

**Table S1.** Metabolites identified and fragment ions (m/z) in *Amaranthus palmeri* GS and GR plants by GC-MS. ID level: Compound was Identified by Authentic Reference standard (1), MS data base search (2) or database-search with striking hits; thus interpretation of MS peaks was done (3).

Metabolites	Abbreviation in Heatmap	ID level	Fragment Ions (m/z)
2-Amino adipate	2-Amino adipate	1	260
2-Isopropylmalate	2-Isopropylmalate	1	275
2-Keto-l-gluconic acid	2-Keto-l-gluconic acid	1	292
2-Oxoglutarate	2-Oxoglutarate	1	198
Adenine	Adenine	1	264
Adenosine	Adenosine	1	236
Adenosine-5-monophosphate	Adenosine-5-MP	2	169
Alanine	Alanine	1	116
Allantoin	Allantoin	2	189, 259, 359
Arabinose	Arabinose	1	307
Arginine	Arginine	1	157
Asparagine	Asparagine	1	231
Aspartate 1	Aspartate 1	1	160
Aspartate 2	Aspartate 2	1	232
Benzoate	Benzoate	1	179
Benzoate derivate	Benzoate der.	3	179, 245
beta-Alanine	beta-Alanine	1	248
Caffeate 1	Caffeate 1	1	219
Caffeate 2	Caffeate 2	1	396
cis-Aconitate	cis-Aconitate	1	229
Citrate / Isocitrate	Citrate	1	257
Dehydroshikimate	Dehydroshikimate	2	296, 402, 417 (386)
Ethanolamine	Ethanolamine	1	174
Ferulic acid / Isoferulic acid	(Iso-)Ferulate	1	338
Fructose 1	Fructose 1	1	307
Fructose 2	Fructose 2	1	307
Fructose-6-Phosphate	Fructose-6-P	1	315
Fumarate	Fumarate	1	245
Galactinol	Galactinol	1	305
Gallic acid	Gallic acid	2	281, 443 (458)
Glucose 1	Glucose 1	1	319
Glucose 2	Glucose 2	1	319
Glucose-6-phosphate	Glucose-6-P	1	387
Glutamate	Glutamate	1	246
Glutamine 1	Glutamine 1	1	RI 1488
Glutamine 2	Glutamine 2	1	RI 1555
Glutaric acid	Glutaric acid	1	261
Glycerate	Glycerate	1	189

Glycerol 3-phosphate	Glycerol 3-P	2	357
Glycine	Glycine	1	174
Glyphosate-Compound RT 19.00	Gly-Cmp 1	3	282
Glyphosate-Compound RT 22.40	Gly-Cmp 2	3	212
Glyphosate-Compound RT 23.00	Gly-Cmp 3	3	155
Hexadecanoic acid	Hexadecanoate	2	313
Isocitric lactone	Isocitric lactone	2	303
Isoleucine	Isoleucine	1	158
Leucine	Leucine	1	158
Lysine	Lysine	1	156
Malate	Malate	1	245
Maleic acid	Maleate	2	245
Methionine	Methionine	1	176
monosaccharide RT 23.20	Monosaccharide 1	3	204
Monosaccharide with modification	Monosaccharide 2	3	319
<i>myo</i> -Inositol	<i>myo</i> -Inositol	1	305
<i>myo</i> -Inositol-1-phosphate	<i>myo</i> -Inositol-1-phosphate	1	318
Octadecadienoic acid	Octadecadienoic acid	2	337
Octadecanoic acid	Octadecanoic acid	2	341
Octadecenoic acid	Octadecenoic acid	2	339
organic acid RT 23.07 galactaric acid	Organic acid 1	3	333
organic acid RT 23.45 Glucaric acid	Organic acid 2	3	333
Oxalate	Oxalate	1	190
Phenylalanine	Phenylalanine	1	192
Phosphate + 2x dihydroxypropyl group	<i>Ukn P+dihydroxypropyl</i>	3	357-503-445-299
Phosphorylated saccharide RT 27.25	Saccharide-P 1	3	387
phosphorylated saccharide RT 29.75	Saccharide-P 2	3	387
Proline	Proline	1	142
Pyrophosphate 4TMS	Pyrophosphate 4TMS	2	451
Pyruvate	Pyruvate	2	174
Quinate	Quinate	1	345
Quinic acid derivative (glycosylated?) RT 31.40 mz	Quinate derivate 1	3	255-204-361 (345)
Quinic acid derivative (glycosylated?) RT 31.80 mz	Quinate derivate 2	3	255-204-361 (345)
Quinic acid derivative (glycosylated?) RT 32.10 mz	Quinate derivate 3	3	255-204-361 (255)
Quinic acid derivative (glycosylated?) RT 32.40 mz	Quinate derivate 4	3	255-204-361 (345)
Ribitol	Ribitol	1	217
Serine	Serine	1	204

Shikimate	Shikimate	1	204
Shikimate-3-phosphate	Shikimate-3-phosphate	2	483
