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## NEW GENERAL CHAPTER ON CHEMOMETRICS IN THE EUROPEAN PHARMACOPOEIA

The chapter on *Chemometric methods applied to analytical data* (5.21) has been published in the European Pharmacopoeia Supplement 8.7 which enters into force on 1 April 2016. The European Pharmacopoeia is the first pharmacopoeia to have elaborated such a chapter. This general chapter is for information only and is not legally binding. It is an introduction to the use of chemometric techniques for processing analytical data sets, providing pointers on good chemometric practices and requirements and presenting a selection of those established chemometric methods which are currently most used. The principles of the selected methods are briefly described along with critical aspects and limitations.

The chapter should encourage the use of chemometric methods for the evaluation of data currently generated mainly by spectroscopic methods like near-infrared, Raman or mass spectroscopy. They may of course also be used to analyse analytical data from e.g. LC-MS or other techniques.

Chemometrics is described as the chemical discipline that uses mathematical and statistical methods to design optimal measurement procedures and to provide maximum chemical information by analysing chemical data. It mainly consists of multivariate modelling techniques that result in empirical mathematical models used for the prediction of properties. It helps to structure data sets and to recognise hidden relationships within the system.

Chemometric methods have revolutionised near infrared spectroscopy and such techniques are now an integral component of process analytical technology (PAT) and quality by design (QbD) in a variety of fields. The new chapter contains the following sections:

- Introduction to chemometric methods
- Good chemometric practice including figures of merit, implementation steps, data considerations and maintenance
- Assessment and validation of chemometric methods
- Description of important chemometric techniques (e.g. PCA, measures between objects, SIMCA, MCR, MLR, PCR, PLSR, SVM and ANNs)
- Glossary

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**Note for the Editor:** Further information is available on the internet site **www.edqm.eu**
The EDQM is a leading organisation that protects public health by enabling development, supporting implementation, and monitoring the application of quality standards for safe medicines and their safe use. Our standards are recognised as a scientific benchmark world-wide. The European Pharmacopeia is legally-binding in Member States[1]. Similarly, the EDQM develops guidance and standards in the areas of blood transfusion, organ transplantation and consumer health issues.

[1]There are thirty-eight members of the European Pharmacopoeia Commission: *Austria, Belgium, Bosnia and Herzegovina, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Malta, Montenegro, Netherlands, Norway, Poland, Portugal, Romania, Serbia, Slovak Republic, Slovenia, Spain, Sweden, Switzerland, the Former Yugoslav Republic of Macedonia, Turkey, Ukraine, United Kingdom and the European Union.*