THE UNIVERSITY OF TOKYO

RISS
Research and Development of Innovative Simulation Software

Biomolecular interaction simulator
BioStation

ABINIT-MP
BioStaion Viewer

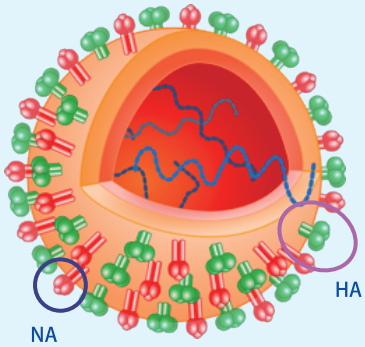
Analysis of interaction between proteins and chemical compounds based on fragment molecular orbital (FMO) method
➡ Efficient search and design of useful molecules!

Innovative and practical software for quantum chemical calculation and analysis
works on from a PC cluster to a vector supercomputer

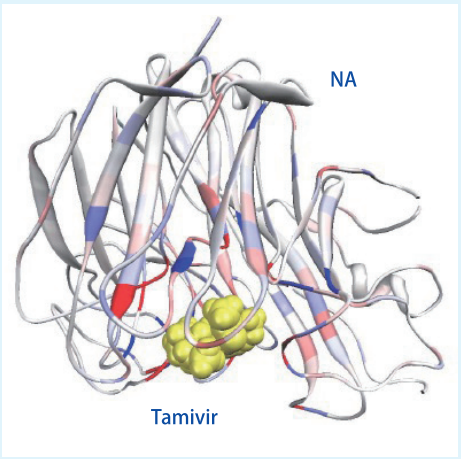
Feasibility Studies

In silico analysis of anti-influenza drug

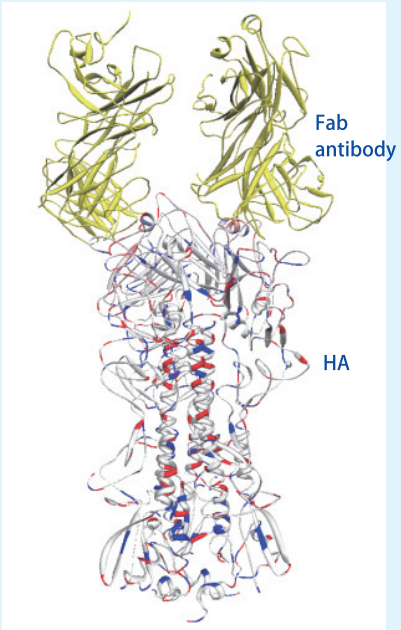
Large scale MP3 level calculations on the Earth Simulator (ES2) for
Hemagglutinin (HA, a protein related to the absorption process of a virus) and
Neuraminidase (NA, a protein related to the desorption process of a grown virus)



Influenza virus



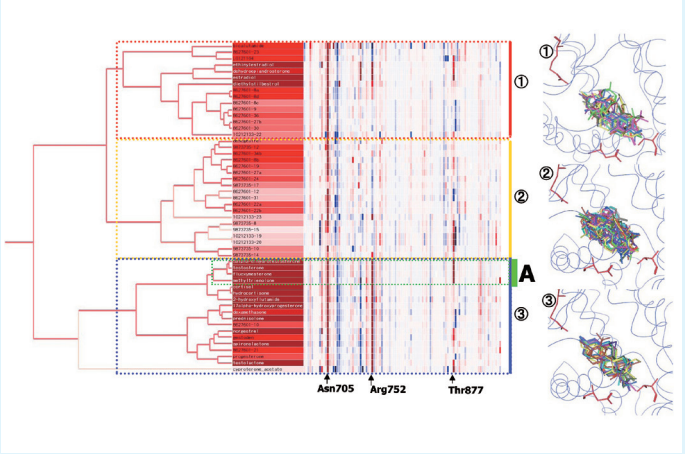
Interaction analysis of NA and Tamivir
is useful for developing an anti-influenza drug



Interaction analysis of HA trimer and
Fab antibody is useful for predicting mutation
or virus and for developing a vaccine

Virtual ligand screening

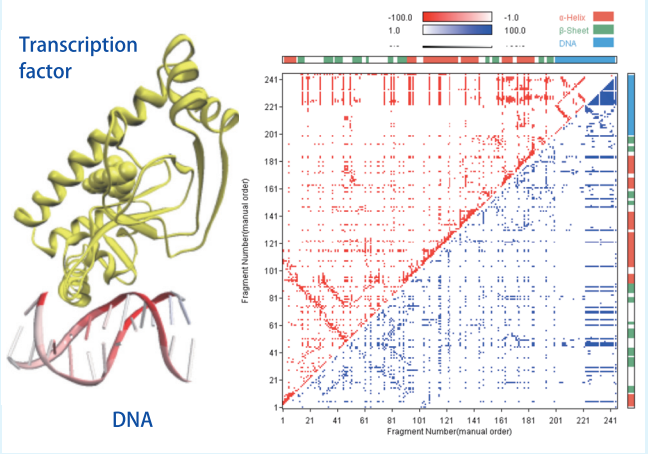
Cluster analysis using dissimilarity between IFIEs of
drugs or their candidates with a protein
⇒Search molecules similar to target one (Region A in figure below)



