# 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.

- Post-test evaluation and comparison with pre-test.