
LIST OF FIGURES

S.No.	Figure	Page No.
1.1	RCSB downloaded shows 3-D structure of Exfoliative toxin A (1DUA)	18
1.2	RCSB downloaded 3-D structure of Exfoliative toxin B (1DT2)	18
1.3	RCSB downloaded 3-D structure of Panton Valentine Leukocidin (1PVL) with ligand 2-(n-morpholino)-ethanesulfonic acid.	19
1.4	The figure shows the secondary structure of 3GBG	20
1.5	RCSB downloaded 3D structure of 3GBG with ToxT and Palmitoleic acid	20
1.6	RCSB downloaded structure of catalytic domain of diphtheria toxin (1DTP) with ligand ApUp attached.	22
1.7	RCSB downloaded structure of New Delhi Metallo-β-lactamase with inhibitors attached.	23
4.1	The figure shows the predicted structure of JCpep7, predicted using Pepfold3	50
4.2	The figure shows the predicted structure of Sesquin, predicted using Pepfold3	51
4.3	The figure shows the predicted structure of Snakin-2, predicted using Pepfold3	51
4.4	The figure shows the predicted structure of Ib-AMP1, predicted using Pepfold3	52
4.5	The figure shows best docked structure of ETA and JCpep7. The residues of ETA are shown in yellow colour and the residues of JCpep7 are shown in magenta. The red coloured residues show the crucial residues of ETA.	53
4.6	The figure shows best docked structure of ETB and JCpep7. The residues of ETB are shown in yellow colour and the residues of JCpep7 are shown in magenta. The red coloured residues show the crucial residues of ETB.	54
4.7	The figure shows best docked structure of PVL and JCpep7. The residues of PVL are shown in yellow colour and the residues of JCpep7 are shown in magenta. The red coloured residues show the crucial residues of PVL	55
4.8	The figure shows best docked structure of ETA and Sesquin. The residues of ETA are shown in yellow colour and the residues of Sesquin are shown in magenta. The red coloured residues show the crucial residues of ETA.	56
4.9	The figure shows best docked structure of ETB and Sesquin. The residues of ETB are shown in yellow colour and the residues of Sesquin are shown in magenta. The red coloured residues show the crucial residues of ETB.	56
4.10	The figure shows best docked structure of PVL and Sesquin. The residues of PVL are shown in yellow colour and the residues of Sesquin are shown in magenta. The red coloured residues show the crucial residues of PVL.	57
4.11	The figure shows best docked structure of ETA and Snakin-2. The residues of ETA are shown in yellow colour and the residues of Snakin-2 are shown in magenta. The red coloured residues show the crucial residues of Snakin-2.	58

	residues of ETA.	
4.12	The figure shows best docked structure of ETB and Snakin-2. The residues of ETB are shown in yellow colour and the residues of Snakin-2 are shown in magenta. The red coloured residues show the crucial residues of ETB.	59
4.13	The figure shows best docked structure of PVL and Snakin-2. The residues of PVL are shown in yellow colour and the residues of Snakin-2 are shown in magenta. The red coloured residues show the crucial residues of PVL.	60
4.14	The figure shows best docked structure of ETA and Ib-AMP1. The residues of ETA are shown in yellow colour and the residues of Ib-AMP1 are shown in magenta. The red coloured residues show the crucial residues of ETA.	61
4.15	The figure shows best docked structure of ETB and Ib-AMP1. The residues of ETB are shown in yellow colour and the residues of Ib-AMP1 are shown in magenta. The red coloured residues show the crucial residues of ETB.	62
4.16	The figure shows best docked structure of PVL and Ib-AMP1. The residues of PVL are shown in yellow colour and the residues of Ib-AMP1 are shown in magenta. The red coloured residues show the crucial residues of PVL.	62
4.17	The modelled structure of ToxT with the missing residues repaired in it	65
4.18	The docked complex of ToxT and Ib-AMP1. The yellow residues represent the residues of ToxT, red residues represent the crucial residues of ToxT and the magenta residues represent the residues of antimicrobial peptide Ib-AMP1	66
4.19	The docked complex of ToxT and Ib-AMP2. The yellow residues represent the residues of ToxT, red residues represent the crucial residues of ToxT and the magenta residues represent the residues of antimicrobial peptide Ib-AMP2.	67
4.20	The docked complex of ToxT and Ib-AMP3. The yellow residues represent the residues of ToxT, red residues represent the crucial residues of ToxT and the magenta residues represent the residues of antimicrobial peptide Ib-AMP3.	68
4.21	The docked complex of ToxT and Ib-AMP4. The yellow residues represent the residues of ToxT, red residues represent the crucial residues of ToxT and the magenta residues represent the residues of antimicrobial peptide Ib-AMP4.	69
4.22	Comparative plot for the RMSD values of ToxT, docked complex of ToxT+Ib-AMP1 and docked complex of ToxT+Ib-AMP3	71
4.23	Comparative plot for the RMSD values of ToxT and docked complex of ToxT+Ib-AMP1	71
4.24	Comparative plot for the RMSF values of ToxT, docked complex of ToxT+Ib-AMP1 and docked complex of ToxT+Ib-AMP3	72
4.25	Comparative plot for the Radius of gyration values of ToxT, docked complex of ToxT+Ib-AMP1 and docked complex of ToxT+Ib-AMP3	73
4.26	Comparative plot for the Radius of gyration values of ToxT and docked complex of ToxT+Ib-AMP1	74
4.27	Predicted 3D structure of Anionic peptide SAAP	76

