

Supplementary Materials

Article title: **Metabolic profile discriminates and predicts *Arabidopsis* susceptibility to virus under field conditions**

Table S1 Spearman correlations between dry biomass (DB), viral accumulation (OD) and 10 primary metabolites content measured on the 26 *A. thaliana* accessions of the '2015' field experiment

	OD	Amino Acids	Proteins	Glutamate	Malate	Fumarate	Starch	Glucose	Fructose	Sucrose	Chla
DB_Mock-inoculated	-	-0.66 ***	-0.42 *	-0.45 *	0.38 *	0.36 .	0.48 **	0.65 ***	0.18	0.3	-0.12 NS
DB_TuMV-inoculated	-0.62 ***	-0.75 ***	-0.27 NS	-0.71 ***	-0.44 *	-0.22 NS	-0.3 NS	-0.38 *	-0.61 ***	-0.52 ***	0.23 NS
OD_TuMV-inoculated	1	0.49 ***	0.35 .	0.63 ***	0.22	0.44 *	0.58 **	0.55 ***	0.42 *	0.70 ***	-0.08 NS

All the significant correlations where showed by asterisks and values (Signif.codes: 0 **** 0.001 *** 0.01 ** 0.05 . 0.1)
- Non tested and NS = Non significant differences

Table S2 List of the *A. thaliana* accessions with their geographic position and their susceptible status to TuMV infection confirmed by OD values and SD in '2017' experiment

Genotype	ID ¹	Latitude	Longitude	Country	Susceptibility Groups ²	OD Means	OD-Standard Deviations
Ra-0	6958	46	3.3	FRA	R	0.0188	0.0174
TOU-A1-84	348	46.6667	4.11667	FRA	R	0.0202	0.02
Bay-0	6899	49	11	GER	R	0.0218	0.0143
Petergof	7296	59	29	RUS	R	0.0406	0.0197
Rak-2	8365	49	16	CZE	R	0.053	0.0037
Col-0	6909	38.3	-92.3	USA	S	0.325	0.165
Mt-0	6939	32.34	22.46	LIB	S	0.379	0.122
Bu-0	8271	50.5	9.5	GER	S	0.621	0.222
CUR-10	79	45	1.75	FRA	S	0.769	0.274
Bs-1	8270	47.5	7.5	SUI	S	0.832	0.364

¹ ID according to [40].

² In 2017, categories have been defined according to the healthy control Col-0 which mean OD value was 0.078 (SD 0.00722). Infected genotypes with mean OD ≤ 0.078 were defined as resistant (R). Infected genotypes with mean OD > 2.5 * 0.078 were defined as susceptible [41].

Table S3 Common Variable Importance in the Projection (VIPs) obtained with the OPLS-DA performed on mock and TuMV-inoculated and on resistant and susceptible accessions of twenty-six accessions in 2015. For each VIP, the comparison between the metabolic content in mock (M) and TuMV-inoculated (I) samples was done and the fold change was represented. Moreover, the comparison, for each VIP, of metabolic content between resistant (R) and susceptible (S) accessions was also represented.

