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Gormley Lab
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Machine Learning Directed Design of Polymer-Protein Hybrids

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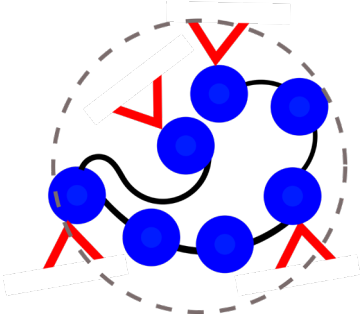
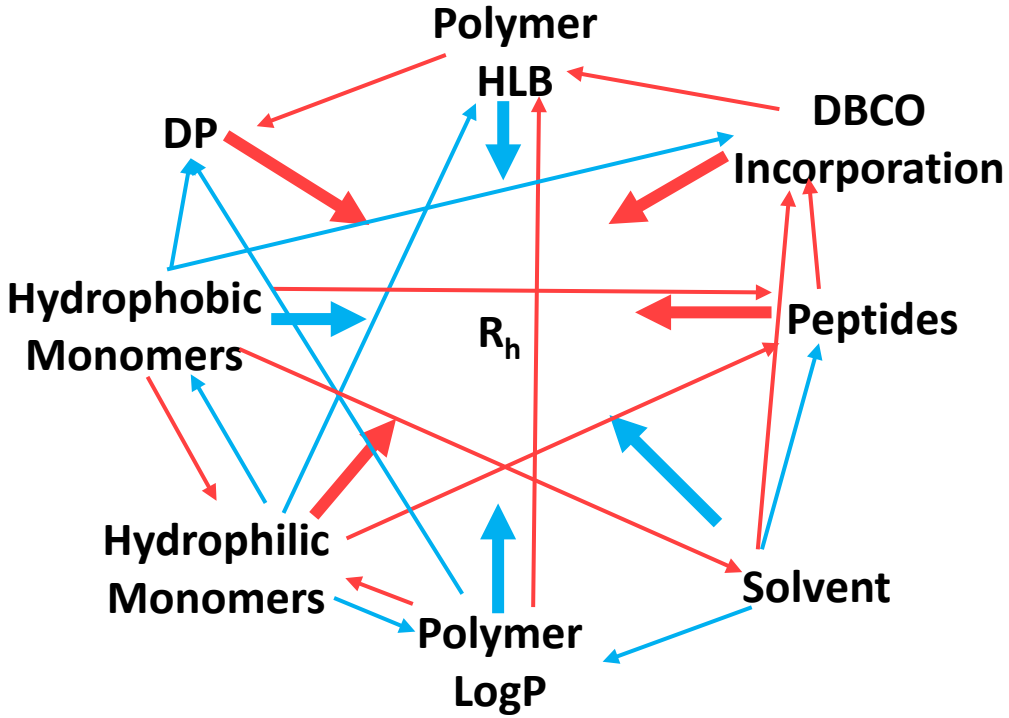
AI+Big Data Session, Controlled Release Society (CRS) 2022 Annual Meeting & Expo

