LIST OF FIGURES

CHAPTER 1

S.No.	Figure	Page No.
D.1 (U.	T iguit	1 450 1101
1.	Stucture of Natural Cytotoxicity receptors in cartoon presentation.	
2.	Structures of NKp46 homologous proteins.	
3.	Charged surface representation of NKp44 and closely related homologues sialoadhesin, pIgR, TLT-1, and TREM-1	
4.	User Interface of T-antigen Database.	
5.	User interface of Phyre2	13
6.	HADDOCK score v/s i-l-RMSD clustering graph for NKp30-Ag002094_TAPBP	15
7.	Clustering of structures obtained after docking of NKp30-Ag002904_TAPBP	18
8.	H-bond forming residues of NKp30-B7H6	20
9.	H-bond forming residues of NKp30-Ag002094_TAPBP	20
10.	RMSD curve of NKp30-Ag002094_TAPBP with reference to initial structure after 3000ps	22
11.	Alignment of NKp30-Ag002094_TAPBP complex before and after 3000ps simulation run.	22
12.	H-bond forming residues of NKp30-Ag_002094_TAPBP after 3000ps of simulation run	23
13.	Result of ASAP and the regions of hemagglutinin protein selected as active site compartments.	25

14.	H-bond forming residues of NKp46-hemagglutinin complex	
15.	RMSD curve of complex NKp46-hemagglutinin for 3000ps simulation run	
16.	H-bond forming residues of NKp46-hemagglutinin complex	28
16.	H-bond forming residues of NKp44-hemagglutinin complex	30
17.	RMSD curve of complex NKp44-hemagglutinin for 3000ps simulation run.	31
18.	H-bond forming residues of NKp44-Hemagglutinin after 3000ps of simulation run.	32

CHAPTER 2

S.No.	Figure	
a)	A potential role for KIR2DL4–HLA-G interactions in early pregnancy	
1.	RMSD plot of KIR2DL4 modeled structure for 15 ns simulation run.	
2.	Ramachandran plot of the KIR2DL4 after 15ns of simulation	
3.	Errat plot of the KIR2DL4 pre and post Molecular Dynamics	45
4.	Alignment of Pre MD and Post MD structure of KIR2DL4.	46
5.	Clustering of structures of KIR2DL4-HLA-G on the basis of HADDOCK Score	48
6.	H bond forming residues of HLA-G and KIR2DL4.	49
7.	H-bond forming residues of HLA-E and KIR2DL4.	51
8.	Clustering of structures of complex HLA-Cw3-KIR2DL4 obtained from HADDOCK	53
9.	Residues of HLA-Cw3 and KIR2DL4 involved in H-bond interaction	54
10.	H-bond forming residues of KIR2DL4 and HLA-Cw4	56

LIST OF TABLES

CHAPTER 1 S.No. Page No. Table legends Showing the structures of Natural Cytotoxicity Receptors 1. 6 available with their resolutions, PDB ID and references. 2. HADDOCK score of top cluster of NKp30-B7H6 complex 15 3. BLAST result of B7H6 with Tumor antigen sequences 17 Statistics of the top cluster with highest energy among all other 4. 17 dockings Residues of B7H6 involved in H bonds with NKp30 5. 18 Residues of Ag002094_TAPBP involved in H bonds with 6. 18 NKp30 Residues of Ag_002094_TAPBP involved in H bonds with 7. 23 NKp30 after 3000ps of simulation run. Residues of the 4 compartments of hemagglutinin and their 8. 24 docking scores and Z scores with NKp46 Residues of hemagglutinin involved in H bond formation with 9. 26 NKp46. Residues of hemagglutinin involved in H bonds with NKp46. 10. 27

11.	Residues of the 4 compartments of hemagglutinin and their HADDOCK and Z scores with NKp46	29
12.	Residues of NKp44 and hemagglutinin involved in H bond formation.	30
13.	Residues of NKp44 and hemagglutinin involved in H bond formation after 3000ps simulation	32

CHAPTER 2

S.No.	Table legends	Page No.
1.	Results obtained from HADDOCK docking of KIR2DL4-HLA-G	47
2.	Residues of KIR2DL4 which forms H bonds with HLA-G along with their H Bond distance	49
3.	Results obtained from HADDOCK docking of KIR2DL4-HLA-E .	50
4.	Residues of KIR2DL4 which forms H bonds with HLA-E along with their H Bond distance	51
5.	Results obtained from HADDOCK for KIR2DL4-HLA-E	53
6.	Residues of KIR2DL4 which forms H bonds with HLA-Cw3 along with their H Bond distance	54
7.	Energy scores of top cluster generated HADDOCK for HLA-Cw4-KIR2DL4 docking	55
8.	H bond forming residues of KIR2DL4 and HLA-Cw4.	56

LIST OF ABBREVIATIONS

A.U.	Atomic Unit
AIR	Ambiguous interaction restraints
ASAP	Accessible Surface Area Predictor
ASAP	Accessible Surface Area Predictor
BLAST	Basic Local Alignment Search Tool
BLOSSUM62	Block Substitution Matrix
CDR3	Cluster of differentiation 3
DAP12	Cytotoxic T lymphocyte
HADDOCK	High Ambiguity Driven biomolecular DOCKing
H-bond	Hydrogen bond
HCV	Hepatitis C virus infection
HLA	Human leukocyte antigen
HLA	Human Leukocyte Antigen
ITAM	Immunoreceptor Tyrosine-based Activation Motif
ITIM	Immunoreceptor Tyrosine-based Inhibitory Motif
K	Kelvin
KIR	Killer cell immunoglobulin-like receptors
MD	Molecular Dynamics
МНС	Major Histocompatibility Complex
NK	Natural Killer
OPLS	Optimized potentials for liquid simulations
PBMC	Peripheral Mononuclear Cells
PDB	Protein Data Bank
RCSB	The Research Collaboratory for Structural Bioinformatics
RMSD	Root Mean Square Deviation

SPC	Simple point charge
TAPBP	TAP Binding Protein
uNK	Uterine Natural Killer Cell