In Silico approach to find out most influential protein of lipopolysaccharide biosynthesis pathway of *Pseudomonas aeruginosa* using a graph theoretic approach and validation of result using KEGG graph packages

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Abstract: *Pseudomonas aeruginosa* is an opportunistic human pathogen that causes chronic infections in patients with cystic fibrosis and is the predominant cause of death by Gram-negative bacteria. Through analyzing the metabolic network of *Pseudomonas aeruginosa*, lipopolysaccharide biosynthesis pathway is one of the virulent pathways of this organism for the reason that it contributes an important function on host-bacterium interactions. Using graph theory, lipopolysaccharide biosynthesis sequence of *Pseudomonas aeruginosa* is examined and consequently the most influential proteins are identified. The digraph representing this biological network provides information in a given pathway as far as the connectivity of each protein or metabolite is concerned, thus offering an insight into the significance of a range of components in the pathway, which can be studied quantitatively. Likewise, the most prominent set of proteins is recognized by making use of a graph theoretic algorithm, which when eliminated could in turn trigger a significant impact on the biosynthesis sequence. Furthermore, this set of proteins can serve as drug targets. In the present study, the metabolic network of *Pseudomonas aeruginosa* is constructed and the lipopolysaccharide biosynthesis sequence is investigated for potential drug targeting. In fact the KEGG PATHWAY database is used to create the metabolic network and is nonetheless subjected to graph theoretical analysis. What is more, the nearness index of a protein is used to determine how dominant the protein is on other components in the network, hence allowing the proteins in a pathway to be ordered according to their nearness indices. As a final point, the KEGG graph package is used to validate the result where the most influential protein is found which is also prevalent in previous work. A method for identifying the most strategic nodes to target for disrupting the metabolic networks is shown, aiding the development of new drugs to combat this deadly disease.

Keywords:
Opportunistic, Lipopolysaccharide biosynthesis pathway, Graph theoretic approach, Metabolic network, Nearness index