VIP-OPLS- DA ¹	VIP values	m/z ²	rt ³	Mock vs. TuMV Infected		Resistant vs. Susceptible	
					Fold change		
193;324	2.201000988	193.13	323.817	I > M	4.54	S > R *** ⁴	
331;329	2.177409793	331.12	328.817	I > M	2.55	S > R ***	
474;107	2.100348101	474.22	107.298	I > M	7.12	S > R ***	
482;101	2.02851797	482.11	101.274	I > M	3.24	S > R ***	
205;242	1.95494017	205.1	242.121	I > M	3.16	S > R ***	
209;488	1.895244441	209.15	488.35	I > M	3.87	S > R ***	
212;284	1.812272811	211.56	283.891	I > M	1.97	S > R ***	
343;345	1.793276838	343.12	345.319	I > M	2.41	S > R ***	
116;100	1.77949346	116.07	100.163	I > M	6.88	S > R ***	
162;357	1.767230127	162.05	356.879	I > M	3.1	S > R ***	
303;463	1.682969043	303.13	463.27	I > M	2.9	S > R ***	
219;311	1.640982077	219.1	311.134	I > M	3.44	S > R ***	
355;306	1.594996482	355.1	306.288	I > M	8.11	S > R ***	
305;210	1.575910966	305.09	210.166	I > M	2.69	S > R ***	
133;296	1.573543164	133.06	295.68	I > M	3.79	S > R ***	
221;216	1.49354017	221.09	215.744	I > M	2.46	S > R ***	
124;346	1.493002053	124.08	346.354	I > M	1.68	S > R ***	
503;391	1.478656897	503.19	391.457	I > M	2.24	S > R ***	
373;344	1.456529478	373.13	343.531	I > M	1.78	S > R ***	
151;359	1.45485619	151.08	359.377	I > M	1.28	S > R ***	
374;322	1.444521384	374.14	321.703	I > M	1.88	S > R ***	
162;249	1.431791986	162.05	249.101	I > M	1.81	S > R ***	
175;402	1.423091039	175.15	401.831	I > M	2.52	S > R ***	
332;430	1.416086097	332.13	430.481	I > M	2.32	S > R ***	
315;448	1.412434025	315.13	447.821	I > M	2.05	S > R ***	
221;230	1.4121623	221.12	230.244	I > M	1.67	S > R ***	
391;774	1.397491479	391.24	774.477	I > M	2.36	S > R ***	
386;278	1.385282143	386.22	277.549	I > M	5.51	S > R ***	
348;319	1.376257143	348.27	318.945	I > M	4.2	S > R ***	
356;452	1.358448769	356.12	452.352	I > M	1.69	S > R ***	
201;344	1.355039751	201.05	343.832	I > M	1.71	S > R ***	

222;216	1.351138929	221.6	215.822	I > M	2.46	S > R **
370;302	1.331366534	370.15	301.519	I > M	5.59	S > R ***
315;370	1.330904866	315.13	370.476	I > M	3.58	S > R ***
367;358	1.251165644	367.1	358.491	I > M	1.62	S > R ***
182;466	1.243641489	182.08	465.796	I > M	3.65	S > R ***
302;407	1.221943812	302.1	406.697	I > M	4.3	S > R ***
191;363	1.219391802	191.07	362.643	I > M	2.37	S > R ***
367;342	1.199530791	367.15	341.908	I > M	2.4	S > R ***
291;259	1.165429681	291.18	259.063	I > M	3.68	S > R ***
178;191	1.128214863	178.09	191.013	I > M	3.11	S > R ***
396;348	1.126209569	396.11	347.739	I > M	7.35	S > R ***
394;517	1.125664243	394.2	517.072	I > M	4.36	S > R ***
543;99	1.122326073	543.13	98.5221	I > M	2.62	S > R ***
212;774	1.113329112	212.09	774.047	I > M	3.14	S > R ***
164;375	1.107007943	164.07	375.012	I > M	2.38	S > R ***
210;465	1.09694612	210.11	464.799	I > M	2.27	S > R ***
379;402	1.091061829	379.09	402.311	I > M	2.47	S > R ***
133;126	1.06741008	133.1	126.347	I > M	2.62	S > R **
409;491	1.066982099	409.17	490.545	I > M	1.46	S > R ***
109;359	1.035812334	109.06	359.34	I > M	1.67	S > R ***
162;402	1.032043124	162.05	402.281	I > M	1.41	S > R ***
227;789	1.023548533	227.16	788.506	I > M	1.71	S > R ***
192;462	1.000060126	192.04	462.37	I > M	1.31	S > R ***
433;700	2.253892757	433.24	700.261	I > M	3	R > S ***
361;491	1.914433317	361.09	490.564	I > M	4.84	R > S ***
512;491	1.813252344	512.13	491.367	I > M	21.08	R > S ***
64;395	1.668700459	63.934	395.047	I > M	1.25	R > S ***
79;396	2.194133112	79.041	395.754	M > I	1.85	S > R ***
105;700	1.816365199	105.07	700.287	M > I	1.88	S > R ***
169;496	1.288454553	169.05	495.5	M > I	1.91	S > R ***
449;442	1.102028381	449.11	442.311	M > I	4.26	R > S ***
137;131	1.036410357	136.93	131.31	M > I	1.35	R > S ***

