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Tomato and other plant-food metabolites for health

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1 BACKGROUND

A diet rich in fruits and vegetables is well known to reduce the risk of several diseases, such as cardiovascular disease and some cancers. Plant foods, including tomato, contain chemical compounds (metabolites or phytochemicals), which are believed to be beneficial for the health of consumers. The metabolite composition within each plant-food type varies by cultivar, climate and production system. Our previous research has shown that some tomato cultivars contain the gold-coloured form of lycopene known as tetra-*cis*-lycopene rather than the usual red form known as all-*trans*-lycopene.

This project has two aims:

1. To identify tomato cultivars that contain substantial amounts of tetra-cis-lycopene by measuring tetra-cis-lycopene in a range of heritage tomato selections. Tetra-*cis*-lycopene will be measured by UHPLC (Ultra High Performance Liquid Chromatography).
2. To measure specific metabolites in various plant foods provided by Mark Christensen, Heritage Food Crops Research Trust.

2 MATERIALS AND METHODS

Table 1 contains a list of the plant foods that were analysed for this project along with the names of the compounds that were measured.

Table 1. Plant foods analysed as part of this project and the target metabolites.

Plant food	# of Samples	Compounds
Tomato	13	tetra-*cis*-lycopene; all-*trans*-lycopene; beta-carotene; lutein
Carrot	30	lutein, alpha-carotene; beta-carotene; all-trans-lycopene; chlorogenic acid; quercetin 3-galactoside; p-coumarylquinnic acid, falcarinol, anthocyanins
Potato	31	alpha-chaconine; alpha-solanine; quercetin 3-galactoside; quercetin 3-rutinoside; kaempferol 3-rutinoside, p-coumarylquinnic acid, anthocyanins
Carrot	30	lutein, alpha-carotene; beta-carotene; all-trans-lycopene; chlorogenic acid; quercetin 3-galactoside; p-coumarylquinnic acid, falcarinol (not detected), anthocyanins

Plant food	# of Samples	Compounds
Capsicums	8	quercetin 3-galactoside; quercetin 3-rhamnoside; quercetin 3-rutinoside
Pears	2	catechin; epicatechin; chlorogenic acid; kaempferol 3-rutinoside; procyanidin B1; procyanidin B2; p-coumarylquinnic acid; quercetin 3-galactoside; quercetin 3-rutinoside
Crab apple	1	catechin; epicatechin; chlorogenic acid; kaempferol 3-rutinoside; procyanidin B1; procyanidin B2; p-coumarylquinnic acid; quercetin 3-galactoside; quercetin 3-rutinoside; phloridzin, triterpenoids
Apple	5	triterpenoids
Choke/ Wolfberry	2	epicatechin; chlorogenic acid; procyanidin B2; kaempferol 3-rutinoside; p-coumarylquinnic acid; quercetin 3-galactoside; quercetin 3-rutinoside; quercetin 3-rhamnoside
Grapefruit	1	hesperidin, neohesperidin, naringin, naringenin,
Medlar jelly	1	quercetin 3-galactoside; quercetin 3-rhamnoside; quercetin 3-rutinoside, phloridzin

3 RESULTS

Each sample type was analysed for the metabolites listed in Table 1 by either Ultra High Performance Liquid Chromatography (UHPLC) or Liquid Chromatography – Mass Spectrometry (LCMS). Quantitative measurement requires authentic analytical standards and in most cases quantitation was achieved using a standard of the target metabolite. In some cases the authentic metabolite is not available, for example the terpenoic acids in apple skin. In these cases, quantitation was achieve using a metabolite of a similar type and the results are reported as an equivalence of the metabolite used.

The results of these analyses are provided without comment or interpretation.

Table 2. Carotenoid concentrations (mg/100g FW) in samples of tomato measured by UHPLC.

Tomato genotype	TC-lyco	AT-lyco	b-caro	lut
‘Moonglow’	3.95	n.d.	n.d.	n.d.
‘Golden Eye’	n.d.	n.d.	15.3	0.1
‘Lemon Eye’	n.d.	n.d.	0.3	0.0
‘Tangerine’ (not covered plant 4)	5.82	n.d.	n.d.	n.d.
‘Tangerine’ (covered plant 2)	4.34	n.d.	n.d.	n.d.
‘Orange Teardrop’	5.31	0.2	n.d.	n.d.
‘Mini Orange’	3.36	n.d.	n.d.	n.d.
‘Olga's Round Golden Chicken Egg’	2.93	n.d.	n.d.	n.d.
‘Orange Crimea’	3.86	n.d.	n.d.	n.d.
‘Orange Queen’	2.41	n.d.	n.d.	n.d.
‘Kellogs Breakfast’	3.42	n.d.	n.d.	n.d.
‘Orange Cherub’	3.44	0.1	n.d.	0.1
‘Amish Yellowish Orange Oxheart’	4.36	0.1	n.d.	n.d.

n.d. = not detected; TC-lyco = tetra-*cis*-lycopene; AT-lyco = all-*trans*-lycopene; b-carotene = beta carotene; lut = lutein.

