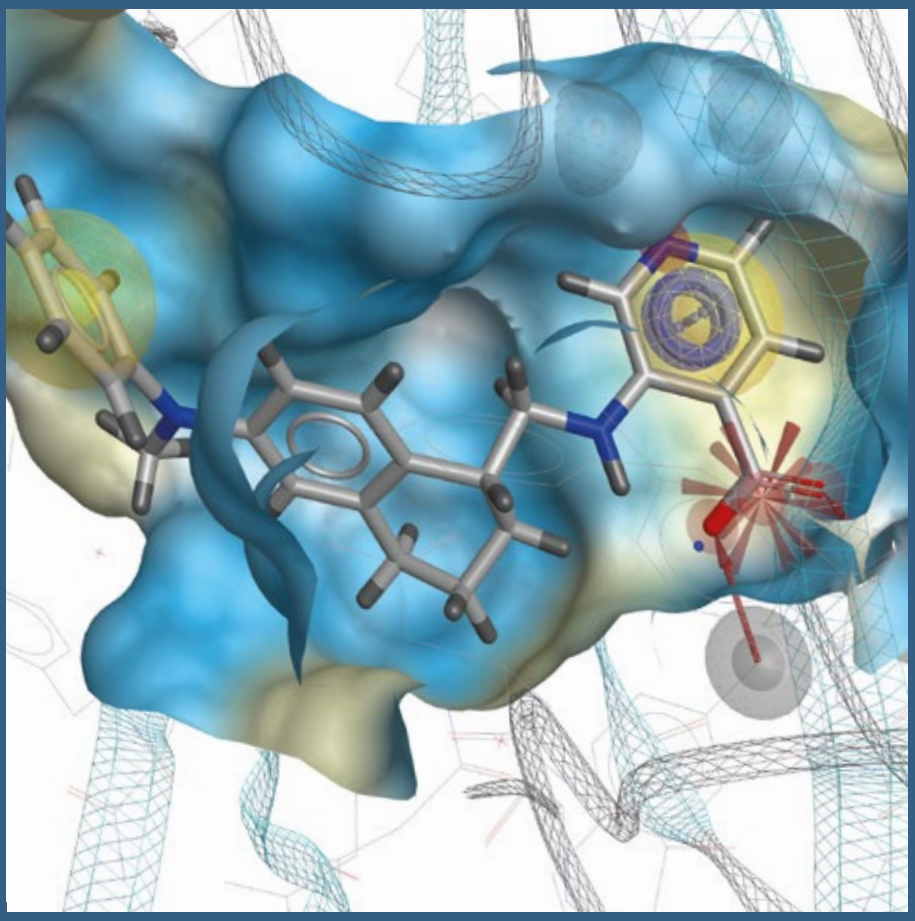
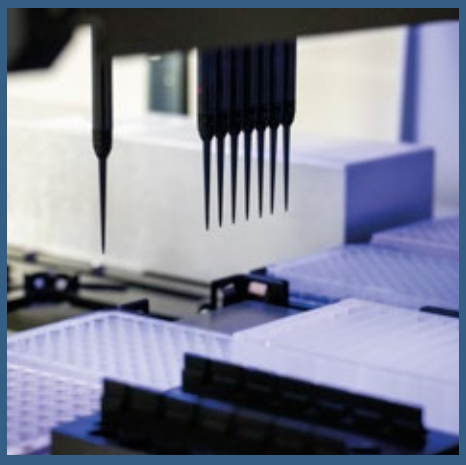
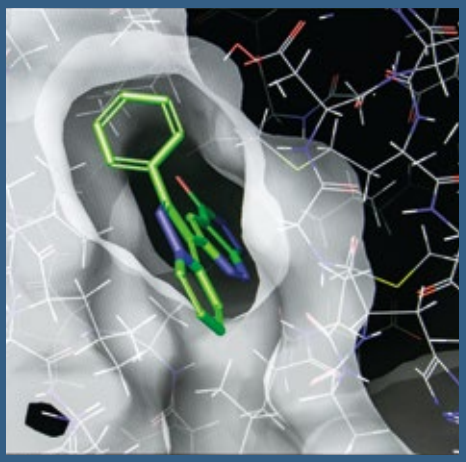
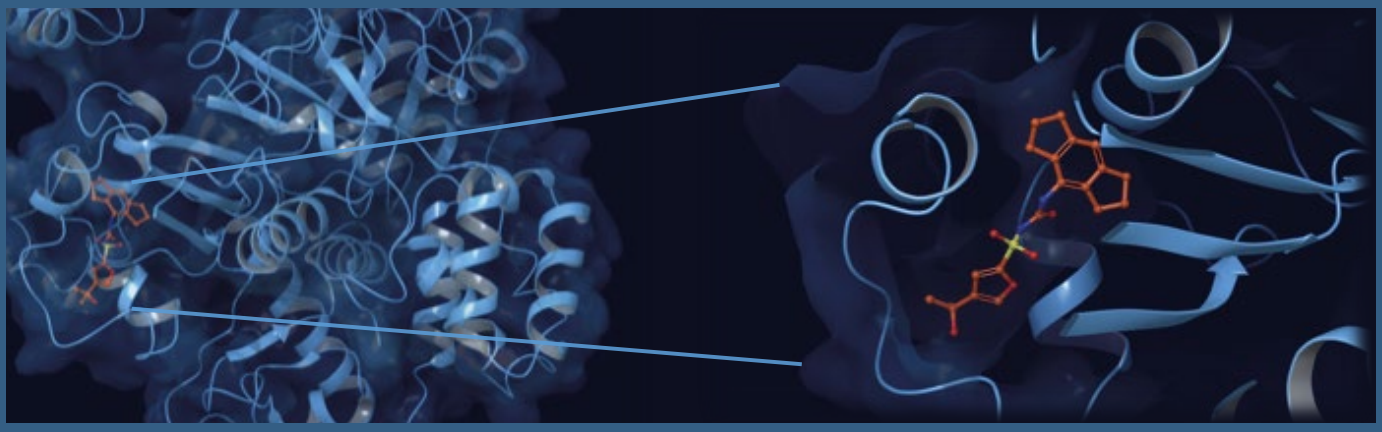
Molecular Informatics Group @ Ri.MED

