-Electronic Supplementary Information-

Chemometric and green metrics strategies for sustainable analytical methods: phenolic compounds in lettuce-NADES extracts

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Table S1. Experiments and responses of the PCs in the BBD design.

Run	A	B	C	Peak area (mAU)					
	Plant/solvent ratio (mg L^{-1})	**Time (min)**	**Temperature (°C)**	**Rut**	**Caf**	**Clor**	**Van**	**Fer**	**Gal**
1	10	60	55	0.0483	1.4417	0.9695	2.8490	9.24680	0.2923
2	60	35	30	0.0796	2.7671	0.6018	2.8881	70.3243	0.1356
3	10	35	80	0.0287	2.1737	0.2785	3.0737	25.9524	0.1969
4	35	35	55	0.0916	3.5689	1.1103	3.4558	70.0788	0.2319
5	60	35	80	0.0940	3.2958	0.8761	3.0462	65.3412	0.2085
6	35	35	55	0.1004	3.5251	1.1812	3.4384	70.0160	0.2157
7	60	10	55	0.0780	3.1702	0.8315	2.9972	37.8805	0.2276
8	35	35	55	0.1227	3.3722	0.9186	3.2299	62.4343	0.2069
9	35	35	55	0.0868	3.7270	1.2101	3.3149	70.5697	0.2233
10	35	60	30	0.0771	3.3240	0.8179	2.6102	42.2561	0.2257
11	60	60	55	0.0101	1.6286	0.9857	2.5044	39.7263	0.2192
12	35	10	30	0.0784	3.3087	0.6390	2.9876	31.0792	0.2003
13	35	35	55	0.0775	2.8150	0.9341	3.1529	26.9130	0.2241
14	10	35	30	0.0273	2.5431	1.2202	2.7902	49.2424	0.2304
15	35	10	80	0.0883	2.8953	0.4931	2.7071	6.54490	0.2117
16	35	60	80	0.0687	3.2712	0.3729	3.1648	5.42800	0.2162
17	10	10	55	0.0191	3.7832	0.5124	2.8153	6.02860	0.1943

Fig S1. Values obtained from the desirability function for each phenolic compound considering the significant variables under study. Optimal condition: A): plant/solvent ratio (35.5 mg mL^{-1}), B): Extraction time (36 min), and C): Extraction temperature (30 °C).

