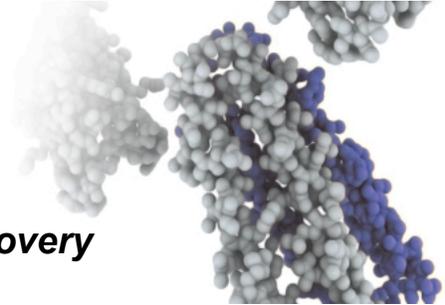


# NANO-D

Algorithms for Modeling and Simulation of Nanosystems

## Development of Formulation for Anisotropic Potential Function for *Computational Drug Discovery*

INRIA Grenoble - Rhône-Alpes  
NANO-D research group



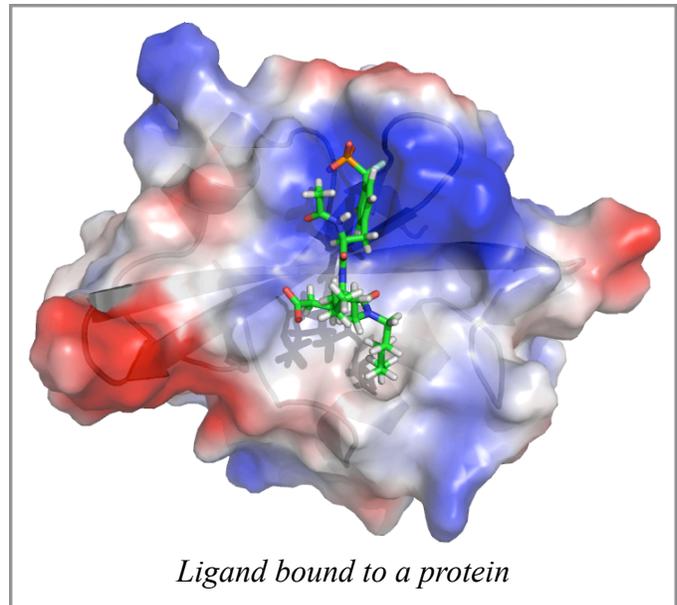
### About NANO-D

The [NANO-D](#) team aims at developing efficient computational methods for modeling and simulation of complex nanosystems, both natural (e.g. the ATPase engine and other complex molecular mechanisms found in biology) and artificial (e.g. NEMS - Nano Electro-Mechanical Systems).

In particular, the group develops novel multiscale, *adaptive* modeling and simulation methods that are used to model and simulate molecular structures. Applications of these methods are molecular structure predictions via folding, docking and refinement algorithms.

### Computational drug discovery

Structure-based [drug discovery](#) relies on knowledge of the [three dimensional structure](#) of the biological target obtained through methods such as [X-ray crystallography](#), which is used as a basis for designing new ligands by applying accepted principles of molecular recognition. The basic assumption underlying structure-based drug discovery is that a good ligand molecule should [bind](#) tightly to its target. Thus, one of the most important principles for designing or obtaining potential new ligands is to predict the [binding affinity](#) of a certain ligand to its target and use it as a criterion for selection. The binding affinity can be [approximated](#) with certain physics-based empirical functions or using knowledge-driven potentials.



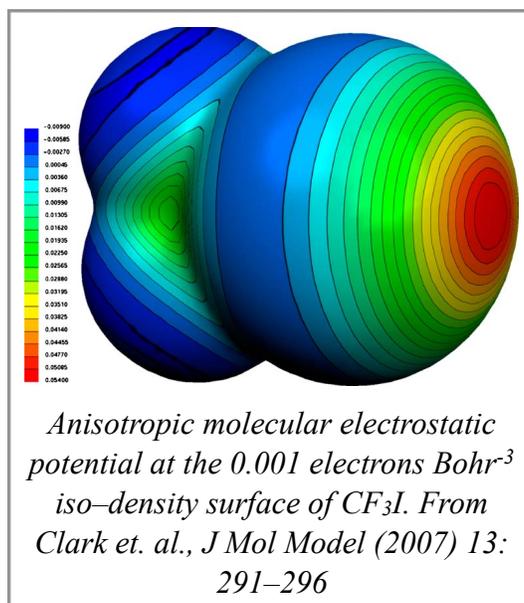
*Ligand bound to a protein*

## Research Internship Details

We have recently developed a new *isotropic* (i.e., direction-independent) formulation for the potential function for interactions between proteins. We would like to extend this formulation to a class of *anisotropic* (i.e., direction-dependent) potential functions.

The goals of the internship are:

- develop a pairwise anisotropic potential function able to describe various types of non-covalent interactions in small molecules, particularly:
  - halogen bonds
  - hydrogen bonds
  - aromatic interactions
- deduce coefficients for the potential from the knowledge-base (i.e., PDBBind data set)
- study the effect of several angular basis sets, as well as several radial basis sets on the quality of the potential
- validate the potential on a set of structures of high resolution extracted from the Protein Data Bank and Cambridge Structural Database



## About Grenoble

Grenoble is the capital city of the French Alps. Combining the urban life-style of southern France with a unique mountain setting, it is ideally situated for outdoor activities. The Grenoble area is today an important centre of industry and science (second largest in France). Dedicated to an ambitious policy in the arts, the city is host to numerous cultural institutions. With 60,000 students (including 6,000 foreign students), Grenoble is the third largest student area in France.

## Contact Information

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