

Supplementary Materials

Table S1. Measured polyphenol concentration (Conc.) and calculated Limit Of Quantification (LOQ) in the 12 rosé wines (n.d.: not detected).

		1		2		3		4	
		Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
Benzoic acids and derivatives	<i>Gallic acid</i>	10.53 ± 0.09	0.08	0.427 ± 0.009	0.2	1.34 ± 0.02	0.2	3.5 ± 0.1	0.08
	<i>Protocatechuic acid</i>	2.46 ± 0.02	0.07	0.54 ± 0.02	0.02	0.572 ± 0.006	0.03	1.51 ± 0.03	0.04
	<i>Syringic acid</i>	1.68 ± 0.06	0.07	1.11 ± 0.05	0.03	0.327 ± 0.008	0.03	0.63 ± 0.03	0.04
	<i>Vanillic acid</i>	1.5 ± 0.2	0.3	1.1 ± 0.3	0.3	0.37 ± 0.06	0.3	0.86 ± 0.05	0.2
	<i>Ethyl gallate</i>	0.9 ± 0.3	0.005	0.06 ± 0.03	0.05	0.18 ± 0.06	0.005	0.4 ± 0.2	0.007
	<i>Ethyl protocatechuate</i>	0.12 ± 0.1	<0.02	0.06 ± 0.05	<0.02	0.03 ± 0.02	0.02	0.21 ± 0.1	<0.02
Hydroxycinnamic acids and derivatives	<i>Caffeic acid</i>	2.88 ± 0.03	0.2	0.69 ± 0.02	0.07	3.4 ± 0.2	0.05	10.5 ± 0.8	0.06
	<i>p-coumaric acid</i>	1.3 ± 0.3	0.5	0.3 ± 0.2	0.5	0.8 ± 0.2	0.3	4.1 ± 0.7	0.3
	<i>Ferulic acid</i>	0.4 ± 0.2	0.05	0.1 ± 0.2	0.2	0.2 ± 0.2	0.2	0.9 ± 0.3	0.4
	<i>Caftaric acid (cis- and trans- isomers)</i>	40.6 ± 0.6	0.3	4.97 ± 0.1	0.5	53.6 ± 0.4	0.3	5.74 ± 0.06	0.4
	<i>Coutaric acid (cis- and trans- isomers)</i>	20.5 ± 0.6	0.02	2.9 ± 0.4	0.02	12.2 ± 0.5	0.06	3 ± 2	0.02
	<i>Fertaric acid</i>	4.4 ± 0.2	0.02	3.91 ± 0.08	0.01	9.7 ± 0.5	0.004	6.5 ± 0.4	0.003
	<i>GRP (cis- and trans- isomers)</i>	6.9 ± 0.3	0.2	10.1 ± 0.2	0.08	23 ± 3	0.06	10 ± 2	0.04
	<i>Ethyl caffeate</i>	0.14 ± 0.07	0.008	0.11 ± 0.02	0.009	1.4 ± 0.3	0.008	6.2 ± 0.3	0.07
<i>Ethyl coumarate</i>	0.08 ± 0.08	0.01	0.014 ± 0.005	0.005	0.23 ± 0.09	0.007	0.67 ± 0.1	0.008	
Stilbens	<i>trans-resveratrol</i>	0.133 ± 0.005	0.05	0.185 ± 0.002	0.02	0.085 ± 0.009	0.02	0.22 ± 0.04	0.04
	<i>cis-resveratrol</i>	0.059 ± 0.008	0.02	0.034 ± 0.005	0.02	0.046 ± 0.007	0.02	0.186 ± 0.009	0.03
	<i>viniferin-1</i>	0.24 ± 0.09	0.4	0.09 ± 0.04	0.3	0.08 ± 0.05	0.2	0.11 ± 0.05	0.2
	<i>viniferin-2</i>	0.01 ± 0.02	0.02	0.029 ± 0.002	0.05	0.018 ± 0.003	0.02	0.021 ± 0.005	0.04
	<i>trans-piceid</i>	1.41 ± 0.09	0.5	0.9 ± 0.2	0.7	0.23 ± 0.05	0.4	0.4 ± 0.04	0.3
	<i>cis-piceid</i>	0.59 ± 0.06	0.3	1.3 ± 0.2	0.09	0.57 ± 0.04	0.06	1.25 ± 0.04	0.3
Flavonols	<i>Quercetin Glc</i>	0.017 ± 0.003	0.03	0.013 ± 0.002	0.02	0.008 ± 0.005	0.02	0.004 ± 0.004	0.01
	<i>Myricetin glucuronide</i>	0.12 ± 0.04	2	0.004 ± 0.002	0.2	0.003 ± 0.003	0.2	0.021 ± 0.006	0.6
	<i>Myricetin Glc</i>	0.19 ± 0.02	0.007	0.012 ± 0.003	0.004	0.01 ± 0.002	0.002	0.051 ± 0.007	0.004
	<i>Quercetin glucuronide</i>	0.44 ± 0.03	0.006	0.12 ± 0.03	0.002	0.26 ± 0.07	0.004	0.31 ± 0.03	0.005
	<i>Quercetin</i>	n.d.	0.2	0.01 ± 0.02	0.2	0.01 ± 0.02	0.02	0.005 ± 0.01	0.03

Table S1. Cont.

	1		2		3		4		
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	
	<i>Catechin</i>	19.9 ± 0.2	0.3	2.8 ± 0.4	0.08	4.6 ± 0.3	0.04	3.177 ± 0.241	0.08
	<i>Galloylated dimer</i>	n.d.	<0.002	n.d.	<0.002	n.d.	<0.002	n.d.	<0.002
	<i>Trimer-1 (1 isomer)</i>	0.44 ± 0.05	0.02	0.02 ± 0.02	<0.007	0.08 ± 0.03	<0.007	0.041 ± 0.008	0.007
	<i>Trimers-2 (several isomers)</i>	0.209 ± 0.004	<0.002	0.001 ± 0.003	0.03	0.024 ± 0.002	0.03	0.035 ± 0.005	0.03
	<i>(epi)cat-ethyl-(epi)cat-1 (1 isomer)</i>	n.d.	<0.08	n.d.	<0.08	n.d.	<0.08	n.d.	<0.08
Flavan-3-ols	<i>(epi)cat-ethyl-(epi)cat-2 (2 isomers)</i>	n.d.	<0.0007	n.d.	0.008	n.d.	0.02	n.d.	0.001
	<i>Epicatechin</i>	5.5 ± 0.3	3	1.8 ± 0.2	0.6	0.8 ± 0.6	0.2	1.9 ± 0.7	0.9
	<i>Dimer B2</i>	2.73 ± 0.07	0.06	0.48 ± 0.02	0.05	0.33 ± 0.02	0.04	0.94 ± 0.03	0.03
	<i>Dimer B1</i>	18.7 ± 0.2	0.05	1.96 ± 0.05	0.05	5.3 ± 0.2	0.03	2.9 ± 0.2	0.03
	<i>Dimer B3</i>	1.04 ± 0.05	0.04	0.165 ± 0.007	0.02	0.17 ± 0.02	0.02	0.218 ± 0.008	0.04
	<i>Dimer B4</i>	0.25 ± 0.08	0.4	0.06 ± 0.04	0.06	n.d.	0.2	0.19 ± 0.06	0.07
	<i>Astilbin</i>	0.84 ± 0.04	0.003	0.75 ± 0.02	0.002	0.488 ± 0.009	0.001	0.98 ± 0.03	0.01
Dihydroflavonols	<i>Taxifolin</i>	0.73 ± 0.03	0.2	0.32 ± 0.02	0.2	0.25 ± 0.05	0.07	0.46 ± 0.04	0.2
	<i>Malvidin 3,5-diGlc</i>	0.045 ± 0.004	0.4	0.38 ± 0.02	0.2	0.03 ± 0.02	0.08	0.067 ± 0.007	0.6
	<i>Delphinidin 3,5-diGlc</i>	0.052 ± 0.014	0.02	0.036 ± 0.01	0.02	n.d.	0.02	0.042 ± 0.006	0.02
	<i>Cyanidin 3,5-diGlc</i>	0.021 ± 0.004	0.02	n.d.	0.02	n.d.	0.02	0.01 ± 0.02	0.02
	<i>Petunidin 3,5-diGlc</i>	n.d.	0.02	n.d.	0.02	n.d.	0.02	n.d.	0.02
	<i>Peonidin 3,5-diGlc</i>	0.04 ± 0.02	0.2	0.21 ± 0.03	0.1	0.005 ± 0.009	0.02	0.036 ± 0.005	0.2
	<i>Malvidin 3-O-Glc</i>	6.68 ± 0.03	0.02	2.88 ± 0.05	0.2	1.6 ± 0.02	0.005	4.38 ± 0.1	0.04
	<i>Delphinidin 3-O-Glc</i>	0.316 ± 0.006	0.03	0.0167 ± 0.0008	0.02	0.0142 ± 0.0004	0.002	0.16 ± 0.02	0.01
Anthocyanins	<i>Cyanidin 3-O-Glc</i>	0.0465 ± 0.0006	0.002	0.0065 ± 0.0005	0.004	0.005 ± 0.002	0.0007	0.021 ± 0.002	0.002
	<i>Petunidin 3-O-Glc</i>	0.8 ± 0.03	0.02	0.036 ± 0.005	0.002	0.07 ± 0.006	0.005	0.41 ± 0.02	0.02
	<i>Peonidin 3-O-Glc</i>	1.25 ± 0.02	0.03	0.9 ± 0.03	0.06	0.203 ± 0.006	0.004	0.56 ± 0.01	0.02
	<i>Delphinidin 3-O-acetyl-Glc</i>	0.0269 ± 0.0004	0.003	0.0027 ± 0.0009	0.002	0.0044 ± 0.0003	0.002	0.086 ± 0.004	0.003
	<i>Cyanidin 3-O-acetyl-Glc</i>	0.0086 ± 0.0004	0.002	0.0009 ± 0.0002	0.0007	0.0068 ± 0.0003	0.0007	0.036 ± 0.003	0.002
	<i>Petunidin 3-O-acetyl-Glc</i>	0.046 ± 0.002	0.002	0.0031 ± 0.0004	0.002	0.0128 ± 0.001	0.002	0.132 ± 0.006	0.0009
	<i>Peonidin 3-O-acetyl-Glc</i>	0.131 ± 0.006	0.0008	0.016 ± 0.002	0.0003	0.161 ± 0.005	0.0005	0.45 ± 0.02	0.002

Table S1. Cont.

