ESRF	**Experiment title:** A quick solution: *ab initio* structure determination of a 19 kDa metalloproteinase using ACORN	**Experiment number**: LS-1673
Beamline: ID14-2	**Date of experiment**: from: 25/03/00 to: 27/03/00	**Date of report**: 30/08/01
Shifts: 1	**Local contact(s)**: Ed Mitchell	*Received at ESRF:*

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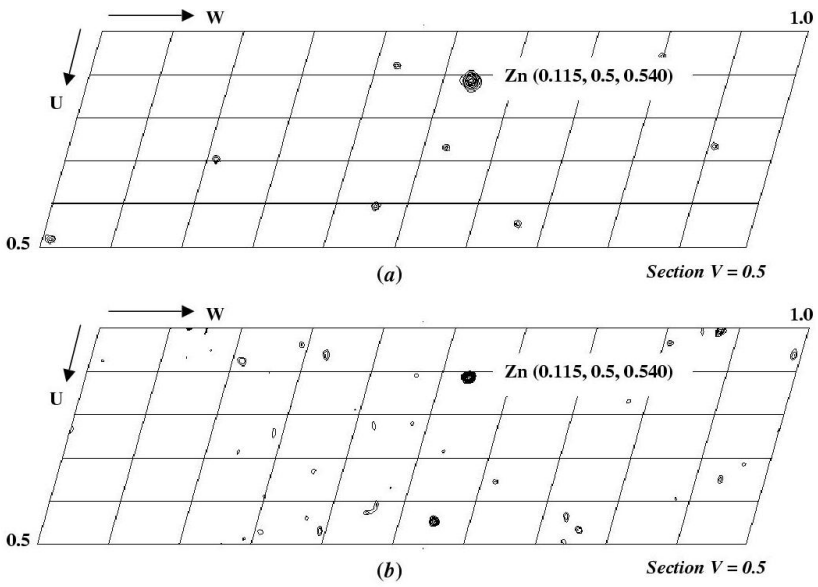
Report:

Deuterolysin from *Aspergillus oryzae* is a zinc metalloproteinase consisting of 177 amino acids, with a molecular weight of approximately 19 kDa. Deuterolysin crystals belong to the space group $P2_1$, with unit cell dimensions a = 38.4, b = 34.8, c = 60.3 Å, β = 106.0°. Data were collected for the enzyme at atomic resolution on beamline ID14-2 in March 2000. The data are 99.6% complete and the overall R_{merge} for data between 30.0 – 1.0Å is 5.2% and 24% in the highest resolution shell.

The high resolution allowed the structure to be solved with the direct methods program ACORN, using the co-ordinates of the Zn atom as a starting point. The position of the zinc atom could be determined either from the anomalous difference Patterson or the sharpened native Patterson.



Anomalous difference Patterson

Sharpened native Patterson

The phases obtained from ACORN were of sufficient quality to allow automated building to be carried out in ARP/wARP. Minimal manual rebuilding of the model was required

and the structure determination was completed using the maximum likelihood refinement program REFMAC. The whole process, starting from the processed and merged data and ending with a refined model, required less than 6 hours of computational time.

The structure has now been accepted for publication in *Acta Crystallogr. Sect D.*