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Supplementary Figures and Tables

Green light drives embryonic photosynthesis and protein accumulation in developing pea (*Pisum sativum* L.) seeds.

Nataliia Stepanova, Elena Tarakhovskaya, Alena Soboleva, Anastasia Orlova, Aditi Basnet, Anastasia Smolenskaya, Nadezhda Frolova, Tatiana Bilova, Anastasia Kamionskaya, Andrej Frolov, Sergei Medvedev and Galina Smolikova

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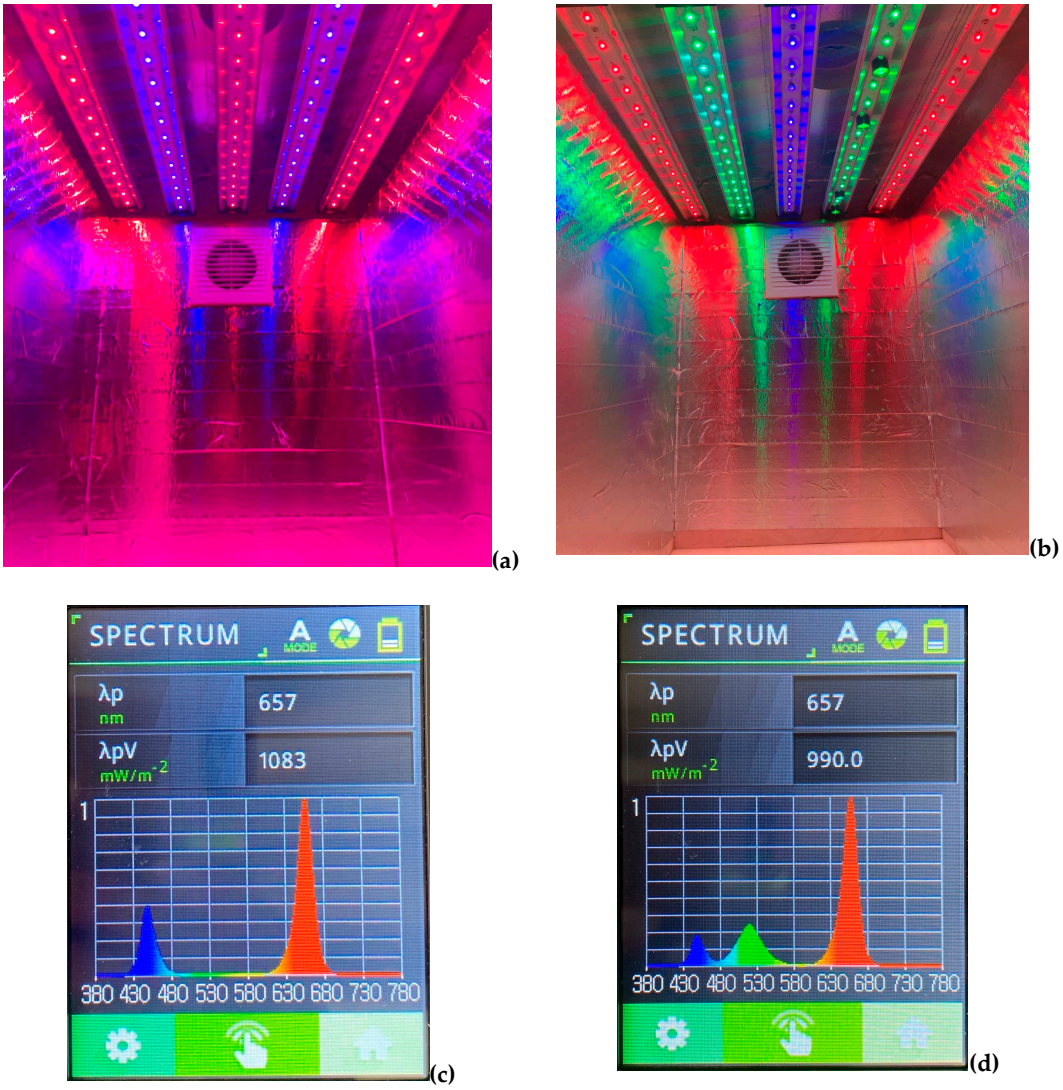

Figure S1. Close-type installation and spectral characteristics of the light for growing the *Pisum sativum* plants: **(a, c)** RB module illuminated with blue LEDs (BL, 400-500 nm, maxima of 450 nm, 42 ± 4 µmol photons m^{-2} s^{-1}) and red LEDs (RL, 600-700 nm, maxima of 660 nm, 165 ± 17 µmol photons m^{-2} s^{-1}); **(b, d)** RGB module illuminated with blue LEDs (BL, 400-500 nm, maxima of 450 nm, 44 ± 4 µmol photons m^{-2} s^{-1}), red LEDs (RL, 600-700 nm, maxima of 660 nm, 155 ± 17 µmol photons m^{-2} s^{-1}) and green LEDs (GL, 500-600 nm, maxima of 520 nm, 32 ± 3 µmol photons m^{-2} s^{-1}). The spectral characteristics of the light were measured using the spectroradiometer UPRtek PG100N (Taiwan, China).

