

## UČNI NAČRT PREDMETA / COURSE SYLLABUS

|                      |                                     |
|----------------------|-------------------------------------|
| <b>Predmet:</b>      | KEMIJA HETEROCIKLIČNIH SPOJIN       |
| <b>Course Title:</b> | CHEMISTRY OF HETEROCYCLIC COMPOUNDS |

| Študijski program in stopnja<br>Study Programme and Level | Študijska smer<br>Study Field | Letnik<br>Academic Year | Semester<br>Semester |
|---|-------------------------------|-------------------------|----------------------|
| UŠP Kemija, 1. stopnja                                    | /                             | 3.                      | 6.                   |
| USP Chemistry, 1 <sup>st</sup> Cycle                      | /                             | 3 <sup>rd</sup>         | 6 <sup>th</sup>      |

**Vrsta predmeta / Course Type:** izbirni strokovni / Elective Professional

**Univerzitetna koda predmeta / University Course Code:** KES19

| Predavanja<br>Lectures | Seminar<br>Seminar | Vaje<br>Tutorial | Klinične vaje<br>Work | Druge oblike študija | Samost. delo<br>Individual Work | ECTS |
|------------------------|--------------------|------------------|-----------------------|----------------------|---------------------------------|------|
| 30                     | 15                 | 30 LV            | /                     | /                    | 75                              | 5    |

**Nosilec predmeta / Lecturer:** doc. dr. Uroš Grošelj / Dr. Uroš Grošelj, Assistant Professor

**Jeziki / Languages:**

|                               |                       |
|-------------------------------|-----------------------|
| <b>Predavanja / Lectures:</b> | slovenski / Slovenian |
| <b>Vaje / Tutorial:</b>       | slovenski / Slovenian |

**Pogoji za vključitev v delo oz. za opravljanje študijskih obveznosti:**

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|---|--|
| Študent oz. kandidat mora imeti predmet opredeljen kot študijsko obveznost. | <b>Prerequisites:</b><br>The course has to be assigned to the student. |
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**Vsebina:**

**Struktura, nomenklatura in lastnosti heterociklov.** Sistematika osnovnih sistemov (velikost, število, in povezava obročev, stopnja nasičenja). Heteroaromati: tautomerija in valenčne izomerizacije. Nasičeni sistemi: napetost malih obročev, konformacijske značilnosti in analiza, anomerni efekt.

**Sinteza heterociklov.** Ciklizacije (ciklosubstitucije, ciklokonkondenzacije, cikloadicije). Značilni gradniki za sintezo heterociklov. Baldwinova pravila.

**Pretvorbe heterociklov.** Reakcije z elektrofilni in nukleofili. Odpiranja in pretvorbe obročev. Metaliranje heterociklov. S paladijem katalizirane reakcije. Periciklične reakcije.

**Pregled kemije osnovnih tipov heterociklov.**

**Content (Syllabus outline):**

**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 heterocycles.** Reactions with electrophiles and nucleophiles. Ring-opening and ring-transformations. Metallation of heterocycles. Palladium in heterocyclic

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 duškovim atomom.  
**Pomen heterociklov v kemiji, biokemiji in farmaciji.**

chemistry. Pericyclic reactions.  
**Survey on the chemistry 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).

#### Cilji in kompetence:

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.

#### Objectives and Competences:

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:

##### 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 heterocikličnih N-oksidov v sintezni kemiji
- elektrofilne in nukleofilne substitucije

#### Intended Learning Outcomes:

##### 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,

|   |  |
|---|--|
| - reaktivnost petčlenskih in šestčlenskih heterociklov, podobnosti in razlike<br>- selektivne reaktivnosti, transformacije funkcionalnih skupin   | - reactivity of five- and six-membered heterocycles, similarity and differences,<br>- selective reactivity, transformations of functional groups   |
| <u>Uporaba</u><br>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. | <u>Application</u><br>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, pharmaceutical chemistry, and coordination chemistry etc. |
| <u>Refleksija</u><br>Predmet je osnova za delo na ostalih področjih kemije predvsem nekaterih predmetov izbirnega sklopa organske kemije in biokemije.<br>Posebnega pomena je tovrstno znanje za delo v kemijski in farmacevtski industriji   | <u>Analysis</u><br>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.                                       |
| <u>Prenosljive spretnosti</u><br>Znanje heterociklične kemije zagotavlja zaradi prisotnosti heteroatomov v organskem skeletu najširše strukturne in reakcijske možnosti na celotnem področju kemije.  | <u>Skill-transference Ability</u><br>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:

Predavanja; seminarji, individualni in skupinski projekti, laboratorijske vaje, individualni in skupinski sintezni projekti.

#### Learning and Teaching Methods:

Lectures, seminars, seminar projects, and laboratory trainings

Delež (v %) /

#### Načini ocenjevanja:

Weight (in %) **Assessment:**

|                                       |             |                                     |
|---------------------------------------|-------------|-------------------------------------|
| Pisni izpit                           | <b>70 %</b> | Written exam                        |
| Seminarska naloga                     | <b>30 %</b> | Seminar project                     |
| Ocene: pozitivno 6-10; negativno 1-5. |             | Grades: positive 6-10, negative 1-5 |

#### Reference nosilca / Lecturer's references:

1. E. Pušavec Kirar, M. Drev, J. Mirnik, U. Grošel, A. Golobič, G. Dahmann, F. Požgan, B. Štefane, J. Svete, Synthesis of 3D-Rich Heterocycles: Hexahydropyrazolo[1,5-a]pyridin-2(1H)-ones and Octahydro-2H-2a,2a1-diazacyclopenta[cd]inden-2-ones, J. Org. Chem. 2016, 81, 8920–8933. DOI: 10.1021/acs.joc.6b01608. [COBISS.SI-ID 1537115331]
2. U. Grošel, E. Pušavec, A. Golobič, G. Dahmann, B. Stanovnik, J. Svete, Synthesis of 1,5-

disubstituted-4-oxo-4,5-dihydro-1H-pyrazolo[4,3-c]pyridine-7-carboxamides, *Tetrahedron* 2015, 71, 109–123. DOI: 10.1016/j.tet.2014.11.034. [COBISS.SI-ID 1536061891]

3. U. Grošelj, A. Beck, W. B. Schweizer, D. Seebach, Preparation and Structures of 2-Substituted 5-Benzyl-3-methylimidazolidin-4-one-Derived Iminium Salts, Reactive Intermediates in Organocatalytic Transformations Involving  $\alpha,\beta$ -Unsaturated Aldehydes, *Helv. Chim. Acta* 2014, 97, 751–796. DOI: 10.1002/hlca.201400110. [COBISS.SI-ID 1536179139]

4. U. Grošelj, M. Žorž, A. Golobič, B. Stanovnik, J. Svete,  $\alpha$ -Amino acid derived enaminones and their application in the synthesis of N-protected methyl 5-substituted-4-hydroxypyrrole-3-carboxylates and other heterocycles, *Tetrahedron* 2013, 69, 11092–11108. DOI: 10.1016/j.tet.2013.11.008. [COBISS.SI-ID 1650735]

5. U. Grošelj, A. Podlogar, A. Novak, G. Dahmann, A. Golobič, B. Stanovnik, J. Svete, Synthesis of tetrahydropyrazolo[1,5-c]pyrimidine-2,7(1H,3H)-diones, *Synthesis* 2013, 45, 639–650. DOI: 10.1055/s-0032-1318107. [COBISS.SI-ID 36543749]

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