Sinapic acid derivate	Sinapic acid derivate	3	227, 301, 329 (344)
Stearic acid	Stearic acid	2	311, 453
Succinate	Succinate	1	247
Sucrose	Sucrose	1	361
Threitol	Threitol	2	217
Threonic acid	Threonic acid	2	292
Threonine	Threonine	1	291
Tyramine	Tyramine	1	174
Tyrosine	Tyrosine	1	280
Uracil	Uracil	2	255
Valine	Valine	1	144
Xylitol	Xylitol	1	307
Xylitol or similar monosaccharide / alcohol	Xylitol-like	3	307
<i>Unknown 1</i>	<i>Unknown 1</i>		245, 308, 410, 424
<i>Unknown 2</i>	<i>Unknown 2</i>		224, 296, 386
<i>Unknown amin RT 15.65</i>	<i>Ukn amin 1</i>		174, 156
<i>unknown amin RT 17.30</i>	<i>Ukn amin 2</i>		174
<i>unknown phosphorylated compound RT 32.90</i>	<i>Ukn-P</i>	3	169, 450, 384
<i>unknown RT 17.70</i>	<i>Ukn RT 17.70 1</i>		275
<i>unknown RT 17.70</i>	<i>Ukn RT 17.70 2</i>		244, 275
<i>unknown RT 18.60</i>	<i>Ukn RT 18.60</i>		230, 257, 359, 374
<i>unknown RT 22.40</i>	<i>Ukn RT 22.40</i>		424
<i>unknown RT 22.70</i>	<i>Ukn RT 22.70</i>		155, 271, 299, 447
<i>unknown RT 25.30</i>	<i>Ukn RT 25.30 1</i>		204, 210, 235
<i>Unknown RT 25.30</i>	<i>Ukn RT 25.30 2</i>		204, 217, 235
<i>unknown RT 33.60</i>	<i>Ukn RT 33.60</i>		307, 375, 219, 714
<i>unknown RT 34.90</i>	<i>Ukn RT 34.90</i>		307, 375, 219, 714
<i>unknown RT 35.12</i>	<i>Ukn RT 35.12</i>		307, 375, 219, 714
<i>unknown RT 35.46</i>	<i>Ukn RT 35.46</i>		204, 217, 361, 597
<i>unknown steroid-like compound isomer 1 RT 28.40</i>	<i>Steroid-like 1</i>	3	245, 360, 430, 520, 592
<i>unknown steroid-like compound isomer 2 RT 28.55</i>	<i>Steroid-like 2</i>	3	245, 360, 430, 520, 592

**Table S2.** Metabolites identified in *Amaranthus palmeri* GS and GR plants by LC-MS. Confidence level of annotation (According to Matern et al., 2019) is as follows: 1, verified with mass, retention time, and CID spectrum of a commercial standard or a synthesized standard; 2, putatively annotated compounds based on CID spectrum interpretation, data base hits, and literature; 3, possible structure or metabolite family based on hits in data bases; 4, unknown.

Annotation	Elemental composition	RT [min]	Quantifier ion		Ann. level
			Type	m/z meas.	
Pipecolic acid	C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub>	0.37	[M+H] <sup>+</sup>	130.09266	2
L-Histidine	C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub>	0.37	[M+H] <sup>+</sup>	156.0744	1
L-Proline	C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub>	0.4	[M+H] <sup>+</sup>	116.07113	1
Ribulose 1,5-bisphosphate	C <sub>4</sub> H <sub>4</sub> O <sub>7</sub> P <sub>2</sub>	0.42	[M+H] <sup>+</sup>	226.95123	1
Cytosine	C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O	0.43	[M+H] <sup>+</sup>	112.05308	1
D-Ribose 5-phosphate	C <sub>5</sub> H <sub>11</sub> O <sub>8</sub> P	0.43	[M+K] <sup>+</sup>	268.9814	1
L-Valine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	0.43	[2M+Na] <sup>+</sup>	257.14615	1
unknown ubiquitous metabolite	C <sub>4</sub> HO <sub>2</sub> PS <sub>4</sub>	0.44	[M+H] <sup>+</sup>	240.86606	4
D-Xylitol	C <sub>5</sub> H <sub>11</sub> NaO <sub>5</sub>	0.45	[M+Na] <sup>+</sup>	175.05737	1
Betaine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	0.47	[2M+H] <sup>+</sup>	235.16485	1
Trigonelline	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	0.47	[M+H] <sup>+</sup>	138.05513	1
Nicotinic acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	0.48	[2M+H] <sup>+</sup>	247.07745	1
