Supporting information

Combined metabonomic and quantitative RT-PCR analyses revealed metabolic reprogramming associated with *Fusarium graminearum* resistance in transgenic *Arabidopsis thaliana*

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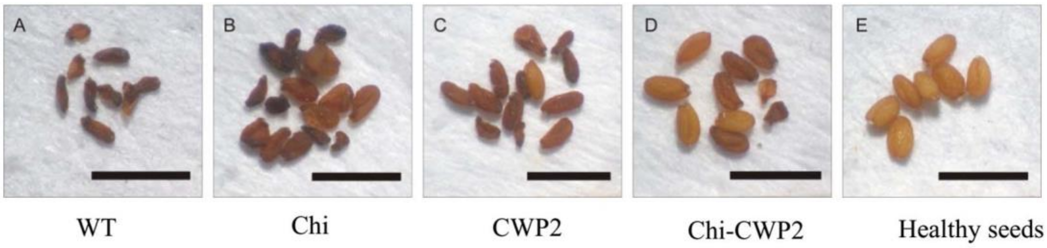
Figure S1. Phenotype for mature seeds of the *F. graminearum* inoculated *A. thaliana*.



A, WT; B, Chi; C, CWP2; D, Chi-CWP2; E, Healthy seeds; Bar=1 mm.

Figure S2. Differential metabograms for wild-type (WT) and transgenic *A. thaliana* expressing Chi, CWP2 and Chi-CWP2, respectively, treated with water (but without FG). Only the red-colored metabolites had significant inter-group differences. Keys for metabolites are given in Table S4.

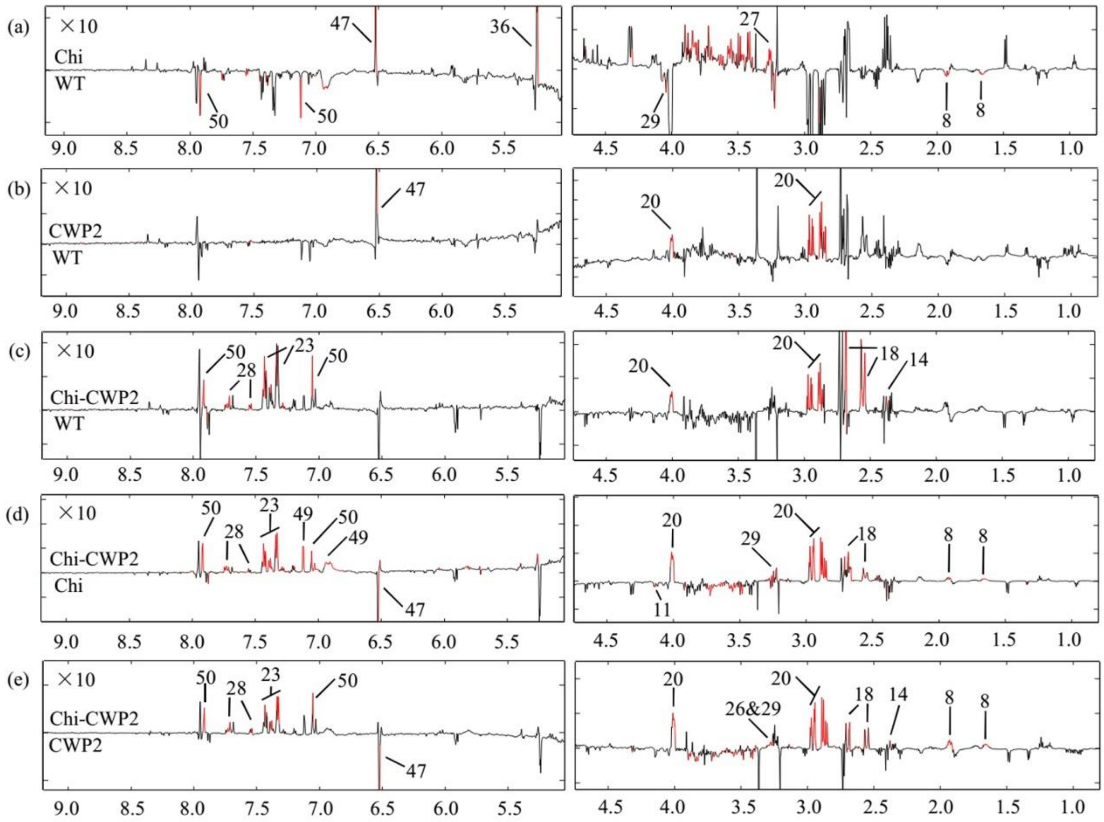


Figure S3. Differential metabograms for wild-type (WT) and transgenic *A. thaliana* expressing Chi, CWP2 and Chi-CWP2, respectively, with FG challenge. Only the red-colored metabolites had significant inter-group differences. Keys for metabolites are given in Table S4.

