

# Four prenylflavone derivatives with antiplasmodial activities from the stems of *Tephrosia purpurea* subsp. *leptostachya*

Yoseph Atilaw, Lois Muiva-Mutisya, Albert Ndakala, Hoseah M. Akala, Redemptah Yeda, Yu J. Wu, Paolo Coghi, Vincent K.W. Wong, Máté Erdélyi, Abiy Yenesew

## Table of Contents

Figure	Content Page
Figs. S1 –S6 <sup>1</sup> H & <sup>13</sup> C NMR; COSY; NOESY; HSQC & HMBC correlations of compound <b>1</b>	3-8
Fig. S7 HRMS of compound <b>1</b>	9
Fig. S8 UV spectrum of compound <b>1</b>	10
Figs. S9 –S13 <sup>1</sup> H & <sup>13</sup> C NMR; NOESY; HSQC & HMBC correlations of compound <b>2</b>	11-15
Fig. S14 HRMS of compound <b>2</b>	16
Fig. S15 UV spectrum of compound <b>2</b>	17
Fig. S16-S21 <sup>1</sup> H; <sup>13</sup> C; COSY; NOESY; HSQC & HMBC correlations of compound <b>3</b>	18-23
Fig. S22 HRMS of compound <b>3</b>	24
Fig. S23 UV spectrum of compound <b>3</b>	25
Fig. S24-S29 <sup>1</sup> H and <sup>13</sup> C; COSY; NOESY; HSQC & HMBC correlations of compound <b>4</b>	26-31
Fig. S30 HRMS of compound <b>4</b>	32
Fig. S31 UV spectrum of compound <b>4</b>	33
Table S11H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>5</b> , CDCl <sub>3</sub>	34
Table S21H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>6</b> , CDCl <sub>3</sub>	35
Table S31H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>7</b> , CDCl <sub>3</sub>	36
Table S41H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>8</b> , CDCl <sub>3</sub>	37
Table S51H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>9</b> , CDCl <sub>3</sub>	38
Table S61H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>10</b> , CDCl <sub>3</sub>	39
Table S71H (800 MHz) and <sup>13</sup> C (200 MHz) NMR spectroscopic data for compound <b>11</b> , CDCl <sub>3</sub>	40

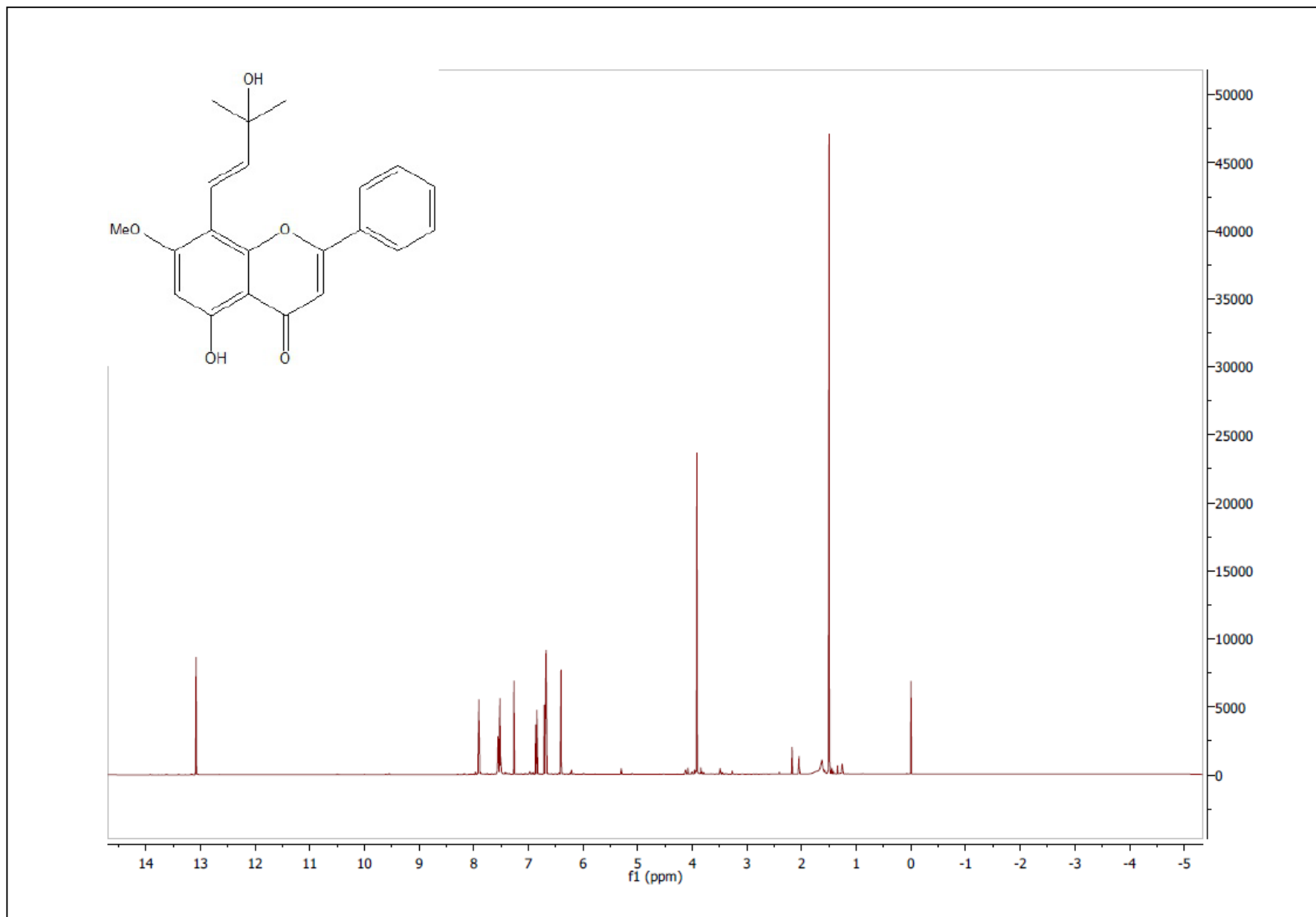


Fig. S1: <sup>1</sup>H NMR spectrum of compound 1 (800 MHz; CDCl<sub>3</sub>)

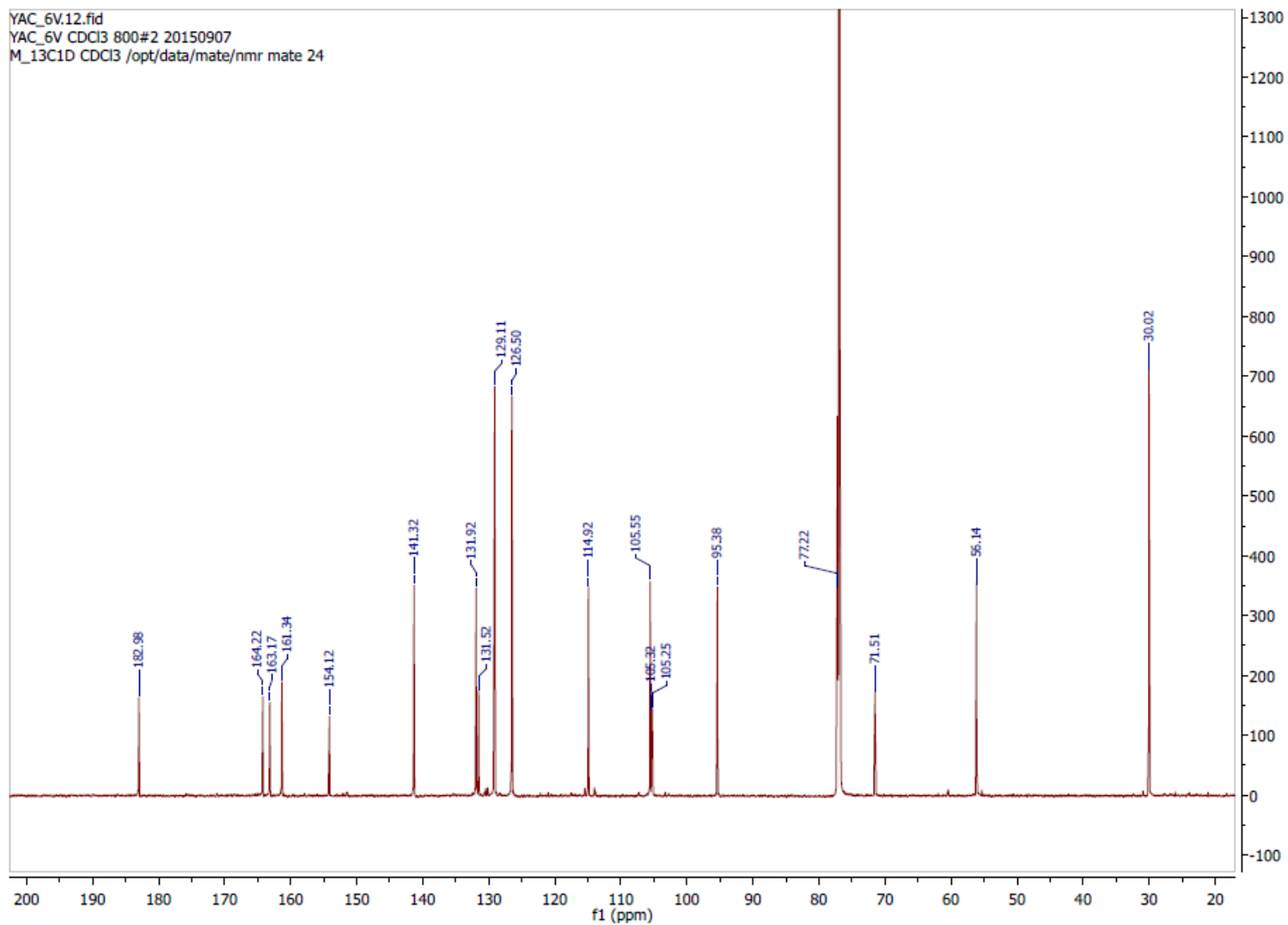


Fig. S2:  $^{13}\text{C}$  NMR spectrum of compound 1 (200 MHz;  $\text{CDCl}_3$ )

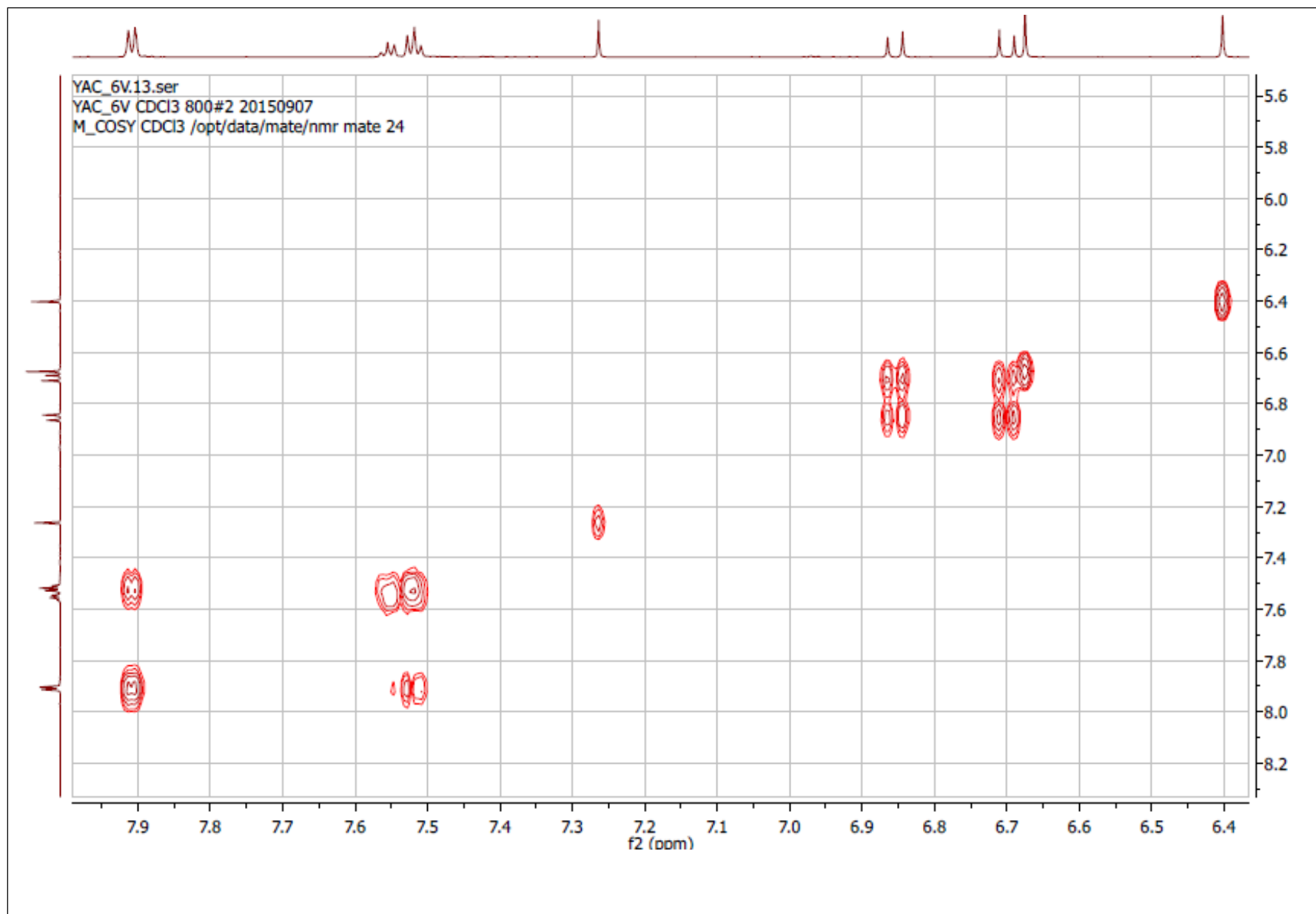


Fig. S3: COSY spectrum of compound **1** (CDCl<sub>3</sub>)

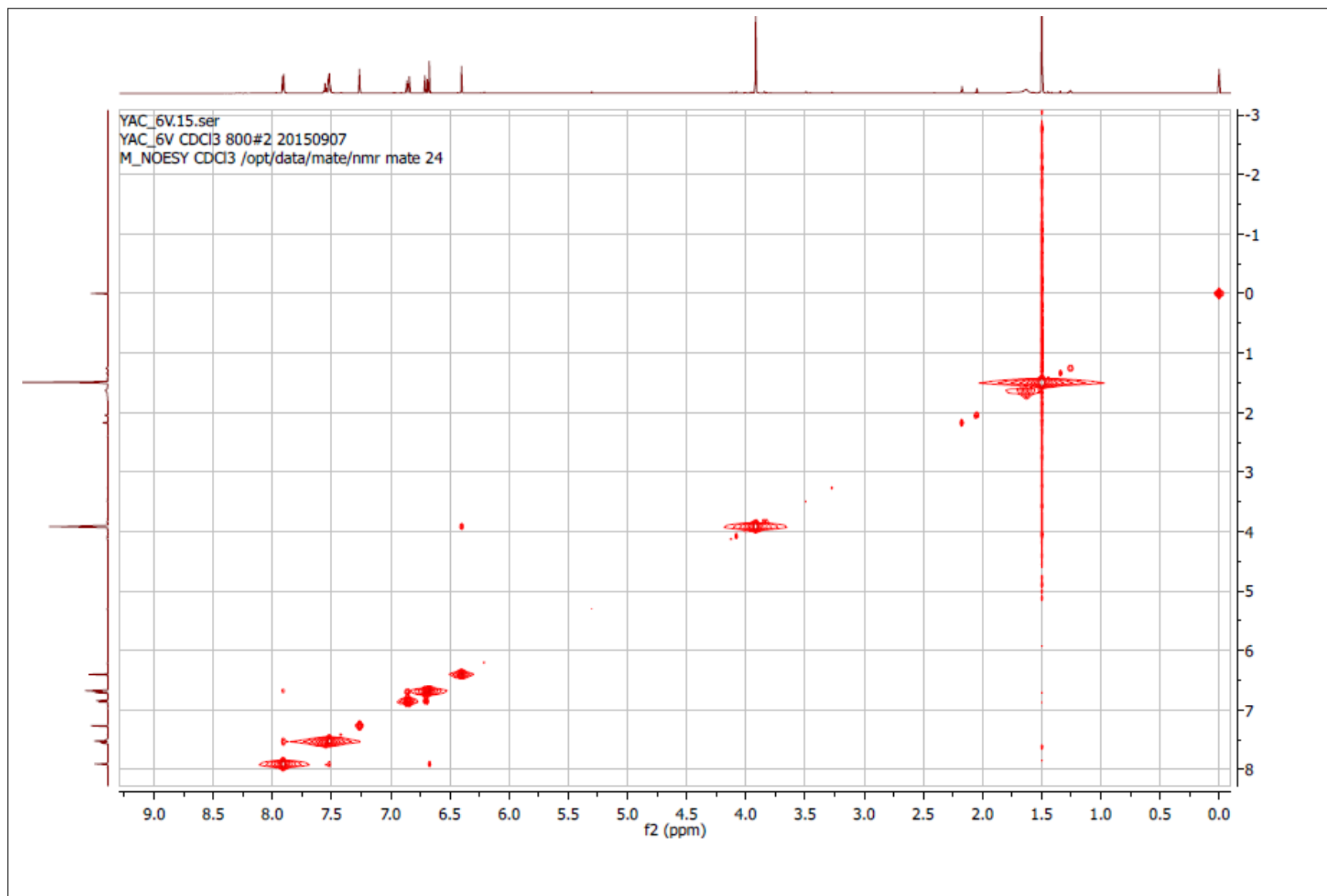


Fig. S4: NOESY spectrum of compound **1** (CDCl<sub>3</sub>)

