

ANALYSIS OF STABILITY OF COMPLEXES OF ISONICOTINIC ACID HYDRAZID DERIVATIVES WITH BETA-CYCLODEKSTRIN

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System containing isonicotinic acid N'-[4-(4-chlorobenzylidene)-5-oxoimidazolidin-2-yl]-hydrazid and beta-cyclodekstrin have been analyzed to find the possible mechanism of creation and stabilization of complexes. Experimental attempts failed to create stable systems. Theoretical analysis could be helpful in explaining factors originating instability of the complexes, and propose modifications in experimental procedures. Docking scheme was performed to find the most probable conformations of possible complexes and was followed by molecular dynamics simulations. To compare obtained results the whole procedure was also repeated for compounds found to create stable complexes with cyclodextrin and having similar structure motives to analyzed anti-tuberculosis agent.