Supplementary material 2

Short Chain Peptide (Focus in LEU, MET, PRO)

Table X1.1: Binding interaction of pancreatic lipase inhibitory peptides-MMML

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
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
M**M**ML	MET2			C - NA CA - NA CB - NA CE - Gly77, Phe78, Asp80, His152 CG - Phe78 O - Phe216 N - NA SD - Gly77, Phe78, His152, Ser153	NA	NA	NA

MMML	MET3			C - NA CA - NA CB - NA CE - Val260 CG - NA O - Phe78 N - Phe78 SD – NA	NA	NA	NA
MMML	LEU4			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

Table X1.2: Binding interaction of pancreatic lipase inhibitory peptides-FDML

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
Short chain peptide FD**<u>M</u>**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
FDM**<u>L</u>**	LEU4			C - NA CA - NA CB - Ile79 CD_1 - NA CD_2 - NA CG - NA N - Ile79 O - Ile79	NA	NA	NA

Table X1.3: Binding interaction of pancreatic lipase inhibitory peptides-MSNYF

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
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

Table X1.4: Binding interaction of pancreatic lipase inhibitory peptides-LRFPL

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
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
LRFP**L**	LEU5			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Gly114, Tyr115	NA	NA	O - Tyr115
LRF**P**L	PRO4			C - NA CA -NA CB - NA CD - Phe216 CG - Phe216 N- NA O - Phe78, Tyr115	NA	NA	NA

Table X1.5: Binding interaction of pancreatic lipase inhibitory peptides-LQR

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
Short chain peptide **L**QR	LEU1	cluster1_4	-9.6	C - Phe78 CA - NA CB - NA CD_1 - Val260 CD_2 - Arg257, Val260, Ala261, Leu265 CG - NA N - Leu265 O - Phe78	NA	NA	NA

Table X1.6: Binding interaction of pancreatic lipase inhibitory peptides-RLLP

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
Short chain peptide R**L**LP	LEU2	cluster8_1	-7.2	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Val260	NA	NA	NA
RL**L**P	LEU3			C - NA CA - NA CB - Ile79 CD_1 - Phe78, Ile79 CD_2 - NA CG - NA N - NA O - Ile79	NA	NA	NA
RLL**P**	PRO4			C - NA CA -NA CB - NA CD - Val260 CG -Thr256 N- NA O - Trp253	NA	NA	NA

Table X1.7: Binding interaction of pancreatic lipase inhibitory peptides-VIAPW

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
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

Medium Chain Peptide (Focus in PRO, LEU)

Table X2.1: Binding interaction of pancreatic lipase inhibitory peptides-RLARAGLAQ

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
Medium chain peptide R**L**ARAGLAQ	LEU2	cluster1_4	-7.9	C - NA CA - NA CB - NA CD_1 - Phe78 CD_2 - Ile79 CG - Phe78 N - NA O - NA	NA	NA	NA
RLARAG**L**AQ	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O – NA	NA	NA	NA

Table X2.2: Binding interaction of pancreatic lipase inhibitory peptides-IIAPPER

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
Medium chain peptide IIA**P**PER	PRO4	cluster9_3	-7.3	C - Val260 CA - Val260 CB - Val260 CD - Val260 CG - Val260 N - Val260 O -NA	NA	NA	NA
Medium chain peptide IIAP**P**ER	PRO5			C - NA CA - NA CB -NA CD - Ile79 CG - Ile79 N- NA O - NA	NA	NA	NA

Table X2.3: Binding interaction of pancreatic lipase inhibitory peptides-LAPSTIK

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
Medium chain peptide **L**APSTIK	LEU1	cluster1_2	-8.0	C - NA CA - Val260 CB - NA CD_1 - NA CD_2 - Phe259 CG - NA N - Val260 O - NA	NA	NA	NA
LA**P**STIK	PRO3			C - NA CA - NA CB - NA CD - Val260 CG - Ile79, Val260 N - NA O - NA	NA	NA	NA

Table X2.4: Binding interaction of pancreatic lipase inhibitory peptides-VAPEEHPV

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
Medium chain peptide VA**P**EEHPV	PRO3	cluster2_4	-7.6	C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - Gly114, Tyr115	NA	NA	O- Tyr115
VAPEEH**P**V	PRO7			C - NA CA -NA CB - Tyr115 CD - NA CG - Phe216 N- NA O - Ile210, Phe216	NA	NA	NA

Table X2.5: Binding interaction of pancreatic lipase inhibitory peptides-KVEGDLK

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
Medium chain peptide KVEGD**L**K	LEU6	cluster1_2	-7.9	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Tyr115	NA	NA	NA

Table X2.6: Binding interaction of pancreatic lipase inhibitory peptides-NYVADGLG

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
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

Table X2.7: Binding interaction of pancreatic lipase inhibitory peptides-AAAPVAVAK

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
Medium chain peptide AAA**P**VAVAK	PRO4	cluster2_3	-7.6	C - Pro181 CA - NA CB - Cys182 CD - NA CG - NA N - NA O - Tyr115, Pro181, Cys182	NA	NA	NA

Table X2.8: Binding interaction of pancreatic lipase inhibitory peptides-YDDGSYKPH

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
Medium chain peptide YDDGSYK**P**H	PRO8	cluster1_1	-8.9	C - Ile79 CA - Ile79 CB - NA CD - NA CG - NA N - NA O - Val260	NA	NA	NA

Table X2.9: Binding interaction of pancreatic lipase inhibitory peptides-AGDDAPR

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
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

Table X2.10: Binding interaction of pancreatic lipase inhibitory peptides-FDPFPK

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
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
FDPF**P**K	PRO5			C - NA CA - NA CB - NA CD - Phe216 CG -NA N - NA O - Tyr115	NA	NA	NA

Table X2.11: Binding interaction of pancreatic lipase inhibitory peptides-ELPPHFL

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
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
ELP**P**HFL	PRO4			C - NA CA - NA CB - NA CD - Ile210 CG - Ile211 N - NA O – NA	NA	NA	NA
E**L**PPHFL	LEU2			C - NA CA - NA CB - NA CD_1 - Thr116 CD_2 - NA CG - Thr116 N - NA O – NA	NA	NA	NA

