The Advanced Machine Learning for Innovative Drug Discovery (AIDD) project

Newsletter 6, May 2023

The **Advanced Machine Learning for Innovative Drug Discovery** (AIDD) project is a Marie-Skłodowska-Curie Innovative Training Network (ITN) for Early Stage Researchers (ESRs) funded by the European Commission under the Horizon 2020 Programme, Marie Skłodowska-Curie grant agreement No 956832. The project brings together fifteen academic and industry beneficiaries from ten European countries and the University of British Columbia (Canada) to train sixteen PhD students in close collaboration with partners from the USA, Australia, China, Israel, and other countries.

Project development

The **AIDD project started on 01.01.2022**.

Fourth AIDD School - Spring School on Advanced Machine Learning in Helsinki

The 4th AIDD school was organised by Aalto University from March 20th to 23rd. The event took place at the Otaniemi campus adjacent to Helsinki, Finland. Aalto University is the premier technical university of Finland that combines technology, business and art with over 17,000 students and 4000 staff. The university is located on the Otaniemi campus, surrounded by nature and the Baltic Sea.

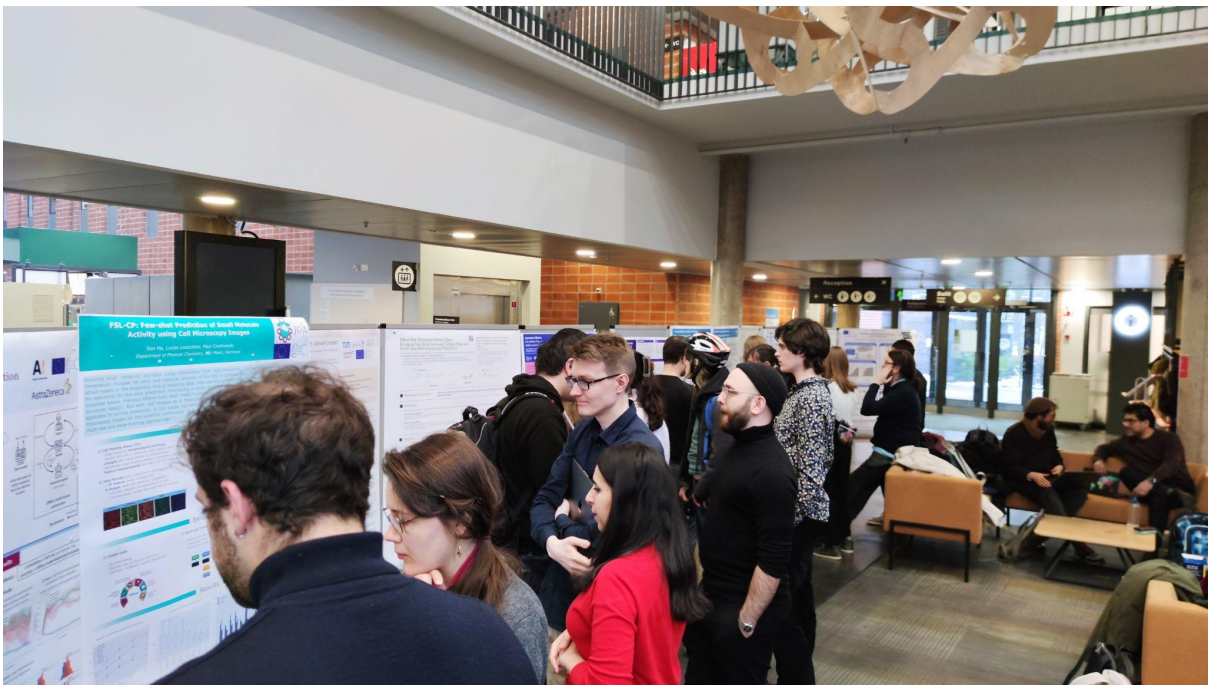
Photo: Aalto University / Mikko Raskinen

The school welcomed attendees including fellows and PIs from various locations around Europe. The program focused on statistical methods relevant to drug discovery and featured 13 speakers from Finland and various consortium partners. The school was complemented by poster presentations and pitch talks from the fellows. Zoom broadcasts were organized for increased outreach, and almost all speakers presented lectures on-site. Audience members also included local students who attended several talks.

Prof. Kaski starts the scientific program of the School.

The school started on Monday 20th March with a welcome by local organisers Prof. Samuel Kaski and Markus Heinonen. The scientific program began with a tutorial by Prof. Samuel Kaski on collaborative modelling, design and decision making in artificial intelligence. This was complemented by a practical tutorial on AI-assisted drug design, at the end of the day, organised by local PhD students Elena Shaw, Alex Hämäläinen and Sebastiaan de Peuter, and fellow Yasmine Nahal. The second talk of the day was by Prof. Juho Rousu on the topic of predicting drug combination responses in cancer, followed by Prof. Harri Lähdesmäki discussing deep latent variable models for longitudinal biomedical data. In the afternoon there was the first pitching session, a speciality of the spring school, where each fellow gave a 5-minute spotlight talk about their research with feedback from both fellows and PIs.

On the second day, the talks started with a description of efficient uncertainty estimation with node-based BNNs by local PhD student Trung Trinh. The talks were continued by Kristof Schutt from Pfizer about neural network potentials. Lewis Marvin from AstraZeneca presented Qptuna for easy, automated QSAR model building. After lunch, the second pitching session gave the floor to five more fellows to present their research to the participants. The day ended with a final talk by Tianyu Cui from Imperial College London about priors in Bayesian deep learning.



