F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

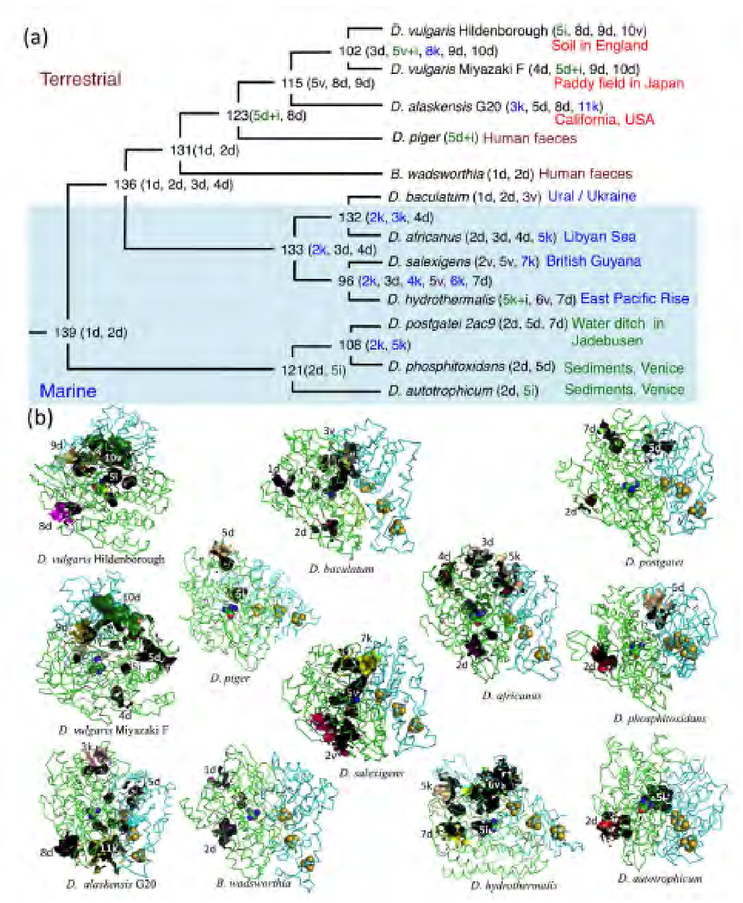
Computational Biomolecular Science

Mechanical Engineering department

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

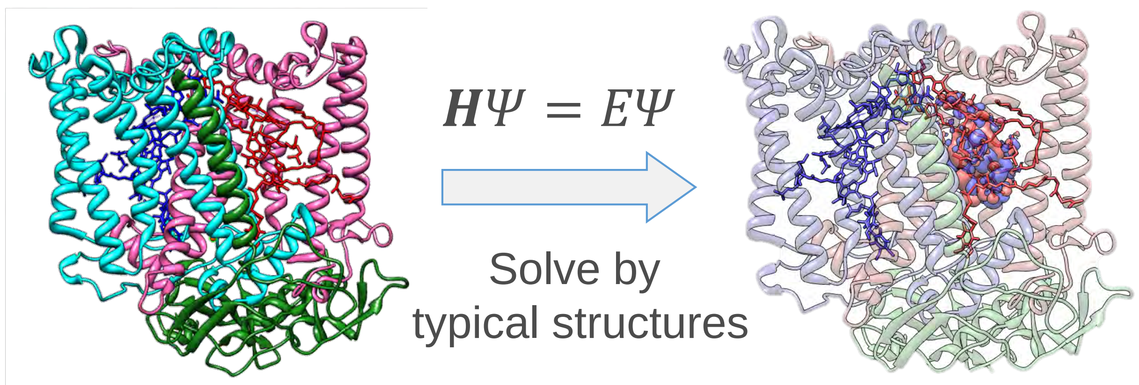
Protein Design by Quantum Chemical Calculation

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.

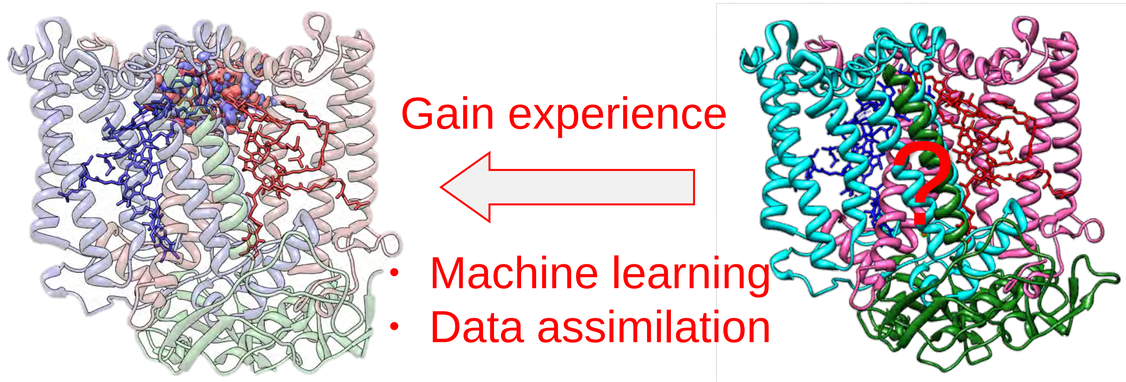


The conventional methods;
Phylogenetic traits, homology modeling,
and molecular dynamics methods

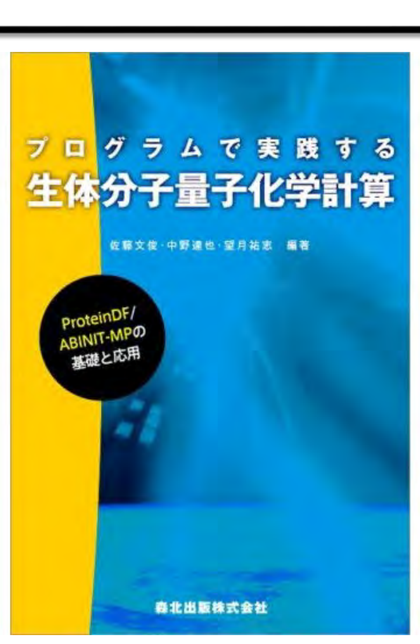
The deductive method; Which residues already have impacts on reaction mechanism?



The Inductive method; Which residues newly give impacts?



This work;
Protein canonical molecular orbitals analysis



Textbooks (in Japanese)