	Experiment title: The structure of human phosphoserine phosphatase in complex with its ligands	**Experiment number**: MX-38
Beamline: ID14-1	**Date of experiment**: from: 4/11/2002 to: 5/11/2002	**Date of report**: 6/1/2003
Shifts: 3	**Local contact(s)**: Dr. Joanne McCarthy	*Received at ESRF:*

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Report:

Human phosphoserine phosphatase (HPSP) is a 25 kDa enzyme responsible for the third and last step of the L-serine biosynthesis pathway. It catalyses the Mg^{2+}-dependent hydrolysis of L-phosphoserine. HPSP belongs to a class of phosphotransferases forming a phosphoaspartate intermediate during catalysis. Other enzymes forming a phosphoaspartate intermediate include e.g. P-type ATPases and phosphomannomutases.

Previously a selenomethionyl derivative was prepared and we collected a MAD dataset at the DESY synchrotron, Hamburg. The structure of HPSP was solved using this three wavelength MAD dataset. The ribbon diagram in figure 1 shows the structure of HPSP. An article about this structure was send to a journal and the coordinates will be deposited in the Protein Data Bank upon acceptance of the article.

Figure 1: The structure of Human Phosphoserine Phosphatase

The structure of HPSP as presented here is in a completely open conformation. HPSP is in this open conformation when no substrate or inhibitor is bound to the active site.

Since we want to study the working mechanism of HPSP in detail we want to have some ligands bound to the active site. Previously we collected a data set of a HPSP-crystal soaked with L-serine at the BM30A beamline at ESRF, Grenoble (France), but this attempt failed.

Now, we tried co-crystallization of HPSP with several ligands and we collected data sets of four different co-crystallization experiments. The first was the co-crystallization of HPSP with L-serine and phosphate. The data collection statistics are given in table 1.

Table 1: Data collection statistics for HPSP with L-serine and phosphate	
Space group	$C2221$
Cell parameters	$a = 49.102$ Å $b = 130.631$ Å $c = 156.915$ Å
	$\alpha = \beta = \gamma = 90.00°$
Resolution	2.30 Å
Wilson B	35.11 Å^2
Number of reflections	22893
Completeness (%)	99.7
Multiplicity	3.6
R-sym (%)	5.5

The data collection statistics for the co-crystallization experiment of HPSP with $NaVO_3$ are summarized in table 2.

Table 2: Data collection statistics for HPSP with $NaVO_3$	
Space group	$C2221$
Cell parameters	$a = 51.628$ Å $b = 135.341$ Å $c = 157.082$ Å
	$\alpha = \beta = \gamma = 90.00°$
Resolution	2.30 Å
Wilson B	54.60 $Å^2$
Number of reflections	23084
Completeness (%)	98.8
Multiplicity	4.2
R-sym (%)	6.4

The other two experiments were co-crystallizations of HPSP with L-serine and with phosphate alone. These data set still have to be further processed.

For a final conclusion and results some further analysis of these data have to be done. We hope that one of the ligands is bound to the active site of HPSP and this leads to a better understanding of the working mechanism of H PSP.