

Table S1. UHPLC-HRMS characteristics of the polyphenols identified in pistachio varieties

RT (min)	Compound	Chemical Formula	[m/z]- Theoretical	Error (ppm)	MSIMI level ^a
<i>Hydroxybenzoic acids</i>					
2.88	3,4,5-Trihydroxybenzoic acid	C ₇ H ₆ O ₅	169.0131	-0.59	1
3.15	Benzene-1,2-diol	C ₆ H ₅ O ₃	125.0233	-1.60	1
3.38	Theogallin	C ₁₄ H ₁₆ O ₁₀	343.0663	-0.87	2
6.6	Galloylshikimic acid	C ₁₄ H ₁₄ O ₉	325.0554	3.38	2
8.69	3,4-Dihydroxy-5-((3,4,5-trihydroxybenzoyl)oxy)benzoic acid	C ₁₄ H ₁₀ O ₉	321.0241	2.18	2
8.69	Methylgallic acid I	C ₈ H ₇ O ₅	183.0287	1.64	2
11.72	Methylgallic acid II	C ₈ H ₇ O ₆	183.0287	1.64	2
9.28	Vanillic acid	C ₈ H ₇ O ₄	167.0339	1.80	1
9.87	Vanillic acid hexoside	C ₁₄ H ₁₈ O ₉	329.0867	3.34	2
10.9	Ellagic acid	C ₁₄ H ₆ O ₈	300.9978	4.32	1
12.31	Benzoic acid	C ₇ H ₅ O ₂	121.0284	0.00	1
9.88	Benzoic acid I	C ₈ H ₇ O ₄	167.0338	2.39	2
11.71	Benzoic acid II	C ₈ H ₇ O ₄	167.0338	2.39	2
13.82	Benzoic acid III	C ₈ H ₇ O ₄	167.0338	2.39	2
6.02	3,4-Dihydroxybenzoic acid	C ₇ H ₆ O ₄	153.0182	-1.31	1
<i>Galloyl derivatives</i>					
2.29	Mono-galloyl-glucose I	C ₁₃ H ₁₆ O ₁₀	331.0659	3.02	2
6.25	Mono-galloyl-glucose II	C ₁₃ H ₁₆ O ₁₀	331.0659	3.02	2
3.09	Galloyl dihexose	C ₁₉ H ₂₆ O ₁₅	493.1188	0.20	2
8.39	Digalloyl hexose I	C ₂₀ H ₂₀ O ₁₄	483.0769	2.28	2
8.92	Digalloyl hexose II	C ₂₀ H ₂₀ O ₁₄	483.0769	2.28	2
8.94	Hydroxy-methoxyphenylgalloyl hexoside I	C ₂₀ H ₂₂ O ₁₂	453.1027	2.43	2
9.63	Hydroxy-methoxyphenylgalloyl hexoside II	C ₂₀ H ₂₂ O ₁₂	453.1027	2.43	2
9.89	Tetra-O-galloyl glucoside I	C ₃₄ H ₂₈ O ₁₉	787.0994	1.40	2
10.65	Tetra-O-galloyl glucoside II	C ₃₄ H ₂₈ O ₁₉	787.0994	1.40	2
11.4	Pentagalloylglucose	C ₄₁ H ₃₂ O ₂₆	939.1098	0.64	2
<i>Hydroxycinnamic acids</i>					
8.07	5-O-caffeoylquinic acid	C ₁₆ H ₁₈ O ₉	353.0867	0.28	1
9.17	O-caffeoylquinic acid II	C ₁₆ H ₁₈ O ₉	353.0867	0.28	2
11.37	Sinapic acid	C ₁₁ H ₁₂ O ₅	223.0600	2.24	1
8.93	Sinapic acid derivative	C ₁₁ H ₁₂ O ₅	223.0600	2.24	2
10.61	4'-Hydroxycinnamic acid	C ₉ H ₈ O ₃	163.0395	-2.45	1
8.51	4'-Hydroxy-3'-methoxycinnamic acid derivative	C ₁₀ H ₁₀ O ₄	193.0495	1.55	2
7.67	3-(3',4'-Dihydroxyphenyl)propanoic acid	C ₉ H ₉ O ₄	181.0495	0.55	1

