Bachelor / Master Thesis Proposal

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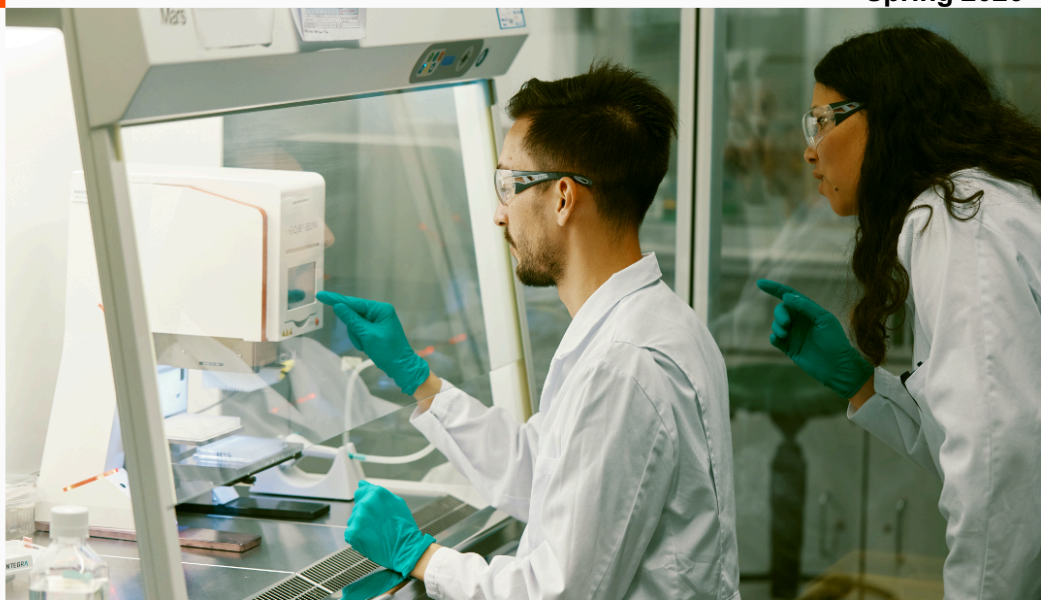

Explainable AI for Molecules to Understand Drivers of Property Predictions

Machine learning (ML) models are widely used in drug discovery to predict key properties of molecules, such as how quickly a compound is eliminated from the body. These predictions help scientists decide which molecules should be tested experimentally. However, many ML models act as “black boxes” and the reasons why a molecule is predicted to have favorable or unfavorable properties are often unclear.

This project focuses on applying explainable artificial intelligence (XAI) methods to better understand how ML models relate molecular structure to property predictions. By analyzing the patterns learned by these ML models, one could identify which parts of a molecule influence predicted properties and make hypothesis for compound design.

The student will investigate state-of-the-art XAI techniques for molecular ML models, assess their robustness, and validate XAI results in collaboration with chemists and pharmacokinetic experts. The project offers hands-on experience at the interface of AI/ML, chemistry and drug discovery and it is recommended for BSc or MSc students in a quantitative field or life sciences, preferably with multidisciplinary background (chemoinformatics, bioinformatics, biomedical data science). Understanding of ML methods and Python programming are required.

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Desired project start: Q2 2026

Project duration: approx. 8 months

This proposal does not entail any future financial compensation as it is part of a BSc/MSc framework program to foster educational collaboration in accordance with specific terms and regulations of both Novartis and its academic partners.