ELPPHF**L**	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.12: Binding interaction of pancreatic lipase inhibitory peptides-APFPLR

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
Medium chain peptide A**P**FPLR	PRO2	cluster1_3	-7.0	C - NA CA - NA CB - Leu214 CD - NA CG - Leu214 N - NA O - NA	NA	NA	NA
APF**P**LR	PRO4			C - NA CA - Tyr115 CB - Tyr115 CD - NA CG - NA N- NA O - Phe78	NA	NA	NA
APFP**L**R	LEU5			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.13: Binding interaction of pancreatic lipase inhibitory peptides-LNLDLLR

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
Medium chain peptide **L**NLDLLR	LEU1	cluster11_2	-8.1	C - NA CA - NA CB - NA CD_1 - Arg112 CD_2 - NA CG - NA N - Ile79 O - Phe78	NA	NA	NA
LN**L**DLLR	LEU3			C - NA CA - NA CB - NA CD_1 - Thr113 CD_2 - NA CG - NA N - Gly114 O - NA	NA	NA	NA
LNLD**L**LR	LEU5			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

LNLDL**L**R	LEU6			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.14: Binding interaction of pancreatic lipase inhibitory peptides-LNFEPR

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
Medium chain peptide **L**NFEPR	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
LNFE**P**R	PRO5			C - NA CA - NA CB - Ile210 CD - NA CG - NA N- NA O - NA	NA	NA	NA

Table X2.15: Binding interaction of pancreatic lipase inhibitory peptides-TTDVLR

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
Medium chain peptide TTDV**L**R	LEU5	cluster2_4	-8.3	C - NA CA - NA CB - Tyr115 CD_1 - NA CD_2 - NA CG - NA N - NA O - Tyr115	NA	NA	NA

Table X2.16: Binding interaction of pancreatic lipase inhibitory peptides-MANLQR

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
Medium chain peptide MAN**L**QR	LEU4	cluster2_2	-9.0	C - NA CA - NA CB - Phe216 CD_1 - Tyr115, Pro181 CD_2 - NA CG - NA N - Phe216 O - NA	NA	NA	NA

Table X2.17: Binding interaction of pancreatic lipase inhibitory peptides-HLPGRG

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
Medium chain peptide H**L**PGRG	LEU2	cluster5_3	-7.5	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - Phe216 N - Phe216 O - NA	NA	NA	NA
HL**P**GRG	PRO3			C - NA CA - NA CB - NA CD - Tyr115 CG - Tyr115 N- NA O - NA	NA	NA	NA

Table X2.18: Binding interaction of pancreatic lipase inhibitory peptides-FLWPEYGAL

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
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
FLW**P**EYGAL	PRO4			C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
FLWPEYGA**L**	LEU9			C - NA CA - NA CB - NA CD_1 - NA CD_2 - Leu25 CG - NA N - NA O - Pro24	NA	NA	NA

Table X2.19: Binding interaction of pancreatic lipase inhibitory peptides-PAGNFLP

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
Medium chain peptide **P**AGNFLP	PRO1	cluster1_3	-8.8	C - NA CA - Phe78 CB - Phe78 CD - Phe78, Asp80 CG - Phe78, His152, Leu265 N- NA O - NA	NA	NA	NA
PAGNF**L**P	LEU6			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
PAGNFL**P**	PRO7			C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA

Table X2.20: Binding interaction of pancreatic lipase inhibitory peptides-FYLGYCDY

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
Medium chain peptide FY**L**GYCDY	LEU3	cluster1_3 (1)	-6.4	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.21: Binding interaction of pancreatic lipase inhibitory peptides-SPFWNINAH

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
Medium chain peptide S**P**FWNINAH	PRO2	cluster1_4	-8.8	C - NA CA - NA CB - Val260 CD - Leu214, Phe216 CG - Phe216, Val260 N- NA O - NA	NA	NA	NA

Table X2.22: Binding interaction of pancreatic lipase inhibitory peptides-AQMACPHL

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
Medium chain peptide AQMAC**P**HL	PRO6	cluster9_2	-8.9	C - Phe259 CA - Phe259 CB - Phe259 CD - NA CG - NA N- NA O - NA	NA	NA	NA
AQMACPH**L**	LEU8			C - Cys238 CA - NA CB - NA CD_1 - NA CD_2 - Gln254, Phe259 CG - NA N - NA O - NA	NA	NA	NA

Table X2.23: Binding interaction of pancreatic lipase inhibitory peptides-VAPAGHAVT

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
Medium chain peptide VA**P**AGHAVT	PRO3	cluster9_2	-8.9	C - NA CA - NA CB - NA CD - NA CG - Ala261, His264, Leu265 N- NA O - Phe216, Val260, Ala261	NA	NA	NA

Table X2.24: Binding interaction of pancreatic lipase inhibitory peptides-PHHCDAEAI

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
Medium chain peptide **P**HHCDAEAI	PRO1	cluster13_1	-8.9	C - Ile79 CA - Arg257 CB - Trp253 CD - Ile79, Lys81, Trp253 CG - Ile79, Trp253 N - Trp253 O - Ile79, Asp80	NA	NA	NA

Table X2.25: Binding interaction of pancreatic lipase inhibitory peptides-INEGSLLLPH

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
Medium chain peptide INEGS**L**LLPH	LEU6	cluster3_3	-9.8	C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - Trp253	NA	NA	NA
INEGSL**L**LPH	LEU7			C - Trp253 CA - Trp253 CB - Ile79, Arg112 CD_1 - Lys81, Glu84, Arg112 CD_2 - Ile79, Asp80, Glu84, Try253, Arg257 CG - Ile79, Asp80, Arg112 N - NA O - NA	NA	NA	NA
INEGSLL**L**PH	LEU8			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - Trp253 N - Trp253 O - Lys81, Trp253	NA	NA	O - Lys81

INEGSLLL**P**H	PRO9			C - Lys81 CA - Lys81 CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA

Table X2.26: Binding interaction of pancreatic lipase inhibitory peptides-HTVMILFK

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**
Medium chain peptide HTVMI**L**FK	LEU6	cluster1_1	-9.0	C - Arg112 CA - NA CB - Ile79 CD_1 - Arg257 CD_2 - Arg257 CG - NA N - Ile79 O - Arg112	NA	NA	O - Arg112