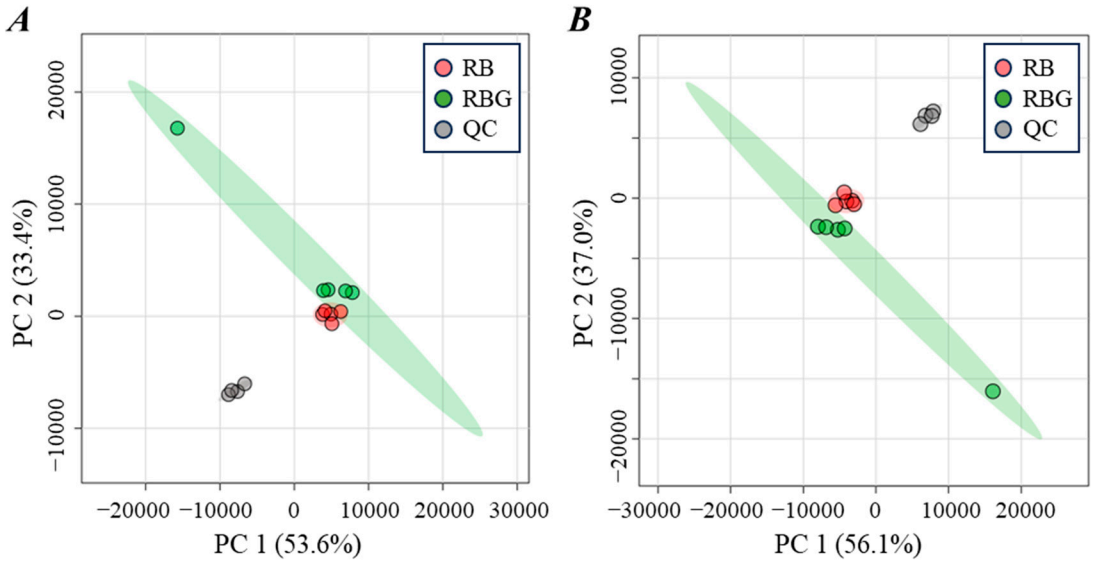

Figure S2. Sample scores for the first two principal components derived from PCA of the thermally stable (*A*) and thermally labile (*B*) polar metabolite profiles of *P. sativum* cotyledons developed under red-blue (RB) or red-green-blue (RGB) light and quality control (QC) samples. Images were generated using MetaboAnalyst 6.0 (http://www.metaboanalyst.ca).

