

## ***Supporting Information***

### **Cytotoxic Scalarane Sesterterpenes from the Sponge *Hyrtios erectus***

Oh-Seok Kwon <sup>1</sup>, Donghwa Kim <sup>1</sup>, Chang-Kwon Kim <sup>1</sup>, Jeongyoon Sun <sup>2</sup>, Chung J. Sim <sup>3</sup>,  
Dong-Chan Oh <sup>1</sup>, Sang Kook Lee <sup>1</sup>, Ki-Bong Oh <sup>2,\*</sup>, and Jongheon Shin <sup>1,\*</sup>

<sup>1</sup> *Natural Products Research Institute, College of Pharmacy, Seoul National University,  
San 56-1, Sillim, Gwanak, Seoul 151-742, Korea*

<sup>2</sup> *Department of Agricultural Biotechnology, College of Agriculture and Life Science,  
Seoul National University, San 56-1, Sillim, Gwanak, Seoul 151-921, Korea*

<sup>3</sup> *Department of Biological Sciences, College of Life Science and Nano Technology,  
Hannam University, 461-6 Jeonmin, Yuseong, Daejeon 305-811, Korea*

*shinj@snu.ac.kr*

## Contents

<b>Table S1.</b> $^{13}\text{C}$ NMR (ppm, type) Assignments for Compounds <b>3-8</b> , <b>10</b> , and <b>11</b> at 150 MHz	S5
<b>Table S2.</b> $^1\text{H}$ NMR ( $\delta$ , mult ( $J$ in Hz)) Assignments for Compounds <b>3-8</b> , <b>10</b> , and <b>11</b> at 600 MHz	S6
<b>Table S3.</b> Results of Antibacterial Tests	S7
<b>Table S4.</b> Isolated amount of each compounds	S7
<b>Figure S1.</b> Key correlations of COSY (bold), and HMBC (arrows) experiments for compounds <b>2-8</b>	S8
<b>Figure S2.</b> Key correlations of NOESY (blue arrows) experiments for compounds <b>2-8</b>	S9
<b>Figure S3.</b> The $^1\text{H}$ NMR (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S10
<b>Figure S4.</b> The $^{13}\text{C}$ NMR (150 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S11
<b>Figure S5.</b> The COSY (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S12
<b>Figure S6.</b> The eHSQC (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S13
<b>Figure S7.</b> The HMBC (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S14
<b>Figure S8.</b> The LR-HSQMBC (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S15
<b>Figure S9.</b> The NOESY (600 MHz, $\text{MeOH-}d_3$ ) spectrum of <b>1</b>	S16
<b>Figure S10.</b> ESI/MS isotopic cluster patterns of compound <b>1</b> in positive and negative ion modes	S17
<b>Figure S11.</b> The $^1\text{H}$ NMR (600 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S18
<b>Figure S12.</b> The $^{13}\text{C}$ NMR (150 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S19
<b>Figure S13.</b> The COSY (600 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S20
<b>Figure S14.</b> The eHSQC (600 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S21
<b>Figure S15.</b> The HMBC (600 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S22
<b>Figure S16.</b> The NOESY (600 MHz, $\text{MeOH-}d_4$ ) spectrum of <b>2</b>	S23
<b>Figure S17.</b> The $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S24
<b>Figure S18.</b> The $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S25
<b>Figure S19.</b> The COSY (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S26
<b>Figure S20.</b> The eHSQC (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S27
<b>Figure S21.</b> The HMBC (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S28
<b>Figure S22.</b> The NOESY (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>3</b>	S29
<b>Figure S23.</b> The $^1\text{H}$ NMR (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>4</b>	S30
<b>Figure S24.</b> The $^{13}\text{C}$ NMR (150 MHz, $\text{CDCl}_3$ ) spectrum of <b>4</b>	S31
<b>Figure S25.</b> The COSY (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>4</b>	S32
<b>Figure S26.</b> The eHSQC (600 MHz, $\text{CDCl}_3$ ) spectrum of <b>4</b>	S33

<b>Figure S27.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>4</b>	S34
<b>Figure S28.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>4</b>	S35
<b>Figure S29.</b> The <sup>1</sup> H NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S36
<b>Figure S30.</b> The <sup>13</sup> C NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S37
<b>Figure S31.</b> The COSY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S38
<b>Figure S32.</b> The eHSQC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S39
<b>Figure S33.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S40
<b>Figure S34.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>5</b>	S41
<b>Figure S35.</b> The <sup>1</sup> H NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S42
<b>Figure S36.</b> The <sup>13</sup> C NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S43
<b>Figure S37.</b> The COSY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S44
<b>Figure S38.</b> The eHSQC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S45
<b>Figure S39.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S46
<b>Figure S40.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>6</b>	S47
<b>Figure S41.</b> The <sup>1</sup> H NMR (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S48
<b>Figure S42.</b> The <sup>13</sup> C NMR (150 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S49
<b>Figure S43.</b> The COSY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S50
<b>Figure S44.</b> The eHSQC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S51
<b>Figure S45.</b> The HMBC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S52
<b>Figure S46.</b> The NOESY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>7</b>	S53
<b>Figure S47.</b> The <sup>1</sup> H NMR (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S54
<b>Figure S48.</b> The <sup>13</sup> C NMR (150 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S55
<b>Figure S49.</b> The COSY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S56
<b>Figure S50.</b> The eHSQC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S57
<b>Figure S51.</b> The HMBC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S58
<b>Figure S52.</b> The NOESY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>8</b>	S59
<b>Figure S53.</b> The <sup>1</sup> H NMR (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S60
<b>Figure S54.</b> The <sup>13</sup> C NMR (150 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S61
<b>Figure S55.</b> The COSY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S62
<b>Figure S56.</b> The HSQC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S63
<b>Figure S57.</b> The HMBC (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S64
<b>Figure S58.</b> The NOESY (600 MHz, MeOH- <i>d</i> <sub>4</sub> ) spectrum of <b>9</b>	S65
<b>Figure S59.</b> The <sup>1</sup> H NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S66
<b>Figure S60.</b> The <sup>13</sup> C NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S67

<b>Figure S61.</b> The COSY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S68
<b>Figure S62.</b> The HSQC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S69
<b>Figure S63.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S70
<b>Figure S64.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>10</b>	S71
<b>Figure S65.</b> The <sup>1</sup> H NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S72
<b>Figure S66.</b> The <sup>13</sup> C NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S73
<b>Figure S67.</b> The COSY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S74
<b>Figure S68.</b> The HSQC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S75
<b>Figure S69.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S76
<b>Figure S70.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>11</b>	S77
<b>Figure S71.</b> The <sup>1</sup> H NMR (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S78
<b>Figure S72.</b> The <sup>13</sup> C NMR (150 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S79
<b>Figure S73.</b> The COSY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S80
<b>Figure S74.</b> The HSQC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S81
<b>Figure S75.</b> The HMBC (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S82
<b>Figure S76.</b> The NOESY (600 MHz, CDCl <sub>3</sub> ) spectrum of <b>12</b>	S83
<b>Figure S77.</b> The results of DP4 analyses of <b>12</b>	S84
<b>Figure S78.</b> Isolated known compounds from <i>Hyrtios erectus</i>	S85
<b>Figure S79.</b> Calculated and experimental ECD spectra of <b>4</b> , <b>8</b> and <b>13</b>	S87

**Table S1.**  $^{13}\text{C}$  NMR (ppm, type) Assignments for Compounds **3-8**, **10**, and **11** at 150 MHz

position	<b>3</b> <sup>a</sup>	<b>4</b> <sup>a</sup>	<b>5</b> <sup>a</sup>	<b>6</b> <sup>a</sup>	<b>7</b> <sup>b</sup>	<b>8</b> <sup>b</sup>	<b>10</b> <sup>a</sup>	<b>11</b> <sup>a</sup>
1	39.6, CH <sub>2</sub>	39.6, CH <sub>2</sub>	39.8, CH <sub>2</sub>	39.8, CH <sub>2</sub>	41.4, CH <sub>2</sub>	41.4, CH <sub>2</sub>	39.7, CH <sub>2</sub>	39.8, CH <sub>2</sub>
2	18.5, CH <sub>2</sub>	18.5, CH <sub>2</sub>	18.6, CH <sub>2</sub>	18.2, CH <sub>2</sub>	20.1, CH <sub>2</sub>	20.1, CH <sub>2</sub>	18.5, CH <sub>2</sub>	18.5, CH <sub>2</sub>
3	42.0, CH <sub>2</sub>	42.0, CH <sub>2</sub>	42.0, CH <sub>2</sub>	42.1, CH <sub>2</sub>	43.7, CH <sub>2</sub>	43.7, CH <sub>2</sub>	42.0, CH <sub>2</sub>	42.0, CH <sub>2</sub>
4	33.2, C	33.2, C	33.2, C	33.3, C	34.7, C	34.7, C	33.2, C	33.3, C
5	56.6, CH	56.3, CH	56.6, CH	56.5, CH	58.5, CH	58.4, CH	56.3, CH	56.4, CH
6	18.1, CH <sub>2</sub>	18.1, CH <sub>2</sub>	18.1, CH <sub>2</sub>	18.6, CH <sub>2</sub>	19.8, CH <sub>2</sub>	19.8, CH <sub>2</sub>	18.2, CH <sub>2</sub>	18.2, CH <sub>2</sub>
7	41.5, CH <sub>2</sub>	41.1, CH <sub>2</sub>	41.5, CH <sub>2</sub>	41.2, CH <sub>2</sub>	43.0, CH <sub>2</sub>	43.1, CH <sub>2</sub>	41.8, CH <sub>2</sub>	41.8, CH <sub>2</sub>
8	37.2, C	36.7, C	37.5, C	37.0, C	38.7, C	38.5, C	37.7, C	37.9, C
9	57.7, CH	57.5, CH	58.7, CH	58.6, CH	59.8, CH	59.9, CH	57.6, CH	57.9, CH
10	37.4, C	37.3, C	37.4, C	37.4, C	39.1, C	39.0, C	37.2, C	37.3, C
11	25.4, CH <sub>2</sub>	25.3, CH <sub>2</sub>	25.5, CH <sub>2</sub>	25.6, CH <sub>2</sub>	24.5, CH <sub>2</sub>	27.0, CH <sub>2</sub>	27.2, CH <sub>2</sub>	27.4, CH <sub>2</sub>
12	74.4, CH	74.1, CH	75.0, CH	79.4, CH	79.0, CH	77.1, CH	74.4, CH	75.0, CH
13	44.1, C	44.3, C	44.7, C	45.3, C	43.9, C	45.1, C	45.4, C	46.1, C
14	53.5, CH	48.9, CH	53.0, CH	48.6, CH	51.4, CH	51.2, CH	49.4, CH	50.0, CH
15	24.3, CH <sub>2</sub>	22.6, CH <sub>2</sub>	24.4, CH <sub>2</sub>	22.6, CH <sub>2</sub>	23.7, CH <sub>2</sub>	23.0, CH <sub>2</sub>	24.9, CH <sub>2</sub>	28.0, CH <sub>2</sub>
16	73.6, CH	68.4, CH	73.9, CH	68.7, CH	70.8, CH	71.9, CH	74.2, CH	76.6, CH
17	140.4, C	138.7, C	133.9, C	133.6, C	131.7, C	151.8, C	81.0, C	81.8, C
18	152.4, C	152.8, C	160.3, C	160.6, C	165.1, C	147.4, C	83.1, C	82.2, C
19	171.8, C	172.0, C	84.8, CH	84.5, CH	83.0, C	173.3, C	106.1, CH	106.0, CH
20	167.9, C	168.7, C	169.0, C	169.6, C	171.3, C	88.4, C	103.2, CH	110.7, CH
21	33.2, CH <sub>3</sub>	33.2, CH <sub>3</sub>	33.2, CH <sub>3</sub>	33.3, CH <sub>3</sub>	34.2, CH <sub>3</sub>	34.2, CH <sub>3</sub>	33.2, CH <sub>3</sub>	33.3, CH <sub>3</sub>
22	21.3, CH <sub>3</sub>	21.2, CH <sub>3</sub>	21.2, CH <sub>3</sub>	21.2, CH <sub>3</sub>	22.2, CH <sub>3</sub>	22.3, CH <sub>3</sub>	21.2, CH <sub>3</sub>	21.2, CH <sub>3</sub>
23	15.9, CH <sub>3</sub>	15.9, CH <sub>3</sub>	16.2, CH <sub>3</sub>	16.1, CH <sub>3</sub>	17.2, CH <sub>3</sub>	17.1, CH <sub>3</sub>	16.3, CH <sub>3</sub>	16.4, CH <sub>3</sub>
24	17.1, CH <sub>3</sub>	17.3, CH <sub>3</sub>	17.4, CH <sub>3</sub>	17.7, CH <sub>3</sub>	18.4, CH <sub>3</sub>	18.3, CH <sub>3</sub>	18.2, CH <sub>3</sub>	18.0, CH <sub>3</sub>
25	16.4, CH <sub>3</sub>	15.1, CH <sub>3</sub>	17.4, CH <sub>3</sub>	16.1, CH <sub>3</sub>	17.9, CH <sub>3</sub>	16.0, CH <sub>3</sub>	11.1, CH <sub>3</sub>	10.4, CH <sub>3</sub>
1'	38.5, CH <sub>2</sub>	38.6, CH <sub>2</sub>	40.3, CH <sub>2</sub>	40.3, CH <sub>2</sub>	41.5, CH <sub>2</sub>	42.4, CH <sub>2</sub>		
2'	170.1, C	170.3, C	171.1, C	171.4, C	173.6, C	172.2, C		
12-OAc					173.4, C			
					22.2, CH <sub>3</sub>			
16-OMe	58.1, CH <sub>3</sub>	57.8, CH <sub>3</sub>	57.3, CH <sub>3</sub>	57.3, CH <sub>3</sub>	57.9, CH <sub>3</sub>	58.0, CH <sub>3</sub>		
19-OMe			50.3, CH <sub>3</sub>	50.1, CH <sub>3</sub>			55.6, CH <sub>3</sub>	56.9, CH <sub>3</sub>
20-OMe						51.7, CH <sub>3</sub>	56.0, CH <sub>3</sub>	55.6, CH <sub>3</sub>

<sup>a, b</sup>Data were measured at CDCl<sub>3</sub>, and MeOH-*d*<sub>4</sub>, respectively.

**Table S2.**  $^1\text{H}$  NMR ( $\delta$ , mult ( $J$  in Hz)) Assignments for Compounds **3-8**, **10**, and **11** at 600 MHz

position	<b>3</b> <sup>a</sup>	<b>4</b> <sup>a</sup>	<b>5</b> <sup>a</sup>	<b>6</b> <sup>a</sup>
1 $\alpha$	0.76, m	0.78, m	0.81, m	0.81, m
1 $\beta$	1.71, br d (12.7)	1.71, br d (12.5)	1.71, br d (12.8)	1.69, br d (12.5)
2 $\alpha$	1.41, m	1.45, m	1.44, m	1.39, m
2 $\beta$	1.58, m	1.57, m	1.63, m	1.62, m
3 $\alpha$	1.12, m	1.12, m	1.11, m	1.10, m
3 $\beta$	1.37, br d (12.8)	1.36, br d (13.0)	1.37, br d (13.1)	1.37, br d (13.0)
5	0.78, m	0.81, m	0.80, m	0.82, m
6 $\alpha$	1.60, m	1.61, m	1.58, m	1.57, m
6 $\beta$	1.42, m	1.41, m	1.39, m	1.43, m
7 $\alpha$	0.88, m	0.96, m	0.90, m	0.96, m
7 $\beta$	1.82, m	1.76, br d (11.5)	1.84, ddd (12.8, 2.8, 2.8)	1.78, m
9	0.86, m	0.95, m	0.86, m	0.96, m
11 $\alpha$	1.86, m	1.89, br d (11.9)	1.80, dd (12.8, 2.3)	1.80, m
11 $\beta$	1.52, m	1.52, m	1.55, m	1.54, m
12	3.70, dd (10.5, 3.8)	3.74, br d (9.3)	3.58, dd (11.0, 4.0)	3.64, dd (11.2, 4.1)
14	1.13, m	1.50, m	1.13, m	1.55, m
15 $\alpha$	2.32, dd (12.7, 7.3)	2.12, br d (12.5)	2.25, dd (12.4, 6.8)	2.04, br d (12.0)
15 $\beta$	1.65, m	1.60, m	1.65, m	1.53, m
16	4.18, dd (9.2, 6.7)	4.10, br d (2.3)	4.21, dd (9.3, 7.2)	3.99, br d (1.7)
19			5.75, s	5.69, s
21	0.84, s	0.84, s	0.84, s	0.82, s
22	0.81, s	0.81, s	0.81, s	0.79, s
23	0.84, s	0.84, s	0.85, s	0.84, s
24	0.91, s	0.89, s	0.91, s	0.88, s
25	1.22, s	1.11, s	1.21, s	1.09, s
1'	4.26, br s	4.27, br s	4.50, d (17.9) 3.65, d (17.9)	4.52, d (17.9) 3.69, d (17.9)
16-OMe	3.55, s	3.45, s	3.52, s	3.42, s
19-OMe			3.09, s	3.12, s

position	<b>7</b> <sup>b</sup>	<b>8</b> <sup>b</sup>	<b>10</b> <sup>a</sup>	<b>11</b> <sup>a</sup>
1 $\alpha$	0.88, m	0.86, m	0.82, m	0.82, m
1 $\beta$	1.65, m	1.72, m	1.67, m	1.66, m
2 $\alpha$	1.44, m	1.44, m	1.43, m	1.44, m
2 $\beta$	1.66, m	1.67, m	1.60, m	1.60, m
3 $\alpha$	1.18, ddd (13.8, 13.6, 3.9)	1.17, ddd (13.5, 13.3, 4.2)	1.12, m	1.12, m
3 $\beta$	1.38, br d (13.6)	1.38, m	1.34, br d (12.4)	1.33, br d (12.4)
5	0.87, m	0.87, m	0.82, m	0.80, m
6 $\alpha$	1.62, m	1.62, m	1.53, m	1.53, m
6 $\beta$	1.48, m	1.49, m	1.38, m	1.38, m
7 $\alpha$	0.96, m	0.93, m	0.92, br d (12.3)	0.91, br d (12.3)
7 $\beta$	1.89, ddd (12.6, 3.2, 3.2)	1.87, br d (12.8)	1.78, m	1.77, m
9	1.00, dd (12.6, 1.5)	0.94, m	0.93, m	0.92, m
11 $\alpha$	2.02, dd (4.6, 1.9)	1.78, ddd (13.3, 4.1, 1.9)	1.60, m	1.61, m
11 $\beta$	1.50, m	1.50, m	1.50, m	1.50, m
12	4.83, dd (11.3, 4.5)	3.62, dd (10.9, 4.3)	4.34, m	4.34, m
14	1.58, dd (12.7, 1.3)	1.37, m	1.32, m	1.26, m
15 $\alpha$	2.09, br d (14.3)	2.16, br d (14.7)	1.79, m	1.74, m
15 $\beta$	1.71, m	1.71, m	1.44, m	1.65, m
16	3.98, dd (2.7, 1.3)	3.93, dd (4.2, 1.0)	3.72, dd (12.0, 5.7)	3.57, dd (11.5, 6.0)
19	5.40, s		5.22, s	5.40, s
20		5.49, s	4.99, s	5.10, s
21	0.87, s	0.87, s	0.83, s	0.83, s
22	0.84, s	0.84, s	0.79, s	0.80, s
23	0.88, s	0.89, s	0.82, s	0.83, s
24	0.97, s	0.93, s	0.88, s	0.87, s
25	1.22, s	1.09, s	1.00, s	1.12, s
1'	4.27, d (18.0) 3.88, d (18.0)	4.32, d (18.0) 3.87, d (18.0)		
12-OAc	2.03, s			
16-OMe	3.41, s	3.41, s		
16-OH			2.32, br s	2.57, br d (10.3)
17-OH			3.47, br s	3.13, br s
18-OH			3.87, br s	3.68, br s
19-OMe			3.40, s	3.49, s
20-OMe		3.09, s	3.56, s	3.46, s

<sup>a, b</sup>Data were measured at CDCl<sub>3</sub>, and MeOH-*d*<sub>4</sub>, respectively.

**Table S3.** Results of Antibacterial Tests <sup>a</sup>

Compound	MIC (µg/mL)					
	Gram (+) bacteria			Gram (-) bacteria		
	A	B	C	D	E	F
<b>1</b>	>64	8	>64	>64	2	>64
<b>2</b>	>64	>64	>64	>64	>64	>64
<b>3</b>	>64	>64	>64	64	>64	>64
<b>4</b>	>64	>64	>64	64	>64	>64
<b>5</b>	>64	>64	>64	>64	>64	>64
<b>6</b>	>64	>64	>64	64	>64	>64
<b>7</b>	64	>64	>64	64	>64	>64
<b>8</b>	64	64	16	32	>64	>64
<b>9</b>	>64	>64	>64	64	>64	>64
<b>10</b>	>64	>64	>64	>64	>64	>64
<b>11</b>	>64	>64	>64	64	>64	>64
<b>12</b>	8	8	>64	4	>64	>64
<b>13</b>	>64	>64	>64	2	>64	>64
ampicillin	0.13	0.50	0.50		0.13	4
tetracyclin				0.25		

<sup>a</sup>A: *Staphylococcus aureus* (ATCC6538p), B: *Enterococcus faecalis* (ATCC19433), C: *Enterococcus faecium* (ATCC 19434), D: *Klebsiella pneumoniae* (ATCC10031), E: *Salmonella enterica* (ATCC14028), F: *Escherichia coli* (ATCC25922)

**Table S4.** Isolated amount of each compound

Compound	overall yields (mg)	percent yields (%)	retention time (min)
<b>1</b>	2.8	0.0012	44.2 <sup>a</sup>
<b>2</b>	6.1	0.0027	23.0 <sup>b</sup>
<b>3</b>	7.0	0.0031	20.5 <sup>b</sup>
<b>4</b>	2.2	0.00097	21.9 <sup>b</sup>
<b>5</b>	4.6	0.0020	10.1 <sup>b</sup>
<b>6</b>	1.9	0.00084	16.7 <sup>b</sup>
<b>7</b>	1.8	0.00079	12.5 <sup>b</sup>
<b>8</b>	3.0	0.0013	20.0 <sup>b</sup>
<b>9</b>	0.8	0.00035	8.2 <sup>b</sup>
<b>10</b>	5.2	0.0023	35.1 <sup>b</sup>
<b>11</b>	3.7	0.0016	38.7 <sup>b</sup>
<b>12</b>	2.3	0.0010	19.7 <sup>b</sup>
<b>13</b>	110	0.048	23.0 <sup>d</sup>
<b>14</b>	1.8	0.00079	44.1 <sup>c</sup>
<b>15</b>	9.8	0.0043	28.6 <sup>c</sup>
<b>16</b>	0.9	0.00039	18.0 <sup>c</sup>
<b>17</b>	1.2	0.00053	46.9 <sup>c</sup>
<b>18</b>	1.6	0.00070	22.8 <sup>c</sup>
<b>19</b>	4.7	0.0020	50.4 <sup>c</sup>
<b>20</b>	2.2	0.00097	38.3 <sup>c</sup>

semipreparative reversed-phase HPLC (YMC-ODS column, 10 × 250 mm; 2.0 mL/min)

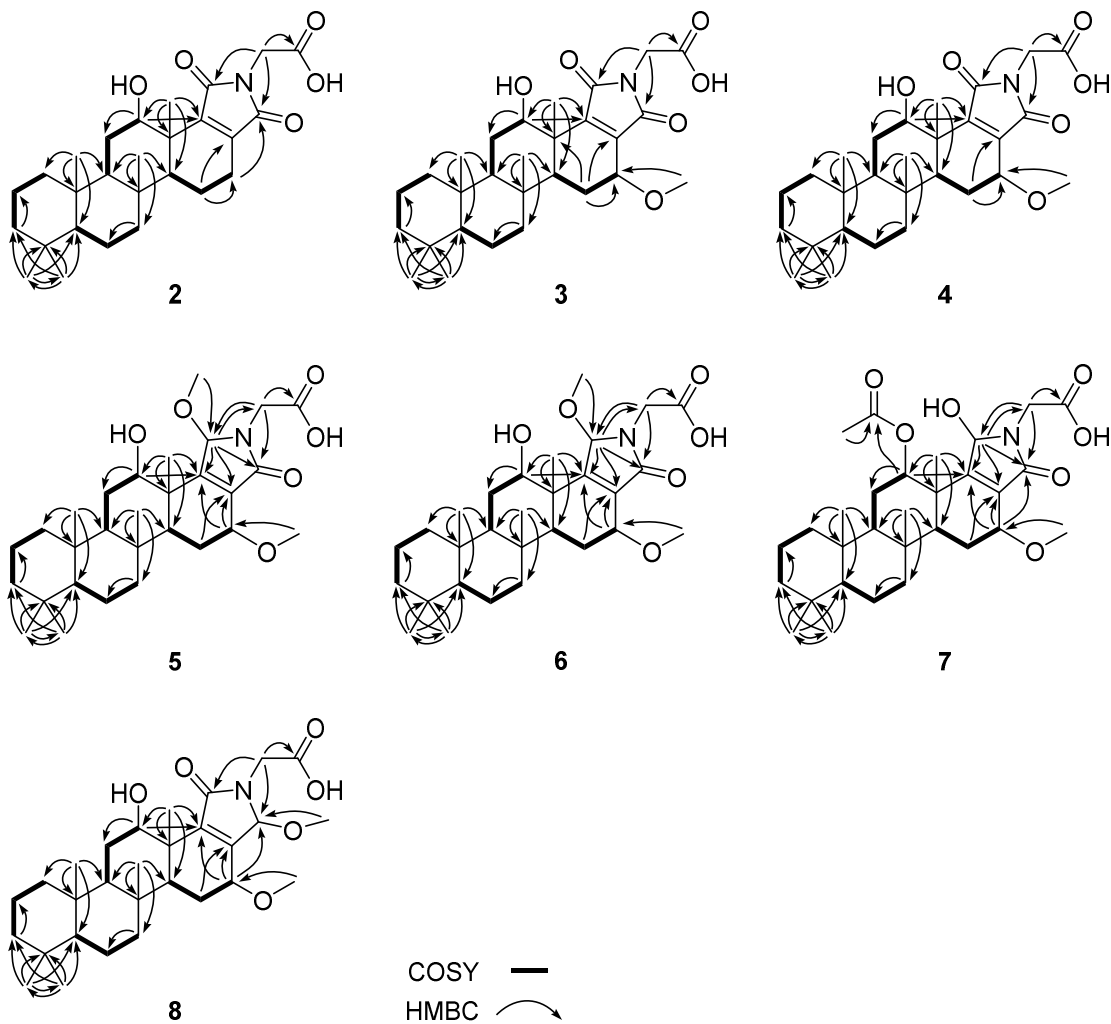
<sup>a</sup> (H<sub>2</sub>O-MeOH, 65:35)

<sup>b</sup> (H<sub>2</sub>O-MeOH, 30:70 with 0.1% TFA)

<sup>c</sup> (H<sub>2</sub>O-MeOH, 25:65)

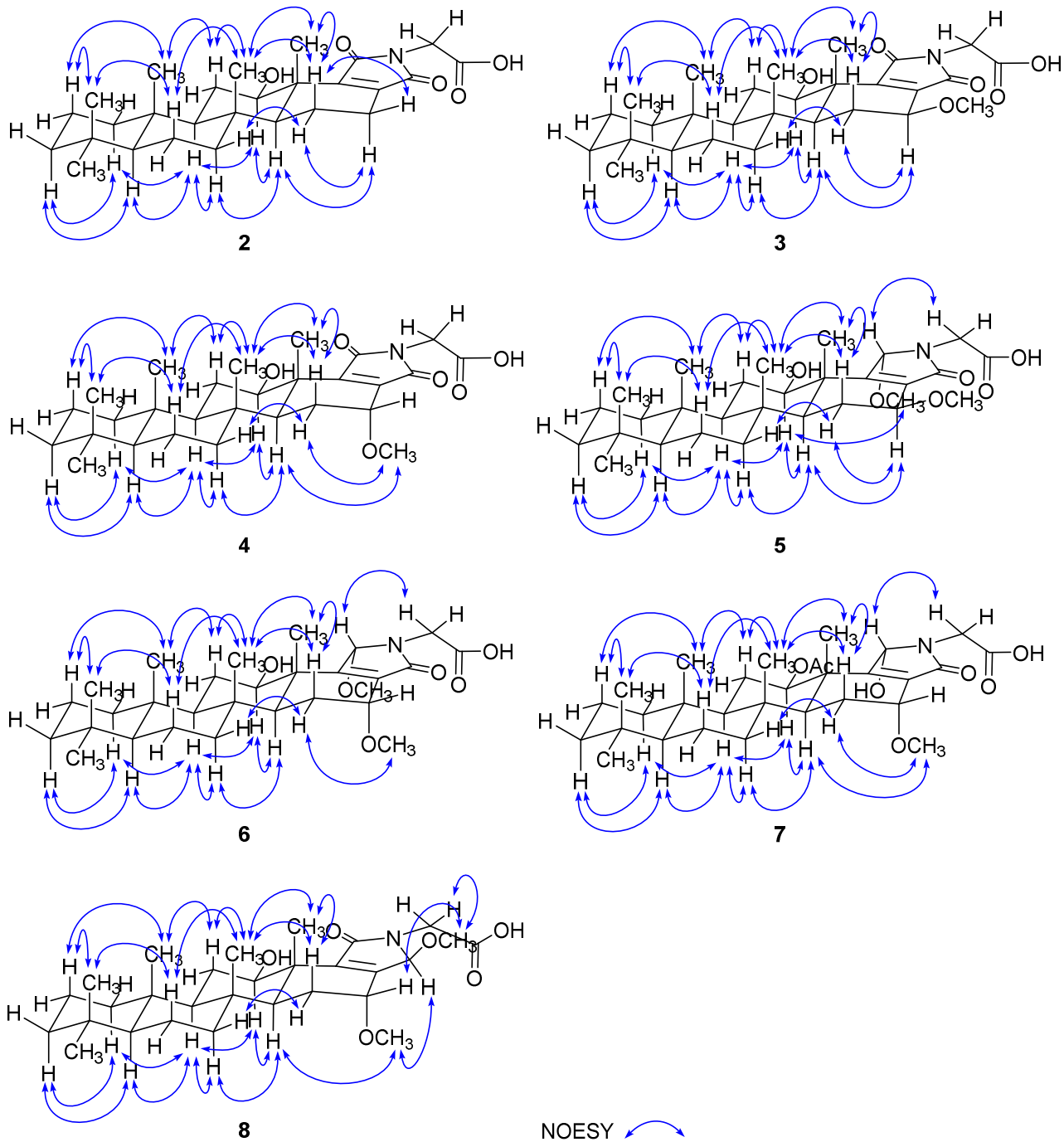
<sup>d</sup> (H<sub>2</sub>O-MeOH, 10:65)

Extract = 225.8 g

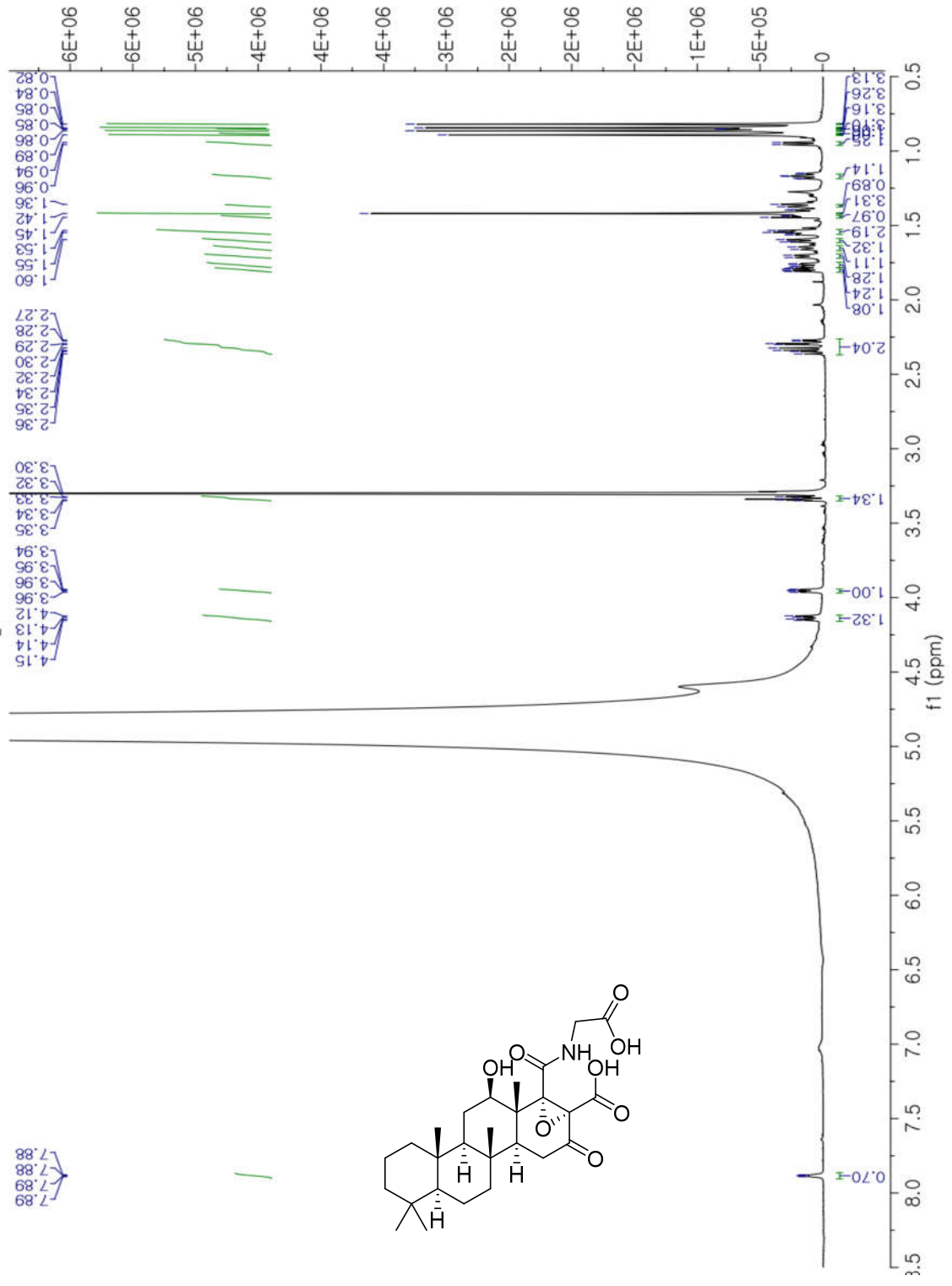


**Figure S1.** Key correlations of COSY (bold), and HMBC (arrows) experiments for compounds 2-8

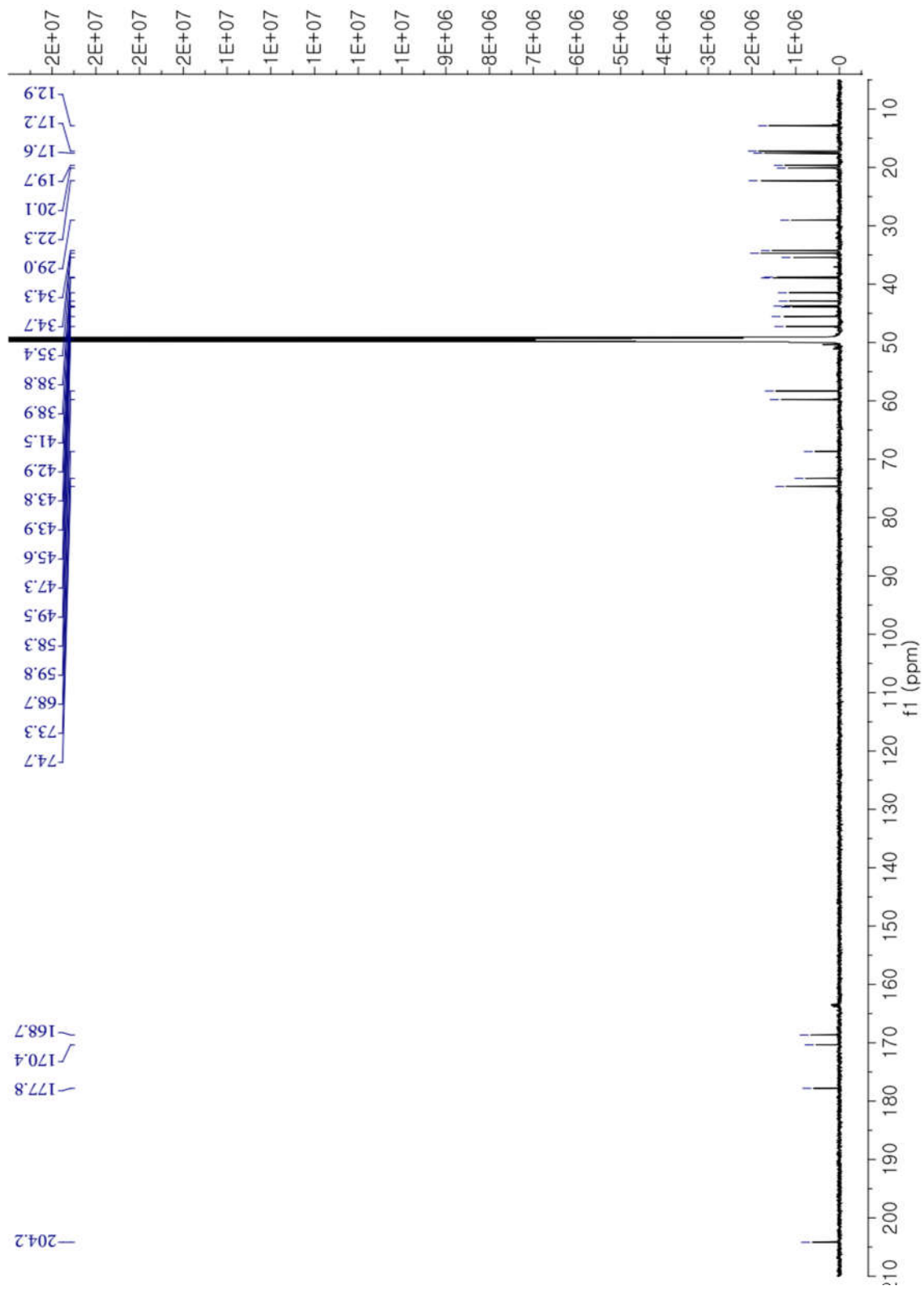




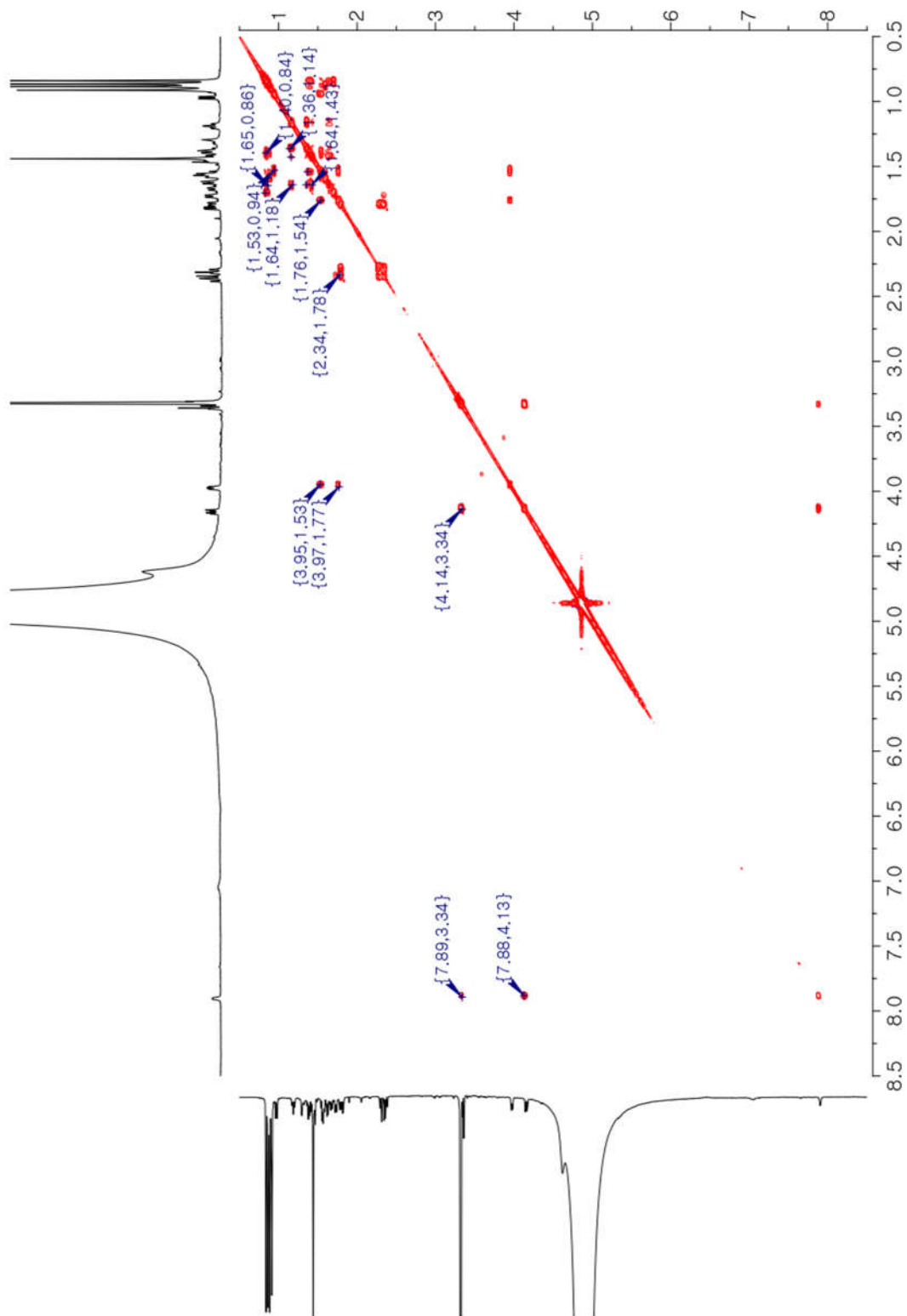
**Figure S2.** Key correlations of NOESY (blue arrows) experiments for compounds 2-8



