THIAZOLO[3,2-a]QUINOLINIUM 1-OXIDE DERIVATIVES

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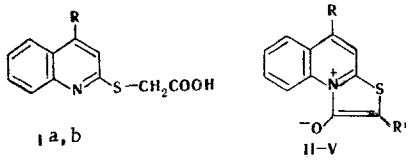
It was found that acetyl derivatives IIa,b [IIa, 66% yield, mp 255°C (from pyridine), λ_{max} (log ε) in CH_3CN: 293 (3.79) and 452 (4.04); IIb, 72% yield, mp 250°C (from pyridine), λ_{max} (log ε): 288 (4.18) and 452 (4.28)] rather than compounds of the III type, as was assumed in [1], are formed when a mixture of 1 mmole of (2-quinolylthio)acetic acids (Ia,b) and 5 ml of acetic anhydride is heated to the boiling point. Compounds III were obtained when the reaction was carried out in a mixture of 1 ml of acetic anhydride and 2 ml of acetic acid [IIIa, 60% yield, mp 209-210°C (from Ac_2O), λ_{max} (log ε): 297 (3.96), 328 (3.87), and 455 nm (4.22); IIIb, 65% yield, mp 205°C (from pyridine), λ_{max} (log ε): 297 (4.05), 328 (3.93), and 452 nm (4.30)].



Ia,b

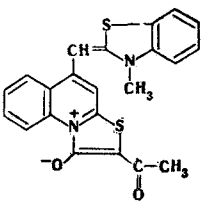
II–V

II R' = —COCH3;
III R' = —(CO)CH2S—
IV R' = —H;
V R' = —CH=CH—

I– C2H5

I–V a R=H; b R=CH3

The initial products are evidently the unstable thiazolo[3,2-a]quinolinium 1-oxide (IVa,b), which, depending on the conditions, are acetylated or undergo dimerization. In fact, if one carries out the cyclization of 1 mmole of Ia in 10 ml of acetic acid and 0.3 ml of acetic anhydride in the presence of an electrophilic agent such as 3-ethyl-2-(acetanilidovinyl)benzothiazolium iodide, 2-substituted thiazolo[3,2-a]quinolinium 1-oxides [V, 62% yield, mp 256°C (from Ac_2O), λ_{max} 588 nm (log ε 4.80)] can be isolated. A dye of a different type (VI) was obtained from acetyl derivative IIb (1 mmole) and 2-methylthio-3-methylbenzothiazolium methylsulfate (1 mmole) in a mixture of 3 ml of pyridine, 3 ml of acetic anhydride, and 0.25 ml of triethylamine [68% yield, mp 250°C (from Ac_2O), λ_{max} 566 nm (log ε 4.63) (in nitromethane)].



VI

The compounds obtained are stable substances. The tendency of thiazolo[3,2-a]quinolinium 1-oxide to undergo reactions with electrophilic agents and dimerization follows from its molecular diagram calculated by the MO LCAO method within the Pariser–Parr–Pople approximation.

The structure of the synthesized compounds were confirmed by the PMR and mass spectra. The results of elementary analysis for N and S were in agreement with the calculated values.

LITERATURE CITED

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