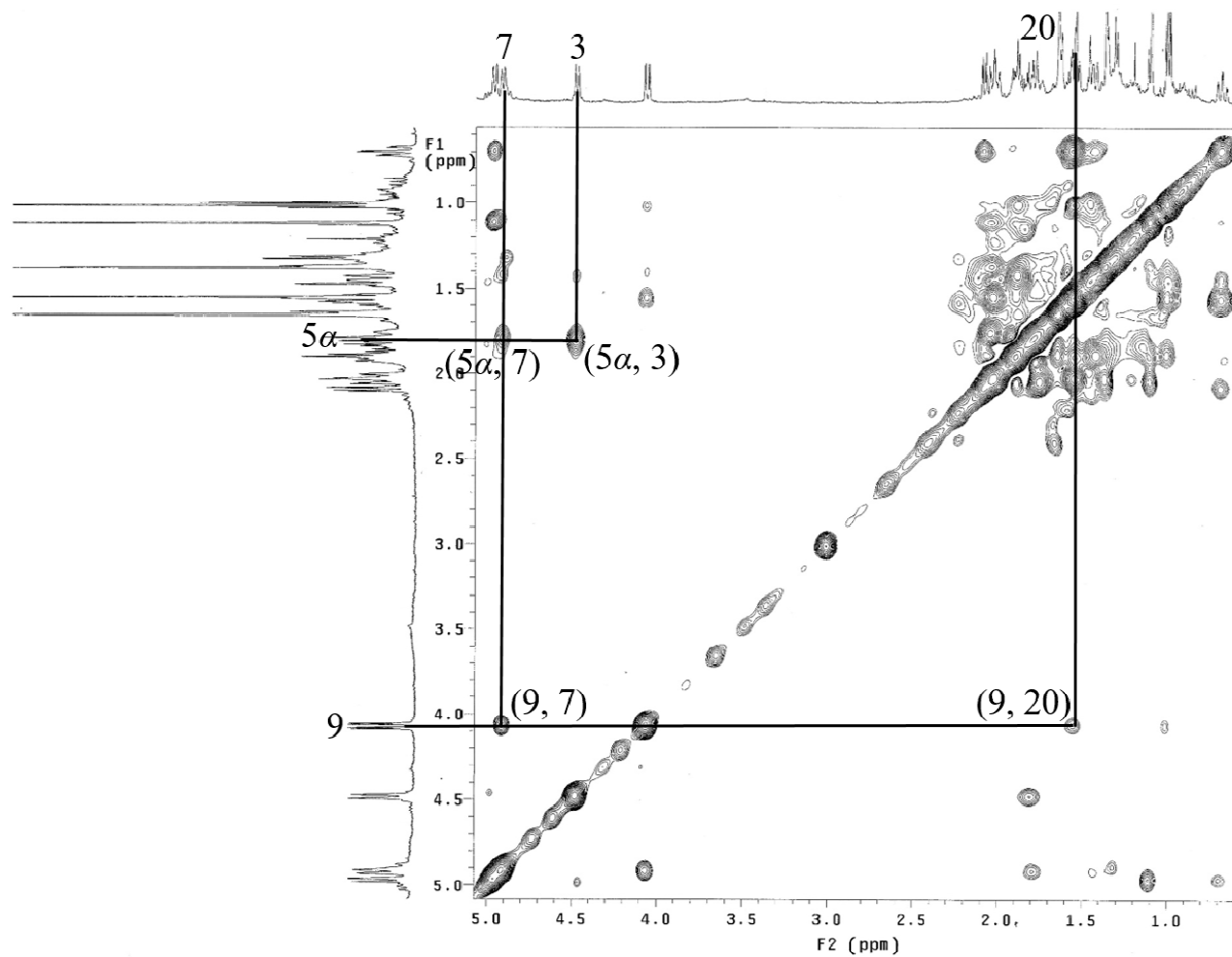
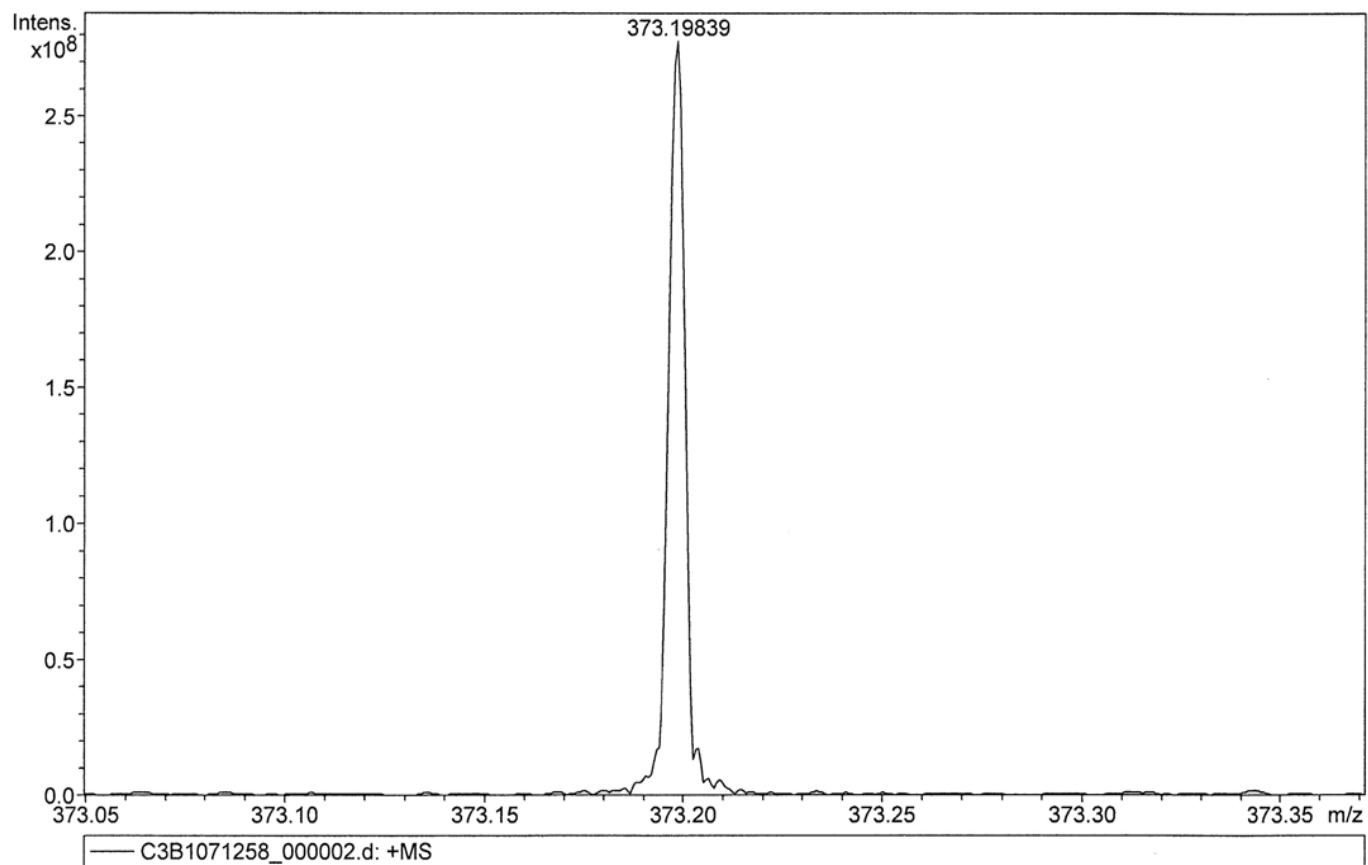


Figure S28. NOESY spectrum of 4 in  $C_6D_6$



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
373.19839	1	C <sub>20</sub> H <sub>30</sub> NaO <sub>5</sub>	100.00	373.19855	0.16	0.43	7.9	5.5	even	ok

