



	<b>Experiment title:</b> Structure analysis of methanogenic enzymes	<b>Experiment number:</b> LS-2189
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## Report:

### 1. Methylene-tetrahydromethanopterin reductase (Mtd)

Mtd is an enzyme of the methanogenic pathways isolated from *Methanopyrus kandleri*. Crystals obtained from MPD as precipitant adopted the space group  $C222_1$  with unit cell parameters of 120 Å, 151 Å and 220 Å for the native enzyme and 120 Å, 151 Å and 110 Å for the selenomethionine labelled enzyme. We collected a native data set to 1.9 Å resolution with an overall  $R_{sym}$  value of 7.6%. Moreover, we measured a complete MAD experiments at the selenium edge to 2 Å resolution with  $R_{sym}$  values between 4.3 % and 7.6 %. The peak data set of a second crystals was measured. However, the selenium sites could not detected. Finally, we measured a high resolution data set of the selenomethionine- labelled enzyme crystals up to 1.5 Å resolution with an  $R_{sym}$  of 7.6%.

### 2. ATP sulfurylase

ATP sulfurylase is the final enzyme sulfide or sulfur oxidation to sulfate. Crystals from *Allochromaticum vinosum* obtained from sodium citrate had the space group  $P2_1$  and the cell parameter were 73 Å, 97 Å, 73 Å and 118°. A complete data set was collected with an  $R_{sym}$  of 6.1% in the resolution range 30.0 - 1.6 Å.

### 3. 4-Hydroxybenzoyl-CoA reductase (4-OH)

4-OH is involved in the anaerobic degradation of aromatic compounds. Crystals from *Thauera aromatica* grew in the space group  $P2_12_12_1$  with cell parameters of 113 Å, 115 Å and 174 Å. The resolution of the data was 1.65 Å and their quality was excellent ( $R_{sym} = 6.3$  %).

#### **4. ATP-binding subunit of the sulfate ABC transporter (CysA)**

CysA is involved in the sulfate transport into the inner membrane of bacteria. CysA from *Alicyclobacillus acidocaldarius* was crystallized in the space group  $P2_1$  with the cell parameters of 155 Å, 56 Å and 92 Å. Native data up to 1.9 Å resolution were collected. The  $R_{\text{sym}}$  value was 5.8 %.

#### **5. Formaldehyde-activating enzyme (FAE)**

FAE is an enzyme of the methylotrophic pathway and converts formaldehyde to methylenetetrahydromethanopterin. Crystals from *Methylobacterium extorquens* grew in the space group  $P4_x2_x2$  with cell parameters of 120.8 Å and 206.2 Å. Native data were collected up to 1.9 Å resolution; the  $R_{\text{sym}}$  was 5.4%.

#### **6. $\gamma$ -subunit of the sulfite reductase (DsvC)**

Sulfite reductase is involved in sulfate reduction to sulfide, DsvC might playing a role by transporting electrons. DsvC from *Archaeoglobus fulgidus* was crystallized in the space group  $P2_12_12_1$ , the cell parameters were 39.9 Å, 46.5 Å and 57.2 Å. A complete data set was collected at 1.1 Å resolution. The  $R_{\text{sym}}$  value was 7.8 %.