

Supplementary Table S7

Putatively identified metabolites that were statistically significantly different between DH and ACE seeds treated with PEG for 4 weeks.

Putative ID	Target Mass	Formula	Metabolite Class	Error	Detected Mass	Analysis Mode	ratio of DH / ACE	ratio t-test
Indole-carboxylic acid	161.0477	C9H7NO2	Indole derivative	0.75	161.0478	1202	3.26	0.0166
gluconate / gulonate / galactonate/mannonate/gluco-hexonic acid	196.0583	C6H12O7	sugar acid	0.5	196.0584	1102	1.55	0.0005
[[2,5-dimethyl-1-(4-methylphenyl)pyrrole-3-carbonyl]amino] phosphonic acid	308.09259	C14H17N2O4P	unusual	0.99	308.0929	1102	1.43	0.054
Trihydroxycycloartan-24-one; 16-O-Arabinopyranoside / 12-Oleanene-3,21,22,28-tetrol; 28-b-D-Xylopyranoside	606.4132	C35H58O8	triterpene	1.27	606.4124	1202	1.35	0.0035
Diacylglycerol (e.g. DG(18:2/18:3)	614.491	C39H66O5	lipids	1.75	614.4921	1203	1.34	0.0628
Arginine	174.1117	C6H14N4O2	aminoacid	0.14	174.1117	1102	1.32	0.0143
2-[2-[2-(2-methylprop-2-enoyloxy)ethoxy]ethoxy]ethyl 3,4,5-tridodecoxybenzoate	874.68979	C53H94O9	unusual	0.9	874.689	1204	1.31	0.0213
[[1-(carbamoithiylhydrazinylidene)-3,4,5-trihydroxy-pentan-2-ylidene]amino]thiourea	294.0568	C7H14N6O3S2	unusual	2.65	294.0561	1102	1.25	0.0612
1-(4-Chlorobenzoyl)-1,2-dihydro-2-quinolinecarbonitrile, 9Cl	294.056	C17H11ClN2O	unusual	0.37	294.0561	1102	1.25	0.0612
Lignoceric acid / 2,4-dimethyl-docosanoic acid	368.3654	C24H48O2	fatty acid	1.09	368.3658	1204	1.24	0.0069

Sitosterol-3-O-beta-D-glucoside-6'-O-eicosanate	870.73126	C55H98O7	sterol	0.74	870.7319	1204	1.19	0.0364
PEG diacrylate / 3-[1-(2-cyclohexylethoxycarbonyloxy)ethoxy]-3-oxo-propanoic acid / methyl 8-hydroxy-8-(2-methoxycarbonylethyl)-1,4-dioxaspiro[4.5]decane-7-carboxylate / roridinic acid	302.1366	C14H22O7	ambiguous	0.84	302.1363	1202	1.17	0.0902
Triacylglycerol (e.g. TG(18:0/18:3/20:0); TG(16:0/18:3/22:0))	912.8146	C59H108O6	storage lipids	4.83	912.8193	1203	0.93	0.0818
2a-(Hydroxymethyl)-17-methyl-5a-androstane-3beta,17beta-diol / Pregnane-triol	336.2664	C21H36O3	sterol	0.59	336.2666	1203	0.88	0.0852
Triacylglycerol (e.g. TG(18:1/18:2/18:3) TG(16:0/18:2/20:4))	878.73634	C57H98O6	storage lipid	5.3	878.741	1203	0.88	0.0096
Triacylglycerol (e.g. TG(18:1/18:2/18:2); TG(18:0/18:2/18:3); TG(18:1/18:1/18:3))	880.75199	C57H100O6	storage lipids	4.21	880.7557	1203	0.86	0.0411
3-(3,4-Dihydroxyphenyl)-2-propenoic acid, Triacetyl ester / tert-butyl (2R)-2-[(1R)-7-methyl-1-phenylmethoxy-oct-6-enyl]docosanoate	600.5118	C39H68O4	unusual	3.23	600.5137	1203	0.77	0.051
disaccharide (e.g. Galactinol ; cellobiose ; lactose ; maltose ; galactosylmyoinositol ; trehalose)	342.1162	C12H22O11	carbohydrate	1.2	342.1158	1102	0.73	0.0807
N-(2-Cyanoethyl)-2-(1,1-dimethylethyl)-6-nitro-4-quinolinecarbothioamidel	342.115	C17H18N4O2S	unusual	2.2	342.1158	1102	0.73	0.0807

