MOLECULAR DYNAMICS SIMULATION OF ETORICOXIB UNDER CONFINED GEOMETRY CONDITIONS OF NANOCRYSTALLINE CELLULOSE-BASED AEROGEL IN A SUPERCRITICAL CARBON DIOXIDE MEDIUM

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Aerogels possess a number of unique physicochemical properties, such as low thermal conductivity, very low density, and high porosity, which make them highly attractive for use in various technologies. In pharmaceuticals, aerogels are promising delivery systems for active pharmaceutical ingredients, among which aerogels based on nanocrystalline cellulose have great potential for application. The use of carrier matrices such as aerogels makes it possible to increase the bioavailability of an active pharmaceutical ingredient through its amorphization in the pores. Furthermore, drug formulations based on aerogels allow for the controlled release rate of medicinal compounds.

This work studies the impregnation of nanocrystalline cellulose-based aerogel with etoricoxib, a nonsteroidal anti-inflammatory drug.

The report discusses molecular dynamics modeling of the impregnation of nanocrystalline cellulose-based aerogel with etoricoxib in a supercritical carbon dioxide medium. The modeling was performed at various temperatures and carbon dioxide densities equal to 1.1 times the critical density of CO_2. The metadynamics method was applied to calculate the free energy of conformers and the entire free energy landscape as a function of the dihedral angles of etoricoxib. This method enables accurate calculation of the free energy of conformational transitions between states separated by high energy barriers. The results of the performed calculations are discussed in the report.

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