

UniCat Colloquium

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The combination of resonance Raman spectroscopy and Molecular Dynamics Simulations to understand the role of the distal polar cavity residues of Thermobifida fusca hemoglobin

The truncated hemoglobin of *Thermobifida fusca* (Tf-trHb) is the first thermostable truncated hemoglobin to be identified (1). In common with other bacterial truncated hemoglobins, this protein displays genuine peroxidase activity (2). The polarity of the Tf-trHb distal cavity is intermediate between that of vertebrate hemoglobins and heme-containing peroxidases (3), being characterized by a highly polar distal environment in which TrpG8, TyrCD1, and TyrB10 provide three potential H-bond interactions to stabilize the incoming ligands. The role of these residues has been recently addressed by studying the interaction of different exogenous ligands with the WT protein and a combinatorial set of mutants, involving these distal polar residues. While CO (3), F- (4,5), and HS- (6) ligands are stabilized by TrpG8 and TyrCD1 via strong H-bonds, TyrB10 is involved, albeit through an indirect H-bond, only in the stabilization of the OH- ligand (7). In fact, UV-Vis, RR, and EPR spectroscopy together with MD simulations of the mutated proteins, allowed us to conclude that the OH- anion establishes three H-bonds at alkaline pH, with TrpG8, TyrCD1 and with a water molecule H-bonded to TyrB10. In the present work, the data obtained for different anionic ligands will be compared and discussed in terms of the different capability of the TyrB10 and TyrCD1 residues to act as hydrogen bond donor or acceptor, and therefore, in their possible roles in the peroxidase activity.

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TU Berlin, Institute of Chemistry
Straße des 17. Juni 115, 10623 Berlin

Building C, Lecture Hall C 264

Prof. Hildebrandt (TUB)

Organizer

Coffee and cake will be served 30 minutes before the lecture. Guests are cordially invited to attend!
Prof. Dr. Matthias Driess - Chair of the Cluster of Excellence UniCat - www.unicat.tu-berlin.de



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