**Atomistic model for nearly quantitative simulations of Langmuir monolayers**

Lung surfactant and a tear film lipid layer are examples of biologically relevant macromolecular structures found at the air–water interface. Because of their complexity, they are often studied in terms of simplified lipid layers, the simplest example being a Langmuir monolayer. Given the profound biological significance of these lipid assemblies, there is a need to understand their structure and dynamics on the nanoscale, yet there are not many techniques able to provide this information. Atomistic molecular dynamics simulations would be a tool fit for this purpose; however, the simulation models suggested until now have been qualitative instead of quantitative. This limitation has mainly stemmed from the challenge to correctly describe the surface tension of water with simulation parameters compatible with other biomolecules. In this work, we show that this limitation can be overcome by using the recently introduced four-point OPC water model, whose surface tension for water is demonstrated to be quantitatively consistent with experimental data and which is also shown to be compatible with the commonly employed lipid models. We further establish that the approach of combining the OPC four-point water model with the CHARMM36 lipid force field provides nearly quantitative agreement with experiments for the surface pressure–area isotherm for POPC and DPPC monolayers, also including the experimentally observed phase coexistence in a DPPC monolayer. The simulation models reported in this work pave the way for nearly quantitative atomistic studies of lipid-rich biological structures at air–water interfaces.

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**Investigation of the structural anisotropy in a self-assembling glycinate layer on Cu(100) by scanning tunneling microscopy and density functional theory calculations**

Self-assembling organic molecule-metal interfaces exhibiting free-electron like (FEL) states offers an attractive bottom-up approach to fabricating materials for molecular electronics. Accomplishing this, however, requires detailed understanding of the fundamental driving mechanisms behind the self-assembly process. For instance, it is still unresolved as to why the adsorption of glycine ([NH2(CH2)COOH]) on isotropic Cu(100) single crystal surface leads, via deprotonation and self-assembly, to a glycinate ([NH2(CH2)COO−]) layer that exhibits anisotropic FEL behavior. Here, we report on bias-dependent scanning tunneling microscopy (STM) experiments and density functional theory (DFT) calculations for glycine
adsorption on Cu(100) single crystal surface. We find that after physical vapor deposition (PVD) of glycine on Cu(100),
glycinate self-assembles into an overlayer exhibiting c(2x4) and p(2x4) symmetries with non-identical adsorption sites. Our
findings underscore the intricacy of electrical conductivity in nanomolecular organic overlayers and the critical role the
structural anisotropy at molecule-metal interface plays in the fabrication of materials for molecular electronics.

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Scopus rating (2012): SJR 0.918 SNIP 1.373 CiteScore 2.26
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Scopus rating (2010): SJR 0.924 SNIP 1.141
Scopus rating (2009): SJR 0.842 SNIP 1.023
Scopus rating (2008): SJR 0.899 SNIP 1.087
Scopus rating (2007): SJR 0.795 SNIP 0.945
Scopus rating (2006): SJR 0.852 SNIP 1.052
Scopus rating (2005): SJR 0.679 SNIP 0.946
Scopus rating (2004): SJR 0.964 SNIP 1.126
Scopus rating (2003): SJR 0.988 SNIP 1.027
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Key steps in unconventional secretion of fibroblast growth factor 2 reconstituted with purified components
FGF2 is secreted from cells by an unconventional secretory pathway. This process is mediated by direct translocation
across the plasma membrane. Here, we define the minimal molecular machinery required for FGF2 membrane
translocation in a fully reconstituted inside-out vesicle system. FGF2 membrane translocation is thermodynamically driven
by PI(4,5)P2-induced membrane insertion of FGF2 oligomers. The latter serve as dynamic translocation intermediates
of FGF2 with a subunit number in the range of 8-12 FGF2 molecules. Vectorial translocation of FGF2 across the membrane
is governed by sequential and mutually exclusive interactions with PI(4,5)P2 and heparan sulfates on opposing sides of
the membrane. Based on atomistic molecular dynamics simulations, we propose a mechanism that drives PI(4,5)P2
dependent oligomerization of FGF2. Our combined findings establish a novel type of self-sustained protein translocation
across membranes revealing the molecular basis of the unconventional secretory pathway of FGF2.
Lipid membranes: Theory and simulations bridged to experiments

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Cholesterol oxidation products and their biological importance

The main biological cause of oxysterols is the oxidation of cholesterol. They differ from cholesterol by the presence of additional polar groups that are typically hydroxyl, keto, hydroperoxy, epoxy, or carboxyl moieties. Under typical conditions, oxysterol concentration is maintained at a very low and precisely regulated level, with an excess of cholesterol. Like cholesterol, many oxysterols are hydrophobic and hence confined to cell membranes. However, small chemical differences between the sterols can significantly affect how they interact with other membrane components, and this in turn can have a substantial effect on membrane properties. In this spirit, this review describes the biological importance and the roles of oxysterols in the human body. We focus primarily on the effect of oxysterols on lipid membranes, but we also consider other issues such as enzymatic and nonenzymatic synthesis processes of oxysterols as well as pathological conditions induced by oxysterols.

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Scopus rating (2008): SJR 1.114 SNIP 1.057
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Scopus rating (2002): SJR 1.005 SNIP 0.813
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Exercise loading history and femoral neck strength in a sideways fall: A three-dimensional finite element modeling study.

Over 90% of hip fractures are caused by falls. Due to a fall-induced impact on the greater trochanter, the posterior part of the thin superolateral cortex of the femoral neck is known to experience the highest stress, making it a fracture-prone region. Cortical geometry of the proximal femur, in turn, reflects a mechanically appropriate form with respect to habitual exercise loading. In this finite element (FE) modeling study, we investigated whether specific exercise loading history is associated with femoral neck structural strength and estimated fall-induced stresses along the femoral neck. One hundred and eleven three-dimensional (3D) proximal femur FE models for a sideways falling situation were constructed from magnetic resonance (MR) images of 91 female athletes (aged 24.7±6.1 years, >8 years competitive career) and 20 non-competitive habitually active women (aged 23.7±3.8 years) that served as a control group. The athletes were divided into five distinct groups based on the typical loading pattern of their sports: high-impact (H-I: triple-jumpers and high-jumpers), odd-impact (O-I: soccer and squash players), high-magnitude (H-M: power-lifters), repetitive-impact (R-I: endurance runners), and repetitive non-impact (R-NI: swimmers). The von Mises stresses obtained from the FE models were used to estimate mean fall-induced stresses in eight anatomical octants of the cortical bone cross-sections at the proximal, middle, and distal sites along the femoral neck axis. Significantly (p<0.05) lower stresses compared to the control group were observed: the H-I group - in the superoposterior (10%) and posterior (19%) octants at the middle site, and in the superoposterior (13%) and posterior (22%) octants at the distal site; the O-I group - in the superior (16%), superoposterior (16%), and posterior (12%) octants at the middle site, and in the superoposterior (14%) octant at the distal site; the H-M group - in the superior (13%) and superoposterior (15%) octants at the middle site, and a trend (p=0.07, 9%) in the superoposterior octant at the distal site; the R-I group - in the superior (14%), superoposterior (23%) and posterior (22%) octants at the middle site, and in the superoposterior (19%) and posterior (20%) octants at the distal site. The R-NI group did not differ significantly from the control group. These results suggest that exercise loading history comprising various impacts in particular is associated with a stronger femoral neck in a falling situation and may have potential to reduce hip fragility.
Hydrophobisation of wood surfaces by combining liquid flame spray (LFS) and plasma treatment: Dynamic wetting properties

