

## Department of Civil Engineering Seminar

# Big data, AI and intelligent modeling for modern computational toxicology

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**Friday November 15, 2019, 12:45-1:45PM @ Bingham 103**  
**Lunch and discussion at 12:00PM at Bingham 102 (Vose Room)**

### Abstract

Addressing the safety aspects of new chemicals has historically been undertaken through animal testing studies, which are expensive and time-consuming. Alternative models, such as those based on high-throughput screening (HTS) techniques, lowered the toxicity testing cost but were not able to provide reliable evaluations of chemical toxicity *in vivo*. Due to the massive available data for known chemicals, modern toxicology has been advanced to the “big data” era. Central to this shift is the development of artificial intelligence approaches to implementing innovative modeling based on the dynamic, heterogeneous, and large nature of public toxicity data sets. As a result, our recently developed artificial intelligence approaches and relevant modeling studies answered this challenge by providing new solutions to chemical toxicity evaluations based on big data modeling and mechanistic analysis. The resulted read-across study provided deep insights to the continuum from chemical structure, *in vitro*, to animal toxicity outcomes. The relevant novel big data mining, analysis, and modeling techniques provided critical support to the recent toxicity read-across studies. In summary, the new advancement of artificial intelligence in the big data era has paved the road to future computational toxicology, which will have a significant impact on the risk assessment procedure and eventually public health.

**About the speaker:** Dr. Hao Zhu is an Associate Professor and Graduate Program Director in the Department of Chemistry, as well as a member of the Rutgers Center for Computational & Integrative Biology at Rutgers University at Camden. His major research interest is to use cheminformatics tools to develop predictive toxicity models and design biocompatible biomaterials. His pioneering research of using big data modeling in the computational toxicology studies has attracted great attentions from research communities. Dr. Zhu is author/co-author of 69 publications in the fields of cheminformatics, computational toxicology, medicinal chemistry and biomaterials, including 63 peer-reviewed articles, one book and five book chapters (Total citations ca. 3,000 and h-index = 29). Dr. Zhu has been a NIEHS grant awardee since 2013. His recent computational toxicology paper (*Environ. Health Perspect.* 2019, (127) 47001) was featured as NIEHS Extramural Paper of the Month (June, 2019). Dr. Zhu gave over 30 oral presentations worldwide, including several keynote seminars in international conferences.