¹ When undetermined, VIP are identified through m/z;rt values. VIP values are classified in decreasing order.

² mass to charge ratio

³ retention time

⁴ The significance was assessed through a Wilcoxon test at *** P < 0.001, ** 0.001 < P < 0.01

Table S4 Comparisons between the Variable Importance in the Projection (VIPs) identify by OPLS-DA analysis and those identify by PLS analysis performed with resistant and susceptible twenty-six accessions in 2015. The same results of metabolic content comparisons were found between resistant (R) and susceptible (S) accessions. The fold change was also represented for each VIP. Primary metabolites are light-grey highlighted. Metabolites that accumulate significantly more in resistant accessions are at the bottom of the table.

VIP PLS ¹	VIP-PLS value	VIP-OPLS- DA value	m/z ²	rt ³	Resistant vs Susceptible metabolic contents	Fold change
356;45			356.1	452.		
2	2.1040	1.9580	202	352	S > R *** ⁴	2.17
Gluta mate	2.0854	1.5902	NA	NA	S > R ***	1.47
Sucros e	1.9944	2.2126	NA	NA	S > R ***	2.89
219;31			219.1	311.		
1	1.9753	1.9395	011	134	S > R ***	4.81
385;21			385.1	210.		
0	1.9524	1.7380	055	083	S > R ***	45.77
373;45			373.1	452.		
3	1.9059	1.2900	273	6	S > R ***	1.81
270;58			270.1	587.		
7	1.8532	1.5343	33	091	S > R ***	43.68
315;37			315.1	370.		
0	1.8277	1.5236	333	476	S > R ***	3.93
348;31			348.2	318.		
9	1.8190	1.3963	736	945	S > R ***	3.61
394;51			394.2	517.		
7	1.8096	1.4897	045	072	S > R ***	17.28
191;36			191.0	362.		
3	1.7958	1.3599	699	643	S > R ***	2.76
474;10			474.2	107.		
7	1.7890	1.6748	178	298	S > R ***	2.68
226;40			226.1	406.		
6	1.7712	1.5540	066	369	S > R ***	7.97
420;27			419.6	275.		
6	1.7295	1.2167	949	797	S > R ***	1.77
367;34			367.1	341.		
2	1.7210	1.0107	531	908	S > R ***	1.96
302;40			302.1	406.		
7	1.6916	1.4864	013	697	S > R ***	7.16

