human cancers and mutation breeding of crops and microbes by means of ion-beam technology. However, the underlying mechanism for the energetic particle induced biological effects is still elusive because the interacting system involves radiolysis of different biomolecules such as DNA, proteins, sugar and lipids, and moreover, there are cross-correlations among these varied substances due to their interactions and signal transductions in living cells. A new trend of research is therefore to investigate the interaction between energetic particles and organisms with consideration of the entire cellar micro-environment and the entangled processes occurring in a whole cell, and to scrutinize the changes of cellular structure and compositions on the micro-scale and also monitor the dynamic and kinetic processes for the interactions. In this context, it is very useful and powful to apply micro-spectral imaging technology such as FTIR and Raman confocal microscopy because it can provide not only good time and spatial resolution, but also non-invasive measurement. In this work, we utilized the high spatial resolution FTIR and Raman microscopy to study the cellular changes of some model microbes and cells by mapping and monitoring the fingerprint bands of the cellular components such as lipids, carbohydrates, polyunsaturated fatty acids, proteins and nucleic acids under the irradiation of energetic particles. Correspondingly, the cell activity, the intracellular content of ROS, the level of MDA and GSH, the activity of CAT and SOD were measured to explain the biological effect induced by energetic particles. This work is supported by NSFC (No. 10975152, No. 11175204), CAS Innovative Project (KJX2-YW-N34-1) and Hundred Talents Program of CAS, China.

3001-Pos Board B771

Simulating the Amide I IR Signal of a Peptide in Solution using a Classical Implicit Water Approximation

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Behavior of the amide I IR signal of peptides has been the object of much study because it can provide valuable information about the environments and conformations of peptides in solution. Numerous models have been proposed to predict the amide I band shape, the most successful of which may have limited utility in studying dynamic processes due to high computational cost. Here a new, simple method is employed to predict the effects that the aqueous environment and side chains have on the shape of the amide I IR signal for a polypeptide in water. Using GEPOL to generate a solute cavity, apparent charges at the solvent accessible surface are generated considering a conductor like response from the solvent to partial charges on atoms (AMBER, or CHARMM). Potentials on the atoms in amide groups resulting from the surface charges and from the side groups are then used along with an electrostatic potential map to predict how the amide I signals are perturbed from gas phase signals. Effects of cavity size and atomic partial charges on the integrity of predicted band shapes are examined. The method gives results comparable to much more computationally intensive methods.

3002-Pos Board B772

Measuring Moments of Protein Conformation Distributions using Infrared Spectroscopy

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Infrared spectroscopy is often used to characterize the concentration and secondary structures of proteins in a variety of static and dynamics samples. Our work develops new methods to compare the structure, dynamics and function of nearly identical protein samples, in order to help characterize bio-similar protein therapeutics. We have developed a method to describe protein conformational variations around the average molecular values. By comparing the moments of the protein structural distributions and amide hydrogen/deuterium exchange methods, we explore the relationships between protein stability and dynamics. Examples include lysozyme and albumin in solution, cytochrome c interacting with lipid membranes of varying net-negative surface charge density, and bacteriorhodopsin during its photocycle.

3003-Pos Board B773

Isotope-Edited FT-IR Spectra of Isotopmers of Helical Hexamers of Alpha-Aminoisobutyric Acid

