SUPPLEMENTARY MATERIAL

A new indole-type alkaloid from the roots of *Clematis florida var. plena*

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A new indole-type alkaloid from the roots of *Clematis florida var. plena*

Abstract: One new indole-type alkaloid, *α*-L-rhamnopyranosyl-(1→6)-*β*-D-glucopyranosyl 6-methoxy-3-indolecarbonate (**1**), together with three known alkaloids (**2-4**), one aromatic acid (**5**) and five known saponins (**6-10**), was isolated from the roots of *Clematis florida var. plena*. Their structures were established by NMR spectroscopic analysis and acid hydrolysis. In *in vivo* anti-inflammatory activity, *n*-butanol extract was found to be potent against ear edema in mice, with inhibition rate of 48.7% at a dose of 800 mg/kg. Furthermore, compounds **8** and **9** obtained from the *n*-butanol extract exhibited significant anti-inflammatory activities with inhibition rates of 50.9% and 54.7% at a dose of 200 mg/kg.

Keywords: *Clematis florida var. plena*; alkaloid; saponins; anti-inflammatory

List of Supporting Information

Table S1. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectral data of compounds **1-5** in CD_3OD.

No.	**1**		**2**		**3**		**4**		**5**	
	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1										129.1
2	7.87 s	133.3	7.98 s	134.2	7.86 s	133.0	7.85 s	132.3	7.02 d (2.1)	114.9
3		107.5		107.5		108.2		108.4		151.5
4	7.86 d (8.8)	122.6	8.01 m	122.0	7.91 d (8.7)	122.4	7.90 d (8.8)	121.5		148.2
5	6.76 dd (2.2, 8.8)	112.8	7.12 m	122.7	6.99 dd (2.1, 8.7)	114.4	6.74 dd (2.2, 8.8)	112.8	6.92 d (8.3)	112.7
6		158.3	7.12 m	123.9		156.0		158.5	7.04 dd (2.1, 8.3)	122.8
7	6.87 d (2.2)	96.0	7.36 m	113.0	7.17 d (2.1)	100.4	6.85 d (2.2)	96.1		
8		121.5		127.5		122.9		122.6		
9		138.9		138.2		138.4		139.0		
α									6.26 d (15.9)	116.9
β									7.54 d (15.9)	146.7
Glc										
1’	5.60 d (7.8)	95.2	5.62 d (7.7)	95.3	4.84 d (7.7)	103.3				
2’	3.41 m	74.0	3.42 m	74.2	3.40 m	75.0				
3’	3.41 m	72.3	3.42 m	78.2	3.44 m	78.0				
4’	3.75 m	71.2	3.45 m	72.1	3.34 m	71.7				

5’	3.50 m	77.6	3.50 m	77.7	3.56 m	77.0				
6’	3.90 dd (1.5, 11.2)	67.8	3.90 dd (1.5, 11.0)	67.8	4.02 dd (1.5, 11.0)	68.5				
	3.59-3.53 m		3.58 dd (1.5, 11.0)		3.64 dd (1.5, 11.0)					
Rha										
1”	4.63 d (1.6)	102.2	4.63 d (1.2)	102.3	4.72 d (1.2)	102.5				
2”	3.32 m	72.1	3.33 m	71.3	3.82 m	72.2				
3”	3.59-3.53 m	72.3	3.58 m	72.3	3.72 m	72.3				
4”	3.26 br. s	74.1	3.25 m	74.0	3.44 m	74.1				
5”	3.59-3.53 m	69.8	3.56 m	69.8	3.72 m	70.0				
6”	1.10 d (6.2)	17.9	1.10 d (6.2)	17.9	1.21 d (6.2)	17.9				
C=O		165.5		165.4		167.8		168.0		171.0
6-OCH_3	3.73 s	55.9					3.88 s	56.1	3.87 s	56.5
$COOCH_3$					3.84 s	51.4	3.83 s	51.5		

Table S2. ^{1}H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectral data of compounds **6-10** in C_5D_5N.