D-Mannitol	C <sub>6</sub> H <sub>14</sub> O <sub>6</sub>	0.48	[M+CO <sub>2</sub> H <sub>2</sub> +H] <sup>+</sup>	229.09487	1
Betaine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub>	0.48	[M+H] <sup>+</sup>	118.08674	1
D-Sucrose	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	0.5	[M+Na] <sup>+</sup>	365.10311	1
Fructose/Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	0.5	[M+Na] <sup>+</sup>	203.0513	3
L-Asparagine	C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub>	0.5	[2M+Na] <sup>+</sup>	287.10002	1
Adenine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	0.5	[M+H] <sup>+</sup>	136.06184	1
Quinate	C <sub>7</sub> H <sub>12</sub> O <sub>6</sub>	0.51	[M+Na] <sup>+</sup>	215.05107	1
L-Arginine	C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub>	0.51	[M+CH <sub>2</sub> O <sub>2</sub> Na] <sup>+</sup>	243.11056	1

L-Glutamine	C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub>	0.54	[M+H] <sup>+</sup>	147.07496	1
Glutamic acid	C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub>	0.55	[M+H] <sup>+</sup>	148.06083	1
Inosine 5'-monophosphate	C <sub>10</sub> H <sub>13</sub> N <sub>4</sub> O <sub>8</sub> P	0.57	[M+H] <sup>+</sup>	349.06017	1
L-Ureidosuccinic acid	C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub>	0.62	[M-CHNO+H] <sup>+</sup>	134.04472	1
Glutathione	C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> S	0.64	[M] <sup>+</sup>	307.08285	1
Citric acid	C <sub>6</sub> H <sub>8</sub> O <sub>7</sub>	0.64	[M+K] <sup>+</sup>	230.99227	1
2-maleylacetate	C <sub>6</sub> H <sub>4</sub> O <sub>5</sub>	0.64	[M-2H] <sup>+</sup>	157.01305	3
Adenosine 5'-monophosphate	C <sub>10</sub> H <sub>14</sub> N <sub>5</sub> O <sub>7</sub> P	0.64	[M+H] <sup>+</sup>	348.06929	1
Nicotinic acid	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	0.64	[M+H] <sup>+</sup>	124.03988	1
Methionine	C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S	0.64	[M+H] <sup>+</sup>	150.0567	1
Succinic acid	C <sub>4</sub> H <sub>6</sub> O <sub>4</sub>	0.65	[M+H] <sup>+</sup>	119.03968	1
Aminoundecanoic acid	C <sub>11</sub> H <sub>23</sub> NO <sub>2</sub>	0.66	[M+H] <sup>+</sup>	202.17957	3
Uridine	C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub>	0.66	[M+H] <sup>+</sup>	245.07566	1
Adenine	C <sub>5</sub> H <sub>5</sub> N <sub>5</sub>	0.66	[M+H] <sup>+</sup>	136.06284	1
Nicotinamide	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O	0.67	[M+H] <sup>+</sup>	123.04904	1
L-Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	0.68	[M-NH <sub>2</sub> ] <sup>+</sup>	165.05422	1
L-Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	0.68	[M+H] <sup>+</sup>	182.08059	1
Adenosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub>	0.69	[M+H] <sup>+</sup>	268.10259	1
Tyramine	C <sub>8</sub> H <sub>11</sub> NO	0.73	[M-NH <sub>2</sub> ] <sup>+</sup>	121.06483	1
Guanosine	C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>5</sub>	0.74	[M+H] <sup>+</sup>	284.09886	2
Tyramine	C <sub>8</sub> H <sub>11</sub> NO	0.74	[M+H] <sup>+</sup>	138.08954	1
Inosine	C <sub>10</sub> H <sub>12</sub> N <sub>4</sub> O <sub>5</sub>	0.76	[M+H] <sup>+</sup>	269.09141	1
Hypoxanthine	C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O	0.76	[M+H] <sup>+</sup>	137.04988	1
