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Influence of ester structures on kinetics of piperidine and morfoline *N*-acylation in aqueous-organic solvents

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Abstract

The kinetics of piperidine and morfoline reactions with mono- and dinitrosubstituted phenyl benzoates in phenoxide ring is investigated in binary solvents water–2-propanol and water–1,4-dioxane. It is shown that Hammet's equation is true for the compounds of this class. Linearity is established between logarithms of the reactions rate constants and pK_a values of the ester leaving groups. Linearity is established between logarithms of rate constants of the amines reactions with 4-nitrophenyl benzoate and phenyl salicilate. Values of activation parameters of piperidine reactions with esters agree with results of investigations of temperature dependence of dibutyl amine and diethyl amine reactions with 4-NPhB in the same conditions. It is shown that E_{LUMO} values of the substituted phenyl benzoates can be descriptors of their reactivity in reaction with piperidine.