

Online Tool for the Estimation of Measurement Uncertainty

Hubert Zipper, Daniela Dörk, Anja Barth, Ellen Scherbaum and Michelangelo Anastassiades

E-Mail: Hubert.Zipper@cvuas.bwl.de; Michelangelo.Anastassiades@cvuas.bwl.de



Introduction

One important requirement of ISO/IEC 17025 for the competence of a testing laboratory is that its analytical results should include an estimation of the (expanded) measurement uncertainty (MU), which describes an interval near the result, within which the true value can be expected to lie with a defined level of confidence. There are two well-known concepts for the estimation of MU in the field of pesticide residue analysis:

(a) The **bottom-up approach** breaks up the analytical procedure into single steps. Then the individual MU-contributions are estimated for each step and combined to the uncertainty of the final result. From a practical point of view, this approach is too laborious for pesticide residue laboratories.

(b) The **top-down approach** is based on the estimation of MU by using the variability of within-laboratory data (method validation and/or long-term precision data derived from laboratory control samples) and proficiency test (PT) results. At first glance, this approach reduces the workload and seems feasible for pesticide residue laboratories, as laboratories accredited under ISO/IEC 17025 must participate in PTs and produce validation as well as long-term precision data.

The Problem

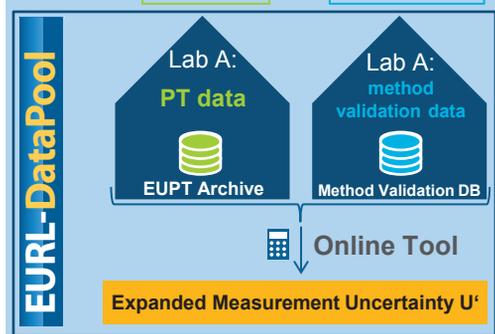
The main problem with estimating the MU is that many pesticide residue laboratories do not have the necessary data readily available to perform the appropriate calculations for hundreds of pesticides in many different foodstuffs within a reasonable timeframe.

The Solution

To help the official laboratories estimate the MU more easily, the EURLs for Pesticide Residues offer an **infrastructure** for management of PT and method validation data within the EURL Data Pool-website (www.eurl-pesticides-test.eu). In addition, an **online tool** was recently introduced into the website that enables the estimation of the expanded MU based on rules described in document No. SANTE 11945/2015 (Eq. 1, Eq. 2):

Eq. 1 $U' = 2 * u'$

Eq. 2 $u' = \sqrt{u'(bias)^2 + u'(RSD_{WR})^2}$



Lab-specific PT-data (extracted from EUPPT-Archive) is used to compute the contribution of the method/lab bias to the overall measurement uncertainty. In-house validation (from Method Validation database) may be used to calculate the standard uncertainty due to within-laboratory imprecision.

How to use the MU Online-Tool

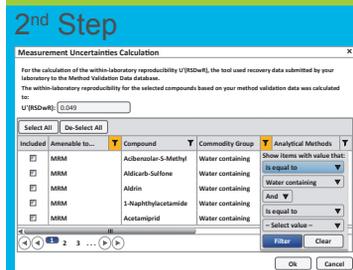
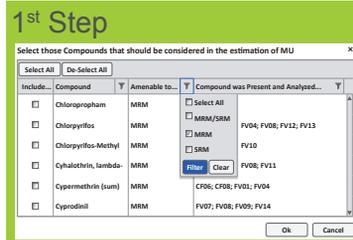
The online tool offers various filter options allowing the labs conveniently select their PT and validation data to be considered in the MU calculation.

1st step (filter your PT data): Select among individual PTs or pesticides or pesticide groups (e.g. MRM-amenable pesticides).

2nd step (filter your validation data): Choose among various criteria (e.g. only acidic commodities) in order to calculate the within-laboratory reproducibility. In case no validation data is available within the EURL DataPool a user-calculated value for the within-laboratory reproducibility can be entered by the user.

3rd step (generate result): The final and all intermediate results are presented in a synoptical table (e.g. estimation of U' using FV12-, FV13- and FV14-data).

Watch this Demo for more Details!



3rd Step

Comment	Parameter	Result
Number of EUPPT results used in the calculation procedure	m	51
Sum of squares of the bias	$\sum (bias)_i^2$ where bias = $\frac{lab\ result - assigned\ value}{assigned\ value}$	1,719
Sum of quotients between Qn and square roots of number of submitted lab results	$\sum \frac{Qn_i}{\sqrt{No.\ of\ lab\ results}}$	1,164
Uncertainty component arising from method and laboratory bias (estimated from your EUPPT data)	$u'(bias) = \sqrt{(RMS_{bias})^2 + u'(c_{eq})^2}$	
Root mean square of the sum of squared bias(i) divided by number of EUPPT results used in the calculation	$RMS_{bias(i)} = \sqrt{\frac{\sum (bias)_i^2}{m}}$	0,183
Laboratory bias (estimated from your EUPPT data)	$u'(c_{eq}) = \frac{\sum Qn_i}{m \cdot \sqrt{No.\ of\ lab\ results}} + 1,253$	0,029
By applying the results of RMS bias and u'(c _{eq}) to u'(bias) is calculated to:	$u'(bias) =$	0,186
Estimation of the within-laboratory reproducibility		0,088
Combined standard uncertainty	$u' = \sqrt{u'(bias)^2 + u'(RSD_{WR})^2}$	0,206
Expanded Measurement Uncertainty (in %)	U' = 2 * u'	41,1

Summary

The EURL DataPool offers the infrastructure that allows pesticide residue laboratories to systematically collect PT-results organized by various PT-providers and results from in-house method validation. An easy-to-use online tool uses this lab-specific data to estimate the expanded MU and significantly reduces the workload to determine this important parameter. The tool is currently being tested by the EURLs and NRLs. After testing, the official EU pesticide laboratories will have the possibility to conveniently estimate the expanded MU based on their PT and method validation data and to demonstrate that their own expanded MU is less than 50% which is the prerequisite of SANTE 11945/2015 for the usage of the 50% default expanded MU in case of enforcement decisions.

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