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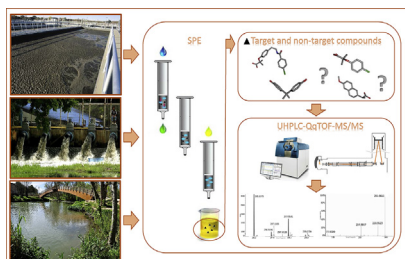
Universal method to determine acidic licit and illicit drugs and personal care products in water by liquid chromatography quadrupole time-of-flight



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GRAPHICAL ABSTRACT



ABSTRACT

Pharmaceuticals, illicit drugs and personal care products are emerging contaminants widely distributed in water. Currently, a number of solid-phase extraction (SPE) procedures followed by liquid chromatography tandem mass spectrometry (LC–MS/MS) have been reported. However, target analysis of selected compounds is commonly used whereas other related contaminants present in the sample remain invisible. Carmona et al. [1] described a method for determining 21 emerging contaminants by LC–MS/MS with improved mobile phases. We tested this protocol in combination with high resolution mass spectrometry using a quadrupole time-of-flight (QqTOF) instrument to get a wide non-target screening approach in order to have a broader scope and more practical method for detecting licit and illicit drugs and personal care products than traditional target methods. The essential points in the method are:

- The screening capabilities of QqTOF (ABSciex Triple TOF™) are used for detecting and identifying non-target pharmaceuticals and a large number of other emerging contaminants in water.

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- The quantitative features of the instrument, the Achilles heel of the QqTOF mass spectrometers, are established for few selected compounds.
- The method may be applied to identify a large number of emerging contaminants in water. However, pre-validation will be needed to quantify them.

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ARTICLE INFO

Method name: Non-target screening by SPE and UHPLC quadrupole time-of-flight

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Method details

Many different types of pollutants have been found in environmental compartments as water. Licit and illicit drugs or personal care products are some of the so-called emerging contaminants extensively used by humans [1,2]. A number of analytical methods are already available [3–9] to determine emerging contaminants in environmental matrices at low concentrations. However, these methods are only reported for one type of instrument. In this study, we proposed a procedure to analyse pharmaceuticals, illicit drugs, personal care products and others contaminants on different water matrices through a common method for a triple quadrupole (QqQ) and a quadrupole time-of-flight (QqTOF) mass spectrometers.

Reagents and materials

Acetaminophen, bezafibrate, bisphenol A, butylparaben, chloramphenicol, clofibrac acid, diclofenac, ethylparaben, flufenamic acid, gemfibrozil, ibuprofen, indomethacin, methylparaben, naproxen, propylparaben, salicylic acid, thiamphenicol, triclocarban, triclosan and warfarin from Sigma-Aldrich (The Woodlands, Texas, USA) and tetrahydrocannabinol (THC) and 11-nor-9-carboxy- Δ^9 -tetrahydrocannabinol (THC-COOH) from LoGiCal (Luckenwalde, Germany) were used as target analytes for QqQ analysis. Calibration standards were prepared by serial dilution of the mixed working solution. Stock and working solutions were stored at -20°C in the dark [10].

Water used for preparation of calibration standards and LC-MS mobile phase was purified by an Elix Milli-Q system (Millipore, Billerica, MA, USA). Methanol was purchased from Panreac (Castellar del Vallès, Barcelona, Spain) and formic acid was purchased from Amresco (Solon, OH, USA). Ammonium fluoride was acquired from Alfa Aesar GmbH & Co KG (Karlsruhe, Germany).

Extraction procedure

- (1) Vacuum filter the samples (250 mL) through 0.45 μm retention capacity glass fiber filter of 90 mm diameter by Advantec (Toyo Roshi Kaisha, Ltd., Japan) using a Bücher funnel (with the filter) over a 250 mL Kitasato flask with 400 mbar h^{-1} Pa^{-1} of vacuum, to remove solid particles before the solid phase extraction (SPE).
- (2) Put the Phenomenex Strata-X 33u Polymeric Reversed Phase (200 mg/6 mL) cartridges (Phenomenex, Torrance, Ca, USA) into a 12 port vacuum manifold Supelco Visiprep 57030-U of Sigma-Aldrich (St. Louis, MO, EEUU).
- (3) Condition the cartridge with 6 mL methanol and 6 mL of Milli-Q water both with 400 mba h^{-1} Pa^{-1} vacuum.
- (4) Pass the samples through the cartridges under previous vacuum at a flow rate of 10 mL min^{-1} .
- (5) Wash the cartridges with 6 mL of Milli-Q water.
- (6) Dry the cartridges under vacuum for 15 min.
- (7) Elute the analytes on a 15 mL Falcon tube VWR (Radnor, PA, USA) with 6 mL of methanol and then 3 mL of a methanol-dichloromethane solution (1:1, v/v) at gravity flow.

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