Informações Suplementares

Article

Low-Temperature Partitioning Without Freezing in Liquid-Liquid Extraction: Determination of Thiamethoxam Residues in Percolation Water

Partição à Baixa Temperatura Sem Congelamento em Extração Líquido-Líquido: Determinação de Resíduos de Tiametoxam em Águas de Percolação

João Pedro M. Silva,[a] Anizio M. Faria[a,b,*]

[a]Universidade Federal de Uberlândia, Chemistry Institute, Separation Materials and Chromatography Research Laboratory, Zip Code 38400-902, Uberlândia-MG, Brazil

[b]Universidade Federal de Uberlândia, Pontal Institute of Exact and Natural Sciences, Separation Materials and Chromatography Research Laboratory, Zip Code 38304-402, Ituiutaba-MG, Brazil

*anizio@ufu.br

This is an open-access article distributed under the terms of the Creative Commons Attribution Licence.

Table S1. Textural and chemical properties of the red latosol used in this work

Soil Properties	
Depth collected (cm)	5-20
Coarse sand (g/kg)	256
Fine sand (g/kg)	528
Silt (g/kg)	31
Clay (g/kg)	185
Texture	medium
pH (in water)	4.93
Residual phosphorus [a] (mg/L)	34.59
Mehlich phosphorus [b] (mg/L)	18.94
Potassium [b] (mg/dm^3)	34.35
Calcium [c] (cmol$_c$/dm^3)	1.66
Magnesium [c] (cmol$_c$/dm^3)	0.75
Aluminum [c] (cmol$_c$/dm^3)	1.90
H + Al [d] (cmol$_c$/dm^3)	3.05
Effective cation exchange capacity (cmol$_c$/dm^3)	4.40
Total cation exchange capacity (cmol$_c$/dm^3)	5.55
Base saturation (cmol$_c$/dm^3)	45.13
m [e] (cmol$_c$/dm^3)	43.10
Some of the bases (cmol$_c$/dm^3)	2.51
Organic Matter [f] (cmol$_c$/dm^3)	0.04
Organic carbon (cmol$_c$/dm^3)	0.02
Cu [b] (cmol$_c$/dm^3)	1.35
Zn [b] (cmol$_c$/dm^3)	0.37
Mn [b] (cmol$_c$/dm^3)	0.15
Fe [b] (cmol$_c$/dm^3)	4.40
B [g] (cmol$_c$/dm^3)	0.09
S [h] (cmol$_c$/dm^3)	8.77

[a]: Residual phosphorus in a 10 mmol/L $CaCl_2$ solution containing 60 mg/L of P; [b]: Mehlich I extractor; [c]: KCl extractor at 1 mol/L; [d]: calcium acetate; [e]: aluminum Saturation; [f]: organic carbon x 1.724; [g]: extractor S - monocalcium phosphate in acetic acid; [h]: extractor B - hot water extractor.

This is an open-access article distributed under the terms of the Creative Commons Attribution Licence.

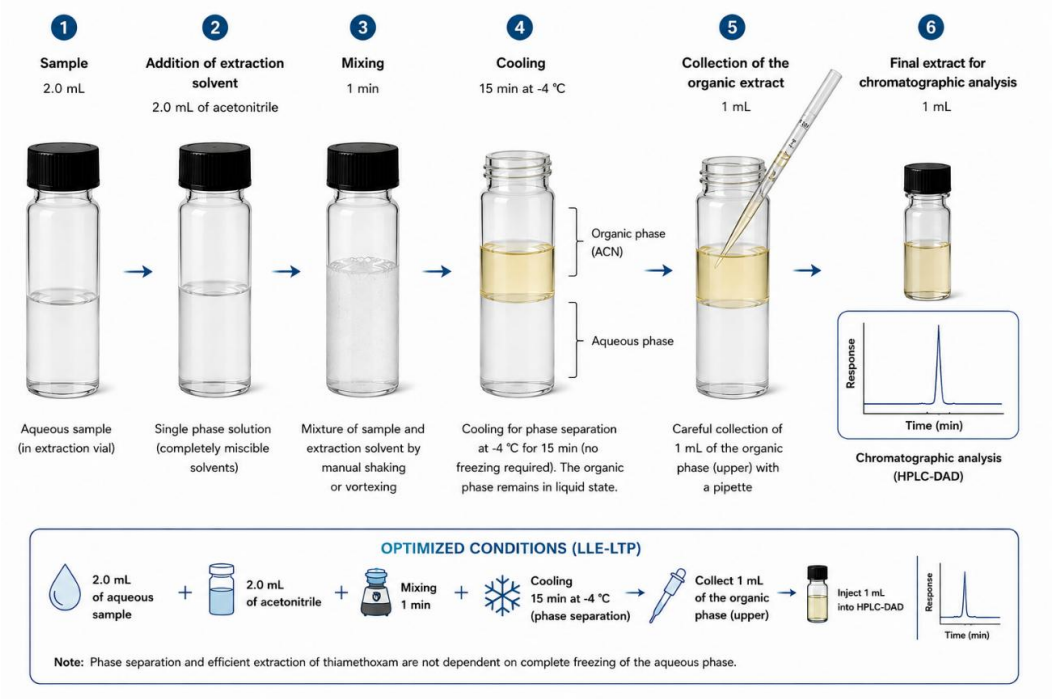


Figure S1. Scheme of the optimized procedure for liquid-liquid extraction with low-temperature partitioning of thiamethoxam in percolate water samples

#	Criterion		Score	Weight
1.	Sample preparation placement:	Ex situ	0.00	1
2.	Hazardous materials:	2 [g or mL]	0.23	5
3.	Sustainability, renewability, and reusability of materials:	> 75% of reagents and materials are sustainable or renewable	0.75	2
4.	Waste:	2 [g or mL]	0.52	4
5.	Size economy of the sample	Mass or volume of the sample: 2 [g or mL]	0.57	2
6.	Sample throughput:	120 [samples/h]	1.00	5
7.	Integration and automation	Sample prep. steps: 2 steps or fewer, Semi-automated systems	0.50	2
8.	Energy consumption:	0.1 [W]	1.00	4
9.	Post-sample preparation configuration for analysis:	GC and HPLC with non-MS detection, atomic absorption spectroscopy, capillary electrophoresis, etc.	0.50	2
10.	Operator's safety:	1 hazard	0.75	3

Figure S2. Evaluation of the analytical sustainability of the LLE-LTP/HPLC-DAD method using the AGREEprep metric,[1] considering criteria related to sample preparation, use of hazardous materials, waste generation, energy consumption, automation, analytical productivity, and operator safety

Bibliographic References

1. Pena-Pereira, F.; Tobiszewski, M.; Wojnowski, W.; Psillakis, E.; A tutorial on AGREEprep an analytical greenness metric for sample preparation. *Advances in Sample Preparation* **2022**, *3*, 100025. [Crossref]

This is an open-access article distributed under the terms of the Creative Commons Attribution Licence.