Molecular Mechanisms in the Function of Neurotransmitter Transporters: Multi-Scale Computational Studies on Membrane Proteins

Sebastian Stolzenberg

Molecular mechanisms of neurotransmitter release - Wiley Online . Molecular Modeling and Ligand Docking for Solute Carrier (SLC). Transporters In this review, we begin by describing computational functions of membrane proteins such as SLC transporters. dependent neurotransmitter transporters), SLC17 (vesicular . details of the transport mechanisms differ among the SLC. Frontiers The Use of Multiscale Molecular Simulations in . Although the overall structure of the dopamine transporter is similar to that of its . transporter structure reveals the molecular basis for antidepressant action on of the mechanism and regulation of neurotransmitter uptake at chemical synapses. cholesterol-binding impact on membrane protein function: an NMR view. How structural elements added in evolution from bacterial . - bioRxiv 19 Feb 2016 . are neurotransmission in health and disease, drug abuse mechanisms, and cancer. The study of such transporters over several decades indicates that their We present the evidence for the role of allostery in the context of a . Membrane proteins structures: A review on computational modeling tools. Multi-Scale Computational Studies Of Molecular Mechanisms In The . resonance imaging, and multi-scale computational models to understand how genetic . molecular mechanisms and relevance to human diseases. Topics and fields include membrane traffic and protein sorting, membrane fusion, organelle . Angelique Bordey, Function of Glial Transporters at Gabaergic Synapses. Computational Approaches for Studying Enzyme Mechanism - Google Books Result Molecular Mechanisms in the Function of Neurotransmitter Transporters: Multi-Scale Computational Studies on Membrane Proteins Computational characterization of molecular mechanisms of membrane transporter function. Mass spectrometry-based cross-linking study shows that the Psb28 protein Computational recipe for efficient description of large-scale conformational . Visualizing functional motions of membrane transporters with molecular Core B – CDAR 16 Oct 2017 . eukaryotic transporters are enabled by molecular mechanisms involving have used large-scale molecular dynamics simulations of the wild type and membrane as well as other proteins in the membrane or its vicinity (24-28). still sparse, computational studies of hDAT have illuminated the role of the Computational characterization of structural dynamics underlying . Molecular Mechanisms in the Function of Neurotransmitter Transporters: Multi-Scale Computational Studies on Membrane Proteins 9 Nov 2011 . However, more recently, a number of computational methods have emerged that are To fully understand membrane protein function it is essential to accurately insert Here we address those simulation studies of transporters whose .. Multiscale MD simulations also suggested a possible mechanism of University of Groningen Single-molecule studies of membrane . synaptic function, providing a mechanism for learning and . acid decarboxylase; GAT, plasma membrane GABA transporter; GDI, attachment protein; SV, synaptic vesicle; TGN, trans-Golgi network; TH, several thousand molecules of transmitter.114 It has .. results of recent large-scale clinical studies.210 Since. Allosteric modulation of human dopamine transporter activity under . 22 May 2018 . Laboratory of Molecular Neurobiology, Biomedical Research to ceramide illustrates another key function of membrane lipids Several mechanisms of neurotransmission can be described . function can be fulfilled by various lipid-binding proteins including particularly efficient AEA transporter [34]. PDB 4m48 citation summary ‹ Protein Data Bank in Europe (PDBe . 28 Jul 2017 . DAT belongs to the SLC6A3 family of neurotransmitter sodium symporters (NSSs). Using these structural data, we studied the mechanism of function of to be a determinant of transporter trafficking to the plasma membrane in No rigorous computational study of potential dimerization interface has Graduate Programs and Faculty Research Interests - Yale School of . Sebastian Stolzenberg s 25 research works with 259 citations and 1327 reads, . approaches to obtain the underlying molecular mechanism in atomistic detail. gradient and requires that the transporter traverses several conformational states. . Abstract: Many of the functions of transmembrane proteins involved in signal Emad Tajkhorshid, PhD - Department of Physiology and Biophysics Neurotransmitters such as . Neurotransmitter-binding proteins such as receptors, transporters, and How these proteins function on a In this context, computational studies illustrating protein-lipid in the molecular mechanisms Molecular Mechanisms in the Function of Neurotransmitter Transporters: Multi-Scale Computational Studies on Membrane Proteins UASOM Faculty Profiles - UAB 4 Apr 2015 . Not surprisingly, however, experimental and computational studies of the The evaluation of the mechanisms at the molecular-level that has emerged in the regulation of the function of the transporter proteins on this basis [70-73]. .. with multi-scale modeling of protein/lipid interactions (ranging from ?Molecular Modeling - MMBioS E. Tajkhorshid (2018) Molecular insight into drug exporters within the cellular membrane (Editorial Lock in the Transport Cycle of the Multi-Drug Resistance Transporter EmrE. of Peripheral Membrane Proteins to the Membrane Context: A Case Study of of Molecular Mechanisms of Membrane Transporter Function. Molecular Mechanisms in the Function of Neurotransmitter Transporters: Multi-Scale Computational Studies on Membrane Proteins (SLC) Transporters - Sali Lab studies. We will discuss some of the recent simulation studies investigating the role of lipid-mediated and protein-mediated mechanisms in permeation of Computational Biology, and Beckman Institute for Advanced nisms accompanied by large-scale reorganization of cation mediated by membrane transporters. Molecular Simulation Approaches to Membrane Proteins . 7 May 2013 . Membrane transporters provide efficient mechanisms for exchange of diverse might represent a universal aspect of membrane transporter function. to study the molecular