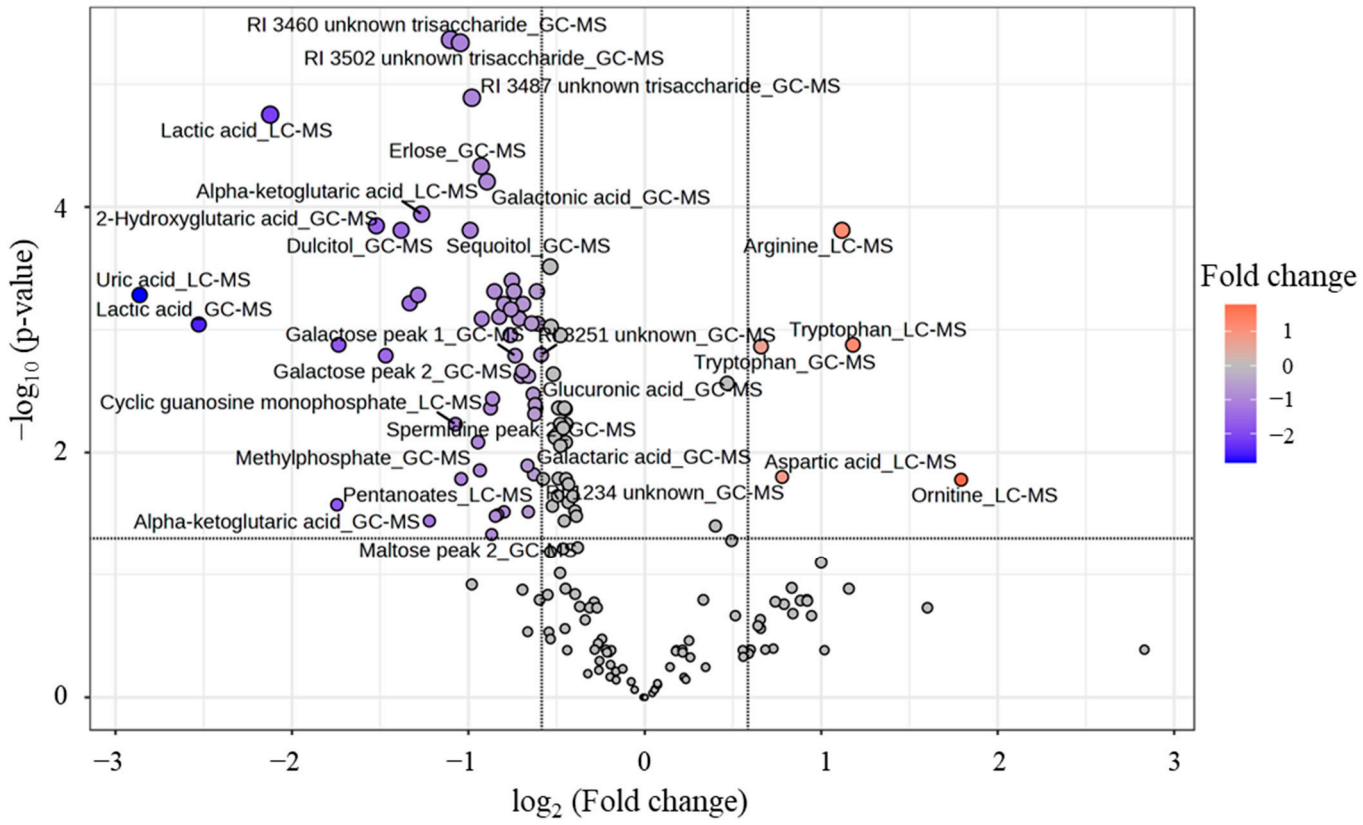

Figure S3. Volcano plot showing the metabolites of *P. sativum* cotyledons developed under red-blue (RB) or red-green-blue (RGB) light. The plot includes compounds with significantly ($p < 0.05$, FDR-adjusted) different abundances in the tested experimental conditions (RB light vs RGB light) with fold changes ≥ 1.5. Data analysis was performed using MetaboAnalyst 6.0 (https://www.metaboanalyst.ca).

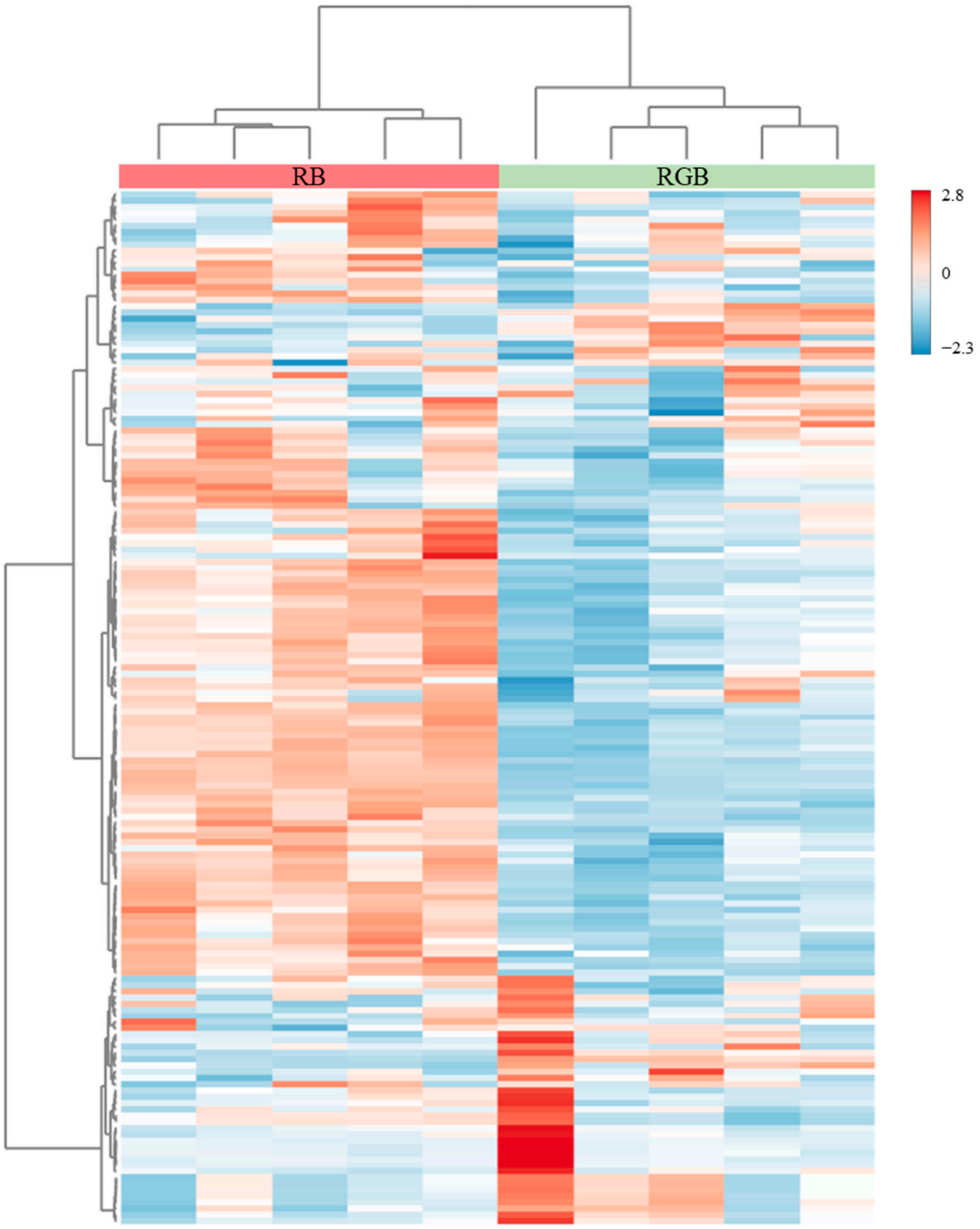

Figure S4. Heatmap showing the metabolite profiles of *P. sativum* cotyledons developed under red-blue (RB) or red-green-blue (RGB) light. The metabolite list includes all compounds detected by GC-MS or HPLC-MS approach, both identified and unknown (Tables S4–S5). Heatmap was generated using MetaboAnalyst 6.0 (https://www.metaboanalyst.ca).

