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Modeling Ionization Events iduced by Protein Protein Binding[1]

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— The association of two or more biological macromolecules dramatically change the environment of the amino acids situated at binding interface and could change ionization states of titratable groups. The change of ionization due to the binding results in proton uptake/release and causes pH-dependence of the binding free energy. We apply computational method, as implemented in Multi Conformation Continuum Electrostatics (MCCE) algorithm, to study protonation evens on a large set of protein-protein complexes. Our results indicate that proton uptake/release is a common phenomena in protein binding since in vast majority of the cases (70%) the binding caused at least 0.5 units proton change. The proton uptake/release was further investigated with respect to interfacial area and charges of the monomers and it was found that macroscopic characteristics are not important determinants. Instead, charge complementarity across the interface and the number of unpaired ionizable groups at the interface are the primary source of proton uptake/release.

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