Table S2. Identification and annotation of detected purine metabolite peaks.

Reporting metabolite data was presented according to the recommendation by Fernie et al., 2011			
Level	**Aspect**	**Information**	**Fill in**
general aspect	Type of metabolome analysis	targeted metabolite analysis	TRUE
		non-targeted metabolite class scale profiling	FALSE
		non-targeted metabolome scale profiling	FALSE
		non-targeted finger printing of mass features	FALSE
	Type of quantification	absolute or quantification	Relative quantification
	Type of reference samples	chemically defined	standard reference compounds aquired in chemical companies
		biologically defined	-
	Type of replication	analytical (same analytical sample preparation)	1
		technological (same biological preparation)	1
		biological (same experimental condition)	5
		full experiment	10
	Type of technology	reference publication	Lisec et al (2006)
	Sample preparation		chemical derivatized
		method of chromatography/separation	Lisec et al (2006)
		method of ionization	- 70 MeVolt hard ionization
		method of detection	electron impact ionization
metabolite/mass feature	Metabolite	metabolite name	see below
		metabolite sum formula	see below
		metabolite structure and public source of metabolite identifier	Metabolites were identified in comparison to database entries of authentic standards (Kopka *et al.*, 2005; Schauer *et al.*, 2005).
	Identification	identification process	manually supervized with Xculibar
		by authentic mass isotopomer added to one or all biological sample(s)	FALSE
		by authentic reference compound within a co-processed reference mixture	FALSE
		by authentic reference compound previously mapped to the analytical system	TRUE
		reference library	Metabolites were identified in comparison to spectrum of authentic standards analyzed with samples.

		type of mass spectrum	
		by match of molecular mass (single mass fragment)	YES
		by match of fragments	YES
		by match of fragmentation pattern	YES
		type of retention index	min/sec
		by match of retention time (index) to reference library	FALSE
	Quantification	type of quantification	relative peak area quantification by internal standard and sample fresh weight
	Validity testing	Recovery testing (chemical analog)	not performed
		Recovery testing (internally added mass isotopomer)	not performed
		Recovery testing (mixture of most divergent samples from the experiment)	not performed
		Test for linear range	not performed
		Limit of quantification (LOQ)	not performed
		Limit of detection (LOD)	not performed

Experiment title:	Metabolite profiles of Arabidopsis thaliana seedling, grxs mutant line
Organism/Plant species:	*Arabidopsis thaliana*
Organ/tissue:	seedling
Analytical tool:	GC/TOF-MS

Peak/compound no.- number of compound found

Ret . Time- Time expected, Tag Time Index and Time deviation

Putative Name- putative identification of the metabolite/derivative

Corresponding metabolite name in literature

Mol. Formula- molecular formula of the metabolite or its FA adduct;

Mass to charge ratio (m/z)

(S)- identification confirmed by a standard compound

I, II, III- different isomers

Identification level (A; B; C; D)- (A) standard or NMR; (B) MS/MS; (C) MS^E; (D) MS only

Experiment title:	Metabolite changes in *grxs17* mutants	
Organism/Plant species:	*Arabidopsis thaliana*	
Organ/tissue:	seedlings	
Analytical tool:	GC-TOF-MS	

Peak/compound no.- number referenced back to the main text
Ret . Time- Time expected, Tag Time Index and Time deviation
Putative Name- putative identification of the metabolite/derivative
Corresponding metabolite name in literature
Mol. Formula- molecular formula of the metabolite or its FA adduct;
Mass to charge ratio (m/z)
(S)- identification confirmed by a standard compound
I, II, III- different isomers
Identification level (A; B; C; D)- (A) standard or NMR; (B) MS/MS; (C) MS^{E}; (D) MS only

Peak/Compound no.	**Time Expected (min)**	**Putative metabolite name**	**Mol formula**	**g mol−1**	**Mass to charge ratio (m/z)**	**Identification level (A-D)**
Peak no. 1	3,83	Urea	CH4N2O	60,06	261	A
Peak no. 2	5,49	Allantoic acid	C4H8N4O4	176,13	189	A
Peak no. 3	9,9	Allantoin	C4H6N4O3	158,12	188	A
Peak no. 4	10,68	Hypoxanthine	C5H4N4O	136,11	192	A
Peak no. 5	12,01	Uric acid	C5H4N4O3	168,11	441	A
Peak no. 6	12,05	Xanthine	C5H4N4O2	152,11	353	A
Peak no. 7	15,09	Xanthosine	C10H12N4O6	284,23	245	A

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