Supplementary material 1

Table S1a: Binding interaction of pancreatic lipase inhibitory peptides-MMML at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide **M**MML	MET1	cluster10_1	-7.3	C - NA CA - Val260 CB - NA CE - Thr256 CG - Thr256 O - NA N - Val260, Ala261 SD - Arg257	NA	NA	N - Arg257
Total number of bonds					34	0	0	1
Total no of interactive residues					6	0	0	1
Overall percentage of bonding					18%	0%	0%	100%

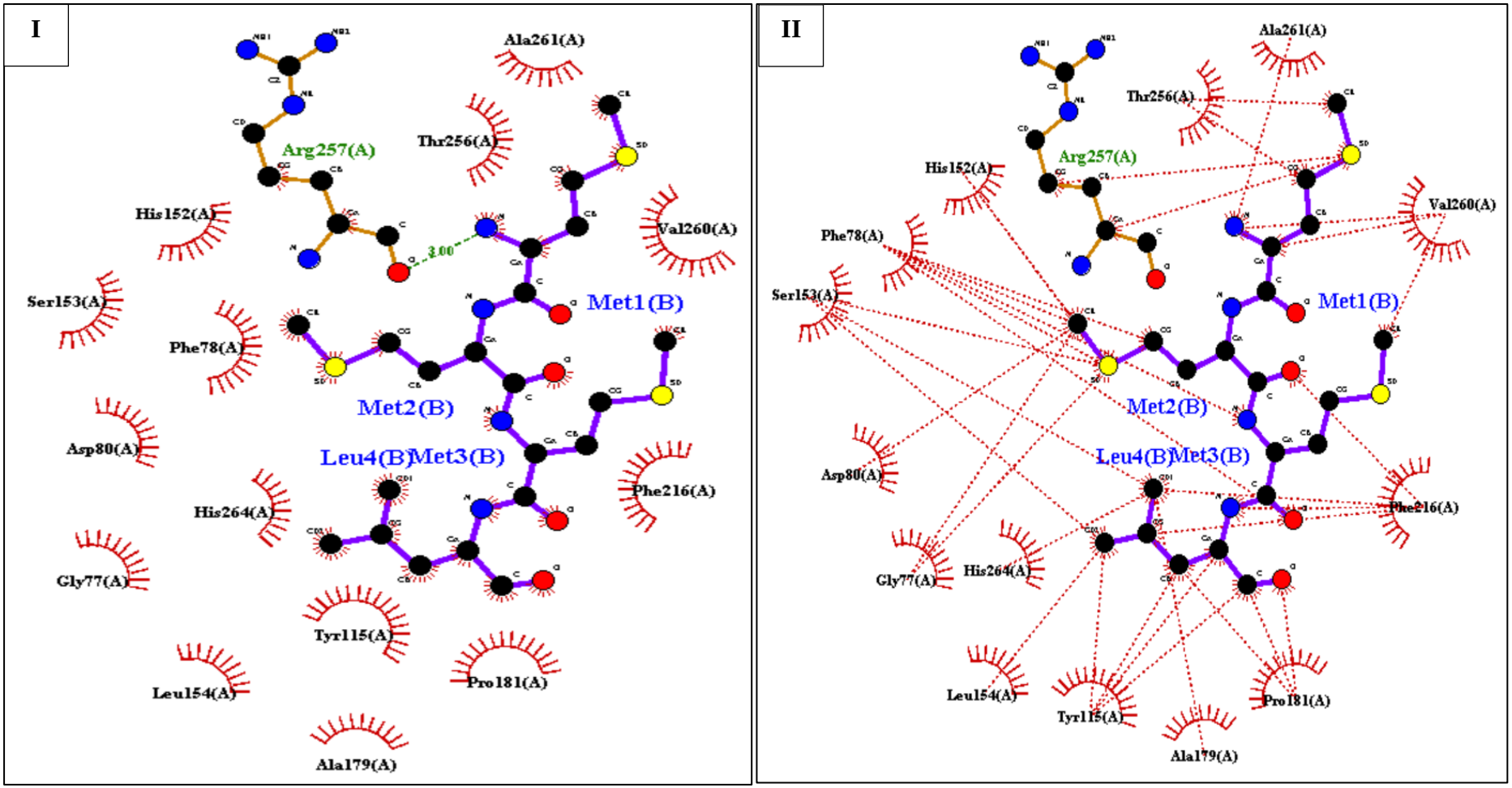

Figure S1a: Binding interaction of **MMML** inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S1b: Binding interaction of pancreatic lipase inhibitory peptides-MSNYF at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide **M**SNYF	MET1	cluster 1_4	-7.7	C - Phe216 CA - NA CB - Phe216 CE - Pro181 CG - Pro181, Tyr115 O - Phe216 N - Tyr115, Phe78 SD - Pro181, Tyr115	NA	NA	NA
Total number of bonds					27	0	0	0
Total no of interactive residues					10	0	0	0
Overall percentage of bonding					37%	0%	0%	0%

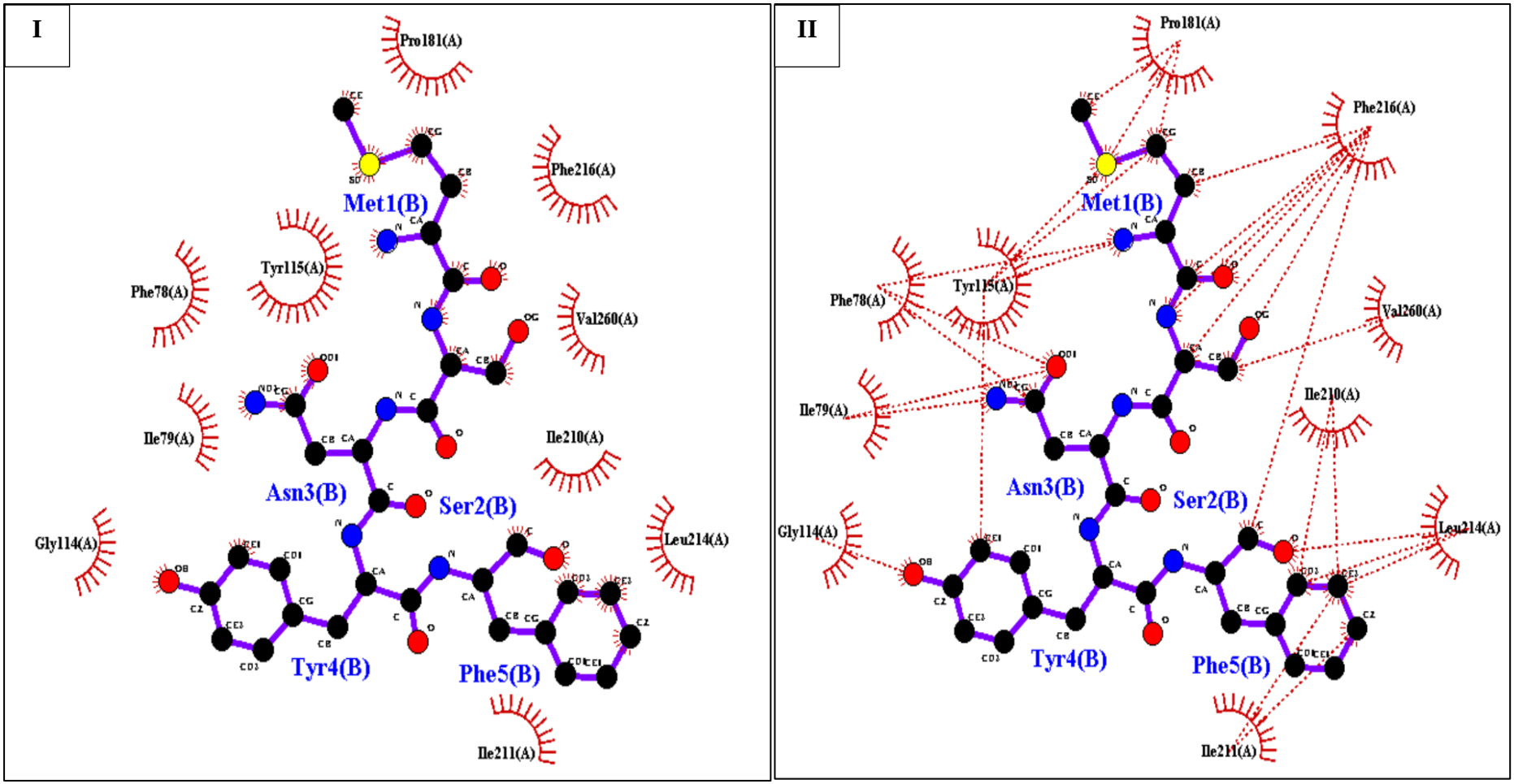

Figure S1b: Binding interaction of **M**SNYF inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S1c: Binding interaction of pancreatic lipase inhibitory peptides-AAGF at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide **A**AGF	ALA1	cluster1_3	-6.5	C - Pro181 CA - NA CB - NA N - NA O - Pro181	NA	NA	O - Cys182
Total number of bonds					18	0	0	1
Total no of interactive residues					2	0	0	1
Overall percentage of bonding					11%	0%	0%	100%

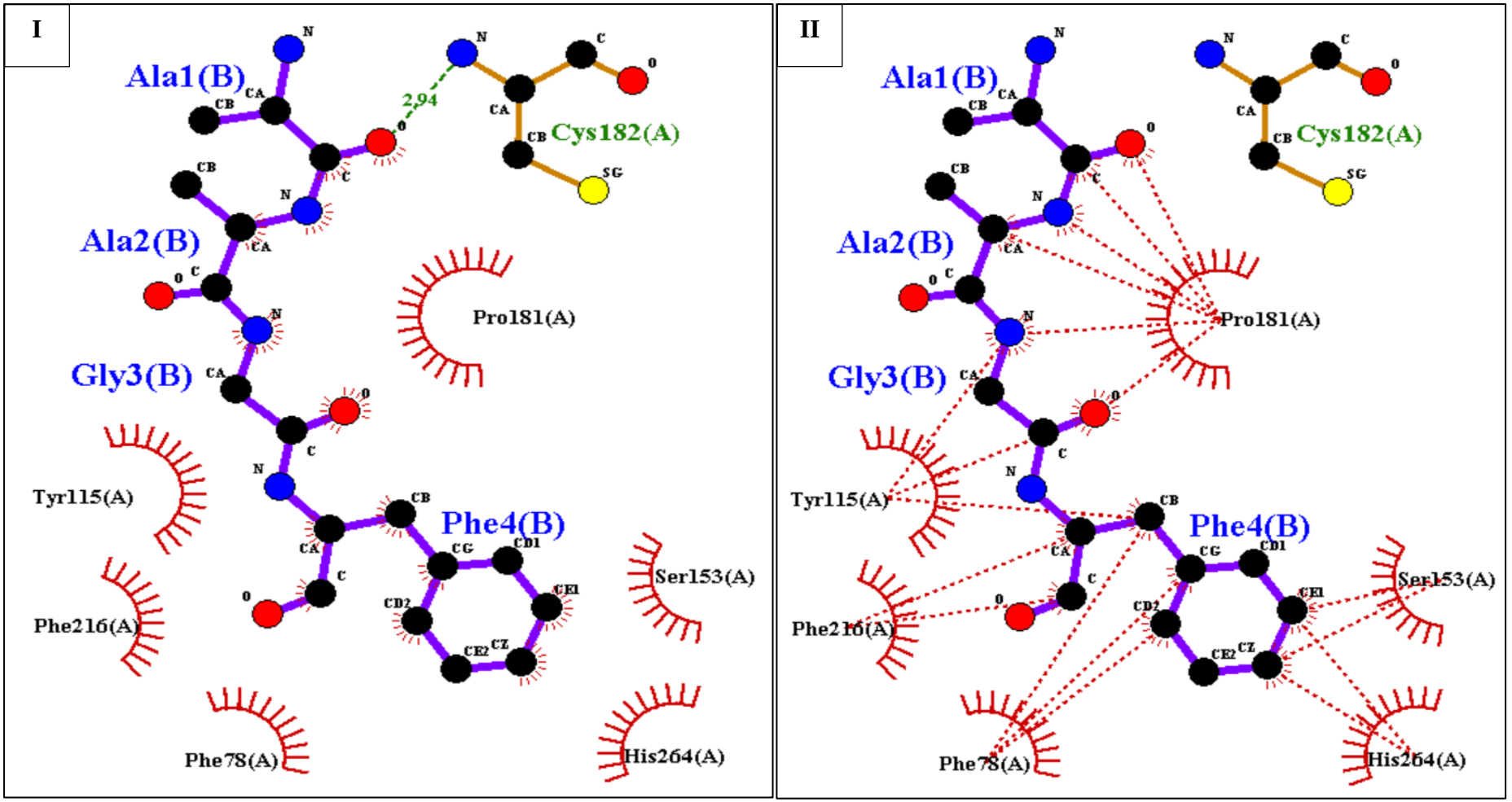

Figure S1c: Binding interaction of **A**AGF inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S1d: Binding interaction of pancreatic lipase inhibitory peptides- LRFPL at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide **L**RFPL	LEU1	cluster1_1	-7.4	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - Leu214, Phe261 O - NA	NA	NA	NA
Total number of bonds					24	0	0	2
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					8%	0%	0%	0%

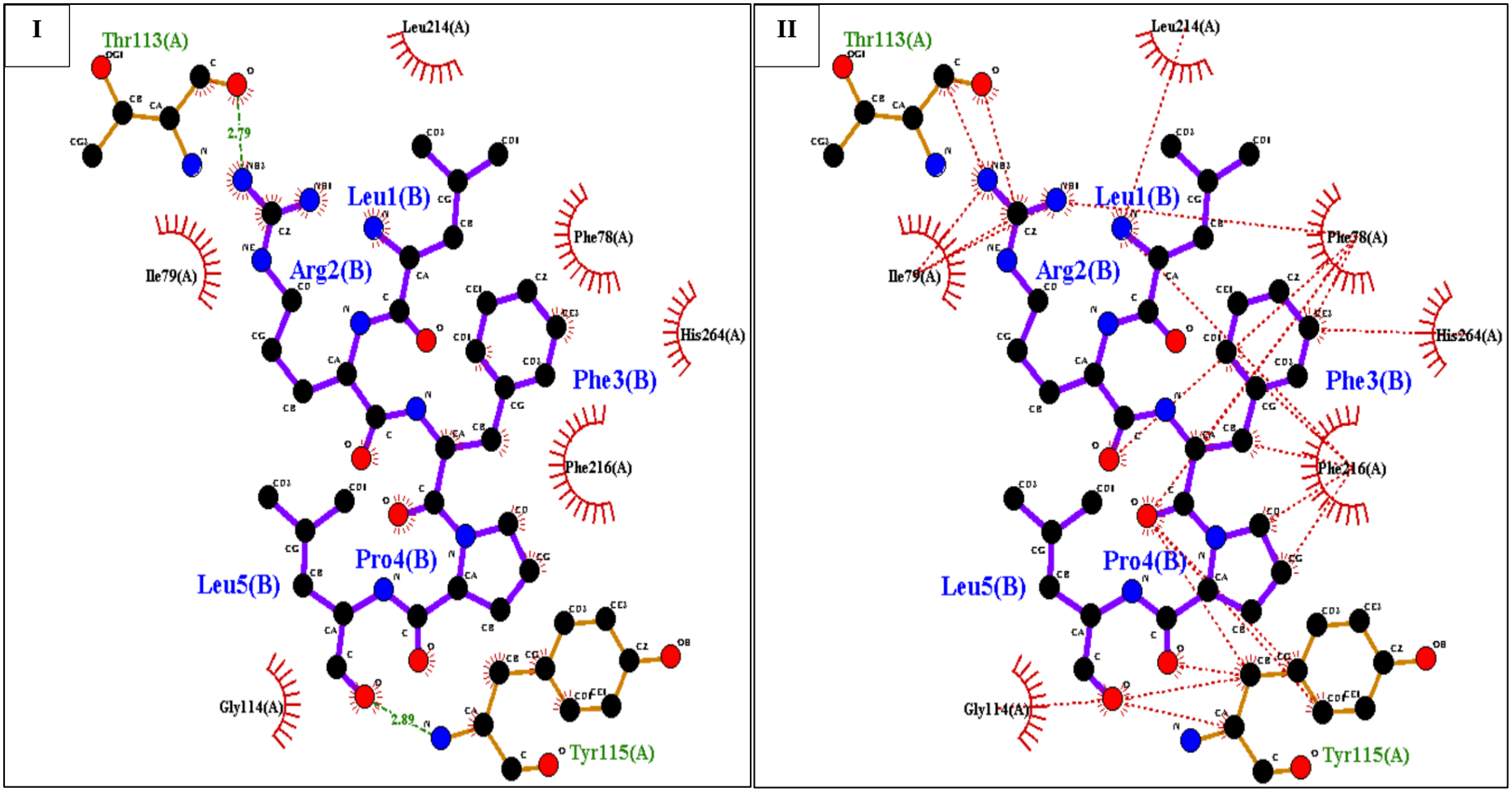

Figure S1d: Binding interaction of **L**RFPL inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S1e: Binding interaction of pancreatic lipase inhibitory peptides-NVQR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide **N**VQR	ASN1	cluster8_1	-7.7	C - Trp253 CA - NA CB - NA CG - NA N- Trp253 ND_2 - NA O - NA OD_1 - NA	NA	NA	NA
Total number of bonds					23	1	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

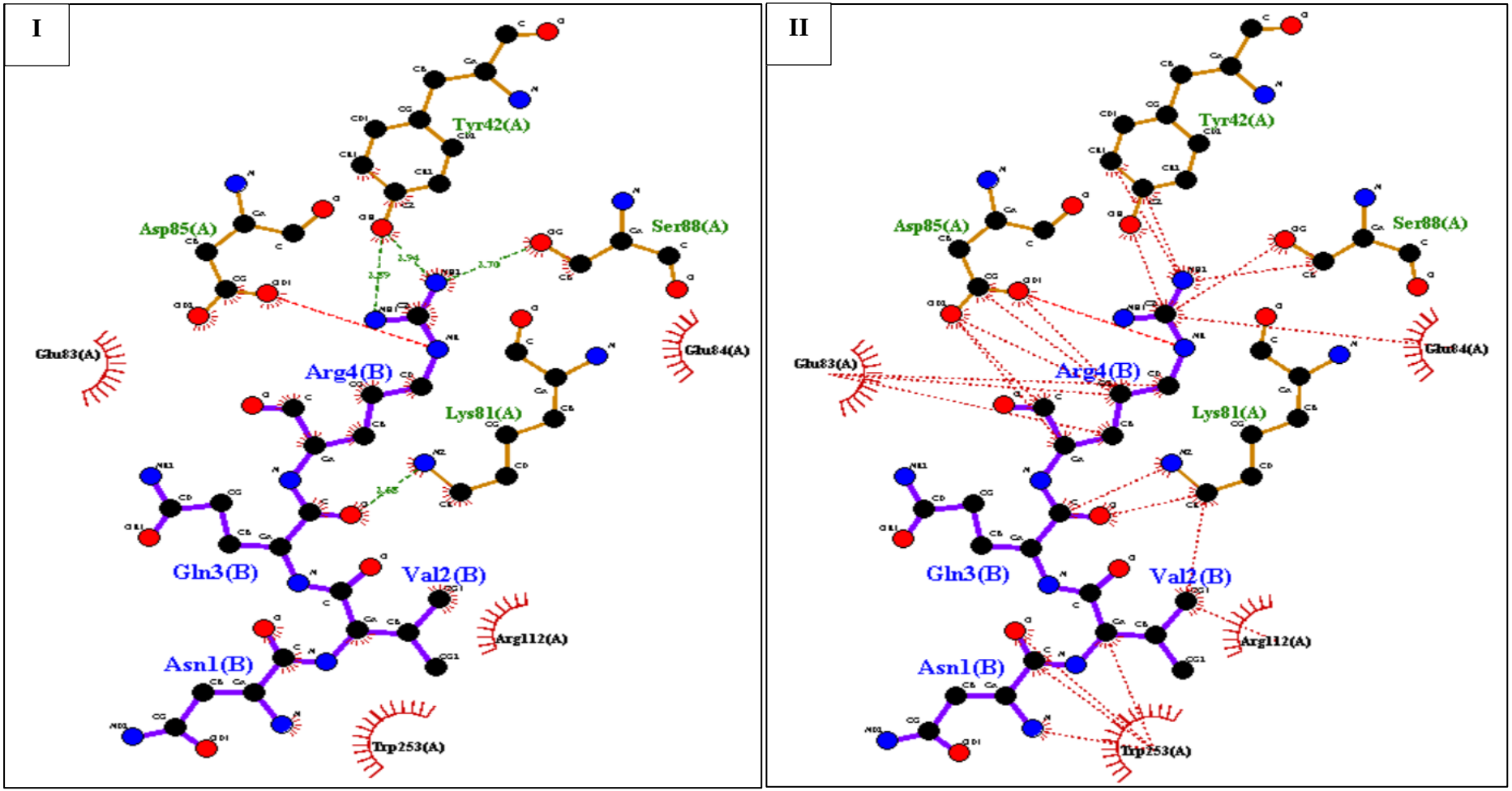

Figure S1e: Binding interaction of **N**VQR inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2a: Binding interaction of pancreatic lipase inhibitory peptides-FDPFPK at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **F**DPFPK	PHE1	cluster2_1	-7.1	C - Phe216 CA - Phe216 CB - Val260 CD_1 - Val260 CD_2 - Leu214 CE_1 - NA CE_2 - Leu214 CG - Val260 CZ - NA N - Val260 O - Phe216	NA	NA	NA
Total number of bonds					33	0	0	0
Total no of interactive residues					9	0	0	0
Overall percentage of bonding					27%	0%	0%	0%

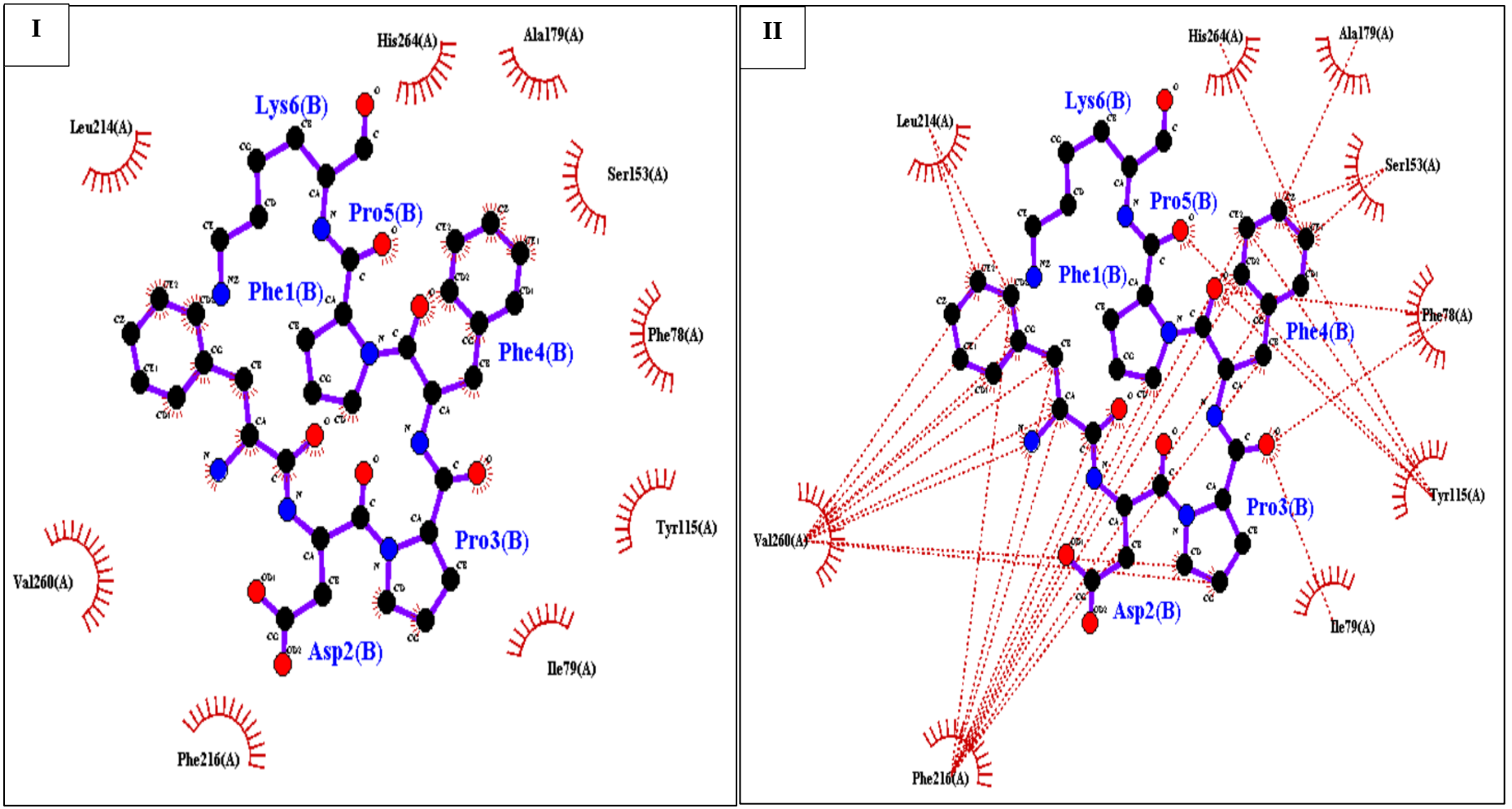

Figure S2a: Binding interaction of **F**DPFPK inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2b: Binding interaction of pancreatic lipase inhibitory peptides-FYLGYCDY at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **F**YLGYCDY	PHE1	cluster1_3	-6.4	C - NA CA - Phe78 CB - NA CD_1 - Phe78, Ser153, His264 CD_2 - Phe216 CE_1 - Ser153, His264 CE_2 - Phe216 CG - NA CZ -Tyr115 N - Ile79 O - Phe78	NA	NA	NA
Total number of bonds					23	0	0	1
Total no of interactive residues					11	0	0	0
Overall percentage of bonding					48%	0%	0%	0%

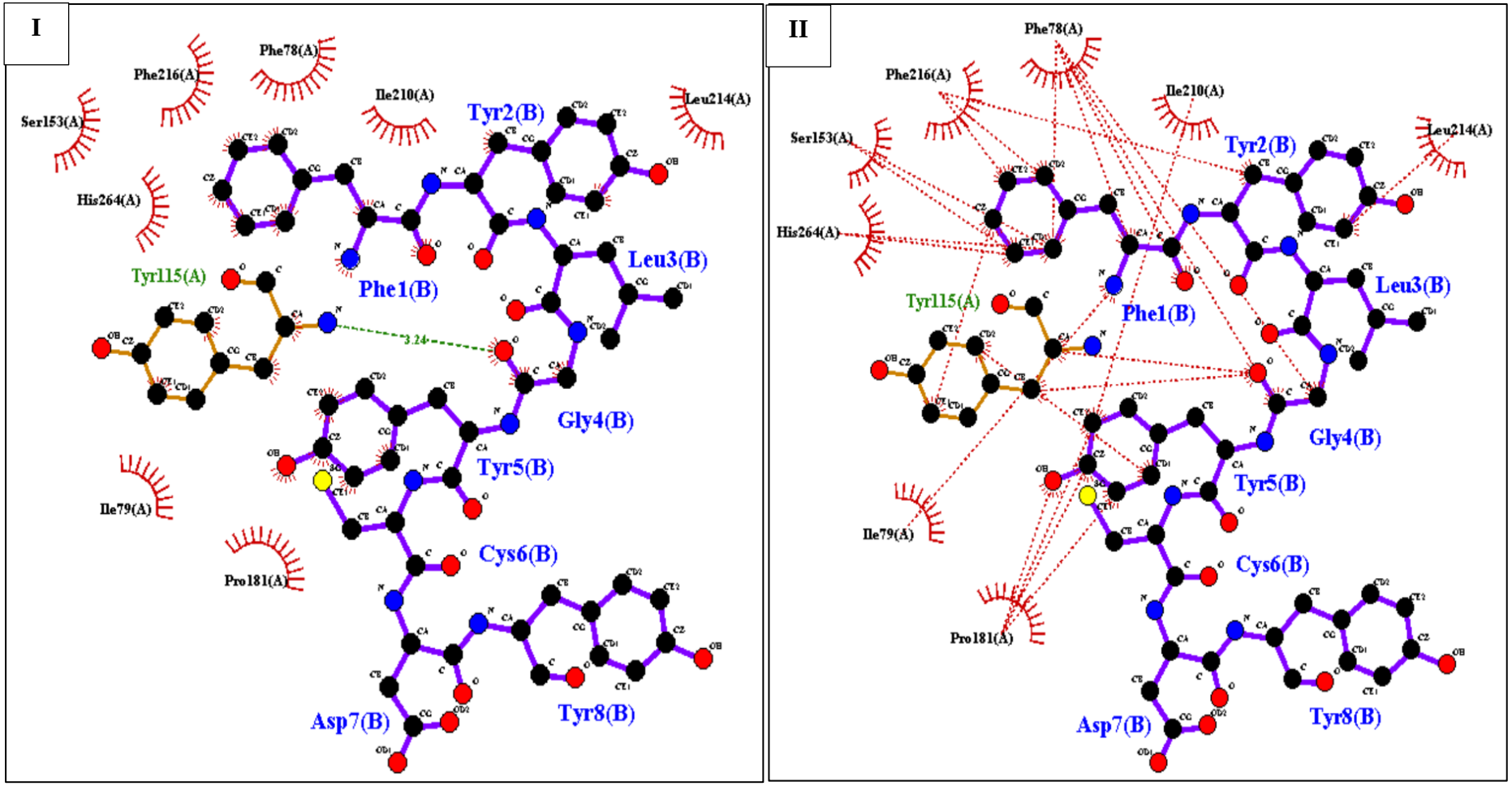

Figure S2b: Binding interaction of **F**YLGYCDY inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2c: Binding interaction of pancreatic lipase inhibitory peptides-NPVWKR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **N**PVWKR	ASN1	cluster1_2	-7.1	C - NA CA - Thr116 CB - NA CG - Thr116 N- NA ND_2 - Gly114 O - NA OD_1 - Gly114, Thr116	NA	NA	OD_1 - Thr116
Total number of bonds					32	1	0	3
Total no of interactive residues					5	0	0	1
Overall percentage of bonding					16%	0%	0%	33%

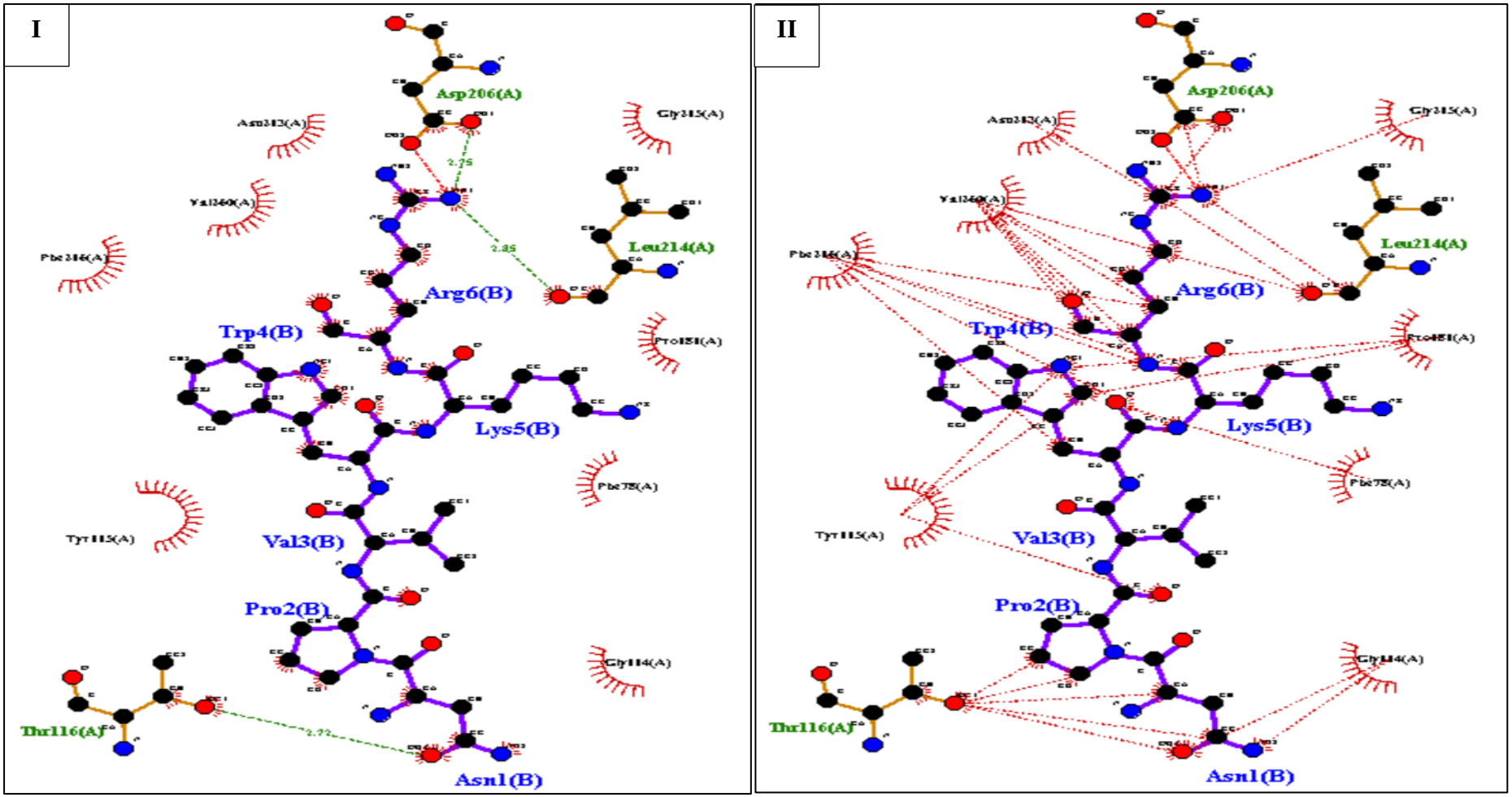

Figure S2c: Binding interaction of NPVWKR inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2d: Binding interaction of pancreatic lipase inhibitory peptides-NPVWKRK at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **N**PVWKRK	ASN1	cluster3_4	-7.0	C - NA CA - NA CB - Arg112, Thr113 CG - Arg112, Thr113 N- NA ND_2 - Arg112, Thr113 O - NA OD_1 - NA	NA	NA	ND_2 - Arg112
Total number of bonds					27	0	0	2
Total no of interactive residues					6	0	0	1
Overall percentage of bonding					22%	0%	0%	50%

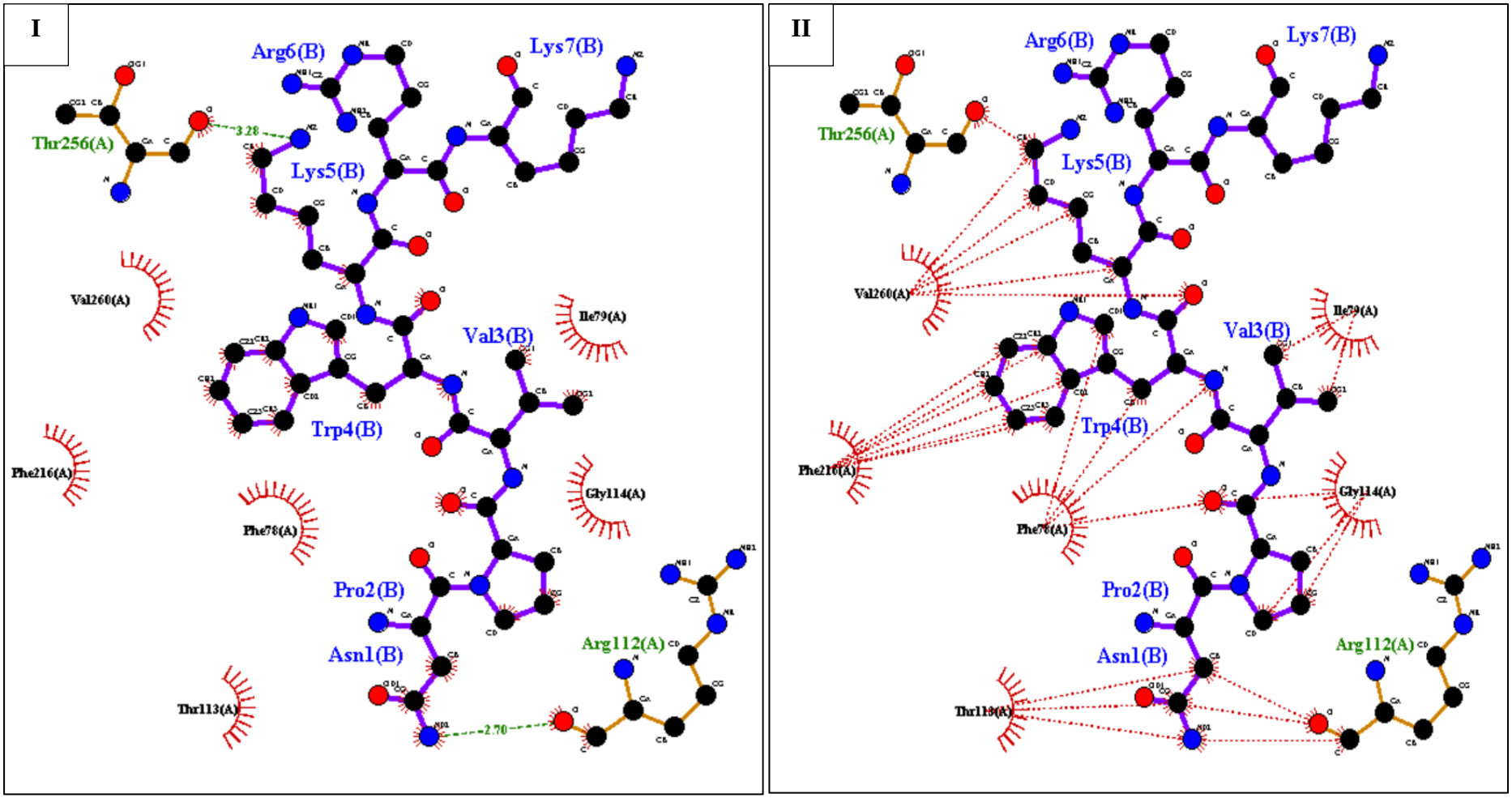

Figure S2d: Binding interaction of NPVWKRK inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2e: Binding interaction of pancreatic lipase inhibitory peptides-AGDDAPR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **A**GDDAPR	ALA1	cluster 3_4	-6.9	C - Phe78 CA - Phe78 CB - Phe78 N - NA O - Phe78, Tyr115	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					20%	0%	0%	0%

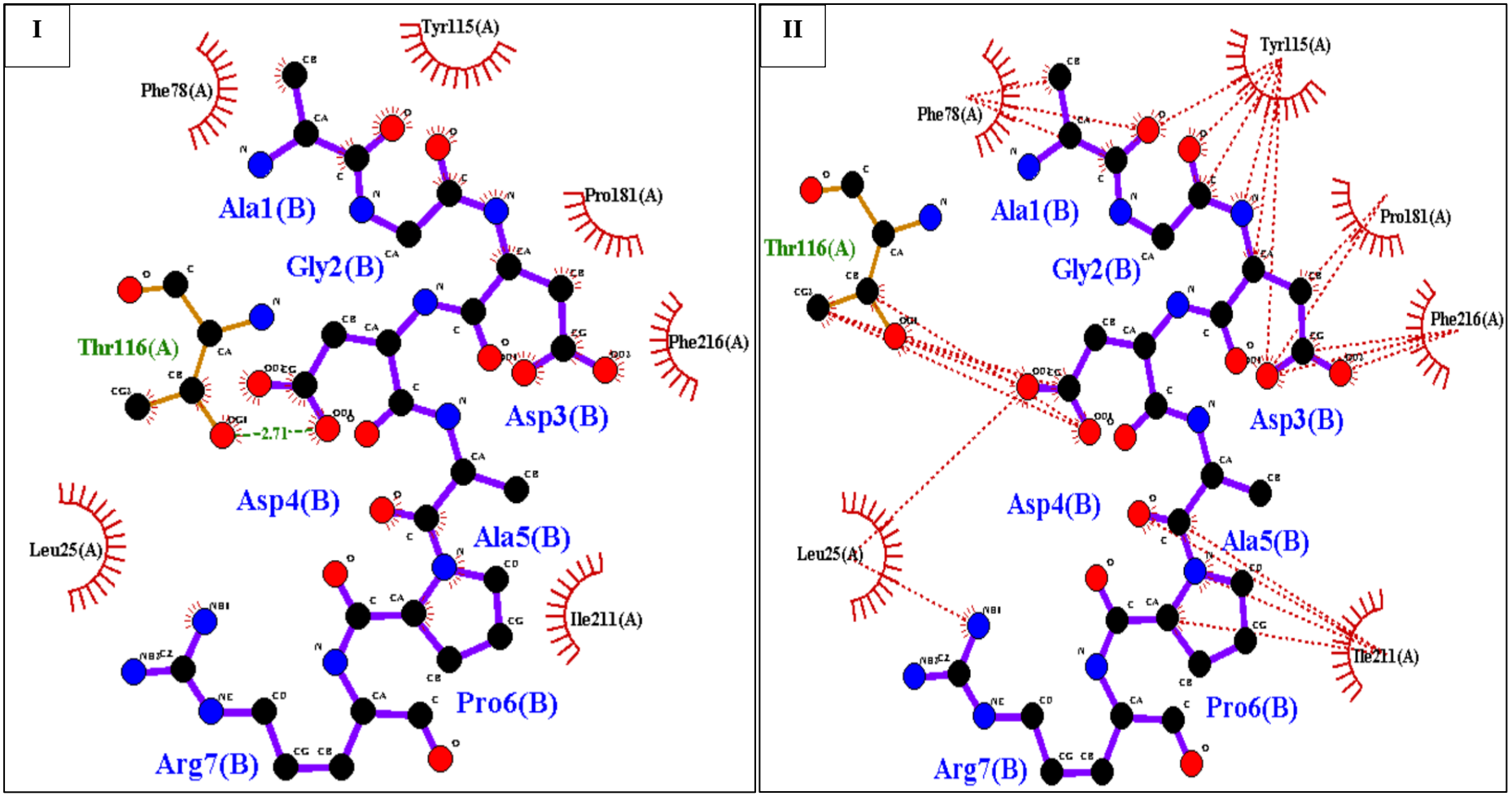

Figure S2e: Binding interaction of **A**GDDAPR inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2f Binding interaction of pancreatic lipase inhibitory peptides-APFPLR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **A**PFPLR	PRO4	cluster1_3	-7.0	C - NA CA - NA CB - NA N - NA O - NA	NA	NA	NA
Total number of bonds					16	0	0	0
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

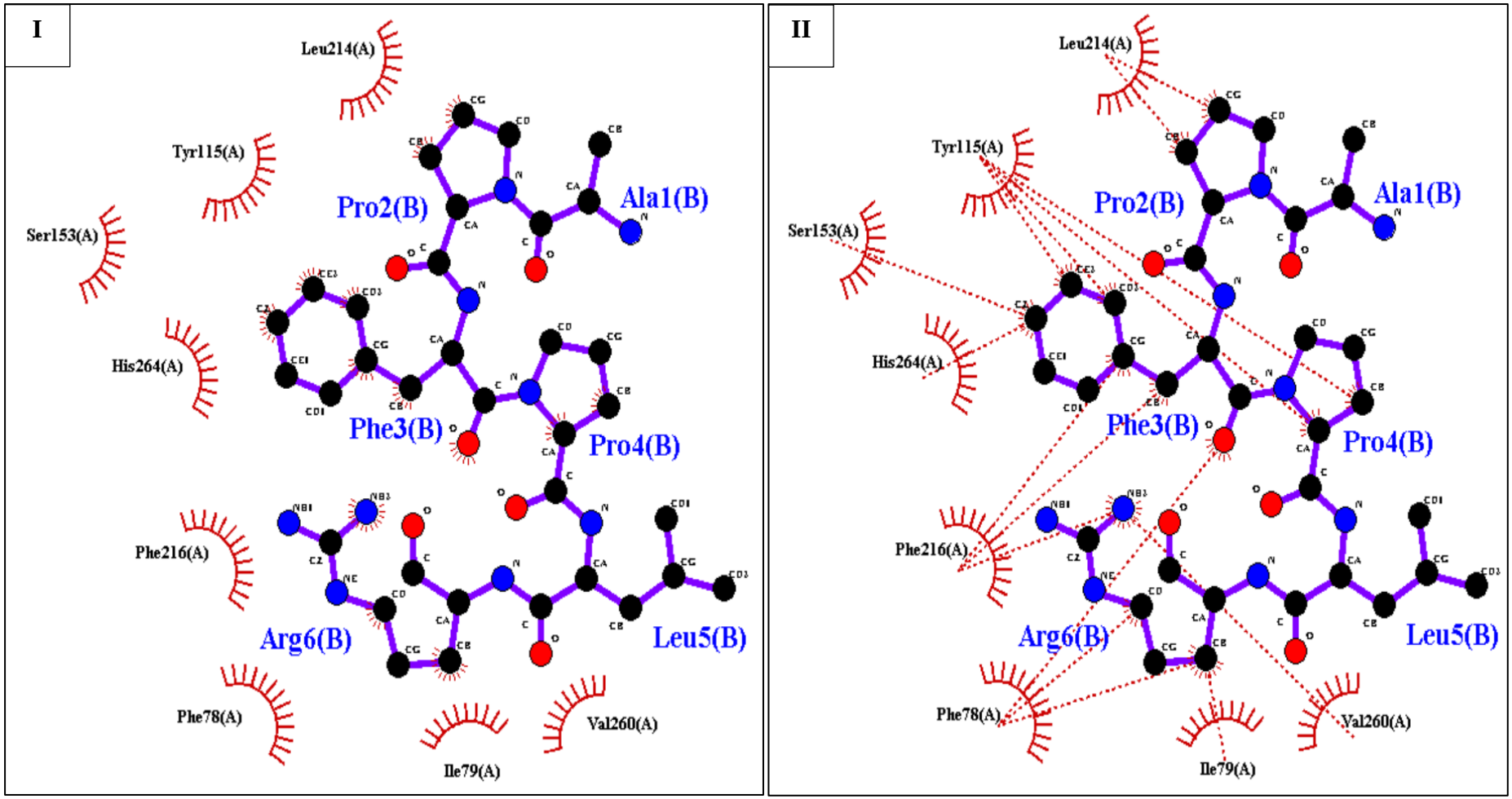

Figure S2f: Binding interaction of **A**PFPLR inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2g: Binding interaction of pancreatic lipase inhibitory peptides-LNLDLLR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide **L**NLDLLR	LEU1	cluster11_2	-8.1	C - NA CA - NA CB - NA CD_1 - Ile79, Arg112 CD_2 - NA CG - NA N - Ile79 O - Phe78, Thr113	NA	NA	NA
Total number of bonds					20	0	0	2
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					20%	0%	0%	0%

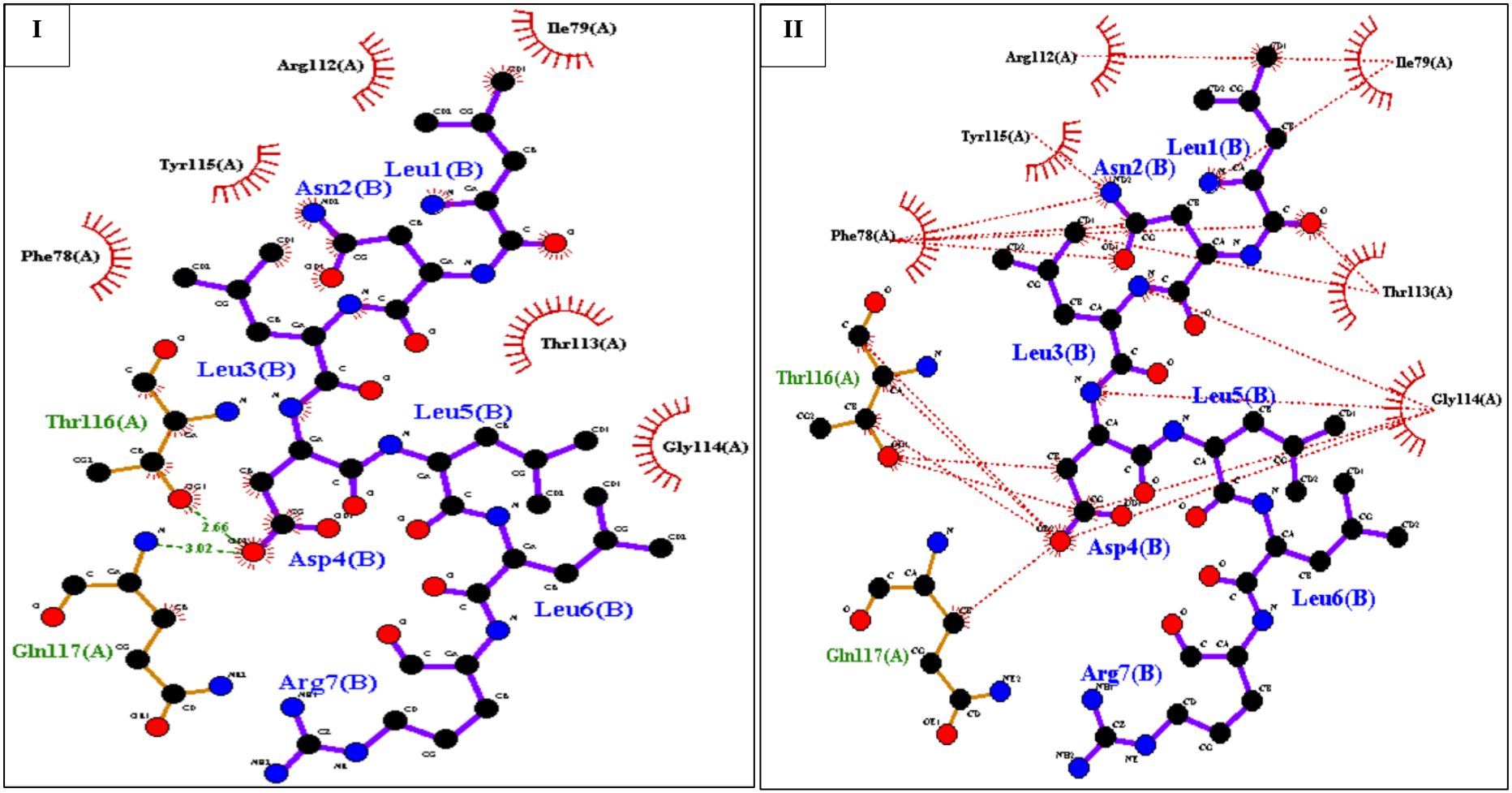

Figure S2g: Binding interaction of **L**NLDLLR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S2h: Binding interaction of pancreatic lipase inhibitory peptides- LNFEPR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide LNFEPR	LEU1	cluster2_2	-8.0	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

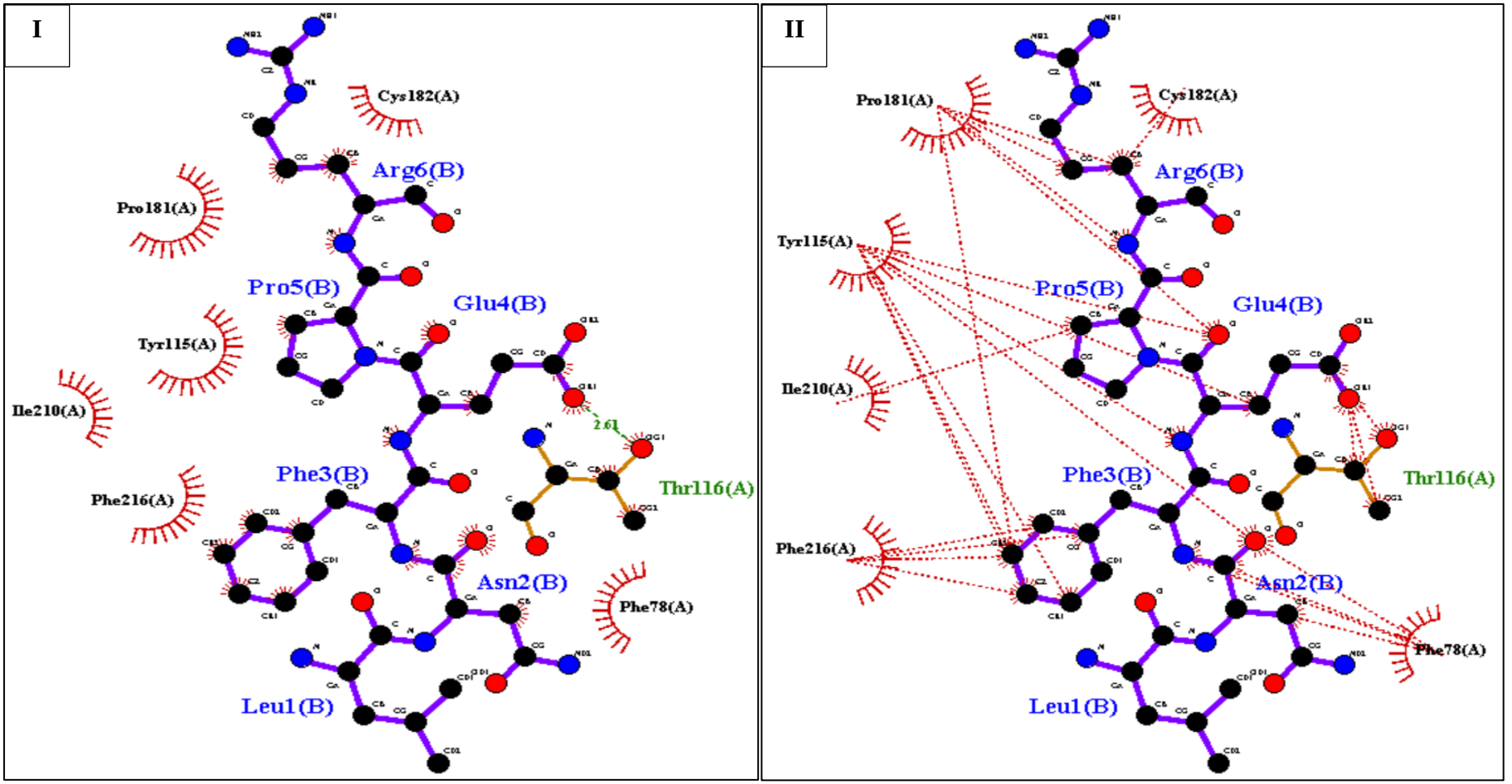

Figure S2h: Binding interaction of LNFEPR inhibitory peptide at N1position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3a: Binding interaction of pancreatic lipase inhibitory peptides-GNPVGGVGHGTTGT at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide GNPVGGVGHG TTGT	GLY1	cluster5_1	-8.9	C - NA CA - NA N - NA O - NA	NA	NA	NA
Total number of bonds					36	1	0	4
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

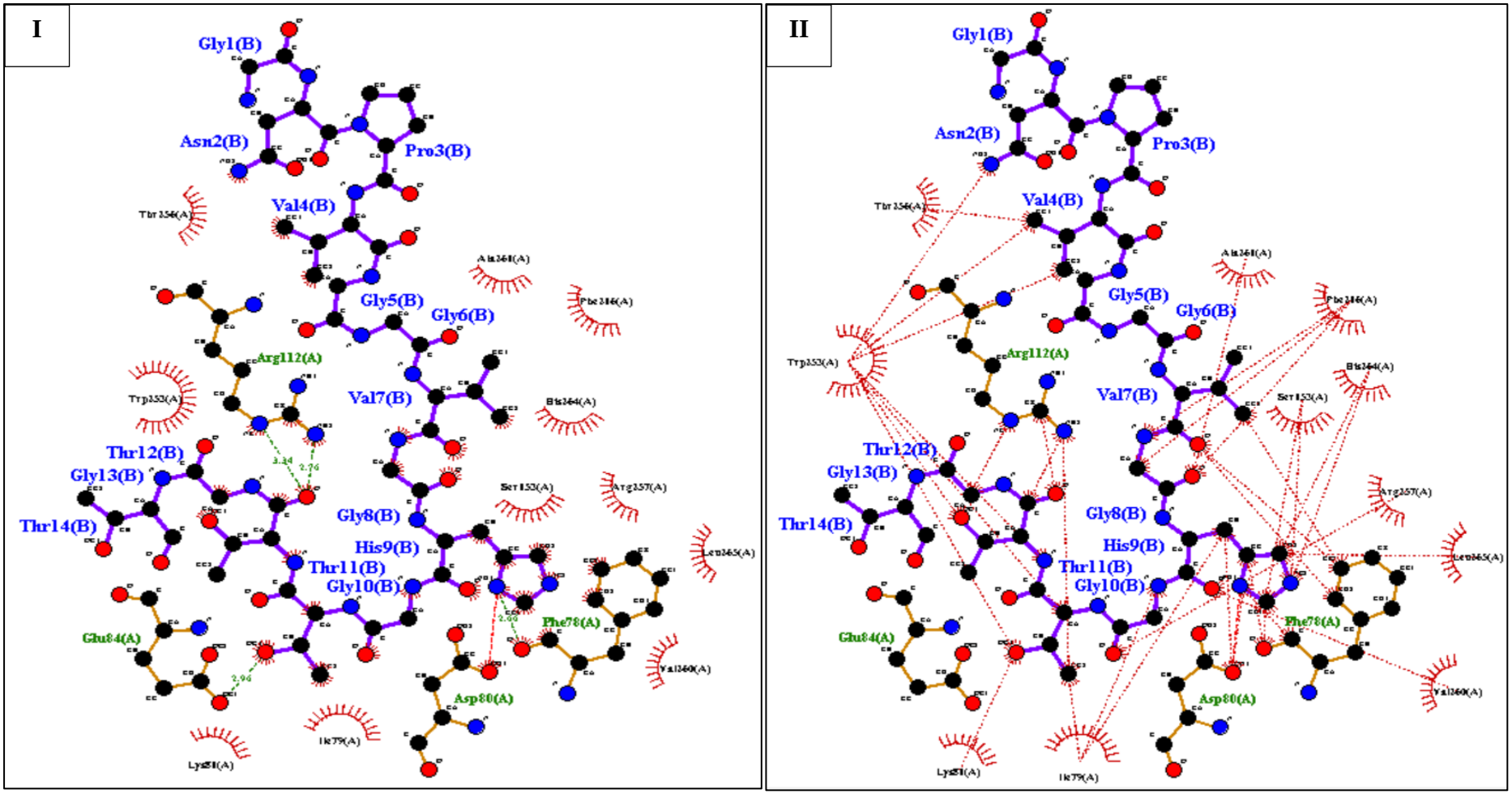

Figure S3a: Binding interaction of GNPVGGVGHGTTGT inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3b: Binding interaction of pancreatic lipase inhibitory peptides-GQLGEHGGAGMG at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **G**QLGEHGGAG MG	GLY1	cluster1_1	-8.5	C - Phe78 CA - Tyr115 N - Phe78, Tyr115 O - Phe78	NA	NA	NA
Total number of bonds					24	0	0	0
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					21%	0%	0%	0%

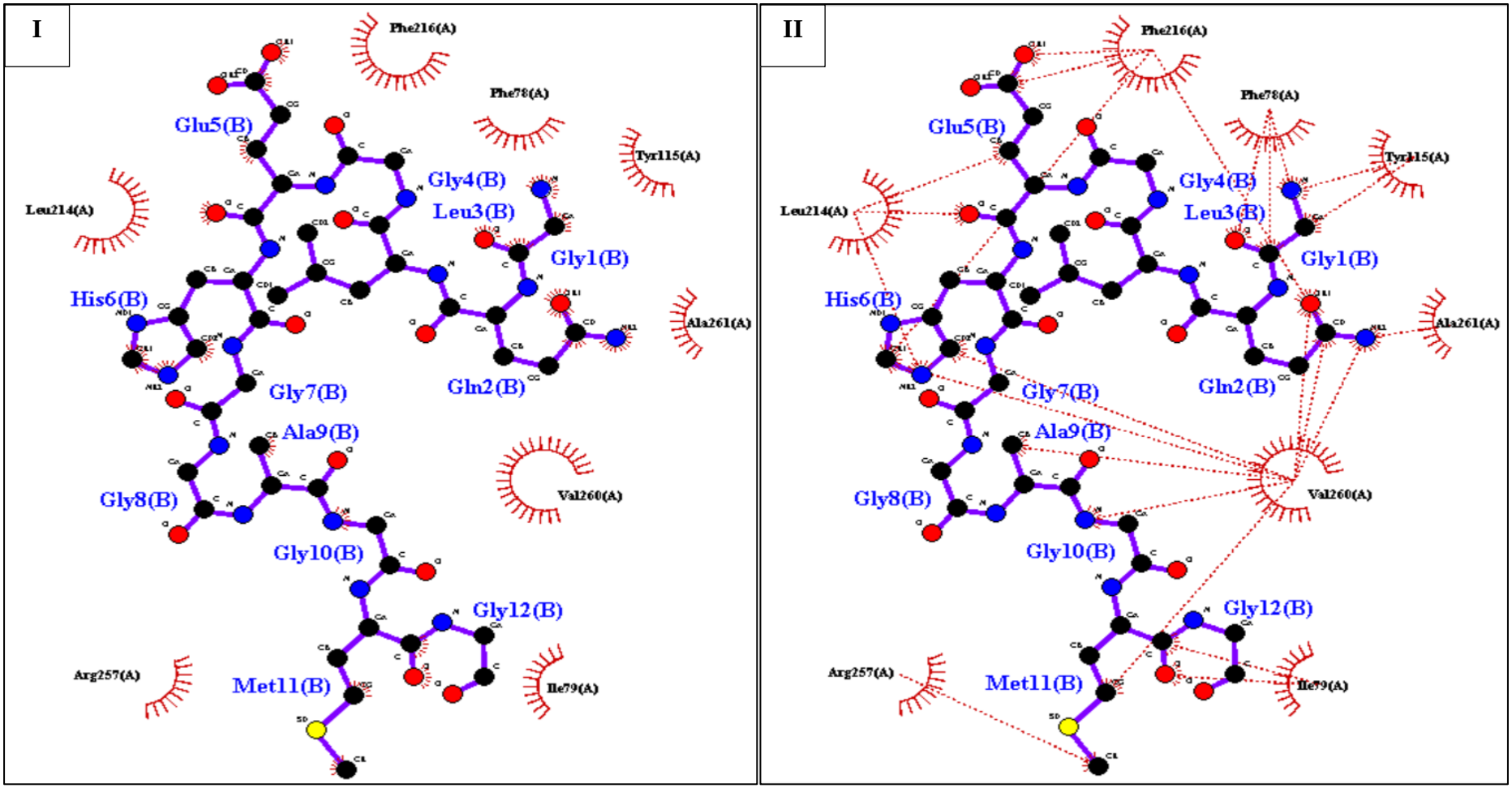

Figure S3b: Binding interaction of **G**QLGEHGGAGMG inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3c: Binding interaction of pancreatic lipase inhibitory peptides-FFRSKLLSRGAAAAKGALLPQYW at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **F**FRSKLLSRG AAAAKGALLP QYW	PHE1	cluster1_3	-9.2	C - Thr116 CA - Thr116 CB - NA CD_1 - Gly114 CD_2 - NA CE_1 - NA CE_2 - NA CG - NA CZ -NA N - Thr116 O - NA	NA	NA	NA
Total number of bonds					45	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

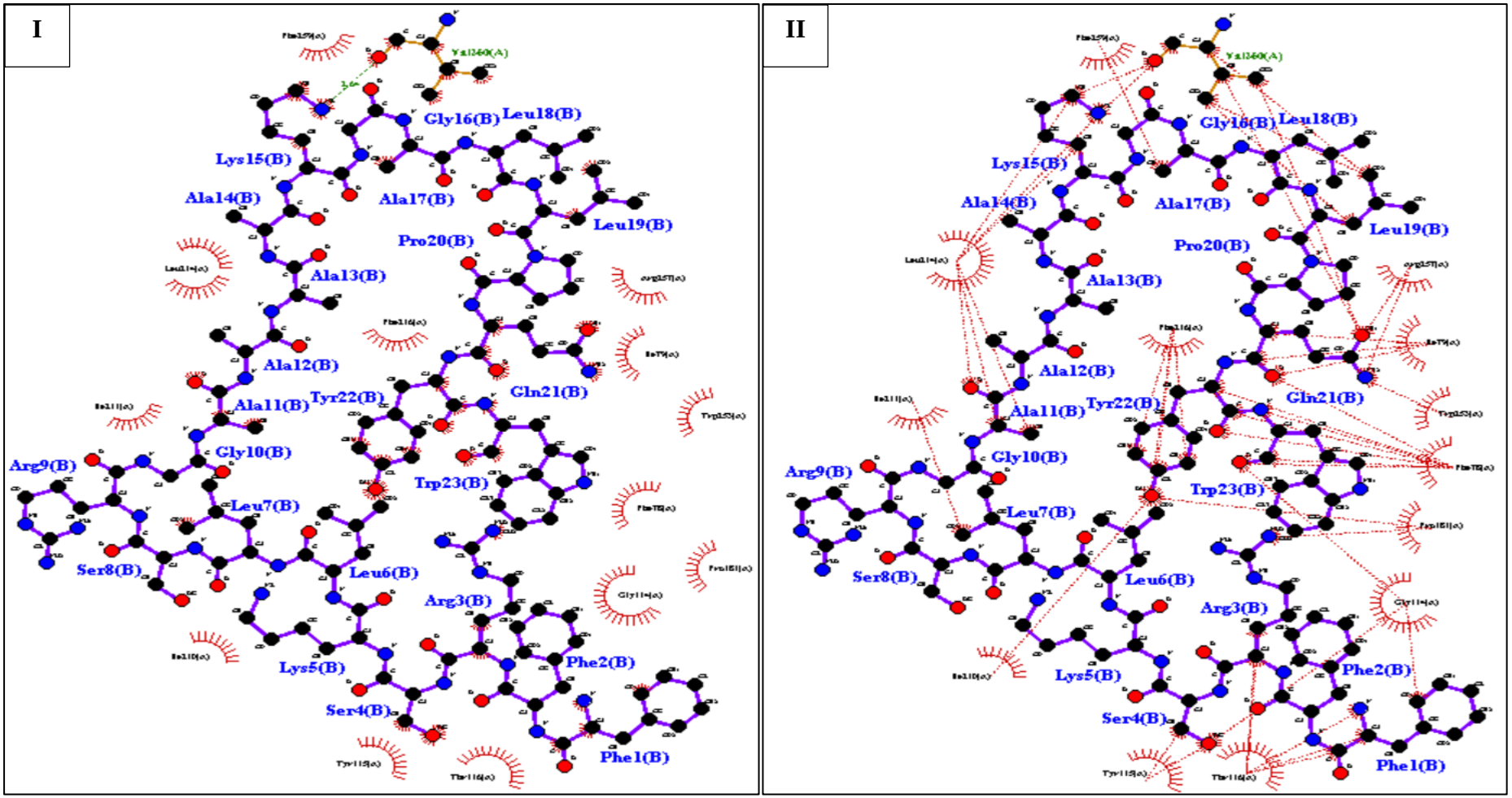

Figure S3c: Binding interaction of **FFRSKLLSRGAAAAKGALLPQYW** inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3d: Binding interaction of pancreatic lipase inhibitory peptides- FVVAEQAGNEEGFE at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **F**VVAEQAGNE EGFE	PHE1	cluster3_4	-8.8	C - NA CA - NA CB - NA CD_1 - NA CD_2 - Cys182 CE_1 - Glu180, Ile210 CE_2 - Glu180, Cys182 CG - NA CZ - Glu180, Ile210 N - NA O - NA	NA	NA	NA
Total number of bonds					45	1	0	2
Total no of interactive residues					7	0	0	0
Overall percentage of bonding					16%	0%	0%	0%