VISCANA analysis for interaction of protein-chemical compounds

Transcription mechanism of DNA

Exhaustive analysis for interaction of DNA and protein

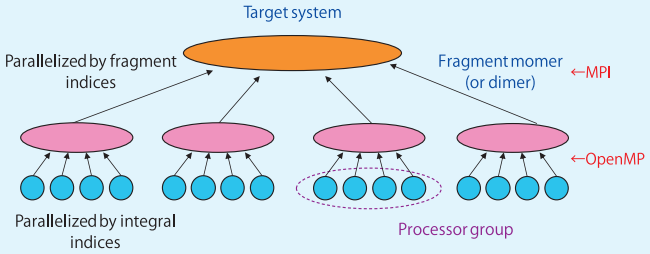


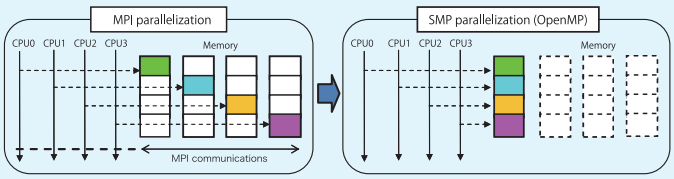
IFIE map analysis for interaction of DNA-protein

Feature works

Parallel computing with fragmentation

Hybrid parallelization with MPI for inter-fragment and with OpenMP for intra-fragment



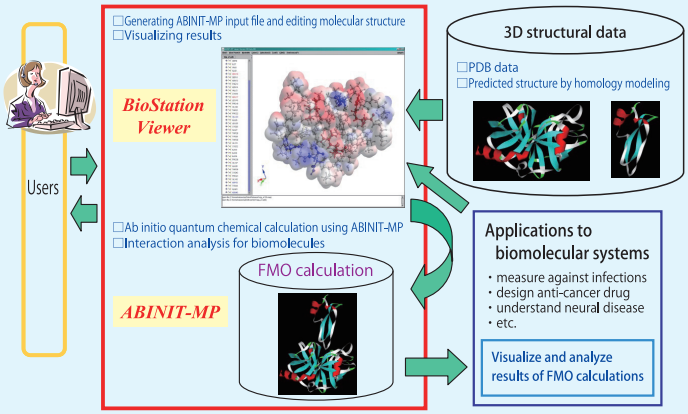


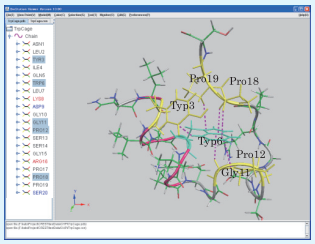
Molecule	Machine	Level	Basis	Time (h)	Core (Node)
HIV-1PR + Lopinavir	PC cluster	FMO-MP2/6-31G	17423	3.8	64 (16)
	PC cluster	FMO-MP3/6-31G	17423	15.4	64 (16)
NA monomer + Tamivir	PC cluster	FMO-MP3/6-31G	32549	41.5	64 (16)
HA trimer + Fab	ES2	FMO-MP3/6-31G	201276	5.8	1024 (128)
NA monomer + Tamivir	ES2	FMO-MP3/6-31G	32549	1.1	512 (64)
	ES2	FMO-MP3/6-31G*	50447	4.4	512 (64)

Vectorization for ABINIT-MP also shows high execution efficiency; ABINIT-MP had the highest performance of all public-used programs on ES2 in 2010.

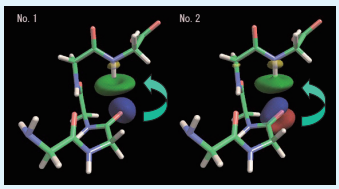
Pre-/Post-visualization program for FMO BioStation Viewer

Editing molecular structure, making ABINIT-MP input files, and visualizing FMO results





CH/π interaction analysis



Orbital-wise interaction analysis (CAFI)

Functions

Functions	Contents
FMO	FMO2, FMO3
Energy calculation	HF, MP2, MP3
Energy gradient	HF, MP2
Optimization	BFGS, CG, PRCG, Partial optimization
Local interaction analysis	CAFI, FILM
Population analysis	Mulliken charge, NPA charge
BSSE correction	Counterpoise method

Analyses*	Details
Inter-fragment interaction energy (IFIE)	Quantitative investigation of interaction between fragments
IFIE map	Exhaustive analysis of 2-body interaction with 2D map on IFIE
VISCANA	Visualized cluster analysis of protein−ligand interaction for virtual ligand screening
CAFI	Orbital-wise charge transfer and polarization interaction analysis
FILM	Orbital-wise dispersion interaction analysis (CH/π, π/π interaction, etc.)
CHPI	Analysis and visualization of CH/π interaction

*All of analyses are visualized by using BioStation viewer.

Platforms

■ ABINIT-MP

Language : Fortran90, MPI
OS : Linux (64 bit), executable binary
Compiler : Intel Fortran, PGI Fortran
Supercomputer : Earth simulator (ES2), PC cluster (HA8000)
Can work even on a 1-processor PC without MPI

■ BioStation Viewer

Language : Java, Java3D
OS : Windows (XP/Vista/7), Linux, Mac OS (10 or higher)
Installer for Windows

Documents/Examples

User manual/Example data（Tutorial for modeling in BioStation Viewer）

BioStation is supported by the project "Research and Development of Innovative Simulation Software (RISS)". BioStation and ABINIT-MP are a registered trademark of the Center for Research on Innovative Simulation Software (CISS), IIS, The University of Tokyo. All registered trademarks belong to their individual owners.

Please contact us if you would like to use or customize this software.
Center for Research on Innovative Simulation Software, Institute of Industrial Science (IIS), The University of Tokyo.
http://www.ciss.iis.u-tokyo.ac.jp/riss/project/molecule/
E-mail : software@ciss.iis.u-tokyo.ac.jp /

November, 2012