

Code: QO427								
Name: Química Orgânica 1								
Name in English: Organic Chemistry 1								
Name in Spanish: Química Orgánica 1								
Subject type: Weekly								
Approval Type: Grades and Frequency								
Characteristic: Regular								
Frequency: minimum of 75%								
Period Type / Offering period: Semestral/ Every year								
Requires Final Exam: Yes								
Vectors								
T	L	P	O	PE	OE	SL	WEEKS	CREDITS
4	-	-	-	-	-	4	15	4
Occurrence on curriculum: 09, 13, 39, 43								
Pre requirement: QG101 or QI242								
<p>Summary:</p> <ol style="list-style-type: none"> 1) Reactions of acids and bases (Arrhenius, Brønsted and Lewis) 2) Alkanes and conformational analysis 3) Stereochemistry 4) Addition, substitution and elimination reactions 5) Properties and reactivities of nucleophiles (alcohols, amines, enols, enamines, Grignard reagents, organolithium compounds and carbanions) 6) Properties and reactivities of electrophiles (aldehydes, ketones, imines, carboxylic acids and their derivatives, alkyl halides and carbocations) 7) Conjugations and aromaticity (benzene derivatives and heteroarenes) 								
<p>Program:</p> <ol style="list-style-type: none"> 1) Reactions of acids and bases (Arrhenius, Brønsted and Lewis) <ol style="list-style-type: none"> a) Acids and bases of Arrhenius, Brønsted and Lewis; b) Chemical equilibrium; c) Acid-base reactions; d) Strength of acids and bases, K_a and pK_a; e) Relationships between acid/base properties and chemical structure 2) Alkanes and conformational analysis <ol style="list-style-type: none"> a) Alkanes occurrence; b) n-Alkanes: rotations around C-C bonds and their conformations; c) Cycloalkanes: ring, torsional and steric strain d) Conformations of cycloalkanes; e) Reactions of alkanes: pyrolysis, radical halogenation, and stability of their radicals. 3) Stereochemistry <ol style="list-style-type: none"> a) General overview and definitions; b) Constitutional isomers and stereoisomers; c) Chirality and its importance to biological systems; d) Enantiomers: definitions and absolute configuration assignments (R and S, cf. Cahn-Ingold-Prelog rules); e) Racemic mixtures and properties of chiral molecules; f) Diastereoisomers; g) E and Z geometries in alkenes; h) Fischer projections. 								

4) Addition, substitution and elimination reactions

- a) Definitions;
- b) Addition reactions to alkenes, alkynes and to the carbonyl group;
- b) The Markovnikov rule;
- c) Stability of carbocations and rearrangements;
- d) Hyperconjugation;
- e) Oxidation of alkenes: di-hydroxylation, oxidative cleavage, epoxidation,
- f) S_N2 and S_N1 reactions: mechanism, kinetics, free energy diagrams, transition states, stereochemistry, influence of the nature of reagents and the reaction medium (polarity of solvents and temperature);
- g) E_2 , E_1 e E_{1cB} reactions: mechanism, kinetics, free energy diagrams, transitions states, stereochemistry and influence of the nature of reagents and the reaction medium (polarity of solvents and temperature);
- h) Basicity versus nucleophilicity.

5) Properties and reactivities of nucleophiles (alcohols, amines, enols, enamines, Grignard reagents, organolithium compounds and carbanions)

- a) Structure and properties of alcohols and ethers;
- b) Reactions of alcohols: dehydrations, substitutions, additions and oxidations;
- c) Structures and properties of amines;
- d) Nucleophilicity, basicity and formation of salts using amines;
- e) Preparation of imines and enamines;
- f) Alkylation of amines;
- g) Reductive amination;
- h) Reactions of deprotonated terminal alkynes as nucleophiles.

6) Properties and reactivities of electrophiles (aldehydes, ketones, imines, carboxylic acids and their derivatives, alkyl halides and carbocations)

- a) Structures and Properties of carbonyl compounds (aldehydes, ketones, and carboxylic acid derivatives);
- b) General methods for the preparation of carbonyl compounds;
- c) Preparation of hydrates, ketals and hemi-ketals, imines and enamines starting from aldehydes and ketones;
- d) Enolization of carbonyl compounds;
- e) Racemization at the alpha position of carbonyl compounds;
- f) Nucleophilic addition to the carbonyl group vs enolate formation;
- g) Addition of carbon nucleophiles to carbonyl compounds: HCN, Grignard reagents, organolithium compounds, phosphorus ylides (Wittig reaction)
- h) Reduction and oxidation methods for carbonyl compounds: Baeyer-Villiger oxidation, reductions using metal hydrides, catalytic hydrogenation
- i) Formation of salts, soaps, detergents and emulsions using carboxylic acids;
- j) Reactions of nucleophilic substitution using carboxylic acid derivatives: formation of esters, amides, acyl halides, thioesters, and anhydrides.

7) Conjugation and aromaticity (benzene derivatives and heteroarenes)

- a) Structures and Properties of alkenes and alkynes;
- b) Relative stability of alkenes: hydrogenation heats;
- c) Structures and reactivities of dienes;
- d) alpha,beta-unsaturated carbonyl compounds
- e) Conjugate addition;
- f) Definition of aromaticity by Hückel;
- g) Electrophilic substitution of arenes;
- h) Nucleophilic substitutions of arenes;
- i) Birch reduction.

Basic Bibliography

- 1) J. Clayden, N. Greeves, S. Warren, P. Wothers, "**Organic Chemistry**", Oxford, 1a. edição, Oxford University Press, 2000.
- 2) T. W. G. Solomons, C. B. Fryhle, "**Química Orgânica – Volumes 1 e 2**", 10ª. edição, LTC, 2012.

Supplementary Bibliography

- 1) John Macmurry, "**Química Orgânica**", 3ª. Edição, Cengage Learning, 2016.
- 2) M. G. Constantino, "**Química Orgânica – Curso Básico Universitário (volumes 1, 2 e 3)**", 1ª. edição, LTC - Livros Técnicos e Científicos, 2008.
- 3) F. A. Carey, R. J. Sundberg, "**Advanced Organic Chemistry - Parts A and B**", 5a. edição, Springer, 2008.
- 4) J. March, M. B. Smith, "**March's Advanced Organic Chemistry: Reactions, Mechanisms, 3 and Structure**", 6a. edição, John Wiley & Sons, 2007.
- 5) M. B. Smith, "**Organic Synthesis**", 4a. edição, McGraw-Hill Science, 2001.