

Iktos and Bayer collaborate to leverage AI to design novel Sustainable Crop Protection solutions

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Iktos, a company specialized in Artificial Intelligence (AI) for new drug design, and Bayer's Crop Science division with its industry-leading R&D pipeline and portfolio of seeds & traits, crop protection and digital farming solutions, today announced a collaboration to expand the use of AI in the discovery and development of new sustainable crop protection products.

Iktos's *de novo* generative design software Makya will be deployed by Bayer scientists to facilitate the design of novel molecules according to pre-defined profiles and accelerate hit-to-lead/lead optimization, whereby potential molecular candidates are further optimized and developed into lead compounds.

Makya is based on deep learning generative models which design and optimize, in-silico, novel molecules that satisfy multiple parameters, such as efficacy, selectivity, safety, and sustainability. The technology brings new insights and directions into the molecular discovery process based on a comprehensive data-driven chemical structure generation technology. It also allows scientists to analyse billions of molecules in a virtual environment, enabling the exploration of new and larger chemical spaces than previously possible. The Makya Software as a Service (SaaS) platform enables researchers to benefit from the technology thanks to its user-friendly interface and a secure and scalable technical implementation in the cloud.

This approach to innovation, validated through multiple collaborations in pharmaceutical research and development, is now being used for the first time to help solve a key challenge in crop protection discovery: the rapid and efficient identification and

optimization of successful and safe molecules and holds great potential to support Bayer's sustainability objective to reduce the environmental impact of agriculture, via lower application rates and favourable safety profiles of its solutions.

Rachel Rama, Head of Small Molecules at Bayer's Crop Science division said "Bayer's CropKey approach to crop protection innovation is made possible by data-driven breakthrough technologies such as those made accessible by Iktos. They will allow us to unlock a new way to protect crops, food security and the environment and, in doing so, set a new benchmark in the industry."