使用基於高解析質譜之可疑物篩查策略針對人類毛髮中暴露體進行特徵分析

Characterization of human exposome in hair using a high-resolution mass spectrometry-based suspect screening strategy

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Abstract

Urine is commonly used for assessing human exposure to toxicants, while it can only reflect short-term toxicant exposure. Hair analysis can be used for the long-term and retrospective determinations; however, using hair as the alternative biospecimen for exposure assessments is lacking. This study aimed to apply hair for profiling human exposome using an ultra-high performance liquid chromatography coupled with high-resolution mass spectrometry (UHPLC-HRMS) based suspect screening strategy. We generated an in-house human exposome suspect list (n=1154) collected from National Report on Human Exposure to Environmental Chemicals published by the U.S. CDC and the Exposome-Explorer 3.0 database developed by the WHO for suspect screening. We prepared 990 mg pooled hair samples from 3-cm hair segments collected from 66 participants (including 22 elderly subjects and 44 young adult subjects) and underwent a sample preparation procedure, including decontamination, homogenization, and extraction. The hair extracts were further analyzed by UHPLC-HRMS with full scan, and the raw data was processed with MS-DIAL software. We annotated the features as the suspect hits by comparing the experimental m/z values in HRMS dataset with the theoretical m/z values within 5 ppm. To further identify the chemical structures of suspect hits, the corresponding MS/MS spectra were collected by data-dependent acquisition (DDA) mode and annotated within Massbank of north America (MoNA) database for identification. The feature number in average were 24,279 in positive mode and 13,602 in negative mode, respectively. There were 332 suspects in positive mode matched with the in-house suspect list, 485 suspects in negative mode, respectively. 182 suspects were identified with MS/MS spectrum by annotation in MoNA database. Among them, there were 14 suspects identified with authentic chemical standards, including 8 phthalate metabolites, 4 parabens metabolites, and perfluorohexanoic acid (PFHxA). Furthermore, 8 phthalate metabolites identified in hair have been previously reported in the urine. Overall, hair may be a suitable biospecimen for characterization of the human exposome.

關鍵字：暴露體、頭髮、特徵分析、可疑物篩查、液相層析高解析質譜法
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