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Preface

NMR spectroscopy for atomistic views of biomembranes and cell surfaces

NMR spectroscopy is an important analytical tool for probing complex heterogeneous environments such as biomembranes and cell surfaces. The articles in this special issue on "NMR Spectroscopy for Atomistic Views of Biomembranes and Cell Surfaces" highlight the power of NMR spectroscopy in problem-solving efforts of biological importance involving membranes and cell surfaces. The authors discuss opportunities that are ripe for future research and, collectively, inspire the continued development and application of NMR approaches to dissect the structure and function of intact cellular systems, membranes, membrane proteins, and cell surfaces. Articles are organized thematically as contributions either in: (i) membranes and membrane proteins or (ii) whole cells and cell surfaces.

Within the realm of membrane and membrane–protein systems, articles include solution-state and solid-state NMR experimental approaches, computational strategies, and biochemical developments. The more membrane-focused articles include investigations of the structure and dynamics of lipids, fusion events, peptide interactions and influence on membrane environments. Long and coworkers present NMR-derived details of structure and motion of specific lipids in lung surfactant extract. A review from the Wassall group discusses efforts to understand how some bioactive marine long chain polyunsaturated fatty acids under biomedical and clinical investigations influence plasma membrane phospholipid organization. Epand and coworkers review the contributions of NMR methods in understanding of how membrane curvature influences membrane–protein insertion, interactions with membranes, and protein activity. Das, Park, and Opella review the NMR methodology involved in the determination of membrane protein structures from rotationally aligned membrane protein preparations and emphasize the importance of rapid rotational diffusion of proteins with as many as seven transmembrane helices. Advances in examining stress-induced deformations of lipid bilayers using solid-state ^{2}H NMR measurements and how such deformations may influence protein conformations are reviewed by Brown and coworkers. McDermott and coworkers describe NMR-observed specific contact between the c subunit of ATP synthase and cardiolipin which co-purifies with the protein. Yau, Schulte, and Qiang report on the fibrillation of the Alzheimer's Aβ peptide in a membrane and use NMR to detect changes in membrane morphology that may also occur in neuronal membranes in the disease state. Vogel and coworkers present studies of the anti-microbial peptide tritrpticin with 5-hydroxytryptophan replacing tryptophan and show that at least for one derivative, permeabilization of the inner membrane is not responsible for cell killing. Finally, Weliky and coworkers present the electrostatic and hydrophobic bases for the kinetics of membrane fusion induced by the HIV gp41 protein and show by NMR that the membrane-interacting fusion peptide domain has a β sheet structure.

There are also important contributions focused on membrane proteins. The Marassi Lab reports on the structure of the membrane protein FXYD2 by solution NMR in detergent micelles and employs solid-state NMR to examine the protein in lipid bilayers, together providing support for how the protein may influence the membrane to regulate Na,K-ATPase activity in kidney epithelial cells. Tang and Xu and their colleagues describe the structures of the Cys-loop pentameric ligand-gated ion channel and NMR investigation of protein motion induced by drug binding to the protein. Veglia and coworkers present NMR results of a disease-correlated phospholamban mutant and detected increased motion of the mutant relative to the wild-type protein. Gill, Wang, and Tian investigate LR11, a transmembrane sorting receptor important in trafficking and processing the amyloid precursor protein (APP) with implications for Alzheimer's disease, and identify a cytosolic amphipathic helix that may be involved in LR11 function. In addition, there are contributions describing developments in NMR methodology related to membranes and membrane environments. Lorigan and coworkers demonstrate the ability to control the size of nanometer-diameter lipodisqs using the lipid-to-polymer ratio. Banigan, Gayen, and Traaseth report on the influence of sample temperature on MAS NMR signal intensity and spectral resolution of lipid bilayer preparations in the context of related bilayer fluidity estimates and they tested the implications for optimal solid-state NMR preparations with two membrane transporters. Concluding this section, Ramamoorthy and coworkers report on the16-fold NMR signal enhancement of the membrane-anchored cytochrome b5 protein in bacterial cells using dynamic nuclear polarization.

The whole-cell and cell-surface division includes solid-state NMR approaches to bacterial and algal whole cells, bacterial cell walls, and bacterial biofilms. Chang, Singh, and Kim review the development and implementation of methods to examine bacterial cell-wall composition and architecture in Gram-positive bacteria and to dissect the modes of action of key cell-wall inhibitors including oritavancin which recently received FDA approval for the treatment of bacterial infections. Schaefer and coworkers describe new labeling strategies and an NMR approach using REDOR, frequency-selective pulse schemes, and spin diffusion to examine cell-wall architecture in *S. aureus* and the clinically important *femA* mutant. Marcotte and coworkers provide NMR data on microalgal cells that can be simplified by separately detecting more rigid or mobile components, together highlighting cell wall constituents, storage sugars, and phospholipids. Finally, Cegelski and coworkers present a top-down NMR approach to characterize the composition of the complex extracellular matrix produced by *Vibrio cholerae* beyond the cell surface during biofilm formation.

We hope you enjoy this special collection of original research and review articles. We would like to thank all of the contributors for their

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outstanding papers and also the Editors and staff at BBA-Biomembranes for their ideas and assistance in the compilation and editing of this Special Issue.

Lynette Cegelski is an Assistant Professor in the Department of Chemistry at Stanford University. She received her BS degree in Chemistry summa cum laude from Binghamton University, Binghamton, NY. She earned her PhD degree in Chemistry from Washington University in St. Louis, MO and she performed postdoctoral research in Microbiology and Infectious Diseases at the Washington University School of Medicine. Her laboratory is engaged in developing new strategies using solid-state NMR spectroscopy to define composition and structure in assemblies including bacterial cell walls and biofilms, and is working to identify small molecules to interfere with assembly processes to drive the development of new therapeutics. Lynette is the recipient of the Burroughs Wellcome Career Award at the Scientific Interface, the NIH Director's New Innovator Award, the Stanford Terman Fellowship, and the Hellman Faculty Scholar Award.

David P. Weliky received a B.A. with High Honors in Chemistry and Physics from Swarthmore College and a Ph. D. in Chemistry from University of Chicago with a thesis on ultra-high-resolution infrared spectroscopy of crystalline solid hydrogen. He became interested in solid-state NMR during a summer spent working with Rob Tycko at AT&T Bell Laboratories and then went to work with Rob as a post-doc in the NIH intramural program doing NMR method development as well as structural measurements on an antibody-bound peptide. As a professor at Michigan State University, he has worked on the development of NMR-based structural models of membrane-associated viral fusion proteins and on the development of experimentally-based structure-function models for these proteins. He has also applied NMR to quantitation and molecular structure of recombinant protein in bacterial inclusion bodies and showed that 100–400 mg recombinant protein per L culture is typical for standard growth and expression conditions.

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