the structure and the known mutations establish the molecular basis for MPS IV A and for the larger MPS family of diseases.

2913-Pos Board B68
On the Structural and Biochemical Properties of the Human Septins: SEPT3
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Septins constitute a family of conserved guanine nucleotide binding proteins that are found in different organisms. The human septins comprise 13 genes which encode proteins involved in important cellular processes, such as cytokinesis, exocytosis, membrane compartmentalization. They can be divided into 4 groups based on sequence similarity. Septins from different groups have showed to interact with each other assembling into heteromeric complexes that can polymerize to form filaments. Currently, only one of these possible heterocomplexes had its structure solved, but it did not include any member of the SEPT3 group. Recent publications suggest SEPT9, a member of the SEPT3 group, can occupy the terminal position in the assembly of octameric complexes. Here, we present the first determination of the crystallographic structure and biochemical properties of the SEPT3. The analysis of this structure shows unique features that can be useful in understanding the assembling of septin octamer units and the polymerization control of the septin filaments. A truncated version of SEPT3 lacking the N-terminal domain (SEPT3-GC) was found to be a monomer in solution, and the dimerization was dependent on salt concentration and the presence of GTPS. Additional site-directed mutagenesis experiments proved that the SEPT3-GC monomeric state is related to a tyrosine residue which is present in all human septins, except in the SEPT3 group. The SEPT3-GC affinity by GTPS was Mg^{2+} dependent and this septin was also active and able to hydrolyze GTP in vitro. The crystal structure of SEPT3-GC forms foreshortened filaments which employ the same NC and G interfaces observed in the hexameric complex of human septins 2, 6 and 7, reinforcing the notion of 'promiscuous' interactions described previously.

2914-Pos Board B69
Characterization of Novel Influenza Vaccines by Transmission Electron Microscopy
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A novel panel of influenza vaccines contain modules that target both the innate and adaptive immune system on a continuous polypeptide. These modules produce a more immunogenic vaccine than if they are co-administered as separate molecules. The immunogenicity also varies with the particular arrangement (and stoichiometry) of modules in the construct. We present and interpret volume maps of (some of) the panel, derived from electron micrographs. Recognition elements of the innate and adaptive immune system are used as fiducials to inform map interpretation and biological significance.

2915-Pos Board B70
Characterization and Structural Analysis of the Ig1 Domain of Obscurin
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Obscurin (700-800 kD) is a giant modular protein involved in many aspects of muscle cell organization and maintenance. Disregulation of obscurin leads to supermolecular deformities of the sarcomeric cytoskeleton, and mutations of obscurin and its targets cause cardiomyopathies and muscular dystrophies. The extreme N-terminal domain of obscurin (Ig1) interacts with the extreme C-terminal domain (M10) of the ''molecular ruler'' protein Titin, and mutations in M10 lead to LGMD2J. While the structure of M10 has been solved through X-ray crystallographic techniques, the high-resolution structure of obscurin's Ig1 domain remains elusive and unknown. In an attempt to better characterize the biophysical parameters of the M10-Ig1 interaction, here we present NMR assignments of Ig1. This work is the first step in solving the high-resolution structure of Ig-1 and eventually the M10-Ig1 complex.

2916-Pos Board B71
Structure of NEMO through EPR Spectroscopy and Multiscale Modelling
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NEMO is a key eukaryotic protein interaction hub involved in NFkappaB signalling. The structure has been proposed to be dominated by two extended coiled coil domains, but high resolution data on the complete structure and information on the mechanism of signalling has remained unclear. Here we describe the use of multiscale modelling with electron paramagnetic resonance to propose an all atom model of the structure. We find that the protein behaves as a single rod like coiled coil, with a short connecting region which allows a change in the register of the coiled coil packing. We discuss the impact of the structure on proposed mechanisms of signalling and the role of frustrated coiled coils in signal processing in biology.

2917-Pos Board B72
The Protein Circular Dichroism Data Bank: A Resource for Data Sharing
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The Protein Circular Dichroism Data Bank (PCDDB) (http://pcddb.cryst.bbk.ac.uk) is a resource for circular dichroism (CD) spectroscopic data and metadata, with links to sequence and structure databases and citation references. For depositors it provides a means of fulfilling granting body and journal data sharing requirements. For users it enables access to raw and processed data associated with published studies.The PCDDB website also includes software for spectral matching and analyses, as well as a format-conversion website that produces versions of the data in a wide variety of formats, including the new instrument-independent JCAMP-DX-CD format. It also includes validation software (ValiDichro) for verification of the quality of data measurement and processing, including providing to the depositor a validation report that can be included in publication submissions as evidence of data quality and the availability of the data that will be released on publication. In many cases the entries in the PCDDB contain additional information to that included in the publication, which will be of particular value to the biophysics and bioinformatics communities. Making these data available for meta-analyses opens the potential for their use in a wide range of applications, including methodology development, comparisons of modelled and experimental structures, identification of new protein folds, and comparisons of wild type and mutant proteins.
From the initial release of the 71 proteins that comprise the SP175 reference dataset that is widely used for CD analyses, the holdings have grown to include a wide range of soluble and membrane proteins, as well as thermal denaturation series; more than 90000 files have been downloaded thus far by users across a wide range of disciplines.
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2918-Pos Board B73
Improved Secondary Structure Determination and Fold Prediction by Circular Dichroism Spectroscopy
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Circular dichroism (CD) spectroscopy is a well known technique for the study of the secondary structure of proteins. Although the presently available algorithms reliably estimate the secondary structure of the α-helical proteins, the prediction of β-sheet structure is much less accurate. In the case of proteins with unique β-structures, such as membrane proteins and amyloid fibrils, the secondary structure prediction results are unacceptable. The problem arises from the diversity of β-structures, which results large spectral differences even between proteins with similar overall β-sheet content. We have developed a new algorithm for the accurate estimation of secondary structure contents for a broader range of protein folds with special interest to β-structure rich proteins including amyloid fibrils. The reference spectrum database was expanded with high quality spectra of globular proteins and amyloid fibrils recorded down to 175 nm using synchrotron radiation CD. Our algorithm takes into account the diverse twist of the β-sheets that has a great influence on the spectral features. For the first time, we can reliably distinguish parallel and antiparallel β-structure using CD spectroscopy. Moreover, it performs better than any other algorithms for any secondary structure types. With its improved accuracy and more detailed structural information, the method is capable of predicting the protein fold to the level of topology in the CATH classification with good reliability. A web server was constructed to make the algorithm available for the protein science research community.