

Table S1: Compounds identified from control and β CC treated tomato plants by LC-MS/MS. A total of 57 compounds were identified based on the fragment ion spectra in both positive and negative ionization modes. 1-32 compounds are present in positive mode, and 33-57 in negative mode. RT, retention time; #, metabolites identified by matching the molecular and daughter ions from the predicted spectra from HMDB.

Sr. No.	Molecular formula	Abundance (%)	Adducts	Mass	m/z	RT	Score	Compound Name
1	C ₁₁ H ₁₀ O ₅	149(100), 160(56.02), 159(0.46)	(M+H)+	222.0528	223	10.696	79.18	2-Succinylbenzoate
2	C ₁₆ H ₁₈ O ₉	192.05(100), 191.05(41.23), 173.04(5.06)	(M+H)+	354.0951	355.08	10.603	84.08	Chlorogenic acid
3	C ₉ H ₈ O ₂	119.04(78.23), 117.03(54.87), 103.05(23.78)	(M+H)+	148.0524	149.04	14.911	89.04	Cinnamic acid
4	C ₆ H ₈ O ₇	191(100), 175(36.14), 170(18.03)	(M+H)+	192.027	193.0343	6.582	96.46	Citric acid
5	C ₆ H ₆ O ₆	142.99(82.09), 112(26.78), 99.007(1.62)	(M+H)+	174.0164	175.0084	6.54	93.14	Dehydroascorbic acid
6	C ₅₀ H ₈₁ NO ₂₁	1032.541(100), 1030.522(72.19), 898.485(25.63)	(M+H)+	1031.53	1076.532	11.903	86018	Dehydrotomatine
7	C ₈ H ₁₁ NO ₂	154.086(100), 154(89.06), 153(38.74)	(M+H)+	153.079	154.0863	4.917	76.02	Dopamine
8	C ₆ H ₁₂ O ₆	163.06(92.64), 145.04(63.74), 127.039(9.34)	(M+Na)+	180.0634	198.0972	4.509	95.59	Galactose
9	C ₄ H ₉ NO ₂	102.07(100), 87.04(6.47), 86.06(2.58)	(M+H)+	103.0633	104.07	4.427	87.57	γ amino butyric acid
10	C ₆ H ₁₂ O ₆	118.9(36.4), 113(13.98), 89(0.64)	(M+H)+	180.0634	179	4.549	91.68	Glucose
11	C ₆ H ₁₃ O ₉ P	199(78.02), 138.979(37.51), 96.96 (2.78)	(M+H)+	260.0297	261.022	4.308	88.57	Glucose-6-phosphate
12	C ₅ H ₉ NO ₄	130.05(82.63), 102.07(46.32), 85.047(2.78)	(M+H)+	147.0532	148.06	4.438	86.84	Glutamate
13	C ₅ H ₁₀ N ₂ O ₃	169.05(100), 130.04(25.33), 101.07(17.69)	(M+H)+	146.0691	147.06	4.346	85.26	Glutamine
14	C ₄ H ₉ NO ₃	119.99(100), 102.04(65.42), 74.125(3.74)	(M+H)+	119.0582	120.065	7.392	80.85	Homoserine
15	C ₁₈ H ₃₂ O ₂	281(100), 280(80.14), 265(23.87)	(M+H)+	280.2402	281.247	19.73	75.37	Linoleic acid
16	C ₆ H ₁₄ N ₂ O ₂	145.1(100), 130.08(3.61), 119.08(076)	(M+H)+	146.1055	147.11	4.023	78	Lysine
17	C ₅₂ H ₈₅ NO ₂₃	1092(100), 1013(56.13), 383(17.85)	(M+H)+	1091.551	1092	4.143	18.06	Lycoperside A

