Supplementary material 1

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

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			Selected from PRODIGY	(Kcai mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N1	Short chain peptide <u>M</u> 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 num	ber of bonds			34	0	0	1	
	Total no of interactive residues				6	0	0	1	
	Overall perce	ntage of bond	ling		18%	0%	0%	100%	



Figure S1a: Binding interaction of <u>M</u>MML 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction			
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Short chain peptide <u>M</u> 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 num	ber of bonds	•		27	0	0	0
	Total no of interactive residues				10	0	0	0
	Overall perce	ntage of bond	ling		37%	0%	0%	0%

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



Figure S1b: Binding interaction of <u>M</u>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) representing the amino acid that present in the inhibitory peptides.

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

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



Figure S1c: Binding interaction of <u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic	lipase involve in p position	Covolont	teraction and its
terminal			from PRODIGY		interaction	Bridge	bond	bond
N1	Short chain peptide	LEU1	cluster1_1	-7.4	C - NA CA - NA	NA	NA	NA
	<u>L</u> RFPL				CB - NA CD ₁ - NA CD ₂ - NA CG - NA N - Leu214, Phe261 O - NA			
	Total num	ber of bond	s		24	0	0	2
	Total no of interactive residues				2	0	0	0
	Overall perce	ntage of bon	ding		8%	0%	0%	0%

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



Figure S1d: Binding interaction of <u>LRFPL</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre	eatic lipase involv Salt Bridge	e in protein peptide Covalent bond	e interaction Hydrogen bond
			PRODIGY		micraction	Druge	Jonu	Jona
N1	Short chain peptide	ASN1	cluster8_1	-7.7	C - Trp253	NA	NA	NA
	<u>N</u> VQR				CB - NA CB - NA CG - NA N- Trp253 ND ₂ - NA O - NA OD ₁ - NA			
	Total num	ber of bonds			23	1	0	4
	Total no of interactive residues				2	0	0	0
	Overall perce	ntage of bond	ling		9%	0%	0%	0%

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



Figure S1e: Binding interaction of <u>N</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pance	reatic lipase involv	e in protein peptide	e interaction
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide	PHE1	cluster2_1	-7.1	C - Phe216 CA - Phe216	NA	NA	NA
	<u>F</u> DPFPK				$\begin{array}{l} CB &- Val260\\ CD_1 &- Val260\\ CD_2 &- Leu214\\ CE_1 &- NA\\ CE_2 &- Leu214\\ CG &- Val260\\ CZ &- NA\\ N &- Val260\\ O &- Phe216 \end{array}$			
	Total num	ber of bonds			33	0	0	0
	Total no of interactive residues				9	0	0	0
	Overall percer	ntage of bond	ling		27%	0%	0%	0%

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



Figure S2a: Binding interaction of <u>FDPFPK</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancre	atic lipase involve	in protein peptide	e interaction
N-and C- terminal			from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide <u>F</u> YLGYCDY	PHE1	cluster1_3	-6.4	$ \begin{array}{c} 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 \\ \end{array} $	NA	NA	NA
	Total num	ber of bond	s	1	23	0	0	1
	Total no of interactive residues				11	0	0	0
	Overall perce	ntage of bon	ding		48%	0%	0%	0%

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



Figure S2b: Binding interaction of <u>FYLGYCDY</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Peptide length and sequence Target Amino HADDOCK Binding affinity Acids Cluster ΔG Selected (Kcal mol ⁻¹)		Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide	ASN1	cluster1_2	-7.1	C - NA CA - Thr116	NA	NA	OD_1 - Thr116
	<u>N</u> PVWKR				CB - NA CG - Thr116 N- NA ND ₂ - Gly114 O - NA OD ₁ - Gly114, Thr116			
	Total num	ber of bond	S		32	1	0	3
	Total no of interactive residues				5	0	0	1
	Overall perce		16%	0%	0%	33%		

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	lipase involve in position	protein peptide inf 1	eraction and its
N-and C- terminal			Selected (K from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide	ASN1	cluster3_4	-7.0	C - NA CA - NA	NA	NA	ND ₂ - Arg112
	<u>N</u> PVWKRK				CB - Arg112, Thr113 CG - Arg112, Thr113 N- NA ND ₂ - Arg112, Thr113 O - NA OD ₁ - NA			
	Total num	ber of bond	S		27	0	0	2
	Total no of interactive residues				6	0	0	1
	Overall perce	ntage of bon	ding		22%	0%	0%	50%

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	lipase involve in p position	protein peptide int I	eraction and its
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide	ALA1	cluster 3_4	-6.9	C - Phe78 CA - Phe78	NA	NA	NA
	<u>A</u> GDDAPR				CB - Phe78 N - NA O - Phe78, Tyr115			
	Total num	ber of bond	S		25	0	0	1
	Total no of int	5	0	0	0			
	Overall perce	ntage of bon	ding		20%	0%	0%	0%

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



Figure S2e: Binding interaction of <u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N and C	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Keal mal ⁻¹)	Residues of pancreation	lipase involve in p position	protein peptide int	eraction and its
terminal			from PRODIGY	(Kcai mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Medium chain peptide	PRO4	cluster1_3	-7.0	C - NA CA - NA	NA	NA	NA
	<u>A</u> PFPLR				CB - NA N - NA O - NA			
	Total num	ber of bond	S		16	0	0	0
	Total no of int		0	0	0	0		
	Overall percer	ntage of bon	ding		0%	0%	0%	0%

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



Figure S2f: Binding interaction of <u>APFPLR</u> 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) representing the amino acid that present in the inhibitory peptides.

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 Hydrophobic interaction	lipase involve in p position Salt Bridge	rotein peptide int Covalent bond	eraction and its Hydrogen bond
N1	Medium chain peptide <u>L</u> 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					0%	0%	0%

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



Figure S2g: Binding interaction of <u>LNLDLLR</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein pep position			eraction and its
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide	LEU1	cluster2_2	-8.0	C - NA CA - NA	NA	NA	NA
	LNFEPR				CB - NA CD ₁ - NA CD ₂ - NA CG - NA N - NA O - NA			
Total number of bonds				25	0	0	1	
	Total no of int	eractive res	idues		0	0	0	0
Overall percentage of bonding				0%	0%	0%	0%	

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



Figure S2h: Binding interaction of <u>LNFEPR</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre	Salt	in protein peptide Covalent	interaction Hydrogen bond
			PRODIGY		interaction	Druge	DOILG	Dona
N1	Long chain peptide	GLY1	cluster5_1	-8.9	C - NA CA - NA	NA	NA	NA
	GNPVGGVGHG				N - NA			
	TTGT				O - NA			
Total number of bonds				36	1	0	4	
	Total no of int	eractive resi	idues		0	0	0	0
	Overall perce	ntage of bon	ding		0%	0%	0%	0%

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N and C	Peptide length and sequence	Target Amino Acids	HADDOCK Binding 2.4 affinity Cluster ΔG Sciented (Keel model)		Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide	GLY1	cluster1_1	-8.5	C - Phe78 CA - Tvr115	NA	NA	NA
	<u>G</u> QLGEHGGAG MG	QLGEHGGAG MG			N - Phe78, Tyr115 O - Phe78			
Total number of bonds				24	0	0	0	
	Total no of interactive residues				5	0	0	0
	Overall percer	ntage of bon	ding		21%	0%	0%	0%

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



Figure S3b: Binding interaction of <u>GQLGEHGGAGMG</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N1	Long chain peptide <u>F</u> 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					0%	0%	0%	

