

**A Metabolomics Study at the Postharvest Conditions of Cold Storage
and Fungicide (Imazalil Sulfate) Treatment in Navel Oranges and
Clementine Mandarins.**

Supporting Information

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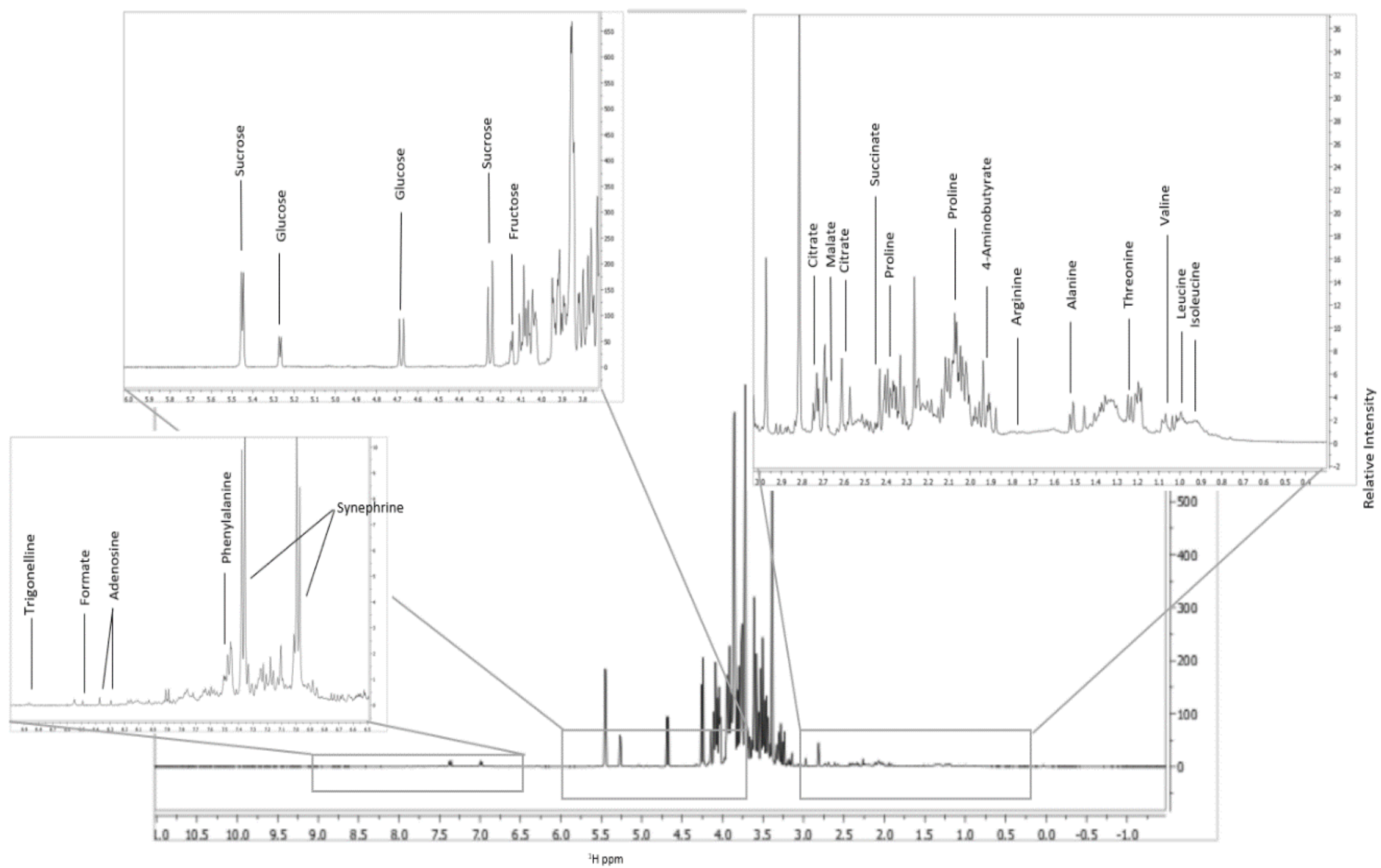
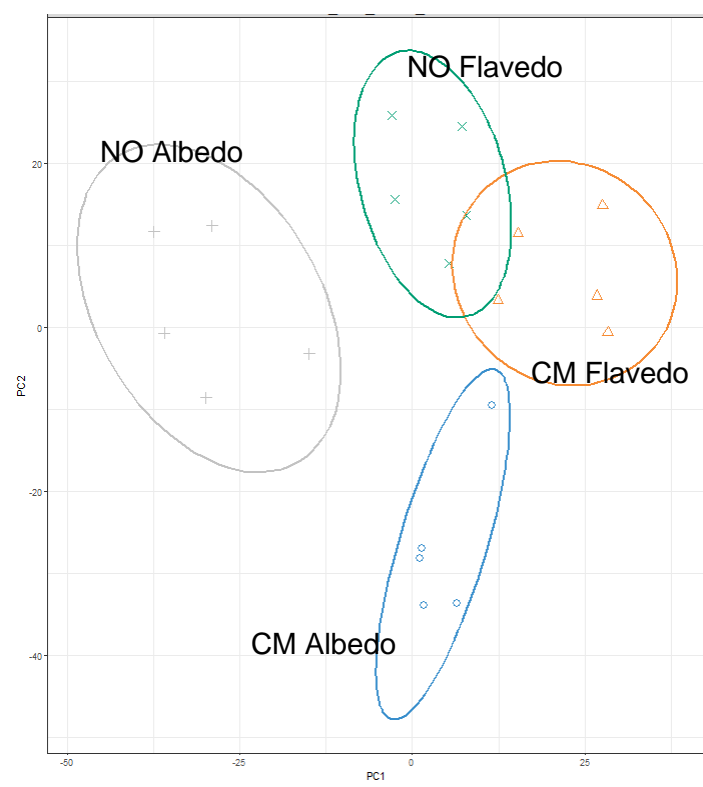
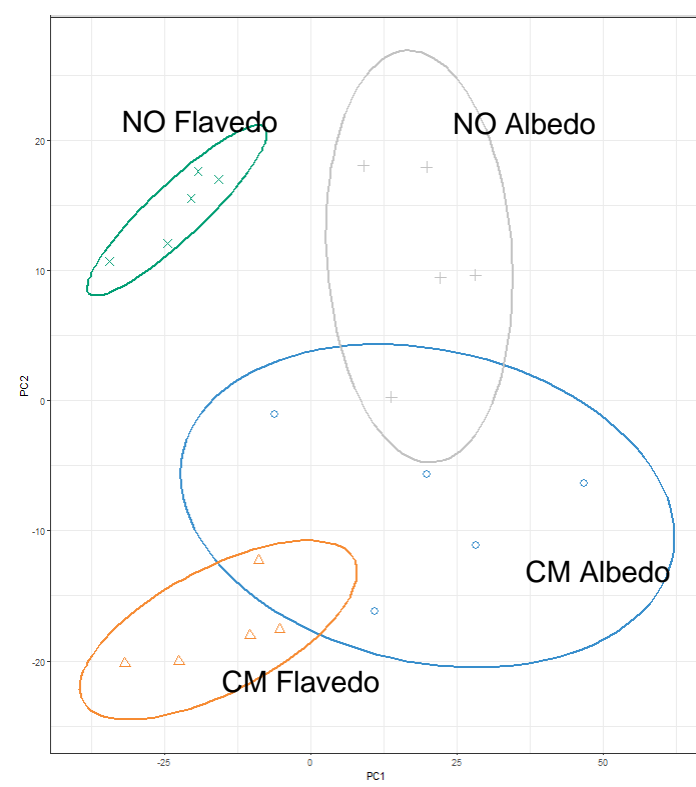


