Publications:

MGmapper: Reference based mapping and taxonomy annotation of metagenomics sequence reads

An increasing amount of species and gene identification studies rely on the use of next generation sequence analysis of either single isolate or metagenomics samples. Several methods are available to perform taxonomic annotations and a previous metagenomics benchmark study has shown that a vast number of false positive species annotations are a problem unless thresholds or post-processing are applied to differentiate between correct and false annotations. MGmapper is a package to process raw next generation sequence data and perform reference based sequence assignment, followed by a post-processing analysis to produce reliable taxonomy annotation at species and strain level resolution. An in-vitro bacterial mock community sample comprised of 8 genuses, 11 species and 12 strains was previously used to benchmark metagenomics classification methods. After applying a post-processing filter, we obtained 100% correct taxonomy assignments at species and genus level. A sensitivity and precision at 75% was obtained for strain level annotations. A comparison between MGmapper and Kraken at species level, shows MGmapper assigns taxonomy at species level using 84.8% of the sequence reads, compared to 70.5% for Kraken and both methods identified all species with no false positives. Extensive read count statistics are provided in plain text and excel sheets for both rejected and accepted taxonomy annotations. The use of custom databases is possible for the command-line version of MGmapper, and the complete pipeline is freely available as a bitbucked package (https://bitbucket.org/genomicepidemiology/mgmapper). A web-version (https://cge.cbs.dtu.dk/services/MGmapper) provides the basic functionality for analysis of small fastq datasets.
Phase behavior of supported lipid bilayers: A systematic study by coarse-grained molecular dynamics simulations

Solid-supported lipid bilayers are utilized by experimental scientists as models for biological membranes because of their stability. However, compared to free standing bilayers, their close proximity to the substrate may affect their phase behavior. As this is still poorly understood, and few computational studies have been performed on such systems thus far, here we present the results from a systematic study based on molecular dynamics simulations of an implicit-solvent model for solid-supported lipid bilayers with varying lipid-substrate interactions. The attractive interaction between the substrate and the lipid head groups that are closest to the substrate leads to an increased translocation of the lipids from the distal to the proximal bilayer-leaflet. This thereby leads to a transbilayer imbalance of the lipid density, with the lipid density of the proximal leaflet higher than that of the distal leaflet. Consequently, the order parameter of the proximal leaflet is found to be higher than that of the distal leaflet, the higher the strength of lipid interaction is, the stronger the effect. The proximal leaflet exhibits gel and fluid phases with an abrupt melting transition between the two phases. In contrast, below the
melting temperature of the proximal leaflet, the distal leaflet is inhomogeneous with coexisting gel and fluid domains. The size of the fluid domains increases with increasing the strength of the lipid interaction. At low temperatures, the inhomogeneity of the distal leaflet is due to its reduced lipid density.

**General information**

State: Published
Organisations: Department of Systems Biology, Center for Biological Sequence Analysis, University of Memphis
Authors: Poursoroush, A. (Ekstern), Sperotto, M. M. (Intern), Laradji, M. (Ekstern)
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Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
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BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.532 SNIP 1.17 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.787 SNIP 1.118 CiteScore 2.86
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.805 SNIP 1.207 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.73 SNIP 1.052
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.003 SNIP 1.104
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.189 SNIP 1.12
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.163 SNIP 1.108
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.176 SNIP 1.266
Web of Science (2006): Indexed yes
Spontaneous Lipid Flip-Flop in Membranes: A Still Unsettled Picture from Experiments and Simulations

Biomembrane asymmetry, whose regulation is important for function, is maintained by the movement of lipids from one bilayer leaflet to the other (flip-flop). During the last decades a number of studies have been done to characterize this process, and it was found that it can be spontaneous or assisted by protein transporters. It can be accelerated or inhibited by various factors, e.g., it can be induced by mechanical stresses. It was also found that flip-flop rate and mechanism strongly depend on the molecular structure of the flipping lipid and on the composition and physical state of the membrane. Yet, large discrepancies exist among the data available in the literature, and a quantitative and comprehensive understanding of this process is still missing. This chapter reviews our current knowledge of the molecular aspects of spontaneous (or passive) flip-flop. An overview of experimental studies is presented, together with a summary of the state of the art of computer simulation studies, which enable a direct insight at the molecular level. The achievements and limitations of experimental and computational approaches are pointed out, as well as the challenges that remain to be addressed.
Model studies of lipid flip-flop in membranes

