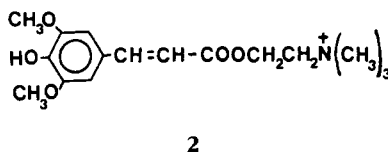
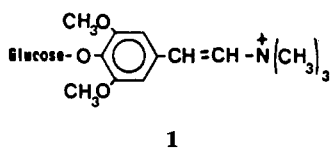


A NOVEL QUATERNARY BASE FROM *BRASSICA NAPUS*

A. BELKHIRI and G.B. LOCKWOOD*

Department of Pharmacy, University of Manchester, Manchester M13 9PL, UK

Brassica napus L. (Cruciferae) is an important crop grown mainly for its high fixed oil content. During an investigation on glucosinolate content of seeds of this species, a new quaternary base has been isolated. The structure, 2,6-dimethoxy-4-(2'-trimethylammonium ethenyl)-phenyl α -D-glucopyranoside [**1**] is proposed. The occurrence of sinapine [**2**], a rather widely distributed quaternary base, has been found in the Cruciferae and as the cationic moiety in combination with *p*-hydroxybenzylglucosinolate (1).



EXPERIMENTAL

PLANT MATERIAL.—Seeds of *B. napus* were obtained from Kenneth Wilson Ltd., UK. A voucher specimen (#071) is deposited in the Department of Pharmacy, University of Manchester.

EXTRACTION, ISOLATION, AND IDENTIFICATION.—Freshly powdered, defatted seeds (10 g) were introduced into boiling MeOH (50 ml), boiled for 5 min, and filtered off on Whatman paper no. 1. The plant material was homogenized and re-extracted with boiling MeOH. Both extracts were combined, concentrated to about 5 ml using a Rotavapor (40°), and applied to the top of a microcrystalline cellulose (Avicel MN100) column (200 × 20 mm i.d.).

The column was thoroughly washed with

MeOH, and 5-ml fractions were collected, checked by tlc in *n*-BuOH-HOAc-H₂O (4:1:5), and combined according to their tlc behavior. The novel compound was eluted within the first 20 ml. Further purification was carried out by hplc using Hypersil ODS, eluted with MeOH-MeCN (1:1).

Uv λ max (MeOH), 208, 224 sh, 248, 254, 260, 274 sh; ir ν max (film) 3373, 2930, 1516, 1451, 1230, 1057, 798 cm^{-1} ; ¹H nmr (80 MHz, D₂O) δ 3.18 (9H, s, -N⁺Me₃), 3.54–3.73 (10H, m, H-sugar), 3.83 (6H, s, 2-OMe), 5.33 (1H, d, *J* = 3 Hz, H-anomeric), 6.94 (2H, s, 3-H, 5-H), 6.39 and 7.60 both (1H, d, 16 Hz). The coupling constant in the latter case and the absence of any further coupling (decoupling experiments) indicate an AB system of a *trans* disubstituted

double bond attached to the aromatic ring; eims *m/z* (rel. int.) [M]⁺ (0), [M - glucose]⁺ 238 (28), 223 (20), 180 (30), 165 (20), 137 (20).

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