



## IDENTIFYING DATA

### Computing Techniques for Chemistry

Subject	Computing Techniques for Chemistry			
Code	V11G201V01415			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Optional	4th	2nd
Teaching language	#EnglishFriendly Spanish Galician			
Department				
Coordinator	Hermida Ramón, José Manuel			
Lecturers	Hermida Ramón, José Manuel			
E-mail	jose_hermida@uvigo.es			
Web	<a href="http://moovi.uvigo.gal/">http://moovi.uvigo.gal/</a>			
General description	The subject "Computer Techniques in Chemistry" aims to introduce students to the use of advanced computer tools, based on free software, beyond office automation packages already used during the previous courses of the degree, thus expanding skills for work and/or or research.			

The subject is divided into four blocks in which the general aspects of the GNU/Linux operating system and how to install it, creation of documents in LaTeX with chemical applications, Fortran and Python will be considered. They will be taught combining small theoretical sessions together with practical examples that the students will verify in situ, and always supervised by the professors responsible for the subject.

The evaluation will consist of carrying out some written tasks (programs and documents in LaTeX) with a weight of 50% together with the preparation of reports explaining how the aforementioned tasks have been implemented (with a weight of 30%) and systematic observation of the work done during the practical sessions in a presentation at the end of the course (20%). There will also be the possibility of not using continuous assessment with a written exam whose weight will be 100% if requested.

English Friendly subject: International students may request from the teachers: a) resources and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.

## Training and Learning Results

Code	
A1	Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study
A5	Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy
B1	Ability for autonomous learning
B2	Organization and planning capacity
B3	Ability to manage information
C37	Acquire basic knowledge of programming and be able to use appropriate computer packages to solve problems of chemical interest
D1	Ability to solve problems

## Expected results from this subject

Expected results from this subject	Training and Learning Results		
Python/Fortran program creation	B1 B2	C37	D1
Utilization of a distribution of the GNU/Linux operative system	A1 A5		

**Contents**

Topic	
GNU/Linux operative system	<ul style="list-style-type: none"> <li>- Installation of a distribution.</li> <li>- Graphic environment.</li> <li>- Introduction to the command line.</li> <li>- Installation of programs.</li> <li>- Installation and configuration of an integrated development environment.</li> </ul>
Introduction to LaTeX	<ul style="list-style-type: none"> <li>- Structure of the documents.</li> <li>- Common elements of all types of documents or classes.</li> <li>- Tools for technical texts.</li> <li>- Presentations (Beamer).</li> <li>- Applications for chemicals.</li> </ul>
Python 3	<ul style="list-style-type: none"> <li>- Structure of the source code of the programs and fundamentals of Python.</li> <li>- Variables and strings.</li> <li>- Type of data.</li> <li>- Syntax and basic commands.</li> <li>- Programming some practical examples.</li> </ul>
Modern Fortran	<ul style="list-style-type: none"> <li>- Structure of the source code of the programs and fundamentals of Fortran.</li> <li>- Variables and arrays.</li> <li>- Syntax and basic commands.</li> <li>- Programming some practical examples.</li> </ul>

**Planning**

	Class hours	Hours outside the classroom	Total hours
Lecturing	12	12	24
Problem solving	12	27	39
Practices through ICT	14	28	42
Autonomous problem solving	12	27	39
Essay	2	4	6

\*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

**Methodologies**

	Description
Lecturing	Theoretical classes given through an on-screen presentation (available to students on the Moovi platform). In these classes the basic contents will be introduced, emphasizing the most important and difficult issues. Practical examples will be shown.
Problem solving	Aimed at solving problems and/or tasks and discussing them. The necessary material will be provided through the Moovi platform.
Practices through ICT	Application from what is discussed in the lecture and in the problem solving sessions to more general, but related, cases to the subject. Through the Moovi platform, the practice scripts and the work rules in the laboratory will be provided.
Autonomous problem solving	(*)Destinados á resolución de tarifas que integren os contados dados e exerciten as competencias a adquirir. A través da plataforma Moovi proporcionarase o material necesario.

**Personalized assistance**

Methodologies	Description
Lecturing	The student that need help will have the possibility of attend to "special tutorial sessions to solve doubts, mainly following the schedules indicated previously. To optimize the time, it is convenient that the student contacts with the professor with previously enough.
Practices through ICT	The student that need help will have the possibility of attend to "special tutorial sessions to solve doubts, mainly following the schedules indicated previously. To optimize the time, it is convenient that the student contacts with the professor with previously enough.
Problem solving	The student that need help will have the possibility of attend to "special tutorial sessions to solve doubts, mainly following the schedules indicated previously. To optimize the time, it is convenient that the student contacts with the professor with previously enough.
Autonomous problem solving	

<b>Assessment</b>					
	Description	Qualification	Training and Learning Results		
Problem solving	The students will give all the written work made in the session, such as creation of documents in LaTeX and Fortran/Python source code.	20	B1	C37	D1
Practices through ICT	The students will give all the written work made in the session, such as creation of documents in LaTeX and Fortran/Python source code.	30	A1 A5	B1 B3	C37 D1
Autonomous problem solving	(*)Presentación da resolución de tarefas complexas que integren o coñecementos e competencias da materia.	30	A1	B1	C37 D1
Essay	The students will present the results of their practices made using LaTeX and explaining the design of his applications of Fortran/Python.	20	A1 A5	B1 B2 B3	C37 D1

### Other comments on the Evaluation

### Sources of information

#### Basic Bibliography

Jay LaCroix, **Learn Linux TV**, Youtube, 2022

#### Complementary Bibliography

Jay LaCroix, **Mastering Ubuntu Server : explore the versatile, powerful Linux Server distribution Ubuntu 22.04 with this comprehensive guide**, 4, Packt Publishing Limited, 2022

Richard Blum, Christine Bresnahan, **Linux command line and shell scripting bible**, 3, John Wiley & Sons, 2015

Collaboratively writing open-content textbook, **LaTeX**, <https://en.m.wikibooks.org/wiki/LaTeX>, 2022

J. Mulero, J.M. Sepulcre, **LATEX con palabras clave**, Publicacions de la Universitat d'Alacant, 2016

Collaboratively writing open-content textbook, **Python Programming**, [https://en.m.wikibooks.org/wiki/Python\\_Programming](https://en.m.wikibooks.org/wiki/Python_Programming),

**Python 3 Tutorial**, <https://www.tutorialspoint.com/python3/>,

Alberto Cuevas Álvarez, **Python 3**, RA-MA Editorial, 2016

David Beazley, Brian K. Jones, **Python Cookbook**, 3, O'Reilly, 2013

**Fortran Tutorial**, <https://www.tutorialspoint.com/fortran/index.htm>,

Collaboratively writing open-content textbook, **Fortran**, <https://en.m.wikibooks.org/wiki/Fortran>,

Michael Metcalf, John Reid, Malcolm Cohen, **Modern Fortran Explained (Numerical Mathematics and Scientific Computation)**, 4, Oxford University Press, 2011

William H. Press, Brian P. Flannery, Saul A. Teukolsky, William T. Vetterling, **Numerical Recipes in Fortran 77: The Art of Scientific Computing**, 2, University Press, 1992-1996

### Recommendations

#### Subjects that it is recommended to have taken before

Mathematics: Mathematics 1/V11G201V01103

Mathematics: Mathematics 2/V11G201V01108

Chemistry: Chemistry 1/V11G201V01104

Chemistry: Chemistry 2/V11G201V01109