503;39			503.1	391.		
1	1.6879	1.6947	902	457	S > R ***	2.51
116;10			116.0	100.		
0	1.6790	1.8669	701	163	S > R ***	6.05
396;25			396.1	256.		
7	1.6725	1.1064	854	51	S > R ***	1.43
303;46			303.1	463.		
3	1.6577	1.9734	334	27	S > R ***	3.69
355;30			355.1	306.		
6	1.6414	1.4506	015	288	S > R ***	3.29
370;30			370.1	301.		
2	1.6342	1.6097	486	519	S > R ***	28.49
343;34			343.1	345.		
5	1.6096	1.6930	168	319	S > R ***	2.08
533;39			533.1	391.		
2	1.6000	1.9258	549	765	S > R ***	4.98
201;45			201.0	451.		
1	1.5993	1.0635	543	123	S > R ***	1.75
757;31			757.2	319.		
9	1.5938	1.5374	171	13	S > R ***	1.69
386;27			386.2	277.		
8	1.5899	1.2560	198	549	S > R ***	3.48
903;31			903.2	318.		
9	1.5874	1.7102	769	889	S > R ***	8.48
449;31			449.1	318.		
9	1.5823	1.5451	063	949	S > R ***	1.75
182;46			182.0	465.		
6	1.5645	1.4146	808	796	S > R ***	4.21
175;40			175.1	401.		
2	1.5414	1.7128	478	831	S > R ***	3.77
305;21			305.0	210.		
0	1.5354	1.4081	861	166	S > R ***	2.24
195;45			195.0	452.		
3	1.5352	1.1541	648	614	S > R ***	1.55
221;21			221.0	215.		
6	1.5350	1.7483	915	744	S > R ***	3.13
374;32			374.1	321.		
2	1.5256	1.3048	436	703	S > R ***	1.77
Glucos						
e	1.5212	1.7342	NA	NA	S > R ***	2.49
179;60			179.1	603.		
4	1.5211	1.3057	063	961	S > R ***	1.64

161;44			161.0	441.		
2	1.5180	1.2744	957	797	S > R ***	1.79
394;10			394.2	108.		
8	1.7935	1.5477	001	419	R > S ***	1.93
351;18			351.0	184.		
4	1.7480	2.0467	062	222	R > S ***	2.88
324;18			323.9	183.		
4	1.7384	1.2634	889	797	R > S ***	106.8
280;18			280.0	183.		
4	1.7056	1.2289	842	768	R > S ***	5.9
432;18			431.9	183.		
4	1.6488	1.8309	707	776	R > S ***	3.44
			86.05	184.		
86;184	1.6112	1.0146	939	278	R > S ***	1.87

¹ When undetermined, VIP are identified through m/z;rt values. VIP values are classified in decreasing order.

² mass to charge ratio

³ retention time

⁴ The significance was assessed through a Wilcoxon test at *** $P < 0.001$, ** $0.001 < P < 0.01$

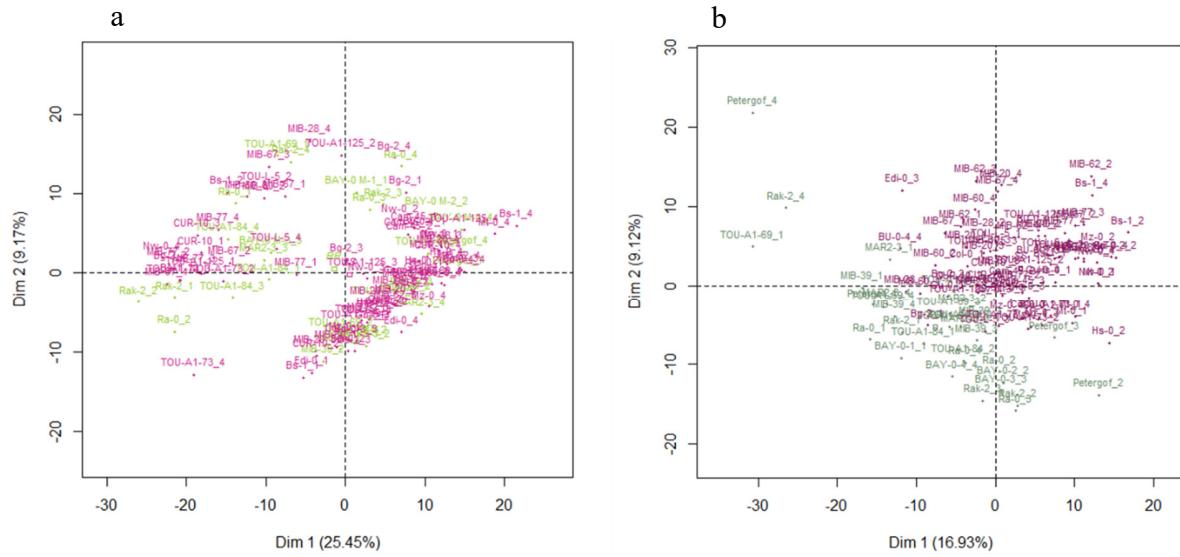


Figure S1. Principal component analysis performed on the 505 metabolic signatures (m/z) measured on 26 *A. thaliana* accessions in the '2015' field experiment

