edge (XANES) and extended (XAFS) at the Zn K-edge have been explored. We will present further insights into the divalent metal ions regulation of the hut operon in Bacillus subtilis, by combining both crystallography and X-ray absorption spectroscopic studies.
1)Kumarevel et al., Nature 434, 183-191 (2005), 2)Kumarevel et al., Nucleic Acids Res. 33, 5494-5502 (2005)

Keywords: X-ray absorption fine structure, protein crystallography with synchrotron radiation, protein refinement

MS.63.5

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The structure of the Amyloid β-peptide high affinity copper II binding site in Alzheimer's disease

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A major source of neurodegeneration observed in Alzheimer's disease (AD) is believed to be related to the toxicity from reactive oxygen species (ROS) produced in the brain by the Amyloid-β (Aβ) protein bound primarily to copper ions. The evidence for an oxidative stress role of Aβ-Cu redox chemistry is still incomplete. Details of the copper binding site in Aβ may be critical to the etiology of AD. Here we present the structure determined by combining X-ray absorption fine structure (XAFS) and Density Functional Theory analysis of truncated Aβ(1-16) peptide complexed with Cu(II) in solution under a range of buffer conditions. PBS buffer salt (NaCl) concentration does not affect the copper binding mode. The XAFS spectra for truncated Aβ(1-16)-Cu(II) and full length Aβ(1-40/42)-Cu(II) peptides are similar. The novel six-coordinated (3N3O) geometry around copper in the Aβ-Cu(II) complex includes three histidines, glutamic or/and aspartic acid and axial water. The structure of high affinity Cu2+ binding site is consistent with the hypothesis that the redox activity of the metal ion bound to Aβ can lead to the formation of di-tyrosine linked dimers found in AD. X-ray absorption near-edge spectroscopy (XANES) has been used to probe the substrate mediated reduction of Cu(II) to Cu(I) in Aβ-Cu(II) complexes by ascorbate and the neurotoxin 6-hydroxydopamine (6-OHDA), however dopamine and, in particular, cholesterol are incapable of reducing soluble monomeric Aβ-Cu(II) complexes. The results are in agreement with assignment of the redox potentials for Aβ-Cu(II), ascorbic acid and dopamine.

Keywords: beta-amyloids, Alzheimer's proteins, X-ray absorption

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Structural basis of a plant photosystem I sunlight conversion

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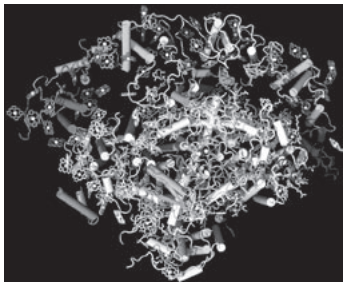
A plant Photosystem I (PSI) is a large membrane super-complex that drives photosynthesis. PSI captures sunlight through sophisticated pigment network and uses the energy to perform transmembrane electron transfer. It consists of the reaction center complex (RC), where the charge separation reaction takes place and the light harvesting complex (LHCI), which serves as an additional antenna system. PSI performs a photochemical activity with the unprecedented quantum yield of close to 1.0, being the most efficient light capturing and energy conversion device. We determined the X-ray structure of intact PSI at 3.4 Å resolution [1]. The crystal structure provides a picture at near atomic detail of 17 protein subunits; 3038 amino acids were assigned, as well as 168 chlorophylls, 2 phyloquinones, 3 Fe4S4 clusters and 5 carotenoids. The remarkable feature of PSI is the unprecedented high content of non-protein components, approximately one third of the total mass of about 650 KDa consists of different co-factors. The structure reveals intriguing insights regarding unique interactions between the RC and the LHCI complexes.
[1] Amunts, A., Drory, O. & Nelson, N. (2007) Nature, 447, 58-63.



Keywords: photosynthesis, membrane protein, electron transfer

MS.64.2

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Inhibitor complexed structures of the Cyt bc1 from the photosynthetic bacterium *R. sphaeroides*

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The cytochrome bc1 complex (bc1) is a major contributor to the proton motive force across the membrane by coupling electron transfer to proton translocation. The crystal structures of wild type and mutant bc1 complexes from the photosynthetic purple bacterium Rhodobacter sphaeroides (Rsbc1), stabilized with the quinol oxidation (QP) site inhibitor stigmatellin alone or in combination of with the quinone reduction (QN) site inhibitor antimycin, were determined. The high quality electron density permitted assignments of a new metal-binding site to the cytochrome c1 subunit and a number of lipid and detergent molecules. Structural differences between Rsbc1 and its mitochondrial counterparts are mostly extra membranous and provide a basis for understanding the function of the predominantly longer sequences in the bacterial subunits. Functional implications for the bc1 complex are derived from analyses of 10 independent molecules in various crystal forms and from comparisons with mitochondrial complexes.

Keywords: membrane protein crystallization, cytochrome bc1 complex, mechanism of proton pumping

MS.64.3

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Structure and mechanism of the DsbB-DsbA protein disulfide generation system in *E. coli*

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