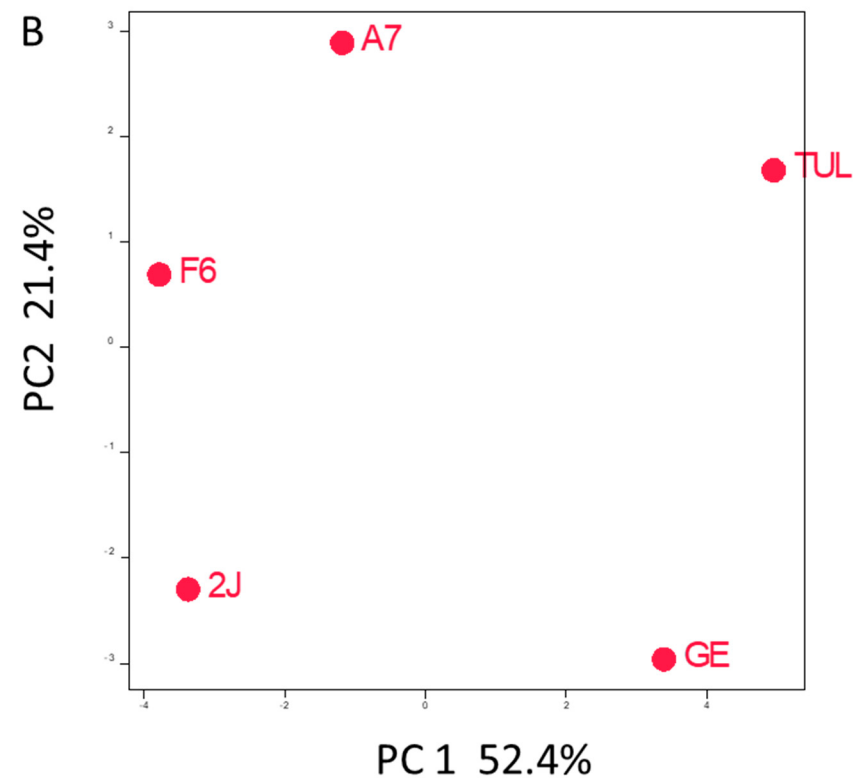
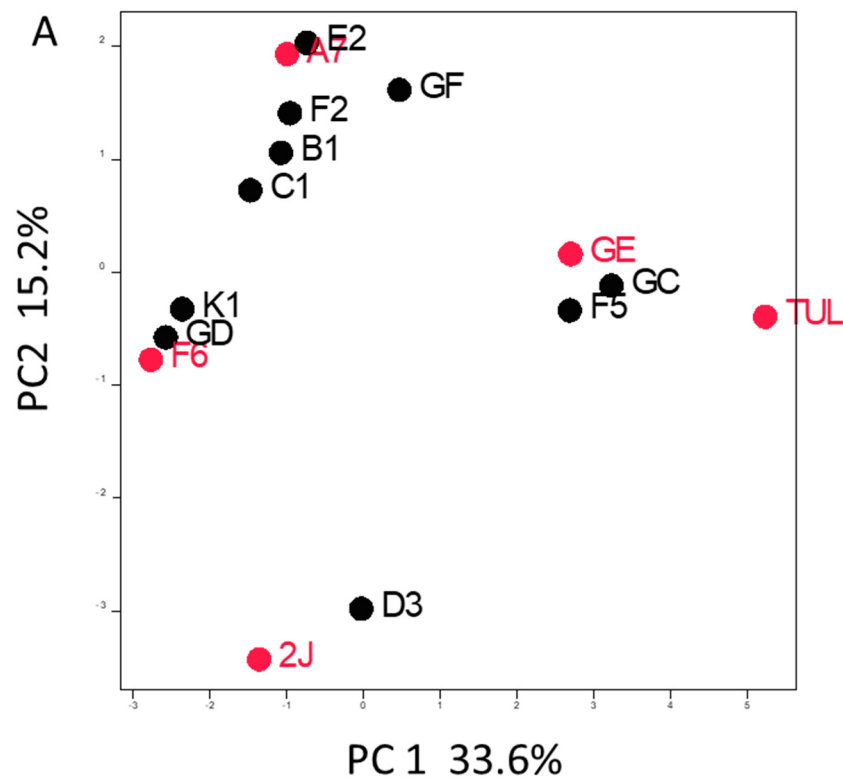
