Center for Molecular Spectroscopy and Dynamics, IBS-Korea University

IBS Center for Molecular Spectroscopy and Dynamics

Seminar

- **SPEAKER**
  Prof. Jinhee Choi (University of Seoul)

- **TITLE**
  Artificial intelligence-based toxicity prediction of environmental chemicals: Perspective in next generation risk assessment

- **ABSTRACT**
  Recently, research on the development of artificial intelligence (AI)-based computational toxicology models that predict toxicity without the use of animal testing has emerged, because of the rapid development of computer technology. Various computational toxicology techniques that predict toxicity based on the structure of chemical substances are gaining attention, including the quantitative structure–activity relationship. Based on a systemic review of recent publications, we found that AI models have been developed to predict approximately 30 different toxicity endpoints using more than 20 toxicity databases. For model development, molecular access system and extended-connectivity fingerprints are the most commonly used molecular descriptors. The most used algorithm among the used machine learning techniques is the random forest, while the most used algorithm among deep learning techniques is a deep neural network. The use of AI technology in the development of toxicity prediction models is a new concept that will aid in achieving a scientific accord and meet regulatory applications. To understand the recent development of AI-based toxicity prediction models, in this seminar I will introduce the current status of databases, molecular descriptors and fingerprints, and algorithms used in recent studies for the development of toxicity prediction models. I will also introduce a toxicity prediction studies based on the pathway of toxicity that are being carried out in our group. The comprehensive overview provided in this seminar will provide an insight for the further development of toxicity prediction models as well as their application in next generation risk assessment.

- **DATE AND VENUE**
  March 30, 2022 (Wednesday, 16:00 - 17:00)
  Virtual Seminar

- **LANGUAGE**
  Korean

- **INVITED BY**
  Dr. Jin-Sung Park