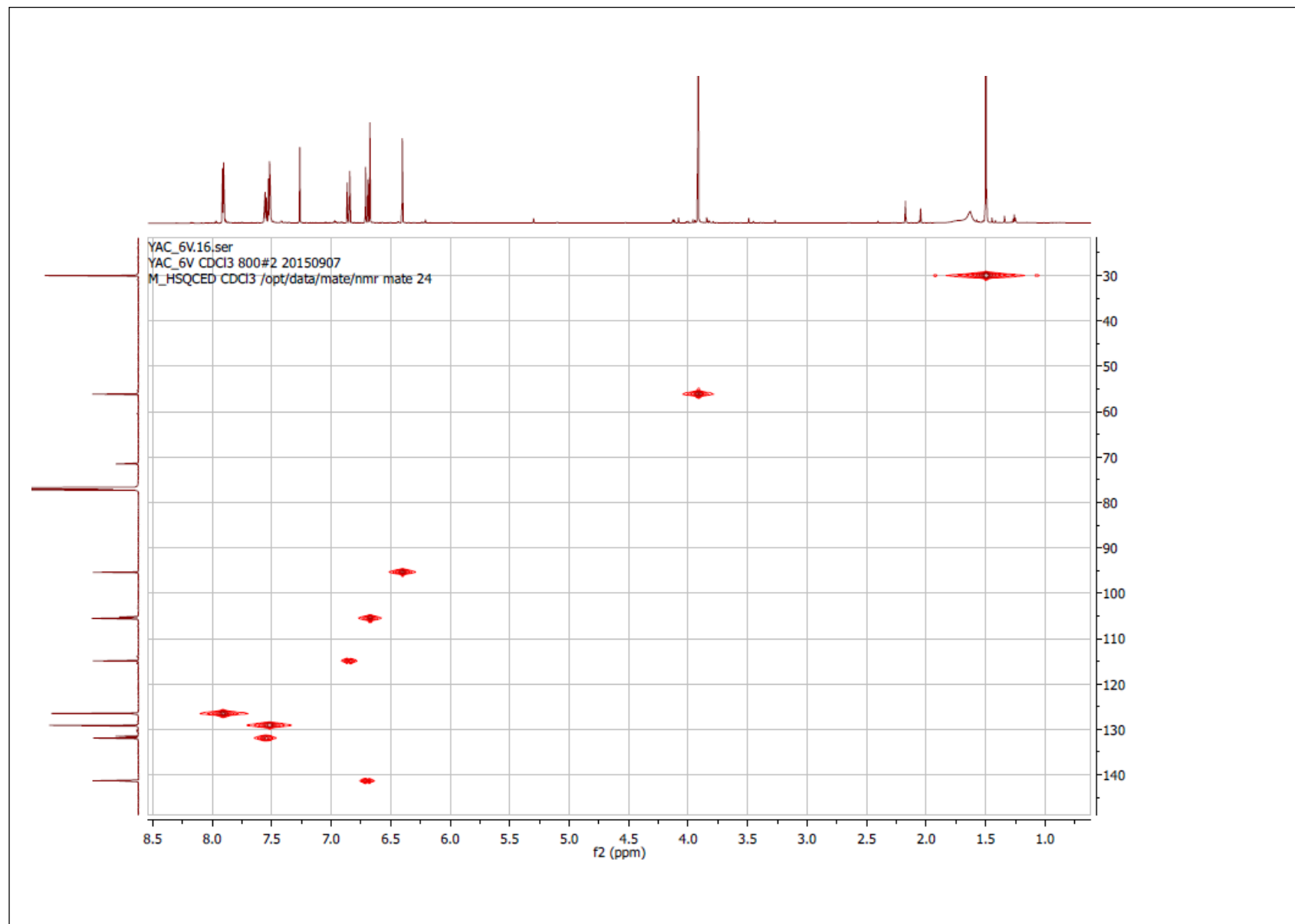


Fig. S5: HSQC spectrum of compound **1** (CDCl<sub>3</sub>)

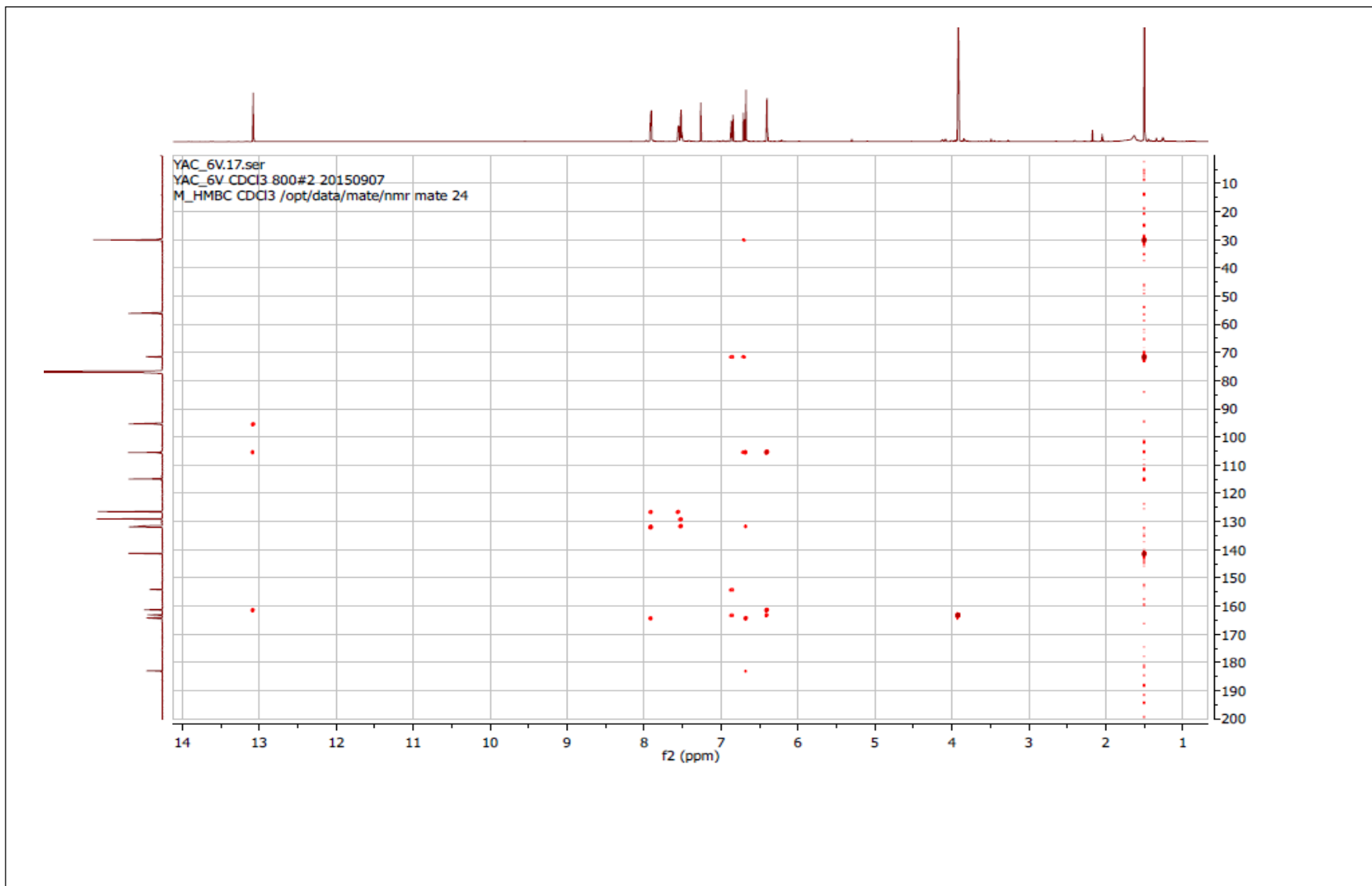


Fig. S6: HMBC spectrum of compound **1** (CDCl<sub>3</sub>)

Yoseph\_08 #164-167 RT: 0.60-0.61 AV: 4 NL: 1.05E4  
T: + c Full ms [ 35.00-500.00]

