SynSilico B.V. launches AI-based enzyme and inhibitor discovery service

Fully automated pipeline allows for 500.000 binding energy predictions per month to speed up in silico enzyme and inhibitor screening and discovery projects

GELEEN, NETHERLANDS, October 31, 2024 /EINPresswire.com/ -- SynSilico launches its first AI-based enzyme and inhibitor discovery service for Life Science and Pharma customers. This service is based on a fully automated pipeline which combines the latest peer-reviewed AI-based structure, binding site, docking and binding energy prediction models. The predictive performance of this pipeline

Tomorrow's AI applications. Today.

was validated for virtual screening of enzymes, starting from enzyme sequence libraries and given target substrates using SMILES representations. This workflow, together with other predictive tools, will accelerate the discovery of enzymes as well as process development which can directly start validating identified enzyme targets at more relevant scales.

In addition to applications in enzyme discovery this workflow was validated for inhibitor screening of huge small molecule libraries against pharma relevant protein targets. Customers involved in drug discovery can benefit from those developments by co-creating tailor-made pipelines that can combine other predictive tools relevant for their development. SynSilico's AI service targets customers that don't want to invest in own computational capabilities or resources but want to benefit from increasingly powerful AI models to accelerate their developments.

Martin Schürmann (Chief Scientific Officer) stated that "with our current pipeline and own computational power 500.000 small/large molecule combinations can be screened in-silico per month. Even more impressive than the achieved throughput (which is easy to scale) is the quality of our predicted results. For both our enzyme as well as our inhibitor screening test case, 7 out of 10 wet lab confirmed top ranking candidates could be confirmed."

Oliver May (Managing Director) mentioned that "those impressive results encouraged us to launch our first services while we will still add additional predictive tools and services to our portfolio."

SynSilico is a NL-based joint venture of Genzai and InnoSyn which provides AI-based services to accelerate innovations of their Life Science and Material Science customers.

Oliver May
SynSilico
oliver.may@synsilico.com
Visit us on social media:
LinkedIn