

## *Supporting Information*

# **Biotransformation of two guaiane-type sesquiterpene lactones with filamentous fungi and extremophile bacteria.**

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Table 1S: <sup>1</sup>H NMR and <sup>13</sup>C NMR Data of Compounds **1**, **3–6** in CDCl<sub>3</sub><sup>a</sup>

	<b>1</b>		<b>3</b>		<b>4</b>		<b>5</b>		<b>6</b>	
Position	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)	$\delta_C$	$\delta_H$ (J in Hz)
<b>1</b>	133.8	-	134.5	-	133.5	-	134.4	-	85.9	-
<b>2a</b>	33.6	2.71 brd (17.7)	39.3	2.83 m	33.5	2.64 brd (17.5)	39.1	2.80 m	44.1	2.60 dd (14.7,3.8)
<b>2b</b>		2.44 dq (17.7,1.7)		2.36 d (17.3)		2.36 brd (17.5)		2.35 brd (16.5)		1.64 d (14.7)
<b>3</b>	63.8	3.38 brs	79.0	3.87 brd (4.0)	63.8	3.31 brs	79.0	3.84 d (4.0)	83.0	3.82 brs
<b>4</b>	67.1	-	83.1	-	67.2	-	83.1	-	81.9	-
<b>5</b>	52.5	3.09 brd (10.7)	51.5	2.78 m	51.9	2.93 brd (10.8)	53.7	2.73 m	64.2	2.50 m
<b>6</b>	80.7	3.64 dd (10.5,10.0)	82.9	3.95 t (10.1)	80.5	3.58 t (10.2)	82.5	3.94 t (10.0)	80.9	4.62 dd (10.7,9.5)
<b>7</b>	54.5	2.77 m	54.2	2.83 m	57.7	1.78 m	55.2	1.85 m	44.8	2.88 m
<b>8a</b>	25.8	2.12 m	25.8	2.08 m	27.5	1.80 m	27.2	1.86 m	24.6	1.89 m
<b>8b</b>		1.30 m		1.33 m		1.13 m		1.26 m		1.61 m
<b>9a</b>	33.9	2.25 brt (13.5)	34.4	2.28 brd (14.0)	34.3	2.10 m	34.6	2.18 m	35.1	2.29 td (14.1,4.0)
<b>9b</b>		2.06 m		2.19 ddd (14.0,5.4,2.2)		1.98 ddd (14.2,5.6,1.1)		2.11 m		1.56 m
<b>10</b>	134.9	-	132.3	-	135.3	-	132.6	-	76.9	-
<b>11</b>	139.4	-	139.3	-	41.3	2.13 m	41.6	2.22 m	139.4	-
<b>12</b>	169.5	-	170.0	-	177.7	-	178.5	-	170.6	-
<b>13a</b>	117.8	6.12 d (3.3)	118.8	6.17 d (3.2)	12.3	1.16 d (7.0)	12.3	1.23 d (7.0)	118.9	6.15 d (3.5)
<b>13b</b>		5.38 d (3.0)		5.45 d (3.2)						5.44 d (3.1)
<b>14</b>	22.6	1.66 brs	24.1	1.75 brs	22.6	1.62 brs	23.8	1.73 brs	22.0	1.28 s
<b>15</b>	19.0	1.69 brs	23.9	1.59	19.1	1.57 s	24.0	1.55	28.8	1.48 s

<sup>a</sup>Chemical shifts ( $\delta$ ) downfield from TMS, *J* couplings (in parentheses) in Hz run at 400.13 MHz.

Table 2S: <sup>1</sup>H NMR and <sup>13</sup>C NMR Data of Compounds **2**, **7–9** in CDCl<sub>3</sub><sup>a</sup>

	<b>2</b>		<b>7</b>		<b>8</b>		<b>9</b>	
Position	$\delta_c$	$\delta_H$ (J in Hz)	$\delta_c$	$\delta_H$ (J in Hz)	$\delta_c$	$\delta_H(\text{ppm})$ (J in Hz)	$\delta_c$	$\delta_H(\text{ppm})$ (J in Hz)
<b>1</b>	44.9	2.98 ddd (10.5,8.5,7.5)	44.4	3.11 m	44.2	2.79 c (7.8)	44.4	3.07 m
<b>2a</b>	33.0	2.07 dd (14.0,7.5)	36.1	2.30 m	32.6	2.01 m	36.0	2.27 m
<b>2b</b>		1.81 ddd (14.0,10.5,1.2)		1.72 ddd (13.4,6.9,0.9)		1.70 dd (13.2,10.9)		1.70 m
<b>3</b>	63.2	3.38 brs	80.6	3.89 brd (3.6)	63.1	3.27 s	80.4	3.86 brd (3.1)
<b>4</b>	65.8	-	83.1	-	66.0	-	82.7	-
<b>5</b>	50.8	2.32 dd (11.0,8.5)	52.4	2.35 t (11.0)	50.4	2.18 m	52.3	2.23 m
<b>6</b>	80.5	4.08 dd (11.0,8.9)	82.6	4.18 dd (11.0,9.3)	80.7	3.87 t (10.2)	82.5	4.15 t (10.6)
<b>7</b>	44.1	2.87 m	48.4	2.72 m	49.9	1.81 m	52.7	1.79 m
<b>8a</b>	29.2	2.22 m	31.5	2.20 dd (13.1,3.9)	30.88	1.98 m	33.1	2.05 dd (13.1,3.7)
<b>8b</b>		1.53 m		1.32 dd (13.1,3.7)		1.26 dd (11.3,6.2)		1.21 m
<b>9a</b>	28.6	2.28 m	37.8	2.60 dt (13.0,3.9)	30.99	2.21 m	38.0	2.57 m
<b>9b</b>		2.19 m		1.88 td (13.0,3.7)		2.04 m		1.79 m
<b>10</b>	146.0	-	148.3	-	147.6	-	148.5	-
<b>11</b>	139.6	-	139.2	-	41.9	2.12 m	41.7	2.12 m
<b>12</b>	169.7	-	169.9	-	178.3	-	178.5	-
<b>13a</b>	120.2	6.21 d (3.6)	120.2	6.14 d (3.4)	13.2	1.12 d (6.8)	13.2	1.16 d (7.0)
<b>13b</b>		5.48 d (3.2)		5.43 d (3.1)				
<b>14a</b>	115.3	4.95 brs	112.8	4.89 brs	114.1	4.78 brs	112.12	4.85 brs
<b>14b</b>		4.86 d (1.7)				4.74 brs		4.85 brs
<b>15</b>	18.5	1.62 s	24.4	1.46 s	18.7	1.49 s	24.6	1.42 s

<sup>a</sup>Chemical shifts ( $\delta$ ) downfield from TMS, *J* couplings (in parentheses) in Hz run at 400.13 MHz

