Supporting Information for:

On the Mechanism of the Quorum-Quenching Lactonase (AiiA) *from Bacillus thuringiensis*: 1. Product-Bound Structures

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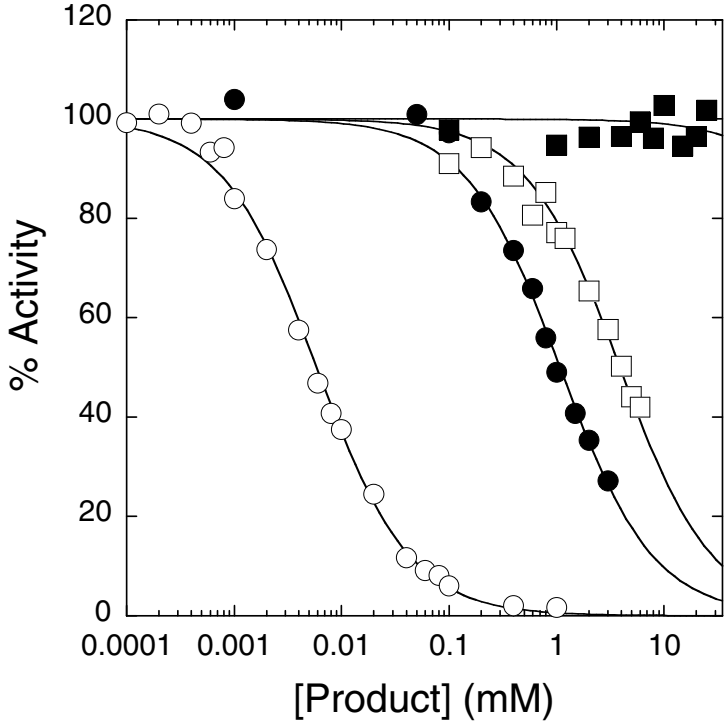
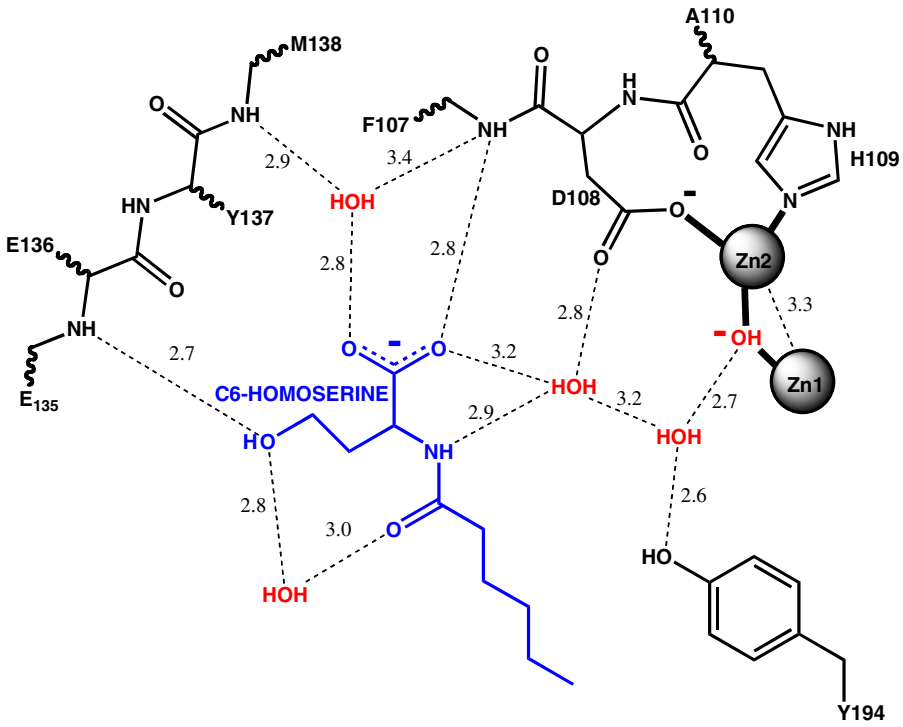
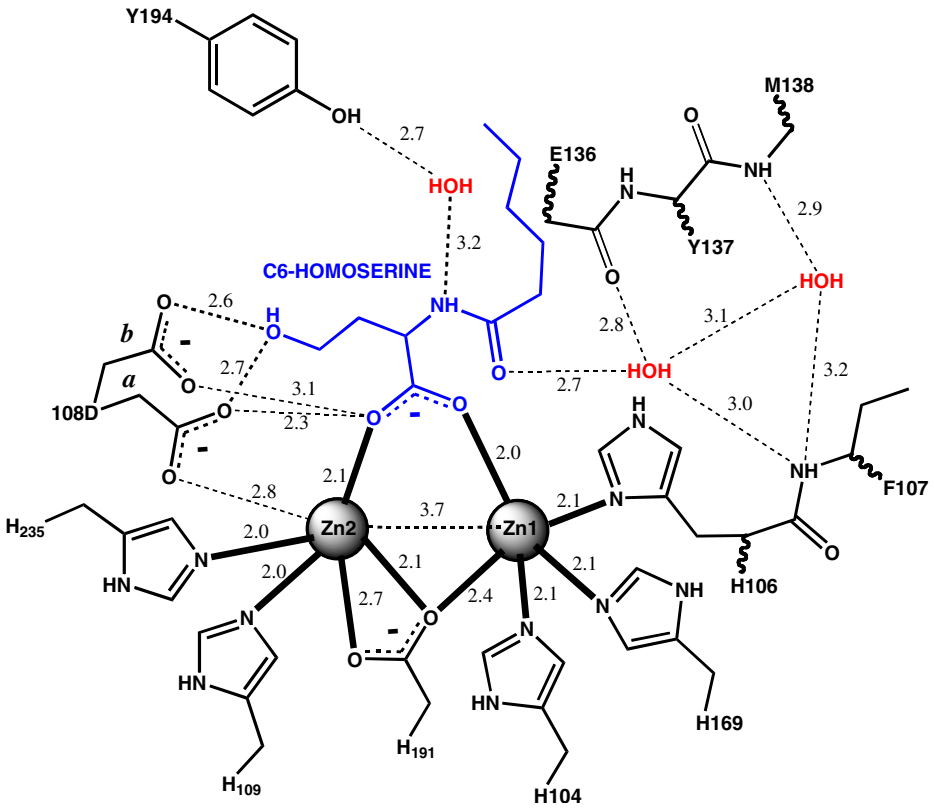


