

**OFFER AN INTERNSHIP**  
**Academic Year 2014 – 2015**

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**Name of training supervisors: Dr. Laura Belvisi (researcher) and Dr. Monica Civera (post doc)**

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Specialty training : Research ☒ Professional ☐

a few key words to describe the subject of training :

molecular modeling – protein-protein interactions – peptide mimics – structure-based drug design

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**Title of internship:**

Computational modeling of peptidomimetic molecules targeting protein-protein interactions

this subject is a first step towards a thesis: No

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**Short texte describing your project**

The training project will comprise the application of various computational techniques to design peptidomimetics that are able to modulate protein-protein interactions of therapeutic relevance in cancer, such as the interactions involving adhesion molecules (like integrins and cadherins) or other specific cell surface receptors (e.g. growth factor receptors), identified as relevant in tumor progression.

In particular, the combined use of molecular mechanics, molecular dynamics simulations and docking calculations with available structural information (x-ray, NMR) will be exploited in:

- designing peptidomimetics promoting specific peptide conformations involved in binding through the insertion of non natural amino acids or rigid scaffolds
- defining the conformational equilibrium of peptidomimetics simulating structural motifs of protein-protein interfaces
- evaluating the stability of protein-peptidomimetic complexes.

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