Table X2.27: Binding interaction of pancreatic lipase inhibitory peptides-APYVMILF

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
Medium chain peptide A**P**YVMILF	PRO2	cluster2_1	-8.3	C - NA CA - Val21 CB - Pro24 CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
APYVMI**L**F	LEU7			C - NA CA - NA CB - Phe216 CD_1 - NA CD_2 - NA CG - NA N - NA O - Phe78	NA	NA	NA

Table X2.28: Binding interaction of pancreatic lipase inhibitory peptides-AEWLHDWKL

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
Medium chain peptide AEW**L**HDWKL	LEU4	cluster1_1	-7.0	C - NA CA - NA CB - Ile79 CD_1 - Phe78, Ile79 CD_2 - NA CG - NA N - Ile79 O - NA	NA	NA	NA
AEWLHDWK**L**	LEU9			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.29: Binding interaction of pancreatic lipase inhibitory peptides-AVVSPLKPCC

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
Medium chain peptide AVVS**P**LKPCC	PRO5	cluster1_3	-8.1	C - Phe78 CA - NA CB - NA CD - Phe78, Ile79 CG - Phe78 N - Phe78 O - Phe78	NA	NA	NA
AVVSP**L**KPCC	LEU6			C - Phe216 CA - NA CB - Phe216 CD_1 – Val260 CD_2 - Phe216 CG - NA N - NA O - Phe216	NA	NA	NA
AVVSPLK**P**CC	PRO8			C - Ile210 CA - lle210, Phe216 CB - Ile219 CD_1 - NA CD_2 - NA CG - NA N - Phe216 O - Ile211	NA	NA	NA

Table X2.30: Binding interaction of pancreatic lipase inhibitory peptides-CFLPLPLLK

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
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
CFL**P**LPLLK	PRO4			C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
CFLP**L**PLLK	LEU5			C - NA CA - NA CB - Val260 CD_1 - Thr257, Arg257 CD_2 - NA CG - Thr256 N - Val260 O - NA	NA	NA	NA

CFLPL**P**LLK	PRO6			C - NA CA - Ile79 CB - NA CD - NA CG - NA N- NA O - Ile79	NA	NA	NA
CFLPLP**L**LK	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
CFLPLPL**L**K	LEU8			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.31: Binding interaction of pancreatic lipase inhibitory peptides-DNLMPQFM

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
Medium chain peptide DN**L**MPQFM	LEU3	cluster8_1	-9.5	C - Phe78 CA - Phe78 CB - NA CD_1 - Phe216, Val260 CD_2 - Phe78 CG - NA N - Phe78 O - Phe78	NA	NA	NA
DNLM**P**QFM	PRO5			C - NA CA - Ile210 CB - Ile210 CD - NA CG - NA N- NA O - Ile210, Ile211	NA	NA	NA

Table X2.32: Binding interaction of pancreatic lipase inhibitory peptides-FCLPLPLLK

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
Medium chain peptide FC**L**PLPLLK	LEU3	cluster2_3	-7.6	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - Phe78 O - Phe78, Ile79	NA	NA	NA
FCL**P**LPLLK	PRO4			C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
FCLP**L**PLLK	LEU5			C - NA CA - NA CB - Ile79 CD_1 - Val260 CD_2 - NA CG - NA N - NA O - Ile79	NA	NA	NA

FCLPL**P**LLK	PRO6			C - NA CA - NA CB - NA CD - NA CG - NA N- NA O - NA	NA	NA	NA
FCLPLP**L**LK	LEU7			C - Lys81, Arg112 CA - NA CB - Arg112 CD_1 - Ile79, Arg257 CD_2 - Trp253 CG - Ile79 N - NA O - Lys81, Arg112	NA	NA	NA
FCLPLPL**L**K	LEU8			C - Lys81 CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - Trp253 O - Lys81, Trp253	NA	NA	O - Lys81

Table X2.33: Binding interaction of pancreatic lipase inhibitory peptides-FMFFGPQ

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
Medium chain peptide FMFFG**P**Q	PRO6	cluster1_4	-7.7	C - NA CA - Val21 CB - Val21, Gln22 CD - Cys182 CG - Gln22 N- NA O - NA	NA	NA	NA

Table X2.34: Binding interaction of pancreatic lipase inhibitory peptides-GMAGGPPLL

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
Medium chain peptide GMAGG**P**PLL	PRO6	cluster8_1	-7.5	C - NA CA - NA CB - Phe216 CD - NA CG - NA N- NA O - Phe78	NA	NA	NA
GMAGGP**P**LL	PRO7			C - NA CA - NA CB - Val260 CD - Phe216 CG - Phe216 N- NA O - Phe216, Val260	NA	NA	NA
GMAGGPP**L**L	LEU8			C - Phe78 CA - NA CB - Phe78 CD_1 -Ser153 CD_2 - Phe216, His264 CG - NA N - NA O - Ile79	NA	NA	NA

GMAGGPPL**L**	LEU9			C - Phe78, His264 CA - Phe78, Ile79 CB - NA CD_1 - Arg257, Val260 CD_2 - Ile79 CG - NA N - NA O - Leu265	NA	NA	NA

Table X2.35: Binding interaction of pancreatic lipase inhibitory peptides-KDLWDDFKGL

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
Medium chain peptide KD**L**WDDFKGL	LEU3	cluster2_1	-8.5	C - NA CA - Trp253 CB - NA CD_1 - NA CD_2 - Trp253 CG - NA N - Trp253 O - NA	NA	NA	NA
KDLWDDFKG**L**	LEU10			C - NA CA - NA CB - Pro181 CD_1 - Tyr115 CD_2 - NA CG - NA N - Pro181 O - Pro181, Ile210	NA	NA	NA

Table X2.36: Binding interaction of pancreatic lipase inhibitory peptides-LLPAPPLL

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
Medium chain peptide **L**LPAPPLL	LEU1	cluster11_3	-6.7	C - NA CA - NA CB - NA CD_1 - Gln181 CD_2 - Glu180, Gln181 CG - NA N - NA O - NA	NA	NA	NA
L**L**PAPPLL	LEU2			C - NA CA - NA CB - NA CD_1 - Ile211 CD_2 - NA CG - Ile211 N - Ile210 O - Pro181, Ile210	NA	NA	NA
LL**P**APPLL	PRO3			C - NA CA - Pro181 CB - Cys182 CD - NA CG - NA N- NA O - Tyr115	NA	NA	NA