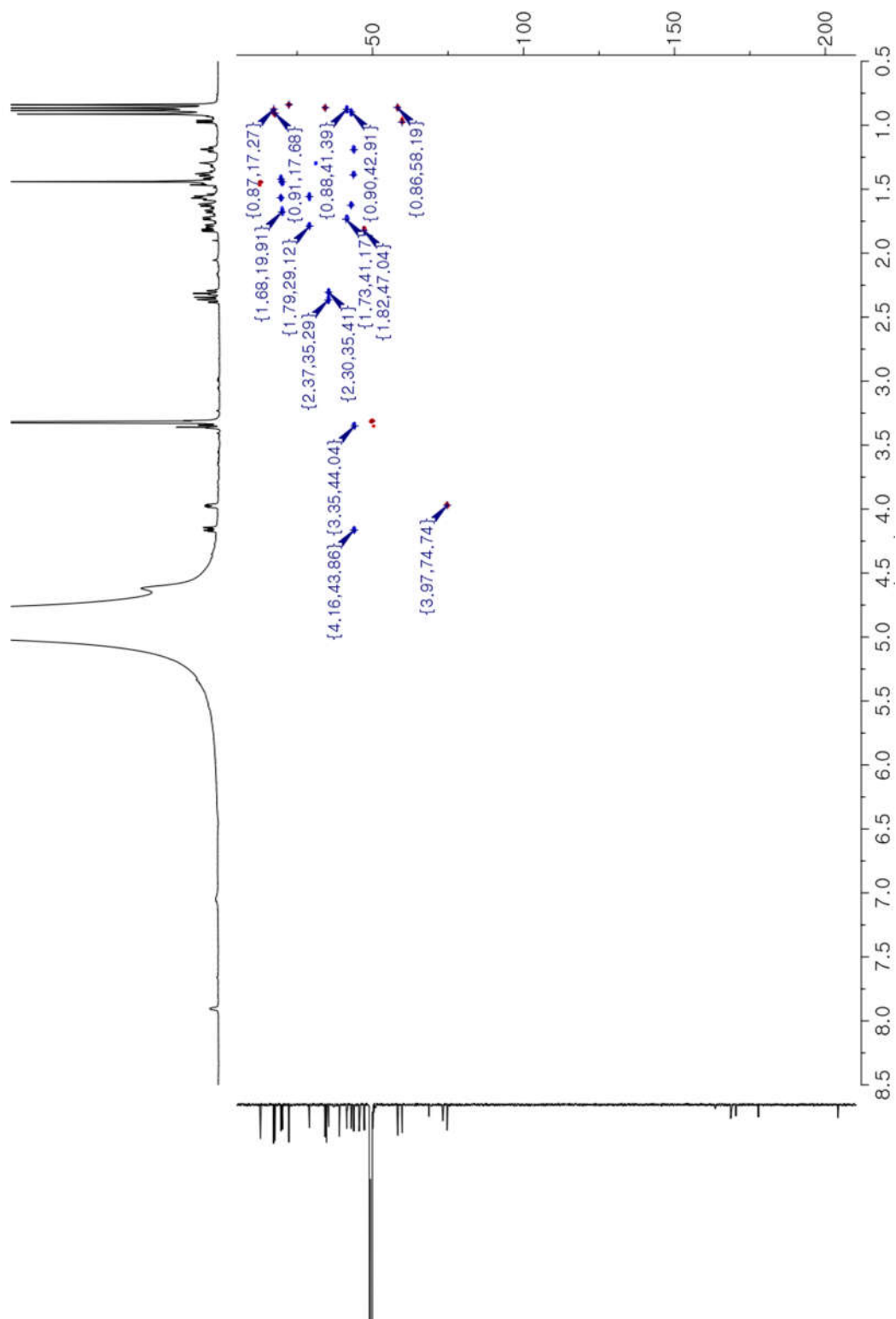
**Figure S3.** The <sup>1</sup>H NMR (600 MHz, MeOH-*d*<sub>3</sub>) spectrum of **1**



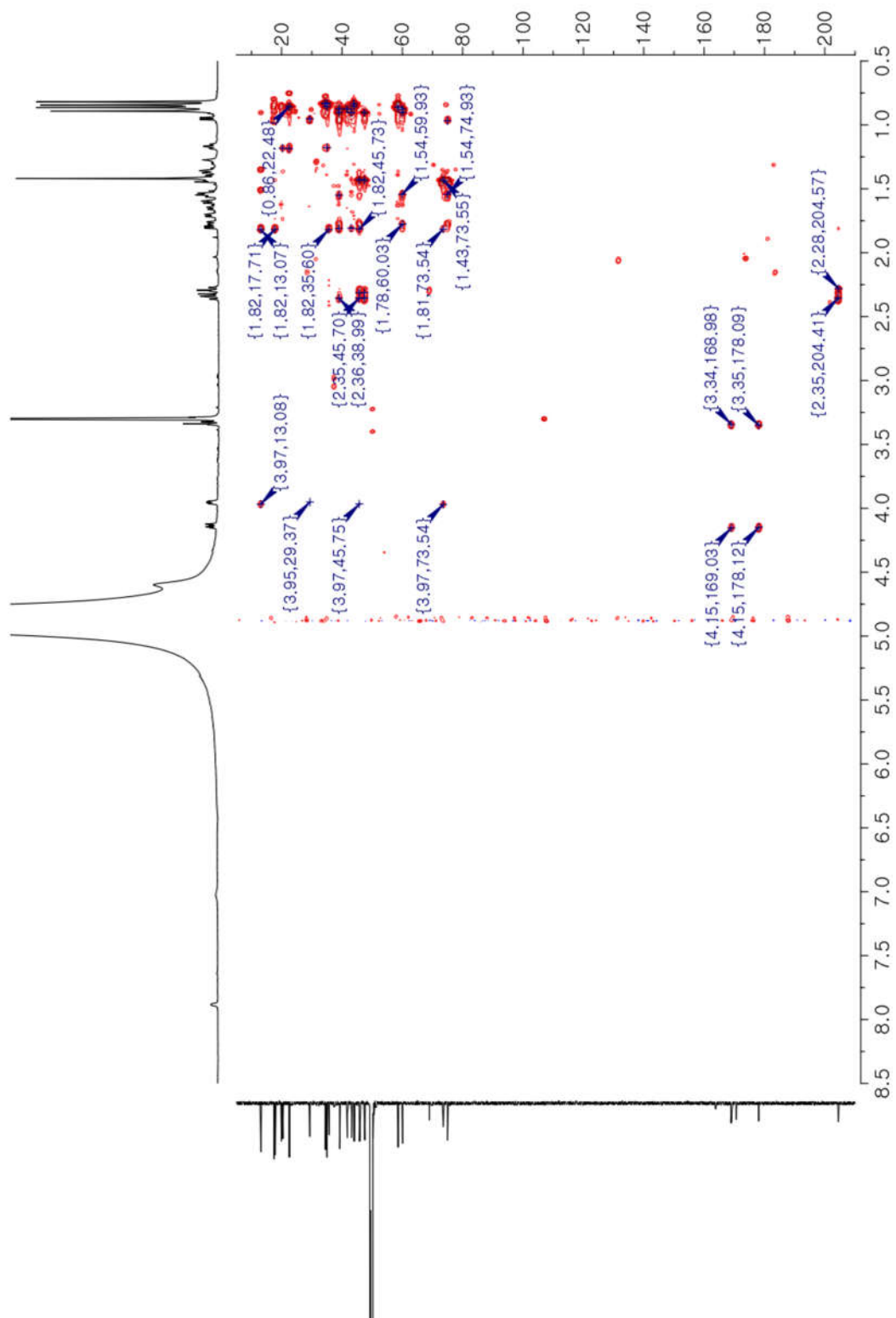
**Figure S4.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_3$ ) spectrum of **1**



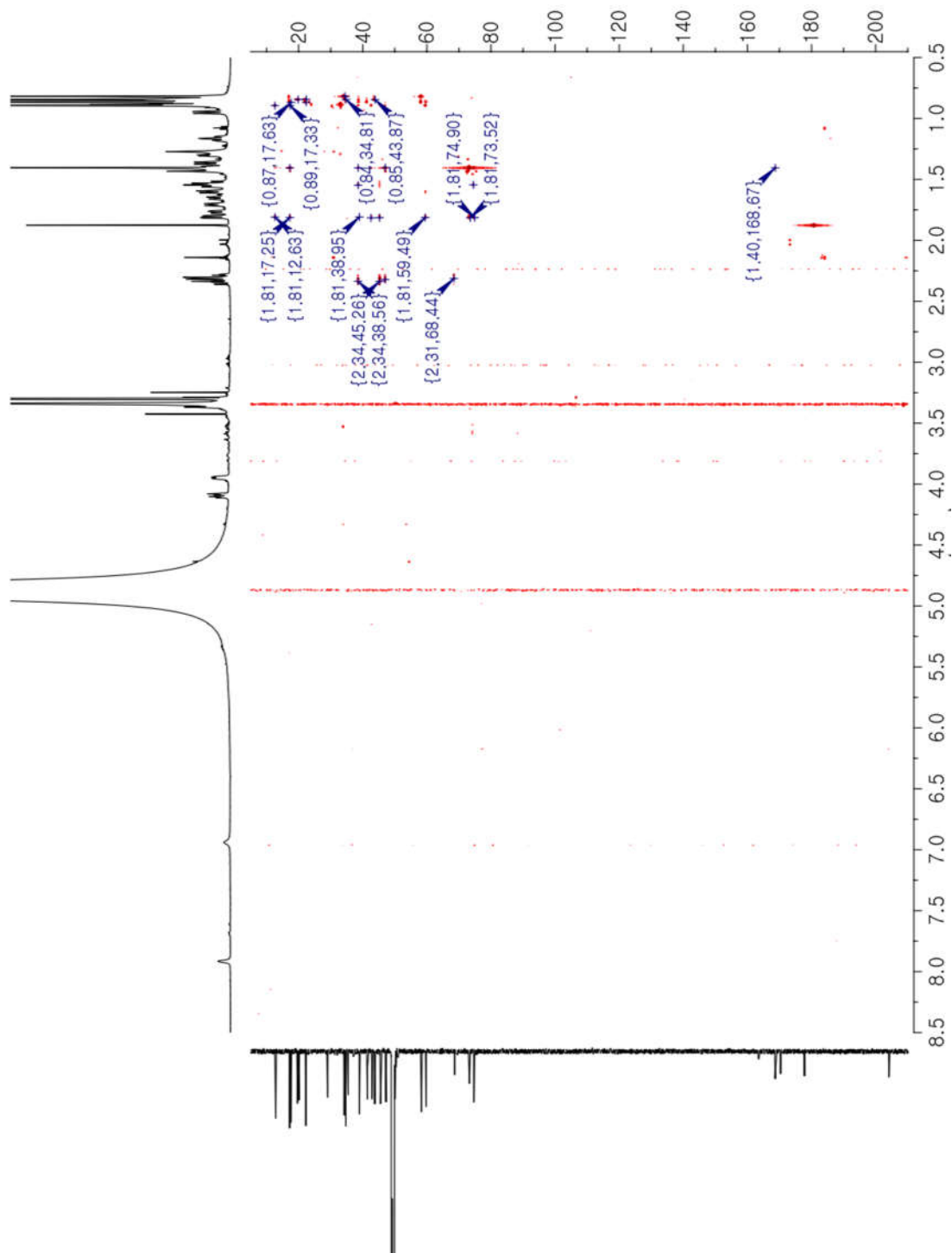
**Figure S5.** The COSY (600 MHz, MeOH-*d*<sub>3</sub>) spectrum of **1**



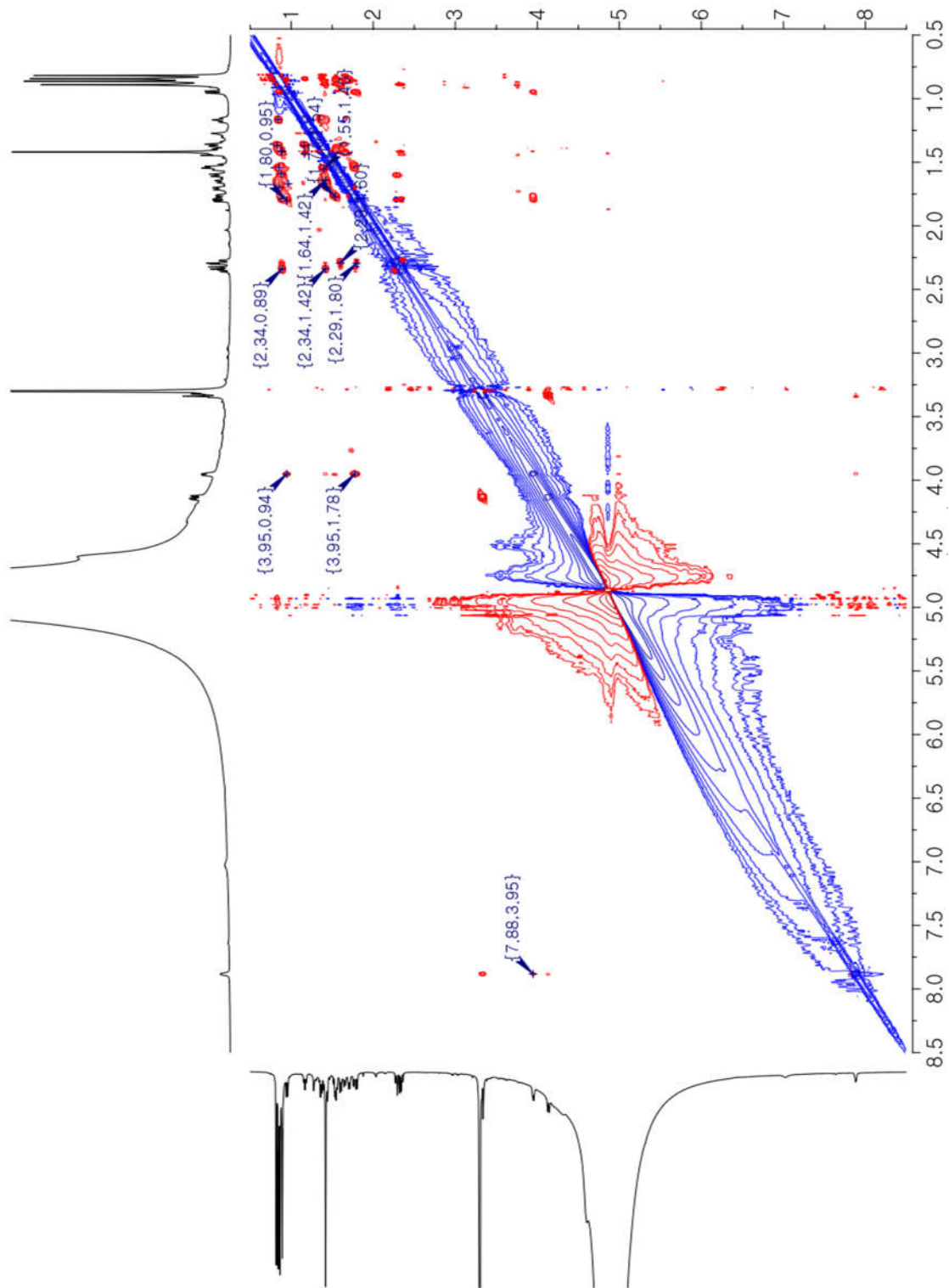
**Figure S6.** The eHSQC (600 MHz,  $\text{MeOH-}d_3$ ) spectrum of **1**



**Figure S7.** The HMBC (600 MHz, MeOH-*d*<sub>3</sub>) spectrum of **1**

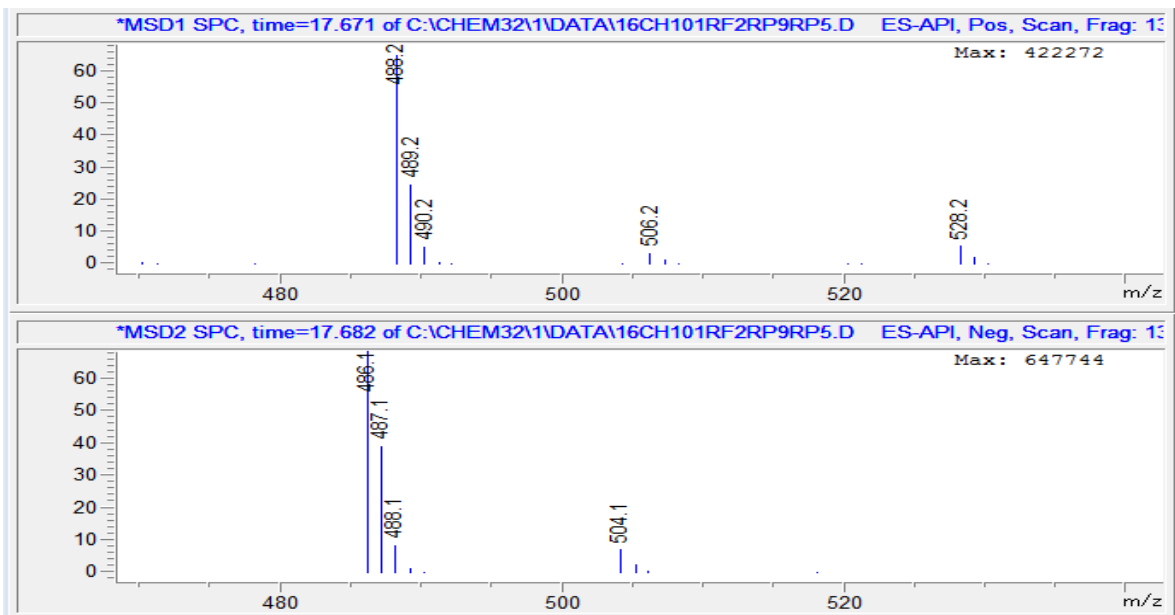


**Figure S8.** The LR-HSQC (600 MHz,  $\text{MeOH-}d_3$ ) spectrum of **1**

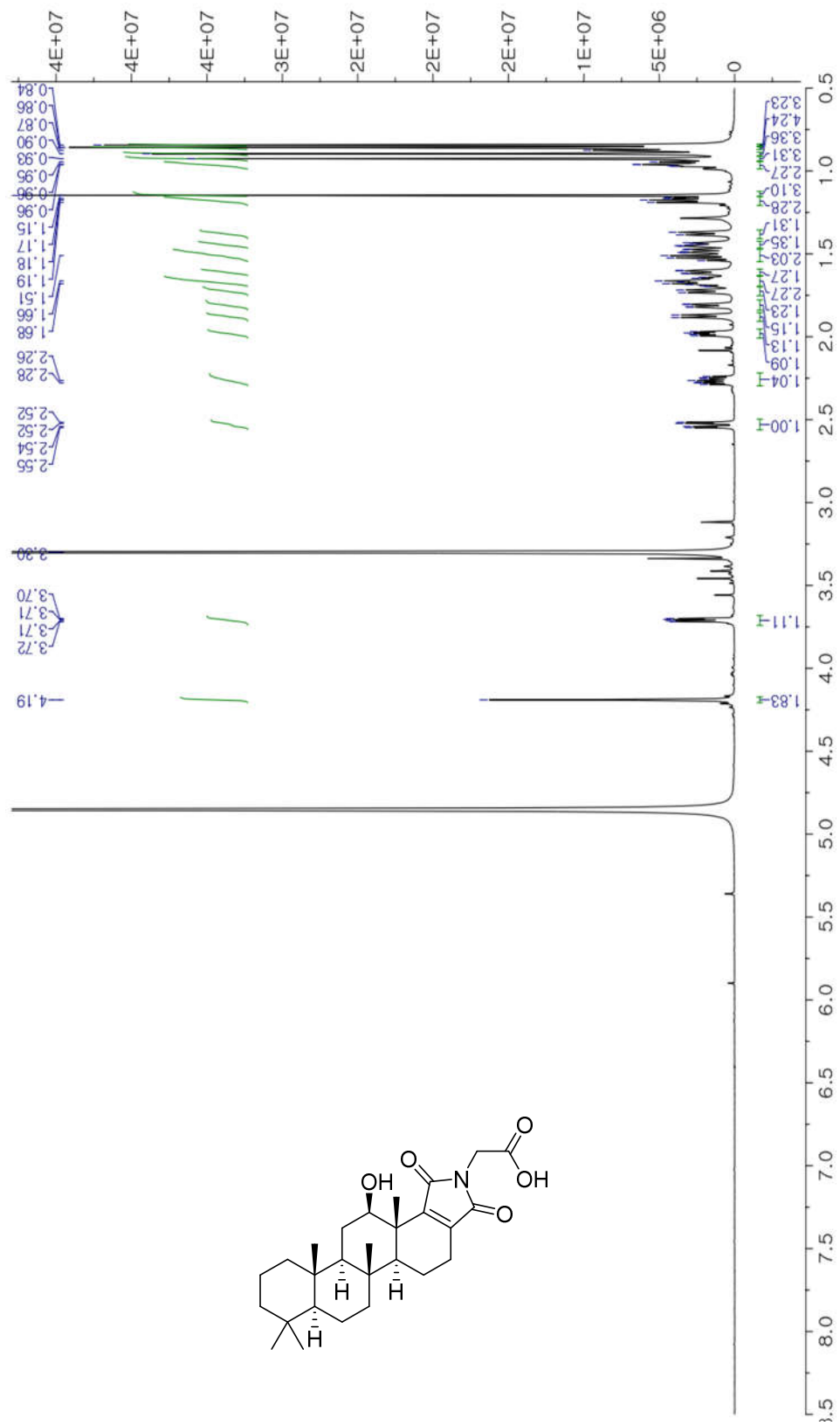


**Figure S9.** The NOESY (600 MHz, MeOH- $d_3$ ) spectrum of **1**

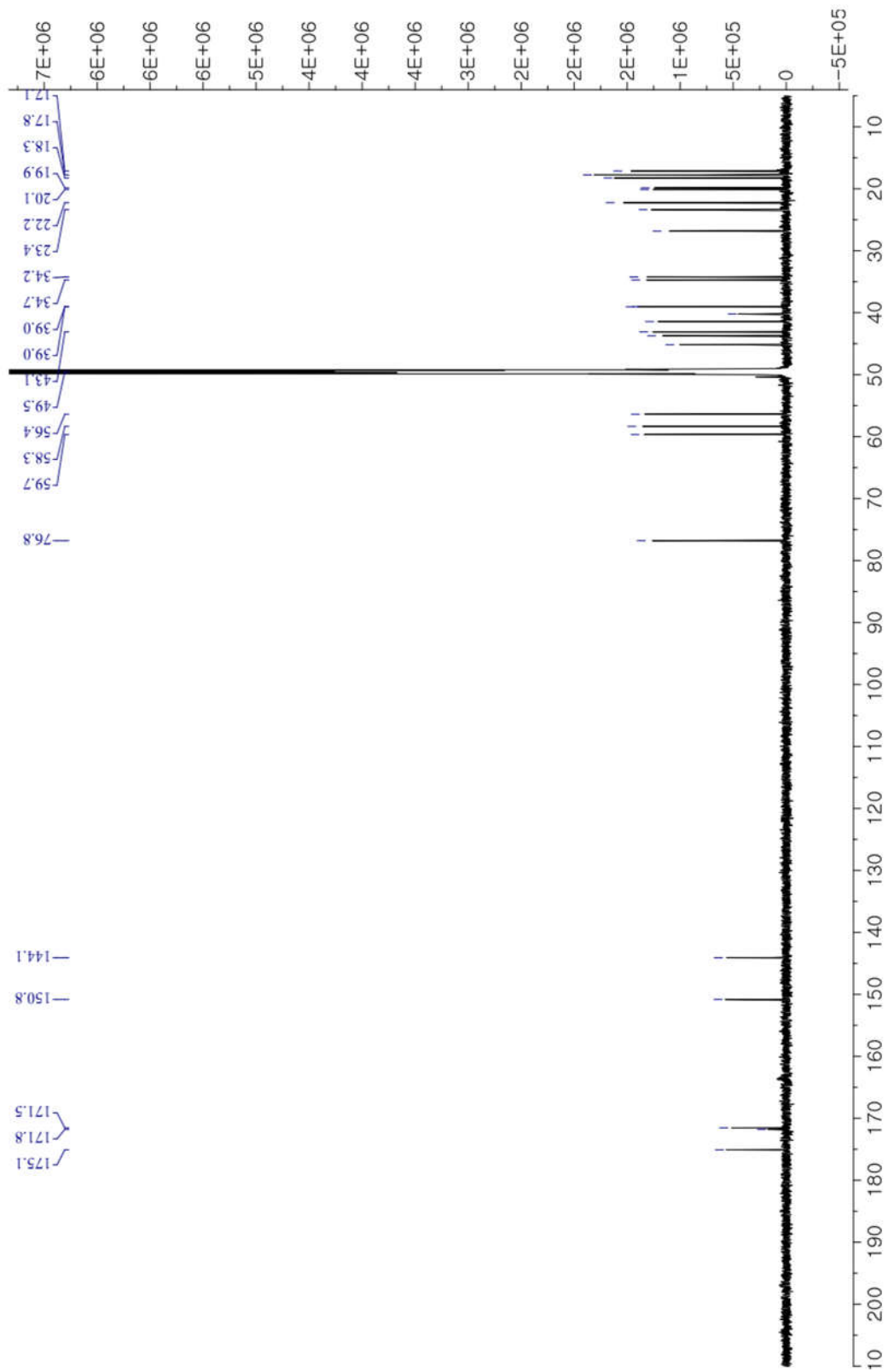




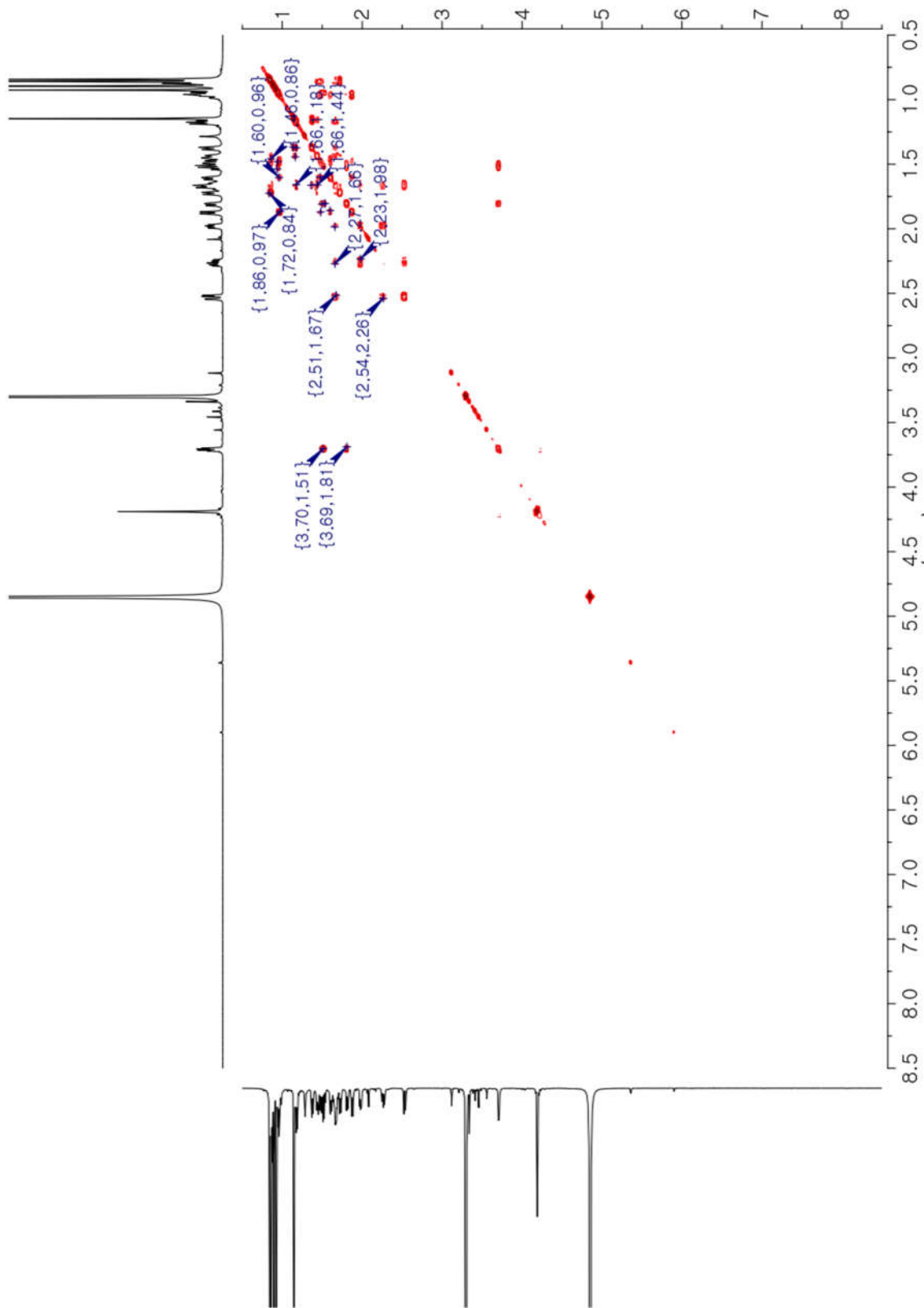
**Figure S10.** ESI/MS isotopic cluster patterns of compound **1** in positive and negative ion modes



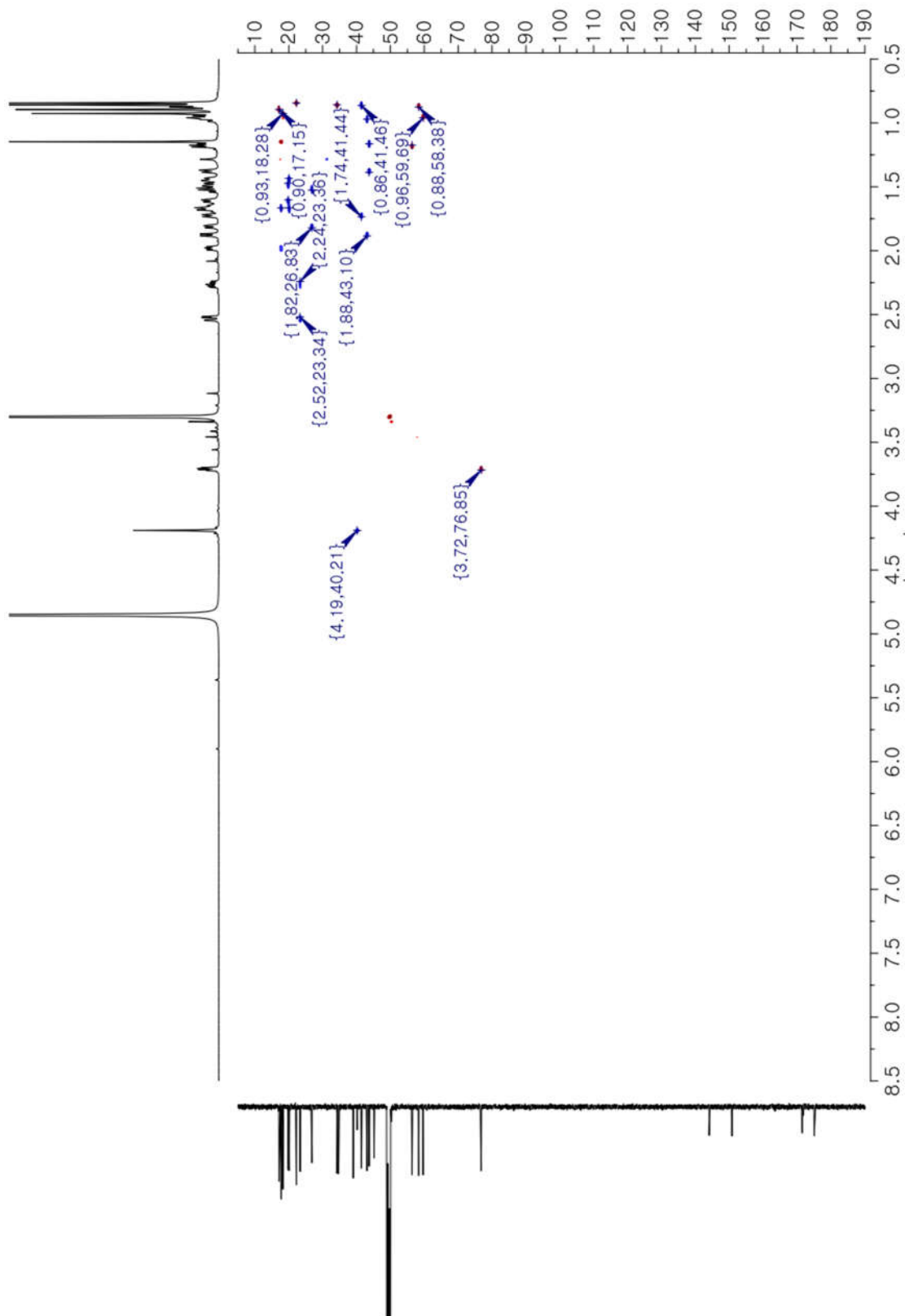
**Figure S11.** The <sup>1</sup>H NMR (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **2**



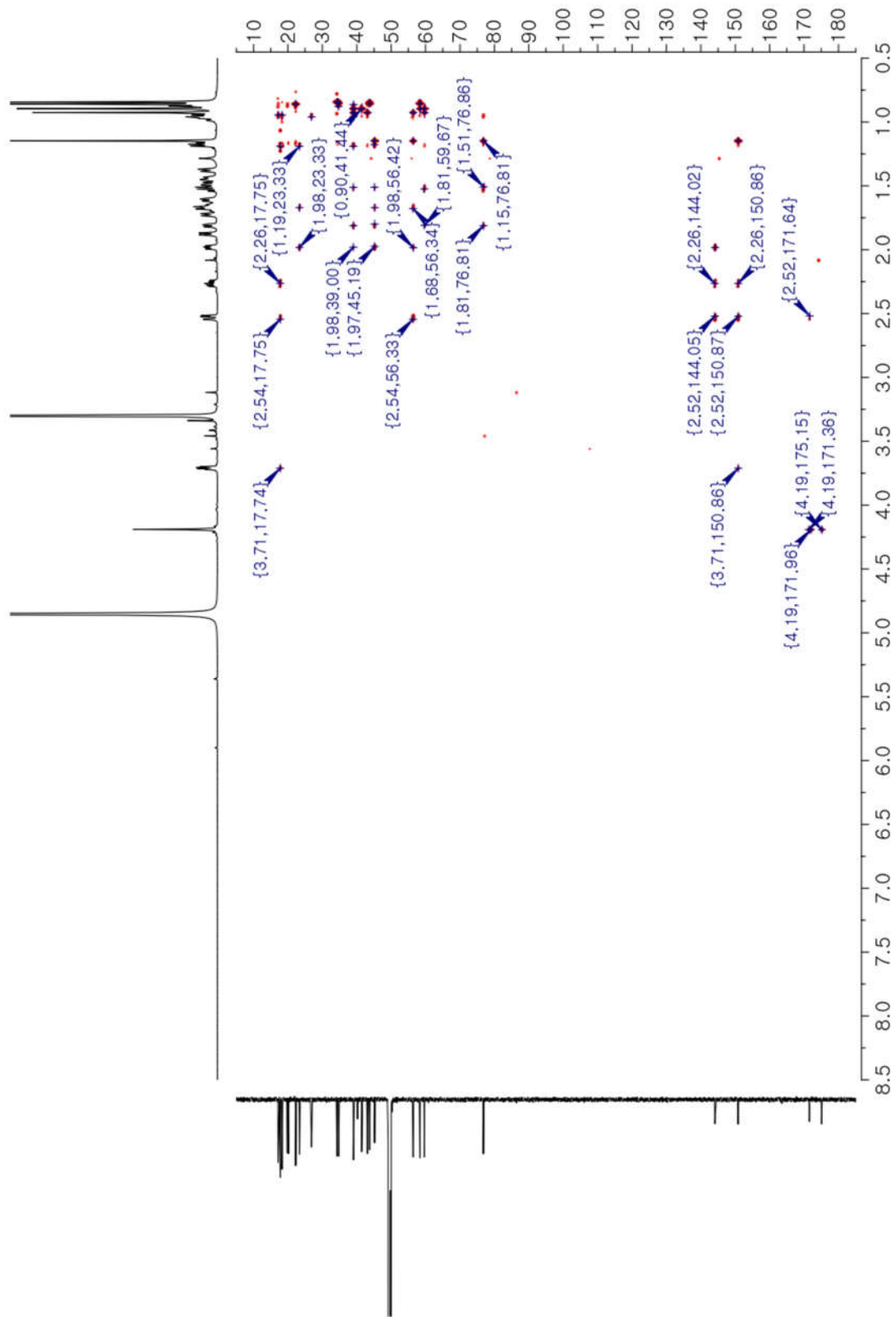
**Figure S12.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of **2**



