

Supplementary Material Tables

Application of dynamic colonic gastrointestinal digestion model to high-flavanol red wines: kinetics of colonic flavanol metabolism, gut microbiota transformation and cardioprotective effects

Table S1. Optimized MRM conditions for analysing the (poly)phenolic compounds determined in the different samples.

Table S2. Concentration of the main (wine precursors) and their colonic metabolites quantified in the ascending colon section (AC) during the digestion of wine 2020.

Table S3. Concentration of the main (wine precursors) and their colonic metabolites quantified in transversal colon section (TC) during digestion of 2020 wine.

Table S4. Concentration of the main (wine precursors) and their colonic metabolites quantified in descending colon section (DC) during digestion of 2020 wine.

Table S5. Concentration of the main (wine precursors) and their colonic metabolites quantified in ascending colon section (AC) during digestion of 2021 wine.

Table S6. Concentration of the main (wine precursors) and their colonic metabolites quantified in transversal colon section (TC) during digestion of 2021 wine.

Table S7. Concentration of the main (wine precursors) and their colonic metabolites quantified in descending colon section (DC) during digestion of 2021 wine.

Table S1. Optimized MRM conditions for analysing the (poly)phenolic compounds determined in the different samples.

<u>Compound</u>	<u>RT (min)</u>	<u>MRM transitions for quantification</u>						<u>MRM transitions for identification</u>						<u>Standart used to quantify</u>
		<u>Q1 / Q3</u>	<u>DP</u>	<u>EP</u>	<u>CEP</u>	<u>CE</u>	<u>CXP</u>	<u>Q1 / Q3</u>	<u>DP</u>	<u>EP</u>	<u>CEP</u>	<u>CE</u>	<u>CXP</u>	
Catechin	4.80	288.9 / 108.9	-40	-10	-22	-50	-2	288.9 / 122.7	-40	-10	-28	-50	-2	Catechin
Epicatechin	6.60	288.9 / 108.9	-40	-10	-22	-50	-2	288.9 / 122.7	-40	-10	-22	-50	-2	Epicatechin
Gallic acid	3.10	305.0 / 125.0	-40	-10	-23	-50	-2	305.0 / 109.1	-40	-10	-23	-50	-2	Gallic acid
Epigallocatechin	4.30	305.0 / 125.0	-40	-10	-23	-50	-2	305.0 / 109.1	-40	-10	-23	-50	-2	Epicatechin
Epigallocatechin gallate	5.30	457.0 / 169.0	-40	-10	-29	-50	-2	457.0 / 125.0	-40	-10	-29	-50	-2	Epicatechin
Procyanidin B1	4.20	577.1 / 124.9	-70	-10	-26	-50	-2	577.2 / 289.2	-70	-10	-33	-34	-4	Procyanidin B1
Procyanidin B2	6.00	577.1 / 124.9	-70	-10	-33	-50	-2	577.2 / 289.2	-70	-10	-33	-34	-4	Procyanidin B2
Procyanidin B3	7.60	577.1 / 124.9	-70	-10	-33	-50	-2	577.2 / 289.2	-70	-10	-33	-34	-4	Procyanidin B1
Procyanidin T	5.60	577.1 / 124.9	-70	-10	-33	-50	-2	577.1 / 289.2	-70	-10	-33	-34	-4	Procyanidin B1
