Development of analytical methods for rapid and comprehensive identification of chemical substances

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We developed a rapid, accurate and comprehensive method to detect a wide range of volatile substances typically released during industrial accidents or disasters. This method uses portable analyzers to quickly measure a wide range of volatile organic compounds in combination with laboratory analyzers capable of performing exhaustive analysis.

In subtheme 1, we developed a portable analyzer that can simultaneously measure a wide range of substances with sufficient sensitivity and comprehensiveness, mainly for volatile organic compounds.

In subtheme 2, we developed a simultaneous analysis method for semi-volatile organic compounds that can be used in the event of chemical spills or leaks due to accidents or disasters and created a support tool.

We selected substances to be measured during disasters, collected data such as relative retention time, detection intensity, and calibration curves, and added 179 substances that could be identified and quantified to the AIQS database. We then confirmed the measurement accuracy by AIQS and proposed a highly accurate identification method using GC/QTofMS. Furthermore, we developed a manufacturer-independent AIQS (MI-AIQS) that can be analyzed by any manufacturer's GCMS and started operating a Web version of MI-AIQS. We also developed a field survey support site available to environmental research departments and provided information on the Web-based version of AIQS to D.ChemCore, the information infrastructure for Theme 1. In collaboration with local environmental research institutions, we promoted the dissemination of the AIQS and conducted field surveys during several disasters to verify the effectiveness of the AIQS.

In subtheme 3, we have registered accurate mass and collision cross-section information in the database built into liquid chromatograph quadrupole time-of-flight mass spectrometer (LC-QTOFMS), mainly for organic chemicals with low volatility. Subsequently, we developed a comprehensive analysis method for river water and wastewater samples, in Japan. To strengthen our analysis techniques, we conducted screening analyses for chemicals in river water and wastewater and confirmed the accuracy of quantification. The chemicals most detected in the samples were pharmaceuticals and personal care products, derived from daily consumption or usage by humans. Analysis of samples from the influent and effluent of a sewage treatment plant revealed caffeine to be present only in the influent, indicating a caffeine removal efficiency of 100% by the sewage treatment.

Furthermore, dilution of samples before solid-phase extraction or their direct injection

into LC-QTOFMS without pretreatment paired the quantification accuracy.

[References]

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