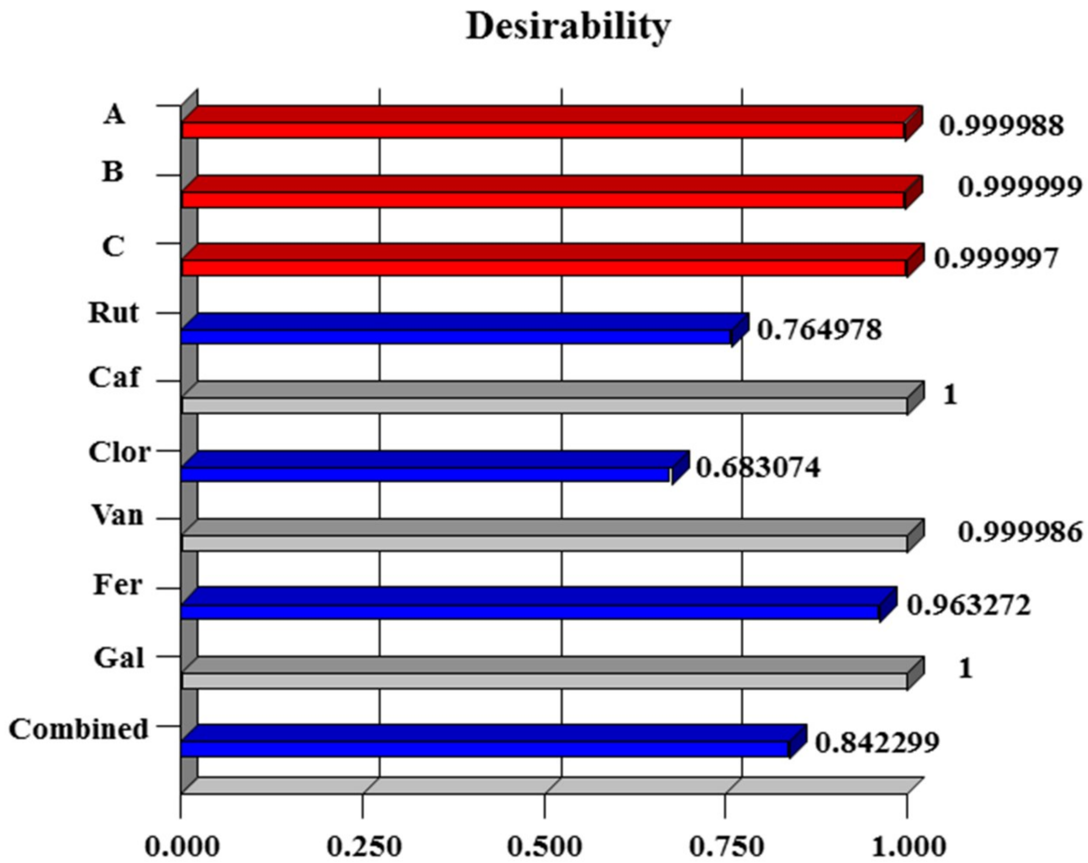

Fig. S2A. Analytical Greenness report summary of the present work.

Criteria	Score	Weight
1. Direct analytical techniques should be applied to avoid sample treatment.	0.48	2
2. Minimal sample size and minimal number of samples are goals.	0.85	2
3. If possible, measurements should be performed in situ.	0.66	2
4. Integration of analytical processes and operations saves energy and reduces the use of reagents.	0.8	2
5. Automated and miniaturized methods should be selected.	0.75	2
6. Derivatization should be avoided.	1.0	2
7. Generation of a large volume of analytical waste should be avoided, and proper management of analytical waste should be provided.	0.31	2
8. Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.	0.82	2
9. The use of energy should be minimized.	1.0	2
10. Reagents obtained from renewable sources should be preferred.	0.5	2
11. Toxic reagents should be eliminated or replaced.	0.31	1
12. Operator's safety should be increased.	0.8	2

Fig. S2B. Analytical Greenness report summary of Viacava et al. 2018.

Criteria	Score	Weight
1. Direct analytical techniques should be applied to avoid sample treatment.	0.48	2
2. Minimal sample size and minimal number of samples are goals.	0.98	2
3. If possible, measurements should be performed in situ.	0.66	2
4. Integration of analytical processes and operations saves energy and reduces the use of reagents.	0.8	2
5. Automated and miniaturized methods should be selected.	0.75	2
6. Derivatization should be avoided.	1.0	2
7. Generation of a large volume of analytical waste should be avoided, and proper management of analytical waste should be provided.	0.31	2
8. Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.	1.0	2
9. The use of energy should be minimized.	0.0	2
10. Reagents obtained from renewable sources should be preferred.	0.0	2
11. Toxic reagents should be eliminated or replaced.	0.25	1
12. Operator's safety should be increased.	0.6	2

Fig. S2C. Analytical Greenness report summary of Yang et al. 2018.

Criteria	Score	Weight
1. Direct analytical techniques should be applied to avoid sample treatment.	0.48	2
2. Minimal sample size and minimal number of samples are goals.	0.88	2
3. If possible, measurements should be performed in situ.	0.66	2
4. Integration of analytical processes and operations saves energy and reduces the use of reagents.	0.8	2
5. Automated and miniaturized methods should be selected.	0.75	2
6. Derivatization should be avoided.	1.0	2
7. Generation of a large volume of analytical waste should be avoided, and proper management of analytical waste should be provided.	0.39	2
8. Multi-analyte or multi-parameter methods are preferred versus methods using one analyte at a time.	1.0	2
9. The use of energy should be minimized.	0.0	2
10. Reagents obtained from renewable sources should be preferred.	0.0	2
11. Toxic reagents should be eliminated or replaced.	0.27	1
12. Operator's safety should be increased.	0.4	2