Anal Bioanal Chem
DOI 10.1007/s00216-014-7614-1

RESEARCH PAPER

Elucidation of transformation pathway of ketoprofen, ibuprofen, and furosemide in surface water and their occurrence in the aqueous environment using UHPLC-QTOF-MS

A. Jakimska · M. Śliwka-Kaszyńska · J. Reszczyńska · J. Namieśnik · A. Kot-Wasik

Received: 30 September 2013 / Revised: 31 December 2013 / Accepted: 2 January 2014

Abstract
The identification and determination of transformation products (TPs) of pharmaceuticals is essential nowadays, in order to track their fate in the aqueous environment and, thus, to estimate the actual pollution. However, this is a challenging task due to the necessity to apply high-resolution instruments enable to detect known and unknown compounds. This work presents the use of liquid chromatography quadrupole time-of-flight mass spectrometry (LC-QTOF-MS) as a powerful tool for the identification of three selected pharmaceuticals, furosemide (FUR), ibuprofen (IBP), and ketoprofen (KET), and their TPs in various water samples. Laboratory degradation experiments were performed using xenon lamp as a source of the irradiation in order to simulate phototransformation processes which may occur in the environment. Furthermore, the photodegradation kinetics of three selected compounds were assessed in a reactor equipped with xenon lamp in river water samples. Five TPs of IBP, seven of KET, and five of FUR were identified; some of them are presented here for the first time. Accurate mass measurements and fragmentation pattern obtained during an LC-QTOF-MS analysis allowed for structure elucidation of TPs followed by the creation of transformation pathway of selected pharmaceuticals. Finally, different water samples (wastewater influent and effluent, river water, untreated and treated water) were analyzed in order to estimate the presence of parent and transformed compounds. Only KET was detected in untransformed form in considered samples. Most of the TPs of selected drugs were found at least once in all water samples. Although IBP and FUR were not present in water samples as parent compounds, their different TPs occur. A great potential of LC-QTOF-MS in the identification and structural elucidation of TPs in the environment, allowing the recognition of the fate of pharmaceuticals in the environment through the determination of transformation pathway, has been presented.

Keywords Pharmaceuticals · Irradiation · Aqueous environment · Transformation products · Transformation pathway

Published in the topical collection *Euroanalysis XVII* (The European Conference on Analytical Chemistry) with guest editor Ewa Bulska.

Electronic supplementary material The online version of this article (doi:10.1007/s00216-014-7614-1) contains supplementary material, which is available to authorized users.

A. Jakimska (✉) · J. Namieśnik · A. Kot-Wasik
Department of Analytical Chemistry, Chemical Faculty, Gdańsk University of Technology (GUT), G. Narutowicza Street 11/12, 80-233 Gdańsk, Poland
e-mail: anik.jakimus@interia.pl

M. Śliwka-Kaszyńska
Department of Organic Chemistry, Chemical Faculty, Gdańsk University of Technology (GUT), G. Narutowicza Street 11/12, 80-233 Gdańsk, Poland

J. Reszczyńska
Department of Chemical Technology, Chemical Faculty, Gdańsk University of Technology (GUT), G. Narutowicza Street 11/12, 80-233 Gdańsk, Poland

Introduction

Pharmaceutically active compounds (PhACs) have become an increasingly serious problem in recent years due to their continuous introduction to environmental waters from wastewater treatment plants (WWTPs) [1, 2]. Global consumption

Published online: 23 January 2014