Gamma-methyl L-glutamate	C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub>	0.92	[M-H <sub>2</sub> O+H] <sup>+</sup>	144.06494	3
L-Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	1.21	[M+H] <sup>+</sup>	166.08536	1
Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	1.23	[M-CH <sub>2</sub> O+H] <sup>+</sup>	120.08096	1
L-Phenylalanine	C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub>	1.3	[M+CH <sub>2</sub> O <sub>2</sub> Na] <sup>+</sup>	234.07395	1
Phenylalanylglutamate	C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub>	1.47	[M+H] <sup>+</sup>	295.13017	3
D-pantothenic acid	C <sub>9</sub> H <sub>17</sub> NO <sub>5</sub>	1.59	[M+H] <sup>+</sup>	220.11212	1
HDMBOA, 2-Hydroxy-4,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	C <sub>10</sub> H <sub>11</sub> NO <sub>5</sub>	1.64	[M+H] <sup>+</sup>	226.0706	3
Protocatechuic acid	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	1.79	[M+H] <sup>+</sup>	155.03549	1
L-Tryptophan	C <sub>22</sub> H <sub>24</sub> N <sub>4</sub> O <sub>4</sub>	2.33	[2M+H] <sup>+</sup>	409.1869	1
3,4-Dimethoxyphenethylamine	C <sub>10</sub> H <sub>15</sub> NO <sub>2</sub>	2.34	[M+H] <sup>+</sup>	182.11745	1
Tryptophan, in-source fragment	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	2.35	[M-CHO <sub>2</sub> ] <sup>+</sup>	159.09081	1
Tryptophan, in-source fragment	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	2.36	[M-C <sub>2</sub> H <sub>4</sub> NO] <sup>+</sup>	146.06003	1
L-Tryptophan	C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	2.37	[M+H] <sup>+</sup>	205.09657	1
5-S-Methyl-5-thioadenosine	C <sub>11</sub> H <sub>15</sub> N <sub>5</sub> O <sub>3</sub> S	2.48	[M+H] <sup>+</sup>	298.09673	3
Gentisic acid	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	2.52	[M-H <sub>2</sub> O+H] <sup>+</sup>	137.0248	1
Anthranilate	C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub>	2.52	[M+H] <sup>+</sup>	138.05398	3
Leucyl-Proline	C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub>	2.57	[M+H] <sup>+</sup>	229.15289	1
Esculin	C <sub>15</sub> H <sub>16</sub> O <sub>9</sub>	2.71	[M+H] <sup>+</sup>	341.08723	1
3-Amino-4-hydroxybenzoic acid, 5-amino salicylic acid	C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub>	2.77	[M+H] <sup>+</sup>	154.04987	3
2-Hydroxybenzoic acid, Salicylic acid	C <sub>7</sub> H <sub>6</sub> O <sub>3</sub>	2.78	[M-H <sub>2</sub> O+H] <sup>+</sup>	121.02945	1
Tryptamine	C <sub>10</sub> H <sub>12</sub> N <sub>2</sub>	2.79	[M+H] <sup>+</sup>	161.10689	1

2,4 Dihydroxybenzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>4</sub>	2.9	[M-H <sub>2</sub> O+H] <sup>+</sup>	137.02384	2
β-Carbocine-3-carboxylic acid	C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub>	3	[M+H] <sup>+</sup>	217.09646	2
Hydroxycoumarin 1	C <sub>9</sub> H <sub>6</sub> O <sub>3</sub>	3.09	[M+H] <sup>+</sup>	163.04201	3
Methyl 4-methoxycinnamate	C <sub>11</sub> H <sub>12</sub> O <sub>3</sub>	3.15	[M+H] <sup>+</sup>	193.0832	3
ubiquitous metabolite	C <sub>11</sub> H <sub>28</sub> N <sub>2</sub> O <sub>12</sub>	3.17	[M+H] <sup>+</sup>	381.17402	4
Scopoletin hexose-pentose	C <sub>21</sub> H <sub>26</sub> O <sub>13</sub>	3.19	[M+H] <sup>+</sup>	487.14409	3
Scopolin	C <sub>16</sub> H <sub>18</sub> O <sub>9</sub>	3.2	[M+H] <sup>+</sup>	355.10117	1
L-Tyrosyl-L-leucine	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>4</sub>	3.27	[M+H] <sup>+</sup>	295.17048	2