The Curse of Dimensionality

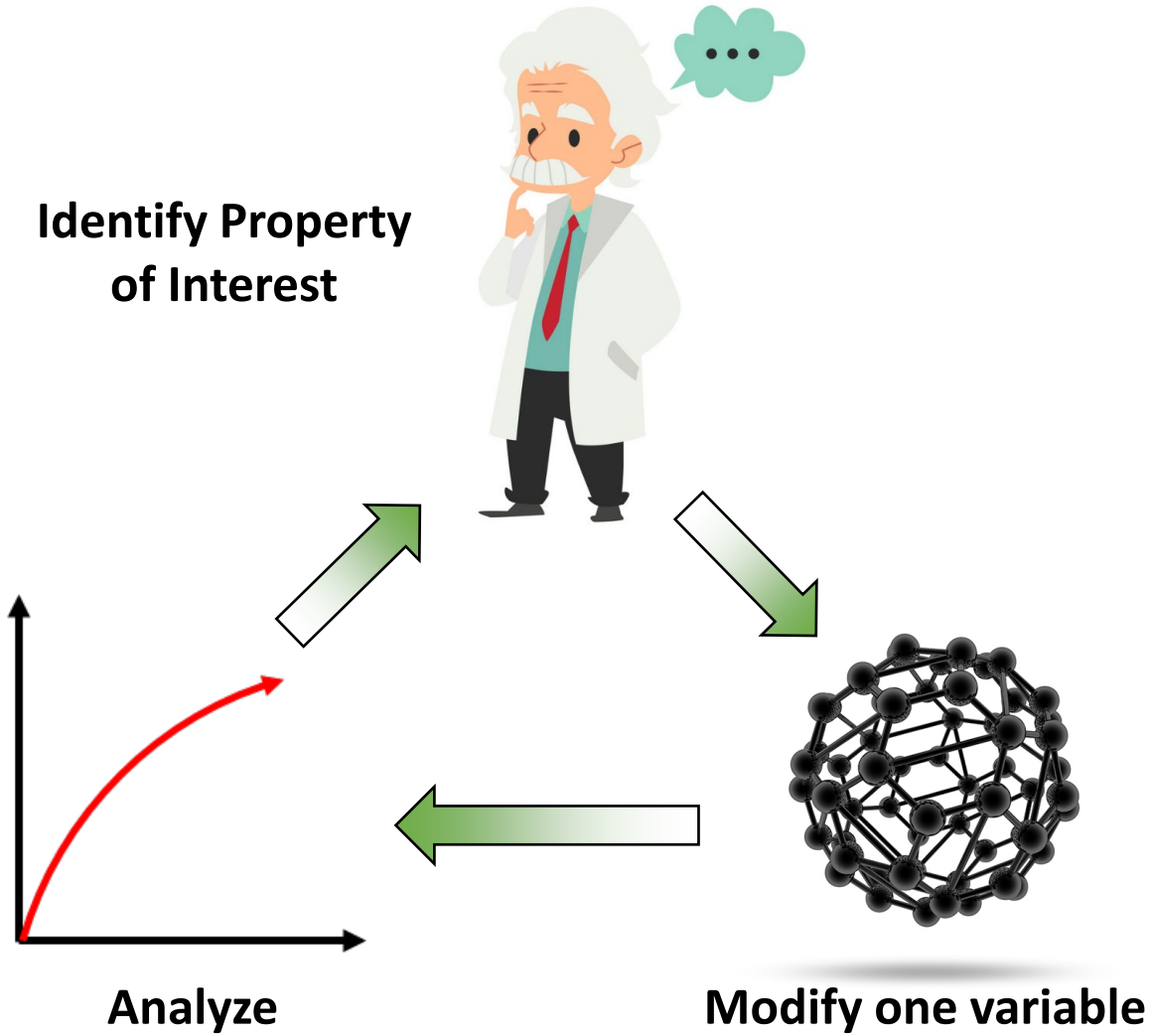


Protein Inspired
Single-Chain Polymer
Nanoparticles

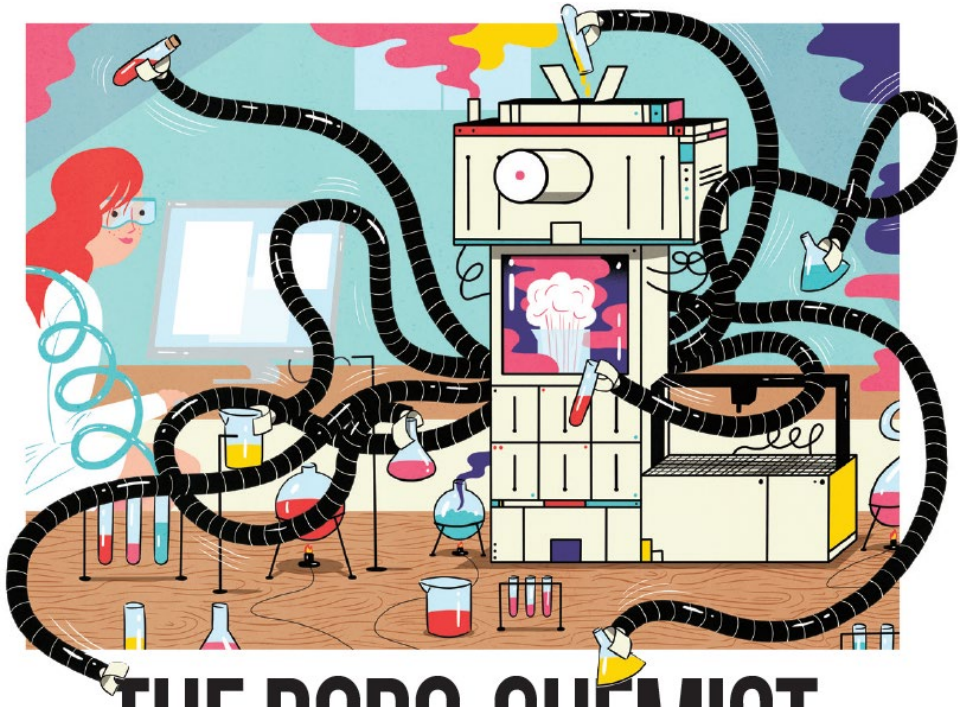


Many interacting parameters challenge
the discovery process

Identify Property
of Interest



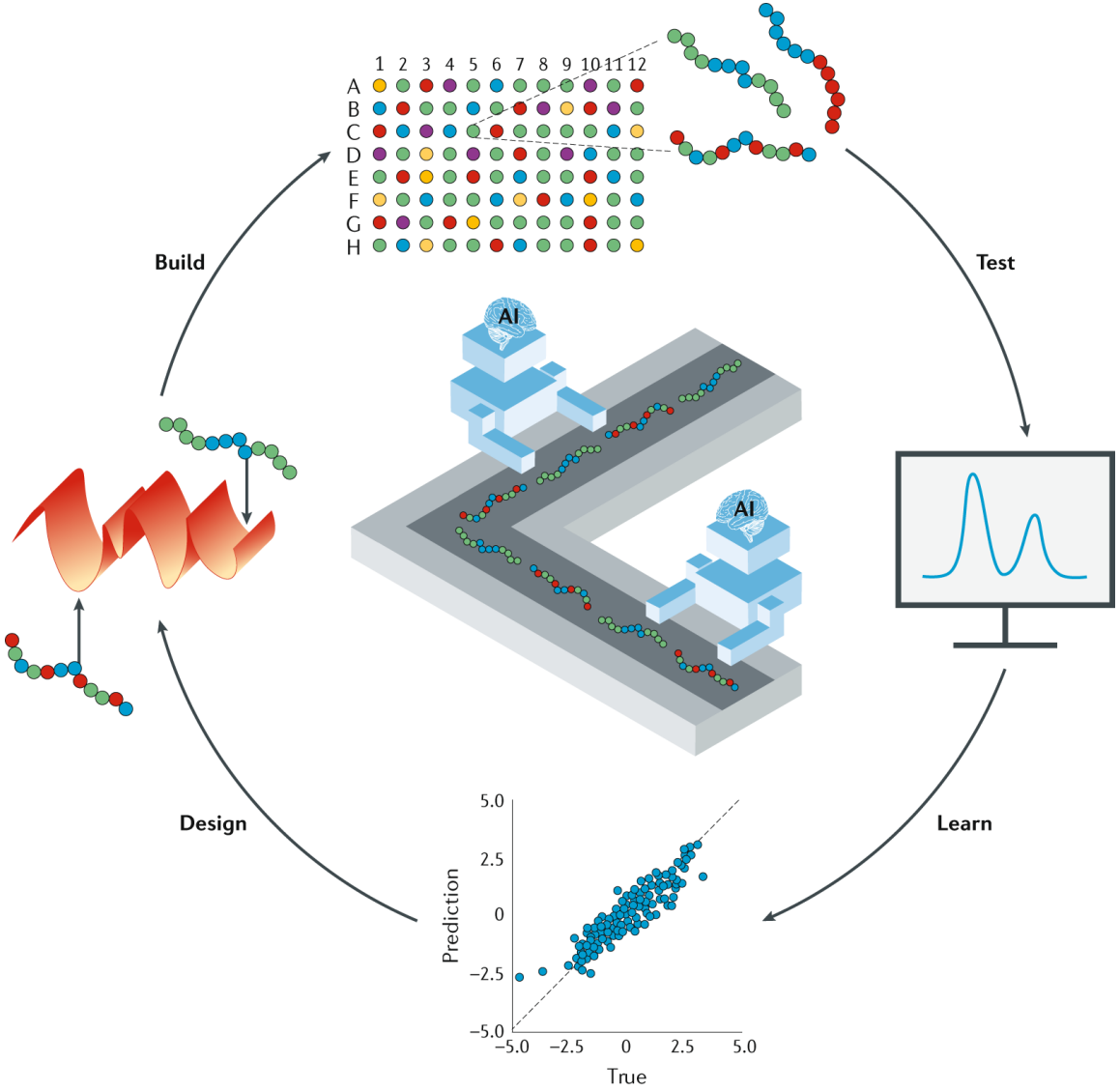
AI and Robotics for Autonomous Material Discovery



