Eurachem

CITAC

Co-Operation on International Traceability in Analytical Chemistry

Guide: Traceability in Chemical Measurement

Overview

- **Why traceability is important**
- **Principles of traceability**
- **Application of these principles to chemical measurements**
- **Establishing traceability**

Traceability

- **Traceability is a fundamental property of a result**
- **Not an optional extra**
- **Not just an additional burden**
- **It enables results to be compared**

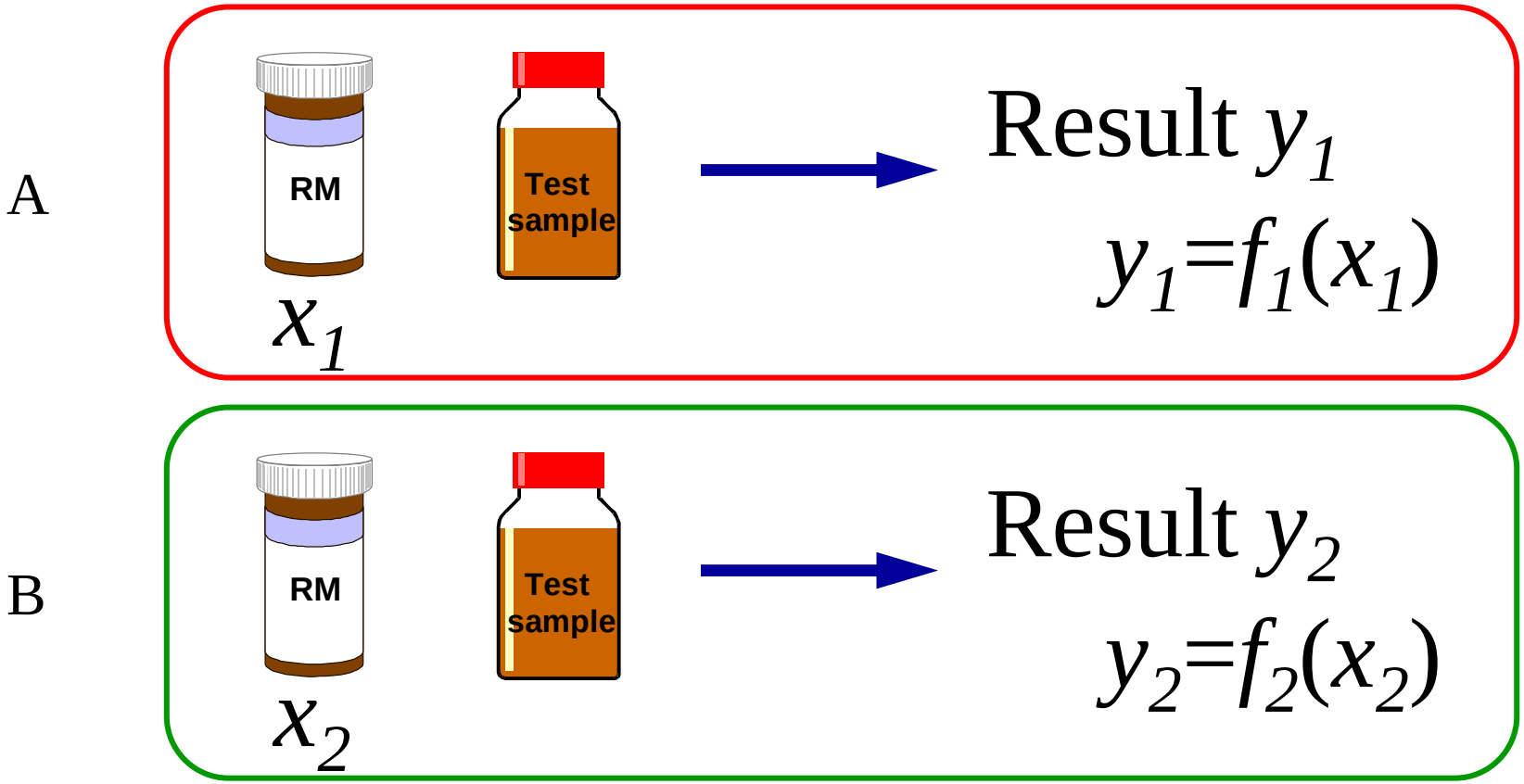
Principles Of Measurement

- **Value of the result is obtained from a comparison with the value of a standard**

