Chiral Naphthalenediimides: From Synthesis to Applications

Recently, we have synthesized chiral naphthalenediimides (NDI), based on which we have constructed the enantioselective sensors for teratogenic (*S*)- and terpeutic (*R*)-*Thalidomide* in blood plasma. The atropisomeric NDI derivatives synthesized by us, which exhibited intramolecular charge-transfer bonding, enabled us to observe the induced chirality phenomenon in an achiral solvent which was only rarely observed in the Raman Optical Activity (ROA) spectra. For the first time in Poland, for chiral NDI derivatives, we performed the spectroelectrochemical electronic circular dichroism (SEC ECD) studies. They allowed us to develop the interpretation of electrochemical processes in chiral compounds, and supplement the conclusions from the UV-Vis SEC and EPR-SEC measurements. Our investigations were supported by molecular spectroscopy, X-ray structure determination and quantum-chemical calculations. In the new project, we intend to break new barriers.

We have three main goals of the project:

(**1**) To construct new enantioselective electrochemical sensors for chiral drugs.
(**2**) To explain the role of the range of the resonance energy transfer (RET) in the ROA-observed induced chirality.
(**3**) To perform the Circular Magnetic Dichroism spectroelectrochemical (MCD SEC) measurements which have been reported only few times in the world literature and to juxtapose them with the SEC ECD, UV-Vis and EPR measurements of the chiral NDI derivatives.

To achieve these goals:

(**1**) We will synthesize new chiral NDI derivatives [UPH Siedlce], which, due to their semiconductivity (*n*, *p*, or ambipolar type), will find further applications as electrochemical sensors.
(**2**) We will construct new enantioselective electrochemical sensors for chiral drugs or bioactive substances [UW].
(**3**) We will perform comprehensive spectroscopic measurements (ECD, VCD, MCD) [IChTJ], ROA [UJ], NMR [UPH Siedlce], X-ray structure determination [IChTJ], electrochemical [PŚ Gliwice] and quantum-chemical [IChTJ], [CMDiK PAN] characterizing new chiral NDIs and their intermolecular interactions [IChTJ, CMDiK PAN] with chiral sensor targets [UW, MUW].
(**4**) We will measure the ROA spectra of a series of synthesized chiral naphthalenediimides [UJ] to verify various hypotheses about the type and range of the resonance energy transfer accompanying the induced chirality phenomenon in ROA spectroscopy [UJ, IChTJ].
(**5**) We will measure the MCD SEC characteristics of a series of model compounds and synthesized chiral naphthalenediimides and compare them with results of the SEC ECD, UV-Vis and EPR measurements [PŚ Gliwice, IChTJ].

The expected effect of the project:

(**1**) We will construct new sensors of chiral drugs/biomolecules to control the level of therapeutic and/or toxic substances in body fluids.
(**2**) We will fully understand the phenomenon of chiral induction from a dissolved chiral molecule to achiral solvent observed in the ROA spectroscopy, and we will explain the role of the short-, medium- and long-range RET.
(**3**) We will obtain the MCD spectroelectrochemical characteristics which will provide information complementary to those obtained from the ECD SEC, UV-Vis SEC and EPR SEC measurements.