

SUPPLEMENTARY INFORMATION

Bioactive phytochemical composition of grape pomace resulted from different white and red grape cultivars

Petronela Anca Oneche ¹, Elisabeta-Irina GEANĂ^{2,*}, Corina Teodora CIUCURE², Alina FLOREA^{1,*}, Dorin Ioan SUMEDREA¹, Roxana Elena IONETE², Ovidiu TIȚA ³

¹National Research&Development Institute for Biotechnology in Horticulture Stefanesti - Arges, Romania, Sos. București-Pitești no 37; anca27il@yahoo.com , alinaflorea964@yahoo.com, dsunedrea@yahoo.com

²National Research&Development Institute for Cryogenic and Isotopic Technologies-Râmnicu Vâlcea Romania, strada Uzinei nr.4 , 240050; : irina.geana@icsi.ro, corina.ciucure@icsi.ro , roxana.ionete@icsi.ro

³ "Lucian Blaga" Sibiu University Romania, blv Victoriei no 10, 550024, ovidiu.tita@ulbsibiu.ro

*Correspondence: irina.geana@icsi.ro , alinaflorea964@gmail.com; Tel.: +40745752559,+40747813151 (E.I.G., A.F.)

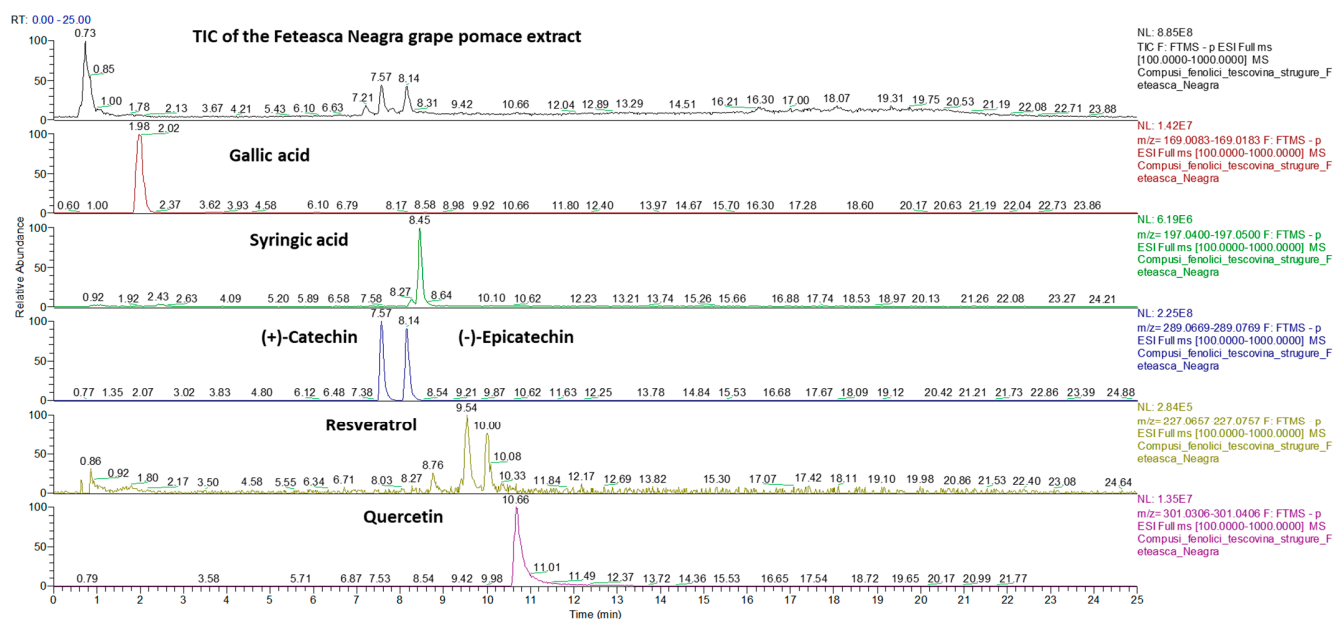
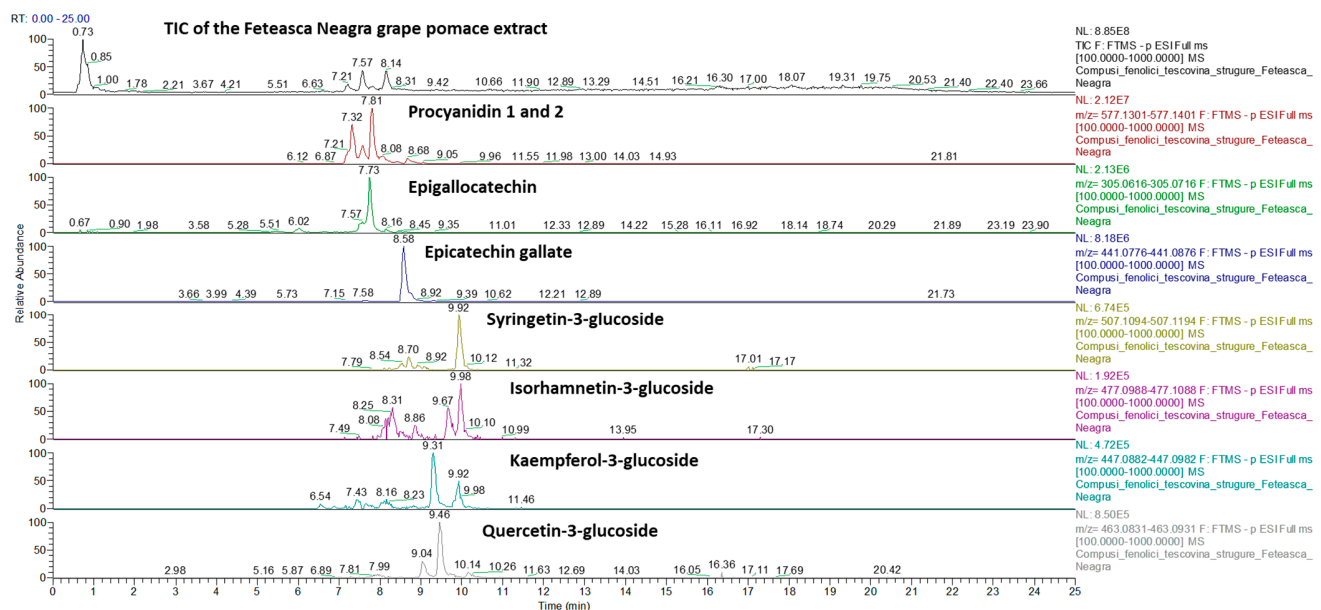
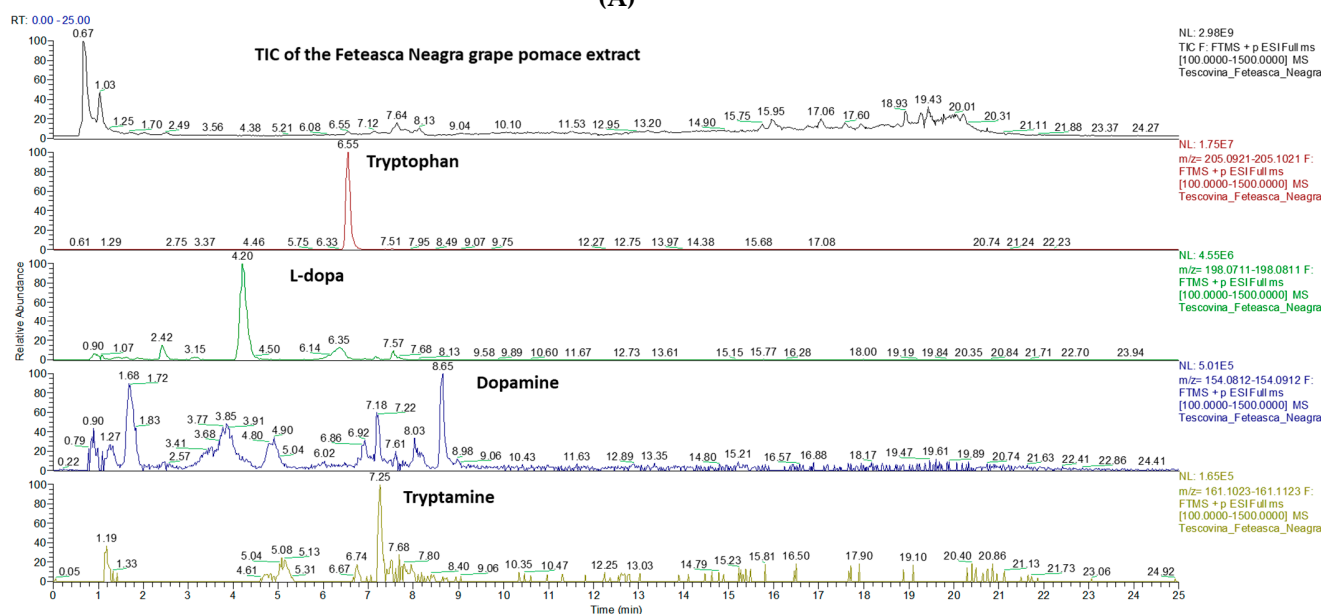


