

## Supplementary Materials

### Bioactive abietane-type diterpenoid glycosides from leaves of *Clerodendrum infortunatum* (Lamiaceae)

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<b>List of contents</b>	
<b>Content</b>	<b>Page</b>
Figure S1-A. 1D- <sup>1</sup> H NMR (600 MHz) spectrum of compound <b>1</b> in Methanol- <i>d</i> <sub>4</sub> .	3
Figure S1-B. 1D- <sup>1</sup> H NMR (600 MHz) spectrum of compound <b>1</b> in DMSO- <i>d</i> <sub>6</sub> .	4
Figure S2-A. 1D- <sup>13</sup> C NMR (150 MHz) spectrum of compound <b>1</b> in Methanol- <i>d</i> <sub>4</sub> .	5
Figure S2-B. 1D- <sup>13</sup> C NMR (150 MHz) spectrum of compound <b>1</b> in DMSO- <i>d</i> <sub>6</sub> .	6
Figure S3-A. COSY spectrum of compound <b>1</b> in Methanol- <i>d</i> <sub>4</sub> .	7
Figure S3-B. COSY spectrum of compound <b>1</b> in DMSO- <i>d</i> <sub>6</sub> .	8
Figure S4-A. HSQC spectrum of compound <b>1</b> in Methanol- <i>d</i> <sub>4</sub> .	9
Figure S4-B. HSQC spectrum of compound <b>1</b> in DMSO- <i>d</i> <sub>6</sub> .	10
Figure S5-A. HMBC spectrum of compound <b>1</b> in Methanol- <i>d</i> <sub>4</sub> .	11
Figure S5-B. HMBC spectrum of compound <b>1</b> in DMSO- <i>d</i> <sub>6</sub> .	12
Figure S6. HR mass spectrum of compound <b>1</b> in methanol.	13
Figure S7-A. 1D- <sup>1</sup> H NMR (600 MHz) spectrum of compound <b>2</b> in Methanol- <i>d</i> <sub>4</sub> .	14
Figure S7-B. 1D- <sup>1</sup> H NMR (600 MHz) spectrum of compound <b>2</b> in DMSO- <i>d</i> <sub>6</sub> .	15
Figure S7-C. 1D- <sup>1</sup> H NMR (600 MHz) spectrum of compound <b>2</b> in D <sub>2</sub> O.	16
Figure S8-A. 1D- <sup>13</sup> C NMR (150 MHz) spectrum of compound <b>2</b> in Methanol- <i>d</i> <sub>4</sub> .	17
Figure S8-B. 1D- <sup>13</sup> C NMR (150 MHz) spectrum of compound <b>2</b> in DMSO- <i>d</i> <sub>6</sub> .	18
Figure S8-C. 1D- <sup>13</sup> C NMR (150 MHz) spectrum of compound <b>2</b> in D <sub>2</sub> O.	19
Figure S9-A. COSY spectrum of compound <b>2</b> in Methanol- <i>d</i> <sub>4</sub> .	20
Figure S9-B. COSY spectrum of compound <b>2</b> in DMSO- <i>d</i> <sub>6</sub> .	21
Figure S9-C. COSY spectrum of compound <b>2</b> in D <sub>2</sub> O.	22
Figure S10-A. HSQC spectrum of compound <b>2</b> in Methanol- <i>d</i> <sub>4</sub> .	23
Figure S10-B. HSQC spectrum of compound <b>2</b> in DMSO- <i>d</i> <sub>6</sub> .	24
Figure S10-C. HSQC spectrum of compound <b>2</b> in D <sub>2</sub> O.	25
Figure S11-A. HMBC spectrum of compound <b>2</b> in Methanol- <i>d</i> <sub>4</sub> .	26
Figure S11-B. HMBC spectrum of compound <b>2</b> in DMSO- <i>d</i> <sub>6</sub> .	27
Figure S11-C. HMBC spectrum of compound <b>2</b> in D <sub>2</sub> O.	28
Figure S12. HR mass spectrum of compound <b>2</b> in methanol.	29
Figure S13. HR mass spectrum of compound <b>3</b> in methanol.	30
Figure S14. UHPLC (λ = 330 nm) chromatogram of <i>n</i> -butanol fraction from leaves of <i>Clerodendrum infortunatum</i>	31
Table S1. 1D ( <sup>1</sup> H, 600 MHz and <sup>13</sup> C, 150 MHz) NMR spectroscopic data for compound <b>3</b> in CD <sub>3</sub> OD and (CD <sub>3</sub> ) <sub>2</sub> SO	32

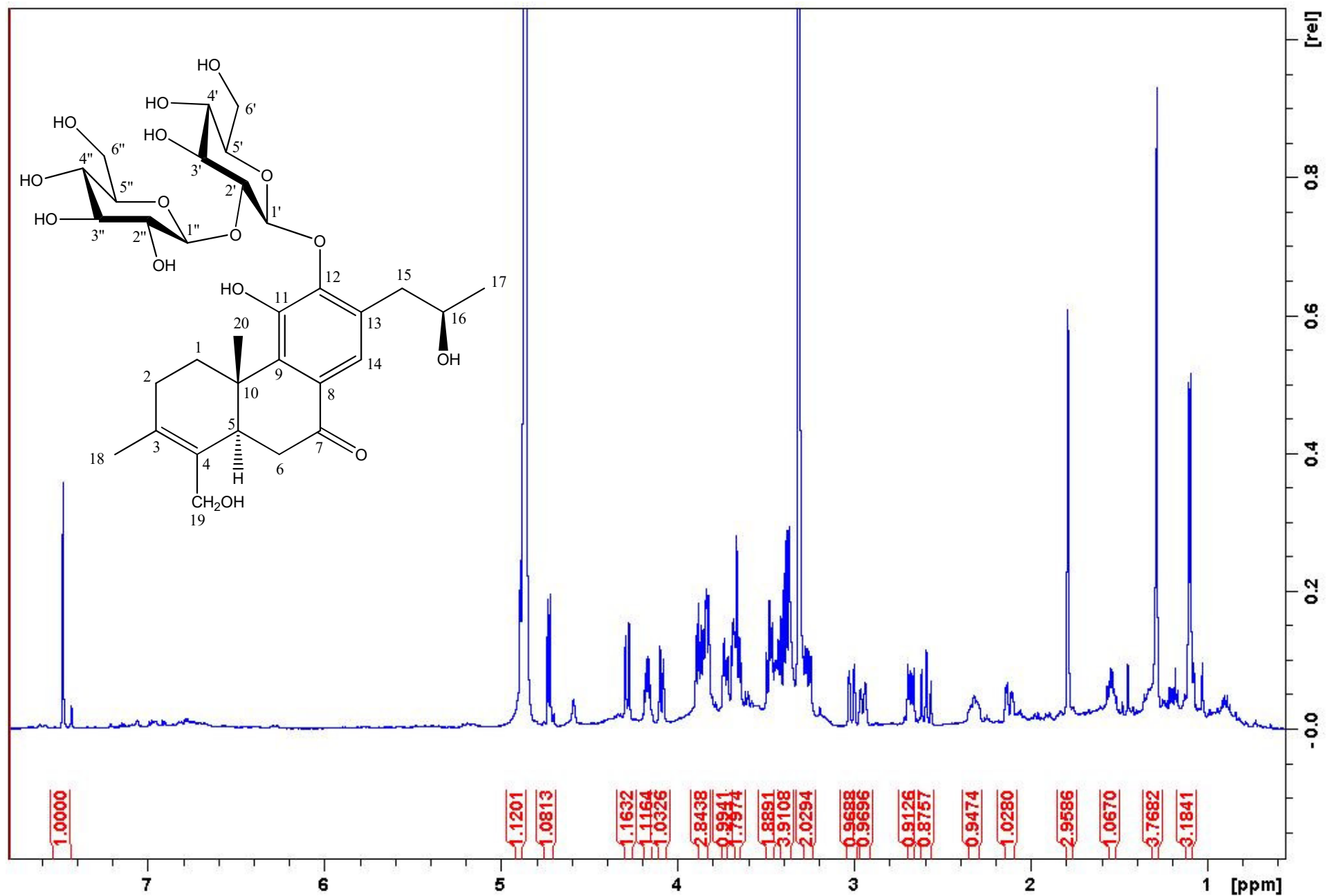


Figure S1-A.  $^1\text{H}$  NMR spectrum of compound **1** in  $\text{Methanol-}d_4$ .

