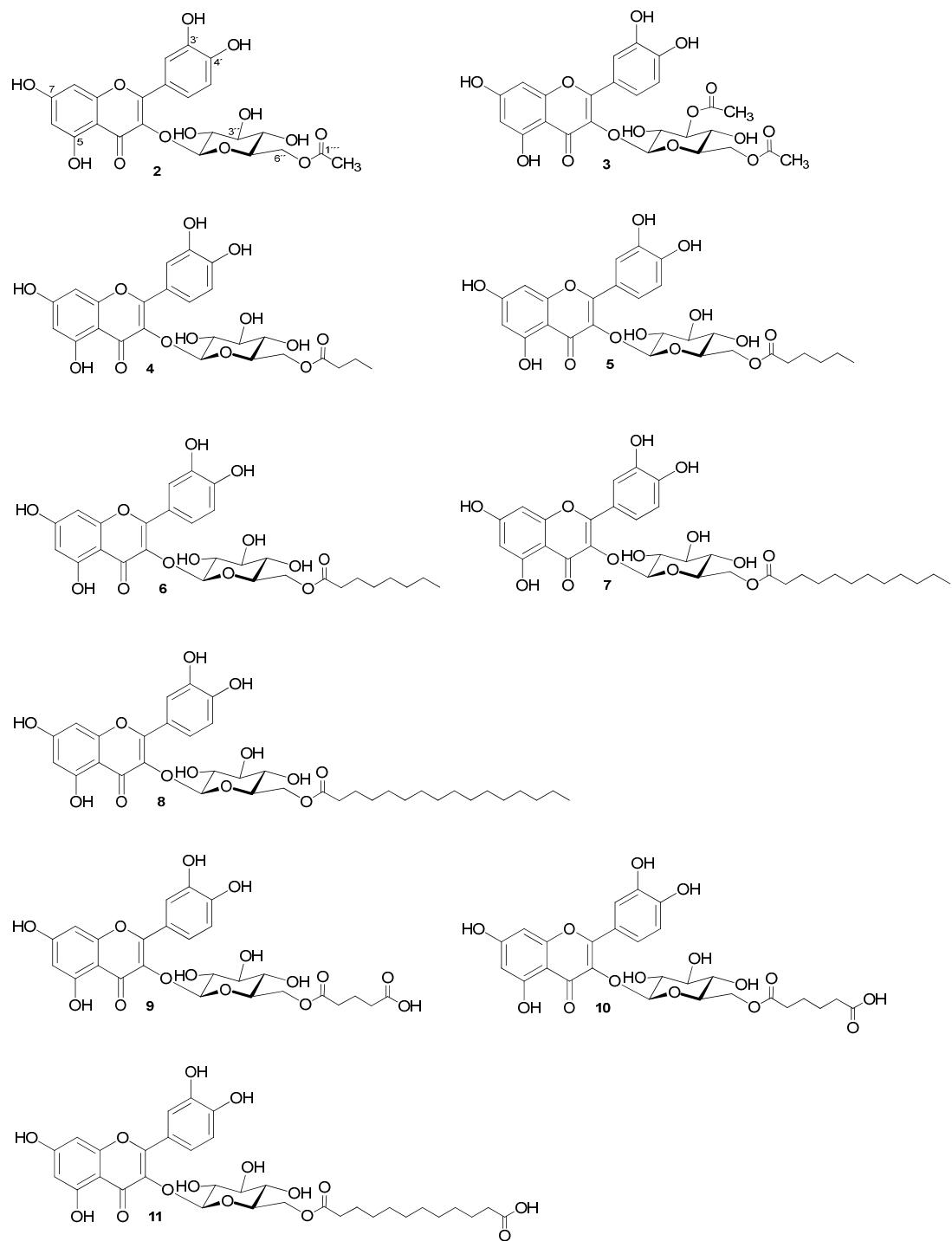


# Supplementary Materials: Isoquercitrin Esters with Mono- or Dicarboxylic Acids: Enzymatic Preparation and Properties

Eva Vavříková, Fanny Langschwager, Lubica Jezova-Kalachová, Alena Křenková, Barbora Mikulová, Marek Kuzma, Vladimír Křen and Kateřina Valentová

Content	Page
<b>Figure S1</b> Structures of compounds 2–11 .....	S3
<b>Table S1</b> $^{13}\text{C}$ NMR data of prepared compounds 2–8 .....	S4
<b>Table S2</b> $^1\text{H}$ NMR data of prepared compounds 2 and 3 .....	S6
<b>Table S3</b> $^1\text{H}$ NMR data of prepared compounds 4–8 .....	S7
<b>Table S4</b> $^{13}\text{C}$ NMR data of prepared compounds 9–11 .....	S9
<b>Table S5</b> $^1\text{H}$ NMR data of prepared compounds 9–11 .....	S10
<b>Figure S2</b> $^{13}\text{C}$ NMR spectrum of compound 2 .....	S11
<b>Figure S3</b> $^1\text{H}$ NMR spectrum of compound 2 .....	S12
<b>Figure S4</b> HPLC chromatogram of compound 2 .....	S13
<b>Figure S5</b> $^{13}\text{C}$ NMR spectrum of compound 3 .....	S14
<b>Figure S6</b> $^1\text{H}$ NMR spectrum of compound 3 .....	S15
<b>Figure S7</b> HPLC chromatogram of compound 3 .....	S16
<b>Figure S8</b> $^{13}\text{C}$ NMR spectrum of compound 4 .....	S17
<b>Figure S9</b> $^1\text{H}$ NMR spectrum of compound 4 .....	S18
<b>Figure S10</b> HPLC chromatogram of compound 4 .....	S19
<b>Figure S11</b> $^{13}\text{C}$ NMR spectrum of compound 5 .....	S20
<b>Figure S12</b> $^1\text{H}$ NMR spectrum of compound 5 .....	S21
<b>Figure S13</b> HPLC chromatogram of compound 5 .....	S22
<b>Figure S14</b> $^{13}\text{C}$ NMR spectrum of compound 6 .....	S23
<b>Figure S15</b> $^1\text{H}$ NMR spectrum of compound 6 .....	S24
<b>Figure S16</b> HPLC chromatogram of compound 6 .....	S25
<b>Figure S17</b> $^{13}\text{C}$ NMR spectrum of compound 7 .....	S26
<b>Figure S18</b> $^1\text{H}$ NMR spectrum of compound 7 .....	S27
<b>Figure S19</b> HPLC chromatogram of compound 7 .....	S28
<b>Figure S20</b> $^{13}\text{C}$ NMR spectrum of compound 8 .....	S29
<b>Figure S21</b> $^1\text{H}$ NMR spectrum of compound 8 .....	S30
<b>Figure S22</b> HPLC chromatogram of compound 8 .....	S31
<b>Figure S23</b> $^{13}\text{C}$ NMR spectrum of compound 9 .....	S32
<b>Figure S24</b> $^1\text{H}$ NMR spectrum of compound 9 .....	S33
<b>Figure S25–27</b> Details of $^1\text{H}$ NMR spectrum of compound 9 .....	S34–S36
<b>Figure S28</b> HSQC NMR spectrum of compound 9 .....	S37
<b>Figure S29–31</b> Details of HSQC NMR spectrum of compound 9 .....	S38–S40
<b>Figure S32</b> HMBC NMR spectrum of compound 9 .....	S41
<b>Figure S33–36</b> Details of HMBC NMR spectrum of compound 9 .....	S42–S45
<b>Figure S37</b> COSY NMR spectrum of compound 9 .....	S46
<b>Figure S38–40</b> Details of COSY NMR spectrum of compound 9 .....	S47–S49
<b>Figure S41</b> HPLC chromatogram of compound 9 .....	S50
<b>Figure S42</b> $^{13}\text{C}$ NMR spectrum of compound 10 .....	S51
<b>Figure S43–45</b> Details of $^{13}\text{C}$ NMR spectrum of compound 10 .....	S52–S54
<b>Figure S46</b> $^1\text{H}$ NMR spectrum of compound 10 .....	S55
<b>Figure S47–49</b> Details of $^1\text{H}$ NMR spectrum of compound 10 .....	S56–S58
<b>Figure S50</b> HSQC NMR spectrum of compound 10 .....	S59
<b>Figure S51–54</b> Details of HSQC NMR spectrum of compound 10 .....	S60–S63

<b>Figure S55</b> HMBC NMR spectrum of compound <b>10</b> .....	S64
<b>Figure S56–62</b> Details of HMBC NMR spectrum of compound <b>10</b> .....	S65–S71
<b>Figure S63</b> COSY NMR spectrum of compound <b>10</b> .....	S72
<b>Figure S64–66</b> Details of COSY NMR spectrum of compound <b>10</b> .....	S73–S75
<b>Figure S67</b> HPLC chromatogram of compound <b>10</b> .....	S76
<b>Figure S68</b> <sup>1</sup> H NMR spectrum of compound <b>11</b> .....	S77
<b>Figure S69</b> <sup>1</sup> H NMR spectrum WET of compound <b>11</b> .....	S78
<b>Figure S70–72</b> Details of <sup>1</sup> H NMR spectrum WET of compound <b>11</b> .....	S79–S81
<b>Figure S73</b> HSQC NMR spectrum of compound <b>11</b> .....	S82
<b>Figure S74–76</b> Details of HSQC NMR spectrum of compound <b>11</b> .....	S83–S85
<b>Figure S77</b> HMBC NMR spectrum of compound <b>11</b> .....	S86
<b>Figure S78–82</b> Details of HMBC NMR spectrum of compound <b>11</b> .....	S87–S91
<b>Figure S83</b> COSY NMR spectrum of compound <b>11</b> .....	S92
<b>Figure S84–86</b> Details of COSY NMR spectrum of compound <b>11</b> .....	S93–S95
<b>Figure S87</b> HPLC chromatogram of compound <b>11</b> .....	S96
<b>Figure S88</b> HPLC chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the presence of Novozym 435® .....	S97
<b>Figure S89</b> HPLC chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the absence of Novozym 435® .....	S98
<b>Figure S90</b> HPLC-MS (–) chromatogram of the monosuccinate of isoquercitrin .....	S99
<b>Figure S91</b> HPLC-MS (–) chromatogram of the disuccinate of isoquercitrin.....	S100
<b>Figure S92</b> HPLC-MS (–) chromatogram of the trisuccinate of isoquercitrin .....	S101



**Figure S1.** Structures of compounds 2–11.

**Table S1.**  $^{13}\text{C}$  NMR data of prepared compounds 2–8 (DMSO- $d_6$ , 30 °C).

**Table S1.** *Cont.*

<b>Comp.</b>	<b>2</b>	<b>3</b>	<b>4</b>	<b>5</b>	<b>6</b>	<b>7</b>	<b>8</b>					
<b>Atom Number</b>	<b><math>\delta</math> C</b>	<b>m C</b>										
1'''	169.88	s	-	-	172.29	s	172.42	s	172.43	s	172.44	s
2'''	20.12	q	-	-	35.25	t	33.19	t	33.24	t	33.24	t
3'''	-	-	-	-	17.81	t	23.92	t	24.24	t	24.23	t
4'''	-	-	-	-	13.19	q	30.51	t	28.27	t	28.31	t
5'''	-	-	-	-	-	-	21.61	t	28.18	t	28.52	t
6'''	-	-	-	-	-	-	13.75	d	31.09	t	28.73	t
7'''	-	-	-	-	-	-	-	-	22.03	t	28.86	t
8'''	-	-	-	-	-	-	-	-	13.95	q	29.00	t
9'''	-	-	-	-	-	-	-	-	-	-	29.02	t
10'''	-	-	-	-	-	-	-	-	-	-	31.33	t
11'''	-	-	-	-	-	-	-	-	-	-	22.12	t
12'''	-	-	-	-	-	-	-	-	-	-	13.98	q
13'''	-	-	-	-	-	-	-	-	-	-	-	29.09 <sup>3C</sup>
14'''	-	-	-	-	-	-	-	-	-	-	-	31.33
15'''	-	-	-	-	-	-	-	-	-	-	-	22.12
16'''	-	-	-	-	-	-	-	-	-	-	-	13.97

<sup>3C</sup> ... three overlapped carbon signals.

**Table S2.**  $^1\text{H}$  NMR data of prepared compounds **2** and **3** (DMSO- $d_6$ , 30 °C).

Comp.	2					3				
Atom Number	$\delta$ H	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]		
2	-	-	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-	-	-
4	-	-	-	-	-	-	-	-	-	-
4a	-	-	-	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-	-	-	-
6	6.201	1	d	2.1	6.210	1	d	2.0		
7	-	-	-	-	-	-	-	-	-	-
8	6.409	1	d	2.1	6.414	1	d	2.0		
8a	-	-	-	-	-	-	-	-	-	-
1'	-	-	-	-	-	-	-	-	-	-
2'	-	-	-	-	-	-	-	-	-	-
3'	7.528	1	d	2.2	7.543	1	d	2.2		
4'	-	-	-	-	-	-	-	-	-	-
5'	7.531	1	dd	9.0, 2.2	7.509	1	dd	2.2, 8.4		
6'	6.832	1	d	9.0	6.841	1	d	8.4		
1''	5.372	1	d	7.5	5.482	1	d	7.7		
2''	3.27 H	1	m	-	3.47 *	1	ddd	7.7, 4.9, 9.3		
3''	3.25 H	1	m	-	4.849	1	dd	9.3, 9.3		
4''	3.147	1	t	9.0	3.389	1	ddd	6.2, 9.3, 9.5		
5''	3.30 H	1	m	-	3.46 *	1	ddd	2.2, 5.6, 9.5		
6''	4.125	1	dd	11.8, 2.2	4.115	1	dd	2.2, 11.9		
	3.941	1	dd	11.8, 6.1	3.983	1	dd	5.6, 11.9		
5-OH	12.595	1	s	-	12.566	1	s	-		
7-OH	n.a.	-	-	-	n.a.	-	-	-		
1'-OH	n.a.	-	-	-	n.a.	-	-	-		
2'-OH	n.a.	-	-	-	n.a.	-	-	-		
2''-OH	n.a.	-	-	-	5.649	1	d	4.9		
4''-OH	n.a.	-	-	-	5.400	1	d	6.2		
3''-CO	-	-	-	-	-	-	-	-		
3''-Ac	-	-	-	-	2.056	3	s	-		
6''-CO	-	-	-	-	-	-	-	-		
6''-Ac	1.730	3	s	-	1.757	3	s	-		

n.a.—not assigned due to lack of conclusive correlation from broadened OH signals; \*—HSQC readout.

**Table S3.**  $^1\text{H}$  NMR data of prepared compounds **4–8** (DMSO- $d_6$ , 30 °C).

Comp.	4					5					6					7					8				
Atom Number	$\delta$ H	n H	m	J [Hz]	$\delta$ H [ppm]	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]					
2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
4a	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
6	6.216	1	dd	2.0, 0.2	6.192	1	d	2.0	6.189	1	d	2.0	6.185	1	d	2.0	6.183	1	d	2.1					
7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
8	6.441	1	dd	2.0, 0.9	6.839	1	d	2.0	6.384	1	d	2.0	6.379	1	d	2.0	6.381	1	d	2.1					
8a	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
1'	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
2'	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
3'	7.542	1	d	2.2	7.516	1	d	2.2	7.515	1	d	2.1	7.516	1	d	2.2	7.520	1	m	-					
4'	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
5'	7.521	1	dd	8.3, 2.2	7.521	1	dd	2.2, 8.7	7.518	1	dd	2.1, 9.1	7.514	1	dd	2.2, 9.0	7.512	1	dd	2.2, 8.2					
6'	6.845	1	d	8.3	6.825	1	d	8.7	6.824	1	d	9.1	6.821	1	d	9.0	6.822	1	m	-					
1''	5.436	1	d	7.6	5.436	1	d	7.4	5.434	1	d	7.6	5.429	1	d	7.6	5.428	1	d	7.6					
2''	3.26 H	1	m	-	3.265	1	m	-	3.27 H	1	m	-	3.26 H	1	m	-	3.256	1	m	-					
3''	3.26 H	1	m	-	3.256	1	m	-	3.26 H	1	m	-	3.25 H	1	m	-	3.242	1	m	-					
4''	3.123	1	br.t.	7.5	3.126	1	m	-	3.126	1	m	-	3.12 H	1	m	-	3.125	1	dd	9.7, 8.5					
5''	3.29 H	1	m	-	3.298	1	m	-	3.30 H	1	m	-	3.300	1	m	-	3.297	1	ddd	9.7, 7.1, 2.2					
	4.157	1	dd	11.8, 2.2	4.155	1	dd	1.8, 11.8	4.155	1	dd	2.2, 11.7	4.152	1	dd	2.4, 11.7	4.149	1	dd	11.7, 2.2					
6''	3.940	1	dd	11.8, 7.0	3.949	1	dd	7.0, 11.8	3.950	1	dd	7.1, 11.7	3.947	1	dd	7.1, 11.7	3.948	1	dd	11.7, 7.1					
5-OH	12.612	1	s	-	12.612	1	s	-	12.610	-	-	-	12.608	1	s	-	12.60 7	1	s	-					
7-OH/ 1'-OH/ 2'-OH	10.962 *	1	br.s.	-	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	10.81 9	1	s	-					
2''-OH	9.725 *	1	br.s.	-	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	9.655	1	s	-					
3''-OH	9.249 *	1	br.s.	-	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	9.183	1	s	-					
2''-OH	5.173	1	br.s.	-	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	5.341	1	s	-					
3''-OH	5.377	1	br.d	2.6	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	5.147	1	s	-					
4''-OH	5.173	1	br.s.	-	n.a.	-	-	-	n.a.	-	-	-	n.a.	-	-	-	5.147	1	s	-					

**Table S3.** Cont.

Comp.	4					5					6					7					8				
Atom Number	$\delta$ H	n H	m	J [Hz]	$\delta$ H [ppm]	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]					
1'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-			
2'''	1.961	2	m	-	1.968	2	m	-	1.971	2	m	-	1.970	2	m	-	1.969	2	m	-					
3'''	1.246	2	m	-	1.238 H	2	m	-	1.24 H	2	m	-	1.23 H	2	m	-	1.233	2	m	-					
4'''	0.649	3	t	7.4	1.030	2	m	-	1.05 H	2	m	-	1.04 H	2	m	-	1.035	2	m	-					
5'''	-	-	-	-	1.118	2	m	-	1.09 H	2	m	-	-	-	-	-	1.078	2	m	-					
6'''	-	-	-	-	0.778	3	t	7.0	1.12 H	2	m	-	-	-	-	-	1.236	2	m	-					
7'''	-	-	-	-	-	-	-	-	1.21 H	2	m	-	1.05–1.22 H	10	m	-	1.142	2	m	-					
8'''	-	-	-	-	-	-	-	-	0.837	3	t	7.2	-	-	-	-	1.191	2	m	-					
9'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.210	2	m	-					
10'''	-	-	-	-	-	-	-	-	-	-	-	-	1.23 H	2	m	-	1.233	2	m	-					
11'''	-	-	-	-	-	-	-	-	-	-	-	-	1.25 H	2	m	-	-	-	-	-	-				
12'''	-	-	-	-	-	-	-	-	-	-	-	-	0.857	3	t	7.1	1.233	6	m	-					
13'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-				
14'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.233	2	m	-					
15'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.250	2	m	-					
16'''	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.849	3	t	7.1					

n.a.—not assigned due to lack of conclusive correlation from broadened OH signals;  $^{3C}$  ... three overlapped carbon signals; \*—HSQC readout.

**Table S4.**  $^{13}\text{C}$  NMR data of prepared compounds 9–11.

Comp.	9 <sup>a</sup>		10 <sup>b</sup>		11 <sup>c</sup>	
Atom Number	$\delta$ C	m C	$\delta$ C	m C	$\delta$ C	m C
2	157.33	s	158.47	s	158.1 <sup>M</sup>	s
3	133.35	s	135.65	s	135.4 <sup>M</sup>	s
4	177.08	s	179.18	s	179.0 <sup>M</sup>	s
4a	103.53	s	105.63	s	105.2 <sup>M</sup>	s
5	159.53	s	163.23	S	163.1 <sup>M</sup>	s
6	99.22	d	100.33	d	100.6 <sup>H</sup>	d
7	164.68	s	166.51	s	167.6 <sup>M</sup>	s
8	94.62	d	95.09	d	95.2 <sup>H</sup>	d
8a	156.11	s	158.12	s	158.2 <sup>M</sup>	s
9	147.40	s	151.27	s	151.4 <sup>M</sup>	s
10	143.22	s	147.38	s	147.4 <sup>M</sup>	s
11	116.42	d	118.13	d	118.0 <sup>H</sup>	d
12	121.38	s	122.83	s	122.6 <sup>M</sup>	s
13	122.26	d	123.28	d	123.1 <sup>H</sup>	d
14	114.99	d	116.62	d	116.6 <sup>H</sup>	d
1'	102.07	d	104.77	d	104.5 <sup>H</sup>	d
2'	73.56	d	76.46	d	76.3 <sup>H</sup>	d
3'	75.34	d	78.91	d	78.9 <sup>H</sup>	d
4'	69.24	d	71.65	d	71.8 <sup>H</sup>	d
5'	73.18	d	76.29	d	76.2 <sup>H</sup>	d
6'	62.66	t	64.69	t	64.7 <sup>H</sup>	t
5-OH	-	-	-	-	-	-
7-OH	-	-	-	-	-	-
9-OH	-	-	-	-	-	-
10-OH	-	-	-	-	-	-
2'-OH	-	-	-	-	-	-
3'-OH	-	-	-	-	-	-
4'-OH	-	-	-	-	-	-
1''	175.30	s	173.77	s	174.0 <sup>M</sup>	s
2''	32.96	t	34.42	t	34.7 <sup>H</sup>	t
3''	20.85	t	25.30	t	25.5 <sup>H</sup>	t
4''	36.37	t	25.53	t	29.6 <sup>H</sup>	t
5''	182.31	s	34.95	t	29.7 <sup>H</sup>	t
6''			176.29	s	29.8 <sup>H</sup>	t
7''	-	-	-	-	30.0 <sup>H</sup>	t
8''	-	-	-	-	29.9 <sup>H</sup>	t
9''	-	-	-	-	30.0 <sup>H</sup>	t
10''	-	-	-	-	26.7 <sup>H</sup>	t
11''	-	-	-	-	37.1 <sup>H</sup>	t
12''	-	-	-	-	179.3 <sup>H</sup>	s
5''-OH	-	-	-	-	-	-
6''-OH	-	-	n.d.	-	-	-
12''-OH	-	-	-	-	-	-

<sup>a</sup> D<sub>2</sub>O, 293.2 K, 150.94 MHz for  $^{13}\text{C}$ ; <sup>b</sup> pyridin, 293.2 K, 150.94 MHz for  $^{13}\text{C}$ ; <sup>c</sup> pyridin, 293.2 K, 150.94 MHz for  $^{13}\text{C}$ ; H—HSQC readout; M—HMBC readout; n.d.—not detected.

**Table S5.**  $^1\text{H}$  NMR data of prepared compounds 9–11.

Comp.	9 <sup>a</sup>				10 <sup>b</sup>				11 <sup>c</sup>				
	Atom Number	$\delta$ H	n H	m	J [Hz]	$\delta$ H [ppm]	n H	m	J [Hz]	$\delta$ H	n H	m	J [Hz]
2	-	-	-	-	-	-	-	-	-	-	-	-	-
3	-	-	-	-	-	-	-	-	-	-	-	-	-
4	-	-	-	-	-	-	-	-	-	-	-	-	-
4a	-	-	-	-	-	-	-	-	-	-	-	-	-
5	-	-	-	-	-	-	-	-	-	-	-	-	-
6	5.874	1	br.s.	-	6.731	1	d	2.0	6.738	1	br.s.	-	-
7	-	-	-	-	-	-	-	-	-	-	-	-	-
8	5.852	1	br.s.	-	6.694	1	d	2.0	6.787	1	br.s.	-	-
8a	-	-	-	-	-	-	-	-	-	-	-	-	-
9	-	-	-	-	-	-	-	-	-	-	-	-	-
10	-	-	-	-	-	-	-	-	-	-	-	-	-
11	7.251	1	br.s.	-	8.361	1	d	2.1	8.361	1	br.s.	-	-
12	-	-	-	-	-	-	-	-	-	-	-	-	-
13	7.032	1	br.d	8.4	8.113	1	dd	8.4, 2.1	8.144	1	br.d.	8.1	-
14	6.546	1	d	8.4	7.313	1	d	8.4	7.328	1	br.d.	8.1	-
1'	4.726	1	d	7.8	6.157	1	m	-	6.206	1	br.d.	4.8	-
2'	3.420	1	dd	7.8, 9.2	4.346	1	m	-	4.355	1	m	-	-
3'	3.344	1	dd	9.2, 9.0	4.346	1	m	-	4.355	1	m	-	-
4'	3.283	1	m	-	4.059	1	ddd	9.8, 6.0, 2.8	4.042	1	m	-	-
5'	3.283	1	m	-	4.128	1	ddd	9.8, 6.1, 1.9	4.169	1	m	-	-
6'	3.952	2	m	-	4.841	1	dd	11.6, 1.9	4.886	1	br.d.	11.6	-
					4.685	1	dd	11.6, 6.1	4.720	1	dd	11.6, 5.8	-
5-OH	n.d.	-	-	-	13.205	1	br.s.	-	n.d.	-	-	-	-
7-OH/	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
9-OH/	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
10-OH	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
2'-OH	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
3'-OH	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
4'-OH	n.d.	-	-	-	-	-	-	-	n.d.	-	-	-	-
1''	-	-	-	-	-	-	-	-	n.d.	-	-	-	-
2''	1.911	2	m	-	2.332	1	m	-	-	-	-	-	-
					2.269	1	m	-					-
3''	1.441	2	m	-	1.672	2	m	-	2.269	2	m	-	-
4''	1.898	2	m	-	1.733	2	m	-	1.534	2	m	-	-
5''	-	-	-	-	2.424	2	t	7.5	1.171	2	m	-	-
6''	-	-	-	-	-	-	-	-	1.124	2	m	-	-
7''	-	-	-	-	-	-	-	-	1.138	2	m	-	-
8''	-	-	-	-	-	-	-	-	1.211	2	m	-	-
9''	-	-	-	-	-	-	-	-	1.291	2	m	-	-
10''	-	-	-	-	-	-	-	-	1.473	2	m	-	-
11''	-	-	-	-	-	-	-	-	1.901	2	m	-	-
12''	-	-	-	-	-	-	-	-	2.634	2	m	-	-
5''-OH	n.d.	-	-	-	n.d.	-	-	-	-	-	-	-	-
6''-OH	-	-	-	-	-	-	-	-	-	-	-	-	-
12''-OH	-	-	-	-	-	-	-	-	n.d.	-	-	-	-

<sup>a</sup> D<sub>2</sub>O, 293.2 K, 600.23 MHz for  $^1\text{H}$ ; <sup>b</sup> pyridin, 293.2 K, 600.23 MHz for  $^1\text{H}$ ; <sup>c</sup> pyridin, 293.2 K, 600.23 MHz for  $^1\text{H}$ ; H—HSQC readout; M—HMBC readout; n.d.—not detected.

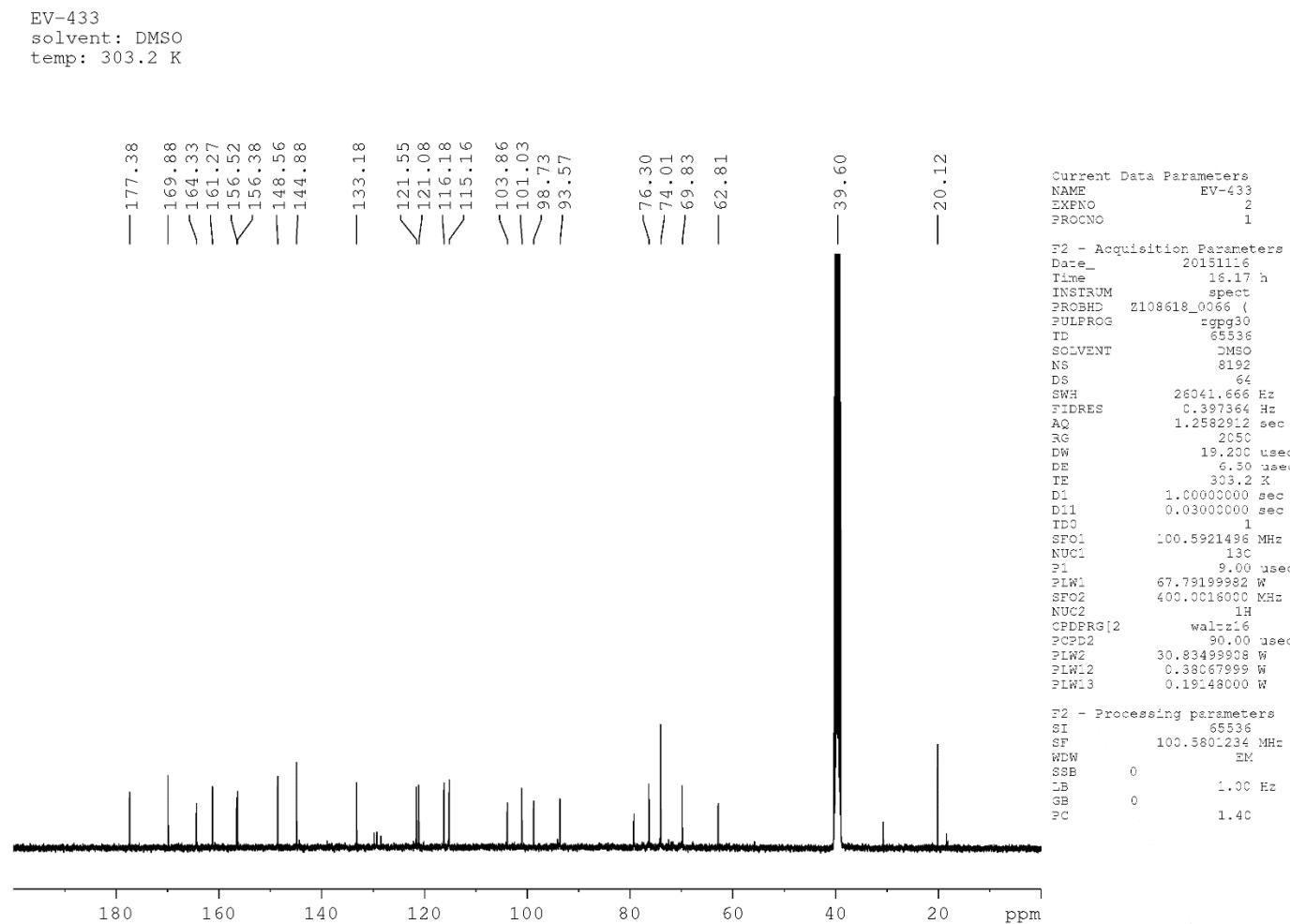


Figure S2.  $^{13}\text{C}$  NMR spectrum of compound 2.

EV-433  
solvent: DMSO  
temp: 303.2 K

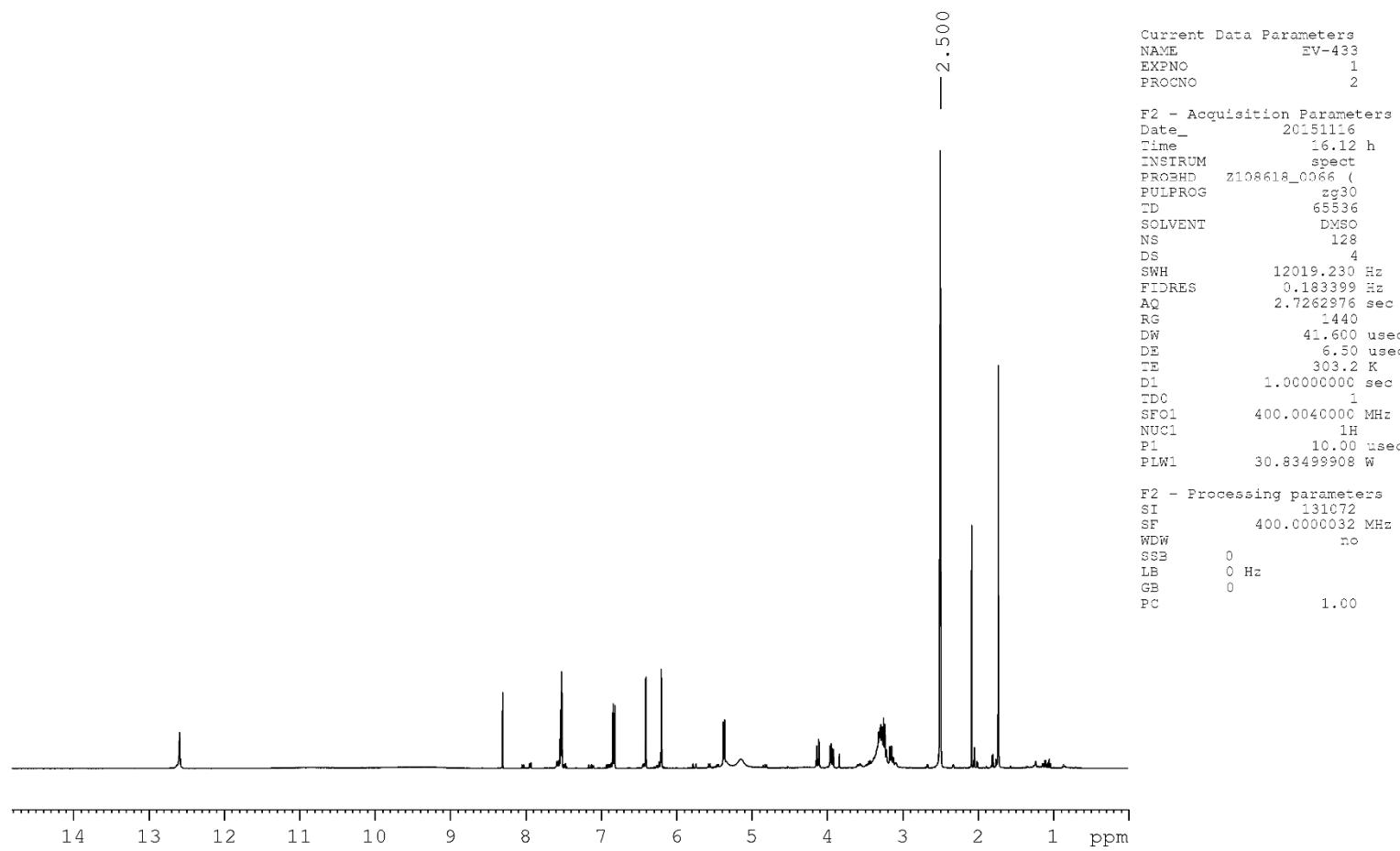
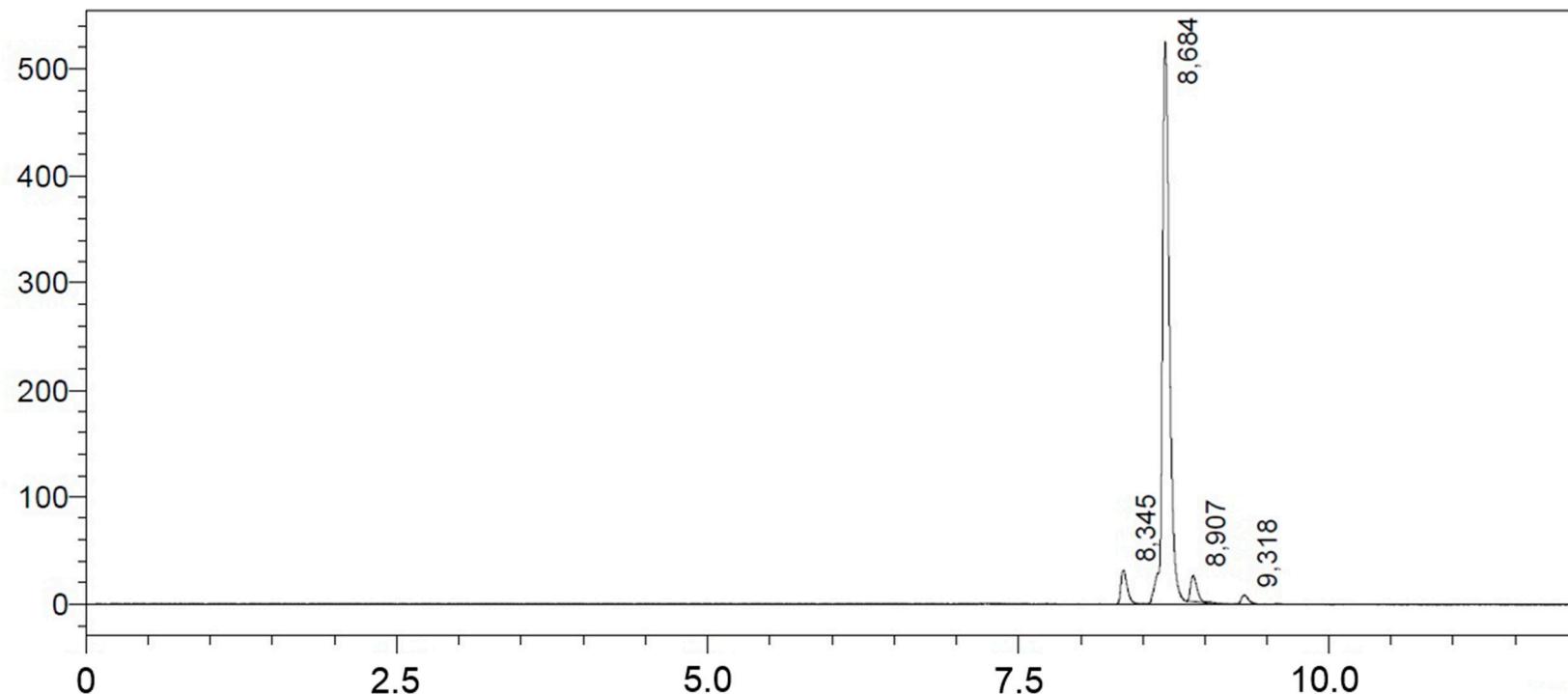


Figure S3.  $^1\text{H}$  NMR spectrum of compound 2.

mAU



**Figure S4.** HPLC chromatogram of compound 2.

FL-002  
solvent: DMSO  
temp: 303.2 K  
date: 28 Oct 2013

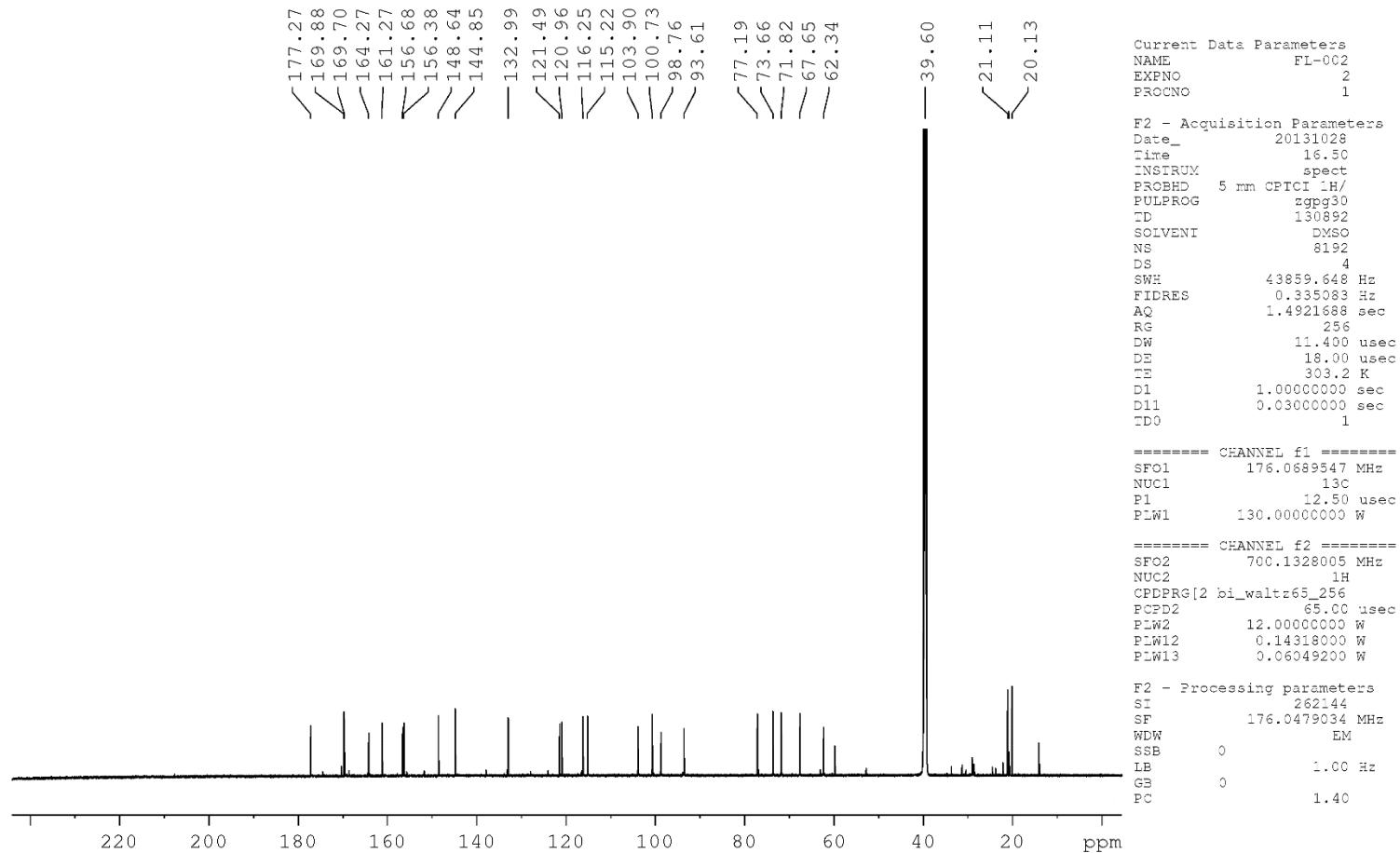
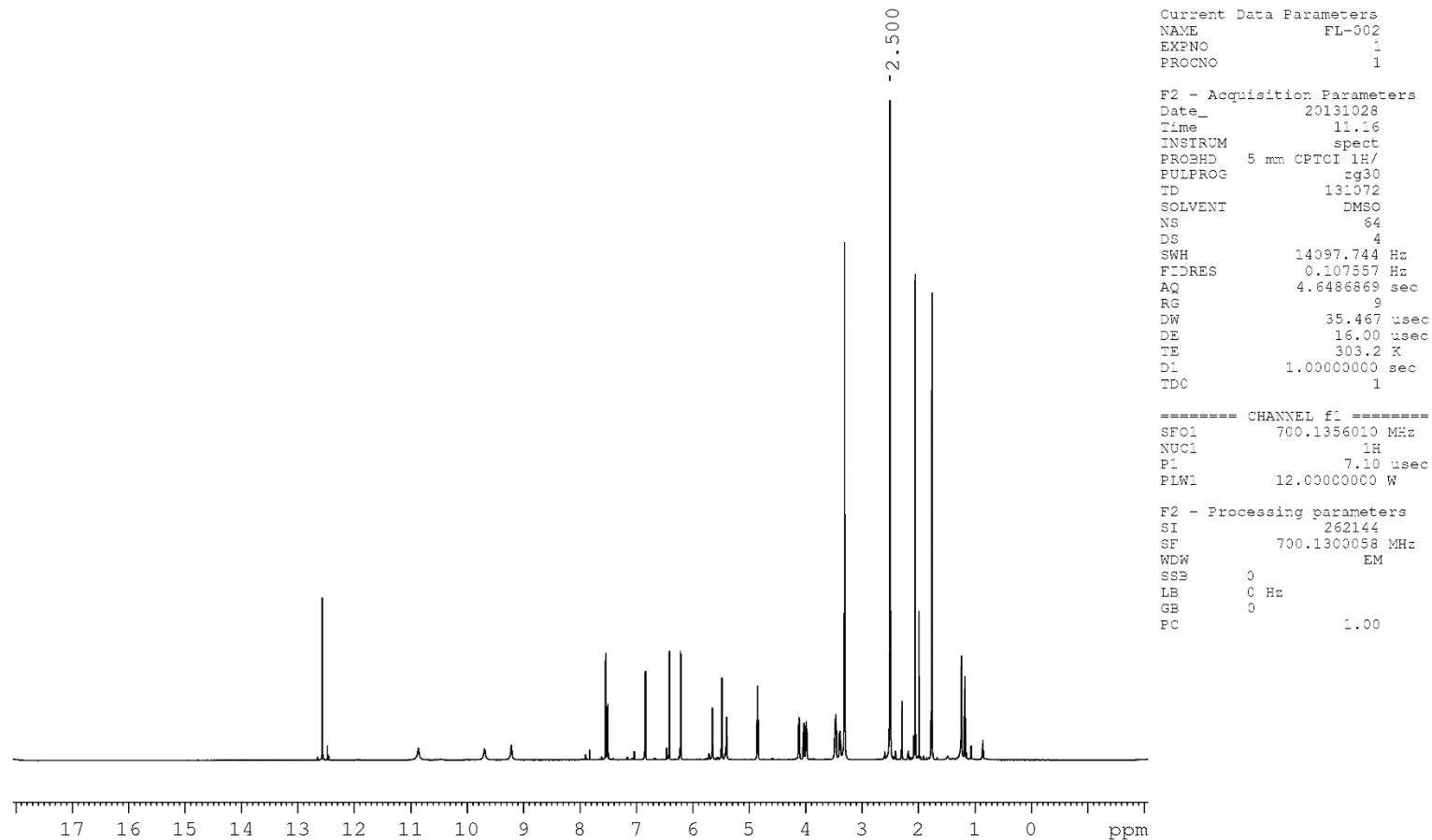
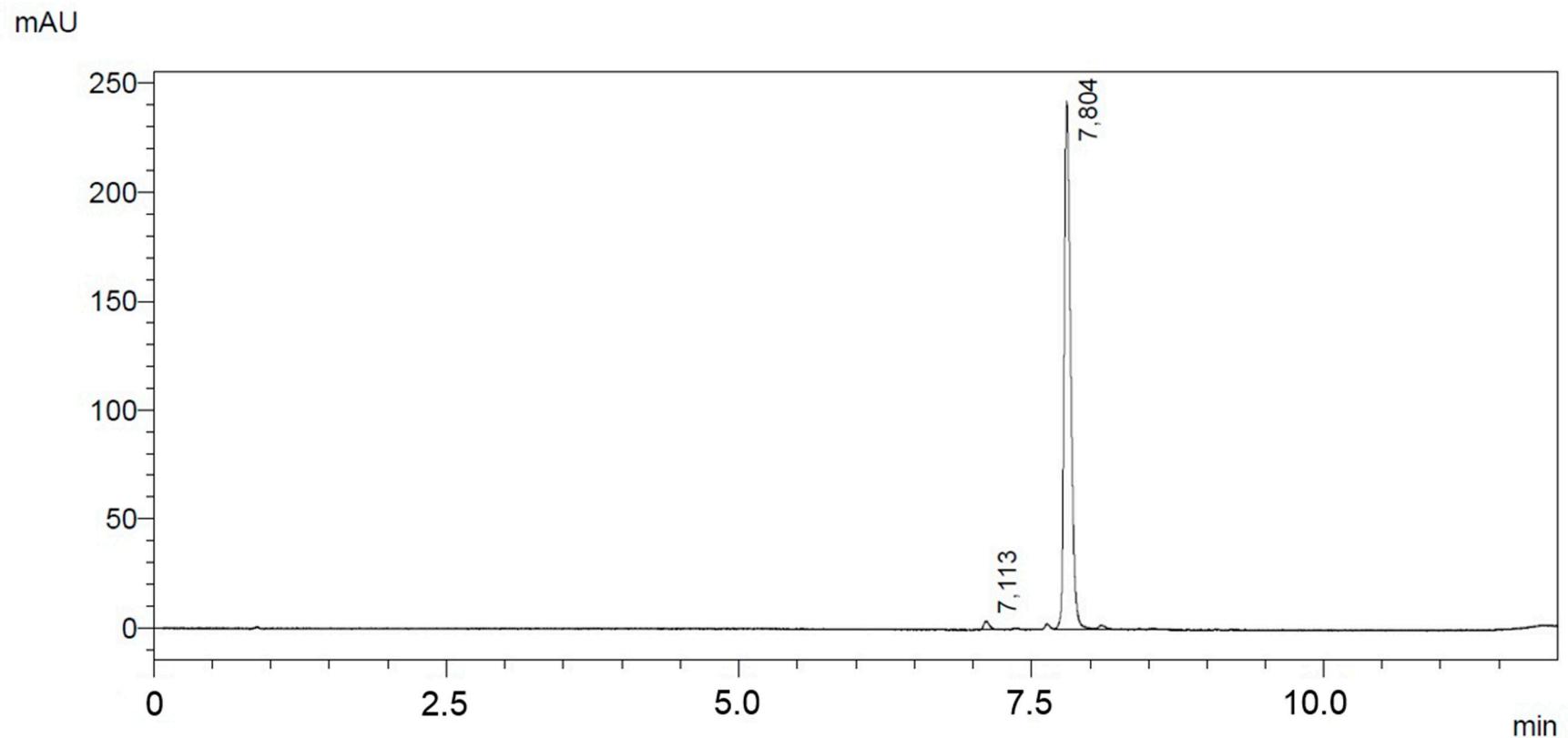


Figure S5.  $^{13}\text{C}$  NMR spectrum of compound 3.