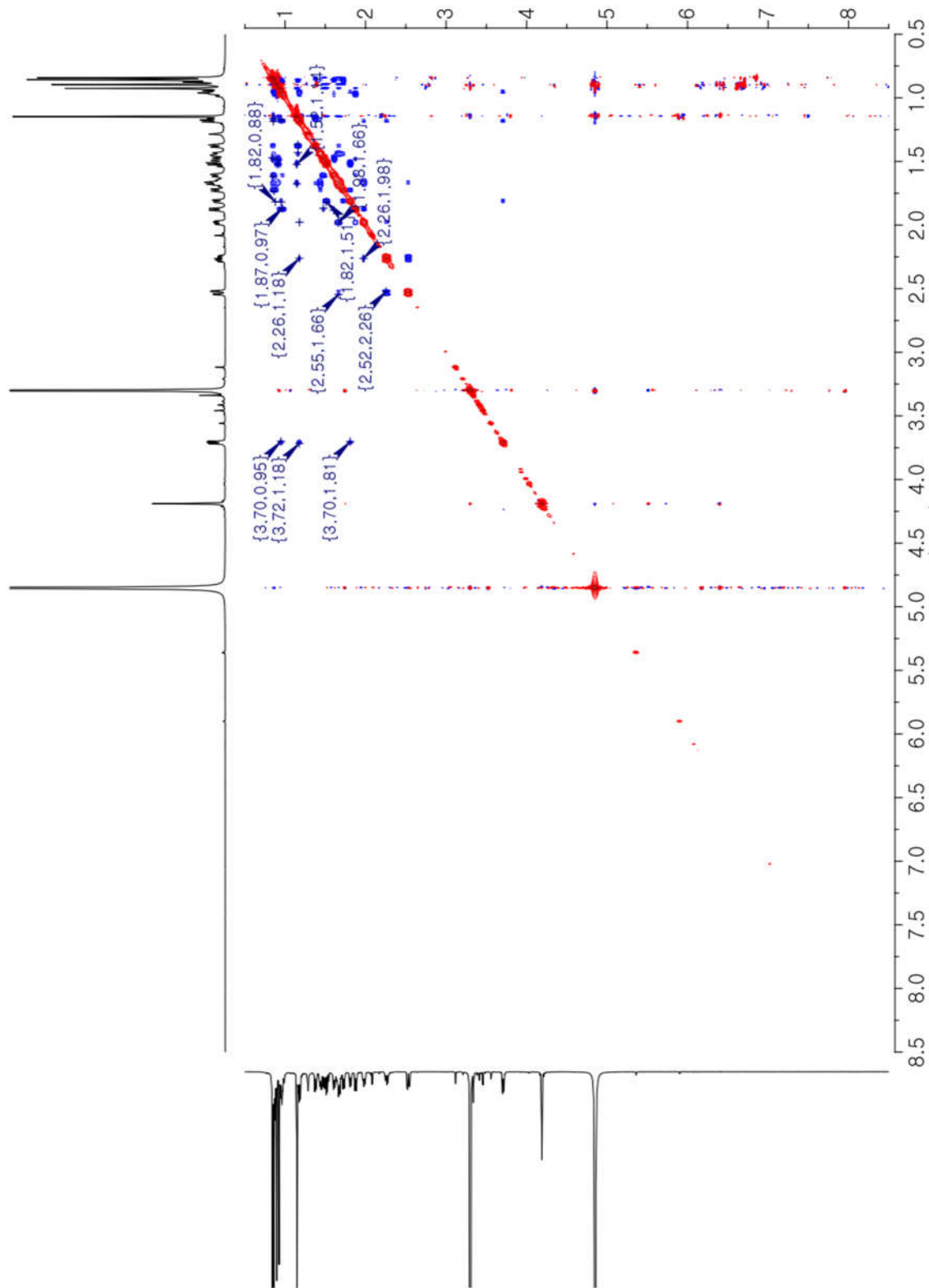
**Figure S13.** The COSY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **2**



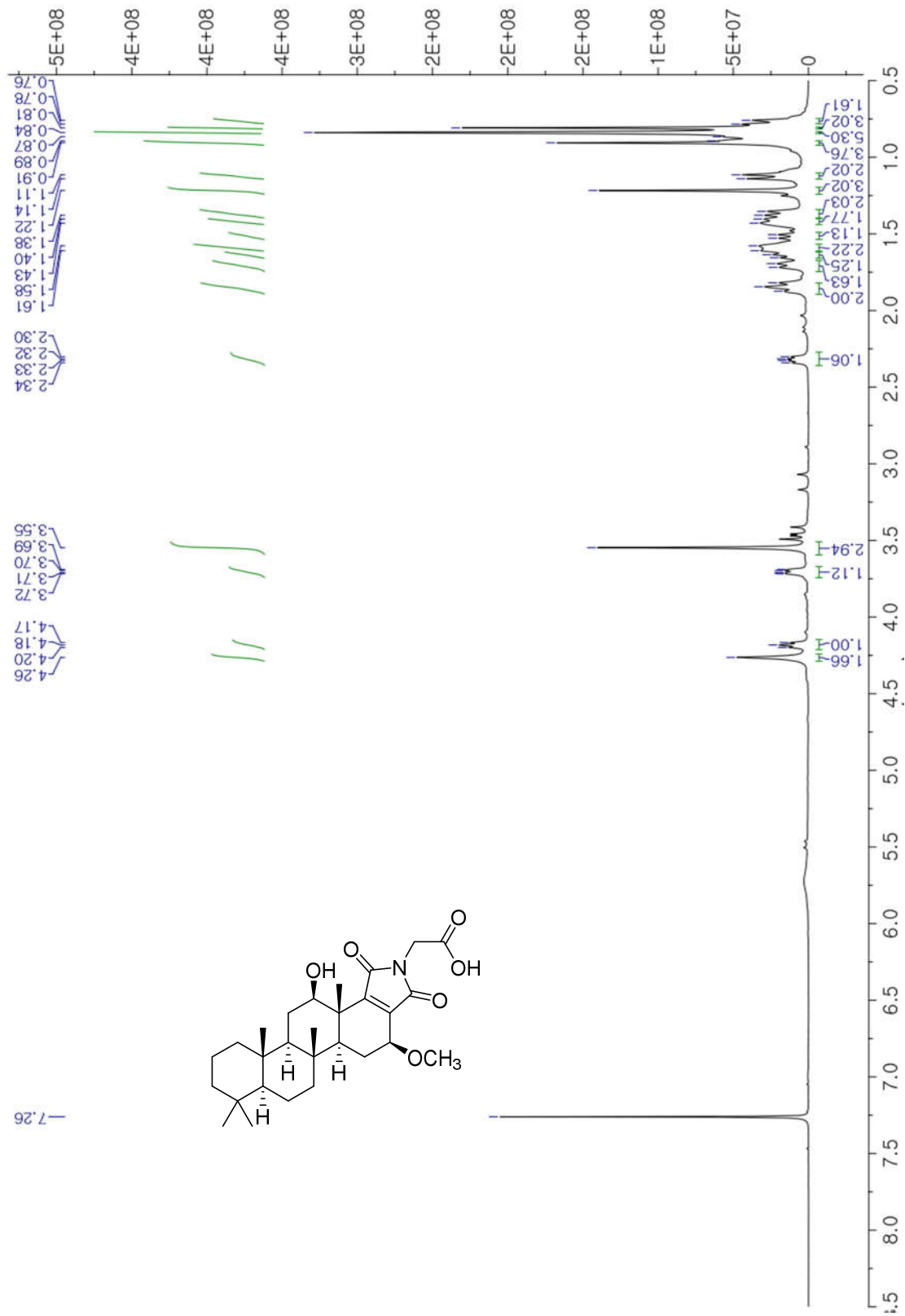
**Figure S14.** The eHSQC (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of **2**



**Figure S15.** The HMBC (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **2**

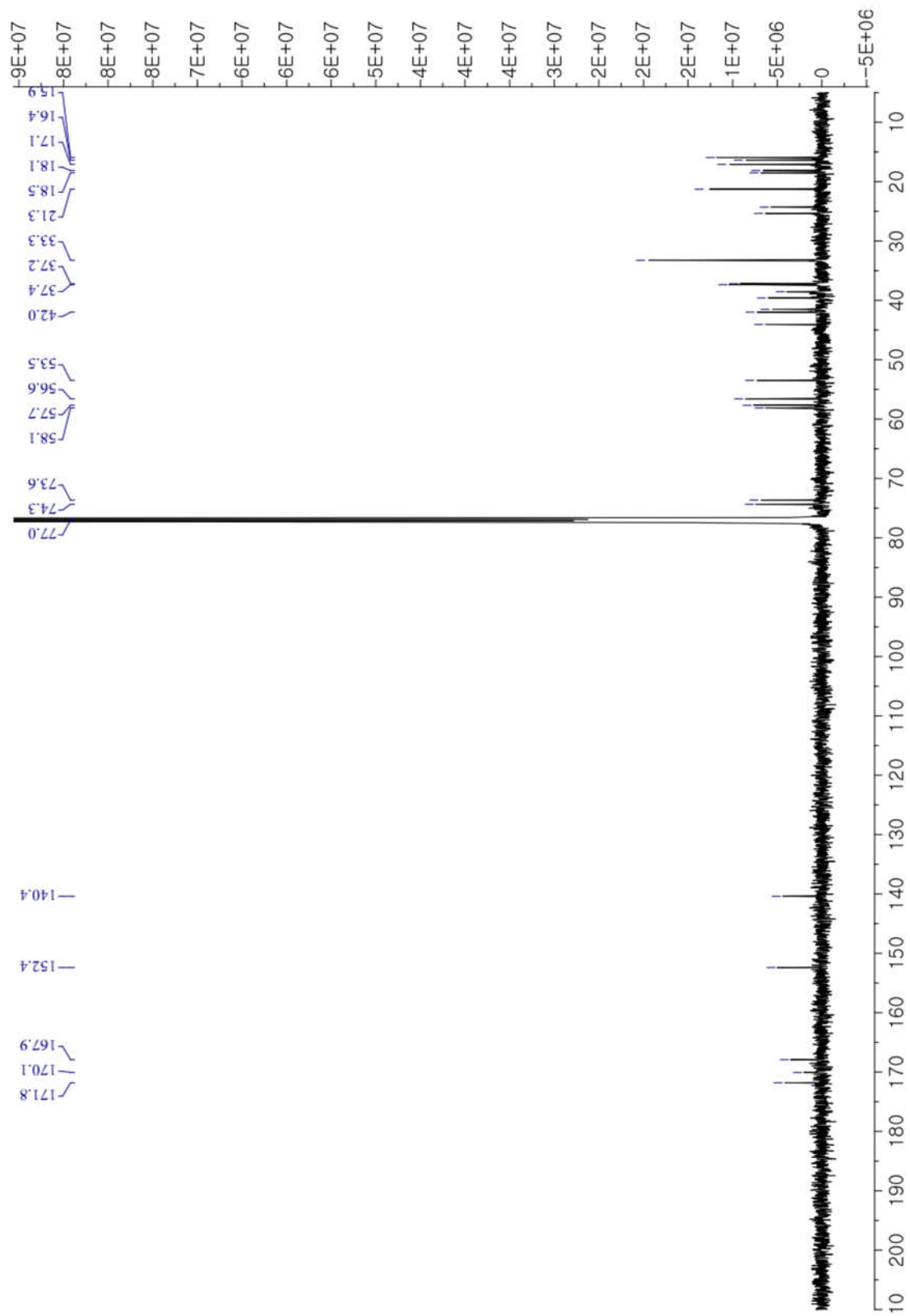


**Figure S16.** The NOESY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **2**

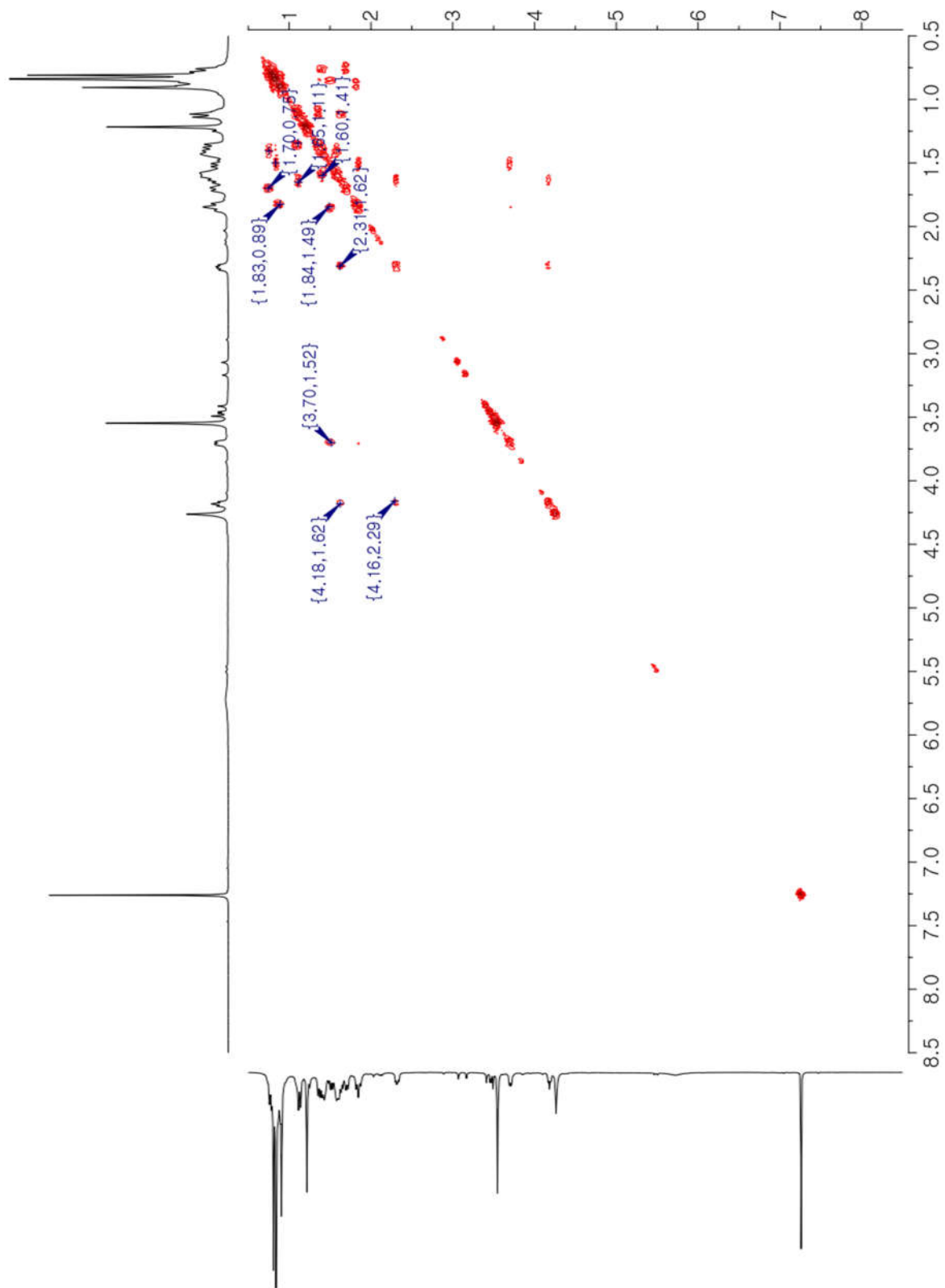


**Figure S17.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of **3**





**Figure S18.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **3**



**Figure S19.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **3**

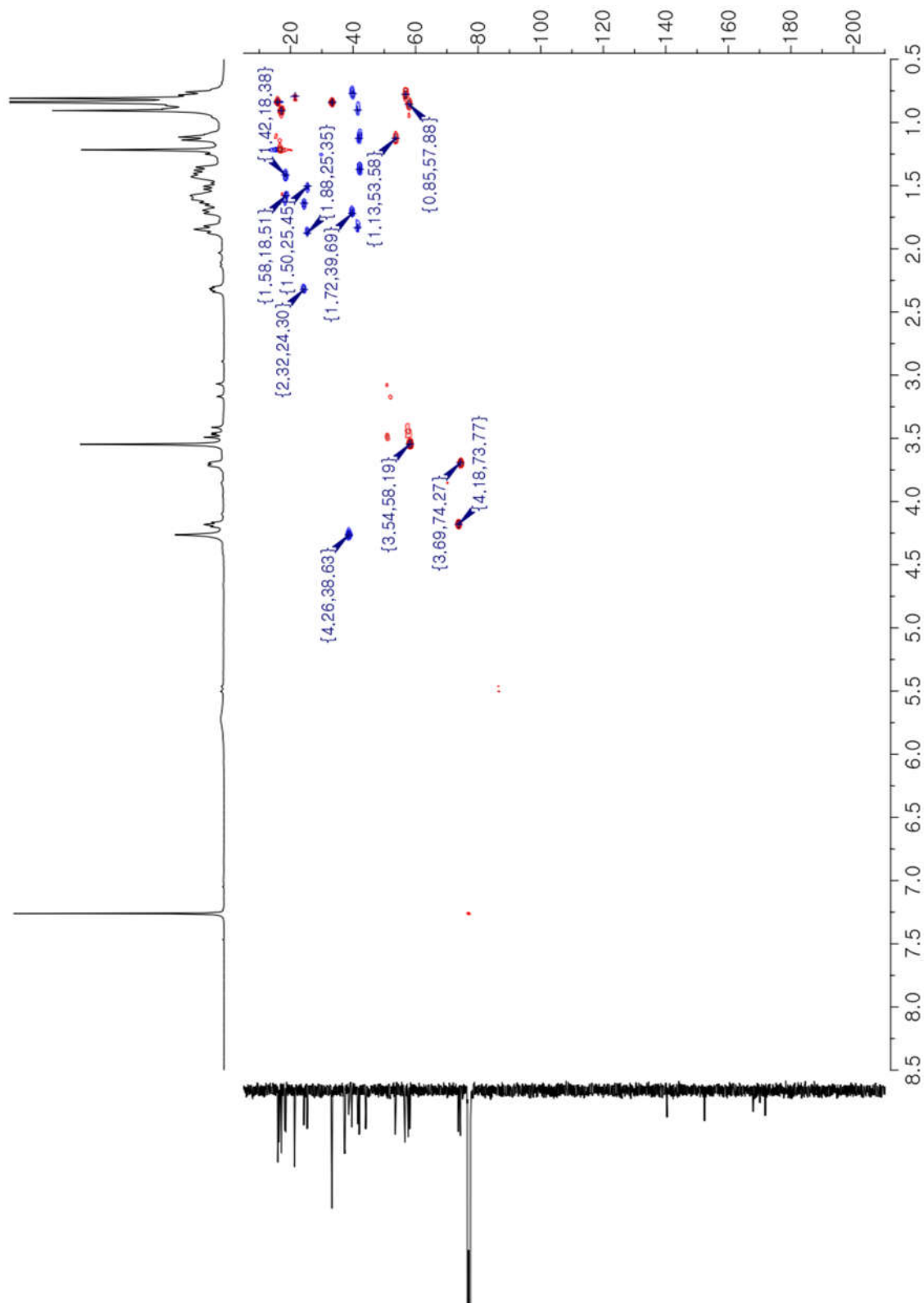


Figure S20. The eHSQC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **3**

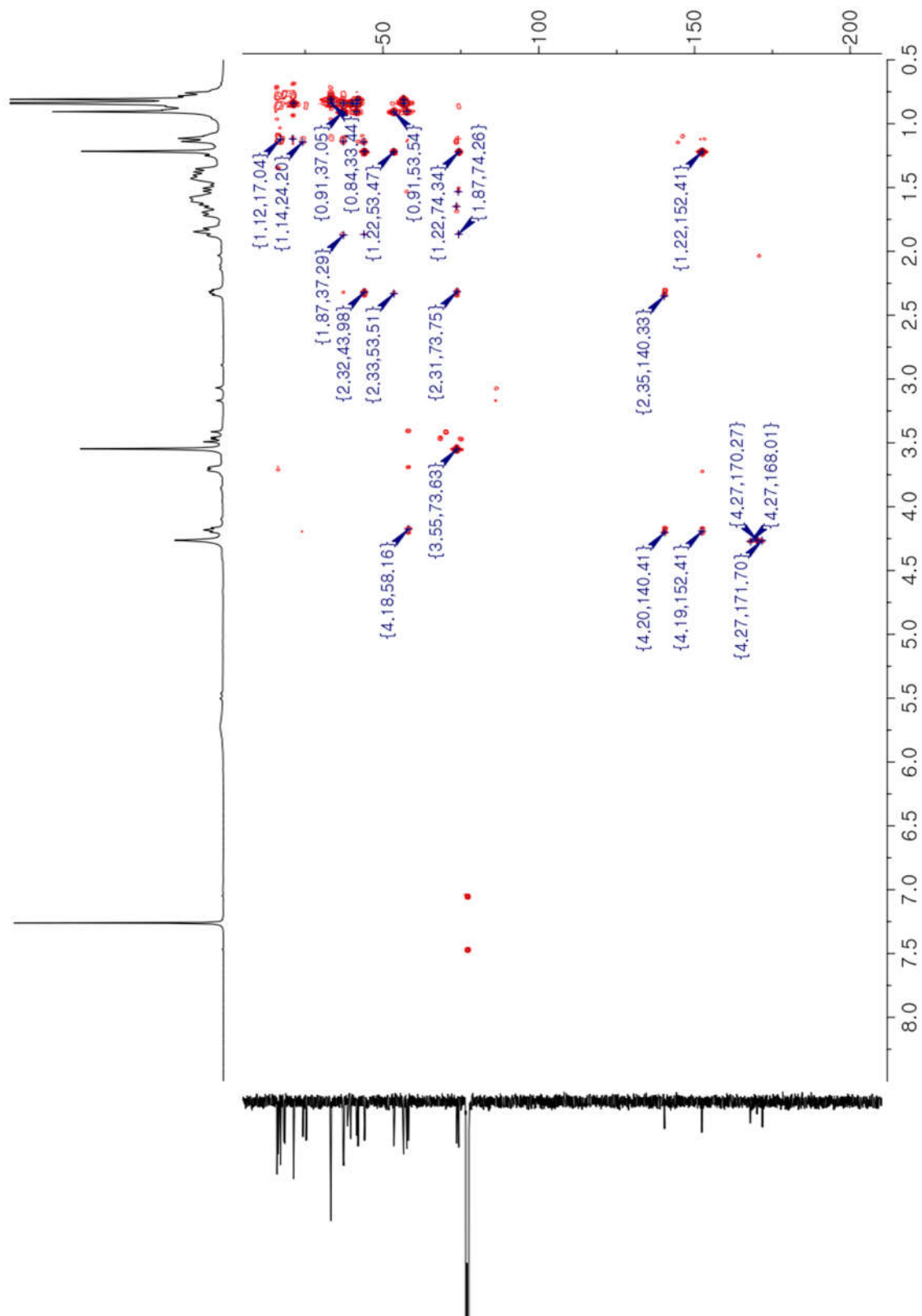
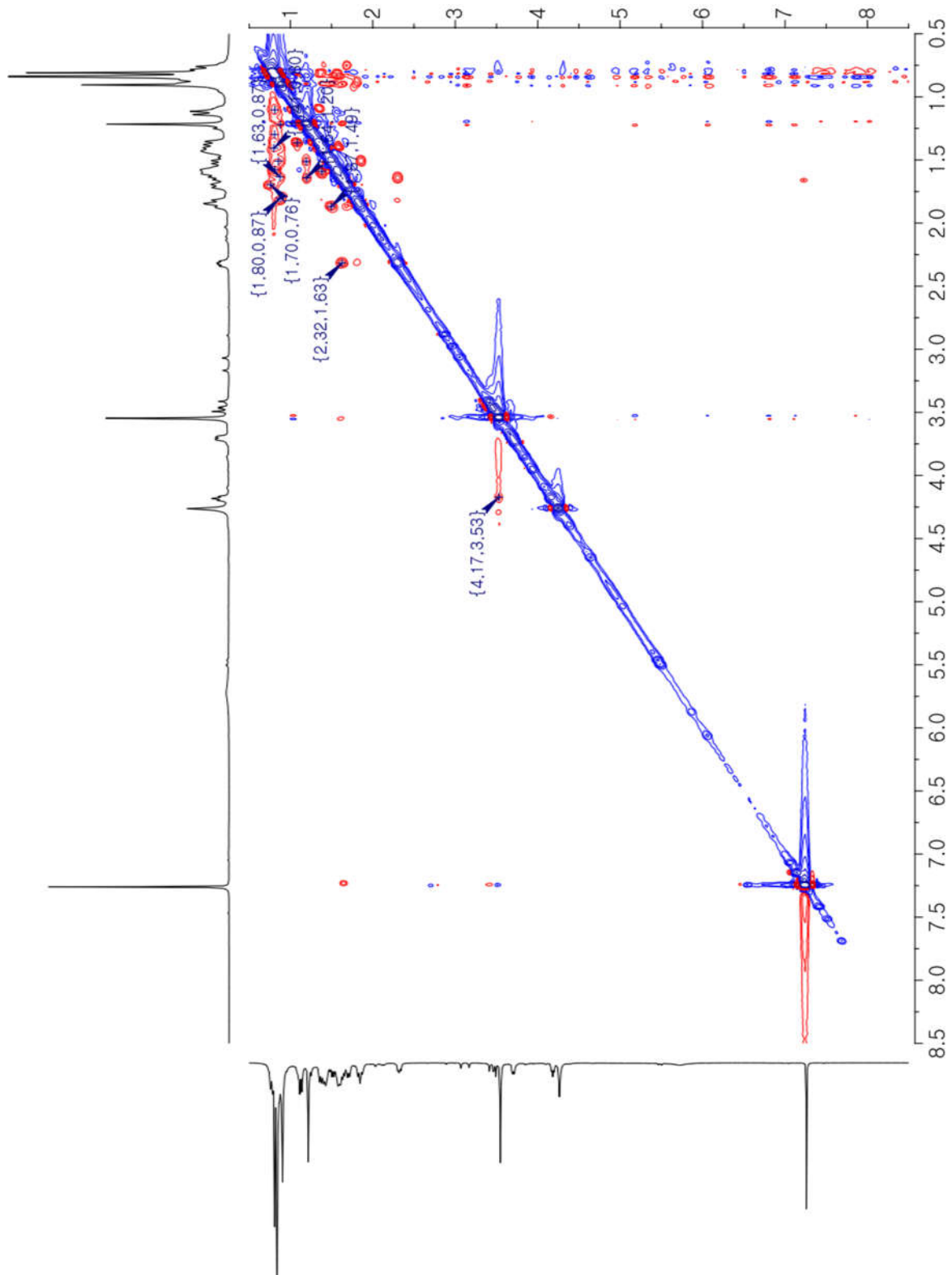
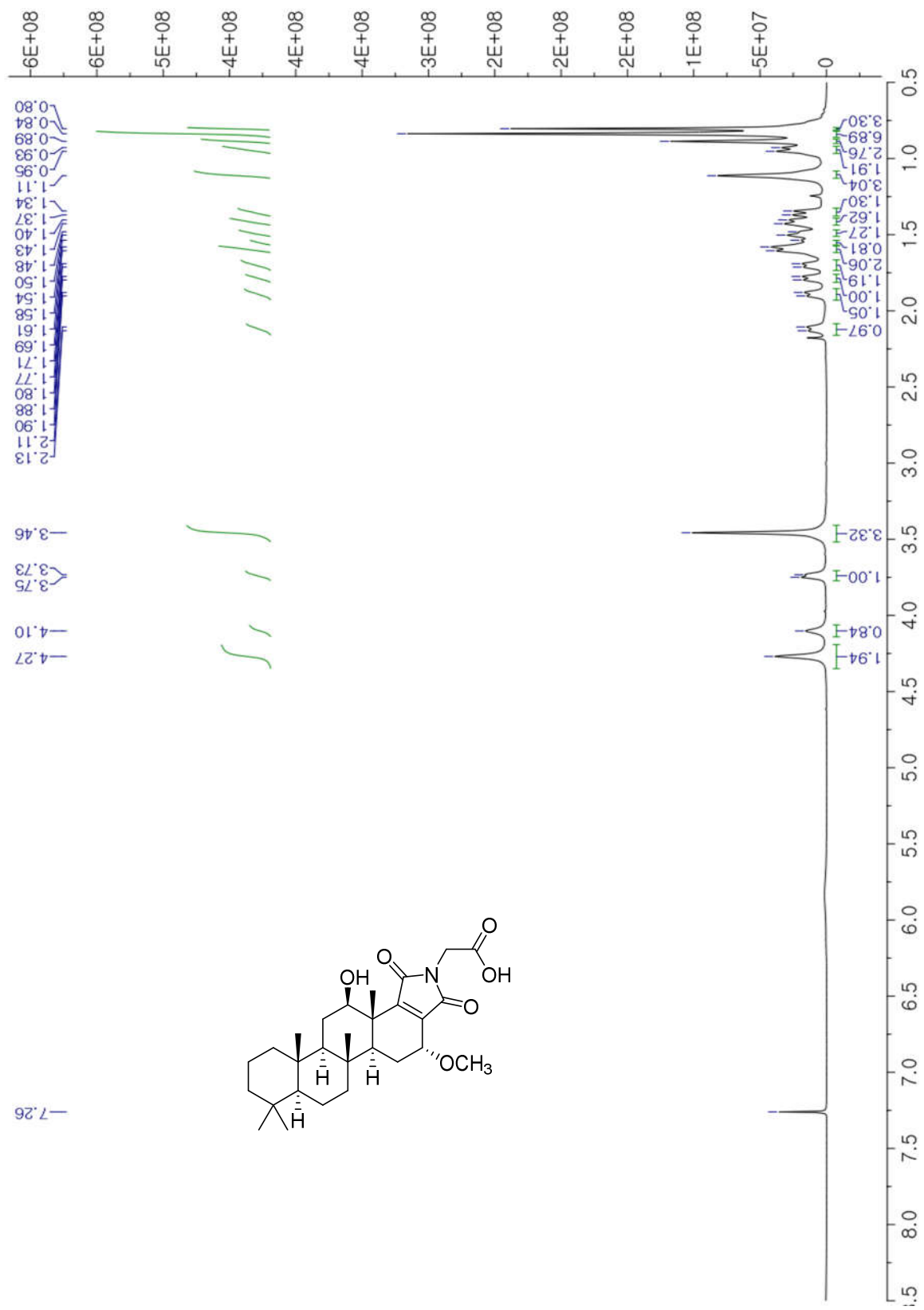


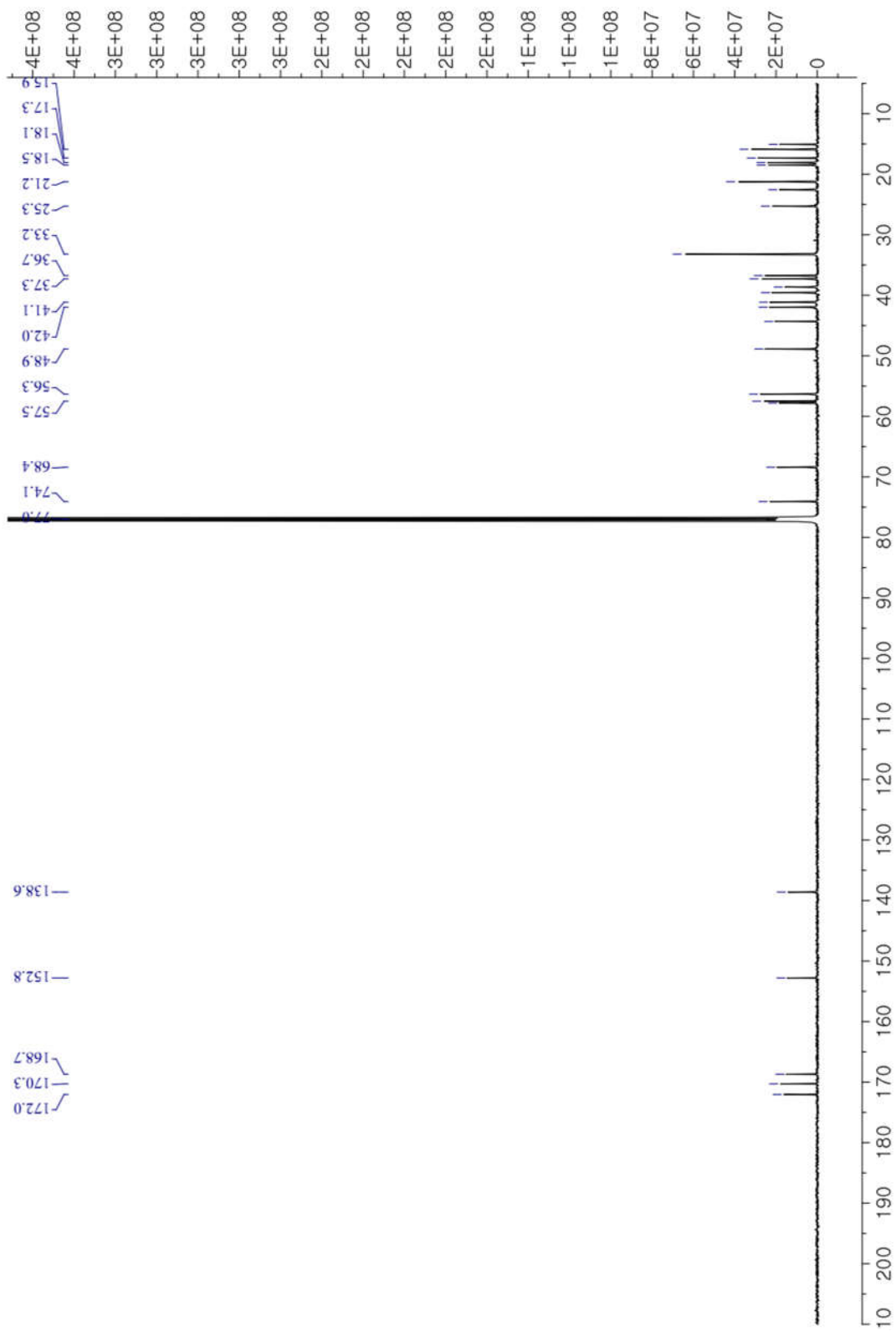
Figure S21. The HMBC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **3**



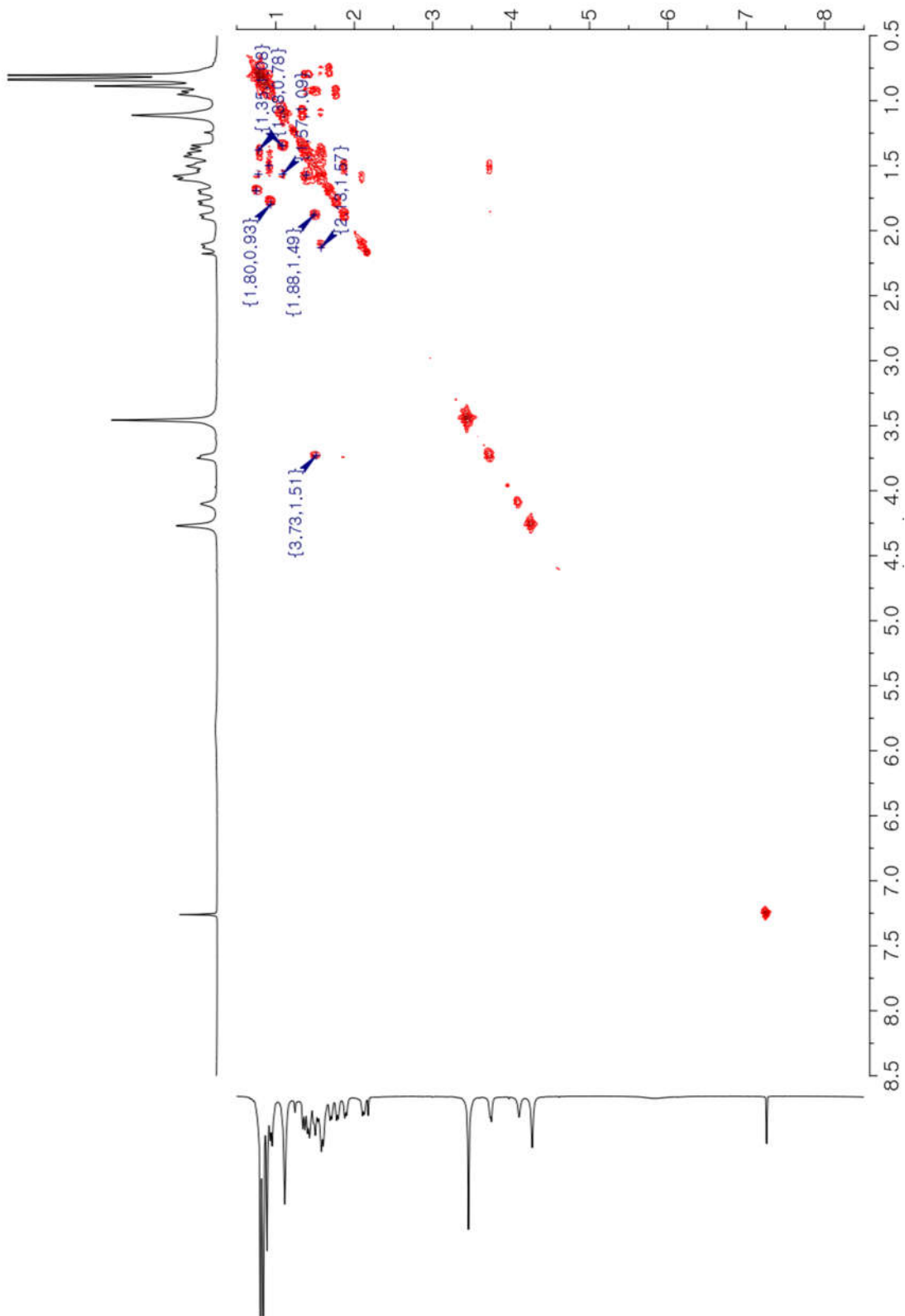
**Figure S22.** The NOESY (600 MHz, CDCl<sub>3</sub>) spectrum of **3**