$$C_{sample} = C_{std}\, I_{sample}/I_{std}$$

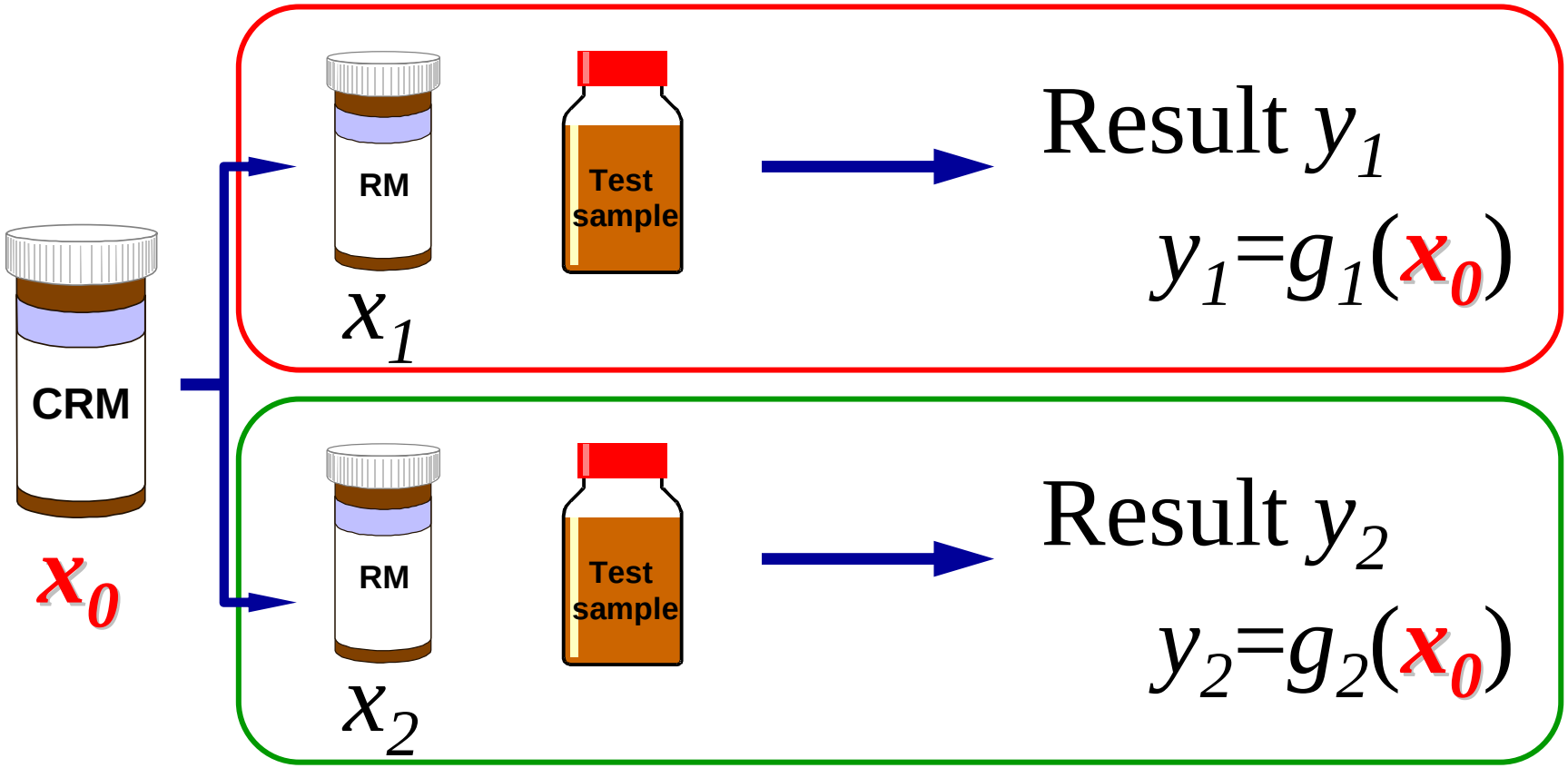
- **Value of the result is traceable to the value of the standard**
- **Uncertainty on the result is the uncertainty on this comparison plus the uncertainty on the standard**

Principles of Traceability



Relationship between y_1 and y_2?

