

Green Chemistry TechHub – A Trilateral Doctoral Program

Position 6:

Sustainable approaches to isotopic labelling: application to the Biotin C-H postulate



In collaboration with Boehringer Ingelheim, this project aims to develop sustainable strategies for targeted isotopic labeling as well as for the degradation of pharmaceutical residues in the environment. A starting point is a novel approach to the deuteration of carbonyl compounds at the α -position, based on a retro-En reaction triggered by the addition of [d6]DMSO to activated amides. Mechanistic investigations and DFT analyses have shown that this process tolerates a broad range of functional groups and tertiary amides, consistently delivers high yields, and achieves a high degree of deuterium incorporation. Successful demonstration of chemoselective bis-deuteration further highlights the potential of this method for mechanistic studies and applications in the life sciences.

In parallel, the project pursues the development of photocleavable bioisosteres that can be incorporated into active pharmaceutical ingredients without compromising their therapeutic efficacy. After administration, many drugs are not fully metabolized and are excreted into wastewater, where they accumulate and pose ecological and human health risks. By incorporating such bioisosteres, drug residues can be made selectively degradable: upon exposure to visible light — for example, sunlight — the bioisosteres undergo cleavage, causing the parent drug to break down into biologically inactive fragments.

The combination of these concepts opens new opportunities both for the development of isotopically labeled biomolecules for high-resolution spectroscopic analysis of molecular interactions and for the design of environmentally friendly pharmaceuticals with controlled degradability.

Host Institution:

University of Vienna

Industrial Partner:

Boehringer Ingelheim


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