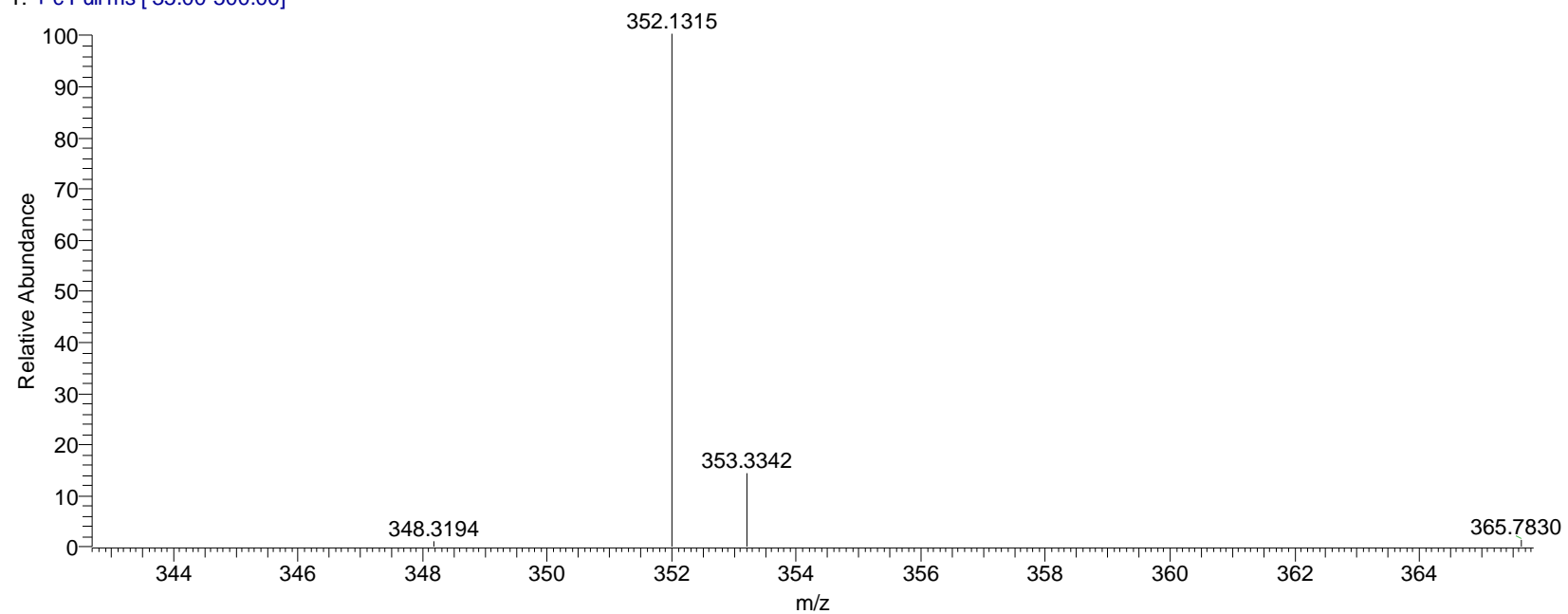


Fig. S7: HRMS of compound 1



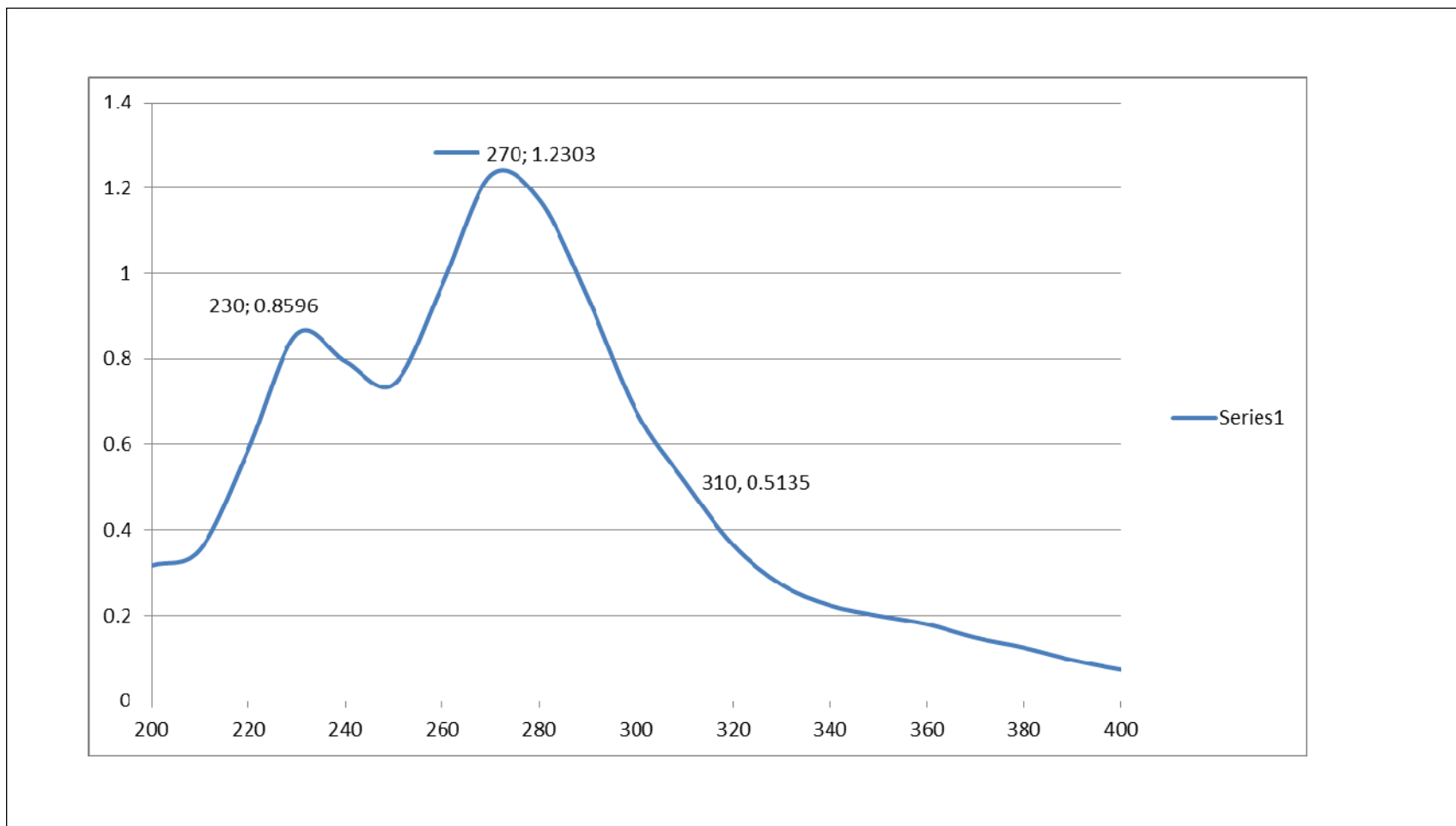


Fig. S8: UV spectrum of compound **1**

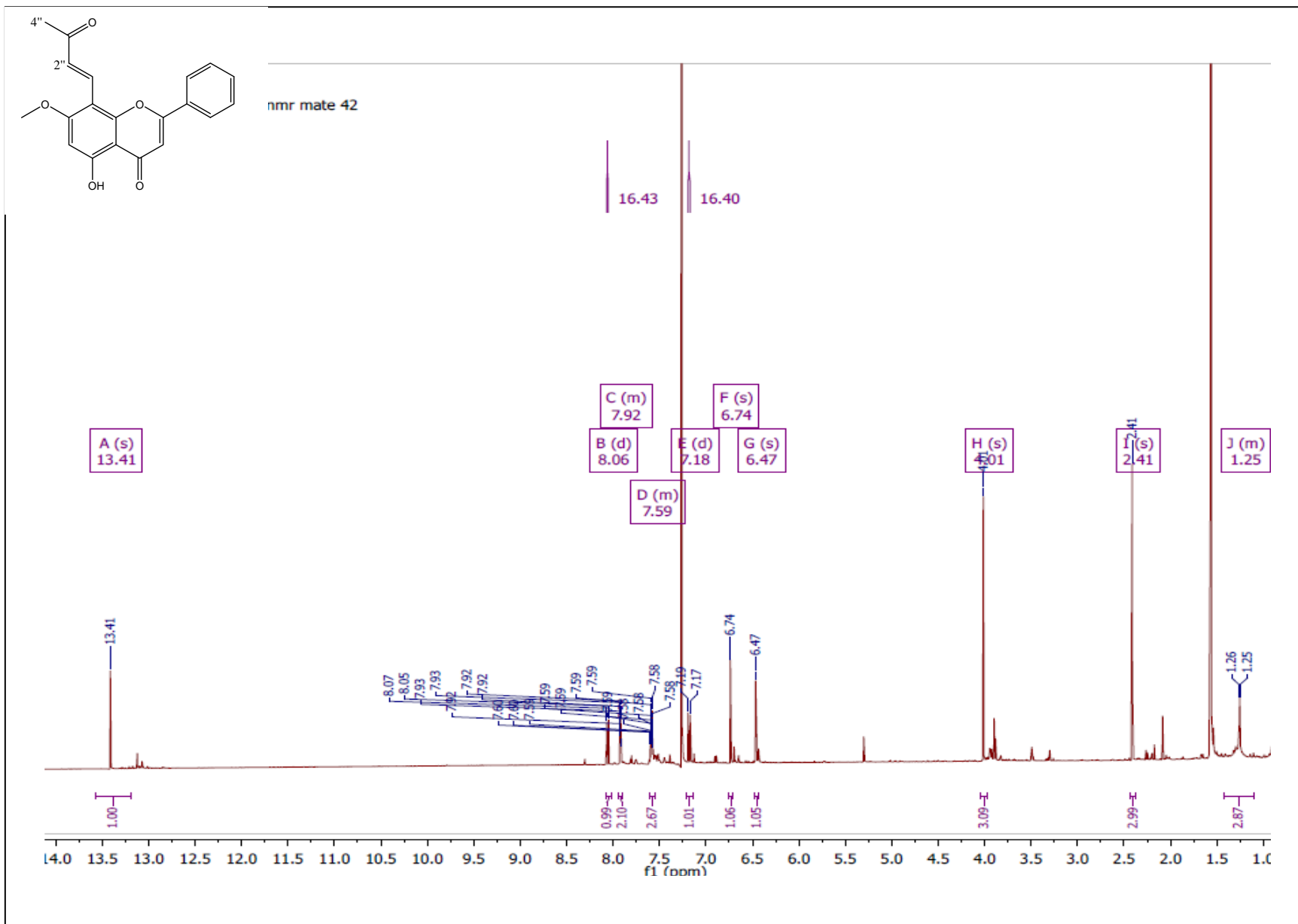


Fig. S9:  $^1\text{H}$  NMR spectrum of compound 2 (800 MHz;  $\text{CDCl}_3$ )

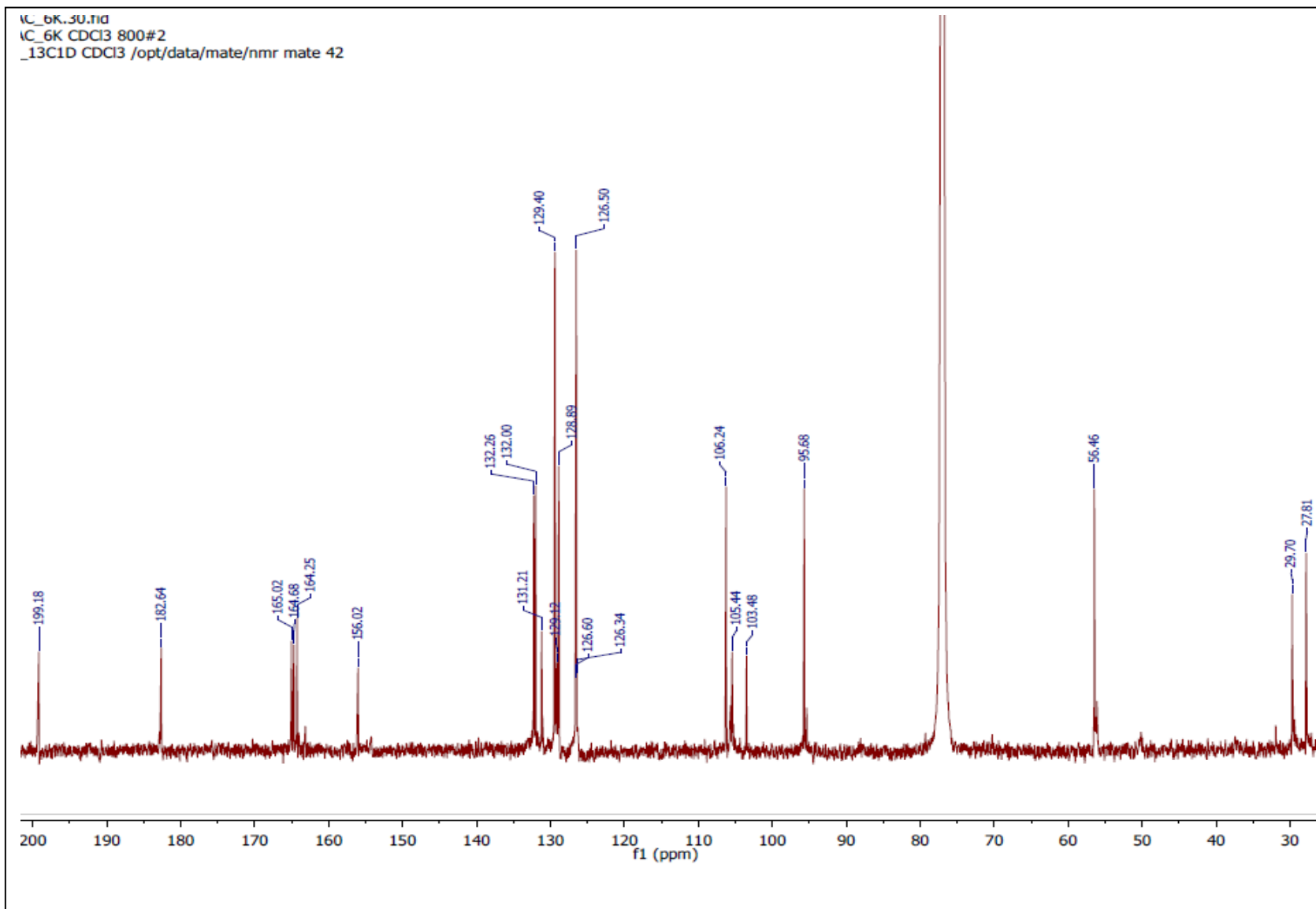


Fig. S10:  $^{13}\text{C}$  NMR spectrum of compound **2** (200 MHz;  $\text{CDCl}_3$ )

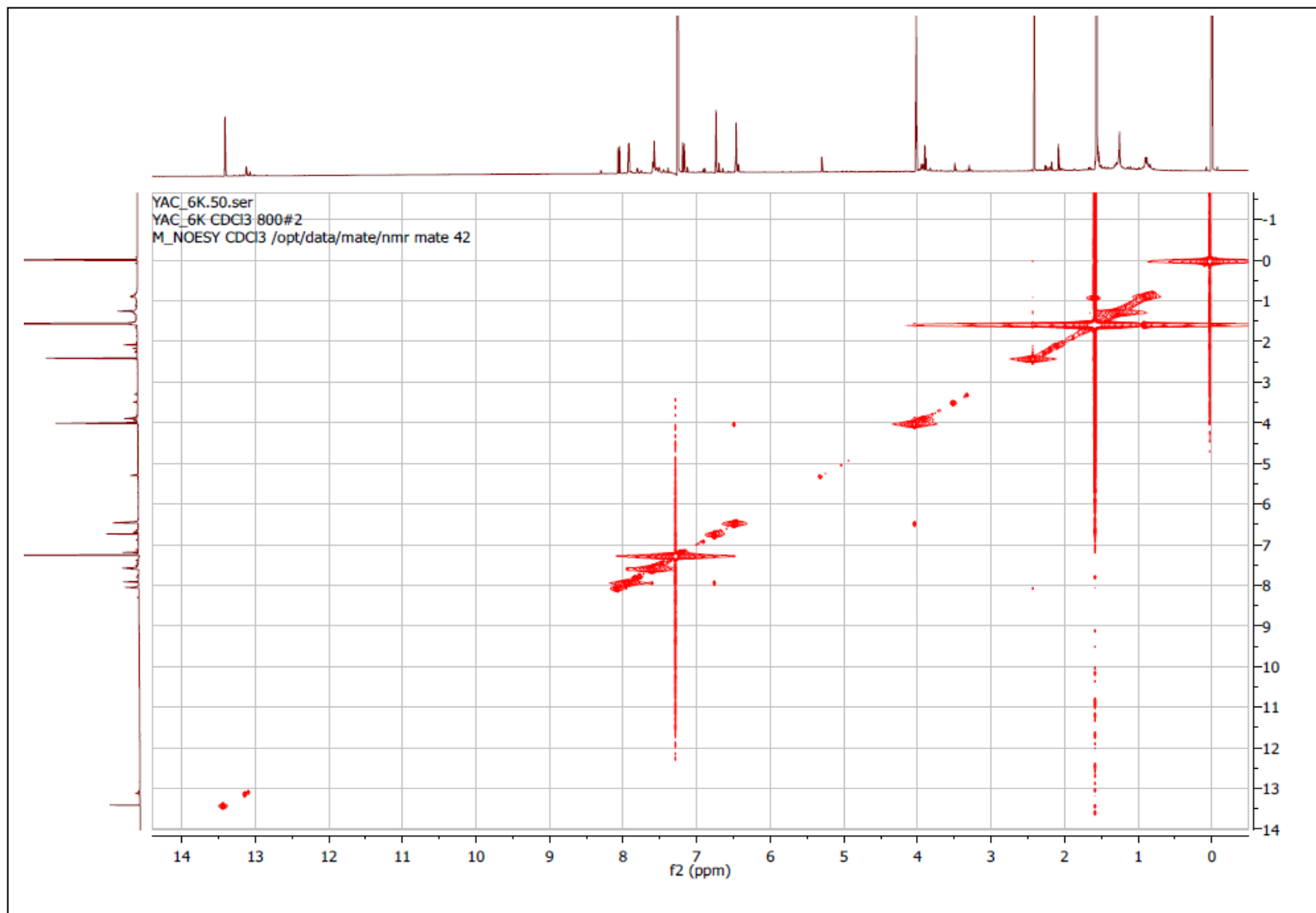


Fig. S11: NOESY spectrum of compound **2** (CDCl<sub>3</sub>)

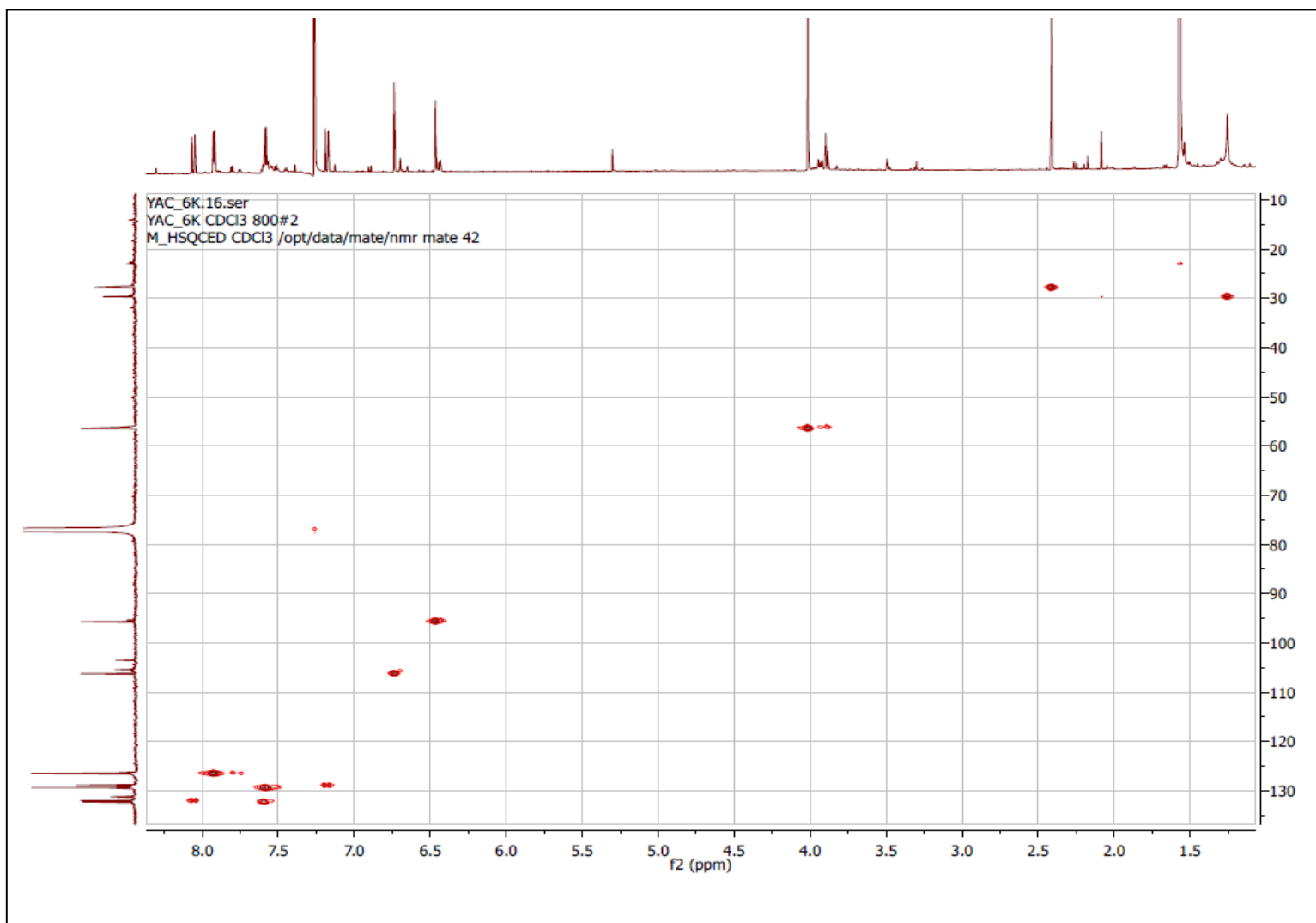


Fig. S12: HSQC spectrum of compound **2** (CDCl<sub>3</sub>)

