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A homology model of *Staphylococcus aureus* phenylalanine tRNA synthetase: Active site analysis and docking interactions

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Increased resistance of MRSA (Multidrug Resistance Staphylococcus Aureus) to anti-infective drugs is a threat to global health. So anti-infectives with novel mechanisms must be developed. Aminoacyl-tRNA Synthetases (aaRSs) are essential enzymes to protein biosynthesis as they catalyze the attachment of amino acid to its cognate tRNA molecule. Phenylalanine tRNA Synthetase (PheRS) is a unique enzyme of aaRSs family, it is an (αβ)2 tetrameric enzyme composed of two alpha subunits (PheS) and two larger beta subunit (PheT). Our potential target in the drug development for the treatment of MRSA infections is the phenylalanine tRNA synthetase alpha subunit that contains the binding site for the natural substrate. There is no crystal structure available to *S. aureus* PheRS enzyme, therefore comparative structure modeling is required to establish a putative 3D structure for the required enzyme enabling development of new inhibitors with greater selectivity. The *S. aureus* PheRS alpha subunit homology model was constructed using Molecular Operating Environment (MOE) software. *Staphylococcus haemolyticus* PheRS was the main template while Thermus thermophilus PheRS was utilized to predict the enzyme binding with tRNA. The model has been evaluated and compared with the main template through Ramachandran plots, Verify 3D and ProSA. The query protein active site has been predicted from its sequence using a conservation analysis tool. Docking suitable ligands using MOE into the constructed model was used to assess the predicted active site. The docked ligands involved the PheRS natural substrate (phenylalanine), several described *S. aureus* PheRS inhibitors and phenylalanyl-adenylate analogue.

Biography

Samar Said Mahmoud Mohamed Elbaramawi has completed her Master degree in 2014 from Faculty of Pharmacy, Zagazig University, Egypt. She is an Assistant Lecturer of Medicinal Chemistry, Faculty of Pharmacy, Zagazig University, Egypt. Currently, she is a PhD student at School of Pharmacy and Pharmaceutical Sciences, Cardiff University, Cardiff, United Kingdom through a joint supervision scholarship between Zagazig University and Cardiff University. She has published five papers in reputed journals

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