

Supplementary Data

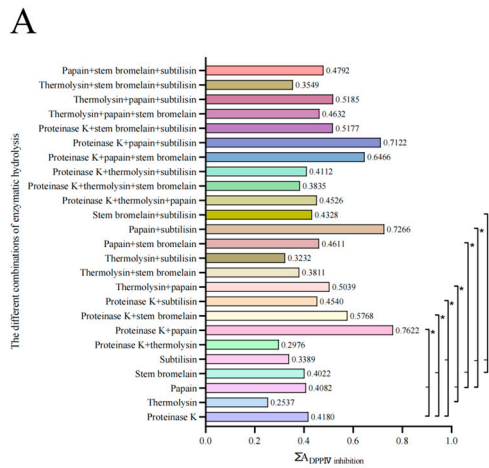


Figure S1. The total frequency of DPP-IV inhibitory peptides (ΣA_{DPP-IV} inhibition value) in goat casein and whey protein by *in silico* proteolysis using single enzymes or enzyme combinations. The * represents significant differences among different enzyme combinations ($p < 0.05$).

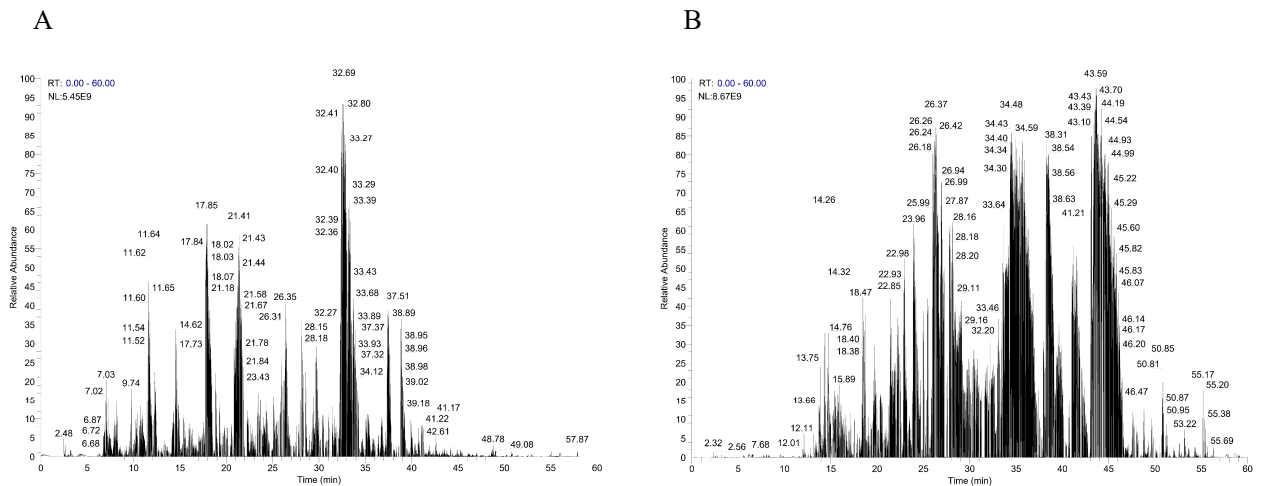


Figure S2. Basepeak plot obtained by LC-MS/MS for casein and whey protein in goat milk. A, basepeak plot of whey protein. B, basepeak plot of casein.

