Solid state NMR characterization of lipid membrane and organic solvent induced effects

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https://cmb.ornl.gov/dynamic-visualization-of-lignocellulose/

Project Goals: The development of renewable biofuels is a key mission of the DOE Genomic Science program. Lignocellulosic biomass has the potential to be an abundant, renewable source material for production of biofuels and other bioproducts. The use of organic solvents to optimize biomass pretreatment has shown considerable promise, but their disruption of microbial membranes is key to toxic effects limiting fermentation titers. The Oak Ridge National Laboratory (ORNL) Scientific Focus Area (SFA) Biofuels Program utilizes multi-length scale imaging with neutron scattering complemented by high performance computer simulations, NMR, biochemistry and targeted deuteration to provide fundamental knowledge about the molecular forces that drive solvent disruption of the critical assemblies of biomolecules that comprise plant cell walls and microbial biomembranes.

Organic solvent is widely acknowledged as a major determinant of product titer limitations of fermentations due to its disruption and induced destabilization of microbial cellular membranes. Amphiphilic solvents disrupt the molecular packing and organization of lipid membranes, causing fluidity alteration and reducing structural integrity. In this study, solid state nuclear magnetic resonance (NMR) was employed to investigate the effects of organic solvents on phase and dynamics of lipid membranes. Model lipid 1-palmitoyl-2-oleoylglycerophosphoglycerol (POPG) was used to prepare a multilamellar lipid vesicle (MLV) and two organic solvents, i.e., n-butanol and tetrahydrofuran (THF), were used. High resolution solid state ^{1}H, ^{31}P and ^{13}C NMR experiments with various pulse sequences including cross-polarization (CP), direct-polarization (DP), and insensitive nuclei enhancement by polarization transfer (INEPT) under magic-angle spinning (MAS) were used to investigate the phase behavior of membrane in the presence of solvents. The interaction of POPG with the solvent molecules was examined by using two-dimensional nuclear Overhauser effect spectroscopy (NOESY) spectra. The static solid state ^{31}P NMR spectra showed that the phospholipids had a combination of phases with powder distribution and isotropic peaks. The lipid membrane was also observed to adapt to various orientations depending on the solvents. For example, butanol addition caused the lipid molecules to orient both parallel and perpendicular to the magnetic field, while the presence of THF changed the orientation of the lipid molecules to be primarily perpendicular to the magnetic field. In this work, we are extending the use of Solid state NMR to provide fundamental insights on solvent-membrane interaction and dynamics and phase behavior of membranes.

Funding Statement:
This research is supported by the U. S. Department of Energy, Office of Science, through the Genomic Science Program, Office of Biological and Environmental Research, under FWP ERKP752. Oak Ridge National Laboratory is managed by UT-Battelle, LLC for the U.S. Department of Energy under contract no. DE-AC05-00OR22725.