

## IUPAC Project Progress Report

**Date:** 16 October 2008

**Task Group Leader:** Christoph von Holst

**Project number:** 2005-024-2-600

**Project Title:** Establishment of guidelines for the validation of qualitative and semi-quantitative (screening) methods by collaborative trial: a harmonized protocol

**Important information:** Since 2007 this project is working together with a corresponding working group of the European project "MoniQA" ([www.moniqua.org](http://www.moniqua.org))

### Report:

#### 1. Current status of project:

Based on the decisions of the last working group meeting of the European project "MoniQA", the current activities are focused on statistical simulations. As pointed out in a former document, the critical factor of the validation of *qualitative* methods is the number of available data, since the result is exclusively expressed as "present/non-present" decision. In consequence, traditional approaches that are applicable to *quantitative* methods such as the calculation of the standard deviation are not applicable. The objective of the current research is to establish a link between the number of available results of measurements (=number of laboratories × the number replicates × number concentration levels) and the precision of the estimate of the limit of detection (LOD). Based on these information simulations were started, to establish regressions curves from percentage rate of correct positive results plotted against the known concentration of the target analytes in the samples. The calculated regression line were used to estimate the LOD and the corresponding uncertainty range of the estimate.

#### 2. Progress relative to 'milestones':

There is still a delay considering the planned deadline of the project. However, the very recent results are very promising.

#### 3. Difficulties encountered (or concerns):

The main difficulty was related to the fact that the colleagues from the "MoniQA" project who were supposed to contribute with their specific statistical expertise, did not start with the work on-time.

#### 4. Projected completion date (documents ready for external review):

5. Please list all of the intended outputs and the dissemination plan for this project (viz. articles, CD, conference presentations; etc.). These may have been expanded since project approval: The first results have been presented in the last conference from the project "MoniQA" (<http://www.icc.or.at/events/moniqua2008/>). The presentation is attached. It is planned to write at least one publication about the results of the simulations and in addition the final guideline

6. If your project is within 6 months of completion, how do you plan to utilise any remaining budget for this project?

7. Work on this project may have identified new problems, issues, challenges, emerging topics, opportunities for related projects, etc. Please indicate these here so that the Division can follow up on them:

**I would like to ask for a prolongation of the project by at least one year. The prolongation does not require an additional budget.**