Table 3. Carotenoid concentrations (mg/100g FW) in samples of carrot measured by UHPLC.

Carrot genotype	a-caro	b-caro	lut	AT-lyco
'Jaune Obtuse du Doubs' (Baker Creek)	n.d.	0.49	1.09	n.d.
'Synsdu Violette' ('Syrian Violet')	n.d.	n.d.	0.29	n.d.
'Limburgse Gele Van Mollenstaart'	n.d.	0.45	0.87	n.d.
'Gniff' (Swiss variety)	n.d.	n.d.	0.09	n.d.
'Lillisse'	n.d.	n.d.	n.d.	n.d.
'Lunar White'	n.d.	n.d.	n.d.	n.d.
'Jaune du Doubs'	n.d.	0.62	1.01	n.d.
'Pfalzer Gelbe'	n.d.	1.08	0.90	n.d.
'Purple Dragon'	2.92	6.08	1.15	n.d.
'Weibe Kuttiger'	n.d.	n.d.	n.d.	n.d.
'Rouge Sang Violet'	1.30	4.62	0.53	n.d.
'Black Anatolean'	0.09	0.53	1.52	n.d.
'Autumn King'	4.11	6.22	0.56	n.d.
'Cosmic Purple'	1.65	5.93	0.64	n.d.
'Black Anatolean'	n.d.	3.28	0.61	n.d.
'Purple Dragon'	2.02	9.27	0.28	n.d.
'Royal Chantenay'	2.71	10.60	0.39	n.d.
'Lubyana'	n.d.	0.71	0.45	n.d.
'Touchon'	1.58	9.80	0.16	n.d.
'Yellow Austrian Lobbericher'	n.d.	0.32	0.16	n.d.
'Top Weight'	4.25	9.17	0.68	n.d.
'St. Valery'	1.20	7.24	0.17	n.d.
'Atomic Red'	n.d.	3.31	n.d.	6.67
'Danvers 126 Half Long'	2.84	13.87	0.35	n.d.
'White Belgium'	n.d.	n.d.	n.d.	n.d.
'James Scarlet Intermediate'	1.97	10.23	0.30	n.d.
'Amarillo Yellow'	n.d.	0.22	0.29	n.d.
'Autumn King'	2.37	15.19	0.50	n.d.

n.d. = not detected; TC-lyco = tetra-*cis*-lycopene; AT-lyco = all-*trans*-lycopene; b-carotene = beta carotene; lut = lutein.

Table 4. Polyphenol concentrations (mg/100g FW) in samples of carrot measured by LCMS.

Carrot genotype	Chlorogenic acid	Quercetin 3-galactoside	*p*-Coumarlyquinic acid
'Synsdu Violette'	n.d.	0.08	n.d.
'Gniff'	46.53	0.03	n.d.
'Purple Dragon'	8.52	0.05	n.d.
'Rouge Sang Violet'	0.06	n.d.	n.d.
'Black Anatolean'	0.25	0.06	0.27
'Cosmic Purple'	n.d.	0.04	0.34
'Black Anatolean'	6.65	0.16	0.30
'Purple Dragon'	9.63	0.01	1.31
'Atomic Red'	n.d.	n.d.	n.d.

n.d. = not detected.

Table 5. Anthocyanin concentrations (mg cyanidin 3-glucoside equiv./100g FW) in samples of carrot measured by UHPLC.

