Multi-Conformation Continuum Electrostatics - MCCE

MCCE is a biophysics simulation program developed at Gunner Lab at City College of New York.

MCCE combines continuum electrostatics and molecular mechanics. In this program, the protein side chain motions are simulated explicitly while the dielectric effect of solvent and bulk protein material is modeled by continuum electrostatics.

What can MCCE do?

MCCE can calculate:

- residue pka, cofactor Em and protein PI in protein-solvent systems;
- protein structural responses to changes in charge;
- residue ionization changes in response to protein structural changes;
- location and stoichiometry of proton transfers coupled to electron transfer;

References

Cite these papers if you use MCCE for publications:

- Song Y., J. Mao, Gunner M.R. (2009). MCCE2: Improving Protein pK_a Calculations with Extensive Side Chain Rotamer Sampling. J. Comp. Chem 30(14): 2231–2247
- Georgescu R.E., Alexov E.G., Gunner M.R.(2002). Combining conformational flexibility and continuum electrostatics for calculating pKa's in proteins. Biophys J. 83, 1731-1748
- Alexov, E. and Gunner, M.R. (1997) Incorporating protein conformational flexibility into pH- titration calculations: Results on T4 Lysozyme. Biophys. J. 74, 2075-2093

Contact

Need to contact us?

- About issues with this program: Submit an issue from Github
- About Physics of MCCE: Email to Marilyn Gunner
- Not sure? Email to Junjun Mao

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