Molecular docking evaluation of celecoxib on the boron nitride nanostructures for alleviation of cardiovascular risk and inflammatory

ABSTRACT

Celecoxib (CXB) is a nonsteroidal anti-inflammatory drug (NSAID) that can be used to treat rheumatoid arthritis and ischemic heart disease. In this research, density functional theory (DFT) and molecular docking simulations were performed to study the interaction of boron nitride nanotube (BNNT) and boron nitride nanosheet (BNNS) with CXB and its inhibitor effect on pro-inflammatory cytokines. The calculated adsorption energies of CXB with the BNNT were determined in aqueous phase. The results revealed that adsorption of CXB molecule via its SO_2 group on BNNT is thermodynamically favored than the NH_2 and CF_3 groups in the solvent environment. Adsorption of CXB on BN nanomaterials are weak physisorption in nature. This can be attributed to the fact that both phenyl groups in CXB are not on the same plane and require significant activation energies for conformational changes to obtain greater H-π interaction. Both BNNT and BNNS materials had huge sensitivity in electronic change and short recovery time during CXB interaction, thus having potential as molecular sensor and biomedical carrier for the delivery of CXB drug. IL-1A and TNF-α were implicated as vital cytokines in diverse diseases, and they have been a validated therapeutic target to manage cardiovascular risk in patients with inflammatory bowel disease. A molecular docking simulation confirms that the BNNT loaded CXB could inhibit more pro-inflammatory cytokines including IL-1A and TNF-α receptors as compared to BNNS loaded to CXB.