

Supplementary Material

Combinatorial transcriptomics and metabolomics analysis reveals the effects of the harvesting stages on the accumulation of phenylpropanoid metabolites in *Lonicera japonica*

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Table S1. Primers used for qRT-PCR analysis of selected glycolysis/gluconeogenesis and phenylpropanoid biosynthesis related genes.

Gene Name	Primer sequence
<i>LjALDO</i>	F : 5'-GACTTCACTATCTTGCTCAATC-3' R:5'-GACTTCACTATCTTGCTCAATC-3'
<i>LjpckA</i>	F:5'-CCAAGGAGAGGACCAGAA-3' R:5'-CCAAGGAGAGGACCAGAA-3'
<i>LjCAD</i>	F:5'-GAGACGCAAGAAGTATTG-3' R:5'-ACTCAGGCATCTTACTAC-3'
<i>LjCSE</i>	F:5'-TTGACCAACCAAAGGAAAGG-3' R:5'-CCAACCAGATCCGTTTTCTATC-3'
<i>LjCOMT</i>	F:5'-AGATGAATGGGTGGATTCGTGTG-3' R:5'-CTCCAGAAAATGATCCAAGTAAAAT-3'

Table S2. Quality estimation of raw reads in all transcriptome.

sample	raw_reads	clean_reads	clean_bases	error_rate	Q20	Q30	GC_pct
GB_1	22597599	21285518	6.39G	0.03	97.84	93.58	43.79
GB_2	22987350	21528990	6.46G	0.02	98.11	94.31	43.68
GB_3	23049403	21810770	6.54G	0.03	97.8	93.48	43.69
WB_1	23324860	21957778	6.59G	0.03	97.94	93.86	43.12
WB_2	22886999	21404163	6.42G	0.02	98.16	94.41	43.07
WB_3	24639578	22875270	6.86G	0.02	98.09	94.24	42.92

Table S3. Splicing length and frequency distribution.

	300bp-500b	500bp-1kb	1kb-2kb	> 2kb	Mean_lengt	N50	Total
	p	p	p		h		
Number of transcripts	36645	40210	45710	48190	1552	2323	170755
Number of Unigenes	21696	20252	14845	14640	1278	2071	71433

Table S4. Enrichment results of DEGs in glycolysis/gluconeogenesis pathway of *L. japonica*.

Enzyme	KO ID	KO Description	P-value	log2FC	FPKM		Up/Down
					WB	GB	
PGM	K01835	phosphoglucomutase	0.046242	-7.3903	3.92	0	down
HK	K00844	hexokinase	5.13E-05	3.2192	6.0067	62.2933	up
PFP	K00895	diphosphate-dependent phosphofructokinase	0.0065068	1.2184	0.7767	2.01	up
PFP	K00895	diphosphate-dependent phosphofructokinase	0.0495	-2.5927	3.36	0.6167	down
ALDO	K01623	fructose-bisphosphate aldolase	0.017874	-3.1608	120.2767	12.6067	down
ALDO	K01623	fructose-bisphosphate aldolase	7.28E-06	-7.4989	51.8867	0.2633	down
GAPDH	K00134	glyceraldehyde 3-phosphate dehydrogenase	0.02582	-4.0476	3.4033	0.1867	down
ENO	K01689	enolase	0.00034036	1.9681	16.16	68.0233	up
pckA	K01610	phosphoenolpyruvate carboxykinase	0.025807	-1.2842	31.96	14.1133	down
pckA	K01610	phosphoenolpyruvate carboxykinase	0.00045228	-3.3094	57.7867	6.56	down
DLAT	K00627	dihydrolipoamide acetyltransferase	0.00015826	1.2263	13.23	32.0533	up
PDC	K01568	pyruvate decarboxylase	4.28E-11	4.3526	2.0233	45.7567	up
LDH	K00016	L-lactate dehydrogenase	0.049639	1.9264	1.4633	5.5367	up
DLD	K00382	dihydrolipoamide	7.28E-06	2.1089	8.0967	37.6867	up

		dehydrogenase					
ADH	K00121	alcohol dehydrogenase	2.78E-09	2.4404	0.7	3.94	up
		aldehyde					
ALDH	K00128	dehydrogenase	0.00042374	1.8727	2.9633	11.81	up
		aldehyde					
ALDH	K00128	dehydrogenase	0.028499	-1.2632	13.02	5.4667	down

Genes with an adjusted P-value <0.05 found by DESeq were assigned as differentially expressed.

$|\log_2(\text{foldchange})| > 1$ was set as the threshold for significantly differential expression. Expected

number of fragments per kilobase of transcript sequence per millions base pairs sequenced

(FPKM) >0.3 was means significantly differential expression.

Table S5. Enrichment results of DEGs in phenylpropanoid biosynthetic pathway of *L.**japonica.*

Enzyme	KO ID	KO Description	P-value	log2FC	FPKM		Up/Down
					WB	GB	
CSE	K18368	caffeoylshikimate esterase	0.028675	1.5096	5.01	14.9067	up
COMT	K13066	caffeic acid 3-O-methyltransferase	0.00035208	-8.5148	33.6667	0.0833	down
CAD	K00083	cinnamyl-alcohol dehydrogenase	3.57E-16	4.489	1.3733	33.6167	up
CAD	K00083	cinnamyl-alcohol dehydrogenase	7.78E-05	6.9607	0	2.16	up
CAD	K00083	cinnamyl-alcohol dehydrogenase	2.17E-05	1.7807	17.5	62.4367	up
CAD	K00083	cinnamyl-alcohol dehydrogenase	0.00014903	-2.5436	74.3233	14.05	down
CAD	K00083	cinnamyl-alcohol dehydrogenase	8.79E-07	-7.9363	357.897	1.6867	down
CAD	K00083	cinnamyl-alcohol dehydrogenase	8.12E-09	-2.0477	15.6433	3.8933	down
bgl	K01188	beta-glucosidase	5.84E-05	2.0774	0.7733	3.3933	up
bgl	K01188	beta-glucosidase	0.00037202	-8.674	7.88	0.02	down
bgl	K01188	beta-glucosidase	0.0040595	-8.4018	43.0033	0.1133	down
bglX	K05349	beta-glucosidase	0.0061101	1.1755	8.9	21.3933	up
bglX	K05349	beta-glucosidase	0.023593	1.621	4.6233	15.3567	up
POD	K00430	peroxidase	0.0086415	3.5238	0.2067	2.6	up
POD	K00430	peroxidase	6.09E-05	4.1956	0.2233	4.51	up
POD	K00430	peroxidase	3.20E-05	3.0117	7.4567	60.89	up
POD	K00430	peroxidase	0.0042876	1.8398	1.1867	4.4467	up
POD	K00430	peroxidase	0.049359	3.5915	0.27	3.7567	up
POD	K00430	peroxidase	0.00013107	1.9991	1.4867	6.2867	up
POD	K00430	peroxidase	0.021702	-3.5282	2.46	0.2433	down
POD	K00430	peroxidase	0.00022357	-1.5428	7.3867	2.6733	down

Table S6. Enrichment results of DETFs in different harvesting stages (main part)

No.	Family	TF	P-value	log2FC	FPKM		Up/Down
					WB	GB	
1	MYB	MYB5	0.033156	1.2938	0.7767	2.01	up
2	MYB	MYB6	0.036041	2.4377	0.3867	2.2467	up
3	MYB	MYB12	0.00066076	5.7112	0.6433	39.49	up
4	MYB	MYB44	0.020621	-4.0377	22.5267	1.5733	down
5	MYB	MYB52	0.0033795	3.7117	0.4333	6.11	up
6	MYB	MYB60	0.027094	-3.8898	15.1633	0.9333	down
7	MYB	MYB61	0.00092711	-2.8837	9.7633	1.48	down
8	MYB	MYB63	1.42E-07	-6.0777	2.7467	0.0433	down
9	MYB	MYB77	0.0011671	-3.3531	19.99	2.1867	down
10	MYB	MYB111	0.0017486	4.7532	0.41	12.7167	up
11	MYB	MYB308	0.00067253	-3.9222	273.0333	20.5267	down
12	MYB	MYB1R1	3.60E-06	-1.8579	15.36	4.3267	down
13	bHLH	bHLH10	0.0068109	3.6305	0.0633	0.7933	up
14	bHLH	bHLH25	1.42E-12	4.5608	0.3133	7.6533	up
15	bHLH	bHLH71	0.0057875	3.1993	1.0333	10.8233	up
16	bHLH	bHLH78	0.00010465	-1.3276	14.3233	6.0667	down
17	bHLH	bHLH122	0.001252	-1.1372	7.9667	3.8	down
18	AP2/ERF	ERF003	0.0002489	2.4449	3.24	18.9367	up
19	AP2/ERF	ERF008	0.020182	-2.168	56.3867	13.9933	down
20	AP2/ERF	ERF010	0.0013079	-2.6397	17.3133	3.0833	down
21	AP2/ERF	ERF039	0.02437	-2.6921	2.6233	0.41	down
22	AP2/ERF	ERF060	3.14E-07	-1.2474	106.8767	47.46	down
23	AP2/ERF	ERF095	0.00033969	-6.8235	3.76	0	down
24	AP2/ERF	ERF110	0.031437	-3.4541	20.4367	2.1367	down

25	AP2/ERF	RAP2-3	5.95E-12	3.2322	4.6	45.59	up
26	AP2/ERF	RAP2-7	0.00020971	-1.6236	6.4033	2.1367	down
27	AP2/ERF	AIL5	1.16E-05	8.0014	0	2.07	up
28	AP2/ERF	PTI6	0.00055295	1.4222	11.5467	32.0633	up
29	NAC	NAC002	3.03E-05	-3.0506	25.2433	2.9933	down
30	NAC	NAC021	0.0014725	-3.2756	4.5233	0.4633	down
31	NAC	NAC071	2.45E-05	2.3081	2.44	12.8	up
32	NAC	NAC073	0.029176	1.871	0.6733	2.6133	up
33	NAC	NAC076	0.014452	1.9672	1.76	7.5667	up
34	NAC	NAC104	2.36E-06	-5.24	4.1067	0.1233	down
35	NAC	JA2L	0.036492	-2.1443	93.7033	23.7267	down

TFs with an adjusted P-value <0.05 found by DESeq were assigned as differentially expressed. $|\log_2(\text{fold change})| > 1$ was set as the threshold for significantly differential expression. Expected number of fragments per kilobase of transcript sequence per millions base pairs sequenced (FPKM) > 0.3 was means significantly differential expression.