The hydrophilic nature of wood surfaces is a major cause for water uptake and subsequent biological degradation and dimensional changes. In the present paper, a thin transparent superhydrophobic layer on pine veneer surfaces has been created for controlling surface wettability and water repellency. This effect was achieved by means of the liquid flame spray (LFS) technique, in the course of which the nanoparticulate titanium dioxide (TiO2) was brought to the surface, followed by plasma polymerisation. Plasma polymerised perfluorohexane (PFH)

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Authors: Moghammad, M. S., Heydari, G., Tuominen, M., Fielden, M., Haapanen, J., Mäkelä, J. M., Wålinder, M. E., Claesson, P. M., Swerin, A.
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Scopus rating (2013): SJR 0.89 SNIP 1.295 CiteScore 2.21
Scopus rating (2012): SJR 1.023 SNIP 1.721 CiteScore 2.5
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Interdigitation of long-chain sphingomyelin induces coupling of membrane leaflets in a cholesterol dependent manner

It has been a long-standing question how the two leaflets in a lipid bilayer modulate each others' physical properties. In this paper, we discuss how this interaction may take place through interdigitation. We use atomistic molecular dynamics simulations to consider asymmetric lipid membrane models whose compositions are based on the lipidomics data determined for exosomes released by PC-3 prostate cancer cells. The simulations show interdigitation to be exceptionally strong for long-chain sphingomyelin (SM) molecules. In asymmetric membranes the amide-linked chain of SM is observed to extend deep into the opposing membrane leaflet. Interestingly, we find that the conformational order of the amide-linked SM chain increases the deeper it penetrates to the opposing leaflet. Analysis of this finding reveals that the amide-linked SM chain interacts favorably with the lipid chains in the opposite leaflet, and that cholesterol modulates the effect of SM interdigitation by influencing the conformational order of lipid hydrocarbon chains in the opposing (cytosolic) leaflet.
Role of charged lipids in membrane structures: Insight given by simulations

Lipids and proteins are the main components of cell membranes. It is becoming increasingly clear that lipids, in addition to providing an environment for proteins to work in, are in many cases also able to modulate the structure and function of those proteins. Particularly charged lipids such as phosphatidylinositol and phosphatidylserine are involved in several examples of such effects. Molecular dynamics simulations have proved an invaluable tool in exploring these aspects. This so-called computational microscope can provide both complementing explanations for the experimental results and guide experiments to fruitful directions. In this paper, we review studies that have utilized molecular dynamics simulations to unravel the roles of charged lipids in membrane structures. We focus on lipids as active constituents of the membranes, affecting both general membrane properties as well as non-lipid membrane components, mainly proteins. This article is part of a Special Issue entitled: Biosimulations edited by Ilpo Vattulainen and Tomasz Róg.

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The biophysical properties of ethanolamine plasmalogens revealed by atomistic molecular dynamics simulations

Given the importance of plasmalogens in cellular membranes and neurodegenerative diseases, a better understanding of how plasmalogens affect the lipid membrane properties is needed. Here we carried out molecular dynamics simulations to study a lipid membrane comprised of ethanolamine plasmalogens (PE-plasmalogens). We compared the results to the PE-diacyl counterpart and palmitoyl-oleyl-phosphatidylcholine (POPC) bilayers. Results show that PE-plasmalogens form more compressed, thicker, and rigid lipid bilayers in comparison with the PE-diacyl and POPC membranes. The results also point out that the vinyl-ether linkage increases the ordering of sn-1 chain substantially and the ordering of the sn-2
What can we learn about cholesterol's transmembrane distribution based on cholesterol-induced changes in membrane potential?

Cholesterol is abundant in the plasma membranes of animal cells and is known to regulate a variety of membrane properties. Despite decades of research, the transmembrane distribution of cholesterol is still a matter of debate. Here we consider this outstanding issue through atomistic simulations of asymmetric lipid membranes, whose composition is largely consistent with eukaryotic plasma membranes. We show that the membrane dipole potential changes in a cholesterol-dependent manner. Remarkably, moving cholesterol from the extracellular to the cytosolic leaflet increases the dipole potential on the cytosolic side, and vice versa. Biologically this implies that by altering the dipole potential, cholesterol can provide a driving force for cholesterol molecules to favor the cytosolic leaflet, in order to compensate for the intramembrane field that arises from the resting potential.

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Mutually Exclusive Roles of SHARPIN in Integrin Inactivation and NF-κB Signaling

SHANK-associated RH domain interactor (SHARPIN) inhibits integrins through interaction with the integrin α-subunit. In addition, SHARPIN enhances nuclear factor-kappaB (NF-κB) activity as a component of the linear ubiquitin chain assembly complex (LUBAC). However, it is currently unclear how regulation of these seemingly different roles is coordinated. Here, we show that SHARPIN binds integrin and LUBAC in a mutually exclusive manner. We map the integrin binding site on SHARPIN to the ubiquitin-like (UBL) domain, the same domain implicated in SHARPIN interaction with LUBAC component RNF31 (ring finger protein 31), and identify two SHARPIN residues (V267, L276) required for both integrin and RNF31 regulation. Accordingly, the integrin α-tail is capable of competing with RNF31 for SHARPIN binding in vitro. Importantly, the full SHARPIN RNF31-binding site contains residues (F263A/I272A) that are dispensable for SHARPIN-integrin interaction. Importantly, disrupting SHARPIN interaction with integrin or RNF31 abolishes SHARPIN-mediated regulation of integrin or NF-κB activity, respectively. Altogether these data suggest that the roles of SHARPIN in inhibiting integrin activity and supporting linear ubiquitination are (molecularly) distinct.
Redox-induced activation of the proton pump in the respiratory complex I

Complex I functions as a redox-linked proton pump in the respiratory chains of mitochondria and bacteria, driven by the reduction of quinone (Q) by NADH. Remarkably, the distance between the Q reduction site and the most distant proton channels extends nearly 200 Å. To elucidate the molecular origin of this long-range coupling, we apply a combination of large-scale molecular simulations and a site-directed mutagenesis experiment of a key residue. In hybrid quantum mechanics/molecular mechanics simulations, we observe that reduction of Q is coupled to its local protonation by the His-38/Asp-139 ion pair and Tyr-87 of subunit Nqo4. Atomicistic classical molecular dynamics simulations further suggest that formation of quinol (QH2) triggers rapid dissociation of the anionic Asp-139 toward the membrane domain that couples to conformational changes in a network of conserved charged residues. Site-directed mutagenesis data confirm the importance of Asp-139; upon mutation to asparagine the Q reductase activity is inhibited by 75%. The current results, together with earlier biochemical data, suggest that the proton pumping in complex I is activated by a unique combination of electrostatic and conformational transitions.
How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: beta(2)-Adrenergic Receptor in the Spotlight