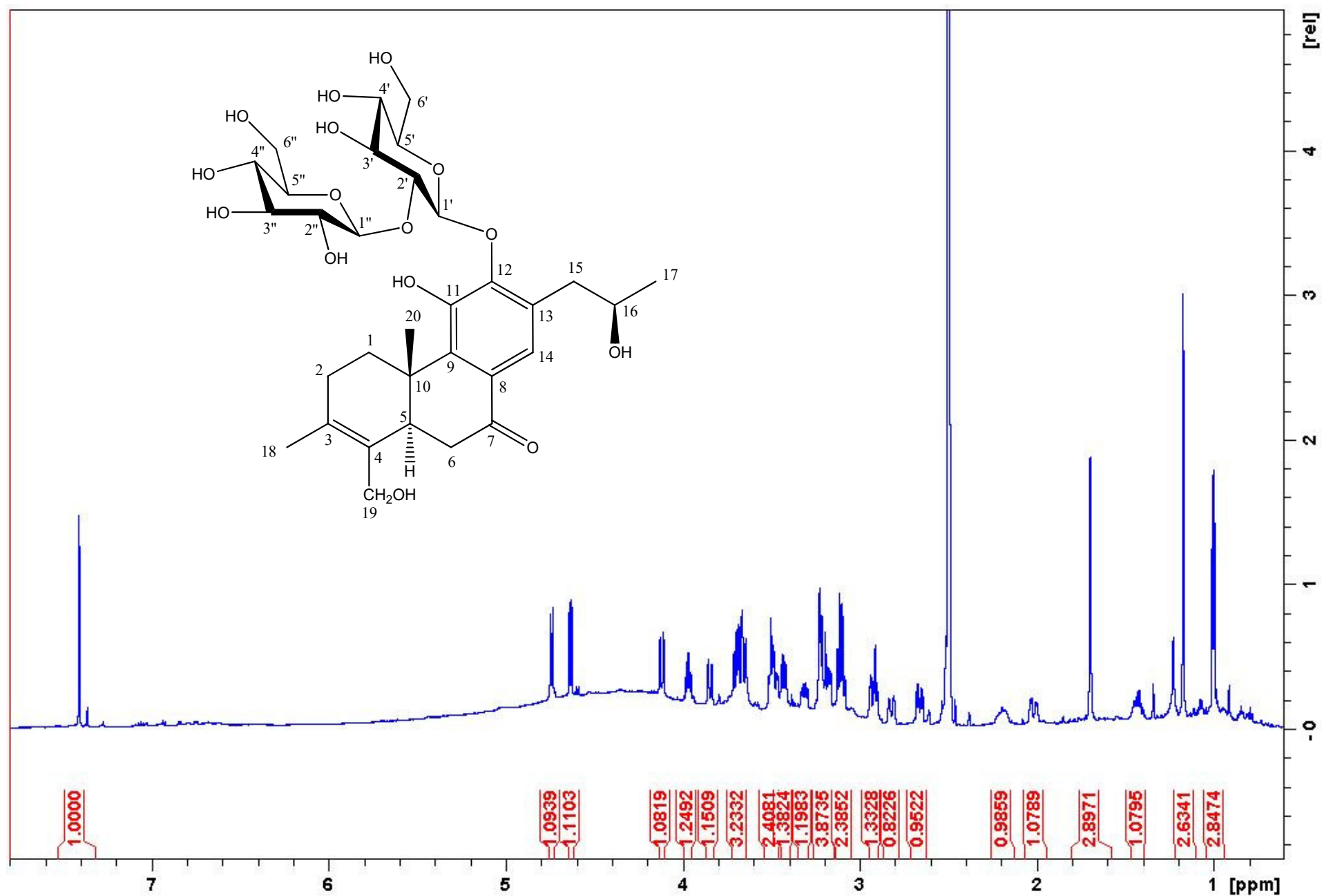


Figure S1-B.  $^1\text{H}$  NMR spectrum of compound 1 in  $\text{DMSO}-d_6$

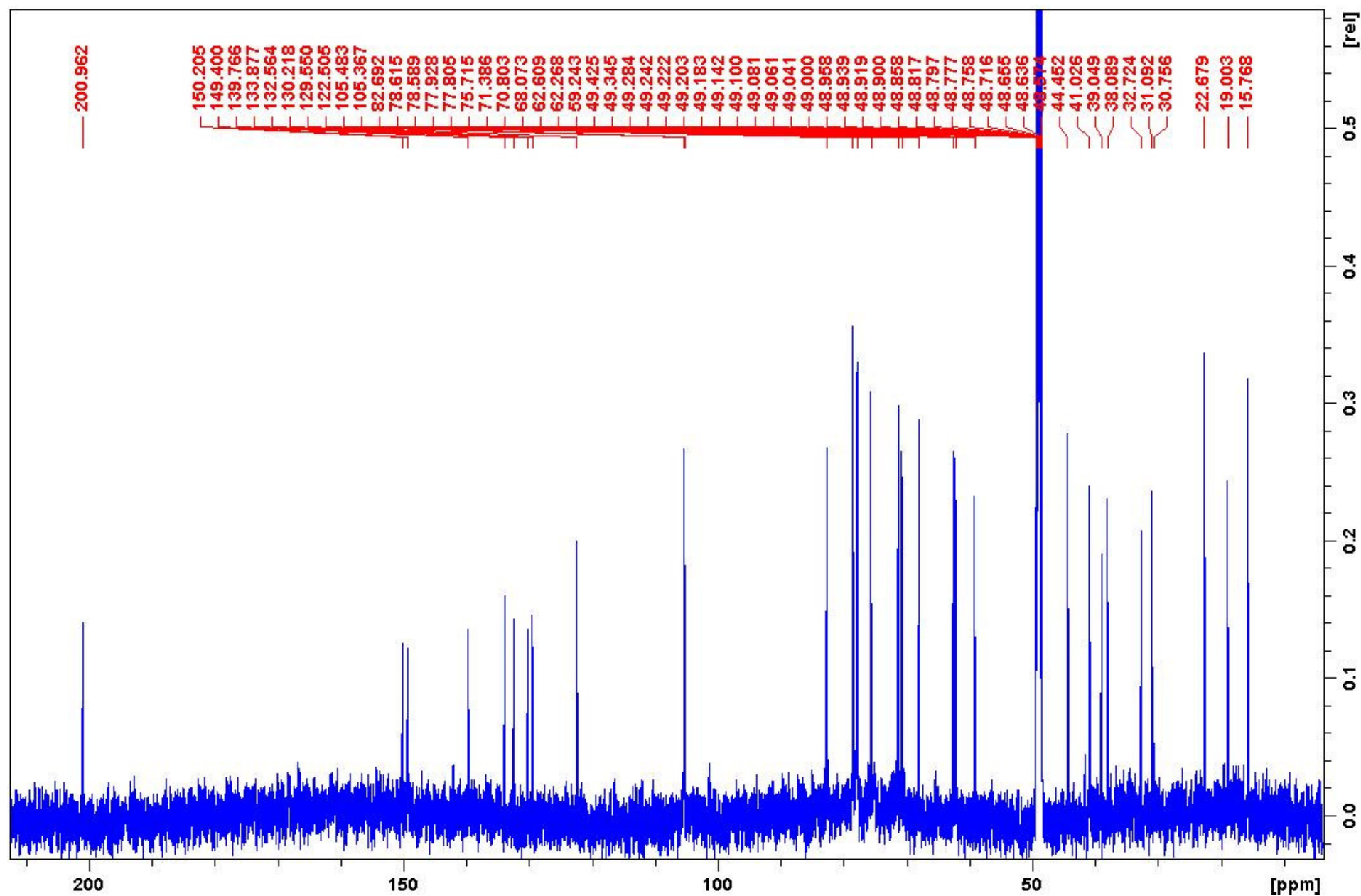
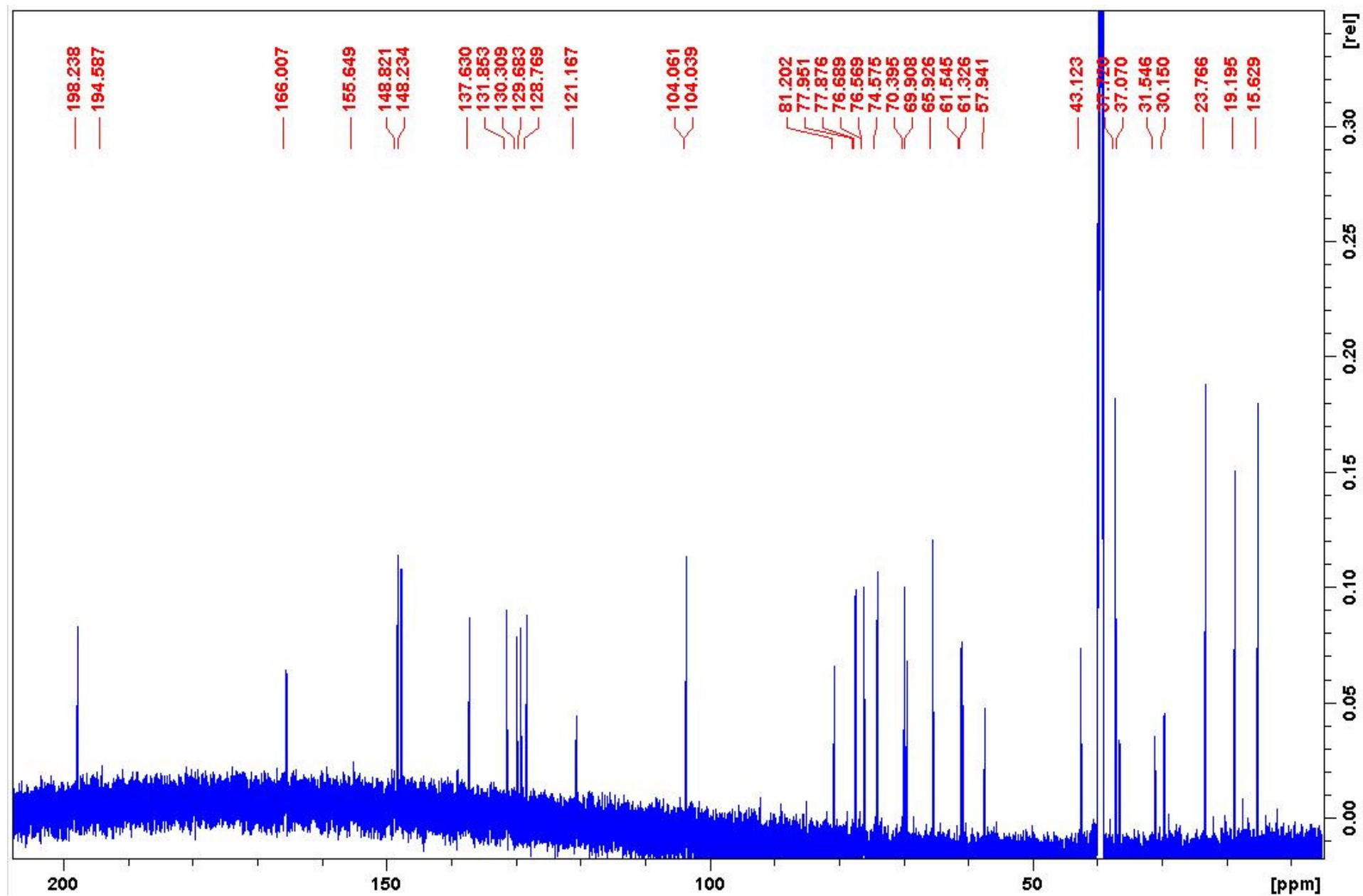


Figure S2-A.  $^{13}\text{C}$  NMR spectrum of compound **1** in Methanol- $d_4$ .



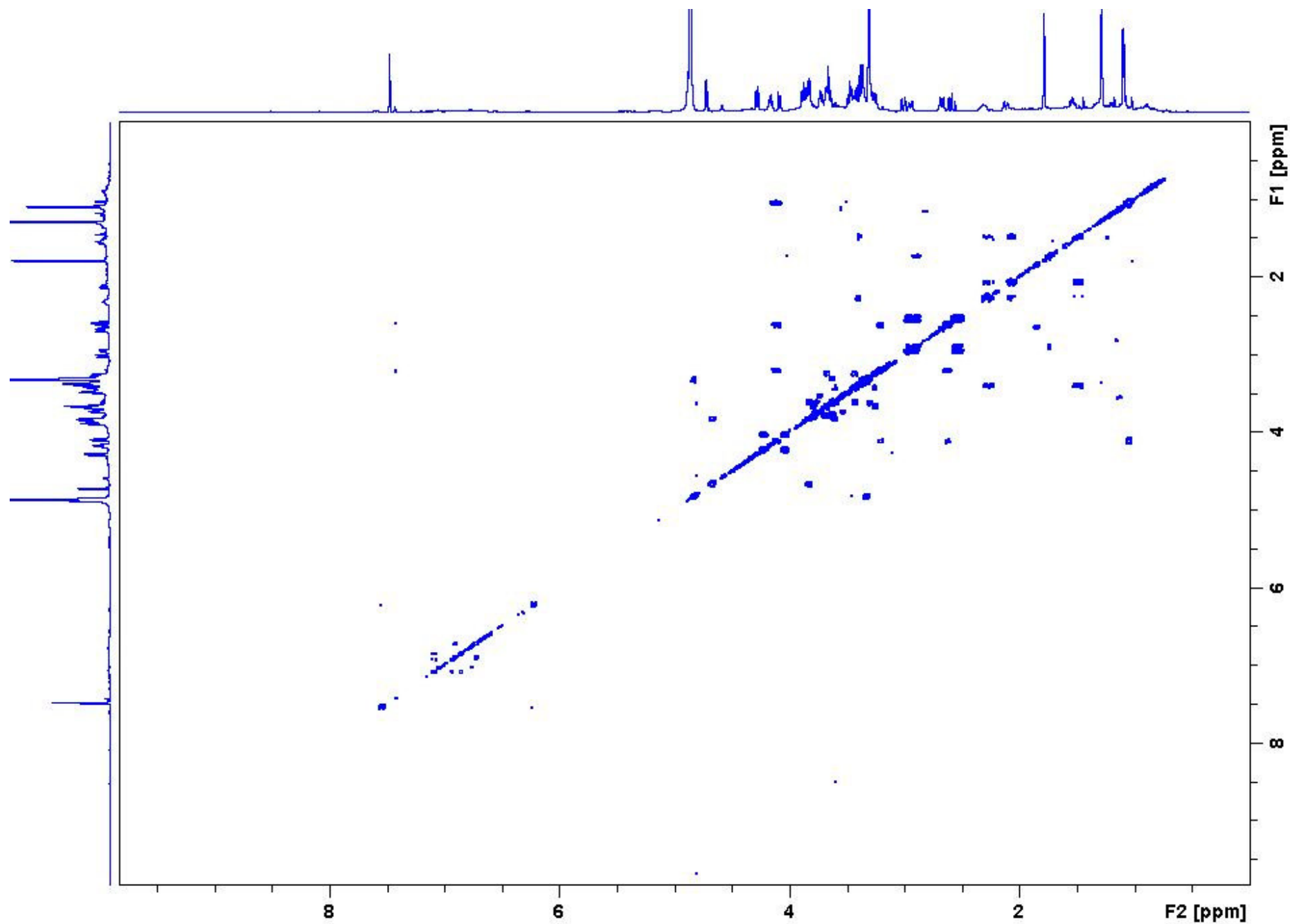


Figure S3-A. COSY spectrum of compound 1 in Methanol- $d_4$ .

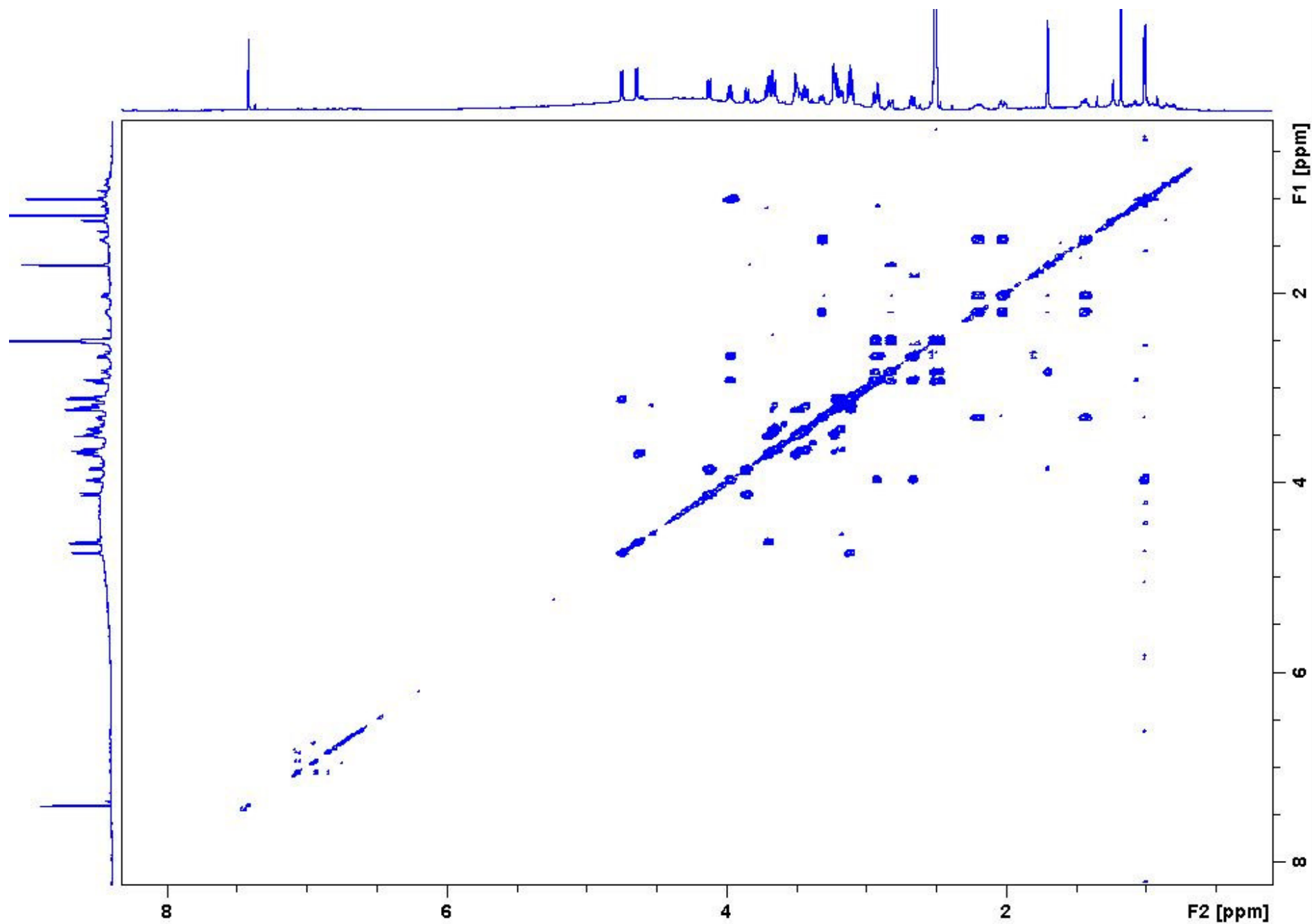


Figure S3-B. COSY spectrum of compound 1 in DMSO- $d_6$ .



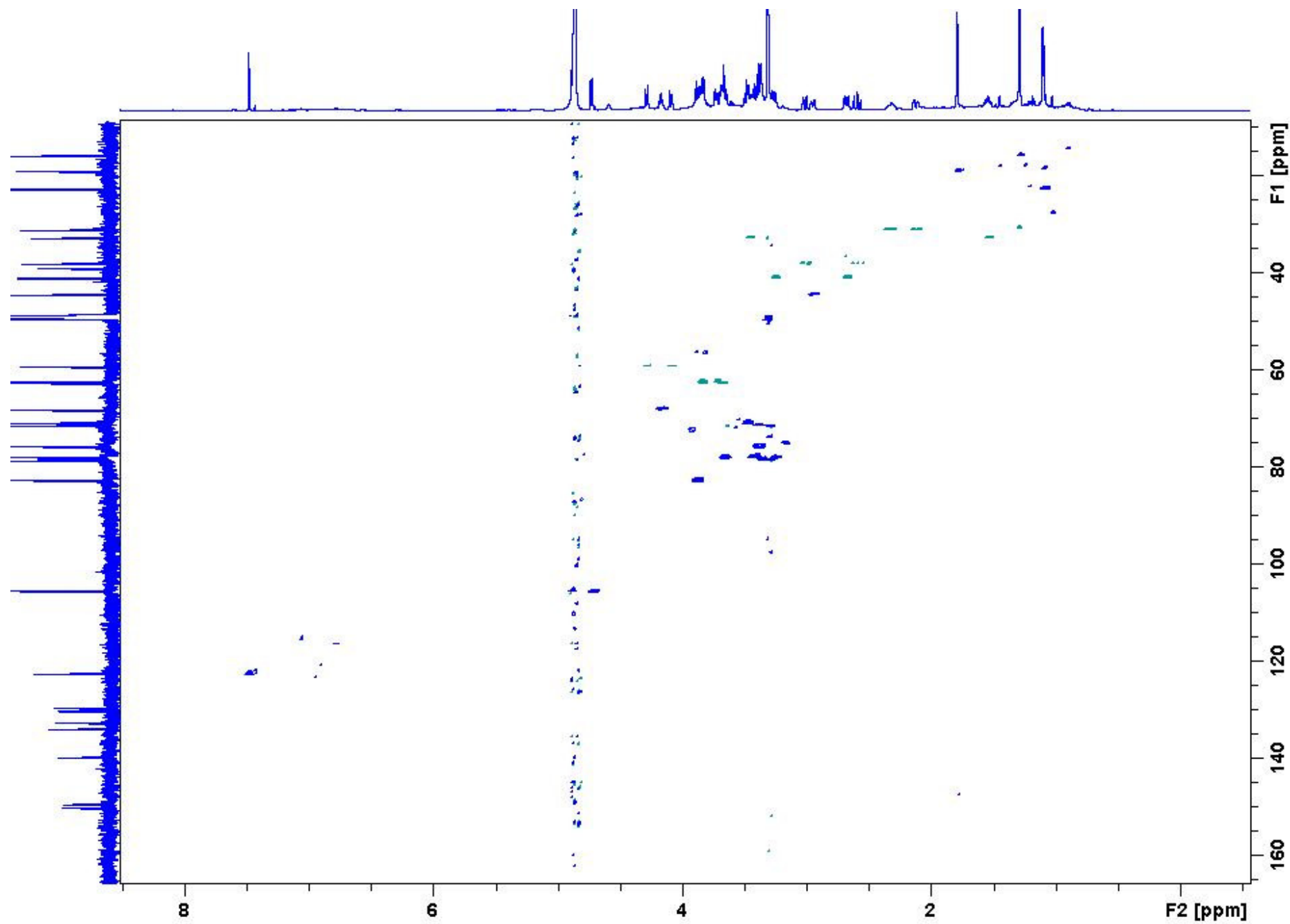


Figure S4-A. HSQC spectrum of compound **1** in Methanol- $d_4$ .