Table S7. Differential metabolites detected in GB vs WB stage.

Compound_ID	Name	Pvalue	VIP	Up/Down
Com_4854_pos	4-oxododecanedioic acid	6.13E-10	1.405595634	down
Com_708_pos	4,6,8-trihydroxy-7-methoxy-3-methyl-3,4-dihydro-2H-1-benzopyran-1-one	1.80E-09	1.390114098	down
Com_739_pos	D-(+)-Camphor	4.65E-09	1.387272726	down
Com_6767_pos	2-(carboxymethoxy)-4-methoxybenzoic acid	1.45E-08	1.381551051	down
Com_5140_neg	Carnosic acid	1.69E-08	1.378858956	up
Com_3909_neg	Cucurbitacin I	3.06E-08	1.3851036	down
Com_8183_pos	Angiotensin IV	5.38E-08	1.381434242	up
Com_2132_pos	Olivetol	6.35E-08	1.374749331	down
Com_1105_pos	Stachyose	7.65E-08	1.370592378	down
Com_123_neg	Glutaric Acid	9.47E-08	1.377796924	down
Com_2005_pos	Ethyl paraben	9.70E-08	1.394197665	down
Com_1508_neg	Xanthosine Dihydrate	9.84E-08	1.368112449	down
Com_2567_pos	(-)-Epigallocatechin	1.16E-07	1.378120231	up
Com_1278_pos	Neomangiferin	1.40E-07	1.377311109	down
Com_1449_pos	Lawsone	1.53E-07	1.364131192	up
Com_1890_pos	N-2-Hydroxycyclopentyladenosine	1.55E-07	1.373997297	up
Com_260_pos	Gardenin B	1.71E-07	1.380615199	up
Com_30_pos	3-Hydroxy-3-Methylpentane-1,5-Dioic Acid	2.17E-07	1.361349872	down
Com_3055_neg	Stevioside	2.21E-07	1.362690945	down
Com_5851_neg	Akebia saponin D	2.28E-07	1.369328419	up
Com_4263_neg	Hesperetin	2.43E-07	1.36344128	up
Com_1149_neg	Sclareolide	2.48E-07	1.377296156	up
Com_4399_neg	Ganoderic acid C6	4.23E-07	1.356895699	down
Com_425_pos	1-(3,4-dihydroxyphenyl)-7-(4-hydroxyphenyl)heptan-3-one	5.41E-07	1.352898252	up
Com_5271_pos	Ajugol	6.56E-07	1.375777512	down
Com_50_neg	D-Erythrose 4-phosphate	7.05E-07	1.36937534	down
Com_3230_pos	Bevirimat	7.24E-07	1.359089835	up
Com_1555_pos	PC (6:0/16:3)	7.77E-07	1.348273337	up
Com_912_pos	Nicotinamide adenine dinucleotide (NAD ⁺)	8.02E-07	1.354518903	down
Com_815_neg	Hydroxytyrosol	8.08E-07	1.351648695	up
Com_365_neg	Caffeic acid	8.80E-07	1.349319419	up
Com_296_pos	Pantothenic acid	1.07E-06	1.348363184	down
Com_5337_pos	iP9G	1.10E-06	1.385559181	down

Com_6170_pos	Tetrahydrojatrorrhizine	1.13E-06	1.344347247	up
Com_6461_pos	Dutasteride	1.17E-06	1.343791142	down
Com_311_neg	Yuheinoside	1.30E-06	1.34918805	down
Com_1469_pos	tetranor-12(R)-HETE	1.30E-06	1.353174766	up
Com_614_neg	Eriodictyol-7-O-glucoside	1.67E-06	1.341297021	down
Com_3549_pos	N-(2,3-dihydro-1,4-benzodioxin-6-yl)-2,5-dimethyl-3-furamide	1.68E-06	1.350854589	up
Com_478_pos	Sweroside	1.69E-06	1.363867922	down
Com_782_neg	Sibiricose A6	1.83E-06	1.342193829	down
Com_4385_pos	4-Hydroxymephenytoin	1.85E-06	1.361614649	up
Com_1845_pos	2-aminoethyl (allylamino)methanedithioate hydrochloride	1.86E-06	1.342326936	up
Com_4517_pos	Cafestol	1.96E-06	1.336892105	down
Com_4020_pos	Tetranor-12(S)-HETE	2.33E-06	1.335735661	up
Com_1892_neg	Ixoside	2.58E-06	1.334360586	down
Com_6657_pos	1-Methylnicotinamide	2.61E-06	1.379022534	up
Com_6418_pos	Picramnioside F	2.69E-06	1.33553907	down
Com_1281_pos	5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	2.70E-06	1.34238081	up
Com_3987_pos	N-[(Tert-butoxy)carbonyl]-L-tryptophan	2.82E-06	1.340684876	up
Com_2995_pos	di-C,C-pentosyl-luteolin	2.88E-06	1.339827062	up
Com_2713_neg	Tricin	3.13E-06	1.363124702	up
Com_903_neg	MGDG (2:0/5:0)	3.16E-06	1.344708946	down
Com_6403_pos	LPC 16:3	3.65E-06	1.327433558	up
Com_1091_pos	Lycorine	3.83E-06	1.36894355	up
Com_335_neg	Maltotriitol	3.84E-06	1.34379287	down
Com_8933_pos	1-[(3S)-3-(1,3-Benzothiazol-2-yl)-1-pyrrolidinyl]-2-phenoxyethanone	4.69E-06	1.342953898	down
Com_3526_neg	1-O-Palmitoylhexitol	4.90E-06	1.323898957	down
Com_5985_neg	Ganoderic acid A	6.03E-06	1.376296128	down
Com_347_pos	Nicotianamine	6.98E-06	1.328450423	down
Com_7065_pos	(-)-chimonanthine	7.25E-06	1.320210693	down
Com_3949_neg	Gracillin	7.27E-06	1.325828584	down
Com_525_neg	Dodecanedioic acid	7.49E-06	1.324711396	up
Com_2546_pos	Sauchinone	7.65E-06	1.338890097	up
Com_876_neg	4-Hydroxyphenylpyruvic acid	8.10E-06	1.324751493	up
Com_7507_pos	4-Demethylepipodophyllotoxin	8.51E-06	1.323414917	down
Com_2024_neg	L-Ornithine	8.69E-06	1.317784299	up
Com_949_pos	D-Raffinose	9.03E-06	1.312403202	down
Com_1383_neg	Leucoside	9.90E-06	1.31180476	down
Com_1124_pos	Methyl indole-3-acetate	1.03E-05	1.327452571	down
Com_5300_pos	Testosterone	1.08E-05	1.309197701	up
Com_511_pos	Coniferin	1.08E-05	1.348693555	up
Com_6771_pos	N-Benzoyl-(2R,3S)-3-phenylisoserine	1.09E-05	1.350816169	up

Com_5471_neg	Timosaponin A3	1.10E-05	1.319384036	down
Com_2289_pos	L-Saccharopine	1.12E-05	1.3124502	down
Com_26_pos	5-hydroxy-4-methoxy-5,6-dihydro-2H-pyran-2-one	1.15E-05	1.341218033	down
Com_2127_pos	alpha-Ionone	1.16E-05	1.322979406	down
Com_1362_neg	Eupatilin	1.19E-05	1.319812219	up
Com_2910_pos	WLH	1.25E-05	1.311345318	down
Com_5636_pos	13,14-dihydro-15-keto-tetranor Prostaglandin E2	1.28E-05	1.313254965	up
Com_6583_pos	11-Deoxy prostaglandin F1 α	1.30E-05	1.327655939	up
Com_926_neg	Pinoresinol 4-O-glucoside	1.33E-05	1.307667549	up
Com_828_pos	7-(2-thienyl)[1,2,4]triazolo[4,3-a]pyrimidine	1.38E-05	1.358202039	down
Com_5235_pos	Osalmide	1.39E-05	1.362337146	down
Com_4875_pos	Stylopine	1.48E-05	1.313111191	up
Com_2396_pos	Fructose 1,6-diphosphate	1.48E-05	1.36799401	down
Com_2867_pos	8,8-dimethyl-2-phenyl-4H,8H-pyrano[2,3-h]chromen-4-one	1.50E-05	1.349708433	up
Com_2473_pos	Esculin	1.51E-05	1.316388431	down
Com_259_neg	Camelliaside A	1.54E-05	1.333043802	up
Com_3815_pos	Arachidonic acid	1.56E-05	1.318201384	up
Com_3164_pos	Phellodensin F	1.59E-05	1.305784542	up
Com_7708_pos	Danshenol C	1.60E-05	1.306903301	up
Com_516_neg	Narcissoside	1.61E-05	1.302578014	up
Com_1497_pos	PE (6:0/16:3)	1.62E-05	1.319176212	up
Com_3075_neg	Malonic acid	1.68E-05	1.343695658	down
Com_3464_pos	(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid	1.74E-05	1.31865593	up
Com_5149_neg	Kolavic acid	1.74E-05	1.343590712	up
Com_361_neg	(+)-Dihydrojasmonic acid	1.79E-05	1.320458116	up
Com_2697_pos	N-Acetyl-D-lactosamine	1.84E-05	1.34199562	down
Com_8036_pos	Asp-phe	1.84E-05	1.299052762	up
Com_80_neg	Acetylharpagide	1.85E-05	1.309825154	down
Com_227_neg	L-Allothreonine	1.88E-05	1.302336175	up
Com_671_pos	Avocadyne 1-acetate	1.99E-05	1.31148943	up
Com_4656_pos	UDP-N-acetylglucosamine	2.00E-05	1.295156119	down
Com_969_neg	Uridine diphosphate-N-acetylglucosamine	2.00E-05	1.304374485	up
Com_5175_neg	FAHFA (2:0/18:1)	2.07E-05	1.294348936	up
Com_1554_pos	Indole-3-propionic acid	2.13E-05	1.293926522	down
Com_420_neg	D-Fructose 1,6-bisphosphate	2.14E-05	1.308562257	down
Com_101_neg	9-Hydroxy-(10E,12Z,15Z)-Octadecatrienoic Acid	2.16E-05	1.304978952	up
Com_425_neg	Methyl jasmonate	2.32E-05	1.30602006	up
Com_1192_pos	4-Ethylbenzaldehyde	2.34E-05	1.344906847	down
Com_2533_neg	Ginkgolic Acid (C13:0)	2.36E-05	1.325655497	up
Com_2019_pos	N-Sinapoylagmatine	2.40E-05	1.293815091	up
Com_2838_pos	N-Acetylneuraminic acid	2.42E-05	1.297416191	down