	1		2		3		4	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Malvidin 3-O-acetyl-Glc</i>	0.565 ± 0.005	0.003	0.049 ± 0.002	0.0008	0.451 ± 0.003	0.004	1.73 ± 0.06	0.002
<i>Delphinidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.05 ± 0.02	0.002	0.001 ± 0.002	0.004	0 ± 0.0001	0.002	0.018 ± 0.005	0.0006
<i>Cyanidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.032 ± 0.006	0.004	0.002 ± 0.003	0.0009	0.008 ± 0.003	0.002	0.007 ± 0.004	0.0004
<i>Petunidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.095 ± 0.006	0.005	0.005 ± 0.002	0.002	0.011 ± 0.002	0.0005	0.023 ± 0.005	0.002
<i>Peonidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.271 ± 0.006	0.003	0.0113 ± 0.0006	0.0002	0.09 ± 0.002	0.002	0.076 ± 0.002	0.002
<i>Malvidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.93 ± 0.03	0.004	0.076 ± 0.002	0.0004	0.213 ± 0.003	0.0009	0.282 ± 0.008	0.003
<i>Delphinidin 3-O-caffeoyl-Glc</i>	n.d.	0.0009	n.d.	0.002	n.d.	0.003	n.d.	0.03
<i>Cyanidin 3-O-caffeoyl-Glc</i>	n.d.	0.0005	n.d.	0.0005	n.d.	0.0006	n.d.	0.002
<i>Petunidin 3-O-caffeoyl-Glc</i>	n.d.	0.0006	n.d.	0.0009	n.d.	0.0005	n.d.	0.0006
<i>Peonidin 3-O-caffeoyl-Glc</i>	0.006 ± 0.005	0.0007	n.d.	0.0003	0.002 ± 0.002	0.0006	0.002 ± 0.003	0.0008
<i>Malvidin 3-O-caffeoyl-Glc</i>	0.012 ± 0.004	0.002	0.006 ± 0.008	0.0008	0.005 ± 0.007	0.0009	0.003 ± 0.002	0.002
<i>(epi)cat-ethyl-peonidin 3-O-Glc-1</i>	n.d.	0.002	n.d.	0.0007	n.d.	0.0008	n.d.	0.003
<i>(epi)cat-ethyl-peonidin 3-O-Glc-2</i>	n.d.	0.002	n.d.	0.0007	n.d.	0.0008	n.d.	0.003
<i>(epi)cat-ethyl-peonidin 3-O-Glc-3</i>	0.0005 ± 0.0009	0.002	n.d.	0.0007	n.d.	0.0008	n.d.	0.003
<i>(epi)cat-ethyl-peonidin 3-O-Glc-4</i>	n.d.	0.002	n.d.	0.0007	n.d.	0.0008	n.d.	0.003
<i>(epi)cat-ethyl-malvidin 3-O-Glc-1</i>	n.d.	0.002	n.d.	0.003	n.d.	0.003	n.d.	0.003
<i>(epi)cat-ethyl-malvidin 3-O-Glc-2</i>	n.d.	0.002	n.d.	0.003	n.d.	0.003	n.d.	0.003
<i>(epi)cat-ethyl-malvidin 3-O-Glc-3 and 4</i>	0.001 ± 0.002	0.002	n.d.	0.003	n.d.	0.003	n.d.	0.003
<i>(epi)cat-ethyl-malvidin</i> <i>3-O-coumaroyl-Glc (2 co-eluted isomers)</i>	0.005 ± 0.008	0.003	n.d.	0.0004	0.002 ± 0.004	0.0004	n.d.	0.0006
<i>Delphinidin 3-O-Glc-(epi)cat</i>	n.d.	0.002	n.d.	0.003	n.d.	0.003	n.d.	0.003
<i>Cyanidin 3-O-Glc-(epi)cat</i>	0.003 ± 0.003	0.04	n.d.	0.002	n.d.	0.004	n.d.	0.002
<i>Petunidin 3-O-Glc-(epi)cat</i>	0.015 ± 0.008	0.06	n.d.	0.003	n.d.	0.003	n.d.	0.005

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	1		2		3		4	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Peonidin 3-O-Glc-(epi)cat</i>	0.07 ± 0.04	0.002	0.005 ± 0.006	0.002	0.0004 ± 0.0008	0.002	0.02 ± 0.02	0.003
<i>Malvidin 3-O-Glc-(epi)cat (2 isomers)</i>	0.16 ± 0.009	0.005	0.014 ± 0.001	0.002	0.007 ± 0.002	0.001	0.044 ± 0.004	0.02
<i>Malvidin 3-O-coumaroyl-Glc-(epi)cat (2 isomers)</i>	0.0004 ± 0.0004	0.005	n.d.	0.003	n.d.	0.0008	n.d.	0.002
<i>(epi)cat-delphinidin 3-O-Glc A-F bicyclic</i>	0.001 ± 0.003	0.002	n.d.	0.002	n.d.	0.005	n.d.	0.007
<i>(epi)cat-cyanidin 3-O-Glc A-F bicyclic</i>	n.d.	0.002	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>(epi)cat-petunidin 3-O-Glc A-F bicyclic</i>	0.006 ± 0.009	0.005	n.d.	0.004	n.d.	0.005	n.d.	0.006
<i>(epi)cat-peonidin 3-O-Glc A-F bicyclic</i>	0.004 ± 0.004	0.002	n.d.	0.007	n.d.	0.006	0.002 ± 0.004	0.003
<i>(epi)cat-malvidin 3-O-Glc A-F bicyclic</i>	0.005 ± 0.004	0.04	n.d.	0.002	0.0004 ± 0.0008	0.002	0.0005 ± 0.0009	0.002
<i>Caftaric-peonidin 3-O-Glc (2 isomers)</i>	0.005 ± 0.006	0.002	0.03 ± 0.02	0.002	0.0003 ± 0.0002	0.002	0.003 ± 0.003	0.002
<i>Caftaric-malvidin 3-O-Glc (2 isomers)</i>	0.026 ± 0.008	0.002	0.04 ± 0.008	0.002	0.009 ± 0.002	0.001	0.006 ± 0.006	0.001
<i>Coutaric-malvidin 3-O-Glc (2 isomers)</i>	n.d.	0.02	n.d.	0.002	n.d.	0.002	n.d.	0.002
<i>Pyranodelphinidin 3-O-Glc</i>	0.001 ± 0.002	0.03	n.d.	0.006	n.d.	0.0009	n.d.	0.002
<i>Pyranocyanidin 3-O-Glc</i>	0.0004 ± 0.0007	0.02	n.d.	0.02	n.d.	0.06	n.d.	0.03
<i>Pyranopetunidin 3-O-Glc</i>	0.0001 ± 0.0003	0.008	n.d.	0.03	0 ± 0.0001	0.02	0.001 ± 0.002	0.02
<i>Pyranopeonidin 3-O-Glc</i>	0.003 ± 0.002	0.003	0.0008 ± 0.0009	0.003	0.0004 ± 0.0003	0.003	0.0003 ± 0.0006	0.005
<i>Pyranomalvidin 3-O-Glc (vitisin B)</i>	0.014 ± 0.003	0.007	0.0009 ± 0.0009	0.005	0.0021 ± 0.0004	0.002	0.006 ± 0.002	0.005
<i>Carboxypyranodelphinidin 3-O-Glc</i>	0.01 ± 0.01	0.02	0.0002 ± 0.0004	0.003	n.d.	0.002	0.004 ± 0.002	0.005
<i>Carboxypyranocyanidin 3-O-Glc</i>	n.d.	0.02	n.d.	0.0003	n.d.	0.009	n.d.	0.03
<i>Carboxypyranopetunidin 3-O-Glc</i>	0.005 ± 0.006	0.0008	n.d.	0.03	n.d.	0.009	0.001 ± 0.002	0.02
<i>Carboxypyranopeonidin 3-O-Glc</i>	0.027 ± 0.008	0.0004	0.0034 ± 0.001	0.0004	0.0013 ± 0.0008	0.0004	0.007 ± 0.003	0.0005
<i>Carboxypyranomalvidin 3-O-Glc (vitisin A)</i>	0.12 ± 0.02	0.003	0.012 ± 0.003	0.002	0.0114 ± 0.0009	0.0004	0.086 ± 0.01	0.005
<i>Pyranodelphinidin 3-O-acetyl-Glc</i>	n.d.	0.003	n.d.	0.0006	n.d.	0.0006	n.d.	0.005
<i>Pyranocyanidin 3-O-acetyl-Glc</i>	0.0003 ± 0.0003	0.008	0.0001 ± 0.0002	0.0007	n.d.	0.0009	0.0001 ± 0.0002	0.002
<i>Pyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.0002	n.d.	0.0005	n.d.	0.0005	n.d.	0.0007
<i>Pyranopeonidin 3-O-acetyl-Glc</i>	n.d.	0.001	n.d.	0.001	n.d.	0.0006	n.d.	0.0003
<i>Pyranomalvidin 3-O-acetyl-Glc</i>	n.d.	0.0004	n.d.	0.0005	n.d.	0.002	n.d.	0.0004
<i>Carboxypyranodelphinidin 3-O-acetyl-Glc</i>	n.d.	0.001	n.d.	0.0005	n.d.	0.0008	n.d.	0.0008