Biomembranes, which are made of a lipid bilayer matrix where proteins are embedded or attached, constitute a physical barrier for cell and its internal organelles. With regard to the distribution of their molecular components, biomembranes are both laterally heterogeneous and transversally asymmetric, and because of this they are sites of vital biochemical activities. Lipids may translocate from one leaflet of the bilayer to the opposite either spontaneously or facilitated by proteins, hence they contribute to the regulation of membrane asymmetry on which cell functioning, differentiation, and growth heavily depend. Such transverse motion—commonly called flip-flop—has been studied both experimentally and computationally. Experimental investigations face difficulties related to time-scales and probe-induced membrane perturbation issues. Molecular dynamics simulations play an important role for the molecular-level understanding of flip-flop. In this review we present a summary of the state of the art of computational studies of spontaneous flip-flop of phospholipids, sterols and fatty acids. Also, we highlight critical issues and strategies that have been developed to solve them, and what remains to be solved.

General information

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Source: FindIt
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Tools and data services registry: a community effort to document bioinformatics resources

Life sciences are yielding huge data sets that underpin scientific discoveries fundamental to improvement in human health, agriculture and the environment. In support of these discoveries, a plethora of databases and tools are deployed, in technically complex and diverse implementations, across a spectrum of scientific disciplines. The corpus of documentation of these resources is fragmented across the Web, with much redundancy, and has lacked a common standard of information. The outcome is that scientists must often struggle to find, understand, compare and use the best resources for the task at hand. Here we present a community-driven curation effort, supported by ELIXIR—the European infrastructure for biological information—that aspires to a comprehensive and consistent registry of information about bioinformatics resources. The sustainable upkeep of this Tools and Data Services Registry is assured by a curation effort driven by and tailored to local needs, and shared amongst a network of engaged partners. As of September 2015, the registry includes 1633 resources, with depositions from 91 individual registrations including 40 institutional providers and 51 individuals. With community support, the registry can become a standard for dissemination of information about bioinformatics resources: we welcome everyone to join us in this common endeavour. The registry is freely available at https://bio.tools.

General information

State: Published
Organisations: Department of Systems Biology, Center for Biological Sequence Analysis, Institut Pasteur, University of Copenhagen, University of Manchester, Palacky University, European Bioinformatics Institute, Centre for Ecology and Hydrology, National Institute for Agronomic Research, University of Bologna, University of Roma ‘Tor Vergata’, VIB - Flanders Institute for Biotechnology, CRS4-Bioinformatics Laboratory, University of Milano Bicocca, Swiss Institute of Bioinformatics, Bielefeld University, Albert Ludwigs Universität Freiburg, Technical University of Munich, French Institute of Bioinformatics, University of Ljubljana, Chinese University of Hong Kong, University of Padua, Bioinformatics Research Centre, Daresbury Laboratory, University of Lübeck, University of Tartu, Imperial College London, IRCCS AOU San Martino-IST, University of Southern Denmark, Wellcome Trust Centre for Human Genetics, Central European Institute of Technology, Fundación Centro Nacional de Investigaciones Cardiovasculares, Sapienza University of Rome, University of Milan, Radboud University Nijmegen, Masaryk University, University of Bergen
Authors: Ison, J. (Intern), Rapacki, K. (Intern), Ménager, H. (Ekstern), Kalaš, M. (Ekstern), Rydza, E. K. (Intern), Chmura, P. J. (Intern), Anthon, C. (Ekstern), Beard, N. (Ekstern), Berka, K. (Ekstern), Bolser, D. (Ekstern), Booth, T. (Ekstern),
Protein raftophilicity. How bioinformatics can help membranologists

Protein raftophilicity is the affinity of proteins for lipid ‘rafts’. Rafts denote nano- and submicro-sized biomembrane domains that are enriched in cholesterol and sphingolipids. These domains are considered relevant for maintaining specialized structures that constitute suitable sites for bioprocesses. Protein raftophilicity depends on features such as lipidation and GPI-anchoring. Can this affinity be inferred solely by knowing such features, without knowing the physical and physico-chemical properties of biomembranes? We tried to answer the question by an artificial neural network (ANN)-based bioinformatics approach. The ANN was trained to recognize feature-based patterns in proteins that are considered to be associated with lipid rafts. The trained ANN was then used to predict protein raftophilicity. We found that, in the case of α-helical membrane proteins, their hydrophobic length does not affect their raftophilicity. This is in agreement with confocal microscopy experiments on DOPC/SM/cholesterol bilayers with reconstituted model peptides, P-23 and P-29.

