



# IKTOS

## Artificial Intelligence for *de novo* drug discovery

Welcome to the latest edition of our newsletter

Iktos newsletter is back with new content and latest updates for our readers: webinar, articles, videos and more...see what we have in store for you this quarter!

Spaya Video

Interested in finding the best synthetic routes to your compounds? Watch our latest video on Spaya: Iktos's AI-powered retrosynthesis tool: <https://iktos.ai/spaya-overview/>

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



## Makya Webinar

Our CSO, Dr. Quentin Perron and VP, Head of BD- EU, RoW Dr. Sree Vadlamudi presented a webinar on 'Makya™: Iktos technology platform for AI-driven *de novo* drug design and multi-parametric optimization' on 13<sup>th</sup> September 2022. Follow the link to access the recording if you missed the webinar: <https://iktos.ai/makya-webinar-2022/>

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

**IKTOS**  
Artificial Intelligence  
for new drug design

**makya**

# Makya Webinar

Tuesday, 13th September 2022

Session 1: 10:00-11:00 CET  
Session 2: 17:00-18:00 CET

Dr. Quentin Perron    Dr. Sree Vadlamudi

## Latest publication

Our research paper on 'A molecular assays simulator to unravel predictors hacking in goal-directed molecular generations' was published by ChemRxiv.

Follow the link to read the full paper: <https://iktos.ai/2022/06/13/a-molecular-assays-simulator-to-unravel-predictors-hacking-in-goal-directed-molecular-generations/>

Working Paper Joseph-André Turk Iktos, Philippe Gendreau Iktos, Nicolas Drizard Iktos, Yann Gaston-Mathé Iktos

## Abstract

Generative models are being increasingly used in drug discovery campaigns, with either coupled with QSAR or the similar quantitative structure-activity relationship (QSAR) models to optimize a given set of properties. The molecules generated by these algorithms are often considered to be false positives, i.e. outside the true candidate drug target space (DTS). Because the conditions are being learned by the generative model during the optimization, by feeding an iteratively updated set of generated molecules to the model, it can learn to generate molecules that are more likely to be true positives. This is done by a combination of generative models in iterative learning, and it can be done in a more robust manner by using a more advanced generative model. In this work, we introduce a combination of multi-target models using a multi-target neural network (MTNN) which returns continuous values for any target molecule. We use this model to optimize a real-world generative model optimization example. Thus, we have generated molecules in an iteratively updated set of molecules aimed at predicting their real world values. Second, we generate new optimized molecules using the open-source generative package coupled with the previously built models. Thirdly, we select compounds which match the DTS according to the predicted values and evaluate them by comparing the real world values. We observe that even when the generative models have excellent performance metrics, the final selection and validation steps are essential according to the observed values. We evaluate the optimization behavior in terms of an iterative selection using either a logistic regression or a random forest prediction model. We also propose and evaluate several methods to help integrate the learning loop.

[Click to read the full article](#)

## Blog

In this blog, Dr. Sree Vadlamudi, Vice President, BD- EU & RoW, Iktos, talks about how we can adopt AI to help foster productivity within pharmaceutical research, as well as the current challenges faced by the drug discovery sector. Read the full interview here: <https://iktos.ai/2022/08/26/using-ai-to-foster-productivity-in-pharmaceutical-research-and-development/>

## insights from industry

Sree Vadlamudi

Vice President, Head of Business Development EU, RoW  
Iktos



Profile of the month: Christopher Houssemann, Head of Medicinal Chemistry Iktos

Christopher is the Head of Medicinal Chemistry at Iktos. With a Ph.D. in organic synthesis from ICSN-Gif-sur-Yvette and over 12 years of experience in several blue-chip pharma companies, he is leading a team of talented scientists, dedicated towards finding the next breakthrough drug.

Christopher started his career as a pure organic chemist, but thanks to his medchem mentors, got drawn towards medicinal chemistry. Over the years, he realized the need to explore wider chemical space, improve quality of designed molecules and use cutting-edge technology to accelerate drug discovery. Working as a medicinal chemist allows him to be within reach of



different disciplines, such as chemistry (back to the basics), biology, structure based, DMPK and pharmacology. It is the ability to innovate and solve complex projects that he enjoys the most about his job. At the end of the day, finding a new drug candidate that would benefit mankind is a rewarding satisfaction.

Outside of work, Christopher enjoys diving and swimming in the deep blue sea. He is also a talented photographer, fascinated by how different the world looks through the lens of his camera. With a simple motto of “full speed ahead and never give up, love will make the rest”, Christopher starts his day with a big smile on his face!

## Newest Additions to the Iktos Family

We are thrilled to welcome the newest members of the Iktos family. Their skills and experiences are a great asset to the company, and we wish them all the best in their new roles!



**Ronan Lami**  
Chief Operating Officer



**Vincent Bouttier**  
Senior Data Scientist



**Thibaut Danvers**  
DevOps Engineer



**Victoire Cachoux**  
Application Scientist,  
Japan



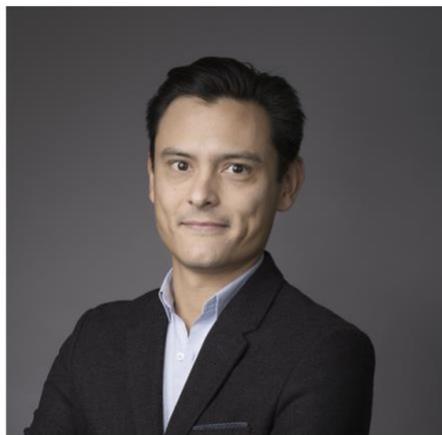
**Nikolaii Lodenos**  
Software Developer  
Full stack



**Benjamin Bouillet**  
Dev Ops  
Engineer

AWS re:Invent 2022

Our Co-founder and CTO, Dr. Nicolas Do Huu will be giving a talk on 'Dock AI Against Malaria' on 30<sup>th</sup> November at the AWS re:Invent 2022 conference in Las Vegas. Follow the link to the conference: <https://reinvent.awsevents.com/>



## Upcoming Conferences

You can also catch us at the following events next quarter:

- Boulder Peptide Symposium: Colorado, USA; 7<sup>th</sup>-10<sup>th</sup> November 2022
- 7<sup>th</sup> Annual Drug Discovery Summit: Madrid, Spain; 16<sup>th</sup>- 17<sup>th</sup> November 2022

### Contact Information:

Iktos,  
65 rue de Prony  
75017 Paris  
Tel: +33(0)973584548  
Email: [contact@iktos.com](mailto:contact@iktos.com)  
Web: <https://iktos.ai>