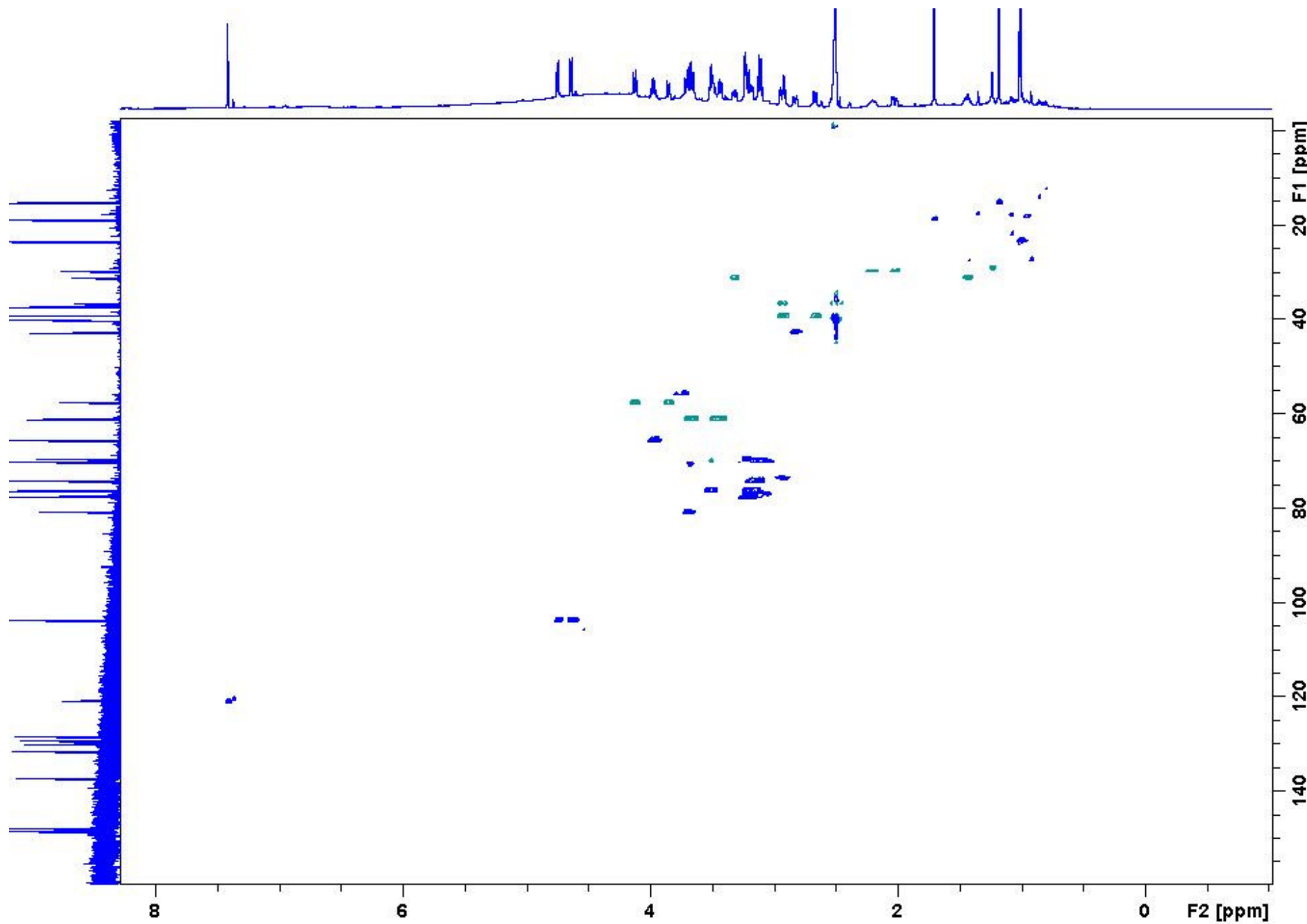


Figure S4-B. HSQC spectrum of compound **1** in DMSO- $d_6$ .

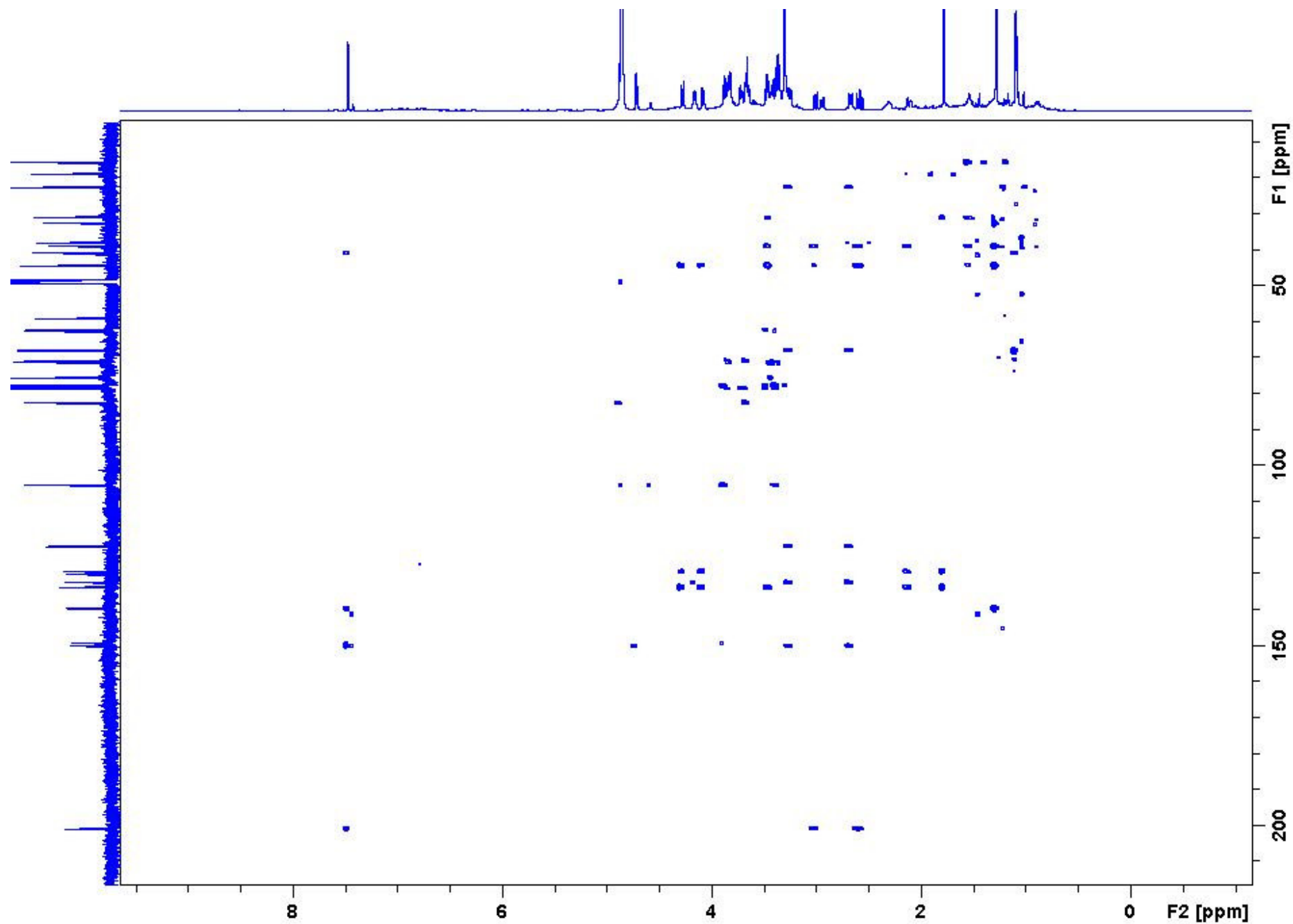


Figure S5-A. HMBC spectrum of compound **1** in Methanol- $d_4$ .

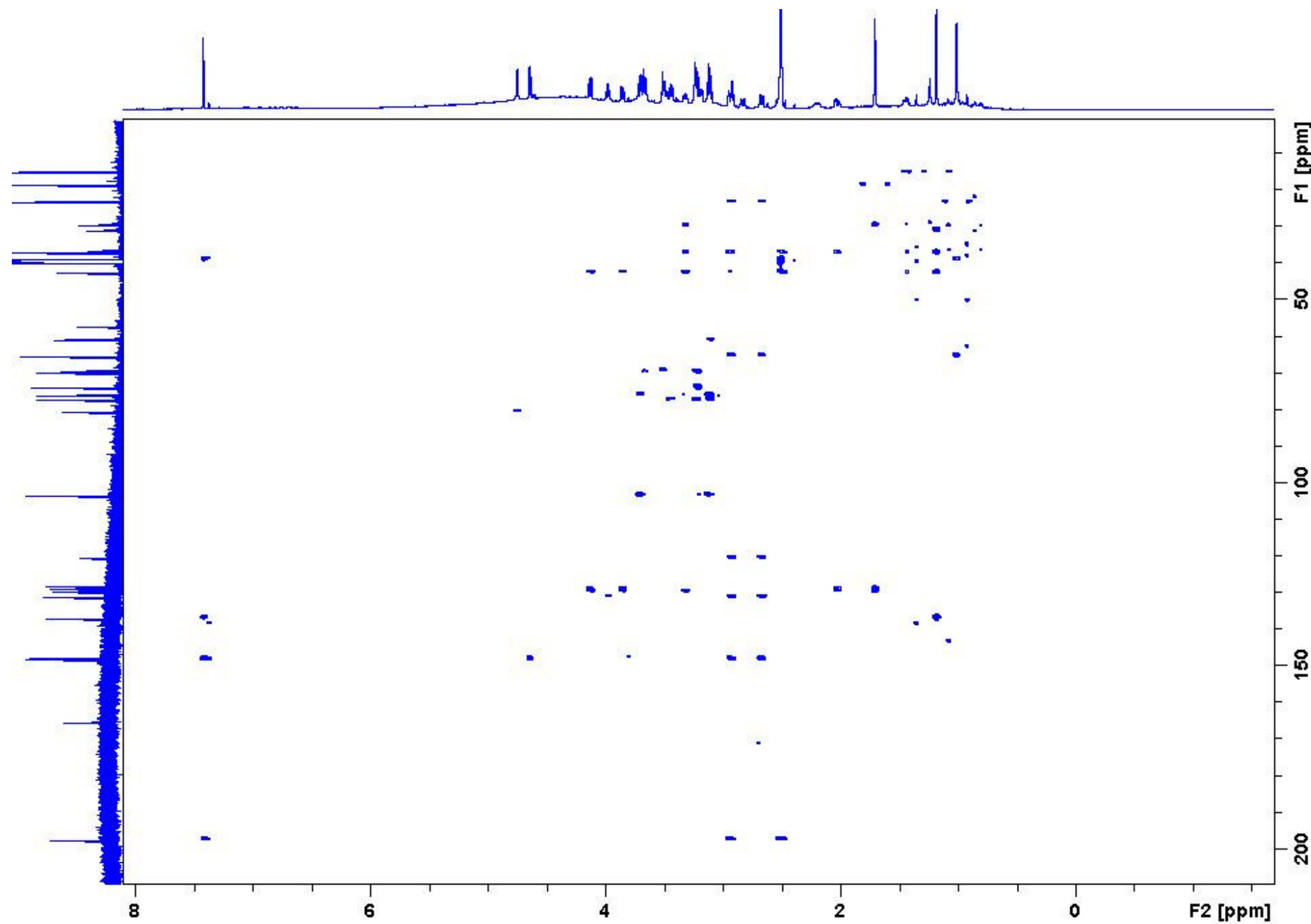
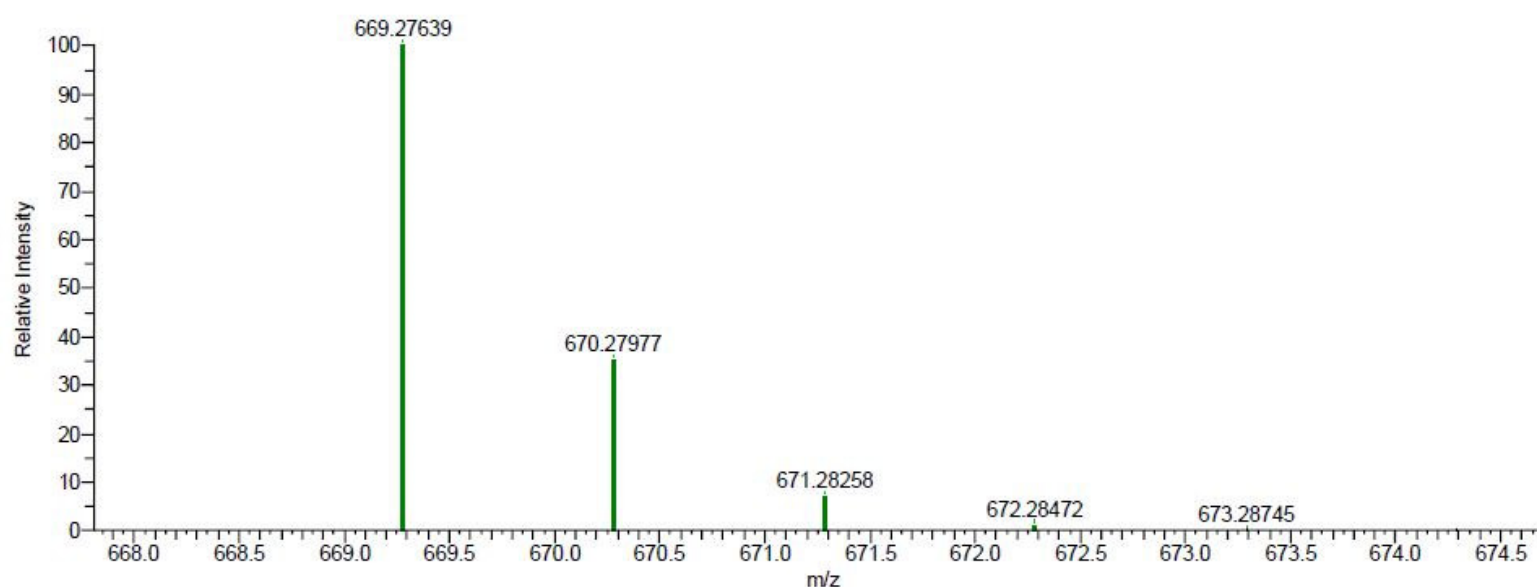
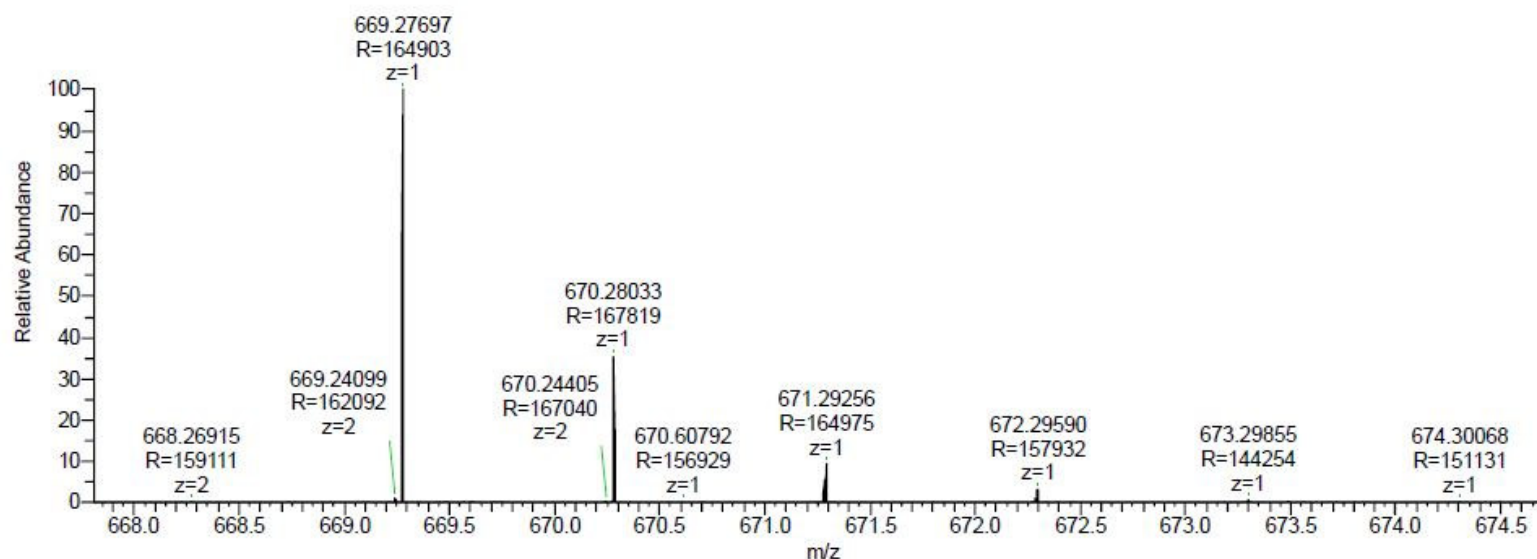


Figure S5-B. HMBC spectrum of compound **1** in  $\text{DMSO}-d_6$ .

