

TAMÁS HEGEDŰS



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RESEARCH AREA

Our research focuses on transmembrane proteins, which are associated with many diseases and are the targets of most available drugs. We are investigating ABC proteins acting as multidrug transporters to protect cells from toxic substances. We use theoretical and computational methods to understand their mechanism of function and substrate recognition. We also investigate how cystic fibrosis causing mutations in the CFTR/ABCC7 chloride channel affect protein unfolding, dynamics and function. CFTR channel opening requires phosphorylation of its disordered regulatory region. In order to understand the associated regulatory processes, we determine the intramolecular interactions of the disordered region and design a protein to counteract these interactions to achieve activation. In a similar manner, we design a small protein that binds to the C-terminus of the SARS Cov-2 Envelope transmembrane protein, inhibiting its binding to the human Pals1 protein, thus the degradation of cell-cell contacts and the development of inflammation.

TECHNIQUES AVAILABLE IN THE LAB

Bioinformatics, 3D-bioinformatics, AlphaFold2, computational biology, molecular dynamics, High Performance Computing, Python, web application development, molecular biology, protein expression and purification, biochemistry, florescent microscopy, atomic force microscopy.

SELECTED PUBLICATIONS

Hegedűs, T., Geisler, M., Lukács, G.L., Farkas, B. (2022) Ins and Outs of AlphaFold2 Transmembrane Protein Structure Predictions. **Cell Mol Life Sci** **79**: 73.

Nagy, T., Tóth, Á., Telbisz, Á., Sarkadi, B., Tordai, H., Tordai, A., **Hegedűs, T.** (2021) The Transport Pathway in the ABCG2 Protein and Its Regulation Revealed by Molecular Dynamics Simulations. **Cell Mol Life Sci** **78**: 2329–2339.

Csizmadia, G., Erdős, G., Tordai, H., Padányi, R., Tosatto, S., Dosztányi, Z., **Hegedűs, T.** (2020) The MemMoRF Database for Recognizing Disordered Protein Regions Interacting with Cellular Membranes. **Nucleic Acids Res** **49**: D355–D360.

Veit, G., Avramescu, R., Perdomo, D., Phuan, P., Bagdany, M., Apaja, P., Borot, F., Szollosi, D., Wu, Y., Finkbeiner, W., **Hegedus, T.**, Verkman, A., és Lukacs, G. (2014) Some Gating Potentiators, Including VX-770, Diminish $\Delta F508$ -CFTR Functional Expression. **Sci Transl Med** **6**: 246ra97.