Developing Nanometer Scale, Atomically Precise Metallo-catalysts with Molecular Lego

DE-EE0008321
Temple University
Summer 2018-Summer 2020

Prof. Christian Schafmeister Temple University
Prof. Graham Dobereiner Temple University

U.S. DOE Advanced Manufacturing Office Program Review Meeting
Washington, D.C.
July 17-19, 2018

Overview

Timeline

- Award is being issued imminently
- Projected End date August 2020
- Project 1% complete (this meeting)

Barriers

- Because the foundational technology of molecular Lego building blocks has been proven, and because chemical synthesis is straightforward, the principal barrier is effective design of the reaction site to synthesize stereospecific polyester polymers

Budget

	FY 16 Costs	FY 17 Costs	FY 18 Costs	Total Planned Funding (FY 19-Project End Date)
DOE Funded	_	_	$66.3k	$729k
Project Cost Share	_	_	$13.3k	$186k

Partners

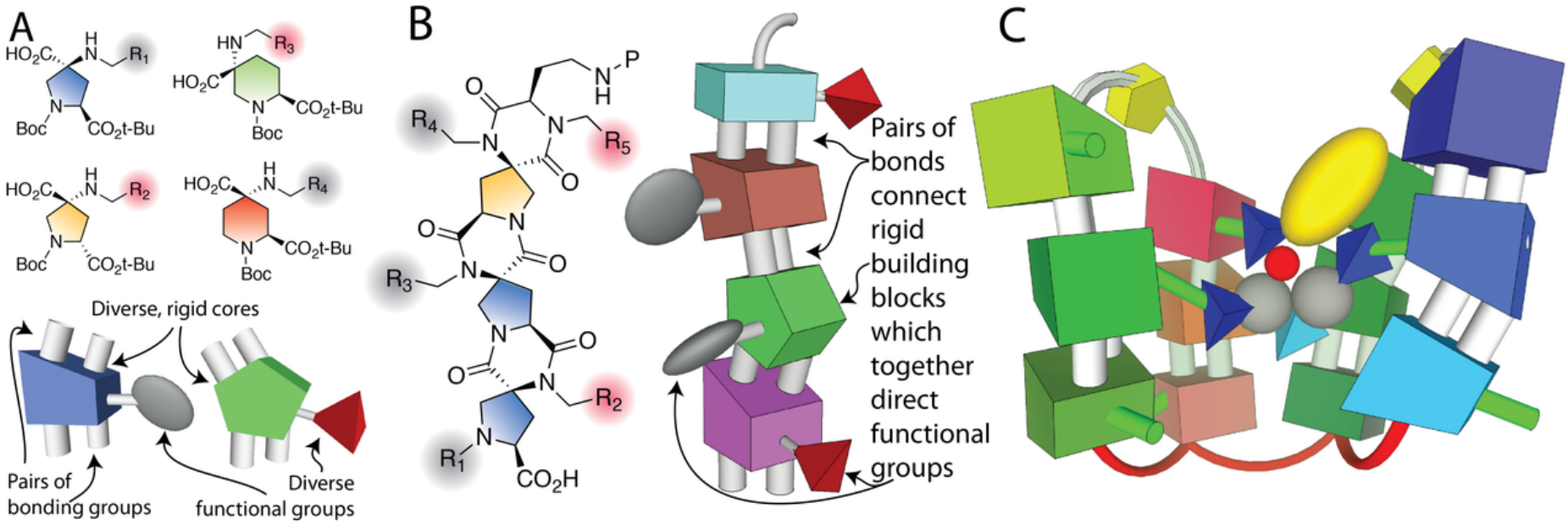
- We will be exploring potential industrial partners who would be interested in licensing the technology during the course of the project

Project Objective(s)

- AMO MYPP alignment: "Develop a new class of **atomically precise catalysts** for 10,000x improvements in catalytic selectivity/activity compared to state-of-the-art catalysts"
- Develop a cross-cutting, general approach for making **atomically precise catalysts** that assemble **atomically precise polymers** with excellent physical properties
- Advanced catalysts are essential for achieving the AMO goal of advanced materials and manufacturing technologies for a 50% reduction in lifecycle energy impact
- Temple University to synthesize atomically precise catalysts to achieve highly selective polyester formation
- Enzymes teach us that **atomically precise, nanometer scale active sites** are many orders of magnitude more active and selective than existing small molecule catalysts

