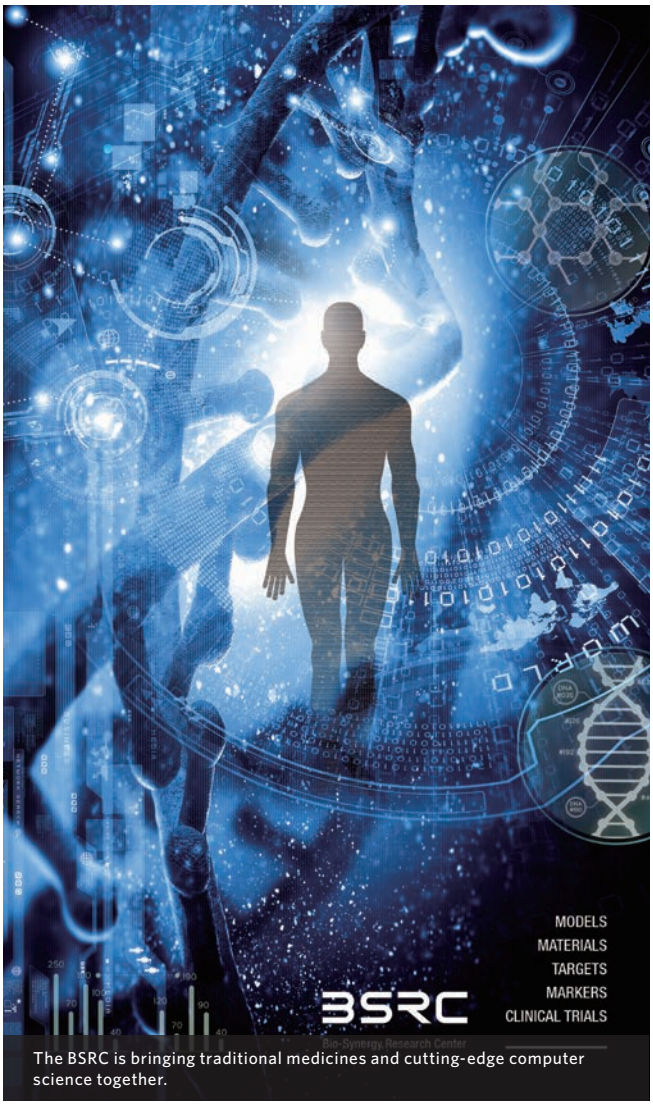
Traditional medicine meets artificial intelligence

CODA is a powerful tool that can change the future of DRUG DEVELOPMENT



The BSRC is bringing traditional medicines and cutting-edge computer science together.

A computer program that acts as a virtual human body could help predict how people will react to new therapeutic drugs. It will enable more chemical combinations to be tested with fewer human trials, making drug development faster, cheaper, and safer.

Researchers at the Bio-Synergy Research Center in Daejeon, South Korea, recently developed CODA (Context-Oriented Directed Associations), software that draws on recent advances in artificial intelligence and biotechnology. The team plans to use CODA to explore the therapeutic potential of chemical compounds found in traditional medicines, such as Samul-Tang — a combination of extracts from four Asian plants used to treat blood disorders such as anaemia. The work is guided by a comprehensive account of Korea's rich medicinal heritage from a 400-year-old book called *Dongui Bogam*.

Doheon Lee, a professor of bio- and brain engineering at KAIST, and the director of the Bio-Synergy Research Project, believes that CODA could speed up personalized drug development — tailored medicines based on a patient's genetic and physiological characteristics — by reducing the number of superfluous trials. He says, "CODA's prediction power can save time and money by providing important biological information that will enable us to conduct experiments efficiently."

Previous drug development strategies have focussed on producing chemicals designed to react only with the proteins involved in a disease, reducing the risk of side effects. But these drugs can still react with unintended targets. As Lee explains, "some serious diseases, such as cancer, can cause many complex interactions, so a multi-target approach that regulates them entirely can be effective". It is impossible to test every possible combination of drug on a broad range of patients. CODA aims to find a solution.

To build CODA, the researchers first developed a computer language to represent biological interactions. They then gathered information from public databases and the scientific literature to construct a network of potential interactions between chemicals, proteins and genes within, and between, organs.

"Identifying unexpected drug interactions is an essential step in drug development," says Lee. His team has recently developed a method to test the effects and interactions of drug pairs, rather than single drugs, using CODA. "The CODA system can be used to predict and analyze the efficacy, toxicity and mechanism of action of multiple components," Lee concludes. When tested using drugs with verified effects, CODA successfully identified both therapeutic and adverse effects.

Lee hopes to make CODA into an online service that will "enable users to easily perform various drug analyses, and predict the effects of single and complex drugs". The research centre will continue to investigate the molecular activity of natural compounds extracted from traditional medicines. "With CODA, we can discover new healthcare materials, including botanical drugs, and functional foods". ■

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