Using AI to accelerate drug discovery

An innovative young company, Standigm Inc., is creating CUTTING-EDGE AI TECHNOLOGY for discovering and developing new therapeutics.

Drug discovery and development has always been subject to a large degree of chance and serendipity. Now, artificial intelligence (AI) is promising to substantially boost the odds of identifying new drug candidates that can be commercialized. Fewer than 10% of drug candidates that make it to clinical trials progress beyond the first of the four phases. And for each drug candidate that does go all the way to become a commercial product, the entire process takes about 10-15 years and costs more than US$2 billion, on average. By eliminating some of the guesswork from the process, AI promises to cut the cost and timeline.

Standigm is one of the early pioneers to apply the power of AI technologies to drug discovery and development. The company hopes to eliminate some of the false guesswork from the drug-discovery process. So far, Standigm is employing its unique AI algorithms throughout the drug discovery and development process. By eliminating some of the false guesswork from the process, AI promises to cut the cost and timeline.

Standigm employs AI to detect patterns and trends relevant to human biology across vast biomedical databases. It uses three main proprietary AI models, including hit generation, lead optimization, and drug repurposing and target discovery, and then applies novel design solutions to go from new disease targets to innovative molecules in record time.

The process begins with dataset parsing to interpret and sort all available information in a usable way. After rapidly exploring these datasets in detail, Standigm’s technologies can generate drug candidates by applying AI modeling, which automatically analyzes the innumerable ways the data can be combined and configured to create weight-optimized, deep-learning models based on rules hidden in the data. By using a virtual landscape, the AI technology then assesses biological performances of drug candidates — examining how they would probably interact with real patients and how effective a particular drug might be in treating certain diseases. Thus, the technology can optimize the structure of lead compounds in drug discovery concerning desired chemical properties such as binding affinity or absorption, distribution, metabolism, excretion and toxicity. Researchers can use this information to inform choices about which drug candidates to investigate further.

The company initially explored new potential uses for already-marketed drugs and possible applications for different combinations of established drugs. But now, in collaboration with several leading international pharmaceutical companies, Standigm is focusing on the earliest stages of drug discovery, with the identification of useful novel compounds at the core of its business. Thus, Standigm seeks to produce highly targeted opportunities for potentially successful new drugs.

In collaboration with an IT firm, Standigm has recently developed a searchable online platform called iCLUE&ASK™ where researchers can prioritize potential protein targets for diseases. The AI-aided target discovery platform offers protein targets by producing a huge knowledge graph database from the context of all the scientific data, which can be used to rank targets for various disease areas. Targets provided by iCLUE&ASK™ are being experimentally validated and used for lead generation with global collaboration partners.

Kim adds that another of Standigm’s strengths lies in the company’s commitment to continually revisit and re-evaluate its processes, monitoring and fine-tuning its algorithms, retaining what works and discarding what doesn’t. “If we fail, we update our model to make a better decision,” Kim explains. “In this way, we keep learning from our experience and cutting the time it takes to reach the end product.”