THE ROBO-CHEMIST

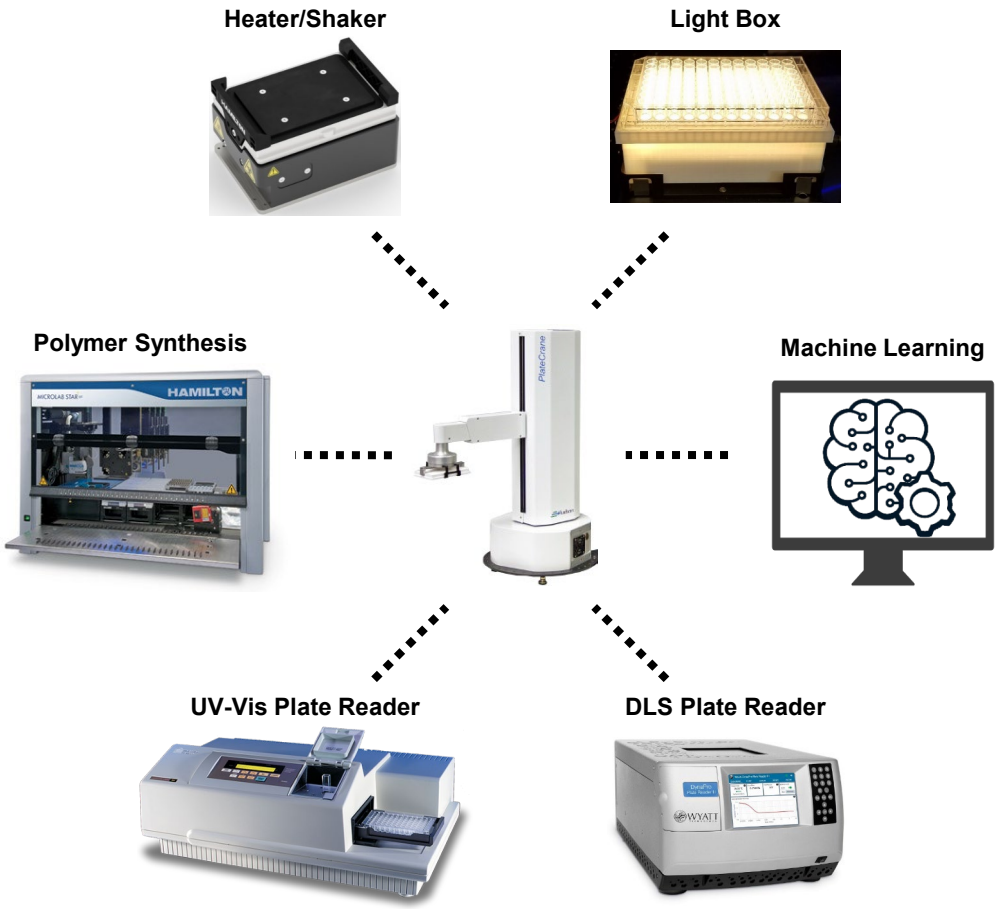
The race is on to build a machine that can synthesize any organic compound. It could transform chemistry.

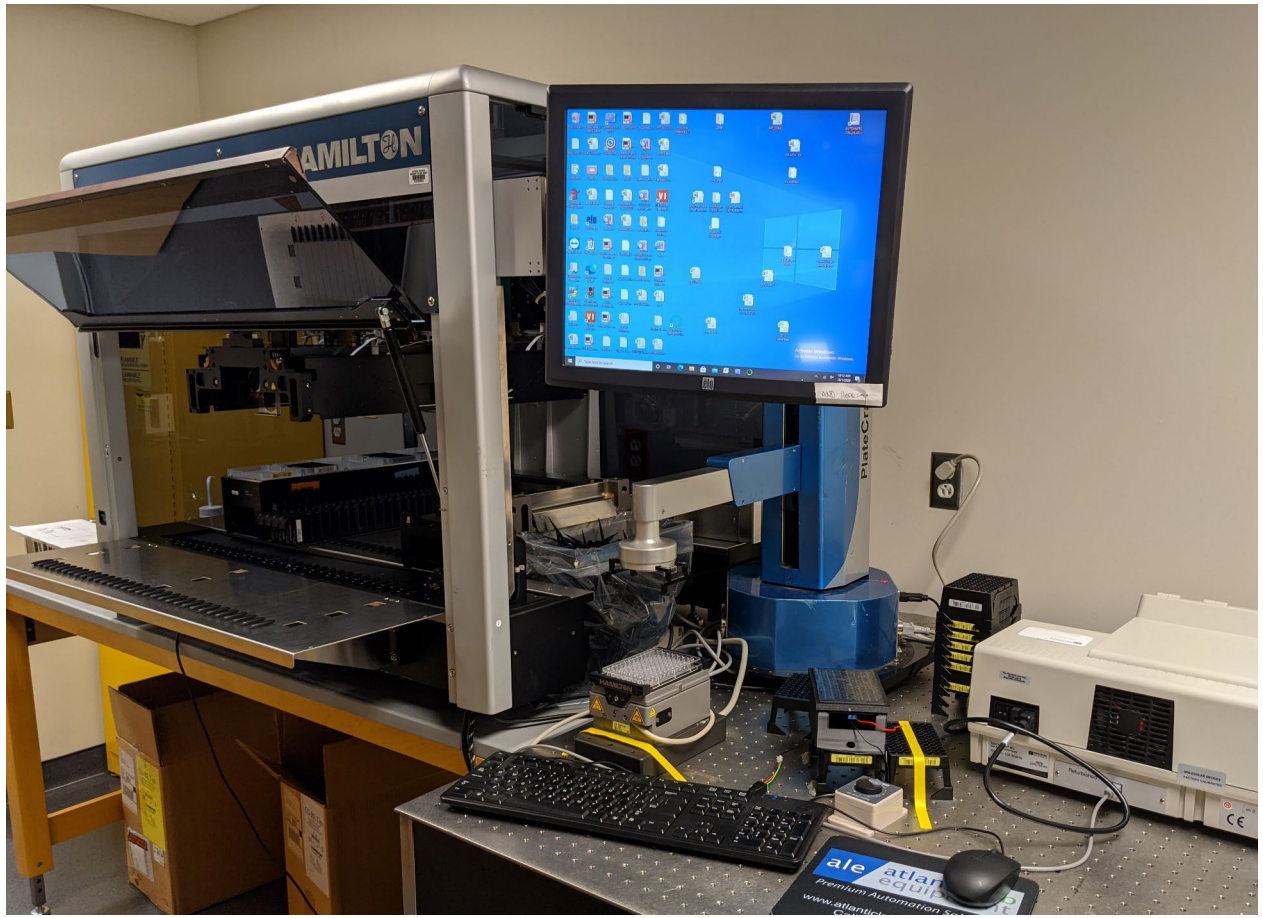
Peplow, M., 2014. **Nature News**, 512 (7512), 20



A.J. Gormley & M.A. Webb, 2021. **Nature Reviews Materials,** 6: 642-644.

