White paper

Polarity-Extended Chromatography:

A holistic solution for the analysis of organic molecules in the aqueous environment

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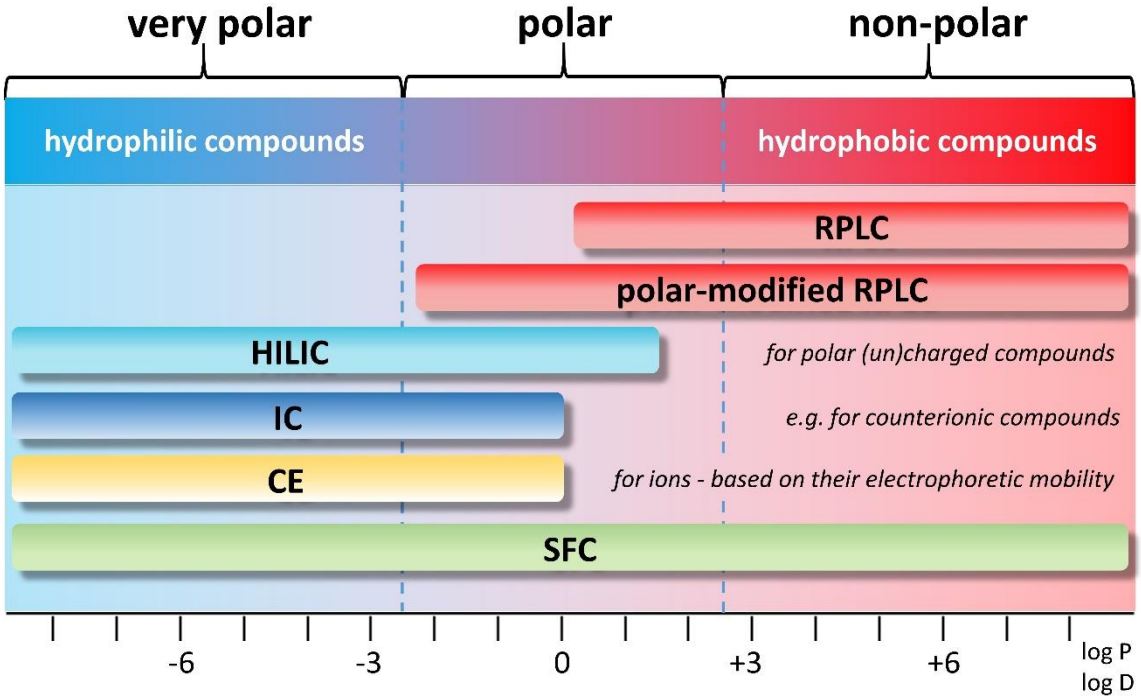
The gaining interest in persistent, mobile and toxic (PMT) and very persistent and very mobile (vPvM) substances in waterbodies resulted in the requirement to adjust the applied analytical techniques towards these compounds, which are often (very) polar, i.e. mostly with a logD (pH) ≤ 0 and some of them ionic. On the molecular level these (organic) compounds are perfectly suitable to analytical techniques like mass spectrometric detection and a prior chromatographic/electrophoretic separation.

This comment is a contribution to the special issue 'Persistent and Mobile Organic Compounds – An Environmental Challenge' of the Journal 'Analytical and Bioanalytical Chemistry' which we recommend to read [1]. Herewith, we would like to address and point towards chromatographic techniques which are available and useable for analyzing (simultaneously and combined) non-polar, polar and very polar molecules in one single run with so called 'polarity-extended chromatography'.

Commonly applied chromatographic techniques like gas chromatography and reversed phase liquid chromatography (RPLC) can be used for a chromatographic separation of non-polar and polar molecules. However, they reach their limits in analyzing very polar molecules. For such molecules, techniques like polar-modified RPLC, Hydrophilic Interaction Liquid Chromatography (HILIC), Ion Chromatography (IC), Capillary Electrophoresis (CE) and Supercritical Fluid Chromatography (SFC) can be applied to close the 'analytical gap' in the very polar region (see Figure below).



Polarity scheme for chromatographic (electrophoretic) separation techniques regarding the logD (logP) values of separable molecules and molecule characteristics.

For several years we apply now two very robust polarity-extended chromatographic separation techniques in research studies as well as in routine applications, i.e. the serial RPLC-HILIC coupling and the (polar stationary phase) SFC [2]. These two techniques provide orthogonal and complementary separations [3] and cover the full spectrum of polarity from non-polar to very polar compounds. As a consequence, the use of these techniques in environmental analysis closes the often-observed 'monitoring gap'. Both techniques offer the chance to widen the analytical scope significantly towards very polar compounds and to complement already used analytical techniques for polar and non-polar compounds such as RPLC without the requirement of two individual analysis of a sample.

Impressive examples using this chromatographic strategy presented the studies of sulfamethoxazole [4], diclofenac [5], and bisphenol A [6] degradation (in wastewater treatment) by electrochemical oxidation (in which very polar molecules like oxalic acid, fumaric acid, and/or inorganic by-products emerged).

The benefits of this 'polarity extended chromatography' have also been reported in various further matrices like red wine [7], plant metabolome [8] and house dust [9]. This gives hope for the global and fast usage of polarity extended analysis of PMTs and vPvMs monitoring in close future (especially in environmental non-target screening [10]).

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please cite as:
Bieber S and Letzel T (2020) White Paper – Polarity-Extended Chromatography, AFIN-TS Forum; February (1): 1-4.

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