Figure S1

Ctrl



Cold Storage



Cold Storage + IMZ

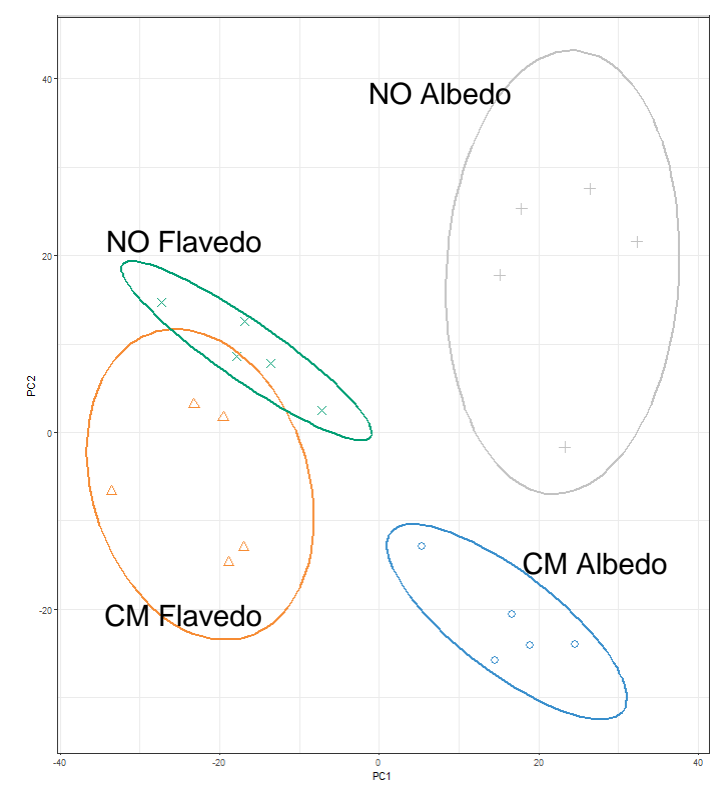


Table S1. Average Metabolite Concentration in Albedo Tissues

Metabolites	Clementine			Navel		
	Control	Cold Storage	Cold Storage + IMZ	Control	Cold Storage	Cold Storage + IMZ
Sugars						
Fructose	36.96 ± 5.50	28.61 ± 11.36	32.92 ± 3.10	57.59 ± 14.51	56.83 ± 6.97	57.26 ± 10.65
Glucose	39.27 ± 3.60	30.78 ± 11.28	35.25 ± 2.87	71.72 ± 7.92	79.52 ± 18.14	78.01 ± 14.79
Sucrose	33.49 ± 6.92	20.83 ± 6.63	23.46 ± 2.45	18.32 ± 8.65	12.27 ± 0.58	11.11 ± 1.35
myo-Inositol	8.98 ± 0.87	7.51 ± 2.63	10.29 ± 0.78	6.45 ± 0.70	7.07 ± 0.33	6.74 ± 1.73
Amino Acids						
Alanine	0.36 ± 0.09	0.26 ± 0.09	0.41 ± 0.08	0.28 ± 0.05	0.23 ± 0.01	0.22 ± 0.03
Arginine	2.19 ± 0.16	1.31 ± 0.08	1.32 ± 0.11	2.98 ± 0.11	2.45 ± 0.08	2.28 ± 0.05
Asparagine	ND	ND	ND	ND	ND	ND
Aspartate	ND	ND	ND	ND	ND	ND
Isoleucine	0.16 ± 0.04	0.09 ± 0.03	0.09 ± 0.02	0.06 ± 0.02	0.09 ± 0.03	0.10 ± 0.03
Leucine	0.12 ± 0.05	0.11 ± 0.04	0.15 ± 0.02	0.16 ± 0.03	0.10 ± 0.02	0.09 ± 0.01
Phenylalanine	0.44 ± 0.03	0.29 ± 0.11	0.40 ± 0.13	0.57 ± 0.07	0.60 ± 0.14	0.49 ± 0.13
Proline	3.97 ± 0.91	3.61 ± 1.03	3.48 ± 0.85	3.91 ± 2.07	2.97 ± 0.29	3.26 ± 0.69
Threonine	0.47 ± 0.07	0.35 ± 0.17	0.41 ± 0.08	0.32 ± 0.07	0.34 ± 0.04	0.30 ± 0.05
Valine	0.21 ± 0.06	0.13 ± 0.05	0.24 ± 0.10	0.23 ± 0.04	0.26 ± 0.06	0.28 ± 0.02
Organic Acids						
2-Phosphoglycerate	ND	ND	ND	ND	ND	ND
4-Aminobutyrate	0.71 ± 0.14	0.74 ± 0.12	0.75 ± 0.15	0.82 ± 0.48	0.74 ± 0.11	0.81 ± 0.20
Citrate	0.78 ± 0.45	0.79 ± 0.53	0.50 ± 0.26	0.59 ± 0.21	0.33 ± 0.17	0.45 ± 0.32
Formate	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.00	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.00
Malate	1.36 ± 0.52	1.33 ± 0.32	1.18 ± 0.21	1.17 ± 0.65	0.49 ± 0.21	0.92 ± 0.52
Malonate	1.01 ± 0.24	0.84 ± 0.14	0.95 ± 0.24	0.40 ± 0.20	0.50 ± 0.17	0.63 ± 0.25
Succinate	0.15 ± 0.02	0.11 ± 0.03	0.12 ± 0.04	0.10 ± 0.01	0.07 ± 0.01	0.09 ± 0.03
Others						
Adenosine	0.03 ± 0.01	0.03 ± 0.01	0.04 ± 0.00	0.03 ± 0.01	0.03 ± 0.00	0.03 ± 0.00
Choline	1.31 ± 0.25	1.16 ± 0.38	1.38 ± 0.24	0.48 ± 0.27	0.71 ± 0.09	0.74 ± 0.19
Proline betaine	0.63 ± 0.05	0.62 ± 0.08	0.65 ± 0.10	0.35 ± 0.08	0.44 ± 0.06	0.43 ± 0.10
Synephrine	2.48 ± 0.07	1.73 ± 0.53	2.31 ± 0.37	1.18 ± 0.14	1.06 ± 0.12	0.91 ± 0.14
Trigonelline	0.02 ± 0.01	0.02 ± 0.00	0.02 ± 0.01	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00

