

# Poster Presentations

**[MS25-P16] A comparative study of transferable theoretical aspherical pseudoatom data bank and classical force field in predicting the electrostatic interaction in molecular dimers.**

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Accurate and fast evaluation of electrostatic interactions in molecular systems is one of the most challenging tasks in the rapidly advancing field of macromolecular chemistry, including molecular recognition, protein modeling and drug design. Electrostatic interactions are extremely essential in biological system and it is also well known that ab-initio calculations are very expensive and time consuming. In this study we have evaluated electrostatic interaction energy of S66 (1) and JSCH-2005(2) data sets, total 203 molecular complexes. These complexes are representative of a range of chemical and biological systems for which hydrogen bonding, electrostatic,  $\pi$  stacking and van der waals interactions play important role. Reference benchmark energies were obtained directly from wavefunctions at the level of theory (DFT/B3LYP/aug-cc-pVTZ)(3; 4) using SAPT: Symmetry-Adapted Perturbation Theory (5). Electrostatic energy calculated on the basis of UBDB databank(6)-Exact Potential Multipole Method(EPMM)(7) of aspherical models and force fields were compared with corresponding reference results. Root mean square error's (RSMEs) and regression coefficient's were used as a quantitative measure of the quality of the analyzed properties. The energy trends are well consistent ( $R^2 \approx 0.98$ ) for the UBDB-EPMM method as compared to AMBER(8) and CHARMM force field methods (9) ( $R^2 \approx 0.95$ ). RSMEs are about 1-3 and 8-15 Kcal mol<sup>-1</sup> for the UBDB and force field methods, respectively.

This study shows that estimation of electrostatic interaction energy using UBDB databank is more accurate and fast when compared to other known methods and open new possibility of applying on macromolecules.

## References

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**Keywords:** UBDB Database, Pseudatom model, Charge density, electrostatic interaction energy