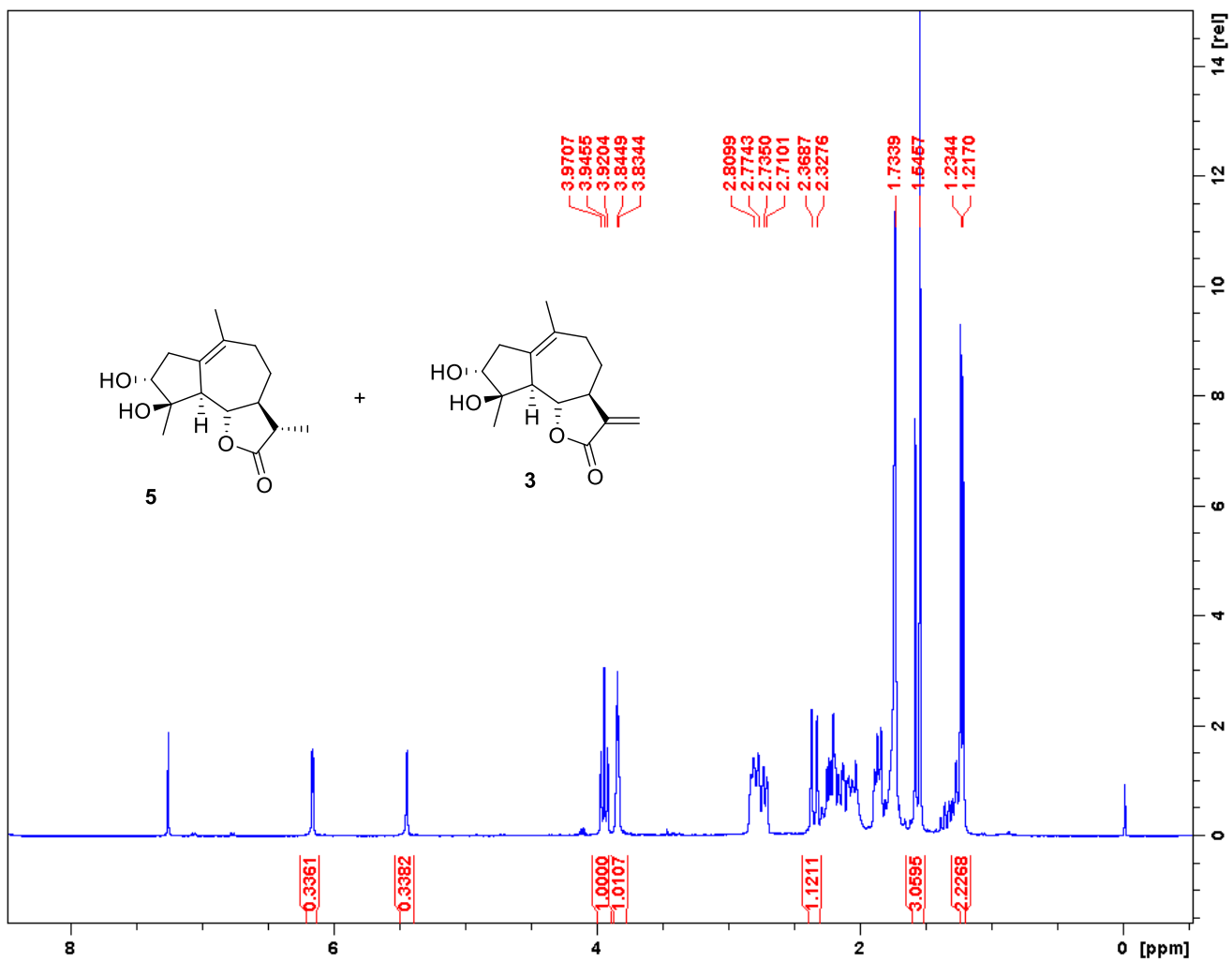
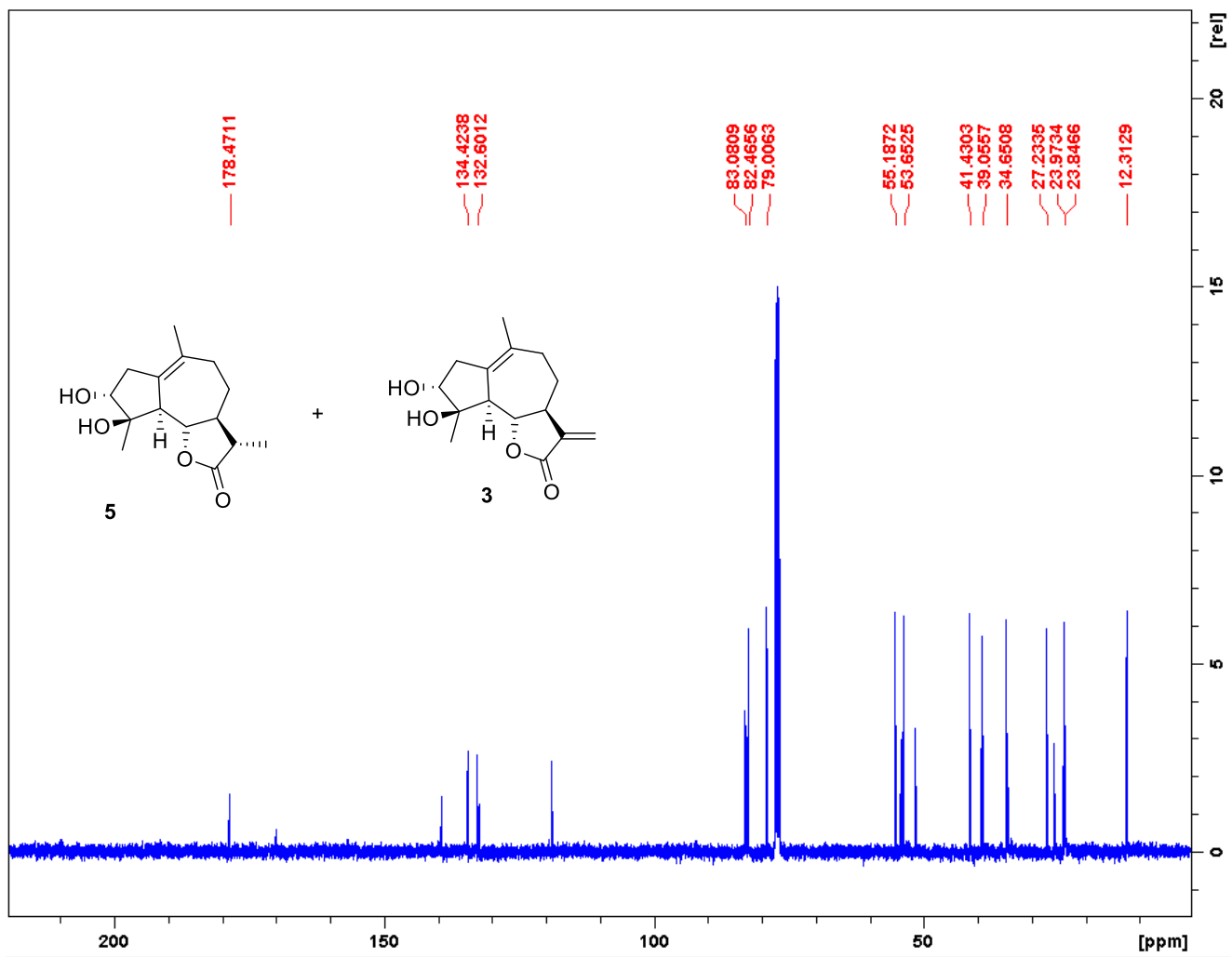
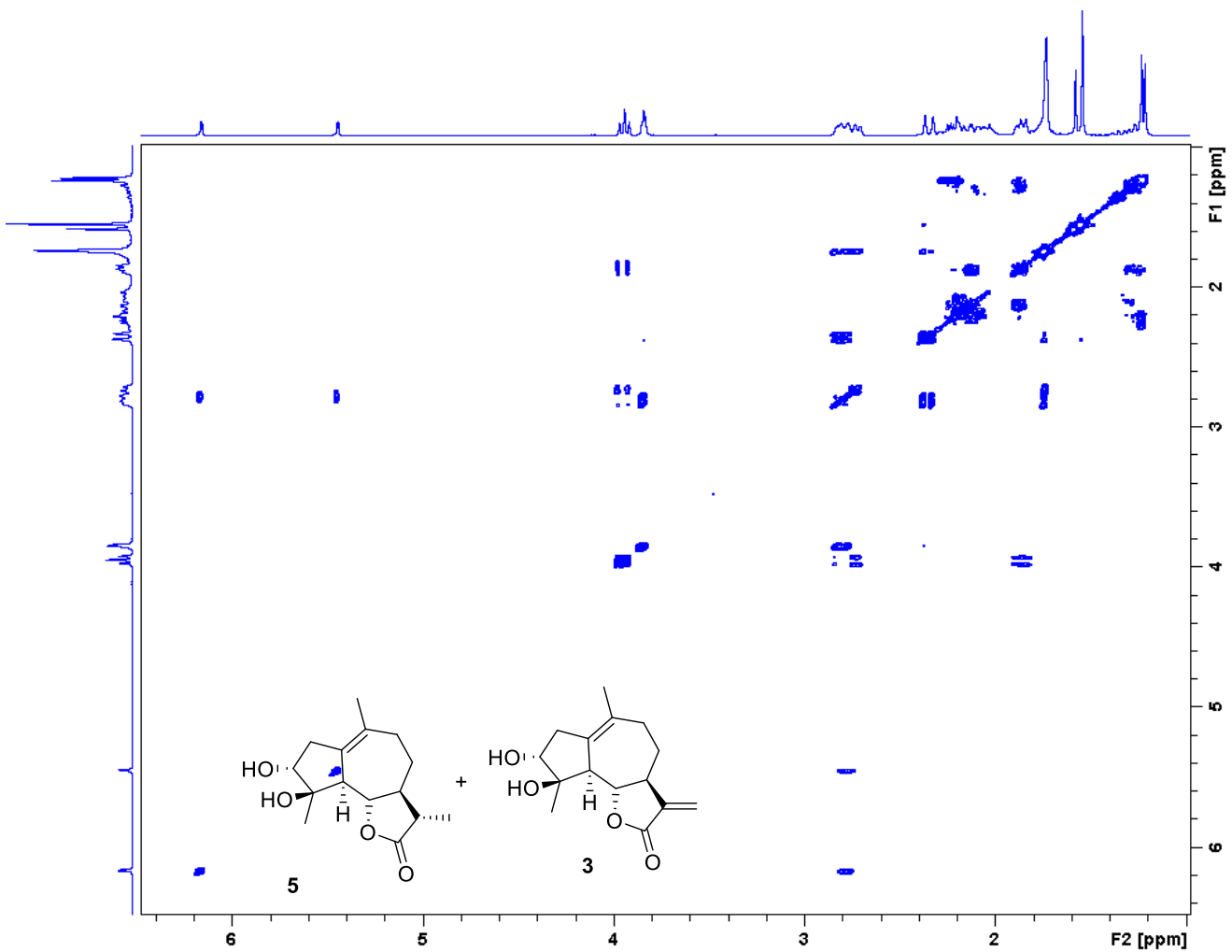


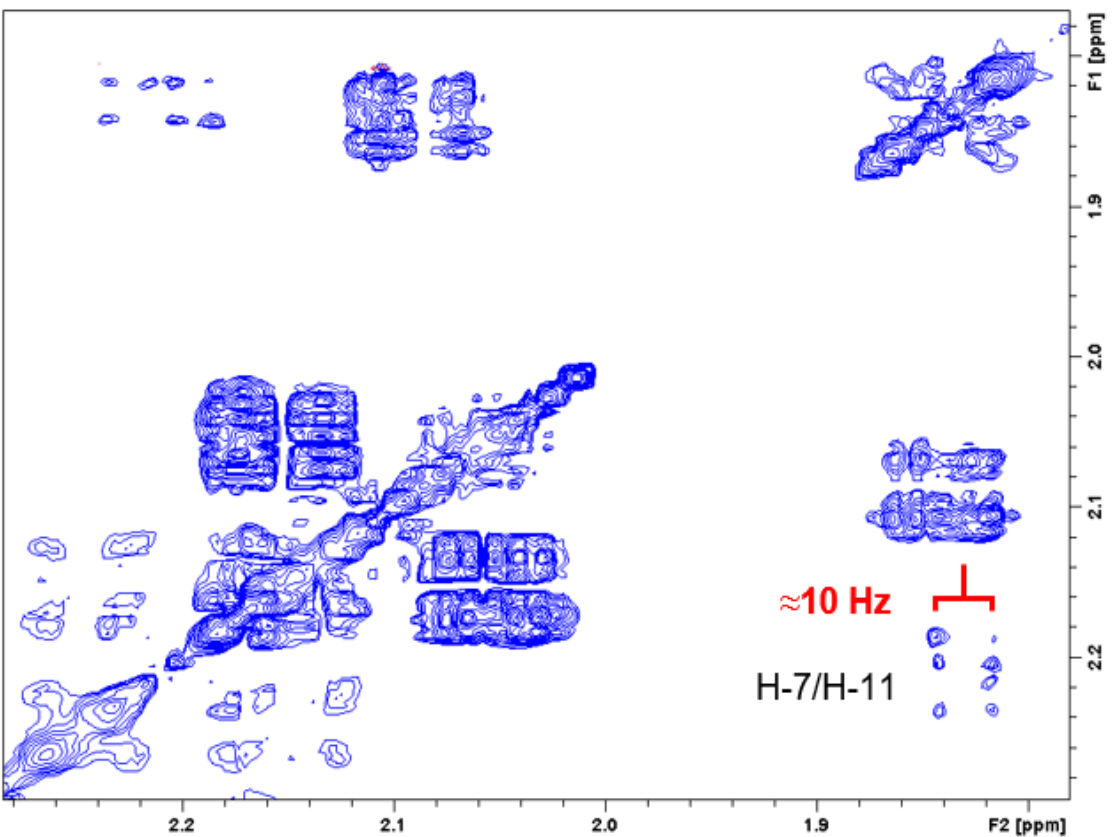
Figure 1S. <sup>1</sup>H NMR spectrum of a mixture composed of compounds 5 and 3 (CDCl<sub>3</sub>, 400.13 MHz)