Expressed in mM with ± Standard Deviation, ND: Not Detected

Table S2. Average Metabolite Concentration in Flavedo Tissue

Metabolites	Clementine			Navel		
	Control	Cold Storage	Cold Storage + IMZ	Control	Cold Storage	Cold Storage + IMZ
Sugars						
Fructose	57.87 ± 8.35	62.97 ± 6.30	64.10 ± 5.76	60.96 ± 10.08	65.56 ± 4.95	70.62 ± 10.19
Glucose	54.78 ± 8.07	64.17 ± 5.18	61.79 ± 5.39	63.52 ± 10.91	67.88 ± 9.04	72.77 ± 11.93
Sucrose	29.78 ± 4.55	21.49 ± 4.51	22.61 ± 6.12	24.34 ± 11.28	17.77 ± 2.54	15.64 ± 3.23
myo-Inositol	6.89 ± 1.39	7.73 ± 2.21	8.38 ± 0.76	6.09 ± 1.18	6.02 ± 1.16	6.19 ± 0.55
Amino Acids						
Alanine	0.36 ± 0.06	0.31 ± 0.07	0.37 ± 0.03	0.67 ± 0.17	0.49 ± 0.11	0.48 ± 0.05
Arginine	3.93 ± 0.18	4.07 ± 0.34	5.44 ± 0.20	5.85 ± 0.32	6.34 ± 0.39	6.54 ± 0.35
Asparagine	0.91 ± 0.46	0.67 ± 0.44	0.48 ± 0.26	5.84 ± 6.59	4.72 ± 5.39	8.44 ± 6.85
Aspartate	ND	ND	ND	ND	ND	ND
Isoleucine	0.21 ± 0.09	0.26 ± 0.12	0.25 ± 0.04	0.20 ± 0.06	0.30 ± 0.08	0.28 ± 0.08
Leucine	0.24 ± 0.05	0.22 ± 0.05	0.27 ± 0.05	0.28 ± 0.04	0.18 ± 0.03	0.20 ± 0.06
Phenylalanine	0.45 ± 0.05	0.43 ± 0.04	0.40 ± 0.06	0.46 ± 0.07	0.48 ± 0.06	0.44 ± 0.05
Proline	6.04 ± 1.48	4.58 ± 0.72	4.03 ± 1.50	6.19 ± 1.37	5.81 ± 1.28	7.34 ± 2.01
Threonine	0.76 ± 0.13	0.79 ± 0.32	0.75 ± 0.19	0.86 ± 0.26	0.87 ± 0.13	0.87 ± 0.12
Valine	0.32 ± 0.06	0.37 ± 0.14	0.40 ± 0.09	0.51 ± 0.14	0.60 ± 0.04	0.60 ± 0.13
Organic Acids						
2-Phosphoglycerate	ND	ND	ND	ND	ND	ND
4-Aminobutyrate	0.78 ± 0.23	0.81 ± 0.08	0.73 ± 0.24	1.16 ± 0.23	1.23 ± 0.34	1.30 ± 0.41
Citrate	0.58 ± 0.35	0.34 ± 0.07	0.29 ± 0.21	0.31 ± 0.10	0.22 ± 0.06	0.31 ± 0.13
Formate	0.02 ± 0.00	0.02 ± 0.00	0.03 ± 0.01	0.03 ± 0.00	0.03 ± 0.01	0.04 ± 0.01
Malate	0.71 ± 0.20	0.85 ± 0.28	0.90 ± 0.64	2.00 ± 0.52	1.20 ± 0.55	2.16 ± 1.19
Malonate	0.82 ± 0.18	0.75 ± 0.15	0.70 ± 0.24	0.23 ± 0.07	0.28 ± 0.13	0.33 ± 0.06
Succinate	0.09 ± 0.03	0.10 ± 0.01	0.08 ± 0.05	0.10 ± 0.04	0.11 ± 0.06	0.19 ± 0.07
Others						
Adenosine	0.04 ± 0.01	0.04 ± 0.01	0.05 ± 0.00	0.06 ± 0.01	0.05 ± 0.01	0.05 ± 0.00
Choline	0.77 ± 0.34	0.88 ± 0.32	0.81 ± 0.17	0.47 ± 0.09	0.58 ± 0.11	0.70 ± 0.21
Proline betaine	1.08 ± 0.13	1.13 ± 0.26	0.88 ± 0.38	0.62 ± 0.25	0.67 ± 0.21	0.95 ± 0.38
Synephrine	4.10 ± 0.65	3.96 ± 0.93	3.66 ± 0.26	1.29 ± 0.05	1.43 ± 0.39	1.34 ± 0.27
Trigonelline	0.02 ± 0.00	0.02 ± 0.01	0.03 ± 0.02	0.00 ± 0.00	0.00 ± 0.00	0.00 ± 0.00