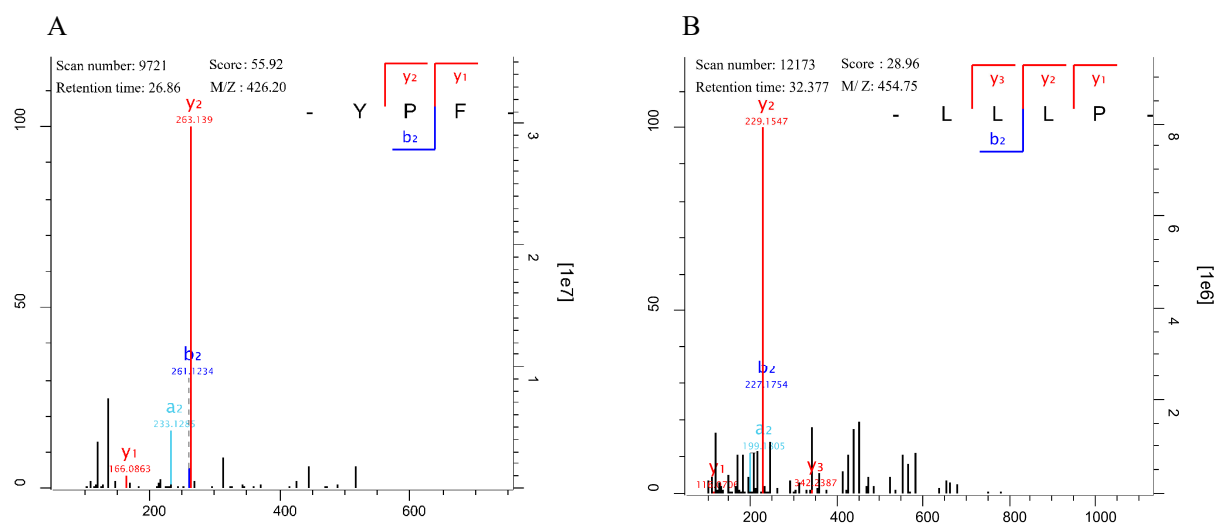


Figure S3. Mass spectrogram obtained by LC-MS/MS for YPF and LLLP in goat milk. A, mass spectrogram of YPF. B, mass spectrogram of LLLP.

Table S1 Source of identified peptides

Number	Whey protein	Casein protein	Whey protein and casein protein
1	RVY	YPF	YPF
2	KYL	WKK	WKK
3	FLF	YLY	YLY
4	WLQ	YLL	YLL
5	VLW	YLM	YLM
6	VVW	YVM	YVM
7	NEW	YVF	YVF
8	LLW	VLW	VLW
9	YLF	WYL	WYL
10	LKF	LFF	LFF
11	LYL	MLY	MLY
12	YVF	LSW	LSW
13	VWF	LEY	LEY
14	WTL	LLW	LLW
15	KLF	HPF	HPF
16	LRL	WSF	WSF
17	WLE	SWL	SWL
18	YLL	FFK	FFK
19	WSL	YAY	YAY
20	WVY	LQW	LQW
21	LEY	YQL	EFR
22	LFW	EFR	LWV
23	WYL	LWV	TLW
24	LFF	TLW	FEL
25	FEL	FEL	VVW
26	FSW	VVW	EYL
27	FLQ	EYL	VFY
28	TLW	VFY	FLF
29	LWF	FLF	LWF
30	VWE	WFK	FLQ
31	YVY	RLF	LYQ
32	RWL	LWF	WTL
33	YVE	FLQ	KDF
34	LVW	LYQ	RFL
35	DYL	WTL	WLQ
36	EYL	SWE	HFL
37	YLY	KDF	VTW
38	KLY	RFL	LWK
39	VYW	WLQ	MFF
40	FVY	HFL	AFY
41	FLK	YYV	DYL
42	WKK	VTW	NLY

Number	Whey protein	Casein protein	Whey protein and casein protein
43	VEW	LWK	YTF
44	YRL	WEV	LLR
45	VFY	MFF	WLM
46	LFE	AFY	YYF
47	HFL	DYL	FEK
48	FFK	YPY	FVY
49	LSW	NLY	TWY
50	LLR	NYY	LEF
51	WDL	YTF	LFW
52	TWY	LLR	KLY
53	HPF	WLM	VEW
54	WLM	TYF	YSF
55	LTW	YYF	TFF
56	LEF	WKP	WAE
57	TFF	FRY	YLR
58	YLE	FEK	FLK
59	VTW	FVY	VWF
60	SWL	TWY	WVL
61	YPF	LEF	YVR
62	WRQ	TWL	YWL
63	YSF	LFW	WVY
64	YVQ	WAY	RWL
65	WVL	FLE	VWY
66	AWY	KLY	QVY
67	PFR	VEW	LRL
68	WQL	YSF	FKF
69	FDF	TFF	LHY
70	YHR	WAE	YFS
71	QDF	YLR	FTR
72	LYQ	WYA	HYL
73	YAY	FLK	YLK
74	YLK	VWF	MEY
75	LHY	SYF	YLE
76	RLQ	WVL	SKW
77	KDF	YVR	YVE
78	RFL	YWL	YRL
79	LHW	WVY	RSF
80	MFF	RWL	NEW
81	NFF	KEY	FNQ
82	TFW	VWY	YYK
83	LQW	QVY	QFE
84	YTF	FEY	WAH
85	HYL	RDW	REL

