

Figure S1 Base peak chromatogram in positive and negative ion modes of WT and T51
Note: a is positive ion mode; b is negative ion mode.

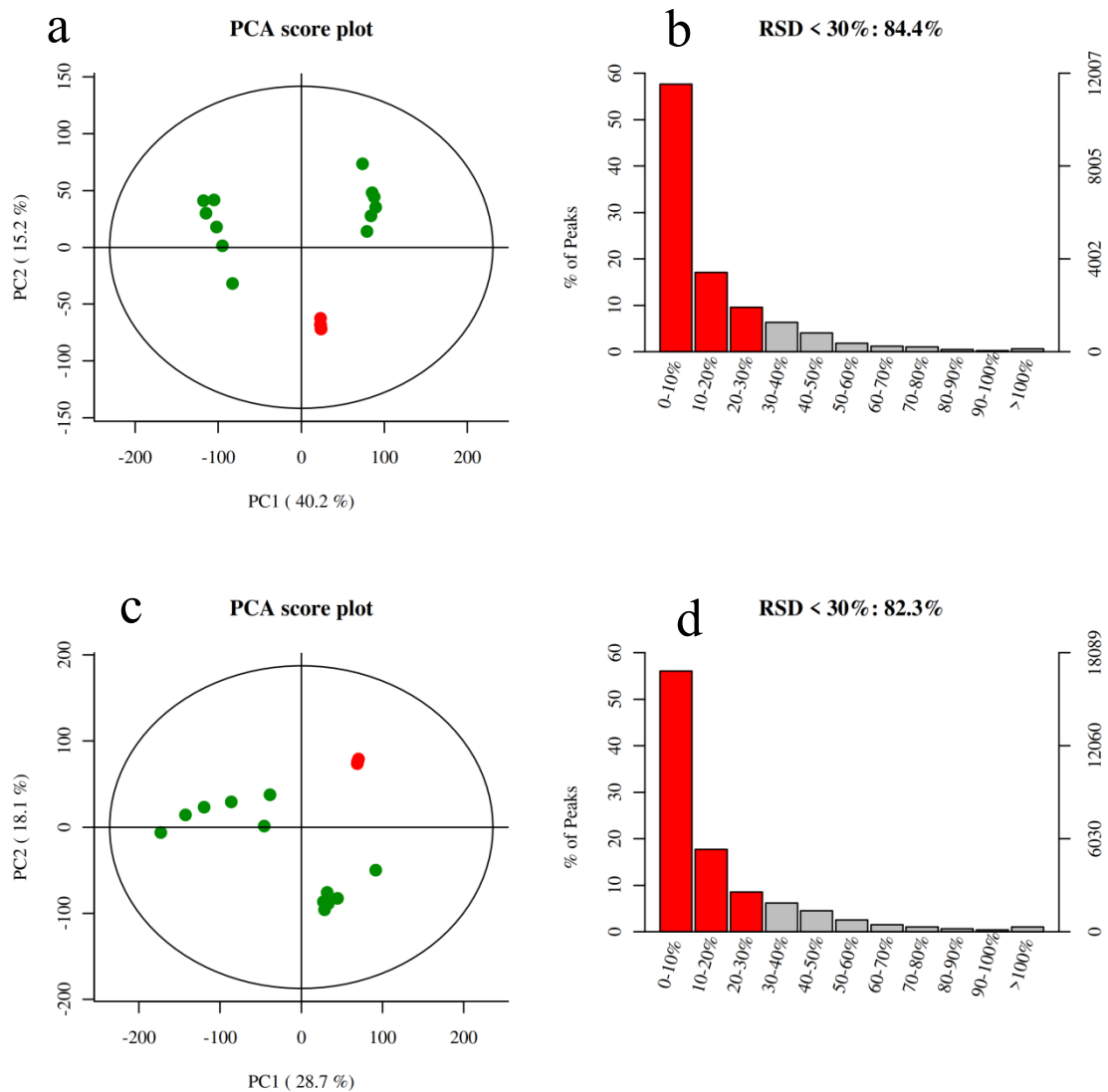


Figure S2 QC and QA scores plot in positive and negative ion modes of WT and T51
 Note: A is QC scores in positive ion mode; C is QC scores of negative ion mode; B is QA scores of positive ion mode; D is QA scores of negative ion mode.