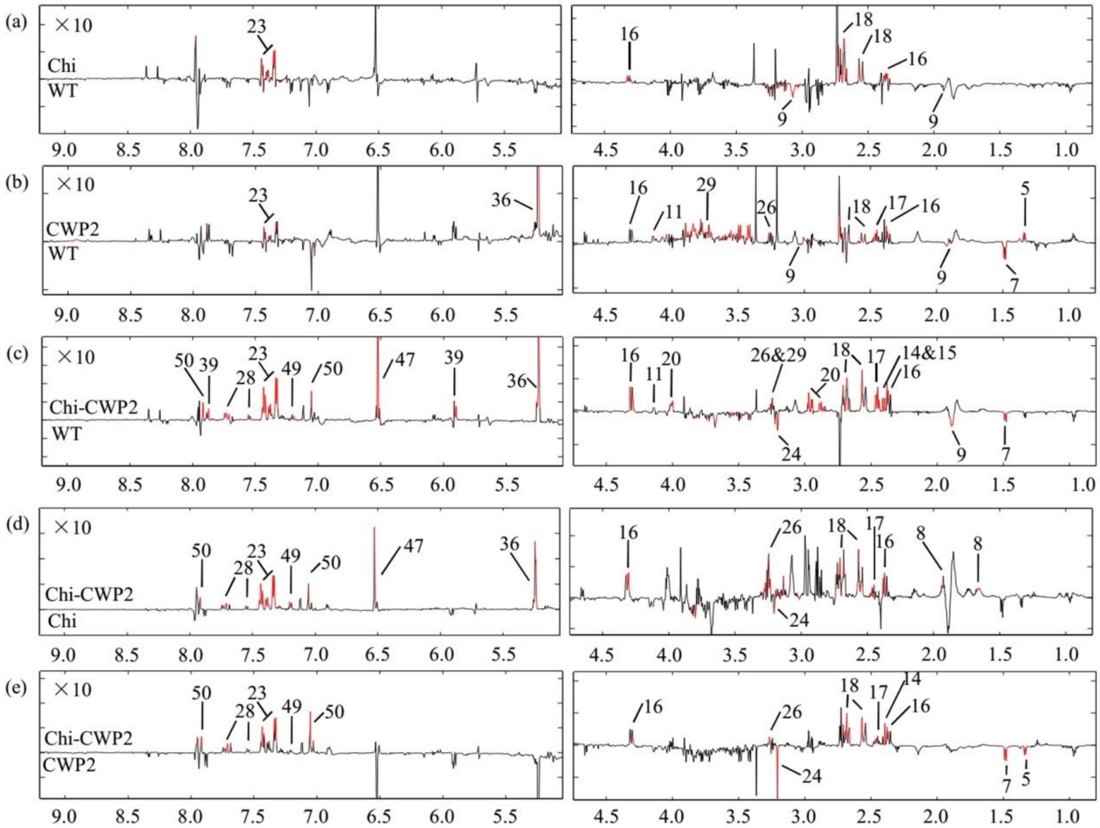


Figure S4. Heatmaps showing correlations of mycotoxin contents with the FG-induced significant changes of metabolites (a) and mRNA levels of seven genes (b) for wild-type (WT) and transgenic *A. thaliana* expressing Chi, CWP2 and Chi-CWP2 respectively. The correlation coefficients were color-coded with hot color (e.g., red) denoting positive correlations whereas the cool one (e.g., green) indicating negative ones. *TAT*, tyr aminotransferase; *ACS*, acetyl-CoA synthetase; *α-KGDH*, α-ketoglutarate dehydrogenase; *IDH*, isocitrate dehydrogenase; *BADH*, betaine-aldehyde dehydrogenase; *OAT*, ornithine aminotransferase; *SSADH*, succinic-semialdehyde dehydrogenase; *XS*, xylan synthase; *G6PD*, glucose-6-phosphate -1-dehydrogenase; *IDO*, indoleamine 2,3-dioxygenase; *PAL*, phenylalanine ammonia-lyase; *SS*, strictosidine synthase.

