using Far UV CD and FTIR revealed that the helix conformation induced at higher concentrations of TFE is non-specific. Additionally, the role of the charged amino and carboxyl groups at the ends of the peptides were studied to determine if these groups affect helix induction by TFE. 15-mers of poly-L-glutamic acid and poly-L-lysine were synthesized from amide resins and their C-terminals were acetylated. The protected poly-L-glutamic acid and poly-L-lysine were titrated with TFE at pH 2, 7 and 13, and the secondary structures were determined using CD: no significant difference was found when compared to the non-protected homopolypeptides. The results obtained in this study clearly question the validity of structures of short peptides characterized in high concentrations of organic solvents.

3004-Pos Board B51

Kinetics of Film Formation of Poly-L-Proline at High Temperatures

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At room temperature and in aqueous solution, poly-L-proline predominantly adopts a relatively open left-handed 3_1-helix termed polyproline II (PPII). The corresponding far UV electronic circular dichroism (ECD) spectrum exhibits a couplet with a pronounced minimum at ~ 204 nm, and a much less intense maximum at ~ 228 nm. When poly-L-proline is incubated in a quartz cell for two hours at temperatures above 60°C, a gradual decay of the PPII signal is observed. It is replaced by a spectrum which displays a strong negative signal at ~220 nm (?), thus being indicative of a right handed conformation. This PPII signal decay is thought to be caused by the formation of a film on the inner surface of the cell. After removal of the poly-L-proline solution from the cell, the ECD was measured on both the liquid and cell individually. The ECD of the removed liquid portion resembles a typical PPII spectrum, while that of the cell results in the aforementioned spectrum, with a significant minimum at ~220 nm, and a minor minimum at ~204 nm. The rate of film formation depends strongly on the incubation temperature. Bi-exponential rise and decay modeled the disappearance of the PPII signal in aqueous solution and growth of the film, respectively. The respective relaxation constants were determined to be 10^{-3} s^{-1} and 10^{-4} s^{-1} for the PPII signal disappearance and film formation, respectively, at T= 65C ? (Laura?). The analysis of the kinetics measured at different temperatures between 60° and 75° C reveals a non- Arrhenius behavior. A further structural characterization of the obtained poly-L-proline film and a thermodynamic analysis are currently being carried out in our laboratory.

3005-Pos Board B52

Thermophilic protein structure adaptation examined with Burial Depth and Travel Depth

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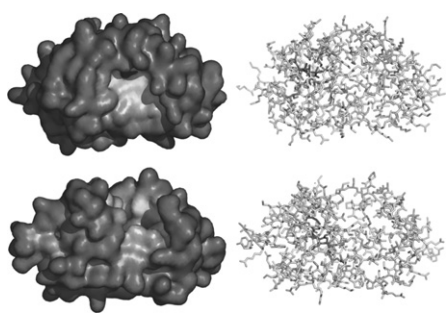
Organisms evolved at extreme temperatures (above 80° C) have constraints on their protein structures. These constraints result in differences in residue utilization and overall structure. By studying thermophile/mesophile pairs of homologous structures, we have examined these differences.

Geometric measures, specifically Burial Depth (distance from the molecular surface to each atom) and Travel Depth (distance from the convex hull to the molecular surface that avoids the protein interior), along with common metrics like packing are used to gain insight into the constraints experienced by thermophiles.

Our results show that extreme thermophiles show significant trends towards becoming more ''ball-like''. Their mean Travel Depth is less than their mesophilic counterparts, indicating smaller, less numerous and less deep pockets. Their mean Burial Depth is higher indicating that they bury more surface area and are more compact. This can be tracked on the individual residue level, for instance Alanine becomes more significantly buried under thermophilic conditions, and charged residues become less buried.

Shown is an example pair with the thermophile at top. At left are Travel Depth surfaces, at right Burial Depth. Note the fewer, smaller pockets and the deeper core in the thermophile.



3006-Pos Board B53

Small Conformational Changes Detected For Short Lived Transient Species During A Photoreaction

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he focus of the present study is firstly to investigate the origin of global conformational change during the photoreaction. Secondly, how such changes are transduced and spread to all over the protein molecule was investigated by studying the photoreaction of the site directed mutants. The diffusion of pG and pB of E46Q mutant showed the small difference, suggesting that the absence of negative charge at 46 position is responsible for the lack of partial unfolding in structure of PYP upon pB formation. The role of N-terminal region was further studied by replacing phenylalanine by alanine at position 6 (F6A). The diffusion constant of pB of F6A was not very different from that of pG, which is explained by a small conformational change in N-terminal tail upon pB formation. Previously, creation of a disulfide bond between position 6 (Phe6) and 121 (Phe121) showed the restricted movements of N-termius and less structural fluctuation upon pB formation. These results argued the more ordered and folded structure of pB of mutants lacking Phe6

3007-Pos Board B54

Probing the Dynamics and Conformations of Free and Ligand-bound Gamma-synuclein

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The synucleins are a family of natively unstructured, soluble proteins consisting of α-, β-, and γ -synuclein. They are primarily expressed in neurons, though they differ in their localization. Relatively little is known about the physiological roles of any of the synucleins, although the most studied of the group, α-synuclein, has been linked to Parkinson's disease. γ-synuclein was first identified in breast cancer cells, and was later found to be overly expressed in several other types of cancer, including ovarian cancer and retinoblastoma. Furthermore, subsequent studies found that γ-synuclein overexpression in breast carcinomas interferes with the activity of commonly used chemotherapeutic drugs, such as taxol and nocodazole. In the current study, we use a combination of single molecule Förster resonance energy transfer (FRET) and fluorescence correlation spectroscopy (FCS) to examine the conformations and dynamics of γ-synuclein alone and bound to potential ligands. Our findings will not only help understand the structural properties of a disordered protein, but will also lead to a better understanding of the mechanisms through which γ-synuclein alters the efficacy of antitumor drugs.

3008-Pos Board B55

Conformational Motion of Biological Macromolecules

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The beauty of biological macromolecules as a dancer in solution can be seen if we manage to understand graceful movements of the dancers. Biological macromolecules are dynamic machines so for proper functionality they need changing of shape, dancing through each other and non-contacting communicating to execute their ''understanding'' on distances. However there is no single theory to explain encountered experimental data and increase our understanding on the conformational motion. The problem is a suggestion of non-equilibrium nature of the macromolecules. Does it mean that non-equilibrium system like biological macromolecules can act as the dancer and can function properly? Does it mean that there is some rule that non-equilibrium macromolecules follow? Can the rule be generalized for any kind of non-equilibrium systems or not? My attempt to give a mathematical definition of the problems and point to their solution will be presented. Let consider bonded n point and correspond to the system some geometric figure with $V=n$ vertexes, virtual F,E faces and edges correspondingly. The conformational motion of the system is a changing the shape of the figure so we have two possibilities 1) the Euler Characteristic of the figure is changing in time as well as F,E changes; and 2) the Euler Characteristic of the figure is constant but F,E changes. Set of all possible {F,E} gives us the group with undefined operator f where f is operator which transfers elements of the set in each other $f:(F_i,E_j)\in\{F,E\}\rightarrow(F_g,E_k)$. The tusk could be solved if we manage to find the operator f. The value of the f can be immediately found by adding some physical conditions to the operator. The physical conditions and the equation of conformational motion will be presented at