

Supplementary Information

Table S1. The characteristics of known AMPs derived from milk proteins.

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life		Boman Index (kcal/mol)
RPKHPIK	f(1–7) of α_{S1} -casein	3.1	11.17	875.0	−2.029	19.84	55.71	Mamalian	1 h	3.68
								Yeast	2 min	
								E.coli	2 min	
RPKHPIKHQGLPQEVLENLLRF	Isracidin f(1–23) of α_{S1} -casein	2.2	9.99	2764.2	−0.987	46.49	97.39	Mamalian	1 h	2.42
								Yeast	2 min	
								E.coli	2 min	
GLPQE	f(10–14) of α_{S1} -casein	−1.0	4.00	542.5	−1.040	123.56	78.00	Mamalian	10 h	1.29
								Yeast	>20 h	
								E.coli	>20 h	
IKHQGLPQE	f(6–14) of α_{S1} -casein	0.1	6.75	1049.1	−1.256	63.66	86.67	Mamalian	20 h	1.92
								Yeast	30 min	
								E.coli	>10 h	
VLNENLLR	f(15–22) of α_{S1} -casein	0.0	5.97	970.1	0.075	32.83	182.5	Mamalian	100 h	2.02
								Yeast	>20 h	
								E.coli	>10 h	
LRLKKYKVPQL	α_{S1} -casein, gen. var. B-8P f(99–109)	4	10.46	1385.7	−0.636	46.18	132.73	Mamalian	5.5 h	1.67
								Yeast	3 min	
								E.coli	2 min	
SDIPNPIGSENSEK	f(180–193) of α_{S1} -casein	−2	4.14	1486.5	−1.314	32.69	55.71	Mamalian	1.9 h	2.89
								Yeast	>20 h	
								E.coli	>10 h	
KTKLTEEEKNRLNFLK KISQRYQKFALPQYLK TVYQHQQK	casocidin-I f(150–188) of α_{S2} -casein gen. var. A	7.1	10.08	4869.6	−1.323	27.85	70.00	Mamalian	1.3 h	2.83
								Yeast	3 min	
								E.coli	2 min	
VYQHQQAMKPWIQPK TKVIPYVRY	f(183–206) α_{S2} -casein gen. var. A	5.1	10.12	3002.6	−0.783	2.25	72.92	Mamalian	100 h	1.37
								Yeast	>20 h	
								E.coli	>10 h	
LKKISQ	f(165–170) of ovine α_{S2} -casein	2.0	10.00	715.8	−0.633	12.13	130.00	Mamalian	5.5 h	1.7
								Yeast	3 min	
								E.coli	2 min	
VYQHQQAMKPWIQPK TKVIPYVRYL	f(183–207) of bovine α_{S2} -casein	5.1	10.12	3115.7	−0.600	2.56	85.60	Mamalian	100 h	1.12
								Yeast	>20 h	
								E.coli	>10 h	

Table S1. Cont.

