




Supplementary Material

Title: Multi-mechanistic antihyperglycemic assessment of three Indian red rice cultivars: In silico, in vitro and in vivo analyses

Table S1. Morphological details of traditional experimental red rice varieties.

Sample name	Sample code	Rice grains with bran	Bran %	Grain length (mm)	Grain breadth (mm)	Morphological * classification
Kattuyanam	KA		13 %	5.0	2.0	Short & Bold
Chennangi	GS		10 %	4.0	2.0	Short & Bold
Karungkuvai	KU		11 %	5.0	3.0	Short & Round

* As per the Food and Agriculture Organization (FAO) of the United Nations, Rome, Italy.

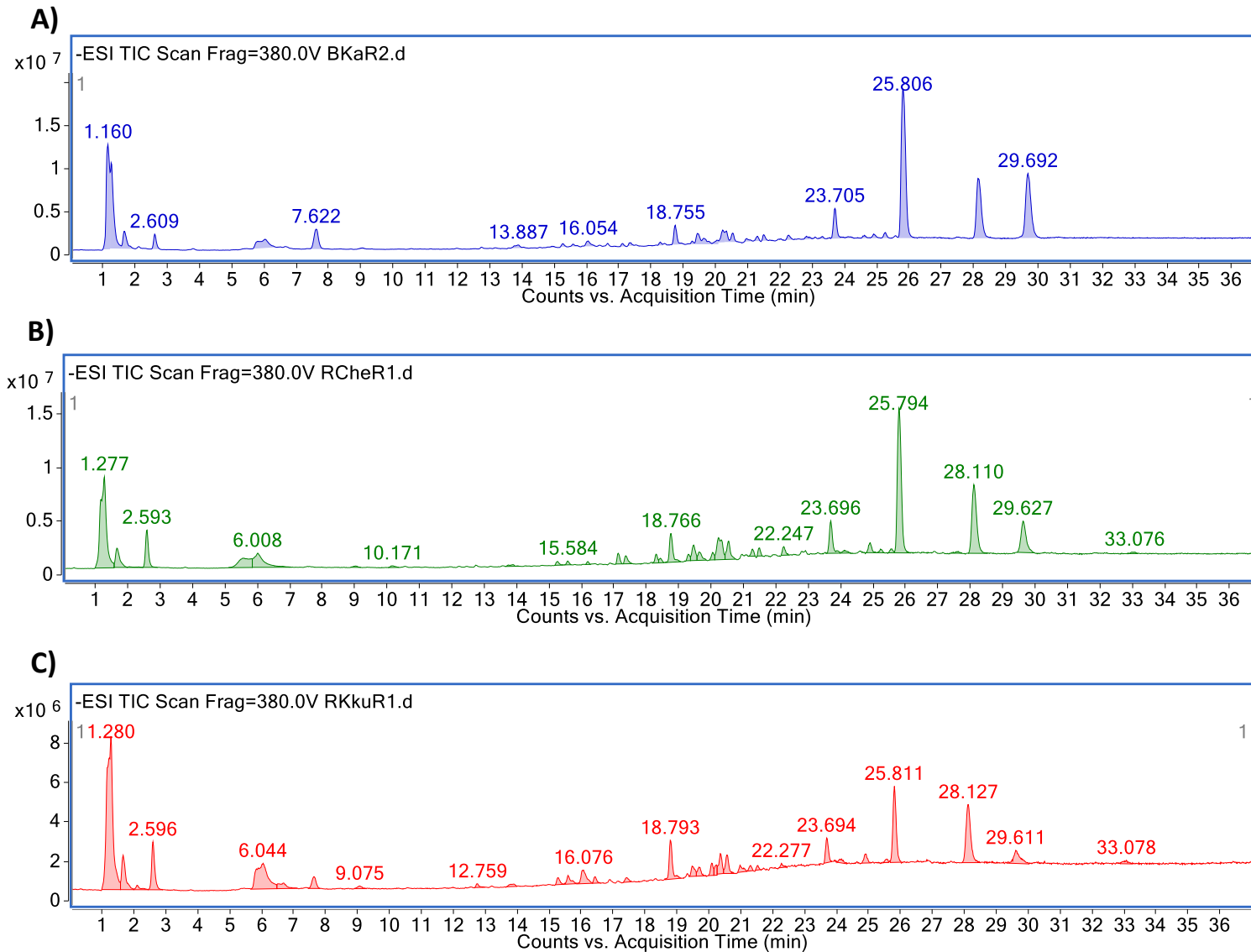


Figure S1. Total ion chromatograms of (A) Kattuyanam (B) Chennangi (C) Karungkuruvai.

