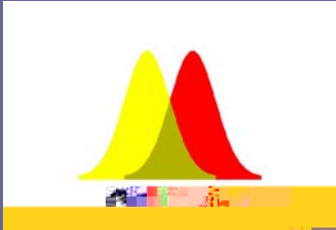
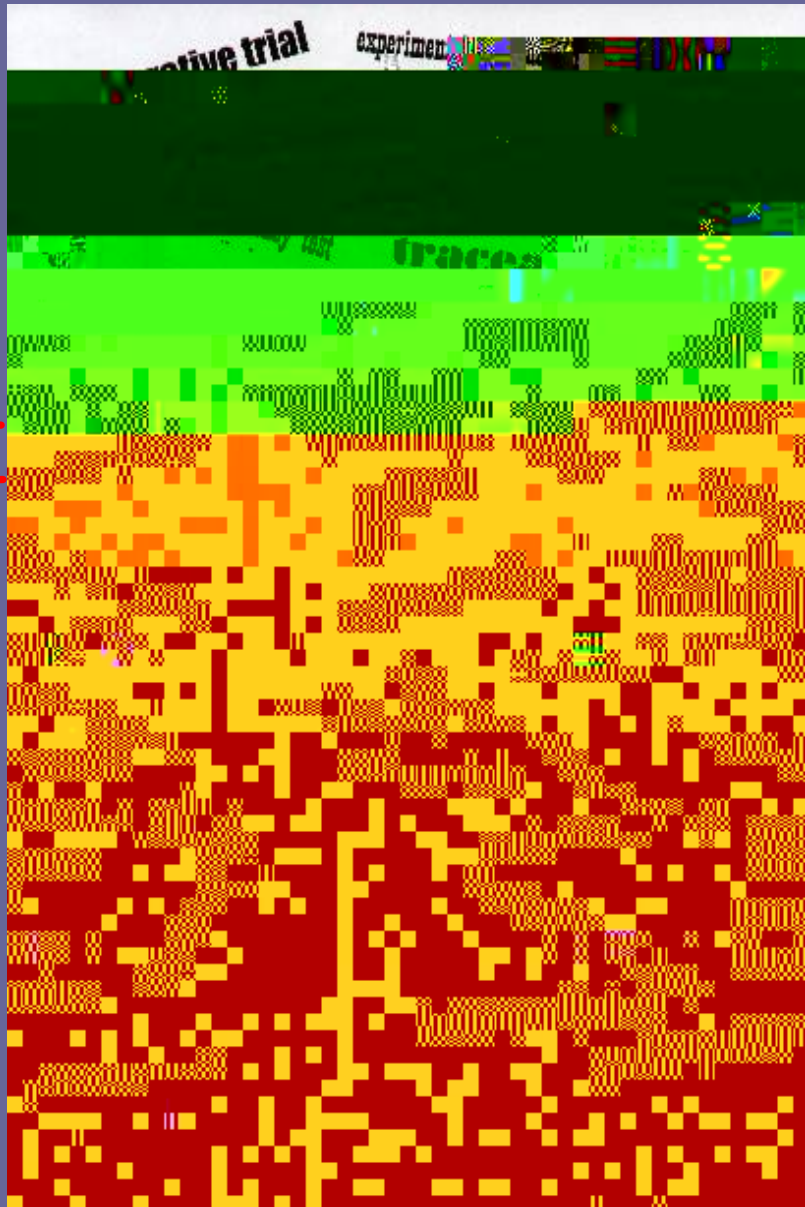


Big Issues in Analytical Chemistry—the Work of the Analytical Methods Committee

Michael Thompson

Birkbeck University of London

(Editor of *AMC Technical Briefs*)



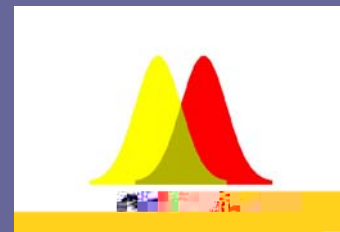
Help!

Aims

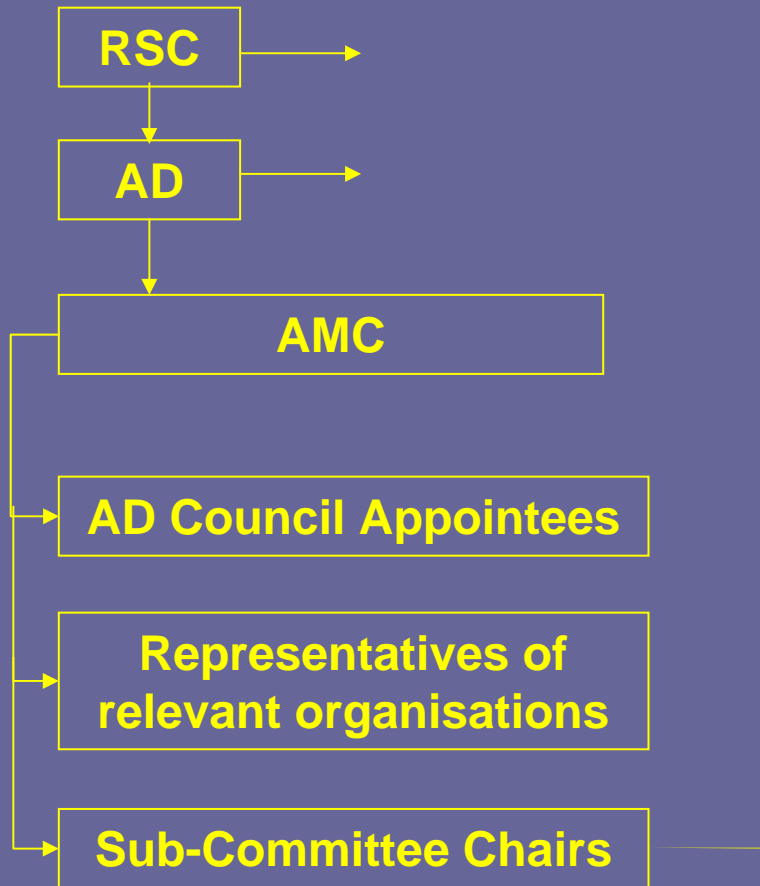
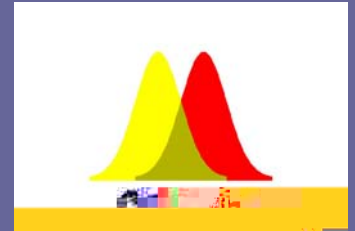


- The broad aim of the AMC is to participate in national and international efforts to establish a comprehensive framework for appropriate quality in chemical measurement, and to keep the analytical science community informed of developments.

