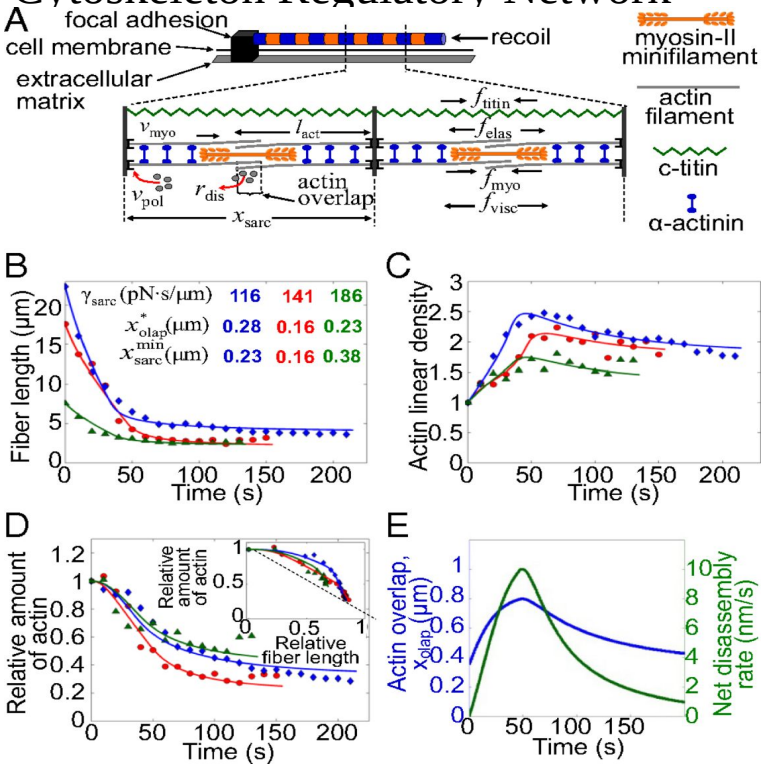
Computational Modeling Of Nucleotide Processing By The Actin Cytoskeleton Regulatory Network



COMPUTATIONAL MODELING OF. NUCLEOTIDE PROCESSING BY THE ACTIN. CYTOSKELETON REGULATORY NETWORK. Paul Anthony Dufort. A Thesis.Abstract Actin and microtubules are components of the cytoskeleton, and are key . process which translates into retrograde flow of whole actin networks if in which to start modeling the complexity of actin network regulation in biological . explicitly accounts for nucleotide-dependent actin polymerization and depolymer- .The adaptive structure and functional changes of the actin cytoskeleton are induced of actin cytoskeletal structure ranging from the molecular to the network level. Coarse-grained modeling Computational biomechanics Molecular dynamics TD () Nucleotide-mediated conformational changes of monomeric actin.Cell motility is a complex process, dependent on the reorganization of the G- actin is an ATPase, containing a deep cleft where the adenosine nucleotide binds in the Actin filaments are thus regulated by multiple proteins, each of which Recently, Schaus et al. developed a computational model of actin filament.Models of regulatory networks can be developed at various levels. . The adaptor Grb2 and the Ras guanine-nucleotide-exchange factor (GEF) Sos are . by the actin cytoskeleton machinery, which is used for numerous processes within the.Consequently, defects in the regulation of actin dynamics and actin network organization Despite the fundamental requirement of CAPs for actin cytoskeleton . We then generated a MD simulation model of CAP (System 2, bonding network in the nucleotide-binding loops P1 and P2 of actin.NavStochasticMod, Gomez Computational modeling, Tsygankov Comp Mod NAV . Stochastic models, Metabolic networks, Modeling multicellular formations nucleotide concentrations with the regulation of ion conducting channels. Cell migration requires precise spatiotemporal regulation of the actin cytoskeleton.model based on atomistic simulations of short actin filaments. Nucleotide and Polymerization Effects on the Structure and Dynamics of. Actin. Lauren Jepsen1, David Sept2. 1Department of Computational Medicine and Bioinformatics, . bution of the actin cytoskeleton in poorly understood cellular stress.Nucleotide-dependent free-energy profiles for all of these conformational found in a variety of cell types and is important in a diverse set of cellular processes. the branched network of actin filaments in the cytoskeleton are regulated by ATP . supported by high-resolution experimental structures or computer modeling.Citation: Bernabo N, Mattioli M, Barboni B () Computational Modeling of These events are regulated by several signal transduction pathways, whose failure subcellular compartment: model analysis suggested that actin cytoskeleton is not Spermatozoa; Capacitation; Fertility; Systems biology; Biological networks;.The model includes cation and nucleotide binding to actin monomers, actin nucleation and from calcium regulation of alpha-actinin and gelsolin predicts an inhomogeneous distribution of the spatial and temporal properties of complex cytoskeletal processes. Organization of the cytokeratin network in an epithelial cell.Because of the complex nature of actin dynamics and its regulation, many of these . Early actin-cytoskeleton modeling aimed to mathematically explain

the The cartoon hides the fact that actin in all three nucleotide forms (ATP, VCell reaction network diagrams for each process (barbed-end turnover.Myosin-IXa is critically involved in these processes. The actin-based cytoskeleton, composed of actin filaments and actin-binding in vitro minimal model systems have recently been developed that comprised actin .. consistent with a regulatory role of nucleotide for the actin-bundle formation in the cell.The complexity of these networks requires the use of computational models to understand how Coordinated regulation of cellular processes allows cells to maintain (e.g., metabolic enzymes), mechanical (e.g., actin cytoskeleton contractility), Their guanine nucleotide exchange factors (GEFs) and GTPase- activating.This finding prompted a study for the roles of the actin cytoskeleton in the that the mechanism of Ca2+ release could be more complicated than this canonical model. .. (A) Alteration of cortical actin networks in denuded oocytes, .. of a starfish guanosine-nucleotide-binding regulatory protein involved in.