Phytochemistry, Vol. 24, No. 10, pp. 2473–2474, 1985.
Printed in Great Britain.

0031–9422/85 $3.00 + 0.00

ERVATININE, AN INDOLE ALKALOID FROM *ERVATAMIA CORONARIA*

ATTA-UR-RAHMAN, ANJUM MUZAFFAR and NADER DAULATABADI

H. E. J. Research Institute of Chemistry, University of Karachi, Karachi-32, Pakistan

(*Received* 2 *November* 1984)

Key Word Index—*Ervatamia coronaria*; Apocynaceae; indole alkaloids; ervatinine; structural determination.

Abstract—An indole alkaloid, ervatinine, has been isolated from the leaves of *Ervatamia coronaria* and its structure has been elucidated.

INTRODUCTION

Ervatamia coronaria (Stapf.) is a glabrous, evergreen tree commonly grown in gardens of West Pakistan. Various parts of the plant are used in the indigenous system of medicine for the treatment of ophthalmia, for application on wounds and inflamed parts of the body, as an anthelmintic, etc. A number of indole alkaloids have been reported previously from the leaves, stem bark and roots of the plant [1–13].

RESULTS AND DISCUSSION

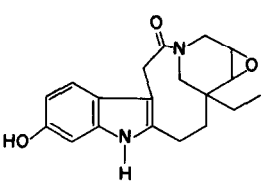
The crude alkaloids obtained from an ethanolic extract of fresh leaves were fractionated at different pH values. The fraction obtained at pH 7 afforded a mixture of alkaloids which was further purified by prep. TLC to afford a new alkaloid, named ervatinine, as a colourless amorphous material $[\alpha]_D$ +74° ($CHCl_3$).

The compound exhibited a UV spectrum showing absorption maxima at UV λ_{max} nm (log ε): 205 (4.2), 227 (4.5) and 300 (3.80) and minima at UV λ_{max} nm (log ε): 225 (3.5) and 252 (3.6) which was consistent with the presence of a hydroxyl group at the 11-position on an indole nucleus [14]. The IR spectrum showed peaks at IR ν_{max} cm^{-1}: 3500 (–OH), 3425 (N–H), 2920 (C–H), 1690 (–C=O, amide), 1600, 1465, 1380, 1220 (–C–O–C of epoxide), 1130, 900, 840 and 760.

The mass spectrum indicated the presence of the Aspidosperma skeleton and gave the $[M]^+$ at *m/z* 326.1626, which was consistent with the molecular formula $C_{19}H_{22}N_2O_3$. This showed the presence of 10 double bond equivalents in ervatinine. Six of these were accounted for by the presence of the indolic ring system, one by the amide carbonyl group and two by the two rings of the cleaved Aspidosperma skeleton. Since the IR and ^1H NMR spectra did not show the presence of any additional olefinic linkages, it seemed plausible that the second oxygen atom was in the form of a ketonic, epoxide or ether group. Failure of attempted reduction with sodium borohydride and the absence of corresponding signals in the IR spectrum showed that there was no ketonic group in the molecule. The mass fragmentation indicated that one of the oxygen atoms was present as an epoxide or ether in the piperidine ring of the Aspidosperma skeleton while another oxygen was present as a hydroxyl group on the benzene ring of the indole nucleus. Ervatinine showed the following major peaks in its mass spectrum: MS *m/z* (rel. int.): 326.1626 $[M]^+$ ($C_{19}H_{22}N_2O_3$) (100), 309.16009 $[M-OH]^+$ ($C_{19}H_{21}N_2O_2$) (14), 298.1679 $[M-CO]^+$ ($C_{18}H_{22}N_2O_2$) (6), 297.1243 $[M-C_2H_5]^+$ ($C_{17}H_{17}N_2O_3$) (9), 281.1639 ($C_{18}H_{21}N_2O$) (15), 270.1121 $[M-C_3H_6N]^+$ ($C_{16}H_{16}NO_3$) (12), 251.1309 ($C_{13}H_{10}NO$) (10), 175.0633 ($C_{10}H_9NO_2$) (24), 173.0841 ($C_{11}H_{11}NO$) (17), 159.0683 ($C_{10}H_9NO$) (31), 152.1073 ($C_9H_{10}NO$) (21), 110.0970 ($C_7H_{12}N$) (18), 111.1046 ($C_7H_{13}N$) (8), 108.0815 ($C_7H_{10}NO$) (41) and 96.0813 ($C_6H_{10}N$) (28). The formulae of the ions were established by computer monitored high resolution mass measurements and confirmed by peak matching experiments on important ions.