FL-002  
solvent: DMSO  
temp: 303.2 K  
date: 28 Oct 2013

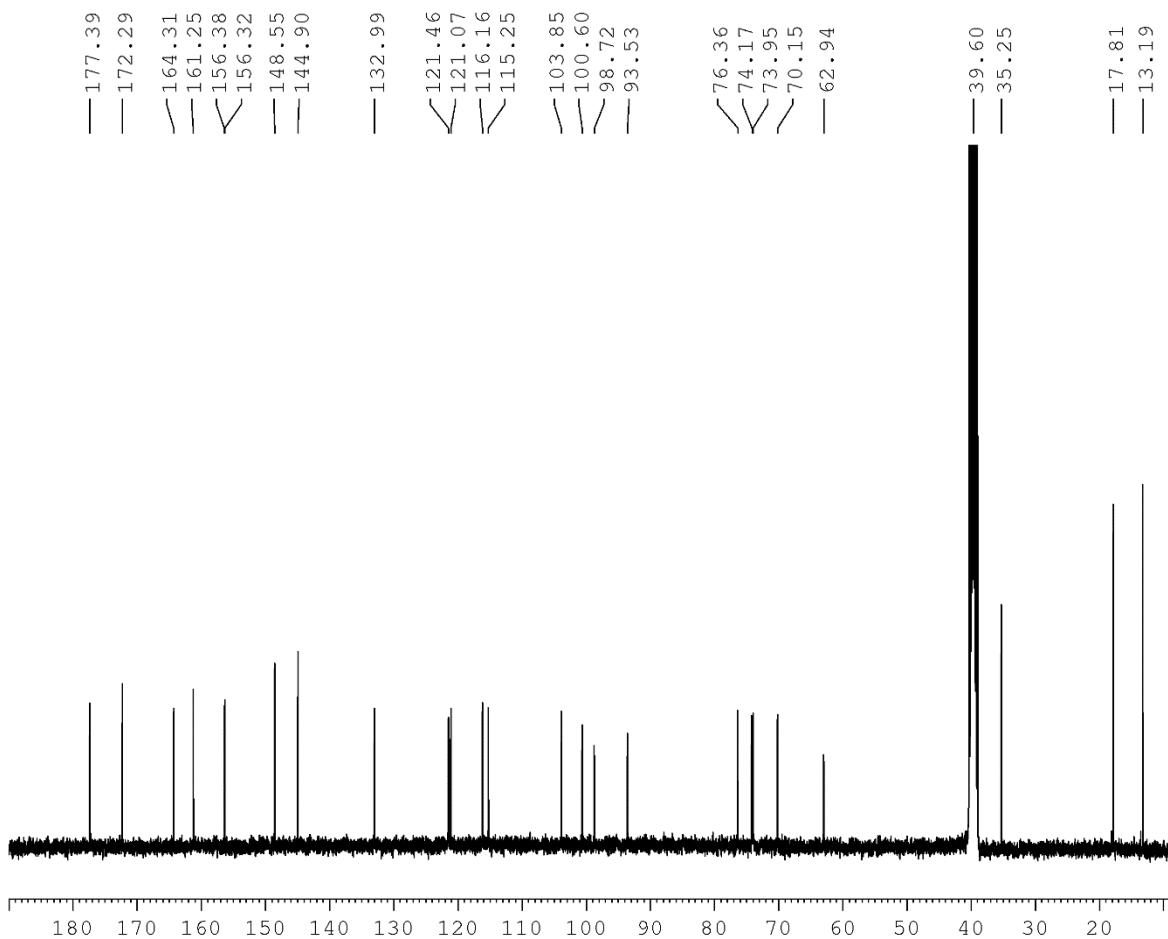


**Figure S6.** <sup>1</sup>H NMR spectrum of compound 3.



**Figure S7.** HPLC chromatogram of compound 3.

EV-415  
solvent: DMSO  
temp: 303.2 K



Current Data Parameters  
NAME EV-415  
EXPNO 2  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 20151014  
Time 16.40 h  
INSTRUM spect  
PROBHD Z108618\_0066 (   
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 8192  
DS 32  
SWH 26041.666 Hz  
FIDRES 0.397364 Hz  
AQ 1.2582912 sec  
RG 2050  
DW 19.200 usec  
DE 6.50 usec  
TE 303.2 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
IDC 1  
SF01 100.5916467 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 67.79199982 W  
SF02 400.0016000 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
FCPD2 90.00 usec  
PLW2 30.83499908 W  
PLW12 0.38067999 W  
PLW13 0.19148000 W  
  
F2 - Processing parameters  
SI 131072  
SF 100.5801233 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

Figure S8. <sup>13</sup>C NMR spectrum of compound 4.

EV-415  
solvent: DMSO  
temp: 303.2 K

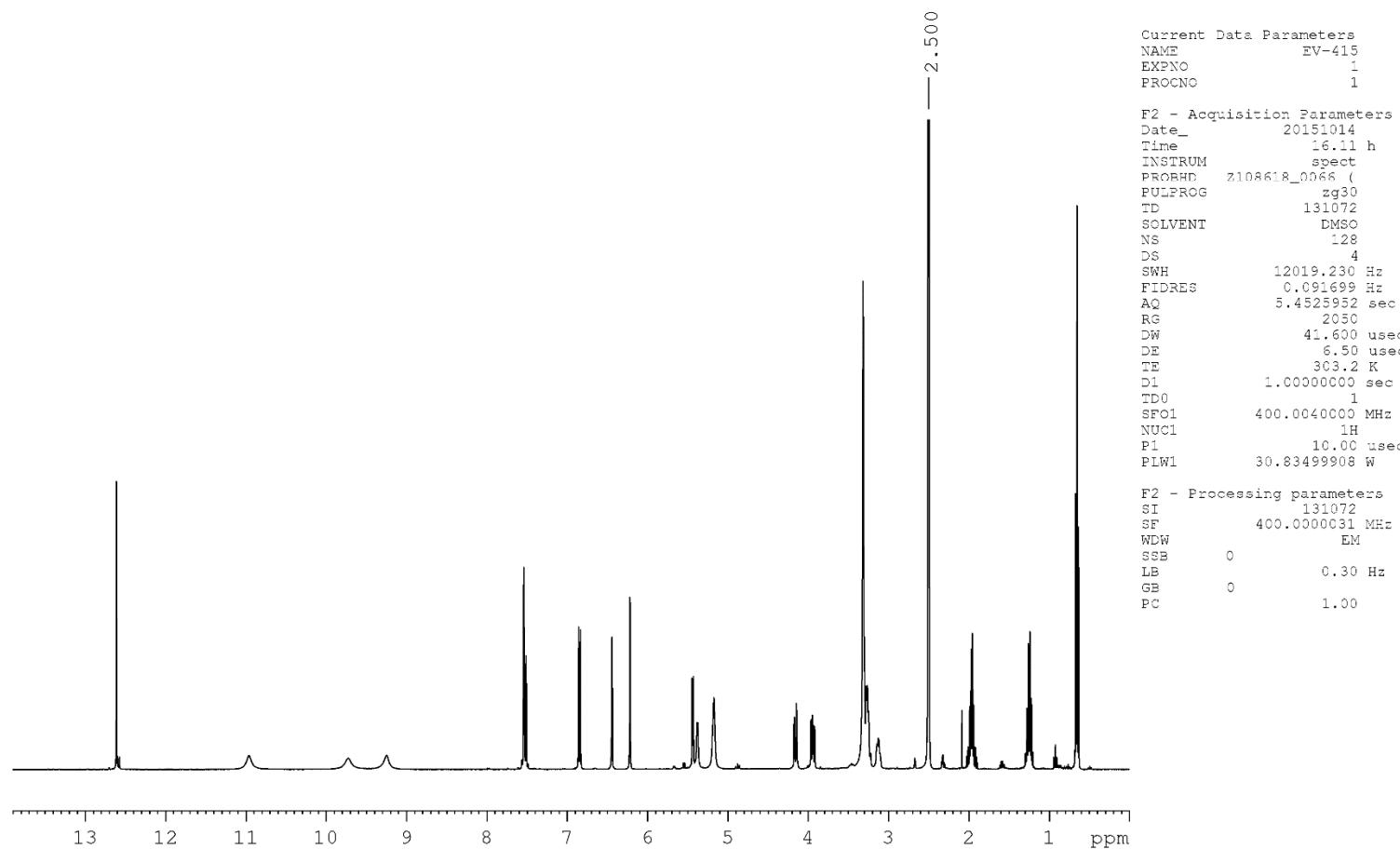
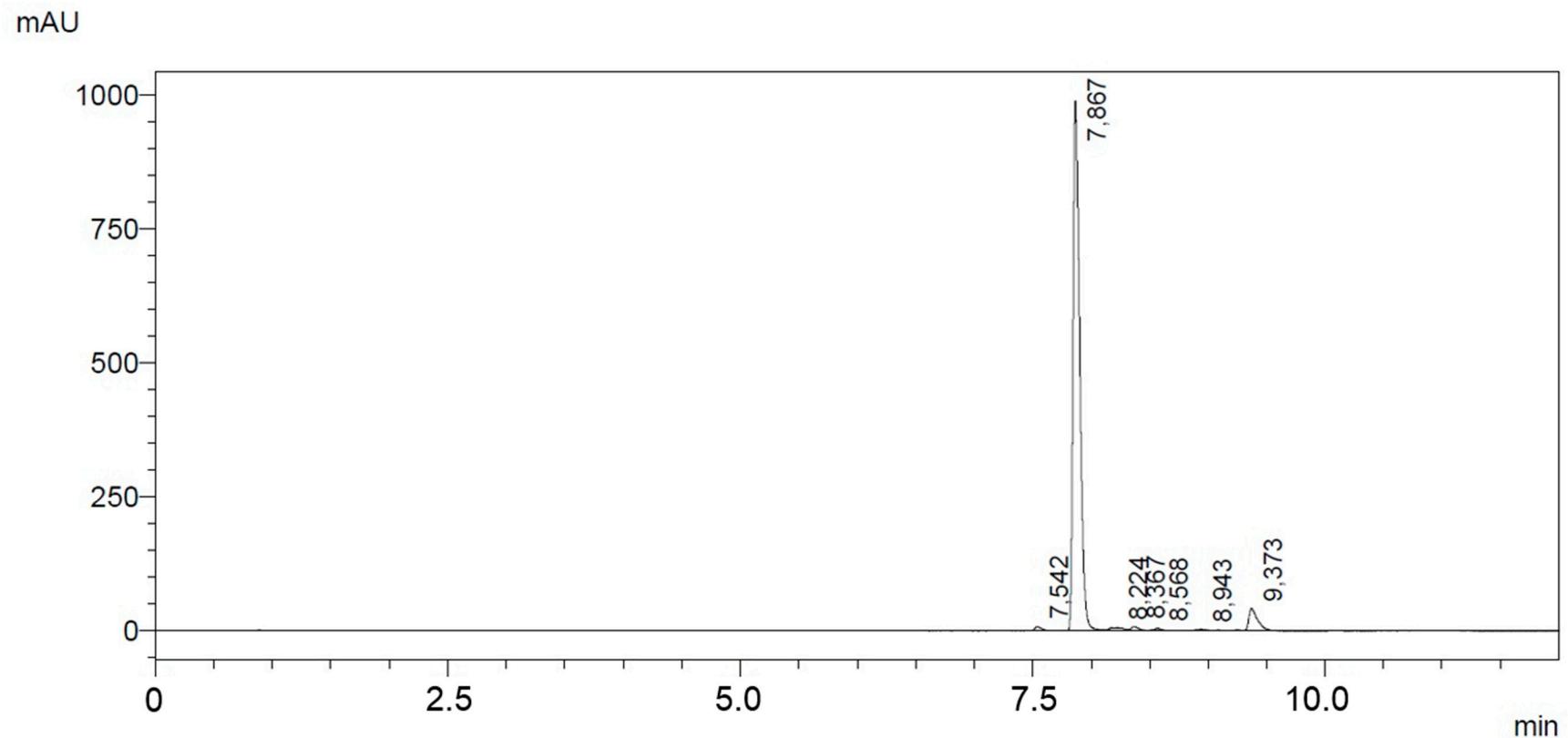


Figure S9.  $^1\text{H}$  NMR spectrum of compound 4.



**Figure S10.** HPLC chromatogram of compound 4.

FL-005  
solvent: DMSO  
temp: 303.2 K  
date: 31 Jan 2014

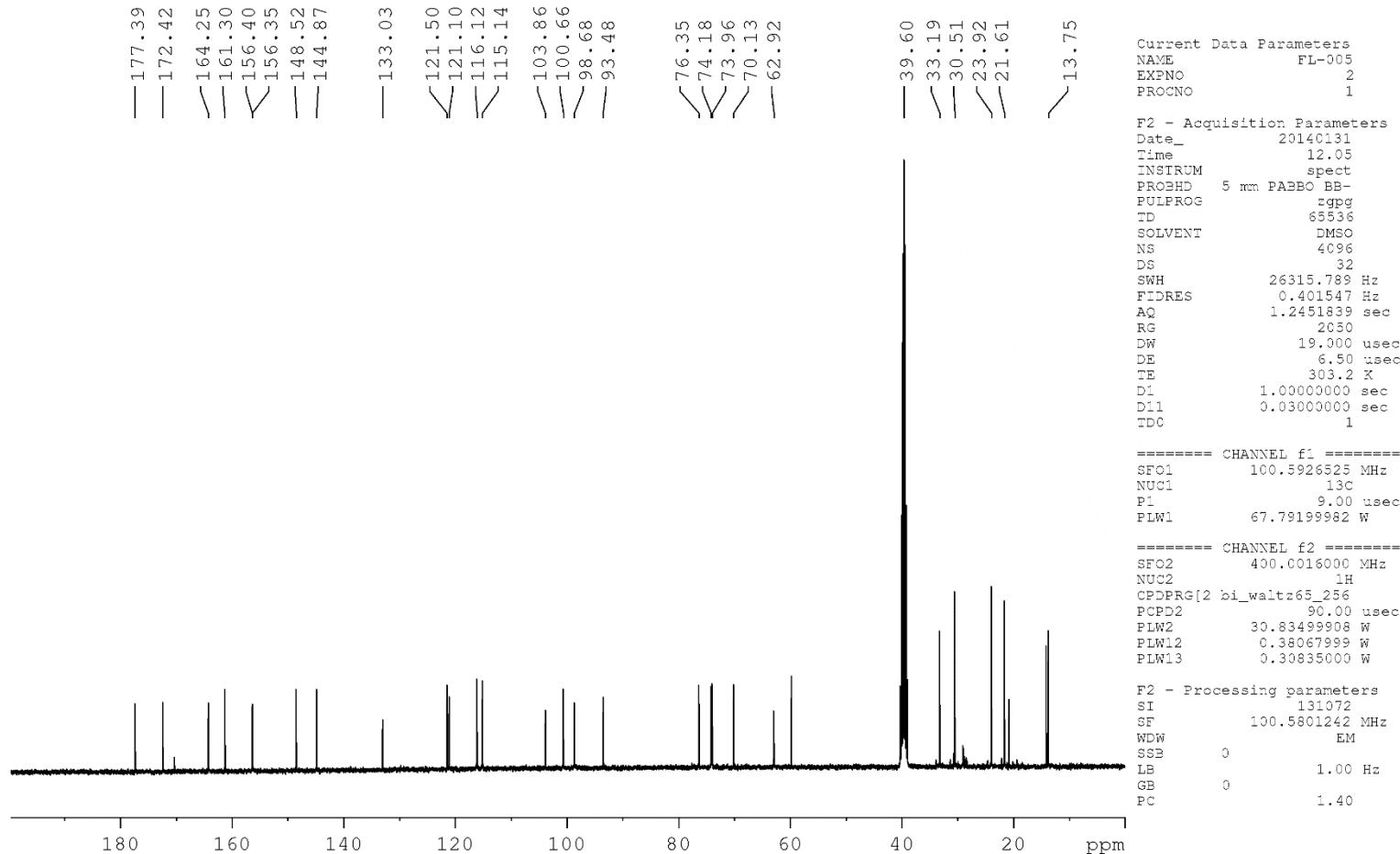


Figure S11. <sup>13</sup>C NMR spectrum of compound 5.

FL-005  
solvent: DMSO  
temp: 303.2 K  
date: 31 Jan 2014

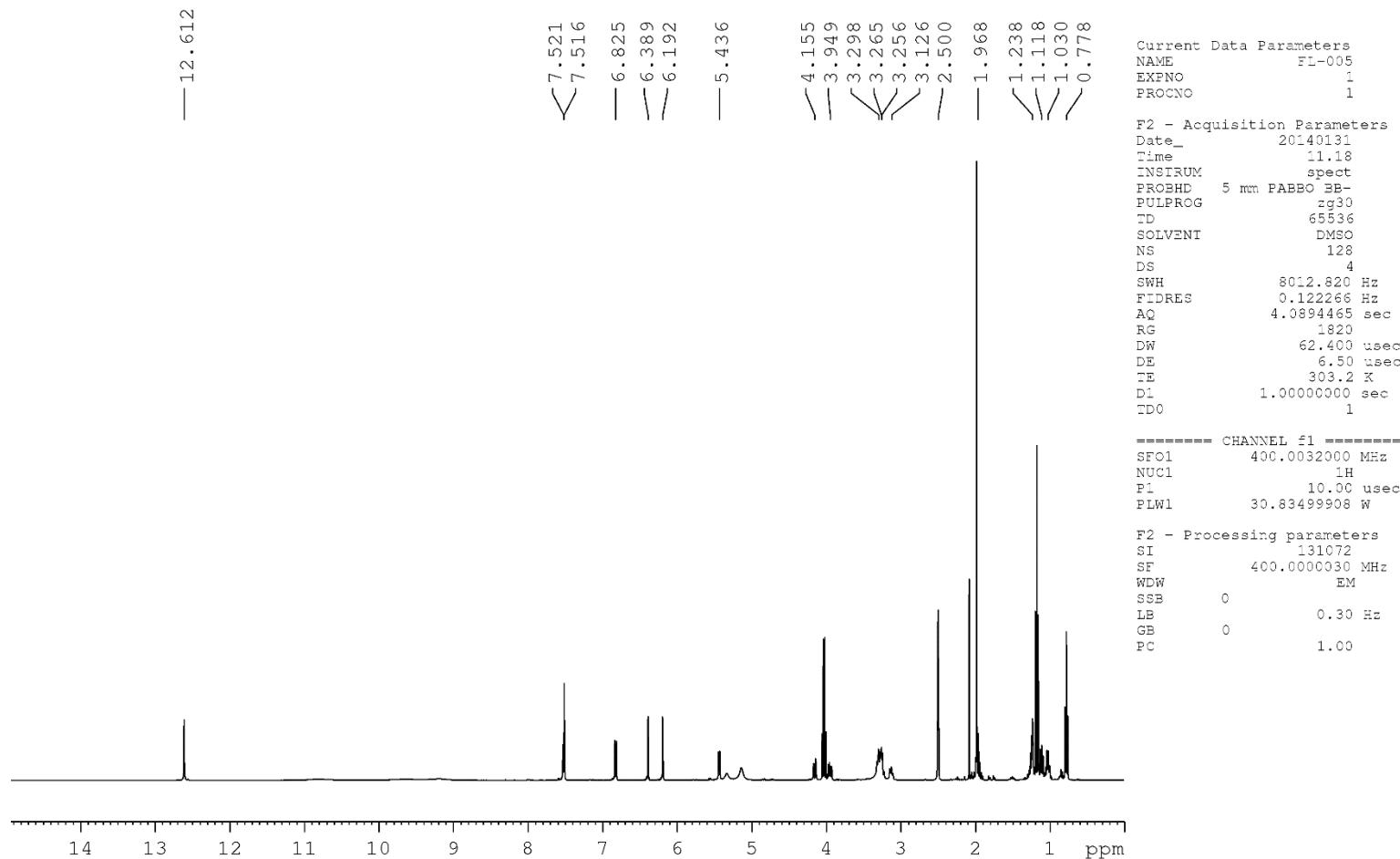
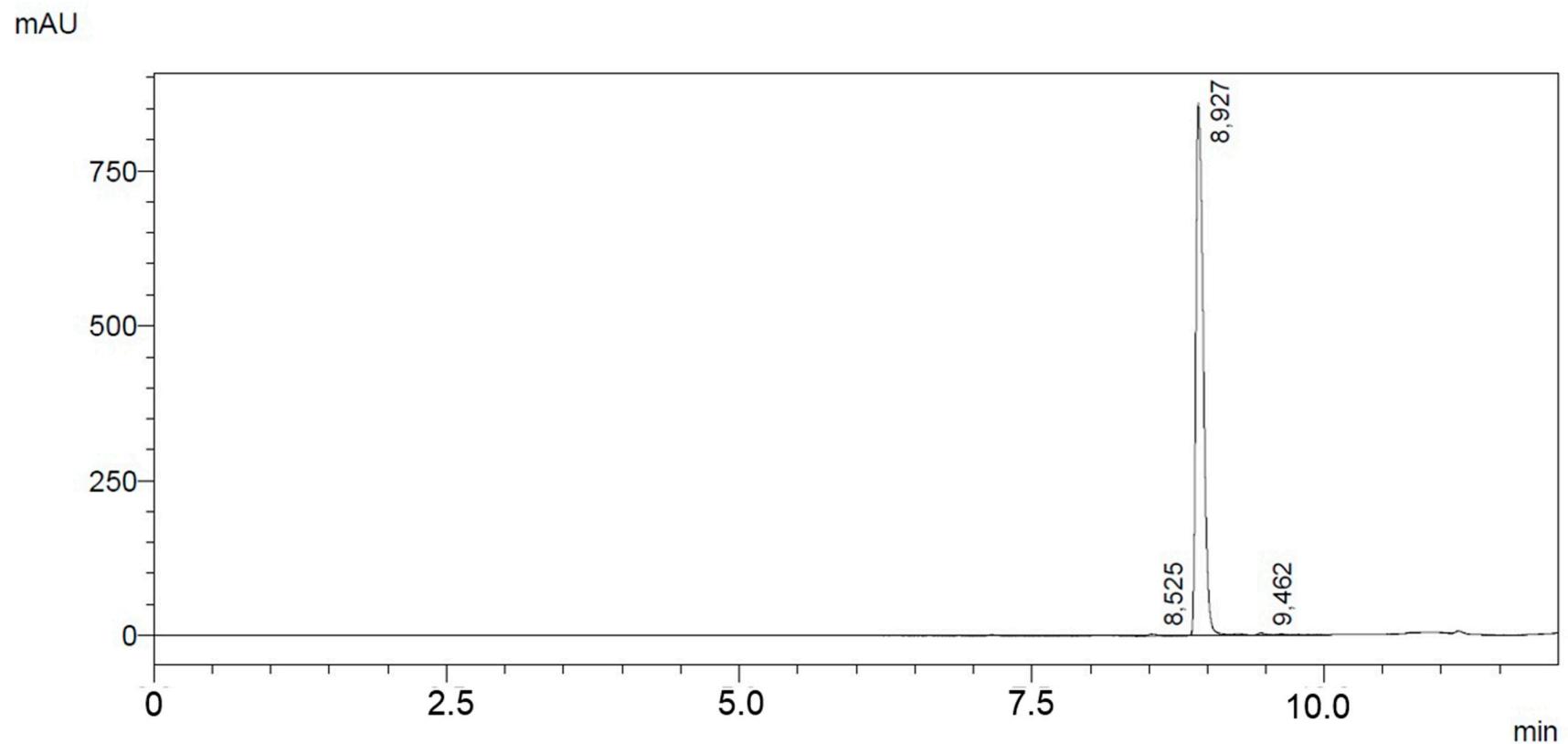


Figure S12.  $^1\text{H}$  NMR spectrum of compound 5.



**Figure S13.** HPLC chromatogram of compound 5.

FL-004  
solvent: DMSO  
temp: 303.2 K  
date: 22 Jan 2014

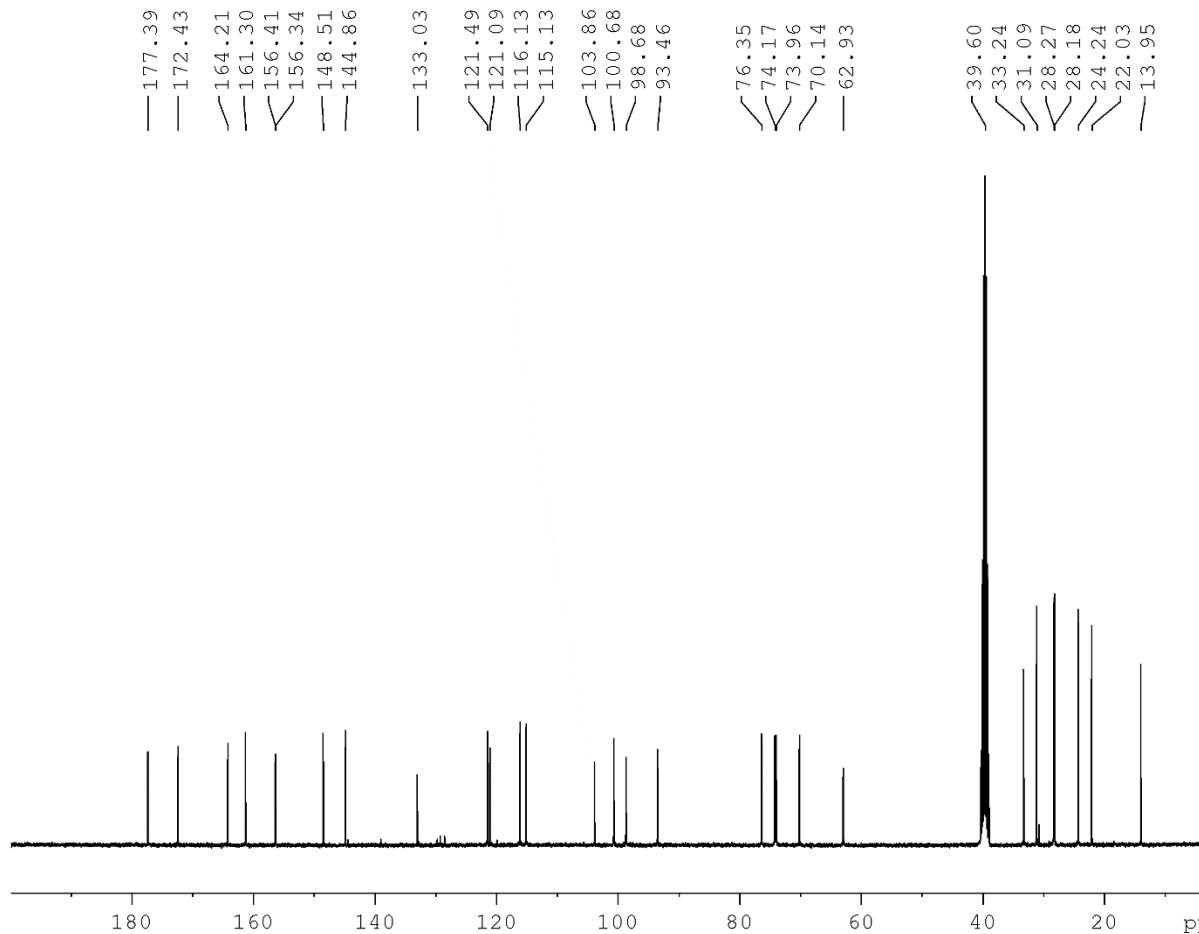


Figure S14. <sup>13</sup>C NMR spectrum of compound 6.

Current Data Parameters  
NAME FL-004  
EXPNO 2  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 20140122  
Time 17.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgppg  
TD 65536  
SOLVENT DMSO  
NS 7885  
DS 32  
SWH 26315.789 Hz  
FIDRES 0.401547 Hz  
AQ 1.2451839 sec  
RG 2030  
DW 19.000 usec  
DE 6.50 usec  
TE 303.2 K  
D1 1.0000000 sec  
D11 0.0300000 sec  
TDC 1  
  
===== CHANNEL f1 =====  
SFC1 100.5926525 MHz  
NUC1 13C  
P1 9.00 usec  
PLW1 67.79199982 W  
  
===== CHANNEL f2 =====  
SFC2 400.0016000 MHz  
NUC2 1H  
CPDPRG[2 bi\_waltz65\_256  
PCPD2 90.00 usec  
PLW2 30.83499908 W  
PLW12 0.38067999 W  
PLW13 0.30835000 W  
  
F2 - Processing parameters  
SI 131972  
SF 100.5801249 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

FL-004  
solvent: DMSO  
temp: 303.2 K  
date: 22 Jan 2014

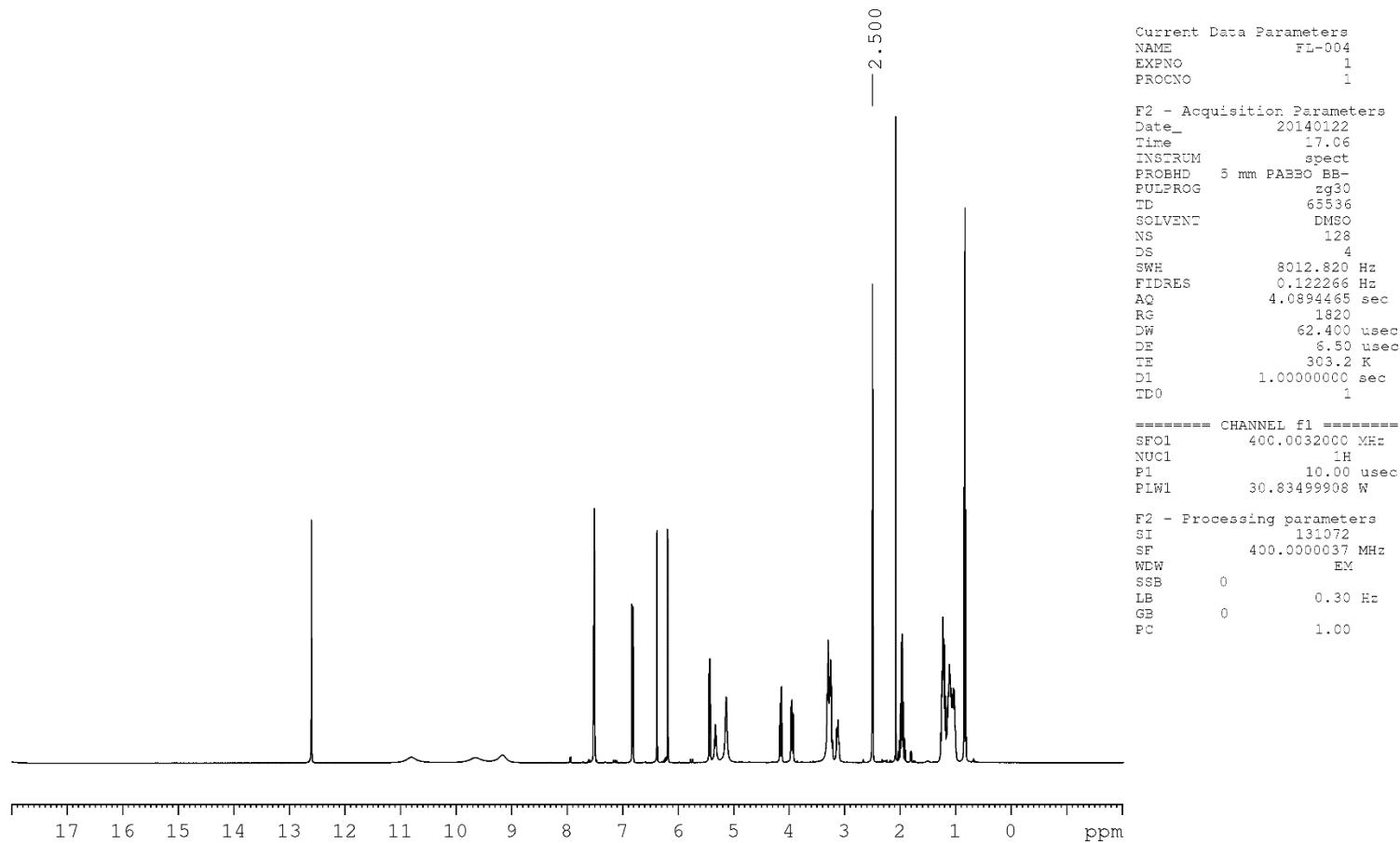
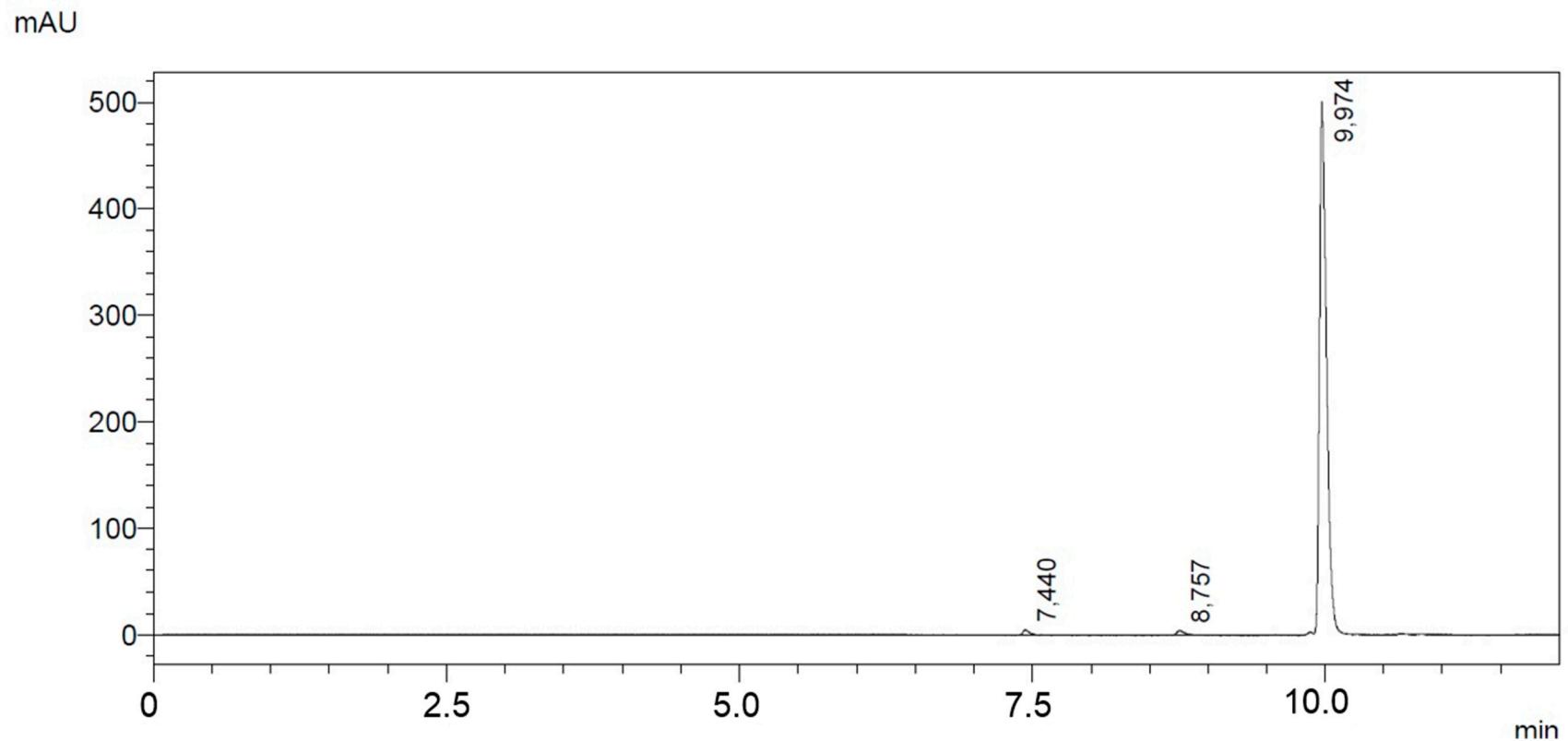


Figure S15. <sup>1</sup>H NMR spectrum of compound 6.



**Figure S16.** HPLC chromatogram of compound 6.

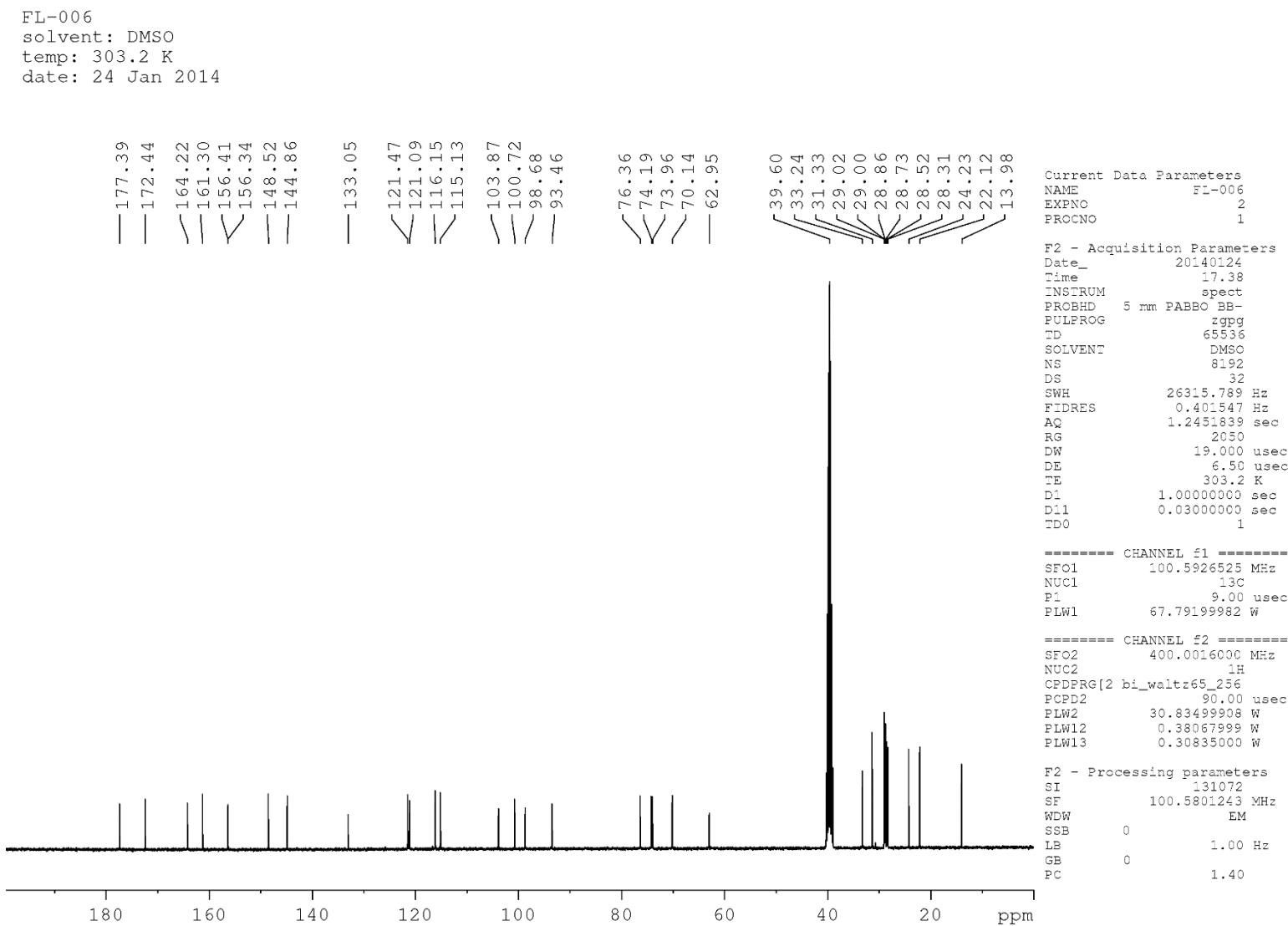


Figure S17.  $^{13}\text{C}$  NMR spectrum of compound 7.

