

Supplementary material – Table S2

Phenolic compounds and biopotential of grape pomace extracts from Prokupac red grape variety

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Table S2. Characterization of phenolic compounds in the aqueous extracts of grape pomace and its constituents of Prokupac red grape variety using UHPLC-MS/MS Orbitrap.

<i>t_R</i> , min	Compound name	Parent ions, <i>m/z</i>	MS ² Fragments, (% Base Peak)	MS ³ Fragments, (% Base Peak)	MS ⁴ Fragments, (% Base Peak)
Hydroxybenzoic acids and derivatives					
1.90	Gallic acid dihexoside	493	332(10), 331 (100)	169 (100), 125(20)	125 (100)
2.04	Gallic acid hexoside isomer 1	331	271(20), 241(10), 169 (100), 125(5)	125 (100)	107 (100), 81(10)
2.52	Gallic acid	169	125 (100)	107 (100)	–
3.81	Gallic acid hexoside isomer 2	331	169 (100), 125(5)	125 (100)	110(10), 97(30), 81 (100), 53(30)
3.86	Dihydroxybenzoic acid hexoside	315	153 (100), 152(50), 109(15), 108(10)	109 (100)	123(25), 109(10), 85(10), 81 (100)
4.33	Protocatechuic acid	153	109 (100), 95(75), 79(20), 59(10)	81 (100), 68(25), 65(15)	–
5.08	Hydroxybenzoic acid hexoside	299	137 (100)	93 (100)	–
5.20	Galloyl-HHDP-hexose*	633	463(10), 301 (100)	301(50), 284(25), 257 (100), 229(50), 185(40)	257(10), 240(10), 229 (100), 213(20), 185(50)
5.37	<i>p</i> -Hydroxybenzoic acid	137	109(10), 93 (100)	93 (10)	–
5.44	Gentisic acid	153	136(5), 125(10), 109 (100), 95(20), 79(10)	81(85), 67 (100), 63(60)	–
6.81	Ethyl gallate	197	169 (100), 151(20), 125(15)	125 (100)	81 (100)
6.82	Vanillic acid	167	153(10), 152(80), 124(10), 123 (100), 108(20)	108 (100)	79 (100)
6.84	Ellagic acid	301	284(40), 271(60), 257 (100), 229(85), 185(40)	229 (100), 213(20), 185(85)	201 (100), 185(95), 157(30), 145(20), 129(10)
Hydroxycinnamic acids and derivatives					
4.73	Caffeoyltartaric acid	311	179(40), 177(15), 149 (100)	131(50), 103(90), 87 (100), 59(25)	59 (100)
4.74	Caffeic acid	179	135 (100), 117(10), 91(20), 59(15)	107 (100), 59(50)	–
5.26	Chlorogenic acid	353	191 (100), 179(5)	173(75), 127 (100), 111(40), 93(60), 85(90)	109(40), 99(50), 85 (100)
5.77	Feruloyltartaric acid	325	265(20), 235(15), 193 (100), 149(10), 113(5)	178(65), 149 (100), 134(40)	134 (100)
6.37	<i>p</i> -Coumaric acid	163	119 (100)	119(60), 101(20), 93(25), 91 (100), 72(10)	–
7.02	Ferulic acid	193	178(70), 149 (100), 134(50)	134 (100)	106 (100)
Flavan-3-ols and procyanidins					
3.10	Procyanidin trimer B type isomer 1	865	695 (100), 577(60), 425(30), 407(30), 287(30)	543 (100), 451(45), 243(60)	525 (100), 391(40)
3.66	Procyanidin trimer B type isomer 2	865	695 (100), 577(80), 425(30), 407(40), 287(35)	543 (100), 451(45), 243(60)	525 (100), 391(40)
4.90	Procyanidin dimer B type isomer 1	577	451(30), 425 (100), 407(50), 289(25), 287(10)	407 (100), 381(5), 273(10)	389(30), 297(30), 285 (100), 243(70)
5.25	Procyanidin trimer B type isomer 3	865	695 (100), 577(70), 425(30), 407(40), 287(30)	543 (100), 451(45), 243(60)	525 (100), 391(40)
5.35	Catechin	289	271(5), 245 (100), 205(40), 179(15), 125(5)	227(30), 203 (100), 187(25), 175(10), 161(20)	188(70), 185(20), 175 (100), 161(40), 157(10)
5.57	Procyanidin dimer B type isomer 2	577	451(30), 425 (100), 407(50), 289(25), 287(10)	407 (100), 381(5), 273(10)	389(30), 297(30), 285 (100), 243(70)
5.82	Procyanidin dimer B type gallate isomer 1	729	577 (100), 559(50), 425(30), 407(50), 289(5)	559(50), 421(70), 425(50), 407 (100), 289(40)	389(25), 297(30), 285 (100), 255(20), 243(20)
5.83	Epicatechin	289	271(5), 245 (100), 205(40), 179(15), 125(5)	227(35), 203 (100), 187(30), 175(15), 161(25)	188(60), 185(20), 175 (100), 161(35), 157(15)
5.85	Procyanidin trimer B type isomer 4	865	695 (100), 577(80), 425(35), 407(35), 287(30)	543 (100), 451(45), 243(60)	525 (100), 391(40)
6.08	Procyanidin dimer B type gallate isomer 2	729	711(10), 603(30), 577(90), 559(90), 407 (100)	389(25), 297(30), 285 (100), 255(20), 243(20)	257 (100), 241(10), 213(5)
6.47	Procyanidin dimer B type digallate isomer 1	881	729 (100), 711(30), 577(20), 559(25), 407(30)	711(20), 603(70), 577(65), 559(50), 407 (100)	389(15), 297(20), 285 (100), 255(30)