Intentions



- Development, revision and promulgation of validated, standardised and official methods of analysis
- Development and establishment of suitable performance criteria for methods and instruments
- Use and development of appropriate statistical methods
- Identification and promulgation of best analytical practice, including aspects relating to sampling, equipment, instrumentation and materials
- Generation of validated compositional data of natural products for interpretative purposes.



Animal Feeding Stuffs



Mass Spectrometry



Nitrogen Factors



Statistical Methods

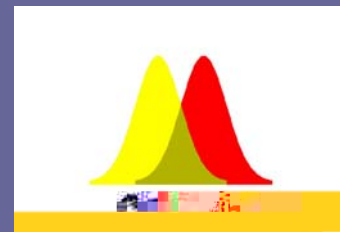


Sampling Uncertainty



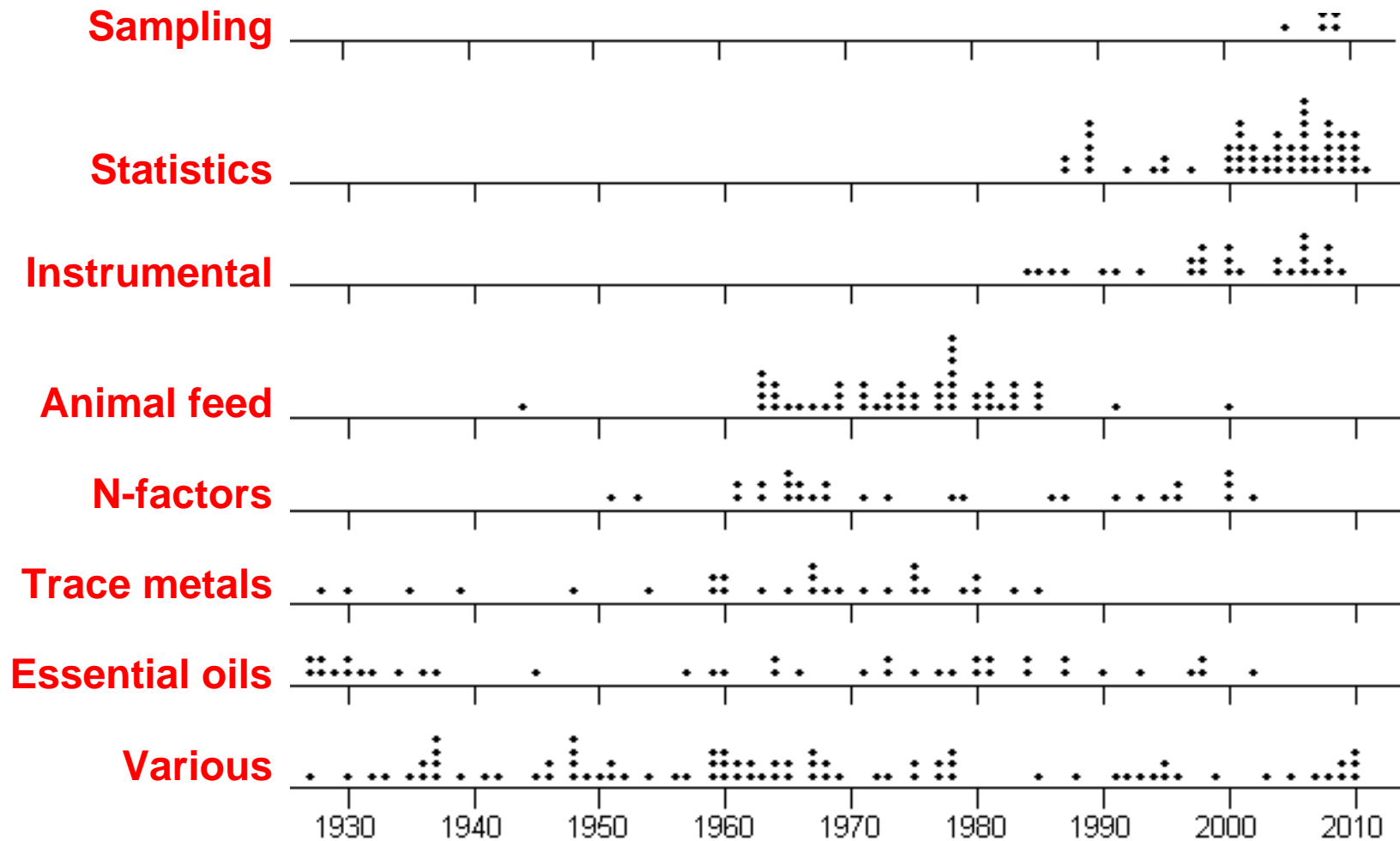
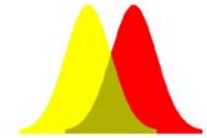
Method Validation

AMC outputs

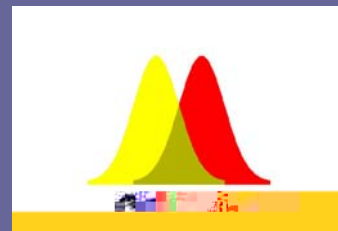


- Reports
 - AMC Technical Briefs
 - Datasets
 - Presentations
 - Software?
- www.rsc.org/amc

AMC Reports and TBs by year



Analyst, 1959, 84, 214-216



Analytical Methods Committee

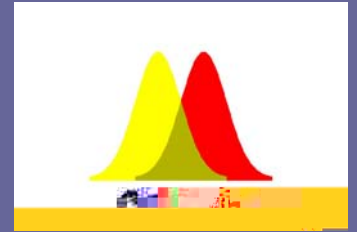
REPORT PREPARED BY THE METALLIC IMPURITIES IN
ORGANIC MATTER SUB-COMMITTEE

Notes on Perchloric Acid and its Handling in Analytical Work

The Analytical Methods Committee has received the following report from its Metallic Impurities in Organic Matter Sub-Committee. The Report has been approved by the

