Table S1. Detection of secondary metabolites in fermented wheatgrass juice using LC-MS-MALDI-TOF/TOF and their characteristics

RT	Observed m/z value	Metabolite detected	Identity of compound	Activities	References (Compound identity)	References (Biological property)
1.4	122.9	M+H	2,4- Dimethylphenol	Anti-oxidant	[1]	[2]
30.6	149.0	M+H	Cinnamic acid	Anti-cancer Anti-diabetic Anti-microbial Cardioprotective Hepatoprotective Neuroprotective	[3]	[4]
1.3	170.9	M-H	Gallic acid	Anti-cancer Anti-oxidant	[5]	[6]
1.3	182.9	$M+NH_4$	Eugenol	Anti-inflammatory	[7]	[7]
27.0	191.0	M-H	Quinic acid	Anti-diabetic Anti-inflammatory Anti-oxidant	[8]	[9]
1.4	198.9	Fragment M+3H	2-Methyl 4,6- dinitrophenol, Hydroxymethoxydimethyl benzoic acid	Anti-oxidant Anti-inflammatory	[1,10]	[11]
30.6	245.0	M-H Fragment Fragment Fragment Fragment Fragment Fragment Fragment	3-or 4-Hydroxyphenyl propionic acid sulphate, Catechin, Catechin gallate, Epicatechin, Epicatechin gallate, Procyanidin B1, Procyanidin B2, Prodelphinidin A	Anti-cancer Anti-diabetic Anti-inflammatory Anti-oxidant Anti-tumorigenic	[12,13]	[14]
19.0	246.2	M-H	Vanillic acid 4-sulfate	Anti-inflammatory Anti-oxidatnt Neuroprotective	[15]	[16]
1.4	257.1	Fragment	Ellagic acid	Anti-oxidant	[17]	[18]
33.3	271.2	Fragment	Pinobanksin arabinose	Anti-bacterial Anti-inflammatory Anti-oxidant Anti-parasitic Anti-proliferative Immunomodulatory	[19]	[20]
33.3	272.2	M+H	Piperyline	Anti-cancerous Anti-tumorigenic	[21]	[21]
21.8	274.2	M+3H	Pelarogonidin	Anti-oxidant Anti- cancerous	[22]	[22]
21.8	275.2	M-H	Dihydroxyferulic acid sulphate	Anti-cancer Anti-diabetic Anti-inflammatory Anti-microbial Anti-oxidant	[12]	[23]
1.6	277.0	M+H	Linoleic acid isomer 1 or 2	Anti-atherogenic Anti-cancer	[24]	[25]
34.6	282.2	M+2H	Rhein	Anti-cancer Anti-inflammatory Anti-microbial Anti-oxidant	[26]	[27]

1.4	288.9	M+H	Fraxetin-7-O-sulfate	Anti-bacterial Anti-osteoporosis Anti-oxidant	[10]	[28]
18.9	291.2	M+H	Catechin	Anti-inflammatory Growth inhibitory	[10]	[14]
30.6	301.1	Fragment M-3H	Delphinidin-3-glucoside, Quercetin	Anti-bacterial Anti-inflammatory Anti-oxidant Anti-viral Gastroprotective Immunomodulatory	[13]	[29]
30.6	302.2	M+H Fragment Fragment Fragment Fragment	Peonidin, Peonidin-3-O-glucoside, Peonidin-3-O-rutinoside-5-glucoside, Peonidin-3-O-sambioside-5-O-glucoside, Peonidin-3-O-rutinoside	Anti-bacterial Anti-inflammatory Anti-oxidant Anti-viral Gastroprotective Immunomodulatory	[13,10]	[29]
30.6	303.3	Fragment M-H Fragment Fragment	Myricetin-3-O-glucoside, Taxifolin, Taxifolin-O-pentoside, Taxifolin-3-O-rhamnoside	Anti-bacterial Anti-inflammatory Anti-oxidant Anti-viral Gastroprotective Immunomodulatory	[13]	[29]
26.4	315.1	Fragment M-H Fragment M-H	Malvidin-3-(6-O-acetyl) glucoside, Protocatechuic acid 4-O-glucoside, Petunidin-3-O-glucoside, Violanone	Anti-ageing Anti-asthmatic Anti-athrogenic Anti-bacterial Anti-cancer Anti-diabetic Anti-inflammatory Anti-oxidant Anti-tumorigenic Anti-ulcer Neuroprotective	[13,30]	[31]
27.0	319.0	M+H Fragment	Myricetin, Riboflavin	Anti-cancer Anti-oxidant Anti-viral	[3]	[22]
26.0	330.3	Fragment	Syringetin 3-O-hexoside	Anti-bacterial Anti-inflammatory Anti-oxidant	[32]	[33]
26.0	331.3	M+H M+H Fragment Fragment M-H M-H	Cirsiliol, Tricin, Malvidin-3-rutinoside, Malvidin-acetyl-glucoside, Carnosic acid, Gallic acid 4-O-glucoside	Anti-inflammatory Anti-neoplastic Anti-oxidant Cardioprotective Neuroprotective	[10,34,35]	[6,22]
26.4	337.1	M-H	3-p-Coumaroylquinic acid	Anti-inflammatory Anti-microbial Cardioprotective	[36]	[37]
35.1	338.3	Fragment	Ferulic acid	Anti-cancer Anti-diabetic Anti-inflammatory Anti-microbial Anti-oxidant	[38]	[23]