Number	Whey protein	Casein protein	Whey protein and casein protein
86	TQW	LNK	YVH
87	SKW	LRL	FDQ
88	WRK	FKF	WLH
89	FEK	LHY	RVY
90	SEW	YRY	YHT
91	VMY	WSR	FYK
92	ELF	NWT	HER
93	YHL	YFS	VYPF
94	RFQ	LYR	VPPF
95	WLD	FYA	YLPL
96	YYF	FTR	VTVL
97	WFT	HYL	TLVF
98	LWV	YLK	TLLA
99	VWY	MEY	PEVL
100	LWK	YLE	TSVL
101	WTQ	SKW	LLPL
102	MWL	YVE	PAAF
103	EFR	YRL	TLTL
104	MLY	YYH	VTTL
105	MSW	RSF	YVLA
106	RAW	NEW	VTPQ
107	YYK	FNQ	YVYP
108	RSF	YHV	QLPE
109	WLH	YYK	VTEL
110	QVY	QFE	TLAL
111	KMF	WAH	LLLL
112	LYK	REL	TDVL
113	VWK	YVH	LFSL
114	EFM	FDQ	TPVV
115	TTW	WLH	VTLY
116	FWV	RVY	LLLP
117	YWL	YHT	VSVL
118	YHF	FYK	VKPE
119	FNQ	HER	VTLV
120	PWL	VYPF	YVVT
121	LRQ	VPPF	VLLK
122	YLD	FTVP	LLTV
123	YFS	YLPL	VLTV
124	WAE	FPPQ	VPVQ
125	FKF	VTVL	TLLL
126	AFY	TLVF	VATL
127	VYR	TLLA	VTLF
128	MHF	PEVL	YLAV

Number	Whey protein	Casein protein	Whey protein and casein protein
129	NLY	TSVL	FEVS
130	EDF	LLPL	LLKL
131	YLM	PAYT	VTLQ
132	QFE	PAAF	VTAF
133	YLR	TLTL	YTTL
134	QFF	VTTL	TLTV
135	WAQ	YVLA	TLLT
136	RMF	VTPQ	SLTF
137	TPW	TDVE	RHVP
138	HER	YVYP	TPTK
139	YWS	QLPE	YVLT
140	FYK	TLDV	GEDF
141	KFH	VTEL	SKLL
142	FQF	TLAL	LEPL
143	RDF	LLLL	FEVQ
144	LEW	TDVL	VTVQ
145	YVH	LFSL	VLLT
146	QPY	TPVV	YESL
147	YTM	VTLY	SFAL
148	YVR	VTAL	TLAV
149	YVM	LEYS	VFTV
150	QQF	LLLP	VLVE
151	EEF	VSVL	LELA
152	TVW	VKPE	VELY
153	YRV	VTLV	YVLL
154	FTR	YVVT	YTLV
155	WKE	TQDT	VTEF
156	RRH	VLLK	VTKE
157	RRQ	LLTV	VTLP
158	RHN	ATSY	NETV
159	FDQ	LLLG	LATF
160	HFT	VLTV	YVVE
161	REL	VPVQ	LLVT
162	TDW	TLLL	LAVQ
163	WTN	VATL	PEVK
164	YHT	VTLF	VTKP
165	MEY	FYPD	VPSK
166	RFK	YLAV	LELF
167	EFH	VFVG	VGAW
168	YLQ	FEVS	GELF
169	THW	LLKL	LEGF
170	QFQ	VTLQ	LEVT
171	RQT	VTAF	LKLE