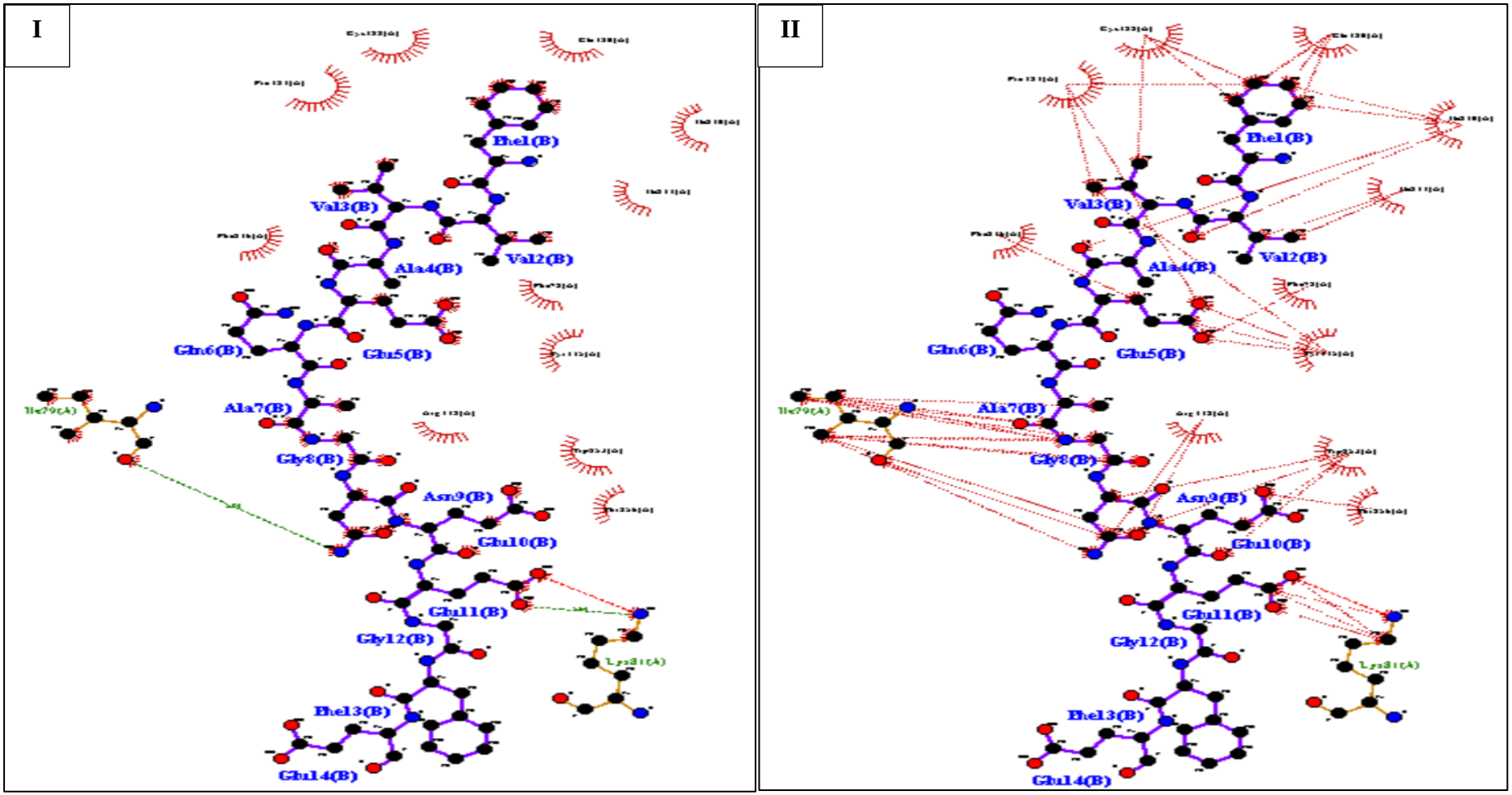

Figure S3d: Binding interaction of **F**VVAEQAGNEEGFE inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3e: Binding interaction of pancreatic lipase inhibitory peptides-MLPLMLPFTMGY at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **M**LPLMLPFTM GY	MET1	cluster2_1	-8.4	C - NA CA - NA CB - Phe259 CE – Thr256 CG - Thr256 O - NA N - NA SD - Thr256	NA	NA	NA
Total number of bonds					41	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

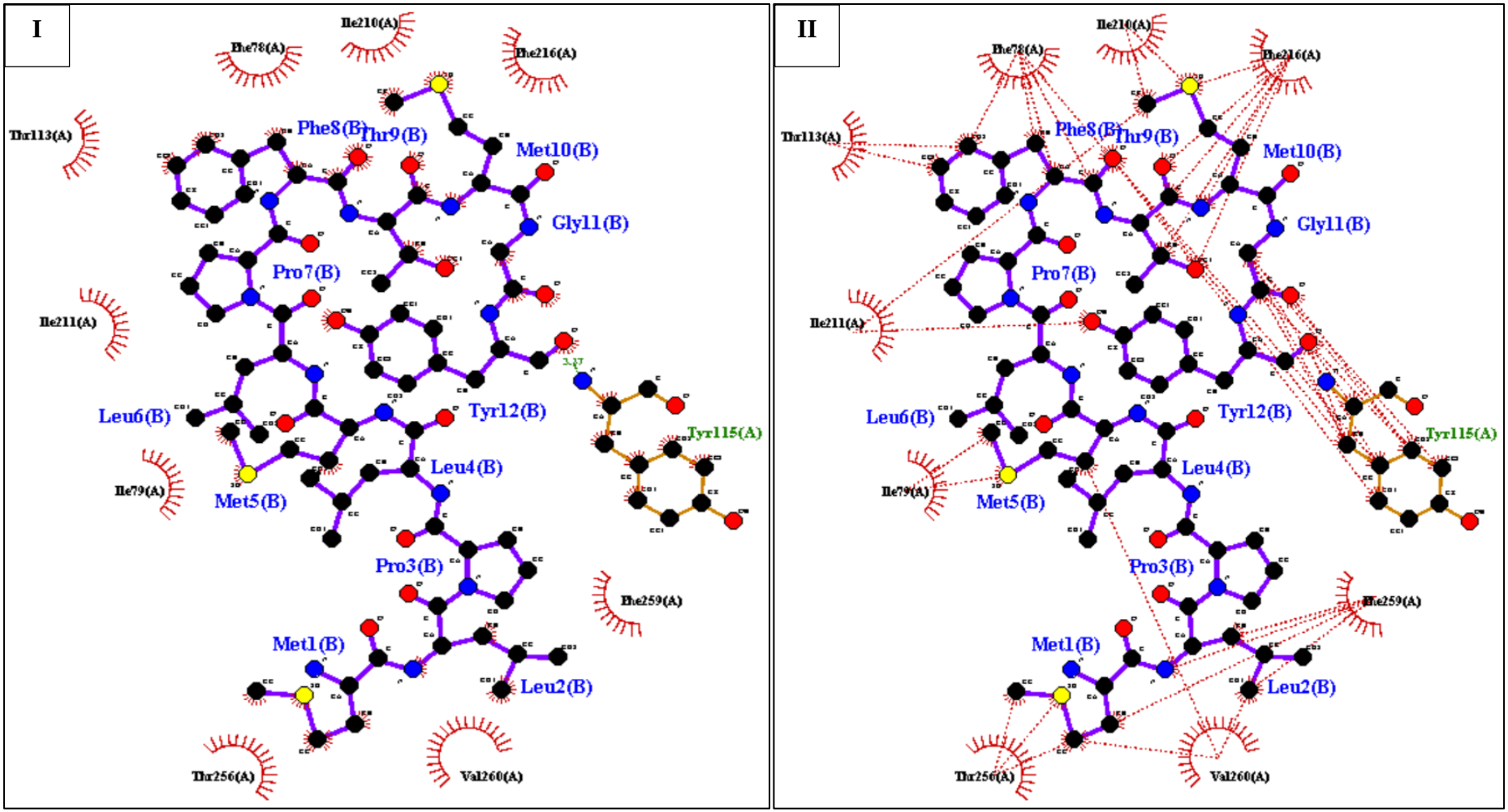

Figure S3e: Binding interaction of **M**LPLMLPFTMGY inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3f: Binding interaction of pancreatic lipase inhibitory peptides-MSKFLPLPLMFY at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **M**SKFLPLPLM FY	MET1	cluster1_4	-7.4	C - NA CA - NA CB - NA CE -Phe216 CG - NA O - NA N - Ile79 SD - Phe78	NA	NA	NA
Total number of bonds					45	0	0	2
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					7%	0%	0%	0%

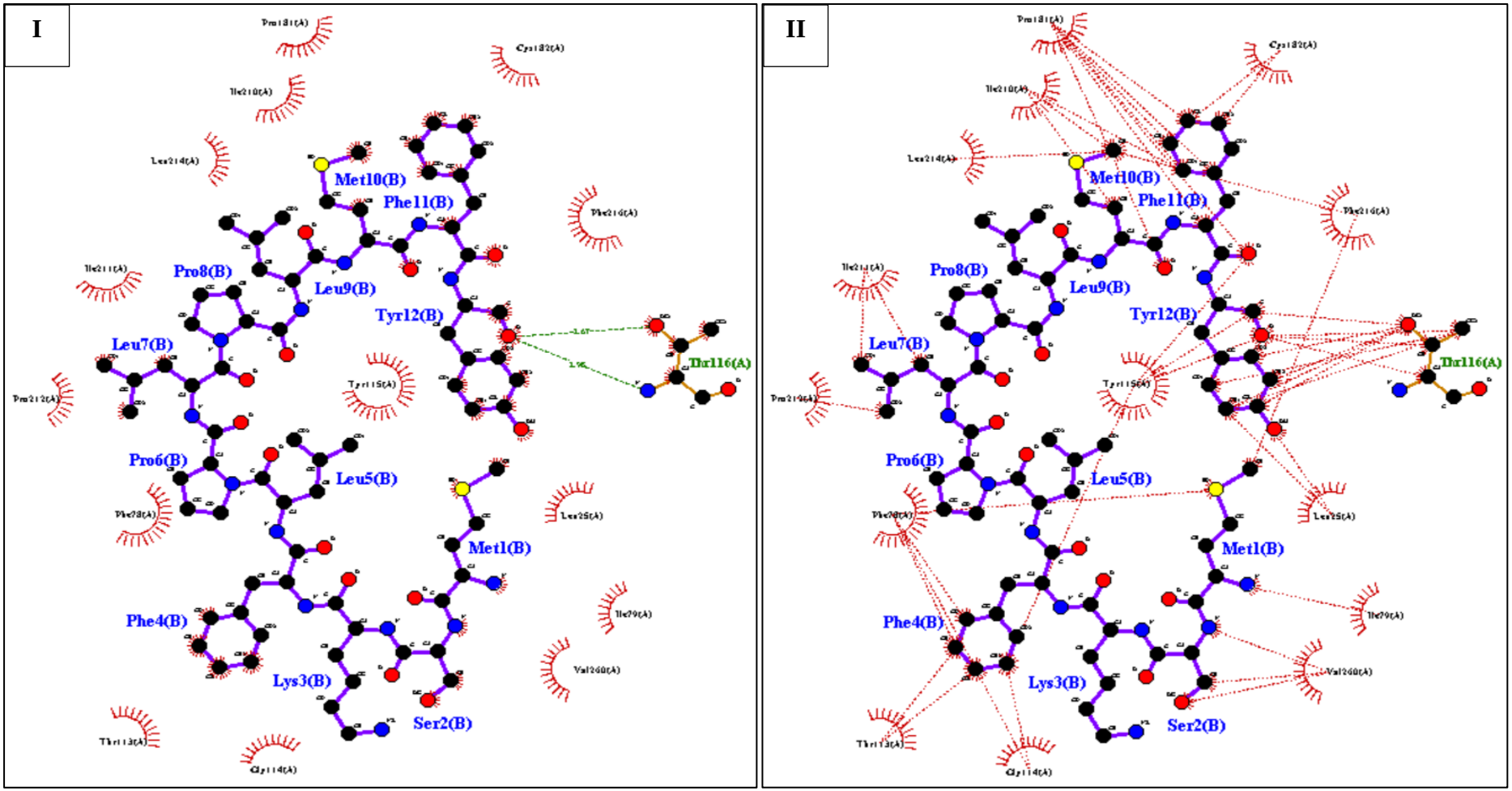

Figure S3f: Binding interaction of **M**SKFLPLPLMFY inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3g: Binding interaction of pancreatic lipase inhibitory peptides-LAAVEALSTNG at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **L**AAVEALSTN G	LEU1	cluster1_1	-8.4	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					31	0	0	3
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

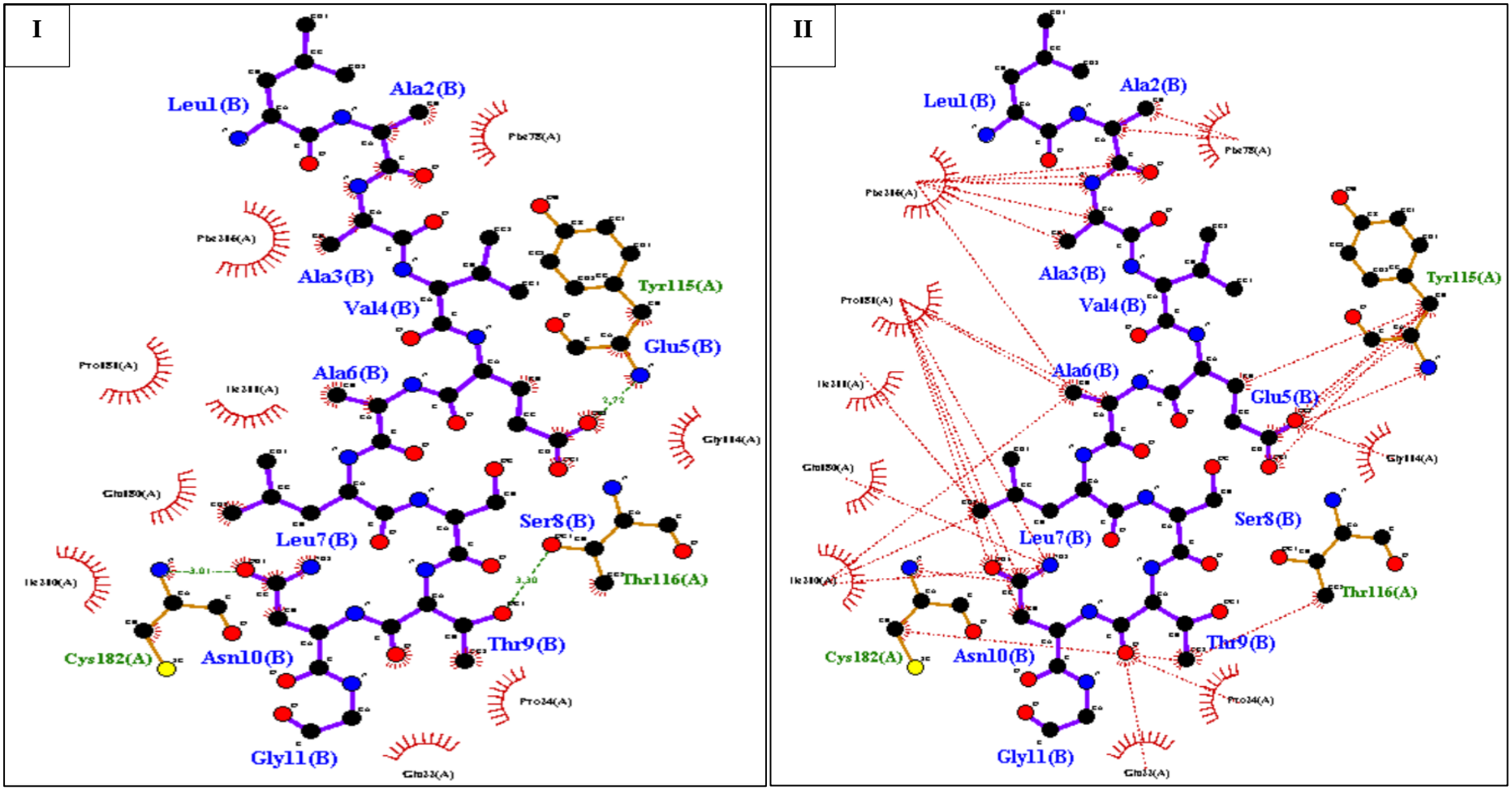

Figure S3g: Binding interaction of **L**AAVEALSTNG inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3h: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **L**NNPSVCDCD CMMKAAR	LEU1	cluster3_4	-9.8	C - NA CA -Phe216 CB - Phe78 CD_1 -Phe78 CD_2 - Phe216 CG - Phe78 N - Phe216 O - NA	NA	NA	NA
Total number of bonds					45	0	0	3
Total no of interactive residues					6	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

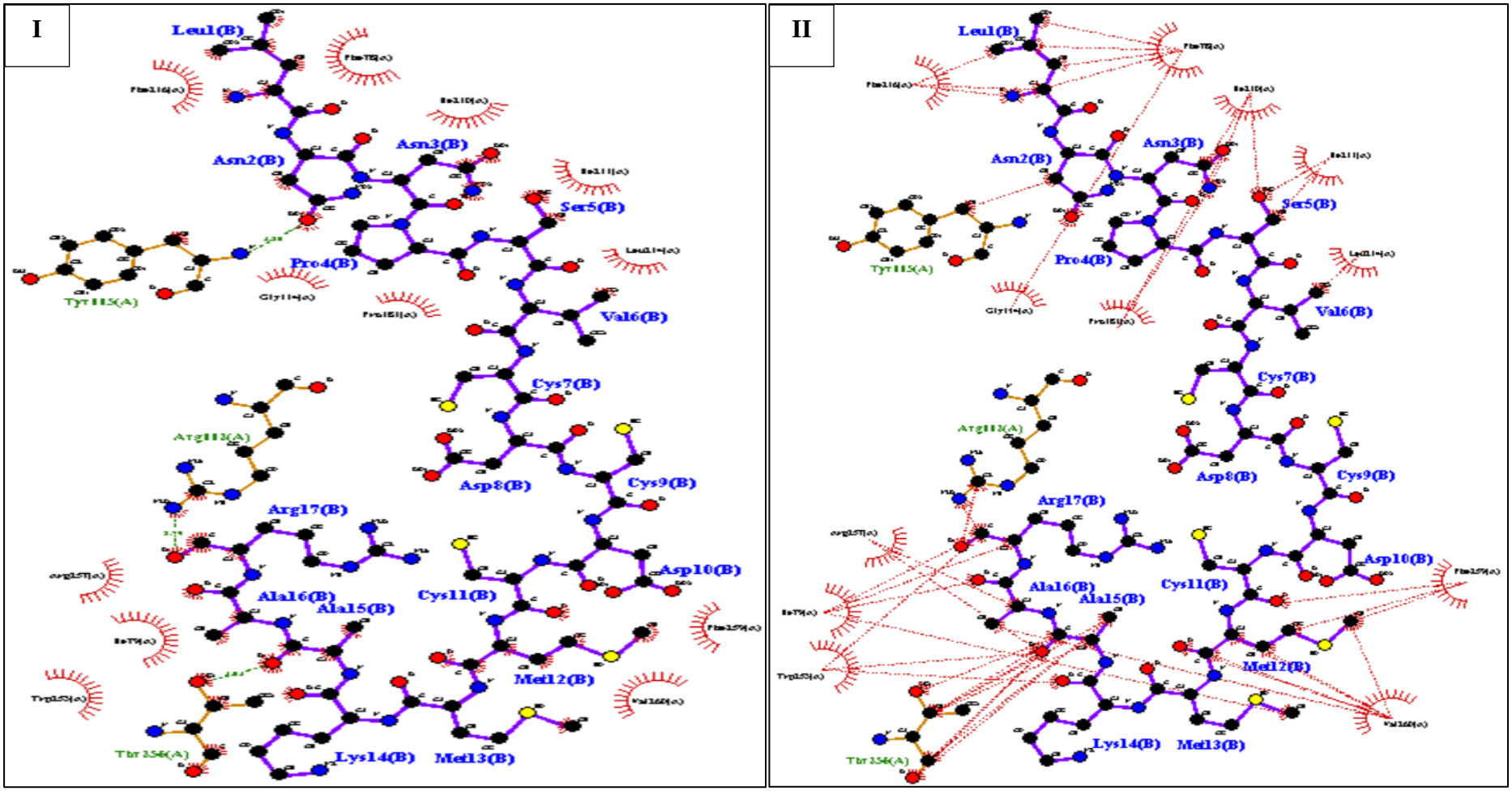

Figure S3h: Binding interaction of LNNPSVCDCDCMMKAAR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S3i: Binding interaction of pancreatic lipase inhibitory peptides- NALKCCHSCPA at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **N**ALKCCHSCP A	ASN1	cluster1_3	-10.4	C - Val260 CA - Val260 CB - NA CG - NA N - Val260 ND_2 - NA O - Val260 OD_1 - NA	NA	NA	NA
Total number of bonds					47	0	0	2
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

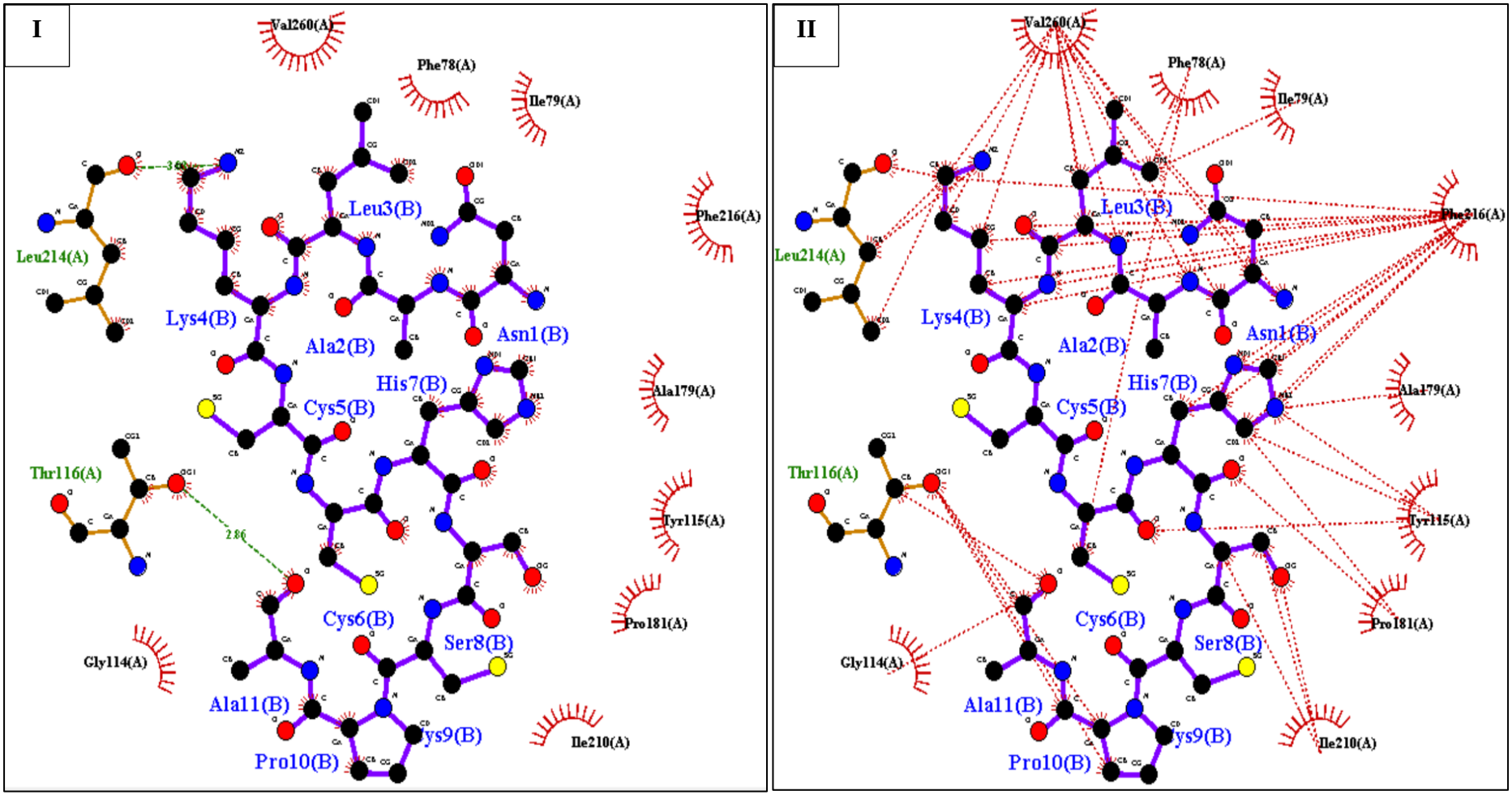

Figure S3i: Binding interaction of NALKCCHSCPA inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides

Table S3j: Binding interaction of pancreatic lipase inhibitory peptides- ALWGAGGGGLGLSSGR at N1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide **A**LWGAGGGGL GLSSGR	ALA1	cluster1_4	-7.6	C - NA CA - NA CB - NA N - NA O - NA	NA	NA	NA
Total number of bonds					45	0	0	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

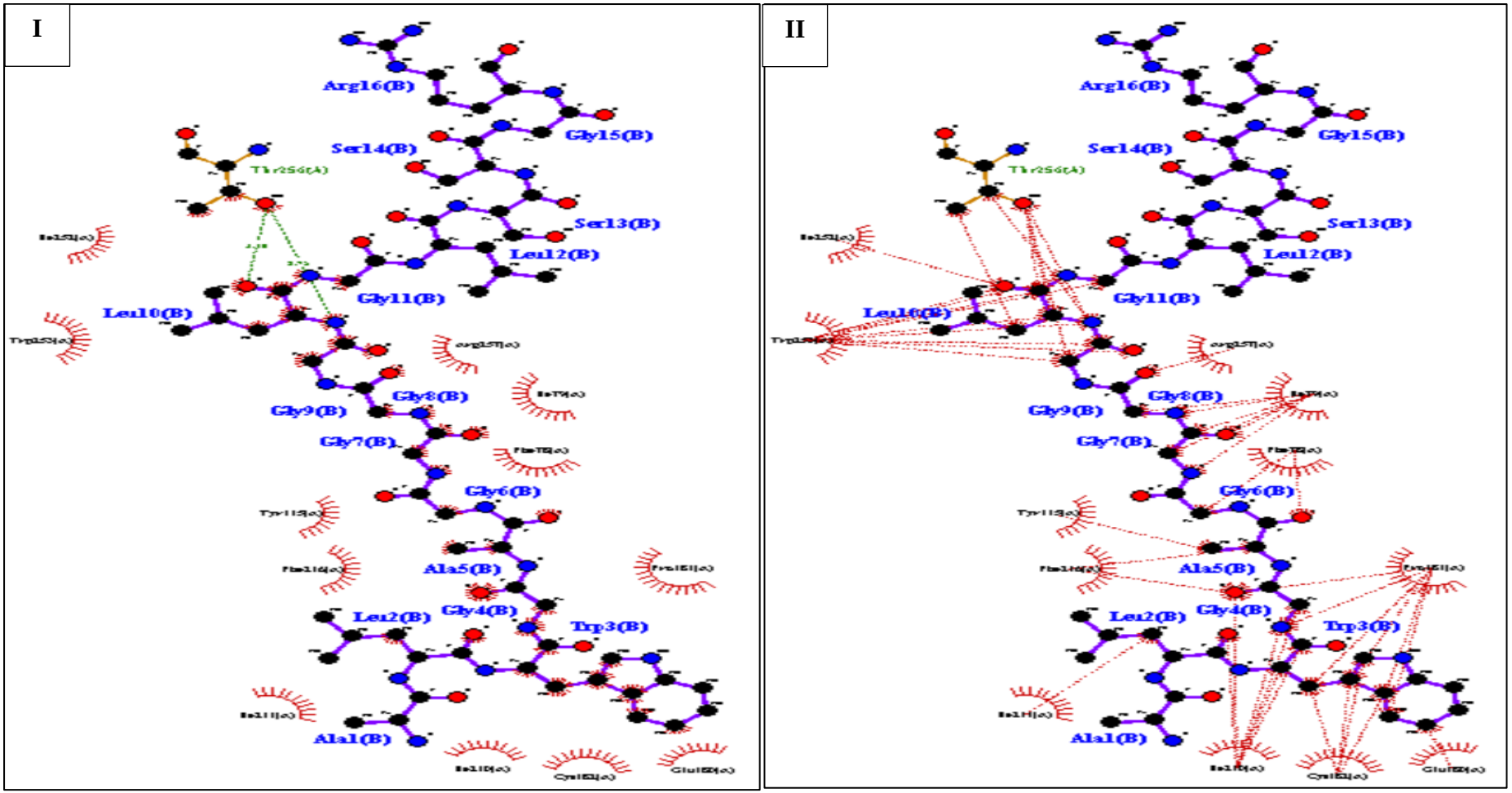

Figure S3j: Binding interaction of ALWGAGGGGLGLSSGR inhibitory peptide at N1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S4a: Binding interaction of pancreatic lipase inhibitory peptides-MMML at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Short chain peptide MMM**L**	LEU4	cluster10_1	-7.3	C - Tyr115, Pro181 CA - Tyr115 CB - Tyr115, Pro181 CD_1 - Ser153, Ala179 Phe216, His264 CD_2 - Tyr115, Ser153 Leu154, Phe216 CG - Phe216 N - Phe216 O - Pro181	NA	NA	NA
Total number of bonds					34	0	0	1
Total no of interactive residues					16	0	0	0
Overall percentage of bonding					47%	0%	0%	0%

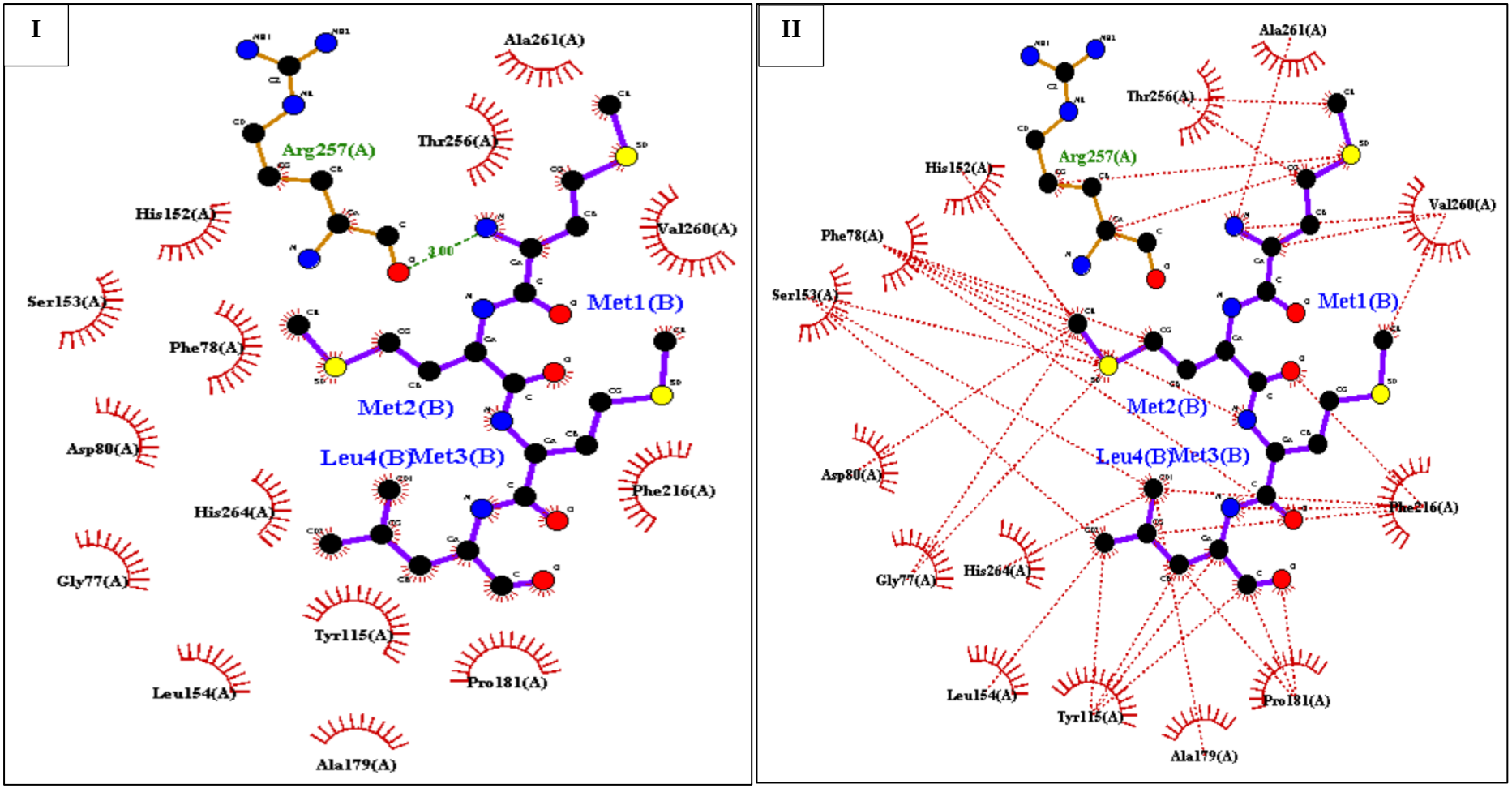

Figure S4a: Binding interaction of MMM**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S4b: Binding interaction of pancreatic lipase inhibitory peptides-FDML at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Short chain peptide FDM**L**	LEU4	cluster4_3	-7.1	C - NA CA - NA CB - Ile79 CD_1 - NA CD_2 - NA CG - NA N - Ile79 O – Ile79	NA	NA	NA
Total number of bonds					21	0	0	0
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					14%	0%	0%	0%

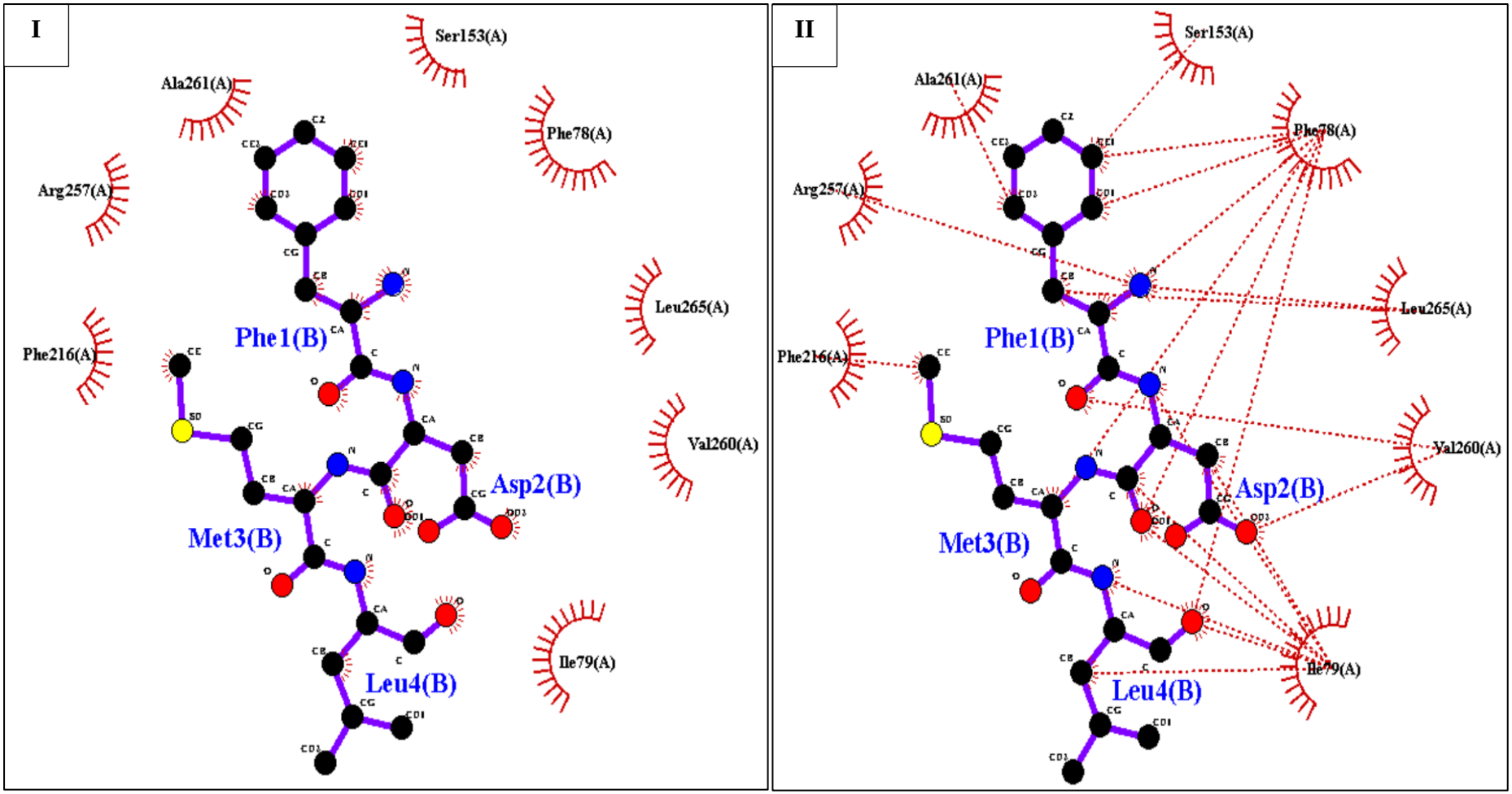

Figure S4b: Binding interaction of FDM**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S4c: Binding interaction of pancreatic lipase inhibitory peptides-RLLP at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Short chain peptide RLL**P**	PRO4	cluster8_1	-7.2	C - NA CA -NA CB - NA CD - Val260 CG -Thr256 N- NA O - Trp253	NA	NA	NA
Total number of bonds					21	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					14%	0%	0%	0%

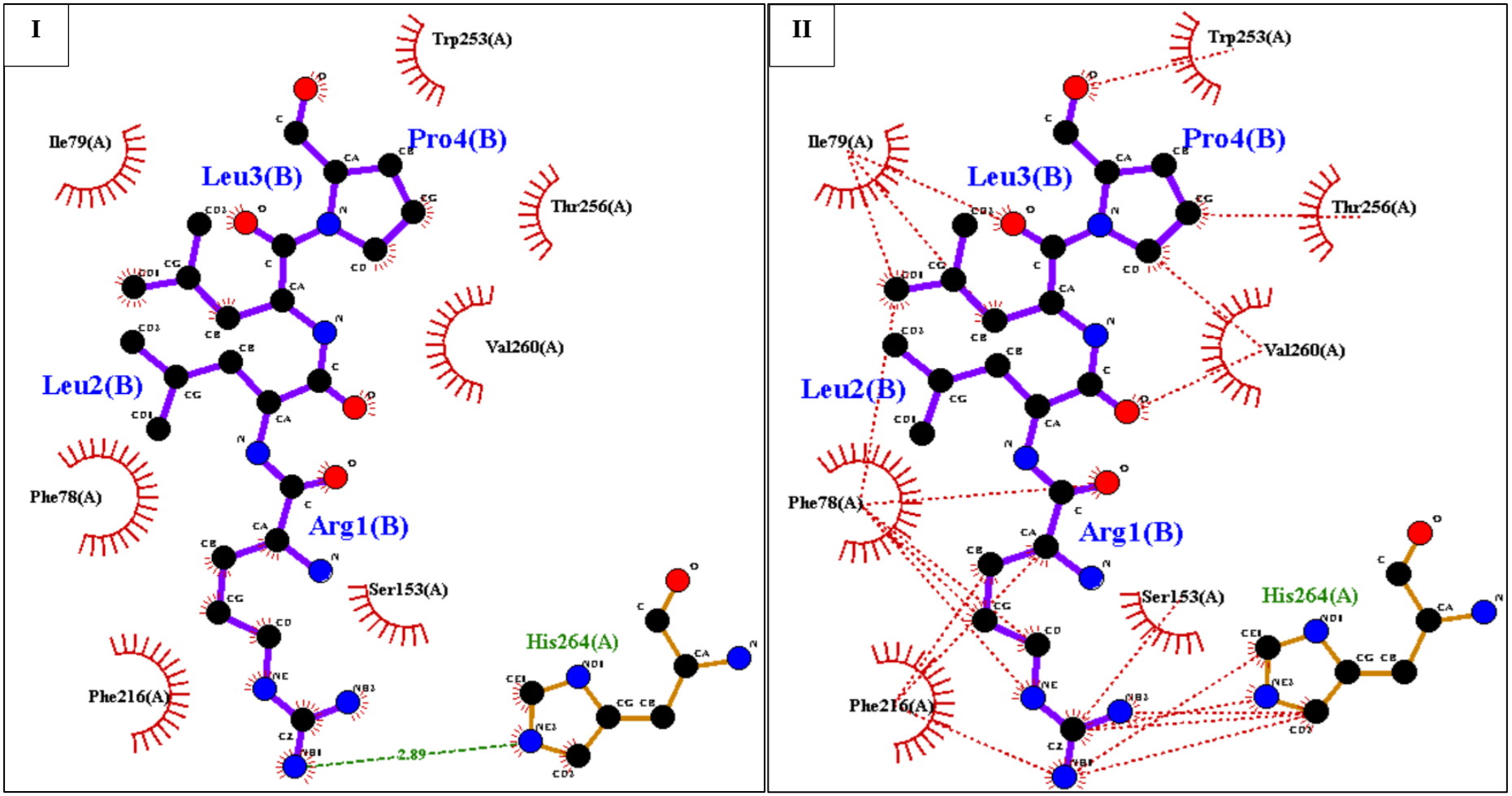

Figure S4c: Binding interaction of RLL**P** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5a: Binding interaction of pancreatic lipase inhibitory peptides-LAPSTIK at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide LAPSTI**K**	LYS7	cluster1_2	-8.0	C - NA CA - NA CB - Phe216 CD - Pro181, Phe216 CE - Tyr115 CG - Phe216 NZ - Ala179, Pro181, Phe216 O - NA	NA	NA	NZ - Tyr115
Total number of bonds					28	0	0	1
Total no of interactive residues					8	0	0	1
Overall percentage of bonding					29%	0%	0%	100%

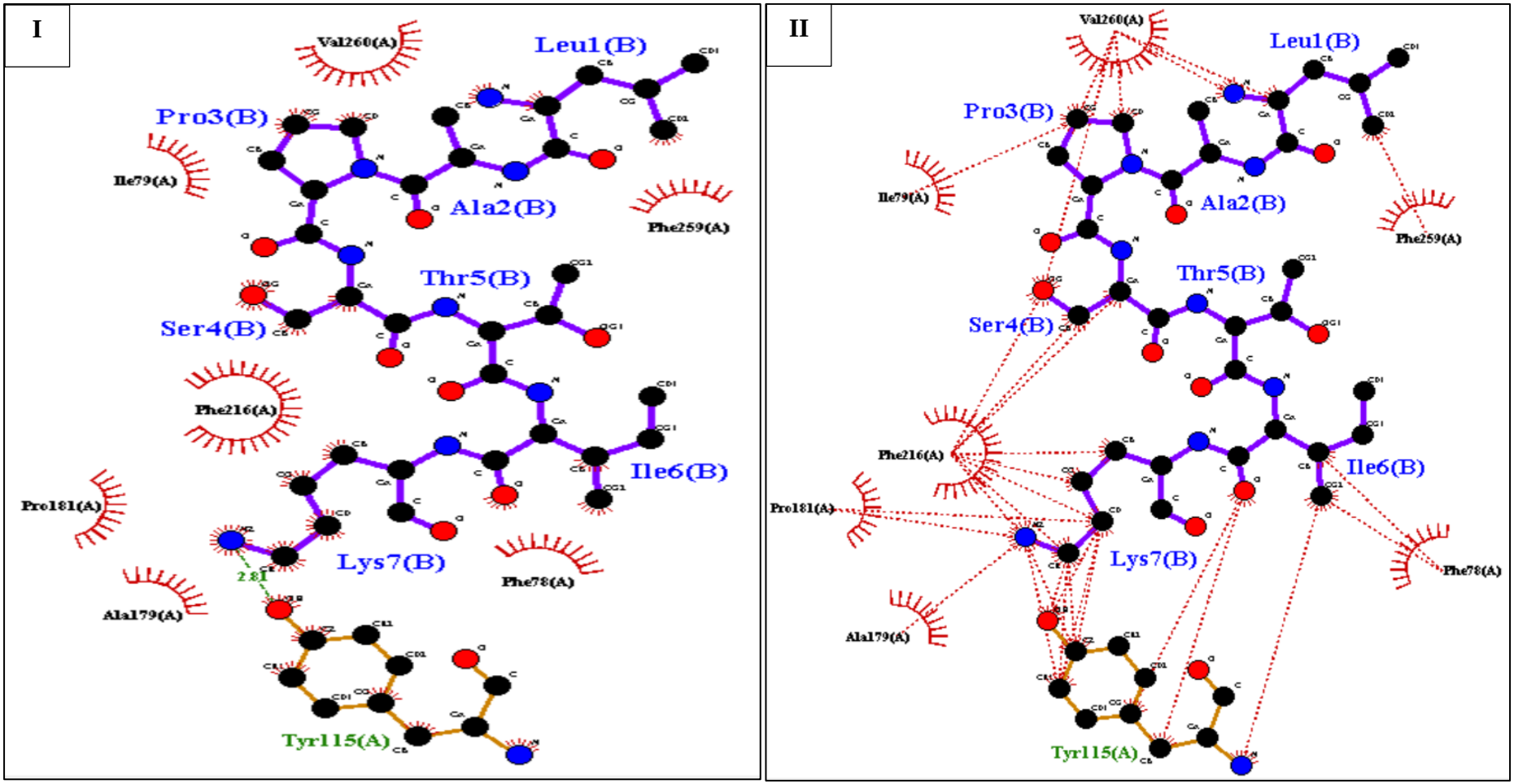

Figure S5a: Binding interaction of LAPSTI**K** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5b: Binding interaction of pancreatic lipase inhibitory peptides-KVEGDLK at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide KVEGDL**K**	LYS7	cluster1_2	-7.9	C - Phe216 CA - NA CB - Phe216 CD - Phe78, Phe216 CE - His 264 CG - Phe78 NZ - Ala261, His264 O - Tyr115, Pro181, Ile210, Phe216	NA	NA	NA
Total number of bonds					22	0	0	0
Total no of interactive residues					12	0	0	0
Overall percentage of bonding					55%	0%	0%	0%

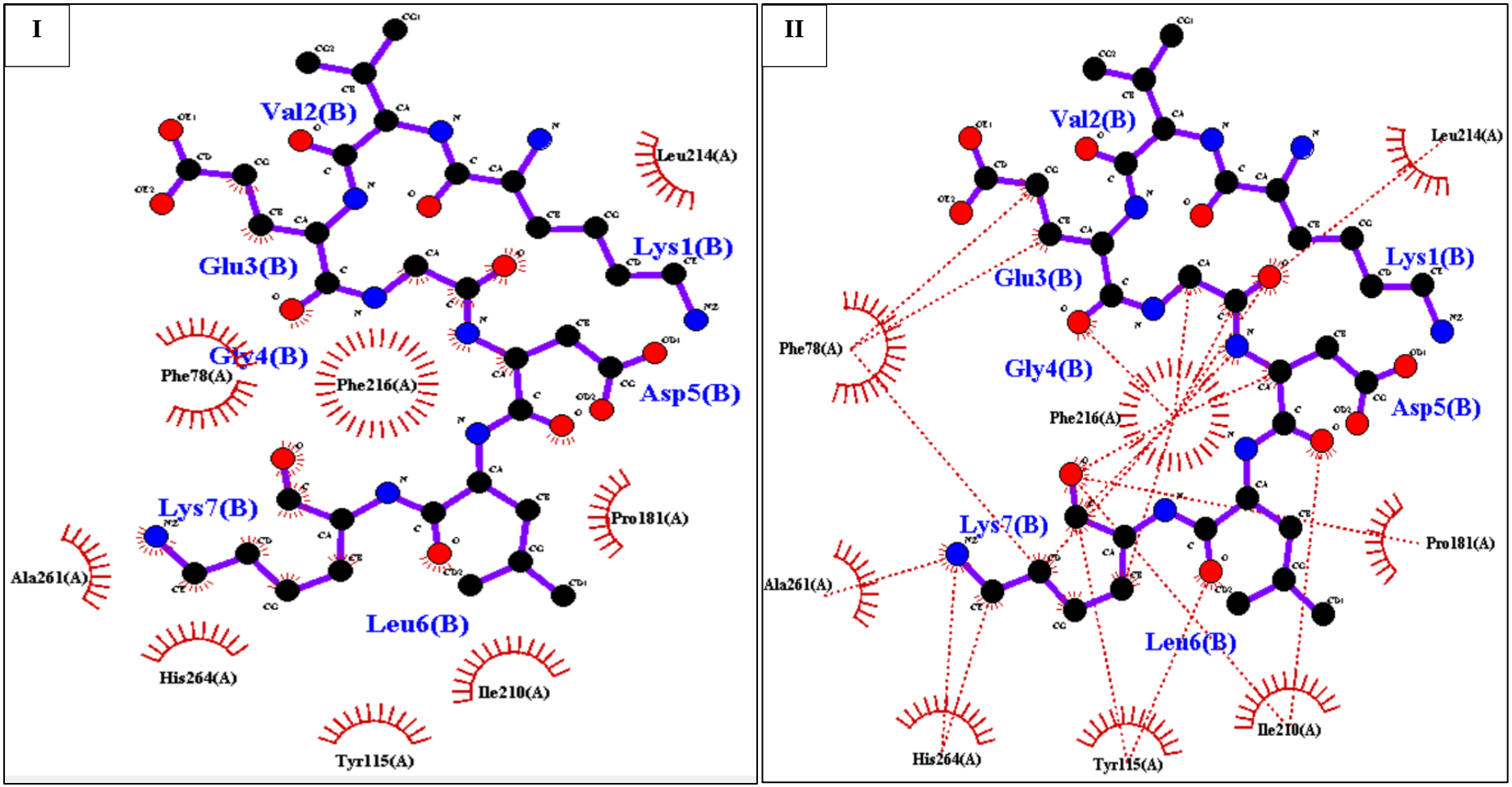

Figure S5b: Binding interaction of KVEGDL**K** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5c: Binding interaction of pancreatic lipase inhibitory peptides-ELPPHFL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide ELPPHF**L**	LEU7	cluster5_2	-6.8	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					33	0	0	4
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

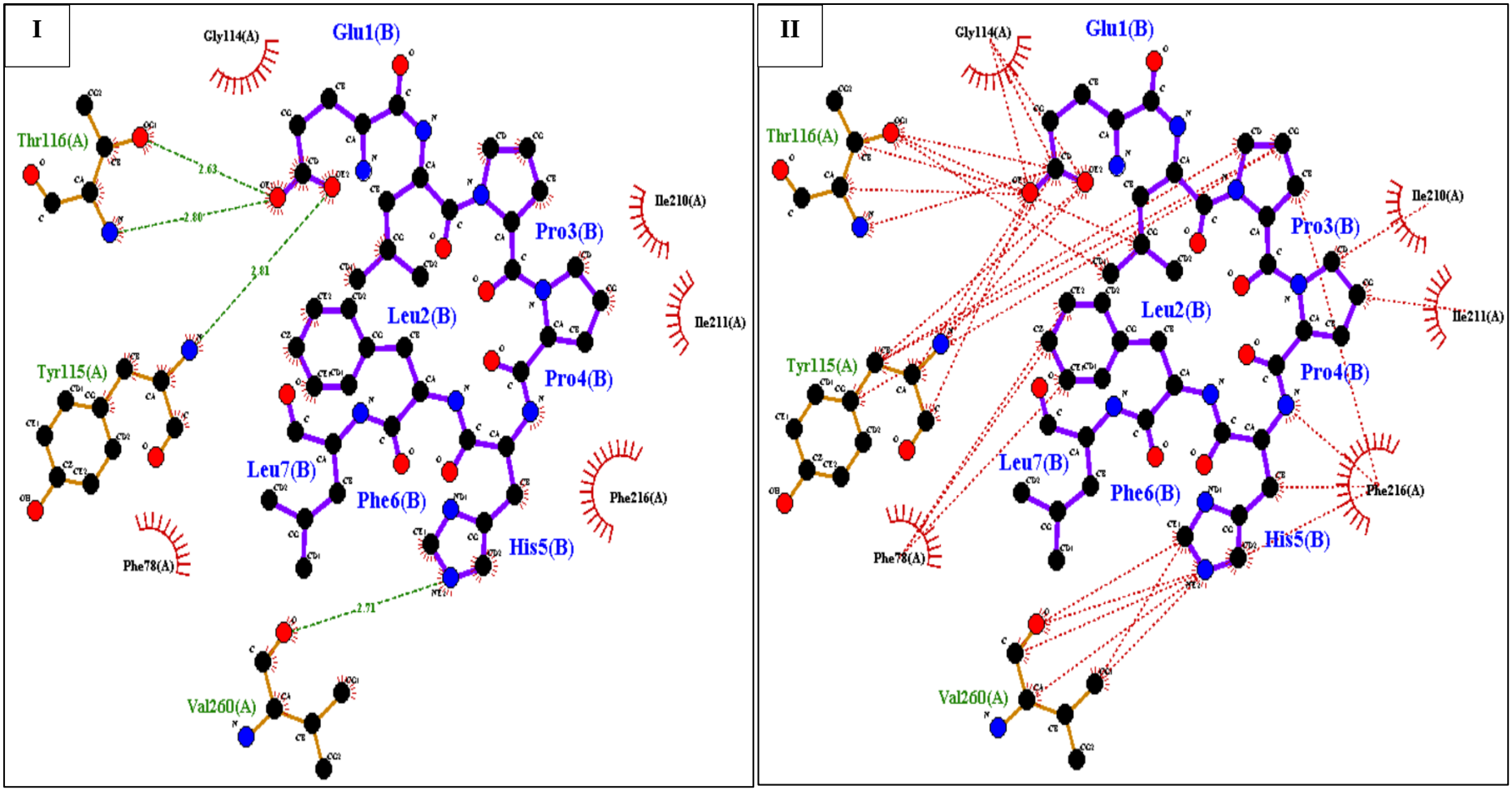

Figure S5c: Binding interaction of ELPPHF**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5d: Binding interaction of pancreatic lipase inhibitory peptides-FLWPEYGAL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide FLWPEYGA**L**	LEU9	cluster11_3	-7.6	C - NA CA - NA CB - NA CD_1 - NA CD_2 - Leu25 CG - NA N - NA O - Pro24	NA	NA	NA
Total number of bonds					30	0	0	3
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					7%	0%	0%	0%

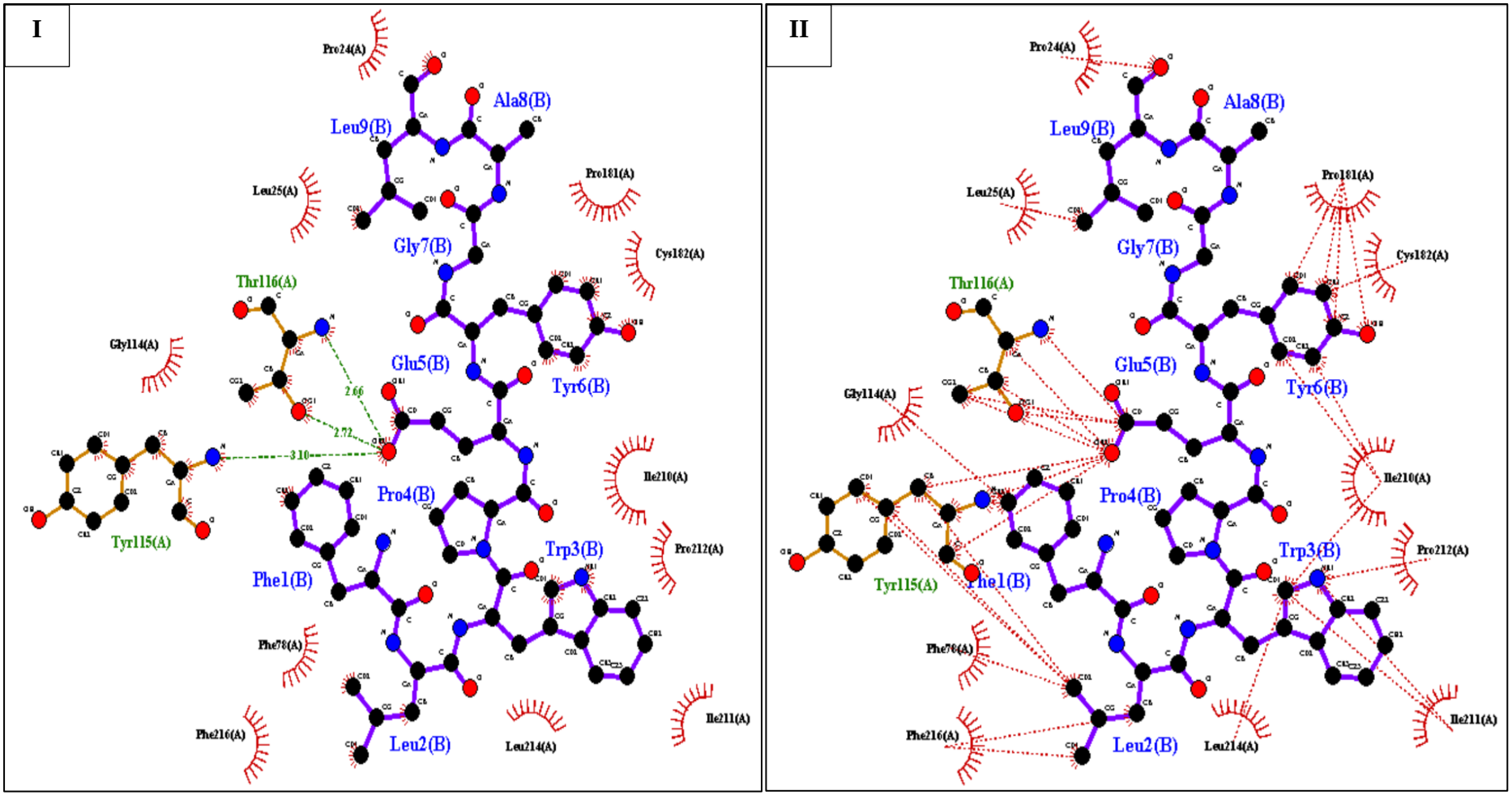

Figure S5d: Binding interaction of FLWPEYGA**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5e: Binding interaction of pancreatic lipase inhibitory peptides-AQMACPHL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide AQMACPH**L**	LEU8	cluster9_2	-8.9	C - Cys238 CA - NA CB - NA CD_1 - NA CD_2 - Gln254, Phe259 CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					44	2	0	4
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					7%	0%	0%	0%

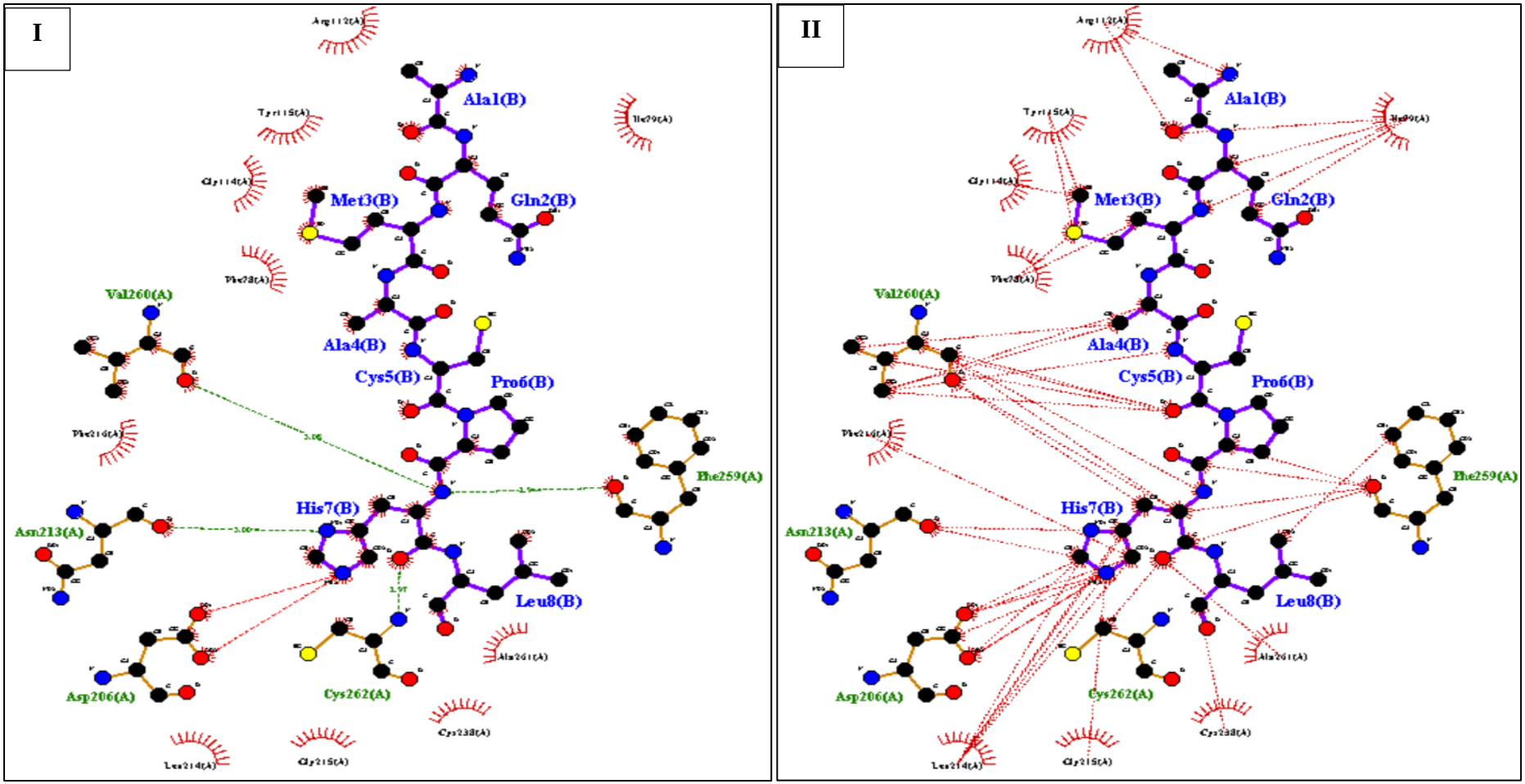

Figure S5e: Binding interaction of AQMACPH**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5f: Binding interaction of pancreatic lipase inhibitory peptides-AEWLHDWKL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide AEWLHDWK**L**	LEU9	cluster1_1	-7.0	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					21	0	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

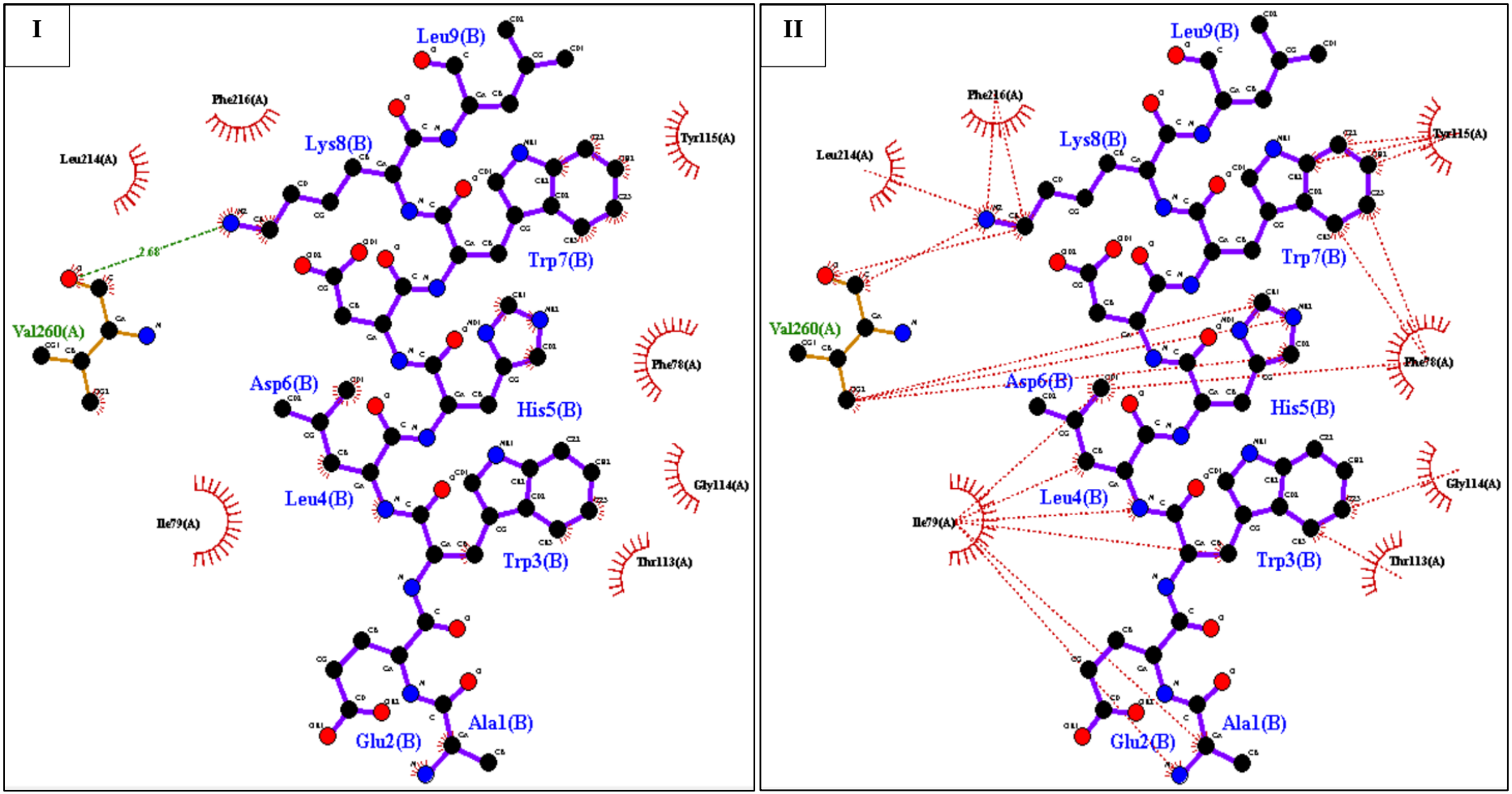

Figure S5f: Binding interaction of AEWLHDWK**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5g: Binding interaction of pancreatic lipase inhibitory peptides-GMAGGPPLL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide GMAGGPPL**L**	LEU9	cluster8_1	-7.5	C - Phe78, His264 CA - Phe78, Ile79 CB - NA CD_1 - Arg257, Val260 CD_2 - Ile79 CG - NA N - NA O - Leu265	NA	NA	NA
Total number of bonds					29	0	0	1
Total no of interactive residues					8	0	0	0
Overall percentage of bonding					28%	0%	0%	0%

