Opportunity Title: Development of Cheminformatics Tools for Prediction of Molecular Properties, Chemical Structure, and Spectroscopy Fellowship
Opportunity Reference Code: ICPD-2024-08

Organization Office of the Director of National Intelligence (ODNI)

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How to Apply **Create and release your Profile on Zintellect** – Postdoctoral applicants must create an account and complete a profile in the on-line application system. **Please note: your resume/CV may not exceed 3 pages.**

Complete your application – Enter the rest of the information required for the IC Postdoc Program Research Opportunity. The application itself contains detailed instructions for each one of these components: availability, citizenship, transcripts, dissertation abstract, publication and presentation plan, and information about your Research Advisor co-applicant.

Additional information about the IC Postdoctoral Research Fellowship Program is available on the program website located at: https://orise.orau.gov/icpostdoc/index.html.

If you have questions, send an email to ICPostdoc@orau.org. Please include the reference code for this opportunity in your email.

Application Deadline 2/28/2024 6:00:00 PM Eastern Time Zone

Description **Research Topic Description, including Problem Statement:**

Cheminformatics is a relatively new field of science that brings together chemistry, computer science, and data analysis, *1. While cheminformatics has seen significant applicability in drug discovery and pharmaceutical development, this may be only the tip of the iceberg in terms of how these tools could be used by researchers and the Intelligence Community. By harnessing the power of advanced analytical tools, such as AI and machine learning, cheminformatics enables researchers to predict molecular properties, design new compounds, and characterize those compounds in new and insightful ways.*2,*3,*4.

The pharmaceutical industry uses cheminformatics tools in drug discovery as described in the review article by Lawless, et al from 2016, *5. These models use chemical properties such as solubility, permeability, metabolic stability, and structure to determine likely candidates for particular bioactivities. Building on a similar framework, cheminformatics tools can be used to predict a number of molecular and spectral properties. Identification of novel materials, understanding the potential synthesis pathways for novel materials, and characterizing the spectra derived from novel materials are three types of information that can be time consuming and/or expensive to compile using traditional laboratory methods. Cheminformatics may be able to greatly improve the time and cost related to these tasks, *6.

A key aspect of all cheminformatics tools are the libraries of data they are able to pull from. Developing new methods, or augmenting existing methods, for parsing large and diverse datasets is a critical component of developing the cheminformatics tools of the future.

References:

1. Wishart DS. Introduction to cheminformatics. Curr Protoc Bioinformatics.

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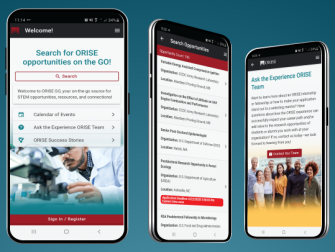
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2007 Jun; Chapter 14: Unit 14.1. doi: 10.1002/0471250953.bi1401s18. PMID: 18428788.
2. Deng, J., Yang, Z., Wang, H. et al. A systematic study of key elements underlying molecular property prediction. Nat Commun 14, 6395 (2023). DOI: 10.1038/s41467-023-41948-6.
3. Wu, Z., Wang, J., Du, H. et al. Chemistry-intuitive explanation of graph neural networks for molecular property prediction with substructure masking. Nat Commun 14, 2585 (2023). DOI: 10.1038/s41467-023- 38192-3.
4. Y. Chen, J. Kirchmair. Cheminformatics in Natural Product-based Drug Discovery. Mol. Inf. 2020, 39, 2000171.
5. Lawless MS, Waldman M, Fraczkiewicz R, Clark RD. Using Cheminformatics in Drug Discovery. Handb Exp Pharmacol. 2016;232:139-68. doi: 10.1007/164_2015_23. PMID: 26318607.
6. Ljoncheva, M., Stepisnik, T., Dzeroski, S. et al. Cheminformatics in MS-based environmental exposomics: Current achievements and future directions. Trends in Env. Analytical Chem 28, e00099 (2020). DOI: 10.1016/j.teac.2020.e00099.

Example Approaches:

Researchers seeking to reply to this topic should seek to develop new cheminformatics tools or apply currently existing tools to new applications, such as:

- Prediction of chemical structure of novel materials
- Prediction of synthesis pathways for novel materials
- Novel methods for spectral modeling of existing materials
- Characterization of molecular properties through computational methods

Through these studies, it is hoped that the academic and intelligence communities will have an enhanced understanding of what is possible through cheminformatics and how to apply these tools to new and evolving threat materials. While the focus of the effort should be on computational chemistry and modeling tools, collaboration with experimental scientists and/or laboratories is encouraged.

Relevance to the Intelligence Community:

The S&T priority AI and Machine Learning directly aligns with this research topic.

– Develop/enhance agile, scalable, accessible, and reliable methods of processing disparate data. (Category Zero)
– Develop/enhance capabilities to flag anomalies within massive data sets (Category Zero)
– Develop/enhance understanding of global dual-use technologies that may be used for chemical, biological, radiological, and nuclear weapons programs. (Category One)
– Develop/enhance methods to discriminate offensive biological activities from defensive programs or other non-offensive research (Category Two).

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– Develop/enhance methods to detect, assess, and/or evaluate current and emerging threats that cause death, disease, or other biological malfunction of the neurological system. (Category Two)
– Develop/enhance capabilities to detect and identify chemical agents, and associated delivery systems (Category Two) 2N051 – Develop/enhance detection and monitoring of chemical weapon program activities, including Schedule 1 chemicals or precursors (Category Two)
– Develop/enhance detection capabilities to identify chemical weaponization (Category Two)

Key Words: cheminformatics, chemoinformatic, computational chemistry, chemical sensing, predictive modeling, spectral modeling, molecular modeling, chemical structure, data mining, mathematical modeling, database development

Qualifications

Postdoc Eligibility

- U.S. citizens only
- Ph.D. in a relevant field must be completed before beginning the appointment and within five years of the appointment start date
- Proposal must be associated with an accredited U.S. university, college, or U.S. government laboratory
- Eligible candidates may only receive one award from the IC Postdoctoral Research Fellowship Program

Research Advisor Eligibility

- Must be an employee of an accredited U.S. university, college or U.S. government laboratory
- Are not required to be U.S. citizens

Eligibility Requirements

- **Citizenship:** U.S. Citizen Only
- **Degree:** Doctoral Degree.
- **Discipline(s):**
  - **Chemistry and Materials Sciences** (12)
  - **Communications and Graphics Design** (4)
  - **Computer, Information, and Data Sciences** (17)
  - **Earth and Geosciences** (21)
  - **Engineering** (27)
  - **Environmental and Marine Sciences** (14)
  - **Life Health and Medical Sciences** (45)
  - **Mathematics and Statistics** (11)
  - **Other Non-Science & Engineering** (2)
  - **Physics** (16)
  - **Science & Engineering-related** (1)
  - **Social and Behavioral Sciences** (30)