



Artificial Intelligence for *de novo* drug discovery

Welcome to the latest edition of our newsletter

As we kick start the new year, we would like to wish you all a very happy and prosperous 2022. The last quarter of 2021 was very busy and exciting for Iktos. Below we have shared with you a few of our favourite highlights:

Latest publication

Our research paper on 'Integrating synthetic accessibility with AI-based generative drug design' was recently published by ChemRxiv. If you are a fan of artificial intelligence just like us, [follow the link to read the full paper: https://bit.ly/35S9ngN](https://bit.ly/35S9ngN)

ChemRxivTM

Generative models are frequently used for *de novo* design in drug discovery projects to propose new molecules. However, the question of whether or not the generated molecules can be synthesized is not systematically taken into account during generation, even though being able to synthesize the generated molecules is a fundamental requirement for such methods to be useful in practice. Methods have been developed to estimate molecule synthesizability, but, so far, there is no consensus on whether or not a molecule is synthesizable. In this paper we introduce the Retro-Score (RScore), which computes a synthetic feasibility score of molecules by performing a full retrosynthetic analysis through our data-driven synthetic planning software Speks, and its derivatives (1). After a comparison of RScore with other synthetic scores from the literature, we describe a pipeline to generate molecules that validate a lot of targets while still being easy to synthesize. We further this idea by performing experiments comparing molecular generator outputs across a range of constraints and conditions. We show that the RScore can be learned by a Neural Network, which leads to a new score: RSPred. We demonstrate that using the RScore or RSPred as a constraint during molecular generation enables to obtain more synthesizable solutions, with higher diversity. The open-source Python code containing all the scores and the experiments can be found on <https://github.com/Iktos/generation-under-synthetic-constraint>.

[Click to read](#)

Makya Webinar

Our CSO, Dr. Quentin Perron and Senior Director & Head of BD, Dr. Sree Vadlamudi presented a webinar on 'Makya™: Iktos technology platform for AI-driven de novo drug design and multi-parametric optimisation' on 7th December 2021. [Follow the link to access the recording: https://iktos.ai/makya-webinar-2021-2/](https://iktos.ai/makya-webinar-2021-2/)

IKTOS
Artificial Intelligence
for new drug design

Makya Webinar

Tuesday, 7th December 2021
Session 1: 10:00-11:00 CET
Session 2: 17:00-18:00 CET

Dr. Quentin Perron Dr. Sree Vadlamudi

makya
AI-driven de novo drug design

Makya Poster Video

Interested in learning more about applications of Makya to a structure-based project? Here is a short video, explaining our poster on 'Discovery of Novel Inhibitors of PIM-1 Kinase Enabled by Generative AI': <https://iktos.ai/poster-video-discovery-of-novel-inhibitors-of-pim-1-kinase-enabled-by-generative-ai/>

Discovery of Novel Inhibitors of PIM-1 Kinase Enabled by Generative AI

onco design

KEYNOTE

The poster details the discovery of novel PIM-1 kinase inhibitors using generative AI. It includes sections for: **GENERATIVE AI SETUP**, **RESULTS**, **CONCLUSIONS AND TAKEAWAYS**, **ACKNOWLEDGEMENTS**, and **IKTOS PRODUCTS**. The poster also features chemical structures and data tables.

Latest Collaborations

We are delighted to share with you our latest collaborations with Chiesi Group, Jiangsu Hengrui Pharmaceuticals, The University of Dundee, Drug Discovery Unit (DDU) and Astrogen, who will be using Iktos technology to expedite their drug discovery process. *Follow the link for our latest press releases: <https://iktos.ai/news-2/>*



Profile of the month: Abderraouf El Gasser, Head of Software Development, Iktos

Abderraouf (Abdel) is the Head of Software Development at Iktos, responsible for implementing, integrating, and deploying the work produced by our R&D teams into production ready features in our SaaS application Makya. With a strong background in software engineering, and nearly 20 years of diverse experience, Abdel is in charge of finding ways to improve the efficiency and usability of Makya, as well as making sure developers can work effectively.

Though initially wanting to make a career in electronics, Abdel has an interesting story of how he migrated towards software development.

During his Bachelor's, he was given a piece of software to develop (in C; back in 1998), to visualise data from a device that was used to detect levels of CO₂, Ozone, and temperature in a room through a bunch of sensors. He realised that this project was more exciting than the device itself, as he could draw charts to follow the temperature and CO₂, Ozone levels over time, which opened a whole new world of possibilities for him. When asked what he loves the most about his role, he says, "the same thing that made me move from



electronics to software development: the idea that the sky is the limit.” He explains that just with the help of a keyboard, CPU, and display, he can set-up whatever he needs to simplify and optimise his day-to-day life. He shows the same passion at Iktos, where he is full of new ideas and technical inputs. With a simple mantra of “If you can think it, I can build it,” Abdel is determined to help our pharmaceutical and biotech clients in their drug discovery journey.

Newest Additions to the Iktos Family

We are thrilled to welcome Payash, Pierre, Massina, Yanyuan, Auriane and Elenora, who have joined Iktos in the last quarter. Their skills and experiences are a great asset to the company, and we wish them all the best in their new roles!



Payash Bahuguna
Marketing &
Communications
Manager



Pierre Grenut
Business Development
Analyst



**Massina
Abderrahmane**
Data Scientist



Yanyuan Zhang
Intern



Auriane Riou
Intern



Eleonora Serra
Intern

SLAS: AI Powered Drug Discovery Symposium

Our Senior Director & Head of BD, Europe, Dr. Sree Vadlamudi and Marketing Manager, Payash Bahuguna exhibited and presented two posters at the SLAS: AI Powered Drug Discovery Symposium in November 2021. Additionally, Dr. Sree Vadlamudi delivered a talk on ‘Generative AI: Application to Drug Discovery’ and took

part in a panel discussion as well. *Contact us if you would like a copy of the posters that the team presented:*
<https://iktos.ai/contact/>



Upcoming Conferences

Catch us at the following events next quarter:

- SLAS 2022: Boston, USA; 5th-9th February 2022
- ACS Spring: San Diego, USA; 20th- 24th March 2022

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