the presentation. Conformational motion theory is believed to be found in group theory.

3009-Pos Board B56

Extension of the Tryptophan Dihedral Angle - W3 Band Frequency Relationship to a Full Rotation

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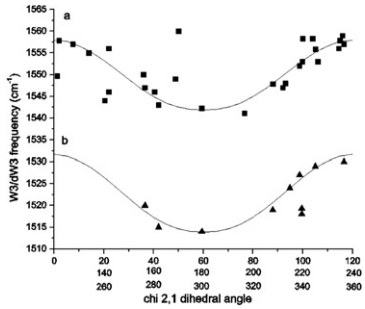
The correlation of the UVRR νW3 mode with the tryptophan $\chi^{2,1}$ dihedral angle (T. Miura et al. 1989, T. Maruyama & H. Takeuchi 1995, H. Takeuchi 2003) has been extended to a full, 360° rotation. The three-fold periodicity of the relationship (cos $3\chi^{2,1}$) over 360° results in up to six dihedral angles for a given νW3. Consideration of a circular plot of dihedral angles for proteinaceous tryptophans taken from the Protein Data Bank along with a Newman projection shows that steric hindrance limits the range of preferred dihedral angles, and reduces the possible $\chi^{2,1}$ to one or two, reasserting the general utility of the νW3 - $\chi^{2,1}$ relationship. However, not all proteinaceous tryptophans follow the relationship. DFT based calculations suggest that the discrepancies observed for the PGA-ligated mutant enzyme, *S. cerevisiae* TIM Trp90Tyr Trp157Phe, are due to electrostatic interaction between the indole ring of Trp-168 and the Glu-129 carboxyl.



3010-Pos Board B57

The Residue Network Architecture of a Protein-Protein Complex Reveals the Linkage between Dynamics and Energetics

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Among the toxins secreted by *Bacillus anthracis* the edema factor EF, an adenylate cyclase, provokes severe cellular dysfunction by accumulating cAMP from ATP. EF is activated by calmodulin (CaM), involved in many calcium signaling pathways. The stability of the EF-CaM complex depends on the level of calcium bound to CaM while the architecture of the complex loaded with 2, 3 or 4 Ca^{2+} ions remains practically unchanged. That is why modeling the electrostatic effect of Calcium through EF-CaM structure is challenging.

Here, we aim at describing the calcium-induced changes in EF-CaM dynamics and energetics through a consensual view of its residue network organization. The analysis of molecular dynamics (MD) simulations of EF-CaM with 0, 2 and 4 Ca^{2+} ions helped characterize CaM conformational plasticity and led to a model of the EF-CaM interaction, in which CaM acts as a spring that maintains EF in an open active conformation (Laine et al., 2008).

The computation of various dynamical covariances and energetic dependency maps from the MD trajectories further raised the concept of residue network connectedness. This connectedness quality provides a frame for unifying the dynamics and energetics of the complex and a criterion for assessing its stability (Laine et al., under revision).

Laine E., JD. Yoneda, A. Blondel and TE. Malliavin (2008). *Proteins*. 71: 1813-29.
Laine E., A. Blondel and TE. Malliavin. *Biophys. J. (under revision)*

3011-Pos Board B58

Picosecond Dynamics Evolution During Function For Photoactive Yellow Protein

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Picosecond protein dynamics refer to both diffusive motion at the protein surface and adjacent solvent as well as possible underdamped structural vibrational modes. Functional protein structure changes result in possible changes in both these diffusive and collective dynamics which can lead to either an increase or decrease in flexibility in the active state. In the case of photoactive yellow protein (PYP), a large conformational change occurs as one proceeds from the resting pG state to the active pB state with partial molten globule formation. Previous terahertz dielectric response has been used to monitor changes in picosecond dynamics for the photoactive protein PYP with opposing results [1, 2]. While in one set of measurements, hydrated films were used and the pG/pB relative state population was monitored, in another set of measurements low conc PYP solution was used without monitoring of the conversion. In this paper we present THz dielectric response as a function of photocycle state for fully solvated PYP with in situ monitoring of the conversion using UV/Vis absorbance, both at room temperature and below freezing. Freezing reduces the background relaxational absorption of bulk water, and increases conversion to pB by slowing the photocycling time.

