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Fragment Molecular Orbital Method for Large-Scale Biomolecular Systems

Shigenori Tanaka[1]

Summary

Recent developments in ab initio calculations for biomolecular systems such as proteins and nucleic acids are illustrated on the basis of the fragment molecular orbital (FMO) method. Examples of the calculated systems include nuclear receptors with small ligands, cAMP receptor protein complexed with DNA, influenza virus hemagglutinin complexes, and bioluminescent oxyluciferin-luciferase complex. Quantitative calculations with the inclusion of relevant electron correlation effects have well reproduced those experimental results concerning the binding affinity, the mutation effects, the emission spectra, and so on. Feasibility of massively parallel computations with the FMO method is also discussed.

[1]Kobe University