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A New Cycloartane from *Sphaerophysa salsula*

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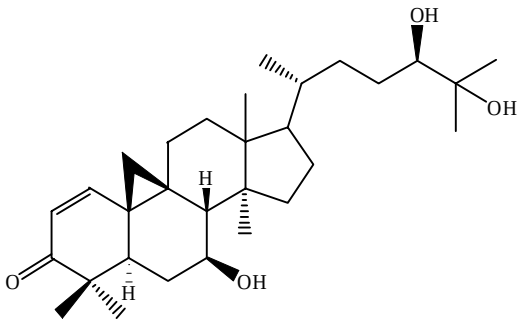
Abstract: A novel cycloartane, named sphaerophysone A, 9, 19-cycloart-7β, 24β, 25-triol-1-en-3-one, was isolated from the ethanol extract of *Sphaerophysa salsula* DC. The structure was elucidated on the basis of spectral evidences and confirmed by X-ray analysis, the stereochemistry of the compound was also defined by X-ray analysis.

Keywords: Leguminosae, *Sphaerophysa salsula*, cycloartane.

Sphaerophysa salsula was a plant widely distributed in the northwest of China. The extract of the plant has the pharmacological action of anti-hypertension[1]. Several kinds of compounds, such as isoflavans, coumarins, flavonoids and sterols were isolated from the plant. We previously reported the isoflavans from *Sphaerophysa salsula* DC[2], in our extended research, we isolated a new cycloartane from the extract of the plant, it is the first time that isolated cycloartane from the whole herbs of *Sphaerophysa salsula* DC. This paper describes the structural elucidation of the compound.

Figure 1 Sphaerophysone A (**1**)



The EtOAc portion derived from the ethanolic extract was separated by silica gel column chromatographies to give one new compound, namely sphaerophysone A (**1**).

Sphaerophysone A (**1**) had a molecular $C_{30}H_{48}O_4$ based on NMR and positive

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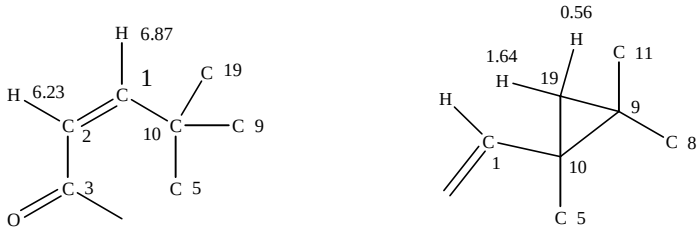
ESI-MS (*m/z* 473.2) spectra. In the ^{1}H NMR spectrum of **1**, two olefinic protons were presented at δ 6.23 (d, 1H, J=10.0 Hz, H-2) and δ 6.87 (d, 1H, J=10.0 Hz, H-1) and in ^{13}C NMR spectrum, it showed two signals at δ 127.1 (C-2) and δ 153.4 (C-1), plus a carbonyl resonance at δ 204.0 (C-3), are characteristics of the conjugated 1-en-3-one system in the structure[3]. The ^{1}H-NMR spectrum (pyridine-d_5) displayed an AB quartet signal at δ 0.56 (d, 1H, J=4.7 Hz, H-19) and δ 1.64 (d, 1H, J=4.7 Hz, H-19), it is not so evident as a 9, 19-cycloartane. This because they are de-shield by the conjugated systems in the 1- en-3-one. In the ^{1}H NMR spectrum of **1**, it showed six tertiary methyls at δ 0.86, 0.96, 0.98, 1.22, 1.51 and δ 1.54. One secondary methyl at δ 1.01 (d, 3H, J=4.5 Hz, H-21).

Table 1 The NMR data of compd. **1**(in pyridine-d_5)

