

LIST OF PUBLICATIONS

- G. Enkavi, J. Li, P.-C. Wen, S. Thangapandian, M. Moradi, T. Jiang, W. Han, and E. Tajkhorshid (2014) A Microscopic View of the Mechanisms of Active Transport Across the Cellular Membrane. **Annual Reviews in Computational Chemistry**, in press.
- J. Li, G. Enkavi, P.-C. Wen, S. A. Shaikh, and E. Tajkhorshid (2013) Transient Formation of Water-conducting States in Membrane Transporters. **Proceedings of the National Academy of Sciences USA**, 110: 7696-7701.
- U. K. Eriksson, G. Fischer, R. Friemann, G. Enkavi, E. Tajkhorshid*, and R. Neutze* (2013) Sub-Angstrom resolution x-ray structure details aquaporin-water interactions. **Science**, 340: 1346-1349.
- S. A. Shaikh, J. Li, G. Enkavi, P.-C. Wen, Z. Huang, and E. Tajkhorshid (2013) Visualizing Functional Motions of Membrane Transporters with Molecular Dynamics Simulations. **Biochemistry** (Current Topic) 52: 569-587.
- R. R. Geyer, R. Musa-Aziz, G. Enkavi, P. Mahinthichaichan, E. Tajkhorshid, and W. Boron (2013) Movement of NH₃ through the Human Urea Transporter B (UT-B): A New Gas Channel. **American Journal of Physiology - Renal Physiology**, 304: F1447-F1457.
- G. Enkavi, J. Li, P. Mahinthichaichan, P.-C. Wen, Z. Huang, S. A. Shaikh, and E. Tajkhorshid (2013) Simulation Studies of the Mechanism of Membrane Transporters. In Editors: Luca Monticelli and Emppu Salonen, "Biomolecular Simulations – Methods and Protocols", Humana Press. **Methods in Molecular Biology**, Vol. 924, Part 2, 361-405.
- E. J. Levin, Y. Cao, G. Enkavi, M. Quick, Y Pan, E. Tajkhorshid*, and M. Zhou* (2012) Structure and permeation mechanism of a mammalian urea transporter. **Proceedings of the National Academy of Sciences USA**, 109: 11194-11199.
- Z. Huang, S. A. Shaikh, P.-C. Wen, G. Enkavi, J. Li, and E. Tajkhorshid (2011) Membrane Transporters - Molecular Machines Coupling Cellular Energy to Vectorial Transport Across the Membrane. **In Editor: Benoit Roux, "Molecular Machines", Chapter 9: pp. 151–182**, World Scientific Publishing, Singapore.
- G. Enkavi and E. Tajkhorshid (2010) Simulation of spontaneous substrate binding revealing the binding pathway and mechanism and initial conformational response of GlpT. **Biochemistry**, 49: 1105-1114.
- P.-C. Wen, Z. Huang, G. Enkavi, Y. Wang, J. C. Gumbart, and E. Tajkhorshid (2010) Molecular mechanisms of active transport across the cellular membrane. **In, Editors: Mark Sansom and Philip Biggin, "Molecular Simulations and Biomembranes: From Biophysics to Function"** pp. 248-286. Royal Society of Chemistry, Cambridge, UK.
- S. Shaikh, P.-C. Wen, G. Enkavi, Z. Huang, and E. Tajkhorshid (2010) Capturing Functional Motions of Membrane Channels and Transporters with Molecular Dynamics Simulation. **Journal of Computational and Theoretical Nanosciences**, 7;2481-2500.
- J. Feng, E. Lucchinetti, G. Enkavi, Y. Wang, P. Gehrig, B. Roschitzki, M. C. Schaub, E. Tajkhorshid, K. Zaugg, and M. Zaugg (2010) Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. **American Journal of Physiology - Cell Physiology**, 298: 740-748.
- Ch. Law*, G. Enkavi*, D.-N. Wang, and E. Tajkhorshid (2009) Structural basis of substrate selectivity in the glycerol-3-phosphate:phosphate antiporter GlpT. **Biophysical Journal**, 97: 1346-1353. *equal contribution