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life	Boman Index (kcal/mol)
LKKISQRYQKFALPQY	f(164–179) of bovine α_{S2} -casein	4.0	10.17	2011.4	−0.938	25.45	79.38	Mamalian Yeast E.coli 5.5 h 3 min 2 min	2.02
PYVRYL	f(203–208) of ovine α_{S2} -casein	1.0	9.00	809.9	−0.117	−4.23	113.33	Mamalian Yeast E.coli >20 h >20 h ?	1.04
KTVYQHQAAMKPWI PKTKVIPYVRYL	f(181–207) of ovine α_{S2} -casein	6.1	10.22	3345.0	−0.726	3.11	79.26	Mamalian Yeast E.coli 1.3 h 3 min 3 min	1.33
LKTVYQHQAAMKPWI QPKTKVIPYVRYL	f(180–207) of ovine α_{S2} -casein	6.1	10.22	3458.22	−0.564	0.32	90.36	Mamalian Yeast E.coli 5.5 3min 3min	1.11
ALPQYLKTVYQHQA MKPWIQPKTKVIPYVR YL	f(175–207) of ovine α_{S2} -casein	6.1	10.1	4030.8	−0.503	11.18	91.52	Mamalian Yeast E.coli 4.4 h >20 min >10 min	0.91
QKFALPQYLKTVYQHQA KAMKPWIQPKTKVIPY VRYL	f(172–207) of ovine α_{S2} -casein	7.1	10.17	4434.3	−0.589	11.08	83.89	Mamalian Yeast E.coli 0.8 h 10 min 10 h	1.06
LKKISQRYQKFALPQY LKTVYQHQAAMKPWI QPKTKVIPYVRYL	f(164–207) of ovine α_{S2} -casein	10.1	10.35	5451.6	−0.700	9.69	86.36	Mamalian Yeast E.coli 5.5 h 2 min 2 min	1.44
LKKISQRYQKFALPQ YL	f(164–180) of ovine α_{S2} -casein	4.0	10.17	2124.5	−0.659	24.54	97.65	Mamalian Yeast E.coli 5.5 h 2 min 2 min	1.61
YQEPVLGPVRGPFPI	β -casein, gen. var. A ² -5P f(193–207)	0	6.00	1668.9	−0.033	80.71	90.67	Mamalian Yeast E.coli 2.8 h 10 min 2 min	0.3
YQEPVLGPVRGPFPIIV	β -casein, genetic variant A ² -5P f(193–209)	0	6.00	1881.2	0.482	67.4	120.00	Mamalian Yeast E.coli 2.8 h 10 min 2 min	−0.25
MAIPPKKNQDKTEIPTI NTIASGEPTSTPTTEAV ESTVATLEDSPEVIESPP EINTVQVTSTAV	Kappacin f(107–169) of κ -casein gen. var. A	−7.0	4.04	6707.4	−0.370	64.17	77.66	Mamalian Yeast E.coli 30 h 20 h 10 h	1.55

Table S1. *Cont.*

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life	Boman Index (kcal/mol)
YYQQKPVA	f(42–49) of bovine κ -casein	1.0	8.50	996.1	−1.137	62.9	48.75	Mamalian Yeast E.coli 2.8 h 10 min 2 min	1.38
VQVTSTAV	f(162–169) of bovine κ -casein	0.0	5.49	803.9	1.087	−11.29	121.25	Mamalian Yeast E.coli 100 h >20 h >10 h	0.01
STVATL	f(141–146) of bovine κ -casein	0.0	5.24	590.6	1.267	8.33	130.00	Mamalian Yeast E.coli 1.9 h >20 h >10 h	−0.37
FSDKIAK	f(18–24) of bovine κ -casein	1.0	8.59	807.9	−0.429	−15.69	70.00	Mamalian Yeast E.coli 1.1 h 3 min 2 min	1.93
IQY	f(28–30) of bovine κ -casein	0.0	6.09	422.79	−0.100	−18.47	130.00	Mamalian Yeast E.coli 20 h >30 min >10 h	0.25
YVL	f(30–32) of bovine κ -casein	0.0	6.09	393.51	2.233	6.67	226.67	Mamalian Yeast E.coli 20 h 30 min >10 h	−2.59
EIPT	f(118–121) of bovine κ -casein	−1.0	3.85	458.54	−0.325	3.85	97.50	Mamalian Yeast E.coli 1 h 30 min >10 h	1.11
VESTVATL	f(139–146) of bovine κ -casein	−1.0	4.00	818.9	1.038	32.83	133.75	Mamalian Yeast E.coli 100 h >20 h >10 h	0.08
PAAVRSPAQILQ	f(64–75) of bovine κ -casein	1.0	10.18	1250.4	0.200	157.72	114.17	Mamalian Yeast E.coli >20 h >20 h ?	0.84
AVESTVATLEDSPEVIE SPPE	f(136–156) of bovine κ -casein	−6.0	3.40	2199.3	−0.243	134.70	88.10	Mamalian Yeast E.coli 4.4 h >20 h >10 h	1.54
EQLTK	LTD1-f(1–5) of α -laktoalbumin, gen. var. B	0.0	6.10	617.7	−1.560	46.52	78.00	Mamalian Yeast E.coli 1h 30 min >10 h	3.11

