Chirality sensing by stereodynamic chromophoric probes

The word *chirality*, originating from Greek word χειρ – "hand", is the property of the object, making it undistinguishable from its mirror image. Chirality of chemical compounds plays the key role in numerous biologically active covalently and non-covalently bound systems, like: enzymes, DNA, drugs etc. The chirality transfer (or chirality sensing) is in fact the transfer of information about three-dimensional structure from one compound to another. This phenomenon may be successfully studied utilizing stereodynamic chromophoric probes. Such probes (reporters) are conformationally labile and they are able to adapt their conformation to chiral environment. Thus, as a result of chirality transfer from chiral non-racemic inductor molecule to dynamic reporter molecule the whole covalently or non-covalently bound system becomes optically active in circular dichroism spectroscopy (Figure 1).

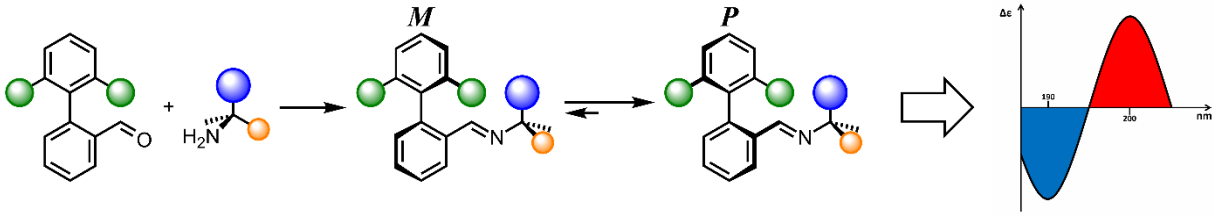

Figure 1. The chirality transfer within covalently bound inductor-reporter system.

The aim of the project is to develop novel bi- and triaryl-based dynamic probes and reveal their application in studies of the chirality transfer phenomenon within covalently bound inductor-reporter systems. To achieve the main tasks of the project, we will synthesize new chromophoric probes using well-known and/or modified methodologies. Subsequently, we are going to test our probes using numerous inductor molecules of different constitution and sterical properties. We expect to observe characteristic bisigned Cotton effects in electric circular dichroism spectra (ECD) induced by adaptation of reporter molecule to chiral inductor molecule. All experimental data will be supported by quantum-chemical calculations at DFT level of theory.

Our research will result in deep understanding of chirality transfer within inductor-reporter systems utilizing yet unknown bi- and triaryl-based probes. Moreover, we will establish mechanism of action of newly developed probes and provide their application for stereochemical assignments.