Quercetin-3-O-glc-1-3-rham-1-6-glucoside	C <sub>33</sub> H <sub>40</sub> O <sub>21</sub>	3.33	[M+H] <sup>+</sup>	773.20921	3
Fraxin	C <sub>16</sub> H <sub>18</sub> O <sub>10</sub>	3.42	[M-C <sub>6</sub> H <sub>10</sub> O <sub>5</sub> +H] <sup>+</sup>	209.0463	1
Derivative of dicaffeoyl quinic acid	C <sub>24</sub> H <sub>18</sub> O <sub>12</sub>	3.57	[M+H] <sup>+</sup>	499.087	3
Unknown Hexoside	C <sub>19</sub> H <sub>30</sub> O <sub>8</sub>	3.64	[M+H] <sup>+</sup>	387.20108	3
7,8-Dihydroxycoumarin	C <sub>9</sub> H <sub>6</sub> O <sub>4</sub>	3.67	[M+H] <sup>+</sup>	179.03724	1
9,10-Dihydrohydroxy-jasmonic acid sulfate	C <sub>12</sub> H <sub>20</sub> O <sub>7</sub> S	3.68	[M+H] <sup>+</sup>	309.10273	2
Riboflavin	C <sub>17</sub> H <sub>20</sub> N <sub>4</sub> O <sub>6</sub>	3.71	[M+H] <sup>+</sup>	377.14348	1
β-d-glucosyl indole-3-carboxylate	C <sub>15</sub> H <sub>17</sub> NO <sub>7</sub>	3.85	[M+H] <sup>+</sup>	324.10978	2
Quercetin + Hex + Hex + Fuc	C <sub>33</sub> H <sub>40</sub> O <sub>21</sub>	3.92	[M+H] <sup>+</sup>	773.20551	3
Quercetin + Hex+Hex	C <sub>27</sub> H <sub>30</sub> O <sub>17</sub>	3.96	[M+H] <sup>+</sup>	627.1529	3
Quercetin Deoxyhex Deoxyhex Hex	C <sub>33</sub> H <sub>40</sub> O <sub>20</sub>	4.01	[M+H] <sup>+</sup>	757.21447	3
Saponarin	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	4.01	[M+H] <sup>+</sup>	595.16569	2
Quercetin Deoxyhex Hex	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	4.02	[M+H] <sup>+</sup>	611.15714	3
Isorientin	C <sub>21</sub> H <sub>20</sub> O <sub>11</sub>	4.02	[M+H] <sup>+</sup>	449.10799	3
1-O-Feruloyl-beta-D-glucose	C <sub>16</sub> H <sub>20</sub> O <sub>9</sub>	4.06	[M+H] <sup>+</sup>	357.11916	3
N-Phenylacetyl-Aspartic acid	C <sub>12</sub> H <sub>13</sub> NO <sub>5</sub>	4.07	[M+H] <sup>+</sup>	252.0869	2
Hydroxyjasmonic acid	C <sub>12</sub> H <sub>18</sub> O <sub>4</sub>	4.11	[M+H] <sup>+</sup>	227.12685	3
Sinapyl alcohol	C <sub>11</sub> H <sub>12</sub> O <sub>3</sub>	4.17	[M-H <sub>2</sub> O+H] <sup>+</sup>	193.08493	1
Phthalide	C <sub>8</sub> H <sub>6</sub> O <sub>2</sub>	4.18	[M+H] <sup>+</sup>	135.04479	1
Leucyl-Phenylalanine	C <sub>15</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub>	4.19	[M+H] <sup>+</sup>	279.16744	1
Carveol	C <sub>10</sub> H <sub>16</sub> O	4.2	[M+H] <sup>+</sup>	135.11612	3
Quercetin+hex+deoxyhex	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	4.23	[M+H] <sup>+</sup>	611.15799	3
fragment of Quercetin+hex+deoxyhex	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	4.24	[M+H] <sup>+</sup>	465.10365	3
fragment of Quercetin+hex+deoxyhex	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	4.24	[M+H] <sup>+</sup>	303.0499	3
Unknown, similar to Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	4.26	[M+H] <sup>+</sup>	182.08109	4
Unknown, similar to Feruloyl glycerol	C <sub>13</sub> H <sub>16</sub> O <sub>6</sub>	4.29	[M+H] <sup>+</sup>	269.10204	4
Methylumbelliferone	C <sub>10</sub> H <sub>8</sub> O <sub>3</sub>	4.39	[M+H] <sup>+</sup>	177.05444	3
Feruloyl dehydrotyramine	C <sub>18</sub> H <sub>17</sub> NO <sub>4</sub>	4.4	[M+H] <sup>+</sup>	312.12362	3
Scopoletin	C <sub>10</sub> H <sub>8</sub> O <sub>4</sub>	4.41	[M+H] <sup>+</sup>	193.05111	1
Methylumbelliferone	C <sub>10</sub> H <sub>8</sub> O <sub>3</sub>	4.44	[M+H] <sup>+</sup>	177.05434	3
