Supplementary Data

Novel insight into the taste mechanism of umami and bitter peptides in low-salt fermented fish sauce based on peptidomics, molecular docking, and molecular dynamics

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Table S1. Sequences and characteristics of 97 peptides with different tastes from LF and Th fish sauces

Number	Peptide sequence	Molecular weight (Da)	Isoelectric point	Charge	Hydropathicity (GRAVY)	Aliphatic index	Bitter AA (%)	Umami AA (%)
U1	EEGDLIE	803.81	3.5	-4	-0.87	111.43	28.57%	57.14%
U2	LEEGDLIE	916.98	3.5	-4	-0.29	146.25	37.50%	50%
U3	VIEEDDEHAI	1169.2	3.83	-4.9	-0.57	117	40%	50%
U4	LEETGEL	789.83	3.67	-3	-0.571	111.43	28.57%	42.86%
U5	SESKEEK	835.86	4.78	-1	-2.843	0	0	42.86%
U6	RDEDLAP	814.84	4.03	-2	-1.571	70	42.86%	42.86%
U7	NELEEIP	842.89	3.67	-3	-1.043	111.43	42.86%	42.86%
U8	VEEGREF	864.91	4.25	-2	-1.2	41.43	28.57%	42.86%
U9	IDGNELEEIP	1128.19	3.5	-4	-0.67	117	40%	40%
U10	EPAEREFEFI	1266.35	4.09	-3	-0.82	49	50%	40%
U11	EGDLIEFP	918.99	3.57	-3	-0.175	97.5	50%	38%
U12	TLELEKEF	1008.12	4.25	-2	-0.588	97.5	37.50%	37.50%
U13	KEESGELP	887.93	4.25	-2	-1.675	48.75	25%	37.50%
U14	TDVDIGDL	864.88	3.42	-3	0.113	133.75	37.50%	37.50%
U15	DIVPADDH	880.9	3.93	-2.9	-0.6	97.5	50%	37.50%
U16	EDEVLSVP	886.94	3.57	-3	-0.087	121.25	50%	37.50%
U17	DEVGTEMI	892.97	3.57	-3	-0.125	85	25%	37.50%
U18	PDEWEVAR	1001.05	4.14	-2	-1.438	48.75	50%	37.50%
U19	DKADDIPGK	958.02	4.43	-1	-1.556	54.44	33.33%	33.33%
U20	SINDELDPP	999.03	3.49	-3	-1.078	86.67	44.44%	33.33%
U21	VEPGEEGLQ	956.99	3.67	-3	-0.933	75.56	33.33%	33.33%
U22	QPGALLEDDQ	1085.12	3.49	-3	-1.01	88	40%	30%
U23	VEETEGVDLR	1146.21	4	-3	-0.74	97	30%	30%
B1	LGFFWAF	887.03	5.52	0	1.814	70	85.71%	0
B2	AGAGLALLV	783.97	5.57	0	2.244	195.56	77.78%	0

