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# Predicting the binding free energy of the inclusion process of cyclodextrin derivatives and small molecules by means of MM/3D-RISM method

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Cyclodextrin is a cyclic molecule formed by six to eight glucopyranose units and includes a small hydrophobic molecule into a cavity. Cyclodextrins are widely used as an additive of foods and drugs, because cyclodextrins have low toxicity and its physicochemical characteristics can be varied by the substitution of hydroxyl group. Although rational design of cyclodextrin derivatives are desired to develop a new pharmaceutical products based on inclusion ability of the cyclodextrins, designing of a functional Cyclodextrin derivative have been practiced in an empirical way so far. In this study, we tried to develop a procedure based on MM/3D-RISM method to screen drug candidate cyclodextrin derivative and assessed the capability of our procedure on the test system, for instance, 2-Hydroxypropyl-β-Cyclodextrin and small molecules. To accomplish this objective, we tried to get appropriate ensemble of the complex state and isolated state and after that, predict the binding free energy. Our procedure reproduce reasonable correlation between the experimental and calculated binding free energy and we conclude MM/3D-RISM method have an ability to distinguish the tightly bind compounds from the candidate molecules if we get an appropriate ensemble. Now we are applying this procedure to screen a functional cyclodextrin derivative. We are also trying to improve our procedure.

## Biography

Masatake Sugita has completed his PhD from Ritsumeikan University in 2014. From 2014-2015, he was a Postdoctoral Fellow at Ritsumeikan University and from 2015 to till date working as an Assistant Professor in the same university. During his PhD, he has worked with Professor Takeshi Kikuchi and tried to apply a course grained simulation for analyzing folding mechanism of proteins. Since 2014, he has been working with Professor Fumio Hirata and trying to apply 3D-RISM theory to the drug screening and to develop new methods based on 3D-RISM theory.

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