A Three-dimensional model of the nitrilase from *Rhodococcus rhodochrous* J1 and highlighting the effect of mutations on structure.

[1]**Thuku R.N** and [1]Sewell B.T.

[1]Electron Microscope Unit, University of Cape Town, Rondebosch 7700, South Africa.

Enzymes in the nitrilase superfamily[1] are expressed widely in prokaryotes and eukaryotes. Nitrilases hydrolyze nitriles to the corresponding carboxylic acid and ammonia. The nitrilase from *R.rhodochrous* J1 is reported to exist as an inactive dimer in absence of substrate, but forms an active oligomer in presence of benzonitrile[2]. Structural alignment of its sequence against known structures in the PDB using GenTHREADER produced four structures of distant homologues with an average sequence identity of 19%, which revealed a conserved $\alpha\beta\beta\alpha$ fold with poor conservation of the loops. Two significantly long insertions in its sequence could contribute to the postulated spiral-forming surface C. Association across this surface is thought to be responsible for the structures of the cyanide degrading enzymes from *Pseudomonas stutzeri* AK61[3], *Bacillus pumilus* C1, and *Gloeocercospora sorghi*, which form spirals of sizes 14, 18, and long fibres respectively. The model has been used to interpret previous site-directed mutagenesis studies on nitrilases. Ultimately, we aim to use it as a basis for interpreting its quaternary structure yet to be solved by single particle reconstruction methods.

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