KEMIJA HETEROCIKLIČNIH SPOJIN

UČNI NAČRT PREDMETA/COURSE SYLLABUS

Predmet:	Kemija heterocikličnih spojin
Course title:	CHEMISTRY OF HETEROCYCLIC COMPOUNDS
Članica nosilka/UL Member:	UL FKKT

Študijski programi in stopnja	Študijska smer	Letnik	Semestri	Izbirnost
Kemija, prva stopnja, univerzitetni	Ni členitve (študijski program)	2. letnik, 3. letnik		izbirni

Univerzitetna koda predmeta/University course code:	0086911
Koda učne enote na članici/UL Member course code:	KESI9

Predavanja /Lectures	Seminar /Seminar	Vaje /Tutorials	Klinične vaje /Clinical tutorials	Druge oblike študija /Other forms of study	Samostojno delo /Individual student work	ECTS
30	15	30 LV			75	5

Nosilec predmeta/Lecturer:	prof. dr. Uroš Grošelj
Vrsta predmeta/Course type:	izbirni/elective

Jeziki/Languages:	Predavanja/Lectures:	Angleščina, Slovenščina
	Vaje/Tutorial:	Angleščina, Slovenščina

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):
Struktura, nomenklatura in lastnosti heterociklov. Sistematika osnovnih sistemov (velikost, število, in povezava obročev, stopnja nasičenja). Heteroaromati: tavtomerija in valenčne izomerizacije. Nasičeni sistemi: napetost malih obročev, konformacijske značilnosti in analiza, anomerni efekt. **Sinteza heterociklov.** Ciklizacije (ciklosubstitucije, ciklokondenzacije, cikloadicije). Značilni gradniki za sintezo heterociklov. Baldwinova pravila. **Pretvorbe heterociklov.** Reakcije z elektrofili in nukleofili. Odpiranja in pretvorbe obročev. Metaliranje heterociklov. S paladijem katalizirane reakcije. Periciklične reakcije. **Pregled kemije osnovnih tipov heterociklov.**	**Structure, nomenclature, and properties of heterocyclic compounds:** Systematic survey on heterocycles (ring size, number of rings, connection of rings). Heteroaromatic systems: tautomerism and valence isomerisation. Saturated heterocycles: ring strain in small rings, conformational properties and analysis, anomeric effect. **Synthesis of heterocycles.** Cyclisations (cyclosubstitutions, cyclocondensations, cycloadditions). Typical building blocks in the synthesis of heterocycles. Baldwin rules. **Transformations of heterocylces.** Reactions with electrophiles and nucleophiles. Ring-opening and ring-transformations. Metallation of heterocycles. Palladium in heterocyclic chemistry. Pericyclic reactions.

Piridini, kinolini in izokinolini. Diazini. Piroli in indoli. Furani in tiofeni. 1,2- in 1,3-diazoli. Heterocikli s tremi in več heteroatomi. Heterocikli z mostnim dušikovim atomom. **Pomen heterociklov v kemiji, biokemiji in farmaciji.**	**Survey on the chemisty of fundamental heterocyclic systems.** Pyridines, quinolines, and isoquinolines. Pyrroles and indoles. Furans and thiophenes. 1,2- and 1,3-diazoles. Systems with three or more heteroatoms. Systems with a bridgehead nitrogen atom. **Importance of heterocycles in chemistry, biochemistry, and pharmacy.**

Temeljna literatura in viri/Readings:

- A. Joule, K. Mills: Heterocyclic Chemistry At A Glance, 2nd Edition, John Wiley & Sons, 2013, 230 strani.

Dodatna literatura:

- Comprehensive Heterocyclic Chemistry III, A. R. Katritzky, C. A. Ramsden, E. F. V. Scriven, R. J. K. Taylor eds., Elsevier Science, Oxford 2008. (izbrana poglavja).
- Pregledni članki, ki pokrivajo posamezne vsebine iz heterociklične kemije (praviloma v zadnjih 10 letih),
- Louis D. Quin, John A. Tyrell, FUNDAMENTALS OF HETEROCYCLIC CHEMISTRY, Importance in Nature and in the Synthesis of Pharmaceuticals, WILEY,
- Peter A. Jacobi, INTRODUCTORY HETEROCYCLIC CHEMISTRY, WILEY.

Cilji in kompetence:	**Objectives and competences:**
Heterociklične spojine predstavljajo zelo pomemben del organske kemije, farmacije in biokemije, saj igrajo bistveno vlogo v osnovnih življenjskih procesih. **Cilj**: Študent se v okviru tega predmeta seznani s sintezami in pretvorbami heterocikličnih sistemov kot pomembnih gradnikov v organski kemiji, biokemiji in farmaciji. **Kompetence**: Poznavanje in uporaba heterocikličnih spojin kot intermediatov v organski sintezi.	Due to essential role of heterocyclic compounds in biological processes, these compounds represent an important topic in chemistry, biochemistry, and pharmacy. *Objectives:* The expected learning outcomes are knowledge and understanding of the synthesis and typical reactivity and transformations of heterocycles as well as their use as building blocks in organic chemistry, biochemistry, and pharmacy. *Competences:* Knowledge of heterocyclic compounds and their application as intermediates in organic synthesis.

