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Metabolomics analysis of mangosteen (*Garcinia mangostana* Linn.) fruit pericarp using different extraction methods and GC-MS

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Supplementary Table 1. Identified metabolites from mangosteen fruit pericarp at the final stage of ripening (dark purple colour) using a GC-MS analysis. The samples were extracted using five different extraction methods; Method 1: methanol acidified with formic acid, Method 2: methanol/chloroform/water with ratio o f 2:1:2, Method 3: methanol/chloroform/water with ratio of 2:1:2 assisted with sonication, Method 4: methanol/chloroform/water with ratio of 3:1:1 and Method 5: methanol/chloroform/water with ratio of 3:1:1 assisted with sonication. KEGG ID represents a code for each metabolite in the KEGG biosynthetic pathway. Relative peak area was calculated from initial sample weight and normalized using D-mannose. SD, standard deviation; nd, not detected

Class	Metabolites	KEGG ID	Relative Peak Area ± SD				
			Method 1	Method 2	Method 3	Method 4	Method 5
Sugar	2-Deoxy-galactopyranose	C00124	nd	nd	nd	nd	7.5105 ± 3.94
	Arabinofuranose	C06115	9.1110 ± 5.26	nd	414.7957 ± 237.79	nd	104.5254 ± 58.24
	Arabinose	C00259	nd	0.04490 ± 0.03	nd	nd	61.5461 ± 30.62
	D-Fructose	C00095	16.7760 ± 7.63	25.0694 ± 6.21	55.2019 ± 30.18	39.9064 ± 17.73	54.8634 ± 12.01
	D-Galactose	C00124	205.3409 ± 114.84	1.4938 ± 0.49	5.8186 ± 3.16	9.9933 ± 5.32	10.1579 ± 2.62
	D-Glucose	C00031	1.0169 ± 0.59	11.6023 ± 4.08	21.6714 ± 7.63	409.6600 ± 235.53	2.2727 ± 1.15
	D-Mannose	C00159	249.6622 ± 142.68	0.0195 ± 0.01	1.5973 ± 0.80	0.0972 ± 0.05	189.1221 ± 100.39
	Dihydroxyacetone dimer	-	nd	nd	nd	nd	3.5698 ± 2.06
	D-Ribofuranose	C16639	nd	nd	121.2284 ± 69.99	nd	5.1522 ± 2.64
	D-Ribose	C00121	2.6853 ± 1.38	116.0368 ± 66.31	7.8612 ± 3.94	1.3585 ± 0.59	10.7110 ± 3.79
	D-Turanose	C19636	nd	nd	283.1452 ± 163.47	nd	nd
	D-Xylofuranose	-	nd	nd	nd	nd	3.4055 ± 1.74
	D-Xylopyranose	-	nd	0.0408 ± 0.02	112.3784 ± 64.87	0.0347 ± 0.02	nd
	D-Xylose	C00181	0.2410 ± 0.14	27.0840 ± 15.43	12.4532 ± 7.19	0.0543 ± 0.03	153.0057 ± 86.32