Reads2Type: a web application for rapid microbial taxonomy identification

Identification of bacteria may be based on sequencing and molecular analysis of a specific locus such as 16S rRNA, or a set of loci such as in multilocus sequence typing. In the near future, healthcare institutions and routine diagnostic microbiology laboratories may need to sequence the entire genome of microbial isolates. Therefore we have developed Reads2Type, a web-based tool for taxonomy identification based on whole bacterial genome sequence data. Raw sequencing data provided by the user are mapped against a set of marker probes that are derived from currently available bacteria complete genomes. Using a dataset of 1003 whole genome sequenced bacteria from various sequencing platforms, Reads2Type was able to identify the species with 99.5 % accuracy and on the minutes time scale. In comparison with other tools, Reads2Type offers the advantage of not needing to transfer sequencing files, as the entire computational analysis is done on the computer of whom utilizes the web application. This also prevents data privacy
issues to arise. The Reads2Type tool is available at http://www.cbs.dtu.dk/~dhany/reads2type.html.

General information
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Organisations: Department of Systems Biology, Center for Biological Sequence Analysis, Metagenomics, Immunological Bioinformatics, National Food Institute, Research Group for Genomic Epidemiology, National Centre for Agricultural Research and Extension
Authors: Saputra, D. (Intern), Rasmussen, S. (Intern), Larsen, M. V. (Intern), Haddad, N. (Ekstern), Sperotto, M. M. (Intern), Aarestrup, F. M. (Intern), Lund, O. (Intern), Sicheritz-Pontén, T. (Intern)
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Scopus rating (2014): SJR 1.836 SNIP 1.202 CiteScore 2.91
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Scopus rating (2013): SJR 1.932 SNIP 1.335 CiteScore 3.38
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Scopus rating (2012): SJR 1.857 SNIP 1.155 CiteScore 3.24
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.655 SNIP 1.215 CiteScore 3.34
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Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 1.756 SNIP 1.15
Web of Science (2010): Indexed yes
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Scopus rating (2008): SJR 1.945 SNIP 1.146
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.971 SNIP 1.129
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Organisations: Department of Systems Biology, Integrative Systems Biology, Center for Biological Sequence Analysis
Authors: Brunak, S. (Intern), Løngreen, P. (Intern), Rapacki, K. (Intern), Sperotto, M. M. (Intern)
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Predictions of Phase Separation in Three-Component Lipid Membranes by the MARTINI Force Field

The phase behavior of the coarse-grained MARTINI model for three-component lipid bilayers composed of dipalmytoyl-phosphatidylcholine (DPPC), cholesterol (Chol), and an unsaturated phosphatidylcholine (PC) was systematically investigated by molecular dynamics simulations. The aim of this study is to understand which types of unsaturated PC induce the formation of thermodynamically stable coexisting phases when added to mixtures of DPPC and Chol and to unravel the mechanisms that drive phase separation in such three-component mixtures. Our simulations indicate that the currently used MARTINI force field does not induce such phase separation in mixtures of DPPC, Chol, and unsaturated PCs with a low unsaturation level, such as palmitoyl-oleoyl-phosphatidylcholine (POPC) or dioleoyl-phosphatidylcholine (DOPC). Also, we found that phase separation does occur in mixtures of DPPC, Chol, and polyunsaturated PCs, such as dilinoleoyl-phosphatidylcholine (DUPC) and diarachidonoyl-phosphatidylcholine (DAPC). Through systematic tweaking of the interactions between the hydrophobic groups of the PC molecules, we show that the appearance of phase separation in three-component lipid bilayers, as modeled through the MARTINI force field, is primarily due to the interactions between the coarse-grained molecules, i.e., the beads, rather than due to the differences between the conformations of saturated and unsaturated lipid acyl chains, namely entropy driven.
Flip-Flop of Steroids in Phospholipid Bilayers: Effects of the Chemical Structure on Transbilayer Diffusion