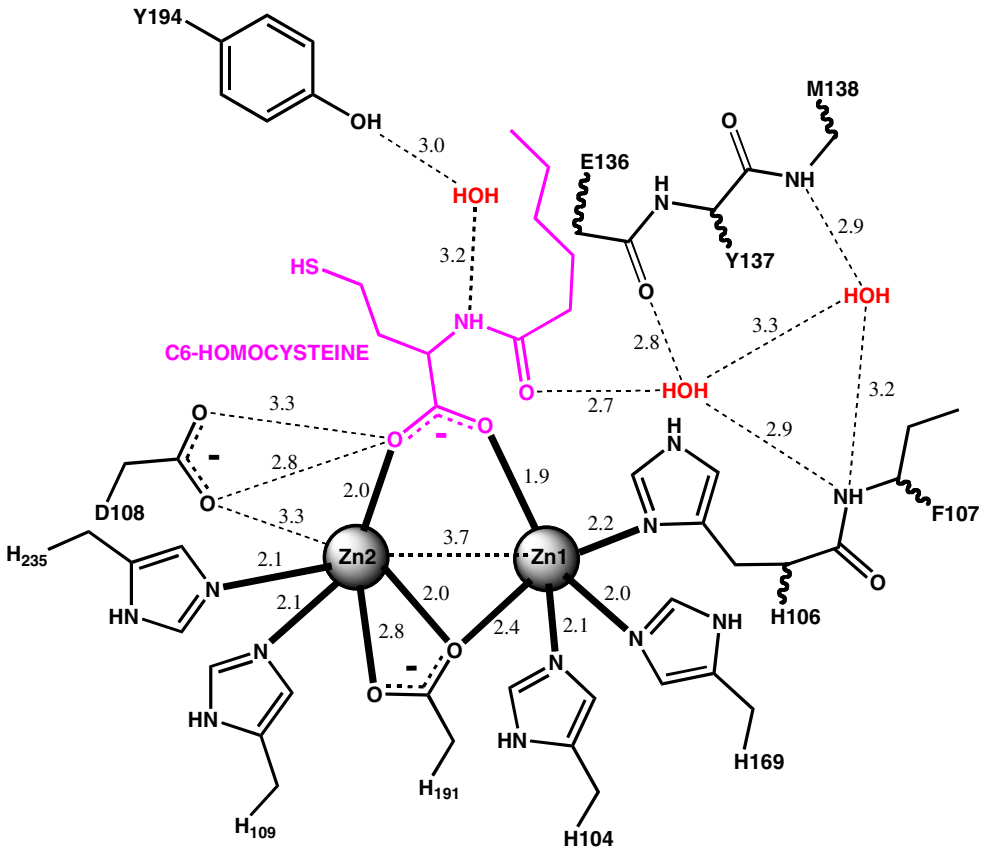
Supplemental Figure 1. Product Inhibition of AHL lactonase. Inhibition of dicadmium substituted AHL lactonase by the ring opened products C6-homocysteine (○) and C6-homoserine (□) is observed, with calculated K_i values of 3 μM and 2 mM, respectively. Inhibition of dizinc substituted AHL lactonase by C6-homocysteine (●) is observed, with an IC_{50} of 1.08 ± 0.05 mM (calculated K_i = 550 ± 25 μM). Dizinc AHL lactonase is not inhibited by C6-homoserine (■) at concentrations as high as 25 mM. The dicadmium AHL lactonase inhibition data and the materials and methods are taken from Momb, J., et al. (2006) *Biochemistry 45*, 13385.



Supplemental Figure 2. Two-dimensional Scheme for The Product-binding Site in Complex I. The C6-homoserine product is shown in blue, protein residues in black and water/hydroxide species in red. Metal coordination bonds are shown as bold lines and hydrogen bonding distances as dashed lines. Key distances are given in angstroms.



Supplemental Figure 3. Two-dimensional Scheme for The Product-Binding Site in Complex II. The C6-homoserine product is shown in blue, the protein residues in black and the water molecules in red. Two alternate conformations of D108 are shown and labeled as *a* and *b* respectively. Metal coordination bonds are shown as bold lines and hydrogen bonds as dashed lines. Key distances are given in angstroms.



Supplemental Figure 4. Two-dimensional Scheme for The Product-Binding Site in Complex III. The C6-homocysteine product is shown in purple, protein residues in black and water molecules in red. Metal coordination bonds are shown as bold lines and hydrogen bonds as dashed lines. Key distances are given in angstroms.