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



Figure S3c: Binding interaction of <u>F</u>FRSKLLSRGAAAAKGALLPQYW 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity AG	Residues of pancreatic lipase involve in protein peptide interaction an position			
N-and C- terminal	sequence	Terus	Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide <u>F</u> 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 int	eractive res	idues		7	0	0	0
Overall percentage of bonding					16%	0%	0%	0%

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



Figure S3d: Binding interaction of \underline{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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHADDOAmino2.4AcidsCluste	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide	MET1	cluster2_1	-8.4	C - NA CA - NA	NA	NA	NA
	M LPLMLPFTM				CB - Phe259			
	GY				CE – Thr256			
					CG - Thr256			
					O - NA			
					N - NA			
					SD - Thr256			
Total number of bonds				41	0	0	1	
	Total no of int	teractive resi	idues		4	0	0	0
	Overall perce	ntage of bon	ding		10%	0%	0%	0%

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



Figure S3e: Binding interaction of <u>MLPLMLPFTMGY</u> 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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	protein peptide int 1	eraction and its	
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N1	Long chain peptide <u>M</u> 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					0	0	0
	Overall perce	ntage of bon	ding	7%	0%	0%	0%	

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



Figure S3f: Binding interaction of <u>M</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	itionPeptide lengthTargetHADDOCKBirminoandAmino2.4affid insequenceAcidsCluster4nd C-Selected(Kca				Residues of pancreatic lipase involve in protein peptide interaction and its positionHydrophobic interactionSaltCovalent bondHydrogen bond			
terminal			from PRODIGY	()	interaction	Salt Bridge	bond	bond
N1	Long chain peptide <u>L</u> 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 num	ber of bond	s		31	0	0	3
	Total no of int	0	0	0	0			
	Overall perce	ntage of bon	ding		0%	0%	0%	0%

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



Figure S3g: Binding interaction of <u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreation	e lipase involve in p position	ase involve in protein peptide interaction and its position		
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N1	Long chain peptide <u>L</u> 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					0	0	0	
	Overall perce	ntage of bon	ding		13%	0%	0%	0%	

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



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) representing the amino acid that present in the inhibitory peptides.

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 pancreatio Hydrophobic interaction	e lipase involve in p positior Salt Bridge	orotein peptide int Covalent bond	eraction and its Hydrogen bond
N1	Long chain peptide <u>N</u> 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 int		4	0	0	0		
	Overall perce	ntage of bon	ding		9%	0%	0%	0%

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



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) representing the amino acid that present in the inhibitory peptides

Position of amino acid in N-and C-	sitionPeptide lengthTargetHADDOCKBinuninoandAmino2.4affid insequenceAcidsClusterAnd CSelected(Kcal			Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction and its positionHydrophobic interactionSalt BridgeCovalent bondHydrogen bondC - NANANANAC - NANANANA			
terminal			from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N1	Long chain peptide	ALA1	cluster1_4	-7.6	C - NA CA - NA	NA	NA	NA
	<u>A</u> LWGAGGGGL GLSSGR				CB - NA N - NA O - NA			
Total number of bonds				45	0	0	2	
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bon	ding	0%	0%	0%	0%	

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kaal mal ⁻¹)	Residues of pancre	e interaction		
terminal			from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Short chain peptide	LEU4	cluster10_1	-7.3	C - Tyr115, Pro181 CA - Tyr115	NA	NA	NA
	MMM <u>L</u>				CB - Tyr115, Pro181 CD ₁ - Ser153, Ala179 Phe216, His264 CD ₂ - Tyr115, Ser153 Leu154, Phe216 CG - Phe216 N - Phe216 O - Pro181			
Total number of bonds				34	0	0	1	
	Total no of interactive residues				16	0	0	0
	Overall perce	ntage of bond	ling		47%	0%	0%	0%

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



Figure S4a: Binding interaction of MMM<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancre	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			Selected from PRODIGY	(Kcai moi ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Short chain peptide	LEU4	cluster4_3	-7.1	C - NA CA - NA	NA	NA	NA	
	FDM <u>L</u>				CB - Ile79				
					$CD_1 - NA$				
					$CD_2 - NA$				
					CG - NA				
					N - He/9				
					O - He /9				
Total number of bonds				•	21	0	0	0	
	Total no of interactive residues					0	0	0	
	Overall perce	ntage of bond	ling	14%	0%	0%	0%		

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



Figure S4b: Binding interaction of FDM<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancr	eatic lipase involv	e in protein peptide	e interaction
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Short chain peptide	PRO4	cluster8_1	-7.2	C - NA	NA	NA	NA
	RLL <u>P</u>				CA - NA CB - NA CD - Val260 CG - Thr256 N- NA O - Trp253			
Total number of bonds					21	0	0	1
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bond	ding	14%	0%	0%	0%	

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



Figure S4c: Binding interaction of RLL<u>P</u> 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) representing the amino acid that present in the inhibitory peptides.

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

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



Figure S5a: Binding interaction of LAPSTI<u>K</u> 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) representing the amino acid that present in the inhibitory peptides.

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 Hydrophobic interaction	lipase involve in p position Salt Bridge	protein peptide int n Covalent bond	eraction and its Hydrogen bond
C1	Medium chain peptide KVEGDL <u>K</u>	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			I	22	0	0	0	
	Total no of int	12	0	0	0			
	Overall percer	ntage of bon	ding	55%	0%	0%	0%	

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



Figure S5b: Binding interaction of KVEGDL<u>K</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kaal mal ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			Selected from PRODIGY	(K cai moi ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide ELPPHF <u>L</u>	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
	Overall percer	ntage of bond	ling	0%	0%	0%	0%	

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



Figure S5c: Binding interaction of ELPPHF<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY	(Ixear mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide FLWPEYGA <u>L</u>	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 int	eractive resid	dues	2	0	0	0	
	Overall percer	ntage of bond	ling		7%	0%	0%	0%

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



Figure S5d: Binding interaction of FLWPEYGA<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Peptide length andTarget AminoHADDOCK 2.4Bind affir affir SequenceSequenceAcidsCluster SelectedΔ(Kcal		Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre	atic lipase involv	e in protein peptide	e interaction
terminal			from PRODIGY		interaction	San Bridge	bond	bond
C1	Medium chain peptide AQMACPH <u>L</u>	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%

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



Figure S5e: Binding interaction of AQMACPH<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	PositionPeptide lengthTargetHADDof aminoandAmino2.acid insequenceAcidsClustorialN and CSetureSetureSeture			Binding affinity ΔG (Kaal mal ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide AEWLHDWK <u>L</u>	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%

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



Figure S5f: Binding interaction of AEWLHDWK<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	IPeptide length andTarget AminoHADDOCK 2.4Binding affinity0and sequenceAcidsCluster SelectedΔG			Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre	atic lipase involv	e in protein peptide	e interaction
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide GMAGGPPL <u>L</u>	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%

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



Figure S5g: Binding interaction of GMAGGPPL<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	ingth Target Amino nce Acids	TargetHADDOCKAmino2.4AcidsClusterSelected		Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
Cl	Medium chain peptide KDLWDDFKG <u>L</u>	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%

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



Figure S5h: Binding interaction of KDLWDDFKG<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	PositionPeptide length andTarget AminoHADDOCKf aminoandAmino2.4acid insequenceAcidsCluster				Residues of pancreatic lipase involve in protein peptide interaction			
N-and C- terminal			from PRODIGY	(Iscai III01 ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide LLPAPPL <u>L</u>	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%

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



Figure S5i: Binding interaction of LLPAPPL<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Peptide length andTarget Amino Acids	TargetHADDOCKBinAmino2.4affAcidsCluster4Selected(Keen		Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide WGLWDDMQG <u>L</u>	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%

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



Figure S5j: Binding interaction of WGLWDDMQG<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre Hydrophobic interaction	atic lipase involv Salt Bridge	e in protein peptide Covalent bond	e interaction Hydrogen bond
C1	Medium chain peptide WNWGWLLWQ <u>L</u>	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 Total no of interactive residues					41	0	0	0
	Overall perce	ntage of bond	ling	5%	0%	0%	0%	

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



Figure S5k: Binding interaction of WNWGWLLWQL 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length andTarget AminoHADDOCK 2.4Bin affr affr ClustersequenceAcidsCluster SelectedΔ		Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction				
terminal			from PRODIGY	(Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Medium chain peptide MPSKPPL <u>L</u>	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					0	0	0
	Overall perce	ntage of bond	ling		12%	0%	0%	0%

 Table S51: Binding interaction of pancreatic lipase inhibitory peptides-MPSKPPLL at C1 position.