No.	**6**		**7**		**8**		**9**		**10**	
	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C
1	0.89 m, 1.41 m	38.6	0.89 m, 1.40 m	39.2	0.82 [a], 1.36 m	38.5	0.92 [a], 1.41 m	38.6	0.87 m, 1.42 m	38.1
2	1.87 m, 2.10m	26.2	2.12 m, 1.98 m	26.6	1.82 m, 1.97 m	26.2	1.89 m, 2.06 m	25.7	1.86 m,2.08 m	25.8
3	3.25 dd (4.6, 11.9)	88.9	4.20 [a]	81.2	3.12 dd (4.2, 11.5)	88.4	4.11 [a]	81.6	3.27 dd (3.6, 11.4)	87.9
4		39.3		43.5		39.1		44.8		39.1
5	0.86 [a]	55.5	1.63 [a]	47.2	0.78 [a]	55.6	1.61 [a]	47.7	0.88 [a]	56.2
6	1.25 m, 1.44 m	18.3	1.61 [a], 1.25 [a]	18.7	1.24 m, 1.45 m	18.0	1.58 [a], 1.23 [a]	18.0	1.27 m, 1.45 m	17.7
7	1.31 m,1.46 m	32.7	1.48 m, 1.25 [a]	33.0	1.33 m, 1.52 m	32.6	1.44 m, 1.23 [a]	32.5	1.30 m, 1.51 m	32.3
8		39.6		39.9		39.4		39.3		39.1
9	1.61 m	47.8	1.70 [a]	48.2	1.61 m	47.6	1.71 [a]	48.5	1.61 m	47.2
10		36.7		36.4		36.5		36.5		36.2
11	1.87 m, 2.07 m	23.4	1.96 m, 1.85 m	23.5	1.89 m, 2.02 m	23.3	1.89 m, 1.72 [a]	23.2	1.87 m, 2.06 m	22.8
12	5.40 m	122.5	5.41 br. s	122.8	5.36 br.s	122.8	5.28 br. s	122.4	5.39 br. s	122.2
13		143.9		144.3		143.8		143.5		143.3
14		41.8		42.2		41.6		41.5		41.3
15	1.13 m, 2.30 m	27.8	1.12 m, 2.30 m	28.5	1.14 m, 2.20 m	27.7	1.41 m, 2.03 m	27.5	1.13 m, 2.28 m	27.4
16	1.07 m, 2.07 m	23.0	1.98 m	23.6	1.03 [a], 2.06 m	22.9	1.83 m, 2.06 m	22.8	1.06 [a], 2.07 m	22.5
17		46.8		47.2		46.6		47.8		46.2
18	3.20 dd (3.9, 13.9)	41.4	3.20 dd (3.9, 13.9)	41.8	3.12 dd (3.2, 13.2)	41.2	2.87 dd (2.7, 12.6)	41.1	3.16 dd (3.2, 12.7)	40.8

19	1.25 m, 1.74 m	45.8	1.25 [a], 1.78 m	46.4	1.22 m, 1.71 m	45.8	1.25 [a], 1.74 m	46.7	1.24 m, 1.73 m	45.4
20		30.5		30.9		30.2		30.2		29.9
21	1.07 [a], 1.32 m	33.6	1.07 [a], 1.31 m	34.2	1.07 [a], 1.38 m	33.5	1.07 [a], 1.33 m	33.5	1.07 [a], 1.42 m	33.2
22	1.85 m, 2.06 m	32.2	1.83 m, 1.74 m	32.8	1.89 m, 2.09 m	32.0	1.86 m, 2.06 m	31.9	1.87 m, 2.08 m	31.7
23	1.28 s	27.7	4.26 [a], 3.90 m	64.0	1.27 s	27.7	3.63 m, 4.04 m	63.4	1.24 s	27.4
24	1.16 s	16.9	1.16 s	14.4	1.18 s	16.6	1.16 s	14.8	1.16 s	16.3
25	0.86 s	15.4	0.86 s	15.8	0.82 s	15.2	0.85 s	15.8	0.87 s	14.8
26	1.07 s	17.2	1.07 s	17.6	1.06 s	17.0	1.03 s	16.7	1.06 s	16.3
27	1.25 s	25.6	1.25 s	26.2	1.28 s	25.6	1.24 s	25.7	1.30 s	25.2
28		176.3		176.7		176.4		176.7		175.7
29	0.89 s	32.7	0.89 s	33.2	0.99 s	32.6	0.95 s	32.5	0.88 s	32.3
30	0.89 s	23.4	0.89 s	23.8	0.99 s	23.2	0.95 s	23.2	0.88 s	23.0
	28-O-GlcI		28-O-GlcI		28-O-GlcI		28-O-GlcI		28-O-GlcI	
1	6.25 d (8.0)	95.4	6.25 d (8.1)	95.7	6.13 d (8.0)	95.1	5.93 d (8.0)	94.4	6.24 d (8.0)	94.8
2	4.11 m	73.4	4.05 m	74.0	4.11 m	73.2	4.37 m	74.4	4.10 m	73.0
3	4.20 m	78.1	4.20 m	78.7	4.22 m	77.9	4.11 m	79.6	4.23 m	77.9
4	4.32 m	70.2	4.28 m	70.9	4.39 m	70.0	4.11 m	71.0	4.31 m	70.0
5	4.05 m	77.6	4.08 m	78.2	4.04 m	77.7	4.04 m	76.8	4.07 m	77.2
6	4.33 m, 4.67 m	68.9	4.68 br. d (11.0), 4.32 m	69.3	4.74 m, 4.37 m	68.5	4.15 [a], 4.49 m	69.3	4.75 m, 4.36 m	68.4
	Glc II (at C-$6_{Glc\ I}$)		Glc II (at C-$6_{Glc\ I}$)		Glc II (at C-$6_{Glc\ I}$)		Glc II (at C-$6_{Glc\ I}$)		Glc II (at C-$6_{Glc\ I}$)	
1	4.93 d (7.6)	104.5	5.00 d (7.4)	105.3	5.02 d (7.3)	104.7	5.05 d (7.8)	103.9	4.99 d (7.9)	104.0
2	3.90 m	74.7	3.92 m	75.5	3.91 m	75.2	3.96 m	75.3	3.94 m	74.5
3	4.14 m	75.9	4.12 m	76.8	4.08 m	75.9	4.08 m	76.3	4.15 m	75.7

