Position in Artificial Intelligence for Drug Discovery at Leiden University

Chair: Artificial Intelligence in Chemistry

**Leiden Academic Centre for Drug Research (LACDR) and
Leiden Institute of Chemistry (LIC), Universiteit Leiden**

1. Description of the Research Area of the Chair

Drug discovery is still largely an empirical process, which is challenging, time consuming, and labor consuming. The design, synthesis, and evaluation of new molecules that modulate protein function in aberrant signaling processes in living systems is of key importance for drug discovery and chemical biology research. Chemical space is vast and can only be explored to a small extent with experimental methods to find suitable hits for drug discovery programs. Artificial Intelligence methods can help searching this vast space intelligently. Once a suitable hit has been identified, a multi-parameter optimization of chemical structures is needed to balance the activity, selectivity, solubility and pharmacokinetic parameters of a drug candidate. This process requires the understanding of high dimensional datasets. Artificial Intelligence (AI) and advanced machine learning models promise to revolutionize the field of drug discovery and chemical biology. Computational chemistry methods are used to analyze and predict a wide range of physicochemical properties and biological activities for compounds by utilizing large high-dimensional datasets generated by high throughput screening, and advanced analytical technologies (e.g. chemical proteomics).

Challenges

Understanding the available high-dimensional datasets and translating these findings to concrete applications in the drug discovery process is challenging. Implementation of artificial intelligence methods in the Leiden drug discovery & chemical biology research and education necessitates the involvement of chemical biologists/medicinal chemists experienced in artificial intelligence for chemistry (or vice versa). Findings should be understandable and usable in existing lab workflows. Hence, a close collaboration with chemical and biological experts in the faculty of science is essential. We expect a wide range of approaches from the field of artificial intelligence to be contributing to the expected revolution in drug discovery and chemical biology.

Goal

The main goal of the chair in Artificial Intelligence and Chemistry is to develop and apply AI methods for chemical biology and drug discovery, specifically in multi-objective optimization, dimensionality reduction, and clustering. The faculty aims to strengthen its position in AI by including further areas including, but not limited to, surrogate modeling, evolutionary computation, graph modeling, decision making, text analytics, predictive analytics, (automatic) machine learning, and high performance computing for large-scale data analytics.

2. Profile of the Full Professor "High-dimensional data analytics"

The Leiden Institute of Chemistry (LIC) and Leiden Academic Center for Drug Research (LACDR) aim to hire a chemical biologist/medicinal chemist pursuing research questions in the field of drug discovery, for example, relating to receptors, enzymes, protein-protein interactions or protein synthesis & folding. The professor shall have:

- experience with computational chemistry approaches from the field of AI (e.g. graph modeling, clustering, network analysis, and machine learning)
- a background in organic chemistry / chemical biology / medicinal chemistry
- a collaborative mindset and an affinity with multidisciplinary research
- the ability to attract prestigious national and international personal grants
- the ability to initiate international research programs and consortia
- experience in establishing research programs and supervising and coordinating scientific research
- the ability to supervise and inspire undergraduate, graduate, and PhD students and researchers
- excellent communication and social skills
- significant teaching experience at the undergraduate and graduate level and the willingness to contribute the LIC and LACDR bachelor programmes "Molecular Science & Technology", "Life Science & Technology", "BioPharmaceutical Sciences" and the master programmes "Chemistry", "Life Science & Technology", and "BioPharmaceutical Sciences"

3. Embedding

SAILS

At the level of Leiden University, the chair will contribute to the recently started initiative on Social Science, Humanities, Law, AI and Life Sciences ("SAILS"), in which multidisciplinary research across different faculties, with AI as a core technology, is conducted. SAILS provides ample opportunities for multidisciplinary collaborations, with application domains for machine learning where new approaches for understanding the decision making in chemistry will be very welcome.

This position will form a bridge between the institutes LIC and LACDR. The chair will interact with several existing groups that focus on Computational Drug Discovery, Molecular Physiology, Medicinal Chemistry, and Bio-Organic Synthesis.

The professor will participate in and initiate research projects of LIC and LACDR and will supervise PhD students.

Facilities

The institutes house state-of-the-art organic synthesis, biochemical, and molecular biology laboratories supported by dedicated technicians. Chemical proteomics, lipidomics, and metabolomics equipment is available. LACDR has made computational approaches a focus point, as such LACDR has established an extended computational chemistry facility. This facility includes both CPU and GPU compute servers, extended storage capabilities, and access to state of the art software. Furthermore, LACDR will hire a dedicated computational technician as of 2020. Finally, Leiden University is establishing a computer cluster "Computational Facility for Excellent Research" scheduled to go online 2nd half of 2019.