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Figure S6. HR mass spectrum of compound 1 in methanol.

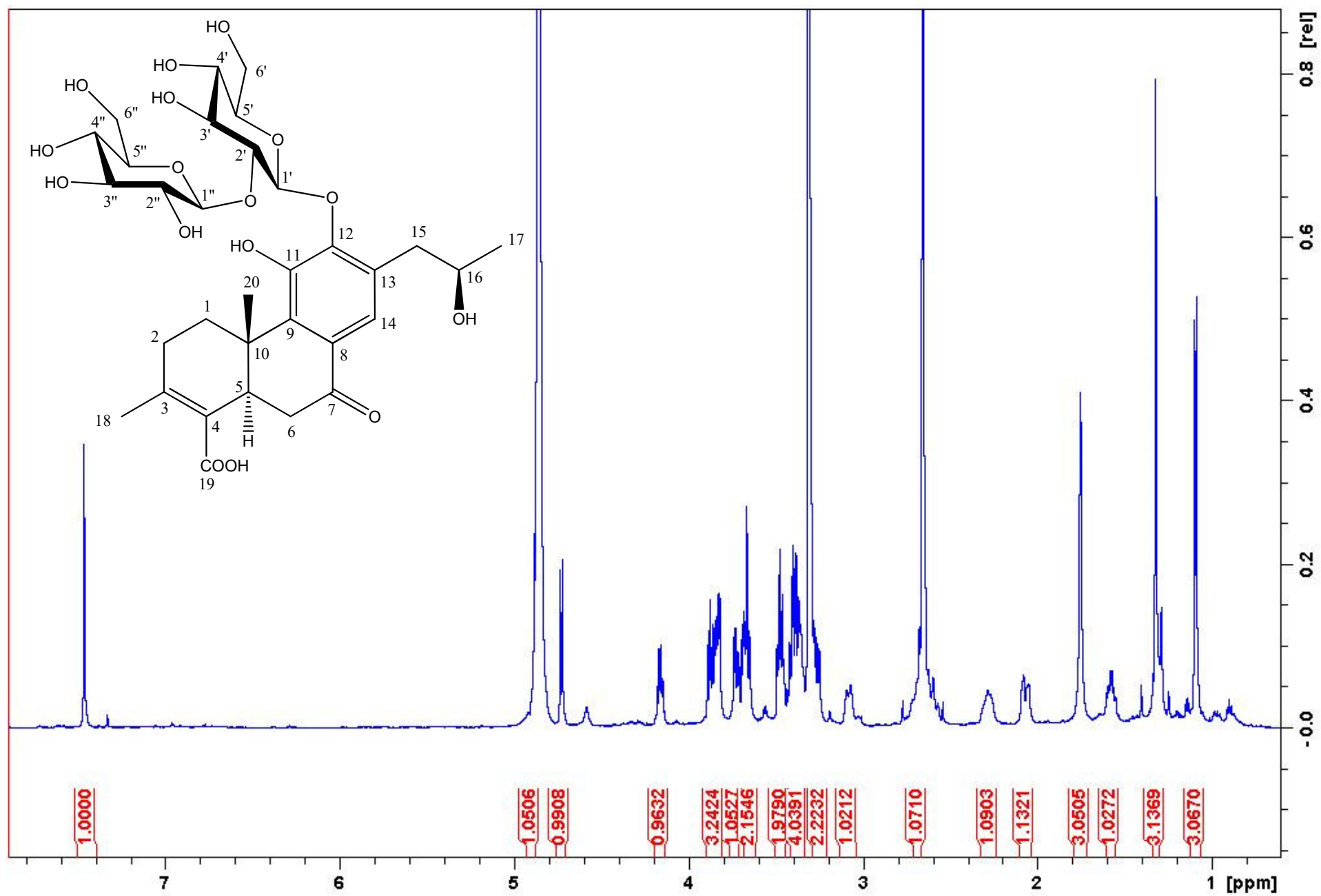


Figure S7-A.  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{Methanol-}d_4$ .

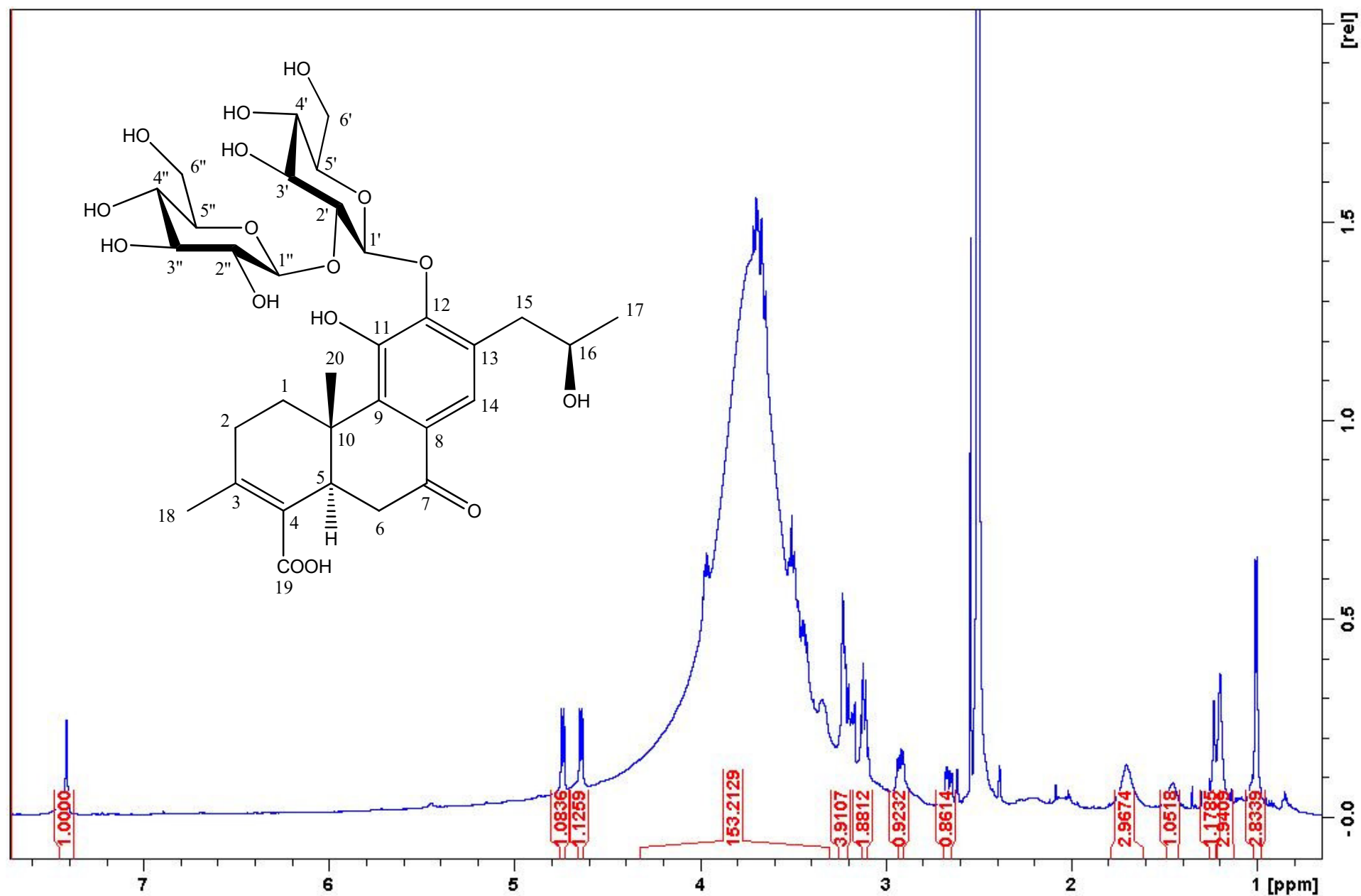


Figure S7-B.  $^1\text{H}$  NMR spectrum of compound **2** in  $\text{DMSO-}d_6$ .

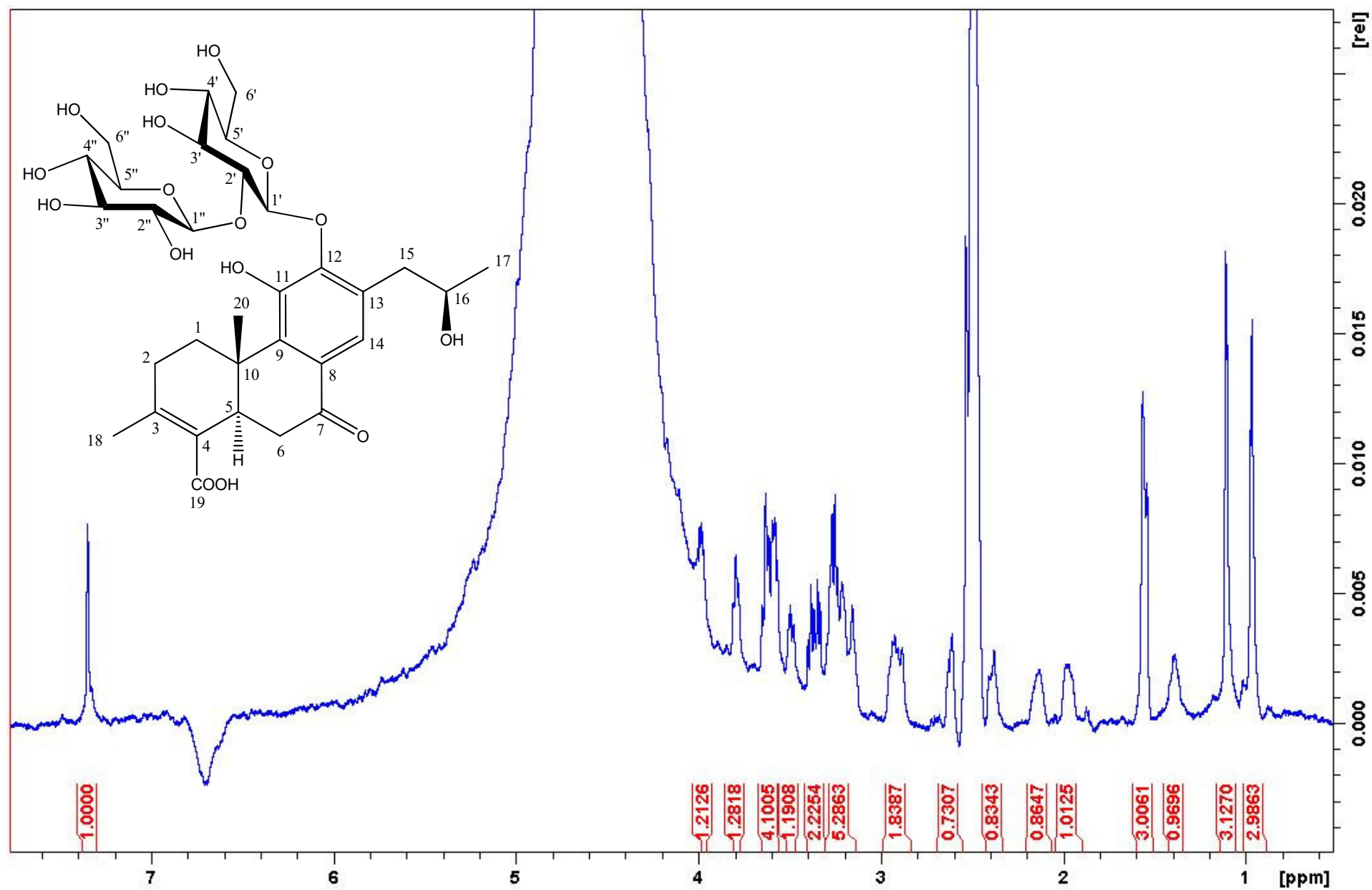
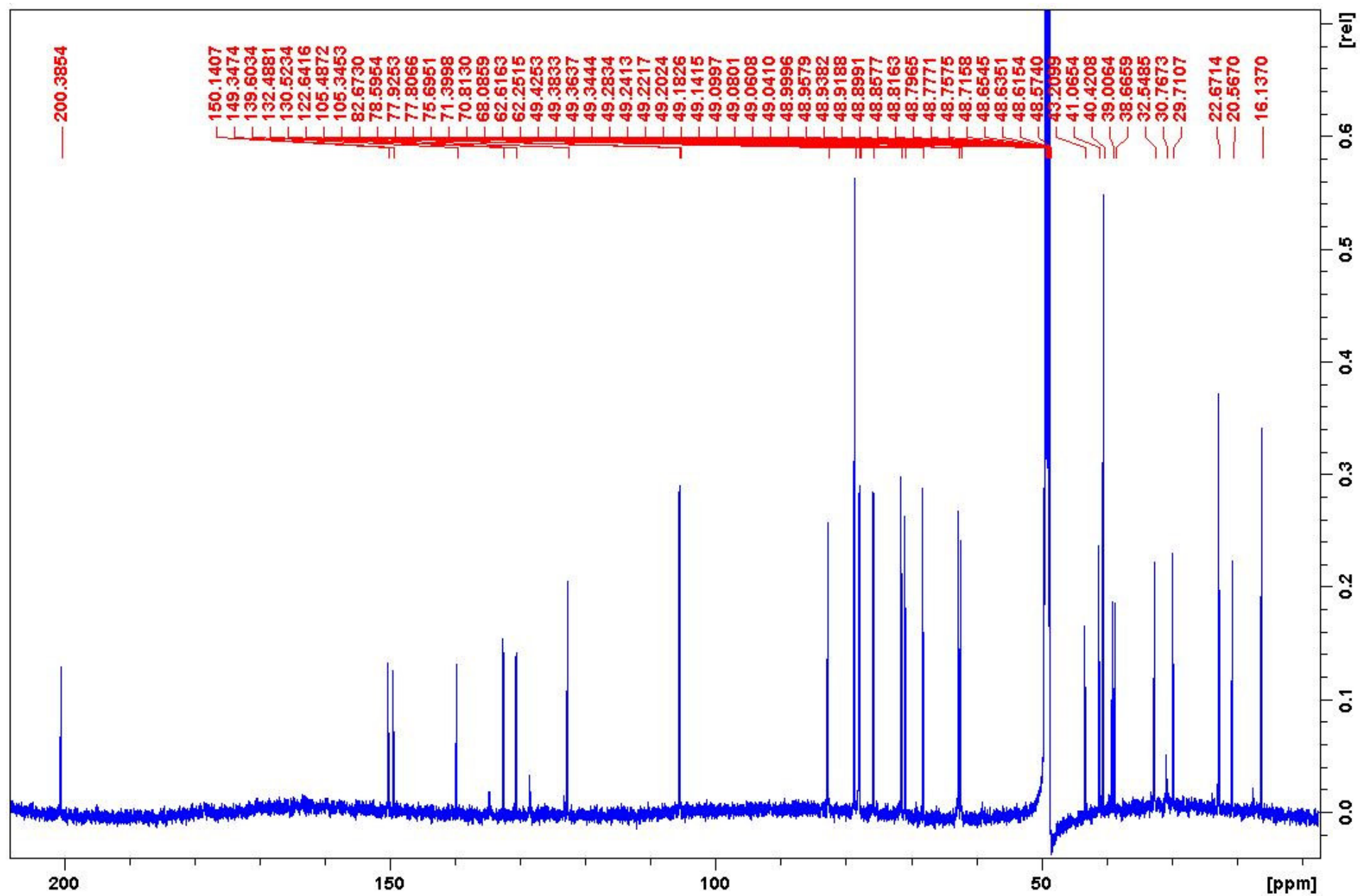


Figure S7-C.  $^1\text{H}$  NMR spectrum of compound 2 in  $\text{D}_2\text{O}$ .





