



<b>Experiment title:</b> BAG CBS Montpellier	<b>Experiment number:</b> MX-446	
<b>Beamline:</b> ID 14-2	<b>Date of experiment:</b> from: 10th April to: 11th April 2006	<b>Date of report:</b> 13/06/06
<b>Shifts:</b> 3	<b>Local contact(s):</b> Olivia SLEATOR	<i>Received at ESRF:</i>
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#### **/ NAD**

Background: LmNADK1, is a tetrameric kinase from *Listeria monocytogenes* involved in the 2' phosphorylation of NAD.

Wild-type form:

Kinetic studies of catalysis using various soaking times of NADK crystal I222 with NAD, ATP and Mn. Four complete datasets collected up to 2.0 Å (I222 form). Best refinement currently with Rwork of 19.0 and Rfree of 22.8. Datasets were also collected for two complexes with a substrate mimic (with and without ATP) at 2.1 and 2.2 Å resolution. Refinement undertaken.

Four purine derivatives crystals in I222 form soaked on wild-type NAD kinase were tested, and four complete datasets were collected (best dataset: max resolution= 2.3 Å).

D45N mutant:

Evaluation of the role of this residue in the catalysis of NADKs. Four complexes studied (ATP/NAD/Mn at various soaking times) with complete datasets collected up to 1.8 Å (I222 form). Best refinement ended with Rwork of 18.6 and Rfree of 22.5.

In conclusion, global improvement in resolution and new complexes obtained.

#### **./Testicular receptor 4**

The nuclear receptor TR4 is an orphan receptor that has no known ligand. It has been crystallized in order to aid ligand identification. We previously collected low and "high" resolution datasets but these data could not be merged properly. Here, a complete 4.0-3.0 Å dataset has been collected (I4122 form). The structure has been solved by molecular replacement and is currently being refined.

#### **./Pregnane X receptor**

The nuclear receptor PXR is a xenosensor involved in the detoxification of the organism. We have identified a new PXR ligand (PXR-4) that has better functional characteristics than the reference ligand. We co-crystallized PXR-4 with PXR and collected a 2.3 Å dataset. The structure has been solved by molecular replacement and is currently being refined (current Rw = 0.20, Rf = 0.27).

#### **./Cyclophilin D**

The Cyp D has been crystallized alone (apo-form) and in complex with a new inhibitor. Datasets at 1.0 Å resolution have been collected for both apo and liganded CypD. The structures have been solved by molecular replacement and are currently being refined (current Rw = 0.27/0.28, Rf = 0.29/0.31).

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