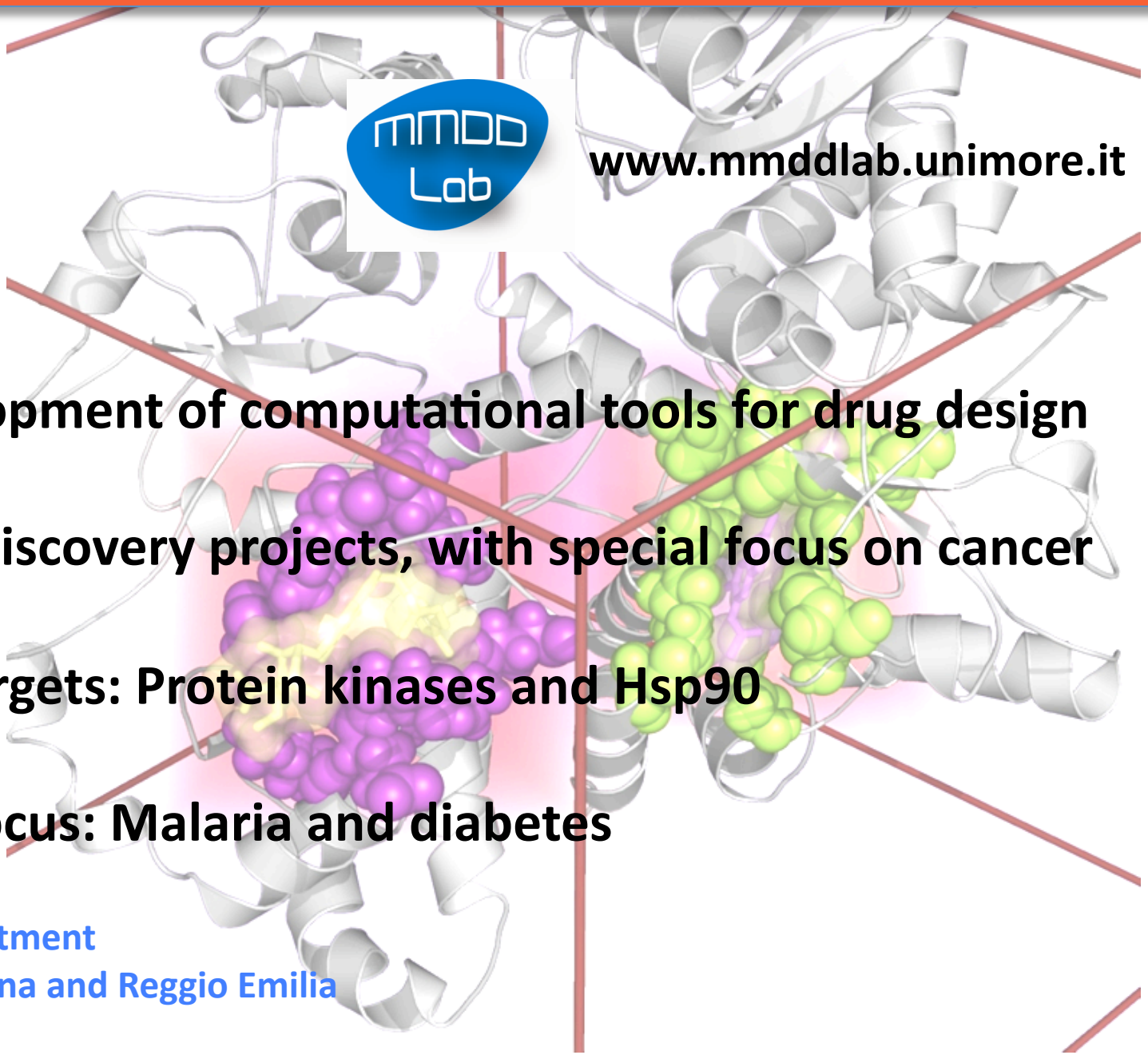
UNIMORE - Molecular Modelling & Drug Design Lab

