1047-Pos Board B802
Selective Refinement and MDR Selection of Near-Native Protein Structures
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In recent years \textit{in silico} protein structure prediction reached a level where a variety of servers can generate large pools of near-native structures. However, the identification and further refinement of the best structures from the pool of decoys remain problematic. To address these issues, we have developed a selective refinement protocol (SRP), and a molecular dynamics (MD) simulation based ranking method (MDR). In SRP the refinement of structures is accomplished by using the relax mode of the Rosetta software package, subject to specific constraints determined by the type and complexity of the target. The final best models are selected with MDR by testing their relative stability against gradual heating during all atom MD simulations. We have implemented the selective refinement protocol and the MDR method in Mufold-MD, our fully automated protein structure prediction server. Mufold-MD was one of the top servers in the CASP10 competition.

1048-Pos Board B803
Structural Analysis of CRIP1a by in Silico Approaches
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The novel protein, Cannabinoid receptor interacting protein (CRIP) is encoded by Cnrip gene, and is found on chromosome number 2 in humans. CRIP1a can modulate CB1 receptor cellular localization and signal transduction. However the structural aspects of CRIP1a and its interaction with CB1 are unknown. Because no sequence or structural homology with other known proteins is currently available, an ab initio modeling approach for prediction CRIP1a structure has been used. The Molecular docking and molecular dynamics simulations have been used to investigate binding and relative stability between CB1 and CRIP1a. The results show compact structure of 12 beta sheets along with small helix and loops, which is supported by secondary structure data, Ramachandram plot, Aggregation analysis, and lesser number of high energy zones. Further the entire protein was refined by 10 ns MD simulation with Gromacs and the structural changes were observed which appear to be related with rearrangement of hydrogen bonds. Molecular docking with CB1 C-terminal peptide revealed binding pocket in CRIP1a. The relationship between Cannabinoid receptor isoform one (CB1) and CRIP1a play significant roles in addiction, diabetes, cardiovascular disease, neurodegenerative disorders and the pain management.
Grant Support:NIH DA03690 and ICMR, India.

1049-Pos Board B804
Protein Model Quality Assessment Prediction by using a Residue Specific Statistical Potential
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A residue specific approach is introduced for enhancing the accuracy of knowledge-based statistical potentials for quality assessment of protein models. The proposed method relies on an assumption that common substructure motifs among different protein folds can still share similar patterns of interactions with neighboring residues.
Instead of using the classic approach, in which a set of non-homologous whole-chain structures are used to derive a potential, we created a potential that was composed of independent sub-potentials; each of them was specific to a certain residue in the target sequence. To achieve that, the target sequence was split into short linear segments, then every segment was threaded through PDB to find proteins that share sequence similarity with this segment. Then, after removal the hits that were homologous to the target sequence, the remaining proteins were used to derive a statistical sub-potential for the residue that was in the center of a certain segment that had been threaded through PDB. This procedure was performed for every residue in the target protein.
We applied this methodology to create a residue-specific variant of the DFIRE statistical potential. For CASP9 single-domain targets, the average Pearson's correlation coefficient per target between the pseudo-energy predicted by the residue-specific DIFIRE potential and the GDT_TS score was 0.656. The classic DFIRE potential achieved the correlation coefficient of 0.561.
We believe that, for the current size (which is still growing) of the PDB database, this methodology can be successfully applied to increase the accuracy of other state-of-the-art statistical potentials.

Biosurface Interactions and Engineered Biosurfaces

1050-Pos Board B805
Molecular Simulation of the Adsorption of Amino Acid Sidechain Analogs to the TiO2 (100) Surface
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Titanium dioxide (TiO2) in the form of nanoparticles (NPs) are found in many common food and health products. TiO2-NPs have been shown to attract biological material, such as proteins and lipids, which form a protective "corona" on the NP surface. This coating is believed to be a key element in determining the toxicity behavior of the nanoparticle, and its potential hazard to human health.
Large-scale computer simulations promise to provide atomistically detailed information on the molecular basis of NP corona formation, but are limited by the absence of suitable interaction parameters for inorganic nanomaterials (such as TiO2) and biomolecules. We have developed forcefield parameters for simulations of TiO2–biomolecular interfaces to alleviate this situation. The new forcefield is based on high-quality experimental data and is directly compatible with the widely used AMBER parameters for biomolecules.
Side chain analogs (SCA) are small molecules designed to mimic the naturally occuring amino acids, and serve as a model system for studies of NP and protein/peptide interactions. We have performed systematic molecular dynamics simulations with our new forcefield parameters to study the adsorption of SCAs to the TiO2 (100) surface. Advanced sampling techniques are employed to determine accurate free energy profiles of SCA binding to TiO2, which are used to map the affinities of individual peptide segments to TiO2. The impact for general protein-surface adsorption are discussed, also in light of recent experimental data.

1051-Pos Board B806
NMR Study of the Interaction between Ti Binding Peptide and TiO_2 Nanoparticles
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In order to improve theTi implant surface, the introduction of both TiO_2 binding sequence and silk is planned. We used the Ti Binding Peptide (TBP)[1], Arg-Lys-Leu-Pro-Asp-Ala, to strengthen the interaction between Ti surface and silk fibroin. The solution structure of TBP was determined in aqueous solution containing TiO_2 nanoparticles by NOE experiments. Then, the site specific interaction between TBP and TiO2 nanoparticles was investigated by $T_{1\rho}$ analysis. Also, the structure of the sequence, RKLPDA in aqueous solution was modified by presence of AGSGAG, the repeated sequence in *Bombyx mori* silk fibroin, in the both sides of the sequence. The solid state structure of AGSG[1-^{13}C]AGGRKLPD[1-^{13}C]AGGAGSGAG adsorbed on the TiO_2 surface was also studied using ^{13}C CP/MAS NMR on the basis of ^{13}C conformation-dependent chemical shift.
Reference:
1. Sano K. and Shiba K., *J. Am. Chem. Soc.*; 125(47) 14234 (**2003**).

1052-Pos Board B807
FTIR-Spectroscopic Analysis of Proteins in Liquid Samples
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Fourier-transform-infrared- (FTIR) spectroscopy has proved to be quite useful for protein detection at low concentrations and determination of protein secondary structures. It has been very successfully applied for detection and structure analysis of soluble and membrane proteins [1]. The surface sensitive total reflection- (ATR) technique has been particularly useful for the analysis of membrane anchored proteins [2,3,4]. Thus, secondary structure analysis of various disease related proteins like Prion Protein (PrP) or Amyloid-beta-(Aß) is achieved. Upon disease progression, these proteins undergo a structural transition from a-helix to ß-sheet conformations.
The modification of the internal reflection element (IRE) renders the surface selective for specific compounds [5]. Further, ATR-spectroscopy is suitable for analysis of protein-protein interactions and their biological function in an aqueous environment. Kinetic analysis of protein-substrate interactions were performed. Additional, the orientation of proteins can also be obtained using polarized infrared radiation. Here, we provide a brief overview of current applications and the potential of the ATR-spectroscopy in the biomedical sector.