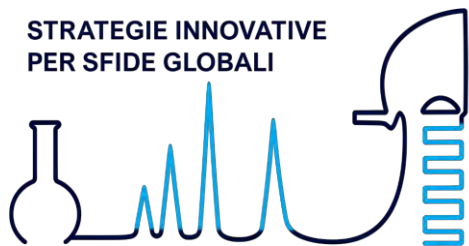


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O-CHEMO-07

Untargeted Screening of Emerging Contaminants in Wastewater: comparing chromatographic methods through a novel ROI-MCR based approach

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3D printing is emerging as a transformative technology in electroanalytical chemistry, The increasing regulatory [1] and scientific attention [2] devoted to emerging contaminants (ECs) in wastewater and reclaimed water calls for analytical strategies capable of extending contaminant monitoring beyond predefined target lists. In this context, untargeted UHPLC-HRMS/MS workflows represent a valuable tool for the screening of both known and previously unrecognized ECs. However, several analytical challenges still limit their broader application, including sample pretreatment, chromatographic selectivity, and, above all, data-processing strategies able to extract chemically meaningful features while minimizing background signals and artefacts.

In this work, we investigated the performance of two different chromatographic stationary phases, namely a biphenyl column and a C18 column, within an untargeted UHPLC-HRMS/MS workflow applied to wastewater and reclaimed water samples. The main objective was to evaluate the suitability of the two chromatographic systems for the detection of the widest possible range of contaminants, while proposing a strategy for feature selection within a Regions of Interest-Multivariate Curve Resolution (ROI-MCR) [2] data-treatment workflow. Particular attention was devoted to the effect of threshold values and to the definition of feature-selection criteria based on blanks, reference standards, and evaluation of ROI and MCR-component quality.

For each selected MCR model, putative assignment was performed on the basis of accurate mass and retention time, and selected features were compared with Compound Discoverer outputs. The proposed strategy allowed assessment of the complementarity of the two chromatographic systems and highlighted the importance of robust ROI-MCR feature-selection criteria for improving interpretability and reducing false-positive signals in untargeted screening workflows.

Acknowledgements

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P-CHEMO-05

A Proof of Concept for the Detection of Emerging Contaminants in Wastewater Using Portable Spectroscopy and MCR-ALS

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Nowadays, water scarcity is a major concern, and the reuse of treated wastewater could be a key strategy to support water conservation within circular economy frameworks. For these reasons timely monitoring of emerging contaminants (ECs), such as pharmaceuticals and personal care products, that may persist after treatment is crucial. This study, developed within the EXWASTER project, explores the integration of portable vibrational spectroscopy (MiniRaman, microNIR) and advanced chemometric modeling as a rapid and solvent-free strategy for the screening of ECs directly on sorbent materials used for sample preconcentration. Spectra were acquired directly on hydrophilic–lipophilic balance (HLB) resins from SPE cartridges and POCIS passive samplers, avoiding solvent extraction prior to analysis.

A multistandard mixture of selected ECs (caffeine, metoprolol, atenolol, diclofenac, and hydrochlorothiazide) was prepared following a structured Design of Experiments (DoE), enabling systematic variation of concentration levels and controlled generation of multicomponent mixtures. Given the strong spectral overlap and the complexity of the sorbent matrix, Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) was adopted as the core data analysis strategy.

MCR-ALS enabled the resolution of latent components attributable to individual ECs and to the sorbent background, despite partial collinearity and overlapping vibrational features. The structured DoE significantly contributed to reducing rotational ambiguity and stabilizing the decomposition. A benchtop Raman spectrometer, enabling spatially resolved Raman mapping was also tested to investigate analyte distribution within the sorbent phase.

Acknowledgements

Funded by the Ministry of University and Research under the Call for Proposals related to the scrolling of the final rankings of the PRIN 2022 call for proposals. Project Title: EXploitation of targeted and untargeted analytical strategies for WASTEwater monitoring: toward a sustainable water management according to the principles of circular economy- EXWASTER. Prot. n° 2022L3AH34. Principal Investigator: C. Durante.

P-ABC-25

Occurrence and environmental monitoring of per- and polyfluoroalkyl substances (PFAS) in groundwater

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Per- and polyfluoroalkyl substances (PFAS) are synthetic contaminants with no natural sources, widely detected in groundwater even in the absence of identified emission points, reflecting their high mobility and persistence in subsurface environments. Their diffuse occurrence, combined with increasingly stringent regulatory limits at the ng/L level, highlights the need for reliable analytical approaches for groundwater monitoring, particularly based on SPE and LC–MS/MS methodologies [2,3]. PFAS contamination in aquifers has been extensively reported in European and Italian groundwater systems [1,2,4,5], where it is often associated with diffuse sources, industrial activities, and long-range transport processes, while regional-scale data remain limited. In this study, the occurrence of seven PFAS (PFBS, PFHxS, PFOS, PFPeA, PFHxA, PFHpA, PFNA) was investigated in groundwater samples collected in the province of Modena (Emilia-Romagna, Italy). Samples were preconcentrated by solid-phase extraction and analyzed by LC–MS/MS operating in electrospray ionization negative mode and multiple reaction monitoring. The analytical performance of the method was assessed according to commonly accepted validation criteria for PFAS determination, confirming its suitability in terms of sensitivity, accuracy, and precision for trace-level analysis in groundwater, with no significant carry-over effects. PFAS were detected at low concentrations, with sporadic occurrence of selected compounds, indicating a generally limited yet diffuse contamination of groundwater. This finding is consistent with literature data [2] and reflects the environmental behavior of PFAS in subsurface systems. Overall, the results provide new data on PFAS occurrence in groundwater in the Emilia-Romagna region and support groundwater quality assessment within the current regulatory framework.

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P-ABC-34

Soil-biodegradable chitosan-cutin coatings for sustainable controlled release fertilizers

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The intensive use of mineral fertilizers has increased crop yields but has also led to environmental and economic concerns, including nutrient leaching, volatilization, and low nutrient use efficiency. Controlled-release fertilizers (CRFs) represent a promising strategy by enabling a gradual release of nutrients according to plant demand [1]. However, conventional coatings are often based on non-biodegradable synthetic polymers that may accumulate in the environment.

This study focuses on the development of a biodegradable coating for CRFs based on chitosan and cutin, two natural polymers with film forming properties. The objectives were to (i) formulate a chitosan-cutin suspension, (ii) optimize its application on fertilizer granules, (iii) identify a suitable substrate, and (iv) perform preliminary nutrient release tests.

Three commercial fertilizers were evaluated, and one formulation showed the best performance in terms of structural stability and coating response. Two solvent systems were investigated, an initial water-rich formulation, which caused partial granule degradation, and a second ethanol-rich formulation, which improved suspension stability, coating applicability, and granule integrity.

Two application methods were compared, immersion and spray coating. Immersion resulted in pigment loss and fragmentation, while spray application preserved granule structure. The optimized process, based on 14 spray cycles with intermediate drying at 40 °C, led to a more uniform and homogeneous coating, as confirmed by stereomicroscopy observations.

Preliminary nutrient release tests (NPK) were conducted in two substrates (25% pumice, 50% coconut fiber, 25% wood fiber; and 70% peat, 30% pumice) under both natural and artificial light conditions; analyses are currently ongoing.

Overall, the results demonstrate the potential of chitosan-cutin biodegradable coatings as a sustainable alternative for CRFs, improving nutrient management while reducing environmental impact.

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