Artificial Intelligence in Drug Discovery (3FF036), 7.5 hp - a new introductory course at the Faculty of Pharmacy

UPPSALA UNIVERSITET

See more info and syllabus at Uppsala University course-portal https://www.uu.se/en/admissions/freestanding-courses/course-syllabus/?kKod=3FF036 - Course administrators: Jonathan Alvarsson, Henry Wittler, Ola Spjuth, et al.

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This course serves as an introduction to the use of artificial intelligence (AI) and machine learning (ML) in drug discovery. Including basic concepts for AI / ML, with commonly used methods for tabular data and different types of deep neural networks. Emphasizing the vast extent and importance of data for modelling. Considering various application areas in drug development where AI can be used, such as ligand-based methods for virtual screening and prediction of properties based on chemical structure, structure-based methods, image-based methods, *de novo* drug design and network / graph-based methods.

The primary focus of course is on making predictions and interpreting the results, but also including the steps for training and validation of AI / ML models.

The course is planned to be held twice per year, that is one time each semester. Being an international distance-based course in English, all material are online at the Studium education portal of Uppsala University.

The course has 6 core weeks (week 1-6), where each week has two lectures alike chapters, to read in PDF format with some explaining videos to concepts and applications, each having two sessions with related quiz (at Studium) and an exercise (to do at Studium) with a couple of questions pertaining to it. Each week has different interesting topics to cover in this field of AI in drug discovery.

The course concludes with two weeks, (week 7-8) where we complement, reflect and look over the core weeks material and have an graded home-exam.

Shown to the right below is an graphical abstract of lecture 5 in week 3. Lecture 5 is about how is about structural biology and how AI improves structure prediction. Basic and graded material denoted here as a cornerstone or cube; there is also optional material in lecture that is not graded.

Week 1-8

- **Week 1:** Course introduction and overview of AI in drug discovery. Orange data mining software and principal component analysis.
- **Week 2:** Unsupervised and supervised learning. Ligand based prediction and quantative structure activity relationship modelling.
- **Week 3:** Structure based ML and introduction to neural networks, including convolutional neural networks and binding site prediction.
- **Week 4:** Potential of ML in physics and simulation understanding in drug design. De novo design and how AI is used in the field, including graph neural networks.
- **Week 5:** Image-based ML and applications. Moreover graph based ML methods and applications.
- **Week 6:** Training and validating models with tabular and neural network data.
- **Week 7:** Complement, study and rehearsal week.
- **Week 8:** Examination week with an home-exam.

Week 3 (Lecture 5 & 6. Lecture 5 shown here)