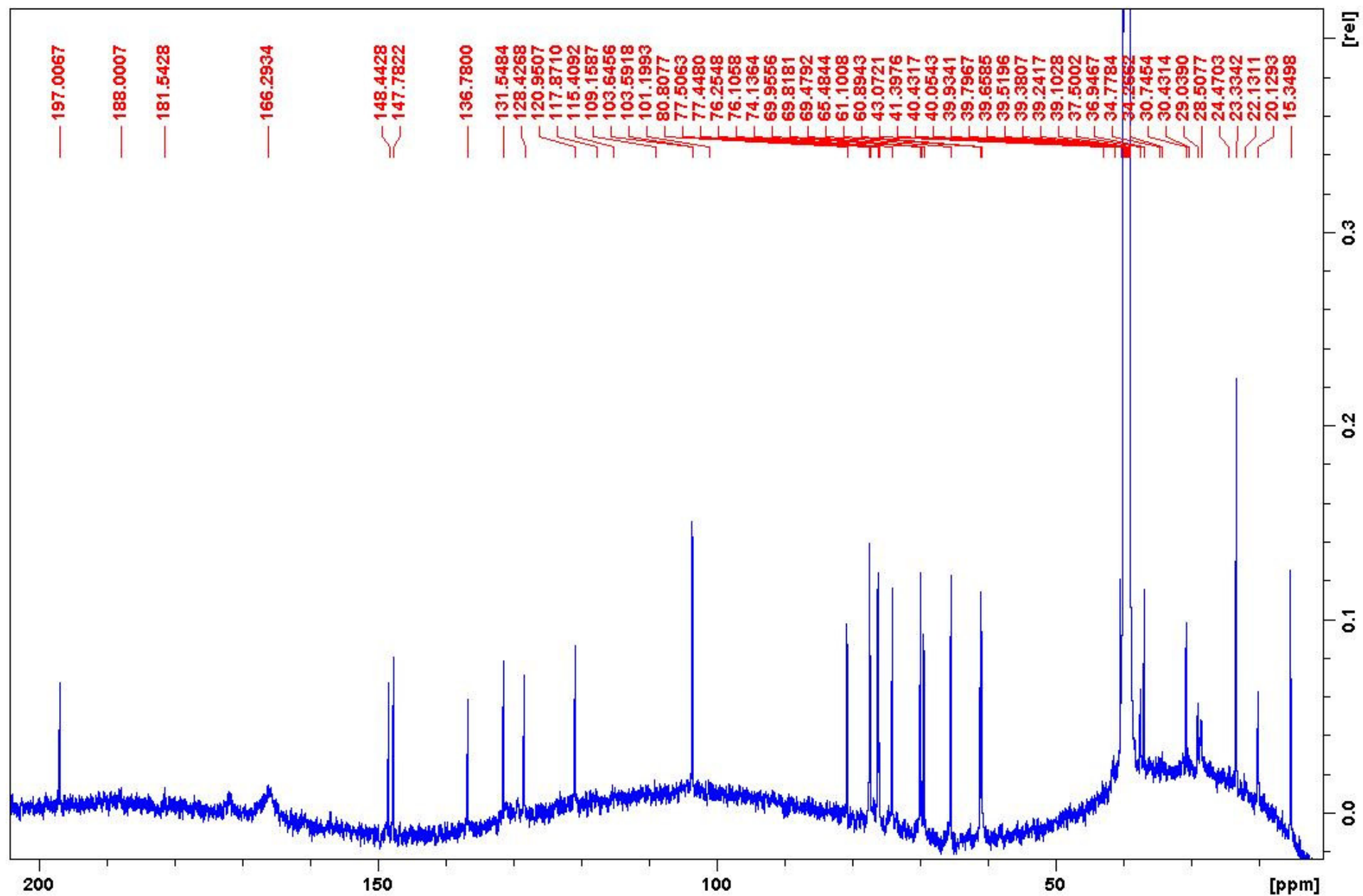
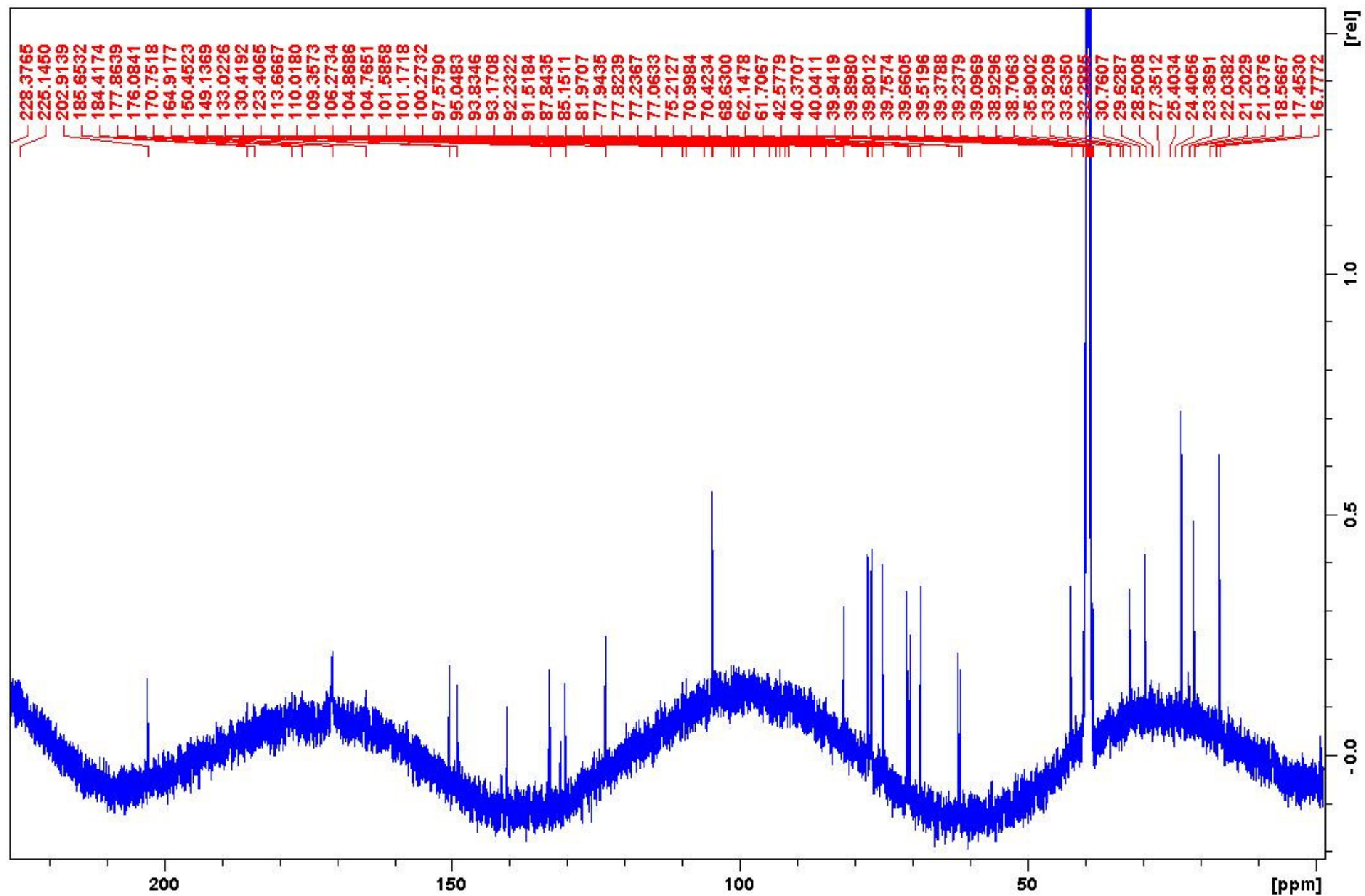


Figure S8-B. <sup>13</sup>C NMR spectrum of compound 2 in DMSO-*d*<sub>6</sub>.

Figure S8-C. <sup>13</sup>C NMR spectrum of compound **2** in D<sub>2</sub>O.

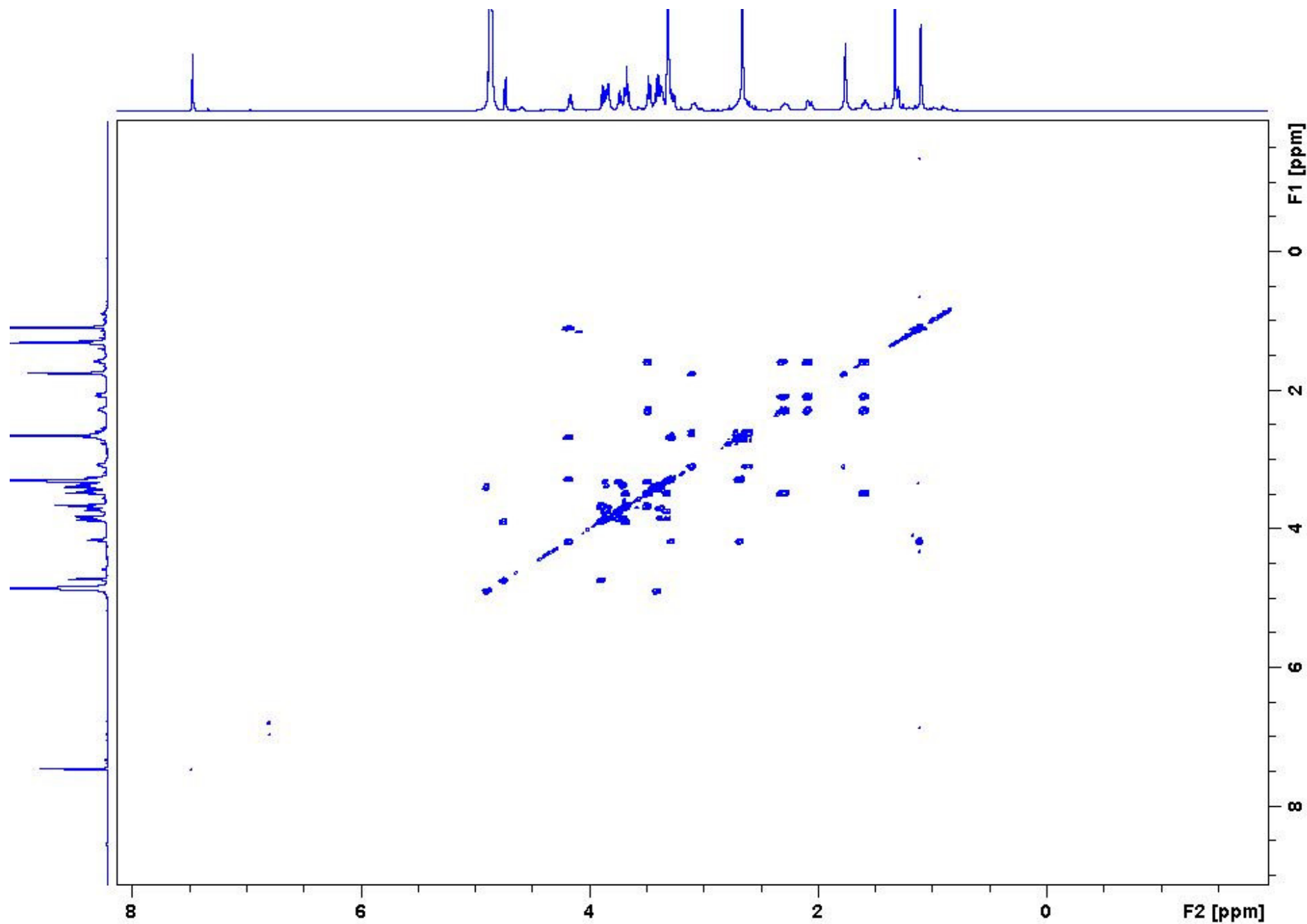


Figure S9-A. COSY spectrum of compound **2** in Methanol- $d_4$ .

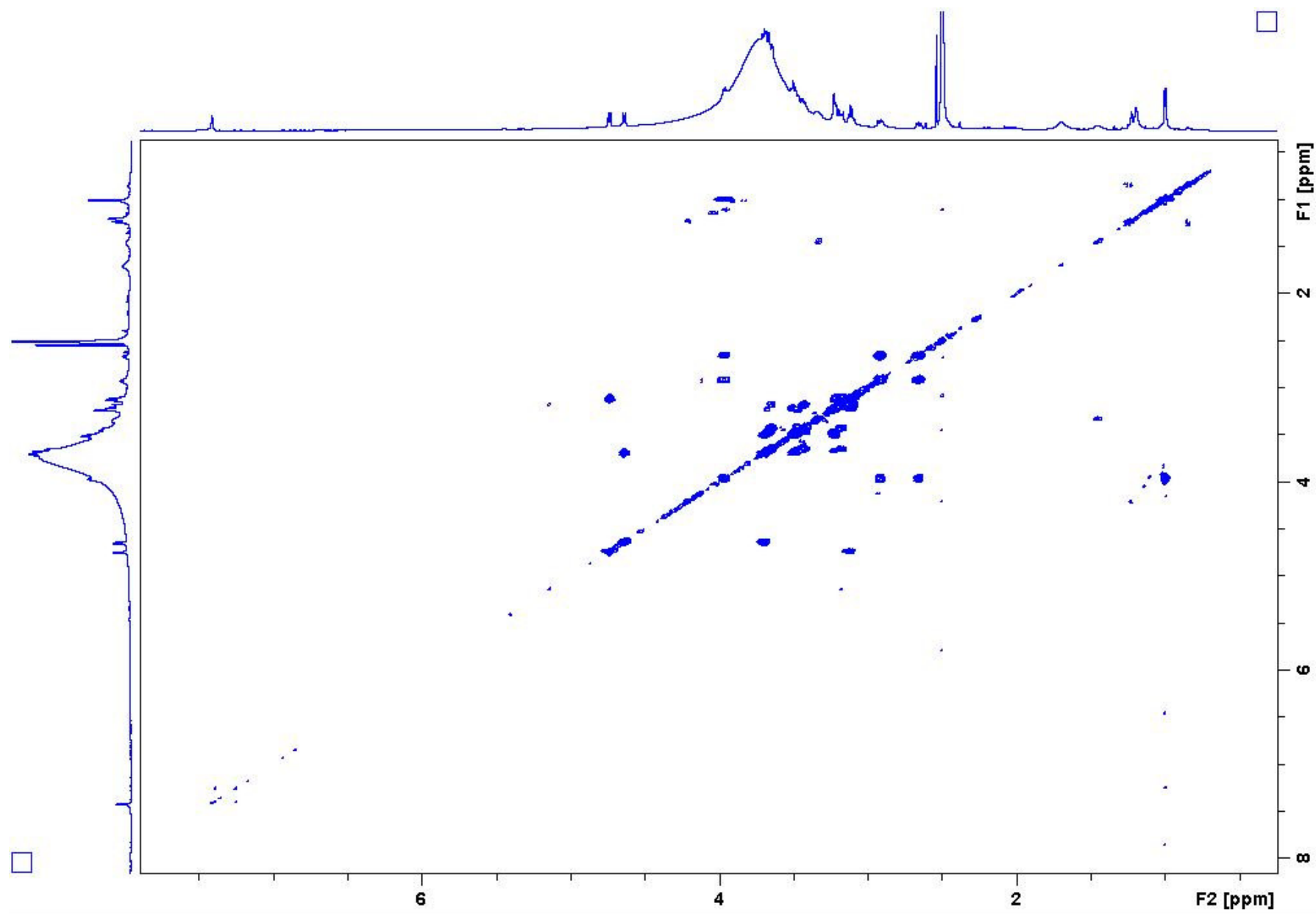


Figure S9-B. COSY spectrum of compound 2 in DMSO- $d_6$ .

