

Computational Approaches to Investigate Ligand Migration Pathways in Proteins

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Small gaseous ligands perform important functions in proteins. Since their discovery in 1984, internal cavities have spurred interest in their role, function, and interconnectivity. Also, the cavities provide interesting possibilities to carry out controlled experiments and better characterize the interior of proteins. In this contribution I will provide an overview of cavities and their networks in a range of globin-proteins and I will discuss means to sample this network ranging from pure-MD to pure-MC approaches. Also, Markov- and Smoluchowski-based strategies and their advantages and disadvantages are assessed.