



	Experiment title: BAG CBS Montpellier	Experiment number: MX-330
	Beamline: ID 14-3	Date of experiment: from: 30 january to: 31 january 2005
	Shifts: 3	Date of report: 27/02/05 <i>Received at ESRF:</i>
Local contact(s): David Richard Hall		
Names and affiliations of applicants (* indicates experimentalists): Stefan Arold, Marie-Line Garron and Guillaume Poncet , CBS, 34060 Montpellier, France		

1/. HIV-1 Nef soaked with cholesterol

Background: HIV1-1 Nef was reported to bind to cholesterol via its C-terminus. 15 cholesterol-soaked crystals were tested, and 3 complete and 3 partial datasets were collected (best dataset: max resolution= 3.0 Å, 150 images collected, $R_{\text{merge}} = 0.11$ completeness = 100%)

2/. HIV-1 Nef soaked with an inhibitory peptide (#5)

20 Nef crystals soaked with different peptide concentrations, and flash-cooled using different cryoprotectants were tested; maximum resolution however was only 7 Å (compared to 2.9 Å for native crystals).

3/. NAD-kinase in complexe with ATP, NAD or NADP

26 NAD kinase crystals soaked with ATP, NAD+ ATP+MgCl₂ or NADP+ADP+MgCl₂ were tested. 6 data sets to maximum resolutions of 3.2-4 Å were recorded. Data processing is currently underway.

5/. MabA C60V-G139A-S144L

Background: MabA (FabG1), is a *Mycobacterium tuberculosis* protein involved in the long-chain fatty acid elongation system FAS-II.

MabA mutants were designed to enhance the interaction with its substrates. One dataset on these mutants has been collected to a resolution of 2.0 Å ($R_{\text{merge}} = 0.048$, completeness = 96%).

6/. PLCR native

Native data has been collected in an attempt to obtain a isomorphous high resolution native data set, to be combined with ongoing efforts to obtain phase information from selenium derivatives. Data processing is currently underway.

7/. CcpN

Background: CcpN represses one of the two gap operons of *B. subtilis* by a yet unknown mechanism.

Native data to 2.0 Å resolution has been collected on crystals of the regulatory domain of CcpN (180 images collectes, $R_{\text{merge}} = 0.074$, completeness = 96 %). Attempts to solve the structure by molecular replacement (templates have less than 20 % sequence identity) are underway. In parallel, crystal trials have been set up using selenium-met derivatives of CcpN.

8/.Protegrin-Apamin peptides:

4 crystals tested. Three datasets collected (100 frames each) with very high resolution around 1 Å. The best dataset (comp 99%, $R_{\text{merge}} 0.06$) was used to resolve the structure by direct method at 1.1 Å. Writing publicaion is on the way.

