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

Newsletter 7th February 2025

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 and will finish on 31.03.2025.

AIDD Closing Conference – "AI in Drug Discovery" Workshop at ICANN2024

In early 2023, members of the AIDD consortium won the bid to organise the 33rd International Conference on Artificial Neural Networks (ICANN2024) – the flagship conference of the European Neural Network Society (ENNS). The conference was hosted by AIDD consortium member Dalle Molle Institute for Artificial Intelligence Research (IDSIA USI-SUPSI) in Lugano, Switzerland in collaboration with both the AIDD (https://ai-dd.eu) and AiChemist (https://aichemist.eu) EU Horizon MSCA projects, with sponsoring from the King Abdullah University of Science and Technology (https://www.kaust.edu.sa/en/) in Saudia Arabia and Artificialy (https://www.artificialy.com/), a Swiss company providing AI-based solutions for businesses, based in Lugano. The conference started on the morning of the 17th of September and ended in the late afternoon on Friday the 20th of September. The "AI in Drug Discovery" Workshop, jointly organised by the AIDD and AiChemist projects, was split across four sessions, with the first two taking place in the morning/afternoon on Thursday the 19th of September and the two remaining sessions on Friday the 20th in the morning/afternoon. In total there were 18 lectures given by AIDD fellows and external participants.

The opening session on Tuesday the 17th started with a keynote by AIDD project PI Jürgen Schmidhuber, on the past, present, future and far future of ML, and how the principles of the G, P and T in ChatGPT emerged in 1991. Followed by parallel sessions on computer vision, reinforcement learning and time-series processing, applications of ML/AI in medicine and physiology, generative modelling in computer vision, brain-inspired computation with applications in music, robotics and human-computer interfaces, cognitive and computational neuroscience, environment and climate applications, graph neural networks + time series and applications, as well as a workshop on explainable AI in human-robot interactions and

a tutorial on FEDn – a scalable federated ML framework for cross-device and cross-silo environments (Uppsala, Sweden). The day was rounded off nicely with an evening drinks reception in the courtyard of the West Campus at USI.

Keynote lecture by Jürgen Schmidhuber (left) and drinks receptions (right) on the first day of the conference.

Day 2, the 18th of September, kicked off with a keynote by Tanja Schultz, Professor of Cognitive Systems at the University of Bremen, on the topic of technical cognitive systems that automatically adapt to users' needs by interpreting their biosignals, presenting illustrative cases ranging from silent and imagined speech interfaces that convert myographic and neural signals directly into audible speech, to interpretation of human attention and decision making in human-robot interaction from multimodal biosignals. Over the course of the day, the conference attendees participated in parallel sessions on theoretical contributions in Machine Learning and Neural Networks, applications of Neural Networks, Multimodality, security in Computer Vision, in addition to special sessions, workshops and tutorials in the areas of Reservoir Computing, Neurorobotics, Federated Learning and Time Series Feature Extraction. The day was rounded off with a second keynote, by Michael Reimann, group leader of the Connectomics division of the Blue Brain Project at EPFL, who presented a model of neocortical micro- and mesocircuitry built up from highly detailed and biologically realistic models of rat non-barrel somatosensory regions under the umbrella of the Blue Brain Project.

