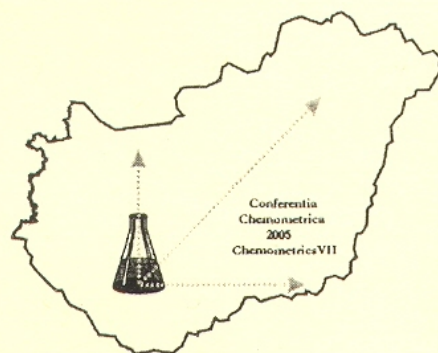


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REFINEMENT OF SMALL MOLECULES DOCKING / MAPPING ON BIOMOLECULES

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Small molecule mapping of biomolecules (peptides, proteins) support the determination of binding site [1-4]. The target molecule is generally rigid, so the effect of the change in side-chains conformations on the docking results can not be estimated. The induced fitting can be find only with a docking/molecular dynamics (MD) combined protocol. DDRP (Dynamically Defined Reaction Path) [5] calculations are used for the determination of the reaction path of conformation transition in small molecule [6]. A protocol was developed – docking/mapping of small ligand molecule on rigid target and DDRP/molecular mechanics (MM) refinement of the target-ligand complex. Ligand can move on the target molecule which is flexible, finding the best position in the complex. The protocol was applied and tested for some examples: small peptide-small molecule ligand complexes. The algorithm try to find the best position on the free energy surface of the association.

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