Atomistic molecular dynamics (MD) simulations are used extensively to elucidate membrane protein properties. These simulations are based on three-dimensional protein structures that in turn are often based on crystallography. The protein structures resolved in crystallographic studies typically do not correspond to pristine proteins, however. Instead the crystallized proteins are commonly engineered, including structural modifications (mutations, replacement of protein sequences by antibodies, bound ligands, etc.) whose impact on protein structure and dynamics is largely unknown. Here we explore this issue through atomistic MD simulations ( ,5 its in total), focusing on the beta(2)-adrenergic receptor (beta(2)AR) that is one of the most studied members of the G-protein coupled receptor superfamily. Starting from an inactive-state crystal structure beta(2)AR, we remove the many modifications in beta(2)AR systematically one at a time, in six consecutive steps. After each step, we equilibrate the system and simulate it quite extensively. The results of this step-by-step approach highlight that the structural modifications used in crystallization can affect ligand and G-protein binding sites, packing at the transmembrane-helix interface region, and the dynamics of connecting loops in beta(2)AR. When the results of the systematic step-by-step approach are compared to an all-at-once technique where all modifications done on beta(2)AR are removed instantaneously at the same time, it turns out that the step-by-step method provides results that are superior in terms of maintaining protein structural stability. The results provide compelling evidence that for membrane proteins whose 3D structure is based on structural engineering, the preparation of protein structure for atomistic MD simulations is a delicate and sensitive process. The results show that most valid results are found when the structural modifications are reverted slowly, one at a time.

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Authors: Manna, M., Kulig, W., Javanainen, M., Tynkkynen, J., Hensen, U., Mueller, D. J., Rog, T., Vattulainen, I.
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Scopus rating (2012): SJR 2.744 SNIP 1.608 CiteScore 5.34
Scopus rating (2011): SJR 2.742 SNIP 1.815 CiteScore 5.82
Scopus rating (2010): SJR 2.372 SNIP 1.46
Scopus rating (2009): SJR 2.616 SNIP 1.273
Scopus rating (2008): SJR 2.367 SNIP 1.173
Scopus rating (2007): SJR 2.3 SNIP 1.401
Dynamics of the peripheral membrane protein P2 from human myelin measured by neutron scattering: A Comparison between wild-type protein and a hinge mutant

Myelin protein P2 is a fatty acid-binding structural component of the myelin sheath in the peripheral nervous system, and its function is related to its membrane binding capacity. Here, the link between P2 protein dynamics and structure and function was studied using elastic incoherent neutron scattering (EINS). The P38G mutation, at the hinge between the β barrel and the α-helical lid, increased the lipid stacking capacity of human P2 in vitro, and the mutated protein was also functional in cultured cells. The P38G mutation did not change the overall structure of the protein. For a deeper insight into P2 structure-function relationships, information on protein dynamics in the 10 ps to 1 ns time scale was obtained using EINS. Values of mean square displacements mainly from protein H atoms were extracted for wild-type P2 and the P38G mutant and compared. Our results show that at physiological temperatures, the P38G mutant is more dynamic than the wild-type P2 protein, especially on a slow 1-ns time scale. Molecular dynamics simulations confirmed the enhanced dynamics of the mutant variant, especially within the portal region in the presence of bound fatty acid. The increased softness of the hinge mutant of human myelin P2 protein is likely related to an enhanced flexibility of the portal region of this fatty acid-binding protein, as well as to its interactions with the lipid bilayer surface requiring conformational adaptations.

General information
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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Oulu, Univ Bergen, University of Bergen, Dept Phys & Technol, Biochemistry and Molecular Medicine and Biocenter Oulu, German Electron Synchrotron (DESY), European Spallation Source (ESS), Max Planck Institute for Experimental Medicine, Institut Laue-Langevin, Department of Biomedicine, CNR-IOM
Authors: Laulumaa, S., Nieminen, T., Lehtimäki, M., Aggarwal, S., Simons, M., Koza, M. M., Vattulainen, I., Kursula, P., Natali, F.
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Scopus rating (2014): SJR 1.545 SNIP 1.141 CiteScore 3.54
Scopus rating (2013): SJR 1.74 SNIP 1.147 CiteScore 3.94
Scopus rating (2012): SJR 1.945 SNIP 1.142 CiteScore 4.15
Scopus rating (2011): SJR 2.369 SNIP 1.23 CiteScore 4.58
Scopus rating (2010): SJR 2.631 SNIP 1.161
Scopus rating (2009): SJR 2.473 SNIP 0.985
Scopus rating (2008): SJR 2.323 SNIP 0.96
Scopus rating (2007): SJR 1.289 SNIP 0.525
Original language: English
ASJC Scopus subject areas: Agricultural and Biological Sciences(all), Biochemistry, Genetics and Molecular Biology(all), Medicine(all)
DOI: 10.1371/journal.pone.0128954
Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis

Polarized membrane morphogenesis is a fundamental activity of eukaryotic cells. This process is essential for the biology of cells and tissues, and its execution demands exquisite temporal coordination of functionally diverse membrane signaling reactions with high spatial resolution. Moreover, mechanisms must exist to establish and preserve such organization in the face of randomizing forces that would diffuse it. Here we identify the conserved AtSfh1 Sec14-nodulin protein as a novel effector of phosphoinositide signaling in the extreme polarized membrane growth program exhibited by growing Arabidopsis root hairs. The data are consistent with Sec14-nodulin proteins controlling the lateral organization of phosphatidylinositol 4,5-bisphosphate (PtdIns(4,5)P<sub>2</sub>) landmarks for polarized membrane morphogenesis in plants. This patterning activity requires both the PtdIns(4,5)P<sub>2</sub> binding and homo-oligomerization activities of the AtSfh1 nodulin domain and is an essential aspect of the polarity signaling program in root hairs. Finally, the data suggest a general principle for how the phosphoinositide signaling landscape is physically bit mapped so that eukaryotic cells are able to convert a membrane surface into a high-definition lipid-signaling screen.