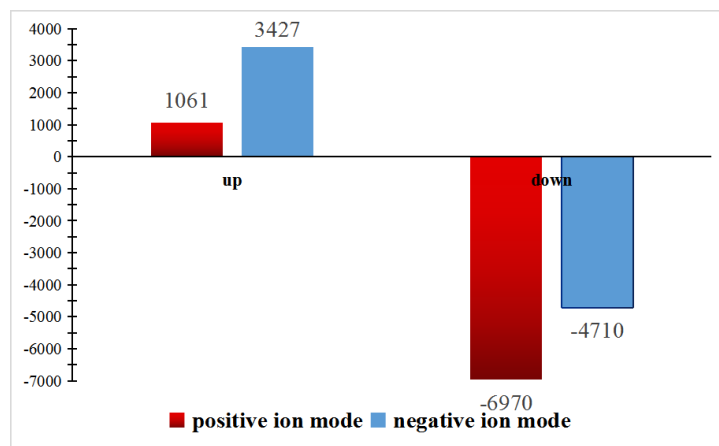


Figure S3 Metabolite statistics in T51 and WT

Table S1 Statistical table of differential metabolites

No.	Metabolite name	VIP	log2(FC)	p.value
1	7-Methyladenine	1.262	14.597	0.005
2	Coniferin	1.457	8.375	0.005
3	3-O-Methylquercetin	1.197	6.122	0.005
4	Etilefrine	1.669	5.404	0.005
5	Phenylephrine	1.558	5.297	0.005
6	Galactitol	1.474	4.924	0.005
7	2-Phenylacetamide	1.764	4.779	0.005
8	Dihydroxyacetone phosphate dilithium salt	1.698	4.757	0.005
9	Aminoadipic acid	1.456	4.025	0.005
10	(S)-Absciscic acid	1.592	3.738	0.005
11	Malvidin 3-glucoside	1.175	3.735	0.005
12	Isoproterenol	1.666	3.659	0.005
13	Coumarin	1.783	3.47	0.005
14	N-Acetyltyramine	1.346	3.216	0.008
15	Apigenin	1.065	3.079	0.005
16	Salidroside	1.468	2.902	0.005
17	Melibiose	1.447	2.833	0.005
18	3-alpha(S)-Strictosidine	1.232	2.814	0.008
19	Oxazepam	1.431	2.642	0.005
20	Quercetin	1.285	2.519	0.005
	3-O-[beta-D-xylosyl-(1->2)-beta-D-glucoside]			
21	Isoquercitrin	1.288	2.261	0.005
22	Tyramine	1.678	2.203	0.005
23	Anserine	1.417	2.117	0.008
24	Azacitidine	1.425	2.114	0.013
25	Glycitein	1.254	2.066	0.031
26	Erythritol	1.347	2.044	0.005
27	Nevadensin	1.239	1.962	0.005
28	Hesperetin	1.412	1.73	0.005
29	2-Aminophenol	1.045	1.723	0.031
30	N-Glucosylnicotinate	1.6	1.684	0.005
31	3-Hydroxyanthranilate	1.432	1.671	0.005
32	Erucic acid	1.109	1.538	0.031
33	Demethylweddelolactone	1.255	1.489	0.005
34	Carbadox	1.378	1.458	0.008
35	Luteolin	1.489	1.453	0.005
36	Hesperetin 7-O-glucoside	1.394	1.392	0.005
37	Methyl jasmonate	1.684	1.131	0.005
38	Geniposidic acid	1.103	1.108	0.02
39	Riboflavin	1.397	1.107	0.005
40	Glutathione	1.415	1.038	0.005
41	Rutin	1.382	1.032	0.005