**Figure S23.** The <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of 4

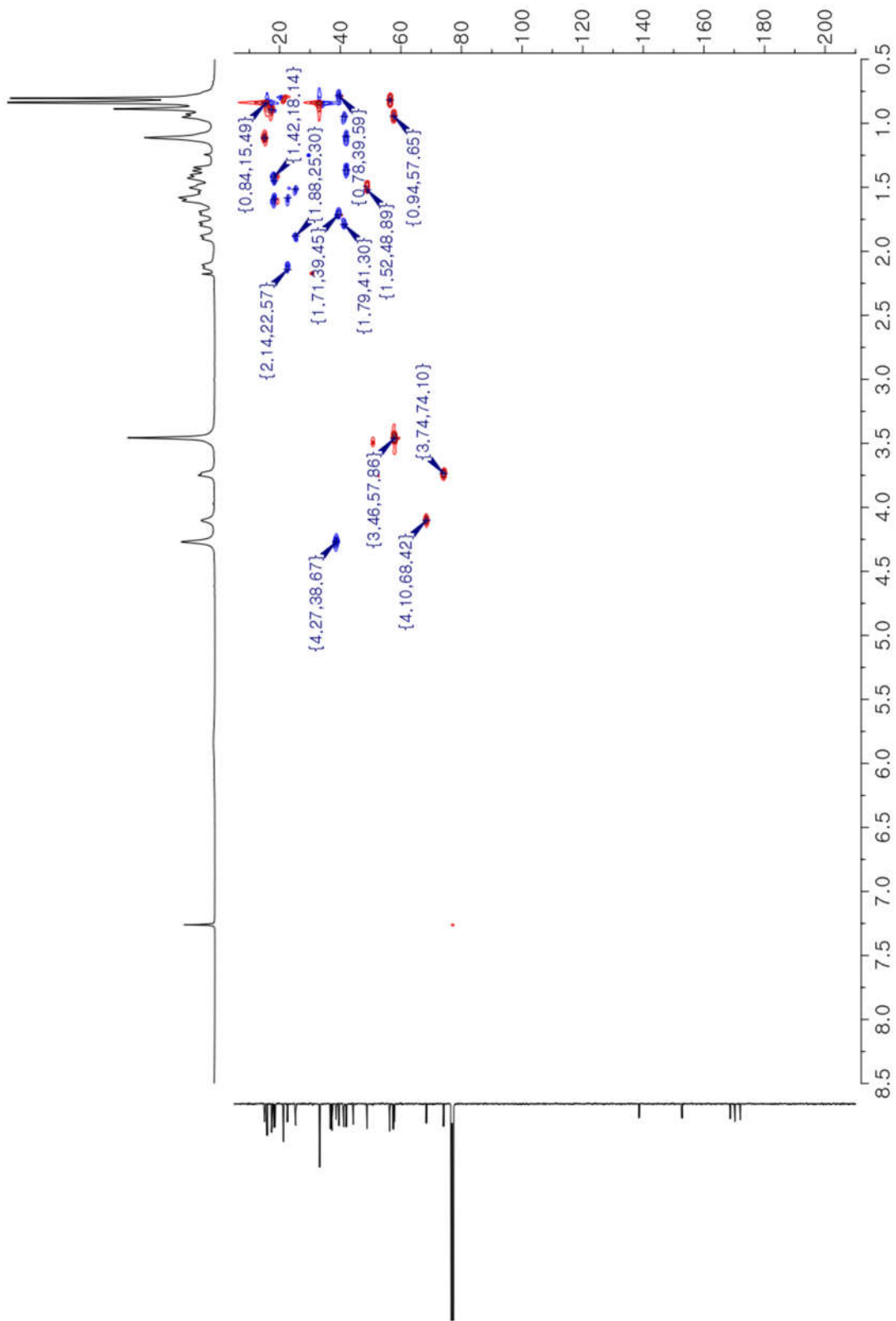


**Figure S24.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **4**



**Figure S25.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **4**





**Figure S26.** The eHSQC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **4**

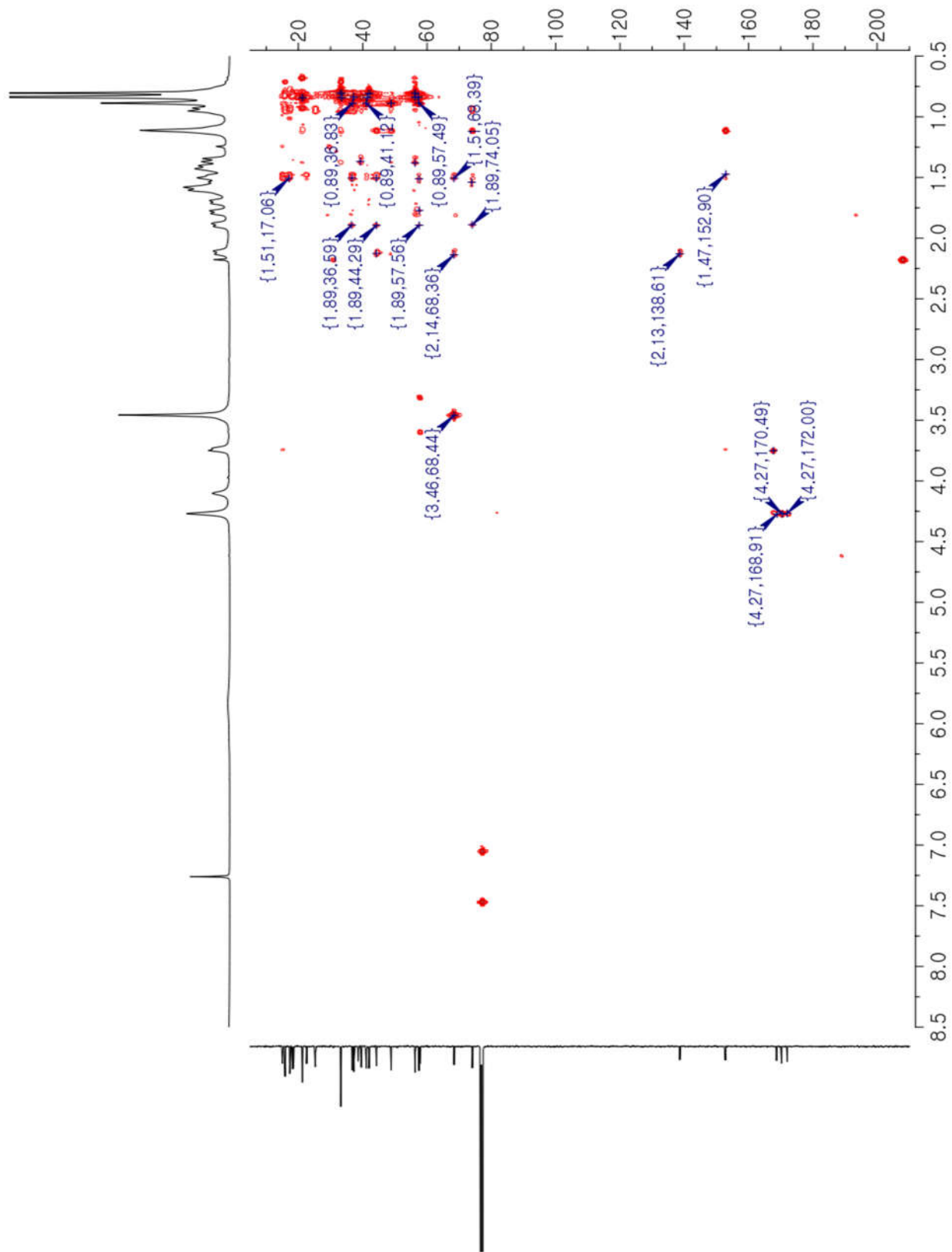
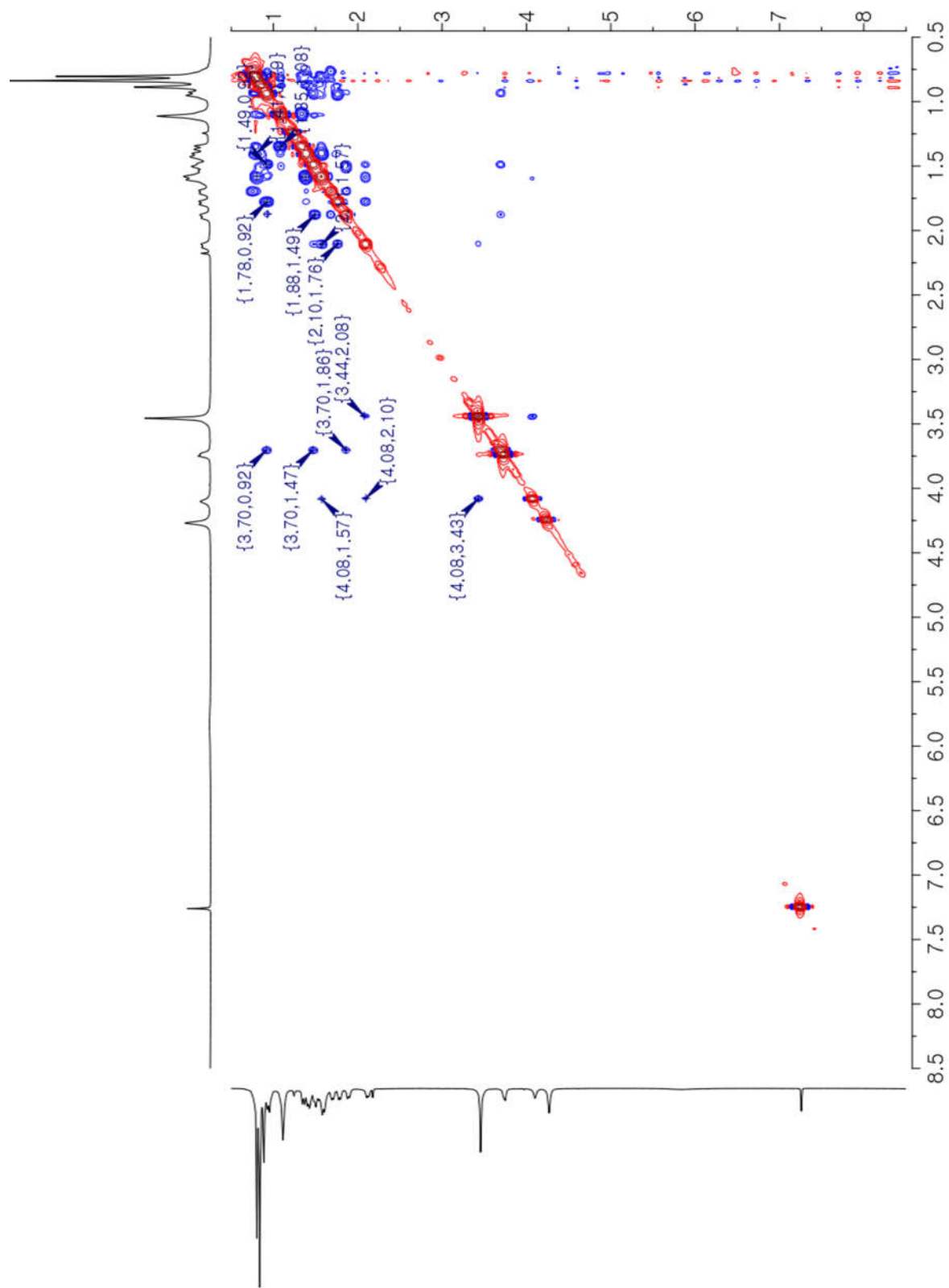
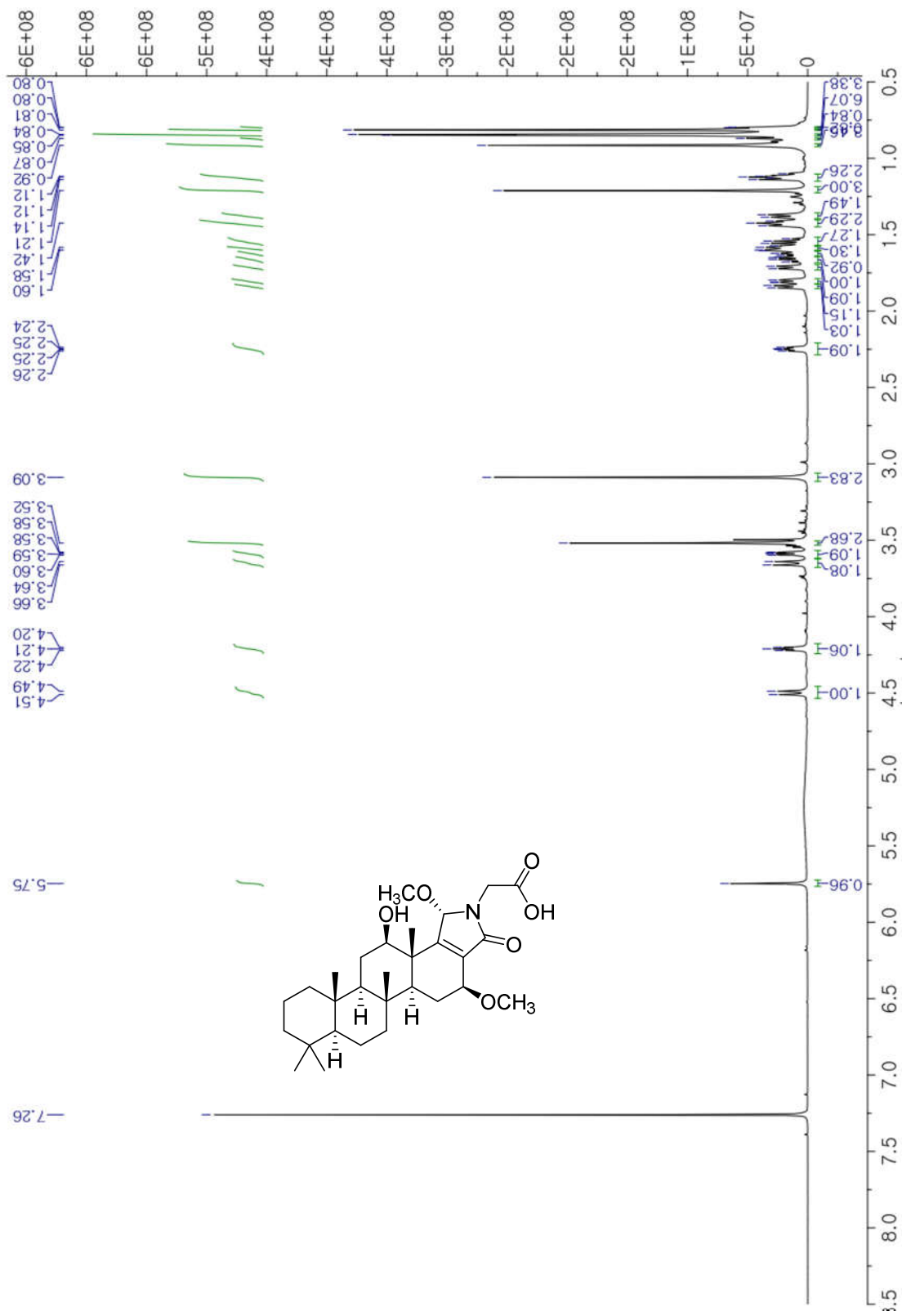


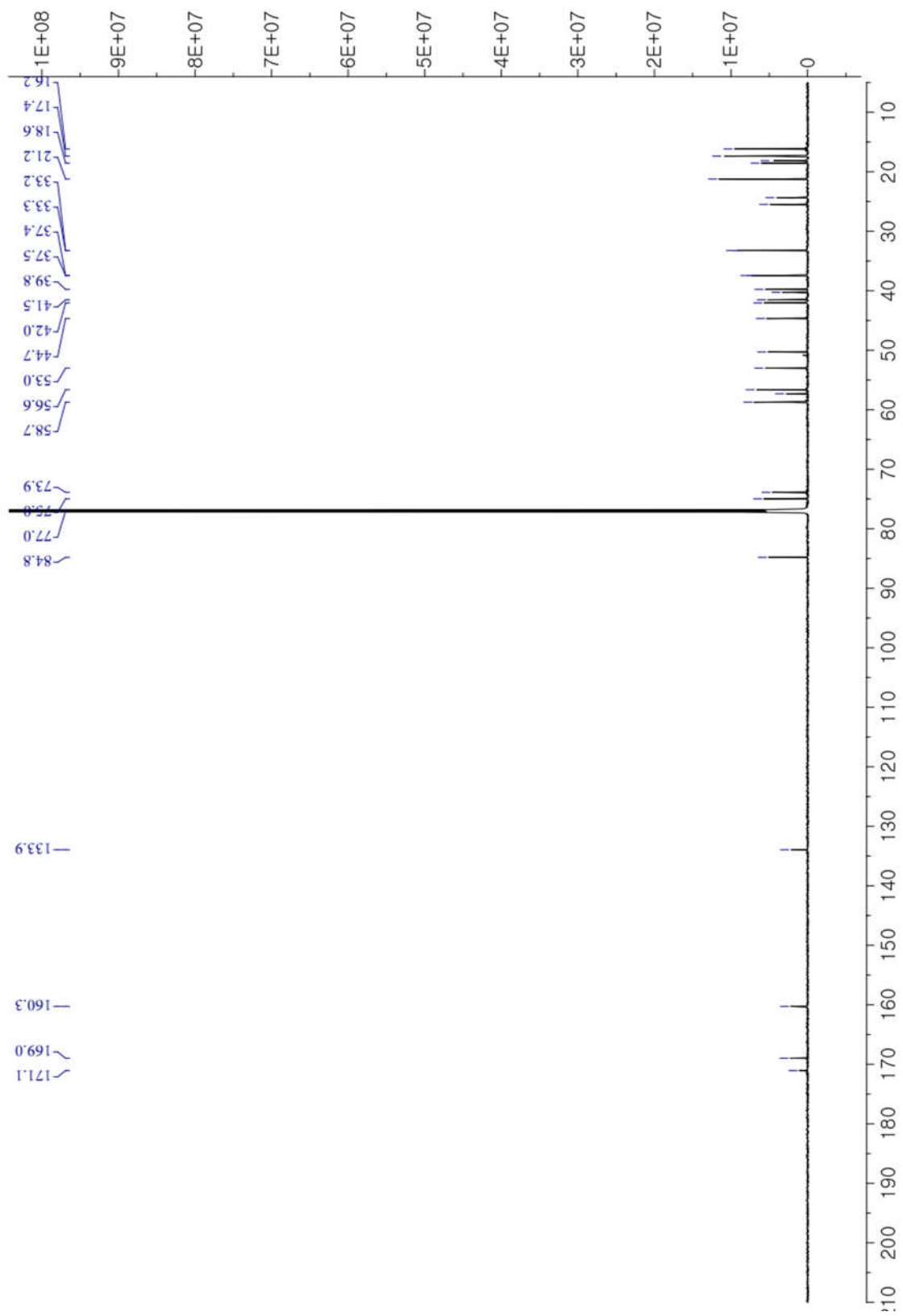
Figure S27. The HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of **4**



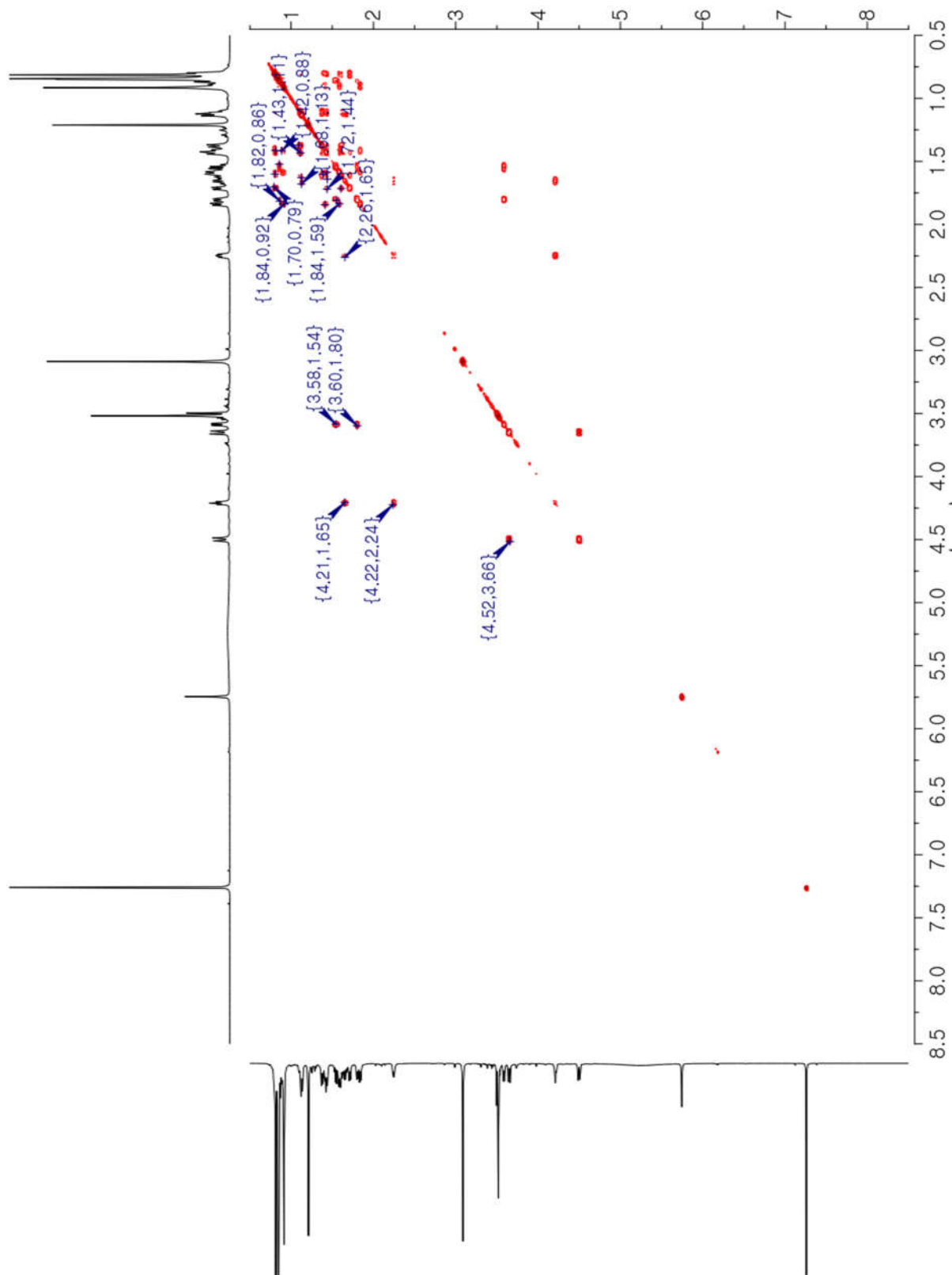
**Figure S28.** The NOESY (600 MHz,  $\text{CDCl}_3$ ) spectrum of **4**



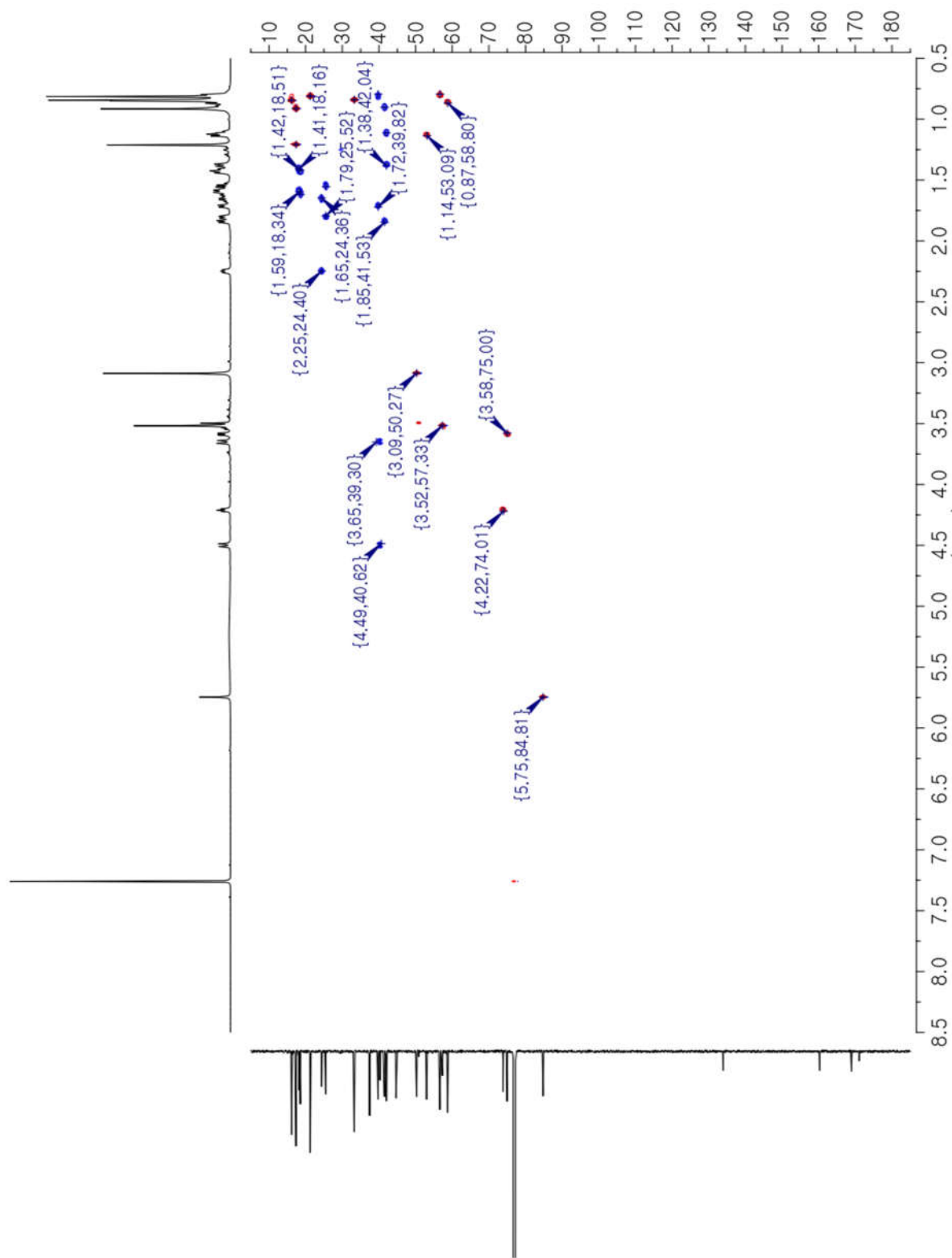
**Figure S29.** The <sup>1</sup>H NMR (600 MHz, CDCl<sub>3</sub>) spectrum of **5**



**Figure S30.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **5**



**Figure S31.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **5**



**Figure S32.** The eHSQC (600 MHz, CDCl<sub>3</sub>) spectrum of **5**

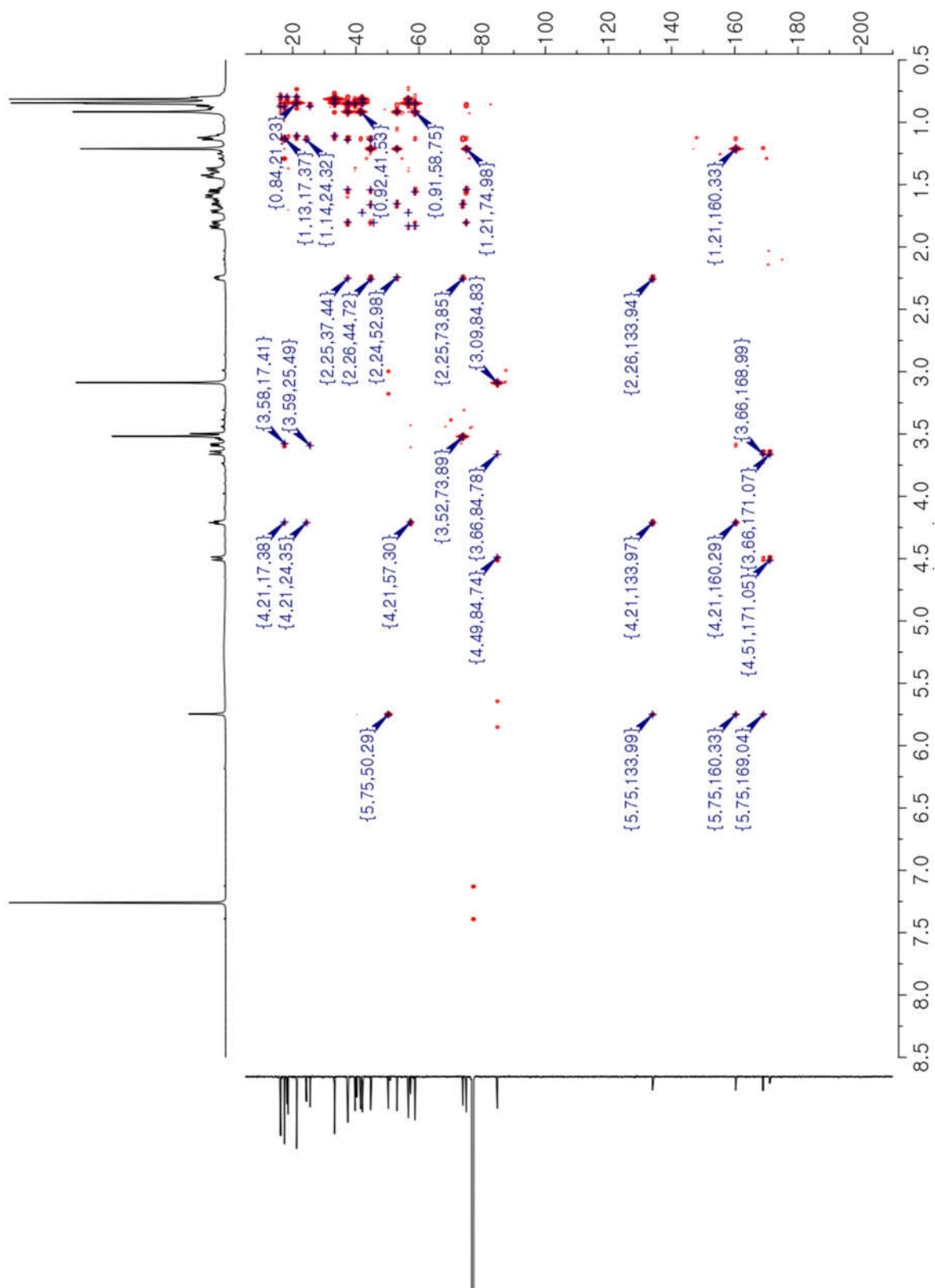
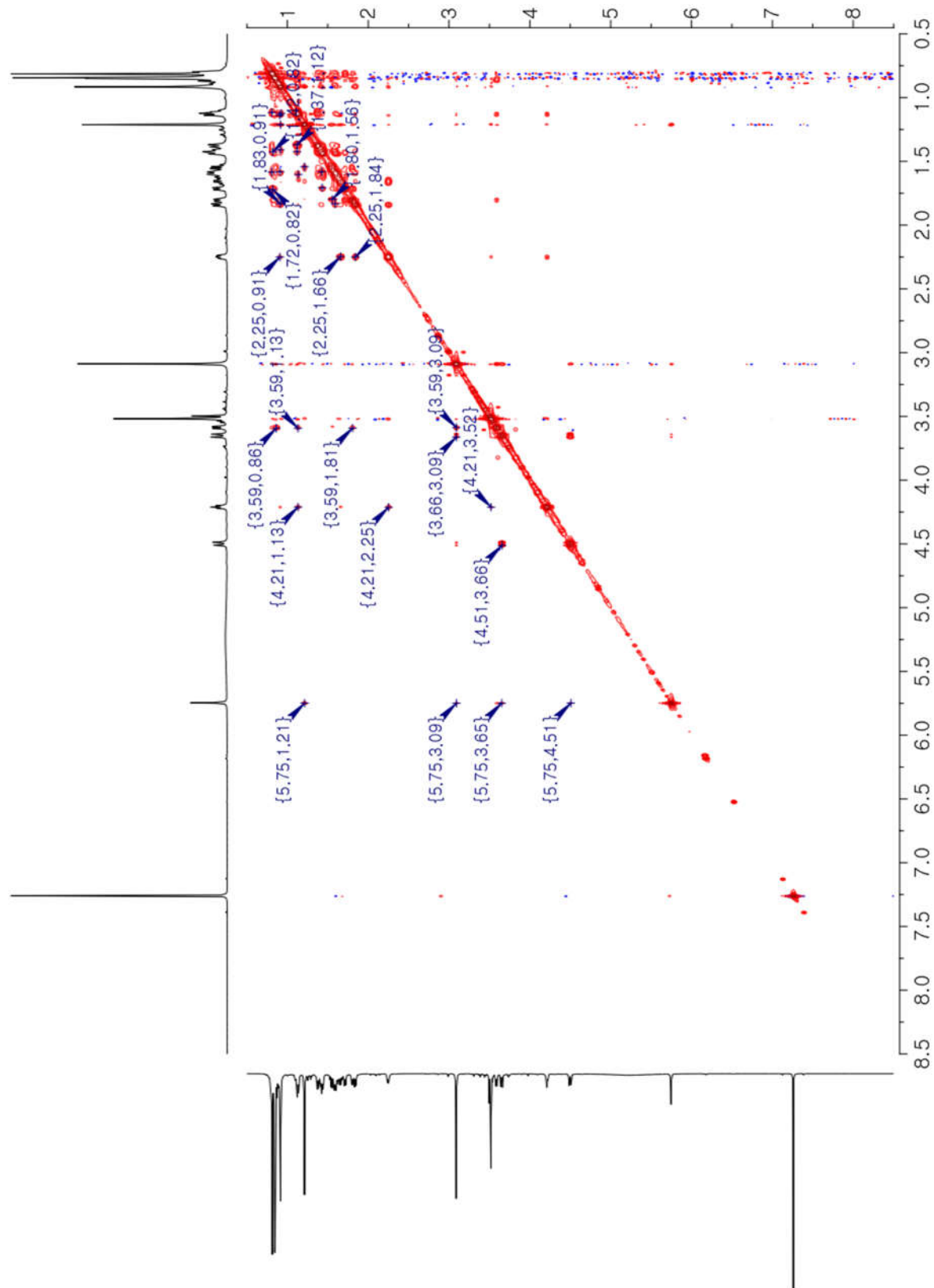
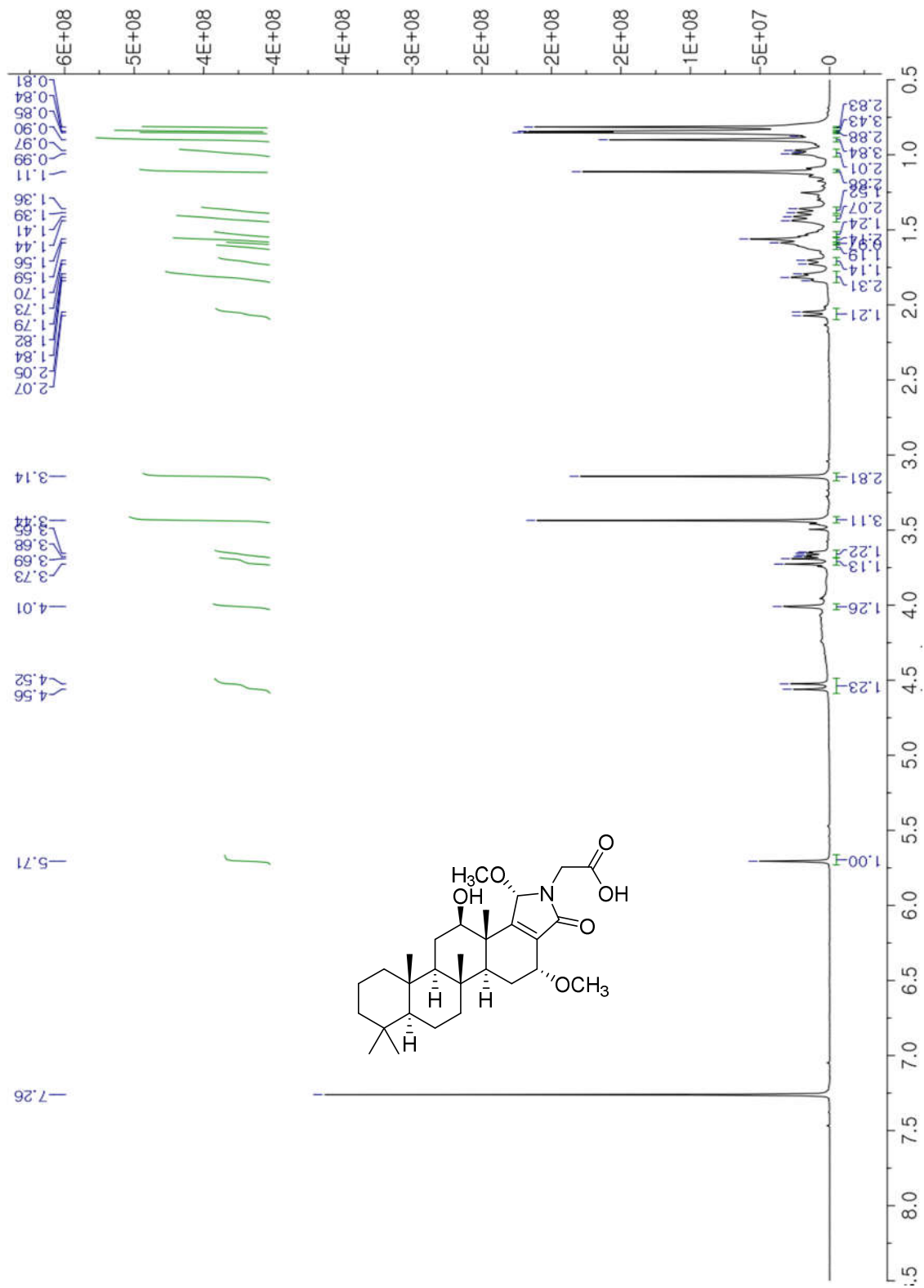


Figure S33. The HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of **5**

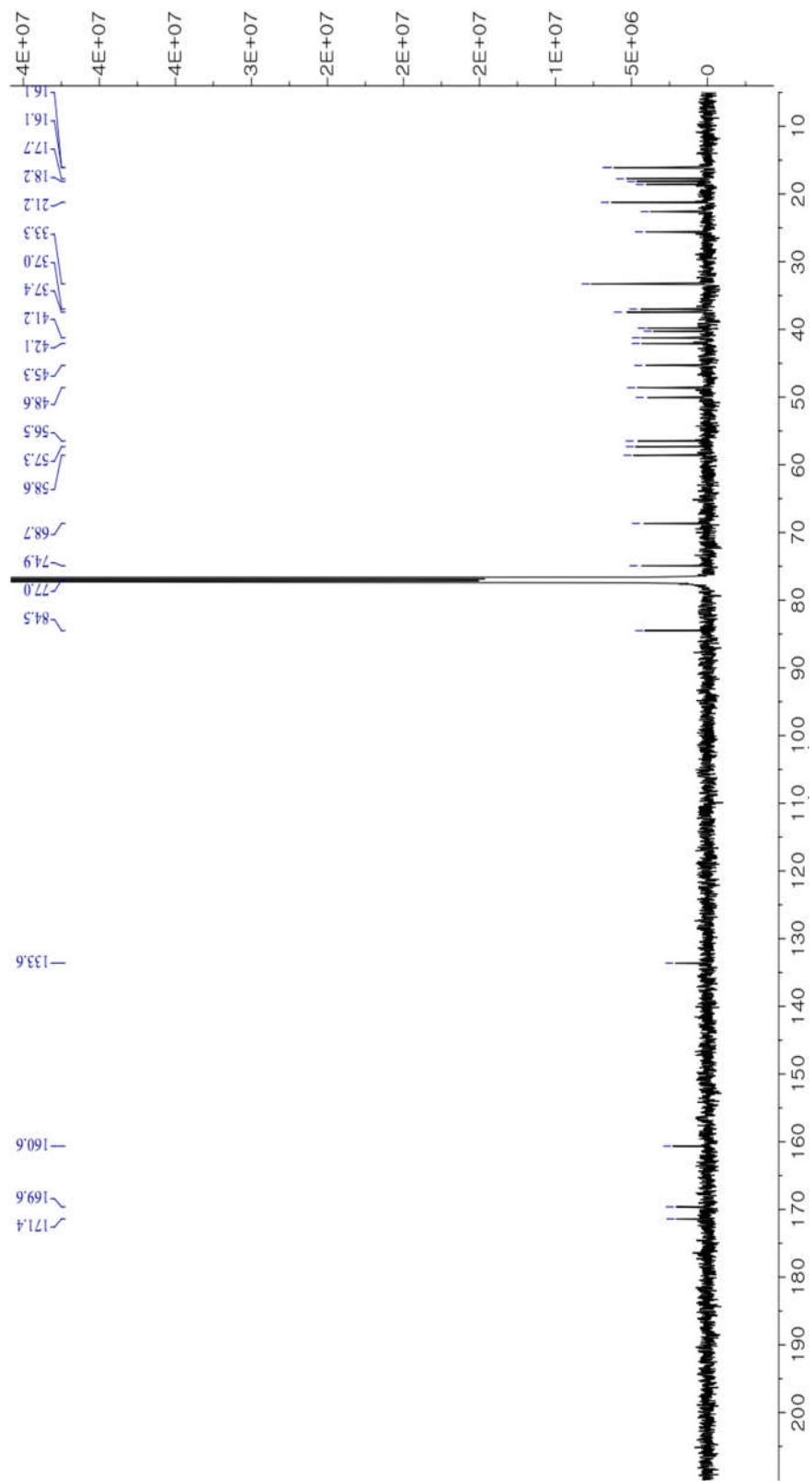




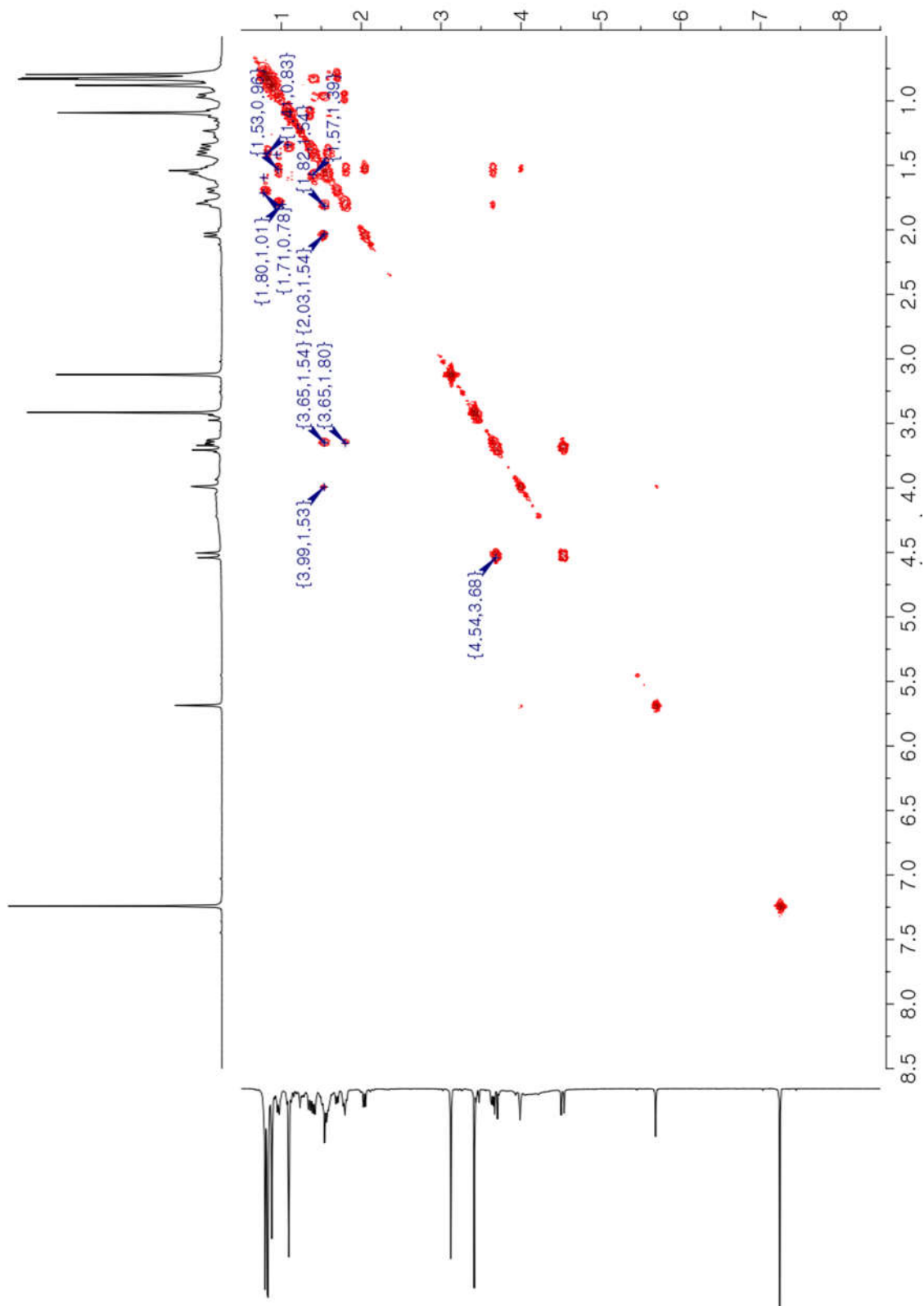
**Figure S34.** The NOESY (600 MHz,  $\text{CDCl}_3$ ) spectrum of **5**