The Molecular Informatics group exploits innovative computational techniques for the design of new chemical or biological entities and the prediction of their therapeutic properties. Powerful computing tools and state-of-the-art infrastructures also allow to elucidate important molecular interactions underlying different pathologies.









Fondazione Ri.MED

AIMS

- Understanding of molecular mechanisms behind different pathologies
- Design of chemical or biological therapeutic agents
- Creation of predictive in silico models to reduce from-bench-to-bedside process duration

FOCUS

- Creation of molecular libraries for biological screening
- Design of chronic inflammation disease modulators
- Design of anticancer agents
- Study of protein-protein interactions in biological processes
- Computational applications for biologics design

OUTCOME

- Completion of the OBIND platform (Oncological therapies through Biological Interaction Network Discovery - https://www.obind.eu/)
- Publication of the recommendation system on protein kinases for the repositioning of anticancer drugs
- Publication of a virtual screening system based on molecular fingerprints (EMBER-Embedding Multiple Molecular Fingerprints for Virtual Screening)

EXPERTISE AND RESOURCES

- Machine Learning models for molecular properties prediction
- Computer-Assisted Molecular Design
- Molecular Dynamics (biased and unbiased)
- CPU and GPU-based virtual screening
- Compound management platform

COLLABORATIONS

- University of Verona, ITA
- University of Palermo, ITA
- University of Milan, ITA
- Université Paris Cité, FRA
- University of Vienna. AUT
- Institute of Translational Pharmacology (IFT) (CNR), ITA

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Molecular Informatics Group
c/o ATeN Center, University of Palermo,
Via Filippo Marini 14, 90128 - Palermo
Group Leader: Ugo Perricone, PhD
uperricone@fondazionerimed.com