From computational pharmacy to modern drug discovery

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Modern drug discovery is a long and tedious process which costs at least 10 years and 2 billion USD in average. How to speed up this expensive process has become one of the most essential topics in pharmaceutical industry. With the progresses in both artificial intelligence and computational biology, advancing modern drug discovery via computational pharmacy plays more and more important roles. In this talk, Prof. Yuan will illustrate applying computational biology and artificial intelligence to answer fundamental questions in life science, especially in the area of G protein-coupled receptors (GPCRs). He will also discuss how to speed up modern drug discovery in an ultimate efficient way. Finally, Prof. Yuan will also talk about his successfully story on how to develop “first-in-class” drug molecules into clinical trials.

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Prof. Shuguang Yuan obtained his master degree in biochemistry and structural biology from the Shanghai Institute of Organic Chemistry (SIOC), Chinese Academy of Sciences in 2009. Following that, his doctoral dissertation was funded by the Maria Curia Fellowship. It was conducted in three different institutes in Europe: EPFL(Switzerland), Polish Academy of Science (Poland) and KULeuven University (Belgium).

In his research, he investigated the principles of various biological systems including enzymes, kinases, ion channels, transporters and, in particular, G protein-coupled receptors (GPCRs). In June 2013, he was awarded with a PhD title with the honor of distinguished thesis. Following that, he was offered the Marie Curie ETH Postdoc Fellowship. In 2014, Dr. Yuan proposed a theory about the activation mechanism and the continuous water channel of GPCRs (Nature Communications, 2014), which has been widely recognized in this area.

Prof. Yuan worked at Idorsia (previously known as Actelion) Pharmaceutical Ltd in Basel as a specialist in computer-aided drug design (CADD) for 5 years. In the past few years, he has advanced two of his designed molecules into clinical trials. In 2018, he was honored with a title of "affiliate professor" by the University of Warsaw. In 2019, Prof. Yuan was offered a full professor position by the Shenzhen Institute of Advanced Technology, CAS. He is also the director of the "Research Center for Computer-aided Drug Discovery" (http://www.cadd2drug.org).

In 2020, Prof. Yuan established the start-up “AlphaMol Science Ltd” with Prof. Horst Vogel together in both Switzerland and China. AlphaMol combines innovative computational methods with newly invented biotechnology to advance modern drug discovery. Currently, there are several “first-in-class” drug discovery pipelines are actively being progressed in AlphaMol.