a. PCA performed on the 505 metabolic signatures (m/z) measured by UHPLC-LTQ Orbitrap on 26 *A. thaliana* mock-inoculated accessions. The two major components that together accounted for 34.62% of the variance. Resistant and susceptible accessions are in light green and light pink, respectively. b. PCA performed on the 505 metabolic signatures (m/z) measured by UHPLC-LTQ Orbitrap on 26 *A. thaliana* TUMV-inoculated accessions. The two major components accounted for 26.05% of the variance. Resistant and susceptible accessions are in dark green and dark pink,

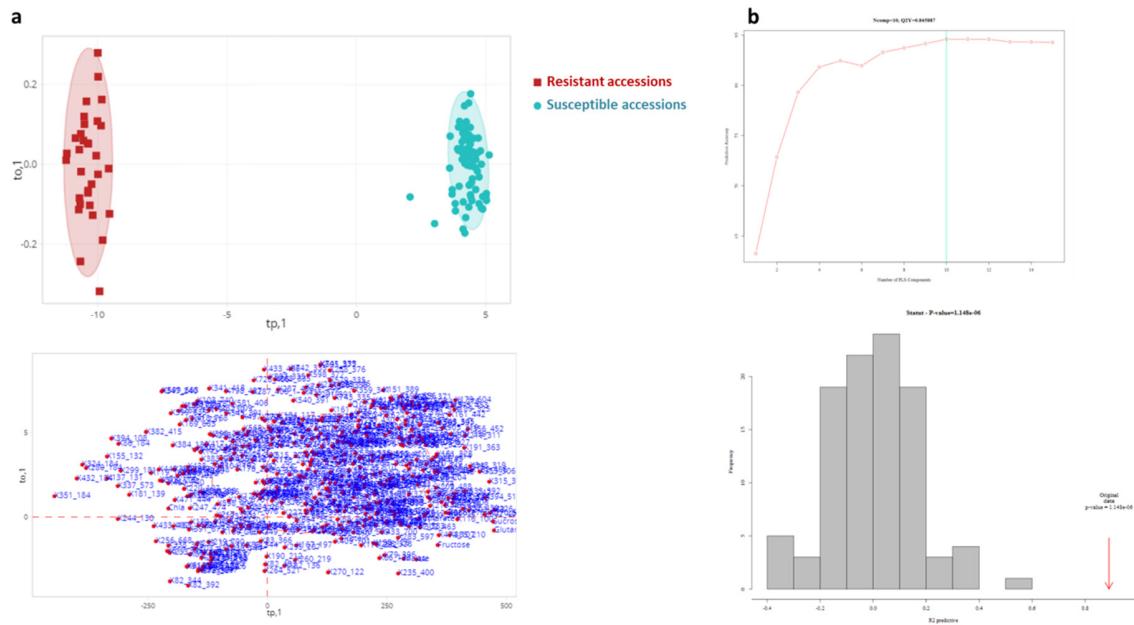
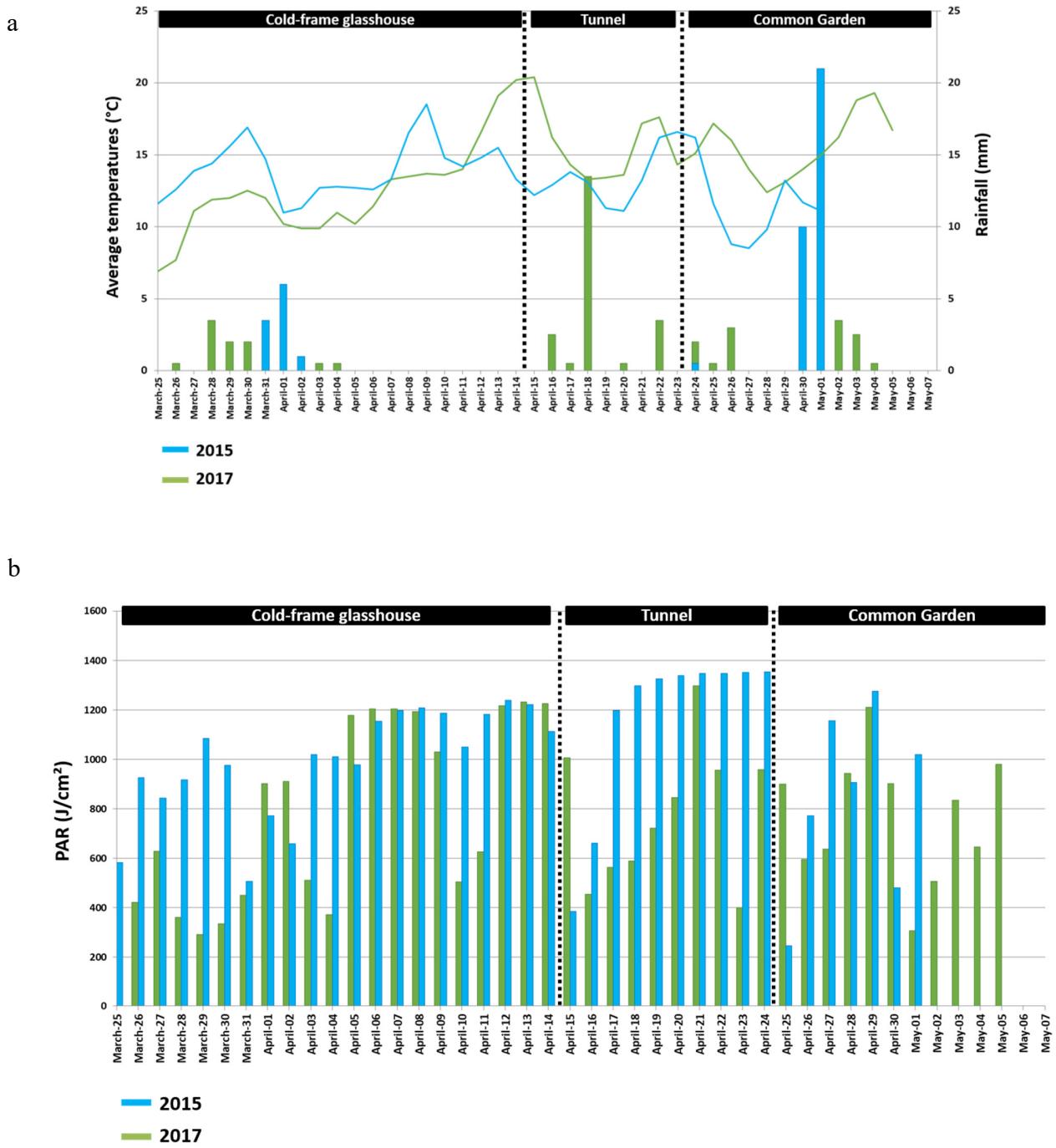
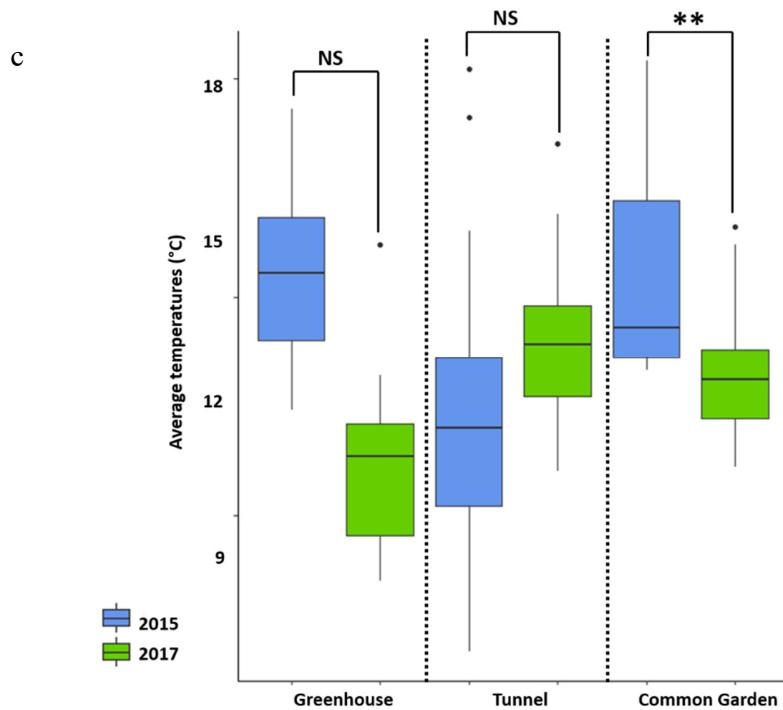


