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Organic solvent desorption from two tegafur polymorphs

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Abstract

Desorption behavior of 8 different solvents from α and β tegafur (5-fluoro-1-(tetrahydro-2-furyl)uracil) has been studied in this work. Solvent desorption from samples stored at 95 % and 50 % relative solvent vapor pressure was studied in isothermal conditions at 30 °C. The results of this study demonstrated that: solvent desorption rate did not differ significantly for both phases; solvent desorption in all cases occurred faster from samples with the largest particle size; and solvent desorption in most cases occurred in two steps. Structure differences and their surface properties were not of great importance on the solvent desorption rates because the main factor affecting desorption rate was sample particle size and sample morphology. Inspection of the structure packing showed that solvent desorption rate and amount of solvent adsorbed were mainly affected by surface molecule arrangement and ability to form short contacts between solvent molecule electron donor groups and freely accessible tegafur tetrahydrofuran group hydrogens, as well as between solvents molecule proton donor groups and fluorouracil ring carbonyl and fluoro groups. Solvent desorption rates of acetone, acetonitrile, ethyl acetate and tetrahydrofuran multilayers from α and β tegafur were approximately 30 times higher than those