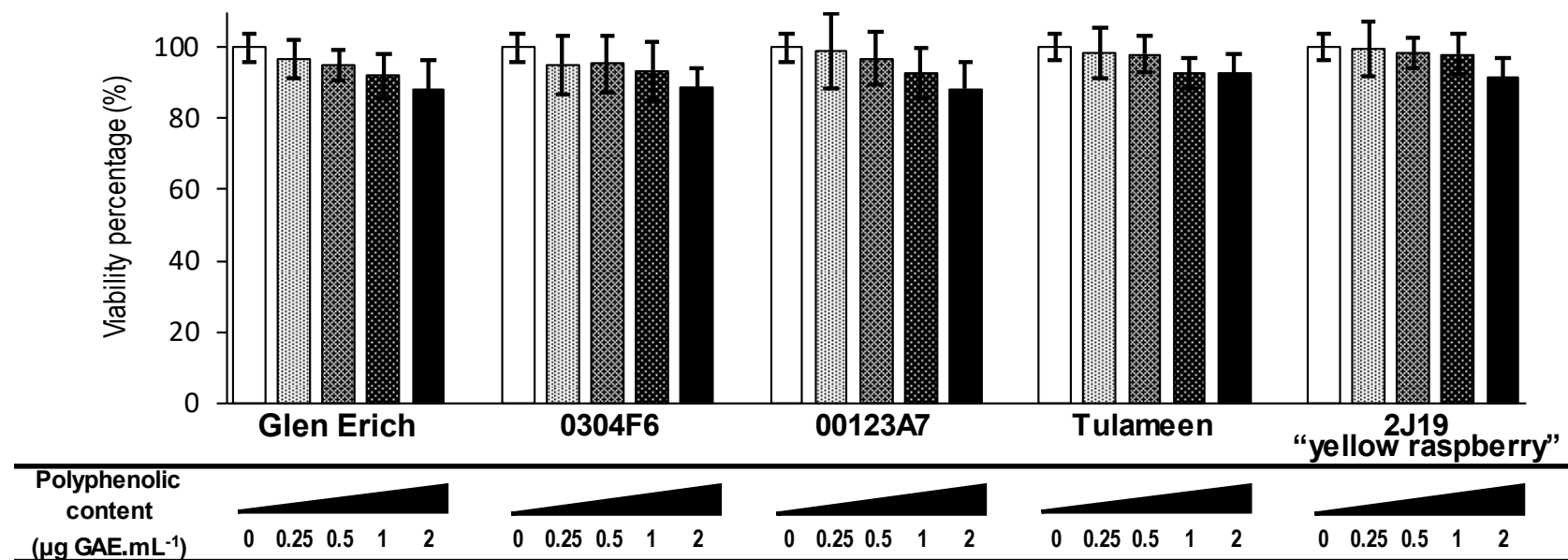