The transverse motion of molecules from one leaflet to the other of a lipid bilayer, or flip-flop, represents a putative mechanism for their transmembrane transport and may contribute to the asymmetric distribution of components in biomembranes. However, a clear understanding of this process is still missing. The scarce knowledge derives from the difficulty of experimental determination. Because of its slow rate on the molecular time scale, flip-flop is challenging also for computational techniques. Here, we report a study of the passive transbilayer diffusion of steroids, based on a kinetic model derived from the analysis of their free energy surface, as a function of their position and orientation in the bilayer. An implicit membrane description is used, where the anisotropy and the nonuniformity of the bilayer environment are taken into account in terms of the gradients of density, dielectric permittivity, acyl chain order parameters, and lateral pressure. The flip-flop rates are determined by solving the Master Equation that governs the time evolution of the system, with transition rates between free energy minima evaluated according to the Kramers theory. Considering various steroids (cholesterol, lanosterol, ketosterone, 5-cholestene, 25-hydroxycholesterol, and testosterone), we can discuss how differences in molecular shape and polarity affect the pathway and the rate of flip-flop in a liquid crystalline 1,2-dipalmitoyl-sn-glycero-3-phosphatidylcholine (DPPC) bilayer, at low steroid concentration. We predict time scales ranging from microseconds to milliseconds, strongly affected by the presence of polar substituents and by their position in the molecular skeleton.
Coarse-grain membrane models

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Organisations: Department of Systems Biology
Authors: Sperotto, M. M. (Intern)
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Mesoscopic models of biological membranes

Phospholipids are the main components of biological membranes and dissolved in water these molecules self-assemble into closed structures, of which bilayers are the most relevant from a biological point of view. Lipid bilayers are often used, both in experimental and by theoretical investigations, as model systems to understand the fundamental properties of biomembranes. The properties of lipid bilayers can be studied at different time and length scales. For some properties it is
sufficient to envision a membrane as an elastic sheet, while for others it is important to take into account the details of the individual atoms. In this review, we focus on an intermediate level, where groups of atoms are lumped into pseudo-particles to arrive at a coarse-grained, or mesoscopic, description of a bilayer, which is subsequently studied using molecular simulation. The aim of this review is to compare various strategies to coarse grain a biological membrane. The conclusion of this comparison is that there can be many valid different strategies, but that the results obtained by the various mesoscopic models are surprisingly consistent. A second objective of this review is to illustrate how mesoscopic models can be used to obtain a better understanding of experimental systems. The advantage of coarse-grained models is that these can be simulated very efficiently, so that phenomena involving large systems, or requiring a large number of simulations, can be studied in detail. This is illustrated with the study of the relation between the phase behavior of a membrane and the structure of the phospholipids, and the membrane structural changes due to molecules (such as alcohols, cholesterol and anesthetics) adsorbed to the membrane. We then discuss the effect of transmembrane peptides on the local structure of a membrane and the mechanism of vesicle fusion and fission.

General information
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Organisations: Department of Systems Biology
Authors: Venturoli, M. (Ekstern), Sperotto, M. M. (Intern), Kranenburg, M. (Ekstern), Smit, B. (Ekstern)
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BFI (2016): BFI-level 2
Scopus rating (2016): SJR 6.933 SNIP 8.393 CiteScore 17.17
BFI (2015): BFI-level 2
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Scopus rating (2013): SJR 11.278 SNIP 12.298 CiteScore 24.21
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 11.443 SNIP 11.173 CiteScore 22.3
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 12.464 SNIP 11.19 CiteScore 20.3
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 9.976 SNIP 9.009
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 8.634 SNIP 8.493
BFI (2008): BFI-level 2
Scopus rating (2006): SJR 7.213 SNIP 5.399
Web of Science (2006): Indexed yes
Scopus rating (2004): SJR 8.12 SNIP 7.117
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Modelling of proteins in membranes

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Organisations: Department of Systems Biology
Authors: Sperotto, M. M. (Intern), May, S. (Ekstern), Baumgaertner, A. (Ekstern)
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Scopus rating (2016): SJR 0.976 SNIP 0.862 CiteScore 2.78
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.957 SNIP 0.957 CiteScore 2.75
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.885 SNIP 1.039 CiteScore 2.62
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.82 SNIP 1.055 CiteScore 2.66
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.803 SNIP 0.974 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.727 SNIP 0.984 CiteScore 2.56
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.874 SNIP 0.964
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.9 SNIP 0.995
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.114 SNIP 1.057
Scopus rating (2007): SJR 1.083 SNIP 1.091
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.808 SNIP 0.881
Web of Science (2006): Indexed yes
Simulation studies of protein-induced bilayer deformations, and lipid-induced protein tilting, on a mesoscopic model for lipid bilayers with embedded proteins