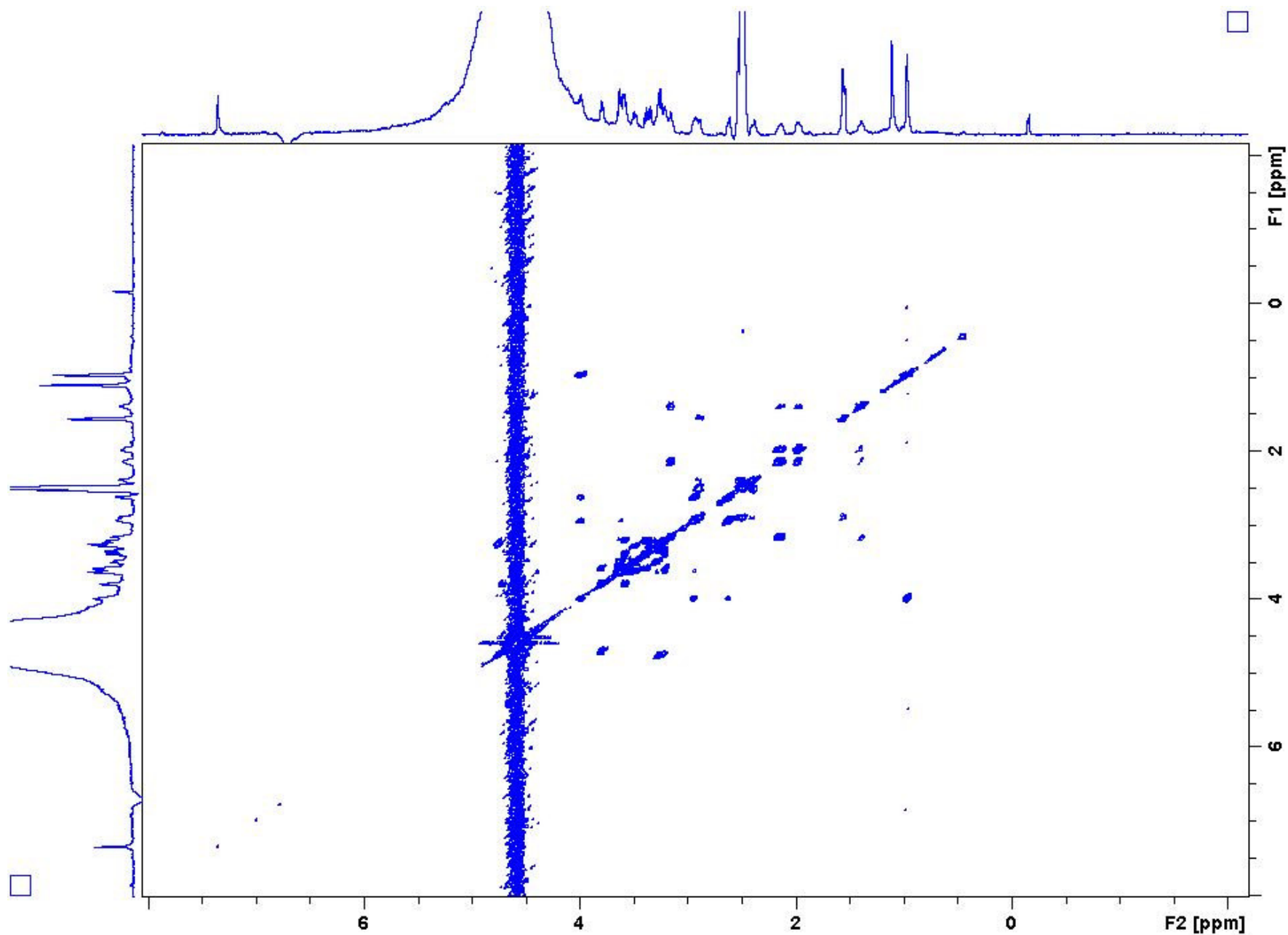


Figure S9-C. COSY spectrum of compound **2** in D<sub>2</sub>O.

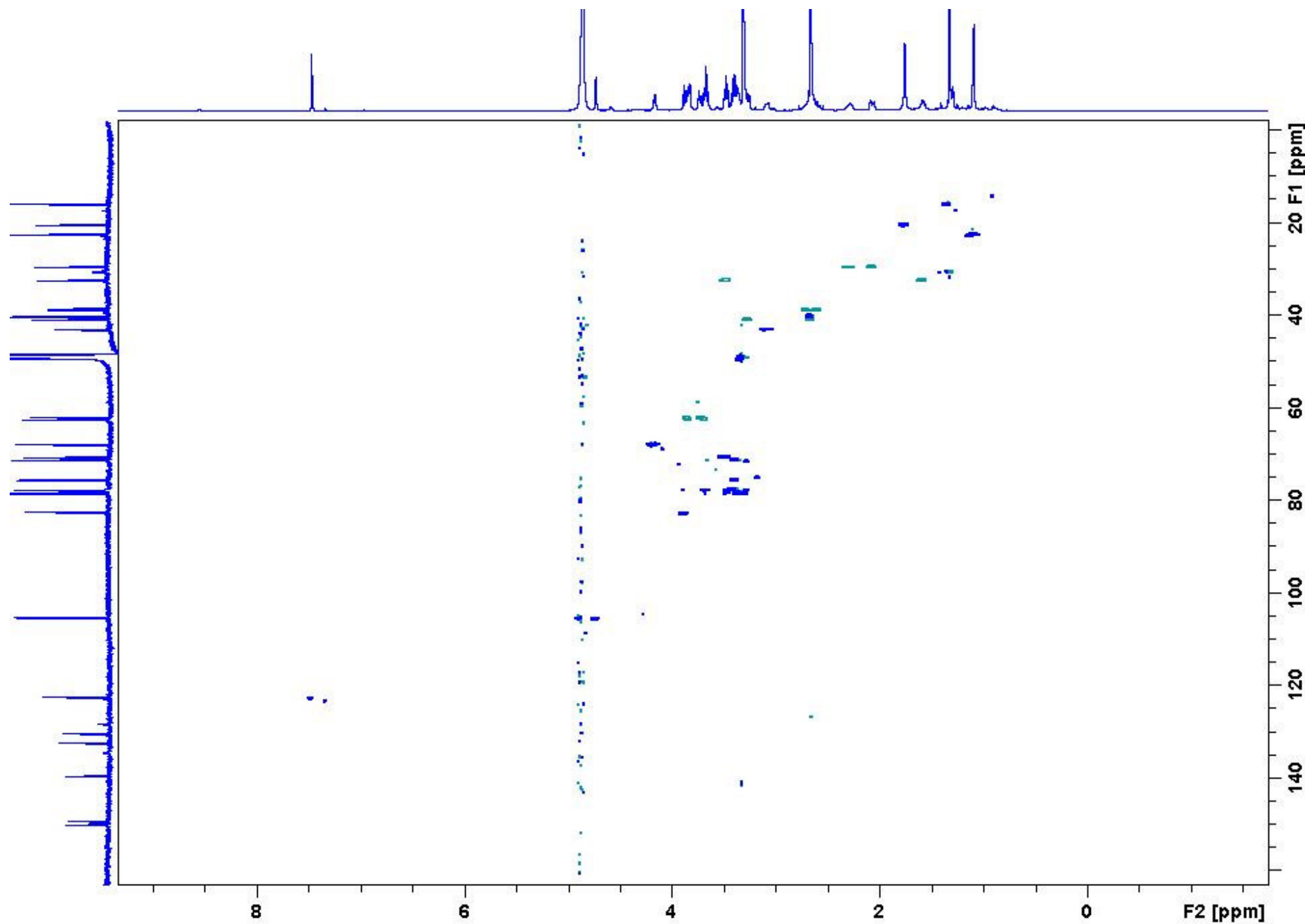


Figure S10-A. HSQC spectrum of compound 2 in Methanol- $d_4$ .



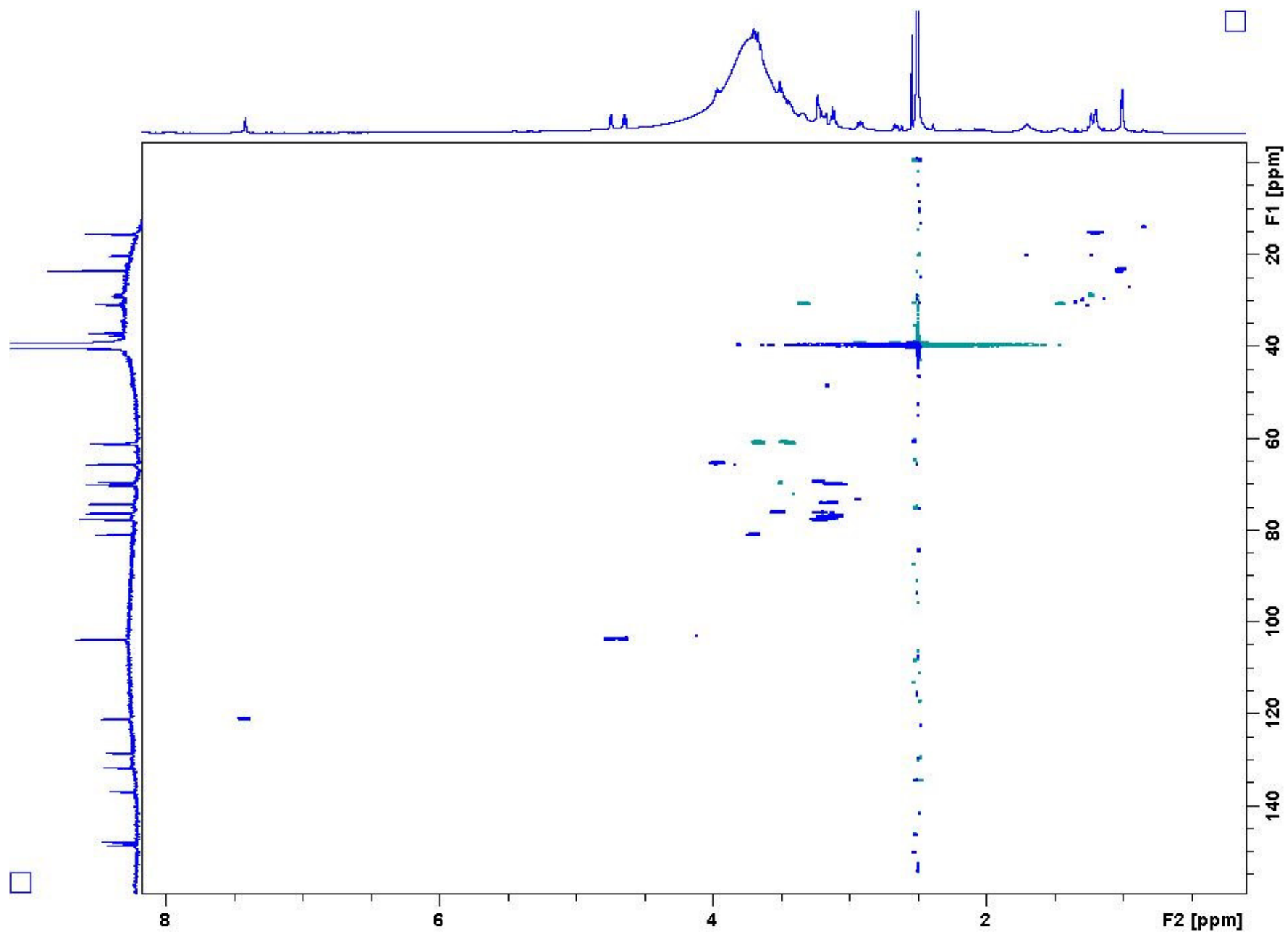


Figure S10-B. HSQC spectrum of compound **2** in DMSO- $d_6$ .



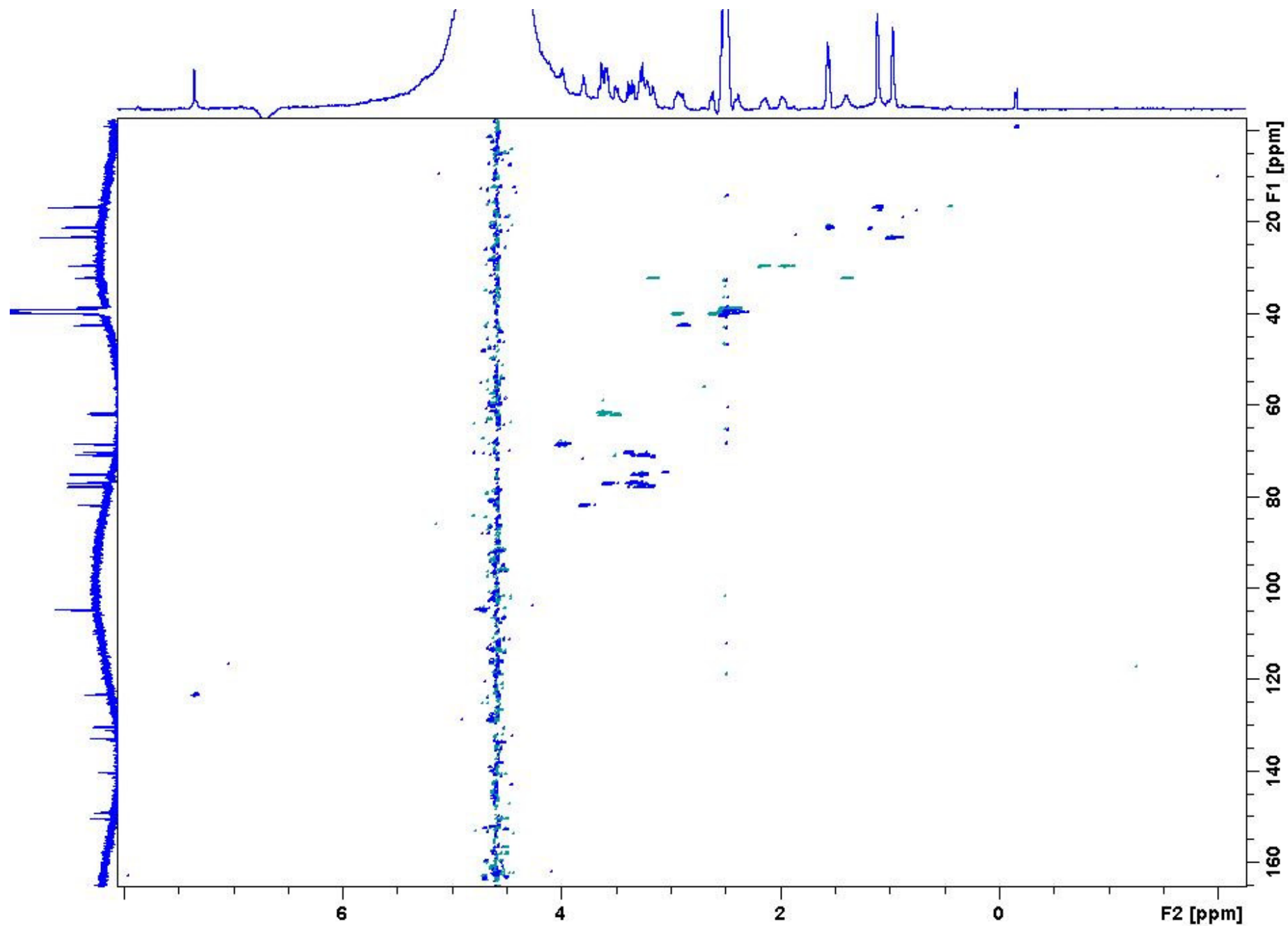


Figure S10-C. HSQC spectrum of compound **2** in  $\text{D}_2\text{O}$ .