	Erythrose	C01796	nd	nd	0.2504 ± 0.13	nd	nd
	Glucofuranoside	-	nd	nd	nd	0.0768 ± 0.04	10.1610 ± 1.85
	Glucopyranose	-	nd	nd	10.6770 ± 5.44	nd	12.6349 ± 4.10
	Glycoside	-	nd	nd	nd	nd	1.0009 ± 0.52
	Gulose	C15923	nd	nd	1298.6308 ± 749.76	nd	nd
	Inososе	-	nd	nd	0.2359 ± 0.14	nd	nd
	Lyxopyranoside	-	nd	nd	nd	nd	117.3190 ± 67.73
	Lyxose	C01508	nd	0.0297 ± 0.02	10.1244 ± 5.85	nd	nd
	Mannopyranose	C21056	nd	nd	nd	nd	11.9671 ± 6.91
	Sorbopyranose	-	nd	nd	438.1043 ± 252.94	nd	nd
	Talose	C06467	nd	nd	nd	nd	167.9375 ± 84.25
	α-D-Galactofuranoside	-	nd	0.0242 ± 0.01	nd	nd	nd
	α-D-Glucopyranoside	-	292.8833 ± 169.10	nd	1241.0133 ± 620.99	6.7862 ± 3.92	588.6889 ± 339.88
	α-DL-Arabinopyranose	C00259	nd	nd	nd	0.1207 ± 0.06	3.3432 ± 1.93
	α-DL-Lyxofuranoside	-	2.6625 ± 1.54	nd	nd	nd	nd
	α-DL-Lyxopyranose	-	nd	nd	nd	0.0399 ± 0.02	nd
	α-D-Mannopyranoside	-	nd	nd	nd	nd	985.6240 ± 569.05
	α-l-Galactofuranoside	-	2.9906 ± 1.73	nd	nd	nd	nd
	α-L-Mannofuranose	-	nd	nd	nd	nd	1.1823 ± 0.68
	β-DL-Lyxofuranoside	-	0.1624 ± 0.09	nd	nd	nd	nd
	β-D-Mannopyranoside	-	nd	0.0439 ± 0.02	nd	nd	nd
	β-l-Galactopyranoside	-	nd	nd	nd	nd	238.8975 ± 137.93
Sugar acids							
	β-D-Galactopyranosiduronic acid	-	nd	nd	0.1739 ± 0.1	nd	nd
	2-Keto-d-gluconic acid	C06473	nd	nd	834.9214 ± 482.04	nd	nd
	Gluconic acid	C00257	0.6254 ± 0.36	nd	nd	nd	nd
	Mannonic acid	-	nd	0.0259 ± 0.01	nd	nd	nd
	Pentonic acid	-	nd	nd	nd	nd	14.7932 ± 8.31
	Ribonic acid	C01685	nd	9.0426 ± 5.22	nd	nd	nd

Organic acids	Butanedioic acid	C00042	nd	0.4687 ± 0.26	nd	nd	nd
	Malic acid	C00149	nd	0.0344 ± 0.02	3.2093 ± 1.80	nd	7.5619 ± 1.03
	Methylmaleic acid	C02226	nd	nd	0.4383 ± 0.25	nd	nd
	Propanedioic acid	C00383	nd	nd	2.3975 ± 1.38	nd	nd
	L-(+)-Tartaric acid	-	nd	0.1632 ± 0.09	0.5778 ± 0.33	nd	nd
Phenolic compounds	Salicylic acid	C00805	12.9489 ± 7.48	nd	nd	nd	nd
	3,4-dihydroxybenzoic acid	C00230	28.7896 ± 16.62	nd	nd	nd	nd
	4-Hydroxyphenylethanol	C06044	1.9647 ± 1.13	nd	nd	nd	nd
	Benzoic acids	C00180	1.1622 ± 0.67	nd	nd	nd	nd
Aromatic compounds	2H-1-Benzopyran	-	nd	nd	28.2234 ± 16.29	nd	97.1145 ± 56.07
	Benzaldehyde	C00261	0.7162 ± 0.41	nd	nd	nd	nd
Alcohols	Adonitol	C00474	nd	9.8687 ± 5.7	55.1888 ± 31.86	nd	6.7446 ± 3.89
	Arabinitol	C00532	40.8558 ± 23.59	0.2527 ± 0.11	0.8005 ± 0.41	0.1316 ± 0.08	76.2847 ± 47.34
	Myo-Inositol	C00137	5.1401 ± 2.97	6.7599 ± 2.95	42.4426 ± 21.28	nd	68.3622 ± 21.25
	Pentitol	-	nd	nd	nd	0.6336 ± 0.37	nd
	Phenol	C00146	0.8247 ± 0.48	nd	nd	nd	nd
	Pyrocatechol	C00090	4.4868 ± 2.59	nd	nd	nd	nd
	Threitol	C16884	nd	nd	nd	0.0966 ± 0.06	nd
Aldehyde	Butanal	C01412	31.7555 ± 18.33	0.0505 ± 0.03	0.0648 ± 0.04	nd	nd
Others	Benzene	-	1.0224 ± 0.59	nd	nd	nd	nd
	1,4-Pentadiene	-	0.4472 ± 0.26	nd	nd	nd	nd
	2-Hydroxymandelic acid	-	0.4334 ± 0.25	nd	nd	nd	nd
	2-Pyridinecarboxylic acid	-	nd	0.0218 ± 0.01	nd	nd	nd
	1,4-cyclohexadiene	-	0.5000 ± 0.29	nd	nd	nd	nd
	3-Mercaptobenzoic acid	-	1.1459 ± 0.66	nd	nd	nd	nd
	Cyclopenta-1,3-diene	-	nd	nd	0.3281 ± 0.19	nd	1.3550 ± 0.78
	α,β-L-idopyranuronic acid	-	nd	nd	1.4814 ± 0.86	nd	nd
	Acetamide	-	nd	nd	nd	nd	0.6451 ± 0.37