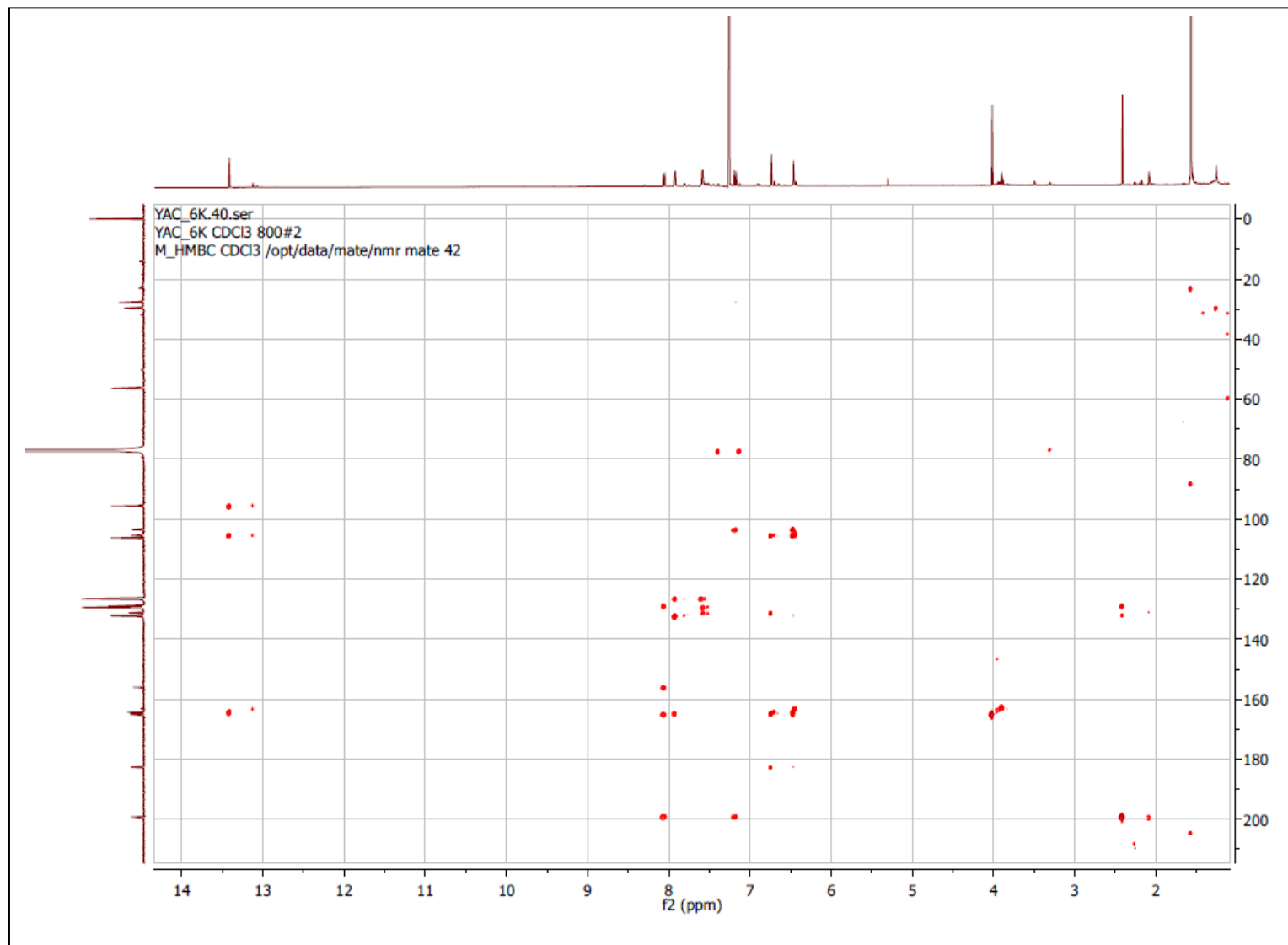


Fig. S13: HMBC spectrum of compound **2** (CDCl<sub>3</sub>)

Yoseph\_07 #160-173 RT: 0.59-0.63 AV: 14 NL: 1.92E2  
T: + c Full ms [ 35.00-500.00]

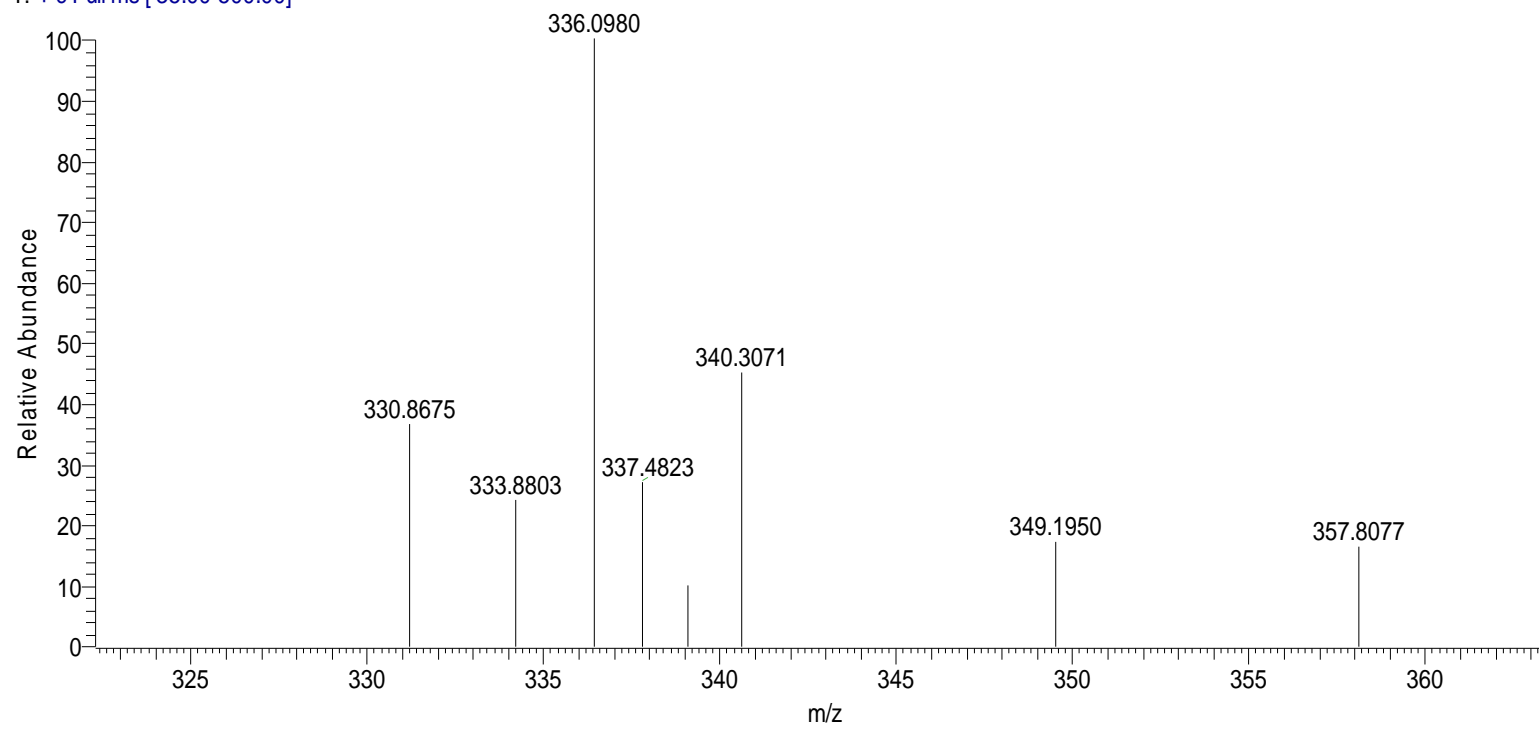


Fig. S14: HRMS of compound 2

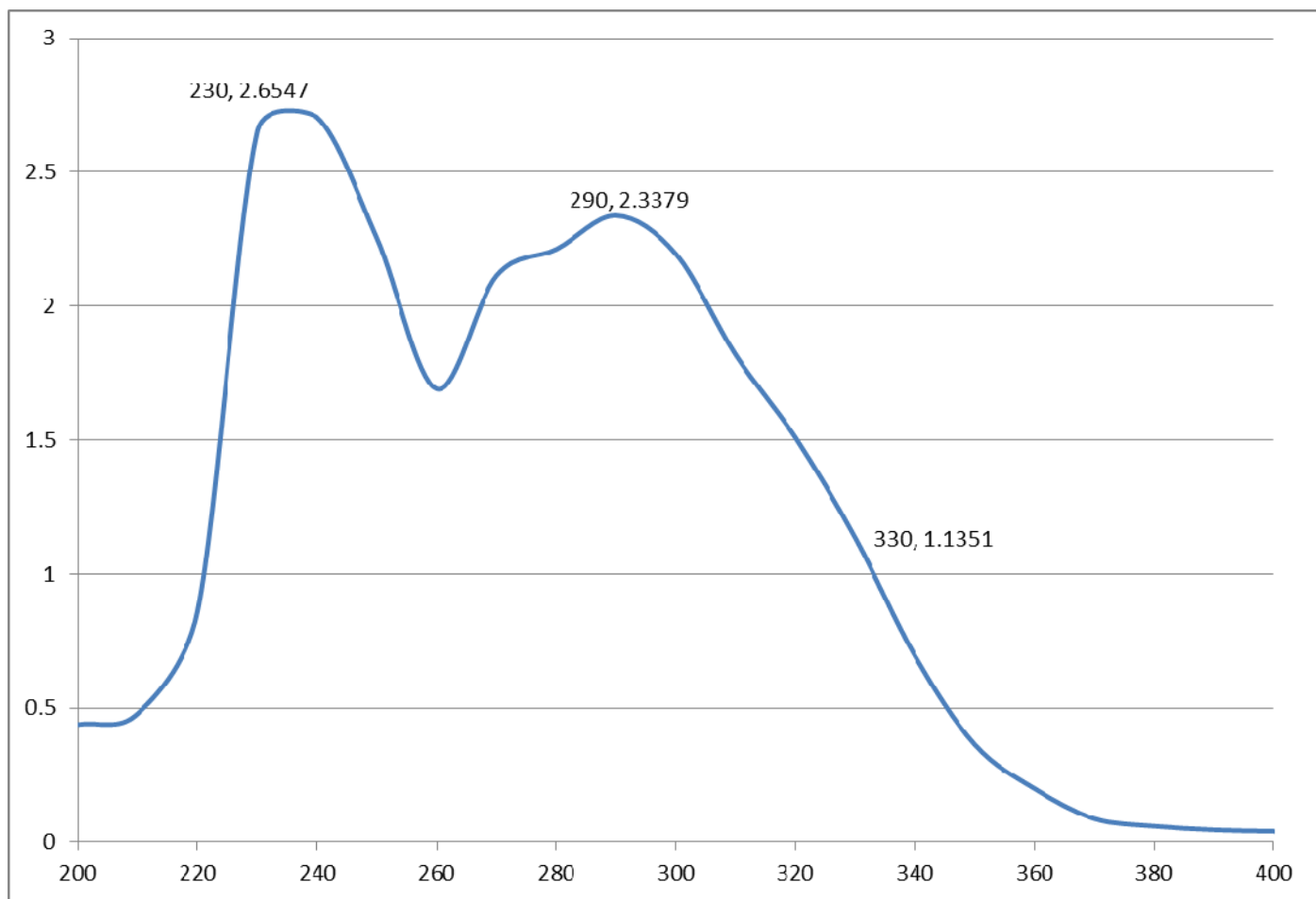


Fig. S15: UV spectrum of compound 2



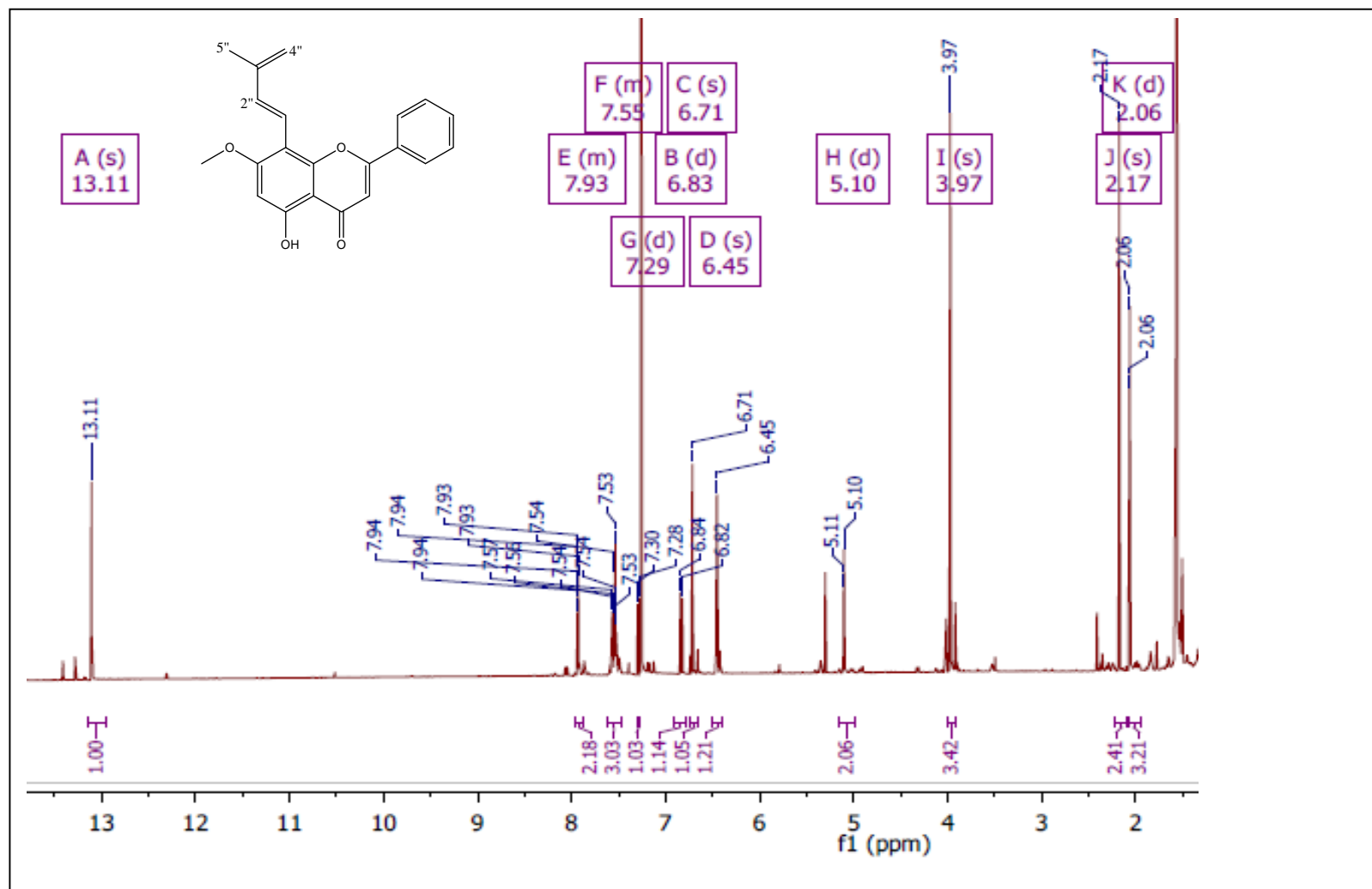


Fig. S16:  $^1\text{H}$  NMR spectrum of compound 3 (800 MHz;  $\text{CDCl}_3$ )