37.5	339.3	M-H M+H	8-Prenylnaringenin, Docosenoic acid	Anti-cancer Anti- inflammatory Anti-microbial Anti-oxidant Anti-viral	[10,39]	[40,41]
27.0	341.0	M-H Fragment M+H M+H	1-O-Caffeoyl glucose, 1-O-Sinapoyl-β-D-glucose, 8-Prenylnaringenin, Esculin	Anti-cancer Anti-inflammatory Anti-oxidant Anti-viral	[13,36]	[42]
32.4	343.1	M+H	Malabaricone B	Anti-inflammatory Anti-microbial	[7]	[7]
23.9	346.3	Fragment	Pallidol	Anti-microbial Anti-oxidant	[13]	[43]
1.3	347.0	M+H	Syringetin	Anti-oxidant	[22]	[44]
1.3	348.0	$M+NH_4$	Dihydroguaiaretic acid	Anti-oxidant	[7]	[7]
18.9	351.2	M-H M-H	Trihydroxy-ent-kauranoic acid, Naringenin sulfate	Anti-bacterial Anti-cancer Anti-convulsant Anti-inflammatory Anti-leishmania Anti-mutagenic	[45,46]	[47,48]
19.0	353.2	M-H M-H	3-Caffeoylquinic acid, Chlorogenic acid	Anti-bacterial Anti-helminthic	[15,49]	[50]
33.7	357.2	M-H	Dihydrocaffeic acid 3-O-glucuronide	Anti-oxidant	[15]	[51]
27.0	358.2	Fragment	Avenasterol	Anti-diabetic Anti-inflammatory Cardioprotective	[10]	[52]
27.0	360.2	$M+NH_4$	Austrobailignan-7	Anti-inflammatory Anti-oxidant Anti-tumorigenic	[7]	[7]
1.6	365.1	M+Na Fragment	Austrobailignan-7, Phloretin-3',5-di-C-β-glucoside	Anti-inflammatory Anti-oxidant Anti-tumorigenic Anti-viral Immunosuppressive Cardioprotective	[7,53]	[7]
25.4	375.3	Fragment	Pentahydroxytrimethoxy flavone	Anti-angiogenic Anti-fungal Anti-tumorigenic Anti-viral Immunomodulatory	[10]	[54]
1.6	381.0	M+H	Pentacosenoic acid	Anti-microbial Anti- thrombotic	[10]	[55]
1.3	391.1	M+H	Monotropein	Anti-apoptotic Anti-catabolic Anti-fungal Anti-inflammatory Anti-nociceptive Anti-oxidant	[7]	[7]
34.6	395.3	M+Na Fragment	1-(2,6-Dihydroxypheny l)-9-(4-hydroxy-3-methoxy phenyl), Catechin gallate	Anti-angiogenic Anti-melanogenic Anti-oxidant Anti-plasmodic	[7,13]	[56]
34.6	399.2	M+H	Campestenone	Anti-cancerous Anti-diabetic Anti-inflammatory	[10]	[57]

