

The importance of water quality in LC-MS/MS

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Introduction

- Chromatographers take great care in the selection of salts and organic solvents used in mobile phase preparation, but selecting the best type of water is sometimes an arduous task.
- LC-MS/MS requires the use of high purity water to prepare the aqueous mobile phase, for method blanks, control sample, precision and recovery measurements.
- The presence of so-called emerging contaminants in the environment is of increasing concern in the scientific community and the general public. In recent years, several studies conducted in Europe and North America have shown the presence of a variety of medications and cosmetic products in environmental waters, as well in some tap waters.
- The high purity water used in analytical laboratories, be it bottled HPLC-grade, LC-MS grade, or from a water purification system, comes from tap water that was purified. This study is aimed at investigating the potential impact of these environmental contaminants for LC-MS/MS users.

Pharmaceuticals and Personal Care Products

The increasing use of pharmaceuticals and personal care products (PPCP) containing persistent organic compounds has led to the contamination of many water sources. Medications such as antibiotics, anti-inflammatory drugs, birth control pills, etc. have been found in environmental waters in many different locations (Table 1).

Compound	Median (Maximum) concentration (ng/L)			
	France	Germany	Austria	Finland
Carbamazepine	78 (800)	25 (110)	75 (294)	70 (370)
Diclofenac	18 (41)	150 (1200)	20 (64)	15 (40)
Ibuprofen	23 (120)	70 (530)	ND	10 (65)
Iopromide	7 (17)	100 (910)	91 (211)	-
Sulfamethoxazole	25 (133)	30 (480)	ND	-

ND: not detected

Adapted from the WHO technical report entitled Pharmaceuticals in drinking-water (2011)

Table 1. Concentrations of selected PPCPs in surface waters of several European countries.

Experimental Methods

In this study, the concentrations of PPCPs were measured in HPLC-grade and LC-MS grade bottled water (from competitors), and after tap water was purified by reverse osmosis.

Sample Preparation

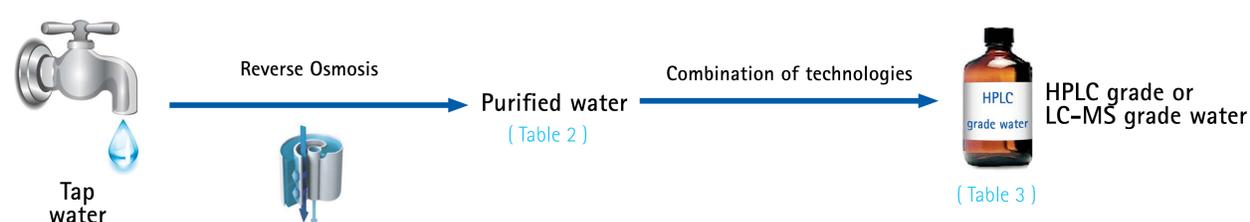
- 250 mL water sample was extracted using Oasis HLB cartridges (conditioned with methanol and Milli-Q® water).
- Cartridge was washed, dried under vacuum, and eluted with methanol.
- Eluent was evaporated to 100 µL and reconstituted with 900 µL of 20% acetonitrile in Milli-Q® water with 0.1% formic acid.

LC-MS/MS conditions

- System LC-MS/MS Agilent 1100, AB SCIEX 4000 QTRAP®
- Column Supelco C-18, 150x2.1 mm
- Flow 0.25 mL/min
- Inj. volume 10 µL
- Eluent A 0.1% formic acid in Milli-Q® water
- Eluent B 0.1% formic acid in acetonitrile

Results and Discussion

- In many locations around the world, tap water contains small amounts of many contaminants, including PPCPs, as shown in Table 2 for Rolla, MO, USA.
- Reverse osmosis is a water purification technique that efficiently removes a wide class of water contaminants. It is used in water treatment plants and desalination plants. Tap water, after it has gone through reverse osmosis, still contains some PPCPs originally present in tap water (Table 2). Thus, additional purification techniques are necessary to further reduce the levels of these contaminants.
- HPLC grade and LC-MS grade bottled waters are usually prepared using several additional purification techniques, such as deionization, UV photo-oxidation, activated carbon and a filter. Deionization reduces ionic species, but most PPCPs are not in their ionized form in water. UV radiation and activated carbon are used to reduce organic contaminants in water. Four PPCPs were still detected in the HPLC grade and LC-MS grade bottles of water tested (Table 3).



Compound	Concentration (ng/L)	
	Tap water	After reverse osmosis
Acetaminophen	2.505	ND
Caffeine	76	9.04
Carbamazepine	12.56	1.38
Erythromycin	ND	ND
Lincomycin	2.39	0.5
Sulfamethoxazole	7.68	1.22
Trimethoprim	9.94	1.02

Table 2. Concentrations of PPCPs in the tap water of Rolla, MO, USA, and after purification by reverse osmosis.

Compound	Concentration in bottled water (ng/L)	
	HPLC grade	LC-MS grade
Acetaminophen	ND	ND
Caffeine	11.24	10.08
Carbamazepine	0.21	0.17
Erythromycin	ND	ND
Lincomycin	0.37	0.44
Sulfamethoxazole	ND	ND
Trimethoprim	0.35	0.37

Table 3. Concentrations of PPCPs in HPLC grade and LC-MS grade bottled water.

Conclusion

- Advances in HPLC and MS technologies have made possible trace quantification of PPCPs in various water sources. In many locations worldwide, tap water has been shown to contain some PPCPs.
- High purity water for laboratories comes from tap water that has been purified. Reverse osmosis does not completely remove the PPCPs found in tap water.
- HPLC grade or LC-MS grade bottled water, which has undergone extensive water purification steps, may still contain some PPCPs.
- There is a need for improved water purification techniques that can deliver high purity water suitable for even the most sensitive LC-MS/MS analyses.