Table S1. *Cont.*

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life	Boman Index (kcal/mol)
GYGGVSLPEWVCTTF	LDT 2, α -chain f(17–31) of α -laktoalbumin, gen. var. B	−1.0	4.00	1615.8	0.453	44.95	64.67	Mamalian >30 h Yeast >20 h E.coli >10 h	−0.46
ALCSEK	LDT 2, β -chain f(109–114) of α -laktoalbumin, . gen. varB	0.0	6.04	649.7	−0.017	40.43	81.67	Mamalian 4.4 h Yeast >20 h E.coli >10 h	1.29
CKDDQNPH	LDC, α -chain f(61–68) of α -laktoalbumin, gen. var. B	−1.0	5.21	956.0	−2.525	5.15	0.00	Mamalian 1.2 h Yeast >20 h E.coli >10 h	4.81
ISCDKF	LDC, β -chain chain f(75–80) of α -laktoalbumin, gen. var. B	0.0	5.83	711.8	0.267	80.62	65.00	Mamalian 20 h Yeast 30 min E.coli >10 h	1.41
VAGTWY	f(15–20) β -laktoglobulin, gen. var. A	0.0	5.49	695.7	0.450	−30.87	65.00	Mamalian 100 h Yeast >20 h E.coli >10 h	−1.06
IPAVFK	f(78–83) β -laktoglobulin, gen. var. A	1.0	8.75	673.8	1.300	10.58	130.00	Mamalian 20 h Yeast 30 min E.coli >10 h	−1.36
AASDISLLDAQSAPLR	f(25–40) β -laktoglobulin, gen. var. A	−1.0	4.21	1627.8	0.256	60.91	122.50	Mamalian 4.4 h Yeast >20 h E.coli >10 h	1.32
VLVLDTDYK	f(92–100) β -laktoglobulin, gen.var. A	−1.0	4.21	1065.2	0.344	−7.81	151.11	Mamalian 100 h Yeast >20 h E.coli >10 h	0.86
FKCRRWQWRMKKLG APSITCVRRAF	bovine lactoferricin B f(17–41) of lactoferrin	7.9	11.84	3125.8	−0.576	77.92	50.80	Mamalian 1.1 h Yeast 3 min E.coli 2 min	2.75
APRKNVRW	f(1–8) of lactoferrin	3.0	12.01	1026.2	−1.613	95.00	48.75	Mamalian 4.4 h Yeast >20 h E.coli >10 h	4.23
FKCRRWQWRMKKLG APSITCVRRFAFA	f(17–42) of lactoferrin	7.9	11.84	3196.9	−0.485	75.31	52.69	Mamalian 1.1 h Yeast 3 min E.coli 2 min	2.57