LLPA**P**PLL	PRO5			C - NA CA - Tyr115 CB - Phe78, Tyr115 CD - NA CG - NA N - Tyr115 O - Pro181	NA	NA	NA
LLPAP**P**LL	PRO6			C - NA CA - Phe216 CB - Phe216 CD - Phe78 CG - Phe78 N- NA O - Val260	NA	NA	NA
LLPAPP**L**L	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
LLPAPPL**L**	LEU8			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.37: Binding interaction of pancreatic lipase inhibitory peptides-LTMPQWW

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
Medium chain peptide **L**TMPQWW	LEU1	cluster4_4	-6.9	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
LTM**P**QWW	PRO4			C - Phe216 CA - Phe216 CB - Leu214, Phe216 CD - Val260 CG - Val260 N- NA O - Leu214, Phe216	NA	NA	NA

Table X2.38: Binding interaction of pancreatic lipase inhibitory peptides-MMHDFLTLCM

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
Medium chain peptide MMHDF**L**TLCM	LEU6	cluster1_1	-8.3	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
MMHDFLT**L**CM	LEU8			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Trp253	NA	NA	NA

Table X2.39: Binding interaction of pancreatic lipase inhibitory peptides-WGLWDDMQGL

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
Medium chain peptide WG**L**WDDMQGL	LEU3	cluster1_2	-7.6	C - NA CA - Ile79 CB - Ile79 CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
WGLWDDMQG**L**	LEU10			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X2.40: Binding interaction of pancreatic lipase inhibitory peptides-WNWGWLLWQL

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
Medium chain peptide WNWGW**L**LWQL	LEU6	cluster8_1	-8.6	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Val260	NA	NA	NA
WNWGWL**L**WQL	LEU7			C - NA CA - NA CB - NA CD_1 -NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
WNWGWLLWQ**L**	LEU10			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - Ile252 N - Ile252 O - NA	NA	NA	NA

Table X2.41: Binding interaction of pancreatic lipase inhibitory peptides-YWYPPK

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
Medium chain peptide YWY**P**PK	PRO4	cluster2_3	-7.4	C - NA CA - NA CB - Phe216 CD - Tyr115 CG - Tyr115 N- NA O - NA	NA	NA	NA
YWYP**P**K	PRO5			C - NA CA - NA CB - NA CD - Phe216 CG - Phe216 N- NA O - Phe216	NA	NA	NA

Table X2.42: Binding interaction of pancreatic lipase inhibitory peptides-YWYPPQ

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
Medium chain peptide YWY**P**PQ	PRO4	cluster1_3	-8.1	C - Phe216 CA - Tyr115 CB - Phe78, Tyr115 CD - NA CG - NA N- NA O - Phe216	NA	NA	NA
YWYP**P**Q	PRO5			C - NA CA - Phe216 CB - Phe216, His264 CD - Tyr115 CG - Phe78, Ser153 N - Phe216 O - Phe78	NA	NA	NA

Table X2.43: Binding interaction of pancreatic lipase inhibitory peptides-TLMPQWW

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
Medium chain peptide T**L**MPQWW	LEU2	cluster1_1	-7.9	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - Val260 O - NA	NA	NA	NA
TLM**P**QWW	PRO5			C - NA CA - Phe216 CB - NA CD - Phe216 CG - Leu214, Phe216 N - Phe216, Val260 O - NA	NA	NA	NA

Table X2.44: Binding interaction of pancreatic lipase inhibitory peptides-MPSKPPLL

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
Medium chain peptide M**P**SKPPLL	PRO2	cluster2_1	-8.8	C - NA CA - Ile79 CB - Ile79 CD - Val260 CG - Val260 N - NA O - NA	NA	NA	NA
MPSK**P**PLL	PRO5			C - NA CA - NA CB - NA CD - Tyr115 CG - NA N - NA O - Tyr115, Pro181	NA	NA	NA
MPSKP**P**LL	PRO6			C - NA CA - Ile210 CB - Ile210, Ile211 CD - NA CG - Ile211 N - NA O - NA	NA	NA	NA

MPSKPPLL	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - Thr116 CG - NA N - Pro181 O - Pro181, Cys182	NA	NA	O - Cys182
MPSKPPLL	LEU8			C - Val21, Gln22 CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - Glu180, Pro181	NA	NA	NA

Table X2.45: Binding interaction of pancreatic lipase inhibitory peptides-AVVSPLKPCC

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
Medium chain peptide AVVS**P**LKPCC	PRO5	cluster1_3	-8.1	C - Phe78 CA - NA CB - NA CD - Phe78 CG - Phe78 N - Phe78 O - Phe78	NA	NA	NA
AVVSP**L**KPCC	LEU6			C - Phe216 CA - NA CB - Phe216 CD_1 - Val260 CD_2 - Phe78 CG - NA N - NA O - Phe216	NA	NA	NA
AVVSPLK**P**CC	PRO8			C - Ile210 CA - Ile210, Phe216 CB - Ile210 CD - NA CG - NA N - Phe216 O - Ile2110	NA	NA	NA

Table X2.46: Binding interaction of pancreatic lipase inhibitory peptides-LKCCHSCPA

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
Medium chain peptide **L**KCCHSCPA	LEU1	cluster1_2	-8.2	C - NA CA - Phe78 CB - NA CD_1 - NA CD_2 - Tyr115 CG - Tyr115 N - Phe216 O - NA	NA	NA	NA
LKCCHSC**P**A	PRO8			C - NA CA - NA CB - NA CD - Trp253 CG - Trp253 N - NA O - NA	NA	NA	NA

Table X2.47: Binding interaction of pancreatic lipase inhibitory peptides-NPVWKRK

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
Medium chain peptide N**P**VWKRK	PRO2	cluster3_4	-7.0	C - NA CA - NA CB - NA CD - Gly114 CG - Gly114 N - NA O - Phe78, Gly114	NA	NA	NA