Tables

Table S1. Gas chromatography (GC) and electron ionization-quadrupole-mass spectrometry (EI-Q-MS) settings used for the analysis of primary polar thermally stable metabolites extracted from *P. sativum* cotyledons.

Parameters	**GC settings**
Separation column	Phenomenex ZB-5MS (30 m × 0.25 mm ID, 0.25 μm film thickness)
Carrier gas / carrier gas flow rate	Helium / 1 mL/min
Injector operation mode	Splitless mode (90 s splitless time)
Injector temperature	250°C
Temperature program	1 min at 40°C ramp 15°C/min to 70°C 1 min at 70°C ramp 6°C/min to 320°C 12 min at 320°C
	MS settings
Ionization mode	Electron ionization (EI)
Electron energy	70 eV
Operation mode	scanning at 0.34 sec $scan^{-1}$
m/*z* range	50 - 700

The GC-MS analysis was accomplished using a Shimadzu GC2010 gas chromatograph with CTC GC PAL liquid injector (Shimadzu Scientific Instruments, Australia) and coupled online to a Shimadzu GCMS QP2010 quadrupole mass selective detector.

Table S2. Composition of the alkane standard mixture used to determine Kovats retention time indices (RI)

Alkane name	**Elemental composition**	**Ref. *m/z***	**RI**	**t_R (min)**
Undecane	$C_{11}H_{24}$	156	1100	9.537
Dodecane	$C_{12}H_{26}$	170	1200	11.904
Tridecane	$C_{13}H_{28}$	184	1300	14.433
Tetradecane	$C_{14}H_{30}$	198	1400	16.957
Pentadecane	$C_{15}H_{32}$	212	1500	19.009
Hexadecane	$C_{16}H_{34}$	226	1600	20.901
Heptadecane	$C_{17}H_{36}$	240	1700	22.675
Octadecane	$C_{18}H_{38}$	254	1800	24.404
Nonadecane	$C_{19}H_{40}$	268	1900	26.053
Eicosane	$C_{20}H_{42}$	282	2000	27.646
Heneicosane	$C_{21}H_{44}$	296	2100	29.169
Docosane	$C_{22}H_{46}$	310	2200	30.657
Tricosane	$C_{23}H_{48}$	324	2300	32.086
Tetracosane	$C_{24}H_{50}$	338	2400	33.462
Pentacosane	$C_{25}H_{52}$	352	2500	34.786
Hexacosane	$C_{26}H_{54}$	366	2600	36.059
Heptacosane	$C_{27}H_{56}$	380	2700	37.289
Octacosane	$C_{28}H_{58}$	394	2800	38.472
Nonacosane	$C_{29}H_{60}$	408	2900	39.624
Triacontane	$C_{30}H_{62}$	422	3000	40.729
Hentriacontane	$C_{31}H_{64}$	436	3100	41.806
Dotriacontane	$C_{32}H_{66}$	450	3200	42.848
Tritriacontane	$C_{33}H_{68}$	464	3300	43.859
Tetratriacontane	$C_{34}H_{70}$	478	3400	44.841
Pentatriacontane	$C_{35}H_{72}$	492	3500	45.792
Hexatriacontane	$C_{36}H_{74}$	506	3600	46.81
Heptatriacontane	$C_{37}H_{76}$	520	3700	47.96
Octatriacontane	$C_{38}H_{78}$	534	3800	49.285
Nonatriacontane	$C_{39}H_{80}$	548	3900	50.848
Tetracontane	$C_{40}H_{82}$	562	4000	52.723

Table S3. Ion pair-reversed phase ultra-high performance liquid chromatography (IP-RP-UHPLC) separation conditions and electrospray ionization-triple quadrupole-tandem mass spectrometry (ESI-QqQ-MS/MS) settings used for the analysis of anionic primary thermolabile metabolites from cotyledons of pea seeds using the Waters ACQUITY UPLC H-Class UPLC system (Waters GmbH, Eschborn, Germany) coupled online to an AB Sciex QTRAP 6500 hybrid triple quadrupole linear ion trap (QqLIT) mass spectrometer (AB Sciex, Darmstadt, Germany).

CHROMATOGRAPHY	
ACQUITY Sample Manager (SM)	
Injection mode	PartialLoop
Injection volume	5 µL
Weak wash solvent	0.3 mmol/L aq. ammonium formate
Weak wash volume	800 µL
Strong wash solvent	Acetonitrile
Strong wash volume	400 µL
Target sample temperature	4.0 C
Needle overfill flush	Automatic
Column conditions	
Separation column	EC 150/2 NUCLEOSHELL RP 18 (150 x 2 mm, particle size 2.7 µm)
Target column temperature	40.0 C
ACQUITY Binary Solvent Manager (BSM)	
Eluent A	0.3 mmol/L aq. ammonium formate
Eluent B	Acetonitrile
Seal wash duration	5 min
Flow rate	0.4 mL/min
Elution program	2% eluent B isocratic - 2 min gradient to 36% eluent B – 16 min gradient to 95% eluent B – 3 min 95% eluent B isocratic – 1.5 min gradient to 2% eluent B – 0.1 min 2% eluent B isocratic – 2.4 min (re-equilibration)
MASS SPECTROMETRY	
General	
Mass analyzer type	triple quadrupole-linear ion trap (QqLIT, QTRAP, operated in QqQ mode)
Ion source	TurboIonSpray®
Experiment type	multiple reaction monitoring (MRM)
Operatinon mode	negative
Cycle time (s)	1.1
Pause between ranges (ms)	5.007
Settling time (s)	0
Duration	24 min
Ion source settings	
Nebulizer gas (psig)	60
Drying gas (psig)	70
Curtain gas (psig)	40
Ion spray voltage (kV)	-4.5

