Supplementary Information

Development of a Process for Hydrolysis of Chicken Blood Meal and Identification of Bioactive Peptides by LC-MS/MS

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Table S1. Analysis of variance of NaOH hydrolysis - degree of hydrolysis

Source of variation	DF	SQ	MS	*F*-value	*P*-value
Mode	4	457.749	114.437	32.79	0
Linear	2	453.38	226.69	64.96	0
Substrate	1	75.232	75.232	21.56	0.001
NaOH	1	378.148	378.148	108.35	0
Interactions	1	0.397	0.397	0.11	0.743
Curvature	1	3.972	3.972	1.14	0.311
Error	10	34.899	3.49		
Total	14	492.648			

DF: degrees of freedom, SQ: sum of squares, MS: mean square.

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Table S2. Model coefficients with standard errors and statistical significance

Predictor	Estimate	Standard error	*t*-Statistic	*P*-value
Intercept	17.90049762	0.485366415	36.88037958	7.02323E-13
Sample	–2.503863702	0.542656149	–4.61408888	0.000747543
NaOH	5.613582406	0.542656149	10.34463982	5.26417E-07
Sample:NaOH	0.181961262	0.542656149	0.335315951	0.743694523

$p < 0.05$ indicates that the effect of the variable is statistically significant. Regression equation: y = 17.9 + 2.5x1 + 5.6 x2 + 0.18x1x2.

Table S3. Analysis of variance of NaOH hydrolysis - nitrogen

Source of variation	DF	SQ	MS	*F*-value	*P*-value
Mode	4	1.91492	0.47873	132.53	0
Linear	2	1.87197	0.93599	259.11	0
Substrate	1	1.79312	1.79312	496.39	0
NaOH	1	0.07885	0.07885	21.83	0.005
Interactions	1	0.03512	0.03512	9.72	0.026
Curvature	1	0.00783	0.00783	2.17	0.201
Error	5	0.01806	0.00361		
Total	9	1.93298			

DF: degrees of freedom, SQ: sum of squares, MS: mean square.

Table S4. Estimated coefficients of the multiple linear regression evaluating the effects of sample and NaOH on the response variable

Predictor	Estimate	Standard Error	*t*-Statistic	*P*-value
Intercept	2.096727993	0.020772884	100.9358169	6.37325E-11
x_1 NaOH	–0.099281729	0.02322479	–4.274817073	0.005235305
x_2 Sample	0.473434265	0.02322479	20.38486733	9.05963E-07
NaOH:Sample	–0.066255762	0.02322479	–2.852803497	0.029074565

$p < 0.05$ indicates that the effect of the variable is statistically significant. Regression equation**:**. y = 2.09 + 0.01x1 + 0.48x2 + 0.06x1x2.

Table S5. Analysis of variance for hydrolysis with Alcalase - degree of hydrolysis

Source of variation	DF	SS	MS	*F*-value	*P*-value
Model	4	51.68	12.92	43.8	0
Linear	2	45.5	22.75	77.12	0
Substrate	1	30.09	30.09	102.02	0
Enzyme	1	15.4	15.4	52.23	0.001
Interactions	1	5.79	5.79	19.63	0.007
Curvature	1	0.39	0.39	1.33	0.301
Error	5	1.47	0.29		
Total	9	53.15			

DF: degrees of freedom, SS: sum of squares, MS: mean square.

Table S6. Model coefficients with standard errors and statistical significance

Predictor	Estimate	Standard deviation	Estat.t	*P*-value
Intercept	9.843928453	0.176428563	55.79554847	2.22593E-09
Sub	1.939515588	0.19725313	9.832622607	6.37667E-05
Enzyme	1.387749749	0.19725313	7.035375039	0.000412053
Sub:Enzyme	0.850800568	0.19725313	4.313242416	0.005019608

$p < 0.05$ indicates that the effect of the variable is statistically significant**.** Regression equation: y = 9.84 + 1.94x1 + 1.39x2 + 0.85x1x2.

Table S7. Analysis of variance for hydrolysis with Alcalase - nitrogen

Source of Variation	DF	SS	MS	*F*-value	*P*-value
Model	4	0.89	0.22	25.82	0.002
Linear	2	0.86	0.43	50.11	0
Substrate	1	0.61	0.61	70.64	0
Enzyme	1	0.25	0.25	29.58	0.003
Interactions	1	0.02	0.02	2.38	0.183
Curvature	1	0.005	0.005	0.69	0.444
Error	5	0.004	0.008		
Total	9	0.94			

DF: degrees of freedom; SS: sum of squares; MS: mean square.

Table S8. Estimated coefficients of the multiple linear regression evaluating the effects of substrate and enzyme on the response variable

Predictor	Estimate	Standard deviation	Estat.t	*P*-value
Intercept	0.970616086	0.02868916	33.83215424	4.43982E-08
x1 Sub	0.276862651	0.032075456	8.631604522	0.000133159
x2 Enzyme	0.179154039	0.032075456	5.58539336	0.00139957
Sub:Enzyme	0.050923037	0.032075456	1.587601351	0.163474658

$p < 0.05$ indicates that the effect of the variable is statistically significant. Regression equation: y = 0.97 + 0.28x1 + 0.18x2 + 0.05x1x2.

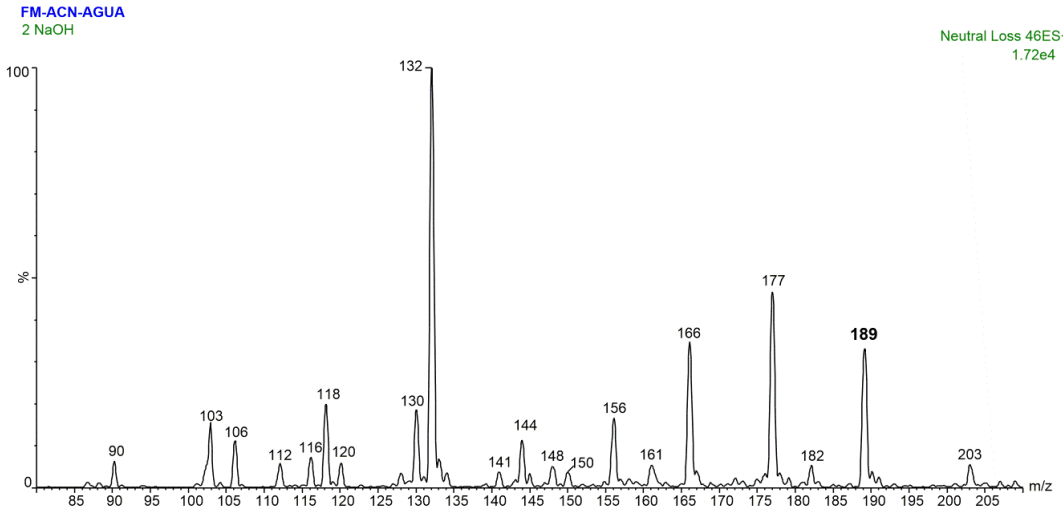

Figure S1. LC-MS/MS of 46 Da neutral loss from experiment 2 (80-210) of the alkaline hydrolysate of chicken blood meal.

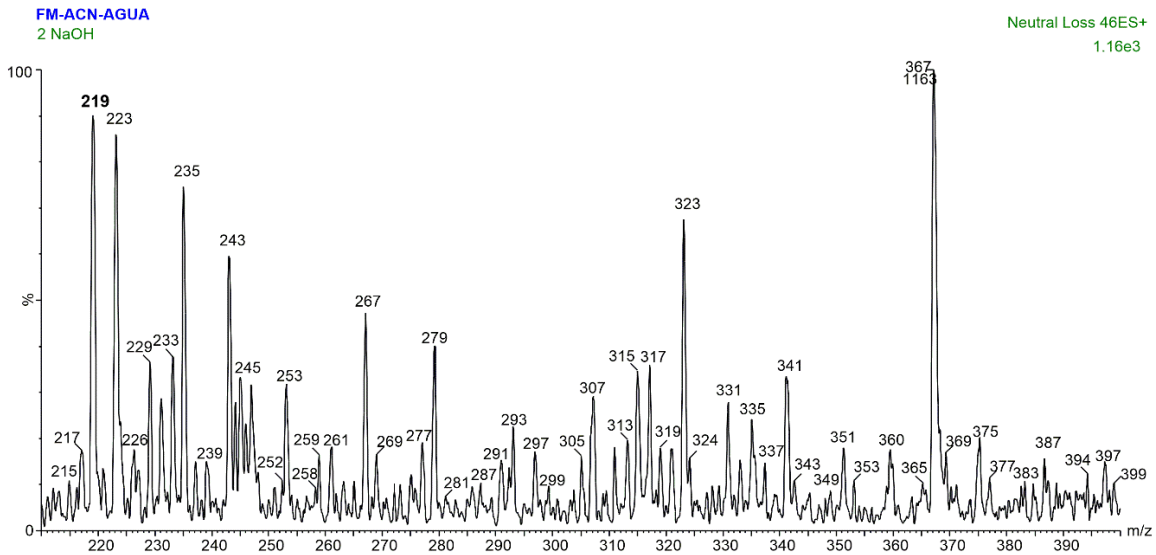

Figure S2. LC-MS/MS of 46 Da neutral loss from experiment 2 (210-400) of the alkaline hydrolysate of chicken blood meal.