FL-006  
solvent: DMSO  
temp: 303.2 K  
date: 24 Jan 2014

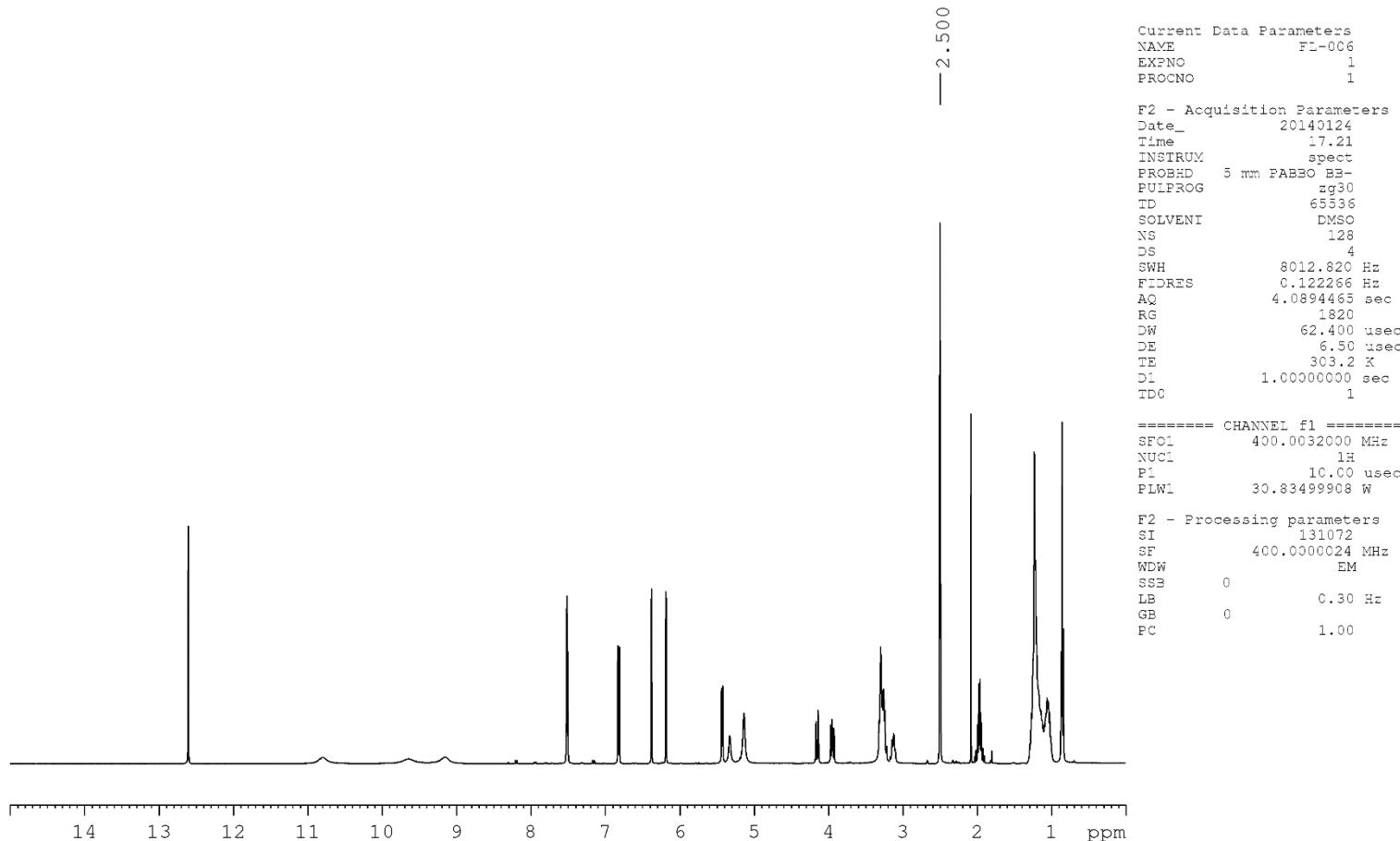
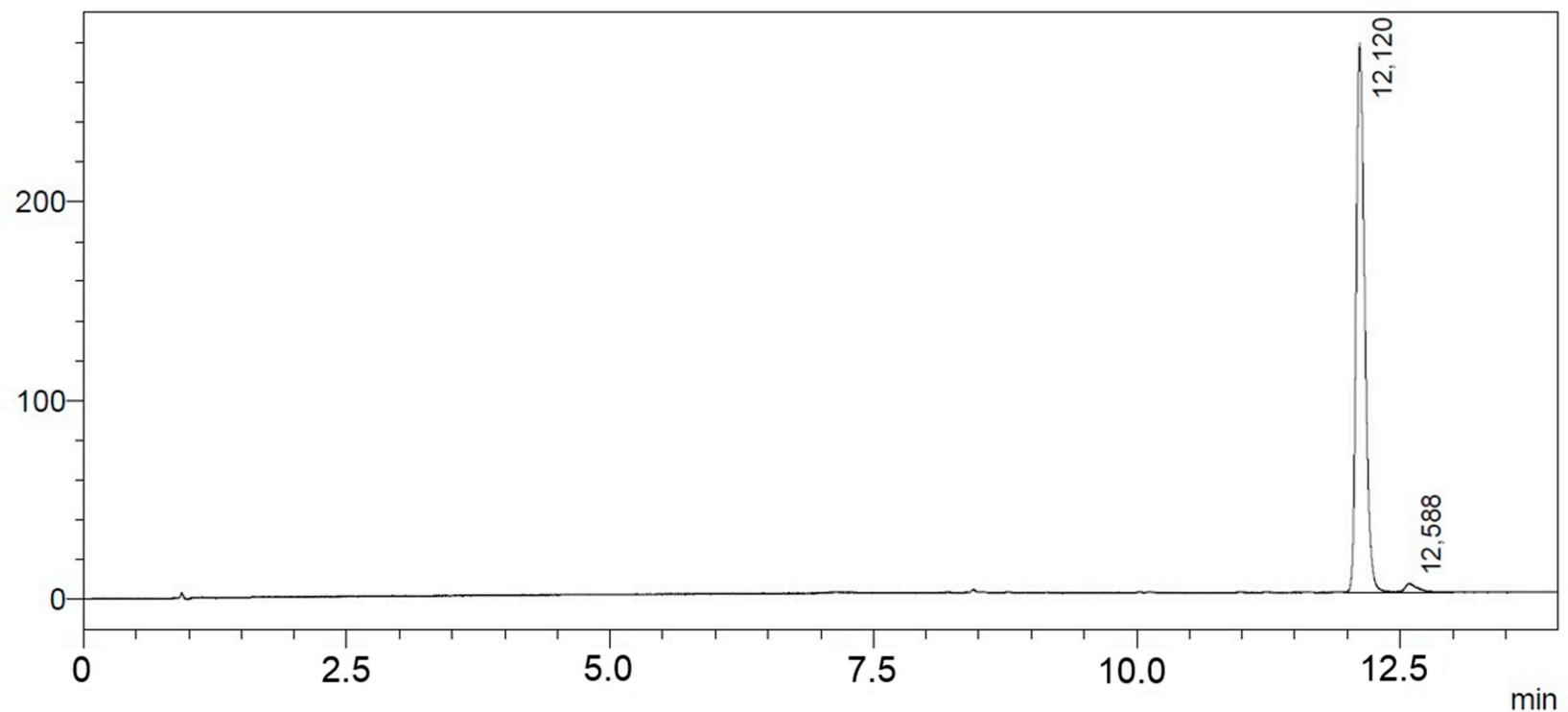


Figure S18.  $^1\text{H}$  NMR spectrum of compound 7.

mAU



**Figure S19.** HPLC chromatogram of compound 7.

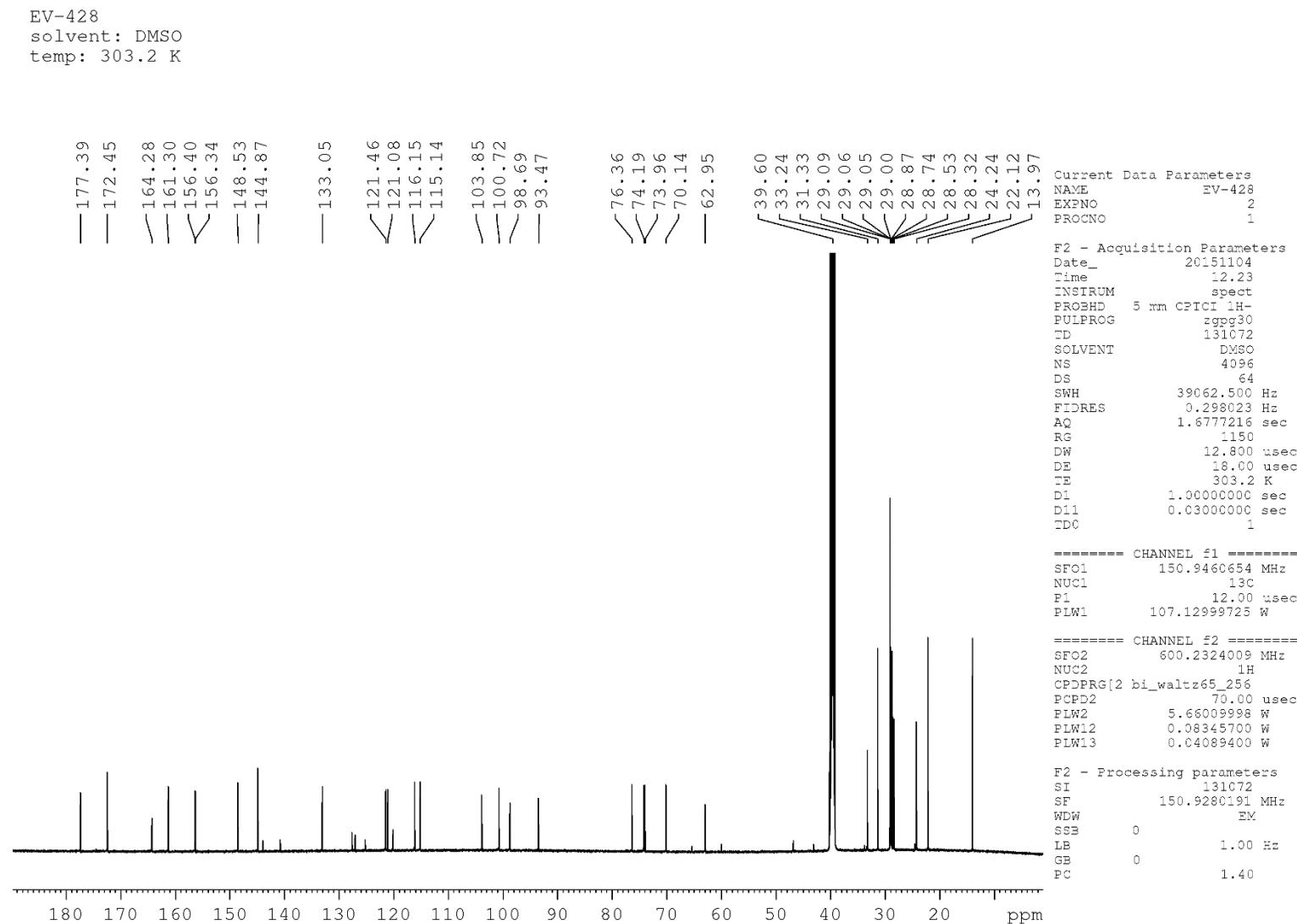


Figure S20.  $^{13}\text{C}$  NMR spectrum of compound 8.

EV-428  
solvent: DMSO  
temp: 303.2 K

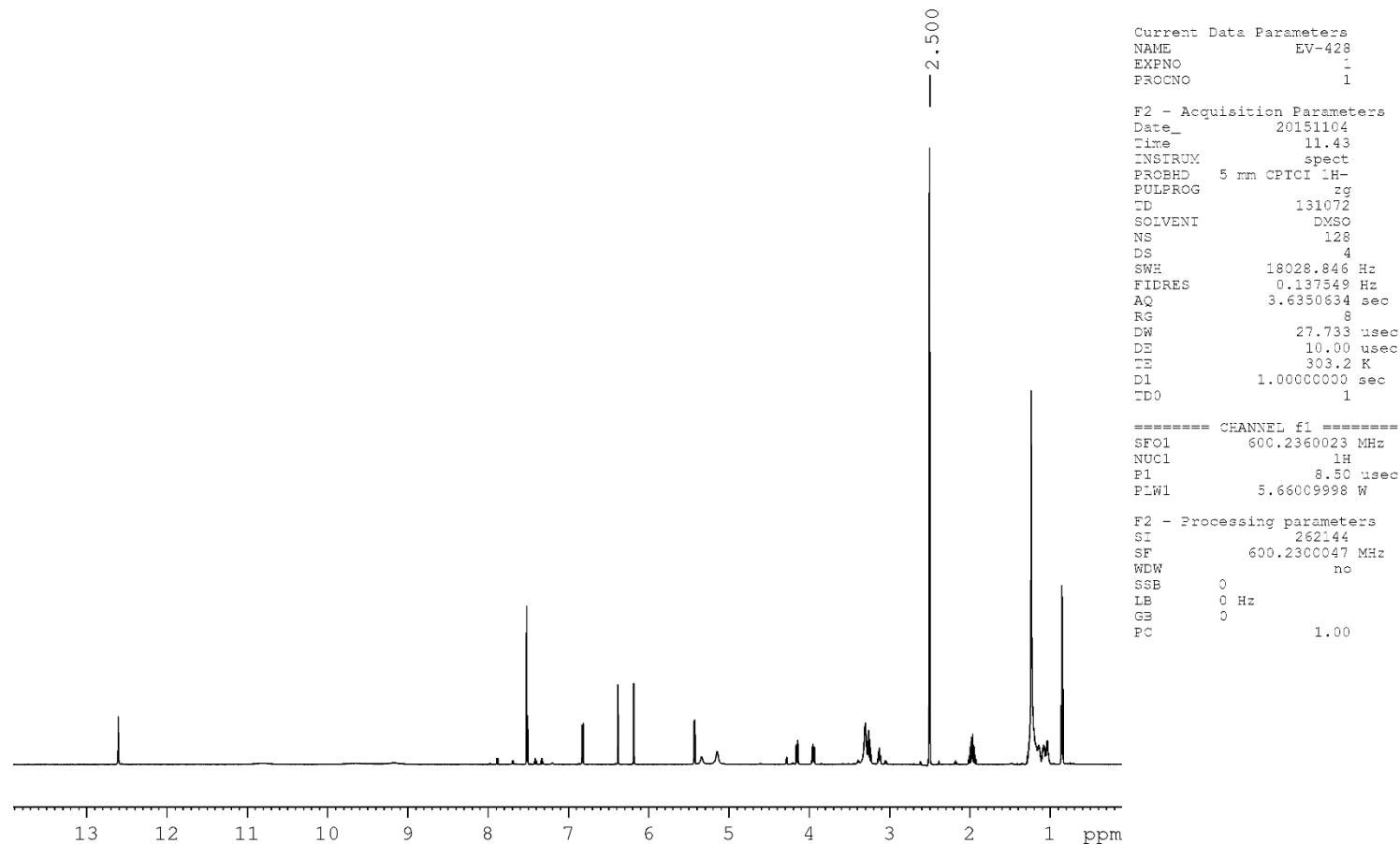
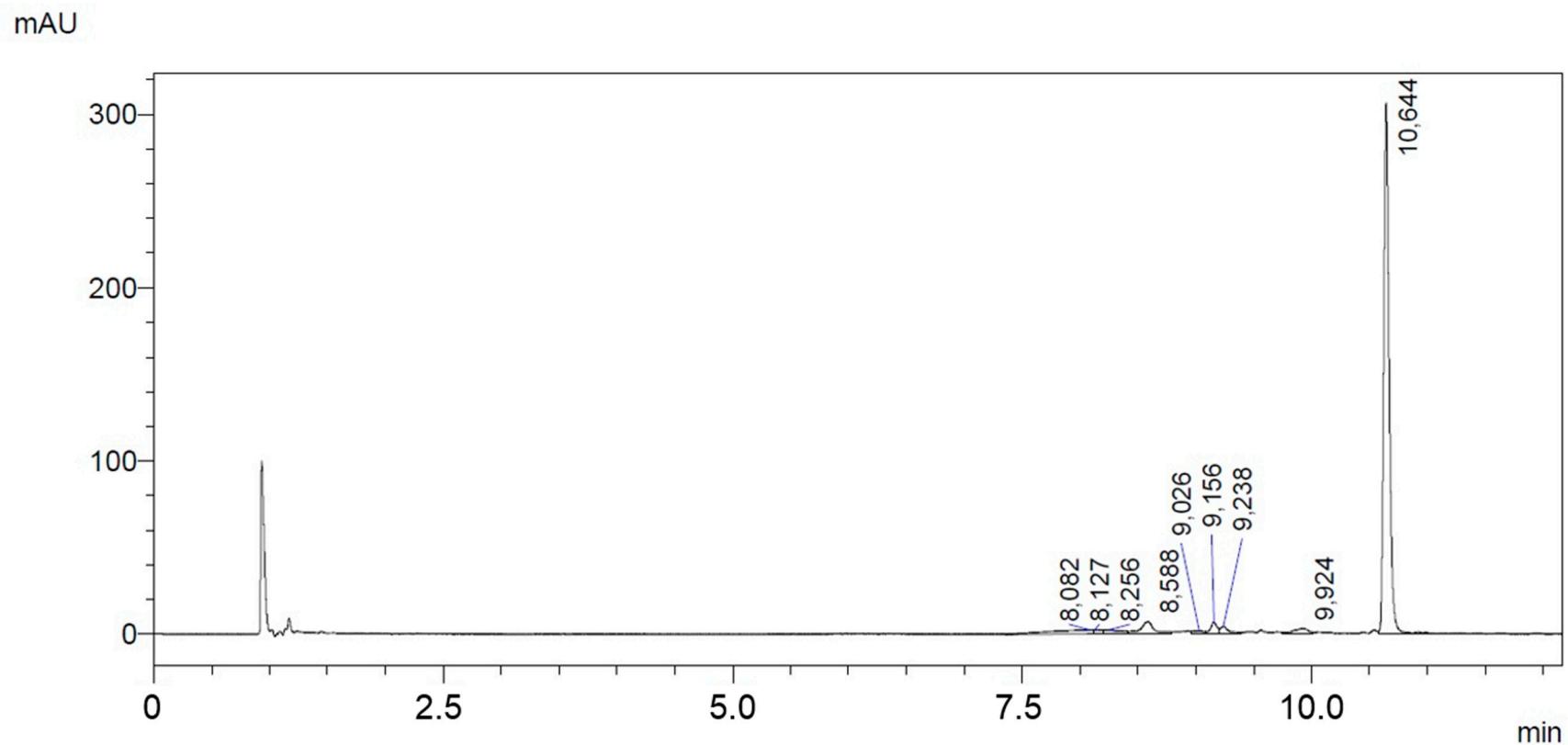


Figure S21.  $^1\text{H}$  NMR spectrum of compound 8.



**Figure S22.** HPLC chromatogram of compound 8.

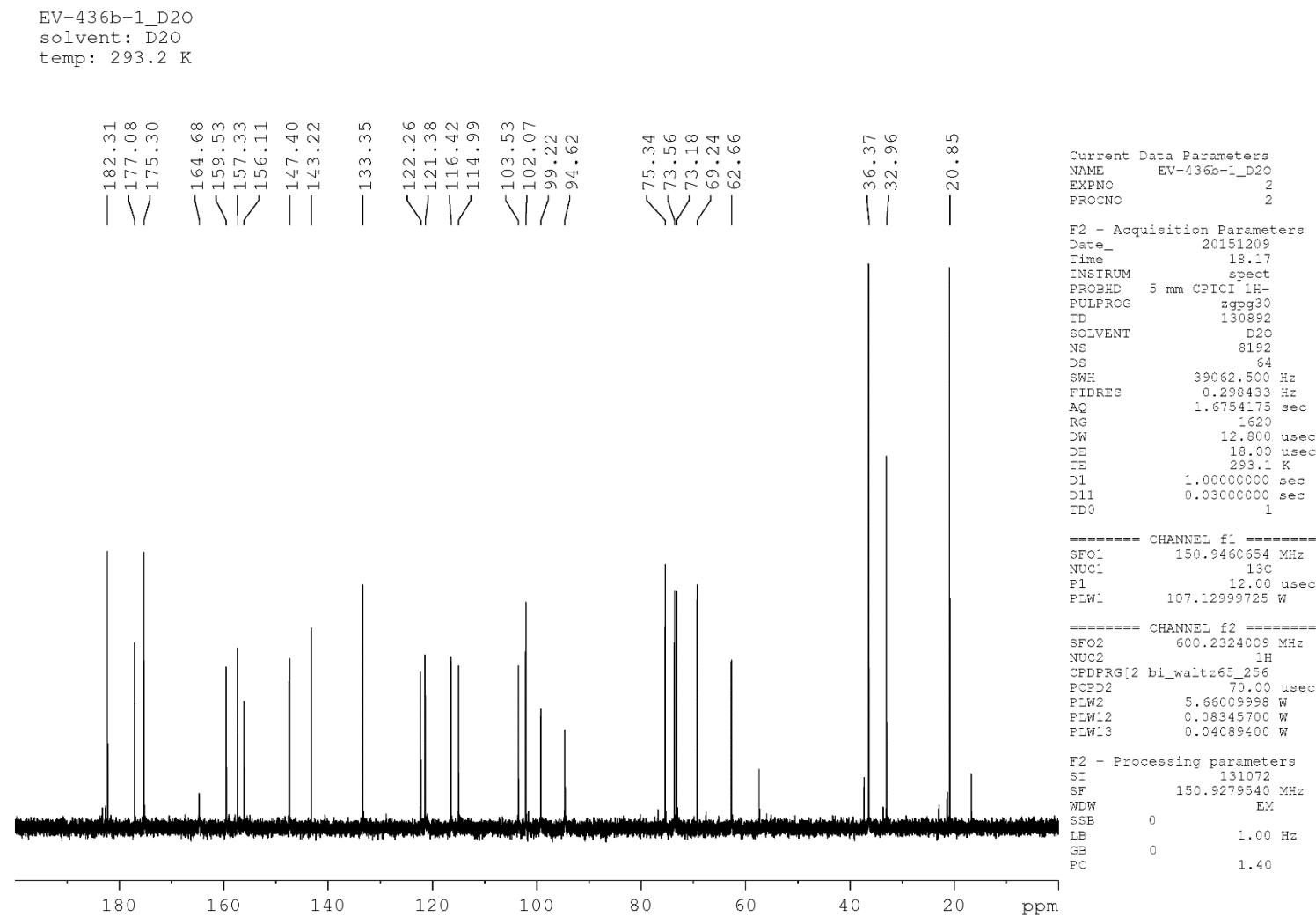


Figure S23.  $^{13}\text{C}$  NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

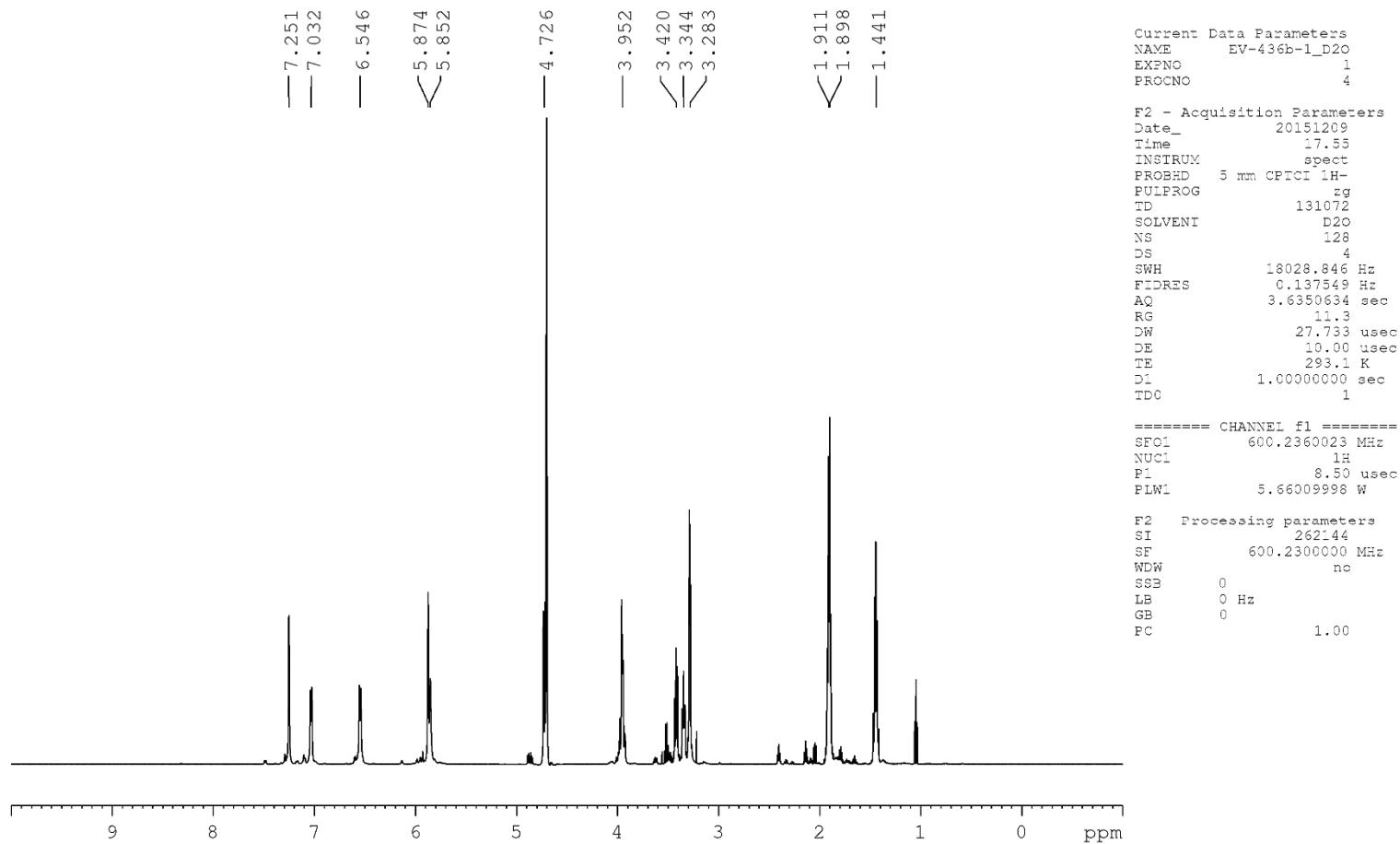
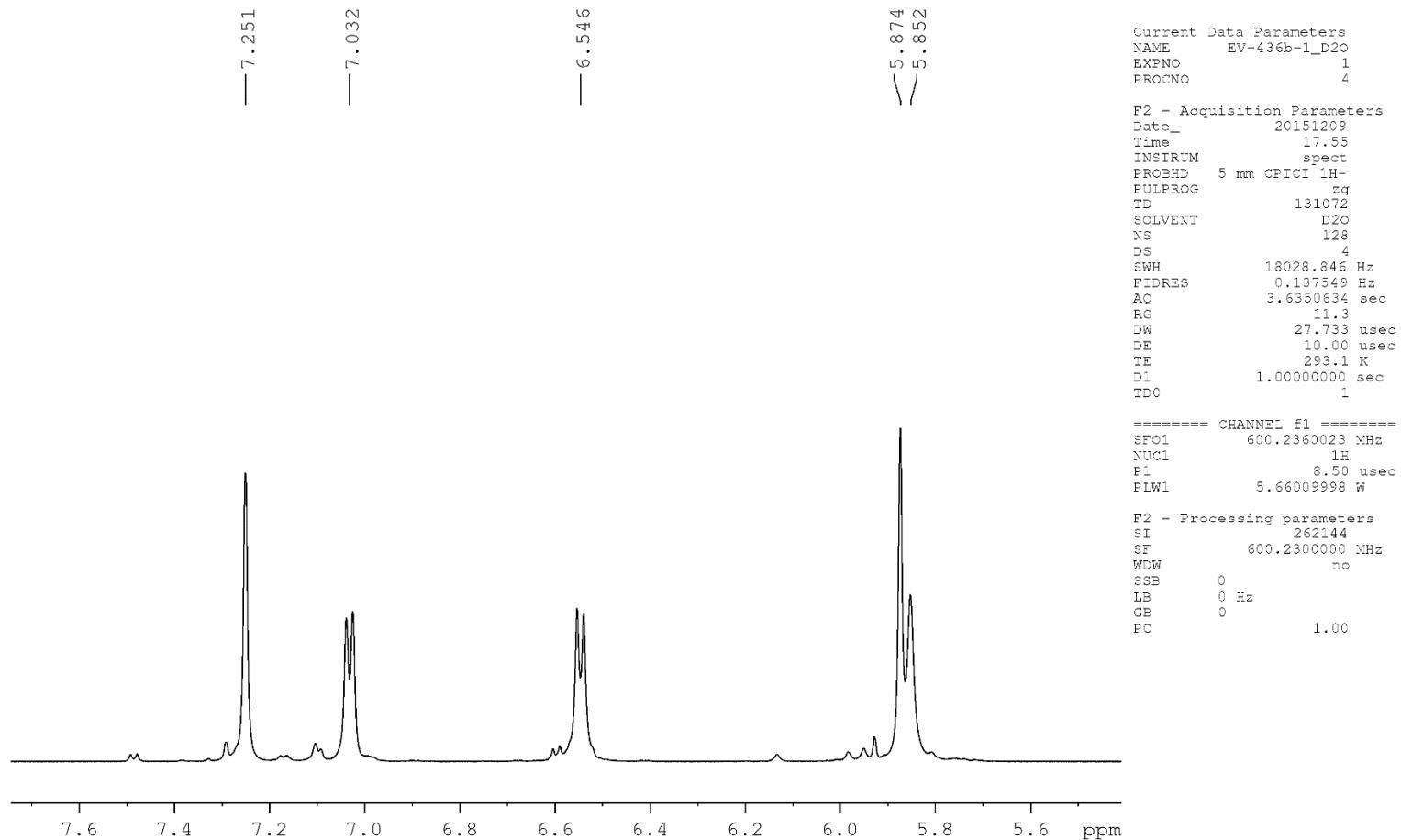


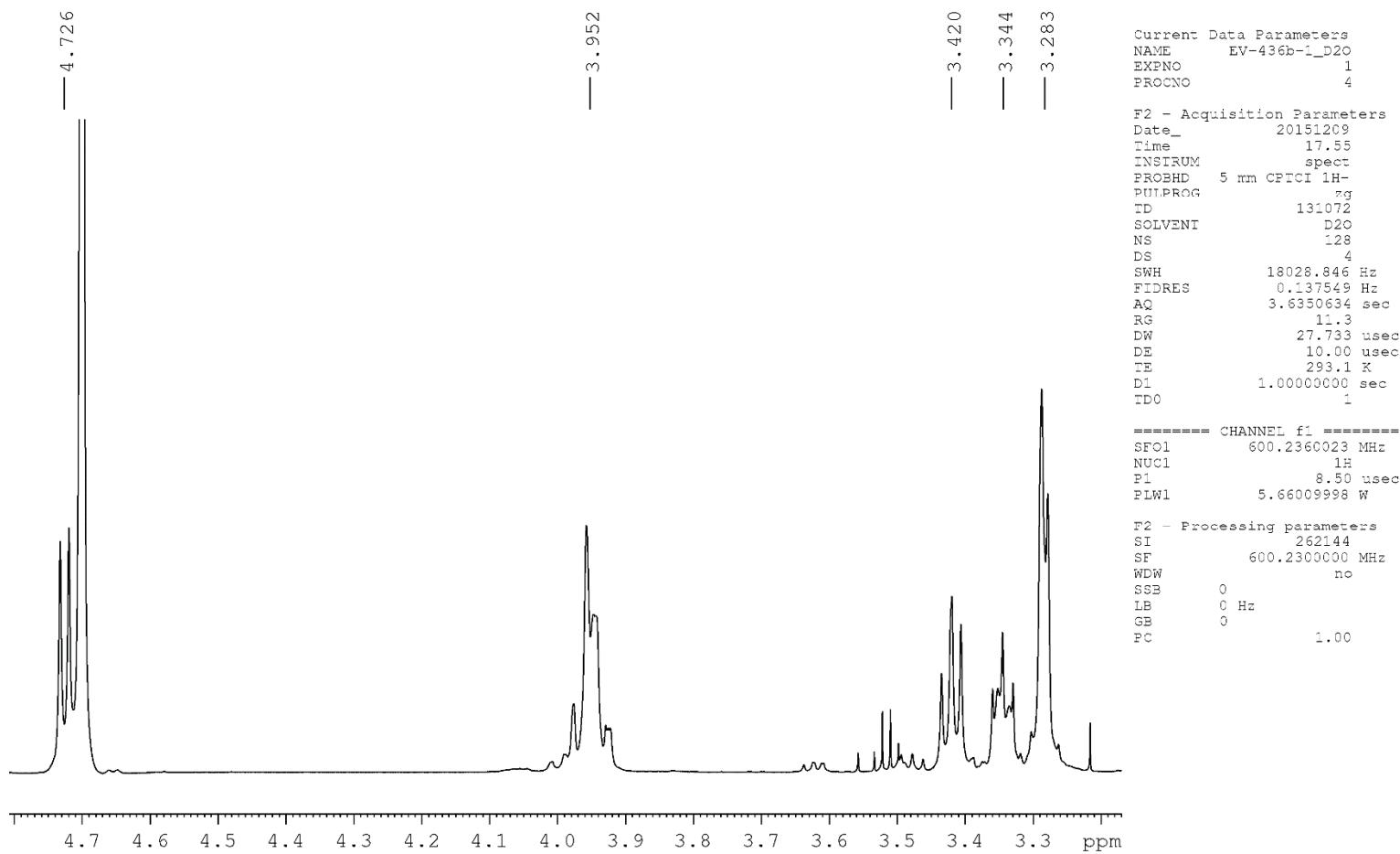
Figure S24.  $^1\text{H}$  NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



**Figure S25.** Detail (1/3) of <sup>1</sup>H NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



**Figure S26.** Detail (2/3) of <sup>1</sup>H NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

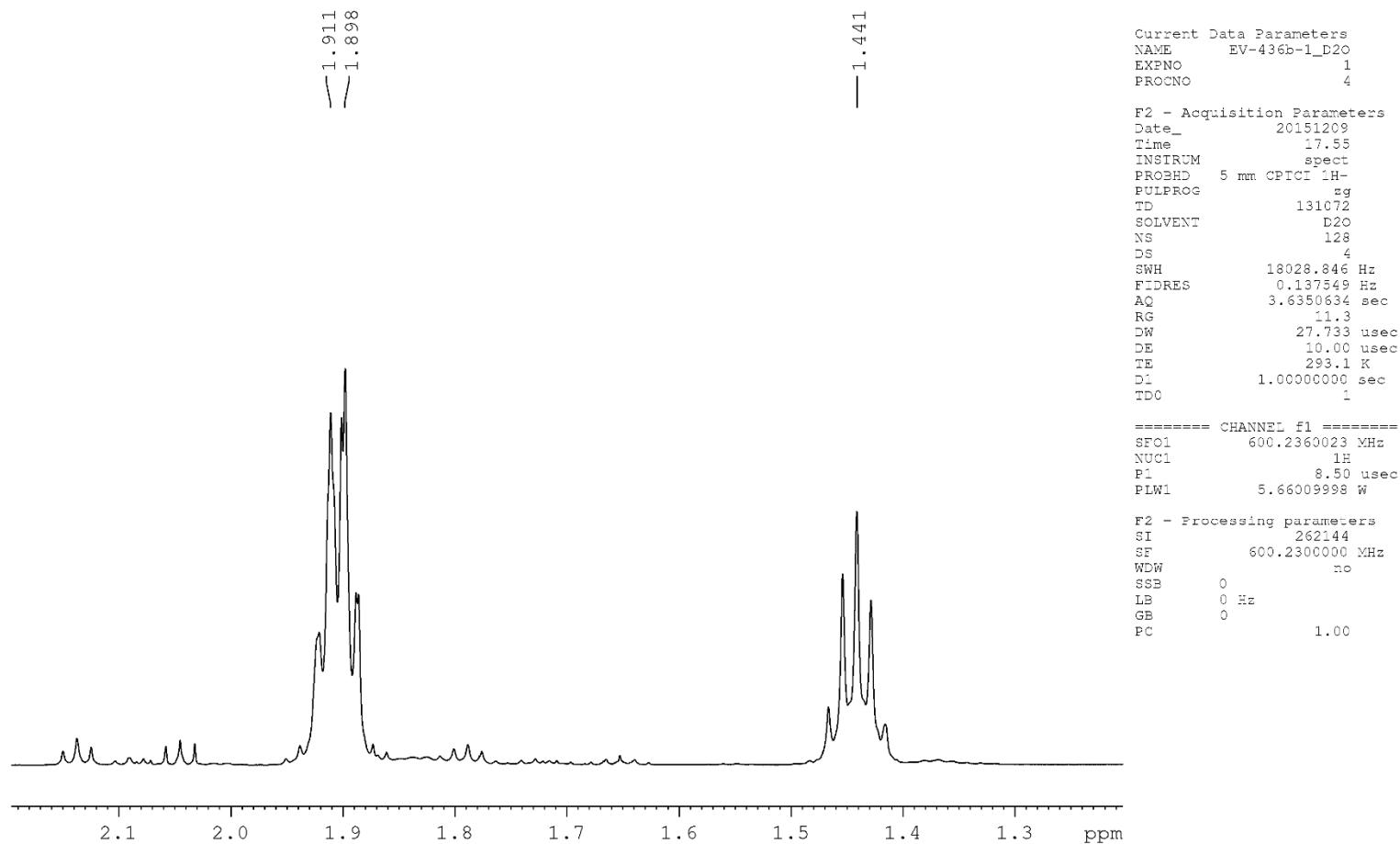


Figure S27. Detail (3/3) of  $^1\text{H}$  NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

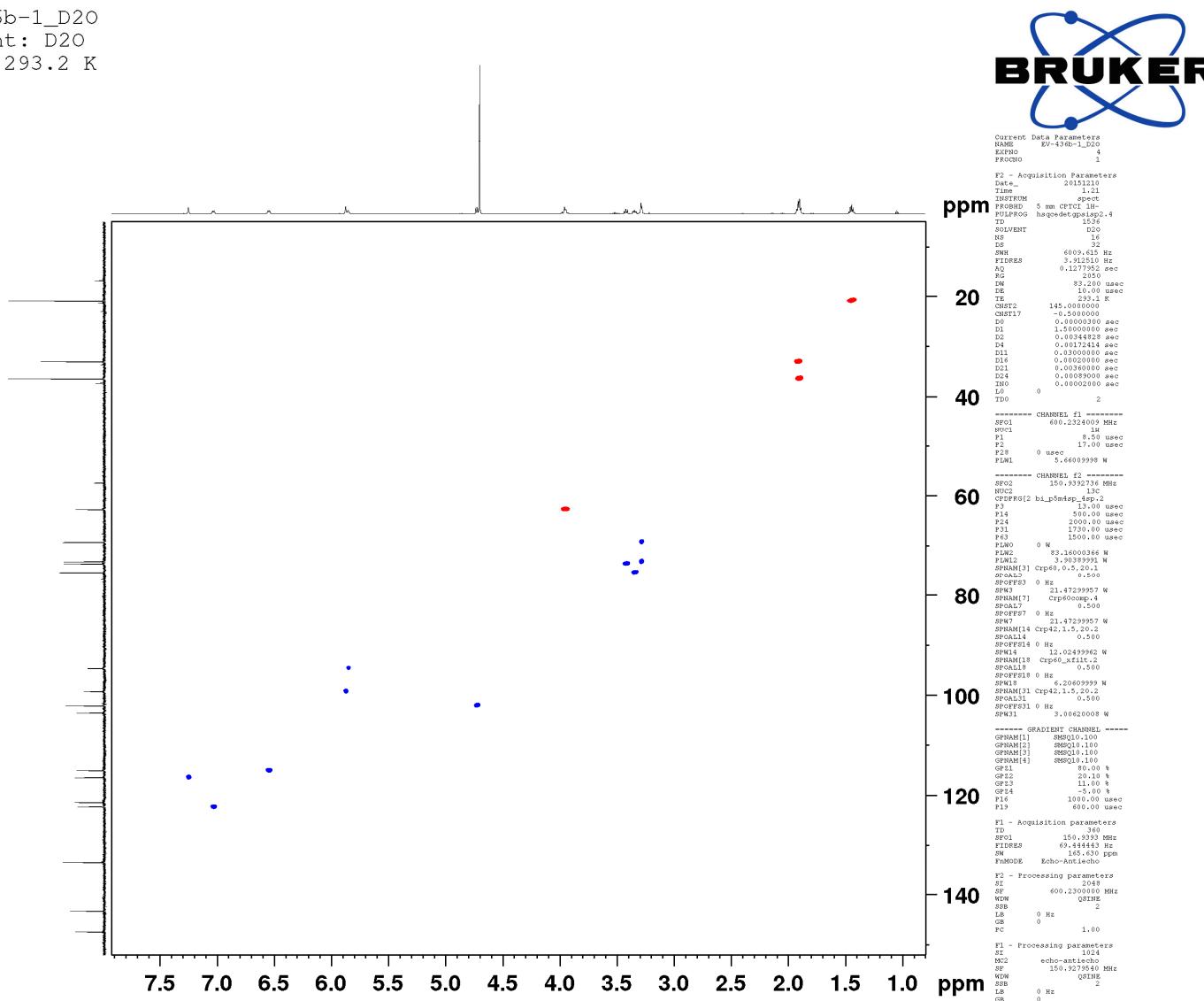
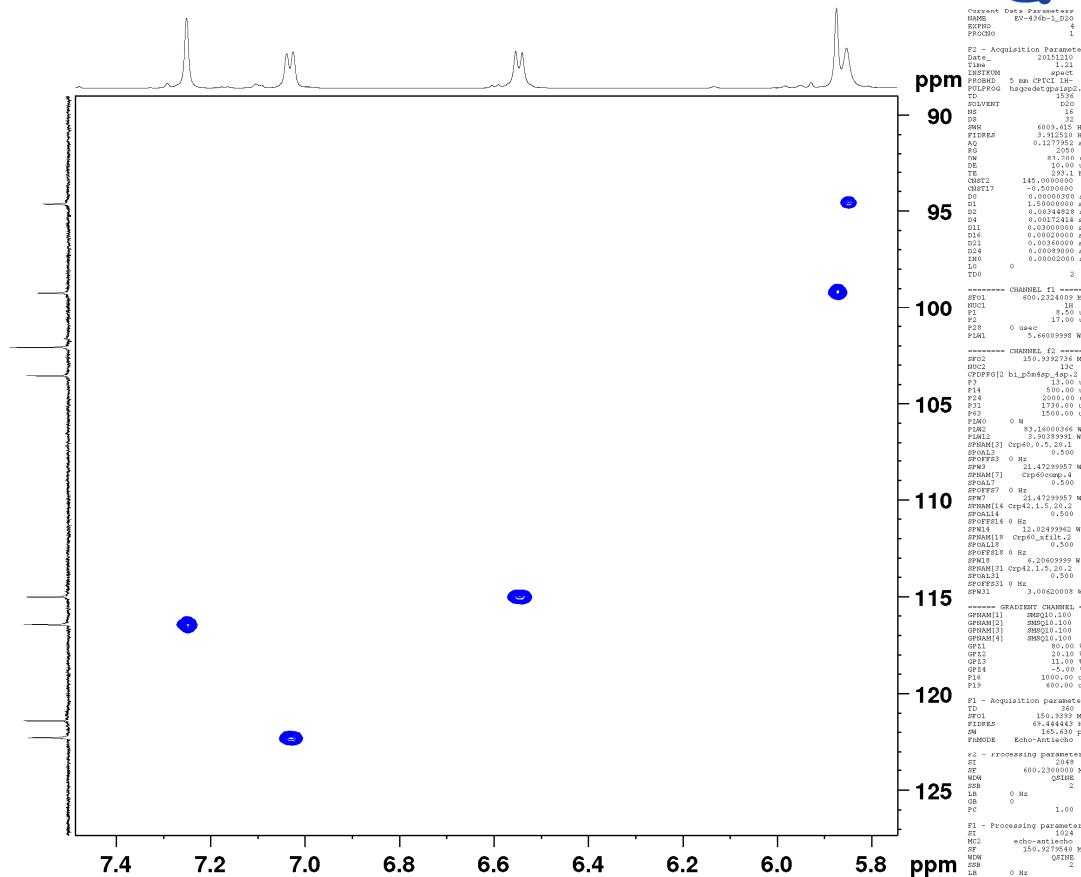


Figure S28. HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



**Figure S29.** Detail (1/3) of HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

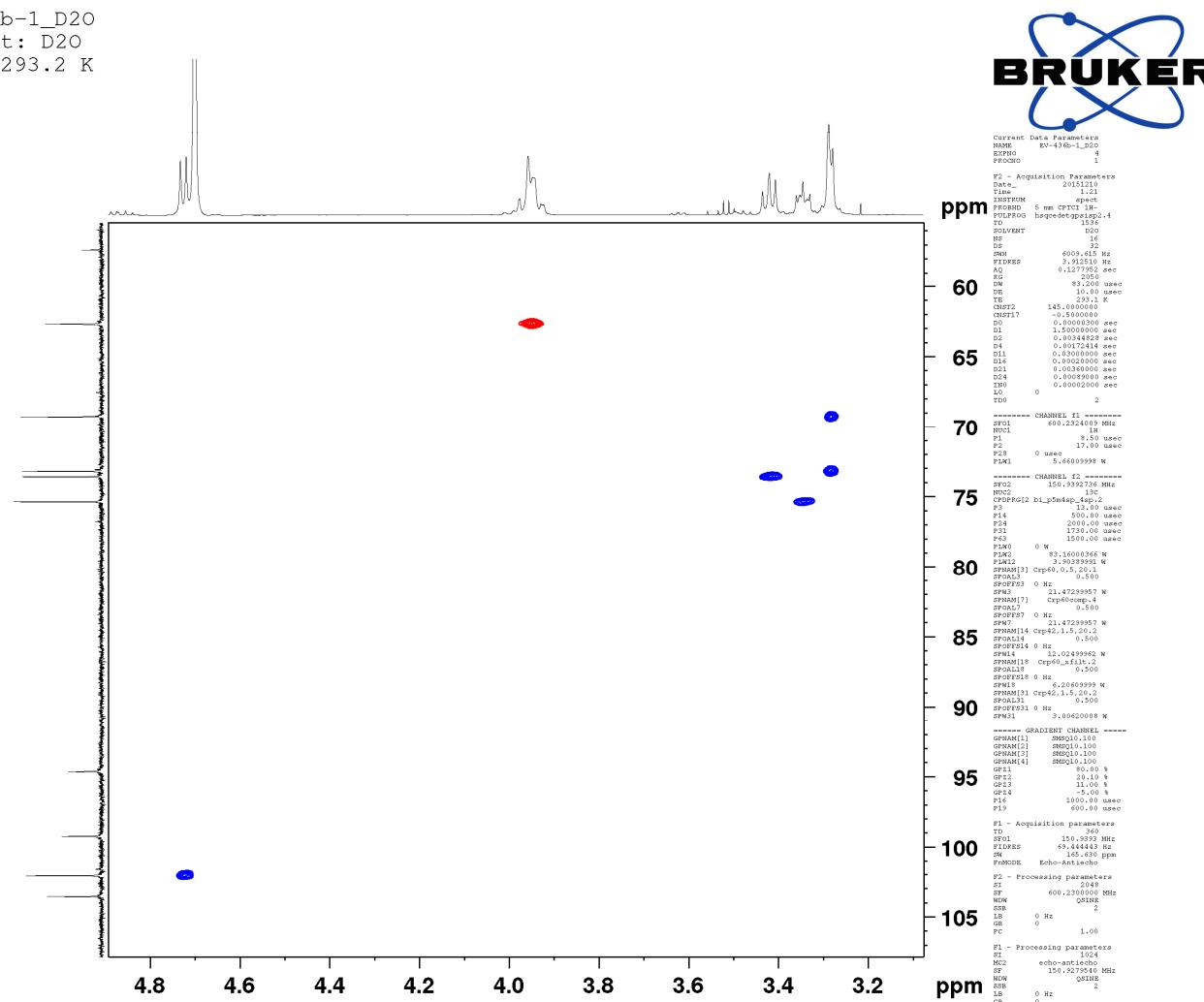
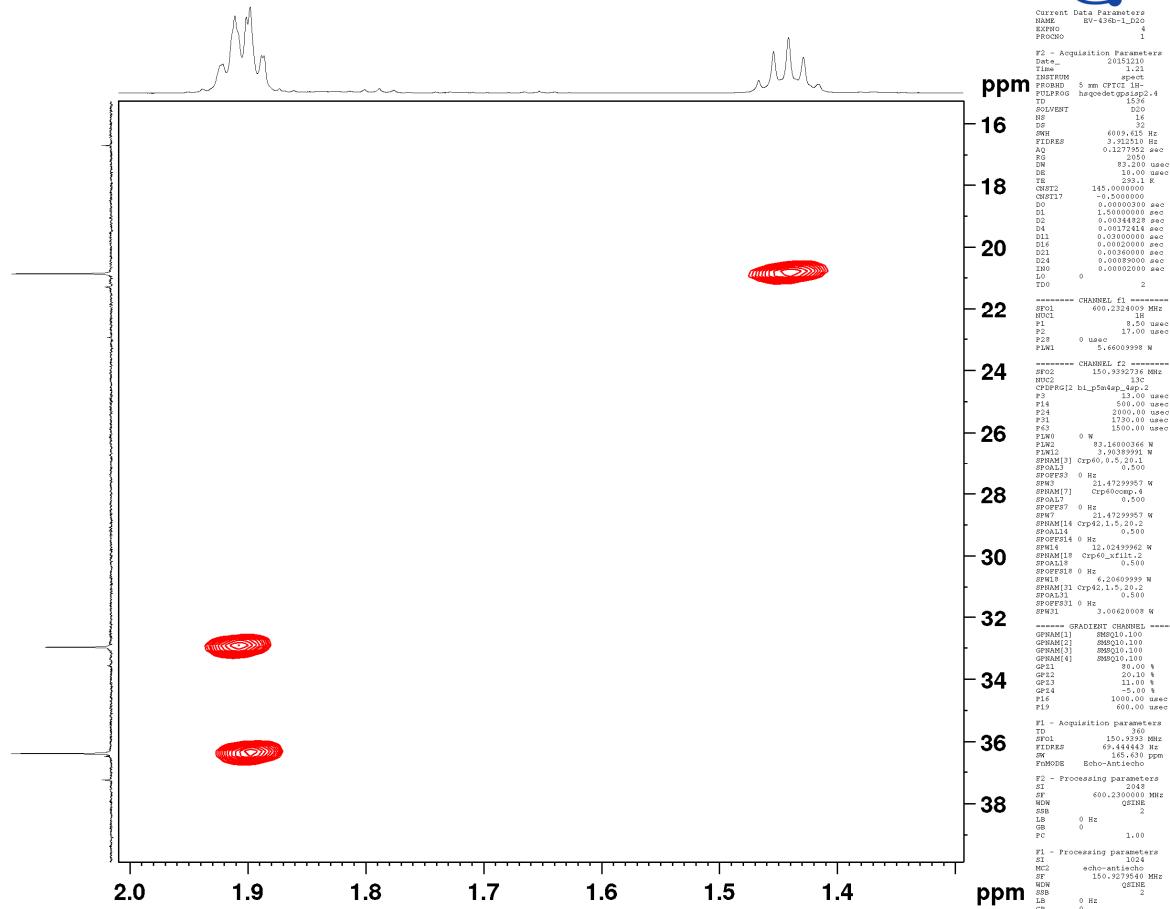