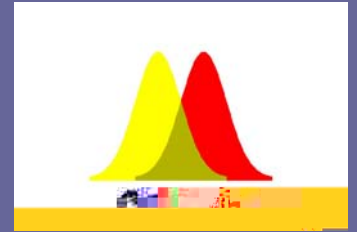
REPORT

When the Metallic Impurities in Organic Matter Sub-Committee was reorganised in 1957, it was realised that one of its first duties would be the recommendation of different methods



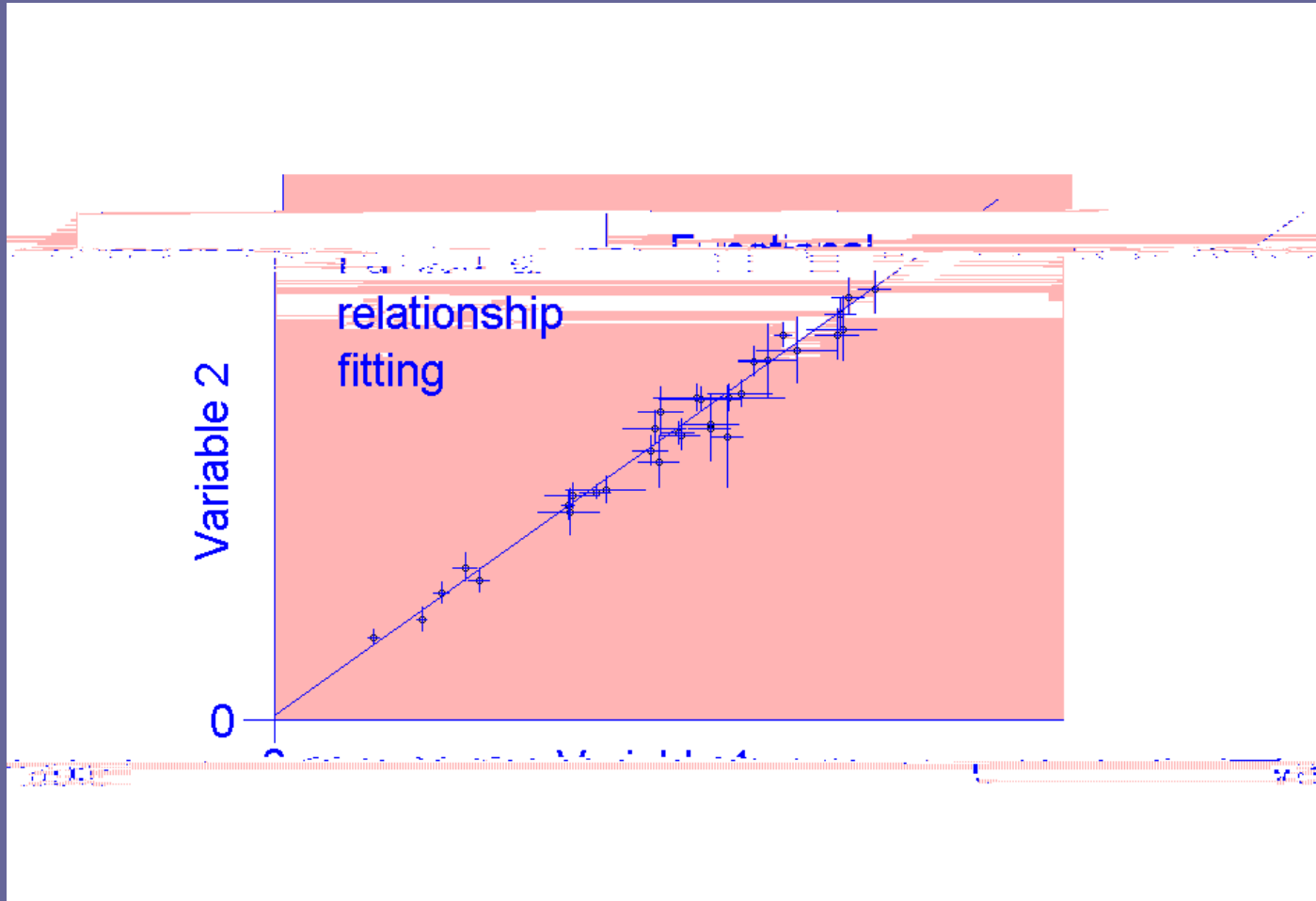
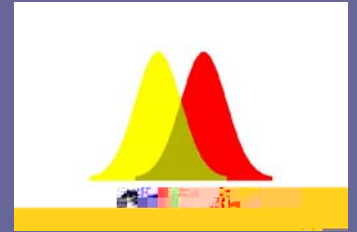
Statistical Subcommittee

Example 1—functional relationship

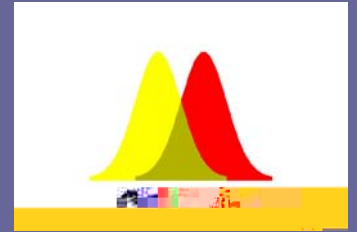


- *AMC Technical Briefs No 10:*
“Fitting a linear functional relationship to data with error on both variables”.
- *AMC Software: Excel Add-in.*
- *AMC Datasets No 24:*
“Dissolved oxygen method comparison”.

Don't use regression!