Figure S51: Binding interaction of MPSKPPL<u>L</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length andTar Am Am sequenceSequenceAc	TargetHADDOCKBindiAmino2.4affiniAcidsClusterΔG	Binding affinity ΔG	Residues of pancreation	lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	ected (Kcal mol ⁻¹) rom DDIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide NALKCCHSCP <u>A</u>	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 int	3	0	0	1			
	Overall perce	ntage of bon	ding	6%	0%	0%	50%	

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



Figure S6a: Binding interaction of NALKCCHSCP<u>A</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTargetandAminosequenceAcids	TargetHADDOCKAmino2.4AcidsCluster		Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected (Kcal mol ⁻¹ from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide GEHGGAGMGG GQFQP <u>V</u>	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
	Overall perce	ntage of bon	ding	0%	0%	0%	0%	

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



Figure S6b: Binding interaction of GEHGGAGMGGGQFQP<u>V</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTarandAmsequenceAci	TargetHADDOCKAmino2.4AcidsCluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	rom DDIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide GQLGEHGGAG M <u>G</u>	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 perce	ntage of bon	ding		0%	0%	0%	0%

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



Figure S6c: Binding interaction of GQLGEHGGAGM<u>G</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide lengthTailandAsequenceA	Target HADDOCK Bin Amino 2.4 affi Acids Cluster Δ Selected (Kcal		Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatio	: lipase involve in protein peptide interaction and its position		
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide LAAVEALSTN <u>G</u>	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
	Overall perce	ntage of bon	ding		0%	0%	0%	0%

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



Figure S6d: Binding interaction of LAAVEALSTN<u>G</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interactio position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Long chain peptide MLPLMLPFTM G <u>¥</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 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					0	0	1	
	Overall perce	ntage of bon	ding	5%	0%	0%	100%		

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



Figure S6e: Binding interaction of MLPLMLPFTMG<u>Y</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction a position				
N-and C- terminal			Selected from PRODIGY	(KCal mol ⁻¹)	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					0	0	2	
	Overall percer	ntage of bon	ding	4%	0%	0%	100%		

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



Figure S6f: Binding interaction of MSKFLPLPLMF<u>Y</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein pept position			e interaction and its	
N-and C- terminal			from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Long chain peptide FFRSKLLSRG AAAAKGALLP QY <u>W</u>	TRP23	cluster1_3	-9.2	$\begin{array}{c} C - Phe78\\ CA - NA\\ CB - NA\\ CD_1 - NA\\ CD_2 - NA\\ CE_2 - NA\\ CE_3 - NA\\ CG - NA\\ CH_2 - NA\\ CZ_2 - NA\\ CZ_3 - NA\\ N - Phe78\\ NE_1 - NA\\ O - Phe78, Gly114 \end{array}$	NA	NA	NA	
	Total number of bonds				45	0	0	1	
	Total no of int	4	0	0	0				
	Overall perce	ntage of bon	ding		9%	0%	0%	0%	

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



Figure S6g: Binding interaction of FFRSKLLSRGAAAAKGALLPQY<u>W</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Long chain peptide RCMAFLLSDG AAAAQQLLPQ Y <u>W</u>	TRP22	cluster3_3	-9.4	C - NA CA - NA CB - NA CD ₁ - NA CD ₂ - NA CE ₂ - NA CE ₂ - NA CE ₃ - Ile211 CG - NA CH ₂ - NA CZ ₂ - NA CZ ₂ - NA CZ ₃ - Ile211 N - NA NE ₁ - NA O - NA	NA	NA	NA	
	Total num	l	32	0	0	2			
	Total no of int		2	0	0	0			
	Overall perce	ntage of bon	ding		6%	0%	0%	0%	

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



Figure S6h: Binding interaction of RCMAFLLSDGAAAAQQLLPQY<u>W</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N and C	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kaal mal ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction a position			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide EQGFLPGPEE SG <u>R</u>	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
	Overall perce	ntage of bon	ding	0%	0%	0%	0%	

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



Figure S6i: Binding interaction of EQGFLPGPEESG<u>R</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interac position			eraction and its
N-and C- terminal			Selected from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide	ARG16	cluster3_1	-7.4	C - NA CA - NA	NA	NA	NA
	SGGGGGGVAG AATAS <u>R</u>				CB - NA CD - Thr256 CG - NA CZ - Thr256 N - NA NH ₁ - Val260 NB ₂ - Arg257 NE - Thr256 O - NA			
Total number of bonds					40	0	0	0
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bon	ding	13%	0%	0%	0%	

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



Figure S6j: Binding interaction of SGGGGGGVAGAATAS<u>R</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino	Peptide length and	Target Amino	HADDOCK 2.4 Chuston	Binding affinity	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal	sequence	Acius	Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide YGNPVGGVG <u>H</u>	HIS10	cluster1_3	-9.0	$ \begin{array}{c} C & - \mbox{Ile79} \\ CA & - \mbox{Ile79} \\ CB & - \mbox{Ile79} \\ CD_2 & - \mbox{Glu84}, \mbox{Trp253} \\ CE_1 & \mbox{Ile79}, \mbox{Asp80} \\ \mbox{Lys81}, \mbox{Glu84} \\ \mbox{Arg257} \\ CG & - \mbox{Ile79} \\ N & - \mbox{Ile79} \\ ND_1 & - \mbox{Ile79}, \mbox{Asp80} \\ NE_2 & - \mbox{Glu84} \\ O & - \mbox{Ile79} \\ \end{array} $	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%	

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



Figure S6k: Binding interaction of YGNPVGGVG<u>H</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	tide lengthTargetIandAminosequenceAcids	Carget Amino HADDOCK Binding affinity Acids 2.4 affinity Cluster ΔG Selected (Kcal mol ⁻¹) from PRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal				(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C1	Long chain peptide RPAQPNYPWT AVLVFR <u>H</u>	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	NA	NA	NA
	Total num	ber of bond	s		0 - NA 56	1	0	1
Total no of interactive residues Overall percentage of bonding					0 0%	0 0%	0	0 0%

 Table S6I: Binding interaction of pancreatic lipase inhibitory peptides-RPAQPNYPWTAVLVFRH at C1 position.



