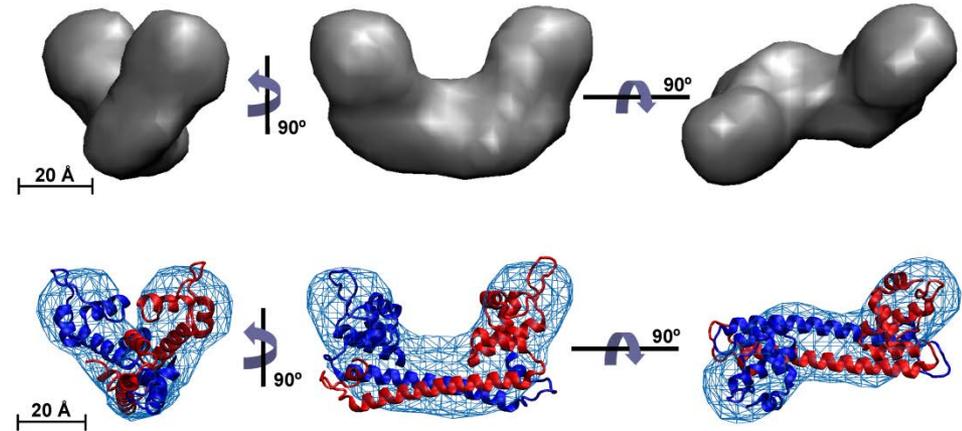


Structure and Conformational Dynamics of the Metalloregulator MerR upon Binding of Hg(II)

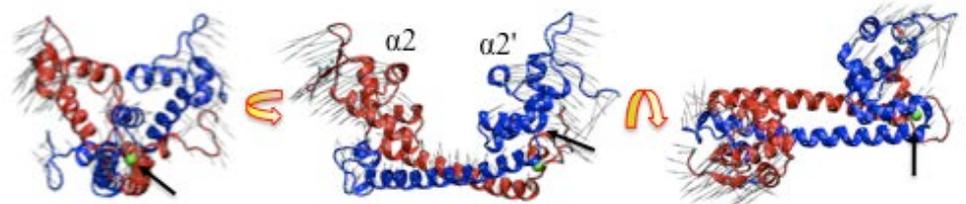
Contact: **Jeremy C. Smith** (smithjc@ornl.gov, 865-574-9635)

DOE/Office of Science/Biological & Environmental Research

- Many bacteria living in contaminated environments possess a mercury resistance (*mer*) system, which is regulated by MerR.
- Combined experimental (small-angle X-ray scattering, SAXS) and computational (molecular dynamics, MD) studies were used to determine the structure and dynamics of MerR bound to mercury.
- MD simulation results agree well with SAXS experiments (top right) and provide atomic detail.
- Simulations reveal large-amplitude domain opening-and-closing of mercury-bound MerR (bottom right).
- Domain motions in MerR are thought to play an important role in initiating DNA transcription of mercury resistance genes in the presence of nanomolar levels of mercury in bacterial cells.



The SAXS envelope shape of Hg(II)-bound form of MerR (top) superimposes well with the atomistic model from the MD simulation (bottom)



Largest-amplitude modes from principal component analysis of the MD trajectories of Hg(II)-MerR

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Scientists at Oak Ridge National Laboratory have used a combined experimental and computational approach to determine the structure and molecular dynamics of a critical component of mercury resistance—the metalloregulator MerR—when mercury binds to it. The studies used small-angle X-ray scattering and molecular dynamics simulations to provide clues on how a single mercury ion can induce a significant change in the structure of MerR. This structural change turns on DNA transcription of the genes for several other proteins and enzymes, which ultimately rid the microbes of toxic mercury species.

Guo, H.-B., A. Johs, J.M. Parks, L. Olliff, S.M. Miller, A.O. Summers, L. Liang and J.C. Smith. 2010. Structure and conformational dynamics of the metalloregulator MerR upon binding of Hg(II). *J. Mol. Biol.* 398:555-568 (doi:10.1016/j.jmb.2010.03.020).