Number	Whey protein	Casein protein	Whey protein and casein protein
172	WAH	LPAF	VLDL
173	WSF	YTTL	LPPL
174	QFH	TLTV	VSTL
175	VTDL	TLLT	TLSW
176	VYPF	LYVP	VTDL
177	LFSL	HLSW	TAYV
178	VESL	SLTF	TPPL
179	VVVL	RHVP	VKVL
180	VPPF	PDPV	VFLN
181	VTVQ	PLLV	VGQL
182	VTPQ	TPTK	VNVK
183	TLLA	YVLT	YLVA
184	VPVQ	GEDF	FALE
185	LLTV	SKLL	TLQA
186	LHLR	LEPL	TLSL
187	VTTL	FEVQ	VEVF
188	VELL	VTVQ	VELV
189	SPPL	VLLT	TLKL
190	WVEA	YESL	YSLQ
191	LLVQ	SFAL	VLEP
192	VEFA	TLAV	NSLL
193	QLPE	VFTV	SKKA
194	LLLL	VLVE	LEVA
195	TLTL	VHVL	TTAE
196	YLAV	TSLM	LLEA
197	LELY	LELA	VEPF
198	TPPL	VELY	VTLK
199	LLKQ	YVLL	VTSV
200	VQLV	YTLV	LAVE
201	NFPA	VTEF	LEGH
202	VTVL	VSLV	NFPA
203	YLPL	VTKE	LHLR
204	TLVF	VTLP	VALK
205	TPTK	YSVS	VELK
206	PLLL	NETV	FEAL
207	TLTV	YEVN	TPPK
208	WLGL	LATF	LKLS
209	VTSL	YVVE	TLVE
210	VQVA	LLVT	VEFA
211	LELF	LRLF	PPLE
212	VEFL	LAVQ	SSVF
213	VTSV	PEVK	FFTK
214	VAPF	VTKP	EDLQ

Number	Whey protein	Casein protein	Whey protein and casein protein
215	TLLT	MLYQ	VQNL
216	LLAN	VELQ	ELYK
217	LLTL	VPSK	VGLD
218	YVLL	LELF	PGKL
219	LLKL	LDVE	SSKV
220	VLTV	VGAW	VTPE
221	VGQL	PFPT	VVPQ
222	LEVL	GELF	VDVT
223	FELL	LMLQ	FAAE
224	THKV	PFSP	TKEP
225	VPDL	VLPL	VEEE
226	TLNL	LEGF	KLLA
227	FEVS	LEVT	LAVR
228	VETD	LKLE	SNVL
229	TEVE	VLDL	SSTF
230	LELK	LPPL	YTGE
231	TLVE	VSTL	VTTE
232	SDLL	VPVT	TDLA
233	VEVL	TLSW	PGLK
234	VTLV	VTDL	VASE
235	VEVT	GQPK	LLTS
236	MELL	TAYV	MFPPQ
237	YSLL	TPPL	TPVVV
238	YTLL	VKVL	PAALE
239	TLLL	VFLN	KEMPFK
240	VLVE	VGQL	LPAPIVR
241	LKLS	VNVK	RGPFILV
242	WLVL	YLVA	TEEEKNRLN
243	VTLQ	PPQP	VEELKPTPEGN
244	LAVE	APAY	GLSPEVPNENLLR
245	LELA	PKPA	ELKPTPEGNLEIL
246	LLEA	FALE	-
247	LLVR	HFLY	-
248	VAKL	TLQA	-
249	TSVL	TLSL	-
250	WLVK	PEPE	-
251	VTLF	PKVL	-
252	VLLT	VEVF	-
253	VTTW	VELV	-
254	LEVT	TLVD	-
255	TKPL	TLKL	-
256	RLLK	YSLQ	-
257	VTEF	VMLY	-

Number	Whey protein	Casein protein	Whey protein and casein protein
258	VTEL	VLEP	-
259	TGLL	SSTK	-
260	VVEQ	VPLL	-
261	VVVK	FHVM	-
262	PEAL	NSLL	-
263	FRPD	SKKA	-
264	LLKV	VFVN	-
265	KCSS	LEVA	-
266	TGLE	TETL	-
267	EALL	PLAD	-
268	TLSL	PLDL	-
269	LFVL	TTAE	-
270	HLPL	LLEA	-
271	VTPE	VEPF	-
272	VLLK	VTLK	-
273	PFVT	VTSV	-
274	VTAE	LAVE	-
275	KLLA	LEGH	-
276	LKLE	TQPL	-
277	PEVL	NFPA	-
278	VTKV	TESF	-
279	LEPL	LHLR	-
280	LPPL	VALK	-
281	ELLK	VELK	-
282	LAVT	FEAL	-
283	NELQ	TPPK	-
284	QPPK	LKLS	-
285	VTDW	SPFQ	-
286	EAVF	TLVE	-
287	LLKD	VEFA	-
288	VEVQ	PPLE	-
289	SLTF	SSVF	-
290	FPEV	FFTK	-
291	KGWS	EDLQ	-
292	YLLK	PKCQ	-
293	LEVA	VQNL	-
294	LLVT	ELYK	-
295	TDLL	VGLD	-
296	QFPF	VPYY	-
297	VSPL	PGKL	-
298	PPGR	VTEA	-
299	VTLP	SSKV	-
300	LLLQ	VTPE	-

