

COMENZE Training Meeting | March 2026

# Workshop on Multiscale Computational Modeling and Design of Polymer-Degrading Enzymes

*Notes: You need to bring your own laptop*

**DAY 1 - 09. MARCH 2026**

Introduction to Computational Modeling of enzymatic systems

Av. Andorra, 28, 17251, Platja d'Aro-Calonge, Spain

Time	Activity
9:30-10:00	<b>Arrival and Welcome</b>
10:00-11:00	<b>S. Osuna</b> - Welcome & Overview of Challenges in computational modeling of plastic-degrading enzymes, especial focus on dynamics
11:00-11:30	<b>TEA BREAK</b>
11:30-13:30	<b>S. Osuna</b> - Hands-on: Software for proteins visualization, Artificial Intelligence supported proteins prediction - AlphaFold, Models validation
13:30-14:30	<b>LUNCH</b>
14:30-15:30	<b>C. Rovira</b> - QM/MM-MD strategies for enzymatic catalysis
15:30-16:00	<b>COFFEE BREAK</b>
16:00-18:00	<b>A. Nin</b> - Hands-on: CPMD QM/MM Tutorial: Proton transfer of malonaldehyde in solution

**DAY 2 - 10. MARCH 2026**

Role of protein dynamics and water in enzyme catalysis

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Time	Activity
9:30-10:30	<b>A. Gora</b> - Role of protein dynamics and water in enzyme catalysis
10:30-11:00	<b>TEA BREAK</b>
11:00-13:00	<b>A. Raczynska</b> - Water network analysis from MD trajectories
13:00-14:00	<b>LUNCH</b>
14:00-15:00	<b>V. Moliner</b> - QM/MM strategies for enzymatic catalysis in plastic degradation
15:00-15:30	<b>COFFEE BREAK</b>
15:30-17:30	<b>K. Świderek</b> - Hands-on: QM/MM Modelling of Biochemical Reactions. Exploring GNMT Catalysis through Potential of Mean Force

**DAY 3 - 11. MARCH 2026**
**Computational investigation of protein-ligand interactions and enzyme design tools**

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Time	Activity
9:30-10:30	M. De Vivo - Enhanced sampling & free energy calculations
10:30-11:00	<b>TEA BREAK</b>
11:00-13:00	P. Vidossich - Hands-on: Computing binding free energy changes due to point mutations via alchemical calculations
13:00-14:00	<b>LUNCH</b>
14:00-15:00	S. Mazurenko- AI-Driven Enzyme Engineering
15:00-15:30	<b>COFFEE BREAK</b>
15:30-17:30	P. Kohout: Hands-on: Enzyme stability prediction using FireProt pipeline
17:30-18:30	S. Osuna - Scientific data presentation
20:00-23:00	<b>GALA DINNER</b>

**DAY 4 - 12. MARCH 2026**
**Computational investigation of protein-ligand interactions and enzyme design tools**

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Time	Activity
9:30-10:30	F. Sancho - Strategies for proteins redesign
10:30-11:00	<b>TEA BREAK</b>
11:00-13:00	F. Sancho - Hands-on: Strategies for proteins redesign
13:00-14:00	<b>LUNCH</b>
14:00-15:00	V. Ferrario - Understanding protein-ligand interactions
15:00-15:30	<b>COFFEE BREAK</b>
15:30-17:30	V. Ferrario - Hands-on: Understanding protein-ligand interactions

## Venue

The training meeting will be held at Park Hotel San Jorge COSTA BRAVA in Platja d'Aro (Girona)  
(<https://www.parkhotelsanjorge.com/en/>)



## How to get to Park Hotel San Jorge

### Travel by air

The most common way to fly to Spain is via **Girona Airport**. From Girona Airport, the easiest way to reach **Platja d'Aro** is to take the **bus to Girona train station** (line 607 – [Sagalés](#)), and then transfer to another bus operated by either **Teisa** ([teisa-bus.com](https://teisa-bus.com)) or **Moventis** ([moventis.es](https://moventis.es)).

Alternatively, you can fly to **Barcelona Airport**, from where there are **direct Moventis buses** departing from both **Terminal 1** and **Terminal 2** ([moventis.es](https://moventis.es)).

### Travel by train

Girona can easily be reached by train. Within RENFE, you can check the trains on the website <https://www.renfe.com/es/en>

### Taxis

Taxi Girona: +34 972 22 23 23 <https://www.gitaxi.cat/en/>

## Map