Com_6160_pos	Pterodin Z	2.46E-05	1.318560056	up
Com_539_neg	LPC 18:1	2.46E-05	1.300994855	up
Com_4251_neg	Ziyuglycoside I	2.49E-05	1.317116581	up
Com_3606_neg	Secoisolariciresinol diglucoside	2.49E-05	1.291091542	up
Com_2878_pos	Taxifolin	2.78E-05	1.297798345	up
Com_4595_pos	Pterostilbene	2.81E-05	1.29068215	up
Com_2937_pos	Eicosapentaenoic acid	2.91E-05	1.291468905	up
Com_1101_neg	Tricin 5-O-hexoside	2.95E-05	1.293132634	down
Com_1475_neg	6-hydroxy-7,8-dimethoxycoumarin	2.96E-05	1.311830485	down
Com_899_pos	Methionine	3.05E-05	1.29346052	up
Com_4318_pos	LPC 17:2	3.11E-05	1.286629369	up
Com_1488_pos	Pheophorbide A	3.13E-05	1.356242922	up
Com_1500_pos	Eucalyptol	3.37E-05	1.285674513	down
Com_111_pos	3-(3,4,5-trimethoxyphenyl)propanoic acid	3.38E-05	1.298258513	up
Com_593_pos	Sedanolid	3.68E-05	1.298629437	up
Com_2982_neg	Kaempferide	3.70E-05	1.304313769	up
Com_1242_pos	Bakuchiol	3.74E-05	1.312319233	up
Com_137_pos	PC (16:1e/2:0)	3.97E-05	1.298030334	up
Com_4546_pos	N-(4-butyl-2-methylphenyl)-N'-[4-(4-methylpiperazino)phenyl]urea	4.02E-05	1.330187578	down
Com_1588_neg	Typhaneoside	4.07E-05	1.282240973	down
Com_1771_neg	Scopolin	4.34E-05	1.346652441	up
Com_517_neg	Raffinose	4.37E-05	1.282959528	down
Com_5358_pos	Catharanthine hemitartrate	4.57E-05	1.317626455	up
Com_4941_neg	FAHFA (2:0/18:3)	4.64E-05	1.348381172	up
Com_3632_pos	LPE 18:4	4.70E-05	1.279533595	up
Com_1705_pos	6-Acetylmorphine	4.72E-05	1.308449938	up
Com_43_neg	9-HpOTrE	4.80E-05	1.308946162	up
Com_3522_pos	1,4-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	4.85E-05	1.311434856	up
Com_8524_pos	PC (4:0/16:3)	4.86E-05	1.341165335	up
Com_1701_pos	2-((2-[(5-methylisoxazol-3-yl)amino]-2-oxoethyl)thio)acetic acid	4.99E-05	1.318105187	down
Com_56_neg	Ribose	5.00E-05	1.315411702	down
Com_349_neg	Tuberonic acid hexoside	5.20E-05	1.303901421	down
Com_7226_pos	Ubenimex	5.73E-05	1.310275953	up
Com_6145_pos	N8-Acetylspermidine	5.84E-05	1.280828638	up
Com_5763_pos	Xanthine	5.97E-05	1.283801031	down
Com_2682_pos	2-(tert-butyl)-6,7-dimethoxy-4H-3,1-benzoxazin-4-one	6.03E-05	1.282949461	up
Com_4503_pos	Alternariol	6.12E-05	1.269858293	up
Com_3461_pos	5-acetyl-2,6-dimethyl-1,2,3,4-tetrahydropyridin-4-one	6.44E-05	1.279406883	up
Com_369_pos	Lactucin	6.49E-05	1.274134162	up

Com_237_neg	12,13-EODE	6.74E-05	1.27117775	up
Com_893_pos	IAA-Glu	6.75E-05	1.352534284	up
Com_5434_neg	Indole-3-acetic acid	6.83E-05	1.273671126	up
Com_1695_pos	(11E,15Z)-9,10,13-trihydroxyoctadeca-11,15-dienoic acid	6.92E-05	1.300068112	down
Com_858_pos	Sepiapterin	7.01E-05	1.296390905	down
Com_4231_pos	(3R)-4,4-Dimethyl-2-oxotetrahydro-3-furanyl beta-D-glucopyranoside	7.09E-05	1.264038734	down
Com_21_neg	3,5-Dicaffeoylquinic acid	7.41E-05	1.270050408	up
Com_2645_pos	Phosphoenolpyruvic acid	7.45E-05	1.309116525	down
Com_2662_pos	C-pentosyl-luteolin O-p-coumaroylhexoside	7.78E-05	1.330635862	up
Com_5290_pos	4-oxo-4-(5,6,7,8-tetrahydronaphthalen-1-ylamino)but-2-enoic acid	8.09E-05	1.270192928	up
Com_3926_pos	Epinephrine	8.40E-05	1.278136511	down
Com_7650_pos	dG-C8-IQ	8.53E-05	1.311488532	down
Com_8160_pos	LPC 14:0	9.09E-05	1.264541335	up
Com_1247_pos	Methyl cinnamate	9.12E-05	1.315705081	up
Com_2583_neg	Cyclic adenosine diphosphate-ribose	9.17E-05	1.274278913	down
Com_1394_pos	Trigonelline	9.21E-05	1.254621112	down
Com_653_pos	Pyridoxine	9.34E-05	1.27340534	up
Com_261_pos	2-[(1-benzothiophen-3-ylmethyl)amino]-1-phenylethanol	9.82E-05	1.300681554	up
Com_214_pos	1-(4-hydroxyphenyl)propane-1,2-diol	9.90E-05	1.298432601	down
Com_258_neg	Bavachalcone	9.93E-05	1.270621696	down
Com_130_pos	L-Aspartic acid	0.000102088	1.324936542	down
Com_400_pos	UDP	0.000103089	1.266202055	down
Com_3574_pos	Curcumenol	0.000103158	1.294099537	down
Com_863_neg	Forsythoside B	0.000103631	1.257300025	up
Com_154_neg	Shikimic acid	0.000104199	1.323081443	up
Com_3013_pos	Neodiosmin	0.000107621	1.255940594	down
Com_5031_pos	8-Hydroxy-2-Deoxyguanosine	0.000107658	1.258359097	down
Com_10032_pos	Nortanshinone	0.000108533	1.263757039	up
Com_3202_pos	Debromohymenialdisine	0.000112777	1.253179474	up
Com_27_pos	PC (16:2e/2:0)	0.000115521	1.286577505	up
Com_4054_pos	PE (2:0/16:3)	0.000115667	1.261054516	up
Com_1386_neg	10-Hydroxydecanoic acid	0.0001179	1.297264673	up
Com_411_pos	D-(+)-Melezitose	0.000118013	1.260529312	down
Com_3011_neg	LPC 16:1	0.000122503	1.271239621	up
Com_3562_pos	PC (14:1e/3:0)	0.00012382	1.250069879	up
Com_1361_pos	Apigenin	0.000126462	1.245200829	down
Com_1453_neg	Triethyl citrate	0.000129506	1.258199965	up
Com_8397_pos	LysoPC 18:0	0.000135997	1.273762434	up
Com_40_pos	5-Hydroxymethylfurfural	0.000137403	1.320835733	down
Com_3195_neg	6-Hydroxynicotinic acid	0.0001381	1.27531236	up

