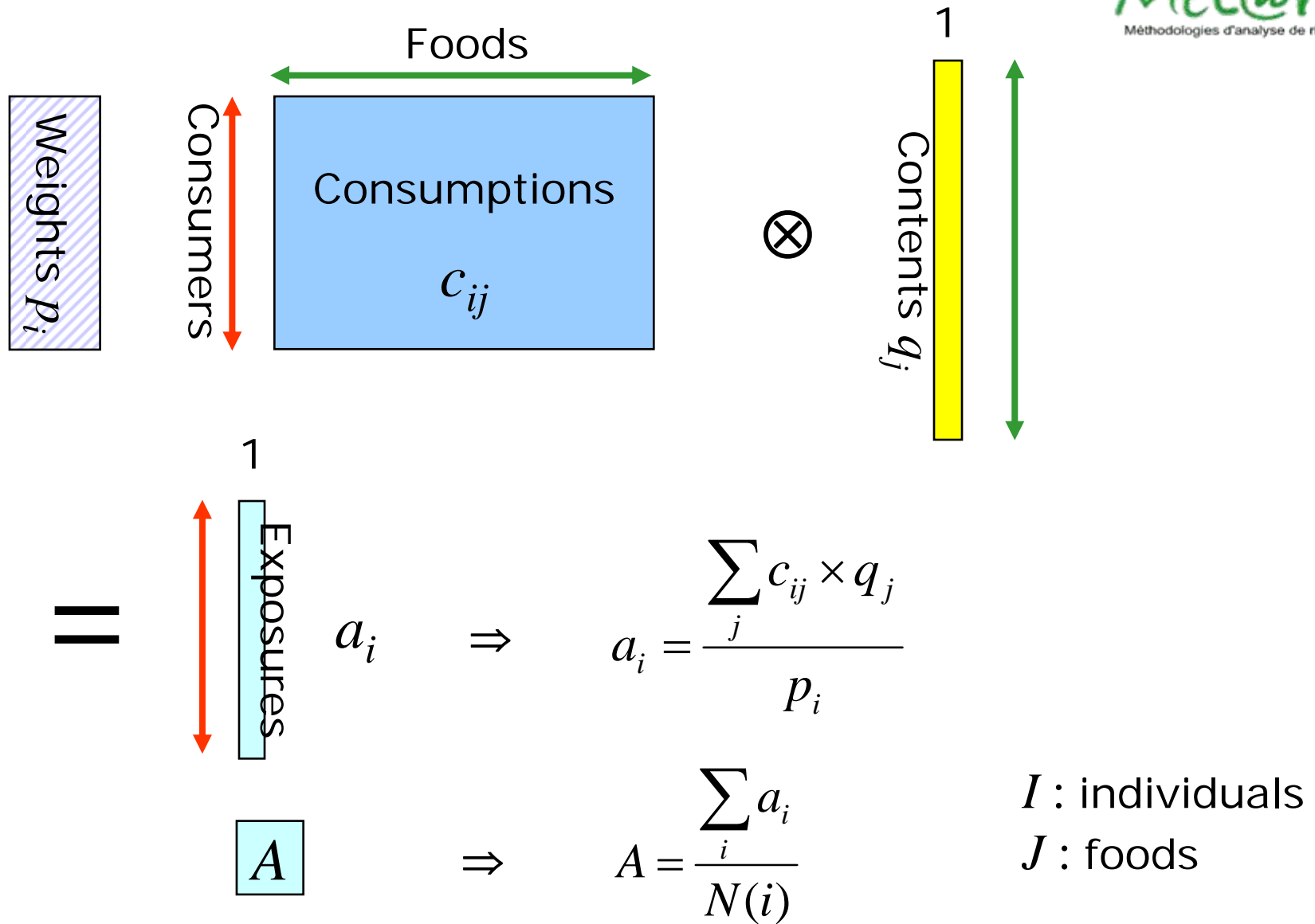
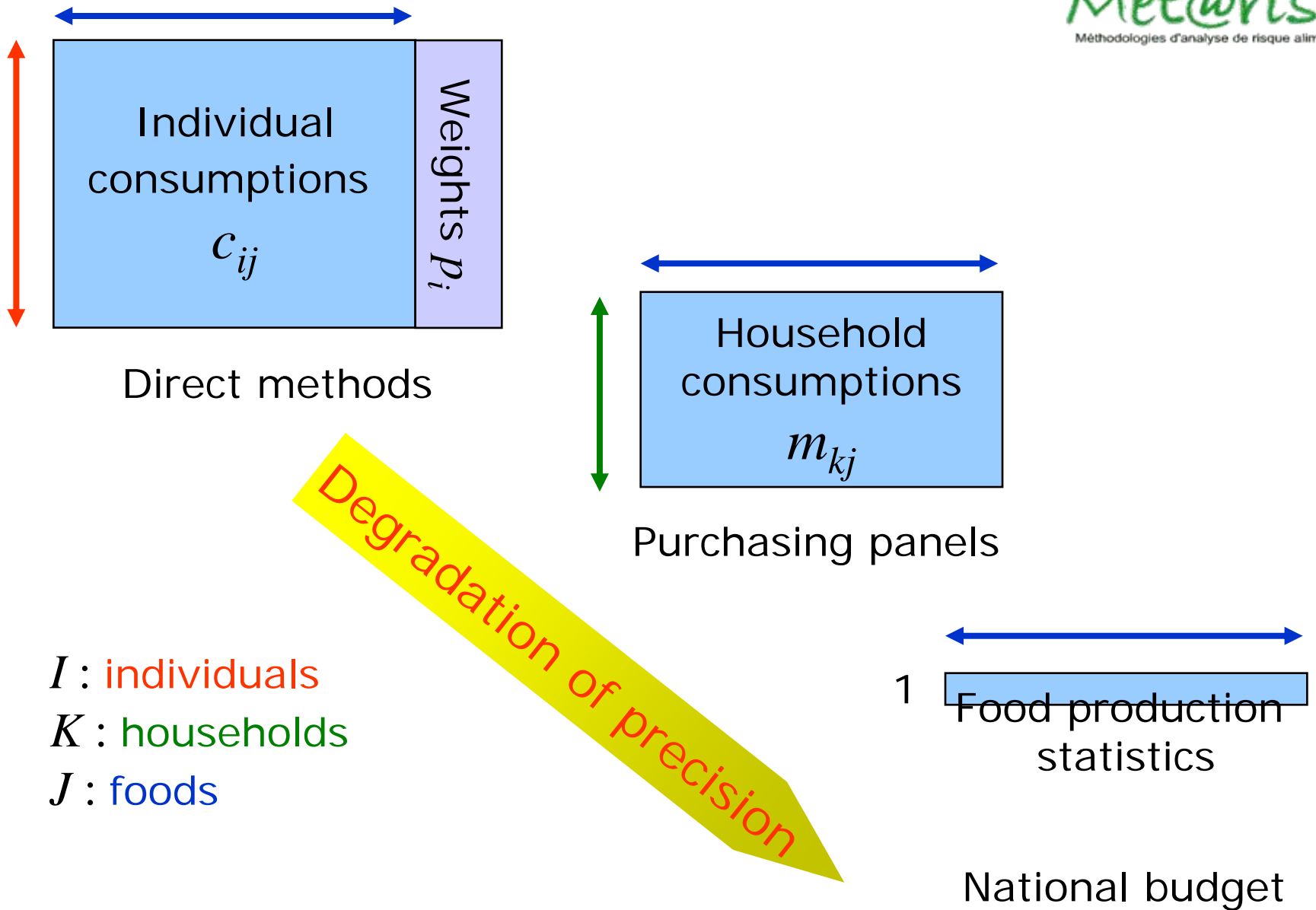


Characterization of the uncertainty in exposure assessment of flavourings

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General method to calculate exposure



I : individuals

K : households

J : foods

Dimension "reduction"

Exposure assessment methods for flavourings

- Maximized Survey derived Daily Intake or Per-Capita Times Ten (PCTT)
- Correction factors
 - Annual production volume is corrected by 60%.
 - 10% population are consumers.

