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il Dr. Shuguang Zhang, Ph.D.

Laboratory of Molecular Architecture, Media Lab
Massachusetts Institute of Technology
Cambridge, Massachusetts, USA

terrà il seminario dal titolo:

The Simple QTY Code for Protein Design

The simple QTY code, for designing hydrophobic protein domains to become water soluble without detergents [1-2], is based on two key molecular structural facts: 1) all 20 amino acids are found in naturally occurring α -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 α -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 [AlphaFold2](#) predictions proved the QTY code validity [3]. 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, and perhaps aggregated proteins.

[1] Zhang, S., et al (2018) QTY code enables design of detergent-free chemokine receptors that retain ligand-binding activities. *Proc. Natl. Acad. Sci. USA* 115 (37) E8652-E8659. <https://doi.org/10.1073/pnas.1811031115>

[2] Qing, R., et al. (2022) Protein design: from the aspect of water solubility. *Chemical Reviews*, 122. <https://doi.org/10.1021/acs.chemrev.1c00757>

[3] Smorodina E, et al (2022) Structural informatic study of determined and AlphaFold2 predicted molecular structures of 13 human solute carrier transporters and their water-soluble QTY variants. *Scientific Reports* 12, 20103. [doi: 10.1038/s41598-022-23764-y](https://doi.org/10.1038/s41598-022-23764-y)

Prof. D. Carbonera
Prof. M. Bortolus

Il Direttore del Dipartimento
Michele Maggini