Figure S6I: Binding interaction of RPAQPNYPWTAVLVFR<u>H</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	ngth Target Amino Ice Acids		Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction			
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide	ALA2	cluster1_3	-6.5	C - NA	NA	NA	NA
	A <u>A</u> GF				CB - NA CB - NA N - Pro181 O - 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%	

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



Figure S7a: Binding interaction of A<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

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 pancre Hydrophobic interaction	eatic lipase involv Salt Bridge	e in protein peptide Covalent bond	e interaction Hydrogen bond
N2	Short chain peptide N <u>V</u> 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%

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



Figure S7b: Binding interaction of N<u>V</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic Hydrophobic interaction	lipase involve in p position Salt Bridge	rotein peptide int Covalent bond	eraction and its Hydrogen bond
			PRODIGY		micraetion	Diluge	oonu	bond
N2	Short chain peptide	ILE2	cluster3_2	-6.7	C - NA CA - NA	NA	NA	NA
	V <u>I</u> APW				CB - NA CD ₁ - Phe78, Val260 CG ₁ - Val260 CG ₂ - NA N - NA O - 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%	

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



Figure S7c: Binding interaction of V<u>I</u>APW 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTargetandAminosequenceAcids	getHADDOCKBindingino2.4affinitydsClusterΔG		Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Short chain peptide	MET2	cluster10_1	-7.3	C - NA CA - NA	NA	NA	NA
	M <u>M</u> ML				CB - NA CE - Gly77, Phe78, Asp80, His152 CG - Phe78 O - Phe216 N - Phe78 SD - Gly77, Phe78, His152, Ser153			
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%	

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



Figure S7d: Binding interaction of MML 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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	e lipase involve in p position	protein peptide int	eraction and its
N-and C- terminal			Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N2	Short chain peptide	SER2	cluster 1_4	-7.7	C - NA CA - Phe216	NA	NA	NA
	M <u>S</u> NYF				CB - Val260 N - Phe216 O - NA OG - NA			
	Total num	ber of bond	s		28	0	0	0
	Total no of interactive residues				3	0	0	0
	Overall perce	ntage of bon	ding		11%	0%	0%	0%

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



Figure S7e: Binding interaction of M<u>S</u>NYF 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N2	Short chain peptide	THR2	cluster9_4	-8.7	C - NA	NA	NA	NA	
	G <u>T</u> IT				CA - NA CB - NA CG ₂ – Phe216 OG ₁ – Phe216 N - NA				
	Total num	ber of bonds			16	0	0	0	
	Total no of interactive residues				2	0	0	0	
	Overall perce	ntage of bond	ling		13%	0%	0%	0%	

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



Figure S7f: Binding interaction of G<u>T</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	ptide length andTarget AminoHADDOCK 2.4Binding affinitysequenceAcidsClusterΔG				Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	ted (Kcal mol ⁻¹) m JIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond		
N2	Short chain peptide	ARG2	cluster1_1	-7.4	C - NA CB - NA	NA	NA	NA		
	L <u>R</u> FPL				CD - NA CG - NA CZ - Thr113 N - NA NE - NA NH ₁ - Phe78, Ile79 NH ₂ - Ile79, Thr113 O - Phe78					
	Total num	ber of bond	s	•	24	0	0	2		
	Total no of interactive residues			6	0	0	0			
	Overall perce	ntage of bon	ding		25%	0%	0%	0%		

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



Figure S7g: Binding interaction of L<u>R</u>FPL 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) representing the amino acid that present in the inhibitory peptides.

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 Hydrophobic interaction	lipase involve in p position Salt Bridge	orotein peptide int Covalent bond	eraction and its Hydrogen bond
N2	Medium chain peptide L <u>N</u> 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 num	ber of bond	s		20	0	0	2
	Total no of interactive residues				5	0	0	0
	Overall perce	ntage of bon	ding		25%	0%	0%	0%

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



Figure S8a: Binding interaction of L<u>N</u>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) representing the amino acid that present in the inhibitory peptides.

Table S	8h: Binding	interaction of	² nancreatic l	inase inhibitorv	nentides-	LNFEPR at N2 i	position.
I able De	Jos Dinaing	, michaethon of	panel calle I	puse minutory	peptices .		position.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreation	lipase involve in position	protein peptide int	eraction and its
terminal			from PRODIGY	(Ktai mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide	ASN2	cluster2_2	-8.0	C - Phe78 CA - NA	NA	NA	NA
	L <u>N</u> FEPR				CB - Phe78 CG - NA N - Phe78 ND ₂ - NA O - Phe78, Tyr115 OD ₁ - NA			
Total number of bonds			25	0	0	1		
	Total no of interactive residues				5	0	0	0
	Overall perce	ntage of bon	ding		20%	0%	0%	0%



Figure S8b: Binding interaction of L<u>N</u>FEPR 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of panc	reatic lipase involv Salt	e in protein peptide Covalent	e interaction Hydrogen
terminal			from PRODIGY		interaction	Bridge	bond	bond
N2	Medium chain peptide	LEU2	cluster5_2	-6.8	C - NA CA - NA	NA	NA	NA
	E <u>L</u> PPHFL				CB - NA CD ₁ - Thr116 CD ₂ - NA CG - Thr116 N - NA O - NA			
	Total num	ber of bonds			33	0	0	4
	Total no of interactive residues				2	0	0	0
	Overall perce	ntage of bond	ling		6%	0%	0%	0%

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



Figure S8c: Binding interaction of E<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein Hydrophobic Salt			e interaction
terminal			from PRODIGY	(Ixear mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide	LEU2	cluster11_3	-7.6	C - NA CA - NA	NA	NA	NA
	F L WPEYGAL				CB - Phe216 CD ₁ - Phe216 CD ₂ - Phe78, Tyr115 CG - NA N - NA O - NA			
	Total num	ber of bonds			30	0	0	3
	Total no of interactive residues			3	0	0	0	
	Overall perce	ntage of bond	ling		10%	0%	0%	0%

Table S8d:	Binding	interaction o	f pancreatic	lipase i	inhibitory	peptides	-FLWPE	YGAL at N2	2 position.



Figure S8d: Binding interaction of F<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity AG	Residues of pancre	eatic lipase involve	in protein peptide	e interaction
N-and C- terminal			from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Medium chain peptide	ALA2	cluster1_2	-8.0	C - NA CA - NA	NA	NA	NA
	L <u>A</u> PSTIK				CB - NA N - NA O - NA			
	Total num	ber of bond	s		28	0	0	1
	Total no of interactive residues				0	0	0	0
	Overall percent	ntage of bon	ding		0%	0%	0%	0%

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



Figure S8e: Binding interaction of L<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction a position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N2	Medium chain peptide	ALA2	cluster2_4	-7.6	C - NA CA - NA	NA	NA	NA	
	V <u>A</u> PEEHPV				CB - NA N - NA O - NA				
	Total num	ber of bond	S		32	0	0	2	
	Total no of interactive residues				0	0	0	0	
	Overall perce	ntage of bon	ding		0%	0%	0%	0%	

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



Figure S8f: Binding interaction of V<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHADIAmino2AcidsClu	HADDOCKBinding2.4affinityClusterΔGSelected(Kcal mol ⁻¹)fromPRODIGY	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal				(Kcai Mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide G <u>N</u> 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 perce	ntage of bon	ding		3%	0%	0%	0%

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



Figure S9a: Binding interaction of G<u>N</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHADAmino2AcidsCh	HADDOCKBinding2.4affinityClusterΔGSelected(Kcal mol ⁻¹)fromPRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal				(Kcai mol [*])	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 num	ber of bond	s		45	0	0	3
Total no of interactive residues					3	0	0	1
	Overall perce	ntage of bon	ding		7%	0%	0%	33%

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



Figure S9b: Binding interaction of L<u>NNPSVCDCDCMMKAAR</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK I 2.4 : Cluster Selected (K from PRODIGY	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide M <u>L</u> 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 perce	ntage of bon	ding		10%	0%	0%	0%

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



Figure S9c: Binding interaction of MLPLMLPFTMGY 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	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			
terminal					interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide N <u>A</u> 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 perce	ntage of bon	ding		2%	0%	0%	0%

