DYCOCA - Dynamic covalent capture: dynamic chemistry for biomolecular recognition and catalysis

Molecular recognition plays a fundamental role in nearly all chemical and biological processes. The objective of this research project is to develop new methodology for studying and utilizing the noncovalent recognition between two molecular entities, focusing on biomolecular receptors and catalysts. A dynamic covalent capture strategy is proposed, characterized by the following strongholds. The target itself self-selects the best component out of a combinatorial library. The approach has a very high sensitivity, because molecular recognition occurs intramolecularly, and is very flexible, which allows for an easy implementation in very diverse research areas simply by changing the target.
The dynamic covalent capture strategy is strongly embedded in the fields of supramolecular chemistry and (physical) organic chemistry. Nonetheless, the different work programmes strongly rely on the input from other areas, such as combinatorial chemistry, bioorganic chemistry, catalysis and computational chemistry, which renders the project highly interdisciplinary. Identified targets are new synthetic catalysts for the selective cleavage of biologically relevant compounds (D-Ala-D-Lac, cocaine and acetylcholine, and in a later stage peptides and DNA/RNA). Applicative work programmes are dedicated to the dynamic imprinting of monolayers on nanoparticles for multivalent recognition and cleavage of biologically relevant targets in vivo and to the development of new screening methodology for measuring chemical equilibria and, specifically, for the discovery of new HIV-1 fusion inhibitors.

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