Com_4916_pos	Arachidonoyl amide	0.000138144	1.244811077	down
Com_5678_pos	Docosatrienoic acid	0.000144369	1.264965048	down
Com_5096_pos	N-p-Coumaroylagmatine	0.00014506	1.275039845	up
Com_636_neg	Monocrotaline	0.000146368	1.24998242	up
Com_3447_neg	6-Phosphogluconic acid	0.000148251	1.242206106	down
Com_168_pos	DL-Arginine	0.000153204	1.296109649	up
Com_7184_pos	Cyanidin O-rutinoside	0.000158739	1.255358638	down
Com_5559_pos	Diosgenin	0.000159414	1.314368464	up
Com_536_neg	D-Ribose 5-phosphate	0.000159874	1.277034087	down
Com_1599_pos	HQH	0.000160225	1.252562224	down
Com_7459_pos	16-Heptadecyne-1,2,4-triol	0.000162459	1.235963953	down
Com_251_pos	5-Aminolevulinic acid	0.000164606	1.308556891	down
Com_82_pos	L-Phenylalanine	0.000164808	1.299784147	up
Com_6568_pos	7-Methoxyflavone	0.000165619	1.283623161	down
Com_977_pos	DL-Lysine	0.000171444	1.24565605	up
Com_900_pos	2-[(3S)-1-Benzyl-3-pyrrolidinyl]-1,3-benzothiazole	0.000171808	1.310473339	up
Com_5194_pos	Anacardic Acid	0.000172233	1.240252431	up
Com_145_neg	Uridine??diphosphate??glucose	0.000173284	1.242094938	up
Com_2_pos	Oleamide	0.000178096	1.242607088	down
Com_1647_pos	Ethyl oleate	0.000184058	1.276441353	down
Com_232_neg	N7-Methylguanosine	0.000186089	1.243276896	up
Com_3374_neg	Methyl-Hesperidin	0.000189178	1.262767406	up
Com_3585_pos	beta-Alanine methyl ester hydrochloride	0.000192624	1.325416845	up
Com_2259_neg	Ligustroflavone	0.000199701	1.235563198	up
Com_4130_pos	PC (2:0/16:3)	0.000201059	1.238002192	up
Com_2353_neg	B Liriopesides B	0.000209724	1.251405733	down
Com_4358_neg	Gallic acid	0.000210624	1.268447249	up
Com_2108_pos	Astaxanthin	0.000212822	1.245202509	up
Com_4474_pos	D-Glucose 1-phosphate	0.000213977	1.270845653	up
Com_104_neg	13-HPODE	0.000218809	1.243532411	up
Com_562_pos	L-Asparagine	0.000219547	1.227635787	down
Com_8879_pos	alpha-Zearalanol	0.000223605	1.224224724	up
Com_6933_pos	Scutellarin	0.000232322	1.302272313	up
Com_5759_pos	Dihydrokavain	0.000239607	1.237888031	down
Com_439_pos	Isomucronulatol	0.000250077	1.280217451	up
Com_716_pos	5 α -Dihydrotestosterone	0.000251468	1.241195525	up
Com_553_neg	Robinin	0.000252246	1.223341645	up
Com_3543_neg	Xanthosine	0.00025369	1.29868069	down
Com_1628_pos	TBHQ	0.000254782	1.274215463	down
Com_1134_neg	Arginine	0.000261008	1.29132903	up
Com_1516_pos	Isoquinoline	0.000264637	1.278754475	down
Com_8109_pos	Homosildenafil	0.000271103	1.2295514	down
Com_302_pos	Glucose 1-phosphate	0.000272207	1.229678052	down

Com_114_pos	Luteolin	0.000278368	1.221072283	up
Com_1567_neg	C-hexosyl-luteolin O-p-coumaroylhexoside	0.000286341	1.217424819	up
Com_247_neg	Linoleic acid	0.000290605	1.288223979	up
Com_289_pos	D-(+)-Maltose	0.000291124	1.296215039	down
Com_6447_pos	Neocnidilide	0.000295631	1.219547828	up
Com_392_pos	L-serine	0.000295806	1.254808977	down
Com_1092_pos	(12Z)-9,10,11-trihydroxyoctadec-12-enoic acid	0.000297141	1.213385876	down
Com_471_pos	trans-Cinnamaldehyde	0.00030019	1.224924702	down
Com_1952_pos	1-(3,4-dimethoxyphenyl)ethan-1-one oxime	0.000300589	1.30378957	up
Com_190_pos	Safrole	0.000303866	1.221325914	up
Com_5178_pos	(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	0.000307773	1.275217359	up
Com_1144_pos	N alpha-Acetyl-L-lysine	0.000320878	1.214710032	up
Com_1399_neg	N-Acetyl-leucine	0.00032133	1.246395096	down
Com_1082_pos	Dihydrojasmonone	0.000324126	1.234571279	up
Com_943_pos	Kirenol	0.00032674	1.272409376	up
Com_4621_pos	Methyl Palmitate	0.000342207	1.227865559	up
Com_10692_pos	PC (22:6e/18:5)	0.000345478	1.24795859	up
Com_4232_pos	5-Methyluridine	0.000347427	1.212002118	up
Com_320_neg	Uridine	0.00035512	1.244259468	down
Com_1333_pos	L-(-)-Methionine	0.000374507	1.228781791	up
Com_1618_neg	Sinapoyl O-hexoside	0.00037934	1.253401148	down
Com_490_pos	N-Acetyl-L-Tyrosine	0.000385378	1.21698575	up
Com_3256_neg	Laricitrin	0.000398431	1.250170369	up
Com_4708_pos	LysoPC 16:1	0.000398541	1.20254329	up
Com_2376_pos	Citrinin	0.000401841	1.256126398	down
Com_7994_pos	4-([[(3-morpholinopropyl)amino]carbothioyl]amino)benzoate	0.000407267	1.23076302	up
Com_3044_neg	C-pentosyl-apeiginin O-feruloylhexoside	0.00040928	1.203155965	up
Com_1427_neg	Hesperetin 5-O-glucoside	0.000415645	1.214561817	up
Com_1447_pos	13(S)-HOTrE	0.000420957	1.210899548	down
Com_1084_neg	Iridin	0.000423109	1.244779052	down
Com_664_pos	β -Nicotinamide mononucleotide	0.000426385	1.204151798	down
Com_836_neg	Aminophylline	0.000426754	1.247826959	down
Com_3_neg	Sucrose	0.000430005	1.229054387	down
Com_5773_pos	4-[1-(dimethylamino)ethylidene]-2-phenyl-1,3-oxazol-5(4H)-one	0.000432357	1.246128152	up
Com_2012_pos	lupinine	0.000435196	1.201589977	down
Com_1015_pos	Cytidine	0.000449715	1.201677637	up
Com_1205_neg	FAHFA (2:0/20:0)	0.00045279	1.269364462	down
Com_1666_pos	2-Deoxy-D-galactose	0.000459474	1.231081807	down
Com_3413_neg	LPC 16:0	0.000459853	1.210058614	up
Com_2764_pos	3-[4-methyl-1-(2-methylpropanoyl)-3-oxocyclohexyl]propanoic acid	0.000467829	1.202826857	up

	exyl]butanoic acid			
Com_1065_pos	(5-L-Glutamyl)-L-amino acid	0.00047094	1.231894903	down
Com_2500_pos	7-Aminoclonazepam-d4	0.000471821	1.222723628	down
Com_385_neg	Pantothenate	0.000472927	1.201162257	down
Com_2854_pos	5-O-Methylvisammioside	0.000482729	1.233281456	down
Com_5637_neg	Polygalaxanthon VIII	0.000490449	1.19251198	down
Com_6456_pos	2-[2-(2-pyridyloxy)ethoxy]pyridine	0.00049718	1.208832694	down
Com_23_neg	Quinic acid	0.00049769	1.259001676	up
Com_3914_pos	S-Methyl-5'-thioadenosine	0.000528236	1.199390678	down
Com_5483_neg	LPE 16:1	0.000538386	1.208934826	up
Com_1708_neg	Antiarol	0.000544068	1.209208259	down
Com_4183_pos	α -Hydroxyalprazolam	0.000592344	1.260912111	up
Com_2076_pos	Adenosine diphosphate (ADP)	0.000620287	1.262968102	down
Com_1951_pos	(2E,4E)-N-(2-methylpropyl)deca-2,4-dienamide	0.00062884	1.237445029	down
Com_436_neg	3-(Hydroxymethyl)phenol	0.000633011	1.276515273	up
Com_3032_pos	gamma-Glutamylleucine	0.000656514	1.195614065	down
Com_135_neg	Alpha-Linolenic acid	0.000680872	1.254489046	up
Com_628_pos	Prunin	0.00068405	1.184246388	down
Com_3269_neg	Eupafolin	0.000687389	1.222001165	up
Com_4110_pos	Momordin Ic	0.000691769	1.191295675	down
Com_148_pos	Sinapinic acid	0.000691793	1.177850583	down
Com_408_pos	Pimpinellin	0.000697115	1.277604958	up
Com_5709_neg	Timosaponin A1	0.000699199	1.21372747	down
Com_5220_pos	C-pentosyl-luteolin-C-hexoside	0.000699239	1.176538007	down
Com_1611_pos	(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-(propan-2-yloxy)oxane-3,4,5-triol	0.000700025	1.206160438	down
Com_1931_pos	(-)-3-(3,4-Dihydroxyphenyl)-2-methylalanine	0.000705994	1.253575778	up
Com_3297_neg	Salvianolic acid A	0.0007069	1.17734967	up
Com_10_pos	octadec-9-ynoic acid	0.000712159	1.190682402	down
Com_3482_pos	4,7,8-trimethoxyfuro[2,3-b]quinoline	0.00071446	1.194183462	up
Com_318_pos	trans-Aconitic acid	0.000729783	1.191769216	up
Com_6401_pos	(\pm)-17(18)-EpETE	0.000738484	1.176336357	down
Com_3600_pos	Cimifugin	0.000739101	1.224190513	up
Com_124_pos	L-Tyrosine	0.000744402	1.235853055	up
Com_10008_pos	Oxypeucedanin	0.000772997	1.23700802	up
Com_1316_pos	(\pm)-Abscisic acid	0.00080387	1.191406043	down
Com_1814_pos	2,6-Diaminoimelic Acid	0.000804306	1.183530455	up
Com_1122_pos	Kynurenic acid	0.000810477	1.215510457	down
Com_663_pos	Sattabacin	0.000814585	1.234038187	down
Com_1885_pos	5-(4-methylphenyl)-2-phenyl-6H-1,3-thiazin-6-one	0.000815225	1.186901562	up
Com_121_pos	Obscurolide A1	0.000821935	1.244723821	up
Com_147_neg	4-O-p-Coumaroylquinic acid	0.000852172	1.183203435	down
Com_3756_pos	Quercetin 3- α -L-arabinofuranoside	0.000861798	1.164755904	up