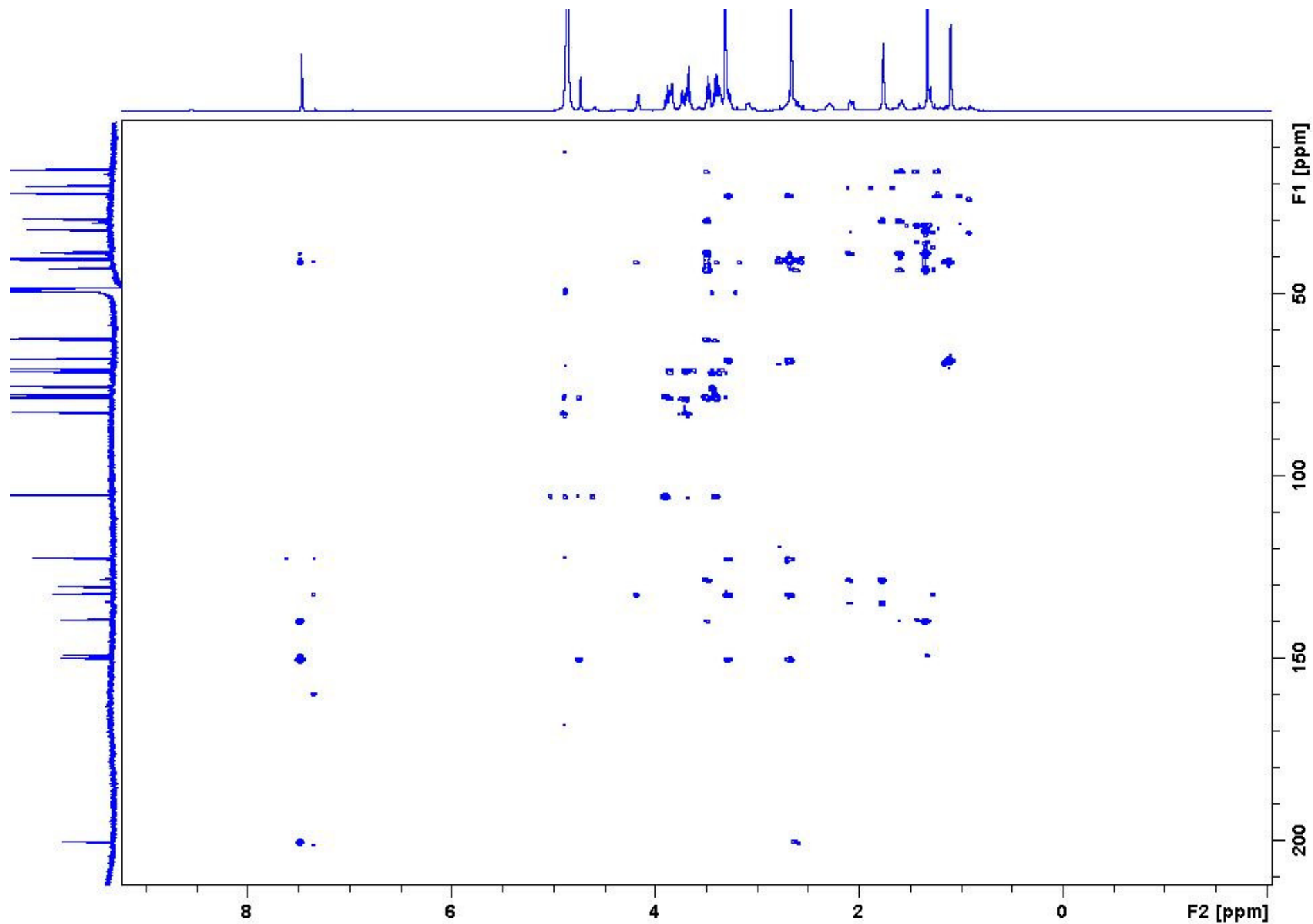


Figure S11-A. HMBC spectrum of compound **2** in Methanol- $d_4$ .

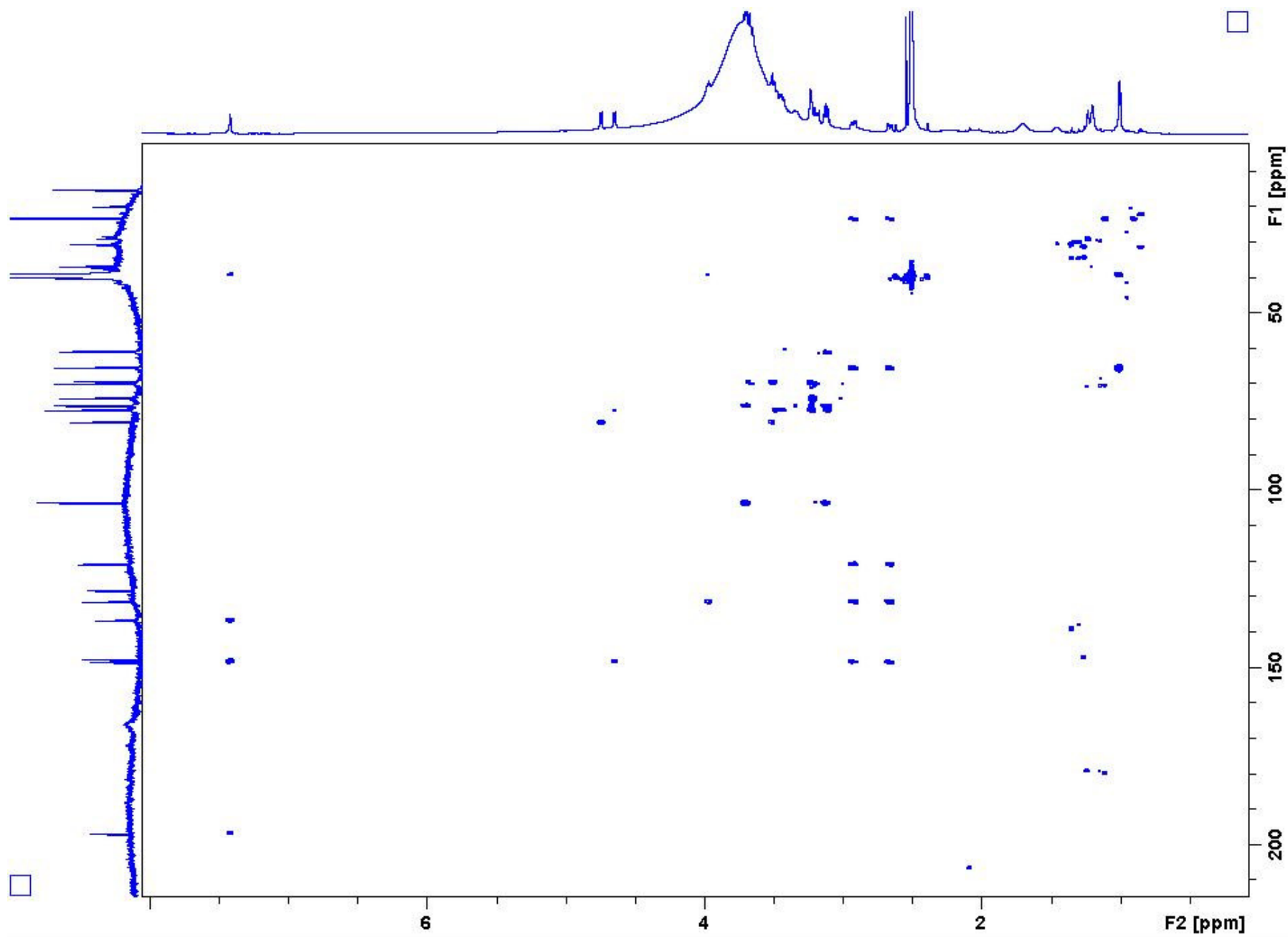


Figure S11-B. HMBC spectrum of compound **2** in DMSO- $d_6$ .

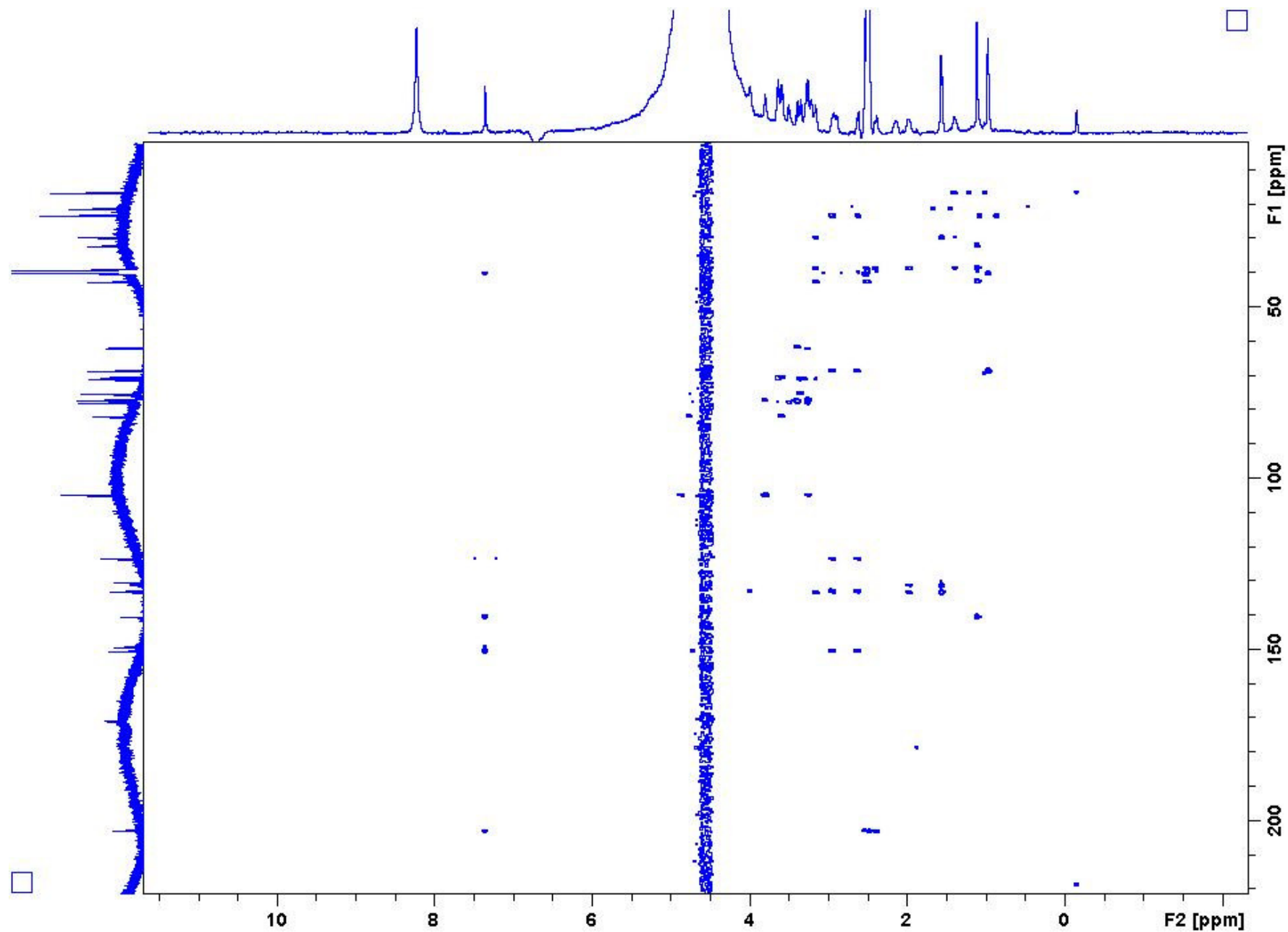
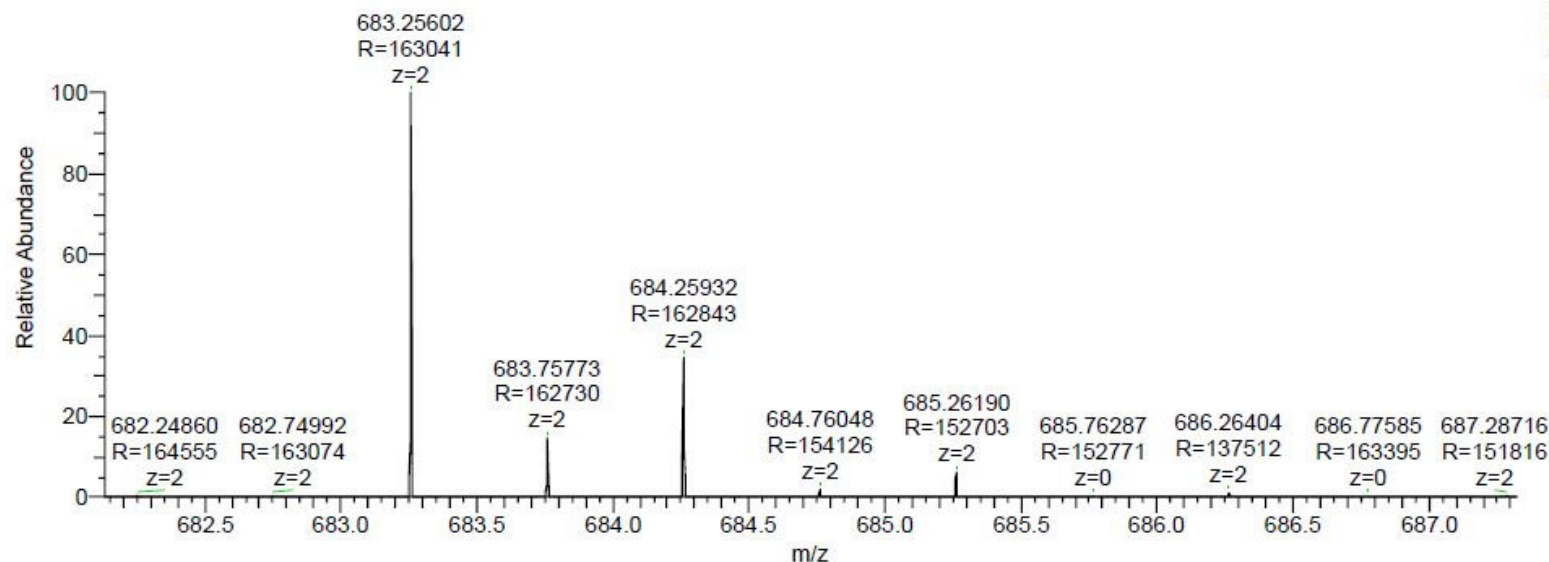


Figure S11-C. HMBC spectrum of compound 2 in D<sub>2</sub>O.