Figure S30. Detail (2/3) of HSQC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D<sub>2</sub>O  
temp: 293.2 K



**Figure S31.** Detail (3/3) of HSQC NMR spectrum of compound 9.

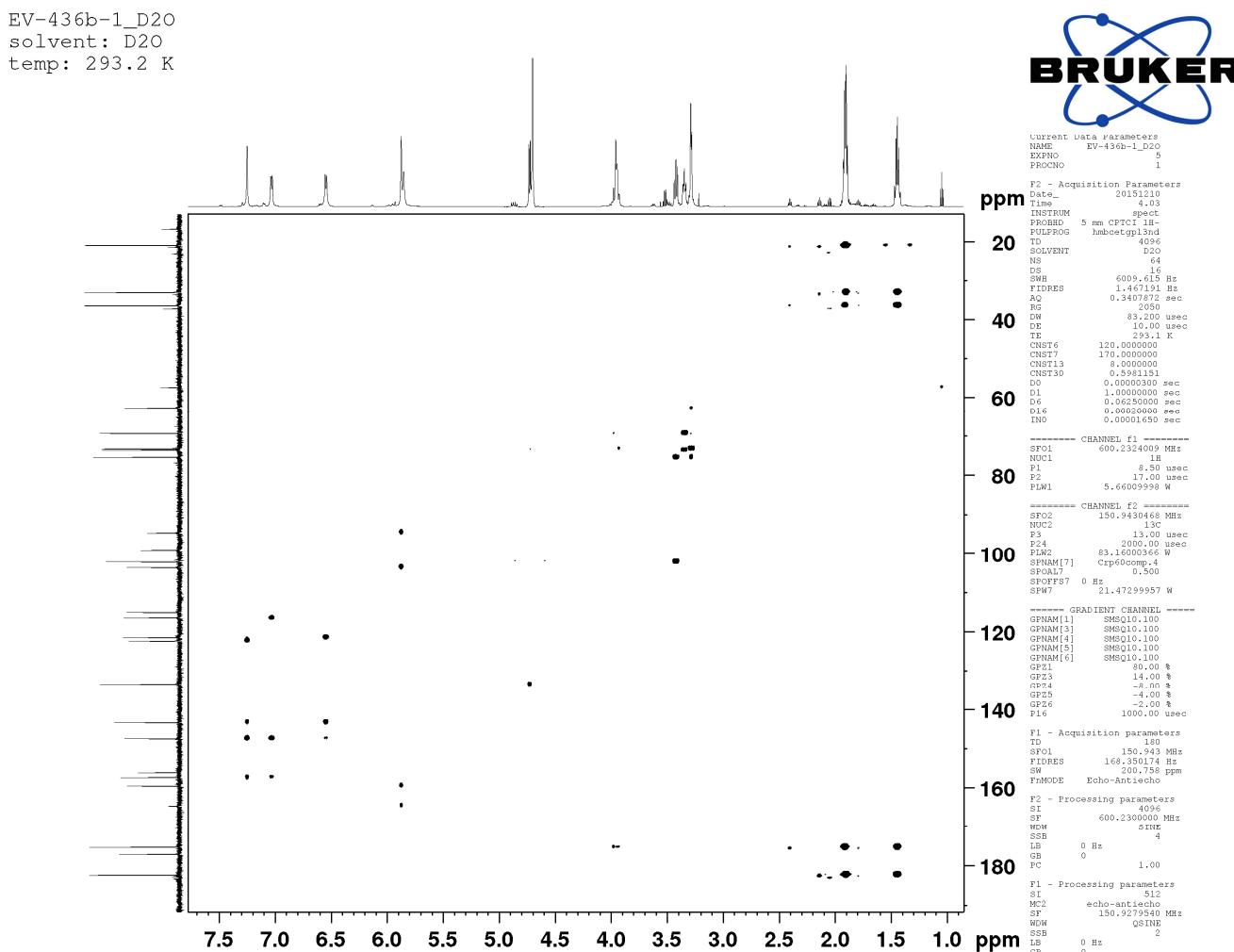


Figure S32. HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

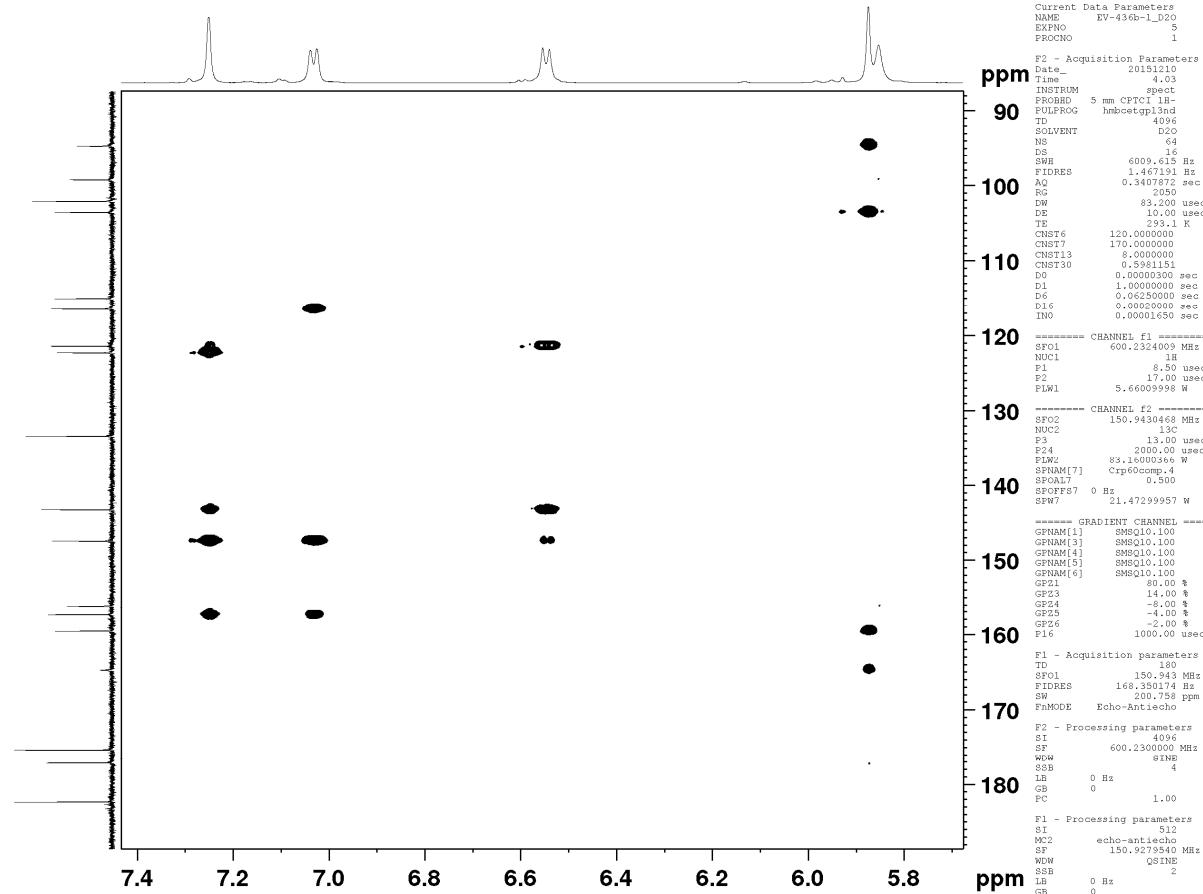


Figure S33. Detail (1/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



Current Data Parameters  
NMR EV-436b-1\_D2O  
EXPNO 5  
PROCNO 1  
  
F2 - Acquisition Parameters  
Data\_ 20151210  
Time 4.03  
DITRUM 894  
F2BDD 5 nm CPT118d  
T2 4096  
SOVENT D2O  
NS 64  
DS 16  
SWH 6009.615 Hz  
FIDRES 1.467191 Hz  
AQ 0.3407872 sec  
RG 2050  
P 83.42 usec  
DE 10.00 usec  
TE 293.1 K  
CNS75 120.000000  
CNS77 170.000000  
CNS713 8.000000  
CNS730 0.5981151  
DO 0.000001300 sec  
D1 1.000000 sec  
D6 0.06250000 sec  
D1G 0.00020000 sec  
IND 0.00001650 sec

CHANNEL f1  
SF01 600.2324009 MHz  
NUC1 13C  
P1 8.1 usec  
F2 17.00 usec  
FLW1 5.66009998 W

CHANNEL F2  
SF02 150.9430468 MHz  
NUC2 13C  
P1 12.00 usec  
P24 2000.00 usec  
FLW2 83.16000366 W  
SPNAM[7] Crp69comp.4  
GP1 0.500  
SPOFFS7 0 Hz  
SPW7 21.47299957 W

GRADIENT CHANNEL

GPNAME[1] SMS910.100

GPNAME[3] SMS910.100

GPNAME[5] SMS910.100

GPNAME[6] SMS910.100

GP21 80.00 %

GP23 10.00 %

GP24 -8.00 %

GP25 -4.00 %

GP26 -2.00 %

P16 1000.00 usec

F1 - Acquisition parameters

TR 150.943 MHz

FID01 168.350174 Hz

SW 200.758 ppm

FMODE Echo-Antiecho

F2 - Processing parameters

SI 4096

SB 600.2300000 MHz

WDW SINE

SSB 4

LB 0 Hz

GB 0

PC 1.00

F1 - Processing parameters

SI 512

MC2 echo-antiecho

SF 150.9279540 MHz

WDW QSINE

SSB 2

LB 0 Hz

GB 0

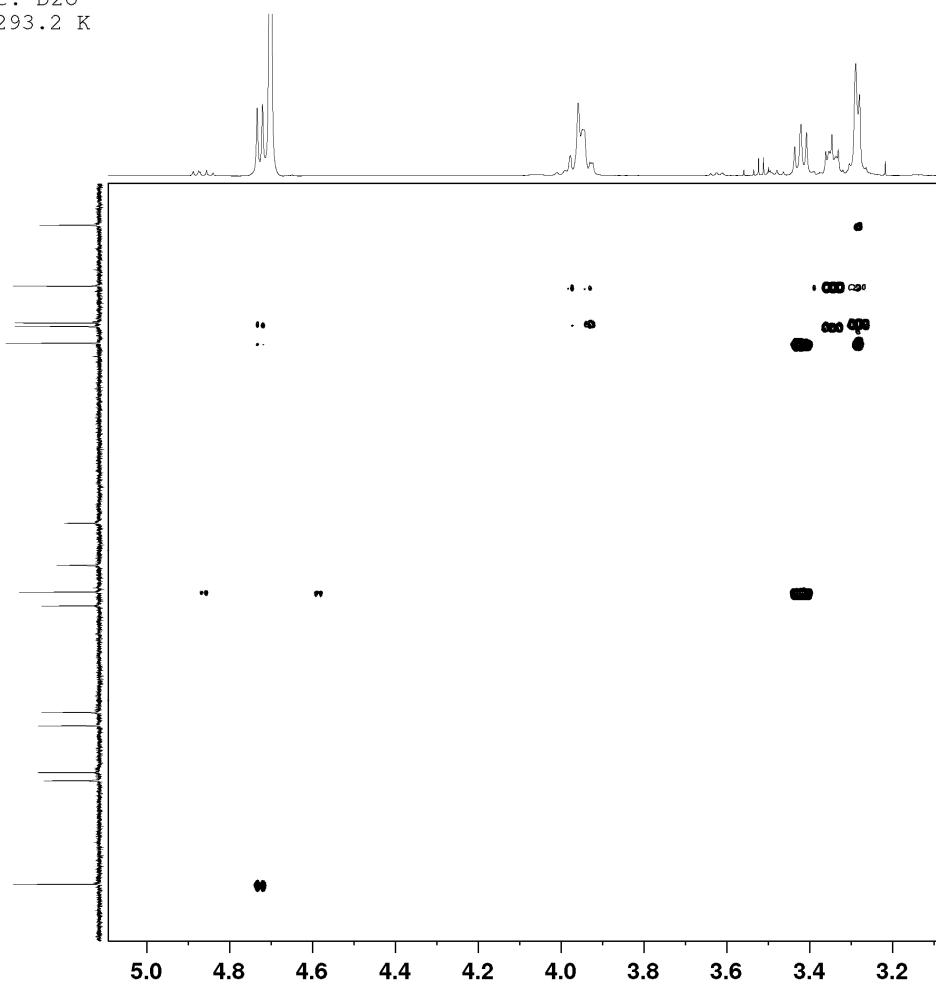
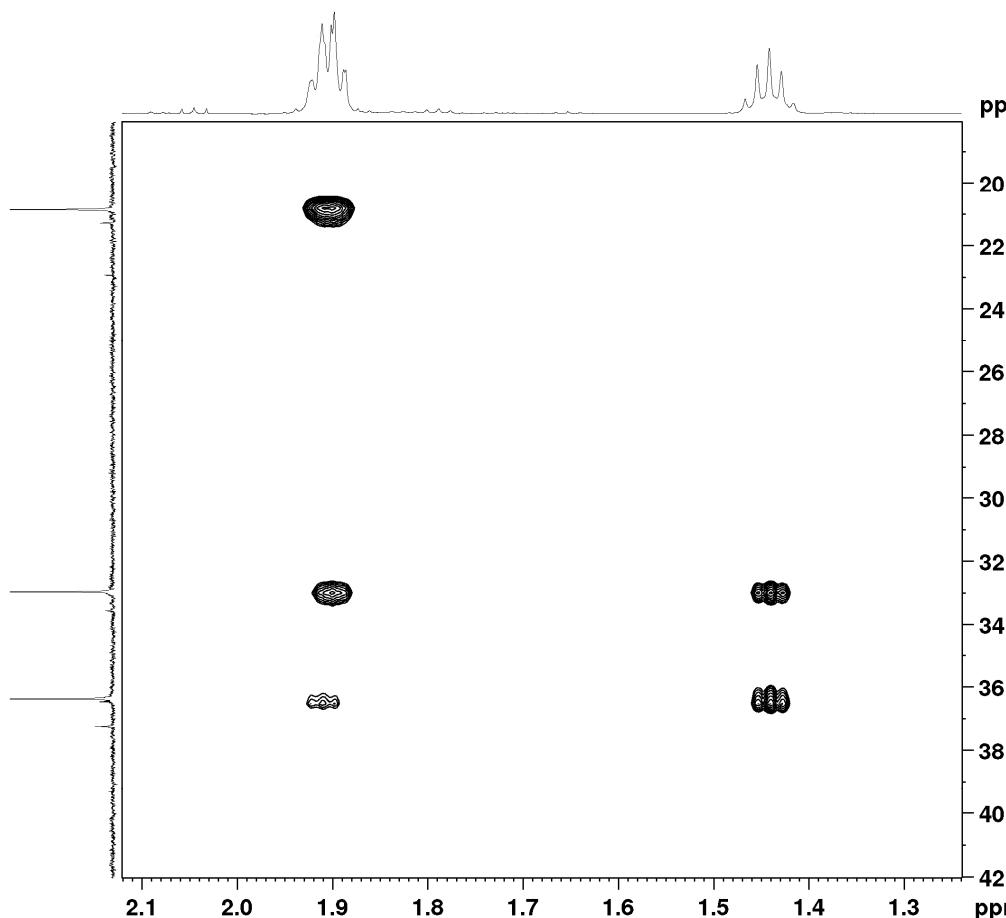


Figure S34. Detail (2/4) of HMBC NMR spectrum of compound 9.

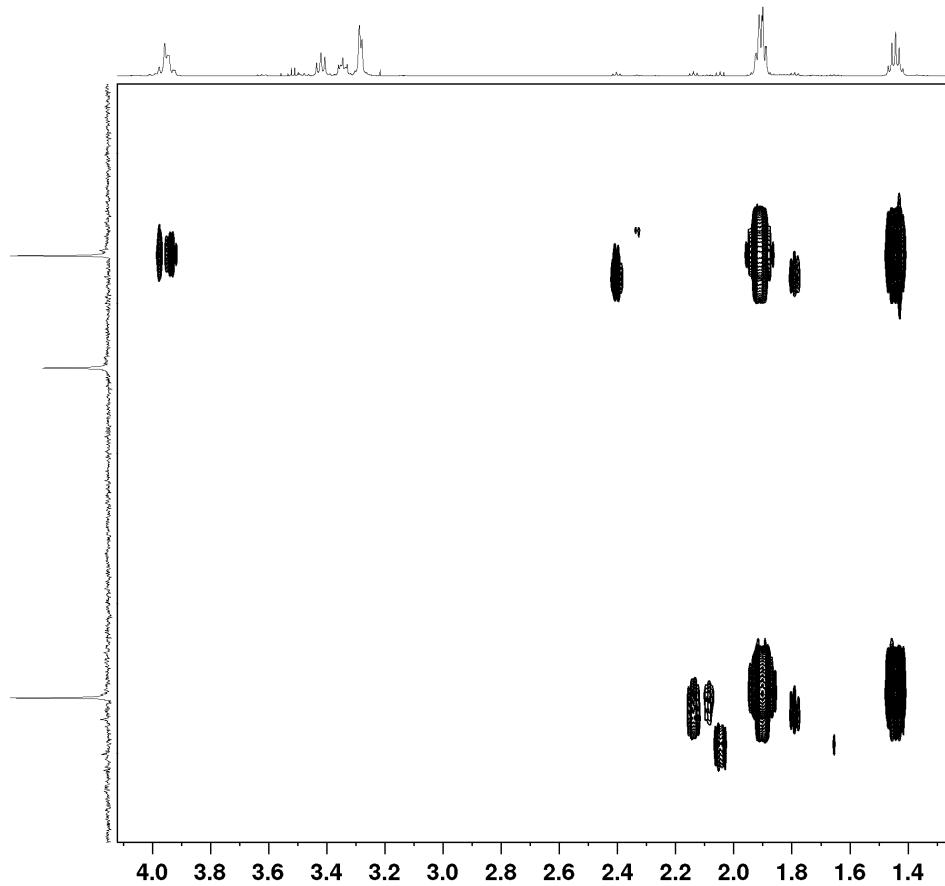
EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



Current Data Parameters  
NAME EV-436b-1\_D2O  
EXPNO 5  
PRCNO 1  
  
F2 - Acquisition Parameters  
Date 20151210  
Time 4.03  
INSTRUM spect  
PROBOD 5 mm CPT-1H  
PULPROG hmbctsgp13d  
TD 4096  
SOLVENT D2O  
NS 64  
DS 16  
SW 6000.015 Hz  
FIDRES 1.4471572 Hz  
AQ 0.3497872 sec  
RG 2050  
DW 83.200 usec  
D1 1.0000000 sec  
TDZ 10.000 usec  
TE 233.14 K  
CNS76 120.000000  
CNS77 170.000000  
CNS713 130.000000  
CNS720 0.5981151  
D0 0.00000300 sec  
D1 1.00000000 sec  
D2 0.1000000 sec  
D16 0.00020000 sec  
IND 0.00012000 sec  
  
===== CHANNEL f1 =====  
SF01 600.2324009 MHz  
NUC1 1H  
D1 8.00 usec  
P2 17.00 usec  
PLW1 5.66009998 W  
  
===== CHANNEL F2 =====  
SF02 150.9430468 MHz  
NUC2 13C  
P3 13.00 usec  
P4 200.000000 usec  
P1M2 83.16000346 W  
SPNAM[7] Crp60comp.4  
SPCAL7 0.500  
SPFF87 0 Hz  
SPW 21.47299957 W  
  
===== GRADIENT CHANNEL =====  
GPNAME[1] SMC910.100  
GPNAME[3] SMC910.100  
GPNAME[4] SMC910.100  
GPNAME[5] SMC910.100  
GPNAME[6] SMC910.100  
GP23 80.00 %  
GP23 14.00 %  
GP24 -8.00 %  
GP23 -4.00 %  
GP26 -2.00 %  
P16 1000.00 usec  
  
F1 - Acquisition parameters  
TD 180  
SF01 150.943 MHz  
L1DRES 169.350000 Hz  
SW 200.758 ppm  
F1MODE Echo-Antiecho  
  
F2 - Processing parameters  
SI 4096  
SF 600.2300000 MHz  
WDW SINE  
SSB 4  
LB 0 Hz  
GB 0  
PC 1.00  
  
F1 - Processing parameters  
SI 512  
MIXING echo-anti-160  
SF 150.9279540 MHz  
WDW QSINE  
SSB 2  
GB 0

Figure S35. Detail (3/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



Current Data Parameters  
NAME EV-436b-1\_D2O  
EXPNO 5  
PROCNO 1  
FID dimension 1  
TD 204800  
Time 1.03  
INSTRUM spect  
PROBHD 5 mm CPTCI 1H  
PULPROG hmcetdpgrd  
TDZ 1096  
SOLVENT D2O  
NS 64  
DW 6000.615 ms  
FIDRES 1.467191 Hz  
AQ 0.340712 sec  
SWR 2050  
DS 83.200 usec  
DE 10.00 usec  
TE 293.2 K  
C18ST6 120.000000  
C18ST7 170.000000  
C18ST13 8.0000000  
C18ST30 0.1-1.1  
DW0 0.00000300 sec  
D1 1.0000000 sec  
D6 0.0625000 sec  
D16 0.0000000 sec  
IM 0.00001450 sec

CHANNEL f1 -----  
SF01 600.232419 MHz  
NUC1 1H  
P1 8.50 usec  
P2 17.00 usec  
P1M1 5.66009998 H

CHANNEL f2 -----  
SF02 150.943013 MHz  
NUC2 13C  
P24 2000.00 usec  
P44 83.12600000 H  
SF03M[7] Csp6000sp.4  
SF04L7 0.500  
SF05FS7 0 Hs  
SF07 21.47299957 H

GRADIENT CHANNEL -----  
GRNM[1] SMSQ10.100  
GRNM[3] SMSQ10.100  
GRNM[4] SMSQ10.100  
GRNM[5] SMSQ10.100  
GRNM[6] SMSQ10.100  
GP21 80.00 %  
GP23 14.00 %  
GP24 -8.00 %  
GP25 -4.00 %  
GP26 -2.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 180  
SF01 150.943 MHz  
FIDRES 168.350174 Hz  
W1W0 20.0000 ppm  
PR1 MODE Echo-antiEch

F2 - Processing parameters  
SI 1024  
SF 600.2300000 MHz  
W1W0 SINE  
SSB 4  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 512  
MC2 echo-antiecho  
SF 150.9279540 MHz  
W1W0 QSBINE  
SSB 2  
LB 0 Hz  
GB 0

Figure S36. Detail (4/4) of HMBC NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K



Current Data Parameters  
NAME EV-436b-1\_D2O  
EXPNO 3  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date 20151210  
Time 0.14  
INSTRUM spect  
PROBHD 5 mm CPTCI 1H-  
PULPROG cosyqpmfgrf  
TD 4096  
SOLVENT D2O  
NS 8  
DS 16  
SWH 6009.615 Hz  
FIDRES 1.467191 Hz  
AQ 0.3407872 sec  
RG 2050  
DW 83.200 usec  
DE 10.00 usec  
TE 293.1 K  
D0 0.00000300 sec  
D1 1.0000000 sec  
D13 0.00000400 sec  
D16 0.0002000 sec  
INO 0.00016660 sec  
  
===== CHANNEL f1 =====  
SF01 600.2324009 MHz  
NUC1 1H  
P1 8.50 usec  
PLW1 5.66009998 W  
  
===== GRADIENT CHANNEL =====  
GPNAME[1] SMSQ10.100  
GPNAME[2] SMSQ10.100  
GPNAME[3] SMSQ10.100  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
PL6 1000.00 usec  
  
F1 - Acquisition parameters  
TD 360  
SF01 600.2324 MHz  
FIDRES 16.673336 Hz  
SW 10.000 ppm  
FmMode QF  
  
F2 - Processing parameters  
SI 4096  
SF 600.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GR 0  
PC 1.00  
  
F1 - Processing parameters  
SI 4096  
MC2 QF  
SF 600.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

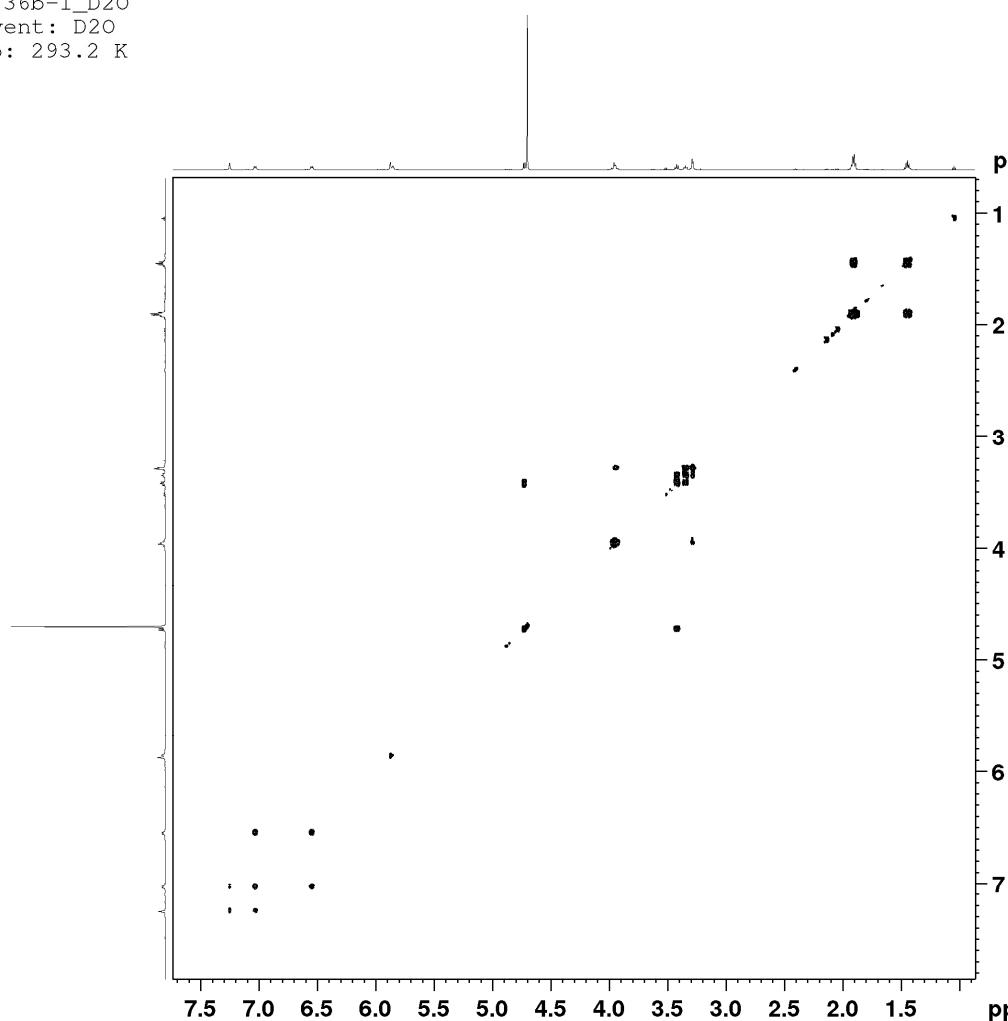


Figure S37. COSY NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D2O  
temp: 293.2 K

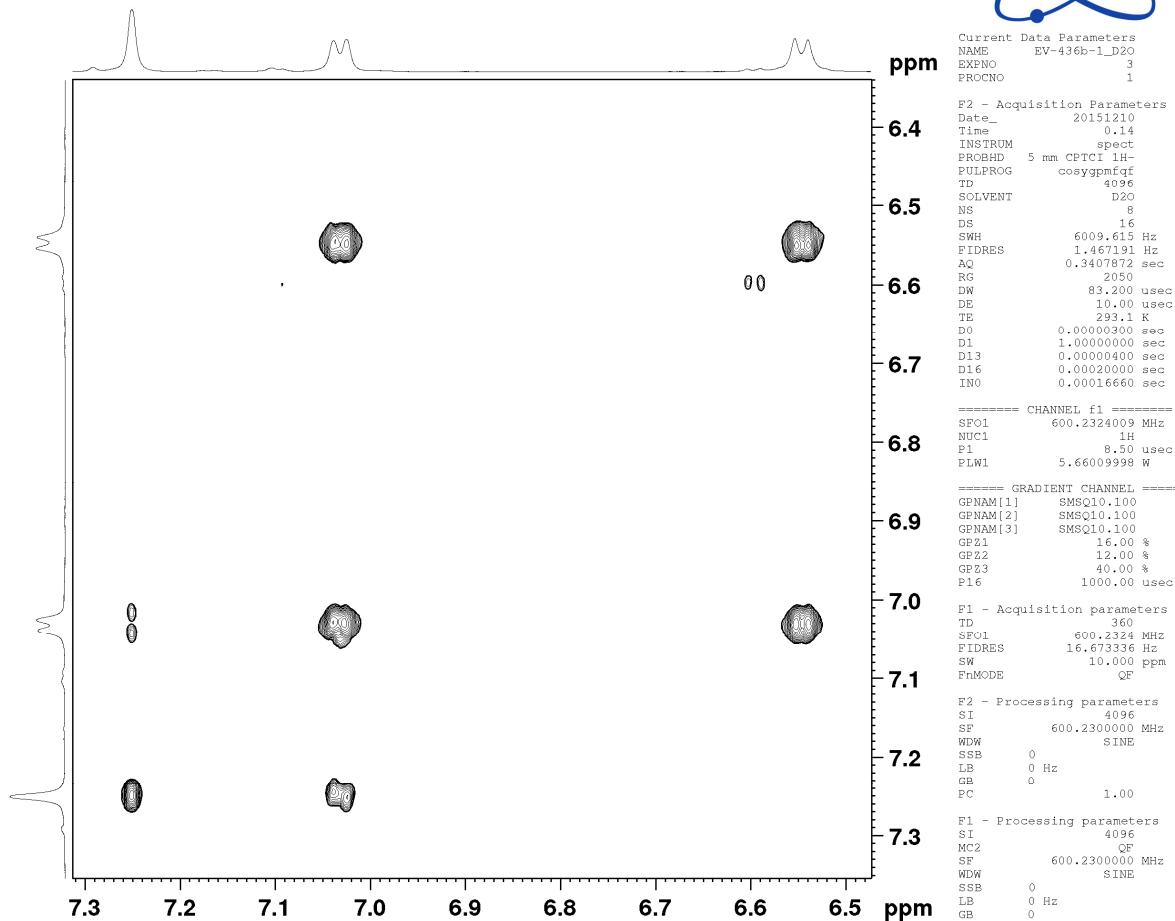


Figure S38. Detail (1/3) of COSY NMR spectrum of compound 9.

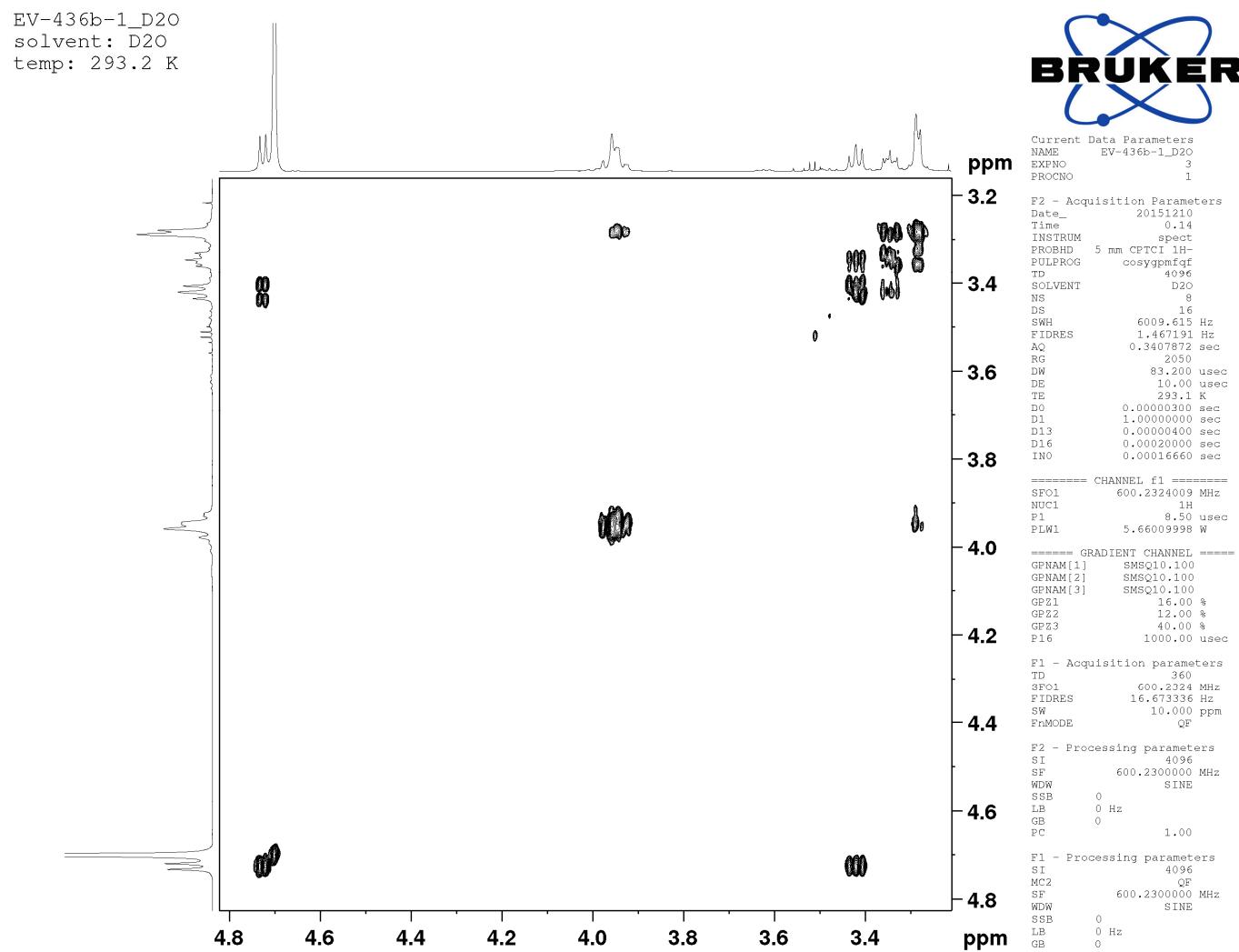
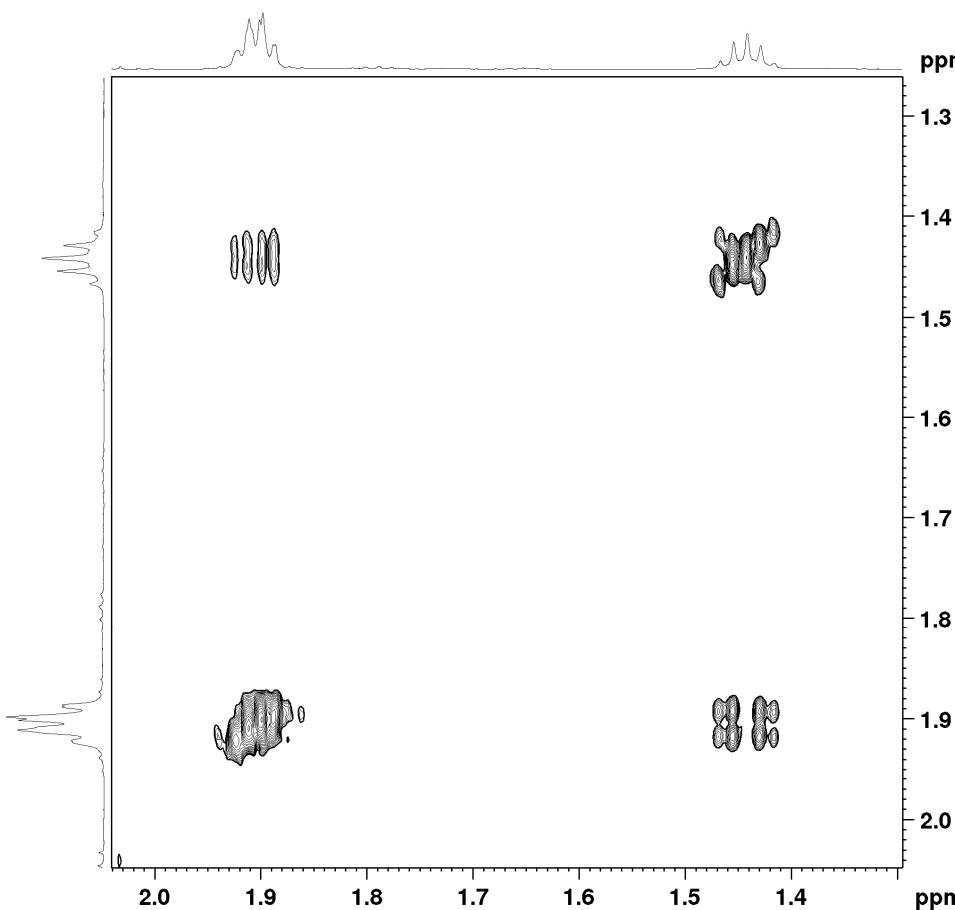


Figure S39. Detail (2/3) of COSY NMR spectrum of compound 9.

EV-436b-1\_D2O  
solvent: D<sub>2</sub>O  
temp: 293.2 K



Current Data Parameters  
NAME EV-436b-1\_D2O  
EXPNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date 20151210  
Time 0.14  
INSTRUM spect  
PROBHD 5 mm CPTCI 1H-  
PULPROG cosygppmfgf  
TD 4096  
SOLVENT D<sub>2</sub>O  
NS 8  
DS 16  
SWH 6009.615 Hz  
FIDRES 1.467191 Hz  
AQ 0.3407872 sec  
RG 2050  
DW 83.200 usec  
DE 10.00 usec  
TE 293.1 K  
D0 0.00000300 sec  
D1 1.00000000 sec  
D13 0.00000400 sec  
D16 0.00020000 sec  
INO 0.00016660 sec

===== CHANNEL f1 ======

SFO1 600.2324009 MHz  
NUC1 1H  
P1 8.50 usec  
PLW1 5.66009998 W

===== GRADIENT CHANNEL =====

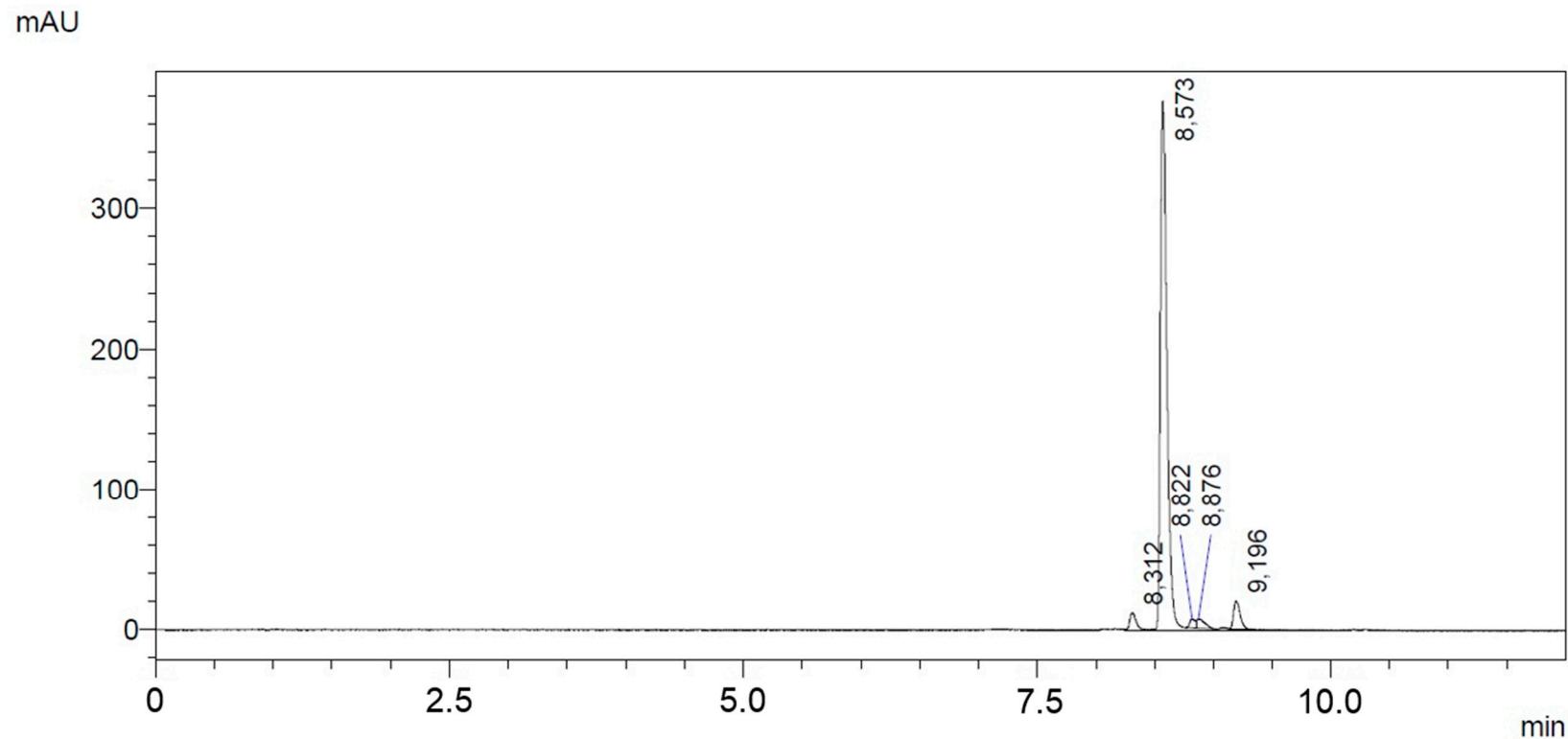
GENAM[1] SMSQ10.100  
GENAM[2] SMSQ10.100  
GENAM[3] SMSQ10.100  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec

F1 - Acquisition parameters  
TD 360  
SFO1 600.2334 MHz  
FIDRES 16.673336 Hz  
SW 10.000 ppm  
FIDMODE QF

F2 - Processing parameters  
SI 4096  
SF 600.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 4096  
MC2 QF  
SF 600.2300000 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

Figure S40. Detail (3/3) of COSY NMR spectrum of compound 9.