	(Avicularin)			
Com_8486_pos	Ginkgolide C	0.000871585	1.202282222	up
Com_4462_neg	Parishin A	0.000884799	1.273795593	up
Com_4330_pos	16,16-Dimethyl prostaglandin A1	0.000904107	1.231991522	up
Com_914_neg	trans-Zeatin-riboside	0.00091251	1.226772368	up
Com_1365_pos	2-Methoxyresorcinol	0.000917984	1.257791675	down
Com_3593_pos	Maltotetraose	0.000924286	1.181481481	down
Com_1040_pos	Glutathione	0.000927512	1.257600185	up
Com_587_pos	methylChrysoeriol C-hexoside	0.00094105	1.161792367	down
Com_4511_pos	Ala-Ile	0.000942369	1.211739984	up
Com_1130_neg	Maltitol	0.000981511	1.185988918	down
Com_8613_pos	HPK	0.000981802	1.243622276	up
Com_4116_neg	Pedunculoides	0.001017404	1.18168092	up
Com_2558_neg	Esculetin	0.00103009	1.170466534	up
Com_517_pos	N-(2,6-Dimethylphenyl)-N-(methoxyacetyl) alanine	0.001043659	1.187863558	up
Com_3340_pos	Quinoline	0.001059935	1.157726302	down
Com_2738_pos	4-acetyl-4-(ethoxycarbonyl)heptanedioic acid	0.001089848	1.200803984	down
Com_4230_pos	2-piperidinobenzoic acid	0.001103053	1.213035809	up
Com_2306_neg	Bergenin	0.001119859	1.170479993	up
Com_476_pos	Palmitoleic Acid	0.001126496	1.170463811	up
Com_7790_pos	Palmatine	0.001166266	1.173823284	up
Com_2129_neg	Toddalolactone	0.001186768	1.165683309	down
Com_2766_neg	Pectolarin	0.001187107	1.157714548	up
Com_1427_pos	2,4-dihydroxyheptadec-16-en-1-yl acetate	0.001201121	1.164341107	up
Com_741_pos	Quercetin	0.001208929	1.218636431	up
Com_3145_neg	Pinosresinol Diglucoside	0.001222129	1.147324146	up
Com_3424_pos	4-amino-2-(2,4-dimethoxyanilino)-5-pyrimidinecarbonitrile	0.001224237	1.171410702	up
Com_4697_pos	N-Acetylglucosamine 1-phosphate	0.001235362	1.241844633	down
Com_2442_pos	LPE 18:1	0.00124602	1.194618655	up
Com_9454_pos	1-O-(3,4,5-Trimethoxybenzoyl)-beta-L-galactopyranose	0.001295632	1.220100227	down
Com_1800_pos	Hypoxanthine	0.001328452	1.163073015	down
Com_1673_pos	D-Panthenate	0.001385799	1.165489537	down
Com_15_pos	Chlorogenic acid	0.001405727	1.230296798	up
Com_4949_neg	Gossypol	0.001518056	1.162642985	up
Com_4852_neg	L-Leucyl-L-alanine Hydrate	0.001570299	1.148999735	up
Com_1230_pos	Bornyl acetate	0.001592615	1.135251771	up
Com_5077_pos	N-Feruloyl putrescine	0.001616339	1.1452347	up
Com_293_pos	2-Phenylacetamide	0.001625655	1.165234689	up
Com_1814_neg	Pantetheine	0.001687093	1.133656358	down
Com_928_neg	5-oxoproline	0.001687124	1.183883104	up
Com_491_pos	6-Hydroxymethylherniarin	0.001737702	1.140136713	down

Com_5032_pos	FPH	0.001743804	1.142187784	up
Com_475_neg	7-Hydroxycoumarin	0.00174752	1.2215885	up
Com_566_pos	4-(2,3-dihydro-1,4-benzodioxin-6-yl)butanoic acid	0.001758901	1.177842132	up
Com_1844_pos	Methyl Dihydrojasmonate	0.00176526	1.211887112	down
Com_6518_pos	AL 8810	0.00176852	1.24336655	up
Com_1010_pos	16H-dinaphtho[2,1-d:1,2-g][1,3]dioxocine	0.001829527	1.243364585	up
Com_5354_pos	3,14-dihydro-15-keto-tetranor Prostaglandin E2	0.00183346	1.141662782	up
Com_1540_pos	Ginkgolic acid C17-1	0.001839902	1.210504149	up
Com_968_neg	Sophoricoside	0.001954371	1.159480941	down
Com_4323_neg	Thymidine	0.001966105	1.164003107	up
Com_8193_pos	2'-Hydroxygenistein	0.002021713	1.165573293	up
Com_37_pos	Hexadecanamide	0.002135977	1.115971147	down
Com_324_pos	N-Acetylphenylalanine	0.002136071	1.127839302	down
Com_3036_neg	Calceolarioside B	0.002152339	1.167504698	up
Com_358_neg	3-[(Carboxycarbonyl)amino]-L-alanine	0.002201955	1.134715416	up
Com_3192_neg	Eriodictyol O-malonylhexoside	0.002209851	1.215106245	down
Com_4361_pos	Dehydroaripiprazole	0.00223502	1.16886506	down
Com_8187_pos	Arachidonoyl ethanolamide phosphate	0.002270877	1.140019964	up
Com_4115_pos	Sphingosine (d18:1)	0.002282178	1.185788347	up
Com_3734_pos	methyl 3,4,5-trihydroxycyclohex-1-ene-1-carboxylate	0.002299112	1.13848307	up
Com_2444_pos	Sorbic acid	0.002314285	1.173438833	down
Com_894_neg	Alisol B	0.002374618	1.152346807	down
Com_5469_pos	Tectochrysin	0.002380938	1.116707603	up
Com_8162_pos	Alnustone	0.002423107	1.117415773	up
Com_915_pos	Isorhamnetin	0.002428389	1.198338777	up
Com_3190_neg	1,4-Cyclohexanedicarboxylic acid	0.002444257	1.172271971	down
Com_6440_pos	Nobiletin	0.002449369	1.167021579	down
Com_2375_pos	N3,N4-Dimethyl-L-arginine	0.002471389	1.104340709	up
Com_207_neg	1-O-Feruloyl quinic acid	0.002602114	1.165888875	up
Com_306_pos	Cantharidin	0.002643359	1.168831964	up
Com_4846_pos	Chrysin	0.002670319	1.118610762	up
Com_3624_neg	Kaempferol-3-gentiobioside	0.002715884	1.108237943	up
Com_357_pos	Coumarin	0.00274449	1.123748121	down
Com_358_pos	p-Aminocinnamic acid	0.00274449	1.123748121	down
Com_445_pos	6-Methylquinoline	0.002828274	1.207646371	down
Com_2078_neg	L-Tryptophan	0.002913894	1.112984134	down
Com_2125_neg	Eriodictyol	0.003003286	1.111129584	up
Com_1895_neg	D-beta-Homophenylalanine	0.003017883	1.122878764	down
Com_3221_neg	Astringin	0.003020313	1.184985886	up
Com_2895_pos	Diosmetin	0.003047524	1.175222745	down
Com_1522_neg	DL-m-Tyrosine	0.003065596	1.169399376	up
Com_192_pos	9-Oxo-ODE	0.003142826	1.13218025	up

Com_362_pos	LPE 18:3	0.00316071	1.153294475	up
Com_3544_neg	Pectolarigenin	0.003269583	1.169030374	down
Com_7928_pos	Sugiol	0.003354397	1.150675726	down
Com_2433_neg	Indolelactic acid	0.003359351	1.167374607	down
Com_618_neg	Diosmetin-7-O-β-D-glucopyranoside	0.003367615	1.174478483	down
Com_6459_pos	S-Adenosyl-L-homocysteine	0.00339976	1.122225372	down
Com_4736_pos	2-morpholino-1-phenyl-1-ethanol	0.003408849	1.148335167	up
Com_3072_pos	Fosfosal	0.00341157	1.187507168	down
Com_2673_pos	PharmaGSID_47333	0.003484468	1.16463016	down
Com_7682_pos	Wilforlide A	0.003512585	1.149435549	down
Com_5904_pos	Oroxylin A	0.003569067	1.118207326	up
Com_1552_pos	PC (14:0e/2:0)	0.00362551	1.163838177	up
Com_348_neg	Lonicerin	0.003782239	1.084362505	down
Com_1710_neg	Abscisic acid	0.003832755	1.08225665	down
Com_3078_pos	5-methoxy-8,8-dimethyl-2-phenyl-4H,8H-pyrano [2,3-h]chromen-4-one	0.003882813	1.164137077	up
Com_9378_pos	Isomaltose	0.003908623	1.166017767	up
Com_2102_neg	O-p-coumaroyl-O-salicyloyl quinic acid	0.003914567	1.103234106	up
Com_558_pos	2,3-Dinor-8-epi-prostaglandin F2α	0.003950349	1.098933943	up
Com_6326_pos	Leonurine Hydrochloride	0.004111445	1.098543069	up
Com_1993_pos	Corticosterone	0.004161051	1.107421539	up
Com_2530_pos	Leucylproline	0.004179574	1.11593169	up
Com_7900_pos	11(Z),14(Z),17(Z)-Eicosatrienoic acid	0.004289541	1.151975581	up
Com_4003_pos	Ganoderiol A	0.004321926	1.176853259	down
Com_329_neg	Roseoside	0.004366746	1.129895479	down
Com_4554_pos	Indole-3-acrylic acid	0.004410713	1.160332113	down
Com_5053_pos	Roburic acid	0.004487206	1.189565152	down
Com_897_pos	Scopoletin	0.00450568	1.08051153	down
Com_782_pos	Succinic anhydride	0.004543932	1.167462491	down
Com_4657_neg	2'-O-acetylpoliumoside	0.00457517	1.067646947	up
Com_251_neg	R-Aminobutyrate	0.004647921	1.08988987	down
Com_342_pos	Prostaglandin K2	0.004889401	1.081759584	up
Com_8197_pos	Ziyuglycoside II	0.004953049	1.145520877	down
Com_3605_pos	Ligustilide	0.004966044	1.124961552	down
Com_6148_pos	2-{2-oxo-2H,8H,9H-furo[2,3-h]chromen-8-yl}pr opan-2-yl acetate	0.005038461	1.073869519	up
Com_5744_pos	N alpha-Acetyl-L-Arginine	0.005081345	1.078417272	down
Com_2266_pos	1,4-dihydroxyheptadec-16-en-2-yl acetate	0.005361353	1.058276493	up
Com_424_pos	Gamma-Aminobutyric acid	0.005392619	1.066693706	down
Com_2613_pos	Methionine sulfoxide	0.005495164	1.14496915	up
Com_1112_neg	Protocatechuic acid	0.005787634	1.149257696	up
Com_2183_pos	3-N-butyl-4,5-dihydrophthalide	0.005934436	1.047788809	down
Com_7258_pos	4-[4-phenyl-3,6-dihydro-1(2H)-pyridinyl]butanoi c acid hydrochloride	0.005981653	1.10063774	up

