InterAx Biotech AG

Accelerate drug discovery by integrating biology, mathematical modelling, and AI

Company's summary

InterAx deciphers the effects of drug candidates on intra-cellular signaling – one of the least understood "black boxes" in biology, and a major point of failure for new medicines.

Main focus of the company are G Protein-Coupled Receptors (GPCRs) – the largest group of drug targets, accounting for more than 30% of all approved drugs. The company generates own quality-controlled experimental data using real-time cellular assays. The data is analyzed with proprietary mathematical models to determine mechanistic parameters of cell signaling activation. These parameters are fed into fit-for-purpose deep learning algorithms trained in drug chemistry – allowing to design drugs which are most effective in reaching desired and avoiding undesired cellular responses, thus reducing the risk of drug failure.

InterAx - Artificial Intelligence drug design

It takes 10-15 years and up to €2.3 billion for a new drug to enter the market. Of all drug discovery programs entering clinical development 90% fail, primarily due to limited biological characterization of drug candidates which manifests in unexpected efficacy and/or safety issues.

The InterAx real-time experimental assays on live cells and systems biology modeling re-creates a part of the *in vivo* biological complexity already during *in vitro* studies. This characterization of drug effects on cellular signaling allows to select drug molecules which are less likely to show unexpected physiological responses later on, and thus have higher chance to succeed in animal and human studies.

The InterAx machine learning / AI algorithms are trained on proprietary systems biology datasets to understand both the biological effects of GPCR drugs on cell signaling, and the chemical-structural rules of drug-target interactions. This union of systems biology and AI enables InterAx technology to guide the design of new chemical entities with desired cellular biology signaling parameters.

In addition to the classic discovery of high affinity binders, InterAx technology opens new dimensions in drug design – enabling selection of high efficacy drug candidates based on cellular biology mechanisms. In other words, this technology helps to move from "ligand discovery" to "drug discovery".

InterAx GPCR systems biology approach has proven itself in several collaborations with pharma partners. To confirm the power of further uniting systems biology with machine learning / AI InterAx focused on beta-2-adrenergic receptor (B2AR) – an anti-asthma target. InterAx systems biology AI computationally designed a set of novel drug candidates for this target, which were then synthesized and experimentally proven to show high efficacy of B2AR activation on a specific signaling pathway.

InterAx AI models learn from drug-target molecular dynamics and systems biology parameters – to predict which drug chemistries will show the desired efficacy and biological response.

Dr. Aurélien Rizk, CEO rizk@interaxbiotech.com
InterAx Biotech AG, PARK innovAARE, 5234 Villigen, Switzerland

Impact

After successful proof-of-concept show-cases, InterAx is now increasing throughput of its technology platform and ramping up own in-house drug discovery program – supported by the new technological advancements. The discovery program for treatment of several solid tumors via a novel target is showing promising results. First in class, high potency, drug molecules are currently under investigation in animals after successful *in vitro* tests to block proliferation and migration of breast cancer cells.

InterAx is setting an industry example of how to better understand and de-risk drug candidates: by leveraging not just large quantities of data with machine learning algorithms, but simultaneously incorporating crucial biological knowledge of the underlying system into the intelligent drug discovery algorithms. Rigorously building such bottom-up understanding of the target systems is a challenging task, which, nevertheless, is an unavoidable milestone on the path to rational design of effective and safe drug candidates.

The AI architecture established at InterAx paves new way to generate *in vivo*-like systems biology knowledge and directly incorporate it into intelligent workflows at the early stages of drug development, thereby designing and selecting more efficient and safer drugs.

Dr. Aurélien Rizk, CEO rizk@interaxbiotech.com
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