6.79	(epi)Catechin gallate	441	331(10), 289 (100), 271(10), 169(25)	271(5), 245 (100), 205(40), 179(20)	227(20), 203 (100), 187(20), 175(10), 161(20)
7.40	Procyanidin dimer B type digallate isomer 2	881	729 (100), 711(35), 589(40), 577(25), 559(20)	711(80), 603 (100), 577(60), 559(70), 407(90)	–
Flavonols aglycones and glycosides					
5.89	Aromadendrin 7- <i>O</i> -hexoside	449	288(15), 287 (100), 269(40), 259(40)	259 (100), 243(15), 201(5)	241(30), 215 (100), 173(35), 125(60)
5.93	Quercetin 3,7-di- <i>O</i> -hexoside	625	463 (100), 301(30)	301 (100), 300(30)	283(20), 273(25), 257(10), 179 (100), 151(75)
6.22	Myricetin 3- <i>O</i> -hexoside	479	317(80), 316 (100), 299(5), 179(10)	287(30), 271 (100), 179(40)	271(15), 243 (100), 227(30)
6.42	Quercetin 3- <i>O</i> -rutinoside	609	343(5), 301 (100), 300(30), 271(10), 255(5)	273(25), 257(20), 179 (100), 151(75)	151 (100)
6.70	Laricitrin 3- <i>O</i> -hexoside	493	331 (100), 330(25), 317(40)	316 (100), 301(15), 285(5), 179(10), 151(10)	299(15), 287(25), 271(80), 179 (100), 151(35)
6.72	Quercetin 3- <i>O</i> -hexuronide	477	302(10), 301 (100)	273(20), 257(20), 179 (100), 151(75)	151 (100)
6.74	Quercetin 3- <i>O</i> -glucoside	463	301 (100), 300(30)	273(25), 257(20), 179 (100), 151(75)	151 (100)
7.05	Quercetin 3- <i>O</i> -rhamnoside	447	301 (100), 300(35), 284(20)	273(25), 257(20), 179 (100), 151(75)	151 (100)
7.12	Syringetin 3- <i>O</i> -hexoside	507	387(20), 345(50), 344 (100), 329(10)	329(90), 316 (100), 301(85), 287(10), 273(80)	301 (100), 300(20), 287(10), 273(60)
7.15	Kaempferol 3- <i>O</i> -glucoside	447	327(20), 285(80), 284 (100), 255(10)	255 (100), 227(10)	227 (100), 211(60)
7.26	Isorhamnetin 3- <i>O</i> -glucoside	477	357(20), 315(50), 314 (100), 300(5), 299(5)	300(30), 285 (100), 271(75), 257(10), 243(25)	270 (100)
7.32	Isorhamnetin 3- <i>O</i> -hexuronide	491	473(10), 315(90), 301 (100), 300(60)	283(15), 272(20), 256(10), 179 (100), 151(75)	151 (100)
7.98	Aromodendrin	287	269(10), 259 (100), 243(15), 201(10)	241(25), 215 (100), 173(30), 151(20), 125(65)	200(25), 187(10), 173 (100), 158(15)
8.79	Quercetin	301	283(15), 271(60), 257(25), 179 (100), 151(80)	151 (100)	107 (100), 83(10)
9.73	Kaempferol	285	255 (100), 227(10)	211 (100), 195(5), 167(15)	211(40), 137 (100)
9.95	Isorhamnetin	315	301(20), 300 (100)	283(30), 271 (100), 255(50), 227(52), 151(90)	243 (100), 227(70), 216(10), 199(20)
Stilbenoids					
6.62	Resveratrol	227	185 (100), 159(30), 143(20)	157(10), 143 (100), 117(5)	115 (100)
7.35	Resveratrol 3- <i>O</i> -glucoside	389	227 (100)	185 (100), 183(40), 159(35), 157(30), 143(20)	–
8.97	Resveratrol dimer isomer 1	453	417(30), 407(40), 359(90), 341 (100), 300(20)	323(10), 297(15), 282(30), 231(15), 217 (100)	–
8.39	Resveratrol tetramer isomer 1	905	811 (100), 717(50), 451(10), 359(15)	717 (100), 611(5), 451(5), 358(10)	699(20), 675 (100), 623(30), 611(80), 357(60)
8.64	Resveratrol tetramer isomer 2	905	811 (100), 717(60), 451(15), 359(15)	717 (100), 675(5), 611(5), 451(5), 357(10)	699(50), 675(90), 623(15), 611(65), 357 (100)
9.17	Resveratrol dimer isomer 2	453	435(10), 369(10), 359(30), 347 (100), 333(40)	329(10), 305(20), 253 (100), 240(30), 225(10)	225 (100), 209(10)
9.24	Resveratrol trimer isomer 1	679	585 (100), 491(10)	491 (100), 479(20), 385(10)	473(40), 447(30), 421(20), 397(25), 385 (100)
9.55	Resveratrol trimer (like α -viniferin)	677	571 (100), 529(10), 501(20), 465(30), 437(20)	529(30), 501(70), 465 (100), 437(30), 423(20)	447(10), 437(30), 423 (100), 421(60), 371(40)
9.72	Resveratrol trimer isomer 2	679	661(70), 637(20), 585 (100), 573(90), 451(35)	567(90), 543(50), 491(70), 479 (100), 347(20)	461(70), 435(75), 385 (100), 355(40), 327(30)
Anthocyanins					
4.64	Delphinidin 3- <i>O</i> -glucoside	465	304(15), 303 (100)	303(50), 285(5), 257 (100), 247(10), 229(30)	229 (100), 213(15), 201(25), 173(15)
4.65	Malvidin 3,5-di- <i>O</i> -glucoside	655	494(15), 493 (100), 332(10), 331(70)	331 (100)	316(80), 315 (100), 299(90), 298(30), 287(70)
4.78	Cyanidin 3- <i>O</i> -glucoside	449	288(10), 287 (100)	287 (100), 259(15), 241(20), 231(20), 213(30)	195(10), 185 (100), 167(10), 157(25), 141(20)
4.82	Cyanidin 3- <i>O</i> -sambubioside	581	288(10), 287 (100)	287(60), 259(40), 241(50), 231(70), 213 (100)	195(10), 185(100), 167(10), 157(20), 141(20)
5.07	Petunidin 3- <i>O</i> -hexoside	479	318(10), 317 (100)	302 (100), 274(10)	274 (100), 246(15), 228(10), 218(15)
5.04	Cyanidin 3- <i>O</i> -arabinoside	419	288(10), 287 (100)	287(60), 259(40), 241(50), 231(70), 213 (100)	195(10), 185(100), 167(10), 157(20), 141(20)
5.15	Pelargonidin 3- <i>O</i> -glucoside	433	272(10), 271 (100)	271 (100), 243(50), 225(60), 215(70), 197(80)	197(5), 169(100), 153(5), 141(30)
5.42	Peonidin 3- <i>O</i> -glucoside	463	302(10), 301 (100)	287(10), 286 (100)	268(20), 258 (100), 230(25), 202(10)
5.47	Malvidin 3- <i>O</i> -glucoside	493	332(15), 331 (100)	316(80), 315 (100), 299(90), 287(75), 270(50)	313 (100), 287(80), 285(60), 257(50)
5.97	Malvidin 3- <i>O</i> -hexoside-acetaldehyde	517	356(15), 355 (100)	339 (100), 322(30), 311(15), 294(40), 266(20)	337(70), 321(30), 311 (100), 309(80), 281(30)

