

Title: Peptides in biology and materials: bridging simulation and experimental data

Dates: 30th-31st August 2024

Venue: Plesso Didattico Morgagni - University of Florence (Italy)

Webpage: <https://www.cecarn.org/workshop-details/1333>

Expected participants: 30-40; senior and young researchers.

Organizing Committee:

Gianfranco Bocchinfuso (Rome Tor Vergata University)

Paolo Calligari (University of Rome "Tor Vergata")

Anela Ivanova (Sofia University "St. Kliment Ohridski")

Manuel N. Melo (Instituto de Tecnologia Química e Biológica - Universidade NOVA de Lisboa)

Marco Pagliai (University of Florence)

Lorenzo Stella (University of Rome Tor Vergata)

Description

This workshop is a **satellite event of the joint 37th European Peptide Symposium and 14th International Peptide Symposium and is also a CECAM (Centre Européen de Calcul Atomique et Moléculaire) flagship event.**

The workshop's primary objective is to critically evaluate the state-of-the-art in-silico methods and explore their potential integration with experimental data to outline methodological approaches to solve problems specifically related to peptide systems.

The workshop will address specific subjects and associated challenges related to in-silico studies of peptides. These topics span from **design methods** (such as integrative structural methods, improvements in force fields, and design tailored for specific functions) to the exploration of **bioactive peptides** (e.g. membrane-active peptides and inhibitors of protein-protein interactions) and **nanomaterials** (including the investigation of peptide aggregates and functionalized nanoparticles).

Taking advantage of the concomitant joint EPS/IPS Symposium, we aim to attract scientists from different fields to promote a thorough discussion and define possible future strategies. This workshop will be an opportunity to bring together computational biophysicists, peptide modelers, bioinformaticians, and experimentalists involved in studying peptides in different contexts, providing a unique opportunity to bridge the gap between these approaches. The exchange of knowledge, techniques, and data can contribute to advancements in peptide research, leading to new discoveries and insights. For this reason, the workshop will welcome participants from both the scientific community and the industry.

Participation in the workshop is free of charge.

To enhance discussion among attendees, the number of participants will be limited.