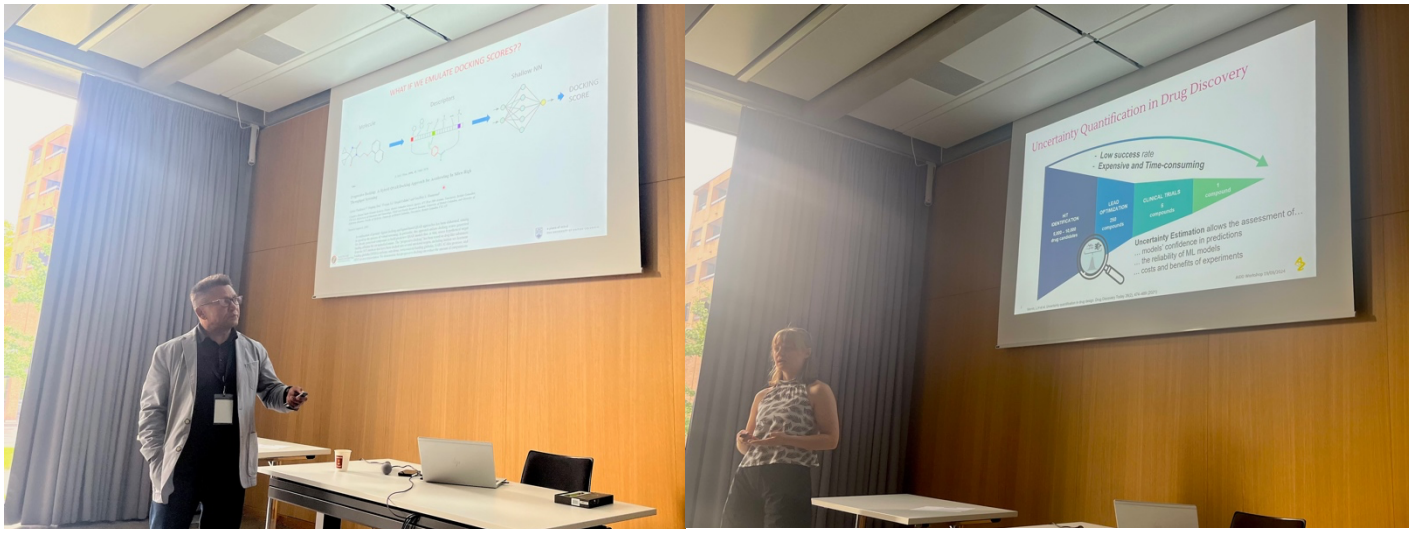
Keynote lectures by Tanja Schultz (left) and Michael Reimann (right) on the second day of the conference

The two-day-long “AI in Drug Discovery” (AIDD) Workshop, jointly organised by the AIDD and AiChemist projects, commenced in the morning of the 19th of September, shortly after the opening keynote of the day, given by Walter Senn, Professor for Computational Neuroscience at the University of Bern, discussing functional models of the brain inspired by the unprecented successes of modeling cognitive processes with AI and exploring the parallels between cortical attention mechanisms and context-dependent gating in the brain and recent advances in AI. The AIDD Workshop sessions ran alongside a dense and varied schedule of sessions dedicated Computer Vision, Neural Architectures, Sentiment Analysis, Spiking Neural Networks, Graph Neural Network Medical Image Processing, Accuracy and Robustness in Deep Neural Networks and Human-Centered Applications of Neural Networks, Novel Methods in Machine Learning, Language Modeling and Topics in Speech and Language, which ran over the course of the last two days of ICANN2024.

Walter Senn at the podium, delivering the final keynote of ICANN2024 on its penultimate day

The AIDD Workshop brought together leading researchers and practitioners (including all of the AIDD fellows and many of the AIDD and AiChemist consortium PIs) to discuss advancements and applications of artificial intelligence in pharmaceutical research and drug development. The workshop provided a platform to explore cutting-edge methodologies and real-world case studies in the domain, encouraging lively scientific exchange and giving the AIDD fellows a unique opportunity to disseminate their findings and receive constructive feedback from experts in the field. The first session was opened with a short keynote by invited speaker Artem Cherkasov, Professor in the Department of Urologic Sciences at the University of British Columbia gave an overview on the use of Active Learning for effective exploration of the chemical universe. This was followed by talks by AIDD fellows Rosa Friesacher, Alessio Fallani, Mathias Hilfiker, Muhammad Arslan Masood and Mikhail Andronov, on a range of topics, including uncertainty quantification in ML models, leveraging quantum mechanical information in ML for drug discovery, toxicity prediction and reagent space mapping.

Getting ready for the AIDD Workshop



Invited speaker Artem Cherkasov and AIDD fellow Rosa Friesacher giving talks during the first session of the AIDD Workshop.

