Since January 2020 Elsevier has created a COVID-19 resource centre with free information in English and Mandarin on the novel coronavirus COVID-19. The COVID-19 resource centre is hosted on Elsevier Connect, the company's public news and information website.

122-Pos
Working Towards Cryo-Em Structures of Mitochondrial Dynamin-Like GTPases
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Dynamins are a class of GTPase enzymes responsible for the fusion, fission, and vesiculation of cellular lipid membranes throughout the cell. The dynamin-like proteins Mitofusin (Mfn1/2) and Optic Atrophy 1 (Opa1) are responsible for the fusion of the outer and inner mitochondrial membranes, respectively. Unlike other dynamin-like proteins, Mfn1/2 and Opa1 are transmembrane proteins. Currently, structural data for Mfn1/2 in association with membranes is limited and any structural or biochemical data for Opa1 is even more so. We have developed protocols for systematically expressing Mfn1/2 and are working towards purification in a lipid bilayer. Additionally, expression and purification of biologically relevant and biochemically active shortened isoforms of Opa1 in sufficient quantity to conduct biochemical assays have also been achieved. Furthermore, we are optimizing sample preparation and have begun reconstructions of a proteolytically processed short form, s-Opa1, by cryo-EM on a lipid surface and are examining the role nucleotide states play in structural rearrangements.

123-Pos
Modelling Long Loops of Membrane Proteins using Pretzel
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Beta-barrel membrane proteins are found in the outer membrane of gram-negative bacteria, mitochondria, and chloroplasts. They play important roles in membrane anchoring, pore formation and enzyme activities. The extracellular loops (ECLs) of outer membrane proteins (OMPs) are highly variable, and often little is known about their functional roles. in this work, we study the extracellular loop regions of the protein LptD, an essential OMP that inserts lipopolysaccharide endotoxins into the outer membrane of Escherichia coli. LptD contains 26 strands and 13 loops. We model the longer loops of LptD using the Pretzel (Protein Topology of Zoetic Loops) method and generate a conformational ensemble of these loops which can help to understand their functionality. Pretzel provides a novel computational framework that combines Monte Carlo conformational sampling, structure clustering, and ensemble energy evaluation. It was developed to investigate gating behavior of OMPs under different pH conditions. While successfully applied to decipher the pH-regulated control mechanism of OmpG gating, our results show that Pretzel can be applied to broadly model the conformational ensembles of extracellular loops.

124-Pos
Molecular Mechanism of Potassium (K^+) Ion Sensing Histidine Kinase Involved in Biofilm Formation
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Eighty percent of human infections are caused from persistent biofilm communities that have become resistant to antibiotics. Pathogenesis as simple as dental plaque buildup to medical device transplant complications are in need of novel antimicrobial endeavors to combat persistent bacterial infections. The objective of this study is to elucidate the activation mechanism of a bacterial Histidine Kinase from *Bacillus subtilis*, KinC, which initiates a signal transduction cascade leading to biofilm formation. Wildtype KinC has been successfully recombinantly expressed and purified along with the first mutant construct targeting the autophosphorylation site to disrupt phosphorylation activity. initial functional assays demonstrate that radiolabeled ATP can be used to study KinC's phosphorylation activity. This project will utilize a biochemical approach to elucidate the mechanism of a bacterial potassium-sensing enzyme putatively involved in initiating a signal transduction cascade inside the cell. with current antimicrobial methods being defeated, continuation of elucidating various bacterial communication mechanisms can assist in development of novel antimicrobial methods.

125-Pos
Investigating SARS-CoV-2 Orf7B Homodimerization by Molecular Dynamics Simulations
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ORF7b is a 43-amino-acid single-pass transmembrane protein that is associated with the virulence of SARS-CoV-2 and localizes to the endoplasmic reticulum-Golgi intermediate compartment. Its homodimer associates to suppress host immune response; however, a structural model of protein-protein interface within the homodimer is unknown. This work aims to investigate the ORF7b homodimerization through molecular dynamics (MD) and provide insights into molecular interactions to assist the design of inhibitions. A multi-scale MD simulation with coarse-grained (CG) and all-atom (AA) models was conducted to simulate the formation of dimer and identify the key dimer interactions. initially separated AA monomers of the wild-type ORF7b were used to simulate homodimers in parallel or anti-parallel orientations based on the N-terminus placement of each monomer. The dimers were taken as initial conformations for five microsecond CG MD simulations by using the Martini force field (FF) with explicit solvent, and a bilayer of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) lipids. The structures obtained from the last step of CG MD simulations were used to covert to initial configurations for 400 ns AA MD simulations by using the CHARMM36 FF. The result of MD simulations shows different molecular conformations for the two orientations, whose residue-residue interactions were identified in different sections and intensities through hydrogen bonding, π-π stacking, and other hydrophobic contacts. The preliminary results indicate two potential configurations for homodimerization with different levels of binding intensity, which requires confirmation from our experimental collaborators (Dr. Bryan Berger's Lab at UVA). This study will further construct the mutated ORF7b at the identified residue pairs to better understand the homodimerization while the specific interactions are enhanced or reduced.

126-Pos
Interplay between Leakage and Fusion of Phosphatidylcholine Liposomes Induced by the Macrolittins, a Synthetically Evolved Family of Pore-Forming Peptides
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Peptides that form pores in lipid bilayer membranes can be used in a variety of biotechnological and clinical applications including drug delivery and targeted cancer therapy. According to the results from our previous peptide library screening, novel peptides called ''macrolittins'' were discovered that release macromolecules from phosphatidylcholine vesicles at low concentration by forming large pores. Here we explore how the uniquely potent functions of an example macrolittin, M159, depend on bilayer properties. We found that M159 causes dramatic vesicle aggregation and fusion even at low concentration (P:L$<$1:200). We tested whether liposome aggregation and fusion are required for leakage. inclusion of 5 mol % PEG-2k lipids or 5 mol % anionic POPG in POPC liposomes blocked aggregation and fusion almost completely but did not change macromolecular leakage. Thus, the bilayer destabilization that leads to aggregation and fusion is incidental to pore formation. These data show that, in contrast to some cell penetration and antimicrobial peptides where liposomal leakage is an artifact of liposome fusion, the macrolittin M159 permeabilizes liposomes by forming true membrane spanning pores. Next, we tested the effect of cholesterol on M159 macromolecular poration activity and found that the addition of 30% cholesterol causes a large decrease in activity. Finally, we measured macromolecule leakage in fluid phase bilayers that have a thinner or thicker hydrocarbon core, compared to the POPC bilayers used in the screen. M159 activity is blocked by thicker phospholipid bilayers which also inhibited liposomal aggregation or fusion induced by M159. Importantly, the membrane selectivity of M159 may be used to trigger cargo release in vivo from modified liposomes without lipid aggregation and fusion.

127-Pos
Deciphering the Roles of *Yersinia pestis* Outer Membrane Proteins in their Native Environment
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Plasminogen activator (Pla) and Adhesion invasion locus (Ail) are the outer membrane β-barrel proteins from *Yersinia pestis* involved in bacterial dissemination and serum survival within humans. The activities of these virulence factors are regulated by non-proteinaceous components of the asymmetric outer membrane of *Yersinia pestis*. For example, the outer