4	4.41 m	77.8	4.41 m	78.5	4.40 m	77.9	4.39 m	78.2	4.42 m	77.4
5	3.65 m	76.6	3.67 m	77.3	3.65 m	76.4	3.65 m	76.8	3.64 m	76.3
6	4.08 m, 4.20 m	60.7	4.08 m, 4.16 m	61.4	4.08 m, 4.18 m	60.7	4.00 m, 4.18 m	61.1	4.10 m, 4.22 m	60.4
	Rha I (at C-4$_{Glc\ II}$)		Rha I (at C-4$_{Glc\ II}$)		RhaI(at C-4$_{Glc\ II}$)		Rha I (at C-4$_{Glc\ II}$)		Rha I (at C-4$_{Glc\ II}$)	
1	5.88 br. s	102.5	5.87 br. s	103.0	5.94 br. s	102.1	5.84 br. s	101.6	5.88 br. s	101.9
2	4.67 m	72.0	4.66 br. s	72.7	4.67 m	71.9	4.60 m	71.5	4.66 m	71.7
3	4.54 m	72.2	4.55 m	72.9	4.55 m	72.2	4.48 m	72.4	4.54 m	71.9
4	4.33 m	73.6	4.32 m	74.0	4.33 m	73.3	4.39 m	73.3	4.33 m	73.2
5	5.00 m	70.1	5.00 m	70.5	5.03 m	69.6	4.96 m	69.6	4.98 m	69.5
6	1.71 d (6.1)	18.1	1.71 d (6.1)	18.7	1.72 d (6.2)	17.9	1.70 d (6.2)	18.0	1.70 d (5.9)	17.6
							Rha II (at C-2$_{Glc\ I}$)			
1							6.45 br. s	102.9		
2							4.60 br. s	72.4		
3							4.42 [a]	72.4		
4							4.37 [a]	73.9		
5							4.49 [a]	70.0		
6							1.72 d (6.4)	18.0		
	3-O-Ara		3-O-Ara		3-O-xyl		3-O-Ara		3-O-Ara	
1	4.66 d (6.7)	105.0	4.67 d (6.5)	104.7	4.91 d (8.0)	105.8	4.73 d (6.6)	103.5	4.65 d (6.2)	104.5
2	4.51 m	75.4	4.43 m	75.9	4.23 m	74.9	4.48 m	75.4	4.44 m	74.4
3	4.23 m	74.6	4.20 [a]	75.7	4.18 m	74.7	4.04 m	75.3	4.23 m	74.5
4	4.23 m	80.0	4.20 [a]	81.1	4.15 m	69.4	4.10 m	69.6	4.22 m	68.6
5	3.77 d (10.5), 4.38 m	65.1	3.69 d (11.0), 4.35 m	66.2	3.72 [a], 4.37 m	64.8	3.64 d (11.1), 4.39 m	66.2	3.80 d (11.7), 4.40 m	64.8

	Rha II (at C-2$_{Ara}$)		Rha II (at C-2$_{Ara}$)		RhaII(at C-2$_{Xyl}$)		Rha III (at C-2$_{Ara}$)		Rha II (at C-2$_{Ara}$)	
1	6.29 br. s	101.9	6.29 br. s	101.5	6.60 br. s	100.8	6.27 br. s	101.5	6.32 br. s	100.6
2	4.87 br. s	71.5	4.87 br. s	72.1	4.81 br. s	71.3	4.73 br. s	72.4	4.87 br. s	71.2
3	4.71 d (10.6)	79.7	4.71 d (10.6)	81.3	4.62 [a]	80.4	4.60 m	72.4	4.75 d (10.3)	80.4
4	4.41 m	72.5	4.41 m	73.1	4.45m	72.2	4.38 m	73.9	4.42 m	72.0
5	4.61 m	69.4	4.71 [a]	70.0	4.54m	69.4	4.64 m	69.6	4.65 m	69.0
6	1.56 d (5.2)	18.3	1.55 d (5.8)	18.7	1.65 d (5.8)	17.9	1.68 d (5.5)	17.9	1.53 d (6.0)	17.7
	Rib (at C-3$_{Rha\ II}$)		Rib (at C-3$_{Rha\ II}$)		Rib (at C-3$_{Rha\ II}$)				Rib (at C-3$_{Rha\ II}$)	
1	5.84 d (4.8)	104.5	5.84 d (4.8)	104.8	5.86 d (4.7)	103.9			5.82 d (5.5)	103.8
2	4.29 [a]	75.1	4.28 [a]	72.9	4.30 [a]	72.0			4.30 [a]	72.0
3	4.46 m	78.1	4.51 m	69.0	4.51 br. s	68.4			4.54 m	68.4
4	4.14 m	69.9	4.12 m	70.5	4.19 m	69.8			4.13 m	69.4
5	4.32 m, 4.16 m	62.3	4.32 m, 4.14 m	65.5	4.21 m	64.6			4.32 m, 4.15 m	64.4
	Glc (at C-4$_{Ara}$)		Glc (at C-4$_{Ara}$)							
1	5.14 d (7.6)	106.4	5.13 d (7.6)	107.2						
2	4.03 m	75.1	4.03 m	75.6						
3	4.19 m	78.5	4.16 m	79.0						
4	4.23 m	71.1	4.23 m	71.4						
5	3.90 m	78.7	3.93 m	78.7						
6	4.46 m, 4.35 m	62.3	4.46 m, 4.35 m	62.7						

[a] Overlapped with other signals.

