

Supplementary material – Table S1

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

Danijel D. MILINČIĆ¹, Nemanja S. STANISAVLJEVIĆ², Aleksandar Ž. KOSTIĆ¹, Svetlana SOKOVIĆ BAJIĆ², Milan O. KOJIĆ², Uroš M. GAŠIĆ³, Miroljub B. BARAĆ¹, Sladjana P. STANOJEVIĆ¹, Živoslav Lj. TEŠIĆ⁴, Mirjana B. PEŠIĆ^{1*}

¹*University of Belgrade, Faculty of Agriculture, Department of Food Technology and Biochemistry, Nemanjina 6, 11081 Belgrade, Serbia*

² *University of Belgrade, Institute of Molecular Genetics and Genetic Engineering, P.O. Box 23, 11 010 Belgrade, Serbia*

³ *University of Belgrade, Institute for Biological Research “Siniša Stanković”, National Institute of Republic of Serbia, Department of Plant Physiology, Bulevar despota Stefana 142, 11060 Belgrade, Serbia*

⁴ *University of Belgrade, Faculty of Chemistry, P.O. Box 51, 11158, Belgrade, Serbia*

*Corresponding author: Tel./Fax: +381 11 21 99 711

E-mail address: mpesic@agrif.bg.ac.rs (M. Pešić)

Table S1. Calibration curves, correlation coefficients (r^2), limits of detection (LOD), limits of quantification (LOQ), and linear ranges for 28 standards used for UHPLC-Orbitrap MS⁴ qualitative analysis of phenolic compounds in aqueous grape pomace extracts of Prokupac variety

Compound name	Linear regression ($y=a+b*x$)	r^2	LOD (mg/L)	LOQ (mg/L)	Linear range (mg/L)
<i>Hydroxybenzoic acids and derivatives</i>					
Gallic acid	$y = -2.08E+7 + 3.86E+7*x$	0.9908	0.17	0.56	0.50 - 2.00
Protocatechuic acid	$y = 3.73E+5 + 1.72E+5*x$	0.9993	0.06	0.20	0.01 - 2.00
<i>p</i> -Hydroxybenzoic acid	$y = 9.83E+5 + 2.71E+7*x$	0.9948	0.08	0.27	0.01 - 1.11
Gentisic acid	$y = -1.76E+4 + 8.65E+5*x$	0.9907	0.21	0.71	0.10 - 2.00
Vanillic acid	$y = -1.08E+5 + 1.24E+7*x$	0.9922	0.09	0.30	0.01 - 0.95
<i>Hydroxycinnamic acids and derivatives</i>					
Caffeic acid	$y = -1.30E+6 + 2.43E+7*x$	0.9939	0.17	0.58	0.01 - 1.90
Chlorogenic acid	$y = -6.67E+6 + 1.70E+7*x$	0.9982	0.10	0.32	0.01 - 2.10
<i>p</i> -Coumaric acid	$y = 7.85E+5 + 5.44E+6*x$	0.9937	0.16	0.53	0.05 - 1.90
Ferulic acid	$y = 5.24E+3 + 1.04E+7*x$	0.9910	0.11	0.36	0.01 - 1.00
<i>Flavan-3-ols and procyanidins</i>					
Catechin	$y = -3.56E+4 + 3.60E+5*x$	0.9977	0.08	0.26	0.15 - 1.50
<i>Flavonols aglycones and glycosides</i>					
Quercetin 3- <i>O</i> -rutinoside	$y = -3.72E+5 + 1.98E+7*x$	0.9994	0.06	0.18	0.01 - 2.00
Quercetin 3- <i>O</i> -glucoside	$y = 7.13E+5 + 3.33E+7*x$	0.9986	0.08	0.28	0.01 - 2.00
Quercetin 3- <i>O</i> -rhamnoside	$y = 9.31E+5 + 3.69E+7*x$	0.9919	0.14	0.48	0.03 - 1.50
Kaempferol 3- <i>O</i> -glucoside	$y = -1.07E+5 + 1.33E+7*x$	0.9984	0.02	0.07	0.01 - 0.50
Isorhamnetin 3- <i>O</i> -glucoside	$y = 6.45E+5 + 2.06E+7*x$	0.9933	0.21	0.71	0.03 - 2.00
Quercetin	$y = -1.31E+6 + 1.70E+7*x$	0.9911	0.11	0.36	0.05 - 1.00
Kaempferol	$y = -1.21E+6 + 3.18E+7*x$	0.9983	0.09	0.31	0.10 - 1.10
Isorhamnetin	$y = -5.51E+6 + 8.99E+6*x$	0.9974	0.10	0.34	0.25 - 2.00
<i>Stilbenoids</i>					
Resveratrol	$y = -1.36E+5 + 4.50E+6*x$	0.9985	0.08	0.27	0.01 - 2.00
Resveratrol 3- <i>O</i> -glucoside	$y = 3.84E+4 + 2.85E+6*x$	0.9965	0.12	0.41	0.01 - 2.00
<i>Anthocyanins</i>					
Delphinidin 3- <i>O</i> -glucoside	$y = -1.73E+4 + 4.26E+5*x$	0.9988	0.04	0.13	0.05 - 1.00
Malvidin 3,5-di- <i>O</i> -glucoside	$y = -6.79E+3 + 4.09E+5*x$	0.9983	0.04	0.13	0.10 - 1.00
Cyanidin 3- <i>O</i> -glucoside	$y = -1.61E+4 + 6.21E+5*x$	0.9988	0.04	0.13	0.03 - 1.00
Cyanidin 3- <i>O</i> -sambubioside	$y = -4.98E+3 + 4.32E+5*x$	0.9994	0.03	0.10	0.05 - 1.00
Cyanidin 3- <i>O</i> -arabinoside	$y = -1.96E+4 + 5.98E+5*x$	0.9994	0.03	0.10	0.05 - 1.00
Pelargonidin 3- <i>O</i> -glucoside	$y = -8.57E+3 + 8.09E+5*x$	0.9988	0.04	0.14	0.03 - 1.00

Peonidin 3- <i>O</i> -glucoside	$y = -7.44E+3 + 2.86E+5*x$	0.9916	0.10	0.33	0.05 - 1.00
Malvidin 3- <i>O</i> -glucoside	$y = -1.04E+4 + 6.94E+5*x$	0.9931	0.09	0.31	0.05 - 1.00