Rutin, Quercetin 3-o-rutinoside	C <sub>27</sub> H <sub>30</sub> O <sub>16</sub>	4.45	[M+H] <sup>+</sup>	611.15984	1
Rutin, in-source fragment 302	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	4.45	[M+H] <sup>+</sup>	303.0498	1
Rutin, in-source fragment 464	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	4.45	[M+H] <sup>+</sup>	465.10349	1
Gibberellic acid	C <sub>19</sub> H <sub>18</sub> O <sub>4</sub>	4.49	[M-H <sub>4</sub> O <sub>2</sub> +H] <sup>+</sup>	311.12722	1
Leuko-DOPA-chrome	C <sub>9</sub> H <sub>9</sub> NO <sub>4</sub>	4.56	[M+H] <sup>+</sup>	196.06113	3
Quercetin-3-o-glucoside, in-source fragment -Glc	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub>	4.59	[M+H] <sup>+</sup>	303.04987	1

Quercetin-3-glucoside, Isoquercitrin	C <sub>21</sub> H <sub>20</sub> O <sub>12</sub>	4.59	[M+H] <sup>+</sup>	465.10251	1
Benzoic acid	C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>	4.64	[M+H] <sup>+</sup>	123.04509	1
N-(3-Hydroxypropyl)-phthalimide; 1H-Isoindole-1,3(2H)-dione	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>	4.76	[M+H] <sup>+</sup>	206.0799	1
Guaiacylglycerol β-coniferyl ether (G(8-O-4)G)	C <sub>20</sub> H <sub>24</sub> O <sub>7</sub>	4.81	[M+H] <sup>+</sup>	377.16009	3
Kaempferol 3-O-beta-Glc-7-O-alpha-Rha	C <sub>27</sub> H <sub>30</sub> O <sub>15</sub>	4.81	[M+H] <sup>+</sup>	595.1655	2
4-Hydroxy-3,5-dimethylbenzoic acid	C <sub>9</sub> H <sub>10</sub> O <sub>3</sub>	4.85	[M+H] <sup>+</sup>	167.07077	2
Unknown, similar to Tyrosine	C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub>	4.86	[M+H] <sup>+</sup>	182.08115	4
5-Methoxyindole-3-acetic acid	C <sub>11</sub> H <sub>11</sub> NO <sub>3</sub>	4.98	[M+H] <sup>+</sup>	206.07929	1
Unknown polysaccharide	C <sub>12</sub> H <sub>22</sub> O <sub>11</sub>	5.31	[M+H] <sup>+</sup>	365.10049	4
Kaempferin	C <sub>21</sub> H <sub>20</sub> O <sub>10</sub>	5.41	[M+H] <sup>+</sup>	433.1236	3
3,4-dimethoxycinnamic acid	C <sub>11</sub> H <sub>12</sub> O <sub>4</sub>	5.6	[M+H] <sup>+</sup>	209.08191	1
Simulanol (S(8-5)G)	C <sub>21</sub> H <sub>24</sub> O <sub>7</sub>	5.67	[M+H] <sup>+</sup>	389.16803	2
N-feruloyltyramine	C <sub>18</sub> H <sub>19</sub> NO <sub>4</sub>	5.84	[M+H] <sup>+</sup>	314.13753	2
Glyphosate constituent 1	C <sub>16</sub> H <sub>33</sub> NO <sub>3</sub>	5.89	[M+H] <sup>+</sup>	288.2528	4
Abscisic acid	C <sub>15</sub> H <sub>18</sub> O <sub>3</sub>	5.9	[M+H] <sup>+</sup>	247.13147	1
Glycosmistic acid	C <sub>20</sub> H <sub>20</sub> O <sub>7</sub>	5.91	[M+H] <sup>+</sup>	373.13667	2
p-Coumaric acid-O-dihydroxy-cinnamoyl methyl ester	C <sub>19</sub> H <sub>16</sub> O <sub>6</sub>	5.92	[M+H] <sup>+</sup>	341.10174	3
Glyphosate constituent 2	C <sub>16</sub> H <sub>33</sub> NO <sub>3</sub>	6.06	[M+H] <sup>+</sup>	288.25272	4
(E)-Cinnamic acid	C <sub>9</sub> H <sub>8</sub> O <sub>2</sub>	6.09	[M+H] <sup>+</sup>	131.04966	1
Herniarin	C <sub>10</sub> H <sub>8</sub> O <sub>3</sub>	6.17	[M+H] <sup>+</sup>	177.05415	1
Glyphosate constituent 3	C <sub>16</sub> H <sub>33</sub> NO <sub>3</sub>	6.3	[M+H] <sup>+</sup>	288.25232	4
Amaranthus triterpenoid, 1258 (fragment 502)	C <sub>30</sub> H <sub>46</sub> O <sub>6</sub>	6.64	[M+H] <sup>+</sup>	503.33567	3
Genistein	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	6.77	[M+H] <sup>+</sup>	271.06077	1
Amaranthus triterpenoid, 792	C <sub>40</sub> H <sub>56</sub> O <sub>16</sub>	6.79	[M+H] <sup>+</sup>	793.36031	3