Table S3. Effects of *Clematis florida var. plena* on ear edema induced by xylene in mice.

Extracts/Fractions	Dose (mg/kg)	Edema Degree ($\bar{x}$ ±SD, mg)	Inhibition Rate (%)
Control group		7.47±0.26	
Aspirin	200	4.85±0.25*	35.1
Methanol extract	600	6.48±0.42*	13.2
	800	5.55±0.35*	25.7
Petroleum ether fraction	600	5.78±0.46*	22.6
	800	4.75±0.27*	36.4
Ethyl acetate fraction	600	5.35±0.48*	28.4
	800	4.68±0.18*	37.3
n-Butanol fraction	600	5.87±0.71*	21.5
	800	3.83±1.07*	48.7
Fr. B2	600	4.57±0.62*	38.9
Fr. B3	600	4.77±0.33*	36.2
Fr. B4	600	3.92±1.60*	47.6
Fr. B5	600	5.65±0.63*	20.3
Compound **1**	200	5.45±0.56*	27.0
Compound **8**	200	3.67±0.31*	50.9
Compound **9**	200	3.53±0.80*	54.7

* ***P*** < 0.01 *vs*. Control group

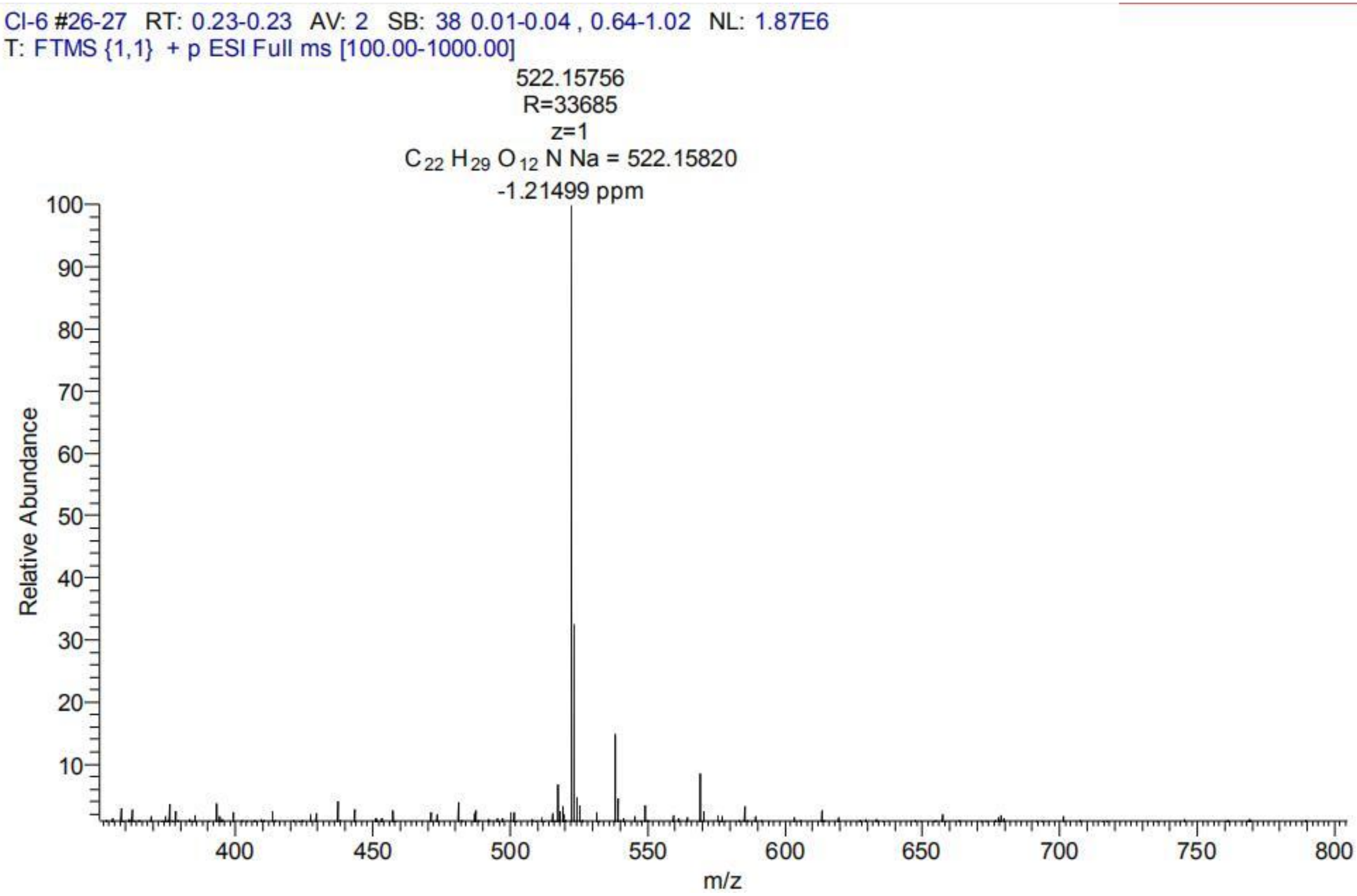

Figure S1. HRESIMS spectrum of compound **1**.