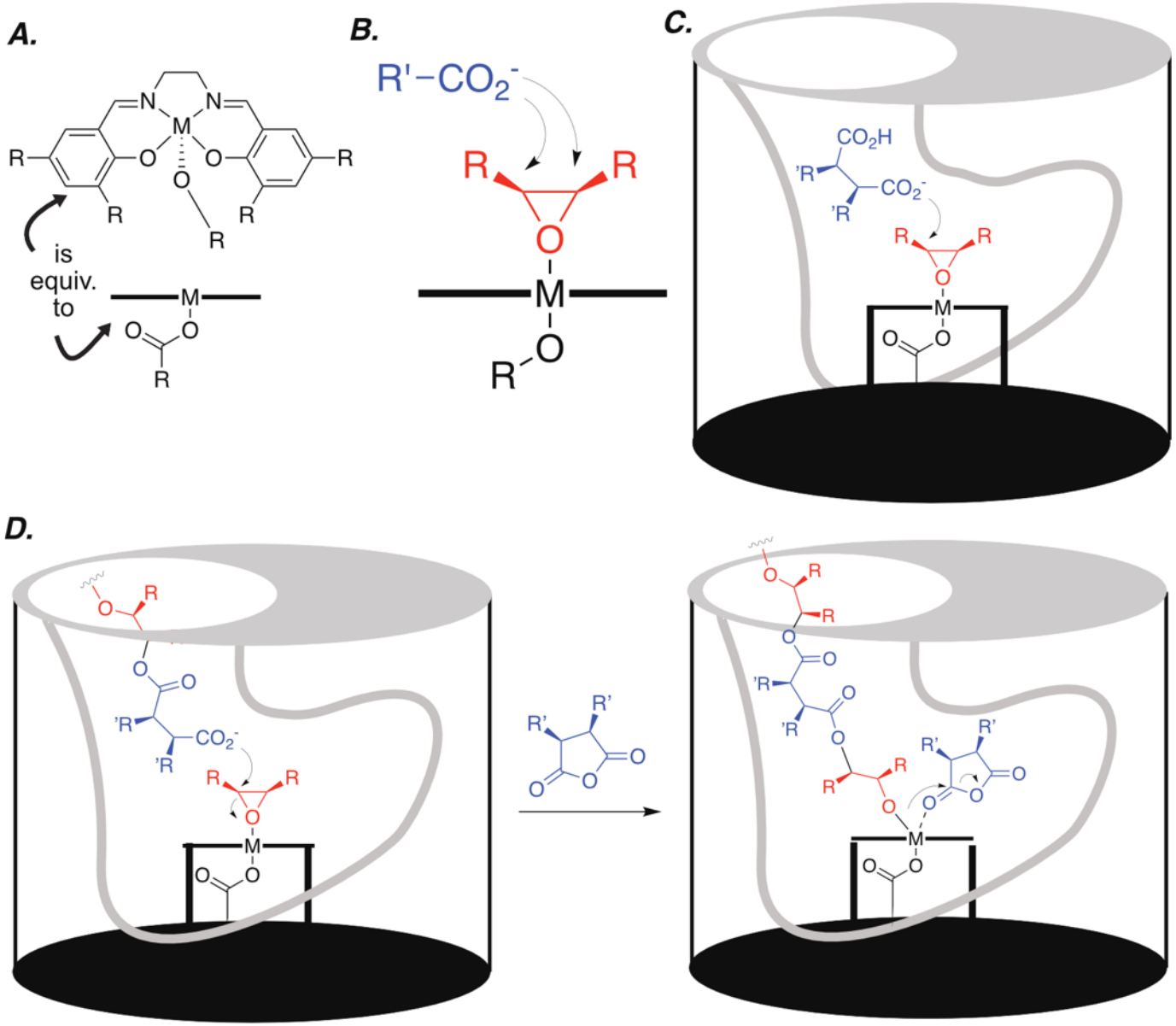
Technical Innovation

- **Current catalysts** are materials or small molecules with **poorly controlled active sites**.
- Our **molecular Lego** "**second shell**" around the metal center will combine the **selectivity of enzymes** – with the **rugged nature** of inorganic material catalysts.