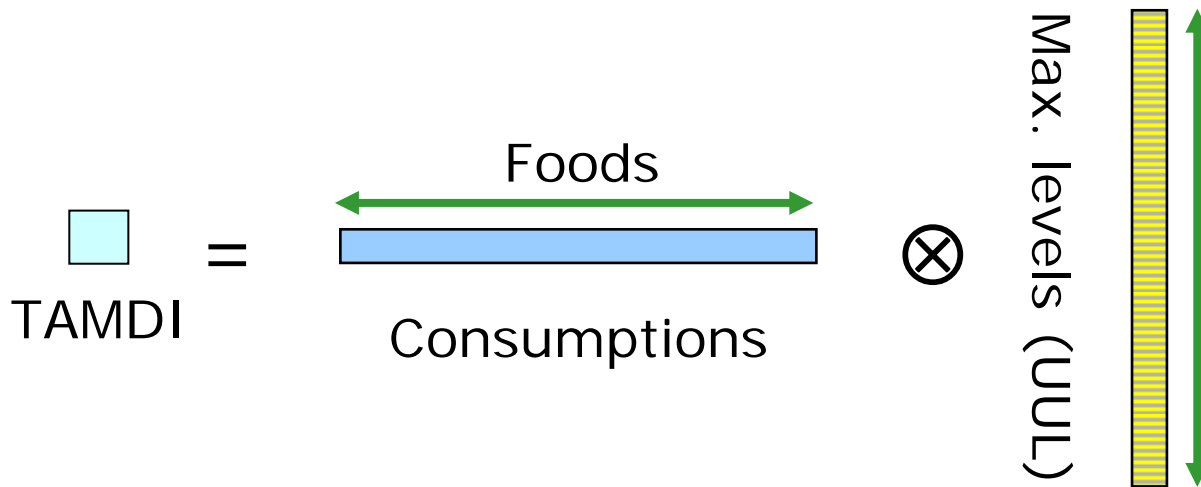
$$\text{MSDI} = \frac{\text{Flavour production volume } v}{\text{Consumers population } p} \times \text{Correction factors}$$

$$MSDI = C_f \times \frac{v}{p}$$

MSDI

Theoretical Added Maximum Daily Intake

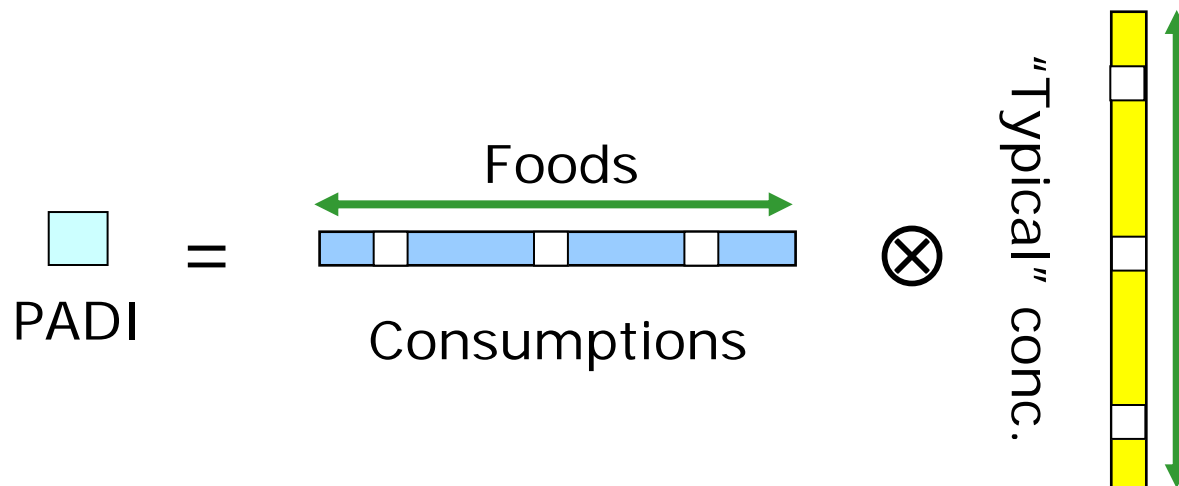
- “Maximal” Concentration. Upper Use Level (UUL)
- Consumer consumes a fixed amount of flavoured food and beverages that contains the flavouring at its specified level.



