Molecular simulations of protein/ligand interactions

Julien Michel

EastCHEM School of Chemistry,
Joseph Black Building,
The King's Buildings,
Edinburgh, EH9 3JJ,
United Kingdom
mail@julienmichel.net

Monte Carlo and molecular dynamics simulations of protein/ligand interactions have been around for decades, but it is only in recent years that the methodologies have started to find regular use in structure-based drug design programs; primarily to predict binding affinities. Although a clear statistical thermodynamics framework to compute binding affinities exists, several technical issues and pitfalls limit the predictive power of the approach and have hindered widespread adoption. In this talk I will outline challenges faced by practitioners and discuss possible solutions. Some the problems likely to be covered will include: polarization effects, hydration in binding sites and extreme protein dynamics.