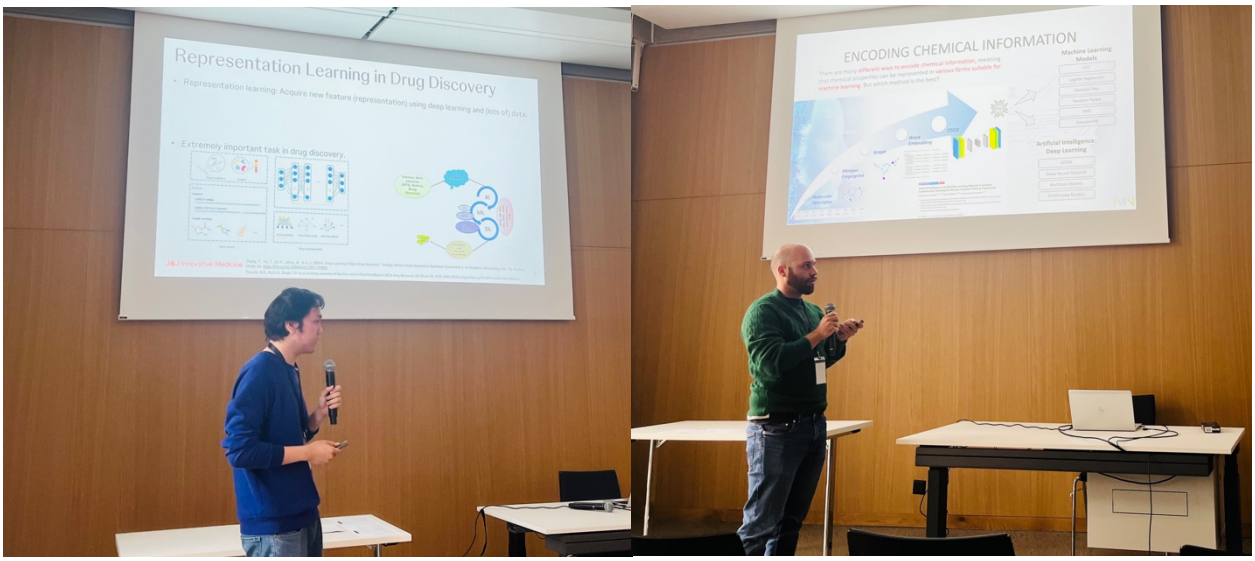
The second session began shortly after lunch, and featured talks on retrosynthesis planning, human-in-the-loop assisted drug discovery and *de novo* ligand generation from AIDD fellows Paula Torren-Peraire, Yasmine Nahal and Julian Cremer, in addition to talks on a range of topics from speakers outside of the AIDD consortium. The second session was rounded off with a short poster session, with contributions from both AIDD and AiChemist consortium members, as well as external workshop attendees.

AIDD fellows Paula Torren-Peraire (left) and Yasmine Nahal (right) delivering their presentations at the workshop

		Thursday 19th September - Foyer on Floor 0 of Corpus A, East Campus, Via La Santa 1, 6962 Lugano-Viganello	
10:30 – 10:50	Artem Cherkasov (invited speaker)	University of British Columbia	The Use of Active Learning for Effective Exploration of Chemical Universe
10:50 - 11:10	Rosa Friesacher	AstraZeneca, Katholieke Universiteit Leuven	Temporal Evaluation of Probability Calibration with Experimental Errors
11:10 - 11:30	Alessio Fallani	Janssen, University of Luxembourg	Atom-level Quantum Pretraining Enhances the Spectral Perception of Molecular Graphs in Graphormer
11:30 - 11:50	Mathias Hilfiker	AstraZeneca, University of Luxembourg	Leveraging quantum mechanical properties to predict solvent effects on large drug-like molecules
11:50 - 12:10	Muhammad Arslan Masood	Janssen, Aalto University	Balancing Imbalanced Toxicity predictor: Using MolBERT with Focal Loss
12:10 - 12:30	Mikhail Andronov	Pfizer, SUPSI	Curating reagents in chemical reaction data with an interactive reagent space map
12:30 - 14:00			**Lunch break**
14:00 - 14:20	Paula Torren Peraire	Janssen, Helmholtz Zentrum München	Improving Route Development Using Convergent Retrosynthesis Planning
14:20 - 14:40	Yasmine Nahal	Aalto University , AstraZeneca	Towards Interpretable Models of Chemist Preferences for Human-in-the-loop Assisted Drug Discovery
14:40 - 15:00	Marco Bertolini	Pfizer	Enhancing Interpretability in Molecular Property Prediction with Contextual Explanations of Molecular Graphical Depictions
15:00 - 15:20	Pedro Ballester	Imperial College	Scaffold Splits Overestimate Virtual Screening Performance
15:20 - 15:40	Justin Diamond	Universität Basel	Geometrically Guided Diffusion for Molecular Generation
15:40 - 16:00	Julian Cremer	Pfizer, Universitat Pompeu Fabra	Latent-Conditioned Equivariant Diffusion for Structure-Based De Novo Ligand Generation
16:00 – 16:30			**Poster session with coffee**

Agenda of the first two AIDD workshop sessions

On the morning of the final day of ICANN2024, the AIDD workshop reconvened with a talk from AIDD fellow Son Ha, who gave a talk based on his work on cross-multimodal learning of cell painting and transcriptomics data, which was followed by a second short poster session. During the last set of talks, AIDD fellow Emma Svensson spoke about her work on uncertainty quantification under distribution shift and external speakers, including representatives from the AiChemist consortium, gave taks based on their most recent work.



