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Development of Automated Identification and Quantification System (AIQS) for Target Screening and Its Application to Environmental Samples

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Chemical substances are indispensable materials for modern society. The number and production volume of them therefore have been rapidly increasing. Since some of them however give adverse effects on human health and the ecosystem, a lot of survey has been carried out for clarifying occurrence of them and has found that the environment is polluted by a large number of chemicals. However, the number of surveyed chemicals and survey frequency are not sufficient due to limitation of the existing analytical methods, indicating needs of novel comprehensive analytical methods.

The objectives of this study were to develop 1) a novel automated identification and quantification system (AIQS) that can measure a large number of chemicals without the use of standard substances and 2) comprehensive target screening methods using AIQS by which we can simultaneously analyse a large number of chemicals in a short time and with low cost.

Nowadays GC-MS is one of the most frequently used analytical instruments for analysing organic substances due to high sensitivity and selectivity. So we have developed AIQS for GC-MS. AIQS consists of retention times, mass spectra and calibration curves of nearly 1000 semi-volatile organic compounds (SVOCs). Retention times (RTs) of them when analysing samples are predicted by using their programmed temperature retention indexes and retention times of n-alkanes. Differences between actual and predicted RTs are less than 3s, which is the same level as differences obtained by the conventional method measuring standard substances before sample measurement. Slopes of calibration curves are maintained using the designated GC-MS conditions. As a result, correct identification and quantification are performed without the use of standard substances.

Two comprehensive target screening methods that can accurately determine the SVOCs registered in AIQS have been developed. SVOCs in water samples were extracted liquid-liquid extraction with CH_2Cl_2 or tandem solid-phase extraction (SPE) using Sep Pak PS-2 and AC-2 cartridges. Results of recovery tests showed that almost SVOCs except for polar substances were quantitatively extracted. Method detection limits of most substances were less than 10 μg/L. In addition, since 110 substances such as PCBs and organochlorine pesticides were measured by SIM, their MDLs were one-tenth of MDLs obtained by scan mode.

As a result of application of the developed methods, the combination of extraction methods and AIQS, to actual environmental samples, rivers in China, Vietnam and Japan, substances detected in three countries were almost the same, indicating that chemical pollution has spread globally by globalization of the economy. Whereas, detected concentrations between three countries were quite different from each other; concentrations in Japan were lower than in China and Vietnam. This difference may be due to difference of use and management of chemical substances and also due to the penetration rate of wastewater treatment facilities. From these results, it was confirmed that comprehensive target screening using AIQS is a useful tool for grasping a whole pollution picture by chemicals.