B3	SLANLALPP	895.05	5.24	0	0.833	152.22	77.78%	0
B4	SIFLIMLP	933.21	5.24	0	2.362	195	75%	0
B5	SIMPAVAV	786.98	5.24	0	2	146.25	75%	0
B6	APPLTQLL	852.03	5.57	0	0.725	158.75	75%	0
B7	KWSPPVFP	957.12	8.75	1	-0.425	36.25	75%	0
B8	IVTAHAF	757.88	6.74	0.1	1.6	125.71	71.43%	0
B9	TPEFVAL	775.89	4	-1	0.971	111.43	71.43%	14.28%
B10	YHPPPPP	803.9	6.74	0.1	-1.786	0	71.43%	0
B11	LAGICFV	721.91	5.52	-0.1	2.743	167.14	71.43%	0
B12	PTLMLIP	784.02	5.96	0	1.443	167.14	71.43%	0
B13	PLSQFLF	851	5.96	0	1.043	111.43	71.43%	0
B14	PSDVAPP	681.73	3.8	-1	-0.443	55.71	71.43%	14.28%
B15	STALACIPAP	943.12	5.24	-0.1	1.15	108	70%	0
B16	IMAPTLMLIP	1099.45	5.52	0	1.83	166	70%	0
B17	TAAAMLLFAS	995.2	5.19	0	1.8	118	70%	0
B18	TLAPSDVAP	869.96	3.8	-1	0.378	97.78	66.67%	11.11%
B19	GLDPAGPLF	886.02	3.8	-1	0.522	97.78	66.67%	22.22%
B20	TSLANLALP	899.04	5.19	0	0.933	152.22	66.67%	0
B21	AIPTGVKVF	931.13	8.8	1	1.211	118.89	66.67%	0
B22	STDPAVVPP	881.97	3.8	-1	0.044	75.56	66.67%	0
B23	EIPAGLLDP	924.05	3.67	-2	0.367	141.11	66.67%	22.22%
B24	TSLALFSP	834.96	5.19	0	1.038	110	62.50%	0
B25	ANPMVTPP	825.97	5.57	0	-0.138	48.75	62.50%	0
B26	IGVNLTFF	910.07	5.52	0	1.688	133.75	62.50%	0
B27	SPTLFWGL	920.06	5.24	0	0.75	97.5	62.50%	0
B28	TLWWIGIK	1016.23	8.41	1	0.75	146.25	62.50%	0
B29	GLDPAGPL	738.83	3.8	-1	0.237	110	62.50%	12.50%
B30	VPMMIGAP	815.06	5.49	0	1.337	97.5	62.50%	0
B31	TLSLFSQFAP	1110.26	5.19	0	0.76	88	60%	0

B32	QLVCLLFDSL	1150.39	3.8	-1.1	1.69	185	60%	10%
B33	GLDPAGP	625.67	3.8	-1	-0.271	70	57.14%	14.28%
B34	TIPVLTS	729.86	5.19	0	1.243	152.86	57.14%	0
B35	TSAVCPP	673.78	5.18	-0.1	0.543	55.71	57.14%	0
B36	TPSLPPQ	738.83	5.19	0	-0.857	55.71	57.14%	0
B37	LQTPPSP	738.83	5.52	0	-0.857	55.71	57.14%	0
B38	SATEAWI	776.83	4	-1	0.314	84.29	57.14%	14.28%
B39	ASETWLA	776.83	4	-1	0.214	84.29	57.14%	14.28%
B40	GIMSFLL	779.99	5.52	0	2.229	167.14	57.14%	0
B41	PMEPYPP	829.96	4	-1	-1.329	0	57.14%	14.28%
B42	SIHLFID	843.97	5.06	-0.9	1.157	167.14	57.14%	14.28%
B43	RVPAFQQ	844.96	9.75	1	-0.614	55.71	57.14%	0
B44	DFYITVP	853.96	3.8	-1	0.629	97.14	57.14%	14.28%
B45	WLQGCPP	799.94	5.52	-0.1	-0.243	55.71	57.14%	0
B46	SLPHFLY	876.01	6.46	0.1	0.5	111.43	57.14%	0
B47	TCHFLLP	830.01	6.4	0	1.057	111.43	57.14%	0
B48	PMMIGAP	715.93	5.96	0	0.929	70	57.14%	0
B49	TPNLSPP	724.8	5.19	0	-0.857	55.71	57.14%	0
B50	GAINFIT	734.84	5.52	0	1.286	125.71	57.14%	0
B51	PEAEARP	768.82	4.53	-1	-1.586	28.57	57.14%	28.57%
B52	TLAPTWK	815.96	8.41	1	-0.314	70	57.14%	0
B53	APVNCRI	771.93	8.29	0.9	0.486	111.43	57.14%	0
B54	TYILCIP	822.03	5.18	-0.1	1.671	167.14	57.14%	0
B55	AGGTPPP	595.65	5.57	0	-0.643	14.29	57.14%	0
B56	TTPSLPP	711.8	5.19	0	-0.457	55.71	57.14%	0
B57	TLAGSLP	657.76	5.19	0	0.843	125.71	57.14%	0
B58	PTKSPPP	722.83	9.18	1	-1.686	0	57.14%	0
B59	LEHLGAP	735.83	5.24	-0.9	0.1	125.71	57.14%	14.28%
B60	PAHYTLP	797.9	7.17	0.1	-0.4	70	57.14%	0

