

idad
a



Universidad
Europea



Cofinanciado por
la Unión Europea

Blended Intensive Program BIP

Computational Tools in
Biopharma: Driving Innovation in
Drug Discovery

October 26-30, 2026

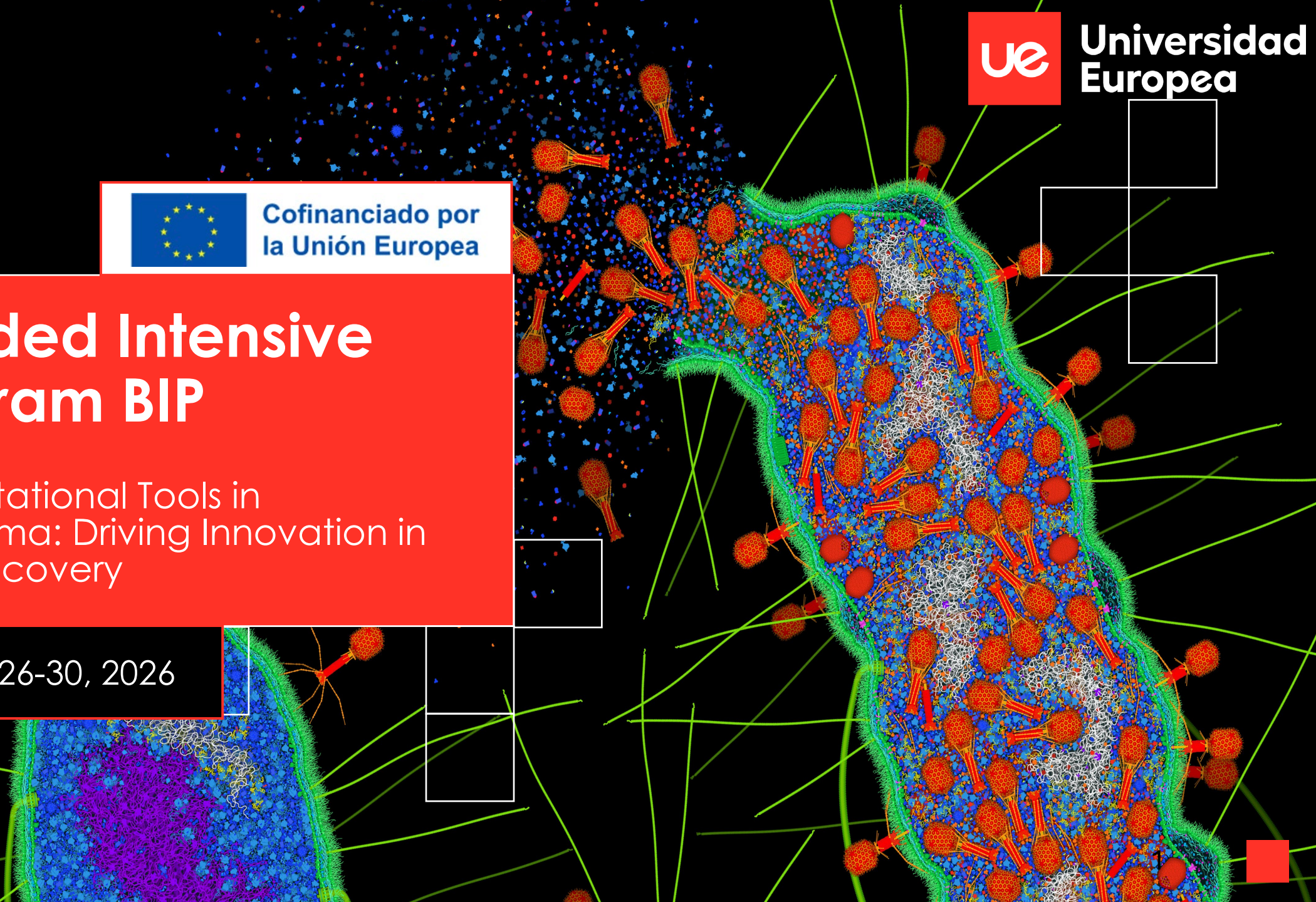







Table of contents

	1	Learning objectives
	2	Working plan: <ul style="list-style-type: none">• Phase 1. Online sessions• Phase 2. In-person sessions
	3	Working plan detailed schedule
	4	Evaluation
	5	Practical information