Table S2. Retention time, m/z ratio, formula, diff, MS fragments and scores of the phenolic compounds identified in the experimental samples.

S. No.	RT	[M-H] ⁻ m/z	Formula	Diff (mDa)	Score	MS fragments	Compound	Class	Sub class
1.	1.105	205.036	C ₇ H ₁₀ O ₇	1.94	85.72	125.0124	2-methyl citric acid	Other polyphenols	
2.	1.147	479.11895	C ₂₂ H ₂₃ O ₁₂	2.06	84.6	87.0076,123.0440	4-O-Methyl delphinidin 3-O-D-glucoside	Flavonoids	Anthocyanins
3.	1.152	271.0983	C ₁₆ H ₁₆ O ₄	0.55	85.67	225.0557	3'-O-Methylequol	Flavonoids	Isoflavonoids
4.	1.155	480.4188	C ₂₂ H ₂₄ O ₁₂	-4.07	97.25	303.0874, 261.0768, 141.0557	3'-O-Methyl(-)-epicatechin 7-O-glucuronide	Flavonoids	Flavanols
5.	1.169	304.2946	C ₁₆ H ₁₆ O ₆	-0.86	94.45	149.0244, 123.0451, 111.0451	3'-O-Methylcatechin	Flavonoids	Flavanols
6.	1.205	208.0674	C ₁₁ H ₁₂ O ₄	-0.23	86.94	159.0446, 133.0289	Sinapaldehyde	Other polyphenols	Hydroxycinnamaldehydes
7.	1.222	637.1526	C ₂₉ H ₃₂ O ₁₆	1.41	91.51	325.0348, 269.0449, 147.0293	Kaempferol 3-O-(6''-acetyl-galactoside) 7-O-rhamnoside	Flavonoids	Flavonols
8.	1.231	435.0927	C ₂₀ H ₁₉ O ₁₁	4.32	89.51	101.0238, 115.0395	Delphinidin 3-O-arabinoside	Flavonoids	Anthocyanins
9.	1.233	145.0501	C ₉ H ₆ O ₂	-0.36	86.48	129.045	Coumarin	Phenolic acids	Hydroxycinnamic acids
10.	1.238	306.0726	C ₁₅ H ₁₄ O ₇	1.24	87.27	286.0452, 260.0663	Epigallocatechin	Flavonoids	Flavanols
11.	1.282	419.09782	C ₂₀ H ₁₉ O ₁₀	-8.51	87.45	101.0238, 129.0551	Cyanidin 3-O-arabinoside	Flavonoids	Anthocyanins
12.	1.355	134.0143	C ₄ H ₆ O ₅	0.02	98.93	84.9926	Malic acid	Flavonoids	Flavonols
13.	1.705	124.1372	C ₇ H ₈ O ₂	-0.68	87.23	123.0446, 65.0027	3-Methylcatechol	Other polyphenols	Alkylphenols
14.	1.771	167.0342	C ₈ H ₈ O ₄	-0.67	85.07	168.0376, 125.0231	3,4-Dihydroxyphenylacetic acid	Phenolic acids	Hydroxyphenylacetic acids