Supplementary Figure S1. PCA plot of polyphenol composition of: A. Extracts from raspberry cultivars and genotypes **B.** GIB fractions of selected raspberry cultivars and genotypes. Raspberry cultivars Glen Cally (GC), Glen Doll (GD), Glen Ericht (GE), Glen Fyne (GF), Tulameen (TUL) and genotypes 2J19 (2J), 00123A7 (A7), 0019E2 (E2), 0304F6 (F6), 0435D-3 (D3), 0460F-5 (F5), 0485K-1 (K1), 0534RB-1 (B1) & 9455F-2 (F2), 9911C-1 (C1). Cultivars and genotypes in red were selected for *in vitro* digestion.



Supplementary Figure S2. Cytotoxicity of the five raspberry GIB fractions under physiological concentrations. None of the five GIB fractions demonstrated significant cytotoxic effects at 0.25, 0.5, 1 and 2 $\mu\text{g GAE.mL}^{-1}$, even after 24 h of incubation.

Supplementary Table S1. Major polyphenols in raspberry cultivars and genotypes

Compound	R _t (min)	Glen Cally	Glen Doll	Glen Ericht	Glen Fyne	Tulameen	00123A7	0019E2	0304F6
Anthocyanin (µg g⁻¹ FDW)									
Cyanidin 3-sophoroside	16.36	3582.7	2781.2	3437.9	2579.0	3671.0	1831.8	2573.5	1213.7
Cyanidin 3-sophoroside-5-rhamnoside	17.04	975.3	16.2	913.5	1245.8	1191.8	410.8	633.2	24.3
Cyanidin 3-glucoside	17.20	535.0	700.3	527.4	441.6	606.7	650.5	756.3	261.1
Pelargonidin3-sophoroside / cyanidin 3-rutinoside	17.98	499.0	187.1	511.6	507.8	558.5	212.7	325.5	68.1
Total		5592.0	3684.8	5390.4	4774.1	6028.0	3105.9	4288.5	1567.2
Flavonol (µg g⁻¹ FDW)									
Quercetin 3-glucosylrutinoside	20.16	40.73	2.10	40.03	37.79	46.30	12.64	22.10	0.56
Quercetin diglucoside	21.02	10.15	30.78	9.54	5.75	14.21	7.15	8.37	13.55
Quercetin 3-galactoside	24.11	16.11	0.00	12.93	0.00	19.85	26.90	15.50	6.12
Quercetin 3-glucuronide	24.34	12.10	9.51	9.90	12.29	34.73	108.68	25.77	4.29
Quercetin 3-glucoside	24.44	4.09	11.33	3.41	4.03	6.34	11.13	8.84	2.71
Total		83.2	53.7	75.8	59.9	121.4	166.5	80.6	27.2
Ellagic acid conjugates (µg g⁻¹ FDW)									
Ellagic acid pentoside A	23.15	37.66	12.50	33.60	17.69	40.72	13.24	14.16	11.25
Ellagic acid pentoside B	23.64	29.71	20.52	27.35	17.55	5.48	14.41	18.62	20.13
Ellagic acid	24.01	10.16	4.29	8.54	9.34	16.70	5.01	3.83	9.73
Methyl ellagic acid pentoside A	26.53	13.83	5.73	13.31	4.51	22.88	4.85	4.75	4.04
Ellagic acid acetylpentoside A	26.67	5.27	6.76	5.20	10.39	4.50	6.16	7.17	6.36
Ellagic acid acetylpentoside B	27.68	7.30	17.83	7.43	14.65	1.66	12.09	15.38	19.93
Total		103.9	67.6	95.4	74.1	91.9	55.8	63.9	71.4
Ellagitannins (relative levels)									
Lambertianin C	21.01	100.0	45.6	86.9	55.4	48.2	85.3	98.0	39.9
Sanguiin H6	21.60	100.0	77.5	89.6	81.6	87.8	77.3	81.4	70.5

Compound	Rt (min)	0435D-3	0485K-1	0534RB-1	0460F-5	9455F-2	9911C-1	2J19
Anthocyanin ($\mu\text{g g}^{-1}$ FDW)								
Cyanidin 3-sophoroside	16.36	3224.8	2754.7	1696.3	4473.1	2632.4	3210.4	20.7
Cyanidin 3-sophoroside-5-rhamnoside	17.04	0.0	21.8	573.2	758.4	565.9	1.3	0.6
Cyanidin 3-glucoside	17.20	534.4	459.3	465.6	819.0	618.1	805.0	18.2
Pelargonidin3-sophoroside / cyanidin 3-rutinoside	17.98	125.1	140.9	297.1	451.6	268.9	147.8	0.0
Total		3884.3	3376.7	3032.1	6502.2	4085.3	4164.4	39.5
Flavonol ($\mu\text{g g}^{-1}$ FDW)								
Quercetin 3-glucosylrutinoside	20.16	0.00	3.30	17.86	33.58	15.45	0.00	0.00
Quercetin diglucoside	21.02	28.38	28.07	7.97	12.16	7.37	17.75	2.63
Quercetin 3-galactoside	24.11	3.59	0.00	5.85	0.00	5.98	10.40	0.00
Quercetin 3-glucuronide	24.34	4.34	26.48	1.85	20.88	3.42	6.62	24.06
Quercetin 3-glucoside	24.44	5.51	6.24	1.39	5.97	2.23	3.05	13.94
Total		41.8	64.1	34.9	72.6	34.5	37.8	40.6
Ellagic acid conjugates ($\mu\text{g g}^{-1}$ FDW)								
Ellagic acid pentoside	23.15	28.97	19.29	17.17	32.85	18.34	18.47	25.75
Ellagic acid pentoside	23.64	30.36	16.26	13.78	17.93	20.62	16.70	20.05
Ellagic acid	24.01	8.39	6.43	7.21	7.03	5.09	6.30	10.08
Methyl ellagic acid pentoside	26.53	10.81	5.15	6.57	16.64	6.23	4.61	13.96
Ellagic acid 4-acetylxyloside	26.67	2.96	11.17	11.75	2.59	8.29	8.64	5.77
Ellagic acid 4-acetylarabinoside	27.68	5.32	16.46	13.44	2.21	15.89	11.92	6.49
Total		86.8	74.8	69.9	79.3	74.5	66.6	82.1
Ellagitannins (relative levels)								
Lambertianin C	21.01	60.2	65.8	40.4	13.9	93.6	89.0	61.9
Sanguin H6	21.60	97.4	88.0	75.3	57.7	75.4	82.0	86.0

