**Level**: PhD

**Course title:** Chemical Structure and Properties of Chemical Compounds (DSH-701)

**Status**: Elective

**ECTS**: 15

**Requirements**: None

**Learning objectives**

Introduce students to the connection that exists between the structure and properties of chemical compounds.

**Learning outcomes**

Upon successful completion of this course, the student should be able to apply different chemometrical methods in the treatment of experimental data and drawing conclusions from the correlations obtained.

**Syllabus**

*Theoretical and practical instruction*

Correlation between chemical structure, properties and physico-chemical characteristics of molecules. Molecular descriptors, atomic, group and fragmentary. Methods for the determination and calculation of descriptors. The connection between descriptors and property (QSPR - Quantitative Structure-Property Relationships). Application of MLR (Multiple Linear Regression), PCA (Principal Component Analysis), HCA (Hierarchical Cluster Analysis), PLS (Partial Least Square) and other chemometric tools in the treatment of experimental data and drawing conclusions from dataset.

| **Weekly teaching load** | | | | Other: |
|---|---|---|---|---|
| Lectures: 5 | Exercises: | Other forms of teaching: | Student research: 5 | |