

	Fanny MATHIAUX (2025 - 2028)
	Characterization of Chemical Pressure Fingerprints in Streams of Small Catchments: Development of Non-Targeted Analytical Strategies for Organic Compounds
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Project description

The quality of surface waters is deteriorating due to various anthropogenic pressures exerted on catchments, whether direct (discharges of treated or untreated wastewater, industrial activities, agriculture, etc.) or indirect (climate warming, eutrophication, etc.) (European Environment Agency et al., 2015; Johnes et al., 2023). The artificial alteration of watercourses and the release of uncontrolled synthetic substances into the environment constitute two of the six planetary boundaries already exceeded (out of nine in total) (Richardson et al., 2023). Organic micropollutants—such as pesticides, pharmaceuticals and personal care products, plasticizers, surfactants, and flame retardants—are now ubiquitous in aquatic systems and contribute, even at very low concentrations, to their degradation (Finckh et al., 2024). However, their monitoring alone is not sufficient to characterize the full range of chemical pressures acting on catchments.

Dissolved Organic Matter (DOM), defined purely technically as the fraction of organic matter not retained by a filter with porosity $< 0.45 \mu\text{m}$ (Artifon et al., 2019), plays a crucial role in the hydrosphere, particularly as a source of nutrients, UV shield, and thermal regulator (Johnes et al., 2023; Minor and Oyler, 2023; Rose et al., 2009). Its alteration could have serious consequences for flora and fauna, as well as for overall water quality. Years of watershed studies and monitoring have revealed changes in the concentration and composition of natural DOM in surface waters attributable to human activities, with largely unexplored consequences for ecosystem functioning and the global carbon cycle (Chen et al., 2023; Evans et al., 2006; Williams et al., 2016).

To better characterize organic contamination in watercourses (DOM and micropollutants), new analytical strategies must be developed. Over the past fifteen years, non-target screening (NTS) approaches based on high-resolution mass spectrometry (HR-MS) coupled with chromatography—generally liquid chromatography (LC)—have become key techniques in environmental analysis due to their ability to detect signals from thousands of organic micropollutants (Hollender et al., 2023; Krauss et al., 2010). Despite their great potential, these strategies have not yet found their place in the field of DOM characterization, which remains scarcely explored in the literature (Ribeiro et al., 2017; Uehara et al., 2025). Therefore, the primary objective of this PhD is to improve acquisition and data-processing strategies (workflows), along with sampling strategies (passive or active), sample preparation (direct injection, solid-phase extraction, etc.), and LC-HR-MS methods, to characterize chemical pressures acting on small catchments.

A bank of samples collected at the outlets of small (sub-) catchments—already the subject of previous studies and for which metadata (hydro-climatic conditions, type of drained sub-catchment, land use, anthropogenic activities, etc.) are available—will be established. Sampling will also account for temporal variability (e.g., high-flow/low-flow cycles, seasonality of agricultural practices). Since NTS data are intrinsically dependent on the reprocessing steps implemented in workflows, substantial optimization work will be required to ensure data quality and robustness. Only then can these data be interpreted through multivariate analyses comparing them with (1) more conventional DOM characterization results (dissolved organic carbon, UV-visible spectrophotometry, HPSEC) and (2) catchment metadata (land use and land cover, hydro-climatic conditions, etc.). These comparisons will enable the development of new indicators of chemical pressures on watercourses, which may support decision-makers (public authorities, managers, users, etc.) in better assessing the health of aquatic environments under human influence and in optimizing actions for improved management and protection (Hernández et al., 2019; Johnes et al., 2023).

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