SS03-2 **Structure Modeling and Binding Energy Calculation by Fragment Molecular Orbital Method for Protein-Ligand Complex**

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A reliable protein-ligand complex structure is required for the accurate prediction of binding energy between a protein and a ligand. We have developed a hybrid quantum mechanical/molecular mechanical method, FMOMM, in which the fragment molecular orbital (FMO) method was employed as a QM method. Using the FMOMM method, the geometry optimizations were carried out on the complexes of protein kinase 2 (CK2) and its four ligands. For the FMO calculations, we employed HF-D (the Hartree-Fock theory augmented with an empirical dispersion term) and the 6-31G basis set (FMO-HF-D/6-31G). The optimized complex structures agreed well with experimental ones. FMO-MP2/6-31G* and FMO/PCM calculations were performed to estimate the binding free energies between the protein and the ligands. A good correlation between the calculated and the experimental binding energies was obtained.