

Supplementary file

The Different Metabolic Responses of Resistant and Susceptible Wheats to *Fusarium graminearum* Inoculation

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Table S1. Assignment of NMR data for metabolites in FHB-resistant (Sumai 3) and -susceptible (Annong 8455) wheat varieties inoculated with ddH₂O, wild type (WT), *TPS1*⁻ and *TPS2*⁻.

no.	metabolites	moieties	$\delta^1\text{H}$ (ppm)	$\delta^{13}\text{C}$ (ppm)
1	isoleucine (Ile)	$\delta\text{-CH}_3$	0.94 (t) ^a	13.7
		$\gamma\text{-CH}_3$	1.01 (d)	17.5
		$\beta\text{-CH}$	1.97 (m)	38.7
2	leucine (Leu)	$\delta'\text{-CH}_3$	0.96 (d)	23.5
		$\delta\text{-CH}_3$	0.97 (d)	24.8
		$\gamma\text{-CH}$	1.69 (m)	26.9
		$\beta\text{-CH}_2$	1.72 (m)	42.9
3	valine (Val)	$\gamma'\text{-CH}_3$	0.99 (d)	19.8
		$\gamma\text{-CH}_3$	1.04 (d)	20.9
		$\beta\text{-CH}$	2.27 (m)	31.7
		$\alpha\text{-CH}$	3.61 (d)	63.4
4	threonine (Thr)	$\gamma\text{-CH}_3$	1.33 (d)	20.8
		$\beta\text{-CH}$	4.24 (m)	68.6
		$\alpha\text{-CH}$	3.57 (d)	63.4
		COOH		175.6
5	alanine (Ala)	$\beta\text{-CH}_3$	1.48 (d)	17.9
		$\alpha\text{-CH}$	3.78 (q)	53.4
		COOH		178.7
6	arginine (Arg)	$\delta\text{-CH}_2$	3.23 (t)	43.3
		$\gamma\text{-CH}_2$	1.68 (m)	26.5
		$\beta\text{-CH}_2$	1.90 (c)	29.3
		$\alpha\text{-CH}$	3.77 (t)	57.3
7	methionine (Met)	$\gamma\text{-CH}_2$	2.65 (t, 7.5)	32.0
		$\beta\text{-CH}_2$	2.17 (m)	32.5
		$\alpha\text{-CH}$	3.78 (m)	56.7
		S-CH ₃	2.14 (s)	16.7
8	γ -aminobutyrate (GABA)	$\gamma\text{-CH}_2$	3.02 (t)	42.3
		$\beta\text{-CH}_2$	1.91 (qu)	26.7
		$\alpha\text{-CH}_2$	2.30 (t)	37.3
		COOH		184.2
9	glutamate (Glu)	$\gamma\text{-CH}_2$	2.36 (m)	34.7
		$\beta\text{-CH}_2$	2.02, 2.08 (m)	29.8
		$\alpha\text{-CH}$	3.76 (t)	57.6
10	glutamine (Gln)	$\gamma\text{-CH}_2$	2.45 (m)	32.3
		$\beta\text{-CH}_2$	2.14 (m)	27.5

		α -CH	3.76 (t)	55.1
		COOH		175.0
11	aspartate (Asp)	β' -CH	2.82 (dd)	37.6
		β -CH	2.67 (dd)	43.2
		α -CH	3.90 (dd)	53.2
		COOH		175.2,178.1
12	asparagine (Asn)	β' -CH	2.96 (dd)	36.1
		β -CH	2.86 (dd)	35.9
		α -CH	4.01 (dd)	53.2
		COOH		174.5,174.2
13	phenylalanine (Phe)	C2, 6, ring	7.33 (m)	124.3
		C3, 5, ring	7.43 (t)	127.5
		C4, ring	7.38 (m)	127.1
14	tryptophan (Trp)	C7H, ring	7.55 (d)	111.1
		C6H, ring	7.29 (t)	121.1
		C5H, ring	7.20 (t)	118.5
		C4H, ring	7.74 (d)	117.6
		C2H, ring	7.33(s)	126.2
		COOH		175.1
15	tyrosine (Tyr)	C2, 6H, ring	7.19 (d)	131.1
		C3, 5H, ring	6.90 (d)	115.4
		COOH		175.3
16	histidine (His)	5-CH	7.07 (s)	119.1
		3-CH	7.85 (s)	137.6
17	sucrose	Glc-C1H	5.41 (d)	96.2
		Glc-C2H	3.57 (dd)	72.1
		Glc-C5H	3.83 (c)	63.3
		Fru- C3H	4.22 (d)	77.3
		Fru- C4H	4.06 (t)	75.1
		Fru- C6H	3.83 (c)	63.2
18	α -glucose	C1H	5.24 (d)	95.9
		C2H	3.55 (dd)	74.3
		C4H	3.42 (dd)	72.8
19	β -glucose	C1H	4.65 (d)	98.7
		C2H	3.25 (t)	77.3
		C3H	3.49 (t)	78.9
		C4H	3.41 (dd)	72.8
		C6H	3.90 (dd)	64.3
20	raffinose	Gal-C1H	5.01 (d)	101.8
		Gal-C4H	4.01 (d)	72.6