Ion source temperature (°C)	450
MS/MS settings	
Fragmentation mode	CAD
MS/MS experiment type	MRM
Collision gas	nitrogen
Collision gas pressure	3 psig (medium)
Entrance potential (V)	-10.0
Scheduled MRM	enabled
Scheduled MRM type	basic
MRM detection window (s)	500
Target scan time (s)	1
Dwell time	adjusted by scheduled MRM algorithm
Q1 resolution	unit
Q3 resolution	unit

Table S4. Thermally stable metabolites detected by GC-MS analysis in aqueous methanolic extracts of *P. sativum* cotyledons developed under red-blue (RB) or red-green-blue (RGB) light.

No	Annotated metabolite features[a]	Derivatization groups[b]	t_R[c] exp	RI[d]	*m/z* quant.[e]	Library, match factor[f]
1	Lactic acid	2TMS	9.04	1079.1	117	NIST (962), ASL
2	Glycolic acid	2TMS	9.40	1094.0	177	NIST (939), ASL
3	Oxalic acid	2TMS	10.57	1143.5	190	NIST (890), ASL
4	RI 1166 unknown		11.09	1165.6	205	
5	Beta-Hydroxybutyric acid	2TMS	11.16	1168.4	117	NIST (788)
6	Leucine peak 1	1TMS	11.38	1178.0	86	NIST (703)
7	Methylphosphate	2TMS	11.54	1184.8	241	NIST (849)
8	3-Hydroxy-3-methylbutyric acid	2TMS	12.23	1212.9	131	NIST (754)
9	Valine	2TMS	12.34	1217.4	144	NIST (896), ASL
10	RI 1234 unknown		12.76	1233.7	159	
11	Urea	2TMS	13.12	1248.1	189	NIST (932)
12	Ethanolamine	3TMS	13.41	1259.5	174	NIST (902)
13	Leucine peak 2	2TMS	13.57	1266.1	158	NIST (712), ASL
14	Phosphoric acid	3TMS	13.58	1266.4	299	NIST (962), ASL
15	Glycerol	3TMS	13.63	1268.5	218	NIST (934), ASL
16	Isoleucine	2TMS	14.05	1285.0	158	NIST (870), ASL
17	Proline	2TMS	14.12	1287.8	142	NIST (794), ASL
18	Threonine peak 1	2TMS	14.14	1288.6	219	NIST (867), ASL
19	Glycine	3TMS	14.30	1294.8	174	NIST (941), ASL
20	Succinic acid	2TMS	14.57	1305.4	247	NIST (951), ASL
21	Ethylmalonic acid	2TMS	14.83	1315.7	261	NIST (853)
22	Glyceric acid	3TMS	14.91	1318.9	189	NIST (724), ASL
23	Uracil	2TMS	15.06	1325.0	241	NIST (921)
24	Fumaric acid	2TMS	15.38	1337.4	245	NIST (838), ASL
25	2,5-Hydroxypyrazine	2TMS	15.52	1343.0	241	NIST (829)
26	Serine	3TMS	15.56	1344.6	204	NIST (805), ASL
27	Nonanoic acid	1TMS	15.67	1349.1	215	NIST (700)
28	Threonine peak 2	3TMS	16.10	1365.9	218	NIST (906), ASL
29	2,4-Hydroxybutyric acid	3TMS	16.67	1388.8	103	NIST (817)
30	Beta-alanine	3TMS	16.97	1400.6	248	NIST (864), ASL
31	Aspartic acid peak 1	2TMS	16.98	1401.2	160	NIST (920), ASL
32	RI 1414 unknown		17.25	1414.1	243	
33	Homoserine	3TMS	17.44	1423.8	128	GMD (649), ASL
34	Malic acid	3TMS	18.28	1457.6	233	NIST (958), ASL
35	Erythritol	4TMS	18.53	1476.4	217	NIST (742), ASL
36	Pyroglutamic acid	2TMS	18.89	1494.2	156	NIST (947), ASL
37	Aspartic acid peak 2	3TMS	18.93	1496.0	232	GMD (835), ASL
38	Gamma-aminobutyric acid	3TMS	19.05	1502.5	174	NIST (873), ASL
39	RI 1506 sugar		19.11	1505.8	217	
40	Glutamic acid peak 1	2TMS	19.22	1511.0	174	NIST (856), ASL
41	RI 1511 phenol	3TMS	19.23	1511.4	239	NIST (750)
42	Threonic acid	4TMS	19.38	1519.6	292	NIST (730)
43	RI 1528 unknown		19.54	1528.0	219	
44	Erythronic acid	4TMS	19.72	1537.7	292	NIST (917), ASL

