Structures of Enzymes and Drug Discovery

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Many enzyme inhibitors have been widely used as therapeutics. Moreover, it is well known that they bind to their target enzymes in a three dimensional manner to exert their pharmacological effects. Thus, studies to understand 3D-structural characteristics of the binding between enzymes and chemicals are highly important for the drug discovery. Usually, 3D-structures of active sites of enzymes in the same family are highly similar since they have similar molecular function and substrates with a similar chemical type. Thus, if we know the common structural elements of the active site of some proteins in a family, we can design scaffolds that can bind to other proteins in this family. Namely, it is possible in drug discovery to target all the disease proteins of a family at the same time instead of targeting only one enzyme. Such studies are conceptually different from the existing structure-based-drug-discovery. Thus, in this presentation, we will discuss concepts, technologies and results of this new approach.