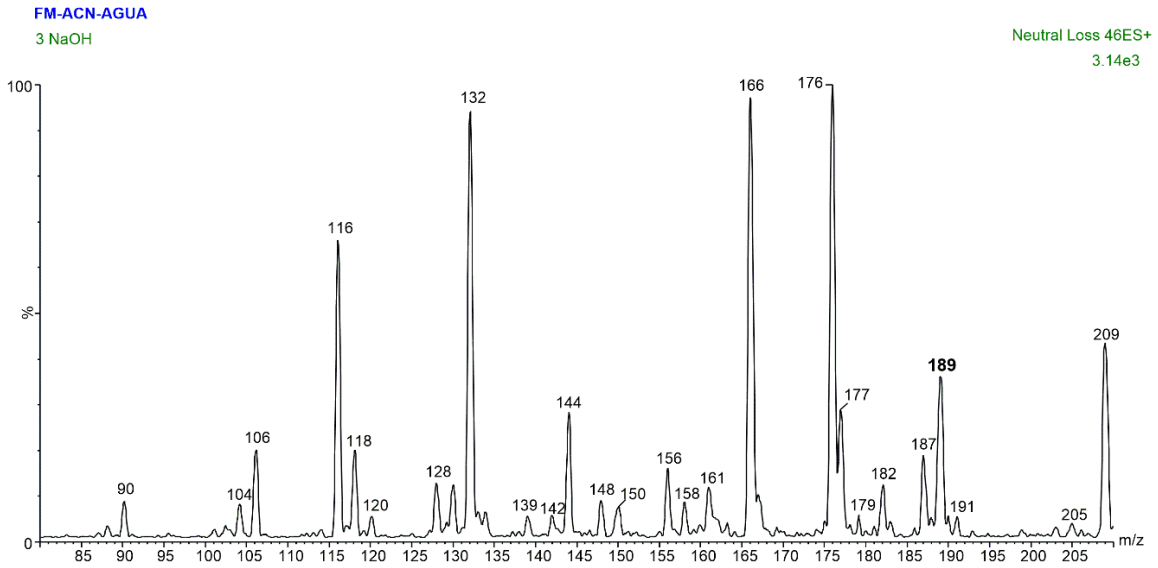

Figure S3. LC-MS/MS of 46 Da neutral loss from experiment 3 (80-210) of the alkaline hydrolysate of chicken blood meal.

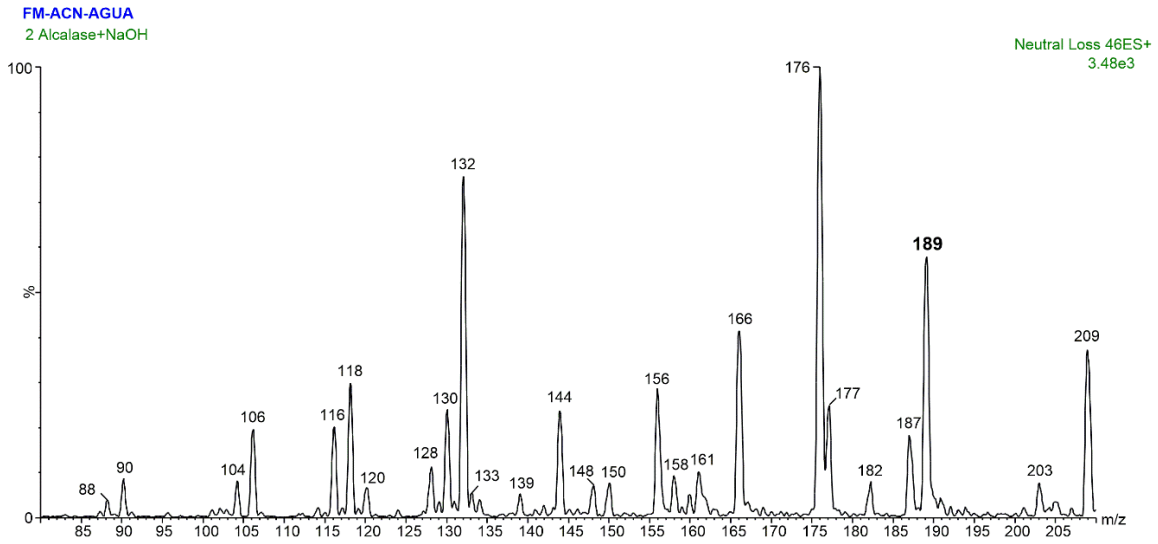

Figure S4. LC-MS/MS of 46 Da neutral loss from experiment 2 (80-210) of the hydrolysate combined with Alcalase and NaOH from chicken blood meal.

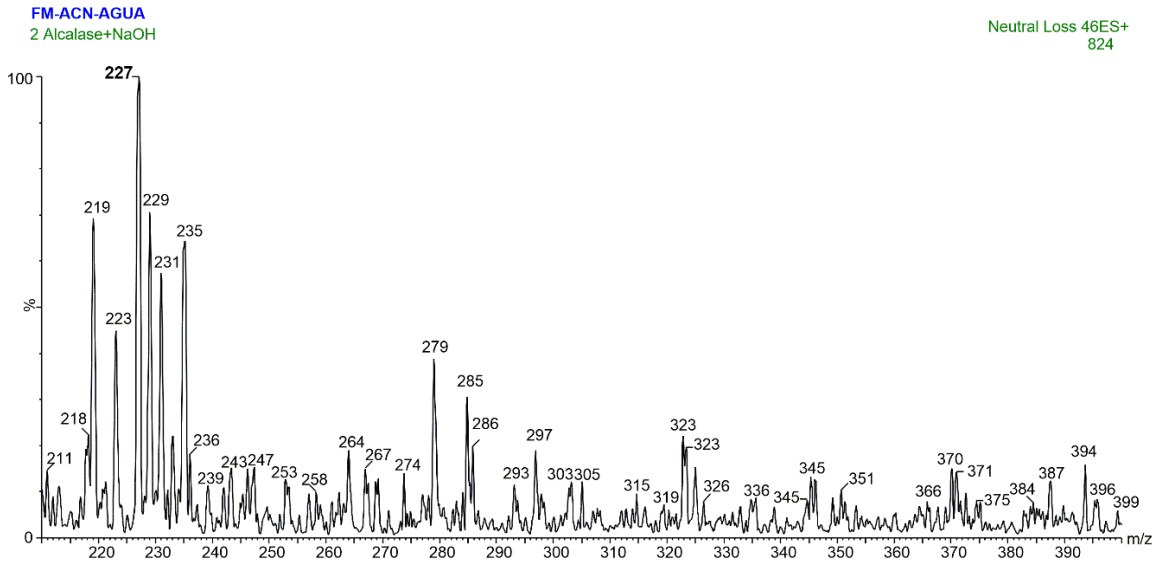

Figure S5. LC-MS/MS of 46 Da neutral loss from experiment 2 (210-400) of the hydrolysate combined with Alcalase and NaOH from chicken blood meal.

