Merucathine, A New Phenylalkylamine from *Catha edulis*

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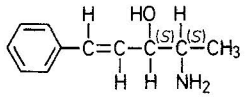
In the course of our analytical studies (1) of the CNS-active khatamines from *Catha edulis* Forsk. (Celastraceae), a popular stimulant in Yemen and East Africa (2,3), chromatographic and spectroscopic data indicated the presence of further amines in addition to the known phenylpropylamines cathinone, norephedrine and norpseudoephedrine.

The isolation of the khatamines was carried out by extraction with hydrochloric acid of fresh plant material and subsequent precipitation as oxalates. The separation of the new compound was achieved by column chromatography on silica gel. The structure of merucathine was elucidated as 4(*S*)-amino-3(*S*)-hydroxy-1-phenyl-*trans*-pentene (CA: 1-pentene-3(*S*)-ol-1-phenyl-4-(*S*)-amine) by HPLC, GC-MS, ^{1}H-NMR, IR, CD and UV.



Merucathine

The *cis*-isomer occurs only as an artefact in GC-separation and due to UV-irradiation. Its mass spectrum is identical to that of the *trans*-isomer. Contrary to the cathines (norephedrine, norpseudoephedrine) the analogous diastereomer for merucathine could not yet be found.

The cathinone-corresponding keto-compound, merucathinone, which has already been suggested earlier (4) could be confirmed by GC-MS in our khat-sample. It seems that these phenylpentylamines can be found particularly in khat originating from Kenya. Pharmacological investigations with synthesized substances will show whether these new compounds have a psychoactive effect.

Merucathine was isolated from fresh plant material which is cultivated in the Meru area (North Kenya) and sold in Nairobi's streetmarket.

The extraction was performed as reported earlier (1) with Ultraturrax and 0.1 N hydrochloric acid, followed by precipitation of the khatamines as oxalate with oxalic acid in ether (1 % w/v). Subsequent fractionation by column chromatography (60 × 3 cm) using silica gel 60 and $CHCl_3$ – MeOH 9 : 1 (v/v), from fraction 8 on with an addition of 10 % acetone, yielded 16 fractions of 90 ml each. Fraction 11 was used for the further identification.

HPLC: standard method for khatamines (1): t_R (min) *cis*-merucathine = 12.2; t_R *trans*-merucathine = 13.7.

GC: derivatization with TFAA (trifluoroacetic acid anhydride) in benzene; OV-1701 fused silica, 170° C (16 min), 15°/min → 230°: t_R (min) *cis*-merucathine = 22.2; t_R *trans*-merucathine = 22.7.

(GC-)MS: EI (32 eV): *m/e* (rel. int.) 140 (5), 133 (70), 115 (20), 105 (10), 91 (5), 79 (15), 77 (10), 55 (100). CI-NH_3 (60 eV): 291 (100), 275 (10), 256 (5). ^{1}H-NMR (100.1 MHz/80° C/D_2O): δ 1.80 ppm (d, J = 6.5 Hz); 4.14 (m, J = 7 Hz); 4.68 (t, J = 6 Hz); 6.76 (dd, J_1 = 16 Hz, J_2 = 6 Hz); 7.31 (dd, J_1 = 16 Hz, J_2 = 1.5 Hz); 7.97 (m). CD (H_2O): $\Psi_{290} = -50$; (+)-norpseudoephedrine $\Psi_{266} = -146$. UV: λ_{max}^{H2O} nm (log ε): 249 (4.15), 281 (2.85), 291 (2.70). IR (KBr, base): 1590 cm^{-1}, 1490, 1450, 1045, 1025, 970 (*trans*-olefin), 750, 700.

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