Molecular Lego

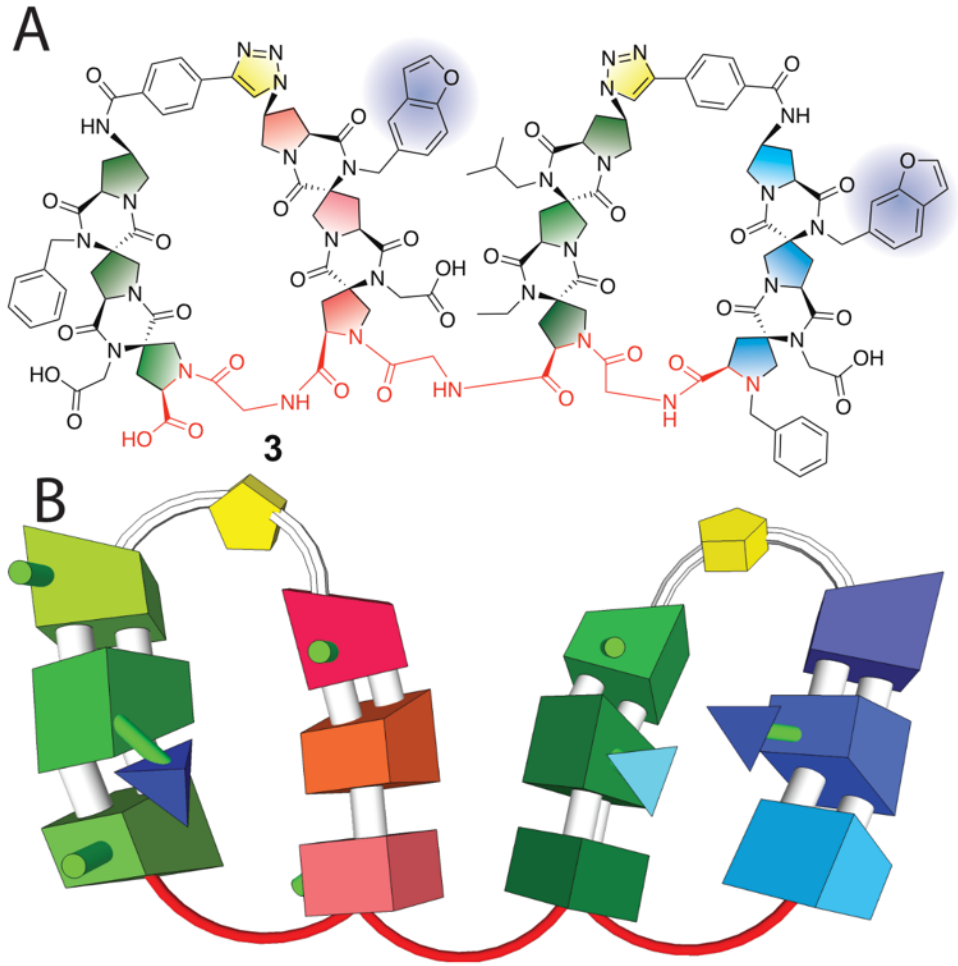
Technical Innovation

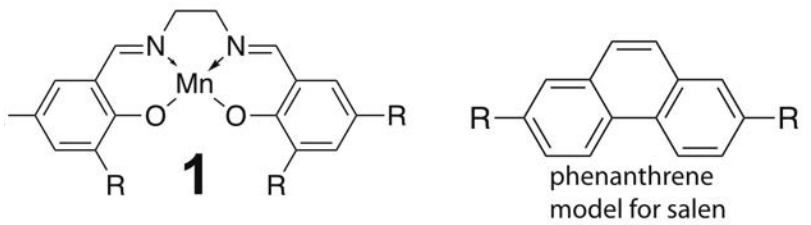


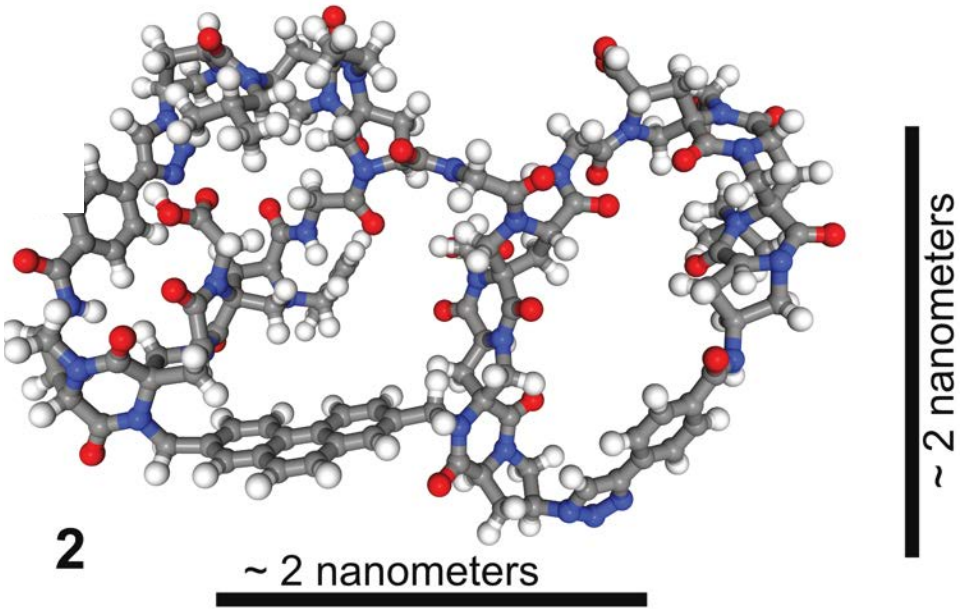
Our catalysts (cartoon) are just 10x larger than current catalysts and will create enzyme-like pockets that control substrate geometry.

Technical Approach

- We are working on the synthesis of macromolecular metal binding catalysts wherein the scaffold will control polyester formation.

