

Unveiling low-abundance ACE inhibitory peptides in not-from-concentrate orange juice processed by high-pressure processing and pasteurization

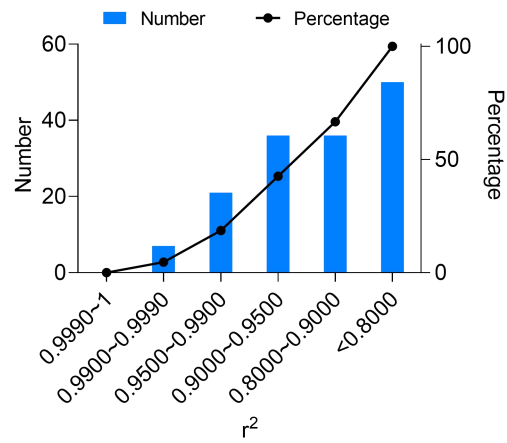
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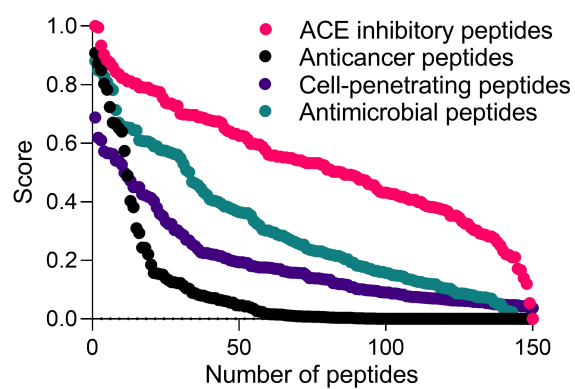
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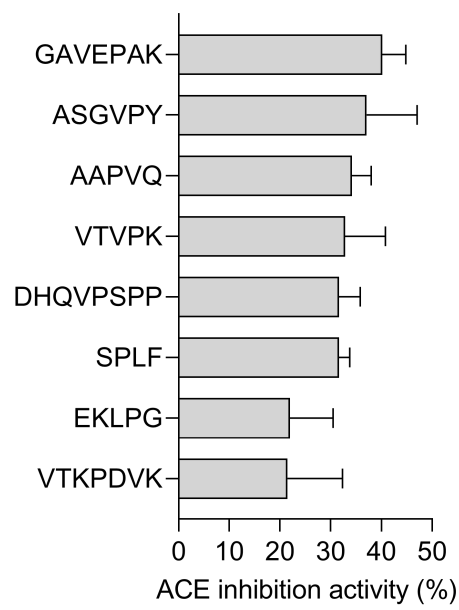
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Supplementary Figure 1. Linearity results of the untargeted peptidomics approach.



Supplementary Figure 2. Prediction scores for bioactivities of peptides.



Supplementary Figure 3. Angiotensin converting enzyme (ACE) inhibition activity of peptides.

Supplementary Table 1 Ion pairs and charge number of 150 peptides in pseudotargeted peptidomics.

ID	Charge number	Theoretical MS1 <i>m/z</i>	MS1 <i>m/z</i>	MS2 <i>m/z</i>
ECACG	1	482.1058	482.1056	353.0651
EALH	1	469.2388	469.2389	156.0763
ASMEN	1	551.2103	551.2109	419.1570
AVVVA	1	458.3340	458.3335	143.1184
GAVEPAK	1	671.3698	671.3697	315.2025
GLKPGPH	1	705.4024	705.4021	407.2029
STLK	1	448.2618	448.2618	260.1605
AAPVQ	1	485.2699	485.2707	343.1994
DSDGS	1	480.1612	480.1621	163.0387
DTLAG	1	476.2328	476.2328	458.2206
SQFAN	1	566.2552	566.2549	216.0985
EAAPVQ	1	614.3113	614.3130	343.1969
EKLPG	1	543.3121	543.3126	371.2297
VTVPK	1	543.3496	543.3496	244.1652
QKLPG	1	542.2925	542.2907	370.2085
TSPIS	1	504.2664	504.2673	316.1863
ADLPG	1	472.2397	472.2394	173.0924
NGVLT	1	503.2806	503.2806	271.1399
HCGPGSGS	1	701.2263	701.2282	539.1736
SIFGK	1	551.3171	551.3156	351.2041
ASGVPI	1	593.2911	593.2919	279.1351
LSVEVQ	1	674.3318	674.3320	528.2661
QGAIGPR	1	698.3819	698.3819	329.1826
EQTVVLK	1	816.4815	816.4815	440.2161
PLCGNSAC	1	764.2417	764.2452	572.1672
EILSN	1	575.3042	575.2986	356.2170
VFDPVS	1	663.3372	663.3349	302.1706
LVVLG	1	500.3425	500.3425	312.2296
EQIPFE	1	762.3660	762.3659	392.1819
SSPLF	1	550.2853	550.2892	376.2231
SSSNGNGS	1	709.1945	709.1987	433.1123
SPLF	1	463.2536	463.2539	298.1771
VAPIL	1	512.3436	512.3434	342.2378
LPLV	1	441.3044	441.3052	328.2215
ELLPS	1	558.3110	558.3110	356.2182
SGGASGSGS G	1	723.2147	723.2126	433.1377
VFDPFS	1	711.3317	711.3331	350.1699
DADVDPYV	1	893.3649	893.3651	378.1671
PVSAVNQ	1	714.3824	714.3827	696.3744