Figure S2 OPLS-DA analysis and its parameters of validation for the TuMV-inoculated resistant and susceptible 26 *A. thaliana* accessions of the '2015' field experiment a. OPLS-DA results with the score plot and the loading plot containing all the metabolic variables tested. The resistant (in red) and susceptible (in blue) accessions were represented. b. Parameters for validation of the OPLS-DA analysis.





d

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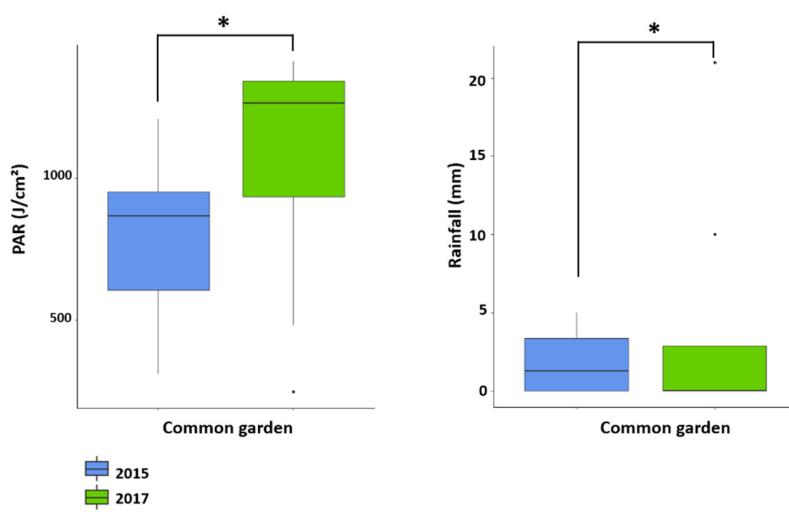


Figure S3 Climate raw data and comparison between the 2015 and 2017 field experiment
a. Rainfall and average temperature in 2015 and 2017 b. PAR in 2015 and 2017 recorded under the three successive conditions of the experiment, cold-frame glasshouse, tunnel and

common garden. c. Comparison of the average temperatures between 2015 and 2017 under the 3 successive conditions of the experiments. d. Comparison of PAR between 2015 and 2017 under common garden conditions. e. Comparison of rainfall between 2015 and 2017 under common garden conditions. The significance was assessed through a Wilcoxon test at *p-value* = 0.05 indicated by a *, NS: non-significant.