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Supplementary Table 1. Comparison of various enzymatic digestion conditions for deconjugating phenolic compounds in breastmilk.

Analyte	Conditions, %Yield[I], %RSD[II]			
	3.85 kU, 60 min	3.85 kU, 120 min	1.93 kU, 60 min	1.93 kU, 120 min
QUE	97.9, 3.8	95.8, 5.2	74.9, 4.1	81.3, 6.4
EC	85.1, 7.4	81.0, 26.4	100.0, 5.9	74.5, 34.4
KPF	84.5, 13.0	100.0, 4.5	69.6, 9.1	77.0, 4.3
NRG	100.0, 4.0	97.0, 4.6	61.1, 9.1	68.4, 1.9
GA	100.0, 4.7	96.7, 5.9	76.0, 8.1	75.2, 5.3
CRA	100.0, 3.0	96.2, 6.9	86.4, 9.7	92.6, 8.0
FA	96.0, 2.3	100.0, 12.0	73.6, 8.6	79.9, 3.1
DOPAC	99.3, 0.3	99.3, 0.6	98.7, 0.0	98.9, 0.7
CA	100.0, 5.1	84.1, 6.7	54.7, 11.7	79.7, 18.1
DAI	100.0, 4.4	92.0, 2.9	53.9, 12.8	57.5, 10.6
DOBA	98.4, 1.1	94.6, 10.1	43.5, 9.1	38.7, 9.8
Equol	92.4, 2.7	85.1, 9.9	78.7, 10.2	79.4, 5.4

[I]%Yield: percent of the mean maximum analyte recovered by each method, which was calculated as the ratio of mean analyte area under the curve to internal standard area under the curve compared to the highest ratio (A/IS) recovered and expressed in percentage; [II]%RSD: percent relative standard deviation; Compounds abbreviations: epicatechin (EC), gallic acid (GA), ferulic acid (FA), kaempferol (KPF), naringenin (NRG), quercetin (QUE), caffeic acid (CA), chlorogenic acid (CRA), 3,4-dyhydroxyphenylacetic aicd (DOPAC), 3,4-dihydroxybenzoic acid (DOBA), daidzein (DAI), and (*S*)-3-(4-hydroxyphenyl)chroman-7-ol) (Equol).

Supplementary Table 2. Calibration parameters, limits of detection, recoveries, intra-day variations and inter-day variations of the optimized analytical method with optimized MRM parameters and retention times for the phenolic analytes and the internal standard in QqQ.

Analyte	LOD[I] (nmol/L)	LDR[II] (nmol/L)	R^2	Spiked amount (ng/mL)	Recovery[III] (%)	Intra-day RSD[III] (%)	Inter-day RSD[III] (%)	Retention time (min)	Precursor ion (*m/z*)	Fragmentor (V)	Quantifier		Qualifier	
											Product ion (*m/z*)	Collision energy (V)	Product ion (*m/z*)	Collision energy (V)
QUE	4.0	15.4-984.3	0.9980	100	71.74 (4.33)	0.31	1.70	5.93	301.0	110	151.0	15	121.0	22
				500	84.42 (9.87)									
				1000	96.67 (6.36)									
EC	8.6	17.1-437.5	0.9959	100	68.04 (5.00)	1.76	2.94	4.16	289.1	133	245.2	6	109.1	20
				500	77.87 (12.32)									
				1000	89.99 (11.85)									
KPF	7.7	15.3-391.3	0.9991	100	97.72 (16.52)	0.79	3.37	6.49	285.1	130	117.1	43	143.2	30
				500	98.10 (10.55)									
				1000	105.59 (9.18)									
NRG	15.4	17.2-2203.8	0.9990	100	110.00 (8.98)	2.18	1.42	6.40	271.1	110	119.2	24	151.2	10

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				500	96.27 (10.49)									
				1000	89.68 (14.60)									
				100	73.08 (6.17)									
GA	27.0	27.0-345.3	0.9961	500	89.12 (14.25)	1.59	2.31	0.84	169.1	85	125.1	10	79.1	23
				1000	113.74 (3.73)									
				100	65.59 (16.60)									
CRA	3.1	3.1-316.1	0.9986	500	68.47 (11.81)	1.29	2.06	3.76	353.1	100	190.9	9	84.9	43
				1000	86.16 (10.07)									
				100	110.49 (9.18)									
FA	9.8	19.7-1009.4	0.9979	500	107.75 (6.15)	0.63	1.16	4.75	193.2	95	133.9	12	178.2	7
				1000	103.75 (8.99)									
				100	102.30 (2.68)									
DOPAC	25.2	50.3-1610.5	0.9979	500	75.12 (12.00)	1.78	1.13	0.84	167.0	50	123.2	5	95.2	20
				1000	73.07									