Number	Whey protein	Casein protein	Whey protein and casein protein
301	FEFL	VVPQ	-
302	VDPL	VDVT	-
303	VFAE	FAAE	-
304	VLNL	TKEP	-
305	YSLQ	VEEE	-
306	SSLL	KLLA	-
307	VQLS	LAVR	-
308	SFLE	VPSR	-
309	VHKL	SNVL	-
310	YRVY	SSTF	-
311	VPSK	YTGE	-
312	LLAE	VTTE	-
313	VTAF	TDLA	-
314	PLVR	PGLK	-
315	PAAF	VASE	-
316	VEVF	LLTS	-
317	YESL	MFPPQ	-
318	VVLE	MPFPK	-
319	VRLQ	TPVVV	-
320	VLDL	VDVPF	-
321	EDLQ	PAALE	-
322	LKLK	KEMPPFK	-
323	VVTL	LPAPIVR	-
324	VEGL	TPVVVPPF	-
325	YVVA	RGFPILV	-
326	TLAV	EEKNRLN	-
327	PLVL	TEDELQDK	-
328	YVYP	TEEKNRLN	-
329	VVTF	HPHPLSFM	-
330	VDPP	VASLLGLSL	-
331	VKLD	SPEVPNENLL	-
332	TSQL	EKDERFFDDK	-
333	FDVD	SPEVPNENLLR	-
334	TLDP	MNKLLSPIVPQ	-
335	TKLL	FSDIPNPIGSE	-
336	VNFL	VEELKPTPEGN	-
337	VDVT	KDERFFDDKIA	-
338	EELL	KPTPEGNLEIL	-
339	SKLL	EMPPFKYPVEPF	-
340	YAVA	TPVVVPPFLQPE	-
341	QKLL	TEDELQDKIHPF	-
342	TLAL	LSPEVPNENLLR	-
343	YVLA	PTVVVEDLRLCT	-

Number	Whey protein	Casein protein	Whey protein and casein protein
344	RGQF	SLSQPKVLPVPQ	-
345	LHSL	PILVTPSLDPLQ	-
346	TDVL	GLSPEVPNENLLR	-
347	VGAW	KEMPFPKYPVEPF	-
348	REDF	ELKPTPEGNLEIL	-
349	TLVY	HKEMPFPKYPVEPF	-
350	VAFN	-	-
351	TTSL	-	-
352	VELY	-	-
353	TLKL	-	-
354	VKVL	-	-
355	VALE	-	-
356	GELF	-	-
357	VTLY	-	-
358	VQNL	-	-
359	FAAE	-	-
360	LEVS	-	-
361	VFTV	-	-
362	VTVE	-	-
363	TEVK	-	-
364	WLTl	-	-
365	VATL	-	-
366	KRVL	-	-
367	YPSP	-	-
368	PEVK	-	-
369	LLPL	-	-
370	VMLL	-	-
371	VLAw	-	-
372	GFDL	-	-
373	TSLF	-	-
374	VAVL	-	-
375	FEAL	-	-
376	TDLA	-	-
377	TLSW	-	-
378	YEFK	-	-
379	VALL	-	-
380	YLLE	-	-
381	LFSE	-	-
382	SSML	-	-
383	LSDD	-	-
384	GEDF	-	-
385	VSVL	-	-
386	VELV	-	-

Number	Whey protein	Casein protein	Whey protein and casein protein
387	PFAQ	-	-
388	AYLK	-	-
389	FFTK	-	-
390	MKVL	-	-
391	YVVE	-	-
392	VTKP	-	-
393	VALK	-	-
394	TPVV	-	-
395	PAYV	-	-
396	VKSP	-	-
397	TLLW	-	-
398	RSKC	-	-
399	VTVN	-	-
400	VEPF	-	-
401	VKAE	-	-
402	KAYS	-	-
403	VLSL	-	-
404	SPLL	-	-
405	LETK	-	-
406	PFVL	-	-
407	VVPK	-	-
408	YTLV	-	-
409	YSAE	-	-
410	SFAL	-	-
411	LEKG	-	-
412	LLSA	-	-
413	LLTS	-	-
414	QALL	-	-
415	VTWD	-	-
416	LQQN	-	-
417	YVLT	-	-
418	LAVR	-	-
419	DFGL	-	-
420	SSVF	-	-
421	SPVL	-	-
422	VEPL	-	-
423	SSQL	-	-
424	VFTQ	-	-
425	LEGF	-	-
426	VTLK	-	-
427	FALE	-	-
428	TWAR	-	-
429	TFLE	-	-