42	Diosmin	1.044	1.011	0.02
43	Ascorbate	1.1	0.772	0.013
44	Piceatannol	1.325	0.756	0.005
45	Squalene	1.087	0.712	0.008
46	N-Acetylleucine	1.467	0.694	0.005
47	1,3-Benzenediol	1.316	0.642	0.005
48	Gardenoside	1.116	0.567	0.031
49	Salicylic acid	1.003	0.497	0.02
50	Paxilline	1.109	0.484	0.045
51	Cytidine, cyclic 2,3-(hydrogen phosphate), monosodium salt	1.394	0.48	0.005
52	Adenine	1.356	0.467	0.005
53	Forsythoside E	1.045	0.398	0.02
54	Fructose 1,6-bisphosphate	1.061	0.318	0.013
55	Glycylleucine	1.155	0.182	0.008
56	m-Cresol	1.05	-0.086	0.031
57	Betaine	1.484	-0.274	0.005
58	Agmatine	1.026	-0.286	0.045
59	L-Homocysteic acid	1.393	-0.294	0.005
60	Stearidonic acid	1.146	-0.311	0.008
61	5,7-Dihydroxyflavone	1.16	-0.375	0.02
62	CID 234817	1.385	-0.377	0.005
63	Rimantadine	1.653	-0.388	0.005
64	2,6-Dihydroxy-4-methoxyacetophenone	1.4	-0.405	0.005
65	Uridine-5-diphosphate disodium salt	1.027	-0.421	0.008
66	cis-Aconitic acid	1.062	-0.431	0.005
67	Androsterone	1.198	-0.519	0.031
68	8-O-Acetylharpagide	1.157	-0.535	0.02
69	6-Acetyl-D-glucose	1.246	-0.539	0.005
70	Sodium 3-methyl-2-oxopentanoate	1.446	-0.552	0.005
71	Deoxycytidine	1.083	-0.56	0.005
72	D-Arabitol	1.463	-0.563	0.005
73	Neocnidilide	1.1	-0.572	0.005
74	S-Adenosylmethionine	1.554	-0.587	0.005
75	Prostaglandin J2	1.278	-0.59	0.005
76	11,12,15-THETA	1.502	-0.617	0.005
77	alpha-Tocopherol	1.188	-0.62	0.02
78	Vanillic acid	1.33	-0.652	0.005
79	Melibiitol	1.016	-0.661	0.045
80	Isovitexin	1.126	-0.688	0.008
81	5,6-DHET	1.184	-0.707	0.031
82	N-Acetyl-DL-methionine	1.242	-0.708	0.031
83	Esculin	1.224	-0.709	0.005
84	Cortisol	1.208	-0.712	0.013

85	1H-Indole-3-carboxaldehyde	1.453	-0.719	0.005
86	4-Hydroxy-3-methoxy-benzaldehyde	1.571	-0.72	0.005
87	Sodium deoxycholate	1.274	-0.784	0.031
88	Niacinamide	1.386	-0.785	0.005
89	Limonin	1.139	-0.786	0.008
90	Fumaric acid	1.196	-0.788	0.005
91	Metoclopramide	1.46	-0.79	0.005
92	Trehalose	1.39	-0.792	0.02
93	2,4-Dinitrophenol	1.455	-0.792	0.005
94	Pyridoxal	1.623	-0.795	0.005
95	Prostaglandin F2a	1.534	-0.803	0.008
96	Pantothenic acid	1.527	-0.817	0.005
97	Sorbitol	1.563	-0.828	0.005
98	3,4-Dihydroxymandelic acid	1.198	-0.835	0.031
99	Azelaic acid	1.687	-0.84	0.005
100	2-O-(alpha-D-Mannosyl)-D-glycerate	1.186	-0.843	0.008
101	Tetrahydrocorticosterone	1.6	-0.847	0.008
102	Rosmarinic acid	1.366	-0.867	0.005
103	(+)-Syringaresinol O-beta-D-glucoside	1.13	-0.886	0.008
104	Palmitoylethanolamide	1.19	-0.918	0.02
105	Sucrose	1.119	-0.919	0.045
106	Nandrolone phenpropionate	1.352	-0.935	0.013
107	Alpha-Linolenic acid	1.25	-0.943	0.031
108	Safrole	1.518	-0.958	0.005
109	Xanthoxylin	1.451	-0.967	0.005
110	6beta-Hydroxytestosterone	1.659	-1.006	0.005
111	Deoxycholic acid	1.674	-1.006	0.005
112	Apigenin 7-O-neohesperidoside	1.149	-1.008	0.031
113	Nicotinamide riboside	1.32	-1.009	0.031
114	Leukotriene D4	1.17	-1.015	0.005
115	L-Isoleucine	1.546	-1.051	0.005
116	Uracil	1.694	-1.094	0.005
117	(9Z,11E,13E)-Octadecatrienoic acid	1.402	-1.1	0.013
118	Zedoarondiol	1.424	-1.111	0.013
119	Dihydrotestosterone	1.138	-1.124	0.045
120	Stachyose	1.332	-1.155	0.005
121	Indolepyruvic acid	1.209	-1.156	0.005
122	Potassium;(3,4,5,6-tetrahydroxyoxan-2-yl)methyl hydrogen phosphate	1.014	-1.175	0.005
123	Lonicerin	1.084	-1.183	0.031
124	Mirtazapine	1.507	-1.185	0.008
125	Calcitriol	1.494	-1.186	0.005
126	Stearidonoyl glycine	1.355	-1.213	0.02
127	L-Proline	1.807	-1.218	0.005