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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Mahidol Univ, Mahidol University, Phramongkutklao College of Medicine, Fac Dent, Dept Anat, University of Southern Denmark, Department of Molecular and Cellular Medicine, Texas A AndM Health Sciences Center, Center for Plant Molecular Biology, Plant Physiology, Universität Tübingen, Zentrum für Datenverarbeitung, Unidad de Biofísica (CSIC, UPV/EHU), Departamento de Bioquímica, Universidad del País Vasco, Institut de Formation Aux Carrieres de Sante de Rabat, Department of Biochemistry and Biophysics, Texas A AndM University
Number of pages: 18
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Scopus rating (2015): SJR 3.573 SNIP 1.11 CiteScore 4.03
Scopus rating (2014): SJR 3.693 SNIP 1.145 CiteScore 4.33
Scopus rating (2013): SJR 4.008 SNIP 1.212 CiteScore 4.57
Scopus rating (2012): SJR 4.132 SNIP 1.192 CiteScore 4.97
Scopus rating (2011): SJR 4.83 SNIP 1.221 CiteScore 5.26
Scopus rating (2010): SJR 5.605 SNIP 1.286
Scopus rating (2009): SJR 5.779 SNIP 1.288
Scopus rating (2008): SJR 5.798 SNIP 1.284
Scopus rating (2007): SJR 6.031 SNIP 1.335
Scopus rating (2006): SJR 6.074 SNIP 1.379
Scopus rating (2005): SJR 5.965 SNIP 1.416
Scopus rating (2004): SJR 6.469 SNIP 1.439
Scopus rating (2003): SJR 6.879 SNIP 1.396
Scopus rating (2002): SJR 6.345 SNIP 1.386
Scopus rating (2001): SJR 6.283 SNIP 1.359
Scopus rating (1999): SJR 7.456 SNIP 1.337
Role of subunit III and its lipids in the molecular mechanism of cytochrome c oxidase

The terminal respiratory enzyme cytochrome c oxidase (CcO) reduces molecular oxygen to water, and pumps protons across the inner mitochondrial membrane, or the plasma membrane of bacteria. A two-subunit CcO harbors all the elements necessary for oxygen reduction and proton pumping. However, it rapidly undergoes turnover-induced irreversible damage, which is effectively prevented by the presence of subunit III and its tightly bound lipids. We have performed classical atomistic molecular dynamics (MD) simulations on a three-subunit CcO, which show the formation of water wires between the polar head groups of lipid molecules bound to subunit III and the proton uptake site Asp91 (Bos taurus enzyme numbering). Continuum electrostatic calculations suggest that these lipids directly influence the proton affinity of Asp91 by 1-2 pK units. We surmise that lipids bound to subunit III influence the rate of proton uptake through the D-pathway, and therefore play a key role in preventing turnover-induced inactivation. Atomistic MD simulations show that subunit III is rapidly hydrated in the absence of internally bound lipids, which is likely to affect the rate of O<sub>2</sub> diffusion into the active-site. The role of subunit III with its indigenous lipids in the molecular mechanism of CcO is discussed.

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Organisations: Department of Physics, Research area: Computational Physics, Tampere University of Technology, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Institute of Molecular Biotechnology, Jena, Germany, Helsinki Bioenergetics Group, University of Helsinki Institute of Biotechnology
Authors: Sharma, V., Ala-Vannesluoma, P., Vattulainen, I., Wikström, M., Róg, T.
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Volume: 1847
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Scopus rating (2014): SJR 2.441 SNIP 1.441 CiteScore 4.94
Scopus rating (2013): SJR 2.569 SNIP 1.371 CiteScore 4.79
Scopus rating (2012): SJR 2.816 SNIP 1.531 CiteScore 5.17
Scopus rating (2011): SJR 2.375 SNIP 1.373 CiteScore 4.56
Scopus rating (2010): SJR 2.562 SNIP 1.38
Scopus rating (2008): SJR 2.329 SNIP 1.301
Scopus rating (2007): SJR 2.558 SNIP 1.19
Scopus rating (2006): SJR 2.354 SNIP 1.184
Scopus rating (2005): SJR 2.448 SNIP 1.301
Scopus rating (2004): SJR 2.42 SNIP 1.411
Scopus rating (2003): SJR 2.923 SNIP 1.214
Scopus rating (2002): SJR 2.864 SNIP 1.547
Scopus rating (2001): SJR 3.148 SNIP 1.66
Scopus rating (2000): SJR 3.09 SNIP 1.457
N-Glycosylation as determinant of epidermal growth factor receptor conformation in membranes

The epidermal growth factor receptor (EGFR) regulates several critical cellular processes and is an important target for cancer therapy. In lieu of a crystalllographic structure of the complete receptor, atomistic molecular dynamics (MD) simulations have recently shown that they can excel in studies of the full-length receptor. Here we present atomistic MD simulations of the monomeric N-glycosylated human EGFR in biomimetic lipid bilayers that are, in parallel, also used for the reconstitution of full-length receptors. This combination enabled us to experimentally validate our simulations, using ligand binding assays and antibodies to monitor the conformational properties of the receptor reconstituted into membranes. We find that N-glycosylation is a critical determinant of EGFR conformation, and specifically the orientation of the EGFR ectodomain relative to the membrane. In the absence of a structure for full-length, posttranslationally modified membrane receptors, our approach offers new means to structurally define and experimentally validate functional properties of cell surface receptors in biomimetic membrane environments.

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Organisations: Department of Physics, Tampere University of Technology, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Paul Langerhans Institute Dresden of the Helmholtz Centre Munich, University Clinic Carl Gustav Carus, TU Dresden, German Center for Diabetes Research (DZD e.V.), Max Planck Institute for Molecular Cell Biology and Genetics
Authors: Kaszuba, K., Grzybek, M., Orłowski, A., Danne, R., Róg, T., Simons, K., Coskun, Ü., Vattulainen, I.
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Scopus rating (2015): SJR 6.767 SNIP 2.682 CiteScore 8.84
Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86
Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5
Scopus rating (2012): SJR 6.792 SNIP 2.682 CiteScore 9.49
Scopus rating (2011): SJR 6.771 SNIP 2.636 CiteScore 9.31
Scopus rating (2010): SJR 6.769 SNIP 2.529
Scopus rating (2009): SJR 6.913 SNIP 2.544
Scopus rating (2008): SJR 6.899 SNIP 2.445
Scopus rating (2007): SJR 6.766 SNIP 2.441
Scopus rating (2006): SJR 6.734 SNIP 2.434
Scopus rating (2005): SJR 6.784 SNIP 2.551
Scopus rating (2004): SJR 7.026 SNIP 2.622
Scopus rating (2003): SJR 7.018 SNIP 2.501
Scopus rating (2002): SJR 7.183 SNIP 2.471
Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles

Using replica exchange umbrella sampling we calculated free energy profiles for uptake of cholesterol and one of its oxysterols (7-ketocholesterol) from an aqueous solution into a high-density lipoprotein particle. These atomistic molecular dynamics simulations show that both sterols are readily taken up from the aqueous solution with comparable free energy minima at the surface of the particle of -17 kcal/mol for cholesterol and -14 kcal/mol for 7-ketocholesterol. Moreover, given its preferred position at the particle surface, 7-ketocholesterol is expected to be able to participate directly in biological signaling processes.
Proton-coupled electron transfer and the role of water molecules in proton pumping by cytochrome c oxidase

