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METAS UncLib – A Measurement Uncertainty Calculator in Chemical Analysis

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Evaluation of measurement uncertainty (MU) in chemical analysis is essential to make measurement results comparable and to fulfill the requirement of metrological traceability to reference values obtained by agreed realizations of the SI units. It is therefore also a requirement for all accredited laboratories working under ISO/IEC 17025:2017. With the Guide to the Expression of Uncertainty in Measurement (GUM)[1], an internationally accepted and uniform procedure for the evaluation of MU was established. However, without the help of an uncertainty propagation software, it can be very challenging and time-consuming to implement this approach in a mathematically correct way, especially for complicated analytical methods.

METAS UncLib[2], a software library that facilitates the linear propagation of uncertainties through a measurement model is in full accordance with the GUM and is one of the most versatile MU calculators available. METAS UncLib can be downloaded free of charge at [3]. It is written in C#, and MATLAB and Python wrappers exist. So far, METAS UncLib has been mainly known in the physical community. We think that it can be of great use for chemists as well for establishing their MU budgets.

In our laboratory, we use METAS UncLib together with Python for the evaluation of the MU in the determination of polycyclic aromatic hydrocarbons (PAHs) in food matrices, for example. The analytical method is composed of solvent extraction of the test material, multi-stage purification by solid-phase extraction (SPE) and/or gel permeation chromatography (GPC), and measurement with GC-MS/MS using isotopically labelled internal standards. It currently includes the 16 PAHs listed in EPA610. For each PAH, our measurement model relates more than 45 input quantities, each exhibiting uncertainties, to the output quantity, the mass fraction of the PAH in the tested food. As an example, the figure shows the results of a measurement of contaminated infant formula. While for PAH4 (sum of benz[a]anthracene (BaA), benzo[a]pyrene (BaP), benzo[b]fluoranthene (BbF), and chrysene (Chr)), the lower bound of the MU at the 95 % level (k = 2) is clearly above the regulated maximum level, there is an overlap of the MU range for BaP. In this case, MU is a key factor for conformity assessment.

In conclusion, METAS UncLib is perfectly suited as a measurement uncertainty calculator in chemical analysis, especially for complicated analytical methods including a large number of chemical compounds.

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[1] BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP, OIML, Evaluation of Measurement Data - Guide to the Expression of Uncertainty in Measurement, *JCGM/WG1* **2008**, *100*.
[2] M. Zeier, J. Hoffmann, M. Wollensack, *Metrologia* **2012**, *49*, 809, https://doi.org/10.1088/0026-1394/49/6/809.
[3] https://www.metas.ch/unclib

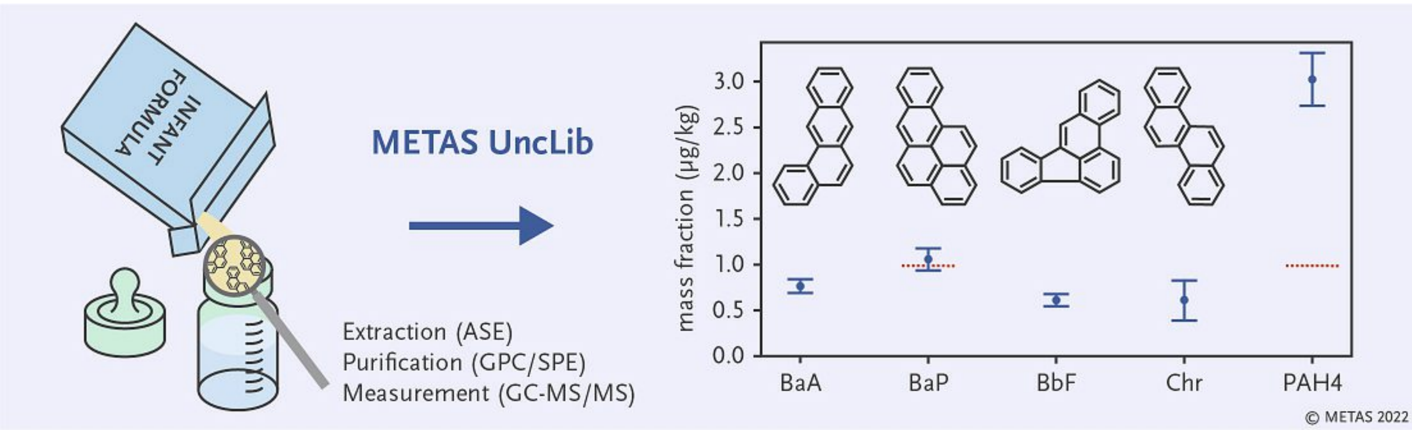

Fig. 1: Selected mass fractions and uncertainties (95 %, k = 2) for the PAHs benz[a]anthracene (BaA), benzo[a]pyrene (BaP), benzo[b]fluoranthene (BbF) and chrysene (Chr) determined in contaminated infant formula (proficiency test material, BIPEA 09-2344). Maximum levels (1 µg/kg) of BaP and the sum of BaA, BaP, BbF and Chr (PAH4) listed in the Swiss contaminants regulation (SR 817.022.15) are indicated with red dotted lines.

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