



	<b>Experiment title:</b> Block Allocation Group Italy (BAG)	<b>Experiment number:</b> LS-2183
<b>Beamline:</b> ID14-4	<b>Date of experiment:</b> from: 19/9/2002                      to: 21/9/2002	<b>Date of report:</b> 4/10/2002
<b>Shifts:</b> 6	<b>Local contact(s):</b> Dr Steffi Arzt (e-mail: arzt@esrf.fr)	<i>Received at ESRF:</i>
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## Report:

The nickel-containing Superoxide Dismutase (NiSOD) is a new class of the Superoxide Dismutase family. This metallo-enzyme catalyses the dismutation of superoxide radicals to molecular oxygen and peroxide and thus plays an important role in the protection of biomolecules from harmful byproducts of oxidative stress. We have recently solved the crystal structure of NiSOD. As suggested by low amino acid sequence homology and differing spectroscopic features to other members of the SOD family, the NiSOD shows a unique quaternary, tertiary and active site structure.

With the data collection of this experimental session we aim at studying the inhibition mechanism of NiSOD. Two small anionic molecules (CN<sup>-</sup> and N<sub>3</sub><sup>-</sup>) have been shown previously to inhibit NiSOD, indicating that the active site should be accessible for them.

During this experimental session we collected datasets on NiSOD crystals soaked in different concentrations of either NaCN, KCN or NaN<sub>3</sub>.

Table 1.: Summary of data collection statistics on (20-21/9/2001, beamline ID14-4)

**10 mM NaCN soak**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell (A)	a=112.184 b=113.921 c= 128.764
Resolution (A)	1.75
No. observed reflections	2278829
No. unique	163661
Completeness (%)	98.6
Mosaicity (deg)	0.4
Rsym (%)	7.7

**150 mM NaN<sub>3</sub> soak**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell (A)	a=112.091 b=113.513 c=128.684
Resolution (A)	1.75
No. observed reflections	1840309
No. unique	162205
Completeness (%)	98.7
Mosaicity (deg)	0.5
Rsym (%)	8.4

**50 mM KCN soak**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell (A)	a=112.014 b=113.777 c=128.645
Resolution (A)	1.75
No. observed reflections	1762178
No. unique	155693
Completeness (%)	94.3
Mosaicity (deg)	0.4
Rsym (%)	7.3

**10 mM NaCN soak**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell (Å)	a=112.201 b=113.556 c=128.643
Resolution (Å)	1.75
No. observed reflections	1254643
No. unique	142539
Completeness (%)	86.4
Mosaicity (deg)	0.6
Rsym (%)	10.9

**150 mM NaN<sub>3</sub> soak**

Space group	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Unit cell (Å)	a=112.369 b=113.691 c=128.736
Resolution (Å)	1.81
No. observed reflections	1321406
No. unique	142135
Completeness (%)	94.7
Mosaicity (deg)	0.55
Rsym (%)	8.0