Example 2: Robust methods



- A robust method for the estimation of mean and standard deviation is “Huber’s H15” .
- The statistics (e.g., mean and standard deviation) are defined by an *algorithm*, not by equations.
- *AMC Technical Briefs No 6: “Robust statistics: a method of coping with outliers”*.
- *AMC Software: Excel add-in for mean, standard deviation, and ANOVA.*

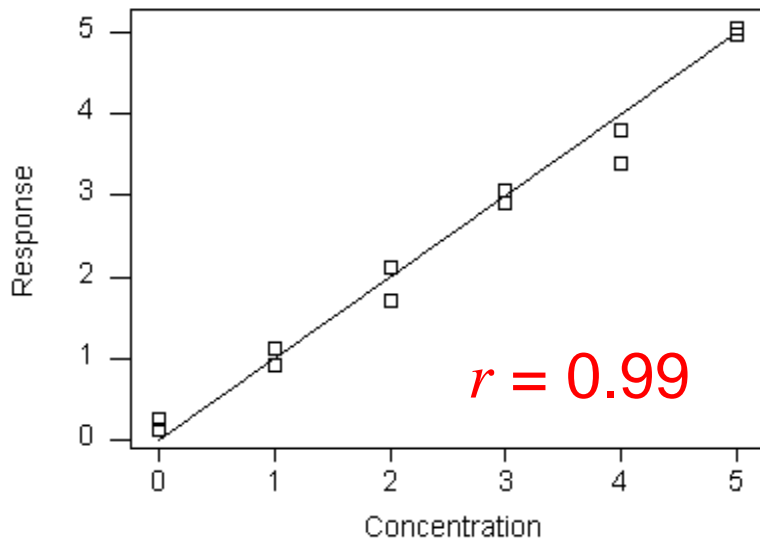
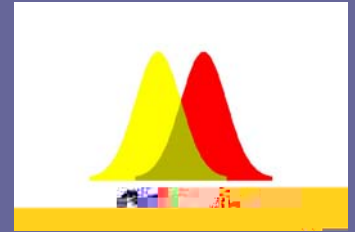
$$\mathbf{x}^T = [x_1 \quad x_2 \quad \cdots \quad x_n]$$

Set $1 < \alpha < 2$, $\mu_0 = 0$, $\hat{\mu}_0 = \text{median}$, $\hat{\sigma}_0 = 1.5 \times \text{MAD}$

Example 3—

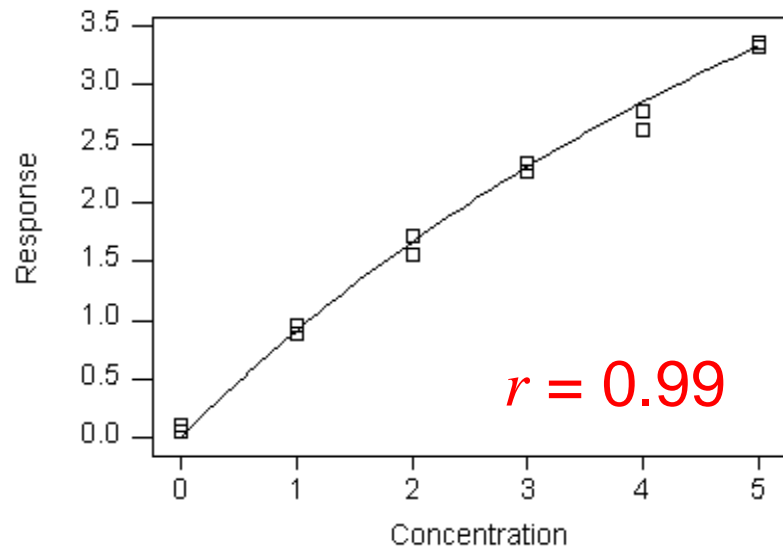
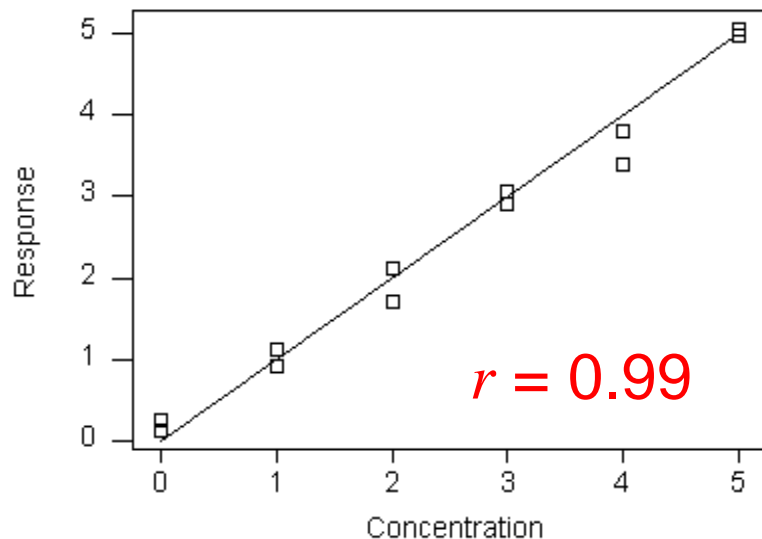
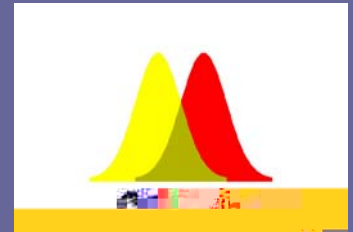
Is my calibration linear?

