SUBJECT GUIDE

Academic year 2013-2014

INSTRUMENTAL TECHNIQUES

MODULE	CONTENT	YEAR	TERM	CREDITS	TYPE
Chemistry	Instrumental Techniques	1st	1st	6	Compulsory

LECTURER(S)	Postal address, telephone nº, e-mail address
Concepción López Martínez, Pedro J. Martínez de las Parras, Mª Isabel Martínez Puentedura, Mª José Ruedas Rama	Department of Physical Chemistry. Faculty of Pharmacy. Campus Cartuja. 18071-Granada (Spain) Tel.:0034 958-243823. mclopezm@ugr.es, 958-243829 martinez@ugr.es, 958-243824 pparras@ugr.es, 958-243824 mjruedas@ugr.es, 958243825
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. Cromatrographic theories. Cromatographic parameters.

Practical Sessions in the laboratory:

Session 1. Construction of spectrophotometric absorption graphic. Calculation of molar extintion coefficients. Spectrophotometric determination of a mixture of B_2 and B_{12}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 acetilsalicitic acid.

READING

Basics:
Principios de Análisis Instrumental. (5ª Edición) Skoog-Holler-Nieman. Editorial Mc Graw Hill.
Espectroscopia Atomica 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 Fisicoquímicas. 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.
Fisicoquímica: Problemas y Soluciones. L. Labowitz. Editorial Paraninfo.
Fisicoquímica. (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/fotoelectrico/fotoelectrico.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.astbury.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/~jruiz27/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/gaschrm.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.