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Use of MM-PBSA in reproducing the binding free energy of NSAIDs to b-cyclodextrin

Sabrina Pricl, Marco Ferrone, Maurizio Fermeglia, Alessia Lodi, and Alessandra Mazzurco. Department of Chemical Engineering, University of Trieste, Piazzale Europa 1, Trieste, 34127, Italy

The understanding of noncovalent interactions is of paramount importance in supramolecular and biological chemistry. Towards this goal, the molecular recognition of many simple host molecules, such as cyclodextrins, has been extensively studied. Unlike the natural systems, the synthetic host-guest complexes have better defined conformations and therefore can be analyzed both experimentally and theoretically in great detail. Non steroidal anti-inflammatory drugs (NSAIDs) are used widely in the community for several inflammatory conditions. Nonetheless, there is a concern over the widespread use of NSAIDs, mainly bound to their side-effects, which include adverse reactions in the gastrointestinal tract, kidney, liver, dermis and central nervous system. In this work we applied MM-PBSA (Molecular Mechanics-Poisson-Boltzmann/Surface Area) combined with molecular docking to determine the binding mode and the relevant free energy of binding of the most common NSAIDs with beta-cyclodextrin and 2-hydroxypropy-beta-cyclodextrin, in order to characterize the corresponding most suitable drug delivery host-guest supermolecular complex.

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