Expressed in mM with ± Standard Deviation, ND: Not Detected

Table S3. Average Metabolite Concentration in Juice

Metabolites	Clementine			Navel		
	Control	Cold Storage	Cold Storage + IMZ	Control	Cold Storage	Cold Storage + IMZ
Sugars						
Fructose	294.33 ± 13.24	300.78 ± 7.62	276.04 ± 16.61	244.63 ± 46.93	248.29 ± 40.44	227.36 ± 26.46
Glucose	271.42 ± 8.71	260.57 ± 17.82	248.01 ± 4.48	213.44 ± 40.30	219.39 ± 38.42	207.42 ± 29.98
Sucrose	387.03 ± 15.36	385.59 ± 29.26	389.41 ± 16.22	211.18 ± 19.47	208.90 ± 18.21	222.87 ± 9.29
myo-Inositol	98.75 ± 9.64	99.48 ± 7.95	97.46 ± 10.73	88.83 ± 7.43	79.86 ± 22.06	89.10 ± 10.62
Amino Acids						
Alanine	0.94 ± 0.06	0.92 ± 0.05	1.04 ± 0.32	1.21 ± 0.20	1.10 ± 0.20	1.42 ± 0.43
Arginine	45.04 ± 0.98	53.97 ± 1.84	54.19 ± 1.18	58.34 ± 2.12	63.78 ± 1.54	73.60 ± 2.33
Asparagine	ND	ND	ND	ND	ND	ND
Aspartate	32.98 ± 2.58	32.76 ± 1.75	36.15 ± 4.38	27.85 ± 4.60	26.31 ± 2.60	25.60 ± 3.49
Isoleucine	0.14 ± 0.02	0.12 ± 0.03	0.13 ± 0.02	0.15 ± 0.03	0.15 ± 0.01	0.19 ± 0.04
Leucine	0.26 ± 0.07	0.24 ± 0.06	0.26 ± 0.03	0.23 ± 0.03	0.22 ± 0.02	0.28 ± 0.04
Phenylalanine	0.11 ± 0.02	0.13 ± 0.02	0.14 ± 0.01	0.20 ± 0.06	0.20 ± 0.05	0.20 ± 0.03
Proline	7.21 ± 1.33	7.50 ± 0.74	7.38 ± 2.45	5.77 ± 1.89	8.70 ± 1.76	10.71 ± 3.15
Threonine	0.30 ± 0.03	0.27 ± 0.04	0.29 ± 0.04	0.35 ± 0.06	0.37 ± 0.06	0.47 ± 0.09
Valine	0.30 ± 0.02	0.29 ± 0.02	0.28 ± 0.04	0.29 ± 0.05	0.29 ± 0.04	0.32 ± 0.07
Organic Acids						
2-Phosphoglycerate	63.44 ± 9.57	66.24 ± 12.33	74.20 ± 3.91	67.88 ± 8.20	63.33 ± 7.43	67.48 ± 10.87
4-Aminobutyrate	ND	ND	ND	ND	ND	ND
Citrate	107.85 ± 12.79	113.96 ± 19.86	112.09 ± 13.27	90.22 ± 22.61	97.85 ± 19.85	91.31 ± 9.13
Formate	0.03 ± 0.01	0.02 ± 0.01	0.03 ± 0.01	0.05 ± 0.02	0.04 ± 0.01	0.06 ± 0.02
Malate	ND	ND	ND	ND	ND	ND
Malonate	0.93 ± 0.11	0.96 ± 0.13	0.91 ± 0.33	0.44 ± 0.21	0.75 ± 0.14	1.23 ± 0.69
Succinate	0.10 ± 0.01	0.12 ± 0.01	0.12 ± 0.04	0.12 ± 0.04	0.18 ± 0.03	0.29 ± 0.12
Others						
