

Assessing the universe of solid phase extraction (SPE) of polydisperse dissolved organic matter (DOM)

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Dissolved organic matter (DOM) is a complex mixture of organic molecules with ~50% carbon content and various proportions of oxygen, nitrogen, phosphorus and sulfur [1]. DOM is one of the most abundant contributors to the global carbon pool, and is actively involved in many diverse key aquatic ecosystem processes.

DOM isolation is essential as it directly affects both dissolved organic carbon (DOC) recovery and the selectivity of isolated molecules, upon which all consecutive evaluation has to exclusively rely. For any characterization of polydisperse and molecularly heterogeneous DOM, consequences of erroneous sampling always exceed those resulting from inattentive analysis.

Meanwhile, DOM isolation should provide high yield for providing representative materials with limited bias to ensure authenticity. In sharp contrast to even the most complex mixtures of biomolecules extracted from living organisms, polydisperse biogeochemical supermixtures such as freshwater and marine DOM from water bodies cannot be resolved into individual molecules at present as a result of the huge number ($>10^6$) of diverse molecules present in any fraction [1].

Solid phase extraction (SPE) employs sample-, sorbent- and solvent-dependent interactions to temporarily retain DOM; eluted fractions commonly show beneficial properties in organic structural spectroscopy such as FTICR mass spectrometry, NMR and EEM spectroscopy [2]. We have mapped the solid phase extraction (SPE) process of freshwater and marine DOM, using 24 types of commercially available SPE materials and systematic variation of elution conditions (loading, flow rate, loading, up-scaling) and investigating eluates, permeates and wash fluids by complementary NMR, FTMS and EEM spectroscopy [3, 4, 5]. The findings obtained are significant to enable dependable isolation of representative fractions of polydisperse DOM from different sources. These findings will aid in development of reproducible and standardized DOM isolation protocols enabling large scale studies of DOM while minimizing the inconsistencies among laboratories.

[1] Hertkorn *et al* (2007) *Anal. Bioanal. Chem.* **389**, 1311-1327. [2] Hertkorn *et al* (2013) *Biogeosciences* **10**, 1583-1624. [3] Li *et al* (2016) *Anal. Chem.* **88**, 6680-6688. [4] Li *et al* (2016) *Water Research* **106**, 477-487. [5] Li *et al* (2017) *Water Research* **107**, in press.