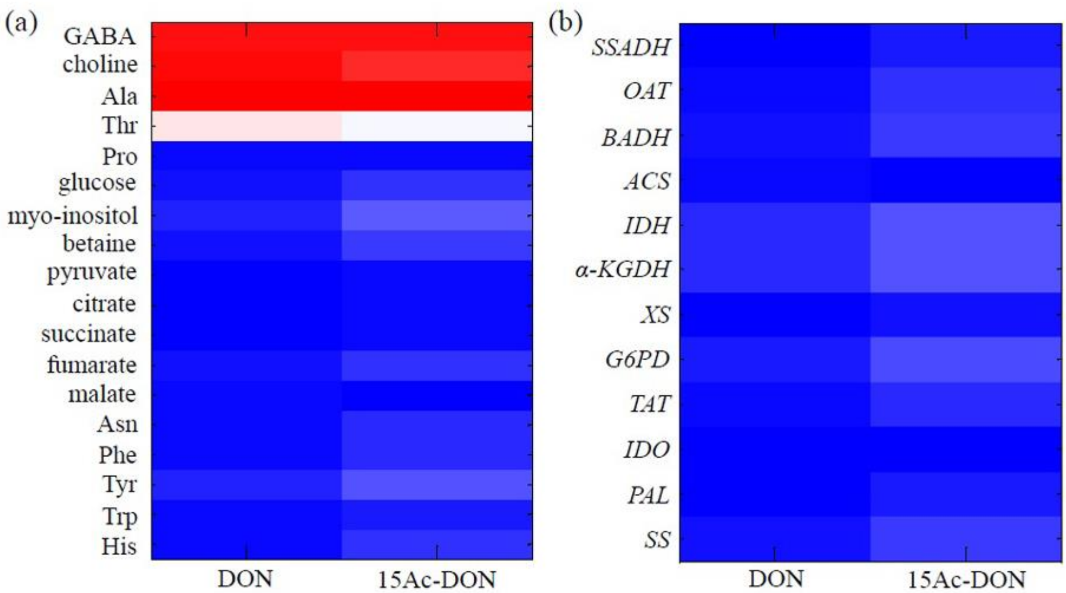


Table S1. T_1 values (seconds) for protons of some selected metabolites in *A. thaliana*.

metabolites	δ (multiplets)[a]	T_1 Values	
		Mean	SD
Tsp	0.00 (s)	2.03	0.01
alanine	1.48 (d)	2.42	0.01
isoleucine	1.01 (d)	0.85	0.01
valine	1.04 (d)	1.01	0.01
threonine	1.33 (d)	0.94	0.01
γ-aminobutyrate	2.30 (t)	1.47	0.01
pyruvate	2.37 (s)	1.46	0.06
succinate	2.41 (s)	1.07	0.01
glutamine	2.45 (m)	1.22	0.01
citrate	2.56 (d)	0.18	0.02
aspartate	2.80 (dd)	0.63	0.01
asparagine	2.88 (dd)	1.13	0.01
ethanolamine	3.14 (t)	2.42	0.02
choline	3.19 (s)	2.33	0.01
betaine	3.26 (s)	1.51	0.02
myo-insitol	3.27 (t)	1.51	0.01
fructose	4.11 (d)	1.07	0.01
proline	4.14 (m)	ND	ND
malate	4.32 (dd)	0.25	0.01
galactose	5.26 (d)	1.93	0.02
α-glucose	5.23 (d)	2.42	0.01
sucrose	5.40 (d)	1.07	0.01
fumarate	6.52 (s)	1.98	0.01
histidine	7.11 (s)	1.70	0.01
phenylalanine	7.42 (m)	2.50	0.01
trytophan	7.53 (d)	2.09	0.02
tyrosine	6.90 (d)	2.59	0.02
uridine	7.85 (d)	1.48	0.01
inosine	8.22 (s)	ND	ND
hypoxanthine	8.24 (s)	2.70	0.01
adenosine	8.32 (s)	1.27	0.01

ND: T_1 value was not determined because of signal overlapping; [a] δ: chemical shifts.

Table S2. Primers for quantitative real-time PCR (qRT-PCR) analysis of gene expressions.

