Improved anti-inflammatory and anticancer properties of celecoxib loaded zinc oxide and magnesium oxide nanoclusters: A molecular docking and density functional theory simulation

ABSTRACT

Present study offers great prospects for the adsorption of anti-inflammatory celecoxib molecule (CXB) over the surface of zinc oxide ($Zn_{12}O_{12}$) and magnesium oxide ($Mg_{12}O_{12}$) nanoclusters in several environments by performing robust theoretical calculations. Density functional theory (DFT), time-dependent density functional theory (TDDFT) and molecular docking calculations have been extensively carried out to predict the foremost optimum site of CXB adsorption. It has been observed that the CXB molecule prefers to be adsorbed by its SO_2 site on the Zn-O and Mg-O bonds of the $Zn_{12}O_{12}$ and $Mg_{12}O_{12}$ nanoclusters instead of NH2 and NH sites, where electrostatic interactions dominate over the bonding characteristics of the conjugate complexes. Furthermore, the presence of interactions between the CXB molecule and nanoclusters has also been evidenced by the UV–Vis absorption spectra and IR spectra. Molecular docking analysis has revealed that both adsorption states including CXB/$Zn_{12}O_{12}$ and CXB/$Mg_{12}O_{12}$ have good inhibitory potential against protein tumor necrosis factor alpha (TNF-α) and Interleukin-1 (IL-1), and human epidermal growth factor receptor 2 (HER2). Hence they might be explored as efficient TNF-α, IL-1, and HER2 inhibitors. Hence from the study, it can be anticipated that these nanoclusters can behave as an appropriate biomedical carrier for the CXB drug delivery.