Figure S29. HREIMS spectrum of 5



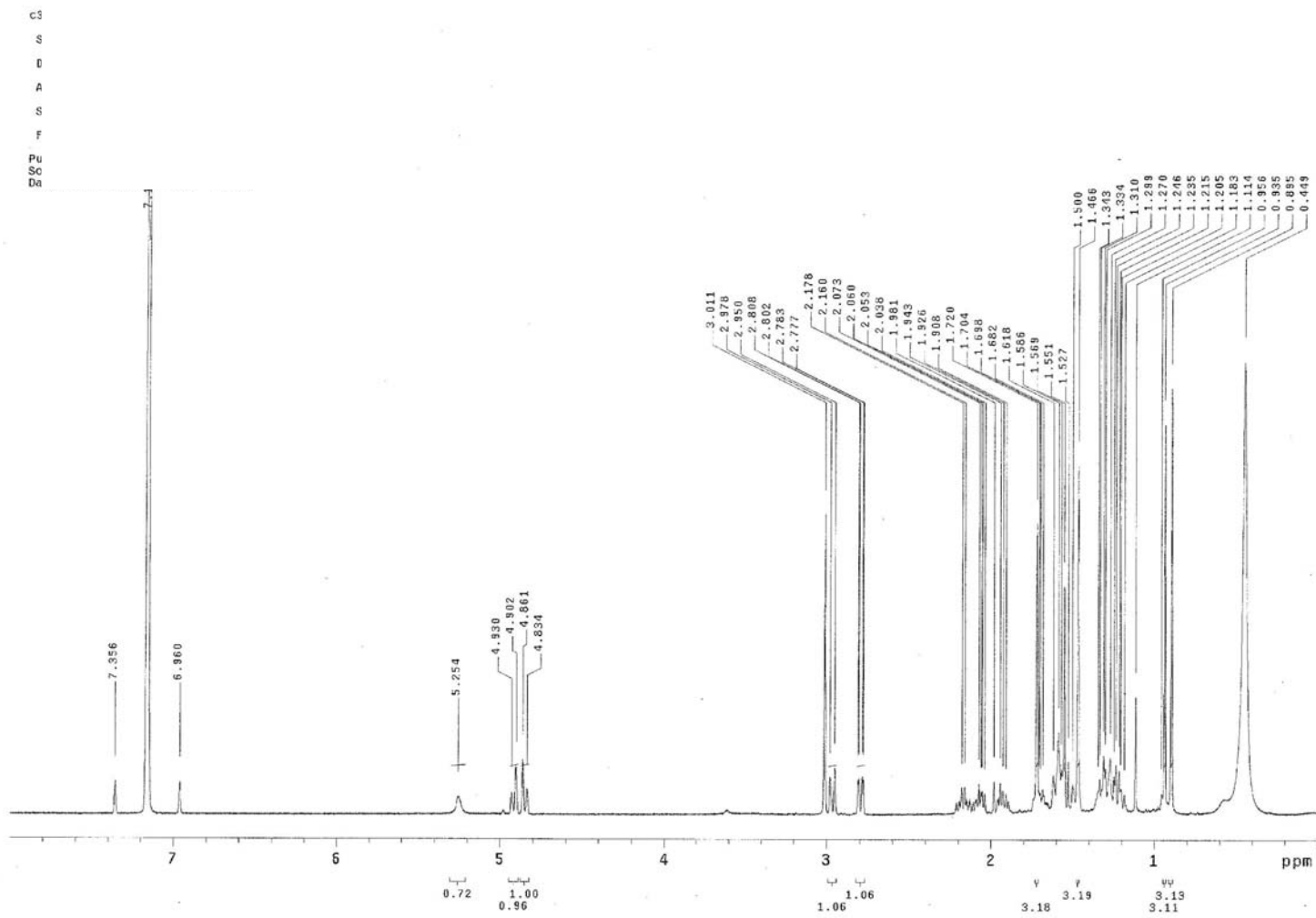


Figure S30.  $^1\text{H}$  NMR spectrum of **5** in  $\text{C}_6\text{D}_6$

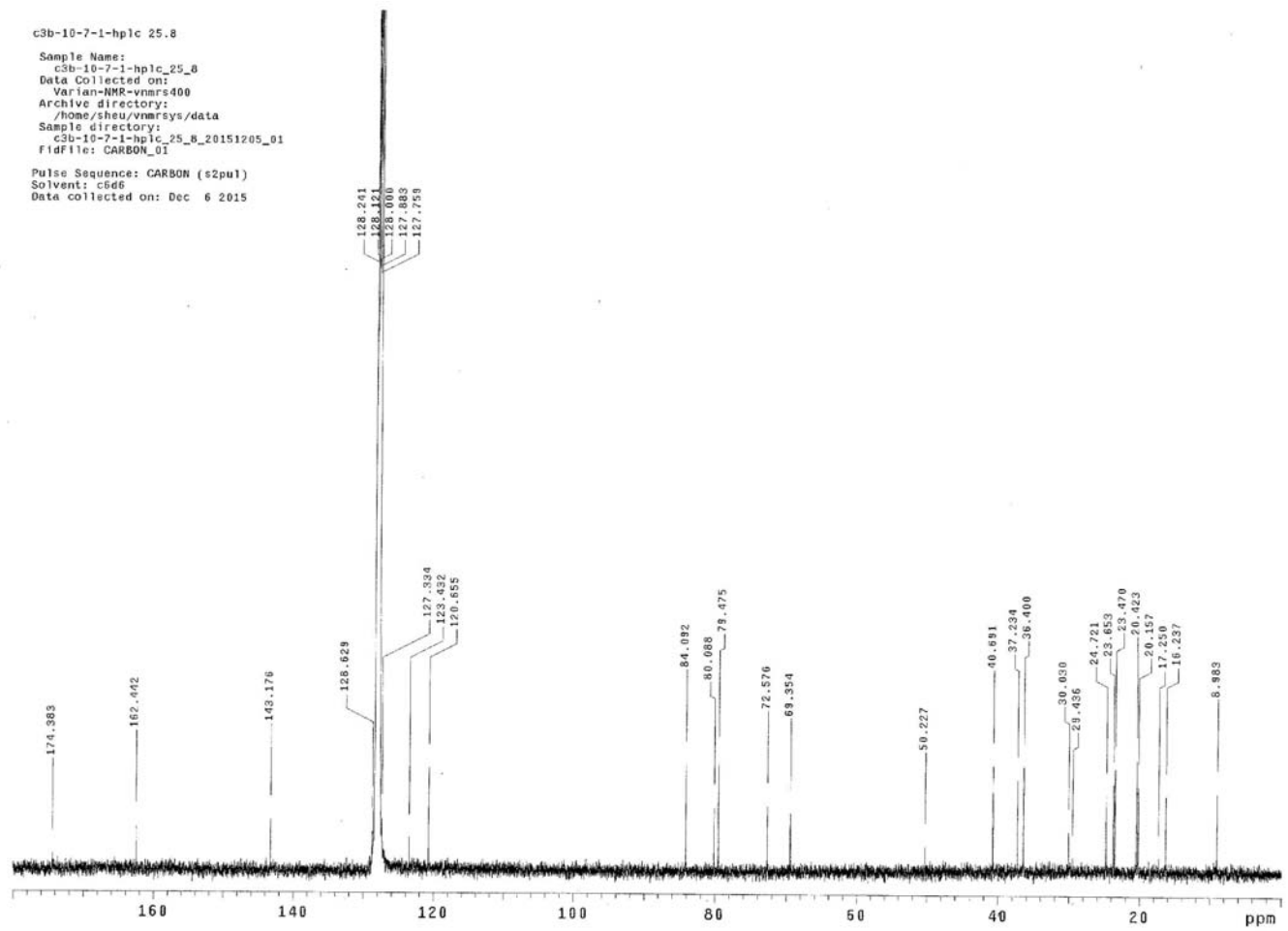


Figure S31.  $^{13}\text{C}$  NMR spectrum of 5 in  $\text{C}_6\text{D}_6$

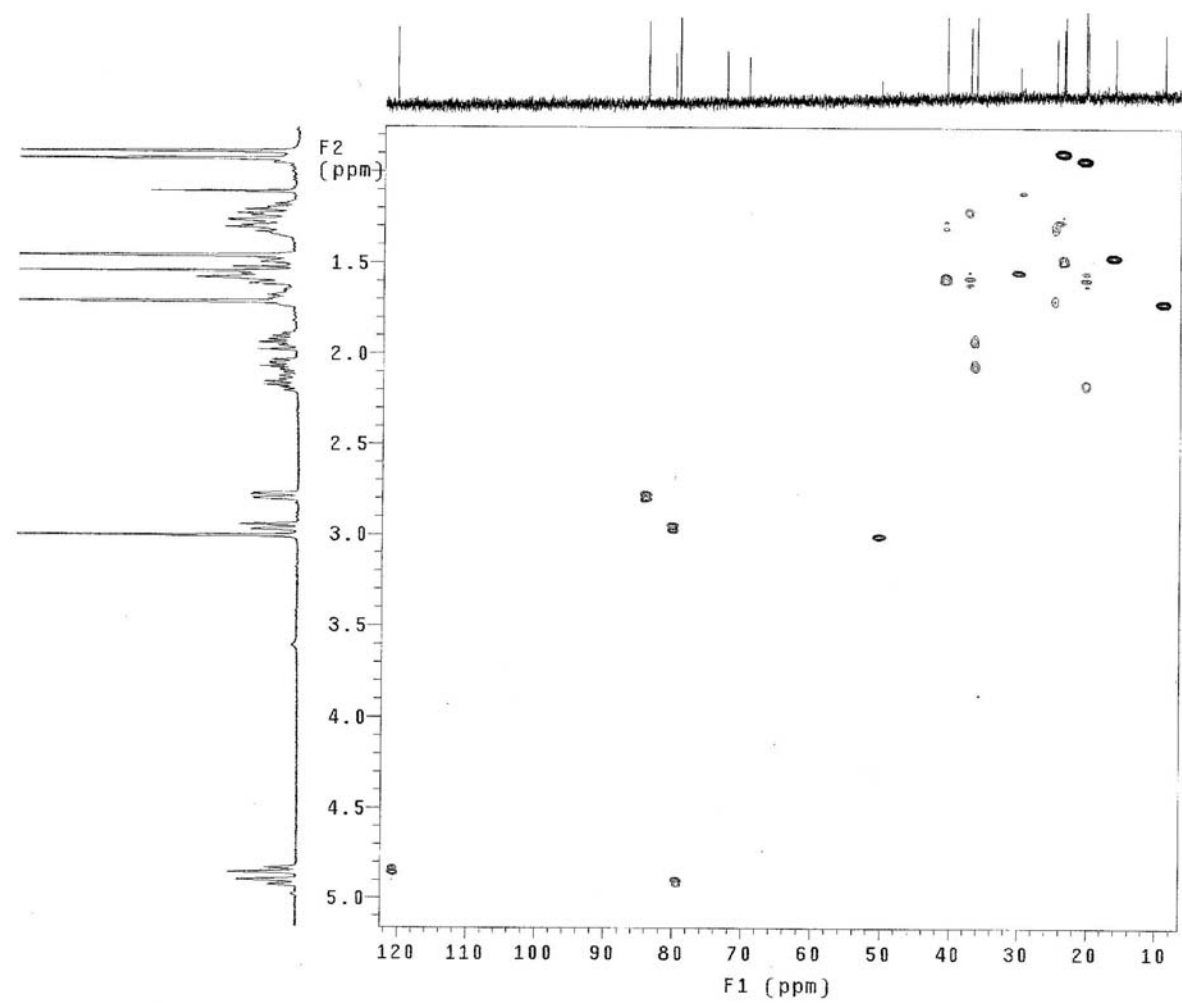


Figure S32. HSQC spectrum of 5 in  $\text{C}_6\text{D}_6$