No standards were available for quantification of the major ellagitannins, so they were expressed as % levels relative to Glen Cally which had the highest levels.

Supplementary Table S2. Detailed polyphenol composition of the selected raspberry genotypes

Compound	R _t (min)	[M+H] ⁺ (m/z)		MS ² (m/z)	00123A7		0304F6		2J19	Glen Ericht	Tulameen
Anthocyanins (µg g⁻¹ FDW)		Observed	Actual								
Cyanidin 3,5-diglucoside	13.55	611.1614	611.1612	449, 287	14.4±0.6b		15.5±2.3b		0±0a	58.4±14.7d	22.6±2.1c
Cyanidin 3-sophoroside	16.27	611.1609	611.1612	287	1723.3±88.3c		936.8±72b		12.7±0.8a	3482.5±986.1d	3509.3±174d
Cyanidin 3-sophoroside-5-rhamnoside	16.86	757.2195	757.2191	611, 433, 287	317.5±15.2 c		16.7±1.3b		0.1±0.1a	609.2±110.1d	771.3±23e
Cyanidin 3-glucoside	17.06	449.1082	449.1084	287	637.1±36.6d		229.1±18.5b		9±0.9a	435.4±93.5c	491.1±18.3c
Cyanidin 3-sambubioside	17.33	581.1510	581.1507	287	63.9±2.6e		49.6±3.3d		0±0a	28.5±6b	36.3±1.5c
Pelargonidin 3-sophoroside / Cyanidin 3-rutinoside	17.47	595.1669	595.1663	449, 271 / 287	180.3±7.3c		49.5±3.4b		0.4±0a	369.2±71.1d	392.8±20.4d
Cyanidin 3-sambubioside-5-rhamnoside	17.72	727.2093	727.2086	581, 433, 287	13.9±0.5cd		12.7±1c		0±0a	8.7±1.5b	15.5±0.8d
Pelargonidin 3-sophoroside-5-rhamnoside	18.07	741.2252	741.2242	595, 417, 271	12.2±0.4c		2.1±0.2b		0±0a	52.3±9.4d	51.8±2.6d
Pelargonidin 3-glucoside	18.37	433.1133	433.1135	271	34.6±2.3d		10.3±0.5b		0.1±0a	49.8±11e	26.1±1.3c
Pelargonidin 3-sambubioside	18.94	565.1559	565.1557	ND	1.7±0.1c		2±0.1c		0±0a	1.3±0.3b	1.3±0b
Pelargonidin 3-rutinoside	19.12	579.1714	579.1714	433, 271	3.5±0.3c		1.2±0b		0±0a	17.5±3.5e	10.5±0.4d
Total Anthocyanins					3002.5±152.2c		1325.4±100.8b		22.4±1.7a	5112.7±1303.5d	5328.6±237.7d
Flavonols (µg g⁻¹ FDW)		[M-H] ⁻ (m/z)									
Quercetin 3-glucosylrutinoside	20.33	771.2001	771.1984	591, 301	8.64±1.3c		0.5±0.03b		0±0a	24.67±19.23c	37.71±27.21c
Quercetin diglucoside	21.26	625.1414	625.1405	300	3.44±0.28b		10.54±0.91d		1.17±0.26a	6.24±1.89c	9.14±4.09cd
Quercetin 3-galactosylrhamnoside* ¹	23.81	609.1473	609.1456	301	2.46±0.22bc		0.01±0a		0.01±0.02a	1±0.47b	4.8±2.12c
Quercetin 3-rutinoside* ¹	24.04	609.1469	609.1456	301	3.31±0.28c		0.64±0.04b		0.02±0.01a	2.95±1.67c	4±1.94c
Quercetin 3-galactoside	24.53	463.0893	463.0877	301	32.44±7.56d		6.28±0.79b		0±0A	11.47±1.63c	26.94±1.01d
Quercetin 3-glucuronide	24.82	477.0684	477.0669	301	137.04±22.14e		4.28±0.65a		26.91±8.05C	7.52±1.4b	39.53±4.43d
Quercetin 3-glucoside	24.87	463.0891	463.0877	301	8.12±0.43c		2.32±0.16a		12.98±2.38D	2.46±0.32a	4.67±0.23b
Quercetin HMG* ²	26.11	607.1311	607.1299	545, 505, 463 , 301	0.36±0.05c		0±0a		0±0A	0.05±0.01b	16.69±1.12d
Kaempferol 3-galactoside	26.26	447.0944	447.0927	285	1.43±0.25c		0.29±0.06b		0±0A	1.79±0.18cd	2.07±0.14d
Kaempferol 3-glucuronide	27.17	461.0736	461.0720	285	7.51±1.52e		0.24±0.05a		0.94±0.19B	1.45±0.2c	2.79±0.32d
Kaempferol 3-glucoside	27.08	447.0940	447.0927		1.33±0.2d		0.15±0.01a		0.36±0.03B	0.56±0.06c	1.22±0.08d
Total Flavonols					206.06±31.02c		25.26±2.43a		42.37±10.91B	60.17±25.99b	149.57±39.2c
Compound	R _t (min)	[M+H] ⁺ (m/z)		MS ² (m/z)	00123A7		0304F6		2J19	Glen Ericht	Tulameen
Ellagic acid derivatives (µg g⁻¹ FDW)		[M-H] ⁻ (m/z)									
Ellagic acid pentoside A	23.00	433.0420	433.0407	301	12.2±1.2a		8.5±0.3a		23.4±4.6B	24.3±9.2b	35.1±7.3b
Ellagic acid pentoside B	23.59	433.0422	433.0407	301	13.4±1.7b		18.4±0.6cd		16.1±1.6bc	22.2±3.3d	4.5±0.4a

