



***Ph.D. School in Chemical Sciences
Cycle XXXVIII***

Proposer/Company: Professor Maria Monti/Dompè farmaceutici S.p.A.

Research project title: Interaction studies between molecules with potential pharmacological activity and protein targets *in vitro* and *ex vivo* experimental systems

Key words: Drug-proteins interactions; drug repurposing; proteomics; Surface Plasmon Resonance; hit identification, target engagement and profiling

Research project abstract: The project proposal relies on the following tasks: Task 1. Identification of new protein targets for the treatment of diseases associated with strong fibrotic and / or inflammatory states, such as liver fibrosis. Through label free differential proteomics experiments, proteins whose expression levels are significantly altered in the pathological state will be identified as potential and specific markers of the pathology. Task 2. Screening of libraries of molecules with potential pharmacological activity (repurposing) on the basis of the new potential protein targets identified by proteomics and predictive *in silico* data generation; Virtual screening and molecular dynamics will provide new evidences in target-drug interaction giving new insights into target identification and/or repositioning of known drug for new therapeutic areas Task 3. Structural and functional validation of drug-protein interaction The potential target proteins of the disease will be expressed in recombinant form and used for *in vitro* functional and structural assays.