Table S1. *Cont.*

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life	Boman Index (kcal/mol)
FKCRRWQWRMKKLGAPSITCVR RAFAL	f(17–43) of lactoferrin	7.9	11.84	3310.0	−0.326	72.89	65.19	Mamalian 1.1 h Yeast 3 min E.coli 2 min	2.29
APRKNNRWCTISQPEW	f(1–16) of lactoferrin	2.0	9.51	1971.2	−1.056	98.42	48.75	Mamalian 4.4 h Yeast >20 h E.coli >10 h	2.72
CIRA	f(45–48) of lactoferrin	1.0	8.55	461.61	1.075	7.50	122.5	Mamalian 1.2 h Yeast >20 h E.coli >10 h	3.69
FKCRRWQWRMKKLGAPSITCVR RAFALECIR	f(17–47) of lactoferrin	7.9	11.37	3811.6	−0.316	78.95	69.35	Mamalian 1.1 h Yeast 3 min E.coli 2 min	2.5
APRKNNRWCTI	f(1–11) of lactoferrin	3.0	10.86	1343.6	−0.600	101.45	70.91	Mamalian 4.4 h Yeast >20 h E.coli >10 h	2.74
CRRWQWRMKKLGAPSITCV	f(19–37) of lactoferrin	4.9	10.93	2319.8	−0.468	77.14	61.58	Mamalian 1.2 h Yeast >20 h E.coli >10 h	2.16
FKCRRWQWRMKKLG	f(17–30) of lactoferrin	6.0	11.74	1923.3	−1.421	74.31	27.86	Mamalian 1.1 h Yeast 3 min E.coli 2 min	3.55
LECIRA	f(43–48) of lactoferrin	0.0	5.99	703.8	0.767	81.57	146.67	Mamalian 5.5 h Yeast 3 min E.coli 2 min	1.46
APRKNNRWCTISQPEWFKCRRW QWRMKKLGAPSITCVRRAFA	f(1–42) of lactoferrin	9.9	11.63	5150.1	−0.702	84.35	51.19	Mamalian 4.4 h Yeast >20 h E.coli >10 h	2.63
FKCRRWQWRMKKLGAPSITCVR RAFALECIRA	f(17–48) of lactoferrin	7.9	11.37	3883.7	−0.250	76.80	70.31	Mamalian 1.1 h Yeast 3 min E.coli 2 min	2.36
WKLLSKAQEKFGKNKSR	Lactoferrampin f(268–284) of lactoferrin	5.0	10.58	2048.4	−1.482	36.01	51.73	Mamalian 2.8 h Yeast 3 min E.coli 2 min	2.97

Table S1. Cont.

Sequence	AMP Origin/Position	Net Charge	Isoelectric Point (pH)	Molecular Mass (Da)	GRAVY	Instability Index	Aliphatic Index	Half Life		Boman Index (kcal/mol)
ADRDQYELL	Antiviral f(241–249) of lactoferrin	−2.0	4.03	1122.2	−1.156	−25.68	97.78	Mamalian	4.4 h	3.68
								Yeast	>20 h	
								E.coli	>10 h	
TRVVWCAVG	Lactoferrin (fr. 343–351)	1	9.01	990.1	1.156	−0.54	107.78	Mamalian	7.2 h	−0.11
GRDPYKLRPV	Lactoferrin (fr. 68–77)	2	9.99	1200.4	−1.33	58.29	68.00	Yeast	>20 h	3.43
EDLIWK	Antiviral f(263–268) of lactoferrin	−1.0	4.37	802.9	−0.583	40.43	130.00	Mamalian	1 h	1.48
								Yeast	30 min	
								E.coli	>10 h	

Table S2. The characteristics of potential AMPs from milk proteins released during in silico proteolysis according to positive prediction scores of two or more statistical models available in CAMP database (SVM, RF, ANN and DA).

