UČNI NAČRT PREDMETA / COURSE SYLLABUS	
Predmet:	KEMOMETRIJA
Course Title:	CHEMOMETRICS

Študijski program in stopnja Study Programme and Level	Študijska smer Study Field	Letnik Academic Year	Semester Semester
MAG Kemija, 2. stopnja	**/**	**1.**	**2.**
USP Chemistry, 2nd Cycle	**/**	**1st**	**2nd**

Vrsta predmeta / Course Type: izbirni strokovni / Elective Professional

Univerzitetna koda predmeta / University Course Code: K2I11

Predavanja Lectures	Seminar Seminar	Vaje Tutorial	Klinične vaje Work	Druge oblike študija	Samost. delo Individual Work	ECTS
45	15	15 SV	/	/	75	5

Nosilec predmeta / Lecturer: prof. dr. Matevž Pompe / Dr. Matevž Pompe, Full Professor

Jeziki / Languages:

Predavanja / Lectures:	**slovenski / Slovenian**
Vaje / Tutorial:	**slovenski / Slovenian**

Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:	Prerequisites:
Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost.	The course has to be assigned to the student.

Vsebina:	Content (Syllabus outline):
Definicija merskega prostora (skalarji, vektorji, razdalje) Predstavili bomo definicije merskega prostora ter opisov populacije ter vzorca. **Osnove napovedne statistike** Študenti se bodo spoznali z osnovnimi porazdelitvami, ki jih srečamo pri statističnih testih. Prav tako bodo dobili vpogled v predpostavke na katerih temeljijo obravnavani test. Detekcija izvenležečih točk. **Kalibracijska premica**, meja zaznavnosti Obravnavali bomo kalibracijsko premico na	**Definition of the measurement space** (scalar , vector , distance) We will present the definition of the measurement area and descriptions of the population and the sample. **Basics of predictive statistics** Students will learn the basic distributions encountered in statistical tests. They will also get an insight into the assumptions underlying the present test. Detection of outliers. **The calibration line** , the limit of detection The procedure to obtain calibration line will be explained in the case of equal or unequal

primeru enakih ali neenakih varianc v merskem prostoru. Poudarek bo na kasnejšem testiranju modela ter izračunu
merske negotovosti ob upoštevanju enačbe premice.

Izdelava modelov (linearni, nelinearni)
V okviru tega poglavja bodo študenti spoznali osnove večkratne linearne regresije, PLS, PCR kot primeri linearne regresije, med nelinearnimi tehnikami pa bomo predstavili različne umetne nevronske mreže.

Transformacije merskega prostora
Predstavili bomo nekatere pogoste transformacije merskega prostora (npr. PCA,...), ki jih uporabljamo za boljšo predstavitev več dimenzionalnih merskih prostorov.

Optimizacija (genetski algoritem) ter eksperimentalni načrt
Študenti bodo spoznali oba navedena postopka optimizacije v večdimenzionalnem merskem sistemu, kot tudi postopke večnivojskega načrtovanja eksperimentov z namenov zmanjšanja potrebnega števila meritev.

Grupiranje
Predstavili bomo enostavne postopke grupiranja podatkov v večdimenzionalnem merskem prostoru, kot tudi uporabo umetnih nevronskih mrež v te namene.

Vrednotenje modelov
Spoznali bomo osnovne postopke za delitev podatkov v več setov potrebnih za učenje in testiranje modela. Prav tako bomo obravnavali metode, ki jih uporabljamo pri testiranju različnih modelov.

Matematične reprezentacije kemijskih struktur
Spoznali bomo nekatere enostavne reprezentacije kemijskih struktur, ki jih lahko uporabljamo pri modeliranju povezav med

variances in metric space. The focus will be on model validation and measurement uncertainty calculation taking into account the calibration line equation.

Modeling (linear and nonlinear)
In this chapter, students will learn the basics of multiple linear regression , PLS, PCR as examples of the linear regression. As example of the non-linear techniques various artificial neural networks will be presented.

Transformation of the measurement space
Some common measurement space transformation will be presented (eg PCA , ...), which are used to enable the graphical presentation of the multi-dimensional metric spaces .
6 Filtering of noise
Students will learn simple procedures for noise filtrations in the experimental measurements.

Optimization (genetic algorithm) and experimental design
Students will learn about both procedures for optimization in multi-dimensional measurement system. They will gain knowledge on multi-level experimental design in order to reduce the number of required experiments.

Clustering
We will present a simple procedure for clustering of data in a multidimensional space of measurements, as well as the use of artificial neural networks for the same purpose.

Model validation
We will learn the basic procedures for dividing data in different sets needed for model validation (learning and testing set). We will also discuss the methods used in various model validation.