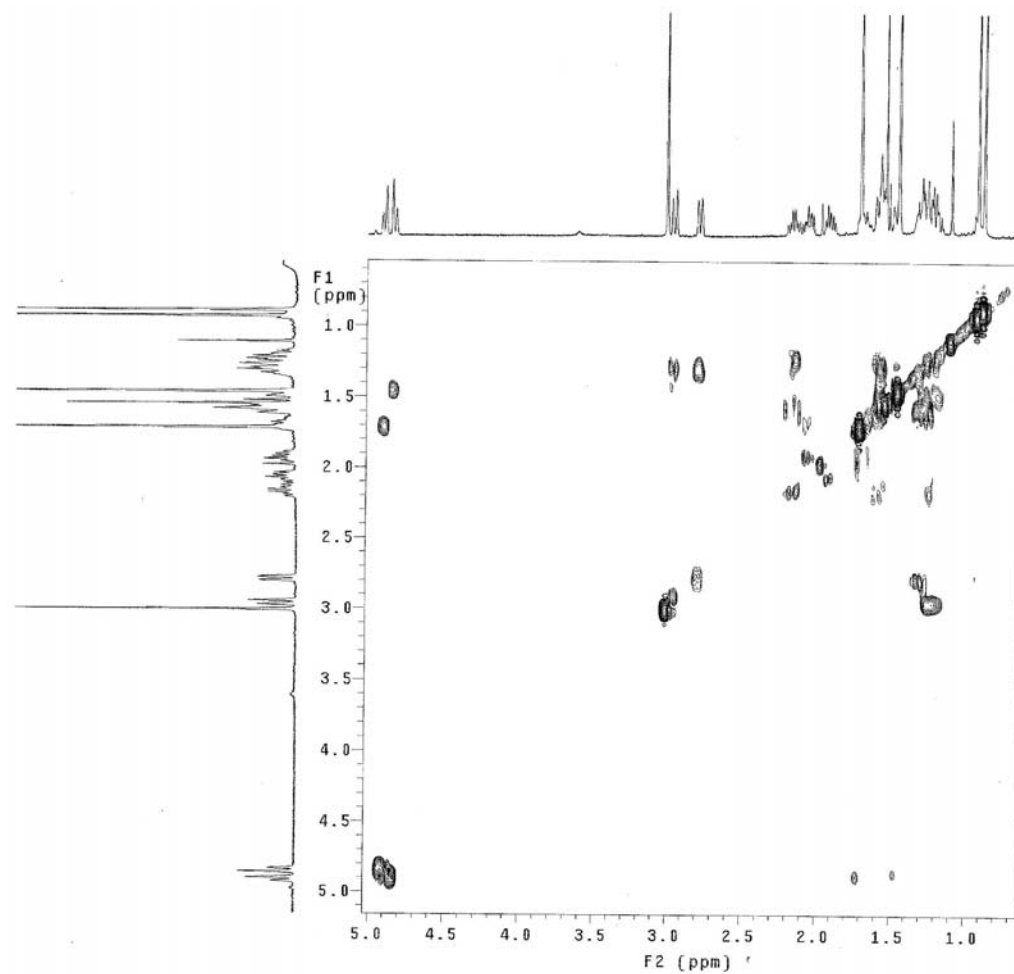


Figure S33.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of 5 in  $\text{C}_6\text{D}_6$

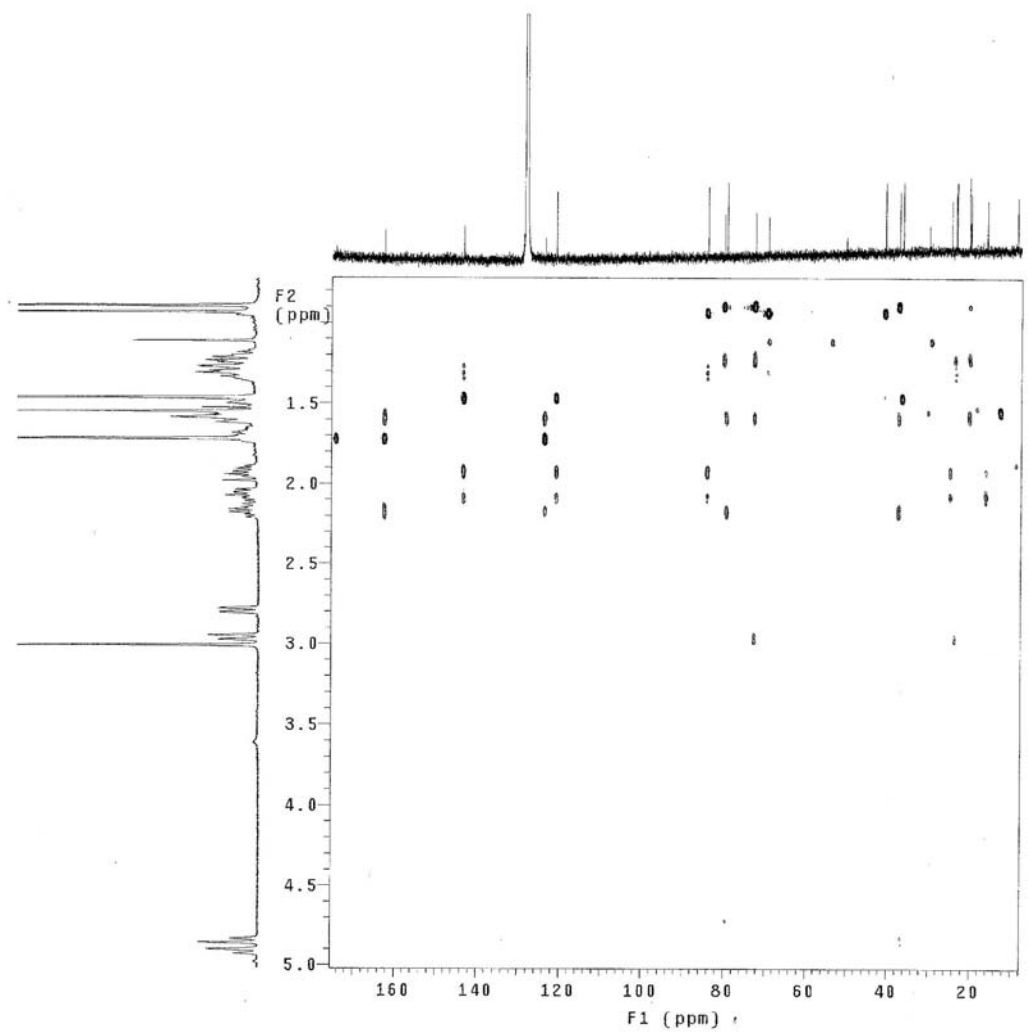


Figure S34. HMBC spectrum of 5 in  $\text{C}_6\text{D}_6$

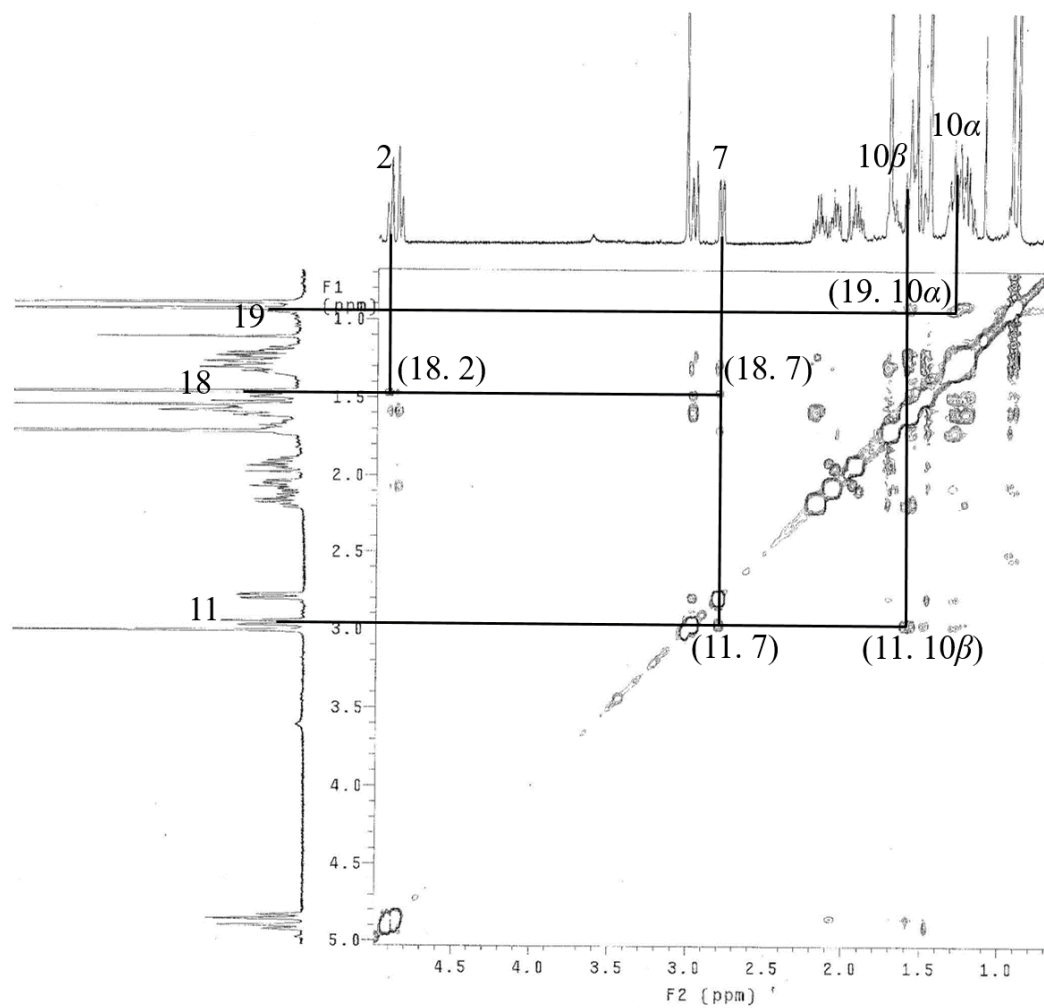
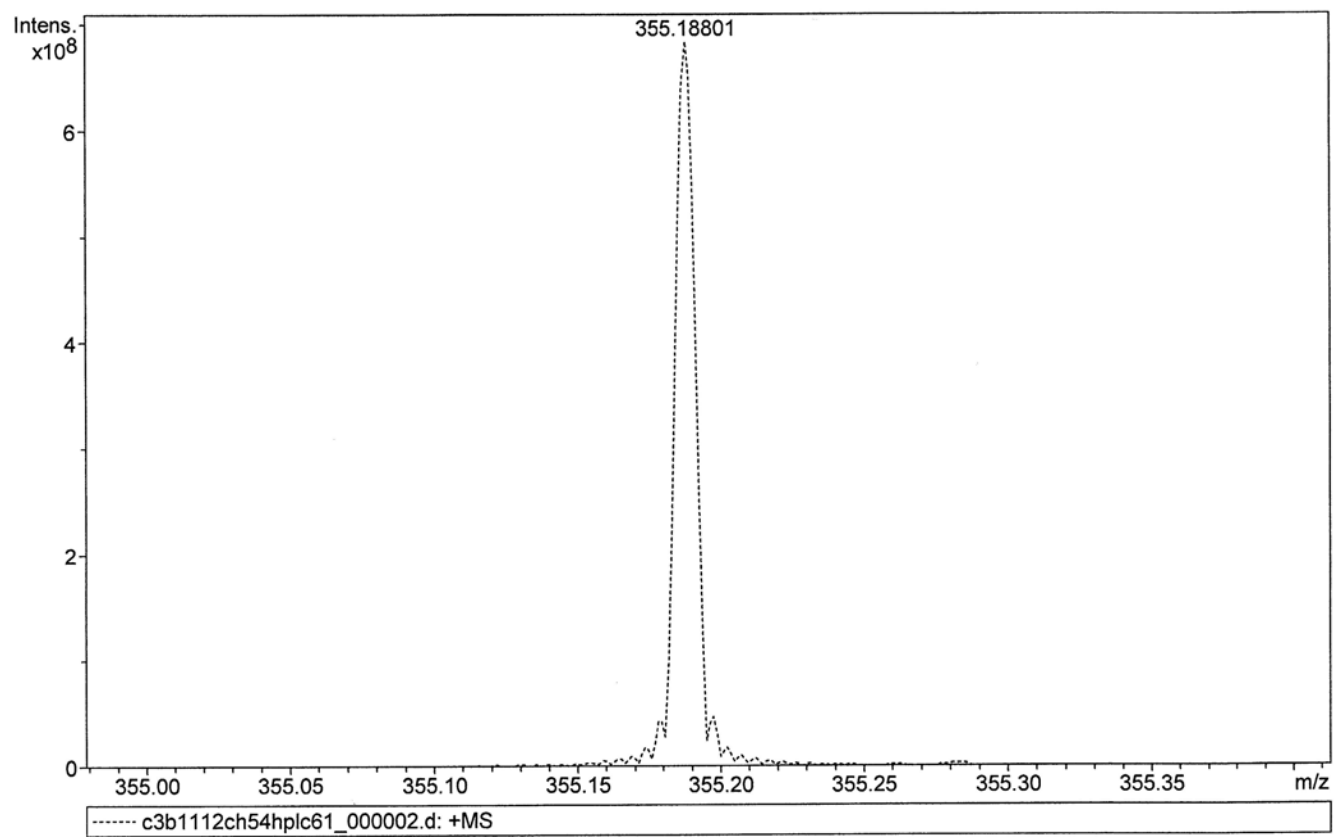