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					(5.39)									
				100	67.35 (7.75)									
CA	2.7	21.7-1387.7	0.9998	500	71.47 (7.08)	1.56	2.68	3.92	179.1	83	135.2	13	89.4	36
				1000	83.37 (15.49)									
				100	101.64 (6.38)									
DAI	1.9	15.4-983.4	0.9988	500	70.69 (7.17)	1.77	2.45	5.72	253.1	120	132.2	40	91.1	35
				1000	91.28 (11.62)									
				100	79.88 (16.16)									
DOBA	5.1	10.1-2595.4	0.9987	500	72.76 (9.28)	1.29	1.52	1.84	153.1	80	109.2	14	108.2	25
				1000	82.83 (3.81)									
				100	81.32 (5.45)									
Equol	8.1	16.1-206.4	0.9962	500	81.97 (5.56)	1.28	1.71	6.44	241.1	70	119.3	15	135.1	10
				1000	101.76 (9.46)									
IS	/	/	/	/	/	/	/	6.11	154.2	70	110.2	7	82.3	20

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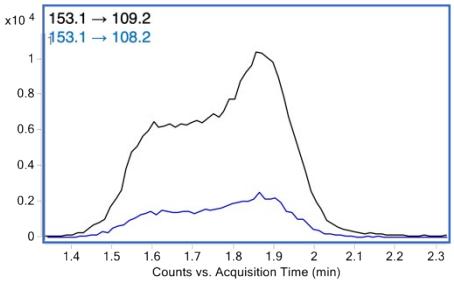
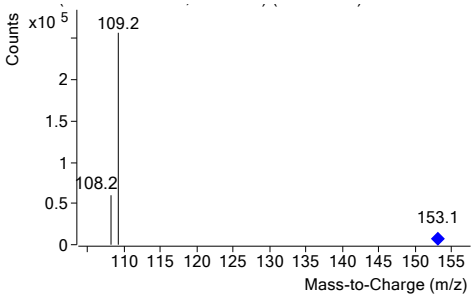
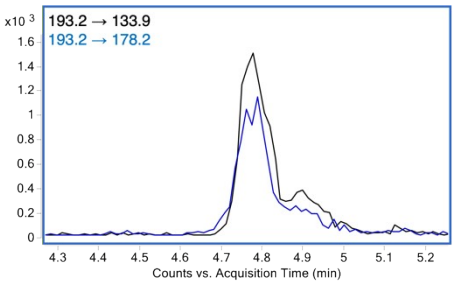
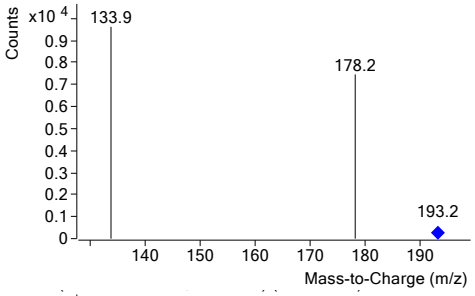
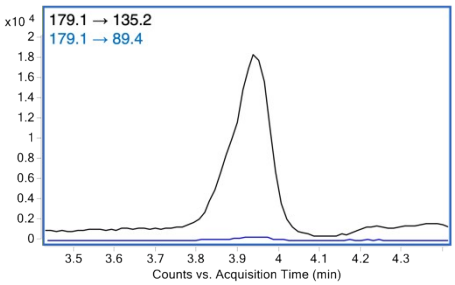
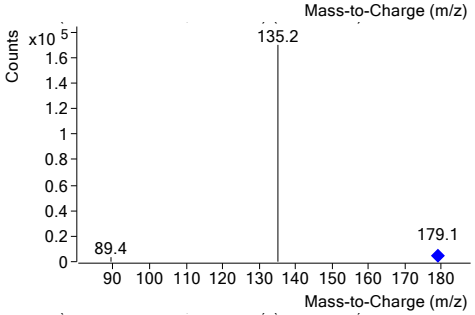
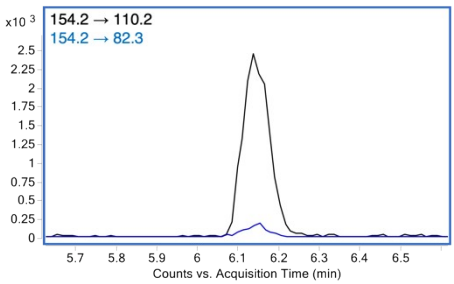
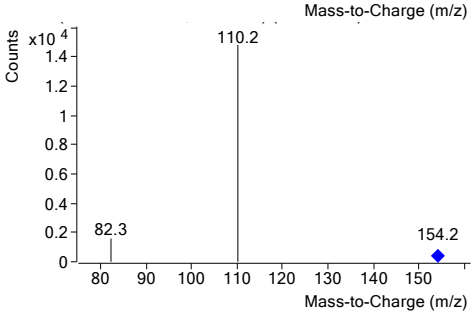
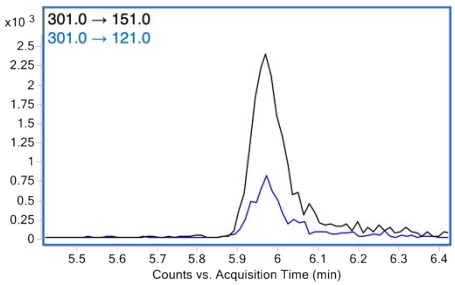
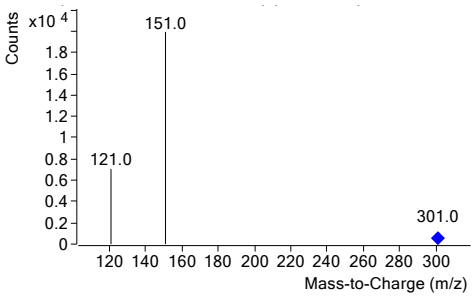
[I]LOD: limit of detection; [II]LDR: linear dynamic range;
[III]Data were expressed as means of 6 independent replicates, and %RSDs for recoveries were shown in parentheses. Compounds abbreviations refer to Supplementary Table 1.