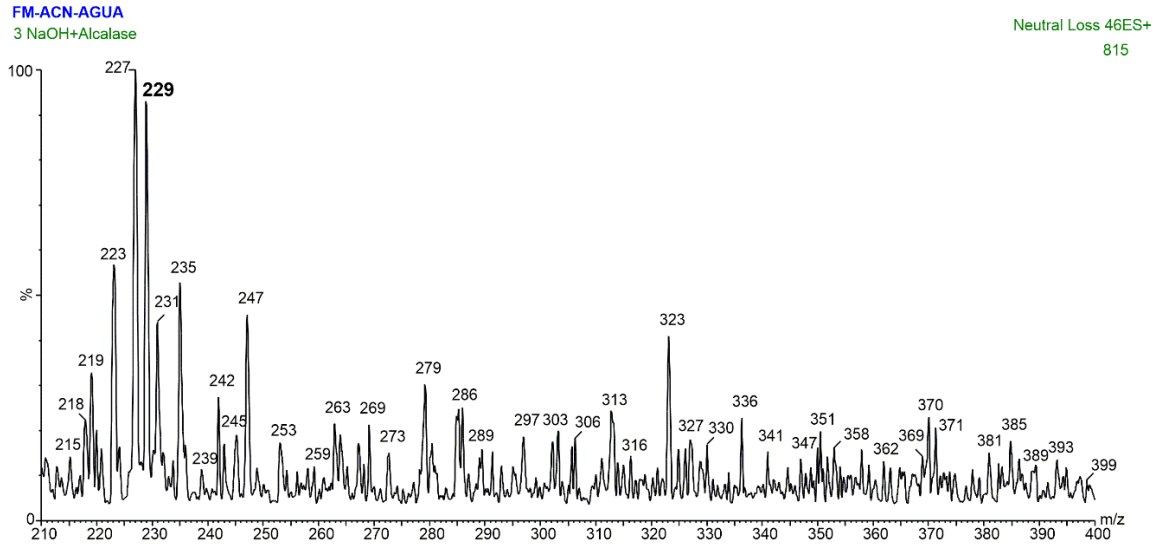

Figure S6. LC-MS/MS of 46 Da neutral loss from experiment 3 (210-400) of the hydrolysate combined with NaOH and Alcalase from chicken blood meal.

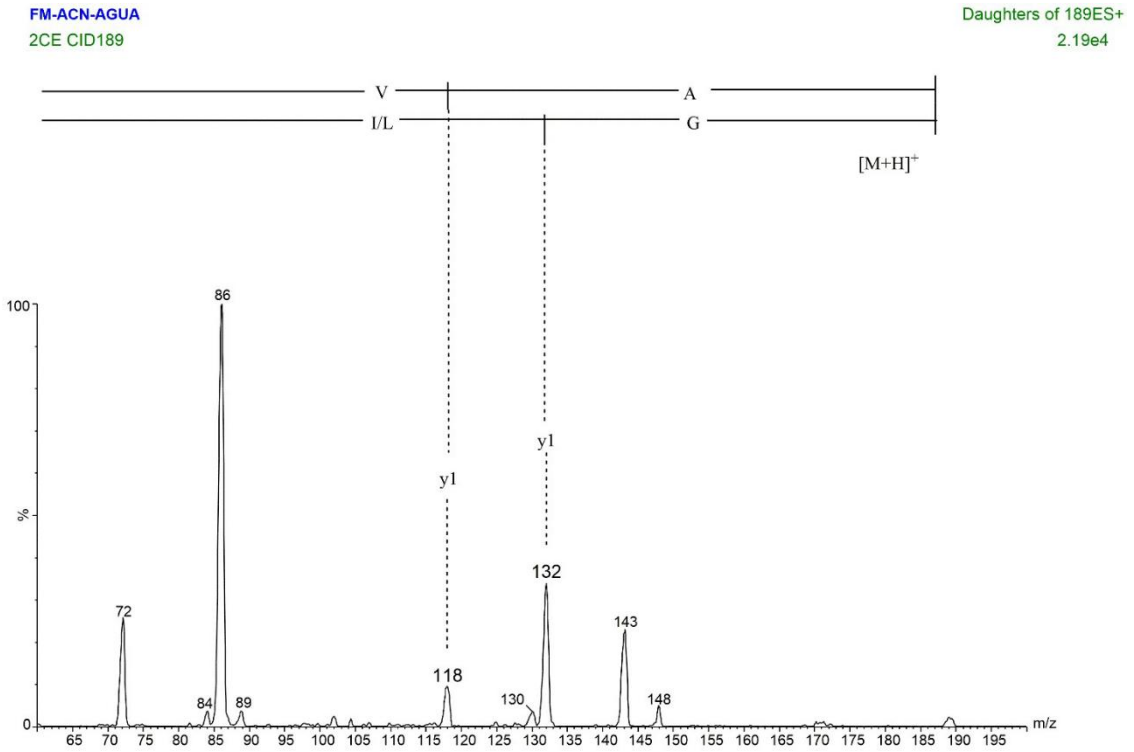

Figure S7. LC-MS/MS (189) with a neutral loss of 46 Da from the sample of experiment 2, combined hydrolysis: Alcalase + NaOH.

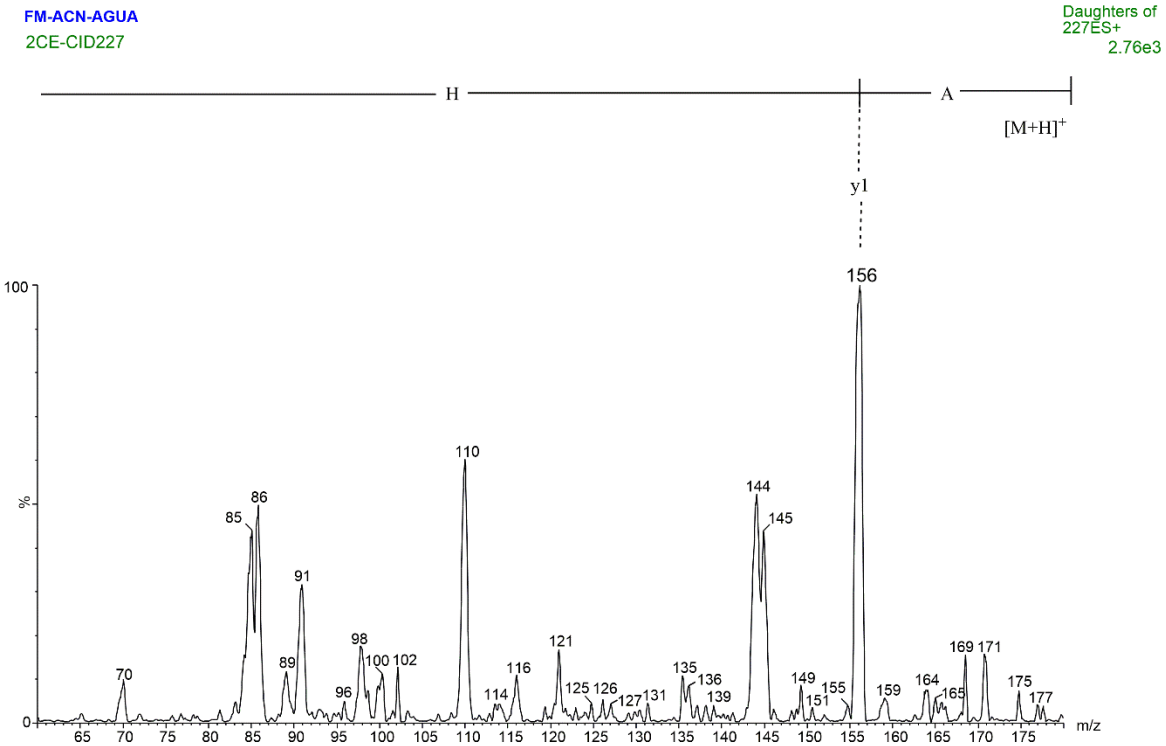

Figure S8. LC-MS/MS (227) with a neutral loss of 46 Da from the sample of experiment 2, combined hydrolysis: Alcalase + NaOH.