Figure S35. NOESY spectrum of 5 in C<sub>6</sub>D<sub>6</sub>



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
355.18801	1	C <sub>20</sub> H <sub>28</sub> NaO <sub>4</sub>	100.00	355.18798	-0.03	-0.10	17.9	6.5	even	ok

Figure S36. HRESIMS spectrum of 6

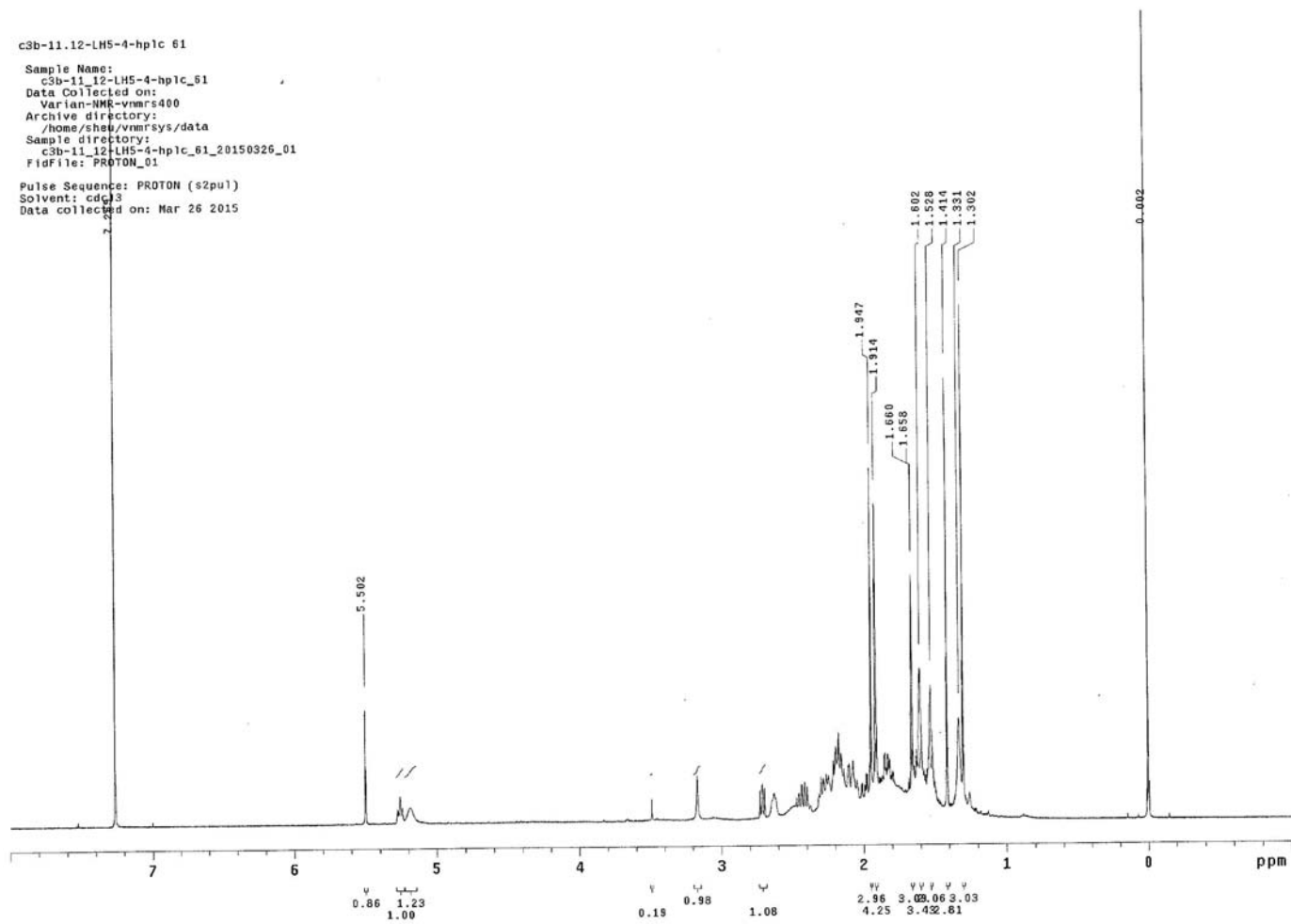


Figure S37.  $^1\text{H}$  NMR spectrum of **6** in  $\text{CDCl}_3$



c3b-11.12-LH5-4-hplc 61  
Sample Name:  
c3b-11.12-LH5-4-hplc\_61  
Data Collected on:  
Varian-NMR-vnmrs400  
Archive directory:  
/home/sheu/vnmrsys/data  
Sample directory:  
c3b-11.12-LH5-4-hplc\_61\_20150326\_01  
FidFile: CARBON\_01  
Pulse Sequence: CARBON (s2pul)  
Solvent: cdc13  
Data collected on: Mar 27 2015