<i>trans</i> -Coumaric acid	7.20	162.9 / 119.0	-20	-10	-14	-12	-2	162.9 / 92.8	-20	-10	-18	-38	-2	<i>trans</i> -Coumaric acid
<i>cis</i> -Coumaric acid	7.80	162.9 / 119.0	-20	-10	-14	-12	-2	162.9 / 92.8	-20	-10	-18	-38	-2	<i>trans</i> -Coumaric acid
Benzoic acid	9.00	121.0 / 77.0	-35	-9	-16	-22	0	121.0 / 64.9	-35	-9	-16	-42	0	4-Hydroxybenzoic acid
3-Hydroxybenzoic acid	5.40	137.0 / 93.0	-35	-9	-17	-22	0	137.0 / 64.9	-35	-9	-17	-42	0	4-Hydroxybenzoic acid
4-Hydroxybenzoic acid	4.10	137.0 / 93.0	-35	-9	-17	-22	0	137.0 / 64.9	-35	-9	-17	-42	0	4-Hydroxybenzoic acid
Protocatechuic acid	3.20	153.0 / 107.6	-35	-10	-17	-38	-1	153.0 / 109.0	-35	-10	-17	-20	-2	Protocatechuic acid
(3,4-Dihydroxybenzoic acid)														
3,5-Dihydroxybenzoic acid	3.00	152.9 / 109.0	-35	-10	-17	-20	-2	152.9 / 107.6	-35	-10	-17	-38	-1	Protocatechuic acid
x,x-Dihydroxybenzoic acid	3.70	152.9 / 109.0	-35	-10	-17	-20	-2	152.9 / 107.6	-35	-10	-17	-38	-1	Protocatechuic acid
x,y-Dihydroxybenzoic acid	4.10	152.9 / 109.0	-35	-10	-17	-20	-2	152.9 / 107.6	-35	-10	-17	-38	-1	Protocatechuic acid
x,z-Dihydroxybenzoic acid	5.20	152.9 / 109.0	-35	-10	-17	-20	-2	152.9 / 107.6	-35	-10	-17	-38	-1	Protocatechuic acid
Gallic acid	2.20	168.9 / 124.9	-40	-4	-18	-16	0	168.9 / 79.0	-40	-4	-18	-34	0	Gallic acid
Phenylacetic acid	9.20	135.0 / 91.0	-30	-9	-17	-12	-2	135.0 / 107.0	-30	-9	-17	-24	-2	4-Hydroxyphenylacetic acid
2-Hydroxyphenylacetic acid	6.40	151.0 / 106.9	-30	-9	-17	-15	-2	151.0 / 64.7	-30	-9	-17	-28	-2	4-Hydroxyphenylacetic acid
3-Hydroxyphenylacetic acid	5.80	151.0 / 106.9	-30	-9	-17	-15	-2	151.0 / 64.7	-30	-9	-17	-28	-2	4-Hydroxyphenylacetic acid
4-Hydroxyphenylacetic acid	4.90	151.0 / 106.9	-30	-9	-17	-15	-2	151.0 / 64.7	-30	-9	-17	-28	-2	4-Hydroxyphenylacetic acid
3,4-Dihydroxyphenylacetic acid	3.70	167.0 / 123.0	-30	-10	-18	-15	-4	167.0 / 95.0	-30	-10	-18	-26	-2	3,4-Dihydroxyphenylacetic acid
Hippuric acid	5.00	178.0 / 134.0	-40	-10	-18	-15	-2	178.0 / 77.0	-40	-10	-18	-20	0	Hippuric acid
Phenylpropionic acid	11.8	149.0 / 105.0	-45	-7	-17	-13	-2	149.0 / 77.0	-45	-7	-17	-32	-2	3-Phenylpropionic acid
3-(3'-Hydroxyphenyl)propionic acid	7.70	164.8 / 121.2	-65	-10	-18	-14	-4	164.8 / 105.8	-65	-10	-18	-32	-2	3-(3'-Hydroxyphenyl)propionic acid
3-(4'-Hydroxyphenyl)propionic acid	7.30	164.8 / 119.1	-65	-10	-18	-37	-2	164.8 / 121.2	-65	-10	-18	-14	-4	3-(3'-Hydroxyphenyl)propionic acid
3-(3',4'-Dihydroxyphenyl)propionic acid	5.00	181.0 / 59.0	-55	-9	-18	-16	-2	181.0 / 137.0	-55	-9	-18	-14	0	3-(3',4'-Dihydroxyphenyl)propionic acid

