Protein Simulations at constant pH.

Sometimes a pKa is not a pKa

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I will present a methodology to simulated protein dynamics and ensemble properties under a constant pH constraint, instead of the usual constant protonation paradigm. The method will be used to predict pKas of proteins, but more importantly, I will show that experimental pKas are to be taken with a somewhat skeptical view, as that they sometimes report conformational effects rather than simple energetics. This new view can have repercussions in our understanding of buried charged residues in proteins.