	2-[3-[(4-Amino-2-methylpyrimidin-5-yl)methyl]			
128	-4-methyl-1,3-thiazol-3-ium-5-yl]ethyl	1.191	-1.262	0.045
	dihydrogen phosphate;chloride;dihydrate			
129	Syringic acid	1.74	-1.275	0.005
130	10-Nitrolinoleic acid	1.53	-1.282	0.005
131	Linoleic acid	1.606	-1.294	0.005
132	21-Hydroxypregnenolone	1.502	-1.315	0.013
133	trans-Ferulic acid	1.713	-1.316	0.005
134	Fludrocortisone	1.672	-1.321	0.005
135	Xanthoxic acid	1.676	-1.321	0.005
136	Progesterone	1.207	-1.341	0.013
137	3-Indoleacetic acid	1.138	-1.342	0.02
138	Uric acid	1.376	-1.348	0.02
139	Cirsilineol	1.145	-1.353	0.031
140	Scopoletin	1.467	-1.358	0.005
141	Pelargonic acid	1.084	-1.38	0.045
142	Carnosol	1.726	-1.39	0.005
143	Arbutin	1.429	-1.405	0.005
144	19(R)-HETE	1.564	-1.407	0.005
145	Costunolide	1.155	-1.419	0.045
146	Palmitoleic acid	1.507	-1.423	0.005
147	Swertiajaponin	1.572	-1.433	0.005
148	(+)-(S)-Carvone (+)	1.808	-1.441	0.005
149	Dodecanedioic acid	1.796	-1.446	0.005
150	Phenylethyl primeveroside	1.565	-1.455	0.005
151	Xanthine	1.666	-1.456	0.005
152	LysoPA(16:0/0:0)	1.078	-1.461	0.013
153	Cinnamaldehyde	1.13	-1.469	0.045
154	Cytidine	1.422	-1.477	0.005
155	3alpha,20alpha,21-Trihydroxy-5beta-pregnan-11-one	1.247	-1.499	0.029
156	3-Methoxycinnamic acid	1.561	-1.506	0.005
157	Prephytoene diphosphate	1.217	-1.521	0.02
158	Luteolin 7-galactoside	1.431	-1.535	0.005
159	Ethyl oleate	1.258	-1.539	0.045
160	5-Hydroxymethylfurfural	1.343	-1.578	0.013
161	Sinapyl alcohol	1.743	-1.586	0.005
162	Citrinin	1.62	-1.633	0.005
163	2,3-Cyclic CMP	1.418	-1.634	0.005
164	12,13-DHOME	1.543	-1.729	0.013
165	Ethyl ferulate	1.761	-1.734	0.005
166	FMN	1.255	-1.741	0.005
167	Cyanidin 3-glucoside	1.575	-1.769	0.008
168	UMP	1.36	-1.777	0.005