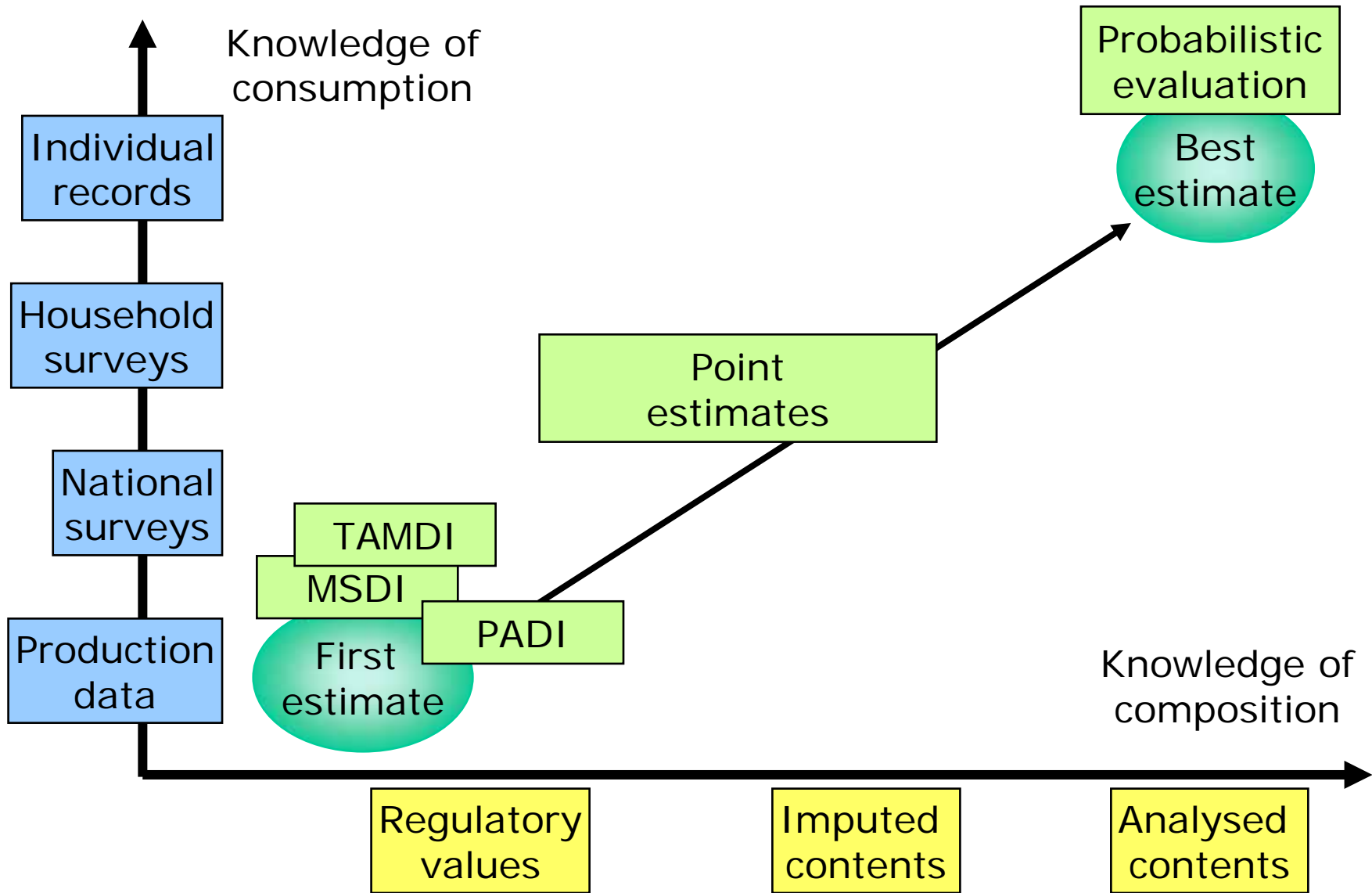
TAMDI

● Possible Average Daily Intake

- (“Typical” concentration of the flavour agent within specific food categories) × (Daily mean consumption of those food categories). Median values ?
- Proposed by Flavour and Extract Manufacturers’ Association (FEMA, USA).