B61	PDFHSPL	811.88	5.08	-0.9	-0.586	55.71	57.14%	14.28%
B62	KITFICP	821.04	8.22	0.9	1.157	111.43	57.14%	0
B63	ALGVTAGAH	795.88	6.79	0.1	0.967	108.89	55.56%	0
B64	PSPSSEAPP	867.9	4	-1	-1.167	11.11	55.56%	11.11%
B65	TTVTSAPLP	886	5.19	0	0.411	86.67	55.56%	0
B66	SVTTPSLPP	898.01	5.24	0	0.022	75.56	55.56%	0
B67	TAAACVLSK	863.04	7.89	0.9	1.167	108.89	55.56%	0
B68	KTGPDPIPP	921.05	5.84	0	-1.156	43.33	55.56%	11.11%
B69	SSYHPPPPP	978.07	6.46	0.1	-1.567	0	55.56%	0
B70	TDAFTAFHP	1006.07	5.05	-0.9	-0.056	22.22	55.56%	11.11%
B71	TAVRPEVFE	1047.16	4.53	-1	-0.089	75.56	55.56%	22.22%
B72	TGLDPAGP	726.78	3.8	-1	-0.325	61.25	50%	12.50%
B73	TSAPLPTT	786.87	5.19	0	-0.062	61.25	50%	0
B74	WVPGGQSF	876.95	5.52	0	-0.075	36.25	50%	0

Note: Thresholds of umami and bitter were>30% and >50%, respectively. Umami peptides and bitter peptides were marked as U and B, respectively

