

MOLECULE  
MAKER LAB  
INSTITUTE



# MOLECULE MAKER LAB INSTITUTE (MMLI) INDUSTRIAL PARTNERSHIP PROGRAM

*MANY OF THE GREATEST CHALLENGES FACING SOCIETY TODAY LIKELY HAVE MOLECULAR SOLUTIONS THAT AWAIT DISCOVERY.*

The MMLI is an interdisciplinary initiative with leaders in AI and organic synthesis collaborating to create frontier AI tools, dynamic open access databases, and fast and broadly accessible small molecule manufacturing and discovery platforms. The MMLI is a collaboration between the **University of Illinois-Urbana Champaign**, **Rochester Institute of Technology**, and **Pennsylvania State University**. The MMLI is an AI Institute for Molecular Discovery, Synthesis Strategy, and Manufacturing supported by the National Science Foundation.

## Innovations:

- **Digital Molecule Maker:** Education tool for building molecules using Lego-like virtual molecular blocks.
- **AlphaSynthesis (CLEAN, ChemScraper, and Mollie):** Research platform of click-and-go AI tools for molecule synthesis with a user-friendly interface containing tutorials and example data.

## Impact:

- Over 1,900 students reached through curriculum and outreach activities.
- 7,600+ prediction tasks processed on the **CLEAN** tool in 4 months.
- **AI tools** for identifying how structural components of kinase inhibitors could impact blood brain barrier penetration.



**Johnson & Johnson**  
Innovative Medicine

**LanzaTech**



**IBM**

**abbvie**

**AMGEN**

# OUR EXPERTISE

The MMLI has brought together a world-leading team of researchers with highly complementary expertise in AI and ML, chemical and biological catalysis, enzyme engineering, materials synthesis and characterization, and outreach and workforce development.

## TECHNICAL CAPABILITIES

- Cyberinfrastructure for creating and maintaining databases at the National Center for Supercomputing Applications
- Molecule Maker Lab in the Beckman Institute
- Automated synthesizers
- Illinois Biological Foundry for Advanced Biomanufacturing (iBioFAB)



## INFRASTRUCTURE

- Advanced ML algorithms for catalyst discovery, molecular function prediction, and process optimization
- Advanced text and image mining tools for data curation and knowledge extraction
- Advanced synthesis planning tools
- Dynamic databases of chemical and biological reactions
- A Lego-like platform for small molecule synthesis
- Rapid biocatalyst discovery, engineering, and optimization

## OUR RESEARCH

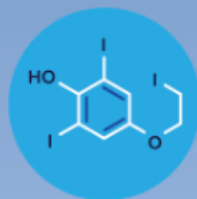


Thrust 1: AI-Enabled Synthesis Planning

Thrust 2: AI-Enabled Catalyst Development



Thrust 4: AI-Enabled Molecule Discovery



Thrust 3: AI-Enabled Molecule Manufacturing



Thrust 5: Education and Workforce Development

# INDUSTRIAL PARTNERSHIP PROGRAM

The goal of the MMLI Industrial Partnership Program is to provide the opportunity for the two-way exchange of information between the MMLI and industry researchers. This program is a way for MMLI researchers to share the tools and databases being developed for more efficient synthesis and discovery of chemical and materials for a wide-range of applications. Industry researchers can provide perspective on which projects will most benefit society.

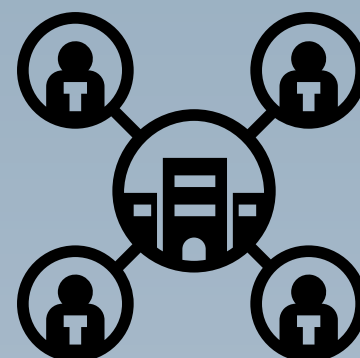
## ADD ON | ALL LEVELS



- Personalized collaborations with MMLI researchers.
- Option to hand off projects, work hand-in-hand, or utilize MMLI resources.
- Cost varies based on requested experience.

## ASSOCIATE LEVEL MEMBERS | \$10,000

- Advanced ML algorithms for catalyst discovery, molecular function prediction, and process optimization
- Advanced text and image mining tools for data curation and knowledge extraction
- Advanced synthesis planning tools
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- A Lego-like platform for small molecule synthesis
- Rapid biocatalyst discovery, engineering, and optimization



## ADDITIONAL BENEFITS FOR PARTNER LEVEL MEMBERS | \$50,000

### All of the above PLUS:

- Non-exclusive, royalty-free non-commercial license of materials developed under the seed grant program
- Quarterly meetings on Zoom to exchange research ideas with MMLI researchers
- A role in selecting which proof-of-concept projects are funded from the seed grant program



## GET STARTED:

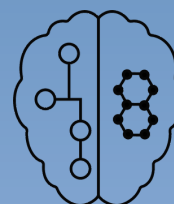
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