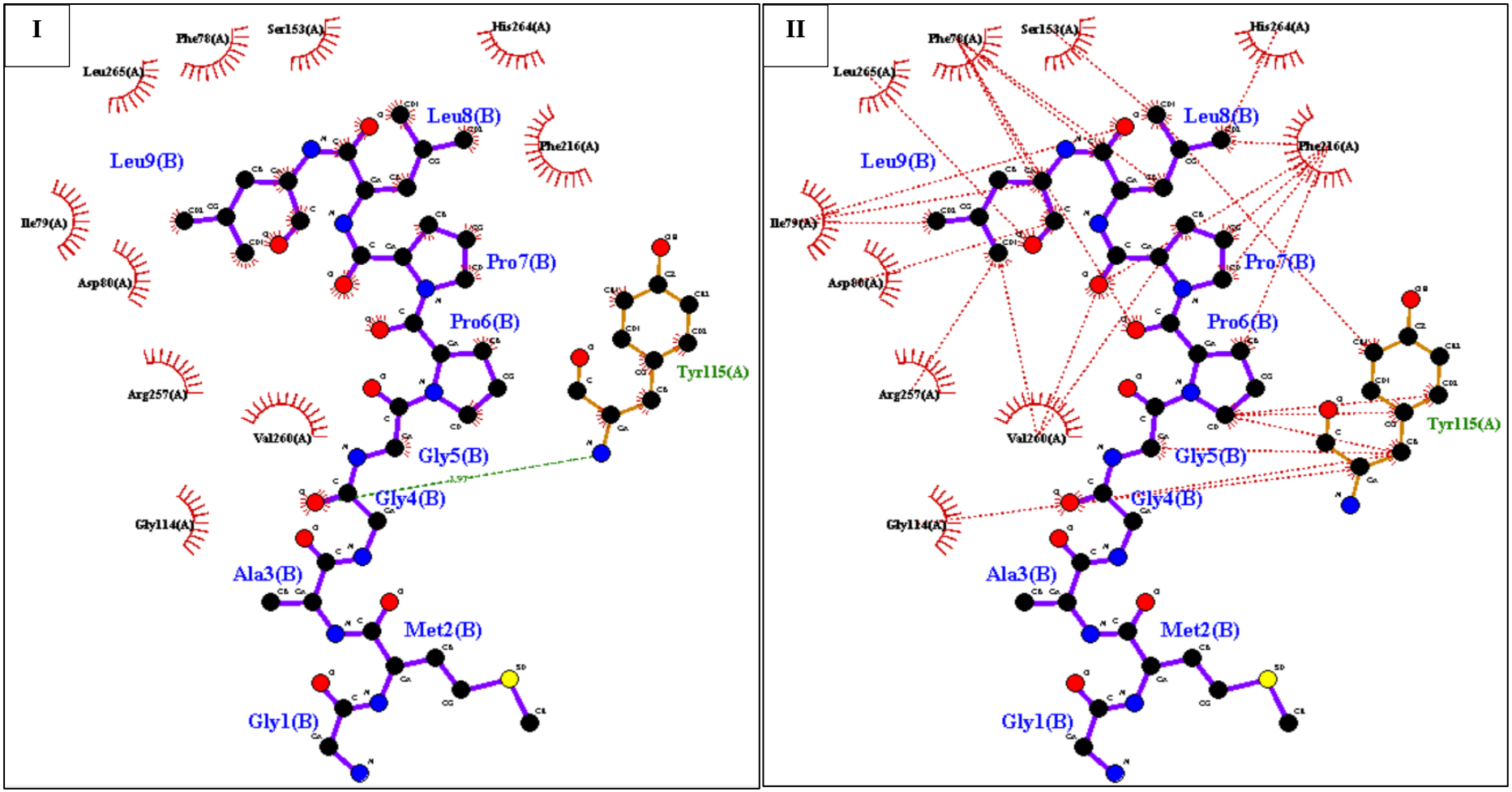

Figure S5g: Binding interaction of GMAGGPPL**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5h: Binding interaction of pancreatic lipase inhibitory peptides-KDLWDDFKGL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide KDLWDDFKG**L**	LEU10	cluster2_1	-8.5	C - NA CA - NA CB - Pro181 CD_1 - Tyr115 CD_2 - NA CG - NA N - Pro181 O - Pro181, Ile210	NA	NA	NA
Total number of bonds					48	0	0	2
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

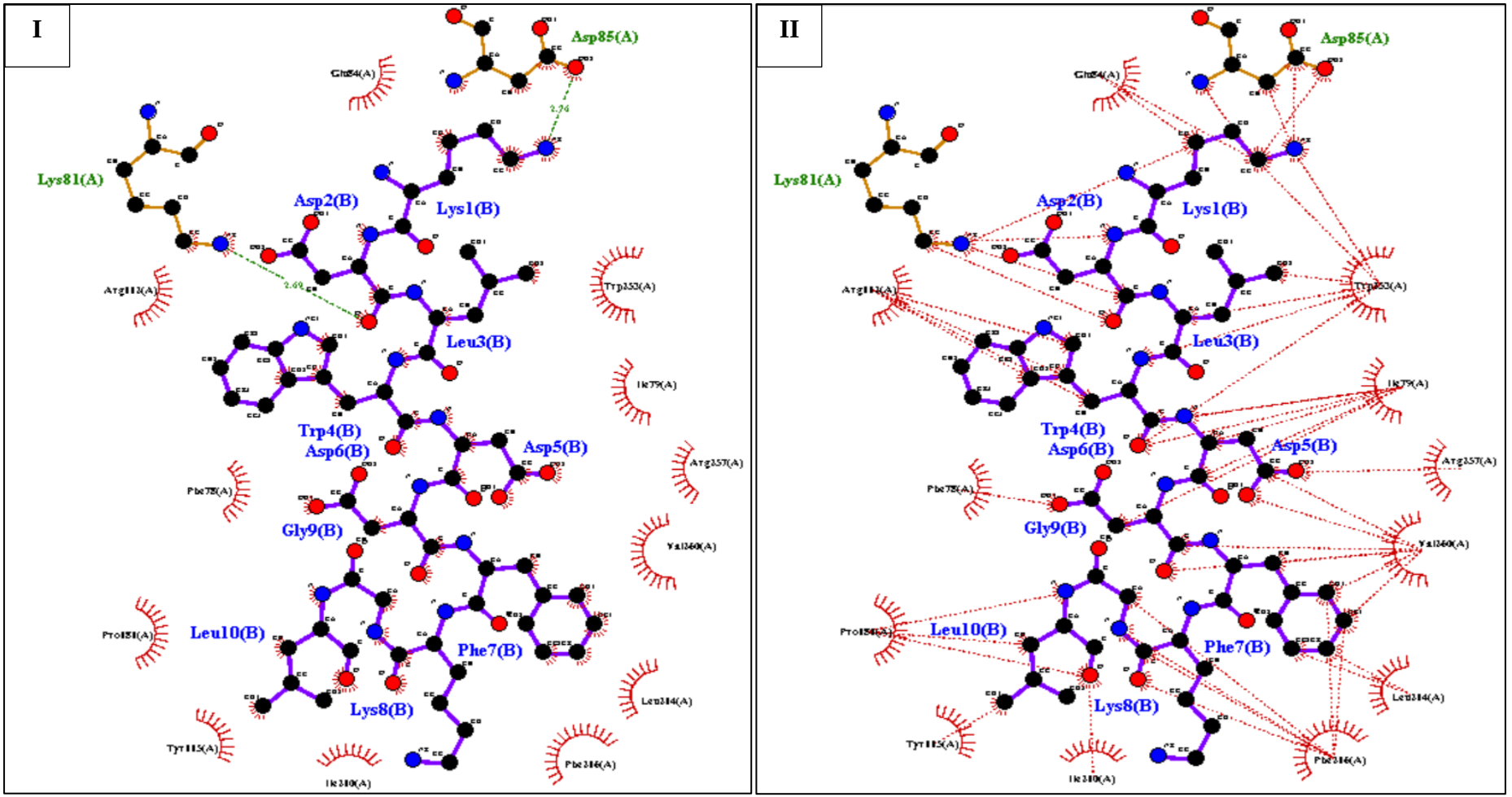

Figure S5h: Binding interaction of KDLWDDFKG**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5i: Binding interaction of pancreatic lipase inhibitory peptides-LLPAPPLL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide LLPAPPL**L**	LEU8	cluster11_3	-6.7	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					23	0	0	0
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

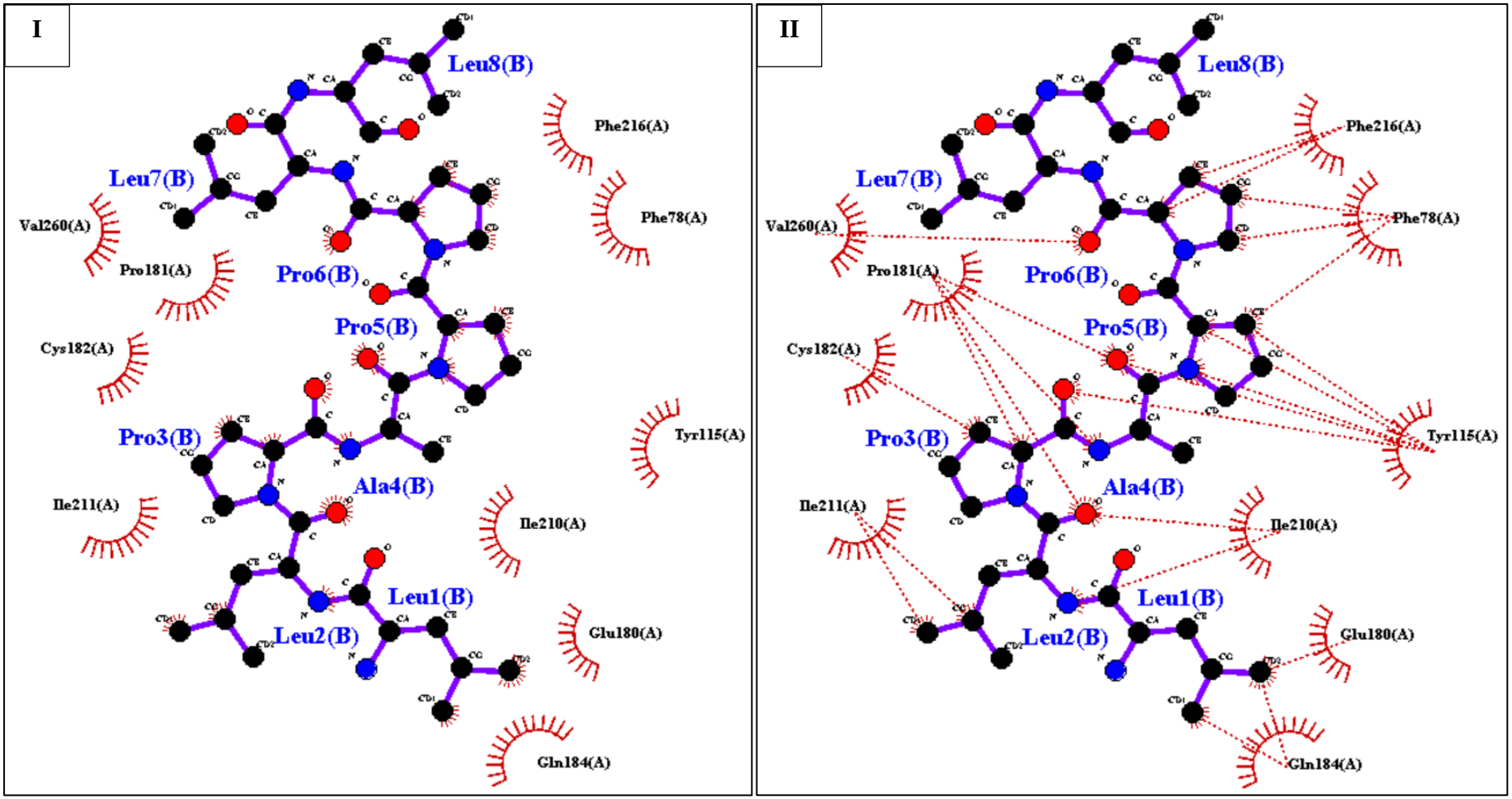

Figure S5i: Binding interaction of LLPAPPL**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5j: Binding interaction of pancreatic lipase inhibitory peptides-WGLWDDMQGL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide WGLWDDMQG**L**	LEU10	cluster1_2	-7.6	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					39	2	0	3
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

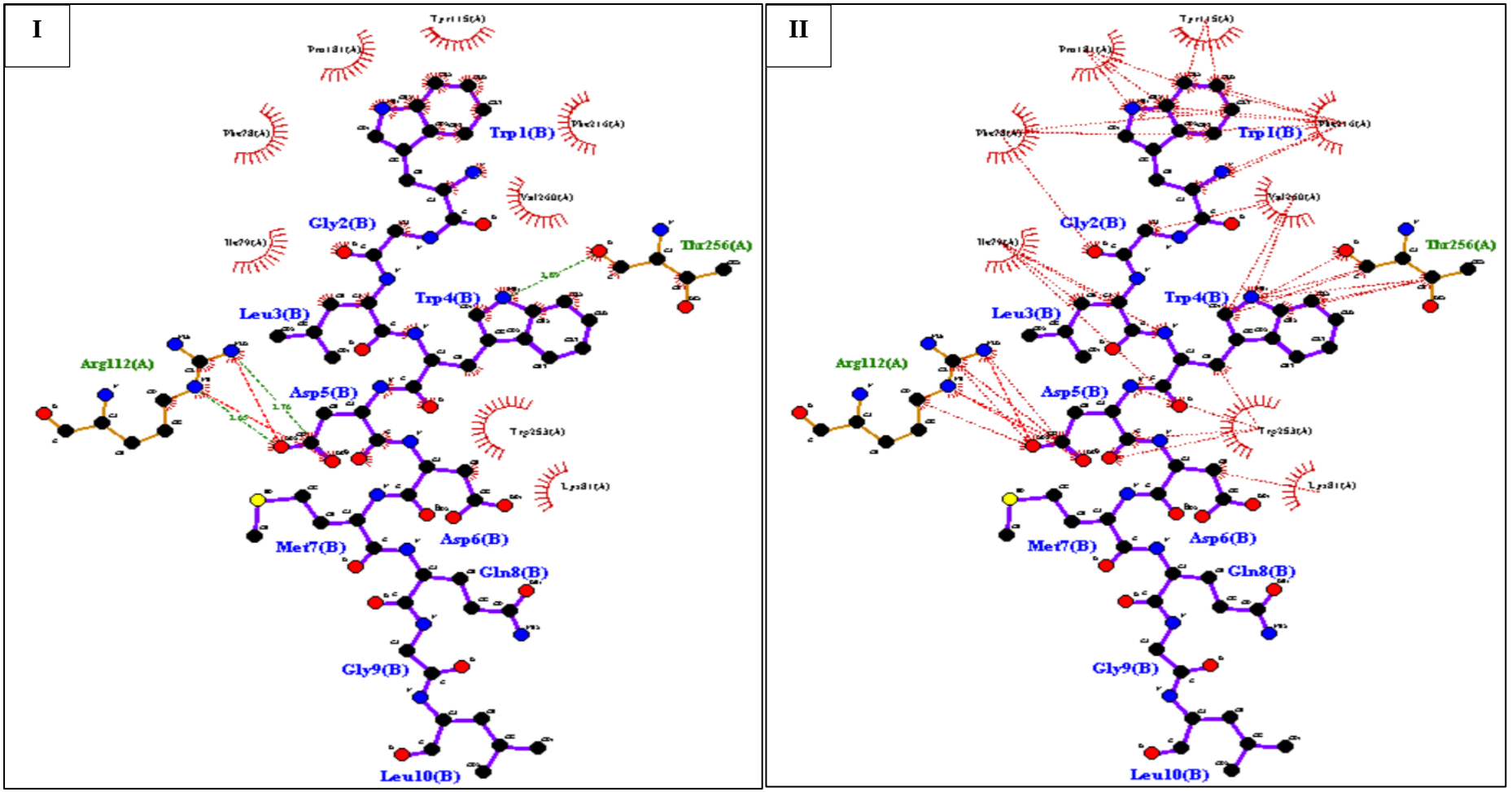

Figure S5j: Binding interaction of WGLWDDMQG**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5k: Binding interaction of pancreatic lipase inhibitory peptides-WNWGWLLWQL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide WNWGWLLWQ**L**	LEU10	cluster8_1	-8.6	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - Ile252 N - Ile252 O - NA	NA	NA	NA
Total number of bonds					41	0	0	0
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					5%	0%	0%	0%

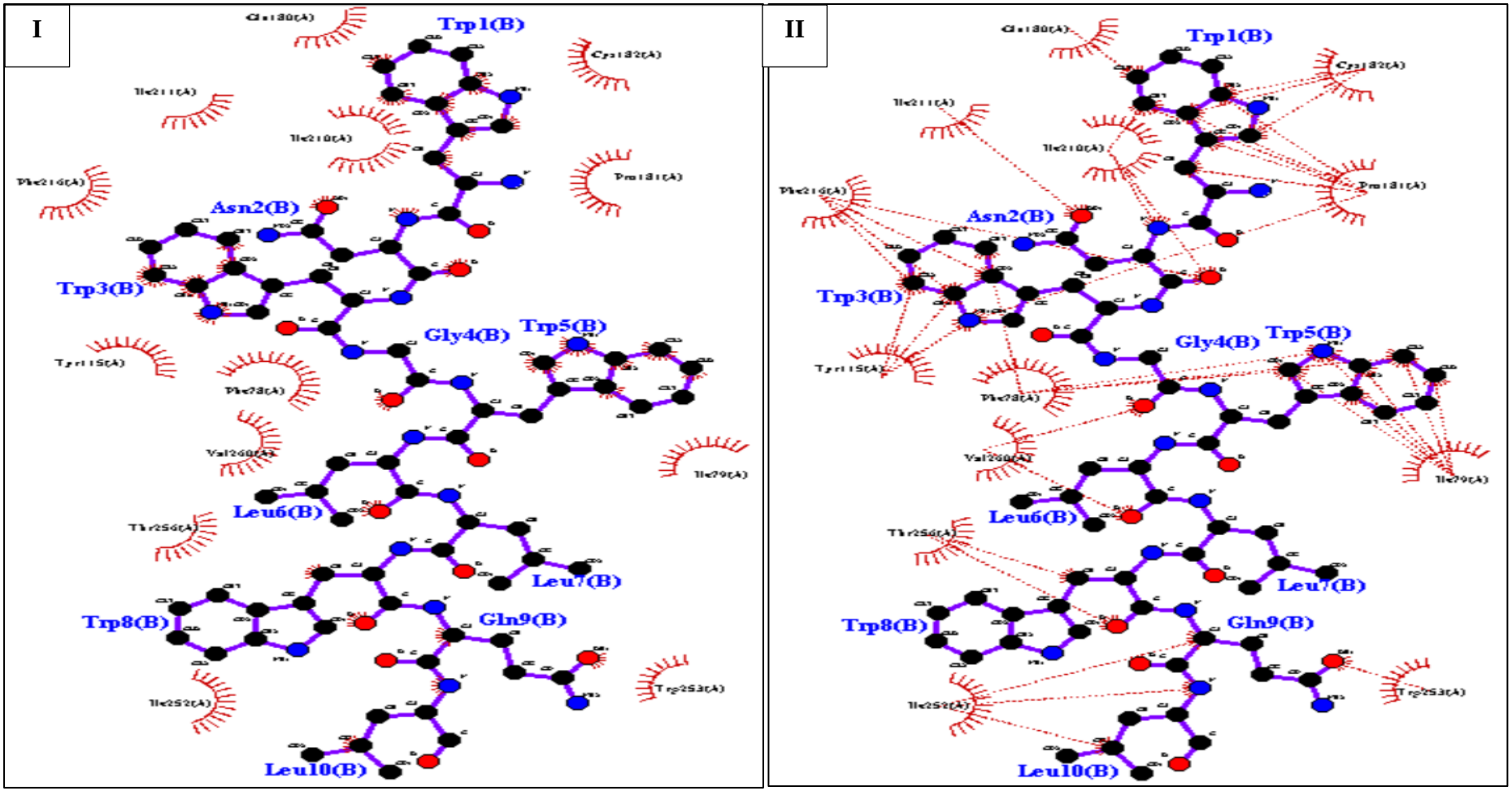

Figure S5k: Binding interaction of WNWGWLLWQ**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S5l: Binding interaction of pancreatic lipase inhibitory peptides-MPSKPPLL at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide MPSKPPL**L**	LEU8	cluster2_1	-8.8	C - Val21, Gln22 CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Glu180, Pro181	NA	NA	NA
Total number of bonds					33	0	0	2
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					12%	0%	0%	0%

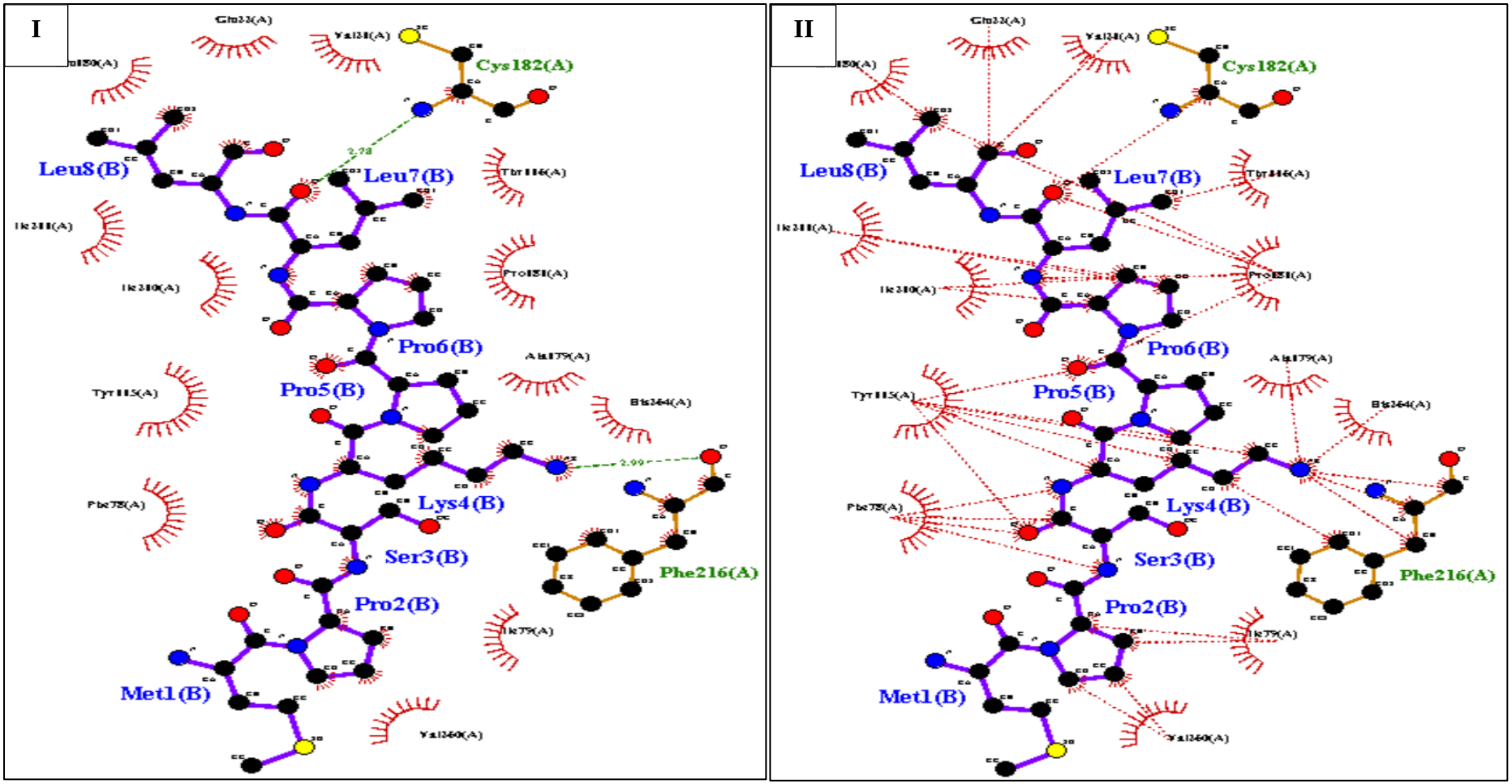

Figure S5l: Binding interaction of MPSKPPL**L** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6a: Binding interaction of pancreatic lipase inhibitory peptides- NALKCCHSCPA at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide NALKCCHSCP **A**	ALA11	cluster1_3	-10.4	C - Thr116 CA - NA CB - NA N - NA O - Gly114, Thr116	NA	NA	O - Thr116
Total number of bonds					47	0	0	2
Total no of interactive residues					3	0	0	1
Overall percentage of bonding					6%	0%	0%	50%

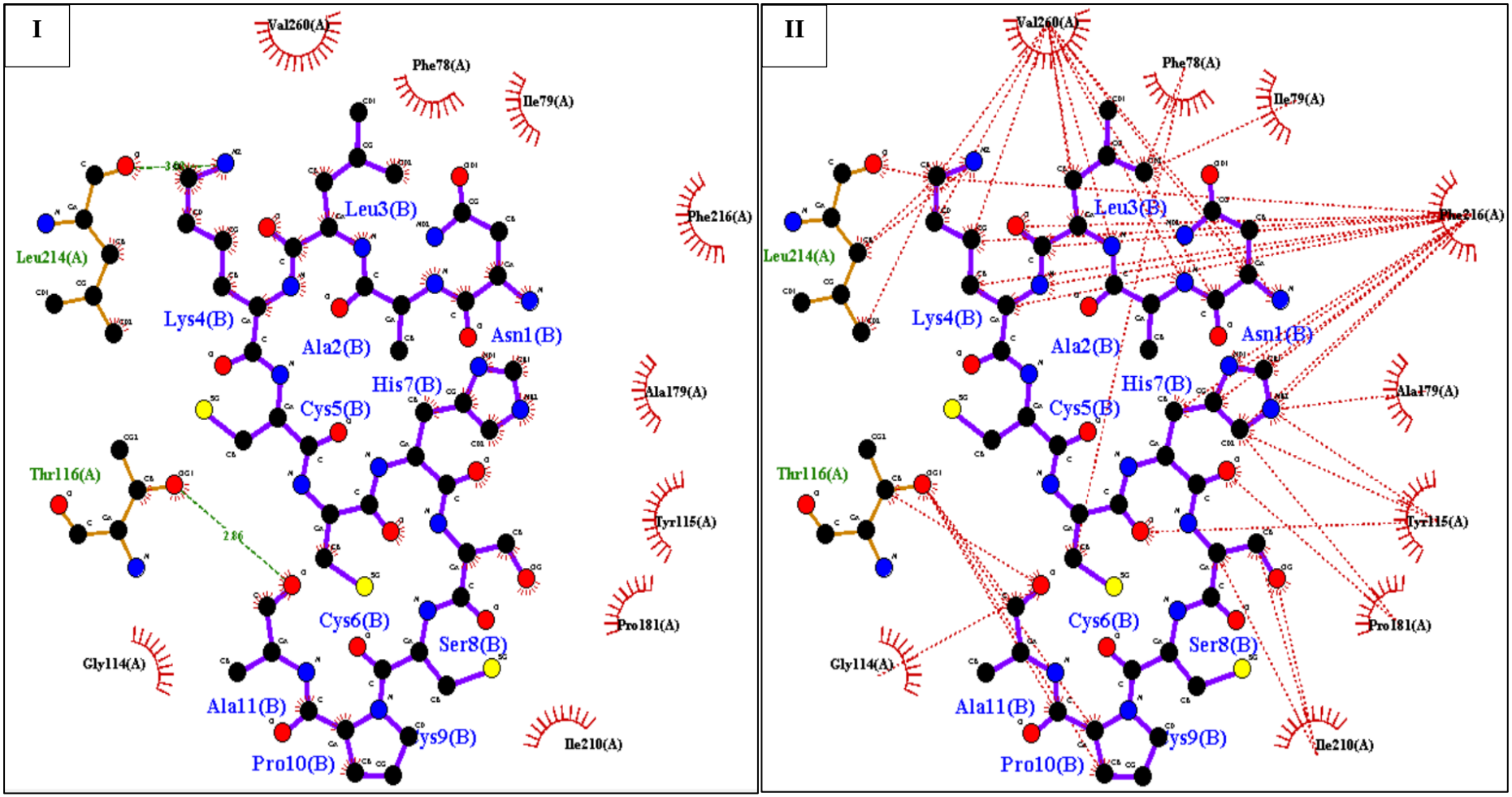

Figure S6a: Binding interaction of NALKCCHSCP**A** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6b: Binding interaction of pancreatic lipase inhibitory peptides-GEHGGAGMGGGQFQPV at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide GEHGGAGMGG GQFQP**V**	VAL16	cluster1_2	-9.1	C - NA CA - NA CB - NA CG_1 - NA CG_2 - NA N - NA O - NA	NA	NA	NA
Total number of bonds					40	0	3	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

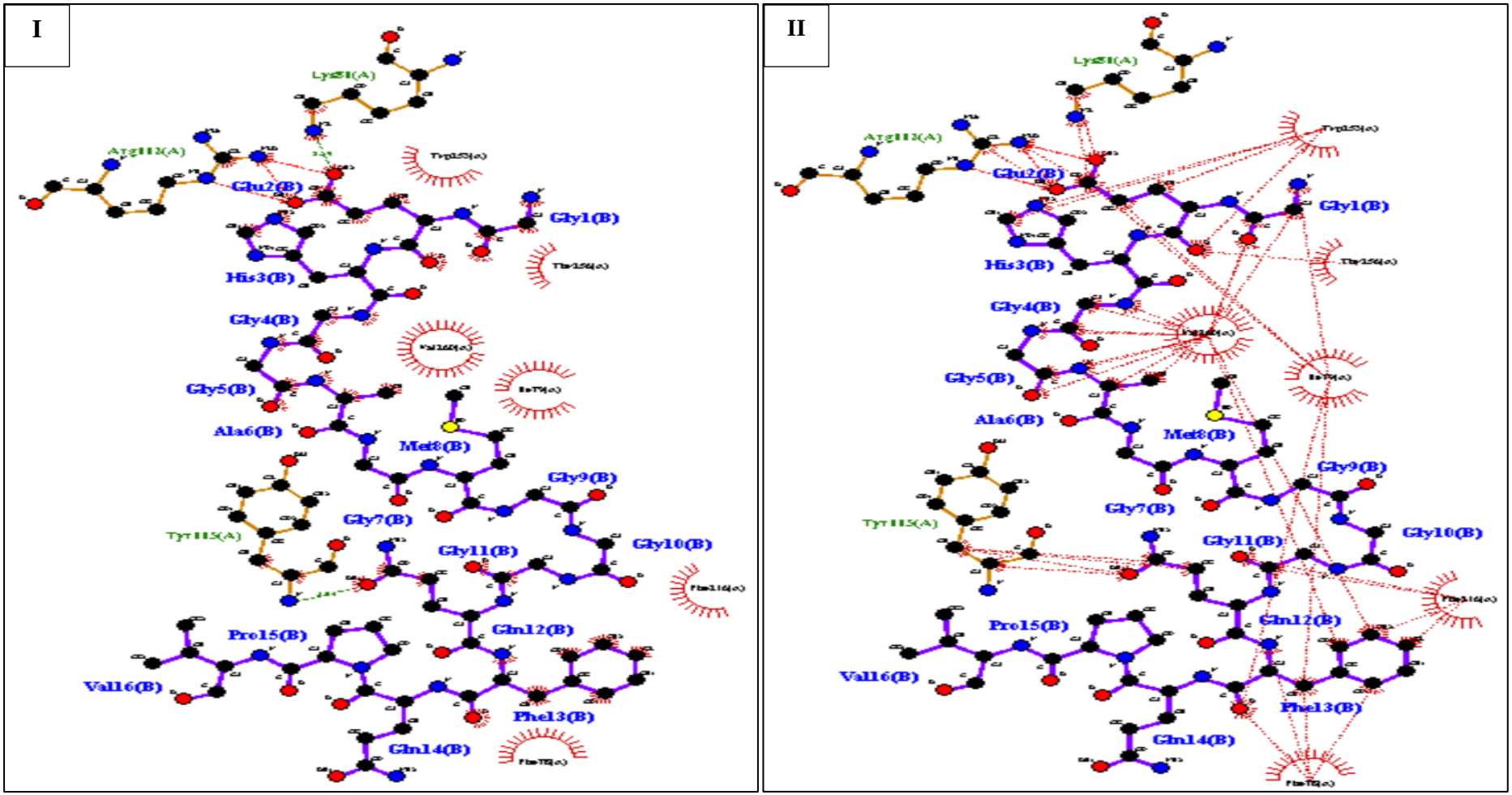

Figure S6b: Binding interaction of GEHGGAGMGGGQFQP**V** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6c: Binding interaction of pancreatic lipase inhibitory peptides-GQLGEHGGAGMG at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide GQLGEHGGAG M**G**	GLY12	cluster1_1	-8.5	C - NA CA - NA N - NA O - NA	NA	NA	NA
Total number of bonds					24	0	0	0
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

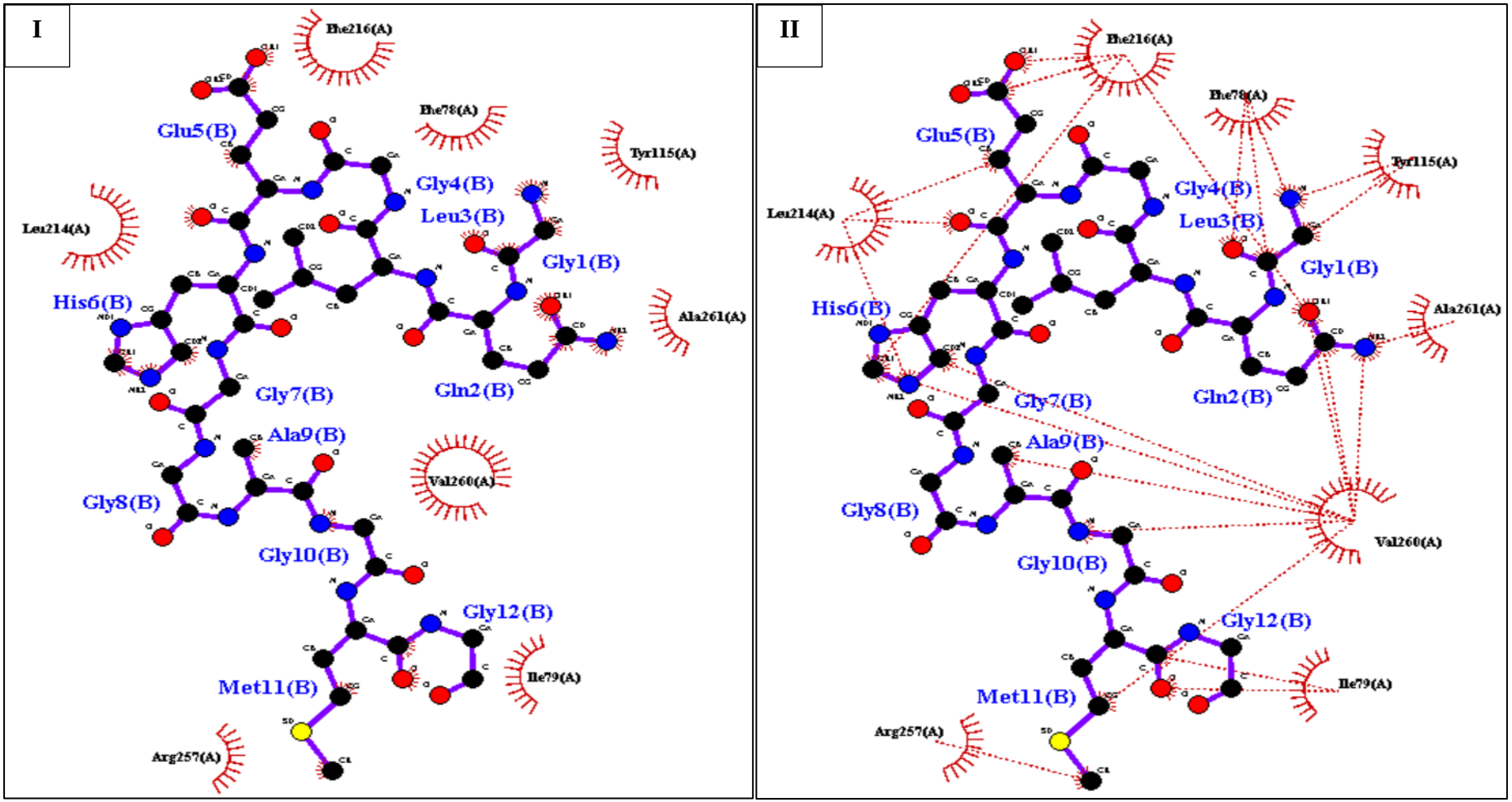

Figure S6c: Binding interaction of GQLGEHGGAGM**G** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6d: Binding interaction of pancreatic lipase inhibitory peptides-LAAVEALSTNG at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide LAAVEALSTN **G**	GLY11	cluster1_1	-8.4	C - NA CA - NA N - NA O - NA	NA	NA	NA
Total number of bonds					31	0	0	3
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

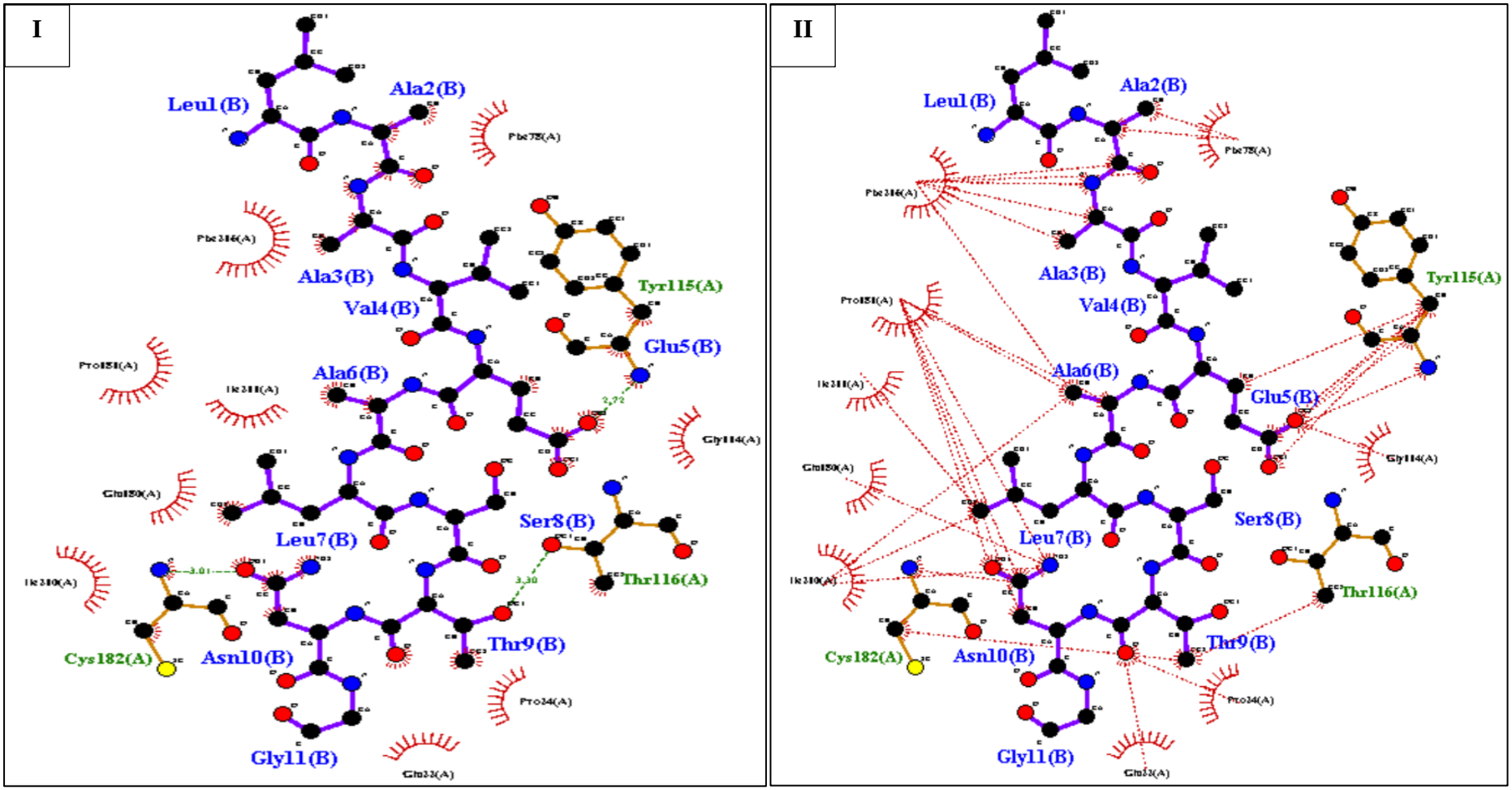

Figure S6d: Binding interaction of LAAVEALSTN**G** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6e: Binding interaction of pancreatic lipase inhibitory peptides-MLPLMLPFTMGY at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide MLPLMLPFTM G**<u>Y</u>**	TYR12	cluster2_1	-8.4	C - NA CA- NA CB - NA CD_1 - NA CD_2 - NA CE_1 - NA CE_2 - NA CG - NA CZ - NA N - NA O - Tyr115 OH - Ile211	NA	NA	O - Tyr115
Total number of bonds					41	0	0	1
Total no of interactive residues					2	0	0	1
Overall percentage of bonding					5%	0%	0%	100%

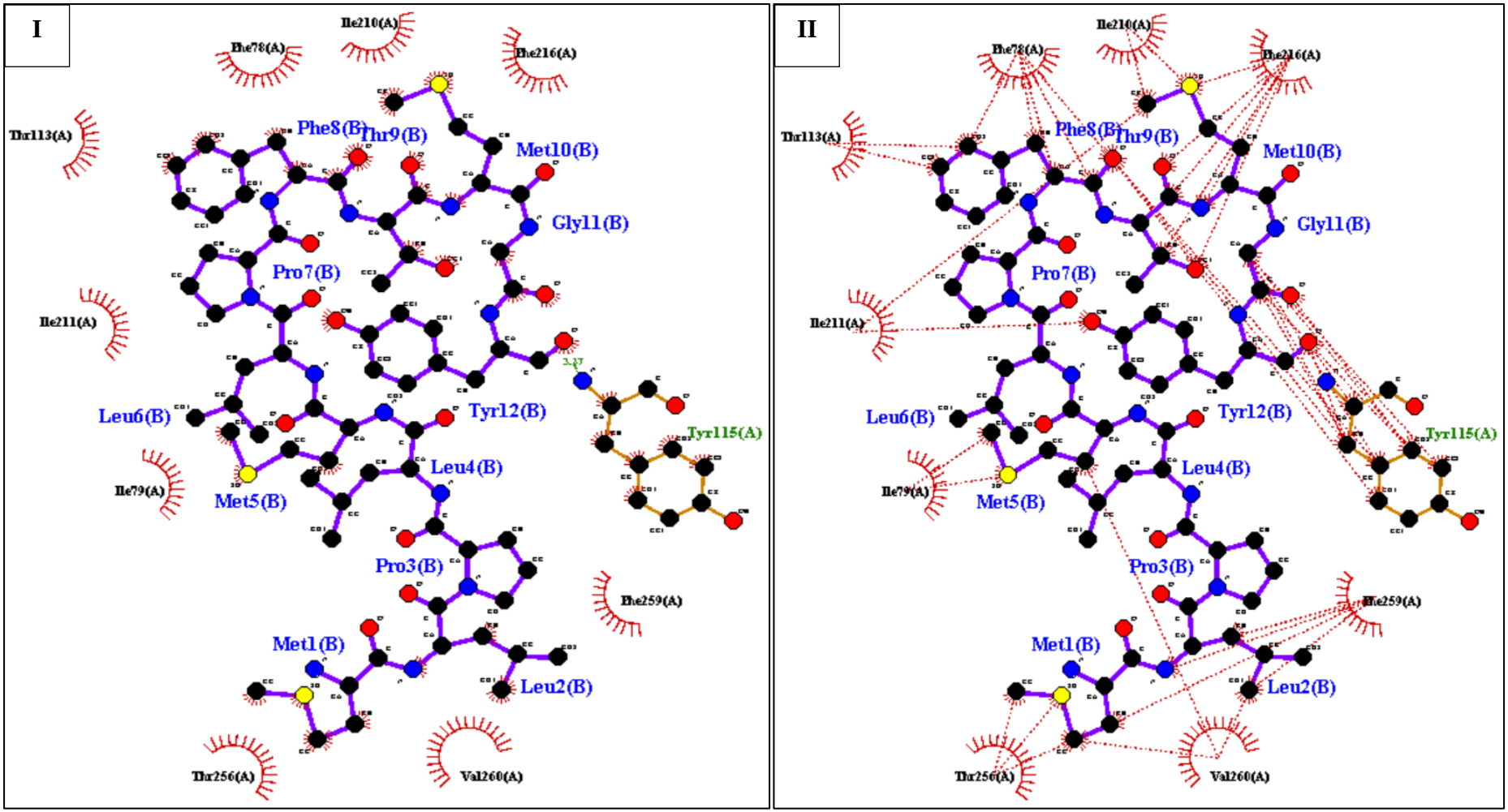

Figure S6e: Binding interaction of MLPLMLPFTMG**Y** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6f: Binding interaction of pancreatic lipase inhibitory peptides-MSKFLPLPLMFY at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide MSKFLPLPLM F**<u>Y</u>**	TYR12	cluster1_4	-7.4	C - Tyr116, Thr116 CA- NA CB - NA CD_1 - Thr116 CD_2 - Thr116 CE_1 - Leu25, Thr116 CE_2 - Thr116 CG - NA CZ - Thr116 N - NA O - Tyr116, Thr116 OH - Leu25	NA	NA	O - Thr116
Total number of bonds					45	0	0	2
Total no of interactive residues					2	0	0	2
Overall percentage of bonding					4%	0%	0%	100%

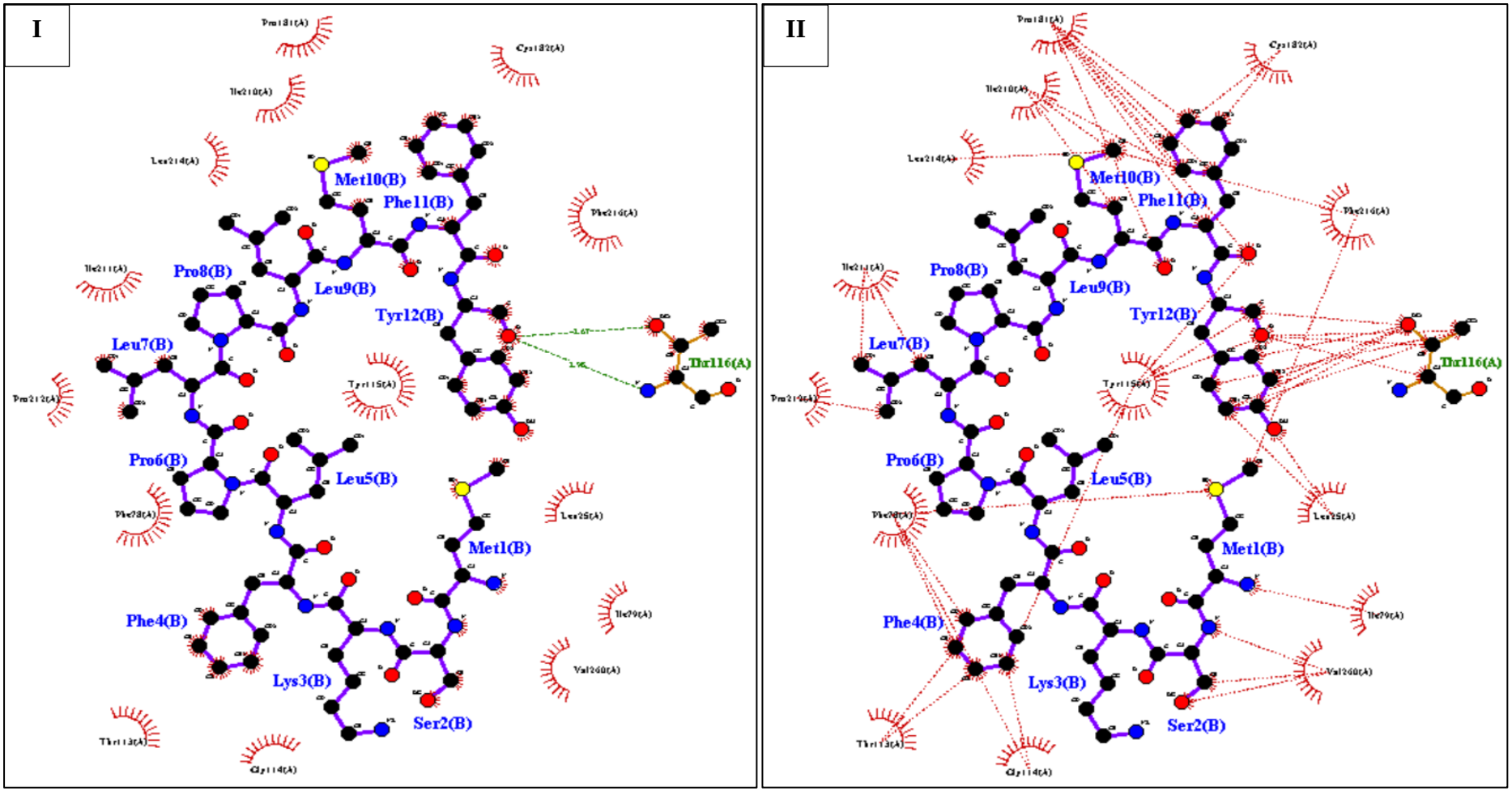

Figure S6f: Binding interaction of MSKFLPLPLMF**Y** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6g: Binding interaction of pancreatic lipase inhibitory peptides-FFRSKLLSRGAAAAKGALLPQYW at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide FFRSKLLSRG AAAAKGALLP QY**W**	TRP23	cluster1_3	-9.2	C - Phe78 CA - NA CB - NA CD_1 - NA CD_2 - NA CE_2 - NA CE_3 - NA CG - NA CH_2 - NA CZ_2 - NA CZ_3 - NA N - Phe78 NE_1 - NA O - Phe78, Gly114	NA	NA	NA
Total number of bonds					45	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

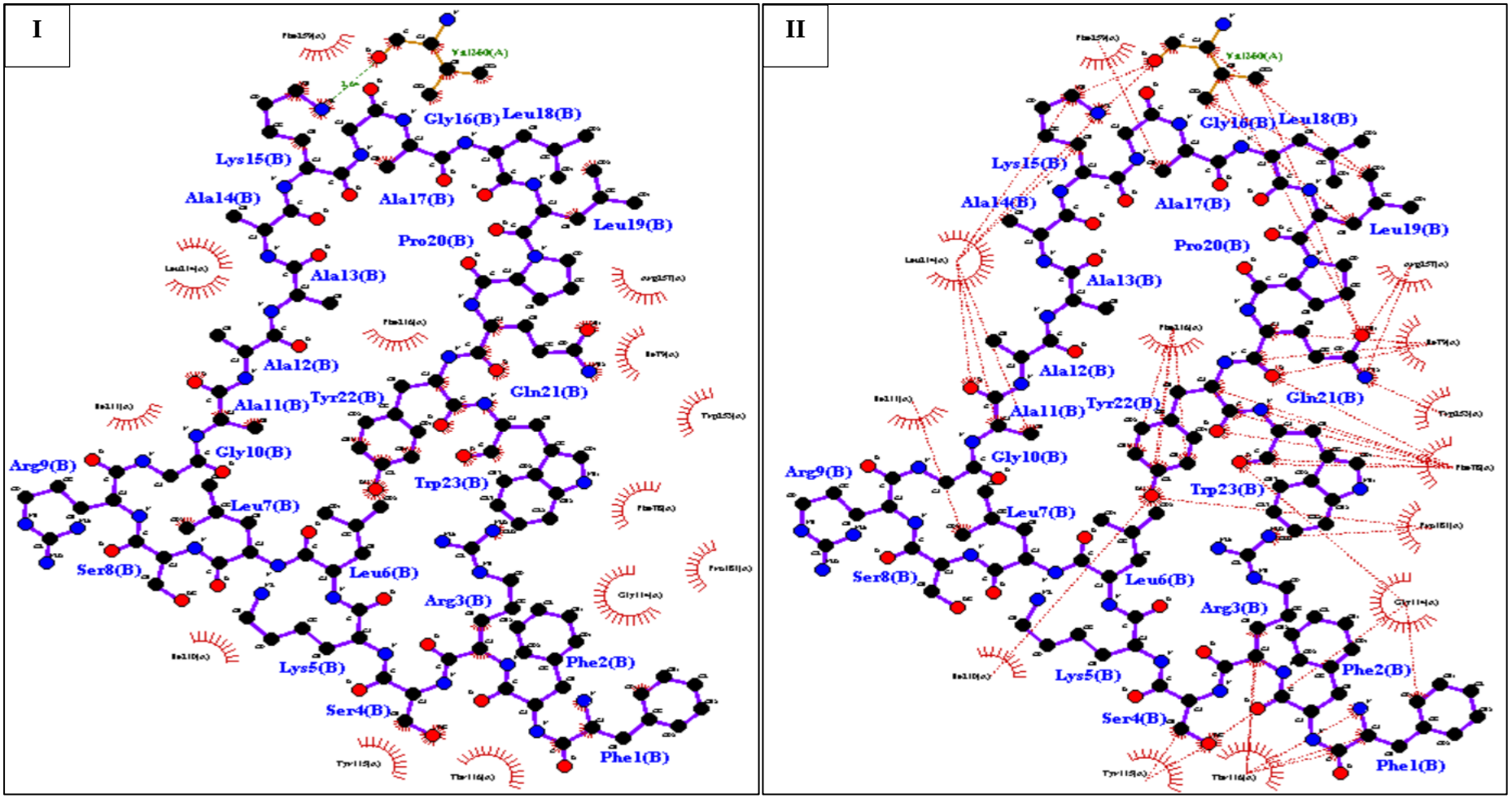

Figure S6g: Binding interaction of FFRSKLLSRGAAAAKGALLPQY**W** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6h: Binding interaction of pancreatic lipase inhibitory peptides-RCMAFLLSDGAAAAQQLLPQYW at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide RCMAFLLSDG AAAAQQLLPQ Y**W**	TRP22	cluster3_3	-9.4	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CE_2 - NA CE_3 - Ile211 CG - NA CH_2 - NA CZ_2 - NA CZ_3 - Ile211 N - NA NE_1 - NA O – NA	NA	NA	NA
Total number of bonds					32	0	0	2
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					6%	0%	0%	0%

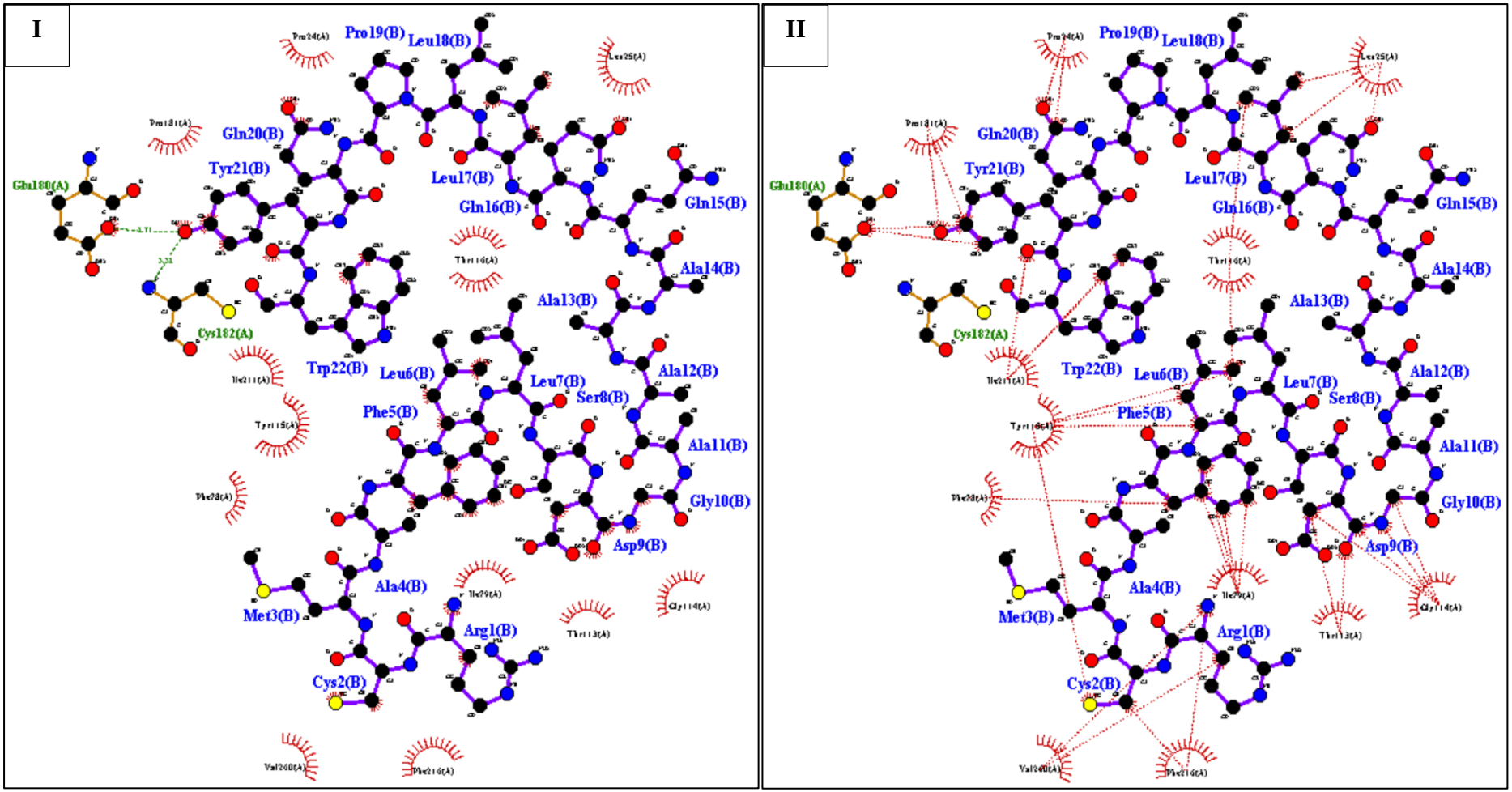

Figure S6h: Binding interaction of RCMAFLLSDGAAAAQQLLPQY**W** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6i: Binding interaction of pancreatic lipase inhibitory peptides-EQGFLPGPEESGR at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide EQGFLPGPEE SG**R**	ARG13	cluster1_2	-8.9	C - NA CA - NA CB - NA CD - NA CG - NA CZ - NA N - NA NB_1 - NA NB_2 - NA NE - NA O - NA	NA	NA	NA
Total number of bonds					44	0	2	4
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

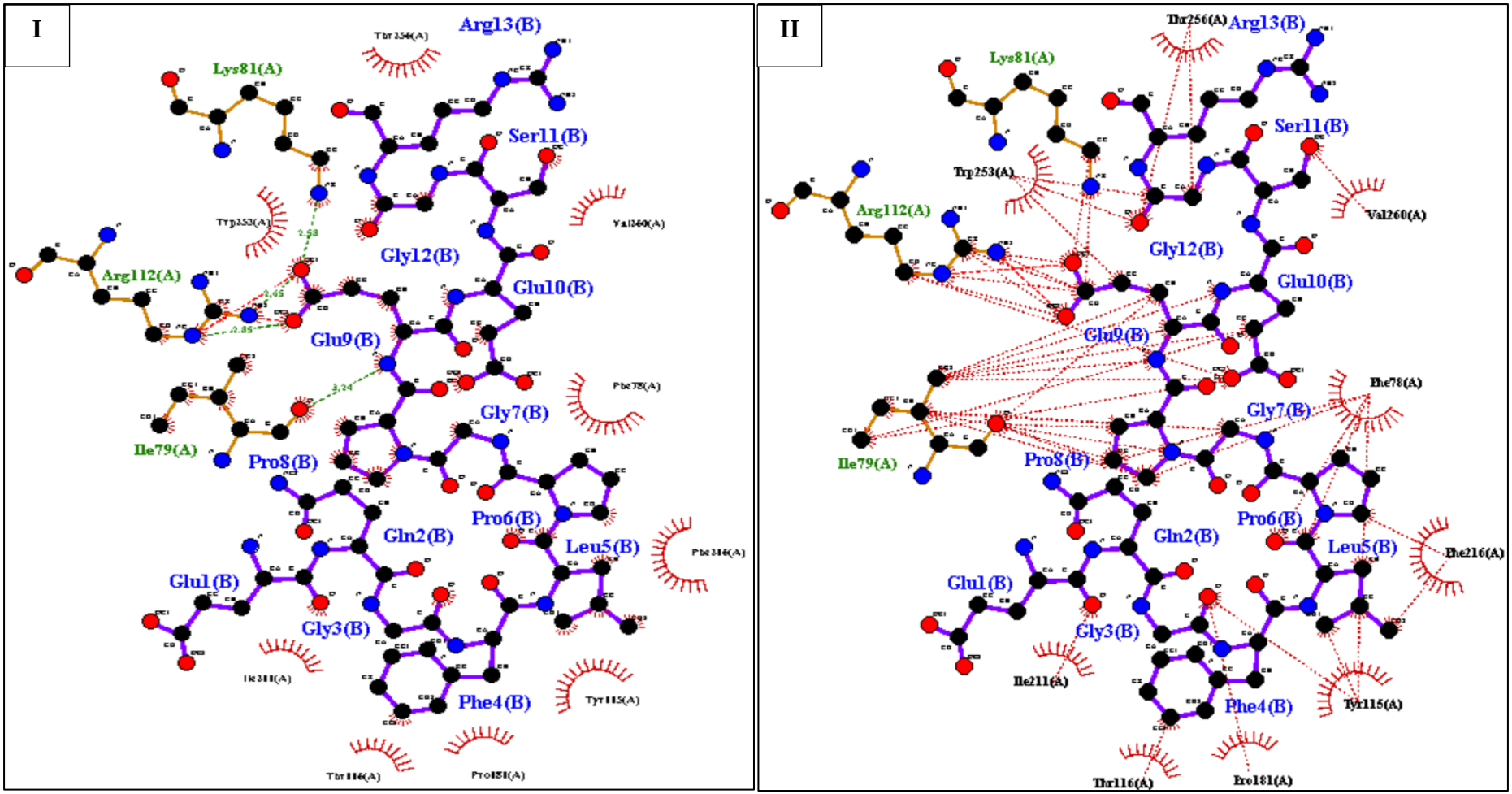

Figure S6i: Binding interaction of EQGFLPGPEESG**R** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6j: Binding interaction of pancreatic lipase inhibitory peptides-SGGGGGGVAGAATASR at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide SGGGGGGVAG AATAS**R**	ARG16	cluster3_1	-7.4	C - NA CA - NA CB - NA CD - Thr256 CG - NA CZ - Thr256 N - NA NH_1 - Val260 NB_2 - Arg257 NE - Thr256 O - NA	NA	NA	NA
Total number of bonds					40	0	0	0
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

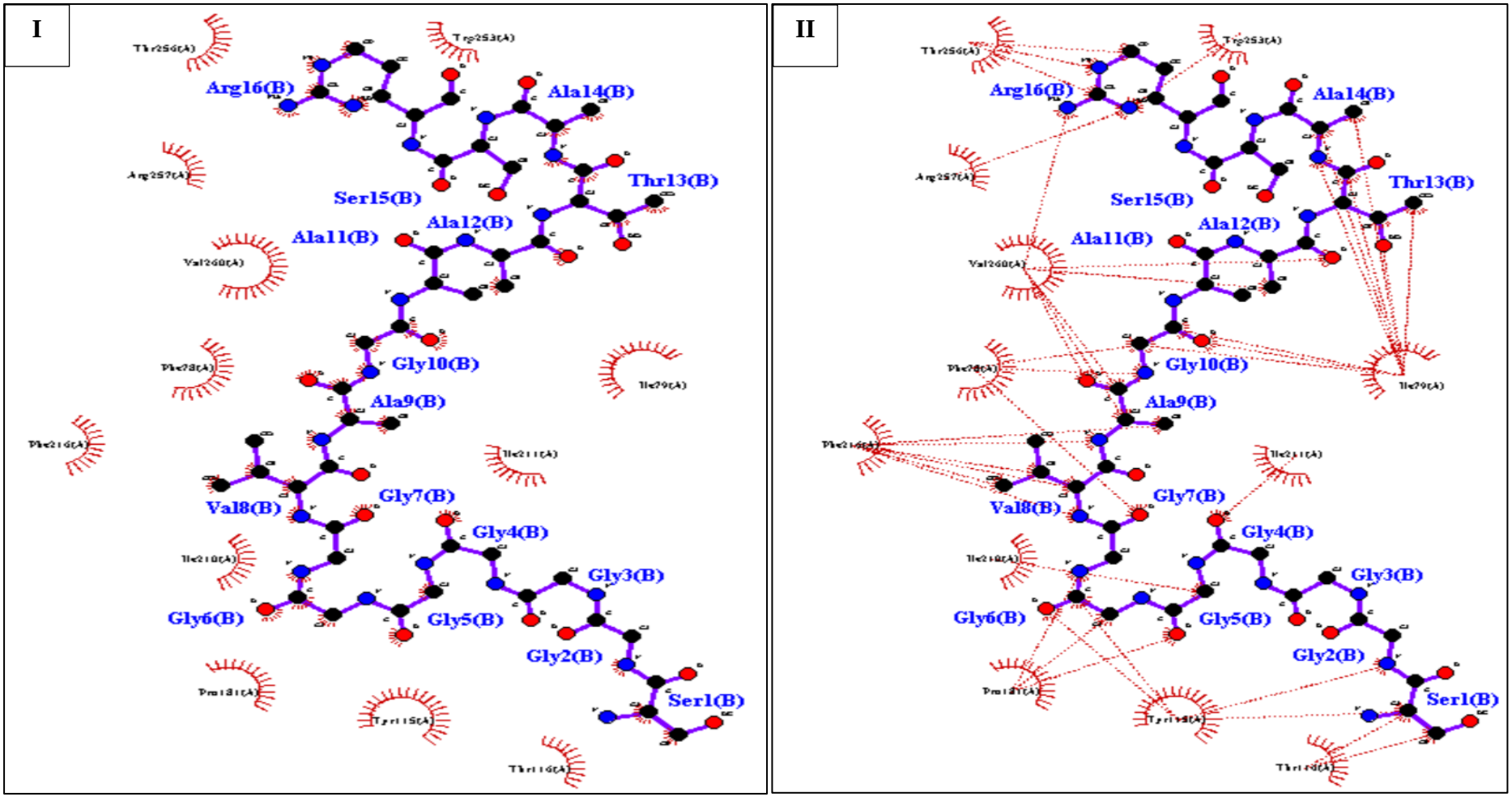

Figure S6j: Binding interaction of SGGGGGGVAGAATAS**R** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6k: Binding interaction of pancreatic lipase inhibitory peptides-YGNPVGGVGH at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide YGNPVGGVG**H**	HIS10	cluster1_3	-9.0	C - Ile79 CA - Ile79 CB - Ile79 CD_2 - Glu84, Trp253 CE_1- Ile79, Asp80 Lys81, Glu84 Arg257 CG - Ile79 N - Ile79 ND_1 - Ile79, Asp80 NE_2 - Glu84 O - Ile79	NE_2 - Asp80, Glu84	NA	ND_1 - Ile79 NE_2 - Glu78
Total number of bonds					57	2	0	4
Total no of interactive residues					16	2	0	2
Overall percentage of bonding					28%	100%	0%	50%