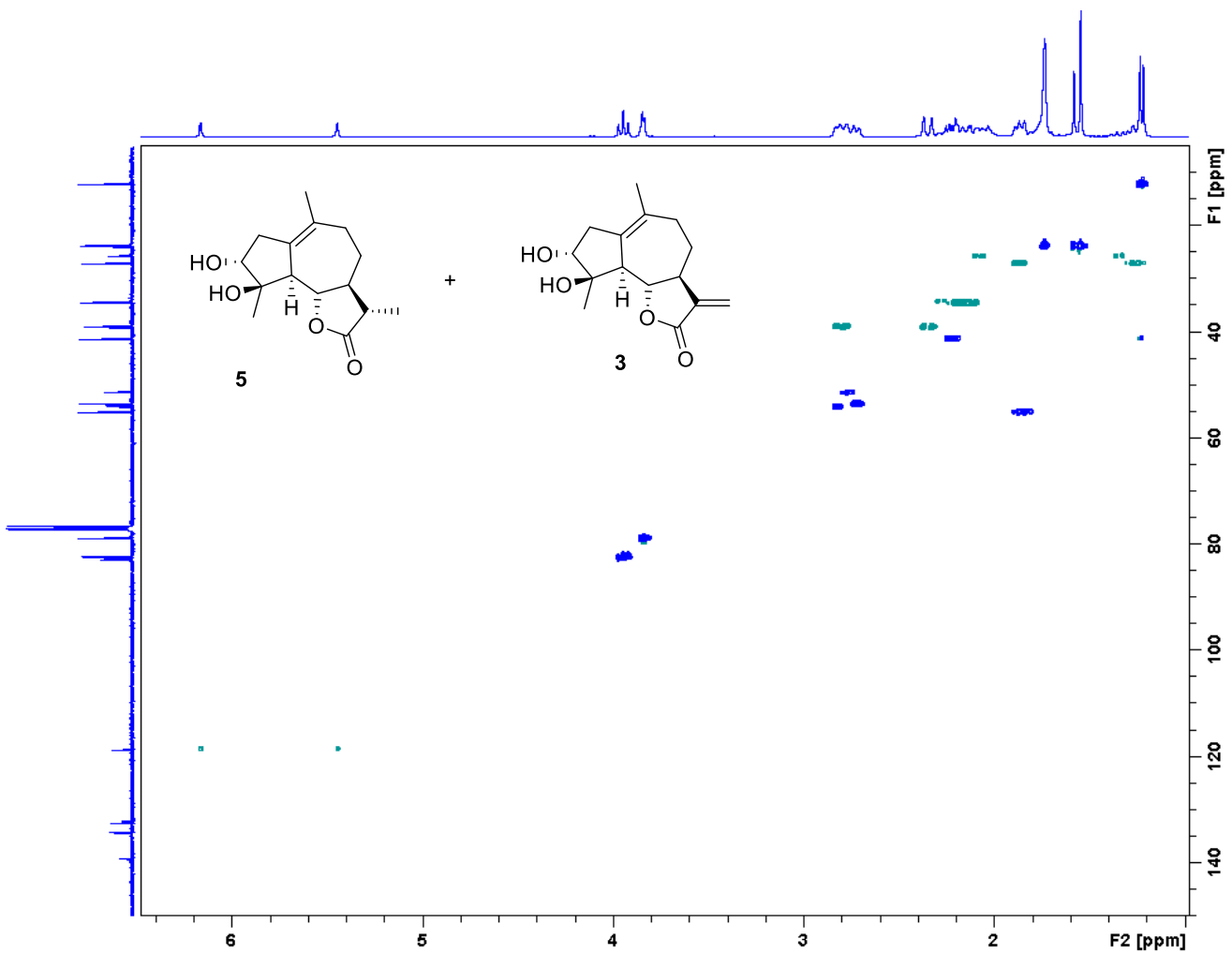
**Figure 2S.**  $^{13}\text{C}$  NMR spectrum of a mixture composed of compounds 5 and 3 ( $\text{CDCl}_3$ , 100.03 MHz)



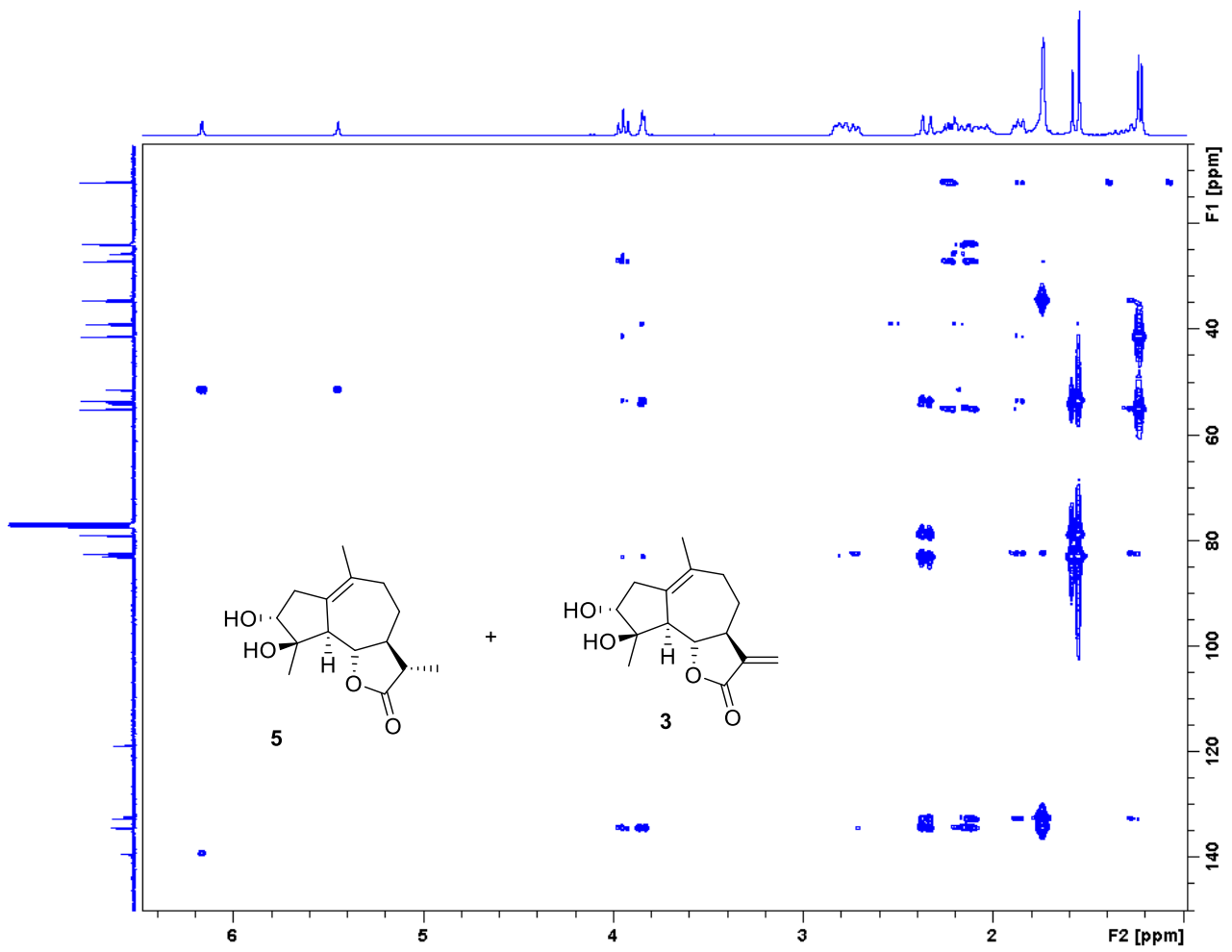
**Figure 3S.** COSY spectrum of a mixture composed of compounds **5** and **3** (CDCl<sub>3</sub>, 400.13 MHz)