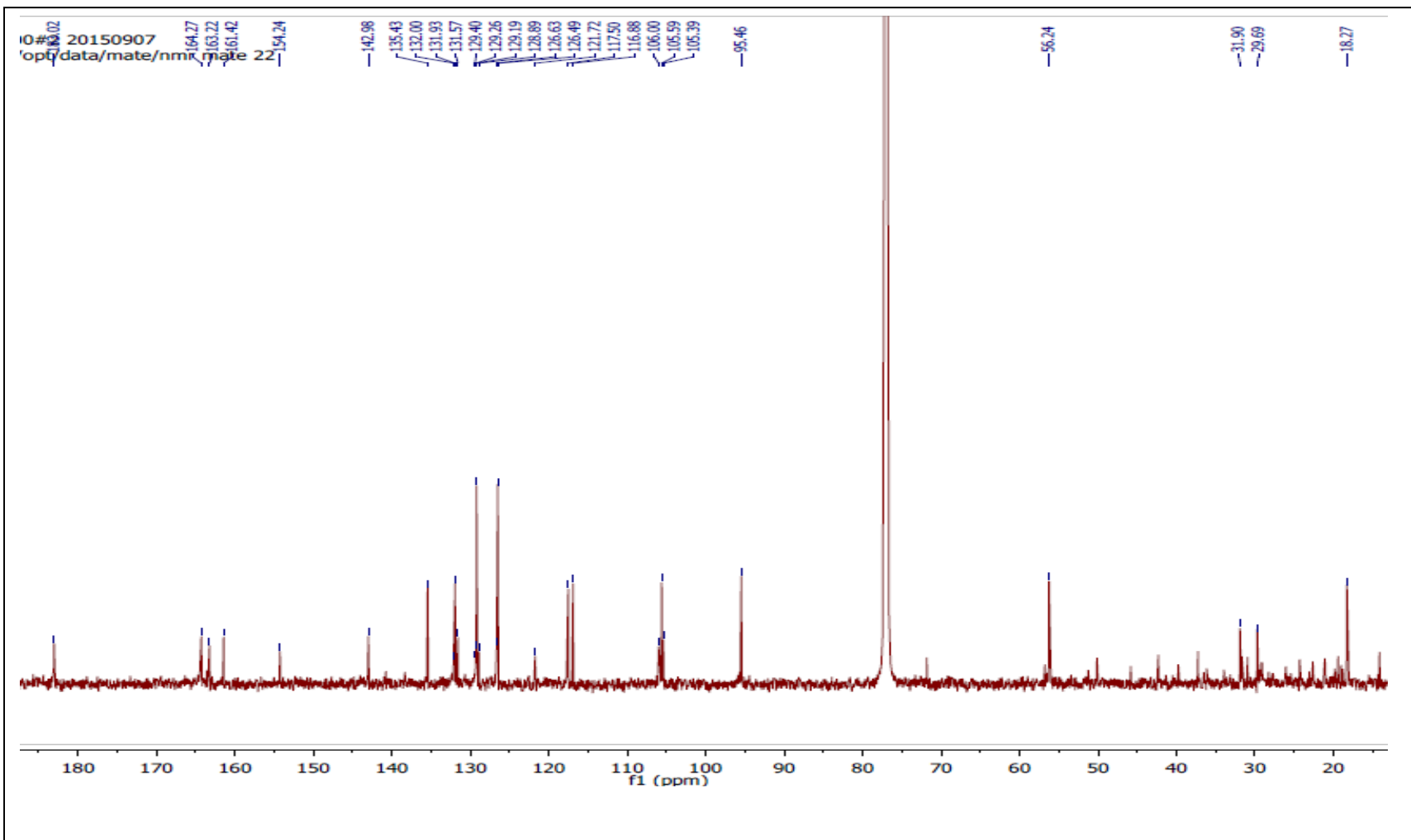


Fig. S17:  $^{13}\text{C}$  NMR spectrum of compound **3** (200 MHz;  $\text{CDCl}_3$ )

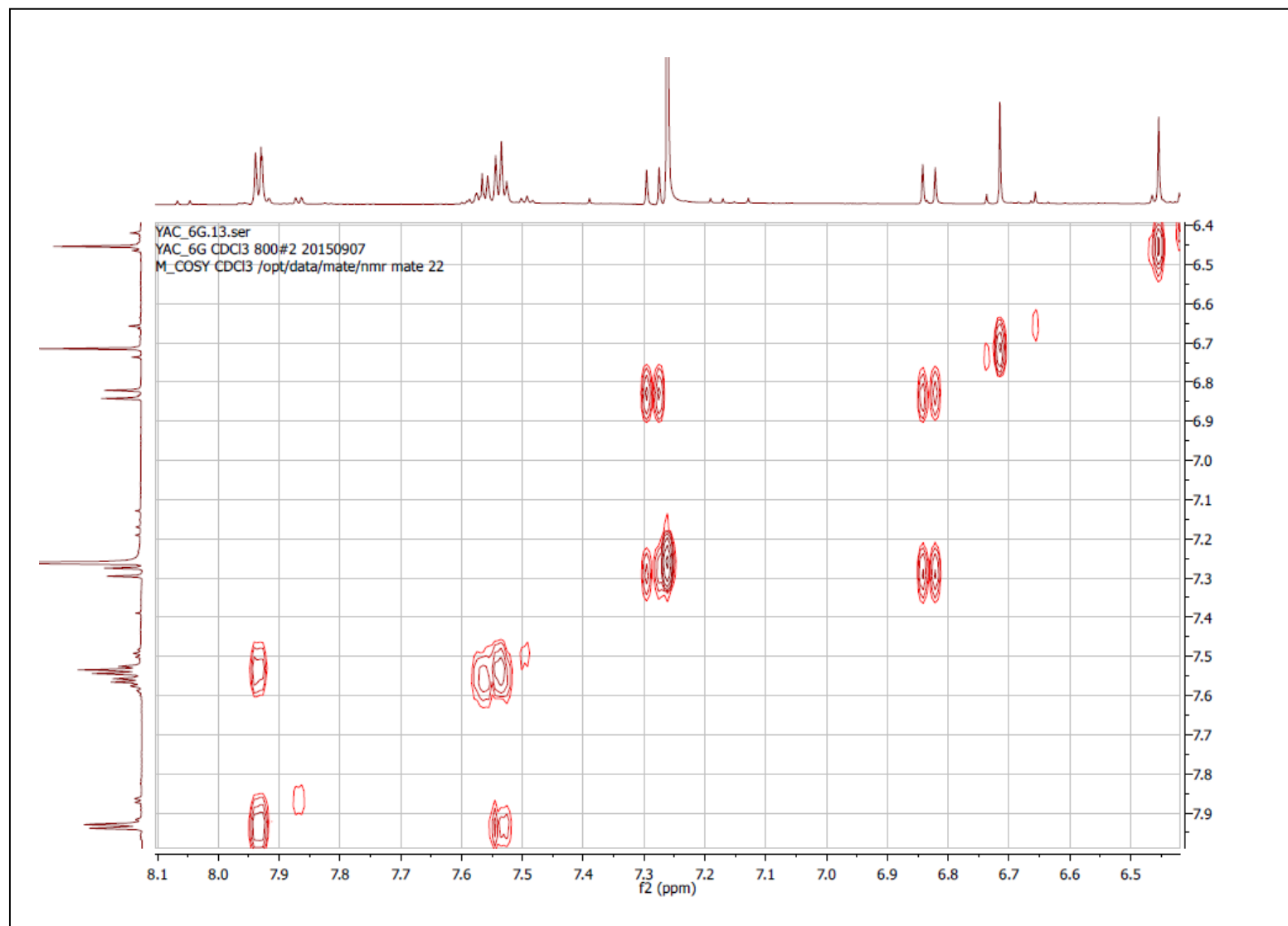


Fig. S18: COSY NMR spectrum of compound **3** (CDCl<sub>3</sub>)

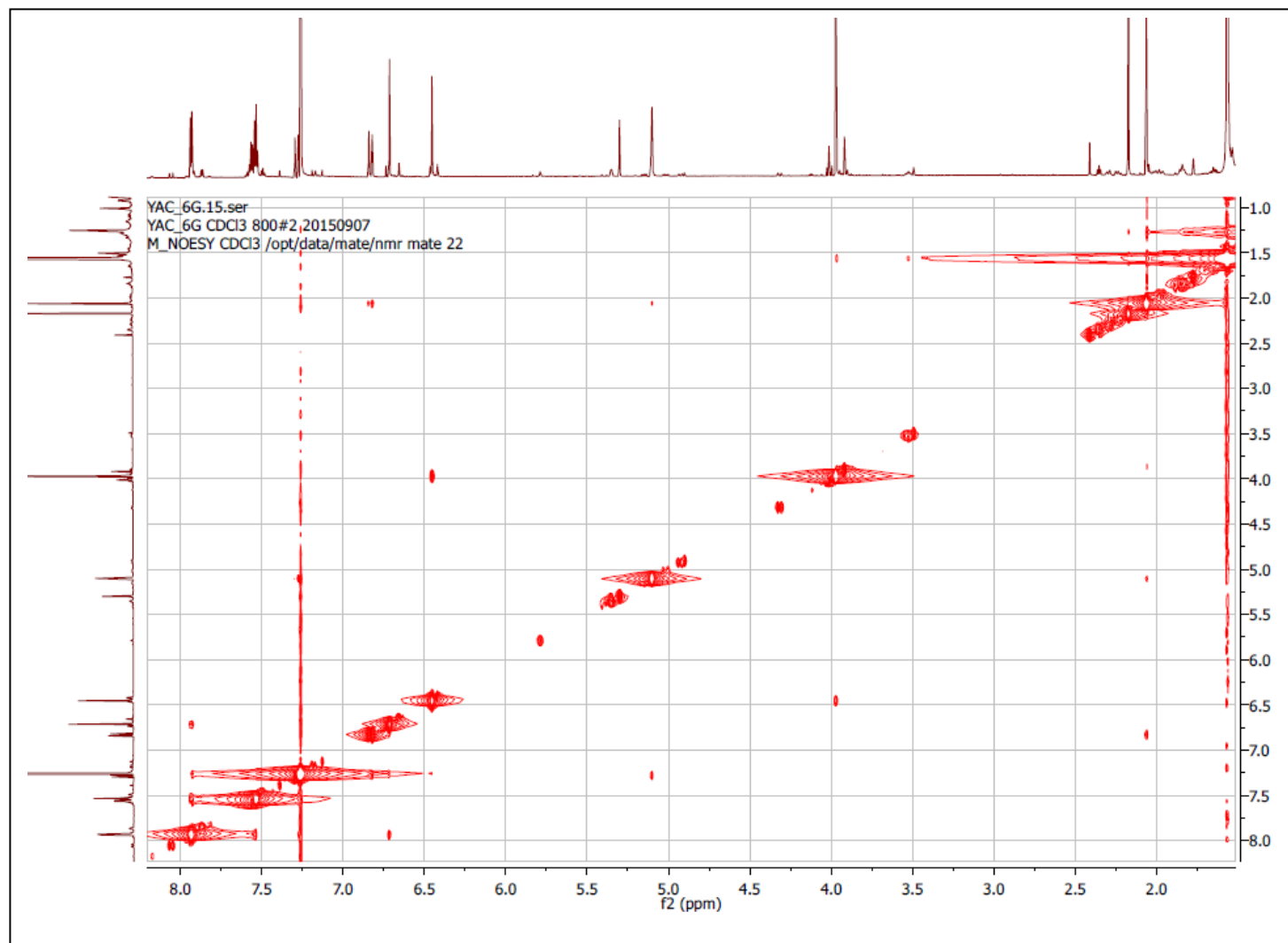


Fig. S19: NOESY spectrum of compound **3** (CDCl<sub>3</sub>)

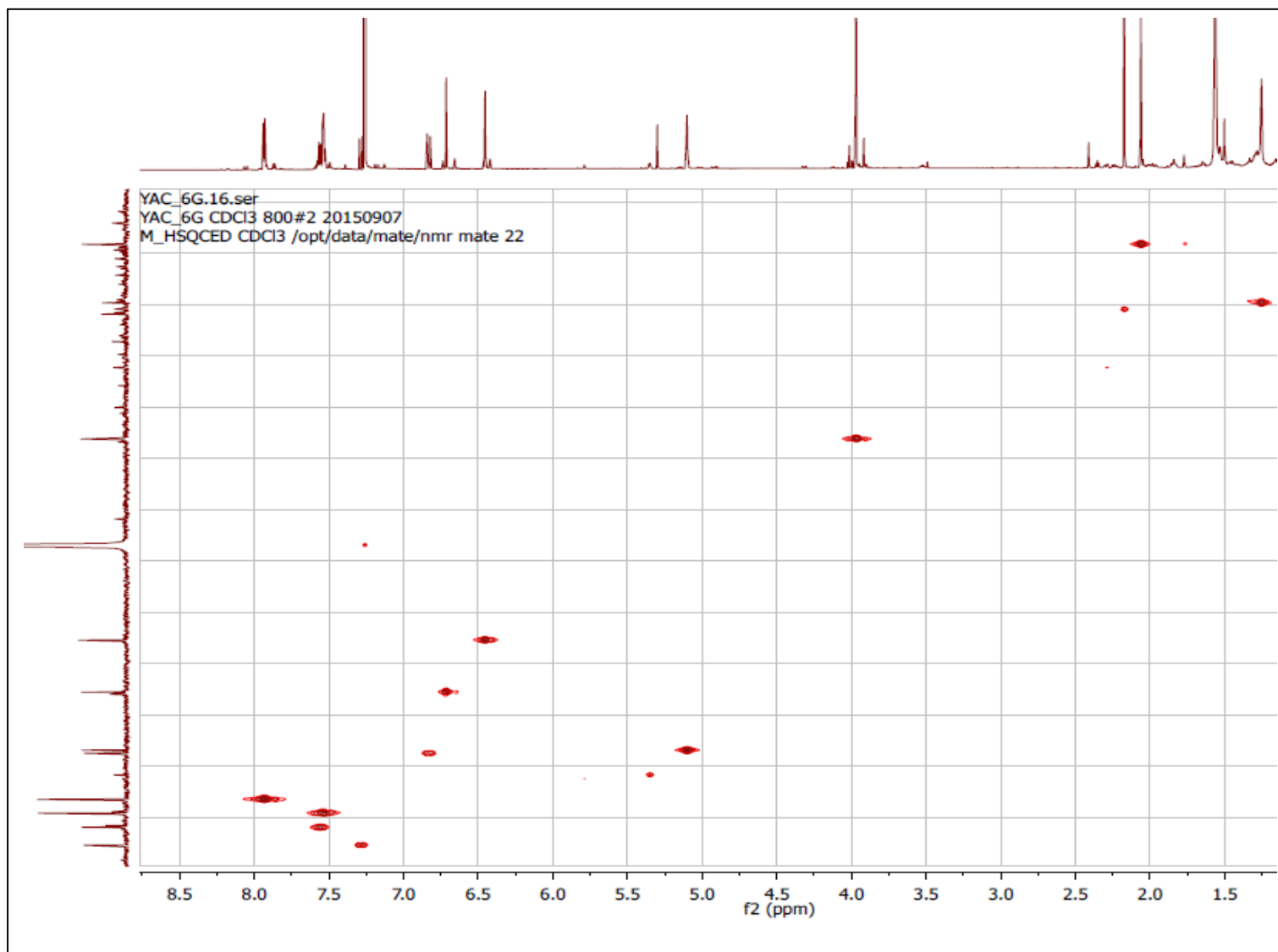


Fig. S20: HSQC NMR spectrum of compound **3** (CDCl<sub>3</sub>)

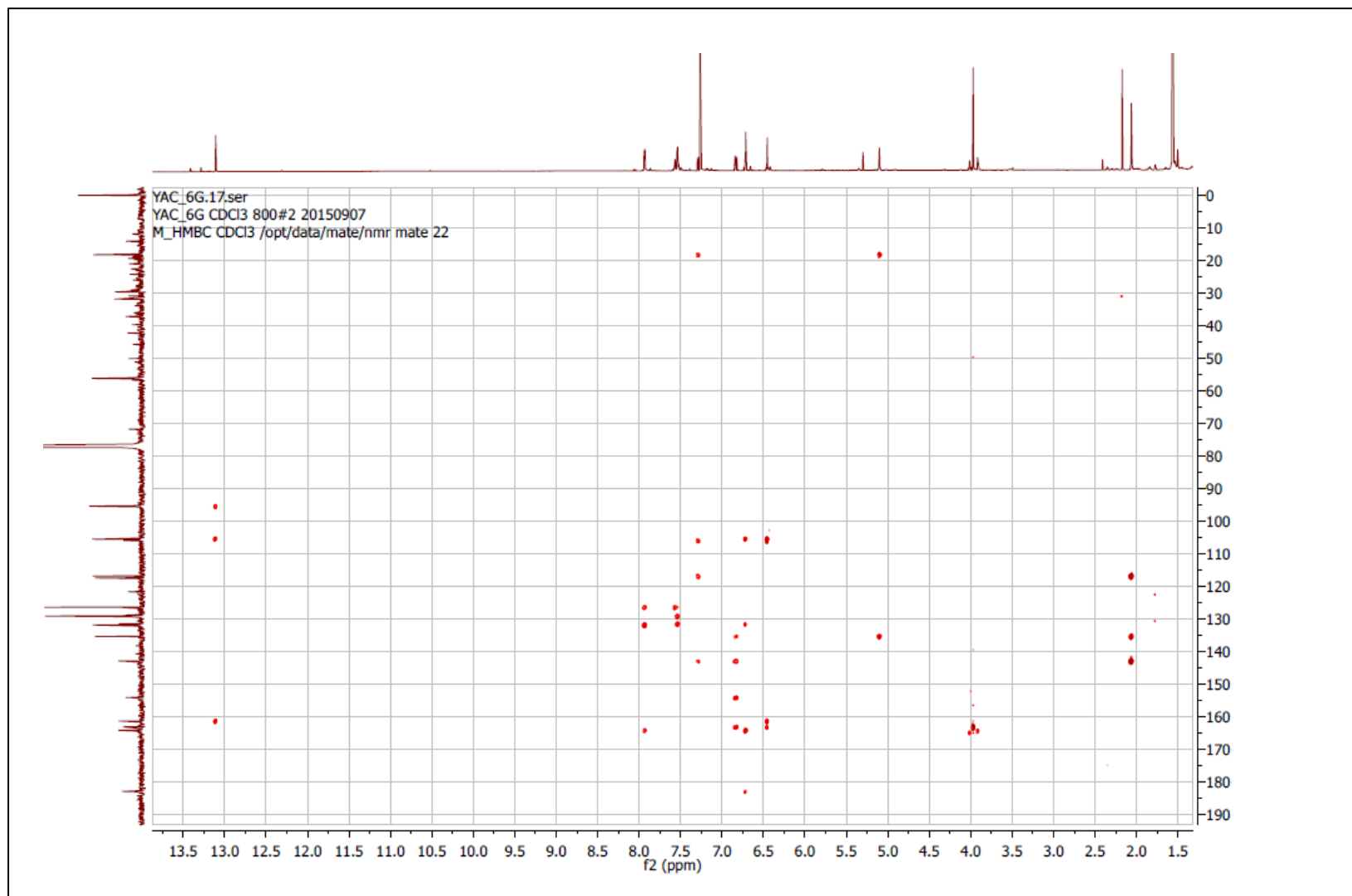


Fig. S21: HBMC spectrum of compound **3** (CDCl<sub>3</sub>)