Table X2.48: Binding interaction of pancreatic lipase inhibitory peptides-CANPHELPN

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
Medium chain peptide CAN**P**HELPN	PRO4	cluster1_2	-10.0	C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
CANPHE**L**PN	LEU7			C - NA CA - NA CB - Ile79 CD_1 - Phe78 CD_2 - NA CG - NA N - Phe78 O - Ile79	NA	NA	NA
CANPHEL**P**N	PRO8			C - NA CA - NA CB - NA CD - Val260 CG - Val260 N - NA O - Val260	NA	NA	NA

Table X2.49: Binding interaction of pancreatic lipase inhibitory peptides-NPVWKR

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
Medium chain peptide N**P**VWKR	PRO2	cluster1_3	-8.2	C - NA CA - NA CB - NA CD - NA CG - Gly114, Tyr115, Thr116 N - NA O - Gly114, Tyr115	NA	NA	O - Tyr115

Table X2.50: Binding interaction of pancreatic lipase inhibitory peptides-YGNPVGGVGH

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
Long chain peptide YGN**P**VGGVGH	PRO4	cluster1_3	-9.0	C - NA CA - NA CB - NA CD - Phe216 CG - Phe216 N - NA O - NA	NA	NA	NA

Long Chain Peptide (Focus in ALA, GLY, LEU, PRO)

Table X3.1: Binding interaction of pancreatic lipase inhibitory peptides-EQGFLPGPEESGR

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
Long chain peptide EQ**G**FLPGPEE SGR	GLY3	cluster1_2	-8.9	C - NA CA - NA N - NA O - NA	NA	NA	NA
EQGF**L**PGPEE SGR	LEU5			C - Phe78 CA - NA CB - Phe78 CD_1 - Tyr115 CD_2 - Phe216 CG - Tyr115 N - NA O - Phe78	NA	NA	NA
EQGFL**P**GPEE SGR	PRO6			C - NA CA - NA CB - NA CD - Phe216 CG - NA N - NA O - NA	NA	NA	NA

EQGFLPG**P**EE SGR	PRO8			C - NA CA - NA CB - Ile79 CD - Ile79, Phe78 CG - Ile79 N - Ile79 O - NA			
EQGFLPGPEE S**G**R	GLY12			C - Trp253 CA - Thr256 N - NA O - Trp253			

Table X3.2: Binding interaction of pancreatic lipase inhibitory peptides- GNPVGGVGHGTTGT

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
Long chain peptide **G**NPVGGVGHG TTGT	GLY1	cluster5_1	-8.9	C - NA CA - NA N - NA O - NA	NA	NA	NA
GN**P**VGGVGHG TTGT	PRO3			C - NA CA - NA CB - NA CD - Phe216 CG - NA N - NA O - NA	NA	NA	NA
GNPV**G**GVGHG TTGT	GLY5			C - NA CA - NA N - NA O - NA	NA	NA	NA
GNPVG**G**VGHG TTGT	GLY6			C - NA CA - NA N - NA O - NA	NA	NA	NA

GNPVGGV**G**HG TTGT	GLY8			C - NA CA - Phe216 N - NA O - Phe216	NA	NA	NA
GNPVGGVGH**G** TTGT	GLY10			C - NA CA - NA N - NA O - Arg257	NA	NA	NA
GNPVGGVGHG TT**G**T	GLY13			C - NA CA - Arg112 N - NA O - NA	NA	NA	NA

Table X3.3: Binding interaction of pancreatic lipase inhibitory peptides-GEHGGAGMGGGQFQPV

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
Long chain peptide **G**EHGGAGMGG GQFQPV	GLY1	cluster1_2	-9.1	C - Val260 CA - Val260 N - Ile79 O - Val260	NA	NA	NA
GEH**G**GAGMGG GQFQPV	GLY4			C - NA CA - NA N - NA O - Phe259	NA	NA	NA
GEHGG**A**GMGG GQFQPV	ALA6			C - NA CA - Val260 CB - Val260 N - Val260 O - NA	NA	NA	NA
GEHG**G**AGMGG GQFQPV	GLY5			C - NA CA - NA N - NA O - NA	NA	NA	NA
GEHGGA**G**MGG GQFQPV	GLY7			C - NA CA - NA N - NA O - NA	NA	NA	NA

GEHGGAGM**G**G GQFQPV	GLY9			C - NA CA - NA N - NA O - NA	NA	NA	NA
GEHGGAGMG**G** GQFQPV	GLY10			C - NA CA - NA N - NA O - NA	NA	NA	NA
GEHGGAGMGG **G**QFQPV	GLY11			C - NA CA - NA N - NA O - NA	NA	NA	NA
GEHGGAGMGG GQFQ**P**V	PRO15			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.4: Binding interaction of pancreatic lipase inhibitory peptides-GQLGEHGGAGMG

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
Long chain peptide **G**QLGEHGGAG MG	GLY1	cluster1_1	-8.5	C - Phe78 CA - Tyr115 N - Phe78, Tyr115 O - Phe78	NA	NA	NA
GQ**L**GEHGGAG MG	LEU3			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
GQL**G**EHGGAG MG	GLY4			C - NA CA - NA N - NA O - NA	NA	NA	NA
GQLGEH**G**GAG MG	GLY7			C - NA CA - NA N - NA O - NA	NA	NA	NA

GQLGEHG**G**AG MG	GLY8			C - NA CA - NA N - NA O - NA	NA	NA	NA
GQLGEHGG**A**G MG	ALA9			C - NA CA - NA CB -Val260 N - NA O - NA	NA	NA	NA
GQLGEHGGA**G** MG	GLY10			C - NA CA - NA N - Val260 O - NA	NA	NA	NA
GQLGEHGGAG M**G**	GLY12			C - NA CA - NA N - NA O - NA	NA	NA	NA

Table X3.5: Binding interaction of pancreatic lipase inhibitory peptides-MLPLMLPFTMGY

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
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 - NA O - NA	NA	NA	NA
ML**P**LMLPFTM GY	PRO3			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
MLP**L**MLPFTM GY	LEU4			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

MLPLM**L**PFTM GY	LEU6			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
MLPLML**P**FTM GY	PRO7			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
MLPLMLPFTM **G**Y	GLY11			C - Tyr115 CA - Tyr115 N - NA O - Tyr115	NA	NA	NA