Number	Whey protein	Casein protein	Whey protein and casein protein
430	VPKP	-	-
431	VQWL	-	-
432	TLMC	-	-
433	VVPQ	-	-
434	FAVP	-	-
435	TPPK	-	-
436	SNVL	-	-
437	AKLL	-	-
438	LFKV	-	-
439	VTWQ	-	-
440	VELK	-	-
441	FALT	-	-
442	QLKF	-	-
443	EAPF	-	-
444	PALF	-	-
445	YTTL	-	-
446	PEKV	-	-
447	VTTE	-	-
448	ELYK	-	-
449	SDVF	-	-
450	YVVT	-	-
451	VEEE	-	-
452	LRPL	-	-
453	NVTV	-	-
454	SSYT	-	-
455	VLEP	-	-
456	PKPK	-	-
457	VTLH	-	-
458	NSLL	-	-
459	TKEP	-	-
460	LATF	-	-
461	VLVS	-	-
462	VAVR	-	-
463	RHVP	-	-
464	LAVQ	-	-
465	TPEP	-	-
466	VTLT	-	-
467	FDVW	-	-
468	VASE	-	-
469	LLLP	-	-
470	VSTL	-	-
471	LEYQ	-	-
472	QKGW	-	-

Number	Whey protein	Casein protein	Whey protein and casein protein
473	YTGE	-	-
474	YGTD	-	-
475	FEVQ	-	-
476	RFVS	-	-
477	LKEY	-	-
478	VGLD	-	-
479	LAWL	-	-
480	YVHE	-	-
481	SRTT	-	-
482	HKVT	-	-
483	QNLE	-	-
484	VPLK	-	-
485	RPAE	-	-
486	VFLN	-	-
487	TLLK	-	-
488	KAVF	-	-
489	PPLE	-	-
490	VGTY	-	-
491	TLKW	-	-
492	YLVA	-	-
493	VMLE	-	-
494	AAQL	-	-
495	EPYA	-	-
496	YAVK	-	-
497	FDTD	-	-
498	TEPP	-	-
499	TKPE	-	-
500	PNLV	-	-
501	VEDE	-	-
502	PGKL	-	-
503	RLAW	-	-
504	GDTY	-	-
505	EAPT	-	-
506	LKPP	-	-
507	PEFH	-	-
508	LETE	-	-
509	LLRA	-	-
510	NYVV	-	-
511	HEAL	-	-
512	PGWL	-	-
513	VKPE	-	-
514	TTVT	-	-
515	TAYV	-	-

Number	Whey protein	Casein protein	Whey protein and casein protein
516	NETV	-	-
517	LLSK	-	-
518	VERR	-	-
519	EDVS	-	-
520	PGLK	-	-
521	VNVK	-	-
522	VTTK	-	-
523	TTAE	-	-
524	VRKQ	-	-
525	LHTS	-	-
526	SSTF	-	-
527	KGTE	-	-
528	SKKA	-	-
529	PLPP	-	-
530	SSVR	-	-
531	VAKF	-	-
532	LRVK	-	-
533	LDHA	-	-
534	VTSK	-	-
535	YVYK	-	-
536	TLQA	-	-
537	EPVL	-	-
538	VAWF	-	-
539	RQGG	-	-
540	LEGH	-	-
541	LVAK	-	-
542	LVRQ	-	-
543	NVRF	-	-
544	VTKE	-	-
545	VETH	-	-
546	SSKV	-	-
547	VELSN	-	-
548	MFPPQ	-	-
549	TLLTV	-	-
550	VEGLE	-	-
551	TPVVV	-	-
552	THKLE	-	-
553	PAALE	-	-
554	VLPLV	-	-
555	VSVPE	-	-
556	LPAPIVR	-	-
557	KEMPFPK	-	-
558	SPRDVLVR	-	-

