

## Supplementary material

# Multicomponent polyphenolic extracts from *Vaccinium corymbosum* at lab and pilot scale. Characterization and effectivity against nosocomial pathogens

Eva Gato <sup>1</sup>, Astrid Perez<sup>1\*</sup>, Alicja Rosalowska <sup>2</sup>, Maria Celeiro <sup>3</sup>, German Bou <sup>1</sup> and Marta Lores <sup>2,\*</sup>

<sup>1</sup> Departamento de Microbiología, Complejo Hospitalario Universitario A Coruña (CHUAC), Instituto de Investigación Biomédica A Coruña (INIBIC), Universidad de A Coruña (UDC), A Coruña (Spain); eva.gato.corral@sergas.es; astrid.perez.gomez@gmail.com; german.bou.arevalo@sergas.es

<sup>2</sup> LIDSA, Department of Analytical Chemistry, Nutrition and Food Science, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Spain; marta.lores@usc.es; ally.rosalowska@gmail.com

<sup>3</sup> CRETUS, Department of Analytical Chemistry, Nutrition and Food Science, Universidade de Santiago de Compostela, E-15782 Santiago de Compostela, Spain; maria.celeiro.montero@usc.es

\* Correspondence: astrid.perez.gomez@gmail.com (A.P.); marta.lores@usc.es (M.L.)

**Table S1.** Studied compounds. CAS number, ionization mode, retention time, MS/MS transitions and suppliers.

Compound	CAS	Ionization mode	Retention time (min)	MS/MS transitions (Collision energy, eV) <sup>a</sup>
Gallic acid <sup>b</sup>	149-91-7	-	2.25	<u>169.02 → 125.04 (17)</u> 169.02 → 153.1 (15)
2,4,6-trihydrobenzoic acid <sup>b</sup>	487-70-7	+	3.23	<u>168.98 → 150.99 (17)</u> 168.98 → 83.02 (23) 168.98 → 107.02 (22)
2,4-dihydroxybenzoic acid <sup>b</sup>	89-86-1	+	3.69	<u>153.00 → 109.05 (16)</u> 153.00 → 65.09 (19) 153.00 → 67.07 (23)
3,4-dihydroxybenzoic acid <sup>b</sup>	99-50-3	+	3.70	<u>152.98 → 109.04 (17)</u> 152.98 → 91.04 (28) 152.98 → 108.03 (26)
Caftaric Acid <sup>b</sup>	67879-58-7	-	4.21	<u>310.96 → 178.97 (17)</u> 310.96 → 148.96 (14)
3,4-dihydroxybenzaldehyde <sup>b</sup>	139-85-5	+	4.55	<u>137.07 → 136.11 (21)</u> 137.07 → 91.09 (24) 137.07 → 92.13 (25)
2,5-dihydroxybenzoic acid <sup>b</sup>	490-79-9	+	4.74	<u>152.96 → 108.00 (24)</u> 152.96 → 81.02 (21) 152.96 → 109.01 (16)
Procyanidin B1 <sup>c</sup>	20315-25-7	-	4.76	<u>577.03 → 407.06 (26)</u> 577.03 → 288.93 (25) 577.03 → 424.97 (26)

