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<http://jglobal.jst.go.jp/public/20090422/200901030856290730>

■ Researcher information

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Major

Quantum Chemistry, Computational Chemistry, Computer Simulation

■ Research topics

Theoretical Study Applied to Glycoscience

Keywords

sugar chain, geometry, intermolecular interaction, sugar-binding specificity, fragment molecular orbital theory (FMO)

Contents

■ Overview (background, goal, detail)

Geometries and biological functions of polysaccharide are of great interest as the third biological chain. The ultimate goal of this research is to interpret the recognition mechanism and the specific interaction between proteins and polysaccharides based on quantum mechanics. Fragment molecular orbital (FMO) theory is applied to clarify the recognition sites and to elucidate the specific interaction among them.

■ Process, case study

- 1) Theoretical analysis of the intermolecular interaction between protein and polysaccharide, which has inhibitory effect on enzymes
- 2) Three-dimensional structure and intermolecular interaction of glycolipids to form micro domain in the membrane
- 3) Quantum chemical description of the interaction between glycan ligand and Siglec-7 using ab initio FMO method (Figs.1&2)

■ Potential (applications, future goals)

Drug design
Development of new materials with novel functions

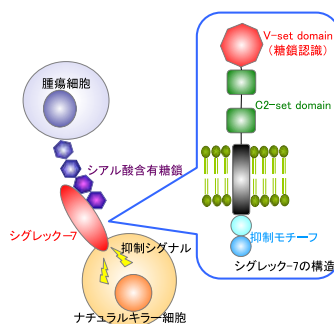


Fig. 1 Function of Siglec-7

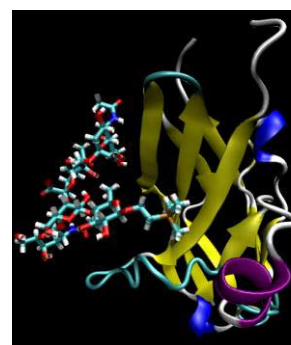


Fig.2 X-ray structure of the complex of Siglec-7(V-set domain) and glycan ligand (PDB ID:2HRL)

Intellectual properties (Patents, computer programs), productization, publications and social/industrial contributions

- 1) The 2nd Regional Meeting in Tokyo area of the Chemical Society of Japan, Aug. 2008, Kiryu, Japan (Invited talk)
- 2) The 71st Okazaki Conference, "New perspectives on molecular science of glycoconjugates" Nov. 2011, Okazaki, Japan (Invited talk)

Potential of social/industrial contribution

■ Joint research/ technical consulting

Joint projects with experimentalists in company and national institutes could be possible in biochemistry. Technical consulting to them could be provided.

■ knowledge sharing (open courses, workshops)

Introductory courses of computational chemistry with exercises will be available.