	Gene encoded protein	Sequence (F: Forward, 5'-3'; R: Reverse, 5'-3')	Gene
1	beta-tubulin	F: TGCTATTCTGCGTTTGGACCTTG R: ATCCCTTACGATTTCACGCTCTG	At3g12110
2	tyrosine aminotransferase (TAT)	F: GGGAATGTTTTCTCTCGCCAA R: CACCATCCAACCAAGTCTCCA	At5g36160
3	acetyl-CoA synthetase (ACS)	F: TAAACGCCGTCGTGTTAGGAGA R: TATCAGACCAAAAAGCAGCAGGG	At5g36880
4	α-ketoglutarate dehydrogenase(α-KGDH)	F: TCTTCTTCTGCTTCGGGATTGG R: TGGACACCCTGGACAAGAACG	At5g55070
5	isocitrate dehydrogenase subunit (IDH)	F: ACTGCTGCTGGTATTGCTGGA R: TGCTCTTCCGTTGTATCCTTCC	At2g17130
6	betaine-aldehyde dehydrogenase(BADH)	F: CCACCGAGGATGAGGCAATT R: GCCTGGAAAGCCTTACTAACACG	At3g48170
7	ornithine aminotransferase (OAT)	F: ATGATGCTACTCGTGGATTCGG R: TTTCAAGTAACCGTCGGGAGG	At5g46180
8	succinic-semialdehyde dehydrogenase (SSADH)	F: GCGGCAACGCACCCTCTAT R: CCCATCCCTAAACCCATCTCCT	At1g79440
9	phenylalanine ammonia-lyase (PAL)	F:AAGTGAAGAGAATGGTTGCTGAG R:GAAGTGCGACACCGTTTTTG	At2g37040
10	indoleamine 2,3-dioxygenase (IDO)	F: CACAACACCCACAACTCCAAAAG R: TATGCCAAATCCAACTGCCACTG	At4g02610
11	xylan synthase (XS)	F: AACGAGCAGTTCTGGGTCATAGG R: CGCAAACTCATCGTCTCCATCT	At1g02730
12	glucose-6-phosphate -1-dehydrogenase (G6PD)	F: GAAGGACGTGGAGGGTACTTTG R: TCGGTGTAGGCAGGATATGTGA	At5g13110
13	strictosidine synthase (SS)	F:TTTGTCTCGTTGATTTCTCTTCTCC R:CGTTAGTGGTTCCAAGTGCTCC	At1g74000

Table S3. Tail-PCR primers used in this study.

Primers	Sequence (5'-3')
LAD1	ACGATGGACTCCAGAGCGGCCGC (G /C /A) N (G /C /A) NNNGGAA
LAD2	ACGATGGACTCCAGAGCGGCCGC (G /C /T) N (G /C /T) NNNGGTT
LAD3	ACGATGGACTCCAGAGCGGCCGC (G /C /A) (G /C /A) N (G /C /A) NNNCCAA
LAD4	ACGATGGACTCCAGAGCGGCCGC (G /C /T) (G /A /T) N (G /C /T) NNNCGGT
AC	ACGATGGACTCCAGAG
LB0a	CGCGCGATATAAAACAAAAGATAGCTCATAA
LB1a	ACGATGGACTCCAGTCCGGCCTTAAATAGGATCAAACGCG
LB2a	ATGGTCTATAGTCGAACGTACGGCC

Table S4. NMR data and signal assignments for metabolites in wild-type and transgenic *A. thaliana* expressing Chi, CWP2 and Chi-CWP2.

NO	metabolites	moiety	δ^1 H (multiplicity)[a]	δ^{13} C	experiments
1	Leucine (Leu)	δ-CH_3	0.94 (t, 7.2 Hz)	24.4	TOCSY, HSQC,
		δ′-CH_3	0.96 (t, 6.3 Hz)	26.3	HMBC
		γ-CH_2	1.69 (m)	26.4	
		β-CH_2	1.72 (m)	42.6	
		α-CH	3.69 (t, 8.7 Hz)	56.9	
2	Isoleucine (Ile)	δCH_3	0.94 (t, 7.2 Hz)	16.2	TOCSY, HSQC,
		β-CH_3	1.01 (d, 7.0 Hz)	18.9	HMBC
		γ-CH_2	1.25 (m)	27.1	
		β-CH	1.98 (m)	38.4	
		α-CH	3.65 (m)	63.3	
3	Valine (Val)	γ-CH_3	1.04 (d, 7.2 Hz)	20.4	TOCSY, HSQC,
		γ′-CH_3	0.99 (d, 7.0 Hz）	19.2	HMBC
		β-CH	2.27 (m)	31.8	
		α-CH	3.61 (d, 5.0 Hz)	63.3	
		COOH	\	175.6	
4	Ethanol	CH3	1.17 (t, 6.1 Hz)	19.4	TOCSY, HSQC,
		CH2	3.66 (q, 2.0 Hz)	60.1	HMBC
5	Threonine (Thr)	CH_3	1.33 (d, 6.6 Hz)	21.9	TOCSY, HSQC,
		α-CH	3.59 (q, 4.7 Hz)	63.2	HMBC
		β-CH	4.27 (m)	68.7	
		COOH	\	185.1	
6	Lysine (Lys)	γ-CH_2	1.45, 1.51 (m)	24.2	TOCSY, HSQC,
		δ-CH_2	1.73 (m)	26.6	HMBC
		β-CH_2	1.91 (m)	30.2	
		ε-CH_2	3.03 (t, 7.5 Hz)	43.1	
		α-CH	3.76 (t, 5.0 Hz)	56.9	
7	Alanine (Ala)	CH_3	1.48 (d, 7.3 Hz)	18.9	TOCSY, HSQC,
		CH	3.79 (q, 6.3 Hz)	53.6	HMBC
		COOH	\	178.7	
8	Arginine (Arg)	γ-CH	1.68, 1.72 (m)	26.5	TOCSY, HSQC,
		β-CH2	1.91 (m)	30.0	HMBC
		δ-CH2	3.25 (m)	43.1	
		α-CH	3.78 (t, 4.7 Hz)	56.9	
9	γ-aminobutyrate (GABA)	β-CH_2	1.91 (m)	26.3	TOCSY, HSQC,
		α-CH_2	2.30 (t, 7.4 Hz)	36.7	HMBC
		γ-CH2	3.02 (t, 7.9 Hz)	42.2	
		COOH	\	184.3	
10	Acetate (Acet)	CH_3	1.92 (s)	26.7	HSQC, HMBC
		COOH	\	177.3	
11	Proline (Pro)	γ-CH_2	2.01 (m)	26.6	TOCSY, HSQC,
		β-CH_2	2.35 (m)	29.6	HMBC

