On the Importance of Physically Correct Models for Describing Protein/Ion/Ligand Binding

Martin Lepšík

ORCID ID: 0000-0003-2607-8132

Affiliation: Institute of Organic Chemistry and Biochemistry (IOCB) of the Czech Academy of Sciences, Prague, Czech Republic, lepsik@uochb.cas.cz

Understanding protein-ligand binding in atomistic details is the key to success in structure-based drug design. Herein, I review i) the progress of corrected semiempirical quantum mechanics (QM)-based scoring function in sampling, ranking and virtual screening[1,2] and ii) application of effective electronic polarization scheme for classical molecular dynamics (MD) which helps explain a rare oligosaccharide conformer in lectin/calcium/carbohydrate complex.[3] In summary, developing and applying physically correct models of protein-ligand binding heads toward an unrivaled qualitative enhancement of the predictive power of computer-aided drug design.

References

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