

Supporting Information

Identification and Relative Quantification of Bioactive Peptides Sequentially Released during Simulated Gastrointestinal Digestion of Commercial Kefir

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Table S1. sMRM Parameters for the Internal Standard (Angiotensin I) and Targeted Bioactive Peptides in Kefir and Digests.

Peptide	Parent ion (m/z)	Parent ion charge state	Fragment ion (m/z) ^a	Fragment Ion charge state	Ion type	Collision energy (V)
Angiotensin I	649.05	2	784.88	1	b6	37
			882.00	1	b7	
			1029.17	1	b8	
α_{S1} -Casein ₁₄₆₋₁₄₉	521.20	1	358.41	1	y3	39
			261.29	1	y2	
			390.41	1	b3	
α_{S1} -Casein ₂₄₋₃₁	453.32	2	788.91	1	b7	25
			562.68	1	b5	
			659.75	1	y6	
α_{S2} -Casein ₈₉₋₉₅	487.28	2	810.92	1	y6	27
			682.79	1	y5	
			792.90	1	b6	
β -Casein ₆₃₋₆₈	594.32	1	365.45	1	b4	43
			252.29	1	b3	
			462.56	1	b5	
β -Casein ₂₀₃₋₂₀₉	742.40	1	441.59	1	y4	52
			399.46	1	b4	
			512.62	1	b5	
β -Casein ₁₀₈₋₁₁₃	748.32	1	619.80	1	y5	53
			488.60	1	y4	
			505.61	1	b5	
β -Casein ₁₁₄₋₁₁₉	751.28	1	489.54	1	b4	53
			588.67	1	y5	
			360.43	1	b3	
β -Casein ₁₆₉₋₁₇₅	780.32	1	537.72	1	b5	55
			440.51	1	y4	
			341.47	1	b3	
β -Casein ₆₋₁₄	969.44	1	643.71	1	y6	65
			723.84	1	b7	
			610.68	1	b6	
β -Casein ₁₈₃₋₁₉₀	489.20	2	613.75	1	b5	30
			741.88	1	b6	
			812.96	1	b7	
β -Casein ₁₃₂₋₁₄₀	515.42	2	688.84	1	b6	28
			899.11	1	b8	
			575.68	1	b5	
β -Casein ₅₉₋₆₈	1100.48	1	594.68	1	y6	73
			872.04	1	b8	
			838.97	1	y8	
β -Casein ₁₃₀₋₁₄₀	629.40	2	916.18	1	y8	33
			1127.36	1	b10	
			706.81	1	b6	
β -Casein ₁₉₃₋₂₀₆	778.41	2	826.96	1	y8	40
			1136.37	1	y11	
			940.12	1	y9	
β -Casein ₁₉₃₋₂₀₇	834.88	2	1441.65	1	b13	42
			1249.53	1	y12	
			940.12	1	y9	
β -Casein ₁₉₃₋₂₀₉	941.05	2	1152.41	1	y11	47
			1461.82	1	y14	
			1095.36	1	y10	
β -Casein ₁₉₂₋₂₀₉	997.55	2	1265.57	1	y12	50
			1461.52	1	y14	
			1152.41	1	y11	

^a The quantifier of peptides were marked in bold.