Learning objectives



- Understand the core principles of molecular structure and computational modeling
- Practice the most commonly used molecular docking techniques to analyze ligand-receptor interactions
- Design molecular modeling and simulation protocols to study macromolecular behavior over time
- Interpret results from molecular dynamics simulations to gain a deeper understanding of complex biological processes
- Develop AI-driven models for drug design by acquiring the necessary knowledge and practical skills



Working plan

Phase 1: online sessions

Provide students with a theoretical foundation in computational drug design and its current and future applications

1. Application of Computational Biology and AI in Drug Design

October 5, 2026. 17:00 - 18:30

2. Computational Tools in Biopharma: From Drug Discovery to

Biocatalyst Design

October 7, 2026. 17:00 - 18:30



Dr. Jon del Arco



Dr. Isabel Oroz Guinea

Working plan

Phase 2: In-Person Sessions (October 26)



Dr. Jon del Arco

Provide students with hands-on experience in omics-based methodologies for target identification

- Live Lecture (10:30 - 12:30): Omics Sciences for Biomarker Discovery and Target Identification
- Lunch break (12:30 - 13:30)
- Hands-on Workshop (13:30 - 16:30): Using Omic Tools for Target Selection

Working plan

What should you bring prepared?

Review what you have studied about Omic Sciences

Think about:

- How can I combine multiple omics layers improve target identification?
- What are the biggest challenges in translating omics discoveries into clinical practice?
- What makes one molecular target more actionable than another?



Working plan

Phase 2: In-Person Sessions (October 27)



Prof. Federico Gago

Provide students with skills in molecular visualization and small molecule construction

- Live Lecture (10:30 - 12:30): Introduction to Molecular Structure
- Lunch break (12:30 - 13:30)
- Hands-on Workshop (13:30 - 16:30): Molecular Visualization of Biological Macromolecules and Small Therapeutic Molecule Construction



Working plan



What should you bring prepared?

Review what you have studied about basic Chemistry fundamentals

Think about:

- How does molecular structure determine biological function?
- Why can small structural changes dramatically alter drug activity?

You can try playing with PyMOL

The image shows a variety of molecular representations: a ball-and-stick model of a complex organic molecule, a purple spherical virus-like structure with green spikes, a surface representation of a protein with a ligand bound in a pocket, and a multi-colored ribbon diagram of a protein structure. A red speech bubble with the text 'Try Me' is positioned above a small PyMOL software icon.

Working plan

Phase 2: In-Person Sessions (October 28)



Dr. Antonio Morreale

Introduce students to molecular docking techniques and ligand-receptor interaction analysis for drug candidate evaluation

- Live Lecture (10:30 - 12:30): Theoretical Considerations of Ligand-Target Docking
- Lunch break (12:30 - 13:30)
- Hands-on Workshop (13:30 - 16:30): Molecular Docking of Drug Candidates into Biological Targets