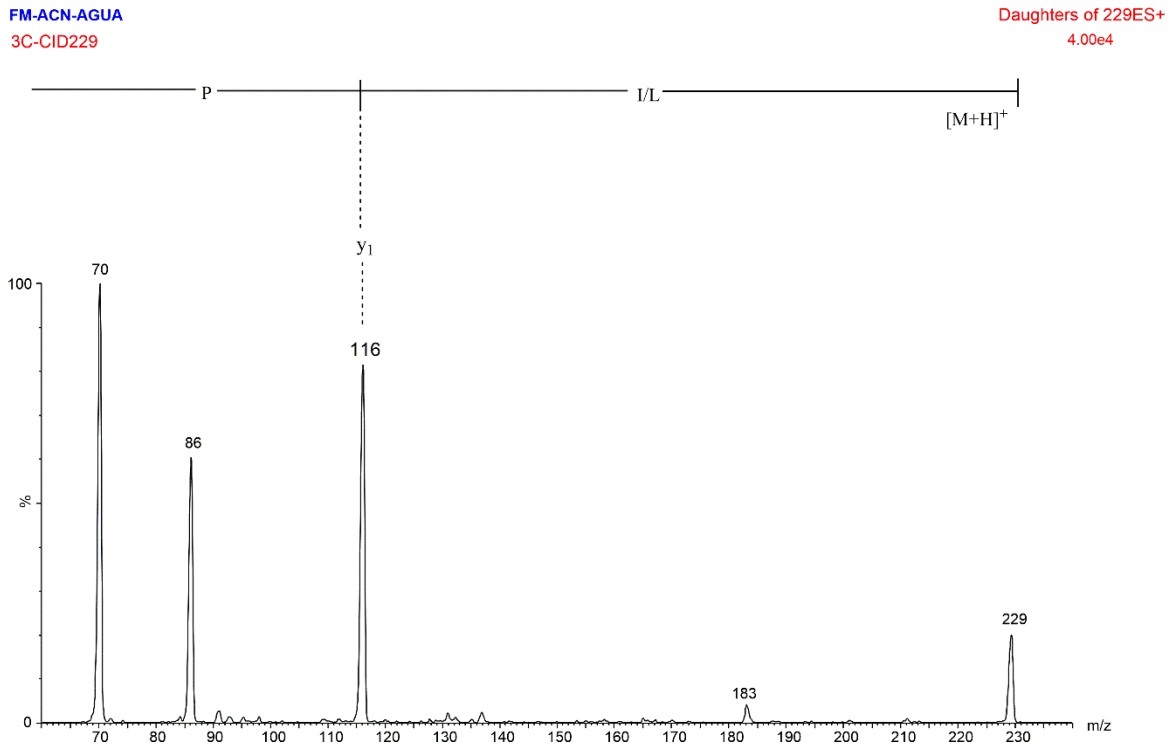

Figure S9. LC-MS/MS (229) with a neutral loss of 46 Da from the sample of experiment 2, combined hydrolysis: NaOH + Alcalase.

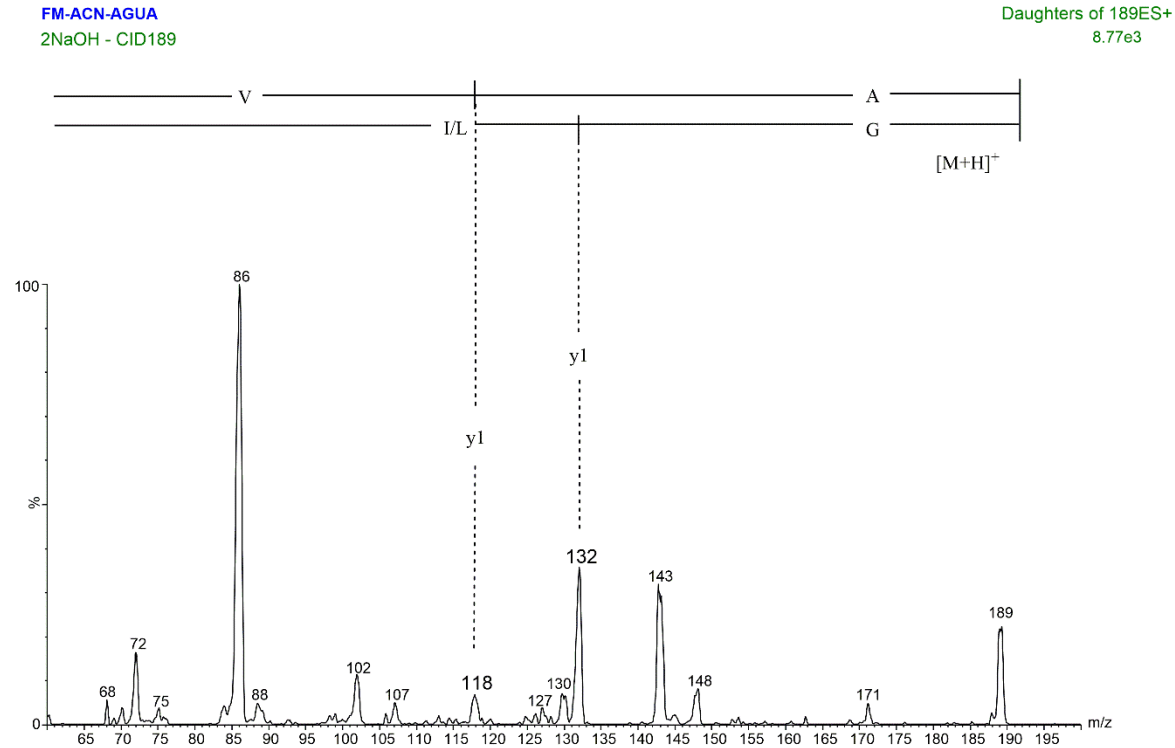

Figure S10. LC-MS/MS (189) with a neutral loss of 46 Da from the sample of experiment 2, hydrolysis: NaOH.

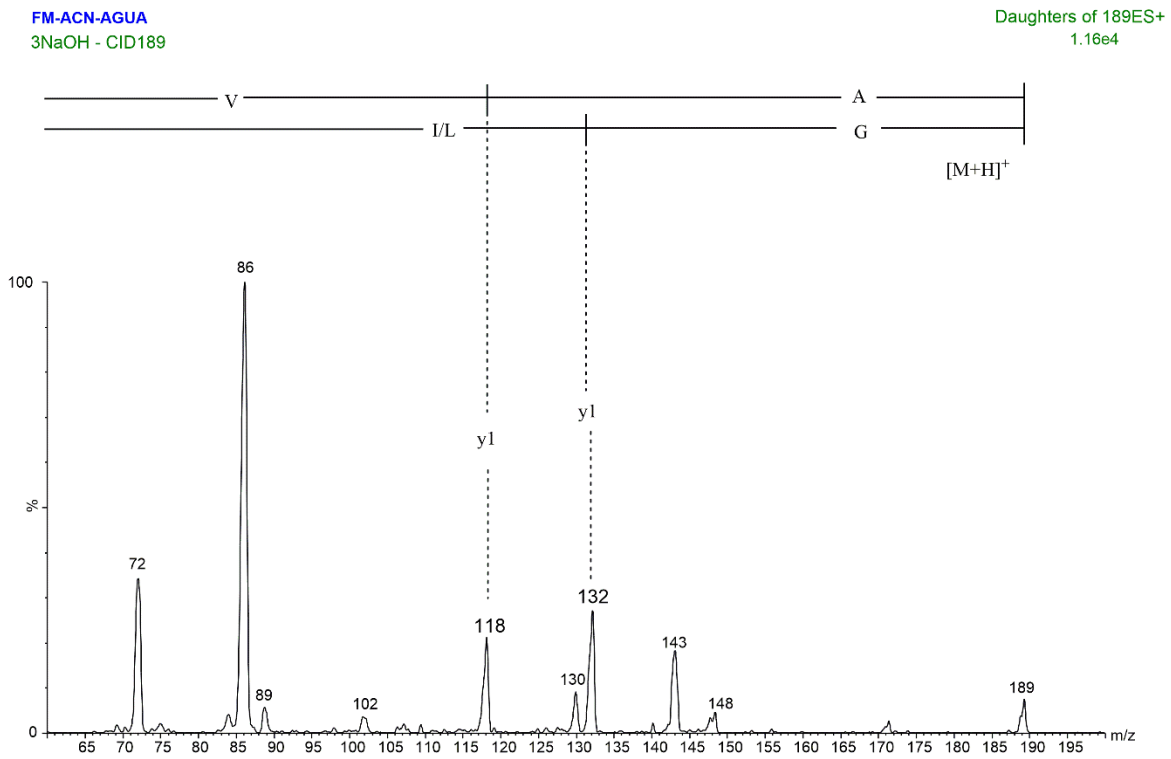

Figure S11. LC-MS/MS (189) with a neutral loss of 46 Da from the sample of experiment 3, hydrolysis: NaOH.

