

Table S1. Identification and quantification of (poly)phenolic compounds in 85% cocoa dark chocolate, green tea, and fruit juice ingested during the experimental period, and mass spectrometric and chromatographic characteristics. Data are expressed as μmol per daily food intake (mean values \pm SD, n = 3).

Compounds	RT (min)	[M-H] ⁻ or [M] ⁺ (m/z)	MS ² fragment ions (m/z)	Standard used for quantification	85% Cocoa dark chocolate	Green tea	Fruit juice	Overall Supplementation
					Daily intake (μmol)			
Hydroxybenzoic acids								
3,4,5-Trihydroxybenzoic acid (gallic acid) ^a	1.45	169 ⁻	125, 107	3,4,5-Trihydroxybenzoic acid	ND	7.78 ± 0.62	17.29 ± 1.21	25.07 ± 1.83
3,4-Dihydroxybenzoic acid (protocatechuic acid) ^b	2.40	153 ⁻	123, 109	3,4,5-Trihydroxybenzoic acid	ND	ND	4.46 ± 0.19	4.46 ± 0.19
4-Hydroxy-3-methoxybenzoic acid (vanillic acid) ^b	3.30	167 ⁻	123,152,125	3,4,5-Trihydroxybenzoic acid	ND	ND	10.50 ± 0.66	10.50 ± 0.66
Total Hydroxybenzoic acids					ND	7.78 ± 4.49	32.25 ± 6.42	40.03 ± 10.59
Hydroxycinnamic acids								
cis-3',4'-Dihydroxycinnamic acid ^b	2.60	179 ⁻	135	3-O-Galloylquinic acid	ND	ND	3.63 ± 0.18	3.63 ± 0.18
trans-3',4'-Dihydroxycinnamic acid ^b	3.20	179 ⁻	121, 135, 109	3-O-Galloylquinic acid	ND	ND	1.78 ± 0.04	1.78 ± 0.04
Total Hydroxycinnamic acids					ND	ND	5.41 ± 1.31	5.41 ± 1.31
Hydrolyzable tannins and ellagic acid derivatives								
Punicalagin-like ^b	0.67	1083 ⁻	601, 721	Punicalin α	ND	ND	5.29 ± 0.27	5.29 ± 0.27
Punicalagin α ^b	2.55	1083 ⁻	601, 781	Punicalagin β	ND	ND	0.92 ± 0.09	0.92 ± 0.09
Punicalagin β ^a	2.72	1083 ⁻	781, 601	Punicalagin β	ND	ND	2.28 ± 0.29	2.28 ± 0.29
Punicalin (α/β) ^a	1.64	781 ⁻	601, 721	Punicalin α	ND	ND	19.89 ± 0.13	19.89 ± 0.13
Pedunculagin I isomer ^b	2.66	783 ⁻	765, 301	Punicalagin β	ND	ND	8.83 ± 0.92	8.83 ± 0.92
Puniglyconin ^b	2.86	801 ⁻	301, 347, 649	3-O-Galloylquinic acid	ND	ND	6.46 ± 0.78	6.46 ± 0.78
Granatin B ^b	3.19	951 ⁻	933, 613	Procyanidin dimer (B1-type)	ND	ND	1.10 ± 0.20	1.10 ± 0.20
Galloyl-hexoside ^b	1.06	331 ⁻	169, 271	3-O-Galloylquinic acid	ND	ND	10.02 ± 0.41	10.02 ± 0.41
Galloyl-HHDP-Hexoside ^b	3.00	633 ⁻	301, 463, 275	3-O-Galloylquinic acid	ND	ND	7.78 ± 0.79	7.78 ± 0.79
3-O-Galloylquinic acid ^a	0.96	343 ⁻	169, 191	3-O-Galloylquinic acid	ND	ND	0.85 ± 0.12	0.85 ± 0.12
4-O-Galloylquinic acid ^b	1.70	343 ⁻	169, 191	3-O-Galloylquinic acid	ND	ND	ND	ND
5-O-Galloylquinic acid ^b	1.41	343 ⁻	191, 196	3-O-Galloylquinic acid	ND	1.53 ± 0.15	ND	1.53 ± 0.15

