Contribution ID: **98** Type: **Poster**

Computational analysis of FecA protein interactions: A docking and molecular dynamics approach

Klebsiella pneumoniae is one of the most common Gram-negative bacteria that cause nosocomial infections, including meningitis, pneumonia, and urinary tract infections. Traditionally, beta-lactam (β-lactam) based antibiotics, such as penicillin, are used to treat K. pneumoniae infections. However, these therapies, including other antibiotics, are losing their effectiveness because the bacteria produce other types of biomolecules that render the medications ineffective. Therefore, new targets are probed in Klebsiella pneumoniae that are essential for microbial survival and pathogenesis. In their microenvironments, microbes produce and release siderophores, which bind and dissolve precipitated or otherwise inaccessible iron. The FecA protein is a desirable target for the development of new treatments because of its involvement in KP pathogenicity. Researchers can potentially lessen the pathogenicity of the bacteria by developing techniques to interfere with the mechanisms of iron uptake in KP. This study focusses on the FecA protein, examining its potential as an inhibitory target and its therapy implications for KP. Lopinavir, Inosine, Famciclovir, Entecavir, and Abacavir were the five small molecule ligands that showed the highest inhibitory potential for the FecA protein. The current study's findings support lopinavir as a possible medication against Klebsiella FecA protein, lopinavir's inhibitory effect on Fec A protein implies that it is more effective at preventing iron from binding to FecA protein. The calculated binding energy of lopinavir to the FecA protein is -10.7 kcal/mol. Further, molecular dynamics studies will be carried out to further support the above results.
Key words: FecA protein, Klebsiella pneumoniae, Iron acquisition, Siderophore, Lopinavir, Molecular docking, Molecular dynamics

Authors: C D, Dr.Vandana (School of Sciences, Jain (Deemed-to-be University), Bangalore); Dr S, Krupa (School of Sciences, Jain (Deemed-to-be University), Bangalore); Dr C, Sandeep Kumar (School of Sciences, Jain (Deemed--to-be University), Bangalore); Mr P S, Sanjeeva (JSS Academy of Higher Education and Research, Mysuru)

Presenter: Mr P S, Sanjeeva (JSS Academy of Higher Education and Research, Mysuru)

Track Classification: Biological Sciences