



Experiment title: Structure Determination of mammalian chitinase YM1		Experiment number: LS1672
Beamline: ID14-1	Date of experiment: from: 19/02/2000 to: 20/02/2000	Date of report: 18/08/2000 <i>Received at ESRF:</i> 28 AOUT 2000
Shifts: 1	Local contact(s): Hassan Berhali	

Names and affiliations of applicants (* indicates experimentalists):

Richard William Stockley *

Neil McDonald

Department of Crystallography

Birkbeck College

London WC1E 7HX

England

Report:

YM1 is a murine chitinase which is over expressed by certain haematopoietic cells in various immuno-deficient mice. This protein can form protein crystals *in vivo* in areas of infection, particularly the gut and lung. We feel that this protein has an important role in the primitive immune response and warranted further study. It is an unusual situation to obtain protein that crystallizes so readily.

Purified material can be readily solubilized at basic pH (>8.5) and easily recrystallized at acidic pH (<7.0). The crystals obtained were hexagonal plates measuring 60um x 40 um x 5um. Since it is expressed *in vivo* this ruled out a seleno-methionine approach and phase determination would involve a MIR approach.

Previous to this trip a native data set had been obtained to 2.2Å at the Daresbury laboratory synchrotron and the space group had been determined to be P2₁. Molecular replacement methods using plant and bacterial chitinase structures had failed so the aim of this trip was to obtain a higher resolution native data set and screen for potential heavy metal atom soaks to aid in structure determination.

Four data sets were obtained during this visit. All were measured over 180° and are summarised below.

Native Data – 1.65 Å resolution

Samarium Chloride derivative – 2.7 Å resolution

Ethyl Mercury Chloride Derivative – 2.9 Å resolution

Platinum Cyanide – 3.3 Å resolution

The native data set was an excellent result and was a great improvement on previous data obtained, unfortunately the mercury and platinum soaks showed low levels of incorporation. The samarium soak was hampered by poor quality crystals (with extensive satellites) but subsequent data sets have shown this to be an excellent derivative.

We hope that the samarium chloride, and mercury chloride derivatives and a recently collected ytterbium derivative in conjunction with the excellent native data set obtained at the ESRF provides sufficient phase information to solve this structure.