1257-Pos Board B27
Novel Ammonium Transport Proteins
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The transport of nitrogen in the reduced form as ammonium/ammonia (NH_3/NH_4^+) is essential for the metabolism of many organisms. Ammonium transport (Amt) proteins form a family of integral membrane proteins that are present in all domains of life. They include the Rhesus proteins in humans and are responsible for the translocation of NH_3/NH_4^+ across biological membranes. Since the first molecular characterization of an Amt protein, MEP1 from *S. cerevisiae*,in 1994 [1], many findings extended the field and led to a better understanding of how these proteins work and how they are regulated. So far, four high resolution crystal structures are available for AmtB from *E. coli* [2], Amt-1 from *A. fulgidus* [3], Rh50 from *N. europaea* [4] and the human RhCG [5]. Nevertheless, a number of mechanistic questions remain to be answered [6].
We are working on the biochemical and biophysical characterization of Amt proteins from different organisms using x-ray diffraction and activity measurements probing the functionality of wild type and variant proteins when overproduced in whole cells or when purified and reconstituted into liposomes.
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[4] D. Lupo *et al, PNAS,* **2007**, 104, 19303; X. Li et al, *PNAS*, **2007**, 104, 19279.
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1258-Pos Board B28
Electrophysiology of Amt Proteins in Planar Lipid Bilayers
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The transport of ammonium/ammonia across biological membranes is mediated by a family of ubiquitous integral membrane proteins, the ammonium transport (Amt) proteins. Although high-resolution crystal structures of four Amt proteins are currently available [1-5], the substrate identity and transport mechanism are still controversially discussed [6].
Current functional data using two-electrode voltage clamp experiments of protein expressed in *Xenopus* oocytes [7,8], measuring the radioactive uptake of methyl ammonium (an alternative substrate) in whole cells [9] or following pH variation with fluorescent probes in proteoliposomes [1], yielded to variable and discrepant results. To conclude on the substrate identity (NH_4^+ or NH_3) and the transport mechanism we are carrying out electrophysiology measurements with reconstituted, pure protein in planar lipid bilayers (PLB). Such experiments have been crucial in identifying transport details in many proteins, among which, the elegant elucidation of Cl^-/H^+ antiport in CLC chloride channels [10] or, more recently, the pH gating mechanism in formate channels [11].
If Amt proteins are electrogenic transporters/channels, charged substrate can be identified and followed by means of electric currents in PLB.
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Protein Structure

1259-Pos Board B29
2D-NMR Peak Assignment of Protein Extracted from Persian Viper's Venon (PPTI) and Structure Determination
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According to several investigation carried out about effective proteins in viper's venoms, two major families of protein, Dendrotoxins and Protease Inhibitors, has been recognized. It seems that they have been derived from the same ancestor gene which has been undergone several mutations. The chosen protein for this investigation, PPTI, has intermediate characteristics which can represent it as an appropriate choice for finding a relation between mentioned family groups.
In this study, in order to achieve the three dimensional structure of PPTI, 2D-NMR spectroscopy was applied in which NOESY, TOCSY and HSQC spectra has been acquired. Conventional peak assignment was applied to identify amino acids and their contacts.

1260-Pos Board B30
Multivariate Analysis of Deep Ultraviolet Resonance Raman Spectra: Secondary Structure Determination
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Studies pertaining to protein or peptide structure, dynamics or function fundamentally require a method for secondary structure measurement. There are four structurally sensitive protein vibrational modes in deep-ultraviolet resonance Raman (DUVRR) spectra, the amide I, II, III and S modes, making it a potentially powerful tool for studying secondary structure changes in even the most difficult peptide samples. Experimental studies reveal that the position and intensity of the four amide modes in UVRR spectra of proteins are correlated with the varying fractions of α-helix, β-sheet and unordered structures of proteins. This relationship has been applied to the prediction of protein secondary structure.
Specifically, multivariate methods have been employed to decompose protein spectral data sets into their underlying pure secondary structure Raman spectra (PSSRS). Ideally, the resolved PSSRS could then be used for prediction of the secondary structure content of unknown proteins from their UVRR spectra. However, previous studies have not examined the performance of multivariate methods on prediction of the structural composition of an unknown test protein. A comparative study of the ability of classical least squares (CLS), principal component regression (PCR), partial least squares (PLS) and multivariate curve resolution- alternating least squares(MCR-ALS) to resolve the pure secondary structure Raman spectra (PSSRS) and predict the structural composition of unknown test proteins will be presented.

1261-Pos Board B31
Solution Structure of the Binuclear Zinc Finger of Cytoplasmic Polyadenylation Element Binding Protein (CPEB)
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Synaptic plasticity, the experience dependent variation in the strength of a synapse, is a means of encoding memory through a network of specific connections between neurons. Cytoplasmic polyadenylation element binding protein (CPEB) is a key factor in establishing the synaptic mark through translational regulation of protein synthesis. A neuronal isoform (CPEB1) participates in sequence specific recognition of a uracil-rich cytoplasmic polyadenylation element (CPE) within the 3' UTR of mRNA. The C-terminal region of CPEB1 binds to mRNA utilizing three structured domains including two RNA recognition motifs and a zinc finger domain. We have characterized the structure of the binuclear zinc finger domain by NMR spectroscopy.

1262-Pos Board B32
Towards the Development of Coarse Grained Multibody Force Fields: A Theoretical Perspective
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Force fields are a computational tool commonly used for a variety of biophysical studies, ranging from structural to dynamic explorations of proteins and nucleic acids. To increase the accessible time scales of those biophysical simulations researchers have recently moved towards structural abstraction or ''coarse-graining'' the systems being studied. However, the process of coarse graining necessarily excludes potentially relevant information from an atomic-level representation. The idea of reintroducing this information back into coarse-grained representation has been explored in a limited sense with the advent of specialized multibody terms to simulate secondary structures such as β-sheets. We here present initial efforts towards developing a generalized statistics-based multibody force field for the coarse grained simulation of biomolecules. In this offering, we describe a statistical exploration of protein structures from the PDB using an information theoretic perspective. We analyze our findings using comparisons to simple theoretical models, such as particles in a box, and protein folding on a grid.