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Thematic course: Theme: Kinetics and mechanism of acyl transfer reactions. Part 10. Reactivity of dipeptides and esters of carboxylic acids at their interaction in aqueous dioxane solutions

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Abstract

An influence of a binary system water - 1,4-dioxane and of esters structure on kinetics of glycyl glycine and L- α -alanyl – L- α -alanine reactions with 4-nitrophenyl acetate and phenyl benzoates activated by nitro group is studied. It is shown that rate constants enhancement at increase of water part in the solvent is connected with specific solvation of the dipeptides. Kinetic data are compared with results of quantum chemical simulation of the reagents molecules. It is established that Hammet's constants, values of leaving groups pK_a and orbital characteristics of the esters molecules can be used as reactivity descriptors in acylation of the dipeptides.