

Supplementary Table 2 KEGG differential metabolite classification.

ID	name	Class I	Class II	log2FC	regulated
NEG_q38	3-(Carboxymethylamino)Propanoic Acid	Amino	aciAlpha Ami	0.644515414	up
NEG_q51	4-Hydroxyisoleucine	Amino	aciOther	0.721401518	up
NEG_q205	L-Glutamic Acid	Amino	aciOther	0.596789872	up
NEG_q242	N-Acetyl-L-Tryptophan	Amino	aciOther	0.553153868	up
NEG_q247	N-Carbamoyl-DL-Aspartic Acid	Amino	aciOther	1.955809988	up
NEG_q250	N-((-)-Jasmonoyl)-S-Isoleucine	Amino	aciDipeptide	-1.263999903	down
NEG_q364	B-Cyano-L-Alanine	Amino	aciOther	1.373087633	up
POS_q5	1-Aminocyclopropane-1-Carboxylic Acid	Amino	aciOther	0.505712997	up
POS_q98	Cis-4-Hydroxy-L-Proline	Amino	aciOther	0.479165708	up
POS_q115	D-Alanine	Amino	aciOther	0.73473115	up
POS_q125	DL-Alanine	Amino	aciOther	0.713007871	up
POS_q130	D-Proline	Amino	aciAlpha Ami	0.727747374	up
POS_q156	H-Abu-Oh	Amino	aciOther	0.259510146	up
POS_q158	H-Asp-Phe-Oh	Amino	aciPeptides	0.750292046	up
POS_q162	H-Leu-Val-Oh	Amino	aciPeptides	-0.296373286	down
POS_q196	L-Alanine	Amino	aciOther	0.816423168	up
POS_q198	L-Alloisoleucine	Amino	aciOther	0.83147109	up
POS_q205	L-Glutamine	Amino	aciOther	1.579675982	up
POS_q206	L-Histidine	Amino	aciOther	2.583124005	up
POS_q209	L-Homoserine	Amino	aciOther	0.866023209	up
POS_q210	L-Homoserine-1	Amino	aciAlpha Ami	0.817725007	up
POS_q216	L-Isoleucine	Amino	aciOther	0.887110716	up
POS_q217	L-Leucine	Amino	aciOther	0.75721556	up
POS_q218	L-Lysine	Amino	aciOther	1.609221552	up
POS_q220	L-Nmma (Acetate)	Amino	aciOther	1.194870248	up
POS_q223	L-Proline	Amino	aciOther	0.747511859	up
POS_q240	Methionine Sulfoxide	Amino	aciOther	0.869199469	up

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POS_q255	Acetylornithine	Amino aciOther	0.84590849 up
POS_q322	Sarcosine (S)-B-	Amino aciPeptides	0.622111896 up
POS_q323	Aminoisobutyric Acid	Amino aciOther	0.718532834 up
POS_q373	Γ-Glu-Phe	Amino aciOther	0.802524309 up
NEG_t119	Tryptophan glutamic acid	Amino aciOther	0.739678759 up
POS_t75	Ile-His 3-O-	Amino aciOther	-0.780925654 down
NEG_q47	Feruloylquinic Acid 5-	PhenylprcOther	0.814716 up
NEG_q54	Feruloylquinic Acid	PhenylprcOther	0.821771897 up
NEG_q86	Caffeic Acid	FPhenylprcSimple Pf	-0.536558446 down
NEG_q108	Danshensu (Soc	PhenylprcSimple Pf	1.541139284 up
NEG_q234	Methyl Sinapate	PhenylprcOther	-15.06365006 down
NEG_q345	Trans-Cinnamic Acid 4-	PhenylprcSimple Pf	-1.438133315 down
POS_q35	Hydroxycinnamic amide 4-	PhenylprcCinnamic	-0.140735488 down
POS_q38	Methoxycinnamic Alcohol	PhenylprcOther	-0.126373407 down
POS_q120	Dehydrodiisoeugenol	PhenylprcOther	-17.35947513 down
POS_t9	Sibirioside A 1-O-Galloyl-	PhenylprcPhenylprc	-0.452603793 down
NEG_q11	6-O-Cinnamoylglucose 2-Cinnamoyl-	PolyphencOther	-1.774079037 down
NEG_q18	1-Galloylglucose	PolyphencOther	-1.791313661 down
NEG_q121	Diacetoxy-6-Gingerdiol	PolyphencOther	-0.657267672 down
NEG_q229	Methyl Gallate (+)-	PolyphencOther	0.864501523 up
NEG_q314	Secoisolariciresinol	PolyphencOther	-3.56763262 down
POS_q361	Urolithin A	PolyphencMonophenc	0.924750742 up

