

Detecting System of Unusual Data for Dioxins

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Introduction

QA/QC is necessary to acquire reliable analytical results of dioxins through each step of collecting the sample, pretreatment, GC/MS analysis, determination, calculation and reporting.

Based on the nation-wide dioxin surveys conducted in Japan, a usual value range and compound composition in each environmental medium can be determined. When an analytical result lies outside of the usual values of the isomer composition, it is often helpful to check the data in order to find out a value with analytical problem.

Sakiyama et al.¹ inspected the results of nation-wide surveys for dioxins and reported a set of criteria to extract unusual data based on statistical consideration and expertise judgment. We report here the GUI-based computer program to help a check of data in these terms. We derived the usual concentration range and isomer composition by processing the results of nation-wide dioxin surveys^{2,3} based on statistical consideration and expertise judgment.

Operating procedure of the system

This system operates on Microsoft® Excel. This system consists of a program file, a data file to be evaluated and a reference data file. We use the aforementioned data^{2,3} as reference data. The number of reference data are following, atmosphere 1548, dust deposition 410, soil 344, groundwater 539, open water 1050, aquatic sediment 750, fish and shellfish 3204.

1) input of the parameter

Before the data processing, it is necessary to input the following parameter.

X : X percentile, criterion for a decision of unusual data.

2) pretreatment of the data

When the data are less than quantification limit (in some cases detection limit), the data in concentration are assigned to zero.

3) comparison of the data with reference data in concentration

When the data to be evaluated are less than X percentile or more than (100-X) percentile of reference data in concentration, the data to be evaluated are judged to be unusual data.

4) comparison of the data with reference data in compound composition ratio

When the data to be evaluated are less than X percentile or more than (100-X) percentile of reference data in compound composition ratio, the data to be evaluated are judged to be unusual data.

5) correlation among isomers, homologue, and toxicity equivalency quantity (TEQ)

At first we calculate correlation factors among isomers, homologue, and TEQ in reference data. If correlation factor is more than 0.95, we extract the pair, calculate the regression line and the distance of each data point to the line. In the same way we calculate the distance of the data to be evaluated and when the distance of the data to be evaluated are more than (100-X) percentile of the distance of reference data, the data to be evaluated are judged to be unusual data.

6) judgment of the data from usual isomer composition

We derived a set of usual isomer compositions from the nation-wide dioxin surveys^{2,3} and decided the boundary between usual and unusual data. We judged whether the data to be evaluated are usual or unusual using the boundary line.

Conclusion

If the data to be evaluated are judged to be unusual data, it is desirable to inspect the data and review the analytical records. But it does not always mean an error in the analytical procedure and also that the data judged to be unusual is wrong data and the usual data is correct data with no problem. It should take notice that there is a possibility these criteria may apply only to Japanese data because they are based on Japanese surveys. It is important to fix the analytical results by noticing the concentration and isomer composition. We would be glad if this system is helpful to QA/QC in your laboratory.

Acknowledgments

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References

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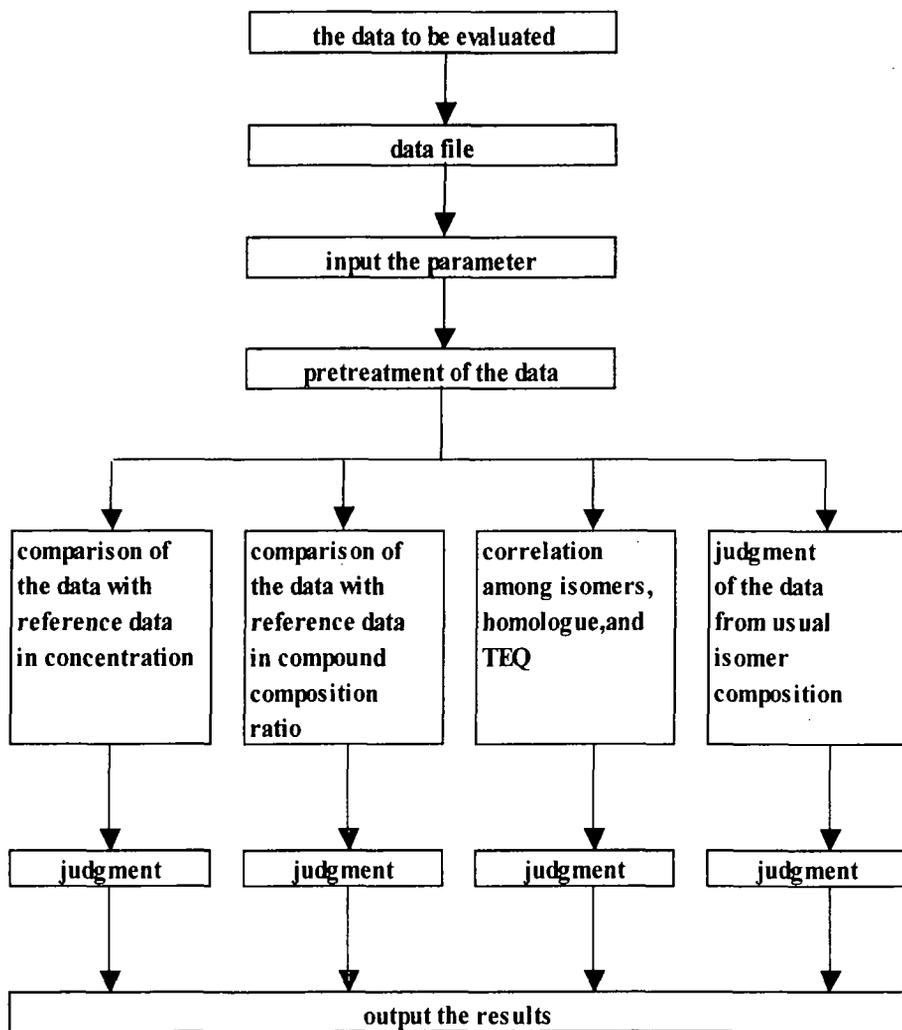


Fig.1 Flowchart of this system