

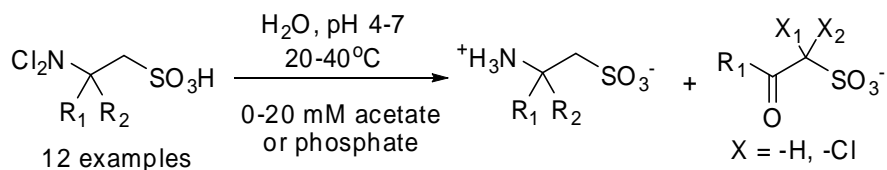
Stieglitz Rearrangement of *N,N*-Dichloro- β,β -Disubstituted Taurines in Mild Aqueous Solution

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Abstract

Among several newly disclosed scaffolds for topical anti-infectives, *N,N*-dichloro- β,β -disubstituted taurines have shown great promise. This study describes the structure-stability relationship (SSR) of various alkyl, heteroalkyl and cycloalkyl β -substitutions which effect order-of-magnitude changes in the aqueous stability of the compounds. These changes are attributed to Stieglitz rearrangement of alkyl groups under extremely mild conditions (H_2O , pH 4-7, 0-20 mM acetate or phosphate buffer, 20-40 °C). The rearrangement products, β -ketosulfonic acids, then destroy the oxidative capacity of the remaining chlorinated compounds through enol-mediated chlorinations.



$\text{R}_1 = \text{-Me, R}_2 = \text{-Me}$ $t_{1/2} (40^\circ\text{C}) > 2$ years

$\text{R}_1 = \text{-Et, R}_2 = \text{-Et}$ $t_{1/2} (40^\circ\text{C}) = 1$ day

$\text{R}_1 = \text{-iPr, R}_2 = \text{-iPr}$ $t_{1/2} (20^\circ\text{C}) < 10$ min