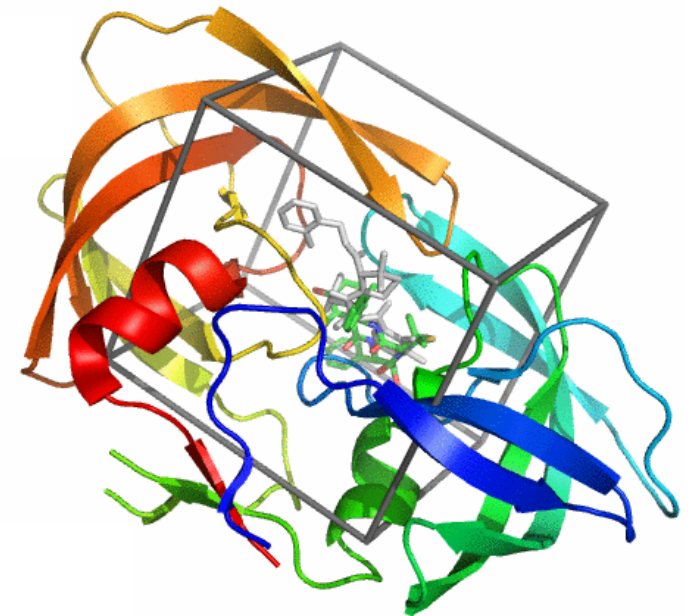
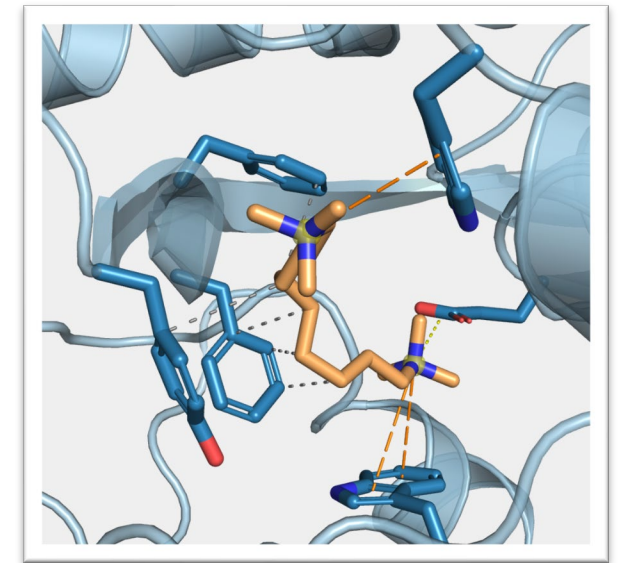
Working plan

What should you bring prepared?



Review what you have studied about fundamentals of molecular interactions

- What types of interactions stabilize ligand binding within a biological target?
- What determines whether a ligand binds strongly to a target?
- Why are some binding pockets more druggable than others?



Working plan

Phase 2: In-Person Sessions (October 29)



Dr. Jon del Arco

Apply molecular dynamics simulations to analyze the stability and interactions of drug candidates with their molecular targets

- Live Lecture (10:30 - 12:30): Theoretical Considerations of Molecular Dynamics Simulations
- Lunch break (12:30 - 13:30)
- Hands-on Workshop (13:30 - 16:30): Molecular Dynamics Simulations for Drug-Target Interaction Analysis