PADI



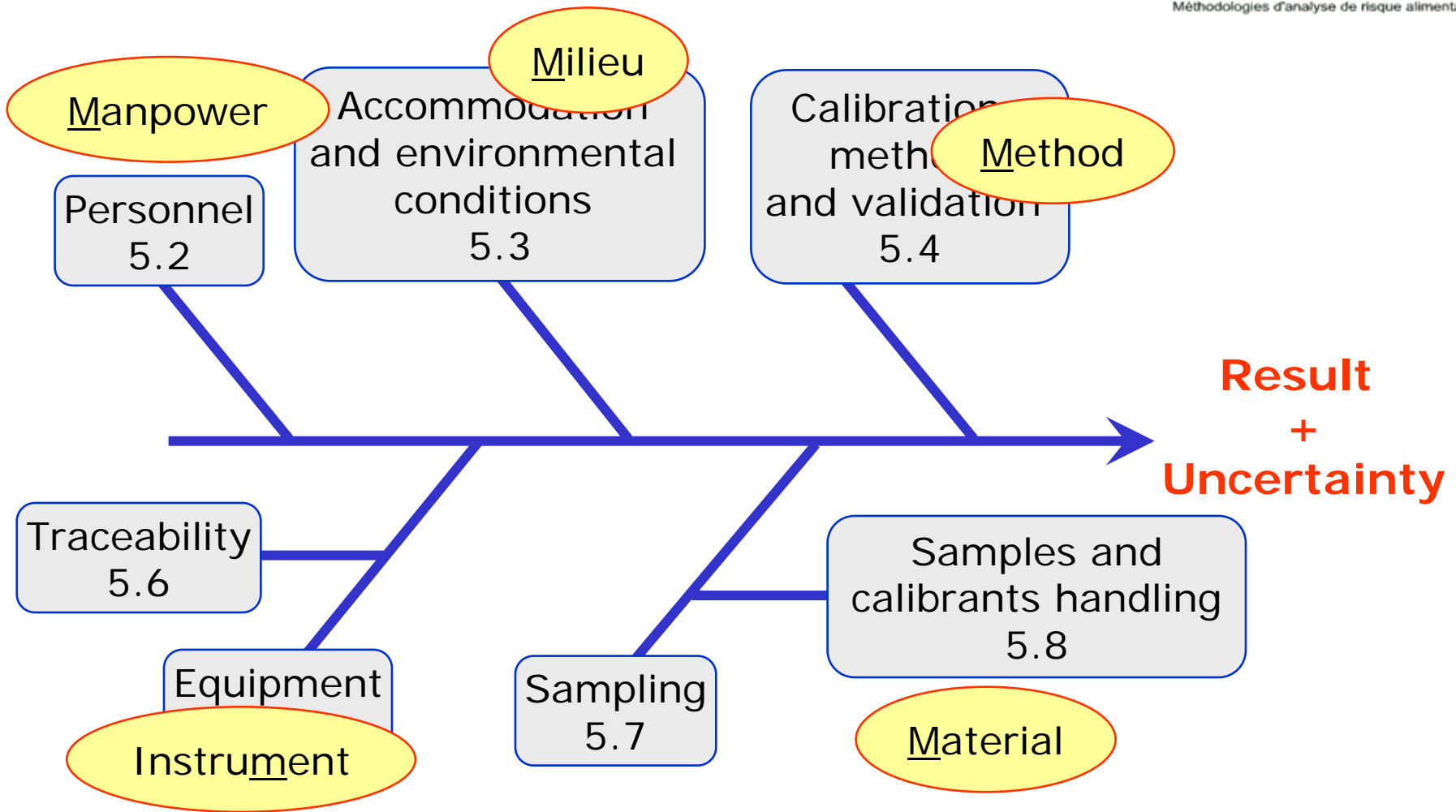
Ranking exposure estimates

Uncertainty and variability

**A proposal to assess
exposure estimate quality**

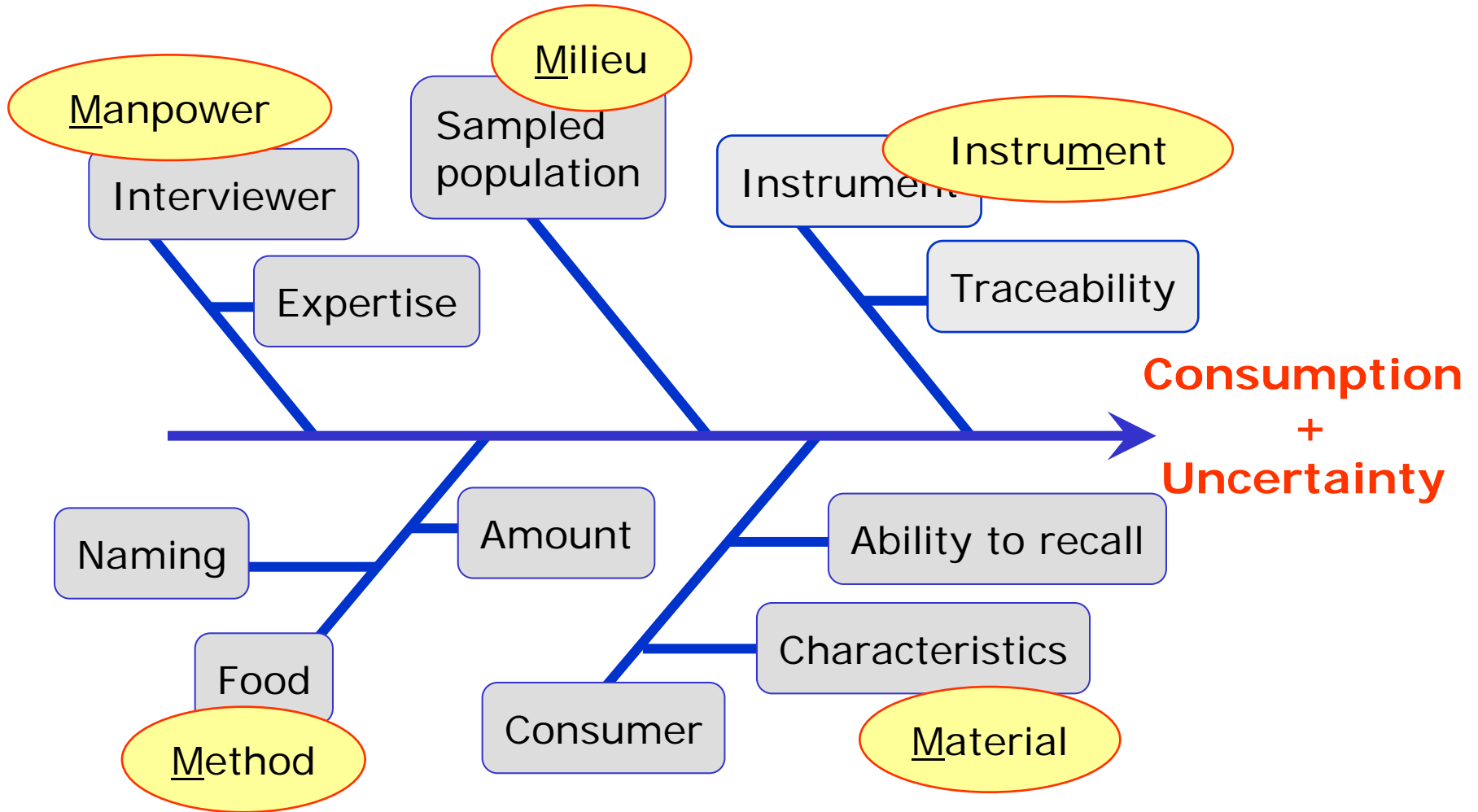
- Uncertainty (of measurement): parameter, associated with the result of a measurement, that characterises the **dispersion** of the values that could reasonably be attributed to the measurand.
 - Measurand: specific quantity subject to measurement.

What is uncertainty?