Table X3.6: Binding interaction of pancreatic lipase inhibitory peptides-FFRSKLLSRGAAAAKGALLPQYW

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
Long chain peptide FFRSK**L**LSRG AAAAKGALLP QYW	LEU6	cluster1_3	-9.2	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
FFRSKL**L**SRG AAAAKGALLP QYW	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - Ile211 CG - NA N - NA O - NA	NA	NA	NA
FFRSKLLSR**G** AAAAKGALLP QYW	GLY10			C - NA CA - NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG **A**AAAKGALLP QYW	ALA11			C - NA CA - Leu214 CB - Leu214 N - NA O - Leu214	NA	NA	NA

FFRSKLLSRG A**A**AAKGALLP QYW	ALA12			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AA**A**AKGALLP QYW	ALA13			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AAA**A**KGALLP QYW	ALA14			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AAAAK**G**ALLP QYW	GLY16			C - NA CA - NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AAAAKG**A**LLP QYW	ALA17			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA

FFRSKLLSRG AAAAKGA**L**LP QYW	LEU18			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AAAAKGAL**L**P QYW	LEU19			C - NA CA - NA CB - Val260 CD_1 - NA CD_2 - Val260 CG - NA N - NA O - NA	NA	NA	NA
FFRSKLLSRG AAAAKGALL**P** QYW	PRO20			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.7: Binding interaction of pancreatic lipase inhibitory peptides-RCMAFLLSDGAAAAQQLLPQYW

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
Long chain peptide RCM**A**FLLSDG AAAAQQLLPQ YW	ALA4	cluster3_3	-9.4	C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
RCMAF**L**LSDG AAAAQQLLPQ YW	LEU6			C - NA CA - Tyr115 CB - Tyr115 CD_1 - Tyr115, Thr116 CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
RCMAFL**L**SDG AAAAQQLLPQ YW	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O – NA	NA	NA	NA

RCMAFLLSD**G** AAAAQQLLPQ YW	GLY10			C - NA CA - Gly114 N - NA O - NA	NA	NA	NA
RCMAFLLSDG **A**AAAQQLLPQ YW	ALA11			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
RCMAFLLSDG A**A**AAQQLLPQ YW	ALA12			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
RCMAFLLSDG AA**A**AQQLLPQ YW	ALA13			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
RCMAFLLSDG AAA**A**QQLLPQ YW	ALA14			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA

RCMAFLLSDG AAAAQQ**L**LPQ YW	LEU17			C - NA CA - NA CB - Leu25 CD_1 - Leu25 CD_2 - Thr116 CG - NA N - NA O - NA	NA	NA	NA
RCMAFLLSDG AAAAQQL**L**PQ YW	LEU18			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
RCMAFLLSDG AAAAQQLL**P**Q YW	PRO19			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.8: Binding interaction of pancreatic lipase inhibitory peptides- RPAQPNYPWTAVLVFRH

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
Long chain peptide R**P**AQPNYPWT AVLVFRH	PRO2	cluster3_1	-9.3	C - NA CA - Ile79 CB - Ile79 CD - Phe78 CG - Ile79, Phe78 N - NA O - NA	NA	NA	NA
RP**A**QPNYPWT AVLVFRH	ALA3			C - Val260 CA - Val260 CB -Thr256, Arg257 N - NA O - Val260	NA	NA	NA
RPAQ**P**NYPWT AVLVFRH	PRO5			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA

RPAQPNY**P**WT AVLVFRH	PRO8			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
RPAQPNYPWT **A**VLVFRH	ALA11			C - NA CA - NA CB -NA N - NA O - NA	NA	NA	NA
RPAQPNYPWT AV**L**VFRH	LEU13			C - NA CA - NA CB - NA CD_1 - Pro181, Ile219 CD_2 - Pro181, Cys182 CG - Pro181 N - NA O - NA	NA	NA	NA

Table X3.9: Binding interaction of pancreatic lipase inhibitory peptides-LAAVEALSTNG

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
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
L**A**AVEALSTN G	ALA2			C - Phe216 CA - Phe78 CB - Phe78 N - NA O - Phe216	NA	NA	NA
LA**A**VEALSTN G	ALA3			C - NA CA - Phe216 CB - Phe216 N - Phe216 O - NA	NA	NA	NA
LAAVE**A**LSTN G	ALA6			C - NA CA - Pro181 CB - Pro181, Phe216 N - NA O - NA	NA	NA	NA

LAAVEA**L**STN G	LEU7			C - NA CA - NA CB - NA CD_1 - NA CD_2 - Ile210, Ile211 CG - NA N - NA O - NA	NA	NA	NA
LAAVEALSTN **G**	GLY11			C - NA CA - NA N - NA O - NA	NA	NA	NA

Table X3.10: Binding interaction of pancreatic lipase inhibitory peptides-EITPEKNPQLR

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
Long chain peptide EIT**<u>P</u>**EKNPQL R	PRO4	cluster1_3	-10.3	C - NA CA - NA CB - Ile210, Phe216 CD - Phe216 CG - Phe216 N - NA O - Ile210	NA	NA	NA
EITPEKN**<u>P</u>**QL R	PRO8			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
EITPEKNPQ**<u>L</u>** R	LEU10			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.11: Binding interaction of pancreatic lipase inhibitory peptides-FVVAEQAGNEEGFE

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
Long chain peptide FVV**A**EQAGNE EGFE	ALA4	cluster3_1	-10.0	C - NA CA - NA CB -NA N - NA O - Ile210, Phe216	NA	NA	NA
FVVAEQ**A**GNE EGFE	ALA7			C - Ile79 CA - NA CB - Ile79 N - Ile79 O - Ile79	NA	NA	NA
FVVAEQA**G**NE EGFE	GLY8			C - Ile79 CA - Ile79 N - Ile79 O - Ile79	NA	NA	NA
FVVAEQAGNE E**G**FE	GLY12			C - NA CA - NA N - NA O - NA	NA	NA	NA

Table X3.12: Binding interaction of pancreatic lipase inhibitory peptides- SGGGGGGVAGAATASR