Molecular oxygen acts as the terminal electron sink in the respiratory chains of aerobic organisms. Cytochrome c oxidase in the inner membrane of mitochondria and the plasma membrane of bacteria catalyzes the reduction of oxygen to water, and couples the free energy of the reaction to proton pumping across the membrane. The proton-pumping activity contributes to the proton electrochemical gradient, which drives the synthesis of ATP. Based on kinetic experiments on the O-O bond splitting transition of the catalytic cycle (A → PR), it has been proposed that the electron transfer to the binuclear iron-copper center of O2 reduction initiates the proton pump mechanism. This key electron transfer event is coupled to an internal proton transfer from a conserved glutamic acid to the proton-loading site of the pump. However, the proton may instead be transferred to the binuclear center to complete the oxygen reduction chemistry, which would constitute a short-circuit. Based on atomistic molecular dynamics simulations of cytochrome c oxidase in an explicit membrane-solvent environment, complemented by related free-energy calculations, we propose that this short-circuit is effectively prevented by a redox-state-dependent organization of water molecules within the protein structure that gates the proton transfer pathway. cell respiration , atomistic molecular dynamics simulations , functional water molecules ,free-energy calculations .

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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Programme for Structural Biology and Biophysics, University of Helsinki Institute of Biotechnology
Authors: Sharma, V., Enkavi, G., Vattulainen, I., Róg, T., Wikström, M.
Number of pages: 6
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Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86
Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5
Scopus rating (2012): SJR 6.792 SNIP 2.682 CiteScore 9.49
Scopus rating (2011): SJR 6.771 SNIP 2.636 CiteScore 9.31
Scopus rating (2010): SJR 6.769 SNIP 2.529
Scopus rating (2009): SJR 6.913 SNIP 2.544
Scopus rating (2008): SJR 6.899 SNIP 2.445
Scopus rating (2007): SJR 6.766 SNIP 2.441
Scopus rating (2006): SJR 6.734 SNIP 2.434
Scopus rating (2005): SJR 6.784 SNIP 2.551
Scopus rating (2004): SJR 7.026 SNIP 2.622
Scopus rating (2003): SJR 7.018 SNIP 2.501
Scopus rating (2002): SJR 7.183 SNIP 2.471
Scopus rating (2001): SJR 7.192 SNIP 2.463
Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate

Cholesteryl hemisuccinate (CHS) is one of the cholesterol-mimicking detergents not observed in nature. It is, however, widely used in protein crystallography, in biochemical studies of proteins, and in pharmacology. Here, we performed an extensive experimental and theoretical study on the behavior of CHS in lipid membranes rich in unsaturated phospholipids. We found that the deprotonated form of CHS (that is the predominant form under physiological conditions) does not mimic cholesterol very well. The protonated form of CHS does better in this regard, but also its ability to mimic the physical effects of cholesterol on lipid membranes is limited. Overall, although ordering and condensing effects characteristic to cholesterol are present in systems containing any form of CHS, their strength is appreciably weaker compared to cholesterol. Based on the considerable amount of experimental and atomistic simulation data, we conclude that these differences originate from the fact that the ester group of CHS does not anchor it in an optimal position at the water-membrane interface. The implications of these findings for considerations of protein-cholesterol interactions are briefly discussed.
How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations

Transformation of cellulose into monosaccharides can be achieved in a chemical process performed by a special group of enzymes known as cellulases. We have used atomistic molecular dynamics simulations to study endoglucanase II (Cel5A) that is one of the proteins in this group. Based on the atomistic simulation results, we discuss how the Cel5A enzyme interacts with cellulose fibrils comprised of both crystalline and amorphous regions. We show that the enzyme’s carbohydrate-binding domain prefers to interact with crystalline regions of cellulose, while the catalytic domain has a high affinity to the amorphous regions of fibrils. In particular, through electrostatic interactions the catalytic domain attracts loose glucose chains to its catalytic cleft. The atomistic details of the enzyme–cellulose interaction are presented and the implications for practical applications are briefly discussed.

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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Lappeenranta University of Technology, University of Jyväskylä, Stora Enso, Department of Physics and Nanoscience Center
Authors: Orłowski, A., Róg, T., Paavilainen, S., Manna, M., Heiskanen, I., Backfolk, K., Timonen, J., Vattulainen, I.
Number of pages: 15
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Scopus rating (2014): SJR 1.071 SNIP 1.334 CiteScore 3.58
Scopus rating (2013): SJR 1.127 SNIP 1.48 CiteScore 3.83
Scopus rating (2012): SJR 1.179 SNIP 1.71 CiteScore 3.74
Scopus rating (2011): SJR 1.354 SNIP 1.795 CiteScore 3.99
Scopus rating (2010): SJR 0.873 SNIP 1.384
Scopus rating (2009): SJR 1.038 SNIP 1.219
Scopus rating (2008): SJR 0.926 SNIP 1.123
Scopus rating (2007): SJR 0.754 SNIP 1.034
Scopus rating (2006): SJR 0.699 SNIP 1.15
Scopus rating (2005): SJR 1.112 SNIP 1.318
Scopus rating (2004): SJR 0.855 SNIP 1.072
Scopus rating (2003): SJR 0.81 SNIP 1.02
How mono-valent cations bend peptide turns and a first-principles database of amino acids and dipeptides

In this contribution we detail our efforts to investigate the structural effects of cations binding to peptides and amino acids. We perform first-principles studies employing long-range dispersion-corrected approximate density-functional theory and compare to gas-phase experiments.

Membrane-associated proteins do care about lipids - perspective based on atomistic molecular dynamics simulations

This thesis consists of three original articles that deal with lipid-protein interactions investigated using atomistic molecular dynamics simulations method, which in some cases were complemented with experimental data. Since very few molecular details of these important interactions are known, the data shown in this thesis can help to understand and develop a broader view on the role of lipids in protein's function. In the first part of this thesis, the membrane-binding part of the COMT protein was studied using the atomistic molecular dynamics simulations. The results indicate that the role of the transmembrane helix and the linker part of this protein is to enclose the enzymatic part of the protein in the close vicinity of the membrane, and therefore to keep it in the specific membrane-water interface environment. Moreover, the particular kind of protein fold, which includes a specific salt bridge in the linker part of the protein, was found in almost all of the
simulations, and this information was evaluated further to reveal that this can be the general folding motif for all similar proteins that possess one transmembrane helix and a short linker part that joins it with the rest of the protein. By continuation of the urge to explain the role of the membrane in enzymatic function of COMT, another idea was also investigated: namely, the suggestion that ligands for that enzyme might have different characteristics in regard to their affinity to how the membrane was evaluated, to check whether the membrane binding part of COMT role is indeed meant to make it more accessible to those ligands which stay close to the membrane. This idea was studied with the atomistic molecular dynamics simulations where two COMT ligands—dopamine and L-dopa—were simulated with the membranes of various compositions, and furthermore the results were validated by experiments. The data from that study was consistent with the suggested idea of preferential binding of some ligands to lipids, but also this finding has been shown to have more possible implications for the neurotransmission process and other highly important physiological processes.