Linked scan measurements on the $[M]^+$ at *m/z* 326 showed that it fragmented directly to the ions at *m/z* 309, 298, 297, 270, 175, 173, 152 and 140. The ion at *m/z* 298 gave rise to that at *m/z* 281 which, in turn, fragmented to the ions at *m/z* 251 and 159. The ion at *m/z* 251 further fragmented to that at *m/z* 196 and the ion at *m/z* 226 was seen to arise directly from that at *m/z* 270. The fragmentation pathway of the ion at *m/z* 140 showed that the ions at *m/z* 111, 110, 108 and 96 arose directly from it. By linked scan measurements it was also confirmed that the ion at *m/z* 124 was derived directly from that at *m/z* 152.

The ^1H NMR spectrum ($CDCl_3$) showed the presence of a triplet centred at δ0.81 (J = 7 Hz) and a quartet centred at δ1.12 (J = 7 Hz) which were assigned to the methyl and methylene protons, respectively, of the ethyl group. The H-15 resonated as a doublet centred at δ2.80 (J = 4.5 Hz). The H-14 resonated as a multiplet centred at δ3.20 ($J_{6\beta,6\alpha}$ = 10 Hz) while H-6β appeared as another



I

doublet at δ3.75 ($J_{6\alpha,6\beta}$ = 10 Hz). A broad peak at δ8.25 was assigned to the N–H group.

On the basis of these spectroscopic data, structure **1** was assigned to ervatinine.

REFERENCES

1. Ratnagiriswaran, A. N. and Venkatachalam, K. (1939) *Quart. J. Pharm. Pharmacol.* **12**, 174.
2. Warsi, S. A. and Ahmad, B. (1949) *Pakistan J. Sci.* **1**, 128.
3. Gorman, M., Neuss, N., Cone, N. J. and Deyrup, J. A. (1960) *J. Am. Chem. Soc.* **82**, 1142.
4. Dutta, T. (1969) *J. Inst. Chem. (India)* **41**, 5.
5. Raj, K., Shoeb, A., Kapil, S. R. and Popli, P. S. (1974) *Phytochemistry* **13**, 1621.
6. Talapatra, B., Patra, A. and Talapatra, K. S. (1975) *Phytochemistry* **14**, 1652.
7. Monache, G. D., D'Albuquerque, I. L., Monache, F. D., Betolo, M. and Battista, G. (1972) *Atti. Acad. Naz. Lincei Cl. Sci. Fis. Mal. Natur. Rend.* **52**, 375.
8. Gonzalez, C. G. and Martinez, J. (1976) *Rev. Cubana Farm.* **10**, 45.
9. Rao, P. G. and Singri, B. P. (1979) *Indian J. Chem. Sect. B*, **17**, 414.
10. Karawya, M. S. and Aboutabl, E. A. (1979) *Egypt. J. Pharm. Sci.* **20**, 241.
11. Rastogi, K., Kapil, S. R. and Popli, S. (1980) *Phytochemistry* **19**, 1209.
12. Jabbar, A. and Hasan, C. M. (1980) *Bangladesh J. Biol. Sci.* **9**, 31.
13. Gonzalez, C. G., Navajaspolo, C., Rodriguez, S. C. and Mendez, L. P. (1981) *Rev. Cubana Farm.* **15**, 192.
14. Gilbert, B., Duarte, A. P., Nakagawa, Y., Joule, J. A., Flores, S. E., Brissolese, J. A., Campello, J., Carrazzoni, E. P., Owellen, R. J., Blossey, E. C., Brown, K. S. and Djerassi, C. (1965) *Tetrahedron* **21**, 1141.