Carrot genotype	ACN1	ACN2	ACN3	ACN4	ACN5	ACN6	ACN7
'Jaune Obtuse du Doubs'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Synsdu Violette' ('Syrian Violet')	n.d.	0.73	1.32	n.d.	n.d.	n.d.	24.16
'Limburgse Gele Van Mollenstaart'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Gniff' (Swiss Variety)	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	3.50
'Lillisse'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Lunar White'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Jaune du Doubs'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Pfalzer Gelbe'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Purple Dragon'	n.d.	n.d.	n.d.	n.d.	n.d.	0.26	0.70
'Weiße Kuttigo'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Rouge Sang Violet'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Black Anatolean'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.24
'Autumn King'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Cosmic Purple'	0.63	0.54	1.18	0.19	0.32	4.66	12.68
'Black Anatolean'	0.89	0.75	1.59	n.d.	n.d.	1.03	30.94
'Purple Dragon'	n.d.	n.d.	0.16	n.d.	n.d.	0.55	1.16
'Royal Chantenay'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Lubyana'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Touchon'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Yellow Austrian Lobbericher'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Top Weight'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'St Valery'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.06
'Atomic Red'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Danvers 126 Half Long'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'White Belgium'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'James Scarlet Intermediate'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Amarillo Yellow'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.
'Autumn King'	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.

n.d. = not detected; ACN7 = likely identification is cyanidin 3-ferulylxylosylglucosylgalactoside. Other anthocyanins were not identified.

Table 6. Polyphenol concentrations (mg/100g FW) in samples of potato measured by LCMS.

Potato genotype	CGQ	K-rut	Q-gal	Q-rut	*p*CQA
'Moeraki Whaler'	106.27	0.06	n.d.	0.08	0.22
'Karupoti'	69.19	0.01	n.d.	0.01	0.10
'Urenika'	229.95	0.09	n.d.	n.d.	0.11
'Raetihi'	12.81	n.d.	n.d.	0.03	0.06
'Pink Fir'	19.57	0.13	n.d.	0.02	0.17
'Kowiniwini'	49.53	n.d.	n.d.	0.04	0.08
'Shetland Black'	51.58	0.08	n.d.	0.03	0.05
'Moe Moe'	16.74	0.01	n.d.	0.02	0.28
'Pawhero'	105.21	0.02	n.d.	0.05	n.d.
'Old Blue'	36.14	0.10	n.d.	0.33	0.16
'Raupi'	75.39	2.01	0.02	4.53	0.05
'Maori 'E'' (Henry Harrington)	8.56	0.05	n.d.	1.01	0.22
'Paraketia'	153.30	n.d.	n.d.	0.04	2.80
'Lumpy Black'	26.29	0.01	n.d.	0.02	1.10
'Waiporoporo'	35.39	0.00	n.d.	n.d.	1.31
'Wherowhero'	41.35	0.10	n.d.	0.01	0.98
'Catriona'	39.96	0.01	n.d.	0.06	2.31
'Huakaroro'	12.29	0.00	n.d.	0.06	0.86
'Waiporoporo'	31.38	n.d.	n.d.	0.04	1.35
'Agria'	44.52	0.03	n.d.	0.84	0.57
'Purple Pride'	280.66	0.03	n.d.	n.d.	0.16
'Purple Prize'	80.09	0.05	n.d.	0.02	2.99
'Purple Promise'	83.62	0.05	n.d.	n.d.	2.31
'Amuri Mystery'	239.22	0.04	n.d.	n.d.	1.69
Purple Skin White Flesh	50.26	0.29	n.d.	1.61	0.07
Pink Skin White Flesh	96.43	0.29	n.d.	0.07	1.26

n.d. = not detected; CGA = chlorogenic acid; K-rut = kaempferol 3-rutinoside; Q-gal = quercetin 3-galactoside; Q-rut = quercetin 3-rutinoside; *p*CQA = *p*-coumarylquinnic acid.

Table 7. Glycoalkaloid concentrations (mg/100g FW) in samples of potato measured by LCMS.

Potato genotype	alpha-chaconine	alpha-solanine
‘Moeraki Whaler’	6.01	2.26
‘Karupoti’	12.64	5.61
‘Urenika’	9.60	7.75
‘Raetihi’	13.79	8.36
‘Pink Fir’	9.10	4.87
‘Kowiniwini’	12.08	8.47
‘Shetland Black’	6.79	3.49
‘Moe Moe’	5.89	3.09
‘Pawhero’	8.29	5.52
‘Old Blue’	3.85	1.95
‘Raupi’	11.10	8.02
‘Maori 'E'' (Henry Harrington)	5.81	3.00
‘Paraketia’	16.88	9.14
‘Lumpy Black’	4.01	1.72
‘Waiporoporo’	9.92	6.04
‘Wherowhero’	4.72	2.17
‘Catriona’	11.44	6.24
‘Huakaroro’	8.77	6.87
‘Waiporoporo’	15.93	10.96
‘Agria’	28.28	20.14
‘Purple Pride’	11.56	8.86
‘Purple Prize’	7.94	3.66
‘Purple Promise’	5.11	1.89
‘Amuri Mystery’	15.67	10.50
Purple Skin White Flesh	28.44	14.34
Pink Skin White Flesh	7.45	3.57

Table 8. Anthocyanin (ug cyanidin 3-glucoside equiv./g DW) in samples of potato measured by UHPLC.