3012-Pos Board B59

Native-Like Structure of Proteins at a Planar PAA Brush

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Applying ATR-FTIR (attenuated total reflection-Fourier transform infrared) and TIRF (total internal reflection fluorescence) spectroscopy, we have studied the secondary structure and aggregation properties of different proteins which are adsorbed at a poly-(acrylic acid) (PAA) brush that covers a macroscopically large, planar surface. The PAA brush has been prepared on the surface of an ATR silicon crystal or a quartz plate. The preparation includes the deposition of a thin poly-(styrene) film by spin-coating and the transfer of the diblock copolymer poly-(styrene)-poly-(acrylic acid) onto the hydrophobic film using the Langmuir-Schäfer technique. It has been found that the proteins hen egg white lysozyme, bovine serum albumin, bovine α-lactalbumin, and bovine insulin adsorb spontaneously at a PAA brush at neutral pD-values, albeit to different degrees. The secondary structure of the proteins was estimated from a decomposition of the amide I'-band in the observed ATR-FTIR spectra. Generally, the fractions of secondary structure elements recovered in this way were almost identical to those found when the proteins are native in solution. In addition, the tendency of insulin to form amyloid fibrils has also been tested when the protein is adsorbed at a planar PAA brush. Insulin is known to form amyloid fibrils in solution at low pH-values and elevated temperatures. The experiments performed in this study suggest that a PAA brush does not promote fibril formation of insulin. Rather, insulin that is adsorbed at a PAA brush seems to be excluded from fibril formation pathways even at pD = 2 and 60 °C, where fibril formation of insulin is triggered in solution. Overall, the results of this study demonstrate that a planar PAA brush may serve as a mild environment for immobilized proteins.

3013-Pos Board B60

Conformation of Beta-Lactoglobulin at an Oil/Water Interface as Determined From Single-Molecule Force Spectroscopy

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Understanding the structure, composition and mechanical properties of adsorbed protein layers is essential for controlling the physico-chemical stability properties of food colloids. We have used atomic force microscopy (AFM)-single molecule force spectroscopy to probe the conformational changes in β-lactoglobulin (β-LG) proteins adsorbed onto the interface of an oil droplet in water, with in situ changes in pH. Single oil droplets were mechanically trapped in the pores of a polycarbonate filter and the AFM tip was used to grab onto and unfold the β-LG molecules. The changes in the contour length upon each unfolding event were determined by fitting the wormlike chain (WLC) model of polymer elasticity to each of the β-LG peaks of the force-extension profiles. Our results show clearly that β-LG on the same oil droplet adopts different conformations for different pH values. At pH 2.5, the unfolded β-LG molecule has a contour length that is similar to the total length of a single monomer with two large unfolding barriers, whereas the molecule exists mainly as a dimer formed of several smaller domains at pH 6.8. Furthermore, at pH 9 the interactions between the AFM tip and the β-LG layer on the oil droplet surface are dominated by an important repulsion due to the highly negatively charged β-LG layer. This study demonstrates a novel application of single molecule force spectroscopy to investigate the underlying mechanisms by which proteins can be used to stabilize food products.

3014-Pos Board B61

Effect of Trifluoperazine on Ca^{2+} -Bound Calmodulin binding to Fas Death Domain for DISC Formation

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Fas death receptor-activated signaling pathway is one important regulating mechanism of apoptosis in a variety of cells. The formation of the death inducing signaling complex (DISC) is a critical step for Fas-mediated signaling of apoptosis. Recent experimental studies showed that calmodulin (CaM) binds to Fas and regulates Fas-mediated DISC formation and the binding of CaM to Fas is inhibited by CaM antagonist, trifluoperazine (TFP). However, the exact molecular mechanisms for the effect of TFP on Fas-mediated DISC formation are still unknown. Knowledge about these is important for identifying new drug candidate to regulate Fas-mediated signaling pathway for apoptosis. In