															acid
	Catechol	3.80	109.0 / 91.0	-60	-10	-16	-35	-1	109.0 / 81.0	-60	-10	-16	-24	0	Catechol
	Pyrogallol	2.10	125.0 / 79.0	-45	-10	-16	-27	-2	125.0 / 81.0	-45	-10	-16	-26	-2	Pyrogallol
	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid	4.50	225.0 / 163.0	-70	-10	-20	-20	-2	225.0 / 181.0	-70	-10	-20	-35	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	4-Hydroxy-5-(4'-hydroxyphenyl)-valeric acid	6.90	209.0 / 147.0	-70	-10	-20	-15	-2	209.0 / 165.0	-70	-10	-20	-15	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid	8.30	209.0 / 147.0	-70	-10	-20	-15	-2	209.0 / 165.0	-70	-10	-20	-15	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	4-Hydroxy-5-(2'-hydroxyphenyl)-valeric acid	10.3	209.0 / 147.0	-70	-10	-20	-15	-2	209.0 / 165.0	-70	-10	-20	-15	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	5-(3'-Hydroxyphenyl)-valeric acid	11.7	193.0 / 165.0	-70	-10	-19	-20	-2	193.0 / 149.0	-70	-10	-19	-25	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	5-(4'-Hydroxyphenyl)-valeric acid	9.30	193.0 / 165.0	-70	-10	-19	-20	-2	193.0 / 149.0	-70	-10	-19	-25	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	5-(3',4'-Dihydroxyphenyl)-valeric acid	9.80	209.0 / 135.0	-75	-6	-20	-28	-4	209.0 / 122.0	-75	-6	-20	-25	-3	4,4-Bis-4-hydroxyphenylvaleric acid
	Phenyl-valeric acid	13.7	177.0 / 133.0	-55	-7	-18	-25	-2	177.0 / 77.0	-55	-7	-18	-40	-2	4,4-Bis-4-hydroxyphenylvaleric acid
	5-(3'-Hydroxyphenyl)-γ-valerolactone	9.40	191.0 / 147.0	-75	-8	-19	-17	-3	191.0 / 106.0	-75	-8	-19	-30	-3	5-(3',4'-Dihydroxyphenyl)-δ-valerolactone
	5-(4'-Hydroxyphenyl)-γ-valerolactone	8.40	191.0 / 147.0	-75	-8	-19	-17	-3	191.0 / 106.0	-75	-8	-19	-30	-3	5-(3',4'-Dihydroxyphenyl)-δ-valerolactone
	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	6.70	207.0 / 163.0	-75	-8	-19	-20	-3	207.0 / 122.0	-75	-8	-19	-25	-3	5-(3',4'-Dihydroxyphenyl)-δ-valerolactone
	1-(3',4'-Dihydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	6.70	291.0 / 122.0	-60	-10	-22	-35	-2	291.0 / 247.0	-60	-10	-22	-25	-2	Catechin
	1-(4'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	6.00	275.0 / 231.0	-40	-10	-22	-20	-2	275.0 / 106.0	-40	-10	-22	-35	-2	Catechin
	1-(3'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	8.30	275.0 / 231.0	-40	-10	-22	-20	-2	275.0 / 106.0	-40	-10	-22	-35	-2	Catechin
	1-(2'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	10.3	275.0 / 231.0	-40	-10	-22	-20	-2	275.0 / 106.0	-40	-10	-22	-35	-2	Catechin

RT: Retention Time; DP: Declustering Potential; EP: Entrance Potential; CEP: Collision Cell Entrance Potential; CE: Collision Energy; CXP: Collision Cell Exit Potential

Table S2. Concentration of the main (wine precursors) and their colonic metabolites quantified in the gastric and intestinal digestates, and in the culture medium of the ascending colon section (AC) during the digestion of wine 2020.

