In search of new metalloporphyrinoid catalysts for functionalization of C(sp^3)–H bonds

Catalysis plays an important role in organic chemistry, allowing usually for obtaining desired yet complicated compounds under mild conditions and without multi-step synthesis. This is crucial for the economy and eco-friendliness of the production of a wide range of chemicals, leading to new materials or medicines. Due to the ubiquity of alkane motif in natural products and common synthetic blocks the possibility of direct functionalization of molecules containing multiple similar C–H bonds would be very useful. It would allow for a facile modification of many existing drugs or other biologically active compounds as well as for potentially creating new active pharmaceutical ingredients. Because of fact that many of them also contain amine and alcohol motifs, our investigations will mainly focus on increasing the selectivity of amination and hydroxylation of C–H bond.

The selective and direct functionalization of C–H bonds represents a powerful approach to the synthesis and modification of nontrivial complex molecules. Moreover, because organic compounds typically contain multiple similar C–H bonds, one of the major challenges is to control the site-selectivity of the reaction.

To achieve this goal we need to find the right catalyst. Based on previous research, we will modify metalloporphyrin catalysts, which work well (but not selectively) in these reactions. Such macrocyclic compounds occur in nature, enabling the functioning of many living organisms. One of the most common derivatives of porphyrin complexes is chlorophyll (containing magnesium), heme (iron), and vitamin B12 (cobalt).

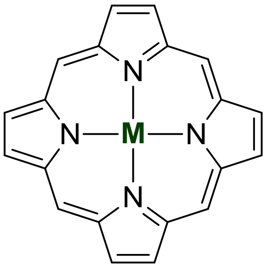

Figure 1. Metalloporphyrin.

The expected effect is the creation of a new class of catalysts which - due to their structure and properties - can help solve the problem of selectivity by proper arrangement of substrates during the reaction, which will enable activation of previously unreactive sites in molecules.

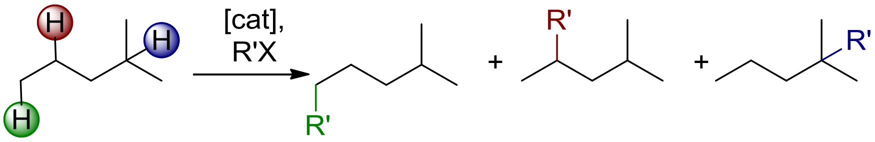

Figure 2. Problem with selectivity in many C-H bond functionalization reactions.