Table S9. List of the 20 most common amino acid residues

Aminoacid			Average mass	M. isotropic	Immonium ion	Related ion
Glycine	Gly	G	57.052	57.02146	30	
Alanine	Ala	A	71.079	71.03711	44	
Serine	Ser	S	87.078	87.03203	60	
Proline	Pro	P	97.117	97.05276	70	
Valine	Val	V	99.133	99.06841	72	
Threonine	Thr	T	101.105	101.04768	74	
Cysteine	Cys	C	103.145	103.00919	76	
Leucine	Leu	L	113.16	113.08406	86	72
Isoleucine	Ile	I	113.16	113.08406	86	72
Asparagine	Asn	N	114.104	114.04293	87	70
Aspartic acid	Asp	D	115.089	115.02694	88	
Glutamine	Gln	Q	128.131	128.05858	101	84, 129
Lysine	Lys	K	128.174	128.09496	101	70, 84, 112, 129
Glutamic acid	Glu	E	129.116	129.04259	102	
Methionine	Met	M	131.199	131.04048	104	61
Histidine	His	H	137.141	137.05891	110	82, 121, 123, 138, 166
Phenylalanine	Phe	F	147.177	147.06841	120	91
Arginine	Arg	R	156.188	156.10111	129	59, 70, 73, 87, 100, 112
Tyrosine	Tyr	Y	163.176	163.06333	136	91, 107
Tryptophane	Trp	W	186.213	186.07931	159	117, 130, 170, 171

Cantú *et al*.[1]

Table S10. Amino acid sequences of peptides identified by LC-MS/MS in chicken blood meal hydrolysates and their biological activities described in the BIOPEP database

Pro-D	$[M+]^+$	y1	Intensity y	Imonium ion	Related ions	b2	Amino acid sequence	Biological activity	Reference
Exp. 2 NaOH	189	118 (V)	1017	44 (A); 72 (V)	–	171	AV	dipeptidyl peptidase IV inhibitor ACE inhibitor	Lan *et al.*;[2] Salampessy *et al.*[3]
Exp. 2 NaOH	189	132 (I/L)	3333	30 (G); 86 (I/L)	72 (I/L)	171	G(I/L)	–	
Exp. 2 NaOH	219	90 (A)	1032	44 (A); 102 (E)	–	259	AE	dipeptidyl peptidase IV inhibitor	Lan *et al.*[2]
Exp. 2 NaOH	219	120 (T)	202	72 (V); 74 (T)	–	201	VT	dipeptidyl peptidase IV inhibitor	Lan *et al.*[2]
Exp. 2 NaOH	219	132 (I/L)	3794	60 (S); 86 (I/L)	72 (I/L)	175	(I/L)S	–	–
Exp. 2 NaOH	219	148 (E)	768	44(A); 102 (E)	-	201	AE	dipeptidyl peptidase IV inhibitor	Lan *et al.*[2]
Exp. 3 NaOH	189	118 (V)	4411	44 (A); 72 (V)	-	171	AV	dipeptidyl peptidase IV inhibitor ACE inhibitor	Lan *et al.*;[2] Salampessy *et al.*[3]
Exp. 3 NaOH	189	132 (I/L)	5094	30 (G); 86 (I/L)	72 (I/L)	171	G(I/L)	–	–
Exp. 3 NaOH + Alcalase	229	116 (P)	33153	70 (P); 86 (I/L)	72 (I/L)	–	(I/L)P	angiotensin-converting enzyme (ACE) inhibitor	Salampessy *et al.*[3]
Exp. 2 Alcalase + NaOH	189	118 (V)	3528	44 (A); 72 (V)	–	171	AV	dipeptidyl peptidase IV inhibitor ACE inhibitor	Lan *et al.*;[2] Salampessy *et al.*[3]
Exp. 2 Alcalase + NaOH	189	132 (I/L)	9915	30 (G); 86 (I/L)	72 (I/L)	171	G(I/L)	–	–
Exp. 2 Alcalase + NaOH	227	156 (H)	3991	44 (E); 110 (H)	82, 121,123,138,166 (H)	209	AH	dipeptidyl peptidase IV inhibitor antioxidant ACE inhibitor	van Platerink *et al.*;[4] Chen *et al.*;[5] Lan *et al.*[2]

Table S11. List of dipeptide masses. The values correspond to the sum of the masses of the amino acid residue from the C-terminal region, plus the mass of the amino acid from the N-terminal region, with the addition of one unit, referring to protonation resulting in [M+H]+

	G	A	S	P	V	T	C	I/L	N	D	Q/K	E	M	H	F/M	R	C	Y	W
G	133																		
A	147	161																	
S	163	177	193																
P	173	187	203	213															
V	175	189	205	215	217														
T	177	191	207	217	219	221													
C	179	193	209	219	221	223	225												
I/L	189	203	219	229	231	233	235	245											
N	190	204	220	230	232	234	236	246	247										
D	191	205	221	231	233	235	237	247	248	249									
Q/K	204	218	234	244	246	248	250	260	261	262	275								
E	205	219	235	245	247	249	251	261	262	263	276	277							
M	207	221	237	247	249	251	253	263	264	265	278	279	281						
H	213	227	243	253	255	257	259	269	270	271	284	285	287	293					
F/M	223	237	253	263	265	267	269	279	280	281	294	295	297	303	313				
R	232	246	262	272	274	276	278	288	289	290	303	304	306	312	322	331			
C	238	252	268	278	280	282	284	294	295	296	309	310	312	318	328	337	343		
Y	239	253	269	279	281	283	285	295	296	297	310	311	313	319	329	338	344	345	
W	243	257	273	283	285	287	289	299	300	301	314	315	317	323	333	342	348	349	353

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S12. List of dipeptide masses useful for the determination of -b2 Ions. The values correspond to the sum of the amino acid residue masses plus one unit

	G	A	S	P	V	T	C	I/L	N	D	Q/K	E	M	H	F/M	R	C	Y	W
G	115																		
A	129	143																	
S	145	159	175																
P	155	169	185	195															
V	157	171	187	197	199														
T	159	173	189	199	201	203													
C	161	175	191	201	203	205	207												
I/L	171	185	201	211	213	215	217	227											
N	172	186	202	212	214	216	218	228	229										
D	173	187	203	213	215	217	219	229	230	231									
Q/K	186	200	216	226	228	230	232	242	243	244	257								
E	187	201	217	227	229	231	233	243	244	245	258	259							
M	189	203	219	229	231	233	235	245	246	247	260	261	263						
H	195	209	225	235	237	239	241	251	252	253	266	267	269	275					
F/M	205	219	235	245	247	249	251	261	262	263	276	277	279	285	295				
R	214	228	244	254	256	258	260	270	271	272	285	286	288	294	304	313			
C	219	233	249	259	261	263	265	275	276	277	290	291	293	299	309	318	323		
Y	221	235	251	261	263	265	267	277	278	279	292	293	295	301	311	320	325	327	
W	244	258	274	284	286	288	290	300	301	302	315	316	318	324	334	343	348	350	373

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S13. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the glycine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-G	A-G	S-G	P-G	V-G	T-G	C-G	I/L-G	N-G	D-G	Q/K-G	E-G	M-G	H-G	F/M-G	R-G	C-G	Y-G	W-G
G	190																		
A	204	218																	
S	220	234	250																
P	230	244	260	270															
V	232	246	262	272	274														
T	234	248	264	274	276	278													
C	236	250	266	276	278	280	282												
I/L	246	260	276	286	288	290	292	302											
N	247	261	277	287	289	291	293	303	304										
D	248	262	278	288	290	292	294	304	305	306									
Q/K	261	275	291	301	303	305	307	317	318	319	332								
E	262	276	292	302	304	306	308	318	319	320	333	334							
M	264	278	294	304	306	308	310	320	321	322	335	336	338						
H	270	284	300	310	312	314	316	326	327	328	341	342	344	350					
F/M	280	294	310	320	322	324	326	336	337	338	351	352	354	360	370				
R	289	303	319	329	331	333	335	345	346	347	360	361	363	369	379	388			
C	295	309	325	335	337	339	341	351	352	353	366	367	369	375	385	394	400		
Y	296	310	326	336	338	340	342	352	353	354	367	368	370	376	386	395	401	402	