Compound (µg/mL media)		Culture medium + wine	Gastric digestate	Intestinal digestate	AC day 12	AC day 13	AC day 14	AC day 15	AC day 16	AC day 18	AC day 20	AC day 23	AC day 26
PRECURSORS	Catechin	4.18	3.02	n.d.	n.d.	0.60	0.85	0.84	0.94	0.91	0.90	1.05	0.82
	Epicatechin	2.13	1.50	n.d.	0.03	0.33	0.49	0.52	0.53	0.54	0.57	0.62	0.51
	Galocatechin	0.74	0.52	n.d.	n.d.	n.d.	n.d.	n.d.	0.02	0.01	0.07	0.08	0.02
	Epigallocatechin	0.80	0.54	n.d.	n.d.	0.05	0.09	0.07	0.11	0.09	0.13	0.16	0.12
	Procyanidin B1	7.72	4.62	n.d.	n.d.	0.81	1.31	1.35	1.60	1.71	1.71	1.77	1.35
	Procyanidin B2	1.89	1.20	n.d.	0.05	0.21	0.29	0.33	0.37	0.40	0.40	0.44	0.33
	Procyanidin B3	0.52	0.42	n.d.	n.d.	0.16	0.19	0.18	0.19	0.20	0.20	0.20	0.18
	Procyanidin T	0.02	0.01	n.d.	n.d.	n.d.	n.d.	n.d.	0.01	n.d.	n.d.	n.d.	n.d.
METABOLITES	trans-Coumaric acid	0.49	0.40	1.52	0.01	0.45	0.18	0.15	0.11	0.16	0.14	0.10	0.17
	cis-Coumaric acid	0.01	n.d.	n.d.	n.d.	n.d.	0.02	0.02	0.03	0.05	0.06	0.08	0.08
	Benzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-Hydroxybenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxybenzoic acid	0.40	0.33	0.30	0.17	0.23	0.29	0.29	0.30	0.25	0.19	0.23	0.22
	Protocatechuic acid	1.26	1.15	0.96	0.09	0.14	0.05	0.04	0.04	0.05	0.05	0.06	0.08
	3,5-Dihydroxybenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	x,x-Dihydroxybenzoic acid	n.d.	n.d.	0.01	n.d.	n.d.	n.d.	0.01	0.01	0.02	0.02	0.03	0.03
	x,y-Dihydroxybenzoic acid	0.06	0.05	0.02	n.d.	0.01	0.02	0.02	0.03	0.05	0.05	0.08	0.08
	x,z-Dihydroxybenzoic acid	0.04	0.03	0.24	0.02	0.04	0.05	0.05	0.08	0.16	0.14	0.15	0.26
	Gallic acid	10.1	9.38	n.d.	n.d.	1.93	2.08	1.74	1.85	1.80	1.85	2.10	1.76
	Phenylacetic acid	n.d.	n.d.	0.20	0.04	0.09	0.12	0.13	0.19	0.18	0.12	0.23	0.24
	2-Hydroxyphenylacetic acid	0.17	0.08	0.13	0.11	0.13	0.13	0.19	0.20	0.20	0.19	0.21	0.29
	3-Hydroxyphenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxyphenylacetic acid	n.d.	n.d.	0.15	0.08	0.12	0.09	0.08	0.11	0.15	0.08	0.12	0.18
	3,4-Dihydroxyphenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Hippuric acid	n.d.	n.d.	0.05	0.18	0.07	0.04	0.03	0.04	0.03	n.d.	n.d.	n.d.
	Phenylpropionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(3'-Hydroxyphenyl)propionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(4'-Hydroxyphenyl)propionic acid	0.20	0.18	0.21	1.18	1.18	1.16	1.37	1.55	1.66	1.59	1.96	2.12
	3-(3',4'-Dihydroxyphenyl)propionic acid	0.58	0.51	n.d.	0.02	0.17	0.49	0.63	0.76	0.80	0.82	1.02	0.86
	Catechol	n.d.	n.d.	n.d.	0.09	0.25	0.48	0.44	0.52	0.50	0.46	0.53	0.44
	Pyrogallol	4.26	4.03	n.d.	n.d.	0.98	1.74	1.99	2.31	2.36	2.14	2.34	1.88
	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(4'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3'-Hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(4'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	1-(3',4'-Dihydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	0.06	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.04	n.d.	0.09	0.04
1-(4'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
1-(3'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
1-(2'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

Table S3. Concentration of the main (wine precursors) and their colonic metabolites quantified in the culture medium of the transversal colon section (TC) during digestion of 2020 wine.

