



Artificial Intelligence for *de novo* drug discovery

We wish all our readers a very happy and prosperous 2023. We are back with renewed enthusiasm as we bring to you some highlights from the last quarter of 2022:

Technical Updates

We are excited to share with you some of our latest technical updates for Makya, our generative AI software and Spaya, our AI-driven retrosynthesis software:

- **Makya:**
 - Fragment Growing Generator introduced
 - Fragment Linking Generator introduced
 - Autoscaling for all types of generators and AutoML
 - Reinforcement learning feature introduced to Novelty generator

Learn more about Makya: <https://iktos.ai/makya/>



- **Spaya:**
 - Regioselectivity issues are now highlighted in the retrosynthesis tree as a Beta feature
 - Substructure can be forbidden or imposed during the Advanced Search
 - Preferred presets can now be saved for the Advanced Search

Learn more about Spaya: <https://iktos.ai/spaya/>



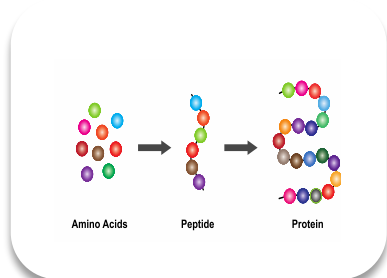
Publications & Media



- **Video: Makya Overview**

Makya is the first user-friendly SaaS platform for AI-driven *de novo* drug design focused on Multi-Parametric Optimisation (MPO). It enables design of novel and easy to make compounds in line with multi-objective blueprint with unprecedented speed, performance, and diversity.

Watch our video for: Introduction to Makya, Generative AI platform, Makya workflow and Generation strategies: <https://iktos.ai/makya-overview-video/>



- **Blog: Peptides**

Peptides are a promising class of therapeutics with unique properties. They share some advantages of proteins, such as their high selectivity but also some of small molecules, like metabolic stability and their low immunogenicity... Read our blog to learn more about representing, predicting, and generating simple and complex peptides:

<https://iktos.ai/2023/01/30/representing-predicting-and-generating-simple-and-complex-peptides/>

Latest Collaboration

- **Medicines for Malaria Venture:**

Iktos announced a collaboration with Medicines for Malaria Venture (MMV), a leading product development partnership (PDP) in the field of antimalarial drug research and development. Under this collaboration agreement, Iktos will apply its new 'DockAI' technology to expedite the discovery of novel antimalarial drug candidates. Follow the link for the full press release:

<https://iktos.ai/2022/11/23/iktos-partners-with-medicines-for-malaria-venture-in-anti-malarial-drug-discovery/>



Profile of the Month: Jean Christophe Meillon



JC is the Head of the Robotics Lab at Iktos. After working for over two decades in medicinal chemistry for various biotech companies and CROs, he decided to get out of his comfort zone and in to the field of robotics and automation. He is currently responsible for setting up the laboratory for Iktos's new chemical robot. He believes robotics and automation to be the future of pharma industry and finds them more fast paced than traditional chemistry. When asked for a word of advice for people just starting their careers, he says "Better be late and miss your train, than be early and jump on the wrong one."

JC's role allows him to interact with brilliant minds from diverse scientific fields, all working towards the same goal- something he finds both thrilling and inspiring. Outside of work, JC loves classical music and luxury wines. He is also an avid traveller and enjoys a good hike before indulging in the finer things in life!

New Additions to the Family



Ganesh Shahane
Application Scientist



Matthew Medcalf
Application Scientist



Brann Joly
Sr. Software
Developer



Luidgi Gromat
Sr. Software
Developer Full stack



Mac Monson
Sr. BD Manager



Alexa Meurant
Chief Legal Counsel



Merveille Eguida
Computational
Chemist

Events



Catch us at the following events next quarter:

- SLAS 2023: San Diego, USA | 25 Feb 2023- 1 March 2023
 - ACS Spring: Indianapolis, USA | 26 March 2023- 30 March 2023
 - ELRIG Research & Innovation: Cambridge, UK | 29 March 2023
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