RESUMO - CONTAMINANTES EMERGENTES E AGROTÓXICOS

RETROSPECTIVE ANALYSIS OF ORGANIC CONTAMINANTS IN DRINKING WATER

Viviane Emi Nakano (viviane.fukasawa@ial.sp.gov.br)

Cibele Nicolaski Pedron (cibelenpedron@gmail.com)

Alan Roberto Costa (alan.costa@ial.sp.gov.br)

Lucas Monteiro Santa Cruz (lucas.cruz@ial.sp.gov.br)

Iracema De Albuquerque Kimura (iracema.kimura@ial.sp.gov.br)

Letícia S. J. Miranda (leticiasilva_33@hotmail.com)

Adriana Palma De Almeida (adriana.almeida@ial.sp.gov.br)

Simone Alves Da Silva (simone.silva@ial.sp.gov.br)

Denise Piccirillo B Da Veiga (denisepiccirillo@gmail.com)

Cristiane Maria Tranquillini Rezende (ctrezende@saude.sp.gov.br)

Janete Alaburda (janete.alaburda@ial.sp.gov.br)

Jose Oscar Vega Bustillos (ovega@ipen.br)

High-resolution Mass Spectrometry (HRMS) is a highly selective qualitative technique that enables retrospective analysis of compounds not targeted in the initial screening. New substances and contaminants are constantly emerging, so this is an important tool that can be used to look for specific compounds at later without re-extraction and re-running samples, or using reference standards

for adjustment and optimization. In this study, screening was carried out to investigate contaminants by LC- HRMS Orbitrap in 160 drinking water samples collected by health authorities of São Paulo state as part of Monitoring Program between February 2021 and April 2023. The researched compounds included pesticides authorized of the 10 main crops in São Paulo state, the most marketed pharmaceutical drugs in Brazil, as well as narcotics and veterinary drugs, totalizing 198 analytes. The HRMS demonstrated good performance in full scan mode for the identification and confirmation of compounds, based on accuracy of mass measurement less than 5 ppm, isotope abundances, and MS spectral information. Under these conditions, the retrospective analysis not found residues of narcotics and other medicine drugs, but indicated the presence of three pesticides: Tebuthiuron (N=2), Triadimefon (N=1) and Metalaxyl-M (N=2), which were in accordance with intense local agricultural activity. These results complement previous analyses carried out on these samples during the Monitoring Program, which investigated 91 pesticides and detected Atrazine, 2,4-D, Diuron, Bentazone, and Tebuconazole. The suspect screening analysis demonstrated to be a valuable technique for determining chemical contaminants in Monitoring Programs, providing subsidies for governmental actions to guarantee the quality of water consumed by the population, as well as future discussions to review of legislation.

Palavras-chave: drinking water; lc-hrms orbitrap; non-target screening; pesticides.