Principles of Traceability



Application to chemical measurements

- Method development establishes an optimised procedure
- Validation demonstrates that this procedure is sufficiently complete for the purpose in hand
- Traceability or control has to be established for each parameter specified in the procedure
- Traceability is established by calibration using appropriate measurement standards.

Application to chemical measurements

Assumptions

- An effective quality system is in place
  - Trained Staff
  - Relevant analytical QC and QA in place
  - Documented methods
- Except for
  - Technical elements of traceability

Application to chemical measurements

A measurement result arises from an equation

$$y = f(x_1, x_2 \ldots \quad x_m)\Big|_{x_{m+1}, x_{m+2} \ldots \quad x_n}$$

- **which is assumed to hold, under certain conditions**
- **value of y is traceable to $x_1, x_2, \ldots x_n$**

Thus, if

$$y = f(x_1, x_2 \ldots \quad x_m)\Big|_{x_{m+1}, x_{m+2} \ldots \quad x_n}$$

- **The sole requirement for *y* to be fully traceable* is that $x_1 \ldots x_n$ are traceable or defined values**
- **Calibration for $x_1 \ldots x_n$ is sufficient**

**other than MU requirements*

Establishing Traceability

- Specifying the measurand and the acceptable uncertainty
- Choosing a suitable method of estimating the value - that is, a measurement procedure with associated calculation - an equation - and measurement conditions
- Demonstrating, through validation, that the calculation and measurement conditions include all the “influence quantities” that significantly affect the result, or the value assigned to a standard.
- Identifying the relative importance of each influence quantity
- Choosing and applying appropriate reference standards
- Estimating the uncertainty

Specifying the measurand

- **Identity of the analyte**
- **Implied measurement conditions**
- **Recovery correction**
- **Specification in terms of a method**

Choosing a suitable method

If we assume

$$y = f(x_1, x_2 \ldots \quad x_m)\Big|_{x_{m+1}, x_{m+2} \ldots \quad x_n}$$

- **The assumption(s) involved must be tested and shown to hold**
- **This is an essential part of method validation**
- **Validation is crucial to establishing traceability**

Validation

- **Unbiased**
  - **Test with relevant independent CRM, spiking, intercomparisons, …..**
- **Linear (test *via* linearity checks)**
- **Complete - No other effects**
  - **Robustness/ruggedness; Interlaboratory studies …**

Choosing reference standards - calibration

- **Physical calibrations are well established**
- **Chemical calibrations can be established in the same way**
  - **pure CRM or matrix calibrant**

  ***OR* (for example)**

  - **using a well-characterised pure material**
- **Uncertainty must be appropriate**

Estimating the uncertainty

- **Necessary for the result**
- **Covered in uncertainty Guide**
- **The uncertainties from the measurement procedure and on the values of the standards must be included**

Conclusions

How does this fit in with the definition?

Traceability

“Property of the result of a measurement or the value of a standard whereby it can be related to stated references, usually national or international standards through an unbroken chain of comparisons all having stated uncertainties” (VIM 1993)

Conclusions

If validation has shown that

$$y = f(x_1, x_2 \ldots \quad x_m)\Big|_{x_{m+1}, x_{m+2} \ldots \quad x_n}$$

- **Then the value of y, the result, is traceable to the values of $x_1 \ldots x_n$**

- **The values of $x_1 \ldots x_n$ are traceable to the values of the standards used in calibration**

- **Thus the result is traceable to the values of these standards, which in turn are traceable to higher level standards**