The second part of this work focuses on the role of cholesterol in hydrophobic matching of peptides and the resulting sorting of transmembrane peptides according to their hydrophobic length. Experimental data from collaborating team suggested that under negative mismatch and the presence of cholesterol in membranes, peptides could laterally sort. Nevertheless, molecular mechanisms of that were unclear. Atomistic molecular dynamics simulations performed for this part of the thesis revealed that cholesterol increases the significance of the negative hydrophobic mismatch, and thus it shifts preference of proteins in such conditions to cluster into domains to minimize the mismatch. In the second part of this study, extended atomistic molecular dynamics simulations showed that cholesterol has a preference to stay in the vicinity of the peptide under negative mismatch when compared to a positive mismatch case. Even more strikingly, cholesterol orients around the negatively mismatched peptide in a special geometrical configuration with its rough side exposed in the direction of peptide. In summation, studies for this work demonstrated a view on some aspects of the lipid-protein interactions at the molecular level retrieved through the atomistic molecular dynamics simulations. Importantly, many of the aspects presented here were validated with experiments or suggested explanation for the phenomena observed beforehand by experimental methods. Certainly, lipids are important for the function of proteins, and as it is shown in this thesis, joining experimental and computational approach is a very good way to understand this complicated interplay better and to provide atomistic details of these dynamic processes.

**General information**

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Authors: Orłowski, A.
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Research output: Collection of articles › Doctoral Thesis

**Computational Modeling of Functional Gold Nanoparticles in Biological Environment**

This work focuses on exploring the properties and functions of charged monolayer-protected gold nanoparticles (AuNPs) in biologically relevant environments by use of atomic-scale molecular dynamics (MD) simulations.

The use of nanoparticles (NPs) in modern technology has been increasing rapidly during the last few years. NPs of different kinds have already been employed, e.g., in nanomedicine as cancer treatments, cleaning agents, cosmetics and new materials for industrial purposes. AuNPs are one type of nanoagents that are being employed for such purposes, and according to recent experimental findings they may have cytotoxic properties. In particular, AuNPs of 2-nm diameter or less are known to permeate through plasma membranes and induce cell death. Hence, studying potential harmful effects
of AuNPs is of importance. Understanding the interaction between NPs and cell membranes is relevant also because all trafficking between the cell interior and extracellular space takes place through the cell membrane.

The first study concentrated on the properties of AuNPs in aqueous solution at physiological temperature (310 K). The results showed that electrostatic properties modulate the formation of a complex comprised of the AuNP together with surrounding ions and water, and suggested that electrostatics is one of the central factors in the complexation of AuNPs with other nanomaterials and biological systems. The results highlighted the importance of long-range electrostatic interactions in determining NP properties in aqueous solutions. This observation was concluded to indicate an important role in the interplay between NPs and lipid membranes, which surround cells.

The second part of the research comprises of studying AuNPs in the presence of model cell membranes. The binding of AuNP and membrane reorganization processes were discovered to be governed by co-operative effects where AuNP, counter ions, water and membrane all contribute. The results suggest that a permeation of a cationic AuNP takes place through pore-formation with partial NP neutralization, leading to membrane disruption at higher NP concentrations. The results also suggested a potential mechanism for cytotoxicity as cationic AuNP binding to the extracellular leaflet may trigger apoptosis through translocation of phosphatidylserine.

Summa summarum, the work presented here provides novel aspects on the interactions of functional AuNPs on cellular level by means of atomistic MD simulation.
Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes

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Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Research group: Materials and Molecular Modeling, Department of Physics, Computational Science X (CompX)
Authors: Heikkilä, E., Martinez-Seara, H., Gurtovenko, A. A., Vattulainen, I., Akola, J.

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Scopus rating (2013): SJR 1.592 SNIP 0.975 CiteScore 3.45
Scopus rating (2012): SJR 1.833 SNIP 1.156 CiteScore 3.99
Scopus rating (2011): SJR 1.644 SNIP 1.227 CiteScore 4.17
Scopus rating (2010): SJR 2.179 SNIP 1.291
Scopus rating (2009): SJR 2.152 SNIP 1.298
Scopus rating (2008): SJR 2.035 SNIP 1.123
Scopus rating (2007): SJR 2.021 SNIP 1.158
Scopus rating (2006): SJR 1.922 SNIP 1.212
Scopus rating (2005): SJR 2.037 SNIP 1.231
Scopus rating (2004): SJR 1.5 SNIP 1.147
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Scopus rating (2002): SJR 1.594 SNIP 1.228
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Scopus rating (2000): SJR 1.089 SNIP 0.907
Scopus rating (1999): SJR 0.95 SNIP 0.841
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Cholesterol, sphingolipids and glycolipids: What do we know about their role in raft-like membranes?
Co-exposure with fullerene may strengthen health effects of organic industrial chemicals

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Authors: Lehto, M., Karilainen, T., Rog, T., Cramariuc, O., Vanhala, E., Yorneus, J., Taberman, H., Jänis, J., Alenius, H., Vattulainen, I., Laine, O.
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Scopus rating (2013): SJR 1.74 SNIP 1.147 CiteScore 3.94
Scopus rating (2012): SJR 1.945 SNIP 1.142 CiteScore 4.15
Scopus rating (2011): SJR 2.369 SNIP 1.23 CiteScore 4.58
Scopus rating (2010): SJR 2.631 SNIP 1.161
Scopus rating (2009): SJR 2.473 SNIP 0.985
Scopus rating (2008): SJR 2.323 SNIP 0.96
Scopus rating (2007): SJR 1.289 SNIP 0.525
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Collective dynamics effect transient subdiffusion of inert tracers in flexible gel networks

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Authors: Godec, A., Bauer, M., Metzler, R.
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Critical adsorption of polyelectrolytes onto charged Janus nanospheres

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Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: de Carvalho, S. J., Metzler, R., Cherstvy, A. G.
Number of pages: 12
Pages: 15539-15550
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Deformation propagation in responsive polymer network films

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Ghosh, S. K., Cherstvy, A. G., Metzler, R.
Number of pages: 10
Pages: 1-9
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 141
Issue number: 7
Article number: 074903
ISSN (Print): 0021-9606
Ratings:
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Scopus rating (2014): SJR 1.386 SNIP 0.989 CiteScore 2.54
Scopus rating (2013): SJR 1.532 SNIP 1.17 CiteScore 2.95
Scopus rating (2012): SJR 1.787 SNIP 1.118 CiteScore 2.86
Scopus rating (2011): SJR 1.805 SNIP 1.207 CiteScore 3.07
Scopus rating (2010): SJR 1.73 SNIP 1.052
Scopus rating (2009): SJR 2.003 SNIP 1.104
Scopus rating (2008): SJR 2.189 SNIP 1.12
Scopus rating (2007): SJR 2.163 SNIP 1.108
Scopus rating (2006): SJR 2.176 SNIP 1.266
Scopus rating (2005): SJR 2.27 SNIP 1.359
Scopus rating (2004): SJR 2.229 SNIP 1.369
Scopus rating (2003): SJR 2.121 SNIP 1.322
Scopus rating (2002): SJR 2.256 SNIP 1.341
Scopus rating (2001): SJR 2.381 SNIP 1.362
Scopus rating (2000): SJR 2.576 SNIP 1.423
Scopus rating (1999): SJR 2.133 SNIP 1.419
Original language: English
DOIs:
10.1063/1.4893056

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-04<br/>Publisher name: American Institute of Physics
Dehydroergosterol as an Analogue for Cholesterol: Why It Mimics Cholesterol So Well - or Does It?

