

Supplementary Material

***Path2Green*: Introducing 12 Green Extraction Principles and a Novel Metric for Assessing Sustainability in Biomass Valorization**

Leonardo M. **de Souza Mesquita**^{a*}, Leticia S. **Contieri**^a, Francisca A **e Silva**^b, Rafael Henrique **Bagini**^a, Felipe S. **Bragagnolo**^a, Monique **Strieder**^a, Filipe H. B. **Sosa**^b, Nicolas **Schaeffer**^b, Mara G. **Freire**^b, Sónia P. M. **Ventura**^b, João A. P. **Coutinho**^b, Maurício A. **Rostagno**^a

^a Multidisciplinary Laboratory of Food and Health (LabMAS), School of Applied Sciences (FCA), University of Campinas, Rua Pedro Zaccaria 1300, 13484-350, Limeira, Sao Paulo, Brazil.

^b CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal.

***corresponding author:** Dr. Leonardo M. de Souza Mesquita – mesquitalm@gmail.com

Table S1. List of articles evaluated considering the 12 principles assessed in *Path2Green* metric and their respective carbon footprint (expressed in $g_{CO2}/g_{biomass}$)

Reference	Scenarios	Principle 1	Principle 2	Principle 3	Principle 4	Principle 5	Principle 6	Principle 7	Principle 8	Principle 9	Principle 10	Principle 11	Principle 12	<i>Path2Green</i>	$g_{CO2}/g_{biomass}$
1	Reusing the alternative solvent	1	0.8	-0.2	0	-1	0.5	-0.5	1	-0.5	0.83	1	0.7	0.33	243.00
1	Not reusing the alternative solvent	1	0.8	-0.2	0	-1	0.5	-0.5	1	-0.5	0.83	0.5	-0.4	0.16	486.00
1	Using volatile organic solvent	1	0.8	-0.2	0	-1	-1	-0.5	1	-0.5	0.83	-1	-1	-0.15	814.00
2	Reusing the alternative solvent	1	-0.1	-0.2	1	-1	0	-0.5	1	0.5	0.83	1	1	0.45	423.84
2	Not reusing the alternative solvent	1	-0.1	-0.2	1	-1	0	-0.5	1	0.5	0.83	0.5	0.4	0.33	461.24
2	Using volatile organic solvent	1	-0.1	-0.2	0	-1	-1	-0.5	1	0.5	0.83	-1	-1	-0.15	1028.00
2	Using a biobased solvent	1	-0.1	-0.2	1	-1	-1	-0.5	1	0.5	0.83	-1	-1	-0.04	824.91
3		0.5	1.0	-0.2	1	-1	1	-0.5	1	-0.5	1	1	0.9	0.47	122.00
4		1	1.0	-0.2	0	1	0	-0.5	1	-0.5	0.83	1	0.9	0.54	95.00
5		0	1.0	-0.2	1	-1	0	0.5	1	0.5	1	0.5	1	0.48	44.00
6		0.5	0.7	-0.2	1	-1	-0.5	0.5	1	0.5	0.83	0.5	0.9	0.45	31.40
7		0	0.9	-0.2	0	-1	0.5	-0.5	1	0.5	0.83	0.5	0.8	0.27	550.00
8		1	1.0	-0.2	0	-1	0	-0.5	1	-0.5	0.83	0.5	-1	0.09	599.77
8	Reusing all the raw materials and reagents	1	1.0	-0.2	0	-1	0	-0.5	1	-0.5	0.83	1	1	0.44	464.20
8	Reusing all the raw materials and reagents +	1	1.0	-0.2	0	-1	0	-0.5	1	-0.5	0.83	1	1	0.37	464.20

	alternative drying														
8	Reusing all the raw materials and reagents + conventional high-energy dependence drying	1	1.0	-0.2	0	-1	0	-0.5	1	-1	0.83	1	1	0.15	544.96
9		1	-0.4	-0.2	0	-1	0	1	1	0.5	1	1	1	0.44	87.20
10		1	1.0	-0.2	0	-1	-1	0	1	0.5	0.66	-1	1	0.20	500.00
11		1	1.0	-0.2	1	1	0	-0.5	1	-0.5	0.83	-1	1	0.44	430.00
12		1	0.9	-0.2	1	1	0	-0.5	1	-0.5	0.83	-1	0.3	0.35	312.00
13		1	1.0	-0.2	0	-1	0	-0.5	-0.5	-0.5	0.83	-1	-1	-0.14	827.90
14		-0.5	1.0	-0.2	0	-1	0.5	-0.5	1	-0.5	0.83	-1	-1	-0.22	1052.00
15		0.5	0.7	-0.7	0	0.5	-	-0.5	-0.5	-0.5	0.83	-1	-1	-0.12	789.00
16		0	1.0	1	0	0.5	-	-0.5	-	-0.5	0.83	-1	-1	-0.04	693.00
17		1	-	-0.7	0	0.5	0	-0.5	-	-0.5	0.83	-1	1	0.12	358.00

DOWNLOAD THE APP



NOTES

- DO NOT FORGET TO SCORE ALL THE 12 PRINCIPLES
- (IF YOU WANT) YOU CAN SWITCH THE SUGGESTED WEIGHTS OF EACH PRINCIPLE
- THE FINAL SCORE VARIES BETWEEN:
-1.00 (LOWEST SCORE) TO
+1.00 (HIGHEST SCORE)