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S14. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the alanine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-A	A-A	S-A	P-A	V-A	T-A	C-A	I/L-A	N-A	D-A	Q/K-A	E-A	M-A	H-A	F/M-A	R-A	C-A	Y-A	W-A
G	204																		
A	218	232																	
S	234	248	264																
P	244	258	274	284															
V	246	260	276	286	288														
T	248	262	278	288	290	292													
C	250	264	280	290	292	294	296												
I/L	260	274	290	300	302	304	306	316											
N	261	275	291	301	303	305	307	317	318										
D	262	276	292	302	304	306	308	318	319	320									
Q/K	275	289	305	315	317	319	321	331	332	333	346								
E	276	290	306	316	318	320	322	332	333	334	347	348							
M	278	292	308	318	320	322	324	334	335	336	349	350	352						
H	284	298	314	324	326	328	330	340	341	342	355	356	358	364					
F/M	294	308	324	334	336	338	340	350	351	352	365	366	368	374	384				
R	303	317	333	343	345	347	349	359	360	361	374	375	377	383	393	402			
C	309	323	339	349	351	353	355	365	366	367	380	381	383	389	399	408	414		
Y	310	324	340	350	352	354	356	366	367	368	381	382	384	390	400	409	415	416	
W	314	328	344	354	356	358	360	370	371	372	385	386	388	394	404	413	419	420	424

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S15. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the serine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-S	A-S	S-S	P-S	V-S	T-S	C-S	I/L-S	N-S	D-S	Q/K-S	E-S	M-S	H-S	F/M-S	R-S	C-S	Y-S	W-S
G	220																		
A	234	248																	
S	250	264	280																
P	260	274	290	300															
V	262	276	292	302	304														
T	264	278	294	304	306	308													
C	266	280	296	306	308	310	312												
I/L	276	290	306	316	318	320	322	332											
N	277	291	307	317	319	321	323	333	334										
D	278	292	308	318	320	322	324	334	335	336									
Q/K	291	305	321	331	333	335	337	347	348	349	362								
E	292	306	322	332	334	336	338	348	349	350	363	364							
M	294	308	324	334	336	338	340	350	351	352	365	366	368						
H	300	314	330	340	342	344	346	356	357	358	371	372	374	380					
F/M	310	324	340	350	352	354	356	366	367	368	381	382	384	390	400				
R	319	333	349	359	361	363	365	375	376	377	390	391	393	399	409	418			
C	325	339	355	365	367	369	371	381	382	383	396	397	399	405	415	424	430		
Y	326	340	356	366	368	370	372	382	383	384	397	398	400	406	416	425	431	432	
W	330	344	360	370	372	374	376	386	387	388	401	402	404	410	420	429	435	436	440

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S16. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the proline residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-P	A-P	S-P	P-P	V-P	T-P	C-P	I/L-P	N-P	D-P	Q/K-P	E-P	M-P	H-P	F/M-P	R-P	C-P	Y-P	W-P
G	230																		
A	244	258																	
S	260	274	290																
P	270	284	300	310															
V	272	286	302	312	314														
T	274	288	304	314	316	318													
C	276	290	306	316	318	320	322												
I/L	286	300	316	326	328	330	332	342											
N	287	301	317	327	329	331	333	343	344										
D	288	302	318	328	330	332	334	344	345	346									
Q/K	301	315	331	341	343	345	347	357	358	359	372								
E	302	316	332	342	344	346	348	358	359	360	373	374							
M	304	318	334	344	346	348	350	360	361	362	375	376	378						
H	310	324	340	350	352	354	356	366	367	368	381	382	384	390					
F/M	320	334	350	360	362	364	366	376	377	378	391	392	394	400	410				
R	329	343	359	369	371	373	375	385	386	387	400	401	403	409	419	428			
C	335	349	365	375	377	379	381	391	392	393	406	407	409	415	425	434	440		
Y	336	350	366	376	378	380	382	392	393	394	407	408	410	416	426	435	441	442	
W	340	354	370	380	382	384	386	396	397	398	411	412	414	420	430	439	445	446	450

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S17. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the valine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-V	A-V	S-V	P-V	V-V	T-V	C-V	I/L-V	N-V	D-V	Q/K-V	E-V	M-V	H-V	F/M-V	R-V	C-V	Y-V	W-V
G	232																		
A	246	260																	
S	262	276	292																
P	272	286	302	312															
V	274	288	304	314	316														
T	276	290	306	316	318	320													
C	278	292	308	318	320	322	324												
I/L	288	302	318	328	330	332	334	344											
N	289	303	319	329	331	333	335	345	346										
D	290	304	320	330	332	334	336	346	347	348									
Q/K	303	317	333	343	345	347	349	359	360	361	374								
E	304	318	334	344	346	348	350	360	361	362	375	376							
M	306	320	336	346	348	350	352	362	363	364	377	378	380						
H	312	326	342	352	354	356	358	368	369	370	383	384	386	392					
F/M	322	336	352	362	364	366	368	378	379	380	393	394	396	402	412				
R	331	345	361	371	373	375	377	387	388	389	402	403	405	411	421	430			
C	337	351	367	377	379	381	383	393	394	395	408	409	411	417	427	436	442		
Y	338	352	368	378	380	382	384	394	395	396	409	410	412	418	428	437	443	444	
W	342	356	372	382	384	386	388	398	399	400	413	414	416	422	432	441	447	448	452

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S18. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the threonine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-T	A-T	S-T	P-T	V-T	T-T	C-T	I/L-T	N-T	D-T	Q/K-T	E-T	M-T	H-T	F/M-T	R-T	C-T	Y-T	W-T
G	234																		
A	248	262																	
S	264	278	294																
P	274	288	304	314															
V	276	290	306	316	318														
T	278	292	308	318	320	322													
C	280	294	310	320	322	324	326												
I/L	290	304	320	330	332	334	336	346											
N	291	305	321	331	333	335	337	347	348										
D	292	306	322	332	334	336	338	348	349	350									
Q/K	305	319	335	345	347	349	351	361	362	363	376								
E	306	320	336	346	348	350	352	362	363	364	377	378							
M	308	322	338	348	350	352	354	364	365	366	379	380	382						
H	314	328	344	354	356	358	360	370	371	372	385	386	388	394					
F/M	324	338	354	364	366	368	370	380	381	382	395	396	398	404	414				
R	333	347	363	373	375	377	379	389	390	391	404	405	407	413	423	432			
C	339	353	369	379	381	383	385	395	396	397	410	411	413	419	429	438	444		
Y	340	354	370	380	382	384	386	396	397	398	411	412	414	420	430	439	445	446	
W	344	358	374	384	386	388	390	400	401	402	415	416	418	424	434	443	449	450	454

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S19. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the cysteine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-C	A-C	S-C	P-C	V-C	T-C	C-C	I/L-C	N-C	D-C	Q/K-C	E-C	M-C	H-C	F/M-C	R-C	C-C	Y-C	W-C
G	236																		
A	250	264																	
S	266	280	296																
P	276	290	306	316															
V	278	292	308	318	320														
T	280	294	310	320	322	324													
C	282	296	312	322	324	326	328												
I/L	292	306	322	332	334	336	338	348											
N	293	307	323	333	335	337	339	349	350										
D	294	308	324	334	336	338	340	350	351	352									
Q/K	307	321	337	347	349	351	353	363	364	365	378								
E	308	322	338	348	350	352	354	364	365	366	379	380							
M	310	324	340	350	352	354	356	366	367	368	381	382	384						
H	316	330	346	356	358	360	362	372	373	374	387	388	390	396					
F/M	326	340	356	366	368	370	372	382	383	384	397	398	400	406	416				
R	335	349	365	375	377	379	381	391	392	393	406	407	409	415	425	434			
C	341	355	371	381	383	385	387	397	398	399	412	413	415	421	431	440	446		
Y	342	356	372	382	384	386	388	398	399	400	413	414	416	422	432	441	447	448	
W	346	360	376	386	388	390	392	402	403	404	417	418	420	426	436	445	451	452	456