POS_t23	4-Hydroxymethylphenol 1-O-rhamnoside 2'-	PolyphenolOther	-1.170970495 down
POS_q13	Deoxyadenosine Monohydrate	NucleotidePurine Nu	0.564494104 up
POS_q63	Adenosine-2'-Monophosphate	NucleotideRibonucle	0.823649496 up
POS_q100	Citicoline (Sodium)	NucleotideOther	1.367508754 up
POS_q191	Kojibiose N6-	NucleotideOther	-0.553169618 down
POS_q249	Methyladenosine Succinylaminoimidazole carboxamide riboside	NucleotidePurine Nu	0.396618773 up
NEG_t9		NucleosideOther	-0.570748258 down
NEG_q105	Cynaroside	FlavonoidPolyphenol	-0.606272235 down
NEG_q175	Hyperoside	FlavonoidPolyphenol	-0.696097298 down
NEG_q185	Isoquercitrin	FlavonoidFlavonols	-0.541467825 down
NEG_q187	Isovitexin	FlavonoidPolyphenol	-1.033711927 down
NEG_q245	Naringin	FlavonoidFlavonone	-2.02577247 down
NEG_q248	Neohesperidin	FlavonoidHydroxyfl	-2.95595001 down
NEG_q281	Plantagoside	Flavonoidflavanone	-1.141719653 down
NEG_q297	Rhamnazin	FlavonoidFlavonols	-18.68969939 down
NEG_q302	Rutin (Hydrate)	FlavonoidFlavonols	-1.161842026 down
NEG_q303	Rutin (Trihydrate)	FlavonoidOther	-1.070314465 down
NEG_q310	Saponaretin	FlavonoidOther	-0.979528463 down
NEG_q311	Schaftoside	FlavonoidOther	-1.114637364 down
NEG_q347	Tricetin	FlavonoidOther	-0.784004651 down
NEG_q358	Vicenin 2	FlavonoidOther	-1.018827086 down
POS_q19	2'',-O-B-L-Galorientin	FlavonoidOther	-1.160395175 down
POS_q225	Lucenin Ii	FlavonoidHydroxyfl	23.25182847 up
POS_q256	Naringenin Chalcone-1	FlavonoidOther	-1.318902732 down
POS_q277	Orientin Quercetin 3-O-	FlavonoidOther	-2.008726602 down
POS_q308	Neohesperidin	FlavonoidFlavonols	-1.884110266 down
POS_q321	Saponarin	FlavonoidOther	-1.115166163 down
POS_q352	Tilianin	FlavonoidMonophenol	-1.161843384 down
POS_q367	Vicenin 3 prim-O-	FlavonoidHydroxyfl	-0.844517725 down
NEG_t101	Glucosylangelic acid	FlavonoidOther	-0.59802133 down