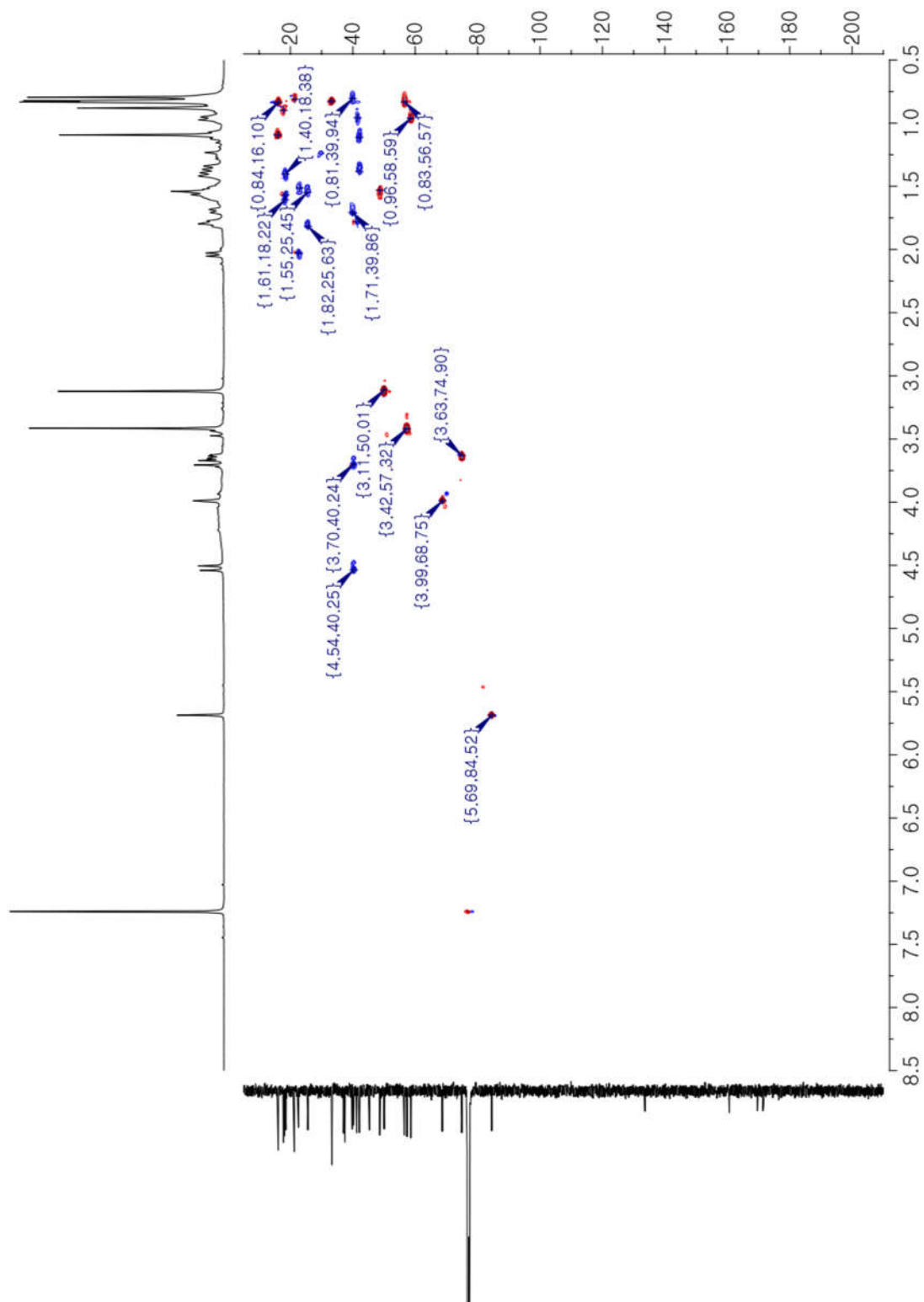
**Figure S35.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of **6**



**Figure S36.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **6**



**Figure S37.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **6**



**Figure S38.** The eHSQC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **6**

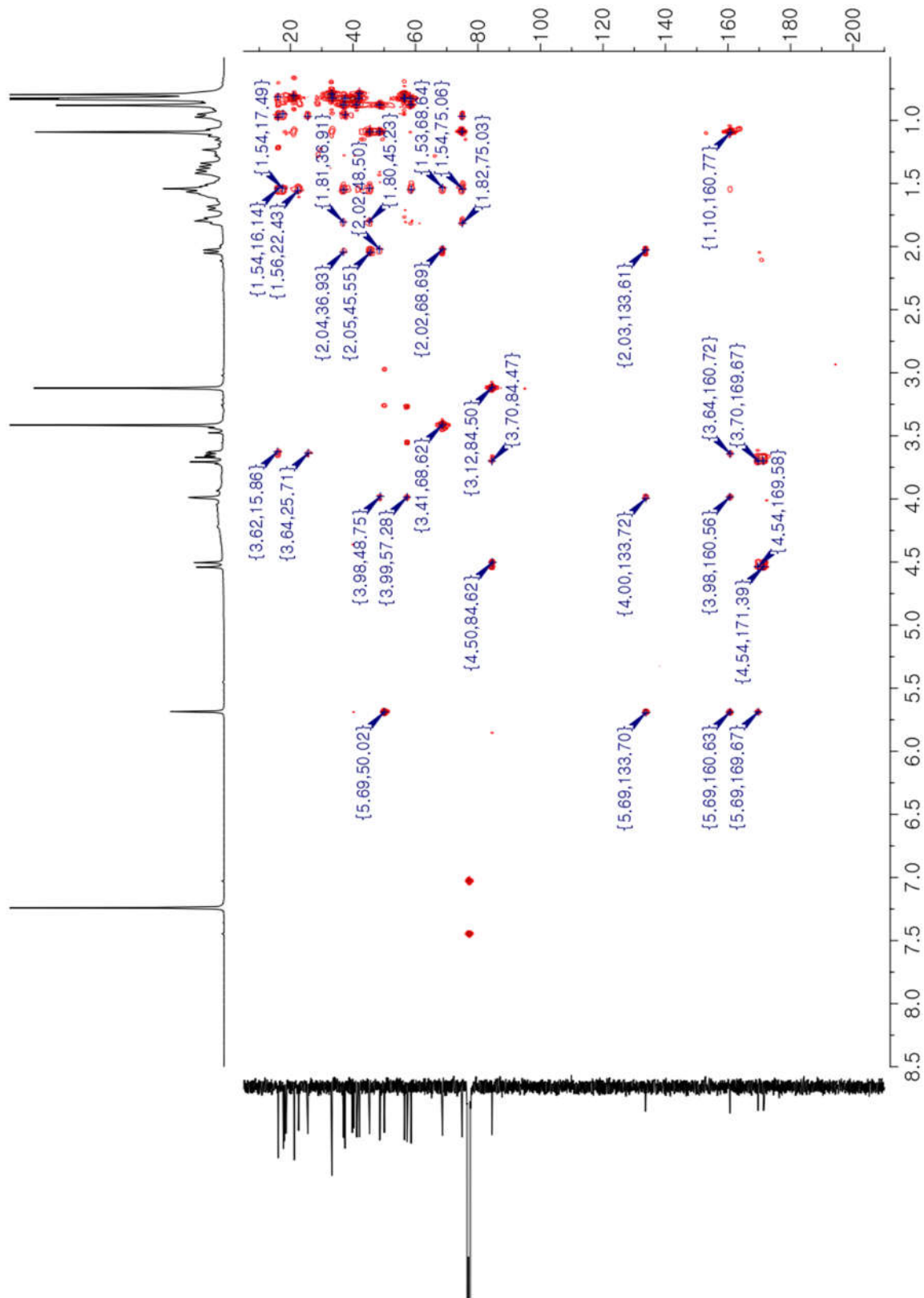
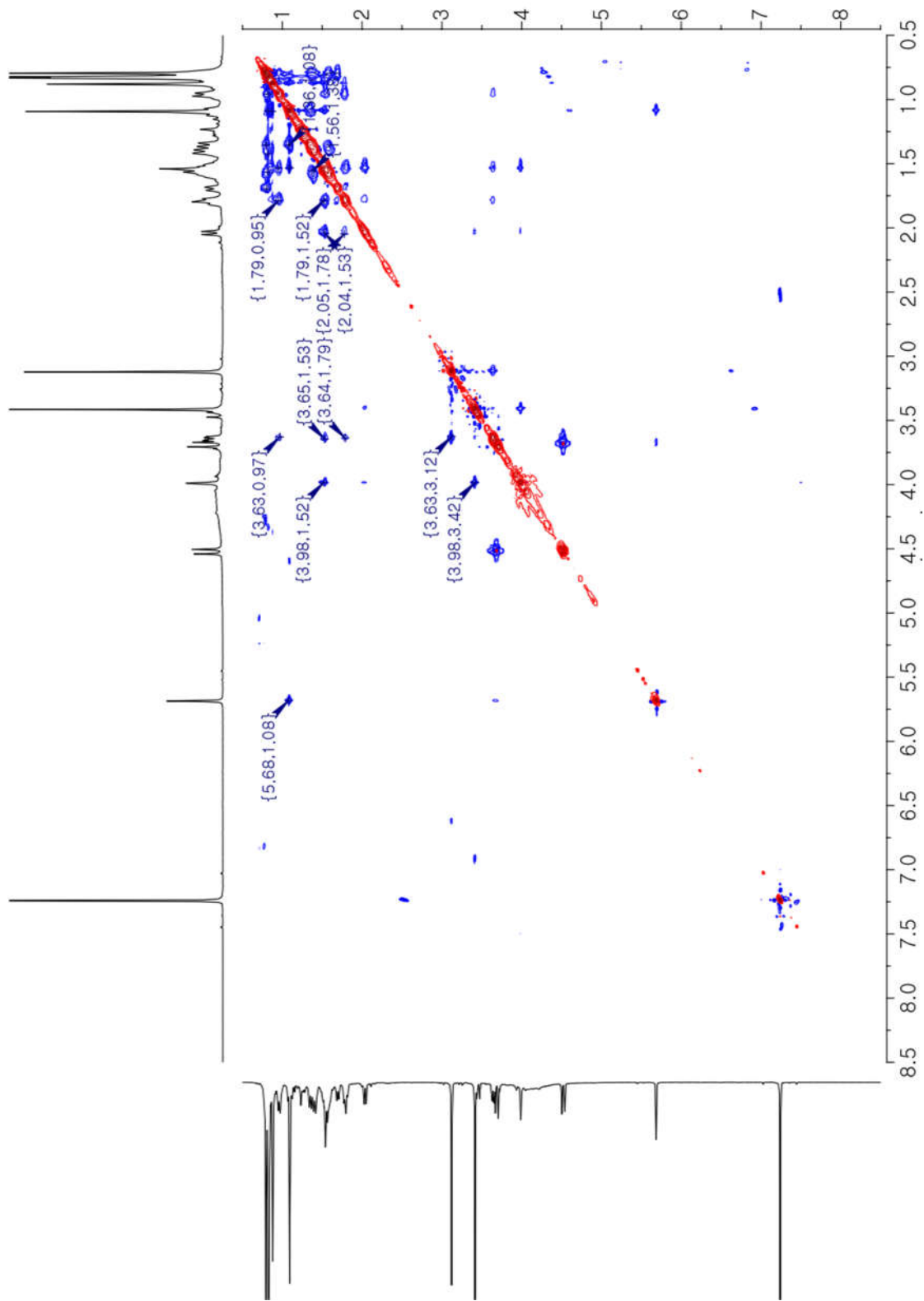
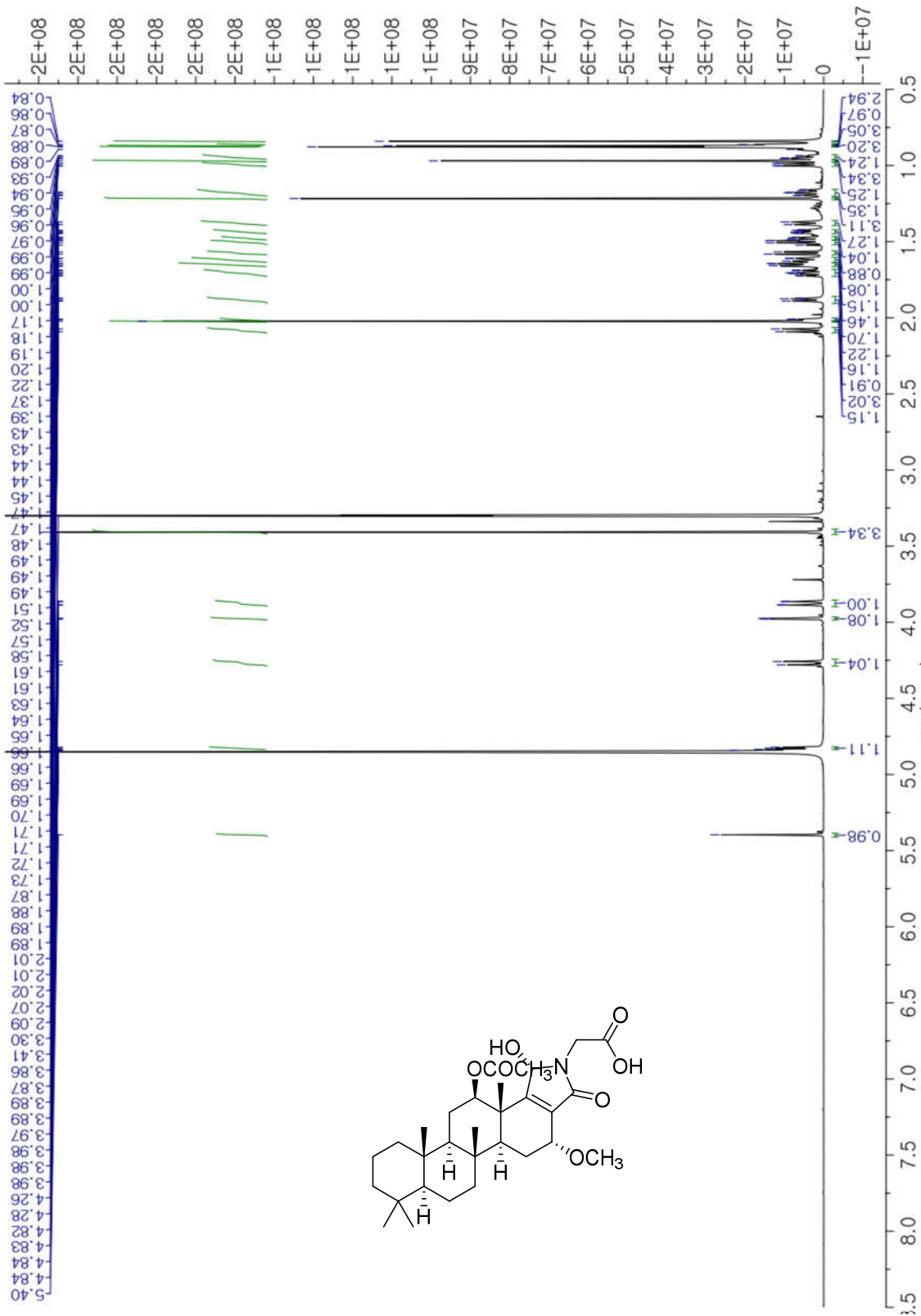


Figure S39. The HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of **6**



**Figure S40.** The NOESY (600 MHz, CDCl<sub>3</sub>) spectrum of **6**



**Figure S41.** The  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of **7**



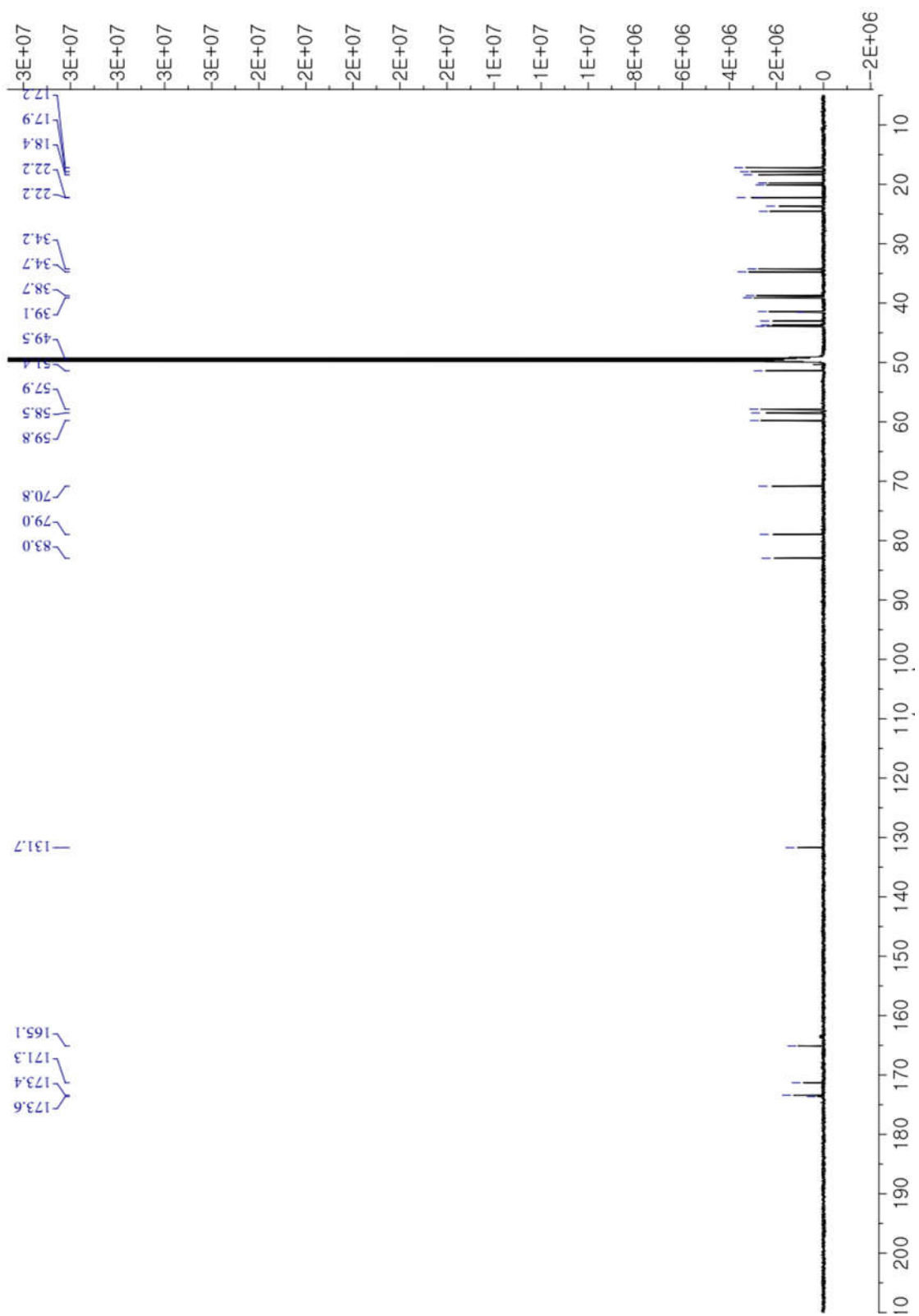
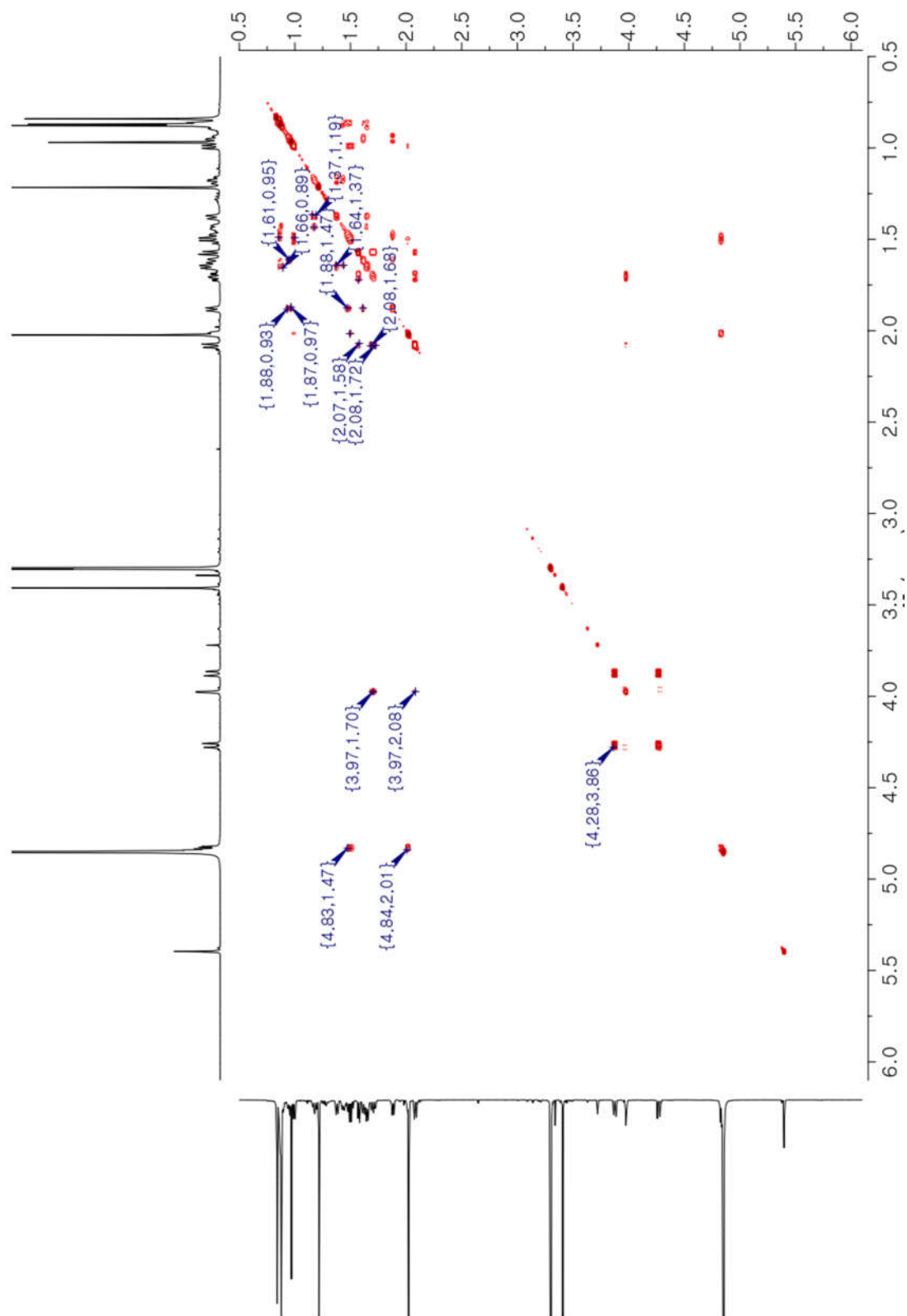
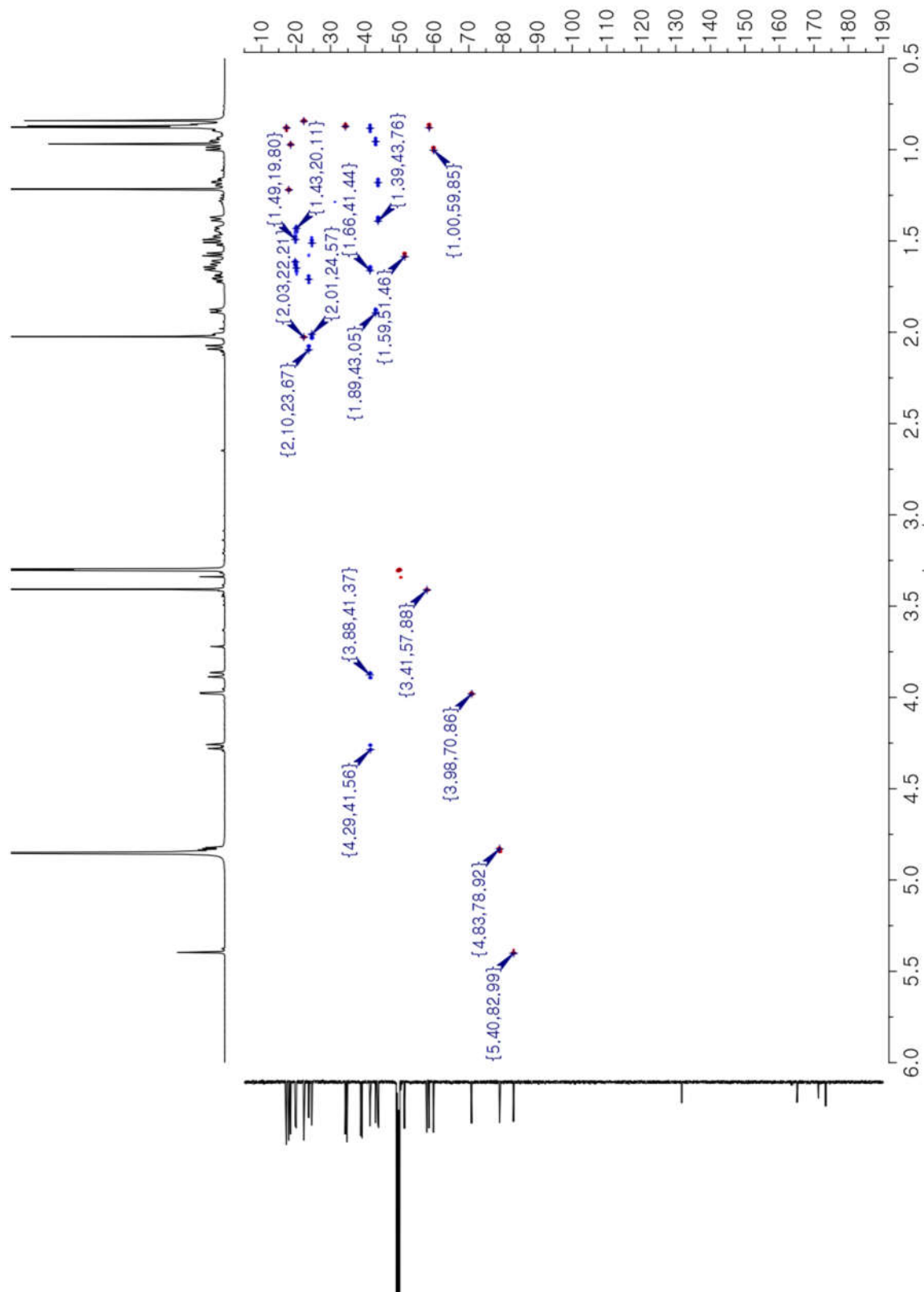


Figure S42. The  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of **7**



**Figure S43.** The COSY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **7**



**Figure S44.** The eHMQC (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **7**

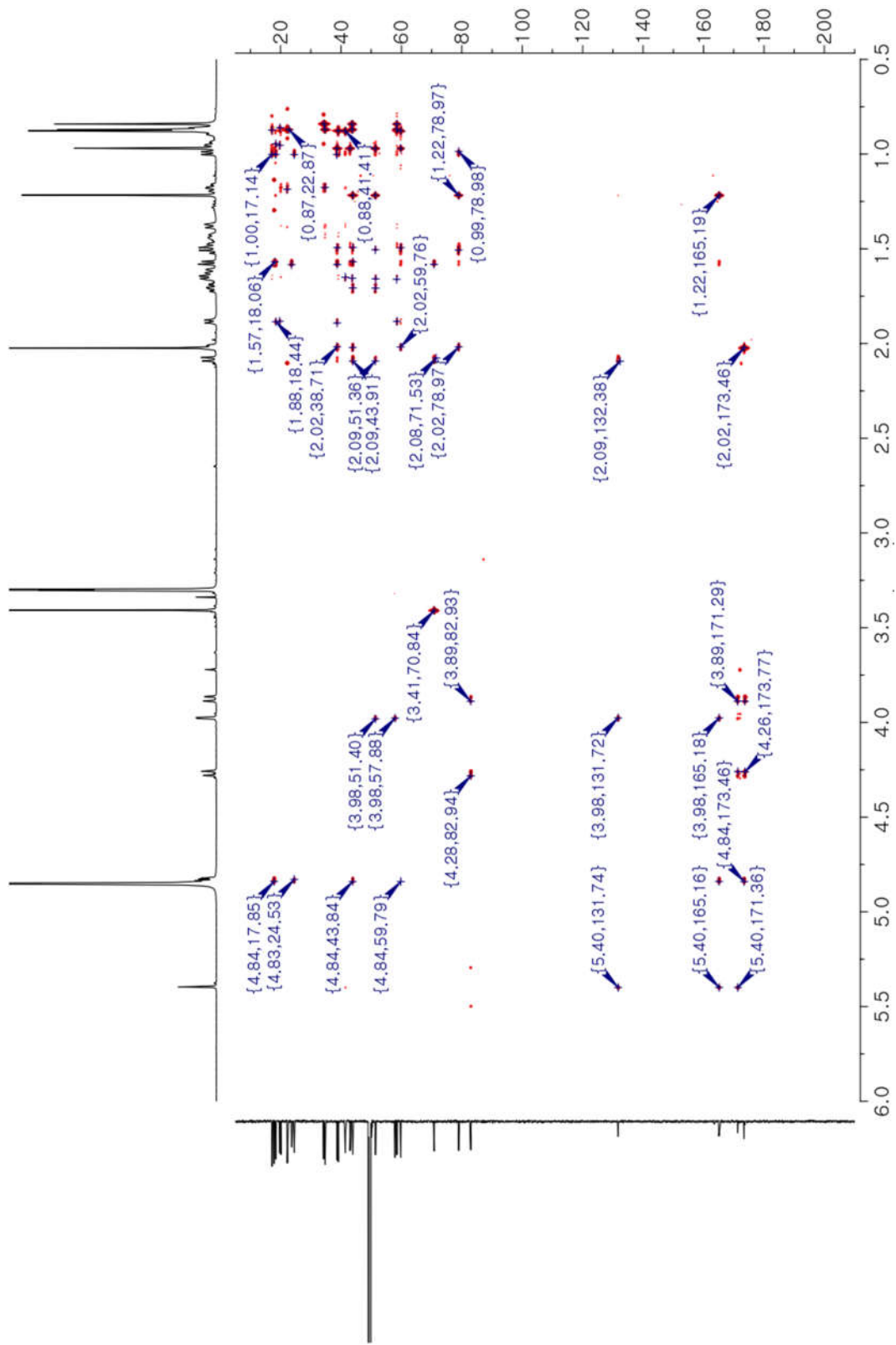
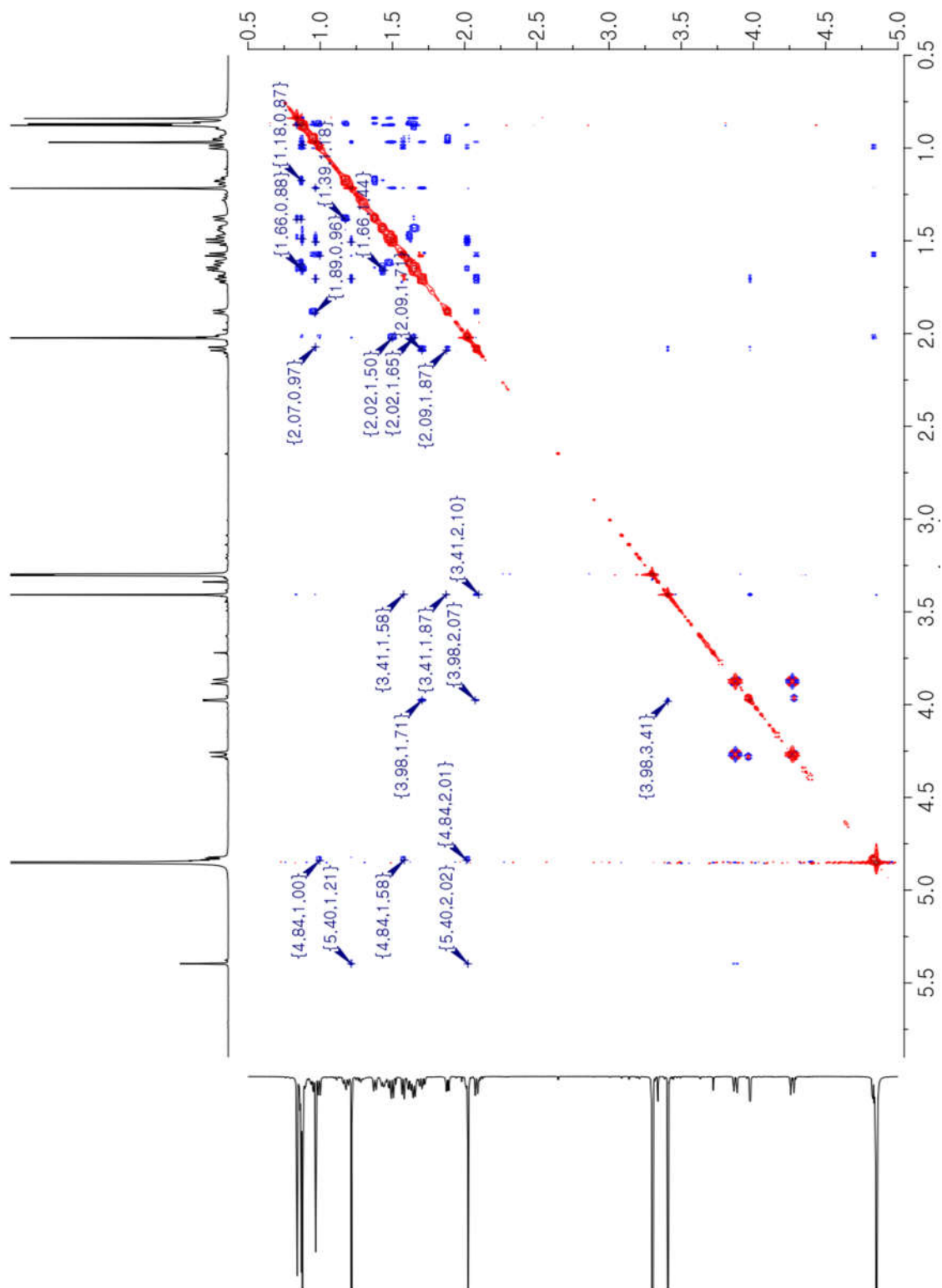
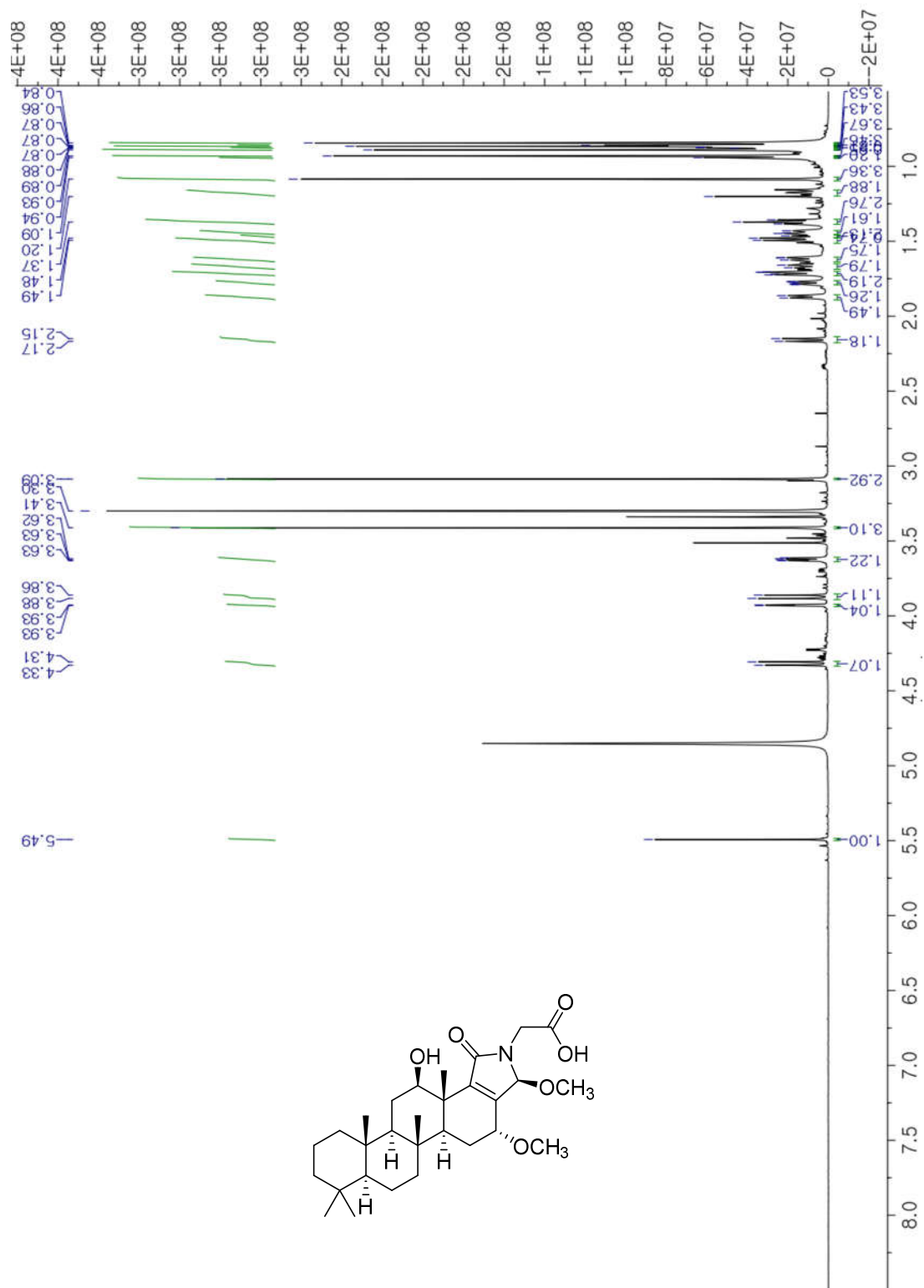


