



XXVII ENCONTRO NACIONAL

Sociedade Portuguesa de Química

Braga, 14-16 julho 2021



Chemistry and Opportunities in a Global Society

Book of abstracts

14-16th July 2021

Building II

Campus of Gualtar

University of Minho



SOCIEDADE PORTUGUESA DE QUÍMICA



Universidade do Minho
Escola de Ciências

Title

Livro de resumos do XXVII Encontro Nacional da Sociedade Portuguesa de Química
Book of abstracts of the XXVII National Meeting of the Portuguese Chemical Society

Editors

Ana Paula Estevão
Luís Monteiro
Maria Manuela Raposo
Sílvia Pereira-Lima
Susana Costa

Edition

Sociedade Portuguesa de Química

Graphic design

Renato Gonçalves
Sílvia Pereira-Lima

Date

July 2021

ISBN

978-989-8124-33-3 (digital edition)

Recommended cataloging

Livro de resumos do XXVII Encontro Nacional da Sociedade Portuguesa de Química
Departamento de Química, Universidade do Minho, 2021 – 345 p.
ISBN 978-989-8124-33-3

This book was produced from the abstracts submitted directly by the authors, in accordance with the rules publicly disclosed in the event's announcements. Only small formatting changes were introduced that did not modify the scientific contents, which are the sole responsibility of the respective authors.



- P23** *Gas-phase standard molar enthalpies of formation of some anthranilate derivatives.*
C. A. O. Silva, Centro de investigação em Química (CIQUP), Department of Chemistry and Biochemistry, Faculty of Sciences – University of Porto, Portugal.
- P24** *Development of innovative materials for antibiotics removal.*
A. Saraiva, CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal.
- P25** *New strategies for the removal of cytostatics from urine.*
R. Francisco, CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal.
- P26** *Determination of sertraline antidepressant drug in aqueous effluents by SPE/HPLC-DAD.*
V. Machado, Mountain Research Centre (CIMO), Polytechnic Institute of Bragança, Portugal.
- P27** *Effect of zeolite nanomaterials in methanogenic communities.*
J. F. Faria, Centre/Department of Chemistry, University of Minho, Portugal.
- P28** *Complexos heterolépticos de cobre (I) como catalisadores da CuAAC.*
M. S. Viana, LAQV-REQUIMTE, Departamento de Química, NOVA School of Science and Technology (FCT NOVA), Portugal.
- P29** *Heterogeneous photocatalysis and photo-Fenton as integrated water treatment.*
A. Torres-Pinto, Laboratory of Separation and Reaction Engineering - Laboratory of Catalysis and Materials (LSRE-LCM), Faculdade de Engenharia, Universidade do Porto, Portugal.
- P30** *Evaluation of a triphenylamine-derived thiosemicarbazone as an optical chemosensor for anions.*
Â. B. M. P. Leite, Centre/Department of Chemistry, University of Minho, Portugal.
- P31** *Biodegradation potential of microplastics by bacteria recovered from the marine environment.*
N. F. de Villalobos, Centro de Ciências do Mar do Algarve, Universidade do Algarve, Portugal.
- P32** *Optimization of SPME/GC-MS analytical method using response surface methodology for pesticides monitoring in aqueous matrices.*
F. Cáceres, Mountain Research Centre (CIMO), Polytechnic Institute of Bragança, Portugal.

Posters

P1	T. F. P. Alves	P39	C. Q. V. da Costa	P77	A. Seco
P2	C. Rodrigues	P40	I. I. Afonso	P78	M. Rocha
P3	F. Chamorro	P41	B. L. C. Santos	P79	I. S. Oliveira
P4	R. Lopes	P43	L. A. S. Cavaca	P80	A. Camuenho
P5	M. S. T. Gonçalves	P44	A.C.S. Ferreira	P81	A. C. Santos
P6	J. R. A. Coelho	P45	D. R. P. Loureiro	P82	G. Colucci
P7	A. G. Fortes	P46	A. Dias	P83	M. Nunes
P8	L. V. Cavichi	P47	S. Sousa	P84	H. Boumeriame
P9	M. Barral-Martinez	P48	D. Pereira	P85	F. F. Roman
P10	P. Garcia-Oliveira	P49	B. Ferreira	P86	R. Rua
P11	F. Campos	P50	C. Machado	P87	D. X. Moreira
P12	I. Pereira	P51	F. Durães	P88	D. M. Fernandes
P13	D. Leithardt	P52	F. Carvalhal	P89	F. M. Almeida
P14	M. Jesus	P53	J. Moreira	P90	E. R. F. P. Pereira
P15	J. S. Amaral	P54	R. Lima	P91	I. S. O. Barbosa
P16	A. Otmani	P55	J. L. Serrano	P92	F. Monteiro
P17	T. B. Schreiner	P56	A. C. Amorim	P93	M. Colaço
P18	S. Hussien	P57	A. Lopes	P94	F. Leitão
P19	J. M. Fernandes	P58	V. Lobo	P95	S. C. Barros
P20	C. V. Boas	P59	A. Dias	P96	R. Rebelo
P21	G. S. Catalão	P60	D. Dantas	P97	I. F. M. Costa
P22	A. R. R. P. Almeida	P61	S. Pêra	P98	Y. Gué
P23	C. A. O. Silva	P62	L. Filipe	P99	B.D.D. Cruz
P24	A. Saraiva	P63	V. S. D. Gomes	P100	T. A. Fernandes
P25	R. Francisco	P64	C. A. S. Almeida	P101	M. P. Loureiro
P26	V. Machado	P65	A. T. Silva	P102	H. M. Rafael
P27	J. F. Faria	P66	S. C. Silva-Reis	P103	R. Gonçalves
P28	M. S. Viana	P67	D. S. P. Cardoso	P104	H. T. Gomes
P29	A. Torres-Pinto	P68	R. Padanha	P105	J. F. Martinho
P30	A. B. M. P. Leite	P69	S. D. C. Ferreira	P106	D. Gago
P31	N. F. de Villalobos	P70	M. Fonte	P107	L. G. Teixeira
P32	F. Cáceres	P71	J. P. Costa	P108	R. Anastácio
P33	I. M. Beltrán	P72	R. M. Durão	P109	T. I. de Menezes
P34	A. Nobahar	P73	A. C. M. O. Lima	P110	A. I. Costa
P35	R. Abreu	P74	B. R. Gomes	P111	P. D. Barata
P36	J. Teixeira	P75	V. Gomes	P112	F. C. Rodrigues
P37	P. M.S. Sousa	P76	M. M. Silva	P113	L. B. Silva