15.	1.788	167.0334	C ₈ H ₈ O ₄	-1.37	82.26	479.0909, 357.0583	<i>Vanillic acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
16.	1.822	197.0446	C ₉ H ₁₀ O ₅	-0.59	97.71	166.9980, 108.9925, 80.9976	<i>Ethyl Gallate</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
17.	1.855	179.0337	C ₉ H ₈ O ₄	-1.26	84.57	181.0438, 145.0244	<i>Caffeic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
18.	1.922	191.019	C ₆ H ₈ O ₇	-0.78	90.56	111.121	<i>Citric acid</i>		
19.	2.105	169.0133	C ₇ H ₆ O ₅	-0.97	93.34	169.0218, 126.0337, 124.0225	<i>Gallic acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
20.	2.138	163.0394	C ₉ H ₈ O ₃	-0.57	97.65	163.0395, 119.3241, 93.0354	<i>p-Coumaric acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
21.	2.455	449.1087	C ₂₁ H ₂₂ O ₁₁	-0.13	80.51	285.0399, 149.0238, 107.0133	<i>Eriodictyol 7-O-glucoside</i>	<i>Flavonoids</i>	<i>Flavanones</i>
22.	3.005	343.1078	C ₁₉ H ₁₈ O ₆	-0.99	91.17	285.0762, 199.0395	<i>Tetramethylscutellarein</i>	<i>Flavonoids</i>	<i>Flavones</i>
23.	3.215	178.0629	C ₁₀ H ₁₂ O ₃	0.33	84.63	123.0446, 79.0183	<i>Ferulaldehyde</i>	<i>Other polyphenols</i>	<i>Hydroxycinnamaldehydes</i>
24.	3.805	138.0234	C ₇ H ₆ O ₃	-1	91.13	137.0239, 93.0341	<i>p-Hydroxybenzoic acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
25.	4.005	178.0508	C ₉ H ₉ NO ₃	-0.17	93.02	178.0499, 134.0943	<i>Hippuric acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
26.	4.272	367.1038	C ₁₇ H ₂₀ O ₉	0.29	87.43	173.0449, 143.0344, 59.0133	<i>Feruloylquinic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
27.	4.555	193.0502	C ₁₀ H ₁₀ O ₄	-0.72	84.6	147.0451, 119.0502	<i>Ferulic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
28.	5.089	195.0286	C ₉ H ₈ O ₅	-1.27	90.82	147.0082, 121.0289, 107.0133	<i>Hydroxycaffeic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
29.	5.414	389.1227	C ₁₈ H ₁₈ O ₆	-1.45	92.83	243.0662	<i>3'-O-Methylviolanone</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
30.	6.044	595.1451	C ₃₀ H ₂₇ O ₁₃	-2.12	85.24	83.0133, 125.0966	<i>Cyanidin 3-O-(6"-p-coumaroyl-glucoside)</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
31.	6.289	153.0192	C ₇ H ₆ O ₄	-0.14	99.64	108.9925, 84.9925, 68.9976	<i>2,4-Dihydroxybenzoic acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>

