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Theoretical evaluation of boronic acids as inhibitors of carbonic anhydrase through docking simulations

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Carbonic anhydrase (CA) is an enzyme with multiple features which does it attractive in medicinal chemistry field. The modulation of its activity is useful to regulate biological responses. Thus, CA-inhibitors have many applications as antibiotics, anti-neoplastics, diuretics, etc. Consequently, several compounds have been tested in their ability for inhibiting this enzyme. Among the tested compounds as CA-inhibitors are boronic acids. However, the approaches for studying the boronic acids-ability to inhibit CA are limited to *in vitro* assays. In this work, we analyzed the binding pose and Gibbs free energy (ΔG) of boronic acids on human and murine CA (Isoform II). The enzymes models were obtained from Protein Data Bank. Then, the docking assays were performed by AutoDock 4.2 and the ligand-protein complexes were analyzed by AutoDock tools and visual molecular dynamics. Results from our theoretical evaluation are in good agreement with those observed in experimental solved structures, similar to that observed in the crystal of CA with a boron-containing aromatic sulfamide (PDB code: 3MNU). The presence of boron atom in ligand is related to binding pose and the calculated value of affinity (pKd) comparatively to boron-free related structures. Also, the role of zinc atom in this enzyme seems to be the key for interactions and predicted energy values. Nevertheless, the relationship between previously reported experimental data and calculated affinity values is poor judged from the co-efficient of determination for these data.

Biography

Soriano-Ursúa M A has completed his PhD from Escuela Superior de Medicina del Instituto Politénico Nacional, México. He is a member of the National System of Researchers, and he is Head of the Physiology Laboratory. He has focused on the rational drug design having boron-containing compounds as main moiety, as well as, the different effects of these compounds on human physiology. He has authored more than 30 publications and has been serving as an Editorial Board Member of repute.

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