



Artificial Intelligence for *de novo* drug discovery

Series A Funding, new product offering and much more ...we are back this quarter with the latest updates from Iktos for you:

Series A Funding

Iktos announces the closing of a € 15.5m Series A financing co-led by new investors M Ventures and Debiopharm Innovation Fund with participation from Omnes Capital. The financing will enable us to expand our artificial intelligence-based drug discovery technologies and solutions. Follow the links for:

- Full press release: <https://bit.ly/3n90qbX>
- Good morning business interview: <bit.ly/446wuOe>
- Sifted article: <bit.ly/41XpuRY>



Technical Updates



- **Dock AI:**

We are pleased to introduce DockAI, a new technology that combines docking with a state-of-the-art active learning methodology to significantly improve the efficiency and effectiveness of this process.

Screen several billions of commercially available molecules in just a few days at low cost with DockAI



- **Makya:**

Coming soon:

- Docking and 3D visualisation
- Electrostatic similarity



- **Spaya:**

What's new?

- Integration of a new clustering method - clustering by key disconnections in a molecule
- Integration of the 1st disconnection feature into the Advanced Search



We are excited to share with you that Iktos is participating in the **CACHE (Critical Assessment of Chemical Encodings) challenge** designed towards combatting the ongoing COVID-19 crisis. Iktos will be leveraging our proprietary technology, DockAI, to help provide quality computational hit-finding predictions.



Exploring isofunctional molecules: Design of a benchmark and evaluation of prediction performance

Identification of novel chemotypes with biological activity similar to a known active molecule is an important challenge in drug discovery called 'scaffold hopping'. Small-, medium-, and large-step scaffold hopping efforts may lead to increasing degrees of chemical...Read the full article: bit.ly/3LB3dnU



Makya Videos:

- Hit-to-lead through fragment growing in Makya: <https://youtu.be/aYWxGHRuVls>
- Dataset upload Makya: <https://youtu.be/cnDVBhF-k-k>
- Lead optimization using the fine-tuning generator in Makya: https://youtu.be/GCILN_SZgdc

Subscribe to our YouTube channel for all our videos: bit.ly/3V8os3u



Podcasts:

- AI for new drug design- Dr. Quentin Perron: bit.ly/3NeTpB9
- Careers in discovery- Dr. Sree Vadlamudi: bit.ly/424x3Gu



Profile of the Month: Alexis Denis



Alexis is the SVP, Head of Drug Discovery at Iktos, responsible for driving and developing Iktos's portfolio of drug discovery programs. With a doctorate in organic chemistry and decades of experience working in blue chip pharma companies such as GSK and Pfizer, his goal is to move faster from the hit generation to the clinical drug candidate and to bring new drugs to the patient using Iktos technologies.

Alexis has always been fascinated by the impact of small molecules in living organisms and finds being at the interface of the AI/in silico technologies and the more traditional approaches of medicinal chemistry very exciting. Expanding more on his passion, he says "I like the concept of 'serendipity' a lot: looking by curiosity somewhere else than expected, always brings you to discoveries and creativity. I always recommend going beyond the comfort zone to explore new areas and disciplines."

Outside of work, Alexis is very fond of reading, cooking, and fine wines! He is also a big fan of rock concerts...so catch him at the next gig!

New Additions to the Family



Alexis Denis
Senior VP, Head of
Drug Discovery



**Jean-Baptiste
Cheron**
Research Software
Engineer

Events



Catch us at the following events next quarter:

- Anglo Nordic Life Science Conference: London, UK | 20 April 2023
- 11th Annual Advances in Chemical Sciences Symposium: Cambridge, USA | 5 May 2023
- IDDST-2023: Tokyo, Japan | 08-10 May 2023
- GGMM 2023: Toulouse, France | 05-08 June 2023
- Bio 2023: Boston, USA | 15-17 May 2023
- Medchem Meet 2023: Paris, France | 08-10 June 2023
- Medicen Day - Drug design and AI: Paris, France | 09 June 2023
- 3rd RSC Anglo-Nordic Medicinal Chemistry Symposium: Snekkersten, Denmark | 13-16 June 2023

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