Com_869_pos	PC (5:0/13:1)	0.005997176	1.102207692	up
Com_3040_pos	Methyl Eugenol	0.006014197	1.05726726	up
Com_3343_pos	Skatole	0.006079737	1.060513184	down
Com_4726_pos	Tetranor-12R-HETE	0.00613104	1.116435381	up
Com_218_neg	Lumichrome	0.006136801	1.0446919	down
Com_9267_pos	2-(2-hydroxy-3-methylbutanamido)-4-methylpentanoic acid	0.006228747	1.153801119	up
Com_2239_neg	Rhein 8-Glucoside	0.006324482	1.043585923	up
Com_4346_neg	Tricin 5-O-hexosyl-O-hexoside	0.006406226	1.093907081	up
Com_6448_pos	Dihydroartemisinic acid	0.006461559	1.033840523	up
Com_195_neg	Attractyloside A	0.006477635	1.152780062	down
Com_2026_neg	Nicotinamide adenine dinucleotide	0.006596369	1.030998133	down
Com_2524_pos	2-acetamido-3-(4-methoxyphenyl)propanoic acid	0.006826029	1.081842289	up
Com_147_pos	trans-3-Indoleacrylic acid	0.006966216	1.054321172	down
Com_4125_pos	PC (14:1e/2:0)	0.006966705	1.05177685	down
Com_8379_pos	Indirubin	0.00701388	1.042438591	down
Com_45_neg	L-Asparate	0.007247141	1.053085606	down
Com_5609_neg	Epimedin C	0.00732969	1.151030329	down
Com_954_pos	methyl 2-[(2-acetyl-3-oxo-1-butenyl)amino]acetate	0.007436663	1.104860346	up
Com_268_pos	N-Acetylglucosamine	0.00749841	1.079864094	down
Com_3799_pos	Nicotinamide adenine dinucleotide phosphate (NADP+)	0.007550038	1.037894971	up
Com_3802_pos	Lithocholic acid	0.007630593	1.027027805	up
Com_659_neg	Parishin E	0.007657278	1.047475744	down
Com_3770_pos	Neonuezhenide	0.007681175	1.064177488	down
Com_110_pos	1-(3-acetyl-2,4,6-trihydroxyphenyl)ethan-1-one	0.007731455	1.025350707	down
Com_1399_pos	3-Methoxy prostaglandin F1 α	0.007790956	1.046485063	up
Com_127_neg	Methylenesuccinic acid	0.007903792	1.01997652	up
Com_2018_pos	TriacetonaMine	0.007937628	1.048142332	down
Com_6516_pos	Methyl oleate	0.008130154	1.013180616	down
Com_7_pos	D-(+)-Proline	0.008141275	1.112335002	up
Com_10296_pos	Geranylgeraniol	0.008215495	1.094831173	down
Com_4754_pos	Glabrolide	0.008247098	1.025594849	down
Com_8764_pos	gamma-Glutamate-Cysteine	0.008264927	1.103187348	up
Com_442_neg	Selgin C-hexoside	0.008376751	1.054845439	up
Com_220_pos	N-Methyl-a-aminoisobutyric acid	0.008677748	1.039804937	up
Com_964_pos	9,17-Octadecadiene-12,14-diyne-1,11,16-triol	0.008752431	1.021246657	up
Com_2815_pos	Tropine	0.008815467	1.016649976	down
Com_69_neg	D-Erythronolactone	0.008817845	1.06930353	down
Com_10007_pos	Eupalinolide A	0.009190763	1.084672884	down
Com_468_neg	Leucinic acid	0.009350497	1.079223889	down
Com_6275_pos	Levodopa	0.009650472	1.092140813	down
Com_1579_pos	3-(1,3-benzoxazol-2-ylthio)-5,5-dimethylcyclohe	0.009679367	1.047950133	down

	x-2-en-1-one			
Com_8298_pos	PC (18:5e/22:5)	0.009689639	1.031679294	up
Com_2287_neg	Adenosine 3',5'-cyclic monophosphate	0.00983227	1.063226894	up
Com_6103_neg	Lancerin	0.009916249	1.011755971	down
Com_2845_pos	N-Acetyl-L-carnosine	0.01007164	1.102395725	up
Com_4506_pos	gamma-Glu-Leu	0.010100315	1.017211309	up
Com_1804_pos	Prim-O-glucosylcimifugin	0.0101777	1.029915325	down
Com_1098_pos	Linoleoyl ethanolamide	0.01025373	1.107629742	up
Com_6448_neg	Gelsemine	0.010393597	1.122738647	down
Com_1101_pos	N-Acetyl-DL-glutamic acid	0.010410205	1.057574081	down
Com_1300_pos	8-Hydroxyquinoline	0.010415614	1.027651143	down
Com_859_neg	Plantagoside	0.010993234	1.022997131	up
Com_277_neg	Isoliquiritin apioside	0.01133168	1.076338893	up
Com_4264_neg	di-C,C-pentosyl-apigenin	0.011370078	1.008137703	up
Com_10523_pos	Protobioside	0.011575506	1.016621046	down
Com_3063_pos	Linderane	0.011647785	1.02953378	up
Com_2862_pos	2-{2-[(4-chlorophenyl)sulfonyl]ethyl}cyclohexan-1-one	0.011811129	1.092005547	down
Com_619_neg	Octanedioic acid	0.012116164	1.06138319	down
Com_3255_neg	Eleutheroside E	0.012214394	1.068550816	down
Com_2732_pos	Irisfloreantin	0.012290685	1.001919586	up
Com_597_pos	2-[(3S)-1-(2-Chlorobenzyl)-3-pyrrolidinyl]-5-methyl-1,3,4-oxadiazole	0.012433724	1.084427739	up
Com_10181_pos	Dihydrocapsaicin	0.013006969	1.011836362	up
Com_847_pos	4-(4-methoxyphenyl)-6-pyridin-4-yl-1,3,5-triazin-2(3H)-one	0.013320579	1.03735302	up
Com_567_pos	4-(3,4-dihydro-2H-1,5-benzodioxepin-7-ylamino)-4-oxobutanoic acid	0.014011942	1.001411059	up
Com_219_neg	Apigenin-7-O-β-D-glucoside	0.015696674	1.0475457	down
Com_1782_pos	6-Sialyllactose	0.01609101	1.042521092	down
Com_6593_pos	Moslosooflavone	0.016216093	1.03931382	down
Com_9500_pos	Arenobufagin	0.016722937	1.018568236	up
Com_811_pos	5'-S-Methyl-5'-thioadenosine	0.018794384	1.023260143	down
Com_3690_pos	N1-isopropyl-2-(1H-2-pyrrolylcarbonyl)-1-hydrazinecarboxamide	0.022826807	1.020443125	down

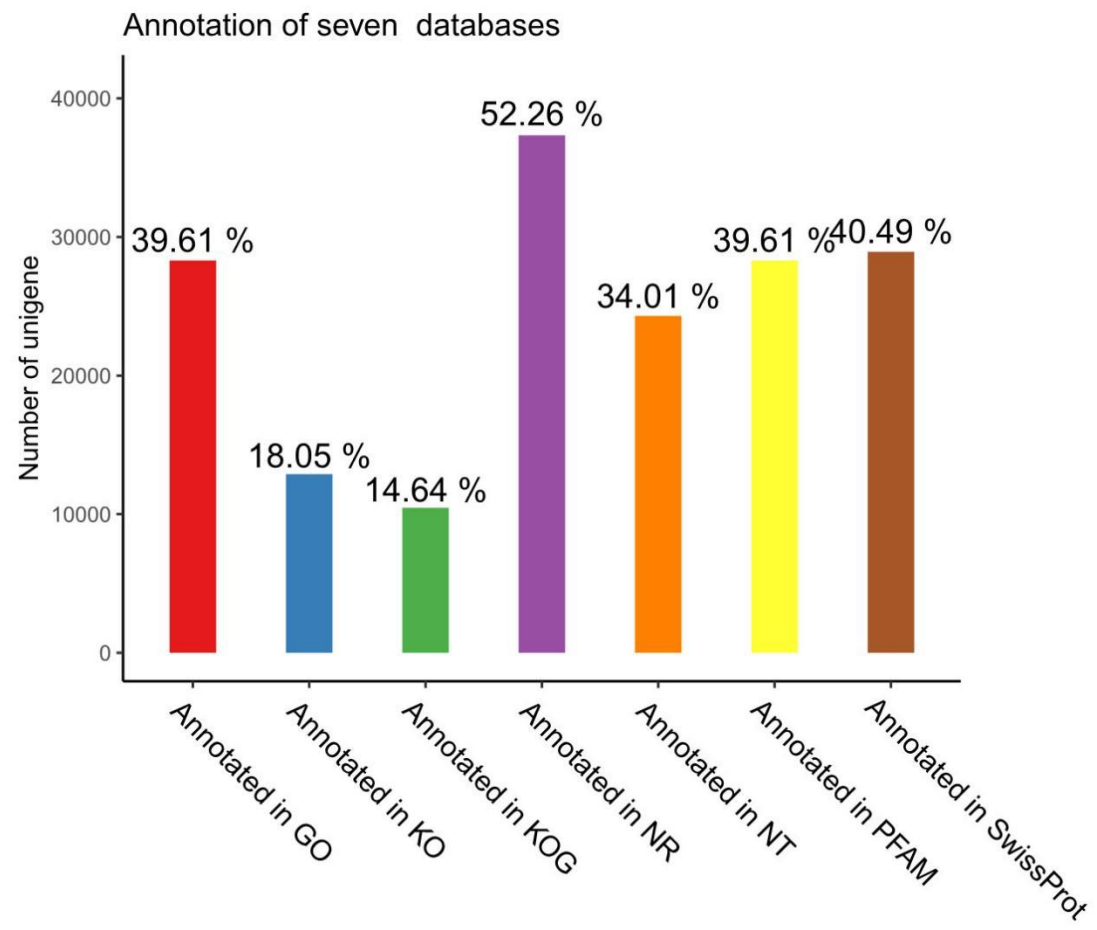


Fig S1. The number of unigenes annotated by NR, Swissprot, PFAM, GO, NT, KO and KOG databases.

