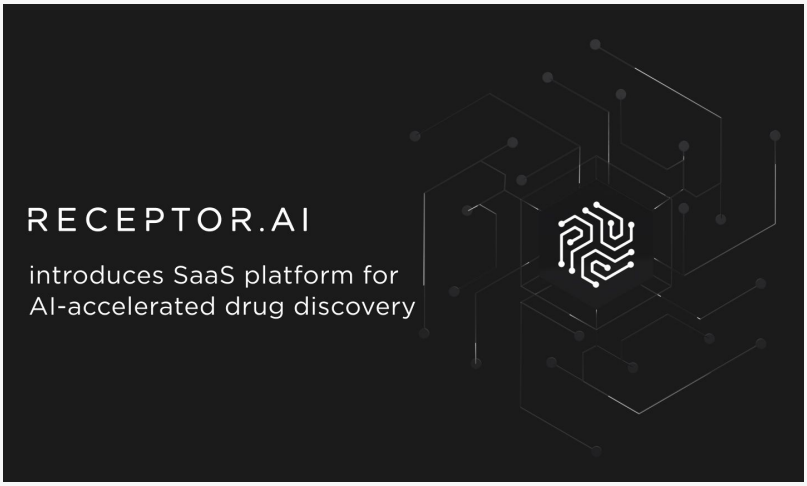
RECEPTOR.AI introduces SaaS platform for rapid and precise drug design

Receptor.AI announces the latest version of our AI-accelerated SaaS platform to disrupt drug discovery.



LONDON, UNITED KINGDOM, August 14, 2022 /EINPresswire.com/ -- Receptor.AI is delighted to announce the launch of the SaaS platform for AI-accelerated virtual screening of multi-billion chemical spaces within an hour.

Our platform has been used internally for several months and has shown experimentally validated results in several case studies and ongoing research collaborations. Moreover, the comparative testing of our technologies with other state-of-the-art algorithms has shown an overwhelming predictive capability of our platform. Now we are ready to provide it for our customers for very competitive prices and with a flexible subscription model.

Currently, our platform includes the following modules:

- AI-based ultra-fast virtual screening module for multi-billion chemical spaces. The module can operate with commercial chemical spaces provided by our partners as well as generate molecules based on novel scaffolds with desired parameters. These chemical spaces offer remarkable diversity and novelty while having a size of more than 30B synthesisable molecules. Moreover, we have created our own synthesisable combinatorial space of 10^16 molecules based on the building blocks and reactions provided by our partners.

- The AI-based ADME-Tox prediction module assessing ADME and toxicity profiles of the possible toxicity of selected hit candidates. The module incorporates more than 40 elaborate AI models, which simultaneously evaluate various pharmacokinetic parameters and potential modes of toxicity for every hit candidate produced by virtual screening;

- The AI-automated molecular docking module performing high-sensitive filtering and ranking of

the hit candidates. Applying this technique following our AI-based virtual screening provides the accuracy of binding affinity predictions, which is superior to existing competing approaches.

These modules provide a seamless automated experience in finding the hit candidates in case of insufficient ligand data for any human protein which is currently added to the platform. Moreover, our platform shows an ultimate average hit rate of 10%, saving time and costs for iterative experimental validation of results.

Our SaaS platform will quickly evolve to incorporate the lead discovery and lead optimisation modules in the next version. New and improved AI models will be integrated continuously. Stay tuned!

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