Figure S1. TIC and the extracted chromatograms of the main phenolic compounds quantified in Feteasca Neagra grape pomace (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75-1000 m/z)



(A)



(B)

Figure S2. TIC and the extracted chromatograms of the main phenolic compounds (A) and amino acids (B) identified in Feteasca Neagra grape pomace (the chromatograms were extracted from TIC using a 5 ppm mass accuracy window; negative ion mode, full scan, base peak in the range 75-1000 m/z)

Table S1. Content of total phenolic compounds (TPC, expressed as GAE), total anthocyanins (TAC, expressed in mg/g), tannins (expressed in mg/g), antioxidant activity (AA, expressed in μmol Trolox/g), content of total flavonoids (TFC, expressed as QE) in grape pomace

Grape Pomace	TPC	AA	TAC	TFC	Tannins	references
Malbec	196,2 \pm 22,7 mg GAE/ g	2756,0 \pm 109,1 μmol TE/g	-	-	-	(Antoniolli et al., 2015)
Pinot noir	-	-	50.616 - 131.868 mg/g DW	-	-	(Kammerer et al., 2004)
Romy	10.79 \pm 0.23 mg GAE/ g	-	-	10.15 \pm 0.14 mg QE/g	3.32 \pm 0.04 mg TE/g	(Gaafar et al., 2019)
Banaty	5.81 \pm 0.09 mg GAE/ g	-	-	5.89 \pm 0.20 mg QE/g	1.60 \pm 0.03 mg TE/g	
Rare Georgian red grape varieties (Simonaseuli, Adreuli Shavi Sreluri, Gabasha)	2.79 \pm 0.02 g/100g dry	79 \pm 0.9 %	737.0 \pm 0.9 mg/100 g	2.32 \pm 0.04 g 100 g-1 dry	10.51 \pm 0.8 mg 100 g-1 productivity	(Gurgenidze et al., 2022)
Merlot	2360.99 \pm 0.77 mg GAE 100 g-1 dw	-	8.96 \pm 0.02 mg cya-3- glu 100 g-1 dw	1793.38 \pm 0.53 mg CTE 100 g-1 dw	-	(Ribeiro et al., 2022)
70% Isabel, 15% Bordo, 10% Carmem and 5% Nagara	8.58 \pm 0.02 mg GAE/g	35.94 \pm 0.23 μmol TE g ⁻¹	1.540 \pm 0.031 mg malvi-3,5- diglu/g	-	-	(da Rocha and Noreña, 2021)
Riesling	47.94 \pm 0.11 mg GAE/g-1	57.45 \pm 0.42 mg AAE.g-1	-	-	-	(Vojáčková et al., 2020)
Cabernet Sauvignon	5.5 g GAE/100g DM	393 mgAAE/L	70.3 mg/100g DM	5.4 g QE/ 100 g DM	12.3 g/L	(Rajha et al., 2014)
Tempranillo	26,8 \div 71,8 mg GAE g-1 dw	300 \div 800 μmol TE/g	-	-	-	(Ayuda-Durán et al., 2019)
Cabernet Sauvignon	69.83 \pm 4.53mg GAE/g	62.74 \pm 1.34 %	133.79 \pm 6.74 mg CE/g	43.89 \pm 1.22 mg RE/g	-	(MJ, 2015)
Chardonnay	58.15 \pm 5.21mg GAE/g	68.28 \pm 0.52 %	92.10 \pm 6.00 mg CE/g	14.32 \pm 1.67 mg RE/g	-	
Viognier	99.1 \pm 0.29mg GAE/g	3.54 \pm 0.06 μmol TE/g	0.02 \pm 0.01 mgCyd-3- glu/g	75.0 \pm 0.42 mg CE/g	98.6 \pm 0.17mg GAE/g	(Xu et al., 2016a)