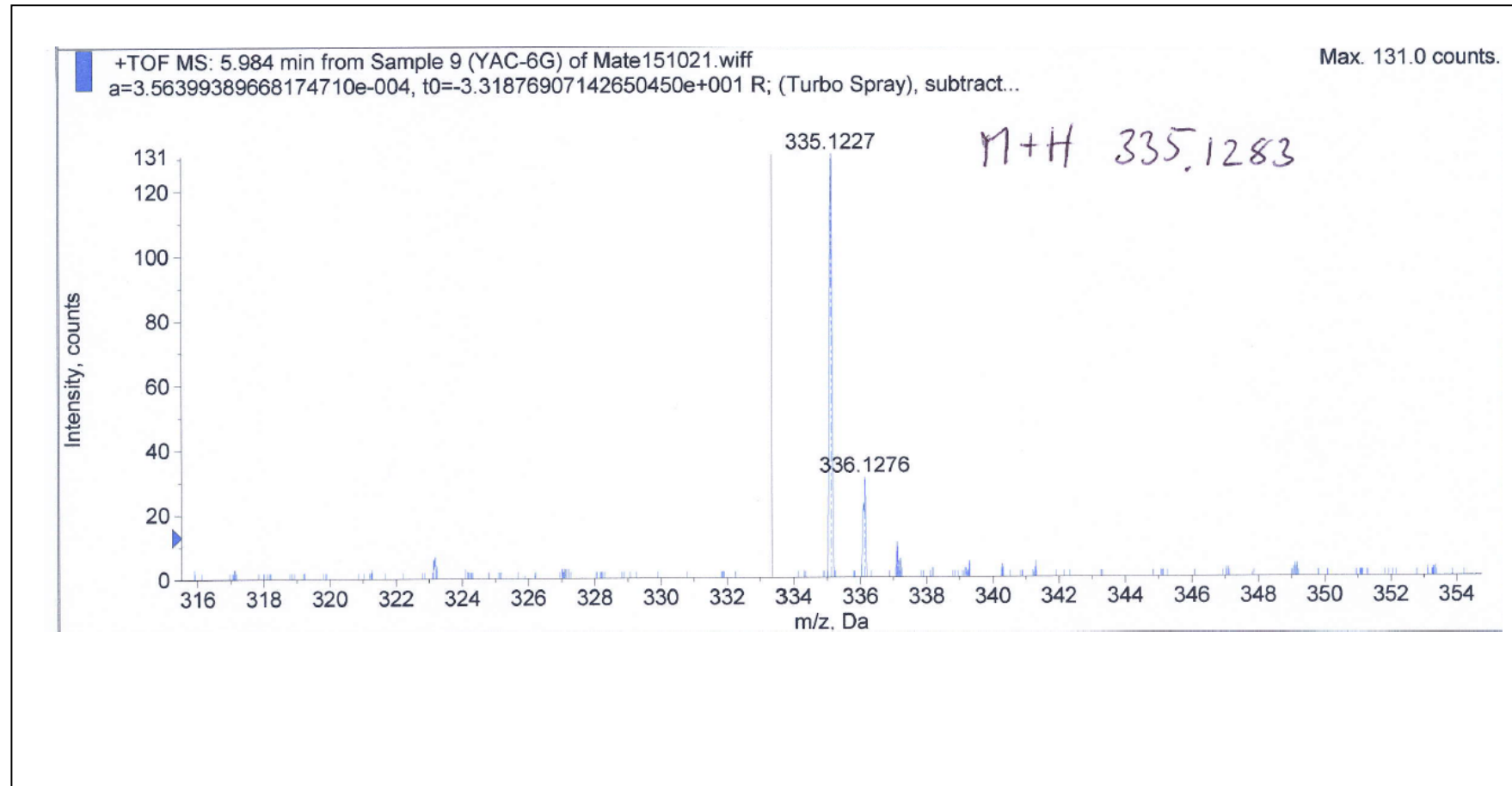


Fig. S22: HRMS of compound **3**

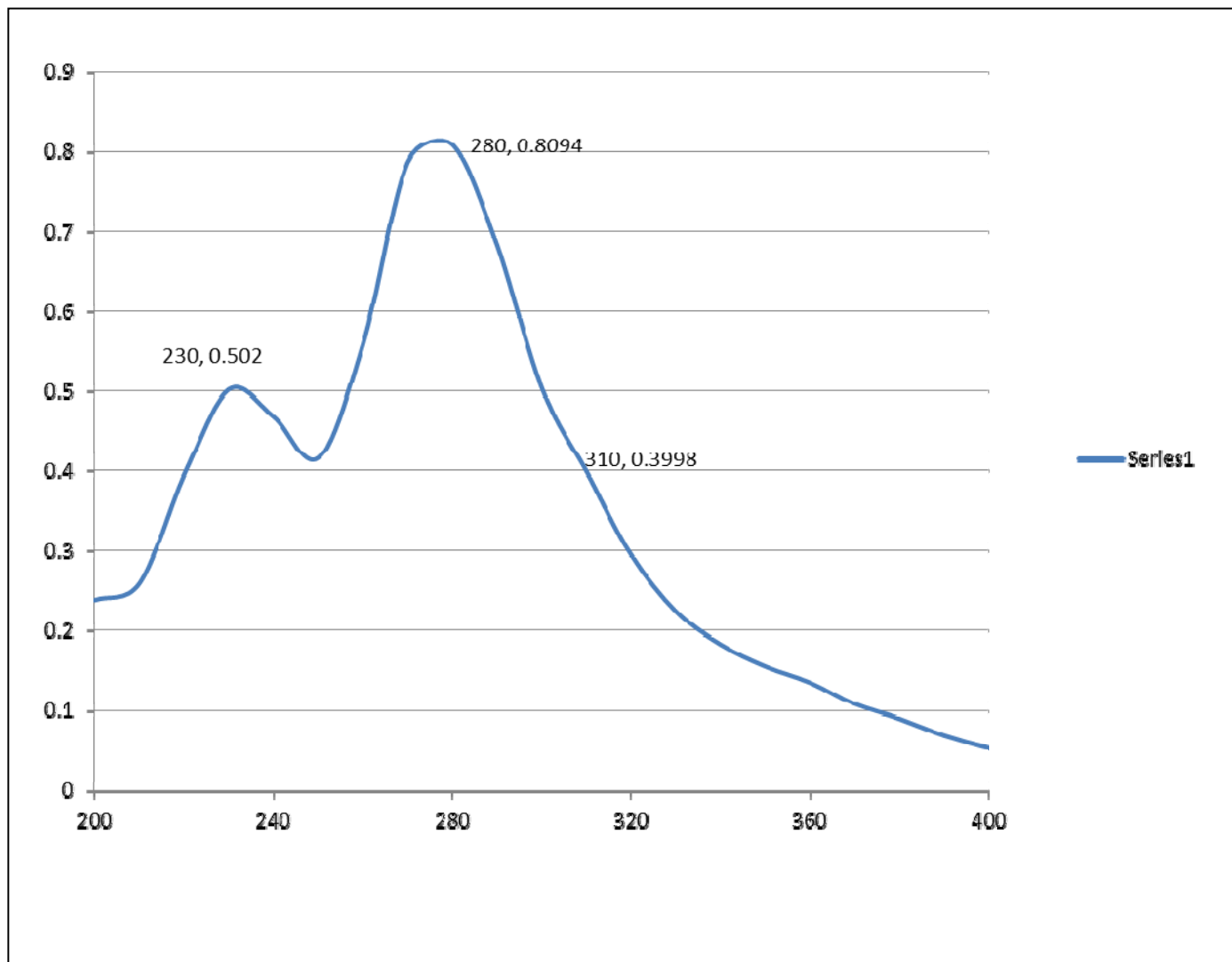


Fig. S23: UV spectrum of compound 3



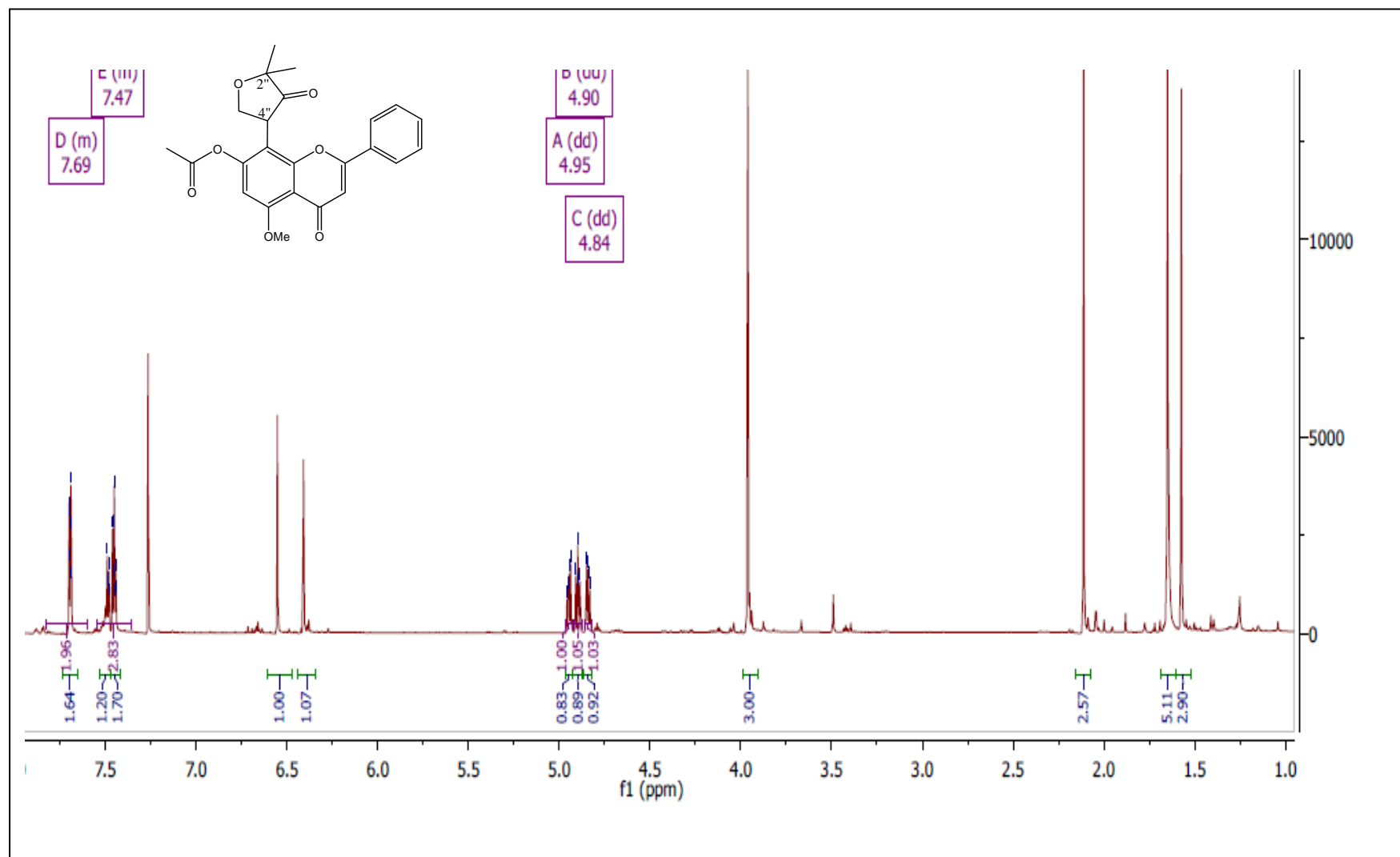


Fig. S24: <sup>1</sup>H NMR spectrum of compound 4 (800 MHz; CDCl<sub>3</sub>)

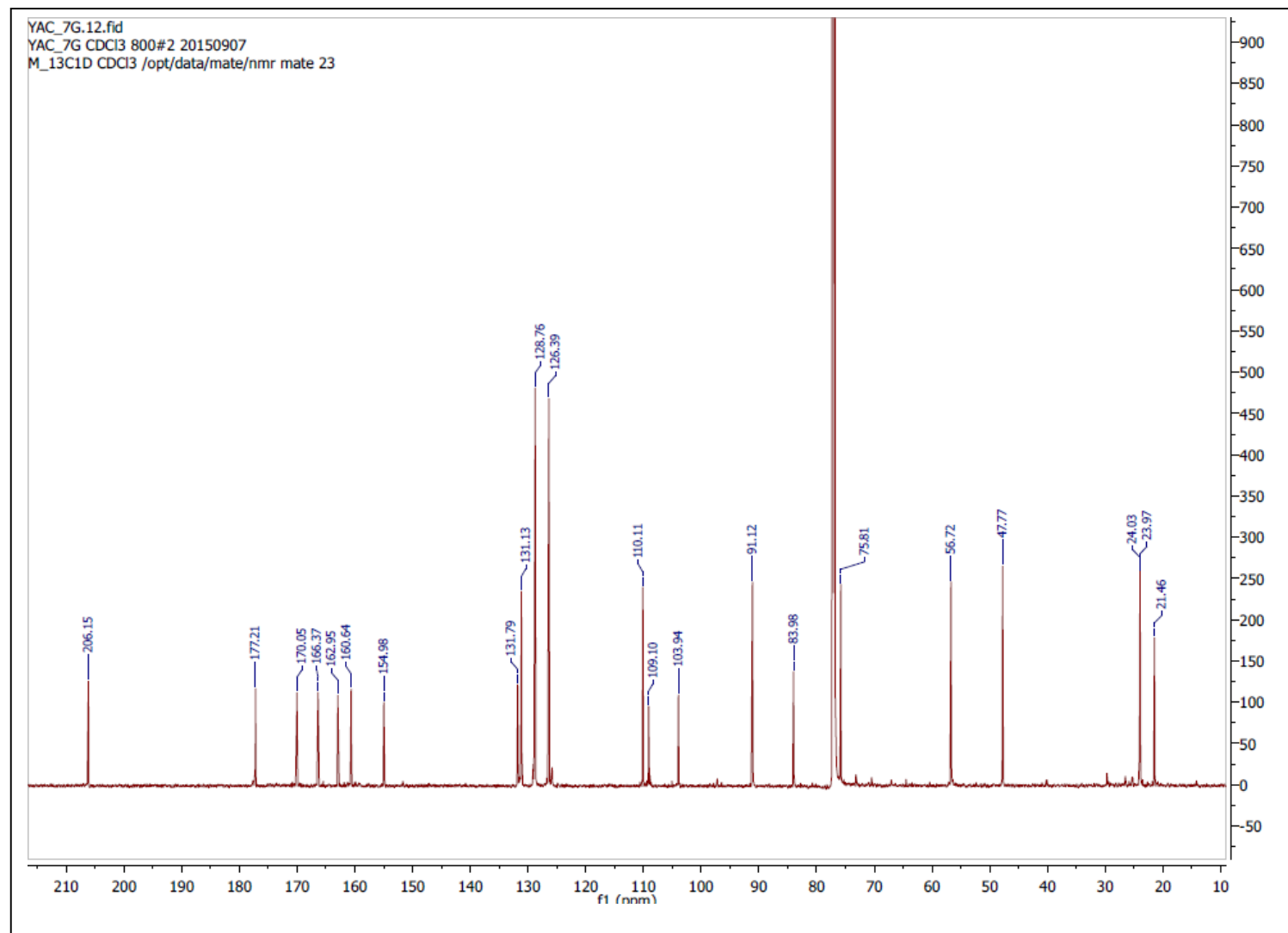


Fig. S25:  $^{13}\text{C}$  NMR spectrum of compound **4** (200 MHz;  $\text{CDCl}_3$ )

