Reg. No: 2016/21/B/ST5/00100; Principal Investigator: dr hab. Marcin Grzegorz Kwit

Design and construction of single molecules or supermolecules that resemble shape and/or the mechanism of action of the macroscopic objects is one of the most important goal of modern chemistry. These molecules or supramolecules bearing the name of molecular machines. Such molecular devices are able to perform mechanical work, collect or process information at the single molecule level. Depending on the role these molecules can be further divided to molecular motors (capable of performing one-way motion under the influence of an external stimulus), switches (able to switch from one stationary state to another under the influence of external stimuli), sensors, receptors or reporters (specifically responding to stimuli), gears (where there is a correlated motion between parts of the molecule), propellers (representing one-way synchronized movement). The same molecule (or molecular fragment) may be classified to different sub-classes depend on the function playing in a given system.

The fascinating stereochemistry of molecular propellers of the general formula YXAr₃ have attracted a lot of attention in the last two decades. Triphenylmethyl group (trityl, Tr) – the simplest C_3 -symmetrical propeller is commonly used in organic synthesis for protection OH and NH functionalities. Trityl cation was the first stable carbocation ever recognized. The shape and structural dynamic of the trityl group can be described as propeller or three-leaved clover (depending on the imagination of the person describing it). On the other hand, lowering the propeller molecular symmetry converts the propeller into a bevel gear.

This project is an attempt at the comprehensive approach to the efficient use of high structural diversity of triarylmethane derivatives in supramolecular chemistry and stereoselective synthesis. The aim of this project is to demonstrate the usability and versatility of triarylmethyl derivatives as stereochemical probes, molecular receptors, chiral selectors, ligands, catalysts, auxiliaries in stereoselective synthesis and inclusion-forming compounds.

We will demonstrate that selected triarylmethyl derivatives of cinchona alkaloids and artificial purpose-designed tripodal receptors can act as chiral selectors for small organic molecules, with particular emphasis on non-modified amino acids and chiral anions. The tripodal receptors of modular structure and great conformational freedom resemble sea anemones with reduced to three the number of arms.

Interest in mechanisms of chirality transfer is a result of our earlier work on a chromophoric probes, molecular propellers, molecular motors and catalytic asymmetric synthesis. It is interesting to explain how the chirality is transferred in systems in which the receptor is linked to a chiral substituent either non-covalently or through a fragment also capable to dynamically adapt to the chiral environment.

Cascade chirality induction, understood as sequential induction of helicity in molecular propeller and then in prochiral substrate, the possibility for "chirality remembering" by the catalysts generated from inherently chiral triarylmethane derivatives as well as the possibility of absolute asymmetric synthesis were never a subject of in depth studies.

The ability to molecular recognition by receptor systems is the decisive factor for the biological activity of a chemical compound, including diverse biological activity of enantiomers. One, well known, example is thalidomide, where one of the enantiomers showed teratogenic properties. Transfer (or induction) of chirality is the concept covering both the process of the transfer of information about the three-dimensional structure to the substrate molecule in case of synthesis, mainly biosynthesis, and process of adaptation of conformationally labile environment to chiral inductor.

In addition, we want to point that mutual cooperation on two levels: experimental and theoretical will lead to a successful collaboration of experts from both areas. Thus, the mutual experimental and theoretical approach to study the mechanism of induction of chirality, the way in which large molecules can create superstructures and recognition mechanism of polar molecules, mainly amino acids by receptor systems will provide an insight into the mechanism of certain phenomena of fundamental importance in chemistry and biochemistry.