**Figure S41.** HPLC chromatogram of compound 9.

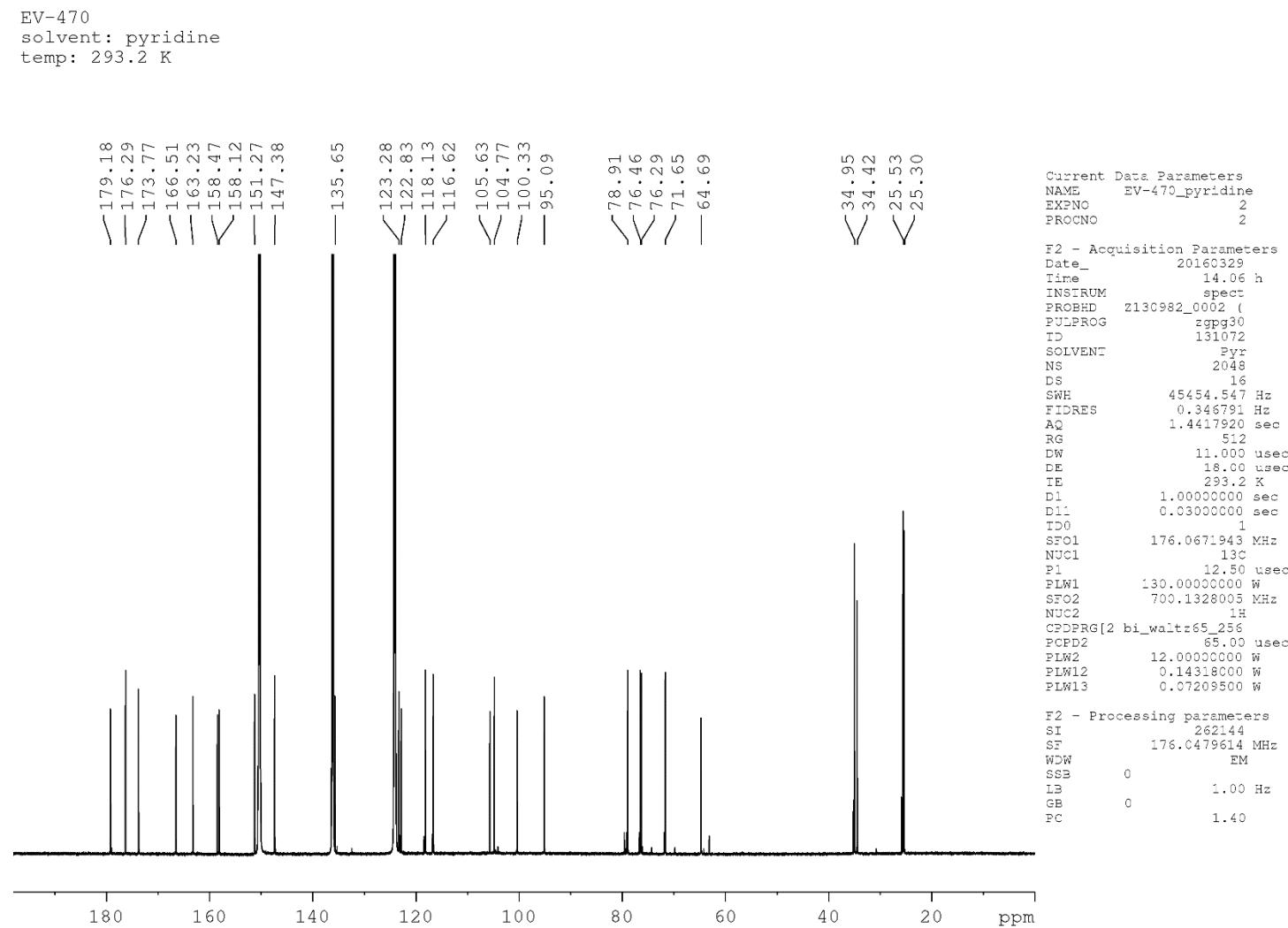


Figure S42.  $^{13}\text{C}$  NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

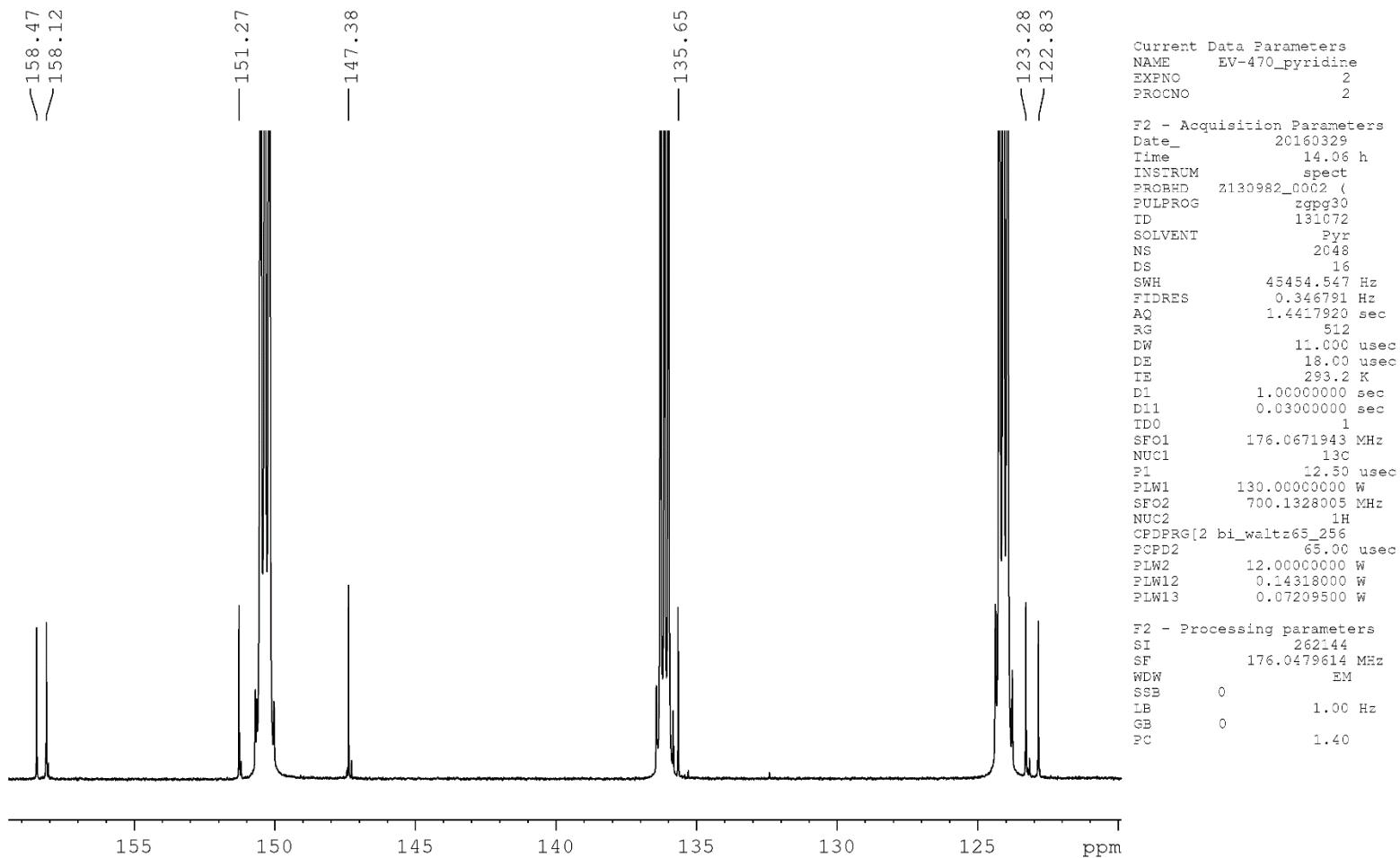


Figure S43. Detail (1/3) of <sup>13</sup>C NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

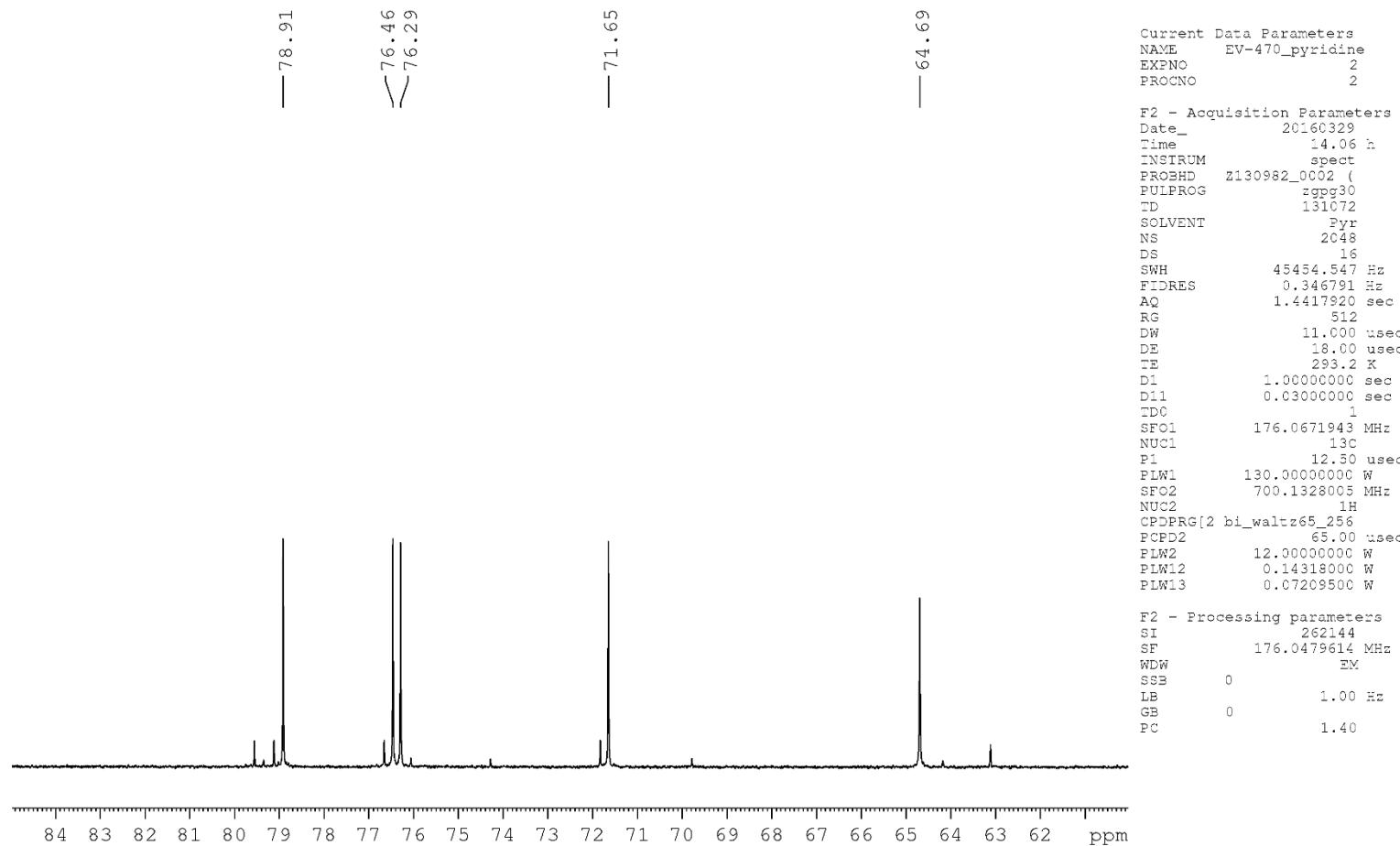


Figure S44. Detail (2/3) of  $^{13}\text{C}$  NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

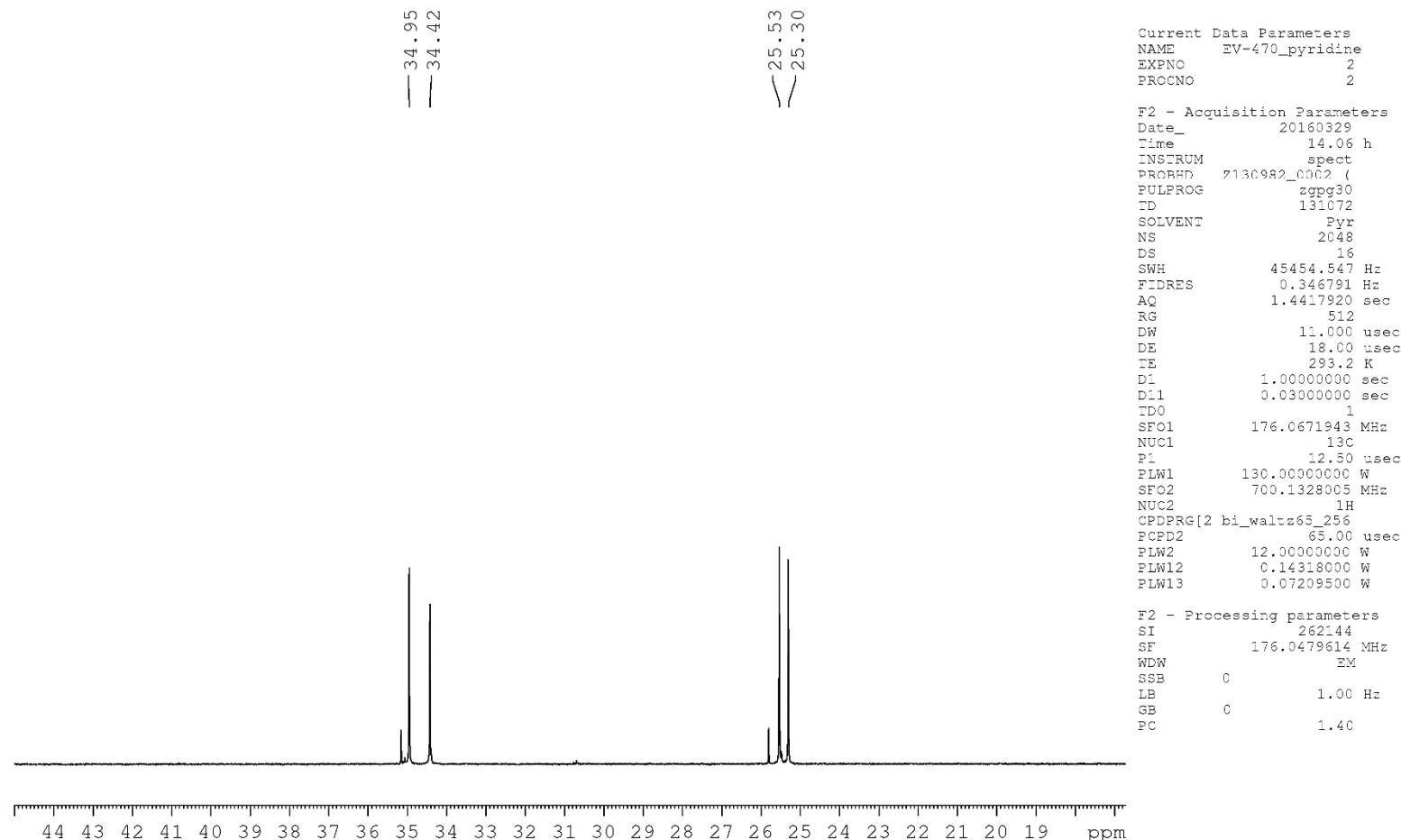


Figure S45. Detail (3/3) of <sup>13</sup>C NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

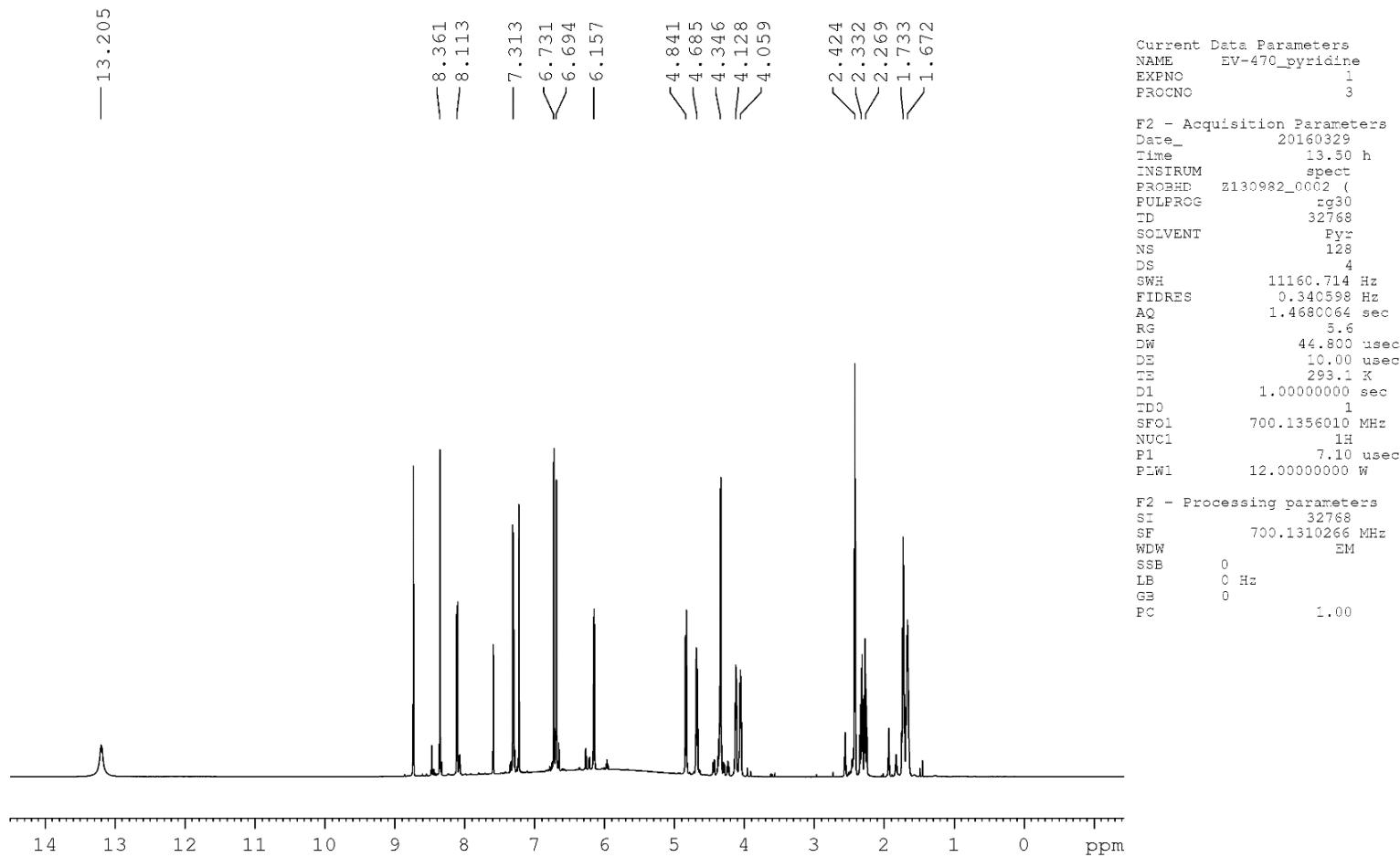


Figure S46.  $^1\text{H}$  NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

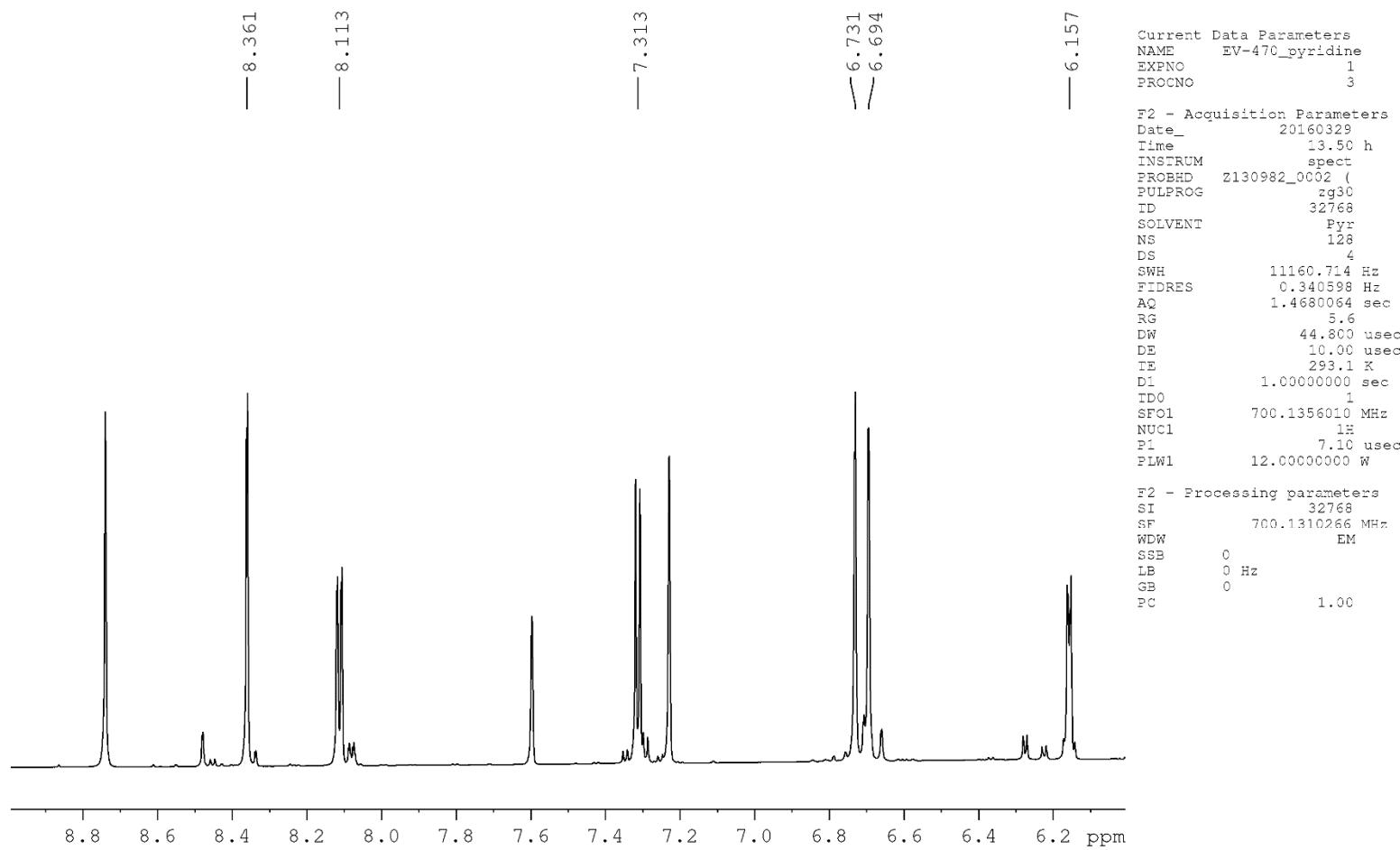


Figure S47. Detail (1/3) of <sup>1</sup>H NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

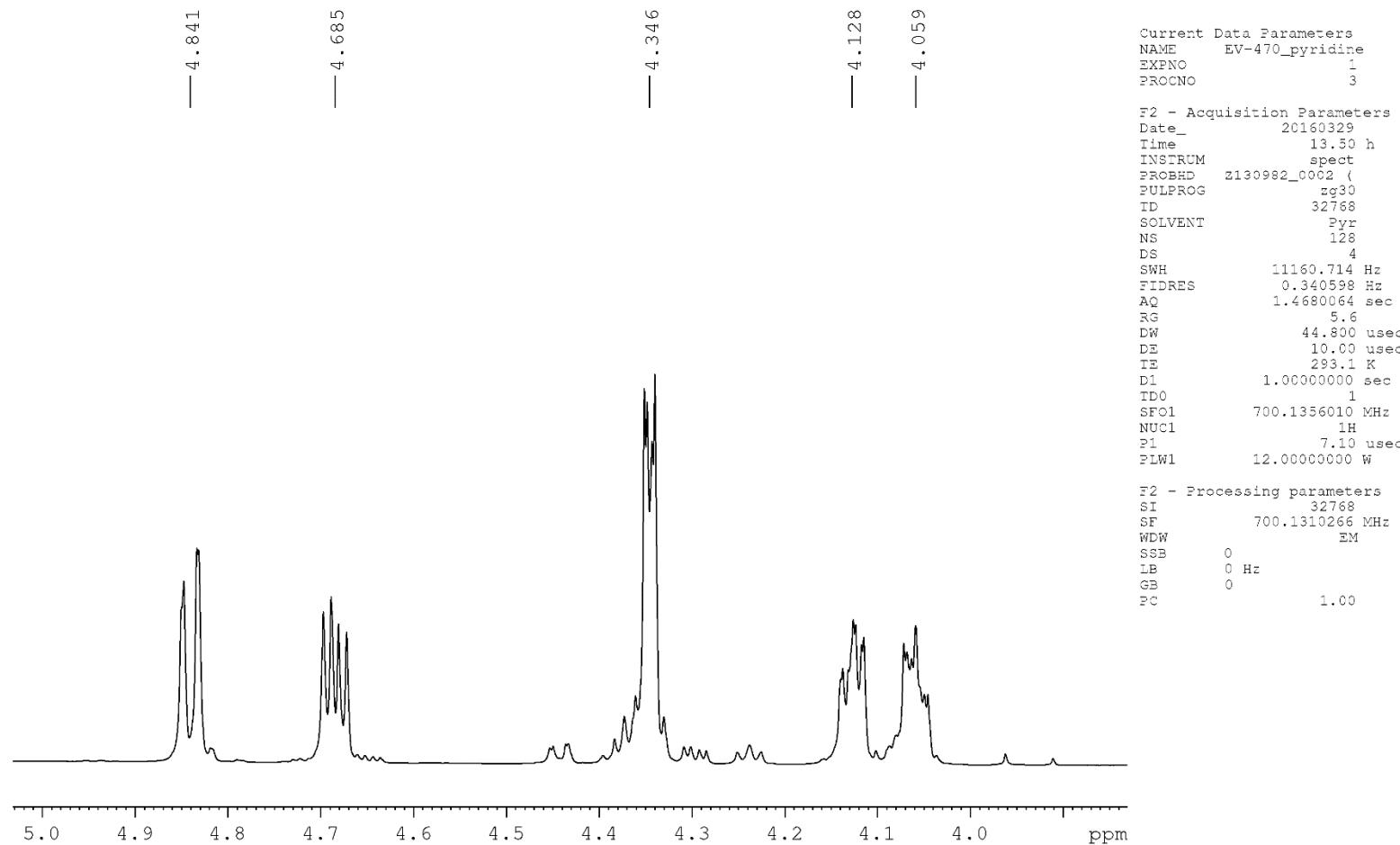


Figure S48. Detail (2/3) of <sup>1</sup>H NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

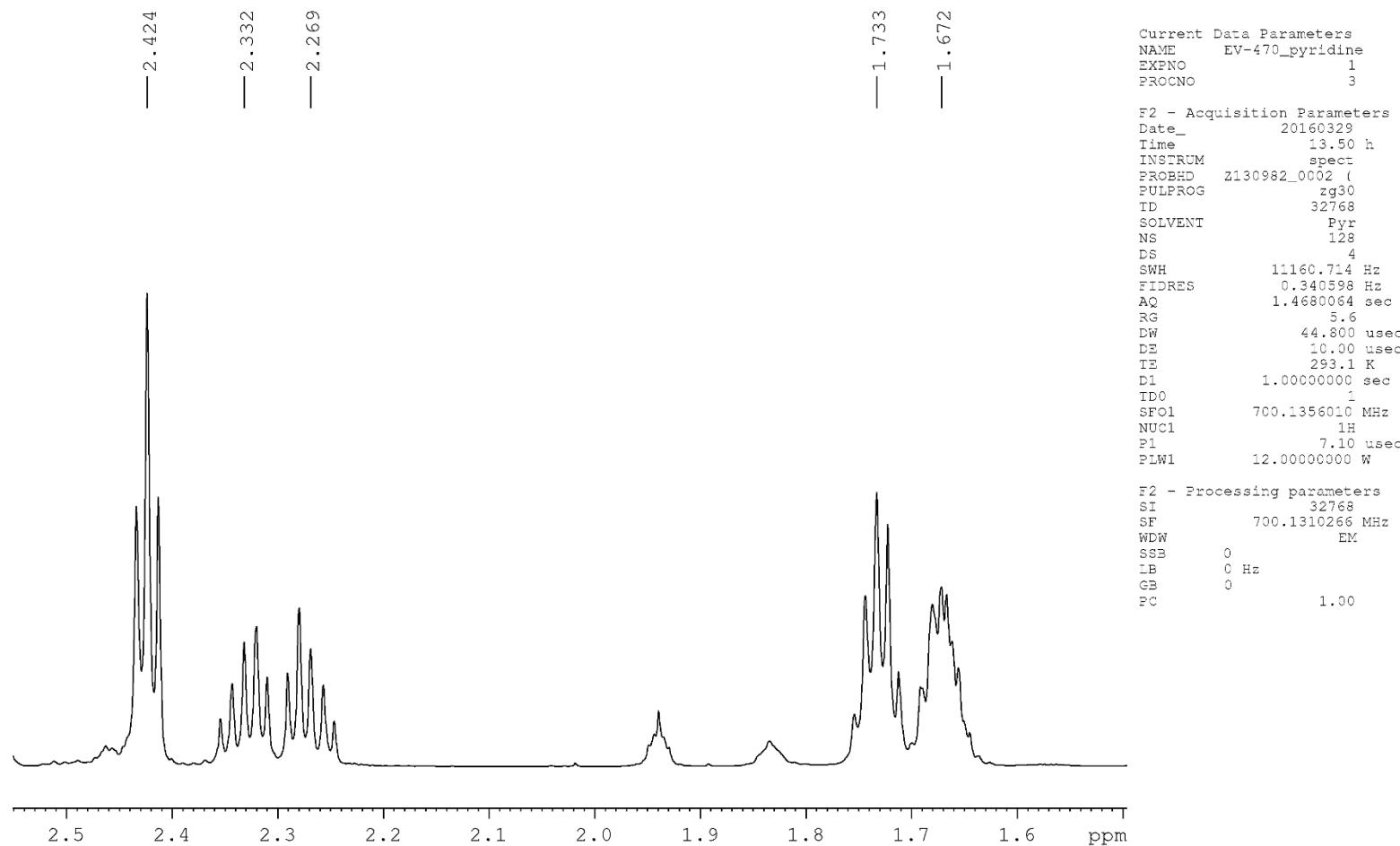


Figure S49. Detail (3/3) of  $^1\text{H}$  NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

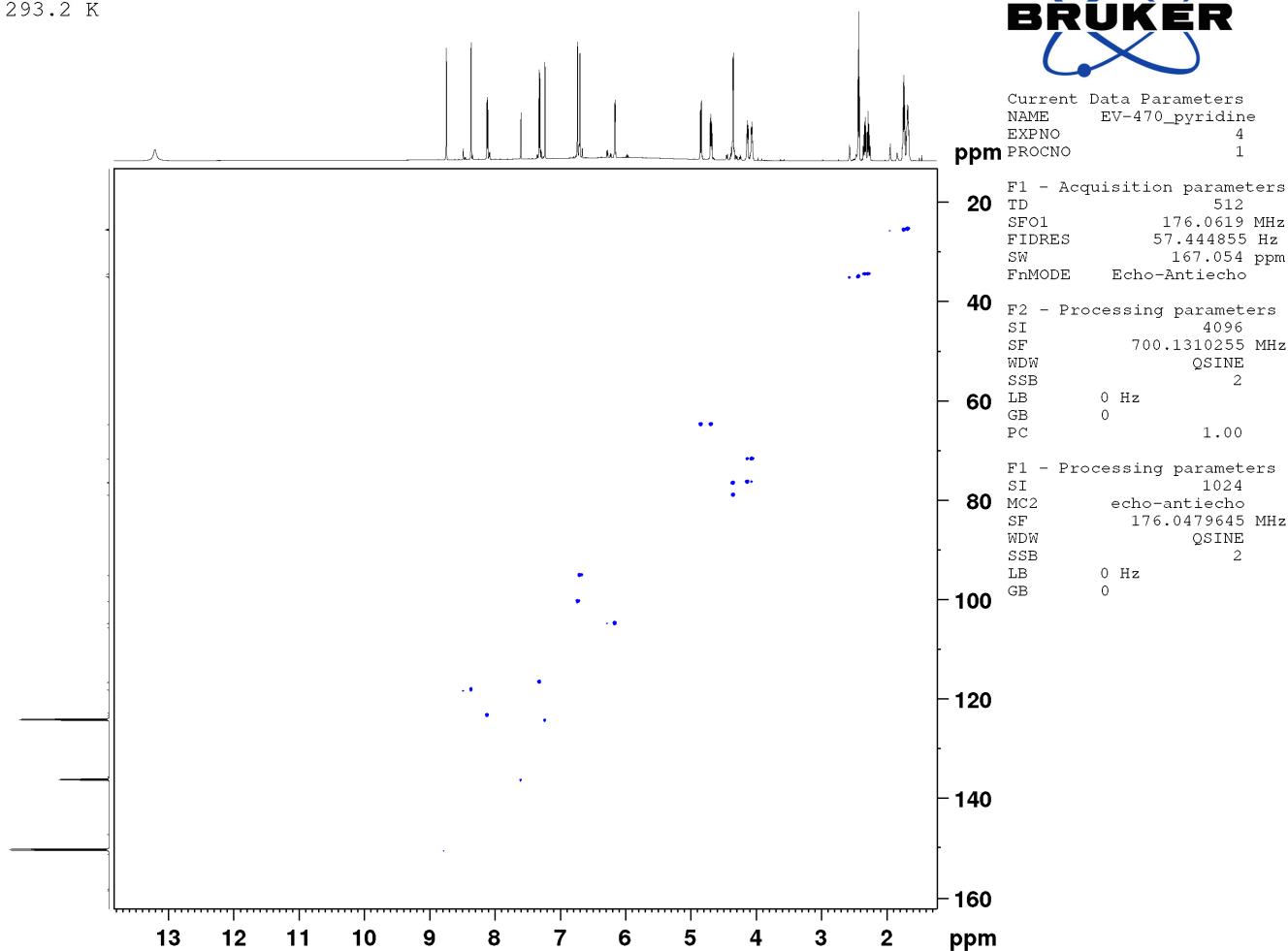
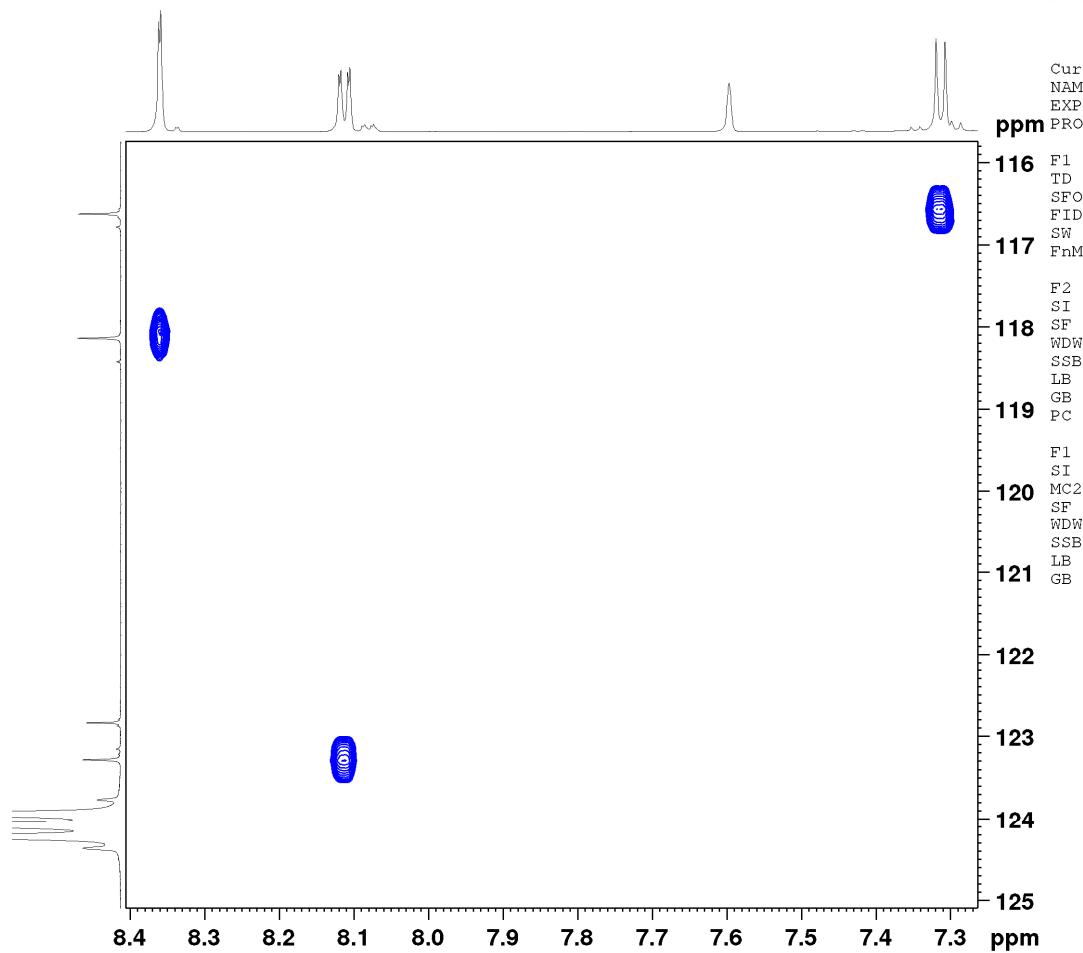


Figure S50. HSQC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 4  
PROCNO 1

**116** F1 - Acquisition parameters  
TD 512  
SF01 176.0619 MHz  
FIDRES 57.444855 Hz  
SW 167.054 ppm  
**117** FnMODE Echo-Antiecho

F2 - Processing parameters  
**118** SI 4096  
SF 700.1310255 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
**119** PC 1.00

F1 - Processing parameters  
**120** SI 1024  
MC2 echo-antiecho  
SF 176.0479645 MHz  
WDW QSINE  
SSB 2  
**121** LB 0 Hz  
GB 0

**122**

**123**

**124**

**125**

Figure S51. Detail (1/4) of HSQC NMR spectrum of compound 10.

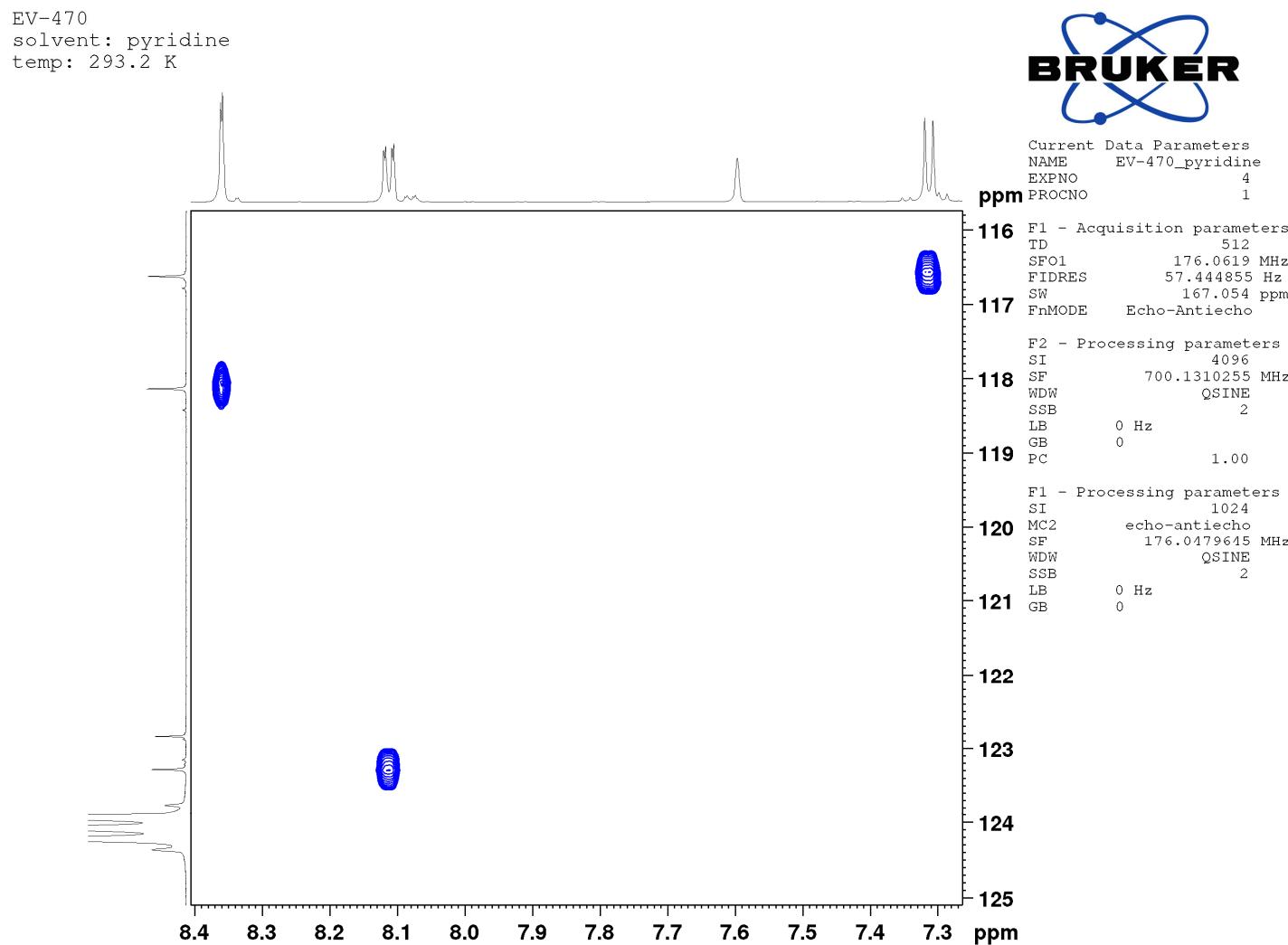


Figure S52. Detail (2/4) of HSQC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 4  
PROCNO 1

60 F1 - Acquisition parameters  
TD 512  
SF 176.0619 MHz  
FIDRES 57.444855 Hz  
SW 167.054 ppm  
FnMODE Echo-Antiecho

70 F2 - Processing parameters  
SI 4096  
SF 700.1310255 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

75 80 F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0479645 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

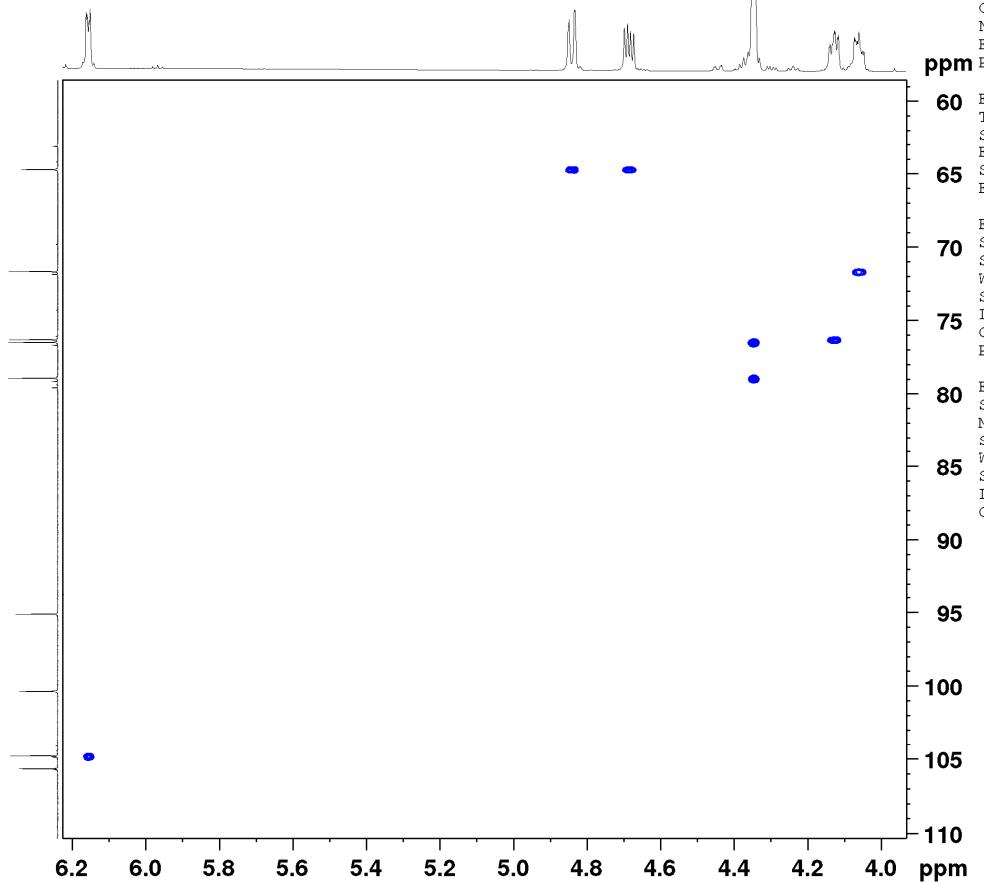


Figure S53. Detail (3/4) of HSQC NMR spectrum of compound 10.

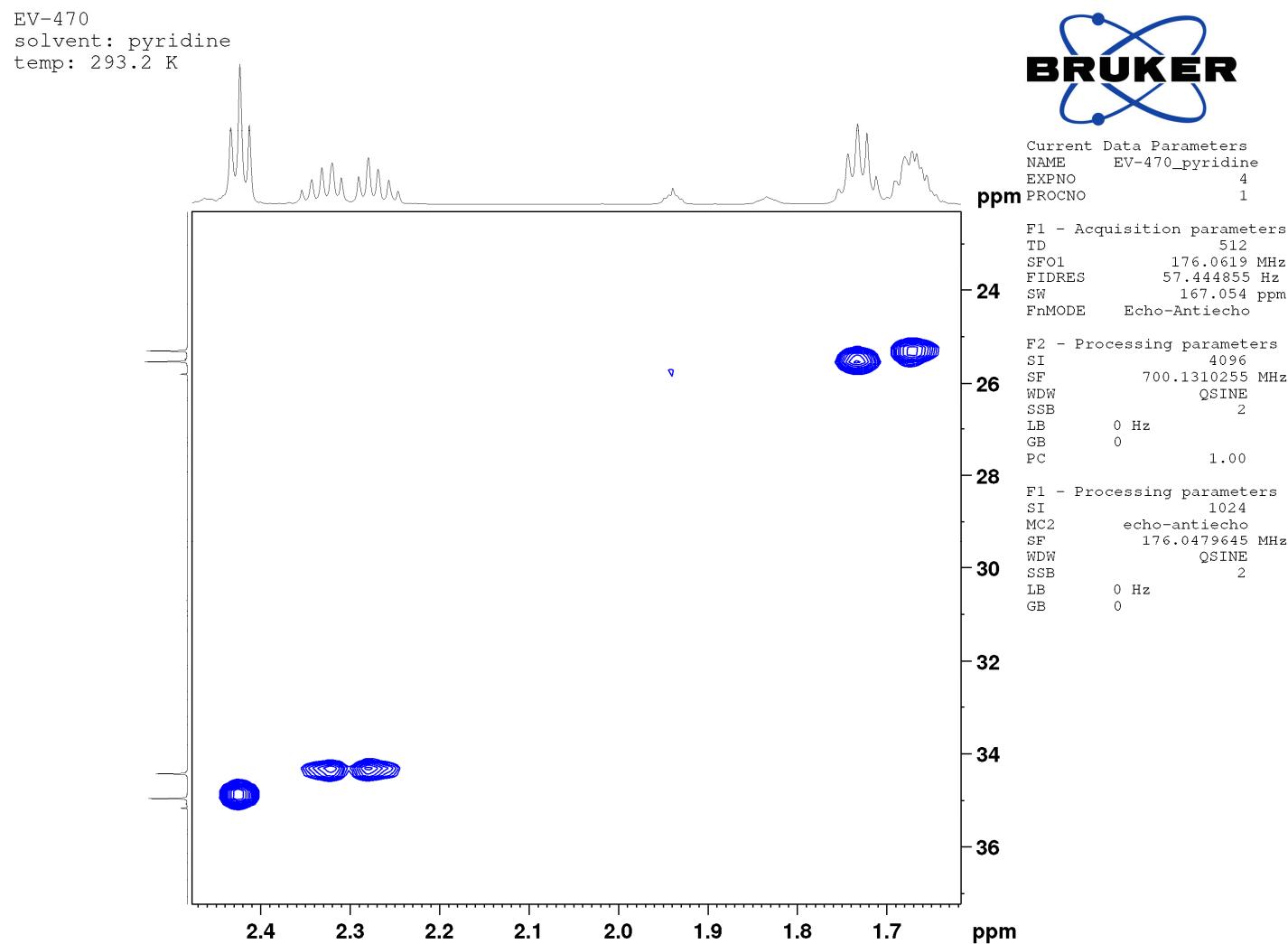


Figure S54. Detail (4/4) of HSQC NMR spectrum of compound 10.