2,3,4,5,6-pentahydroxy-7-[(2S,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-heptanoic acid	388.12169	C13H24O13	unusual	0.75	388.1214	1102	0.71	0.0691
Diacylglycerophosphoethanolamines (e.g. N,N-dimethyl,GPEtn(22:0/24:0); GPEtn(26:0/22:0); GPEtn(24:0/24:0))	915.7656	C53H106NO8P	phospholipid	3.91	915.762	1204	0.71	0.059
9-Hydroxy-2,8-dimethyl-3-oxo-4,6-undecadienoic acid	240.1362	C13H20O4	fatty acid	0.25	240.1361	1202	0.67	0.0876
Diacylglycerophosphoethanolamines (e.g. GPEtn(18:1/18:1); GPEtn(16:1/20:1); GPEtn(16:0/20:2))	743.5466	C41H78NO8P	phospholipid	0.74	743.546	1202	0.67	0.0814
Diacylglycerol (e.g. DG(16:1/17:0/0:0); DG(16:0/17:1/0:0))	580.5066	C36H68O5	lipid	0.99	580.5061	1204	0.65	0.0221
tetrasaccharide (e.g. Stachyose ; Mannose ; Cellotetraose)	666.2216	C24H42O21	carbohydrate	0.3	666.2218	1102	0.6	1.73E-02
Diacylglycerophosphoethanolamines (e.g. GPEtn(20:1/20:1), dihydroxy ; GPEtn(20:0/20:2),dihydroxy;GPEtn (20:0/20:1), epoxy, hydroxyl)	831.5981	C45H86NO10P	phospholipid	0.97	831.5981	1202	0.58	0.0837
Diacylglycerophosphoethanolamines (e.g. GPEtn(10:0/12:0), hydroxyl)	567.3532	C27H54NO9P	phospholipid	0.81	567.3532	1202	0.57	0.0379
Diacylglycerophosphoethanolamines (e.g. N,N-dimethyl,GPEtn(18:3/16:0);GPEtn(18:1/18:2);GPEtn (18:3/18:0))	741.5308	C41H76NO8P	Phospholipid	1.28	741.5299	1202	0.57	4.82E-02
Flavomannin; (+)-form, 5,5'-Dioxo, 10,10'-dihydroxy, 3,3'-di-Me ether	634.1323	C32H26O14	unusual	0.4	634.132	1102	0.54	0.004
Diacylglycerophosphoethanolamines (e.g. GPEtn(20:2/20:1), dihydroxy ; GPEtn(20:2/20:0),epoxy,hydroxy)	829.5833	C45H84NO10P	phospholipid	0.34	829.583	1202	0.52	6.90E-03
Citbismine B; N10'-Me	684.2319	C37H36N2O11	acridone alkaloid	2.79	684.2317	1102	0.5	3.88E-02
UDP-Glucose / UDP-Galactose	566.055	C15H24N2O17P2	precursor carbohydrate	1.63	566.0541	1102	0.5	6.20E-03

trisaccharide (e.g. Raffinose / Cellobiose /Galactotriose)	504.1688	C18H32O16	carbohydrate	1.66	504.1682	1102	0.48	9.60E-03
Tetrahydroxy-3',6-dimethoxyflavone; 3-O-[4-Hydroxy-3-methoxy-E-cinnamoyl-D-xylopyranosyl-(1a2)-[D-glucopyranosyl-(1?3)]-D-glucopyranoside]	978.2641	C44H50O25	flavonoid	2.98	978.2612	1102	0.48	6.32E-02
Sinapate	224.0685	C11H12O5	flavonoid	0.33	224.0684	1202	0.44	5.85E-02
4,7-Dihydroxy-2,3-dimethyl-6-benzofuraldehyde / 10-Hydroxy-2,8-decadiene-4,6-diyonic acid; 8,9-Epoxyde, Me ester / 2,3-Dihydro-3,5-dihydroxy-2-methylnaphthoquinone	206.0579	C11H10O4	ambiguous	0	206.0579	1201	0.33	9.49E-02
Malic acid, O-(4-Hydroxy-3-methoxycinnamoyl)	310.0689	C14H14O8	precursor metabolite and flavonoid	2.04	310.0695	1202	0.32	0.0778
Sinapoyl malate	340.0794	C15H16O9	flavonoid and precursor metabolite	2.35	340.0802	1202	0.29	3.73E-02

Note: Analysis mode codes: 1102, aqueous-negative ESI; 1201, organic-positive ESI; 1202, organic-negative ESI; 1203, organic-positive APCI; 1024, organic-negative APCI. In some case, alternate compound IDs are listed that have similar ionization properties and identical masses. For lipids, multiple fatty acid compositions may produce identical masses. Where appropriate, examples of some of the different fatty acid combinations that could produce the specific target mass are given but an exhaustive list of all possible combinations is not provided.