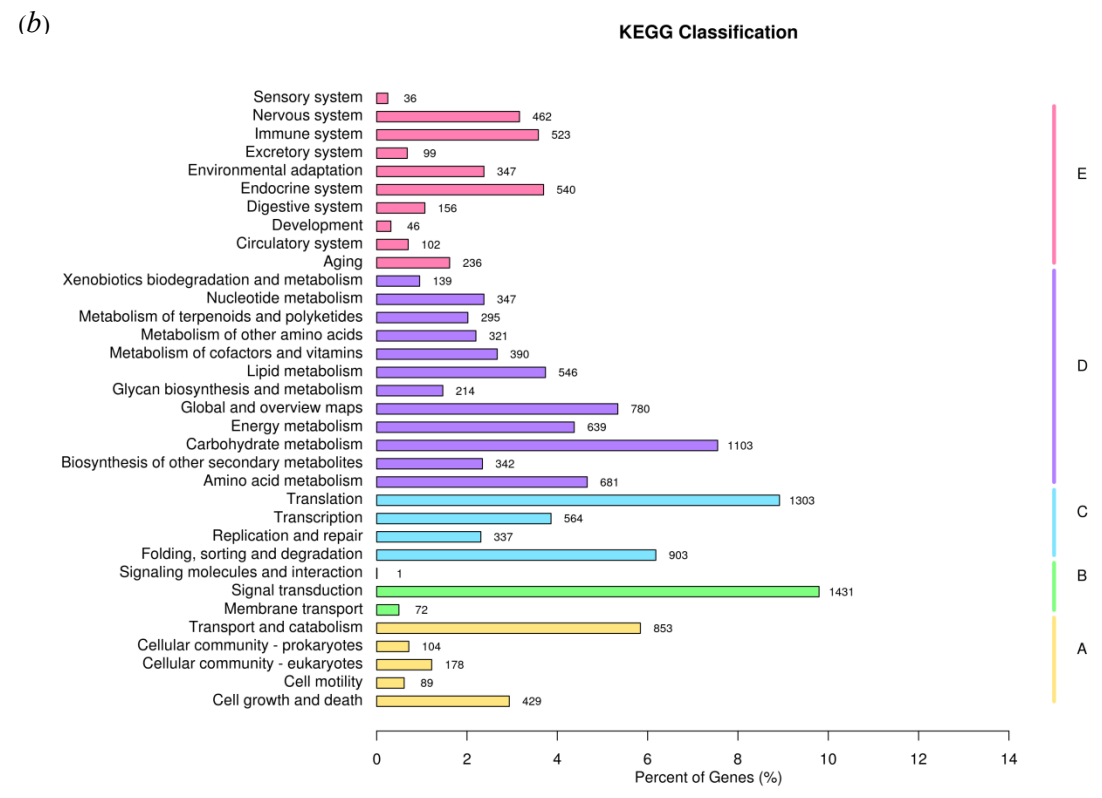
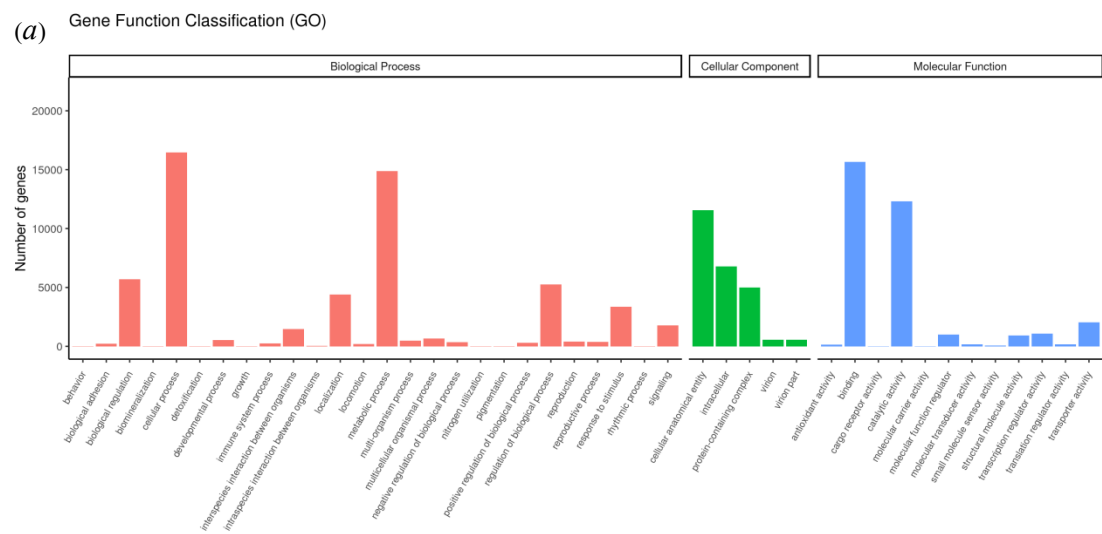


Fig S2. Classification of annotated GO and KEGG terms. (a) All unigenes were assigned to different GO terms. (b) All unigenes were assigned to different KEGG terms, including A cellular processes; B environmental information processing; C genetic information processing; D metabolism; E organismal systems.

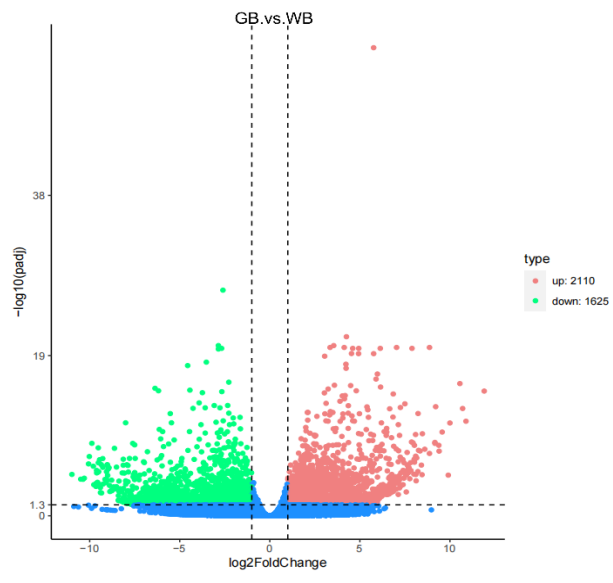


Fig S3. The volcano plots of the DEGs in GB and WB stages.

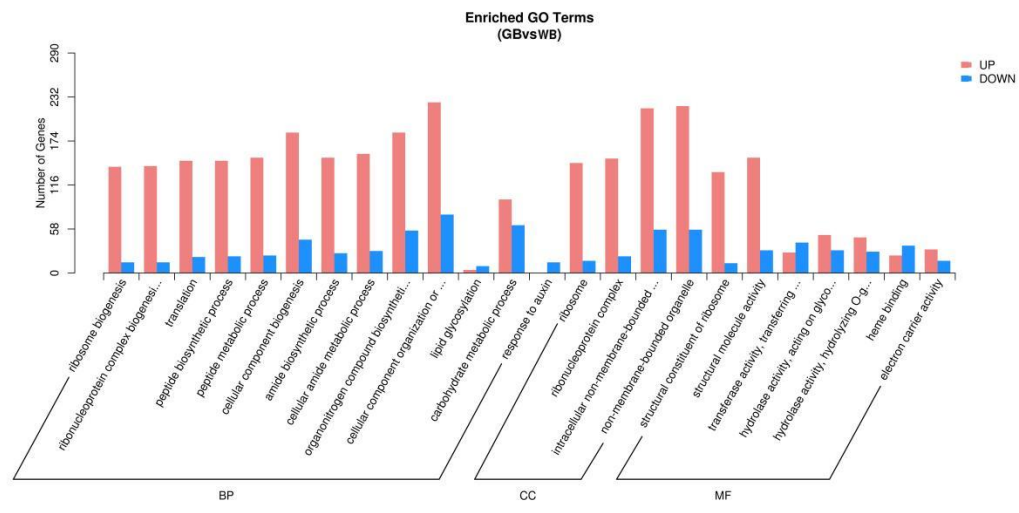


Fig S4. GO enrichment analysis of DEGs in the different harvesting stages of *L. japonica*.