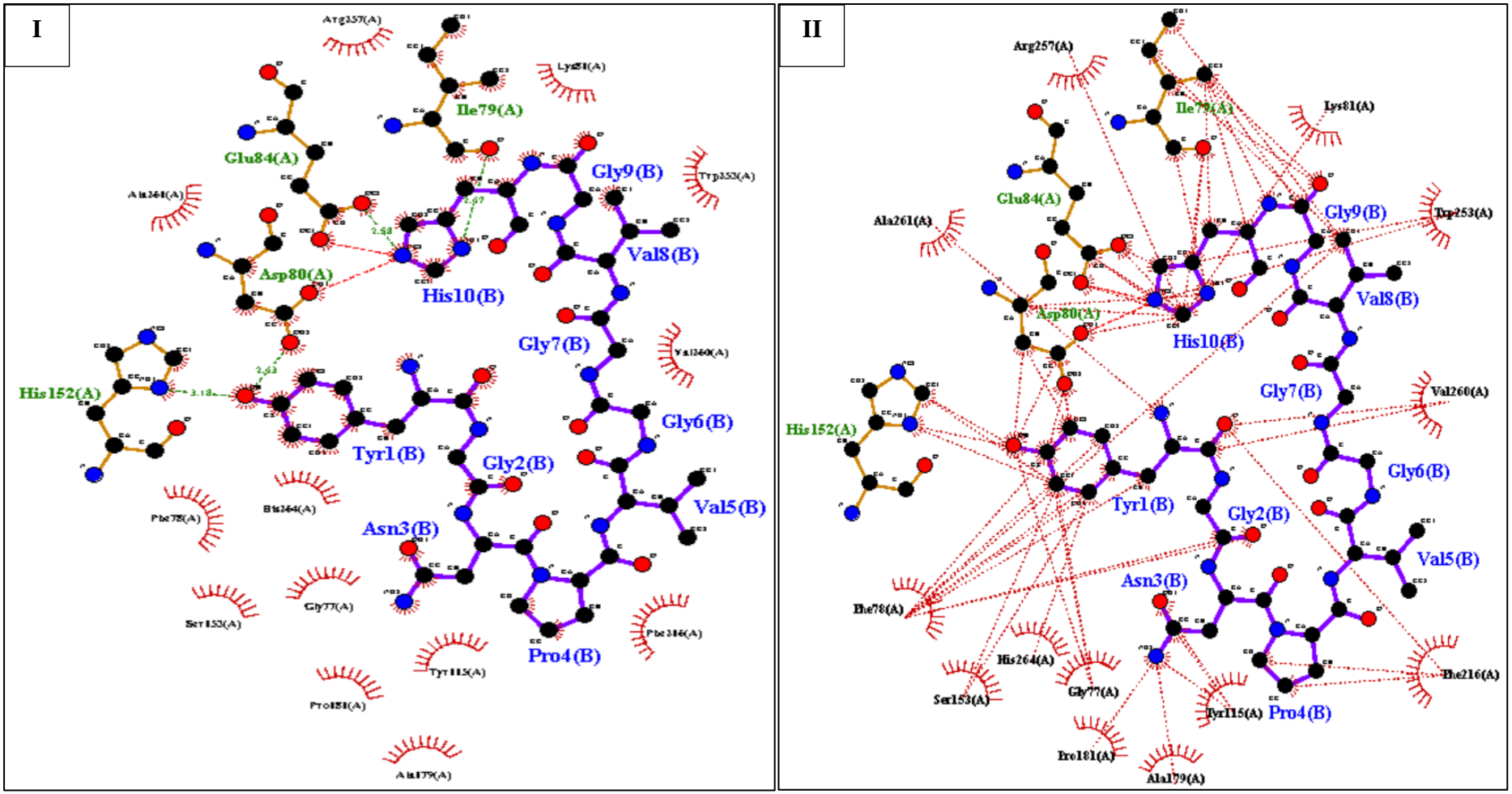

Figure S6k: Binding interaction of YGNPVGGVG**H** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S6l: Binding interaction of pancreatic lipase inhibitory peptides-RPAQPNYPWTAVLVFRH at C1 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide RPAQPNYPWT AVLVFR**H**	HIS17	cluster3_1	-9.3	C - NA CA - NA CB - NA CD_2 - NA CE_1- NA CG - NA N - NA ND_1 - NA NE_2 - NA O - NA	NA	NA	NA
Total number of bonds					56	1	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

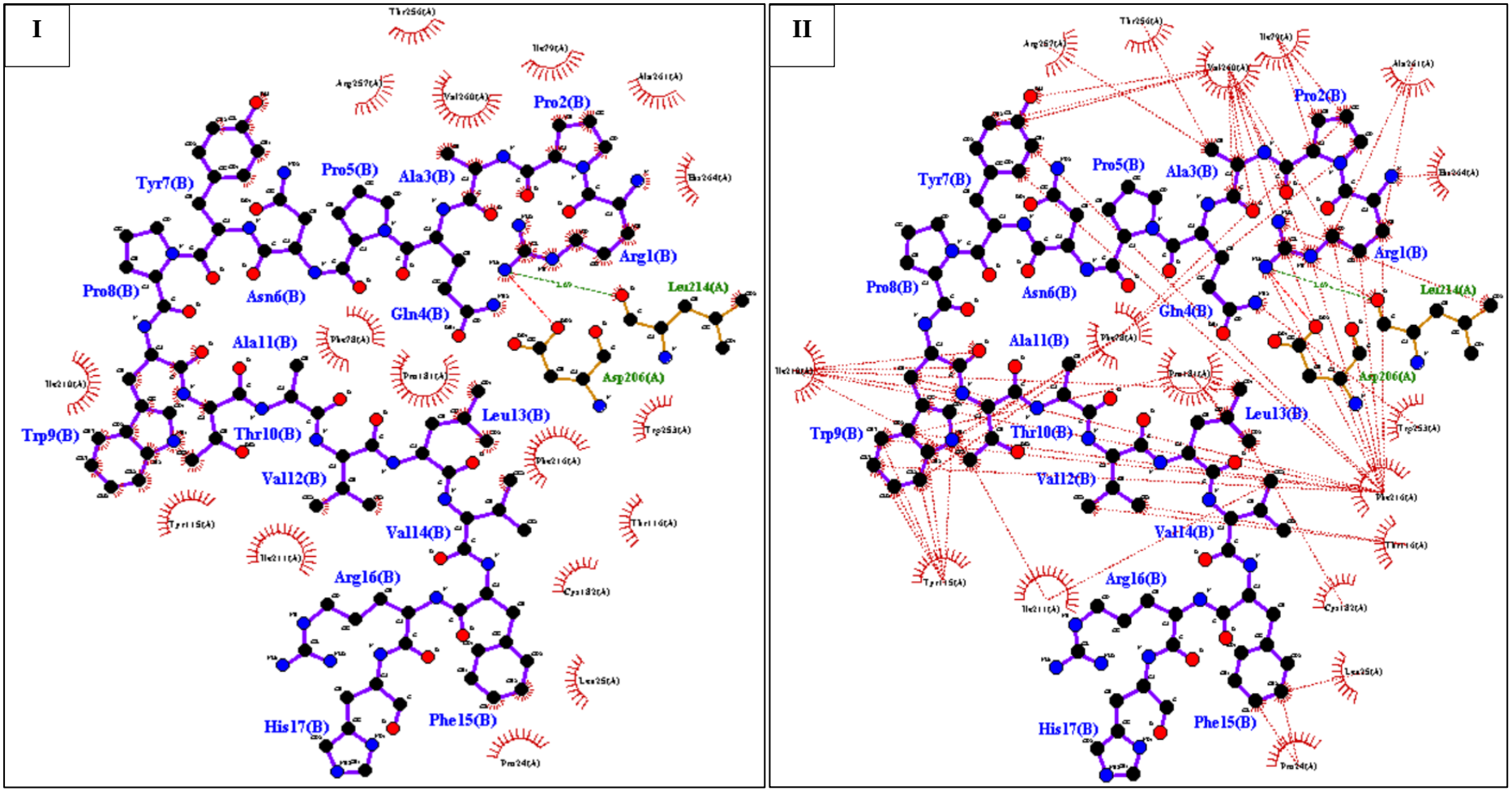

Figure S6l: Binding interaction of RPAQPNYPWTAVLVFR**H** inhibitory peptide at C1 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7a: Binding interaction of pancreatic lipase inhibitory peptides-AAGF at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide A**A**GF	ALA2	cluster1_3	-6.5	C - NA CA - Pro181 CB - NA N - Pro181 O - NA	NA	NA	NA
Total number of bonds					18	0	0	1
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					11%	0%	0%	0%

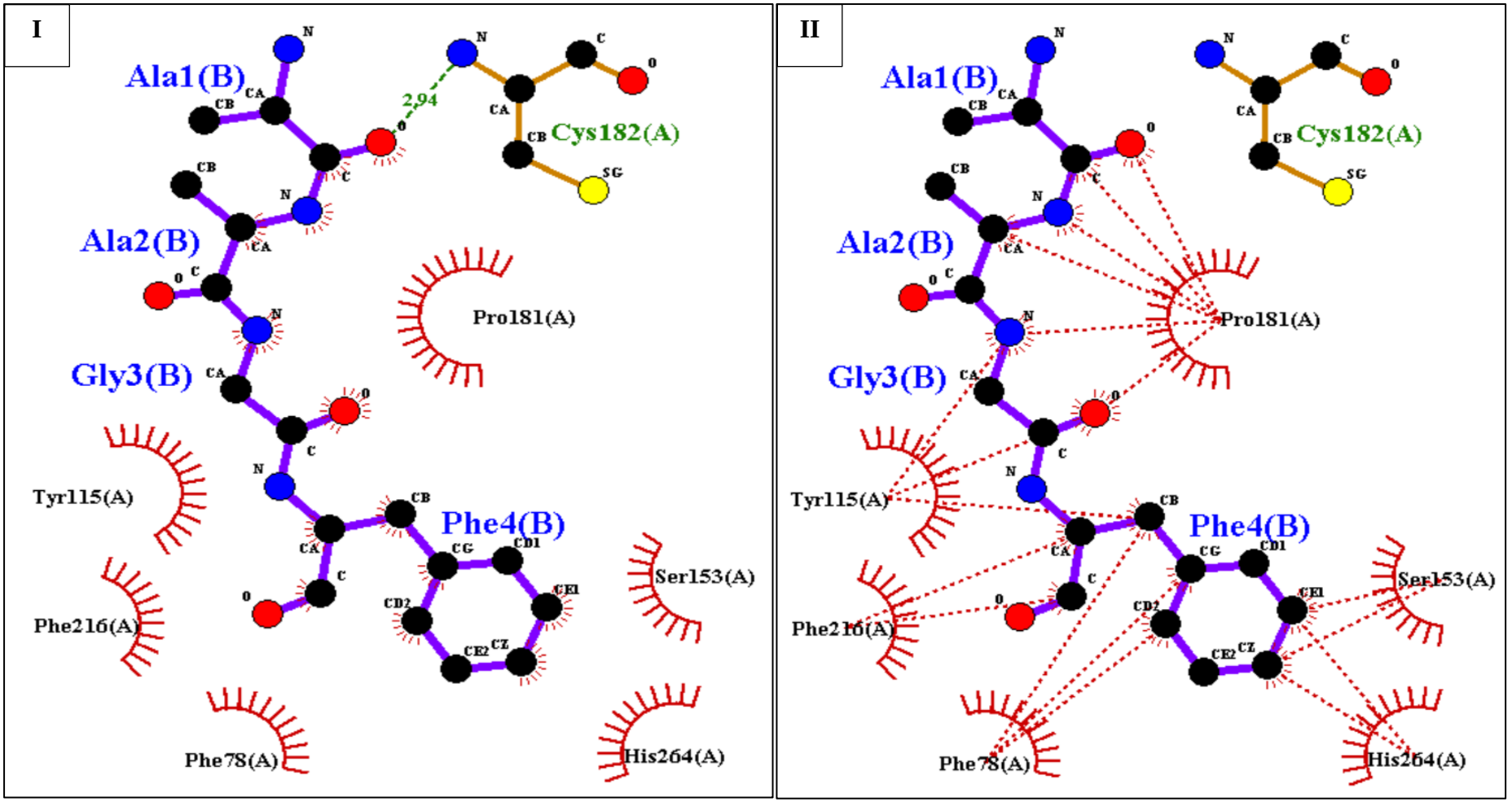

Figure S7a: Binding interaction of A**A**GF inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7b: Binding interaction of pancreatic lipase inhibitory peptides-NVQR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide N**V**QR	VAL2	cluster8_1	-7.7	C - NA CA – Trp253 CB - NA CG_1 – Arg112 CG_2 - NA N - NA O - NA	NA	NA	NA
Total number of bonds					23	1	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

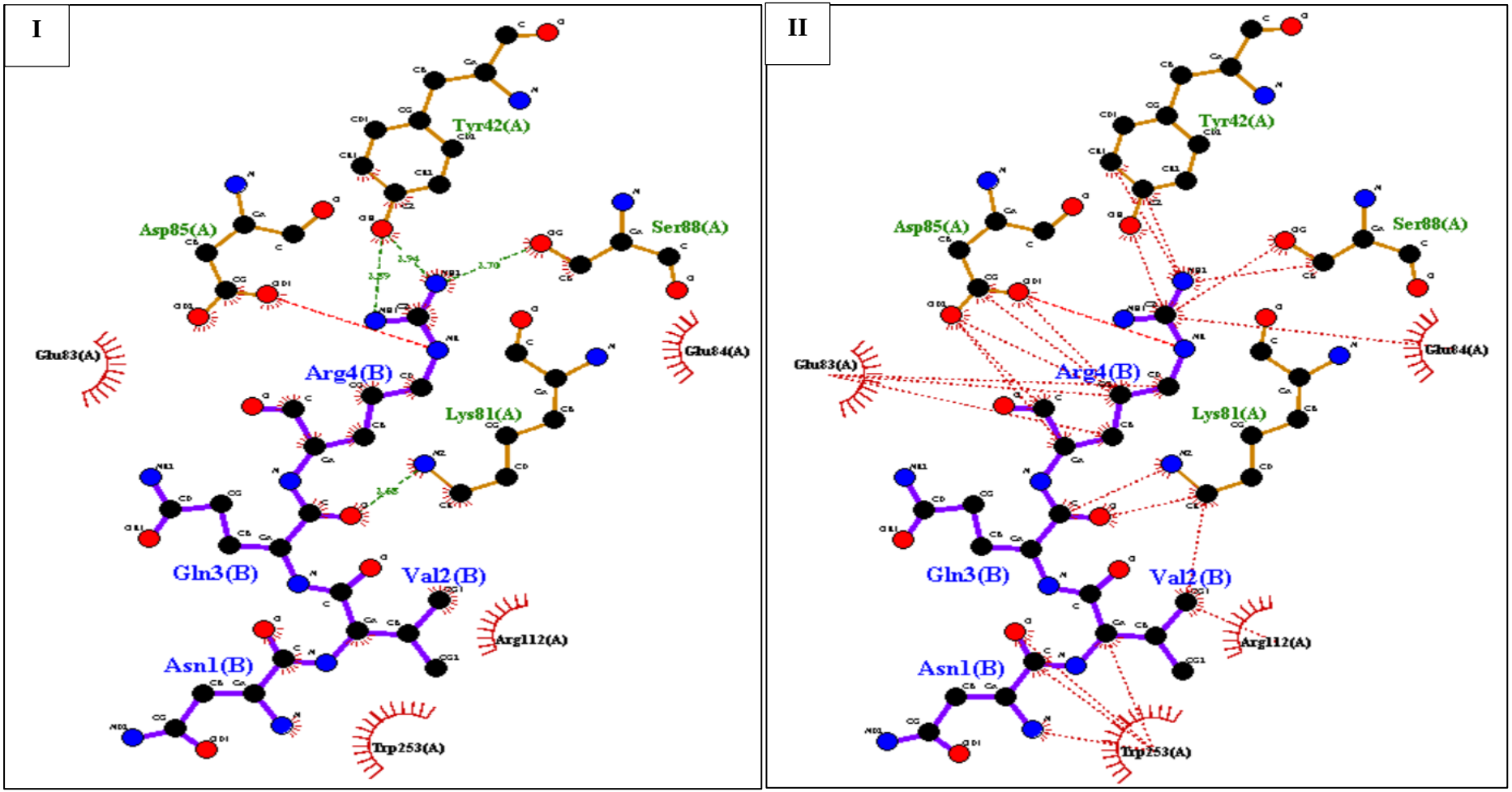

Figure S7b: Binding interaction of N**V**QR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7c: Binding interaction of pancreatic lipase inhibitory peptides-VIAPW at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide V**I**APW	ILE2	cluster3_2	-6.7	C - NA CA - NA CB - NA CD_1 - Phe78, Val260 CG_1 - Val260 CG_2 - NA N - NA O - NA	NA	NA	NA
Total number of bonds					26	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					12%	0%	0%	0%

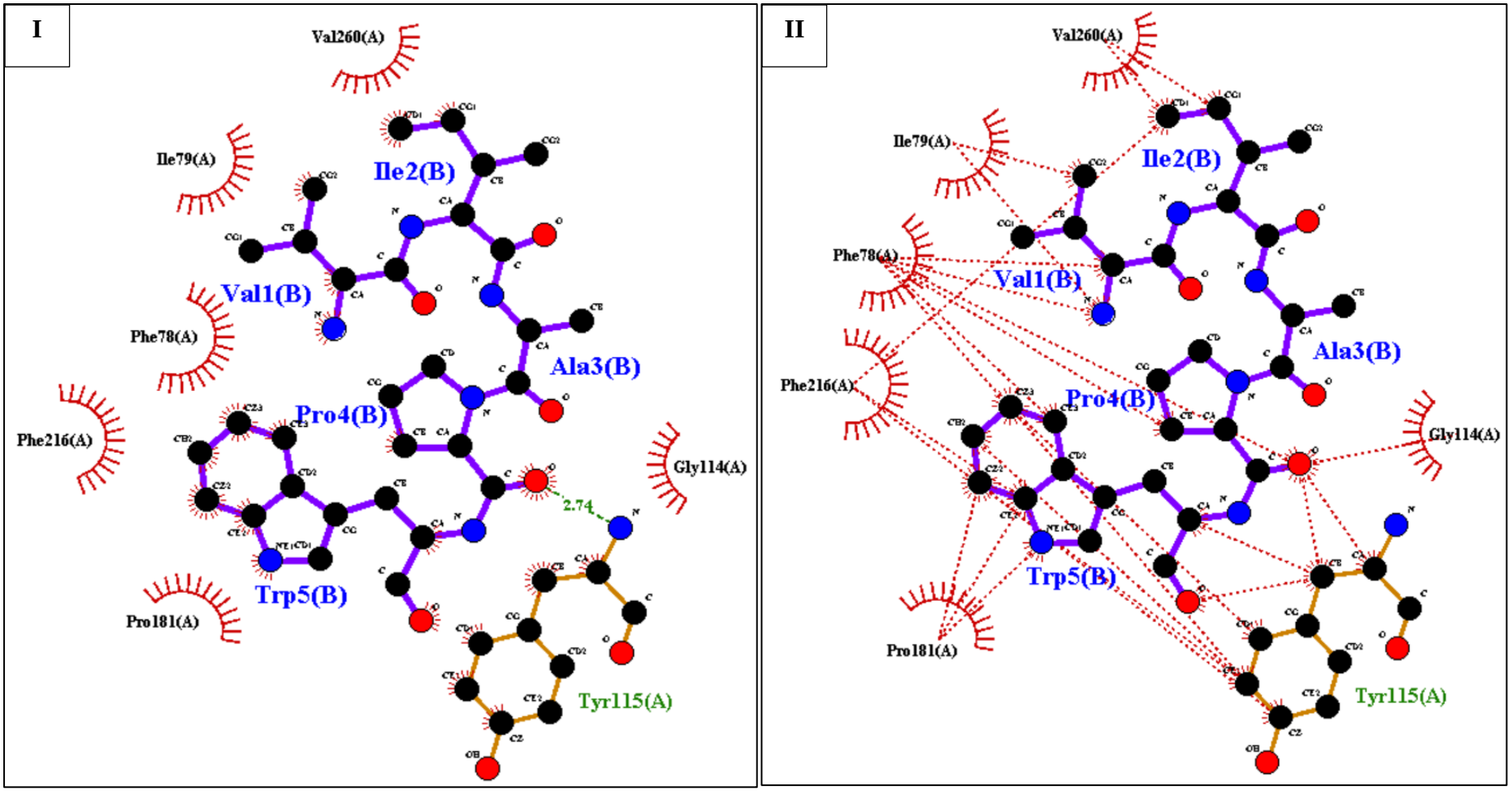

Figure S7c: Binding interaction of VIAPW inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7d: Binding interaction of pancreatic lipase inhibitory peptides-MMML at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide M**M**ML	MET2	cluster10_1	-7.3	C - NA CA - NA CB - NA CE - Gly77, Phe78, Asp80, His152 CG - Phe78 O - Phe216 N - Phe78 SD - Gly77, Phe78, His152, Ser153	NA	NA	NA
Total number of bonds					34	0	0	1
Total no of interactive residues					11	0	0	0
Overall percentage of bonding					32%	0%	0%	0%

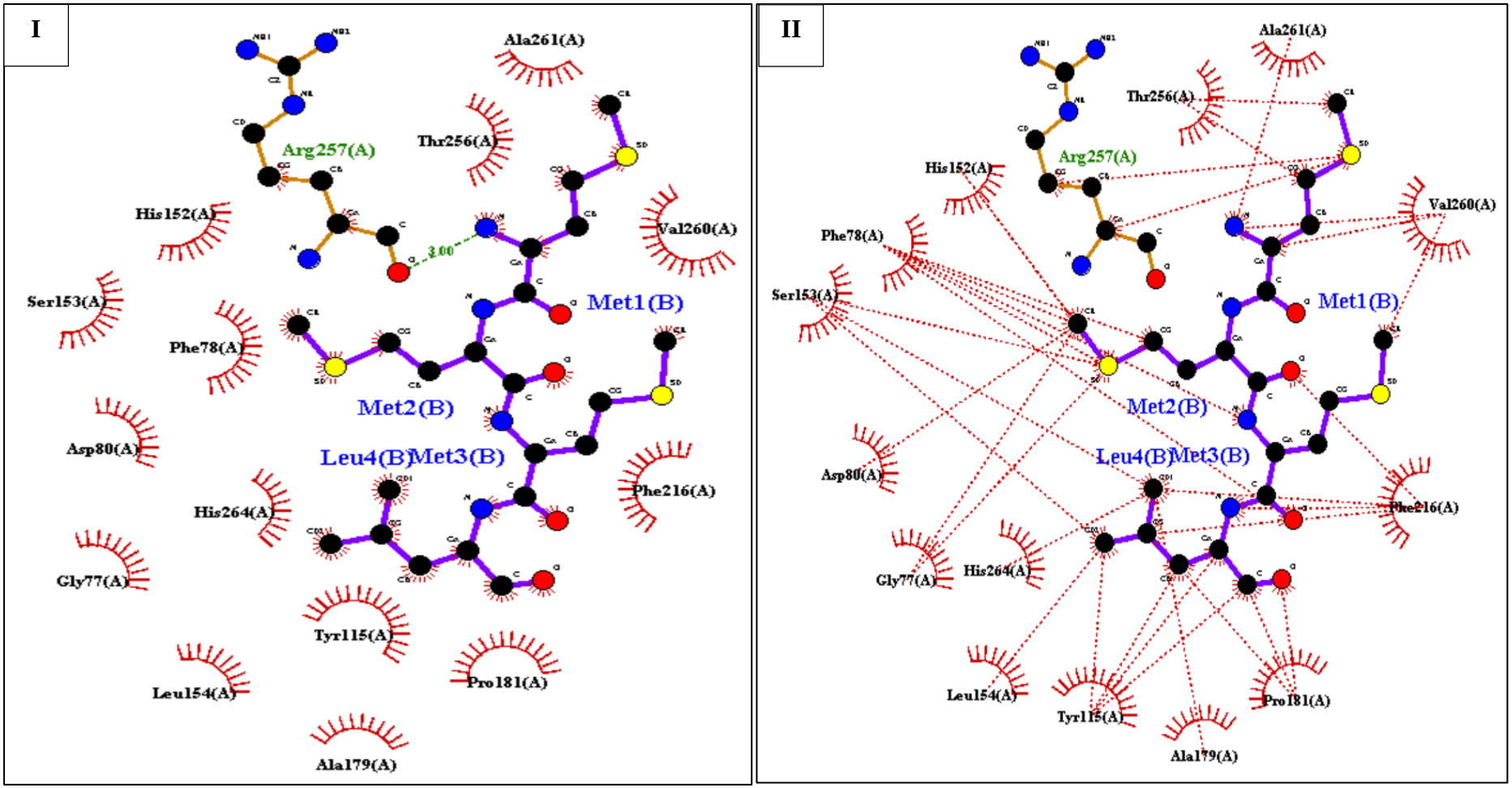

Figure S7d: Binding interaction of M**M**ML inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7e: Binding interaction of pancreatic lipase inhibitory peptides-MSNYF at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide M**S**NYF	SER2	cluster 1_4	-7.7	C - NA CA - Phe216 CB - Val260 N - Phe216 O - NA OG - NA	NA	NA	NA
Total number of bonds					28	0	0	0
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					11%	0%	0%	0%

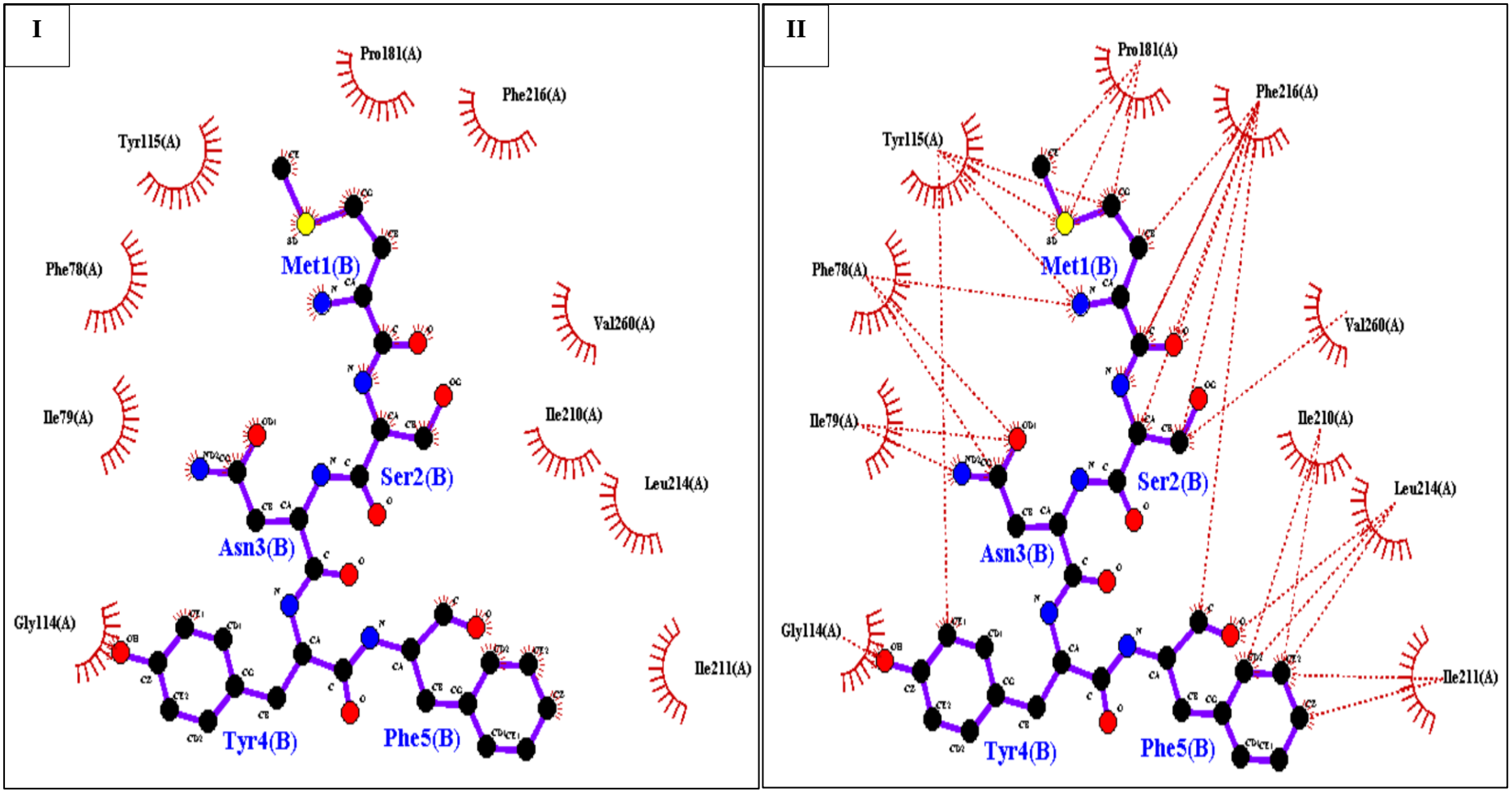

Figure S7e: Binding interaction of MSNYF inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7f: Binding interaction of pancreatic lipase inhibitory peptides-GTIT at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide G**T**IT	THR2	cluster9_4	-8.7	C - NA CA - NA CB - NA CG_2 – Phe216 OG_1 – Phe216 N - NA	NA	NA	NA
Total number of bonds					16	0	0	0
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

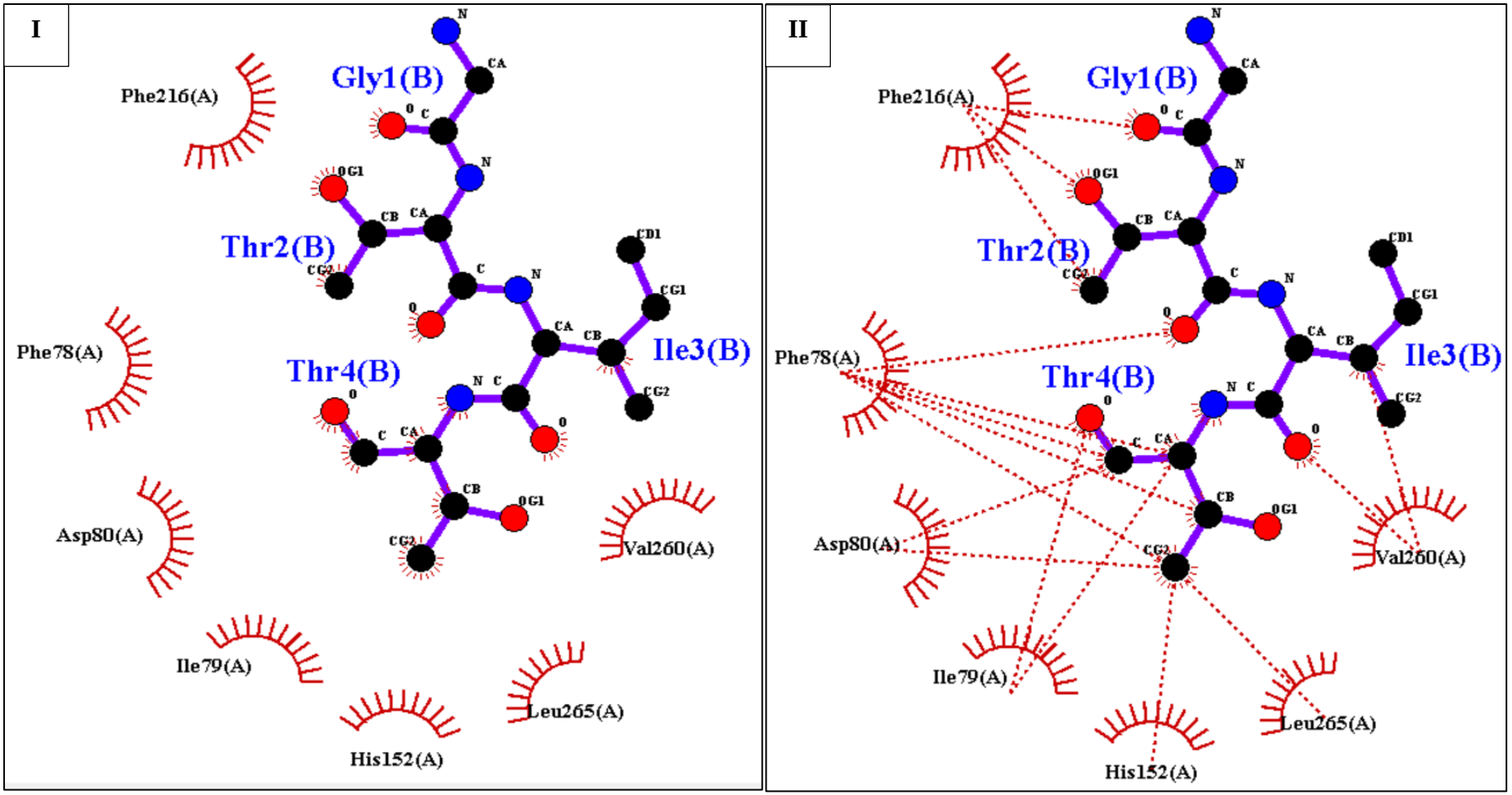

Figure S7f: Binding interaction of G**T**IT inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S7g: Binding interaction of pancreatic lipase inhibitory peptides-LRFPL at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide L**R**FPL	ARG2	cluster1_1	-7.4	C - NA CB - NA CD - NA CG - NA CZ - Thr113 N - NA NE - NA NH_1 - Phe78, Ile79 NH_2 - Ile79, Thr113 O - Phe78	NA	NA	NA
Total number of bonds					24	0	0	2
Total no of interactive residues					6	0	0	0
Overall percentage of bonding					25%	0%	0%	0%

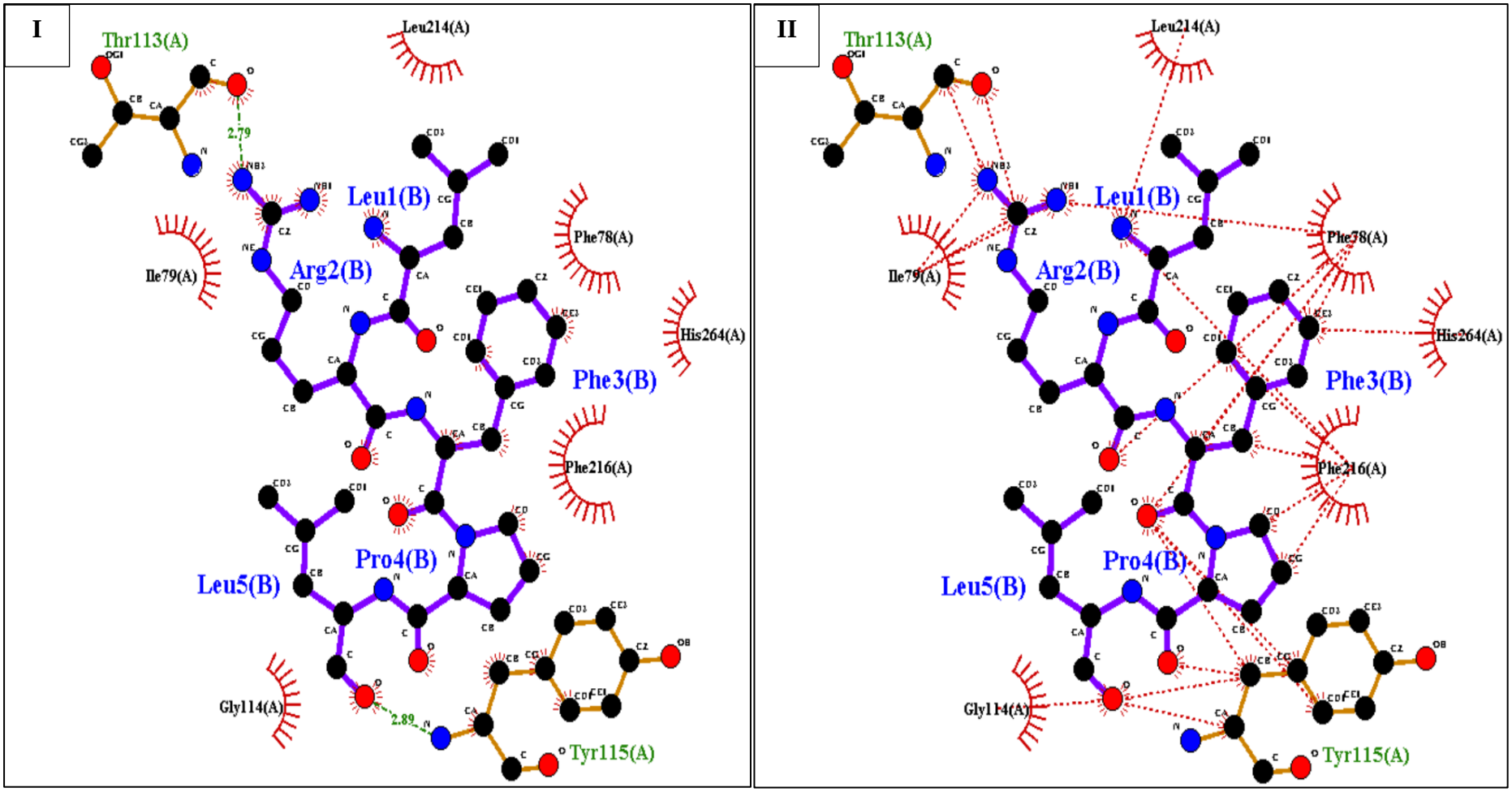

Figure S7g: Binding interaction of LRFPL inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8a: Binding interaction of pancreatic lipase inhibitory peptides-LNLDLLR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide L**N**LDLLR	ASN2	cluster11_2	-8.1	C - NA CA - NA CB - NA CG - Phe78 N- Gly114 ND_2 - Phe78, Tyr115 O - NA OD_1 - Phe78	NA	NA	NA
Total number of bonds					20	0	0	2
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					25%	0%	0%	0%

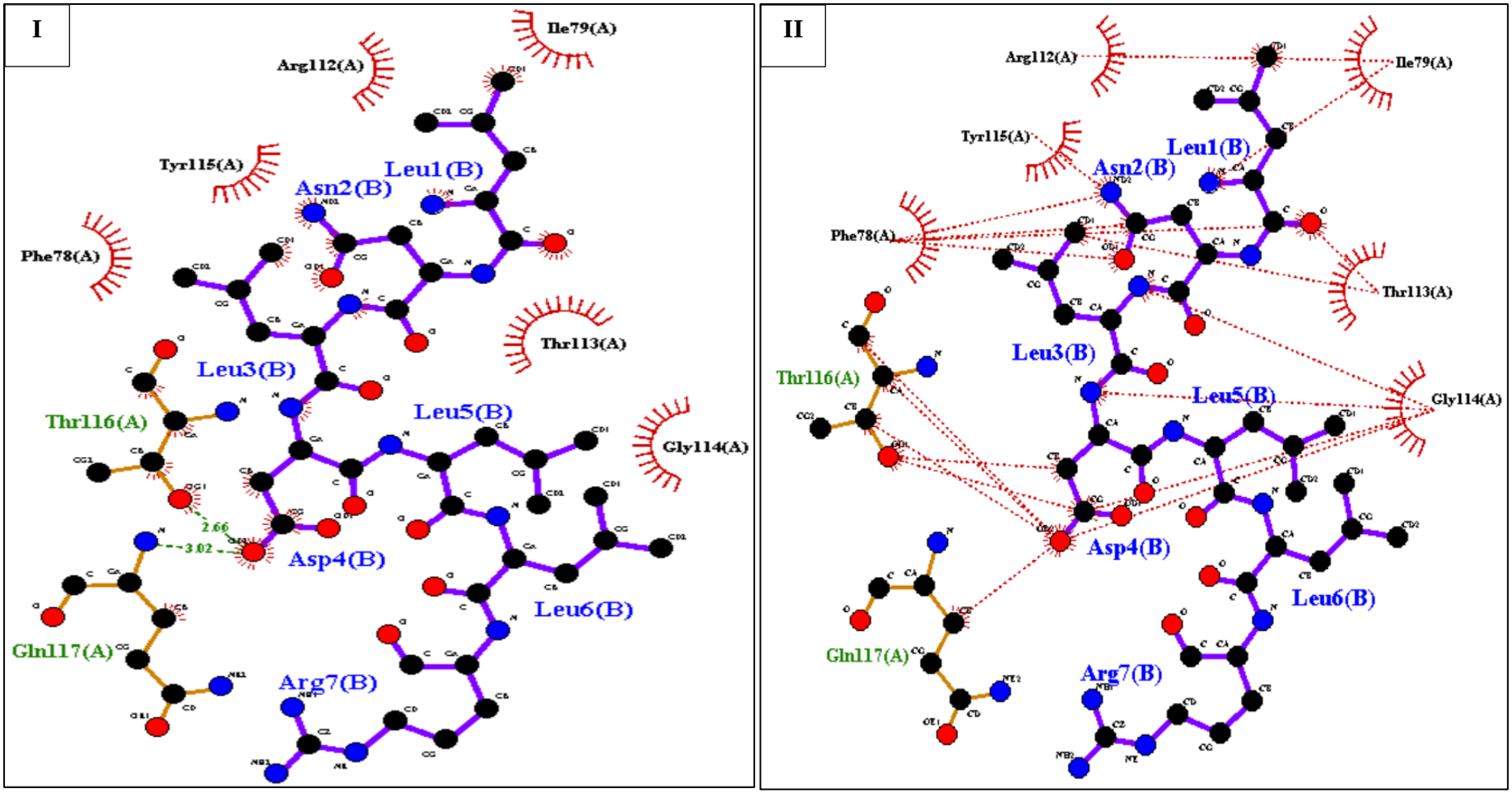

Figure S8a: Binding interaction of L**N**LDLLR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8b: Binding interaction of pancreatic lipase inhibitory peptides- LNFEPR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide L**N**FEPR	ASN2	cluster2_2	-8.0	C - Phe78 CA - NA CB - Phe78 CG - NA N - Phe78 ND_2 - NA O - Phe78, Tyr115 OD_1 - NA	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					20%	0%	0%	0%

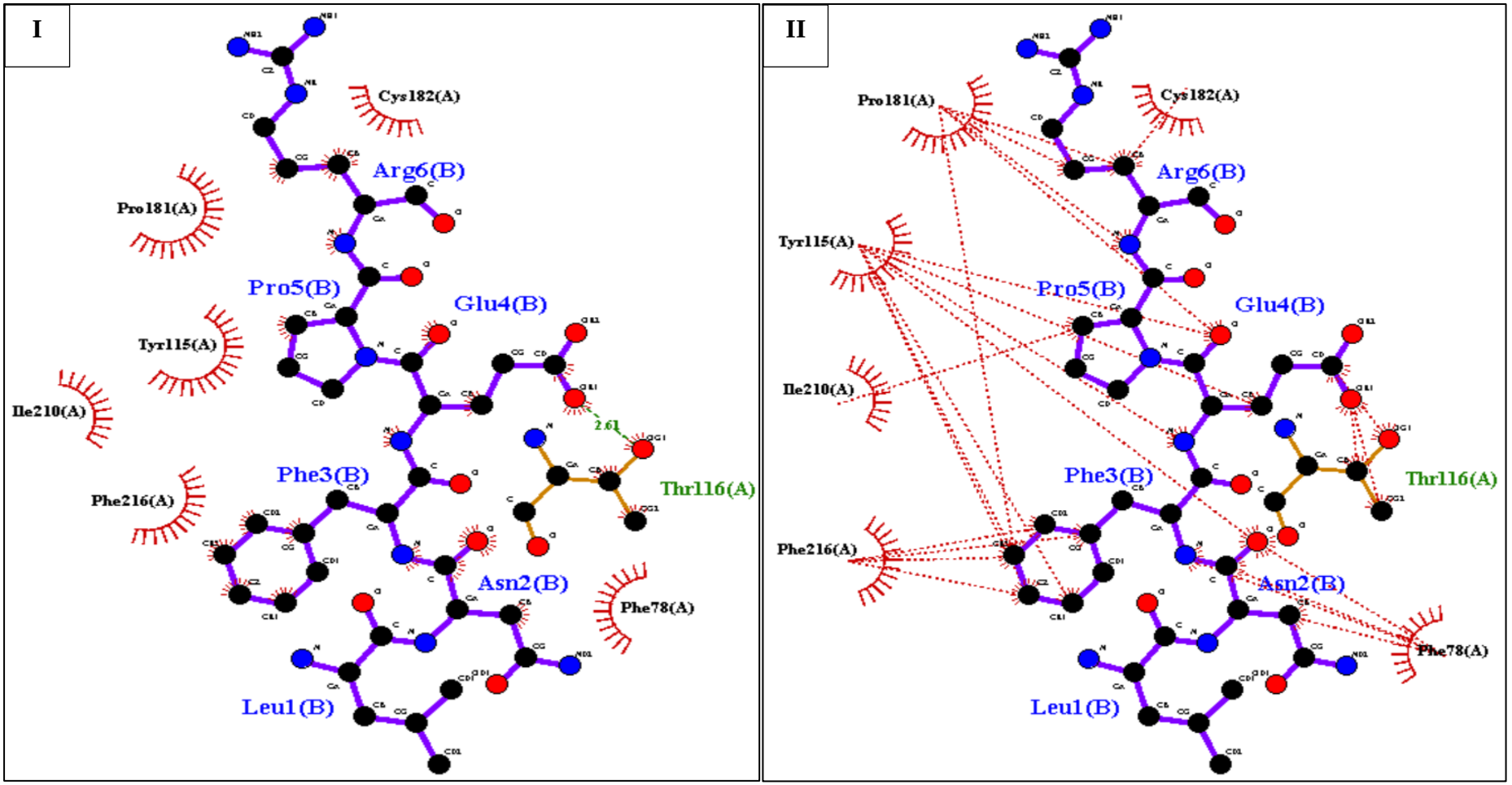

Figure S8b: Binding interaction of LNFEPR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8c: Binding interaction of pancreatic lipase inhibitory peptides-ELPPHFL at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide E**L**PPHFL	LEU2	cluster5_2	-6.8	C - NA CA - NA CB - NA CD_1 - Thr116 CD_2 - NA CG - Thr116 N - NA O - NA	NA	NA	NA
Total number of bonds					33	0	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					6%	0%	0%	0%

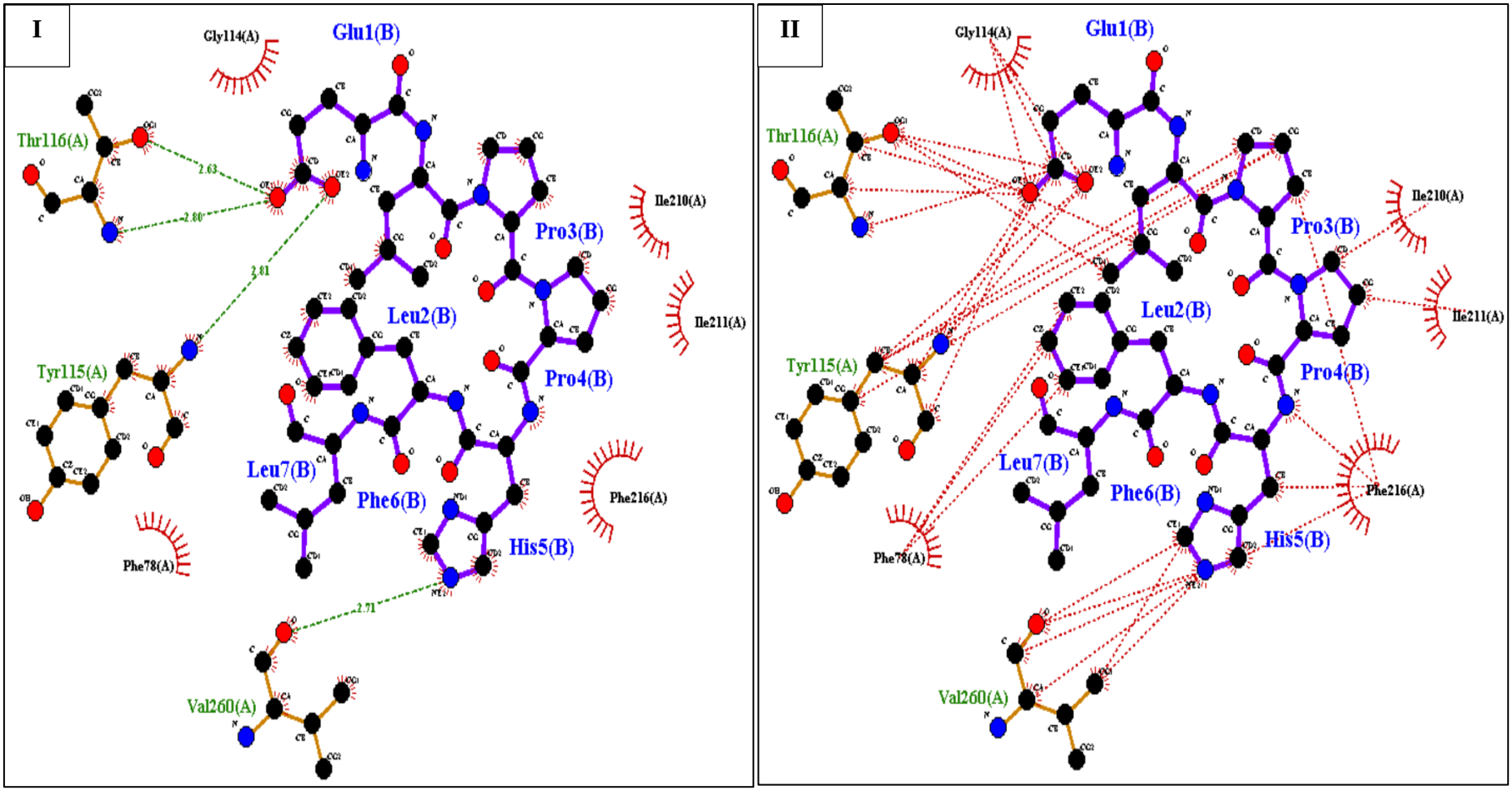

Figure S8c: Binding interaction of E**L**PPHFL inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8d: Binding interaction of pancreatic lipase inhibitory peptides-FLWPEYGAL at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide F**L**WPEYGAL	LEU2	cluster11_3	-7.6	C - NA CA - NA CB - Phe216 CD_1 - Phe216 CD_2 - Phe78, Tyr115 CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					30	0	0	3
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

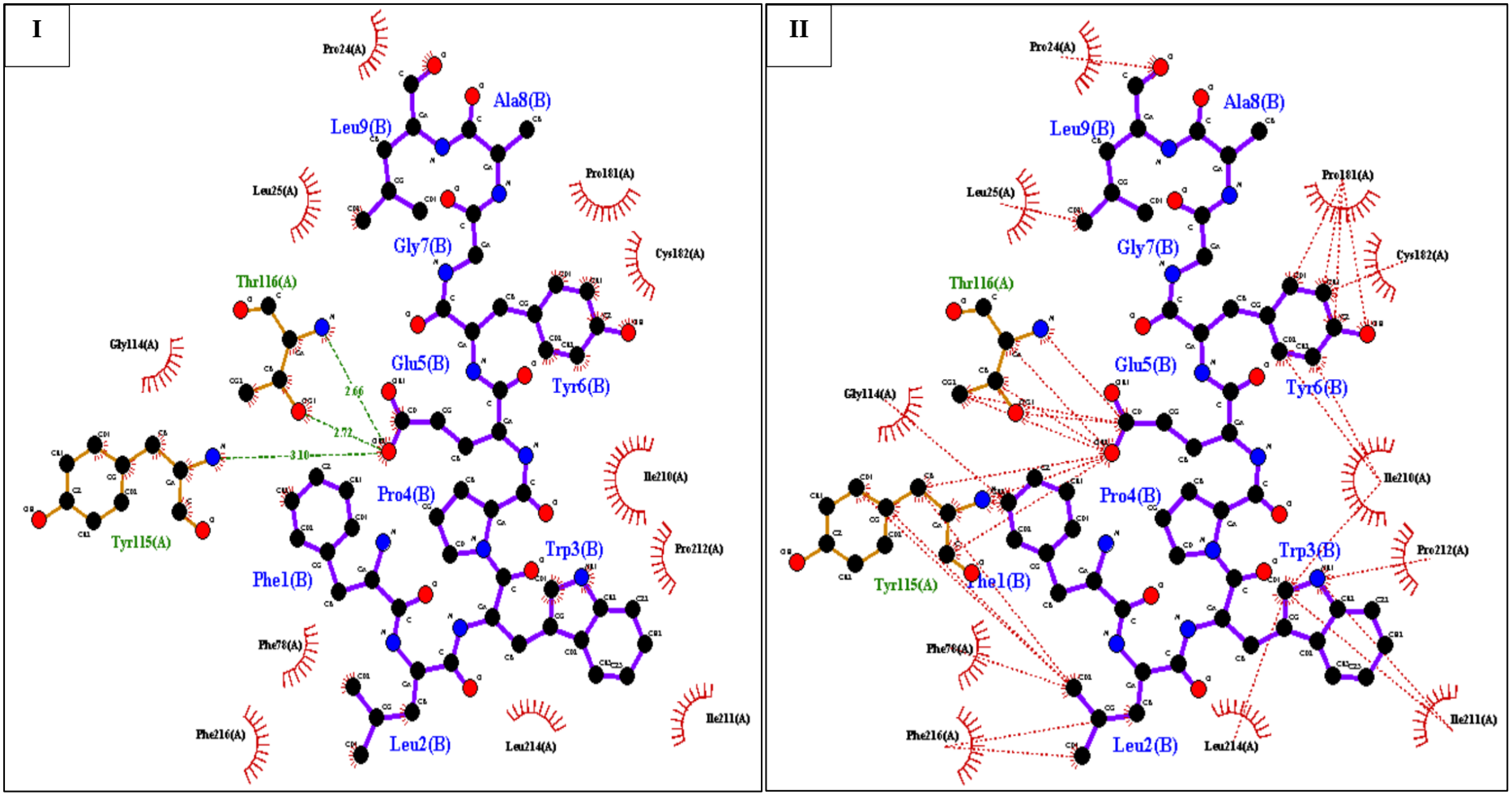

Figure S8d: Binding interaction of F**L**WPEYGAL inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8e: Binding interaction of pancreatic lipase inhibitory peptides-LAPSTIK at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide L**A**PSTIK	ALA2	cluster1_2	-8.0	C - NA CA - NA CB - NA N - NA O - NA	NA	NA	NA
Total number of bonds					28	0	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

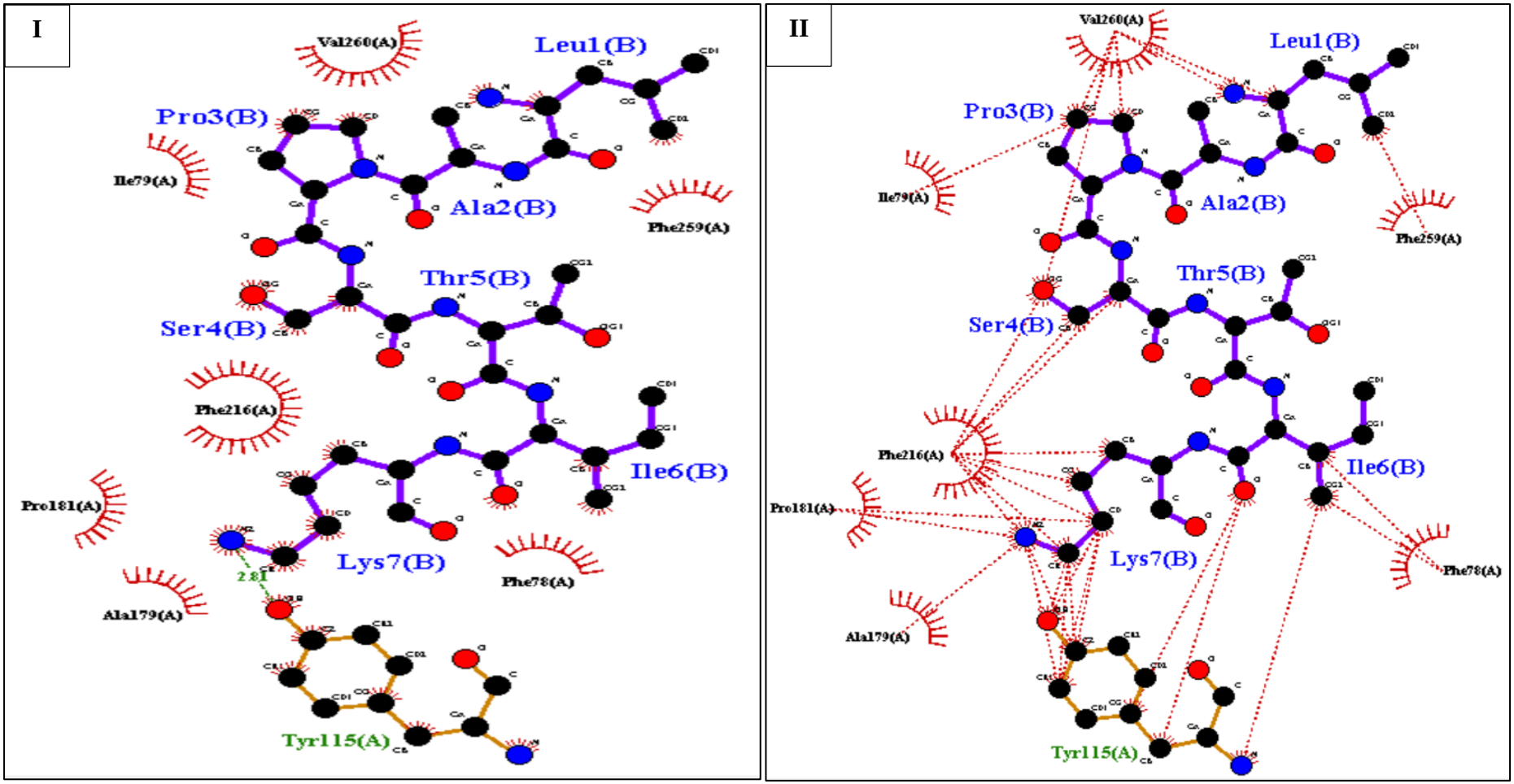

Figure S8e: Binding interaction of L**A**PSTIK inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S8f: Binding interaction of pancreatic lipase inhibitory peptides-VAPEEHPV at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide V**A**PEEHPV	ALA2	cluster2_4	-7.6	C - NA CA - NA CB - NA N - NA O - NA	NA	NA	NA
Total number of bonds					32	0	0	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

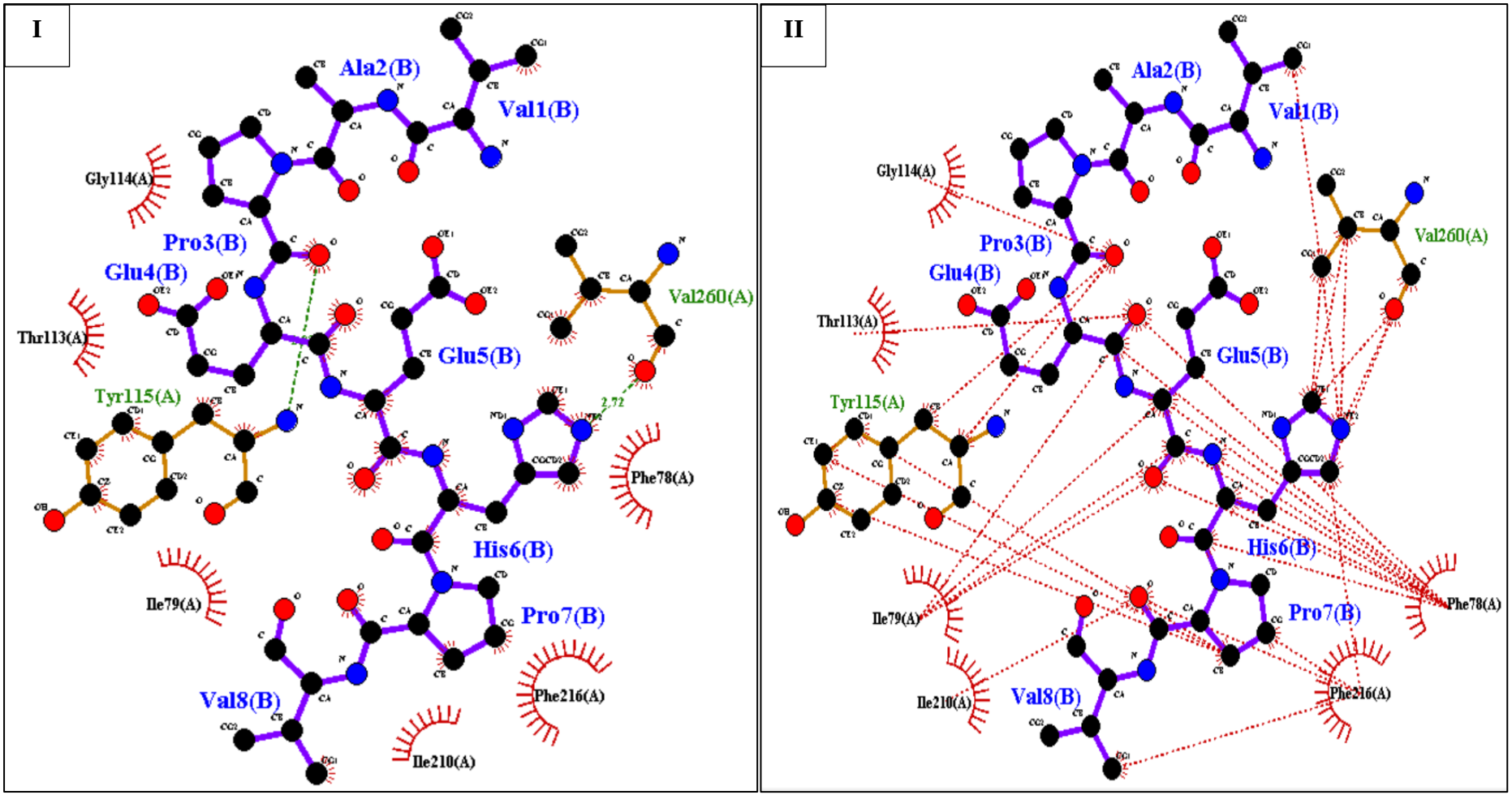

Figure S8f: Binding interaction of V**A**PEEHPV inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9a: Binding interaction of pancreatic lipase inhibitory peptides-GNPVGGVGHGTTGT at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide G**N**PVGGVGHG TTGT	ASN2	cluster5_1	-8.9	C - NA CA - NA CB - NA CG - NA N - NA ND_2 - Trp253 O - NA OD_1 - NA	NA	NA	NA
Total number of bonds					36	1	0	1
Total no of interactive residues					1	0	0	0
Overall percentage of bonding					3%	0%	0%	0%

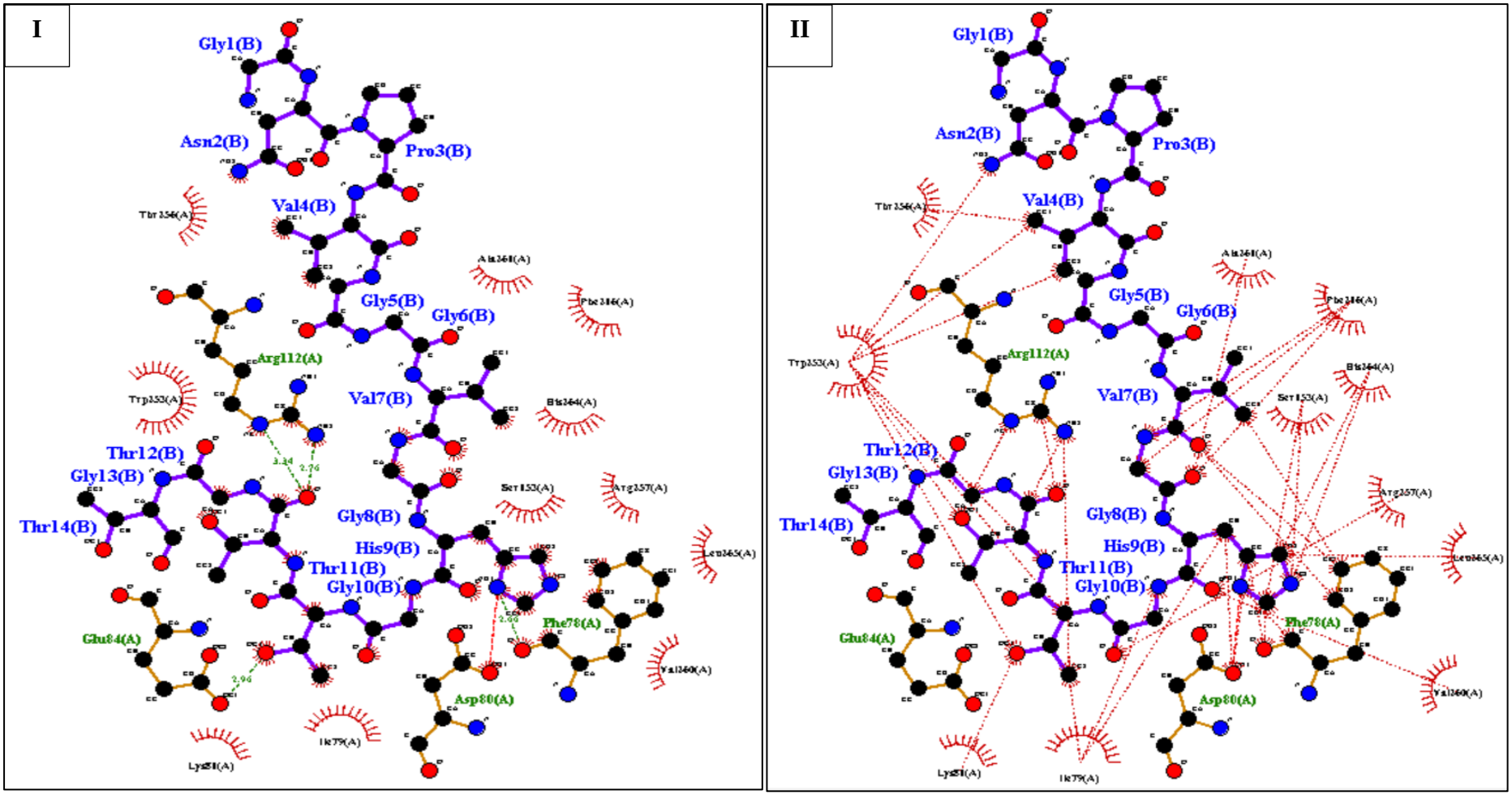

Figure S9a: Binding interaction of G**N**PVGGVGHGTTGT inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9b: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide LNNPSVCDCD CMMKAAR	ASN2	cluster3_4	-9.8	C - NA CA - NA CB - Tyr115 CG - NA N - NA ND_2 - NA O - NA OD_1 - Phe78, Gly114	NA	NA	OD_1 - Tyr115
Total number of bonds					45	0	0	3
Total no of interactive residues					3	0	0	1
Overall percentage of bonding					7%	0%	0%	33%

