

Impact of Eutectic Solvents Utilization in the Microwave Assisted Extraction of Proanthocyanidins from grape pomace

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Figure S1 – Representative chromatogram of phloroglucinolysis products for proanthocyanidin mean degree of polymerization determination. 1 – phloroglucinol adduct of catechin/epicatechin; 2 – phloroglucinol adduct of catechin/epicatechin; 3 – catechin; 4 – phloroglucinol adduct of catechin gallate/epicatechin gallate; 5 – epicatechin; 6 – catechin gallate/epicatechin gallate

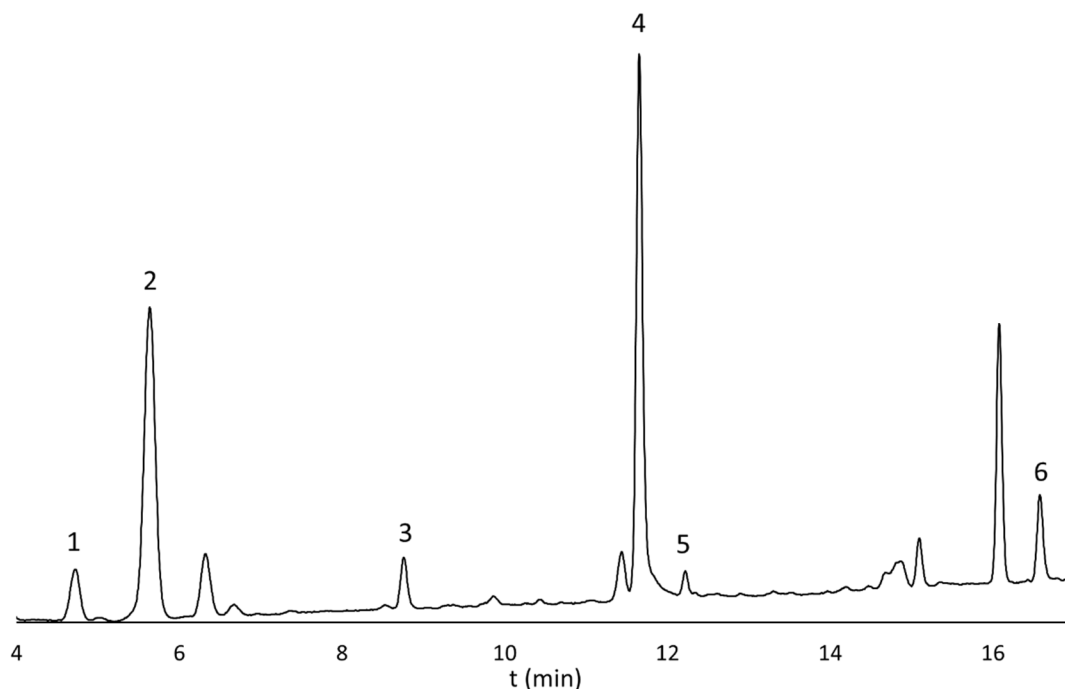


Table S1 – Compounds identified from phloroglucinolysis products and the respective retention times and molecular ions masses.

No	Compound	t_R (min)	$[M-H]^-$ (m/z)
1	phloroglucinol adduct of catechin/epicatechin	4.72	413.19
2	phloroglucinol adduct of catechin/epicatechin	5.64	413.19
3	Catechin	8.76	289.08
4	phloroglucinol adduct of catechin gallate/epicatechin gallate	11.65	565.20
5	epicatechin	12.22	289.08
6	catechin gallate/epicatechin gallate	16.58	441.09

Table S2 – Solvent composition and experimental results of solvent composition optimization of ChCl-LacA-water.

Run				Y_{PAC} (mg _{PAC} /g _{GP})		mDP		%Gal		Y_{CH} (mg _{CH} /g _{GP})	
	x_{ChCl}	x_{LacA}	x_{H_2O}	Measured	Predicted	Measured	Predicted	Measured	Predicted	Measured	Predicted
1	0.490	0.408	0.102	101.7	113.7	9.94	10.60	38.11	38.32	60.9	66.2
2	0.248	0.602	0.150	113.0	115.1	9.52	10.23	38.03	38.19	68.8	63.6
3	0.492	0.201	0.307	114.7	116.4	10.79	10.39	34.86	35.54	82.0	79.1
4	0.700	0.240	0.060	72.8	77.2	9.18	8.70	33.58	35.73	52.0	55.8
5	0.698	0.000	0.302	70.8	71.0	7.57	7.75	31.00	31.52	62.5	60.0
6	0.505	0.000	0.495	73.2	80.5	7.47	7.85	31.37	31.49	65.3	73.3
7	0.502	0.000	0.498	74.5	80.3	7.40	7.83	31.24	31.47	66.8	73.5
8	0.700	0.237	0.063	89.4	77.5	8.82	8.70	38.04	35.69	56.8	56.0