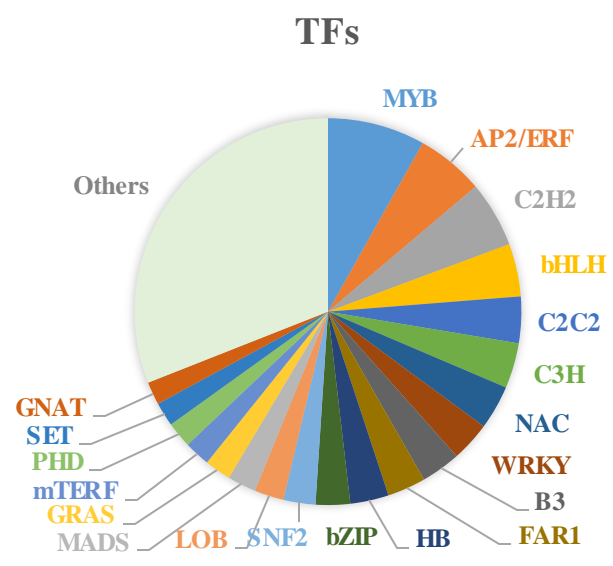


Fig S5. Family distribution of TFs in GB stage and WB stage. The TFs family that the members in it less than forty was considered as others.

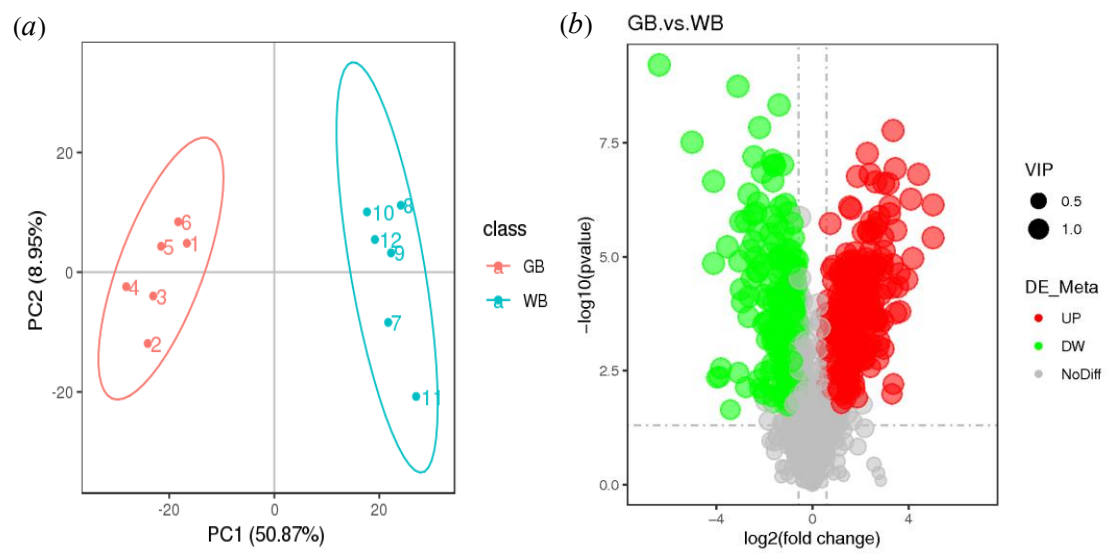


Fig S6. Metabolomics data analysis. (a) PCA score plot metabolite profiles from different harvesting stages. (b) Volcano plots of different metabolites in GB stage and WB stage (up-regulation of different metabolites in GB stage was described to be “up”).

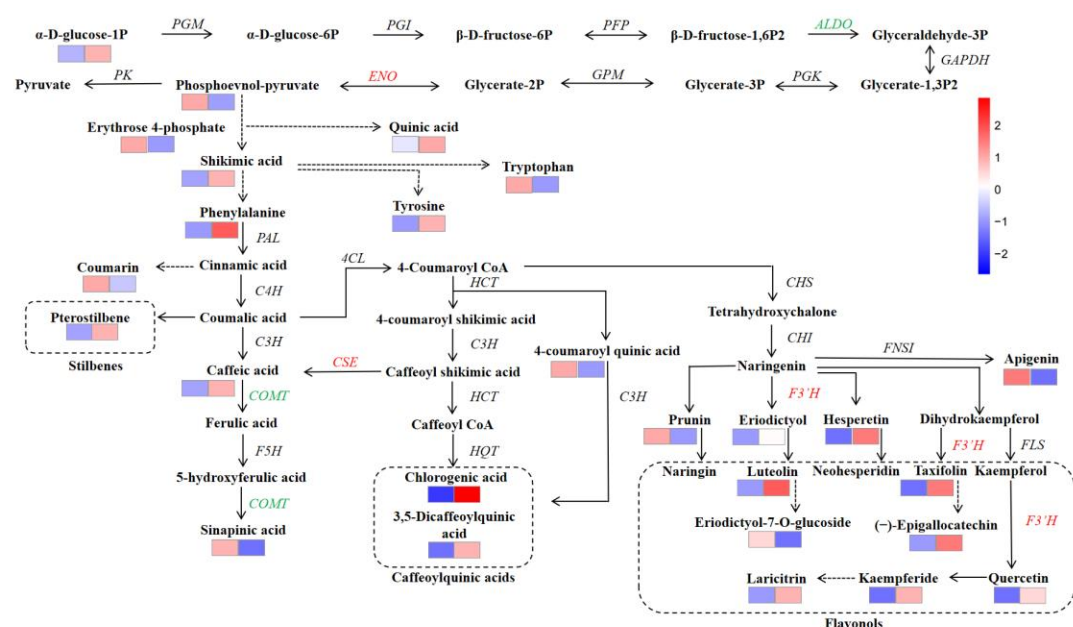


Fig S7. Effects of different harvesting stages on the glycolysis/gluconeogenesis and phenylpropanoid biosynthesis pathways. The changes of metabolites are represented by color blocks, the red color blocks indicate the up-regulation of metabolites and blue color blocks indicate down-regulated of metabolites. Changes in gene expression are shown in italics, red font indicates up-regulation, while green font indicates down-regulation.

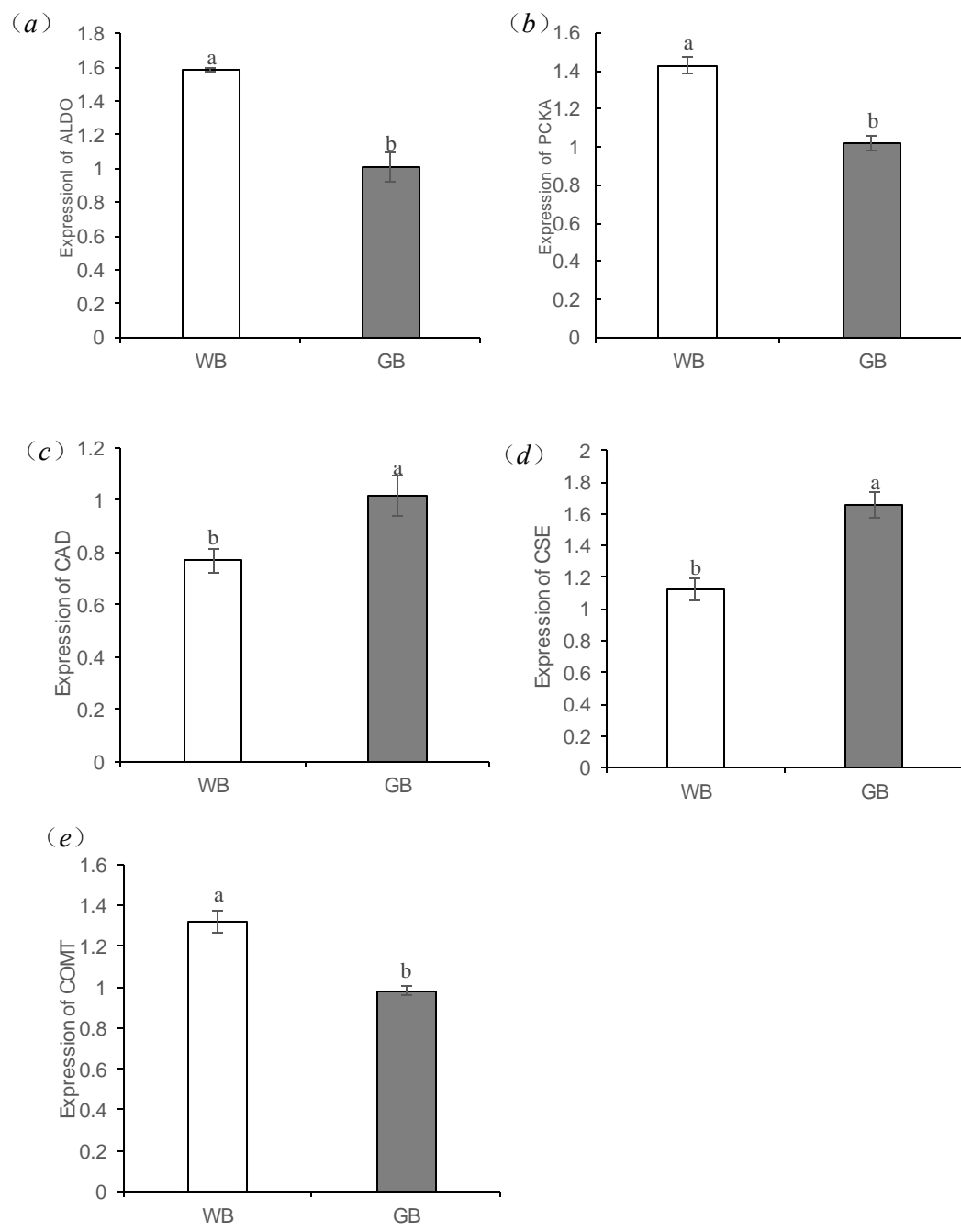


Fig S8. Relative expression of genes involved in glycolysis/gluconeogenesis and phenylpropanoid biosynthesis in two stages. (a) ALDO. (b) PCKA. (c) CAD. (d) CSE. (e) COMT. Different letters indicate significant differences at $P < 0.05$.