folding/unfolding region by obtaining atomic scale detail of core hydrophobic interactions.

1644-Pos Board B488
Functional Dynamics in Chlorella virus DNA Ligase
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DNA ligases specifically recognize and seal double stranded nicked DNA by catalyzing the formation of a phospho-diester bond between the 3′OH and 5′ phosphate termini. In physiological conditions these ubiquitous enzymes are essential for DNA replication, repair and recombination, while in tumor cells they can play a critical role in apoptosis resistance.
Chlorella virus ligase is a pluripotent ATP-dependent ligase composed by two domains, a N-terminal nucleotidyltransferase domain, hosting the catalytic site, and a C-terminal OB-domain, both of which participate to DNA binding. A number of crystallographic studies have elucidated important structural details of the nick-sealing process. DNA binding, in particular, appears to require a large reorientation of the two domains, as well as relevant structural rearrangements localized mainly in the N-terminal region (1). Indeed this protein appears to be a highly dynamic system whose internal motions are closely linked to both the DNA recognition and to the catalytic process. So far, however, the actual nature of these motions is still largely unknown, not only for Chlorella virus ligase, but also for the entire protein family.
We therefore tried to close this gap by undertaking the analysis of the dynamic properties of Chlorella virus liagase by solution NMR spectroscopy.
Reference:
(1) Nair P.A., Nandakumar J., Smith P., Odell M., Lima C.D., Shuman S. (2008) Nat Struct Mol Biol. 14, 770-8.

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Investigating Protein Dynamics Via A Multivariate Frequency Domain Analysis
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A novel method, which is based on a multivariate frequency domain analysis (MFDA), is proposed to extract collective vibrational modes of protein. The idea of the MFDA is to perform band-pass filtering of multivariate time-series using the multitaper Fourier transformation technique before multivariate analyses (e.g., singular-value decomposition) are carried out. The MFDA is compared with the standard multivariate analysis, principal component analysis (PCA), which solely utilizes the information of the equilibrium distribution of protein dynamics. It is found that, compared with the PCA, the MFDA well represents the vibrational behavior of protein and gives us an insight into the high-dimensional vibrational motion of protein. In our poster, we will show the recent extension of the MFDA on the time-frequency domain. Using the time-frequency domain extension of the MFDA, the anharmonic aspects of vibrational motion of protein will be discussed.

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Role of Cationic Residues in Fine Tuning the Flexibility of Charged Single α-helices
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A few highly charged natural peptide sequences have recently been suggested to form stable α-helical structures in aqueous solution. Here we show that these sequences represent a more widespread structural motif called 'charged single α-helix' (CSAH). We have developed two conceptually different computational methods capable of scanning large databases: SCAN4CSAH is based on sequence features characteristic for salt bridge stabilized single α-helices, while FT_CHARGE applies Fourier transformation to charges along sequences. Using the consensus of the two approaches, a remarkable number of proteins were found to contain putative CSAH domains. Recombinant fragments of 50-60 residues in length corresponding to selected hits (from myosin 6, Golgi complex associated protein-60, and mitogen-activated protein kinase M4K4) were found to adopt a highly stable α-helical structure in water. Molecular dynamic simulations of five CSAH peptides (the above three plus peptides from caldesmon and myosin 10) showed that the formation of dynamic ion-pair clusters significantly contribute to the stability of the helices. Furthermore, cationic residues were found to play a differential role in tuning the local flexibility of the CSAH domains. We conclude that sequence specific tuning of flexibility of CSAH peptides could have important role in the mechanical performance of CSAH-containing myosin motors, such as myosin 6 and 10, or in other protein functions.
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Multidimensional IR Study Of The Structure And Dynamics Of Elastin Protein
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Elastin protein is responsible for the elasticity of organs including the skin, lungs, and arterial tissues. Upon heating to physiological temperature the elastic region undergoes an inverse temperature transition (ITT) from an extended to a folded state. It is hypothesized that the ITT results from changes in water structure around the elastic regions hydrophobic side chains. To investigate this hypothesis we have performed temperature dependent FTIR and 2D IR experiments on the amide I, amide A, and water OH stretching vibrations of bovine neck elastin and synthetic peptide mimics. FTIR spectra of hydrated films in the OH stretch region show spectral signatures which are indicative of water molecules interacting with the protein. This spectral signature displays a large absorption band centered at 3450cm-1, extending as far as 3600cm-1. This band is suggestive of weakly hydrogen bound water and may be an indicator of hydrophobic hydration. In 2D IR experiments we have observed a vibrational coupling between the high frequency water band and absorption bands at lower frequency that correspond to the amide A vibration of the protein backbone. Vibrational coupling between these modes may be an indicator of water molecules located at the protein water interface. Finally, 2D IR spectra on the amide 1 vibration of the protein backbone display a cross peak between a well resolved proline vibration centered at 1610cm-1 that originates from the elastic region of the protein, and a vibration centered at 1675cm-1 whose associated secondary structure is currently undetermined. From this data we hope to determine water's role in the ITT and propose a secondary structure for the elastic region of the protein.

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Dynamical Studies Of A Temperature-Sensitive Mutant Of The Tryptophan Repressor Protein, L75F-TrpR
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The overall research goal of these NMR dynamic studies is to enhance our knowledge of the dynamical properties of the tryptophan repressor (TrpR) protein and to establish the origin of flexibility changes that take place in TrpR mutants which exhibit conservative single point amino acid replacements that lead to altered L-trp and/or DNA binding properties.
A second objective is to understand how differential flexibility modulates L-tryptophan (L-trp) co-repressor binding to TrpR, and may be at the origin of the non-local long-range effects observed in the temperature-sensitive (ts) mutant of the tryptophan repressor protein, L75F-TrpR, which cannot simply be rationalized by small structural changes in the 3D fold of L75F-TrpR when compared to the 3D structure of wild-type (WT) TrpR.
We have undertaken 15N NMR relaxation studies to investigate the motional properties of backbone amides in the apo and L-trp bound (holo) forms of L75F-TrpR in solution and to compare the dynamical properties of mutant TrpR to that of wild type repressor. We have identified interesting differences between the flexibility profile of WT-TrpR vs. L75F-TrpR. The overall picture that emerges is that although both proteins exhibit similar ps-ns motion patterns for many residues in the core helices (i.e. helices A, B, C, and F) differences are detected in the DNA binding region (i.e. helix D-turn-helix E motif).

1649-Pos Board B493
Universal Scaling Law for Polypeptide Backbone Dynamics on the Pico- to Millisecond Time Scale
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UV-photolysis of an aromatic disulfide bond which holds a protein or peptide in a non-native conformation has been used to trigger polypeptide backbone relaxation. Geminate recombination of the disulfide bond was used as probe