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
DDKHYQKA (Pancreatic elastase EC 3.4.21.36, Leukocyte elastase EC 3.4.21.37)	α_{s2} -casein, gen. var. A-11P f(74–81)	0.1	7.72	1004.07	4.63	53.06	12.50	−2.625	1.000	0.622	NAMP	0.507
FTK KT KL (Pancreatic elastase EC 3.4.21.36)	α_{s2} -casein, gen. var. A-11P f(147–153)	3.0	10.84	865.08	1.98	−3.56	55.71	−0.929	0.998	0.5215	AMP	0.940
DTDYK KYL (Pancreatic elastase EC 3.4.21.36, Pepsin 1.3 EC 3.4.23.1, Pancreatic elastase EC 3.4.21.71)	β -lactoglobulin, gen. var. B f(96–103)	0.0	6.75	1045.16	3.3	−10.04	48.75	−1.788	1.000	0.4615	NAMP	0.556
KNTMEHV (Pancreatic elastase EC 3.4.21.36, Leukocyte elastase EC 3.4.21.37, Proteinase P1 (lactocepin) EC 3.4.21.96)	α_{s2} -casein, gen. var. A-11P f(1–7)	0.1	6.75	857.9	2.83	−14.33	41.43	−1.243	0.928	0.609	NAMP	0.029
NEEEYSI (Pancreatic elastase EC 3.4.21.36)	α_{s2} -casein, gen. var. A-11P f(48–54)	−3	3.67	882.8	3.66	101.71	55.71	−1.657	1.000	0.5665	NAMP	0.152
QNNDSTEYG (Pancreatic elastase EC 3.4.21.36)	α -lactalbumin, gen. var. B f(43–51)	−2	3.67	1026.9	4.39	42.26	0.00	−2.300	1.000	0.5875	NAMP	0.027
TKESPQTHYYA (Pancreatic elastase EC 3.4.21.36)	Lactoferrin f(84–94)	0.1	6.41	1324.4	2.68	156.75	9.09	−1.700	0.999	0.524	NAMP	0.027
PNSKEKYYG (Pancreatic elastase EC 3.4.21.36)	Lactoferrin f(517–525)	1.0	9.47	1085.18	3.03	13.17	0.00	−2.244	1.000	0.252	NAMP	0.873
LQGAVAKFFSASCVP (Prolyl oligopeptidase EC 3.4.21.26) Poor water solubility	Lactoferrin f(145–159)	1.0	8.97	1524.81	−0.58	54.95	84.67	0.980	0.785	0.2385	AMP	0.716
GQRDLLFKDSALGFLRIP (Prolyl oligopeptidase EC 3.4.21.26)	Lactoferrin f(294–311)	1.0	10.08	2046.41	1.52	20.89	113.89	0.028	0.659	0.4835	AMP	0.834
QEQNQEQP (Prolyl oligopeptidase EC 3.4.21.26), Thermolysin EC 3.4.24.27)	κ -casein, gen. var. A f(1–8)	−2	3.79	999.9	5.3	119.70	0.00	−3.263	0.976	0.5845	AMP	0.000

Table S2. *Cont.*

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
ADALNLDGGYIYTAGKCGLVPLAE (V-8 proteaza EC 3.4.21.19)	Lactoferrin f(389–413)	−2.0	3.7	2523.89	−0.22	16.36	117.20	0.536	0.568	0.5215	NAMP	0.816
GYLAVAVVKKAN (Glutamyl endopeptidase II EC 3.4.21.82)	Lactoferrin f(432–443)	2.0	10.18	1232.49	−0.46	−0.31	130.0	0.733	0.893	0.4395	AMP	0.928
KKYKVPQL (Pepsin 1.3 EC 3.4.23.1, Pancreatic elastase EC 3.4.21.71)	α_{s1} -casein, gen. var. B-8P f(102–109)	3.0	10.45	1003.25	1.67	46.29	85.00	−1.262	0.952	0.509	NAMP	0.916
NVPGEIVESL (Pepsin 1.3 EC 3.4.23.1, Cathepsin G EC 3.4.21.20, Metridin EC 3.4.21.3, Pancreatic elastase II EC 3.4.21.71)	β -casein gen. var. B f(7–17)	−2	3.79	1056.1	0.47	50.75	136.00	0.340	0.586	0.516	NAMP	0.001
GRSAGWIIPMGIL (Pepsin 1.3 EC 3.4.23.1) Poor water solubility	Lactoferrin f(120–132)	1.0	11.04	1370.68	−0.82	52.79	127.69	0.923	0.171	0.564	AMP	0.645
FTK KTK (Thermolysin EC 3.4.24.27)	α_{s2} -casein, gen. var. A-11P f(147–152)	3.0	10.84	751.92	3.13	8.33	0.00	−1.717	1.000	0.5285	AMP	0.986
ANEEEYS (Thermolysin EC 3.4.24.27)	α_{s2} -casein, gen. var. A-11P (fr 47–53)	−3	3.67	840.8	4.11	101.71	14.29	−2.043	0.933	0.6535	NAMP	0.002
AGDDQG (Thermolysin EC 3.4.24.27)	Lactoferrin f(506–511)	−2	3.56	561.5	3.21	8.33	16.67	−1.583	0.624	0.551	NAMP	0.000
ESTEVSF (Cathepsin G EC 3.4.21.20, Pancreatic elastase II EC 3.4.21.71),	α_{s2} -casein, gen. var. A-8P f(152–147)	−2	3.80	710.7	2.09	72.53	48.33	−0.250	1.000	0.531	NAMP	0.005
PYPYYAK (Cathepsin G EC 3.4.21.20) Poor water solubility	κ -casein, gen. var. A f(57–63)	1.0	9.39	901.03	0.59	77.66	14.29	−1.314	0.999	0.3085	NAMP	0.719