AMC Technical Briefs No 3



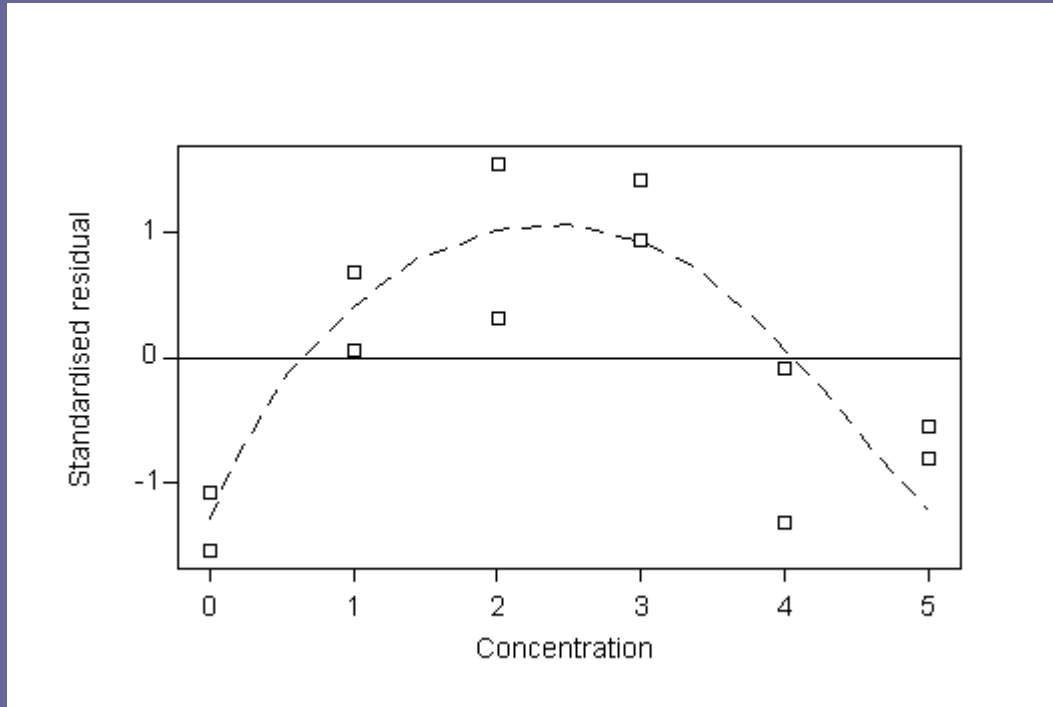
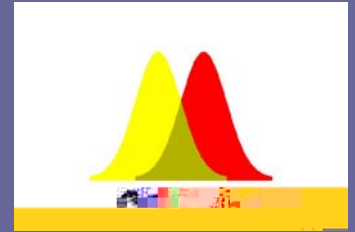
Is my calibration linear?

AMC Technical Briefs No 3



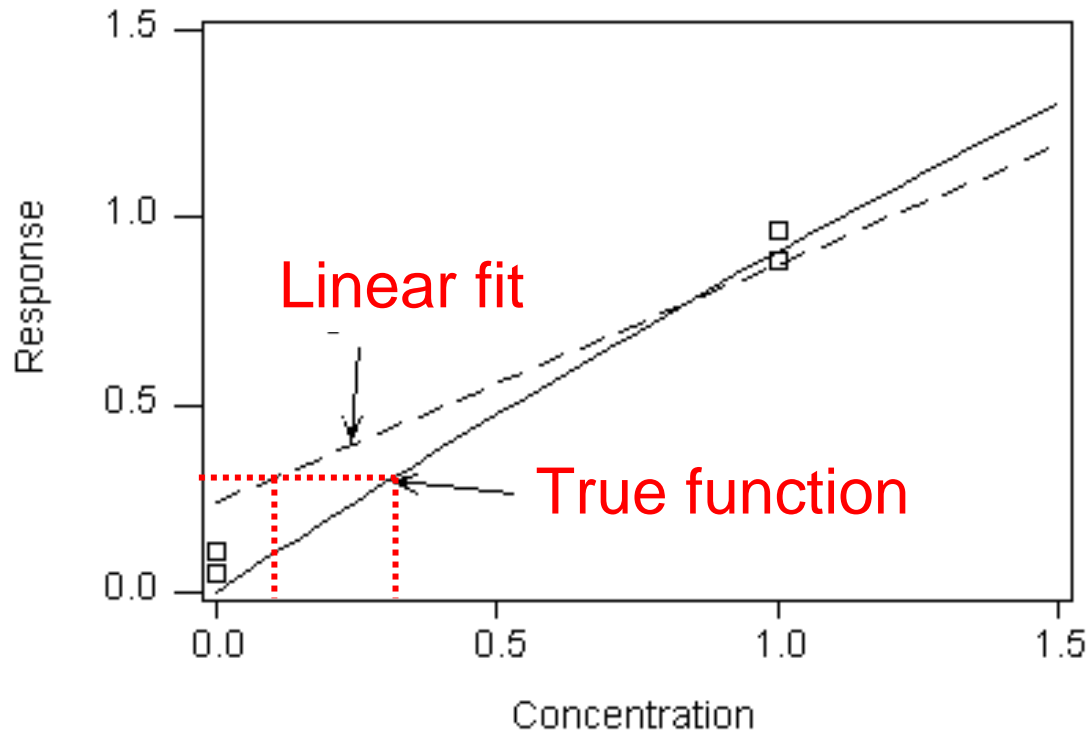
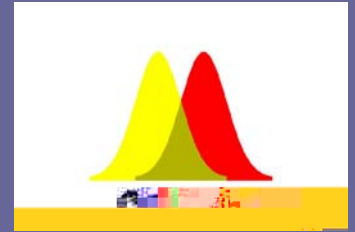
Problem with the correlation coefficient

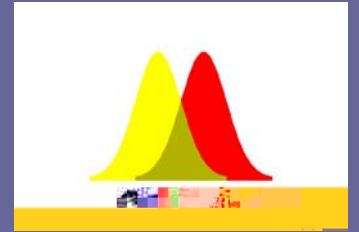
Always look at a residual plot



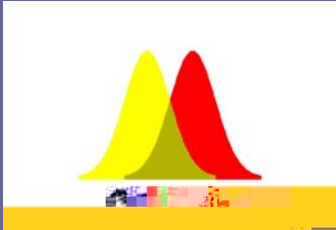
Duplicate readings and use a significance test for lack of fit