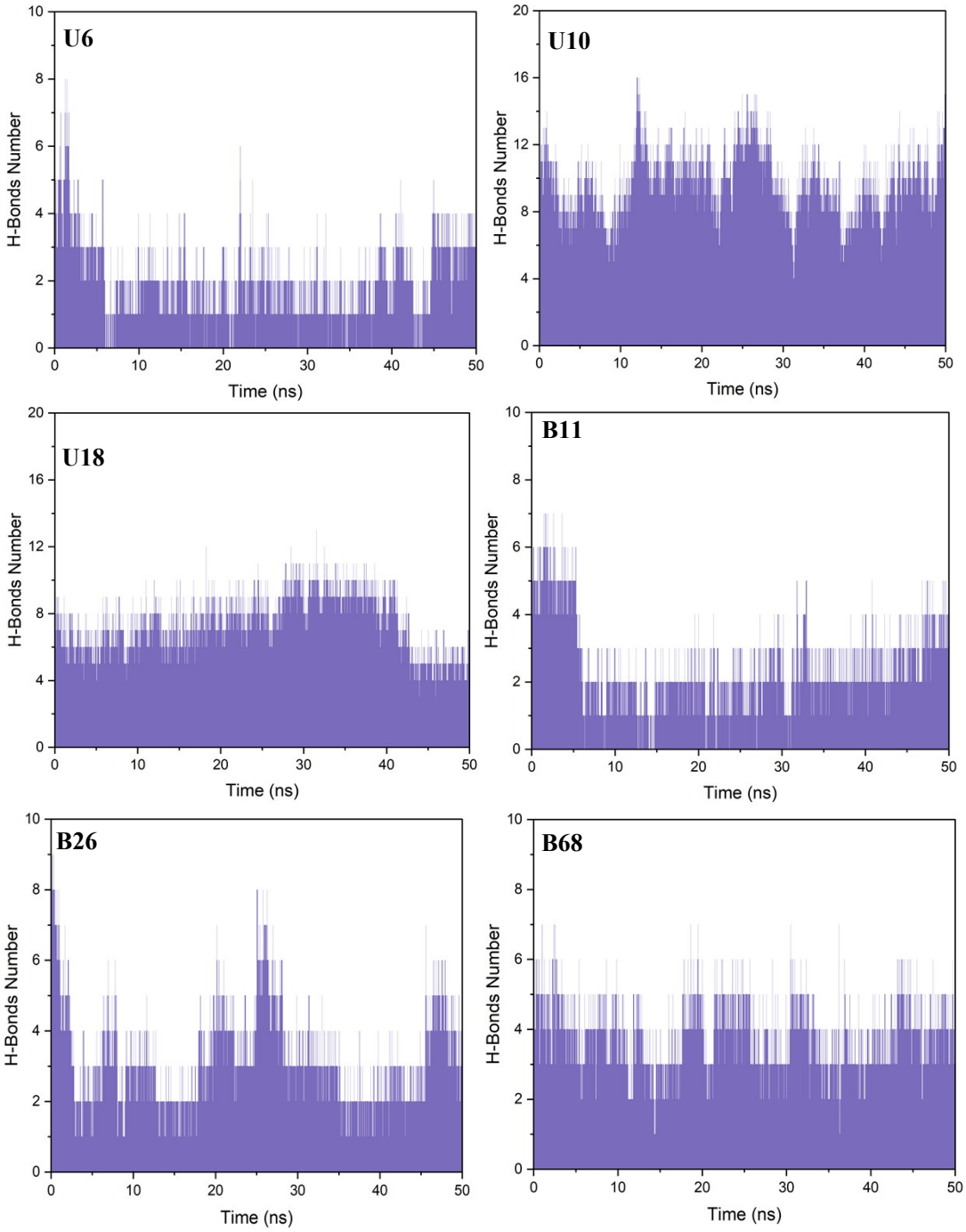


Fig. S1. Diagram of the number of hydrogen bonds in different T1R1/T1R3-umami peptides and TAS2R14-bitter peptides system