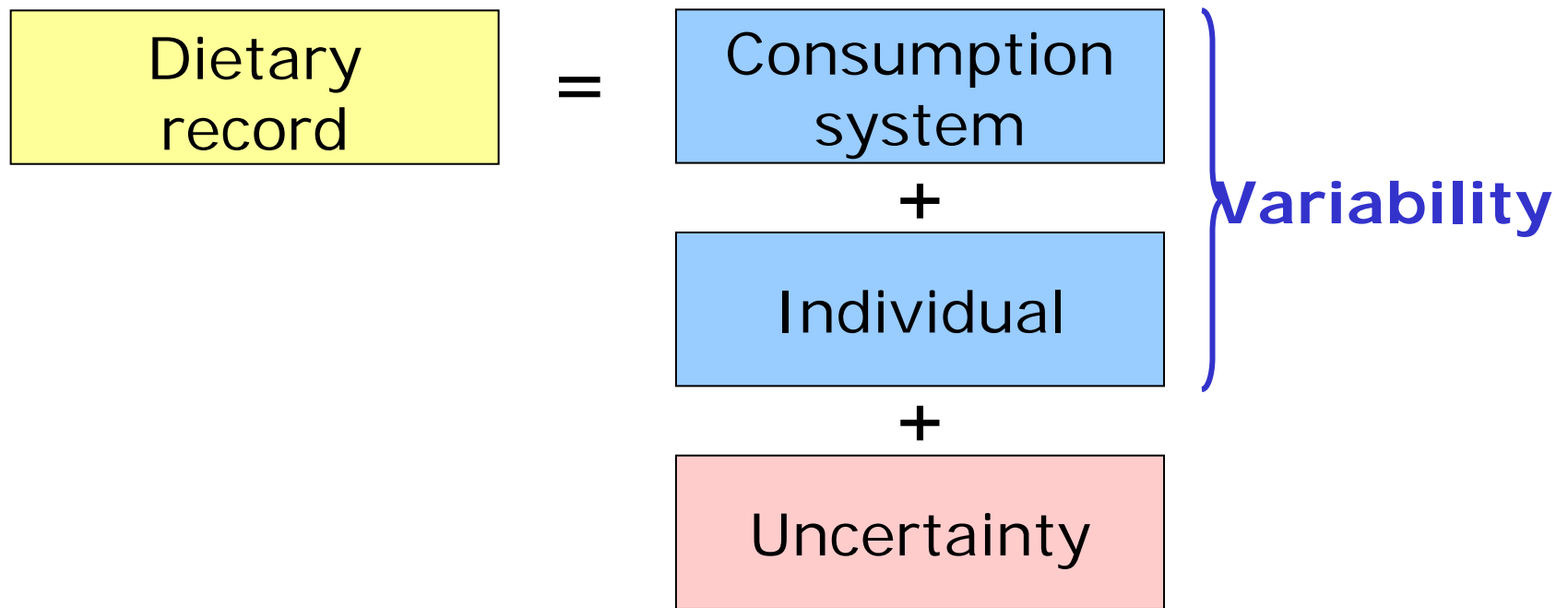
ISO 17025, §5. Technical requirements

Uncertainty for analytical measurement

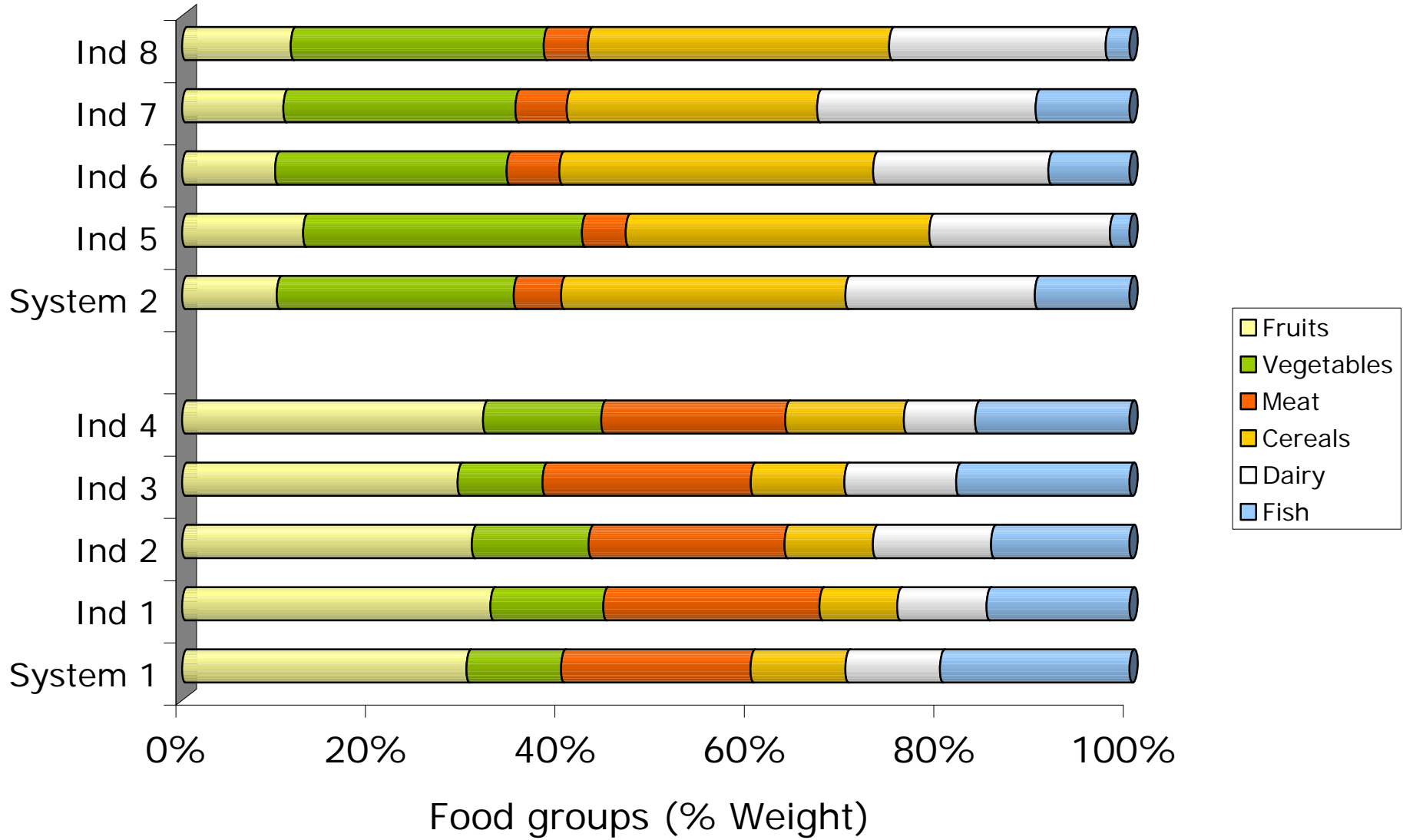


Uncertainty sources for dietary recalls

- Existence of consumption systems inside dietary patterns.