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM)
Authors: Pourmousa, M., Rog, T., Mikkeli, R., Vattulainen, I., Solanko, L. M., Wustner, D., Holmgaard List, N., Kongsted, J., Karttunen, M.
Number of pages: 13
Pages: 7345-7357
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 118
Issue number: 26
ISSN (Print): 1520-6106
Ratings:
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Scopus rating (2014): SJR 1.44 SNIP 1.14 CiteScore 3.28
Scopus rating (2013): SJR 1.494 SNIP 1.2 CiteScore 3.53
Scopus rating (2012): SJR 1.92 SNIP 1.251 CiteScore 3.66
Scopus rating (2011): SJR 1.78 SNIP 1.226 CiteScore 3.62
Scopus rating (2010): SJR 1.849 SNIP 1.214
Scopus rating (2009): SJR 2.232 SNIP 1.349
Scopus rating (2008): SJR 2.543 SNIP 1.381
Scopus rating (2007): SJR 2.346 SNIP 1.282
Scopus rating (2006): SJR 2.369 SNIP 1.415
Scopus rating (2005): SJR 2.275 SNIP 1.474
Scopus rating (2004): SJR 2.148 SNIP 1.511
Scopus rating (2003): SJR 2.034 SNIP 1.47
Scopus rating (2002): SJR 2.118 SNIP 1.496
Scopus rating (2001): SJR 2.053 SNIP 1.508
Scopus rating (2000): SJR 2.145 SNIP 1.527
Scopus rating (1999): SJR 1.713 SNIP 1.8
Original language: English
DOIs: 10.1021/jp406883k

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-09-30<br/>Publisher name: American Chemical Society
Source: researchoutputwizard
Source-ID: 1296
Research output: Scientific - peer-review › Article

Enzymatic oxidation of cholesterol: Properties and functional effects of cholestenone in cell membranes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
First-passage statistics for aging diffusion in systems with annealed and quenched disorder

**General information**
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Krusemann, H., Godec, A., Metzler, R.
Number of pages: 5
Pages: 1-5
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Physical Review E
Volume: 89
Issue number: 4
Article number: 040101
ISSN (Print): 1539-3755
Ratings:
Scopus rating (2016): CiteScore 1.95 SJR 0.993 SNIP 0.896
Scopus rating (2015): SJR 1.047 SNIP 0.978 CiteScore 1.89
Scopus rating (2014): SJR 1.22 SNIP 1.123 CiteScore 2.05
Scopus rating (2013): SJR 1.311 SNIP 1.239 CiteScore 2.28
Scopus rating (2012): SJR 1.42 SNIP 1.226 CiteScore 2.28
Scopus rating (2011): SJR 1.485 SNIP 1.225 CiteScore 2.28
Scopus rating (2010): SJR 1.69 SNIP 1.215
Scopus rating (2009): SJR 1.694 SNIP 1.259
Scopus rating (2008): SJR 1.96 SNIP 1.314
How Anacetrapib Inhibits the Activity of the Cholesteryl Ester Transfer Protein? Perspective through Atomistic Simulations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Äijänen, T., Koivuniemi, A., Javanainen, M., Rissanen, S., Rog, T., Vattulainen, I.
Number of pages: 14
Pages: 1-14
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: PLOS Computational Biology
Volume: 10
Issue number: 11
Article number: e1003987
ISSN (Print): 1553-7358

Ratings:
Scopus rating (2016): CiteScore 4.41 SJR 3.144 SNIP 1.342
Scopus rating (2015): SJR 3.43 SNIP 1.447 CiteScore 4.69
Scopus rating (2014): SJR 3.359 SNIP 1.44 CiteScore 4.74
Scopus rating (2013): SJR 3.295 SNIP 1.457 CiteScore 4.91
Scopus rating (2012): SJR 3.329 SNIP 1.642 CiteScore 5.36
Scopus rating (2011): SJR 3.381 SNIP 1.603 CiteScore 5.25
Scopus rating (2010): SJR 3.523 SNIP 1.554
Scopus rating (2009): SJR 3.273 SNIP 1.44
Scopus rating (2008): SJR 3.58 SNIP 1.371
Scopus rating (2007): SJR 3.09 SNIP 1.264
Scopus rating (2006): SJR 1.988 SNIP 1.018
Original language: English
DOIs:
10.1371/journal.pcbi.1003987

Bibliographical note
Contribution: organisation=fys,FACT1=1
Portfolio EDEND: 2014-12-15
Publisher name: American Physical Society
Source: researchoutputwizard
Source-ID: 814
Research output: Scientific - peer-review › Article
Mixing and segregation of ring polymers: spatial confinement and molecular crowding effects

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Shin, J., Cherstvy, A., Metzler, R.
Number of pages: 19
Pages: 1-19
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: New Journal of Physics
Volume: 16
Article number: 053047
ISSN (Print): 1367-2630
Ratings:
Scopus rating (2016): CiteScore 2.97 SJR 1.788 SNIP 1.031
Scopus rating (2015): SJR 1.938 SNIP 1.047 CiteScore 2.8
Scopus rating (2014): SJR 2.806 SNIP 1.307 CiteScore 2.89
Scopus rating (2013): SJR 2.871 SNIP 1.372 CiteScore 2.77
Scopus rating (2012): SJR 3.352 SNIP 1.533 CiteScore 3.4
Scopus rating (2011): SJR 3.47 SNIP 1.634 CiteScore 3.99
Scopus rating (2010): SJR 3.395 SNIP 1.421
Scopus rating (2009): SJR 3.215 SNIP 1.503
Scopus rating (2008): SJR 2.913 SNIP 1.396
Scopus rating (2007): SJR 2.825 SNIP 1.354
Scopus rating (2006): SJR 2.2 SNIP 1.296
Scopus rating (2005): SJR 1.641 SNIP 1.116
Scopus rating (2004): SJR 1.211 SNIP 1.009
Scopus rating (2003): SJR 1.057 SNIP 0.75
Scopus rating (2002): SJR 0.77 SNIP 0.666
Scopus rating (2001): SJR 1.033 SNIP 0.843
Scopus rating (2000): SJR 1.326 SNIP 1.307
Scopus rating (1999): SJR 0.737 SNIP 0.26
Original language: English
DOIs: 10.1088/1367-2630/16/5/053047