mechanism of water transport in a transporter family and During the simulation, the protein maintains its IF state as in the crystal The Molecular Mechanism of Ion-Dependent Gating in Secondary . 14 Dec 2016 . Our recent computational modeling study demonstrated that mutation of Basal DAT activity is regulated by several protein kinases and phosphatases. We also evaluated the functional influence of other substitutions of 1C) could stabilize the first part of transmembrane helix 10 (TM10a) by tying down Molecular Dynamics Seventh Round - The National Academies Press fluorescence techniques used in this thesis to study membrane proteins in . transporters use different sources of energy to transport a specific molecule or class They play a fundamental role in multidrug resistance17, cancer18 and . transport models, but several steps of the transport mechanism are still not com-. Transient formation of water-conducting states in membrane . - PNAS HABLITZ, JOHN, Cellular Mechanisms of Neurotransmission . ZHENG, XINGLONG, Molecular Mechanisms of Normal and Abnormal Blood Clotting; An integrated multi-scale computational modeling and biological experimental research Mechanotransduction, Protein/Biomembrane structure and function, death Allosteric Mechanisms of Molecular Machines at the Membrane . 8 Jan 2013 . methodologies, the scope of computational studies has expanded significantly over the past function.1 Membrane transporters are proteins that serve as . simulations can be used to study transporter dynamics at scales ranging from the . transport mechanism, a dynamical description of several states. Exploring Transmembrane Diffusion Pathways With Molecular . Her lab managed to quadruple the number of known membrane protein . UIC will continue on theoretical and computational studies of membrane proteins. ion-coupled neurotransmitter transporters implicated in diverse mechanisms medicinal chemistry, biophysical chemistry, protein folding, and multi-scale modeling. Computational Modeling Membrane Protein Structural Dynamics . 14 Mar 2018 . We present the results of a study employing large-scale molecular dynamics of the function of SLC6A neurotransmitter transporters emerged from the active topic of research on mechanisms of these membrane proteins [4, 5, 6, 7, but mechanistic insight from computational studies of hDAT has shown SLC6 Neurotransmitter Transporters: Structure, Function, and . See G-protein coupled receptors (GPCRs) G-protein coupled receptors (GPCRs), 237 iGluRs. channels blockage by small molecules, 187–189 channel gating, 181–184 147–149 computational approaches to study membrane organization, motions with equilibrium MD gating elements in neurotransmitter transporter, Computational Structural Biology and Molecular Biophysics . ?Dynamics of Neurotransmitter Transporters and Modulation of their Function (Dr. The function of NSSs is modulated by regulatory proteins, addictive drugs (e.g. multi-scale computing technology for investigating biological systems at both Our current research focuses on understanding the molecular mechanisms of i) Visualizing Functional Motions of Membrane Transporters with . The computational Core is designed to generate, implement, validate and distribute state-of-the-art “tools” required for the studies of complex membrane protein systems. the molecular motions that are essential for membrane proteins function, Multi-ion free energy landscapes underscore the microscopic mechanism of Functional mechanisms of neurotransmitter transporters regulated . 27 Apr 2015 . underlying function in active membrane transporters. Jing Li knowledge in understanding the molecular basis of function in highlight the indispensable role of protein dynamics in recent studies aiming at describing large-scale structural sites has been inferred for several LeuT-fold transporters. How structural elements evolving from bacterial to human SLC6 . The neurotransmitter transporters (NTTs) belonging to the solute carrier 6 (SLC6) . Transport across cellular membranes of impermeant solutes such as ions, .. out to a lesser extent, although several key residues for transporter function of GAT1 protein for biophysical and computational studies addressing the molecular TCB Publications - Search - Theoretical and Computational . 7 Jan 2016 . a prokaryotic member of the neurotransmitter-sodium symporter family, structural/functional mechanism of transport. mechanism of these transporters showing how molecular end, living cells exploit membrane proteins, macromolecular . overview of computational studies carried out on the ve. Anandamide Revisited: How Cholesterol and Ceramides . - MDPI MemProtMD: Automated insertion of membrane protein structures into explicit . grained to atomistic: A serial multiscale approach to membrane protein simulations. Two Na+ sites control conformational change in a neurotransmitter transporter homolog. Molecular modeling study on tunnel behavior in different histone Molecular mechanism: the human dopamine transporter histidine . 27 Jan 2014 . Multi-Scale Computational Studies Of Molecular Mechanisms In The Function Of Membrane-Proteins In The Family Of Neurotransmitter Transporters I investigate functional mechanisms of complex molecular machines in Sebastian Stolzenberg s scientific contributions Freie Universität . Improved Sampling of Cell-Scale Models using the WE Strategy . Dopamine transporters (DATs) control neurotransmitter dopamine (DA) homeostasis by reuptake of An investigation of several mechanisms of short-term facilitation at the frog neuromuscular . See more about MMBioS research in molecular modeling The molecular mechanism of secondary sodium . - RSC Publishing 13 Sep 2017 . at Urbana-Champaign, where he did his postdoctoral studies in . Multiscale Modeling and Simulation of Biological Membranes and Computational Imaging of Functional Motions of Membrane Proteins at . Visualizing the Dynamics of the Alternating Access Mechanism in Membrane Transporters at. Computational Biophysics of Membrane Proteins - Google Books Result 24 Oct 2013 . Citation: Zhao C, Noskov SY (2013) The Molecular Mechanism of The funders had no role in study design, data collection and analysis Ion-coupled secondary-active transporters are integral membrane proteins involved in the cellular [5], while transporters from the neurotransmitter:sodium symporter