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S20. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the leucine or isoleucine residues from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-I/L	A-I/L	S-I/L	P-I/L	V-I/L	T-I/L	C-I/L	I/L-I/L	N-I/L	D-I/L	Q/K-I/L	E-I/L	M-I/L	H-I/L	F/M-I/L	R-I/L	C-I/L	Y-I/L	W-I/L
G	246																		
A	260	274																	
S	276	290	306																
P	286	300	316	326															
V	288	302	318	328	330														
T	290	304	320	330	332	334													
C	292	306	322	332	334	336	338												
I/L	302	316	332	342	344	346	348	358											
N	303	317	333	343	345	347	349	359	360										
D	304	318	334	344	346	348	350	360	361	362									
Q/K	317	331	347	357	359	361	363	373	374	375	388								
E	318	332	348	358	360	362	364	374	375	376	389	390							
M	320	334	350	360	362	364	366	376	377	378	391	392	394						
H	326	340	356	366	368	370	372	382	383	384	397	398	400	406					
F/M	336	350	366	376	378	380	382	392	393	394	407	408	410	416	426				
R	345	359	375	385	387	389	391	401	402	403	416	417	419	425	435	444			
C	351	365	381	391	393	395	397	407	408	409	422	423	425	431	441	450	456		
Y	352	366	382	392	394	396	398	408	409	410	423	424	426	432	442	451	457	458	
W	356	370	386	396	398	400	402	412	413	414	427	428	430	436	446	455	461	462	466

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S21. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the asparagine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-N	A-N	S-N	P-N	V-N	T-N	C-N	I/L-N	N-N	D-N	Q/K-N	E-N	M-N	H-N	F/M-N	R-N	C-N	Y-N	W-N
G	247																		
A	261	275																	
S	277	291	307																
P	287	301	317	327															
V	289	303	319	329	331														
T	291	305	321	331	333	335													
C	293	307	323	333	335	337	339												
I/L	303	317	333	343	345	347	349	359											
N	304	318	334	344	346	348	350	360	361										
D	305	319	335	345	347	349	351	361	362	363									
Q/K	318	332	348	358	360	362	364	374	375	376	389								
E	319	333	349	359	361	363	365	375	376	377	390	391							
M	321	335	351	361	363	365	367	377	378	379	392	393	395						
H	327	341	357	367	369	371	373	383	384	385	398	399	401	407					
F/M	337	351	367	377	379	381	383	393	394	395	408	409	411	417	427				
R	346	360	376	386	388	390	392	402	403	404	417	418	420	426	436	445			
C	352	366	382	392	394	396	398	408	409	410	423	424	426	432	442	451	457		
Y	353	367	383	393	395	397	399	409	410	411	424	425	427	433	443	452	458	459	
W	357	371	387	397	399	401	403	413	414	415	428	429	431	437	447	456	462	463	467

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S22. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the aspartic acid residue from the N-terminal region, with the addition of one unit,

referring to protonation, resulting in $[M + H]^+$

	G-D	A-D	S-D	P-D	V-D	T-D	C-D	I/L-D	N-D	D-D	Q/K-D	E-D	M-D	H-D	F/M-D	R-D	C-D	Y-D	W-D
G	248																		
A	262	276																	
S	278	292	308																
P	288	302	318	328															
V	290	304	320	330	332														
T	292	306	322	332	334	336													
C	294	308	324	334	336	338	340												
I/L	304	318	334	344	346	348	350	360											
N	305	319	335	345	347	349	351	361	362										
D	306	320	336	346	348	350	352	362	363	364									
Q/K	319	333	349	359	361	363	365	375	376	377	390								
E	320	334	350	360	362	364	366	376	377	378	391	392							
M	322	336	352	362	364	366	368	378	379	380	393	394	396						
H	328	342	358	368	370	372	374	384	385	386	399	400	402	408					
F/M	338	352	368	378	380	382	384	394	395	396	409	410	412	418	428				
R	347	361	377	387	389	391	393	403	404	405	418	419	421	427	437	446			
C	353	367	383	393	395	397	399	409	410	411	424	425	427	433	443	452	458		
Y	354	368	384	394	396	398	400	410	411	412	425	426	428	434	444	453	459	460	
W	358	372	388	398	400	402	404	414	415	416	429	430	432	438	448	457	463	464	468

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S23. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the glutamine or lysine residues from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-Q/K	A-Q/K	S-Q/K	P-Q/K	V-Q/K	T-Q/K	C-Q/K	I/L-Q/K	N-Q/K	D-Q/K	Q/K-Q/K	E-Q/K	M-Q/K	H-Q/K	F/M-Q/K	R-Q/K	C-Q/K	Y-Q/K	W-Q/K
G	261																		
A	275	289																	
S	291	305	321																
P	301	315	331	341															
V	303	317	333	343	345														
T	305	319	335	345	347	349													
C	307	321	337	347	349	351	353												
I/L	317	331	347	357	359	361	363	373											
N	318	332	348	358	360	362	364	374	375										
D	319	333	349	359	361	363	365	375	376	377									
Q/K	332	346	362	372	374	376	378	388	389	390	403								
E	333	347	363	373	375	377	379	389	390	391	404	405							
M	335	349	365	375	377	379	381	391	392	393	406	407	409						
H	341	355	371	381	383	385	387	397	398	399	412	413	415	421					
F/M	351	365	381	391	393	395	397	407	408	409	422	423	425	431	441				
R	360	374	390	400	402	404	406	416	417	418	431	432	434	440	450	459			
C	366	380	396	406	408	410	412	422	423	424	437	438	440	446	456	465	471		
Y	367	381	397	407	409	411	413	423	424	425	438	439	441	447	457	466	472	473	
W	371	385	401	411	413	415	417	427	428	429	442	443	445	451	461	470	476	477	481

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S24. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the glutamic acid residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-E	A-E	S-E	P-E	V-E	T-E	C-E	I/L-E	N-E	D-E	Q/K-E	E-E	M-E	H-E	F/M-E	R-E	C-E	Y-E	W-E
G	262																		
A	276	290																	
S	292	306	322																
P	302	316	332	342															
V	304	318	334	344	346														
T	306	320	336	346	348	350													
C	308	322	338	348	350	352	354												
I/L	318	332	348	358	360	362	364	374											
N	319	333	349	359	361	363	365	375	376										
D	320	334	350	360	362	364	366	376	377	378									
Q/K	333	347	363	373	375	377	379	389	390	391	404								
E	334	348	364	374	376	378	380	390	391	392	405	406							
M	336	350	366	376	378	380	382	392	393	394	407	408	410						
H	342	356	372	382	384	386	388	398	399	400	413	414	416	422					
F/M	352	366	382	392	394	396	398	408	409	410	423	424	426	432	442				
R	361	375	391	401	403	405	407	417	418	419	432	433	435	441	451	460			
C	367	381	397	407	409	411	413	423	424	425	438	439	441	447	457	466	472		
Y	368	382	398	408	410	412	414	424	425	426	439	440	442	448	458	467	473	474	
W	372	386	402	412	414	416	418	428	429	430	443	444	446	452	462	471	477	478	482

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S25. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the methionine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-M	A-M	S-M	P-M	V-M	T-M	C-M	I/L-M	N-M	D-M	Q/K-M	E-M	M-M	H-M	F/M-M	R-M	C-M	Y-M	W-M
G	264																		
A	278	292																	
S	294	308	324																
P	304	318	334	344															
V	306	320	336	346	348														
T	308	322	338	348	350	352													
C	310	324	340	350	352	354	356												
I/L	320	334	350	360	362	364	366	376											
N	321	335	351	361	363	365	367	377	378										
D	322	336	352	362	364	366	368	378	379	380									
Q/K	335	349	365	375	377	379	381	391	392	393	406								
E	336	350	366	376	378	380	382	392	393	394	407	408							
M	338	352	368	378	380	382	384	394	395	396	409	410	412						
H	344	358	374	384	386	388	390	400	401	402	415	416	418	424					
F/M	354	368	384	394	396	398	400	410	411	412	425	426	428	434	444				
R	363	377	393	403	405	407	409	419	420	421	434	435	437	443	453	462			
C	369	383	399	409	411	413	415	425	426	427	440	441	443	449	459	468	474		
Y	370	384	400	410	412	414	416	426	427	428	441	442	444	450	460	469	475	476	
W	374	388	404	414	416	418	420	430	431	432	445	446	448	454	464	473	479	480	484