Amaranthus triterpenoid, 840 (fragment 502)	C <sub>30</sub> H <sub>46</sub> O <sub>6</sub>	6.79	[M+H] <sup>+</sup>	503.33582	3
Jasmonic acid	C <sub>12</sub> H <sub>18</sub> O <sub>3</sub>	6.82	[M+H] <sup>+</sup>	211.13316	1
Amaranthus triterpenoid, 840	C <sub>41</sub> H <sub>60</sub> O <sub>18</sub>	6.82	[M+H] <sup>+</sup>	841.38418	3
Amaranthus triterpenoid, 1216 (fragment 810)	C <sub>40</sub> H <sub>58</sub> O <sub>17</sub>	6.89	[M+H] <sup>+</sup>	811.38031	3
Amaranthus triterpenoid, 1216 (fragment 764)	C <sub>39</sub> H <sub>56</sub> O <sub>15</sub>	6.89	[M+H] <sup>+</sup>	765.37209	3
Amaranthus triterpenoid, 1216 (fragment 810)	C <sub>40</sub> H <sub>58</sub> O <sub>17</sub>	6.98	[M+H] <sup>+</sup>	811.37071	3
Amaranthus triterpenoid, 1216 (fragment 502)	C <sub>30</sub> H <sub>46</sub> O <sub>6</sub>	6.98	[M+H] <sup>+</sup>	503.3365	3
Farnesal	C <sub>15</sub> H <sub>24</sub> O	7.16	[M+H] <sup>+</sup>	203.17828	2
Amaranthus triterpenoid, 794 (fragment 486)	C <sub>30</sub> H <sub>46</sub> O <sub>5</sub>	7.26	[M+H] <sup>+</sup>	487.33998	3
Amaranthus triterpenoid, 794 (fragment 308)	C <sub>10</sub> H <sub>12</sub> O <sub>11</sub>	7.27	[M+H] <sup>+</sup>	309.04793	3
Amaranthus triterpenoid, 1405 (fragment 808)	C <sub>41</sub> H <sub>60</sub> O <sub>16</sub>	7.59	[M+H] <sup>+</sup>	809.39309	3
Amaranthus triterpenoid, 824 (fragment 780)	C <sub>40</sub> H <sub>60</sub> O <sub>15</sub>	7.84	[M+H] <sup>+</sup>	781.39422	3
Biochanin A, 5,7-Dihydroxy-4'-methoxyisoflavone (internal standard)	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	8.79	[M+Na] <sup>+</sup>	307.05808	1
Biochanin A, 5,7-Dihydroxy-4'-methoxyisoflavone (internal standard)	C <sub>16</sub> H <sub>12</sub> O <sub>5</sub>	8.79	[M+H] <sup>+</sup>	285.07614	1
Phytosphingosine	C <sub>18</sub> H <sub>37</sub> NO <sub>3</sub>	9.32	[M+H] <sup>+</sup>	316.28323	3
Methyl octanoate	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	9.35	[M+H] <sup>+</sup>	159.13763	3
Dioscin	C <sub>39</sub> H <sub>63</sub> O <sub>12</sub>	9.7	[M+H] <sup>+</sup>	724.44094	3
Lauric acid diethanolamide	C <sub>16</sub> H <sub>33</sub> NO <sub>3</sub>	9.72	[M+H] <sup>+</sup>	288.25262	3
Glc-Glc-octadecatrienoyl-sn-glycerol (isomer 1)	C <sub>33</sub> H <sub>56</sub> O <sub>14</sub>	9.8	[M+H] <sup>+</sup>	659.36079	3

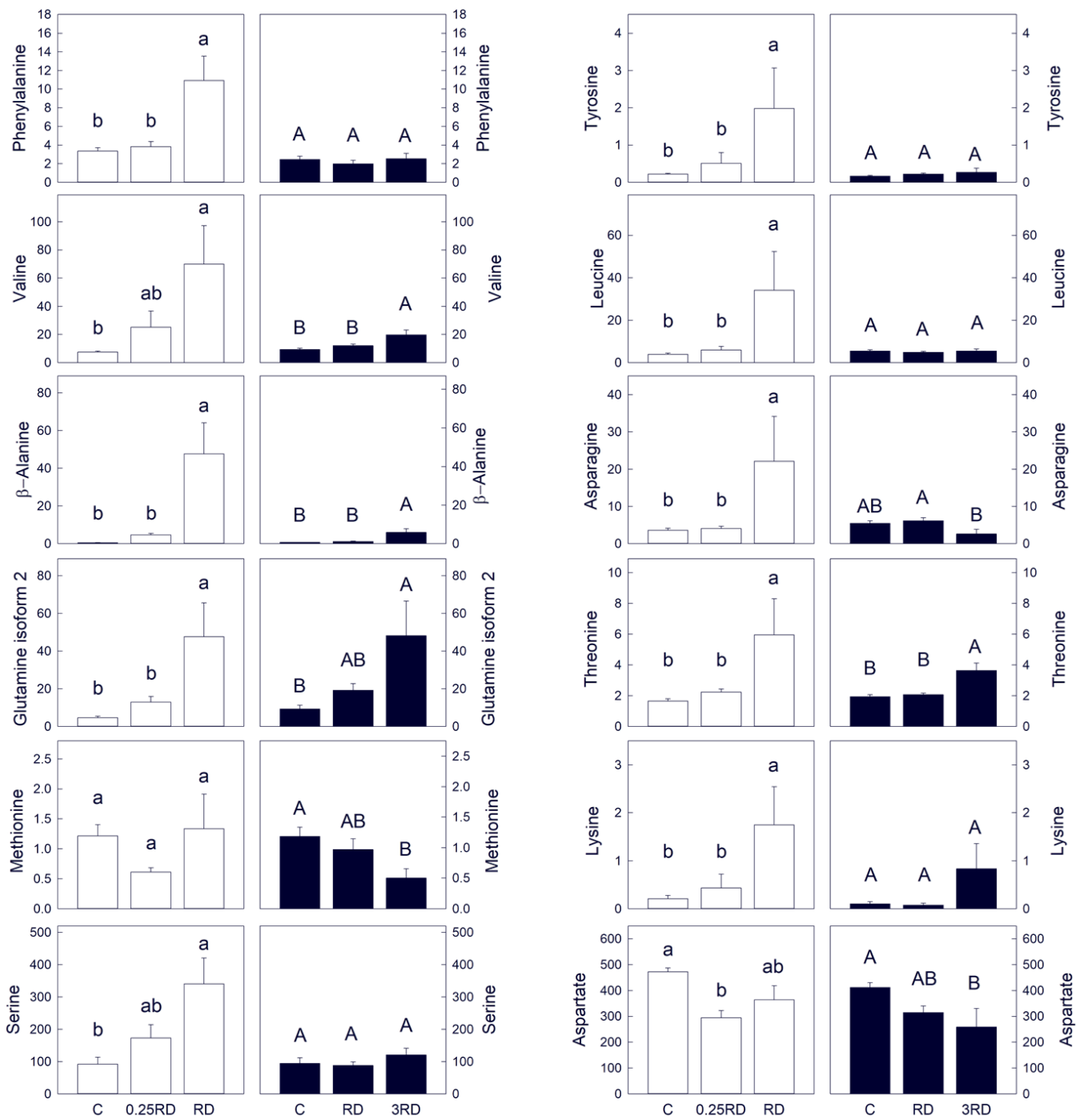
Monolinolenin (isomer 1)	C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>	9.8	[M+H] <sup>+</sup>	353.26758	3
Glc-octadecatrienoyl-sn-glycerol (isomer 1)	C <sub>27</sub> H <sub>46</sub> O <sub>9</sub>	10.03	[M+H] <sup>+</sup>	515.31914	3
Monolinolenin (isomer 2)	C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>	10.03	[M+H] <sup>+</sup>	353.26763	3
Glc-Glc-octadecatrienoyl-sn-glycerol (isomer 2)	C <sub>33</sub> H <sub>56</sub> O <sub>14</sub>	10.04	[M+H] <sup>+</sup>	699.35227	3
Oxo-phytodienoic acid	C <sub>18</sub> H <sub>28</sub> O <sub>3</sub>	10.24	[M+H] <sup>+</sup>	315.1929	2
Capric acid	C <sub>10</sub> H <sub>20</sub> O <sub>2</sub>	10.32	[M+H] <sup>+</sup>	173.15204	1
Lysophosphatidylcholine (isomer 1)	C <sub>26</sub> H <sub>50</sub> NO <sub>7</sub> P	10.62	[M+H] <sup>+</sup>	520.33946	3
Glc-octadecatrienoyl-sn-glycerol (isomer 2)	C <sub>27</sub> H <sub>46</sub> O <sub>9</sub>	10.75	[M+H] <sup>+</sup>	497.31063	3