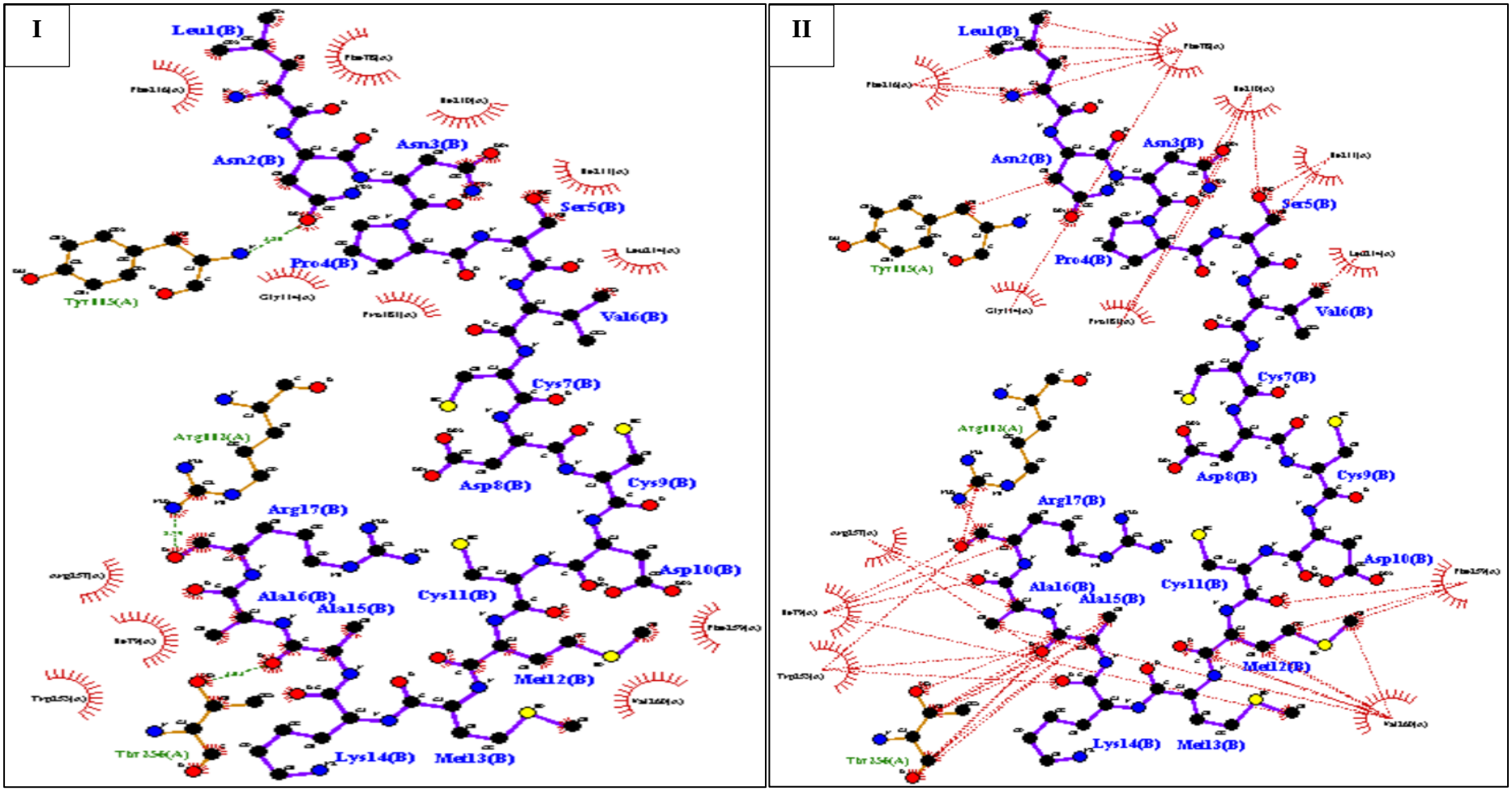

Figure S9b: Binding interaction of L**N**NPSVCDCDCMMKAAR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9c: Binding interaction of pancreatic lipase inhibitory peptides-MLPLMLPFTMGY at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide M**L**PLMLPFTM GY	LEU2	cluster2_1	-8.4	C - NA CA - NA CB - Phe259 CD_1 - Phe259, Val260 CD_2 - NA CG - NA N - Phe259 O - NA	NA	NA	NA
Total number of bonds					41	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

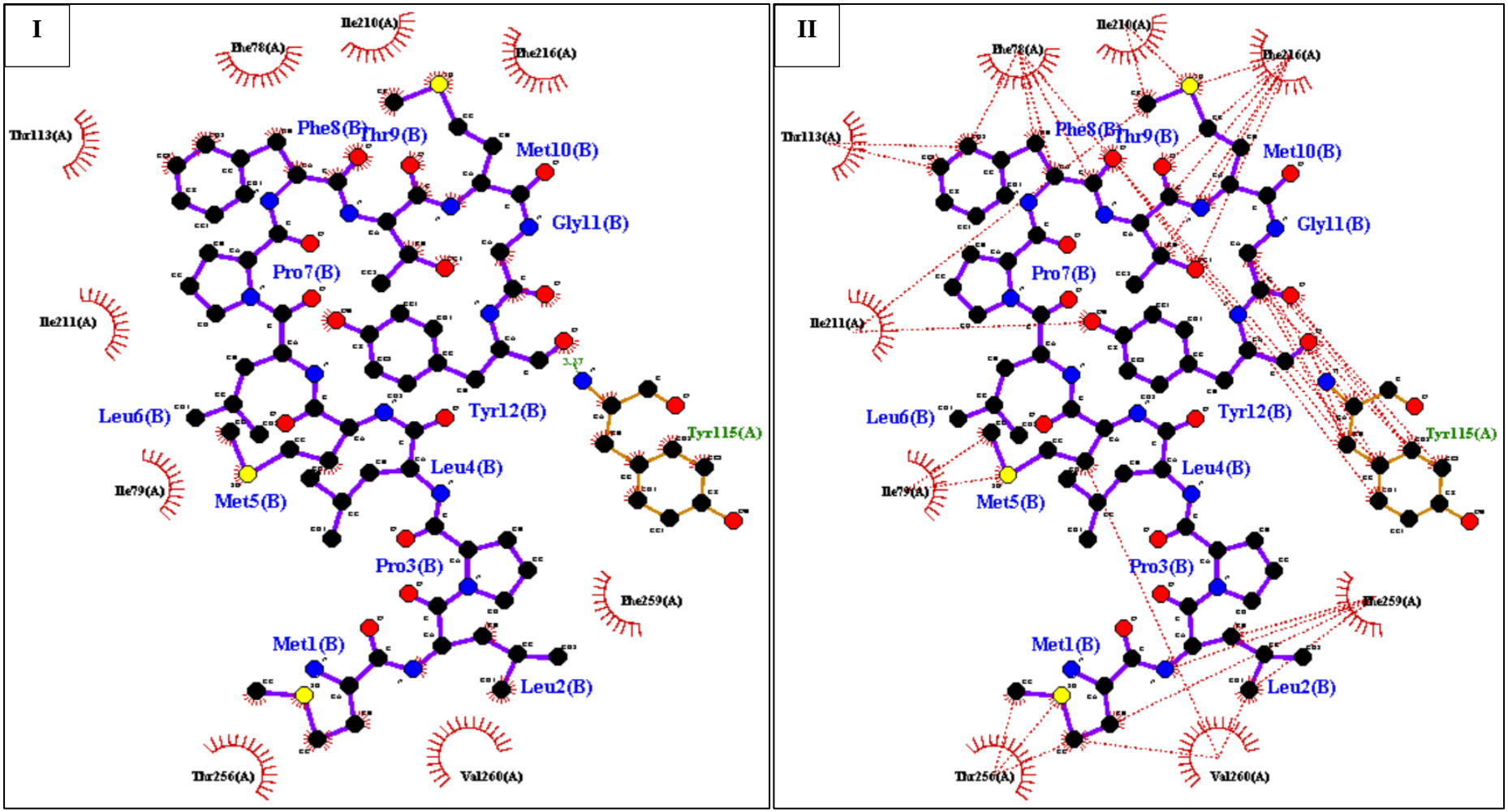

Figure S9c: Binding interaction of M**L**PLMLPFTMGY inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9d: Binding interaction of pancreatic lipase inhibitory peptides- NALKCCHSCPA at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide N**A**LKCCHSCP A	ALA2	cluster1_3	-10.4	C - NA CA - NA CB - NA N - Val260 O - NA	NA	NA	NA
Total number of bonds					47	0	0	2
Total no of interactive residues					1	0	0	0
Overall percentage of bonding					2%	0%	0%	0%

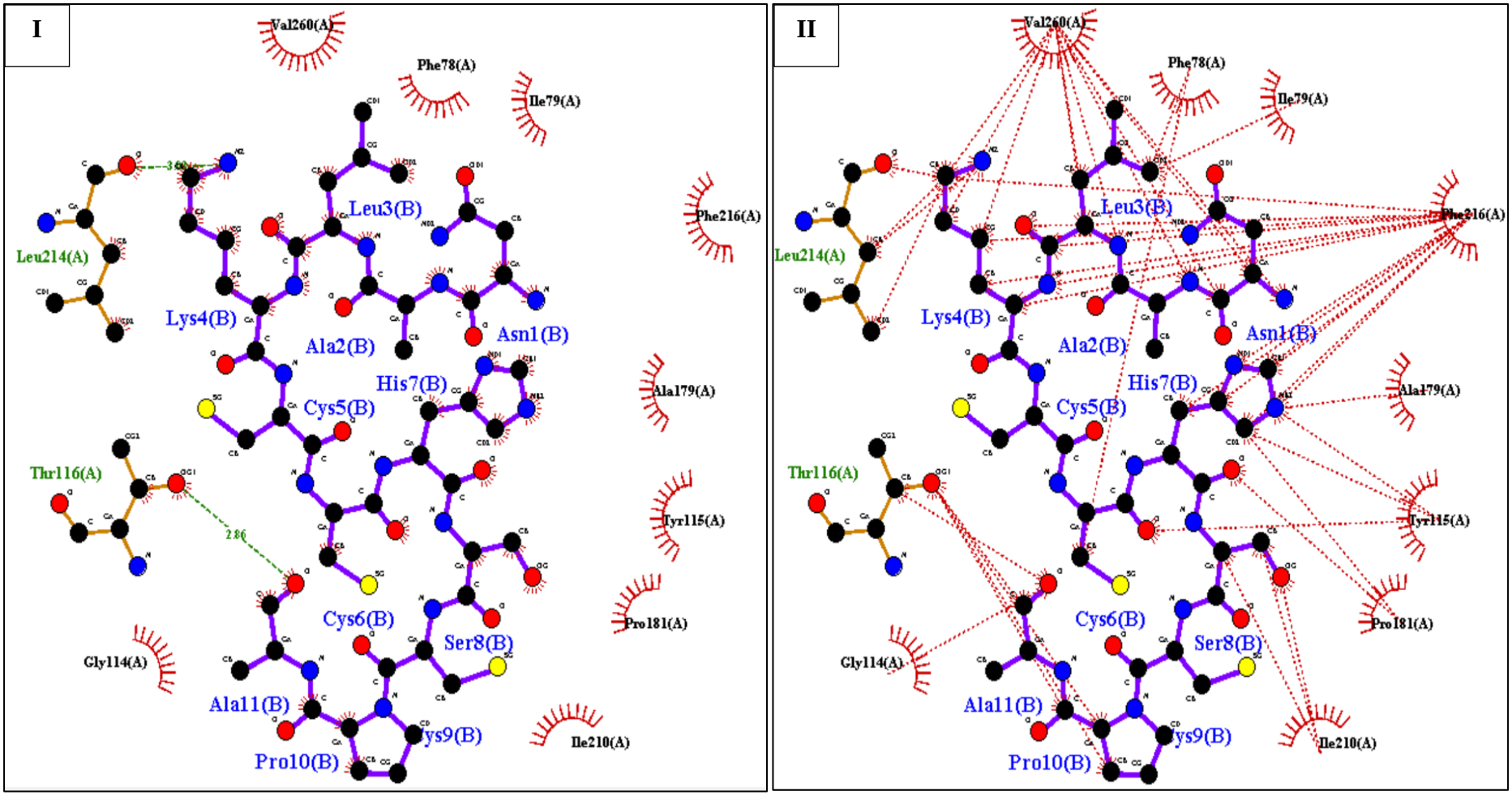

Figure S9d: Binding interaction of N**A**LKCCHSCPA inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9e: Binding interaction of pancreatic lipase inhibitory peptides-LAAVEALSTNG at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide L**A**AVEALSTN G	ALA2	cluster1_1	-8.4	C - Phe216 CA - Phe78 CB - Phe78 N - NA O - Phe216	NA	NA	NA
Total number of bonds					31	0	0	3
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

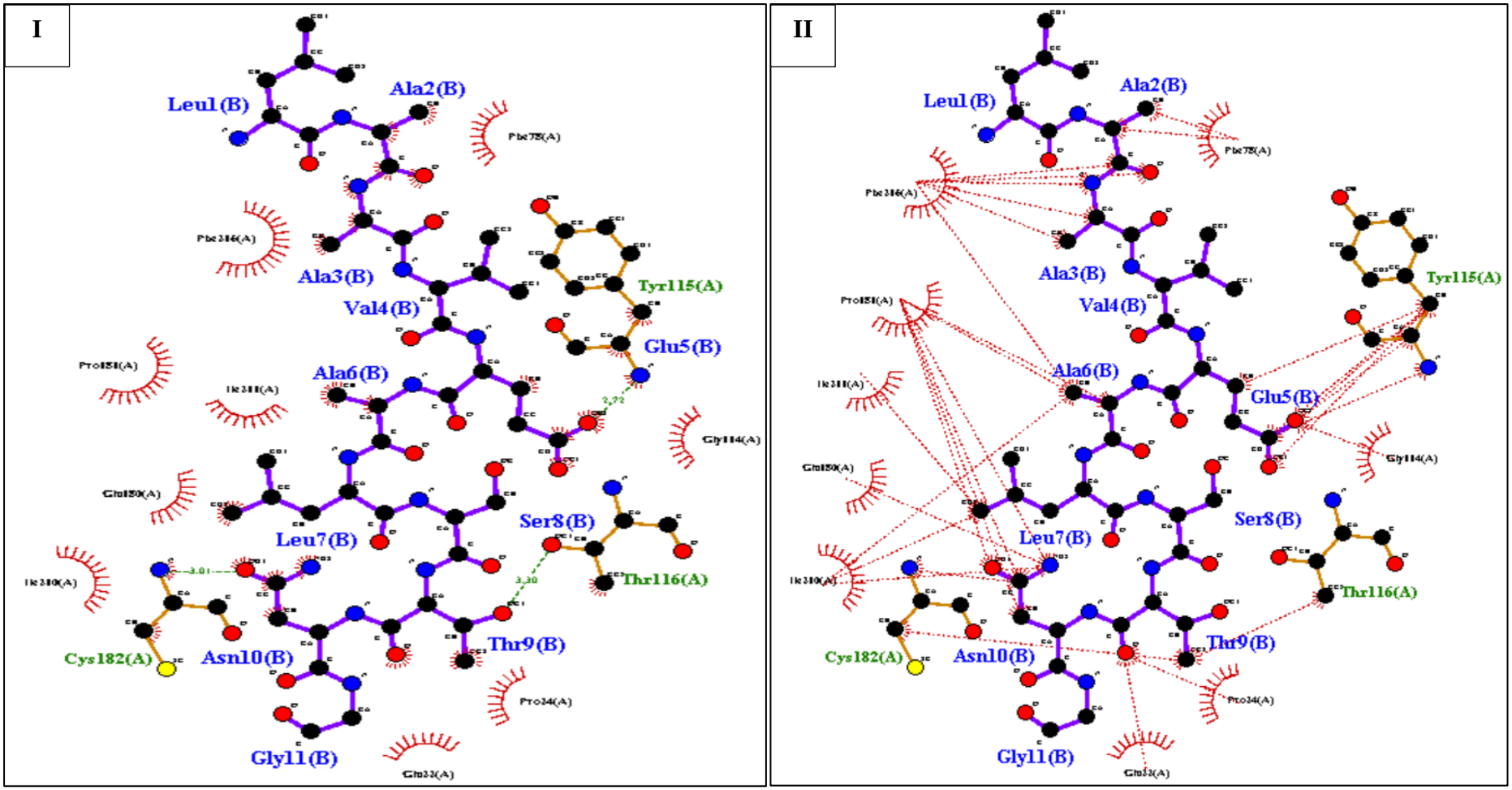

Figure S9e: Binding interaction of L**A**AVEALSTNG inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9f: Binding interaction of pancreatic lipase inhibitory peptides-SGGGGGGVAGAATASR at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide S**G**GGGGGVAG AATASR	GLY2	cluster3_1	-7.4	C - NA CA - NA N - Tyr115 O - NA	NA	NA	NA
Total number of bonds					40	0	0	0
Total no of interactive residues					1	0	0	0
Overall percentage of bonding					3%	0%	0%	0%

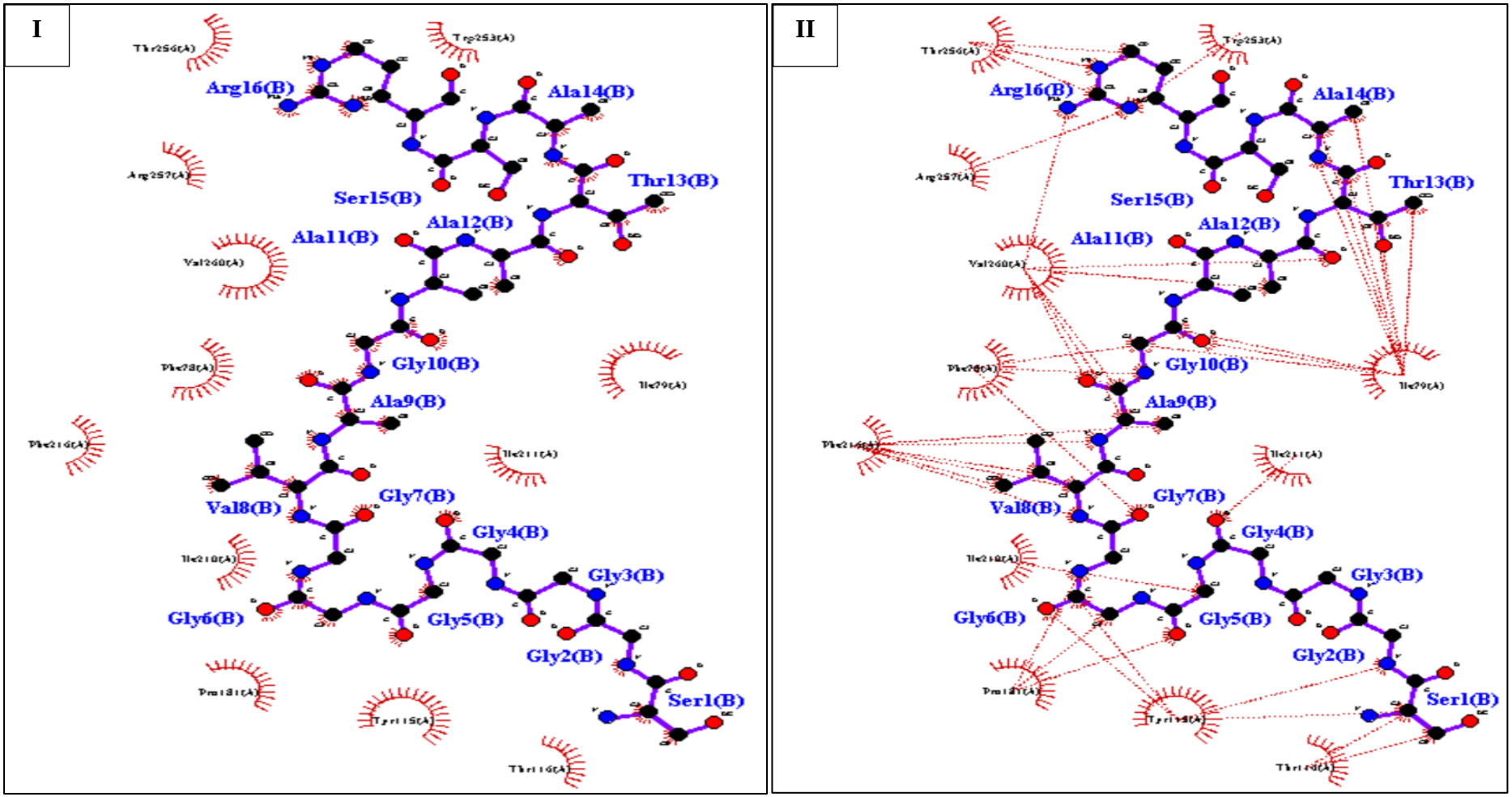

Figure S9f: Binding interaction of S**G**GGGGGVAGAATASR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S9g: Binding interaction of pancreatic lipase inhibitory peptides-YGNPVGGVGH at N2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide Y**G**NPVGGVGH	GLY2	cluster1_3	-9.0	C - Phe78 CA - NA N - NA O - Phe78	NA	NA	NA
Total number of bonds					57	2	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					4%	0%	0%	0%

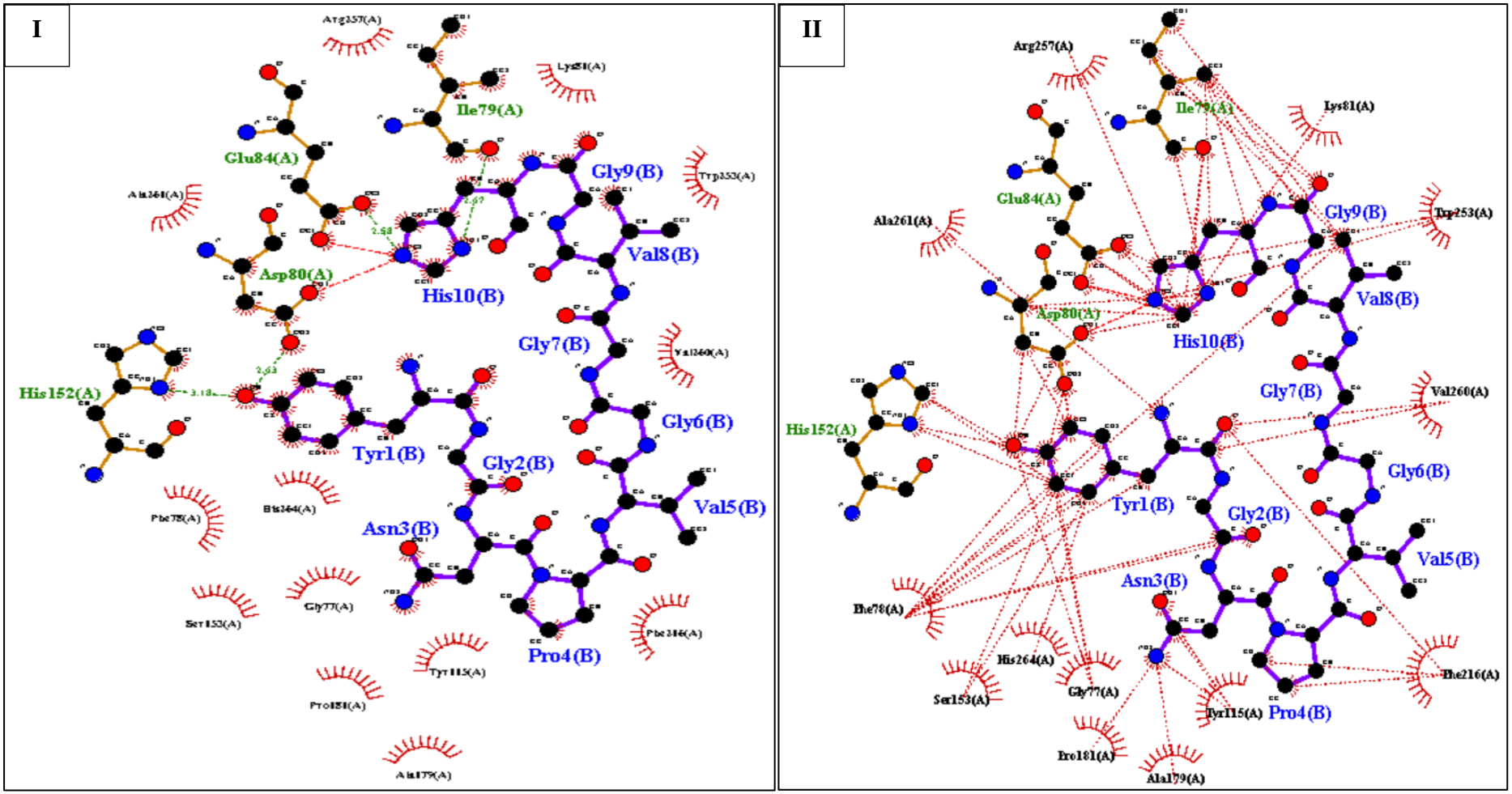

Figure S9g: Binding interaction of Y**G**NPVGGVGH inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10a: Binding interaction of pancreatic lipase inhibitory peptides-MMML at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide MM**M**L	MET3	cluster10_1	-7.3	C - NA CA - NA CB - NA CE - Val260 CG - NA O - Phe78 N - Phe78 SD - NA	NA	NA	NA
Total number of bonds					34	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

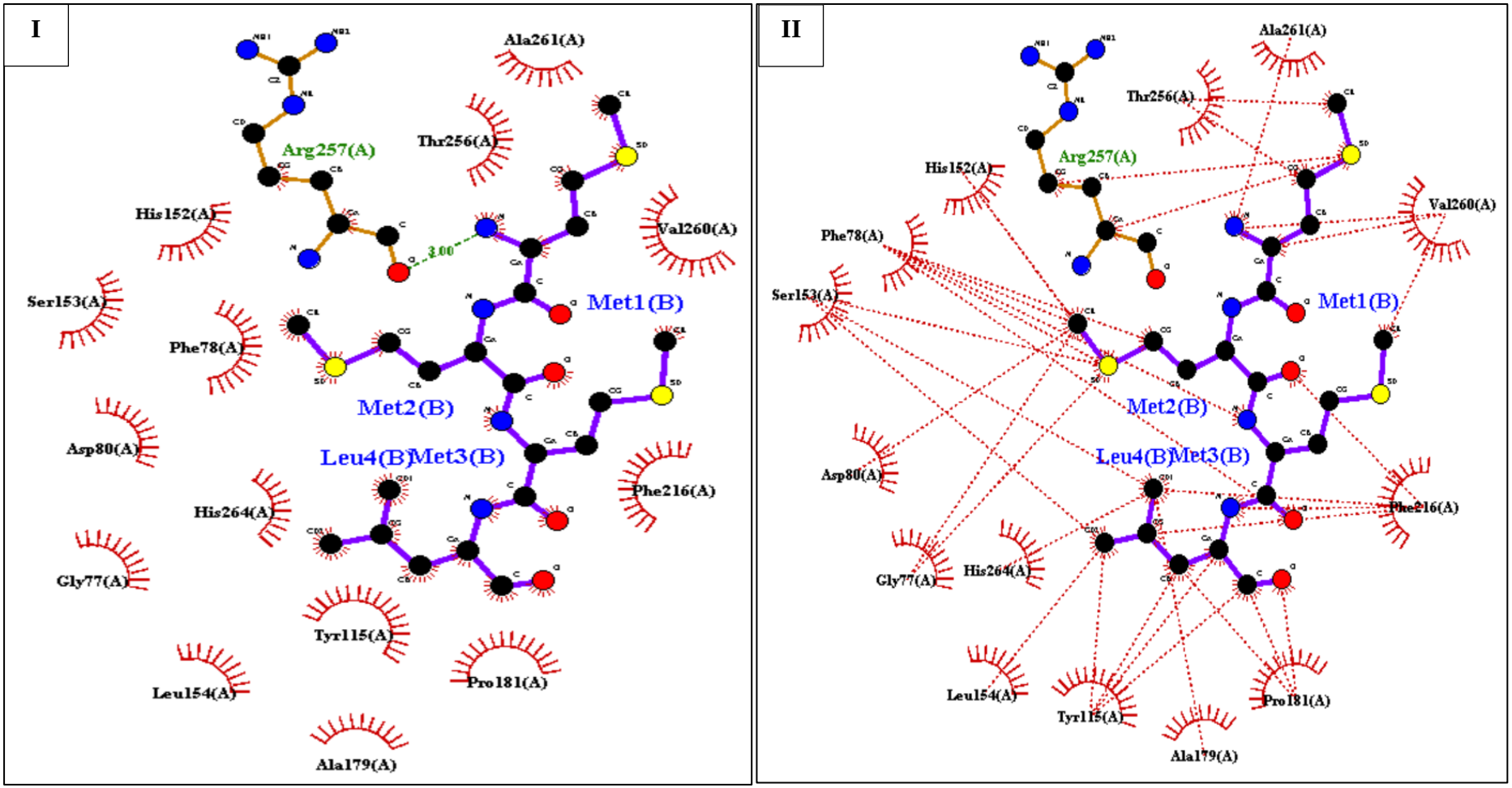

Figure S10a: Binding interaction of MM**M**L inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10b: Binding interaction of pancreatic lipase inhibitory peptides-FDML at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide FD**M**L	MET3	cluster4_3	-7.1	C - NA CA - Phe78 CB - NA CE - Phe216 CG - NA O - NA N - NA SD – NA	NA	NA	NA
Total number of bonds					21	0	0	0
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

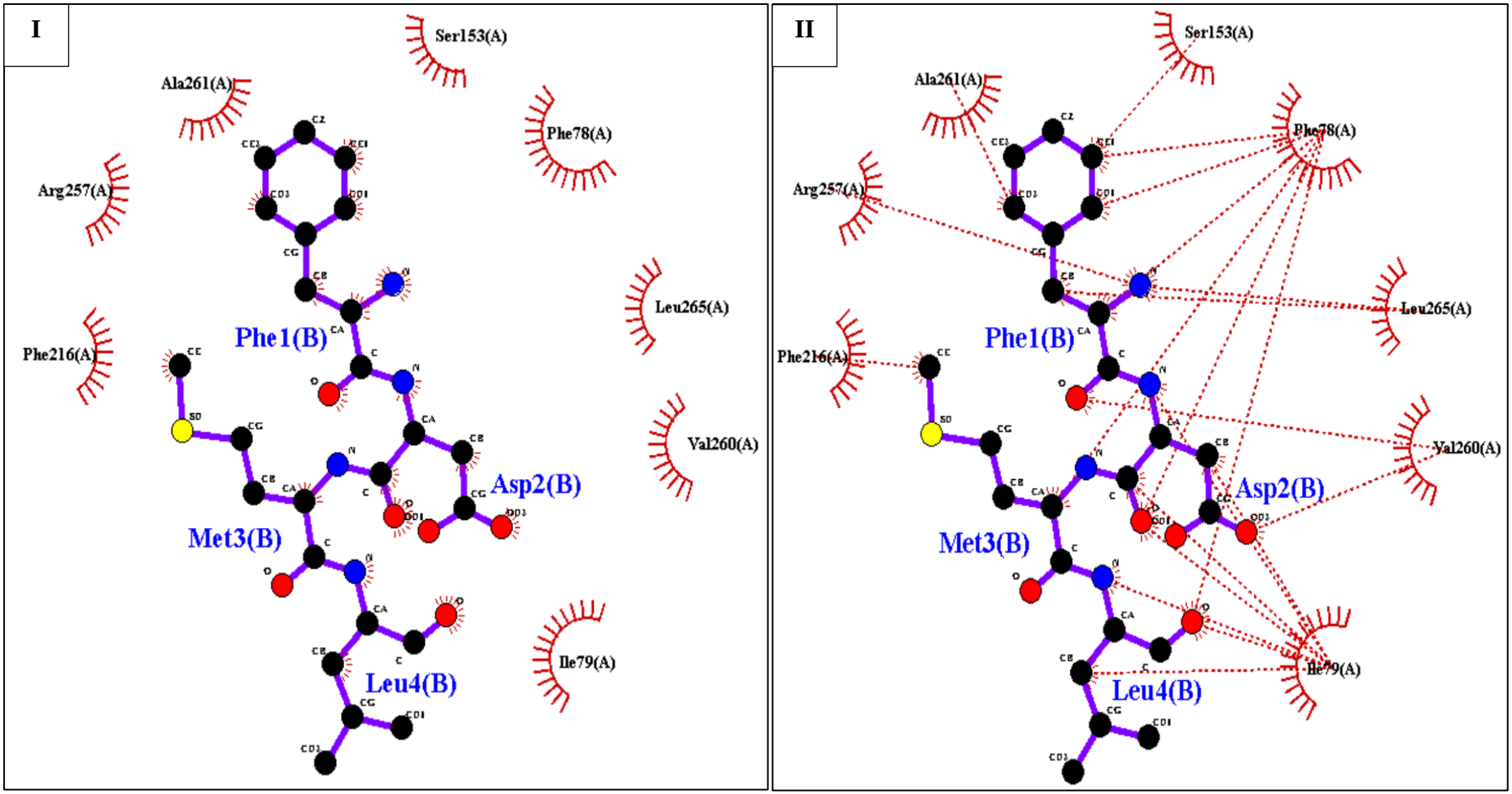

Figure S10b: Binding interaction of FD**M**L inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10c: Binding interaction of pancreatic lipase inhibitory peptides-LRFPL at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide LRF**P**L	PRO4	cluster1_1	-7.4	C - NA CA -NA CB - NA CD - Phe216 CG - Phe216 N- NA O - Phe78, Tyr115	NA	NA	NA
Total number of bonds					24	0	0	2
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					17%	0%	0%	0%

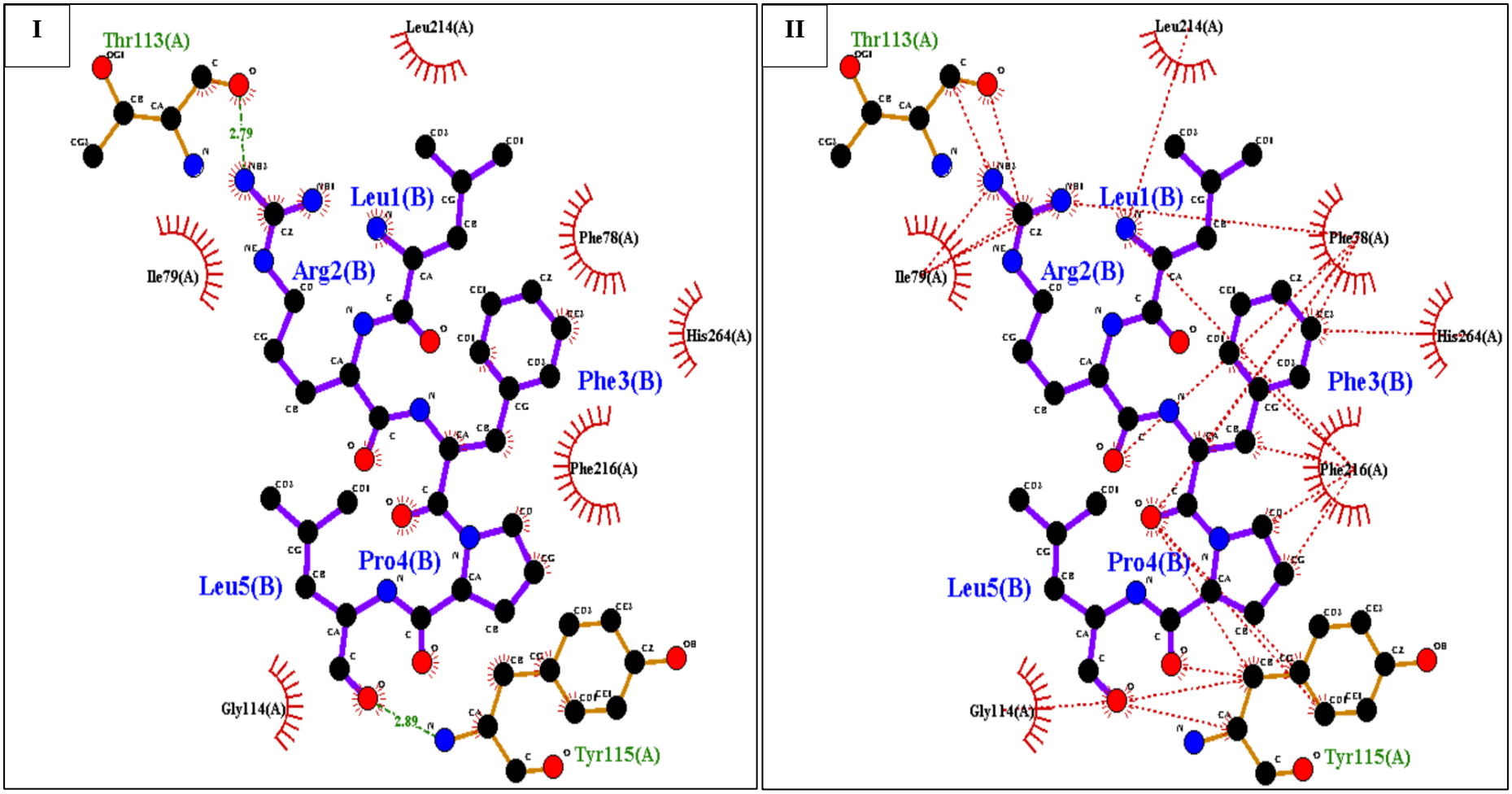

Figure S10c: Binding interaction of LRFPL inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10d: Binding interaction of pancreatic lipase inhibitory peptides-VIAPW at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide VIA**P**W	PRO4	cluster3_2	-6.7	C - NA CA -NA CB - Phe78 CD - NA CG - NA N- NA O - Gly114, Tyr115	NA	NA	O - Tyr115
Total number of bonds					26	0	0	1
Total no of interactive residues					3	0	0	1
Overall percentage of bonding					12%	0%	0%	100%

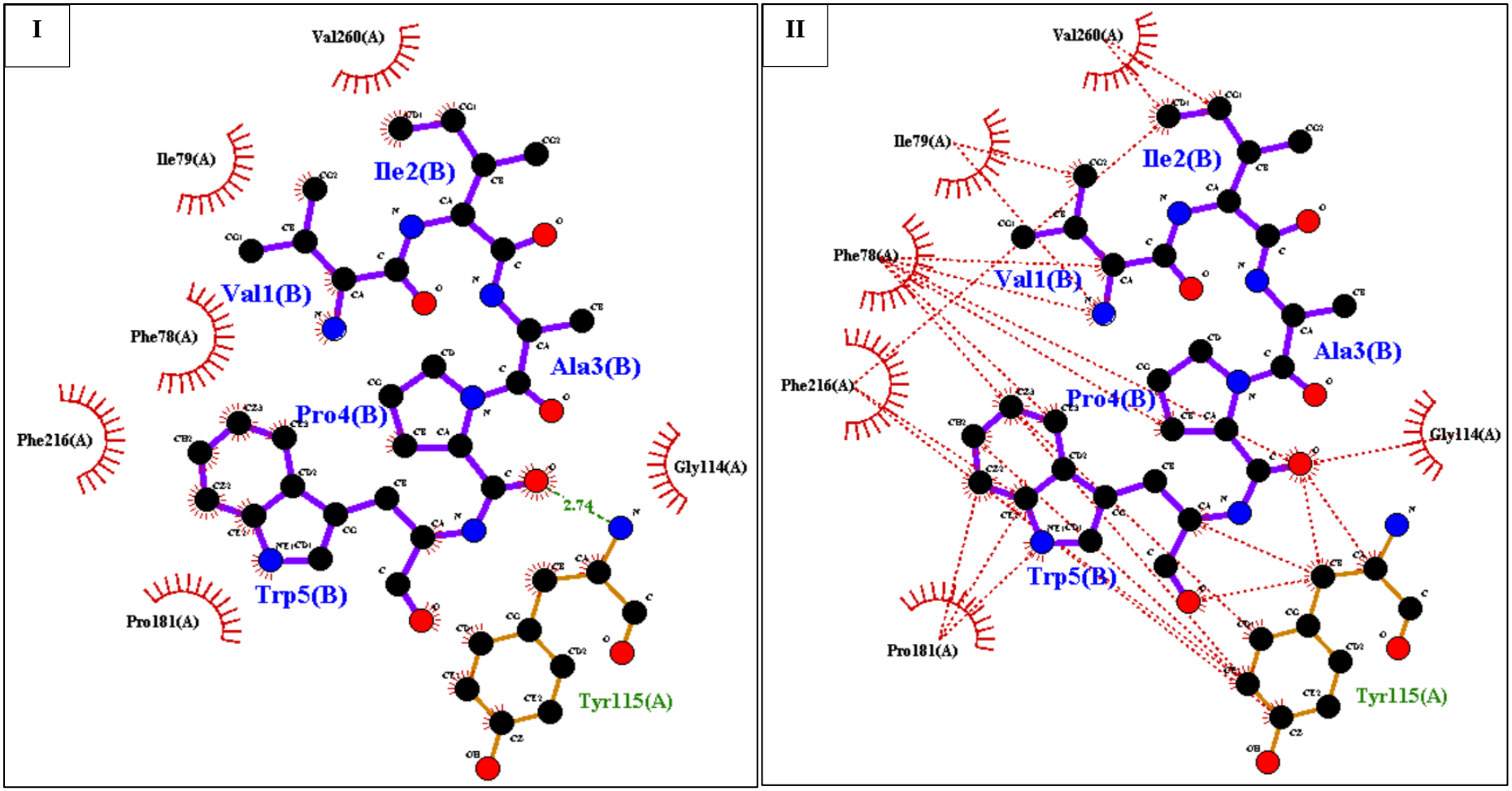

Figure S10d: Binding interaction of VIA**P**W inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10e: Binding interaction of pancreatic lipase inhibitory peptides-RLLP at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide RL**L**P	LEU3	cluster8_1	-7.2	C - NA CA - NA CB - Ile79 CD_1 - Phe78, Ile79 CD_2 - NA CG - NA N - NA O - Ile79	NA	NA	NA
Total number of bonds					21	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					19%	0%	0%	0%

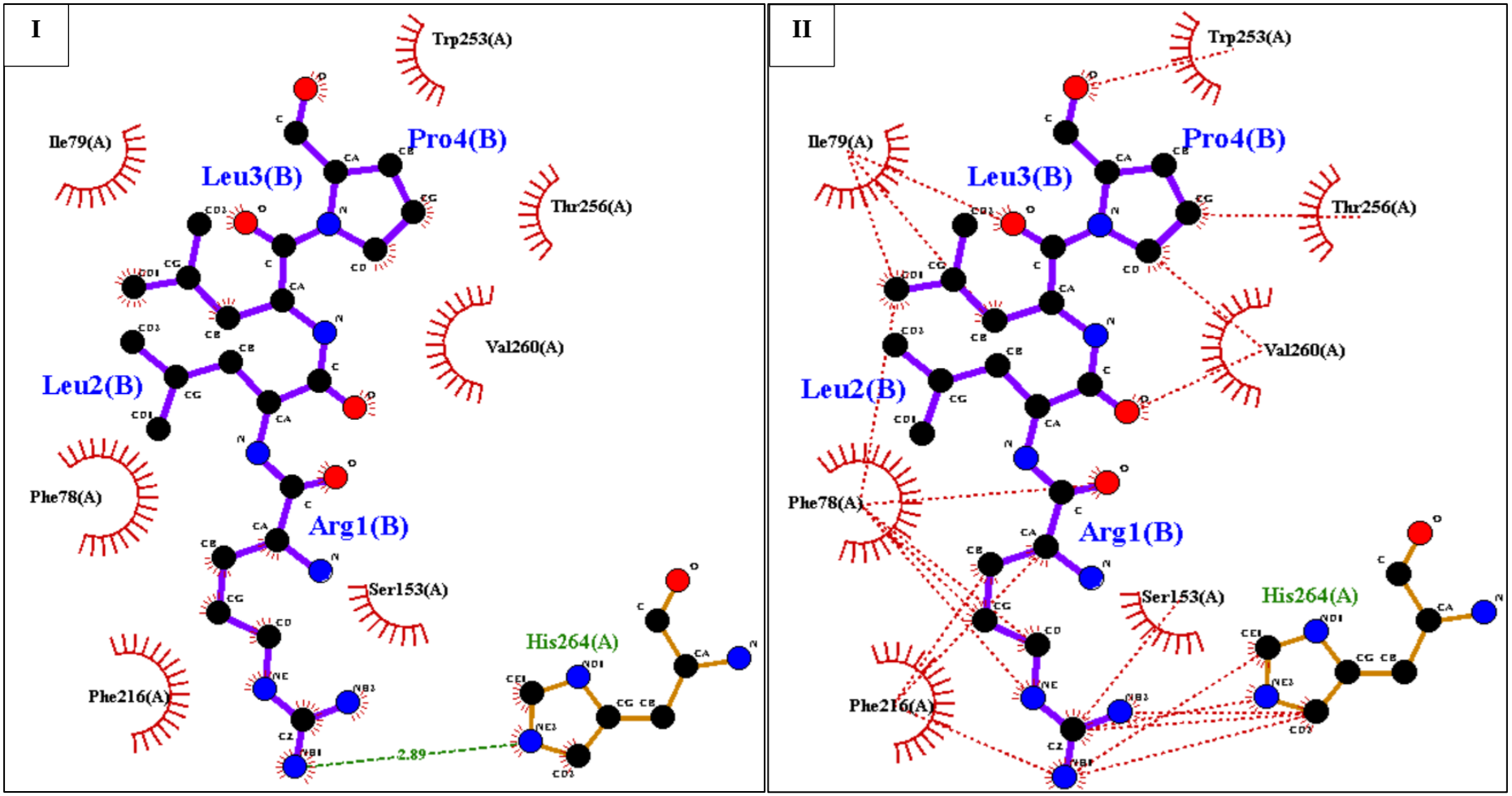

Figure S10e: Binding interaction of RL**L**P inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10f: Binding interaction of pancreatic lipase inhibitory peptides-GTIT at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide GT**I**T	ILE3	cluster9_4	-8.7	C - NA CA - NA CB - Val260 CD_1 - NA CG_1 - NA CG_2 - NA N - NA O - Val260	NA	NA	NA
Total number of bonds					16	0	0	0
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

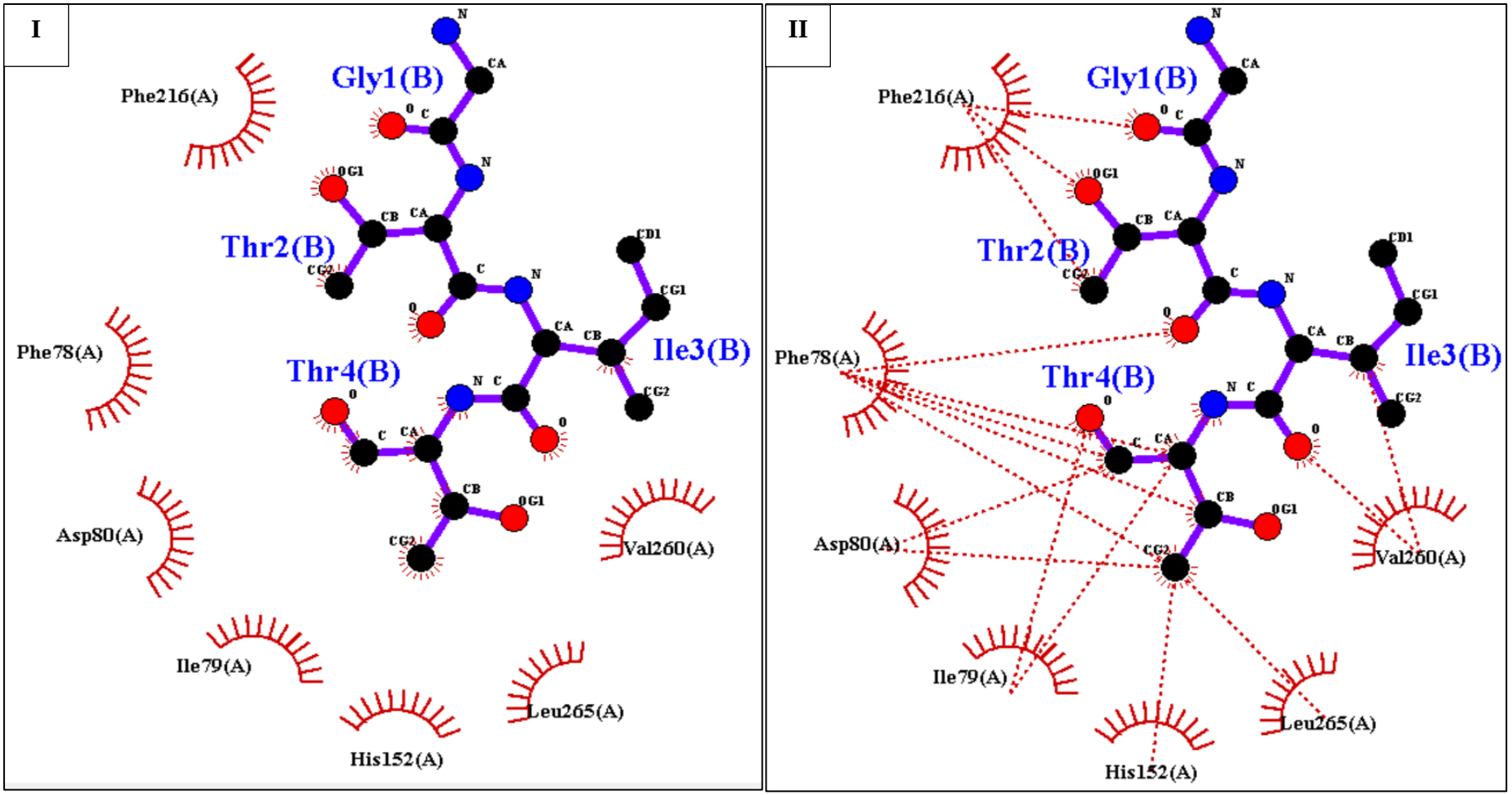

Figure S10f: Binding interaction of GT**I**T inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10g: Binding interaction of pancreatic lipase inhibitory peptides-IRWWW at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide IRW**W**W	TRP4	cluster13_4	-7.2	C - NA CA - NA CB - Phe216 CD_1 - Phe216, Val260 CD_2 - NA CE_2 - NA CE_3 - NA CG - NA CH_2 - NA CZ_2 - NA CZ_3 - NA N - NA NE_1 - Phe216, Val260 O - NA	NA	NA	NA
Total number of bonds					20	3	0	2
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					20%	0%	0%	0%

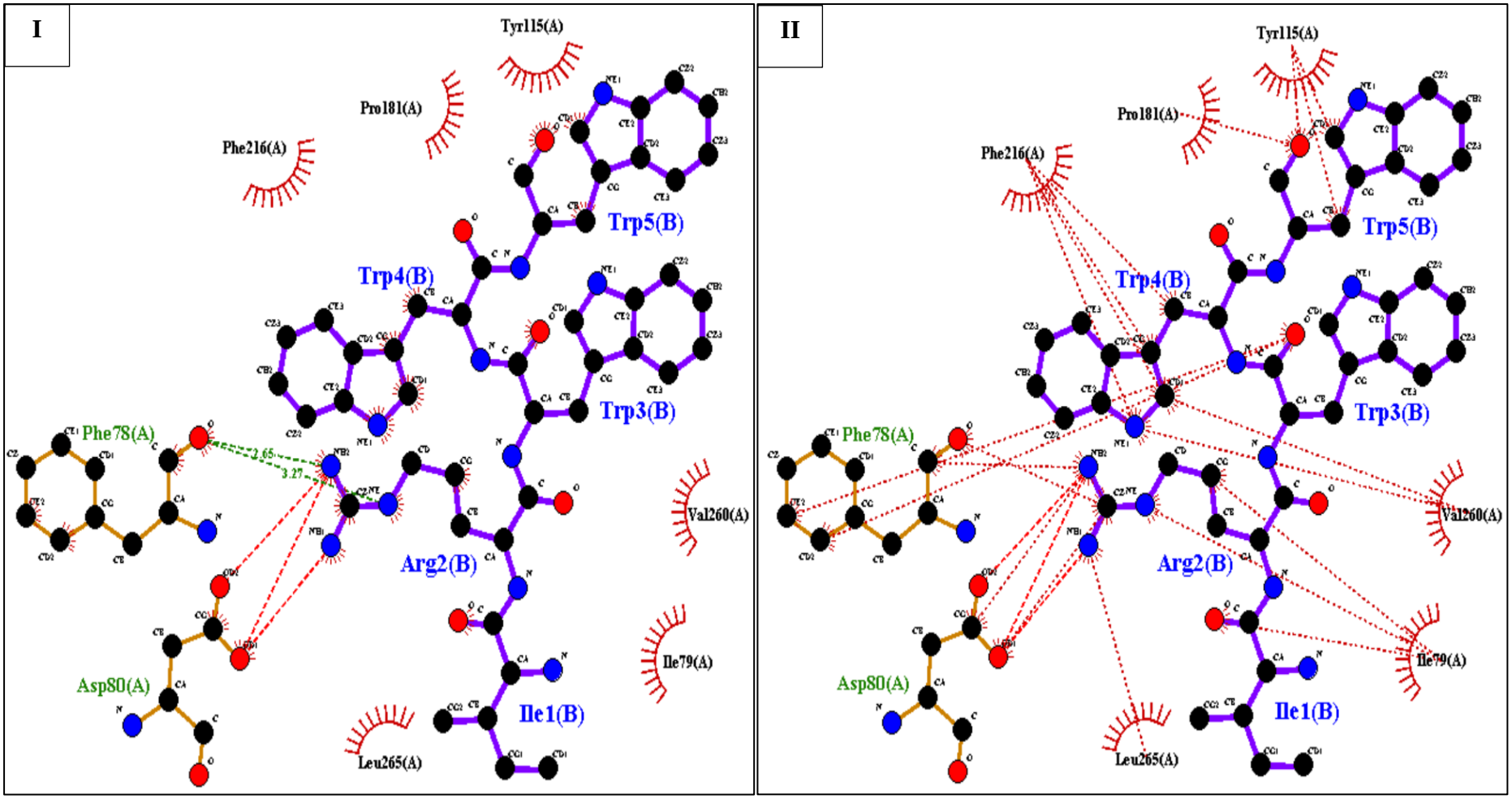

Figure S10g: Binding interaction of IRW**W**W inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S10h: Binding interaction of pancreatic lipase inhibitory peptides-AAGF at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide AA**G**F	GLY3	cluster1_3	-6.5	C - NA CA - NA N - Tyr115, Pro181 O - Tyr115, Pro181	NA	NA	NA
Total number of bonds					18	0	0	1
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					22%	0%	0%	0%

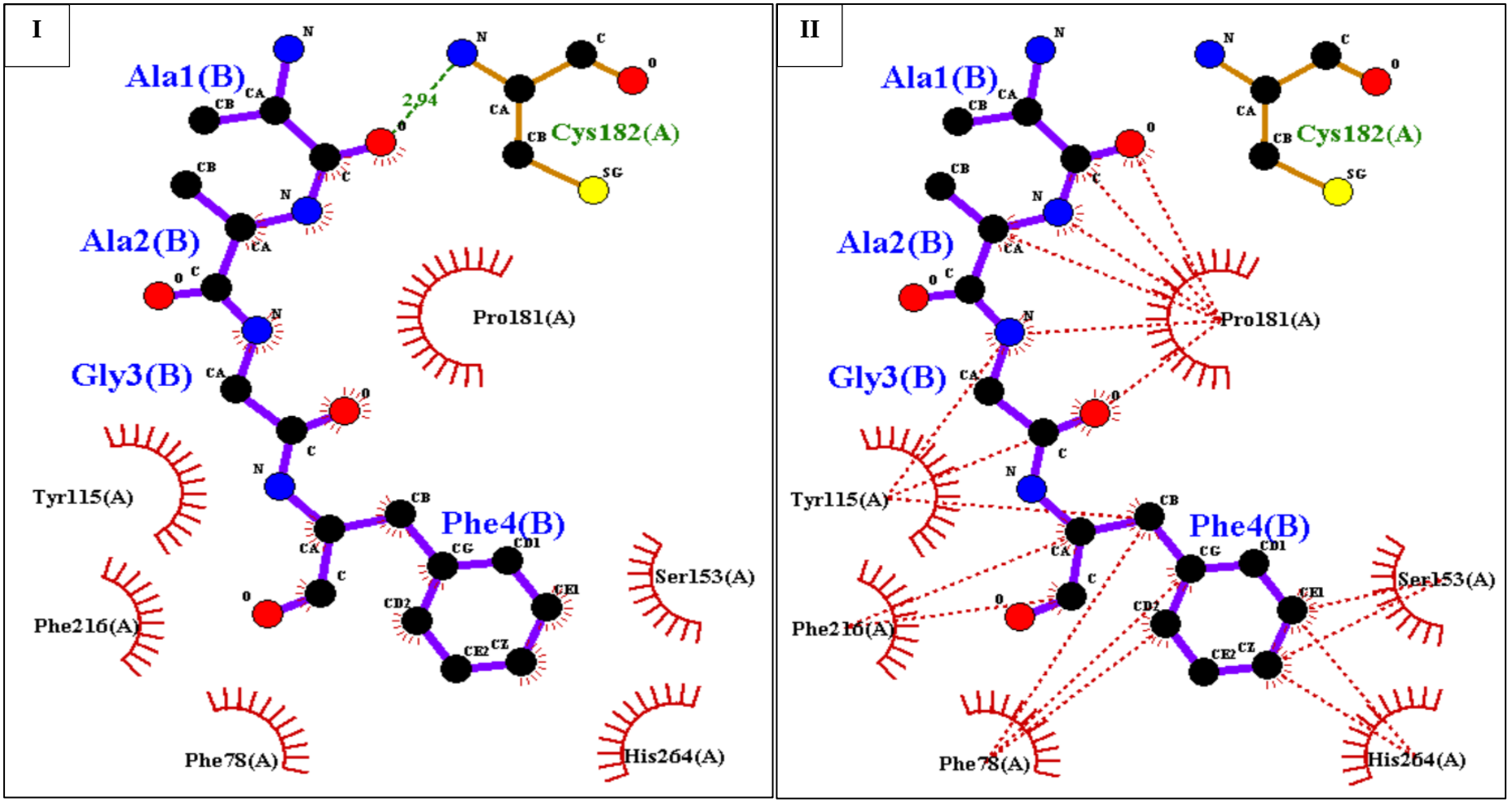

Figure S10h: Binding interaction of AA**G**F inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å),(II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S11a: Binding interaction of pancreatic lipase inhibitory peptides-VAPEEHPV at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide VAPEEH**P**V	PRO7	cluster2_4	-7.6	C - NA CA -NA CB - Tyr115 CD - NA CG - Phe216 N- NA O - Ile210, Phe216	NA	NA	NA
Total number of bonds					32	0	0	2
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					13%	0%	0%	0%

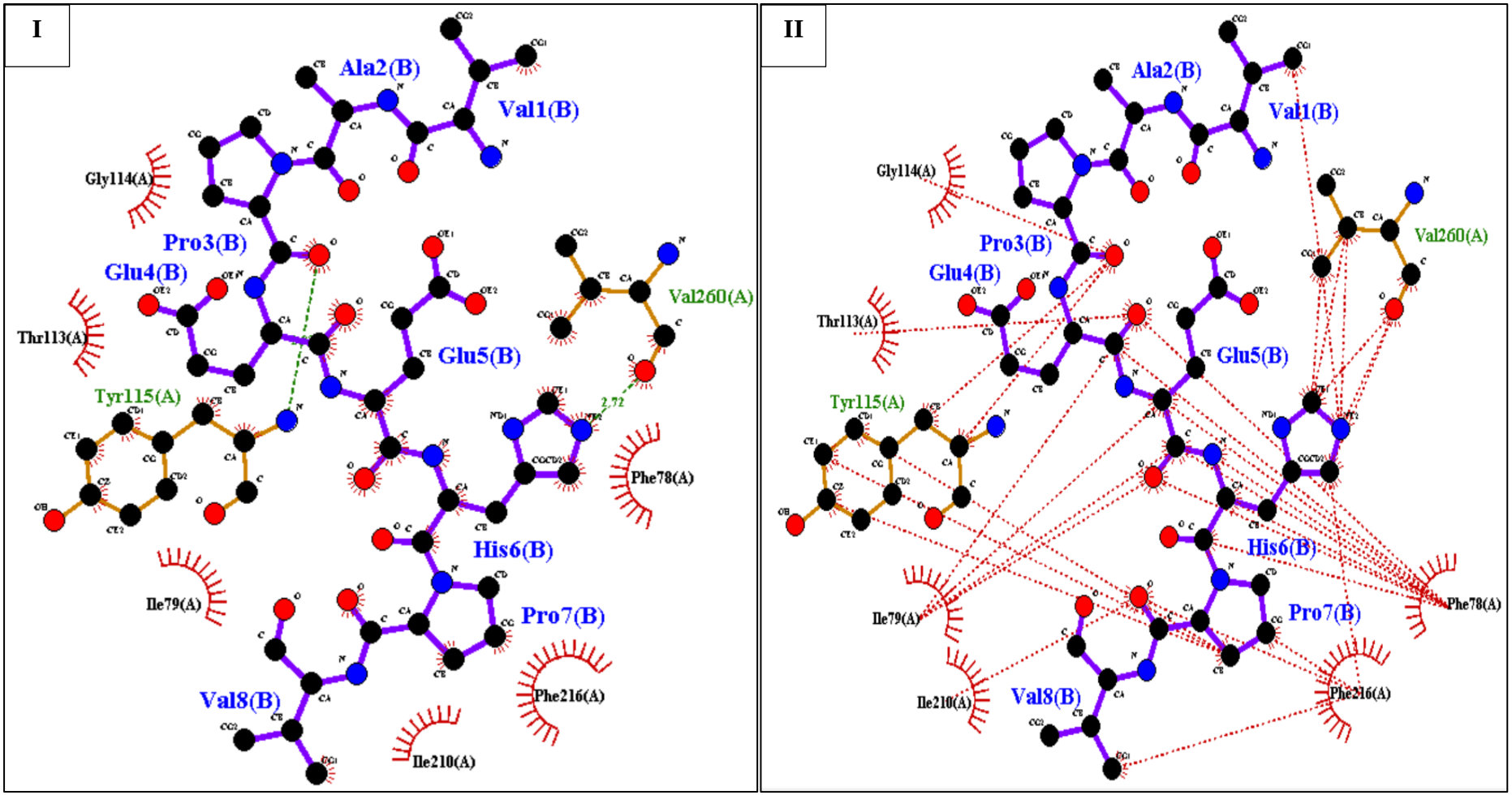

Figure S11a: Binding interaction of VAPEEH**P**V inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S11b: Binding interaction of pancreatic lipase inhibitory peptides-AGDDAPR at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide AGDDA**P**R	PRO6	Cluster3_4	-6.9	C - NA CA - Ile211 CB - NA CD - NA CG - NA N- Ile211 O - NA	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					8%	0%	0%	0%

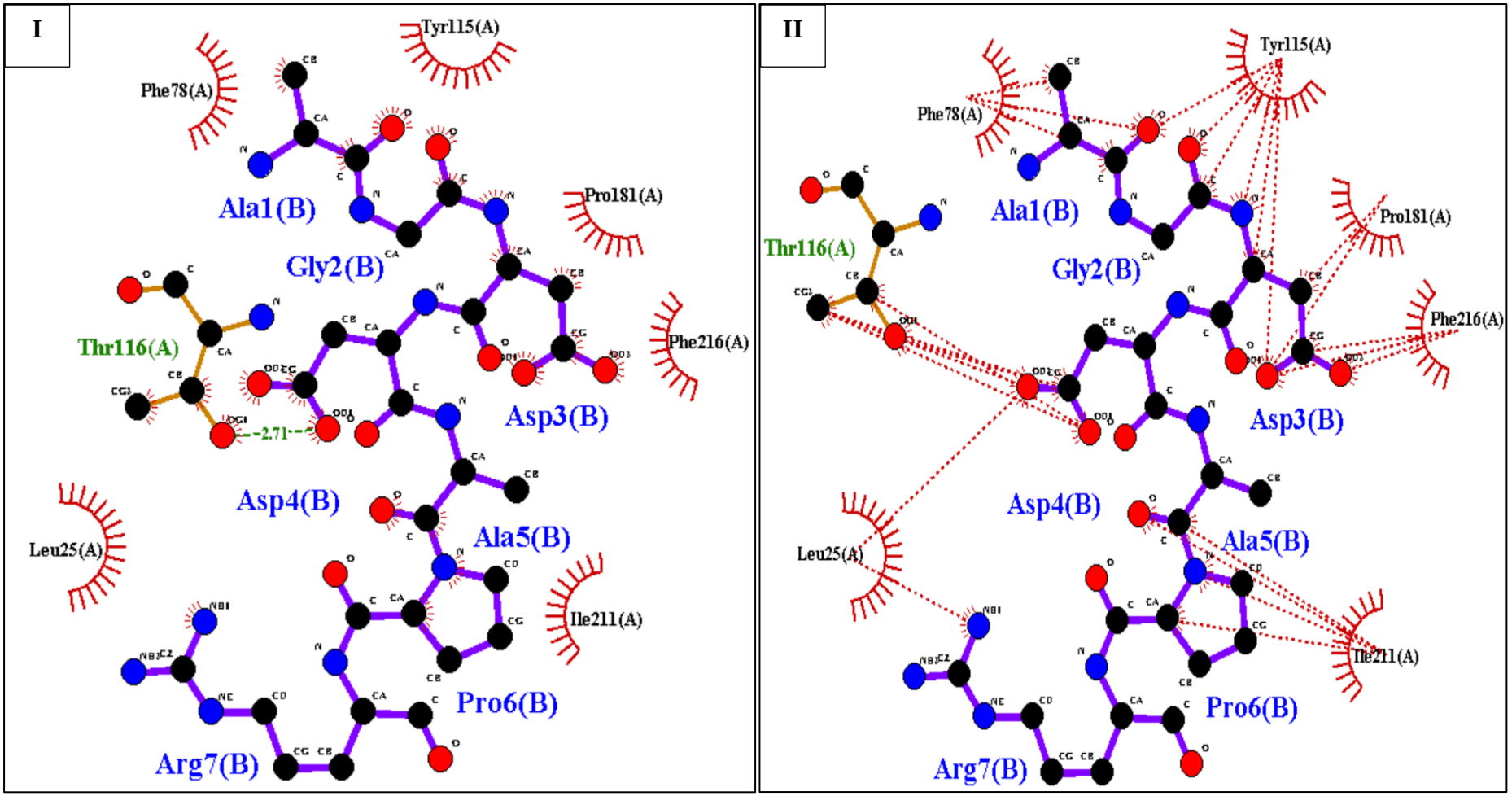

Figure S11b: Binding interaction of AGDDA**P**R inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S11c: Binding interaction of pancreatic lipase inhibitory peptides-NYVADGLG at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide NYVADG**L**G	LEU7	cluster1_1	-7.2	C - Phe216 CA - Phe216 CB - NA CD_1 - NA CD_2 - Phe216, Val 260 CG - NA N - NA O - Phe216	NA	NA	NA
Total number of bonds					29	0	0	3
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					17%	0%	0%	0%

