

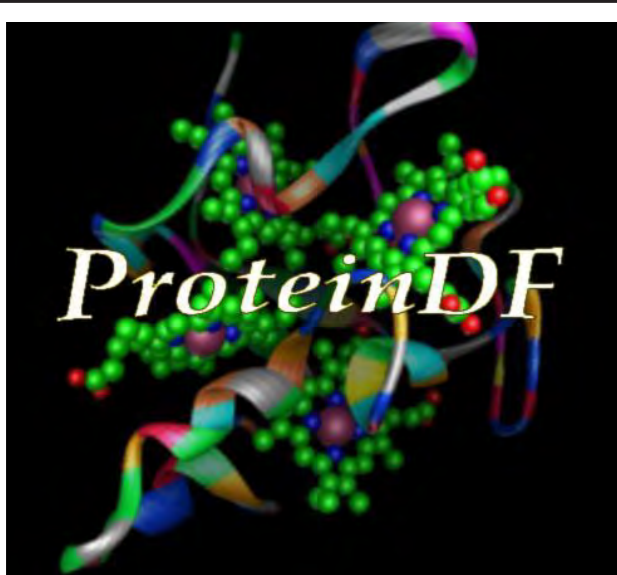
F. SATO LAB.

Innovative Simulation of Bio and Nano Molecules



Center for Research on Innovative Simulation Software
Center for Research on Engineering in Medicine and Biology

Department of Mechanical Engineering, Graduate School of Engineering
Computational Biomolecular Science
<http://www.satolab.iis.u-tokyo.ac.jp/>
<http://www.ciss.iis.u-tokyo.ac.jp/english/> <https://www.remb-utokyo.jp/en/>



Protein Design Using Quantum Chemical Calculation



Our group has been developing the quantum chemical calculation software "ProteinDF/QCLObot" which can calculate **all canonical molecular orbitals of proteins**.

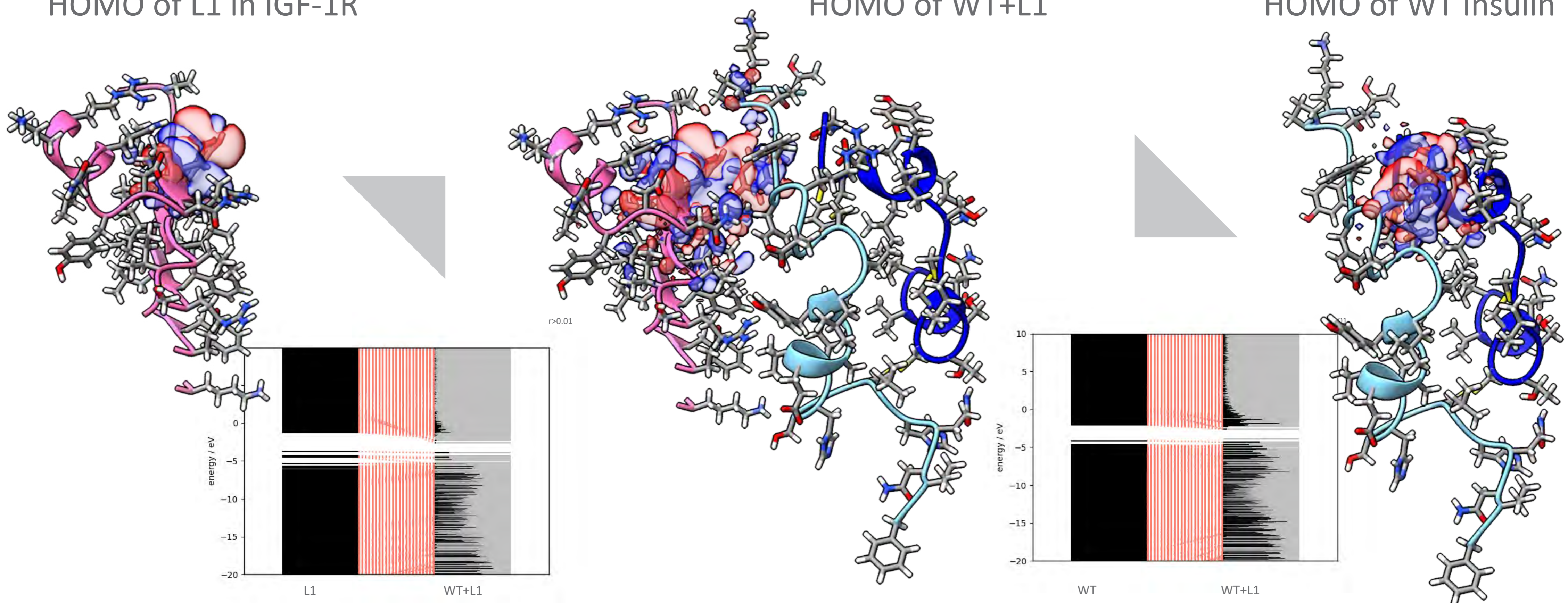
<https://proteindf.github.io/>

We are using these software to analyze and design the electronic structure proteins.

HOMO of L1 in IGF-1R

HOMO of WT+L1

HOMO of WT Insulin



Molecular orbital overlap analysis of the WT insulin/IGF-1 receptor complex



Textbooks (in Japanese)