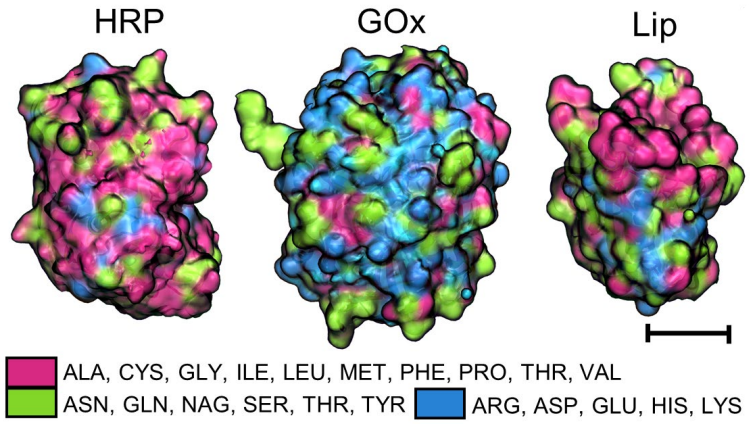
Developments Towards a Self-Driving Lab

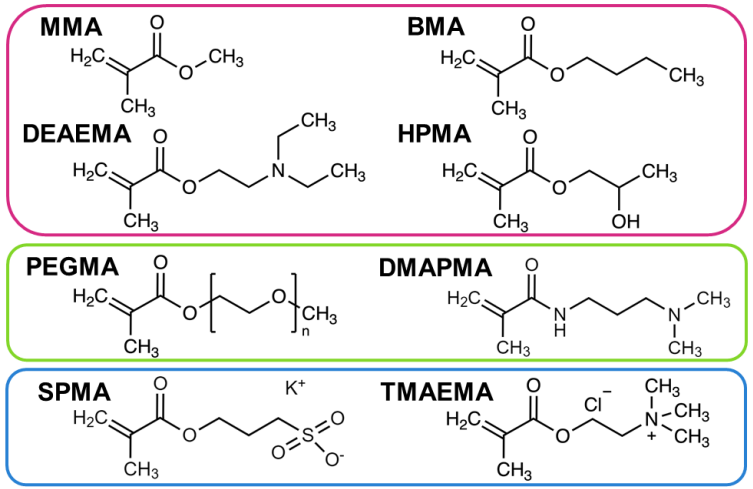




We have closed the hardware and software loop for a fully automated discovery workflow using a custom-built Python interface