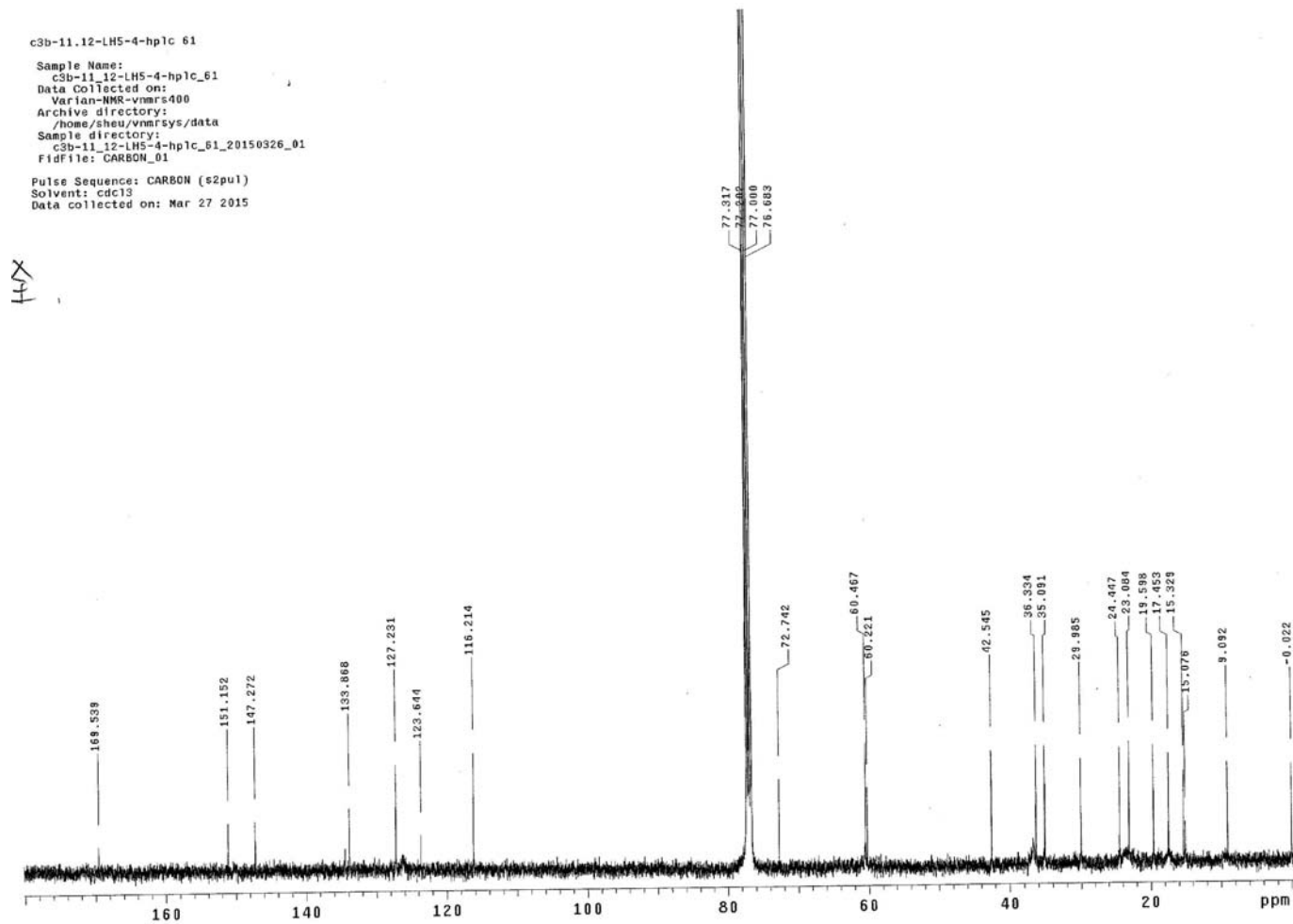


Figure S38.  $^{13}\text{C}$  NMR spectrum of **6** in  $\text{CDCl}_3$

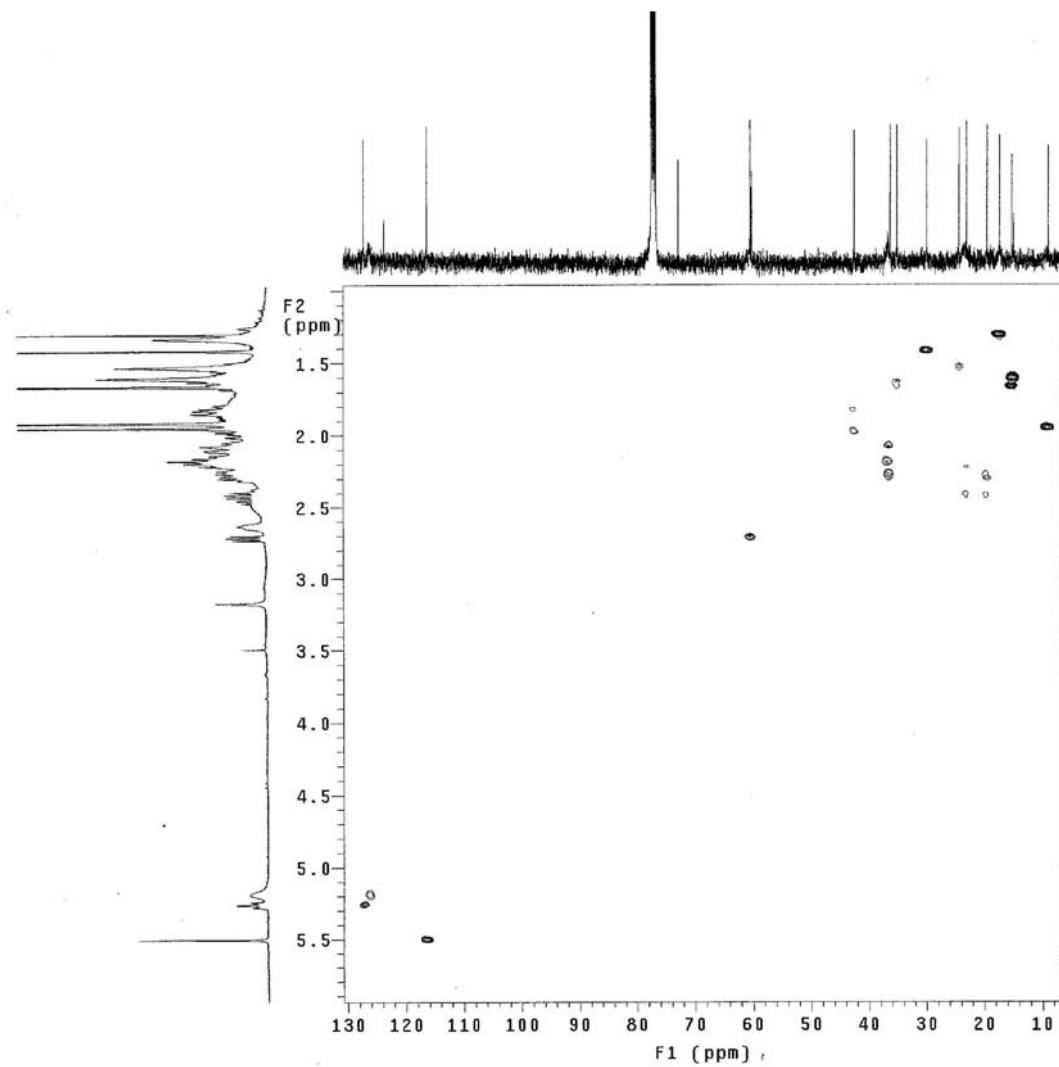


Figure S39. HSQC spectrum of 6 in CDCl<sub>3</sub>

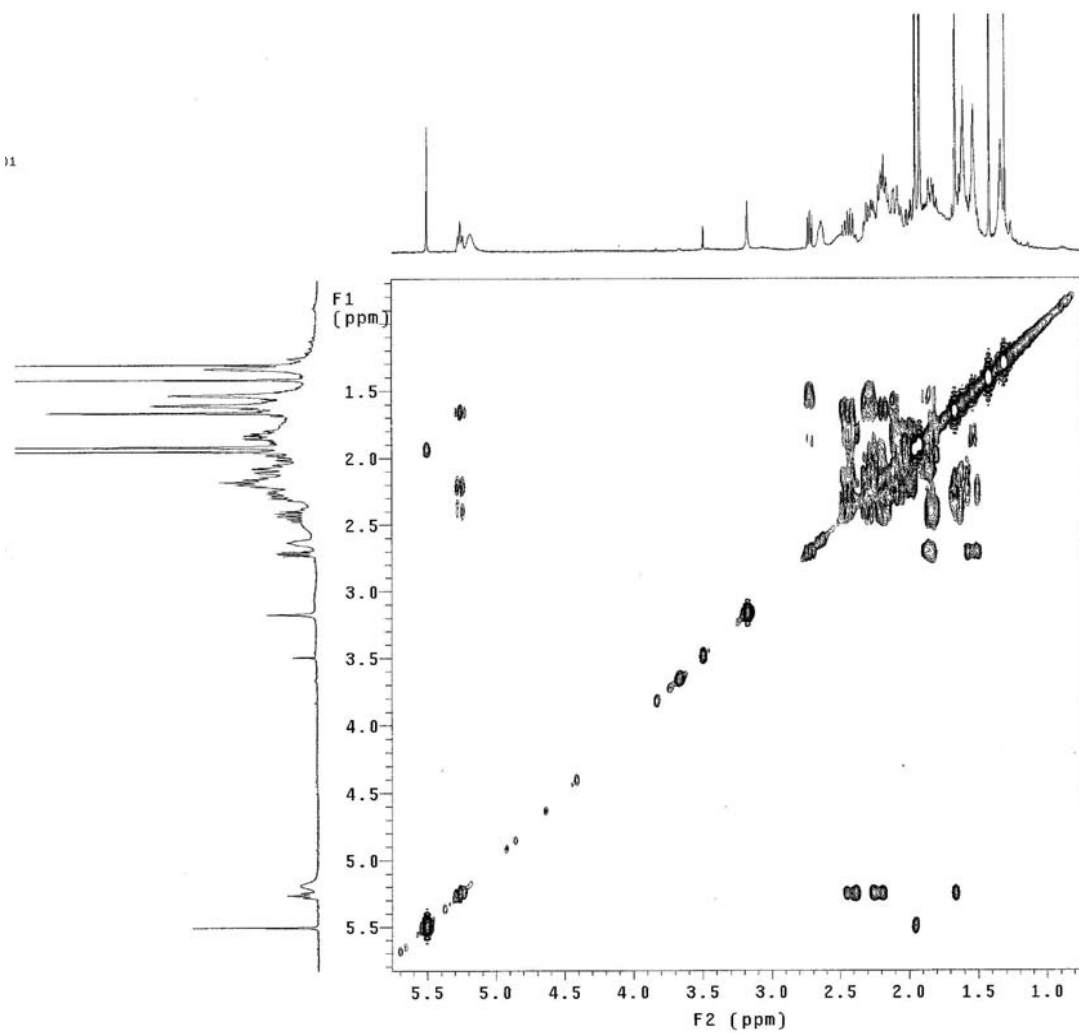


Figure S40.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **6** in  $\text{CDCl}_3$

