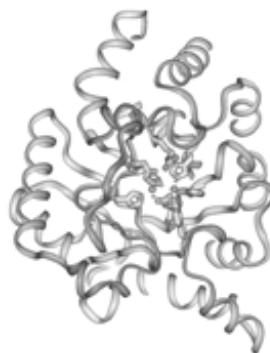


A Comparison of Bromide Ion "Quick-Soak" and Se-Met Derivatives for Structure Determination of a Novel Hydrolase. B. D. Santarsiero, K. Ratia, and A. D. Mesecar, The Center for Pharmaceutical Biotechnology, University of Illinois at Chicago, Chicago, IL 60607 USA.

Organophosphorus Hydrolases (OPH) degrade a number of compounds, including neurotoxins used as chemical warfare agents. A novel OPH has been studied as a target for site-directed and random mutagenesis. The native enzyme, with 333 residues, crystallizes in space group $P3_121$ with the cell dimensions of $a=61\text{\AA}$ and $c=207\text{\AA}$. In addition, a quick soak of a native crystal with KBr was used to generate a bromide ion heavy atom derivative. A MAD dataset was collected to 2.2\AA for the Se-Met derivative, and to 1.9\AA for the Br derivative. Seven Se atoms (figure-of-merit 0.59) were found using SOLVE in the first, and four partially-occupied bromide ions (figure-of-merit 0.30) were found in the latter. Both SOLVE maps are excellent, and allowed for tracing of a significant part of the structure in each: RESOLVE traced 80% of the Se-Met structure, and 67% of the Br structure. The best model has refined to $R(\text{cryst}) = 0.178$, $R(\text{free}) = 0.212$, and a FOM of 0.877 using one of the Br-derivative data sets.



We thank BioCARS for access to beamline 14. This research is supported by Office of Naval Research award N000140210956.