32.	6.289	577.1352	C ₃₀ H ₂₆ O ₁₂	0	90.2	578.1407, 425.0862	<i>Procyanidin dimer B1</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
33.	6.325	595.1663	C ₂₇ H ₃₁ O ₁₅	1.23	88.06	105.0334, 147.0651	<i>Pelargonidin 3-O-sophoroside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
34.	6.455	165.0557	C ₉ H ₁₀ O ₃	-0.04	87.61	111.4031, 83.1211	<i>Dihydro-p-coumaric acid</i>	<i>Phenolic acids</i>	<i>Hydroxyphenylpropanoic acids</i>
35.	6.465	315.1135	C ₁₅ H ₁₈ O ₈	-0.56	90.23	147.0293, 119.0344, 55.0183	<i>1-O-p-Coumaroyl-beta-D-glucose</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
36.	6.539	347.0919	C ₁₅ H ₁₈ O ₉	-1.47	90.88	149.0238, 121.0289, 71.0133	<i>Caffeic acid 4-O-glucoside</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
37.	6.601	355.0652	C ₁₅ H ₁₆ O ₁₀	-1.82	90.3	161.0244, 121.0295	<i>Caffeic acid 3-O-glucuronide</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
38.	6.672	289.0703	C ₁₅ H ₁₄ O ₆	-1.5	92.29	289.0712, 187.0411, 123.0456	<i>Catechin</i>	<i>Flavonoids</i>	<i>Flavanols</i>
39.	7.272	288.2522	C ₁₅ H ₁₂ O ₆	0.41	89.43	179.0344, 161.0238, 135.0446, 121.0289	<i>3',4',5,7-Tetrahydroxyisoflavanone</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
40.	7.372	274.2367	C ₁₅ H ₁₄ O ₅	-0.68	93.94	217.087, 161.0608, 125.0244	<i>3'-Hydroxy-O-desmethylan-golensin</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
41.	7.572	286.1252	C ₁₅ H ₁₀ O ₆	0.25	92.72	201.0193, 149.0244	<i>3'-Hydroxygenistein</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
42.	7.584	121.0289	C ₇ H ₆ O ₂	-0.61	97.34	92.2042, 64.9181	<i>Benzoic acid</i>	<i>Phenolic acids</i>	<i>Hydroxybenzoic acids</i>
43.	7.605	121.0289	C ₇ H ₆ O ₂	-0.64	97.09	121.0294, 108.0218, 93.0345	<i>4-Hydroxybenzaldehyde</i>	<i>Other polyphenols</i>	<i>Hydroxybenzaldehydes</i>
44.	7.672	195.0649	C ₁₀ H ₁₂ O ₄	-1.41	90.72	151.0759, 149.0238, 121.0653	<i>Dihydroferulic acid</i>	<i>Phenolic acids</i>	<i>Hydroxyphenylpropanoic acids</i>
45.	7.739	465.1024	C ₂₁ H ₂₂ O ₁₂	-1.41	90.93	289.0353, 261.0404, 165.0193	<i>Dihydromyricetin 3-O-rhamnoside</i>	<i>Flavonoids</i>	<i>Dihydroflavonols</i>
46.	8.889	563.1408	C ₂₆ H ₂₈ O ₁₄	0.12	99.52	383.2032	<i>Apigenin-6-C-pentosyl-8-C-hexoside</i>	<i>Flavonoids</i>	<i>Flavones</i>

47.	9.389	434.397	C ₂₁ H ₂₂ O ₁₀	1.03	77.66	255.0657, 135.0446, 89.0238	<i>Naringin 4'-glucoside</i>	<i>Flavonoids</i>	<i>Flavanones</i>
48.	9.422	447.0941	C ₂₁ H ₂₀ O ₁₁	0.84	98.04	283.0242, 201.0187, 109.0289, 71.0133	<i>6-Hydroxyluteolin 7-O-rhamnoside</i>	<i>Flavonoids</i>	<i>Flavones</i>
49.	9.789	595.1669	C ₂₇ H ₃₂ O ₁₅	0.25	89.67	287.0555, 135.0082	<i>Eriocitrin</i>	<i>Flavonoids</i>	<i>Flavanones</i>
50.	10.122	303.0517	C ₁₅ H ₁₂ O ₇	0.6	98.41	229.0492, 178.9978	<i>Dihydroquercetin</i>	<i>Flavonoids</i>	<i>Dihydroflavonols</i>
51.	10.406	611.1476	C ₂₇ H ₃₁ O ₁₆	1.55	95.06	177.0399, 131.0344	<i>Cyanidin 3-O-sophoroside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
52.	10.567	431.0992	C ₂₁ H ₂₀ O ₁₀	0.6	76.39	385.0923	<i>3-Methoxynobiletin</i>	<i>Flavonoids</i>	<i>Flavonols</i>
53.	10.575	433.11347	C ₂₁ H ₂₁ O ₁₀	-3.52	89.94	121.0284, 137.0233	<i>Isopeonidin 3-O-arabinoside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
54.	10.806	463.0892	C ₂₁ H ₂₀ O ₁₂	0.93	97.43	301.0388, 243.0328	<i>Isoquercetin</i>	<i>Flavonoids</i>	<i>Flavonols</i>
55.	10.833	482.1004	C ₂₁ H ₂₂ O ₁₃	0.27	98.76	263.0561, 137.0244, 109.0295	<i>Epigallocatechin 3'-O-glucuronide</i>	<i>Flavonoids</i>	<i>Flavanols</i>
56.	10.906	177.0197	C ₉ H ₆ O ₄	0.42	93.19	133.0213, 105.1213, 89.4351	<i>Esculetin</i>	<i>Other polyphenols</i>	<i>Hydroxycoumarins</i>
57.	11.123	740.2155	C ₃₃ H ₄₀ O ₁₉	1.03	83.97	283.0242, 219.086, 135.0082	<i>Kaempferol 3-O-xylosyl-rutinoside</i>	<i>Flavonoids</i>	<i>Flavonols</i>
58.	11.175	403.10291	C ₂₀ H ₁₉ O ₉	-3.47	88.25	99.0082, 113.0238	<i>Pelargonidin 3-O-arabinoside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
59.	11.356	258.0892	C ₁₅ H ₁₄ O ₄	2.38	93.15	119.0502, 109.0295, 93.0345, 77.0396	<i>3',4',7-Trihydroxyisoflavan</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
60.	11.506	147.0453	C ₉ H ₈ O ₂	0.08	99.53	147.0446, 145.8880, 102.9346	<i>Cinnamic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
61.	11.806	624.1627	C ₂₈ H ₃₂ O ₁₆	0.97	97.42	357.0621, 163.0606	<i>Isorhamnetin 3-O-glucoside 7-O-rhamnoside</i>	<i>Flavonoids</i>	<i>Flavonols</i>
62.	12.189	432.1043	C ₂₁ H ₂₀ O ₁₀	0.45	98.95	323.0563, 284.0662	<i>Apigenin 6-C-glucoside</i>	<i>Flavonoids</i>	<i>Flavones</i>