Biological membranes are complex and highly cooperative structures. To relate biomembrane structure to their biological function it is often necessary to consider simpler systems. Lipid bilayers composed of one or two lipid species, and with embedded proteins, provide a model system for biological membranes. Here we present a mesoscopic model for lipid bilayers with embedded proteins, which we have studied with the help of the dissipative particle dynamics simulation technique. Because hydrophobic matching is believed to be one of the main physical mechanisms regulating lipid-protein interactions in membranes, we considered proteins of different hydrophobic length (as well as different sizes). We studied the cooperative behavior of the lipid-protein system at mesoscopic time-and length-scales. In particular, we correlated in a systematic way the protein-induced bilayer perturbation, and the lipid-induced protein tilt, with the hydrophobic mismatch (positive and negative) between the protein hydrophobic length and the pure lipid bilayer hydrophobic thickness. The protein-induced bilayer perturbation was quantified in terms of a coherence length, $x(P)$, of the lipid bilayer hydrophobic thickness profile around the protein. The dependence on temperature of $x(P)$, and the protein tilt-angle, were studied above the main-transition temperature of the pure system, i.e., in the fluid phase. We found that $x(P)$ depends on mismatch, i.e., the higher the mismatch is, the longer $x(P)$ becomes, at least for positive values of mismatch; a dependence on the protein size appears as well. In the case of large model proteins experiencing extreme mismatch conditions, in the region next to the so-called lipid annulus, there appears an undershooting (or overshooting) region where the bilayer hydrophobic thickness is locally lower (or higher) than in the unperturbed bilayer, depending on whether the protein hydrophobic length is longer (or shorter) than the pure lipid bilayer hydrophobic thickness. Proteins may tilt when embedded in a too-thin bilayer. Our simulation data suggest that, when the embedded protein has a small size, the main mechanism to compensate for a large hydrophobic mismatch is the tilt, whereas large proteins react to negative mismatch by causing an increase of the hydrophobic thickness of the nearby bilayer. Furthermore, for the case of small, peptidelike proteins, we found the same type of functional dependence of the protein tilt-angle on mismatch, as was recently detected by fluorescence spectroscopy measurements.

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Authors: Venturoli, M. (Ekstern), Smit, B. (Ekstern), Sperotto, M. M. (Intern)
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Characterization of the thermotropic behavior and lateral organization of lipid-peptide mixtures by a combined experimental and theoretical approach: Effects of hydrophobic mismatch and role of flanking residues

A combined experimental and theoretical study was performed on a series of mixtures of dipalmitoylphosphatidylcholine (DPPC) and synthetic peptides to investigate their thermotropic behavior and lateral organization. The experimental study
was based on differential scanning calorimetry (DSC) and phosphorous nuclear magnetic resonance (P-31-NMR) techniques; the theoretical study was based on calculations on a microscopic molecular interaction model, where the lipid-peptide interaction is built on the hydrophobic matching principle. The chosen peptides, WALP and KALP, consist of a hydrophobic stretch, of variable length, of alternating leucine and alanine residues, flanked on both ends with tryptophan and lysine residues, respectively. By systematically varying the peptide hydrophobic length it was thus possible to explore different matching conditions between the peptide's hydrophobic length and the lipid bilayer hydrophobic thickness, and to investigate the potential role of flanking residues. The results show that both the WALP and the KALP peptides tend to favor the liquid-crystal line (or fluid) phase of the system; i.e., they tend to depress the main-transition temperature, T-m, of pure DPPC. However, the detailed effects of both peptides on the lateral phase behavior of the lipid-peptide system are dependent on the peptide length and the type of flanking residues. The results suggest that below T-m, the shortest among the WALP and KALP peptides induce gel-fluid phase separation in the system within an extensive temperature-composition region. The longer the hydrophobic length of the peptides is, the more narrow this region appears to become.
Variety identification of wheat using mass spectrometry with neural networks and the influence of mass spectra processing prior to neural network analysis

The performance of matrix-assisted laser desorption/ionisation time-of-flight mass spectrometry with neural networks in wheat variety classification is further evaluated.(1) Two principal issues were studied: (a) the number of varieties that could be classified correctly; and (b) various means of preprocessing mass spectrometric data. The number of wheat varieties tested was increased from 10 to 30. The main pre-processing method investigated was based on Gaussian smoothing of the spectra, but other methods based on normalisation procedures and multiplicative scatter correction of data were also used. With the final method, it was possible to classify 30 wheat varieties with 87% correctly classified mass spectra and a correlation coefficient of 0.90.