UNIVERSITÀ DEGLI STUDI
DI MODENA E REGGIO EMILIA

MMDD Lab

www.mmddlab.unimore.it

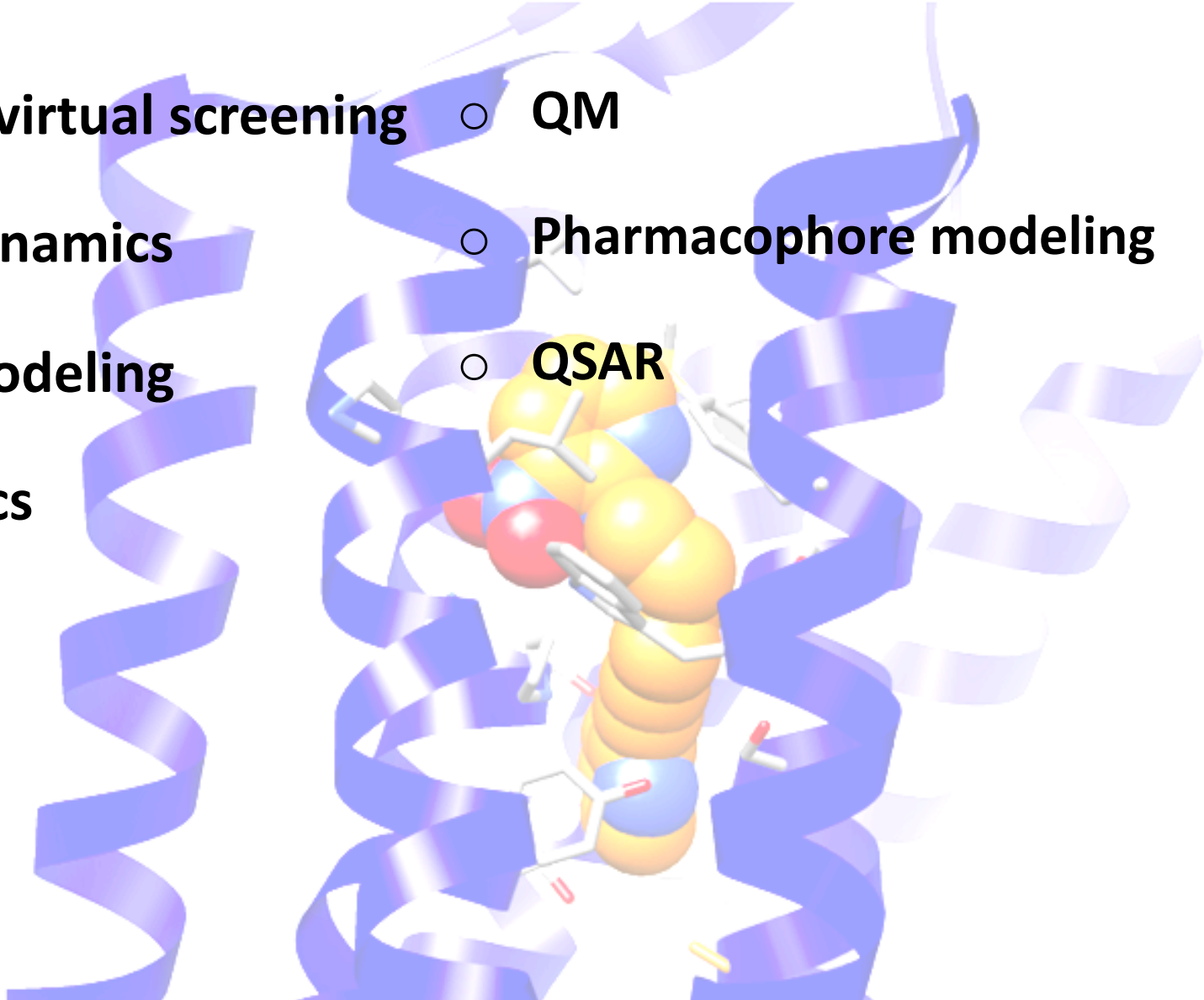


- ✓ **Development of computational tools for drug design**
- ✓ **Drug discovery projects, with special focus on cancer**
- ✓ **Key targets: Protein kinases and Hsp90**
- ✓ **Past focus: Malaria and diabetes**

