

INSTRUMENTAL TECHNIQUES

MODULE	CONTENT	YEAR	TERM	CREDITS	TYPE
Chemistry	Instrumental Techniques	1 st	1 st	6	Compulsory
LECTURER(S)			Postal address, telephone nº, e-mail address		
Luis Crovetto Gonzalez M ^a Isabel Martínez Puentedura, Ángel Orte Gutiérrez José Manuel Paredes Martínez			Department of Physical Chemistry. Faculty of Pharmacy. University of Granada Campus Universitario de Cartuja. 18071 -Granada (Spain) Telf.:+34 958-243823. luiscrovetto@ugr.es , 958-249473 martinez@ugr.es , 958-243824 angelort@ugr.es , 958243825 jparedes@ugr.es , 958243829		
DEGREE WITHIN WHICH THE SUBJECT IS TAUGHT					
Pharmacy Degree					
PREREQUISITES and/or RECOMMENDATIONS (if necessary)					
Proper knowledge about: - Maths - General Chemistry - Basic Physics and Physical Chemistry					
BRIEF ACCOUNT OF THE SUBJECT PROGRAMME (ACCORDING TO THE DEGREE)					
Study of the most employed Instrumental Techniques in Pharmaceutical laboratory and Pharmaceutical research. The study will be theoretical and practical, and it will be applied to the resolution and interpretation of problems.					
GENERAL AND PARTICULAR ABILITIES					
OBJECTIVES (EXPRESSED IN TERMS OF EXPECTED RESULTS OF THE TEACHING PROGRAMME)					



- To show the importance of the Instrumental Techniques in the pharmaceutical field.
- To show the most employed techniques for the identification and quantification of pharmaceutical products.
- To give the physicochemical principles which the Techniques are based on.
- Description of the basic components of the employed instruments.
- Running of the instruments.
- Basis of the employed methodology.
- To select the most suitable technique for the analysis and control of pharmaceuticals, and water, food and environmental analysis.
- To know and apply the main techniques for research, from the point of view of their basis and from the instrumentation.

DETAILED SUBJECT SYLLABUS

Theoretical syllabus:

Lesson 1. Concept, interest and classification of the Instrumental Techniques.

Concept of the Instrumental Techniques in Pharmaceutical Sciences. Advantages and disadvantages of the instrumental methods. Pharmaceutical interest of Instrumental Techniques. Classification of Instrumental Techniques. Choice of a Technique.

Lesson 2. Introduction to Spectroscopy

General concepts. Nature and properties of the electromagnetic radiation: Photoelectric effect. Energy levels of atoms and molecules. Regions of the electromagnetic spectrum. Selection rules.

Lesson 3. Components of the instruments for Optical Spectroscopy

Set up and components of the instruments employed for Optical Spectroscopy. Radiation sources (continuous and discontinuous). Wavelength selectors (monochromators and filters). Detectors of radiation.

Lesson 4. Absorption of light

Lamber-Beer law about radiation absorption. Limitations and deviations of Lamber-Beer law. Absorbance and Transmittance range of minimum error.

Lesson 5. Atomic Spectroscopy

5.1. Introduction to Atomic Spectroscopy: Atomic spectra and selection rules. Effect of temperature in the Atomic Spectra. Atomization of the sample. Introduction of the sample.

5.2. Atomic Absorption Spectroscopy: Radiation sources. Flame atomization. Electrotermic atomization. Types of spectrophotometers. Interferences.

5.3. Atomic Emission Spectroscopy: Atomization instruments. Plasma techniques. Types of spectrophotometers. Applications. Flame emission spectroscopy. Clinic applications of Flame emission spectroscopy. Comparison between both atomic techniques.

Lesson 6. Vibrational or Infrared Spectroscopy

Infrared region of the electromagnetic spectrum. Vibration of diatomic molecules and potential energy curve. Mechanisms of IR radiation absorption. Selection rules. Vibrational Spectra and strength constant in diatomic molecules. Anarmonicity. Vibration of polyatomic molecules. Instrumentation in IR spectroscopy. Applications of the IR spectroscopy: Identification of substances.

