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Structure of the Bi-functional ATP Sulfurylase/APS Kinase from *Aquifex aeolicus*, a Chemolithotrophic Thermophile. Z. Yu, I. MacRae, E. Lansdon, I. Segel, A. Fisher, Univ. of California, Davis, CA 95616.

The chemolithotroph *Aquifex aeolicus* derives its energy from reduced sulfur in the environment. ATP sulfurylase catalyzes the last step in the sulfur oxidation pathway to produce ATP and sulfate. Our lab recently demonstrated that this enzyme also possesses APS kinase activity making it a bifunctional enzyme. APS kinase phosphorylates APS to produce PAPS, the universal sulfate donor. The arrangement of domains in *Aquifex* is reminiscent of fungal ATP sulfurylase where the APS kinase-like domain allosterically regulates the ATP sulfurylase but has no kinase activity. The fungal ATP sulfurylase catalyzes the sulfur assimilatory reaction to produce APS and PP_i, which is the opposite direction to the *Aquifex* enzyme. To better understand the structural and functional differences between the different physiological roles of this enzyme in diverse organisms, we determined the structures of these enzymes from a number of sources. This poster presents the 2.3Å resolution structure of ATP sulfurylase/APS kinase from *Aquifex*. The enzyme forms a homodimer through the APS kinase domain. ADP molecules bound in both ATP sulfurylase and APS kinase active sites. In the APS kinase active site, the P-loop substitution S381P and a non-conserved disulfide bond explains the low kinase activity.