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



Figure S9d: Binding interaction of N<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	TargetHAminoAcids	HADDOCK Binding 2.4 affinity Cluster ΔG Selected (Kcal mol ⁻¹) from PRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal				Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N2	Long chain peptide	ALA2	cluster1_1	-8.4	C - Phe216 CA - Phe78	NA	NA	NA
	L <u>A</u> AVEALSTN				CB - Phe78			
	G				N - NA O - Phe216			
Total number of bonds					31	0	0	3
Total no of interactive residues					4	0	0	0
	Overall perce	ntage of bon	ding		13%	0%	0%	0%

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



Figure S9e: Binding interaction of L<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Table S9f: Binding interaction of	pancreatic lipase inhibitory	peptides-SGGGGGGGVAGAATASR at N2	position.
8	1 1 1	1 1	4

Position of amino acid in N and C	Peptide length and sequence	TargetHADDOCKAmino2.4AcidsClusterClusterCluster	Binding affinity AG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
terminal			from PRODIGY	(iscai iiioi)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide	GLY2	cluster3_1	-7.4	C - NA CA - NA	NA	NA	NA
	S <u>G</u> GGGGGVAG AATASR				N - Tyr115 O - NA			
Total number of bonds					40	0	0	0
Total no of interactive residues					1	0	0	0
	Overall perce	ntage of bon	ding		3%	0%	0%	0%



Figure S9f: Binding interaction of S<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHAAminoAcidsAcids(HADDOCKBinding2.4affinityClusterΔGSelected(Kcal molfromPRODIGY	Binding affinity ΔG	inding ffinityResidues of pancreatic lipase involve in protein peptide positionΔG hL			
N-and C- terminal					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N2	Long chain peptide	GLY2	cluster1_3	-9.0	C - Phe78 CA - NA	NA	NA	NA
	Y <u>G</u> NPVGGVGH				N - NA O - Phe78			
Total number of bonds					57	2	0	4
Total no of interactive residues					2	0	0	0
	Overall perce	ntage of bon	ding		4%	0%	0%	0%

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



Figure S9g: Binding interaction of Y<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target AminoHADDOCKAcids2.4Cluster Sclusterd	CK Binding affinity c AG	Residues of pancreatic lipase involve in protein peptide interaction				
terminal			from PRODIGY	7	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide	MET3	cluster10_1	-7.3	C - NA CA - NA	NA	NA	NA
	MM <u>M</u> L	MM <u>M</u> L		CB - NA CE - Val260 CG - NA O - Phe78 N - Phe78 SD - NA				
Total number of bonds					34	0	0	1
Total no of interactive residues					3	0	0	0
	Overall percent	ntage of bond	ling		9%	0%	0%	0%

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



Figure S10a: Binding interaction of MM<u>M</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from PRODICY	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre Hydrophobic interaction	eatic lipase involv Salt Bridge	e in protein peptide Covalent bond	e interaction Hydrogen bond
C2	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
Total number of bonds					21	0	0	0
Total no of interactive residues					2	0	0	0
	Overall percer	ntage of bond	ling		10%	0%	0%	0%

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



Figure S10b: Binding interaction of FD<u>M</u>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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	Peptide lengthTargandAmirsequenceAcid	TargetHADDOCKAmino2.4AcidsCluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide	PRO4	cluster1_1	-7.4	C - NA CA -NA	NA	NA	NA
	LRF <u>P</u> L				CB - NA CD - Phe216 CG - Phe216 N- NA O - Phe78, Tyr115			
	Total number of bonds				24	0	0	2
	Total no of int		4	0	0	0		
	Overall perce	ntage of bon	ding		17%	0%	0%	0%

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	ide length andTarget AminoHADDOCK 2.4Binding affinity affinityequenceAcidsClusterΔG		Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	1 (Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide	PRO4	cluster3_2	-6.7	C - NA CA -NA	NA	NA	O - Tyr115
	VIA <u>P</u> W				CB - Phe78 CD - NA CG - NA N- NA O - Gly114, Tyr115			
	Total number of bonds				26	0	0	1
	Total no of int		3	0	0	1		
	Overall perce	ntage of bon	ding		12%	0%	0%	100%

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



Figure S10d: Binding interaction of VIA<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N and C	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Keal mal ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction			
terminal			from PRODIGY	(Kcai mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide	LEU3	cluster8_1	-7.2	C - NA CA - NA	NA	NA	NA
	RL <u>L</u> P				CB - Ile79 CD ₁ - Phe78, Ile79 CD ₂ - NA CG - NA N - NA O - Ile79			
Total number of bonds				21	0	0	1	
	Total no of int	4	0	0	0			
	Overall perce	ntage of bond	ling		19%	0%	0%	0%

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



Figure S10e: Binding interaction of RL<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

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 panc Hydrophobic interaction	reatic lipase involv Salt Bridge	e in protein peptido Covalent bond	e interaction Hydrogen bond
C2	Short chain peptide GT <u>I</u> T	ILE3	cluster9_4	-8.7	$\begin{array}{c} C - NA \\ CA - NA \\ CB - Val260 \\ CD_1 - NA \\ CG_1 - NA \\ CG_2 - NA \\ N - NA \\ O - Val260 \end{array}$	NA	NA	NA
Total number of bonds				16	0	0	0	
	Total no of interactive residues					0	0	0
	Overall percer	ntage of bond	ling		13%	0%	0%	0%

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



Figure S10f: Binding interaction of GT<u>I</u>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) representing 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	Peptide length and	Target Amino	HADDOCK 2.4	Binding affinity	Residues of pancreatic	lipase involve in p position	rotein peptide int	eraction and its
acid in N-and C- terminal	sequence	Acids	Cluster Selected from PRODIGY	r AG d (Kcal mol ⁻¹) GY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide IRW <u>W</u> 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 ₂ - NA N - NA NE ₁ - Phe216, Val260 O - NA	NA	NA	NA
	Total num	ber of bond	s	20	3	0	2	
	Total no of int		4	0	0	0		
	Overall perce	ntage of bon	ding	20%	0%	0%	0%	



Figure S10g: Binding interaction of IRW<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	PositionPeptide lengthTarf aminoandAmiacid insequenceAci		HADDOCK Binding 2.4 affinity Cluster ΔG		Residues of pancreatic lipase involve in protein peptide interaction			
N-and C- terminal			Selected from PRODIGY	(Kcai mor)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Short chain peptide	GLY3	cluster1_3	-6.5	C - NA	NA	NA	NA
	АА <u>G</u> F				N - Tyr115, Pro181 O - Tyr115, Pro181			
Total number of bonds					18	0	0	1
	Total no of int		4	0	0	0		
	Overall perce	ntage of bon	ding		22%	0%	0%	0%

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



Figure S10h: Binding interaction of AA<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTaandAnsequenceAc	TargetHADDOCKAmino2.4AcidsCluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	1 (Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide	PRO7	cluster2_4	-7.6	C - NA CA -NA	NA	NA	NA
	VAPEEH <u>P</u> V				CB - Tyr115 CD - NA CG - Phe216 N- NA O - Ile210, Phe216			
	Total number of bonds				32	0	0	2
	Total no of int		4	0	0	0		
	Overall perce	ntage of bon	ding		13%	0%	0%	0%

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



Figure S11a: Binding interaction of VAPEEH<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	e lipase involve in p position	rotein peptide interaction and its			
N-and C- terminal			Selected from PRODIGY	ed (Kcal mol ⁻¹) 1 GY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond		
C2	Medium chain peptide	PRO6	Cluster3_4	-6.9	C - NA CA - Ile211	NA	NA	NA		
	AGDDA <u>P</u> R				CB - NA CD - NA CG - NA N- Ile211 O - NA					
	Total num	nber of bond	s	25	0	0	1			
	Total no of int	2	0	0	0					
	Overall perce	ntage of bon	ding	8%	0%	0%	0%			