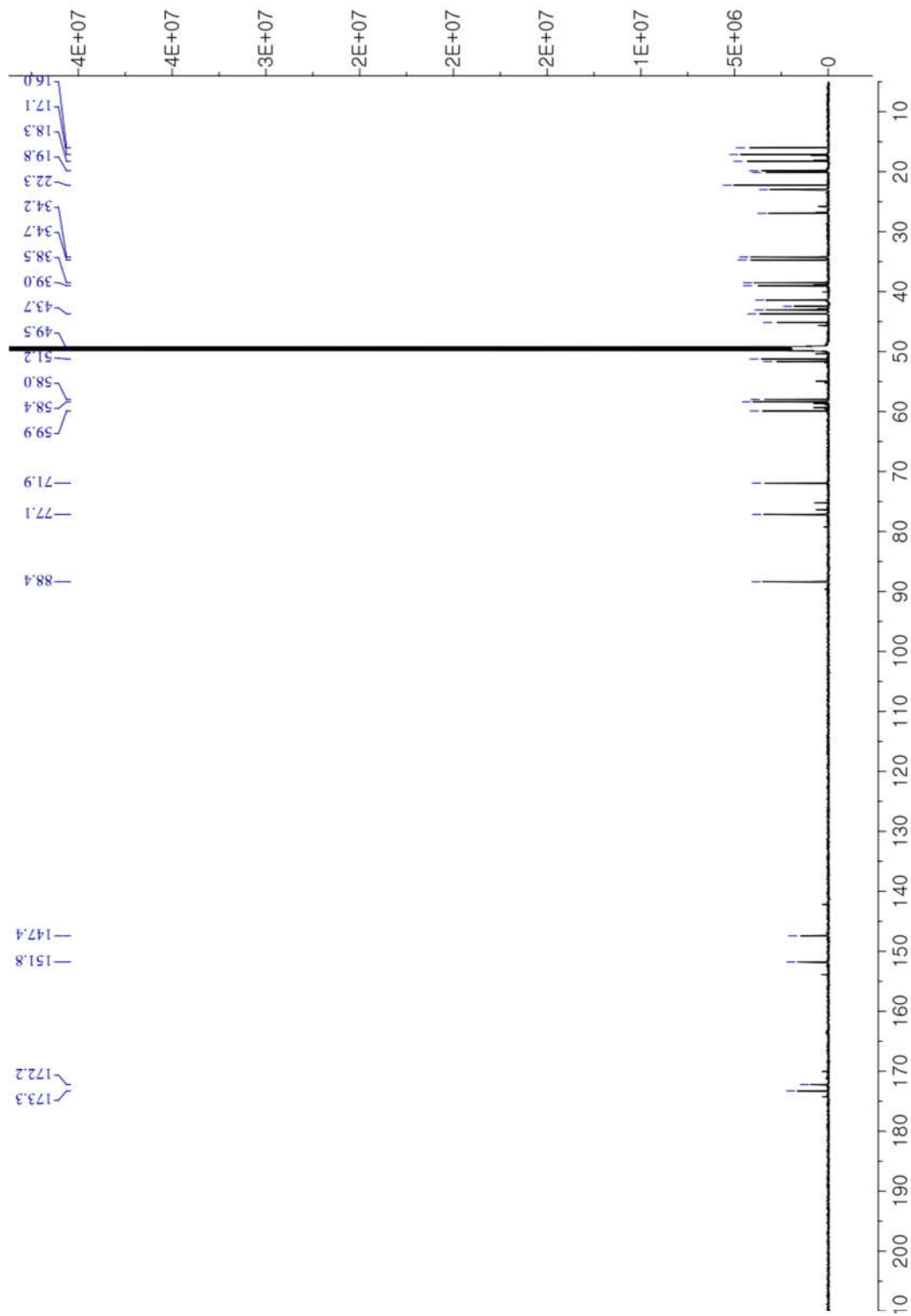
Figure S45. The HMBC (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of 7



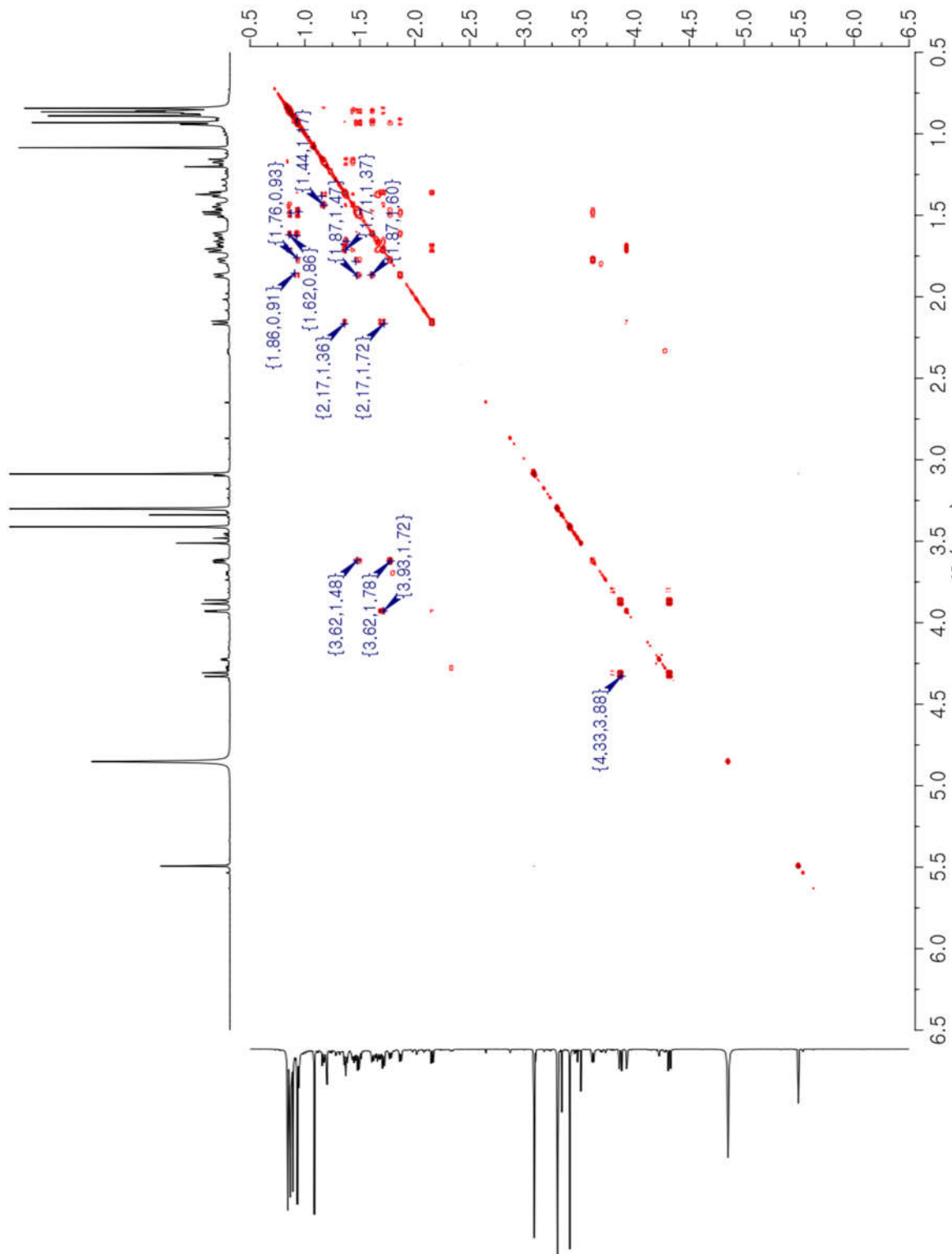
**Figure S46.** The NOESY (600 MHz, MeOH- $d_4$ ) spectrum of **7**



**Figure S47.** The <sup>1</sup>H NMR (600 MHz, MeOH-d<sub>4</sub>) spectrum of **8**

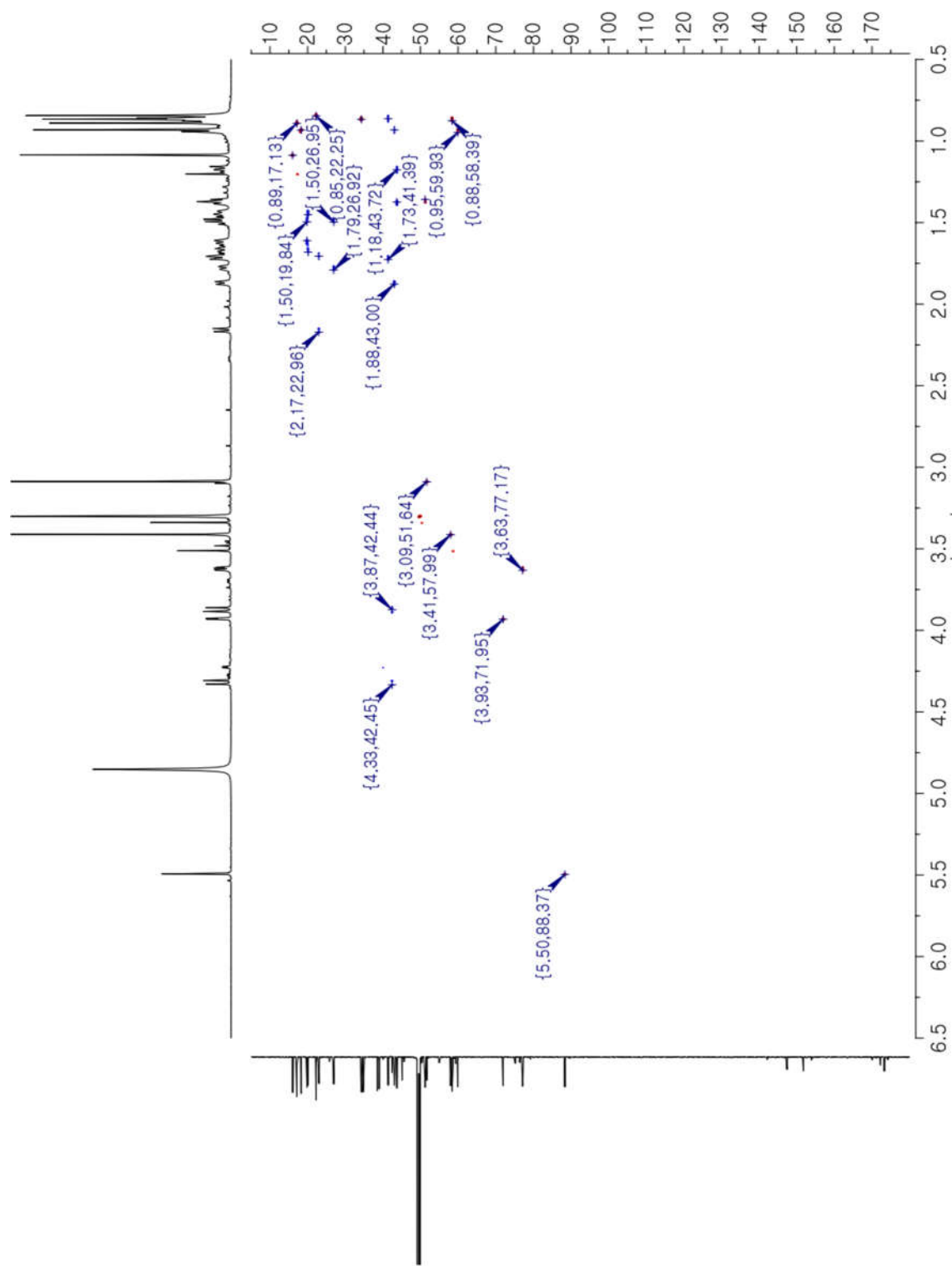


**Figure S48.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of **8**

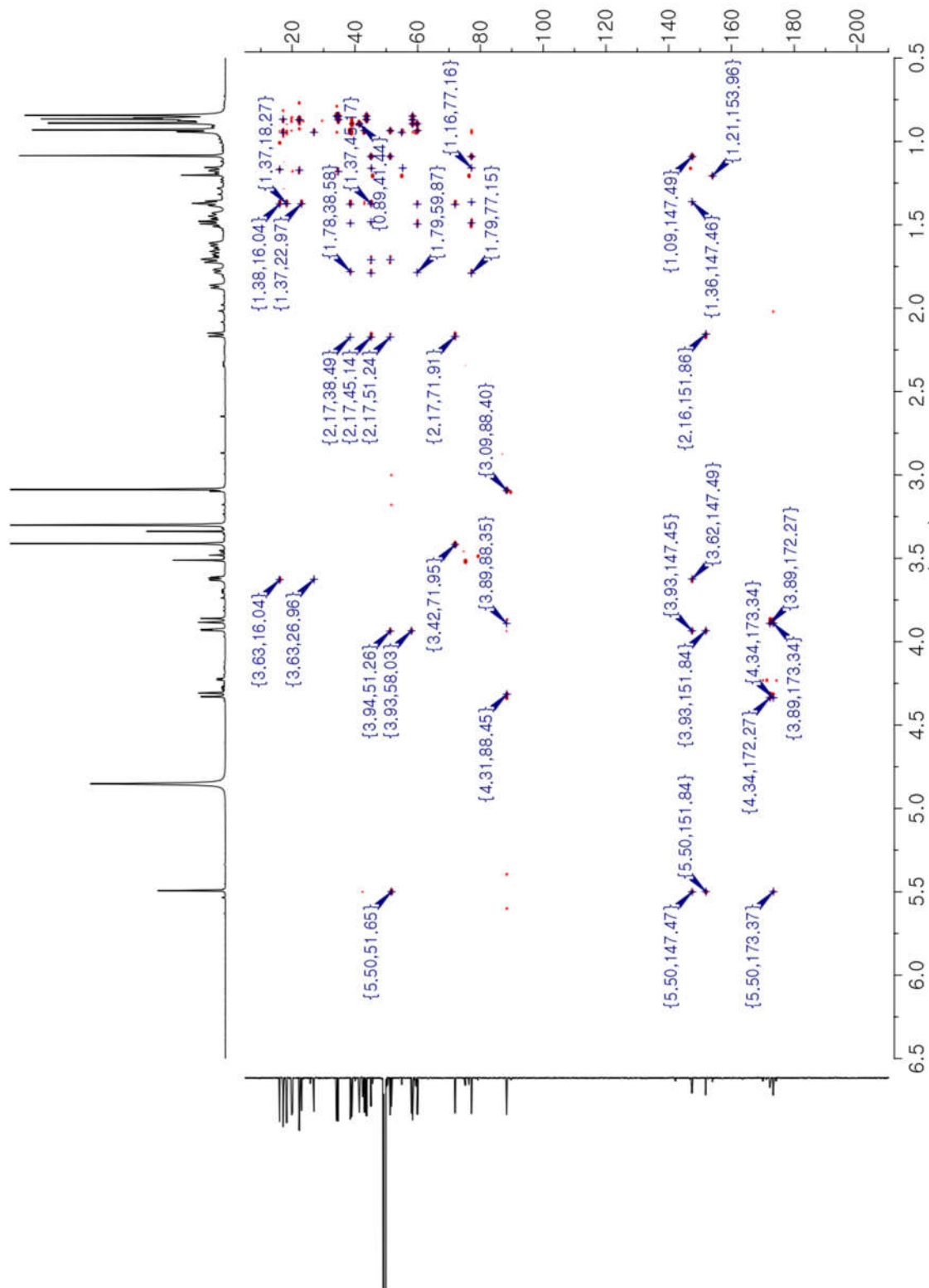


**Figure S49.** The COSY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **8**

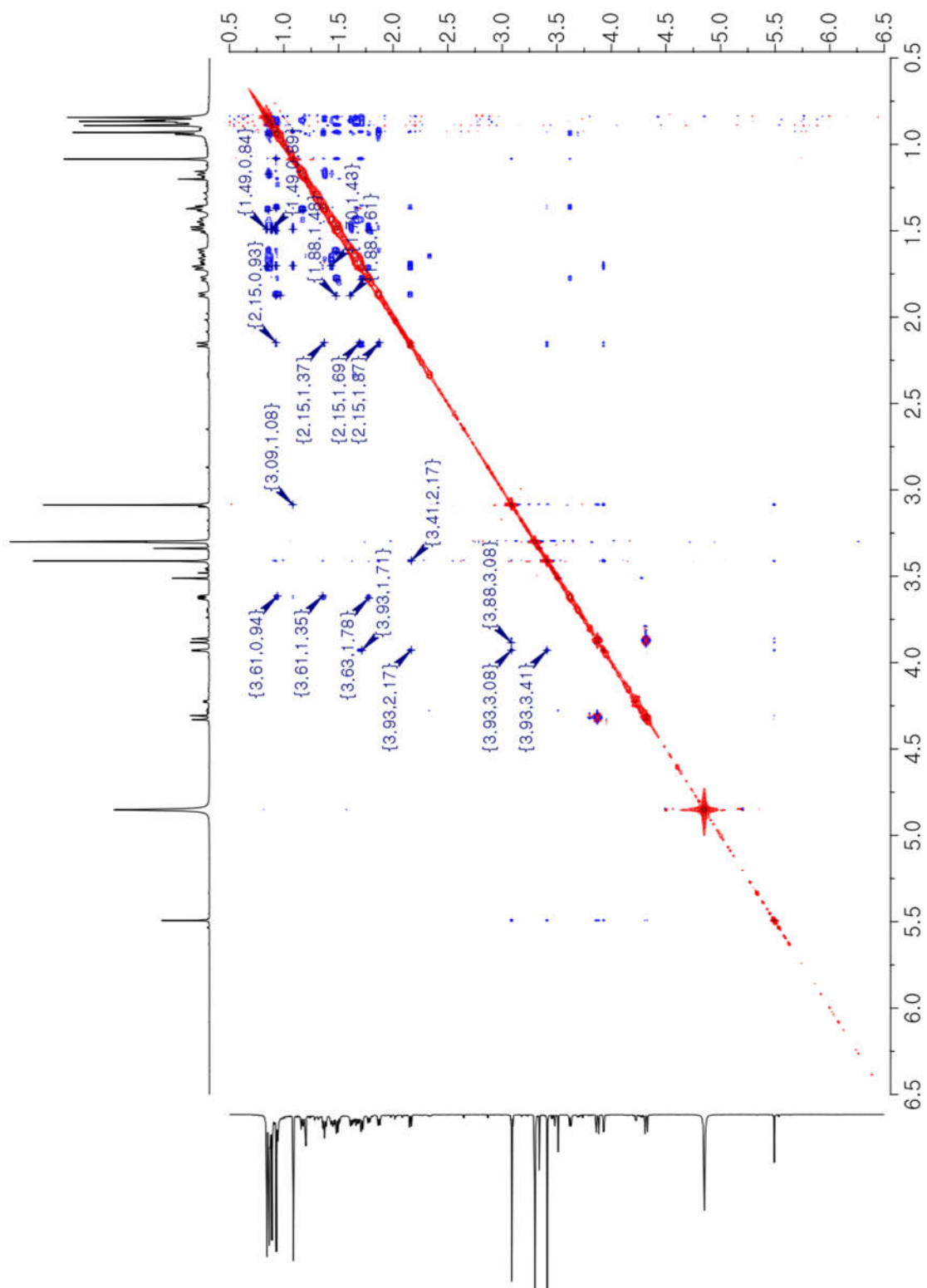




**Figure S50.** The eHSQC (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of **8**



**Figure S51.** The HMBC (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **8**



**Figure S52.** The NOESY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **8**

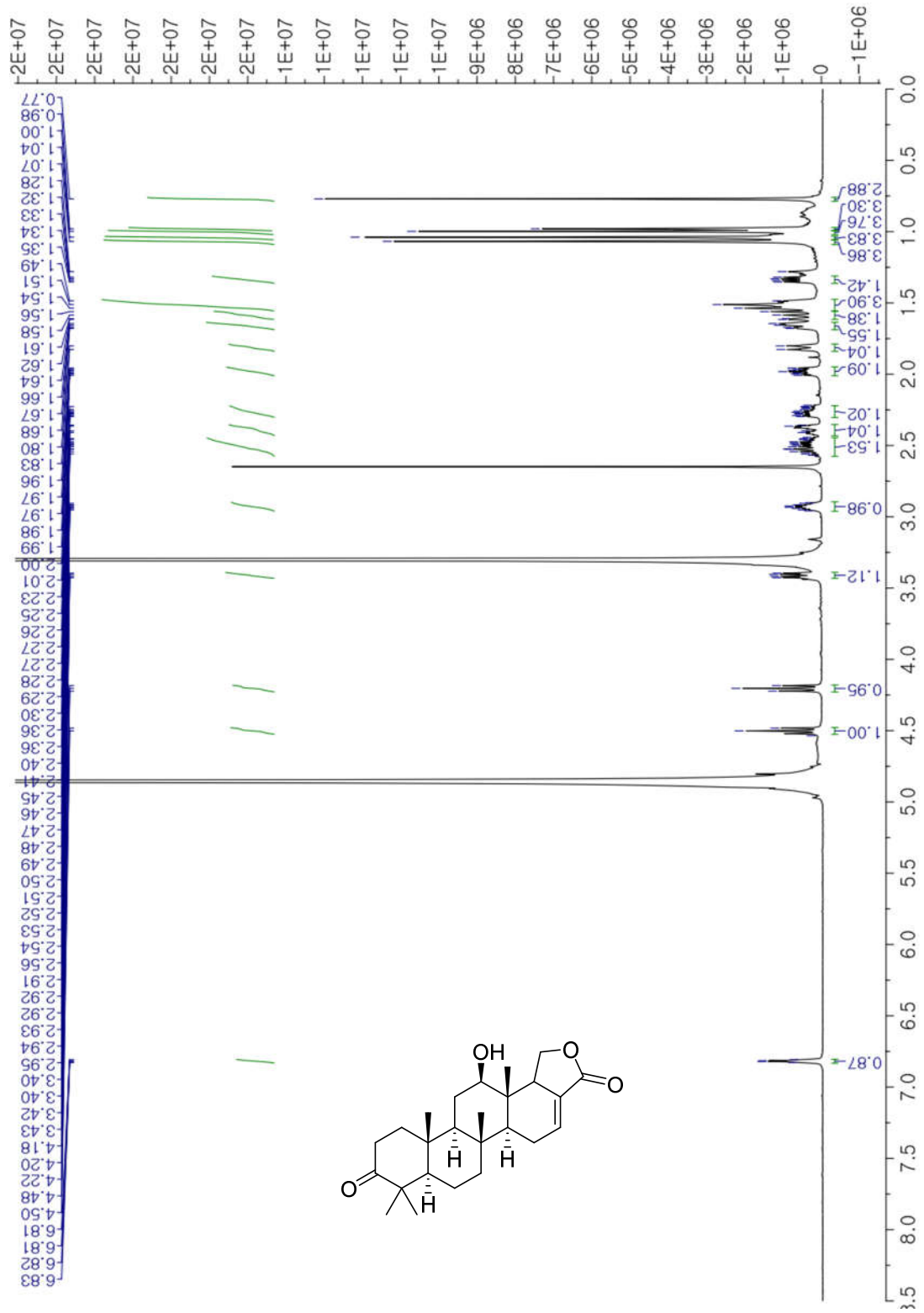
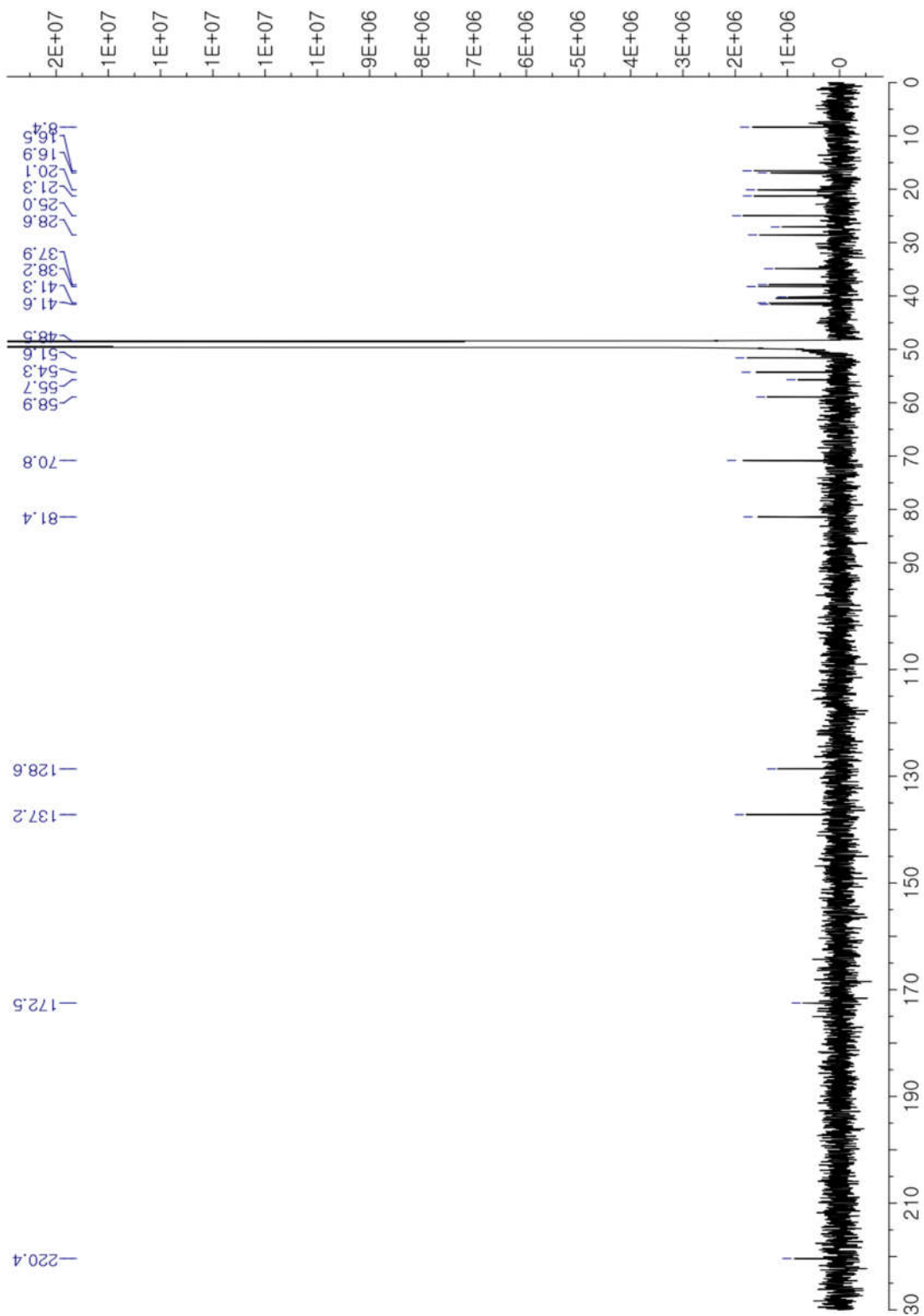
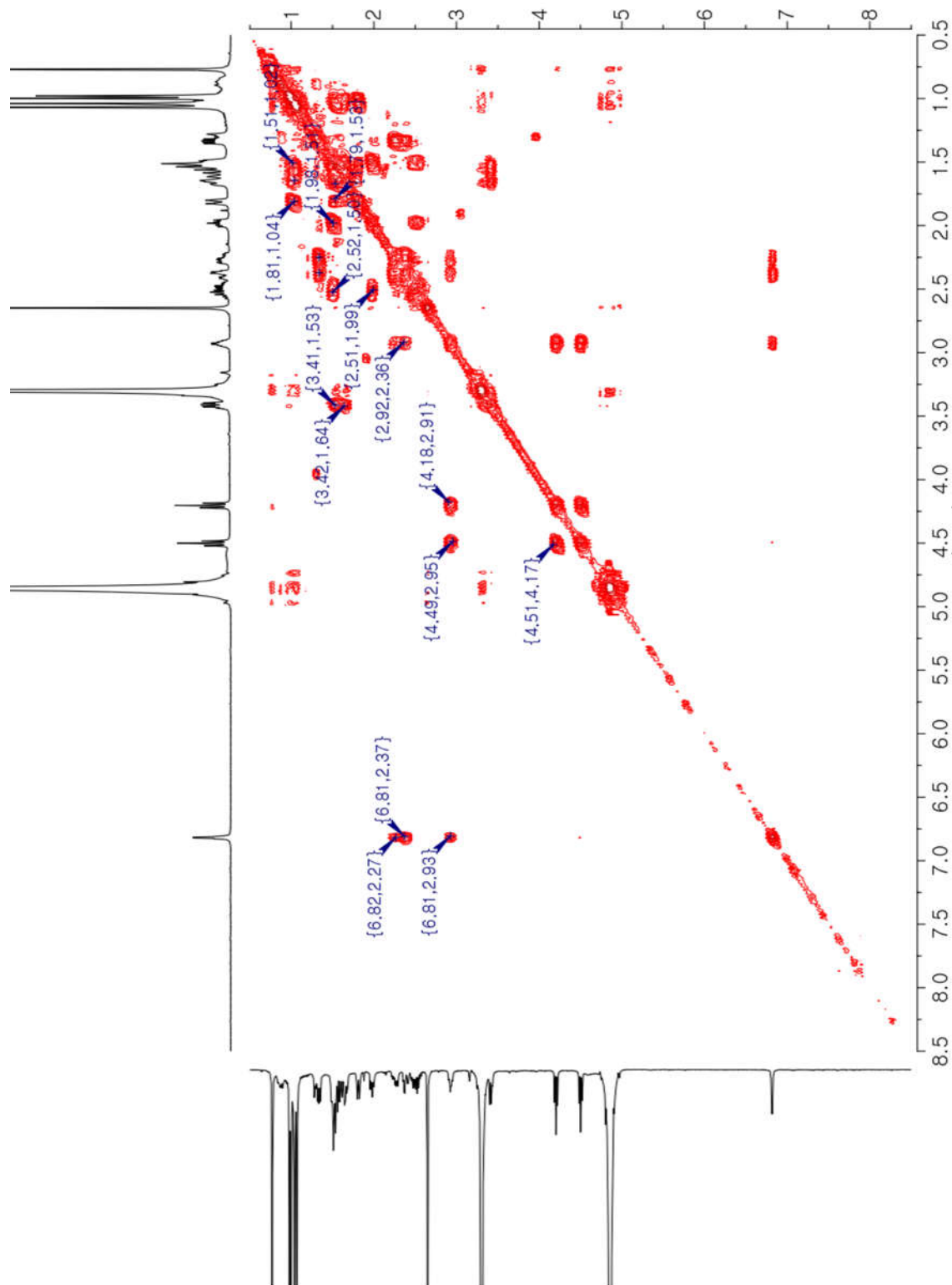


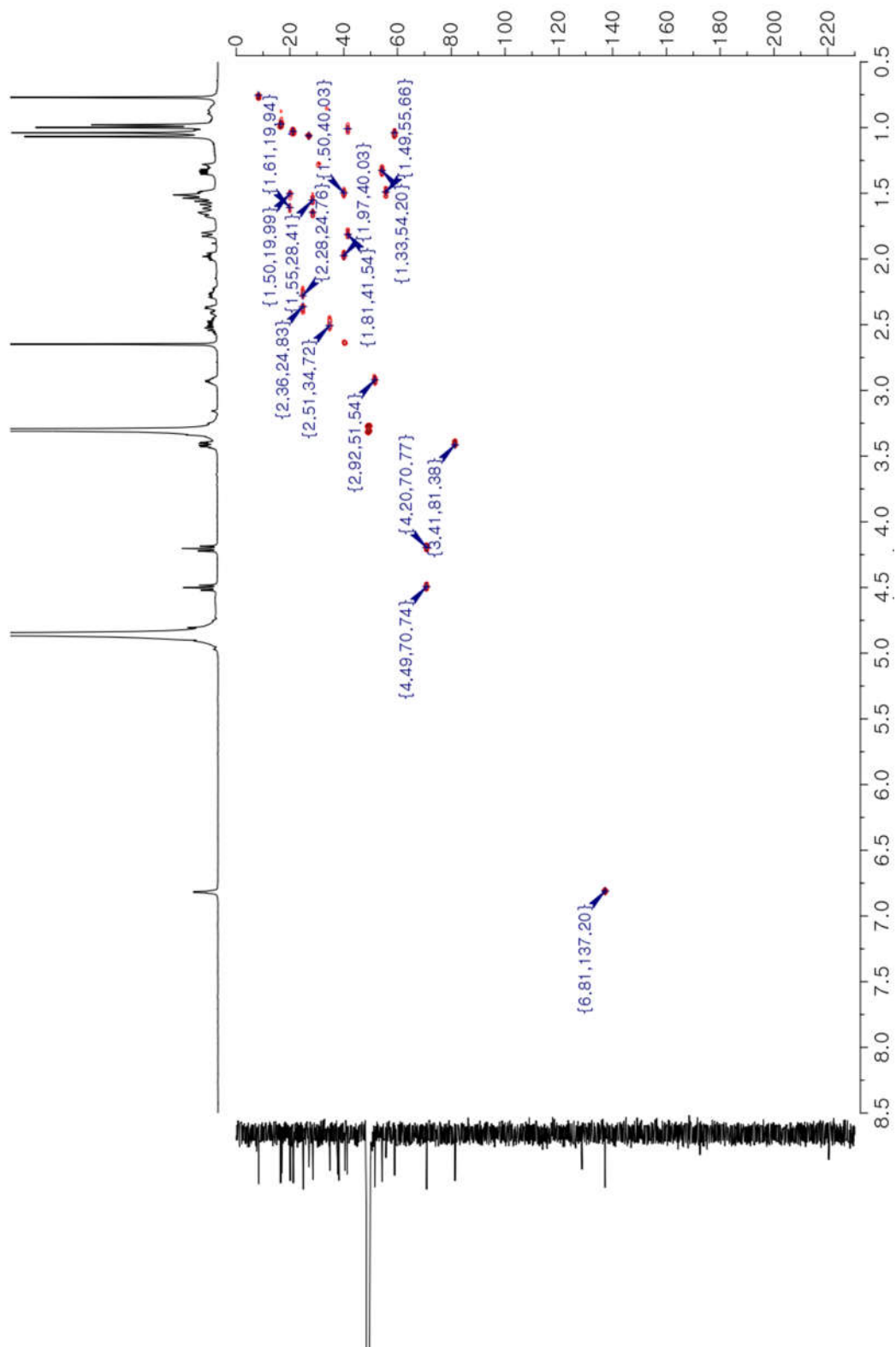
Figure S53. The  $^1\text{H}$  NMR (600 MHz,  $\text{MeOH-}d_4$ ) spectrum of **9**



**Figure S54.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{MeOH-}d_4$ ) spectrum of **9**



**Figure S55.** The COSY (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **9**



**Figure S56.** The HSQC (600 MHz, MeOH-*d*<sub>4</sub>) spectrum of **9**

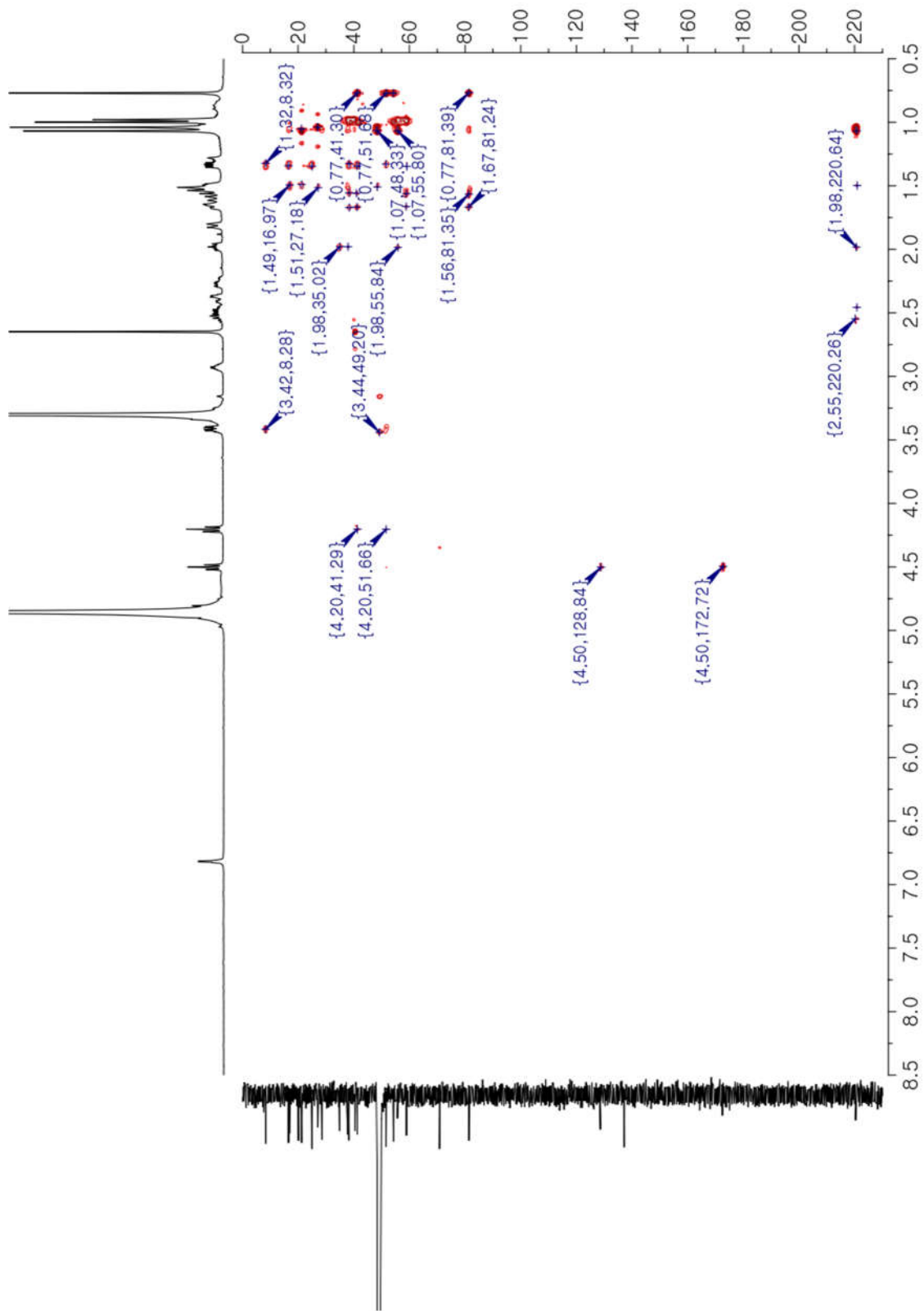
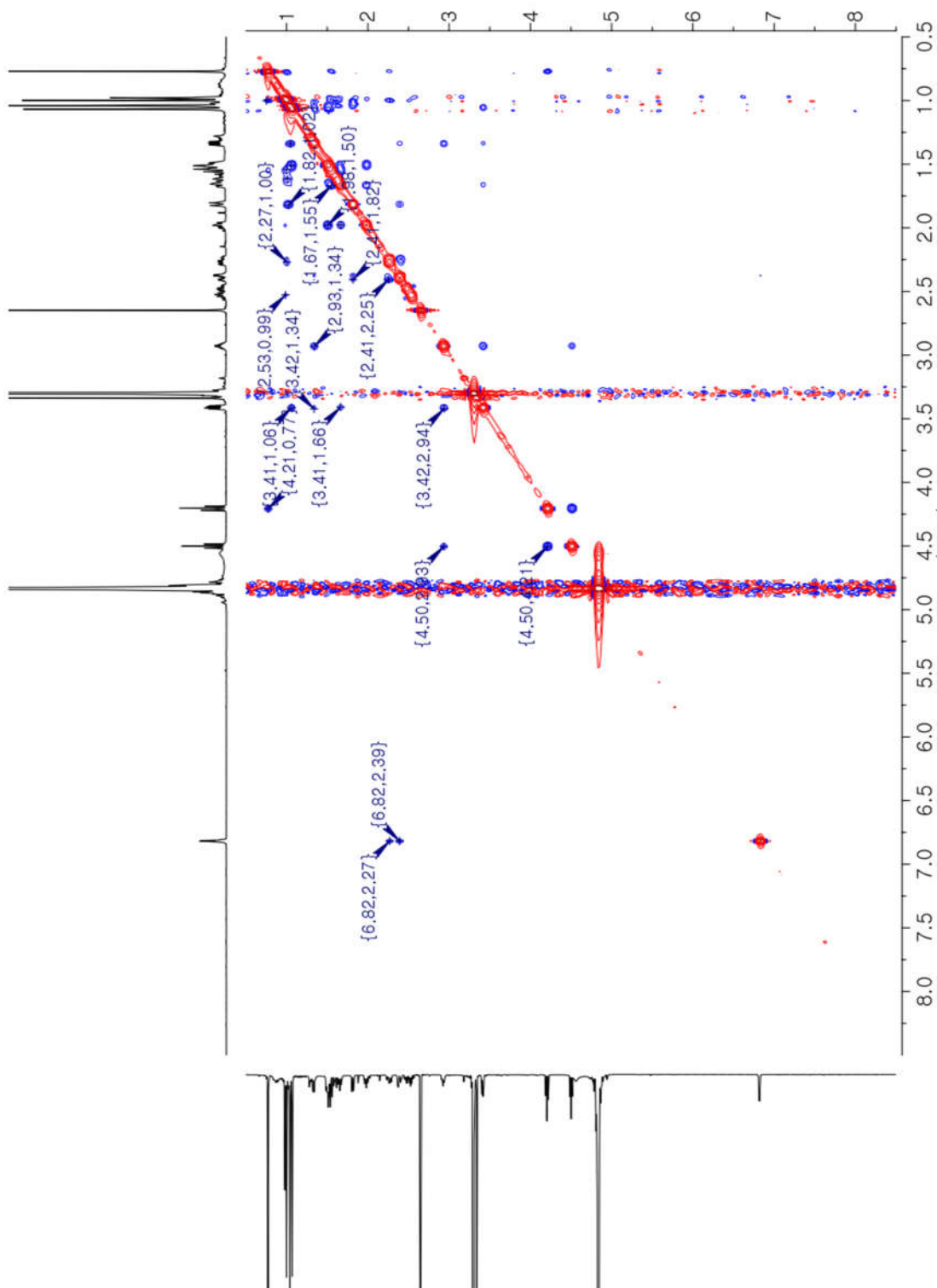