		δ-CH_2	3.34, 3.41 (m)	48.7	
		α-CH_2	4.14 (m)	63.5	
		COOH	\	177.6	
12	Glutamate (Glu)	β-CH_2	2.02, 2.09 (m)	29.4	TOCSY, HSQC,
		γ-CH_2	2.36 (m)	35.9	HMBC
		α-CH	3.75 (m)	57.4	
		COOH	\	182.5	
		COOH	\	177.7	
13	Glutamine (Gln)	β-CH_2	2.14 (m)	29.1	TOCSY, HSQC,
		γ-CH_2	2.45 (m)	33.5	HMBC
		α-CH	3.75 (m)	56.9	
		COOH	\	208.2	
		C=O	\	184.1	
14	Pyruvate (Pyr)	CH_3	2.37 (s)	29.5	HSQC
15	Succinate (Succ)	CH_3	2.41 (s)	36.2	HSQC
		COOH	\	183.4	
16	Malate (Mal)	β’-CH	2.37 (dd, 10.1, 15.3 Hz)	45.9	TOCSY, HSQC, HMBC
		β-CH	2.68 (dd, 3.1, 15.4 Hz)	45.9	
		CH	4.31 (dd, 3.0, 10.1 Hz)	72.6	
		COOH	\	183.9	
17	α-ketoglutarate (α-KG)	γ-CH_2	2.45 (t, 7.9 Hz)	35.9	TOCSY, HSQC
		β-CH_2	3.02 (t, 8.3 Hz)	41.6	
18	Citrate (Cit)	1/2CH_2	2.55 (d, 15.8 Hz）	51.5	TOCSY, HSQC,
		1/2CH_2	2.68 (d, 15.8 Hz）	51.5	HMBC
		3 C	\	78.3	
		COOH	\	177.3	
		COOH	\	180.4	
19	Aspartate (Asp)	β-CH_2	2.68 (dd,7.6, 16.5 Hz)	39.0	TOCSY, HSQC,
		β'-CH_2	2.80 (dd,4.4, 17.5 Hz)	39.0	HMBC
		α-CH	3.89 (dd, 4.3, 7.6 Hz)	55.0	
		COOH	\	176.9	
20	Asparagine (Asn)	β-CH	2.87 (dd,7.6, 16.5 Hz)	37.1	TOCSY, HSQC,
		β'-CH	2.95 (dd,4.6, 16.5 Hz)	37.1	HMBC
		α-CH	4.00 (dd, 4.6, 7.6 Hz)	54.0	
		γ-$CONH_2$	\	177.1	
		COOH	\	176.9	
21	Dimethylamine	CH_3	2.72(s)	39.2	HSQC
22	Ethanolamine (EA)	N-CH_2	3.15 (t, 5.2 Hz)	44.0	TOCSY, HSQC,
		O-CH_2	3.83 (t, 5.1 Hz)	60.1	HMBC
23	Phenylalanine (Phe)	β-CH_2	3.12 (dd,7.8, 14.9 Hz), 3.25 (dd, 5.3, 14.7 Hz)	38.9	TOCSY, HSQC, HMBC
		α-CH	4.00 (m)	58.9	
		3,5CH,	7.33 (m)	131.8	