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	1		2		3		4	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Carboxypyranocyanidin 3-O-acetyl-Glc</i>	0.0002 ± 0.0004	0.002	n.d.	0.01	n.d.	0.0003	0.0002 ± 0.0004	0.0006
<i>Carboxypyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.003	n.d.	0.0004	n.d.	0.0006	0.0002 ± 0.0003	0.0004
<i>Carboxypyranopeonidin 3-O-acetyl-Glc</i>	n.d.	0.005	n.d.	0.002	n.d.	0.04	0.0008 ± 0.0007	0.003
<i>Carboxypyranomalvidin 3-O-acetyl-Glc</i>	0.008 ± 0.004	0.001	n.d.	0.002	0.002 ± 0.004	0.002	0.017 ± 0.003	0.002
<i>Pyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.0007	n.d.	0.0003	n.d.	0.0004	n.d.	0.0005
<i>Pyranopeonidin 3-O-coumaroyl-Glc</i>	n.d.	0.008	n.d.	0.0008	n.d.	0.003	n.d.	0.002
<i>Pyranomalvidin 3-O-coumaroyl-Glc</i>	0.001 ± 0.003	0.0007	n.d.	0.002	n.d.	0.003	n.d.	0.0009
<i>Carboxypyranopetunidin 3-O-coumaroyl-Glc</i>	0.001 ± 0.002	0.002	n.d.	0.002	n.d.	0.002	n.d.	0.002
<i>Carboxypyranopeonidin 3-O-coumaroyl-Glc</i>	0.004 ± 0.004	0.0005	n.d.	0.0005	n.d.	0.0004	0.001 ± 0.002	0.002
<i>Carboxypyranomalvidin 3-O-coumaroyl-Glc</i>	0.008 ± 0.002	0.0004	n.d.	0.0004	n.d.	0.0004	0.002 ± 0.004	0.0002
<i>p-hydroxyphenylpyranopeonidin 3-O-Glc</i>	0.006 ± 0.003	0.004	0.011 ± 0.002	0.02	0.006 ± 0.005	0.004	0.05 ± 0.02	0.05
<i>p-hydroxyphenylpyranomalvidin 3-O-Glc</i>	0.04 ± 0.02	0.0005	0.05 ± 0.02	0.0003	0.055 ± 0.005	0.0002	0.49 ± 0.03	0.0003
<i>p-hydroxyphenylpyranopeonidin 3-O-acetyl-Glc</i>	0.0003 ± 0.0006	0.0004	n.d.	0.0005	0.005 ± 0.002	0.0003	0.027 ± 0.008	0.0002
<i>p-hydroxyphenylpyranomalvidin 3-O-acetyl-Glc</i>	0.0026 ± 0.0004	0.0	0.001 ± 0.002	0.0002	0.012 ± 0.005	0.0002	0.13 ± 0.04	0.0002
<i>p-hydroxyphenylpyranopeonidin 3-O-coumaroyl-Glc</i>	0.0006 ± 0.0003	0.0004	n.d.	0.0002	0.001 ± 0.002	0.0004	0.0191 ± 0.0004	0.0004
<i>p-hydroxyphenylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.007 ± 0.002	0.0006	0.0004 ± 0.0007	0.0004	0.018 ± 0.009	0.0005	0.08 ± 0.02	0.0002
<i>Catechylpyranopeonidin 3-O-Glc</i>	0.013 ± 0.003	0.0003	0.001 ± 0.002	0.0002	0.002 ± 0.002	0.0004	0.06 ± 0.02	0.0004
<i>Catechylpyranomalvidin 3-O-Glc (pinotin A)</i>	0.07 ± 0.02	0.005	0.003 ± 0.002	0.0006	0.026 ± 0.009	0.0005	0.108 ± 0.01	0.0003
<i>Catechylpyranopetunidin 3-O-acetyl-Glc</i>	0.0004 ± 0.0007	0.0002	n.d.	0.0007	n.d.	0.0002	0.013 ± 0.007	0.0002
<i>Catechylpyranopeonidin 3-O-acetyl-Glc</i>	n.d.	0.0002	n.d.	0.0007	0.0002 ± 0.0003	0.0003	0.015 ± 0.007	0.0004
<i>Catechylpyranomalvidin 3-O-acetyl-Glc</i>	0.002 ± 0.003	0.0005	0.0001 ± 0.0002	0.0005	0.005 ± 0.003	0.0005	0.054 ± 0.007	0.0006
<i>Catechylpyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.0004	n.d.	0.0004	0.0001 ± 0.0002	0.0002	0.005 ± 0.005	0.0002
<i>Catechylpyranopeonidin 3-O-coumaroyl-Glc</i>	0.003 ± 0.002	0.0002	n.d.	0.0002	0.003 ± 0.003	0.0003	0.015 ± 0.006	0.00
<i>Catechylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.018 ± 0.008	0.0005	n.d.	0.0002	0.004 ± 0.003	0.0003	0.019 ± 0.006	0.003
<i>Guaiacylpyranomalvidin 3-O-Glc</i>	0.01 ± 0.009	0.0006	0.049 ± 0.01	0.0002	0.059 ± 0.016	0.0002	0.19 ± 0.03	0.0003
<i>Guaiacylpyranomalvidin 3-O-acetyl-Glc</i>	0.0002 ± 0.0003	0.0002	0.001 ± 0.002	0.0002	0.0096 ± 0.0009	0.0003	0.057 ± 0.009	0.0003

Table S1. Cont.

	1		2		3		4		
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	
Anthocyanins	<i>Guaiacylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.003 ± 0.002	0.0003	0.0001 ± 0.0003	0.0009	0.016 ± 0.004	0.0003	0.022 ± 0.004	0.002
	<i>Syringylpyranomalvidin 3-O-Glc</i>	n.d.	0.007	n.d.	0.002	n.d.	0.0009	0 ± 0.0001	0.002
	<i>Petunidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.003	n.d.	0.003	n.d.	0.002	n.d.	0.04
	<i>Peonidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.002	n.d.	0.005	n.d.	0.003	n.d.	0.002
	<i>Malvidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.002	n.d.	0.002	n.d.	0.0004	n.d.	0.001
	<i>Pyranopeonidin 3-O-Glc-(epi)cat</i>	0.0021 ± 0.0004	0.0005	n.d.	0.0010	n.d.	0.0007	0.0008 ± 0.0008	0.0005
	<i>Pyranomalvidin 3-O-Glc-(epi)cat</i>	0.004 ± 0.004	0.0004	n.d.	0.0003	n.d.	0.0002	0.001 ± 0.002	0.0003
	<i>Pyranomalvidin 3-O-coumaroyl-Glc-(epi)cat</i>	n.d.	0.002	n.d.	0.002	n.d.	0.002	n.d.	0.002
	<i>Unknown "551"</i>	0.014 ± 0.01	0.02	0.003 ± 0.003	0.0006	n.d.	0.003	0.002 ± 0.004	0.002
	<i>Unknown "581"</i>	0.032 ± 0.01	0.004	0.004 ± 0.002	0.002	0.001 ± 0.002	0.003	0.021 ± 0.006	0.004
	<i>Unknown "1095"</i>	n.d.	0.02	n.d.	0.02	n.d.	0.03	n.d.	0.02
<i>Unknown "1099"</i>	n.d.	0.02	n.d.	0.004	n.d.	0.002	0.001 ± 0.0003	0.007	
Others (aminoacids and alcohols)	<i>Tyrosine</i>	12.68 ± 0.02	0.4	8.62 ± 0.06	0.6	8.15 ± 0.07	0.7	7.81 ± 0.074	0.7
	<i>Tyrosol</i>	7.97 ± 0.139	4	6.585 ± 0.143	2	9.9 ± 0.3	2	10.3 ± 0.6	4
	<i>Hydroxytyrosol</i>	0.4 ± 0.04	0.07	0.08 ± 0.02	0.2	0.12 ± 0.02	0.03	0.77 ± 0.03	0.2
	<i>Tryptophol</i>	0.2 ± 0.1	0.2	0.17 ± 0.03	0.3	0.4 ± 0.2	0.2	0.5 ± 0.3	0.2
	<i>Tryptophan</i>	1.2 ± 0.2	0	1.6 ± 0.5	0	0.8 ± 0.3	0	1 ± 0.2	0

Table S1. Cont.

		5		6		7		8	
		Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
Benzoic acids and derivatives	<i>Gallic acid</i>	1.71 ± 0.06	0.1	13.8 ± 0.4	0.07	1.48 ± 0.04	0.04	2.36 ± 0.06	0.08
	<i>Protocatechuic acid</i>	1.27 ± 0.05	0.06	2.2 ± 0.02	0.07	0.67 ± 0.02	0.02	1.4 ± 0.2	0.05
	<i>Syringic acid</i>	2.7 ± 0.6	0.05	2.07 ± 0.03	0.05	0.48 ± 0.02	0.08	0.55 ± 0.003	0.04
	<i>Vanillic acid</i>	1.72 ± 0.1	0.2	1.55 ± 0.03	0.2	0.3 ± 0.2	0.05	0.86 ± 0.06	0.05
	<i>Ethyl gallate</i>	0.25 ± 0.1	0.006	2 ± 0.3	0.006	0.11 ± 0.03	0.01	0.37 ± 0.03	0.005
	<i>Ethyl protocatechuate</i>	0.3 ± 0.09	<0.02	0.7 ± 0.2	<0.02	0.07 ± 0.04	<0.02	0.3 ± 0.2	<0.02
Hydroxycinnamic acids and derivatives	<i>Caffeic acid</i>	2.33 ± 0.07	0.09	3.4 ± 0.2	0.06	1.69 ± 0.04	0.2	2.2 ± 0.4	0.06
	<i>p-coumaric acid</i>	1.6 ± 0.2	0.3	1.3 ± 0.1	0.5	1.21 ± 0.08	0.4	0.7 ± 0.2	0.3
	<i>Ferulic acid</i>	0.93 ± 0.07	0.02	0.11 ± 0.08	0.06	0.5 ± 0.2	0.02	0.2 ± 0.2	0.04
	<i>Caftaric acid (cis- and trans- isomers)</i>	30.9 ± 0.7	0.3	23.8 ± 0.4	0.3	26.3 ± 0.4	0.5	48 ± 3	0.2
	<i>Coutaric acid (cis- and trans- isomers)</i>	10 ± 2	0.03	7.705 ± 0.783	0.02	12.5 ± 0.3	0.07	13 ± 0.9	0.03
	<i>Fertaric acid</i>	6.3 ± 0.2	0.006	3.75 ± 0.1	0.008	5.23 ± 0.06	0.007	6.8 ± 0.3	0.02
	<i>GRP (cis- and trans- isomers)</i>	9 ± 2	0.2	0.44 ± 0.08	0.4	15.5 ± 0.3	0.2	11 ± 2	0.2
	<i>Ethyl caffeate</i>	0.5 ± 0.2	0.006	0.22 ± 0.05	0.03	0.5 ± 0.2	0.04	0.39 ± 0.08	0.008
<i>Ethyl coumarate</i>	0.15 ± 0.07	0.02	0.087 ± 0.009	0.02	0.3 ± 0.2	0.01	0.14 ± 0.04	0.05	
Stilbens	<i>trans-resveratrol</i>	0.57 ± 0.04	0.04	0.264 ± 0.008	0.02	0.15 ± 0.009	0.03	0.16 ± 0.02	0.02
	<i>cis-resveratrol</i>	0.53 ± 0.04	0.04	0.416 ± 0.005	0.03	0.049 ± 0.007	0.04	0.11 ± 0.02	0.04
	<i>viniferin-1</i>	0.17 ± 0.09	0.3	0.22 ± 0.03	0.3	0.098 ± 0.007	0.2	0.042 ± 0.008	0.07
	<i>viniferin-2</i>	0.029 ± 0.007	0.04	n.d.	0.02	n.d.	0.03	0.011 ± 0.01	0.03
	<i>trans-piceid</i>	0.93 ± 0.03	0.3	0.38 ± 0.03	0.8	0.43 ± 0.07	0.7	0.4 ± 0.2	0.8
	<i>cis-piceid</i>	2 ± 0.2	0.4	1.4 ± 0.2	0.06	1.04 ± 0.05	0.2	1 ± 0.2	0.2
Flavonols	<i>Quercetin Glc</i>	0.009 ± 0.006	0.02	0.02 ± 0.005	0.009	0.01 ± 0.009	0.008	0.013 ± 0.003	0.02
	<i>Myricetin glucuronide</i>	0.028 ± 0.004	0.6	0.12 ± 0.05	4	0.016 ± 0.006	0.8	0.049 ± 0.003	0.5
	<i>Myricetin Glc</i>	0.052 ± 0.008	0.007	0.33 ± 0.07	0.0008	0.071 ± 0.009	0.002	0.044 ± 0.009	0.006
	<i>Quercetin glucuronide</i>	0.443 ± 0.006	0.007	1.39 ± 0.05	0.003	0.84 ± 0.04	0.003	0.68 ± 0.04	0.009
	<i>Quercetin</i>	n.d.	0.04	n.d.	0.02	n.d.	0.07	0.1 ± 0.05	0.03

Table S1. Cont.