Ellagic acid ^b	3.55	301	257, 229	3-O-Galloylquinic acid	ND	ND	119.20 ± 12.70	119.20 ± 12.70
Ellagic acid-pentoside ^b	3.37	433	301, 415, 433 447, 285	3-O-Galloylquinic acid	ND	3.64 ± 0.36	8.07 ± 0.67	11.72 ± 0.60
Ellagic acid-hexoside ^b	3.04	463	301, 257, 229	3-O-Galloylquinic acid	ND	ND	53.33 ± 1.85	53.33 ± 1.85
Ellagic acid-deoxyhexoside ^b	3.37	447	300, 301	3-O-Galloylquinic acid	ND	ND	19.46 ± 0.73	19.46 ± 0.73
<i>Total Hydrolyzable tannins and ellagic acid derivatives</i>					ND	5.17 ± 0.96	263.49 ± 30.41	268.66 ± 30.30
Flavan-3-ols								
(+)-Catechin ^a	2.92	289	245, 205	(+)-Catechin	87.76 ± 7.66	15.83 ± 0.97	2.20 ± 0.09	105.79 ± 7.26
(-)-Epicatechin ^a	3.15	289	245, 205	(-)-Epicatechin	221.45 ± 9.97	12.98 ± 0.59	0.33 ± 0.01	234.77 ± 9.37
Gallocatechin ^b	2.34	305	179, 221	(-)-Epicatechin	ND	9.50 ± 0.23	0.24 ± 0.03	9.74 ± 0.22
Epigallocatechin ^b	2.75	305	179, 221	(-)-Epicatechin	ND	15.28 ± 1.16	ND	15.28 ± 1.16
Gallocatechin-3'-O-gallate ^b	3.16	457	169, 331	Epigallocatechin-3'-O-gallate	ND	55.34 ± 2.40	ND	55.34 ± 2.40
Epicatechin-3'-O-gallate ^a	3.57	441	301, 300	Epicatechin-3'-O-gallate	ND	37.77 ± 2.27	ND	37.77 ± 2.27
Epigallocatechin-3'-O-gallate ^a	3.24	457	169, 331	Epigallocatechin-3'-O-gallate	ND	5.29 ± 0.26	ND	5.29 ± 0.26
Procyanidin dimer (A2-type) ^b	4.13	575	449, 423	Procyanidin dimer (B2-type)	20.98 ± 0.28	ND	ND	20.98 ± 0.28
Procyanidin dimer (B1-type) ^a	2.99	577	425, 407	Procyanidin dimer (B1-type)	81.07 ± 3.81	2.32 ± 0.23	ND	83.39 ± 3.57
Procyanidin dimer (B2-type) ^a	3.46	577	425, 407	Procyanidin dimer (B2-type)	129.32 ± 8.99	12.79 ± 0.68	ND	142.11 ± 9.69
Procyanidin trimer (A-type) ^a	3.32	863	711, 411	Procyanidin trimer (A-type)	26.53 ± 1.74	ND	ND	26.53 ± 1.74
Procyanidin trimer (C1-type) ^a	3.09	865	695, 739	Procyanidin trimer (C1-type)	43.26 ± 1.20	0.22 ± 0.01	ND	43.48 ± 1.22
<i>Total Flavan-3-ols</i>					610.37 ± 68.76	167.32 ± 16.78	2.77 ± 0.63	780.46 ± 67.81
Flavanones								
Hesperetin-7-O-rutinoside (hesperidin) ^a	3.84	609	301, 285	Hesperetin-7-O-rutinoside	ND	1.59 ± 0.28	12.59 ± 0.32	14.17 ± 0.14
Naringenin-7-O-rutinoside ^b	3.69	579	271, 151	Naringenin	ND	ND	5.91 ± 0.30	5.91 ± 0.30
Isosakuranetin-7-O-rutinoside ^b	4.39	593	285, 270	Hesperetin-7-O-neohesperoside	ND	ND	16.55 ± 0.42	16.55 ± 0.42
Eriodictyol-7-O-rutinoside ^b	3.43	595	287, 269	Hesperetin-7-O-rutinoside	ND	ND	0.25 ± 0.01	0.25 ± 0.01
Naringenin-4'-O-glucoside ^b	3.10	433	271, 301	Hesperetin-7-O-neohesperoside	ND	ND	5.28 ± 0.24	5.28 ± 0.24
Hesperidin-3'-O-glucoside ^b	3.28	771	463, 301	Hesperetin-7-O-neohesperoside	ND	ND	2.27 ± 0.25	2.27 ± 0.25
Hesperetin-7-O-neohesperoside-3'-O-glucoside ^b	2.77	771	609, 463	Hesperetin-7-O-neohesperoside	ND	ND	2.24 ± 0.20	2.24 ± 0.20

