Reg. No: 2015/18/M/NZ2/00423; Principal Investigator: mgr Stefan Mateusz Mordalski

The aim of the project is to develop a method for searching novel bioactive compounds based on fragments extracted from crystal structures. Basing on the assumption, that similar fragments interact with the same amino acids in similar manner, we create a set of those residues with interacting fragments of ligands. Superposing them onto corresponding amino acids in different receptor we can deduct how should their active compounds be composed (in general).

We will use this method to search for active structures for orphan receptors (for which we do not know neither physiological function nor endogenous ligands) from G protein coupled receptors family (GPCRs). GPCRs are membrane proteins responsible for communication with the environment, including sight, taste, smell, or perception of pain.

Together with our Partners from University of Copenhagen we want to discover ligands for twenty orphan receptors, which will push our understanding of GPCRs further, and so our knowledge about functioning of human organism.