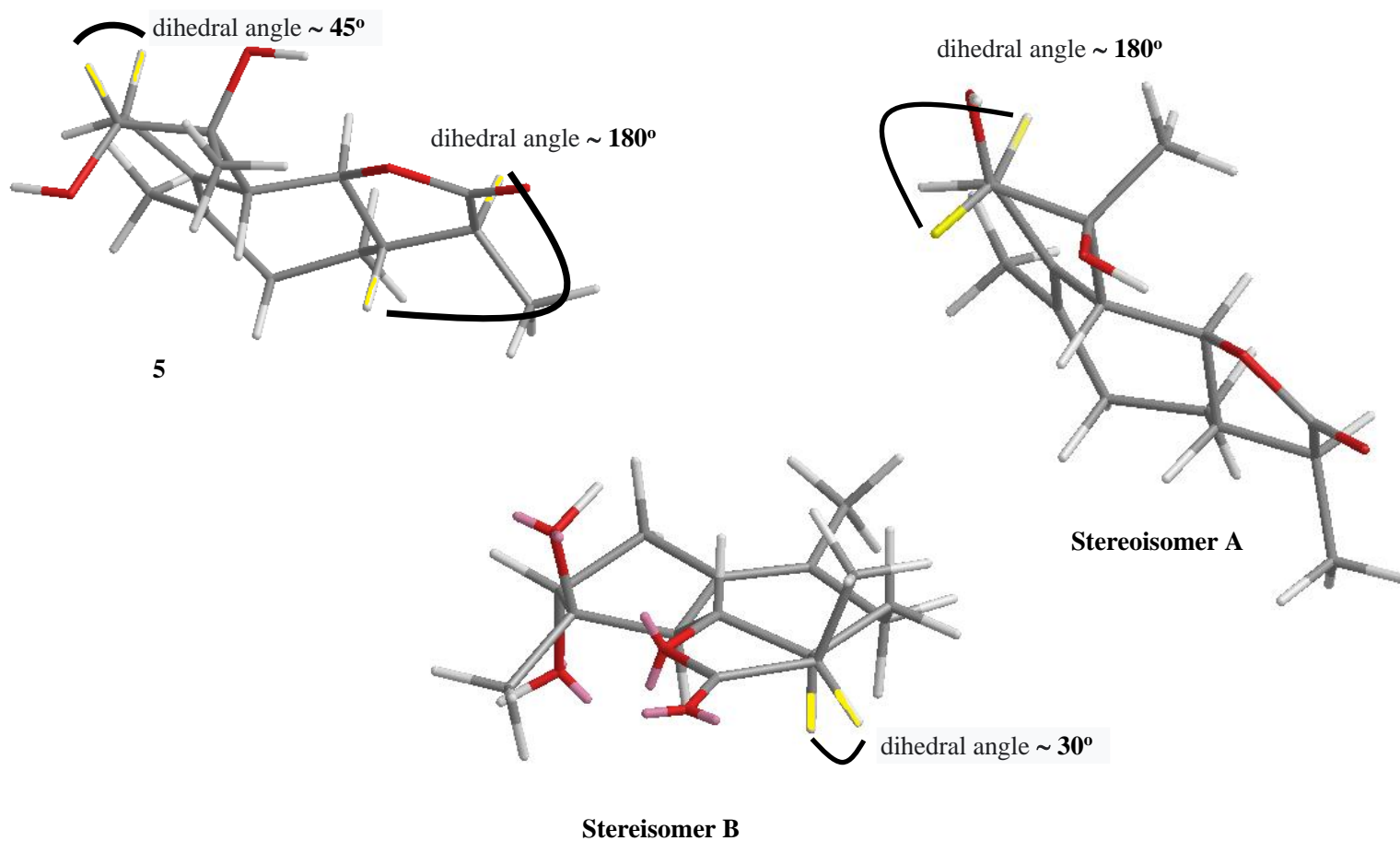
**Figure 4S.** Expanded COSY correlation spectrum of a mixture composed of compounds **5** and **3** (region 2.28–1.78 ppm), (CDCl<sub>3</sub>, 400.13 MHz)



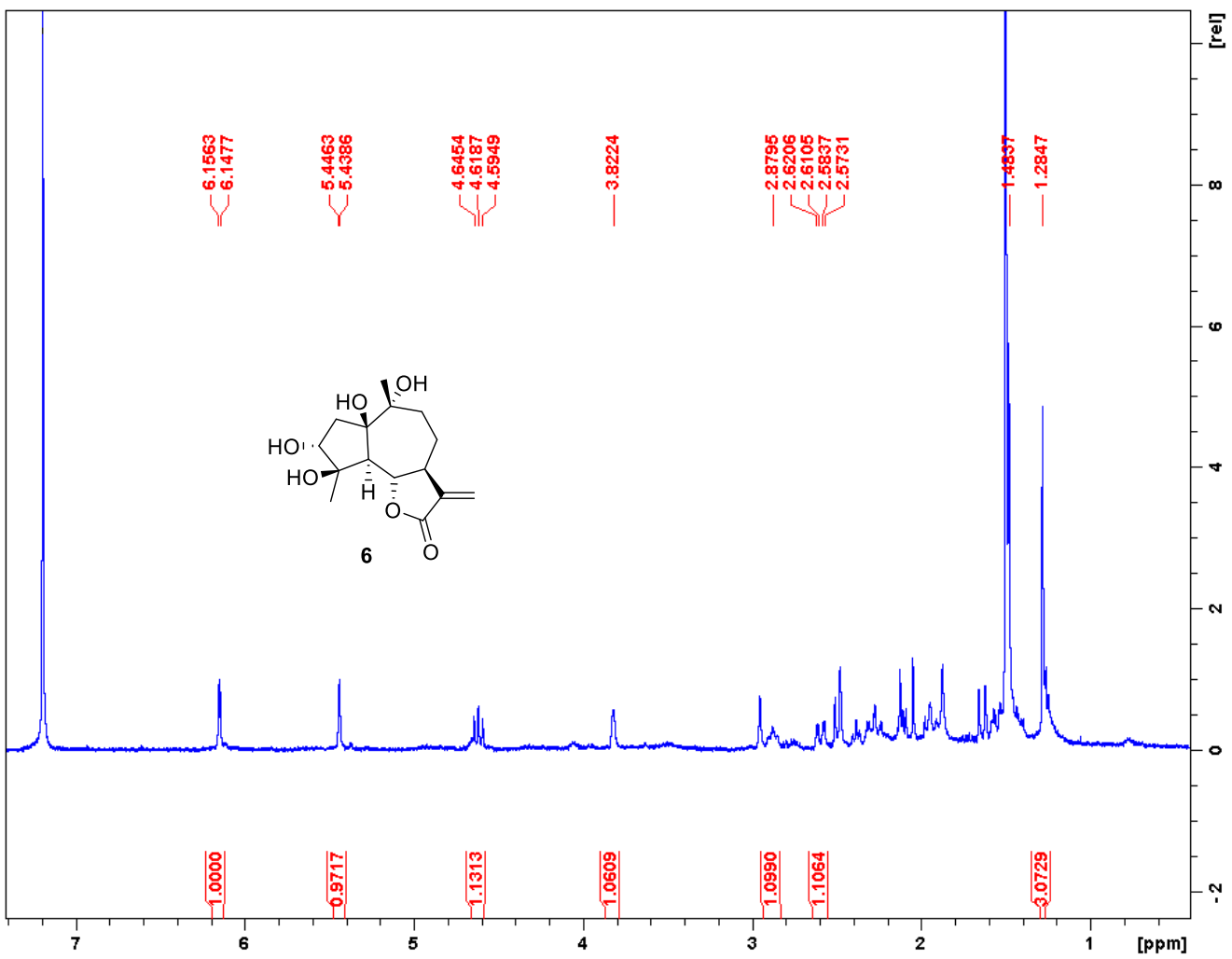
**Figure 5S.** HSQC spectrum of a mixture composed of compounds **5** and **3** (CDCl<sub>3</sub>, 400.13 MHz)



**Figure 6S.** HMBC spectrum of compound **5** ( $\text{CDCl}_3$ , 400.13 MHz)



**Figure 7S.** Minimized structure of compound **5** ( $3\alpha,4\beta$ -dihydroxy, C-11*S* derivative), the stereoisomer A ( $3\beta,4\alpha$ -dihydroxy, C-11*S* isomer), and the stereoisomer B ( $3\alpha,4\beta$ -dihydroxy and C-11*R* isomer)



**Figure 8S.** <sup>1</sup>H NMR spectrum of compound **6** (CDCl<sub>3</sub>, 400.13 MHz)

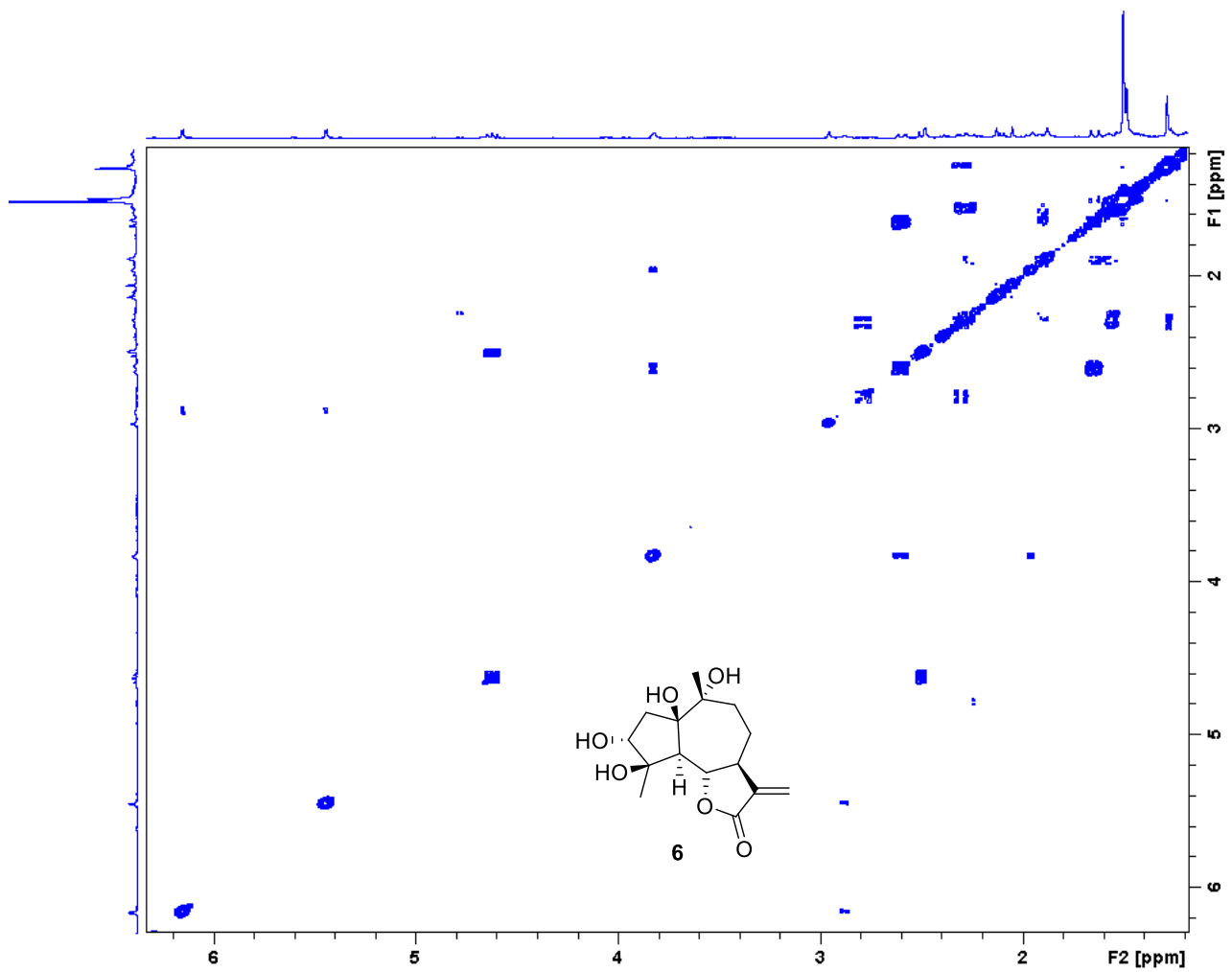


Figure 9S. COSY spectrum of compound 6 (CDCl<sub>3</sub>, 400.13 MHz)