Compound (µg/mL culture medium)		TC day 12	TC day 13	TC day 14	TC day 15	TC day 16	TC day 18	TC day 20	TC day 23	TC day 26
PRECURSORS	Catechin	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Epicatechin	n.d.	0.04	0.02	n.d.	n.d.	n.d.	n.d.	0.02	n.d.
	Gallocatechin	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Epigallocatechin	n.d.	n.d.	0.04	0.03	0.02	n.d.	n.d.	n.d.	n.d.
	Procyanidin B1	0.14	0.57	0.24	0.21	0.22	0.20	0.21	0.24	0.18
	Procyanidin B2	n.d.	0.06	0.02	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Procyanidin B3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Procyanidin T	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
METABOLITES	<i>trans</i> -Coumaric acid	n.d.	0.10	0.18	0.20	0.25	0.29	0.31	0.23	0.21
	<i>cis</i> -Coumaric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Benzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-Hydroxybenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxybenzoic acid	0.18	0.26	0.28	0.19	0.18	0.13	0.25	0.30	0.14
	Protocatechuic acid	0.31	0.51	0.42	0.37	0.40	0.36	0.59	0.80	0.46
	3,5-Dihydroxybenzoic acid	n.d.	0.01	0.01	0.02	0.02	0.01	0.01	0.01	0.01
	x,x-Dihydroxybenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	x,y-Dihydroxybenzoic acid	0.03	0.05	0.09	0.09	0.09	0.10	0.10	0.08	0.07
	x,z-Dihydroxybenzoic acid	0.03	0.05	0.08	0.09	0.10	0.22	0.32	0.37	0.46
	Gallic acid	0.02	0.97	1.34	0.68	0.67	0.36	0.65	0.25	0.17
	Phenylacetic acid	16.2	17.9	17.8	15.7	16.8	19.6	21.4	21.5	22.5
	2-Hydroxyphenylacetic acid	1.50	1.96	2.51	2.38	2.61	3.38	8.14	8.14	9.11
	3-Hydroxyphenylacetic acid	0.43	0.46	0.48	0.47	0.54	0.79	1.37	1.45	1.63
	4-Hydroxyphenylacetic acid	0.97	1.24	0.77	0.84	0.73	0.26	n.d.	0.17	0.07
	3,4-Dihydroxyphenylacetic acid	0.16	0.35	0.55	0.59	0.65	0.60	0.74	1.00	0.72
	Hippuric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Phenylpropionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(3'-Hydroxyphenyl)propionic acid	0.44	0.65	1.45	2.13	2.88	4.07	5.28	4.98	5.23
	3-(4'-Hydroxyphenyl)propionic acid	1.57	1.46	1.76	2.04	1.94	1.87	1.95	1.79	1.78
	3-(3',4'-Dihydroxyphenyl)propionic acid	0.16	1.04	1.72	1.45	1.20	0.21	0.15	0.05	0.03
	Catechol	0.31	0.59	1.08	1.20	1.28	0.83	0.94	1.41	1.46
	Pyrogallol	n.d.	0.46	0.90	0.73	0.48	0.15	0.23	0.17	0.06
	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid	n.d.	0.11	0.09	0.09	0.02	0.19	0.21	0.23	0.13
	4-Hydroxy-5-(4'-hydroxyphenyl)-valeric acid	0.02	0.04	n.d.	n.d.	n.d.	0.07	0.22	0.16	0.13
	4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	0.06	0.08	0.04	0.04	0.02	n.d.
	5-(3'-Hydroxyphenyl)-valeric acid	0.01	0.02	0.07	0.04	0.04	0.07	0.09	0.04	0.01
	5-(3',4'-Dihydroxyphenyl)-valeric acid	n.d.	0.06	0.58	0.86	0.77	0.09	0.06	0.04	0.01
	5-(3'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	0.08	0.16	0.16	0.16
	5-(4'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	0.01	0.01	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	0.07	0.59	1.31	1.29	0.99	1.91	1.61	2.41	1.98
	1-(3',4'-Dihydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
1-(4'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
1-(3'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	
1-(2'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	

Table S5. Concentration of the main (wine precursors) and their colonic metabolites quantified in the gastric and intestinal digestates, and in the culture medium of the ascending colon