Lesson 7. Electronic Spectroscopy: Ultraviolet-visible

Electronic spectra: Vibrational structure of the electronic bands. Franck-Condon Principle. Dissociation Energy. Main electronic transitions in polyatomic molecules. Chromophore and auxochrome groups. Instrumentation.



Applications of the Molecular Absorption Spectroscopy UV-visible.

Lesson 8. Fluorescence Spectroscopy

Theoretical basis of the fluorescence Spectroscopy. Molecular relaxation processes form molecules in excited state: Radiative and non-radiative processes. Types of spectra. Factors affecting the emission intensity. Kavanagh Law. Instrumentation. Quenching. Stern-Volmer equation. Energy transfer processes between molecules. Applications.

Lesson 9. Nuclear Magnetic Resonance (NMR) Spectroscopy

General concepts. Physicochemical basis of NMR. Proton- NMR. Chemical shift. Multiplicity: spin-spin coupling. Instrumentation. Applications. Interpretation of spectra.

Lesson 10. Mass Spectrometry

Physicochemical basis. Types of mass spectra. Components of the instrumentation. Introduction of the sample. Ionization techniques (EI, CI, DI, FI, MALDI, FAB, APcI and ESI). Mass analyzers (Magnetic sector, Quadruplex, TOF, ion trap, FTMS). Detectors. Information from a mass spectrum. Applications. Interpretation of spectra.

Lesson 11. Chromatography techniques

Concept of chromatography. Classification: according to physicochemical basis, phase combination and instrument. General methodologies. Chromatographic theories. Chromatographic parameters.

Practical Sessions in the laboratory:

Session 1. Construction of spectrophotometric absorption graphic. Calculation of molar extinction coefficients. Spectrophotometric determination of a mixture of B₂ and B₁₂ vitamins.

Session 2. Fluorescence spectra of quinine. Kavanahg law. Effect of a quencher.

Session 3. Separation of pharmaceuticals by chromatography.

Session 4. Obtaining and interpretation of the infrared spectrum of acetilsalicylic acid.

READING

Basics:

Principios de Análisis Instrumental. (5ª Edición) Skoog-Holler-Nieman. Editorial Mc Graw Hill.

Espectroscopia Atómica y Molecular. J. Zúñiga Román. Pearson Educación.

Fundamentos de Espectroscopía Molecular. C.N. Banwell. Ediciones del Castillo.

Análisis Instrumental. K.A. Rubinson- J.F. Rubinson. Editorial Prentice Hall.

Métodos Instrumentales de Análisis. H.H. Willard y col. Grupo Editorial Iberoamérica.

Técnicas Instrumentales de Análisis en Bioquímica. J.M. García-Segura y col. Editorial Síntesis.

Métodos Ópticos de Análisis. E. Olsen. Editorial Reverté, 1995.

Monographs:

Química Física. Problemas de espectroscopia. Fundamentos. A. Requena. Prentice Hall.

Espectroscopía molecular. V. Luaña. Servicio de publicaciones de la Universidad de Oviedo.



Espectroscopía Infrarroja. Robert Conley. Editorial Alambra.
Espectroscopia ultravioleta y visible. C.N. Rao. Ed. Alambra.
Fluorescente Spectroscopy. A.J. Pesce. Marcel Dekker. New Cork.
Espectroscopia de Resonancia Magnética. F. J. López. Addison Wesley Iberoamericana S.A.
Introducción a la cromatografía. Abbott y Andrews, Exedra, Ed. Alhambra.
Cromatografía en papel y placa delgada, J.A. Domínguez, OEA.
Fundamentos de la cromatografía de gases. J. M. Storch de García, Exedra, Ed. Alhambra.
Cromatografía de gases. I, Dabrio, Ed. Alhambra.

