Chemical catalysis is the increase in the rate of a chemical reaction due to the participation of an additional substance called a catalyst. The use of a catalyst yields faster reactions and/or lowers the temperature needed for the reaction to occur. As a result, catalytic reactions are preferred in environmentally friendly green chemistry due to the reduced amount of waste generated and power and/or time consumed. Nowadays, the production of most industrially important chemicals involves catalysis and similarly, most biochemically significant processes are also catalyzed. From the chemical point of view, catalyst lowers the free energy barrier of the reaction, meaning that less free energy is required for the substrate to reach the transition state. Catalyzed reactions have a lower activation energy (rate-limiting free energy of activation) than the corresponding non-catalyzed reaction, resulting in a higher reaction rate at the same temperature and for the same reactant concentrations. In most cases, the detailed mechanisms of action of catalysts are complex and catalysis is often a multi-step process. Clearly there are no universal catalysts, but each chemical reaction can be catalyzed by a unique catalyst.

The main goal of this research project is to obtain new knowledge about rational design of new metathesis catalysts. This reaction has been named as "emerging green technology" by the Royal Academy of Science during the 2005 Nobel Prize award and was quickly adopted by research groups as a basic strategy for the synthesis of carbon-carbon bonds. The ability of this method for the selective substitution of atoms between two molecules allows the generation of chemical systems with the desired properties. This is particularly important for complex compounds such as natural compounds and new heterocyclic compounds and macrocyclic compounds. The synthesis of numerous complex organic molecules and materials, such as pharmaceuticals, polymers, agrochemicals, and natural products, has been facilitated by well-defined catalysts. The use of cross-metathesis, ring-opening and ring-closing metathesis, and acyclic diene metathesis polymerization allows the synthesis of compounds via simpler pathways and starting from cheaper raw materials. Currently, there are several different families of catalysts for this reaction known which are based on ruthenium, molybdenum or tungsten compounds. Unfortunately, there are some demanding catalytic reactions, particularly in the chemistry of polymers and pharmaceuticals for which commonly-used catalysts fail or give very poor results. The purpose of this project is also to find such new catalysts.