45	Phenylalanine peak 1	1TMS	19.75	1539	120	NIST (700)
46	2-Hydroxyglutaric acid	2TMS	19.89	1546.5	267	NIST (801)
47	Alpha-ketoglutaric acid	1MEOX 2TMS	20.11	1557.0	198	NIST (700), ASL
48	RI 1576 amine		20.44	1575.7	174	
49	Pyrogallol	3TMS	20.49	1578.2	342	NIST (830)
50	Glutamic acid peak 2	3TMS	20.89	1599.3	246	NIST (866), ASL
51	Phenylalanine peak 2	2TMS	20.97	1603.8	218	NIST (891), ASL
52	RI 1610 phenolic acid		21.07	1609.8	267	
53	Tartaric acid	4TMS	21.21	1617.2	292	NIST (842), ASL
54	Xylose	1MEOX 4TMS	21.54	1635.8	103	NIST (634), ASL
55	Arabinose	1MEOX 4TMS	21.67	1643.3	103	NIST (707), ASL
56	RI 1650 unknown		21.79	1650.2	140	
57	Ribose	1MEOX 4TMS	21.94	1658.9	103	NIST (700)
58	RI 1677 pentitol		22.27	1677.0	319	
59	Xylitol	5TMS	22.43	1686.4	217	NIST (700)
60	Arabitol	5TMS	22.69	1701.0	217	NIST (840), ASL
61	Ribitol	5TMS	22.78	1706.2	217	NIST (970), ASL
62	Glycerol-2-phosphate	4TMS	22.86	1710.5	299	NIST (700), ASL
63	Putrescine	4TMS	22.97	1717.1	174	NIST (731), ASL
64	RI 1734 unknown		23.27	1734.4	333	
65	RI 1745 sugar acid		23.45	1744.9	292	
66	Glycerol-3-phosphate	4TMS	23.47	1746.0	357	NIST (939), ASL
67	RI 1752 sugar		23.58	1752.2	217	
68	RI 1763 sugar acid		23.77	1763.4	292	
69	Phosphoethanolamine	4TMS	23.8	1765.2	299	NIST (792)
70	RI 1786 sugar acid		24.17	1786.4	333	
71	Shikimic acid	4TMS	24.37	1798.0	255	NIST (786)
72	Ornithine	4TMS	24.41	1800.3	142	GMD (700)
73	Citric acid	4TMS	24.49	1805.5	375	NIST (911), ASL
74	Lysine peak 1	3TMS	25.08	1841.1	174	NIST (738), ASL
75	Pinitol	5TMS	25.2	1848.3	260	NIST (800), ASL
76	Fructose peak 1	1MEOX 5TMS	25.36	1857.8	307	NIST (950), ASL
77	Adenine	2TMS	25.37	1858.2	264	NIST (700)
78	RI 1862 unknown		25.43	1862.5	275	
79	Fructose peak 2	1MEOX 5TMS	25.53	1868.4	307	NIST (945), ASL
80	Mannose	1MEOX 5TMS	25.61	1873.0	319	NIST (700)
81	Galactose peak 1	1MEOX 5TMS	25.67	1876.8	319	NIST (798), ASL
82	Glucose	1MEOX 5TMS	25.77	1883.3	319	NIST (727), ASL
83	Methyl-galactopyranoside	4TMS	25.83	1886.3	204	NIST (840)
84	Galactose peak 2	1MEOX 5TMS	26.03	1898.6	319	NIST (924), ASL
85	Lysine peak 2	4TMS	26.21	1909.7	174	NIST (914), ASL
86	Mannitol	6TMS	26.30	1915.5	319	NIST (926), ASL
87	Glucuronic acid	1MEOX 5TMS	26.39	1921.4	333	GMD (700), ASL
88	Sorbitol	6TMS	26.41	1922.4	319	NIST (936), ASL
89	Dulcitol	6TMS	26.49	1927.5	319	NIST (703), ASL
90	Sequoitol	5TMS	26.69	1940.3	318	NIST (724), ASL
91	RI 1950 sugar acid		26.85	1949.9	333	
92	RI 1953 sugar acid		26.90	1953.5	333	