Potato genotype	Unk-1	Pt-courutglu	Unk-2	Mv-courutglu	Mv-ferrtglu
'Waiporoporo'	n.d.	9.2	3.0	n.d.	n.d.
'Agria'	n.d.	16.7	5.1	n.d.	n.d.
'Purple Pride'	n.d.	n.d.	n.d.	n.d.	n.d.
'Purple Prize'	n.d.	n.d.	10.7	1.9	n.d.
'Purple Promise'	n.d.	11.2	3.2	n.d.	n.d.
'Amuri Mystery'	2.0	31.6	12.2	3.8	2.8
Purple skin white flesh	n.d.	n.d.	n.d.	n.d.	n.d.
Pink skin white flesh	53.1	940.4	59.6	272.6	12.7
'Moeraki Whaler'	47.6	297.9	80.8	26.4	12.8
'Karupoti'	82.5	736.4	49.2	188.2	24.2
'Urenika'	42.6	439.9	11.5	891.9	78.4
'Raetihi'	n.d.	39.3	7.5	n.d.	n.d.
'Pink Fir'	n.d.	n.d.	7.0	n.d.	n.d.
'Kowiniwini'	38.4	512.8	49.1	111.8	17.8
'Shetland Black'	n.d.	36.4	7.5	n.d.	n.d.
'Moe Moe'	66.4	776.6	19.2	1824.6	161.4
'Pawhero'	n.d.	n.d.	n.d.	n.d.	n.d.
'Old Blue'	n.d.	n.d.	n.d.	n.d.	n.d.
'Raupi'	n.d.	25.9	n.d.	n.d.	n.d.
'Maori 'E'' (Henry Harrington)	8.5	78.7	10.9	16.8	n.d.
'Paraketia'	n.d.	10.8	n.d.	n.d.	n.d.
'Lumpy Black'	n.d.	9.3	n.d.	19.8	n.d.
'Waiporoporo'	25.1	228.0	16.6	48.9	8.8
'Wherowhero'	n.d.	7.7	n.d.	n.d.	n.d.
'Catriona'	n.d.	n.d.	n.d.	n.d.	n.d.
'Huakaroro'	6.0	162.4	16.5	12.3	5.1
'Scotts'	4.9	37.9	4.1	8.2	n.d.
'Peru Peru'	n.d.	37.8	12.9	5.5	n.d.
'Nadine'	n.d.	n.d.	12.0	7.2	n.d.
'Uwhi'	n.d.	n.d.	n.d.	n.d.	n.d.
'Chatham Island' ('Whataroa')	n.d.	n.d.	n.d.	n.d.	n.d.

n.d. = not detected; Unk-1 = this anthocyanin could not be identified; Pt-courutglu = tentatively identified as petunidin 3-coumarylrutinyl-glucoside; Unk-2 = this anthocyanin could not be identified; Mv-courutglu = tentatively identified as malvidin 3-coumarylrutinyl-glucoside; Mv-ferrutglu = tentatively identified as malvidin 3-ferulylrutinyl-glucoside.

Table 9. Flavanone concentrations (mg/100g FW) in samples of grapefruit measured by LCMS.

Sample name	Hesperidin	Naringin	neoHesperidin	Naringenin
'Ellis' (Peel)[#]	32.9	46.3	46.2	n.d.
'Ellis' (Pith)[#]	37.9	36.9	35.6	n.d.
'Ellis' (Peel)[$]	36.3	41.5	46.8	n.d.
'Ellis' (Pith)[$]	35.6	38.1	35.6	n.d.

n.d. = not detected; [#] = sample obtained using a peeler; [$] = sample obtained using a peeler.

Table 10. Triterpenoid (ug betulinic acid equiv./g DW) in skin samples of apple measured by LCMS.

Terpenoic acid	MS – mother[&]	MS – grafted[#]	MS – AA4[$]	MS – AA12[$]	Takapuna Russet
coum-diOH-urs	48	146	215	100	72
coum-OH-urs_1	15	75	149	84	71
coum-OH-urs_2	28	124	116	107	14
coum-OH-urs_3	29	65	142	73	42
coum-OH-urs_4	31	106	102	101	42
coum-triOH-urs	54	20	28	3	42
oxo-OH-urs_1	37	40	129	245	49
oxo-OH-urs_2	106	115	225	461	49
oxo-diOH-urs	2990	4332	7700	8173	1694
3-OH-lup	178	176	185	196	857
diOH-urs_1	722	602	848	600	225
diOH-urs_2	304	379	568	409	125
diOH-urs_3	498	755	779	671	57
tetra-OH-urs	13	117	48	152	67
tri-OH-urs	361	609	914	617	531
3-OH-urs/olean	973	964	985	944	191

[&] = Original mother tree (over 100 years old); [#] = From a grafted tree; [$] = Seedling grown from seed from the mother tree.

