Level: master

Course title: Correlation Analysis in Chemistry

Status: elective

**ECTS**: 7

## Requirements: none

## Learning objectives

Since the correlation analysis resulted from the development and wide use of computers in all areas of research, including the chemistry, it is now an integral part of theoretical chemistry. Therefore, the aim of this course is to introduce students to the fundamental correlations between the different characteristics and properties of molecules, ranging from chemical structure, to the complex interactions that occur in biomolecules.

## Learning outcomes

Students will be familiar with the basic mathematical correlations and equations that are used in correlation analysis, as well as current trends in the treatment and interpretation of experimental data.

## Syllabus

Theoretical instruction

The concept of Linear Free Energy Relationships (LFER). Theoretical and practical aspects of LFER correlation. Theoretical models used in the interpretation of linear correlation.

Hammett equation. Multi-parameter form of Hammett equation. Molecular descriptors. Connection between chemical structure, molecular descriptors and molecular activity (QSAR

- Quantitative Structure-Activity Relationships) - application.

Practical instruction

The application of statistical methods in the treatment the experimental data.

Weekly teaching load				Other:
Lectures:	Exercises:	Other forms of	Student research:	
2	1	teaching: 2		