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
Long chain peptide S**G**GGGGGVAG AATASR	GLY2	cluster3_1	-7.4	C - NA CA - NA N - Tyr115 O - NA	NA	NA	NA
SG**G**GGGGVAG AATASR	GLY3			C - NA CA - NA N - NA O - NA	NA	NA	NA
SGG**G**GGGVAG AATASR	GLY4			C - NA CA - NA N - NA O - Ile211	NA	NA	NA
SGGG**G**GGVAG AATASR	GLY5			C - NA CA - NA N - NA O - Pro181	NA	NA	NA
SGGGG**G**GVAG AATASR	GLY6			C - Tyr115 CA - Pro181 N - NA O - Tyr115	NA	NA	NA

SGGGGG**G**VAG AATASR	GLY7			C - NA CA - NA N - NA O - Phe78	NA	NA	NA
SGGGGGGV**A**G AATASR	ALA9			C - Val260 CA - Val260 CB - Phe216 N - Phe216 O - Val260	NA	NA	NA
SGGGGGGVA**G** AATASR	GLY10			C - Ile79 CA - Phe78, Ile79 N - Phe78 O - Ile79	NA	NA	NA
SGGGGGGVAG **A**ATASR	ALA11			C - NA CA - NA CB - NA N - NA O - NA	NA	NA	NA
SGGGGGGVAG A**A**TASR	ALA12			C - NA CA - NA CB - Val260 N - NA O - Val260	NA	NA	NA
SGGGGGGVAG AAT**A**SR	ALA14			C - NA CA - Ile79 CB - Ile79 N - Ile79 O - NA	NA	NA	NA

Table X3.13: Binding interaction of pancreatic lipase inhibitory peptides-GSGGGGGGGGGPRR

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
Long chain peptide **G**SGGGGGGGG GPRR	GLY1	cluster4_1	-9.2	C - NA CA - NA N - NA O - NA	NA	NA	NA
GS**G**GGGGGGG GPRR	GLY3			C - NA CA - NA N - NA O - NA	NA	NA	NA
GSG**G**GGGGGG GPRR	GLY4			C - NA CA - NA N - NA O - NA	NA	NA	NA
GSGG**G**GGGGG GPRR	GLY5			C - NA CA - NA N - NA O - NA	NA	NA	NA
GSGGG**G**GGGG GPRR	GLY6			C - Val21 CA - Val21 N - NA O - NA	NA	NA	NA

GSGGGG**G**GGG GPRR	GLY7			C - Val21 CA - Val21 N - Val21 O - Pro24	NA	NA	N - Val21
GSGGGGG**G**GG GPRR	GLY8			C - Cys182 CA - Gln22 N - Gln22 O - Pro181, Cys182	NA	NA	O - Cys182
GSGGGGGG**G**G GPRR	GLY9			C - Pro181 CA - NA N - NA O - NA	NA	NA	NA
GSGGGGGGG**G** GPRR	GLY10			C - Pro181 CA -Tyr115, Pro181 N - Pro181 O - Pro181, Ile210	NA	NA	NA
GSGGGGGGGG **G**PRR	GLY11			C - NA CA - Phe216 N - Tyr115 O - Tyr115	NA	NA	NA
GSGGGGGGGG G**P**RR	PRO12			C - NA CA - Phe78 CB - NA CD - Phe216 CG - NA N - Phe216 O - Phe216	NA	NA	NA

Table X3.14: Binding interaction of pancreatic lipase inhibitory peptides-GGYQGGGYGGNSGGGYGNRG

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
Long chain peptide **G**GYQGGGYGG NSGGGYGNRG	GLY1	cluster1_1	-9.0	C - NA CA - NA N - NA O - NA	NA	NA	NA
G**G**YQGGGYGG NSGGGYGNRG	GLY2			C - NA CA - NA N - NA O - NA	NA	NA	NA
GGYQ**G**GGYGG NSGGGYGNRG	GLY5			C - NA CA - NA N - NA O - NA	NA	NA	NA
GGYQG**G**GYGG NSGGGYGNRG	GLY6			C - NA CA - NA N - NA O - NA	NA	NA	NA
GGYQGG**G**YGG NSGGGYGNRG	GLY7			C - NA CA - NA N - NA O - NA	NA	NA	NA

GGYQGGGY**G**G NSGGGYGNRG	GLY9			C - NA CA - NA N - NA O - Trp253	NA	NA	NA
GGYQGGGYG**G** NSGGGYGNRG	GLY10			C - Trp253 CA - Trp253 N - NA O - NA	NA	NA	NA
GGYQGGGYGG NS**G**GGYGNRG	GLY13			C - Ile79 CA - NA N - Ile79 O - Ile79	NA	NA	NA
GGYQGGGYGG NSG**G**GYGNRG	GLY14			C - Phe78 CA - Phe78 N - NA O - NA	NA	NA	NA
GGYQGGGYGG NSGG**G**YGNRG	GLY15			C - NA CA - NA N - Tyr115 O - Tyr115	NA	NA	NA
GGYQGGGYGG NSGGGY**G**NRG	GLY17			C - NA CA - NA N - NA O - NA	NA	NA	NA
GGYQGGGYGG NSGGGYGNR**G**	GLY20			C - NA CA - NA N - NA O - NA	NA	NA	NA

Table X3.15: Binding interaction of pancreatic lipase inhibitory peptides-GGSGGGGGSSSGRRP

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
Long chain peptide **G**GSGGGGGSS SGRRP	GLY1	cluster1_1	-8.7	C - Trp253 CA - Trp253, Ile252 N - Trp253, Ile252 O - Trp253	NA	NA	NA
G**G**SGGGGGSS SGRRP	GLY2			C - NA CA - Trp253 N - Trp253 O - Thr256	NA	NA	NA
GGS**G**GGGGSS SGRRP	GLY4			C - Ile79 CA - NA N - NA O - Val260	NA	NA	NA
GGSG**G**GGGSS SGRRP	GLY5			C - Ile79 CA - NA N - Ile79 O - Ile79	NA	NA	NA
GGSGG**G**GGSS SGRRP	GLY6			C - Phe78 CA - Phe78 N - Phe78 O - Phe78, Phe216	NA	NA	NA