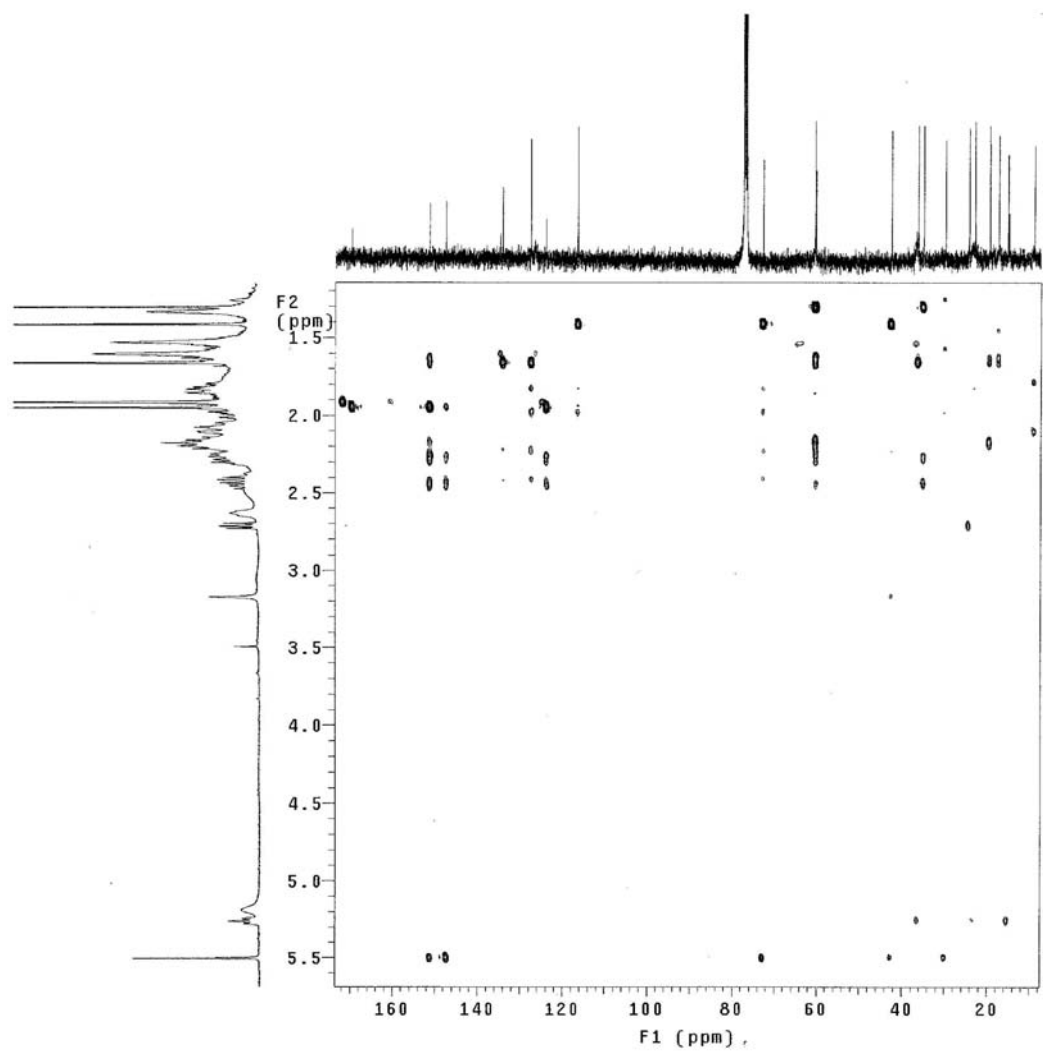


Figure S41. HMBC spectrum of 6 in CDCl<sub>3</sub>

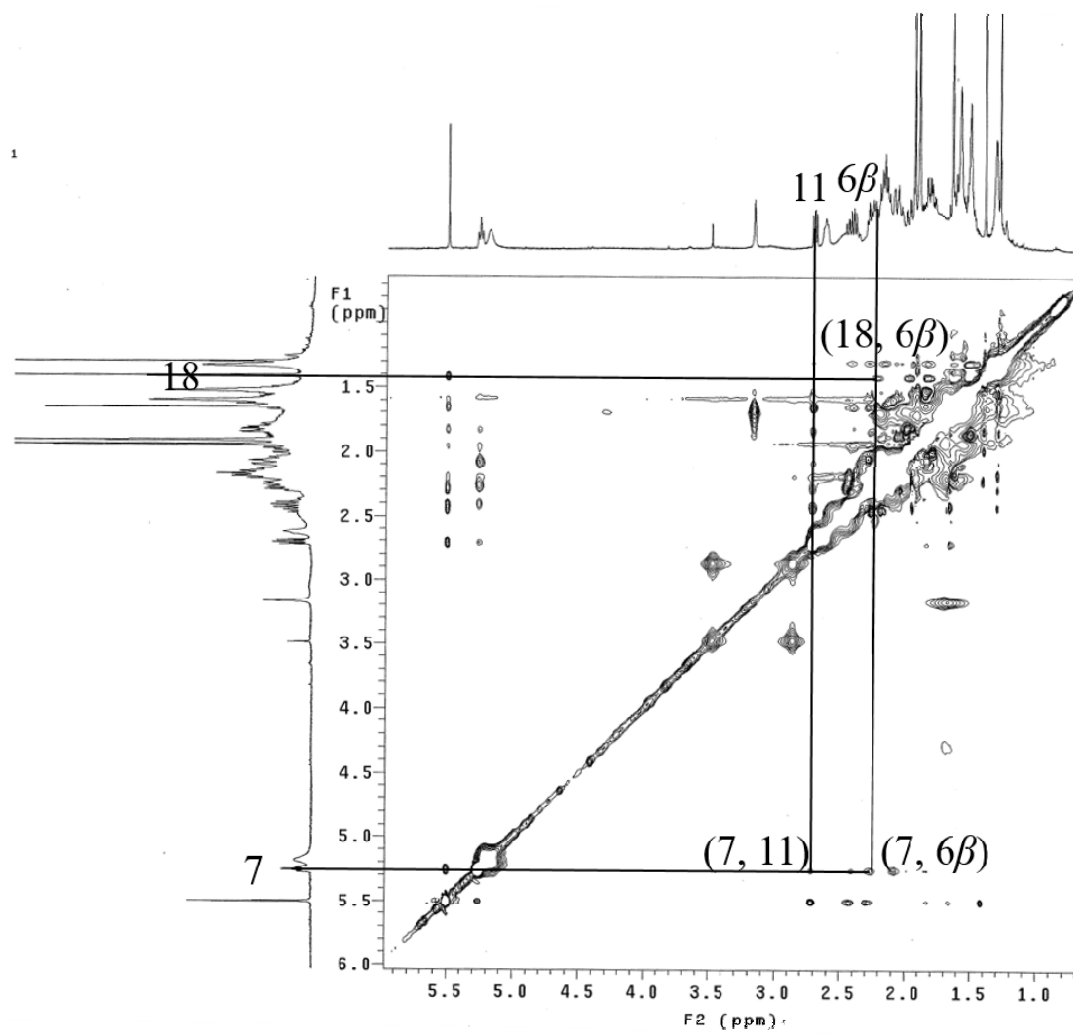
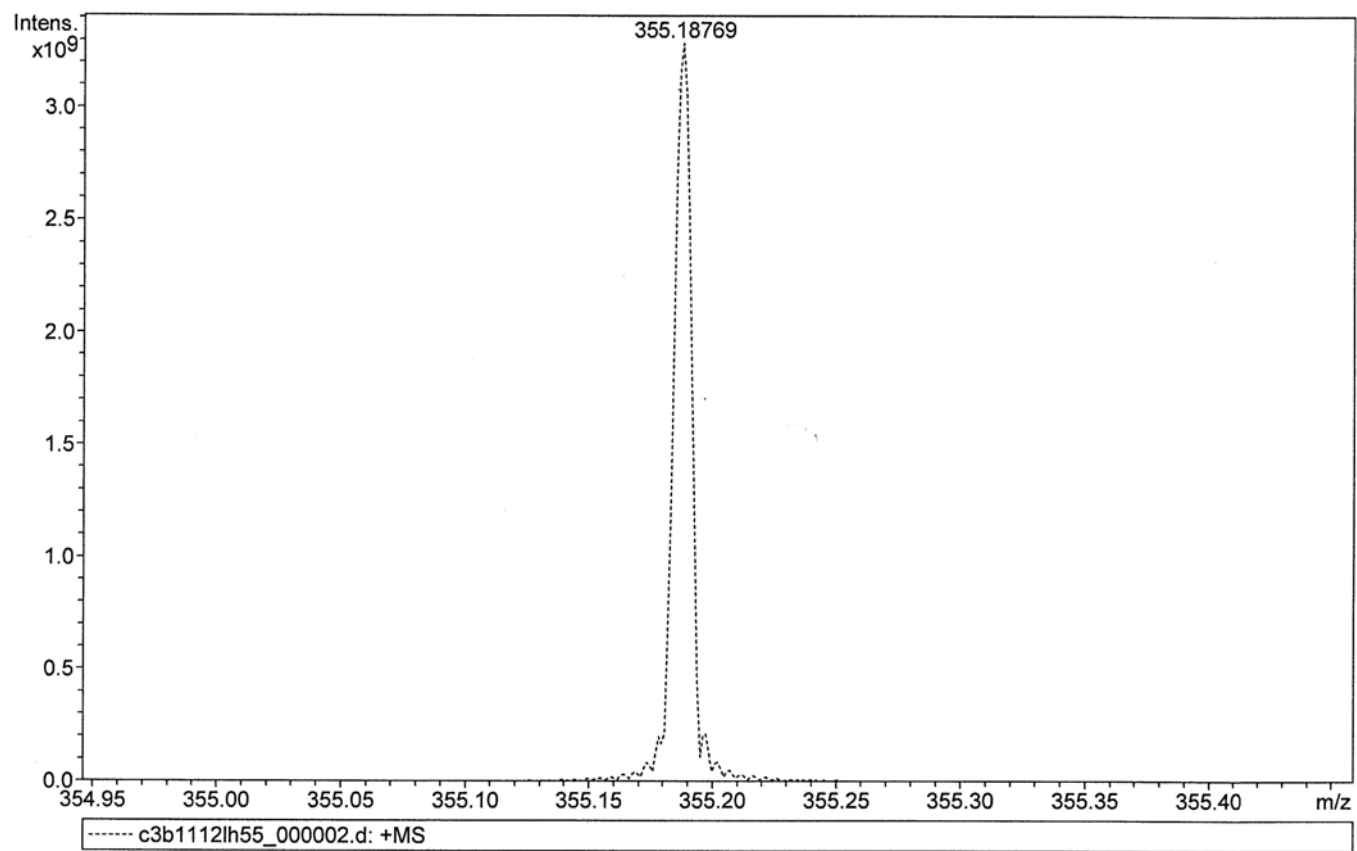


Figure S42. NOESY spectrum of **6** in CDCl<sub>3</sub>



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e <sup>-</sup> Conf	N-Rule
355.18769	1	C <sub>20</sub> H <sub>28</sub> NaO <sub>4</sub>	100.00	355.18798	0.30	0.83	20.8	6.5	even	ok