Bibliographical note
Contribution: organisation=fys,FACT1=1
Portfolio EDEND: 2014-12-18
Publisher name: Institute of Physics Publishing Ltd.; Deutsche Physikalische Gesellschaft
Source: researchoutputwizard
Source-ID: 1494
Research output: Scientific - peer-review » Article

Molecular Dynamics Simulation of Inverse-Phosphocholine Lipids

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Magarkar, A., Rog, T., Bunker, A.
Number of pages: 6
Pages: 19444-19449
Molecular Dynamics Simulation of PEGylated Membranes with Cholesterol: Building Toward the DOXIL Formulation

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Magarkar, A., Rog, T., Bunker, A.
Number of pages: 9
Pages: 15541-15549
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 28
ISSN (Print): 1932-7447
Ratings:
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
DOIs:
10.1021/jp504962m
Molecular motors pulling cargos in the viscoelastic cytosol: how power strokes beat subdiffusion

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Goychuk, I., Kharchenko, V. O., Metzler, R.
Number of pages: 12
Pages: 16524-16535
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
Issue number: 31
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Scopus rating (2003): SJR 1.093 SNIP 0.925
Scopus rating (2002): SJR 1.122 SNIP 0.973
Scopus rating (2001): SJR 1.09 SNIP 0.914
Scopus rating (2000): SJR 0.948 SNIP 1.068
Scopus rating (1999): SJR 0.121 SNIP 0
Original language: English
DOIs:
10.1039/c4co01234h

Nonergodicity, fluctuations, and criticality in heterogeneous diffusion processes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Polymer translocation: the first two decades and the recent diversification

General information
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Palyulin, V. V., Ala-Nissilä, T., Metzler, R.
Pages: 9016-9037
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Soft Matter
Volume: 10
Issue number: 45
ISSN (Print): 1744-683X
Ratings:
Scopus rating (2016): SJR 1.573 SNIP 1.219 CiteScore 3.7
Scopus rating (2015): SJR 1.67 SNIP 1.33 CiteScore 3.97
Scopus rating (2014): SJR 1.751 SNIP 1.267 CiteScore 4.11
Scopus rating (2013): SJR 1.745 SNIP 1.208 CiteScore 4.2
Scopus rating (2012): SJR 1.898 SNIP 1.155 CiteScore 3.96
Scopus rating (2011): SJR 2.006 SNIP 1.314 CiteScore 4.56
Scopus rating (2010): SJR 2.165 SNIP 1.376
Scopus rating (2009): SJR 2.516 SNIP 1.534
Scopus rating (2008): SJR 2.562 SNIP 1.392
Scopus rating (2007): SJR 2.482 SNIP 1.458
Scopus rating (2006): SJR 1.899 SNIP 0.981
Original language: English
DOIs:
10.1039/c4sm01819b

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-17<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1226
Research output: Scientific › peer-review › Review Article

Refined OPLS All-Atom Force Field for Saturated Phosphatidylcholine Bilayers at Full Hydration

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM)
Authors: Maciejewski, A., Pasenkiewicz-Gierula, M., Cramariuc, O., Vattulainen, I., Rog, T.
Number of pages: 11
Pages: 4571-4581
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 17
ISSN (Print): 1932-7447
Ratings:
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Scaled Brownian motion: a paradoxical process with a time dependent diffusivity for the description of anomalous diffusion

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Jeon, J., Chechkin, A. V., Metzler, R.
Number of pages: 7
Pages: 15811-15817
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
Issue number: 30
ISSN (Print): 1463-9076
Ratings:
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
Scopus rating (2010): SJR 1.802 SNIP 1.196
Scopus rating (2009): SJR 2.127 SNIP 1.369
Scopus rating (2008): SJR 2.158 SNIP 1.211
Scopus rating (2007): SJR 1.84 SNIP 1.138
Scopus rating (2006): SJR 1.467 SNIP 1.128
Scopus rating (2005): SJR 1.389 SNIP 1.104
Scopus rating (2004): SJR 1.173 SNIP 1.007
Scopus rating (2003): SJR 1.093 SNIP 0.925
Scopus rating (2002): SJR 1.122 SNIP 0.973
Scopus rating (2001): SJR 1.09 SNIP 0.914
Scopus rating (2000): SJR 0.948 SNIP 1.068
Scopus rating (1999): SJR 0.121 SNIP 0
Original language: English
DOI: 10.1021/jp5016627

Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-09-30<br/>Publisher name: American Chemical Society
Source: researchoutputwizard
Source-ID: 983
Research output: Scientific - peer-review › Article
Single Lipid Extraction: The Anchoring Strength of Cholesterol in Liquid-Ordered and Liquid-Disordered Phases

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Stetter, F., Cwiklic, L., Jungwirth, P., Hugel, T.
Number of pages: 9
Pages: 1167-1175
Publication date: 2014
Peer-reviewed: Yes

Publication Information
Journal: Biophysical Journal
Volume: 107
Issue number: 5
ISSN (Print): 0006-3495
Ratings:
Scopus rating (2016): SJR 1.946 SNIP 1.018 CiteScore 3.06
Scopus rating (2015): SJR 2.145 SNIP 1.173 CiteScore 3.3
Scopus rating (2014): SJR 2.203 SNIP 1.166 CiteScore 3.33
Scopus rating (2013): SJR 2.229 SNIP 1.165 CiteScore 3.64
Scopus rating (2012): SJR 2.343 SNIP 1.154 CiteScore 3.57
Scopus rating (2011): SJR 2.322 SNIP 1.204 CiteScore 3.75
Scopus rating (2010): SJR 2.646 SNIP 1.303
Scopus rating (2009): SJR 2.953 SNIP 1.361
Scopus rating (2008): SJR 3.222 SNIP 1.416
Scopus rating (2007): SJR 3.119 SNIP 1.422
Scopus rating (2006): SJR 2.807 SNIP 1.416
Scopus rating (2005): SJR 2.659 SNIP 1.403
Scopus rating (2004): SJR 2.494 SNIP 1.491
Scopus rating (2003): SJR 2.617 SNIP 1.428
Scopus rating (2002): SJR 2.508 SNIP 1.45
Scopus rating (2001): SJR 2.428 SNIP 1.386
Scopus rating (2000): SJR 2.603 SNIP 1.395
Scopus rating (1999): SJR 2.775 SNIP 1.437
Original language: English
DOIs:
10.1016/j.bpj.2014.07.018

The challenges of understanding glycolipid functions: An open outlook based on molecular simulations

General information
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Universal Method for Embedding Proteins into Complex Lipid Bilayers for Molecular Dynamics Simulations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Javanainen, M.
Number of pages: 6
Pages: 2577-2582
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Theory and Computation
Volume: 10
Issue number: 6
ISSN (Print): 1549-9618
Ratings:
Scopus rating (2016): SJR 2.801 SNIP 1.589 CiteScore 5.37