P-COUMAROYLCHOLINE, A NEW NATURAL CHOLINE ESTER FROM *IBERIS UMBELLATA* SEEDS

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In the course of studies on the *p*-hydroxycinnamic acids derivatives of some Rhoedales species spontaneous or acclimatized in Liguria, our attention was drawn to strongly fluorescent constituents present in the seeds of *Iberis umbellata* L. (Cruciferae). Monitoring by tlc and pc, we isolated by column chromatography on anionotropic and neutral alumina *p*-coumaroylcholine, a new natural choline ester. Identification of this phytoconstituent was obtained by comparison of the ir, nmr and mass spectra and by mmp determination with the same compound synthetically obtained (1).

Some Order Rhoedales species seem to share a rather peculiar chemotaxonomic feature of synthesizing and accumulating choline esters of substituted *p*-hydroxycinnamic and phenolic acids; sinapoylcholine from many Cruciferae species seeds (2), veratroylcholine from *Hesperis matronalis* L. (Cruciferae) seeds (3), feruloylcholine from *Cleome pungens* Willd. (Capparidaceae) seeds (4,5), and isoferulic acid choline ester from *Sibara virginica* L. Rollins (Cruciferae) seeds (6).

EXPERIMENTAL

PLANT MATERIAL.—*Iberis umbellata* L. is a rather widespread species occurring in many areas in Appennino Ligure (7). Collections were made in stony regions of Savona province in July and August 1976, 1977, 1978 and 1979.

EXTRACTION AND ISOLATION.—Seeds (400 g) were ground in a Waring blendor and continuously extracted with carbon tetrachloride (Soxhlet apparatus) for about ten hours. The dried, defatted material (270 g) was extracted by maceration with methanol. The bulk extracts were combined and methanol was evaporated under vacuum. The solution obtained was chromatographed on anionotropic and then on neutral alumina, following a procedure already described for feruloylcholine isolation (4,5). *p*-Coumaroylcholine iodide (mg 90) was obtained as bright, colorless leaflets (from methanol) mp 232° (dec.) (Kofler); mmp 231–232° (d) with authentic synthetic compound (1). The substance has R_f=0.78 [pc, n-butanol-acetic acid-water (4:1:2)], descending, Whatman No 1) and shows a pale blue-violet fluorescence in uv, turning to bright blue after exposure to ammonia vapors; ir (Perkin-Elmer 398), νmax (KBr): 3200 cm^{-1}; 1705; 1280, 1020; 1600, 1510; 1630, 978; 3000~2200; 2960, 2870, 1454, 1375; 2918, 2850, 1474, 724; 825, 810; nmr (Perkin-Elmer R 12), (d$_6$DMSO) δ 7,68 (1H, d, –C(H)–C(=O)–; J=13 Hz), 6,45 (1H, d, =C(H)-ar.; J=12 Hz), 4,67 (2H, m, –O–CH_2), 3,88 (2H, m, –CH_2–<), 3,27 (9H, s, N(CH_3)$_3$); ms (Varian MAT-III; 70 eV); *m/e* (%) 147 (62); 119 (11); 93 (15).

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