Compound (µg/mL media)		Culture medium+wine	Gastric digestate	Intestinal digestate	AC day 12	AC day 13	AC day 14	AC day 15	AC day 16	AC day 18	AC day 20	AC day 23	AC day 26
PRECURSORS	Catechin	5.92	3.34	0.32	0.11	1.13	1.17	1.11	1.20	1.33	1.12	1.11	0.78
	Epicatechin	2.51	1.35	0.09	0.04	0.46	0.40	0.34	0.37	0.43	0.32	0.36	0.23
	Gallocatechin	1.30	0.78	n.d.	n.d.	0.28	0.37	0.34	0.37	0.33	0.33	0.32	0.30
	Epigallocatechin	0.72	0.40	n.d.	n.d.	0.09	0.13	0.12	0.13	0.09	0.11	0.13	0.09
	Epigallocatechin gallate	0.04	0.07	n.d.	n.d.	0.02	0.03	0.02	0.02	0.01	0.02	0.02	0.02
	Procyanidin B1	9.80	4.10	0.46	n.d.	1.37	2.03	2.02	1.69	1.33	1.85	2.26	1.79
	Procyanidin B2	2.43	1.21	n.d.	0.04	0.37	0.46	0.44	0.40	0.36	0.46	0.54	0.42
	Procyanidin B3	0.55	0.29	n.d.	n.d.	0.07	0.08	0.08	0.07	0.07	0.08	0.07	0.06
	Procyanidin T	0.08	0.06	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
METABOLITES	<i>trans</i> -Coumaric acid	0.99	0.86	2.16	n.d.	0.24	0.20	0.21	0.22	0.19	0.24	0.21	0.12
	<i>cis</i> -Coumaric acid	0.05	0.05	0.03	n.d.	0.03	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Benzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-Hydroxybenzoic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxybenzoic acid	0.27	0.22	0.22	0.08	0.11	0.12	0.12	0.14	0.11	0.14	0.16	0.16
	Protocatechuic acid	1.02	0.90	1.00	0.07	0.10	0.07	0.07	0.08	0.11	0.15	0.17	0.14
	3,5-Dihydroxybenzoic acid	1.55	1.50	1.72	0.14	0.20	0.12	0.15	0.14	0.21	0.30	0.34	0.27
	x,x-Dihydroxybenzoic acid	0.01	0.02	0.03	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.05
	x,y-Dihydroxybenzoic acid	0.12	0.10	0.06	0.03	0.04	0.05	0.06	0.07	0.07	0.09	0.17	0.17
	x,z-Dihydroxybenzoic acid	0.06	0.05	0.26	0.16	0.16	0.20	0.22	0.21	0.23	0.24	0.22	0.26
	Gallic acid	14.0	13.4	0.19	n.d.	2.57	3.04	3.04	3.02	2.88	3.73	4.01	3.91
	Phenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	2-Hydroxyphenylacetic acid	1.56	1.50	1.03	0.95	1.22	1.16	1.05	1.16	1.12	1.08	1.14	1.50
	3-Hydroxyphenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxyphenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.19	0.20
	3,4-Dihydroxyphenylacetic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Hippuric acid	n.d.	n.d.	0.10	0.03	0.01	0.00	0.01	0.02	0.02	0.04	0.07	0.04
	Phenylpropionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(3'-Hydroxyphenyl)propionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(4'-Hydroxyphenyl)propionic acid	0.71	0.54	0.52	2.73	2.71	2.66	2.62	2.67	2.08	2.31	2.43	2.55
	3-(3',4'-Dihydroxyphenyl)propionic acid	0.66	0.56	0.02	0.16	1.87	2.72	2.99	3.18	3.19	3.56	3.45	3.62
	Catechol	n.d.	n.d.	n.d.	0.08	0.25	0.46	0.36	0.35	0.25	0.36	0.34	0.46
	Pyrogallol	7.31	6.97	n.d.	n.d.	2.15	3.01	3.32	3.50	3.44	3.25	2.90	2.72
	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(4'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(2'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	0.12	0.11	0.10	0.10	0.10	0.10	0.11	0.12	0.13
	5-(3'-Hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(4'-Hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Phenyl-valeric acid	n.d.	n.d.	n.d.	0.13	0.13	0.14	0.11	0.14	0.05	0.07	0.05	0.08
	5-(3'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(4'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.01
	1-(3',4'-Dihydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	0.42	0.69	0.50	0.17	0.71	0.76	0.97
	1-(4'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	0.19	0.15	0.11	0.11	0.13	0.13	0.11	0.12	0.12	0.13	0.13	0.12
	1-(3'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	1-(2'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	0.09	0.09	0.10	0.09	0.09	0.09	0.09	0.09	0.10	0.10

section (AC) during digestion of 2021 wine.

[illegible]

Table S7. Concentration of the main (wine precursors) and their colonic metabolites quantified in the culture medium descending colon section (DC) during digestion of 2021 wine.

