# Selected Topics in Experimental Design and Chemometrics

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Experimentation is one of the foundational pillars of science. Any theoretical hypothesis that is formulated must ultimately be proved or disproved by experiments. While the scientific method is generally intuitively understood by researchers, not all of them fully realize how various controllable and uncontrollable factors might affect their results. Also, the approach to experimentation is often far from optimal. The course will try to fill these voids by exploring the areas mentioned above. It will begin by introducing the tools needed to evaluate the sources of variation in data through the analysis of variance (ANOVA). This will be followed by a discussion of calibration approaches, method ruggedness and sensitivity. Once these issues are understood, the focus will shift towards experimental designs that allow gaining a multitude of insights in a minimum number of experiments. Approaches discussed will include block designs with all their variants (randomized block designs, Latin square designs, Graeco-Latin squares, etc.), factorial and fractional factorial designs, composite designs, mixture designs and Plackett-Burman designs. In the last part of the course issues related to experimental optimization will be discussed. Approaches ranging from sequential "one-factor-at-a-time" through evolutionary operation to response surface methods will be covered. Finally, purely experimental simplex optimization will be introduced.

## *Course Outline*

- Evaluation of sources of variation in data (analysis of variance)
- Calibration
- Reliability and drift
- Sensitivity and limit of detection
- Experimental design
  - The origins of experimental design
  - Block designs
  - Latin square designs
  - Graeco-Latin square designs
  - Hyper-Graeco-Latin squares
  - Factorial designs
  - Fractional factorial designs
  - Composite designs
  - Mixture designs
  - Placket-Burman design
- Experimental optimization
  - Response surfaces
  - Sequential approach
  - Evolutionary operation

Simplex optimization

## **References***:*

G.E.P. Box, J.S. Hunter, W.G. Hunter, "Statistics for Experimenters", 2nd Ed., Wiley Interscience, 2005

D.L. Massart, B.G.M. Vandeginste, S.M. Deming, Y. Michotte, L. Kaufman, "Chemometrics: a textbook", Elsevier, 2003

R.G. Brereton, "Applied Chemometrics for Scientists". J. Wiley & Sons, 2007

| Termin | Dzień tygodnia | Godzina | Miejsce |
|:---:|:---:|:---:|:---:|
| 27.04.2015 | Poniedziałek | 9.15 – 12.35 | Minicentrum Konferencyjne (Luwr) |
| 28.04.2015 | Wtorek | 9.15 – 12.35 | Minicentrum Konferencyjne (Luwr) |
| 29.04.2015 | Środa | 9.15 – 12.35 | Minicentrum Konferencyjne (Luwr) |
| 30.04.2015 | Czwartek | 9.15 – 12.30 | Minicentrum Konferencyjne (Luwr) |