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



Figure S11b: Binding interaction of AGDDA<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length andTarget AminosequenceAcids	Target Amino Acids	TargetHADDOCKBindingAmino2.4affinityAcidsClusterΔG		Binding affinity ΔG Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide	LEU7	cluster1_1	-7.2	C - Phe216 CA - Phe216	NA	NA	NA
	NYVADG <u>L</u> G				CB - NA CD ₁ - NA CD ₂ - Phe216, Val 260 CG - NA N - NA O - Phe216			
Total number of bonds					29	0	0	3
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bon	ding	17%	0%	0%	0%	

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



Figure S11c: Binding interaction of NYVADG<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length andTarget AminosequenceAcids	Target Amino Acids	getHADDOCKBindingino2.4affinityidsClusterΔG		Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	(Kcai mol ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Medium chain peptide	LEU8	cluster1_3	-7.1	C - NA CA - NA	NA	NA	NA
	CFLPLPL <u>L</u> K				CB - NA CD ₁ - NA CD ₂ - NA CG - NA N - NA O - NA			
Total number of bonds					34	0	0	3
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bon	ding	0%	0%	0%	0%	

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



Figure S11d: Binding interaction of CFLPLPL<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

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 pancre Hydrophobic interaction	atic lipase involve Salt Bridge	in protein peptide Covalent bond	e interaction Hydrogen bond
C2	Medium chain peptide LAPST <u>I</u> 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 int		3	0	0	0		
	Overall perce	ntage of bon	ding		11%	0%	0%	0%

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



Figure S11e: Binding interaction of LAPST<u>I</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Peptide length Target and Amino sequence Acids	TargetHADDOCKAmino2.4AcidsCluster		Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C2	Long chain peptide	GLY12	cluster1_2	-8.9	C - Trp253 CA - Thr256	NA	NA	NA	
	EQGFLPGPEE S <u>G</u> R				N - NA O - Trp253, Thr256				
Total number of bonds					44	0	2	4	
	Total no of interactive residues					0	0	0	
	Overall perce	ntage of bon	ding	9%	0%	0%	0%		

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



Figure S12a: Binding interaction of EQGFLPGPEES<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	otide length andTarget AminosequenceAcids	TargetHADDOCKAmino2.4AcidsClusterSelected(fromPRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal				(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide	GLY9	cluster1_3	-9.0	C - Ile79 CA - NA	NA	NA	NA
	YGNPVGGV <u>G</u> H				N - NA O - Ile79			
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%

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



Figure S12b: Binding interaction of YGNPVGGV<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	TargetHADDOCKAmino2.4AcidsClusterSelectedfromPRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal				(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide	ALA16	cluster3_4	-9.8	C - Thr116 CA - NA	NA	NA	NA
					CB - NA			
	CMMKA <u>A</u> K				$\mathbf{N} - \mathbf{N}\mathbf{A}$ $\mathbf{O} = \mathbf{G}\mathbf{V}114$ Thr116			
					0 - Giyii4, imiio			
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%

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



Figure S12c: Binding interaction of LNNPSVCDCDCMMKA<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHADAmino2AcidsCh	HADDOCKBinding2.4affinityClusterΔG		Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C2	Long chain peptide FFRSKLLSRG AAAAKGALLP Q <u>Y</u> 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 perce	ntage of bon	ding	22%	0%	0%	0%		

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



Figure S12d: Binding interaction of FFRSKLLSRGAAAAKGALLPQ<u>Y</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C2	Long chain peptide	TYR21	cluster3_3	-9.4	C - NA CA- NA	NA	NA	OH - Glu180, Cys182
	RCMAFLLSDG				CB - NA			
	AAAAQQLLPQ				$CD_1 - NA$			
	$\underline{\mathbf{Y}}\mathbf{W}$				$CD_2 - NA$			
					$CE_1 - NA$			
					CE ₂ - Glu180, Pro181			
					CG - NA			
					CZ - Glu180, Pro181			
					N - NA			
					O - lle211			
					OH - Pro181			
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%	

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



Figure S12e: Binding interaction of RCMAFLLSDGAAAAQQLLPQ<u>Y</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C2	Long chain peptide GSGGGGGGGG GP <u>R</u> R	ARG13	cluster4_1	-9.2	$ \begin{array}{c} 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 \\ \end{array} $	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%	

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



Figure S12f: Binding interaction of GSGGGGGGGGGGGGGGGGGGR<u>R</u> 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction				
terminal			from PRODIGY	(KCal Mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C2	Long chain peptide RKQEEDEDEE QQ <u>R</u> 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%		

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



Figure S12g: Binding interaction of RKQEEDEDEEQQ<u>R</u>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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	lipase involve in p position	protein peptide interaction and its I		
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C1	Long chain peptide GEHGGAGMGG GQFQ <u>P</u> 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 perce	ntage of bon	ding		0%	0%	0%	0%	

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



Figure S12h: Binding interaction of GEHGGAGMGGGQFQ<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	protein peptide interaction and its		
N-and C- terminal			Selected from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide	VAL3	cluster1_1	-7.2	C - NA CA - Val260	NA	NA	NA
	NY <u>V</u> ADGLG				CB - NA CG ₁ - Val260 CG ₂ - NA N - NA O - Val260			
Total number of bonds					29	0	0	3
Total no of interactive residues				3	0	0	0	
	Overall perce	ntage of bon	ding		10%	0%	0%	0%

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



Figure S13a: Binding interaction of NY<u>V</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	protein peptide int	eraction and its	
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide	VAL3	cluster3_2	-7.0	C - NA CA - Phe216	NA	NA	NA
	DI <u>V</u> DKIEI				CB - NA CG ₁ - Phe216 CG ₂ - Phe216 N - NA O - NA			
Total number of bonds					17	0	0	1
Total no of interactive residues					3	0	0	0
	Overall perce	ntage of bon	ding		18%	0%	0%	0%

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



Figure S13b: Binding interaction of DI<u>V</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity AG	Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			from PRODIGY	(Kcal mol ⁻⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Medium chain peptide	PRO3	cluster2_1	-7.1	C - NA CA - NA	NA	NA	NA	
	FD <u>P</u> FPK				CB - NA CD - Val260 CG -Val260 N - NA O - NA				
	Total num	ber of bonds			33	0	0	0	
Total no of interactive residues			2	0	0	0			
	Overall perce	ntage of bond	ling		6%	0%	0%	0%	

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



Figure S13c: Binding interaction of FD<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of panc	reatic lipase involv Salt Bridge	e in protein peptide Covalent bond	e interaction Hydrogen bond
			PRODIGY		meraction	Dridge	boliu	bond
N3	Medium chain peptide	PRO3	cluster5_2	-6.8	C - NA CA - NA	NA	NA	NA
	EL <u>P</u> PHFL				CB - NA CD - Ile210 CG - Ile211 N - NA O - NA			
	Total num	ber of bonds			33	0	0	4
Total no of interactive residues				2	0	0	0	
	Overall perce	ntage of bond	ling		6%	0%	0%	0%

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



Figure S13d: Binding interaction of EL<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Medium chain peptide FL <u>W</u> 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 num	ber of bonds	5	L	30	0	0	3	
Total no of interactive residues			5	0	0	0			
	Overall perce	ntage of bond	ding		17%	0%	0%	0%	

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



Figure S13e: Binding interaction of FL<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Medium chain peptide AE <u>W</u> 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 ₂ - NA CZ ₃ - Gly114 N - NA NE ₁ - NA O - NA	NA	NA	NA	
	Total num	ber of bonds			21	0	0	1	
Total no of interactive residues					3	0	0	0	
	Overall perce	ntage of bond	ling		14%	0%	0%	0%	

