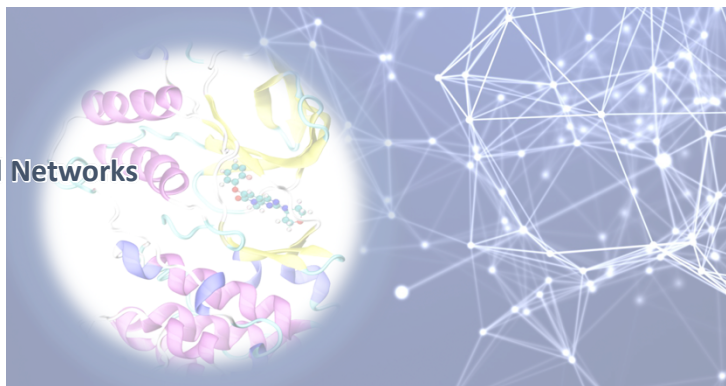


Workshop on

AI in Drug Discovery at the

33rd International Conference on Artificial Neural Networks

ICANN24



The Workshop on AI in Drug Discovery, to be held within the esteemed 33rd International Conference on Artificial Neural Networks (ICANN 2024), invites cutting-edge contributions in the rapidly evolving field of AI-driven drug discovery. We are seeking submissions encompassing various facets such as generative models, explainable AI, model distillation, uncertainty quantification, reaction informatics and synthetic route prediction, quantum machine learning for reactivity, methodologies for mining very large compound data sets, federated learning, analysis of HTS data and identification of frequent hitters and other topics related to the use of ML in chemistry. This workshop aims to bring together machine learning experts, computational chemists and chemoinformaticians working on the development and application of ML in chemistry, environmental health and (eco)toxicology.

WORKSHOP TOPICS

We look forward to receiving contributions from all researchers active in the field, whether they are developing novel methodologies or expanding the scope of established methodologies. A non-exhaustive list of topics includes:

- Big Data and Advanced Machine Learning in Chemistry
- Use of Deep Learning to Predict Molecular Properties
- Modeling and Predication of Chemical Reaction Data
- eXplainable AI (XAI) in Chemistry
- Chemoinformatics
- Generative Models

SUBMISSION INSTRUCTIONS

Contributions (full/short papers or extended abstracts) should be submitted through the regular ICANN submission system at <https://icann2024.org>. Select track "Workshop: AI in Drug Discovery". Accepted papers will appear in the proceedings of the ICANN 2024. The authors of accepted articles/abstracts will be invited to submit new or updated papers to a special issue of a journal before end of September 2024 with a discount (negotiations ongoing).

IMPORTANT DATES

- Deadline for full, short papers and extended abstracts via submission system: 15th of March
- Deadline for extended abstract submission by e-mail to aidd@icann2024.org: 15th of April
- Notification of acceptance: 15th of May
- Conference dates: 17 – 20 September 2024

PROGRAM COMMITTEE

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