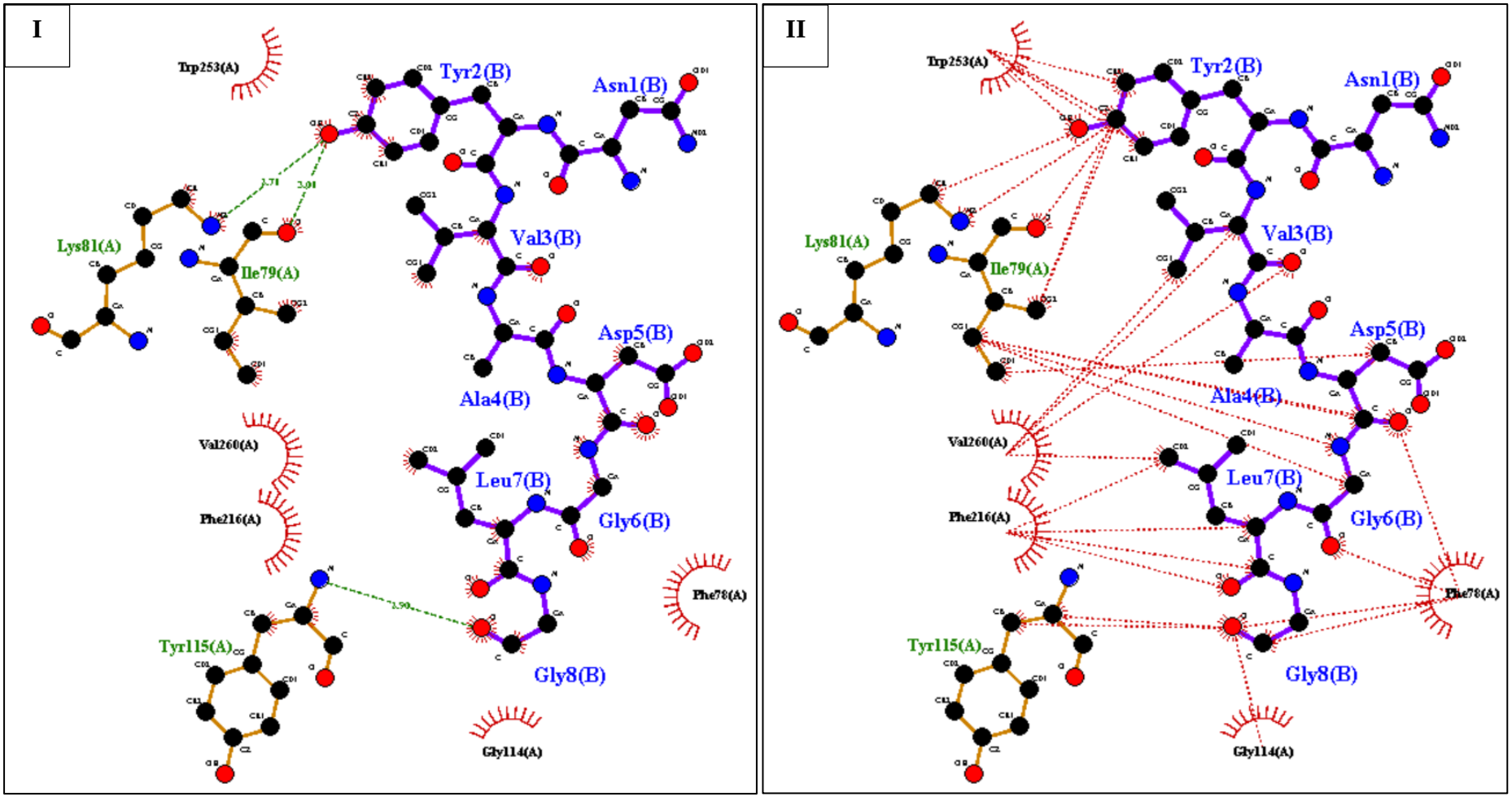

Figure S11c: Binding interaction of NYVADG**L**G inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S11d: Binding interaction of pancreatic lipase inhibitory peptides- CFLPLPLLK at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide CFLPLPL**L**K	LEU8	cluster1_3	-7.1	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					34	0	0	3
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

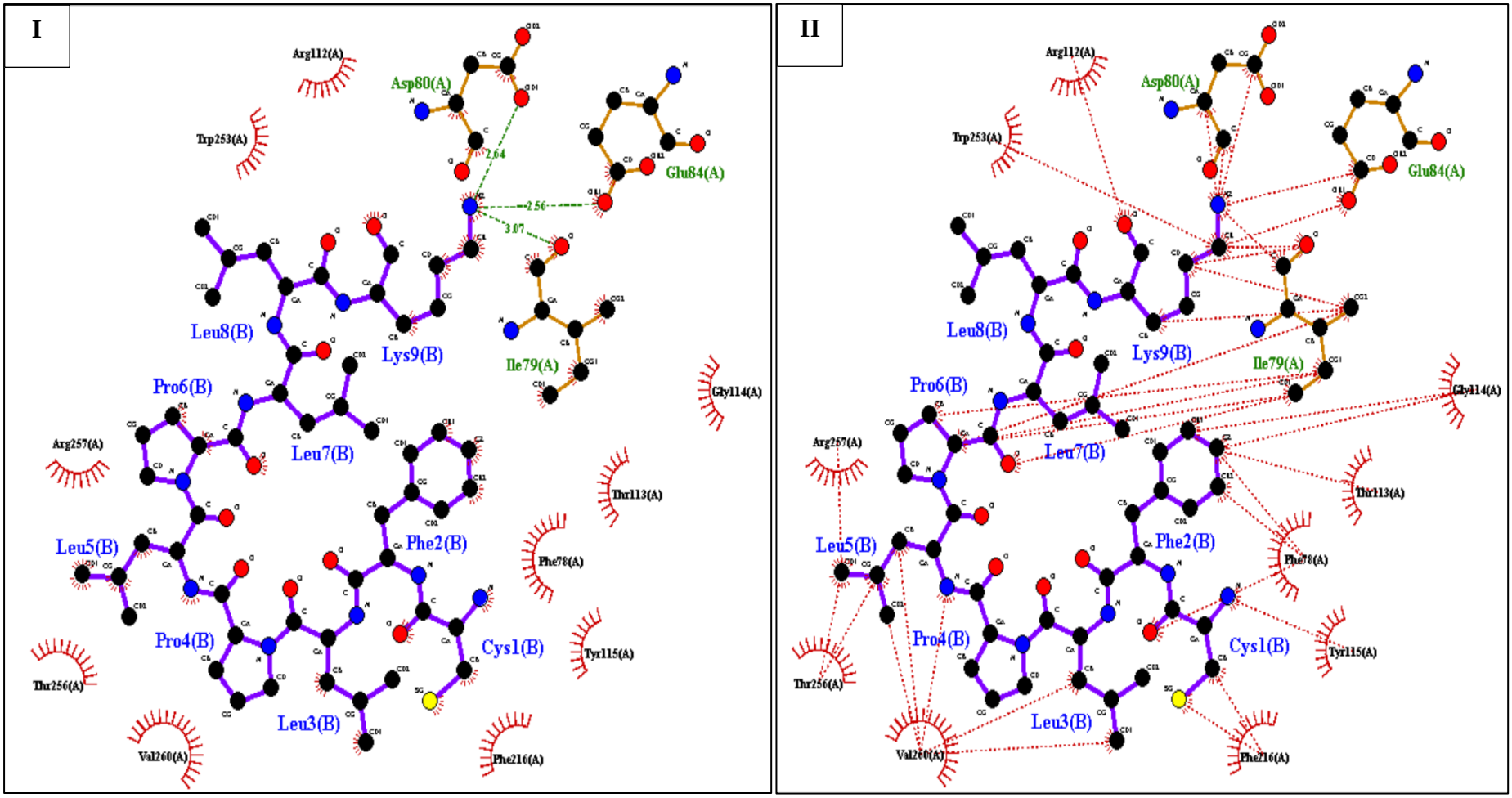

Figure S11d: Binding interaction of CFLPLPL**L**K inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S11e: Binding interaction of pancreatic lipase inhibitory peptides-LAPSTIK at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide LAPST**I**K	ILE6	cluster1_2	-8.0	C - NA CA - NA CB - Phe78 CD_1 - NA CG_1 - Phe78, Tyr115 CG_2 - NA N - NA O -Tyr115	NA	NA	NA
Total number of bonds					28	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					11%	0%	0%	0%

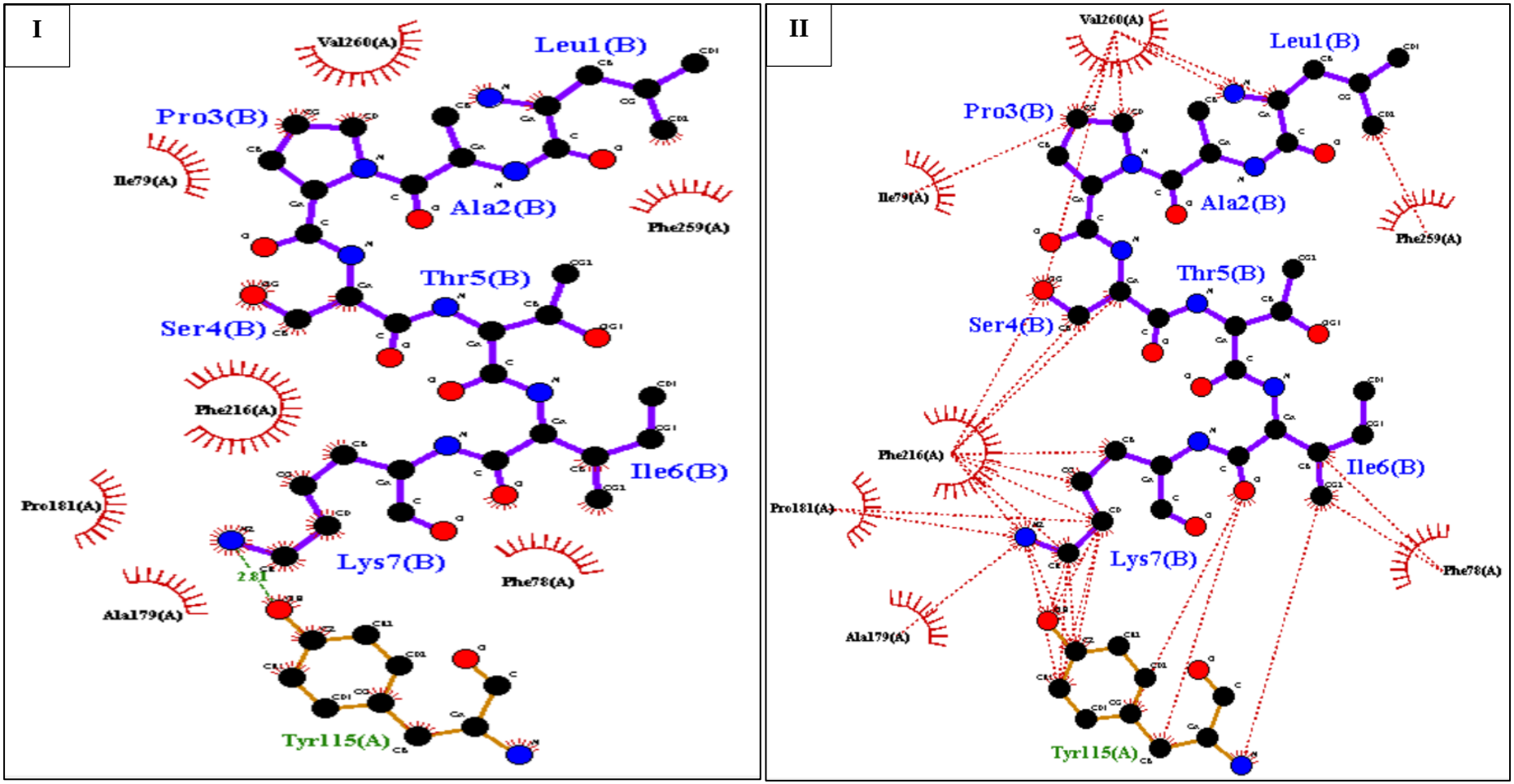

Figure S11e: Binding interaction of LAPST**I**K inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12a: Binding interaction of pancreatic lipase inhibitory peptides-EQGFLPGPEESGR at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide EQGFLPGPEE S**G**R	GLY12	cluster1_2	-8.9	C - Trp253 CA - Thr256 N - NA O - Trp253, Thr256	NA	NA	NA
Total number of bonds					44	0	2	4
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

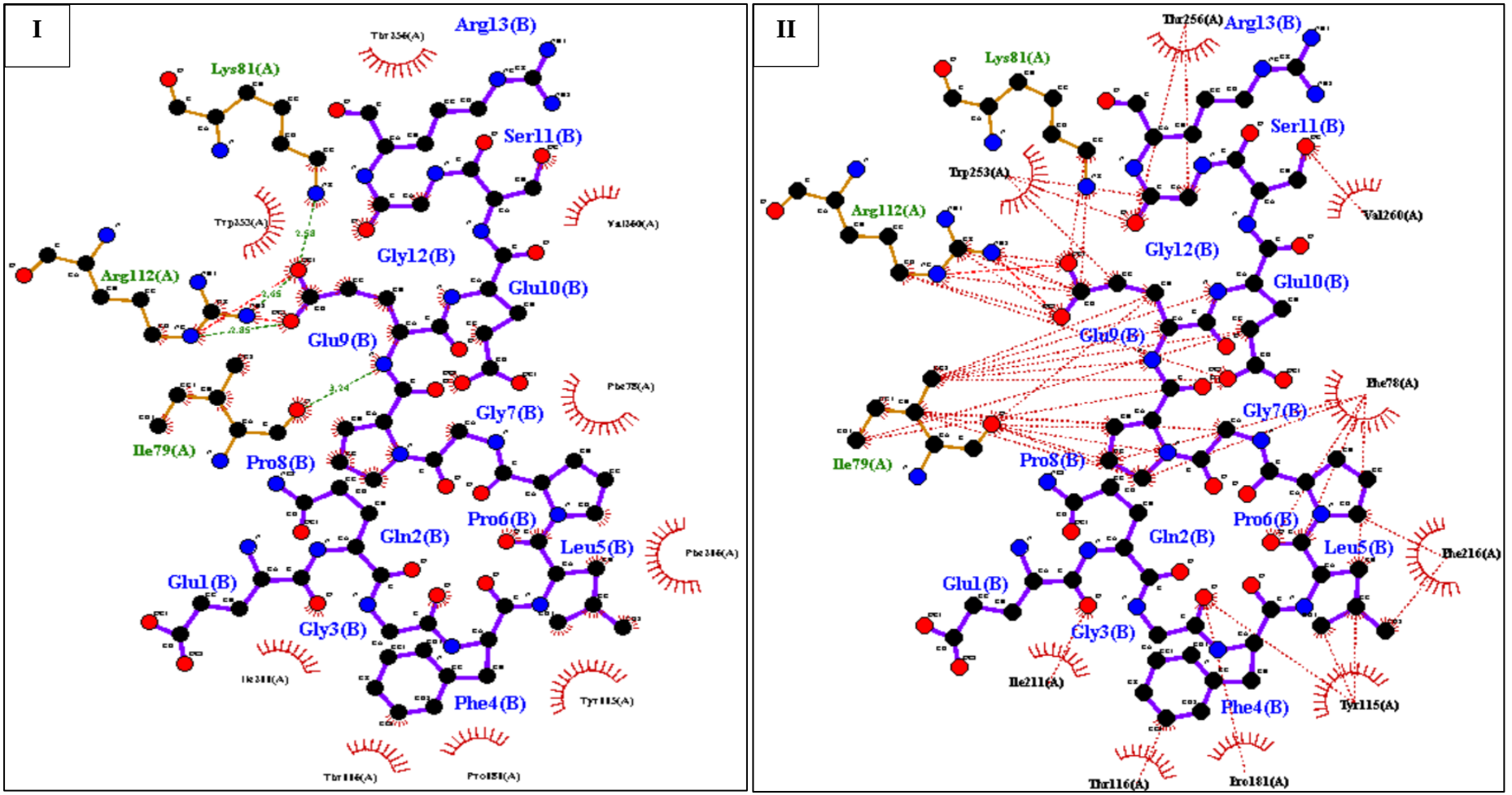

Figure S12a: Binding interaction of EQGFLPGPEES**G**R inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12b: Binding interaction of pancreatic lipase inhibitory peptides-YGNPVGGVGH at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide YGNPVGGV**G**H	GLY9	cluster1_3	-9.0	C - Ile79 CA - NA N - NA O - Ile79	NA	NA	NA
Total number of bonds					57	2	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					4%	0%	0%	0%

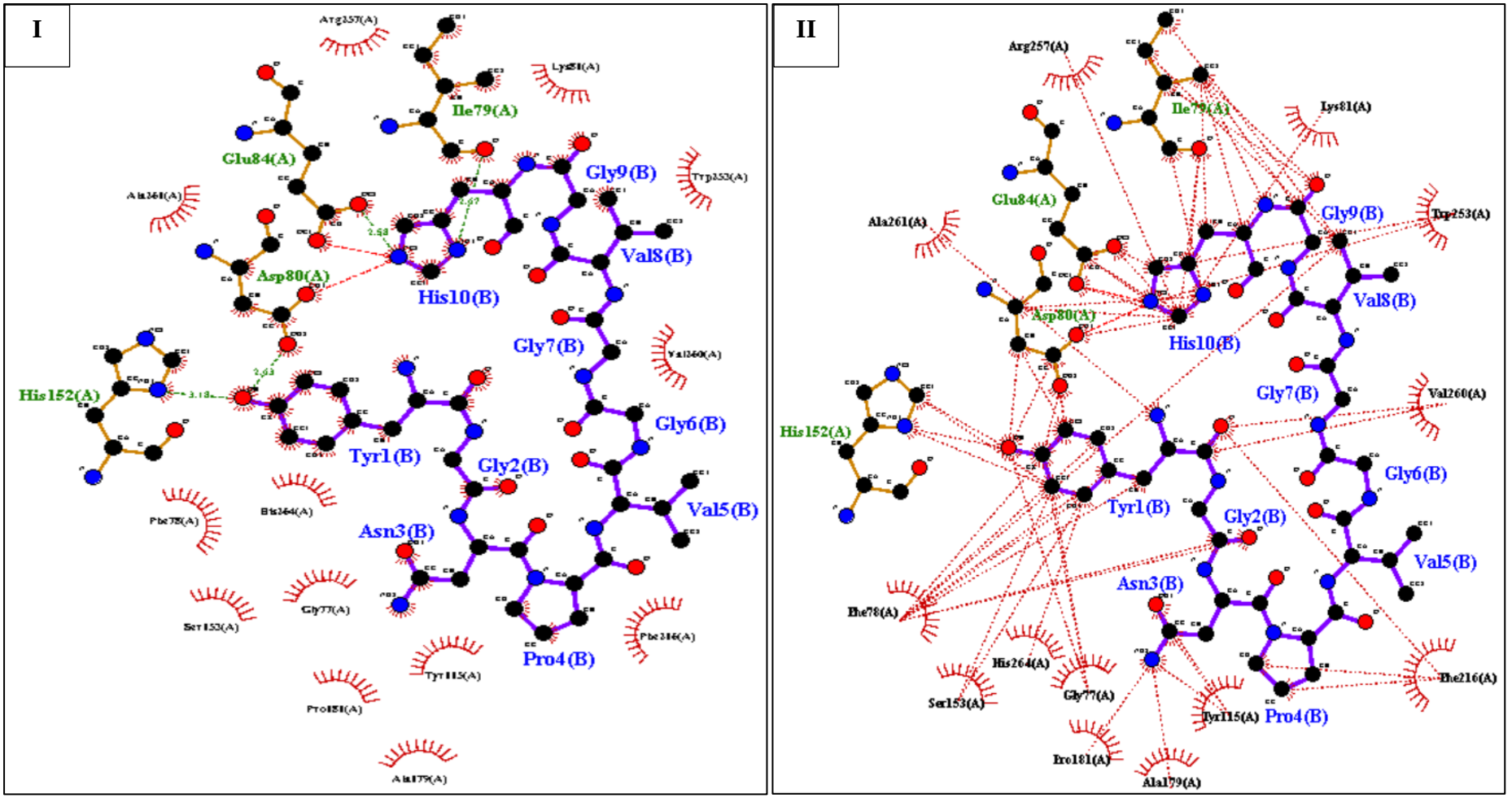

Figure S12b: Binding interaction of YGNPVGGV**G**H inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12c: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide LNNPSVCDCD CMMKA**A**R	ALA16	cluster3_4	-9.8	C - Thr116 CA - NA CB - NA N - NA O - Gly114, Thr116	NA	NA	NA
Total number of bonds					45	0	0	3
Total no of interactive residues					3	0	0	1
Overall percentage of bonding					7%	0%	0%	33%

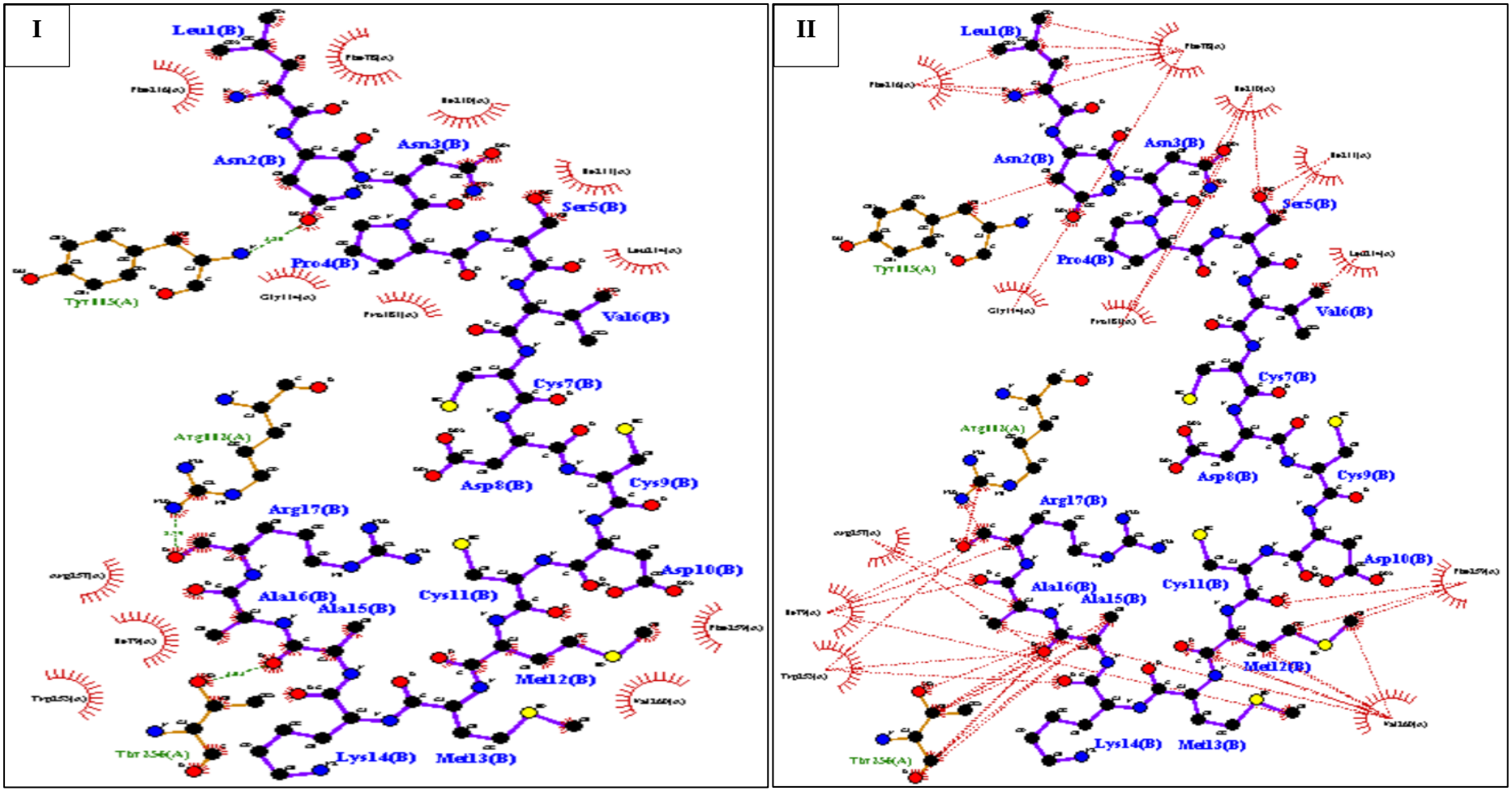

Figure S12c: Binding interaction of LNNPSVCDCDCMMKA**A**R inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12d: Binding interaction of pancreatic lipase inhibitory peptides-FFRSKLLSRGAAAAKGALLPQYW at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide FFRSKLLSRG AAAAKGALLP Q**Y**W	TYR22	cluster1_3	-9.2	C - Phe78 CA- Phe78 CB - NA CD_1 - NA CD_2 - NA CE_1 - Phe216 CE_2 - Phe216 CG - NA CZ - Phe216 N - Phe78 O - Phe78 OH - Pro181, Ile210 Phe216	NA	NA	NA
Total number of bonds					45	0	0	1
Total no of interactive residues					10	0	0	0
Overall percentage of bonding					22%	0%	0%	0%

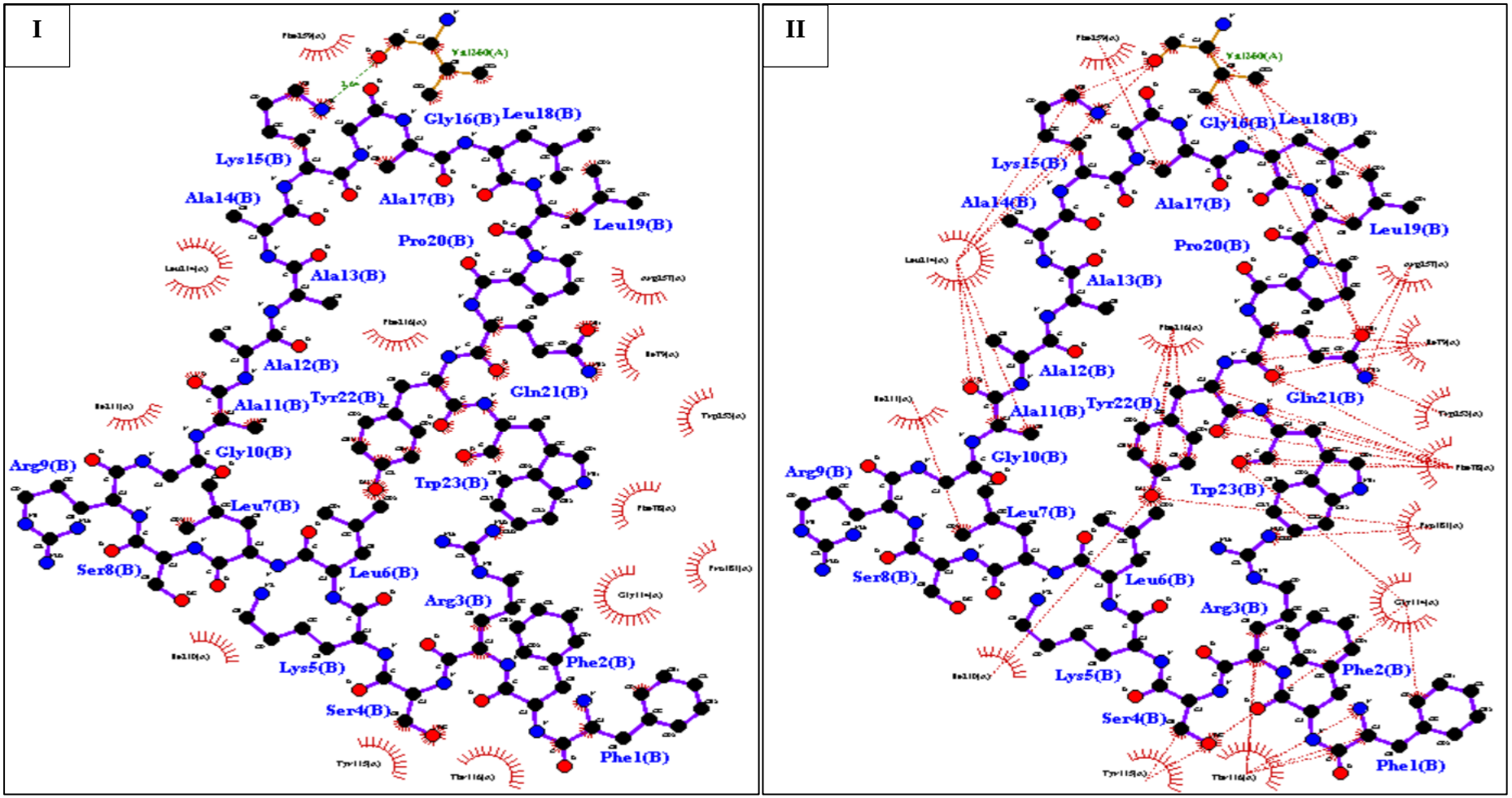

Figure S12d: Binding interaction of FFRSKLLSRGAAAAKGALLPQ**Y**W inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table 12e: Binding interaction of pancreatic lipase inhibitory peptides-RCMAFLLSDGAAAAQQLLPQYW at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide RCMAFLLSDG AAAAQQLLPQ **<u>Y</u>**W	TYR21	cluster3_3	-9.4	C - NA CA- NA CB - NA CD_1 - NA CD_2 - NA CE_1 - NA CE_2 - Glu180, Pro181 CG - NA CZ - Glu180, Pro181 N - NA O - lle211 OH - Pro181	NA	NA	OH - Glu180, Cys182
Total number of bonds					32	0	0	2
Total no of interactive residues					6	0	0	2
Overall percentage of bonding					19%	0%	0%	100%

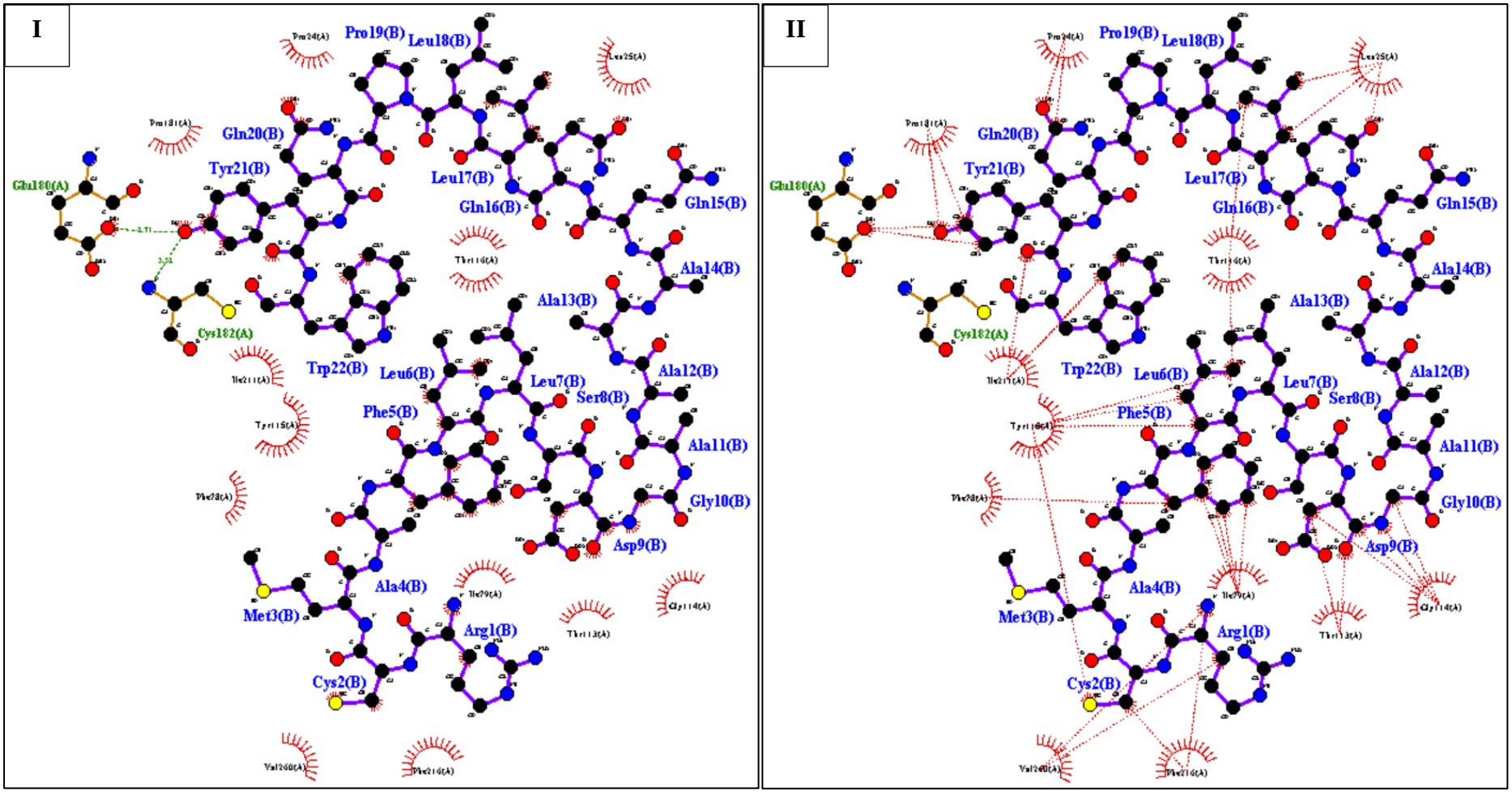

Figure S12e: Binding interaction of RCMAFLLSDGAAAAQQLLPQ**Y**W inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12f: Binding interaction of pancreatic lipase inhibitory peptides- GSGGGGGGGGGPRR at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide GSGGGGGGGG GP**R**R	ARG13	cluster4_1	-9.2	C - NA CA - NA CB - Phe78 CD - Phe78 CG - Phe78 CZ - Gly77, His152 N - Phe78 NH_1 - Gly77, His152 Ser153 NH_2 - Gly77, Asp80 Trp86 NE - Asp80 O - Ile79	NE - Asp80	NA	NH_1 - His152 NH_2 - Asp80
Total number of bonds						1	0	4
Total no of interactive residues					14	1	0	2
Overall percentage of bonding					%	100%	0%	50%

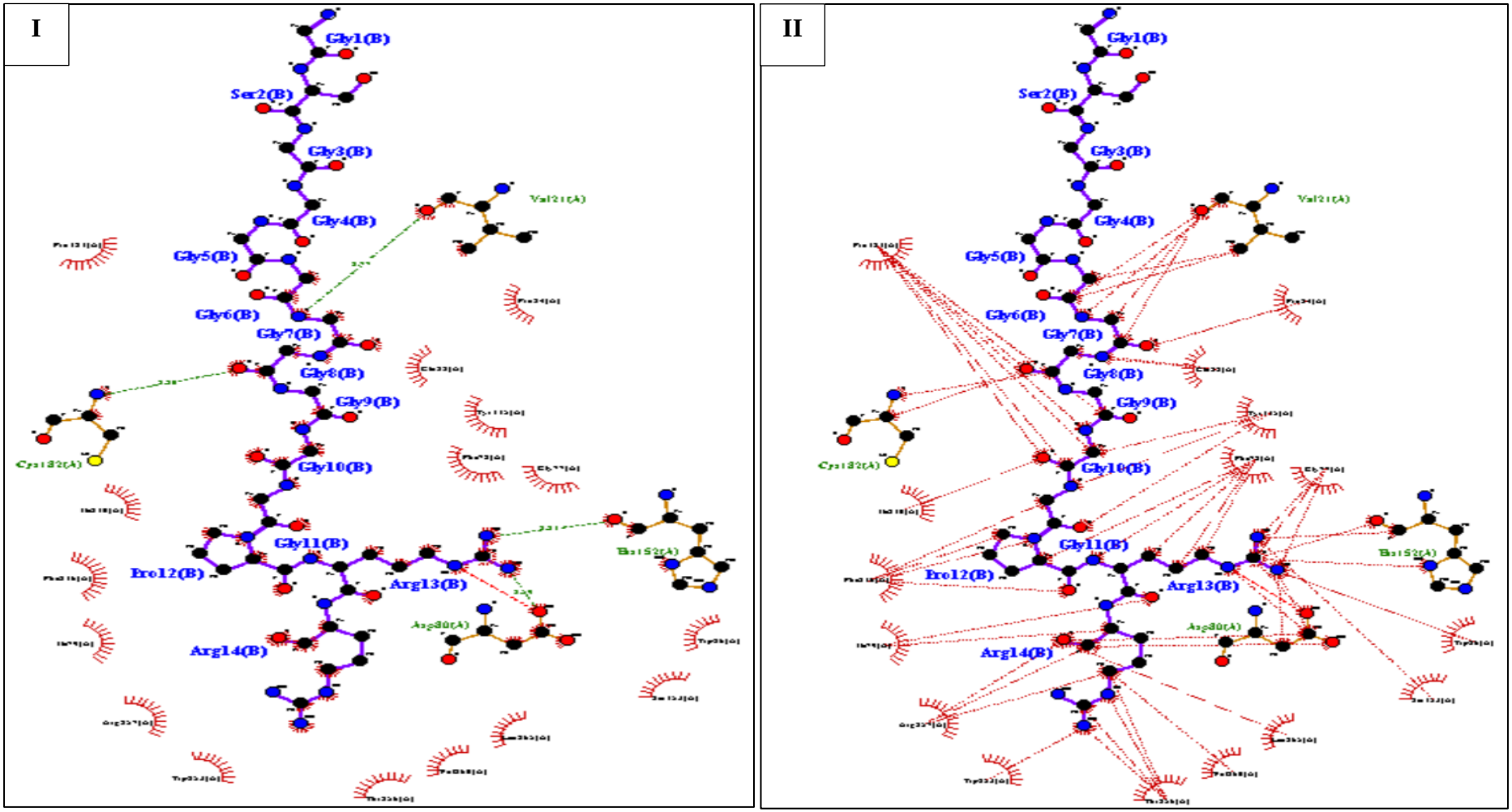

Figure S12f: Binding interaction of GSGGGGGGGGGPRR inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12g: Binding interaction of pancreatic lipase inhibitory peptides-RKQEEDEDEEQQRE at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide RKQEEDEDEE QQ**R**E	ARG13	cluster1_2	-9.8	C - NA CA - NA CB - NA CD - NA CG - NA CZ - NA N - NA NH_1 - NA NB_2 - NA NE - NA O - NA	NA	NA	NA
Total number of bonds					33	3	0	4
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

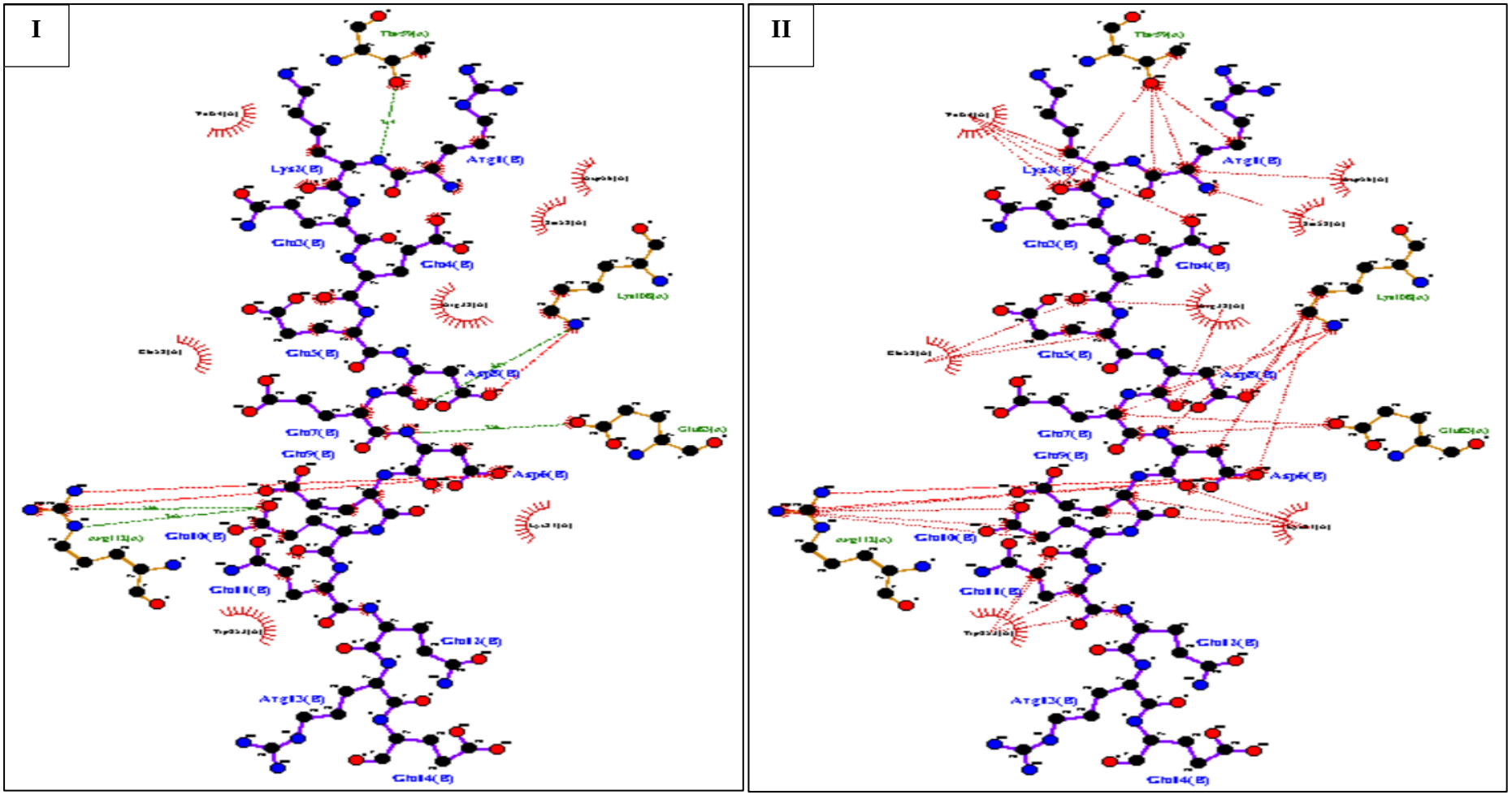

Figure S12g: Binding interaction of RKQEEDEDEEQQ**R**E inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S12h: Binding interaction of pancreatic lipase inhibitory peptides-GEHGGAGMGGGQFQPV at C2 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide GEHGGAGMGG GQFQ**P**V	PRO15	cluster1_2	-9.1	C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
Total number of bonds					40	0	3	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

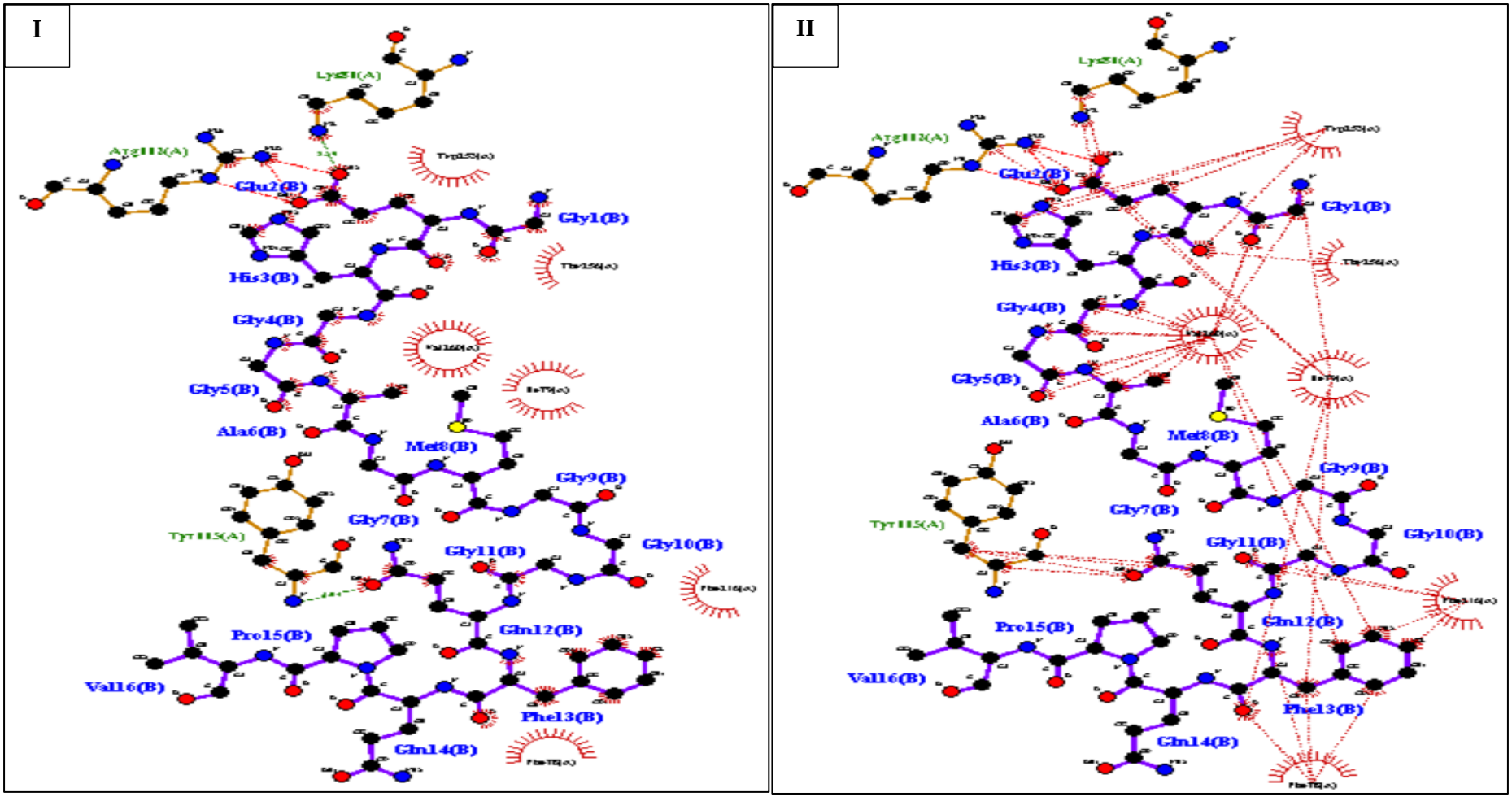

Figure S12h: Binding interaction of GEHGGAGMGGGQFQ**P**V inhibitory peptide at C2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13a: Binding interaction of pancreatic lipase inhibitory peptides-NYVADGLG at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide NY**V**ADGLG	VAL3	cluster1_1	-7.2	C - NA CA - Val260 CB - NA CG_1 - Val260 CG_2 - NA N - NA O - Val260	NA	NA	NA
Total number of bonds					29	0	0	3
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

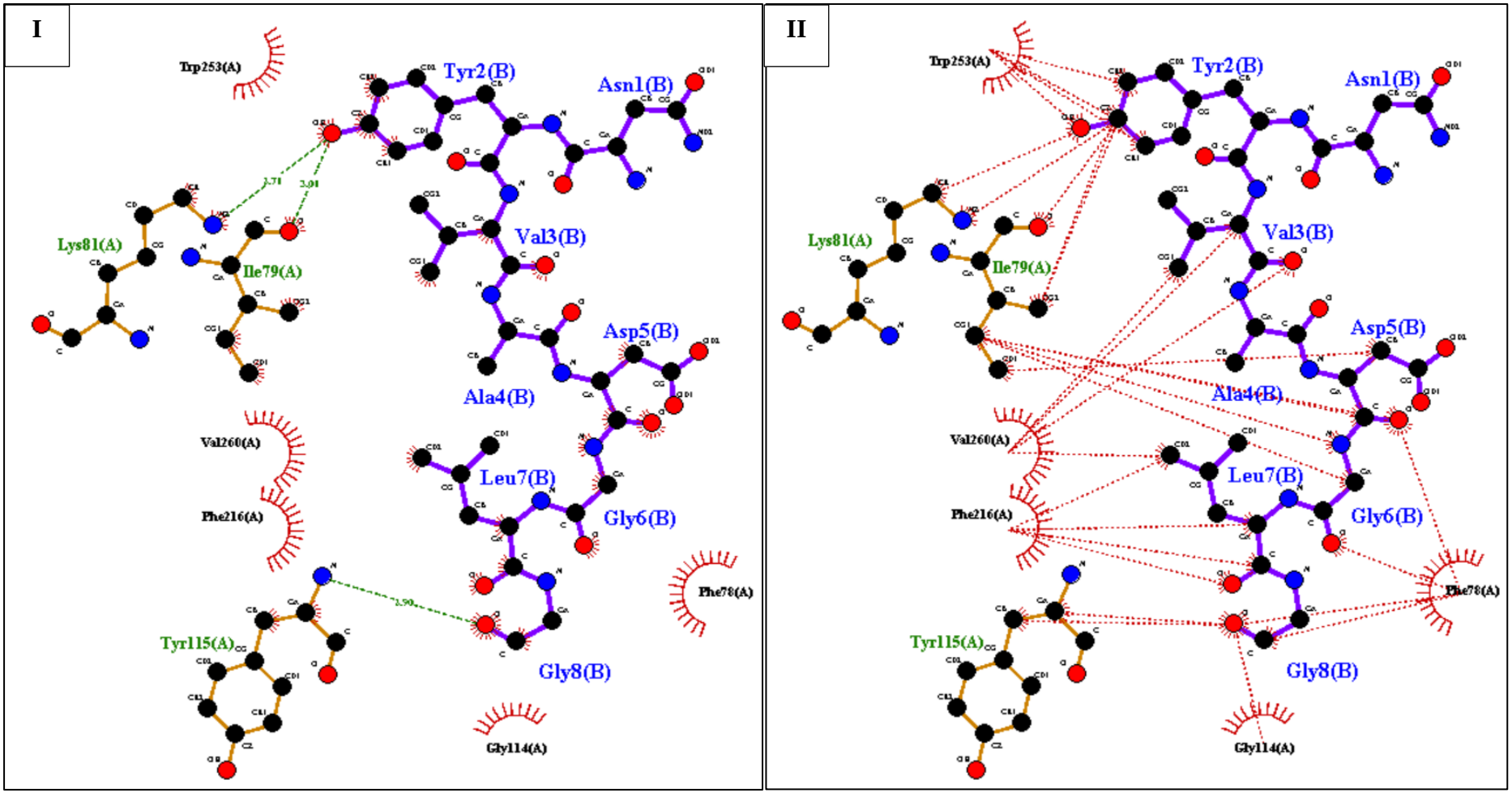

Figure S13a: Binding interaction of NY**V**ADGLG inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13b: Binding interaction of pancreatic lipase inhibitory peptides-DIVDKIEI at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide DI**V**DKIEI	VAL3	cluster3_2	-7.0	C - NA CA - Phe216 CB - NA CG_1 - Phe216 CG_2 - Phe216 N - NA O - NA	NA	NA	NA
Total number of bonds					17	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					18%	0%	0%	0%

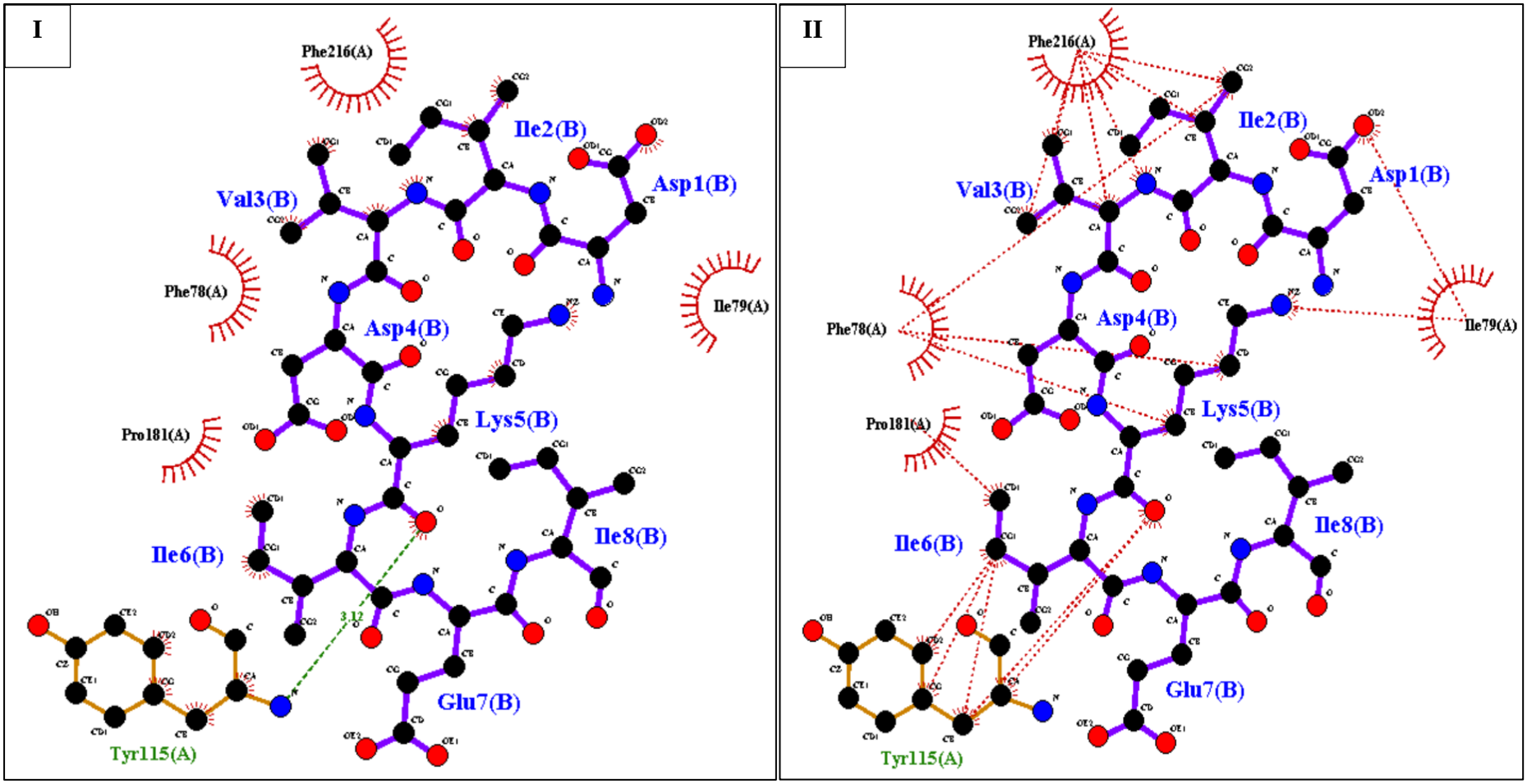

Figure S13b: Binding interaction of DI**V**DKIEI inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13c: Binding interaction of pancreatic lipase inhibitory peptides-FDPFPK at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide FD**P**FPK	PRO3	cluster2_1	-7.1	C - NA CA - NA CB - NA CD - Val260 CG -Val260 N - NA O - NA	NA	NA	NA
Total number of bonds					33	0	0	0
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					6%	0%	0%	0%

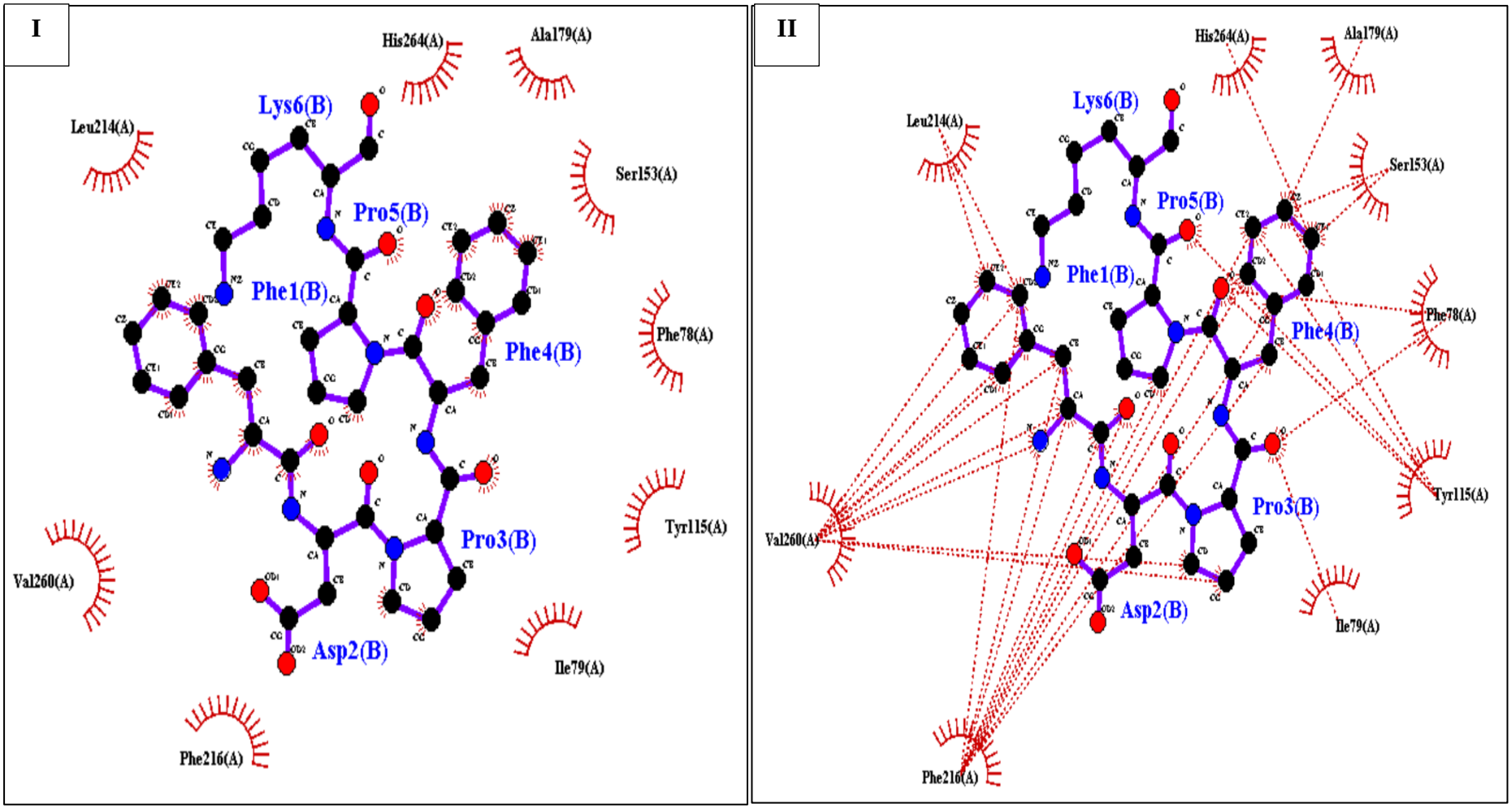

Figure S13c: Binding interaction of FD**P**FPK inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13d: Binding interaction of pancreatic lipase inhibitory peptides- ELPPHFL at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide EL**P**PHFL	PRO3	cluster5_2	-6.8	C - NA CA - NA CB - NA CD - Ile210 CG - Ile211 N - NA O - NA	NA	NA	NA
Total number of bonds					33	0	0	4
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					6%	0%	0%	0%

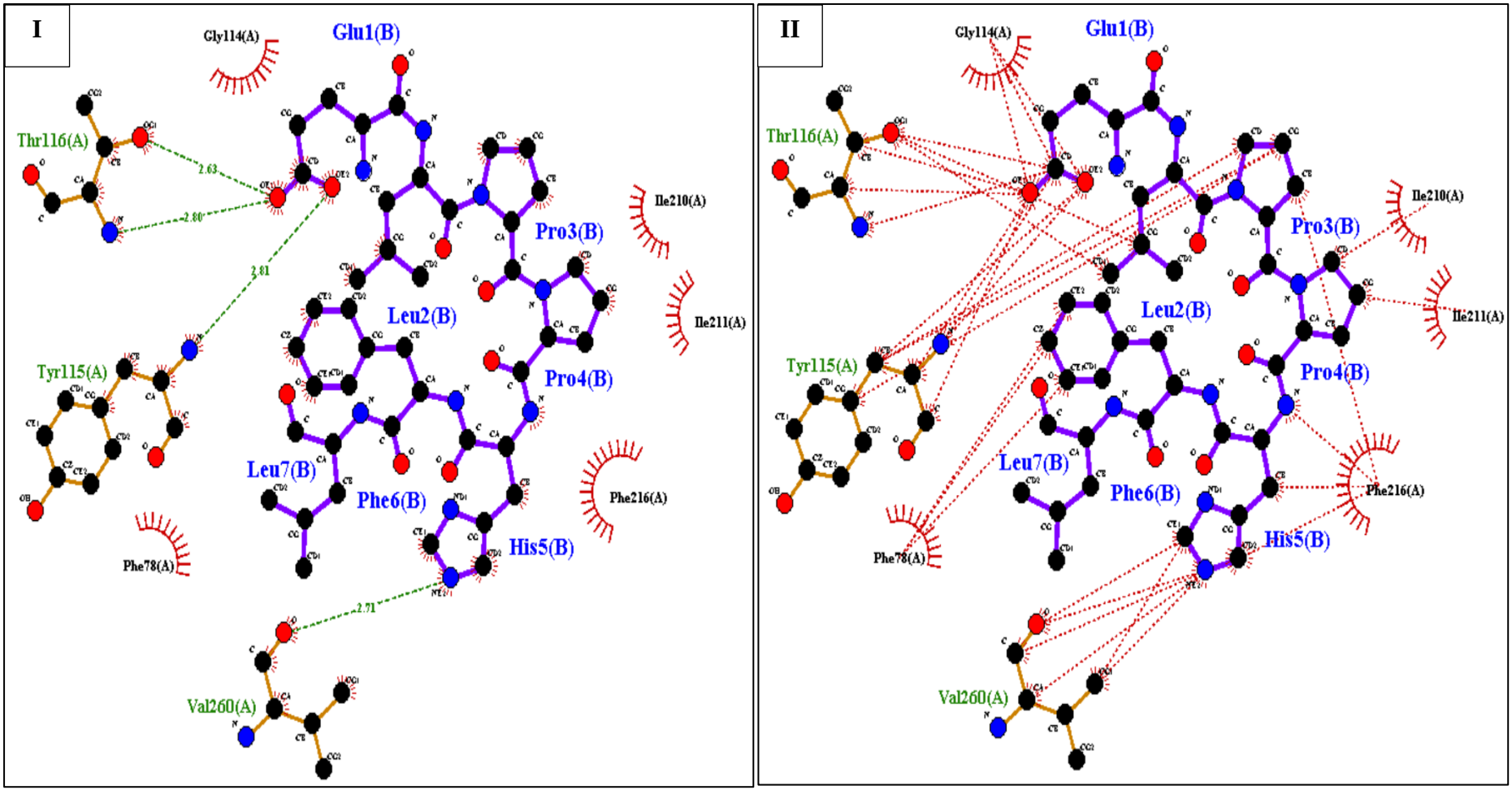

Figure S13d: Binding interaction of EL**P**PHFL inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13e: Binding interaction of pancreatic lipase inhibitory peptides-FLWPEYGAL at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide FL**W**PEYGAL	TRP3	cluster11_3	-7.6	C - NA CA - NA CB - NA CD_1 - Ile210, Leu214 CD_2 - NA CE_2 - NA CE_3 - NA CG - NA CH_2 - NA CZ_2 - NA CZ_3 - Ile211 N - NA NE1 - Ile211, Pro212 O - NA	NA	NA	NA
Total number of bonds					30	0	0	3
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					17%	0%	0%	0%

