Code: QO424								
Name: Fundamentos em Espectroscopia e Ressonância Magnética Nuclear								
Name in English: Fundamentals of Nuclear Magnetic Resonance Spectroscopy								
Name in Spanish: Fundamentos de Espectroscopia y Resonancia Magnética Nuclear								
Subject type: Weekly								
Approval Type: Grade and Frequency								
Characteristic: Regular								
Frequency: 75%								
Period Type / Offering period: Semester/All periods								
Requires Final Exam: Yes								
Vectors								
T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2	**0**	**0**	**0**	**0**	**0**	**2**	**15**	**2**
Occurrence on curriculum: 05, 50, 63								
Pre requirement: QO321								
Summary: fundamental concepts, spectra assignment, and applications of Nuclear Magnetic Resonance Spectroscopy.								

Program:

1 - Fundamental principles

Spin-active nuclei; angular momentum; magnetic moment; nuclei in static magnetic field; population of levels; resonance condition.

2- Nuclear Magnetic Resonance Spectrometer

Basic electronic components of the spectrometer; probe; NMR signal detection; Fourier transform; sample preparation; deuterated solvents.

3- Spectral parameters

Chemical Shift (δ)

Nuclear shielding and chemical shift (chemical environment); diamagnetic shielding; paramagnetic shielding; reference compounds; chemical shift scale; signal intensity.

Scalar Coupling Constant (J)

Origin of the scalar coupling constant (J) spin-spin; 2nI + 1 rule, intensity of multiplet components; Pascal's triangle; homonuclear and heteronuclear couplings.

4- Homonuclear coupling constant ($^{n}J_{HH}$)

Geminal couplings ($^{2}J_{HH}$) positive and negative; vicinal coupling ($^{3}J_{HH}$); Karplus relationship; long-range coupling (allylics); coupling in rigid molecules; coupling in flexible molecules (conformational equilibrium); keto-enol tautomerism; diastereotopic hydrogens; chemical and magnetic equivalence and nonequivalence.

5- ^{13}C NMR spectrum

^{13}C nucleus; coupled spectrum; decoupled spectrum; ^{13}C chemical shift.

6- Spectra assignment

Assignment of ^{1}H and ^{13}C NMR spectra signals and structural determination of saturated and unsaturated aliphatics organic compounds, aromatic and heteroaromatic systems.

7- NMR of other nuclei

^{1}H and ^{13}C NMR spectra for compounds containing ^{19}F and/or ^{31}P; effect of quadrupole nuclei (^{14}N) on ^{1}H NMR spectra; comparison with molecules enriched in ^{15}N.

8- Other NMR techniques

^{13}C DEPT NMR spectra; 2D homonuclear (COSY, TOCSY, and NOESY) and heteronuclear (HSQC and HMBC) contour maps.

Basic Bibliography

1) SILVERSTEIN, R. M. et al. **Identificação espectrométrica de compostos orgânicos**. 8. ed. Rio de Janeiro: LTC, 2019.
2) FRIEBOLIN, H. **Basic one- and two-dimensional NMR spectroscopy**. 5. ed. Weinheim: Wiley-VCH, 2011.
3) PAVIA, D. L.; LAMPMAN, G. M.; KRIZ, G. S. **Introduction to spectroscopy: a guide for students of organic chemistry.** 3. ed. South Melborne: Brooks/Cole, 2001.

Supplementary Bibliography

1) MITCHELL, T. N.; COSTISELLA, B. **NMR – From spectra to structures: An experimental approach,** 2. Ed, Springer Nature ebook 2007
2) MOHAN**,** J. **Organic Spectroscopy:** Principles and applications*,* 2nd edition, Alpha Science (2004)
3) KEELER, J. **Understanding NMR spectroscopy**, 2nd edition; Wiley, 2010.
4) LEVITT, M. H. **Spin Dynamics: Basic of NMR,** 2nd ed., Wiley (2008)
5) CARBAJO, R. J.; NEIRA, J. L. **NMR for chemists and biologists,** 1 ed. Springer nature ebook 2013.