4.28	Predicted 3D structure of Bacteriocin	76
4.29	Predicted 3D structure of Curvalicin-28c	77
4.30	Predicted 3D structure of NRWC	77
4.31	Predicted 3D structure of JCpep7	77
4.32	Predicted 3D structure of Antimicrobial peptide 1	78
4.33	Predicted 3D structure of Cr-ACP1	78
4.34	Predicted 3D structure of Sesquin	78
4.35	Predicted 3D structure of Allumin	79
4.36	The docked complex of DT and SAAP. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide SAAP	79
4.37	The docked complex of DT and Microcin C7. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Microcin C7	80
4.38	The docked complex of DT and Bacteriocin. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Bacteriocin	81
4.39	The docked complex of DT and Curvalicin-28c. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Curvalicin-28c	82
4.40	The docked complex of DT and NRWC. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide NRWC	83
4.41	The docked complex of DT and JCpep7. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide JCpep7	84
4.42	The docked complex of DT and Antimicrobial peptide 1. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Antimicrobial peptide 1	85
4.43	The docked complex of DT and Cr-ACP1. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Cr-ACP1	86
4.44	The docked complex of DT and Sesquin. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Sesquin	87
4.45	The docked complex of DT and Allumin. The yellow residues represent the residues of DT, red residues represent the crucial residues of DT and the magenta residues represent the residues of antimicrobial peptide Allumin	88
4.46	Comparative plot for the RMSD values of DT, docked complex of	90

	DT+Microcin C7 and docked complex of DT+Allumin	
4.47	Comparative plot for the RMSF values of DT, docked complex of DT+Microcin C7 and docked complex of DT+Allumin	91
4.48	Comparative plot for the Radius of gyration values of DT and docked complex of DT+Allumin	92
4.49	Number of hydrogen bonds formed between catalytic domain of diphtheria toxin and Allumin throughout simulation of 20ns.	92
4.50	The docked complex of ToxT and Allumin. The yellow residues represent the residues of ToxT, red residues represent the crucial residues of ToxT and the magenta residues represent the residues of antimicrobial peptide Allumin.	95
4.51	Comparative plot for the RMSD values of ToxT and docked complex of ToxT+Allumin	97
4.52	Comparative plot for the RMSF values of ToxT and docked complex of ToxT+Allumin	98
4.53	Plot for the intermolecular hydrogen bond values for docked complex of ToxT+Allumin	98
4.54	Comparative plot for the Radius of gyration values of ToxT and docked complex of ToxT+Allumin	99
4.55	Modelled structure of NDM-1.	101
4.56	The docked complex of NDM-1 and Allumin. The yellow residues represent the residues of NDM-1, red residues represent the crucial residues of NDM-1 and the magenta residues represent the residues of antimicrobial peptide Allumin	102
4.57	Comparative plot for the RMSD values of NDM-1 and docked complex of NDM-1+Allumin	103
4.58	Comparative plot for the RMSF values of NDM-1 and docked complex of NDM-1+Allumin	104
4.59	Plot for the intermolecular hydrogen bond values for docked complex of NDM-1+Allumin	105
4.60	Comparative plot for the Radius of gyration values of NDM-1 and docked complex of NDM-1+Allumin	105
4.61	The synthesized peptide Allumin procured from USV (P) Ltd Custom Peptide	107
4.62	MS data of synthesized Allumin sent by USV (P) Ltd.	108
4.63	Zone of inhibition of Synthesised Allumin against <i>Staphylococcus aureus</i> (A) and <i>Escherichia coli</i> (B). The controls C and D show do not show any zones of inhibition.	109
