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B2.3

Structural Insight into Dilute Acid Pretreatment Effect of Lignocellulosic Biomass using Small-Angle Neutron Scattering. Sai Venkatesh Pingali[1,2], Volker S. Urban[1,2,3], William T Heller[1,2], Joseph McGaughey[1], Hugh M O'Neill[1,2], Marcus B. Foston[4], Dean A Myles[1,2,3], Arthur Ragauskas[4] and Barbara R Evans[1]; [1]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]Center for Structural Molecular Biology, CSMB, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [3]Neutron Scattering Sciences Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]Institute of Paper Science and Technology, School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, Georgia.

Lignocellulosic biomass comprises the vast majority of biomass on Earth and has the potential to play a major role in generation of renewable biofuels through its conversion to bio-ethanol. Unfortunately, lignocellulosic biomass is a complex biological composite material that shows significant recalcitrance towards the structural breakdown into sugars that is necessary for fermentation to bio-ethanol, making it a cost-ineffective feedstock. Small-angle neutron scattering and X-ray powder diffraction were used to obtain a better understanding of the morphology of the cellulose/lignin composite to aid in understanding and ultimately selecting biomass pretreatment methods that are required to prepare lignocellulosic biomass for conversion to ethanol. In this talk, I will present results from the pretreatment of switch grass using two different chemical processes: (a) the dilute acid pretreatment method used to break down lignocellulosic biomass and (b) the extraction treatment for removing one component at a time from the biomass without disrupting its overall structure. Dilute acid pretreatment: (1) increases the cross-sectional radius of gyration of the individual cellulose fibrils while decreasing the interconnectivity of the fibrils; (2) results in the appearance of an additional length scale most probably due to aggregation of lignin onto the fibrils in lumps; and (3) does not change the surface scattering of the micron-sized particles or pores. In addition, X-ray powder diffraction was used to probe the changes in the crystalline order of the cellulose fibrils. The changes in the cross-sectional fibril radius as measured by the changes in the diffraction line width were in close agreement with the small-angle neutron scattering results. In contrast to the dilute acid pretreatment, the extraction treatment: (1) did not result in an additional length scale assigned to the lignin lumps; and (2) produced a smaller increase in the cross-sectional radius of gyration of the fibrils. This research is funded by the Genomics: GTL Program, Office of Biological and Environmental Research, US DoE, under FWP ERKP704. This research at Oak Ridge National Laboratory's Center for Structural Molecular Biology (CSMB) was supported by the Office of Biological and Environmental Research, using facilities supported by the U. S. Department of Energy, managed by UT-Battelle, LLC under contract No. DE-AC05-00OR22725. The X-ray diffraction laboratory facility funded by the Department of Energy, BES to the Division of Material Sciences and Engineering at Oak Ridge National Laboratory under Project# ERKCC01.

B2.4

Proteins Remain Soft at Lower Temperatures under Pressure. Xiang-qiang Chu[1], Antonio Faraone[2,3], Chansoo Kim[1], Emiliano Fratini[4], Piero Baglioni[4], Juscelino B Leao[2] and Sow-Hsin Chen[1]; [1]Department of Nuclear Science and Engineering, MIT, Cambridge, Massachusetts; [2]NIST Center for Neutron Research, Gaithersburg, Maryland; [3]Department of Material Science and Engineering, University of Maryland, College Park, Maryland; [4]Department of Chemistry and CSGI, University of Florence, Florence, Italy.

The low temperature behavior of proteins under high pressure is not as extensively investigated as that at ambient pressure. In this paper, we study the dynamics of a hydrated protein under moderately high pressures at low temperatures using quasi-elastic neutron scattering method. We show that when applying pressure to the protein-water system, the dynamics of the protein hydration water does not slow down, but becomes faster instead. The degree of "softness" of the protein, which is intimately related to the enzymatic activity of the protein, shows the same trend as its hydration water as a function of temperature at different pressures. These two results taken together suggest that at lower temperatures, the protein remains soft and active under pressure.

B2.5

Neutron Reflectometry Reveals Structure of Bio-Toxins Interacting With Lipid Membranes. Jaroslaw Majewski[1], Mike Kent[2], Tonya Kuhl[3] and Chad Miller[4]; [1]Los Alamos Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico; [2]Sandia National Laboratory, Albuquerque, New Mexico; [3]Department of Chemical Engineering, UC Davis, Davis, California; [4]LANSCE, Los Alamos, New Mexico.