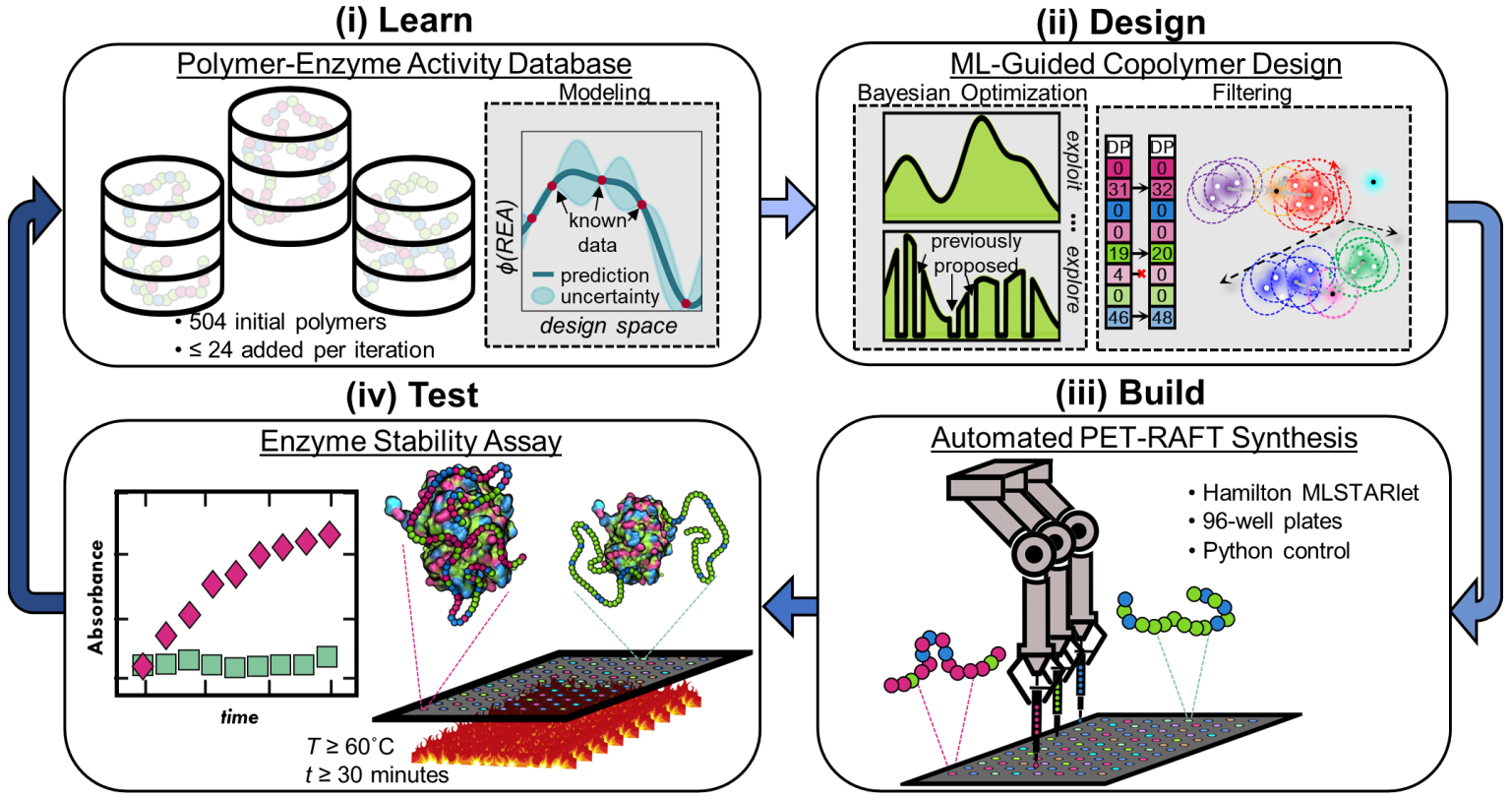
Active Learning Discovery Pipeline





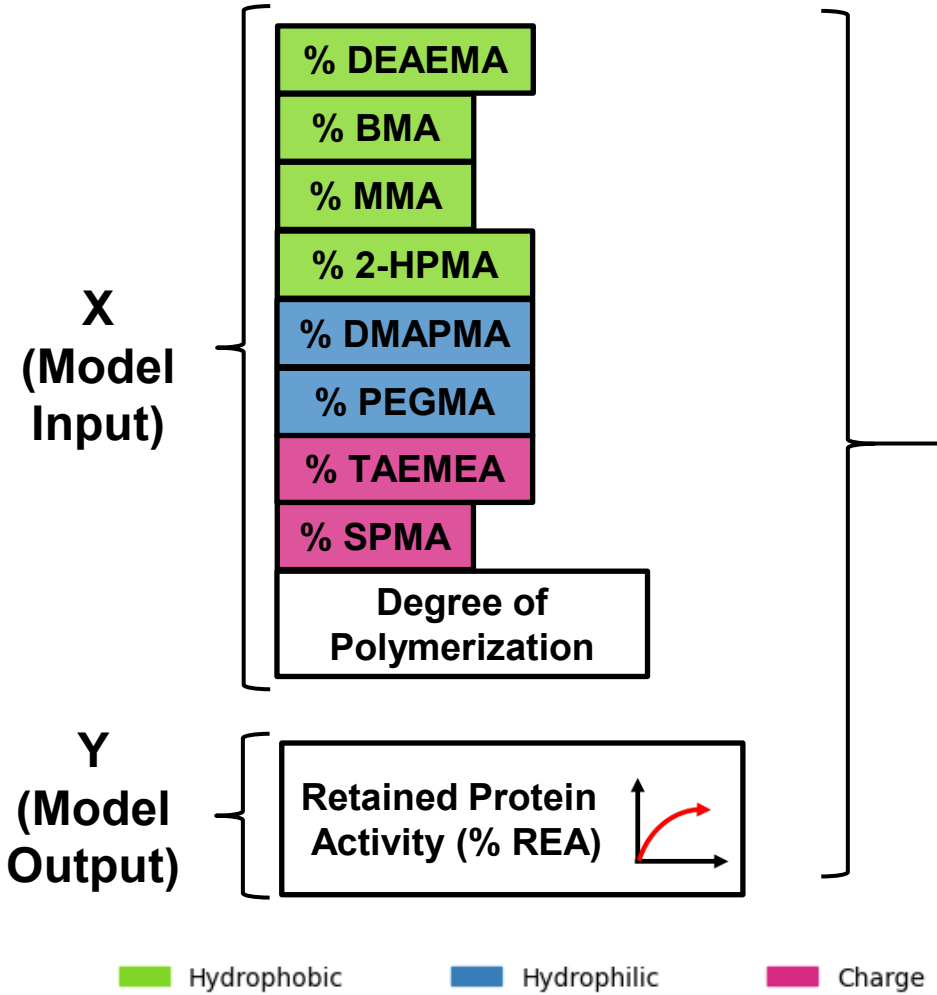
We utilized an iterative learning approach to inform the design of polymer-protein hybrids from direct experimental data.

