F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

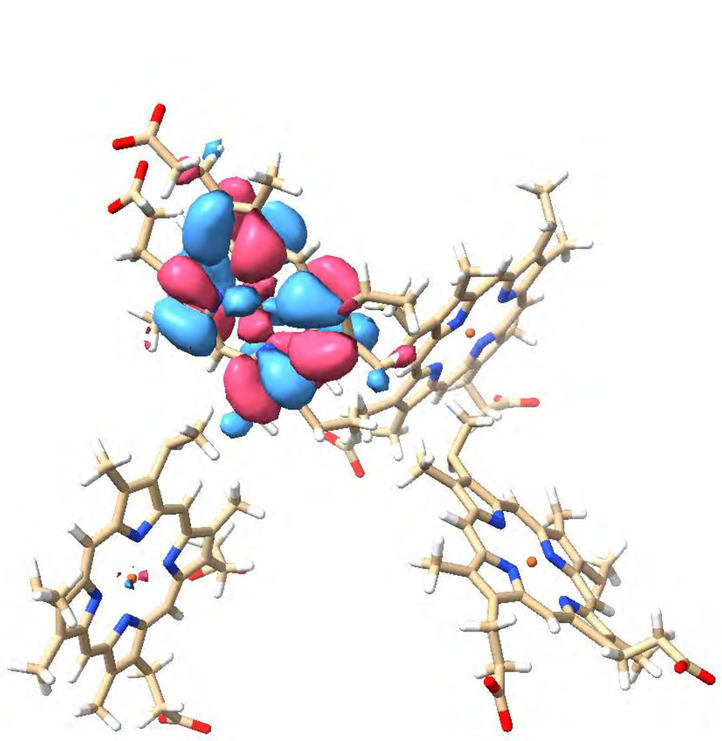
Computational Biomolecular Science

Mechanical Engineering department

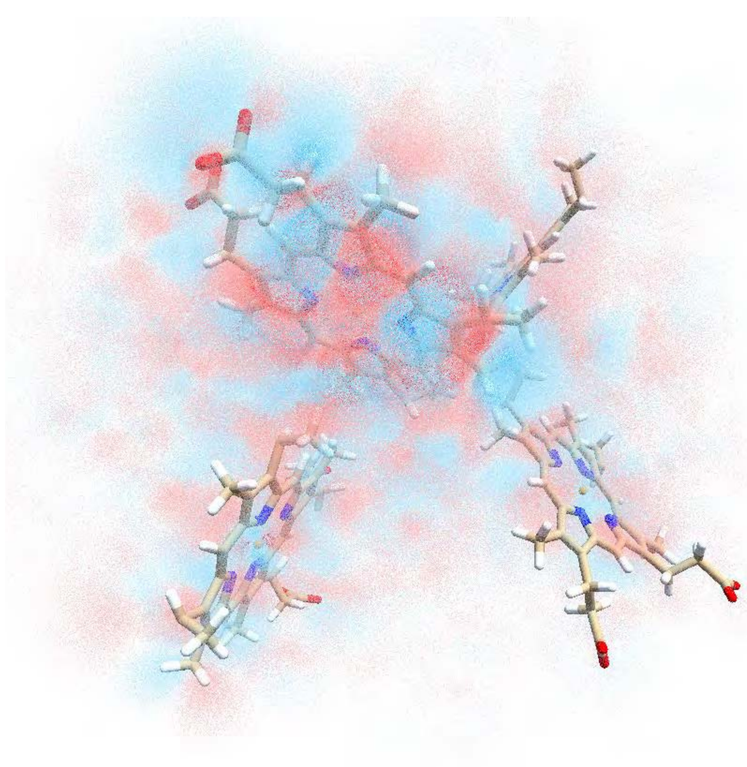
http://www.ciss.iis.u-tokyo.ac.jp, http://www.satolab.iis.u-tokyo.ac.jp

Protein Design by Quantum Chemical Calculation

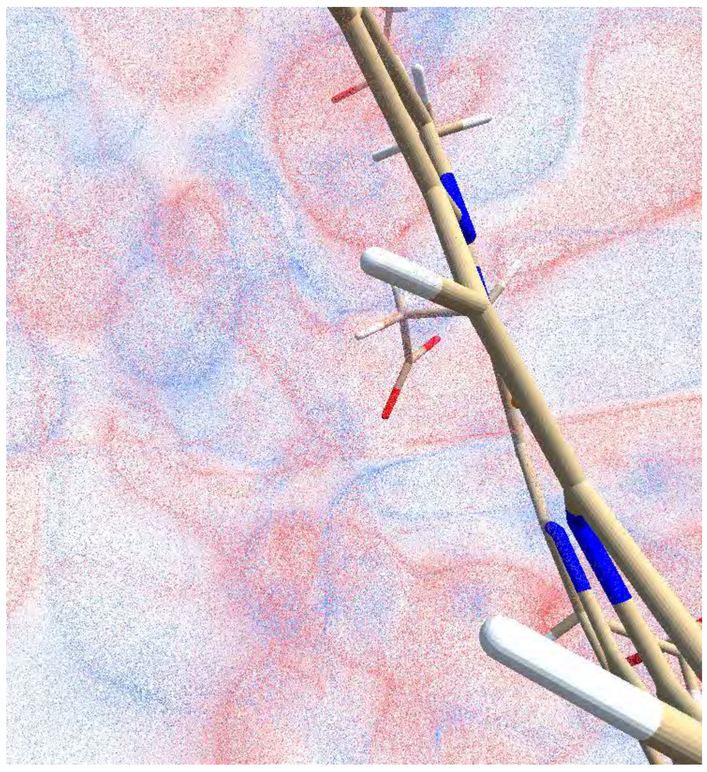
Quantum chemical calculation software “ProteinDF/QCLO” has been developed,
where canonical molecular orbitals of protein are computable.
https://proteindf.github.io/
Protein design is now performed by these methods.



Isosurface model

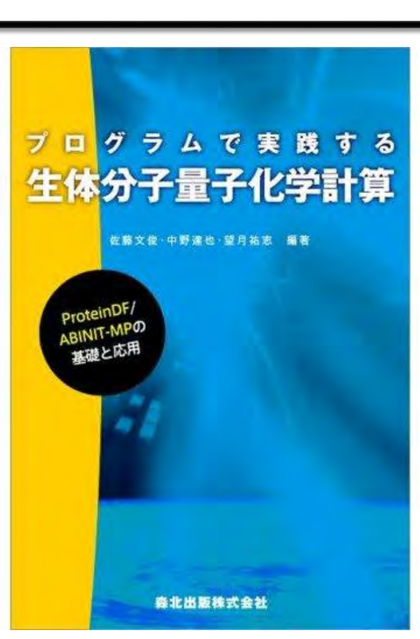


Cloud-like model



Protein internal exploration

Molecular orbital of cytochrome c_3 (Only 4 hemes are drawn as a backbone.)



Textbooks (in Japanese)