PCL3107H – Foundations of Artificial Intelligence for Drug Development Scientists

Topic	Artificial Intelligence Foundations Applied to Drug Development
Prerequisite	N/A. Note: this course is a prerequisite for PCL3108H- Launchpad for Collaborative Projects in Artificial Intelligence and Drug Development
Term	Winter term, first session: Jan - Feb (6 weeks)
Coordinator(s)	Rebecca Laposa, Martin Beaulieu
Day & Time	TBD. 2 x 1h/week
Location	TBD
Course Description	The course is the first of two modules that will allow students from life sciences graduate programs to acquire foundational knowledge for the development and critical evaluation of artificial intelligence (AI) approaches in drug development. The course will introduce students to fundamental concepts in AI and machine learning and demonstrate their application to drug development. Students will examine foundational papers at the intersection of AI and drug development in depth to understand the conceptual framework of the AI models that underlie the findings. The scope of the course includes structural biology, chemistry of druglike molecules, translational research and clinical pharmacology. With facilitation, students will conduct hands-on active learning assignments using simplified datasets to solidify their understanding of AI approaches. To develop collaborative multidisciplinary skills, life science students will meet with Computer Science students and design drug development research questions that can be answered by AI approaches.
Learning Outcomes	By the end of the course, students should be able to: • Have a critical understanding of the foundational AI approaches underlying several high-impact scientific papers at the intersection of AI and drug development • Appreciate the potential and limits of the different AI approaches • Formulate specific research questions in the realm of drug development that could be addressed by AI approaches • Design the key elements and data architecture of a research project that is compatible with AI approaches • Appreciate the perspectives of AI scientists to be able to work productively with AI collaborators

Evaluation	• Participation: 20% • Hands-on Dataset Assignments: 3 X 10% • Research Design Assignment (Letter of Intent): 30% • Oral presentation of Research Design: 10%

Course Plan:

Date	Instructors	Session Topics (1 hr/session)
Jan	Chris Maddison, Martin Beaulieu, Rebecca Laposa	• Setting the stage and context: Overview of the current state of artificial intelligence in drug development, and a vision of what is possible.
Jan	Chris Maddison	• AI Foundations 1: **Prediction**. Understand the underlying models behind predictions of interactions between proteins and chemicals
Jan	Chris Maddison and TAs	• AI Foundations 1: **Prediction.** • Hands-on *Dataset Assignment 1* to familiarize yourself with what data scientists do in a prediction model
Jan	Maddison/Beaulieu/Laposa	• Discussion of high-impact paper focused on the use of **Prediction** in drug development • Meeting 1 with Computer Science students
Jan	Chris Maddison	• AI Foundations 2: **Generative Modeling**. Understand the approaches of models that generate structural information
Jan	Chris Maddison and TAs	• AI Foundations 2: **Generative Modeling.** • Hands-on *Dataset Assignment 2* to familiarize yourself with what data scientists do in a generative model
Jan	Maddison/Beaulieu/Laposa	• Discussion of high-impact paper focused on the use of **Generative Modeling** in drug development • Meeting 2 with Computer Science students
Jan	Chris Maddison	• AI Foundations 3: **Large Language Models**. Understand the approaches of large language models (LLMs)
Feb	Chris Maddison and TAs	• AI Foundations 3: **Large Language Models.** • Hands-on *Dataset Assignment 3* to familiarize yourself with what data scientists do in a large language model

Feb	Maddison/Beaulieu/Laposa	• Discussion of high-impact paper focused on the use of **Large Language Models** in drug development • Meeting 3 with Computer Science Students
Feb	Chris Maddison and TAs	• Designing AI-addressable research questions using AI-relevant datasets: understanding data architecture and constraints • Consolidate Research Design Plans
Feb	Maddison/Beaulieu/Laposa	• *Oral Presentations of Research Designs* • *with Computer Science Students Attending* • *Submit Letter of Intent*