



**UNIVERSITÀ  
DI PARMA**

PhD Course in Drugs, Biomolecules and Health Products

### **Chemometrics and chemoinformatics: basic multivariate statistics**

2 ECTS

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The course includes lessons (4 h) and training in the computer room.

It gives introduction to the basics of multivariate statistical analysis and to its main applications to some problems related to the design, discovery, analysis and development of drugs and other bioactive chemicals. Principal component analysis (PCA) and partial least squares analysis (PLS) are described and discussed, Training is performed with an open-source statistical program (R) and is based on PCA of data measured for pharmaceutical samples and on multivariate calibration of spectral data by PLS.