	5		6		7		8		
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	
Flavan-3-ols	<i>Catechin</i>	6.3 ± 1	0.09	10.8 ± 0.2	0.3	5.2 ± 0.8	0.08	4.7 ± 0.5	0.06
	<i>Galloylated dimer</i>	n.d.	<0.002	n.d.	0.002	n.d.	<0.002	n.d.	<0.002
	<i>Trimer-1 (1 isomer)</i>	0.17 ± 0.03	<0.007	0.46 ± 0.06	<0.007	0.14 ± 0.04	<0.007	0.106 ± 0.007	<0.007
	<i>Trimers-2 (several isomers)</i>	0.07 ± 0.02	0.002	0.64 ± 0.04	0.06	0.07 ± 0.002	<0.002	0.024 ± 0.01	0.04
	<i>(epi)cat-ethyl-(epi)cat-1 (1 isomer)</i>	n.d.	0.2	n.d.	< 0.08	n.d.	<0.08	n.d.	<0.08
	<i>(epi)cat-ethyl-(epi)cat-2 (2 isomers)</i>	n.d.	0.003	n.d.	<0.0007	n.d.	<0.0007	n.d.	0.005
	<i>Epicatechin</i>	2.6 ± 0.2	1	6.3 ± 0.7	4	2.8 ± 1	0.7	3 ± 2	1
	<i>Dimer B2</i>	1.12 ± 0.03	0.04	5.04 ± 0.02	0.04	0.8 ± 0.05	0.06	1.22 ± 0.03	0.03
	<i>Dimer B1</i>	6.05 ± 0.05	0.04	12.6 ± 0.2	0.04	9.5 ± 0.2	0.04	5.9 ± 0.3	0.03
	<i>Dimer B3</i>	0.41 ± 0.02	0.02	1.59 ± 0.04	0.8	0.2 ± 0.02	0.04	0.29 ± 0.03	0.04
<i>Dimer B4</i>	0.4 ± 0.2	0.08	1.5 ± 0.4	0.7	0.05 ± 0.03	0.4	0.12 ± 0.08	0.2	
Dihydroflavonols	<i>Astilbin</i>	2.89 ± 0.04	0.03	0.2 ± 0.05	0.008	0.98 ± 0.02	0.002	0.1 ± 0.03	0.002
	<i>Taxifolin</i>	0.98 ± 0.03	0.3	0.18 ± 0.08	0.05	0.41 ± 0.05	0.3	0.19 ± 0.02	0.2
Anthocyanins	<i>Malvidin 3,5-diGlc</i>	0.23 ± 0.03	0.6	0.14 ± 0.03	2	0.053 ± 0.004	0.1	0.047 ± 0.008	0.6
	<i>Delphinidin 3,5-diGlc</i>	0.04 ± 0.02	0.02	0.063 ± 0.014	0.02	n.d.	0.02	0.06 ± 0.02	0.02
	<i>Cyanidin 3,5-diGlc</i>	n.d.	0.02	0.0191 ± 0.0009	0.02	n.d.	0.02	0.0226 ± 0.0005	0.02
	<i>Petunidin 3,5-diGlc</i>	n.d.	0.02	0.01 ± 0.02	0.03	n.d.	0.02	0.01 ± 0.02	0.05
	<i>Peonidin 3,5-diGlc</i>	0.112 ± 0.006	0.4	0.05 ± 0.02	0.2	0.028 ± 0.005	0.04	0.032 ± 0.002	0.2
	<i>Malvidin 3-O-Glc</i>	13.09 ± 0.1	0.05	17.3 ± 0.2	0.07	4.49 ± 0.1	0.02	11.6 ± 0.2	0.04
	<i>Delphinidin 3-O-Glc</i>	0.09 ± 0.006	0.02	0.47 ± 0.04	0.03	0.075 ± 0.003	0.002	0.432 ± 0.008	0.03
	<i>Cyanidin 3-O-Glc</i>	0.022 ± 0.001	0.002	0.052 ± 0.001	0.002	0.015 ± 0.002	0.005	0.06 ± 0.002	0.003
	<i>Petunidin 3-O-Glc</i>	0.42 ± 0.02	0.007	1.4 ± 0.2	0.02	0.28 ± 0.008	0.004	1.24 ± 0.03	0.02
	<i>Peonidin 3-O-Glc</i>	1.34 ± 0.02	0.04	0.967 ± 0.008	0.02	0.544 ± 0.004	0.008	1.28 ± 0.02	0.03
	<i>Delphinidin 3-O-acetyl-Glc</i>	0.01 ± 0.002	0.003	0.387 ± 0.004	0.004	0.0167 ± 0.0004	0.002	0.141 ± 0.003	0.0005
	<i>Cyanidin 3-O-acetyl-Glc</i>	0.0046 ± 0.0003	0.002	0.143 ± 0.003	0.004	0.0158 ± 0.0002	0.001	0.0771 ± 0.0002	0.002
	<i>Petunidin 3-O-acetyl-Glc</i>	0.0184 ± 0.0007	0.0006	0.593 ± 0.002	0.002	0.045 ± 0.002	0.003	0.245 ± 0.004	0.004
<i>Peonidin 3-O-acetyl-Glc</i>	0.158 ± 0.003	0.001	1.71 ± 0.03	0.006	0.3497 ± 0.0007	0.002	0.911 ± 0.006	0.003	

Table S1. Cont.

	5		6		7		8	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Malvidin 3-O-acetyl-Glc</i>	0.55 ± 0.02	0.003	11.509 ± 0.101	0.04	1.48 ± 0.02	0.004	3.259 ± 0.005	0.01
<i>Delphinidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.01 ± 0.02	0.001	0.12 ± 0.04	0.0009	0.03 ± 0.02	0.0006	0.04 ± 0.02	0.02
<i>Cyanidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.011 ± 0.006	0.0006	0.08 ± 0.02	0.003	0.022 ± 0.007	0.002	0.046 ± 0.005	0.0005
<i>Petunidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.033 ± 0.004	0.0004	0.16 ± 0.03	0.007	0.0568 ± 0.0007	0.002	0.1 ± 0.02	0.005
<i>Peonidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.21 ± 0.06	0.002	0.5 ± 0.2	0.006	0.214 ± 0.003	0.0009	0.34 ± 0.08	0.002
<i>Malvidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.81 ± 0.02	0.002	2.5 ± 0.04	0.03	0.93 ± 0.02	0.002	1.15 ± 0.02	0.004
<i>Delphinidin 3-O-caffeoyl-Glc</i>	n.d.	0.003	n.d.	0.002	n.d.	0.004	n.d.	0.003
<i>Cyanidin 3-O-caffeoyl-Glc</i>	n.d.	0.0004	0.0006 ± 0.0002	0.002	n.d.	0.0008	n.d.	0.0008
<i>Petunidin 3-O-caffeoyl-Glc</i>	n.d.	0.0007	n.d.	0.003	n.d.	0.002	n.d.	0.002
<i>Peonidin 3-O-caffeoyl-Glc</i>	0.007 ± 0.007	0.004	0.01 ± 0.02	0.002	0.005 ± 0.005	0.0007	0.014 ± 0.008	0.0008
<i>Malvidin 3-O-caffeoyl-Glc</i>	0.011 ± 0.006	0.0005	0.03 ± 0.02	0.02	0.026 ± 0.005	0.0007	0.025 ± 0.009	0.0008
<i>(epi)cat-ethyl-peonidin 3-O-Glc-1</i>	n.d.	0.002	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>(epi)cat-ethyl-peonidin 3-O-Glc-2</i>	n.d.	0.002	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>(epi)cat-ethyl-peonidin 3-O-Glc-3</i>	n.d.	0.002	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>(epi)cat-ethyl-peonidin 3-O-Glc-4</i>	n.d.	0.002	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>(epi)cat-ethyl-malvidin 3-O-Glc-1</i>	n.d.	0.002	0.0003 ± 0.0006	0.002	0.0001 ± 0.0002	0.002	0.0002 ± 0.0003	0.004
<i>(epi)cat-ethyl-malvidin 3-O-Glc-2</i>	n.d.	0.002	0.013 ± 0.002	0.002	0.001 ± 0.002	0.002	n.d.	0.004
<i>(epi)cat-ethyl-malvidin 3-O-Glc-3 and 4</i>	n.d.	0.002	0.02 ± 0.006	0.002	0.001 ± 0.003	0.002	0.004 ± 0.007	0.004
<i>(epi)cat-ethyl-malvidin 3-O-coumaroyl-Glc (2 co-eluted isomers)</i>	0.0005 ± 0.001	0.0005	0.03 ± 0.02	0.0008	0.0004 ± 0.0008	0.007	0.001 ± 0.002	0.0006
<i>Delphinidin 3-O-Glc-(epi)cat</i>	n.d.	0.003	n.d.	0.003	n.d.	0.003	n.d.	0.005
<i>Cyanidin 3-O-Glc-(epi)cat</i>	n.d.	0.004	0.003 ± 0.003	0.02	0.0003 ± 0.0005	0.004	n.d.	0.003
<i>Petunidin 3-O-Glc-(epi)cat</i>	0.002 ± 0.003	0.03	0.015 ± 0.003	0.04	n.d.	0.03	0.004 ± 0.005	0.03

Table S1. Cont.

