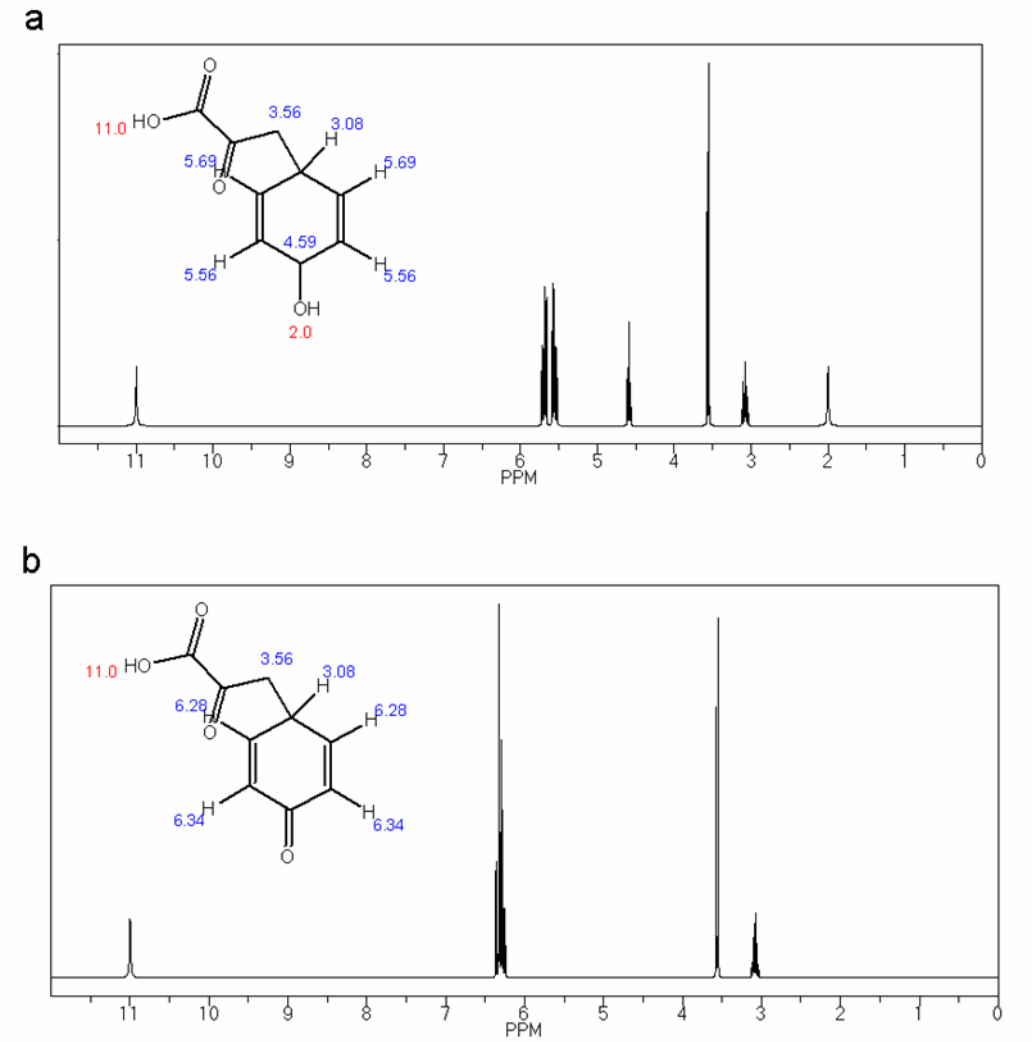
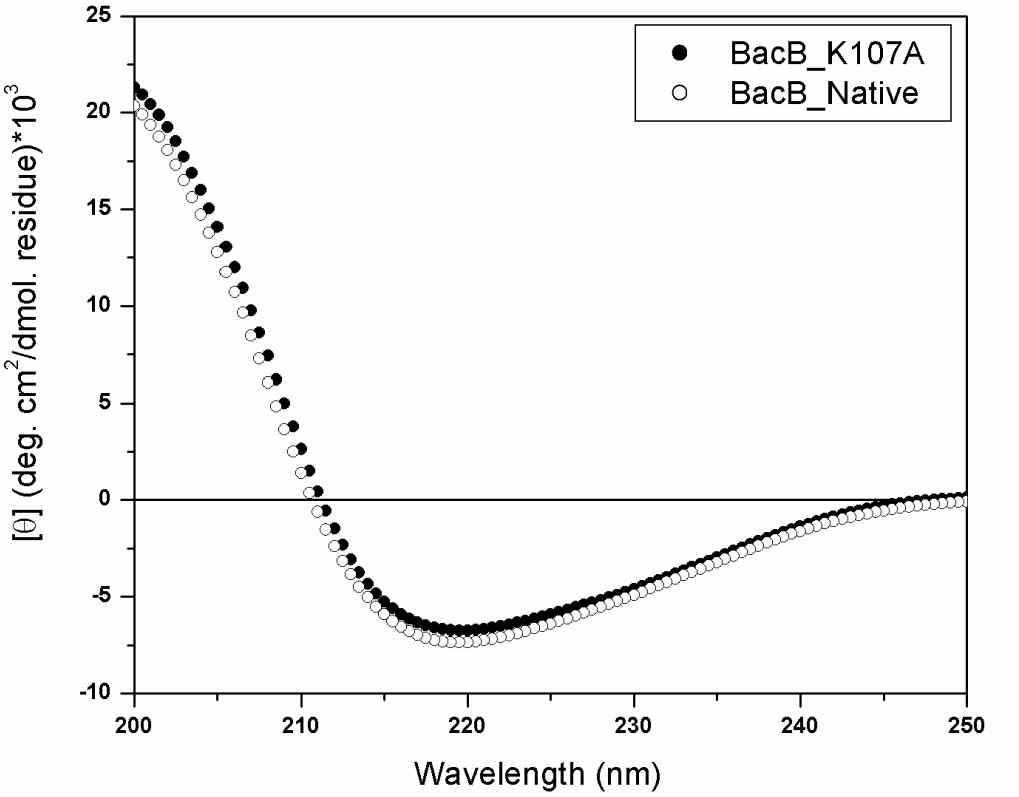
Supplementary Figure S1.



