

**COURSE DATA****Data Subject**

<b>Code</b>	43027
<b>Name</b>	Guided isolation and identification of bioactive natural products
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2021 - 2022

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2138 - Master's Degree in Research in and Rational Use of Medicines	Faculty of Pharmacy and Food Sciences	1	First term
3103 - Doctoral Programme in Biomedicine and Pharmacy	Doctoral School	0	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2138 - Master's Degree in Research in and Rational Use of Medicines	5 - Guided isolation and identification of bioactive natural products	Optional

**Coordination**

<b>Name</b>	<b>Department</b>
CABEDO ESCRIG, NURIA	135 - Pharmacology
GINER PONS, ROSA MARIA	135 - Pharmacology

**SUMMARY**

Optional subject belonging to research itinerary of the “Master en Investigación y Uso Racional del Medicamento” focusses on the main aspects of the laboratory methodology used in the field of research on new natural molecules with pharmacology interest. It deals with the plant material selection, extraction, isolation and structural elucidation of active components.

Aims:



Knowledge of the scientific basis of extraction process, isolation of secondary metabolites which constitute the main active principles in plants as sources of potential natural drugs.

Provide solid criteria for the selection of a plant material, as well as the isolation and structural elucidation of metabolites with pharmacologic interest.

## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

Its convenient students have passed Pharmacognosy, Organic Chemistry, Analytical Chemistry and Pharmacology in order to follow and understand the contents.

## COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

### 2138 - Master's Degree in Research in and Rational Use of Medicines

- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.
- Be able to access to information tools in other areas of knowledge and use them properly.
- Be able to apply the research experience acquired to professional practice both in private companies and in public organisations.
- Capacidad de seleccionar y gestionar los recursos disponibles (instrumentales y humanos) para optimizar resultados en investigación.
- Dominar el método científico, el planteamiento de protocolos experimentales y la interpretación de resultados en la búsqueda, desarrollo y evaluación de nuevos fármacos.

## LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

1. Knowledge of localization of different secondary metabolites in the nature.
2. Establish criteria to obtain natural compounds from different biological sources.
3. Knowledge of essential requirements for the active natural drugs.



4. Knowledge of spectroscopic methods for structural determination of natural drugs. Application of nuclear magnetic resonance (RMN).
5. Choose the adequate bioassays to evaluate pharmacologic activities

## DESCRIPTION OF CONTENTS

### 1. Isolation and elucidation of bioactive natural molecules

Importance of living organisms as a source of new drugs. Criteria for investigation. Bases quimiotaonómicas.

Chemical characteristics influencing the extraction and separation processes of organic molecules. Conventional methods and improved. Supercritical fluids.

Separation of macromolecules and other polymers.

Rationale and applications of chromatographic processes. The planar and column chromatography.

High resolution liquid chromatography.

Bioassays in vivo and in vitro.

Structural elucidation of terpenoids, alkaloids, phenolics and other smaller groups.

## WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	30,00	100
Laboratory practices	15,00	100
Tutorials	5,00	100
Study and independent work	15,00	0
Readings supplementary material	15,00	0
Preparation of evaluation activities	15,00	0
Preparing lectures	15,00	0
Preparation of practical classes and problem	15,00	0
<b>TOTAL</b>	<b>125,00</b>	

## TEACHING METHODOLOGY

During the activities, both theoretical and practical, the applications of the subject contents in relation to the Sustainable Development Goals (SDG) will be indicated. This is intended to provide knowledge, skills and motivation to understand and address these SDGs, while promoting reflection and criticism.



In this subject we will make use of different teaching methodologies such as lectures, workshops on structural elucidation and practical sessions focused on extraction, isolation and identification of natural products to understand the phytochemical methods.

Furthermore, a forum in a Virtual learning environment will be employed to promote active learning and to provide complementary materials.

## EVALUATION

Attendance is compulsory to all teaching activities. Active participation of the students is encouraged and may positively evaluated.

Coursework consist on the structural elucidation of natural products, paper exam consist on answering three out of six questions covering all topics.

Formative Evaluation:

Attendance, engagement and active participation 30%

Workshops and assignment 30%

Paper exam 40%

## REFERENCES

### Basic

- Heinrich, M. , Barnes, J., Prieto, J.M., Gibbons, S., Williamson, E.M. Fundamentals of Phamacognosy and Phytotherapy, 3<sup>a</sup> ed. 2018, Elsevier.
- Dewick, P.M. Medicinal Natural Products. A Biosynthetic Approach, 3<sup>a</sup> ed. 2009, J. Wiley & Sons.
- Wagner, H. and Bladt S. Plant drug analysis, 2009, Springer.
- Cannell, R.J.P. (ed.) (1998): Natural Products Isolation, Totowa, Humana Press.
- Colegate, S.M.; Molyneux, R.J. (eds.) (1993): Bioactive Natural Products. Detection, isolation and structural determination, CRC Press, Boca Raton.
- Vogel, H.G.; Vogel, W.H. (eds.) (1997): Drug Discovery and Evaluation. Pharmacological Assays, Berlin, Springer Verlag.
- Wagner, H., Bladt, S. (1996): Plant Drug Analysis. A Thin layer Chromatography Atlas, 2<sup>a</sup> Edició, Berlin, Springer.
- Williamson, E.M., Okpako, D.T., Evans, F.J. (eds.) (1996): Pharmacological methods in Phytoteraphy Research. Selection, Preparation and Pharmacological Evaluation of Plant Material, Chichester, John Wiley & Sons.