Figure S57. The HMBC (600 MHz, MeOH- $d_4$ ) spectrum of **9**





**Figure S58.** The NOESY (600 MHz, MeOH- $d_4$ ) spectrum of **9**

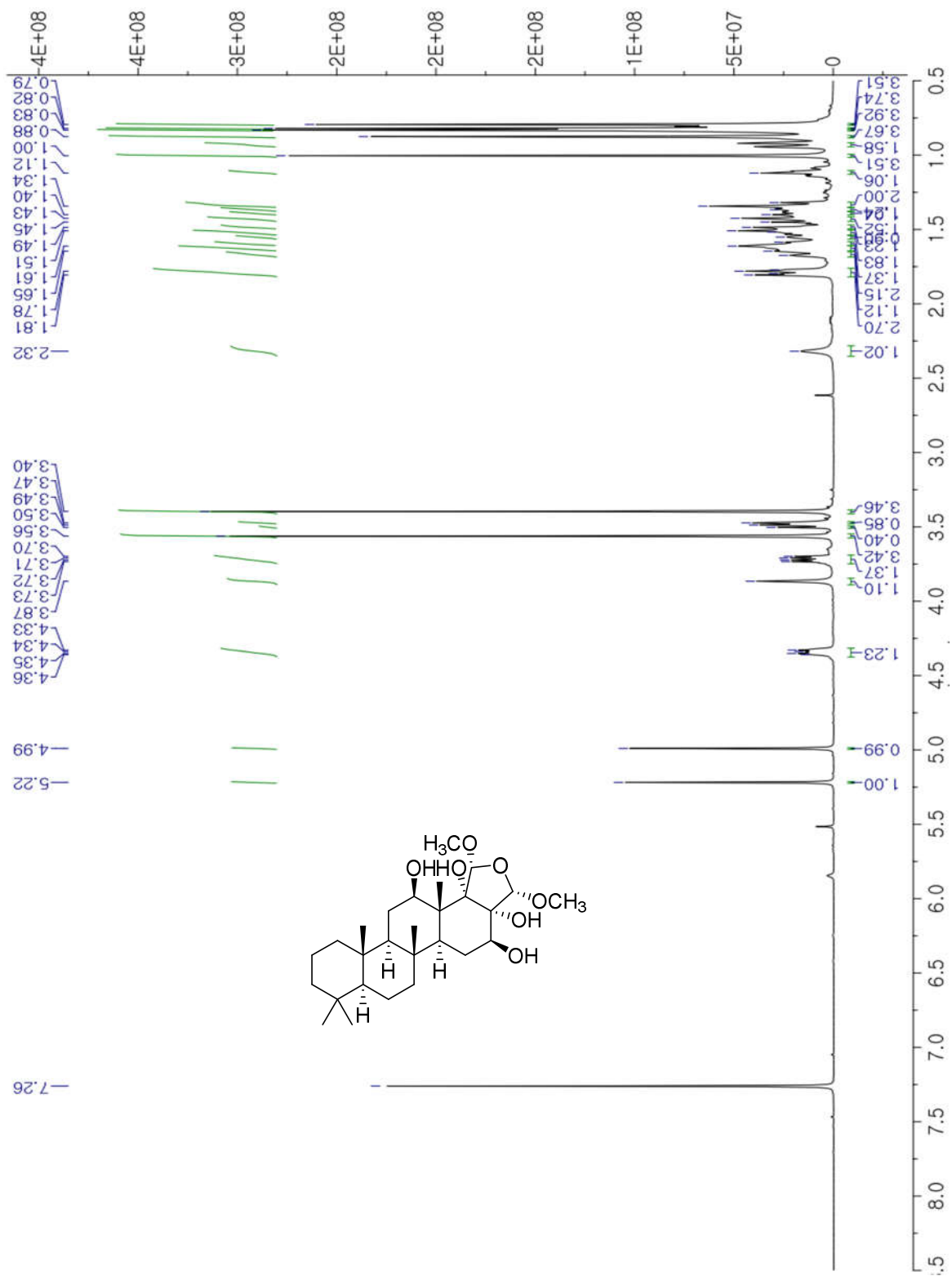
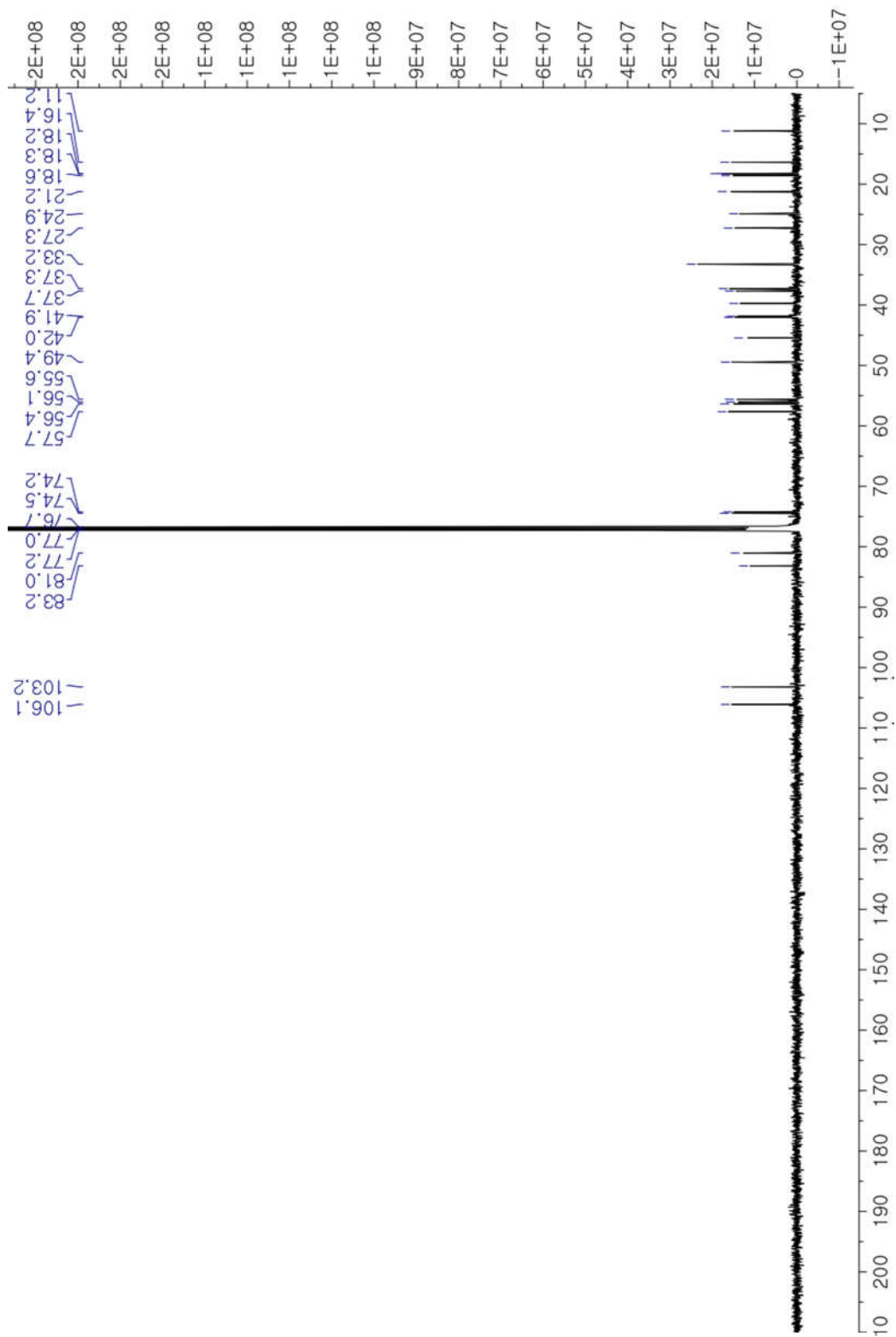
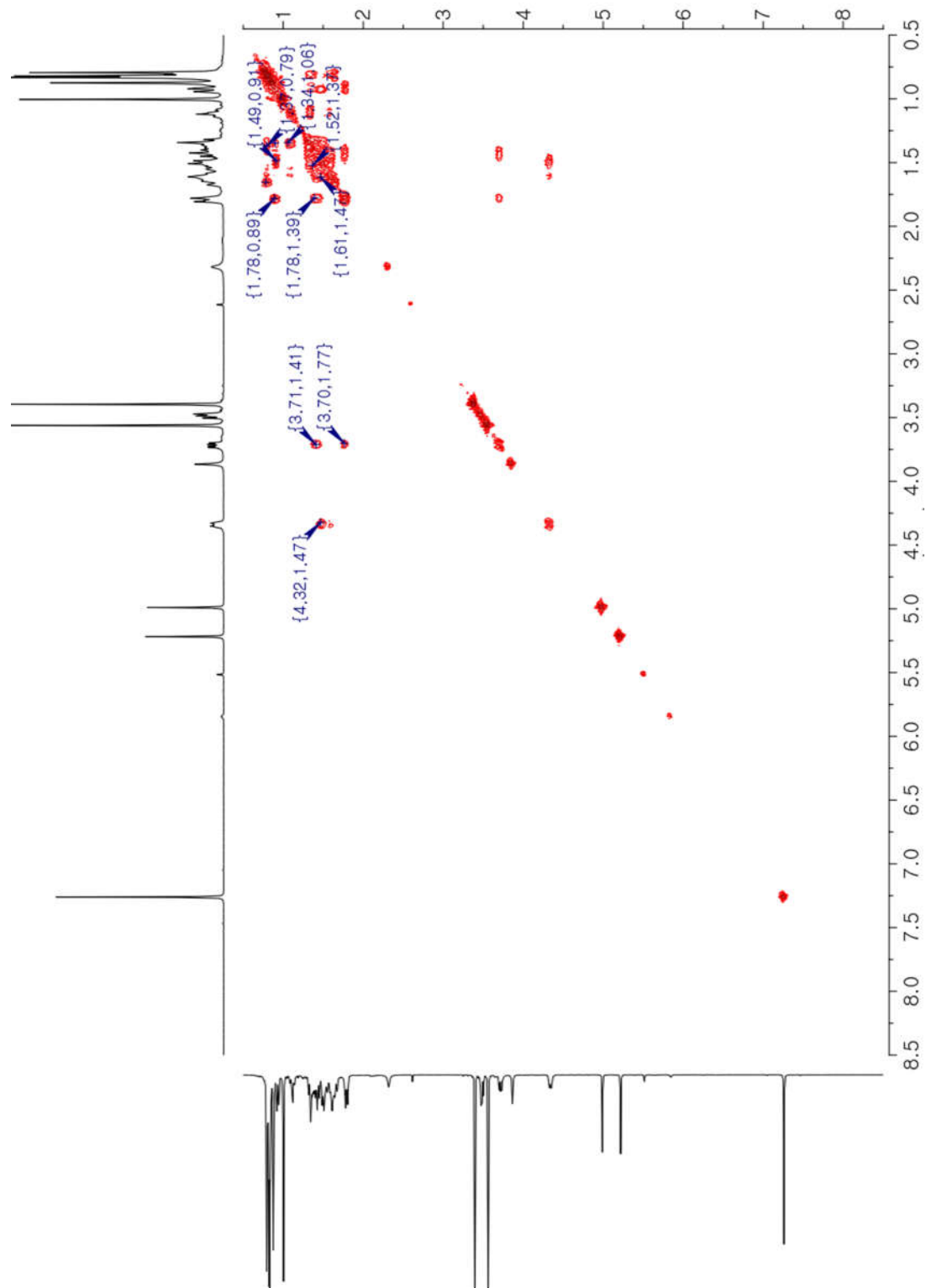


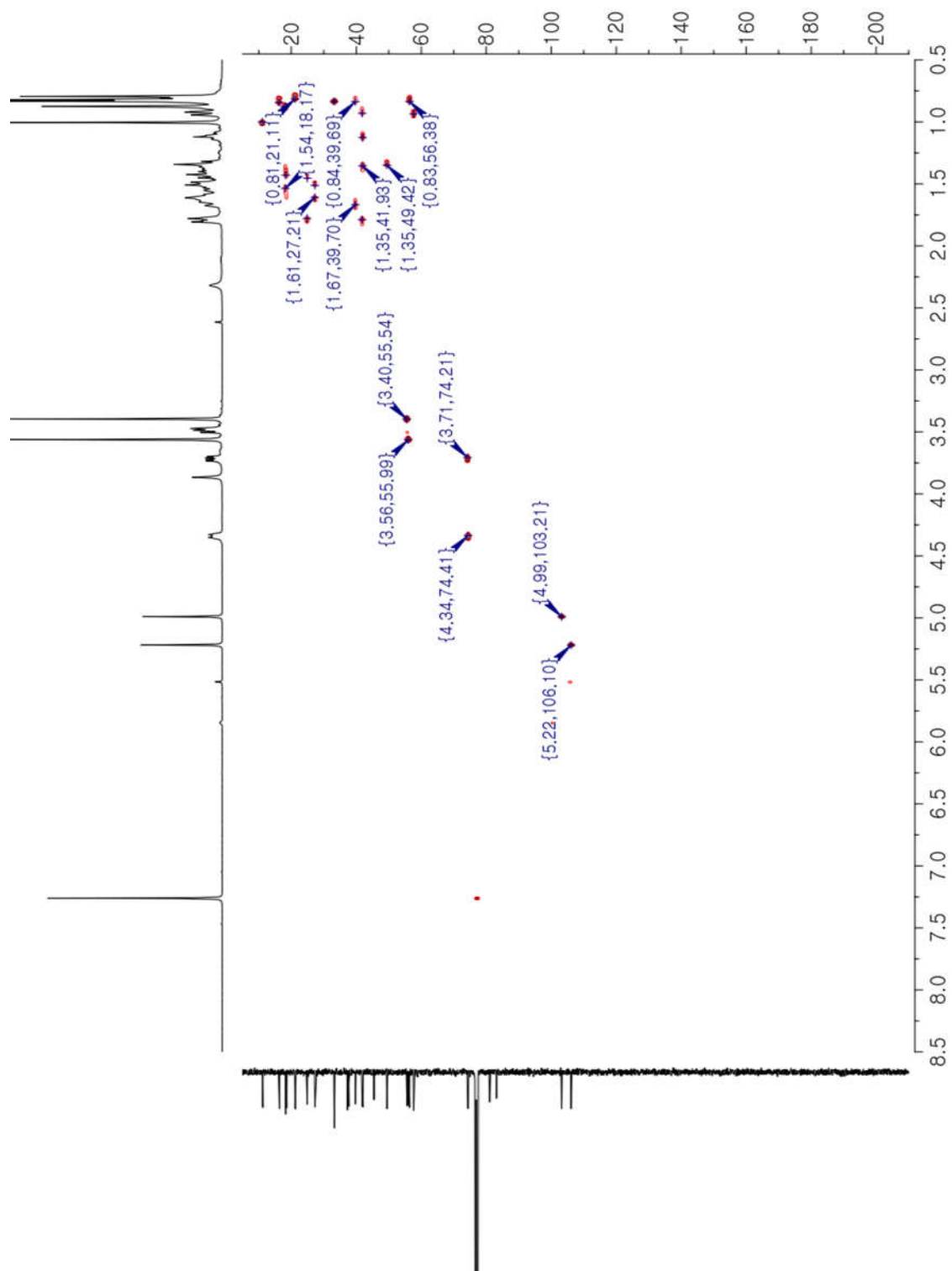
Figure S59. The  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of **10**



**Figure S60.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **10**



**Figure S61.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **10**



**Figure S62.** The HSQC (600 MHz, CDCl<sub>3</sub>) spectrum of **10**

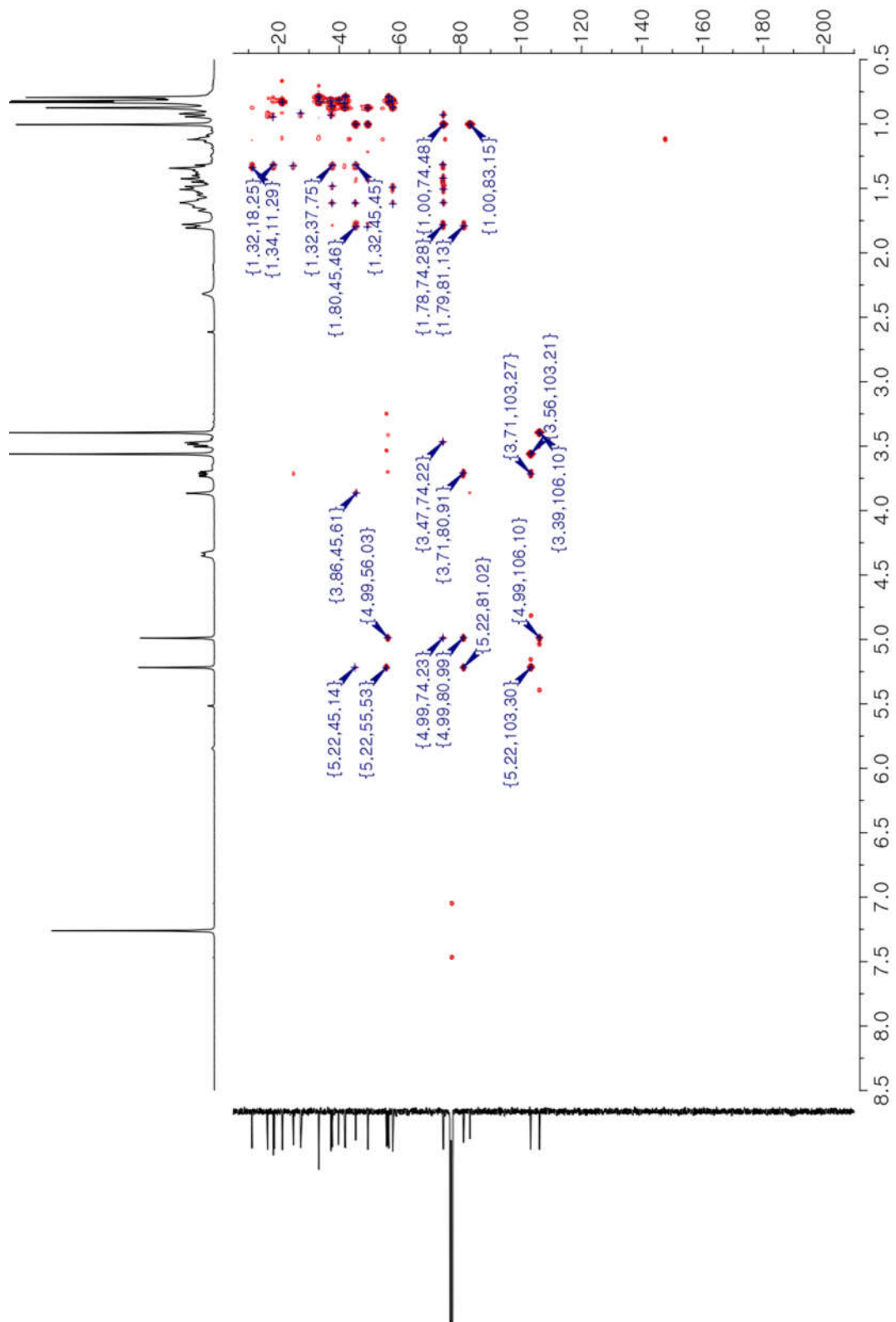
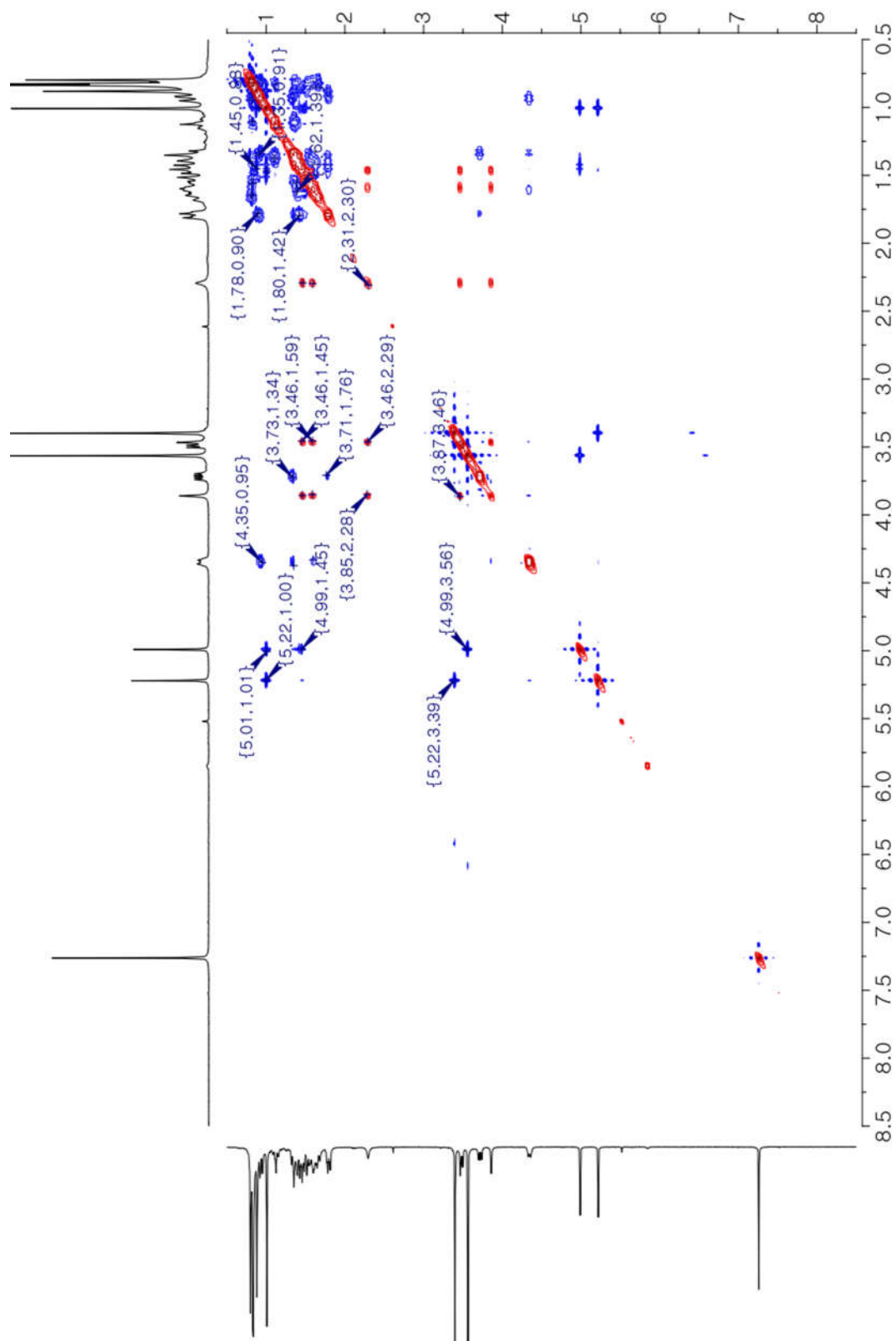
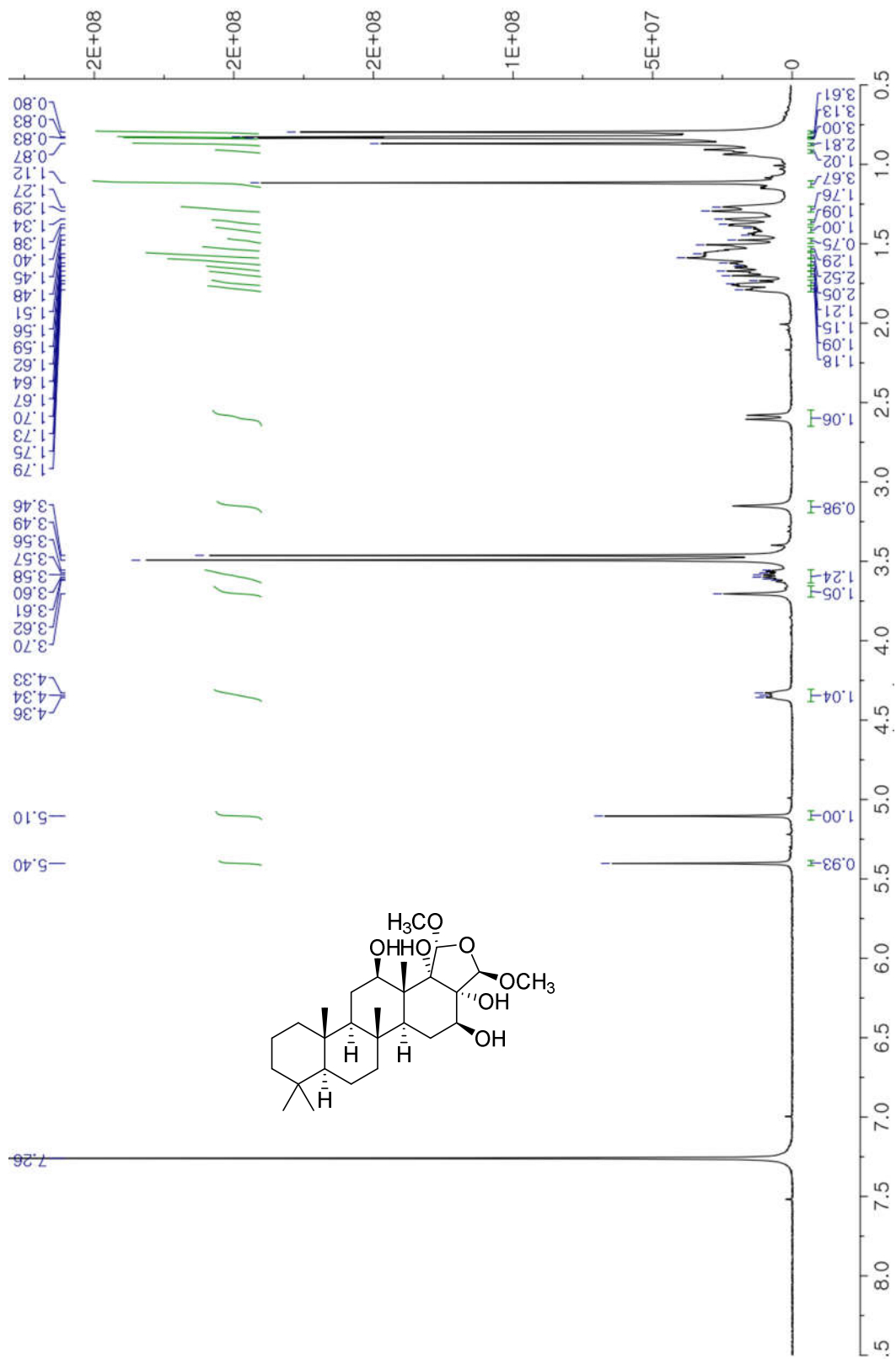


