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Conformational changes of nucleotide-bindings site for the antibiotics development against D-ala-D-ala ligase from *Acinetobactor baumannii*

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Acinetobacter baumannii, which is emerging as a multidrug-resistant nosocomial pathogen, causes a number of diseases, including pneumonia, bacteremia, meningitis and skin infections. With ATP hydrolysis, the D-alanine-D-alanine ligase (DDL) catalyzes the synthesis of D-alanyl-D-alanine, which is an essential component of bacterial peptidoglycan. Structural studies showed the flexible conformational changes in the ATP-binding site, more specifically both the hydrophobic nucleotide base binding site and the hydrophilic triphosphate binding site with the movement of the central domain and serine-loop. The central domain of AbDDL (DDl from *Acinetobacter baumannii*) can have an ensemble of the open and closed conformations before the binding of substrate ATP. In other DDL structures from *Xanthomonas oryzae* pv. *oryzae* and *Yersinia pestis*, the serine-loop and the ω-loop showed flexible conformations, especially the serine-loop is mainly responsible for the conformational change in substrate nucleotide phosphates. Currently, computer-aided drug design method has been actively and efficiently used. The detail catalytic mechanism and structure information will be helpful to apply the CADD method in drug discovery.

Biography

Lin-Woo Kang has completed his PhD at Johns Hopkins University School of Medicine and Post-doctoral studies from Stanford University School of Medicine. He is a Professor at Konkuk University. He has published more than 75 papers in reputed journals in the field of Structural Biology.

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