Sr. No.	Molecular formula	Abundance (%)	Adducts	Mass	m/z	RT	Score	Compound Name
18	C ₄ H ₆ O ₅	135(100), 117(20.02), 89(16.73)	(M+H)+	134.0215	135.0142	5.687	96.78	Malic acid [#]
19	C ₆ H ₁₂ O ₆	180.19(100), 162(81.02), 85.098(24.87)	(M+H)+	180.0634	181.05	4.55	95.33	Mannose
20	C ₅ H ₉ NO ₄	148.06(100), 106.04(43.12), 88.039(2.54)	(M+H)+	147.0532	148.06	4.43	80.7	O-acetylserine
21	C ₉ H ₁₁ NO ₂	165.05(100), 130.96(37.52), 119.96(2.74)	(M+H)+	165.079	166.08	10.037	92.53	Phenylalanine
22	C ₃ H ₄ O ₃	41(100), 43(33.33), 42(8.41)	(M+HCOO) (M+CH ₃ COO)	88.06	89.0088	5.035	96.73	Pyruvic acid
23	C ₇ H ₁₂ O ₆	191.3(100), 126.08(23.45), 156.9(10.87)	(M+H)+	192.0634	193.0707	4.67	98.6	Quinic acid [#]
24	C ₂₇ H ₃₀ O ₁₆	611(100), 610(77.33), 303.04(14.52)	(M+H)+	610.1534	611.16	11.661	81.92	Rutin
25	C ₄₅ H ₇₃ NO ₁₆	884.5(100), 413.33(50.14), 412.33(49.86)	(M+H)+ (M+Na)+	883.4929	884	11.47	85.25	Solasonin
26	C ₃ H ₇ NO ₃	105.037(100), 88.016(41.23), 60.0154(21.87)	(M+H)+	105.0426	106.049	4.308	78.14	Serine
27	C ₄ H ₆ O ₄	116.955(92.14),99.016(26.74), 73.114(10.05)	(M+H)+ (M+CH ₃ COO)	118.0266	119.019	5.484	92.91	Succinic acid [#]
28	C ₁₂ H ₂₂ O ₁₁	324.92(100), 162.96(47.31), 144.94(8.66)	(M+H)+ (M+HCOO)	342.1162	365.1054	4.509	91	Sucrose
29	C ₄ H ₉ NO ₃	118(100), 102.05(32.47), 84.04(1.62)	(M+H)+	119.0582	120.06	4.346	96.23	Threonine
30	C ₅₀ H ₈₃ NO ₂₁	1034.55(100), 1017.54(80.11) 1016.54(73.55)	(M+H)+	1033.546	1034.553	12.108	75.96	Tomatine
31	C ₁₅ H ₂₄ N ₂ O ₁₇ P ₂	566.777(100),565.053(23.84), 542.85(1.64)	(M+H)+	566.055	567.047	4.1	79.51	UDP- Glucose
32	C ₅ H ₁₁ NO ₂	117.99(100), 72.146(20.81), 73.08(2.64)	(M+H)+	117.079	118.0862	6.135	79.91	Valine
33	C ₆ H ₄ N ₂ O ₅	153(100), 123(2.6), 137.01(0.52)	(M-H)-	184.012	183	18.523	76.02	2,4-Dinitrophenol
34	C ₃ H ₇ O ₇ P	166(100), 96.92(25.12), 86.98(2.5)	(M-H)-	185.9929	184.99	4.368	92.98	3-Phosphoglyceric acid
35	C ₆ H ₁₄ N ₄ O ₂	158(100), 157(8.62), 116(5.37)	(M-H)-	174.1117	173.11	4.104	98.74	Arginine
36	C ₆ H ₈ O ₆	147(100), 113.023(27.63), 87.007(5.21)	(M-H)-	176.0321	175.0241	4.351	92.7	Ascorbic acid
37	C ₄ H ₇ NO ₄	132.04(100), 116.03(34.78), 88.03(9.37)	(M-H)-	133.0375	132.044	4.346	81.26	Aspartate