Table S2. *Cont.*

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
TDAPSF (Chymase EC 3.4.21.39), Metridin EC 3.4.21.3)	α_{S1} -casein, gen. var. B-8P f(174–179)	−1	3.80	636.6	1.65	72.53	16.67	−0.333	0.901	0.5085	NAMP	0.011
AVAVVKKGSNF (Chymase EC 3.4.212.39, Metridin EC 3.4.21.3)	Lactoferrin f(94–104)	2.0	10.6	1119.33	0.13	−14.91	97.27	0.591	0.943	0.483	AMP	0.912
IIPMGILRPY (Chymase EC 3.4.21.39) Poor water solubility	Lactoferrin f(126–135)	1.0	9.84	1172.5	−0.79	47.87	156.0	0.980	0.371	0.595	AMP	0.837
VTAIANLKKCSTSPLEACAF (Chymase EC 3.4.21.39) Poor water solubility	Lactoferrin f(666–686)	0.9	8.29	2180.62	0.00	43.29	107.14	0.748	0.685	0.917	AMP	0.852
PQRDMPIQAF (Chymase EC 3.4.21.39, Metridin EC 3.4.21.3)	β -casein gen. var. B f(181–190)	0	6.27	1202.3	2.26	72.20	49.00	−0.720	0.715	0.697	NAMP	0.018
EAGRDPY (Chymase EC 3.4.21.39), Metridin EC 3.4.21.3)	Lactoferrin f(66–72)	−1	4.37	806.8	3.97	8.57	14.29	−1.857	0.848	0.5785	NAMP	0.000
GTKESPQTHY (Chymase EC 3.4.21.39), Metridin EC 3.4.21.3)	Lactoferrin f(83–92)	0.1	6.75	1147.2	3.03	126.91	0.00	−1.96	0.718	0.625	NAMP	0.007
TTMPLW (Papain 3.4.22.2, Bromelain EC 3.4.22.4) Poor water solubility	α_{S1} -casein, gen. var. B-8P f(204–209)	0	5.19	747.9	−0.74	121.03	65.0	0.300	0.976	0.5275	NAMP	0.046
DMPIQA (Papain 3.4.22.2, Bromelain EC 3.4.22.4)	β -casein gen. var. B f(184–189)	−1	3.80	673.7	0.86	81.57	81.67	−0.067	0.768	0.525	NAMP	0.005
QPTTMA (Papain 3.4.22.2, Ficin EC 3.4.22.3, Leukocyte elastase EC 3.4.21.37, Bromelain EC 3.4.22.4) Poor water solubility	κ -casein, gen. var. A f(91–96)	0	5.52	647.7	1.08	61.00	16.67	−0.467	1.000	0.6035	NAMP	0.015

