

**Table S1. Identified metabolites in C5, C6, and LF muscadine ripe berries.**

NO	Compounds identified in ESI+ mode	Compounds identified in ESI- mode	Compounds identified in ESI- &ESI+ mode
1	Trehalose 6-phosphate	16-Hydroxyhexadecanoic acid	12-Hydroxydodecanoic acid
2	2,4,6-Octatriynoic acid	3,5-Digalloylepicatechin	2-Furoic acid
3	2,5-Furandicarboxylic acid	3-Oxo-hexadecanoic acid	2-Methylbenzoic acid
4	2-Deoxymugineic acid	5-Methoxysalicylic acid	4-Acetamidobutanoic acid
5	2-Furanmethanol	6-Chlorocatechin	4-Dodecylbenzenesulfonic Acid
6	2-Isopropyl citrate	6-Epi-7-isocucurbit acid glucoside	4-Hydroxybenzaldehyde
7	2-Methylnicotinate	7-Methylxanthine	4-Pyridoxic acid
8	2-Methylcitric acid	Aesculin	Abscisic acid
9	3-Hydroxycoumarin	Ascorbic acid	Aconitic acid
10	3,4-Dihydroxymandelic acid	Aucubin	Adipic acid
11	3-O-p-Coumaroylquinic acid	Azelaic acid	Arbutin
12	3-Oxododecanoic acid	beta-D-Glucose 6-phosphate	Asiatic acid
13	3-trans-p-Coumaroylrotundic acid	Caryoptosidic acid	Astilbin
14	4-Guanidinobutanoic acid	Cibacic acid	Caffeic acid
15	4-Hydroxynonenal	Citramalic acid	Caffeoylmalic acid
16	5-Aminolevulinic acid	Citrinin	Catechin
17	5-Hydroxy-2-furoic acid	Cyclodopa glucoside	Chlorogenic acid
18	5-Hydroxyindoleacetic acid	Delphinidin 3-lathyruside 5-glucoside	Cinnamic acid
19	8,8-Methylenbiscatechin	Delphinidin 3-sophoroside	Citric acid
20	9-Oxo-nonanoic acid	Deoxyribose	Cysteine
21	Acetophenone	D-Glucuronic acid	Delphinidin 3-arabinoside
22	Acetylornithine	Diethylmalic acid	Deoxyinosine
23	Adenosine	Epiafzelechin 3-gallate	Dicaffeoylquinic acid
24	Alanine	Epigallocatechin 3,5-di-gallate	Ellagic acid
25	Amidosulfonic acid	Epigallocatechin gallate	Epicatechin-3-gallate
26	Aminobutyric acid	Eujambolin	Epigallocatechin
27	Arecoline	Galactaric acid	Epigallocatechin 3-cinnamate
28	Argininosuccinic acid	Gentisic acid	Epigallocatechin 3-glucuronide
29	Asparagine	Gluconic acid	Fertaric acid
30	Benzaldehyde	Glyceric acid	Ferulic acid
31	Benzophenone	Hesperidin	Fumaric acid
32	Caftaric acid	Hydroxypropionic acid	Galactose
33	Capryloylglycine	Isolimoncic acid	Gallic acid
34	Carvone	Isowertin 2-rhamnoside	Glucobrassicin
35	Citral	Kaempferol 3-xylosylglucoside	Glutamine
36	Coumapherine	Kaempferol 7-(6-galloylglucoside)	Glutathione
37	Coumarin	L-Cystine	Glycyrrhetic acid
38	Cyclamic acid	Liquocoumarin	Guanosine
39	Cyclohexylamine	Lucuminic acid	Isochloretin
40	Cytidine	Luteolin	Isochloretin
41	Daucic acid	Malonic acid	Isoferulic acid 3-O-glucuronide
42	Diaminopimelic acid	Methyl acetate	Isolaricresinol 4-O-beta-D-glucoside
43	Dihydroferulic acid	Methylsuccinic acid	Isorhamnetin 3-(6-malonylglucoside)
44	Dihydrojasmonic acid	Naringin	Itaconic acid
45	Dihydromelilotoside	Neuraminic acid	Jasmonic acid
46	Dihydrosinapic acid	N-Undecylbenzenesulfonic acid	Kaempferol 3-glucuronide
47	Dihydrotestosterone	Oxalacetic acid	L-Arginine
48	Dihydrothymine	Oxalic acid	L-Aspartic acid
49	Dihydrouracil	Phenylacetaldehyde	Lepidimonic acid
50	Dopa	p-Hydroxyphenylacetic acid	L-Glutamic acid
51	Dopamine glucuronide	Piceid	L-Histidine
52	Eicosadienoic acid	Pimelic acid	Limocitrin 3-rutinoside
53	Eicosapentaenoic acid	Pyruvic acid	Linamarin

