

Supervisor's contact details

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Title of the project

Development of an efficient platform for macrocycle drug discovery

MSCA-PF Research Panel

- Chemistry (CHE)
- Social Sciences and Humanities (SOC)
- Economic Sciences (ECO)
- Information Science and Engineering (ENG)
- Environment and Geosciences (ENV)
- Life Sciences (LIF)
- Mathematics (MAT)
- Physics (PHY)

Description of the project

All the lowest-hanging "easy drugs" have been found. Yet, there are many diseases without any treatment options. For example, different cancer types and neurological disorders widely lack efficient treatment. This is particularly striking when the biological processes involved in these diseases are based on protein-protein interactions (PPIs). Because PPI surfaces are flat and subjected to significant conformational changes, they have been considered "non-druggable". Thus, the traditional drug discovery approaches fail to produce new drugs efficiently. Our extensive experience discovering PPI modulators drove our general understanding of how PPIs can be rationally targeted. This knowledge, jointly with novel computational tools, combined with synthesis, in vitro measurements, and pharmacokinetics, will now be turned into a systematic discovery of a new type of PPI modulators that have the potential to change the whole field of drug discovery, leading to novel drugs for untreatable diseases. Accordingly, we seek an innovative computational chemist (or similar) to develop and apply novel software tools for molecular discovery. The suitable postdoctoral scientist would have good knowledge of computer-aided drug discovery and machine learning methods and preferably software development skills.

Research objectives or research questions of the project

1. Development and automatization of a novel strategy for the discovery of macrocyclic ligands
2. Identification and development of novel macrocyclic ligands for selected drug discovery targets.