Others:

Técnicas Instrumentales Físicoquímicas. S. Senent. Publicaciones UNED
Química Física (Vol. 1). M. Díaz Peña, A. Roig Muntaner. Editorial Alhambra.
Química Física. P. Atkins. (8ª Ed). Editorial Médica Panamericana.
Química Física. A. Requena. Prentice Hall. Prentice Hall.
Físicoquímica: Problemas y Soluciones. L. Labowitz. Editorial Paraninfo.
Físicoquímica. (Vol. 2). Ira N. Levine. 5ª Ed. Editorial Mc. Graw Hill.
Química Física. J. Morcillo Rubio. 2ª Ed. Publicaciones UNED.

RECOMMENDED INTERNET LINKS

General Spectroscopy:

<http--fisica.usach.cl/~jammann-LabOpticaGuias-G3-PrismaAWEB.pdf>
http://condor.cida.ve/~briceno/cursos/astrof_observ/clase3/
http://jchemed.chem.wisc.edu/JCESoft/Issues/Series_B/9B1/prog3-9B1.html
http://nautilus.fis.uc.pt/wwwfi/hipertextos/espectro/hiper_espectro.html
<http://www.chem.vt.edu/chem-ed/spec/beerslaw.html>
<http://www.chm.davidson.edu/ChemistryApplets/spectrophotometry/BeersLaw.html>
<http://www.inform.umd.edu/EdRes/Topic/Chemistry/ChemConference/Software/Spreadsheets/WWW/BeersLaw.html>
<http://www.sc.ehu.es/sbweb/fisica/cuantica/fotoelectronico/fotoelectronico.htm>
<http://www.shu.ac.uk/schools/sci/chem/tutorials/molspec/beers1.htm>
Prism Applet - Refraction and Dispersion
WebSpectra - Problems in NMR and IR Spectroscopy

IR Spectroscopy:

[IR Absorption Spectrometers](#)
[IR Helper](#)

[Vibración de una molécula diatómica](#)
[Vibraciones de las moléculas diatómicas](#)

Fluorescence Spectroscopy:

http://www.infochembio.ethz.ch/links/en/spectrosc_luminescence.html
<http://www.inform.umd.edu/EdRes/Topic/Chemistry/ChemConference/Software/Spreadsheets/WWW/Fluorescence.html>
<http://teaching.shu.ac.uk/hwb/chemistry/tutorials/molspec/lumin3.htm>

RMN Spectroscopy:

[Basics of NMR](#)
[BCMB-CHEM 8190 Biomolecular NMR](#)
<http--personales.com-espana-madrid-fourier-menu.htm>
<http--www.pharma.ethz.ch-people-oliver.zerbe-Vorlesung-NMR.pdf>



<http://teaching.shu.ac.uk/hwb/chemistry/tutorials/molspec/nmr1.htm>

<http://www.ch.ic.ac.uk/local/organic/nmr.html>

Mass Spectrometry:

<http://www.asibury.leeds.ac.uk/facil/MStut/mstutorial.htm>

Polarimetry. Circular Dichroism:

<http://www.enzim.hu/~szia/cddemo/edemo0.htm>

<http://galeon.hispavista.com/scienceducation/Dicroismo.htm>

<http://library.thinkquest.org/C003776/espanol/book/polarizacion.htm>

<http://www.naoj.org/Observing/Instruments/FOCAS/pol/>

Refractometry:

<http://acacia.pntic.mec.es/~jrui27/dispersion/arcoiris.html>

<http://www.sc.ehu.es/sbweb/fisica/ondas/snell/snell.htm>

<http://enebro.pntic.mec.es/~fmag0006/Prism101.html#a1>

<http://www.um.es/LEQ/laser/Java/Twoangles2.htm>

Chromatography:

<http://www.sci.sdsu.edu/TFrey/Bio750/Chromatography.html>

<http://ull.chemistry.uakron.edu/chemsep/>

<http://www.files.chem.vt.edu/chem-ed/sep/gc/gc.html>

<http://teaching.shu.ac.uk/hwb/chemistry/tutorials/chrom/gaschrn.htm>

<http://www.forumsci.co.il/HPLC/topics.html>

<http://caspar.bgsu.edu/~courses/HPLC/HPLCManual.html>

<http://www.instrumentalchemistry.com/index.htm>

<http://www.science.oas.org/RLQ/tutoriales/cromatografia/croma.htm>