Adenosine	0.20 ± 0.03	0.18 ± 0.03	0.23 ± 0.03	0.24 ± 0.10	0.34 ± 0.05	0.42 ± 0.04
Choline	0.56 ± 0.05	0.62 ± 0.08	0.53 ± 0.13	0.26 ± 0.06	0.38 ± 0.09	0.49 ± 0.13
Proline betaine	3.33 ± 0.38	3.40 ± 0.16	3.37 ± 0.54	3.86 ± 0.96	4.26 ± 1.42	5.12 ± 1.28
Synephrine	0.77 ± 0.08	0.77 ± 0.09	0.66 ± 0.10	0.84 ± 0.18	0.88 ± 0.12	0.91 ± 0.06
Trigonelline	0.08 ± 0.02	0.07 ± 0.00	0.08 ± 0.01	0.04 ± 0.01	0.04 ± 0.02	0.05 ± 0.01

Expressed in mM with ± Standard Deviation, ND: Not Detected

Table S4a: Metabolite Fold Change and p-values of Clementine Control Fruit vs. Cold Storage Fruit

#	metabolites	Navel			Clementine		
		Albedo	Flavedo	Juice	Albedo	Flavedo	Juice
		ctrl vs. 10dC	ctrl vs. 10dC	ctrl vs. 10dC	ctrl vs. 10dC	ctrl vs. 10dC	ctrl vs. 10dC
		FC	FC	FC	FC	FC	FC
1	2-Phosphoglycerate			(1.07)			1.04
2	4-Aminobutyrate	1.00	(1.29)		1.03	1.06	
3	Acetone	(1.09)	(1.28)	1.03	(1.03)	1.00	(1.13)
4	Adenosine	(1.16)	1.09	1.64	(1.21)	(1.12)	(1.08)
5	Alanine	(1.20)	(1.28)	(1.10)	(1.44)	(1.18)	(1.02)
6	Arginine	(1.21)	1.09	1.10	(1.63)	(1.03)	1.19
7	Asparagine		1.04			(1.48)	
8	Aspartate			(1.05)			(1.01)
9	Choline	1.77	1.21	1.48	(1.17)	1.15	1.11
10	Citrate	(1.96)	1.01	1.09	1.00	(1.50)	1.05
11	Formate	1.02	(1.37)	(1.44)	(1.68)	1.25	(1.32)
12	Fructose	1.01	1.07	1.02	(1.38)	1.09	1.02
13	Glucose	1.09	1.09	1.03	(1.35)	1.18	(1.04)
14	Isoleucine	1.52	1.23	1.03	(1.93)	1.19	(1.14)
15	Leucine	(1.53)	(1.77)	(1.02)	(1.09)	(1.08)	(1.04)
16	Malate	(2.36)	(1.01)		1.05	1.18	
17	Malonate	1.35	1.08	1.84	(1.18)	(1.09)	1.03
18	Phenylalanine	1.04	1.05	1.01	(1.58)	(1.03)	1.21
19	Proline	(1.21)	(1.07)	1.54	(1.11)	(1.29)	1.05
20	Proline betaine	1.27	(1.35)	1.09	(1.02)	1.03	1.02
21	Succinate	(1.42)	1.54	1.53	(1.40)	1.11	1.14
22	Sucrose	(1.39)	(1.54)	(1.01)	(1.66)	(1.40)	(1.01)
23	Synephrine	(1.12)	(1.01)	1.06	(1.50)	(1.05)	1.00
24	Threonine	1.09	1.03	1.04	(1.48)	(1.05)	(1.11)
25	Trigonelline			1.08	(1.57)	1.13	(1.09)
26	Valine	1.11	1.07	1.00	(1.62)	1.06	(1.03)
27	myo-Inositol	1.10	1.03	(1.15)	(1.26)	1.10	1.01

