Discngine's 3decision platform to leverage complex protein-ligand 3D data

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Lundbeck will benefit from significantly faster, more efficient structural knowledge analysis, through cloud platform to discover new treatments for brain diseases

Discngine, a French software company specialized in developing applications for life sciences research, on 4 Sep 2019, announces that the Danish international pharmaceutical company Lundbeck has selected its proprietary 3decision® collaborative platform to manage the pharma company's structural knowledge related to protein and ligand 3D structures. Lundbeck is the first customer on Discngine's cloud platform, confirming the advantages it can bring to the pharmaceutical industry. Financial details of the agreement are not disclosed.

Today, rational structure-based drug design (SBDD) techniques are used in the majority of drug discovery projects. However, inconsistent data and complex analysis requirements of structural data hinder a wider uptake. Discngine's 3decision platform was developed to facilitate and accelerate the use of structural data for molecular modelers, structural biologists and medicinal chemists. Lundbeck will use the platform to help with the discovery of new treatments for brain diseases.

The platform transforms raw structural data coming from 3D structures and biomolecular sequences into well-organized and easily accessible knowledge. Thanks to its straightforward web-based interface, it enables both expert and non-expert users to browse, analyze and communicate around complex structural knowledge. Any user can quickly perform tasks such as binding-site comparisons and in-situ idea generation, and retrieve digested information from structures relevant to the project at hand.

Time-consuming and error-prone tasks like searching, retrieving, formatting and analyzing the relevant structural data in the beginning of an SBDD project can be accelerated and done in anything from a few minutes to a few hours, instead of a couple of days. Further down the project pipeline, in the hit-to-lead and the lead optimization stages, the platform allows all users to exploit the structural data to generate and test ideas. For example, both computational and medicinal chemists can quickly edit and re-dock a co-crystalized ligand in a couple of minutes.

"We are delighted that Lundbeck has chosen our cloud platform for handling its structural knowledge. This decision shows the increasing importance of collaboration between medicinal and computational chemists," said Eric Le Roux, founder and CEO of Discngine. "We believe that cloud computing will play an ever increasing role in pharmaceutical

research, bringing significant benefits to drug developers and eventually patients."

"It's important for us to have instant access to all internal and external structural data, and the 3decision platform is an outstanding tool for our purposes," said Lena Tagmose, senior director, Molecular Design and Enabling Technologies at Lundbeck. "It's time- and cost-efficient and brings significant advantages through instant accessibility and a wide range of data modelling options."

The development of the platform began three years ago in a co-operation with Abbvie. It was launched as a commercial product in 2018. In April it received the BioIT World 2019 Innovative Practices Award.

The 3decision platform is available as a Software-as-a-Service offering, on a monthly subscription basis. After initial sales of 3decision as an on-premises version with another customer, Lundbeck is the first pharma company to use 3decision via the cloud.