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Organisations: Department of Systems Biology
Authors: Sørensen, H. A. (Intern), Sperotto, M. M. (Intern), Petersen, M. (Ekstern), Kesmir, C. (Intern), Radzikowski, L. (Intern), Jacobsen, S. (Intern), Søndergaard, I. (Intern)
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BFI (2015): BFI-level 1
Identification of barley and rye varieties using matrix-assisted laser desorption/ionisation time-of-flight mass spectrometry with neural networks

Cereal varieties are normally identified using time-consuming methods such as visual examination of either the intact grain or one-dimensional electrophoretic patterns of the grain storage proteins. A fast method for identification of wheat (Triticum aestivum L.) varieties has previously been developed, which combines analysis of alcohol-soluble wheat proteins (gliadins) using matrix-assisted laser desorption/ionisation time-of-flight mass spectrometry with neural networks. Here we have applied the same method for the identification of both barley (Hordeum vulgare L.) and rye (Secale cereale L.) varieties. For barley, 95% of the mass spectra were correctly classified. This is an encouraging result, since in earlier experiments only a grouping into subsets of varieties was possible. However, the method was not useful in the
classification of rye, due to the strong similarity between mass spectra of different varieties.

**General information**
State: Published
Organisations: Enzyme and Protein Chemistry, Department of Systems Biology, Center for Biological Sequence Analysis
Pages: 440-445
Publication date: 2001
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Rapid Communications in Mass Spectrometry
Volume: 15
Issue number: 6
ISSN (Print): 0951-4198
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.737 SNIP 0.792 CiteScore 2.03
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.806 SNIP 0.807 CiteScore 2.12
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.877 SNIP 0.876 CiteScore 2.26
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.999 SNIP 0.955 CiteScore 2.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.017 SNIP 0.912 CiteScore 2.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.228 SNIP 0.934 CiteScore 2.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.183 SNIP 0.928
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.34 SNIP 0.923
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.333 SNIP 0.959
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.379 SNIP 1.032
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.175 SNIP 0.96
Scopus rating (2005): SJR 1.383 SNIP 1.164
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.247 SNIP 1.083
Consequences of hydrophobic matching on the lateral distribution of lipids around bacteriorhodopsin reconstituted in DLPC/DSPC mixtures

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry
Authors: Dumas, F. (Ekstern), Lebrun, M. (Ekstern), Sperotto, M. M. (Intern), Tocanne, J. (Ekstern), Mouritsen, O. G. (Intern)
Pages: 321-331
Publication date: 1998

Host publication information
Title of host publication: Lipid and Protein Traffic. Pathways and Molecular Mechanisms : NATO ASI Series H:Cell Biology
Volume: 106
Place of publication: Berlin
Publisher: Springer
Main Research Area: Technical/natural sciences
Conference: Lipid and Protein Traffic. Pathways and Molecular Mechanisms, 01/01/1998
Source: orbit
Source-ID: 171193
Publication: Research - peer-review › Article in proceedings – Annual report year: 1998

Theoretical analysis of protein organization in lipid membranes

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry, McGill University
Authors: Ipsen, J. H. (Intern), Gil, T. (Ekstern), Mouritsen, O. G. (Intern), Sabra, M. C. (Intern), Sperotto, M. M. (Intern), Zuckermann, M. J. (Ekstern)
Pages: 245-266
Publication date: 1998
Main Research Area: Technical/natural sciences

Publication information
Journal: Biochimica et Biophysica Acta
Volume: 1376
ISSN (Print): 0006-3002
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.71
Bacteriorhodopsin Carries out a Molecular Sorting in DLPC/DSPC Proteoliposomes

General information
State: Published
Organisations: Department of Chemistry
Authors: Dumas, F. (Ekstern), Lebrun, M. C. (Ekstern), Sperotto, M. M. (Intern), Mouritsen, O. G. (Intern)
Pages: 78
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: European Biophysics Journal
Volume: 26
ISSN (Print): 0175-7571
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.45 SJR 0.672 SNIP 0.619
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.752 SNIP 0.641 CiteScore 1.55
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.098 SNIP 0.924 CiteScore 2.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.119 SNIP 0.912 CiteScore 2.34
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.15 SNIP 0.85 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Lipid Sorting by Bacteriorhodopsin