Sr. No.	Molecular formula	Abundance (%)	Adducts	Mass	m/z	RT	Score	Compound Name
38	C ₇ H ₆ O ₂	123.44(100), 105.045(26.87), 95.049(16.32)	(M-H)-	122.0368	121.0442	13.444	85.43	Benzoic acid
39	C ₉ H ₈ O ₄	163.03(100), 145.02(34.12), 135.04(29.64)	(M-HCOO)-	180.0423	179.04	10.608	85.38	Caffeic acid
40	C ₅ H ₈ O ₅	147.028(100), 129.018(24.85), 87(11.84)	(M-H)- (M+CH ₃ COO)-	148.0372	147.028	7.72	92.8	Citramalic acid
41	C ₉ H ₈ O ₃	163(100), 146(52.63), 123(21.79)	(M-H)-	164.0473	163.0546	13.36	84.85	Coumaric acid
42	C ₁₀ H ₁₀ O ₄	178.026(100), 175.04(84.25), 149.059(52.17)	(M-H)- (M+HCOO)-	194.0579	193.05	14.911	87.68	Ferulic acid
43	C ₄ H ₄ O ₄	115(100), 114.9(8.15), 113.173(0.67)	(M-H)- (M+HCOO)-	116.011	115.0024	5.036	85.63	Fumaric acid
44	C ₆ H ₁₀ O ₇	175.1(100), 131.1(24.81), 113.1(10.67)	(M-H)- (M+CH ₃ COO)-	194.0427	193.035	4.467	92.23	Glucuronic acid
45	C ₅ H ₈ O ₄	130.936(100), 112.97(54.97), 87.075(22.56)	(M+HCOO) (M+CH ₃ COO)-	132.0423	131.03	4.673	99.02	Glutaric acid
46	C ₆ H ₉ N ₃ O ₂	154.903(100), 136.9(63.79), 135.9(14.23)	(M-H)-	155.0695	154.0622	4.346	85.13	Histidine
47	C ₅ H ₉ NO ₃	130.073(100), 132.066(96.42), 114.055(20.14)	(M-H)-	131.0582	130.0655	7.353	80.85	Hydroxyproline
48	C ₁₀ H ₁₀ O ₄	193.16(100), 178.153(54.36), 134.183(8.74)	(M-H)-	194.0579	193.0506	14.993	84.28	Isoferulic acid
49	C ₆ H ₁₃ NO ₂	130.1(100), 129.3(23.64), 86.09(2.69)	(M-Na)-	131.0946	130.1	4.998	75.23	Isoleucine
50	C ₅ H ₆ O ₄	129(100), 113(23.14), 99(0.36)	(M-HCOO) (M-CH ₃ COO)-	130.0266	129.0339	4.958	89.8	Itaconic acid
51	C ₆ H ₁₃ NO ₂	130.506(100), 86.087(24.87), 80.049(1.98)	(M-Na)-	131.0946	130.101	7.957	75.12	Leucine
52	C ₆ H ₅ NO ₂	122.05(100), 106.01(6.87), 80(2.14)	(M-H)- (M+HCOO)-	123.032	122.03	15.62	85.89	Nicotinic acid
53	C ₇ H ₆ O ₃	137.02(100), 98.462(76.84), 112.03(49.54)	(M-H)- (M+HCOO)-	138.12	137.026	15.35	96.58	Salicyclic acid
54	C ₂₇ H ₄₃ NO ₂	412.33(100), 396.324(87.21), 157.099(30.77)	(M-H)-	413.3294	412.33	18.689	77.22	Solasodine [#]
55	C ₇ H ₁₀ O ₅	173(100), 157(63.47), 129(21.49)	(M+HCOO) (M+CH ₃ COO)-	174.0528	173.06	11.05	77.55	Shikimic acid
56	C ₁₁ H ₁₂ N ₂ O ₂	203.89(100), 187.87(54.12), 145.92(8.74)	(M-H)- (M+HCOO)-	204.0899	203.09	10.809	92.89	Tryptophan
57	C ₉ H ₁₁ NO ₃	180.08(100), 165.05(23.74), 136.07(7.64)	(M-H)-	181.0739	180.08	18.64	88.7	Tyrosine

Table S2: Statistical analysis of the levels of discriminant metabolites identified early after β CC treatment. The normalized peak area of the upregulated discriminant metabolites identified after 0, 30, 60, 90, 180, and 240 minutes after β CC treatment was compared with that of control plants. Mean normalized peak area (\pm SE) was analyzed from four replicate plants by one-way ANOVA and Fisher's LSD *post hoc* test. Significant difference is determined at $p \leq 0.05$. ND, not detected.

Sr. No.	Metabolite name	F value ($F_{12,39}$)	0 min	30 min	Mean (\pm SE); <i>p</i> - value			
					60 min	90 min	180 min	240 min
Upregulated metabolites								
1.	Aspartate	2.039	C= 0.045 (± 0.003) B= 0.051 (± 0.005) 0.767	C= 0.028 (± 0.016) B= 0.052 (± 0.018) 0.158	C= 0.030 (± 0.018) B= 0.070 (± 0.009) 0.026	C= 0.014 (± 0.005) B= 0.044 (± 0.011) 0.087	C= 0.011 (± 0.011) B= 0.038 (± 0.005) 0.122	C= 0.023 (± 0.013) B= 0.046 (± 0.015) 0.191
2.	Leucine	9.665	C= ND B= 0.008 (± 0.001) 0.0042	C= ND B= 0.010 (± 0.002) 0.0005	C= ND B= 0.010 (± 0.002) 0.0002	C= ND B= 0.008 (± 0.001) 0.004	C= ND B= 0.010 (± 0.002) 0.0004	C= ND B= 0.015 (± 0.005) <0.0001
3.	Glutamate	2.059	C= 0.137 (± 0.047) B= 0.171 (± 0.011) 0.457	C= 0.165 (± 0.058) B= 0.205 (± 0.017) 0.396	C= 0.154 (± 0.051) B= 0.233 (± 0.023) 0.095	C= 0.107 (± 0.018) B= 0.237 (± 0.040) 0.010	C= 0.185 (± 0.019) B= 0.247 (± 0.032) 0.185	C= 0.164 (± 0.013) B= 0.254 (± 0.014) 0.061
4.	Tryptophan	12.388	C= ND B= 0.103 (± 0.017) <0.0001	C= ND B= 0.122 (± 0.012) <0.0001	C= ND B= 0.077 (± 0.030) 0.0003	C= ND B= 0.080 (± 0.008) 0.0002	C= ND B= 0.067 (± 0.020) 0.0014	C= ND B= 0.081 (± 0.021) 0.0002
5.	Homoserine	49.842	C= ND B= 0.034 (± 0.004) <0.0001	C= ND B= 0.028 (± 0.003) <0.0001	C= ND B= 0.029 (± 0.003) <0.0001	C= ND B= 0.039 (± 0.001) <0.0001	C= ND B= 0.045 (± 0.006) <0.0001	C= ND B= 0.026 (± 0.004) <0.0001
6.	O-acetylserine	45.476	C= ND B= 0.171 (± 0.011) <0.0001	C= ND B= 0.205 (± 0.017) <0.0001	C= ND B= 0.233 (± 0.023) <0.0001	C= ND B= 0.237 (± 0.040) <0.0001	C= ND B= 0.247 (± 0.032) <0.0001	C= ND B= 0.254 (± 0.014) <0.0001
7.	Shikimate	7.444	C= ND B= 0.015 (± 0.005) 0.0221	C= ND B= 0.037 (± 0.005) <0.0001	C= ND B= 0.015 (± 0.006) 0.022	C= ND B= 0.020 (± 0.007) 0.022	C= ND B= 0.016 (± 0.007) 0.0122	C= ND B= 0.018 (± 0.007) 0.005
8.	Coumaric acid	4.166	C= 0.002 (± 0.001) B= 0.009 (± 0.005) 0.186	C= 0.005 (± 0.002) B= 0.011 (± 0.006) 0.243	C= 0.005 (± 0.003) B= 0.017 (± 0.003) 0.024	C= 0.003 (± 0.001) B= 0.001 (± 0.001) 0.74	C= 0.002 (± 0.001) B= 0.025 (± 0.007) <0.0001	C= 0.002 (± 0.001) B= 0.11 (± 0.005) 0.107
9.	Rutin	36.992	C= ND	C= ND	C= ND	C= ND	C= ND	C= ND