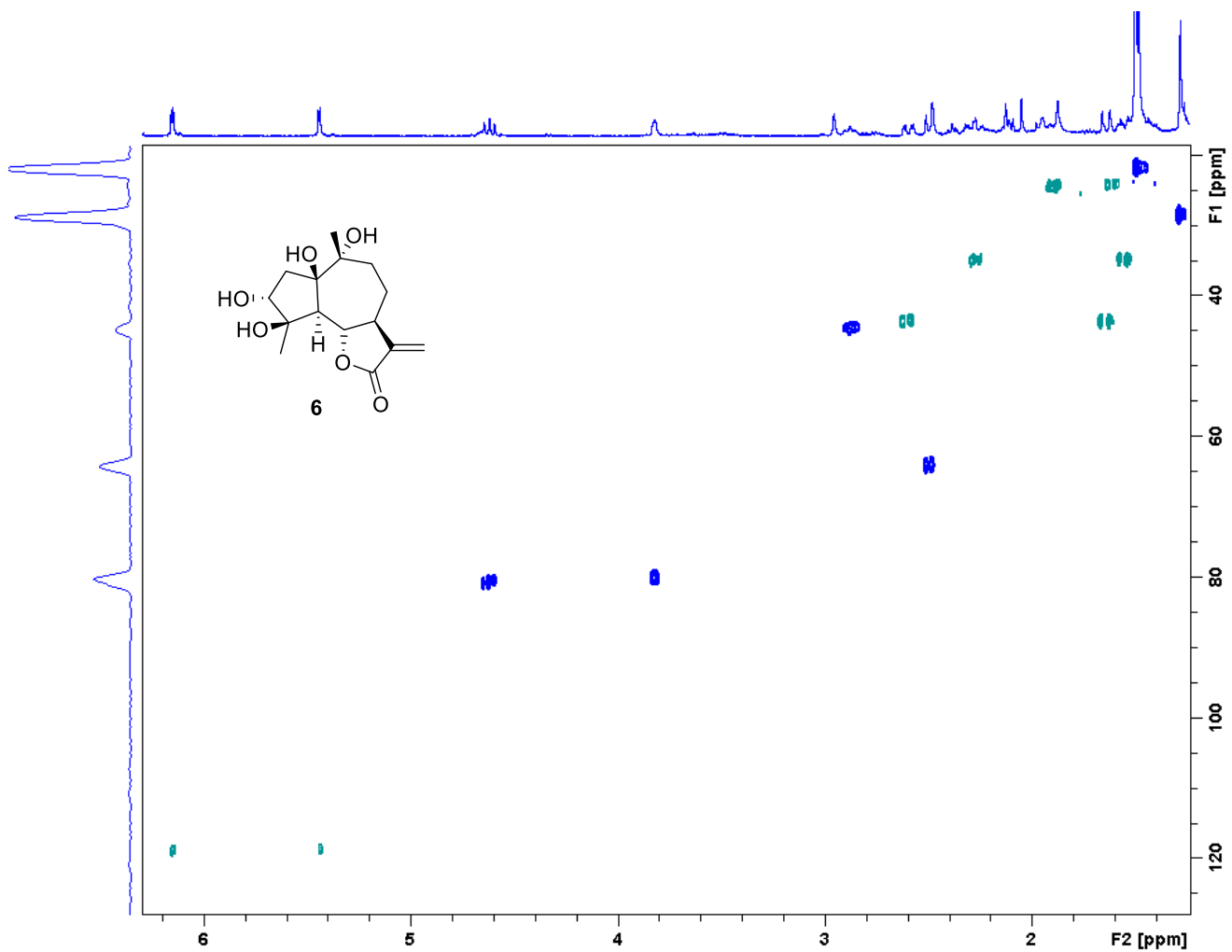


Figure 10S. HSQC spectrum of compound 6 (CDCl<sub>3</sub>, 400.13 MHz)