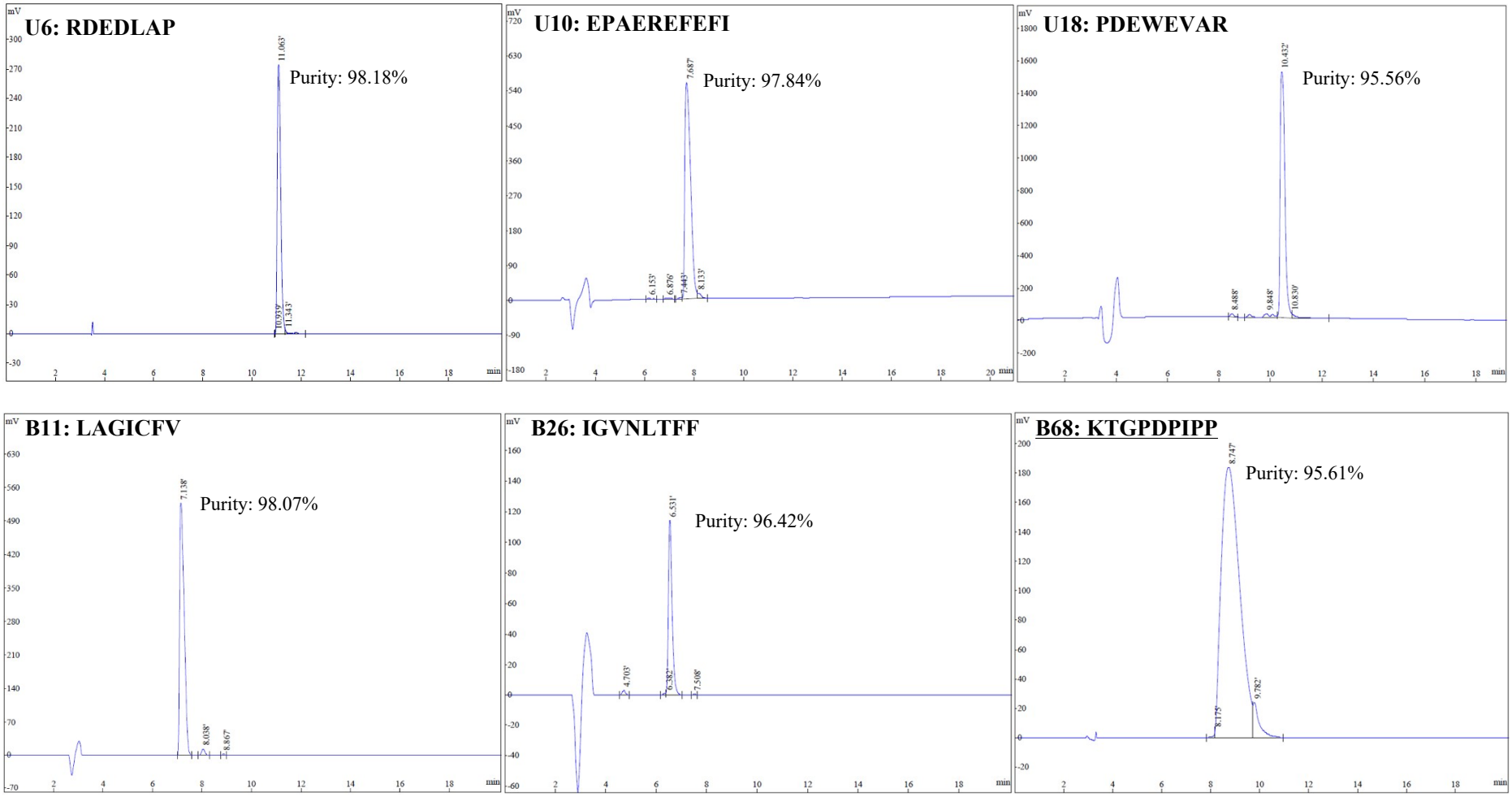
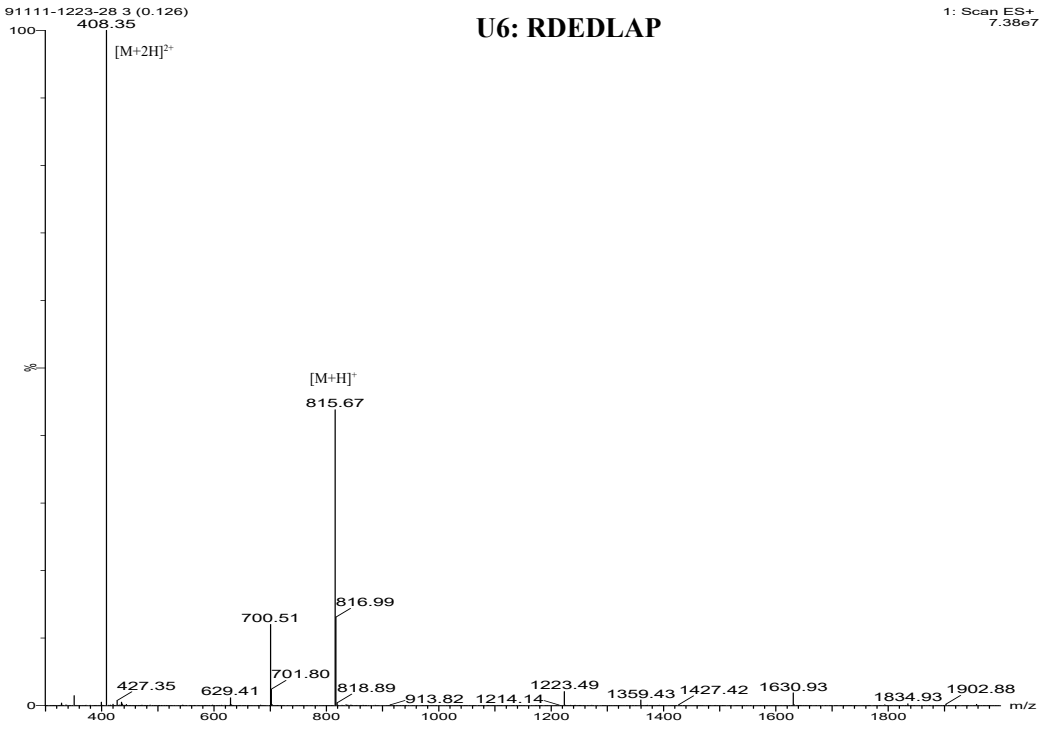