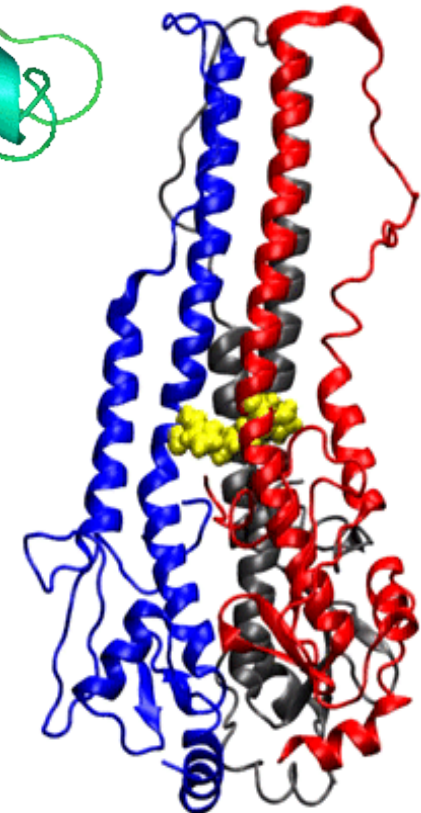
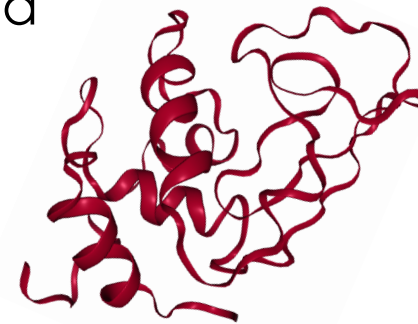
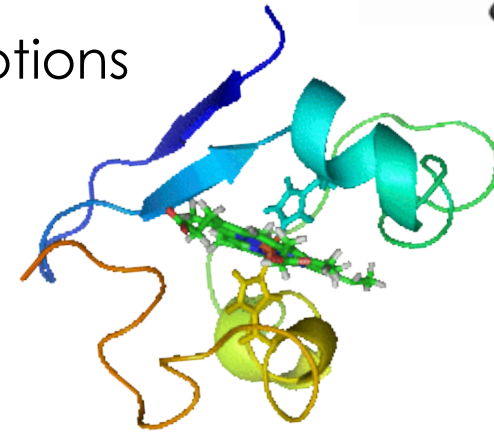
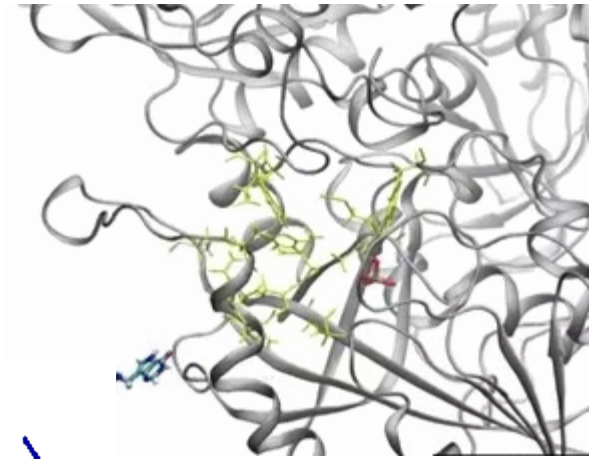
Working plan

What should you bring prepared?

Review what you have studied about macromolecular motions

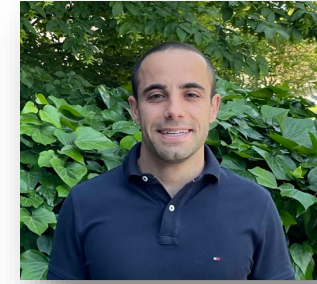
Think about:

- Why are biomolecules dynamic rather than static?
- How do conformational changes affect drug binding?
- What determines whether a ligand remains stable in a binding pocket?



Working plan

Phase 2: In-Person Sessions (October 30)



Dr. Jon del Arco

Provide students with skills to use AI-based tools for identifying and optimizing potential drug candidates

- Live Lecture (10:30 - 12:30): AI for Drug Discovery: Resources, Methods, and Applications
- Lunch break (12:30 - 13:30)
- Final Project defense (13:30 - 16:30)



Working plan: detailed schedule

	MONDAY 26/10/2026	TUESDAY 27/10/2026	WEDNESDAY 28/10/2026	THURSDAY 29/10/2026	FRIDAY 30/10/2026
08:30-09:30					
09:30-10:30					
10:30-11:30	Live lecture	Live lecture	Live lecture	Live lecture	Live lecture
11:30-12:30					
12:30-13:30	Lunch break				
13:30-14:30	Hands-on workshop	Hands-on workshop	Hands-on workshop	Hands-on workshop	Final Project defense
14:30-15:30					
15:30-16:30					

*This calendar only reflects the academic component of the programme. Additional social activities that form part of the programme will be included at a later stage



Evaluation



By the end of the program, students will be able to:

- Learn to construct and visualize molecular structures
- Perform molecular docking simulations to predict ligand-receptor interactions
- Use molecular dynamics simulations to refine docking results and study molecular behavior over time
- Apply AI-driven methodologies for drug candidate selection



Evaluation



Objective tests at the beginning of each session:

- 10-15' quick questions about the content of previous sessions (Kahoot)

FINAL PROJECT

- Throughout the course, students will work in groups on a common Project
- On Friday, October 30th, each group must present their project to the rest of the students
 - 15-minute presentation explaining the main results obtained
 - 10-minute question round

