## MS094.004

## **Microsymposium**

The structure of the cyanide dihydratase (CynD) from Bacillus pumilus

Bryan Trevor Sewell<sup>1</sup>, Achilleas Frangakis<sup>2</sup>, Andani Mulelu<sup>1</sup>, Julian Reitz<sup>1</sup> <sup>1</sup>Centre For Imaging And Analysis, University Of Cape Town, Cape Town, South Africa, <sup>2</sup>Buchmann Institute for Molecular Life Sciences, Goethe University, Frankfurt, Germany E-mail: trevor.sewell@uct.ac.za

We present the first structure of an intact, helical nitrilase. It was determined at a resolution of 3.2Å by cryo-electron microscopy. The locations of residues 3-319 (of a total of 330) were clearly interpretable in the electric potential maps. The enzyme was engineered for increased thermostability by means of the following mutations: Q86R+H305K+H308K+H323K. This combination resulted in stable active fibres that were ideal for image processing.

We have visualized the carboxy-terminal "tail" (residues 278-319) that was absent in the structure of a fragment of a homologous nitrilase from Synechocystis sp. PCC6803 (Zhang et al, 2014). This plays an important role in stabilizing the helical structure through multiple interactions, both at the interfaces between the monomers and with the "tails" of other monomers on the inside of the helix.

The active site is different to that of the homologous amidases and these differences may ultimately give insight into the mechanisms of both nitrilases and amidases.

Zhang, L., Yin, B., Wang C., Jiang, S., Wang, H., Yuan Y.A. & Wei, D. (2014) J Struct Biol, 188, 93–101.



Keywords: Nitrilase, helical reconstruction, cyanide dihydratase