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



Figure S13f: Binding interaction of AE<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	eraction and its		
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide	LEU3	cluster11_2	-8.1	C - NA CA - NA	NA	NA	NA
	LN <u>L</u> DLLR				CB - NA CD ₁ - Thr113 CD ₂ - NA CG - NA N - Gly114 O - NA			
	Total num	ber of bond	s		20	0	0	2
Total no of interactive residues			2	0	0	0		
	Overall perce	ntage of bon	ding		10%	0%	0%	0%

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



Figure S13g: Binding interaction of LNLDLLR 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction position					
N-and C- terminal			Selected from PRODIGY	Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond		
N3	Medium chain peptide	LEU3	cluster1_3	-7.1	C - NA CA - NA	NA	NA	NA		
	CF <u>L</u> PLPLLK				CB - Val260 CD ₁ - NA CD ₂ - Val260 CG - NA N - NA O - NA					
Total number of bonds				34	0	0	3			
Total no of interactive residues				2	0	0	0			
	Overall perce	ntage of bon	ding		6%	0%	0%	0%		

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



Figure S13h: Binding interaction of CF<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Table	S13i:	Binding	interactio	n of pai	ncreatic li	pase inhibite	orv pei	ptides- I	LNFEPR at	t N3 position.
			,							

Position	Peptide length	Target	HADDOCK	Binding	Residues of pancreatic lipase involve in protein peptide interaction and its				
of amino acid in	and sequence	Amino Acids	2.4 Cluster	affinity AG	position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Medium chain peptide	PHE3	cluster2_2	-8.0	C - NA CA - NA	NA	NA	NA	
	LN <u>F</u> EPR				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				
	Total num	ber of bond	S	•	25	0	0	1	
	Total no of int	eractive res	idues		9	0	0	0	
	Overall perce	ntage of bon	ding		36%	0%	0%	0%	



Figure S13i: Binding interaction of LN<u>F</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position			
N-and C- terminal			Selected from PRODIGY	m DIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide AP <u>F</u> 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 perce	ntage of bon	ding		43%	0%	0%	0%

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



Figure S13j: Binding interaction of AP<u>F</u>PLR 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTargetandAminosequenceAcids	Target Amino Acids	TargetHADDOCKBindiAmino2.4affinAcidsClusterΔGSelected(Kcal mfromPRODIGY	Binding affinity ΔG	Residues of pancreation	protein peptide int 1	eptide interaction and its	
N-and C- terminal				(Kcai moi ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide	ASN3	cluster2_2	-9.0	C - NA CA - NA	NA	NA	NA
	MA <u>N</u> LQR				CB - NA CG - NA N - Phe78 ND ₂ - Phe78 O - NA OD ₁ - NA			
	Total number of bonds				37	2	0	6
	Total no of int	teractive res	idues		2	0	0	0
	Overall perce	ntage of bon	nding		5%	0%	0%	0%

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



Figure S13k: Binding interaction of MA<u>N</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide lengthTailandAnsequenceAc	TargetHADDOCKAmino2.4AcidsCluster	Binding affinity ΔG	Residues of pancreation	teraction and its			
N-and C- terminal			Selected (from PRODIGY	(Kcai moi ⁻)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Medium chain peptide CA <u>N</u> 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					0	0	0
	Overall perce	ntage of bon	ding		11%	0%	0%	0%

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



Figure S13I: Binding interaction of CA<u>N</u>PHELPN 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	ncreatic lipase involve in protein peptide interaction and its position			
terminal			from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Long chain peptide YG <u>N</u> 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 perce	ntage of bon	ding		8%	0%	0%	0%	

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



Figure S14a: Binding interaction of YG<u>N</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
N3	Long chain peptide LN <u>N</u> 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 int	teractive res	idues		4	0	0	0	
	Overall perce	ntage of bon	ding		9%	0%	0%	0%	

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



Figure S14b: Binding interaction of LN<u>N</u>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) representing the amino acid that present in the inhibitory peptides.

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 pancre Hydrophobic interaction	atic lipase involve Salt Bridge	in protein peptide Covalent bond	e interaction Hydrogen bond
N3	Long chain peptide HC <u>P</u> 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 int	eractive res	idues		7	0	0	0
	Overall perce	ntage of bon	ding		18%	0%	0%	0%

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



Figure S14c: Binding interaction of HC<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancro Hydrophobic	eatic lipase involve Salt Bridge	in protein peptide Covalent	interaction Hydrogen bond
			PRODIGY		interaction	Druge	Dona	Dona
N3	Long chain peptide	PRO3	cluster2_1	-8.4	C - NA CA - NA	NA	NA	NA
	ML <u>P</u> LMLPFTM				CB - NA			
	GY				CD - NA			
					N- NA			
					O - NA			
Total number of bonds				41	0	0	1	
	Total no of int	eractive resi	idues		0	0	0	0
	Overall perce	ntage of bon	ding		0%	0%	0%	0%

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



Figure S14d: Binding interaction of ML<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C- terminal	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected from	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic Hydrophobic interaction	lipase involve in p position Salt Bridge	orotein peptide int Covalent bond	eraction and its Hydrogen bond
N3	Long chain peptide LA <u>A</u> 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 int	teractive resi	idues		3	0	0	0
	Overall perce	ntage of bon	ding		10%	0%	0%	0%

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



Figure S14e: Binding interaction of LA<u>A</u>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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	e lipase involve in p position	protein peptide int	eraction and its
N-and C- terminal			Selected (from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide RP <u>A</u> 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					0	0	0
	Overall perce	ntage of bon	ding		9%	0%	0%	0%

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



Figure S14f: Binding interaction of RP<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

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 Hydrophobic interaction	lipase involve in p position Salt Bridge	rotein peptide int Covalent bond	eraction and its Hydrogen bond
N3	Long chain peptide NA <u>L</u> 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 int	5	0	0	0			
	Overall perce	ntage of bon	ding	11%	0%	0%	0%	

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



Figure S14g: Binding interaction of NA<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreatic	teraction and its		
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
N3	Long chain peptide AL <u>W</u> 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 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 int	10	0	0	0			
	Overall perce	ntage of bon	ding		22%	0%	0%	0%

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



Figure S14h: Binding interaction of AL<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK Binding 2.4 affinity Cluster ΔG Selected (Kcal mol ⁻¹)		Residues of pancre	Residues of pancreatic lipase involve in protein peptide interact			
terminal			from PRODIGY		interaction	Bridge	bond	bond	
C3	Medium chain peptide	ALA4	cluster5_1	-8.6	C - NA CA - NA	NA	NA	NA	
	TAT <u>A</u> VV				CB - NA N - Phe216 O - Phe216, Val260				
	Total number of bonds				22	0	0	0	
	Total no of interactive residues				3	0	0	0	
	Overall perce		14%	0%	0%	0%			

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



Figure S15a: Binding interaction of TAT<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length andTarget AminoHADDOCK 2.4Binding affinitysequenceAcidsCluster SelectedΔG		Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancre	atic lipase involve	in protein peptide	e interaction	
terminal			from PRODIGY		interaction	Bridge	bond	bond
C3	Medium chain peptide	ALA5	cluster15_1	-8.5	C - NA CA - NA	NA	NA	NA
	DFGI <u>A</u> SF				CB - NA N - Tyr115, Pro181 O - Phe216, Pro181			
	Total number of bonds				26	0	0	0
	Total no of interactive residues				4	0	0	0
	Overall percentage of bonding					0%	0%	0%

