

SUPPLEMENT

Crystal Structure and Mutational Analysis of Aminoacylhistidine Dipeptidase from *Vibrio alginolyticus* Reveal a New Architecture of M20 Metallopeptidases

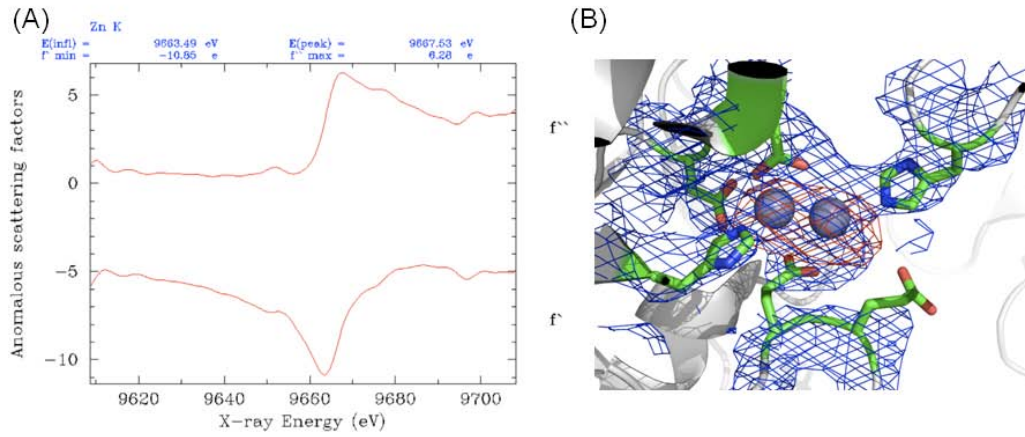
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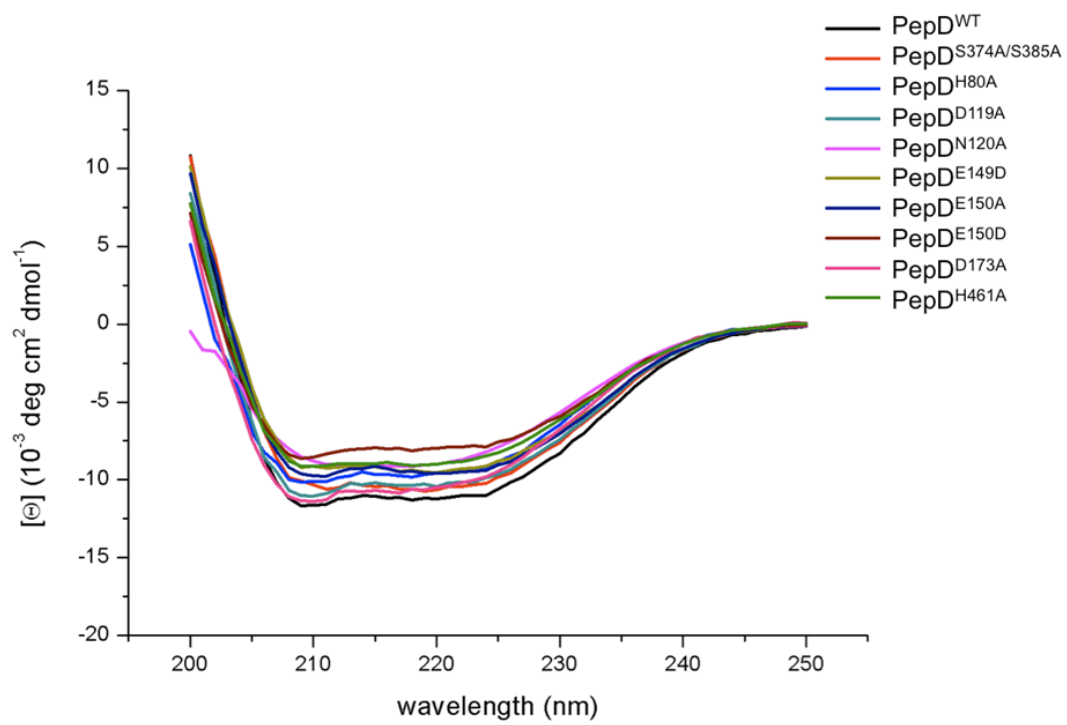
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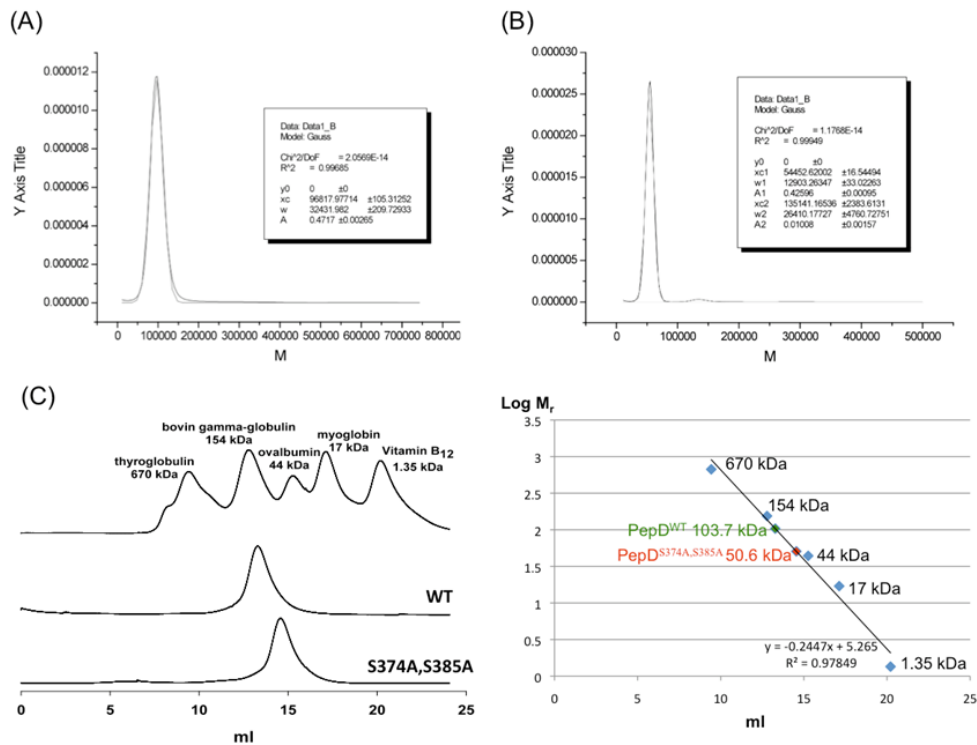
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Supplement Figure 1. The PepD zinc ions determination. (A) The absorption spectra of anomalous scattering factors for zinc ions in PepD as a function of X-ray energy. (B) The electron density map of PepD zinc ions binding site, as part of a composite-omit map contoured at 1.0σ (blue), and anomalous map contoured at 4.0σ (red).



Supplement Figure 2. The CD spectra of *V. alginolyticus* PepD wild-type and various mutants.



Supplement Figure 3. Molecular masses determination of PepD^{WT} and PepD^{S374A/S385A} mutant. Analytical ultracentrifugation determination of (A) PepD^{WT} and (B) PepD^{S374A/S385A} mutant, showing the calculated molecular weight from sedimentation coefficient (s) of approximately 96817.977 ± 105.3 g/mol and 54452.62 ± 16.5 g/mol, respectively. (C) Chromatographic separation and calibration curve for the standard proteins, PepD^{WT} and PepD^{S374A/S385A} on Superdex 200 10/300 GL column (GE HealthcareTM). In the calibration curve, the molecular mass of PepD^{WT} (green dot) and PepD^{S374A/S385A} (red dot) were determined to be 103.7 and 50.6 kDa, respectively.