INNOVATIVE SIMULATION OF BIO AND NANO MOLECULES

De-501, Bldg C Lounge, Bldg E Elevator Hall



F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]



Center for Research on Innovative Simulation Software

Computational Biomolecular Science

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

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

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

Mechanical Engineering department

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 $\alpha 2$ (upper right), Lys23Arg mutant (upper left), and their difference (lower). The ribbon model is a receptor.



Textbooks (in Japanese)