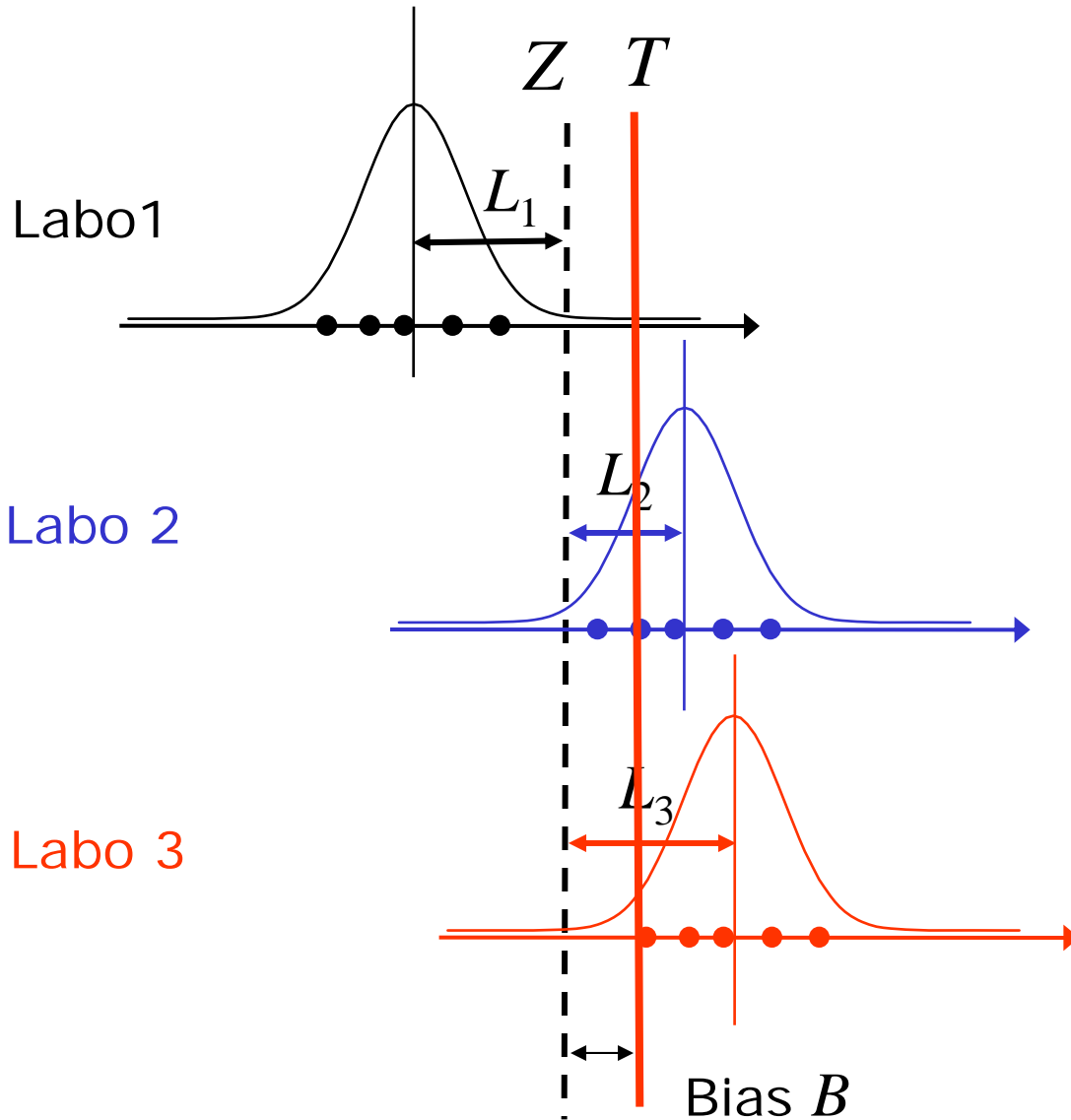
A more complex model



Simulated dietary records

Estimation of uncertainty

Two approaches

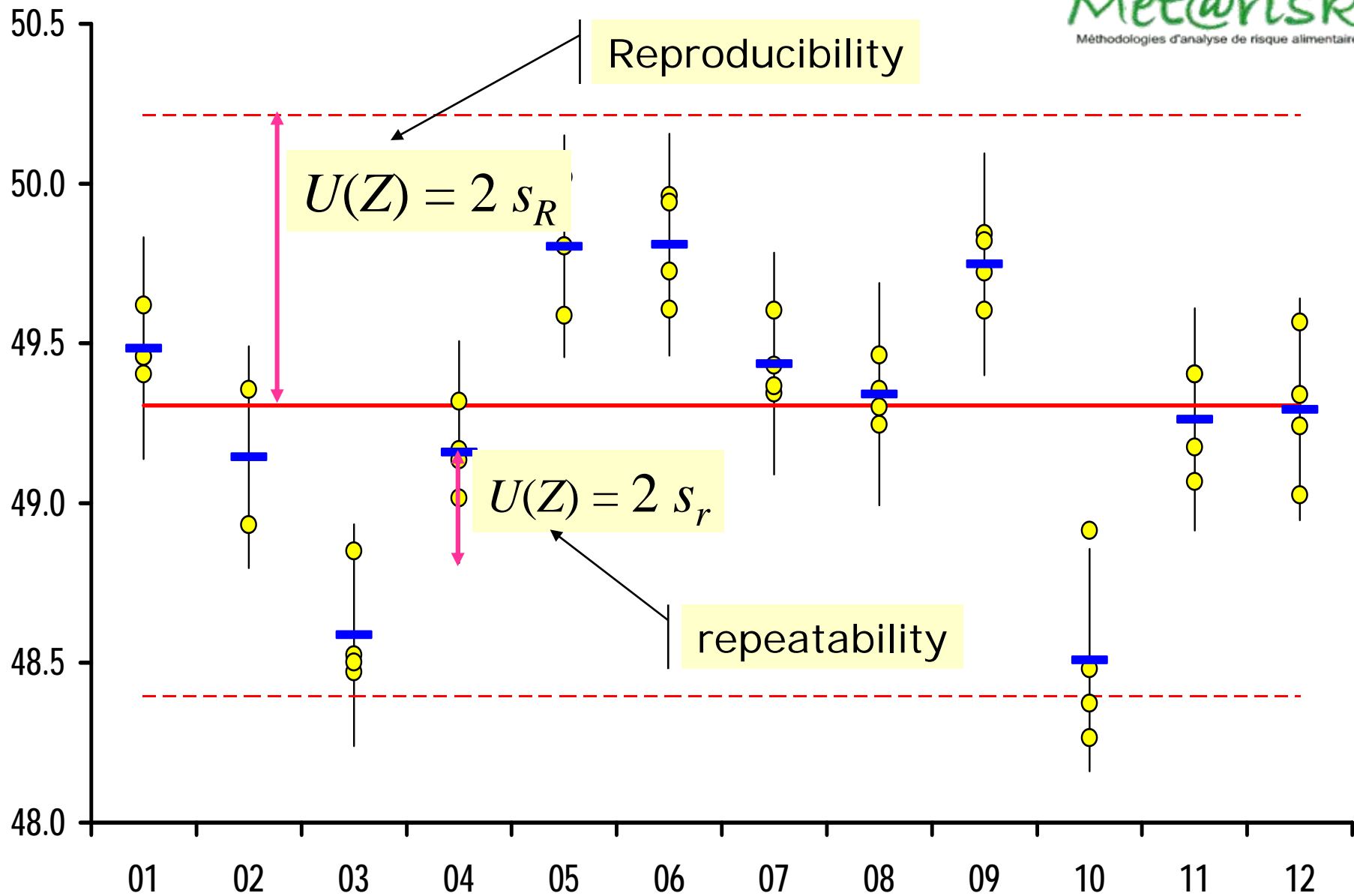


Repeatability S_r
 Inter-labs S_L
 Reproducibility

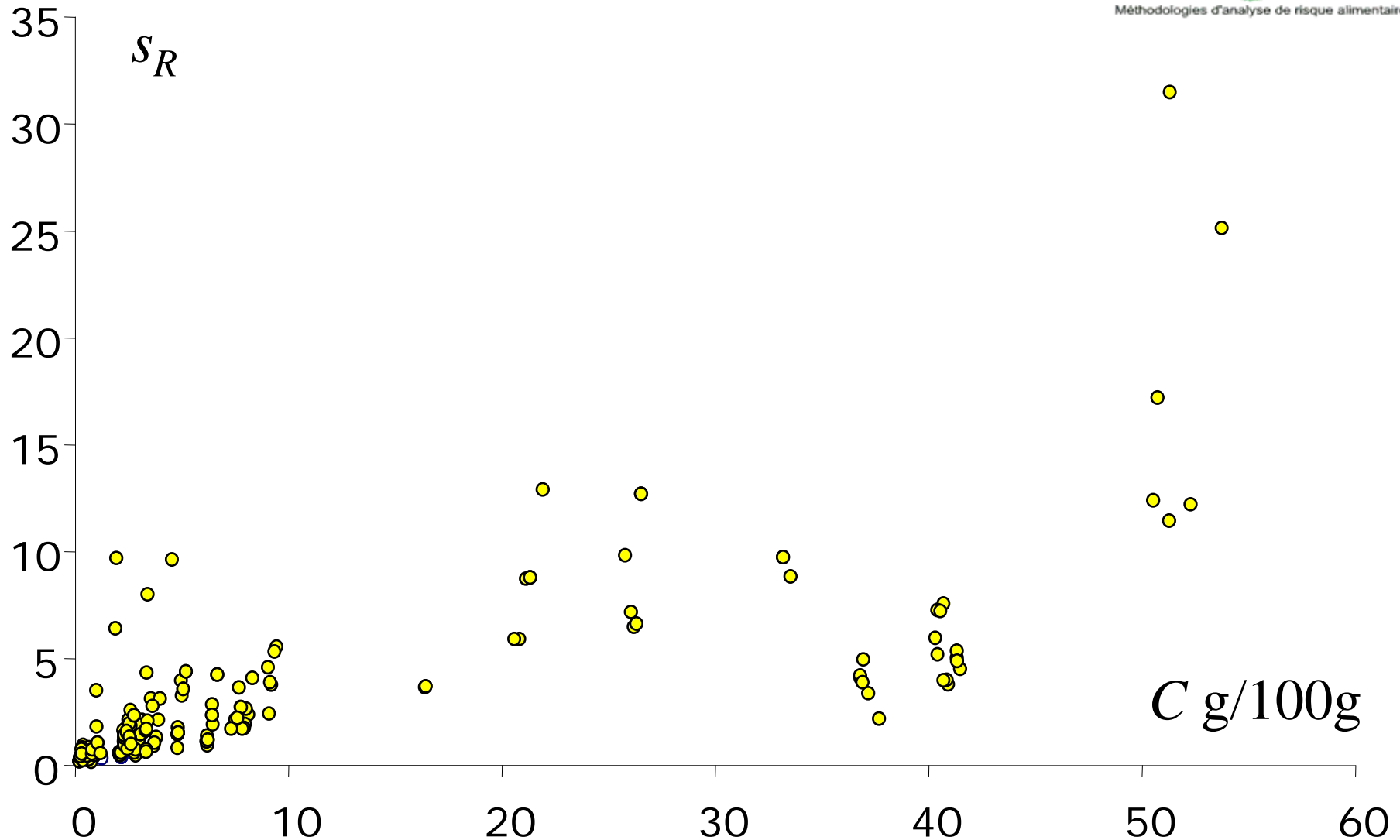
$$S_R = \sqrt{S_L^2 + S_r^2}$$

$$u(Z) = \sqrt{s_F^2 + u^2(T)}$$

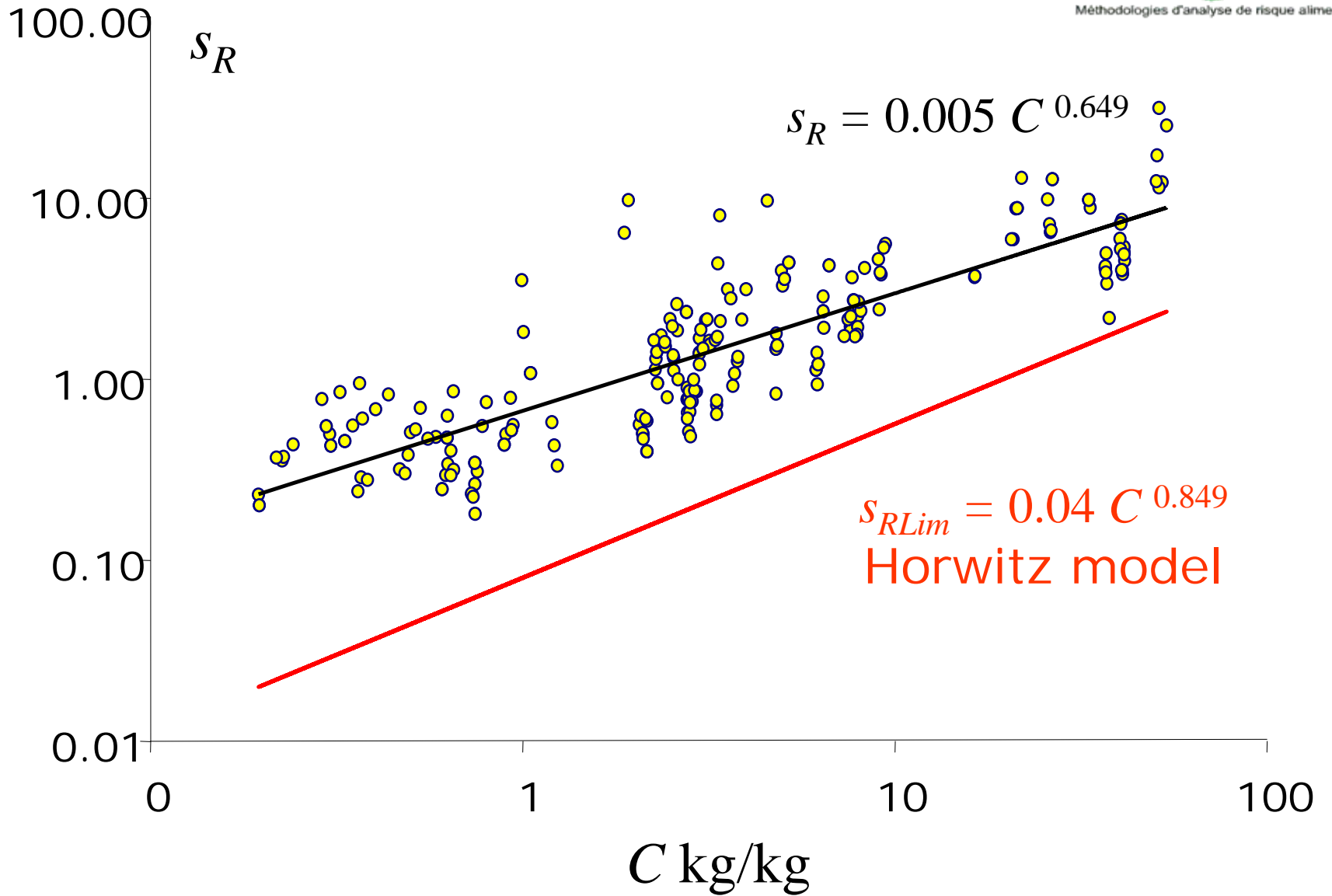
Type A. Inter-lab analysis



Example of an inter-laboratory analysis



Reproducibility and concentration (sugars)



Horwitz's model

- $Z = f(X_1, X_2, X_3, \dots)$.
- Z : reported result.
- X_i : intermediate results, quantities involved in uncertainty, etc...