169	Hypoxanthine	1.673	-1.791	0.005
170	N7-Methylguanosine	1.544	-1.817	0.005
171	Estrone	1.181	-1.836	0.028
172	Asiatic acid	1.761	-1.841	0.005
173	3,4-Dihydroxybenzeneacetic acid	1.046	-1.886	0.013
174	Oleic acid	1.541	-1.9	0.005
175	Hepoxilin	1.695	-1.905	0.005
176	Fucose 1-phosphate	1.438	-1.909	0.005
177	Tectorigenin	1.172	-1.936	0.008
178	3,4-Dihydroxyphenylpropanoate	1.408	-1.943	0.005
179	Deoxyguanosine	1.786	-1.951	0.005
180	Guanosine	1.794	-1.985	0.005
181	2-Phenylethanol	1.709	-2.002	0.005
182	S-Hexyl-glutathione	1.228	-2.032	0.02
183	9,12,13-TriHOME	1.421	-2.034	0.012
184	Punicic acid	1.393	-2.036	0.013
185	(10S)-Juvenile hormone III diol phosphate	1.736	-2.078	0.005
186	Andrographolide	1.199	-2.095	0.008
187	6-Methoxyluteolin	1.48	-2.101	0.005
188	2-Furancarboxaldehyde	1.303	-2.113	0.013
189	Nitrendipine	1.582	-2.13	0.005
190	2-trans,6-trans-Farnesal	1.569	-2.153	0.005
191	1,2,3-Trihydroxybenzene	1.394	-2.177	0.018
192	Menadione	1.8	-2.187	0.005
193	Desaminotyrosine	1.316	-2.21	0.013
194	3-Dehydrosphinganine	1.384	-2.218	0.008
195	6-Methoxymellein	1.7	-2.225	0.005
196	2-Deoxyadenosine monohydrate	1.536	-2.363	0.007
197	Creatine	1.296	-2.378	0.008
198	Isorhamnetin	1.681	-2.434	0.005
199	Orcinol gentiobioside	1.315	-2.435	0.005
200	Phytosphingosine	1.701	-2.466	0.005
201	3-Methylbutanamine	1.813	-2.47	0.005
202	2-Propenal	1.412	-2.505	0.005
203	Gentiopicroside	1.034	-2.553	0.012
204	Pectolarigenin	1.646	-2.562	0.005
205	Deoxyadenosine	1.749	-2.564	0.005
206	Quinoline	1.414	-2.652	0.008
207	Eupatilin	1.447	-2.707	0.005
208	Adenosine	1.642	-2.879	0.005
209	Biotin	1.388	-2.953	0.005
210	Pipecolic acid	1.823	-2.976	0.005
211	Guanosine 3-phosphate	1.777	-2.978	0.005
212	Cortisol 21-acetate	1.432	-3.036	0.008

213	CMP	1.423	-3.045	0.005
214	Sphinganine	1.352	-3.052	0.005
215	3-O-feruloyl-D-quinic acid	1.371	-3.188	0.005
216	13,16,19-Docosatrienoic acid	1.793	-3.286	0.005
217	Clotrimazole	1.442	-3.312	0.013
218	1-O-Feruloyl-beta-D-glucose	1.763	-3.374	0.005
219	(5-L-Glutamyl)-L-glutamate	1.809	-3.378	0.005
220	Cafestol	1.175	-3.569	0.005
221	Phenylacetylglycine	1.83	-3.841	0.005
222	9E-Heptadecenoic acid	1.559	-3.871	0.005
223	GMP	1.571	-4.067	0.005
224	9S-hydroxy-11,15-dioxo-5Z,13E-prostadienoic acid	1.82	-4.285	0.005
225	Palmitic acid	1.812	-5.611	0.005
226	S-Formylglutathione	1.706	-5.692	0.004
227	Ethyl icosapentate	1.829	-5.962	0.005
228	Dimethyl sulfone	1.433	-12.975	0.003
229	Pentadecanoic acid	1.426	-16.31	0.003
230	myo-Inositol	1.16	-17.131	0.003
231	D-Glucose	1.029	-17.304	0.003
232	Glutaric acid	1.208	-17.635	0.003
233	Limonoate A-ring-lactone	1.396	-17.71	0.003
234	D-Fructose	1.282	-17.927	0.003
235	D-Mannose	1.018	-18.221	0.003
236	4-Hydroxybenzoic acid	1.325	-18.81	0.003

Table S2 genes related to tryptophan metabolism and their expression patterns

Gene name	Encoding enzyme (ko id and definition)	Gene expression
<i>TAAI</i>	K16903 // L-tryptophan--pyruvate aminotransferase [EC:2.6.1.99]	3; 1 up , 2 down
<i>YUCCA</i>	K11816 // indole-3-pyruvate monooxygenase [EC:1.14.13.168]	3; 1 up , 2 down
<i>nitrilase</i>	K01501//nitrilase [EC:3.5.5.1]	1; 0 up , 1 down
<i>amiE</i>	K01426 // amidase [EC:3.5.1.4]	1; 0 up , 1 down
<i>ALDH</i>	K00128 // aldehyde dehydrogenase (NAD+) [EC:1.2.1.3]	2; 0 up , 2 down

