ESRF	**Experiment title: Membrane protein structural determination from *Aquifex aeolicus***	**Experiment number**: MX-336
Beamline: ID14 -3	**Date of experiment**: from: 06 November 2004 to: 08 November 2004	
Shifts:1.5	**Local contact(s)**:Celia Romao	*Received at ESRF:*

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Report:

Samples:

Aq1862 crystals from *Aquifex aeolicus*, cytochrome c oxydase mutant crystals from *Parococcus denitrificans*

Background:

Aq1862 protein complex is a relative huge protein, of about 400KD. The sequence of Aq1862 contains no cysteins. We expect it to have low affinity to heavy metals. From a dataset collected at the zink edge, we got no phase information . Therefore, it seems to be necessary to set up screening of different heavy metal derivatives for collecting isomorphous and /or anomalous datasets.

A substitution of Asn 131 in the D-pathway of cytochrome c oxidase with aspartate leads to complete loss of proton-pumping activity while retaining full electron transfer activity. High resolution structure information will help to understand the functional changes.

Results:

5 SAD datasets from Aq1862 crystals:

ldatasets, , Resol (Å)	Rsym(%)	Compl(%)	I/sigma(I)	unit cell (space group R3)
Au, , 3.2,	15.6(36.1),	99.1(100),	7.54(3.84),	a=b=110.43, c =538.04,
Iod, , 2.2,	15.6(44.1),	99.8(100),	6.28(3.01),	a=b=110.36, c =534.15,
KPt, 3.0,	14.5(47.8),	99.1(99.8),	11.60(3.55),	a=b=110.63, c =538.10,
UAc, , 2.0,	18.2(40.7),	98.9(94.7),	5.05(2.98),	a=b=109.09, c =266.62,
Ptre, , 2.8,	10.5(50.0),	99.2(99.4),	12.7(3.63),	a=b=108.10, c =265.86

a cytochrome c oxidase mutant crystal dataset:

Coxmu	7(2.5)	1.3(30.1),	93.7(91.4)	46.58(4.53)	a=83.35, b=150.62, c=155.38