

MS11-05 Structural insights into enzyme catalysis of sulfate reduction in *Desulfovibrio gigas*. Chun-Jung Chen,^a Yin-Cheng Hsieh,^a Sunney I. Chan,^b ^a*Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Center, Taiwan,* ^b*Division of Chemistry and Chemical Engineering, California Institute of Technology, U.S.A.*
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Sulfate-reducing bacteria (SRB), the strict anaerobes, constitute a particular group of prokaryotes that can metabolize sulfate. In dissimilatory sulfate reduction, the activation of sulfate is first catalyzed by ATP sulphurylase to produce adenosine 5'-phosphosulfate (APS), which is then reduced by adenylylsulfate reductase (adenosine 5'-phosphosulfate reductase, APS reductase or APSR) to sulfite. Sulfite is subsequently reduced by dissimilatory sulfite reductase (Dsr) to three products: trithionate ($S_3O_6^{2-}$), thiosulfate ($S_2O_3^{2-}$) or sulfide (S^{2-}). We have determined crystal structures of APSR and Dsr from *Desulfovibrio gigas*, a much studied representatives of SRB. APSR comprises six $\alpha\beta$ -heterodimers that form a hexameric structure. The flavin adenine dinucleotide (FAD) is non-covalently attached to the α -subunit, and two [4Fe-4S] clusters are enveloped by cluster-binding motifs. The C-terminal segment of the β -subunit wraps around the α -subunit to form a functional unit, with the C-terminal loop inserted into the active-site channel of the α -subunit from another $\alpha\beta$ -heterodimer. The structure of APSR, together with its oligomerization properties, suggests that APSR might self-regulate its activity through the C-terminus of the β -subunit [1, 3]. The structures of two active forms of Dsr, Dsr-I and Dsr-II, are also determined and compared. The dimeric $\alpha_2\beta_2\gamma_2$ structure of Dsr-I contains eight [4Fe-4S] clusters, two saddle-shaped sirohemes and two flat sirohydrochlorins. In Dsr-II, the [4Fe-4S] cluster associated with the siroheme in Dsr-I is replaced by a [3Fe-4S] cluster. The γ -subunit C-terminus is inserted into a positively charged channel formed between the α - and β -subunits, with its conserved terminal Cys γ 104 side chain covalently linked to the CHA atom of the siroheme in Dsr-I. In Dsr-II, the thioether bond is broken, and the Cys γ 104 side chain moves closer to the bound sulfite at the siroheme pocket. These different forms of Dsr offer structural insights into a mechanism of sulfite reduction that can lead to $S_3O_6^{2-}$, $S_2O_3^{2-}$ and S^{2-} [2].

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MS12-01 Structural basis of signal peptide recognition by the signal recognition particle. Elisabeth Sauer-Eriksson,^a Shenghua Huang,^a Gitte Meriläinen,^a Kristoffer Brännström,^b Tobias Hainzl,^a ^a*Department of Chemistry, Umeå University, Sweden,* ^b*Department of Medical Biochemistry and Biophysics, Umeå University, Sweden*
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The signal recognition particle (SRP) recognizes and binds to the signal peptide of nascent proteins as they emerge from the ribosome. The conserved core of SRP consists of SRP RNA and the SRP54 protein, and plays the key role in signal-peptide recognition and binding to the SRP receptor. Proper communication between the two SRP54 domains, the GTPase- and the M-domain, is vital for the function of the particle so that signal-peptide binding at the M domain directs SRP receptor binding at the GTPase domain. By studying crystal structures of the SRP RNA in complex with its different protein partners, many of the structural states of the SRP have been revealed. The structures of the *Methanococcus jannaschii* SRP54-SRP19-S domain RNA complex in its free form [1] and in complex with an hydrophobic idealized signal peptide comprising 14 leucine and alanine residues [2] provide an explanation for how signal peptide binding at the M domain triggers a reorientation of the GTPase domain by local structuring and α -helix formation of the GM linker.

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