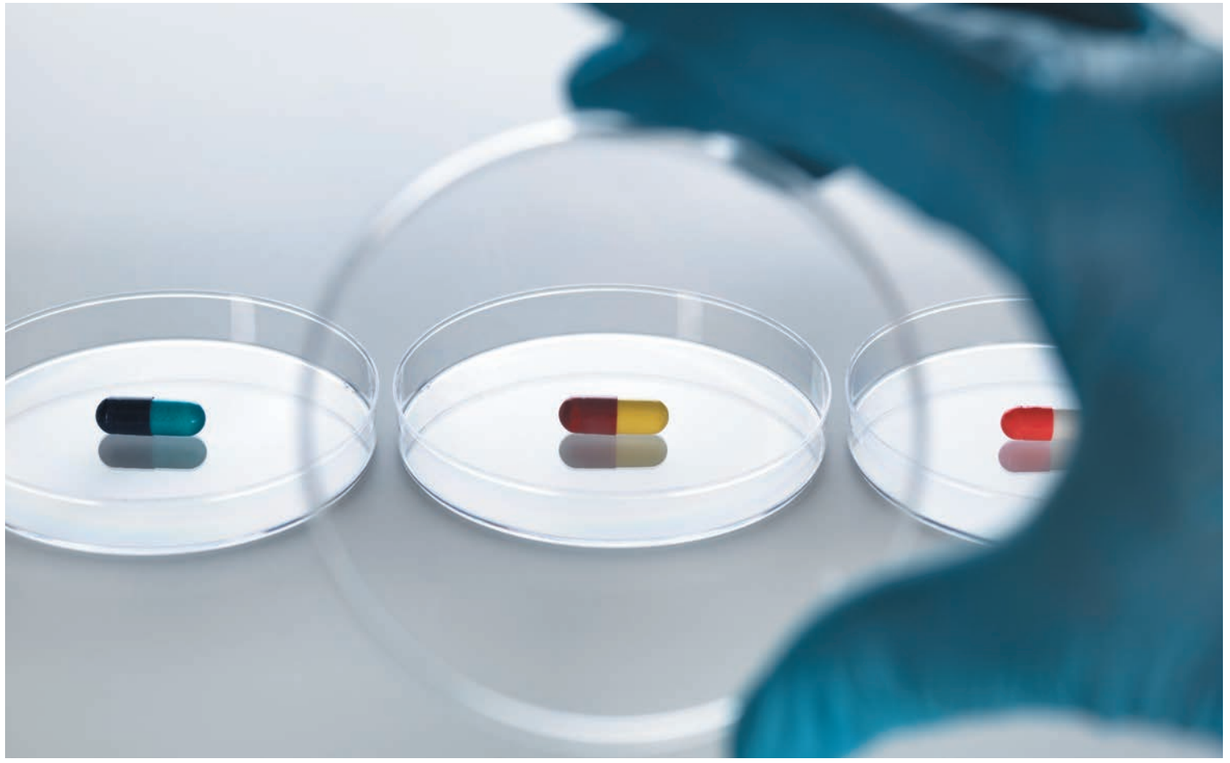
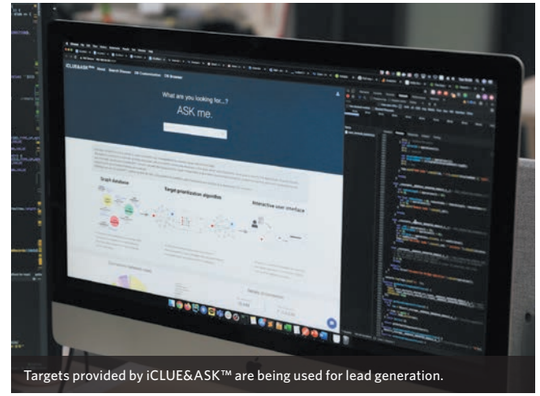
ADVERTISEMENT FEATURE

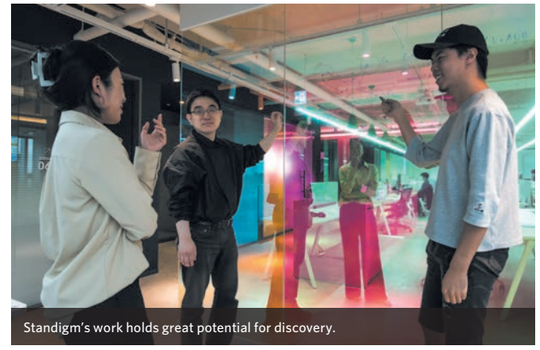
Using AI to accelerate drug discovery

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





Targets provided by iCLUE&ASK™ are being used for lead generation.



Standigm's work holds great potential for discovery.

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 starts in drug development by employing its unique AI algorithms throughout the process. So far, Standigm has produced strong preclinical opportunities for four conditions: Parkinson's disease, autism, mitochondrial diseases, and the liver disease, non-alcoholic steatohepatitis.

But that's just the beginning. "There's no limit to the potential diseases and disorders that could be assessed," says Taeyong Kim, a principal scientist at Standigm with a background in biology. "Standigm is currently using its unique combination of scientific talent and technology to work with drug-discovery teams on several continents."

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A multidisciplined approach to AI

Standigm was founded by three colleagues whose expertise spanned AI, chemical engineering and systems biology. The seemingly disparate range of disciplines that underpinned Standigm's genesis remains a strength of the company today, as exemplified by its multidisciplinary workforce. "We have AI engineers, chemists and biologists all in one place, working together as teams on projects investigating problems at the heart of our business," explains principal scientist Hanjo Kim, a chemist at Standigm. "This collaborative approach is key to the company."

Reducing the guesswork

AI is attractive for drug discovery because it applies the rapid and massive number-crunching capabilities of 21st-century computing technologies, such as machine learning, to data comparison and analysis in the way the human brain would, but in a fraction of the time.

Standigm employs AI to detect patterns and trends relevant to human biology across vast biomedical databases. It uses three main proprietary technologies, including hit generation-lead optimization, 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 modelling, which automatically analyses 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 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.

Intellectual property is at the core of any pharmaceutical business, and hence the ability to assess a potential candidate's novelty is paramount, explains Kim. "We have our own proprietary technology that can be used to score the novelty of a molecule," he says. "That makes it possible to identify, with a high degree of certainty, whether a potential new drug candidate is likely to result in a patentable product, providing pharmaceutical companies with a degree of economic confidence in which potentially marketable products they should invest."

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." ■

Standigm

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