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Interview

How companies will benefit from the first fund for circular bio-economy – ECBF head Michael Brandkamp explains.

THE VOID

COVID-19 Therapeutics

The Green Deal
How biotechnology can change industry in the post-COVID age

Diagnostics
Building a common European framework for antigen tests

Antibodies & Jabs
Industry pipelines full with candidates to ease pandemics

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New Chemical Entities

Existing Drugs

Chemical Scaffolds

Combinations

Pepticmimetics

Novel Targets

Peptides

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Rescue your failed drugs

- By identifying new indications
- By identifying new chemical scafolds for medicinal chemistry
- By combining your drug with another one

Build your own pipeline

- By identifying known drugs/NCEs with novel targets (as a biologic drug/small molecule) in unmet medical indications

Put your R&D process at the forefront

- By identifying novel and known off-target MoAs for the molecules/biologics

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A pioneering real AI drug discovery technology

DRUG DISCOVERY The current COVID-19 pandemic situation has shown that repurposing drugs can be crucial for delivering new treatments to patients with agility. Existing drugs can be developed to bring fast, safe and cost-effective treatments for a wide range of conditions. The improved use of data and the development of advanced AI-based technologies enable the fast and effective identification of drugs, accelerating drug discovery, repurposing and innovation.

› Raúl Insa, MD, PhD, MBA, CEO and Founder of SOM Biotech

The rapid growth of computing power, data availability and the development of advanced genetic algorithms have led to very relevant breakthroughs in artificial intelligence (AI). AI applications are used for a wide range of fields in the life sciences sector. But moreover, AI is revolutionising drug discovery and specially drug repurposing.

SOM Biotech works with a proprietary ligand-based in-silico platform, SOM^{AI} PRO that has proven to be an outstanding tool to successfully identify drugs with similar or better biological activity compared to a reference compound acting on a disease-related target. The drug discovery approach is fundamentally based on molecular structures, and particularly on their structural and physicochemical properties – the "molecular fields" (MFs). SOM^{AI} PRO aligns the MFs of the reference compound with those of a comprehensive Phase II-and-up compound database, using evolutionary algorithms. In this way, SOM^{AI} PRO finds ready-to-repurpose non-structural analogues that can bind to the same target protein as the reference compound, causing the specific desired biological response. As simple as that.

Evolutionary algorithms are inspired by biological evolution. The algorithm proposes solutions to an optimisation problem (in this case, MFs alignment); these solutions are then evaluated by a fitness function and the "fittest" ones are crossed to create the next generation of solutions. This process is iteratively repeated to find the best solution. The number of iterations that SOM^{AI} PRO performs has been optimised through extensive validation. Once the best candidates are selected, their predicted biological response is subsequently verified *in vitro*.

SOM^{AI} PRO is a powerful tool with high predictive power. In 30% of the unmet medical indications selected, the system has been able to find active *in vitro* candidates and in 12% of those projects a drug has successfully reached Phase II positive results. The platform is being continuously improved and updated and today it works not only to identify compounds for a specific disease, but also to identify molecular targets and associated therapeutic areas, indications, or diseases for a given compound. This can be very useful because a compound that failed clinical studies for lack of efficacy can be found to act on a different target and can therefore be repurposed for another indication. In addition, SOM^{AI} PRO can be also applied in early-stage drug discovery projects, when new chemical scaffolds have to be explored, taking special care to retain key molecular physicochemical properties.

The high success rate in SOM Biotech's drug discovery process is clearly linked to the expertise of its team. It is not a routine activity: the process of compound identification to preclinical candidate selection and validation requires significant know-how from scientists and experts of a variety of disciplines. The approach is flexible depending on the characteristics of a specific drug or target discovery program. SOM Biotech screens different Phase II-and-up compound collections and uses a proprietary library of druggable targets, with the ultimate goal being to provide readily available, effective, and safe treatments to patients. ■

Picture: SOM Biotech