93	RI 1963 unknown		27.06	1963.3	394	
94	Galactonic acid	6TMS	27.36	1982.3	292	NIST (887)
95	Gluconic acid	6TMS	27.43	1986.4	333	NIST (823), ASL
96	Glucaric acid	6TMS	27.59	1996.2	333	NIST (779), ASL
97	RI 2001 sugar acid		27.66	2000.7	333	
98	RI 2007 unknown		27.74	2006.3	155	
99	RI 2020 amine		27.95	2019.7	174	
100	Galactaric acid	6TMS	28.11	2030.6	333	NIST (700), ASL
101	Palmitic acid	TMS	28.24	2039.1	313	NIST (948), ASL
102	Myo-inositol	6TMS	28.86	2079.8	305	NIST (957), ASL
103	Ferulic acid	2TMS	29.02	2089.9	338	NIST (700)
104	RI 2100 unknown		29.17	2100.3	245	
105	Caffeic acid	3TMS	29.66	2132.8	396	NIST (715), ASL
106	RI 2178 hexose		30.33	2178.2	204	
107	RI 2183 hexose		30.41	2183.2	204	
108	Spermidine peak 1	4TMS	30.47	2187.3	174	NIST (851)
109	Diglycerol-phosphate	5TMS	30.54	2191.9	357	NIST (774)
110	Linoleic acid	1TMS	30.72	2204.4	337	NIST (731), ASL
111	Tryptophan	3TMS	30.73	2205	202	NIST (882), ASL
112	Oleic acid	1TMS	30.81	2210.7	339	NIST (706), ASL
113	RI 2220 carbohydrate		30.95	2220.5	363	
114	Stearic acid	1TMS	31.21	2238.5	341	NIST (871), ASL
115	Spermidine peak 2	5TMS	31.28	2243.6	144	NIST (815)
116	RI 2294 unknown		32.00	2294.1	204	
117	Fructose-6-phosphate	1MEOX 6TMS	32.09	2300.1	315	NIST (700)
118	Glucose-6-phosphate	1MEOX 6TMS	32.24	2311.2	387	NIST (750), ASL
119	RI 2370 unknown		33.05	2370.0	204	
120	Myo-inositol-1-phosphate	7TMS	33.5	2402.6	318	NIST (896)
121	RI 2428 carbohydrate		33.84	2428.5	204	
122	RI 2438 unknown		33.97	2438.2	340	
123	RI 2487 amine		34.61	2486.6	174	
124	Sucrose	8TMS	36.44	2630.7	437	NIST (888), ASL
125	RI 2687 carbohydrate		37.13	2686.8	204	
126	RI 2719 disaccharide		37.51	2718.9	361	
127	Maltose peak 1	1MEOX 8TMS	37.63	2728.8	361	NIST (921), ASL
128	Maltose peak 2	1MEOX 8TMS	37.95	2756.0	361	NIST (850), ASL
129	RI 2788 fatty acid derivative		38.33	2788.4	311	
130	RI 2816 disaccharide		38.65	2815.7	361	
131	Maltitol	9TMS	38.78	2826.7	361	GMD (700)
132	Melibiose	1MEOX 8TMS	39.13	2857.4	361	NIST (701)
133	RI 2873 carbohydrate		39.32	2873.5	204	
134	RI 2880 carbohydrate		39.39	2879.8	204	
135	RI 2906 disaccharide		39.68	2905.6	204	
136	RI 2908 disaccharide phosphate		39.72	2908.3	315	
137	RI 2938 carbohydrate		40.04	2937.9	204	
138	Galactinol	9TMS	40.46	2975.4	204	NIST (907), ASL
139	Gamma tocopherol	1TMS	40.64	2992.0	488	NIST (871)
140	RI 3121 carbohydrate		42.02	3120.9	597	

141	RI 3139 unknown		42.22	3139.5	259	
142	RI 3143 tryptophane derivative		42.26	3143.4	202	
143	RI 3251 unknown		43.36	3250.9	487	
144	Campesterol	1TMS	43.38	3253.1	382	NIST (841)
145	Sitosterol	1TMS	44.24	3338.6	357	NIST (920)
146	Raffinose	11TMS	44.62	3377.8	437	NIST (940), ASL
147	Erlose	11TMS	44.98	3414.9	361	ASL
148	RI 3460 trisaccharide		45.41	3459.8	361	
149	RI 3487 trisaccharide		45.67	3487.4	361	
150	RI 3502 trisaccharide		45.81	3501.6	361	
151	RI 3802 carbohydrate		49.31	3801.6	204	
152	RI 3810 carbohydrate		49.44	3809.9	204	
153	RI 3863 carbohydrate		50.27	3862.9	204	

a – Metabolite features annotation based on retention times (t_R), retention indices (RI), and EI spectra of co-eluted authentic standards from the in-house spectral library (ASL) as well as RI and EI spectral information from NIST 08 (National Institute of Standards and Technology) and GMD (Golm Metabolome Database). Unidentified metabolites are labeled as "unknown" with an associated retention index (RI). The names of metabolites annotated only to a specific chemical class (for which the exact structure could not be assigned) begin with the RI followed by the name of the annotated chemical class. Annotation to specific chemical classes was confirmed by the presence of characteristic signals in the EI spectra (e.g. saccharide phosphate - *m*/*z* 299, 315, 387; disaccharide - *m*/*z* 361, 204, 319; saccharide derivative acid – *m*/*z* 292, 333, 103). The metabolites are listed in order of increasing retention time (t_R).
b – Numbers of the trimethylsilyl (TMS) and methyloxime (MEOX) groups in the structures of the annotated derivatives.
c – Retention time, min.
d – RI, Kovach Retention Index calculated from the retention times of the alkanes.
e – *m*/*z* value refers to the most characteristic fragment signal selected for quantification by peak areas in characteristic extracted ion chromatograms.
f – EI-MS libraries where metabolite EI mass spectra and RI were used for metabolite annotation: ASL – in-house RI and spectral library of authentic standards, NIST 08 - National Institute of Standards and Technology, GMD – Golm Metabolome Database (http://gmd.mpimp-golm.mpg.de/). The number represents the NIST search match factor of the corresponding library.

Table S5. Thermally labile polar metabolites detected by targeted UHPLC-MS analysis in the acid ethanol-water extracts of *P. sativum* cotyledons developed under red-blue (RB) or red-green-blue (RGB) light.