Ellagic acid	24.22	300.9996	300.9984		7.4±1.7a		8.9±0.4ab		10.6±0.2B		9.9±1.6b		19.7±3.8c
Methyl ellagic acid pentoside A	26.58	447.0579	447.0564	315	4.1±0.5a		3.4±0.1a		11.6±2C		8.5±2.4b		17±2.4d
Ellagic acid acetylxyloside* ³	26.99	475.0528	475.0513	301	6.6±1.3b		5.8±0.7b		5.9±0.1B		4.2±0.5a		4.4±1a
Methyl ellagic acid pentoside B	27.32	447.0578	447.0564	315	1±0.2b		1.7±0.1c		2.9±0.3D		2±0.3c		0.6±0a
Ellagic acid acetylabinoside* ³	28.11	475.0525	475.0513	300	14.6±3.6c		20.6±2.3d		6.4±0.4B		6.8±1.4b		1.8±0.4a
Total EA derivatives					59.3±1.5a		67.3±0.6ab		76.9±1.3b		77.9±2.7b		83.1±2.2b
Ellagitannins (relative levels)	[M-H]⁻² (m/z)												
Lambertianin C	21.46	1401.1081* ³	1401.1069	1401	100.0±2.2a		89.1±3.5a		84.5±10.1a		99.5±11.2a		87.3±7.3a
Sanguin H6	22.07	934.0729* ³	934.0712	1567, 1235 633, 301	95.7±3.2a		92.1±3.4b		91.83±9.1a		99.2±10.6a		100.0±6.0a
Total Ellagitannins*⁴					195.7a		181.2b		176.3a		198.5a		187.3a
Total Phenols*⁵ (mg g⁻¹ FDW)					44124a		33924b		58512c		96024d		52704c

Values are ug g FDW⁻¹ ± standard deviation, except for ellagitannins. Values with the same letter were not significantly different $p < 0.05$.

*¹ Quercetin 3-galactosylrhannoside and quercetin 3-rutinoside have identical mass spectra and were tentatively assigned by elution order (Mullen et al., 2003).

*² Quercetin 3-O-(3-hydroxy-3-methyl-glutaroyl)-galactoside. *³ Quercetin acetylpenosides putatively identified by elution order (Mullen et al., 2003).

*³ Doubly charged ions.

*⁴ No standards were available for quantification of the major ellagitannins, so their peak areas were expressed as % relative to the Lambertianin C peak which had the highest levels. Therefore, total values are only indications of relative content. This explains why the total Ellagitannins value are >100%.

