Study of L-captopril Binding to VIM-20 by X-ray Crystallography Method

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Verona Integron-encoded Metallo-□-lactamase (VIM) is one of the families of B1 subclass of beta-lactamases (BLs) and VIM-20 is one those 74 variants of VIM. We have crystallized the VIM-20 in different crystallization conditions and succeeded in growing crystals large enough for diffraction experiments in MCSG-1 screen. The crystals were soaked into L-captopril and obtained diffraction data at 1.37 Å. The structure of VIM-20/L-captopril complex was solved by using the PHENIX and Coot software packages. The final structure featuring Rwork and Rfree values of 0.185 and 0.218 with 100% ligand occupancy has confirmed that the thiol group of the L-captopril knocks off the catalytic hydroxyl group present in the active site of VIM-20. This finding concluded that the L-captopril can inhibit VIM-20, further supported by the IC50 data.

Key words: MBLs, SBLs, Enzymes, Inhibitors, Activity Assay