In-silico database screening for anti-virulent-inhibitors of *staphylococcus aureus* histidine kinase

Awaad A Radwan

King Saud University, Saudi Arabia

Abstract

Bacterial histidine kinases (HKs) not only govern adaptive responses of the bacteria organisms but also these kinases are unique. So, HKs are attractive drug targets to control bacterial infections. The 3D structure of S. aureus HK was not isolated in high-resolution coordinates. Virtual screening database (VS) search is a modern tools that succeeded to discover several drugs to the market. S. aureus HKs inhibitros are promising antibiotics however, there is no drug in the market and few inhibitor compounds are reported. We were prompted to the use of database VS tools to discover novel HKs/Wak inhibitors. The homology modeling, molecular docking studies and molecular dynamics (MD) simulations were applied to construct target-ligand complex. The obtained complex was applied for VS of small molecules database to get potential active compounds against *S. aureus* HK/Walk as anti-S. aureus agents.

Biography

Awaad A Radwan has completed his PhD from Kitasato University, Tokyo, Japan in 2002. He is the professor of King Saud University, Saudi Arabia. He has over 60 publications that have been cited over 400 times, and his publication H-index is 9 and has been serving as peer reviewer member of reputed Journals.

4th World Conference on Pharmaceutical Research and Drug Management | March 15, 2021