

**Table S1.** Chemical properties of soils before transplanting tomato plants. Mean values of three replicates.

Nutrient condition	pH (1:5)	EC (dS/m)	NO <sub>3</sub> - N (mg/kg)	SOM (g/kg)	Av. P <sub>2</sub> O <sub>5</sub> (mg/kg)	Ex. Cations (cmol <sub>e</sub> /kg)			
						K	Ca	Mg	Na
Low EC soil	6.3	0.8	75	15	172	0.09	2.9	0.6	0.2
High EC soil	5.9	8.6	871	32	791	1.69	13.3	5.0	1.8

**Table S2.** Fertilizer applications for three different nutrient conditions

Fertilizer application	Time	Fertilization for low EC soil (g/kg soil)				Fertilization for high EC soil (g/kg soil)
		Low N		Standard N		High N
		N	K	N	K	K
1 <sup>st</sup> supply	1.5 months after transplant	0	0.14	0.05	0.14	0.05
2 <sup>nd</sup> supply	2 months after transplant	0	0.14	0.05	0.14	0.05
3 <sup>rd</sup> supply	3.5 months after transplant	0	0.14	0.05	0.14	0.05

**Table S3. Differential primary metabolites identified by GC-TOF-MS in tomato fruits cultivated under varied lighting, nutrient, and water conditions**

No.	Ret (min) <sup>a</sup>	Metabolites <sup>b</sup>	Unique Mass (m/z)	MS Fragment pattern (m/z)	ID <sup>c</sup>
<i>Amino acids</i>					
1	7.26	Isoleucine *	158	73, 57, 117, 130, 147, 158, 132, 219, 116	STD/MS
2	7.39	Glycine	174	73, 174, 86, 147, 107, 100, 133, 175, 118	STD/MS
3	7.90	Serine	204	73, 100, 204, 188, 147, 59, 218, 133	STD/MS
4	8.14	Threonine	219	73, 57, 117, 101, 147, 219, 218, 100	STD/MS
5	8.48	β-Alanine *	248	73, 160, 130, 116, 174, 131, 161, 248	STD/MS
6	9.28	Aspartic acid	232	73, 232, 100, 84, 147, 117, 218, 233, 133	STD/MS
7	9.35	Pyroglutamic acid	156	73, 156, 174, 147, 157, 158, 230, 258	STD/MS
8	9.36	GABA	174	73, 174, 84, 147, 86, 175, 157, 100	STD/MS
9	10.16	Phenylalanine	192	73, 218, 100, 192, 147, 84, 59, 219, 130	STD/MS
10	14.14	Tryptophan	202	73, 75, 117, 217, 202, 129, 130	STD/MS
<i>Organic acids</i>					
11	7.43	Succinic acid *	247	73, 147, 107, 77, 55, 69, 84, 247, 256	STD/MS
12	9.02	Malic acid	233	73, 147, 133, 55, 101, 233, 148, 117	STD/MS
13	11.61	Citric acid	273	73, 147, 273, 211, 149, 133, 129	STD/MS
<i>Sugars and sugar derivatives</i>					
14	7.07	Glycerol	205	73, 147, 117, 103, 133, 205, 148, 218	STD/MS
15	7.62	Glyceric acid *	189	73, 147, 189, 133, 103, 117, 130, 148	STD/MS
16	10.42	Xylose	103	73, 103, 217, 147, 133, 117, 307, 189	STD/MS
17	10.94	Ribose *	205	73, 117, 147, 89, 59, 133, 103, 205, 217	STD/MS
18	12.10	Fructose	103	73, 103, 217, 147, 307, 133, 218, 117	STD/MS
19	12.28	Galactose	160	73, 147, 160, 205, 103, 217, 319, 117	STD/MS
20	12.37	Glucose	103	73, 147, 103, 160, 205, 217, 319, 129	STD/MS
21	12.53	Glucuronic acid *	333	73, 147, 103, 160, 217, 333, 133, 129	STD/MS
22	13.44	myo-Inositol *	217	73, 147, 217, 191, 103, 129, 133, 305	STD/MS
23	14.82	Glucose 6-phosphate *	299	73, 147, 103, 299, 129, 387, 160, 217	STD/MS
24	15.35	myo-Inositol phosphate *	299	73, 147, 217, 299, 318, 103, 315, 133	MS
25	16.51	Sucrose	361	73, 147, 103, 217, 129, 169, 361, 271	STD/MS
26	17.03	Maltose	361	73, 147, 103, 361, 217, 191, 129, 204	STD/MS
<i>Fatty acids and lipids</i>					
27	12.97	Palmitic acid *	117	73, 147, 75, 117, 129, 133, 132, 313	STD/MS
28	14.14	Stearic acid **	117	73, 75, 117, 103, 129, 217, 132, 341	STD/MS
29	16.04	Monopalmitin	371	73, 147, 75, 57, 129, 103, 117, 133, 371	STD/MS
30	16.98	Fatty acid derivatives **	129	73, 147, 57, 129, 117, 101, 133, 203, 399	MS
<i>Nucleosides and nucleotides</i>					
31	7.11	Adenosine 5'-diphosphate *	299	73, 299, 133, 193, 211, 300, 207, 191	STD/MS
32	15.49	Uridine	169	73, 217, 130, 174, 147, 169, 129, 259	STD/MS
33	16.40	Adenosine	230	73, 230, 236, 103, 147, 217, 245, 192	STD/MS
34	17.09	Guanosine	324	73, 217, 147, 324, 129, 245, 230, 169	STD/MS

