School of Molecular Sciences

Arizona State University

SMS Fall 2023 Seminar Series

Friday Dec 1| 3pm | Biodesign Auditorium

The Simple QTY Code for Protein Design

The simple QTY code is based on two key molecular structural facts: **1**) all 20 amino acids are found in naturally occurring alpha-helices regardless of their distinct chemical properties: (a) hydrophilic, (b) hydrophobic and (c) amphiphilic; **2**) several amino acids share striking structural similarities despite their different chemical properties; for example, glutamine (Q) *vs* Leucine (L); Threonine (T) *vs* Valine (V) and Isoleucine (I); and Tyrosine (Y) *vs* Phenylalanine (F). Using the simple QTY code, we replace 40%-60% amino acids L, I, V, F in transmembrane a-helices with amino acids Q, T, Y, the water-soluble QTY variants still maintain the stable structures and ligand-binding activities in the chemokine receptors. The AphlaFold2 predictions proved the QTY code validity. The simple QTY code is a likely useful tool and has big impact for designs of water-soluble variants of previously water-insoluble GPCRs, glucose transporters, solute carrier transporters, ABC transporters, potassium ion channels, beta-barrel outer membrane proteins, monoclonal antibodies and perhaps aggregated proteins.

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Shuguang Zhang is at MIT Media Lab, Massachusetts Institute of Technology. His current research focuses on designs of biological molecules, particularly proteins and peptides. He received his B.S from Sichuan University, China and Ph.D. in Biochemistry & Molecular Biology from University of California at Santa Barbara, USA. He was an American Cancer Society Postdoctoral Fellow and a Whitaker Foundation Investigator at MIT. He was a 2003 Fellow of Japan Society for Promotion of Science (JSPS fellow). His work of designer self-assembling peptide scaffold won 2004 R&D100 award. He won a 2006 Guggenheim Fellowship and spent academic sabbatical in University of Cambridge, Cambridge, UK. He won 2006 Wilhelm Exner Medal of Austria. He was elected to Austrian Academy of Sciences in 2010. He was elected to American Institute of Medical and Biological Engineering in 2011 and elected to US National Academy of Inventors in 2013, and elected to the European Academy of Science and Arts in 2021. He won the 2020 Emil Thomas Kaiser Award from the Protein Society. He is a honorary member of the Erwin Schrödinger Society and gave for the 20th Erwin Schrödinger Colloquium at the Austrian Academy of Sciences in 2021. He has published over 200 scientific papers that have been cited over 38,000 with a h-index 93. He is also a board member of Molecular Frontiers Foundation. Molecular Frontiers Foundation organizes annually Molecular Frontiers Symposia in Sweden and around the world. The Foundation encourages young people to ask big and good scientific questions about nature. The selected winners will be awarded for Molecular Frontiers Inquiry Prize.

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