63.	12.189	477.1043	C ₂₂ H ₂₂ O ₁₂	0.45	98.95	151.0036, 109.0295	<i>Hesperetin 3'-O-glucuronide</i>	<i>Flavonoids</i>	<i>Flavanones</i>
64.	12.199	450.1039	C ₂₁ H ₂₂ O ₁₁	0.41	99.51	285.0421, 175.0575, 125.0263	<i>Dihydroquercetin 3-O-rhamnoside</i>	<i>Flavonoids</i>	<i>Dihydroflavonols</i>
65.	12.324	597.1455	C ₂₆ H ₂₉ O ₁₆	0.57	86.28	87.0082, 117.0187	<i>Delphinidin 3-O-sambubioside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
66.	12.439	258.2591	C ₁₅ H ₁₂ O ₅	0.18	98.1	163.04, 145.0295	<i>3',4',7-Trihydroxyisoflavanone</i>	<i>Flavonoids</i>	<i>Isoflavonoids</i>
67.	12.506	178.0556	C ₁₀ H ₁₀ O ₃	-0.26	96.87	133.06533, 115.0547, 91.0547	<i>Mellein</i>	<i>Other polyphenols</i>	<i>Hydroxycoumarins</i>
68.	12.748	609.181	C ₂₈ H ₃₄ O ₁₅	-1.15	91.61	260.0623, 224.0495, 150.0315	<i>Hesperidin</i>	<i>Flavonoids</i>	<i>Flavanones</i>
69.	12.856	151.04	C ₈ H ₈ O ₃	-0.08	87	151.0395, 107.0497	<i>2-Hydroxyphenylacetic acid</i>	<i>Phenolic acids</i>	<i>Hydroxyphenylacetic acids</i>
70.	13.198	318.0295	C ₁₅ H ₁₀ O ₈	-0.77	82.96	165.0496, 151.9063	<i>Myricetin</i>	<i>Flavonoids</i>	<i>Flavonols</i>
71.	13.434	602.4335	C ₄₀ H ₅₈ O ₄	1.21	89.67	177.0187, 313.2531	<i>Gamma oryzanol</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
72.	14.32	609.1608	C ₃₁ H ₂₉ O ₁₃	1.11	88.7	103.0395, 129.0551	<i>Peonidin 3-O-(6''-p-coumaroyl-glucoside)</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
73.	14.84	301.0357	C ₁₅ H ₁₀ O ₇	0.29	85.24	166.9980, 123.0082	<i>6-Hydroxyluteolin</i>	<i>Flavonoids</i>	<i>Flavones</i>
74.	14.942	402.3946	C ₂₂ H ₂₄ O ₉	-0.99	90.06	386.1247, 284.0833	<i>3-Methoxysinensetin</i>	<i>Flavonoids</i>	<i>Flavonols</i>
75.	14.942	358.1052	C ₁₉ H ₁₈ O ₇	-2.99	80.06	327.0868, 243.0293	<i>Gardenin B</i>	<i>Flavonoids</i>	<i>Flavones</i>
76.	14.973	136.0508	C ₈ H ₈ O ₂	-0.01	86.28	136.04763, 134.89358, 108.0204, 92.0492	<i>Phenylacetic acid</i>	<i>Phenolic acids</i>	<i>Hydroxyphenylacetic acids</i>
77.	15.273	151.0755	C ₉ H ₁₂ O ₂	-0.94	82.67	121.0653, 89.0391	<i>4-Ethylguaiaicol</i>	<i>Other polyphenols</i>	<i>Alkylmethoxyphenols</i>
78.	15.35	611.1612	C ₂₇ H ₃₁ O ₁₆	0.65	88.93	103.0395, 131.0344	<i>Cyanidin 3,5-O-diglucoside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
79.	15.47	609.18195	C ₂₈ H ₃₃ O ₁₅	0.27	88.19	87.0446, 103.0395	<i>Peonidin 3-O-rutinoside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>

