Chemotargets announces first AI-Designed drug for Huntington's disease to enter clinical trials

It is a potential first-in-class therapy, the result of the joint efforts between Catalan company Chemotargets and the North American startup Galyan Bio, and is expected to enter the clinical phase in 2022.

Barcelona, 22 April 2021. In less than 12 months, the collaboration between Chemotargets**,** based in the Barcelona Science Park, and Galyan Bio yields a scaffold for first-in-class clinical candidates in difficult area of neurodegenerative disease. Chemotargets employed its proprietary AI-driven *de novo* drug design methods in collaboration with Gaylan Bio to rapidly design novel molecules which would bind to the previously 'undruggable' Huntington's Disease target.

Huntington's Disease (HD) is a neurodegenerative disorder that affects thousands of patients worldwide. There is currently no cure or disease modifying treatment for HD. This is why US-based company Galyan Bio and Barcelona-based Chemotargets joined efforts to design a first in class drug for HD. The result has been the generation of a first-in-class drug candidate for HD. Galyan Bio plans to start clinical trials in HD in 2022. Galyan Bio's new treatment is intended to slow down the disease in symptomatic patients and delay manifestation of HD in symptom-free gene carriers.

"The development of new molecules through medicinal chemistry has always been a laborious and costly process. We used Chemotargets drug discovery platforms to speed up the process considerably. Based on Chemotargets' AI-driven de novo designs, we selected and tested 49 compounds. Our expectations were exceeded as we identified 6 compounds which could actually bind to our drug target. The optimization of one of those hits led to a preclinical drug candidate for HD", says **Dr. Marius Galyan,** CEO of Galyan Bio.

Chemotargets' proprietary ProSurfScan AI-driven de novo drug design platform uses novel methods of agnostically scanning the target protein to perform a virtual fragment-based screening of all possible drug binding areas. Fragments are then automatically linked to design effective binding molecules. The AI-driven methods employed by Chemotargets are particularly suited to novel, difficult, previously unaddressable targets as well as drug targets for which high isoform selectivity is required.

ProSurfScan is part of a complete suite of AI-driven drug discovery tools which are in routine use within Chemotargets that include CLARITY®, the industry-leading software platform for anticipating the safety of new drug molecules CLARITY® (Seal of Excellence project from the European Commission) is currently in use in many of the top pharmaceutical companies worldwide and at the US Food and Drug Administration.

"We are absolutely delighted to have effectively contributed to delivering a first-in-class drug candidate for HD. Having a tangible proof-of-principle that our de novo designs lead to progressible bioactive small molecules in a prospective drug discovery project means a world to us. This means that our in-silico platform is ready to address other novel, difficult, protein targets for which no therapeutic modalities exist", says **Dr. Jordi Mestres**, CSO of Chemotargets.

"First and foremost, we are grateful for the opportunity to contribute to a possible therapeutic alternative for Huntington's Disease patients. I am, quite frankly, not surprised by the experimental activity results of the molecules arising from the de novo design. ProSurfScan has repeatedly demonstrated its ability to design novel, selective molecules which bind to novel and difficult targets in our internal programs and will no doubt continue to do so", says **Dr. Scott Boyer,** CEO of Chemotargets.

"Although artificial intelligence is necessary in nearly everything, we do at Chemotargets, we are a company focused on helping patients. By using AI to aid decision-making in the design and development of novel therapeutics, our mission will always be to facilitate the development of safer, more effective therapeutics in less time and at a lower cost that was possible in the past. We are pleased that, for Huntington's Disease patients, we have been able to demonstrate that potential", he adds.

■ About Chemotargets

Chemotargets was founded in 2006 as a spin-off of the Systems Pharmacology research group of Dr. Jordi Mestres in the framework of the Hospital del Mar Medical Research Institute (IMIM). The company, based in the Barcelona Science Park, offers state-of-the-art methodologies with predictive capabilities in the field of pharmacology and drug safety. Its goal is to help the pharmaceutical industry accelerate drug discovery and development programs, while improving cost-effectiveness and safety. The current shareholders of Chemotargets are Dr. Jordi Mestres, IMIM and Prous Institute for Biomedical Research.

■ About Galyan Bio Inc.

Galyan Bio, Inc. is a startup company located in Berkeley, California (USA). Galyan is developing first-in-class orally available small molecules for neurodegenerative diseases, cancer and aging. It was founded in 2019 by Dr. Marius Galyan.

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