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SYNTHESIS OF 2-PHENYLIMINO-4-OXO-2,3-DIHYDRO-1,3-THIAZINE

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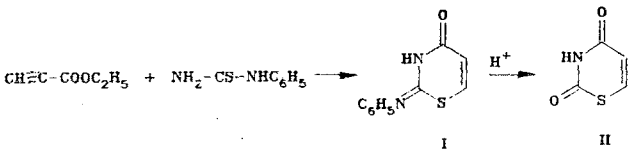
We have established that ethyl propionate and phenylthiourea, in contrast to methylurea, do not enter into a Biginelli cyclocondensation with benzaldehyde, and instead of the expected 2-thiotetrahydropyrimidine derivative, they form 2-phenylimino-4-oxo-2,3-dihydro-1,3-thiazine (I), which when hydrolyzed gives the known [1] 2,4-dioxo-2,3-dihydro-1,3-thiazine (II).



I II

The imine I was produced by boiling equimolar amounts (0.01 mole) of phenylthiourea and ethyl propionate in 30 ml of absolute alcohol, acidified with concentrated hydrochloric acid, for 4 h. Yield 62%. mp 216-218°C (from ethanol), PMR spectrum (DMSO): 5.6 (1H, d, 5-H), 7.42 (5H, s, C_6H_5), 7.66 (1H, d, 6-H), 11.40 ppm (1H, a.s., NH). IR spectrum (in nujol): 1600 (C=C), 1630 (C=O), 3230 cm^{-1} (NH).

The 2,4-dioxo-derivative II is formed when the imine I is boiled in 3% hydrochloric acid for 1 h. Yield 56%. The melting point, IR spectrum, and PMR spectrum of the compound obtained were identical with the characteristics of known 2,4-dioxo-2,3-dihydro-1,3-thiazine [1].

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