



# SUMMER SCHOOL a.a.2022/2023

## Department of Pharmacy - UNIPI

### Summer School Title: Computer-Aided Drug design

July 10<sup>th</sup> – 14<sup>th</sup> 2023

**Scientific manager:** Prof. Tiziano Tuccinardi (tiziano.tuccinardi@unipi.it)

The contribution of computational methodologies to drug discovery is no longer a matter of dispute and the major world's pharmaceutical and biotechnology companies use computational design tools. Computer-aided drug design comprises computational methods and resources that are used to facilitate the design and discovery of new therapeutic solutions.

This summer school will cover all the main computational techniques used in drug discovery, supplying a basic level of knowledge of this research field. This course will be divided into theoretical and practical lessons and will allow the participants to independently develop their own computational studies. At the end of the course participants will receive an Attendance Certificate with a description of the educational objectives of the Summer School and the detail of the activities. 3 credits will be acknowledged by the University of Pisa according to the European Credit Transfer System (ECTS).

#### Who can apply

The school is open to all students that possess a basic background of chemistry, biology or medicinal chemistry. Undergraduates and PhD students, post-doctoral researchers and senior researchers from Universities, research institutes, clinics and industries are welcome.

#### Preliminary program:

- 1) Visualization of a ligand-protein complex.
- 2) Basic linux commands.
- 3) Docking of ligands into target proteins and software reliability evaluation.
- 4) Pharmacophore modeling
- 5) Molecular dynamic simulations of biological systems
- 6) Virtual screening calculations
- 7) Machine Learning in Drug Discovery

**Place:** Department of Pharmacy, University of Pisa

**Website:** <http://www.mmvsl.it/wp/miscellaneous/cadd-summer-school>

**Fee:** 250 €