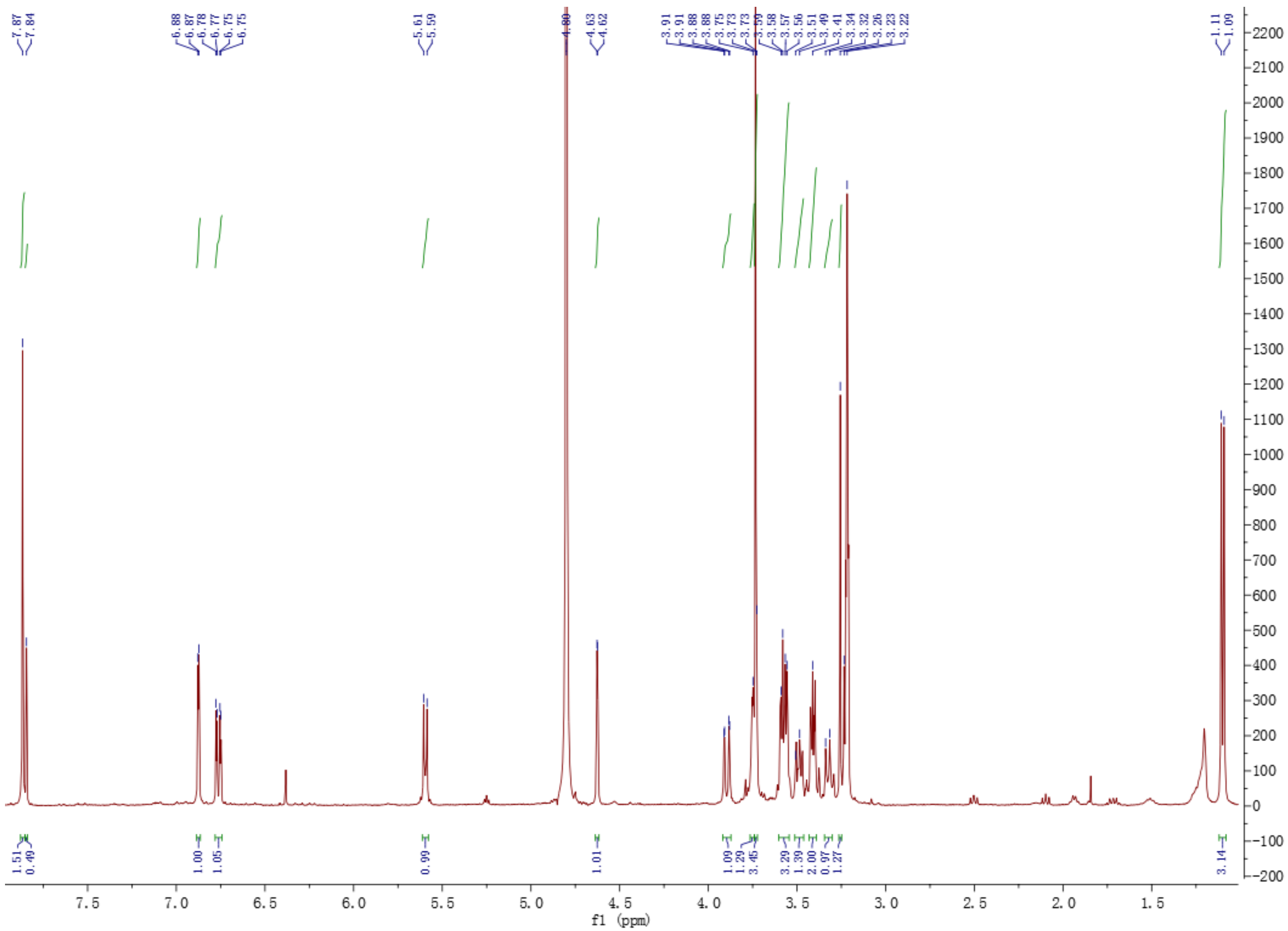

Figure S2. ^{1}H NMR spectrum (400 MHz) of compound **1** in CD_3OD.