Significant metabolites are shown in block letters and underlined. Numbers in red and parenthesis represent down-regulated metabolites

Table S4b: Metabolite Fold Change and p-values of Clementine Cold Storage vs. Cold Storage + Treatment

#	metabolites	Navel			Clementine		
		Albedo	Flavado	Juice	Albedo	Flavado	Juice
		0dC vs. 10dCM	0dC vs. 10dCM	0dC vs. 10dCM	0dC vs. 10dCM	0dC vs. 10dCM	0dC vs. 10dCM
		FC	FC	FC	FC	FC	FC
1	2-Phosphoglycerate			1.06			1.13
2	4-Aminobutyrate	1.07	1.05		1.02	(1.16)	
3	Acetone	(1.08)	(1.27)	(1.02)	(1.11)	(1.17)	1.10
4	Adenosine	(1.05)	(1.00)	1.24	1.36	1.33	1.28
5	Alanine	(1.03)	(1.02)	1.26	1.66	1.19	1.09
6	Arginine	(1.07)	1.04	1.15	(1.03)	1.44	1.01
7	Asparagine		1.48			(1.42)	
8	Aspartate			(1.03)			1.10
9	Choline	1.02	1.19	1.27	1.23	(1.04)	(1.20)
10	Citrate	1.34	1.35	(1.06)	(1.51)	(1.39)	(1.01)
11	Formate		1.38	1.37	1.06	1.09	1.24
12	Fructose	(1.00)	1.07	(1.09)	1.24	1.02	(1.09)
13	Glucose	(1.01)	1.07	(1.05)	1.22	(1.04)	(1.05)
14	Isoleucine	1.10	(1.11)	1.21	1.05	1.08	1.12
15	Leucine	(1.09)	1.08	1.27	1.39	1.24	1.09
16	Malate	1.81	1.66		(1.11)	(1.10)	
17	Malonate	1.25	1.32	1.49	1.11	(1.11)	(1.10)
18	Phenylalanine	(1.24)	(1.09)	1.04	1.38	(1.08)	1.08
19	Proline	1.08	1.25	1.21	(1.02)	(1.19)	(1.06)
20	Proline betaine	(1.02)	1.38	1.22	1.03	(1.35)	(1.02)
21	Succinate	1.30	1.78	1.57	1.09	(1.30)	(1.05)
22	Sucrose	(1.11)	(1.15)	1.07	1.17	1.04	1.01
23	Synephrine	(1.17)	(1.05)	1.04	1.38	(1.06)	(1.18)
24	Threonine	(1.15)	1.00	1.29	1.29	1.00	1.08
25	Trigonelline			1.12	1.26	1.02	1.10
26	Valine	1.10	(1.01)	1.07	1.79	1.15	(1.03)
27	myo-Inositol	(1.07)	1.04	1.16	1.44	1.12	(1.02)

Significant metabolites are shown in block letters and underlined. Numbers in red and parenthesis represent down-regulated metabolites