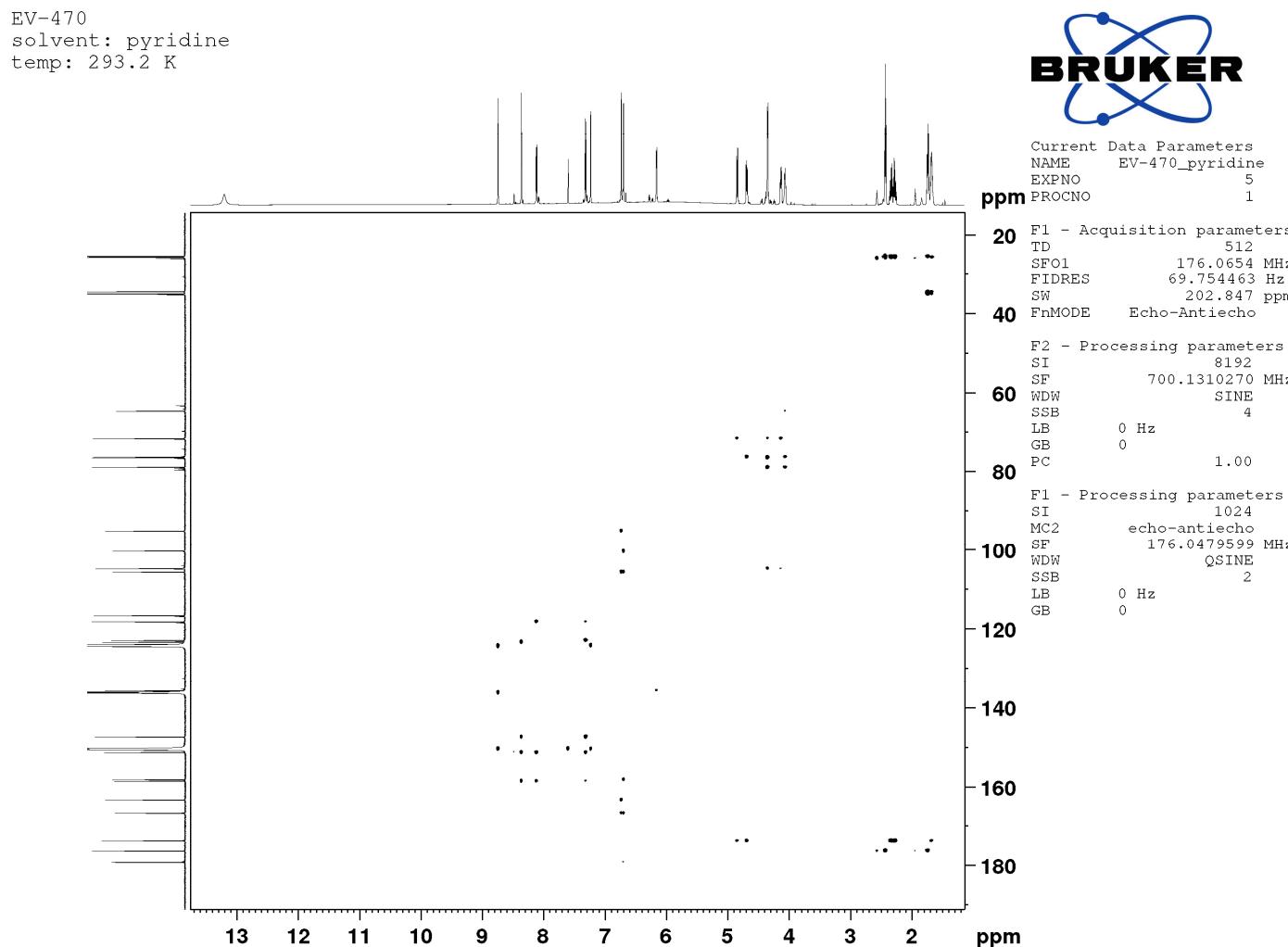


Figure S55. HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 5  
PROCNO 1

F1 - Acquisition parameters  
TD 512  
SF01 176.0654 MHz  
FIDRES 69.754463 Hz  
SW 202.847 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 8192  
SF 700.1310270 MHz  
WDW SINE  
SSB 4  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0479599 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

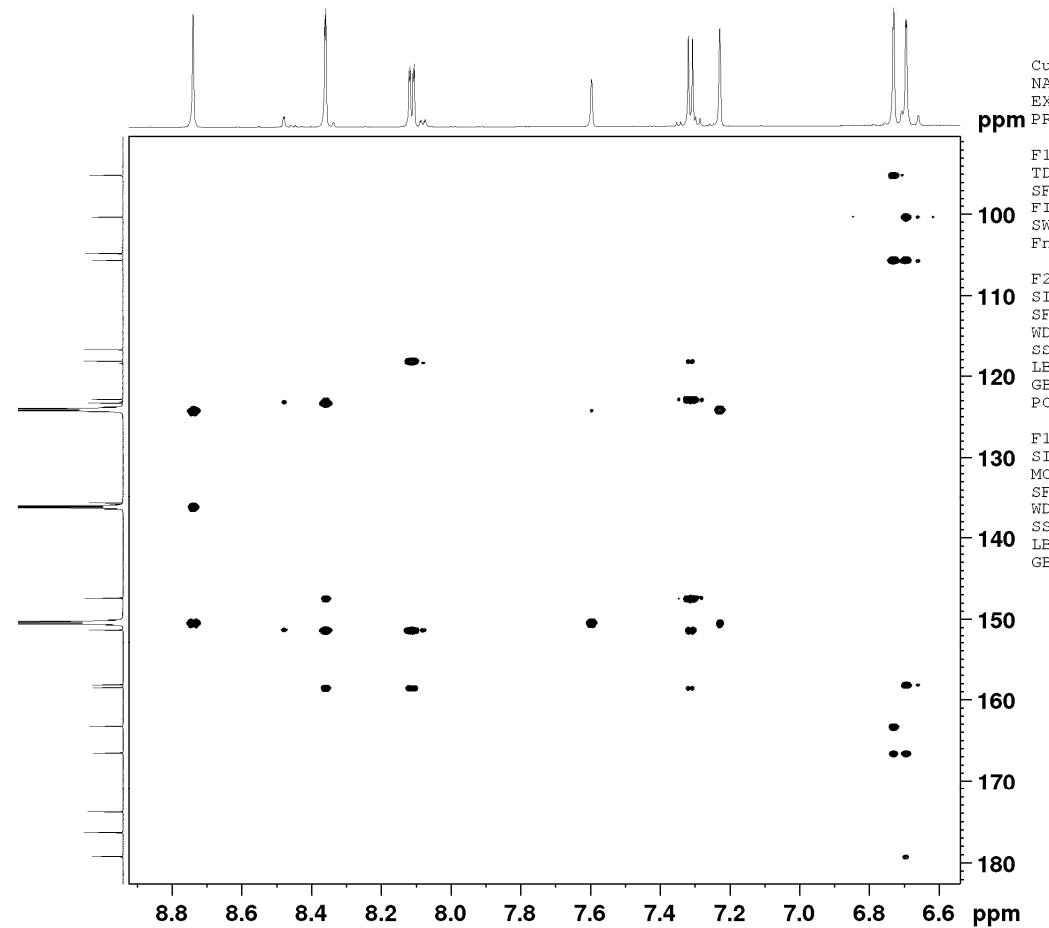


Figure S56. Detail (1/7) of HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

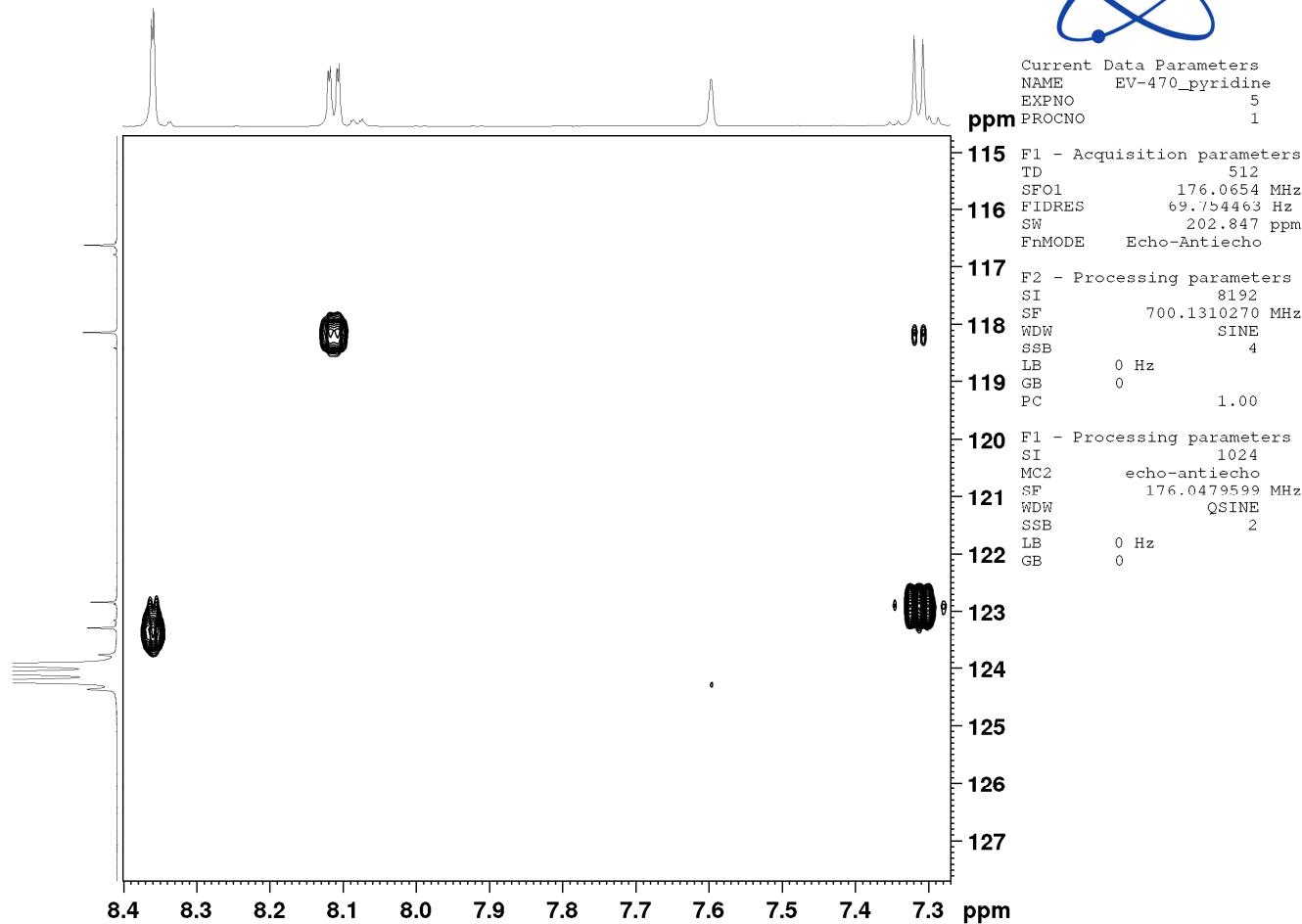


Figure S57. Detail (2/7) of HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 5  
PROCNO 1  
ppm

F1 - Acquisition parameters  
TD 512  
SF01 176.0654 MHz  
FIDRES 69.754463 Hz  
SW 202.847 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 8192  
SF 700.1310270 MHz  
WDW SINE  
SSB 4  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0479599 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

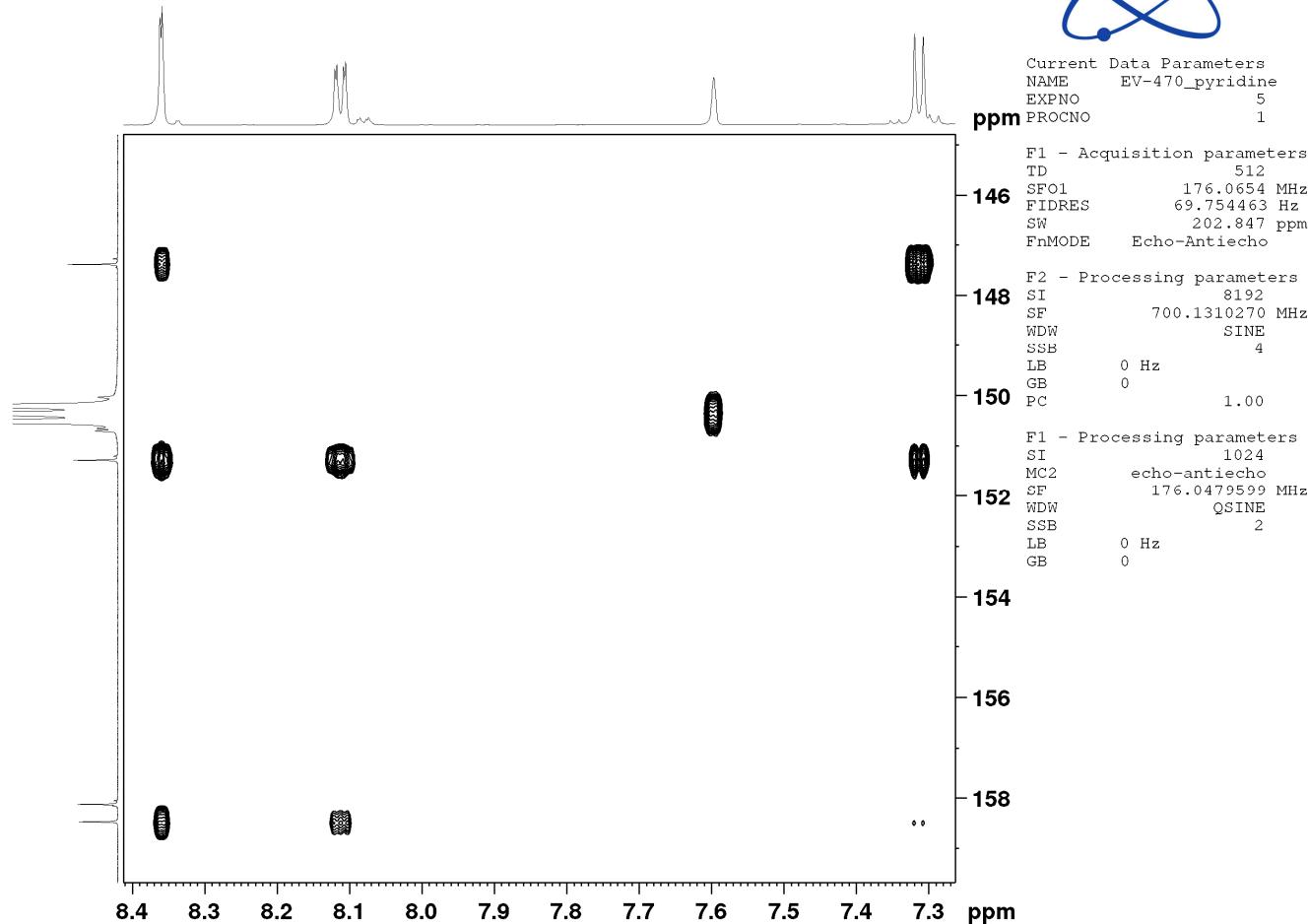


Figure S58. Detail (3/7) of HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 5  
PROCNO 1

ppm F1 - Acquisition parameters  
TD 512  
SF01 176.0654 MHz  
70 FIDRES 69.754463 Hz  
SW 202.847 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 8192  
80 SF 700.1310270 MHz  
WDW SINE  
SSB 4  
LB 0 Hz  
GB 0  
90 PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0479599 MHz  
100 WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

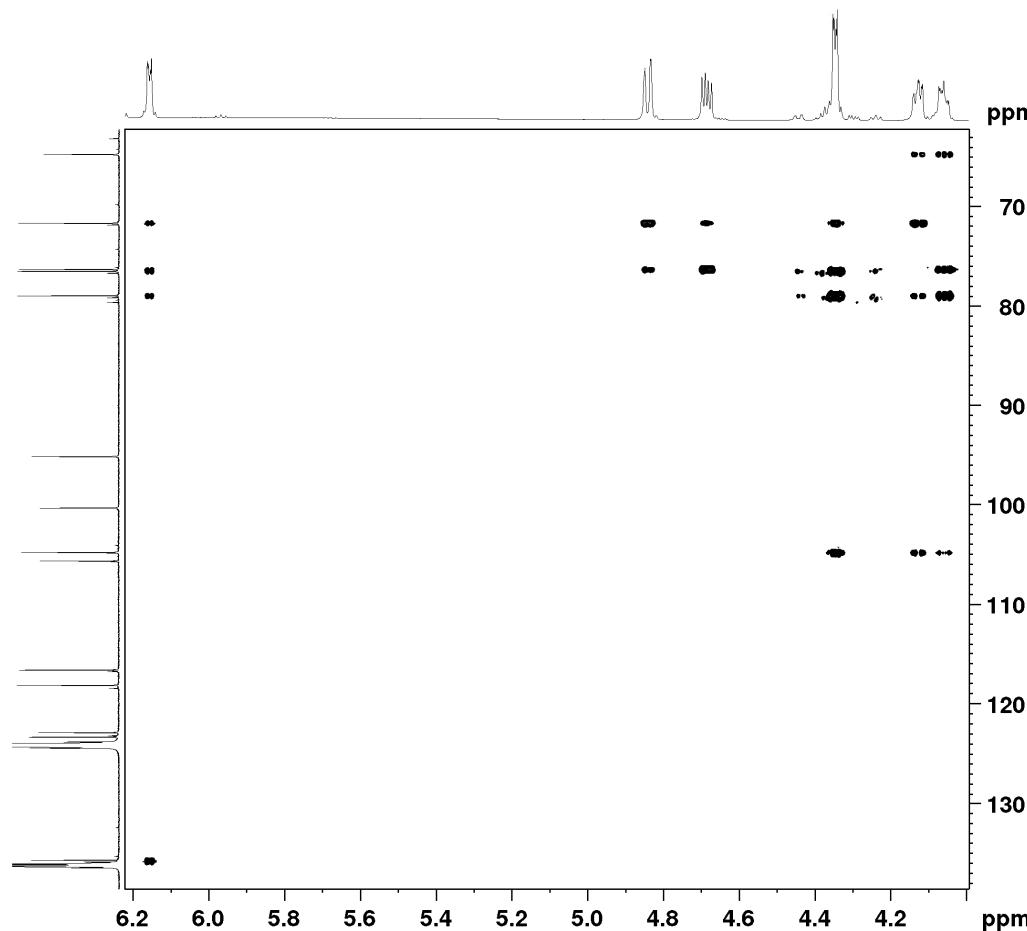


Figure S59. Detail (4/7) of HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-470\_pyridine  
EXPT 5  
PROCNO 1

ppm F1 - Acquisition parameters  
TD 512  
SFO1 176.0654 MHz  
FIDRES 69.754463 Hz  
SW 202.847 ppm  
FnMODE Echo-Antiecho

71 F2 - Processing parameters  
SI 8192  
SF 700.1310270 MHz  
WDW SINE

72 SSB 4  
LB 0 Hz  
GB 0  
PC 1.00

73 F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0479599 MHz  
WDW QSINE

74 SSB 2  
LB 0 Hz  
GB 0

75 76 77 78 79

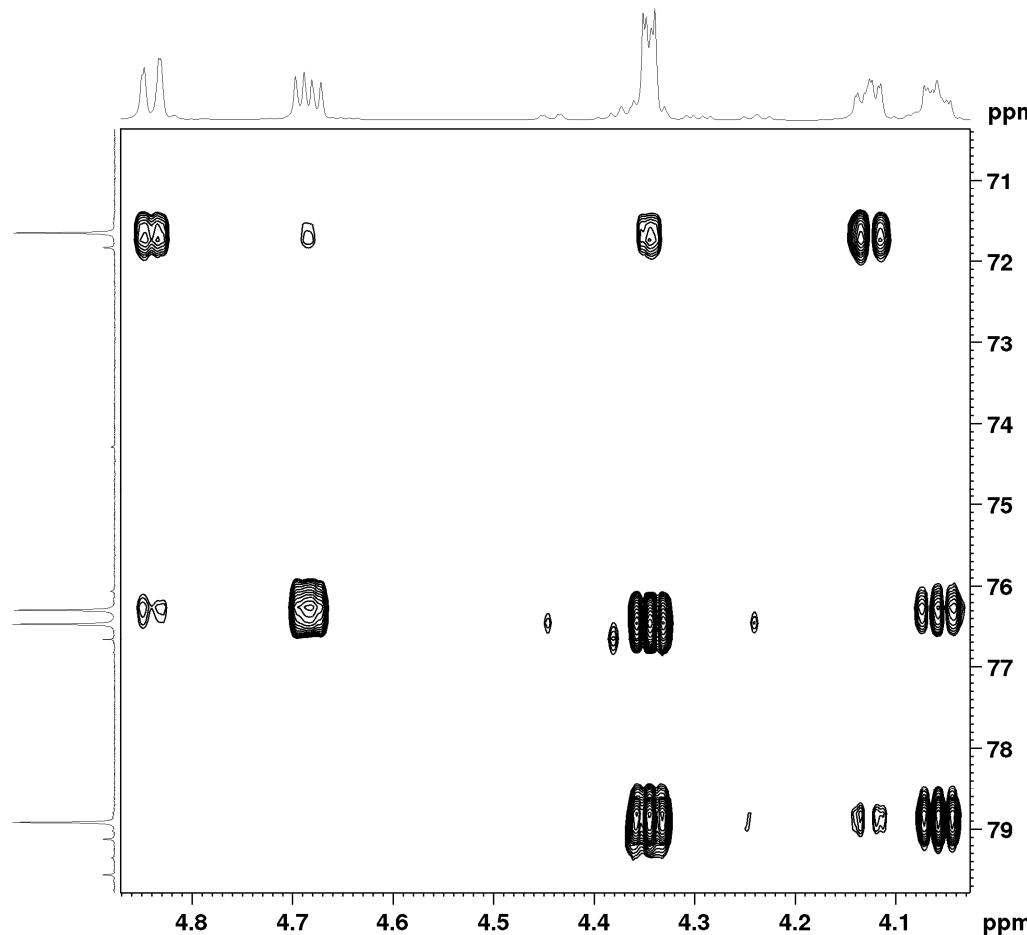
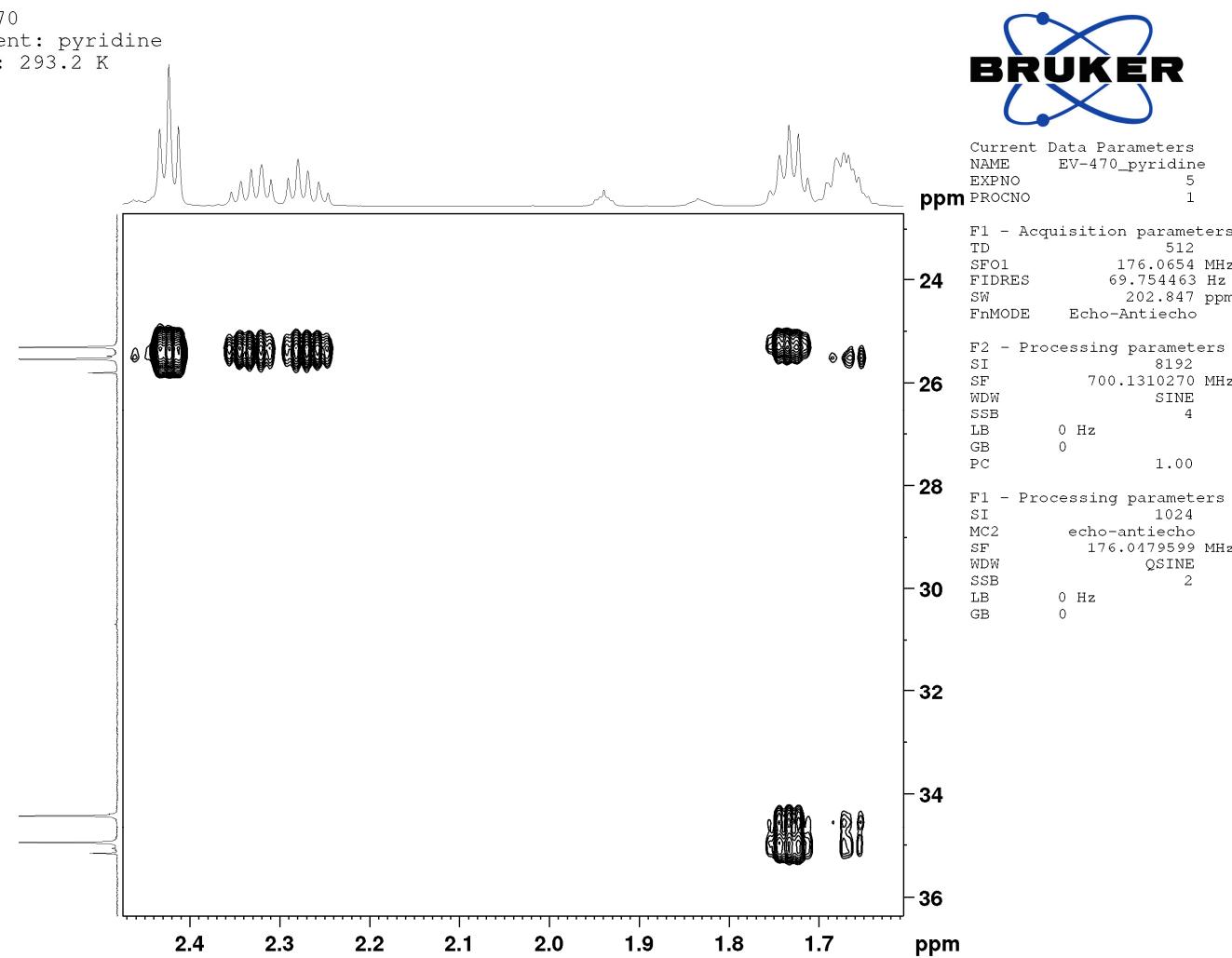


Figure S60. Detail (5/7) of HMBC NMR spectrum of compound 10.



**Figure S61.** Detail (6/7) of HMBC NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

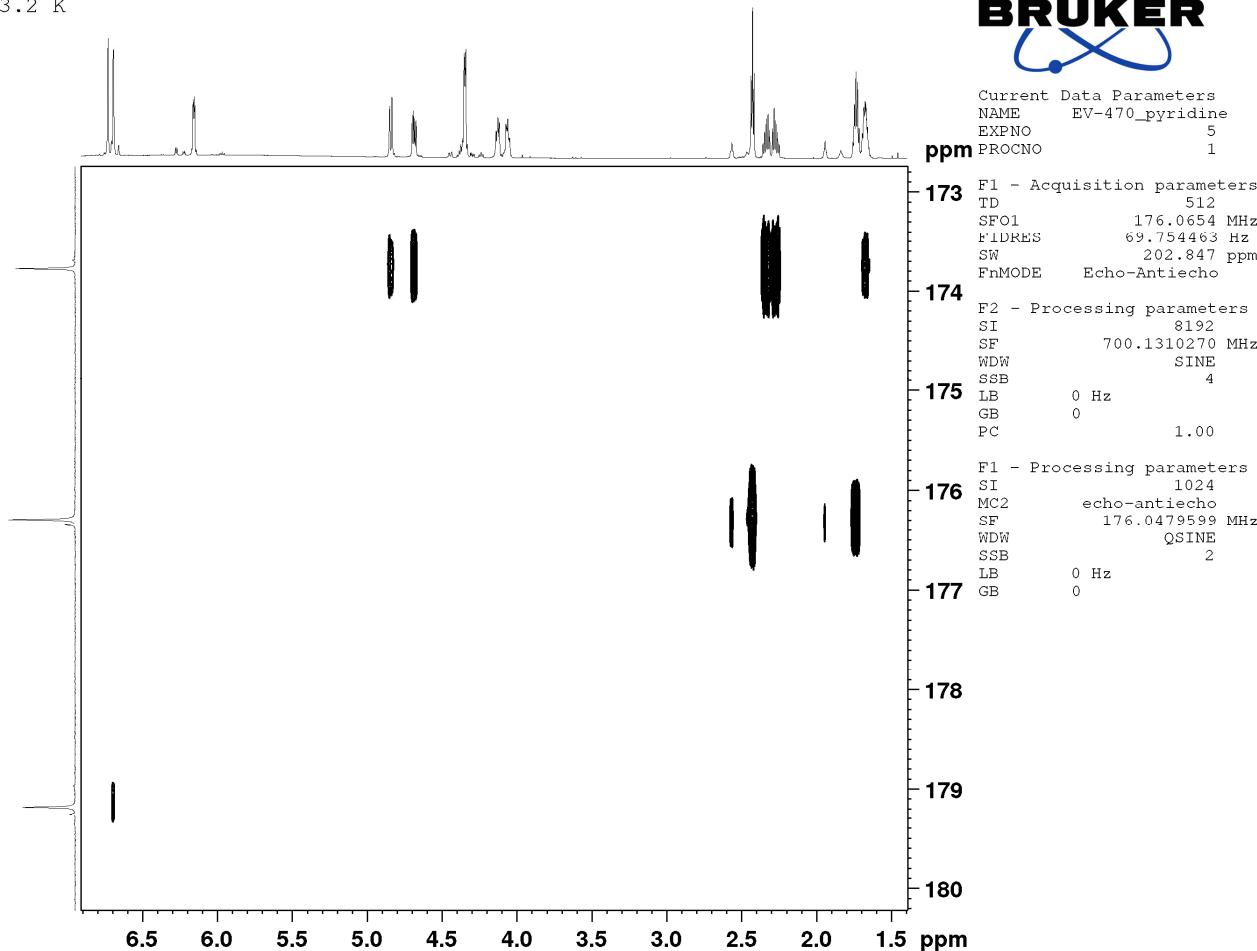


Figure S62. Detail (7/7) of HMBC NMR spectrum of compound 10.

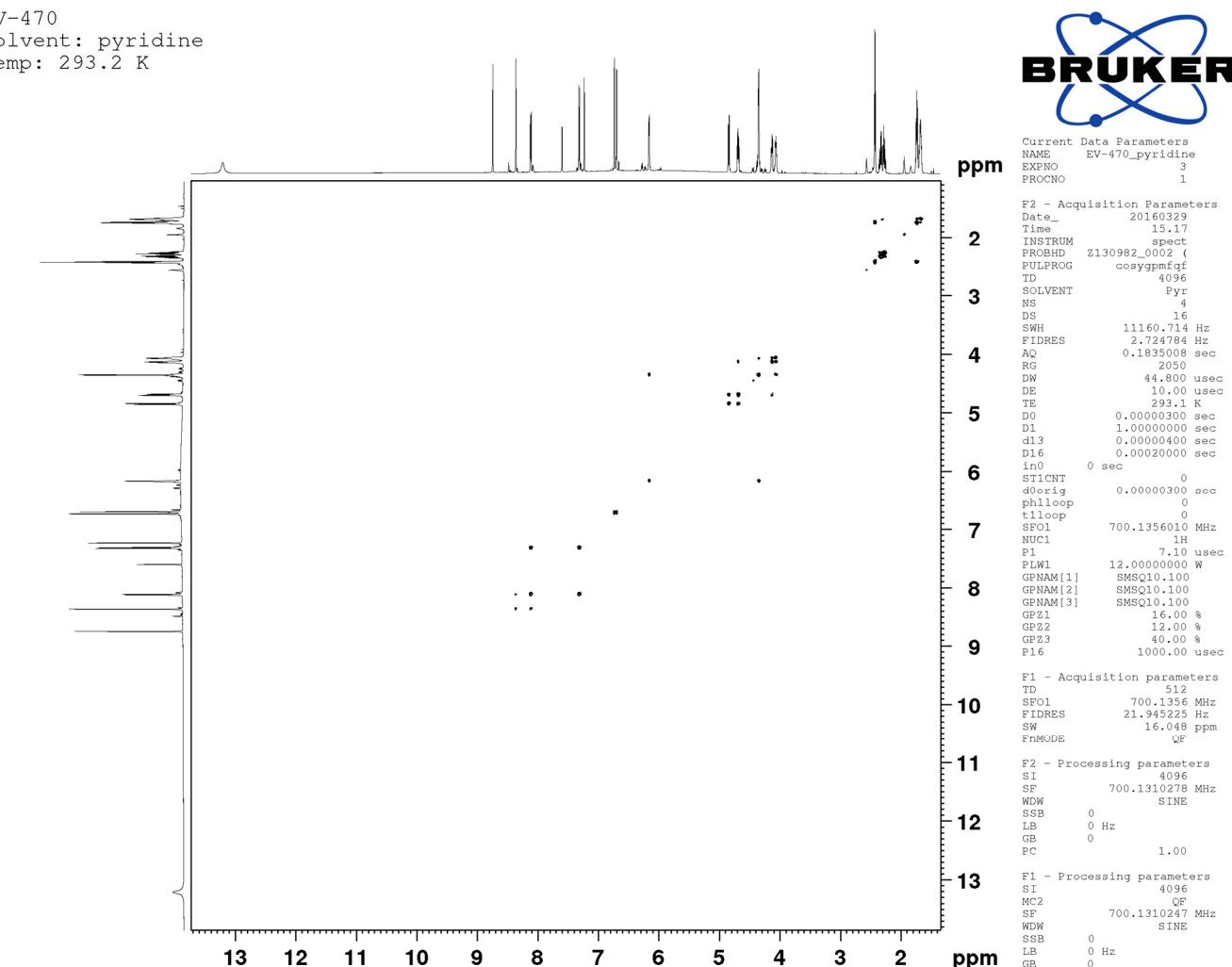


Figure S63. COSY NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

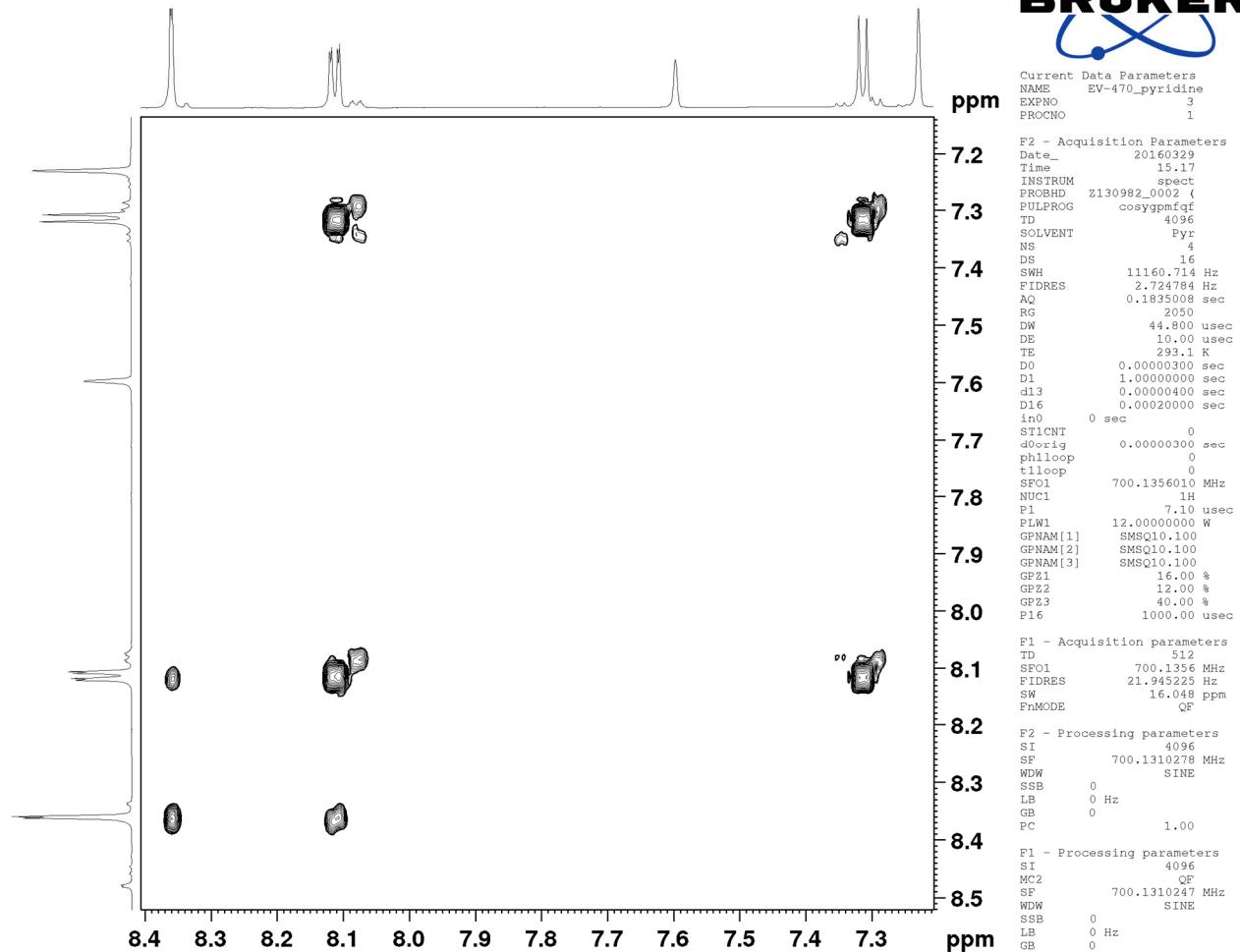


Figure S64. Detail (1/3) of COSY NMR spectrum of compound 10.

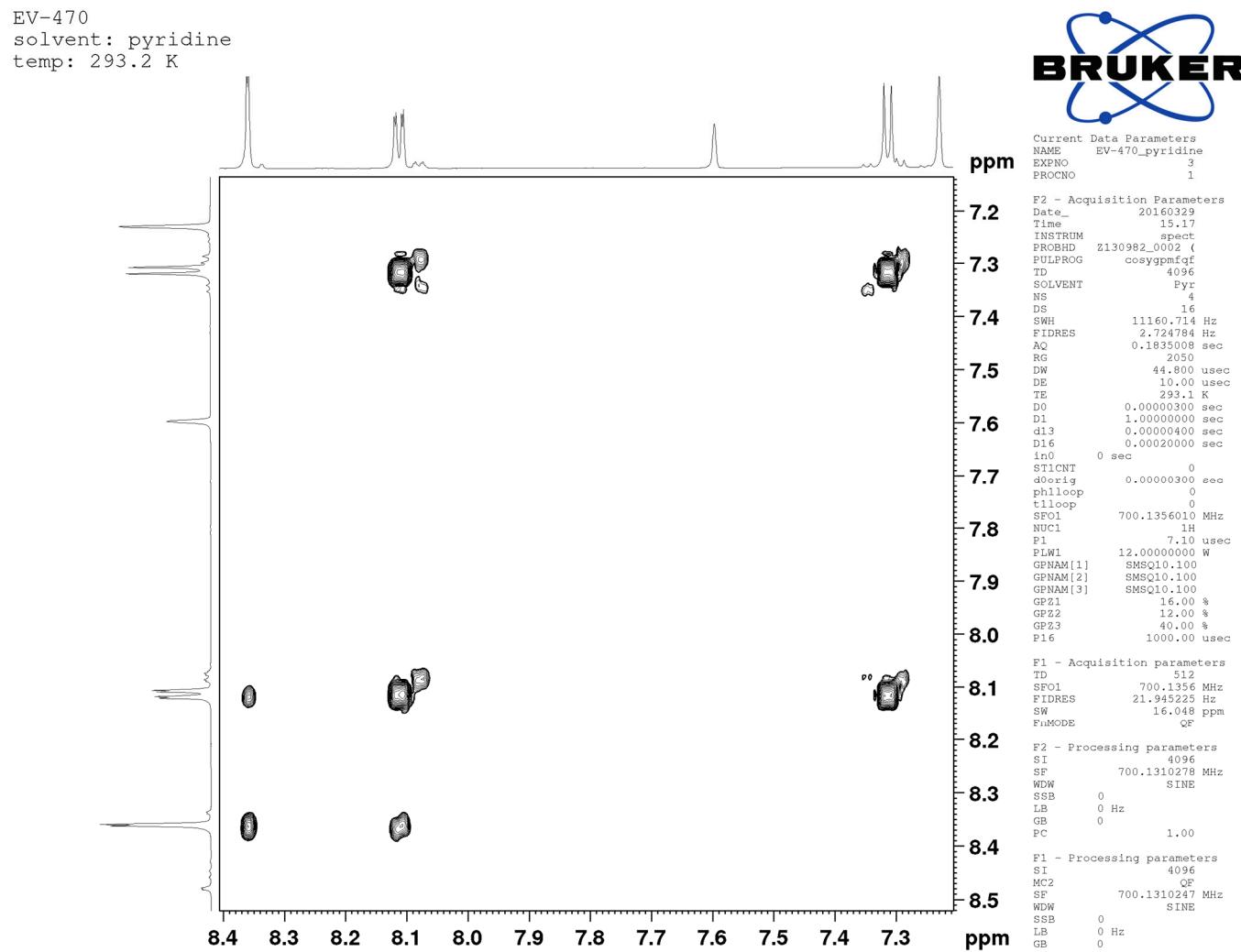
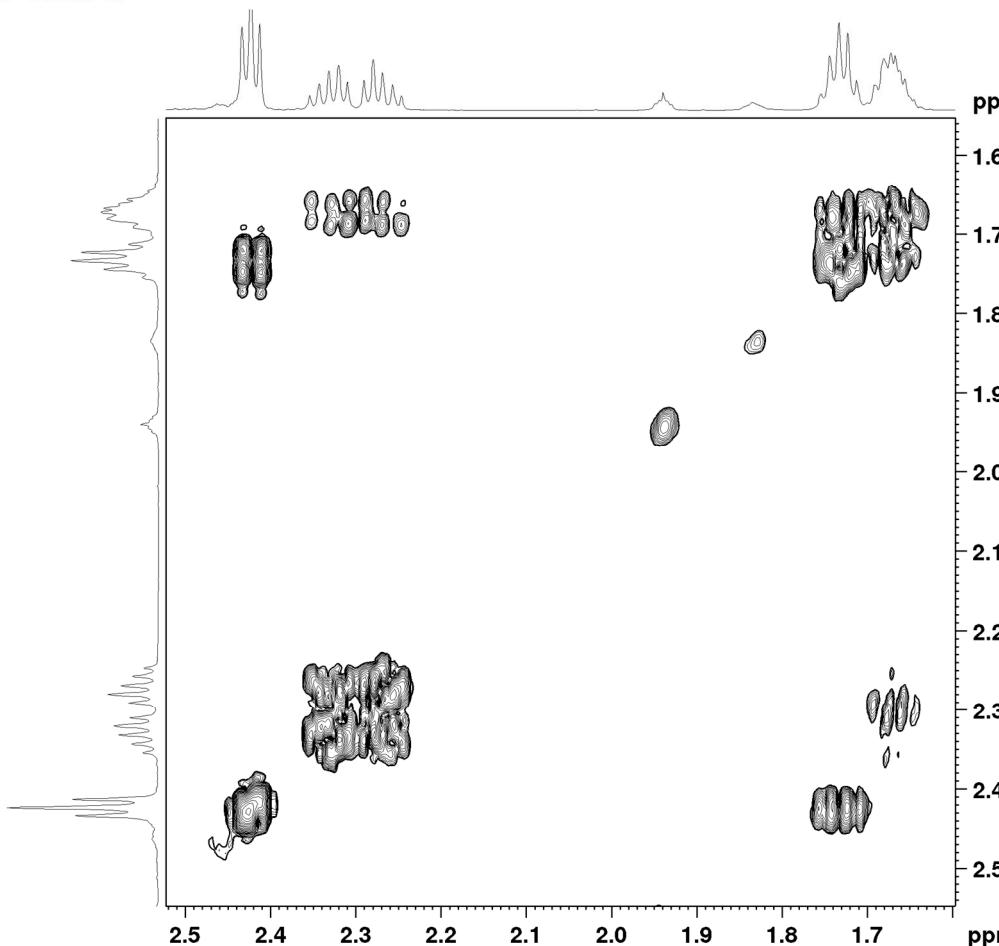


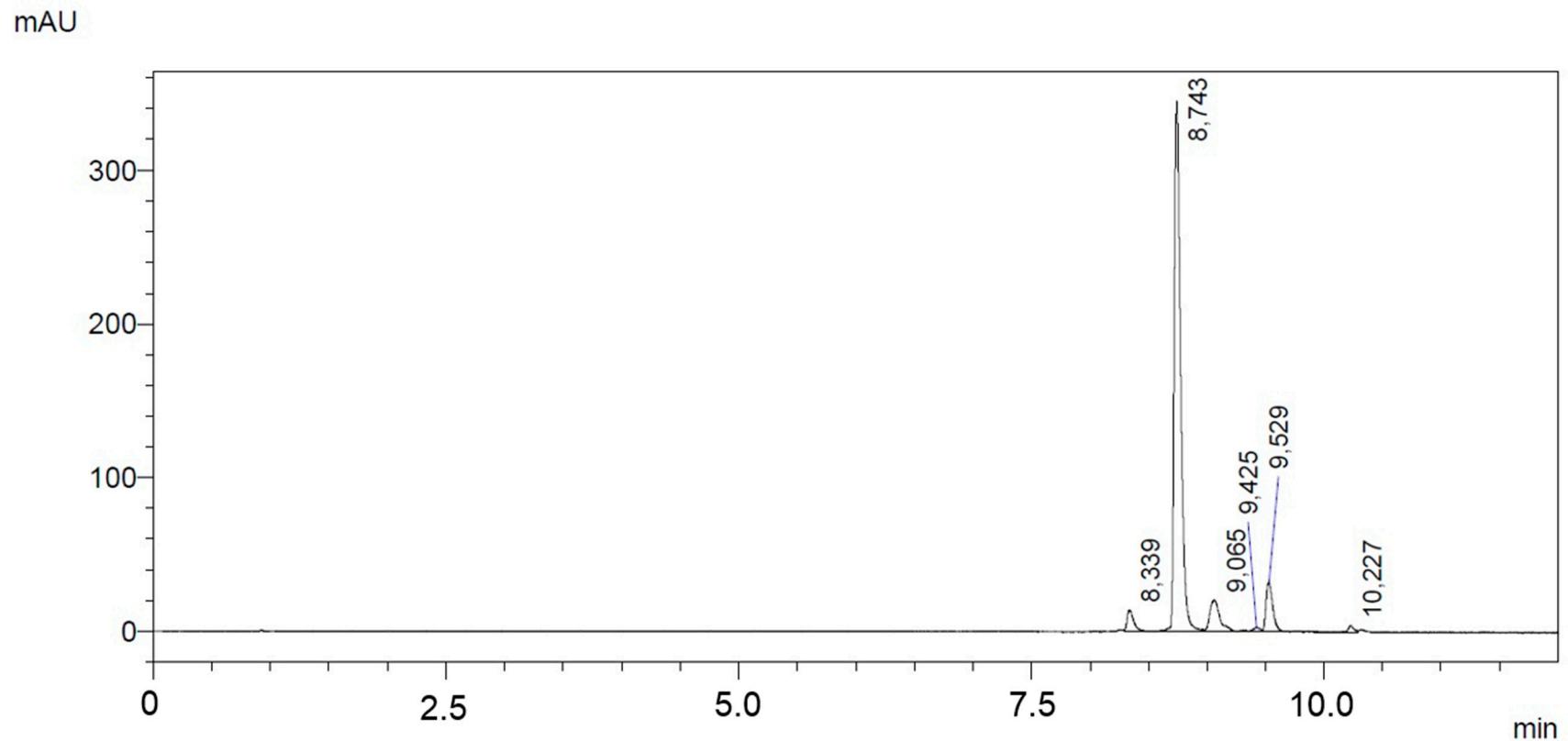
Figure S65. Detail (2/3) of COSY NMR spectrum of compound 10.

