Artificial Intelligence for *de novo* drug discovery

Webinar, collaborations, articles and more! We are back this quarter with our latest updates:

Makya Webinar

Interested in learning about Generative AI for de novo drug design? Iktos hosted a webinar on 'Where do we start if we don't have any data? AI for early-stage projects with Makya on 25th July. If you missed the webinar but would like a recording, please follow the link: *https://iktos.ai/makya-webinar-2023/*

Technical Updates

- **Makya**:

  What's new?
  - A new data preparation step is added to the Dataset Upload
  - Static files are now cached and compressed by default, increasing the initial load speed

- **Spaya**:

  What's new?
  - We can now choose the first disconnections to impose for the retrosynthesis in the advanced search panel.
  - Spaya now groups routes by key disconnections in a first disconnections cluster. The displayed route is the best one found for a given group of key disconnections.

Publications & Media

Research Paper: Molecular Assays Simulator to Unravel Predictors Hacking in Goal-Directed Molecular Generations: Did you know that molecules proposed by generative models can often be false positives, mostly due to overoptimization of the predicted scores, which leads to an actual decrease or stagnation of the real scores, aka 'hacking' of the predictive models?….

Interested in learning more? Follow the link to our research paper: *https://iktos.ai/2023/06/29/article-molecular-assays-simulator-to-unravel-predictors-hacking-in-goal-directed-molecular-generations/*

Videos:

- Peptides: *https://youtu.be/jlefGcHHZf0*
- Spaya GUI: *https://youtu.be/58dUx9O7xKY*
- How to Score a Molecule or Molecules in Makya: *https://youtu.be/9rgo_Mh-6kw*

Subscribe to our YouTube channel for more such videos: https://www.youtube.com/@IktosAI-DrugDiscovery

Interviews/PRs:

- Biotech.info: Iktos offers an integrated drug discovery service: *https://biotechinfo.fr/article/iktos-propose-un-service-de-drug-discovery-integre/*
- Maddyness: After raising 15.5 million euros, Iktos continues to grow in Japan: *https://www.maddyness.com/2023/07/03/iktos-japon/*

Latest Collaborations

- Curreio, Inc:

Iktos announced a collaboration with Curreio, Inc., a Japanese company specializing in structural analysis of biomolecules using cryo-electron microscopy. In this collaboration, Iktos's *de novo* generative design technology in combination with Curreio's state-of-the-art cryo-EM platform will be used to facilitate the rapid and cost-effective design of novel preclinical drug candidates for an undisclosed target: https://iktos.ai/2023/06/08/collaboration-with-curreio-inc-in-new-drug-discovery/

- Kissei Pharmaceutical:

Iktos announced that Kissei Pharmaceutical Co., Ltd., a Japanese pharmaceutical company with approximately 75 years of history, specialized in the field of urology, kidney-dialysis and unmet medical needs, has introduced Makya™, Iktos Software as a Service Platform for AI-driven drug discovery. This will enable the rapid and efficient design of new small molecules, leading to an increase in the speed of drug

discovery and development: *https://iktos.ai/2023/07/03/kissei-introduces-iktos-ai-drug-discovery-system/*

New Additions to the Family

Philip Laut
Head of United States Business Development & Operations

Grégoire Germain
Head of Data Engineering & HPC

Aurélien Demilly
Senior Engineer and Tech Lead, Data Engineering

Clémentine Pescheteau
Junior Scientist

Events

Catch us at the following events next quarter:

- GRS Medicinal Chemistry Strategies and Case Studies in Drug Discovery: New London, USA| 05-06 August 2023
- GRC Medicinal Chemistry: New London, USA| 06-11 August 2023
- ACS Fall: San Francisco, USA | 13-17 August 2023
- EFMC-ASMC 2023: Zagreb, Croatia| 03-07 September 2023
- SCI / RSC 22nd Medicinal Chemistry Symposium: Cambridge, UK | 10-13 September 2023
- 21st Annual Global Healthcare Conference: New York, USA | 11-13 September 2023
- Big Data and AI: Paris, France | 26 September 2023

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