**God is in the detail: On the Importance of Physically Correct Models for Describing Protein/Ion/Ligand Binding**

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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 screening1,2 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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