by binding to the pore of WD domain, a highly conserved region of Gro/TLE protein family. Reliable methods for predicting binding sites would allow a better understanding of protein selective recognition mechanisms. This, in turn, would help developments of new organism-specific medications. To the best of the author's knowledge, this is the first study that uses amino acid sequences to predict binding sites of eh1-like motifs to the WD domain. Three-dimensional models of known eh1-like motifs were generated. Their interactions with the WD domain were studied and optimized using Deep View program and the Swiss-Model server. Spatial distributions of binding sites, residue properties, and bonds' stabilities were used to devise a scoring function. The scoring function was employed to predict and evaluate putative binding sites of randomly generated eh1-like sequences. Bioinformatics database searches were used to check whether the scoring function consistently discriminated between viable and non-viable eh1 candidates and corresponding binding sites. The scoring function expressed well a general relationship between putative motifs' residue sequences and their binding sites with the WD domain. Although the function gave a few false positive findings, it reliably identified sequences that did not form stable bonds with the WD domain. The results of this study should lead to a better understanding of mechanisms of transcriptional regulation and selective protein recognition. The method presented may be used to predict binding sites of other regulatory motifs.

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Genome-wide modeling and analysis of BAR Domains in *Arabidopsis thaliana.*

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The BAR (Bin-Amphiphysin-Rvs) Domain is a conserved dimerization protein domain which senses membrane curvature and binds to the lipid plasma membrane. The Amphiphysin protein family, which contain the BAR domain, are thought to be the modulators of the early phases of endocytosis and intracellular transport. It is theorized that this crescent shaped domain dimer show a preference for binding to highly curved, negatively charged membranes. It has been noted that in mammals and higher organisms, the BAR domain with an N-terminal amphipathic helix and BAR domain (N-BAR) can drive the membrane curvature both *in vivo* and *in vitro*. We have studied the BAR domain in the small flowering plant which is widely used as the model for plant biology, *Arabidopsis thaliana*, where its function remains largely unexplored. We have modeled all the BAR domains of *Arabidopsis thaliana* using an automated modeling pipeline with manual refinement methods and investigated their mechanism relative to other higher organisms. We have identified eight non-redundant domain sequences in *Arabidopsis thaliana*, which can be grouped into three different classes, based on their electrostatic profiles and domain architecture. We provide new insight into the features of plant BAR domains including distinct electrostatic profiles for domain sequences categorized within the same class and atypical electrostatic profiles showing a concentration of positively charged residues at both extremities of the structural fold. Our results are important in understanding the differences in signaling through BAR domains in plants and its implication in plant signaling and membrane trafficking.

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Interactive Visualization of Protein Dynamics in Ribbon Mode

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In recent years, experimental methods have uncovered more and more dynamic properties of molecular systems. Novel techniques for post-processing data from cryo-electron microscopy or small angle X-ray scattering nowadays routinely reveal conformational differences linked to functional states of a biological system. As opposed to molecular dynamics, these methods typically yield information about larger systems, which in effect makes an interactive visualization of the results challenging.

This poster presents an approach that computes a depiction in the more abstract ribbon or cartoon mode, which highlights the secondary structure information of a protein. To accomplish interactive frame rates, the algorithm offloads computational work from a PC's CPU to its graphical processing unit (GPU). This is achieved by separating two phases in the calculation of the geometry representing the protein. The first one involves creating a smooth curve along the protein's backbone, which requires global information and thus has to be computed by the CPU. In the second phase, vertices along that curve are moved to build the geometry for the molecule's depiction. Because local information is sufficient for that, this is handled exclusively by the GPU.

The speed-up factor achieved moves a range of large time-varying proteins into the category of those which can be depicted with interactive frame rates. For intermediate sized molecules, the speed-up results in an even smoother animation and an overall increase of the reactivity of the whole program. Especially simultaneously running processes, e.g. calculations for multi-scale modeling, can benefit from the additionally available CPU resources, too.

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Dynamics-based Alignment: A Novel Tool For Comparing Large-scale Movements In Proteins With Same Or Different Fold

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The biological function of several proteins and enzymes is assisted by large scale conformational changes that are excited in thermal equilibrium. In terms of the traditional logical cascade, sequence -> structure -> function, it is expected that the functional movements of a protein are influenced by the structural architecture. Proteins with similar structures are known to sustain similar large-scale movements; yet it has recently emerged [Carnevale et al. JACS 2006, Capozzi et al. J_Proteome_Res 2007, Zen et al. Prot_Sci 2008] that similar functional movements are shared by proteins with different architecture or topology.

This observation parallels the known paradigm that (i) proteins with similar primary sequences usually attain a similar fold but also that (ii) the same fold is adopted by non-homologous proteins. The sophisticated interplay between sequence and structure has now been extensively characterized thanks to the availability of sequence and structural alignment methods. By analogy, the availability of quantitative methods for comparing the functional-oriented dynamics in proteins would allow to take to a new level the investigation of the structure/function relationship.

We report on a first attempt in this direction by discussing a pairwise alignment scheme that identifies groups of amino acids that undergo similar concerted movements in proteins. The alignment method is based on a coarse-grained elastic network model and requires as input the sole proteins' native structures. No prior detection of structure and sequence correspondence is used. The scheme is first used to perform a dynamics-based alignment (and grouping) of a data set of >70 representative enzymes covering the main functional and structural classes. Finally we discuss an application where the method is used to identify the putative nucleic-acid-binding regions of proteins having AXH-domains [de Chiara et al. Structure 2005].

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Template-Based Modeling of Protein-Protein Interfaces

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Modeling of protein binding sites is important for 3D prediction of protein complexes. Statistical analysis of target-template PSI-BLAST sequence alignments was performed for 329 two-chain target protein complexes selected from DOCKGROUND database. For 214 complexes (~65 %) the alignments contained all interface residues (full interface coverage or FIC alignments) for both complex monomers and 101 (~30 %) complexes had FIC alignments for one of the monomers. The FIC alignments were observed even in the case of poor alignments where only a small portion of the target sequence (as low as 40%) was aligned to template sequence with low alignment identity (40%) alignments, whereas for the low-identity alignments the situation is opposite. Homology models were built based on the FIC alignments with target sequence coverage < 60 %. The results showed that one third of the target sequences with such short FIC alignments produced models with interface RMSD (i-RMSD) < 5 Å, suitable for low-resolution ab initio docking. The proteins with i-RMSD < 5 Å had domain structure, whereas models with 5 Å $<$ i-RMSD < 8 Å (accuracy suitable for structure-alignment methods) were generated for single-domain proteins as well. The results provide guidelines for building 3D protein models for docking studies.

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Homology Modeling and Molecular Dynamics Simulation Studies of the human resistin protein

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Resistin is a member of a secretory protein family, known as resistin-like molecules (RELMs) which were exclusively found in mammalian genomes. Though human resistin molecule has high sequence similarity with mouse, its structural and physiological roles differ considerably from mouse and the