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**Opportunity Title:** Enhancing Drug Discovery by Prediction of Protein “Hot-Spots”
**Opportunity Reference Code:** ORNL-HBCU-MEI-2020-0009

**Organization** Oak Ridge National Laboratory (ORNL)

**Reference Code** ORNL-HBCU-MEI-2020-0009

**How to Apply** All documents must be submitted via Zintellect. All application components **must** be completed and received in the system in order to be considered.

***Application deadline January 10, 2020 at 11:59 pm EST.***

For questions, please contact HBCUMEI@orau.org.

**Application Deadline** 1/10/2020 11:59:00 PM Eastern Time Zone

**Description** ORNL is the largest science and energy laboratory in the Department of Energy system. Areas of research include materials, neutron sciences, energy, high-performance computing, systems biology and national security. Visit http://www.youtube.com/watch?v=NSCdUJ8cavw to discover some exciting reasons why ORNL offers a great internship experience!

**Benefits:**

- Selected faculty spend 10 weeks (Summer Term) at Oak Ridge National Laboratory (ORNL) engaged in a research project under the guidance of a laboratory scientist.
- Faculty members build collaborative relationships with ORNL research scientists, become familiar with ORNL sponsored research programs, scientific user facilities, and potential funding opportunities.
- ORNL may provide laboratory tours, scientific lectures and seminars, workshops on accessing ORNL scientific user facilities.
- Host laboratories provide all required site specific training.

**Project:**

The disruption of protein-protein interactions (PPIs) can lead to cures of various diseases including cancer, heart failure and neurological disorders. Usually only a few residues, so-called "hot-spots", are responsible for the majority of the binding affinity. PPIs can be disrupted with small-molecules that bind strongly to a hot-spot and inhibit the protein complex formation. Currently, in silico docking of small molecules (“ligands”) to proteins is commonly used in early drug discovery to estimate the strength of ligand-protein interactions. However, the ranking of ligands based on docking is not precise enough to allow accurate prediction of drug candidates. The proof-of-principle we will establish is that combination of in silico docking and hot spot prediction can improve the discovery of lead molecules that disrupt protein-protein interactions. The process includes in silico PPI hot spot prediction, large-library docking on supercomputers, followed by running a novel hot-spot-based algorithm for ranking ligand-protein complexes to reduce candidates from thousands to dozens.

**Faculty Mentor/Point of Contact:** Loukas Petridis (petridisl@ornl.gov)

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**Qualifications**

**Applicant must be a faculty member at a HBCU/MEI at the time of application.**

**Faculty Qualifications/Skills Desired:** Some basic computational experience is required, for example using Linux. Familiarity with molecular modeling techniques would be helpful: in silico docking, molecular dynamics simulations, homology modeling. Understanding of molecular biology, biochemistry, biophysics is also encouraged. In general, the software we use is user friendly and research team members come from diverse science backgrounds: biologists, chemists, physicists, chemical engineers.

**Eligibility Requirements**

- **Citizenship:** LPR or U.S. Citizen
- **Degree:** Any degree .
- **Academic Level(s):** Faculty.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12)
  - **Communications and Graphics Design** (2)
  - **Computer, Information, and Data Sciences** (16)
  - **Earth and Geosciences** (21)
  - **Engineering** (27)
  - **Environmental and Marine Sciences** (14)
  - **Life Health and Medical Sciences** (45)
  - **Mathematics and Statistics** (10)
  - **Other Non-Science & Engineering** (2)
  - **Physics** (16)
  - **Science & Engineering-related** (1)
  - **Social and Behavioral Sciences** (27)

**Affirmation**

I am a faculty member at one of the nationally recognized HBCU or MEI institutions. I can provide certification of my faculty position, if requested.