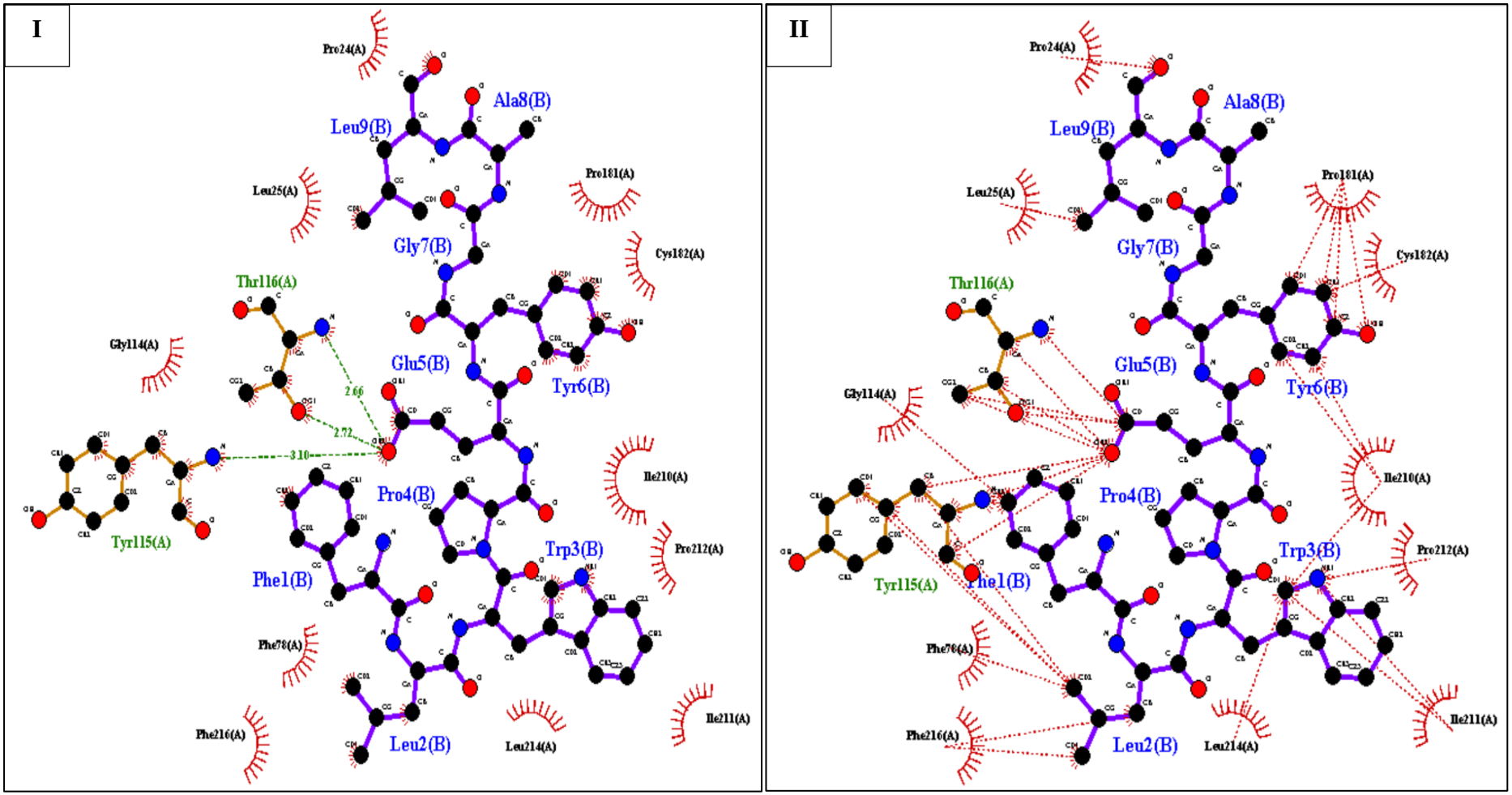

Figure S13e: Binding interaction of FL**W**PEYGAL inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13f: Binding interaction of pancreatic lipase inhibitory peptides-AEWLHDWKL at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide AE**W**LHDWKL	TRP3	cluster1_1	-7.0	C - NA CA - NA CB - Ile79 CD_1 - NA CD_2 - NA CE_2 - NA CE_3 - Thr113 CG - NA CH_2 - NA CZ_2 - NA CZ_3 - Gly114 N - NA NE_1 - NA O - NA	NA	NA	NA
Total number of bonds					21	0	0	1
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					14%	0%	0%	0%

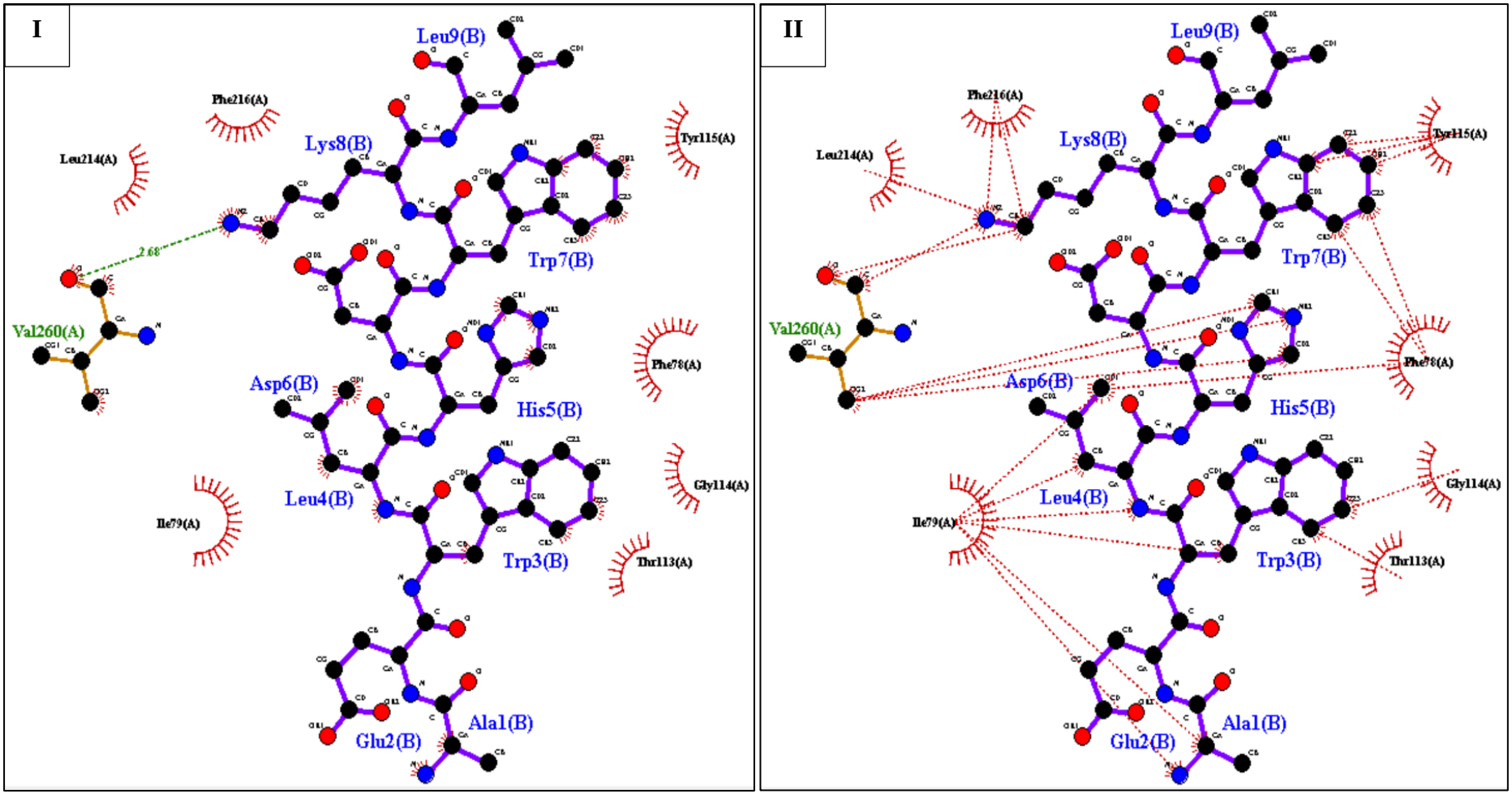

Figure S13f: Binding interaction of AE**W**LHDWKL inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13g: Binding interaction of pancreatic lipase inhibitory peptides-LNLDLLR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide LN**L**DLLR	LEU3	cluster11_2	-8.1	C - NA CA - NA CB - NA CD_1 - Thr113 CD_2 - NA CG - NA N - Gly114 O - NA	NA	NA	NA
Total number of bonds					20	0	0	2
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

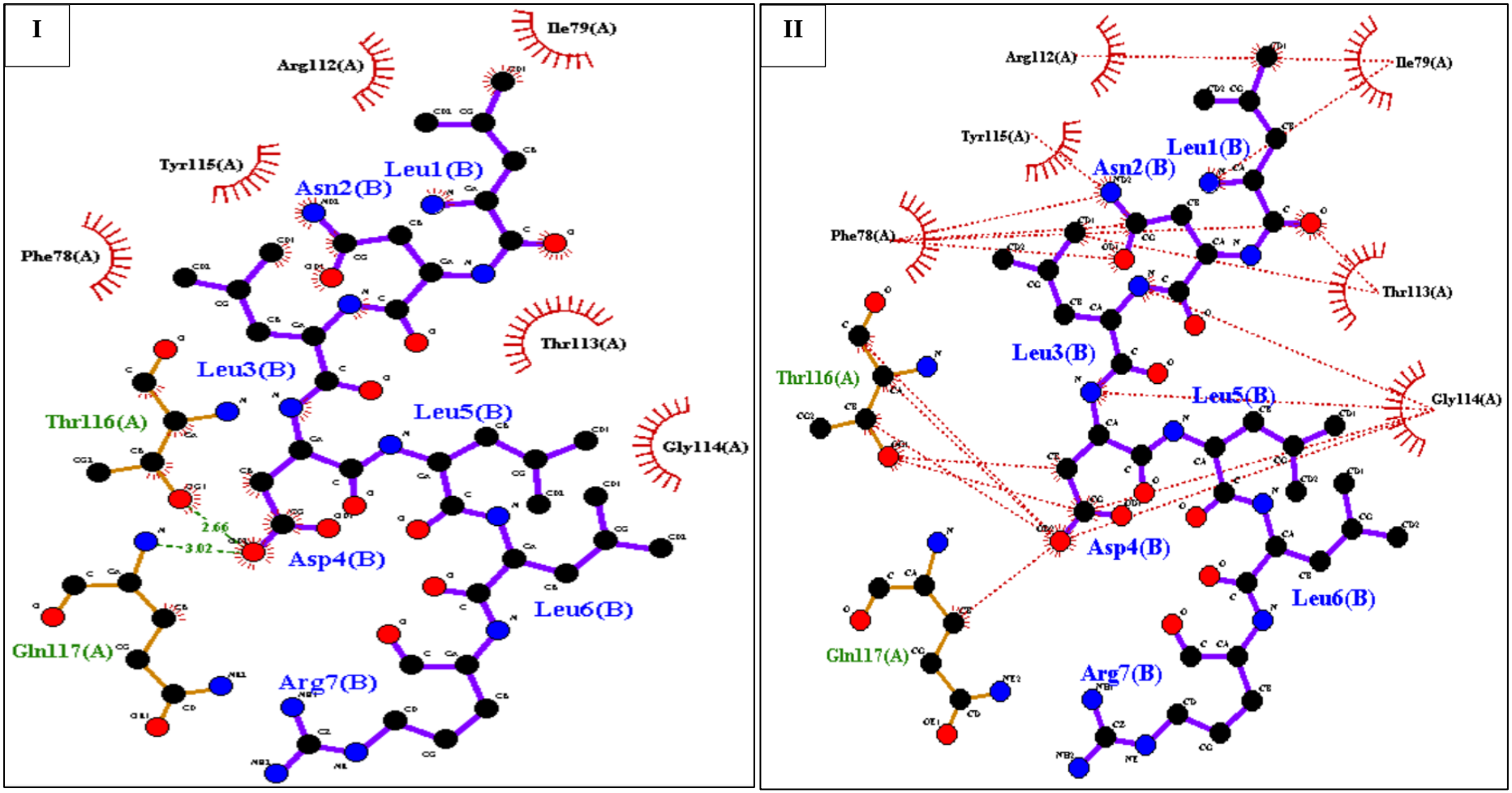

Figure S13g: Binding interaction of LN**L**DLLR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13h: Binding interaction of pancreatic lipase inhibitory peptides-CFLPLPLLK at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide CF**L**PLPLLK	LEU3	cluster1_3	-7.1	C - NA CA - NA CB - Val260 CD_1 - NA CD_2 - Val260 CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					34	0	0	3
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					6%	0%	0%	0%

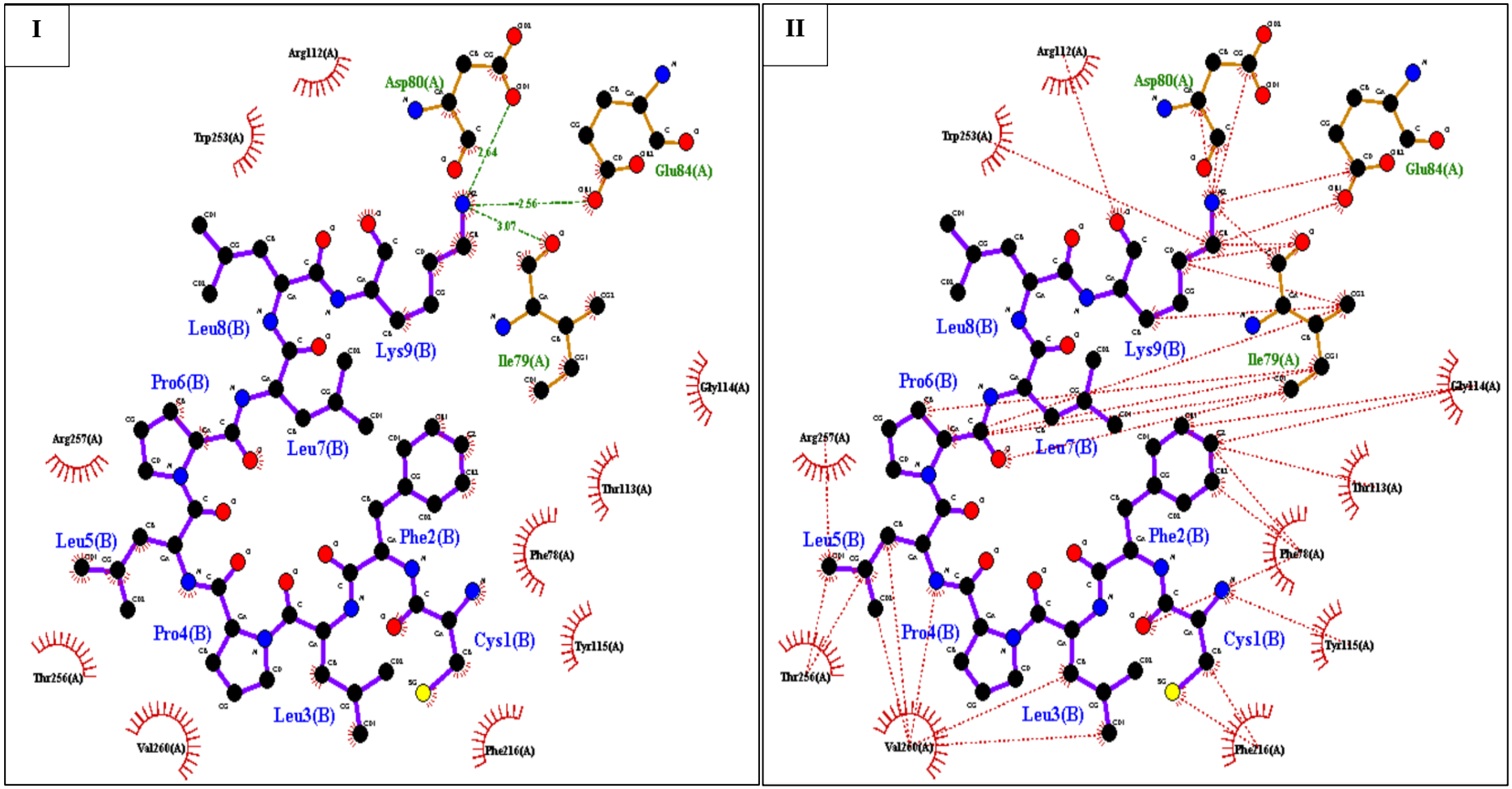

Figure S13h: Binding interaction of CF**L**PLPLLK inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13i: Binding interaction of pancreatic lipase inhibitory peptides- LNFEPR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide LN**F**EPR	PHE3	cluster2_2	-8.0	C - NA CA - NA CB - NA CD_1 - NA CD_2 - Phe216 CE_1 - Tyr115 CE_2 - Tyr115, Pro181, Phe216 CG - Phe216 CZ - Tyr115, Phe216 N - Tyr115 O - NA	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					9	0	0	0
Overall percentage of bonding					36%	0%	0%	0%

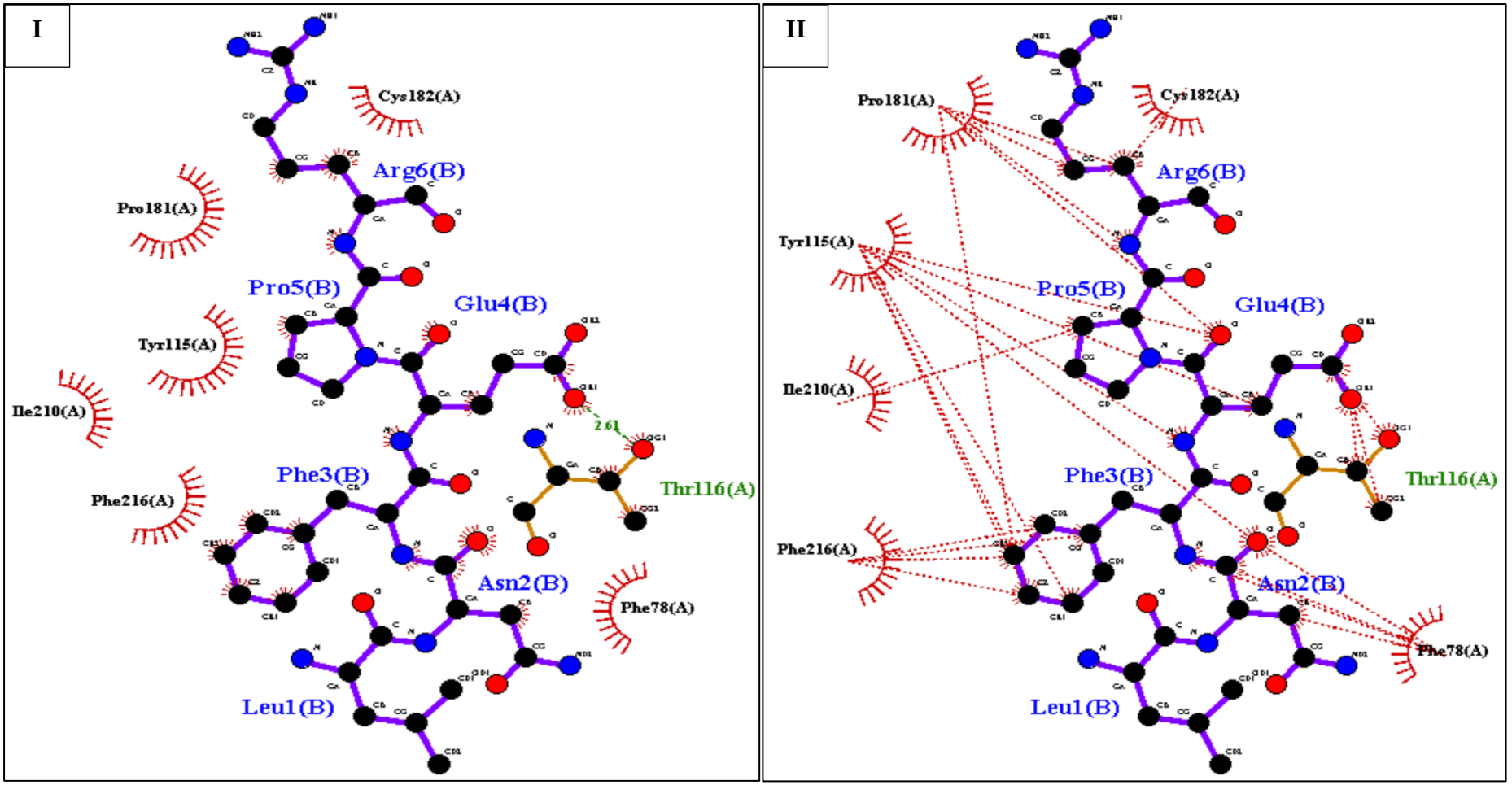

Figure S13i: Binding interaction of LN**F**EPR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13j Binding interaction of pancreatic lipase inhibitory peptides-APFPLR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide AP**F**PLR	PHE3	cluster1_3	-7.0	C - NA CA - NA CB - Phe216 CD_1 - NA CD_2 - Tyr115 CE_1 - NA CE_2 - Tyr115 CG - Phe216 CZ - Ser153, His264 N - NA O - Phe78	NA	NA	NA
Total number of bonds					16	0	0	0
Total no of interactive residues					7	0	0	0
Overall percentage of bonding					43%	0%	0%	0%

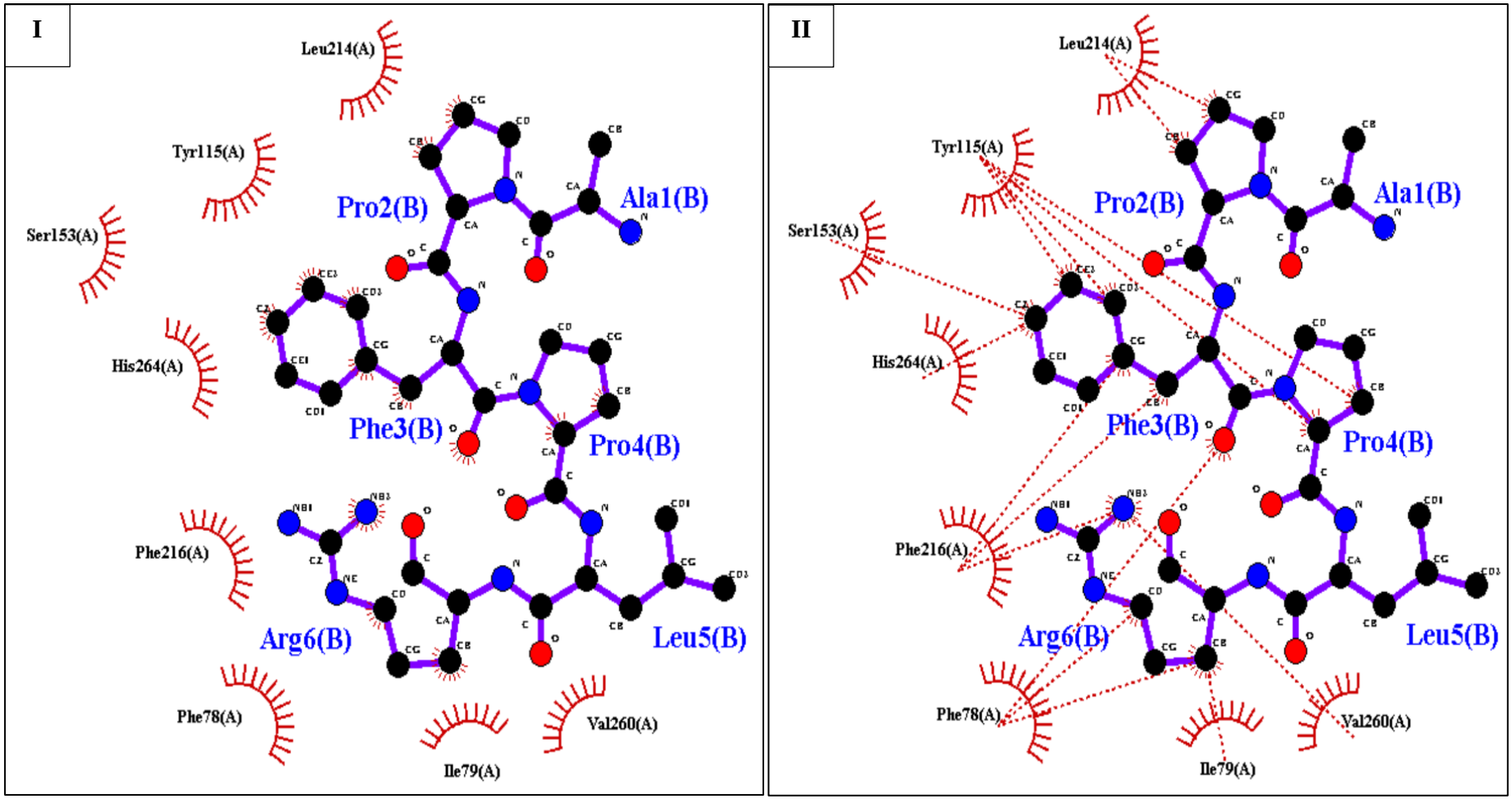

Figure S13j: Binding interaction of APFPLR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13k Binding interaction of pancreatic lipase inhibitory peptides- MANLQR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide MA**N**LQR	ASN3	cluster2_2	-9.0	C - NA CA - NA CB - NA CG - NA N - Phe78 ND_2 - Phe78 O - NA OD_1 - NA	NA	NA	NA
Total number of bonds					37	2	0	6
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					5%	0%	0%	0%

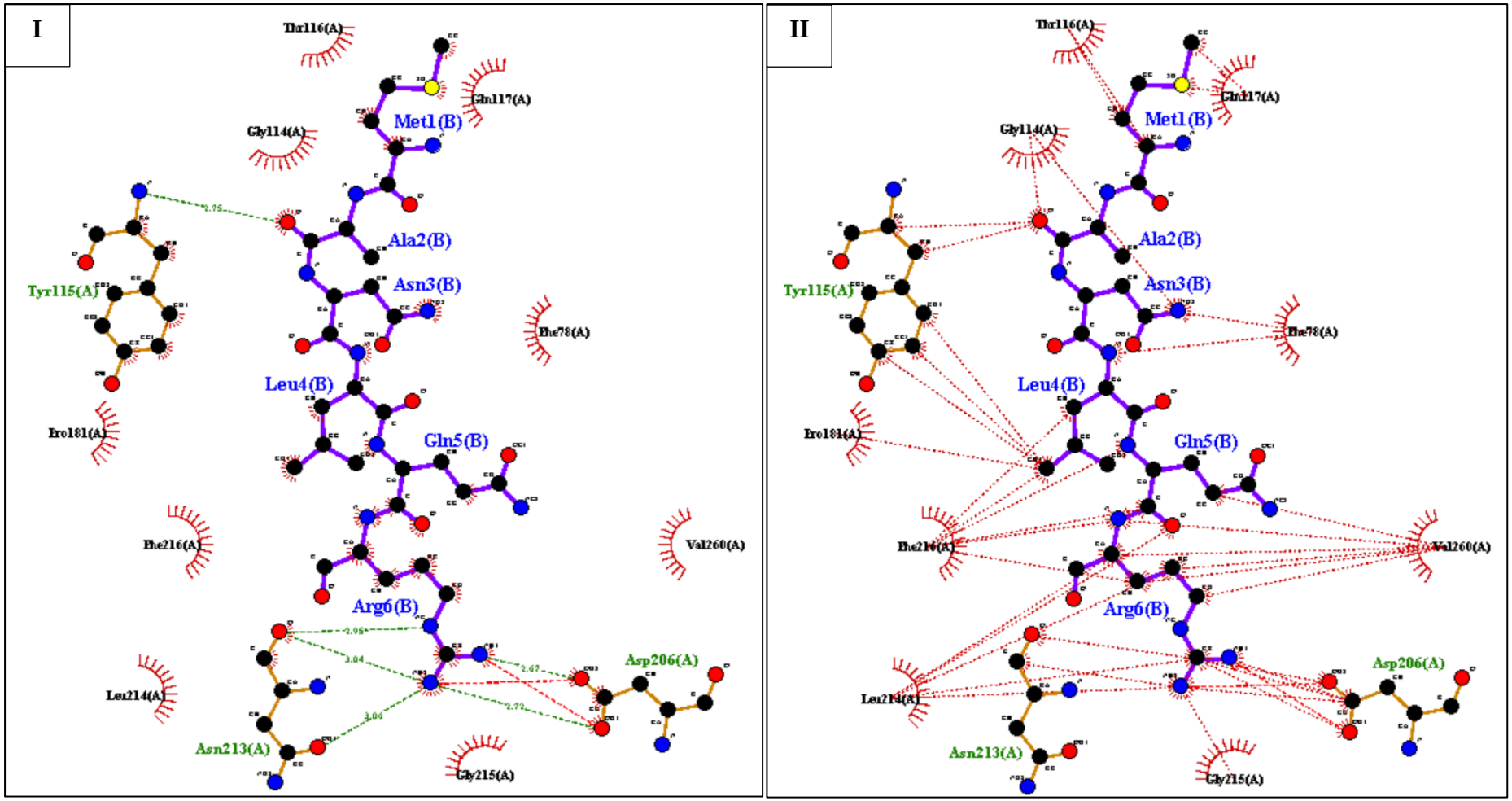

Figure S13k: Binding interaction of MA**N**LQR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S13l Binding interaction of pancreatic lipase inhibitory peptides- CANPHELPN at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide CA**N**PHELPN	ASN3	cluster1_2	-10.0	C - NA CA - NA CB - NA CG - Ile210 N - NA ND_2 - Ile211 O - NA OD_1 - Ile210	NA	NA	NA
Total number of bonds					28	0	0	2
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					11%	0%	0%	0%

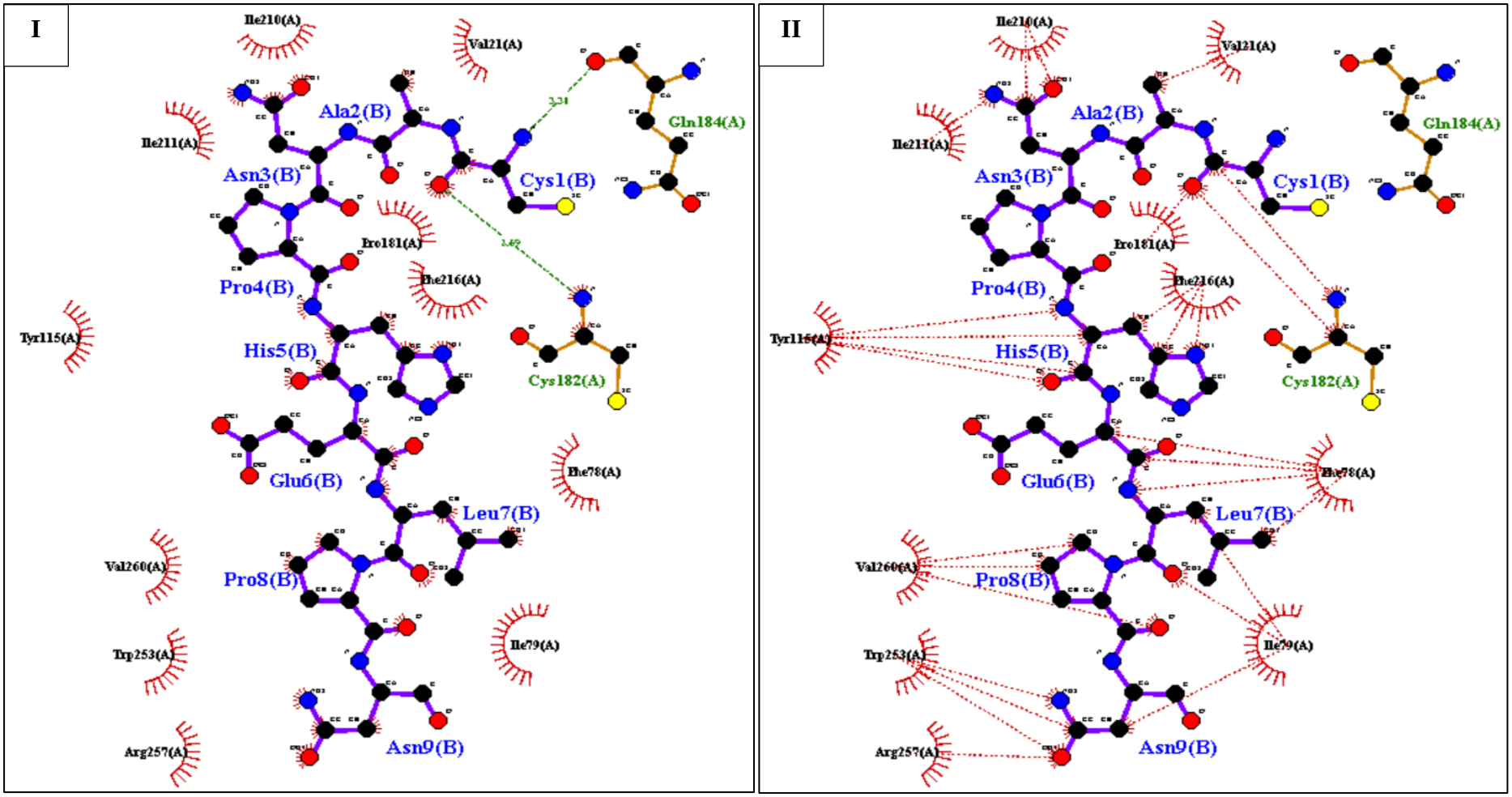

Figure S13l: Binding interaction of CANPHELPN inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14a: Binding interaction of pancreatic lipase inhibitory peptides-YGNPVGGVGH at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide YG**N**PVGGVGH	ASN3	cluster1_3	-9.0	C - NA CA - NA CB - NA CG - Tyr115 N - NA ND_2 - Tyr115, Ala179 Pro181 O - NA OD_1 - NA	NA	NA	NA
Total number of bonds					57	2	0	4
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					8%	0%	0%	0%

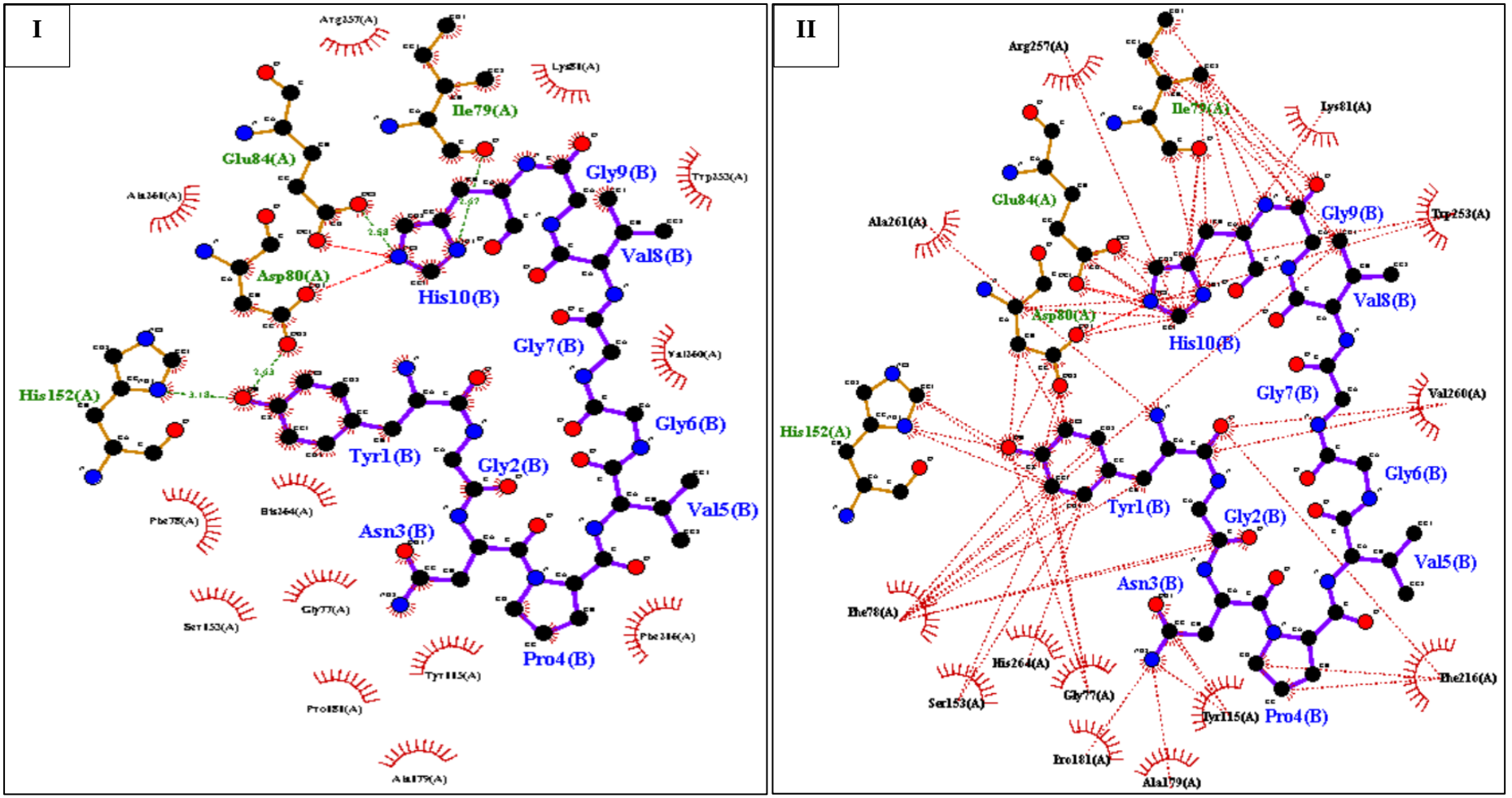

Figure S14a: Binding interaction of YG**N**PVGGVGH inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14b: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide LN**N**PSVCDCD CMMKAAR	ASN3	cluster3_4	-9.8	C - NA CA - NA CB - NA CG - Ile210 N - NA ND_2 - Ile210, Pro181 O - NA OD_1 - Pro181	NA	NA	NA
Total number of bonds					45	0	0	3
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

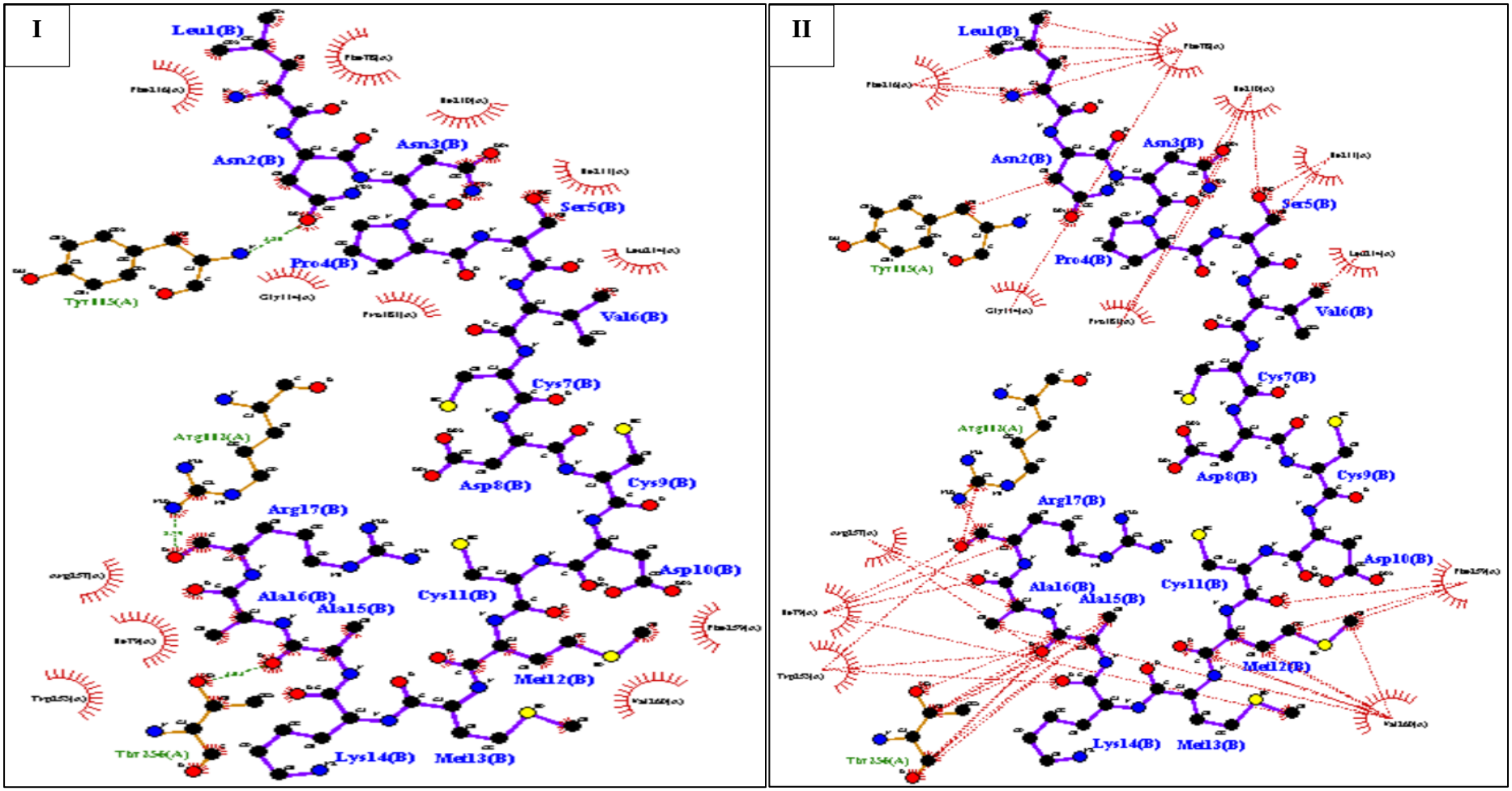

Figure S14b: Binding interaction of LN**N**PSVCDCDCMMKAAR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14c: Binding interaction of pancreatic lipase inhibitory peptides-HCPVPDPVRGL at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide HC**P**VPDPVRG L	PRO3	cluster5_2	-9.0	C - Pro209 CA - Pro209 CB - Glu180, Pro209 CD - NA CG - Gln184, Ser219 N- Pro209 O - NA	NA	NA	NA
Total number of bonds					40	0	0	2
Total no of interactive residues					7	0	0	0
Overall percentage of bonding					18%	0%	0%	0%

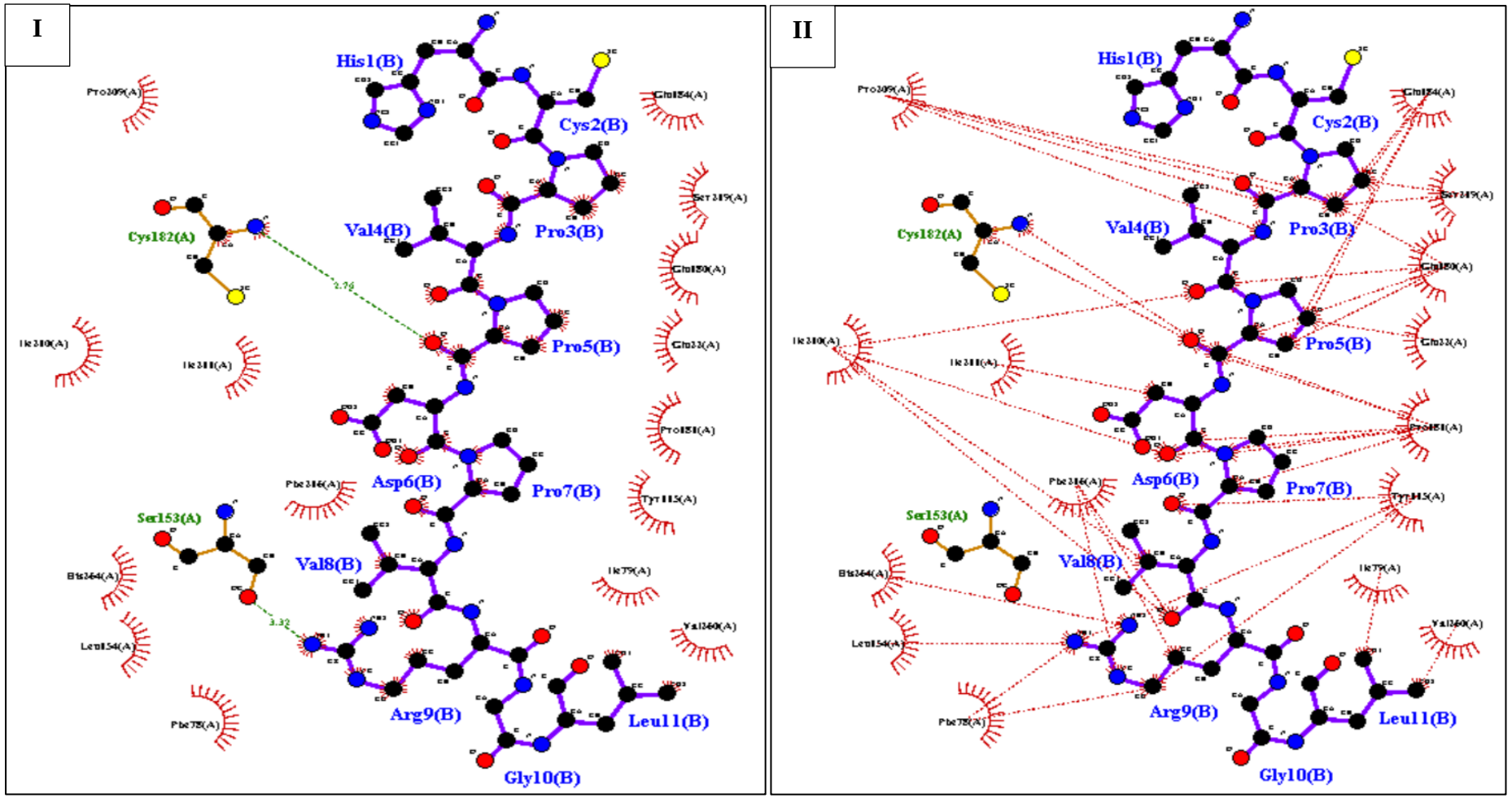

Figure S14c: Binding interaction of HC**P**VPDPVRGL inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14d: Binding interaction of pancreatic lipase inhibitory peptides-MLPLMLPFTMGY at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide ML**P**LMLPFTM GY	PRO3	cluster2_1	-8.4	C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
Total number of bonds					41	0	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

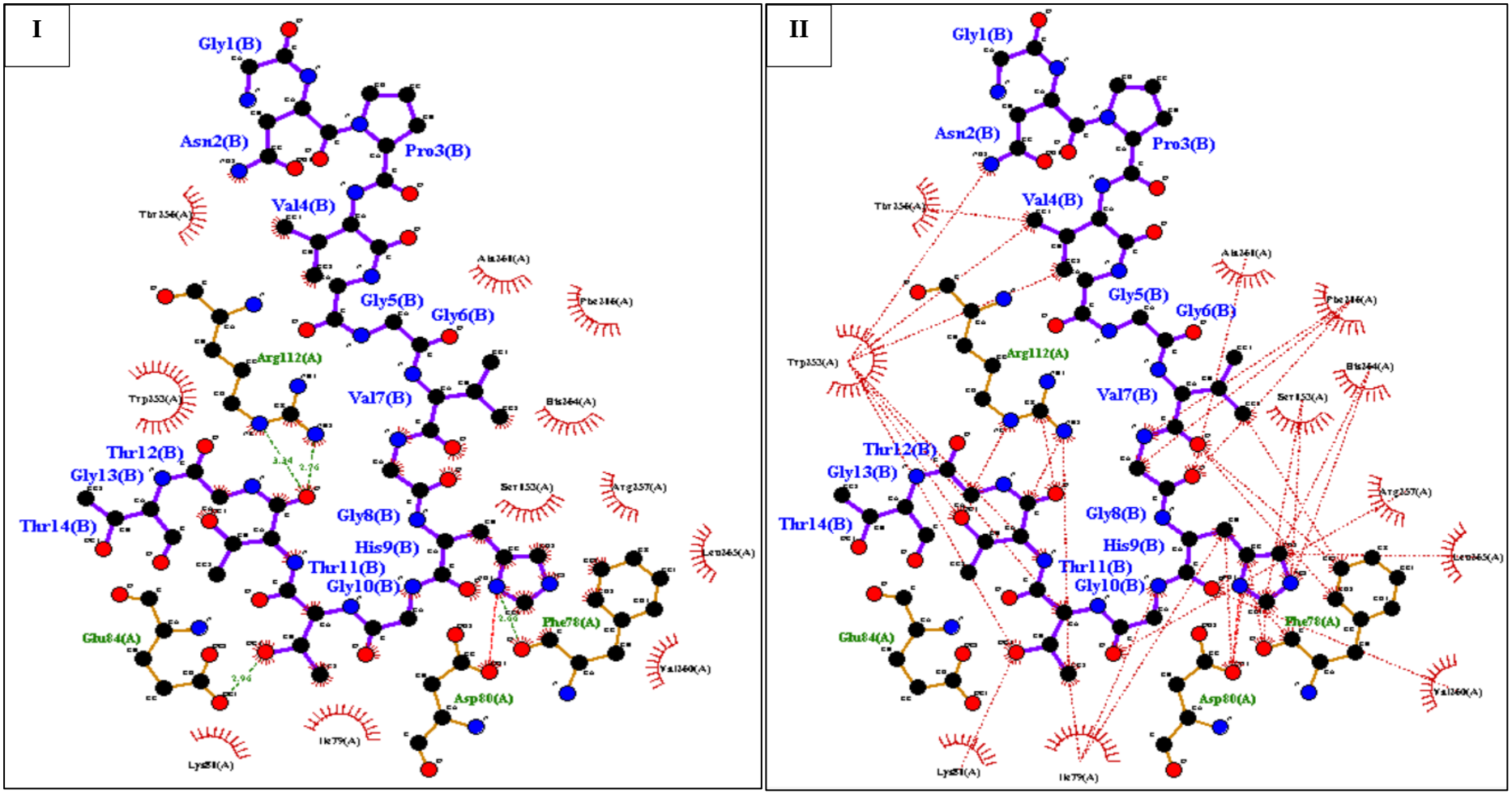

Figure S14d: Binding interaction of ML**P**LMLPFTMGY inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14e: Binding interaction of pancreatic lipase inhibitory peptides-LAAVEALSTNG at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide LA**A**VEALSTN G	ALA3	cluster1_1	-8.4	C - NA CA - Phe216 CB - Phe216 N - Phe216 O - NA	NA	NA	NA
Total number of bonds					31	0	0	3
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

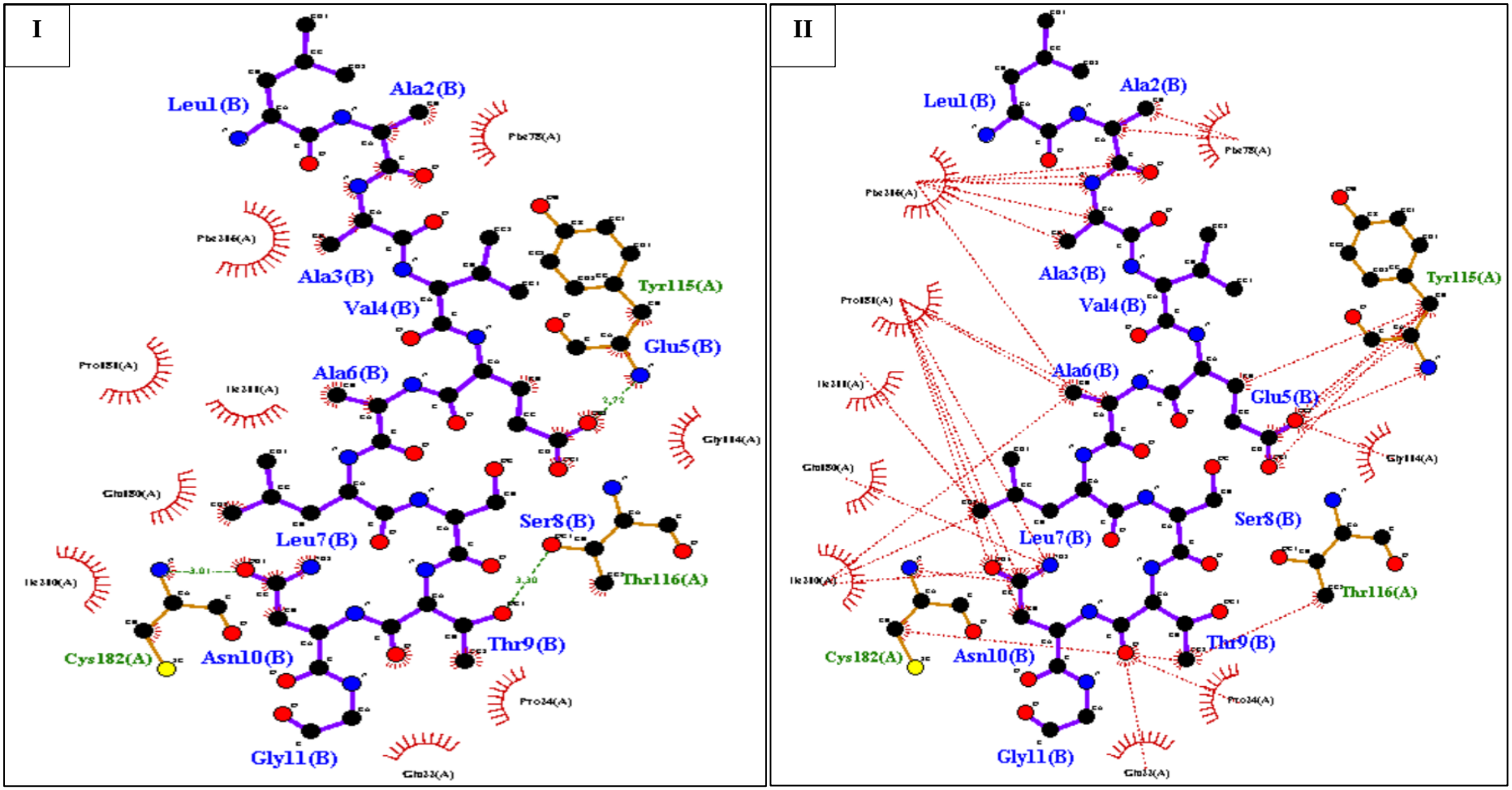

Figure S14e: Binding interaction of LA**A**VEALSTNG inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14f: Binding interaction of pancreatic lipase inhibitory peptides-RPAQPNYPWTAVLVFRH at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide RP**A**QPNYPWT AVLVFRH	ALA3	cluster3_1	-9.3	C - Val260 CA - Val260 CB - Thr256, Arg257 N - NA O - Val260	NA	NA	NA
Total number of bonds					56	1	0	1
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					9%	0%	0%	0%

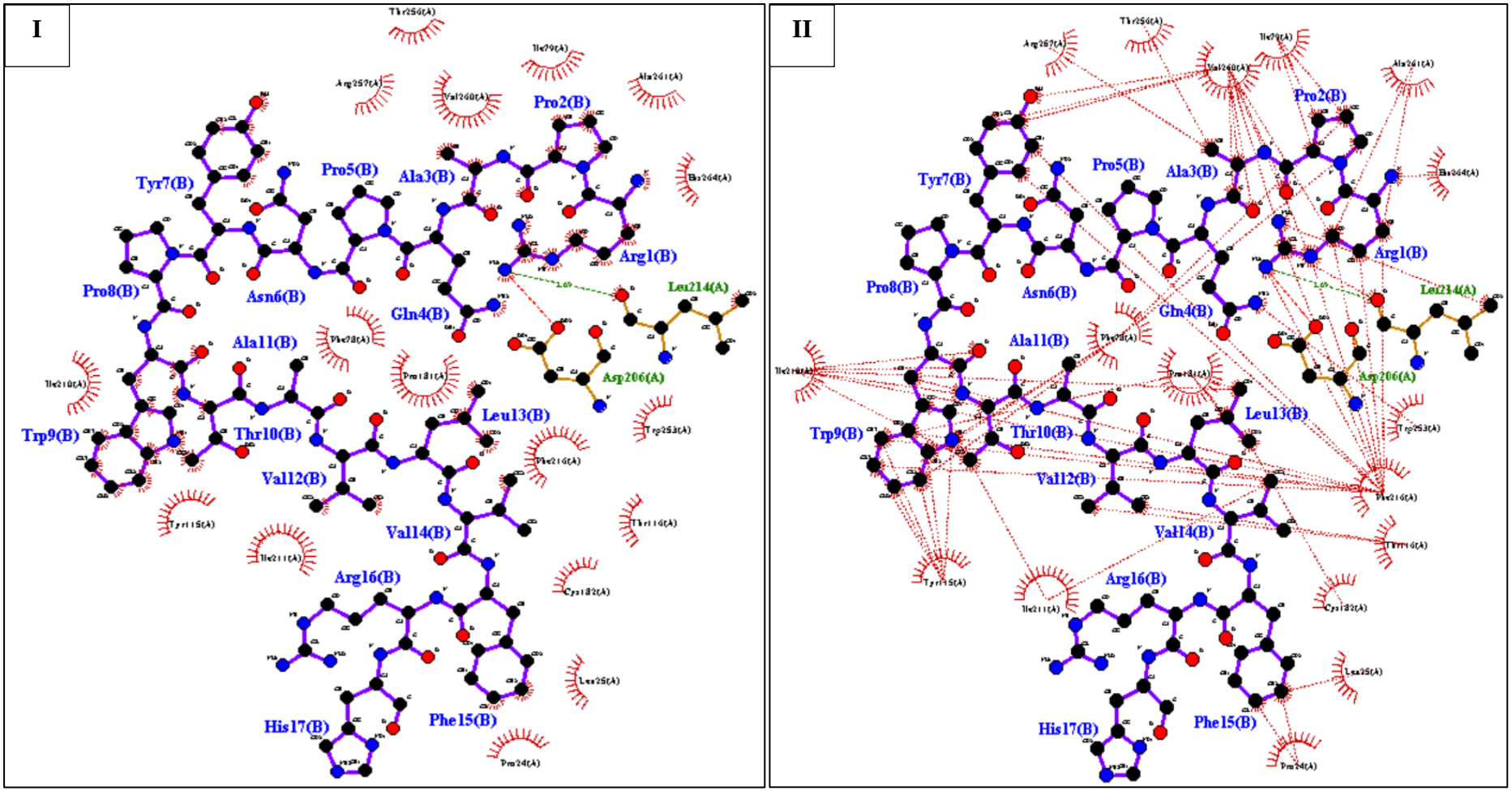

Figure S14f: Binding interaction of RP**A**QPNYPWTAVLVFRH inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14g: Binding interaction of pancreatic lipase inhibitory peptides- NALKCCHSCPA at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide NA**L**KCCHSCP A	LEU3	cluster1_3	-10.4	C - NA CA - Val260 CB - Val260 CD_1 - NA CD_2 - Phe78, Ile79 CG - NA N -Val260 O - NA	NA	NA	NA
Total number of bonds					47	0	0	2
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					11%	0%	0%	0%

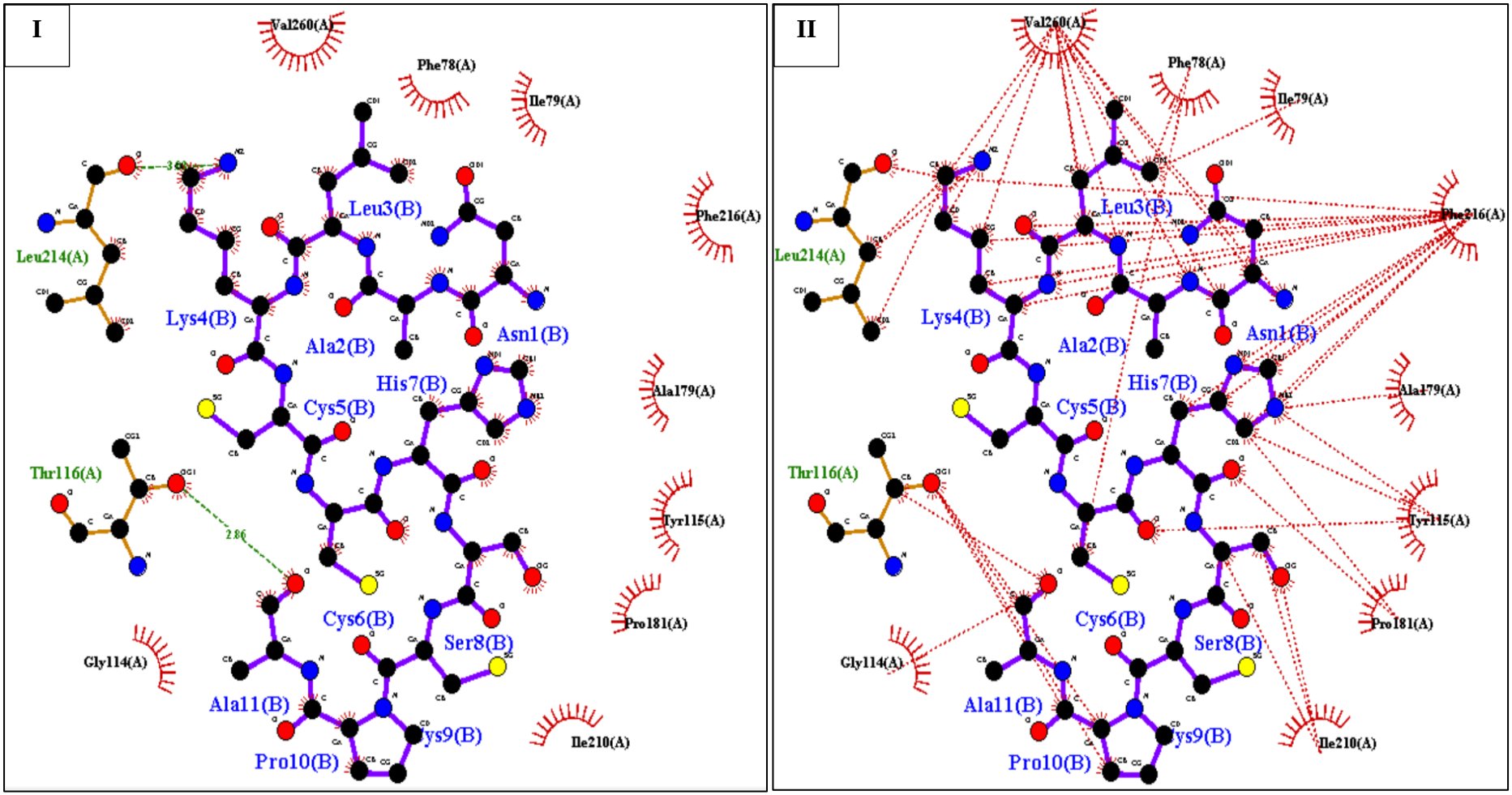

Figure S14g: Binding interaction of NA**L**KCCHSCPA inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S14h: Binding interaction of pancreatic lipase inhibitory peptides- ALWGAGGGGLGLSSGR at N3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide AL**W**GAGGGGL GLSSGR	TRP3	cluster1_4	-7.6	C - Ile210 CA - Ile210 CB - Pro181, Cys182 CD_1 - Cys182 CD_2 - Cys182 CE_2 - NA CE_3 - Pro181 CG - Pro181, Cys182 CH_2 - NA CZ_2 - NA CZ_3 - Glu180 N - NA NE_1 - NA O - NA	NA	NA	NA
Total number of bonds					45	0	0	2
Total no of interactive residues					10	0	0	0
Overall percentage of bonding					22%	0%	0%	0%

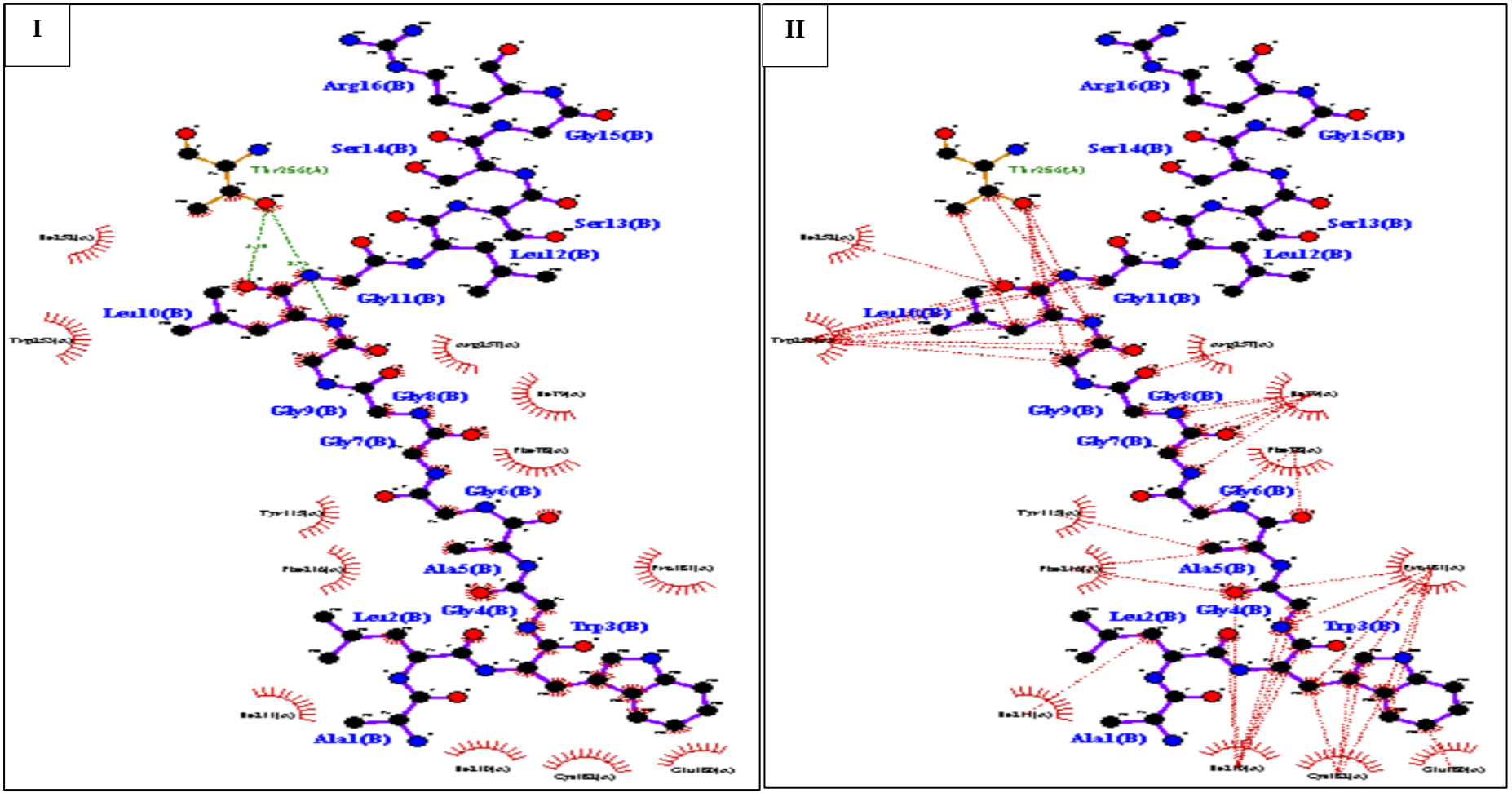

Figure S14h: Binding interaction of AL**W**GAGGGGLGLSSGR inhibitory peptide at N3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15a: Binding interaction of pancreatic lipase inhibitory peptides- TATAVV at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide TAT**A**VV	ALA4	cluster5_1	-8.6	C - NA CA - NA CB - NA N - Phe216 O - Phe216, Val260	NA	NA	NA
Total number of bonds					22	0	0	0
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					14%	0%	0%	0%

