Supporting Information for

Coriatone and Corianlactone, Two Novel Sesquiterpenes from *Coriaria neplalensis*

Yun-Heng Shen¹, Sheng-Hong Li¹, Rong-Tao Li¹, Quan-Bin Han¹, Qin-Shi Zhao¹,
Li Liang¹, Han-Dong Sun^{1*}, Yang Lu², Peng Cao², Qi-Tai Zheng²

¹State Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Sciences, Kunming 650204, Yunnan, P.R. China,

²Institute of Materia Medica, Chinese Academy of Medical Sciences, Beijing 100050, P.R. China

hdsun@mail.kib.ac.cn

*Corresponding author. Phone: (86) 871-5223251. Fax: (86) 871-5216343

1 Coriatone: yellow prism crystals. Mp 219-220°C; $[\alpha]_{\text{D}}^{25.3} -16.13^\circ$ (*c* 0.155, MeOH);

UV (MeOH) λ_{max} (log ϵ) 204 (1.22) nm; IR (KBr) ν_{max} 2997, 2986, 2954 1755, 1627, 1457, 1380, 1252, 1172, 1050, 997, 950, 875 cm^{-1} ; ^1H and ^{13}C NMR data see Table 1; EIMS (70 eV) 322, 294, 234, 155, 127, 95, 67; HRESIMS $[\text{M}+\text{H}]^+ m/z$ 323.1127, calcd 323.1130;

Table 1 ^1H and ^{13}C NMR assignments and HMBC correlations of **Coriatone**

No.	δ_{H} (mult, <i>J</i> , Hz)	δ_{C} (mult.)	HMBC (H-C)	REOSY (H-H)
1		51.3 (s)		
2		192.7 (s)		
3		191.5 (s)		
4	3.51 (d, 4.0)	59.8 (d)	2, 3, 5, 6, 9	5, 9, 10
5	4.27 (d, 4.0)	52.3 (d)	1, 3, 4, 6, 11, 15	4, 9
6		88.7 (s)		
7	1.69 (s)	20.9 (q)	1, 2, 6, 13	10
8		83.9 (s)		
9	1.43 (s)	30.4 (q)	4, 8, 10	4, 5, 10
10	1.28 (s)	25.9 (q)	4, 8, 9	7, 9
11	4.22 (d, 3.0)	57.7 (d)	1, 6, 13	12, 16
12	3.62 (d, 3.0)	57.2 (d)	1, 6, 13	11, 14b
13		64.0 (s)		
14a	3.27 (d, 5.0)	49.4 (t)	12, 13	14b
14b	2.98 (d, 5.0)		12, 13	12, 14a
15		171.2(s)		
16	3.65 (s)	53.0 (q)	15	11 β -H

Data were recorded in $\text{C}_5\text{D}_5\text{N}$ on Bruker AM-400 MHz (^1H , ^{13}C) and Bruker DRX-500 MHz spectrometers (HMBC, REOSY); chemical shifts (δ) are given in parts per million

Figure 1. 400 MHz ^1H NMR spectrum of Coriatone in $\text{C}_5\text{D}_5\text{N}$

Figure 2. 100 MHz ^{13}C NMR and DEPT spectrum of Coriatone in $\text{C}_5\text{D}_5\text{N}$

Figure 3. 500 MHz HMQC spectrum of Coriatone in C_5D_5N

Figure 4. 500 MHz HMBC spectrum of Coriatone in C_5D_5N

Figure 5. 500 MHz REOSY spectrum of Coriatone in C_5D_5N

2 Corianlactone: colorless prism crystals. Mp 244-245°C; $[\alpha]_D^{26.3} -162.5^\circ$ (*c* 0.12, MeOH); UV (MeOH) $\lambda_{\max}$ (log ϵ) 201 (0.30) nm; IR (KBr) $\nu_{\max}$ 2986, 2929, 1762, 1712, 1631, 1492, 1450, 1375, 1295, 1217, 1177, 1115, 1046, 986, 935, 892, 856 cm^{-1} ; ^1H and ^{13}C NMR data see Table 2; EIMS (70 eV) 292, 277, 247, 207, 177, 139, 109, 95, 81, 67; HRESIMS $[\text{M}+\text{H}]^+ m/z$ 293.1033, calcd 293.1025;

Table 2 ^1H and ^{13}C NMR assignments and HMBC correlations of **Corianlactone**

No.	δ_{H} (mult, <i>J</i> , Hz)	δ_{C} (mult.)	COSY	HMBC (H-C)	REOSY (H-H)
1		51.7 (s)			
2		203.4 (s)			
3 α	2.92 (d, 17.1)	44.3 (t)	3 β	2, 4, 8, 10	3 β , 7, 10
3 β	2.63 (d, 17.1)		3 α	1, 2	3 α , 9 β
4	3.13 (m)	50.8 (d)	5, 9	3, 5, 8, 10, 15	5, 7, 9 α
5	4.01 (d, 11.5)	55.1 (d)	4	4, 6, 8, 15	4, 11
6		89.7 (s)			
7	1.83 (s)	22.8 (q)		1, 2, 6, 13	3 α , 4
8		87.8 (s)			
9 α	4.36 (dd, 10.5, 2.5)	66.9 (t)	4, 9 β	8, 15	4
9 β	4.32 (dd, 10.5, 7.5)		4, 9 α	8, 15	3 β
10	1.43 (s)	24.3 (q)		3, 4, 8	3 α
11	4.17 (d, 3.2)	58.4 (d)	12	1, 6	12
12	3.64 (d, 3.2)	57.1 (d)	11	1, 13	11, 14b
13		62.6 (s)			
14a	4.33 (d, 5.0)	51.1 (t)	14b	1, 12, 13	14b
14b	3.25 (d, 5.0)		14a	12, 13	12, 14a
15		173.8 (s)			

Data were recorded in $\text{C}_5\text{D}_5\text{N}$ on Bruker AM-400 MHz (^1H , ^{13}C) and Bruker DRX-500 MHz spectrometers (COSY, HMBC, REOSY); chemical shifts (δ) are given in parts per million

Figure 6. 400 MHz ^1H NMR spectrum of Corianlactone in $\text{C}_5\text{D}_5\text{N}$

Figure 7. 100 MHz ^{13}C NMR and DEPT spectrum of Corianlactone in $\text{C}_5\text{D}_5\text{N}$

Figure 8. 500 MHz COSY spectrum of Corianlactone in C_5D_5N

Figure 9. 500 MHz HMQC spectrum of Corianlactone in C_5D_5N

Figure 10. 500 MHz HMBBC spectrum of Corianlactone in C_5D_5N

Figure 11. 500 MHz REOSY spectrum of Corianlactone in C_5D_5N