EV-470  
solvent: pyridine  
temp: 293.2 K

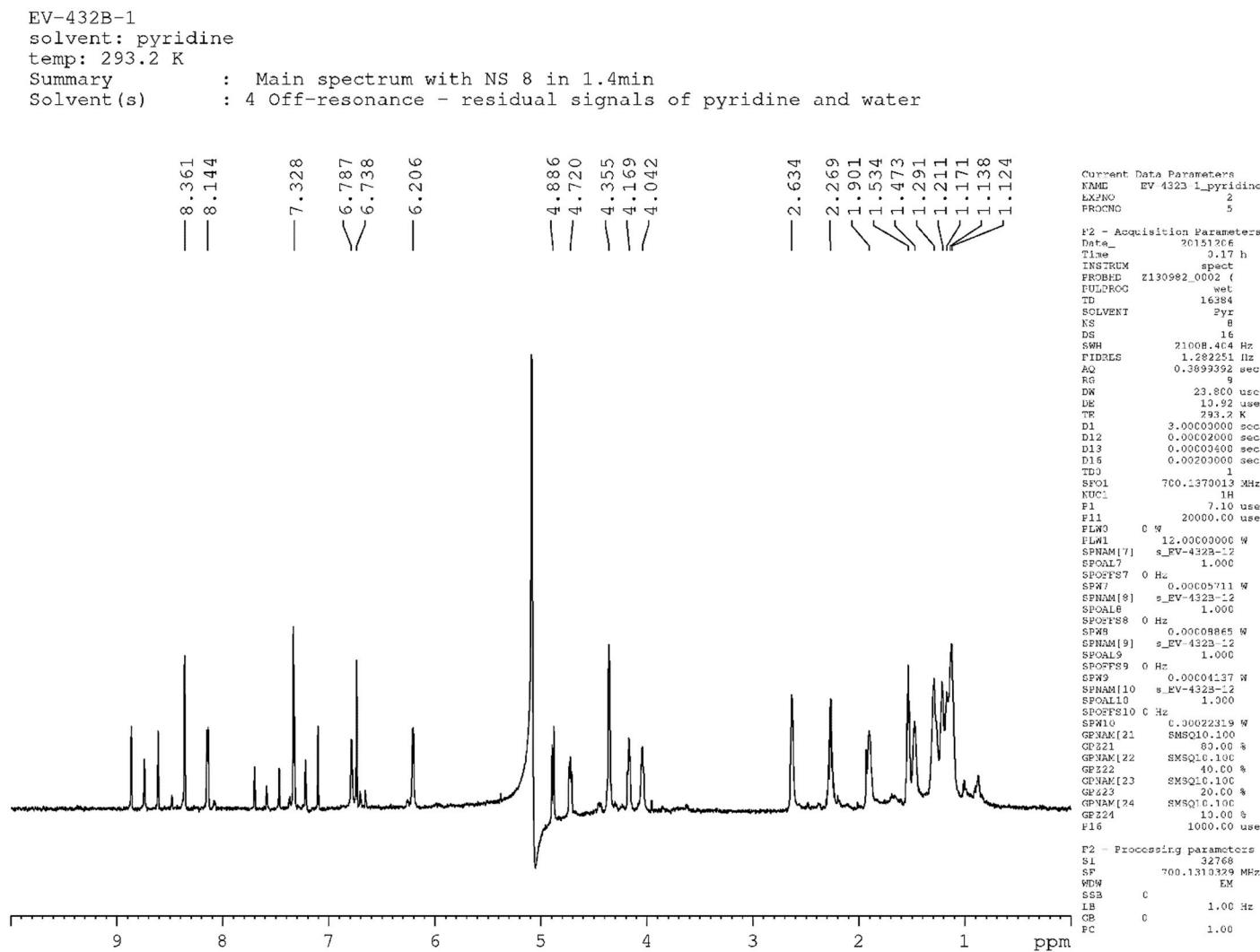


Current Data Parameters  
NAME EV-470\_pyridine  
EXPNO 3  
PROCNO 1  
  
F2 - Acquisition Parameters  
Date\_ 20160329  
Time 15.17  
INSTRUM spect  
PROBHD Z130982\_0002 (cosyqpmgff  
PULPROG 4096  
SOLVENT Pyr  
NS 4  
DS 16  
SWH 11160.714 Hz  
FIDRES 2.724794 Hz  
AQ 0.1835008 sec  
RG 2050  
DW 44.800 usec  
DE 10.00 usec  
TE 293.1 K  
D0 0.00000300 sec  
D1 1.00000000 sec  
d13 0.00000400 sec  
D16 0.00020000 sec  
in0 0 sec  
ST1CNT 0  
d1orig 0.00000300 sec  
phi1loop 0  
t1loop 0  
SFO1 700.1356010 MHz  
NUC1 1H  
P1 7.10 usec  
PLW1 12.00000000 W  
GPNAME[1] SMSQ10.100  
GPNAME[2] SMSQ10.100  
GPNAME[3] SMSQ10.100  
GPZ1 16.00 %  
GPZ2 12.00 %  
GPZ3 40.00 %  
P16 1000.00 usec  
  
F1 - Acquisition parameters  
TD 512  
SFO1 700.1356 MHz  
FIDRES 21.945225 Hz  
SW 16.048 ppm  
FR MODE QF  
  
F2 - Processing parameters  
SI 4096  
SF 700.1310278 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0  
PC 1.00  
  
F1 - Processing parameters  
SI 4096  
MC2 QF  
SF 700.1310247 MHz  
WDW SINE  
SSB 0  
LB 0 Hz  
GB 0

Figure S66. Detail (3/3) of COSY NMR spectrum of compound 10.



**Figure S67.** HPLC chromatogram of compound **10**.



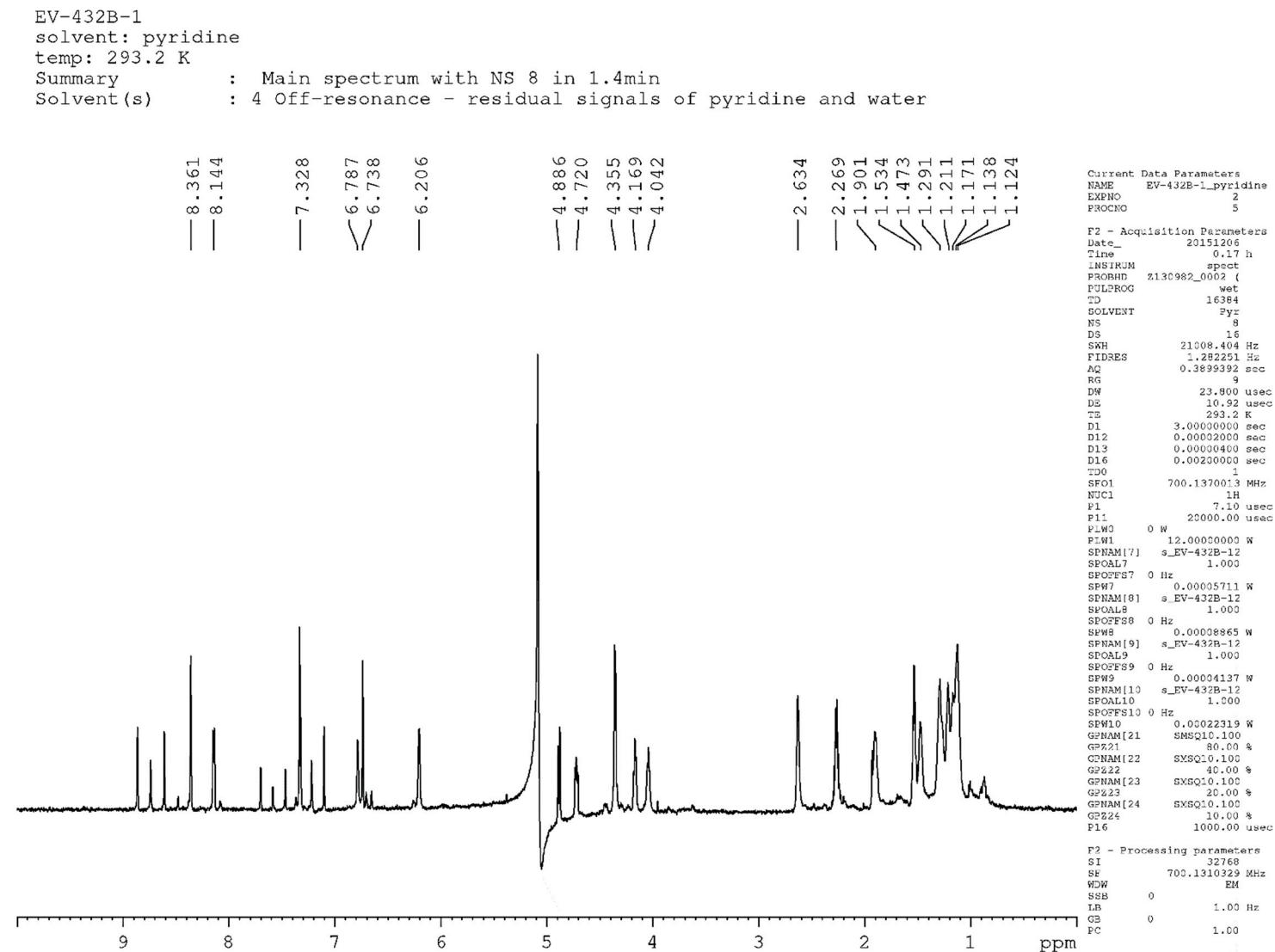


Figure S69.  $^1\text{H}$  NMR spectrum WET of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K  
 Summary : Main spectrum with NS 8 in 1.4min  
 Solvent(s) : 4 Off-resonance - residual signals of pyridine and water

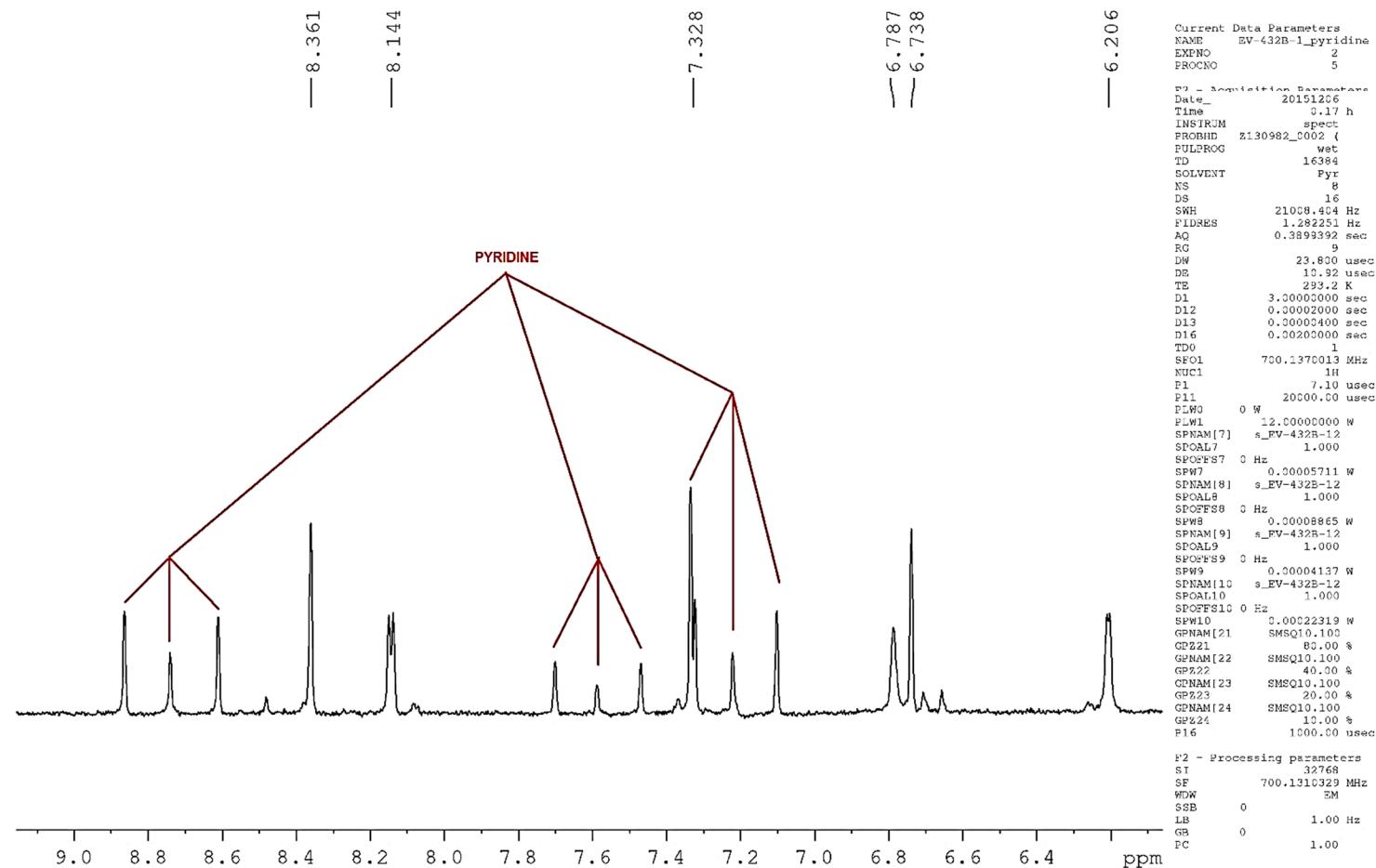
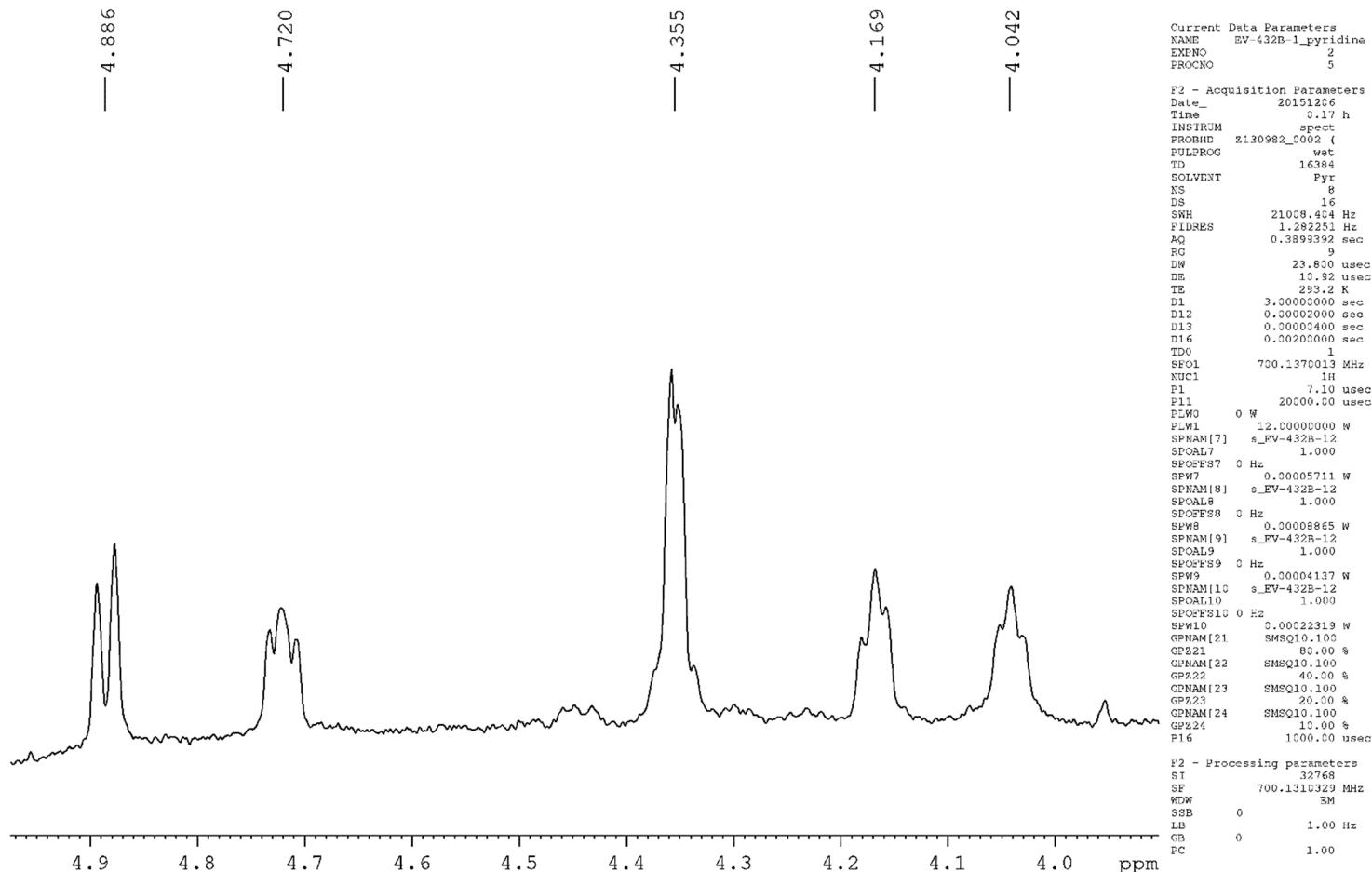


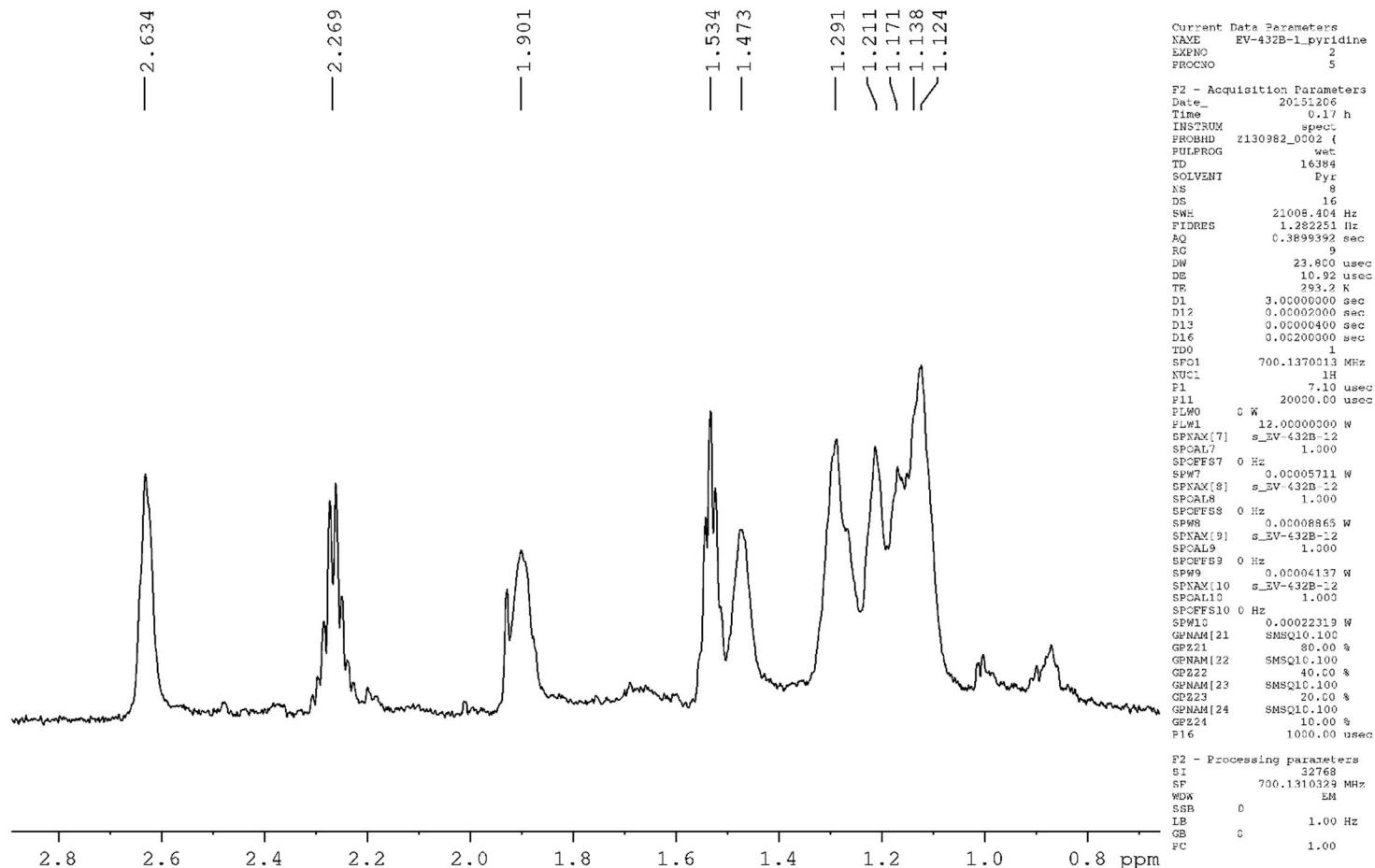
Figure S70. Detail (1/3) of  $^1\text{H}$  NMR spectrum WET of compound 11.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K  
 Summary : Main spectrum with NS 8 in 1.4min  
 Solvent(s) : 4 Off-resonance - residual signals of pyridine and water



**Figure S71.** Detail (2/3) of  $^1\text{H}$  NMR spectrum WET of compound **11**.

EV-432B-1  
 solvent: pyridine  
 temp: 293.2 K  
 Summary : Main spectrum with NS 8 in 1.4min  
 Solvent(s) : 4 Off-resonance - residual signals of pyridine and water



**Figure S72.** Detail (3/3) of <sup>1</sup>H NMR spectrum WET of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K

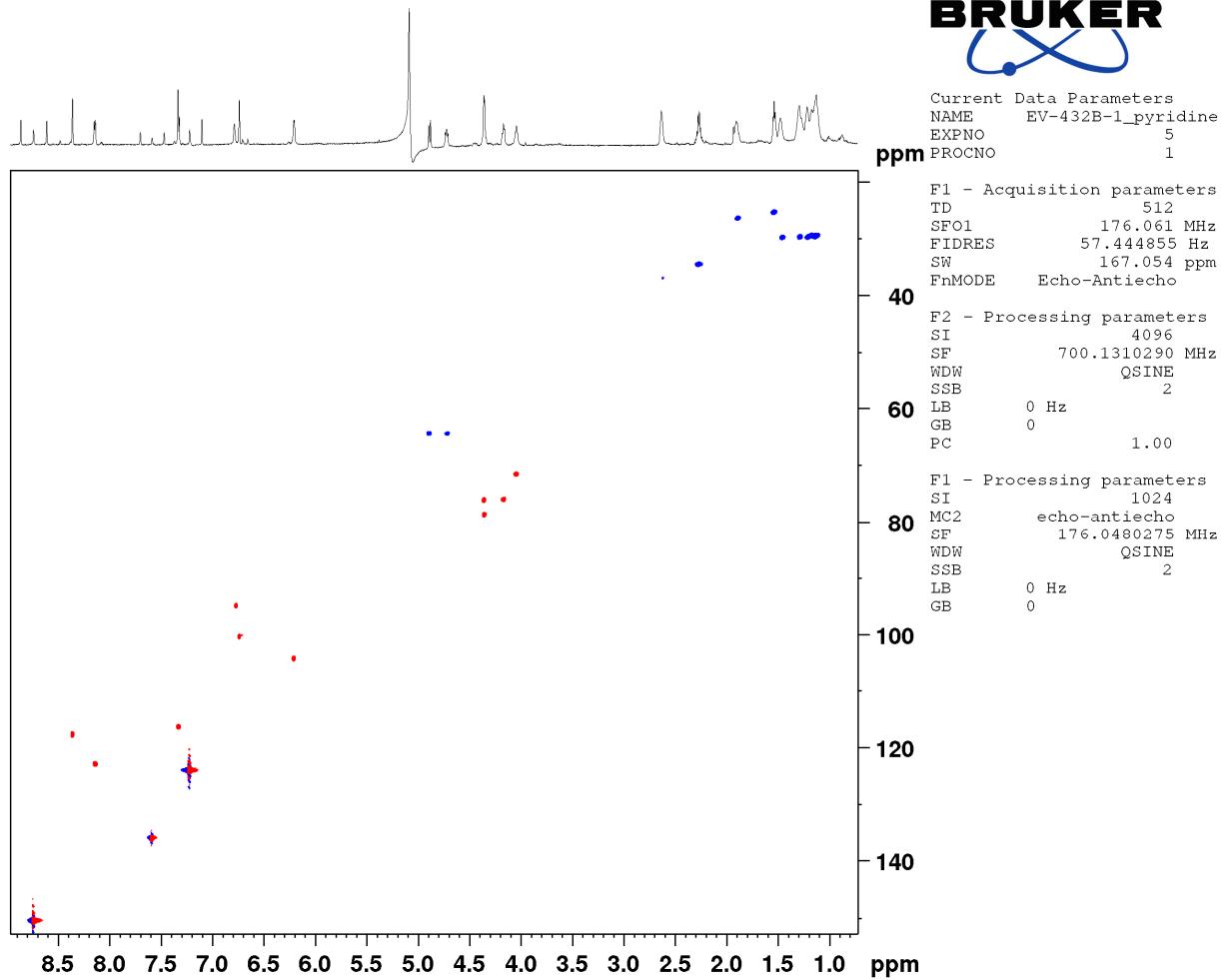


Figure S73. HSQC NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-432B-1\_pyridine  
EXPNO 5  
PROCNO 1

F1 - Acquisition parameters  
TD 512  
SFO1 176.061 MHz  
FIDRES 57.444855 Hz  
SW 167.054 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 4096  
SF 700.1310290 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0480275 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

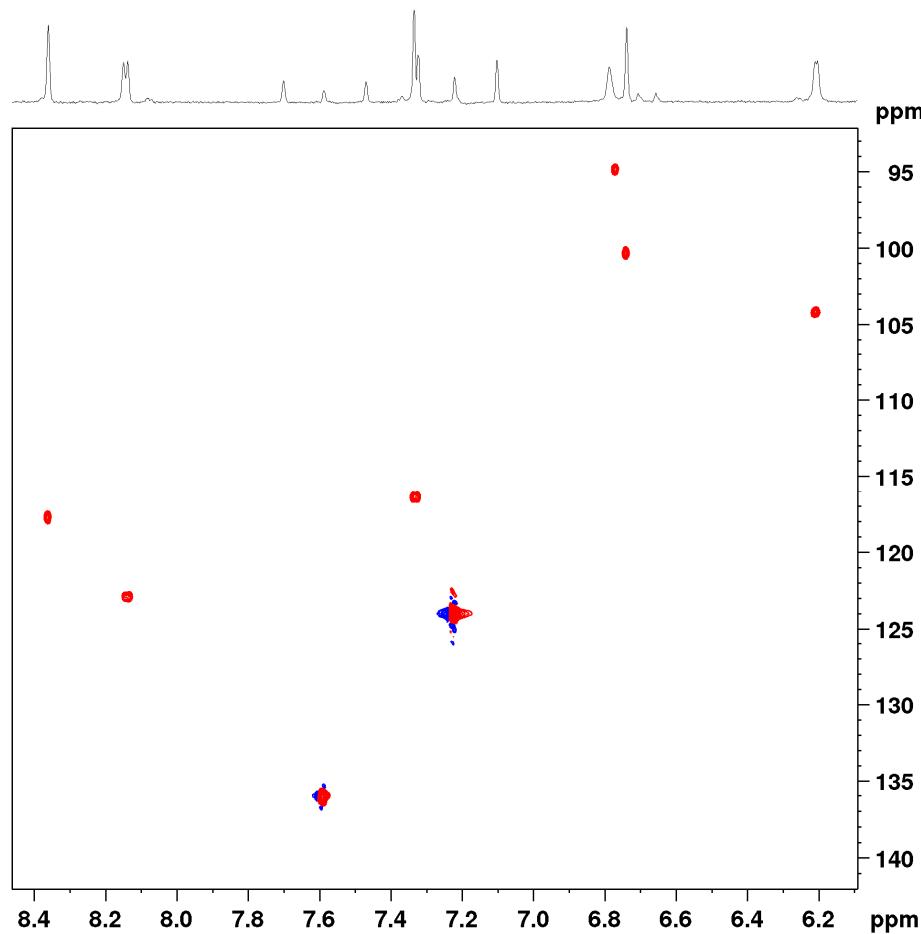


Figure S74. Detail (1/3) of HSQC NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K

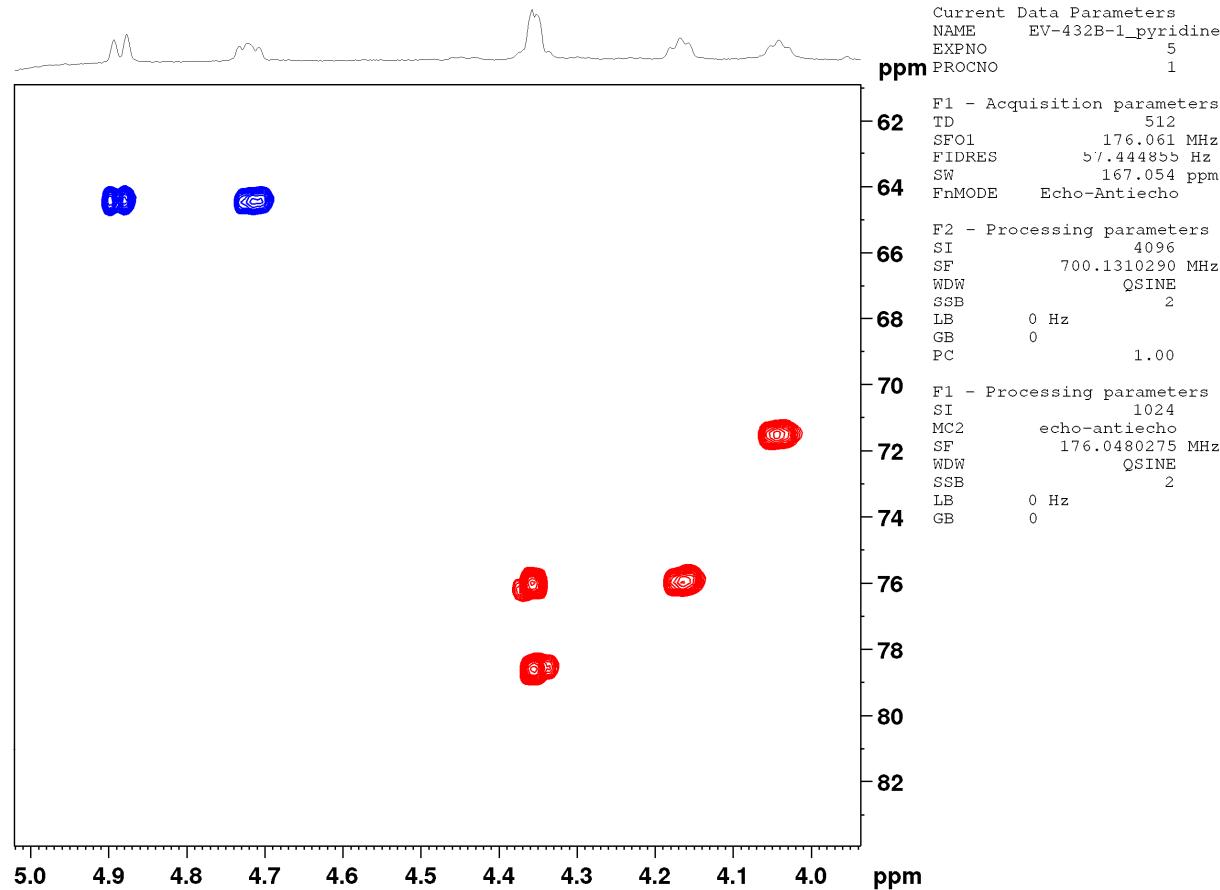


Figure S75. Detail (2/3) of HSQC NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K



Current Data Parameters  
NAME EV-432B-1\_pyridine  
EXPNO 5  
PROCNO 1

F1 - Acquisition parameters  
TD 512  
SFO1 176.061 MHz  
FIDRES 57.444855 Hz  
SW 167.054 ppm  
FnMODE Echo-Antiecho

F2 - Processing parameters  
SI 4096  
SF 700.1310290 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 1024  
MC2 echo-antiecho  
SF 176.0480275 MHz  
WDW QSINE  
SSB 2  
LB 0 Hz  
GB 0

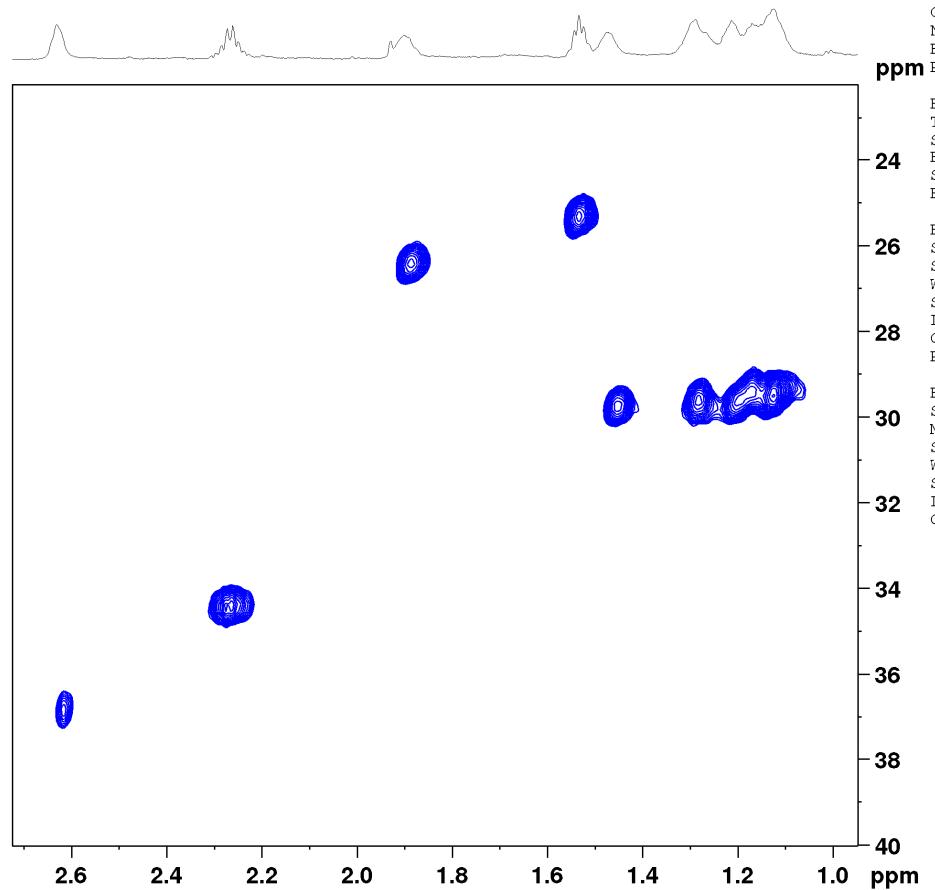


Figure S76. Detail (3/3) of HSQC NMR spectrum of compound 11.

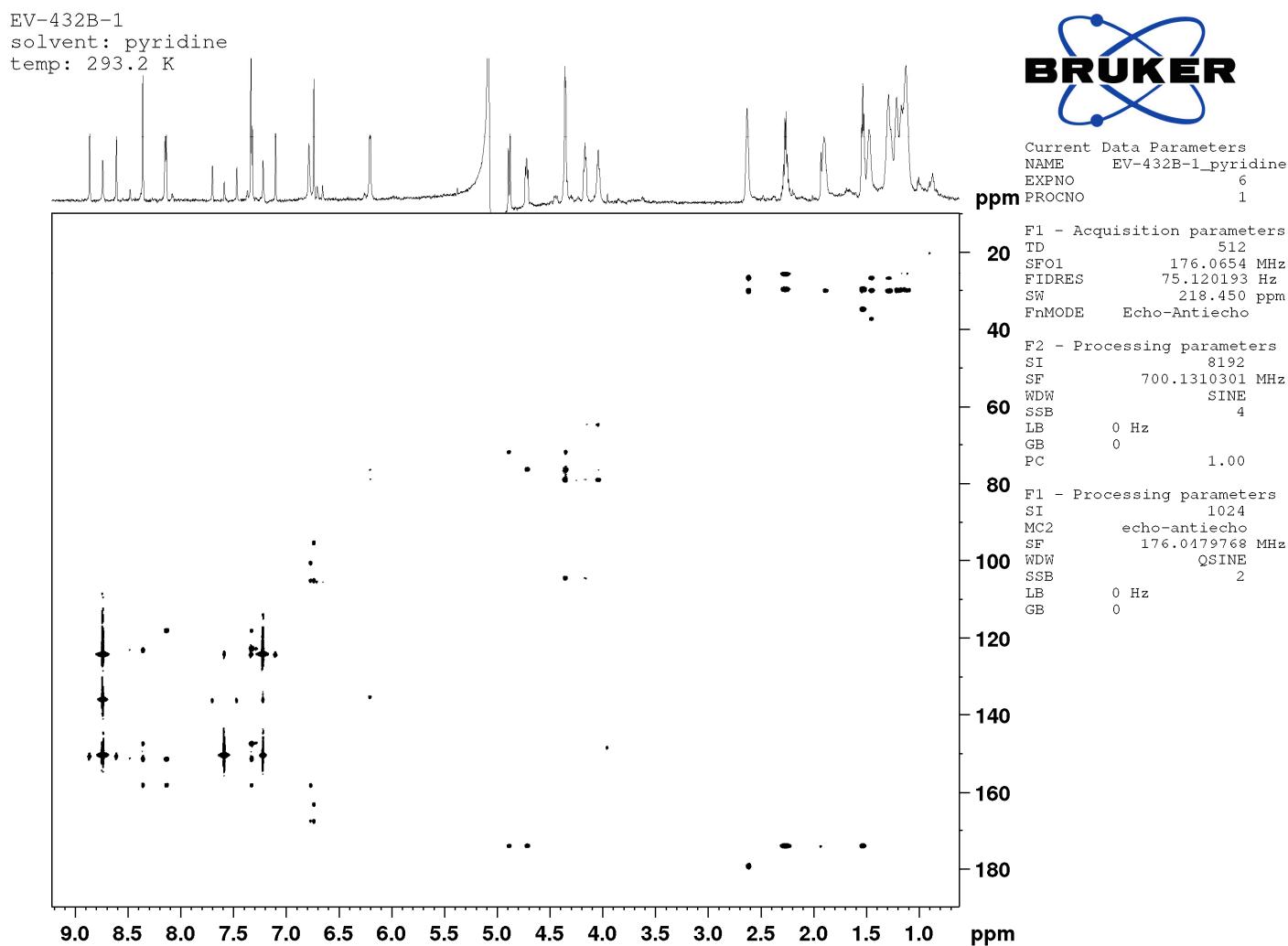


Figure S77. HMBC NMR spectrum of compound 11.

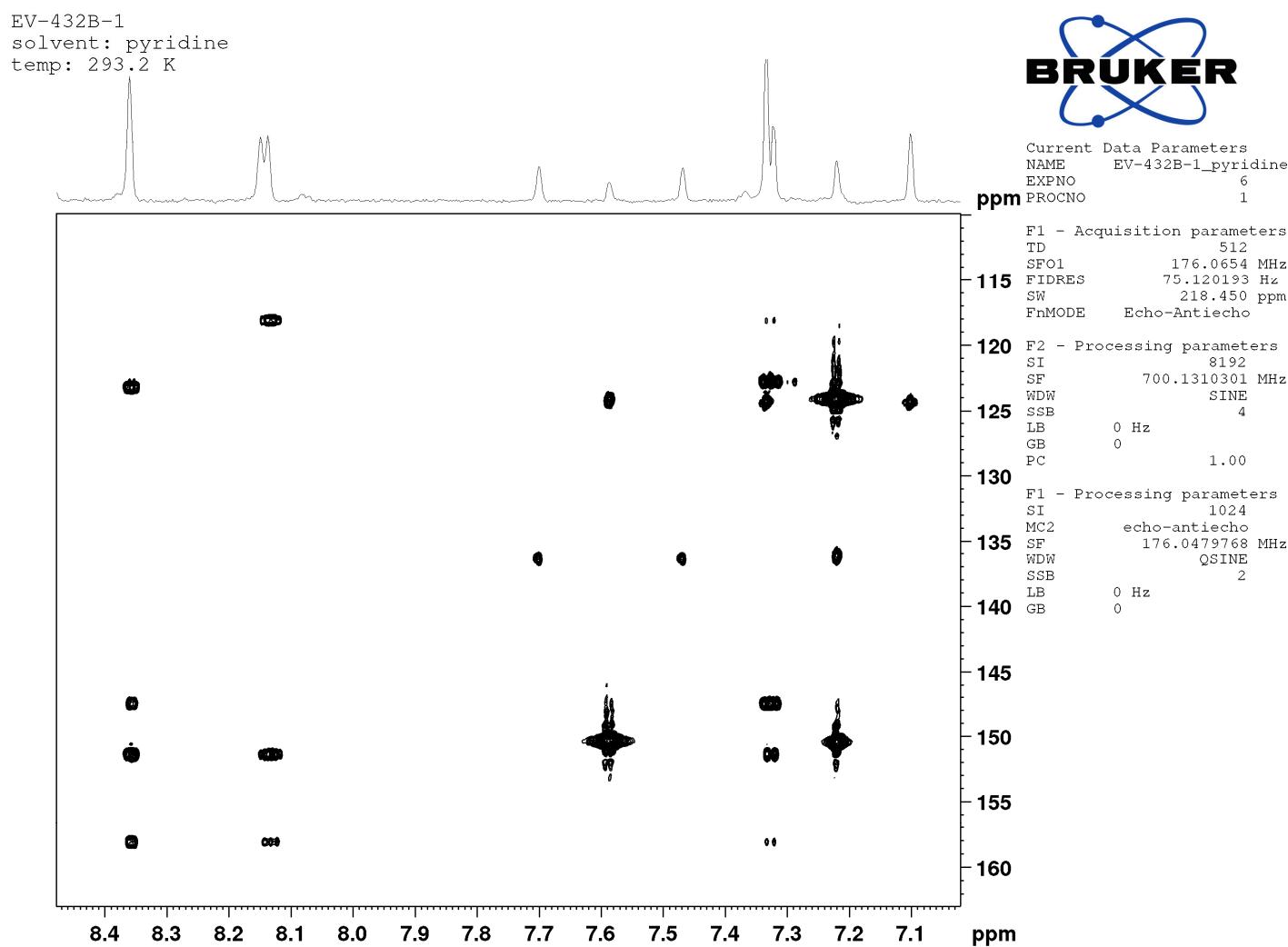


Figure S78. Detail (1/5) of HMBC NMR spectrum of compound 11.

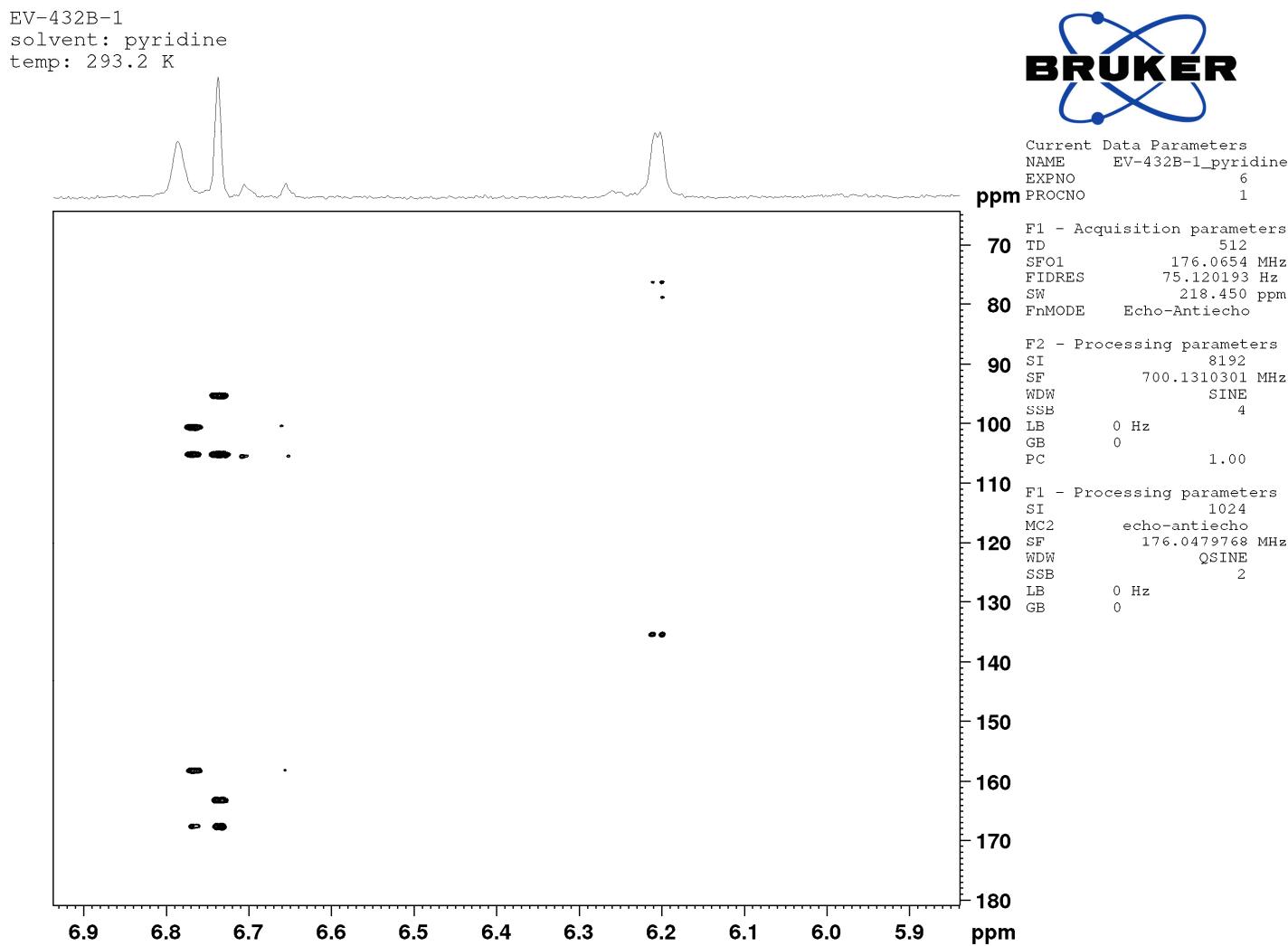


Figure S79. Detail (2/5) of HMBC NMR spectrum of compound 11.

