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Structure-Based Drug Design of Daptomycin, Antimicrobial lipopeptide

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Abstract : Contagious diseases enact severe public health problems and have upsetting consequences. The cyclic lipopeptides explained by bacteria Bacillus, Paenibacillus, Pseudomonas, Streptomyces, Serratia, Propionibacterium and fungus Fusarium are very critical in confining the pathogens. As the degree of drug resistance upsurges in unparalleled manner, the perseverance of searching novel cyclic lipopeptides is being professed. The intense study has shown the implication of these bioactive compounds extending beyond antibacterial and antifungal. Lipopeptides, composed of single units of peptide and fatty acyl moiety, show broad spectrum antimicrobial effects. Among the surplus of cyclic lipopeptides, only few have materialized as strong antibiotics. For their functional vigor, polymyxin, daptomycin, surfactin, iturin and bacillomycin have been integrated in mainstream healthcare. In our work daptomycin has been a major part of antimicrobial resource since the past decade. Daptomycin, a cyclic lipopeptide consists of 13-member amino acid with a decanoyl side-chain. This structure of daptomycin confers it the mechanism of action through which it forms pore in the bacterial cell membrane resulting in the death of cell. Daptomycin is produced by Streptococccus roseoporus and acts against Streptococcus pneumonia (PSRP), methicillin-resistant Staphylococcus aureus (MRSA) and vancomycin-resistant enterococci (VRE). The PDB structure and ligands of daptomycin are available online. The molecular docking studies of these ligands with the lipopeptides were performed and their docking score and glide energy were recorded.

Keywords : daptomycin, molecular docking, structure-based drug design, lipopeptide
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