Supplementary Table 3. Representative peaks and MRM transitions of selected representative compounds.

Compound	Representative chromatogram	MRM transitions
	Phenolic acids	
	Benzoic acid derivative	
DOBA		
	Cinnamic acid derivative	
FA		
CA		
IS (*trans*-cinnamic-d_7 acid)		
	Flavonoids	
	Flavonol	
QUE		
	Flavanone:	

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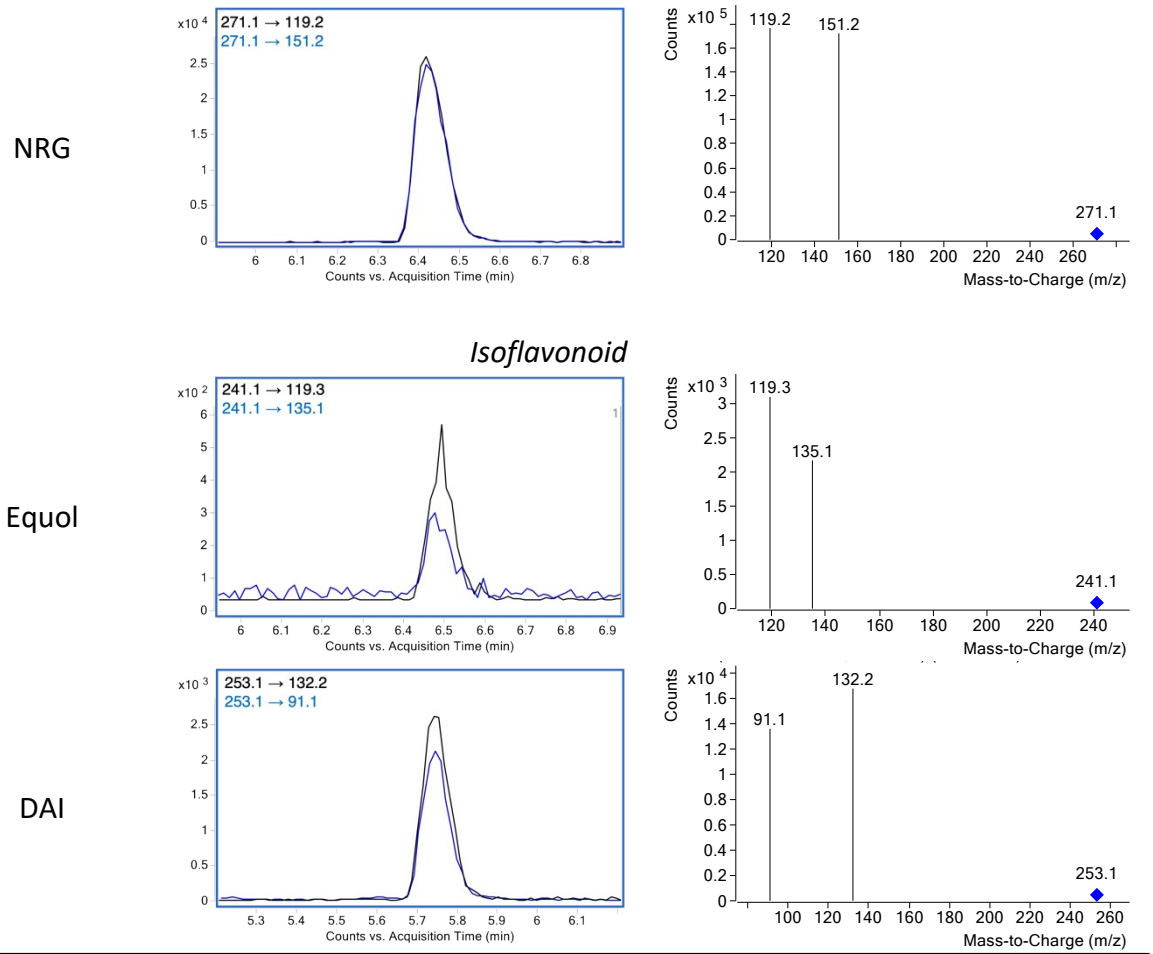