35.1	406.3	$M+NH_4$ Fragment	Fragransin D1, Pallidol	Anti-microbial Anti-oxidant	[7,13]	[43]
30.9	413.2	M+H M+H Fragment	Avenasterol, Fucosterol, Apigenin-7-O-glucoside	Anti-diabetic Anti-inflammatory Cardioprotective	[10,13]	[52]
28.5	414.2	Fragment	Malvidin 3-O-glucoside-4-vinylphenol	Anti-ageing Anti-asthmatic Anti-atherogenic Anti-bacterial Anti-cancer Anti-diabetic Anti-inflammatory Anti-oxidant Anti-tumorigenic Anti-ulcer Neuroprotective	[32]	[31]
24.4	415.2	M-H	Deoxyschisandrin	Anti-cancerous Anti-inflammatory	[30]	[58]
33.7	427.2	M+H Fragment	β-Amyrin, trans-Scirpusin A	Anti-microbial Anti-obesity Anti-parasitic Anti-tumorigenic	[10,13]	[59,60]
33.7	429.2	Fragment	Pinocembrin-O-arabirosyl-glucoside	Anti-cancer Anti-inflammatory Anti-microbial Anti-oxidant	[61]	[62]
34.6	431.1	M-H	Apigenin 6-C-glucoside	Anti-inflammatory Anti-mutagenic Anti-oxidant Anti-viral	[15]	[52]
24.4	437.1	M+H Fragment Fragment Fragment	Phlorizin, Ampelosin D, α-Viniferin, Procyanidin dimer gallate	Anti-inflammatory Anti-microbial Anti-oxidant	[10,13]	[63]
38.8	449.7	M-H M+H	Myricetin 7-O-pentoside, Luteolin-8-C-glucoside	Anti-cancer Anti-inflammatory Anti-osteoporosis Anti-oxidant Anti-thrombotic Cardioprotective	[10,32]	[64]
38.8	453.1	M-H M+H	p-Coumaroyl-hexoside-methylglutarate, Vebonol	Anti-cancer Anti-diabetic Anti-inflammatory Anti-oxidant	[10,65]	[66]
1.4	458.8	M-H	Neotigogenin acetate	Anti-cancer	[5]	[67]
30.0	463.3	Fragment M-H	Peonidin-3-O-rutinoside, Myricetin 3-O-rhamnoside	Anti-Alzheimer's Anti-inflammatory Anti-Parkinson's	[10,30]	[68,69]
24.4	467.1	M+H	Taxifolin-3-O-glucoside	Anti-oxidant	[10]	[70]
33.7	521.3	M-H	Salviaflaside derivatives	Anti-inflammatory	[46]	[71]
1.6	527.1	M+H M-H	Gibberellin acid 8-hexose-gibberellin, Naringenin glucuronide sulfate	Anti-oxidant	[10,45]	[72]
18.9	549.1	M-H	Quercetin-7-O-malonylhexoside	Anti-angiogenic Anti-inflammatory Anti-oxidant Anti-tumorigenic	[65]	[73]

30.0	551.3	M+H	Quercetin 3-O-(6'-malonyl-glucoside), Betanin	Anti-angiogenic Anti-inflammatory Anti-oxidant Anti-tumorigenic	[30]	[73]
33.7	569.5	M+H	Zeaxanthin	Anti-oxidant Anti-inflammatory	[10]	[74]
34.6	573.4	M-H	Viniferal	Neuroprotective	[13]	[75]
30.0	595.3	M-H M+H	Neoeriocitrin, Chrysoeriol C-hexoside-C-pentoside	Anti-oxidant Anti-inflammatory	[10,30]	[61]
1.4	598.8	M-H	Spermidine- N5,10-di-p-coumaric acid-N1-caffeic acid	Anti-fungal Anti-oxidant	[19]	[76]
30.9	614.3	M-H	Spermidine- N1,10-di-caffeic acid-N5-p-coumaric acid	Anti-fungal Anti-oxidant	[19]	[76]
30.0	639.4	M-H	Laricitrin-3-O-rutinose	Anti-allergic Anti-inflammatory Anti-microbial Anti-oxidant	[8]	[77]
30.0	640.4	M+H	Malvidin 3-O-rutinoside	Anti-inflammatory Anti-oxidant	[10]	[22]
1.4	717.9	M+2H	Salvianolic acid B isomer 1 or 2	Anti-cancer Anti-inflammatory Anti-oxidant Cardioprotective	[24]	[28]
30.0	727.4	Fragment	Kaempferol-rha-xyl-gal	Anti-oxidant	[78]	[79]
1.4	758.7	M+H	Peonidin 3-O-sambioside-5-O-glucoside	Anti-oxidant Anti-tumorigenic Cardioprotective	[30]	[80]
34.6	771.4	M+H	6-C-hexosyl-chrysoeriol-O-rhamnoside-O-hexoside	Anti-cancer Anti-inflammatory Anti-microbial Anti-osteoporosis Anti-insect Neuroprotective	[10]	[81]
30.9	805.5	Fragment	Malvidin-3-glucoside-4-vinyl (epi) catechin	Anti-inflammatory Anti-oxidant	[82]	[22]

RT- Retention time

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