Figure S43. HRESIMS spectrum of 7

Solvent: CDCl<sub>3</sub>  
Data collected on: Feb 28 2015

H<sub>2</sub>

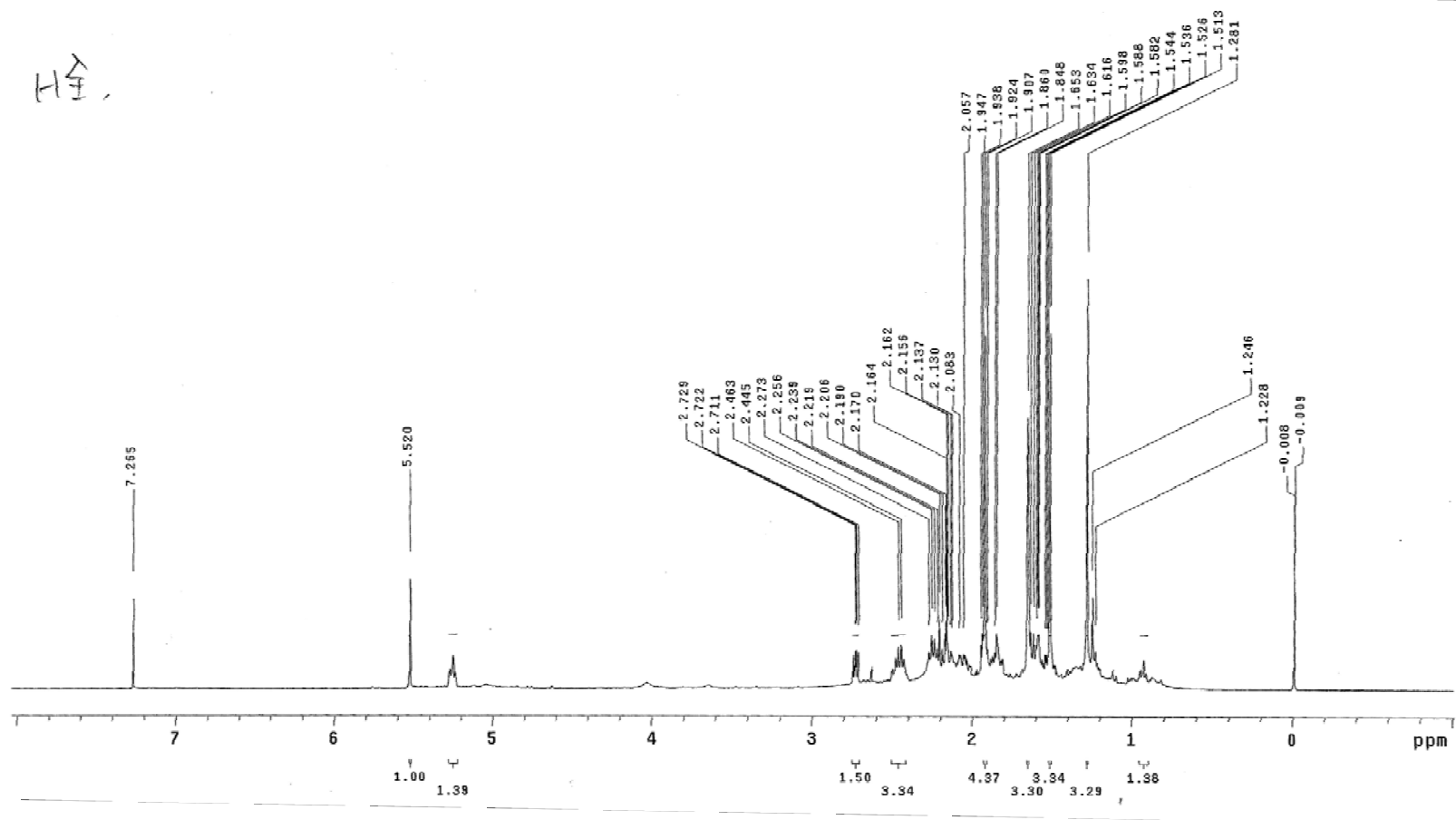


Figure S44. <sup>1</sup>H NMR spectrum of 7 in CDCl<sub>3</sub>  
S47

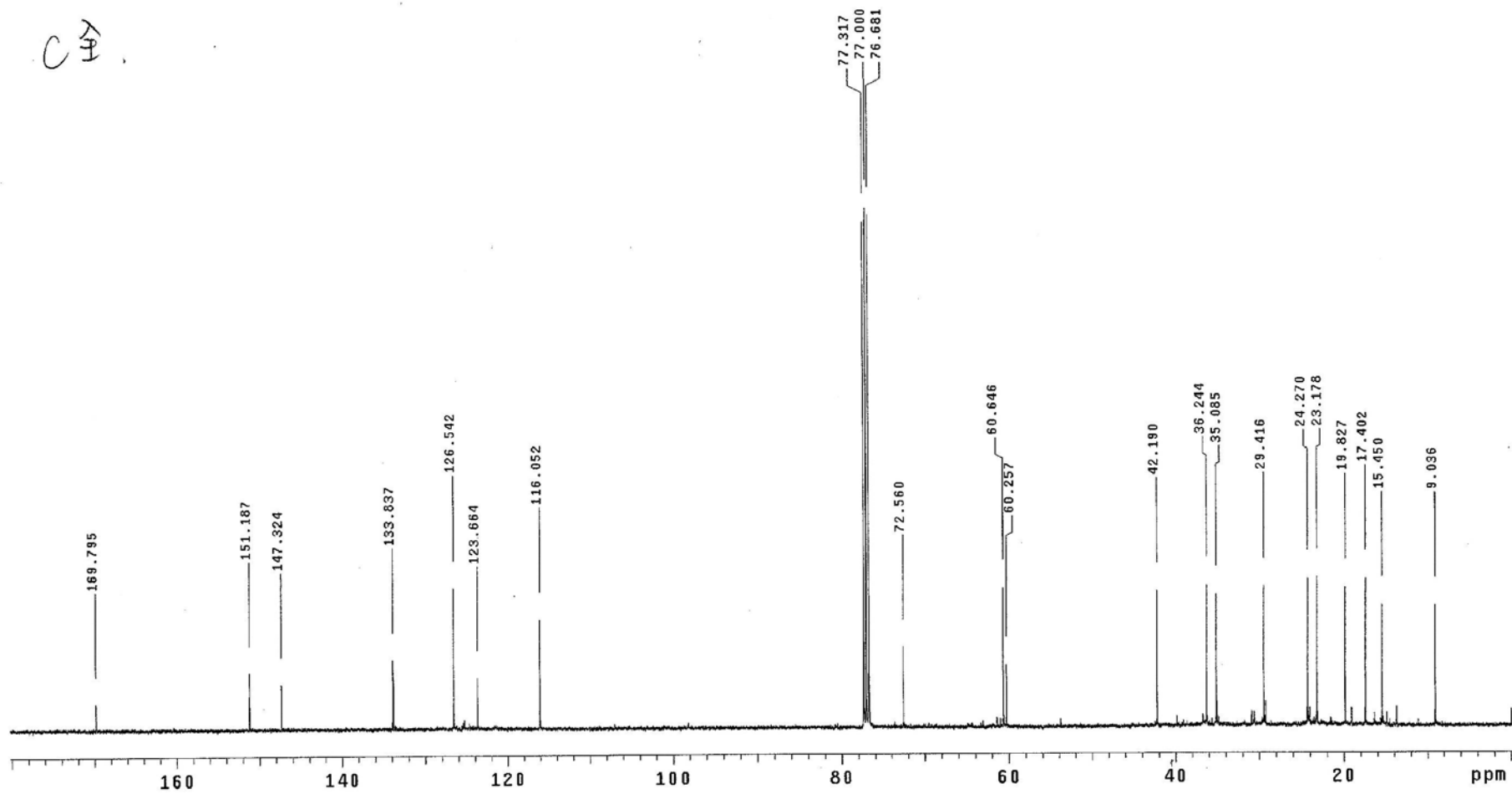


Figure S45. <sup>13</sup>C NMR spectrum of 7 in CDCl<sub>3</sub>



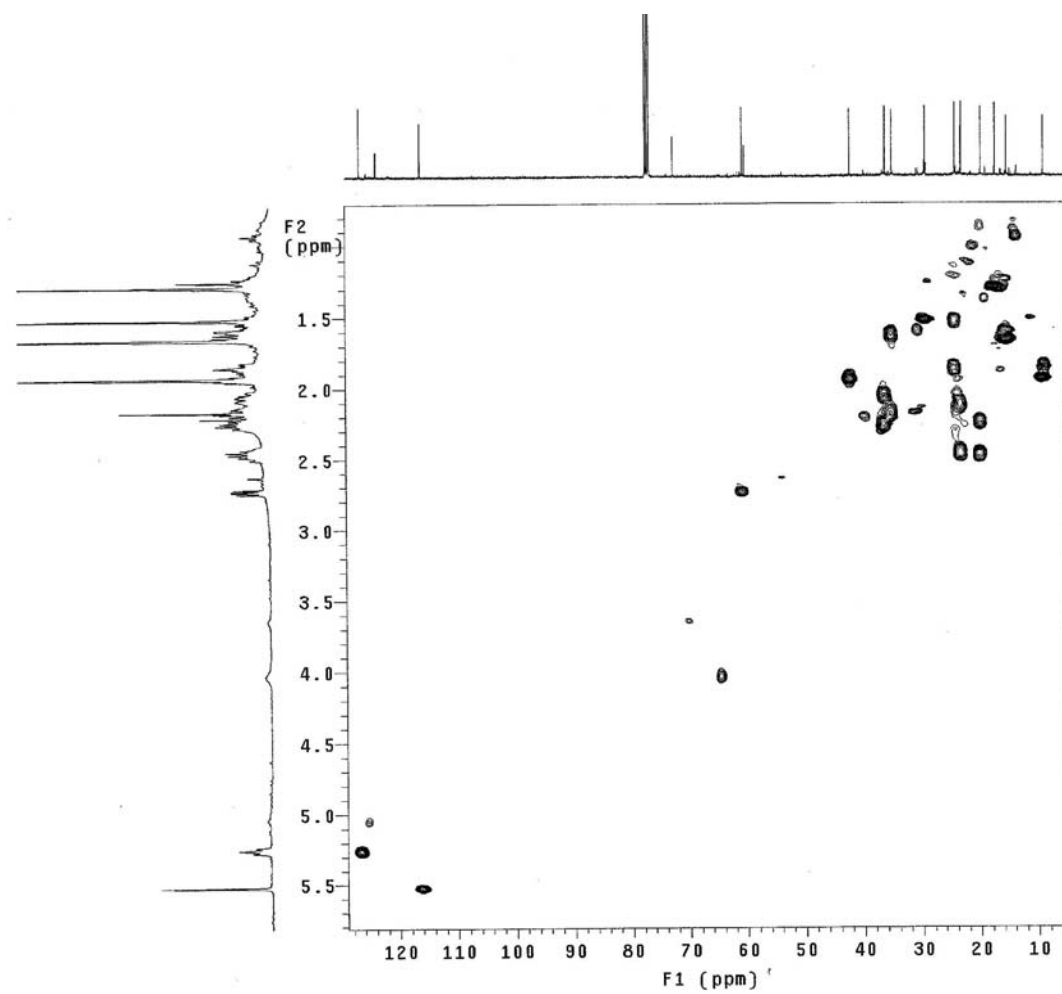