Representative peaks of the quantifier ion (in black) and the qualifier ion (in blue). Compounds abbreviations refer to Supplementary Table 1.

Supplementary Table 4. Maternal plant-based food consumption based on the sensitivity analysis with exclusion of coffee/tea intake.

Food group (unit)	T1 (n = 31)	T2 (n = 31)	T3 (n = 30)	*P*-value
Vegetables (servings/d)	2.1 ± 0.2	2.5 ± 0.2	1.9 ± 0.2	0.14
Fruits (servings/d)	1.6^{a} ± 0.2	0.9^{b} ± 0.2	$1.4^{a,b}$ ± 0.2	0.02*
Grains (servings/d)	6.8 ± 0.3	7.7 ± 0.4	7.9 ± 0.5	0.18
Nuts (g/d)	11.3^{a} ± 2.8	7.9^{a} ± 2.2	3.9^{b} ± 2.0	0.84
Legumes (servings/d)	2.6^{a} ± 0.5	$1.9^{a,b}$ ± 0.4	1.3^{b} ± 0.2	0.00**
Coffee (cups/d)	0.2 ± 0.1	0.1 ± 0.1	0.1 ± 0.0	0.36
Tea (cups/d)	0.7 ± 0.2	1.2 ± 0.3	0.9 ± 0.2	0.33

Data are expressed as mean ± SEM; Different superscript letters indicate a significant difference in food intakes among three groups ($P \leq 0.05$).
* $P \leq 0.05$, ** $P \leq 0.01$; One-way ANOVA test with Bonferroni post-hoc test.

Supplementary Table 5. Breastmilk polyphenol levels based on the sensitivity analysis with exclusion of coffee/tea intake.

Polyphenols	n [I]	T1 (n = 31)	T2 (n = 31)	T3 (n = 30)	*P*-value
EC	91	33.5 ± 2.9	29.5 ± 2.8	29.7 ± 2.1	0.48
QUE	92	128.4 ± 15.9	152.5 ± 15.2	130.8 ± 15.8	0.49
NRG	92	427.8 ± 35.6	419.2 ± 37.3	360.6 ± 23.7	0.30
KPF	92	26.3 ± 1.6	26.1 ± 1.4	28.1 ± 1.2	0.56
GA	82	61.4 ± 7.4	49.9 ± 3.1	52.6 ± 4.5	0.30
DOPAC	84	322.5 ± 63.1	201.9 ± 10.2	228.5 ± 21.4	0.06
CRA	76	5.0 ± 0.3	5.1 ± 0.3	5.2 ± 0.4	0.83
FA	92	119.4 ± 6.7	108.0 ± 5.6	116.3 ± 8.9	0.51
CA	92	178.0 ± 11.1	149.3 ± 9.7	165.9 ± 9.8	0.14
DAI	92	53.6 ± 9.5	57.9 ± 8.9	62.8 ± 8.0	0.76
DOBA	92	723.8 ± 26.7	697.8 ± 30.1	762.0 ± 33.7	0.33
Equol	91	96.9 ± 6.3	96.4 ± 5.9	101.0 ± 5.3	0.85

Data are expressed as mean ± SEM. Compound abbreviations refer to Supplementary Table 1.
[I] Number of samples in which the phenolic compound was detected.

Supplementary Table 6. Concentrations of phenolic compounds in breastmilk reported in other studies.

	Mean concentration (nmol/L)					
Study	17 free-living lactating women at 1, 4 and 13 weeks after delivery[1]			11 lactating women[2]	14 lactating women consuming their normal diet[3]	13 free-living lactating women[4]
Country	United States			Poland	Poland	Poland
Polyphenols	1 week	4 weeks	13 weeks	After onion soup consumption	/	/
QUE	48.1	59.8	50.9	68.0	/	41.0
NRG	252.1	210.4	196.6	/	823.2	6.9
EC	90.5	249.2	95.5	/	/	Not detected
KPF	15.7	23.1	34.8	/	/	Not detected
GA	/	/	/	/	/	186.9
DAI	/	/	/	/	/	14.2
CA	/	/	/	/	/	302.0

Data are expressed as the mean. Compound abbreviations refer to Supplementary Table 1.

References

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