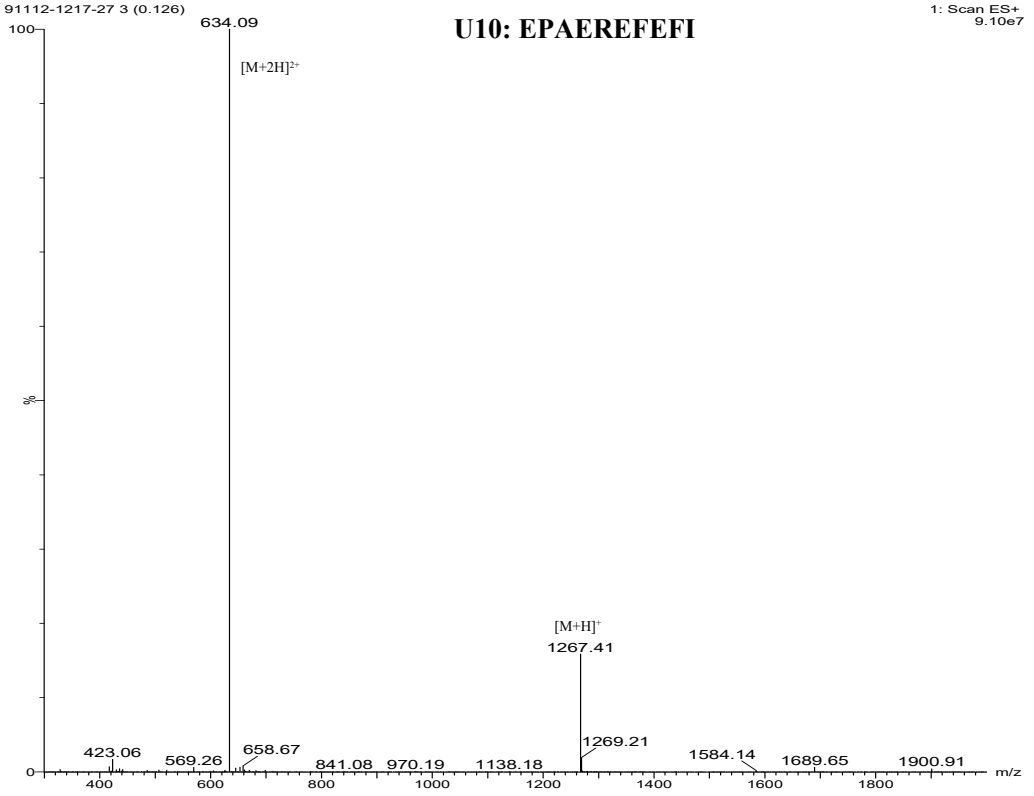