<i>Flavones</i>					
8.54	Luteolin hexoside	C ₂₁ H ₂₀ O ₁₁	447.0921	1.79	2
14.07	Luteolin	C ₁₅ H ₁₀ O ₆	285.0393	3.51	1
11.01	Apigenin hexoside	C ₂₁ H ₂₀ O ₁₀	431.0972	1.16	2
<i>Flavonols</i>					
10.74	Quercetin 3-rutinoside	C ₂₇ H ₃₀ O ₁₆	609.145	0.98	1
10.18	Myricetin hexoside	C ₂₁ H ₂₀ O ₁₃	479.082	1.67	2
12.48	Myricetin	C ₁₅ H ₁₀ O ₈	317.0291	3.47	1
10.55	Quercetin hexoside I	C ₂₁ H ₂₀ O ₁₂	463.0871	1.73	2
10.98	Quercetin hexoside II	C ₂₁ H ₂₀ O ₁₂	463.0871	1.73	2
10.60	Quercetin galloyl glucoside I	C ₂₈ H ₂₄ O ₁₆	615.098	1.46	2
11.43	Quercetin galloyl glucoside II	C ₂₈ H ₂₄ O ₁₆	615.098	1.46	2
14.32	Quercetin	C ₁₅ H ₁₀ O ₇	301.0342	3.65	1
<i>Flavan-3-ols</i>					
6.33	Gallocatechin	C ₁₅ H ₁₄ O ₇	305.0655	3.61	2
8.61	Catechin	C ₁₅ H ₁₄ O ₆	289.0707	4.15	1
9.54	Epicatechin	C ₁₅ H ₁₄ O ₆	289.0707	2.42	1
9.72	Epigallocatechin gallate	C ₂₂ H ₁₈ O ₁₁	457.0765	0.44	1
11.05	Epicatechin gallate	C ₂₂ H ₁₈ O ₁₀	441.0816	0.91	1
11.88	Epiafzelechin 3-gallate	C ₂₂ H ₁₈ O ₉	425.0867	1.88	2
12.42	Afzelechin I	C ₁₅ H ₁₄ O ₅	273.0757	2.93	2
12.94	Afzelechin II	C ₁₅ H ₁₄ O ₅	273.0757	2.93	2
15.23	Afzelechin III	C ₁₅ H ₁₄ O ₅	273.0757	2.93	2
<i>Flavanones</i>					
11.02	Eriodictyol hexoside	C ₂₁ H ₂₂ O ₁₁	449.1078	1.11	2
13.88	Eriodictyol	C ₁₅ H ₁₂ O ₆	287.055	2.79	2
11.98	Naringenin hexoside	C ₂₁ H ₂₂ O ₁₀	433.1129	1.39	2
11.98	Naringenin	C ₁₅ H ₁₂ O ₅	271.0601	2.21	1
<i>Flavanonols</i>					
11.39	Taxifolin	C ₁₅ H ₁₂ O ₇	303.0499	3.30	1
<i>Stilbenes</i>					
10.87	Resveratrol hexoside	C ₂₀ H ₂₂ O ₈	389.1231	2.31	2

^a Annotation from Summer et al. Compounds identified at MSIMI level 1 means there was a commercially available standard. Compounds identified at MSIMS level 2 were tentatively identified. RT: retention time.

Table S2. UHPLC-HRMS Characteristics of Phenolic Acid Catabolites Identified in Pistachio and its by-products Faecal Incubates

Rt (min)	Catabolites	Chemical Formula	[m/z]-Theoretical	Error (ppm)	MSIMI level ^a
7.32	3,4-Dihydroxyphenylacetic acid	C ₈ H ₇ O ₄	167.0338	-2.99	1
8.18	4-Hydroxybenzoic acid	C ₇ H ₅ O ₃	137.0233	0.00	1
8.84	3-(3',4'-Dihydroxyphenyl)propanoic acid	C ₉ H ₉ O ₄	181.0495	0.55	1
8.85	3-(Phenyl)acetic acid	C ₈ H ₇ O ₂	135.0440	0.74	1
10.12	3-Hydroxyphenylacetic acid	C ₉ H ₉ O ₃	151.0389	0.66	2
10.28	3,4-Dihydroxyphenyl-γ-valerolactone	C ₁₁ H ₁₂ O ₄	207.0657	0.415	2
10.91	3-(3-methoxy-4-hydroxyphenyl)propionic acid	C ₁₀ H ₁₁ O ₄	195.0652	3.59	1
10.95	3-(4'-Hydroxyphenyl)propanoic acid	C ₉ H ₉ O ₃	165.0546	0.66	1
11.45	4'-Hydroxy-3'-methoxycinnamic acid	C ₁₀ H ₁₀ O ₄	193.0495	1.04	1
11.6	3'-Hydroxy-4'-methoxycinnamic acid	C ₁₀ H ₉ O ₄	193.0495	2.59	1
11.74	3-(3'-Hydroxyphenyl)propanoic acid	C ₇ H ₆ O ₄	165.0546	0.66	1
14.45	3-(Phenyl)propionic acid	C ₉ H ₉ O ₂	149.0597	0.67	1

^a Annotation from the Summer et al. Compounds identified at MSIMI level 1 means there was a commercially available standard. RT: retention time.

Table S3. Hydroxybenzoic acids group in pistachios during fermentation (nmol/ g)