		ring			
		3,5CH, ring	7.38 (m)	130.2	
		3,5CH, ring	7.43 (m)	131.7	
		COOH	\	174.9	
24	Choline (Cho)	N-$(CH_3)_3$	3.20 (s)	56.6	TOCSY, HSQC, HMBC
		N-CH_2	3.52 (m)	\	
		O-CH_2	4.07 (m)	70.1	
25	Phosphocholine (PC)	N-$(CH_3)_3$	3.23 (s)	56.6	TOCSY, HSQC
		N-CH_2	4.23 (m)	\	
		O-CH_2	3.61 (m)	\	
26	Betaine	CH_3	3.26 (s)	56.6	TOCSY, HSQC, HMBC
		CH_2	3.91 (s)	72.4	
		COOH	\	174.6	
27	Methanol	CH_3	3.36 (s)	51.7	TOCSY, HSQC
28	Tryptophan (Trp)	β-CH_2	3.31 (dd,4.9, 14.3 Hz), 3.48 (dd, 9.1, 14.0 Hz)	27.9	TOCSY, HSQC, HMBC
		α-CH	4.05 (m)	58.4	
		6 CH, ring	7.29 (t, 7.3 Hz)	120.1	
		7 CH, ring	7.53 (d, 8.2 Hz)	114.6	
		4 CH	7.74 (d, 8.0 Hz)	120.7	
		COOH	\	175.8	
29	Myo-inositol (mIno)	2-CH	4.07 (t, 2.5 Hz)	75.1	TOCSY, HSQC, HMBC
		1,3-CH	3.52 (dd, 5.1, 10.9 Hz)	75.3	
		4,6-CH	3.61 (t, 4.9 Hz)	73.9	
		5-CH	3.29 (t, 4.5 Hz)	77.1	
30	Glycine (Gly)	CH_2	3.57 (s)	44.3	TOCSY, HSQC, HMBC
		COOH	\	175.3	
31	Fructose (Fru)	3 CH	3.79, 3.81 (m)	63.8	TOCSY, HSQC
		4 CH	4.01 (m)	54.1	
		3 CH	4.11 (d, 3.7 Hz)	77.8	
32	Sucrose (Suc)	F-1 CH	4.22 (d, 8.8 Hz)	94.8	TOCSY, HSQC
		G-1 CH	5.42 (d, 3.8 Hz)	75.2	
33	Maltose	2 CH	5.22 (d, 3.8 Hz)	102.7	TOCSY, HSQC
		11 CH	5.42 (d, 3.8 Hz)	102.1	
34	NMNA[b]	2 CH	9.13 (s)	148.4	TOCSY, HSQC
		6 CH	8.84 (t)	147.7	
		4 CH	8.85 (t)	145.8	
		CH_3	4.44 (s)	51.0	
35	β-glucose (β-Glc)	2 CH	3.25 (dd, 2.9, 7.0 Hz)	76.8	TOCSY, HSQC
		3 CH	3.49 (m)	78.6	
		4 CH	3.42 (m)	72.6	
		5 CH	3.47 (m)	78.7	

