
COURSE: Informatics for Chemistry

ACADEMIC YEAR: 2016-2017

TYPE OF EDUCATIONAL ACTIVITY: Other

TEACHER: Dr. Sergio Brutti

e-mail: Sergio.brutti@unibas.itwebsite: www2.unibas.it/sbrutti

phone: 0971 205455

mobile (optional):

Language: ITALIAN

ECTS:5 (3 lessons; 2
tutorial/practice)n. of hours: 24 hours of
lessons and 24 hours of
tutorials/practiceCampus: Potenza
Dept./School: DIS
Program:Chemistry L-27Semester: I semester

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

These class lessons are aimed at three main knowledge goals:

1. The use of vectors, matrixes and linear algebra equations to describe the geometry of molecular structures in 3D and basics of molecular mechanics.
 2. The use of computer codes to draw and to manipulate molecular structures in 3D (ChemDraw and Avogadro) as well as to optimize at molecular mechanics level their structure.
 3. The use of spreadsheets to program algorithms for the derivation of structural properties of molecules in 3D and to perform data analysis (linear regressions, plots, etc.)
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PRE-REQUIREMENTSMath 1; Math for Chemists

SYLLABUS

1. Introduction to the use of informatics in chemistry
 2. Matrixes and vectors: simple and complex algebra. Use of spreadsheets to program algorithms capable to solve equations between matrices and vectors.
 3. Linear algebra and molecular geometry in 3D. Mathematical tools to analyze molecular structures in 2D and 3D. Use of spreadsheets to study the structure of complex molecules.
 4. Computational methods to predict molecular structures: molecular mechanics vs. quantum mechanics.
 5. Molecular structure representation: chemdraw vs. Avogadro
 6. Basics of statistics for data analysis: use of spreadsheets to analysis experimental and computational data..
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TEACHING METHODS

The class learning activities are organized in 24h of standard class teaching using the online material provided by the teacher and 8 different practical individual tutorials.

EVALUATION METHODS

During the semester 8 intermediate exams (esoneri) will be organized. Those students able to pass 7/8 esoneri with an average mark >18 will be able to complete the exam in an oral colloquium. Those students unable to pass at least 7/8 esoneri with an average mark >18 will be asked to complete the exam by carrying out a practical and an oral exam.

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

- o DB Hibbert JJ Gooding. Data Analysis for chemistry – Oxford University Press
 - o Online slides downloadable at the webiste www2.unibas.it/sbrutti
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INTERACTION WITH STUDENTS

The teacher is open for discussion and additional teaching during the planned weekly colloquia (tuesday 9-11), by email (sergio.brutti@unibas.it) or by phone (0971 205455).

EXAMINATION SESSIONS (FORECAST)¹January-February-June-July-September-December 2017

¹ Subject to possible changes: check the web site of the Teacher or the Department/School for updates.

SEMINARS BY EXTERNAL EXPERTS YES NO

FURTHER INFORMATION