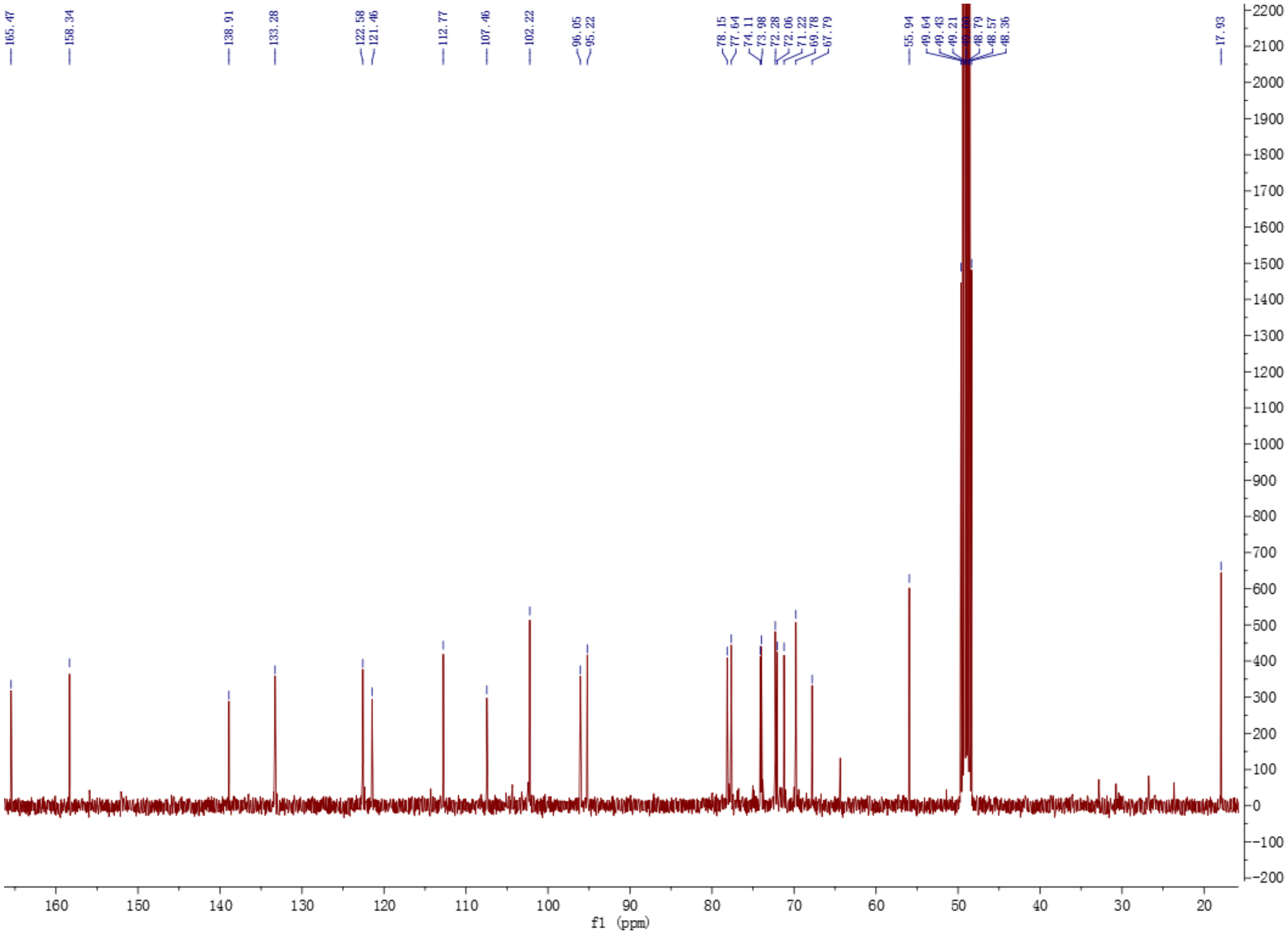

Figure S3. ^{13}C NMR spectrum (100 MHz) of compound **1** in CD$_3$OD.