Table S2. *Cont.*

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
EERLHSMK (Bromelain EC 3.4.22.4)	α_{S1} -casein, gen. var. B-8P f(117–124)	0.1	6.86	1029.1	4.35	49.50	48.75	−1.712	0.717	0.5785	NAMP	0.001
SESTEDQA (Ficain EC 3.4.22.3, Bromelain EC 3.4.22.4)	α_{S1} -casein, gen. var. B-8P f(46–53)	−3	3.57	865.8	4.43	105.05	12.50	−1.812	0.998	0.637	NAMP	0.004
PQRDMPIQA (Ficain EC 3.4.22.3), Bromelain EC 3.4.22.4)	β -casein, gen. var. A-5P f(181–189)	0	6.27	1055.2	2.84	79.11	54.44	−1.111	0.827	0.6745	NAMP	0.010
EMPFPK (Ficain EC 3.4.22.3, Bromelain EC 3.4.22.4)	β -casein, gen. var. A ² -5P f(108–113)	0	6.94	747.91	1.17	145.77	0.00	−0.983	1.000	0.571	AMP	0.190
EPEQSL (Ficain EC 3.4.22.3)	β -lactoglobulin, gen. var. B f(112–117)	−2.0	3.13	701.73	2.94	174.73	65.00	−1.517	1.000	0.4695	NAMP	0.569
ESPQTHY (Ficain EC 3.4.22.3, Bromelain EC 3.4.22.4)	Lactoferrin f(86–92)	−0.9	5.24	860.8	3.3	189.14	0.00	−2.086	0.551	0.658	NAMP	0.004
PQ LEIV (Leukocyte elastase EC 3.4.21.37, Prolidase L.lactis s.cremoris H61 EC 3.4.13.9)	α_{S1} -casein, gen. var. B-8P f(107–112)	−1	4.00	697.8	−0.25	58.38	178.33	0.650	0.945	0.553	NAMP	0.020
EK TTMPLW (Leukocyte elastase EC 3.4.21.37), Proteinase P1 (lactocepin EC 3.4.21.37)	α_{S1} -casein, gen. var. B-8P f(192–199)	0	6.10	1005.2	0.98	93.28	48.75	−0.700	1.000	0.644	NAMP	0.021
NEEEYS (Leukocyte elastase EC 3.4.21.37)	α_{S2} -casein, gen. var. A-11P f(48–53)	−3	3.67	769.7	5.1	117.0	0.00	−2.683	1.000	0.6795	NAMP	0.006

Table S2. *Cont.*

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
QETYSQEKDMA (Leukocyte elastase EC 3.4.21.37)	α_{s2} -casein, gen. var. A-11P f(17–27)	0.0	6.99	1369.52	3.72	76.85	9.09	−2.145	0.697	0.3575	NAMP	0.856
FTK KTKLT EEEEKNRLN FLKKIS (Leukocyte elastase EC 3.4.21.37)	α_{s2} -casein, gen. var. A-11P f(147–168)	4.0	10.53	2696.19	3.06	29.53	70.91	−1.218	0.531	0.497	AMP	0.465
ITRINKKIEKFQS (Leukocyte elastase EC 3.4.21.37)	β -casein, gen. var. A ² -5P f(23–35)	3.0	10.83	1604.92	2.98	88.52	90.00	−0.915	0.492	0.454	AMP	0.739
LTLTDV (Leukocyte elastase EC 3.4.21.37) Poor water solubility	β -casein, gen. var. A ² -5P f(125–130)	−1	3.80	660.7	0.00	8.33	178.33	1.15	0.551	0.5625	NAMP	0.002
GWIPMGILRPYLS (Leukocyte elastase EC 3.4.21.37) Poor water solubility	Lactoferrin f(124–137)	1.0	9.84	1616.01	−0.9	45.86	139.29	0.821	0.501	0.751	AMP	0.619
PPTVMF (Metridin EC 3.4.21.3) Poor water solubility	β -casein, gen. var. A ² -5P f(152–172)	0	5.96	690.8	−1.13	40.43	48.33	0.833	1.000	0.644	NAMP	0.053
RPTEGY (Metridin EC 3.4.21.3)	Lactoferrin f(428–433)	0	6.00	721.7	3.91	58.33	0.00	−2.0	1.000	0.4985	NAMP	0.025
DGGMVF (Metridin EC 3.4.21.3) Poor water solubility	Lactoferrin f(60–65)	−1.0	3.1	624.72	−0.42	28.90	48.33	0.767	0.998	0.644	AMP	0.001
APKHKEM (Pancreatic elastase II EC 3.4.21.71)	β -casein, gen. var. A ² -5P f(103–109)	1.1	8.64	840.0	2.62	69.91	14.29	−1.771	1.000	0.4915	AMP	0.020
KILDKVGINYWLAHK ALCSEK LDQWLCEKL (Calpain EC 3.4.22.17)	α -lactalbumin, gen. var. B f(94–123)	1.0	8.26	3559.26	0.8	12.53	120.33	−0.113	0.691	0.5285	AMP	0.968
INYWLAHK ALCSEK LDQWLCEKL (Glycyl endopeptidase EC 3.4.22.25)	α -lactalbumin, gen. var. B f(101–123)	0.0	7.0	2805.32	0.82	23.38	110.43	−0.183	0.554	0.556	AMP	0.763

