5.1 CONCLUSIONS

The following findings were concluded from the research work-

Ib-AMP1 was predicted to be the potential antimicrobial peptide against toxins of *Staphylococcus aureus,* among the four plant derived antimicrobial peptides JCpep7, Sesquin, Snakin-2 and Ib-AMP1. After docking Ib-AMP1 showed significant interactions and global energies with all the three toxins of *S. aureus* (Enterotoxin A (ETA), Enterotoxin B (ETB) and Panton-Valentine leukocidin (PVL)) taken for the study.

Ib-AMP1 is a 20 amino acid antimicrobial peptide derived from *Impatiens balsamina*. Four 20 amino acid long antimicrobial peptides Ib-AMP1, Ib-AMP2, Ib-AMP3 and Ib-AMP4 are found in *Impatiens balsamina.* Ib-AMP-1 and Ib-AMP3 showed significant docking interactions against the Transcription activator ToxT of *Vibrio cholerae*. The comparative molecular dynamics results of ToxT, docked complex of ToxT+Ib-AMP1 and docked complex of ToxT+Ib-AMP3 predicted the most significant results for docked complex of ToxT and Ib-AMP1. Thus, it was predicted that Ib-AMP1 can be taken for further studies. Further the *In silico* characterization and toxicity prediction of Ib-AMP1 predicted Ib-AMP1 to be toxic. Any alternate drug candidate can never be a toxic compound. Thus, Ib-AMP1 was discarded from further studies to be developed as an alternate drug compound. Thus none of the above four antimicrobial peptides from *Impatiens balamina* were found suitable for being developed as alternate drug. Further studies were done for the prediction of potential antimicrobial peptide.

The docking interaction of Microcin C7 with the catalytic domain of diphtheria toxin was found to be best among all the five selected short length (less than or equal to 10 amino acids) antimicrobial peptides (Anionic peptide SAAP, Microcin C7, Bacteriocin, Curvalicin 28-c and NRWC) from microorganism source. The docking interaction of Alliumin with the

catalytic domain of diphtheria toxin was predicted to be best among all the five short length (less than or equal to 10 amino acids) antimicrobial peptides (JCpep7, Antimicrobial peptide 1, Cr-ACP1, Sesquin and Alliumin) selected from plant source for the study. The molecular dynamics simulation analysis of the RMSD, RMSF, radius of gyration and the number of hydrogen bonds, predicted Alliumin to be the most potential antimicrobial peptide among all the selected antimicrobial peptides against the catalytic domain of diphtheria toxin. Thus, Alliumin was chosen as the most potential antimicrobial peptide for further studies.

Analysis of the docking interactions showed that a significant interaction is found between ToxT and Alliumin. One crucial residue of ToxT interacts with Alliumin and six intermolecular hydrogen bonds formed predict the docking interaction to be significant. The molecular dynamics interactions predict the docked structure to be more stable and compact as compared to the native structure of ToxT. These predict that the confirmation of ToxT becomes more stable after binding to the antimicrobial peptide Alliumin. This predicts that Alliumin interacts quite effectively with the transcription activator ToxT to inhibit it.

The analysis of the docking interactions showed that a significant interaction is found between the superbug protein New Delhi Metallo-β-lactamase (NDM-1) and Alliumin. The protein-peptide interactions were significant; four crucial residue of NDM-1 interacts with Alliumin and four intermolecular hydrogen bonds formed predict the docking interaction to be significant. The molecular dynamics interactions predict the docked structure to be more stable and compact as compared to the native structure of NDM-1. These predict that the confirmation of NDM-1 becomes more stable after binding to the antimicrobial peptide Alliumin. This predicts that Alliumin interacts quite effectively with NDM-1 to inhibit it.

The mass of synthesized Alliumin equals to the *in silico* predicted molecular weight from sequence of Alliumin. Since *in silico* prediction of Alliumin sequence showed it to be non-

toxic and non-hemolytic. Further, the antibacterial assay carried out against *S. aurues* and *E.coli*, showed Alliumin to be effective against these bacteria. Thus, Alliumin showed antibacterial activity. Therefore, Alliumin was predicted as potential antimicrobial peptide to be developed as alternate drug.

5.2 FUTURE SCOPE

The *in silico* studies in the thesis work have predicted Alliumin to be the potential antimicrobial peptide to be developed as an alternate drug. The following studies can be performed further for the development of Alliumin as alternate drug.

Further studies on the effect of Alliumin on resistant pathogens should be done. These studies can help in establishing the mechanism of action of Alliumin against such pathogens.

Studies can be done on developing Alliumin as a lead compound against transcriptional activator ToxT functional deactivation and against the Superbug Beta-lactamases. The exact mechanism of action of Alliumin against these needs to be established.

Alliumin can be established as lead drug compound to be developed as alternate drug for resistant microorganisms and further Clinical trials can be done.