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Druggability analysis and classification of bacterial histidine kinase

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Anti-Microbial Resistance (AMR) is becoming a real threat to humanity with a resistant strains emerging very frequently. The arising of antibiotics resistance is mainly attributed to the misuse of these agents, in addition to the decline in the development of new drugs by the pharmaceutical industry. The development of new novel antibiotics is an emerging necessity to counteract this serious phenomenon. Bacterial Histidine Kinases (HKs) are one of the most promising targets for novel antibacterial drugs. They are part of the bacterial Two-Component Systems (TCSs), the main signal transduction pathways in bacteria, regulating various processes including virulence, secretion systems and antibiotic resistance. Since mammalian histidine kinases signal transduction pathway is different than the prokaryotic one, the inhibition of those pathways could be a potential target for a novel antimicrobial agent. In this study, the druggability of histidine kinase will be assessed for several bacterial species. In this work, different histidine kinases of varies bacterial origins were assed. First we performed some extensive data mining in the Protein Data Bank (PDB) to obtain a large library of crystal structures of histidine kinases, each one of the proteins were then prepared using the Molecular Operating Environment software (MOE). Druggability assessment of the prepared histidine kinases was then carried out using SiteMap module of the Schrödinger molecular modeling suite.

Biography

Mohammad Al sorkhy is an assistant professor of cell and computational biology, Dr Al sorkhy started his career as a cell biologist with interest in protein interactions. Then he started to shift towards computational biology to answer his major question about protein interactions.

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