Life Sciences Department
University of Modena and Reggio Emilia

Main research techniques

- Docking and virtual screening
- Molecular dynamics
- Homology modeling
- Bioinformatics
- QM
- Pharmacophore modeling
- QSAR



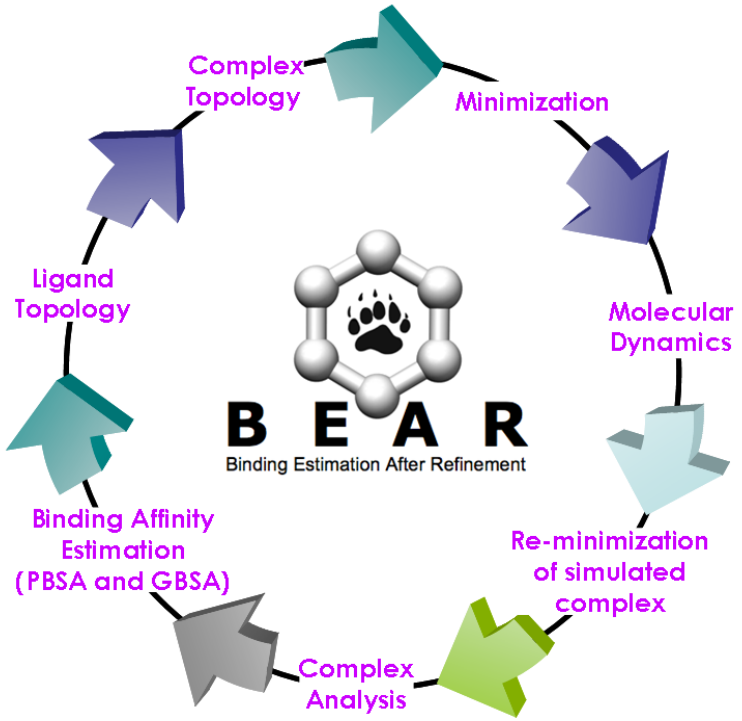
BEAR virtual screening

BEAR (Binding Estimation After Refinement)

We have developed **BEAR** (Binding Estimation After Refinement), an automated post-docking tool based on **molecular dynamics** and **MM-PB(GB)SA** for refining and rescoring virtual screening results.

B E A R
Binding Estimation After Refinement

SPINNER 2013
PERSONE AL FUTURO



Drug discovery on protein kinases

Discovery of allosteric inhibitors of protein kinases as anticancer drugs

Design of small-molecules able to bind distal allosteric pockets of protein kinases and stabilize inactive conformations. Project in collaboration with Istituto di Ricerche Farmacologiche **Mario Negri** in Milan, **University of Milano**, **University of Padova**, **Elettra Sincrotrone Trieste**.

Drug Design

Biology & Pharmacology

Chemical synthesis

Crystallography

Polypharmacology

Targeting the Hsp90 interactome using in silico polypharmacology approaches

Focused on setting up and exploiting ligand-based and structure-based computational protocols for targeting the **Hsp90 interactome** (> 200 proteins) with **polypharmacology** approaches. Project in collaboration with the University of Bonn.

universitätbonn

Development of computational tools for polypharmacology

Computational protocols and approaches for rational polypharmacology and their deployment in drug repurposing, target identification, and prospective drug discovery projects.

Experimental network

	INTERNAL	EXTERNAL
Chemical synthesis	4 groups CIGS	UNIMI, UNIPR
Biology/Pharmacology	Biochem, Mol biol groups, CeIRG (Genomic Research Centre) CMR (Regenerative Medicine Centre)	Mario Negri Institute Europ Institute of Oncology
Crystallography		UNIPD Elettra Synchrotron ScpA
Computing infrastructures	LabCSAI	CINECA