SAGRADO
Universidad del Sagrado Corazón

SCHOOL OF HEALTH AND SCIENCES

SYLLABUS

TITLE:	Organic Chemistry II
CODE:	QUI 302
PREREQUISITE:	QUI 301
CORREQUISITES:	QUI 302L
CREDITS:	4 credits | 45 contact hours | 45 lab hours | 1 term

DESCRIPTION

Study of aromatic systems, aromatic electrophilic substitution mechanisms, nucleophilic addition to carbonyl, acyl nucleophilic substitution, and condensations related to enolates. The IUPAC nomenclature of benzene derivatives, aldehydes, ketones, carboxylic acids and their derivatives, and amines is discussed. An introduction to the chemistry of carbohydrates, lipids, amino acids, and nucleic acids is presented at the end. The course discusses spectroscopic techniques such as ultraviolet-visible, infrared, ^{13}C nuclear magnetic resonance, and mass spectrometry for the elucidation of organic compound structures integrating all these techniques. This course uses web-supported resources, lectures, lab experiences, and teamwork to write a research proposal. This course is aimed at students majoring in Chemistry and health-allied sciences, trained to understand the biological and industrial processes of the world around us.

JUSTIFICATION

Medicines, textiles, plastics, fuels, food, and biological processes occur in the daily life of human beings. Organic chemistry is present in these processes. Therefore, it is important for a student who is training as a scientist to have knowledge about how organic chemistry works. The purpose of the course is to train students to understand organic chemistry and thus have a basis to be able to understand the processes that occur in biological systems or in the environment. This branch of chemistry permeates everything that happens in our daily lives

COMPETENCES

The course develops the following competences in students:

- **Critical questioning**
- **Research and exploration**
- **Communication**

OBJECTIVES

After completion of the course, students will be able to:

1. Explain chemical properties of an aromatic system.
2. Elucidate the molecular structure of an organic compound based on its infrared, mass, nuclear magnetic resonance, and UV-VIS spectra.
3. Explain the chemical properties of aldehydes, ketones, carboxylic acids, and their derivatives and how those properties help carry out organic synthesis.
4. Explain the different condensation reactions that can be carried out in organic compounds and their synthetic use.
5. Explain the chemical properties of amines and how they help carry out organic synthesis.
6. Explain some chemical properties of biologically important organic compounds.

CONTENTS

I. Aromaticity
   A. Resonance
   B. Molecular orbital theory
      1. Fundamentals
         a. Bonding, antibonding, and nonbonding molecular orbitals
         b. Nodes
         c. HOMO & LUMO
      2. Pi molecular orbitals
      3. Allyl system
      4. 1,3-butadiene system
   C. Benzene molecule case
      1. Pi molecular orbitals
      2. Degenerate orbitals
   D. Benzene structure

E. Properties of an aromatic system
    1. Pi electron delocalization
    2. Planar cyclic structure
    3. 4n + 2 pi electrons
    4. Energy diagram of pi molecular orbitals
F. Properties of an antiaromatic system
    1. Definition
    2. 4n pi electrons
    3. Energy diagram of molecular orbitals
G. Ultraviolet-visible spectroscopy (UV-VIS)
    1. Electronic transitions
    2. Instrumentation
    3. Transmittance and absorbance
    4. Absorption spectrum and λMAX
    5. Effect of solvent on λMAX
    6. Woodward-Fieser Rules
        a. Polyenes
        b. Conjugated ketones and aldehydes
        c. Benzene derivatives
H. Electrophilic aromatic substitution
    1. General mechanism
    2. Monosubstitution reactions
        a. Halogenation
        b. Nitration
        c. Sulfonation
        d. Friedel-Crafts alkylation
        e. Friedel-Crafts acylation
    3. Ortho, para, and meta orientation
    4. Resonance and inductive effect on orientation in the product
    5. Reactions of benzene derivatives with R groups and acyl
        a. Oxidation
        b. Reductions
    6. Reactions using diazonium salt

a. Conditions
b. Synthetic routes from diazonium salt

II. Spectroscopic methods
A. Infrared spectroscopy
1. Vibrational modes
a. Symmetrical and asymmetrical elongations
b. Bending
1) Rocking
2) Scissoring
3) Twisting
4) Wagging
2. Oscillator
a. Spring force constant
b. Wavelength
3. Infrared spectrum
a. Useful region
b. Broad bands
c. Sharp bands
4. Functional groups and wavenumber
a. Alkanes
b. Alkenes
c. Alkynes
d. Alcohols
e. Ketones
f. Aldehydes
g. Carboxylic acids and their derivatives
h. Nitriles
i. Amines
j. Benzene derivatives
5. Variations in carbonyl absorption frequency
a. Resonance effect
b. Inductive effect
c. Angular tension

        d. Hydrogen bonds
    6. Examples

B. Mass spectrometry
    1. Instrumentation
        a. Ionization chamber
        b. Mass separator
        c. Mass spectrum
            1) Mass-to-charge ratio (m/z)
            2) Relative abundance
            3) Molecular ion
            4) Base peak
    2. Fragmentation patterns
        a. Alkanes
        b. Alkenes
        c. Alkynes
        d. Alcohols
        e. Ethers
        f. Aromatics
    3. McLafferty rearrangement
        a. Aldehydes
        b. Ketones
        c. Carboxylic acids
        d. Esters
        e. Amides
        f. Anhydrous
    4. Halogenated compounds
        a. Isotopic pattern of chlorinated compounds
        b. Isotopic patterns of brominated compounds
    5. Examples of mass spectra