<i>Others</i>					
35	5.41	Hydroxylamine **	146	73, 133, 146, 119, 59, 86, 147, 130, 100	STD/MS
36	11.92	Quinic acid	345	73, 147, 345, 255, 103, 133, 191, 148	STD/MS
<i>Unknowns</i>					
37	6.46	N.I. 1 **	228	73, 69, 58, 110, 77, 228, 134, 184, 127	— <sup>d</sup>
38	6.92	N.I. 2 *	116	73, 116, 132, 75, 57, 74, 103, 117, 147	—
39	8.45	N.I. 3	160	73, 75, 160, 130, 117, 147, 100, 161, 131	—
40	9.24	N.I. 4 **	83	84, 73, 158, 85, 157, 186, 140, 116, 61	—
41	9.55	N.I. 5 **	120	120, 73, 75, 84, 146, 130, 103, 174	—
42	11.84	N.I. 6 *	173	73, 55, 173, 157, 147, 129, 174, 316	—
43	15.67	N.I. 7 **	103	73, 103, 147, 217, 68, 117, 129, 446	—
44	15.81	N.I. 8	446	73, 103, 147, 156, 68, 217, 117, 446	—

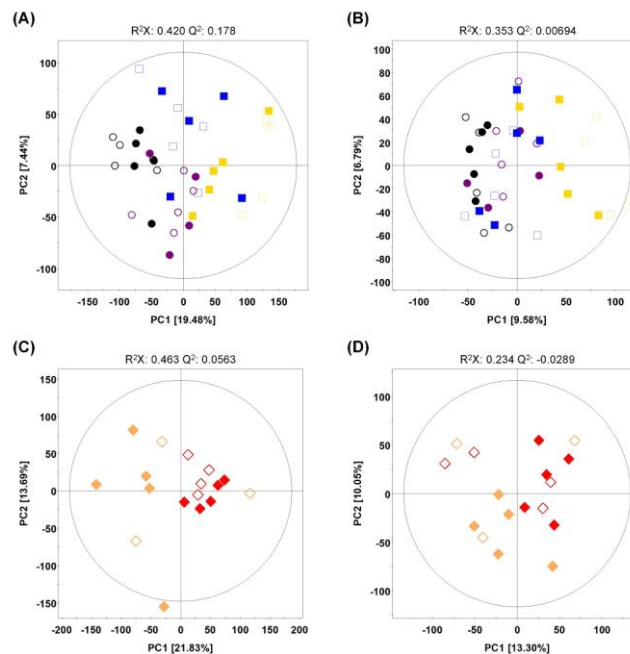
<sup>a</sup> Retention time.; <sup>b</sup> Primary metabolites selected by VIP value (> 1.0) based on PLS-DA model.; <sup>c</sup> Identification. STD/MS, comparing with standard compounds analyzed under same condition and mass spectrum comparison with HMDB, NIST, and wiley 9 database.; <sup>d</sup> not detected.; \* Only selected metabolites in standard and low N soil condition; \*\* Only selected metabolites in high N soil condition.