	5		6		7		8	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Peonidin 3-O-Glc-(epi)cat</i>	0.012 ± 0.009	0.003	0.02 ± 0.02	0.002	0.005 ± 0.003	0.002	0.009 ± 0.002	0.003
<i>Malvidin 3-O-Glc-(epi)cat (2 isomers)</i>	0.092 ± 0.004	0.005	0.279 ± 0.008	0.02	0.03 ± 0.004	0.003	0.077 ± 0.008	0.002
<i>Malvidin 3-O-coumaroyl-Glc-(epi)cat (2 isomers)</i>	0.0002 ± 0.0001	0.002	0.007 ± 0.003	0.03	0.001 ± 0.002	0.005	0.0011 ± 0.0005	0.002
<i>(epi)cat-delphinidin 3-O-Glc A-F bicyclic</i>	n.d.	0.004	0.004 ± 0.002	0.0007	n.d.	0.003	n.d.	0.004
<i>(epi)cat-cyanidin 3-O-Glc A-F bicyclic</i>	n.d.	0.002	n.d.	0.003	n.d.	0.004	n.d.	0.04
<i>(epi)cat-petunidin 3-O-Glc A-F bicyclic</i>	n.d.	0.002	n.d.	0.002	n.d.	0.003	n.d.	0.005
<i>(epi)cat-peonidin 3-O-Glc A-F bicyclic</i>	n.d.	0.004	0.001 ± 0.002	0.003	0.003 ± 0.006	0.007	n.d.	0.006
<i>(epi)cat-malvidin 3-O-Glc A-F bicyclic</i>	0.001 ± 0.002	0.004	0.017 ± 0.009	0.06	0.004 ± 0.007	0.003	0.003 ± 0.004	0.002
<i>Caftaric-peonidin 3-O-Glc (2 isomers)</i>	0.069 ± 0.01	0.002	0.011 ± 0.01	0.002	0.002 ± 0.002	0.0008	0.001 ± 0.001	0.003
<i>Caftaric-malvidin 3-O-Glc (2 isomers)</i>	0.16 ± 0.02	0.002	0.044 ± 0.006	0.08	0.021 ± 0.003	0.003	0.04 ± 0.02	0.002
<i>Coutaric-malvidin 3-O-Glc (2 isomers)</i>	n.d.	0.002	n.d.	0.002	n.d.	0.04	n.d.	0.03
<i>Pyranodelphinidin 3-O-Glc</i>	n.d.	0.004	0.001 ± 0.002	0.002	n.d.	0.004	0.001 ± 0.002	0.03
<i>Pyranocyanidin 3-O-Glc</i>	n.d.	0.02	n.d.	0.07	n.d.	0.02	n.d.	0.001
<i>Pyranopetunidin 3-O-Glc</i>	n.d.	0.002	n.d.	0.006	0.0002 ± 0.0004	0.0005	0.0002 ± 0.0003	0.0007
<i>Pyranopeonidin 3-O-Glc</i>	0.002 ± 0.002	0.003	0.004 ± 0.002	0.002	0.001 ± 0.002	0.004	0.004 ± 0.002	0.003
<i>Pyranomalvidin 3-O-Glc (vitisin B)</i>	0.01 ± 0.002	0.02	0.073 ± 0.006	0.007	0.004 ± 0.002	0.003	0.048 ± 0.004	0.009
<i>Carboxypyranodelphinidin 3-O-Glc</i>	n.d.	0.0008	0.016 ± 0.006	0.03	0.0001 ± 0.0001	0.009	0.012 ± 0.008	0.0008
<i>Carboxypyranocyanidin 3-O-Glc</i>	n.d.	0.005	0.003 ± 0.003	0.02	n.d.	0.02	0.003 ± 0.003	0.02
<i>Carboxypyranopetunidin 3-O-Glc</i>	0.0026 ± 0.0008	0.0008	0.008 ± 0.005	0.0007	n.d.	0.02	0.008 ± 0.005	0.03
<i>Carboxypyranopeonidin 3-O-Glc</i>	0.015 ± 0.004	0.002	0.017 ± 0.003	0.002	0.0015 ± 0.0008	0.0005	0.013 ± 0.0005	0.0003
<i>Carboxypyranomalvidin 3-O-Glc (vitisin A)</i>	0.131 ± 0.009	0.004	0.32 ± 0.03	0.005	0.032 ± 0.008	0.002	0.207 ± 0.007	0.005
<i>Pyranodelphinidin 3-O-acetyl-Glc</i>	n.d.	0.0003	0.0001 ± 0.0001	0.0004	n.d.	0.004	n.d.	0.002
<i>Pyranocyanidin 3-O-acetyl-Glc</i>	0.0002 ± 0.0004	0.0008	0.0004 ± 0.0004	0.002	n.d.	0.0006	0.0003 ± 0.0001	0.0007
<i>Pyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.0005	n.d.	0.0008	0.0001 ± 0.0001	0.0007	n.d.	0.0003
<i>Pyranopeonidin 3-O-acetyl-Glc</i>	n.d.	0.0006	n.d.	0.002	0.0001 ± 0.0002	0.002	n.d.	0.0008
<i>Pyranomalvidin 3-O-acetyl-Glc</i>	0.001 ± 0.002	0.0003	0.03 ± 0.002	0.0002	n.d.	0.002	0.003 ± 0.005	0.002

Table S1. Cont.

	5		6		7		8	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Carboxypyranodelphinidin 3-O-acetyl-Glc</i>	0 ± 0.0001	0.0008	0.001 ± 0.002	0.0007	n.d.	0.0008	n.d.	0.0007
<i>Carboxypyranocyanidin 3-O-acetyl-Glc</i>	0.0005 ± 0.0004	0.02	0.001 ± 0.0006	0.0006	0.0003 ± 0.0003	0.0006	0.0003 ± 0.0001	0.02
<i>Carboxypyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.0006	0.0036 ± 0.0006	0.0002	n.d.	0.0006	0.001 ± 0.002	0.0003
<i>Carboxypyranopeonidin 3-O-acetyl-Glc</i>	0.001 ± 0.002	0.004	0.03 ± 0.02	0.03	0.0009 ± 0.0009	0.008	0.01 ± 0.02	0.004
<i>Carboxypyranomalvidin 3-O-acetyl-Glc</i>	0.007 ± 0.003	0.0006	0.17 ± 0.03	0.002	0.002 ± 0.003	0.0009	0.04 ± 0.02	0.002
<i>Pyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.002	n.d.	0.0003	n.d.	0.0008	n.d.	0.0006
<i>Pyranopeonidin 3-O-coumaroyl-Glc</i>	n.d.	0.002	0.005 ± 0.004	0.0003	n.d.	0.002	0.001 ± 0.002	0.002
<i>Pyranomalvidin 3-O-coumaroyl-Glc</i>	n.d.	0.002	0.02 ± 0.02	0.002	n.d.	0.002	0.006 ± 0.005	0.0005
<i>Carboxypyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.0008	0.002 ± 0.002	0.001	n.d.	0.001	0.001 ± 0.002	0.002
<i>Carboxypyranopeonidin 3-O-coumaroyl-Glc</i>	0.004 ± 0.004	0.0007	0.012 ± 0.009	0.004	0.0005 ± 0.0006	0.0004	0.002 ± 0.003	0.0007
<i>Carboxypyranomalvidin 3-O-coumaroyl-Glc</i>	0.007 ± 0.006	0.003	0.05 ± 0.03	0.002	0.004 ± 0.004	0.0003	0.012 ± 0.006	0.007
<i>p-hydroxyphenylpyranopeonidin 3-O-Glc</i>	0.015 ± 0.01	0.04	0.0019 ± 0.0007	0.008	0.002 ± 0.003	0.0002	0.011 ± 0.006	0.02
<i>p-hydroxyphenylpyranomalvidin 3-O-Glc</i>	0.13 ± 0.02	0.0003	0.07 ± 0.03	0.0003	0.034 ± 0.013	0.0003	0.14 ± 0.04	0.0002
<i>p-hydroxyphenylpyranopeonidin 3-O-acetyl-Glc</i>	0.001 ± 0.001	0.0003	0.003 ± 0.002	0.0003	0.001 ± 0.002	0.0002	0.007 ± 0.004	0.0002
<i>p-hydroxyphenylpyranomalvidin 3-O-acetyl-Glc</i>	0.008 ± 0.004	0.0002	0.03 ± 0.007	0.0004	0.011 ± 0.005	0.0004	0.033 ± 0.009	0.0002
<i>p-hydroxyphenylpyranopeonidin 3-O-coumaroyl-Glc</i>	0.003 ± 0.002	0.0004	0.003 ± 0.001	0.0004	0.003 ± 0.003	0.0004	0.003 ± 0.002	0.0003
<i>p-hydroxyphenylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.03 ± 0.02	0.0003	0.016 ± 0.008	0.0002	0.015 ± 0.004	0.0002	0.021 ± 0.01	0.0003
<i>Catechylpyranopeonidin 3-O-Glc</i>	0.023 ± 0.008	0.0002	0.008 ± 0.005	0.004	0.008 ± 0.001	0.0003	0.03 ± 0.02	0.002
<i>Catechylpyranomalvidin 3-O-Glc (pinotin A)</i>	0.094 ± 0.021	0.0007	0.12 ± 0.02	0.0006	0.06 ± 0.005	0.0003	0.14 ± 0.03	0.0004
<i>Catechylpyranopetunidin 3-O-acetyl-Glc</i>	0.001 ± 0.003	0.0002	0.002 ± 0.002	0.0004	n.d.	0.0004	0.002 ± 0.003	0.0003

Anthocyanins

Table S1. Cont.

