Taifine, a New Alkaloid from *Ruta chalepensis* L.[a]

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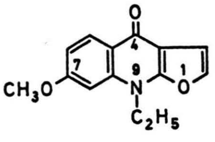
Taifine, Furoquinolone Alkaloid, *Ruta chalepensis*, Rutaceae

From *Ruta chalepensis* L. (Rutaceae) a new alkaloid, taifine, has been isolated. Its structure has been determined as 9-ethyl-7-methoxyfuro[2,3-b]quinolone-4.

From the alcoholic extract of dried plant material of *Ruta chalepensis* L. collected at Taif, Saudi Arabia, a cristalline compound could be isolated, which according to exact mass measurements has an elemental composition of $C_{14}H_{13}NO_3$. In the mass spectrum losses of $CH_3\cdot$, C_2H_4 and $(C_2H_4 + H\cdot)$ are observed followed by eliminations of CO. The IR spectrum shows a carbonyl band at 1625 cm^{-1}, the UV spectrum (CH_3OH) a band at 235 nm (log ε 4,70) and a structured plateau of lower intensity between 280 and 350 nm – in agreement with a N-alkyl-4-quinolone structure [1, 2]. In the NMR spectrum the following signals may be found (δ ppm; J Hz; multiplicity; integration): 1.63; 7; t; 3H and (by decoupling) 4.77; 7; q; 2H: CH_2CH_3 —3.97; 0; s; 3H: CH_3 —7.00; d; 1H and (by decoupling) 7.65; 3; d; 1H: furan α- and β-H —7.38; 9 and 3; dd; 1H, and 7.60; 3; d; 1H, and 8.00; 9; d; 1H: 1,2,4-trisubstituted benzene ring. There are no protons exchangeable with D_2O. These data agree well with those published for furoquinolone alkoloids, esp. acrophyllidine [3] isomaculoridine [4] and the synthetic 9-ethyl-5,7,8-trimethoxyfuroquinolone [5]. The substitution pattern follows from the NMR spectrum: Due to the deshielding effect of the carbonyl group the hydrogen of C-5 occurs at lowest field (8.0 ppm). Since this signal shows *o*-coupling there has to be a hydrogen at C-6 also. The signal at 7.38 ppm (C-6H) is split both by *o*- and by *m*-coupling, that at 7.60 (C-8H) by *m*-coupling only. Hence the benzene ring has to be substituted at C-7. Earlier observations [4] have shown that quinolone N–CH_3 and aromatic O–CH_3 signals hardly differ in their chemical shifts. Thus, a distinction between an NC_2H_5/OCH_3 and an NCH_3/OC_2H_5 pattern is not possible in this way. However, upon addition of CF_3COOD the CH_3 signal is shifted downfield by 0.06 ppm only while that of the ethyl-CH_2 group migrates by 0.26 ppm downfield as expected for protonation of the nitrogen. Structure **1** can, therefore, be attributed to taifine.



1

Experimental

Instruments: IR: Perkin-Elmer Spectrometer 720. UV: Beckmann Spectrometer Model 25. NMR: Varian EM-390 ($CDCl_3$, TMS). MS: Finnigan 3200 with data system 6100 (EI) and Varian MAT 212 (exact mass measurements; results ± 3 ppm).

Isolation of taifine: 950 g dry and powdered plant material was extracted with ethanol under reflux, the concentrated (1 l) extract shaken with an equal volume of a 10% aqueous solution of KOH at room temperature for 1 h and then extracted with ether. The ether extract was washed with H_2O till neutral, dried and evapourated to dryness. The residue was refluxed with ethanolic KOH (5%) for 2 h and extracted with ether. The ether phase was washed with water several times, dried and evapourated to dryness (5,52 g). Chromatography of the residue on neutral alumina (250 g) gave the following fractions: 1. petrol ether (60–80 °C): a colourless liquid. 2. 70% petrol ether, 30% benzene: β-sitosterol, 3. 20% petrol ether, 80% benzene: 30 mg taifine (**1**).

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[a] Constituents of Local Plants, XIII. For XII see: B. A. H. El-Tawil, in press.

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Taifine: White needles, m.p. (from petrol ether) 110 °C.

IR (NaCl): 1625, 1585, 1555, 1515, 1470, 1425, 1375, 1360, 1305, 1240, 1225, 1160, 1110, 1090, 1040, 1020 cm^{-1}. UV (CH_3OH): 235 (4,70), 247 (sh), 282 (sh), 293 (3,92), 305 (3,99), 331 (3,71), 347 (3,71) nm (log ε). The compound shows violet fluorescence. NMR: v. text. MS (elemental compositions indicate exact mass measurements) [6]: [*m/z*]
243 ($C_{14}H_{13}NO_3$, 100%): M^+,
229 (15%): $[M-CH_3]^+$,
215 ($C_{12}H_9NO_3$, 68%): $[M-C_2H_4]^{+\cdot}$,
214 ($C_{12}H_8NO_3$, 81%): $[M-C_2H_4-H^\cdot]^+$,
200 ($C_{11}H_6NO_3$, 32%): $[M-C_2H_4-CH_3^\cdot]^+$,
186 ($C_{11}H_8NO_2$, 30%): [*m/z* 214-CO]$^+$,
172 ($C_{10}H_6NO_2$, 39%): [*m/z* 200-CO]$^+$,
158 (39%), 143 (22%).

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