Domain motions in the mercuric ion reductase MerA

M. Sharp [1], M. Ohl [2], R. Biehl [2], M. Monkenbusch [2], D. Richter [2],
S. Miller [4], I. Harwood[4] , R. Nauss[4]
A. Johs [3], Z. Yi [3], H.B. Guo [3], J. Parks [3], J.C. Smith [3]

[1] European Spallation Source, Sweden;
[2] JCNS-1 & ICS-1, FZJ, Germany;
[3] Oak Ridge National Laboratory, USA
[4] University of California, USA

Bacterial resistance to inorganic and organic mercury compounds is mediated by the *mer* operon, a suite of genes typically located on transposons or plasmids. The *mer* operon consists of several structural genes encoding proteins involved in Hg(II) import, Hg(II) reduction and proteolysis of organomercurials[1,2].

We have chosen to focus on the structure and function of the mercuric ion reductase MerA, an enzyme responsible for catalyzing the NADPH-dependent reduction of Hg(II) to uncharged, and much less harmful, Hg(0). This enzyme consists of a large homodimeric catalytic core unit (MerA) which is connected to two small N-terminal domains (NmerA) by flexible linkers, see Figure 1. The functional role of NmerA domain for the reduction of mercury is not fully understood, but the homology of NmerA to other metallochaperones and its high affinity for Hg(II) mediated by a pair of cysteines suggests that it plays a role in acquiring and transporting Hg(II) to the catalytic core for reduction[2]. For this reason it is important to understand the internal dynamics of this protein, in particular the relative motions of the NmerA domains relative to the core of the enzyme. It is not clear whether statistically random processes or internal modes make up the dominant part of the internal dynamics. We addressed this question using neutron spin echo spectroscopy, a technique which has previously been used to gain valuable insights into the internal dynamics of proteins.[3] Our results reveal long timescale domain motions and shed light on the role of the long flexible linkers for the function of MerA.

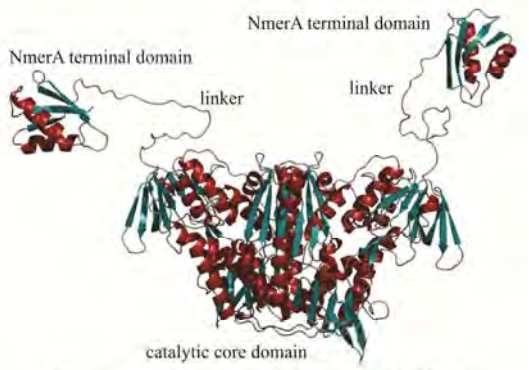

Figure 1: ribbon diagram of full-length MerA

References

1. A.O. Summers, *J. Bac.*, **1992**, *174*, 3097
2. T. Barkay *et al*, *FEMS Microbio. Rev.*, **2003**, *27*, 355
3. R. Biehl *et al*, *Phys. Rev. Letters*, **2008**, *101*, 138102