		6,6′ CH	3.73, 3.90 (m)	63.5	
		1 CH	4.65 (d, 8.0 Hz)	98.7	
36	α-glucose (α-Glc)	4 CH	3.42 (m)	72.2	TOCSY, HSQC
		2 CH	3.53 (dd, 3.8, 9.9 Hz)	74.1	
		3 CH	3.73 (m)	74.8	
		6,6′ CH	3.74, 3.83 (m)	63.5	
		5 CH	3.86 (m)	74.3	
		1 CH	5.23 (d, 3.7 Hz)	94.8	
37a	α-arabinose (α-Arab)	α-1 CH	5.21 (d, 4.0 Hz)	94.5	TOCSY, HSQC
		\	3.87 (m)	63.3	
37 b	β- arabinose (β-Arab)	β-1 CH	4.52 (d, 8.2 Hz)	98.8	TOCSY, HSQC
		\	3.52 (dd, 5.5, 10.2 Hz)	\	
		\	3.69 (m)	\	
38a	α-galactose (α-Galac)	1 CH_2	5.27 (d, 3.8 Hz)	94.9	TOCSY, HSQC
		2 CH	3.81 (dd, 4.7, 8.7 Hz)	73.6	
		3 CH	3.97 (m)		
38 b	β-galactose (β-Galac)	1 CH_2	4.59 (d, 7.7 Hz)	99.2	TOCSY, HSQC
		2 CH	3.49 (dd, 5.3, 10.2 Hz)	78.4	
		3 CH	3.67 (m)	\	
39	Uridine (Uri)	6 CH	4.36 (t, 4.9 Hz)	77.1	TOCSY, HSQC
		12 CH	5.90 (d, 8.1 Hz)	104.9	
		7 CH	5.92 (d, 4.5 Hz)	91.7	
		11 CH	7.88 (d, 8.1 Hz)	144.3	
40	Uracil (Ura)	5 CH	5.80 (d, 7.7 Hz)	103.6	TOCSY, HSQC
		6 CH	7.54 (d, 7.6 Hz)	147.4	
41	Raffinose	G-1 CH	5.44 (d, 3.7 Hz)	95.0	TOCSY, HSQC
		F-1 CH	4.99 (d, 3.6 Hz)	101.1	
		G-1 CH	3.57 (m)	74.1	
42	Guanosine (Guan)	CH	8.01 (s)	138.0	TOCSY, HMBC
		5’-CH_2	5.90 (d, 4.4 Hz)	91.9	
		4’-CH	4.41 (dd, 4.8, 10.4 Hz)	73.8	
		3’-CH	4.22 (m)	88.5	
43	Inosine (Ino)	2 CH	6.08 (d, 6.1 Hz)	92.8	HSQC
		7 CH	8.21 (s)	\	
		12 CH	8.32 (s)	143.3	
44	Hypoxanthine (Hyp)	2 CH	8.20 (s)	\	JRES, TOCSY
		7 CH	8.24 (s)	\	
45	Adenosine (Aden)	14 CH	8.35 (s)	143.2	TOCSY, HSQC
		8 CH	8.26 (s)	155.1	
		1 CH	6.06 (d, 5.7 Hz)	91.0	
46	Sinapate	8 CH	6.50 (d, 15.8 Hz)	117.9	TOCSY, HSQC, HMBC
		7 CH	7.67 (d, 15.8 Hz)	149.1	
		1 CH	\	128.5	
		2,6 CH	7.01 (s)	108.8	

		3,5 CH	\	139.7	
		4 CH	\	151.0	
		4-OCH_3	3.89 (s)	58.7	
		COOH	\	172.0	
47	Fumarate (Fum)	2,3 CH	6.52 (s)	138.0	TOCSY, HSQC,
		COOH	\	177.7	HMBC
48	Polyphenolics	\	6.89 (m)	108.9	TOCSY, HSQC,
		\	7.63 (m)	123.7	HMBC
49	Tyrosine (Tyr)	β-CH_2	3.05 (dd,7.7, 14.9 Hz), 3.15 (dd, 8.5, 14.4 Hz)	39.2	TOCSY, HSQC, HMBC
		α-CH	3.93 (m)	58.7	
		3,5 CH, ring	6.90 (d, 8.6 Hz)	118.3	
		2,6 CH, ring	7.20 (d, 8.4 Hz)	133.2	
		COOH	\	175.1	
50	Histidine (His)	4 CH, ring	7.09 (s)	119.8	TOCSY,HSQC,
		4 CH, ring	7.92 (s)	138.6	HMBC
		β-CH_2	3.20 (dd, 5.1, 14.7 Hz), 3.25 (dd, 9.4, 14.6 Hz)	30.5	
		α-CH	4.00 (m)	56.6	
		COOH	\	174.6	
51	Formate (Form)	CH	8.46 (s)	173.5	HSQC
52	Sarcosine	CH_3	2.75 (s)	38.9	TOCSY, HSQC,
		COOH	\	180.2	HMBC
53	Methionine (Met)	γ-CH2	2.65 (t, 7.5 Hz)	32.6	TOCSY, HSQC
		β-CH2	2.17 (m)	32.9	
		α-CH	3.78 (m)	56.8	
		S-CH3	2.14 (s)	16.1	
		COOH	\	174.3	
54	NAD^{+}[b]	N2 CH	9.47 (s)	143.6	TOCSY,HSQC,
		N4 CH	8.19 (t, 6.9 Hz)	130.5	HMBC
		N5 CH	9.16 (d, 6.2 Hz)	143.8	
		N6 CH	8.95 (d, 7.8 Hz)	149.4	
		N1' CH	6.23 (d, 4.8 Hz)	57.3	
		A2 CH	8.32 (s)	143.7	
		A6 CH	8.23 (s)	155. 0	
		A1' CH	6.06 (d, 5.6 Hz)	90.9	
55	Dimethylglycine	CH_3	2.94 (s)	54.6	TOCSY, HSQC
			\	41.2	
56	D-α-aminobutyrate[b]	2 CH_2	1.89 (m)	27.5	TOCSY, HSQC
		1 CH	3.68 (t, 5.8 Hz)	56.5	
		3 CH_3	0.97 (t, 7.4 Hz)	11.2	
		COOH	\	176.7	

