NIH SciEd24

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| **Project Name:** Adventures in Drug Discovery: Integrating Data Science into the Science Curriculum | |
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| Website: https://intofuture.org/aims.html | **If SEPA project, URL for project on https://nihsepa.org/**<br>https://nihsepa.org/project/adventures-in-drug-discovery-integrating-data-science-into-the-science-curriculum/ |

**Brief Program Description (50 – 60 words)**

In this project, the Institute for Future Intelligence (IFI) and the University of Florida (UF) will collaborate with diverse high schools in several states to develop innovative educational technologies and curriculum materials to help teachers and students teach and learn data science as a method for accelerating scientific inquiry and engineering design in the field of drug discovery.

## Program and Participant Characteristics

**Program type** (Please check all that apply):

☑ Curriculum. __ Out-of-school program

__ Exhibit ☑ Interactive multimedia

☑ Teacher PD

__ Research experiences for students or teachers

__ Other (describe):

**Setting(s):** ☑ Formal ___Informal

**Types of participants**

☑ Students ☑ Teachers __ Scientists

__ Families __ Public

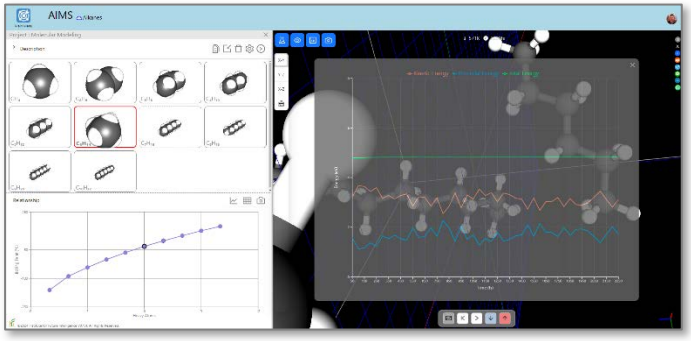
__ Other (describe):

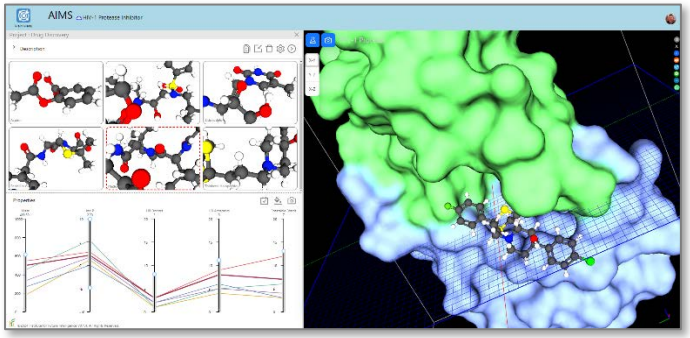
**Grade level(s) of participants**

__ PreK __ Elementary (K-5) __ Middle (6-8)

☑ High (9-12) __ Adult

**Characteristics of the populations you serve relative to DEIA:** General population




## Program Activities

Data science and chemical science can be meaningfully integrated and mutually enhanced if students can make sense of chemical data with molecular models (i.e., connecting bits and atoms). This project is developing an integrated learning platform to infuse data science into the high school science curriculum. This Web-based platform, called *Artificial Intelligence for Molecular Sciences* (AIMS), combines data science and computational science to create visual and interactive scientific inquiry and engineering design tools to empower student learning at the strategically important intersection between data science and molecular sciences.

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## Evaluation

### Constructs measured

☑ Content knowledge ☑ Skills

☑ Nature of science ☑ Career awareness

☑ Attitudes (e.g., interest, identity, belonging)

☑ Quality or fidelity of implementation

__ Other (describe):

### Methods

☑ Tests/surveys ☑ Interviews/focus groups

☑ Observations ☑ Artifacts (e.g., student work)

__ Other (describe):

### Design characteristics

☑ Comparison or control group

☑ Pre/post surveys or assessments

__ Longitudinal tracking of participants

__ Other (describe):

## Project Lessons Learned

The Web-based AIMS platform has turned out to be a successful proof-of-concept, paving the way for this kind of interactive and visual learning technology to reach a vast number of science classrooms (compared with existing cheminformatics and bioinformatics tools developed mainly for professional scientists).

## Key Accomplishments and/or Findings

As this project is still in the first year, there are no findings from a classroom-based study yet. The key accomplishments are:

- Developed a beta version of the AIMS platform to support the integration of data science and molecular sciences.
- Outlined instructional units to infuse data science into chemistry and biology as tools to enhance scientific inquiry and engineering design.
- Recruited five high school science teachers to participate the design-based research as co-designers.

An example of scientific accomplishment:

Equipped with the power of interactive molecular dynamics simulations, AIMS allows students to design and conduct computational experiments to check data science results to close the loop of scientific inquiry. For example, students can build a quantitative structure-property relationship (SQPR) model using machine learning to predict the boiling points of higher alkanes (a well-known example widely used in chemistry education). To explain the relationship, they can then create molecular models of different alkanes and perform molecular dynamics simulations to observe how they boil when temperature is increased. Visualization of van der Waals interactions among the molecules shown in the first figure on Page 1 can draw their attention to the chemical origin of higher boiling points for higher alkanes. Students can also explore similar hydrocarbon families such as cycloalkanes and acenes to test the generalizability of their findings.

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## Questions, Advice Wanted, or Topics of Discussion for the SciEd Community (optional)