	5		6		7		8	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Catechylpyranopeonidin 3-O-acetyl-Glc</i>	0.001 ± 0.002	0.0002	0.006 ± 0.005	0.0003	0.002 ± 0.001	0.0002	0.006 ± 0.004	0.0003
<i>Catechylpyranomalvidin 3-O-acetyl-Glc</i>	0.004 ± 0.004	0.0005	0.083 ± 0.008	0.02	0.013 ± 0.005	0.0003	0.0366 ± 0.0004	0.0003
<i>Catechylpyranopetunidin 3-O-coumaroyl-Glc</i>	0 ± 0.001	0.0002	0 ± 0.001	0.0002	0.0002 ± 0.0004	0.0002	0.002 ± 0.004	0.002
<i>Catechylpyranopeonidin 3-O-coumaroyl-Glc</i>	0.004 ± 0.003	0.0002	0.002 ± 0.003	0.0005	0.0024 ± 0.0006	0.0004	0.009 ± 0.007	0.0002
<i>Catechylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.012 ± 0.006	0.002	0.028 ± 0.005	0.0003	0.034 ± 0.006	0.0002	0.04 ± 0.02	0.005
<i>Guaiacylpyranomalvidin 3-O-Glc</i>	0.073 ± 0.008	0.0005	0.022 ± 0.003	0.006	0.02 ± 0.005	0.0005	0.06 ± 0.02	0.0007
<i>Guaiacylpyranomalvidin 3-O-acetyl-Glc</i>	0.003 ± 0.002	0.0005	0.007 ± 0.003	0.0004	0.005 ± 0.003	0.0004	0.017 ± 0.006	0.0003
<i>Guaiacylpyranomalvidin 3-O-coumaroyl-Glc</i>	0.008 ± 0.006	0.0004	0.003 ± 0.003	0.0004	0.007 ± 0.006	0.0004	0.005 ± 0.005	0.0004
Anthocyanins								
<i>Syringylpyranomalvidin 3-O-Glc</i>	0.0005 ± 0.0008	0.0008	n.d.	0.008	n.d.	0.0009	0.001 ± 0.001	0.002
<i>Petunidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.004	n.d.	0.002	n.d.	0.003	n.d.	0.003
<i>Peonidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.003	0.006 ± 0.005	0.004	n.d.	0.003	n.d.	0.003
<i>Malvidin 3-O-acetyl-Glc-(epi)cat</i>	n.d.	0.002	0.04 ± 0.02	0.002	n.d.	0.0007	0.005 ± 0.005	0.0005
<i>Pyranopeonidin 3-O-Glc-(epi)cat</i>	0.0012 ± 0.0004	0.0006	0.0011 ± 0.0001	0.0005	0.0003 ± 0.0001	0.0008	n.d.	0.002
<i>Pyranomalvidin 3-O-Glc-(epi)cat</i>	0.003 ± 0.003	0.003	0.003 ± 0.003	0.0002	n.d.	0.0002	n.d.	0.0003
<i>Pyranomalvidin 3-O-coumaroyl-Glc-(epi)cat</i>	0.004 ± 0.005	0.05	0 ± 0.001	0.0009	n.d.	0.002	n.d.	0.009
<i>Unknown "551"</i>	0.001 ± 0.002	0.004	0.001 ± 0.002	0.002	0.0004 ± 0.0008	0.0004	0.004 ± 0.007	0.0006
<i>Unknown "581"</i>	0.03 ± 0.02	0.002	0.04 ± 0.03	0.002	0.009 ± 0.008	0.002	0.09 ± 0.04	0.002
<i>Unknown "1095"</i>	n.d.	0.02	n.d.	0.01	n.d.	0.03	n.d.	0.03
<i>Unknown "1099"</i>	n.d.	0.01	0.002 ± 0.0007	< 0.002	0.0004 ± 0.0007	< 0.002	0.0008 ± 0.0008	< 0.002
<i>Tyrosine</i>	10.4 ± 0.2	0.6	4.37 ± 0.07	0.2	5.91 ± 0.05	0.4	5.74 ± 0.06	0.3
<i>Tyrosol</i>	7.85 ± 0.09	6	18.9 ± 0.5	0.9	15.01 ± 0.09	2	15.2 ± 0.3	2
Others (aminoacids and alcohols)								
<i>Hydroxytyrosol</i>	1.1 ± 0.08	0.04	0.44 ± 0.05	0.03	0.07 ± 0.02	0.04	0.261 ± 0.005	0.03
<i>Tryptophol</i>	0.4 ± 0.2	0.3	1.2 ± 0.5	0.2	0.3 ± 0.2	0.3	0.04 ± 0.03	0.2
<i>Tryptophan</i>	1.4 ± 0.3	0	0.65 ± 0.1	0	0.4 ± 0.2	0	0.3 ± 0.2	0

Table S1. Cont.

		9		10		11		12	
		Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
Benzoic acids and derivatives	<i>Gallic acid</i>	5.3 ± 0.2	0.03	3.43 ± 0.09	0.2	21.1 ± 0.5	0.1	1.03 ± 0.02	0.07
	<i>Protocatechuic acid</i>	3 ± 0.3	0.2	1.39 ± 0.03	0.07	0.71 ± 0.06	0.02	0.641 ± 0.003	0.03
	<i>Syringic acid</i>	1.6 ± 0.2	0.06	1.24 ± 0.04	0.03	0.29 ± 0.02	0.04	0.407 ± 0.006	0.05
	<i>Vanillic acid</i>	1.41 ± 0.07	0.2	1.1 ± 0.2	0.2	0.49 ± 0.02	0.2	0.4 ± 0.02	0.08
	<i>Ethyl gallate</i>	0.7 ± 0.3	0.02	0.5 ± 0.3	0.007	4 ± 0.4	0.008	0.14 ± 0.05	0.006
	<i>Ethyl protocatechuate</i>	0.5 ± 0.2	<0.02	0.2 ± 0.2	<0.02	0.06 ± 0.04	<0.02	0.07 ± 0.03	<0.02
Hydroxycinnamic acids and derivatives	<i>Caffeic acid</i>	2.5 ± 0.3	0.2	1.1 ± 0.1	0.03	2.1 ± 0.4	0.2	3.1 ± 0.3	0.08
	<i>p-coumaric acid</i>	2.8 ± 0.5	0.4	1 ± 0.2	0.2	0.52 ± 0.08	0.6	1.1 ± 0.3	0.3
	<i>Ferulic acid</i>	0.48 ± 0.07	0.04	0.3 ± 0.2	0.5	0.2 ± 0.2	0.04	0.2 ± 0.2	0.04
	<i>Caftaric acid (cis- and trans- isomers)</i>	6.4 ± 0.3	0.4	19.4 ± 0.6	0.3	16.4 ± 0.7	0.2	30.1 ± 0.5	0.3
	<i>Coutaric acid (cis- and trans- isomers)</i>	2.64 ± 0.04	0.04	14.4 ± 0.8	0.02	5.5 ± 0.5	0.09	7.1 ± 0.4	0.03
	<i>Fertaric acid</i>	3.49 ± 0.09	0.007	6.7 ± 0.2	0.006	4 ± 0.4	0.02	6.39 ± 0.07	0.009
	<i>GRP (cis- and trans- isomers)</i>	1.9 ± 0.5	0.3	23 ± 2	0.4	12 ± 2	0.05	20 ± 2	0.08
	<i>Ethyl caffeate</i>	0.67 ± 0.03	0.03	0.18 ± 0.03	0.007	0.68 ± 0.06	0.08	0.97 ± 0.09	0.07
	<i>Ethyl coumarate</i>	0.6 ± 0.2	0.03	0.24 ± 0.06	0.03	0.09 ± 0.03	0.02	0.18 ± 0.02	0.006
<i>viniferin-1</i>	<i>trans-resveratrol</i>	0.37 ± 0.05	0.05	0.228 ± 0.007	0.03	0.14 ± 0.03	0.02	0.112 ± 0.008	0.03
	<i>cis-resveratrol</i>	0.68 ± 0.03	0.05	0.17 ± 0.02	0.05	0.23 ± 0.02	0.02	0.12 ± 0.03	0.03
		0.06 ± 0.03	0.6	0.0233 ± 0.0007	0.09	0.1 ± 0.04	0.2	0.1 ± 0.04	0.3
	<i>viniferin-2</i>	0.03 ± 0.02	0.05	0.02 ± 0.002	0.03	n.d.	0.02	0.023 ± 0.002	0.03
	<i>trans-piceid</i>	0.56 ± 0.08	0.7	0.33 ± 0.04	0.4	0.21 ± 0.03	0.8	0.19 ± 0.05	0.8
	<i>cis-piceid</i>	1.84 ± 0.1	0.2	1.4 ± 0.2	0.2	0.62 ± 0.06	0.05	0.52 ± 0.02	0.05
Flavonols	<i>Quercetin Glc</i>	0.01 ± 0.005	0.04	n.d.	0.02	0.008 ± 0.005	0.0009	n.d.	0.02
	<i>Myricetin glucuronide</i>	0.06 ± 0.02	0.3	0.15 ± 0.05	0.9	0.009 ± 0.004	0.03	0.001 ± 0.002	0.03
	<i>Myricetin Glc</i>	0.012 ± 0.007	0.005	0.08 ± 0.04	0.0008	0.003 ± 0.003	0.002	0.003 ± 0.002	0.006
	<i>Quercetin glucuronide</i>	0.008 ± 0.005	0.006	0.554 ± 0.009	0.002	0.1 ± 0.02	0.006	0.0055 ± 0.0006	0.0007
	<i>Quercetin</i>	n.d.	0.02	n.d.	0.2	n.d.	0.04	n.d.	0.03

Table S1. Cont.