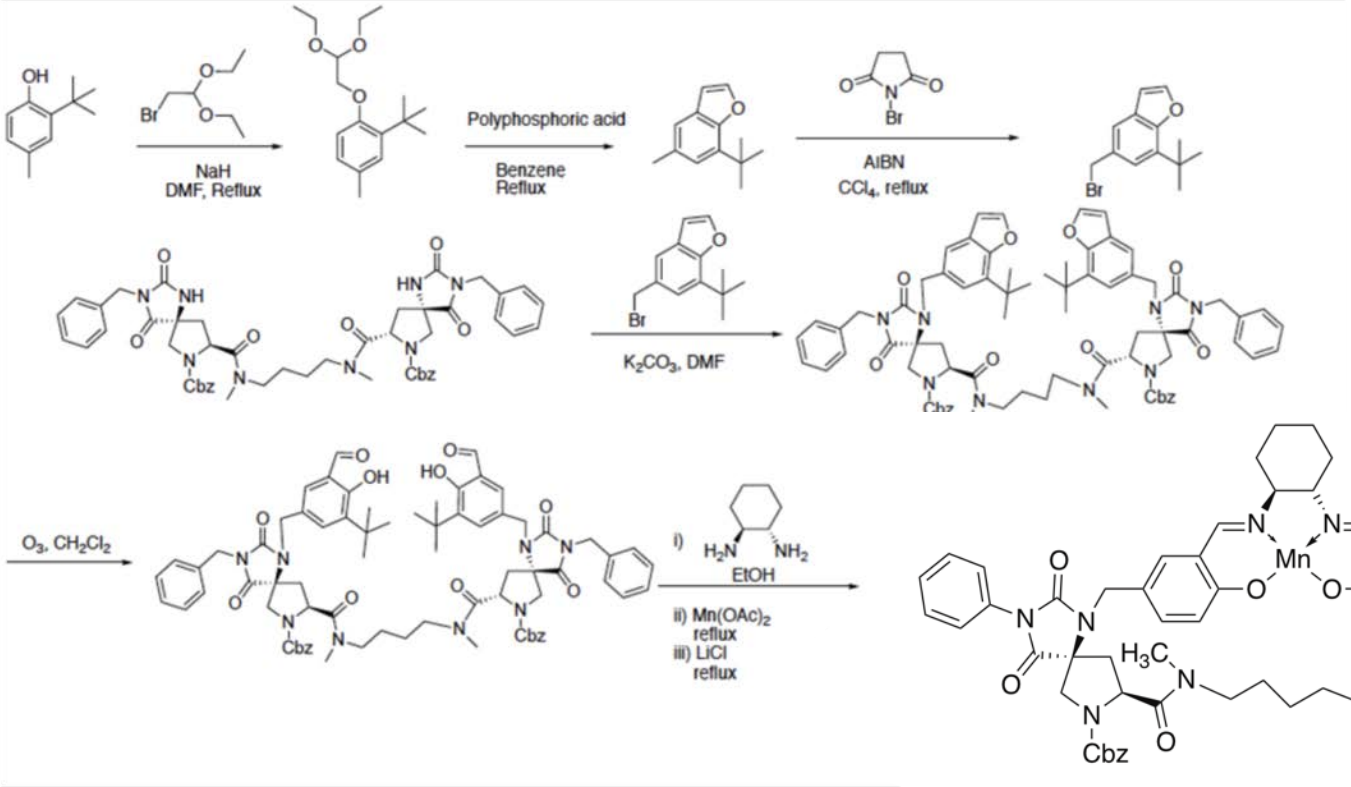






Technical Approach

- Schafmeister group: Catalyst design and synthesis
- Dobereiner group: Catalyst characterization, polymerization kinetics and polymer characterization

