# Post-doc position 2018 – University of Nantes (France)

## Computational design of protein-protein modulators.

**Position:** Post-doc in computational chemistry, bioinformatics – one year as early as possible.
**Location**: University of Nantes (France), CEISAM Laboratory (UMR CNRS 6230), ModES Team.
**Contact:** Dr. Adèle Laurent, Adele.Laurent@univ-nantes.fr

We are looking for motivated candidates for a postdoctoral position funded by the *French National Institute of Cancer* within the framework of a project driven by Dr. Adèle Laurent at the CEISAM laboratory in Nantes (France). This project, conducted in strong collaboration with biologists, is focused on the Computational design of different protein/protein interaction modulators inhibiting different biological targets.

### Research context and program

The present project is embedded into a new regional axis (PIRAMID program) focusing on the design of inhibitors of specific protein-protein interactions (PPI) involved in various medical fields such as (auto)immune diseases or fungal diseases. The aim is to bring relevant and original compounds to be tested by the biologists and optimized by relevant chemical modulations by the organic chemists. The following steps will be carried out to fulfill various goals: homology modeling, virtual screening using “straightforward” and “home-made” libraries of compounds, steered MD and relative binding free energy computations. However, as intrinsically disordered domains have shown their importance in some of the targeted PPI, it will be necessary to deal with such challenging zones using recent molecular modeling advances.

### Applicant

The applicant should have **a PhD in Chemistry, Pharmacy, Biophysics, Biology obtained no more than 4 years ago**. Proven experiences in computational chemistry and molecular simulation techniques are prerequisites, whereas experience in scientific computing and programming are valuable assets. The post-doctoral associate will use a large panel of molecular modeling methodologies (homology modeling, virtual screening, force field parameters, set-up a library of compounds). The candidate should be strongly motivated by topics at the chemistry-biology interface and to work in collaboration with biologists and organic chemists. He/she should show initiative, have the ability to work independently and possess good oral and written communication skills. Applications and informal queries should be addressed to Adele LAURENT (Adele.Laurent@univ-nantes.fr). Interested candidates should send their CV, a cover letter describing their research interests and motivation, and the names of three persons willing to write a recommendation letter.