54	Epidermin	Retinoic acid	Linoleic acid
55	Epsilon-caprolactam	Rhamnazin 3-rutinoside	L-Leucine
56	Erucic acid	S-Lactoylglutathione	L-Phenylalanine
57	Erythrose	Stearic acid	L-Quebrachitol
58	Ethyl lactate	Suberic acid	L-Threonine
59	Ethyl oleate	Sucralose	L-Tyrosine
60	Folinic acid	Tartaric acid	Luteone
61	Fukiic acid	Threonic acid	Malic acid
62	Furaneol	Troloxerutin	Medicagenic acid
63	gamma-Glutamylleucine	Undecanedioic acid	Mevalonic acid
64	Glucogallin	Ureidopropionic acid	Monobutylphthalate
65	Glucosamine	Uridine 5-diphosphate	Myricetin
66	Glucose 1-phosphate	Vanillic acid 4-O-sulfate	Myricetin 3-galactoside
67	Glutaric acid	Xanthylic acid	Myrsinone
68	Glycerol 3-phosphate		N-Acetyl-L-glutamic acid
69	Glycerophosphocholine		Naringenin
70	Guaiacol		Neoglucobrassicin
71	Guanine		N-Undecanoylglycine
72	Heptanal		Oleanolic acid
73	Hexanal		Ornithine
74	Histamine		Oxoadipic acid
75	Homomethionine		Oxoglutaric acid
76	Indole		Pantothenic acid
77	Indole-3-carboxaldehyde		Phaseolic acid
78	Isobutyric acid		Phloretin
79	Isorhamnetin		Phosphate
80	Isovanillic acid		Phosphoenolpyruvic acid
81	Kaempferol		Phthalic acid
82	Kojic acid		Piscidic acid
83	Kynurenic acid		Procyanidin B1
84	Lactosamine		Procyanidin C1
85	L-Agaritine		Protohypericin
86	Levulinic acid		Punicic acid
87	Linoleamide		Pyrocatechol
88	Linoleic acid		Pyroglutamic acid
89	Linoleoyl ethanolamide		Quercetin
90	L-Methionine		Quercetin 3-(6-malonyl-glucoside)
91	Lysine		Quercetin 3-arabinoside
92	Methionine sulfoxide		Quercetin 4-glucoside
93	Methyl cinnamate		Quinic acid
94	Muramic acid		Rutin
95	N-Acetylneuraminic acid		Salicylic acid
96	N-Acetylserotonin		Scopoletin
97	N-Acetylvaline		Serine
98	Neocnidilide		Shikimic acid
99	N-Glycolylneuraminic acid		Sinapic acid
100	Niacinamide		Succinic acid
101	Nicotinic acid		Syringic acid
102	N-Undecanoylglycine		Tocopheronic acid
103	Octadecanamide		Traumatic acid
104	Octadecylamine		Trehalose
105	Oleamide		Trifolin
106	Oleoylethanolamide		Tryptophan
107	Olopatadine		Uridine
108	Palmitic amide		
109	Palmitoleylethanolamde		

110	Panthenol		
111	Pantoyllactone glucoside		
112	p-Coumaric acid		
113	p-Cresol		
114	p-Cymene		
115	Pelargonidin 3-rhamnoside		
116	Penmacric acid		
117	Phenol		
118	Phenylethylamine		
119	Phenylglyoxylic acid		
120	Phosphoglycolic acid		
121	Phosphohydroxypyruvic acid		
122	Phytosphingosine		
123	Pipecolic acid		
124	Piperidine		
125	Pirbuterol		
126	Proanthocyanidin A2		
127	Proline		
128	Prostaglandin B1		
129	protocatechuic acid		
130	Pubescenol		
131	Pyridoxal		
132	Pyruvic acid		
133	Quinolinic acid		
134	Quinone		
135	Resveratrol		
136	Rhamnitol		
137	Rutagravine		
138	Sebacic acid		
139	Spermidine		
140	Sphinganine		
141	Sphingosine		
142	Stearidonic acid		
143	Styrene		
144	Succinylacetone		
145	Targinine		
146	Taurine		
147	Theaflavic acid		
148	Thymine		
149	Tiglic acid		
150	Tridecanoic acid		
151	Triethylamine		
152	Tyrosine methylester		
153	Tyrosol		
154	Urocanic acid		
155	Valine		
156	Valylproline		
157	Vanillin		