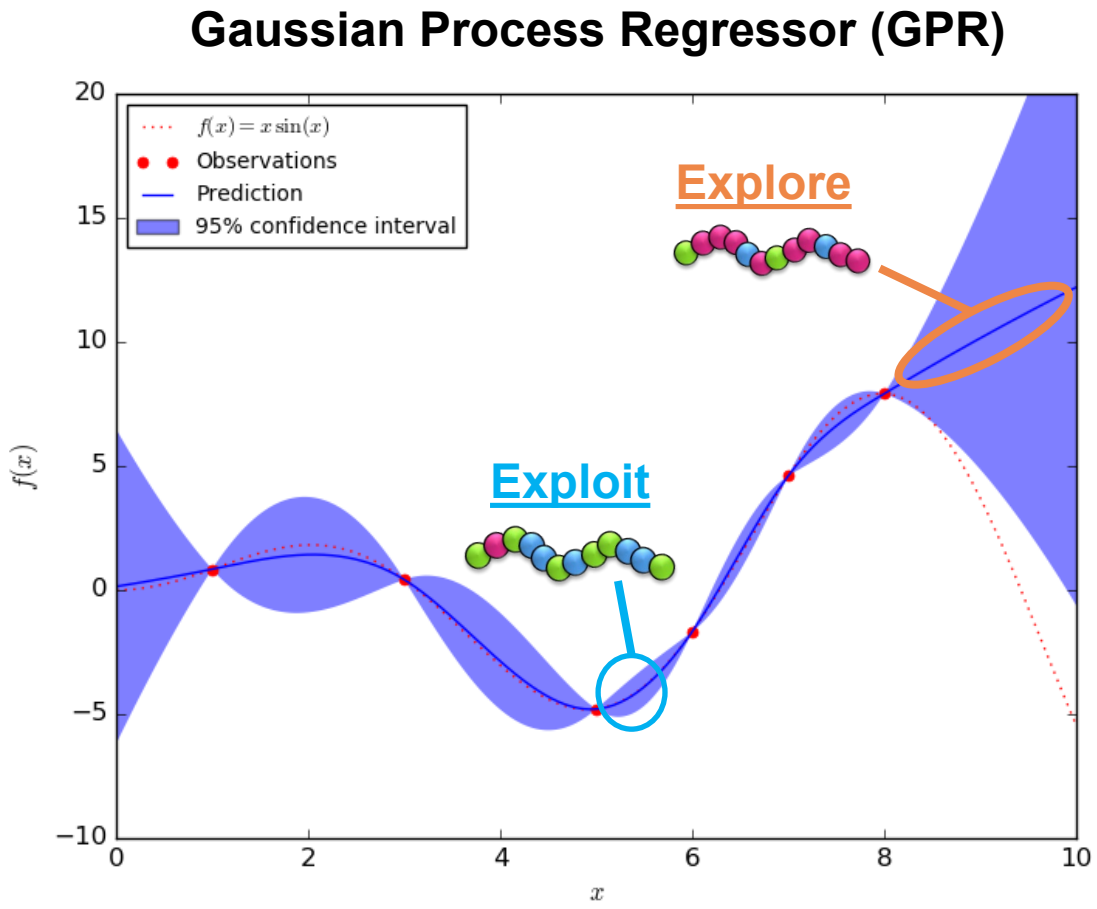
Matt Tamasi



Tamasi, M., et al, Machine learning on a robotic platform for the design of polymer-protein hybrids. **Advanced Materials**. 2201809. DOI: 10.1002/adma.202201809

Explore and Exploit to Find New Polymer Designs





We can use GPR to simultaneously **"exploit"** high performing chemistries, and **"explore"** unknown chemistry intelligently

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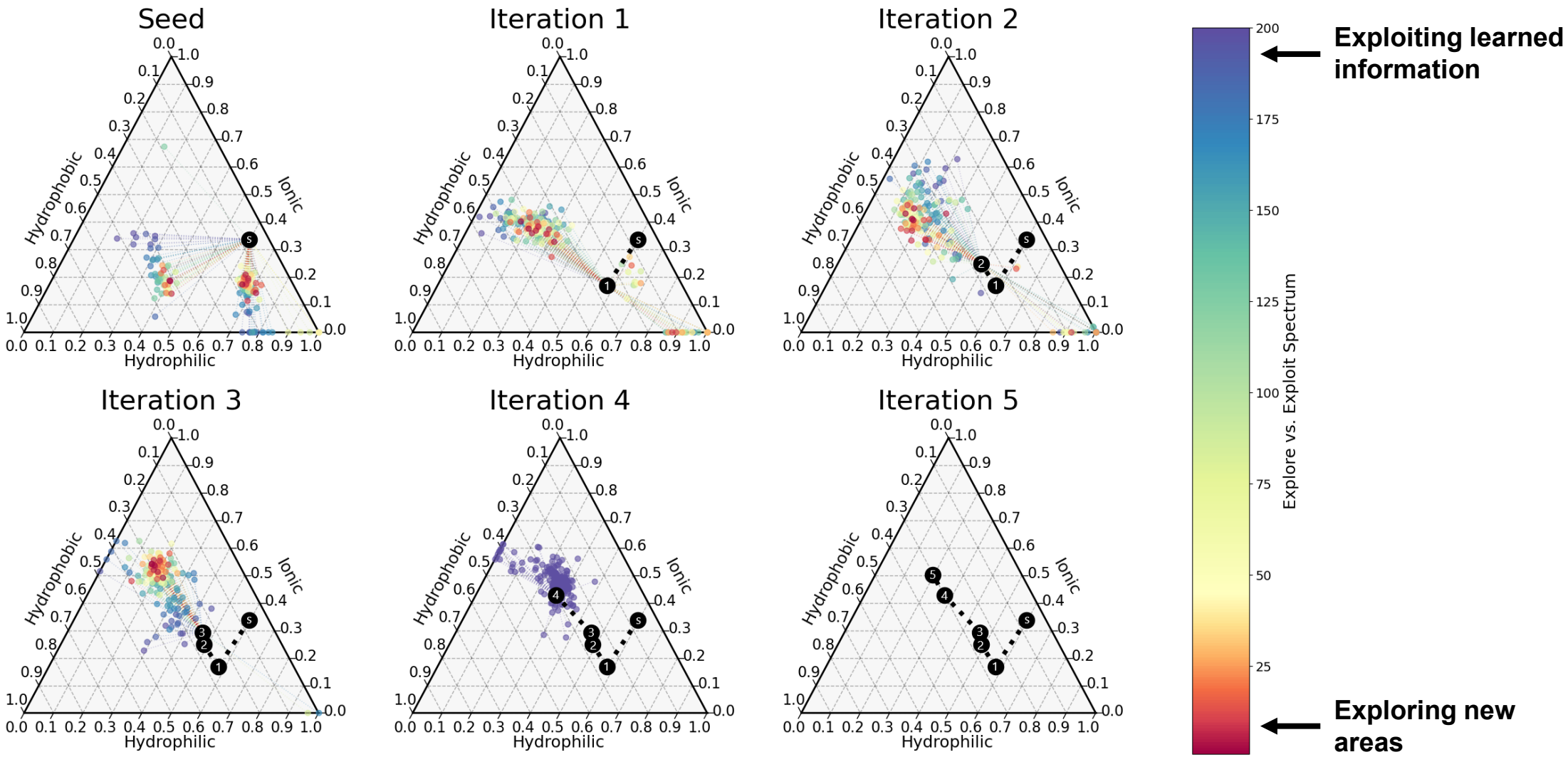
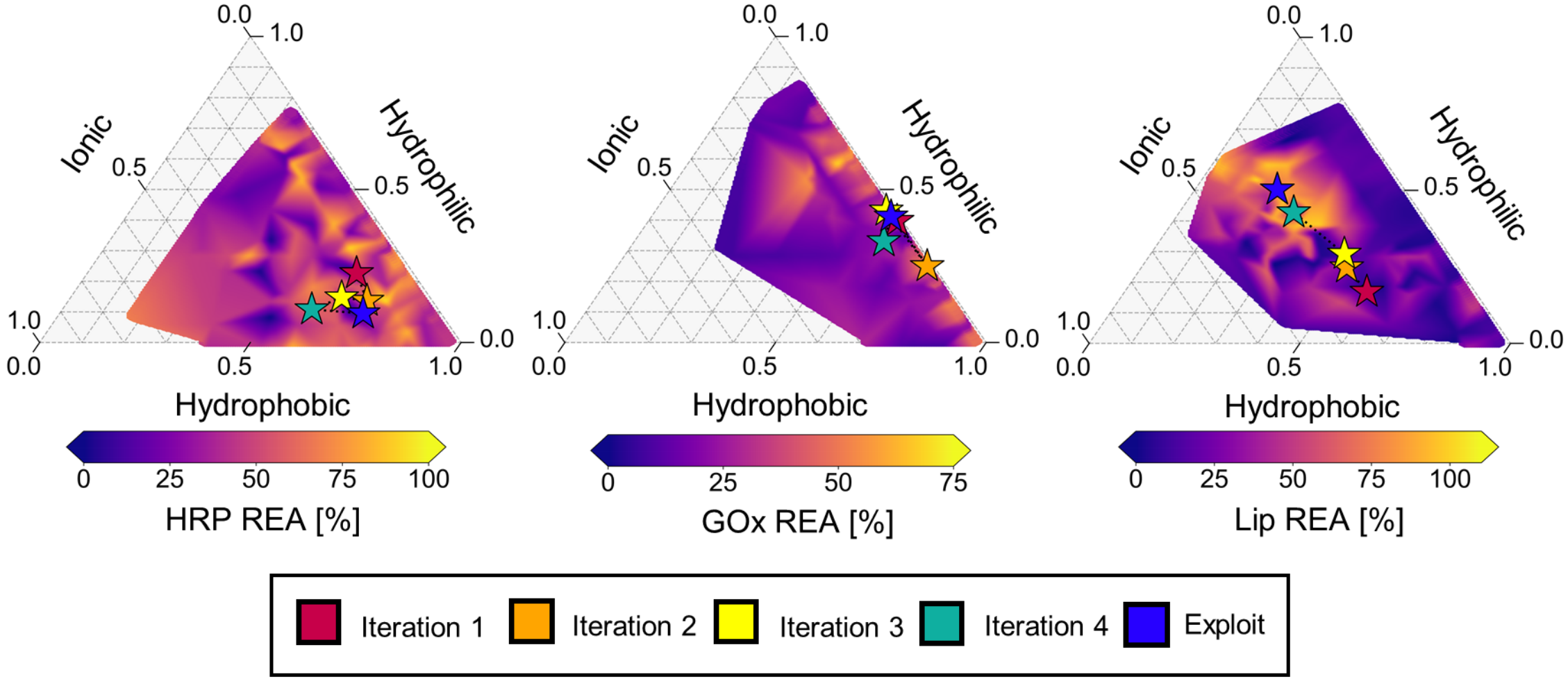
Active Learning Through Chemical Space