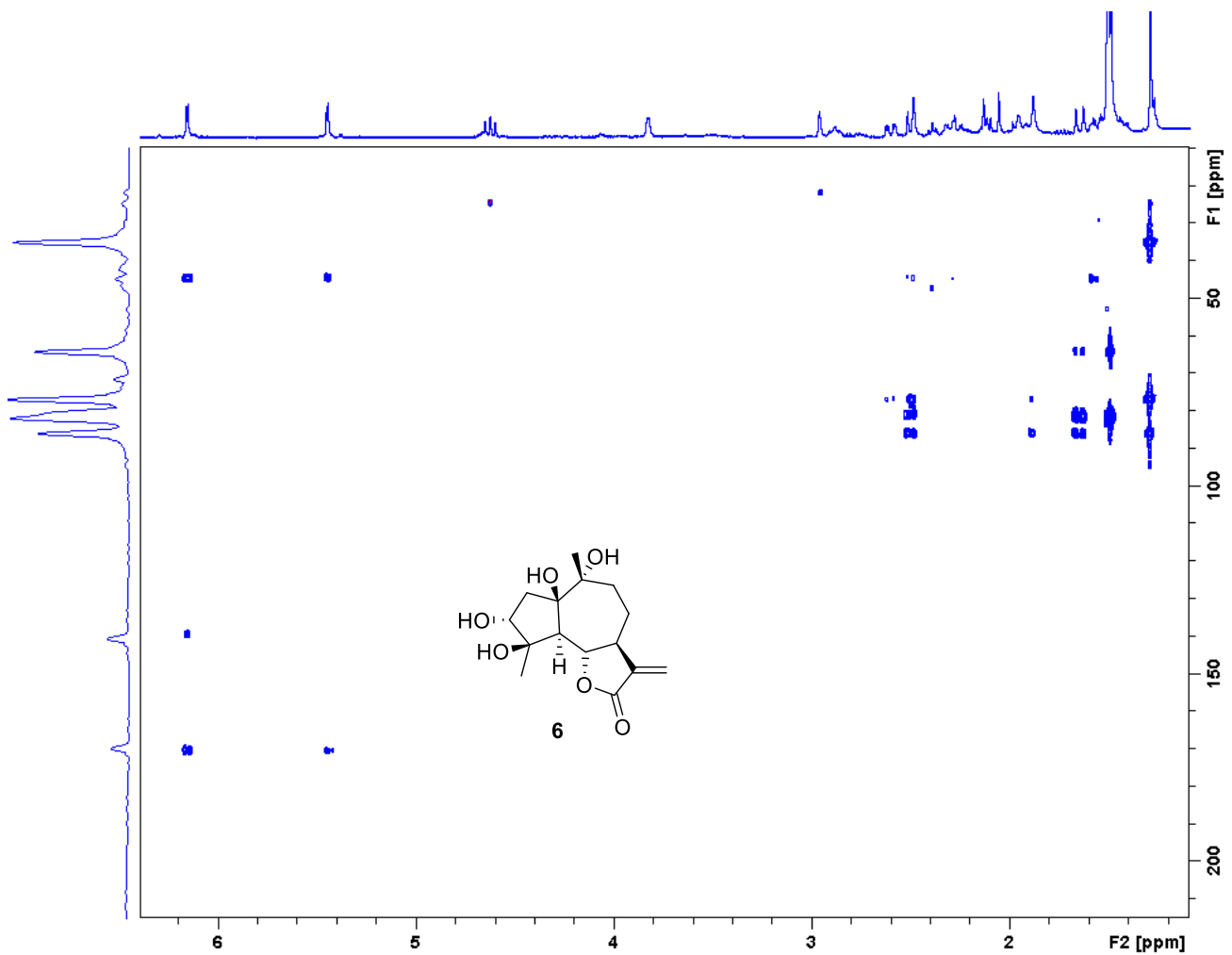
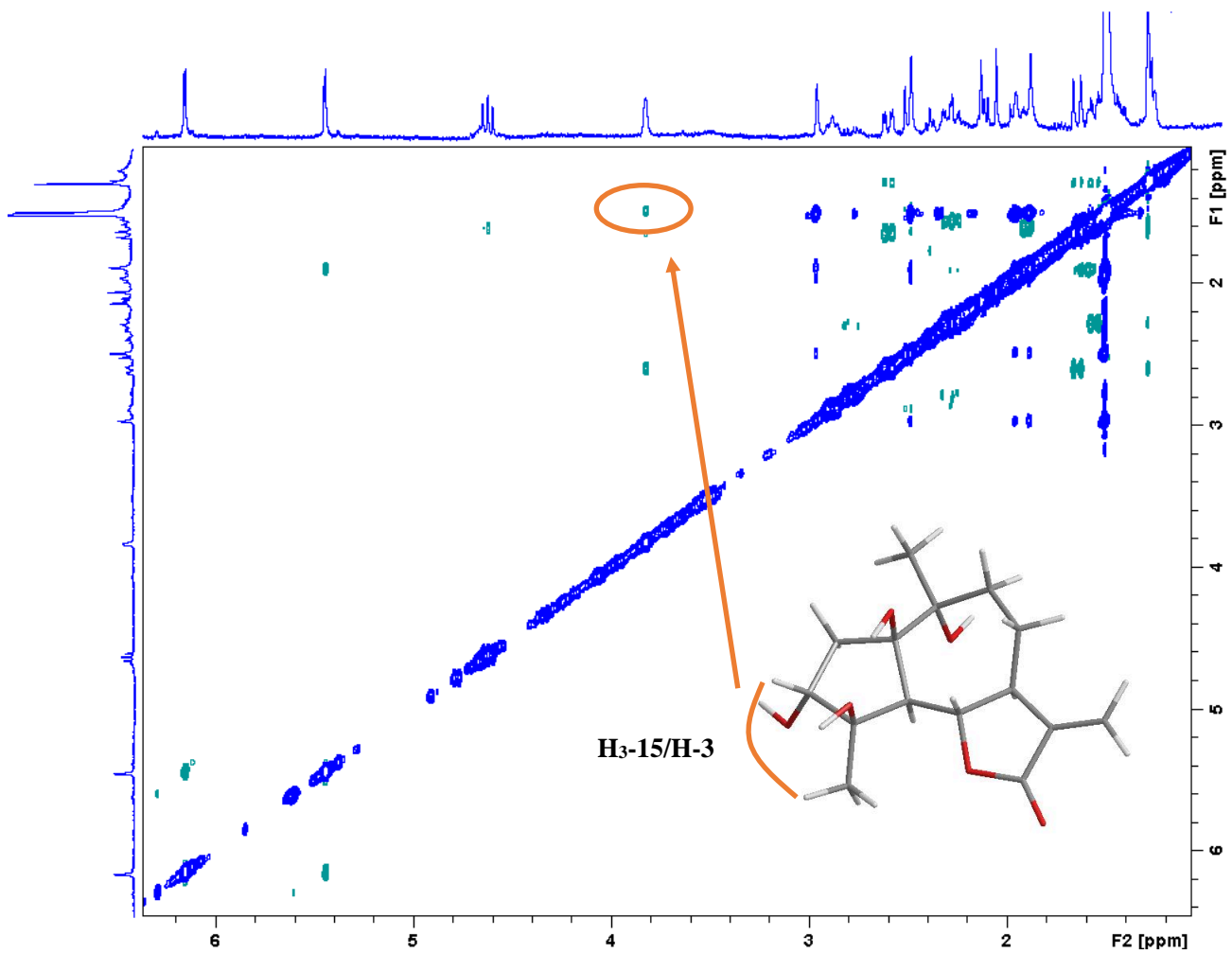
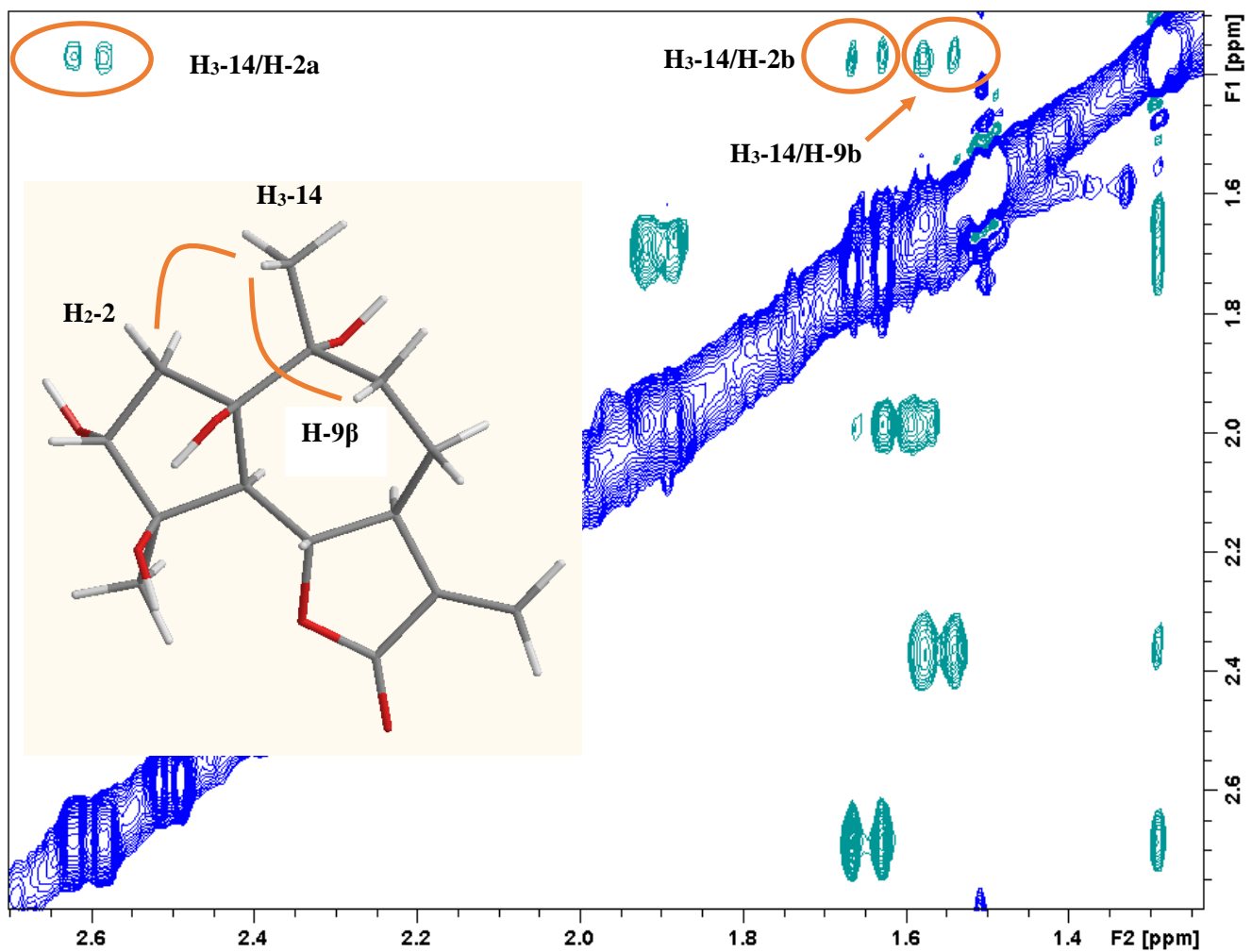


Figure 11S. HMBC spectrum of compound 6 ( $\text{CDCl}_3$ , 400.13 MHz)



**Figure 12S.** NOESY spectrum of compound **6** (CDCl<sub>3</sub>, 400.13 MHz)



**Figure 13S.** Expanded NOESY correlation spectrum of compound **6** (region 2.70–1.25 ppm), (CDCl<sub>3</sub>, 400.13 MHz)