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Isotope-edited FT-infrared spectra of the Amide I region of hexamers of alpha-aminoisobutyric acid (Z-Aib_6-OtBu) have been collected in order to explore the effects of $^{13}C{=}O$ enrichment on the FT-IR spectra in the conformational context of 3_{10} helices. Oligomers of Aib are known to adopt predominantly 3_{10} helical structures, even at short peptide lengths. The Amide I band is sensitive to the details of peptide secondary structure, but the competency of this band to distinguish between alpha- and 3_{10} helical secondary structure remains an open question. The 3_{10} helix is shorter than an alpha-helix of the same number of residues and exhibits an i to i+3 hydrogen bonding pattern, instead of an i to i +4 pattern of the alpha-helix. These differences bring amide oscillators of a 3_{10} helix slightly closer in space and in shorter periodicity of hydrogen-bonding partnership as compared to an alpha-helix. We have collected infrared spectra of isotopomers of hexamers of Aib (e.g., Z-Aib-Aib-Aib-Aib-Aib-Aib-OtBu, Z-Aib*-Aib-Aib*-Aib-Aib-Aib-OtBu, and Z-Aib*-Aib*-Aib-Aib-Aib-Aib-OtBu, Aib* = ^{13}C enrichment at *C=O) in dichloromethane (a nonpolar aprotic solvent) and methanol (a polar, protic solvent) to examine the effects of carbon-13 enrichment on the spectra. Differences among the spectra of peptide isotopomers enriched with one or two ^{13}C labels will be examined, detailing the effects of coupling between pairs of ^{13}C-labeled Amide I oscillators.

3004-Pos Board B774

Under Pressure: Measuring Desolvation of Model α-Helical Peptides

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Model helical peptides have been shown to unfold with temperature, but are stabilized with increased pressure [1-3]. In these peptides, as pressure increases, the solvent environment becomes ordered allowing for an increase of the helical content of the peptide. Our work investigates hydration of the peptide backbone using both temperature and pressure as modifying conditions. The synthetic peptide sequence, $(AAAAK)_3$-AAAAY is well-characterized and ideal for the study of helix properties[3]. To measure the coupling of pressure and temperature, Fourier transform infrared spectroscopy (FTIR) monitors the perturbations in the secondary structure via the amide I' band. FTIR is a sensitive technique for detecting changes in hydrogen bonding and has been used for the estimation of amide photon exchanging with the solvent. Pressure on the peptide is applied using a manually manipulated Diamond Anvil Cell (DAC). Isotopically labeled residues within the peptide have been exploited for probing local interactions due to the shift of the heavier masses of the labeled residues to a lower frequency compared to the global ^{12}C amide I band around 1633 cm^{-1}. Our goal is to compare the location of isotopically edited alanines and the ability to remain desolvated with increasing pressure and temperature. With this technique, it was found that alanines proximal to the lysines were protected from solvent hydrogen interactions due to side chain shielding in the model sequence.

(1) Barber-Armstrong, W.; Donaldson, T.; Wijesooriya, H.; Silva, R. A.; Decatur, S. M. *J Am Chem Soc* **2004**, *126*, 2339.
(2) Gnanakaran, S.; Hochstrasser, R. M.; Garcia, A. E. *Proc Natl Acad Sci U S A* **2004**, *101*, 9229.
(3) Paschek, D.; Gnanakaran, S.; Garcia, A. E. *Proc Natl Acad Sci U S A* **2005**, *102*, 6765.

3005-Pos Board B775

Dependence of Plant Cell Wall Composition and Structure on Cellulose Synthase-Like Knock Out Mutant

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Plant cell walls are a complex mixture of polysaccharides, proteins and the phenolic polymer lignin that have been recently targeted as possible sources of fermentable sugars for the production of biofuels. The development of a biomass-based biofuels industry is partly dependent on genetic engineering and breeding next generation crops containing, among other traits, easily extractable cell wall sugars. Thus, a better understanding of how plants synthesize, deposit and modify their cell walls is necessary for the selection of traits important for biofuel crop improvement. The identification of plants with altered cell wall composition or structure can prove useful in the discovery of novel genes involved in the biosynthesis and modification of the cell wall.
The CELLULOSE SYNTHASE-LIKE 6 (CSL6) gene has been recently shown to mediate the biosynthesis of mixed-linkage glucan (MLG), a cell wall polysaccharide that is thought to be necessary for cell wall expansion in the primary cell wall of young seedlings. A detailed analysis of a loss-of-function MLG rice mutant has been recently conducted revealing surprising results. Though the mutant showed a 99% reduction of MLG content, the rice clsf6 knock out mutant showed only a slight decrease in growth compared to wildtype. The cell wall properties of both mutant and wild type were determined via biochemical and various spectroscopic (Fourier Transform Mid-Infrared spectroscopy)