*⁵ Assayed by Folin method

Supplementary Table S3A. Recovery of polyphenols in raspberry GIB fractions.

Compound		00123A7		0304F6		2J19		Glen Ericht		Tulameen	
		µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec
Anthocyanins	Cyanidin 3,5-diglucoside	1.4	9.6	0.9	6.0	0.0	0.0	11.7	20.1	1.3	5.7
	Cyanidin 3-sophoroside	186.2	10.8	126.6	13.5	1.2	9.8	381.3	11.0	434.9	12.4
	Cyanidin 3-sophoroside-5-rhamnoside	26.0	8.2	1.4	8.1	0.0	0.0	83.5	13.7	111.8	14.5
	Cyanidin 3-glucoside	44.4	7.0	17.5	7.6	2.7	30.1	34.2	7.8	39.1	8.0
	Cyanidin 3-sambubioside	5.1	8.0	4.7	9.4	0.0	0.0	2.7	9.5	3.5	9.7
	Pelargonidin 3-sophoroside / Cyanidin 3-rutinoside	13.4	7.4	4.8	9.7	0.0	4.5	41.8	11.3	45.5	11.6
	Cyanidin 3-sambubioside-5-rhamnoside	0.9	6.7	1.2	9.3	0.0	0.0	0.9	10.5	1.8	11.4
	Pelargonidin 3-sophoroside-5-rhamnoside	0.8	6.2	0.0	1.8	0.0	0.0	6.4	12.2	6.3	12.2
	Pelargonidin 3-glucoside	2.1	6.1	0.6	5.7	0.0	0.0	3.7	7.4	1.8	6.9
	Pelargonidin 3-sambubioside	0.0	0.0	0.0	2.4	0.0	0.0	0.0	0.0	0.0	0.6
	Pelargonidin 3-rutinoside	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total Anthocyanins		280.3	6.36	157.7	6.68	4.0	4.04	566.2	9.41	646.0	8.45
Flavonols	Quercetin 3-glucosylrutinoside	0.76	8.8	0.04	8.4	0.00	0.0	3.64	14.8	5.12	13.6
	Quercetin diglucoside	0.28	8.2	1.52	14.4	0.01	0.6	3.05	48.9	2.39	26.2
	Quercetin 3-galactosylrhamnoside	0.25	10.3	0.00	0.0	0.00	0.0	0.25	25.3	0.88	18.3
	Quercetin 3-rutinoside	0.31	9.3	0.05	7.9	0.01	56.9	0.50	16.8	0.64	16.0
	Quercetin 3-galactoside	0.97	3.0	0.42	6.6	0.07	0.0	0.95	8.3	1.91	7.1
	Quercetin 3-glucuronide	5.48	4.0	0.44	10.3	2.12	7.9	1.11	14.7	3.54	9.0
	Quercetin 3-glucoside	0.66	8.1	0.16	7.0	0.95	7.3	0.25	10.2	0.56	12.0
	Quercetin HMGG	0.01	2.6	0.00	0.0	0.00	0.0	0.00	0.0	1.57	9.4
	Kaempferol 3-galactoside	0.08	5.3	0.02	5.5	0.00	0.0	0.22	12.2	0.23	11.3
	Kaempferol 3-glucuronide	0.44	5.9	0.02	8.7	0.08	8.9	0.21	14.3	0.31	11.2
	Kaempferol 3-glucoside	0.11	8.4	0.01	8.4	0.03	8.7	0.07	11.8	0.16	13.2
Total Flavonols		9.35	6.72	2.68	7.02	3.27	8.21	10.24	16.12	17.33	13.39
Ellagic acid derivatives	Ellagic acid pentoside A	1.23	10.1	0.95	11.2	3.53	15.1	4.48	18.4	5.51	15.7
	Ellagic acid pentoside B	1.35	10.1	1.89	10.3	2.51	15.5	3.52	15.8	0.61	13.6
	Ellagic acid	1.58	21.2	1.68	18.9	3.05	28.7	4.65	47.0	3.52	17.8
	Methyl ellagic acid pentoside A	0.70	17.4	0.52	15.3	2.49	21.4	1.86	22.0	4.56	26.8
	Ellagic acid 4-acetylxyloside A	0.44	6.6	0.43	7.4	0.38	6.5	0.34	8.1	0.35	7.9
	Methyl ellagic acid pentoside B	0.16	17.0	0.24	14.3	0.66	22.9	0.47	23.9	0.42	69.3
	Ellagic acid 4-acetyl-rabinoside B	1.05	7.2	1.54	7.5	0.65	10.2	0.78	11.4	0.34	18.7
Total EA derivatives		6.51	12.8	7.25	12.13	13.27	17.19	16.10	20.94	15.30	24.25
Ellagitannins	Lambertianin C	-	0.07	-	0.03	-	0.01	-	0.49	-	0.08
	Sanguin H6	-	2.35	-	1.89	-	2.61	-	4.39	-	3.05
	Sum of % Ellagitannins*		2.42		1.92		2.62		4.88		3.13

