



## Master project 2021-2022

### Personal Information

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### Project

## Structural bioinformatics

#### Project Title:

Development and testing a protocol for protein-peptide binding using PELE and BCE

#### Keywords:

Computational Chemistry, Molecular Modeling, Protein-Protein Interactions, QM/MM

#### Summary:

This project aims to combine PELE, our proprietary software to explore the potential energy surface of biomolecular systems, with the BCE workflow. BCE stands for Bioactive Conformational Ensemble and it combines a Molecular Mechanics exploration, a clustering technique and a final Quantum Mechanics calculation to obtain a conformational ensemble of drug-like molecules. The goal is to reduce the degrees of freedom to explore with PELE to only cover those conformations that BCE predicts as meaningful. This approach will allow us to study more efficiently protein binding of large peptides or other large molecules like macrocycles.

#### Expected skills::

Biochemistry with programming skills or knowledge

#### Possibility of funding::

Yes

#### Possible continuity with PhD: :

To be discussed

#### Comments:

Initial duration: 4-8 months

