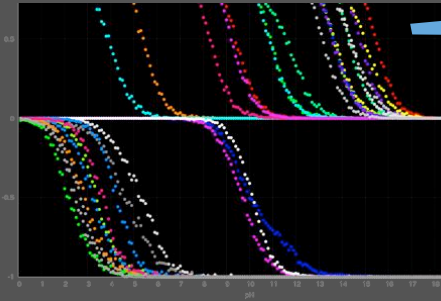


UFFBAPS

A state-of-the-art empirical force field based on FOLD-X. It uses a unified force-field for both stability and binding calculations which increases the consistency of its predictions.

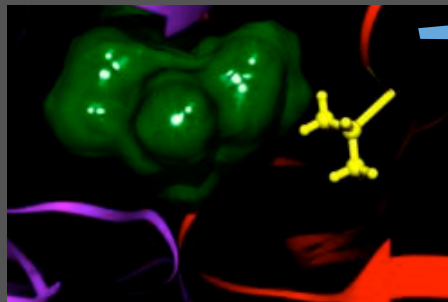
- R. Guerois, J. E. Nielsen, and L. Serrano. Predicting changes in the stability of proteins and protein complexes: a study of more than 1000 mutations. *J Mol Biol*, 320(2):369–387, Jul 2002.



pKD

A Poisson-Boltzmann equation-based algorithm for calculating changes in protein pK_a values. Can also predict mutations that will change the pK_a value of a given residue

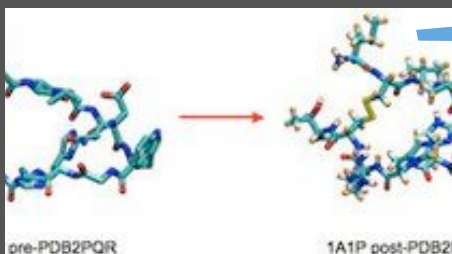
- B. M. Tynan-Connolly and J. E. Nielsen. Redesigning protein pka values. *Protein Sci*, 16(2):239–249, 2007.



Protool

A mutation modeling program developed in-house specifically for PEAT-SA, which uses a backbone specific rotamer library.

- R. L. J. Dunbrack and F. E. Cohen. Bayesian statistical analysis of protein side-chain rotamer preferences. *Protein Sci*, 6(8):1661–1681, Aug 1997



pdb2pqr

pdb2pqr is an open-source packaged used by PEAT-SA to automatically add-hydrogens and correct the structure of proteins submitted to the program.

- T. J. Dolinsky et al. pdb2pqr: expanding and upgrading automated preparation of biomolecular structures for molecular simulations. *Nucleic Acids Res*, 35(Web Server issue):W522–5, Jul 2007