



**Figure 1.** Structure of the Mo-bisPGD substrate of FdhD, or how to transfer a sulfur to the molybdenum atom at the center of the substrate. The GDP moiety of Mo-bisPGD is highlighted in red.

**Keywords:** Enzyme, symmetry, sulfur transfer

## MS5-P57 Crystal structure of Csd3 from *Helicobacter pylori*, a cell-shape determining metallopeptidase

Hye Jin Yoon<sup>1</sup>, Doo Ri An<sup>2</sup>, Hyoun Sook Kim<sup>3</sup>, Se Won Suh<sup>1,2</sup>

1. Department of Chemistry, Seoul National University, Korea
2. Department of Biophysics and Chemical Biology, Seoul National University, Korea
3. College of Pharmacy, Seoul National University, Korea

email: yoonhj@snu.ac.kr

*Helicobacter pylori* is associated with various gastrointestinal diseases such as gastritis, ulcer, and gastric cancer. Its colonization of the human gastric mucosa requires high motility, which depends on the helical cell shape. Seven cell shape-determining genes (*csd1*, *csd2*, *csd3/hdpA*, *ccmA*, *csd4*, *csd5*, and *csd6*) have been identified in *H. pylori*. These proteins play key roles in determining the cell shape through modifications of the cell-wall peptidoglycan by alteration of crosslinking or by trimming of peptidoglycan muropeptides. Among them, Csd3 (also known as HdpA) is a bi-functional enzyme. Its d,d-endopeptidase activity cleaves the d-Ala<sup>4</sup>-mDAP<sup>3</sup> peptide bond between crosslinked muramyl tetra- and penta-peptides. It is also a d,d-carboxypeptidase that cleaves off the terminal d-Ala<sup>5</sup> from the muramyl pentapeptide. Here we have determined the crystal structure for this protein, revealing the organization of its three domains in a latent and inactive state. The N-terminal domain 1 and the core of domain 2 share the same fold despite a very low level of sequence identity and their surface charge distributions are different. The C-terminal LytM domain contains the catalytic site with a Zn<sup>2+</sup> ion, like similar domains of other M23 metallopeptidases. Domain 1 occludes the active site of the LytM domain. The core of domain 2 is held against the LytM domain by the C-terminal tail region that protrudes off the LytM domain. This work could serve as the foundation in discovery of novel inhibitors that would prove helpful in fighting infections by the major human pathogen *H. pylori*.

[1] An, D.R. *et al.* (2015) *Acta Cryst D* **71**, 675-686.

[2] Sycuro, L.K. *et al.* (2010) *Cell* **141**, 822-833.

**Keywords:** *Helicobacter pylori*, *csd3*, cell shape determinant, M23B metallopeptidase