		9		10		11		12	
		Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
Flavan-3-ols	<i>Catechin</i>	8.4 ± 0.8	0.2	4.4 ± 0.3	0.08	5.8 ± 0.5	0.2	2.59 ± 0.05	0.04
	<i>Galloylated dimer</i>	n.d.	<0.002	n.d.	<0.002	n.d.	<0.002	n.d.	<0.002
	<i>Trimer-1 (1 isomer)</i>	0.2 ± 0.07	<0.007	0.08 ± 0.02	<0.007	0.002 ± 0.003	<0.007	0.002 ± 0.004	<0.007
	<i>Trimers-2 (several isomers)</i>	0.24 ± 0.04	0.04	0.08 ± 0.02	0.07	0.1 ± 0.03	0.05	0.0004 ± 0.0007	<0.002
	<i>(epi)cat-ethyl-(epi)cat-1 (1 isomer)</i>	n.d.	<0.08	n.d.	<0.08	n.d.	0.08	n.d.	<0.08
	<i>(epi)cat-ethyl-(epi)cat-2 (2 isomers)</i>	n.d.	0.002	n.d.	0.0007	n.d.	<0.0007	n.d.	0.02
	<i>Epicatechin</i>	7 ± 3	2	1.04 ± 0.05	0.6	3 ± 2	0.6	0.6 ± 0.2	0.2
	<i>Dimer B2</i>	2.37 ± 0.35	0.06	0.61 ± 0.04	0.02	0.3 ± 0.02	0.07	0.11 ± 0.03	0.03
	<i>Dimer B1</i>	9.22 ± 0.09	0.05	5.52 ± 0.07	0.02	0.99 ± 0.02	0.08	1.84 ± 0.05	0.02
	<i>Dimer B3</i>	1.23 ± 0.09	0.3	0.25 ± 0.03	0.2	0.16 ± 0.02	0.03	0.06 ± 0.02	0.03
<i>Dimer B4</i>	1.8 ± 0.3	0.4	0.15 ± 0.1	0.4	0.106 ± 0.009	0.08	0.02 ± 0.02	0.06	
Dihydroflavonols	<i>Astilbin</i>	0.31 ± 0.04	0.002	0.08 ± 0.03	0.006	0.61 ± 0.03	0.02	0.3 ± 0.02	0.003
	<i>Taxifolin</i>	0.5 ± 0.2	0.3	0.12 ± 0.02	0.4	0.32 ± 0.02	0.1	0.23 ± 0.02	0.2
Anthocyanins	<i>Malvidin 3,5-diGlc</i>	0.08 ± 0.02	2	0.08 ± 0.02	0.9	n.d.	0.03	n.d.	0.1
	<i>Delphinidin 3,5-diGlc</i>	n.d.	0.02	0.029 ± 0.003	0.02	n.d.	0.02	n.d.	0.02
	<i>Cyanidin 3,5-diGlc</i>	0.021 ± 0.004	0.04	0.0175 ± 0.0004	0.02	n.d.	0.02	n.d.	0.02
	<i>Petunidin 3,5-diGlc</i>	n.d.	0.02	n.d.	0.03	n.d.	0.02	n.d.	0.02
	<i>Peonidin 3,5-diGlc</i>	0.05 ± 0.02	0.3	0.043 ± 0.006	0.2	n.d.	0.02	n.d.	0.04
	<i>Malvidin 3-O-Glc</i>	13.3 ± 0.3	0.06	11.8 ± 0.2	0.05	0.079 ± 0.007	0.005	0.731 ± 0.007	0.02
	<i>Delphinidin 3-O-Glc</i>	0.19 ± 0.007	0.003	0.422 ± 0.009	0.006	0.0018 ± 0.0009	0.004	0.0014 ± 0.0007	0.002
	<i>Cyanidin 3-O-Glc</i>	0.0395 ± 0.0009	0.003	0.031 ± 0.004	0.003	0.0004 ± 0.0001	0.0008	0.00144 ± 0.00007	0.002
	<i>Petunidin 3-O-Glc</i>	0.78 ± 0.1	0.03	1.61 ± 0.07	0.05	0.0022 ± 0.0008	0.01	0.013 ± 0.003	0.0006
	<i>Peonidin 3-O-Glc</i>	1.04 ± 0.02	0.02	0.43 ± 0.02	0.03	0.015 ± 0.002	0.003	0.074 ± 0.01	0.004
	<i>Delphinidin 3-O-acetyl-Glc</i>	0.094 ± 0.003	0.004	0.085 ± 0.006	0.001	0.0004 ± 0.0005	0.0008	0.0004 ± 0.0004	0.002
	<i>Cyanidin 3-O-acetyl-Glc</i>	0.0731 ± 0.0006	0.003	0.037 ± 0.002	0.0009	n.d.	0.002	0.0014 ± 0.0003	0.0006
	<i>Petunidin 3-O-acetyl-Glc</i>	0.209 ± 0.005	0.002	0.1281 ± 0.0005	0.003	0.0002 ± 0.0005	0.002	0.0028 ± 0.0004	0.0008
<i>Peonidin 3-O-acetyl-Glc</i>	1.23 ± 0.03	0.002	0.222 ± 0.008	0.0009	0 ± 0.001	0.0003	0.059 ± 0.003	0.0007	

Table S1. Cont.

	9		10		11		12	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Malvidin 3-O-acetyl-Glc</i>	6 ± 0.2	0.02	1.29 ± 0.03	0.01	0.0012 ± 0.0005	0.002	0.169 ± 0.004	0.003
<i>Delphinidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.021 ± 0.008	0.008	0.14 ± 0.03	0.009	0.001 ± 0.003	0.0006	0.0002 ± 0.0004	0.002
<i>Cyanidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.029 ± 0.008	0.003	0.08 ± 0.02	0.004	n.d.	0.0004	0.001 ± 0.002	0.0004
<i>Petunidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.051 ± 0.003	0.0006	0.21 ± 0.02	0.009	0.001 ± 0.002	0.0002	0.0021 ± 0.001	0.0003
<i>Peonidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	0.23 ± 0.05	0.006	0.32 ± 0.02	0.005	0.0005 ± 0.0002	0.0003	0.025 ± 0.005	0.002
<i>Malvidin 3-O-coumaroyl-Glc</i> (<i>cis-</i> and <i>trans-</i> isomers)	1.29 ± 0.02	0.04	1.96 ± 0.05	0.02	0.003 ± 0.002	0.0006	0.079 ± 0.002	0.002
<i>Delphinidin 3-O-caffeoyl-Glc</i>	n.d.	0.003	n.d.	0.003	n.d.	0.003	n.d.	0.003
<i>Cyanidin 3-O-caffeoyl-Glc</i>	0.003 ± 0.005	0.001	n.d.	0.0008	n.d.	0.003	n.d.	0.0007
<i>Petunidin 3-O-caffeoyl-Glc</i>	n.d.	0.002	n.d.	0.002	n.d.	0.0006	n.d.	0.002
<i>Peonidin 3-O-caffeoyl-Glc</i>	0.04 ± 0.03	0.006	0.018 ± 0.01	0.0007	n.d.	0.003	n.d.	0.002
<i>Malvidin 3-O-caffeoyl-Glc</i>	0.09 ± 0.04	0.05	0.075 ± 0.009	0.002	n.d.	0.0009	0.0003 ± 0.0006	0.002
<i>(epi)cat-ethyl-peonidin 3-O-Glc-1</i>	n.d.	0.004	n.d.	0.0008	n.d.	0.003	n.d.	0.005
<i>(epi)cat-ethyl-peonidin 3-O-Glc-2</i>	n.d.	0.004	n.d.	0.0008	n.d.	0.003	n.d.	0.005
<i>(epi)cat-ethyl-peonidin 3-O-Glc-3</i>	n.d.	0.004	n.d.	0.0008	0.002 ± 0.003	0.003	n.d.	0.005
<i>(epi)cat-ethyl-peonidin 3-O-Glc-4</i>	n.d.	0.004	n.d.	0.0008	n.d.	0.003	n.d.	0.005
<i>(epi)cat-ethyl-malvidin 3-O-Glc-1</i>	n.d.	0.002	0.00005 ± 0.00009	0.002	0.001 ± 0.002	0.002	n.d.	0.004
<i>(epi)cat-ethyl-malvidin 3-O-Glc-2</i>	n.d.	0.002	0.014 ± 0.006	0.002	0.012 ± 0.009	0.002	n.d.	0.004
<i>(epi)cat-ethyl-malvidin 3-O-Glc-3 and 4</i>	0.01 ± 0.02	0.002	0.051 ± 0.008	0.002	0.03 ± 0.03	0.002	n.d.	0.004
<i>(epi)cat-ethyl-malvidin 3-O-coumaroyl-Glc</i> (2 <i>co-eluted isomers</i>)	0.003 ± 0.005	0.005	0.02 ± 0.01	0.0005	0.001 ± 0.002	0.02	n.d.	0.0006
<i>Delphinidin 3-O-Glc-(epi)cat</i>	n.d.	0.002	n.d.	0.002	n.d.	0.004	n.d.	0.004

Table S1. Cont.

	9		10		11		12	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Cyanidin 3-O-Glc-(epi)cat</i>	0.001 ± 0.002	0.02	0.02 ± 0.02	0.0008	n.d.	0.002	n.d.	0.0009
<i>Petunidin 3-O-Glc-(epi)cat</i>	0.01 ± 0.004	0.07	0.009 ± 0.01	0.06	n.d.	0.0007	n.d.	0.004
<i>Peonidin 3-O-Glc-(epi)cat</i>	0.04 ± 0.02	0.002	0.03 ± 0.02	0.002	n.d.	0.002	0.003 ± 0.005	0.006
<i>Malvidin 3-O-Glc-(epi)cat (2 isomers)</i>	0.34 ± 0.04	0.02	0.14 ± 0.02	0.02	0.0007 ± 0.0002	0.003	0.004 ± 0.003	0.002
<i>Malvidin 3-O-coumaroyl-Glc-(epi)cat (2 isomers)</i>	0.001 ± 0.002	0.006	0.0013 ± 0.0006	0.006	n.d.	0.0006	n.d.	0.003
<i>(epi)cat-delphinidin 3-O-Glc A-F bicyclic</i>	n.d.	0.004	n.d.	0.005	n.d.	0.003	n.d.	0.004
<i>(epi)cat-cyanidin 3-O-Glc A-F bicyclic</i>	n.d.	0.008	n.d.	0.002	n.d.	0.004	n.d.	0.004
<i>(epi)cat-petunidin 3-O-Glc A-F bicyclic</i>	0.001 ± 0.002	0.002	0.002 ± 0.002	0.002	n.d.	0.003	n.d.	0.003
<i>(epi)cat-peonidin 3-O-Glc A-F bicyclic</i>	0.003 ± 0.004	0.002	n.d.	0.003	n.d.	0.005	n.d.	0.003
<i>(epi)cat-malvidin 3-O-Glc A-F bicyclic</i>	0.005 ± 0.005	0.05	0.01 ± 0.02	0.03	0.001 ± 0.002	0.03	n.d.	0.003
<i>Caftaric-peonidin 3-O-Glc (2 isomers)</i>	0.008 ± 0.006	0.003	n.d.	0.02	n.d.	0.001	0.001 ± 0.003	0.002
<i>Caftaric-malvidin 3-O-Glc (2 isomers)</i>	0.019 ± 0.007	0.003	0.012 ± 0.004	0.002	n.d.	0.002	0.007 ± 0.003	0.002
<i>Coutaric-malvidin 3-O-Glc (2 isomers)</i>	n.d.	0.003	n.d.	0.003	n.d.	0.002	n.d.	0.004
<i>Pyranodelphinidin 3-O-Glc</i>	n.d.	0.03	0.002 ± 0.003	0.003	0.0003 ± 0.0006	0.004	n.d.	0.03
<i>Pyranocyanidin 3-O-Glc</i>	n.d.	0.007	n.d.	0.04	n.d.	0.04	n.d.	0.01
<i>Pyranopetunidin 3-O-Glc</i>	0.002 ± 0.002	0.0006	0.006 ± 0.002	0.01	0.0003 ± 0.0006	0.01	n.d.	0.003
<i>Pyranopeonidin 3-O-Glc</i>	0.003 ± 0.002	0.006	0.006 ± 0.002	0.003	0.0061 ± 0.0006	0.002	0.0009 ± 0.0002	0.002
<i>Pyranomalvidin 3-O-Glc (vitisin B)</i>	0.0384 ± 0.001	0.02	0.181 ± 0.006	0.02	0.048 ± 0.004	0.004	0.005 ± 0.002	0.002
<i>Carboxypyranodelphinidin 3-O-Glc</i>	0.001 ± 0.002	0.02	0.011 ± 0.007	0.03	0.001 ± 0.001	0.02	0.001 ± 0.002	0.02
<i>Carboxypyranocyanidin 3-O-Glc</i>	0.002 ± 0.004	0.02	0.003 ± 0.002	0.02	0.001 ± 0.002	0.0005	n.d.	0.003
<i>Carboxypyranopetunidin 3-O-Glc</i>	0.002 ± 0.002	0.02	0.004 ± 0.004	0.02	0.002 ± 0.002	0.004	0.002 ± 0.004	0.002
<i>Carboxypyranopeonidin 3-O-Glc</i>	0.013 ± 0.004	0.002	0.0046 ± 0.0005	0.0003	0.003 ± 0.0002	0.0005	0.0017 ± 0.0007	0.0004
<i>Carboxypyranomalvidin 3-O-Glc (vitisin A)</i>	0.2 ± 0.02	0.003	0.17 ± 0.02	0.005	0.06 ± 0.02	0.002	0.012 ± 0.004	0.0003
<i>Pyranodelphinidin 3-O-acetyl-Glc</i>	n.d.	0.0005	n.d.	0.0003	n.d.	0.005	n.d.	0.0002
<i>Pyranocyanidin 3-O-acetyl-Glc</i>	0.0002 ± 0.0005	0.0009	n.d.	0.0009	n.d.	0.0006	n.d.	0.0005

Table S1. Cont.