Potential errors at low concentrations

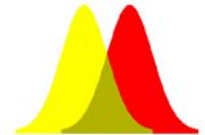




Uncertainty from Sampling



True $\mu = 10\%$



10%

10%

10%

10%

10%

10%

10%

10%

10%

10%

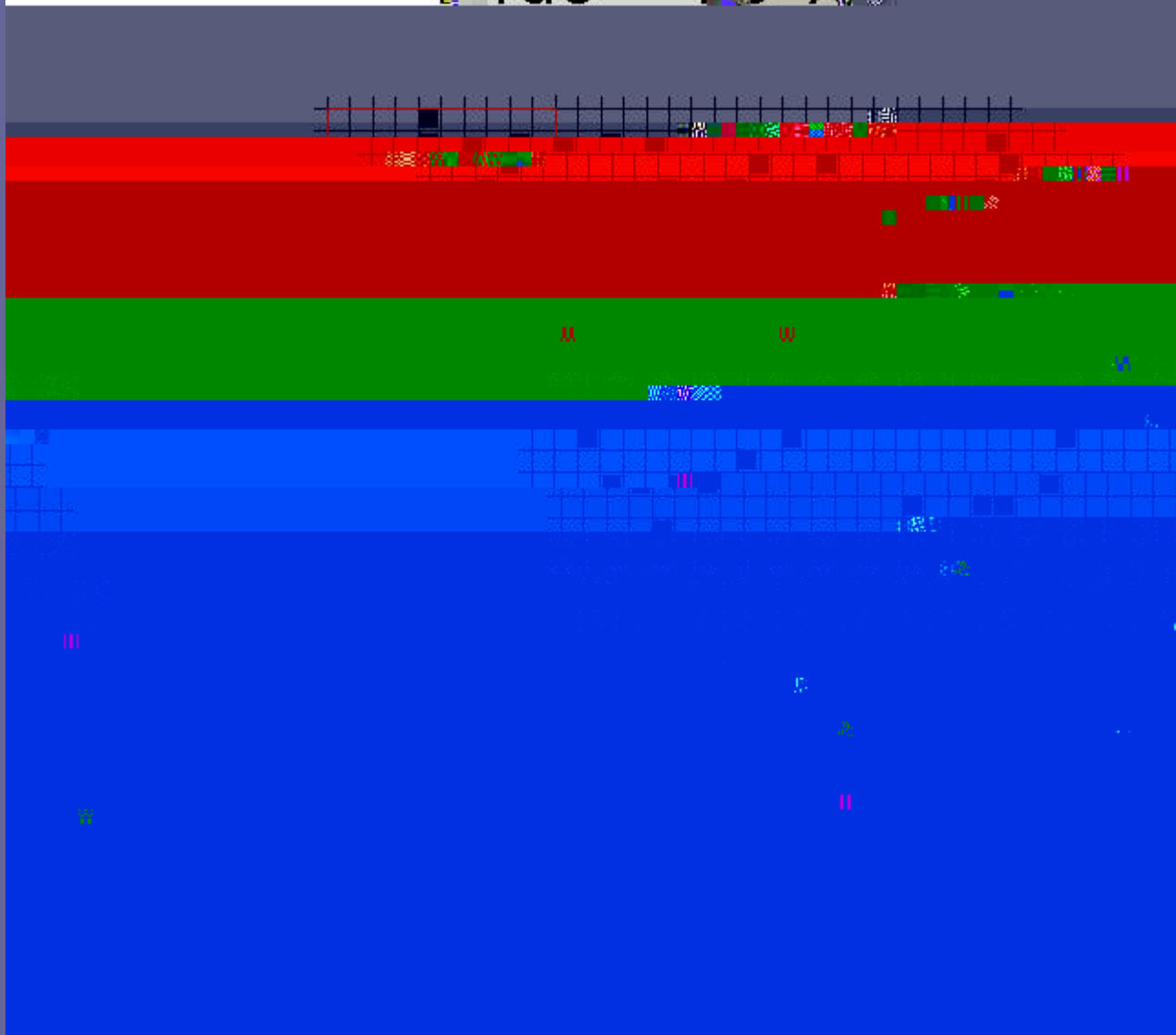
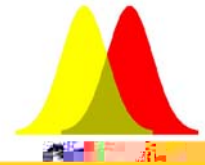
10%

10%

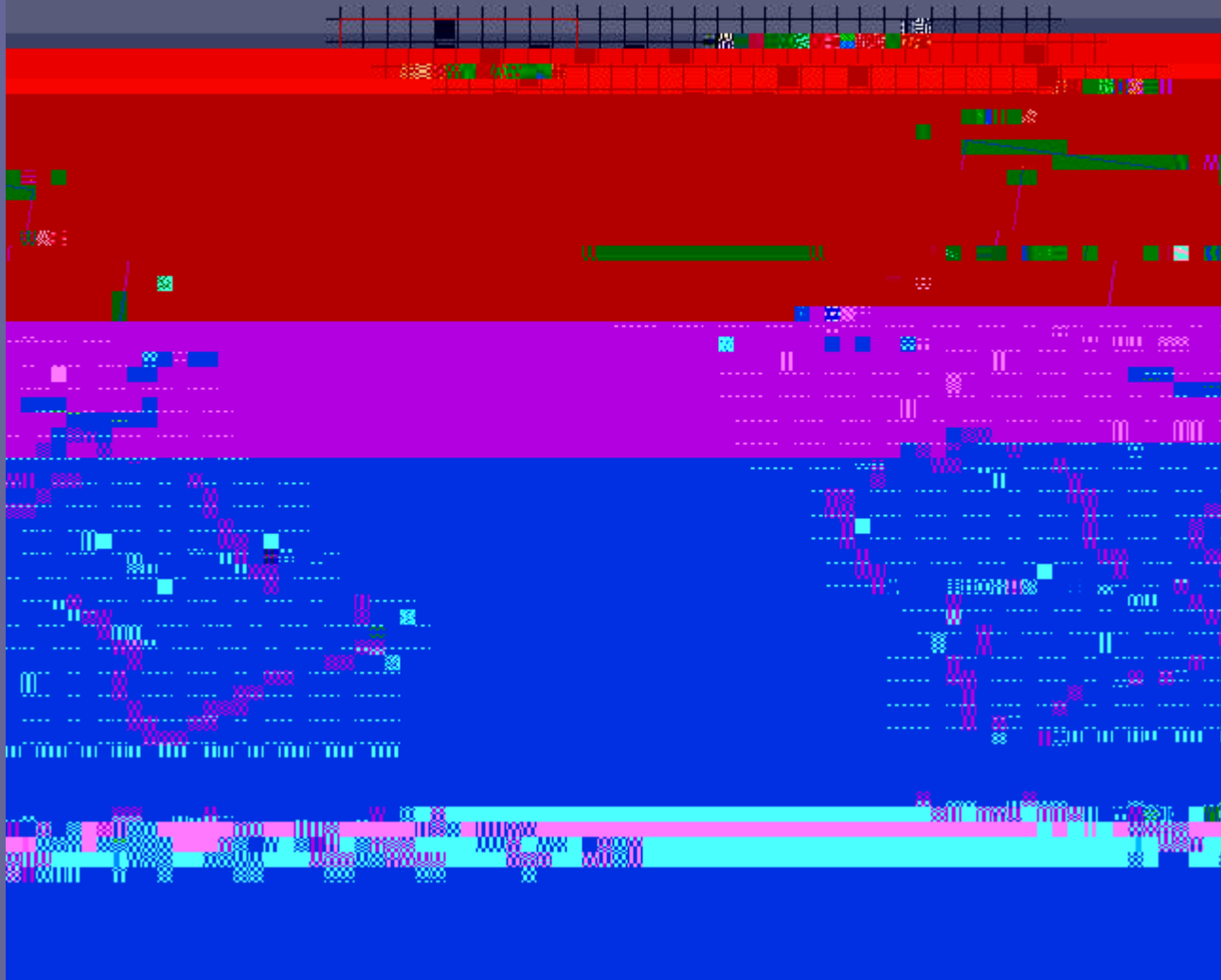
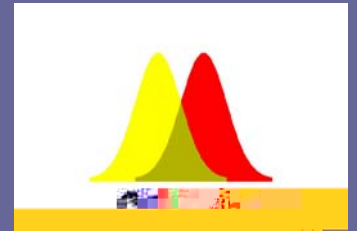
10%