Figure S46. HSQC spectrum of 7 in CDCl<sub>3</sub>

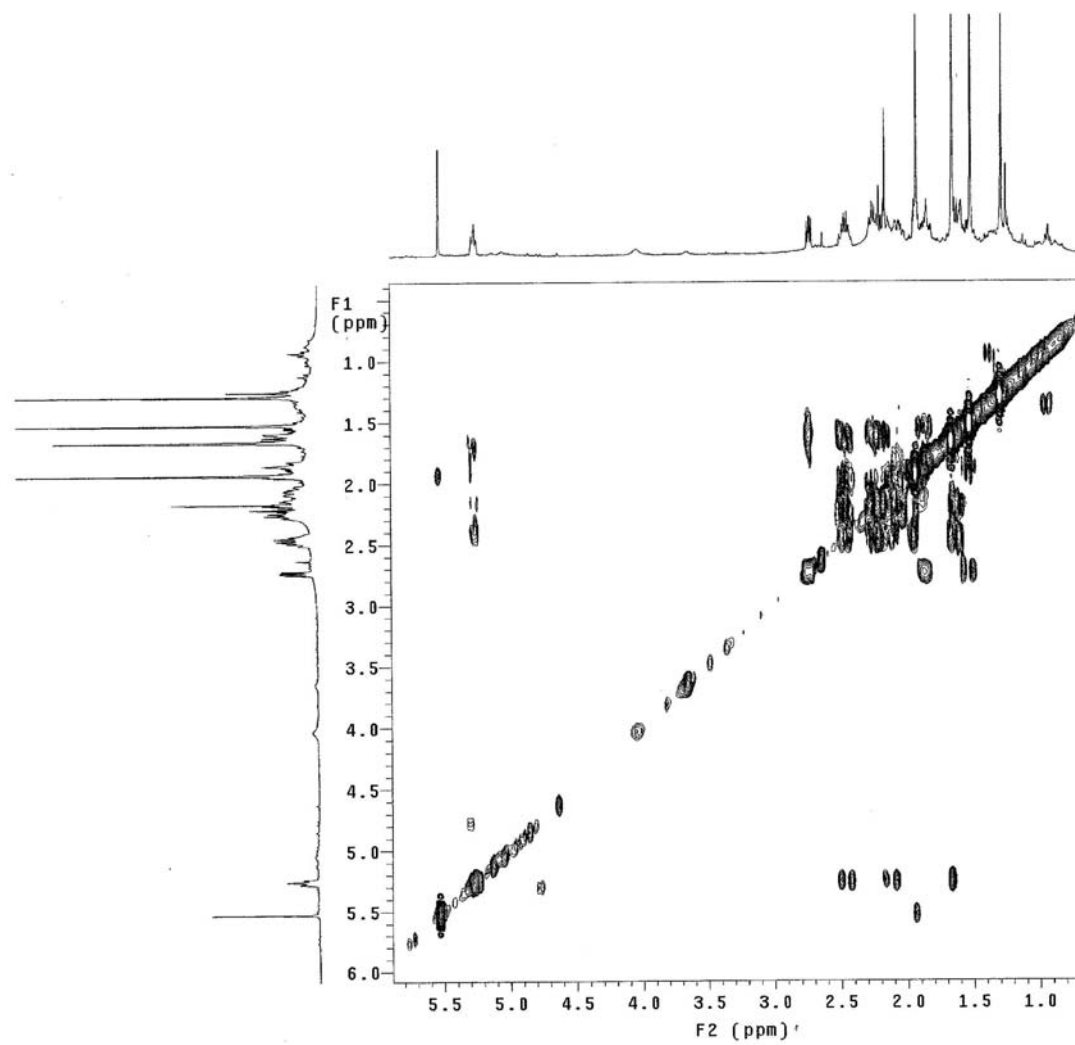


Figure S47.  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of **7** in  $\text{CDCl}_3$

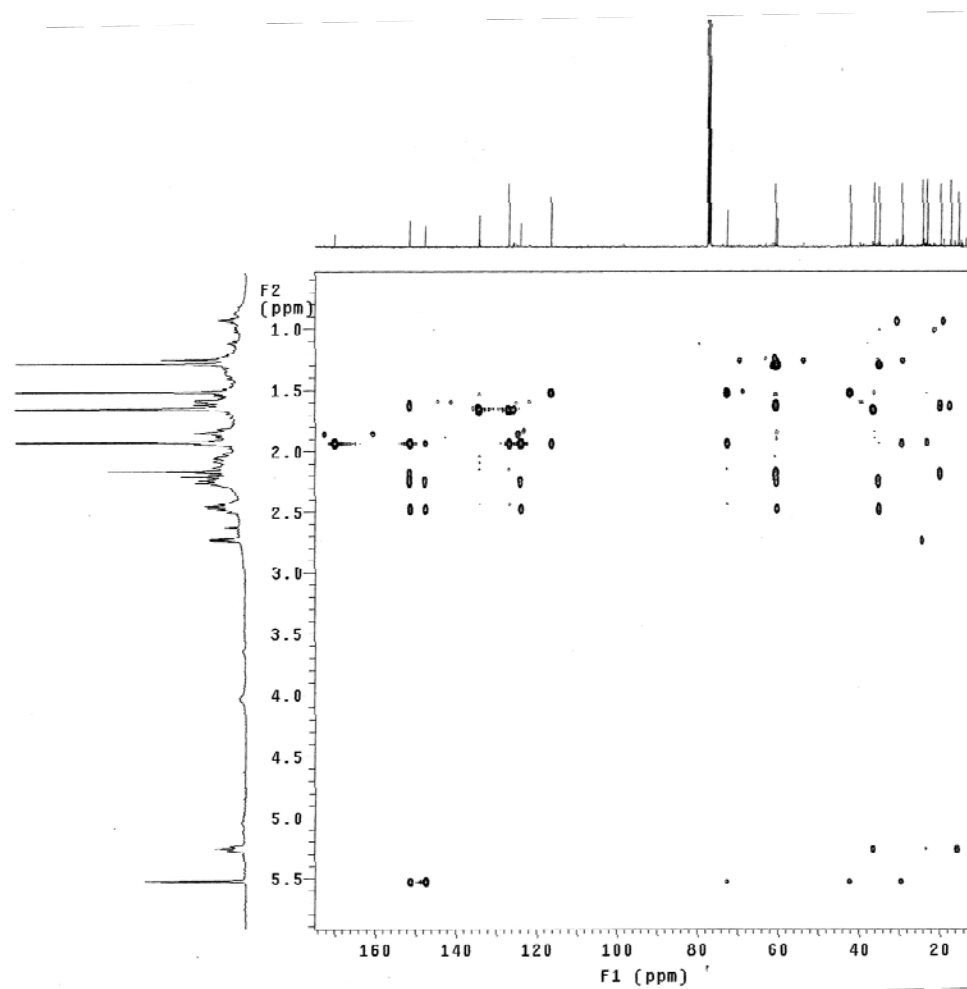


Figure S48. HMBC spectrum of 7 in CDCl<sub>3</sub>

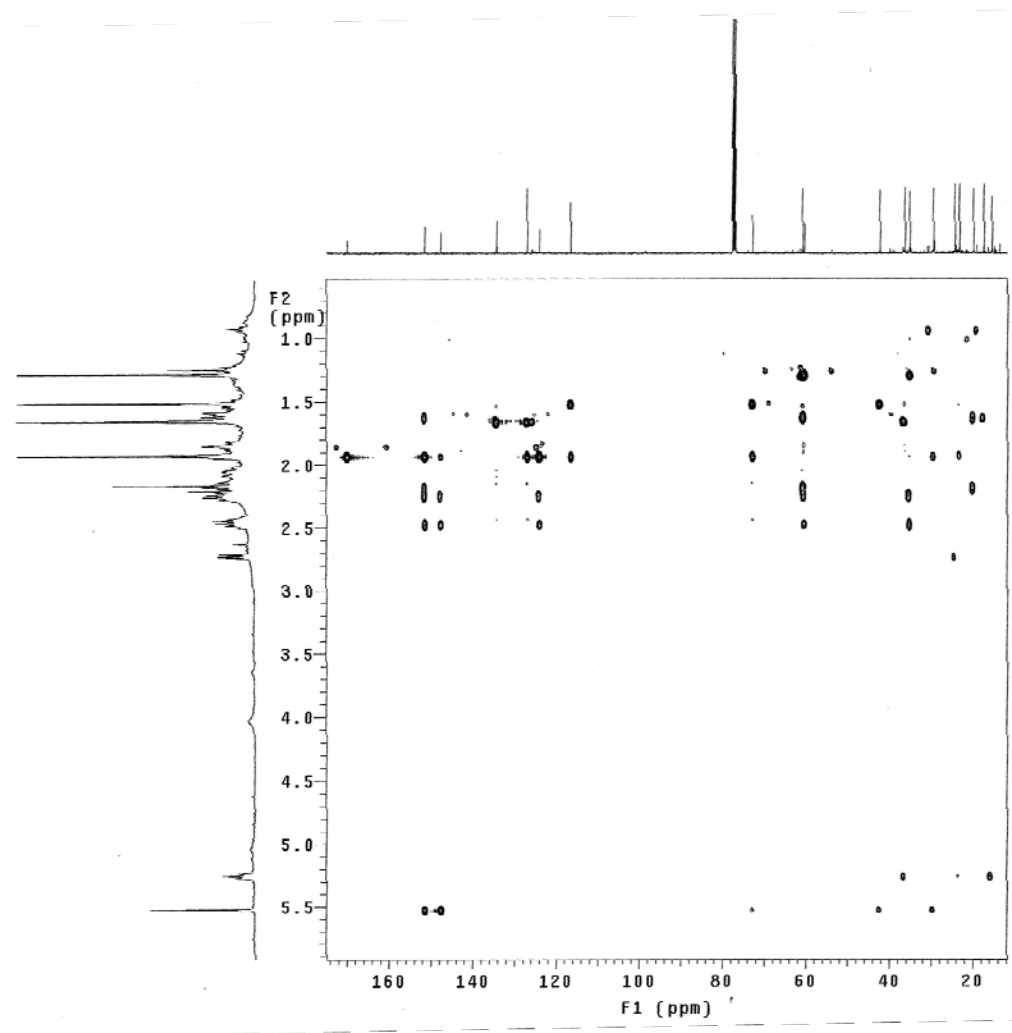


Figure S49. NOESY spectrum of 7 in CDCl<sub>3</sub>