ELLPSF	1	705.3813	705.3839	350.1727
SLIPSIFG				
(Acetyl@N-ter m)	1	875.4834	875.4874	520.2775
AAPPSVPEP	1	864.4972	864.4969	620.3769
LLGGLPEP	1	795.4769	795.4763	767.4837
YMVQ	1	540.2474	540.2448	267.1170
SSIFD	1	568.2630	568.2600	270.1525
TLDAGK	1	604.2822	604.2817	503.1948
AGMIK	2	260.1579	260.1600	147.0764
AGVSSGASA P	2	402.2683	402.2687	210.0608
AVCVR	2	274.1766	274.1768	171.1494
AGVLD	2	237.6377	237.6373	211.1189
VAVAV	2	229.6714	229.6720	359.2663
AGVVE	2	237.6496	237.6492	129.1014
PGQEIH	2	340.7129	340.7136	525.3459
LKMLIK	2	373.2797	373.2797	147.1130
AHVFK	2	301.1762	301.1764	209.1034
VTKPDVK	2	393.7390	393.7385	541.3005
TKQVVE	2	352.2031	352.2029	457.2755
GASVLPGV	2	350.2285	350.2291	484.3199
SHEYEPS	2	424.6740	424.6738	646.2488
EGHGVVE	2	363.6877	363.6880	355.1749
EAHVFK	2	365.6972	365.6976	356.6909
DGSGLLA	2	316.6715	316.6702	258.1459
HLASKS	2	321.6960	321.6928	177.0559
GLVDQ	2	266.1603	266.1595	361.2084
TQSGIIQ	2	373.7124	373.7124	359.2664
SDMSDL	2	334.1678	334.1607	203.0673
DHHVL	2	310.6625	310.6615	390.1529
ELSFSEIE	2	477.2208	477.2208	261.1415
IASEPP	2	307.1879	307.1883	500.2702
SGDLKVK	2	373.7052	373.7064	602.3542
DYMFDE	2	410.2072	410.2066	263.0917
LCLES	2	282.6602	282.6604	235.1198
VTVPQGA	2	336.2081	336.2084	372.2246
SSGKFLR	2	397.7274	397.7278	620.3826
VTVPKQE	2	400.7306	400.7285	501.2659
TAAPDDAAP	2	414.6898	414.6890	585.2560
VGSLDGKIRL	2	529.3482	529.3429	512.3218
VTVPGA	2	272.1804	272.1788	244.1657
LDKSGP	2	308.7046	308.7040	244.1667
TTKPNLT	2	387.7456	387.7445	571.3392