6.30	Peonidin 3- <i>O</i> -(6"-acetyl)hexoside	505	302(10), 301 (100)	287(10), 286 (100)	268(20), 258 (100), 230(25), 202(10)
6.24	Malvidin 3- <i>O</i> -hexoside-(8,8)-methylmethyne-(epi)catechin	809	647(5), 519(20), 357 (100), 341(5)	341 (100), 327(60), 313(10), 296(10), 268(20)	339(90), 313(80), 311 (100), 283(50)
6.32	Malvidin 3- <i>O</i> -(6"-acetyl)hexoside	535	332(15), 331 (100)	316(80), 315 (100), 299(90), 287(75), 270(50)	313 (100), 287(80), 285(60), 257(50)
6.44	Delphinidin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside	611	304(15), 303 (100)	303(50), 285(5), 257 (100), 247(10), 229(30)	229 (100), 213(15), 201(25), 173(15)
6.67	Malvidin 3- <i>O</i> -(6"-caffeoyl)hexoside	655	332(15), 331 (100)	316(80), 315 (100), 299(90), 287(75), 270(50)	313 (100), 287(80), 285(60), 257(50)
6.73	Petunidin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside	625	318(10), 317 (100)	302 (100), 274(10)	274 (100), 246(15), 228(10), 218(15)
7.03	Peonidin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside	609	302(10), 301 (100)	287(10), 286 (100)	268(20), 258 (100), 230(25), 202(10)
7.10	Malvidin 3- <i>O</i> -(6"- <i>p</i> -coumaroyl)hexoside	639	332(15), 331 (100)	316(80), 315 (100), 299(90), 287(75), 270(50)	313 (100), 287(80), 285(60), 257(50)

* Galloyl-hexahydroxydiphenic acid -hexose