Bio-toxins like diphtheria (DT) or cholera (CT) contain separate domains for receptor-specific binding, translocation, and enzymatic activity. Following binding to cells toxin is taken up into endosome-like acidic compartments, where the translocation (T) domain inserts into the endosomal membrane and releases the catalytic (C) domain into the cytosol of the target cell. The process by which the enzyme is translocated across the endosomal membrane is known to involve pH-induced conformational changes, however the molecular mechanisms are not yet understood, in large part due to the difficulty of probing the conformation of the membrane-bound protein. We show here that neutron reflection (NR) provides important conformational information for membrane-bound toxins. For example, NR has revealed that for the DT the bound toxin dimerizes with increasing DT concentration, and that the dimeric form undergoes a conformational change with pH that correlates with deep insertion. Combination of the neutron/x-ray reflectivity and x-ray grazing incidence diffraction allowed characterization of the structure of lipid monolayers before and during the binding of CT. Structural parameters such as density and thickness of the lipid layer, orientation and position of the protein upon binding were obtained.

B2.6

Abstract Withdrawn

B2.7

Internal Dynamics in Proteins Studied by Neutrons and X-rays. Jyotsana Lal[1], Peter Fouquet[2], Marco Maccarini[2], Diane J. Rodi[1] and Lee Makowski[1]; [1]Biosciences Division, Argonne National Laboratory, Argonne, Illinois; [2]Institute Laue-Langevin, Grenoble, Cedex 9, France.

Biomolecular systems are intrinsically dynamic, and a complete understanding of the function of a system requires the characterization of its dynamics. In particular, a complete description of protein motion is critical to an understanding of the function of a protein. Here we will discuss collective internal motions of proteins in solution, an environment that closely resembles the inside of a cell. No single technique is capable of measuring the range of motions needed to develop a complete understanding of such complex systems. To study the dynamics of fluctuations from nanosecond to picosecond time scales we have developed a methodology at Argonne National Laboratory that involves coordinated use of Neutron Spin Echo (NSE) scattering and Wide Angle X-ray solution scattering (WAXS). The X-ray data provides important information about the ensemble of structures present in the scattering volume - and thereby a measure of the spatial extent of internal motions of the protein in solution. NSE is used to characterize the dynamics of the fluctuations observed with the X-ray measurements and determine the rate of relaxation of fluctuations on particular length scales. Results from correlated studies of hemoglobin and myoglobin reveal domain and backbone motion.

B2.8

Cholesterol in Unusual Places. Norbert Kucerka[1], Mu-Ping Nieh[1], Drew Marquardt[2], Thad A. Harroun[2] and John Katsaras[1,2]; [1]Canadian Neutron Beam Centre, National Research Council, Chalk River, Ontario, Canada; [2]Department of Physics, Brock University, St. Catharines, Ontario, Canada.

Cholesterol is an essential component of mammalian cells, and is required for building and maintaining cell membranes, regulating their fluidity, and possibly acting as an antioxidant. Cholesterol has also been implicated in cell signaling processes, where it has been suggested that it forms lipid rafts in the plasma membrane. Aside from cholesterol's physiological roles, what is also becoming clear is its poor affinity for lipids with unsaturated fatty acids as opposed to saturated lipids that more readily form domains. We previously reported the location of cholesterol in membranes with varying degrees of acyl chain unsaturation as determined by neutron diffraction studies [Harroun et al., Biochemistry 45, 1227 (2006); Biochemistry 47, 7090 (2008)]. In bilayers composed of phosphatidylcholine (PC) molecules with a saturated acyl chain at the sn-1 position or a monounsaturated acyl chain at both sn-1 and sn-2 positions, cholesterol was found in its much-accepted "upright" position. However, in dipolyunsaturated 20:4-20:4PC membranes the molecule was found sequestered in the center of the bilayers. Recently, mixing 16:0-18:1 PC (POPC) with 20:4-20:4PC resulted in cholesterol reverting to its upright orientation at approximately 40 mol% POPC. Interestingly, the same effect was achieved with only 5 mol% 14:0-14:0 PC (DMPC), instead of POPC. The biological implications of these results will be discussed.