Resveratrol	0.7 ± 0.04	4.02 ± 0.39	6.40 ± 0.20	nd	1.18 ± 0.08	36.0 ± 4.9	4.54 ± 0.14	-	7.55 ± 0.31
References	(Milinčić et al., 2021)	(Rockenbach et al., 2011)				(Antoniolli et al., 2015)	(Ribeiro et al., 2022)	(Xu et al., 2016b)	Carmines Negro, 2021

Table S2 (continued). Phenolic compounds in grape pomace of different white and red grape cultivars

Compuși	Fetească Neagră	Cabernet Sauvignon (mg/ g DW)	Riesling Italian (μg/g DW)	Fetească Neagră (μg/g DW)	Cabernet Sauvignon (mg/kg)	Shiraz (mg/100 g)
<i>Hydroxybenzoic acids</i>						
Gallic acid	-	0.73± 0.04	-	-	-	4.42 c ± 0.03
Vanillic acid	-	-	-	-	-	-
Acid siringic	-	-	-	-	-	-
<i>Hydroxycinnamic acids</i>						
trans -acid cinamic	-	-	-	-	-	-
Caffeic acid	-	1.03 ± 0.07	-	-	-	0.62 b ± 0.02
Chlorogenic acid	-	-	-	-	-	-
p-Coumaric acid	-	0.51±0.02	-	-	-	-
<i>Flavonoids</i>						
Catechin	2.59 ± 0.01 mg/g d.w.	0.57 ± 0.06	-	-	-	52.30 c ± 1.13
Epicatechin	2.05 ± 0.16 mg/g d.w.	0.50±0.05	-	-	-	27.92c± 1.40
Quercetin	-	0.07 ± 0.02	-	-	122.6±10.0	0.44 ± 0.03
Rutin	-	-	-	-	-	23.70 b ± 0.87
Kaempferol	-	nd	-	-	28.7±2.8	0.16 b ± 0.02
<i>Stilbenoids</i>						
Resveratrol	12.27 ± 3.07 μg/g d.w	0.09 ± 0.04	1.41 ± 0.76	5.38 ± 0.43	-	3.02 ± 0.10
References	Ștefania Silvia Balea, 2018	Carmines Negro, 2021	Maria L. Muncaciu,2017		Ghislaine Hilbert, 2015	L. Butkhupl, 2010

Table S3. Correlation matrix and Pearson coefficients of determination for individual phenolic compounds in grape pomaces