Number	Whey protein	Casein protein	Whey protein and casein protein
559	HKEMPFPK	-	-
560	SGDNVSVR	-	-
561	REVELEDQ	-	-
562	RGPFPILV	-	-
563	VSDDYVGR	-	-
564	TSSEIDRF	-	-
565	VRTPEVDKE	-	-
566	WGPLEPEGQ	-	-
567	TEEEKNRLN	-	-
568	GQSGKDPNHF	-	-
569	LTEEEKNRLN	-	-
570	VEELKPTPEGN	-	-
571	SGKDPNHFRPA	-	-
572	GNQELPREKYL	-	-
573	AEDPSQDIVER	-	-
574	LNPEDETHLE	-	-
575	TYPDSESPLTT	-	-
576	KGGYLPPEEIK	-	-
577	VLAPPQEELSK	-	-
578	EVDDTIQTLQQ	-	-
579	ELTDDKNQRFF	-	-
580	EDPSQDIVERN	-	-
581	SPFPVHPGTPE	-	-
582	RQPQNQNPKLPL	-	-
583	APPQEELSKSTL	-	-
584	GPGAPADPGRPA	-	-
585	AHLHTPMYFFISQ	-	-
586	ELKPTPEGNLEIL	-	-
587	VEELKPTPEGNLE	-	-
588	GLSPEVPNENLLR	-	-
589	QADVIGTETLERL	-	-
590	SPRQPQNQNPKLPL	-	-
591	RSPRQPQNQNPKLPL	-	-
592	ELDPAPNDEVDPGTR	-	-
593	VTYPKVQMLVNMFYVL	-	-
594	YLRSTNWDTRIAAGQAVEAIVK	-	-

Table S2 The pharmacokinetic properties and physicochemical properties of 105 peptides and IPI were further investigated by ADME evaluation

Nu m b e r	Molecule	Canonical SMILES	For m u l a	MW	#H e a v y a t o m s	#Ar o m a t i c h e a v y a t o m s	F r a c t i o n a b l e	#R o t a t i o n a l a c c e p t o r s	#H - b o n d s	#H - b o n d s	M R	T P S A	i L O G P	X L O G P	W L O G P	M L O G P	S il ic o n s e n s i t i v e n e s s	C o n s e n s i t i v e n e s s	ES O L So lu bil ity (m g/ ml)	E S O L So lu bil ity (m ol/ l)	E S O L C l a s s	A l i S o l u b i l i t y (m g/ ml)	Al i S o l u b i l i t y (m ol /l)	Al i S o l u b i l i t y (m ol /l)	Al i S o l u b i l i t y (m ol /l)	Si l i c o s - I T L o g S w	Sili cos -IT Sol ubi lity (m g/ ml)	Sil ico s-IT Sol ubi lity (m ol/l)	Si l i c o s - IT cl a s s	G I a b s o r p t i o n	B B p s u e r m e a n t	P g p s u b s t r a t e	C Y P 1 A 2 i n h i b i t o r	C Y P 2 C 1 9 i n h i b i t o r	C Y P 2 C 9 i n h i b i t o r	C Y P 2 D 6 i n h i b i t o r	C Y P 3 A 4 i n h i b i t o r	l o g K p (c m / s)	Li p i n s k i # v i o l a t i o n s	G h o s e # v i o l a t i o n s	V e b e r # v i o l a t i o n s	E g a n # v i o l a t i o n s	M u e g g e # v i o l a t i o n s	Bi o a v a l i t y S c o r e	P A I N S # a l l e r t s	B r e n k # a l l e r t s	Le a d l i k e n e s s # v i o l a t i o n s	Sy n t h e t i c A c c e s s i b i l i t y																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
1	FRPD	NC(=N)CCCC[C@@H](C(=O)N1CCC[C@H](C(=O)O)CC(=O)O)NC(=O)[C@H](Cc1ccccc1)N	C24H35N7O7	538	36	0.185	1	9	8	13	24	19	10	-5.21	-5.21	-5.03	-5.03	-1.64	68.9	12.9	Highly soluble	0.23	4.34	Highly soluble	0.23	4.34	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly soluble	Highly