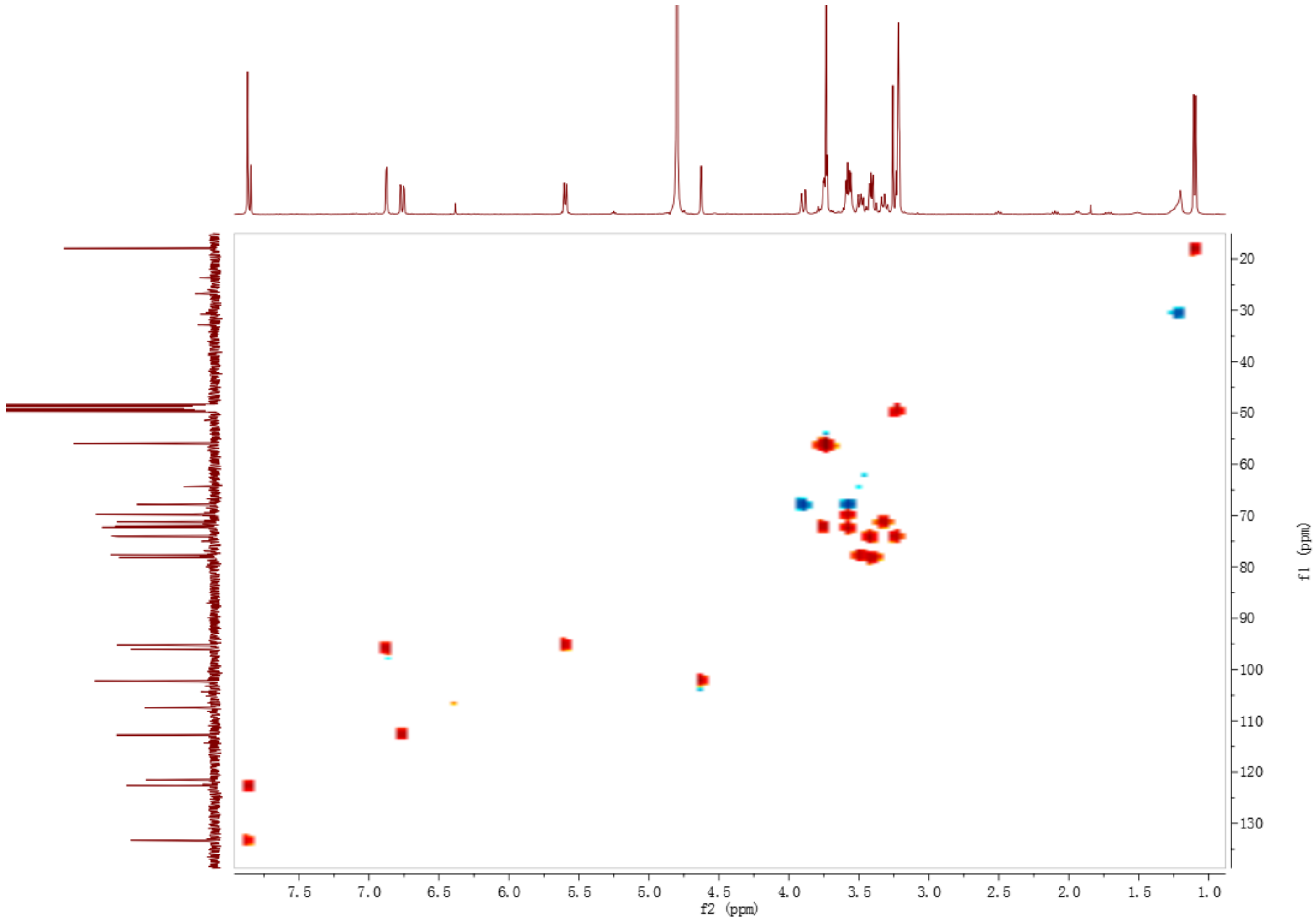

Figure S4. ^{1}H-^{13}C HSQC spectrum of compound **1** in CD_3OD

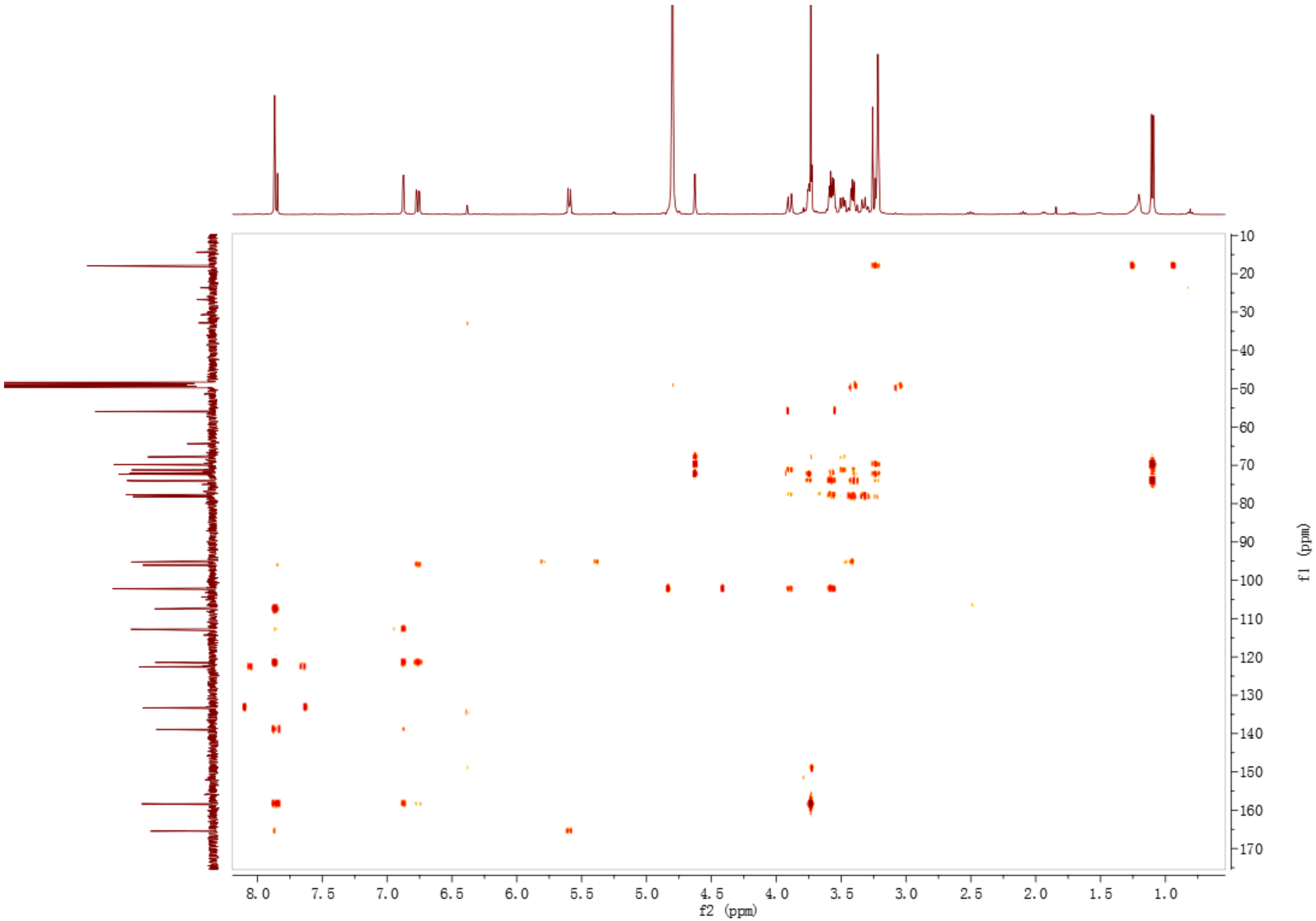

Figure S5. ^{1}H-^{13}C HMBC spectrum of compound **1** in CD_3OD.

