

## **Class Discussion and Assessment on Topic #3: How Can We Responsibly Use AI in Chemistry?**

### **Description**

- Predictive Interactions
  - Quantitative Structure-Activity Relationships (QSAR)
  - Quantitative Structure-Property Relationships (QSPR)
- Nature Journal and Chemical Intelligence articles as background
- Need for (Large) Datasets to train AI
- Must Recognize All Variables
- Use of AI to generate training materials for new researchers?

### **Assessment #3**

- Dropbox document (one-page) outlining an experiment or series of assays they believe would be a good candidate for AI-assisted analysis.
- Discuss some challenges they may face in applying the AI to the problem.
- Role-play based on Integrated research component
  - City Planner, Facilities workers, Budget officer, Public (Consumer), Property owners, Environmental advocate
  - Peer evaluation of roles in each group

### **Wrapping Up**

- As part of review for the final exam, have an in-class discussion about the ethical use of AI and responsible application.
- Potentially include some questions on the exam.
- Encourage students to keep 'playing' with AI and seeing what various models can and cannot do, and where they get their training data from.