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Sampling methods to predict the Gibbs free energy of systems of biological interest

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Abstract: Free energy changes drive mostly chemical processes in nature such as protein–ligand binding, self-assembly, protein folding and denaturation, and reaction pathways.[1,2,3] Being able to reliably predict free energy changes using molecular dynamics simulations has long been extremely attractive as it would enable understand, design, and developing new processes, model reactions, and design materials and drugs with increased efficiency. New methodologies, protocols, and algorithms combined with advances in computation recently leaded to impressive increases in computational power and capacity, and facilitated improvements in both the efficiency and accuracy of free energy calculations, making them useful for prospective applications such as the design of new potential drugs and the understanding of self-assembly in important biological molecules. The developments occurred in the Complex Fluids Lab of PUC-Rio during the covid-19 pandemic have conducted our lab to estimate the octanol-water partition coefficient of important phospholipids in membranes [1,2] and to predict the binding constants of some antiviral peptides with important protein targets of SARSCoV-2 [3] using umbrella sampling and alchemical methods.

Key-words: SARSCoV-2, covid-19, phospholipids, ligand-protein complex, alchemical methods, and umbrella sampling.

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