

基於高解析質譜法對台灣南部污水中之濫用藥物  
進行目標與非目標分析

Profiling of illicit drugs using high-resolution mass spectrometry  
based non-targeted and targeted approaches in wastewater  
in southern Taiwan

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Abstract

The use of illicit drugs is often estimated by measuring the weight of drugs that are intercepted and seized, but it may not provide a comprehensive and accurate investigation of the widespread use of illicit drugs. Wastewater can be used to monitor illicit drug use at the population level. Compared to traditional methods for monitoring illicit drugs, wastewater-based epidemiology (WBE) can determine drug consumption at the population level. The use of high-resolution mass spectrometry (HRMS) is a powerful analytical tool to detect trace amounts of illicit drugs in wastewater. This study aimed to profile the illicit drugs in wastewater by HRMS-based non-targeted analysis and identify the 15 common abused drugs in Taiwan by HRMS-based targeted analysis. Two liters of wastewater samples were collected from Nanzhih wastewater treatment plant. A portion of the sample (240 mL) was filtered through a 0.22 µm glass microfiber filter and subjected to solid phase extraction (SPE). The wastewater samples were then concentrated 1000-fold and subjected to HRMS analysis. The analytical samples were analyzed by HRMS with full scan and data-dependent acquisition (DDA) modes to collect the MS and MS/MS spectra. For targeted analysis, the MS spectra and MS/MS spectra of 15 standards were collected by full scan and DDA mode, which were used for the identification of compounds in wastewater samples. For non-targeted analysis, the MS/MS spectra collected by DDA mode were matched to the mzCloud database using the Compound Discoverer software, and a total of 21 drugs were identified based on the match factor > 70. Based on the source of the drug, they were narcotic drugs, psychoactive drugs, and metabolites of relative drugs. For targeted analysis, 5 of 15 target drugs were identified in the wastewater samples, including amphetamine, ketamine, mephedrone, morphine, and norketamine. To sum up, there were 26 compounds identified in wastewater collected in Nanzhih, including 5 illegal drugs and 6 narcotic drugs, and other painkillers. In the future, WBE can be applied to estimate the consumption of drugs within the service area of Nanzhih wastewater treatment plant.

關鍵字：非法藥物、濫用藥物、污水、非標的物分析、液相層析高解析質譜法

Keywords：Illicit drugs、Drug abuse、Wastewater、Non-targeted analysis、LC-HRMS