Sako Mirzaie et al., Clin Microbiol 2018, Volume 7
DOI: 10.4172/2327-5073-C1-033

Structure-based virtual screening to identify the β-lactamase CTX-M-9 inhibitors: An *in silico* effort to overcome antibiotic resistance in *E. coli*

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Recently, the quick spreads of broad-spectrum β-lactams antibiotic resistance in pathogenic strains of bacteria has become a major global health problem. These new emerging resistances cause ineffectiveness of antibiotics and increasing the severity of diseases and treatment costs. Among different and diverse resistance targets, we chose a class-A β-lactamase, CTX-M-9, with the aim of identifying new chemical entities to be used for further rational drug design. Based on this purpose, a set of 5000 molecules from the Zinc database have been screened by docking experiments using AutoDock Vina software. The best ranked compound with respect of the previously proved inhibitor compound 19 was further tested by molecular dynamics (MD) simulation. Our molecular modeling analysis demonstrates that ZINC33264777 has ideal characteristics a potent β-lactamase CTX-M-9 inhibitor. In the free form of β-lactamase, NMR relaxation studies showed the extensive motions near the active site and in the Ω-loop. However, our molecular dynamics studies revealed that in the compound 1: β-lactamase complex, the flexibility of Ω-loop was restricted.

Biography

Sako Mirzaie has completed his PhD from Science and Research Branch, Azad University. He was an experienced Assistant Professor with a demonstrated history of working in the pharmaceuticals industry. He is also skilled in bioinformatics, animal models, protein chemistry, life sciences and protein purification. He has published more than 23 papers in reputed journals and has been serving as an Editorial Board Member of repute.

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