Son Ha (left) and Eduardo Viganó (right) presenting their work on the second day of the workshop

Friday 20th September - Foyer on Floor 0 of Corpus A, East Campus, Via La Santa 1, 6962 Lugano-Viganello			
10:10 - 10:30	Son Ha	Janssen, Johannes Gutenberg Universität Mainz	Cross Multimodal Learning of Cell Painting and Transcriptomics Data
10:30 - 11:00			**Poster session with coffee**
11:00 - 11:20	Fabrizio Ambrogi / Szymon Czaplak	Selvita	Target-Aware Drug Activity Model: A deep learning approach to virtual HTS
11:20 - 11:40	Emma Svensson	AstraZeneca, Johannes Kepler Universität Linz	Temporal Evaluation of Uncertainty Quantification under Distribution Shift
11:40 - 12:00	Eduardo Viganò	Mario Negri Institute for Pharmacological Research	Artificial Intelligence Methods for Evaluating Mitochondrial Dysfunction: Exploring Various Chemical Notations Suitable for Neural Language Processing Models
12:00 - 12:20	Regina Pikalyova	University of Strasbourg	Combinatorial Library Neural Network (CoLiNN) for Combinatorial Library Visualization without Compound Enumeration
12:20 - 12:40	Dragos Horvath	University of Strasbourg	De novo Drug Design – Do We Really Want To Be "Original"? A real-world case study on colchicine-site tubulin binders.
12:40			**Lunch break**

Agenda of the AIDD workshop sessions on the final day of the conference

The ICANN2024 conference concluded with a closing ceremony, chaired by ICANN2024 organisers Michael Wand and Kristina Malinovska, and ENNS President Stefan Wermter. During the ceremony the Best Paper Awards and the winner of the Tox24 Challenge were announced. The Tox24 Challenge (https://ochem.eu/static/challenge.do) launched in May 2024, was co-organised by the AIDD and AiChemist projects, in collaboration with the US Environmental Protection Agency, and attracted 78 participating teams working to push the boundaries of ML for toxicity prediction. Among the recipients of the Best Paper Awards was AIDD fellow Dr. Julian Cremer - an outstanding achievement which ended the ICANN2024 conference on a particularly high note.

Recipients of awards at the closing conference. Mikhail Andronov (fourth from the left) accepted the Best Paper Award on Julian Cremer's behalf, as Julian unfortunately could not attend the conference in person.

The majority of the workshop proceedings were published open access in the ICANN2024 volume "AI in Drug Discovery, First International Workshop, AIDD 2024, held in conjunction with ICANN2024" https://link.springer.com/book/10.1007/978-3-031-72381-0, while the remainder were published with standard access within Part X of the main ICANN2024 proceedings https://link.springer.com/book/10.1007/978-3-031-72359-9. In addition, all workshop participants were invited to submit extended versions of their articles and/or novel work to the special issue "AI in Drug Discovery" of J. Cheminformatics prepared by guest editors, Dr. D.A. Clevert (Pfizer) and Dr. I.V. Tetko (HMGU), both of whom are PIs of the AIDD project.

Congratulations to our first set of PhD graduates!

Three AIDD students successfully defended their PhD theses in the second half of 2024!

Dr. Mariia Radaeva (centre) defended her PhD on the 30th of August at the University of British Columbia, followed by Dr. Varvara Voinarovska (right of centre), who defended her thesis at the Technical University of Munich on the 17th of October. Dr. Julian Cremer (second from left) defended his PhD on the 28th of November 2024 at Universitat Pompeu Fabra.

Dr. Radaeva joined McKinsey and Company as an Associate shortly after defending her thesis, while Dr. Voinarovska and Dr. Cremer are staying on at their AIDD industrial host organisations (AstraZeneca and Pfizer, respectively) as postdoctoral researchers. Wishing them all the best for what we are sure will be fantastic careers!

Publications from the AIDD Consortium

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