

An accurate method for quantum chemical computations of biomolecules

The fragment molecular orbital method (FMO) delivers the accuracy and generality of *ab initio* quantum chemistry. It can be applied to chemical reactions, excited states and other complicated problems. Using the method on the AIST Super Cluster, we have been able to perform the world record all electron calculation of a system containing more than 20,000 atoms. To facilitate its application in the field of bioscience, it was implemented in a general quantum chemistry program GAMESS and is being distributed free of charge. The intra- and intermolecular interaction analysis is a promising tool for drug design and other applications.

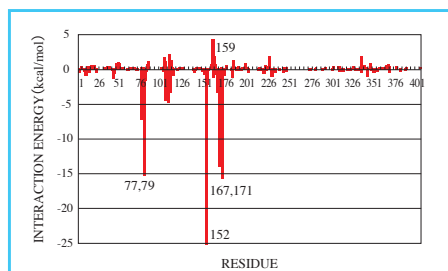


Figure 1: Interaction between thymidine Phosphorylase and its ligand (PDB:1uou). Attractive (residues 77,79,152,167,171) and repulsive (residue 159) interaction between protein and its ligand constitutes useful information for drug design.

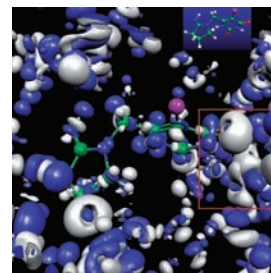


Figure 2: Protein polarisation by the ligand

The difference in the electron density of the protein in vacuum and in the complex with the ligand is plotted. Areas where the density increased are shown as blue and the decreased areas are white. Due to the interaction with the ligand, polarisation is especially large in the area (indicated by the red frame) around the two oxygen atoms (red). Protein atoms are not shown.

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New "Geological Maps of Volcanoes" were Published

New "Geological Maps of Volcanoes", Miyake Jima Volcano and Iwate Volcano, were published. The series of "Geological Maps of Volcanoes" shows geological maps and eruption history of active volcanoes in Japan. These new maps describe new distributions of volcanic ejecta, craters and the development history of the Miyake Jima (Miyake-Jima) and Iwate volcanoes. We hope these maps will help those who are interested in volcanoes, and will be useful to reduce damage from volcanic disaster.

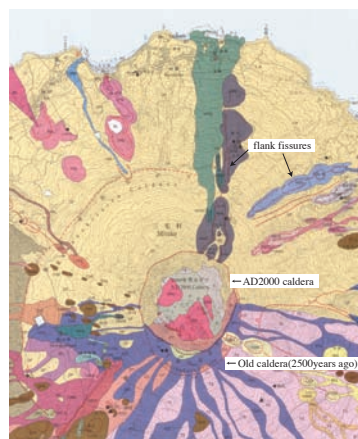


Figure: A part of the geological map of Miyake jima volcano.

There are many fissure vents and pyroclastic cones on the flank of the Miyakejima volcano.

Pyroclastic cones with "C" means newly recognized cones in the study of the geological map.

At the summit area, the map shows the old caldera rim and the new AD2000 caldera.

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