

**P015** Use of computational chemistry techniques to assign chemical species from the reductive half-reaction of AADH  
**Jiayun Pang, Samuel De Visser, Michael Sutcliffe, and Nigel Scrutton**

*Manchester Interdisciplinary Biocentre, 131 Princess Street, Manchester, M1 7DN*

The tryptophan tryptophyl quinone (TTQ)-dependent quinoprotein aromatic amine dehydrogenase (AADH) metabolises primary aromatic amines, with the electrons released transferred from AADH to the type I blue copper protein azurin. The reductive half-reaction of AADH occurs via a multi-step mechanism involving several proton transfers. Previous kinetic studies and computational studies have shown that the substrate oxidation is dominated by ground state hydrogen tunneling, which implicates thermally induced vibrational motion of the protein scaffold in the formation of reaction intermediates. However, there is a lack of kinetic or mechanistic information regarding the interconversion of these intermediates. To characterise the vibrational motions, Gaussian Oniom type quantum mechanical /molecular mechanical (QM/MM) calculations – geometry optimisation and in particular frequency calculations – of the two main intermediates based on high resolution crystallographic structures have been performed. The identified key vibrational frequencies, linked to the information obtained from experimental FTIR spectroscopy, provide a detailed picture at the atomic level of the nature of the reaction intermediates in the reductive half-reaction of AADH.