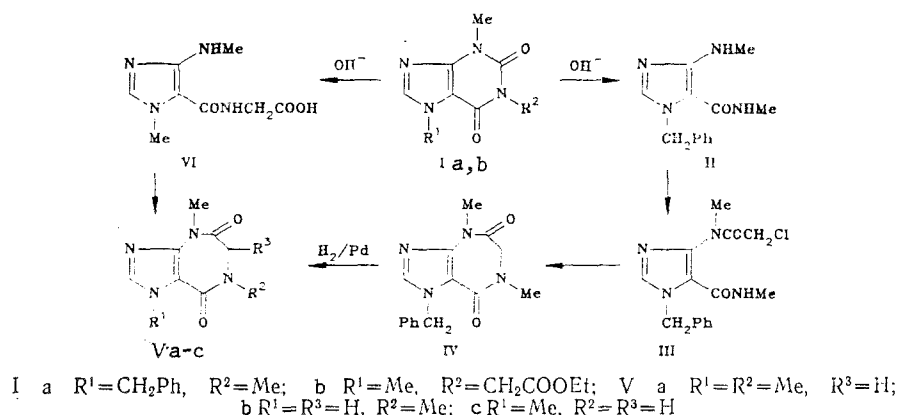


Previously we reported the synthesis of caffeine homolog Va from caffeine [1, 2]. Later this scheme was used by Japanese [3] and American [4] workers to obtain 6-substituted derivatives of the type Va ($R^3 \neq H$) and theophylline homolog Vb.

We showed that homologs of theophylline Vb and theobromine Vc can be obtained from methylated xanthines.



The starting substances were the corresponding derivatives Ia and Ib, obtained by alkylation of the starting alkaloids. Their alkaline hydrolysis occurred with the formation of imidazoles II and VI. Cyclization of VI in the presence of dicyclohexylcarbodiimide or HCl in methanol gave theobromine homolog Vc in quantitative yield. The colorless needles melted at 218-220°C. IR spectrum (KBr): 3275, 3175, 3100, 3030, and 1660 cm^{-1} . PMR spectrum (250 MHz, DMSO- D_6): 8.15 (1H, triplet, 7-H, $J_{67} = 5.3$ Hz), 7.79 (1H, singlet, 2-H), 3.77 (3H, singlet, 1- CH_3), 3.73 (2H, doublet, 6-H, $J_{67} = 5.3$), 3.25 (3H, singlet, 4- CH_3). M^+ 194.

Theophylline homolog Vb was obtained by acylation of derivative II by chloroacetyl chloride with subsequent intramolecular cyclization of chloroacetylamine III in the presence of alcoholates of sodium or alkalies and abstraction of the benzyl group by hydrogenolysis over palladium black. The yield of compound Vb was 98%, with mp 260°C (from methanol). IR spectrum: 3425, 3200-2900, 1660, 1600 cm^{-1} . PMR spectrum (250 MHz, DMSO- D_6): 7.84 (1H, singlet, 1-H), 4.06 (2H, singlet, 6-H), 3.36 (3H, singlet, 4- CH_3), 3.09 (3H, singlet, 7- CH_3). M^+ 194.

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