

ESRF report

Experiment #: MX-367 (ID14-1)

Date: 2<sup>nd</sup> - 3<sup>rd</sup>, February, 2005

### RC-PSII

Crystals of RC-PSII grown by counter-diffusion techniques in three different conditions have been test at ID14-1. Diffraction experiments were done at room temperature in the same capillary where the crystals have been grown avoiding crystal manipulation and at 100K using already known cryo-condition, after extracting the crystals from the capillaries. All crystals show a thin needle shape and clear surface degradation, age. Sixteen crystals were tested for diffraction but only some of them, cryo-cooled, showed diffraction spots at 25-30 Å. Several images were collected for those crystals and the analysis is ongoing to extract the unit cell dimension.

Further efforts are ongoing to obtain better quality crystals and a new proposal will be submitted during the next opening application period for crystal testing.

### HIV-1PR

Crystals of mutant forms of Human Immunodeficiency Virus 1 protease (HIV-1PR) in complex with inhibitor were tested and used to collect diffraction data during the MX-367 experiment at ESRF.

Mutant forms of HIV-1 PR bear mutations typically arise in patients treated with antiviral drug nelfinavir. These mutations cause a reduction in nelfinavir susceptibility and thus contribute to resistance. Crystals of four different mutants bearing combination of mutations D30N, L90M, A71V and N88D in complex with nelfinavir were grown using hanging drop method. Drops contained 2.5mg/ml protease, 100mM Acetate pH 4.5-5, 0.5-1M sodium chloride and 3fold excess of inhibitor. Needle shaped crystals were cryo-cooled in liquid nitrogen using 20-25% glycerol in crystallization buffer as cryoprotecting solution.

Six crystals were tested for diffraction and two of them were used for collecting complete datasets to resolution 1.6 Å and 1.8 Å for D30N/N88D and L90M/A71V mutant complex, at ID14-1 and BM16 respectively. The diffraction data will be used for structure solution using molecular replacement. Analysis of structures will help to understand the structural basis of HIV PR resistance.