80.	15.508	271.06	C ₁₆ H ₁₆ O ₄	-1.28	93.68	225.0551, 123.0451	4',7-Dihydroxy-3'-methoxyisoflavan	Flavonoids	Isoflavonoids
81.	15.723	269.0459	C ₁₅ H ₁₀ O ₅	0.38	99.29	224.0496, 135.0076, 119.0129	3',4',7-Trihydroxyisoflavone	Flavonoids	Isoflavonoids
82.	15.746	471.9983	C ₂₃ H ₂₀ O ₁₁	-2	70.7	287.0561, 123.0451	4''-O-Methylepigallocatechin 3-O-gallate	Flavonoids	Flavanols
83.	15.79	301.0718	C ₁₆ H ₁₄ O ₆	0.08	99.19	243.0297, 196.0011, 151.0042	Hesperetin	Flavonoids	Flavanones
84.	15.79	256.0718	C ₁₅ H ₁₂ O ₄	0.08	99.19	213.0554, 151.0037	Pinocembrin	Flavonoids	Flavanones
85.	16.023	329.0673	C ₁₇ H ₁₄ O ₇	0.62	98.55	271.0242, 147.0082	3,7-Dimethylquercetin	Flavonoids	Flavonols
86.	16.03	288.0654	C ₁₅ H ₁₂ O ₆	-1.17	94.69	151.0395, 109.0289, 83.0133	Eriodictyol	Flavonoids	Flavanones
87.	16.03	329.0655	C ₁₆ H ₁₄ O ₆	-1.3	94.93	243.0293, 149.0238, 107.0133, 91.0183	Homoeriodictyol	Flavonoids	Flavanones
88.	16.09	254.0563	C ₁₅ H ₁₀ O ₄	0.25	99.09	534.0665, 508.1121, 254.0539	7,4'-Dihydroxyflavone	Flavonoids	Flavones
89.	16.09	563.1155	C ₂₉ H ₂₄ O ₁₂	-3.9	82.77	517.0770, 129.0551	Theaflavin	Flavonoids	Flavanols
90.	16.64	315.0511	C ₁₆ H ₁₂ O ₇	0.07	86.81	299.0442, 271.9578, 216.9417, 189.0253	Isorhamnetin	Flavonoids	Flavonols
91.	16.076	621.1091	C ₂₇ H ₂₅ O ₁₇	0.59	89.09	109.0284, 135.0076	Cyanidin 3-O-(3'',6''-O-dimalonyl-glucoside)	Flavonoids	Anthocyanins
92.	16.793	463.1240	C ₂₂ H ₂₃ O ₁₁	-4.95	84.57	121.0284, 145.0495	Isopeonidin 3-O-galactoside	Flavonoids	Anthocyanins

