UNIVERSITY OF PUERTO RICO
RIO PIEDRAS CAMPUS
DEPARTMENT OF CHEMISTRY

A. Course Title/Semester: Structural Problems in Organic Chemistry, First Semester 2018-19

B. Course Code: Chemistry 8445 **When:** MW 2:30-4:00 pm / **Room:** FB-266

C. Professor: José A. Prieto **Office /Hours:** FB 111 / TT 10:00 am-12:00 pm
Email: jose.prieto2@upr.edu

D. Credits/hours: Three credits (three weekly lecture hours, several workshops and student presentations at semester end).

E. Requirements: 12 credits of core chemistry courses.

F. Description: This is a high-level organic spectroscopy course designed for advanced graduate students. It is intended for all graduate students independently of their field of specialization. It will cover, in detail, the aspects of structure elucidation of organic and inorganic compounds, natural products, biopolymers, and reaction intermediates using state-of-the-art **IR**, **NMR** and **MS** techniques. The instrumentation aspects of these techniques will be addressed. Approximately two-thirds of the course will be devoted to NMR. A general knowledge of basic structural organic spectroscopy is expected. An in-depth physical chemical treatment, such as quantum mechanics, is out of the scope of this course.

G. Objectives: After completing the course work and because of the acquired experiences, the student:

a) Should demonstrate command and should be able to explain the basic fundamental principles of NMR and IR spectroscopy, and MS spectrometry.
b) Should be able to apply his knowledge to the solution of spectral problems, in both the mechanistic aspects, as well as the structure elucidation of organic, organometallic, inorganic, biochemical compounds and natural products.
c) Should be able to prepare a sample, set-up the instrument with the appropriate parameters and run IR, and NMR experiments in one and two dimensions.
d) Should determine the structure of an unknown compound after designing and running the appropriate experiments integrating more than one spectroscopic technique.
e) Should be able to unequivocally assign all NMR resonances, extract coupling information and other spectral information after completing the structural assignments on an unknown compound.

I. Teaching Strategies: The general teaching strategies to be used in the course are:

Interactive classroom lecture and discussion: To engage students in the learning process as much as possible during the lectures in the form of frequently asked questions. Student participation is encouraged.

Office hours and participation after the class: To also further interactions between students and class material after class. Cooperative group discussions are also stimulated.

Use of audio- visual and computer tools: To complement the blackboard lecture, various audio-visual tools are used. These include PowerPoint presentations and computer projections of molecular modeling, which are important for allowing the students to graphically understand the three-dimensional complexity and nature of molecules and molecular processes.

Student Feedback: Successful teaching requires feedback mechanisms on how well the teaching is perceived. Four feedback mechanisms are used: questions during lecture, regular problem sets and regular student visits to my office.

Internet: The class home page http://www.organiclab.prof.pr/q8445 will be used to provide all kinds of class-related materials, including problem sets, handouts, spectra, instructions, announcements, etc.

J. Evaluation Strategy: Students will be evaluated based on **2 exams** (100 points each), **problem sets** (25 points), **student presentation** (50 points) and instrument checkouts/**pet compound** (50 points) for a total of 325 points.

Exams: one midterm exam and one comprehensive final exam will be given. These exams cover all the class lectures together with the assigned material, including textbook, handouts and assigned journal articles.

Problem Sets: A set of problems that can contain exercises, problems or literature work will be given on a regular basis. Also hands-on instrument work and computer simulations will be implemented on some problem sets. This is an important pedagogical aspect of this course. You will have two weeks to work on each. They will be browsed by the professor.

Pet Compound: An unknown (or interesting known research compound) will be given to each student or obtained from the student current research project. At the end of the semester, the student should have completed a comprehensive characterization or structure elucidation with all of the spectroscopic signal unambiguous assignments

Instrument checkout: By the end of the course, the student should "checkout" on the available NMR, instruments. Operating the FT-IR and MS is desirable.

Independent short topic: By the end of the course, each student should present a related short topic in spectroscopy (20 min). The topics could be selected from a list provided by the professor or could be related to the student ongoing research or personal interest.

In case of an extended interruption of the class schedule, we will use **non-presential methods** such as videoconferences, instructional modules, among others to cover up to 25% of the course material in compliance with Certification No. 112 (2014-2015) from the UPR Governing Board.

K. Grades: A, B, C, D, F grading system.

L. Bibliography

Text (NMR): *"Basic One- and Two-Dimensional NMR Spectroscopy"*, 5th ed., H. Friebolin, John Wiley & Sons, Inc., 2010. This book can serve as the class NMR textbook.
"*NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*", 3rd Edition, John Wiley & Sons, Inc., 2013.Harald Gunther

Text (IR and MS): There are many books available (modern or classic) in the areas of infrared spectroscopy and mass spectrometry. Any of them will serve as good references books. Some classical titles are:
"Spectrometric Identification of Organic Compounds", R. M. Silverstein, F. X. Webster, 7th edition, John Wiley & Sons, Inc., 2005 and
"Organic Structural Spectroscopy", J. B. Lambert, H. F. Shurvell, D. A. Lightner and R. G. Cooks. 2nd ed., Prentice-Hall, Inc. 1998.

Suggested Readings: There are now many modern books available on 1D- and 2D- NMR. Any of them can be of help for this course.

Recommended Journals: Magnetic Resonance and Journal of Magnetic Resonance.

M. ADA Law and Law 51

"La UPR, Río Piedras cumple con las leyes ADA (**Americans with Disabilities Act**) y 51 (Oficina de Asuntos para Personas con Impedimento del Decanato de Estudiantes) para garantizar igualdad en el acceso a la educación y servicios. Estudiantes con impedimentos o recipientes de servicios de Rehabilitación Vocacional deben informar al profesor(a) sobre sus necesidades especiales y/o de acomodo razonable para el curso durante la primera semana de clases. También deben visitar la Oficina de Asuntos para Personas con Impedimento del Decanato de Estudiantes a la brevedad posible. Se mantendrá la confidencialidad."