Predvideni študijski rezultati:	**Intended learning outcomes:**
Znanje in razumevanje Študent se nauči: - sinteze in pretvorbe osnovnih heterocikličnih sistemov s posebnim poudarkom na sistemih, ki so pomembni v organski sintezi in biokemiji - pretvorbe in premestitve heterocikličnih sistemov, ki so zlasti pomembne v organski sintezni kemiji - uporabnost hetrocikličnih N-oksidov v sintezni kemiji - elektrofilne in nukleofilne substitucije - reaktivnost petčlenskih in šestčlenskih heterociklov, podobnosti in razlike - selektivne reaktivnosti, transformacije funkcionalnih skupin Uporaba Poznavanje heterociklične kemije je eden od temeljev organske kemije, zlasti v sintezni organski kemiji, kjer služijo heterocikli mnogokrat kot reaktivni intermediati. To znanje služi poleg tega še vrsti drugih področij, predvsem biokemiji in farmacevtski industriji, kemiji kompleksov z anorganskimi ioni, itd. Refleksija	Knowledge and Comprehension The student learns*:* -syntheses and transformations of basic heterocyclic systems with emphasis on systems relevant for organic synthesis and biochemistry - transformations and rearrangements of heterocyclic systems relevant in organic synthesis - application of heterocyclic N-oxides in synthetic chemistry - electrophilic and nucleophilic substitutions, - reactivity of five- and six-membered heterocycles, similarity and differences, - selective reactivity, transformations of functional groups Application The knowledge of heterocyclic chemistry belongs to fundamentals of organic chemistry, especially in synthetic organic chemistry, where heterocyclic compounds are frequently used as reactive intermediates. This knowledge is also essential in other related fields, such as biochemistry,

Predmet je osnova za delo na ostalih področjih kemije predvsem nekaterih predmetov izbirnega sklopa organske kemije in biokemije. Posebnega pomena je tovrstno znanje za delo v kemijski in farmacevtski industriji Prenosljive spretnosti Znanje heterociklične kemije zagotavlja zaradi prisotnosti heteroatomov v organskem skeletu najširše strukturne in reakcijske možnosti na celotnem področju kemije.	pharmaceutical chemistry, and coordination chemistry etc. Analysis Knowledge of heterocyclic chemistry is required for practical work in other areas of chemistry. It is also useful if not a prerequisite for elective courses from various specialized topics in organic chemistry. This knowledge is of vital importance for those working in chemical and pharmaceutical industry. Skill-transference Ability Due to presence of heteroatoms in organic structure, the knowledge of heterocyclic chemistry gives wide structural and reaction possibilities within the whole area of chemistry.

Metode poučevanja in učenja:	**Learning and teaching methods:**
Predavanja; seminarji, individualni in skupinski projekti, laboratorijske vaje, individualni in skupinski sintezni projekti.	Lectures, seminars, seminar projects, and laboratory trainings.

Načini ocenjevanja:	**Delež/Weight**	**Assessment:**
Pisni izpit	70,00 %	Written exam
Seminarska naloga	30,00 %	Seminar project
Ocene: pozitivno 6-10; negativno 1-5.		Grades: positive 6-10, negative 1-5

Reference nosilca/Lecturer's references:

L. Ciber, S. Ričko, J. Gregorc, F. Požgan, J. Svete, H. Brodnik, B. Štefane, **U. Grošelj**, Mechanistic Insights into Annulation of Arylidene-Δ²-pyrrolin-4-ones by Cinchona Squaramide-Based Organocatalysts, *Adv. Synth. Catal.* **2022**, *364*, 980-993. https://doi.org/10.1002/adsc.202101369.

U. Grošelj, L. Ciber, J. Gnidovec, Ž. Testen, F. Požgan, B. Štefane, G. Tavčar, J Svete, S. Ričko, Synthesis of Spiro-Δ²-Pyrrolin-4-One Pseudo Enantiomers via an Organocatalyzed Sulfa-Michael/Aldol Domino Sequence, *Adv. Synth. Catal.* **2019**, *361*, 5118–5126. https://doi.org/10.1002/adsc.201900747

S. Ričko, A. Meden, L. Ciber, B. Štefane, F. Požgan, J. Svete, **U. Grošelj**, Construction of Vicinal Tetrasubstituted Stereogenic Centers via a Mannich-Type Organocatalyzed Addition of Δ²-Pyrrolin-4-ones to Isatin Imines, *Adv. Synth. Catal.* **2018**, *360*, 1072–1076. https://doi.org/10.1002/adsc.201701384