HOW TO USE

Home

- Biomass
- Transport
- Pre-treatment
- Solvent
- Scaling
- Purification
- Yield
- Post-treatment
- Energy
- Application
- Repurposing
- Waste
- Score

1ST:
FOR EACH OF THE 12 PRINCIPLES, CHOOSE THE APPROPRIATE SCORE AND WEIGHTS

2ND:
PRINT THE PICTOGRAM WITH THE FINAL SCORE OF YOUR PROCESS AND SHARE

	Path2Green		
	SCORE		
	0.000		

Figure S1. App Path2Green information and usage suggestions

References

- 1 L. M. de Souza Mesquita, S. P. M. Ventura, A. R. C. Braga, L. P. Pisani, A. C. R. V. Dias and V. V. de Rosso, *Green Chem.*, 2019, **21**, 2380–2391.
- 2 L. M. De Souza Mesquita, M. Martins, É. Maricato, C. Nunes, P. S. G. N. Quinteiro, A. C. R. V. Dias, J. A. P. Coutinho, L. P. Pisani, V. V. De Rosso and S. P. M. Ventura, *ACS Sustain. Chem. Eng.*, 2020, **8**, 4085–4095.
- 3 L. S. Contieri, T. B. Ribeiro, F. H. B. Sosa, B. M. C. Vaz, R. S. Pizani, M. Pintado, S. P. M. Ventura, L. M. de S. Mesquita and M. A. Rostagno, *ACS Sustain. Chem. Eng.*, , DOI:10.1021/acssuschemeng.3c03812.
- 4 L. M. de Souza Mesquita, L. S. Contieri, F. H. B. Sosa, R. S. Pizani, J. Chaves, J. Viganó, S. P. M. Ventura and M. A. Rostagno, *Green Chem.*, 2023, **25**, 1884–1897.
- 5 M. Kholany, N. Schaeffer, I. P. E. Macário, T. Veloso, T. Caetano, J. L. Pereira, A. C. R. V. Dias, J. A. P. Coutinho and S. P. M. Ventura, *ACS Sustain. Chem. Eng.*, 2023, **11**, 13594–13605.
- 6 M. Martins, L. M. D. S. Mesquita, B. M. C. Vaz, A. C. R. V. Dias, M. A. Torres-Acosta, B. Quéguineur, J. A. P. Coutinho and S. P. M. Ventura, *ACS Sustain. Chem. Eng.*, 2021, **9**, 6599–6612.
- 7 B. M. C. Vaz, M. Kholany, D. C. G. A. Pinto, I. P. E. Macário, T. Veloso, T. Caetano, J. L. Pereira, J. A. P. Coutinho and S. P. M. Ventura, *RSC Adv.*, 2022, **12**, 30278–30286.
- 8 L. M. de Souza Mesquita, F. H. B. Sosa, L. S. Contieri, P. R. Marques, J. Viganó, J. A. P. Coutinho, A. C. R. V. Dias, S. P. M. Ventura and M. A. Rostagno, *Food Chem.*, 2023, **406**, 135093.
- 9 F. A. Vicente, I. S. Cardoso, M. Martins, C. V. M. Gonçalves, A. C. R. V. Dias, P. Domingues, J. A. P. Coutinho and S. P. M. Ventura, *Green Chem.*, 2019, **2019**, 3816–3826.
- 10 M. Bisht, M. Martins, A. C. R. V. Dias, S. P. M. Ventura and J. A. P. Coutinho, *Green Chem.*, 2021, **23**, 8940–8948.
- 11 F. W. Maciel-Silva, L. E. N. Castro, W. G. Sganzerla, J. M. Costa, M. A. Rostagno and T. Forster-Carneiro, *J. Environ. Chem. Eng.*, 2024, **12**, 111641.
- 12 L. C. Da Silva, J. Viganó, V. L. Sanches, L. M. De Souza Mesquita, R. Pizani and M. A. Rostagno, *Food Chem.*, 2023, **407**, 135117.
- 13 D. C. Murador, A. R. C. Braga, P. L. G. Martins, A. Z. Mercadante and V. V. de Rosso, *Food Res. Int.*, 2019, 108653.
- 14 P. L. Garcia Martins, V. V. de Rosso, P. L. G. Martins and V. V. de Rosso, *Food Res. Int.*, 2016, **82**, 156–164.
- 15 K. Zaghdoudi, S. Pontvianne, X. Framboisier, M. Achard, R. Kudaibergenova, M. Ayadi-Trabelsi, J. Kalthoum-cherif, R. Vanderesse, C. Frochot and Y. Guiavarc'h, *Food Chem.*, 2015, **184**, 131–139.
- 16 R. L. Mendes, H. L. Fernandes, J. Coelho, E. C. Reis, J. M. S. Cabral, J. M. Novais and A. F. Palavra, *Food Chem.*, 1995, **53**, 99–103.
- 17 C. Didaskalou, S. Buyuktiryaki, R. Kecili, C. P. Fonte and G. Szekely, *Green Chem.*, 2017, **19**, 3116–3125.