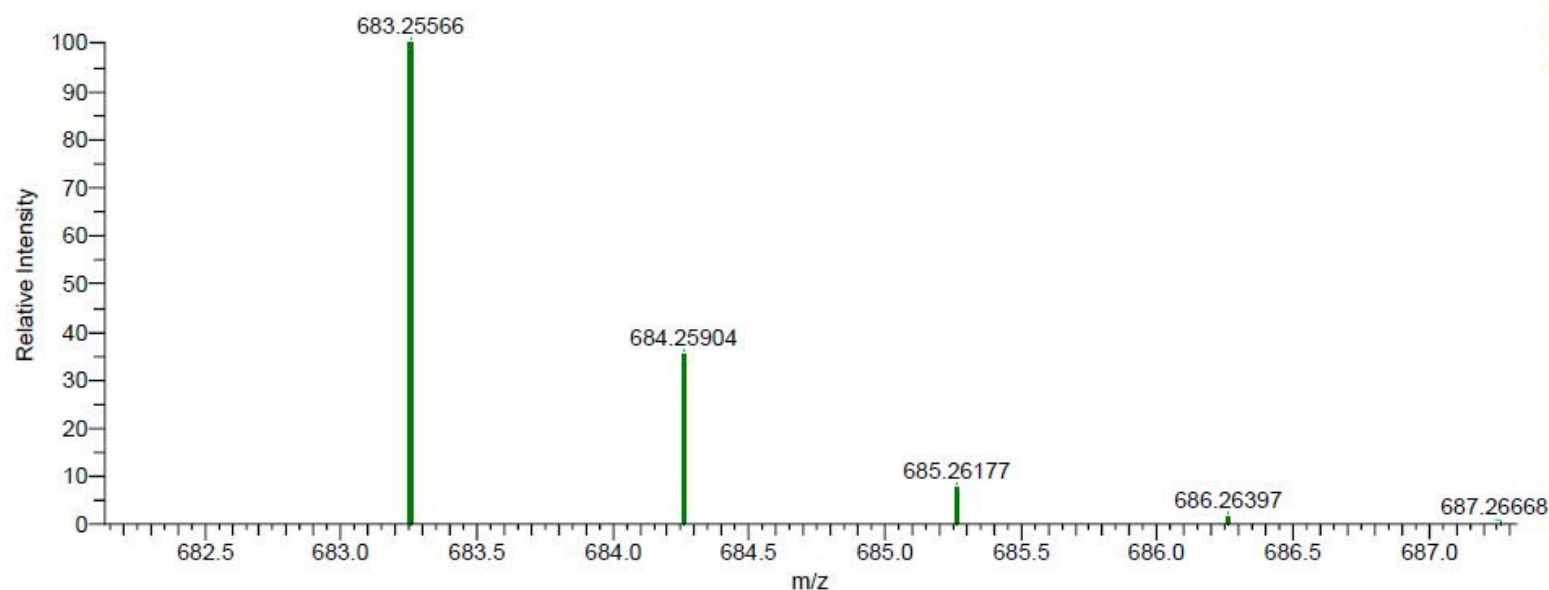
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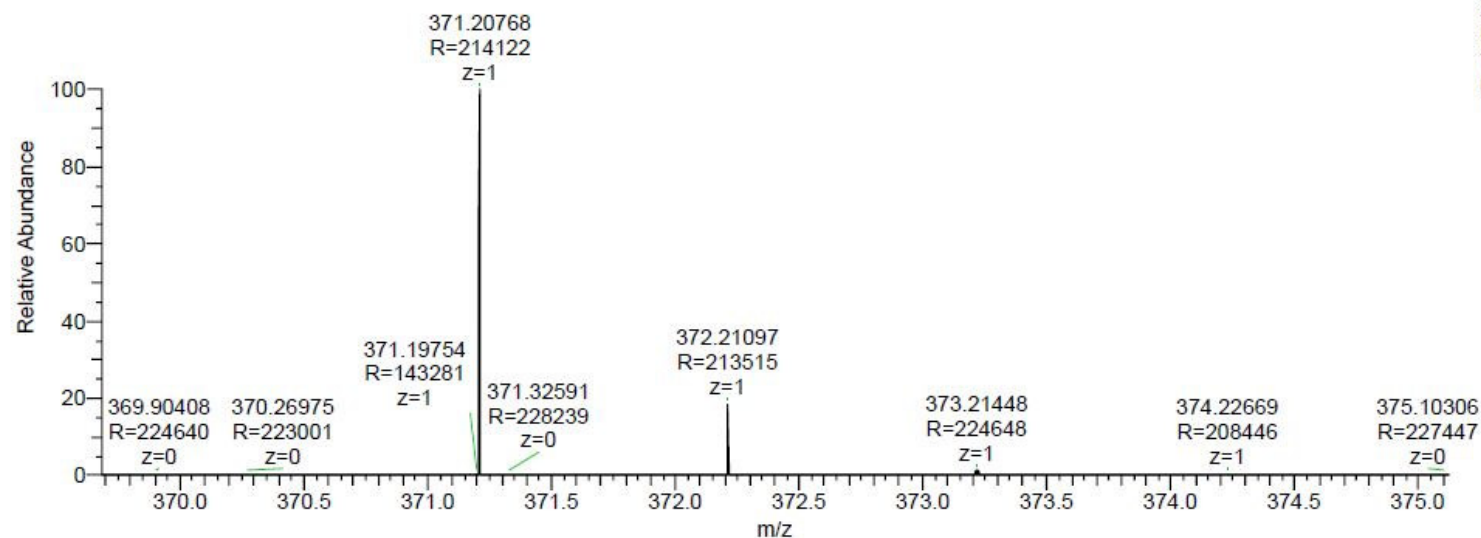
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Figure S12. HR mass spectrum of compound **2** in methanol.

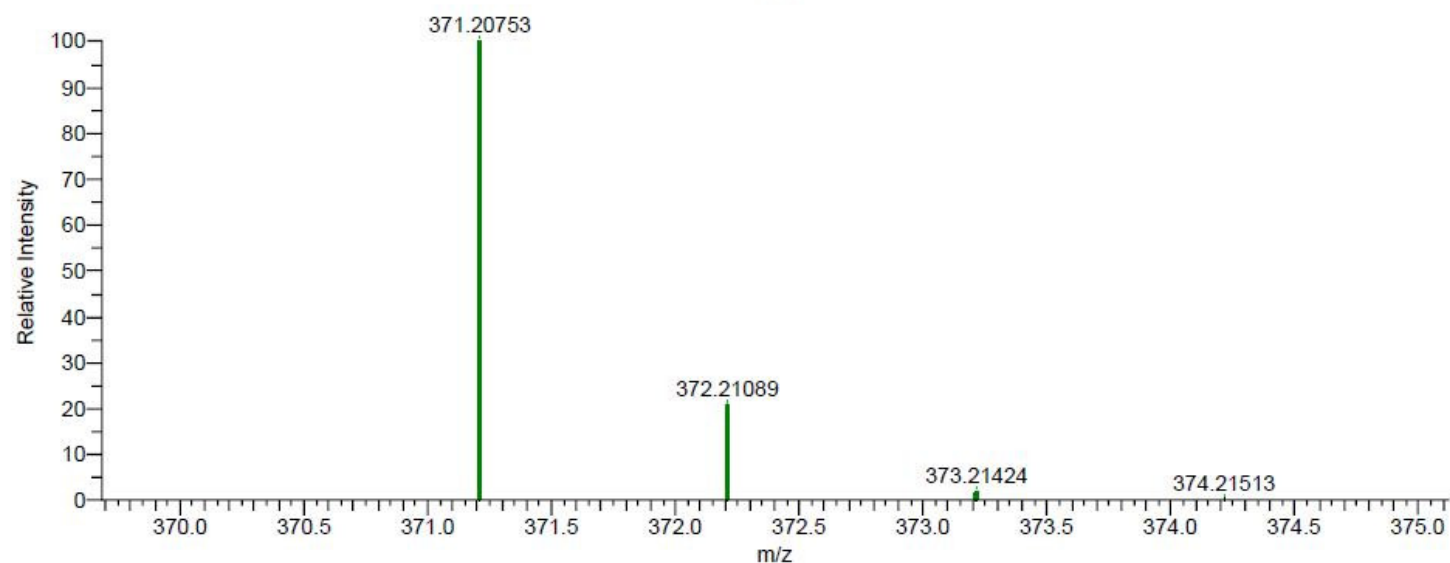
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 @FWHM



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Figure S13. HR mass spectrum of compound **3** in methanol.

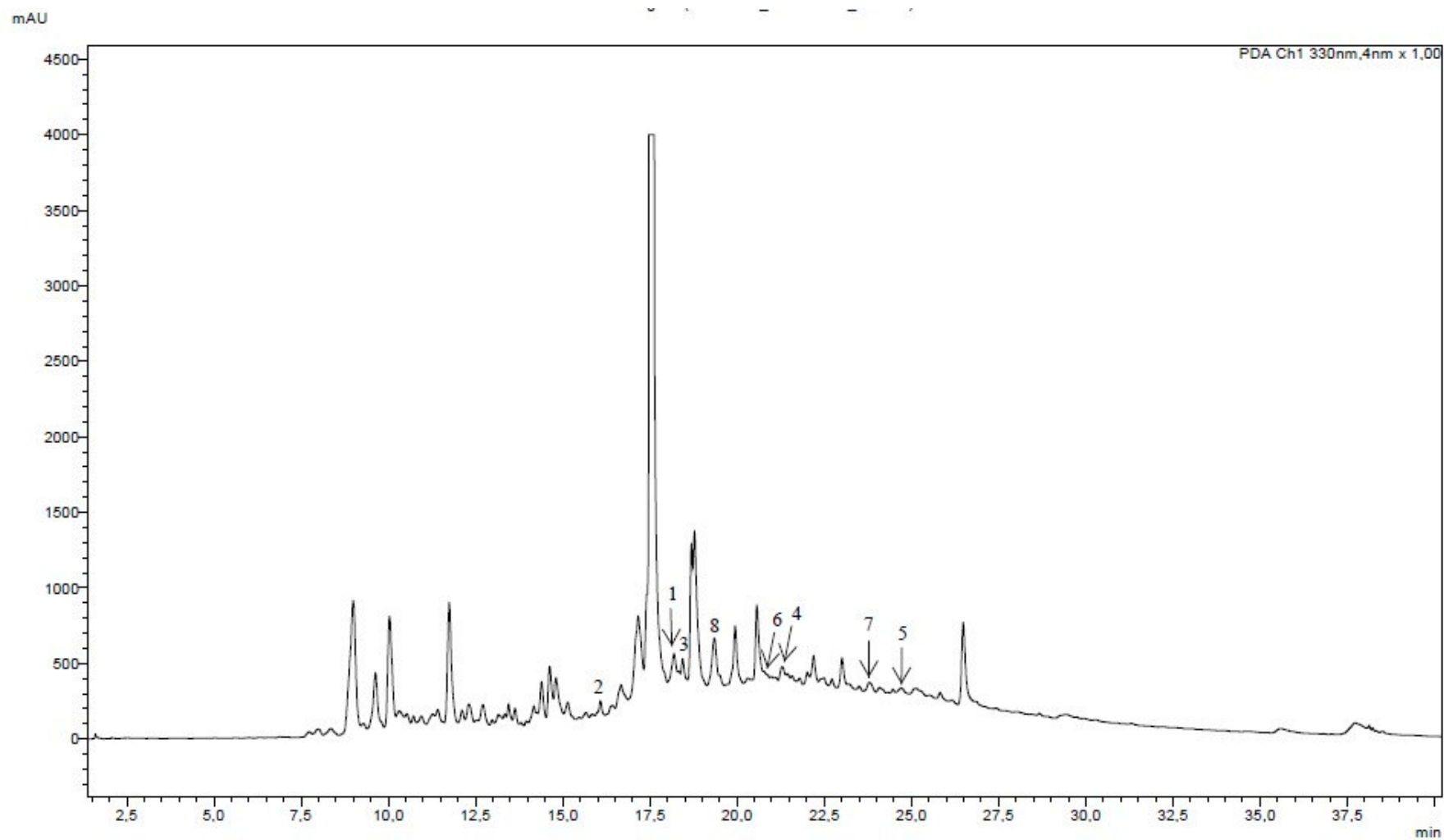


Figure S14. UHPLC ( $\lambda = 330$  nm) chromatogram of *n*-butanol fraction from leaves of *Clerodendrum infortunatum*.

Table S1. 1D ( $^1\text{H}$  and  $^{13}\text{C}$ ) NMR spectroscopic data for compound **3**

	<b>3<sup>a</sup></b>	<b>3<sup>b</sup></b>	<b>3<sup>a</sup></b>	<b>3<sup>b</sup></b>
Position	$\delta_{\text{C}}$ , type	$\delta_{\text{C}}$ , type	$\delta_{\text{H}}$ ( $J$ in Hz)	$\delta_{\text{H}}$ ( $J$ in Hz)
cyclohexanone moiety				
1	37.3, C	35.9, C		
2	48.1, CH <sub>2</sub>	47.0, CH <sub>2</sub>	1.97, d (17.5) 2.46, d (17.5)	1.87, d (17.5) 2.34, d (17.5)
3	202.4, C	198.1, C		
4	125.4, CH	124.2, CH	5.80, s	5.72, s
5	170.1, C	166.1, C		
6	52.4, CH	50.1, CH	1.99, m <sup>b</sup>	1.90, t (5.0)
7	26.8, CH <sub>2</sub>	25.1, CH <sub>2</sub>	1.50, m 1.98, m <sup>b</sup>	1.38, m 1.78, m
8	37.8, CH <sub>2</sub>	36.2, CH <sub>2</sub>	1.61, m 1.67, m	1.50, m
9	75.5, CH	73.3, CH	3.88, m	3.74, dd (12.0, 6.0)
10	19.9, CH <sub>3</sub>	19.5, CH <sub>3</sub>	1.18, d (6.0)	1.1, d (6.0)
11	29.1, CH <sub>3</sub>	26.8, CH <sub>3</sub>	1.01, s	1.00, s
12	27.5, CH <sub>3</sub>	28.5, CH <sub>3</sub>	1.09, s	0.97, s
13	25.0, CH	24.1, CH	2.05, d (1.0)	1.97, m
glucopyranosyl moiety				
1'	102.1, CH	100.7, CH	4.32, d (8.0)	4.16, d (8.0)
2'	75.2, CH	73.5, CH	3.14, dd (9.0, 8.0)	2.89, t (8.5)
3'	78.2, CH	76.9, CH	3.35, dd (9.0, 9.0)	3.12, t (8.5)
4'	71.8, CH	70.3, CH	3.26, m	3.03, m
5'	77.9, CH	76.8, CH	3.25, m	3.05, m
6'	62.9, CH <sub>2</sub>	61.3, CH <sub>2</sub>	3.64, dd (12.00, 5.5) 3.85, dd (12.00, 2.0)	3.41, m 3.64, m

<sup>a</sup>Spectra were referenced to solvent residual and solvent signals of CD<sub>3</sub>OD at 3.31 ppm ( $^1\text{H}$  NMR, 600 MHz) and 49.0 ppm ( $^{13}\text{C}$  NMR, 150 MHz), respectively.

<sup>b</sup>Spectra were referenced to solvent residual and solvent signals of (CD<sub>3</sub>)<sub>2</sub>SO at 2.50 ppm ( $^1\text{H}$  NMR, 600 MHz) and 39.52 ppm ( $^{13}\text{C}$  NMR, 150 MHz), respectively.