

Computational Chemistry And Computer-Aided Drug Design (CADD).

Term: One year with a possibility of a renewal for an additional year.

A one-year immediate postdoctoral position is available in the computational chemistry and drug discovery lab of Dr. Khaled Barakat at the Faculty of Pharmacy, University of Alberta, Canada. Successful applicants will employ state-of-the-art computational techniques and high performance computing facilities accessible by the lab to work on various protein-protein interactions and drug discovery projects.

Applicants must have an outstanding record of research achievements, strong communication skills, and an ability to collaborate effectively. Applicants must hold a PhD in computational chemistry, computer aided drug design or a closely related field. Applicants must have proven expertise in computational tools and approaches for drug design, such as structure-based and ligand-based drug design, homology modeling and molecular dynamics, in silico screening (both structure-based and ligand-based), hit2lead and lead optimization.

The following skills are essential:

1. Understanding the biophysical concepts behind protein-protein interactions and protein-ligand interactions.
2. Familiarity with high performance computing facilities.
3. In depth knowledge of biomolecular simulation techniques, including but not limited to, classical molecular dynamics, ab initio calculations and QM/MM techniques, homology modelling, protein-protein docking and protein-ligand docking.
4. Outstanding experience with the various software packages for atomistic biological simulations, such as AMBER, NAMD, GROMACS, Schrodinger, VMD and MOE, etc.
5. Profound experience with python scripting is a must. Perl or Tcl will be advantageous.
6. At least four first author publications in the aforementioned fields in high impact Journals.
7. Ability to perform effectively and successfully under pressure is significantly important.

The contract will be initially for one year, renewed upon mutual agreement and performance assessment. To apply for this position, please send your most updated CV and a brief statement of research interests, along with the names and contact information of at least three referees, to: Dr. Khaled Barakat ; email:kbarakat_at_ualberta.ca