ESRF	**Experiment title:** BAG CBS Montpellier	**Experiment number**: MX-536
Beamline: ID 14-2	**Date of experiment**: from: 16th to: 17th September 2006	**Date of report**:
Shifts: 3	**Local contact(s)**: Dominique Bougeois	*Received at ESRF:*
Names and affiliations of applicants (* indicates experimentalists): Labesse g., Chaix d. Guichou jf., Bellot g.		

Ccpn(adp atp nad nadp)

15 xl tested, 4 datasets collected for ADP; ATPNH; NAD and NAD complexes.
2 structures resolved up to now, not deposited yet

CCPN-ATPNH: resol 2.26 A R: 0.206 Rf: 0.29485
CCPN-ADP resol:2.45 A; R: 0.198 Rf: 0.27867

Plcr-apo

15 xl tested. No diffraction

Cyclophylin with different ligants tested
10 structures (between 0.9 and 1.5 A) solved
5 structures apo
5 structures with DMF (solvant) at ligant place

p32 (+peptide i3)

2 data sets at 2.5 Å resolution; 1 data set at 2.2 Å resolution; 1 data set at 2.1 Å resolution
Solved structures (molecular replacement) reveal that the peptide is not bound.
Search for new crystallization conditions.

Pxr

During the previous run, PXR crystals ware damaged since no attenuator was used (see report). The crystals carried this run were smaller and only difrracted up to 7 Angstrom. No complete data set was collected.

NAD

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

Novel 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. 8 complete datasets were collected (best dataset: max resolution~ 1.9 Å, R_merge ~ 8 % completeness ~ 98 %).

Two dataset for a soaking of LmNADK1 in quinolinate a suspected allosteric effector. New effector not visible in density despite data quality and resolution (2.26 A; R/Rfree 18.8/23.7).

Data set recorded for NADK mutants W78F and H223E. Diffracted to 2.3 and 2.1 Å, respectively (R/Rfree = 19.2/25.5% I222 form).

Deposited PDB files: 2I1W, *2I29*, *2I2A*, *2I2B*, *2I2D*, *2I2E*, *2I2F*