Table 11. Triterpenoid compound description.

Abbreviation	Compound name
coum-diOH-urs	3-coumaroyloxy-dihydroxy-urs-12-en-28-oic acid
coum-OH-urs_1	3-coumaroyloxy-hydroxy-urs-12-en-28-oic acid_1
coum-OH-urs_2	3-coumaroyloxy-hydroxy-urs-12-en-28-oic acid_2
coum-OH-urs_3	3-coumaroyloxy-hydroxy-urs-12-en-28-oic acid_3
coum-OH-urs_4	3-coumaroyloxy-hydroxy-urs-12-en-28-oic acid_4
coum-triOH-urs	3-coumaroyloxy-trihydroxy-urs-12-en-28-oic acid
oxo-OH-urs_1	3-oxo-hydroxy-urs-12-en-28-oic acid_1
oxo-OH-urs_2	3-oxo-hydroxy-urs-12-en-28-oic acid_2
oxo-diOH-urs	annurcoic acid
3-OH-lup	betulinic acid
diOH-urs_1	dihydroxyurs-12-en-28-oic acid_1
diOH-urs_2	dihydroxyurs-12-en-28-oic acid_2
diOH-urs_3	dihydroxyurs-12-en-28-oic acid_3
tetra-OH-urs	tetrahydroxy-urs-12-en-28-oic acid
tri-OH-urs	trihydroxyurs-12-en-28-oic acid
3-OH-urs/olean	ursolic acid/oleanolic acid

Table 12. Polyphenol concentrations (mg/100g FW) in various sample types measured by LCMS.

Genotype	Cat	epiCat	CGQ	PyB1	PyB2	K-rut	Q-gal	Q-rut	Q-rha	Phlz	*p*CQA	Cy-gal
Pear												
Pyrus nivalis	0.05	0.17	25.6	0.11	2.64	n.d.	0.36	n.d.	n.a.	n.d.	1.97	n.d.
'Roots Cottage'	0.15	1.49	22.1	0.35	2.90	n.d.	0.22	n.d.	n.a.	n.d.	0.21	n.d.
Apple												
Crab apple		1.31	53.4	0.16	3.70	n.d.	4.77	0.29	n.a.		1.96	19.25
Berries												
Wolfberry		n.d.	12.9	n.d.	n.d.	0.01	0.09	n.d.	n.a.	n.d.	n.d.	n.d.
Chokeberry		1.36	31.5	n.d.	1.52	0.37	2.25	4.10	n.a.	n.d.	1.31	46.1
Capsicum												
'Dulce Espana'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	1.46	n.a.	n.a.	n.a.
'Horizon'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	0.30	n.a.	n.a.	n.a.
'Orange Sun'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	0.88	n.a.	n.a.	n.a.
'Special Red'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	0.20	n.a.	n.a.	n.a.
'California Wonder'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	0.04	0.05	0.11	n.a.	n.a.	n.a.
'Zagato'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	1.06	n.a.	n.a.	n.a.
'Banana'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	0.41	0.18	16.6	n.a.	n.a.	n.a.
'Hustler'	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.d.	n.d.	0.98	n.a.	n.a.	n.a.
Medlar Jelly	n.d.	n.d.	n.d.	n.d.	n.d.	n.d.	0.08	0.02	0.06	0.09	n.d.	n.d.

Taranaki small dark red crab apple; n.d. = not detected; n.a. = not analysed; Cat = catechin; epiCat = epicatechin; CGA = chlorogenic acid; PyB1 = procyanidin B1; PyB2 = procyanidin B2; K-rut = kaempferol 3-rutinoside; Q-gal = quercetin 3-galactoside; Q-rut = quercetin 3-rutinoside; Q-rha = quercetin 3-rhamnoside; Phlz = phloridzin; *p*-CQA = *p*-coumarylquinnic acid; Cy-gal = cyanidin 3-galactoside.

Qualifying statement

The results given in this report apply only to the samples provided to Plant & Food Research, which may or may not be representative of all examples of the varieties tested.

This report was prepared for:

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