Code: **QO423**

Name: **Fundamentos da Espectrometria de Massas**

Name in English: **Fundamentals of Mass Spectrometry**

Name in Spanish: **Fundamentos de Espectrometría de Masas**

Subject type: **Weekly**

Approval Type: **Grade and attendance**

Characteristic: **Regular**

Frequency: **75%**

Period Type / Offering period: **Semestral / All periods**

Requires Final Exam: **Yes**

Vectors

T	L	P	O	PE	OE	SL	WEEKS	CREDITS
2						**2**	**15**	**2**

Occurrence on curriculum: **05, 50, 63**

Pre requirement: **QO321 or QO323 or QO427**

Summary: Fundamentals and applications of mass spectrometry

Program:

1. Introduction to the technique and use.
2. Instrumentation: general aspects of a mass spectrometer.
3. Analyzers: magnetic sector, quadrupole, ion trap, time of flight, and gas chromatography/mass spectrometry.
4. Mass spectrum, molecular ion identification, exact mass, isotopic pattern, M+1, M+2, and metastable ions.
5. Use of the Molecular Formula: degree of unsaturation.
6. Fragmentation: homolysis, heterolysis, rules for predicting the most intense fragments.
7. Rearrangements, derivatization, and chemical ionization.
8. Mass spectrum and fragments of the main classes of organic compounds: Hydrocarbons; aliphatic (saturated and unsaturated), aromatic, linear, branched, cyclic, alcohols and phenols, ethers, ketones, aldehydes, carboxylic acids, esters, lactones, amines, amides, nitriles, nitro compounds, nitrates, aliphatic mercaptans, halogenated compounds, aromatics, and some natural products.
9. Gas chromatography/mass spectrometry.

Basic Bibliography

1) SILVERSTEIN, R. M.; BASSLER, G. C. & MORRIL, T. C. "**Spectrometric Identification of Organic Compounds**", fifth edition, John Wiley and Sons, 1991.

2) PAVIA, D. L.; LAMPMAN, G. M. & KRIZ, G. S. "**Introduction to Spectroscopy**" **- A Guide for Students of Organic Chemistry**, Saunders Golden Sunburst Series, 1996.

3) DAVIS, R. & FREARSON, M. **"Mass Spectrometry" - Analytical Chemistry by Open Learning,** John Wiley and Sons, 1989.

Supplementary Bibliography

1) **Journal of Mass Spectrometry** – Wiley Online Library

2) HOFFMANN, E.; STROOBAND, V. "**Mass Spectrometry: Principles and Applications**", 3rd Ed, John Wiley and Sons, 2007

3) GROSS, J. H. "**Mass Spectrometry**", 3rd Ed, Springer, 2017.

4) **Rapid Communications in Mass Spectrometry** - Wiley Online Library

5) Material complementar fornecido pelo docente