- f : represents the measuring process but does express a physical law.
- Z, X_1, X_2, X_3, \dots random variables.

$$u^2(Z) = \sum_{i=1}^p \left(\left(\frac{\partial f}{\partial X_i} \right)^2 u^2(X_i) \right) + 2 \sum_{i=1}^{p-1} \sum_{j=i+1}^p \left(\left(\frac{\partial f}{\partial X_i} \frac{\partial f}{\partial X_j} \right) u(X_i, X_j) \right)$$

Type B. Variance propagation theorem

1. Linear combination.

$$Z = X_1 + X_2 - X_3$$

$$u_c(Z) = \sqrt{u(X_1)^2 + u(X_2)^2 + u(X_3)^2}$$

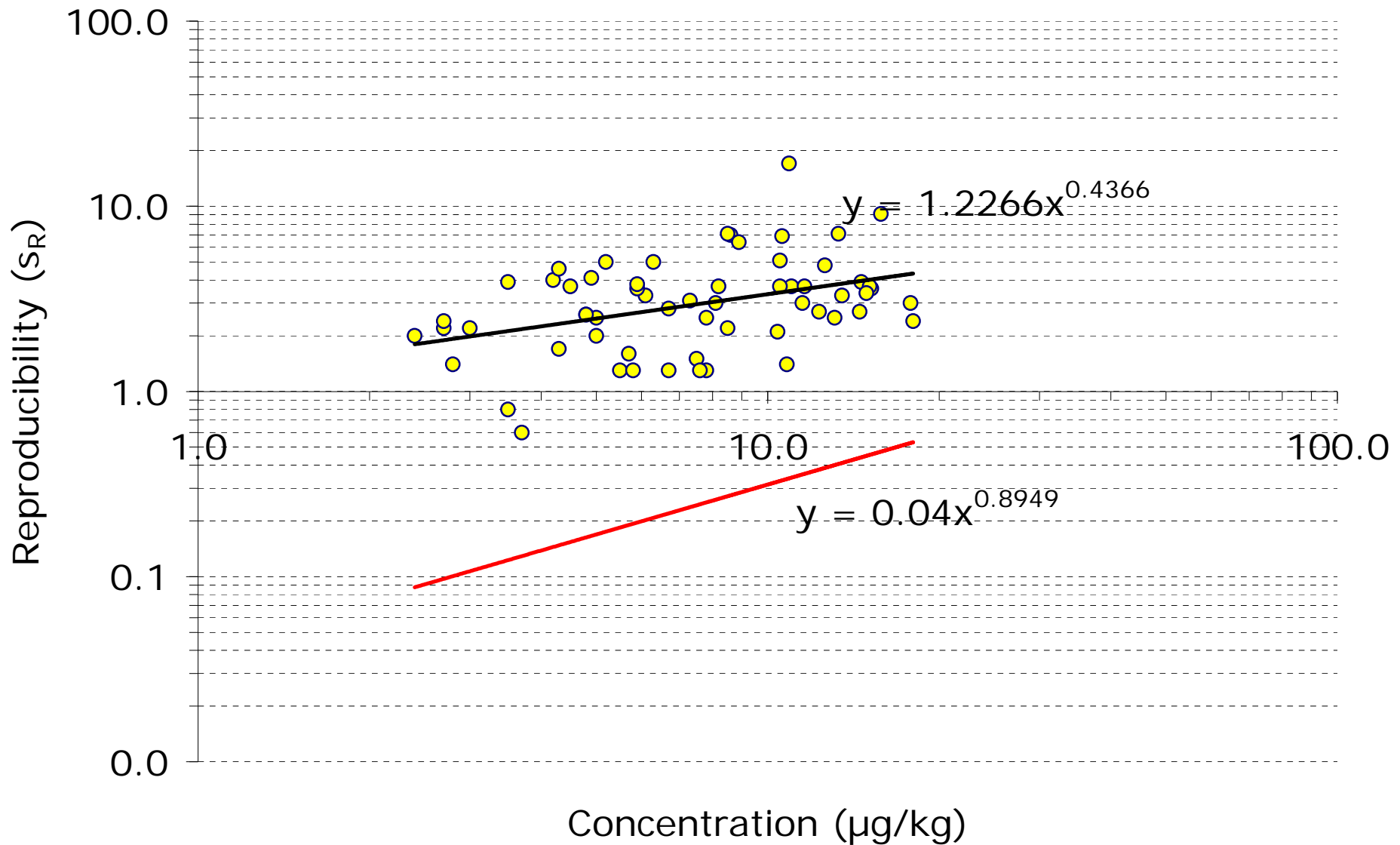
2. Products and/or ratios combination.

