DIPARTIMENTO DI SCIENZE

COURSE: Informatics Methods in Chemistry			
ACADEMIC YEAR: **2019-2020**			
TYPE OF EDUCATIONAL ACTIVITY: others activity			
TEACHER: **Camilla Minichino**			
e-mail: **camilla.minichino@unibas.it**		website:	
phone: **0971-206158**		mobile (optional):	
Language: ITALIAN			
ECTS: 3 (1 lessons e 2 tutorials/practice) 3	n. of hours:32 (8 lessons e 24 tutorials/practice)	Campus:**Potenza** Dept./School:**Dipartimento di Scienze** Program: : **CHIMICA(L27)**	Semester:I **From 02.03.2020 to 31.05- 20.06 2020**

EDUCATIONAL GOALS AND EXPECTED LEARNING OUTCOMES

The course aims to provide an overview of IT tools for collecting, managing, transmitting and processing data of chemical interest.

At the end of the course the student must be able to:

- use software packages to design, visualize and manipulate molecular structures, perform molecular mechanics geometry optimizations;
- find chemical information using the appropriate sources and organize bibliographic information in a database;
- develop simple algorithms and implement computer codes for the numerical resolution of problems.

PRE-REQUIREMENTS

None, but it is strongly recommended to know the contents of the course of Mathematical Methods for Chemistry held in the same semester.

SYLLABUS

Coding and representation of information within a computer.

Computer representation of secondary and tertiary molecular structure. Visualization of molecules and molecular properties, force fields and molecular mechanics methods.

Chemical information retrieval: primary, secondary and tertiary information sources. The main online databases and methods of use. Chemical journals in electronic format. Tools for creating a bibliographic database.

Some applications of numerical methods in chemistry through the use of spreadsheets and / or interpreted programming languages.

TEACHING METHODS

Lectures, computer lab.

EVALUATION METHODS

Oral examination which also includes the discussion of laboratory reports (to be delivered via e-mail at least one week before the exam).

TEXTBOOKS AND ON-LINE EDUCATIONAL MATERIAL

○ Lecture notes and presentation slides (https://cloud.unibas.it/index.php/s/NzkHmHVsWajZbCI and/or https://elearning.unibas.it/).

INTERACTION WITH STUDENTS

At the beginning of the course the instructor, after describing goals, learning objectives, detailed course topics, evaluation method, gives the password for accessing the link where the course material is stored. The lecturer also collects a list of students together with name, family name, e-mail and possibly cell phone number and reminds to be always available for providing help and assistance.

Office hours are normally on Tuesdays and Wednesdays 11 am : 1 pm in room 3D-103B (changes in the schedule

may occur, due to official and institutional duties, therefore send an e-mail in advance) or in different hours/days by appointment.

EXAMINATION SESSIONS (FORECAST)[1]
21/01/2020, 04/02/2020, 20/02/2020, 03/03/2020, 26/05/2020, 09/06/2020, 07/07/2020, 21/07/2020, 15/09/2020, 06/10/2020, 15/12/2020.

SEMINARS BY EXTERNAL EXPERTS YES □ NO X

FURTHER INFORMATION

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