Symposium: Mechanisms of Cell Wall Biopolymer Assembly

94-Symp
BPS2025 - Cellulose biosynthesis and modification: A versatile biomaterial across kingdoms of life
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Cellulose is the most abundant biopolymer on earth as it represents the major component of the cell wall of vascular plants. As a polymer of glucose molecules, its biosynthesis by photosynthetic organisms accounts for a significant annual reduction in atmospheric carbon dioxide. In addition to plant and fungal cell walls, cellulose also serves as a bacterial biofilm component and as a tissue scaffold in some tunicates. Cellulose is synthesized and secreted across the plasma membrane by cellulose synthase, a membrane-embedded, processive glycosyltransferase. While the core biosynthetic machinery is evolutionarily conserved, cellulose biosynthesis shows species-specific variations for the production of tailored cellulosic biomaterials. These include the alignment of cellulose chains into cable-like fibers as the load-bearing components of plant cell walls and the chemical modification of cellulose with small molecules in certain biofilms. We present detailed mechanistic insights into cellulose biosynthesis in plants and bacteria. Combining structural and functional analyses, we explain how cellulose synthase elongates a nascent cellulose polymer, how the elongated chain is translocated across the plasma membrane, and how plant cellulose synthase promotes the alignment of cellulose polymers into fibrillar structures. We also provide insights into the chemical modification of cellulose with lipid-derived phosphoethanolamine by *Enterobacteriaceae*. Here, cellulose synthase is part of a macromolecular complex that catalyzes the synthesis, chemical modification, and secretion of cellulose across the gram-negative cell envelope. Together, our work provides insights into the molecular and mechanistic principles necessary to design novel cellulosic biomaterials.

95-Symp
BPS2025 - The glycoprotein-rich cell wall architecture of *Chlamydomonas reinhardtii*
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Microalgae are of great interest in the context of climate change as they act as carbon sinks, in addition to being a critical renewable biomass for biofuel, food, and nutrients production. However, efficient exploitation of this aquatic resource depends on our understanding of the cell wall composition and structure, as this complex barrier influences access to valuable intracellular molecules. In this work, we used *in situ* and in-cell solid-state as well as sensitivity-enhanced nuclear magnetic resonance methods, complemented by mass spectrometry and electron microscopy, to provide a nanoscale model of the architecture of the glycoprotein-rich cell wall of *Chlamydomonas reinhardtii*. This approach enabled us to gain novel insights into the protein and carbohydrate composition. We found that low-molecular-weight, mannose-rich glycoproteins play a crucial role in maintaining cell wall integrity by interacting with larger protein components, and that the cohesion of the glycoprotein architecture is ensured by short oligosaccharides. In addition, the cell wall exhibits nanoscale heterogeneity, with spatially segregated regions rich in either proteins or carbohydrates, each with distinct dynamics and hydration levels. Water appears to contribute to the overall resiliency and flexibility of *C. reinhardtii*'s cell wall structure. Our approach combining structural, dynamic, and hydration information proves to be valuable for studying cell wall biopolymers.

96-SympSelect
BPS2025 - Shape matters: Toward a molecular understanding of the innate immune recognition of microbial lipids
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The outer-membrane lipopolysaccharide (LPS, endotoxin) of gram-negative bacteria is highly immunostimulatory and induces severe pathology in humans. Investigation of natural and reconstituted membrane systems by small angle X-ray scattering (SAXS) revealed that the supramolecular organization and 3D structure of endotoxin molecules are major determinants for immunological activity. Accordingly, as a general finding, cubic inverted aggregate structures are associated with high inflammatory activity. However, biological activities of LPS are diverse, depending on cell-surface or intracellular receptor sensing. Furthermore, analytical detection of endotoxin as part of contamination in biologicals can be a challenge due to endotoxin masking effects. To provide a better understanding of the different LPS recognition pathways, we have systematically analyzed the structural requirements for LPS sensing/detection. LPS structure and ensemble analysis was performed by DLS, SAXS, and cryo-TEM, providing detailed information on the morphology of LPS aggregates and new insights into the specific rearrangement of LPS in certain solutes that lead to masking effects and loss of biological detection. Comparing reconstituted lipid aggregates made from purified LPS with outer membrane vesicles (OMV) isolated from bacterial cultures we can demonstrate that the interaction mechanisms of both membrane systems with the host cell are quite different. Whereas LPS requires protein mediated transport and activates cell surface receptors, LPS as part of asymmetric organized OMVs can enter the host cell by membrane interaction without transporter and activates intracellular signaling pathways. We have characterized LPS interaction with liposomal membranes and will present lipid traits for docking, fusion and entry into eukaryotic membrane systems. Our data provide a structure-based understanding on how LPS membrane structure and organization can selectively drive or avoid immune recognition pathways.

97-Symp
BPS2025 - Interaction of the *E. coli* cell wall with periplasmic macromolecules: Multiscale MD simulations
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The *E. coli* cell wall is a sugar-peptide polymeric structure that covers the entirety of the cell exterior, residing within the aqueous periplasmic space. While it has been shown to provide structural rigidity and mechanical strength for the cell, the more biochemical aspects of its role in for example, the passage of macromolecules across the periplasm (in either direction; anterograde or retrograde) have been less well explored. Here, we use molecular modelling and simulation to explore the interactions of the cell wall with antimicrobial peptides and osmolytes. We observe that the biochemical composition of the local environment can alter the binding mode of antimicrobials to the cell wall. Based on these observations we posit that incorporation of biological complexity is important in simulations that aim to explore functional modes of action of antimicrobials. Biologically relevant systems also necessitate simulating larger systems than are feasible using atomistic models. As part of an ongoing effort to develop tools to enable simulation of large systems, we will also discuss our preliminary work towards a simplified coarse-grained model of the cell wall that is compatible with the Martini suite of force fields. Overall our approach highlights the computational microbiology approach to studying the *E. coli* cell envelope.

Symposium: Innovations in RNA Therapeutics

98-Symp
BPS2025 - Expanding RNA functions with synthetic biology
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The development of new technologies is crucial for advancing the field of biology. Our objective is to create technologies that enable the control of gene expression, modification, and the expansion of cellular functions, as well as next-generation drug discovery, by artificially designing and evolving RNA and RNA-protein (RNP) complexes with tailored functions. In this presentation, I will introduce our proprietary RNA/RNP technologies, highlighting both their challenges and potential. First, I will discuss our latest research and applications