2,6-dihydroxybenzoic acid <sup>b</sup>	303-07-1	+	4.86	<u>153.00 → 109.05 (17)</u> 153.00 → 65.09 (21) 153.00 → 135.02 (16)
3,5-dihydroxybenzoic acid <sup>b</sup>	99-10-5	+	4.90	<u>152.97 → 109.01 (15)</u> 152.97 → 65.06 (16) 152.97 → 67.05 (20)
Catechin <sup>b</sup>	225937-10-0	+	5.02	<u>289.00 → 245.02 (17)</u> 289.00 → 203.11 (22)
Procyanidin B2 <sup>b</sup>	29106-49-8	-	5.50	<u>577.03 → 407.06 (26)</u> 577.03 → 288.93 (25) 577.03 → 424.97 (26)
2,5-dihydroxybenzaldehyde <sup>b</sup>	1194-98-5	+	5.50	<u>136.99 → 108.02 (21)</u> 136.99 → 81.08 (18) 136.99 → 109.04 (14)
4-hydroxybenzaldehyde <sup>b</sup>	123-08-0	+	5.62	<u>122.97 → 95.05 (13)</u> 122.97 → 51.10 (36) 122.97 → 77.05 (20)
3-hydroxybenzaldehyde <sup>b</sup>	90-02-8	+	5.63	<u>121.02 → 93.05 (20)</u> 121.02 → 92.05 (23) 121.02 → 120.04 (19)
3-hydroxybenzoic acid <sup>b</sup>	99-06-9	+	5.68	<u>136.94 → 93.07 (14)</u> 136.94 → 65.09 (24) 136.94 → 91.01 (32)
Chlorogenic acid <sup>b</sup>	327-97-9	+	5.77	<u>353.00 → 191.07 (22)</u> 353.00 → 85.09 (43) 353.00 → 93.07 (45)
3,4-dimethoxybenzoic acid <sup>d</sup>	93-07-2	+	5.92	<u>182.96 → 137.08 (6)</u> 182.96 → 106.99 (22)
Caffeic Acid <sup>b</sup>	331-39-5	-	5.92	<u>178.98 → 135.03 (19)</u> 178.98 → 134.01 (28)
Epigallocatechingallate <sup>e</sup>	989-51-5	+	6.00	<u>457.15 → 169.05 (21)</u> 457.15 → 125.09 (42) 457.15 → 305.09 (21)
Procyanidin C1 <sup>b</sup>	37064-30-5	-	6.01	<u>577.03 → 288.93 (25)</u> 577.03 → 407.06 (26) 577.03 → 424.97 (26)
Epicatechin <sup>b</sup>	490-46-0	+	6.11	<u>289.00 → 245.02 (17)</u> 289.00 → 203.11 (22)
Petunidin-3-O-glucoside <sup>b</sup>	6988-81-4	+	6.49	<u>303.02 → 115.08 (50)</u> 303.02 → 173.07 (33) 303.02 → 257.07 (27)
Procyanidin A1 <sup>d</sup>	103883-03-0	-	6.50	<u>577.03 → 288.93 (25)</u> 577.03 → 407.06 (26) 577.03 → 424.97 (26)
Gallocatechingallate <sup>b</sup>	4233-96-9	+	6.59	<u>457.15 → 169.05 (21)</u> 457.15 → 125.09 (42) 457.15 → 305.09 (21)
Trans-4-hydroxycinnamic acid <sup>b</sup>	501-98-4	+	7.12	<u>163.02 → 119.07 (18)</u> 163.02 → 93.07 (37) 163.02 → 117.05 (38)
Epicatechingallate <sup>b</sup>	1257-08-5	+	7.13	<u>441.13 → 289.13 (30)</u> 441.13 → 125.08 (42) 441.13 → 169.05 (24)
7-hydroxycoumarin <sup>d</sup>	779-27-1	+	7.14	<u>162.99 → 107.04 (22)</u> 162.99 → 77.05 (34) 162.99 → 91.05 (20)

Catechingallate <sup>b</sup>	130405-40-2	+	7.17	<u>441.13 → 289.13 (20)</u> 441.13 → 125.08 (42) 441.13 → 169.05 (24)
Procyanidin A2 <sup>b</sup>	41743-41-3	-	7.35	<u>577.09 → 287.00 (32)</u> 577.09 → 136.98 (62) 577.09 → 425.08 (13)
Orientin <sup>c</sup>	28608-75-5	-	7.64	<u>447.16 → 327.14 (23)</u> 447.16 → 357.16 (22)
Delphinidin <sup>cf</sup>	528-53-0	+	7.81	<u>303.02 → 229.07 (32)</u> 303.02 → 115.08 (50) 303.02 → 173.07 (33)
3,4-dimethoxybenzaldehyde <sup>b</sup>	120-14-9	+	8.23	<u>167.01 → 139.05 (13)</u> 167.01 → 108.05 (21) 167.01 → 124.03 (18)
Cyanidin <sup>b,f</sup>	528-58-5	+	8.87	<u>287.02 → 128.10 (46)</u> 287.02 → 109.06 (39) 287.02 → 115.08 (45)
4-methoxybenzaldehyde <sup>d</sup>	123-11-5	+	9.05	<u>136.97 → 109.05 (12)</u> 136.97 → 77.05 (23) 136.97 → 94.04 (18)
Quercetin-3-glucuronide <sup>b</sup>	22688-79-5	+	9.21	<u>479.09 → 461.50 (14)</u> 479.09 → 302.96 (18)
Quercetin-3-rutinoside <sup>b</sup>	207671-50-9	-	9.39	<u>609.18 → 270.92 (96)</u> 609.18 → 178.87 (44) 609.18 → 300.01 (37)
Quercetin-3-glucoside <sup>b</sup>	482-35-9	+	9.41	<u>465.07 → 256.90 (41)</u> 465.07 → 302.97 (14)
Petunidin <sup>b,f</sup>	1429-30-7	+	9.43	<u>317.03 → 302.05 (25)</u> 317.03 → 217.03 (40) 317.03 → 245.03 (36)
Pelargonidin <sup>cf</sup>	134-04-3	+	10.09	<u>271.05 → 121.10 (33)</u> 271.05 → 115.14 (45) 271.05 → 141.15 (34)
Myricetin <sup>d</sup>	529-44-2	+	10.30	<u>319.00 → 153.02 (31)</u> 319.00 → 217.06 (31) 319.00 → 245.06 (27)
Peonidin <sup>cf</sup>	134-01-0	+	10.60	<u>301.03 → 286.08 (24)</u> 301.03 → 201.07 (38) 301.03 → 229.07 (38)
Malvidin <sup>cf</sup>	643-84-5	+	10.90	<u>331.11 → 315.14 (30)</u> 331.11 → 242.13 (31) 331.11 → 287.14 (30)
3,4,5-trimethoxycinnamic acid <sup>b</sup>	90-50-6	+	11.08	<u>239.03 → 221.04 (11)</u> 239.03 → 162.99 (27) 239.03 → 190.01 (19)
3,5-dimethoxybenzaldehyde <sup>b</sup>	7311-34-4	+	11.23	<u>167.15 → 124.03 (17)</u> 167.15 → 77.05 (26)
Quercetin <sup>b</sup>	117-39-5	+	11.70	<u>303.09 → 229.10 (28)</u> 303.09 → 153.04 (33)
Kaempferol <sup>b</sup>	520-18-3	-	12.27	<u>285.07 → 184.91 (30)</u> 285.07 → 239.12 (35)
Apigenin <sup>c</sup>	520-36-5	-	12.31	<u>269.09 → 117.12 (37)</u> 269.09 → 149.12 (26) 269.09 → 151.06 (26)
Chrysin <sup>e</sup>	480-40-0	+	13.05	<u>253.13 → 143.18 (30)</u> 253.13 → 63.20 (34)