**Additional**

- Andlauer, W. et al (1999): Determination of selected phytochemicals by reversed-phase high-performance liquid chromatography combined with ultraviolet and mass spectrometric detection. *J. Chromatogr. A* 849, 341-348.
- Bradshaw, J. et al. (2001): A rapid and facile method for the dereplication of purified natural products, *J. Nat. Prod.* 64, 1541-1544.
- Azmir, J., Zaidul, I.S.M. et al. (2013): Techniques for extraction of bioactive compounds from plant materials: A review. *J Food Engineer.* 117, 426-436.
- Broach, J.R.; Thorner, J. (1996): High-throughput screening for drug discovery, *Nature* 384, 14-16
- Bross-Walch, N., Kühn, T., Moskau, D., Zerbe, O. (2005): Strategies and tools for structure determination of natural products using modern methods of NMR spectroscopy (review). *Chemistry and Biodiversity* 2, 147-77.
- Claridge, T.D.W. (2009): High Resolution NMR Techniques in Organic Chemistry, *Tetrahedron Organic Chemistry*, Vol 27, pp 1-383, Elsevier. ISBN-978-0-08-054628-5
- Foucault, A.P., Chevrolet, L. (1998): Counter-current chromatography: instrumentation, solvent selection and some recent applications to natural product purification, *J. Chromatogr. A* 808, 3-22.
- Jarvis, A.P., Morgan E.D. (1997): Isolation of plant products by supercritical-fluid extraction, *Phytochem. Anal.* 8, 217-222.
- Keeler, J. (2010): *Understanding NMR Spectroscopy*, Wiley. ISBN: 978-0-470-74609-7. <http://www.keeler.ch.cam.ac.uk/lectures/Irvine/>
- LaCourse, W.R., Dasenbrock, C.O. (1998): Column liquid chromatography: equipment and instrumentation, *Anal. Chem.* 70, 37R-52R.
- Wickberg, B. (1993): Chemical methods in ethnopharmacology, *J. Ethnopharmacol.* 38, 159-165.
- Wolfender, J.L., Rodríguez, S., Hostettmann, K. (1998): Liquid chromatography coupled to mass spectrometry and nuclear magnetic resonance spectroscopy for the screening of plant constituents, *J. Chromatogr. A* 794, 299-316.
- Schwikkard, S.L., Mulholland, D.A. (2014): Useful methods for targeted plant selection in the discovery of potential new drug candidates. *Planta Med* 80:1154-1160.
- Romanik, G., Gilgenast, E., Przyjazny, A., Kaminski, M. (2007): Techniques of preparing plant material for chromatographic separation and analysis. *J Biochem Biophys Methods* 70: 253-261.
- Renault, JH. (2015): Modern Separation Techniques for the Isolation of Natural Products. *Planta Med.* 81(17):1569.
- Teo CC, Tan SN, Yong JW, Hew CS, Ong ES. (2010): Pressurized hot water extraction (PHWE). *J Chromatogr A.* 1217(16):2484-94.



- Wohlgemuth. R. (2014). Chiral LC-MS/MS of D-and L-2-Hydroxyglutaric Acid Biomarkers. Reporter Appl Newsletter 56:11.

## ADDENDUM COVID-19

**This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council**

- 1. Contents** The content is unequivocally face-to-face, such as the practices initially collected in the teaching guide, since its delivery is impossible. Theoretical contents are prioritized over practical ones. The initial percentage of the theoretical contents is It will add the percentage of the practical contents. With this, we believe that the achievement of the essential learning objectives in the area of foundations.
- 2. Workload** The number of credits assigned to practical activities is reduced, which will be replaced by others activities that will represent in the long run the same volume of work indicated in the original teaching guide. These new activities will have the character of seminars, understood as elaboration tasks, minimally group, and tutored. The scheduled sessions will be taught on the same dates and times, although with a lesser formal duration
- 3. Teaching methodology** The materials will be uploaded in the Virtual Classroom. Theoretical classes will be taught by videoconference synchronous through Blackboard Collaborate. The tutorials will be given by videoconference, and in them the exercises to be solved by the students will be discussed. students.
- 4. Evaluation** It will be evaluated through an open written test of an exercise to be solved by the students distributed in the Classroom Virtual, in addition to answering an objective evaluation test in the Virtual Classroom itself
- 5. Bibliography** The recommended bibliography is kept accessible.