Fig. S2. Purity of the synthetic umami and bitter peptides analyzed by HPLC

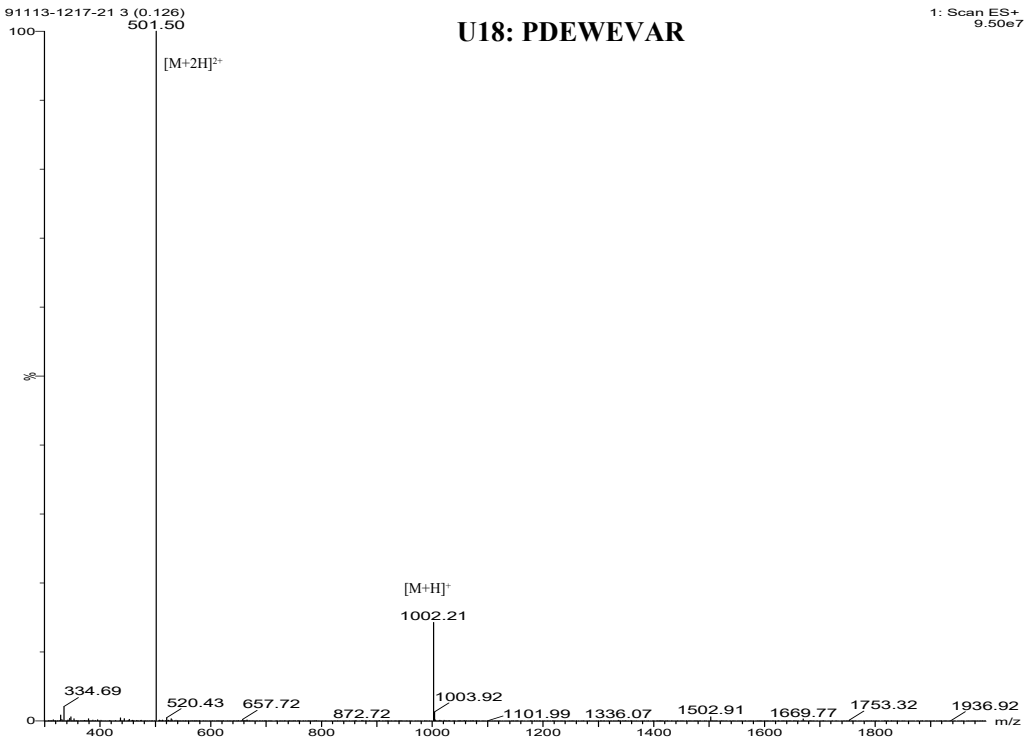
U6: RDEDLAP



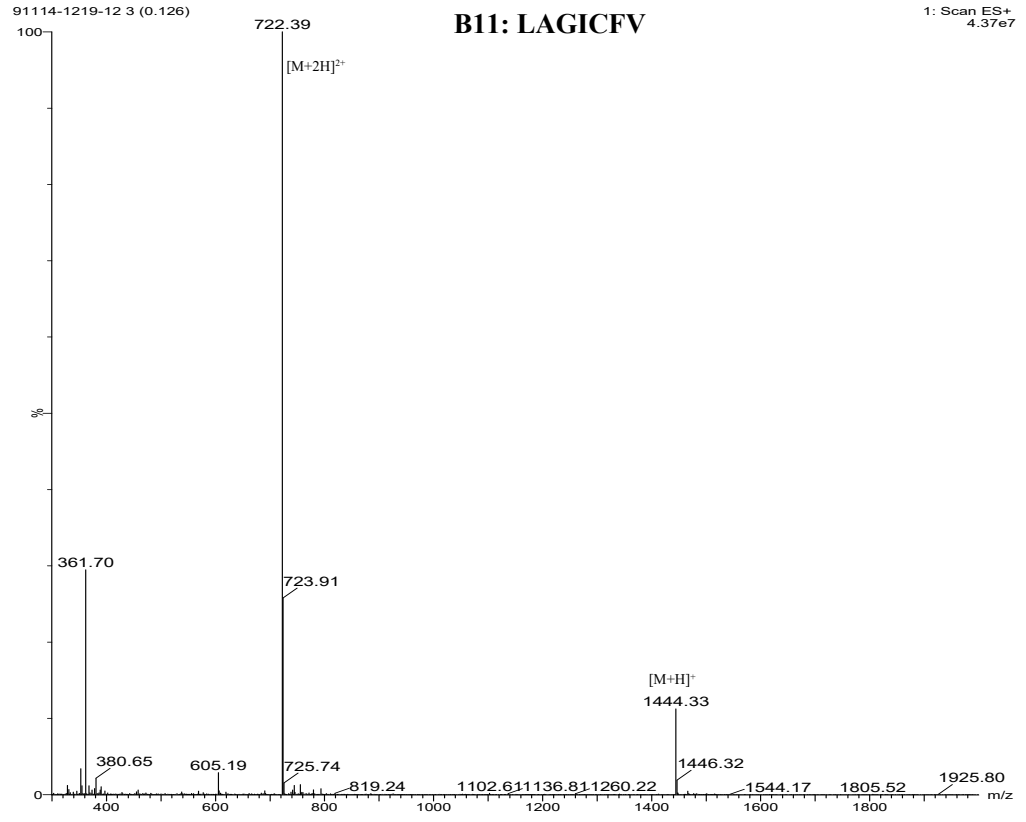
U10: EPAEREFEFI

