Aims | Contents (*Book chapter)*

Varmuza K.:

In Engel T., Gasteiger J. (eds):
Chemoinformatics - Basic Concepts and Methods,
Wiley-VCH, Weinheim, Germany (2018) p. 399-437. ISBN: 978-3-527-33109-3.

Data Analysis and Data Handling (QSPR/QSAR) - Methods for Multivariate Data Analysis.

Aims

This introduction into the use of multivariate data analysis in chemistry has manifold aims:

- It tries to help getting a basic understanding of the most used methods.
- It provides fundamental mathematical concepts for the interested reader.
- It includes some method codes for the ***R*** programming environment for practical numerical experiments.
- It includes examples with the data and the software provided. The examples are considered to support a better understanding and use of the methods.

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