Mathematical representation of chemical structures
Some simple representations of chemical structures that can be used in modeling the

kemijsko strukturo in lastnostmi molekul (QSAR, QSPR). Osnove topoloških indeksov- **Razlike med različnimi tipi QSAR modelov** Modeli za odkrivanje novih zdravil, modeli za regulativo	relationship between chemical structure and properties of molecules (QSAR , QSPR) will be discussed. Basic concepts of topological indices. **Differences between various types of QSAR models.** Models used for drug discovery, models for regulatory purposes

Temeljna literatura in viri / Readings:

- D.L. Massart, B.G.M. Vandeginste, L.C.C. Buydens, S. De Yong, P.J.Lewi, J. Smeyers-Verbeke: handbook of Chemometrics and Qualimetrics, Elsevier, 2003 (700 strani, 30%). Dodatno ZUPAN, Jure. Kemometrija in obdelava eksperimentalnih podatkov. Ljubljana: Kemijski inštitut: Inštitut Nove revije, Zavod za humanistiko, 2009. 368 str., ilustr. ISBN 978-961-92463-3-7.

Cilji in kompetence:	**Objectives and Competences:**
Cilji: a) Seznaniti študente s teorijo in uporabo kemomentričnih metod za: • Pripravo eksperimentov • Predobdelavo merskih podatkov • Vrednotenje podatkov in rezultatov dobljenih pri eksperimentih z večjim številom spremenljivk b) Podati osnove modeliranja, iskanja inverznih modelov ter vrednotenja statistične zanesljivosti dobljenih modelov. c) Omogočiti študentom neposredni dostop do računalnikov ter ustrezne programske opreme za izvedbo naštetih testov. *Kompetence:* Študent bo usposobljen kritično ovrednotiti eksperimentalne podatke, poiskati vzorce v večdimenzionalnih merskih prostorih ter izdelati nekatere enostavne modele, ki povezujejo merski prostor z določeno lastnostjo opazovanega sistema.	**Objectives** a) To acquaint students with the theory and applications of chemometric procedures for: • Preparation of experiments • Pretreatment of experimental data • Evaluation of data and results obtained from experiments with a large number of variables b) Provide the basics of modeling, search for inverse models and the statistical evaluation of the obtained models. c) To allow students direct access to computers and relevant software for carrying out the above tests. **Competences** Student will be able to critically evaluate experimental data to find patterns in multi-dimensional metric spaces, and create some simple models to use measurement space in order to explain some characteristics of the observed system.

Predvideni študijski rezultati:	**Intended Learning Outcomes:**
<u>Znanje in razumevanje</u> Študent se bo naučil kritično uporabljati kemometrične metode. Razumeti bo moral njihovo delovanje. Pri predmetu bo spoznal njihove bistvene prednosti ter omejitve.	<u>Knowledge and Comprehension</u> The students will learn to critically apply chemometric methods. They will understand their operation as well as their main advantages and limitations.

<u>Uporaba</u> Znanja bodo uporabljena v analiznih laboratorijih za zagotavljanje kakovosti rezultatov. Prav tako se bodo znanja uporabljala pri raziskavah v okolju ter analizi živil za razpoznavanje vzorcev ter izdelavi napovednih modelov.	<u>Application</u> Knowledge will be used in analytical laboratories to ensure the quality of the results. The obtained knowledge will be used in the environmental and food research for pattern recognition and the creation of predictive models.
<u>Refleksija</u> Študent bo sposoben samostojno obdelovati eksperimentalne podatke v večdimenzionalnem vektorskem prostoru, v njih poiskati skrite vzorce ter izdelati in validirati enostavne linearne modele.	<u>Analysis</u> Students will be able to independently process the experimental data in multi-dimensional vector space and find the hidden patterns and to establish and validate a simple linear models.
<u>Prenosljive spretnosti</u> Študenti se naučijo kritično podajati in interpretirati eksperimentalne rezultate in izdelati ter validirati enostavne modele.	<u>Skill-transference Ability</u> Students learn to critically present and interpret experimental results and to create and validate simple models.

Metode poučevanja in učenja:	**Learning and Teaching Methods:**
Predavanja s seminarji.	Lectures and seminar work.

Načini ocenjevanja:	Delež (v %) / Weight (in %)	**Assessment:**
Pisni in ustni izpit. ocene od 6-10 (pozitivno) oz. 1-5 (negativno).		Written and oral exam Grades: positive 6-10; negative 1-5.

Reference nosilca / Lecturer's references:

1. **POMPE, Matevž**, DAVIS, Joe M., SAMUEL, Clint D. Prediction of thermodinamic parameters in gas chromatography from molecular structure : hydrocarbons. *J. chem. inf. comput. sci.*, 2004, vol. 44, no. 2, str. 399-409.
2. **POMPE, Matevž**. Variable connectivity index as a tool for solving the 'anti-connectivity' problem. *Chem. Phys. Lett.*. [Print ed.], 2005, vol. 404, no. 4/6, str. 296-299.
3. KOLAR, Jana, ŠTOLFA, Andrej, STRLIČ, Matija, **POMPE, Matevž**, PIHLAR, Boris, BUDNAR, Miloš, SIMČIČ, Jurij, REISSLAND, Birgit. Historical iron gall ink containing documents - properties affecting their condition. *Anal. chim. acta*. [Print ed.], 2006, vol. 555, str. 167-174.