		Gal-C5H	3.90 (m)	70.2
		Glc-C1H	5.43 (d)	95.6
		Fru-C3H	4.22 (t)	77.2
		Fru-C4H	4.06 (t)	75.3
21	fructose	5-CH	4.04, m	84.2
		4-CH	4.01 (m)	79.1
		1-CH	3.68 (d, 3.7)	65.8
22	myo-inositol	2-CH	4.07, t	75.1
		1,3-CH	3.52 (dd)	75.3
		4,6-CH	3.61 (t)	73.9
		5-CH	3.29 (t)	77.1
23	acetate	α -CH ₃	1.92 (s)	26.3
24	pyruvate	CH	2.39 (s)	31.1
		C=O	\	209.9
25	succinate	α -CH ₂	2.41 (s)	37.5
		COOH		184.6
26	lactate	CH ₃	1.33 (d)	22.5
		CH	4.12 (q)	71.5
		COOH		185.2
27	formate	CH	8.46 (s)	169.3
28	fumarate	CH=CH	6.52 (s)	139.2
		COOH		177.5
29	citrate	α' , γ' CH	2.66 (dd)	49.1
		α , γ CH	2.55 (dd)	49.1
		COOH		180.1,184.5
30	α -ketoglutarate (α -KG)	γ -CH ₂	3.02 (t)	40.2
		β -CH ₂	2.44 (t)	32.1
31	malate	β' -CH	2.37 (dd)	43.7
		β -CH	2.67 (dd)	43.3
		α -CH	4.31 (dd)	73.4
32	choline	N-(CH ₃) ₃	3.20 (s)	54.5
		N-CH ₂	3.52 (m)	70.2
		O-CH ₂	4.07 (m)	58.5
33	phosphocholine (PC)	N-(CH ₃) ₃	3.22 (s)	56.7
		N-CH ₂	3.61 (m)	
34	glycine betaine (GB)	N-(CH ₃) ₃	3.27 (s)	54.1
35	ethanolamine (EA)	β -CH ₂	3.83 (t)	56.3
36	dimethylglycine	CH ₃	2.94 (s)	\
37	adenosine	C1'H, ribose	6.06 (d)	

		2-CH	8.33 (s)	
		8-CH	8.24 (s)	155.5
38	uridine	C1'H, ribose	5.90 (d)	104.5
		C6, ring	7.88 (d)	145.8
39	guanosine	8-CH	8.01 (s)	141.0
		5'-CH ₂	5.90 (d)	91.0
40	hypoxanthine	2-CH	8.20 (s)	\
		7-CH	8.22 (s)	\
41	inosine	12-CH	8.32 (s)	
		2-CH	6.10 (d)	
42	deoxy adenosine monophosphate (dAMP)	8-CH	8.27 (s)	\
		C1H of ribose	6.14 (d)	89.9
43	p- hydroxy cinnamic acid (p-HCA)	7-CH	7.55 (d)	132.1
		5-CH	6.97 (d)	118.1
44	chlorogenic acid	8-CH	6.39	124.3
		2, 4-CH	6.93 (d, 8.3)	118.5
		3, 5-CH	7.35 (d, 8.3)	143.2
		6-CH	4.25 (d, 2.90)	73.6
45	thymidine	6-CH	7.65 (s)	140.0
		5'-CH ₂	6.30 (t)	87.0

^a Multiplicity: s, singlet; d, doublet; t, triplet; dd, doublet of doublets; qu, quintet; m, multiplet. \,The signals were not determined.

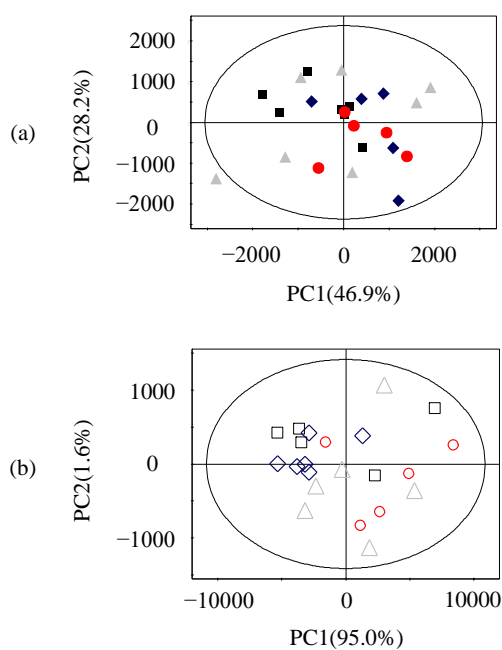


Figure S1. PCA scores plots of the NMR data for FHB-resistant Sumai 3 (a) and -susceptible wheat Annong 8455 (b) respectively. The numbers in parentheses indicate the overall variance explained in the first two principal components. Grey (triangle), black (square), red (circle), and blue (diamond) indicate metabolites in both FHB- resistant (solid symbol) and -susceptible wheat (open symbol) inoculated with ddH₂O, WT, *TPS1*⁻ and *TPS2*⁻ respectively.