Intensive discussions during the AIDD poster session.

On the third day school began with a tutorial by Manuel Haussmann about treatment effect estimation with neural network based models. The fellows continued with a talk by Pedro Reis (Bayer) on hybrid physics and AI methods for pKa predictions in proteins. Next, Prof. Aki Vehtari presented a tutorial on Hamiltonian Monte Carlo. Simultaneously, the PIs participated in the supervisory board and general assembly meetings. After lunch, we continued with the final round of pitching sessions, where the final fellows gave their spotlight talks. This was followed by a poster session, where each fellow presented a poster on their work. The poster session was lively and active discussion filled the hallway. The day finished with a formal dinner at the campus brewery, Fat Lizard.

The final day began with Wenyu Wang presenting an overview of the 1st EUOS/SLAS compound solubility Kaggle challenge, and Igor Tetko continued by describing their winning OCHEM SLAS model. The day ended with a presentation by Bernhard Rohde (Novartis) on how visualising and understanding data helps in modelling the EUOS/SLAS compound solubility challenge. With this final presentation, the spring school was officially finished.

AIDD participants to the BayesComp conference.

Before the spring school, an adjacent meeting was held in Levi, Lapland called BayesComp, a conference series focusing on Bayesian statistics and machine learning. The meeting was relevant for many fellows, and approximately half of them participated in this conference during their trip to Finland. This was followed by an AIDD meeting on Saturday 18th to unpack the conference and discuss new insights.

Voices about the school:

Alan Kai Hassen
"It was great to attend the Bayes Comp 2023 conference in snowy Levi, Lapland, and the 4th AIDD School in Helsinki. During my two-week stay in Finland, I learned new methods like MCMC and deepened my understanding of active learning and uncertainty estimation. It was especially nice to reconnect with fellow AIDD colleagues in Finland and to discuss current projects. I look forward to applying the knowledge I acquired during the conference and AIDD school at Pfizer Germany, where I started the industrial part of my PhD in December 2022. Transitioning from Leiden University, where I was previously based, to Pfizer was a very instructive experience. I am excited to be part of such a dynamic team at Pfizer and can't wait to put my academic skills to use in an industrial setting."

Mathias Hilfiker

"The 4th AIDD School at Aalto University was a really satisfying experience. Having joined the consortium only recently, this was my first school and it was great both from a personal and a scientific point of view. It was a good occasion for networking with other ESRs in the second part of their program, and collecting their personal experiences. The pitch presentations and the poster session were useful to understand the different research carried on in the consortium. The conferences were interesting and they covered a great variety of topics. I also found funny the practical tutorial on AI assistants. Moreover, the mixing with academic and industrial partners allowed me to have more clear how scientific research is carried on in different contexts. In conclusion, it was an experience full of food for thought and I'm happy I participated."

The detailed list of all lecturers, and lecture slides, can be found at: https://ai-dd.eu/lectures.

Next AIDD School will be organised in AstraZeneca, July 3-7 as a hybrid meeting. Zoom access of external participants to selected presentations is currently planned and will be announced on the web site of the project (see https://ai-dd.eu/news).

Meet AIDD partners at (see continuously updated list at AIDD website):

- International Conference on Artificial Intelligence and Statistic, *25 - 27 April*, Valencia, Spain
- The Eleventh International Conference on Learning Representations, *1-5 May*, Kigali, Rwanda, Adam Aramy, Djork-Arné Clevert, Günter Klambauer, Ana Sanchez-Fernandez, Emma Svensson, Alan Kai Hassen
- Helmholtz conference in Drug Discovery, *15-16 May*, Braunschweig, Germany, Ola Engkvist
- Pint of Science Munich, *22-24 May*, Munich, Germany, Paula Torren-Peraire
- QSAR 2023, *5-9 June*, Copenhagen, Denmark, Günter Klambauer, Ana Sanchez-Fernandez, Emma Svensson, Alan Kai Hassen, Varvara Voinarovska
- Helmholtz AI Conference 2023, 12-14 June, Hamburg, Paula Torren-Peraire
- Hybrid Human Artificial Intelligence (HHAI), 26-30 June, Munich, Germany
- AIDD School, 3-7 July, Mölndal, Sweden, AIDD partners
- Gordon Conference in Computer Aided Drug Design, *16 - 21 July*, Vermont, USA, Floriane Montanari, Ola Engkvist
- Intelligent Systems for Molecular Biology / European Conference on Computational Biology, *23-27 July*, Lyon, France, Adam Aramy
- The Fortieth International Conference on Machine Learning, *23-29 July*, Hawaii Convention Center, USA, Adam Aramy

- ELLIS Machine Learning for Molecules Workshop, Summer, on-line, Günter Klambauer, Ana Sanchez-Fernandez, Emma Svensson
- JKU Public PhD Seminars, TBA, on-line, Ana Sanchez-Fernandez, Emma Svensson
- ACS Fall, Harnessing the Power of Data, San Francisco, CA, *27-31 August*, USA, Paula Torren-Peraire
- ICANN2023, *23-26 September*, Cyprus, Igor Tetko
- 17. International Conference on Learning Representations (ICLR), *2-3 December*, Sydney, Australia, Jürgen Schmidhuber
- NIPS 2023, *10-16 December,* New Orleans, USA, Adam Aramy, Günter Klambauer, Alan Kai Hassen

Additional information

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