10%

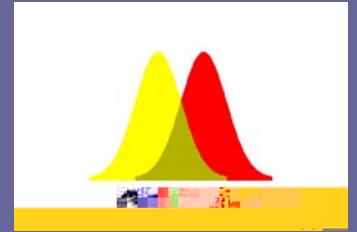
True $\mu = 10\%$



$\text{True} \mu = 10\%$

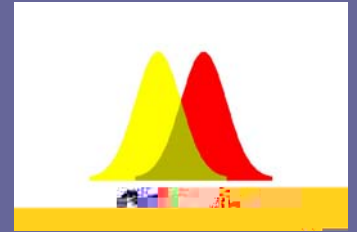


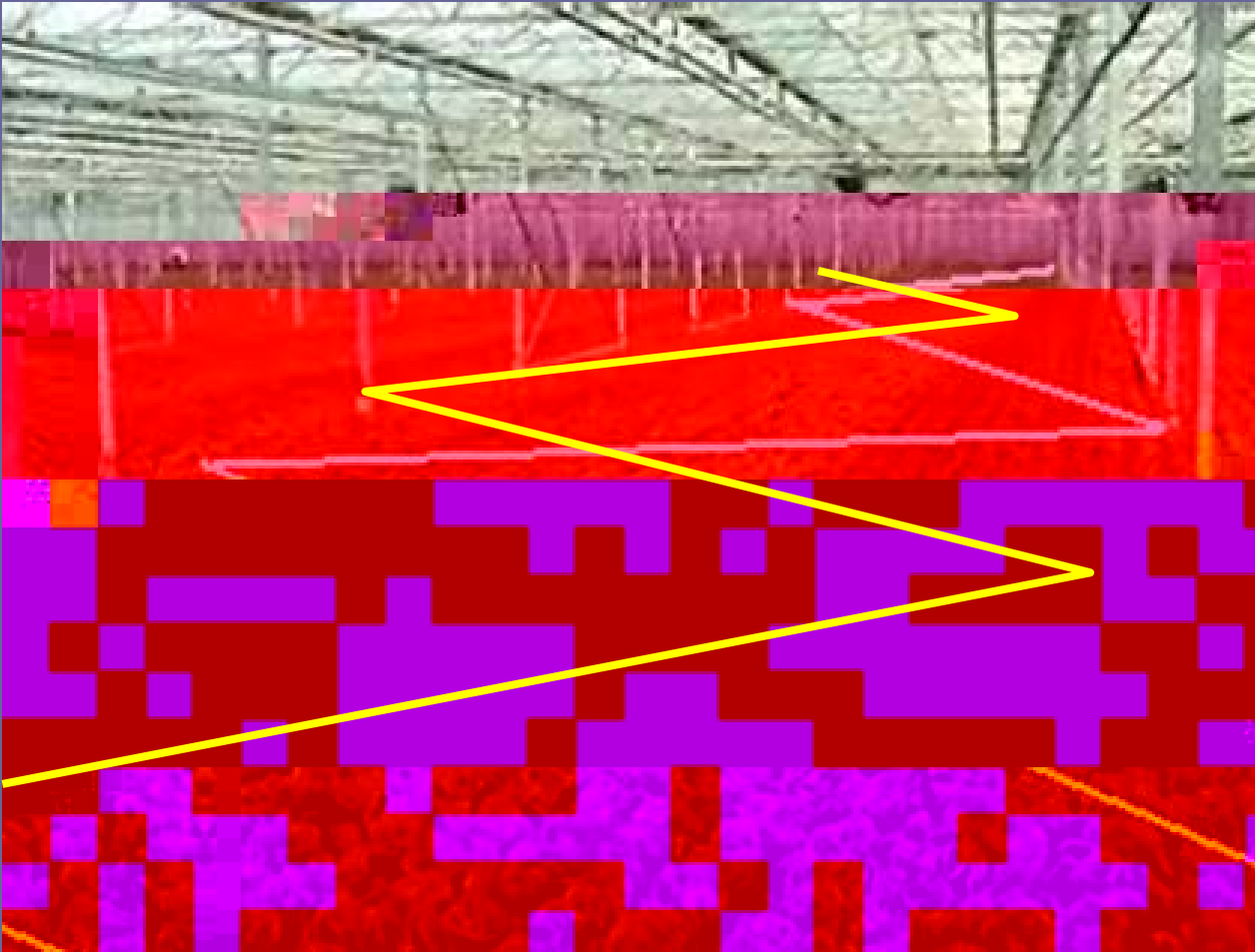
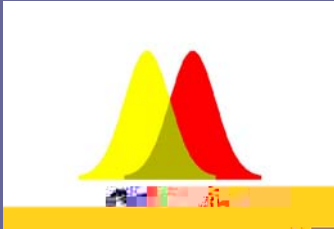
Sampling uncertainty