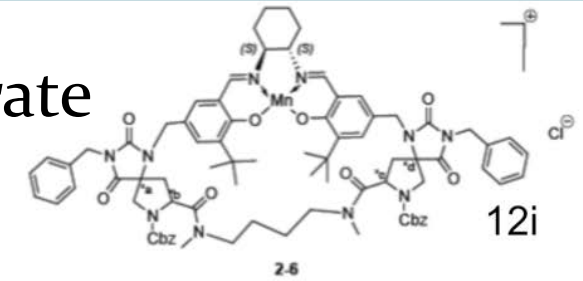


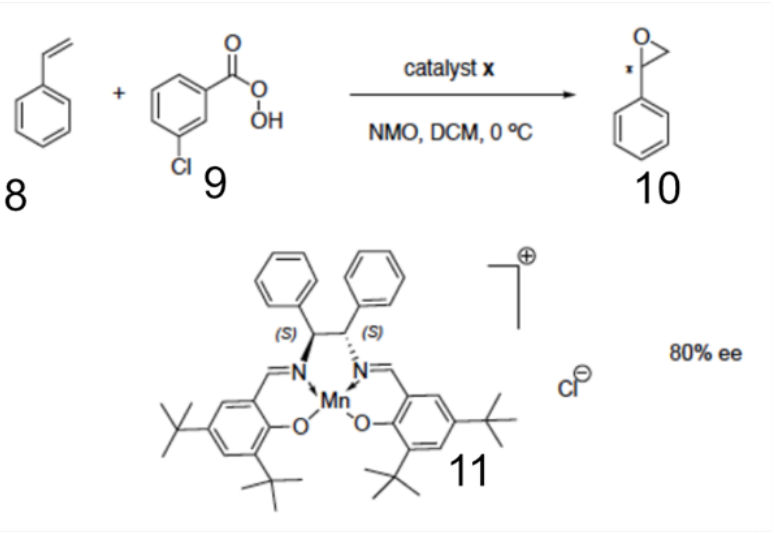
Prototype catalysts

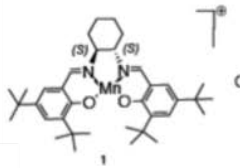
Chemical Formula: $C_{70}H_{70}MnN_{10}O_{12}$
Exact Mass: 1297.46

