# RECYCLIZATION OF 1-(3-OXOBUTYL)ISATINS TO 1,4-DIHYDRO-3-ACETYLQUINOLINE-4-CARBOXYLIC ACIDS

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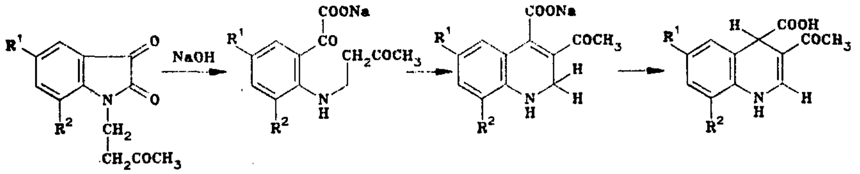
We have shown that 1,4-dihydro-3-acetylquinoline-4-carboxylic acids Ia-c, instead of the expected 1,2-dihydro isomers, are formed from 1-(3-oxobutyl)isatins upon treatment with aqueous alkali.

The pyrrole ring of isatin is readily opened to give N-(3-oxobutyl)-o-aminophenylglyoxylic acid, which, in turn, undergoes cyclization to 1,2-dihydro-3-acetylquinoline-4-carboxylic acid. Subsequent prototropic rearrangement leads to migration of the double bond to the $C_{(2)}-C_{(3)}$ position.



a $R^1=R^2=H$ (mp 238–240°); b $R^1=CH_3$, $R^2=H$ (mp 202–204°); c $R^1=H$, $R^2=CH_3$ (mp 230–232°)

The structure of 1,4-dihydro-3-acetylquinoline-4-carboxylic acid was proved by physicochemical methods. IR spectrum: 3330 (NH); 2500-3000, 1720, 1710, 1445, 1250, 935 (COOH); 1720 (CO); 1645 $cm^{-1}$ (C=C). The mass spectrum of the methyl ester of Ia contains intense peaks of ions with m/z 172, 188, and 189, which are formed when $M^+$ (231) loses, respectively, ester and acetyl groups and a molecule of ketene.

The choice between 1,2- and 1,4-dihydroquinoline structures was made on the basis of the PMR spectrum, which contains signals of two lone 4-H and 2-H protons. PMR spectrum ($d_6$-DMSO): 2.37 (3H, s, $COCH_3$), 4.83 (1H, s, 4-H), 7.80 (1H, d, 2-H, J = 5.7 Hz), and 9.63 ppm (1H, d, NH, J = 5.7 Hz).

The structures of Ib, c were similarly proved.

The results of elementary analysis were in agreement with the calculated values.

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