Compound (µg/mL media)		DC day 12	DC day 13	DC day 14	DC day 15	DC day 16	DC day 18	DC day 20	DC day 23	DC day 26
PRECURSORS	Catechin	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Epicatechin	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Gallocatechin	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Epigallocatechin	n.d.	0.00	0.01	0.02	0.04	0.03	0.04	0.04	0.01
	Epigallocatechin gallate	n.d.	n.d.	n.d.	0.01	0.02	0.02	0.02	0.03	0.03
	Procyanidin B1	n.d.	0.03	0.05	0.03	0.07	n.d.	n.d.	n.d.	n.d.
	Procyanidin B2	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Procyanidin B3	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Procyanidin T	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
METABOLITES	<i>trans</i> -Coumaric acid	n.d.	0.01	0.03	0.09	0.11	0.09	0.05	0.03	0.04
	<i>cis</i> -Coumaric acid	n.d.	n.d.	n.d.	0.00	0.02	0.00	n.d.	n.d.	n.d.
	Benzoic acid	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	3-Hydroxybenzoic acid	0.00	0.00	0.06	0.09	0.11	0.12	0.24	0.25	0.26
	4-Hydroxybenzoic acid	0.25	0.25	0.35	0.27	0.34	0.61	0.65	0.40	0.27
	Protocatechuic acid	0.12	0.15	0.21	0.21	0.23	0.35	0.43	0.46	0.36
	3,5-Dihydroxybenzoic acid	0.27	0.34	0.51	0.48	0.54	0.77	0.95	1.04	0.79
	x,x-Dihydroxybenzoic acid	0.01	0.01	0.01	0.02	0.02	0.02	0.01	0.01	0.02
	x,y-Dihydroxybenzoic acid	0.03	0.05	0.04	0.05	0.06	0.04	0.04	0.04	0.05
	x,z-Dihydroxybenzoic acid	0.22	0.28	0.31	0.27	0.26	0.35	0.45	0.50	0.51
	Gallic acid	n.d.	0.11	0.02	0.04	0.44	0.04	0.04	0.04	0.04
	Phenylacetic acid	13.8	14.7	14.1	14.1	12.2	12.3	13.2	15.6	15.7
	2-Hydroxyphenylacetic acid	24.4	22.7	21.2	18.2	13.3	8.17	8.13	10.2	16.2
	3-Hydroxyphenylacetic acid	0.73	0.59	0.43	0.59	0.45	1.31	8.11	7.02	4.20
	4-Hydroxyphenylacetic acid	4.50	4.45	2.80	3.66	2.49	2.26	3.74	3.26	2.13
	3,4-Dihydroxyphenylacetic acid	0.27	0.76	1.51	2.68	3.33	4.14	3.02	1.84	1.82
	Hippuric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	Phenylpropionic acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	3-(3'-Hydroxyphenyl)propionic acid	0.37	0.60	1.89	4.26	7.13	12.5	13.0	16.9	17.9
	3-(4'-Hydroxyphenyl)propionic acid	1.49	1.22	1.35	1.21	1.26	1.26	1.26	1.93	0.80
	3-(3',4'-Dihydroxyphenyl)propionic acid	0.01	0.10	0.20	0.37	0.52	0.23	0.22	0.22	0.17
	Catechol	0.07	0.09	0.29	0.51	0.70	0.92	0.75	0.95	1.20
	Pyrogallol	n.d.	0.09	n.d.	n.d.	0.47	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid	0.02	0.09	0.16	0.25	0.25	0.27	0.20	0.16	0.30
	4-Hydroxy-5-(4'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	0.03	0.07	0.10	0.13	0.12	0.07
	4-Hydroxy-5-(3'-hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	4-Hydroxy-5-(2'-hydroxyphenyl)-valeric acid	0.25	0.18	0.18	0.16	0.15	0.15	0.14	0.15	0.18
	5-(3'-Hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(4'-Hydroxyphenyl)-valeric acid	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(3',4'-Dihydroxyphenyl)-valeric acid	n.d.	0.04	0.09	0.09	0.14	0.16	0.29	0.29	0.92
	Phenyl-valeric acid	0.05	0.04	0.03	0.02	0.02	0.02	0.02	0.01	0.02
	5-(3'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
	5-(4'-Hydroxyphenyl)-γ-valerolactone	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.01	0.03
	5-(3',4'-Dihydroxyphenyl)-γ-valerolactone	n.d.	0.10	0.85	1.83	4.20	7.45	7.55	8.05	4.72
	1-(3',4'-Dihydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	0.06	0.15	n.d.	0.11	n.d.	n.d.	0.06	n.d.

1-(4'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	0.05	0.06	0.10	0.06
1-(3'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
1-(2'-Hydroxyphenyl)-3-(2',4',6'-trihydroxyphenyl)-propan-2-ol	0.12	0.11	0.11	0.11	0.10	0.10	0.09	0.10	0.11

n.d.: not detected