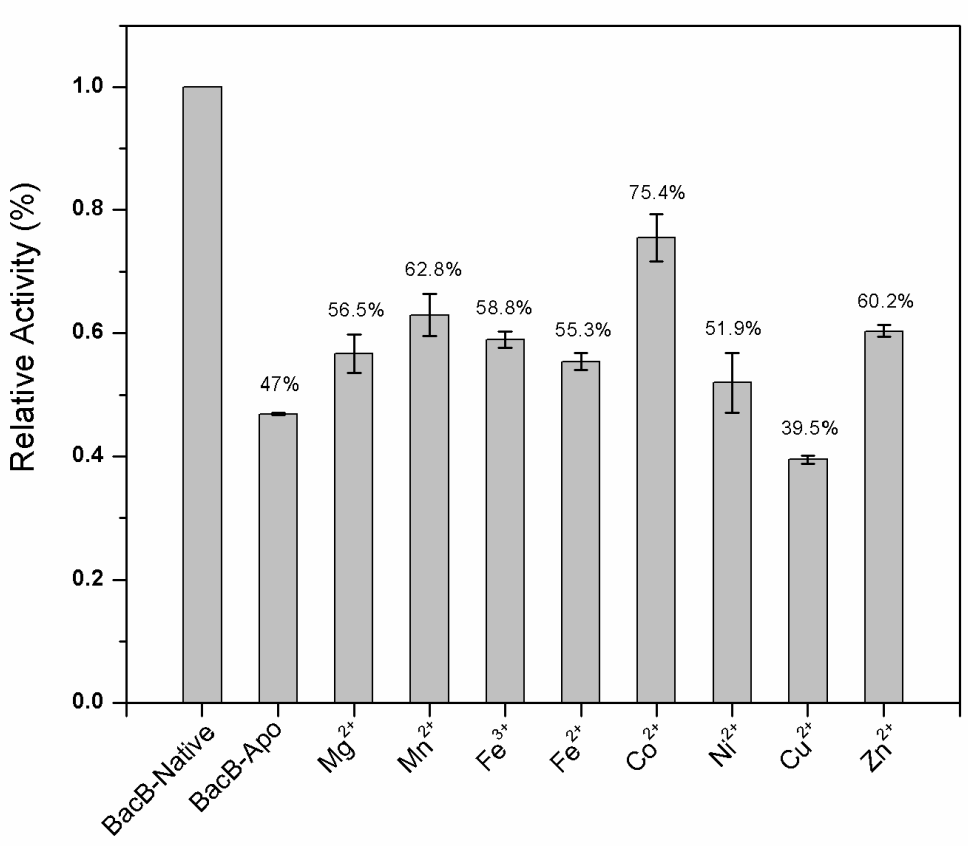
Supplementary Figure S1: Simulated ^{1}H NMR spectrum of the products obtained from BacA and BacB. a. The chemical shifts centered at 3.0 ppm and 5.6-5.7 ppm match those of the product of BacA (3-((1*r*-4*r*)-4-hydroxycyclohexa-2,5-dienyl)-2-oxopropanoic acid). **b.** The chemical shifts centered at 6.2 and 6.3 ppm match those of the product of BacB (2-oxo-3-(4-oxocyclohexa-2,5-dienyl)propanoic acid). The predicted chemical shift values are annotated on the structures.

Supplementary Figure S2.



Supplementary Figure S2. The CD spectra of BacB and the K107A mutant. Lys107 is located at the entrance to the active site of the N-terminal cupin domain. The far UV CD spectrum of the K107A mutant is similar to that of BacB. The loss of catalytic activity of the K107A mutant is thus unlikely to be due to a misfolded protein.

Supplementary Figure S3.



Supplementary Figure S3. The catalytic activity of BacB depends on the metal cofactor. In this experiment, the activity of BacB incubated with different metal ions was compared with that of the freshly purified enzyme. The activity assays were carried out as described in Materials and Methods. This experiment suggests a metal co-factor preference- Co^{2+} > Mn^{2+} > Zn^{2+} > Fe^{3+}.