**Machine learning of energy barriers for reaction network discovery of drug-like molecules**

**Supervisors:** **Primary: Prof. Reinhard Maurer**
**Prof. Scott Habershon**

Why does it take so long to develop a new drug and why do 90% of drugs fail late in clinical trials? Well, it takes time to identify a viable pharmaceutically active molecule and to find a scalable chemical synthesis pathway to make it, but this isn't really the critical problem. The problem is connected to the same reason why many drugs have short shelf lives and strict storage conditions. My name is Reinhard Maurer and I'm supervising a PhD project as part of HetSys CDT that aims to change how we simulate chemical reaction kinetics for drug-like molecules.

The problem is put simply, many large molecules may undergo unforeseen side reactions. Take the drug Agomelatin, which is a common antidepressant. It turns out that many possible impurities can be introduced through unforeseen side reactions that occur during the synthesis or after when the drug is exposed to heat or light.

Often these impurities turn out to cause side effects or worse. Not only are we bad at predicting which possible side reactions can occur, we also can't predict the yield, so how much of that side product is created. This PhD project aims to address this capability gap with multi-scale simulation methods and machine learning techniques.

We want to construct and simulate complex chemical reaction networks that include all possible relevant intermediates and side reactions, allowing us to predict which side products are produced, under which conditions and at which concentration. To achieve this, we will use machine learning methods and quantum chemistry calculations to predict thousands of relevant (1:45) reaction barriers that define the rates of individual chemical reaction steps. This project is co-funded by a leading pharmaceutical company and will provide you with training in scientific machine learning and chemical reaction discovery.

You'll be mentored by a team of experts with complementary expertise and you'll get to work with real-world data and business relevant problems. To top it off, the project will feature a six-month industrial placement at the company. If this sounds interesting to you, please get in touch.

Thank you.