$$Z = \frac{X_1 \cdot X_2}{X_3}$$

$$\frac{u_c(Z)}{Z} = \sqrt{\left(\frac{u(X_1)}{X_1}\right)^2 + \left(\frac{u(X_2)}{X_2}\right)^2 + \left(\frac{u(X_3)}{X_3}\right)^2}$$

Simplifications

Chemistry of flavouring agents



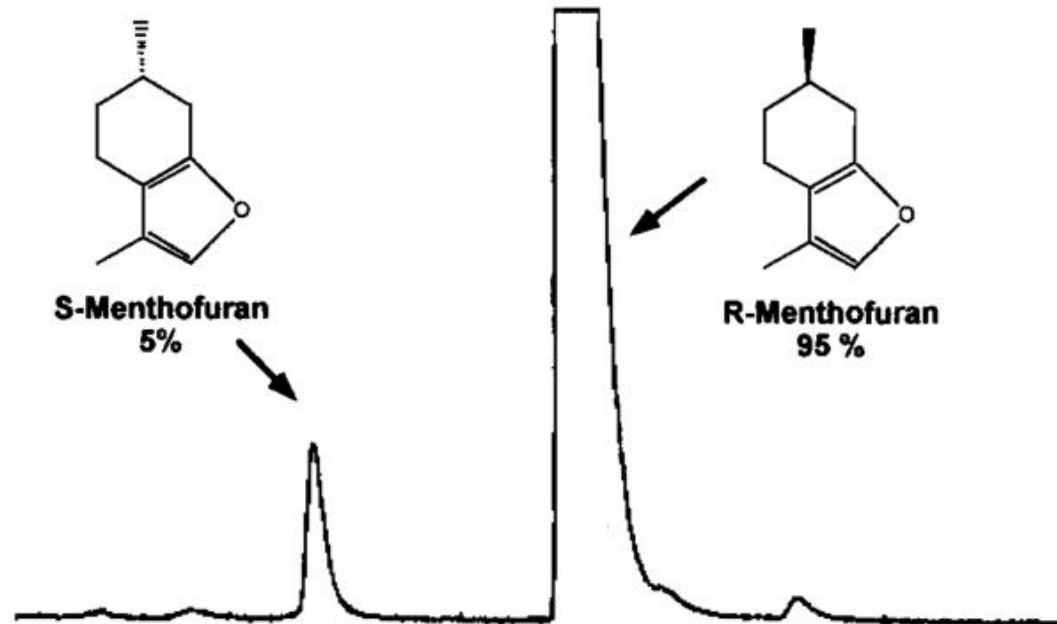
PolyAromatic Hydro. interlaboratory study

- Flavouring categories (Directive 88/388).
 - Natural, natural-identical or artificial flavouring substances, flavouring preparations of plant or animal origin, process flavourings, smoke flavourings.
- Flavouring substance is obtained :
 - by appropriate physical ... or enzymatic or microbiological processes, from material of vegetable or animal origin ...
 - by chemical synthesis or isolated by chemical processes (chemically identical)...
 - by chemical synthesis (not chemically identical).

Extended chemical definition

- 2-methyl butyric acid

- *S*-enantiomer pleasant, sweet, and elegant with a fruity note.
- *R*-enantiomer penetrating, cheesy and sweat-like



Biological activity and chirality

- Hyphenated mass spectrometry coupled to chromatography.
 - GC-MS (quadrupole).
 - GC-MSn (ion trap).
 - LC- MSn (ion trap or TOF).
- Near infrared spectroscopy.
 - GC-FTIR.
- High resolution NMR spectrometry.
- *Sensory analysis coupled to GC.*

Sophisticated analytical techniques

Conclusions

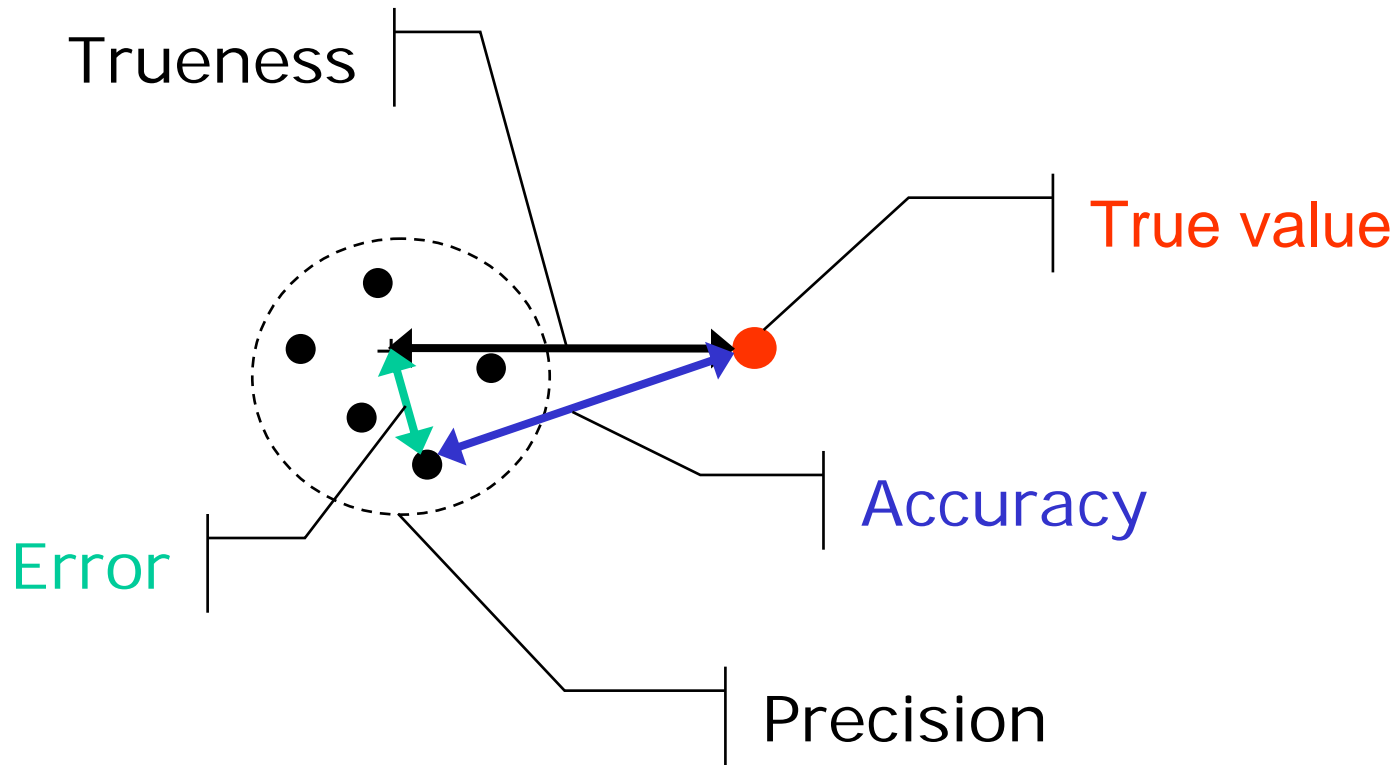
● Flavourings

- Urgent needs for “in-food” measured data.
- Develop analytical methods (standardization).
- Better define some molecules.
- Better relate tolerance and le risk.

● Food consumption

- Needs for harmonisation of dietary records.
- Identification of bias and define traceability.
- A proposal: uncertainty to organise harmonisation.
- Develop methods to assess digestibility.
- A new discipline: “Consumetrics” ?

Conclusions



Trueness and precision