DEGRADATION OF HAZARDOUS CHEMICAL COMPOUNDS INTO VALUABLE BUILDING BLOCKS: FROM COMPUTER-PLANNED ROUTES TO EXPERIMENTAL VALIDATION

Despite of innumerable benefits to the society – in the form of live-saving drugs, fertilizers, useful materials, etc. – chemistry is often perceived as a global polluter responsible for the accumulation of hazardous wastes in the soil and in the oceans. Even though it is not the chemists who are directly responsible, chemistry as a discipline should align better with the policies to strictly control, recycle, and reuse of industrial chemical waste. This project aims to foster such alignment by using modern chemical computing to design new synthetic routes by which chemical wastes are degraded into non-toxic and valuable building blocks. Proposed research aims to automate and streamline the synthetic design for the so-called circular chemistry.

Until recently, the use of computer-assisted synthesis has been limited to rather simple target molecules, this limitation has been overcome only this year with the publication of our papers demonstrating experimental validation of computer-designed syntheses leading to various complex natural products and key molecules involved in the formation of life on primitive Earth.

In the current project, I will use some of these game-changing theoretical tools to enable discovery of new degradation pathways converting harmful substances into structurally smaller yet chemically useful end-products. Specifically, the software I will use will rapidly generate large networks of synthetic possibilities encompassing all possible plans to degrade a substance of interest (Figure 1). Reaction rules used to generate the networks will encompass both chemical and biocatalytic reactions, thereby allowing the computer to plan more environmentally friendly degradation routes. Appropriate scoring functions and AI-based filters will identify the most economical pathways not involving toxic intermediates. These routes will be then subjected to experimental validation. Summarizing, I aim to computer-design and then realize in the laboratory degradation routes commencing with multiple dyes, toxins, pesticides, or biomass-derived compounds. Experimental confirmation and public dissemination of these plans will demonstrate the usefulness of my approach and will be a valuable addition to the current repertoire of waste-degradation technologies.

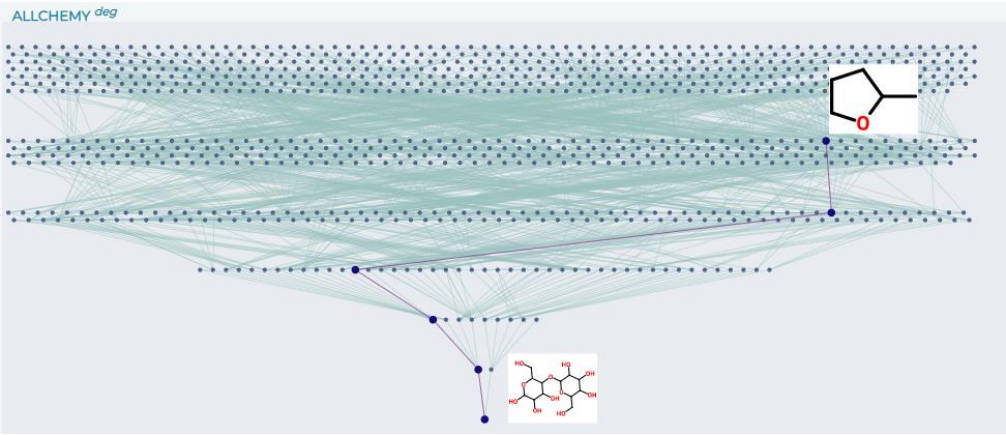

Figure 1. Example of a degradation “tree” illustrating the multitude of possibilities.