Artificial Intelligence for Drug Discovery

A Technology Platform for Deep-Learning-Based de novo Drug Design

Digital tools are a key to shortening the development of active pharmaceutical ingredients and thus market-ready drugs and therapies. Big data and artificial intelligence (AI) can significantly accelerate many processes and make them more efficient. The Paris, France-based start-up Iktos is developing a proprietary AI technology for ligand and structure-based de novo drug design, focusing on multi parametric optimization (MPO). Yann Gaston-Mathé, co-founder and CEO of Iktos, explains the company's technologies and provides an outlook on the further development of the company.

Yann Gaston-Mathé, CEO, Iktos

Personal Profile

Yann Gaston-Mathé holds an engineering degree from Ecole Polytechnique Paris and a master's degree in biology, genetics and biochemistry from AgroParisTech. He held several positions in the pharmaceutical industry (at Servier, Ipsen, Integragen), and in consulting companies Capgemini, BearingPoint and Cepton. With an excellent knowledge of the pharma sector, he has a global vision of the pharmaceutical industry's challenges as well as a broad understanding of methods, approaches and tools of data science. He led Iktos' development since its foundation, incl. capital raising, business development and team recruitment.

CHEManager: Mr. Gaston-Mathé, what was the starting point and motivation for founding Iktos?

Yann Gaston-Mathé: Iktos was founded in 2016 by Quentin Perron, Nicolas Do Huu and myself with the aim of developing an innovative and user-friendly deep learning-based technology platform for de novo drug design. The technology platform was built by leveraging a proprietary algorithm developed by Quentin and Nicolas who initially wanted to apply deep learning generative models to chemistry that were previously used in fields such as image recognition and natural language processing.

Our objective is to make our technology accessible to everyone, and to be the first company to release a user-friendly and high-performance de novo design software for multi-parametric optimization, that can be used by any medicinal or computational chemist, whatever their level of expertise in deep learning and computer programming.

What does the company name Iktos actually stand for?

Y. Gaston-Mathé: The name Iktos stands for 'God of dream catcher' in the native American mythology.

What problem does Iktos's technology specifically solve, or what previously untapped opportunities does it open up?

Y. Gaston-Mathé: We leverage big data and artificial intelligence (AI) to bring radical improvements and efficiencies to drug discovery process. Iktos is developing a proprietary, disruptive, AI-based generative modelling technology for ligand and structure-based de novo drug design, focusing on multi-parametric optimization (MPO). Our proprietary technology is built upon the latest developments in deep learning algorithms, not only for de novo design but also for AI driven synthesis planning.

Our generative modelling technology coupled with synthesis planning can be applied to the early stage drug discovery value chain ranging from hit generation or scaffold hopping projects to lead generation and lead optimization. In a very short timeframe, it can design novel, diverse, druggable and synthesizable molecules, that are optimized to match the target product profile (TPP) of the project.

Iktos has a strong expertise in deep learning based de novo design for medicinal chemistry: superior technology, experience and skills, and technical infrastructure. In a few weeks, we can provide solutions that help to accelerate collaborators research projects.

Who are your customers and in which markets do you find them?

Y. Gaston-Mathé: As a company specializing in AI for drug design, Iktos is developing and commercializing several software products in the field of generative modeling and retrosynthesis. We license our software platforms and interfaces — Makya, Spaya and Spaya API — on an annual SaaS licensing model.

Iktos predominantly operates in the early stage drug discovery sector. Our typical customers are from pharma, biotech, agrochem and academic sectors. Since 2017, our technology has been tested and validated in several real-life projects with bio-pharma collaborators globally. We either have been working or delivered 40 plus projects with bio-pharma collaborators.

What have been the most exciting projects so far?

Y. Gaston-Mathé: We are working with a large number of biopharma collaborators, for us every project is exciting. Here are a few examples where we can share the project details:

Iktos is the first company to report a successful application of deep generative modelling technology in a real-life drug discovery project. We have presented the results of our collaboration with Servier as a poster at the 2018 EFMC meeting and recently published a ChemRxiv preprint.

We have successfully applied our structure-based generative modelling approach to design novel compounds for a kinase target in line with the target-product-profile. Iktos has delivered molecules with well-balanced activity and physio-chemical profile, the MPO project work is progressing well with our collaborator Oncodesign.

What do you see as the main drivers for your success and what is the feedback from the industry?

Y. Gaston-Mathé: Iktos' technology and know-how in generative modelling are key drivers to our success. Our team is composed of 40 talented individuals meeting the key skills required to succeed in our business: medicinal and computational chemistry, machine learning and deep learning, data science, data engineering, open-source big data IT architecture, software development and business development.

Iktos is recognized as one of the key players in this emerging field of generative modelling. Our proprietary technology platform simultaneously tackles de novo design and synthetic planning of the molecules to match the desired blueprint of drug discovery projects. We have been able to sustain long term relationships with existing customers and secure collaborations with new customers on regular basis.

