InterAx Biotech
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INTERAX

Beyond target identification and ligand discovery: connecting artificial intelligence and cell signaling

InterAx Biotech has developed a specialist drug discovery approach that combines artificial intelligence, integrated mathematical models and cell biology experiments to enable the early identification of safe and effective candidates.

Many drug candidates fail in animal and human studies, sometimes as late as phase 3 trials. A more solid knowledge of the effects of drug candidates on the little-understood area of intracellular signaling, like that offered by Switzerland-based InterAx Biotech, will help to de-risk drug development by weeding out unsuitable compounds and result in safer and more effective drugs.

"It is crucial to create better drug candidates, rather than just generate them faster and cheaper. By designing drugs triggering specific intracellular signaling effects, we obtain safer and more efficacious drugs and thus significantly de-risk the development process," said Aurélien Rizk, CEO of InterAx Biotech. "It has been calculated that reducing the failure rate provides by far the biggest benefit, with a 20% decrease in failure rates in clinical trials leading to net savings of more than $500 million."

Early-access programs with partners such as Boehringer Ingelheim, Lundbeck and GPCR Therapeutics have provided strong validation of the approach and market need.

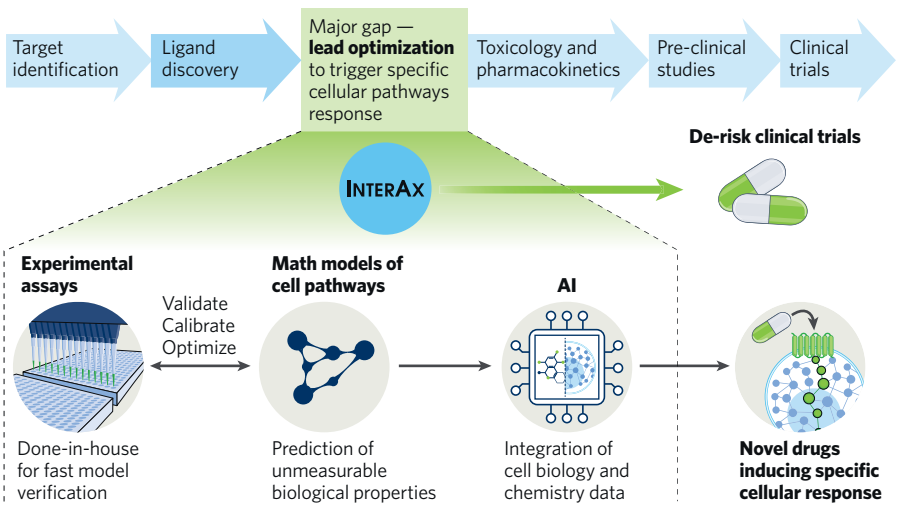

Fig. 1 | Bridging the gap in drug discovery. By combining experimental assays, mathematical modeling and artificial intelligence (AI), InterAx can create novel drugs to induce a specific cellular response, resulting in higher therapeutic efficacy and safety thus de-risking clinical trials.

Applying the technology

InterAx's methodology uses integrated computational methods, artificial intelligence (AI) and state-of-the-art cell biology and pharmacology for G-protein-coupled receptors (GPCRs), the largest class of pharmacological targets. The approach begins with expression of the target in cell lines, followed by assays to understand the kinetic intracellular signaling of the target (Fig. 1).

The next step is to generate a mathematical model that describes the signaling pathways that are modulated by the target. The model incorporates data on the interaction between the target and the signaling pathways, crosstalk between different signaling pathways, and influence of other cell parameters including protein expression levels. Results from the experimental assays and the mathematical model iterate back and forth to validate and calibrate the model and optimize the assays.

The mathematical model is then used to derive comprehensive characterization of drug candidates, independent of assay types and conditions, providing an in-depth view and understanding of the signaling pathways modulated by the drug-target interaction. The model can also determine the signaling properties that are predictive of in vivo behavior. Results from the mathematical model are then fed into machine-learning algorithms, which leverage computational chemistry datasets to design new chemical entities. These compounds are thus designed to induce specific, desired cellular responses, leading to high therapeutic efficacy and safety in vivo.

"We use AI technology, but our core is in systems biology and mathematical modeling, and this is what differentiates us from competitors," said Rizk. "The mathematical models provide a bridge between the experimental cellular assays and the machine-learning algorithms."

For a typical target, characterizing the pathways, selecting hits and optimizing leads takes between two to eight months. The package delivered to the client also includes information on the compounds, such as their effect on the biology of the target and the signaling pathways involved, making it possible to predict the effect of the compounds and understand their mode of action. The InterAx platform can be used to characterize partners' existing drug candidates, helping them to design, select and optimize the best leads. It also allows the unlocking of undruggable drug targets where the cell biology is poorly known.

"We help our partners to create better hits and leads, and we provide data that allows the drug developers to learn more about the drugs up front. In addition to traditional affinity, potency and efficacy parameters, we provide precise information on the response that compounds trigger inside the cell after binding to the target. This information explains why the compound works—or why it doesn't—allowing the drug developers to concentrate on positive traits as they move towards the next stage," said Rizk.

To validate its approach, InterAx initially carried out a retrospective analysis of asthma drugs, successfully showing that the platform predicts therapeutic efficacy at a very early stage, and allows to optimize compounds chemistry to achieve high clinical efficacy. Similar successes followed later in pharma partnerships.

Collaborations and partnerships

InterAx offers access to its unique platform capabilities to biopharma partners and collaborators in need of in-depth insight for the design of high-quality drug candidates that trigger a desired pathway modulation.

"We conducted early-access programs with Boehringer Ingelheim, Lundbeck and GPCR Therapeutics, and just started a new project with Boehringer Ingelheim," said Rizk. "These partnerships validated our technology, and supplied great value to our early partners."

InterAx also has its own in-house discovery program. In mouse studies, InterAx's first-in-class small molecule IAX25663 blocks the biological function of a chemokine receptor responsible for causing tumor growth and metastasis. This target plays a key role in many solid tumors.

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