Scientific Letters

III 1H-TOXRUN International Congress 2024 02-03 May, 2024 | Porto, Portugal

Poster 46

Optimization of the chromatographic conditions of a multi-residue GC-MS method for trace analysis of pesticides and endocrine disruptors in drinking water

Diana Fernandes 1,2,4, Mariana Valente 1,4, Ana Rita Ribeiro 3,4 and Cláudia Ribeiro 1,5,*

Abstract

Background: Nowadays, the presence of pesticide residues and endocrine disruptors in sources for abstraction of drinking water has become a serious concern [1,2]. These classes negatively affect the environment, biodiversity, and public health. In this sense, monitoring these compounds in drinking water is essential to ensure its quality and safety on its use. Therefore, the development of sensitive analytical methods able of detecting the presence of these compounds even at residual concentrations is needed [1-3]. Objective: The aim of this study is to develop an analytical procedure by gas chromatography coupled to mass spectrometry (GC-MS) for the simultaneous quantification of different classes of pesticides and endocrine disruptors in drinking water. **Methods:** A method is being developed to analyze 14 compounds from a wide range of pesticide and endocrine disruptor classes. The latter were derivatized using N-methyl-N-(trimethylsilyl) trifluoroacetamide with 1% trimethylchlorosilane (MSTFA +1% TMCS) reagent and pyridine. Afterwards, the mixture was evaporated, reconstituted in acetate ethyl anhydrous and analyzed by GC-MS. The chromatographic conditions were: a capillary column 5% diphenyl 95% dimethyl polysiloxane (30 m x 0.25 mm x 0.25 mm), the injector temperature set at 280 °C, and a temperature ramp from 70 °C to 280 °C in a total run time of 30 minutes. Results: The target pesticides do not need to be derivatized for analysis, however, since endocrine disruptors require this process, all compounds were subjected to the derivatization step using the optimized conditions for endocrine disruptors, with the aim of including all compounds in the same sample preparation procedure and in a single chromatographic run. Analysis of the results allowed for the distinction and identification of all compounds. Conclusions: Derivatization conditions were optimized, and an analytical chromatographic method was developed allowing the separation and identification of 14 compounds belonging to various classes of pesticides and endocrine disruptors in 30 minutes.

Keywords: water quality assessment; environmental contaminants; chromatographic analysis

Acknowledgments

Diana Fernandes acknowledges the fellowship from project DropH2O (2022.08738.PTDC). Funding: This work is financially supported by national funds through the FCT/MCTES (PIDDAC), under the project 2022.08738.PTDC, PTDC with DOI 10.54499/2022.08738.PTDC (https://doi.org/10.54499/2022.08738.PTDC). ARR acknowledges the

¹ Associate Laboratory i4HB - Institute for Health and Bioeconomy, University Institute of Health Sciences - CESPU, 4585-116 Gandra, Portugal

² UCIBIO - Applied Molecular Biosciences Unit, Forensics and Biomedical Sciences Research Laboratory, University Institute of Health Sciences (1H-TOXRUN, IUCS-CESPU), 4585-116 Gandra, Portugal

³LSRE-LCM – Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials, Faculty of Engineering, University of Porto, 4200-465 Porto, Portugal

⁴ ALICE – Associate Laboratory in Chemical Engineering, Faculty of Engineering, University of Porto, 4200-465 Porto, Portugal ⁵ UCIBIO - Applied Molecular Biosciences Unit, Translational Toxicology Research Laboratory, University Institute of Health Sciences (1H-TOXRUN, IUCS-CESPU), 4585-116 Gandra, Portugal

[‡] these authors contributed equally to this work

^{*} Correspondence: claudia.ribeiro@iucs.cespu.pt

support from FCT funding under the Scientific Employment Stimulus Individual Call (2022.00184.CEECIND) and FCT/MCTES (PIDDAC): LSRE-LCM - UIDB/50020/2020 (DOI: 10.54499/UIDP/50020/2020) and UIDP/50020/2020 (DOI: 10.54499/UIDP/50020/2020); and ALiCE - LA/P/0045/2020 (DOI: 10.54499/LA/P/0045/2020).

References

- 1. Metcalfe, C.D.; Bayen, S.; Desrosiers, M.; Muñoz, G.; Sauvé, S.; Yargeau, V. Methods for the Analysis of Endocrine Disrupting Chemicals in Selected Environmental Matrixes. Environ Res (2022), 206, 112616.
- Rastkari, N.; Ahmadkhaniha, R.; Soleymani, F.; Ravanipour, M. Pesticide Residues in Drinking Water Treatment Plants and Human Health Risk Assessment: A Case Study from Northern Iran. Environ Geochem Health (2024), 46, 68.
- Schwanz, T.G.; Carpilovsky, C.K.; Weis, G.C.C.; Costabeber, I.H. Validation of a Multi-residue Method and Estimation of Measurement Uncertainty of Pesticides in Drinking Water Using Gas Chromatography-Mass Spectrometry and Liquid Chromatography-Tandem Mass Spectrometry. J Chromatogr A (2019), 1585, 10-18.



In Scientific Letters, works are published under a CC-BY license (Creative Commons Attribution 4.0 International License at https://creativecommons.org/licenses/by/4.0/), the most open license available. The users can share (copy and redistribute the material in any medium or format) and adapt (remix, transform, and build upon the material for any purpose, even commercially), as long as they give appropriate credit, provide a link to the license, and indicate if changes were made (read the full text of the license terms and conditions of use at https://creativecommons.org/licenses/by/4.0/legalcode).