

Press Information, August 30, 2022

Harnessing AI to Discover New Drugs

How a visionary scientist established his innovative technology concept in industry

The Schering Stiftung awards the 2022 Ernst Schering Prize to Gisbert Schneider. Through his visionary research, the pioneer in the field of AI-assisted drug development has made it possible to move the idea to industrial application. As a result, active pharmaceutical ingredients can be identified more quickly and tested for potential side effects worldwide.

Gisbert Schneider is considered a pioneer in the field of targeted molecule design using machine learning methods. The biochemist and bioinformatician has broken new ground and advanced artificial intelligence (AI) to the point that it is now possible to reliably predict the efficacy of drugs. His method builds on the knowledge about known active ingredients, natural products, and their effects, and uses AI to develop new drug candidates with desired properties. Through his excellent research and his unflagging commitment to technology transfer, he was able to gain the trust of industry and thus lay the foundations for the use of these methods in modern biomedical practice. Already today, this technology enables a much more efficient identification of potential active ingredients, thus significantly increasing the chances of success when it comes to the development of new drugs.



Prof. Dr. Gisbert Schneider
Photo: Daniel Winkler / ETH Zürich

Prof. Dr. Gisbert Schneider is Professor of Computer-Assisted Drug Design at the Institute of Pharmaceutical Sciences at ETH Zurich and director of the Singapore-ETH Center. For his outstanding research in the field of molecular design, especially the development of machine learning methods to predict drug activity, Gisbert Schneider receives the **Ernst Schering Prize 2022**. The transfer of this innovative concept into medicinal chemistry and chemical biology is recognized as an important contribution to the theory and practice of modern biomedicine.

A seven-member jury composed of international scientists has selected Schneider's research from among a variety of outstanding nominations. The 50,000-euro Ernst Schering Prize is one of the most prestigious German science awards. It is given annually by the Schering Stiftung and honors international scientists whose pioneering research has yielded new, inspiring models or led to fundamental shifts in biomedical knowledge. Prof. Dr. Dr. h.c. Stefan H. E. Kaufmann, Chairman of the Foundation Council of the Schering Stiftung, said: "I have come to know Gisbert Schneider as a visionary who, due to his experiences in both the pharmaceutical industry and academic research, successfully brings together both worlds. At a time when many were still skeptical about the benefits of artificial intelligence for pharmaceutical research, he did not lose faith and improved the technology until it was ready for use."

Gisbert Schneider was nominated for the Ernst Schering Prize by the Office of the President of ETH Zurich. The head of the Strategic Foresight Hub at ETH Zurich, Dr. Chris Luebke, said: "Drug discovery is a long and laborious process. Gisbert Schneider recognized the potential of machine learning to accelerate the discovery of new medicinal agents and increase selection efficiency. His deep belief in and unwavering commitment to this new approach has led, on a sometimes unpopular path, to a paradigm shift in drug research. I am therefore very pleased that Schneider's extraordinary achievements will be honored with the Ernst Schering Prize 2022."

Award Ceremony – Ernst Schering Prize

September 29, 2022, from 5:00 p.m.

Berlin-Brandenburg Academy of Sciences and Humanities | Markgrafenstr. 38 | 10117 Berlin | Leibniz Hall

5:00 p.m. Ernst Schering Prize Lecture

Prof. Dr. Gisbert Schneider:

How artificial intelligence has revolutionized drug research

6:00 p.m. Award Ceremony

Award Presentation: Ulrike Gote, Senator for Higher Education and Research, Health, Long-Term Care and Gender Equality

Attendance by registration only. Please register with Maren Isabel Fritz at fritz@scheringstiftung.de.

Additional Lectures by Prof. Dr. Gisbert Schneider

September 29, 2022, 10:30 a.m.

Public scientific lecture: De novo drug design with machine intelligence
Einstein Center Digital Future, Wilhelmstrasse 67, 10117 Berlin, Event Space
In English | No registration necessary.

September 30, 2022

Lecture to students: Artificial intelligence in modern drug research
Schulfarm Insel Scharfenberg, Berlin-Tegel (not open to the public)

Background Information

The integration of artificial intelligence into medicinal chemistry has changed pharmaceutical drug research forever. Schneider's approach combines machine intelligence with the synthesis of pharmacologically relevant chemical substances, making it possible to significantly facilitate the discovery of new drugs. This process represents a complex multi-dimensional problem, where different properties of active agents – including their chemical synthesizability and pharmacological activity – need to be optimized in tandem in order to design new drug candidates. It uses, for example, automated chemical synthesis, biochemical tests, and especially artificial intelligence methods to continuously improve the design hypothesis through feedback. This way, it is possible to increasingly automate many aspects of this multidimensional process on the path towards potential drugs.

Gisbert Schneider studied biochemistry at the Freie Universität Berlin, where he also received his doctorate in 1994. After several international post-docs, he joined Roche Pharma in Basel. In parallel, he completed his *Habilitation* at the University of Freiburg. In 2002 he moved from industry to the Goethe University Frankfurt where he was awarded the Beilstein Endowed Chair of Chem and Bioinformatics. Since 2010, he has been Full Professor of Computer-Assisted Drug Design at the Institute of Pharmaceutical Sciences in the Department of Chemistry and Applied Biosciences at ETH Zurich. In 2021, he was also appointed director of the Singapore-ETH Center. Schneider is the founder of several startups, and his research has been honored with numerous international awards.

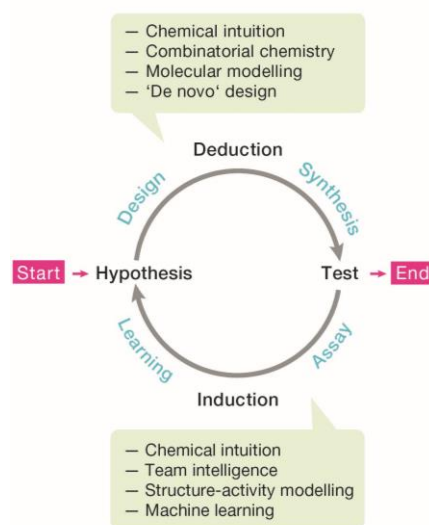
Further Information

This press release as well as images related to the prize recipient, Prof. Dr. Gisbert Schneider, can be found at <https://scheringstiftung.de/presse/>.

Press contact:

Maren Isabel Fritz, Project Manager Science
Schering Stiftung, Unter den Linden 32–34, 10117 Berlin, phone: +49-(0)30-20 62 29-67,
fritz@scheringstiftung.de

Molecular design with collaborative intelligence



Schematic diagram of drug development.
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