<i>Total Flavanonones</i>					ND	1.59 ± 0.60	45.09 ± 5.99	46.68 ± 6.28
Flavones								
Apigenin-6,8-C-diglucoside ^b	3.02	593-	473, 503	Luteolin-4-glucoside	5.17 ± 0.68	1.63 ± 0.17	3.20 ± 0.11	10.00 ± 0.86
<i>Total Flavones</i>					5.17 ± 0.68	1.63 ± 0.17	3.20 ± 0.11	10.00 ± 0.86
Flavonols								
Quercetin ^a	4.56	301-	179, 151	Quercetin	4.88 ± 0.57	ND	0.04 ± 0.01	4.92 ± 0.57
Myricetin-hexoside ^b	3.30	479-	317, 316	Luteolin-glucoside	ND	ND	0.31 ± 0.04	0.31 ± 0.04
Quercetin-3-glucoside ^b	3.54	463-	301, 300	Quercetin-3-rutinoside	13.24 ± 0.91	2.79 ± 0.02	0.35 ± 0.00	16.37 ± 0.93
Dihydrokaempferol-hexoside ^b	3.15	449-	287, 269	Luteolin-glucoside	ND	ND	0.72 ± 0.07	0.72 ± 0.07
Kaempferol-hexoside ^b	2.77	447-	285, 286	Luteolin-glucoside	ND	ND	0.89 ± 0.07	0.89 ± 0.07
Syringetin-hexoside (isomer 1) ^b	3.28	507-	327, 315	Procyanidin dimer (B1-type)	ND	ND	0.33 ± 0.05	0.33 ± 0.05
Syringetin-hexoside (isomer 2) ^b	3.52	507-	345, 323	Procyanidin dimer (B1-type)	ND	ND	0.91 ± 0.01	0.91 ± 0.01
Quercetin-pentoside ^b	3.70	433-	301, 300	Quercetin-3-rutinoside	13.52 ± 0.43	ND	ND	13.52 ± 0.43
Quercetin-3-rutinoside ^a	3.42	609-	301, 300	Quercetin-3-rutinoside	ND	5.12 ± 0.13	ND	5.12 ± 0.13
Kaempferol-rutinoside ^b	4.39	593-	285, 547	Luteolin-glucoside	ND	0.21 ± 0.04	ND	0.21 ± 0.04
<i>Total Flavonols</i>					31.64 ± 5.59	8.12 ± 1.75	3.54 ± 0.37	43.29 ± 5.93
Anthocyanins								
Delphinidin-3',5'-diglucoside ^b	2.27	627+	465, 303	Delphinidin-3'-glucoside	ND	ND	1.57 ± 0.11	1.57 ± 0.11
Cyanidin-3',5'-diglucoside ^b	2.44	611+	449, 287, 177	Cyanidin-3'-glucoside	ND	ND	11.01 ± 0.46	11.01 ± 0.46
Pelargonidin-3',5'-diglucoside ^b	2.61	595+	433, 271	Pelargonidin-3'-glucoside	ND	ND	0.36 ± 0.01	0.36 ± 0.01
Delphinidin-3'-glucoside ^a	2.61	465+	303, 305, 395	Delphinidin-3'-glucoside	ND	ND	1.71 ± 0.29	1.71 ± 0.29
Cyanidin-3'-glucoside ^a	2.77	449+	287, 255, 269	Cyanidin-3'-glucoside	ND	ND	13.90 ± 0.72	13.90 ± 0.72
Pelargonidin-3'-glucoside ^a	2.80	433+	271, 273, 350	Pelargonidin-3'-glucoside	ND	ND	0.64 ± 0.06	0.64 ± 0.06
Peonidin-3'-glucoside ^a	2.95	463+	301, 395	Peonidin-3'-glucoside	ND	ND	0.78 ± 0.02	0.78 ± 0.02
Malvidin-3'-glucoside ^a	2.99	493+	331, 279	Malvidin-3'-glucoside	ND	ND	0.85 ± 0.06	0.85 ± 0.06
Cyanidin-3'-rutinoside ^a	2.80	595+	120, 316	Cyanidin-3'-rutinoside	ND	ND	0.42 ± 0.04	0.42 ± 0.04
<i>Total Anthocyanins</i>					ND	ND	31.24 ± 5.16	31.24 ± 5.16
Total phenolic compounds								
					647.17 ± 24.79	191.60 ± 5.40	387.00 ± 20.46	1226 ± 40

RT: Retention time; ^a: Compounds identified by comparing retention times and MS data with those of reference compounds; ^b: compounds (tentatively) identified; ND: Not detected.