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The greatest strength of Molcure's system is the ability to discover drugs that could never be found by using conventional methods

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Ryu Ogawa and Satoshi Tamaki of Japanese AI-powered drug discovery firm Molcure outline how their technology can supercharge the speed and efficiency of the drug discovery process as well as the wider implications for greater use of artificial intelligence in the biotechnology field.

Can you begin by explaining Molcure's origin story and the initial problem the company set out to solve?

Ryu Ogawa (RO): When I was a student, my focus was on creating artificial intelligence (AI) systems for scientists in the biotechnology field. This research contributed to society but in an indirect way. When my father contracted cancer, I felt powerless because my work was not able to solve that problem. Therefore, I wanted to shift to contributing directly to people's health, using the technology that I had previously studied to help create biotech drugs. This led to the creation of Molcure in 2013.

What have been some of the key milestones since Molcure's founding?

RO: Molcure's first important milestone came in 2012 with the proof of concept of our AI-driven technology. This proof of concept was validated and verified on a small scale before the company

was established.

The second milestone came in 2014 when we received around USD two million in funding from the venture capital (VC) arm of Tokyo University. With this funding, we were able to build up our technology to utilize greater amounts of data and potentially discover more molecules.

In 2016 our third major milestone came when we were selected as a vendor of Japanese next-generation drug discovery technology, which was a big project for a start-up like Molcure. This project was also worth around USD two million in funding, primarily from the Japanese government.

In 2018, we raised USD three million from a large Japanese insurance company, a mid-sized Japanese pharmaceutical company, and the VC branch of GMO Internet, one of the country's most significant internet and software companies. With this funding we were able to open our technology to pharmaceutical companies, having previously only worked on joint research projects with universities and research institutes. Today, five pharmaceutical companies are using our AI technology, one from the US and the other four from Japan.

How do Molcure's two proprietary drug discovery technologies Abtracer, Peptracer and HAIVE work and what is their advantage over more traditional methods of drug discovery?

RO: Molcure's unique proprietary antibody and peptide discovery platform, Abtracer and Peptracer, and newly developed automated drug discovery system, HAIVE, are part of our whole system, which has three functions. The first and second one is to do biological experiments using HAIVE to executes those experiments automatically with high levels of accuracy and reproducibility. The second function is to collect a large amount of data from those experiments. The third one is to analyze those data sets to train the AI. The AI then outputs the molecule structure of the new drug candidate.

The greatest strength of Molcure's system is the ability to discover drugs that could never be found by using conventional methods. Of course, the system's accuracy and speed are significant, but the ability to discover unique molecules is the key selling point.

With the global biomedical community currently scrambling to find COVID-19 treatments and vaccines in record time, what do you see as the potential for greater

integration of artificial intelligence in biotechnology?

RO: There are two major impacts of AI in biotechnology. The first one is to give scientists more time and space to be creative. In the drug discovery field, there are a lot of lab tasks that can, and should, be done by robots rather than humans. This will allow scientists to use their time to create new ideas and methods for biological experiments.

The second major impact is on what AI can teach scientists, as well as what scientists can teach AI. Scientists come up with new ideas, which they then teach to the AI, but also the AI tests many things using robotics that scientists can learn from.

Satoshi Tamaki (ST): This links into some of the work that Molcure is undertaking. Currently, we do scientist-designed experiment protocols. We execute some of these protocols with robots, then the scientists analyze that data and put it to AI. The AI system then comes up with some conclusions before the scientists could make a final decision. In the next stage, our company will try to make this cycle faster by automating some of the processes.

We want to establish an AI system that gives all the orders to the robot system. Then the robot will proceed with the experiment and gain data. The AI system will then take that data automatically and think of new experimental protocols. This cannot be fully automated, but most parts can. We want scientists to focus more on the discussion phase of the R&D process.

We have been hearing about the concept of AI in drug discovery for a while. As a small company, how do you compete with the technology giants also investing in this area?

RO: General-purpose AI that can be used for translation or facial recognition, for example, is dominated by big players like Google and IBM and this is an area where a small company like Molcure is unable to compete. However, we operate in a very specific field for which a lot of deep domain knowledge of biology, chemistry, and physics is required to create AI and AI training datasets.

Small start-ups should focus on their specific niches and create technology that tech giants cannot invent themselves. For example, we have designed many new biological experiments for gathering training datasets as well as creating an original machine to execute those biological experiments.

ST: From an R&D perspective, speed and focus are the most important assets that Molcure possesses. Of course, larger companies can also move quickly, but our ability to focus on one

objective alone is what sets us apart.

How has the Japanese start-up ecosystem evolved since Molcure's founding in 2013 and what barriers to its further evolution remain?

RO: There have been some significant improvements. At the time of our company's first fundraising round in 2014, there were almost no VC funds for deep tech start-up companies with the objective of providing technology-based on substantial scientific advances and high tech engineering innovation in Japan. The only VC that understood technology and had a scientific background was that of Tokyo University, which had PhDs as well as financing experts on its staff.

However, today there are about four such science-focused VC funds related to major universities in Tokyo, Kyoto, and Osaka in Japan. This represents great progress but overall, there are still very few science-focused VCs in Japan. Budgets are also getting bigger, but fund sizes remain comparatively small in relation to other industries.

To make the Japanese start-up ecosystem even better, all stakeholders – not only VC and the start-ups themselves – need to raise awareness of this sector. In Japan, a mindset still exists whereby the only viable and respected career path for scientists is to go to a good university, and upon graduation began working for one of the country's large conglomerates.

Gradually this mindset is shifting, with lifestyles and career paths becoming more diverse and start-ups more accepted as a viable option for young innovators. However, there needs to be a continued push from the Japanese government, media, and education system to ensure that this positive trend continues.

Having previously worked solely with academia, you now count five pharmaceutical companies as partners. How did you acquire these partners and what is your partnership strategy moving forward?

RO: In all honesty, our team is made up almost exclusively of scientists, meaning that we perhaps initially lacked a clear commercial and partnership strategy. However, with the expansion of our business, we have begun to collaborate with sales agents with previous experience in Big Pharma and good connections with the industry to help us in our partnership push. We also attend business conferences on biotechnology, and we will be looking to broaden our strategic efforts to find even

more partners and increase the awareness of Molcure.

Molcure is currently a provider of software but its technology has the potential to take care of the entire drug discovery cycle. What are your ambitions for the company's future?

RO: Our current focus is on designing pharmaceutical drug molecules. In the future, we want to create many kinds of molecules, not only drugs, for the benefit of humanity. We would like to become the de facto standard technology for the design of those molecules at the very early stage of drug discovery.

ST: In the relatively short-term, our company is supporting pharmaceutical companies' drug discovery process. Our technology can help discover various types of drugs, but we are not aiming to become a pharma company and make drugs ourselves, but instead spread our service to lots of pharma companies around the world. We want to become the recognized AI-supported drug discovery platform for all pharma companies.

Then, we want to gather all the data inside our company and use that data to train our AI systems. The more the customer uses our system, the smarter and more accurate the system gets.

What are your priorities for the next five years?

ST: Looking for new drug candidates will remain one of our areas of focus, but my key objective is the incubation of our automation robot and our biotech/AI systems. We are trying to create a new type of ecosystem for pharma companies with stronger links between AI, robotics, and biotech.

RO: In the next five years, we want to engage in joint research with pharma companies and reach a total of 100 projects, meaning that hundreds of new drugs will be designed with our system.

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