			B= 1.424 (±0.135) <0.0001 C= ND B= 0.002 (±0.002) 0.396	B= 1.656 (±0.243) <0.0001 C= ND B= 0.003 (±0.001) 0.089	B= 2.184 (±0.322) <0.0001 C= ND B= 0.003 (±0.001) 0.132	B= 1.240 (±0.322) <0.0001 C= ND B= 0.007 (±0.003) 0.001	B= 1.045 (±0.129) <0.0001 C= ND B= 0.004 (±0.001) 0.049	B= 1.376 (±0.143) <0.0001 C= ND B= 0.004 (±0.001) 0.057
10.	Salicylic acid	2.783						
11.	UDP-glucose	5.999						
			B= 2.457 (±0.522) 0.007	B= 3.637 (±0.833) 0.0002	B= 4.006 (±1.756) <0.0001	B= 0.606 (±0.195) 0.487	B= 0.662 (±0.142) 0.448	B= 1.540 (±0.002) 0.604
12.	Galactose	16.399						
			C= ND B= 0.142 (±0.009) <0.0001	C= ND B= 0.086 (±0.020) 0.0013	C= ND B= 0.130 (±0.024) <0.0001	C= ND B= 0.171 (±0.040) <0.0001	C= ND B= 0.131 (±0.014) <0.0001	C= ND B= 0.123 (±0.029) <0.0001
Downregulated metabolites								
13.	Cinnamic acid	2.947	C= 0.007 (±0.003) B= ND 0.256	C= 0.015 (±0.004) B= ND 0.0218	C= 0.015 (±0.007) B= ND 0.026	C= 0.011 (±0.004) B= ND 0.084	C= 0.021 (±0.011) B= ND 0.0016	C= 0.008 (±0.003) B= ND 0.22
14.	Linoleic acid	10.045						
			C= 0.017 (±0.002) B= ND <0.0001	C= 0.013 (±0.001) B= 0.001 (±0.001) <0.0001	C= 0.006 (±0.004) B= 0.005 (±0.003) 0.533	C= 0.004 (±0.002) B= 0.004 (±0.002) 0.79	C= 0.010 (±0.001) B= ND 0.0005	C= 0.002 (±0.002) B= ND 0.532
15.	Nicotinic acid	7.143						
			C= 0.003 (±0.001) B= ND 0.019	C= 0.003 (±0.001) B= ND 0.036	C= 0.001 (±0.001) B= ND 0.339	C= 0.008 (±0.001) B= ND <0.0001	C= 0.005 (±0.002) B= ND 0.0009	C= 0.001 (±0.001) B= ND 0.437
16.	Sucrose	11.259						
			C= 0.044 (±0.014) B= ND 0.017	C= 0.073 (±0.006) B= ND 0.0002	C= 0.087 (±0.013) B= ND <0.0001	C= 0.059 (±0.019) B= ND 0.0019	C= 0.110 (±0.025) B= ND <0.0001	C= 0.073 (±0.022) B= ND 0.0002