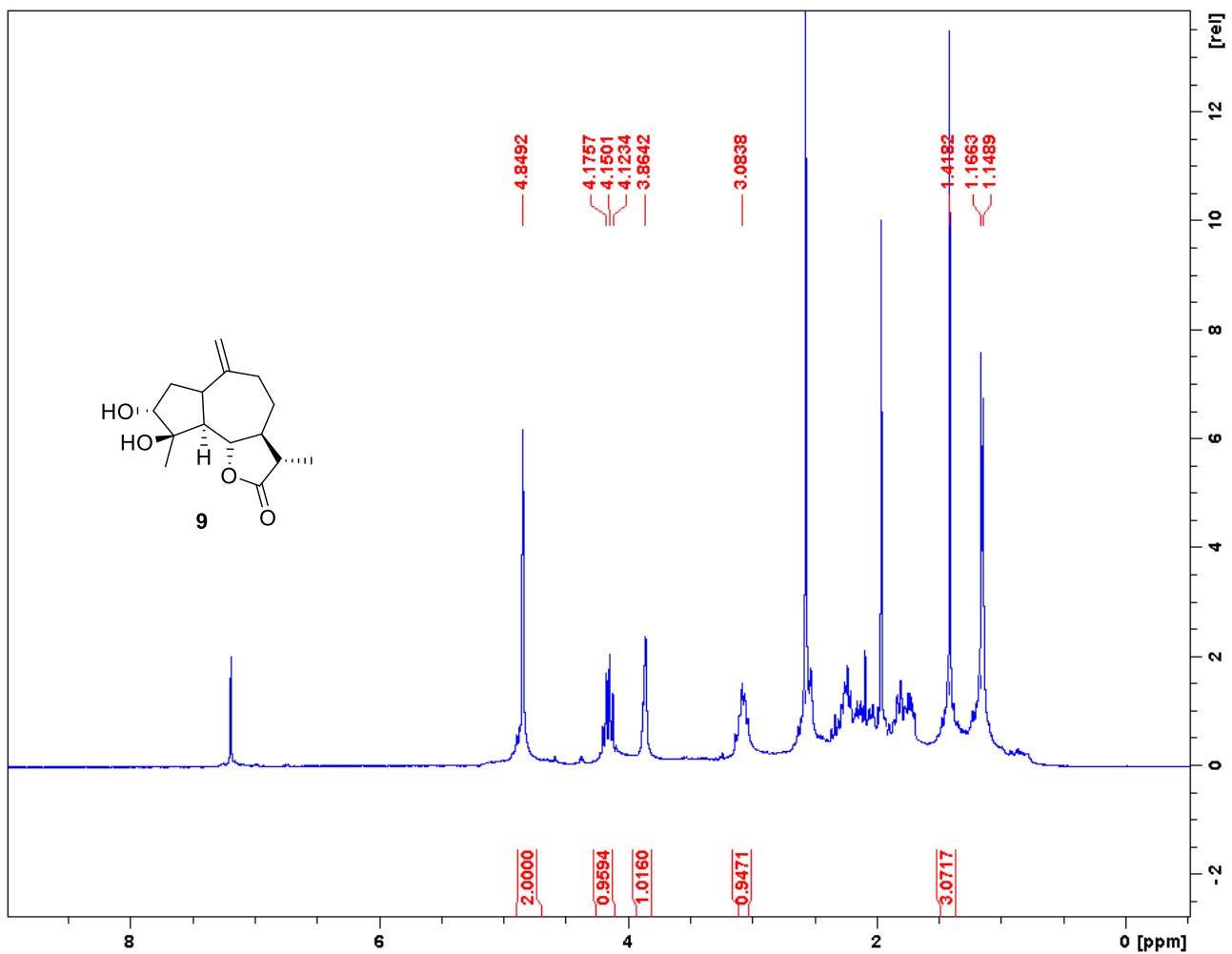
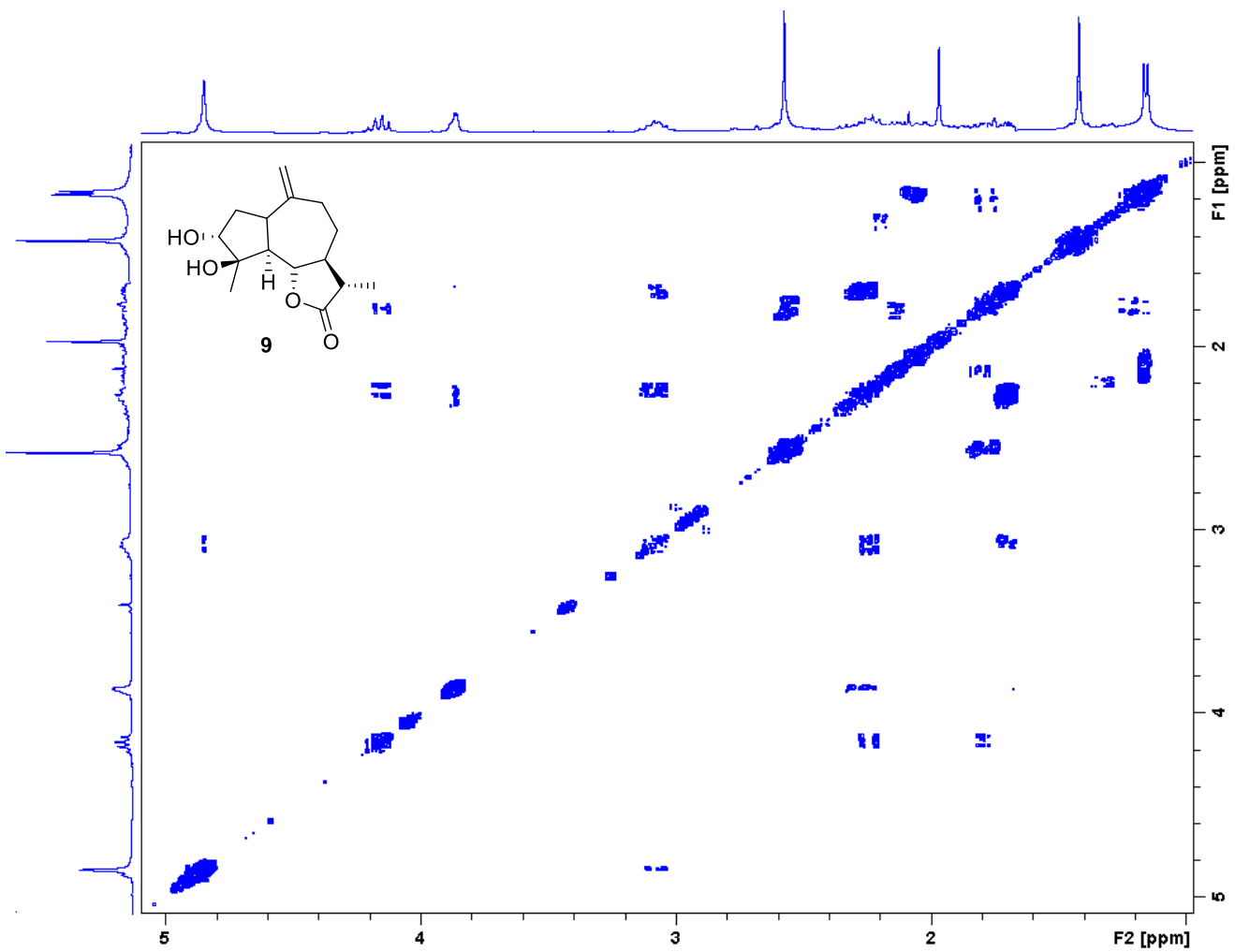
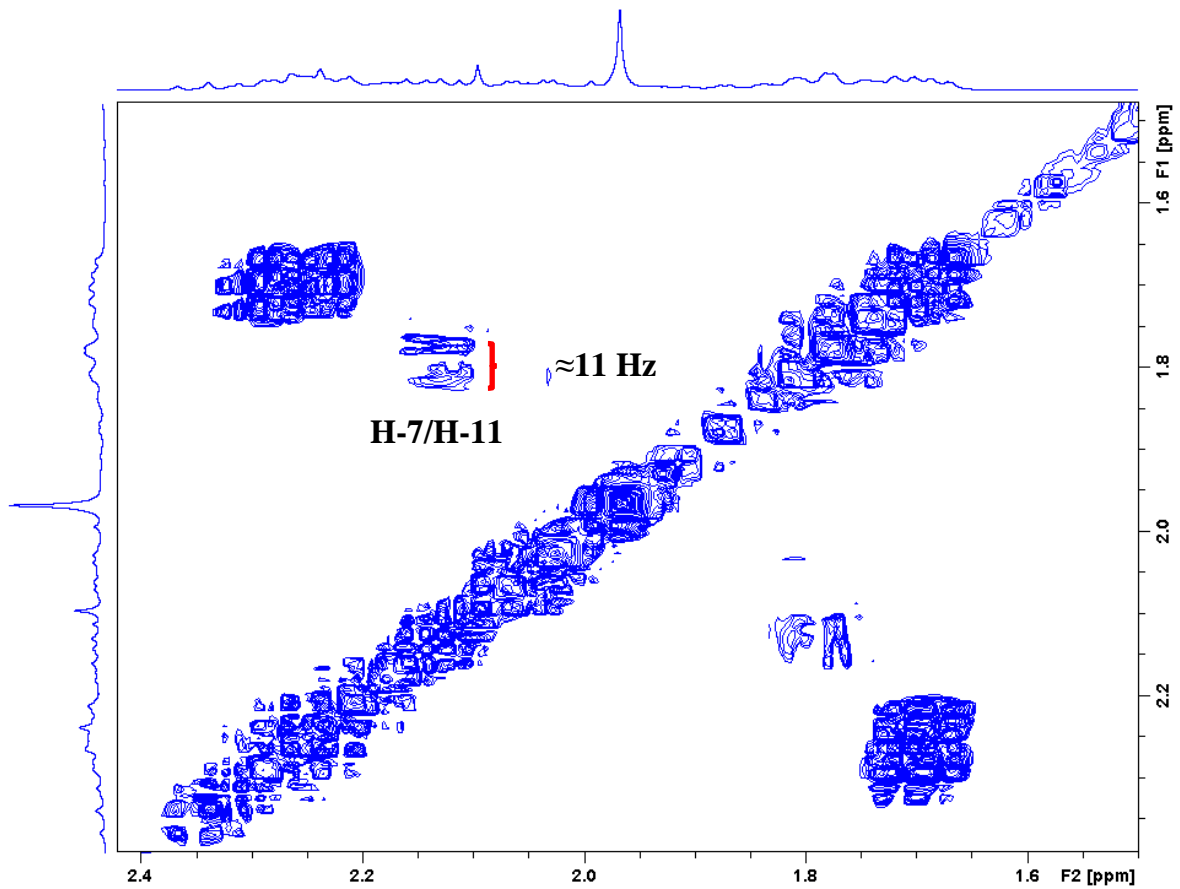