9	RQ	H](C(=O)N[C@H](C(=O)O)CCC(=O)N)NC(=O)[C@H](Cc1c[nH]c2c1cccc2)N	2232N8O5	885		.41	7			28.235	42.81	.48	39186	136	02	1.29	.53	40	36	ighlysoluble	0.58	8	262	erysoluble	4.08	403	000824	oderatelysoluble	o	o	o	o	o	o	o	o	12.06						17					29
20	APAY	Oc1ccc(cc1)C[C@@H](C(=O)O)NC(=O)[C@@H](NC(=O)[C@@H]1CCCN1C(=O)[C@@H](N)C)C	C20H24N4O6	436	0	1	7	5	111	16.21	18.16	-2.83	-1082	0.01	-0.54	-0.18	278	0.66	Verysoluble	-0.17	28	0.671	Verysoluble	-2.23	2.47	0.0587	Soluble	L	N	N	N	N	N	N	N	-10.77	0	1	2	1	2	0.55	0	0	2	3.75		
21	FTR	NC(=N)NCCC[C@@H](C(=O)O)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H](Cc1cccc1)N	C19H23N6O5	436	0	1	7	8	10984	203745	0.47	-107958	-4178	-0.58	-1.396	0	3850	9.11	Hightlysoluble	0.42	1100	2.61	Hightlysoluble	-2.73	0.792	0.0187	Soluble	L	N	Y	N	N	N	N	N	-11.78	2	1	2	1	3	0.17	0	2	2	4.05		
22	WDL	CC(C[C@@H](C(=O)O)NC(=O)[C@@H](NC(=O)[C@H](Cc1c[nH]c2c1cccc2)N)CC(=O)O)C	C21H24N4O6	439	0	1	7	6	11322	17461	1.29	-0.65	1.35	0.54	0.271	-0.8	83194	0.194	Verysoluble	-1.3	21.8	0.0503	Verysoluble	-3.75	0.0773	0.0179	Soluble	L	N	N	N	N	N	N	N	-10.25	1	0	2	1	2	0.11	0	0	2	3.96		

79	WTL	CC(C[C@@H](C(=O)O)NC(=O)[C@H]([C@H](O)C)NC(=O)[C@H](Cc1c[nH]c2c1ccc2)N)C	C211830N4O5	41849	30	9	0.48	12	6	6	112559	112754	11276231	-1.52	0.83	1.03	0.86	58.2	0.139	Very soluble	-1.2	26.5	0.0632	Very soluble	-3.84	0.0599	0.00143	Soluble	Low	No	Yes	No	No	No	No	No	No	-9.99	1	0	2	1	2	0.55	0	0	2	4.01
80	LYL	Oc1ccc(cc1)C[C@@H](C(=O)N[C@H](C(=O)O)CC(C)C)NC(=O)[C@H](CC(C)C)N	C211733N3O5	4209	6	0.57	13	6	5	1112215	114106	2.105	-1.431	1.11	2.05	1.06	-0.82	62	0.152	Very soluble	-1.14	29.7	0.0729	Very soluble	-3.76	0.0708	0.00174	Soluble	High	No	Yes	No	No	No	No	No	-9.74	0	0	2	1	0	0.55	0	0	2	3.74	
81	WVY	Oc1ccc(cc1)C[C@@H](C(=O)O)NC(=O)[C@H](C(C)C)NC(=O)[C@H](Cc1c[nH]c2c1cccc2)N	C25630N4O5	434	15	0.32	12	6	6	128333	125754	2.842	-1.72	0.58	2.12	1.04	-2.48	4.64	0.00995	Soluble	-2.42	1.76	0.00377	Soluble	-5.88	0.00618	0.00132	Moderately soluble	Low	No	Yes	No	No	No	No	No	-9.44	1	0	2	1	2	0.55	0	0	2	4.02	
82	FSW	OC[C@@H](C(=O)N[C@H](C(=O)O)Cc1c[nH]c2c1cccc2)NC(=O)[C@H](Cc1ccccc1)N	C23826N4O5	432	15	0.26	12	6	6	117854	117794	2.709	-2.39	0.031	2.03	0.45	-0.8	70	0.16	Very soluble	-0.69	89.4	0.204	Very soluble	-5.49	0.0143	0.00325	Moderately soluble	Low	No	No	No	No	No	No	No	-10.46	1	0	2	1	3	0.55	0	0	2	3.83	
83	WS	OC[C@@H](C(=O)N[C@H](C(=O)O)Cc1c[nH]c2c1cccc2)N	C232	432	15	0.2	12	6	6	1150	1150	0.2	-0.2	2.0	0.1	-0.0	70	0.16	Ver	-0.4	89.20	0.20	Ver	-5.01	0.00	0.00	Moderately soluble	Low	No	No	No	No	No	No	No	-1	1	0	2	1	3	0.55	0	0	2	3.83		

