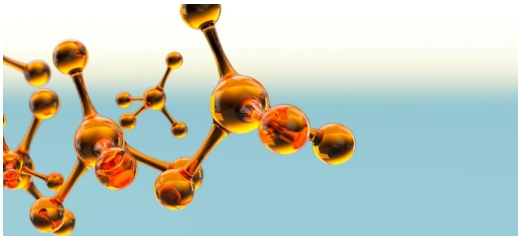
Amber Machine Learning and Free Energy Simulation Workshop (AMBER2026)



Uzt. 13 - Uzt. 17 2026

Kod. Z61-26

Mod.:
Aurrez aurrekoa

Edizioa
2026

Jarduera mota
Workshop

Data
Uzt. 13 - Uzt. 17 2026

Kokalekua
DIPC eta Kimika Fakultatatea

Hizkuntzak
Ingelesa

Balio akademikoa
50 ordu

Antolakuntza Batzordea

Azalpena

Simulation methods used to investigate a wide range of chemical and biological processes, including drug binding, protein folding, protein–protein interactions, allosteric regulation, gas adsorption and diffusion in metal–organic frameworks (MOFs), piezoelectric responses, and catalytic events. Improving the accuracy and efficiency of these simulations remains an active area of research, particularly with the growing integration of machine learning potentials (MLPs) and artificial intelligence (AI) to expand the scope and reliability of free energy methods. As computational resources and theoretical techniques continue to advance, so too does the potential impact of free energy simulations. However, these methods are often technically challenging to set up and execute.

This workshop will equip computational scientists with the knowledge and practical skills to perform robust, accurate, and efficient free energy simulations using the AMBER software suite. AMBER offers an advanced array of free energy simulation and analysis methods with high-throughput enabled by its efficient GPU-accelerated free energy simulation engine. Through a combination of lectures and expert-guided hands-on tutorials, participants will learn best practices and explore the latest features in AMBER, including new enhanced sampling techniques, optimized alchemical transformation pathways, free energy surface and minimum free energy path methods. AMBER further offers a diverse set of generalized hybrid quantum mechanical (QM), molecular mechanical (MM) and machine learning potential (MLP) force fields enabled by interoperable software infrastructure. Free energy workflows provide a framework from which complex networks of simulations can be efficiently set up, executed and analyzed. Emphasis will be placed on driving applications to enzyme design and drug discovery.

ORGANIZING COMMITTEE:

- Xabier Lopez (EHU)
- Jose M. Mercero (EHU)
- Elena Formoso (EHU)
- Jon Uranga (EHU)
- Darrin York (Rutgers University)
- Solen Ekesan (Rutgers University)

Helburuak

Demystify and streamline **free energy (FE) simulations** for challenging chemical/biological problems (drug binding, protein folding, PPIs, allostery, MOFs, catalysis, piezoelectric effects).

Teach participants to run **robust, accurate, and efficient FE calculations** end-to-end using the **AMBER** software suite.

Showcase **GPU-accelerated** engines and **high-throughput workflows** for setting up, executing, and analyzing complex networks of simulations.

Cover **best practices** via lectures plus **expert-guided, hands-on tutorials**.

Introduce **latest AMBER features**: enhanced sampling, optimized alchemical pathways, free-energy surfaces, and minimum free-energy path methods.

Train attendees to leverage **hybrid QM/MM/MLP force fields** and AMBER’s interoperable infrastructure.

Highlight the growing role of **machine learning and AI** in extending FE accuracy, scope, and efficiency.

Emphasize **applications to enzyme design and drug discovery** as primary use cases.

Ikastaroaren laguntzaile espezifikoak

Zuzendaritza

Xabier Lopez Pestaña

UPV/EHU. Facultad de Ciencias Químicas

Matrikula prezioak

REGISTRATION FEES	2026-07-05 ARTE
Fee waiver	0 EUR
Regular Attendant	200,00 EUR
Industry	400,00 EUR

Kokalekua

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Gipuzkoa