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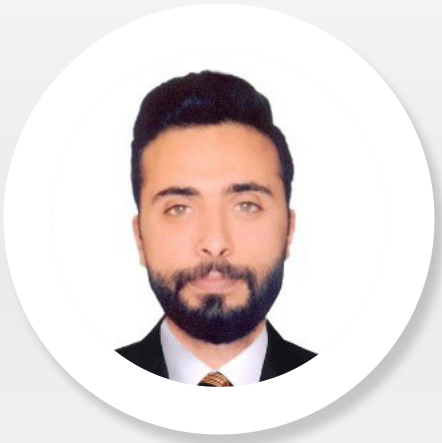
Discovery of natural autoinducers mimics by *Pseudomonas aeruginosa* LasR quorum- sensing signaling receptor via structure based virtual screening



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The human pathogen *Pseudomonas aeruginosa* co-ordinates the expression of virulence factors using quorum sensing, a signaling cascade triggered by the activation of signal receptor by small molecule autoinducers. A molecular study was made for recognition of autoinducers mimics by LasR signaling receptor of *P. aeruginosa* revealed that, the ligand binding domain is N-3-oxo-dedecanoyl homoserine lactone and a new class of triphenyl compounds that are structurally distinct from the binding domain that interact specifically and potently with LasR receptor (Muh et al., 2006). A structure based virtual screening for a database of 5135 isolated and identified natural compounds were docked via three different placement methods and rescored by two different scoring functions and 3D similarity matching against a triphenyl ligand for LasR receptor. The study revealed 42 natural compounds and the majority were tricyclic aromatic that are substituted with one or two isoprene units (fused or separately attached), These compounds present a new class of prenylated cyclic natural autoinducers such as prenylated xanthones, flavones,… etc. that covers the long chain of the binding domain and the aromatic feature of triphenylated compounds. Literature screening showed that 13 compounds were of potent antibacterial activity against resistant strains such as (*Clostridium, MRSA*, and *Mycobacterium*). Molecular binding study was made to confirm the suitability for LasR binding and the required interactions with receptor site amino acids.

Biography

Mohamed Zaineldain is Teaching Assistance in the Department of Medicinal Chemistry at the Faculty of Pharmacy, October 6 University. His research is focused on Drug Design, Virtual Screening and Molecular Modeling. Research projects were in mechanism specifying and finding new targets to address new natural or synthetic drug discovering needs in the areas of cancer therapy and overcoming microbial resistance.

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