C. Introduction to ^{1}H and ^{13}C nuclear magnetic resonance
    1. Degree of unsaturation
        a. Meaning
        b. Formula to calculate it

2. Nuclear spin
3. Magnetic field
4. NMR process
5. Hydrogen shielding
6. Chemical displacement
7. Proton equivalence
    a. Homotopic hydrogens
    b. Enantiotopic hydrogens
    c. Diastereotopic hydrogens
8. Spin-spin coupling
    a. Types of signals
        1) Singlet
        2) Doublet
        3) Triplet
        4) Quartet
        5) Multiplet
    b. Coupling constant
9. Structure elucidation
10. Magnetic anisotropy
    a. Carbonyl
    b. Alkenes
    c. Alkynes
    d. Aromatics
11. Splitting patterns that do not follow the N+1 rule
12. Magnetic resonance of ^{13}C
    a. Principles
    b. Nuclear spin of ^{13}C
    c. Characteristic chemical displacements
    d. Spectrum of NMR ^{13}C
    e. Examples
    f. Elucidation of organic compound structures

III. Aldehydes, Ketones, Carboxylic Acids, and Their Derivatives

A. Aldehydes and ketones

1. Nomenclature of aldehydes and ketones
2. Preparation of aldehydes and ketones
    a. Keto-enol tautomerism
    b. Oxidation of primary alcohols
    c. Adding water to alkynes
    d. Oxidation of primary and secondary alcohols
3. Aldehyde and ketone reactions
4. Mechanism of nucleophilic addition to carbonyl
    a. Reactivity via steric effect
    b. Reactivity via inductive effect
5. Addition of HCN: formation of cyanohydrins
6. Addition of alcohols in acidic medium: formation of ketals and acetals
7. Phosphorane addition: the Wittig reaction
8. Addition of 1,2-ethanediol: protection of carbonyl groups in synthesis
9. Addition of hydroxylamine, hydrazine, phenylhydrazine and phenyl semicarbazone
10. Qualitative testing of aldehydes and ketones
    a. Tollens test
    b. Iodine test

B. Carboxylic acids and their derivatives
1. IUPAC nomenclature of carboxylic acids
2. Preparation of carboxylic acids
    a. Oxidation of alcohols, alkylbenzenes, and aldehydes
    b. Grignard reaction with CO_2
    c. Acid hydrolysis of nitriles
    d. Purification of carboxylic acids
3. Carboxylic acid reactions
    a. Preparation of acyl chlorides from carboxylic acids
    b. Decarboxylation
    c. Dehydration of carboxylic diacids
    d. Formation of acyl chlorides from $SOCl_2$, PCl_3 and PCl_5
4. Preparation of carboxylic acid derivatives
    a. Structure of carboxylic acid derivatives

1) Acyl chlorides
2) Acid anhydrous
3) Nitriles
4) Esters
5) Amides

b. Mechanism of acyl nucleophilic substitution
1) Order of reactivity of the different derivatives
2) Preparation of carboxylic acid derivatives from acyl chlorides
3) Preparation of carboxylic acid derivatives from anhydrous acids
4) Fischer esterification
5) Hydrolysis of esters and amides in acid and basic mediums
6) Nitrile preparation and hydrolysis

IV. Condensation Reactions Using Enolates
A. Aldol condensation
1. Mechanism
2. Formation of the α,β-unsaturated system
3. Synthetic routes from the aldol product and the α,β-unsaturated system
a. Reduction with $NaBH_4$ and $LiAlH_4$
b. Reduction with H_2 in Pd-C and Ni

B. Cross aldol condensation
C. Practical cross-aldol condensation
D. Claisen-Schmidt condensation
E. Cyclization
F. Nucleophilic addition to β carbon from an α,β-unsaturated system
1. The Michael Addition
2. The Robinson Annulation

G. Aldol condensation in an acidic medium
H. Synthesis of monosubstituted and disubstituted ketones

V. Amines
A. Nomenclature of amines

B. Basicity of amines
    1. Basic strength
    2. Amines vs. amides
C. Preparation of amines
    1. S_N2 nucleophilic substitution
    2. Alkyl halide reaction with azide followed by reduction
    3. Reduction of nitro compounds
    4. The Gabriel Synthesis
    5. Substitution with NH_3 derivatives and reduction
    6. Reduction of nitriles and amides
    7. Reduction of oximes
    8. Hofmann rearrangement
D. Purification of amines
E. Amine reactions
    1. Oxidation with H_2O_2
    2. Cope elimination
    3. Hoffman elimination