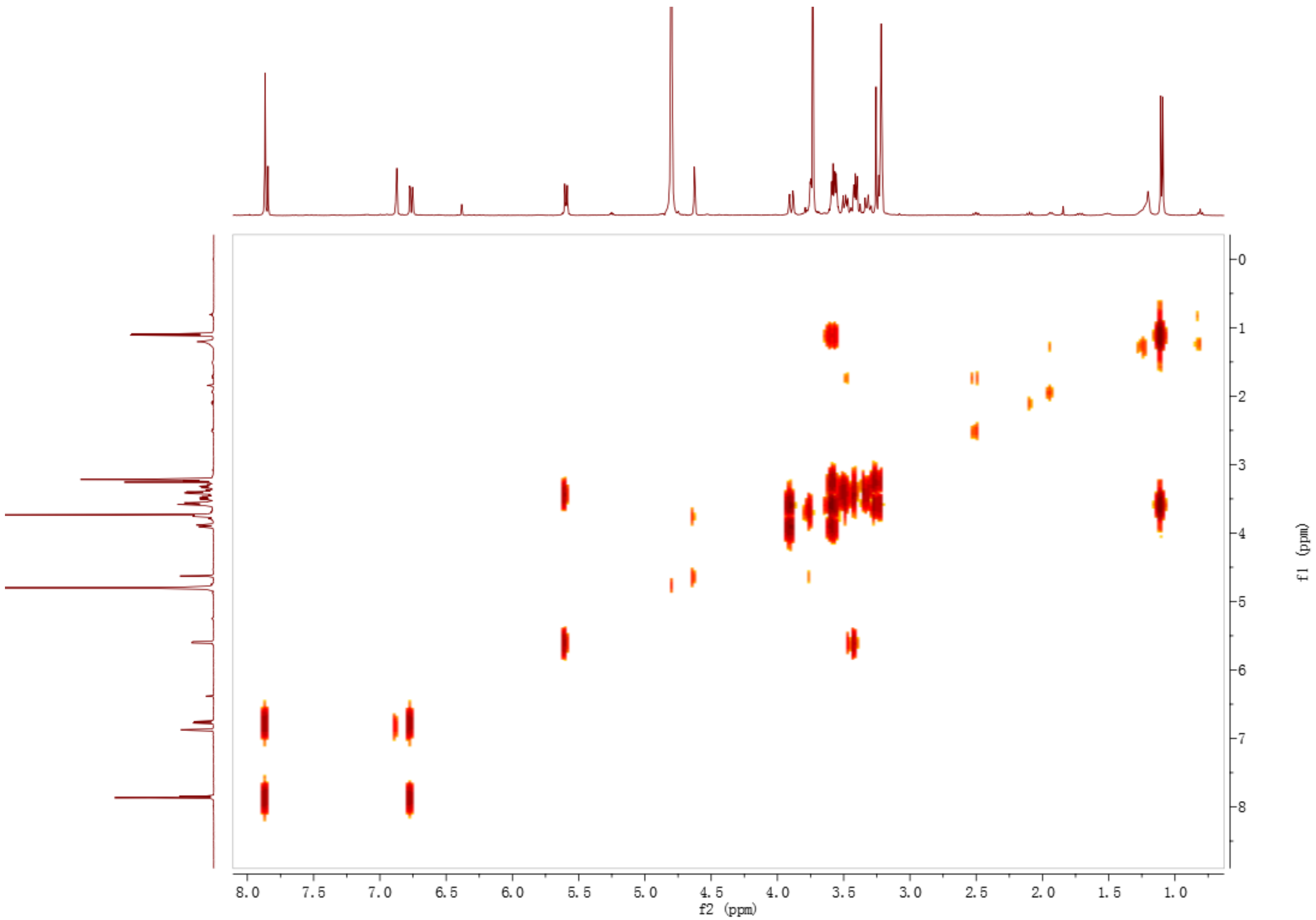

Figure S6. [1]H-[1]H COSY spectrum of compound **1** in CD_3OD.

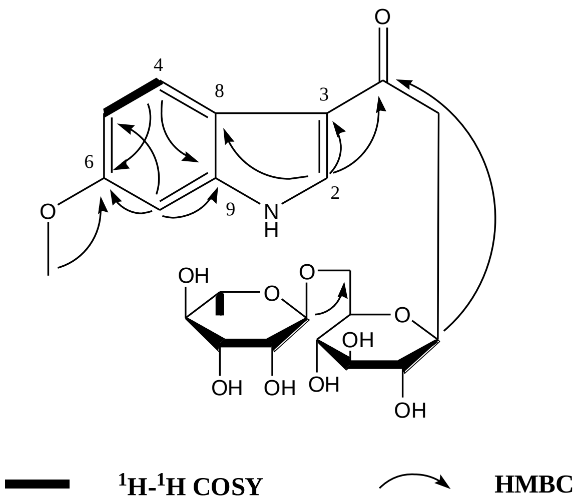

Figure S7. Key ^{1}H-^{1}H COSY and ^{1}H-^{13}C HMBC correlations of compound **1**.