Results and Accomplishments

- Initial oxidation catalysts demonstrate selectivity controlled by scaffold





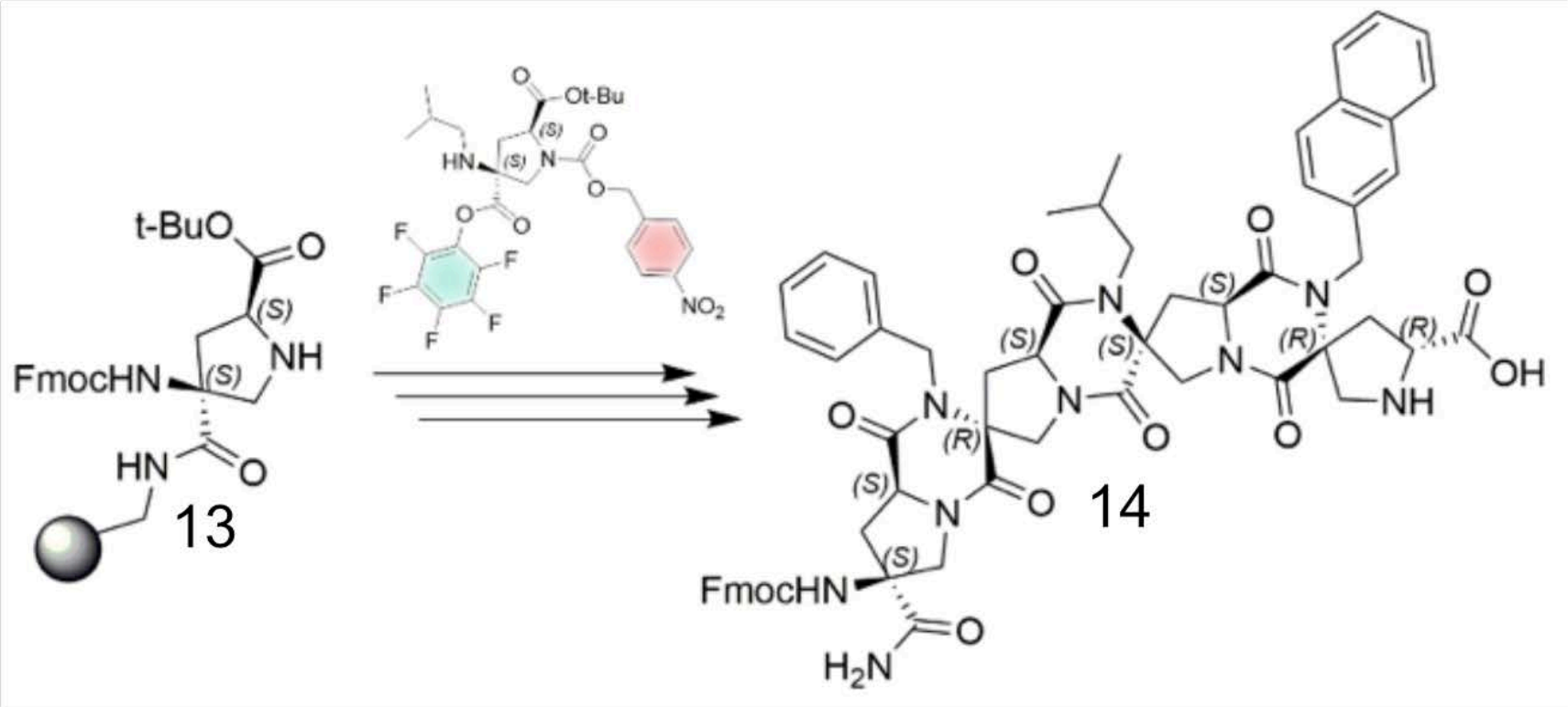


Styrene is a small substrate and the catalysts are large. The selectivity changes are modest at this point.

*Selectivity changes with the catalyst 12i

Results and Accomplishments

- Molecular Lego segment synthesis and catalyst design software is advanced



Transition (beyond DOE assistance)

- We will initially prepare several off-the-shelf catalysts to sell through chemical distributors
  - These products will be used in the research community to demonstrate the utility of this platform technology
- The next stage of commercialization will truly demonstrate the utility of this approach where we will partner with end users to design purpose-built catalysts
  - The catalysts will be designed for specific transformations to improve yield and selectivity
  - The tailored and specialized approach to making catalysts is the game-changing element of this technology