SPECTRAL DATA OF SECOKARACONITINE

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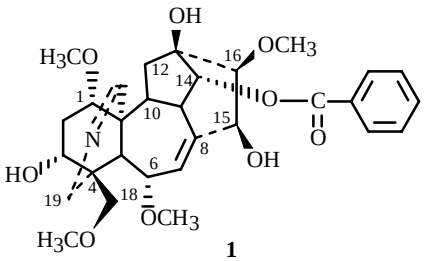
UDC 547.944/945

Recently we isolated from the tubes of *Aconitum karakolicum* Rapaics a new alkaloid secokaraconitine (**1**), and its structure was determined by single-crystal X-ray diffraction analysis [1]. Secokaraconitine (**1**) is the first alkaloid with a lycoctonine skeleton containing N, C-17 and C-7, C-8 double bonds. The spectral data of secokaraconitine have not been recorded earlier because of the small quantity isolated.

In present paper we describe the spectral data of secokaraconitine (**1**).



1

Secokaraconitine has the composition $C_{30}H_{39}NO_9$ (HREIMS), found 557.27503, calc. 557.2814.

IR (ν, cm^{-1}) (Vector 22): 3375, 2930, 2885, 2830, 1727, 1639, 1600, 1491, 1464, 1451, 1414, 1378, 1352, 1319, 1284, 1263, 1223, 1198, 1182, 1106, 1075, 1046, 1080, 986, 962, 933, 915, 873, 717, 668, 640, 612, 594.

Mass spectrum (JMS 600 H), *m/z* (%): M^+ 557 (1.6), 542 (2.6), 526 (22.5), 104 (100), 59 (5.4).

Proton NMR-signal assignments were made by comparison of spectrum **1** with those of secoyesaconitine [2] and related alkaloids. ^{1}H NMR (Bruker, 400 MHz, $CDCl_3$, δ, ppm, J/Hz): 3.20, 3.22, 3.31, 3.7 (each 3H, s, 4′OCH_3), 4.48 (1H, dtd, J = 2.2, 2.3, 2.2, H-6β), 4.82 (1H, dd, J = 2.6, 2.7, H-15β), 5.09 (1H, d, J = 4.2, H-14β), 5.62 (1H, br dd, J = 2.7, 3.9, H-7), 7.83 (1H, br d, J = 1.7, H-17), 7.43 (2H, t, J = 7.7, Ar-H), 7.56 (1H, t, J = 7.4, Ar-H), 8.0 (2H, d, J = 8.1, Ar-H).

The multiplicity of carbon atoms was defined by the DEPT NMR technique and signals assignments were made by comparison with the spectra of related alkaloids. ^{13}C NMR (Bruker, 100.6 MHz, $CDCl_3$, δ): 166.3 (Ar-CO), 165.1 (C-17), 137.8 (C-7), 137.7 (C-8), 133.2 (Ar-C), 131.0 (Ar-C), 129.9 (Ar-C), 129.9 (Ar-C), 128.5 (Ar-C), 92.1 (C-16), 87.0 (C-6), 79.5 (C-1), 79.5 (C-14), 79.2 (C-15), 76.5 (C-18), 73.9 (C-13), 71.0 (C-3), 61.6 (OCH_3-16), 59.0 (OCH_3-6), 57.9 (OCH_3-18), 56.8 (OCH_3-1), 51.5 (C-11), 51.5 (C-11), 51.5 (C-19), 47.9 (C-4), 43.6 (C-5), 42.7 (C-9), 41.5 (C-10), 38.6 (C-12), 33.0 (C-2).

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 0009-3130/03/3905-0512$25.00