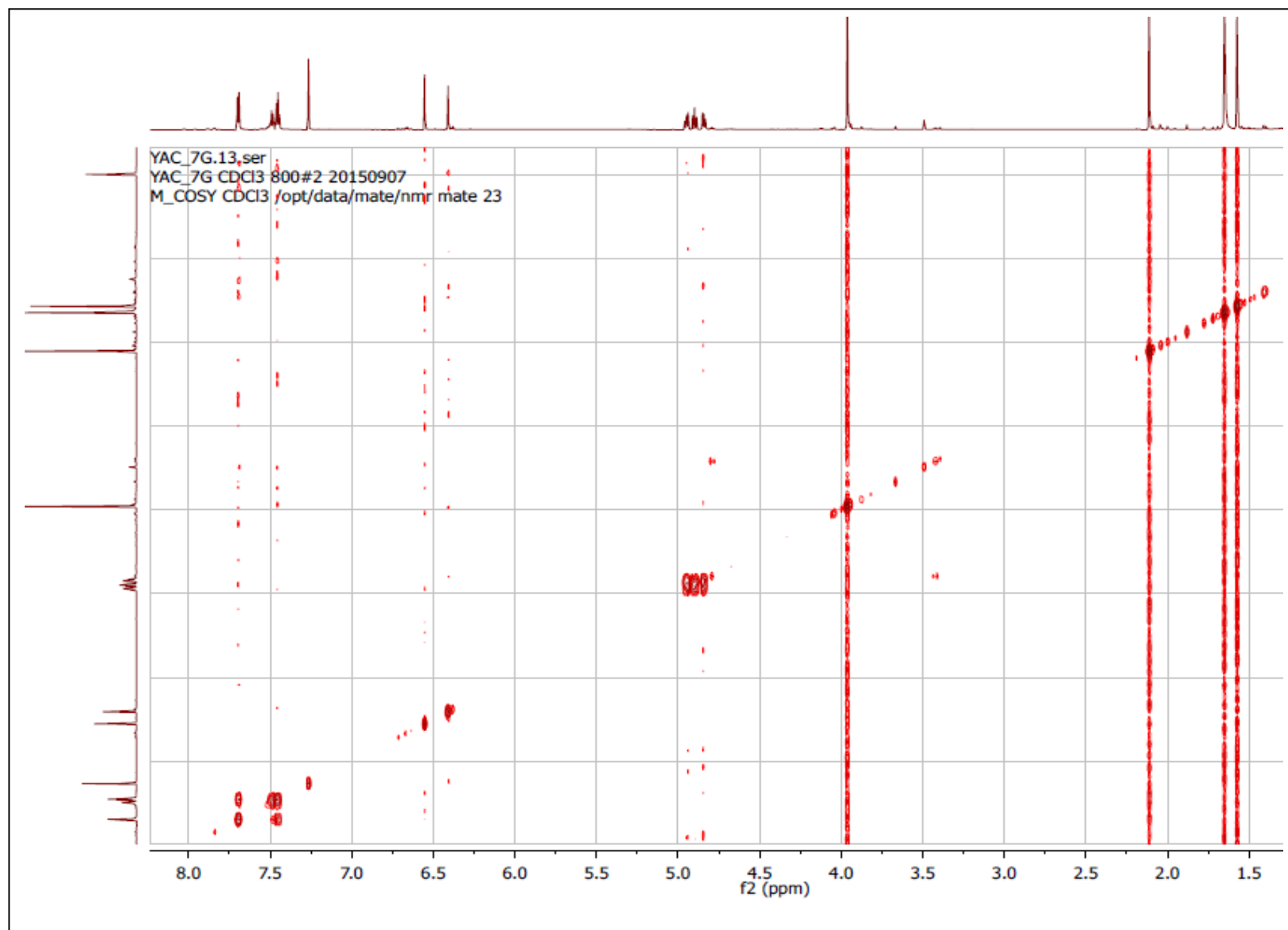


Fig. S26: COSY NMR spectrum of compound 4 (CDCl<sub>3</sub>)

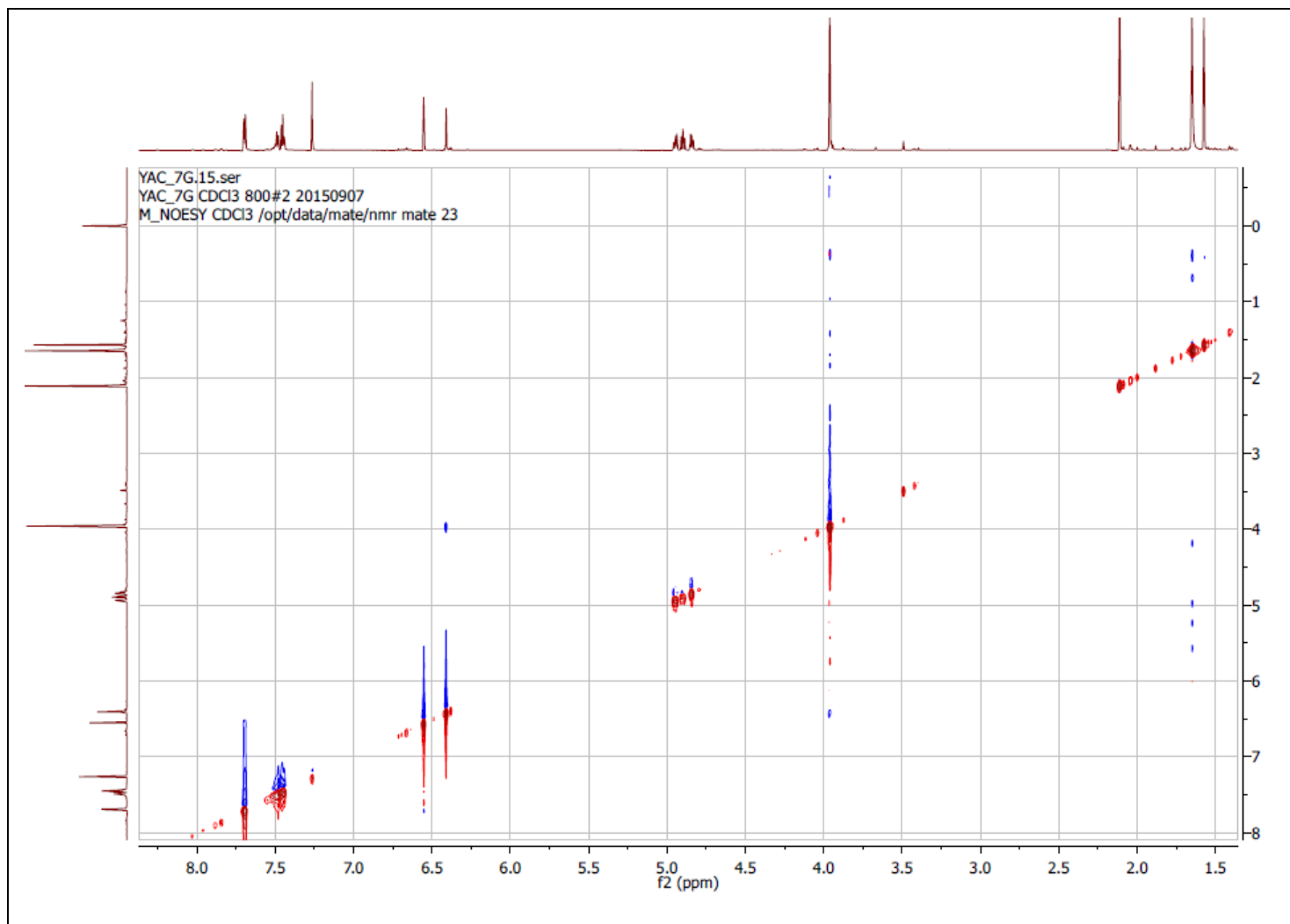


Fig. S27: NOESY spectrum of compound **4** (CDCl<sub>3</sub>)

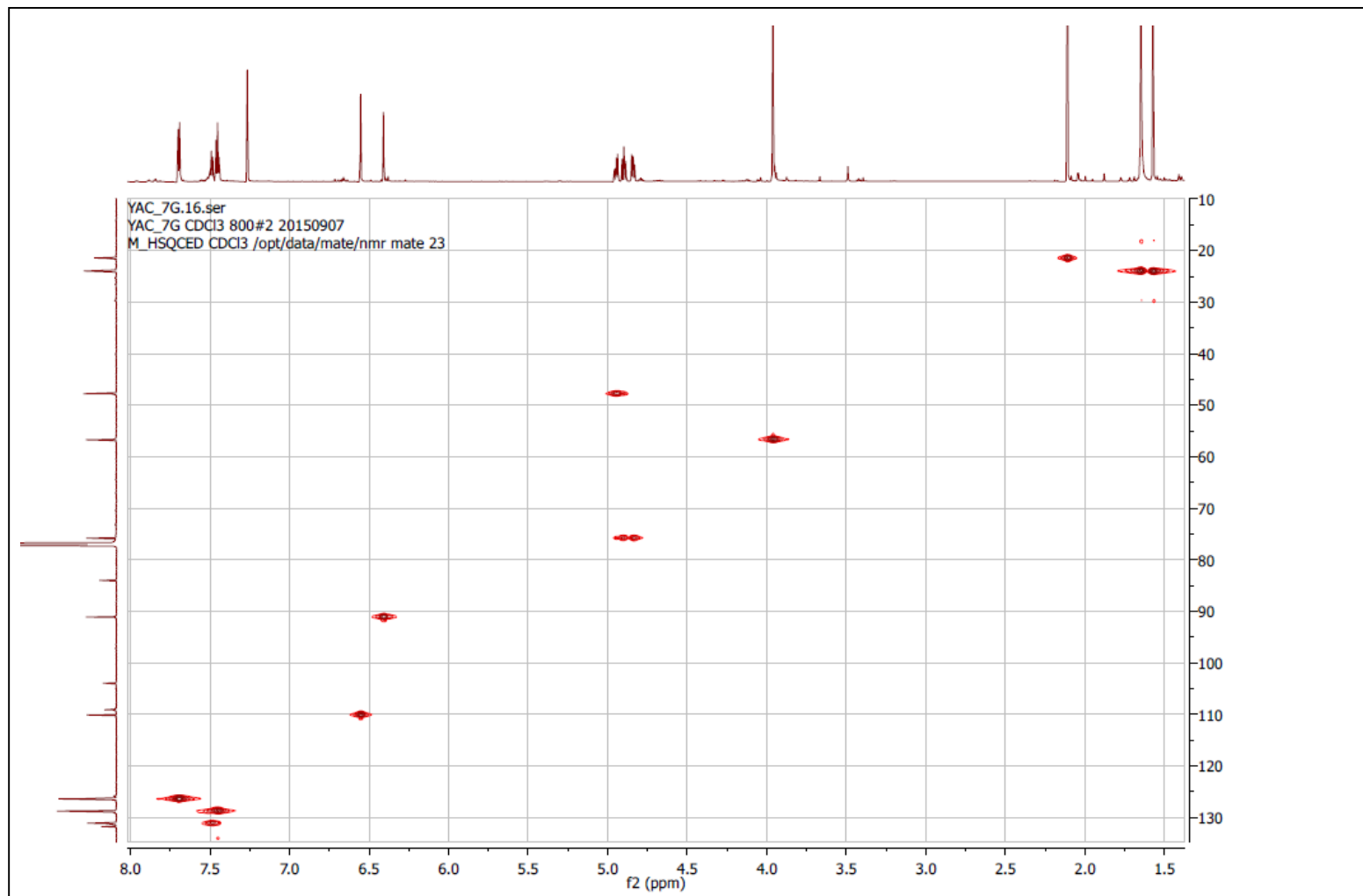


Fig. S28: HSQC NMR spectrum of compound **4** (CDCl<sub>3</sub>)

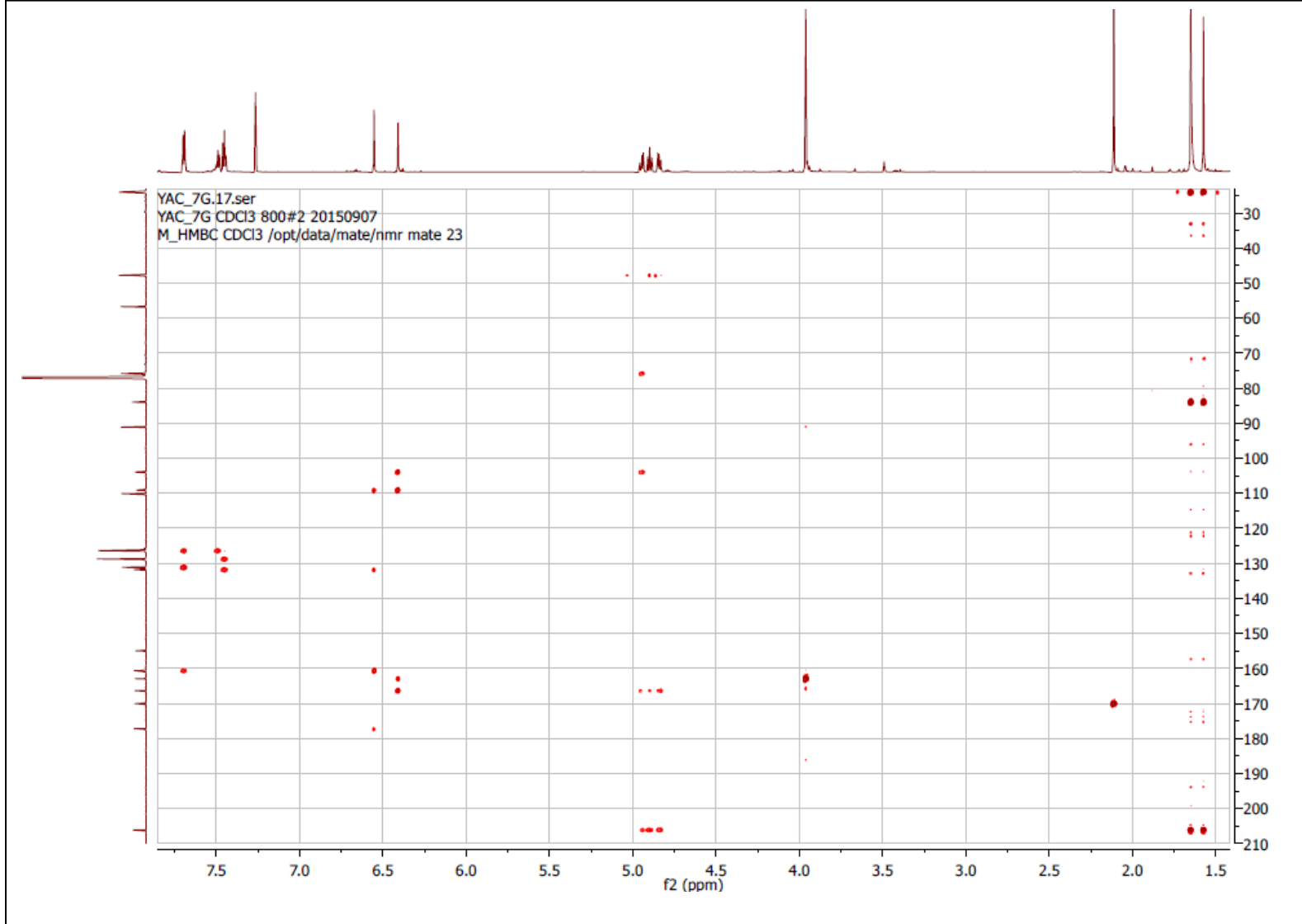


Fig. S29: HMBC NMR spectrum of compound 4 (CDCl<sub>3</sub>)

