

SPME Guidelines

Because of recent confusion and misuse of SPME techniques, the Journal of Chemical Ecology has adopted the following guidelines. We suggest that authors print a copy of these for future reference.

Guidelines for Quantitative Analysis by SPME

1. Determination of absolute quantities

Determination of absolute amounts is possible by SPME when calibrating one's own method with appropriate quantitative standards. Reference compounds must be mixed in relative proportions similar to those that are quantified in the target samples, because high amounts of a main compound A will influence the amounts of a trace component B that elutes shortly after A. Calibration by internal and external standards will be needed; methods must be described in detail. The data obtained this way also can be used to calculate quantities of compounds relative to the total peak area.

Without such calibration, quantitation by SPME requires consideration of the apparatus and equipment, and calculations as described by e.g.

Bartelt, R.J. (1997). *Anal. Chem.* 69: 364-372;

Bartelt, R.J. (1998). *J. Chem. Ecol.* 24: 535-558;

Bartelt, R.J. & Zilkowski, B.W. (1999). *Anal. Chem.* 71: 92-101;

Bartelt, R.J. & Zilkowski, B.W. (2000). *Anal. Chem.* 72: 3949-3955.

2. Determination of relative quantities

(a) Determination of amounts of target compounds relative to total peak area by SPME allows the comparison of quantities of the SAME compound in different samples if constant sampling conditions are used for all samples. All samples need to be collected and analysed exactly the same way. This includes use of the same fiber during all comparative analyses, and controlled, stable temperatures of the sample chambers. Comparisons of these relative peak areas allow one to determine if quantities of peak #1, 2, etc. in species A are x-fold higher/lower than quantities of the SAME peaks in species B.

(b) Determination of relative quantities by SPME does NOT allow one to compare quantities of different compounds in the same sample. For example, species A may release 10 major volatile compounds in its exocrine secretion. Relative quantitation by SPME does NOT allow one to compare relative quantities of peak#1, 2 etc. and does NOT allow one to state that quantities of compound #1 are x-fold higher/ lower than quantities of peak #2 (because of different affinities of different compounds on the fiber, because of different vapor pressures of the target compounds, and because of different response factors of the compounds with the particular detector being used).

In summary, relative quantification of compounds by SPME allows the comparison of amounts of a specific compound across samples/species, whereas comparison of amounts of different compounds within a sample are NOT possible by relative SPME quantification