57	Ethylmalonate[b]	5 CH_3	1.24 (t, 7.1 Hz)	15.3	TOCSY, HSQC,
		6 CH_2	3.28 (s)	42.6	HMBC
		4 CH_2	4.17 (q, 7.2 Hz)	63.1	
		2 COOH	\	169.2	
		7 COOH	\	171.3	
58	α-ketoisovalerate[b]	7,8 CH_3	1.10 (d, 6.7 Hz)	19.8	TOCSY, HSQC,
		6 CH	3.05 (dq, 7.1 Hz)	41.5	HMBC
		COOH	\	178.2	
		COOH	\	196.1	
59	U1	\	1.37	30.6	TOCSY, HSQC
		\	1.85 (m)	23.7	
		\	3.07	56.6	
60	U2	\	0.86 (d, 6.4 Hz)	\	JRES, TOCSY
		\	3.12 (s)	\	
		\	3.36 (m)	\	
		\	3.75 (m)	\	
		\	4.23 (m)	\	
61	U3	\	1.29 (d, 6.0 Hz)	19.5	JRES, TOCSY,
		\	3.55 (dd, 3.7, 11.1 Hz)	30.9	HSQC
		\	3.73 (dd, 5.1, 11.1 Hz)	\	
		\	3.96 (dd, 5.8, 12.5 Hz)	74.5	
		\	4.12 (d, 3.8 Hz)	77.5	
62	U4	\	1.14 (d, 6.1 Hz)	19.0	JRES, TOCSY,
		\	3.47 (m)	72.2	HSQC
		\	3.96 (dd, 5.8, 12.5 Hz)	74.3	
		\	4.15 (m)	\	
63	U5	\	2.65 (dd,11.5, 15.5 Hz)	42.3	JRES, TOCSY,
		\	5.16 (dd, 2.7, 11.2 Hz)	76.6	HSQC
64	U6	\	6.02 (d, 12.5 Hz)	119.6	JRES, TOCSY
		\	7.02 (d, 12.6 Hz)	147.2	
65	U7	\	6.43 (d, 15.8 Hz)	\	JER, TOCSY,
		\	6.64 (d, 15.8 Hz)	97.6	HSQC
66	U8	\	4.19 (dd, 2.5, 8.0 Hz)	78.7	JRES, TOCSY,
		\	4.61 (dd, 2.4, 5.3 Hz)	75.2	HSQC
67	U9	\	7.97 (s)	\	JRES, TOCSY

[a]Multiplicity: s, singlet; d, doublet; dd, doublet of doublets; t, triplet; q, quartet; m, multiplet; U, unidentified signal; \, signals or multiplicities were not determined; [b], tentatively assigned.

Table S5. P-values for inter-group differentiated metabolites in wild-type and transgenic *A. thaliana* expressing Chi, CWP2 and Chi-CWP2 inoculated with water and FG, respectively.

Metabolites	Chi-CWP2 *vs* Chi[a]	Chi-CWP2 *vs* CWP2[a]	**Chi-CWP2 *vs* Chi[b]**	**Chi-CWP2 *vs* CWP2[b]**
Sugars				
myo-inositol	0.038	0.038		
α-glucose			0.020	
Amino acids				
Thr				0.017
Ala				0.025
Arg	0.025	0.038	0.004	
Pro	0.025			
Asn	0.035	0.021		
Phe	0.025	0.023	0.035	0.032
Trp	0.025	0.032	0.023	0.019
Tyr	0.038		0.038	0.040
His	0.002	0.038	0.027	0.038
GABA				
Organic acids				
pyruvate		0.020		0.010
succinate				
malate			0.032	0.038
α-KG			0.028	0.025
citrate	0.028	0.035	0.029	0.027
fumarate	0.028	0.038	0.034	
Nucleoside/tides				
uridine				0.025
Choline metabolites				
choline			0.015	0.018
betaine		0.038	0.004	0.017

[a] inoculated with water; [b] inoculated with FG. [c] red and green signs denote elevation and decrease of metabolites, respectively. Only those with $p < 0.05$ were tabulated.