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A New Benzophenone from *Securidaca inappendiculata*

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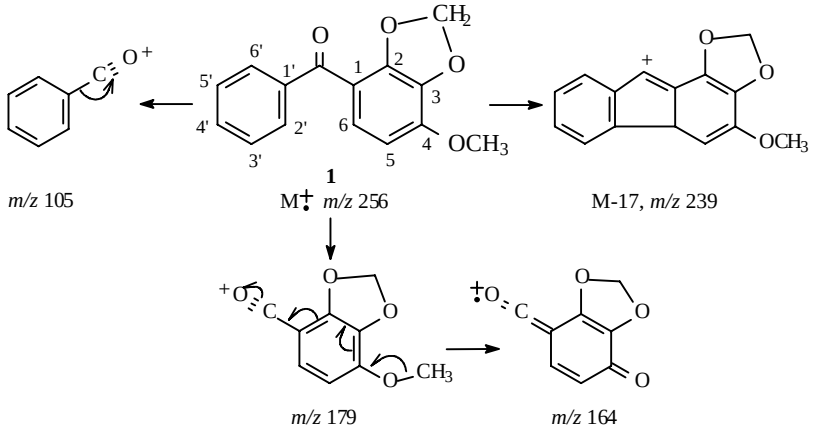
Abstract: A new benzophenone, securiphenone A was isolated from the roots of *Securidaca inappendiculata*. Its structure was determined as 2, 3-methylenedioxy-4-methoxybenzophenone by spectroscopic methods.

Keywords: *Securidaca inappendiculata*, benzophenone, securipheone A.

The roots and stems of *S. inappendiculata* are used as an anti-inflammatory, anti-bacterial and anti-rheumatism agent in Chinese medicine[1]. Previous studies on the stems of this species have revealed the presence of xanthones[2,3,4], organic acids[5], sucrose derivatives[6], hemiterpenic acid glycoside[7], and other compounds[7,8]. We report here the structure elucidation of a new benzophenone, 2, 3-methylenedioxy-4-methoxybenzo-

Figure 1 Structure and EIMS fragmentation of **1**



1

phenone (**1**), isolated from the roots of *S. inappendiculata*.

Compound **1** was obtained as yellow needles, mp 182-184℃. The molecular formula was determined as $C_{15}H_{12}O_4$ by its HREIMS mass spectrum ($[M]^{+\cdot}$, *m/z*

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256.0739, calcd. 256.0736). The IR spectrum of **1** showed absorption bands at 1620 cm^{-1} for a conjugated carbonyl group and no absorption bands for hydroxyl groups. In NMR spectrum of **1** ($CDCl_3$), signals at δ_H 7.79/δ_C 129.6, 7.42/128.1, 7.55/132.7 and δ_C 142.4 indicated a mono-substituted benzene ring (ring A), which was attached to the conjugated carbonyl group (δ_C 195.2). These characteristics indicated a benzophenone skeleton [9]. The NMR spectra of **1** also displayed characteristic signals for a methoxyl group at δ_H 3.84 (3H, s)/ δ_C 60.0, a methylenedioxyl group at δ_H 6.03 (s, 2H)/ δ_C 101.5, and an AB system at δ_H 6.60 (*d*,J= 8.0Hz) and 6.95 (*d*, J= 8.0Hz) in ^{1}H NMR. So, the second benzen ring (ring B) was substituted by one methoxyl and one methylenedioxyl. The methoxyl group was located at C-4, and the methylenedioxyl group at C-2 and C-3 according to the EIMS cleavage patterns of **1** (see **Figure 1**) and its NOE correlations between H-5 and methoxyl protons showed in the NOESY spectrum. Therefore, **1** was identified as 2,3-methylenedioxy-4- methoxybenzophenone, named securiphenone A.

Table 1 ^{13}C NMR (100 MHz) and ^{1}H NMR (400 MHz) data of **1** ($CDCl_3$, TMS, δ, ppm)[a]

No.	^{13}C	^{1}H	No.	^{13}C	^{1}H
1	102.8		3′	128.1[c]	7.42 td (8.0, 1.6)[c]
2	138.5		4′	132.7	7.55 t (8.0)
3	136.9		5′	128.1[c]	7.42 td (8.0, 1.6)[c]
4	151.7		6′	129.6[b]	7.79 dd (8.0, 1.6)[b]
5	124.3	6.60 d (8.0)	MeO-4	60.0	3.84 s
6	126.2	6.95 d (8.0)	CH_2=2, 3	101.5	6.03 s
1′	142.4		C=O	195.2	
2′	129.6[b]	7.79 dd (8.0, 1.6)[b]			

[a] Coupling constants (Hz) in parentheses. [b, c] Overlapping.

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