TTVHSIT	2	379.7051	379.7053	621.3410
SEAGSAGVS	2	382.7003	382.7014	548.2791
TPINADGE	2	408.7431	408.7441	399.7391
DGMATL	2	304.1769	304.1847	173.0917
AGVDVNI	2	344.2234	344.2236	335.2200
TVTVPK	2	322.7022	322.7049	244.1679
VDVHVN	2	341.6799	341.6798	583.2850
VTVTVAVL	2	401.2209	401.2216	502.2508
DTWHRVE	2	471.7247	471.7260	540.2853
AHVFT	2	287.6533	287.6537	308.1743
ESLGSAP	2	330.6715	330.6714	170.0595
LPDNAKVE	2	443.2362	443.2376	386.6941
GEKLYVF	2	428.2072	428.2120	272.1607
EKKGFLN	2	418.2371	418.2361	409.2333
SVDVHVN	2	385.1947	385.1948	583.2825
LLFINK	2	374.2270	374.2270	147.0441
VVKPDQEPV	2	556.3032	556.3022	496.7764
T				
QQSLSFSYK	2	544.2978	544.2952	344.1811
VESDINLA	2	430.7106	430.7109	771.3650
RSSGKFL	2	397.7285	397.7295	516.2885
SGCASA	2	248.1279	248.1280	177.0537
FSDT	2	235.1315	235.1317	120.0821
DHQVPSPPA	2	474.2323	474.2350	664.3062
ISDLSP	2	316.1879	316.1868	116.0688
AGVEVWGA	2	394.7230	394.7233	456.2511
TMLPVVLL	2	443.2467	443.2467	344.1805
GGVLL	2	229.6576	229.6576	197.1035
IFEL	2	261.1255	261.1264	159.0620
ASLNVVAP	2	385.6865	385.6872	584.2706
DHQVPSP	2	438.7128	438.7143	664.3004
QLNPGFK	2	402.2235	402.2331	271.1404
VTVPKVE	2	386.2337	386.2355	472.2759
PNPKVF	2	351.2023	351.2019	490.3066
KEINGPGDL	2	471.7482	471.7485	811.4075
APAPVPEPE	2	453.7304	453.7305	662.3504
ASQLYPDVK	2	510.7715	510.7708	467.1867
IDLQLPIQ	2	470.3282	470.3275	183.1472
SGDAFEACR	2	478.2211	478.2209	460.2173
AERGIAP	2	357.2137	357.2122	414.2694
AGYTGKVVIG	2	482.7765	482.7755	439.1577
ADLPGLR	2	371.2157	371.2168	442.2794
FRLPDN	2	381.1997	381.2005	629.3386
VGMDDIR	2	403.1558	403.1531	317.1275

TPWDIK	2	380.2051	380.2057	561.3092
ERADVDAPA	2	472.2512	472.2532	357.1914
ATYSLSFG	2	423.2219	423.2226	223.1078
IPYVHSDD	2	473.1832	473.1859	416.6384
VLMLVL	2	344.2531	344.2527	213.1595
DYVMAT	2	350.2077	350.2048	191.1184
KINPLVPVD	2	497.7984	497.7981	665.4316
LLMLLL	2	358.2673	358.2676	227.1764
FLWDTIISE	2	562.3257	562.3224	447.2627
DLVLIDPP	2	441.1714	441.1711	397.1807
VGADGGPEG	2	457.7125	457.7106	815.3558
R				
VWDPFR	2	410.2098	410.2103	534.2686
SGHYCAWTG	2	491.1185	491.1199	177.0545
VAGQPQGLE	2	449.7152	449.7145	799.3592
DNNEPFDPF	2	647.7820	647.7868	473.1595
LS				
AEEATMSHQ	2	502.2642	502.2650	219.1744
PIYVLENNIP	2	586.3562	586.3595	473.2747
GLEPGKHLG	2	454.2274	454.2271	189.1490
YETVRSKDD	2	649.3237	649.3242	394.1069
GK				
GSNTANR	2	360.1481	360.1481	163.0604
VWLGP	2	286.1663	286.1755	70.0646
LVDNRAVP	2	442.2070	442.2063	121.0655
KEEVKVE	3	688.4102	688.4101	585.3874
KAVKEAQI	3	296.1954	296.1962	84.0788
AICYAWLLEN	3	451.1862	451.1840	289.1327
R				
SPPFSPPPPF				
IPPPPISSPG	3	728.3974	728.3980	700.4043
GN				
GSNGGGGG	3	360.1499	360.1491	163.0599
GGGGSGSG				

Supplementary Table 2. Angiotensin converting enzyme (ACE) inhibition activity of peptides.

Peptides	Purity	Q1 Mass (Da)	Q3 Mass (Da)	Decluster voltage (V)	Collision energy (eV)
GAVEPAK	98.03%	671.5	315.5	110	45
		671.5	426.3	110	45
VTVPK	98.66%	543.5	244.3	110	35
		543.5	343.4	110	35
AAPVQ	98.00%	485.2	343.2	80	23
		485.2	147.3	85	35
ASGVPI	96.49%	593.3	279.1	90	26
		593.3	315.3	90	27
DHQVPSPP	95.28%	876.5	480.4	150	50
		876.5	381.3	150	60
SPLF	99.38%	463.3	185	110	30
		463.3	157.3	110	38
EKLPG	97.90%	543.4	371.1	100	35
		543.4	258.2	100	35
VTKPDVK	95.66%	786.6	458.2	130	50
		786.6	246.2	120	55