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## MOLECULAR RECOGNITION AS A CRUCIAL STEP IN ENZYMATIC REACTIONS: 3D-RISM/KH STUDY

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**M**olecular Recognition plays a crucial role in an enzymatic reaction, as is implied in the Michaelis-Menten equation for the reaction rate. In order for the reaction to take place, all the players, substrates, ions, and/or co-enzymes, should be bound at proper positions in the active site of protein. Such a process is governed essentially by two physicochemical properties, the free energy change associated with binding of the ligands to active sites, and the structural fluctuation of protein. It is now widely appreciated that water plays essential roles in the both properties, as is represented by the *desolvation free energy*. A great progress has been made in theories of the molecular recognition during the past decade that features use of statistical mechanics of liquids, referred to as 3D-RISM-KH. The theory enables us to find small ligands, such as water molecules, ions, and drug compounds, located at an active site of protein. It also provides the solvation thermodynamics at molecular level, such as the desolvation free energy, that is crucial for the evaluation of binding affinity of a ligand to protein. The theory has been applied successfully to variety processes of molecular recognition, including molecular channels, drug screening, and so on. Recently, we have applied the method to a restriction enzyme, *EcoRV*, which catalyzes the hydrolysis reaction of DNA. The method has been employed to locate the position of water molecules and magnesium ions at the active site, which play crucial roles in the enzymatic reaction.

**Biography**

F Hirata has completed his PhD in 1977 from Hokkaido University, and did his Postdoctoral studies at SUNY, UT and Rutgers in USA. He is a Professor Emeritus of IMS in Japan. He has published more than 250 papers in reputed journals.

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