	3,4,5-Trihydroxybenzoic acid	Benzene-1,2-diol)	3-Galloyl-quinic acid	3,4-Dihydroxybenzoic acid	Galloyl shikimic acid	Vanillic acid hexoside	Ellagic acid	Benzoic acid derivative II	Total
Aegina									
0 h	0.21 bc	nd	nd	0.154 ab	0.0005	0.57	0.244 a	0.198 a	1.38 a
4 h	0.45 a	nd	nd	0.166 a	nd	nd	0.237 b	0.176 b	1.03 b
8 h	0.34 ab	nd	nd	0.148 ab	nd	nd	0.236 b	0.169 b	0.90 c
24 h	0.03 c	0.07	nd	0.039 c	nd	nd	nd	nd	0.14 d
Golden Hills									
0 h	<LOQ	nd	nd	0.046 b	0.0004	0.55	0.243 a	0.13	0.97 a
4 h	0.06 a	nd	nd	0.071 a	nd	nd	0.237 b	0.13	0.50 b
8 h	0.05 a	nd	nd	0.060 ab	nd	nd	0.242 ab	0.13	0.49 c
24 h	<LOQ	0.05	nd	0.024 c	nd	nd	nd	nd	0.07 d
Kastel									
0 h	0.31 a	nd	0.005	0.092 a	0.0004	0.601	0.246	0.174 a	1.43 a
4 h	0.05 c	nd	nd	0.078 a	nd	nd	0.239	0.138 b	0.51 c
8 h	0.11 b	nd	nd	0.082 a	nd	nd	0.241	0.145 ab	0.58 b
24 h	<LOQ	0.04	nd	0.017 b	nd	nd	nd	nd	0.06 d
Kerman									
0 h	<LOQ	nd	0.004	0.036 b	0.0004	0.553	0.238	0.136 b	0.97 a
4 h	0.09 b	nd	nd	0.059 a	nd	nd	0.243	0.149 a	0.54 c
8 h	0.14 a	nd	nd	0.060 a	nd	nd	0.240	0.158 a	0.59 b
24 h	<LOQ	0.06	nd	0.015 c	nd	nd	nd	nd	0.07 d
Larnaka									
0 h	0.26 a	nd	0.01	0.173 a	0.001	0.609	0.238	0.249 a	1.54 a
4 h	0.37 a	nd	nd	0.204 a	nd	nd	0.235	0.175 b	0.98 b
8 h	0.35 a	nd	nd	0.180 a	nd	nd	0.238	0.185 b	0.95 c
24 h	0.04 b	0.11	nd	0.031 b	nd	nd	nd	nd	0.18 d
Sirora									
0 h	0.06 b	nd	0.01	0.113 b	0.0005	0.544	0.236	0.144	1.10 a
4 h	0.12 b	nd	nd	0.140 a	nd	nd	0.239	0.137	0.64 c
8 h	0.29 a	nd	nd	0.167 a	nd	nd	0.235	0.145	0.84 b
24 h	<LOQ	0.04	nd	0.038 c	nd	nd	nd	nd	0.08 d

Values with different letters are significantly different as determined by Tukey test.

Table S4. Flavan-3-ols group in pistachios during fermentation (nmol/ g)

	Catechin	Epi catechin	Epigallo catechin gallate	Epi catechin gallate	Epiafzelechin3 -gallate	Afzelechin III	Total
Aegina							
0 h	0.018 a	0.022 a	nd	0.013	0.013	0.019 a	0.08 c
4 h	0.010 b	0.020 ab	0.13	0.013	0.012	0.018 b	0.21 a
8 h	0.002 c	0.020 ab	0.13	0.012	0.012	0.018 b	0.20 b
24 h	<LOQ	0.019 b	nd	0.012	nd	nd	0.03 d
Golden Hills							
0 h	<LOQ	0.019	nd	0.013	0.013	0.018	0.06 b
4 h	<LOQ	0.018	0.11	0.012	0.012	0.018	0.18 a
8 h	<LOQ	0.019	nd	0.012	0.009	0.018	0.06 c
24 h	<LOQ	0.019	nd	0.012	nd	nd	0.03 d
Kastel							
0 h	0.022	0.026 a	nd	0.014 a	0.014 a	0.020 a	0.10 b
4 h	<LOQ	0.018 b	nd	0.012 b	0.012 b	0.018 b	0.06 c
8 h	<LOQ	0.020 ab	0.12	0.012 b	0.012 b	0.018 b	0.19 a
24 h	<LOQ	0.020 ab	nd	0.012 b	nd	nd	0.03 d
Kerman							
0 h	0.002 a	0.021 a	nd	0.012 a	0.013	0.018	0.07 b
4 h	0.001 b	0.022 a	nd	0.012 a	0.013	0.019	0.07 a
8 h	<LOQ	0.021 a	nd	0.012 a	0.012	0.018	0.06 c
24 h	<LOQ	0.018 b	nd	0.011 b	nd	nd	0.03 d
Larnaka							
0 h	0.057 a	0.025 a	nd	0.014 a	0.013	0.021 a	0.13 b
4 h	0.025 b	0.022 b	0.12	0.012 b	0.012	0.018 b	0.21 a
8 h	0.021 b	0.023 b	0.12	0.012 b	0.012	0.018 b	0.21 a
24 h	<LOQ	0.018 c	nd	0.012 b	nd	nd	0.03 c
Sirora							
0 h	0.007	0.020 a	0.12	0.013	0.013	0.018	0.19 a
4 h	<LOQ	0.019 ab	0.12	0.012	0.012	0.018	0.18 b
8 h	<LOQ	0.020 a	0.12	0.012	0.012	0.018	0.18 b
24 h	<LOQ	0.018 b	nd	0.012	nd	nd	0.03 c

Values with different letters are significantly different as determined by Tukey test.