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Anti-Bacterial Drug Discovery Based on Structural Chemoproteomics

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CrystalGenomics is focused on determining 3-D structures of therapeutic target proteins by X-ray crystallography and NMR. We have developed a systematic approach to increase the solubility of target protein. Based on the 3-D structure of target protein, *in silico screening* has been applied to identify chemical leads that recognize the active site of target proteins. To facilitate the lead discovery, we have developed the active site mapping technology and the drug-like chemical library specifically targeting each protein family.. Here, we determined the complex structures of *E.coli* ENR (enoyl-acyl carrier protein reductase) wild type and its G93V mutant with triclosan. We have also determined the crystal structure of the catalytic domain of *Staphylococcus Aureus* sortase and the bacterial metalloenzyme polypeptide deformylase (PDF). We believe that these results will offer valuable insights for the structure-based design of novel inhibitor.