Free Energy Pertubations in Fragment Based Drug Discovery

The stepwise and systematic nature of the fragment-to-lead process makes FEP (Free energy perturbation) calculations ideally suited to driving the fragment based drug discovery projects. An in press publication by the company Schrodinger demonstrates the value of this technique in fragment based design. The authors used published data to demonstrate how FEP could be used in deciding molecules to be synthesized by expanding a seed fragment.

The project for an internship would involve a retrospective analysis of inhouse fragment projects to see how FEP would have fared in guiding inhouse fragment based projects compared to traditional docking and rescoring methods (eg, WSCORE, HYDE, etc) and prospective work to see if FEP calculations can correctly predict relative binding affinities for growing fragments.

The interested candidate would be working in a multi-disciplinary group and will gain insights into fragment based drug design as well as gaining an overview of early phase drug discovery, and some of the *in silico* methods used in this phase of the discovery process.

A motivated candidate with good command of English and some experience using basic linux commands is sought.

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