No	Metabolite name[a]	t_R (min)	Q1 (*m*/*z*)[b]	Q3 (*m*/*z*)[c]
1	Asparagine	0.56	131	87
2	Allantoin	0.57	157	97.2
3	Ornitine	0.71	131.1	82.9
4	Arginine	0.72	173.1	131
5	Proline	0.8	114	86
6	Serine	0.83	104	74
7	Glutamine	0.84	145.1	108.9
8	Glucose	0.84	179	89
9	Glycine	0.85	74	74
10	Sucrose	0.85	341	89
11	Threonine	0.86	118.1	73.9
12	S-Adenosyl-L-homocysteine	0.87	383.1	133.9
13	Cytidine	0.9	242.1	108.9
14	Lysine	0.9	145.1	99
15	Methionine	0.92	148	47
16	Uridine	0.92	243.1	109.9
17	Tyrosine	0.95	180.1	118.9
18	Leucine/Isoleucine	1.01	261	130
19	Guanosine	1.37	282.1	149.9
20	2-Deoxyguanosine	1.48	266.1	150
21	Phenylalanine	1.65	164.1	103
22	Adenosine	2.33	266.1	133.9
23	Aspartic acid	2.42	132	88
24	Glutamic acid	2.42	146	102
25	5-Deoxyadenosine	2.42	250	134
26	Glucosamine-1-phosphate	2.44	258	78.9
27	D-Galactonic/Gluconic acid	2.44	195.1	129
28	Shikimic acid	2.44	173	92.9
29	Ribonic acid	2.51	165	75
30	Glycolic acid	2.53	75	47
31	3-Dehydroshikimic acid	2.55	171	127
32	Dihydroorotic acid	2.55	157	112.7
33	Uric acid	2.56	167	124
34	Tryptophan	2.58	203.1	116.2
35	Chloride	2.8	35	35
36	Lactic acid	3.1	89	42.9
37	Phosphoric acid	3.65	96.9	78.9
38	Glutathione	3.85	306.1	143
39	Nicotinamide adenine dinucleotide	4.38	662.1	540.1
40	Pyruvic acid	4.61	87	43
41	Sedoheptulose-7-phosphate	5.52	289	97
42	Cyclic guanosine monophosphate	5.54	344	150
43	Fructose-6-phosphate/Glucoso-6-phosphate	5.56	259	96.9
44	Glyceraldehyde-3-phosphate	5.62	169	97
45	Argininosuccinic acid	5.63	289	97
46	Glycerol-3-phosphate	5.7	171	78.8

47	Glucose-1-phosphate	5.88	259	240.8
48	2-C-methylerythritol-4-phosphate	5.96	215	78.9
49	Cytidine monophosphate	6.26	322	79
50	Nicotinic acid	6.42	122	77.9
51	Pantothenic acid	6.45	307	79
52	2-Deoxyribose-5-phosphate	6.46	229	96.8
53	Adenosine-2,3-cyclic monophosphate/Adenosine-3,5-cyclic monophosphate	6.73	328	134
54	Uridine monophosphate	7.10	323	79
55	Dihydroxyacetone phosphate	7.46	169	97
56	Deoxythymidine-5-monophosphate	8.03	321	79
57	2-Deoxyguanosine-5-monophosphate	8.28	346.1	78.8
58	Inosinic acid	8.28	347	134.8
59	Adenosine monophosphate	8.29	346.1	78.8
60	Guanosine-5-monophosphate	8.38	362.1	78.9
61	Glutathione disulfide	8.52	611.1	306.1
62	1-Deoxy-D-xylulose-5-phosphate	8.63	213	97
63	2-Deoxyadenosine-5-monophosphate	8.72	330.1	195
64	3-Hydroxypyruvic acid	9.33	103	59
65	Ureidosuccinic acid	9.4	175	131.8
66	Succinic acid	9.43	117	73
67	Uridine-5-diphosphate-glucose	9.43	565	323
68	Uridine-diphosphate-N-acetylglucosamine	9.54	606	385
69	Fumaric acid	9.65	115	71
70	Malic acid	9.65	133	115
71	Sulphate	9.72	97	97
72	Adenosine diphosphate glucose	10.01	588.1	345.9
73	Adenosine diphosphoribose	10.2	558.1	346
74	Alpha-ketoglutaric acid	10.29	145	101
75	Pentanoates	10.3	101.1	101.1
76	2-C-methyl-D-erythritol 2,4-cyclic diphosphate	10.45	277	79
77	1,4-Dihydronicotinamide adenine dinucleotide	10.72	664.1	78.9
78	(R)-5-phosphomevalonic acid	11.44	227	97
79	Uridine-5-diphosphate	12.9	483	158.8
80	Nicotinamide adenine dinucleotide phosphate	13	743.1	620
81	Aconitic acid	13.02	173	128.7
82	Phosphoenolpyruvic acid	13.4	167	78.8
83	Citric acid	13.75	191	87
84	Isocitric acid	14.1	191	73
85	4-Diphosphocytidyl-2-C-methyl-D-erythritol 2-phosphate	14.7	600	79
86	Fructose-1,6-diphosphate	15.3	339	96.9
87	Adenylosuccinic acid	15.87	462.1	133.9
88	ADP-ribose-2-phosphate	16.25	638	426

Targeted acquisition of UHPLC-MS data was performed in multiple reaction monitoring (MRM) mode.
a – Metabolites are listed in order of increasing retention time (t_R); **b, c** – Analyte-specific combinations of Q1 and Q3 *m*/*z* ranges (transitions); **b** – Q1 is the *m*/*z* of the molecular ion; **c** – Q3 is the *m*/*z* of the characteristic fragment ion.