	9		10		11		12	
	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
<i>Pyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.0005	n.d.	0.0005	n.d.	0.0007	n.d.	0.003
<i>Pyranopeonidin 3-O-acetyl-Glc</i>	0.002 ± 0.004	0.0008	0.0003 ± 0.0005	0.003	n.d.	0.0006	n.d.	0.0005
<i>Pyranomalvidin 3-O-acetyl-Glc</i>	0.009 ± 0.005	0.0008	0.01 ± 0.006	0.0004	0.0002 ± 0.0003	0.0009	n.d.	0.0007
<i>Carboxypyranodelphinidin 3-O-acetyl-Glc</i>	n.d.	0.02	0.0003 ± 0.0005	0.0007	n.d.	0.002	n.d.	0.0006
<i>Carboxypyranocyanidin 3-O-acetyl-Glc</i>	0.0004 ± 0.0003	0.0004	0.0008 ± 0.0008	0.0009	n.d.	0.0005	n.d.	0.002
<i>Carboxypyranopetunidin 3-O-acetyl-Glc</i>	n.d.	0.0004	n.d.	0.008	n.d.	0.0007	n.d.	0.0003
<i>Carboxypyranopeonidin 3-O-acetyl-Glc</i>	0.005 ± 0.005	0.02	n.d.	0.008	n.d.	0.002	0.001 ± 0.002	0.003
<i>Carboxypyranomalvidin 3-O-acetyl-Glc</i>	0.08 ± 0.03	0.02	0.007 ± 0.01	0.001	0.0005 ± 0.0005	0.002	0.0004 ± 0.0008	0.0006
<i>Pyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.003	n.d.	0.002	n.d.	0.0004	n.d.	0.0008
<i>Pyranopeonidin 3-O-coumaroyl-Glc</i>	0.001 ± 0.001	0.0005	0.005 ± 0.005	0.0005	n.d.	0.003	n.d.	0.0007
<i>Pyranomalvidin 3-O-coumaroyl-Glc</i>	0.003 ± 0.003	0.0007	0.041 ± 0.007	0.002	n.d.	0.0008	0.002 ± 0.003	0.0007
<i>Carboxypyranopetunidin 3-O-coumaroyl-Glc</i>	n.d.	0.0007	n.d.	0.002	n.d.	0.0007	n.d.	0.004
<i>Carboxypyranopeonidin 3-O-coumaroyl-Glc</i>	0.002 ± 0.004	0.001	0.003 ± 0.004	0.0005	n.d.	0.001	n.d.	0.0005
<i>Carboxypyranomalvidin 3-O-coumaroyl-Glc</i>	0.009 ± 0.008	0.005	0.012 ± 0.004	0.002	0.004 ± 0.004	0.0004	0.003 ± 0.005	0.003
<i>p-hydroxyphenylpyranopeonidin 3-O-Glc</i>	0.018 ± 0.002	0.008	0.006 ± 0.003	0.002	0.021 ± 0.004	0.0005	0.015 ± 0.002	0.0003
<i>p-hydroxyphenylpyranomalvidin 3-O-Glc</i>	0.26 ± 0.03	0.004	0.25 ± 0.03	0.0003	0.12 ± 0.03	0.0003	0.11 ± 0.04	0.0002
<i>p-hydroxyphenylpyranopeonidin 3-O-acetyl-Glc</i>	0.012 ± 0.005	0.0003	0.002 ± 0.002	0.0002	n.d.	0.0004	0.005 ± 0.004	0.0003
<i>p-hydroxyphenylpyranomalvidin 3-O-acetyl-Glc</i>	0.08 ± 0.02	0.0002	0.01 ± 0.003	0.002	0.0005 ± 0.0009	0.0002	0.028 ± 0.007	0.0003
<i>p-hydroxyphenylpyranopeonidin 3-O-coumaroyl-Glc</i>	0.002 ± 0.001	0.0003	0.01 ± 0.02	0.008	n.d.	0.0003	0.013 ± 0.003	0.0006

Table S1. *Cont.*

		9		10		11		12	
		Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)	Conc. (mg·L ⁻¹)	LOQ (mg·L ⁻¹)
Anthocyanins	<i>Unknown "551"</i>	0.0005 ± 0.0003	0.003	0.0004 ± 0.0003	0.04	0.002 ± 0.003	0.0007	n.d.	0.002
	<i>Unknown "581"</i>	0.024 ± 0.006	0.003	0.072 ± 0.007	0.003	0.006 ± 0.004	0.02	0.007 ± 0.007	0.004
	<i>Unknown "1095"</i>	n.d.	0.02	n.d.	0.02	0.011 ± 0.006	0.02	n.d.	0.02
	<i>Unknown "1099"</i>	0.00135 ± 0.00003	0.002	0.001 ± 0.002	0.03	n.d.	<0.002	n.d.	<0.002
Others (aminoacids and alcohols)	<i>Tyrosine</i>	9 ± 0.08	0.6	6.59 ± 0.07	0.3	14 ± 0.3	0.9	10.92 ± 0.07	1
	<i>Tyrosol</i>	16.07 ± 0.34	4	8 ± 0.2	3	7.3 ± 0.2	0.6	7.1 ± 0.2	0.7
	<i>Hydroxytyrosol</i>	0.95 ± 0.08	0.03	0.2 ± 0.03	0.05	0.82 ± 0.08	0.04	0.1248 ± 0.0005	0.04
	<i>Tryptophol</i>	1.39 ± 0.28	0.4	4.4 ± 0.4	0.3	n.d.	0.4	0.4 ± 0.3	0.34
	<i>Tryptophan</i>	1.65 ± 0.38	0	2.03 ± 0.02	0	n.d.	0	1 ± 0.2	0

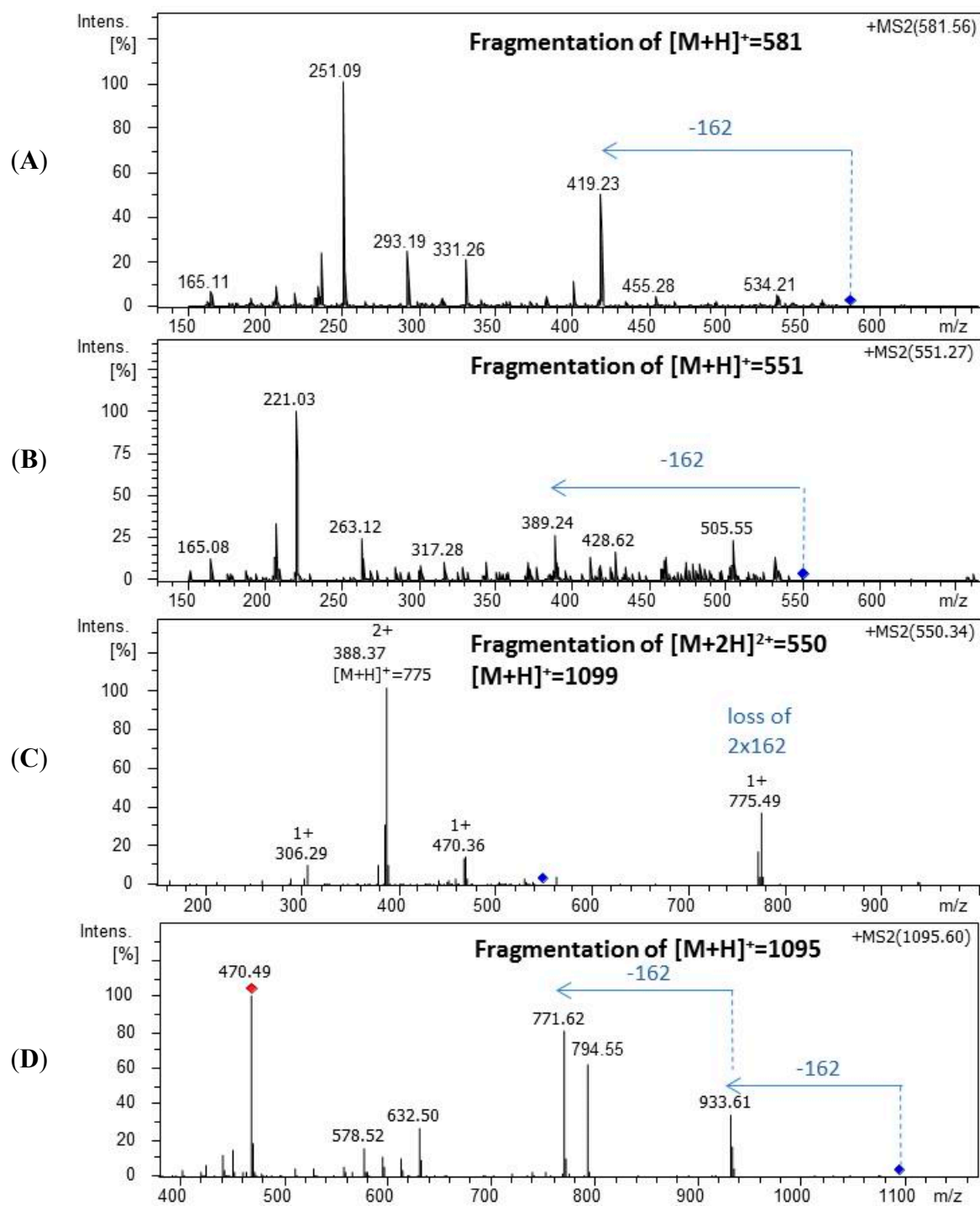


Figure S1. Ion trap MS/MS fragmentation spectra (ESI+ mode) of (A) “unknown581”, (B) “unknown551”, (C) “unknown1099” (from the doubly charged parent ion at m/z 550 Th) and (D) “unknown1095”.