	Glycerol	-	nd	nd	nd	nd	37.9061 ± 16.47
	Methyl 4-methyl-4-nitroso-pentanoate	-	nd	nd	nd	nd	0.4066 ± 0.23
	Thymol-α-d-glucopyranoside	-	2.5371 ± 1.46	6.7076 ± 2.53	24.4155 ± 12.30	3.5428 ± 2.02	7.4949 ± 4.33

Supplementary Table 2. Venn diagram analysis output showing the list of metabolite extracted from the five different extraction methods. Method 1: methanol acidified with formic acid, Method 2: methanol/chloroform/water with ratio of 2:1:2, Method 3: methanol/chloroform/water with ratio of 2:1:2 assisted with sonication, Method 4: metha nol/chloroform/water with ratio of 3:1:1 and Method 5: methanol/chloroform/water with ratio of 3:1:1 assisted with sonication

Metabolites extraction method	Number of metabolites	Elements
Method 1 Method 2 Method 3 Method 4 Method 5	8	Thymol-α-d-glucopyranoside
		Arabinitol
		D-Glucose
		D-Ribose
		Mannose
		D-Fructose
		D-Xylose
		D-Galactose
Method 1 Method 2 Method 3 Method 5	1	Myo-Inositol
Method 1 Method 3 Method 4 Method 5	2	Arabinofuranose
		α-D-Glucopyranoside
Method 1 Method 2 Method 3	1	Butanal
Method 2 Method 3 Method 4	1	D-Xylopyranose
Method 2 Method 3 Method 5	2	Adonitol
		Malic acid
Method 3 Method 4 Method 5	1	D-Ribofuranose
Method 2 Method 3	2	Lyxose
		L-(+)-Tartaric acid
Method 2 Method 5	1	Arabinose
Method 3 Method 4	1	D-Turanose
Method 3 Method 5	3	2H-1-Benzopyran
		Cyclopenta-1,3-diene
		Glucopyranose
Method 4 Method 5	2	Glucofuranoside
		α-DL-Arabinopyranose
Method 1	16	Gluconic acid
		1,4-cyclohexadiene
		Pyrocatechol
		Benzoic acids
		Benzene
		1,4-Pentadiene
		3,4-dihydroxybenzoic acid
		Benzaldehyde
		Salicylic acid
		β-DL-Lyxofuranoside
		2-Hydroxymandelic acid
		α-DL-Lyxofuranoside
		α-l-Galactofuranoside
		3-Mercaptobenzoic acid
		Phenol
		4-Hydroxyphenylethanol

Method 2	6	Ribonic acid
		Butanedioic acid
		Mannonic acid
		β-D-Mannopyranoside
		2-Pyridinecarboxylic acid
		α-D-Galactofuranoside
Method 3	9	β-D-Galactopyranosiduronic acid
		Sorbopyranose
		Propanedioic acid
		Inososе
		2-Keto-d-gluconic acid
		Gulose
		Erythrose
		α,β-L-idopyranuronic acid
		Methylmaleic acid
Method 4	3	Threitol
		Pentitol
		α-DL-Lyxopyranose
Method 5	14	Lyxopyranoside
		Talose Glycoside
		Mannopyranose
		α-L-Mannofuranose
		Acetamide
		Pentonic acid
		2-Deoxy-galactopyranose
		D-Xylofuranose
		Dihydroxyacetone dimer
		Methyl 4-methyl-4-nitroso-pentanoate
		α-D-Mannopyranoside
		Glycerol
		β-l-Galactopyranoside