GGSGGG**G**GSS SGRRP	GLY7			C - Tyr115 CA - Tyr115, Phe216 N - Phe78 O - Tyr115	NA	NA	NA
GGSGGGG**G**SS SGRRP	GLY8			C - Pro181 CA - Pro181 N - Pro181 O - Pro181, Ile210	NA	NA	NA
GGSGGGGGSS S**G**RRP	GLY12			C - Val21 CA - Val21 N - Val21 O - Val21	NA	NA	NA
GGSGGGGGSS SGRR**P**	PRO15			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.16: Binding interaction of pancreatic lipase inhibitory peptides-GDTVTVEFDTFLSR

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
Long chain peptide GDTVTVEFDT FLSR	GLY1	cluster2_3	-10.1	C - NA CA - NA N - NA O - NA	NA	NA	NA
GDTVTVEFDT F**L**SR	LEU12			C - NA CA - NA CB - NA CD_1 - Val260 CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.17: Binding interaction of pancreatic lipase inhibitory peptides-ALWGAGGGGLGLSSGR

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
Long chain peptide **A**LWGAGGGGL GLSSGR	ALA1	cluster1_2	-8.0	C - Val21 CA - Val21 CB - Gln2 N - Val21 O - Gln22	NA	NA	N - Val21
A**L**WGAGGGGL GLSSGR	LEU2			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
ALW**G**AGGGGL GLSSGR	GLY4			C - NA CA - NA N - NA O - Pro181	NA	NA	NA
ALWG**A**GGGGL GLSSGR	ALA5			C - NA CA - NA CB - Try115, Phe216 N - Try115 O - Phe78, Try115	NA	NA	NA

ALWGA**G**GGGL GLSSGR	GLY6			C - Phe78 CA - Phe78 N - NA O - NA	NA	NA	NA
ALWGAG**G**GGL GLSSGR	GLY7			C - Ile79 CA - NA N - Phe78 O - Ile79	NA	NA	NA
ALWGAGG**G**GL GLSSGR	GLY8			C - NA CA - NA N - NA O - Val260	NA	NA	NA
ALWGAGGG**G**L GLSSGR	GLY9			C - Trp253 CA - Trp253 N - NA O - Trp253	NA	NA	NA
ALWGAGGGG**L** GLSSGR	LEU10			C - NA CA - Trp253, Thr256 CB - NA CD_1 - NA CD_2 - NA CG - NA N - Trp253, Thr256 O - Ile252, Trp253, Thr256	NA	NA	N - Thr256 O - Thr256

ALWGAGGGGL **G**LSSGR	GLY11			C - NA CA - Trp253 N - Trp253 O - NA	NA	NA	NA
ALWGAGGGGL G**L**SSGR	LEU12			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - Ile252 O - Ile252	NA	NA	NA
ALWGAGGGGL GLSS**G**R	GLY15			C - NA CA - NA N - NA O - NA	NA	NA	NA

Table X3.18: Binding interaction of pancreatic lipase inhibitory peptides-HCPVPDPVRGL

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
Long chain peptide HC**P**VPDPVRG L	PRO3	cluster5_2	-9.0	C - Pro209 CA - Pro209 CB - Glu180, Gln184, Pro209, Ser219 CD - NA CG - Gln184, Ser219 N - NA O - NA	NA	NA	NA
HCPV**P**DPVRG L	PRO5			C - Pro181, Cys182 CA - Glu180 CB - Gln184 CD - NA CG - Gln22, Gln184 N - NA O - Pro181, Cys182	NA	NA	O - Cys182
HCPVPD**P**VRG L	PRO7			C - NA CA - Pro181 CB - NA CD - NA CG - NA N - Pro181 O - Tyr115	NA	NA	NA

HCPVPDPVR**G** L	GLY10			C - NA CA - NA N - NA O - NA	NA	NA	NA
HCPVPDPVRG **L**	LEU11			C - NA CA - NA CB - NA CD_1 - Ile79 CD_2 - Val260 CG - NA N - NA O - NA	NA	NA	NA

Table X3.18: Binding interaction of pancreatic lipase inhibitory peptides-MSKFLPLPLMFY

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
Long chain peptide MSKF**L**PLPLM FY	LEU5	cluster1_4	-7.4	C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA
MSKFL**P**LPLM FY	PRO6			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
MSKFLP**L**PLM FY	LEU7			C - NA CA - NA CB - Ile211 CD_1 - Ile211 CD_2 - Pro212 CG - NA N - NA O - NA	NA	NA	NA

MSKFLPL**P**LM FY	PRO8			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
MSKFLPLP**L**M FY	LEU9			C - NA CA - NA CB - NA CD_1 - NA CD_2 - NA CG - NA N - NA O - NA	NA	NA	NA

Table X3.19: Binding interaction of pancreatic lipase inhibitory peptides-LNNPSVCDCDCMMKAAR

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
Long chain peptide **L**NNPSVCDCD CMMKAAR	LEU1	cluster3_4	-9.8	C - NA CA - Phe78, Phe216 CB - Phe78 CD_1 - Phe78 CD_2 - Phe216 CG - Phe78 N - Phe216 O - NA	NA	NA	NA
LNN**P**SVCDCD CMMKAAR	PRO4			C - NA CA - NA CB - NA CD - NA CG - NA N - NA O - NA	NA	NA	NA
LNNPSVCDCD CMMK**A**AR	ALA15			C - Thr256 CA - Thr256 CB - Thr256 N - NA O - Thr256, Arg257	NA	NA	O - Thr256

LNNPSVCDCD CMMKA**A**R	ALA16			C - NA CA - Arg257 CB - Val260 N - NA O - Ile79	NA	NA	NA

Table X3.20: Binding interaction of pancreatic lipase inhibitory peptides-NALKCCHSCPA

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
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
NA**L**KCCHSCP A	LEU3			C - Phe216 CA - Val260 CB - Val260 CD_1 - NA CD_2 - Phe78, Ile79 CG - NA N - Val260 O - Phe216	NA	NA	NA
NALKCCHSCP A	PRO10			C - Thr116 CA - Thr116 CB - Thr116 CD - NA CG - NA N - NA O - NA	NA	NA	NA
NALKCCHSCP **A**	ALA11			C - Thr116 CA - NA CB - NA N - NA O - Gly114, Thr116	NA	NA	O - Thr116