



PROGRAMS AND BIBLIOGRAPHY

Subject	
Code	Name
QO423	Fundamentals of Mass Spectrometry

Vector
OF:S-5 T:002 P:000 L:000 O:000 D:000 HS:002 SL:002 C:002 AV:N EX:S FM:75%

Pre requirement
QO321

Summary
Experimental fundamentals, data interpretation and applications.

Program
<ol style="list-style-type: none">1. Introduction to technique and use2. Instrumentation: mass spectrometer overview3. Analyzer: Magnetic sector, quadrupole, ion trap, time of flight and gas chromatograph/mass spectrometer4. Mass spectrum, molecular ion identification, exact mass, isotopic pattern, M+1, M+2, metastable ions5. Use of molecular formula and double bond equivalent6. Fragmentation, homolysis, heterolysis, main fragmentation rules7. Rearrangement and derivatization, chemical ionization8. Mass spectrum and characteristic fragments of main organic functional groups: aliphatic, cyclic and aromatic hydrocarbons, alcohols and phenols, ethers, ketones, aldehydes, carboxylic acids, esters, lactones, amines, amides, nitriles, nitro compounds, mercaptans, halides and natural products.9. Gas chromatography/mass spectrometry

Bibliography
<p>-R. M. Silverstein, G. C. Bassler & T. C. Morrill, "Spectrometric Identification of Organic Compounds", fifth edition, John Wiley and Sons, 1991.</p> <p>-D. L. Pavia, G. M. Lampman & G. S. Kriz, "Introduction to Spectroscopy" - A Guide for Students of Organic Chemistry, Saunders Golden Sunburst Series, 1996.</p> <p>-R. Davis & M. Frearson, "Mass Spectrometry" - Analytical Chemistry by Open Learning, John Wiley and Sons, 1989.</p>

Evaluation criteria
For grading policy, see: Regimento Geral de Graduação, Seção I – Normas Gerais, Capítulo V – Da Avaliação do Aluno na Disciplina. Students are required to attend 75 % of the lectures. For further details, see: Regimento Geral de Graduação, capítulo VI, seção X, artigo 72.