Variables	pinostrobin	resveratrol	p-Coumaric acid	Syringic acid	Gallic acid	Caffeic acid	kaemferol	Absciscic acid	Chlorogenic acid	t-Ferulic acid	4-Hydroxybenzoic acid	Ellagic acid	Cinnamic acid	3,4-Dihydroxybenzoic acid	catechin	quercetin	isorhamnetin	epi-catechin	rutin
pinostrobin	1	0.418	-0.483	-0.190	-0.237	0.027	0.183	-0.143	-0.117	-0.037	-0.283	0.055	-0.010	0.162	-0.389	0.448	0.745	-0.562	-0.429
resveratrol	0.418	1	-0.913	-0.317	-0.024	0.358	0.553	-0.559	0.708	0.385	0.525	0.385	0.295	0.153	-0.506	0.494	0.573	-0.159	0.048
p-Coumaric acid	-0.483	-0.913	1	0.475	0.350	-0.037	-0.371	0.370	-0.495	-0.022	-0.179	-0.104	-0.080	0.077	0.246	-0.205	-0.502	0.113	0.079
Syringic acid	-0.190	-0.317	0.475	1	0.520	0.660	0.456	-0.488	-0.294	-0.124	0.102	0.228	-0.020	0.236	-0.280	0.420	0.208	-0.391	-0.541
Gallic acid	-0.237	-0.024	0.350	0.520	1	0.809	0.574	-0.422	0.443	0.534	0.475	0.403	0.081	0.108	-0.163	0.428	-0.102	0.239	0.155
Caffeic acid	0.027	0.358	-0.037	0.660	0.809	1	0.862	-0.780	0.440	0.456	0.605	0.548	0.195	0.294	-0.552	0.758	0.395	-0.212	-0.175
kaemferol	0.183	0.553	-0.371	0.456	0.574	0.862	1	-0.674	0.424	0.183	0.381	0.191	-0.172	-0.105	-0.328	0.542	0.385	-0.103	-0.189
Absciscic acid	-0.143	-0.559	0.370	-0.488	-0.422	-0.780	-0.674	1	-0.479	-0.248	-0.551	-0.751	-0.481	-0.481	0.653	-0.776	-0.653	0.390	0.489
Chlorogenic acid	-0.117	0.708	-0.495	-0.294	0.443	0.440	0.424	-0.479	1	0.686	0.751	0.532	0.407	0.118	-0.244	0.316	0.038	0.384	0.455
t-Ferulic acid	-0.037	0.385	-0.022	-0.124	0.534	0.456	0.183	-0.248	0.686	1	0.831	0.653	0.626	0.538	-0.563	0.552	0.118	0.035	0.567
4-Hydroxybenzoic acid	-0.283	0.525	-0.179	0.102	0.475	0.605	0.381	-0.551	0.751	0.831	1	0.730	0.671	0.540	-0.631	0.577	0.188	-0.036	0.385
Ellagic acid	0.055	0.385	-0.104	0.228	0.403	0.548	0.191	-0.751	0.532	0.653	0.730	1	0.909	0.861	-0.784	0.794	0.526	-0.369	-0.146
Cinnamic acid	-0.010	0.295	-0.080	-0.020	0.081	0.195	-0.172	-0.481	0.407	0.626	0.671	0.909	1	0.915	-0.730	0.598	0.423	-0.378	0.001
3,4-Dihydroxybenzoic acid	0.162	0.153	0.077	0.236	0.108	0.294	-0.105	-0.481	0.118	0.538	0.540	0.861	0.915	1	-0.860	0.748	0.596	-0.665	-0.216
catechin	-0.389	-0.506	0.246	-0.280	-0.163	-0.552	-0.328	0.653	-0.244	-0.563	-0.631	-0.784	-0.730	-0.860	1	-0.931	-0.825	0.769	0.254
quercetin	0.448	0.494	-0.205	0.420	0.428	0.758	0.542	-0.776	0.316	0.552	0.577	0.794	0.598	0.748	-0.931	1	0.819	-0.670	-0.344
isorhamnetin	0.745	0.573	-0.502	0.208	-0.102	0.395	0.385	-0.653	0.038	0.118	0.188	0.526	0.423	0.596	-0.825	0.819	1	-0.859	-0.625
epi-catechin	-0.562	-0.159	0.113	-0.391	0.239	-0.212	-0.103	0.390	0.384	0.035	-0.036	-0.369	-0.378	-0.665	0.769	-0.670	-0.859	1	0.657
rutin	-0.429	0.048	0.079	-0.541	0.155	-0.175	-0.189	0.489	0.455	0.567	0.385	-0.146	0.001	-0.216	0.254	-0.344	-0.625	0.657	1

Values in bold are different from 0 with a significance level $\alpha=0.05$