Environment and water

Optimization of SPME/GC-MS analytical method using Response Surface Methodology for pesticides monitoring in aqueous matrices

F. Cáceres,^{a,b} R. Pepino,^b P. Brito,^a A.E. Ribeiro,^a A. Queiroz^a

a) Centro de Investigação de Montanha (CIMO), Instituto Politécnico de Bragança, Campus de Santa Apolónia, 5300-253 Bragança, Portugal; b) Universidad Tecnológica Nacional - Facultad Regional Córdoba, Maestro M. López esquina. Cruz Roja Argentina, Ciudad Universitaria, 5016 Córdoba, Argentina

Email: amqueiroz@ipb.pt

Emerging pollutants are a type of contaminants that can occur in water sources. They can be defined as any synthetic or naturally occurring chemical or microorganism that is not usually monitored or regulated in the environment and have the potential to cause detrimental ecological and human health impacts. These compounds can be found in the environment in very low concentrations, at scales ranging from nanograms to micrograms per liter.¹ Pesticides are an important group of emerging pollutants due to the continuous increase in their use in agricultural production process to control diseases, pests and weeds.²

In this work, it will be presented the optimization of solid phase microextraction (SPME), using a response surface methodology (RSM) based on an experimental planification defined using a Box-Behnken Design (BBD). After optimization of the complete analytical methodology (SPME/GC-MS), the method validation is done by monitoring six of the most used pesticides in northeast of Portugal (acetochlor, alachlor, dimethoate, heptachlor, metolachlor and terbuthylazine). The molecular structures of the compounds under study are presented in **Figure 1**. The method is validated through its application using real samples of aqueous matrices collected from different rivers of the region.

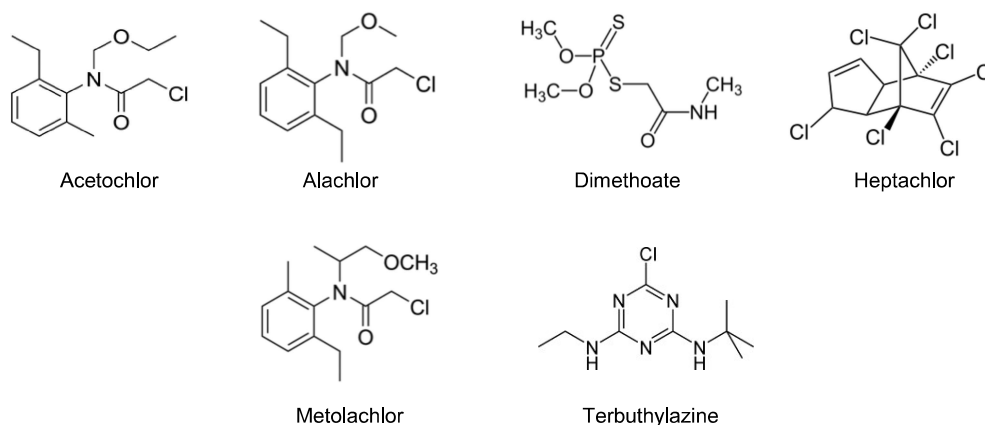


Figure 1: Chemical structures of the studied pesticides.

Acknowledgements: The authors are grateful to the Foundation for Science and Technology (FCT, Portugal) for financial support by national funds FCT/MCTES to CIMO (UIDB/00690/2020).

References:

1. Calvo-Flores, F. G.; Isac-García, J.; Dobado, J. A. *Emerging pollutants: origin, structure, and properties*. Wiley-VCH **2018**, 6-9.
2. Stefanakis A. I.; Becker J. A. *A review of emerging contaminants in water: classification, sources, and potential risks. Impact of Water Pollution on Human Health and Environmental Sustainability* (McKeown A. E., Bugyi G., eds.) **2016**, 55-80.