93.	16.823	313.0772	C ₁₇ H ₁₄ O ₆	0.01	73.75	313.0712, 243.0293, 173.0238, 67.0183	<i>Cirsimaritin</i>	<i>Flavonoids</i>	<i>Flavones</i>
94.	18.722	356.3246	C ₁₆ H ₂₀ O ₉	0.37	98.01	175.0395, 163.0395, 161.0238	<i>1-O-feruloyl-beta-D-glucose</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>
95.	20.106	496.1217	C ₂₂ H ₂₄ O ₁₂	0.71	89.87	289.0717, 181.0506	<i>4'-O-Methyl(-)-epicatechin 3'-O-glucuronide</i>	<i>Flavonoids</i>	<i>Flavanols</i>
96.	20.722	353.1427	C ₂₁ H ₂₂ O ₅	3.25	81.6	353.1438, 233.0848	<i>Isoxanthohumol</i>	<i>Flavonoids</i>	<i>Flavanones</i>
97.	20.943	610.15338	C ₂₇ H ₃₀ O ₁₆	-8.26	87.19	101.0238, 119.0344	<i>Cyanidin 3-O-sophoroside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
98.	22.027	627.1561	C ₂₇ H ₃₁ O ₁₇	0.26	89.87	89.0238, 161.0449	<i>Delphinidin 3,5-O-diglucoside</i>	<i>Flavonoids</i>	<i>Anthocyanins</i>
99.	22.274	338.1008	C ₁₆ H ₁₈ O ₈	1.51	88.6	221.2218, 191.0575, 163.0392, 119.0504	<i>p-Coumaroylquinic acid</i>	<i>Phenolic acids</i>	<i>Hydroxycinnamic acids</i>

Table S3. ADME properties of the abundant red rice phenolic metabolites.

Molecule	MW (< 500 Da)	Lipinski's rule			Water solubility (ESOL)		GI absorption	Bioavailability Score
		LOG P (< 5)	H-bond donors (< 5)	H-bond acceptors (< 10)	Log S	Class		
1-O-feruloyl- β -D-glucose	356.32	1.68	5	9	-1.64	Very soluble	Low	0.55
3',4',7-Trihydroxyisoflavone	362.32	2.65	1	8	-4.28	Moderately soluble	High	0.55
3-methylcatechol	124.14	0.98	2	2	-2.25	Soluble	High	0.55
3'-O-Methylviolanone	330.33	2.79	1	6	-3.65	Soluble	High	0.55
4-Hydroxybenzaldehyde	122.12	0.99	1	2	-1.87	Very soluble	High	0.55
4'-Methyl-epigallocatechin 3'- O-glucuronide	496.42	1.08	8	13	-2.73	Soluble	Low	0.11
4'-O-Methyl(-)-epicatechin 3'- O-glucuronide	480.42	1.04	7	12	-2.87	Soluble	Low	0.11
Apigenin 6-C-glucoside	432.38	1.94	7	10	-2.84	Soluble	Low	0.55
Benzoic acid	122.12	1.11	1	2	-2.2	Soluble	High	0.85
Catechin	290.27	1.47	5	6	-2.22	Soluble	High	0.55
Cirsimaritin	314.29	2.56	2	6	-4.2	Moderately soluble	High	0.55
Dihydroquercetin	304.25	1.3	5	7	-2.66	Soluble	High	0.55
Hesperidin	610.56	2.6	8	15	-3.28	Soluble	Low	0.17
Isoquercetin	464.38	2.11	8	12	-3.04	Soluble	Low	0.17
Isorhamnetin	316.26	2.35	4	7	-3.36	Soluble	High	0.55
Isorhamnetin 3-O-glucoside 7- O-rhamnoside	624.54	3.7	9	16	-3.73	Soluble	Low	0.17
Isoxanthohumol	354.4	3.06	2	5	-4.69	Moderately soluble	High	0.55
Mellein	178.18	1.96	1	3	-2.82	Soluble	Low	0.11
Naringin 4'-glucoside	742.68	4.21	11	19	-2.61	Soluble	Low	0.17
Sinensetin	372.37	3.66	0	7	-4.4	Moderately soluble	High	0.55