Table S4. Differential secondary metabolites identified by UHPLC-LTQ-Orbitrap-MS in tomato fruits cultivated under varied lighting, nutrient, and water conditions

No.	Ret (min)	Tentative Identification <sup>a</sup>	Identified ion ( <i>m/z</i> )		MS <sup>n</sup> fragment pattern ( <i>m/z</i> ) <sup>b</sup>	Elemental composition	Delta ppm	Reference
			[M+H] <sup>+</sup>	[M-H] <sup>-</sup>				
<i>Phenylpropanoids</i>								
1	2.09	Caffeic acid glucose *	—	341.0904	341> 281, 179> 135	C15H17O9 (–)	7.490	REF [24]
2	3.66	Chlologenic acid	355.1014	353.0921	353> 191, 179, 173, 135	C16H17O9 (–)	-2.756	REF [22]
3	3.78	Quercetin rutinoside hexoside	773.2116	771.2064	771> 609, 463> 301> 271, 255, 179	C33H39O21 (–)	-2.683	REF [22]
4	3.84	Guaiacol hexose pentose *	441.1354 <sup>c</sup>	463.1510 <sup>d</sup>	463> 417, 293> 275, 233, 191, 149	C18H26O11Na (+)	-3.066	REF [25]
5	4.43	Quercetin rutinoside pentoside **	743.2014	741.1984	741> 609, 300> 271, 255	C32H39O20 (+)	-2.664	REF [22]
6	4.60	Rutin	611.1593	609.1555	609>301> 271, 255, 179, 151	C27H31O16 (+)	-2.227	REF [22]
7	4.84	Kaempferol rutinoside *	595.1645	593.1558	593> 525, 285> 257, 229, 163	C27H31O15 (+)	-2.111	REF [22]
8	5.36	Tricaffeoylquinic acid *	679.2957	677.3019	677> 353> 335, 191, 173	C34H29O15 (–)	-2.811	REF [22]
9	5.61	Flavonoids derivatives	255.0641	253.0568	253> 224, 209, 197> 165, 153, 139	C15H11O4 (+)	-4.726	LIB <sup>e</sup>
10	6.15	Naringenin *	273.0752	271.0635	271> 225, 177, 151> 107	C15H13O5 (+)	-1.831	REF [S2]
<i>Polyamines</i>								
11	4.01	Feruloylagmatine **	307.1754	305.1656	(+) 307> 247, 230, 177, 145	C15H23N4O3 (+)	-3.311	REF [23]
12	5.51	Coumaroyl tyramine **	284.1272	282.1155	282> 240, 177, 162, 145, 119	C17H18NO3 (+)	-3.238	REF [23]
13	6.63	Grossamide	625.2519	623.2587	623> 460> 297> 282, 175	C36H37N2O8 (+)	-4.082	WebDB <sup>f</sup>
<i>Alkaloids</i>								
14	4.31	Esculeoside B	1228.5942	1272.6053 <sup>e</sup>	1272> 1226> 1094, 932, 770, 608	C56H94NO28 (+)	-1.178	REF [24]
15	4.77	Esculeoside A	1270.6033	1268.6061	1268> 1136, 974, 932> 752, 590	C58H96NO29 (+)	-2.347	REF [22]
16	4.83	Lycoperoside H or Hydroxytomatine	1050.5461	1094.5671 <sup>e</sup>	— <sup>h</sup>	C50H84NO22 (+)	-1.722	REF [24]
17	5.36	Dehydrotomatine **	1032.5355	1076.5585 <sup>e</sup>	—	C50H82NO21 (+)	-1.806	REF [26]
18	5.44	Tomatine *	1034.5493	1078.5707 <sup>e</sup>	—	C50H84NO21 (+)	-3.591	REF [26]
<i>Oxylipins and lipids</i>								