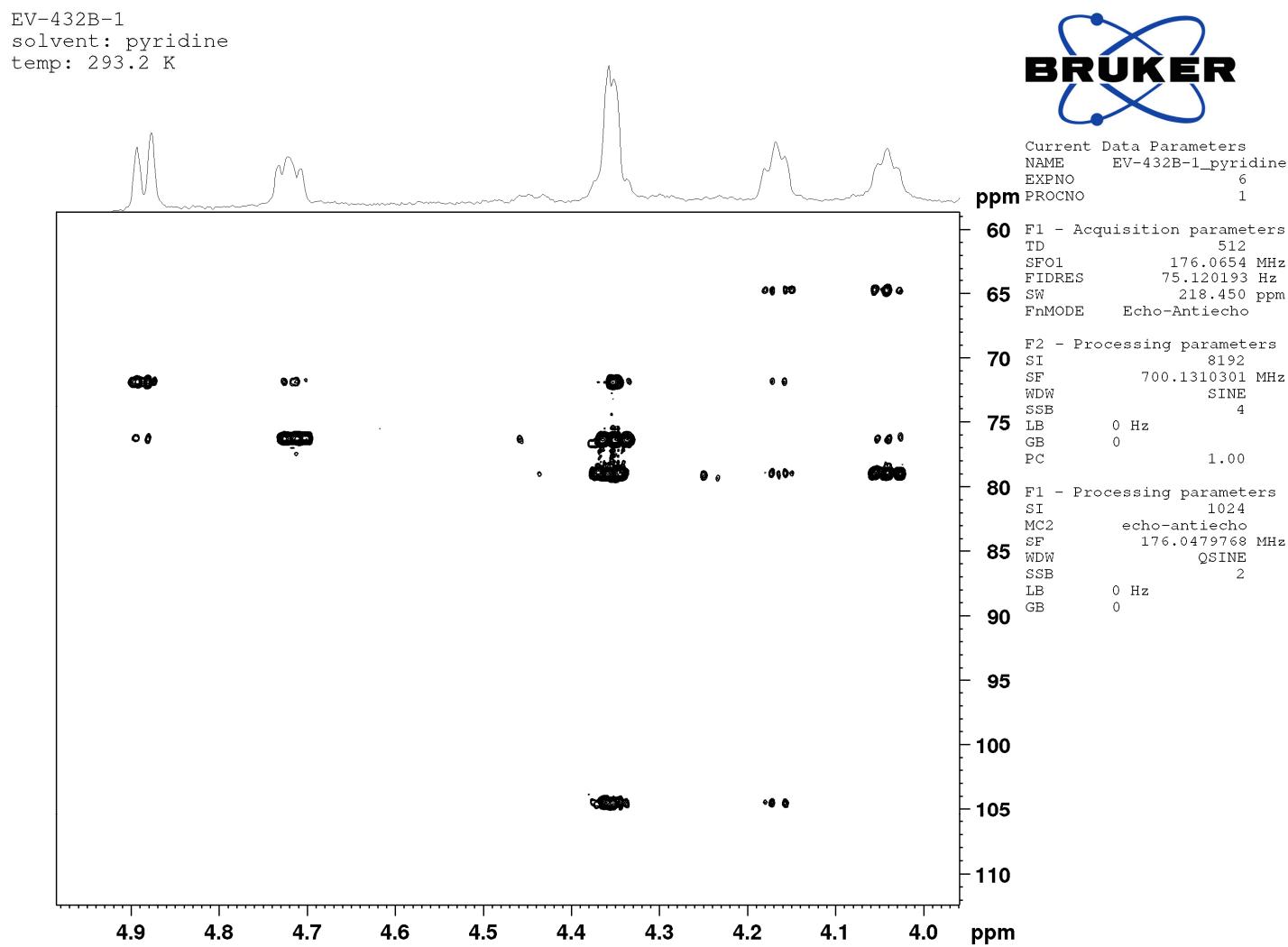


Figure S80. Detail (3/5) of HMBC NMR spectrum of compound 11.

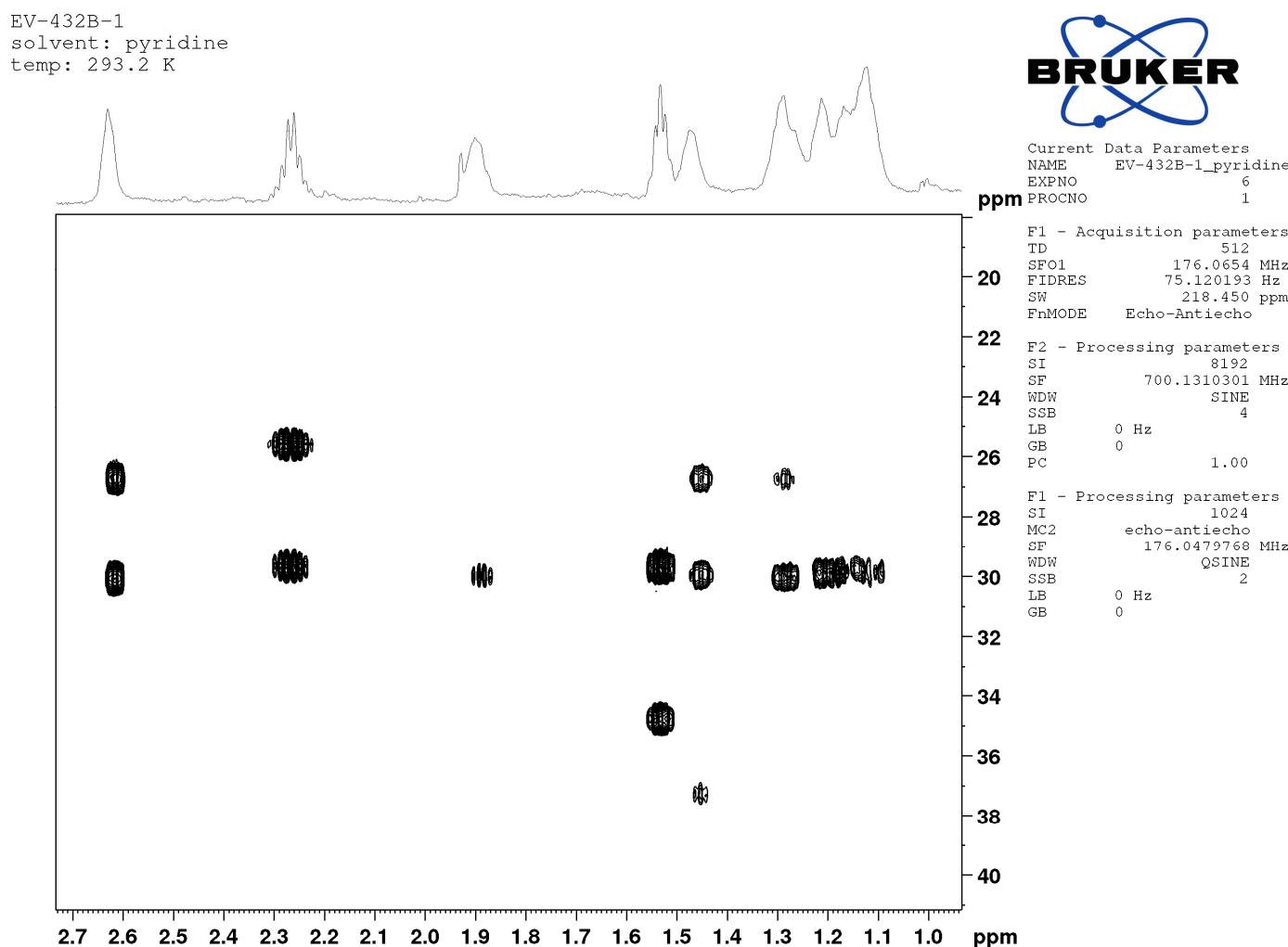


Figure S81. Detail (4/5) of HMBC NMR spectrum of compound 11.

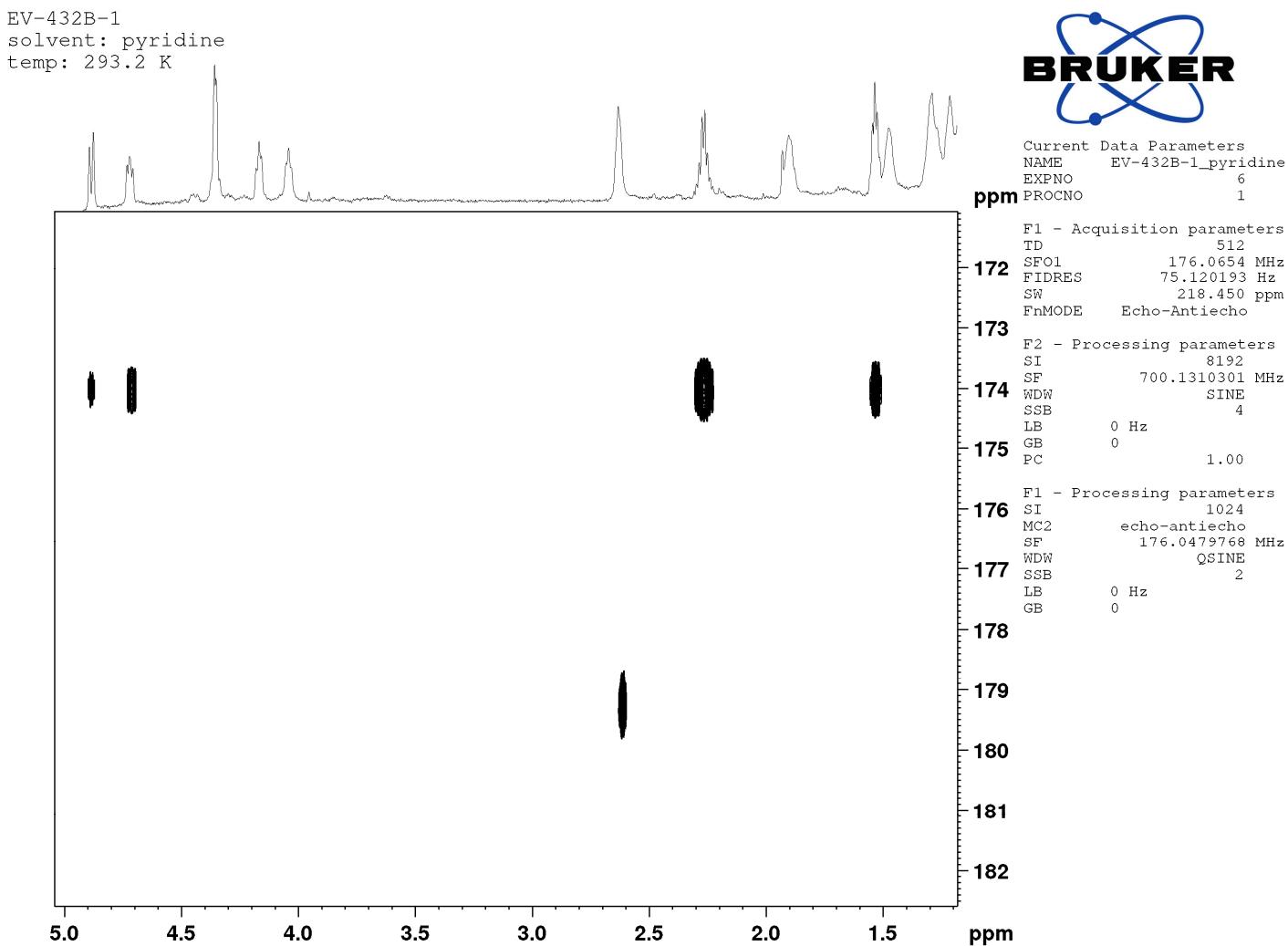


Figure S82. Detail (5/5) of HMBC NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K

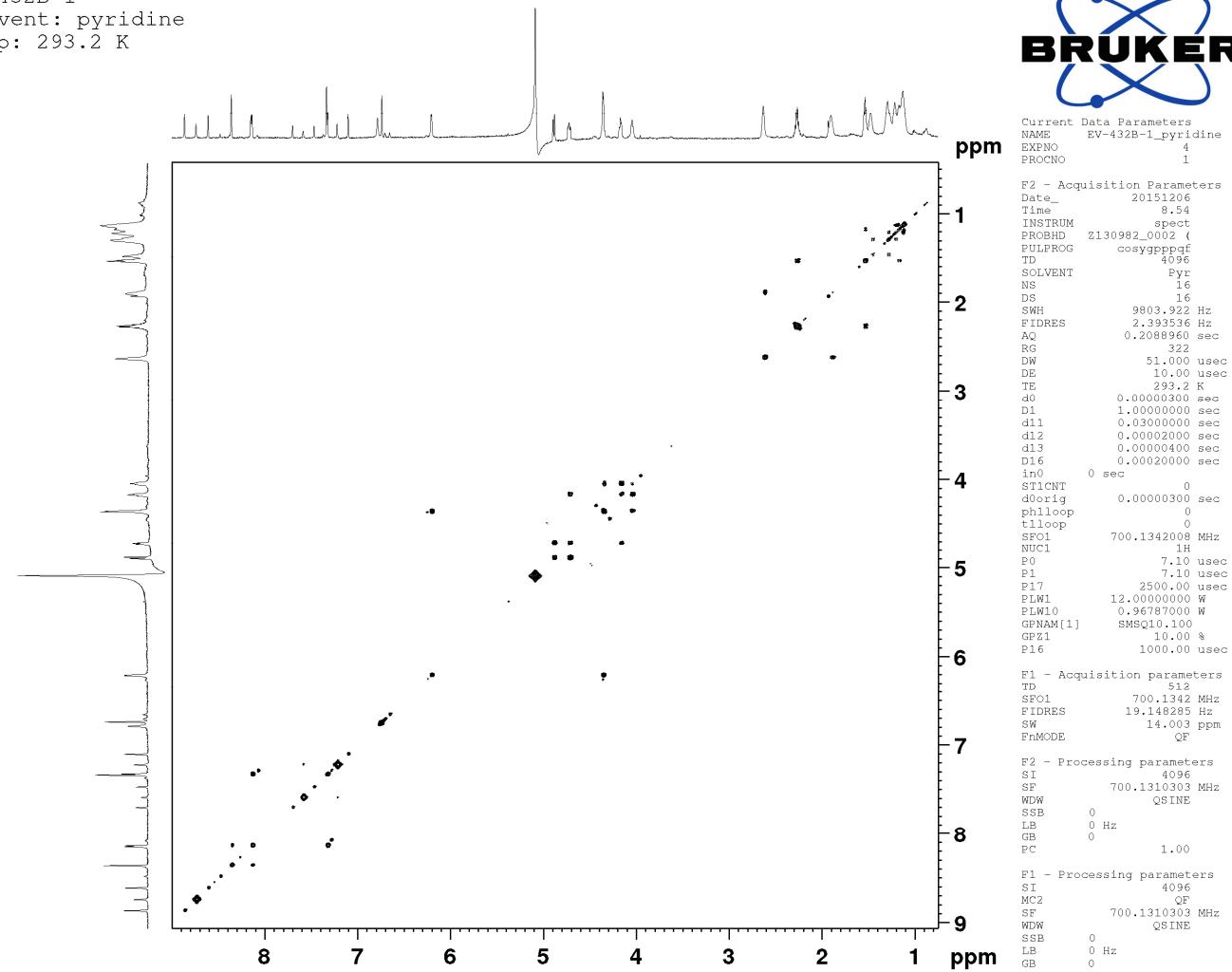


Figure S83. COSY NMR spectrum of compound 11.

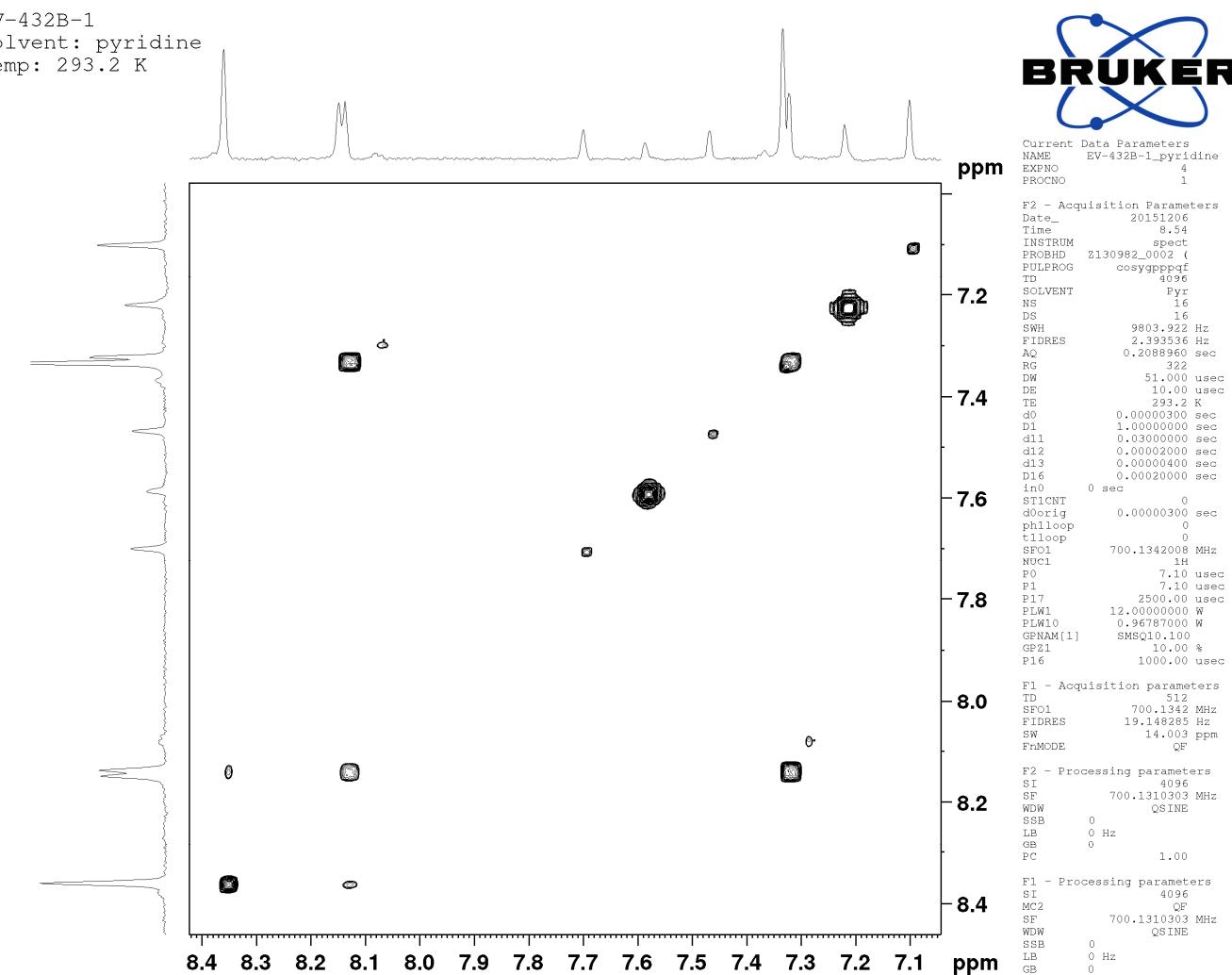


Figure S84. Detail (1/3) of COSY NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K

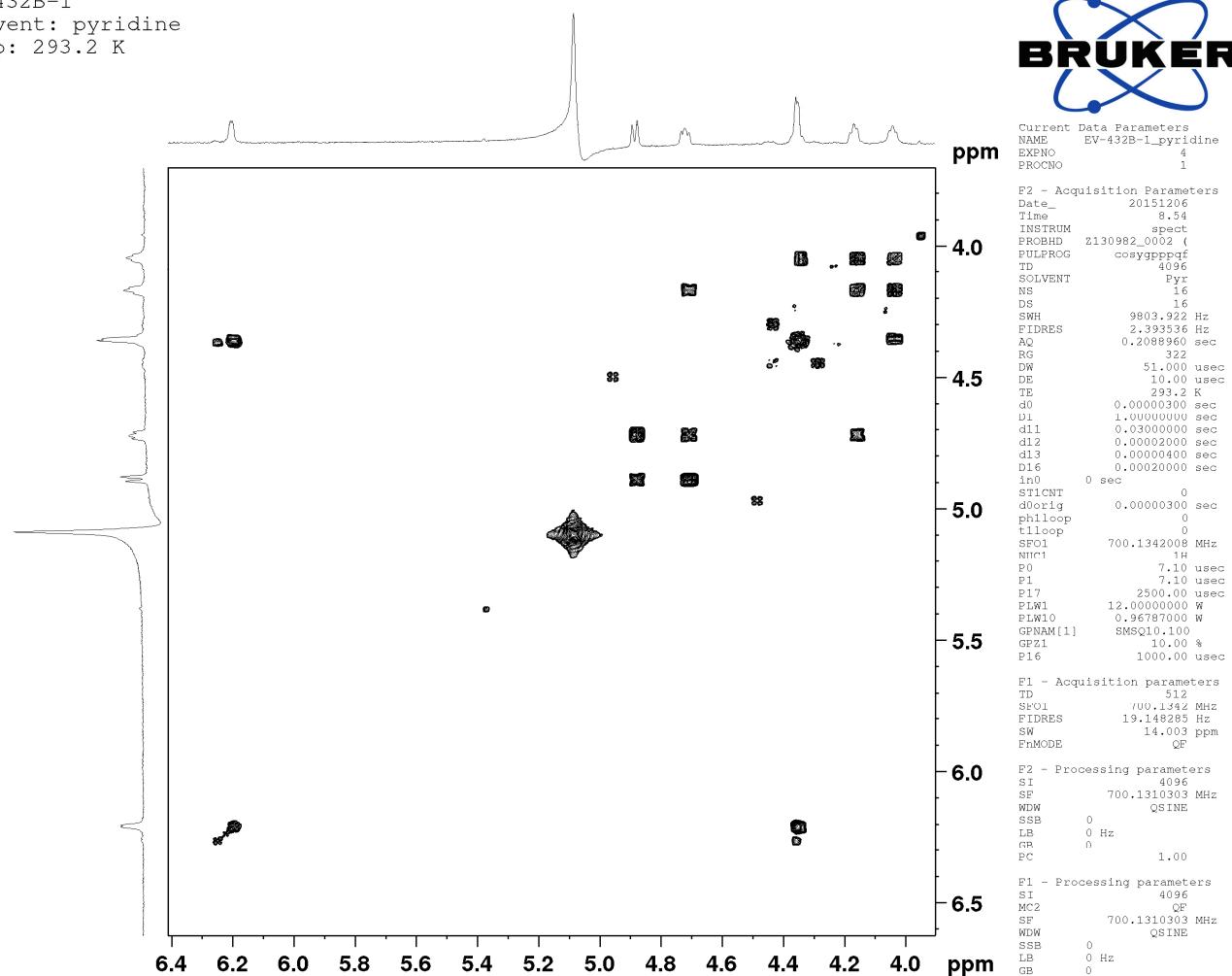


Figure S85. Detail (2/3) of COSY NMR spectrum of compound 11.

EV-432B-1  
solvent: pyridine  
temp: 293.2 K

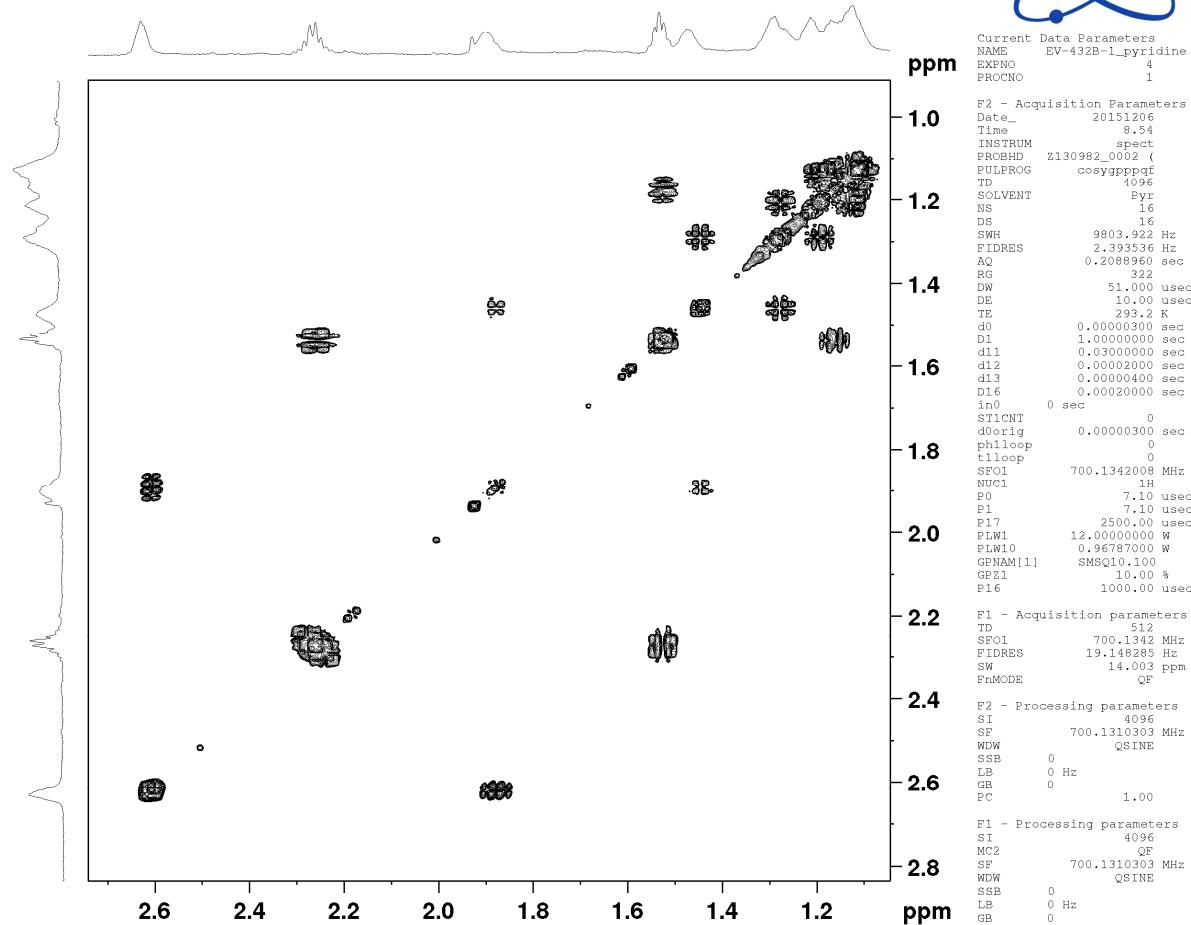
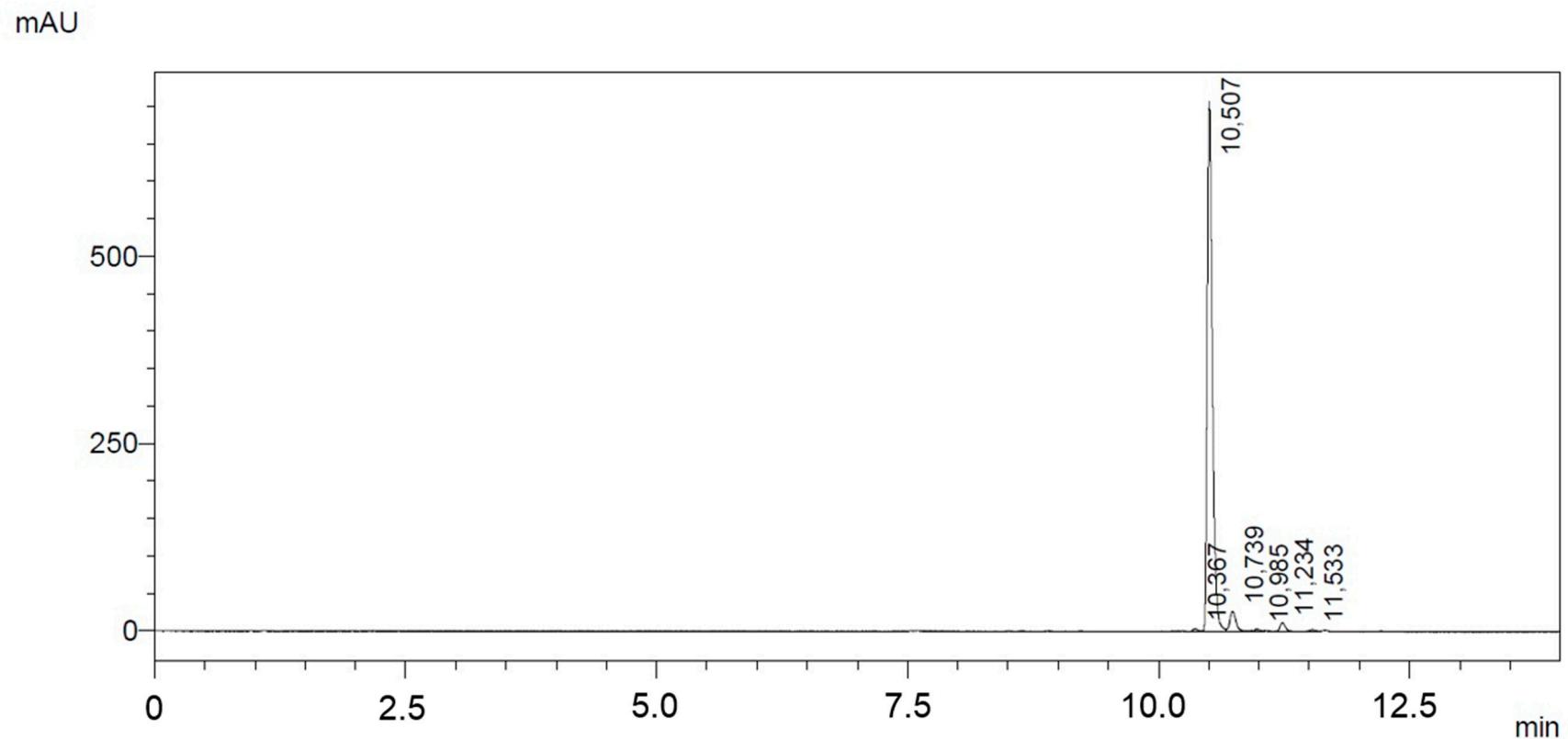
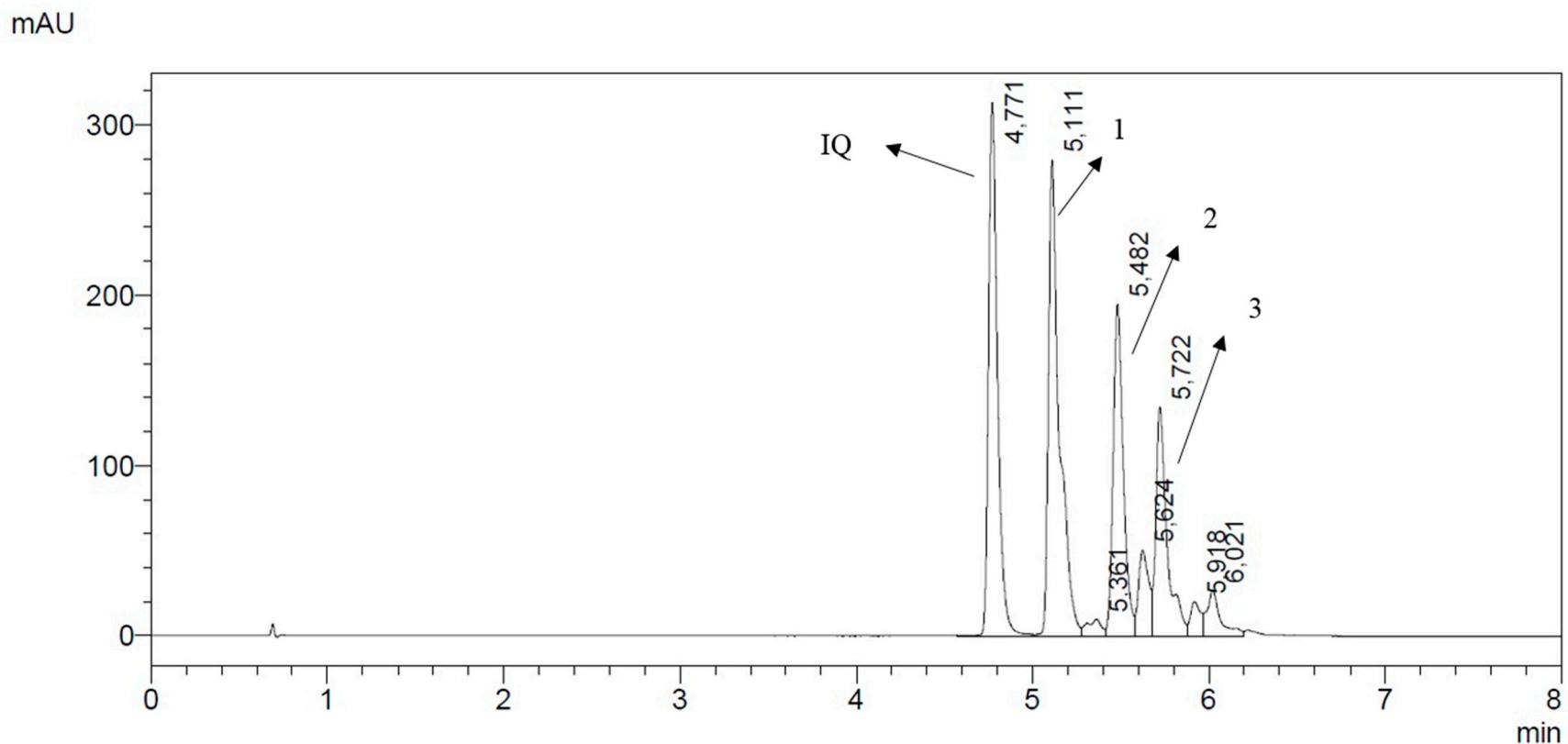


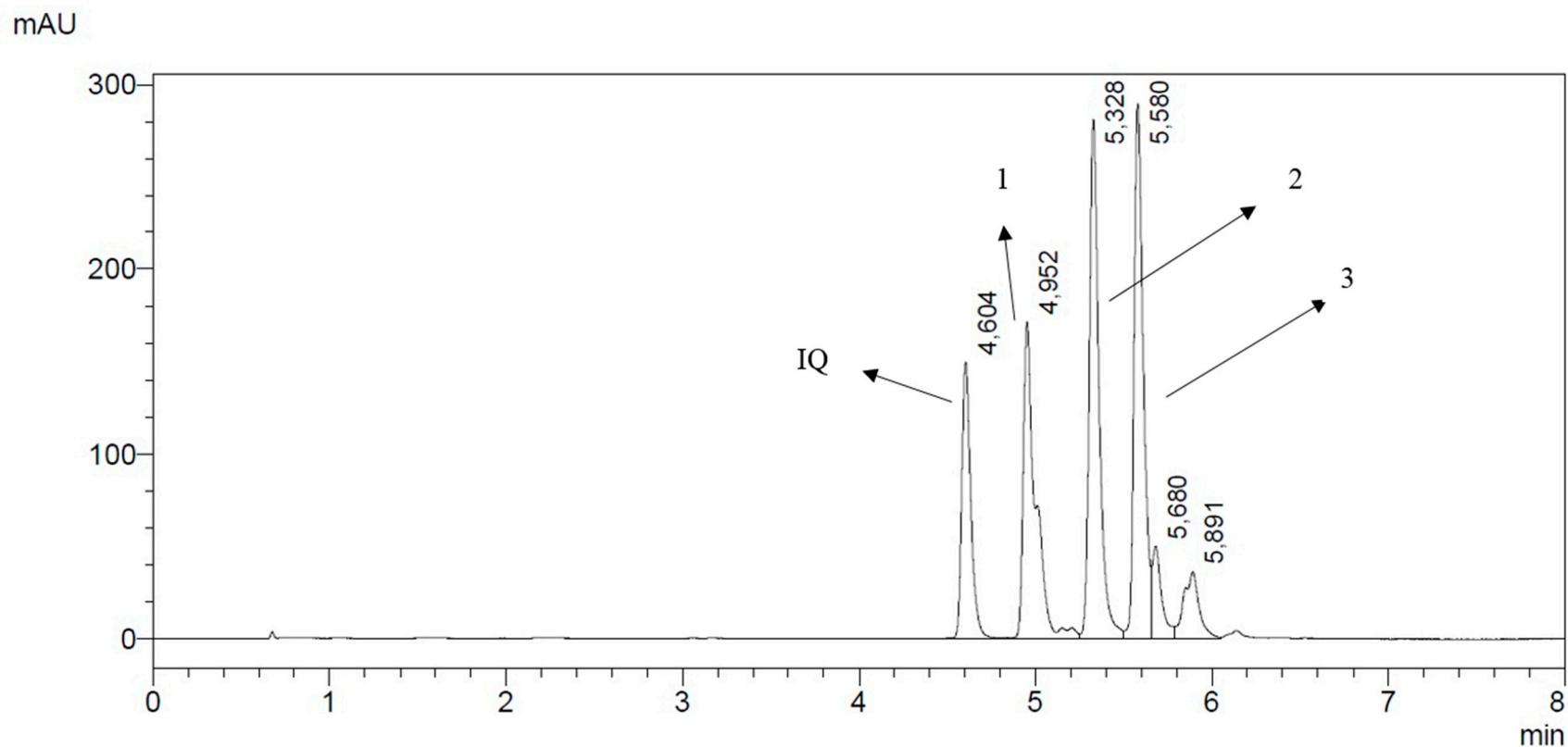
Figure S86. Detail (3/3) of COSY NMR spectrum of compound 11.



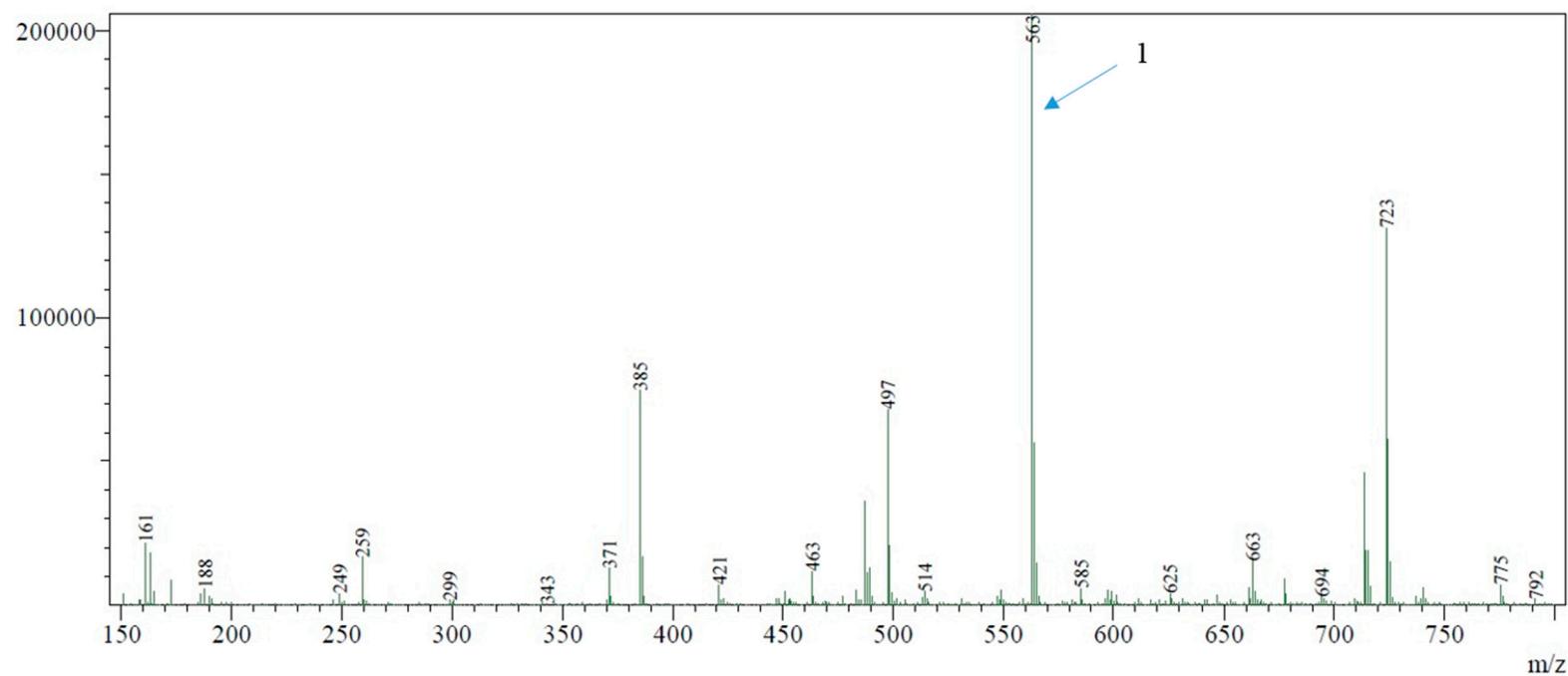
**Figure S87.** HPLC chromatogram of compound **11**.



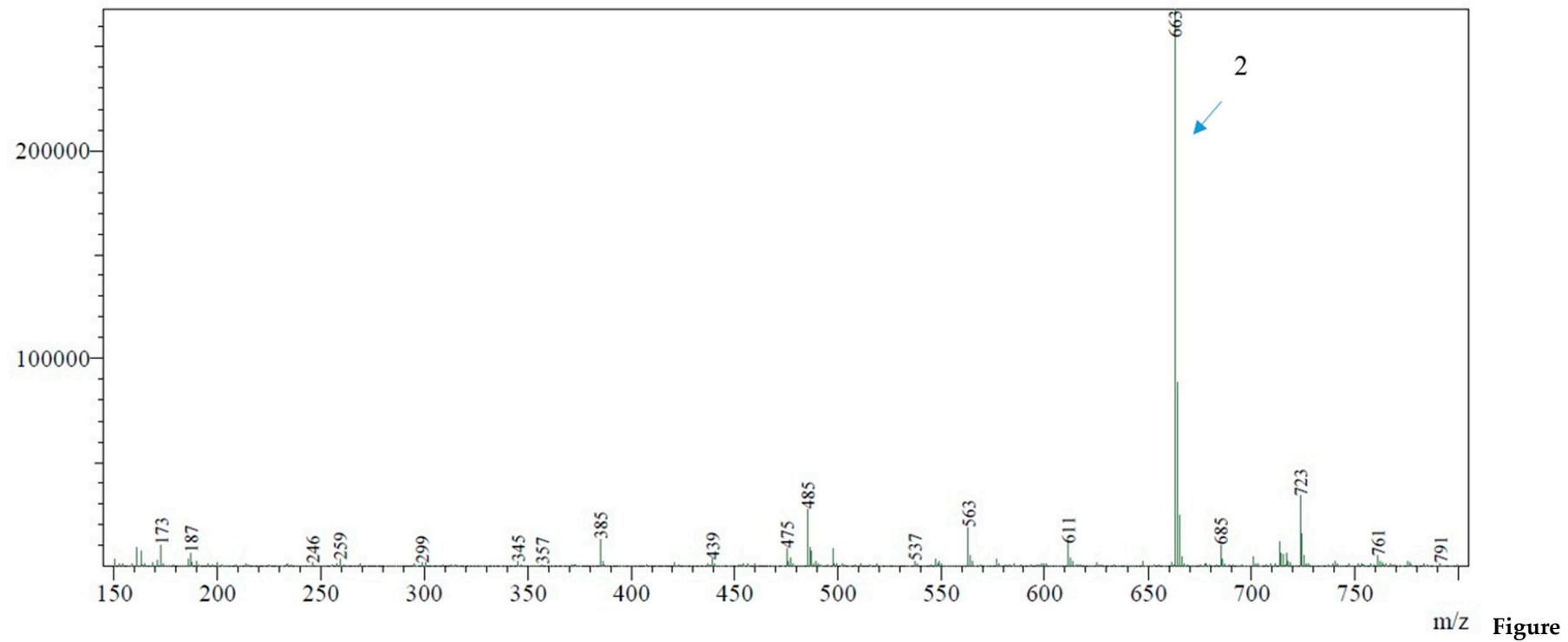
**Figure S88.** HPLC PDA chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the presence of Novozym 435®, acetone, 45 °C, 24 h. Peak 1: monosuccinate of isoquercitrin; Peak 2: disuccinate of isoquercitrin; Peak 3: trisuccinate of isoquercitrin.



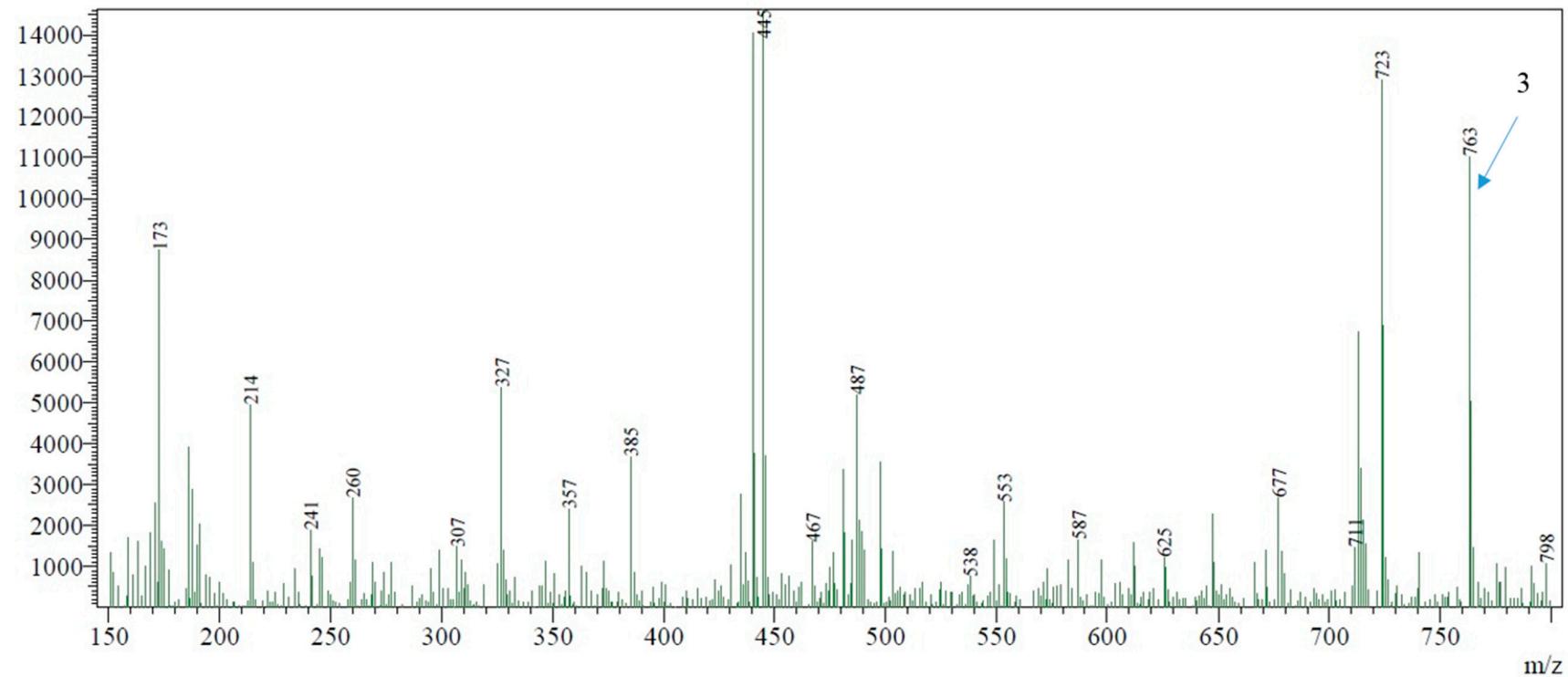
**Figure S89.** HPLC PDA chromatogram of the reaction mixture of isoquercitrin, succinic anhydride in the absence of Novozym 435<sup>®</sup>, acetone, 45 °C, 24 h. Peak 1: monosuccinate of isoquercitrin; Peak 2: disuccinate of isoquercitrin; Peak 3: trisuccinate of isoquercitrin.



**Figure S90.** HPLC-MS (−) chromatogram of the monosuccinate of isoquercitrin (peak 1).



**Figure S91.** HPLC-MS (-) chromatogram of the disuccinate of isoquercitrin (peak 2).



**Figure S92.** HPLC-MS (-) chromatogram of the trisuccinate of isoquercitrin (peak 3).