

### **Project 3.4 Controlling regioselectivity of catalytic transfer hydrofunctionalization reactions by non-covalent interactions**

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#### **Background:**

In recent years, one of the revolutionary concepts, namely shuttle catalysis has been introduced and explored. This strategy enables the formal transfer of small molecules (e.g., HCN, H<sub>2</sub>/CO, HBr) between donor and acceptor molecules and thus can be utilized as a powerful synthetic tool for the functionalization of unsaturated molecules. The process can be directed using simple thermodynamic driving forces (e.g. gas evolution). Therefore, the hydrofunctionalizations of unsaturated molecules can be efficiently carried out using a stoichiometric amount of sacrificial functional group donors. Recently developed transition metal based catalytic systems allow for the transfer of functional groups of great synthetic importance such as nitrile, formyl, chlorocarbonyl or halides. Notably, transfer hydrofunctionalizations of alkenes (and alkynes) can be achieved with cheap, non-toxic, and easy to handle sacrificial donors, eliminating the necessity of direct utilization of toxic and hazardous gases (e.g., HCN, H<sub>2</sub>/CO) or specialized equipment.

The shuttle hydrofunctionalizations would represent a widely applicable powerful tool for organic synthesis. However, when unsymmetrical alkenes (or alkynes) are used in such transformations, mixtures of regioisomers are formed, irrespective of the type of transferred functional groups. This general limitation of shuttle hydrofunctionalization hampers the synthetic utility of the strategy, unless control of regioselectivity is achieved.

#### **Aim:**

The goal of the project is to explore controlling the regioselectivity of transfer hydrofunctionalizations of alkenes and alkynes by non-covalent interactions. We postulate that new classes of precisely designed supramolecular catalysts will selectively promote the formation of one target regioisomer. Therefore, the synthesis of such catalysts will deliver the tools for efficient control of regioselectivity of transfer hydrofunctionalizations.

#### **Requirements:**

- hold an MSc (or equivalent) in Chemistry,
- have an excellent general knowledge of chemistry. Good knowledge of transition metal-based catalysis will be additional asset,
- have some practical experience in synthetic organic chemistry,
- communicate well in English in writing and in oral presentations,
- be a good team player,
- be willing to play a role in keeping the laboratory running by assuming a share of group responsibilities,
- be highly motivated and have a strong commitment to research.