9	0.000	0.405	0.595	58.3	63.4	6.03	6.25	30.72	31.27	95.0	89.5
10	0.000	0.399	0.601	60.6	62.1	5.85	6.17	31.47	31.17	87.8	89.7
11	0.000	0.800	0.200	75.2	71.5	7.45	7.02	34.28	34.59	54.3	45.01
12	0.000	0.599	0.401	78.4	86.3	7.24	7.79	33.34	33.58	63.3	76.2
13	0.306	0.381	0.313	132.2	127.7	11.03	10.87	37.41	36.83	83.1	83.9
14	0.700	0.000	0.300	73.7	70.7	7.74	7.74	32.27	31.51	67.2	59.8
15	0.000	0.800	0.200	75.1	71.4	7.39	7.02	35.10	34.59	39.9	45.01
16	0.247	0.216	0.537	119.2	97.6	10.15	8.66	34.04	33.37	101.0	90.2

Table S3 – Solvent composition and experimental results of solvent composition optimization of ChCl-Glyc-water.

Run	X _{ChCl}	X _{Glyc}	X _{H2O}	Y _{PAC} (mg _{PAC} /g _{GP})		mDP		%Gal		Y _{CH} (mg _{CH} /g _{GP})	
				Measured	Predicted	Measured	Predicted	Measured	Predicted	Measured	Predicted
1	0.000	1.000	0.000	63.3	62	7.62	7.65	39.80	39.48	69.9	63.2
2	0.321	0.479	0.200	74.2	71.1	7.45	7.37	34.90	34.28	70.8	66.0
3	0.000	0.758	0.242	70.0	72.6	7.60	7.67	35.58	36.18	81.1	79.1
4	0.501	0.000	0.499	71.7	76.0	7.13	7.14	31.21	31.97	71.2	66.2
5	0.699	0.000	0.301	66.2	70.7	7.85	7.96	31.00	32.21	69.1	69.5
6	0.242	0.259	0.499	68.2	70.8	6.63	6.66	32.49	31.93	61.5	67.3
7	0.488	0.229	0.283	74.5	73.3	7.47	7.50	33.26	32.92	65.8	67.3
8	0.659	0.281	0.060	47.87	46.94	7.06	7.18	32.33	32.10	54.5	51.1
9	0.502	0.498	0.000	47.11	45.78	6.73	6.79	31.85	33.55	44.03	44.57
10	0.000	0.502	0.498	60.7	62.5	6.57	6.59	31.89	32.24	70.6	74.1
11	0.000	1.000	0.000	63.3	62.0	7.71	7.65	40.00	39.48	58.1	63.2
12	0.000	0.502	0.498	66.1	62.5	6.65	6.59	32.28	32.24	77.2	74.1
13	0.657	0.283	0.060	48.02	47.04	7.33	7.17	33.88	32.11	53.6	51.1
14	0.500	0.000	0.500	81.4	76.0	7.15	7.14	32.83	31.97	69.1	66.1
15	0.246	0.754	0.000	51.5	55.8	7.04	7.03	35.77	36.40	44.86	51.2
16	0.699	0.000	0.301	73.6	70.7	7.80	7.96	32.18	32.21	62.0	69.5

Table S4 – Extraction conditions and experimental results of extraction conditions optimization of ChCl-LacA-water.

Run	temp (°C)	%BM	t (min)	Y _{PAC} (mg _{PAC} /g _{GP})		mDP		%Gal		Y _{CH} (mg _{CH} /g _{GP})	
				Measured	Predicted	Measured	Predicted	Measured	Predicted	Measured	Predicted
1	130	9,84	10	112.8	109.8	3.293	3.415	63.8	61.0	144.1	145.3
2	100	17,51	10	127.8	135.1	7.08	6.74	50.7	53.2	103.3	94.4
3	100	2,621	10	121.7	122.8	2.959	3.524	44.89	42.88	135.3	149.4
4	100	9,99	6	135.8	137.5	8.22	8.72	44.27	43.93	113.0	110.8
5	100	2,471	2	201.4	202.1	3.949	4.280	41.24	38.90	142.6	156.2
6	100	10,22	6	139.3	136.8	9.09	8.77	43.43	44.09	111.4	109.8
7	70	10,63	2	77.4	87.3	6.83	7.97	34.91	37.50	76.3	76.4
8	130	17,72	6	53.9	61.7	2.996	4.543	58.1	57.0	84.9	92.9
9	130	10,30	2	141.3	123.1	5.24	4.386	58.6	56.6	137.4	138.0
10	100	10,30	6	150.2	136.5	8.89	8.79	44.06	44.14	105.6	109.5
11	100	17,47	2	84.3	90.5	8.24	7.63	47.10	49.41	90.4	81.3

12	70	10,01	10	79.8	72.3	7.32	6.98	37.09	39.43	82.3	81.1
13	70	17,46	6	90.3	85.8	8.85	8.15	41.68	36.77	72.0	81.6
14	70	2,569	6	73.8	76.0	4.983	4.878	26.84	26.40	109.2	95.9
15	130	2,626	6	158.0	171.5	2.193	1.398	41.73	46.68	223.3	208.6