Table S2. *Cont.*

Sequence (Enzyme)	AMP Origin/Position	Net Charge	Isoelectric Point pH	Molecular Mass Da	Boman Index kcal/mol	Instability Index	Aliphatic Index	GRAVY	SVM	RFC	ANN	DAC
APSITCVRRFALECI RA IAEKKADAV												
TLDG (Glycyl endopeptidase EC 3.4.22.25)	Lactoferrin f(31–61)	0.9	8.29	3289.88	1.4	46.85	104.19	0.335	0.583	0.490	AMP	0.797
AVAKFFSASCVPCIDRQAYPNLCQLC												
KG (Glycyl endopeptidase EC 3.4.22.25)	Lactoferrin f(149–175)	1.8	8.3	3033.62	0.61	25.65	76.79	0.375	0.903	0.9695	AMP	0.984
Poor water solubility												
L EIVPN (Proteinase P1 (lactocepin) EC 3.4.21.96)	α_{S1} -casein, gen. var. B-8P f(109–114)	−1	4.0	683.6	−0.07	58.38	178.33	0.650	0.556	0.535	NAMP	0.026
Poor water solubility												
RDMP1 Proteinase P1 (lactocepin) EC 3.4.21.96	α_{S1} -casein, gen. var. B-8P f(102–109)	0	5.84	630.7	3.27	95.88	78.00	−0.640	1.000	0.627	NAMP	0.015
ITRINKKIEKF (Proteinase P1 (lactocepin) EC 3.4.21.96)	β -casein, gen. var. A ² -5P f(23–33)	3.0	10.83	1389.71	2.71	62.85	106.36	−0.691	0.694	0.460	AMP	0.879
F MA IPP PK N (Proteinase P1 (lactocepin) EC 3.4.21.96)	κ -casein, gen. var. A f(105–113)	2.0	10.6	1045.32	0.63	40.80	54.44	−0.389	0.890	0.381	AMP	0.684
GAVAKFF (Proteinase P1 (lactocepin) EC 3.4.21.96)	Lactoferrin f(147–153)	1.0	10.1	738.89	−1.28	−3.56	70.0	1.30	0.631	0.4245	AMP	0.597
Poor water solubility												
ALFGKNGKNCPDKFCLFK (Proteinase P1 (lactocepin) EC 3.4.21.96)	Lactoferrin f(616–633)	2.9	9.71	2030.45	1.06	−5.79	48.89	−0.317	0.706	0.7655	AMP	0.987
PKHKEMPF (Prolidase L.lactis s.cremoris H61 EC 3.4.13.9)	β -casein, gen. var. A ² -5P f(104–111)	1.1	9.88	1013.23	2.15	117.35	0.00	−1.625	0.999	0.4065	NAMP	0.552

Fragments of known AMPs are marked in red.