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**COURSE:** Informatics for Chemistry

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**ACADEMIC YEAR:** 2016-2017

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**TYPE OF EDUCATIONAL ACTIVITY:** Other

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**TEACHER:** Dr. Sergio Brutti

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phone: 0971 205455

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Language: ITALIAN

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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

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**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-REQUIREMENTS:** *Math 1; Math for Chemists*

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**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.*

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**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 both practical and an oral exams.*

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**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](http://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 (thuesday 9-11), by email ([sergio.brutti@unibas.it](mailto:sergio.brutti@unibas.it)) or by phone (0971 205455).*

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**EXAMINATION SESSIONS (FORECAST)<sup>1</sup>** *February (2 days); June; July, September; October*

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**SEMINARS BY EXTERNAL EXPERTS** YES  NO **FURTHER INFORMATION**

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