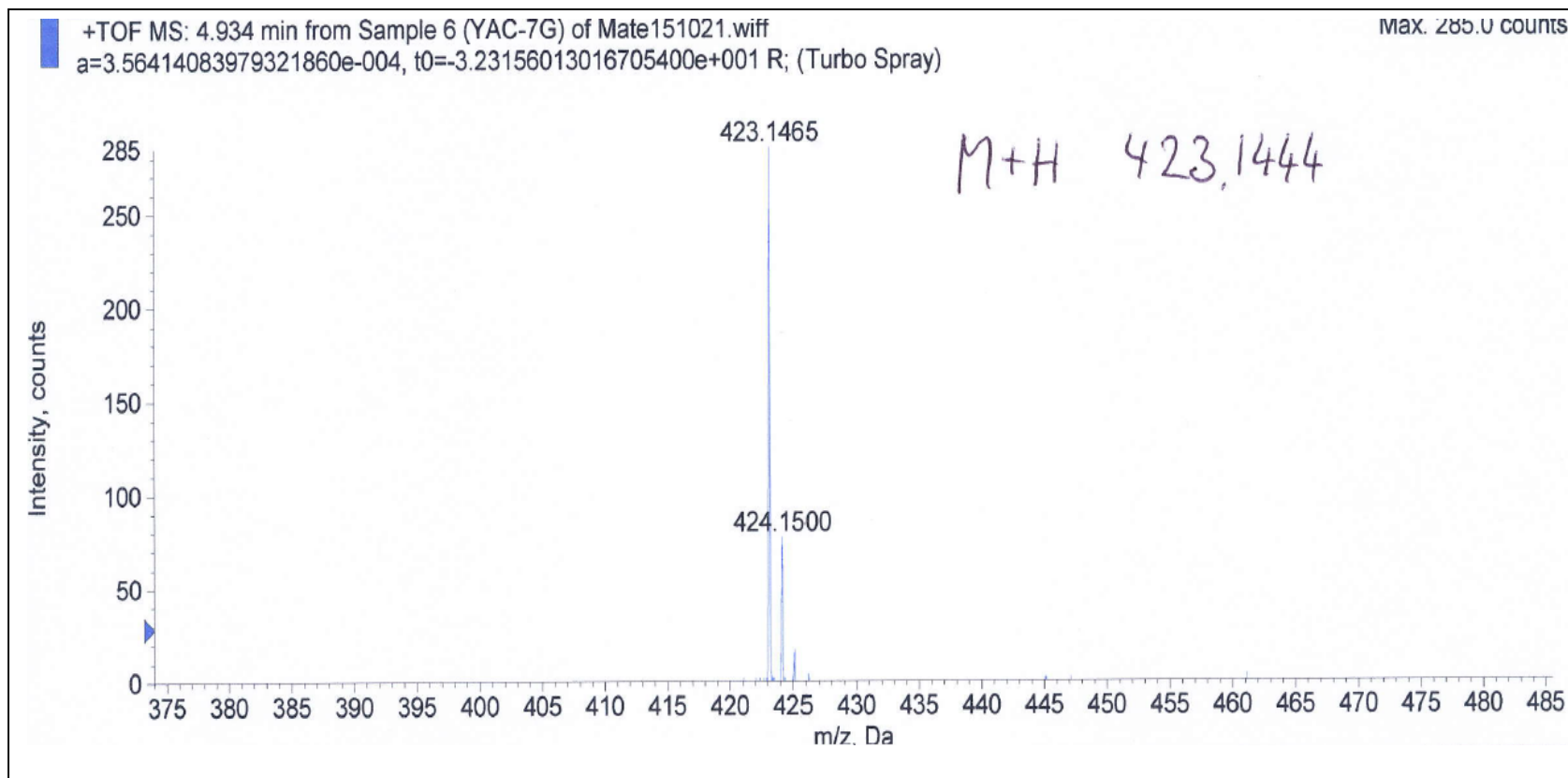


Fig. S30: HRMS of compound 4

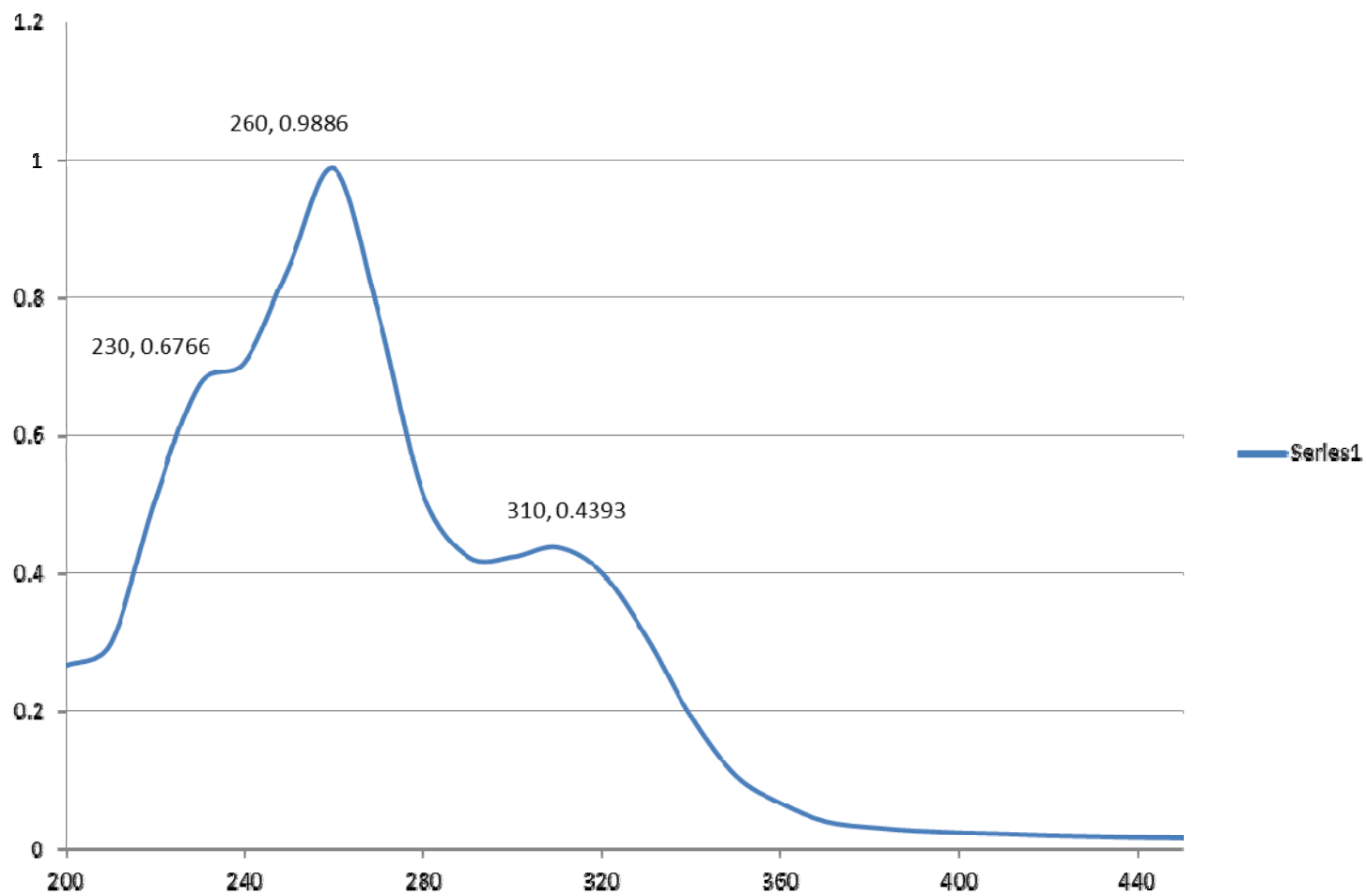


Fig. S31: UV spectrum of compound 4



Table S1.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **5**,  $\text{CDCl}_3$

Position	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>m</i>	HMBC correlations
2	153.91	8.00 <i>s</i>	C-3, C-4, C-8a, C-1'
3	122.94		
4	180.77		
4a	104.97		
5	163.73		
5-OH		12.95 <i>s</i>	
6	99.21	6.26 <i>d</i> (2.11)	C-4a, C-5, C-7, C-8
7	165.12		
8	93.88	6.39 <i>d</i> (2.11)	C-4a, C-6, C-7, C-8a
8a	158.26		
1'	122.60		
2',6'	130.0	7.41 <i>d</i> (8.65)	C-3, C-4', C-2', C-6'
3',5'	115.07	6.90 <i>d</i> (8.65)	C-1', C-3', C-4', C-5'
4'	157.05		

Table S2.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **6**,  $\text{CDCl}_3$

Position	$\delta$ (ppm)		HMBC correlations
	$\delta_{\text{C}}$	$\delta_{\text{H}}$ , <i>m</i> , ( <i>J</i> in Hz)	
<b>2</b>	78.98	5.42 <i>dd</i> (3.04, 13.03)	C-4, C-1', C-2'/6', C-8a
<b>3</b>	43.47	3.05 <i>dd</i> (13.00, 17.10) 2.85 <i>dd</i> (3.09, 17.12)	C-2, C-4, C-1' C-4, C-4a, C-1'
<b>4(C=O)</b>	196.20		
<b>4a</b>	103.19		
<b>5</b>	162.23		
<b>5(OH)</b>		11.99 <i>s</i>	C-5, C-6, C-4a
<b>6</b>	96.92	6.03 <i>s</i>	C-4a, C-5, C-7, C-8
<b>7</b>	163.72		
<b>8</b>	109.02		
<b>8a</b>	159.61		
<b>1'</b>	138.68	-	
<b>2'/6'</b>	125.93	7.46	C-2, C-2'/6', C-3'/5'
<b>3'/5'</b>	128.79	7.45	C-1', C-3'/5'
<b>4'</b>	128.57	7.39	C-2'/6'
<b>1''</b>	21.80	3.33 <i>bt</i>	C-7, C-8, C-8a, C-3'', C-2''
<b>2''</b>	121.56	5.22 <i>btt</i>	C-1'', 3''-Me <sub>2</sub>
<b>3''</b>	134.97		
<b>3''-Me<sub>2</sub></b>	17.84 25.82	1.73 1.73	C-3'', C-2''

Table S3. <sup>1</sup>H (800 MHz) and <sup>13</sup>C (200 MHz) NMR spectroscopic data for compound **7**, CDCl<sub>3</sub>

Position			HMBC correlations
	δ <sub>C</sub> (ppm)	δ <sub>H</sub> (ppm), <i>m</i> , ( <i>J</i> in Hz)	
<b>1</b>			
<b>2</b>	78.95	5.42 <i>dd</i> (13.17, 2.39)	
<b>3</b>	45.64	2.83 <i>dd</i> (16.46, 2.98) 2.99 <i>dd</i> (16.49, 13.16)	C-2, C-4, C-1' C-4, C-4a, C-1'
<b>4(C=O)</b>	176.94		
<b>4a</b>	105.66		
<b>5</b>	162.13		
<b>6</b>	93.79	6.06 <i>s</i>	C-4, C-4a, C-5, C-7, C-8
<b>7</b>	160.01		
<b>8</b>	102.89		
<b>8a</b>	158.79		
<b>1'</b>	138.95	-	
<b>2'/6'</b>	125.93	7.46	C-2, C-2'/6', C-3'/5', C-4'
<b>3'/5'</b>	128.73	7.42	C-3'/5', C-1'
<b>4'</b>	128.90	7.38	C-2'/6'
<b>2''</b>	78.03		
<b>3''</b>	126.32	5.47 <i>d</i> (10.0)	C-8, C-2'', 2''-Me <sub>2</sub>
<b>4''</b>	115.99	6.60 <i>d</i> (10.0)	C-7, C-8, C-8a, C-2''
2''-Me <sub>2</sub>	28.20 28.50	1.45 <i>s</i> 1.46 <i>s</i>	C-3'', C-2'', 2''-Me <sub>2</sub>
<b>OMe (C-5)</b>	56.20	3.90 <i>s</i>	C-5

Table S4.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **8**,  $\text{CDCl}_3$

Position	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>m</i>	HMBC correlations
2	153.91	8.00 <i>s</i>	C-3, C-4, C-8a, C-1'
3	122.94		
4	180.77		
4a	104.97		
5	163.73		
5-OH		12.95 <i>s</i>	
6	99.21	6.26 <i>d</i> (2.11)	C-4a, C-5, C-7, C-8
7	165.12		
8	93.88	6.39 <i>d</i> (2.11)	C-4a, C-6, C-7, C-8a
8a	158.26		
1'	122.60		
2',6'	130.0	7.41 <i>d</i> (8.65)	C-3, C-4', C-2', C-6'
3',5'	115.07	6.90 <i>d</i> (8.65)	C-1', C-3', C-4', C-5'
4'	157.05		

Table S5.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **9**,  $\text{CDCl}_3$

Position	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>m</i>	HMBC correlations
2	161.07		
3	108.86	6.63 <i>s</i>	C-2, C-4, C-4a, C-1'
4	204.51		
4a	109.10		
5	161.23		
6	91.63	6.45 <i>s</i>	C-4, C-4a, C-5, C-7, C-8
7	161.45		
8	98.30		
8a	156.75		
1'	131.84		
2',6'	126.21	7.71 <i>m</i>	C-2, C-4', C- 2', C-6'
3',5'	128.74	7.41 <i>m</i>	C-1', C-3', C-5'
4'	131.11	7.45 <i>m</i>	C-2', C-6'
2''	88.07		
3''	204.51		
4''	109.51		
5''	175.67	6.31, <i>s</i>	C-2'', C-3'', C-4''
2 x Me-2''	23.05	1.57, <i>s</i>	C-3'', C-2''

Table S6.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **10**,  $\text{CDCl}_3$

Position			HMBC correlations
	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>m</i> , ( <i>J</i> in Hz)	
<b>1</b>		-	
<b>2</b>	158.39		
<b>3</b>	135.07		
<b>4(C=O)</b>	178.36		
<b>4a</b>	106.16		
<b>5</b>	161.59		
<b>5(OH)</b>		12.61 <i>s</i>	<b>C-4a, C-6, C-5</b>
<b>6</b>	94.19	6.74 <i>d</i> (2.20)	<b>C-4a, C-6, C-8a, C-7</b>
<b>7</b>	162.13		
<b>8</b>	99.14	6.48 <i>d</i> (2.20)	<b>C-6, C-4a, C-7</b>
<b>8a</b>	156.67		
<b>1'</b>	120.98	-	
<b>2'/6'</b>	130.59	7.81 <i>d</i> (8.69)	<b>C-3'/5', C-2'/6', C-4'</b>
<b>3'/5'</b>	115.18	6.96 <i>d</i> (8.21)	<b>C-3'/5', C-1', C-4'</b>
<b>4'</b>	160.36	-	
<b>2''</b>	98.44	5.58 <i>s</i>	<b>C-7</b>
<b>3''</b>	70.26	3.86 <i>bd</i>	
<b>4''</b>	71.13	3.16 <i>m</i>	
<b>5''</b>	72.04	3.33 <i>t</i>	
<b>6''</b>	70.54	3.44 <i>m</i>	
<b>2'''</b>	102.10	5.42 <i>s</i>	<b>C-3</b>
<b>3'''</b>	70.53	4.00 <i>bd</i>	
<b>4'''</b>	70.78	3.50 <i>bd</i>	
<b>5'''</b>	70.67	3.66 <i>bd</i>	
<b>6'''</b>	71.55	3.15 <i>m</i>	
<b>Me(6'')</b>	18.36	1.15 <i>d</i>	
<b>Me(6''')</b>	17.95	0.82 <i>d</i>	

Table S7.  $^1\text{H}$  (800 MHz) and  $^{13}\text{C}$  (200 MHz) NMR spectroscopic data for compound **11**,  $\text{CDCl}_3$

Position			
	$\delta_{\text{C}}$ (ppm)	$\delta_{\text{H}}$ (ppm), <i>m</i> , ( <i>J</i> in Hz)	HMBC correlations
<b>1</b>	70.96	2.59 <i>d</i> (2.26)	
<b>2</b>	69.25	2.44 <i>dd</i> (2.25, 9.73)	C-5
<b>3</b>	69.78	2.39 <i>dd</i> (2.24, 9.70)	
<b>4</b>	71.54	2.28 <i>t</i> (9.46, 9.46)	C-3, C-5,
<b>5</b>	82.14	1.95 <i>t</i> (9.46, 9.46)	C-3, C-4, OMe-3,
<b>6</b>	70.66	2.59 <i>d</i> (2.26)	
<b>OMe-5</b>	58.10	2.31	