<sup>a</sup> Underlined MS/MS transition used for quantification purpose. <sup>b</sup> Sigma Aldrich GmbH (Steinheim, Germany), <sup>c</sup> Extrasynthese (Genay, France), <sup>d</sup> TCI (Tokyo Chemical Industry) (Tokyo, Japan), <sup>e</sup> Alpha Aesar (Kandel, Germany), <sup>f</sup> Anthocyanidins detection after acid hydrolysis.

**Table S2.** LC-MS/MS performance for the 22 polyphenols identified in the blueberry extracts.

Compound	R <sup>2</sup>	Calibration curve	IDL (µg L <sup>-1</sup> ) <sup>a</sup>
Gallic acid	0.9972	y = 3331.7x + 230025	0.93
3,4-dihydroxybenzoic acid	0.9975	y = 3487.2x - 132653	0.14
3,4-dihydroxybenzaldehyde	9.9982	y = 1967.4x + 1E+6	1.07
Procyanidin B1	0.9960	y = 3184.4x + 140717	0.11
Catechin	0.9995	y = 1496x - 31807	27.6
Procyanidin B2	0.9979	y = 625x - 48344	47.4
Chlorogenic acid	0.9956	y = 16186x - 891959	0.75
Caffeic Acid	0.9953	y = 39450x + 2E+7	1.3
Procyanidin C1	0.9902	y = 42.606x + 17205	16.3
Epicatechin	0.9980	y = 1941.7x + 426449	17.8
Petunidin-3-O-glucoside	0.9998	y = 9E+7x - 1E+7	11.4
Epicatechingallate	0.9901	y = 954.26x - 623942	30.3
Procyanidin A2	0.9993	y = 21030x - 3E+6	1.26
Delphinidin	0.9928	y = 4E+6 + 26225	467.15
Cyanidin	0.9897	y = 4E+6 - 23912	415.6
Quercetin-3-rutinoside	0.9987	y = 1120.7x + 7982.5	1.38
Quercetin-3-glucoside	0.9920	y = 236.35x + 73648	2.68
Petunidin	0.9895	y = 7E+6 + 200420	71.1
Myricetin	0.9974	y = 1279.5x + 189066	25.6
Peonidin	0.9998	y = 3E+7 + 494341	33.1
Malvidin	0.9957	y = 8E+6x - 2E+7	293.3
Quercetin	0.9976	y = 2973.1x - 911531	12.01

<sup>a</sup> IDLs were calculated as the concentration giving a signal-to-noise ratio of three (S/N = 3) in all cases, since none of the target compounds were detected in the mobile phase chromatographic blanks