DEVELOPMENT OF A GC/MS SOFTWARE FOR MULTIPLE COMPOUND SCREENING AND TENTATIVE QUANTIFICATION INCLUDING QUALITY CONTROL PROCEDURES

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Introduction

Due to a significant increase in the number of compounds being monitored under various circumstances, methods of simultaneous analysis are growing in popularity and importance. However, for multiple analysis, particularly in cases with a large number of target compounds, both the analysis itself and the management of standard compounds are complicated and difficult. We developed a GC/MS software for the purpose of enabling multiple compound analysis easily by screening and tentative quantification using databases rather than standard compounds, combined with proper quality control procedures. This report describes the conception and methodology of this software.

Software and database design

For typical GC/MS trace analysis, qualification and quantification are done based upon the retention time and response factor of the target compound. These two values normally vary from one instrument to another, and from day to day. For qualification and quantification, the standard should be analyzed at the same time as sample analysis, followed by revising the compound's information such as the calibration curve. This is the one of the reasons why multiple analysis is so complicated. Also, the target compounds' standard is required every time. To simplify a simultaneous analysis, a new GC/MS method using a database instead of standard compounds was introduced[1)]. The framework of the software we developed basically builds on this method, with several modifications. This software operates by associating with databases which were built aiming to "fix" the values conventionally obtained by standard analysis. As a result, the software enables GC/MS to determine numerous chemicals without standard compounds except for a few internal standard compounds. To make compound information registered in the database applicable to any analysis, the GC/MS parameters were strictly defined in the building of the database and in practical analysis. For this software three kinds of databases were constructed: mass spectra, retention time and relative response factor (RRF). The mass spectra registered were those yielded by DFTPP target tuning according to US EPA method 625. The retention time database was developed based upon the retention time locking (RTL) technique, which was introduced several years ago[2)]. The RRF was calculated in the same way as the general internal standard method using deuterium-labeled PAHs as internal standard. About 1,000 hazardous chemicals were registered in these databases. In this software, determination is done by retention time and RRF databases which work as a "calibration curve", and the mass spectra database is used for confirming identification.

Results and discussion

The key factor for the success of this software and method is consistency of the retention time and the RRF over all instruments any time under the same GC/MS parameters. To check the consistency of the retention time, the RTL was evaluated and demonstrated good reproducibility. Concerning the RRF, a uniform mass spectrum pattern is needed because ions for quantification are normally different between the internal standard and analytes. This is the main reason the MS database is DFTPP tuned. Using DFTPP tuning, relative standard deviations of ion ratios with m/z 69 are 4.88% for m/z 50, 3.45% for m/z 131, 3.83% for m/z 219, 4.13% for m/z 414, and 6.15% for m/z 502 for the six instruments used. This deviation will be added to that derived from conventional internal standard quantification; hence the conventional method essentially has better quantitative accuracy than this method. This additional deviation seemed to be small enough for practical use; however, conventional determination will be helpful when more precise quantification is needed after detection using this software. One more significant factor affecting RRF is the GC/MS chromatographic conditions. To minimize deviation among instruments, proper instrument quality control is very important. This is executed by analyzing a "performance check sample" containing several compounds which tend to be keenly influenced by the

conditions of each GC/MS element: injection port, column or MS. Then each GC/MS part is checked by the chromatographic result, typically a tailing factor or peak ratio. The sample chemicals selected depended upon our practical experience and availability in Japan. For instance, Isoxathion, a pesticide, is characteristically difficult to analyze when the injection liner is dirty, so it was chosen instead of p,p'-DDT. Because of its well-known decomposition due to dirty injection liners, p,p'-DDT may be suitable as a sample for checking GC/MS elements; however, it is regulated under the Stockholm Convention on Persistent Organic Pollutants. All calculations and reporting for performance checks are done by the software automatically. This software can perform "whole analysis", meaning it can analyze all of the compounds registered in the database, without the need to specify a particular target compound, similar to screening. This software can also perform "standard-less" determination, or tentative quantification.

References

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