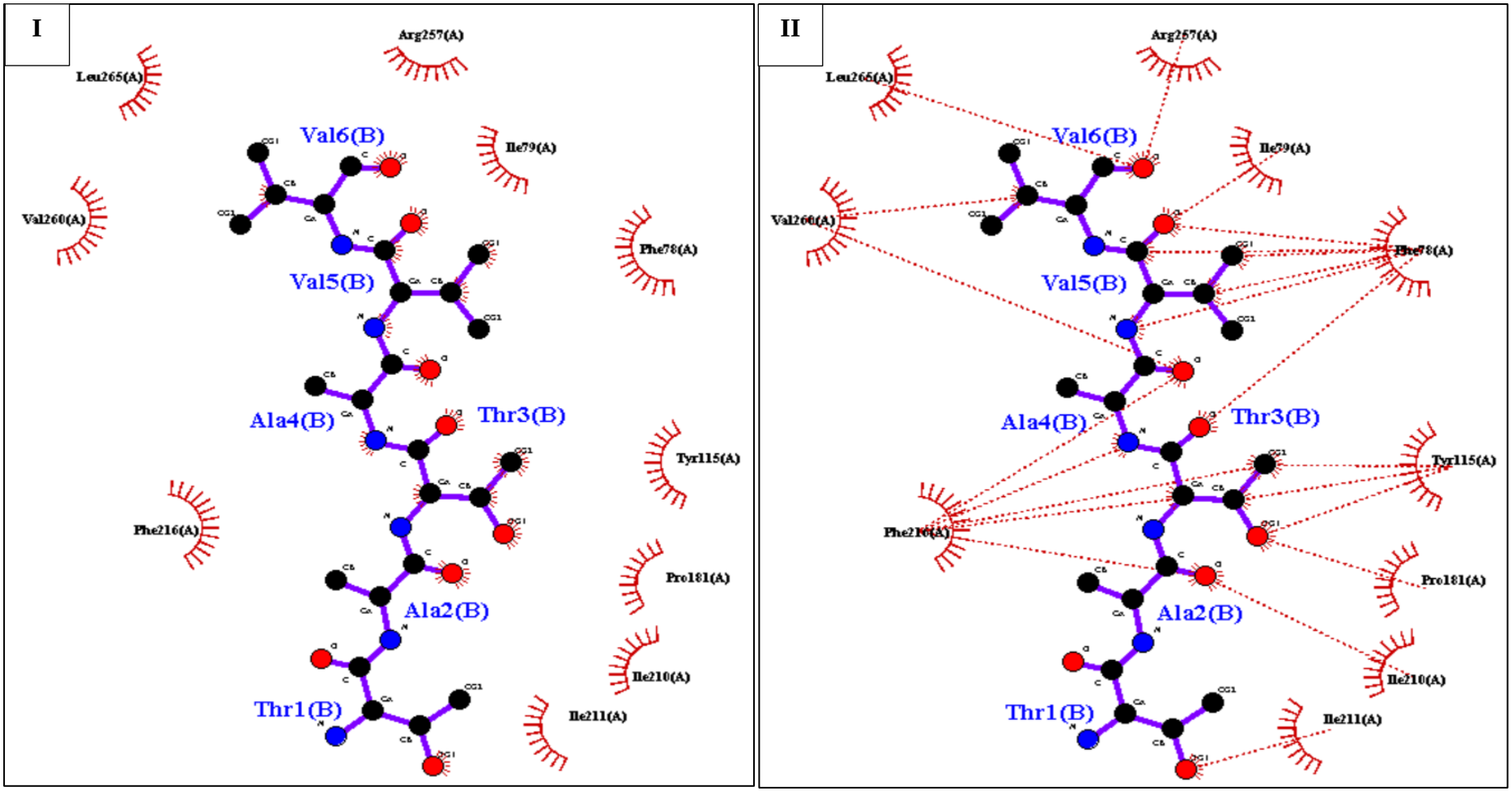

Figure S15a: Binding interaction of TAT**A**VV inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15b: Binding interaction of pancreatic lipase inhibitory peptides- DFGIASF at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide DFGI**A**SF	ALA5	cluster15_1	-8.5	C - NA CA - NA CB - NA N - Tyr115, Pro181 O - Phe216, Pro181	NA	NA	NA
Total number of bonds					26	0	0	0
Total no of interactive residues					4	0	0	0
Overall percentage of bonding					15%	0%	0%	0%

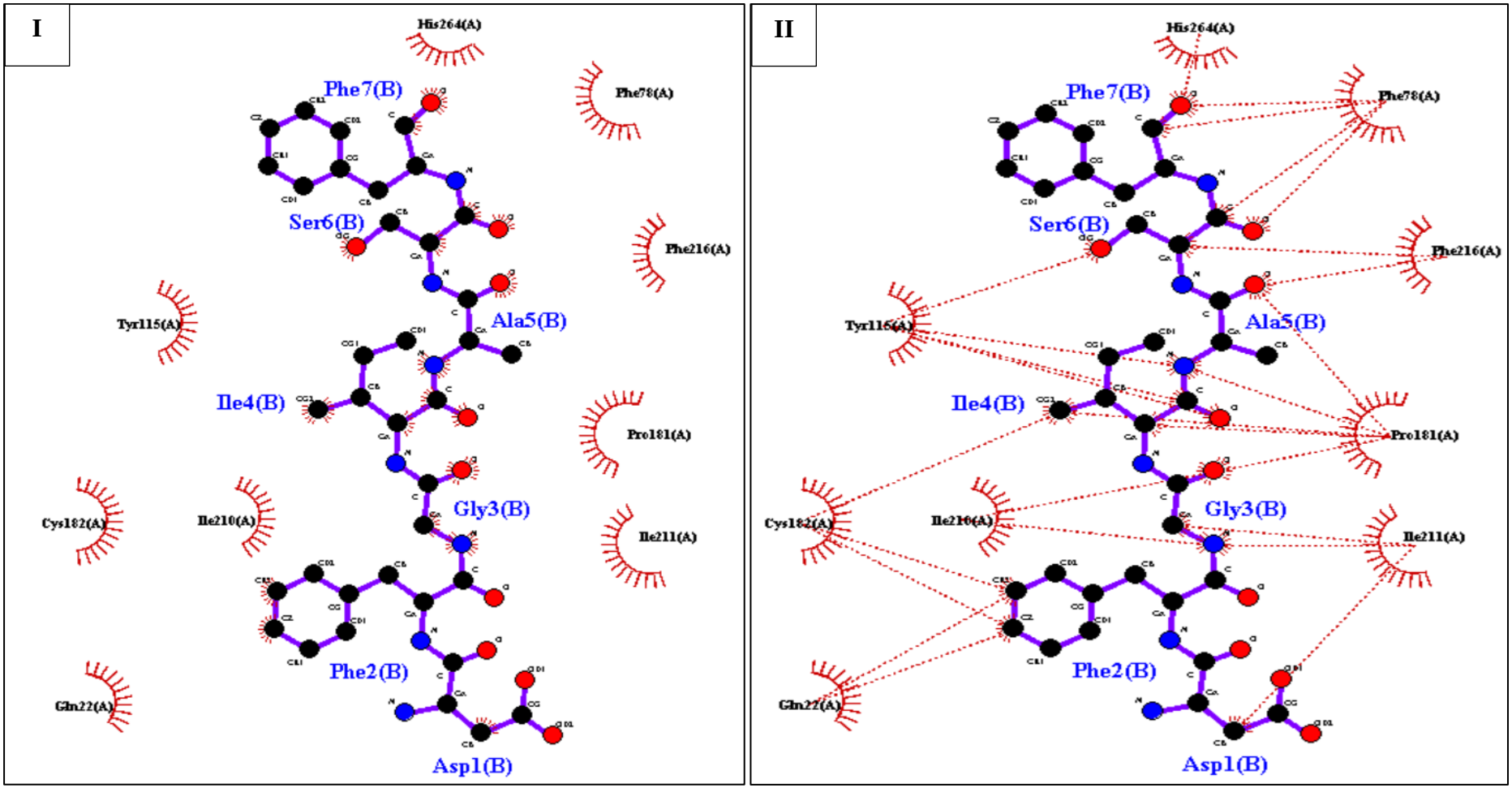

Figure S15b: Binding interaction of DFGI**A**SF inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15c: Binding interaction of pancreatic lipase inhibitory peptides-RLARAGLAQ at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide RLARAG**L**AQ	LEU7	cluster1_4	-7.9	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					23	0	0	3
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

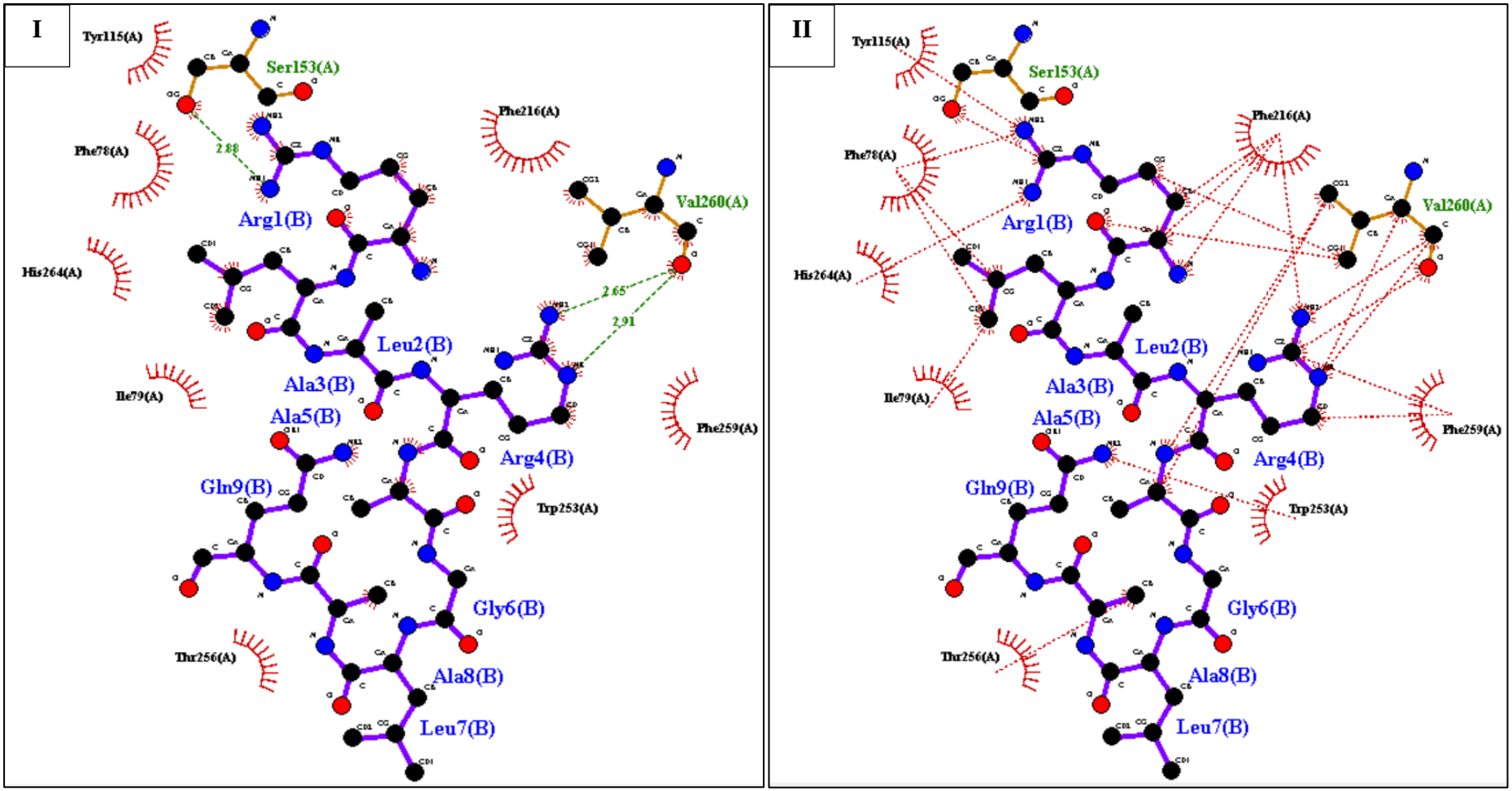

Figure S15c: Binding interaction of RLARAG**L**AQ inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15d: Binding interaction of pancreatic lipase inhibitory peptides-LNLDLLR at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide LNLD**L**LR	LEU5	cluster11_2	-8.1	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
Total number of bonds					20	0	0	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

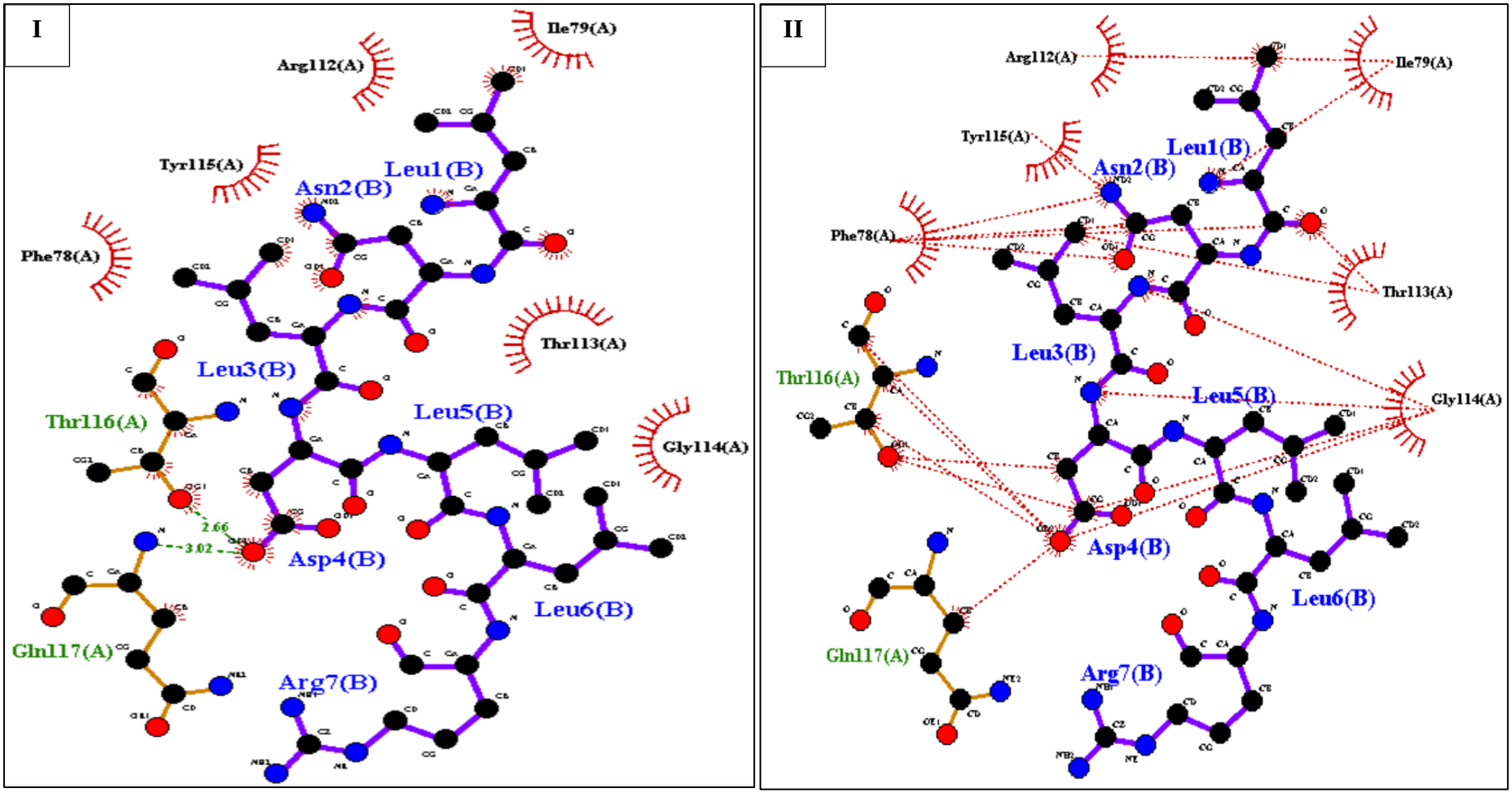

Figure S15d: Binding interaction of LNLD**L**LR inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15e: Binding interaction of pancreatic lipase inhibitory peptides-IIAPPER at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide IIAP**P**ER	PRO5	cluster9_3	-7.3	C - NA CA - NA CB -NA CD - Ile79 CG - Ile79 N- NA O - NA	NA	NA	NA
Total number of bonds					38	0	0	3
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					5%	0%	0%	0%

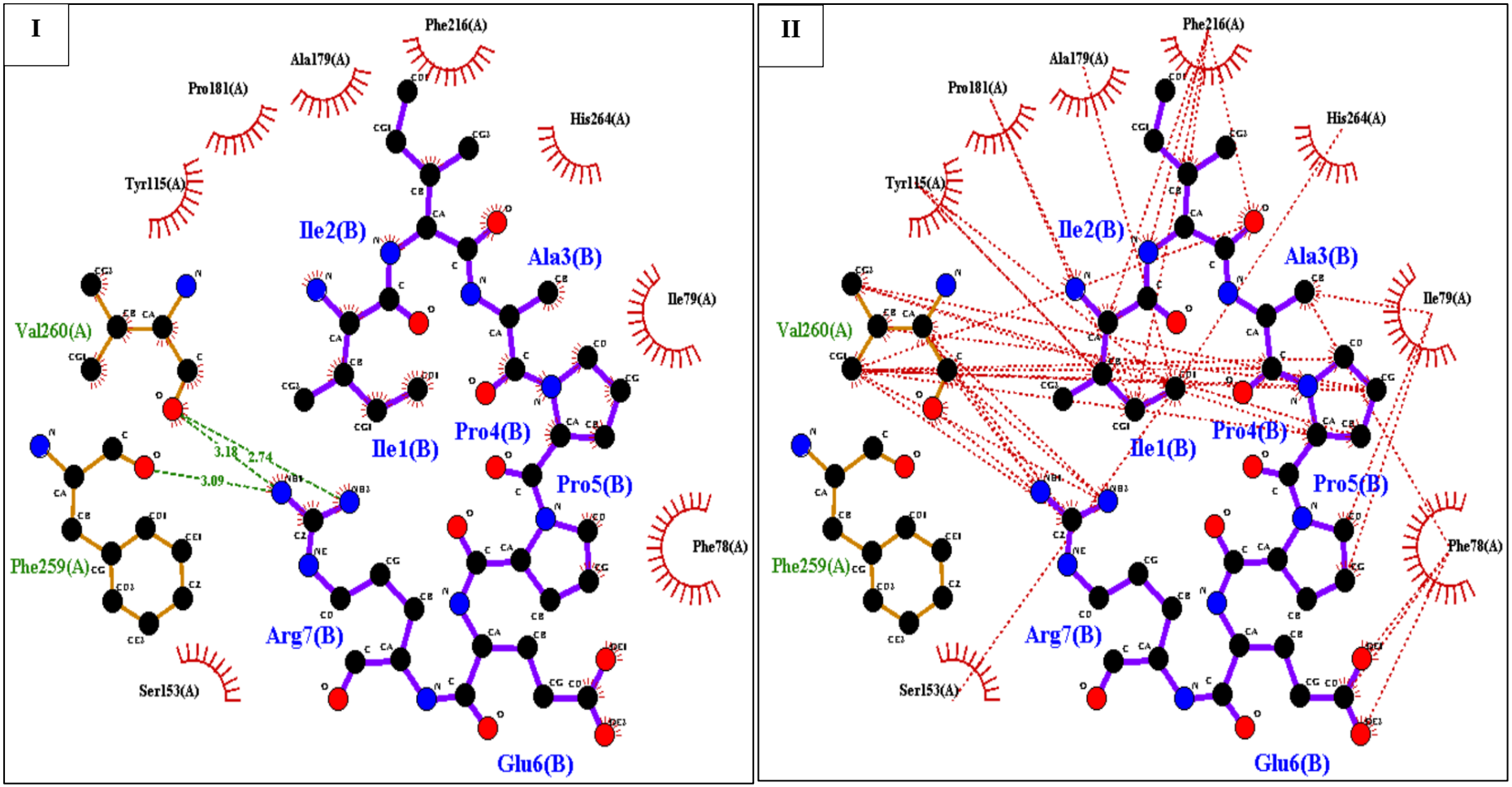

Figure S15e: Binding interaction of IIAPPER inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15f Binding interaction of pancreatic lipase inhibitory peptides-APFPLR at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide APF**P**LR	PRO4	cluster1_3	-7.0	C - NA CA - Tyr115 CB - Tyr115 CD - NA CG - NA N- NA O - Phe78	NA	NA	NA
Total number of bonds					16	0	0	0
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					19%	0%	0%	0%

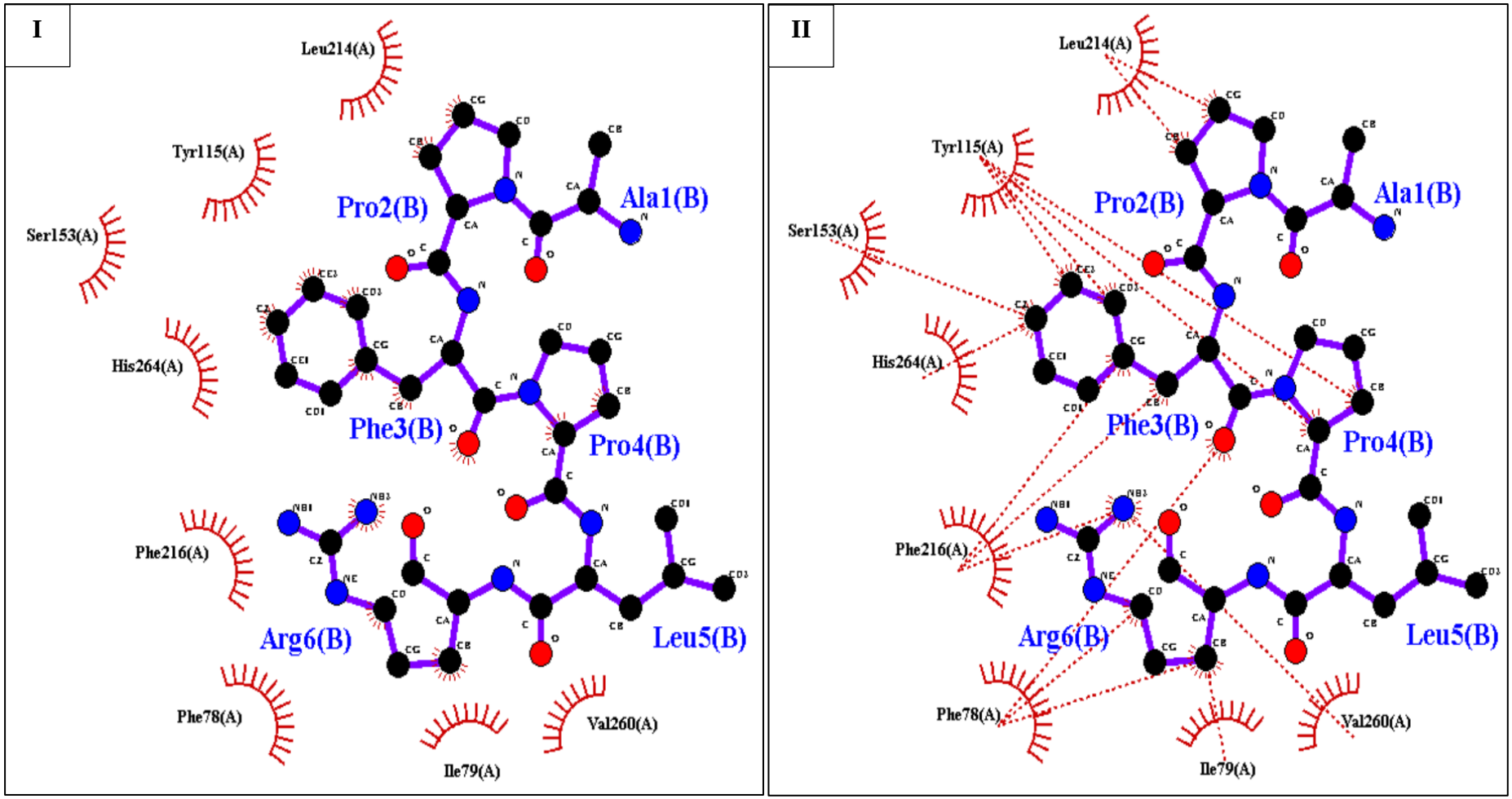

Figure S15f: Binding interaction of APF**P**LR inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15g: Binding interaction of pancreatic lipase inhibitory peptides- NYVADGLG at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide NYVAD**G**LG	GLY6	cluster1_1	-8.4	C - NA CA - Ile79 N - NA O - Phe78	NA	NA	NA
Total number of bonds					29	0	0	3
Total no of interactive residues					2	0	0	0
Overall percentage of bonding					7%	0%	0%	0%

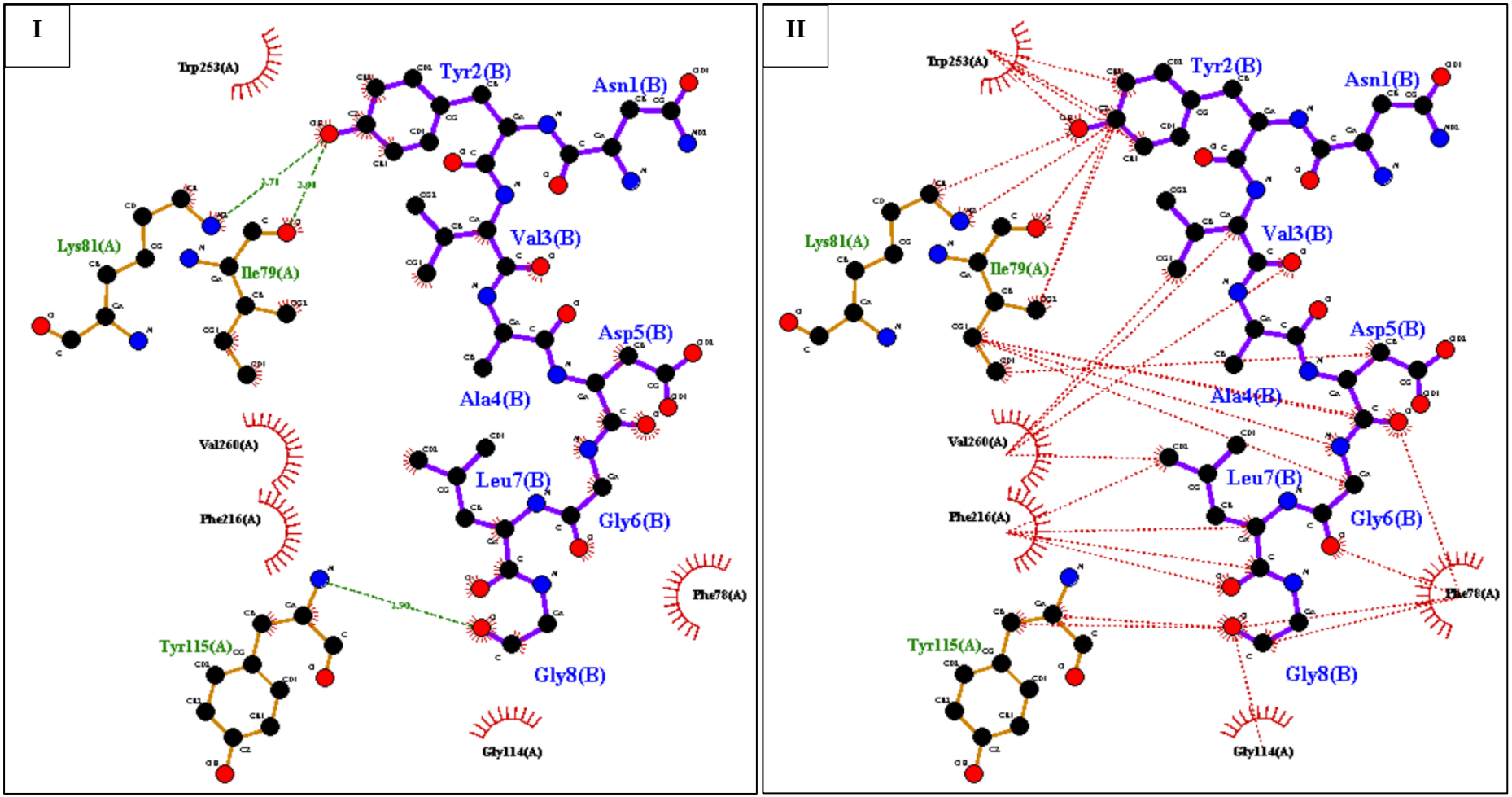

Figure S15g: Binding interaction of NYVAD**G**LG inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15h: Binding interaction of pancreatic lipase inhibitory peptides- HLPGRG at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide HLP**G**RG	GLY4	cluster5_3	-7.5	C - NA CA - NA N - NA O - NA	NA	NA	NA
Total number of bonds					20	0	0	0
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

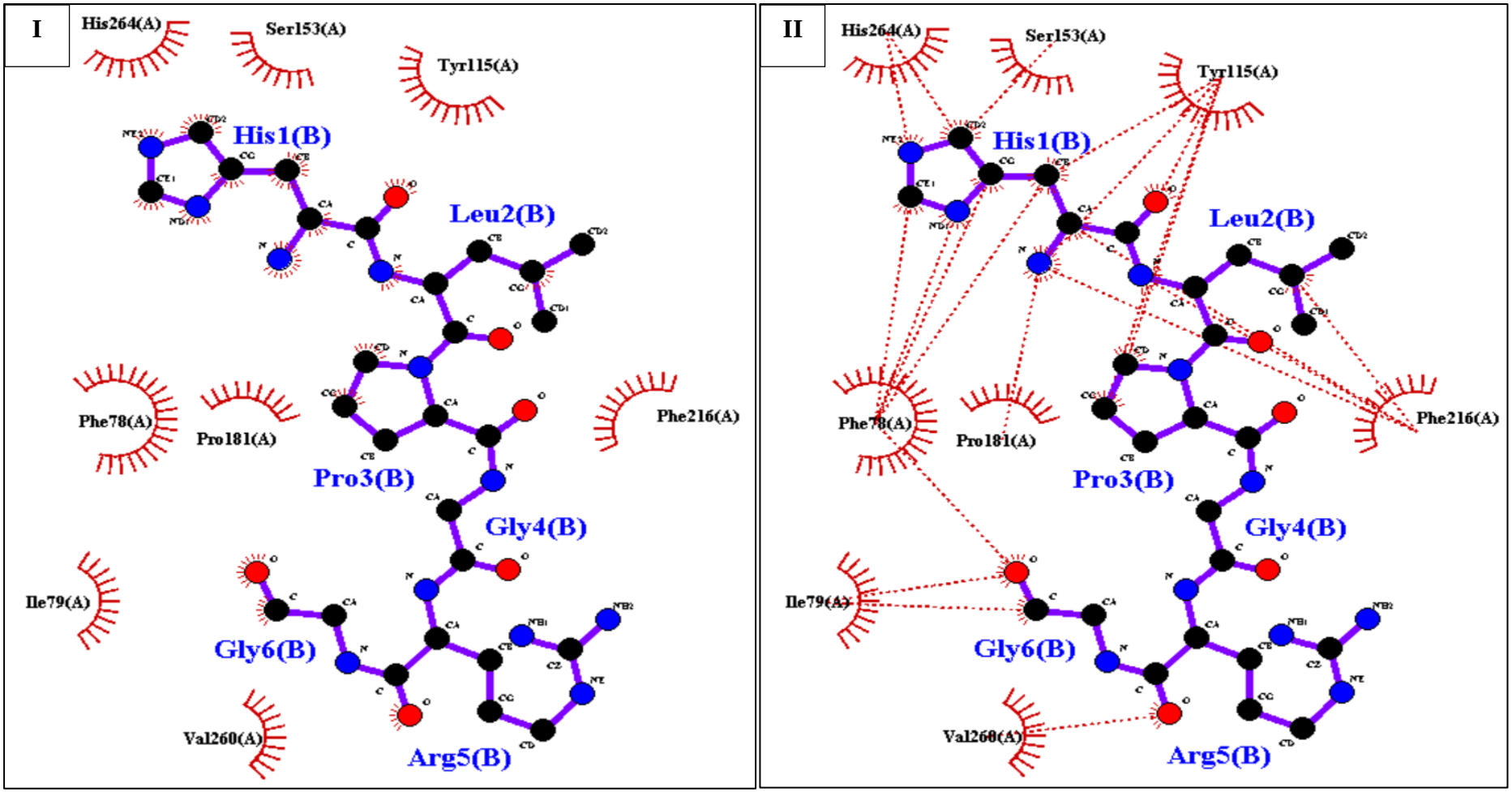

Figure S15h: Binding interaction of HLP**G**RG inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15i: Binding interaction of pancreatic lipase inhibitory peptides-AEWLHDWKL at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide AEWLHD**W**KL	TRP7	cluster1_1	-7.0	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CE_2 - Tyr115 CE_3 - Phe78 CG - NA CH_2 - Try115 CZ_2 - Tyr115 CZ_3 - Phe78 N - NA NE_1 - NA O - NA	NA	NA	NA
Total number of bonds					21	0	0	1
Total no of interactive residues					5	0	0	0
Overall percentage of bonding					24%	0%	0%	0%

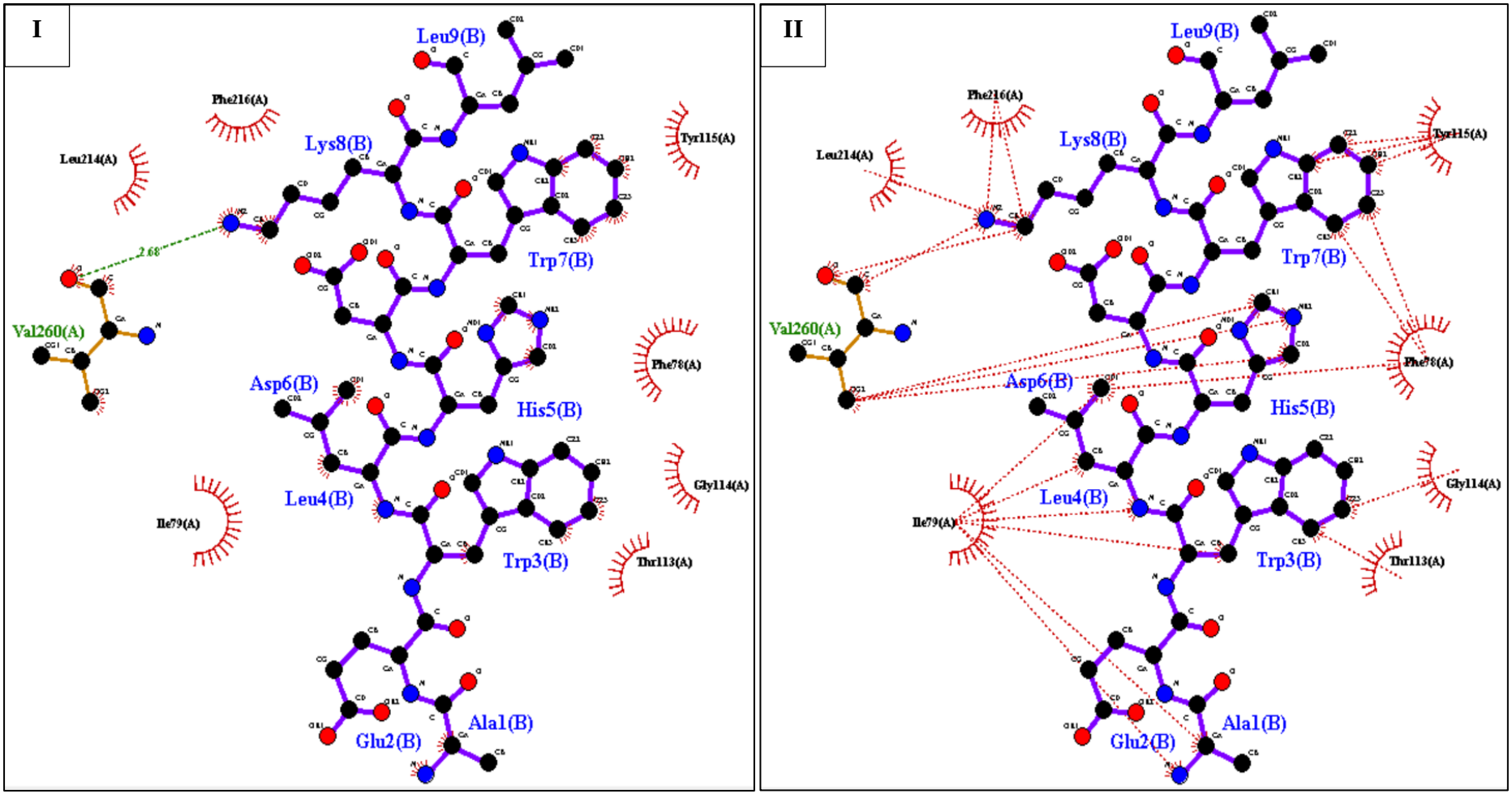

Figure S15i: Binding interaction of AEWLHD**W**KL inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15j: Binding interaction of pancreatic lipase inhibitory peptides- KFQWGY at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide KFQ**W**GY	TRP4	cluster3_1	-7.7	C - Pro181 CA - NA CB - Phe216 CD_1 - Phe216 CD_2 - NA CE_2 - NA CE_3 - Tyr115 CG - Phe216 CH_2 - Phe78, His264 CZ_2 - NA CZ_3 - Phe78, Ser153, His264 N - NA NE_1 - Phe216 O - Tyr115	NA	NA	NA
Total number of bonds					28	0	0	2
Total no of interactive residues					12	0	0	0
Overall percentage of bonding					43%	0%	0%	0%

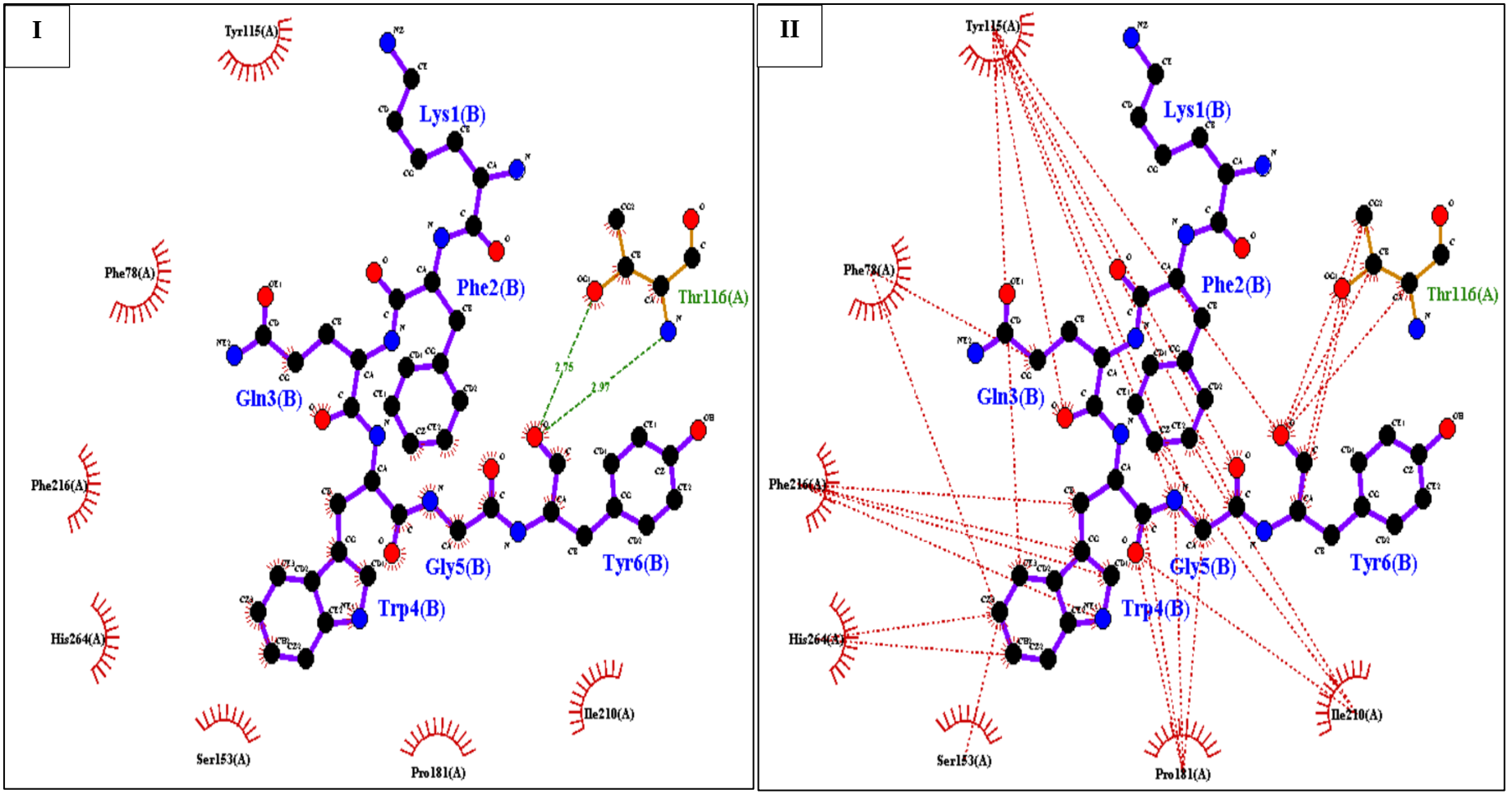

Figure S15j: Binding interaction of KFQ**W**GY inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15k: Binding interaction of pancreatic lipase inhibitory peptides- LTMPQWW at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide LTMP**Q**WW	GLN5	cluster4_4	-6.9	C - NA CA - NA CB - NA CD - NA CG - NA N - NA NE_2 - NA O - NA OE_1 - NA	NA	NA	NA
Total number of bonds					25	0	0	1
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

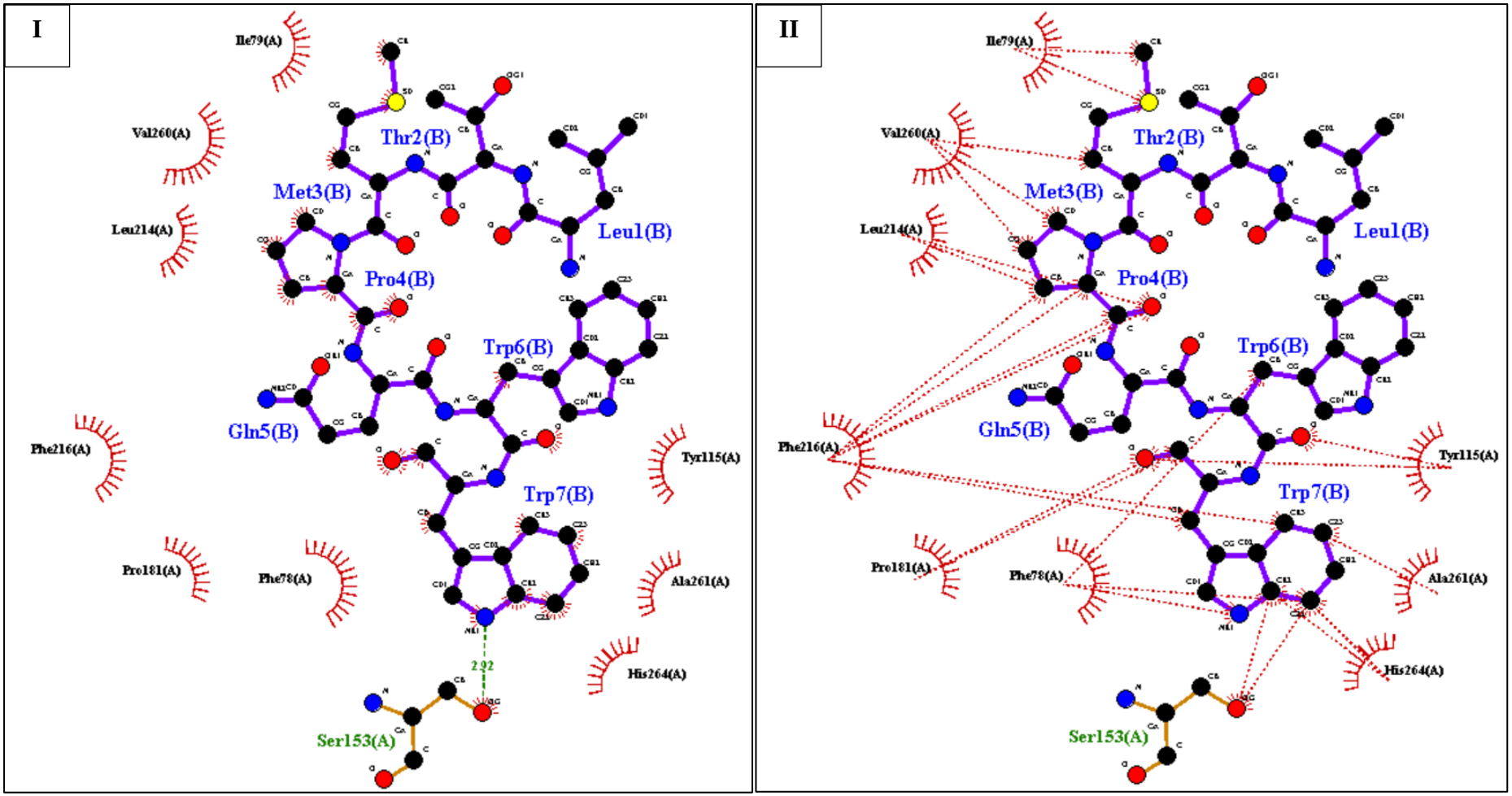

Figure S15k: Binding interaction of LTMP**Q**WW inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S15l: Binding interaction of pancreatic lipase inhibitory peptides-TLMPQWW at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide TLMP**Q**WW	GLN5	cluster1_1	-7.9	C - NA CA - NA CB - NA CD - NA CG - NA N - NA NE_2 - NA O - NA OE_1 - NA	NA	NA	NA
Total number of bonds					29	0	0	0
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

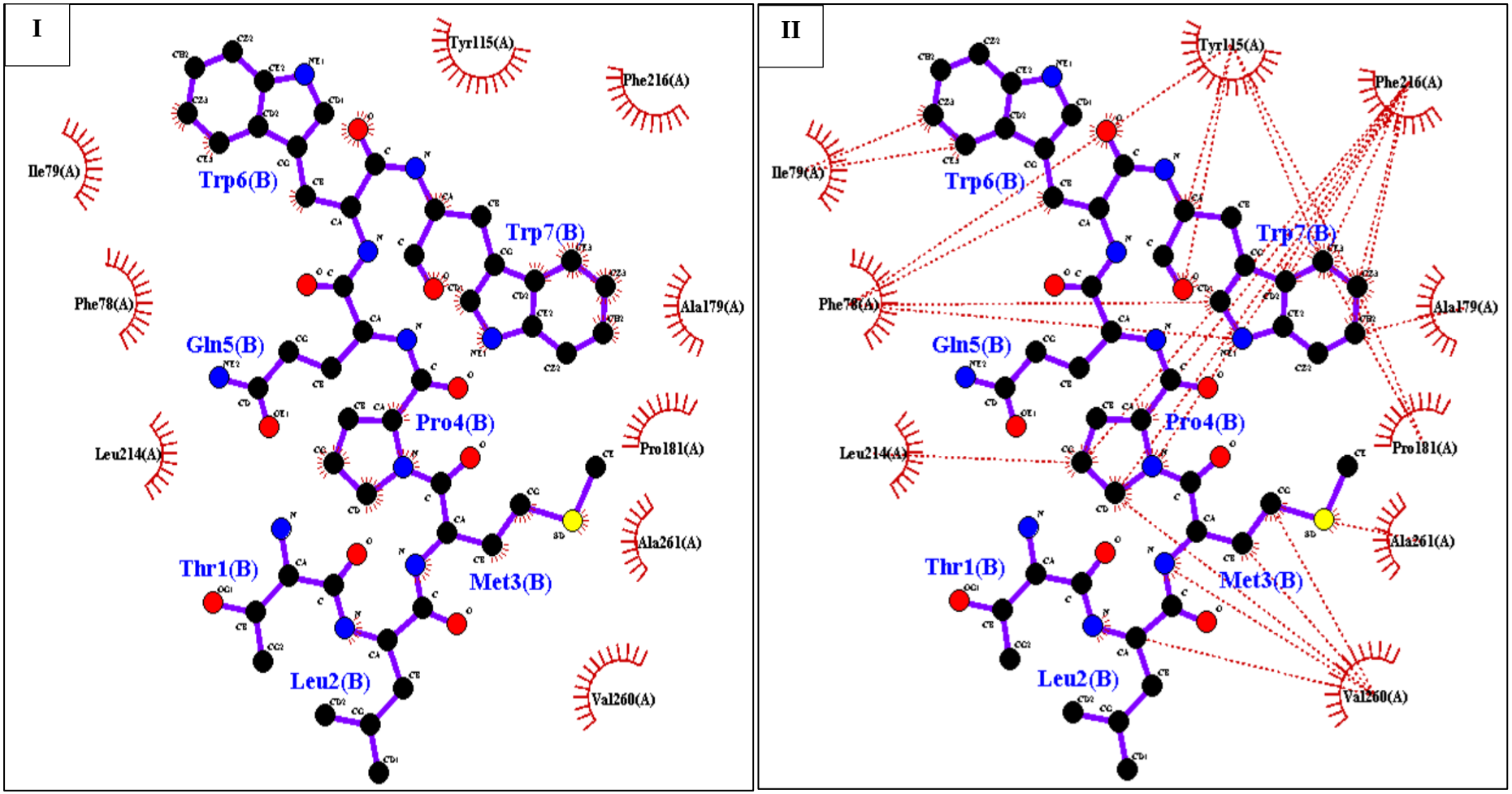

Figure S15l: Binding interaction of TLMP**Q**WW inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line); Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S16a: Binding interaction of pancreatic lipase inhibitory peptides-GEHGGAGMGGGQFQPV at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Long chain peptide GEHGGAGMGG GQF**Q**PV	GLN14	cluster1_2	-9.1	C - NA CA - NA CB - NA CD - NA CG - NA N - NA NE_2 - NA O - NA OE_1 - NA	NA	NA	NA
Total number of bonds					40	0	3	2
Total no of interactive residues					0	0	0	0
Overall percentage of bonding					0%	0%	0%	0%

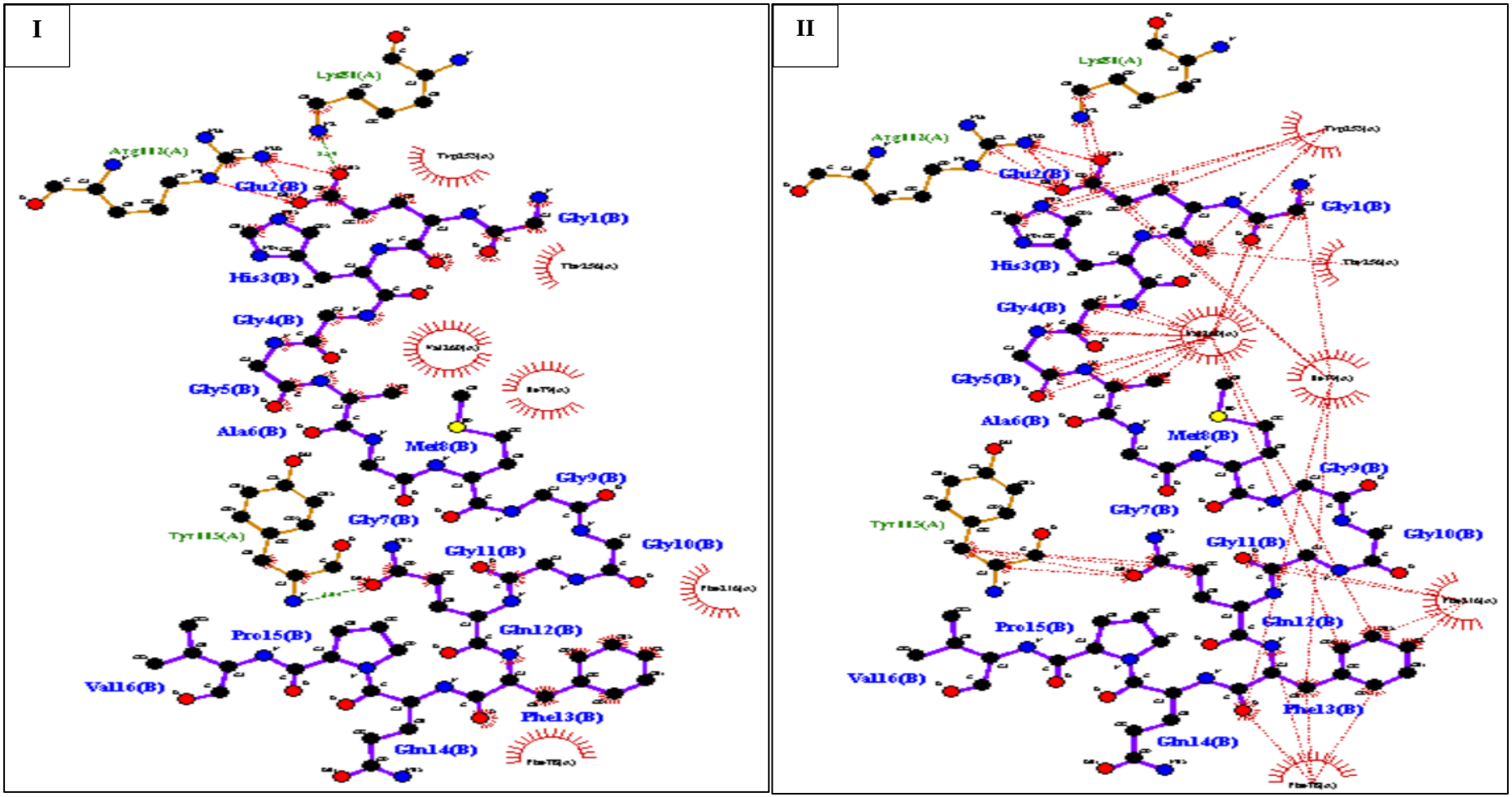

Figure S16a: Binding interaction of GEHGGAGMGGGQF**Q**PV inhibitory peptide at C3position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S16b: Binding interaction of pancreatic lipase inhibitory peptides-FFRSKLLSRGAAAAKGALLPQYW at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Long chain peptide FFRSKLLSRG AAAAKGALLP **Q**YW	GLN21	cluster1_3	-9.2	C - Ile79 CA - Ile79 CB - NA CD - NA CG - NA N - NA NE_2 -Trp253, Arg257 O - Phe78, Ile79 OE_1 - Arg257, Val260	NA	NA	NA
Total number of bonds					45	0	0	1
Total no of interactive residues					8	0	0	0
Overall percentage of bonding					18%	0%	0%	0%

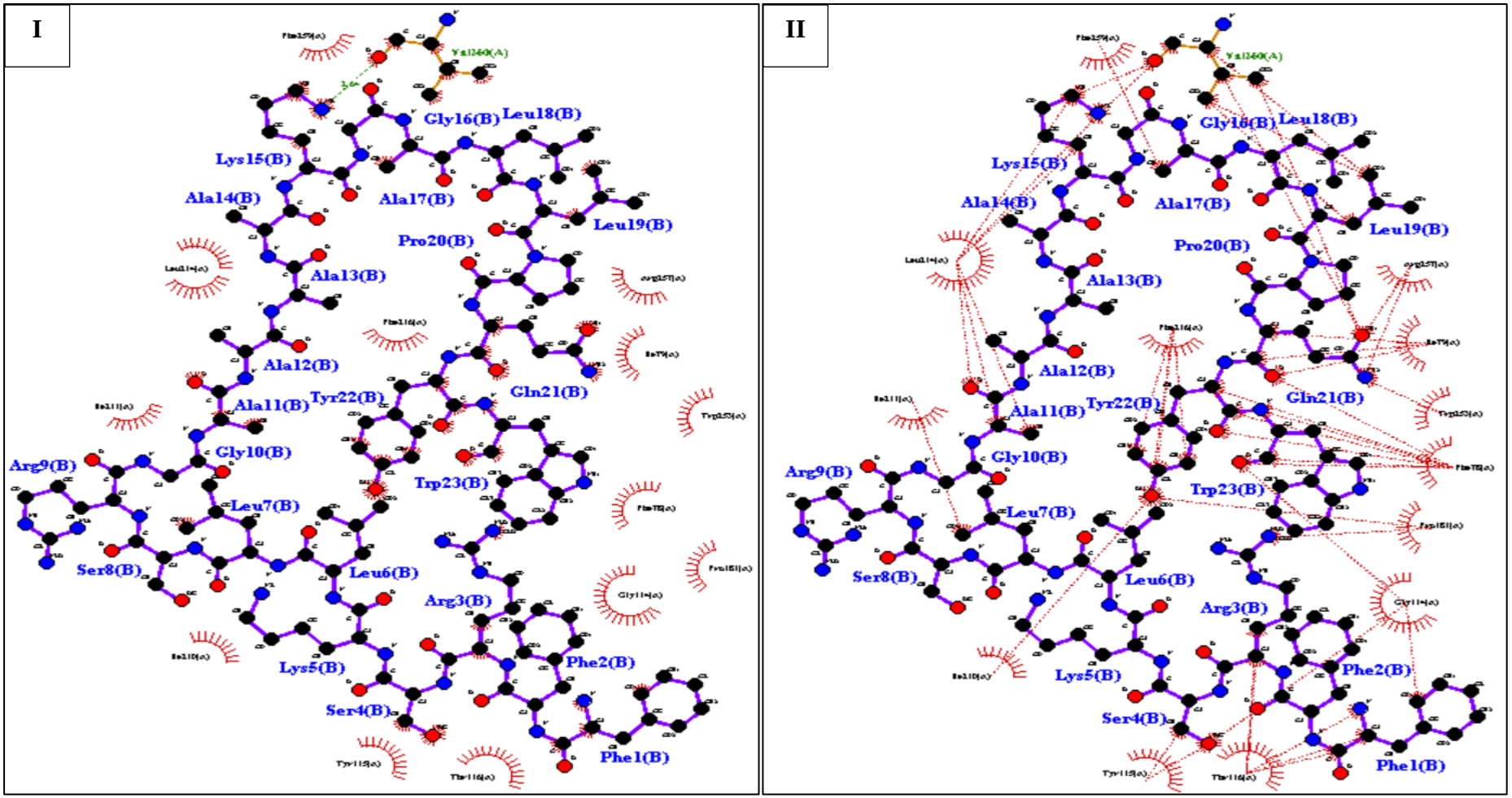

Figure S16b: Binding interaction of FFRSKLLSRGAAAAKGALLP**Q**YW inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S16c: Binding interaction of pancreatic lipase inhibitory peptides-SGGGGGGVAGAATASR at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Long chain peptide SGGGGGGVAG AAT**A**SR	ALA14	cluster3_1	-7.4	C - NA CA - Ile79 CB - Ile79 N - Ile79 O - NA	NA	NA	NA
Total number of bonds					40	0	0	0
Total no of interactive residues					3	0	0	0
Overall percentage of bonding					10%	0%	0%	0%

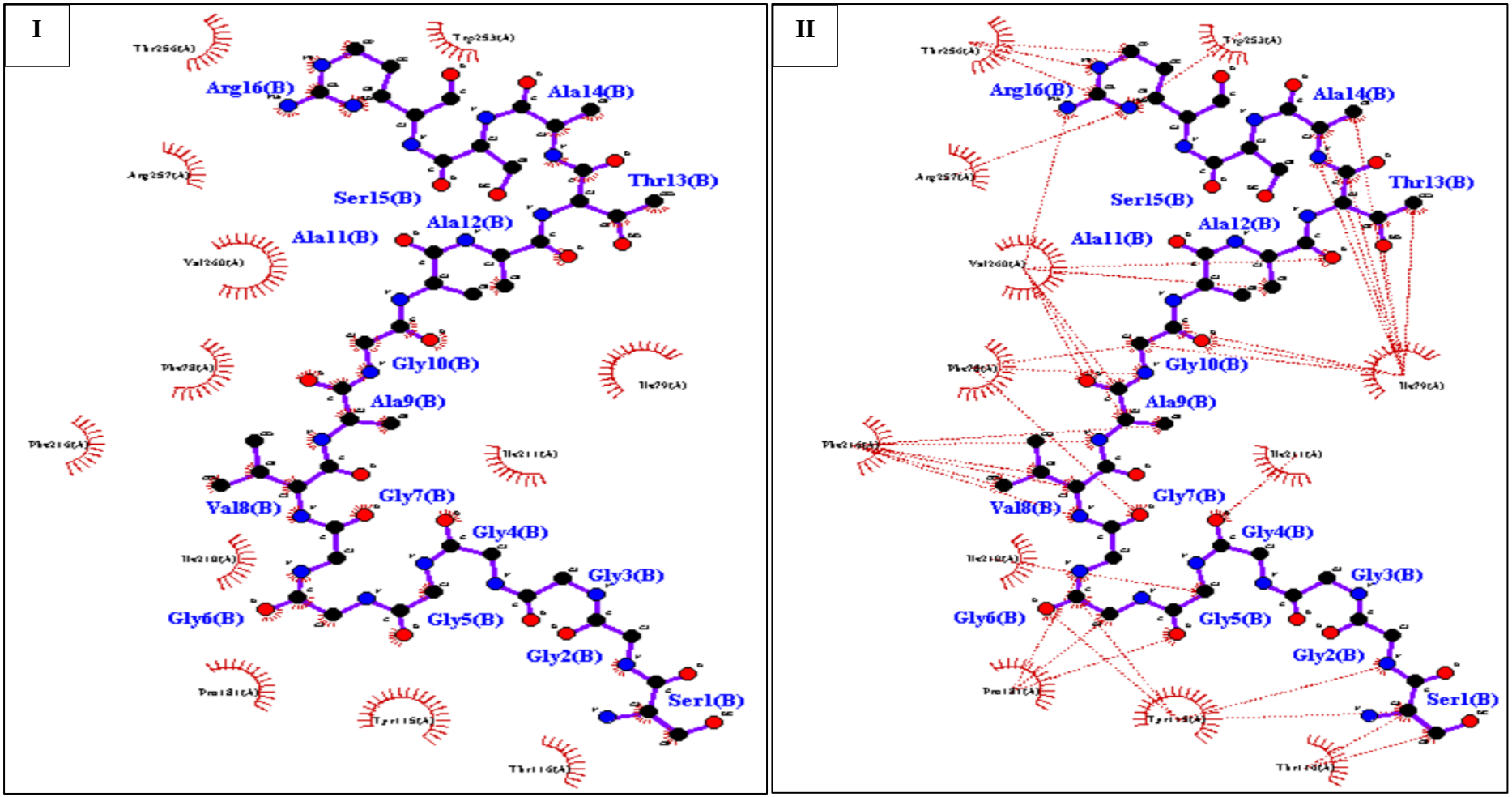

Figure S16c: Binding interaction of SGGGGGGVAGAAT**A**SR inhibitory peptide at N2 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.

Table S16d: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR at C3 position.

Position of amino acid in N-and C-terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODIGY	Binding affinity ΔG (Kcal mol^{-1})	Residues of pancreatic lipase involve in protein peptide interaction and its position			
					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Long chain peptide LNNPSVCDCD CMMK**A**AR	ALA15	cluster3_4	-9.8	C - Thr256 CA - Thr256 CB - Thr256 N - NA O - Trp257, Thr256, Arg257	NA	NA	O - Thr256
Total number of bonds					45	0	0	3
Total no of interactive residues					6	0	0	1
Overall percentage of bonding					13%	0%	0%	33%

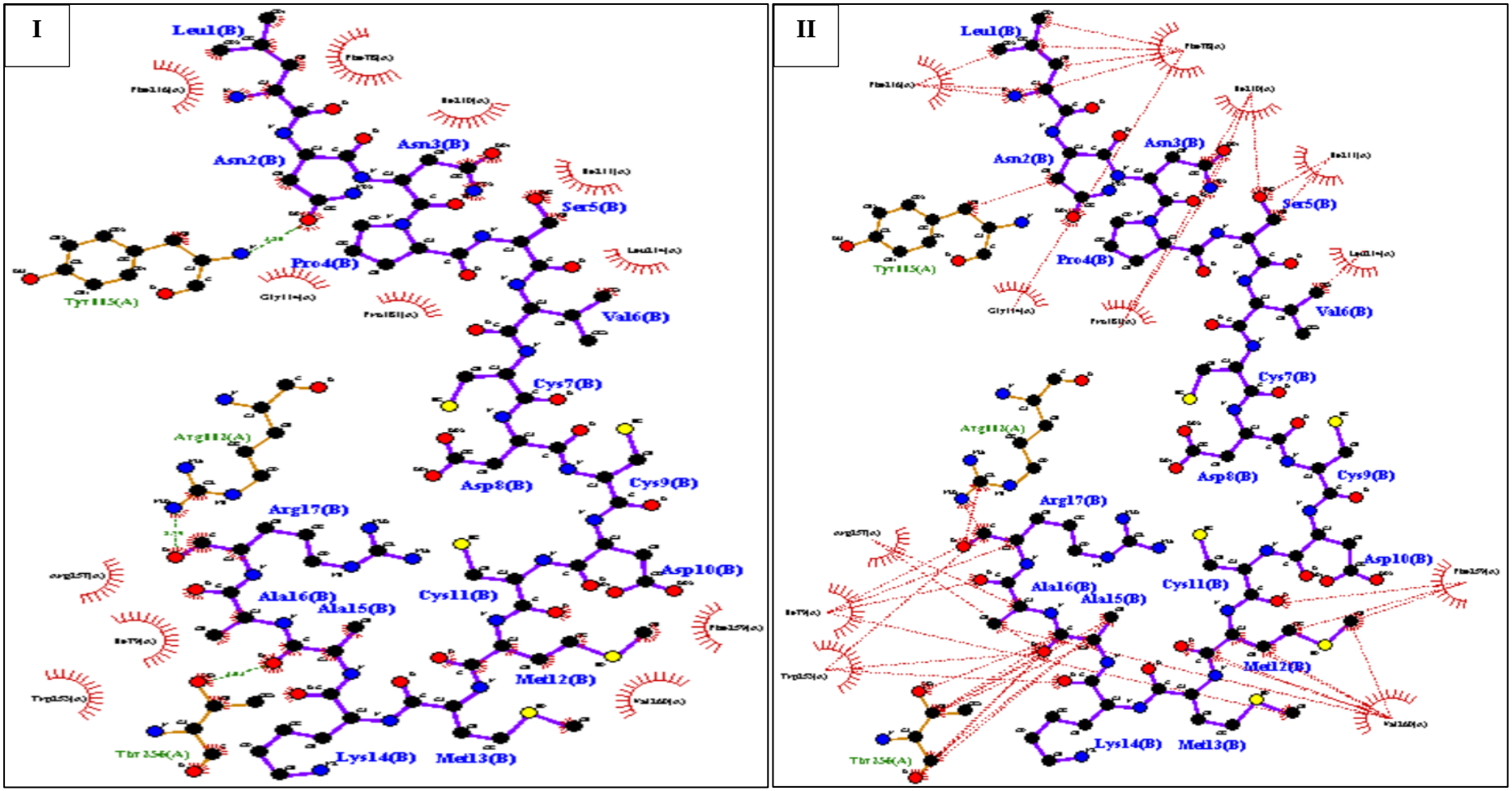

Figure S16d: Binding interaction of LNNPSVCDCDCMMK**A**AR inhibitory peptide at C3 position with pancreatic lipase enzyme. i.e. (I) salt bridge (red dotted line), hydrogen bond and bond distance (olive green dotted line with number in Armstrong, Å), (II) hydrophobic interaction (brick red dotted line interacted with elelashhes), non peptide bond (orange dotted line), ; Nitrogen atom (blue ball), oxygen atom (red ball), carbon atom (black ball) and sulphur atom (yellow ball); (A) representing the interactive amino acid residues of pancreatic lipase enzyme and (B) represnting the amino acid that present in the inhibitory peptides.