[MS11 - 05] Structure of arylamine N-acetyltransferase from *M. tuberculosis*: Triumph over Adversity.

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Arylamine *N*-acetyltransferase from *Mycobacterium. tuberculosis* (TBNAT) plays an important role in the intracellular survival of the microorganism inside macrophages. Medicinal chemistry efforts to optimise TBNAT inhibitors against the enzyme have been hampered by the lack of a 3D-structure of the enzyme. Here we report the first structure of TBNAT determined using a lone crystal produced using cross-seeding with the homologous protein from *Mycobacterium marinum.* Despite the similarity between the two enzymes (74% sequence identity), they show distinct physical and biochemical characteristics. The structure elegantly reveals the characteristic features of the protein surface as well as details of the active site of the TBNAT relevant to drug discovery efforts. The crystallographic analysis of diffraction data presented many challenges, since the crystal was twinned and the habit possessed pseudo-translational symmetry. Molecular replacement was carried out in P1 and 16 molecules in the unit cell. From this, the space group was then found to be $P2_1$ (cell a=96.5 Å, b=139.2 Å, c=96.51 Å, β=91.2º) with a twinning fraction of 0.43 (twin law: l, -k, h).

[1] Abuhammad A., Lowe E.D., McDonough M.A., Shaw Stewart P.D., Kolek S.A., Sim E., Garman E.F. Acta Cryst D (2013): 69 (8).

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