Journal of Cheminformatics

ORAL PRESENTATION Open Access

Non-continuum solvation using the EC-RISM method applied to predict tautomer ratios, pK_a and enantiomeric excess of alkylation reactions

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From 7th German Conference on Chemoinformatics: 25 CIC-Workshop
Goslar, Germany. 6-8 November 2011

The three-dimensional "reference interaction site model" (3D-RISM) integral equation theory is a statistical-mechanical approach to predict liquid state structural and thermodynamic features. It is based on approximate solute-solvent correlation functions to be computed on a 3D grid as a function of the interaction potential between the solute and the solvent sites, circumventing the need of costly sampling of explicit solvent degrees of freedom. In combination with quantum-chemical calculations within the embedded cluster (EC-)RISM framework [1] the theory allows for studying chemical reactions in solution with an accuracy not reached by traditional continuum solvation methods. In particular, it improves upon dielectric continuum solvation by taking solvent granularity into account and also provides a means towards physically cavity formation and dispersion free Energies without introducing artificial boundaries and empirically fitted radii.

We outline the general framework and show application examples from pK_a and tautomeric ratio estimation [2] as well as enantiomeric excess prediction for stereoselective alkylation reactions in organic solvent.

doi:10.1186/1758-2946-4-S1-O9
Cite this article as: Heil *et al.*: Non-continuum solvation using the EC-RISM method applied to predict tautomer ratios, pK_a and enantiomeric excess of alkylation reactions. *Journal of Cheminformatics* 2012 **4**(Suppl 1): O9.

Published: 1 May 2012

References

1. Kloss T, Heil J, Kast SM: **Quantum Chemistry in Solution by Combining 3D Integral Equation Theory with a Cluster Embedding Approach.** *J Phys Chem B* 2008, **112**:4337-4343.
2. Kast SM, Heil J, Güssregen S, Schmidt KF: **Prediction of tautomer ratios by embedded-cluster integral equation theory.** *J Comput-Aided Mol Des* 2010, **24**:343-353.

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