Position	^{13}C	^{1}H	Position	^{13}C	^{1}H
1	153.4	6.87 (d,1H, J=10.0 Hz)	16	28.3	2.00 (m, 2H)[a]
2	127.2	6.23 (d,1H, J=10.0 Hz)	17	52.0	1.62 (m, 1H)
3	204.0		18	15.7	0.98 (s, 3H)
4	45.7		19	25.2	0.56, 1.64 (d,1H, J=4.7 Hz)
5	42.2	2.25 (dd, 1H, J=13.7, 3.8 Hz)	20	37.2	1.51 (m, 1H,)
6	30.5	2.22 (m, 1H), 1.51 (m, 1H)	21	19.1	1.01 (3H, d, J=4.5 Hz)
7	67.6	3.94 (m,1H,)	22	34.6	1.97 (m, 2H)
8	51.1	2.43 (d, 1H, J=4.3 Hz)	23	29.4	2.08 (m, 2H)[a]
9	26.4		24	80.0	3.71 (br, 1H. d, J=9.3 Hz)
10	30.5		25	72.8	
11	28.3	2.02 (m,1H)[a]	26	26.0	1.54 (s, 3H)
12	32.4	1.51 (m, 2H)[b]	27	26.0	1.51 (s, 3H)[b]
13	45.7		28	21.8	1.22 (s, 3H)
14	49.4		29	19.4	0.96 (s, 3H)
15	34.4	1.83 (m, 2H)	30	18.8	0.86 (s, 3H)

[a] interchangable [b] overlapped

Figure 2 Partial structures of **1** as deduced from NMR



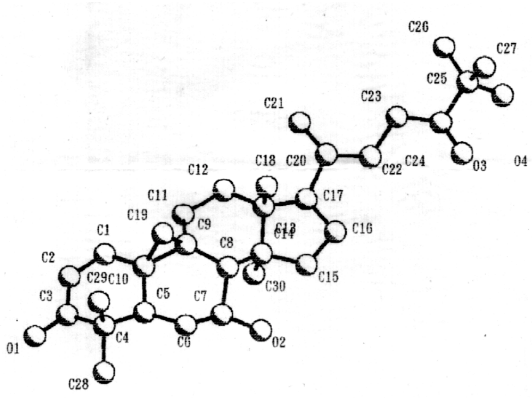
a **b**

There are two methine protons at δ 3.71 (br.d, 1H, J=9.3 Hz, H-24) and δ 3.94 (m, 1H, H-7). It presented 30 carbon signals in the ^{13}C NMR spectrum. It also showed the

corresponding signals due to cyclopropane methylene at δ 25.2. Three carbons bearing hydroxyl at δ 67.6, 72.8 and δ 80.0 were presented. In the ^{1}H-^{1}H COSY spectrum of **1**, it presented the correlated peak between proton δ 3.94 (m, 1H, H-7) and proton δ 2.43 (d, 1H, J= 4.3 Hz, H-8), δ 2.22 (m,1H, H-6), the correlated peaks between proton δ 6.87 (d, 1H, J=10.0 Hz, H-1) and proton δ 6.23 (d,1H, J=10.0 Hz, H-2), proton δ 2.22 (m, 1H, H-6) and proton δ 2.25 (dd, 1H, J=13.7, 3.8 Hz, H-5) were presented. In the HMBC spectr- um of **1**, it showed that proton δ 6.87 (d, 1H, J=10.0 Hz, H-1) in correlation with carbon δ 25.2 (C-19), 30.5 (C-10), 28.3 (C-9), 42.2(C-5), 127.2 (C-2) and δ 204.0 (C-3), the pro- ton δ 6.23 (d, 1H, J=10.0 Hz, H-2) is in correlation with carbon δ 45.7 (C-4) and δ 30.5 (C-10), in combination with ^{1}H-^{1}H COSY spectrum, the moiety a was deduced as **Figure 2**. The proton at δ 0.56 (d, 1H, J=4.7 Hz, H-19) showed long range correlations with carbons δ 153.4 (C-1), 30.5 (C-10), 26.4 (C-9), 51.1 (C -8), 28.3 (C-11) and δ 42.2 (C-5), from above evidences, the moiety b was proposed as **Figure 2**. The rest moieties of the structure were also deduced by DEPT, HMBC, HMQC and ^{1}H-^{1}H COSY spectra. From above evidences, the structure of **1** was formulated as **Figure 1**.

The X-ray analysis of **1** was measured to confirm the structure and determined the stereochemistry of **1** (see **Figure 3**).

Figure 3 Stereoscopic view of compound **1**



Acknowledgments

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References

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4. Compound **1**: Colorless needles from CH_3OH, mp 178~180°C, positive ESI MS: *m/z* 473.2 $[M+H]^+$, UV λ_{Max} (CH_3OH) nm 203, 267. $[\alpha]_D$ –32.3 (*c*0.10, CH_3OH). NMR data see **Table 1**.

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