

## **Iktos Generative AI Technology to Accelerate Drug Design and Discovery**

Hideyoshi Fuji

Iktos SA, 75017 Paris, France

Email: [hideyoshi.fuji@iktos.com](mailto:hideyoshi.fuji@iktos.com)

With the popularity of ChatGPT released in November 2022, generative AI has spread dramatically, and it is expected that generative AI will be used in many fields such as business, art, and science. Iktos is a French AI drug discovery startup company established in October 2016. We specialize in AI development for medicinal chemistry and drug discovery, providing unique and innovative drug discovery solutions based on cutting-edge AI. Iktos believes that it is important for medicinal chemists and other researchers involved in drug discovery to master generative AI, and provides a SaaS software platform that is easy for medicinal chemists to use. In this presentation, after introducing Makya, a de novo drug design platform equipped with Iktos' generative AI, and Spaya, a synthesis planning software based on proprietary AI technology for retrosynthesis analysis, we will introduce the latest active learning methods in docking that we harnessed in DockAI, our solution to perform efficient and cheap virtual screening of ultra-large-scale compound libraries in a matter of days. Finally, we would like to introduce the latest information on Iktos Robotics, Iktos's compound synthesis automation project, and talk about the transformation of the drug discovery process that Iktos is aiming for.