NEG_t102	Catharticin	FlavonoicGlycoside		-0.751581992	down
NEG_t26	Drynachromoside A	FlavonoicGlycoside		-0.455649019	down
NEG_t32	Myricetin-3-O-glucuronide	FlavonoicFlavonols		0.312055787	up
NEG_t36	Quercetin 3-Caffeoylrobino bioside	FlavonoicGlycoside		-0.571526783	down
NEG_t95	Kaempferol-3-O- α -L-rhamnopyranosyl-(1-6)- β -D-glucopyranosyl-(1-2)- β -D-glucopyranoside	FlavonoicOther		-0.7120389	down
NEG_t98	Isohyperoside	FlavonoicFlavonols		-0.362436262	down
POS_t130	Naringin 4'-glucoside	FlavonoicGlycoside		-0.638269214	down
POS_t133	Quercetin-3-O-gentiotetroside	FlavonoicFlavonols		-1.584684107	down
POS_t95	Dodovisone D	FlavonoicOther		0.866757437	up
POS_q95	Chrysoobtusin	Quinones Other		-2.219532024	down
POS_t11	Ruberythric acid	Quinones Anthraqui		-1.089822763	down
NEG_q313	Secoisolariciresinol	Lignans Other		-2.490452675	down
NEG_q79	Benzoxazole	Others Other		-1.069969464	down
NEG_q317	Shikonofuran	Others Other		-0.381975238	down
POS_q27	3-Amino-2-Piperidinone	Others Other		0.732871649	up
POS_q212	Ligustilide	Others Furans		0.379529492	up
POS_q242	Methyl Benzoin N1,N8-Diacetylsperm	Others Other		1.047051255	up
POS_q246	idine (Hydrochloride)	Others Other		1.724945189	up
NEG_t23	Majoroside	Others Other		-1.107563862	down
NEG_t31	5-Methyl-2-furaldehyde	Others Furans		0.576437317	up
NEG_t86	Hellicoside 7-O-	Others Other		-0.831048682	down
NEG_t96	methylaloeresin A	Others Other		0.80250711	up
POS_t20	Fibleucin	Others Other		-0.323178448	down

POS_q42	5-Hydroxy-2-Pyrrolidinone	AlkaloidsOther	-0.765515606 down
POS_q62	Adenine (Hemisulfate)	AlkaloidsOther	-0.563363642 down
POS_q70	Aminophylline	AlkaloidsOther	0.467606744 up
POS_q71	Anatabine	AlkaloidsOther	0.988874243 up
POS_q99	Citicoline	AlkaloidsOther	1.131470322 up
POS_q170	Hydroxy-B-Sanshool	AlkaloidsOther	1.133180776 up
POS_q243	Methyl L-Pyroglutamate	AlkaloidsOther	2.322768936 up
POS_q250	N-Acetyl-5,6-Dehydrololine	AlkaloidsOther	0.280095524 up
POS_q264	Nicotinamide Riboside (Chloride)	AlkaloidsPyridine	0.608237679 up
POS_q266	N-Methylbenzylamine	AlkaloidsOther	-0.58403349 down
POS_q274	Acetylcysteine	AlkaloidsOther	0.916250277 up
POS_q299	Pterolactam	AlkaloidsOrnithine	0.733872036 up
POS_q337	Stachydrine Hydrochloride	AlkaloidsPyrrole	2.419254504 up
NEG_q24	Cinnamoyl-Beta-D-Glucose 3'-	Sugars arGlycoside	-0.570444051 down
NEG_q48	Oxogentamicin A2	Sugars arPolyol	0.976562726 up
NEG_q49	4-Hydroxy-3,5-	Sugars arAromatic	1.196581361 up
NEG_q110	D-Arabinose	Sugars arMonosacch	0.481269975 up
NEG_q200	L-(+)-Arabinose	Sugars arMonosacch	-0.934048072 down
NEG_q287	Progoitrin Uridine 5'-	Sugars arGlycoside	1.740562389 up
NEG_q352	Diphospho-D-Glucose Prim-0-	Sugars arGlycoside	0.555693223 up
POS_q294	Glucosylcimifugin	Sugars arMonosacch	-1.612427264 down
NEG_q82	Betulonic Acid	TerpenoidTriterper	-2.285805979 down
NEG_q83	Bilobalide	TerpenoidSesquiter	-3.052410729 down
NEG_q208	Linalyl Acetate	TerpenoidMonoterpe	-0.668215145 down
POS_q65	Aids031406	TerpenoidTerpene C	-1.377737656 down
POS_q83	Bruceine D	TerpenoidDiterpenc	-1.251854666 down
POS_q366	Verbenalin	TerpenoidIridoids	0.374208967 up