General information
State: Published
Organisations: Department of Chemistry
Authors: Sperotto, M. M. (Intern), Dumas, F. (Ekstern), Lebrun, C. (Ekstern), Tocanne, J. (Ekstern), Mouritsen, O. G. (Intern)
Pages: A307
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Biophysical Journal
Volume: 72
ISSN (Print): 0006-3495
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.946 SNIP 1.018
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.145 SNIP 1.173 CiteScore 3.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.203 SNIP 1.166 CiteScore 3.33
Web of Science (2014): Indexed yes
Molecular Sorting of Lipids by Bacteriorhodopsin in DMPC-DSPC Lipid Bilayers

General information
State: Published
Organisations: Department of Chemistry
Authors: Dumas, F. (Ekstern), Sperotto, M. M. (Intern), Tocanne, J. (Ekstern), Mouritsen, O. G. (Intern)
Pages: 1940-1953
Publication date: 1997
Main Research Area: Technical/natural sciences

Publication information
Journal: Biophysical Journal
Volume: 73
ISSN (Print): 0006-3495
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.946 SNIP 1.018
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.145 SNIP 1.173 CiteScore 3.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.203 SNIP 1.166 CiteScore 3.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.229 SNIP 1.165 CiteScore 3.64
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.343 SNIP 1.154 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.322 SNIP 1.204 CiteScore 3.75
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.646 SNIP 1.303
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.953 SNIP 1.361
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.222 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.119 SNIP 1.422
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.807 SNIP 1.416
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.659 SNIP 1.403
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.494 SNIP 1.491
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.617 SNIP 1.428
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.508 SNIP 1.45
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.428 SNIP 1.386
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.603 SNIP 1.395
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.775 SNIP 1.437
Phase Behavior and Permeability Properties of Phospholipid Bilayers Containing a Short-chain Phospholipid Permeability Enhancer

Theory of phase equilibria and critical mixing points in binary lipid bilayers
The fundamental problem of determining the phase equilibria of binary mixtures is discussed in the context of two-component phospholipid bilayer membranes of saturated phospholipids with different acyl-chain lengths. Results are presented from mean-field calculations and Monte Carlo simulations on a statistical mechanical model in which the interaction between lipid acyl chains of different length is formulated in terms of a hydrophobic mismatch. The model permits a series of binary phase diagrams to be determined in terms of a single "universal" interaction parameter. The part of the free energy necessary to derive phase equilibria is determined from the simulations using distribution functions and histogram techniques, and the nature of the phase equilibria is determined by a finite-size scaling analysis which also permits the interfacial tension to be derived. Results are also presented for the enthalpy and the compositional fluctuations. It is shown, in accordance with experiments, that the nonideal mixing of lipid species due to mismatch in the
hydrophobic lengths leads to a progressively nonideal mixing behavior as the chain-length difference is increased. Moreover, indications are found that a phase transition in a strict thermodynamic sense may be absent in some of the short-chain one-component Lipid bilayers, but a transition can be induced when small amounts of another species are mixed in, leading to a closed phase separation loop with critical points. The physical mechanism of inducing the transition is discussed in terms of the molecular properties of the lipid acyl chains. The results of the numerical model study are expected to have consequences for the interpretation of experimental measurements on lipid bilayer systems in terms of phase diagrams. (C) 1995 American Institute of Physics.
POTTS-MODEL, PHOSPHATIDYLCHOLINES, LIQUID-CRYSTALS, MONTE-CARLO, MEMBRANES, SCATTERING, MIXTURES, CHOLESTEROL, 1ST-ORDER MELTING TRANSITION, LEBWOHL-LASHER MODEL

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Activities:
First Annual Danish Bioinformatics Conference
Maria Maddalena Sperotto (Organizer)
Department of Systems Biology
Center for Biological Sequence Analysis

Description
Member of the Management Committee

Documents:
DKBiC-2015

Links:

Related event
First Annual Danish Bioinformatics Conference
27/08/2015 → 27/11/2015
Odense, Denmark
Activity: Attending an event › Participating in or organising a conference