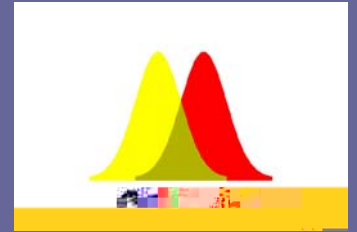


- “Measurement uncertainty arising from sampling—a guide to methods and approaches”.
Eurachem/CITAC/Eurolab/Nordtest/

Lettuce—13-increment sample

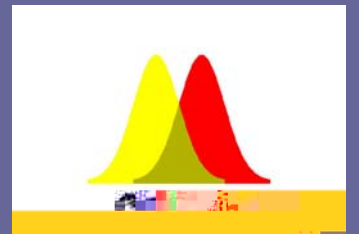


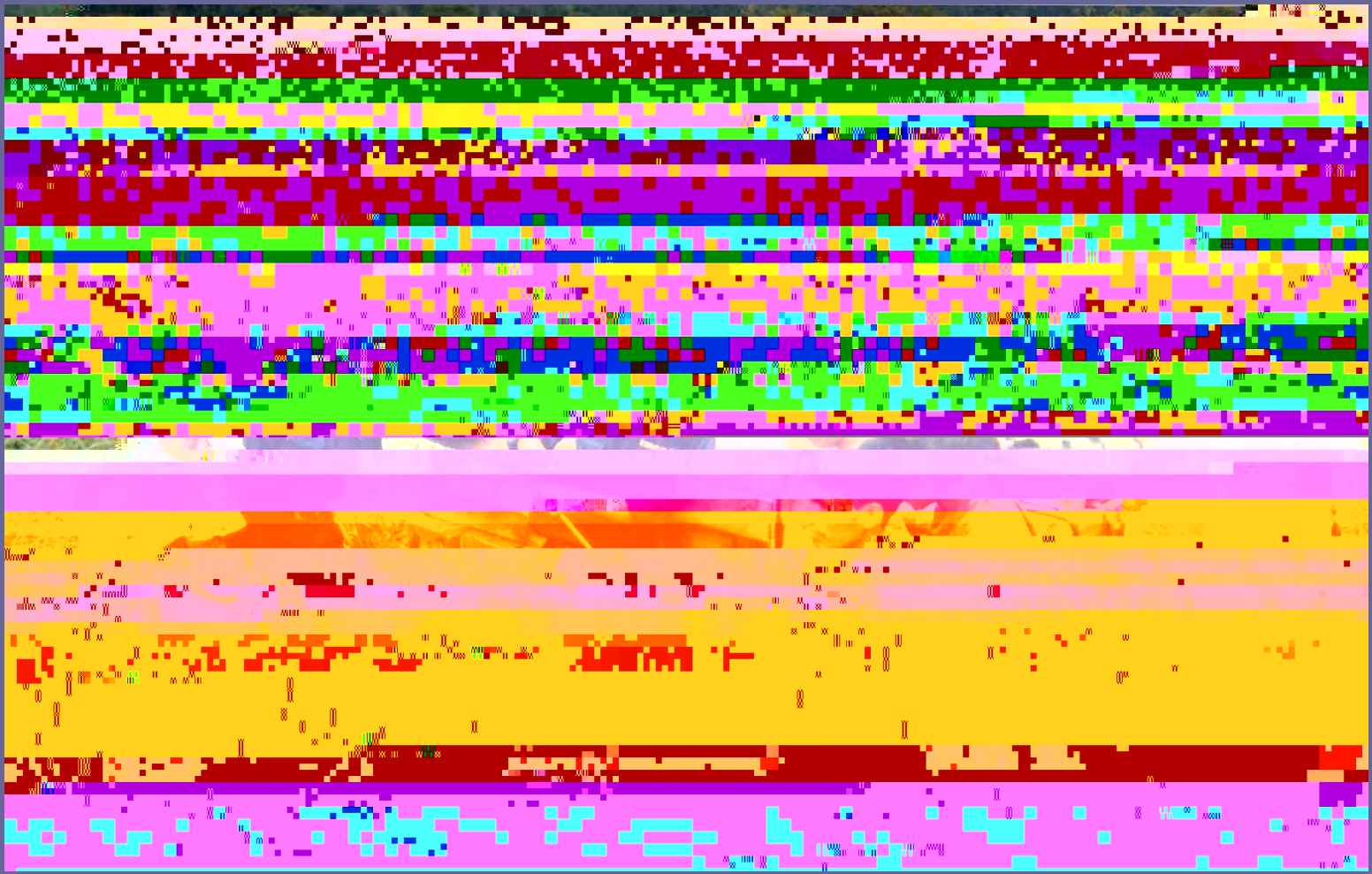
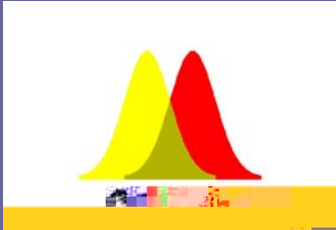




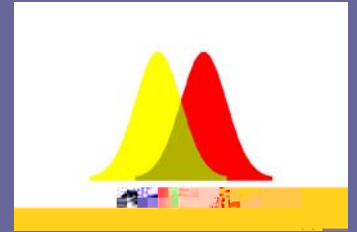
Essential oils

Establishing authenticity via gas chromatograms obtained under standardised conditions.



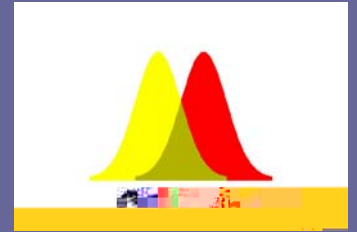


UKAS role of the AMC



- United Kingdom Accreditation Service.
- The AMC has recently been appointed by UKAS as the Advisory Board for chemical measurement.

Could I get involved?



- Contacts via the AMC Chair or Subcommittee Chair.
- Comments, suggestions, ideas *via* MyRSC.