19	6.19	9,12,13-TriHODE *	351.2137 <sup>c</sup>	327.2215	327> 309, 291, 229, 211, 171> 153	C18H32O5Na (+)	-1.467	REF [22]
20	7.85	LysoPC(18:3) *	518.3220	562.3192 <sup>d</sup>	562> 502, 431> 277	C26H49NO7P (+)	-4.043	REF [22]
21	8.14	LysoPE(18:2)	478.2909	476.2819	476> 402, 384> 357	C23H45NO7P (+)	-3.441	REF [22]
22	8.14	LysoPE(20:5)	500.2732	544.2698 <sup>d</sup>	544> 498, 476> 279	C25H43NO7P (+)	-8.007	HMDB <sup>g</sup>
23	8.23	LysoPC(18:2) *	520.3379	564.3346 <sup>d</sup>	564> 504, 391> 279, 242	C26H51NO7P (+)	-3.605	REF [22]
24	8.56	LysoPE(16:0) *	454.2913	452.2807	452> 391, 255> 237	C21H45NO7P (+)	-3.292	REF [22]
25	8.64	LysoPC(16:0) *	496.3377	540.3355 <sup>d</sup>	540> 480, 391> 255, 224	C24H51NO7P (+)	-4.142	REF [22]
26	8.64	Oxylin <sup>**</sup>	311.2205	309.1771	309> 291, 273, 185, 171, 155	C18H31O4 (+)	-3.843	REF [27]
27	8.72	LysoPC(18:1) *	522.3533	566.3500 <sup>d</sup>	566> 506, 415> 281, 242	C26H53NO7P (+)	-3.993	REF [23]
28	8.86	LysoPA(18:2) *	435.2491	433.2386	433> 415, 365, 153> 97, 79	C21H40O7P (+)	-3.461	REF [23]
29	9.50	LysoPC(18:0) *	524.3684	568.3646 <sup>d</sup>	568> 508, 421, 391> 283, 224	C26H55NO7P (+)	-5.065	REF [23]
<b><i>Others</i></b>								
30	3.80	Benzyl alcohol hexose pentose *	425.1406 <sup>c</sup>	447.1559 <sup>d</sup>	447> 401> 269, 233, 161	C18H26O10Na (+)	-2.795	REF [25]
<b><i>Unknowns</i></b>								
31	1.01	N.I. 1	328.1378	326.1264	326> 308, 278, 236, 206, 164	–	–	–
32	3.99	N.I. 2	469.1666 <sup>c</sup>	491.1823 <sup>d</sup>	491> 445> 323, 221, 179	–	–	–
33	4.03	N.I. 3	409.1822 <sup>c</sup>	431.1957 <sup>d</sup>	431> 385> 223, 205, 161, 153	–	–	–
34	4.27	N.I. 4	439.1559 <sup>c</sup>	461.1758 <sup>d</sup>	461> 415, 311> 251, 191, 149	–	–	–
35	6.99	N.I. 5 <sup>**</sup>	449.1473	447.1385	–	–	–	–

<sup>a</sup> Secondary metabolites selected by VIP value (> 1.0) based on PLS-DA model.; <sup>b</sup> MS<sup>n</sup> fragment patterns detected in negative ion mode.; <sup>c</sup> [M+Na]<sup>+</sup>; <sup>d</sup> [M+HCOOH-H]<sup>-</sup>; <sup>e</sup> In house library; <sup>f</sup> Web database (KNAPSAcK core system; [http://www.knapsackfamily.com/knapsack\\_core/top.php](http://www.knapsackfamily.com/knapsack_core/top.php)); <sup>g</sup> The Human Metabolome Database (HMDB; <https://hmdb.ca/>); <sup>h</sup> Not detected.; \* Only selected metabolites in standard and low N soil condition; \*\* Only selected metabolites in high N soil condition.



**Figure S1.** PCA score plots from GC-TOF-MS **(A)** and UHPLC-LTQ-Orbitrap-MS **(B)** analysis of tomato cultivated under different nutrient, water, and light condition. Symbol, SN-SW-OFF (■); SN-LW-OFF (□); LN-SW-OFF (●); LN-LW-OFF (○); SN-SW-ON (■); SN-LW-ON (□); LN-SW-ON (●); LN-LW-ON (○). SN, standard soil; SW, sufficient water; OFF, red light off; LN, Low-N; LW, limited water; ON, red light on. PCA score plots from GC-TOF-MS **(C)** and UHPLC-LTQ-Orbitrap-MS **(D)** analysis of tomato cultivated under water, and light condition for high N soil. Symbol, HN-SW-OFF (◆); HN-LW-OFF (◇); HN-SW-ON (◆); HN-LW-ON (◇). HN, high N soil; SW, sufficient water; OFF, red light off; LW, limited water; ON, red light on.