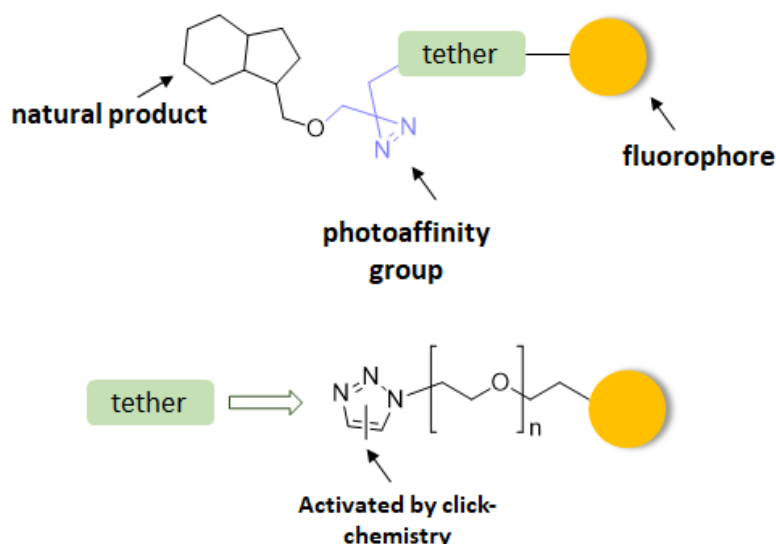# A GENERIC APPROACH FOR TARGET IDENTIFICATION OF NATURAL PRODUCTS EMPLOYING A TANDEM PHOTOAFFINITY-CLICKING STRATEGY

Project related Figures (e.g. photo, schematic, results). For example:

Supervisory Team[1]

Primary Supervisor: *Marko D. Mihovilovic, Institute of Applied Synthetic chemistry, TUW*

TU Wien project partners: *Ruth Birner-Grünberger, Institute of Chemical Technology and Analytics, TUW; Peter Ertl, Institute of Applied Synthetic chemistry, TUW*

External academic partners: *Verena Dirsch, Department of Pharmaceutical Chemistry, University of Vienna; Hermann Stuppner, Department of Pharmacognosy, University of Innsbruck*

External industry partners: *Name and affiliation*

Project Description

This PhD project focuses on the design and synthesis of a platform of pharmacological tool compounds for the identification of biological targets of natural compounds. This involves the incorporation of structural motifs into bioactive natural products bearing multi-functionalizable handles for photoaffinity tagging, photo-switching of biological effects, and

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[1] The Early Stage Researchers (ESRs) will be accompanied during their thesis by an individual "Thesis Advisory Committee" (TAC), which will guide the ESR through the graduate studies. The TAC will consist of the thesis primary supervisor, and two additional members of the Supervisory Team selected by the ESR.

click chemistry to incorporate reporter systems. Within a unified approach, multiple tasks in target identification shall become addressable by installation of functional handles for various purposes. Current natural product scaffolds of interest belong to the class of (neo)lignans; based on already established synthetic strategies towards bioactive molecules, incorporation of the functional handles will be conducted by de-novo synthesis as well as by late-stage functionalization of natural product isolates. Natural product related chemistry will involve advanced concepts of stereoselective synthesis in combination with metal-assisted strategies.

Key Goals and Tasks

The primary aim of this PhD thesis involves the synthetic implementation of the multi-functional platform exemplified on currently worked on natural compound targets in the area of lignans with anti-inflammatory activity. In addition, stereoselective synthetic access to natural product molecules of interest shall be established and optimized in order to also enable structure-activity profiling and scaffold development. Target identification will involve both MS-based approaches as well as computational chemistry

Project-specific Requirements

- Completed master studies in (synthetic) chemistry
- Knowledge on medicinal chemistry, pharmacology, analytical chemistry
- Experience and skills in (asymmetric) organic synthesis, compound purification and characterization (esp. involving NMR and MS)
- Interest in working with biologists and/or pharmacologists
- Enthusiasm for multi-disciplinary research and experimental sciences
- Affinity for automation assisted synthesis
- Willingness to travel to project meetings and scientific conferences
- Excellent English language skills in scientific field
- Personal skills: independent work-style, creativity towards novel ideas, capable to work with multi-disciplinary teams