Linolenoylglycerol	C <sub>21</sub> H <sub>36</sub> O <sub>4</sub>	10.75	[M+H] <sup>+</sup>	353.26762	3
Lysophosphatidylcholine (isomer 2)	C <sub>26</sub> H <sub>50</sub> NO <sub>7</sub> P	10.84	[M+H] <sup>+</sup>	520.33978	3
Lysophosphatidylcholine (isomer 3)	C <sub>24</sub> H <sub>50</sub> NO <sub>7</sub> P	11.03	[M+H] <sup>+</sup>	496.34017	3
Hydroxyoctadecadienoic acid (isomer 1)	C <sub>18</sub> H <sub>32</sub> O <sub>3</sub>	11.33	[M+H] <sup>+</sup>	319.22361	3
Lysophosphatidylcholine (isomer 4)	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	11.44	[M+H] <sup>+</sup>	522.35566	3
1-Oleoyl-sn-glycero-3-phosphocholine	C <sub>26</sub> H <sub>52</sub> NO <sub>7</sub> P	11.67	[M+H] <sup>+</sup>	522.35557	3
Hydroxyoctadecadienoic acid (isomer 2)	C <sub>18</sub> H <sub>30</sub> O <sub>3</sub>	11.68	[M+H] <sup>+</sup>	277.21434	3
Lauric acid	C <sub>12</sub> H <sub>24</sub> O <sub>2</sub>	12.09	[M+H] <sup>+</sup>	201.18435	1
Phthalic anhydride	C <sub>8</sub> H <sub>4</sub> O <sub>3</sub>	12.2	[M+H] <sup>+</sup>	149.02348	3
1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine	C <sub>26</sub> H <sub>54</sub> NO <sub>7</sub> P	12.7	[M+H] <sup>+</sup>	524.37025	3
1-Stearoyl-sn-glycero-3-phosphate	C <sub>21</sub> H <sub>41</sub> O <sub>7</sub> P	13.64	[M+H] <sup>+</sup>	437.2642	3
Linoloylglycerol	C <sub>21</sub> H <sub>38</sub> O <sub>4</sub>	13.7	[M+H] <sup>+</sup>	377.26543	3
Oxylipin	C <sub>36</sub> H <sub>60</sub> O <sub>4</sub>	13.72	[M+H] <sup>+</sup>	557.45365	3
linolenic acid (isomer1 )	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	13.72	[M+H] <sup>+</sup>	279.23108	3
monoglyceride	C <sub>20</sub> H <sub>34</sub> O <sub>3</sub>	13.89	[M+H] <sup>+</sup>	345.23948	3
linolenic acid (isomer 2)	C <sub>18</sub> H <sub>30</sub> O <sub>2</sub>	13.89	[M+H] <sup>+</sup>	279.22526	3
13-apo-β-carotenone	C <sub>18</sub> H <sub>26</sub> O	13.97	[M+H] <sup>+</sup>	259.20489	3
Oleamide	C <sub>18</sub> H <sub>35</sub> NO	14.31	[M+H] <sup>+</sup>	282.27812	3
1-Palmitoylglycerol	C <sub>19</sub> H <sub>38</sub> O <sub>4</sub>	14.36	[M+H] <sup>+</sup>	353.26486	3
17-Octadecynoic acid	C <sub>18</sub> H <sub>32</sub> O <sub>2</sub>	14.58	[M+H] <sup>+</sup>	263.23577	3
1-Stearoyl-rac-glycerol	C <sub>21</sub> H <sub>42</sub> O <sub>4</sub>	15.83	[M+H] <sup>+</sup>	359.31449	3
Diacylglycerine	C <sub>39</sub> H <sub>64</sub> O <sub>5</sub>	17.82	[M+H] <sup>+</sup>	613.481	3

Reference: Matern A, Böttcher C, Eschen-Lippold L, Westermann B, Smolka U, Döll S, Trempel F, Aryal B, Scheel D, Geisler M, Rosahl S (2019). A substrate of the ABC transporter PEN3 stimulates bacterial flagellin (flg22)-induced callose deposition in *Arabidopsis thaliana*. *J Biol Chem.* 294(17):6857-6870. doi: 10.1074/jbc.RA119.007676.

**Figure S1.** Amino acids detected by GC-MS in glyphosate-resistant and sensitive *Amaranthus palmeri* plants. Y-axis: normalized peak intensity. Plants were untreated (control) or treated with glyphosate in two different doses: 0.25 RD (field recommended dose) or RD in GS and RD or 3 RD in GR. Mean ± SE (n=4-6). Different letters within each population indicate significant differences between treatments (p-value ≤ 0.05, Tukey).



AMINO ACIDS



**Figure S2. A.** Treatment application with an aerograph connected to a compressor. **B.** State of the plant at the moment of the treatment.

