ESRF	**Experiment title:** BAG CBS Montpellier	**Experiment number**: MX-446
Beamline: ID 23-1	**Date of experiment**: from: 5th May to: 6th May 2006	**Date of report**: 6/12/06
Shifts: 3	**Local contact(s)**: Joanne MCCARTHY	*Received at ESRF:*
Names and affiliations of applicants (* indicates experimentalists): **Hoh F., Nahoum V. Guichou JF., Chaix D.**		

Cyclophylin with different ligants tested
12 structures (between 0.9 and 1.8 A) solved
7 structures apo
5 structures with DMSO (solvant) at ligant place

TR4

About 10 xl tested but no data collected because of very quickly dying xl (after few frames)

PXR

15 xl tested but no data collected. As TR4, xl were dying very quickly.

Plcr-apo

About 10 xl tested. No diffraction

Ccpn (ATP, ADP)

About 10 xl tested. No diffraction

Phytase

- 10 crystals of complexed phytase with the Six hexasulfate inositol (non hydrolysable ligand) were tested with no diffraction. (max 6A)

- A dataset was collected of the apo form of phytase at 2.3 A . A similar dataset was collected previously on ID14 but the spots were not resolved enough (high diffraction with big unit cell dimension). Structure solved (pdb on hold 2GFI, publication on the way)

- 8 cristals of complexed phytase with phytic acid (obtained by soaking with the apo form) were tested with no diffraction (max 8 A)

p14-akt

2 very tiny crystals were tested with no diffraction (10 A))

BCL

3 complexes with three different ligants were tested.
3 datasets were collected (around 2A) for each complexes (obtained with different conditions of crystallisation). No ligant were visible whatever the complexe.

P3

The protein p3 from Cauliflower mosaic virus (CaMV) mediates virus transmission by aphids. This small protein (15 kDa) associates with the capsid protein in virion shells and binds DNA in a non-sequence specific manner. About 30 crystals were tested. Three datasets of P3 crystals, one native and two derivatives (Hg and Au compounds), have been collected at 6 A resolution (Rsym 6.8, 6.4 and 7.8%, completion 98, 92 and 94 %). They belong to space group $P42_12$ with cell parameters a=b=105 Å, c=80 Å. The Au derivative (Riso=21%) is weakly substituted and the gold derivative is non -isomorphous. We also crystallized the P3 protein in presence of a DNA oligonucleotide (14 bp). The crystal belongs to space group $P2_1$ with cell parameters a=69.5 Å, b=28.9 Å, c=76.6 Å and β=92.4°. Diffraction data on this monoclinic crystal form were measured up to 2.5 Å resolution (completion 98.8%, Rsym=7.6%). There are two P3 molecules in the asymmetric unit. A second native dataset was obtained at 4 A resolution (completion 98.8%, Rsym=7.6%). We are now screening heavy atoms derivatives for the monoclinic form and preparing a selenomethionine labelled protein.

momp

MOMP is the major outer membrane protein from *Campylobacter jejuni and* belongs to the porin family. The MOMP crystals yielded poor quality, highly mosaic diffraction patterns. They belong to space group $P2_12_12$ with unit-cell parameters a = 170.1, b = 101.9, c = 104.9Å. A crystal soaked in $KAu(CN)_2$ that diffract to 4.2 Å (Rsym=11.7 %, completion 92%) and a crystal soaked in uranyl nitrate that diffract to 5.5 – 6 Å but integration – data reduction failed. This gold derivative and the Pt and Pb derivatives previously collected (november 2005) all failed to provide a consistent MIR solution.

NAD

Background: LmNADK1, is a /Listeria monocytogenes/ protein involved in the 2' phosphorylation of NAD.

Various trials of rapid washing/soaking of LmNADK1 (co-crystallized with thioacetyl adenosine) in I222 form failed to remove the endogenous ligand and to replace it by other adenosine derivatives. 16 complete datasets were collected (best dataset: max resolution~ 1.9 Å, R_merge ~ 8 % completeness ~ 98 %).