Recoveries are percentages of the contents in the original material (see Table S1). *-The ellagitannins are only expressed as % recovery values.

Supplementary Table S3B. Identification and recovery of other polyphenols in raspberry GIB fractions

Compound				00123A7		304F6		2J19		Glen Ericht		Tulameen	
	R _t (min)	[M+H] ⁺ (m/z)	MS ² (m/z)	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec	µg g ⁻¹ FDW	%Rec
Phenolic acids (µg g⁻¹ FDW)													
Hydroxybenzoic	1.27	137.0233	93	0.15	NA	0.09	NA	0.17	NA	0.20	NA	0.11	NA
Protocatechuic	1.70	153.0180	109	0.10	NA	0.06	NA	0.01	NA	0.17	NA	0.19	NA
Cinnamic	3.60	147.0440	-	0.02	NA	0.01	NA	0.02	NA	0.03	NA	0.01	NA
Caffeic	3.92	179.0335	135	0.13	NA	0.15	NA	0.04	NA	0.17	NA	0.11	NA
Coumaric	5.45	163.0389	119	0.09	NA	0.04	NA	0.17	NA	0.14	NA	0.15	NA
Ferulic	6.58	193.0491	178, 149 , 134	0.08	NA	0.08	NA	0.08	NA	0.11	NA	0.07	NA
Sinapic	7.02	223.0593	-	0.03	NA	0.02	NA	0.00	NA	0.00	NA	0.03	NA
Ellagitannin degradation products													
Lambertianin C - EA	7.31	1250.5948*	1867, 1567, 1099 , 935, 933, 633	-	0.19	--	0.14	-	0.14	-	0.48	-	0.17
Sanguiin H10 A	6.20	783.0612*	1265 , 933, 633, 301	-	0.41	-	0.63	-	0.86	-	0.98	-	0.94
Sanguiin H10 B	7.07	783.0615*	1265 , 933, 633, 301	-	1.21	-	1.24	-	2.06	-	2.09	-	2.12
Sanguiin H2	7.73	551.0345*	935, 633 , 469	-	0.14	-	0.16	-	0.29	-	0.23	-	0.23
Galloyl glucoside A	1.36	331.0641	313 , 169	--	0.01	-	0.00	-	0.01	-	0.01	-	0.00
Galloyl glucoside B	1.72	331.0640	169	-	0.01	-	0.00	-	0.02	-	0.01	-	0.01
Sanguiin H10 - EA A	2.57	632.0599*	933 , 613, 331, 301	-	0.01	-	0.01	-	0.02	-	0.02	-	0.02
Sanguiin H10 - EA B	3.24	632.0607*	933 , 613, 331, 301	-	0.04	-	0.06	-	0.13	-	0.06	-	0.11
Sanguiin H10 - EA C	3.60	632.0603*	933 , 613, 331, 301	-	0.01	-	0.01	-	0.03	-	0.01	-	0.03
Sanguiin H10 - EA D	3.99	632.0602*	963, 933, 613, 301	--	0.01	-	0.03	-	0.05	-	0.03	-	0.05
Sanguiin H10 - EA E	6.58	632.0604*	935, 933, 551 , 331, 301	-	0.02	-	0.04	-	0.05	-	0.04	-	0.05

Relative levels of phenolic acids assume all phenolic acids have similar ionisation responses.

NA - % recovery not possible as phenolic acids were not quantified in the original samples

Levels of Lambertianin C-ellagic acid derivatives are relative to Lambertianin C peak areas in the original sample assuming similar ionisation responses.

Levels of all other components are relative to Sanguiin H6 assuming similar ionisation responses. * denotes doubly charged ion.