ESRF

ESRF	**Experiment title:** Crystal structure of the *Staphylococcus aureus* leucocidin S component	**Experiment number**: MX-138
Beamline: ID14-EH1	**Date of experiment**: from: 08/11/2002 at 15:00 to: 09/11/2002 at 7:00	**Date of report**: August 1, 2003
Shifts: 2	**Local contact(s)**: Dr Joanne MCCARTHY	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

* Maveyraud Laurent UPS Toulouse

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Report: LukS structure

Two crystal forms were obtained : rather thin needles of the recombinant protein (monoclinic system) appeared in 20 % Jeffamine M-600 at pH 6.5 while bipyramids (tetragonal system) were obtained for the wild-type protein in 30 % Jeffamine M-600 at pH 8.0. Both forms have been totally characterized during these 2 shifts and complete native data sets have been measured. Due to the rather long c axis found in the tetragonal form (306 Å), data were collected to 2.0 Å resolution in order to avoid too much overlaps. The monoclinic form displayed an anisotropic diffraction pattern that nevertheless allowed the collection of a medium resolution data set.

The LukS-PV structure was solved in the tetragonal crystal form (8 mol/asymmetric unit) using molecular replacement with the previously determined 3D-structure of LukF-PV. The R and R_{free} values are 22.0 % and 25.7 %, respectively, and the average temperature factor for all protein atoms is 36.0 $Å^2$. The core of LukS-PV made of the β-sandwich, the prefolded stem and the rim domain is similar to LukF-PV. Major differences occur at the shortened N- and C-terminal β-strands and in the overall structure of the rim domain., which mediates interaction with the the membrane surface of target cells. Manuscript is in preparation.

Space group $P4_3$
Cell parameters a=b=94.8, c=306.2 (Å), α=90, β=90, γ=90 (°)

Data Collection

Δφ= 1° (180 frames) ; exposure time=3x5 s ; XTD=230 mm

Data Processing

Number of unique reflections=169450 ; Completeness=93.6 %
Multiplicity=5.9 ; Rsym=5.5 % ; Resolution limit=2.0 Å

ESRF	**Experiment title:** Crystal structure of the SNA-II lectin from *Sambucus nigra*	**Experiment number**: MX-138
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Report: SNA-II structure

The SNA-II (*Sambucus nigra* agglutinin II) glycoprotein crystallises in 2 M ammonium sulfate, at a pH comprised between 4.5 and 5.2. Two crystal forms occur in these crystallisation conditions : hexagonal and tetragonal crystals that diffract to 1.9 Å and 1.3 Å resolution, respectively. Complete native data sets were collected for both crystal forms during these two shifts. Since the tetragonal crystal form diffracted to very high resolution, two passes were needed in order to measure accurately both high and low resolution data.
The SNA-II structure was solved using the molecular replacement method with the ricin B-chain as a model. For the hexagonal crystal form, the final R and Rfree are 16.2 and 19.3 %, respectively. Four glycan chains are visible in the electron density, accounting for 14 saccharide units. For the structure of the tetragonal crystal form, the final R and Rfree are 17.8 and 20.0 %, respectively. Comparison of the crystal packing in both crystal forms suggests that SNA-II might preferentially exist as a dimer in solution.

Crystal form	Tetragonal	Hexagonal
Spacegroup	$I4_122$	$P6_422$
Cell parameters	a=126.12 Å, c=76.04 Å	a = 120.20 Å, c=177.34 Å
Data collection		
Nb. of frames	94 (high res.), 90 (low res.)	52
Exposure time	6x10s (high res.), 5s (low res.)	6x10s
XTD (mm)	100 (high res.), 230 (low res.)	180
Data Processing		
Resolution range (Å)	64.5 – 1.30	51.3 – 1.90
Nb. of unique reflections	73,310	57,308
Completeness	97.2 %	95.5 %
Multiplicity	8.0	5.0
Rsym	0.081	0.083

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Several crystals of the Gleheda (*Glechoma hederacea* agglutinin) protein that diffract only very weakly on the laboratory source have been tested during this run, giving a maximum resolution of 4 Å. Improvement of the diffraction quality of these crystals is in progress and needs to be estimated.