F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

Computational Biomolecular Science

Mechanical Engineering department

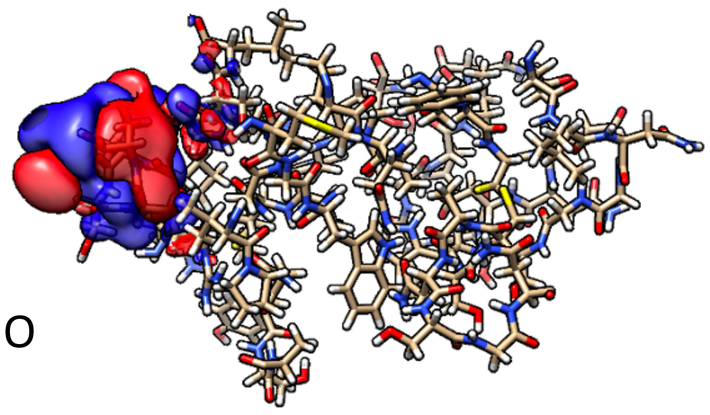
http://www.satolab.iis.u-tokyo.ac.jp/

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

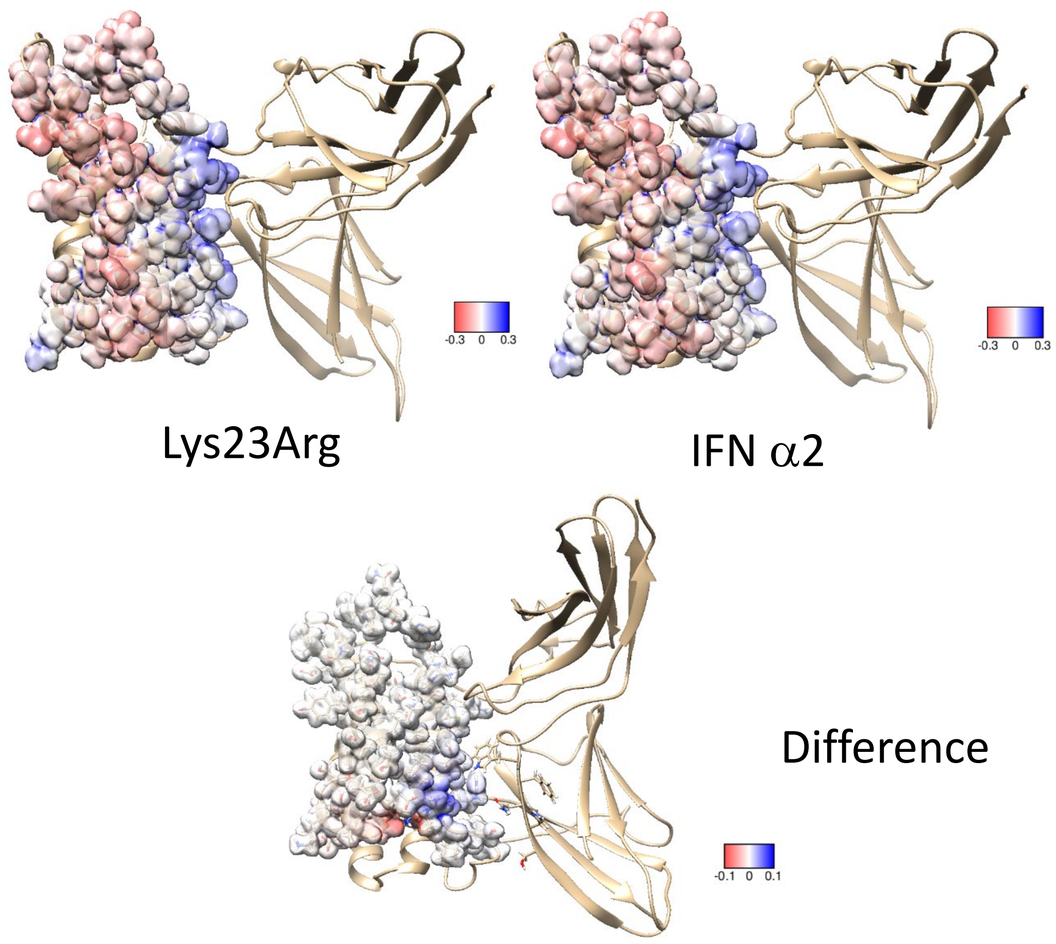
https://npem.iis.u-tokyo.ac.jp/

Protein Design by Quantum Chemical Calculation

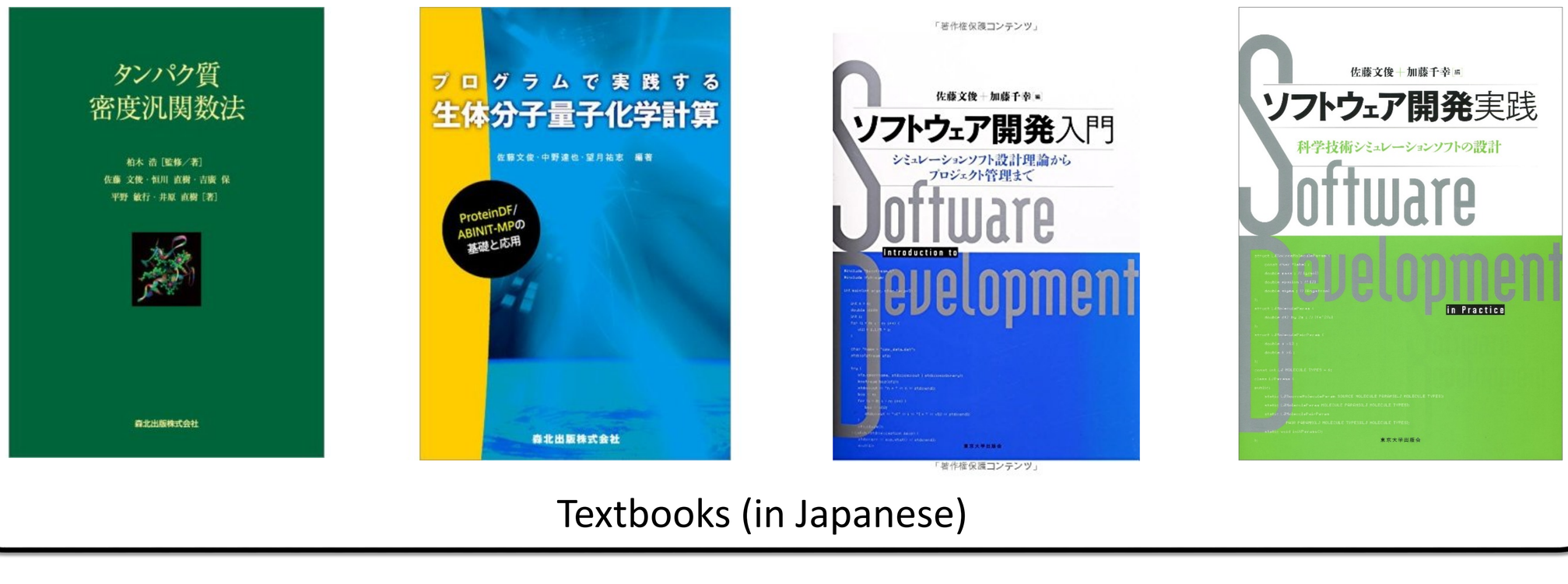
Our group has been developing the quantum chemical calculation software "ProteinDF/QCLObot" which can calculate all canonical molecular orbitals of proteins.
https://proteindf.github.io/
These are used for electronic structure analysis and design of proteins



HOMO (top) and LUMO (bottom) of 57AA model of PETase



Electrostatic potential distributions of interferon α2 (upper right), Lys23Arg mutant (upper left), and their difference (lower). The ribbon model is a receptor.



Textbooks (in Japanese)