Business Idea

Reinventing Medicinal Chemistry

New drug design is long (5 years), costly ($50-100 million) and unproductive (1% success rate from hit to pre-clinical candidate). Iktos leverages big data and artificial intelligence (AI) to bring radical improvements to this process.

Founded in 2016 and located in Paris, France, Iktos is a company specializing in AI technologies and software applied to chemical research, more specifically new drug design, with two proprietary technologies:

- Generative AI technology and software (Makya) for de novo drug design and multi-parameter optimization (MPO)
- AI for synthetic planning with Spaya, a fully data-driven retrosynthesis software which provides plausible synthetic routes for any given compound in a very short time frame.

Iktos has acquired a unique know-how at the interface of AI, medicinal chemistry, and informatics with a solid expertise across multiple areas such as data science, deep learning, machine learning, cheminformatics, molecular modelling, synthetic chemistry, medicinal chemistry, data engineering, high-performance computing, cloud environments and software development. The company has built a talented team of engineer graduates from the French Grandes Ecoles, PhDs in AI, chemistry, specialists in physics and computational chemistry, and computer engineers.

A Tested and Validated Technology

Iktos has been recognized since 2018 as one of the leading players in AI applied to drug discovery.

The company was awarded several competitive grants for innovation and has acquired more than twenty pharma customers, including some of the most prestigious European and USA pharma companies such as Janssen, Merck, MSD, Pfizer, Lundbeck, Servier, UCB and Alkermes.

So far, Iktos's technology has been tested and validated in 40 plus different real-world projects in the pharmaceutical industry. In 2019, the company has established a US subsidiary, Iktos Inc.

- Iktos, Paris, France
  www.iktos.ai

Elevator Pitch

Deep-Learning-Based Drug Design

Iktos is developing a proprietary and innovative AI solution based on deep learning generative models, which enables, using existing data, the design of molecules that are optimized in silico to meet all the success criteria of a small molecule discovery project. The use of Iktos' technology enables major productivity gains in upstream pharmaceutical R&D.

Milestones

2016
- Foundation of Iktos

2017
- Winner of the Innov'Up Proto challenge, sponsored by the Paris region, securing a €100,000 non-dilutive funding
- Raising €700,000 in equity from a pool of private investors

2018
- Winner of the Concours Mondial d'Innovation, a €900,000 competitive innovation grant funded by the French Government

2019
- Research collaboration with Almirall in AI for new drug design
- Research collaboration with Janssen to utilize Iktos' AI technology to increase speed & efficiency of small molecule drug discovery
- Collaboration with Merck for use of Iktos AI technology across three drug discovery projects
- Successful closing of a collaboration with Servier in the field of AI

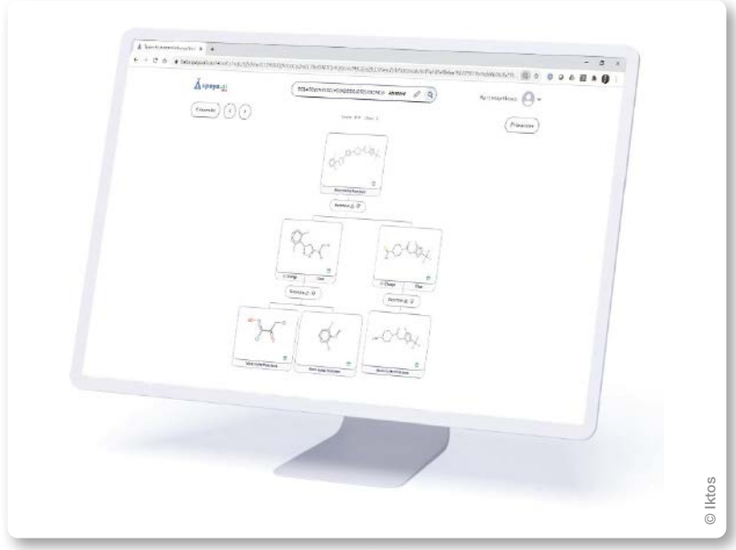
2020
- Additional Collaboration with Merck in AI for new drug design
- Collaboration with SRI International to combine AI and novel automated discovery platform for accelerated development of new anti-viral therapies

2021
- Collaboration with UCB in AI for retrosynthesis
- Collaboration with Kadmon to use AI for new drug design
- Collaboration with Facio Therapies to use AI for FSHD drug design
- Collaboration with Pfizer in AI for drug design

Roadmap

Iktos is seeking to establish new collaborations with pharmaceutical and biotechnology companies interested in the application of its AI technology to their drug discovery projects. It is also developing a SaaS software that aims to make its technology available to medicinal, computational chemistry and informatics groups.

Makya is a web-based SaaS platform for ligand-based generative modeling focusing on multi-parametric optimization (MPO).



Spaya is a web-based retrosynthesis AI SaaS platform which can be licensed as a paid version and/or deployed on customer premises and customized.