F. SATO LAB.

[Innovative Simulation of Bio and Nano Molecules]

Center for Research on Innovative Simulation Software

Computational Biomolecular Science

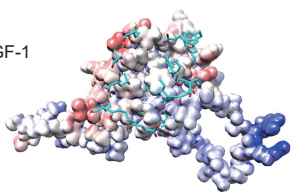
Mechanical Engineering department

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

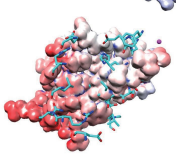
Protein Design by Quantum Chemical Calculation

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.

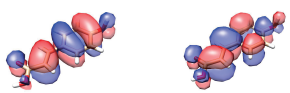
IGF-1



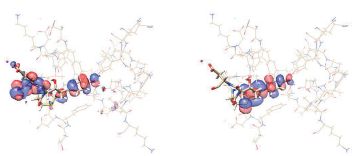
Insulin



Interaction sites between IGF-1 and IGF-1R (above), between insulin and IGF 1R (below). ESP is drawn on each surface.



HOMO (left) and LUMO (right) of optimized structure of pCA



HOMO-3 (left) and LUMO (right) of pCA+35AA model of PYP

Textbooks (in Japanese)