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The virtual screening based on molecular superposition

(Institute of Medicinal Molecular Design, Inc.) ○Harumi Nonaka, Nobuo Tomioka, Akiko Itai

We have newly developed a program system, KeyRecep, which provides almost all program functions for rational drug design when the 3-D structure of target protein is unknown. KeyRecep can automatically superpose several active molecules from literatures and HTS experiments, and then suggest new candidates of biologically-active compounds by virtual screening of 3-D structural databases of commercially-available compounds. One of the features of KeyRecep superposition is that molecules are superposed in terms of specific interaction partner sites in a common receptor presumed from each molecule, while generating all possible combinations of the interaction partner sites between molecules and generating all possible conformations for each molecule exhaustively. The usefulness of KeyRecep system was shown by an example of known inhibitors of cyclin-dependent kinase 2 (CDK2) .