



	Experiment title:	Experiment number LS1924
Beamline: ID29	Date of experiment: from: 14 June 2001 to: 15 June 2001	Date of receipt 21 August 2001
Shifts: 3	Local contact(s): A. Thompson	<i>Received at ESRF</i>
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Report:

The goal of this experiment was to search for heavy atom derivatives of the mitochondrial ADP/ATP carrier crystals and to collect data at a wavelength for which the heavy atom has a high f'' in order to optimise the phasing. The crystals are very thin (max 100 x 10 x a few microns) and cannot be tested on a rotating anode. In our laboratory, on a rotating anode equipped with osmic mirrors, one over ten crystals diffracts to 5 Å, therefore the search for heavy atom derivatives is very difficult (if 1 over 10 soaking conditions does not destroy the crystal, 100 crystals should be tested for one derivative!). In order to optimise the data collection time, we did not change the wavelength for each

derivative but we grouped the derivatives in 2 categories: Pb, Hg and Pt for which we select a wavelength of 0.946 Å and uranyl with a wavelength of 0.72 Å. With these wavelengths all the derivatives have a large f'' .

We prepared 100 crystals soaked in different heavy atoms under different conditions and froze them in advance. We tested 35 crystals. We collected 14 data sets, 6 of which could be integrated correctly.

Derivatives	Unit cell (Å) and space group	Resolution (Å)	Rsym (%)	Completeness (%)	redundan
Uranyl 1	85.2 85.9 102.5 P2 ₁ 2 ₁ 2 ₁	3.1	11.6	99	5
Uranyl 2	85.2 86.8 46.1 P2 ₁ 2 ₁ 2 ₁ or P2 ₁ 2 ₁ 2	2.9	9.5	82	4.5
Uranyl 3	85.0 85.7 100.0 P2 ₁ 2 ₁ 2 ₁	3.0	6.5	99	4.1
Mercuri 1	85.7 85.3 99.4 P2 ₁ 2 ₁ 2 ₁	3.5	11.7	98	5
Mercuri 2	85.4 85.1 48.8 P2 ₁ 2 ₁ 2 ₁ or P2 ₁ 2 ₁ 2	3.5	11.9	97	3
Mercuri 3	85.5 85.9 101.1 P2 ₁ 2 ₁ 2 ₁	2.6	8.8	99.5	8

None of these derivatives show obvious peaks in the Harker sections of anomalous Patterson or isomorphous difference Patterson maps. The data are still analysed.

We had absolutely no problems with ID29. We found the instrument very user friendly and our small crystals diffracted very well compared to their sizes. The number of crystal tested and collected was optimal.