BAKUCHICIN, A NEW SIMPLE FURANOCOUMARIN
FROM PSORALEA CORYLIFOLIA L.

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Abstract — A new simple furanocoumarin, bakuchicin, has been
isolated from the hexane-extract of seeds of Psoralea
corylifolia L. (Leguminosae) alone with stigmasterol, psoralen
and bakuchiol. The structure of bakuchicin has been shown as
8-oxo-8H-furo[2,3-f][1]benzopyran (1) by spectral means.

The seeds of Psoralea corylifolia L. (Leguminosae, Sanskrit name: Bakuchin) is
used as a tonic or an aphrodisiac against impotence and menstruation disorders.
The seed-oil of this plant also is used externally for the treatment of leucodermy,
psoriasis, and leprosy in Indian folkloric remedy.¹ Many studies on the
constituents of the seeds have been reported.² Now the presence of a new simple
furanocoumarin was proved.

The n-hexane extract of the powdered seeds of P. corylifolia yielded an oily
fraction which on silica gel chromatography gave a 0.1% of yield of a crystalline
component (1), mp 138 °C, besides the known compounds, stigmasterol, psoralen (2),
and bakuchiol (3). 1 is a new compound, for which we propose the name bakuchicin.

\[ \text{Table 1. } ^{1}H \text{ Nmr spectral data of 1} \]

\[ \text{Figure 1. } ^{13}C \text{ Nmr spectral data of 1} \]
Bakuchicin (1) was analyzed for C_{11}H_{6}O_{3}, a formula which was confirmed by high-resolution mass spectrometry with a molecular ion peak at 186.0334 (Calcd 186.0317). The ultraviolet absorption spectrum (in 95% EtOH) showed maxima at 242 nm (infl.) (log ε 4.47), 248 nm (log ε 4.48) and 297 nm (log ε 4.13), while the infrared spectrum (in CHCl_{3}) displayed bands at 1722 and 1619 cm^{-1}, suggesting the presence of a furano-coumarin skeleton. This suggestion is supported by spectral data of {^1}H nmr (Table 1), {^{13}}C nmr (Figure 1), and 2D nmr.

Figure 2. Double resonance {^1}H nmr spectra of 1
The COSY spectrum of bakuchicin showed that the signal at 6 7.14 (1H, dd, J=2.0 Hz, 1.25 Hz) is correlated with the signals at 6 7.44 (1H, dd, J=8.75 Hz, 1.25 Hz) and 6 7.70 (1H, d, J=2.0 Hz), but no correlation between the signals 6 7.82 and other aromatic protons. These findings, combined with a double-resonance experiment (Figure 2), showed that another structure (1a) can be ruled out and the structure of bakuchicin is elucidated as 8-oxo-8H-furo[2,3-f][1]benzopyran (1).

Interestingly, previous investigators have been reported isolation of angelicin (4) from seeds of P. corylifolia, however, we proved the presence of bakuchicin (1), a new isomeric simple furanocoumarin, in this paper.

EXPERIMENTAL

Melting points were taken on a Yamato MP-2 melting point apparatus and are uncorrected. Ultraviolet spectra were recorded with a Hitachi U-3200 spectrophotometer. Infrared spectra were determined as CHCl₃ solutions on a Jasco A-100S infrared spectrophotometer. ¹H Nmr and ¹³C nmr spectra were recorded in CDCl₃ on a JEOL FX-500 spectrometer. TMS was used as an internal standard; chemical shifts are reported in 6 ppm units. Mass spectra were determined with a JEOL DX-303 double focusing mass spectrometer operating at 70 eV.

Isolation of substances Dried and powdered seeds of P. corylifolia (1000 g) were exhaustively extracted with n-hexane (2 l x 4) at room temperature for 24 h. The n-hexane solution was evaporated and then subjected to column chromatography on silica gel (6 x 50 cm). Elution was accomplished with n-hexane and increasing quantities of AcOEt. Fractions of about 50 ml were collected and monitored by thin-layer chromatography (tlc). The four major compounds, bakuchiol 3 (52.127 g), stigmasterol (0.050 g), bakuchicin 1 (0.992 g), and psoralen 2 (0.884 g), were obtained from the corresponding fractions 10-16, 28-30, 31-35, and 37-41, respectively.

Bakuchiol (3) Colorless oil, bp 146-147 °C/0.8 mmHg. Ms m/z: 256 (M⁺) (Calcd 256). The identity of this compound was established by comparison of ¹H nmr spectral data.⁴ Bakuchiol 3,5-dinitrobenzoate: Pale yellow plates (acetone-MeOH), mp 130 °C (lit.,⁴ mp 136 °C). Anal. Calcd for C₂₅H₂₆N₂O₆: C, 66.56; H, 5.82; N, 6.22. Found: C, 66.61; H, 5.97; N, 6.14. Fdms m/z: 450 (M⁺).


Bakuchicin (1) Colorless needles (acetone-n-hexane), mp 138 °C. Anal. Calcd for
\[ \text{C}_{11}\text{H}_{6}\text{O}_3: \text{ C}, 70.97; \text{ H}, 3.25. \text{ Found: C}, 70.97; \text{ H}, 3.46. \text{ Ms} m/z: 186.0334 \]
\(\text{Calcd} \ 186.0317\). \text{ Ir (CHCl}_3 \text{) cm}^{-1}: \text{ 1722 (a,\text{\textbeta} unsaturated lactone), 1619 (aromatic). Uv (95\% EtOH) nm (log } \varepsilon \text{): 242 infl. (4.47), 248 (4.48), 297 (4.13).} \]

\(^1\text{H Nmr: Table 1.} \ 13\text{C Nmr: Figure 1.} \)

\textbf{Psoralen (2) Colorless needles (MeOH), mp 155 °C. Anal. Calcd for C}_{11}\text{H}_{6}\text{O}_3: \text{ C}, 70.97; \text{ H}, 3.25. \text{ Found: C}, 71.11; \text{ H}, 3.29. \text{ Ms} m/z: 186 (M^+) \). The identity of this compound with an authentic sample of psoralen was confirmed by comparison of \(^1\text{H nmr, ir, uv spectra, and tlc behavior.} \)

\textbf{REFERENCES}


\textit{Received, 15th November, 1989}