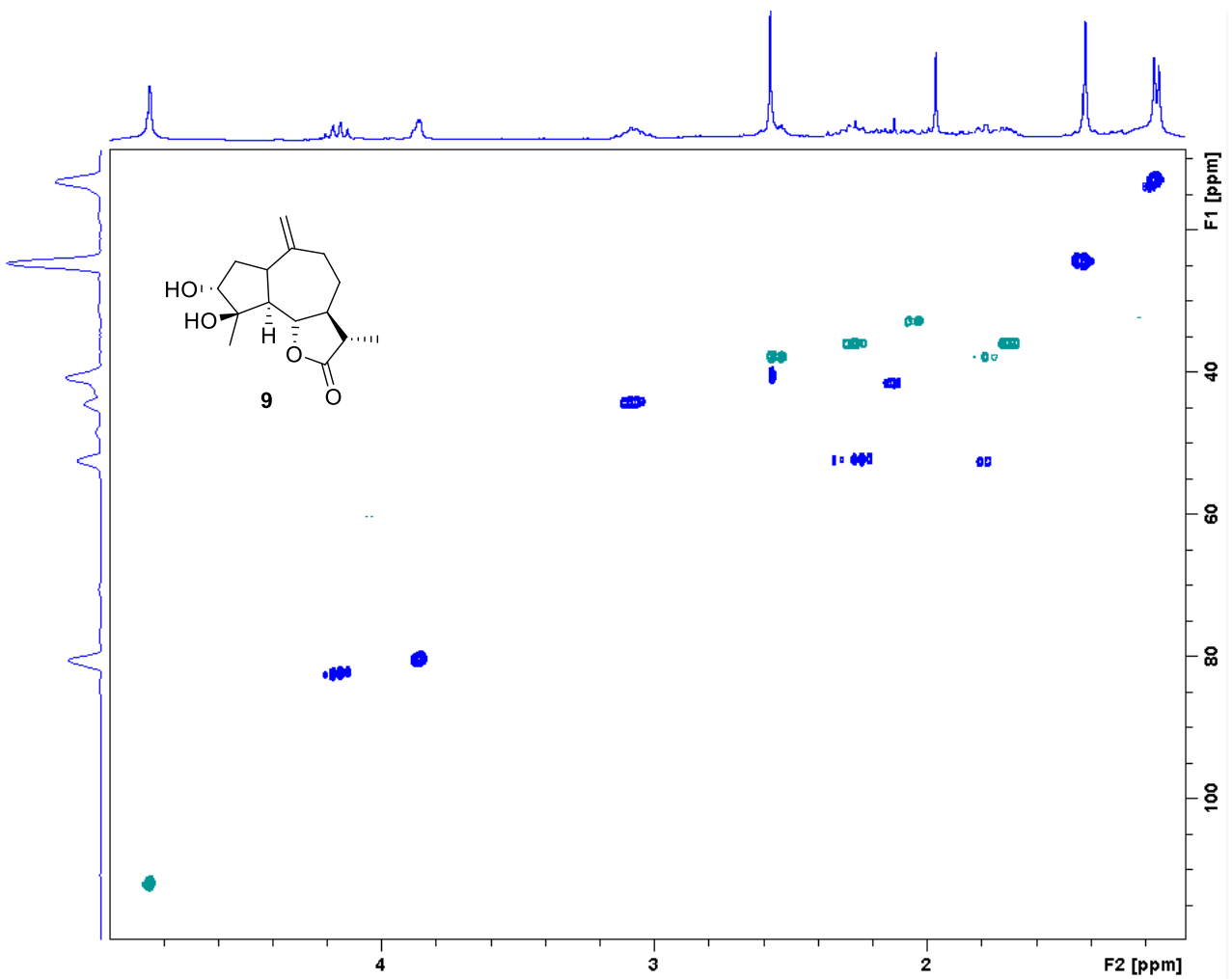
Figure 14S. <sup>1</sup>H NMR spectrum of compound **9** (CDCl<sub>3</sub>, 400.13 MHz)



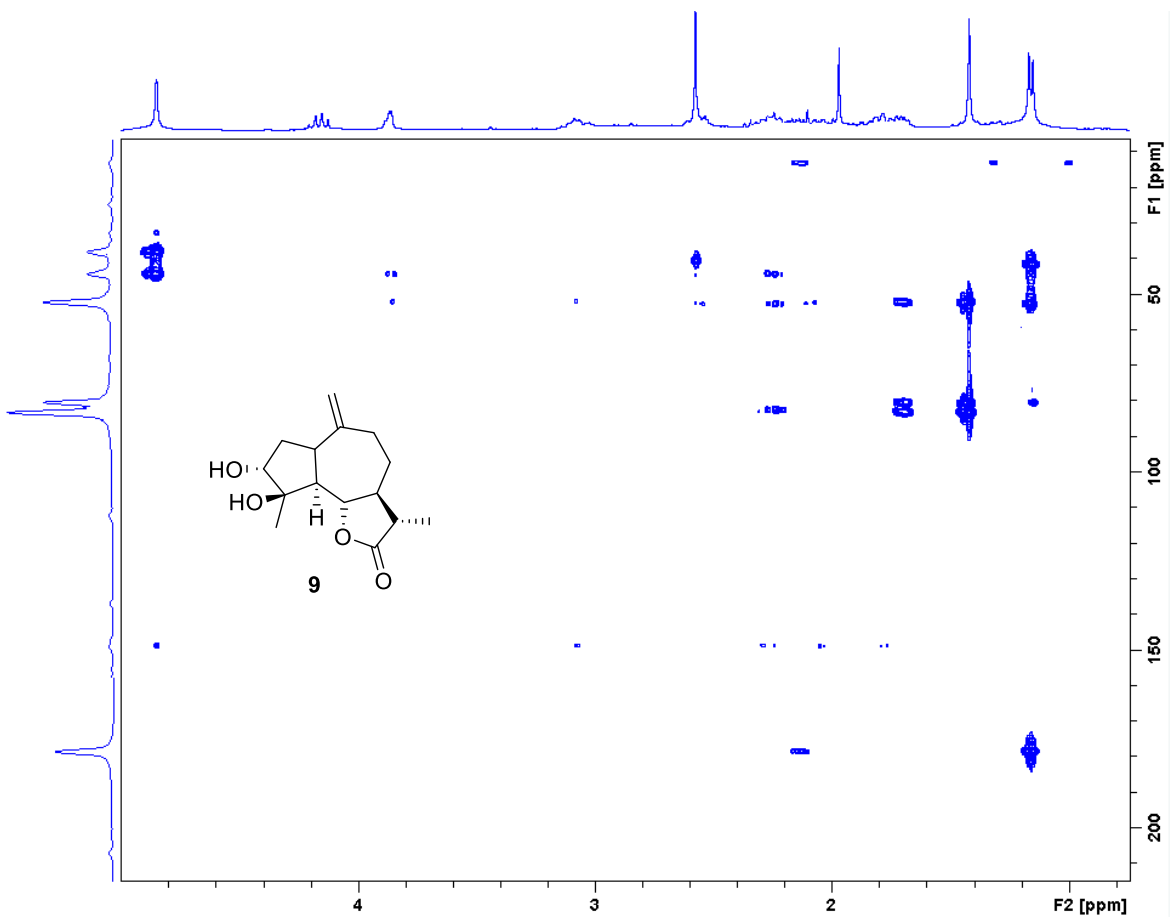
**Figure 15S.** COSY spectrum of compound **9** (CDCl<sub>3</sub>, 400.13 MHz)



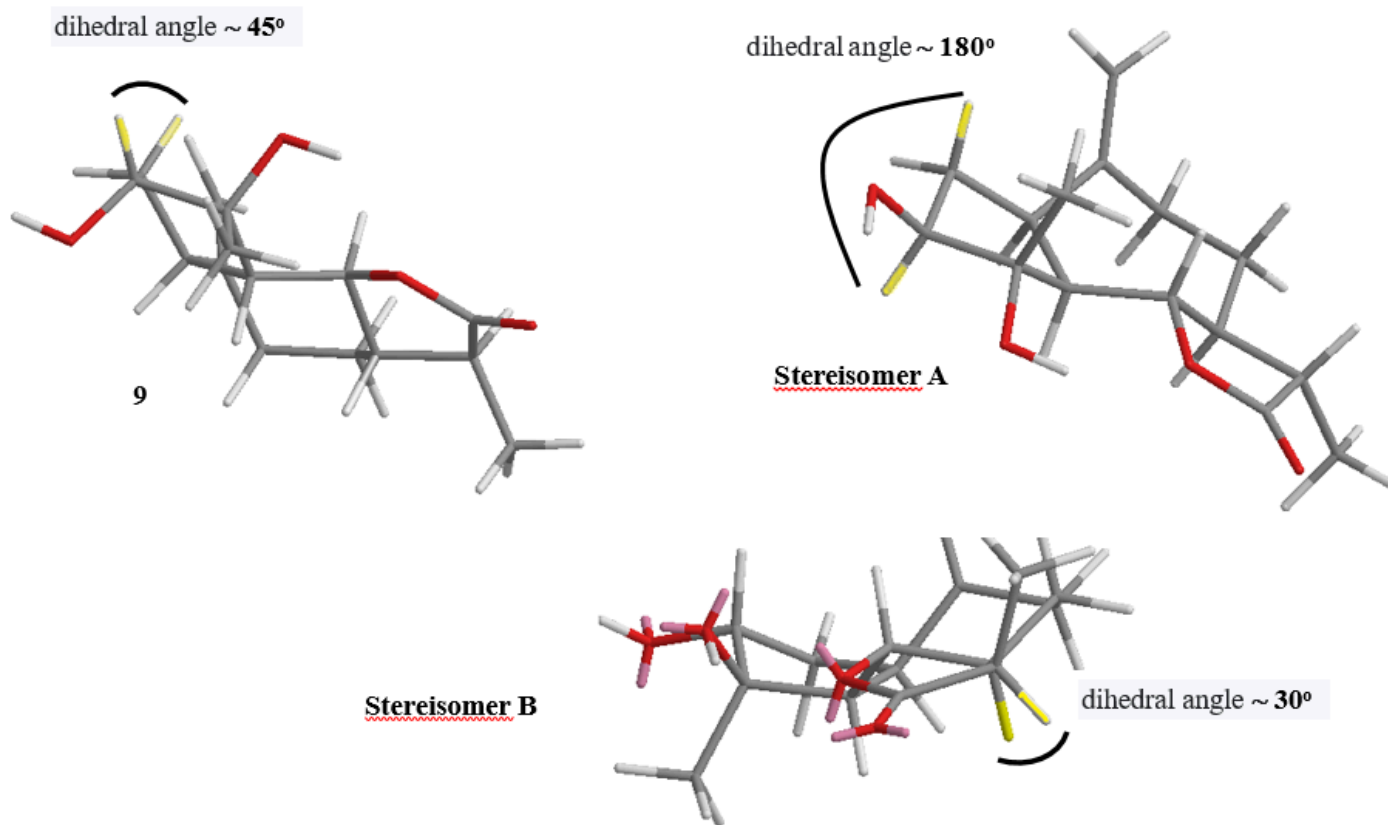
**Figure 16S.** Expanded COSY correlation spectrum of compound **9** (region 2.42–1.50 ppm), (CDCl<sub>3</sub>, 400.13 MHz)



**Figure 17S.** HSQC spectrum of compound **9** (CDCl<sub>3</sub>, 400.13 MHz)



**Figure 18S.** HMBC spectrum of compound **9** (CDCl<sub>3</sub>, 400.13 MHz)



**Figure 19S.** Minimized structure of compound **9** (3 $\alpha$ ,4 $\beta$ -dihydroxy, C-11*S* derivative), the stereoisomer A (3 $\beta$ ,4 $\alpha$  -dihydroxy, C-11*S* isomer), and the stereoisomer B (3 $\alpha$ ,4 $\beta$ -dihydroxy and C-11*R* isomer)