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Ligand docking system in consideration of the induced-fit effect

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We developed ligand doking system in consideration of induced-fit. In this system, induced-fit might be reflected by “torsion angle restrained type MD” and “elastic collision energy evaluation function” based on the normal mode analysys of target protein. In this reseach, we could construct ligand/protein model with high accuracy by this system, while it was able to be shown that “torsion angle restrained type MD “ was uselful tool for induced-fit simulation. Forthermore, we peformed in silico screening using this system. Consequentry, it was able to search for unique ligand in ligand-database. Although many docking systems exist, this system is the new algorithm which used the normal mode analysys results.