Chinese Chemical Letters Vol. 16, No. 7, pp 918-920, 2005
http://www.imm.ac.cn/journal/ccl.html

A New Coumestan from *Arachis hypogaea* L.

Hong Wei FU, Hai Long ZHANG, Yue Hu PEI*

Department of Traditional Chinese Medicines,Shenyang
Pharmaceutical University, Shenyang 110016

Abstract: A new coumestan, 3, 9-dihydroxy-4, 8-dimethoxycoumestan, was isolated from *Arachis hypogaea* L. together with two known compounds: 3, 9-dihydroxy-4-methoxycoumestan and 3, 9-dihydroxy-8-methoxycoumestan. The structure was established by spectroscopic methods.

Keywords: *Arachis hypogaea* L., coumestan, 3, 9-dihydroxy-4, 8-dimethoxycoumestan.

The whole plant of *Arachis hypogaea* L. has been used as traditional Chinese medicine for the treatment of insomnia. In previous study it contained isoflavonoid, 1-pentene-3-ol, geraniol *etc*.[1].

An ethyl acetate extract of *Arachis hypogaea* L. was chromatographed on the silica gel column to afford a new coumestan and two known coumestans using gradient of acetone in chloroform. These three compounds **1-3**, obtained as white needles, gave a positive reaction to the $FeCl_3$ test and exhibited bright blue fluorescence under UV light, a phenomenon commonly noted in coumestans[2]. Compound **2** and **3** are two known compounds. Their structures were established by spectroscopic methods and by comparison with the data of reference[3]. This paper describes the isolation and structural elucidation and bioactivity of the new coumestan.

Compound **1** was obtained as white needles. The high-resolution EIMS showed an M^+ ion peak at *m/z* 328.0582 (calcd. 328.0583), corresponding to the molecular formula $C_{17}H_{12}O_7$ for **1**. In the IR spectrum (KBr) of **1** the absorptions due to the two phenolic hydroxyl (3514, 3480 cm^{-1}), δ-lactone carbonyl (1732 cm^{-1}), aromatic ring (1628, 1603, 1500 cm^{-1}) and aromatic C-O (1280 cm^{-1}) were discernible. The IR (KBr) bands indicated the coumestan nature of **1**[4]. The ^{1}H-NMR spectrum (300MHz, DMSO-d_6) displayed two ortho-coupled aromatic protons at δ 7.60 (d, 1H, *J*=8.7Hz) and 7.00 (d, 1H, *J*=8.7Hz). In Para position were another two protons at δ 7.33 (s, 1H, H-7) and 7.25 (s, 1H, H-10). Other signals were observed: δ 3.89 (s, 6H, 2×OMe) and δ 9.67 (s, 1H), 10.53 (brs, 1H). In a NOESY experiment (**Figure 1**) cross peaks were observed between H-7 and one methoxy signal at δ 3.89, assigned to C-8, while the H-2 signal did not show an NOE. Therefore the location of the other methoxyl group was determinded to be at C-4. The complete structural elucidation of **1** was derived from the chemical

* E-mail: fhw668@yahoo.com.cn

shifts and coupling constant of the ^{1}H-NMR spectrum and from detailed spectral analysis of HMQC, HMBC and NOESY experiments (**Table 2**). Consequently, the structure of **1** was determined as 3, 9-dihydroxy-4, 8-dimethoxycoumestan.

Coumestan, a naturally occurring plant estrogen, is harmful to herbivores due to their estrogenic effects. In our study these three coumestans were tested as inhibitors of lens aldose reductase, which is believed to participate in the initiation of cataract formation in diabetes. Lens aldose reductase was from rat lens with IC_{50} values of 2.6 $\times 10^{-8}$ and 3.6$\times 10^{-8}$ mol/L respectively. The inhibitions (%) were **1:** 38%, 10^{-5} mol/L, 0%, 10^{-6} mol/L, 0%, 10^{-7} mol/L, **2:** 28%, 10^{-5} mol/L, 0%, 10^{-6} mol/L, 0%, 10^{-7} mol/L, **3:** 32%, 10^{-5} mol/L, 0%, 10^{-6} mol/L, 0%, 10^{-7} mol/L respectively.

Figure 1 Key HMBC and NOESY correlations for compound **1**

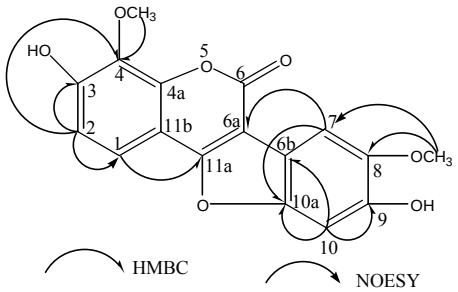

Table 2 ^{1}H-NMR (300MHz), ^{13}C-NMR (75MHz), HMQC, HMBC data of compound **1** (DMSO-d_6, δ ppm)

NO.	δ_H	δ_C	HMQC	HMBC
1	7.60 (d, 1H, *J*=8.7Hz)	116.5	C-1	C-11a
2	7.00 (d, 1H, *J*=8.7Hz)	113.9	C-2	C-3, C-4
3		153.8		
4		135.2		
4a		147.1		
6		157.6		
6a		102.5		
6b		114.3		
7	7.33 (s, 1H, H-7)	102.0	C-7	C-6a, C-10a
8		147.3		
9		149.6		
10	7.25 (s, 1H, H-10)	99.3	C-10	C-6b, C-9, C-10a
10a		146.9		
11a		159.3		
11b		105.4		
OCH_3	3.89 (s, 6H)	60.8		C-4
OCH_3		56.2		C-8

Acknowledgment

We are grateful to Dr. Su Juan WANG of Institute of Materia Medica, Chinese Academy of Medical Sciences for the high-resolution EIMS experiment.

References

1. C. Edwards, R. N. Strange, D. L. Cole, *Plant Pathol.,* **1995** (Pub.1995), *44*(3), 573.
2. S. H. Harper, A. D. Kemp, W. G. E. Underwood, R. V. Campbel, *J. Chem. Soc.,* C **1969,** 1109.
3. D. A. Benson, I. Karsch-Mizrachi, D. J. Lipman., *et al*., *Genbank. Nucl. Acids Res.*, **2000,** *28*(1), 15.
4. D. T. Burns, B. G. Dalgarno, P. E. Gargan, J. Grimshaw, *Phytochemistry,* **1984**, *23*, 167.

Received 16 Augest, 2004