

In silico molecular modelling and docking studies on leukocidin LUKD in *Staphylococcus aureus*

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Methicillin Resistant *Staphylococcus aureus* (MRSA) infection is one of the most prevalent infection among the bacterial infections in animals as well as humans and are resistant to most of the potential antibiotics. The existing drugs are not sufficient to control and cure the infection. Pantone Valentine Leukocidin (PVL), a β -pore forming cytotoxin, of prophage origin that helps MRSA to obtain the nutrient from host cell by oozing out the cell contents, increases its virulence. It targets phagocytes, especially polymorphonuclear neutrophils (PMNs), and also causes necrotising pneumonia. In silico docking provide a platform to study the interaction between the antimicrobial compounds and PVL. But no 3D molecular structure is available for PVL so far. Considering the above, the present study is focused to model a template for the protein and to find out the potential inhibitor for the PVL by interacting the available antibacterial compounds with the predicted active sites. We obtained γ -hemolysin as the template for PVL with 90% query coverage and 77% identity through BLAST. The active sites are predicted by Q-Site Finder and are docked with existing antibacterial compounds using ArgusLab. Based on docking energy and hydrogen bond interaction, diathymosulfone, myrophine, andrimid, beclobrate and probucol are identified as best antibacterial compounds to be used as drugs against PVL containing MRSA.

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Development of ISSR and RAPD markers for authentication of *Centella asiatica* and *Bacopa monnieri*

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Herbal medicine has been enjoying renaissance among the customers throughout the world. Due to the complex nature and inherent variability of the chemical constituents of plant-based drugs, it is difficult to establish quality control parameters. The commercial *Bacopa monnieri* drugs are frequently adulterated with *Centella asiatica* as both are sold in the market by the name of 'Brahmi'. This work using two *Centella asiatica* and one *Bacopa monnieri* accession for development of species specific markers for both species. *Bacopa monnieri* a member of the Scrophulariaceae family is a traditional Ayurvedic herb used as a brain tonic to improve memory and learning, the entire plant is used medicinally *Centella asiatica* belongs to family apiaceae enjoys considerable reputation in Indian system of medicines. Morphological as well as biochemical markers used in the authentication of herbal drugs have many limitations due to the impact of environmental conditions. The molecular approach for the identification of plant varieties/genotypes seems to be more effective than traditional morphological markers because it allows direct access to the hereditary material and makes it possible to understand the relationships between individuals. In this study, the ISSR (Inter simple sequence repeat) and RAPD (Random amplified polymorphic DNA) techniques were employed for authentication of *Centella asiatica* and *Bacopa monnieri*. Thirty primers in the ISSR and thirty eight in RAPD analysis were screened for identification of genuine samples using the DNA isolated from the leaf samples. Out of 30 only sixteen ISSR primers were found amplifiable and in RAPD analysis twenty two were amplified with both species. Among 16 ISSR primers only two were amplified specific alleles for both species and in 22 RAPDs only four gave species-specific reproducible unique amplicons, which could clearly distinguish genuine as well as adulterant samples having similar commercial name 'Brahmi'. ISSR and RAPD could thus, help to serve as complementary tools for quality control of genuine samples sold in the local markets.

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