NEG_t17	Paeonilactone C 6''-O-p-	TerpenoidMonoterpe	-1.523207701 down
NEG_t18	Coumaroylgeni pin gentiobioside 9-O-	TerpenoidMonoterpe	-0.124383802 down
NEG_t27	Ethyldeacetyl orientalide	TerpenoidSesquiter	-0.79648176 down
NEG_t63	Meliasenin E	TerpenoidTriterper	-0.433005519 down
NEG_t73	Eupalinolide I 13-O-p-	TerpenoidSesquiter	-0.458141838 down
NEG_t99	Coumaroylplum ieride	TerpenoidIridoid	-0.357708559 down
POS_t59	Artemisinin B	TerpenoidSesquiter	1.304265527 up
POS_t90	Nudifloside D	TerpenoidIridoid	-1.331347599 down
POS_t93	6- Epiharpagide 3,5-	TerpenoidIridoid	0.297131695 up
NEG_q34	Dimethoxybenz oic Acid 3-	Ketones, Benzoic A	-2.224163035 down
NEG_q42	(Hydroxymethy l)Cyclopentan one	Ketones, Other	-1.433099189 down
NEG_q117	D-Gluconic Acid	Ketones, Sugar Aci	0.608366319 up
NEG_q172	Hydroxyphenyl lactic Acid	Ketones, Other	-17.06018461 down
NEG_q301	Rubinaphthin A (S)-3-(4- Hydroxyphenyl	Ketones, Polyketid	-1.072341197 down
NEG_q305	) -2- Hydroxypropio nic Acid D-Pantothenic Acid (Hemicalcium Salt)	Ketones, Phenylpro	-17.0851541 down
NEG_q139	Riboflavin	Vitamins Vitamin E	-1.546502228 down
POS_q313	Thiamine Pyrophosphate N-(beta-D- Glucosyl)nico tinate 3-	Vitamins Vitamin E	-0.360229868 down
POS_q351	Hydroxycoumar in	Vitamins Other	2.874425544 up
NEG_t7	Herniarin	CoumarinsOther	0.572166088 up
NEG_q41			-21.72070612 down
POS_q161			-2.684000611 down

NEG_q3	1,3-Dicaffeoylquinic Acid	Organic ϵ Carboxylic	-1.874118495	down
NEG_q12	2,3-Dihydroxy-3-Methylbutanoic Acid	Organic ϵ Carboxylic	1.070060526	up
NEG_q13	2,3-Dihydroxy-4-Methoxybenzoic Acid	Organic ϵ Benzoic A	0.942651062	up
NEG_q29	3,4-Dicaffeoylquinic Acid	Organic ϵ Carboxylic	-1.802472214	down
NEG_q66	Adenosine 5' - Diphosphoribose (Sodium)	Organic ϵ Other	14.22390887	up
NEG_q215	Malonic Acid	Organic ϵ Carboxylic	-0.831903125	down
NEG_q263	P-Coumaroyl Quinic Acid	Organic ϵ Carboxylic	-0.636883666	down
NEG_q267	Phenylpyruvic Acid	Organic ϵ Carboxylic	-2.292945518	down
NEG_q275	Phthalic Acid Mono-2-Ethylhexyl Ester	Organic ϵ Carboxylic	-15.02749483	down
NEG_q279	Pinobanksin 3-Acetate	Organic ϵ Other	-0.659279562	down
NEG_q328	Taurine	Organic ϵ Other	4.225866686	up
POS_q58	($\pm$)-Abscissic Acid	Organic ϵ Carboxylic	0.606096563	up
POS_q173	Imidazoleacetic Acid (Hydrochloride)	Organic ϵ Carboxylic	0.340558911	up
POS_q179	Isochlorogenic Acid A	Organic ϵ Carboxylic	-1.812834867	down
POS_q201	L-Azetidine-2-Carboxylic Acid	Organic ϵ Carboxylic	0.527944266	up
POS_q283	Phosphorylcholine	Organic ϵ Other	0.571047569	up
POS_t17	5-O-Caffeoylshikimic acid	Organic ACarboxylic	-1.17020066	down
NEG_q96	Cholic Acid (Sodium)	Steroids Cholestar	-11.26408285	down
NEG_t2	Isophysalin A	Steroids Other	-0.254167866	down

NEG_t62	Methyl protogracilli Steroids Glycoside n			-0.80751699 down
POS_q230	Lysopc (14:0/0:0)	Lipid	Fatty Acy	0.848694608 up