75% Exploration / 25% Exploitation

Tamasi, M., et al, Machine learning on a robotic platform for the design of polymer-protein hybrids. **Advanced Materials**. 2201809. DOI: 10.1002/adma.202201809

Fully Mapped Structure-Activity Profiles



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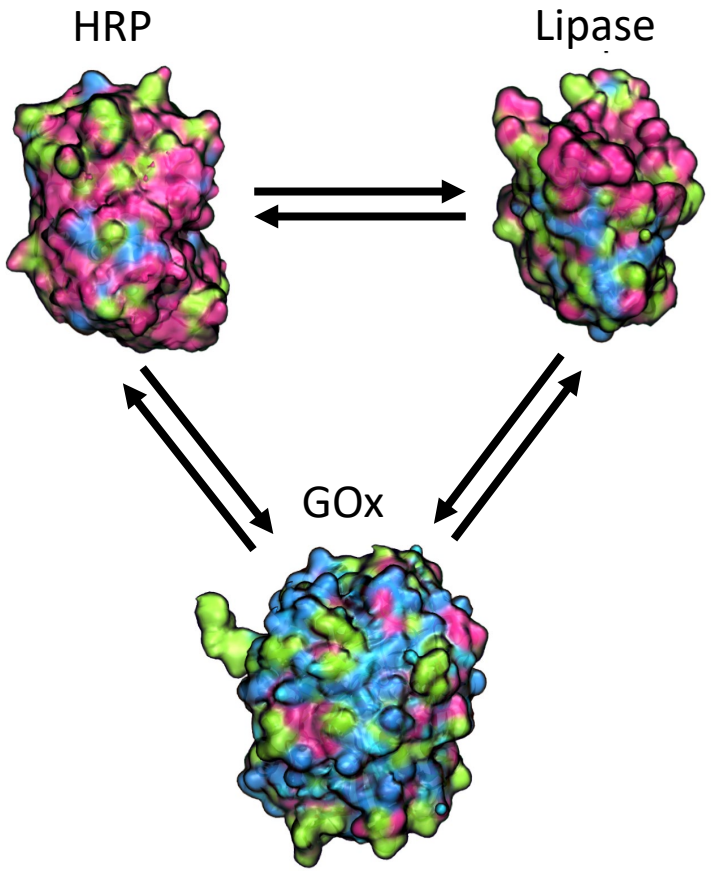
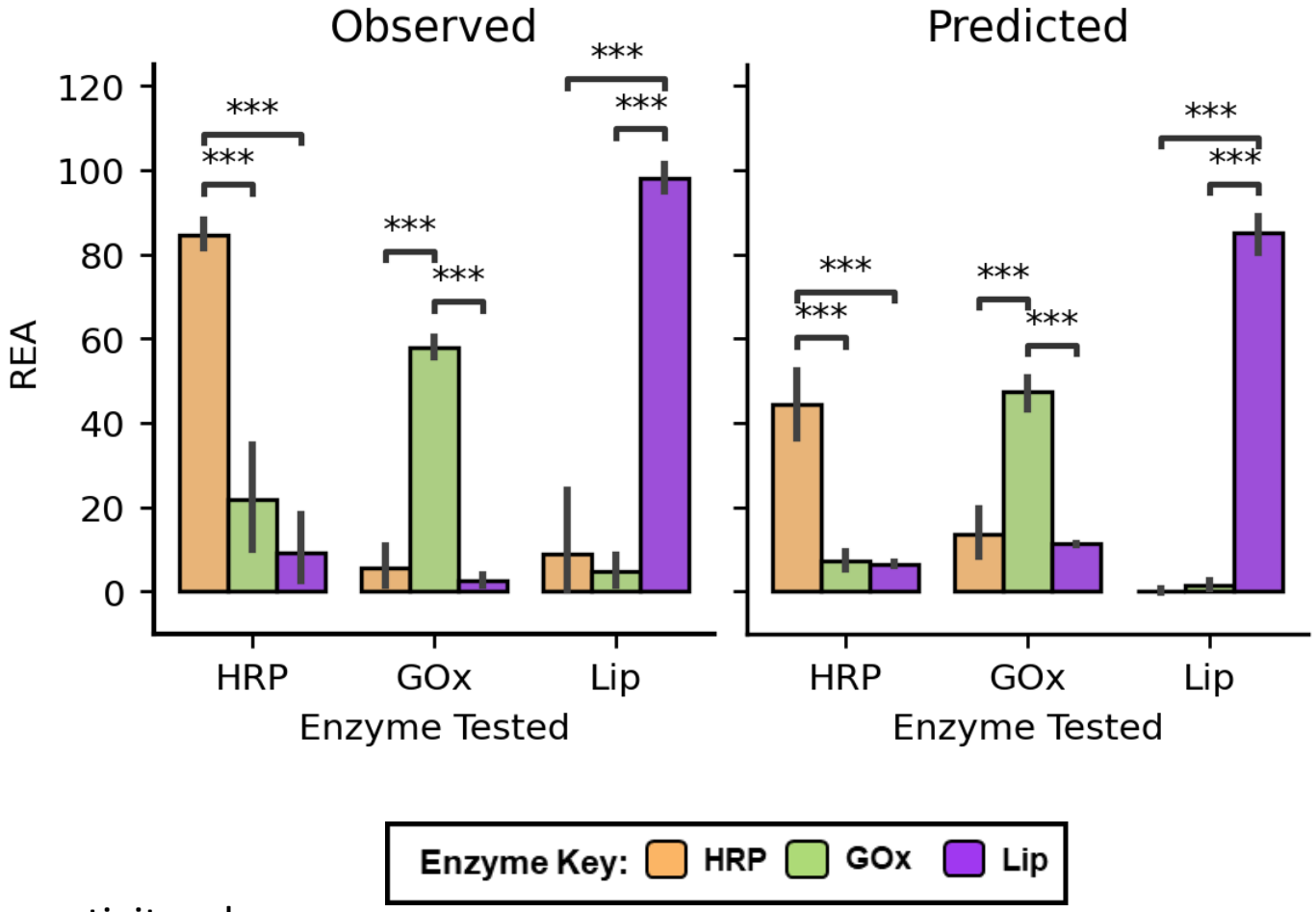
Interactions are Highly Specific