Figure S63. The HMBC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **10**

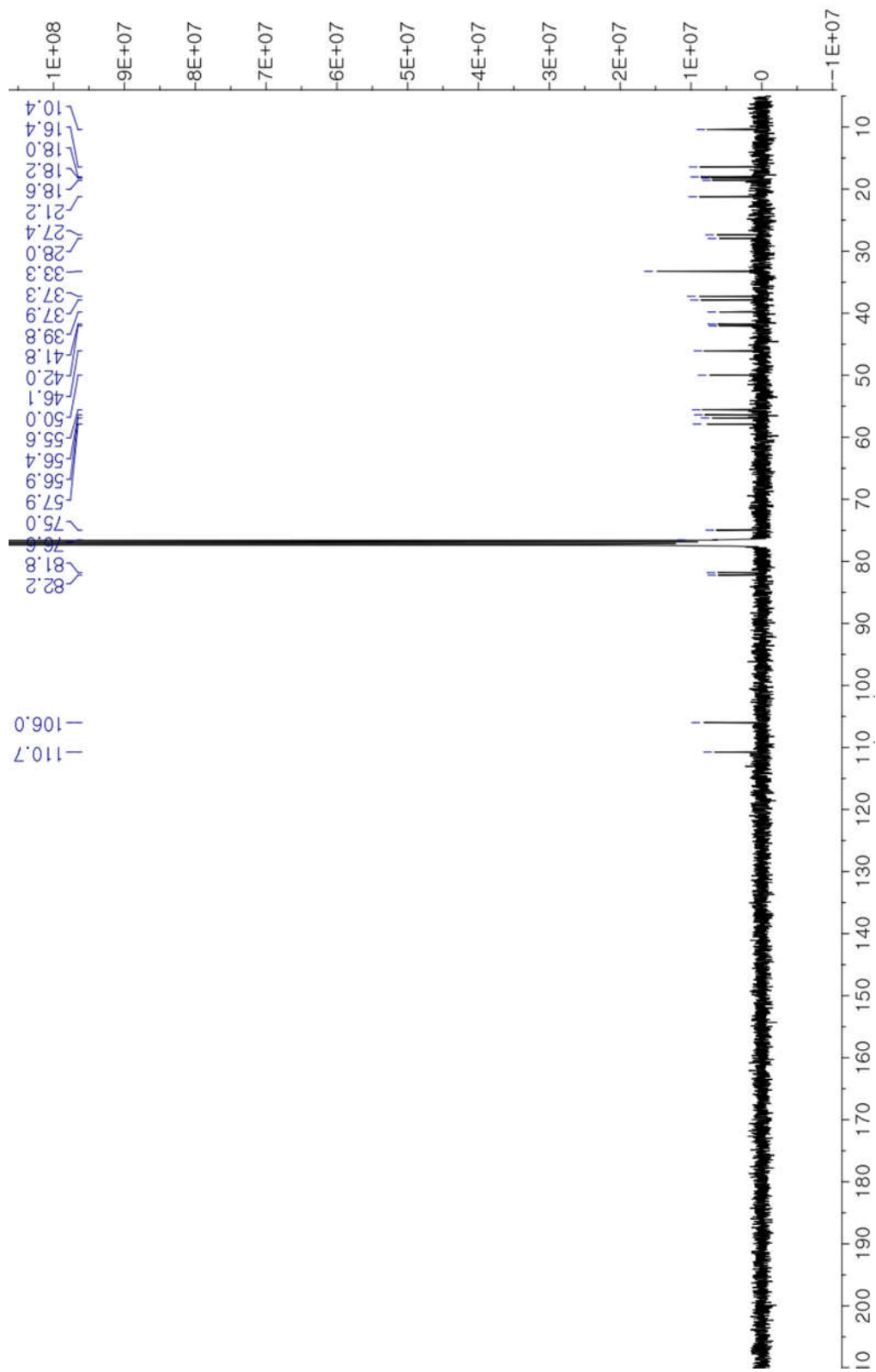


**Figure S64.** The NOESY (600 MHz, CDCl<sub>3</sub>) spectrum of **10**

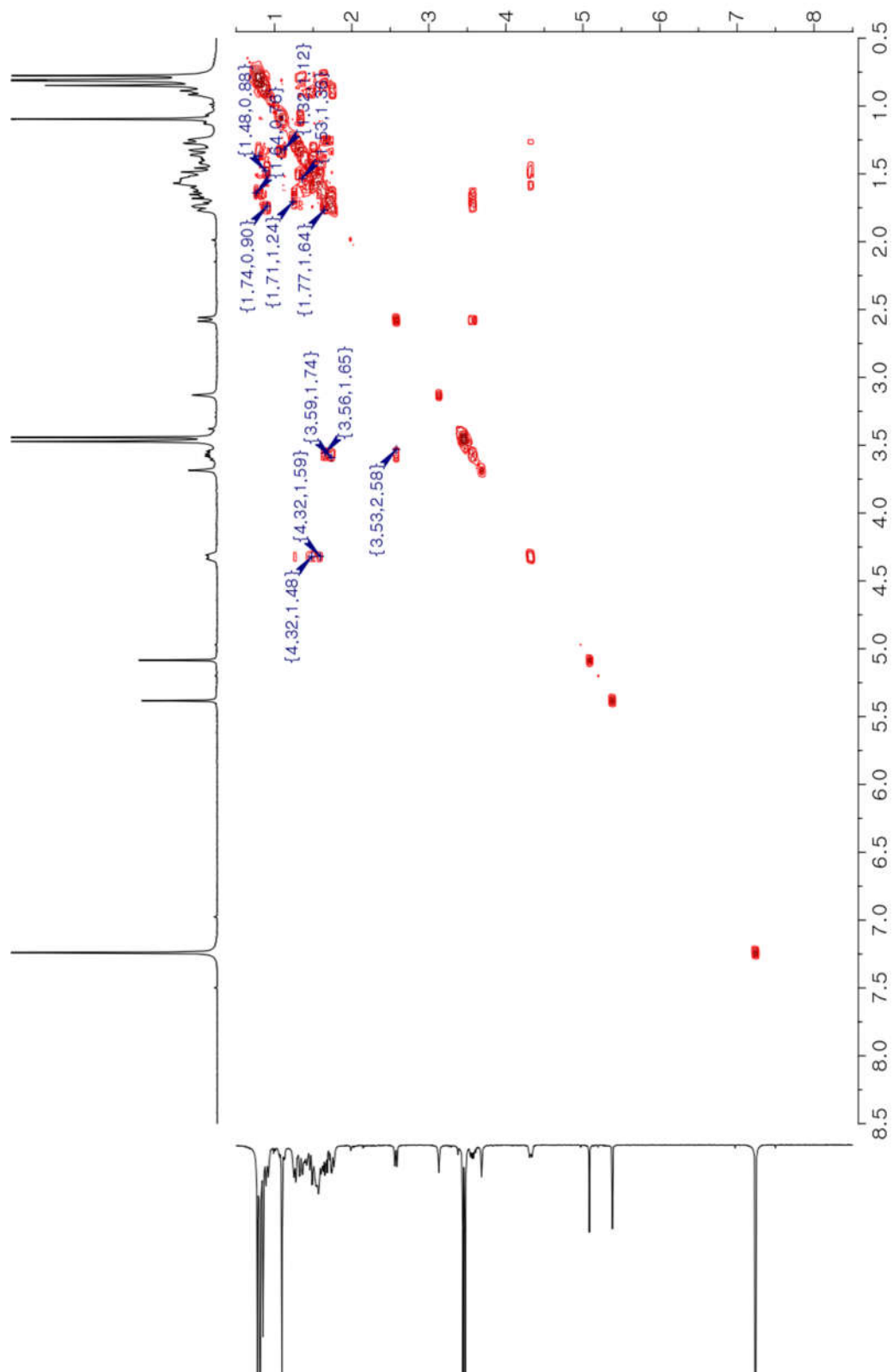


**Figure S65.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of **11**





**Figure S66.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **11**



**Figure S67.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **11**

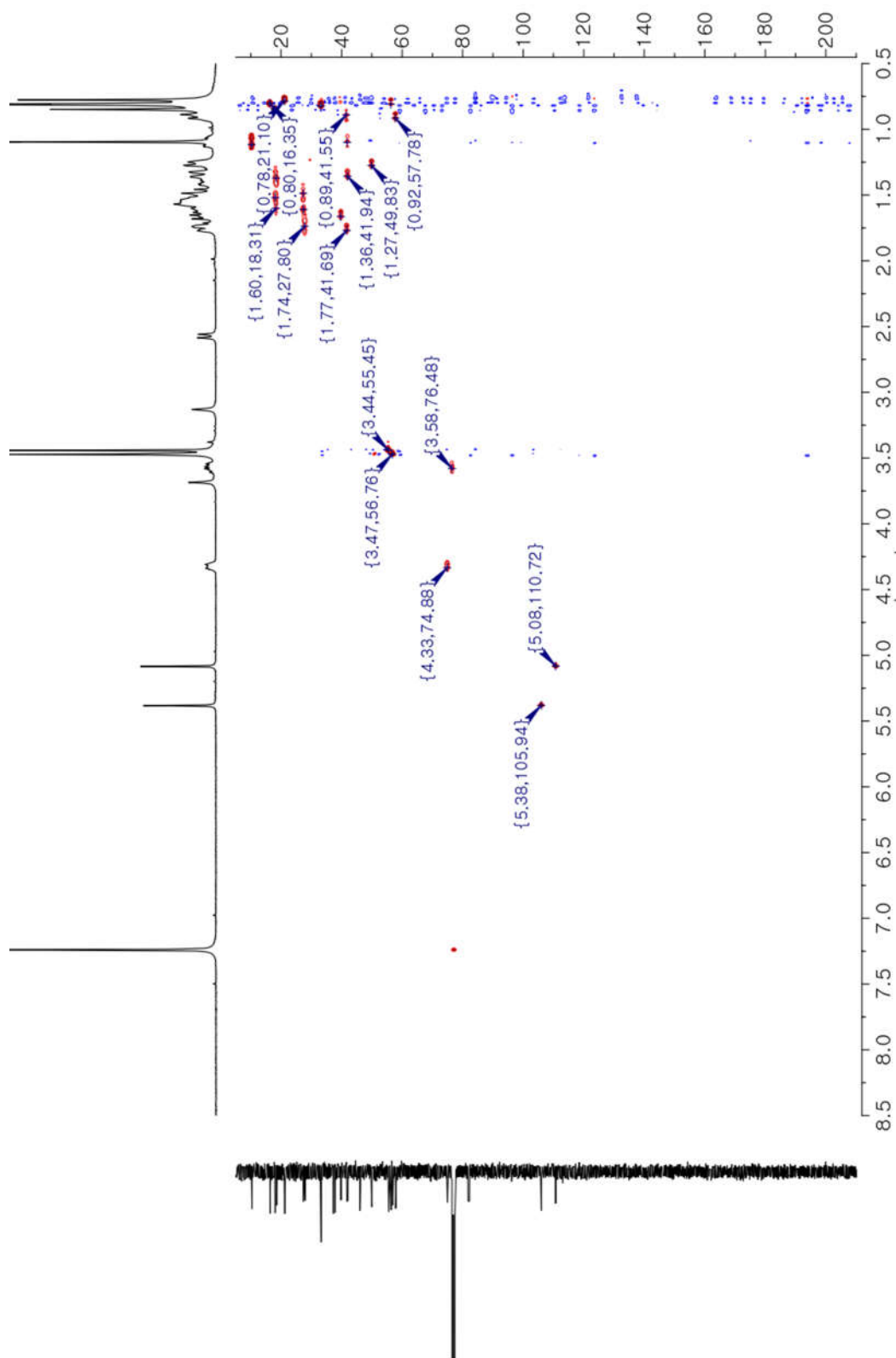
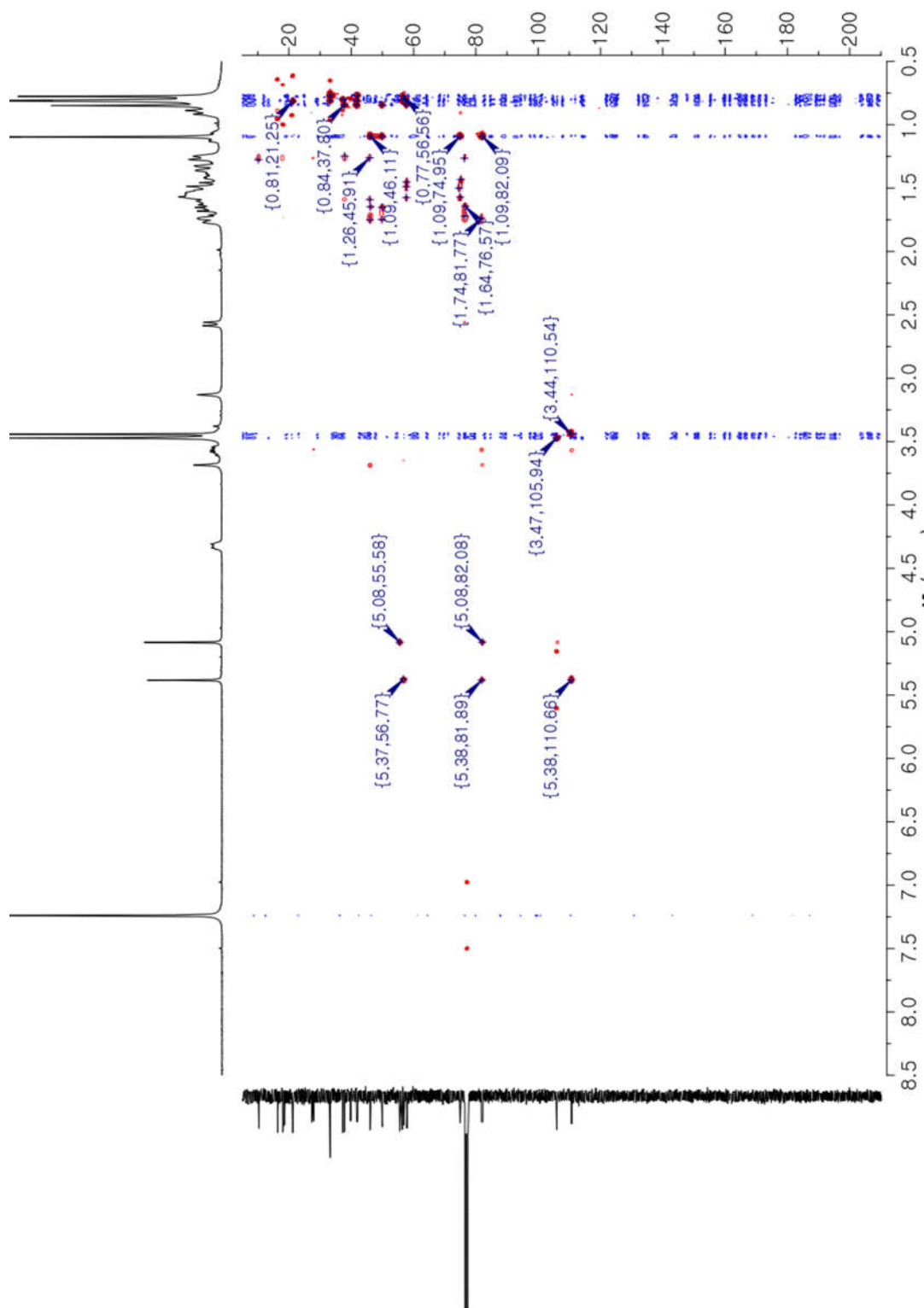
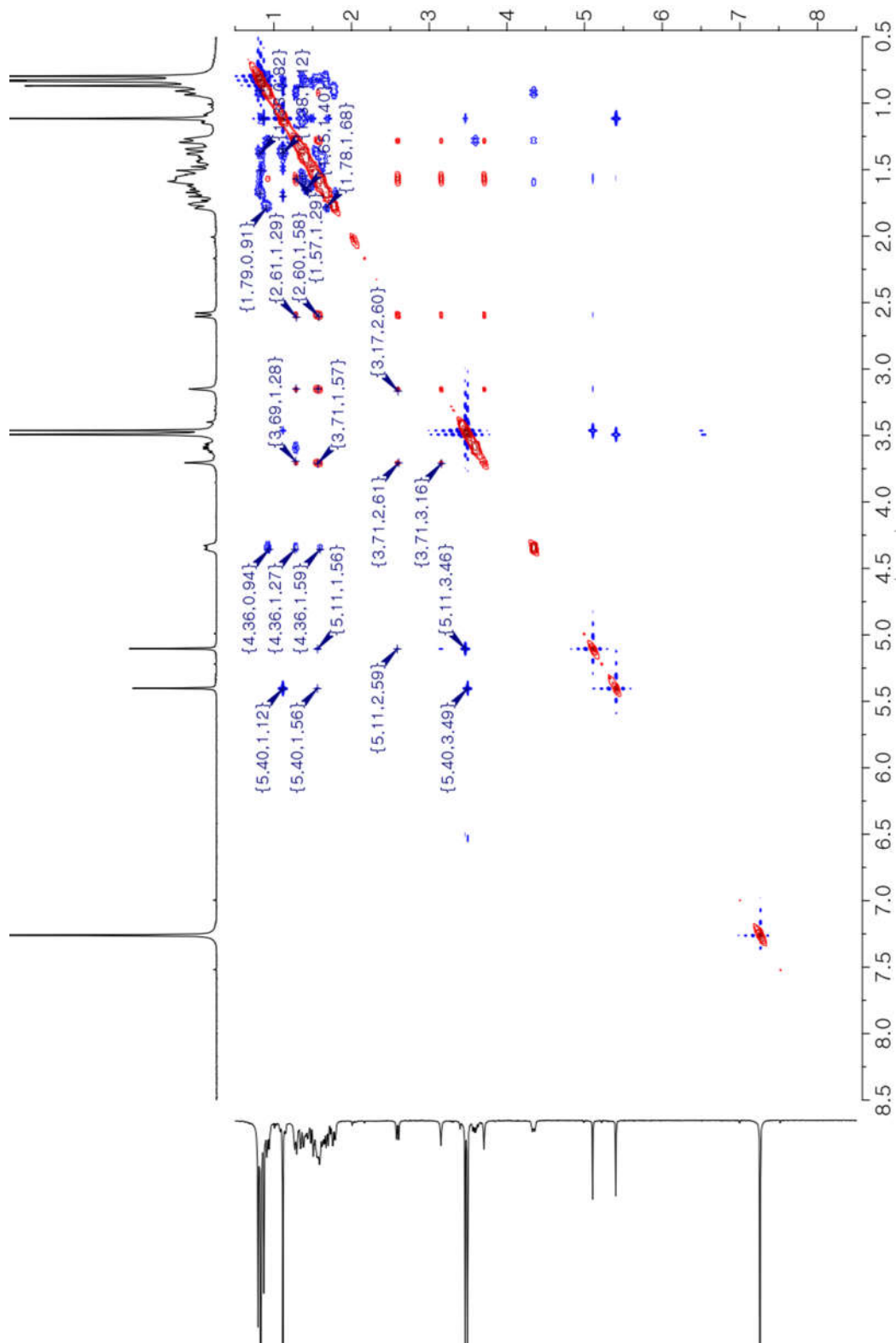


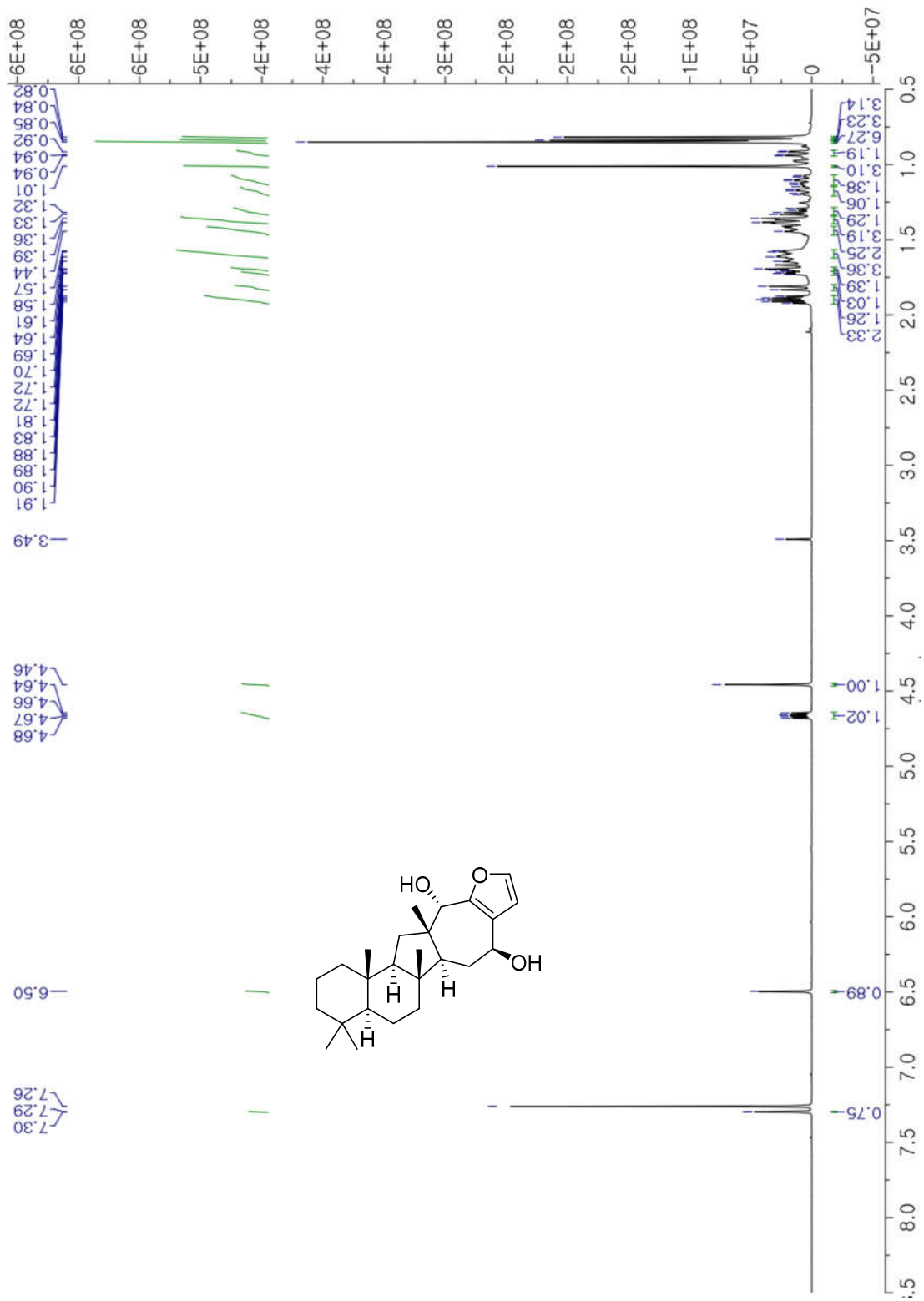
Figure S68. The HSQC (600 MHz, CDCl<sub>3</sub>) spectrum of **11**



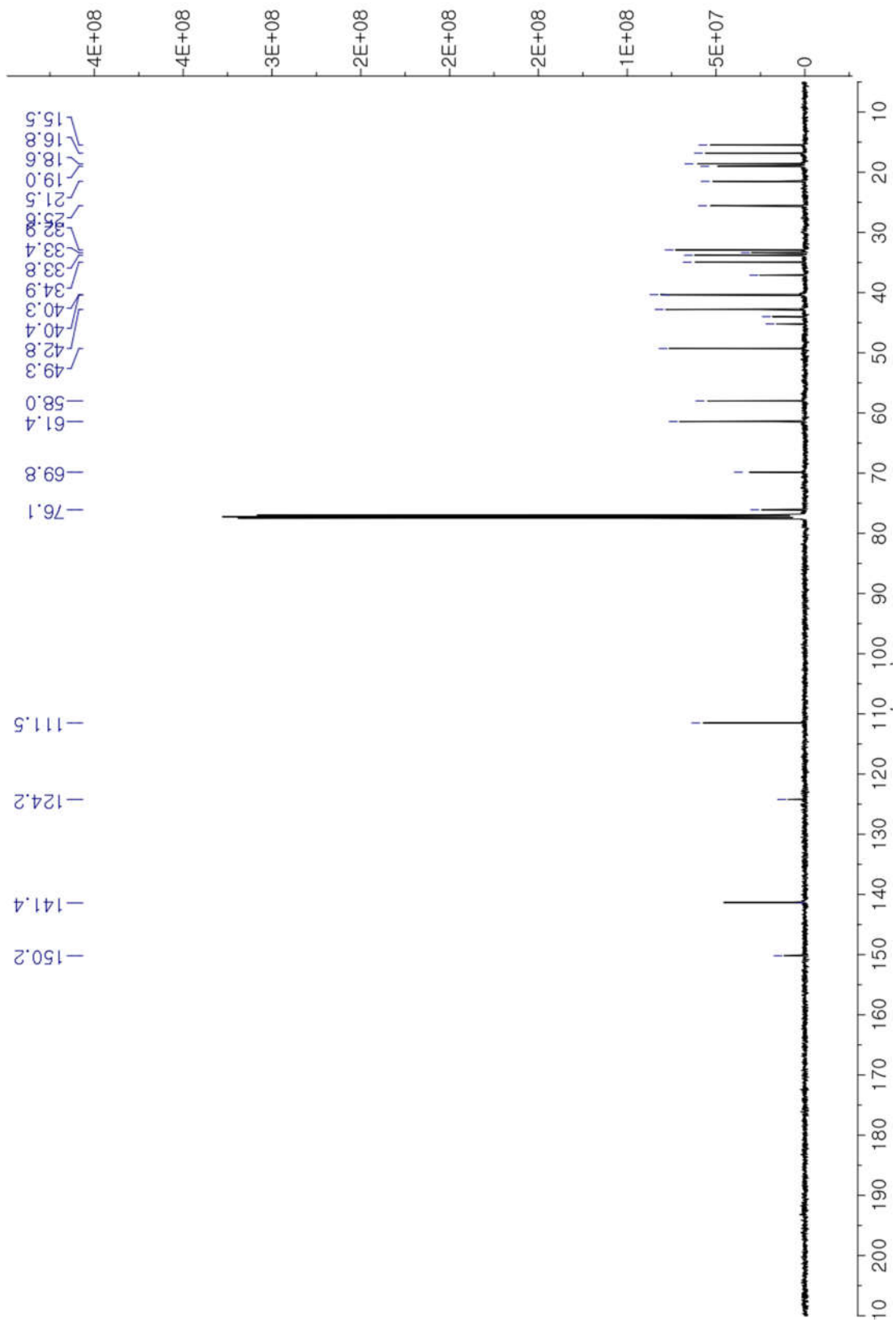
**Figure S69.** The HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of **11**



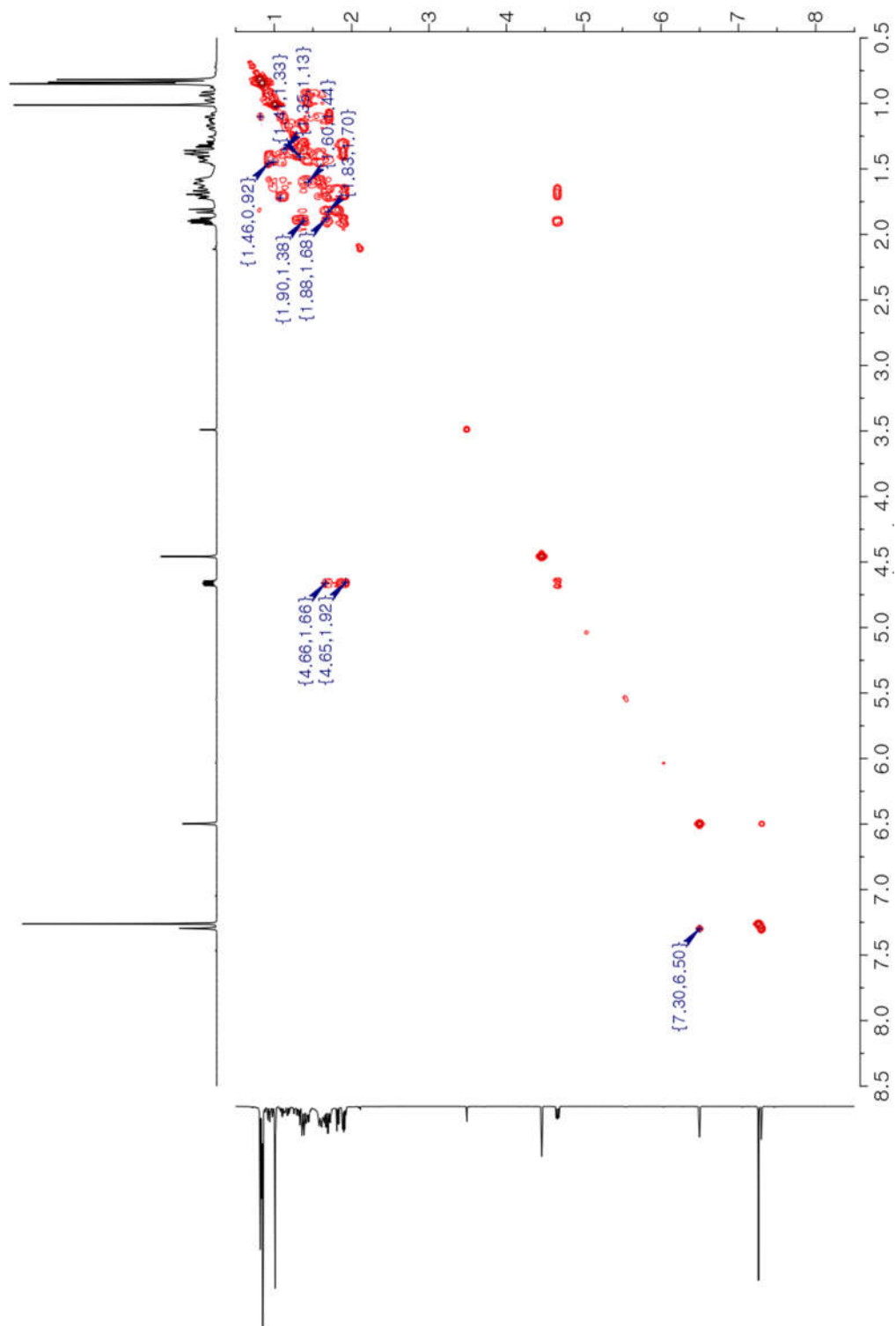
**Figure S70.** The NOESY (600 MHz,  $\text{CDCl}_3$ ) spectrum of **11**



**Figure S71.** The  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) spectrum of **12**

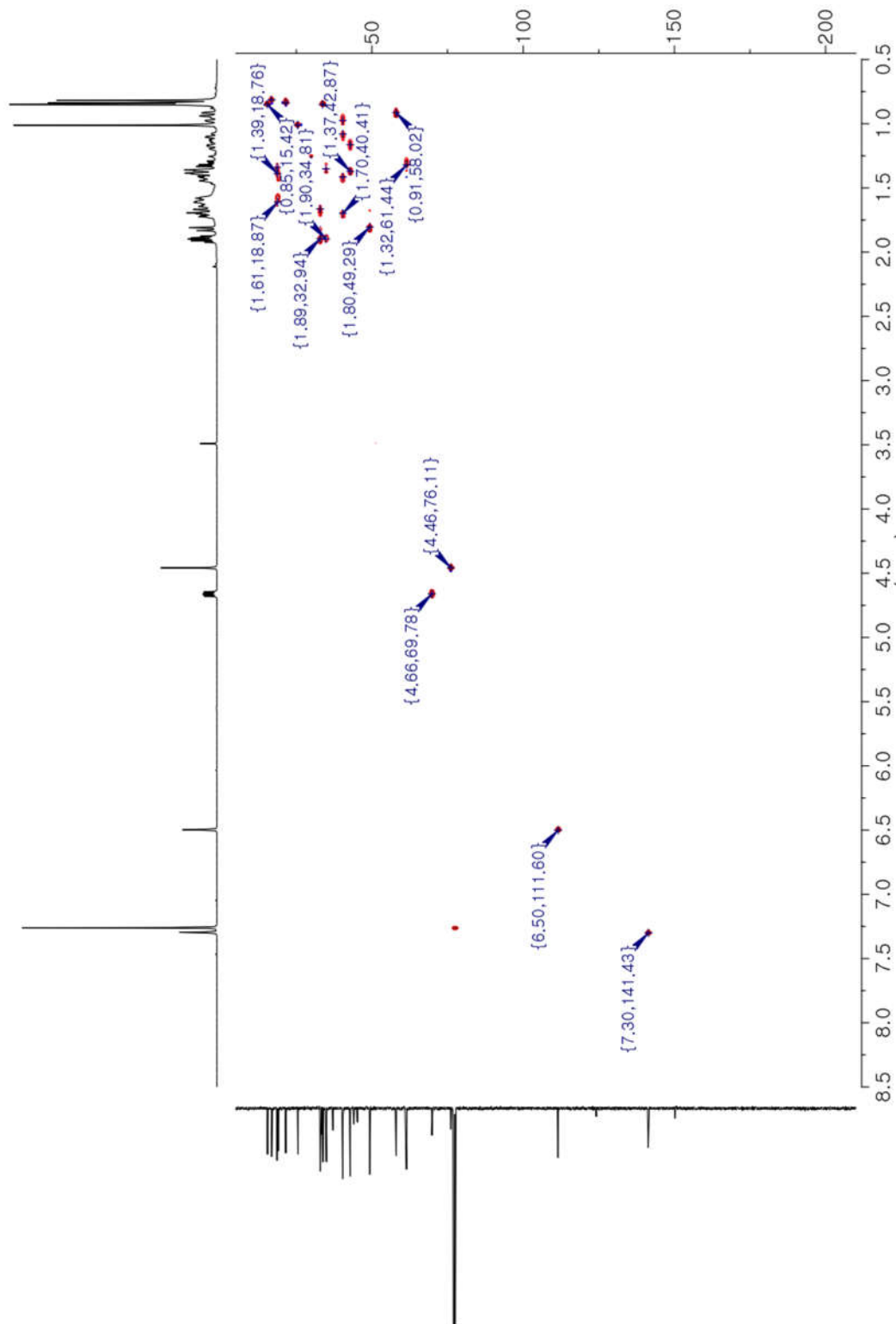


**Figure S72.** The  $^{13}\text{C}$  NMR (150 MHz,  $\text{CDCl}_3$ ) spectrum of **12**



**Figure S73.** The COSY (600 MHz, CDCl<sub>3</sub>) spectrum of **12**





**Figure S74.** The HSQC (600 MHz,  $\text{CDCl}_3$ ) spectrum of **12**

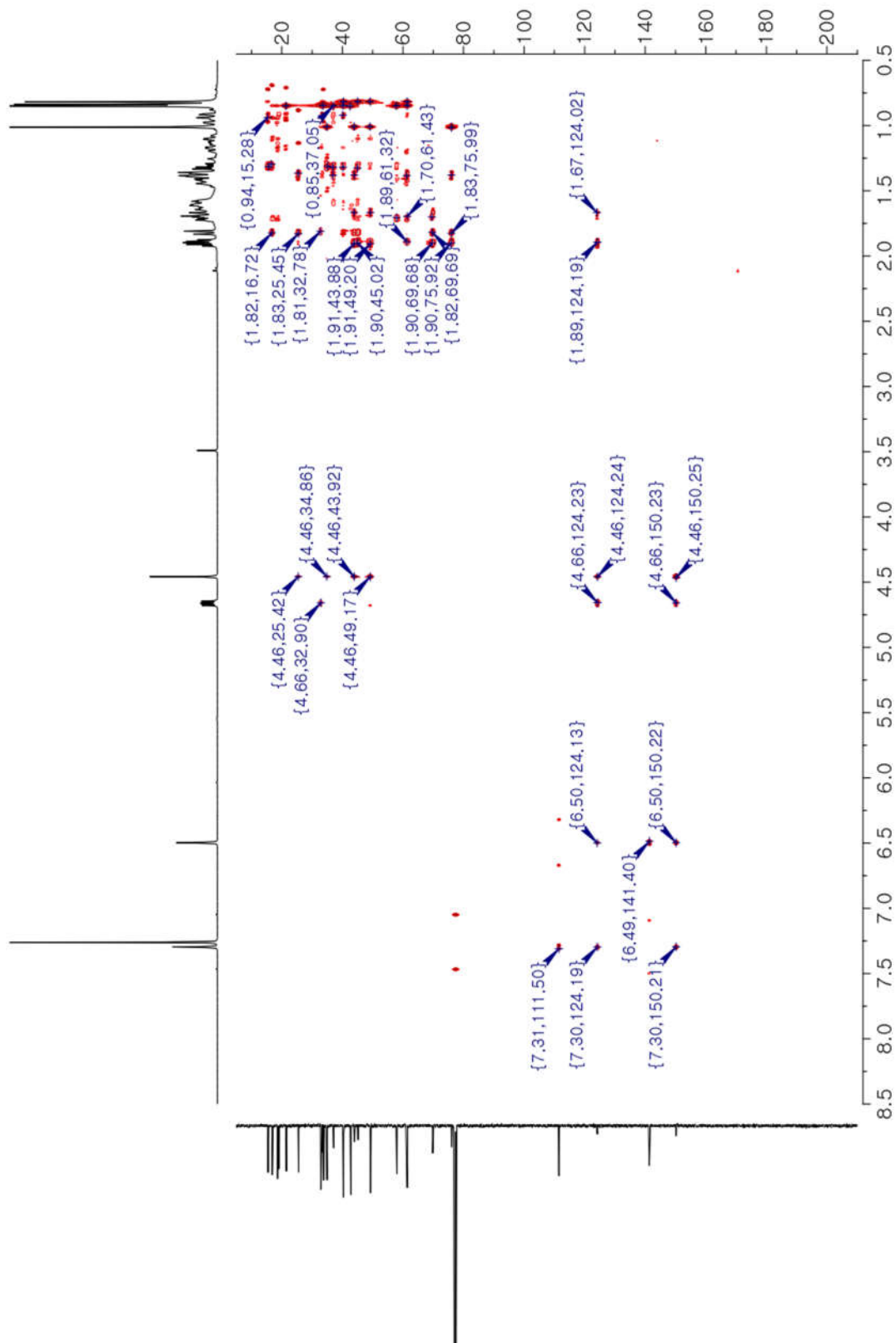
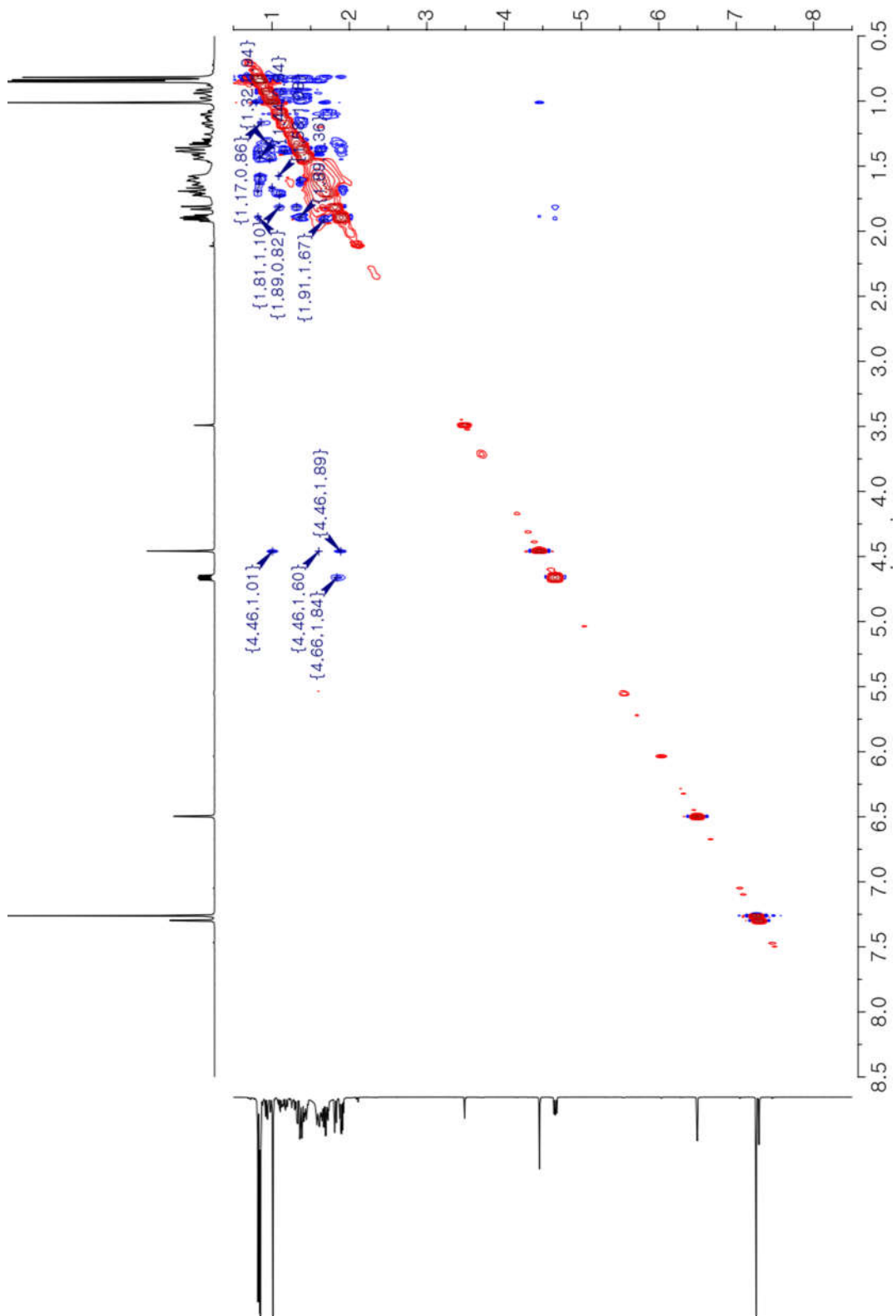


Figure S75. The HMBC (600 MHz, CDCl<sub>3</sub>) spectrum of **12**



**Figure S76.** The NOESY (600 MHz, CDCl<sub>3</sub>) spectrum of **12**

## Assignment of stereochemistry and structure using NMR and DP4

Please select version of database to use:

DP4-original  
DP4-database2

Select probability distribution:

t distribution (recommended)  
 normal distribution

**13C Calc:**

C1,C2,C3,C4,C5,C6,C7,C8,C9,C10,C11,C12,C13,  
154.5,137.2,126.5,112.3,78.2,72.2,64.3,60.2,53.5,4  
153.8,136.3,126.7,113.0,78.6,72.2,64.2,60.4,59.3,4  
158.1,136.3,124.9,113.6,78.9,67.4,64.1,60.5,55.6,4  
157.1,137.4,125.1,115.3,77.8,67.2,64.7,60.3,50.5,4

**1H Calc:**

H1,H2,H3,H4,H5,H6,H7,H8,H9,H10,H11,H12,H13,  
7.1,6.7,4.8,4.6,2.5,2.0,2.0,1.8,1.7,1.7,1.7,1.6,1.5,1.5  
7.2,6.8,4.5,4.5,2.3,2.0,1.8,1.7,1.7,1.6,1.6,1.5,1.4,1.4  
7.1,6.4,4.8,4.7,2.4,2.2,1.9,1.7,1.7,1.7,1.6,1.6,1.6,1.4  
7.0,6.5,4.6,4.5,2.7,2.0,2.0,1.8,1.8,1.7,1.7,1.7,1.6,1.5

**13C Expt:**

150.2(C1), 141.4(C2), 124.2(C3), 111.5(C4), 76.1(C5)

**1H Expt:**

7.3(H1), 6.5(H2), 4.66(H3), 4.46(H4), 1.9(H5), 1.89(H6)

Read Data Show Assignments Calculate Clear

This calculation will use the DP4-database2 version of the database and the t distribution.  
(To change these options select the desired database and distribution from the menus at the top of the applet and then click Calculate).

Results of DP4 using both carbon and proton data:

Isomer 1: 97.5%  
Isomer 2: 2.4%  
Isomer 3: 0.0%  
Isomer 4: 0.0%

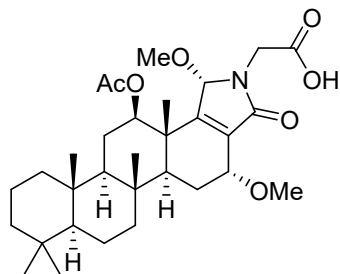
Results of DP4 using the carbon data only:

Isomer 1: 95.5%  
Isomer 2: 3.8%  
Isomer 3: 0.0%  
Isomer 4: 0.6%

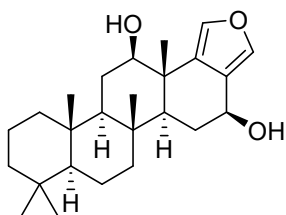
Results of DP4 using the proton data only:

Isomer 1: 59.2%  
Isomer 2: 36.6%  
Isomer 3: 0.0%  
Isomer 4: 4.2%

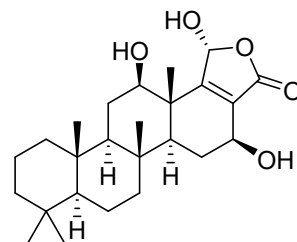
Figure S77. The results of DP4 analyses of 12.



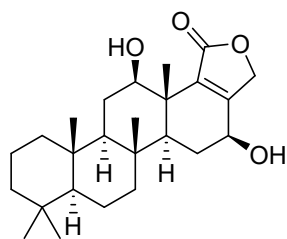
14



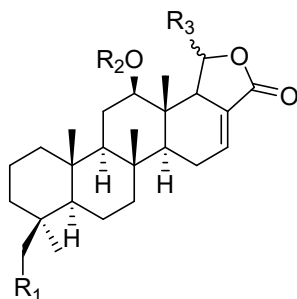
15



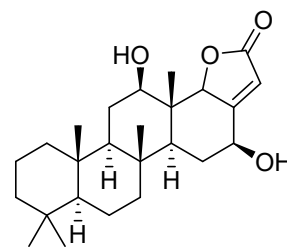
16



17

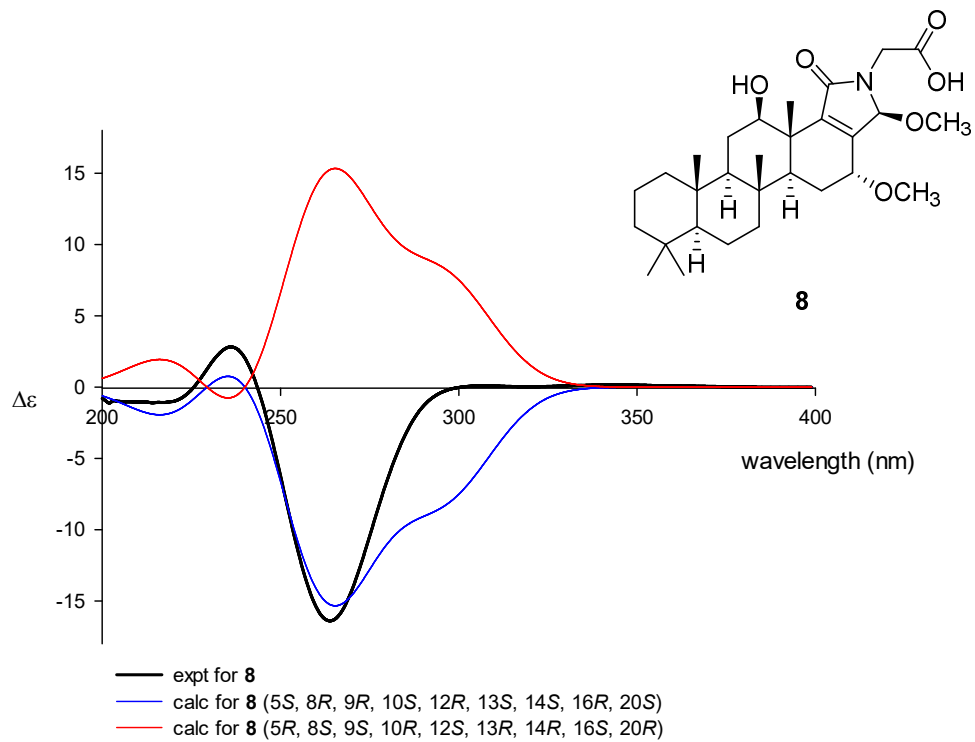
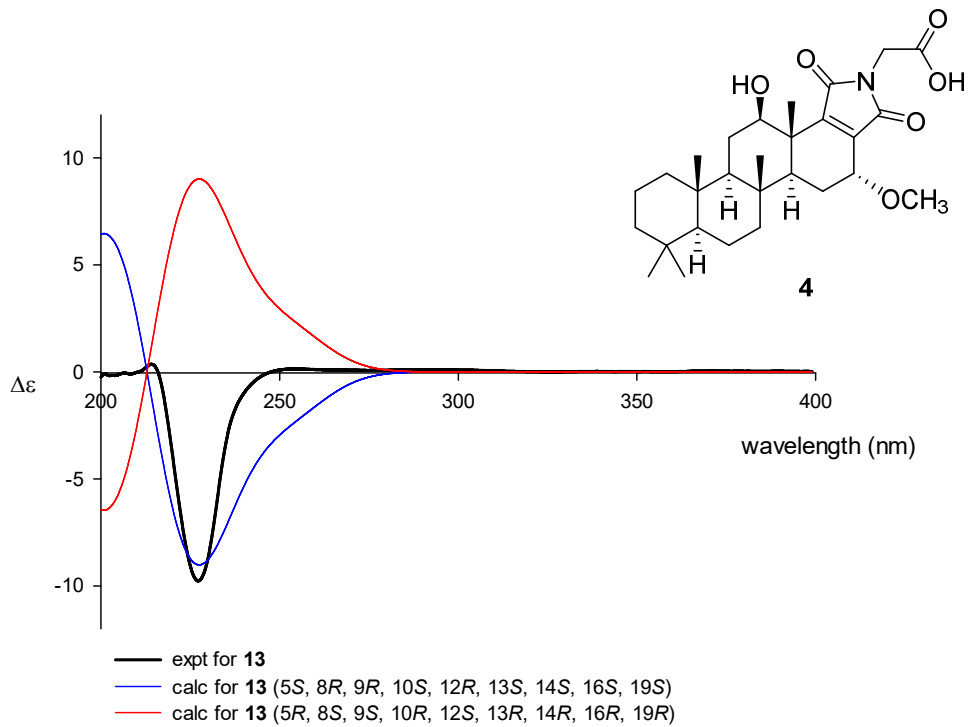


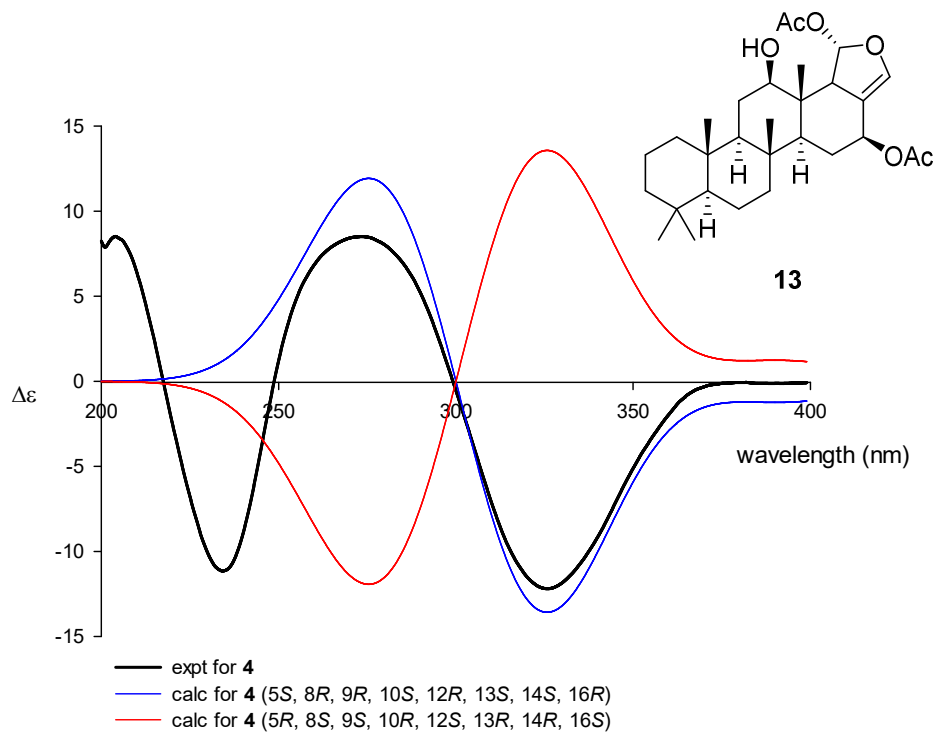
18  $R_1=H$ ,  $R_2=H$ ,  $R_3=OH$  (R)  
 19  $R_1=OCOCH_3$ ,  $R_2=COCH_3$ ,  $R_3=H$



20

Figure S78. Isolated known compounds from *Hyrtilis erectus*





**Figure S79.** Calculated and experimental ECD spectra of **4**, **8** and **13**