RESUMO SIMPLES - CSAU - CIÊNCIAS DA SAÚDE

MOLECULAR MODELING OF SODIUM MONTMORILLONITE AND POLYVINYLPYRROLIDONE AS A CARRIER SYSTEM FOR LITHIUM CARBONATE DELIVERY

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Although it is the standard treatment for bipolar disorder, lithium carbonate has a very narrow therapeutic window. This characteristic leads to severe dose-dependent multi-systemic toxicity and serious adverse reactions, which frequently discourages the clinical use of the drug and hinders patient adherence to the treatment. Carrier systems combining sodium montmorillonite (MMT-Na) and polyvinylpyrrolidone (PVP) are highly promising for controlling the release of the active pharmaceutical ingredient. MMT-Na offers a large surface area and cation exchange capacity, while PVP, being hydrophilic and biodegradable, acts to enhance these carrier properties. The present study aimed to prepare and investigate a molecular model of the drug delivery system

formed by MMT-Na/PVP containing lithium carbonate, to analyze the intermolecular interactions and the dispersion of the Li+ ion within the polymer matrix. The molecular structure of lithium carbonate was prepared using the Avogadro software. The PVP polymer chain containing 40 monomers and the MMT-Na lamellar structure were prepared using the Xenoview software, as well as the water solvation of the molecular system for application in the molecular dynamics simulation. The employed force field was PCFF_interface. Following the 10 ns simulation, the results indicated the interaction of Li+ ions with the MMT lamellae, while Na+ ions interacted with the carbonate molecules, demonstrating the cation exchange activity of MMT-Na. The diffusion coefficient of the Li+ ions in the molecular system was 7.397E-06 cm^2/s, and the Non-Gaussian Parameter (NGP) did not reach zero during the simulation, indicating that the velocities of the Li+ ions were heterogeneous. The Radial Distribution Function (RDF) between Li+ ions at the final moment of the trajectory showed an increase in the distance between the atoms, with the largest computed distance being 19 Å. The molecular dynamics simulation indicated that the Li+ ions can interact with the MMT lamellae and disperse throughout the polymer matrix; therefore, the present study holds the perspective of extending the simulation time to verify the interactions observed in the system in greater detail.

Palavras-chave: lithium carbonate; molecular dynamics simulation; drug carrier system; polyvinylpyrrolidone; montmorillonite.