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



Figure S15b: Binding interaction of DFGI<u>A</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	lipase involve in position	se involve in protein peptide interaction and its position		
N-and C- terminal			Selected from PRODIGY	ected (Kcal mol ⁻¹) om DIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C3	Medium chain peptide	LEU7	cluster1_4	-7.9	C - NA CA - NA	NA	NA	NA	
	RLARAG <u>L</u> AQ				CB - NA CD ₁ - NA CD ₂ - NA CG - NA N - NA O - NA				
Total number of bonds				23	0	0	3		
	Total no of interactive residues					0	0	0	
	Overall perce	ntage of bon	ding	0%	0%	0%	0%		

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



Figure S15c: Binding interaction of RLARAG<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	e lipase involve in p position	n protein peptide interaction and its on		
terminal			Selected (Kcal mol ⁻¹) from PRODIGY	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond		
C3	Medium chain peptide	LEU5	cluster11_2	-8.1	C - NA CA - NA	NA	NA	NA	
	LNLD <u>L</u> LR				CB - NA CD ₁ - NA CD ₂ - NA CG - NA N - NA O - NA				
	Total number of bonds				20	0	0	2	
	Total no of interactive residues					0	0	0	
	Overall perce	ntage of bon	ding	0%	0%	0%	0%		

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



Figure S15d: Binding interaction of LNLD<u>L</u>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) representing the amino acid that present in the inhibitory peptides.

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

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



Figure S15e: Binding interaction of IIAP<u>P</u>ER 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	nPeptide length andTarget AminoHADDOCK 2.4Binding affinity ΔGnandAmino2.4affinity ΔG		Binding affinity ΔG	Residues of pancreatic	Residues of pancreatic lipase involve in protein peptide interaction and its positionHydrophobicSaltCovalentHydrogeninteractionBridgebondbond			
N-and C- terminal			Selected (Kcal mol from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide APF <u>P</u> LR	PRO4	cluster1_3	-7.0	C - NA CA - Tyr115 CB - Tyr115 CD - NA CG - NA N- NA O - Phe78	NA	NA	NA
	Total num	ber of bond	s		16	0	0	0
	Total no of interactive residues					0	0	0
	Overall perce	ntage of bon	ding		19%	0%	0%	0%

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



Figure S15f: Binding interaction of APF<u>P</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of pancreation	e lipase involve in j position	protein peptide int 1	eraction and its	
N-and C- terminal			Selected from PRODIGY	(Kcai mol ⁺)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide NYVAD <u>G</u> 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					0	0	0
	Overall perce	ntage of bon	nding	7%	0%	0%	0%	

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



Figure S15g: Binding interaction of NYVAD<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in N-and C-	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster Selected	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatio	e lipase involve in p position Salt	rotein peptide int Covalent	eraction and its Hydrogen
terminal			from PRODIGY		interaction	Bridge	bond	bond
C3	Medium chain peptide	GLY4	cluster5_3	-7.5	C - NA CA - NA	NA	NA	NA
	HLP <u>G</u> RG				N - NA O - NA			
	Total number of bonds				20	0	0	0
	Total no of interactive residues				0	0	0	0
	Overall perce	0%	0%	0%	0%			

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



Figure S15h: Binding interaction of HLP<u>G</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG	Residues of panc	e in protein peptido	e interaction	
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Medium chain peptide AEWLHD <u>W</u> 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 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 int	dues		5	0	0	0	
	Overall perce	ntage of bond	ling		24%	0%	0%	0%

Table	S15i:	Binding	^y interact	ion of pa	ancreatic li	pase in	hibitory 1	peptides	-AEWLF	IDWKL a	t C3	position.
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Figure S15i: Binding interaction of AEWLHD<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	DOCK Binding .4 affinity ster ΔG cted (Kcal mol ⁻¹) DM DIGY	Residues of pancreatic lipase involve in protein peptide interaction					
N-and C- terminal			Selected from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond		
C3	Medium chain peptide KFQ <u>W</u> 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 num	ber of bonds	5	28	0	0	2			
	Total no of int	teractive resid	dues	12	0	0	0			
	Overall perce	ntage of bond	ding		43%	0%	0%	0%		

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



Figure S15j: Binding interaction of KFQ<u>W</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C3	Medium chain peptide	GLN5	cluster4_4	-6.9	C - NA CA - NA	NA	NA	NA	
	LTMP Q WW				CB - NA CD - NA CG - NA N - NA NE ₂ - NA O - NA OE ₁ - NA				
Total number of bonds					25	0	0	1	
	Total no of int	eractive res	idues	0	0	0	0		
	Overall perce	ntage of bon	ding	0%	0%	0%	0%		

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



Figure S15k: Binding interaction of LTMPQWW 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCK 2.4 Cluster	Binding affinity ΔG (Kcal mol ⁻¹)	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY		Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
С3	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 OE ₁ - NA	NA	NA	NA	
	Total num	ber of bond	s	29	0	0	0		
	Total no of int Overall perce	eractive resi ntage of bon	idues ding	0	0	0	0		

 Table S151: Binding interaction of pancreatic lipase inhibitory peptides-TLMPQWW at C3 position.



Figure S151: Binding interaction of TLMPQWW 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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	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				
N-and C- terminal					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C3	Long chain peptide GEHGGAGMGG GQF <u>Q</u> 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 num	ber of bond	s	40	0	3	2		
	Total no of int	eractive resi	idues	0	0	0	0		
	Overall perce	ntage of bon	ding	0%	0%	0%	0%		

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



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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	Target Amino Acids	HADDOCKBin2.4affCluster\DeltaSelected(KcalfromPRODIGY	Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal				(Kcai mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C3	Long chain peptide	GLN21	cluster1_3	-9.2	C - Ile79 CA - Ile79	NA	NA	NA	
	FFRSKLLSRG				CB - NA				
	AAAAKGALLP				CD - NA				
	<u>Q</u> YW				CG - NA				
					N - NA				
					NE_2 -Irp253, Arg257				
					O = Pne/8, Ile/9 OE = Arc257, Vol260				
					$OE_1 - Arg257, Val200$				
	Total num	ber of bond	S	45	0	0	1		
	Total no of int	eractive res	idues	8	0	0	0		
	Overall perce	ntage of bon	ding	18%	0%	0%	0%		

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



Figure S16b: Binding interaction of FFRSKLLSRGAAAAKGALLP<u>Q</u>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) representing the amino acid that present in the inhibitory peptides.

Position of amino acid in	Peptide length and sequence	TargetHADDOCKAmino2.4AcidsCluster		Binding affinity ΔG	Residues of pancreatic lipase involve in protein peptide interaction and its position				
N-and C- terminal			Selected from PRODIGY	(Kcal mol ⁻¹)	Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond	
C3	Long chain peptide	ALA14	cluster3_1	-7.4	C - NA CA - Ile79	NA	NA	NA	
	SGGGGGGVAG A A T A SR				CB - Ile79 N - Ile79				
	TAT <u>A</u> SIC				O - NA				
	Total num	iber of bond	S	40	0	0	0		
	Total no of int	teractive res	idues	3	0	0	0		
	Overall perce	ntage of bon	ding	10%	0%	0%	0%		

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



Figure S16c: Binding interaction of SGGGGGGVAGAAT<u>A</u>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) representing the amino acid that present in the inhibitory peptides.
Position of amino acid in	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			
N-and C- terminal					Hydrophobic interaction	Salt Bridge	Covalent bond	Hydrogen bond
C3	Long chain peptide LNNPSVCDCD CMMK <u>A</u> 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%

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



Figure S16d: Binding interaction of LNNPSVCDCDCMMK<u>A</u>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) representing the amino acid that present in the inhibitory peptides.