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S26. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the histidine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-H	A-H	S-H	P-H	V-H	T-H	C-H	I/L-H	N-H	D-H	Q/K-H	E-H	M-H	H-H	F/M-H	R-H	C-H	Y-H	W-H
G	270																		
A	284	298																	
S	300	314	330																
P	310	324	340	350															
V	312	326	342	352	354														
T	314	328	344	354	356	358													
C	316	330	346	356	358	360	362												
I/L	326	340	356	366	368	370	372	382											
N	327	341	357	367	369	371	373	383	384										
D	328	342	358	368	370	372	374	384	385	386									
Q/K	341	355	371	381	383	385	387	397	398	399	412								
E	342	356	372	382	384	386	388	398	399	400	413	414							
M	344	358	374	384	386	388	390	400	401	402	415	416	418						
H	350	364	380	390	392	394	396	406	407	408	421	422	424	430					
F/M	360	374	390	400	402	404	406	416	417	418	431	432	434	440	450				
R	369	383	399	409	411	413	415	425	426	427	440	441	443	449	459	468			
C	375	389	405	415	417	419	421	431	432	433	446	447	449	455	465	474	480		
Y	376	390	406	416	418	420	422	432	433	434	447	448	450	456	466	475	481	482	
W	380	394	410	420	422	424	426	436	437	438	451	452	454	460	470	479	485	486	490

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S27. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the phenylalanine residue (or its oxidized version) from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-F/M	A-F/M	S-F/M	P-F/M	V-F/M	T-F/M	C-F/M	I/L-F/M	N-F/M	D-F/M	Q/K-F/M	E-F/M	M-F/M	H-F/M	F/M-F/M	R-F/M	C-F/M	Y-F/M	W-F/M
G	280																		
A	294	308																	
S	310	324	340																
P	320	334	350	360															
V	322	336	352	362	364														
T	324	338	354	364	366	368													
C	326	340	356	366	368	370	372												
I/L	336	350	366	376	378	380	382	392											
N	337	351	367	377	379	381	383	393	394										
D	338	352	368	378	380	382	384	394	395	396									
Q/K	351	365	381	391	393	395	397	407	408	409	422								
E	352	366	382	392	394	396	398	408	409	410	423	424							
M	354	368	384	394	396	398	400	410	411	412	425	426	428						
H	360	374	390	400	402	404	406	416	417	418	431	432	434	440					
F/M	370	384	400	410	412	414	416	426	427	428	441	442	444	450	460				
R	379	393	409	419	421	423	425	435	436	437	450	451	453	459	469	478			
C	385	399	415	425	427	429	431	441	442	443	456	457	459	465	475	484	490		
Y	386	400	416	426	428	430	432	442	443	444	457	458	460	466	476	485	491	492	
W	390	404	420	430	432	434	436	446	447	448	461	462	464	470	480	489	495	496	500

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S28. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the arginine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-R	A-R	S-R	P-R	V-R	T-R	C-R	I/L-R	N-R	D-R	Q/K-R	E-R	M-R	H-R	F/M-R	R-R	C-R	Y-R	W-R
G	289																		
A	303	317																	
S	319	333	349																
P	329	343	359	369															
V	331	345	361	371	373														
T	333	347	363	373	375	377													
C	335	349	365	375	377	379	381												
I/L	345	359	375	385	387	389	391	401											
N	346	360	376	386	388	390	392	402	403										
D	347	361	377	387	389	391	393	403	404	405									
Q/K	360	374	390	400	402	404	406	416	417	418	431								
E	361	375	391	401	403	405	407	417	418	419	432	433							
M	363	377	393	403	405	407	409	419	420	421	434	435	437						
H	369	383	399	409	411	413	415	425	426	427	440	441	443	449					
F/M	379	393	409	419	421	423	425	435	436	437	450	451	453	459	469				
R	388	402	418	428	430	432	434	444	445	446	459	460	462	468	478	487			
C	394	408	424	434	436	438	440	450	451	452	465	466	468	474	484	493	499		
Y	395	409	425	435	437	439	441	451	452	453	466	467	469	475	485	494	500	501	
W	399	413	429	439	441	443	445	455	456	457	470	471	473	479	489	498	504	505	509

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S29. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the carbamidomethylcysteine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-C	A-C	S-C	P-C	V-C	T-C	C-C	I/L-C	N-C	D-C	Q/K-C	E-C	M-C	H-C	F/M-C	R-C	C-C	Y-C	W-C
G	295																		
A	309	323																	
S	325	339	355																
P	335	349	365	375															
V	337	351	367	377	379														
T	339	353	369	379	381	383													
C	341	355	371	381	383	385	387												
I/L	351	365	381	391	393	395	397	407											
N	352	366	382	392	394	396	398	408	409										
D	353	367	383	393	395	397	399	409	410	411									
Q/K	366	380	396	406	408	410	412	422	423	424	437								
E	367	381	397	407	409	411	413	423	424	425	438	439							
M	369	383	399	409	411	413	415	425	426	427	440	441	443						
H	375	389	405	415	417	419	421	431	432	433	446	447	449	455					
F/M	385	399	415	425	427	429	431	441	442	443	456	457	459	465	475				
R	394	408	424	434	436	438	440	450	451	452	465	466	468	474	484	493			
C	400	414	430	440	442	444	446	456	457	458	471	472	474	480	490	499	505		
Y	401	415	431	441	443	445	447	457	458	459	472	473	475	481	491	500	506	507	
W	405	419	435	445	447	449	451	461	462	463	476	477	479	485	495	504	510	511	515

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S30. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the tyrosine residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-Y	A-Y	S-Y	P-Y	V-Y	T-Y	C-Y	I/L-Y	N-Y	D-Y	Q/K-Y	E-Y	M-Y	H-Y	F/M-Y	R-Y	C-Y	Y-Y	W-Y
G	296																		
A	310	324																	
S	326	340	356																
P	336	350	366	376															
V	338	352	368	378	380														
T	340	354	370	380	382	384													
C	342	356	372	382	384	386	388												
I/L	352	366	382	392	394	396	398	408											
N	353	367	383	393	395	397	399	409	410										
D	354	368	384	394	396	398	400	410	411	412									
Q/K	367	381	397	407	409	411	413	423	424	425	438								
E	368	382	398	408	410	412	414	424	425	426	439	440							
M	370	384	400	410	412	414	416	426	427	428	441	442	444						
H	376	390	406	416	418	420	422	432	433	434	447	448	450	456					
F/M	386	400	416	426	428	430	432	442	443	444	457	458	460	466	476				
R	395	409	425	435	437	439	441	451	452	453	466	467	469	475	485	494			
C	401	415	431	441	443	445	447	457	458	459	472	473	475	481	491	500	506		
Y	402	416	432	442	444	446	448	458	459	460	473	474	476	482	492	501	507	508	
W	406	420	436	446	448	450	452	462	463	464	477	478	480	486	496	505	511	512	516

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

Table S31. List of tripeptide masses. The values correspond to the sum of the amino acid residue masses from the C-terminal region, plus the mass of the tryptophan residue from the N-terminal region, with the addition of one unit, referring to protonation, resulting in $[M + H]^+$

	G-W	A-W	S-W	P-W	V-W	T-W	C-W	I/L-W	N-W	D-W	Q/K-W	E-W	M-W	H-W	F/M-W	R-W	C-W	Y-W	W-W
G	300																		
A	314	328																	
S	330	344	360																
P	340	354	370	380															
V	342	356	372	382	384														
T	344	358	374	384	386	388													
C	346	360	376	386	388	390	392												
I/L	356	370	386	396	398	400	402	412											
N	357	371	387	397	399	401	403	413	414										
D	358	372	388	398	400	402	404	414	415	416									
Q/K	371	385	401	411	413	415	417	427	428	429	442								
E	372	386	402	412	414	416	418	428	429	430	443	444							
M	374	388	404	414	416	418	420	430	431	432	445	446	448						
H	380	394	410	420	422	424	426	436	437	438	451	452	454	460					
F/M	390	404	420	430	432	434	436	446	447	448	461	462	464	470	480				
R	399	413	429	439	441	443	445	455	456	457	470	471	473	479	489	498			
C	405	419	435	445	447	449	451	461	462	463	476	477	479	485	495	504	510		
Y	406	420	436	446	448	450	452	462	463	464	477	478	480	486	496	505	511	512	
W	410	424	440	450	452	454	456	466	467	468	481	482	484	490	500	509	515	516	520

A-Ala: alanine; C-Cys: cysteine; D-Asp: aspartic acid; E-Glu: glutamic acid; F-Phe: phenylalanine; G-Gly: glycine; H-His: histidine; I-Ile: isoleucine; K-Lys: lysine; L-Leu: leucine; M-Met: methionine; N-Asn: asparagine; P-Pro: proline; Q-Gln: glutamine; R-Arg: arginine; S-Ser: serine; T-Thr: threonine; V-Val: valine; W-Trp: tryptophan; Y: Tyr: tyrosine.

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