Polymers were highly enzyme specific with little cross-activity when paired with an enzyme outside of the design intention

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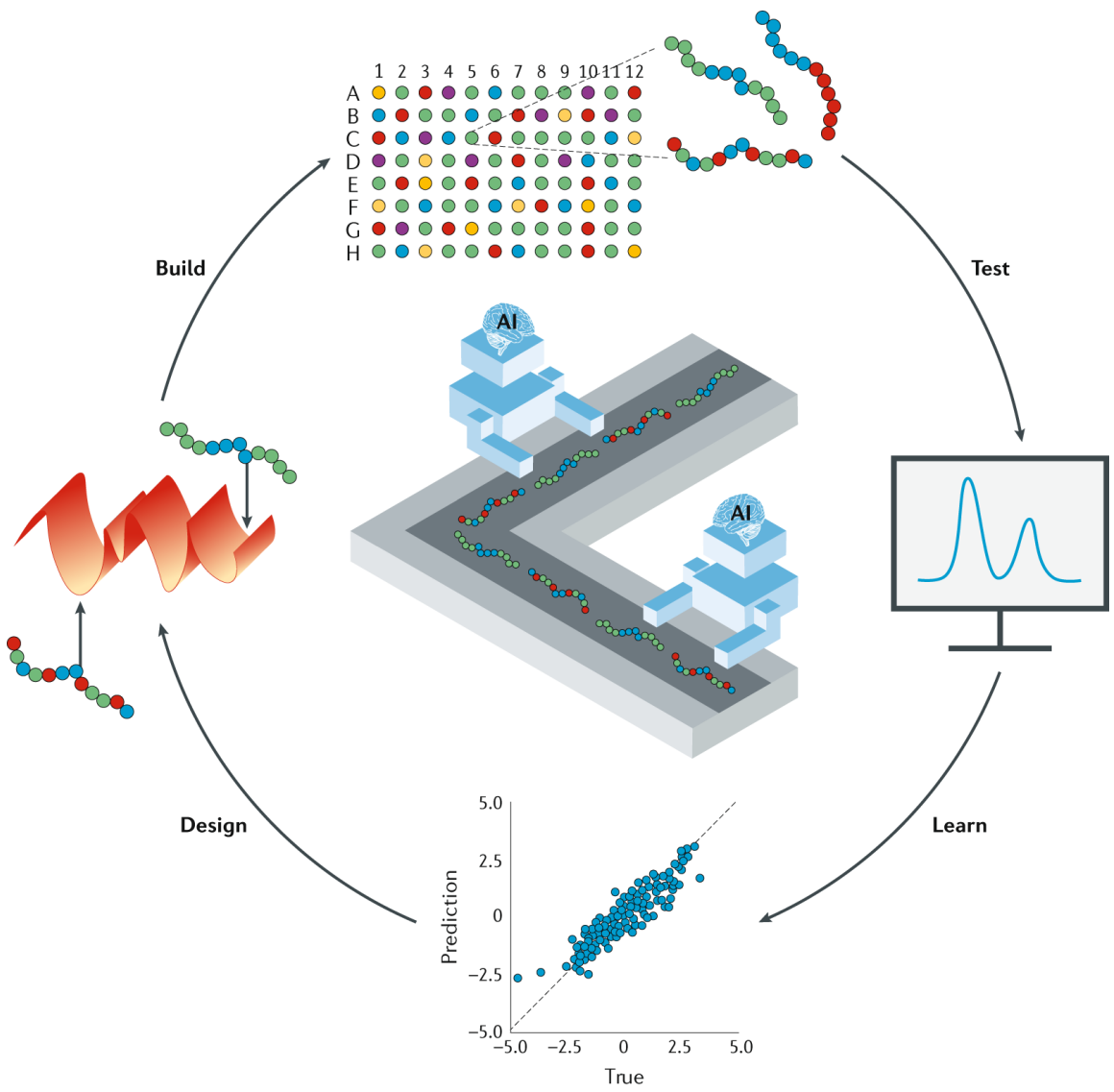
The Future of Self-Driving Labs



A.J. Gormley & M.A. Webb, 2021. **Nature Reviews Materials,** 6: 642-644.

Selected as front cover for next issue of **Advanced Materials**. Artwork by Ella Maru Studio

New Startup in AI for Drug Delivery & Design

PLEXYMER

Novel Excipient Review Pilot Program

September 2021

Conflict of interest

Acknowledgements

Collaborators

@GormleyLab

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Elena Di Mare

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