Deliverables: PowerPoint, PDF or Canva presentation



Your final grade is based on **two components**:



**OBJECTIVE TESTS
MADE EVERY DAY
IN CLASS**

These short daily objective tests completed in class will count for

30%

**OF THE TOTAL
EVALUATION**



**FINAL PRESENTATION
OF THE PROJECT**

The final presentation of your project will count for

70%

**OF THE TOTAL
EVALUATION**

 **In summary:** **30%** from daily objective tests in class | **70%** from the final presentation of the project.



Criteria	Excellent (9–10)	Good (7–8)	Satisfactory (5–6)	Needs Improvement (<5)	Weight
1. Scientific Understanding	Demonstrates deep understanding of biological concepts, computational methodologies, and drug discovery rationale	Shows good understanding with minor conceptual gaps	Basic understanding but limited depth	Major misunderstandings or insufficient knowledge	15%
2. Integration of Course Topics	Effectively integrates omics, molecular modeling, docking, MD simulations, and/or AI approaches into a coherent workflow	Integrates several course components appropriately	Limited integration between methodologies	Methods appear disconnected or incomplete	15%
3. Methodology & Technical Execution	Computational methods are correctly selected, justified, and executed with high rigor	Minor methodological limitations	Methods partially appropriate or insufficiently justified	Significant methodological errors or lack of rigor	15%
4. Data Analysis & Interpretation	Results are critically analyzed with strong scientific reasoning and biological interpretation	Interpretation mostly accurate with some limitations	Descriptive interpretation with limited critical analysis	Weak or incorrect interpretation of results	15%
5. Innovation & Problem-Solving	Demonstrates creativity, critical thinking, and innovative application of computational tools	Good problem-solving with some originality	Limited originality or mostly procedural work	Minimal evidence of independent thinking	10%
6. Quality of Visualizations & Figures	Molecular structures, docking poses, trajectories, graphs, and figures are clear, accurate, and professional	Visual materials mostly clear and appropriate	Visuals understandable but incomplete or inconsistent	Poor-quality or unclear visualizations	10%
7. Presentation & Scientific Communication	Clear, engaging, professional communication with excellent organization and timing	Well-organized presentation with minor communication issues	Adequate communication but uneven clarity or pacing	Difficult to follow or poorly organized	10%
8. Responses to Questions	Answers demonstrate strong understanding, confidence, and critical reasoning	Answers most questions correctly	Answers basic questions but lacks depth	Unable to adequately answer questions	10%

Practical information

Public transportation to our Campus

- The Cuatro Vientos bus station, located in the southwest area of Madrid, is approximately halfway to the university when taking bus line 518. This station can be reached from line 10 of the Madrid Metro, and it is also accessible from the airport by taking Metro line 8 to line 9 and then transferring to line 10
- You can take the C5 commuter train line from Atocha station, in the city center, to Alcorcón Central station. From there, you can continue your journey to the university by taking bus 510 or 510B

Here are the websites for the subway and trains in Madrid:

- [Subway map](#)
- [Commuter train map](#)
- [Useful information about public transport in Madrid](#)
- [Subway prizes](#)



Practical information

Accommodation in Madrid:

You can choose to stay near the campus or opt for accommodation in the city center.

City center:

- [Room Plaza España](#)
- [ApartoHotel Rosales](#)
- [Social hub](#)
- [Hostel Puerta del Ángel](#)

*Many more hotels are available in the city center between Streets Gran via & Princesa.

Near the campus:

- Villaviciosa de Odón village (with 518 bus):
 - [Hostal Las encinas](#)
 - [Hotel Villa Odón](#)
- Alcorcón (with 510 and 510-A bus from Alcorcón central station 10 mins walking):
 - [Hotel NH Alcorcón](#)
- Alcorcón (with 518 bus):
 - [Holiday INN Alcorcón](#)
 - [Ibis Alcorcón](#)





Universidad
Europea

We look forward to
sharing this experience
with you!

Doubts?

erasmus@universidadeuropea.es

Ve más allá