VI. Biologically Important Organic Compounds
A. Carbohydrates
    1. Classification of carbohydrates
        a. Monosaccharides
        b. Polysaccharides
    2. Classification of monosaccharides
        a. Ketoses
        b. Aldoses
    3. D and L configurations of sugars
    4. D-aldose and D-ketose family
    5. Cyclic structures of monosaccharides
        a. The case of glucose
        b. The case of fructose
        c. Pyranoses and furanoses
    6. Anomers in monosaccharides
        a. Anomer α and anomer β

b. Mutarotation

7. Monosaccharide reactions
    a. Epimerization
    b. Reductions: alditols
    c. Oxidation
        1) Bromine water
        2) Nitric Acid
        3) Reactions with HIO_4
    d. The Ruff Degradation
    e. Kiliani-Fischer synthesis

B. Lipids, amino acids, and nucleotides
1. Lipids
    a. Waxes
    b. Fatty acids
    c. Triglycerides
    d. Steroids
    e. Prostaglandins
    f. Terpenes
2. Amino acids
    a. Structure of an amino acid
    b. Stereochemistry
    c. Zwitterionic form
    d. Peptide bond and structure of a polypeptide
3. Nucleic Acids
    a. Nucleotides and ribonucleotides
    b. Nucleosides and ribonucleotides
    c. Nitrogenous bases
    d. Phosphate groups
    e. Polynucleotides

LAB EXPERIENCES

A. Laboratory safety and safety data sheets
B. Synthesis of cyclohexanol by reduction of a ketone

C. Preparation of ethyl butanoate by Fischer's esterification
D. Aspirin synthesis
E. Synthesis of maleanilic acid
F. Synthesis of N-phenylmaleimide
G. Saponification
H. Preparation of dibenzalacetone

METHODOLOGY

The following strategies from the active learning methodology are recommended:

- Written research proposal
- Laboratory
- Solving a problem posed
- Web-supported education
- Literature research
- Simulations
- Lectures
- Collaborative learning and teamwork

EVALUATION

Partial assignments	30%
Compositions	20%
Final project or exam	25%
Immersion experience	25%
Total	**100%**

LEARNING ASSESSMENT

The institutional assessment rubric is applied to the course's core activity.

BIBLIOGRAPHY

TEXTBOOK

Aponte, M., Rivera, Z., & Guntin, M. (2004). *Química Orgánica: Manual de laboratorio* (4th ed.). Librería Universal.

Wade, L.G., Jr., Simek, J. W. (2016). *Organic Chemistry* (9th ed). Pearson.

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Carey, F. (2019). *Organic Chemistry* (11th ed.). McGraw Hill Higher Education.

Karty, J. (2018). *Organic Chemistry: Principles and Mechanisms* (2nd ed.). W. W. Norton& Company.

Klein, D. R. (2016). *Organic Chemistry* (3rd ed.) Wiley.

Klein, D. R. (2016). *Organic Chemistry as a Second Language: First Semester Topics* (4th ed.). Wiley.

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Smith, J. (2018). *General, Organic, and Biological Chemistry* (4th ed.) McGraw Hill Higher Education.

Stoker, H. S. (2015). *General, Organic, and Biological Chemistry* (7th ed.). Cengage Learning.

Valiulin, R. (2020). *Organic Chemistry: 100 Must-Know Mechanisms in Organic Chemistry* (1st ed.). De Gruyter.

Yurkanis, P. (2016). *Organic Chemistry* (8th ed.). Pearson.

ELECTRONIC RESOURCES

American Chemical Society. (n.d.). *ACS Chemistry for Life*. https://www.acs.org/content/acs/en.html

International Union of Pure and Applied Chemistry. https://iupac.org/

For more information resources related to the course's topics, access the library's webpage http://biblioteca.sagrado.edu/

REASONABLE ACCOMMODATION

For detailed information on the process and required documentation you should visit the corresponding office. To ensure equal conditions, in compliance with the ADA Act (1990) and the Rehabilitation Act (1973), as amended, any student in need of reasonable accommodation or special assistance must complete the process established by the Vice Presidency for Academic Affairs.

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This policy applies to all students enrolled at Universidad del Sagrado Corazón to take courses with or without academic credit. A lack of academic integrity is any act or omission that does not demonstrate the honesty, transparency, and responsibility that should characterize all academic activity. Any student who fails to comply with the Honesty, Fraud, and Plagiarism Policy is exposed to the following sanctions: receive a grade of zero in the evaluation and / or repetition of the assignment in the seminar, a grade of F (*) in the seminar, suspension, or expulsion as established in the Academic Integrity Policy effective in November 2022.