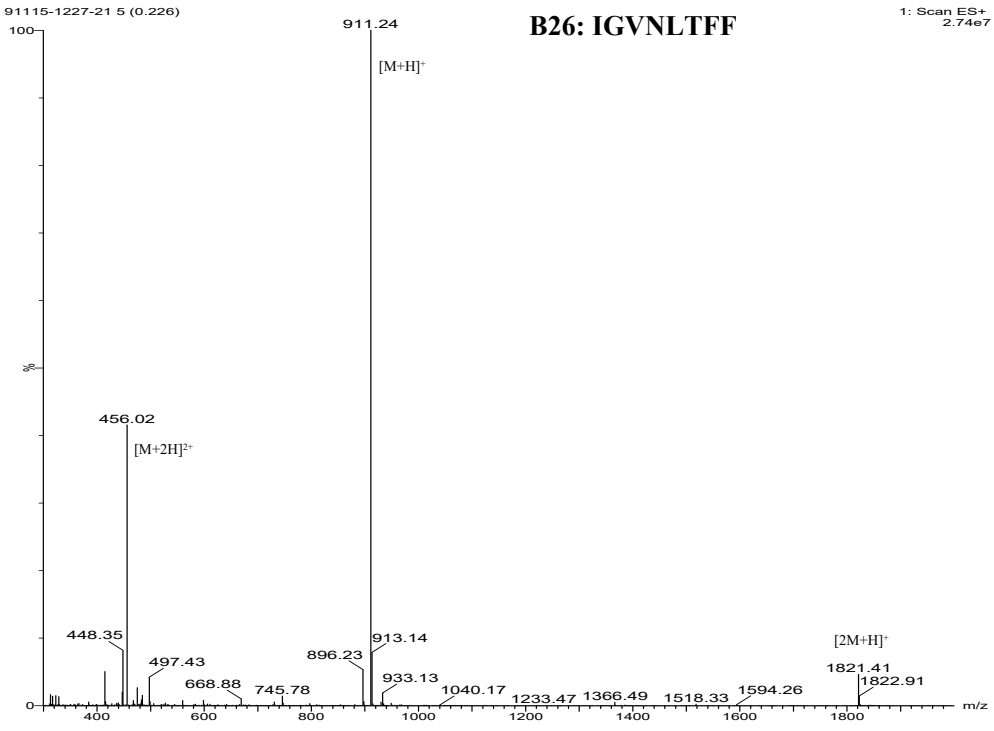


U18: PDEWEVAR



B11: LAGICFV





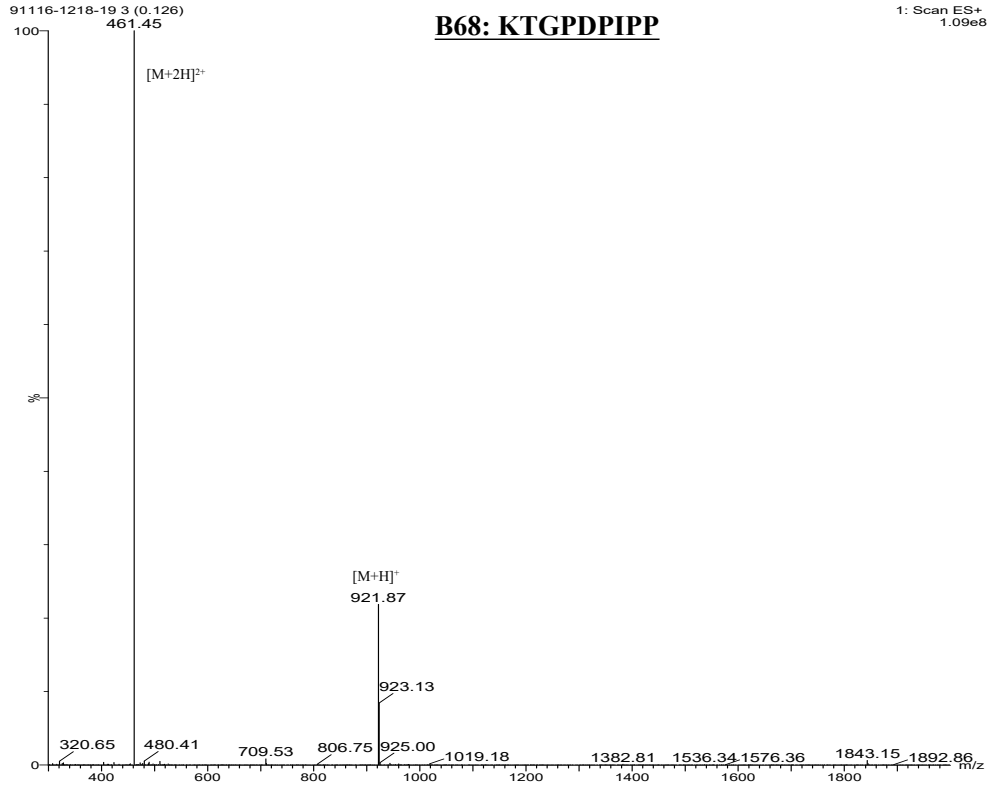


Fig. S3. Secondary MS map of the synthetic umami and bitter peptides