

FROM SIMPLICITY TO COMPLEXITY – GENERATION OF A DYNAMIC NETWORK OF MULTI-CATALYTIC PROCESSES CONTROLLED BY Pd/Ru CATALYSTS AND REACTION CONDITIONS

From biological systems, we recognize the fundamental role of complex reaction networks in orchestrating dynamic interactions and multi-stage transformations, ensuring the efficient transfer of mass, energy, and information. The high precision and efficiency of natural systems arise from their highly ordered sequences of reactions, which remain unparalleled by artificial counterparts. Despite advancements in the construction of artificial complex systems in the past few years, replicating the level of sophistication observed in biological networks remains a significant challenge. Synthetic systems often lack the adaptive and dynamic control mechanisms that characterize natural enzymatic cascades. The development of novel methodologies capable of integrating multiple catalytic events within interconnected reaction networks can therefore be a critical step toward bridging this gap.

The primary objective of this project is to establish strategies that enable the control and management of the complexity of synthetic systems composed of simple molecular components. Through the creation of dynamic and highly flexible networks of chemical reactions, this approach will allow for the selective formation of desired outcomes. Despite the inherent complexity of such systems, they will be presented as valuable tools in modern organic synthesis and catalysis.

Specifically, this project will showcase the strategic design of a network of multi-stage processes using a series of simple starting materials, namely alcohols and aryl halides, with performance governed by a selection of [Ru] and [Pd] catalysts, as well as simple physical or chemical triggers. Along with the development of new pathways, careful analysis of the topology will enable the identification of critical nodes within the artificial system, which operates as an integrated network of distinct reactions. Control over catalytic activities, which enhances certain reaction sequences while inhibiting others, will guide specific synthetic routes (Fig. 1). As a result, it will enable the preferential synthesis of a series of specific products and facilitate their interconversions.

The project aims to merge systems chemistry with aspects of organic chemistry and modern catalysis toward the improved efficiency and sustainable synthesis of fine chemicals and materials. By introducing artificial metabolism-like networks, it seeks to address challenges in organic synthesis that traditional methods cannot easily overcome. These synthetic analogues offer more efficient and flexible approaches to chemical synthesis, improving reaction yields, reducing the need for excess reagents, and minimizing resource and energy consumption, as well as waste generation. This strategy has the potential to revolutionize the synthesis of both simple compounds and advanced materials, providing relatively simple and cost-effective solutions. Additionally, the presented strategy could inspire researchers by opening new avenues for the development of innovative synthetic approaches to various classes of organic compounds.

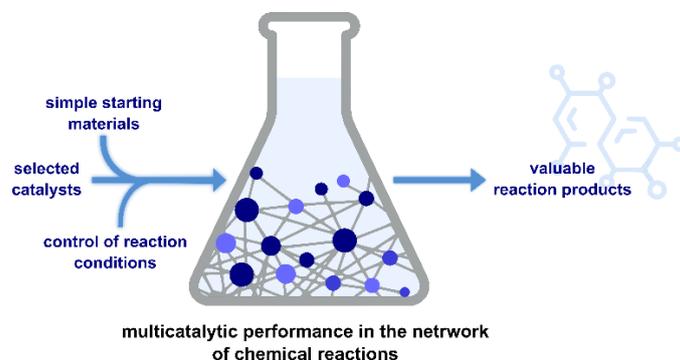


Figure 1. Schematic representation of the project idea – generation of a complex network of chemical reactions using simple starting materials and selected catalysts under strict control of reaction conditions, leading to a range of diverse reaction products.