



Development and Implementation of a Course-Based Undergraduate Research Experience (CURE) in Organic Chemistry

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What is a CURE?

"a project that engages whole classes of students in addressing a research question or problem that is of interest to the scientific community"¹

What do CUREs cure?

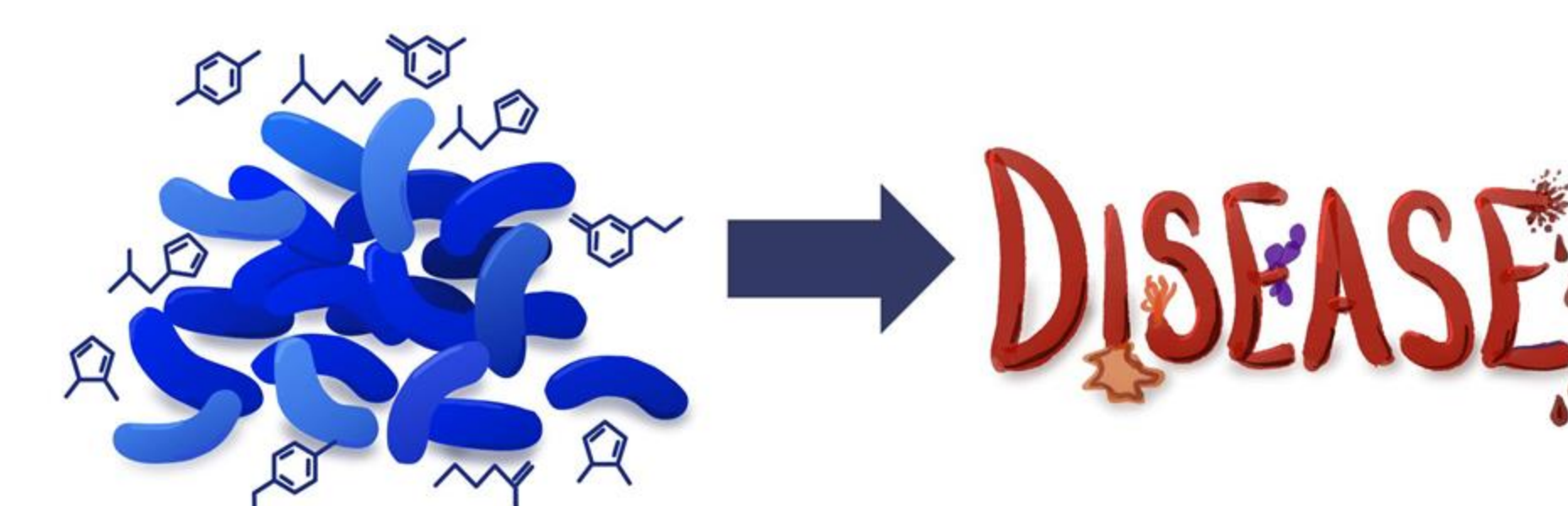
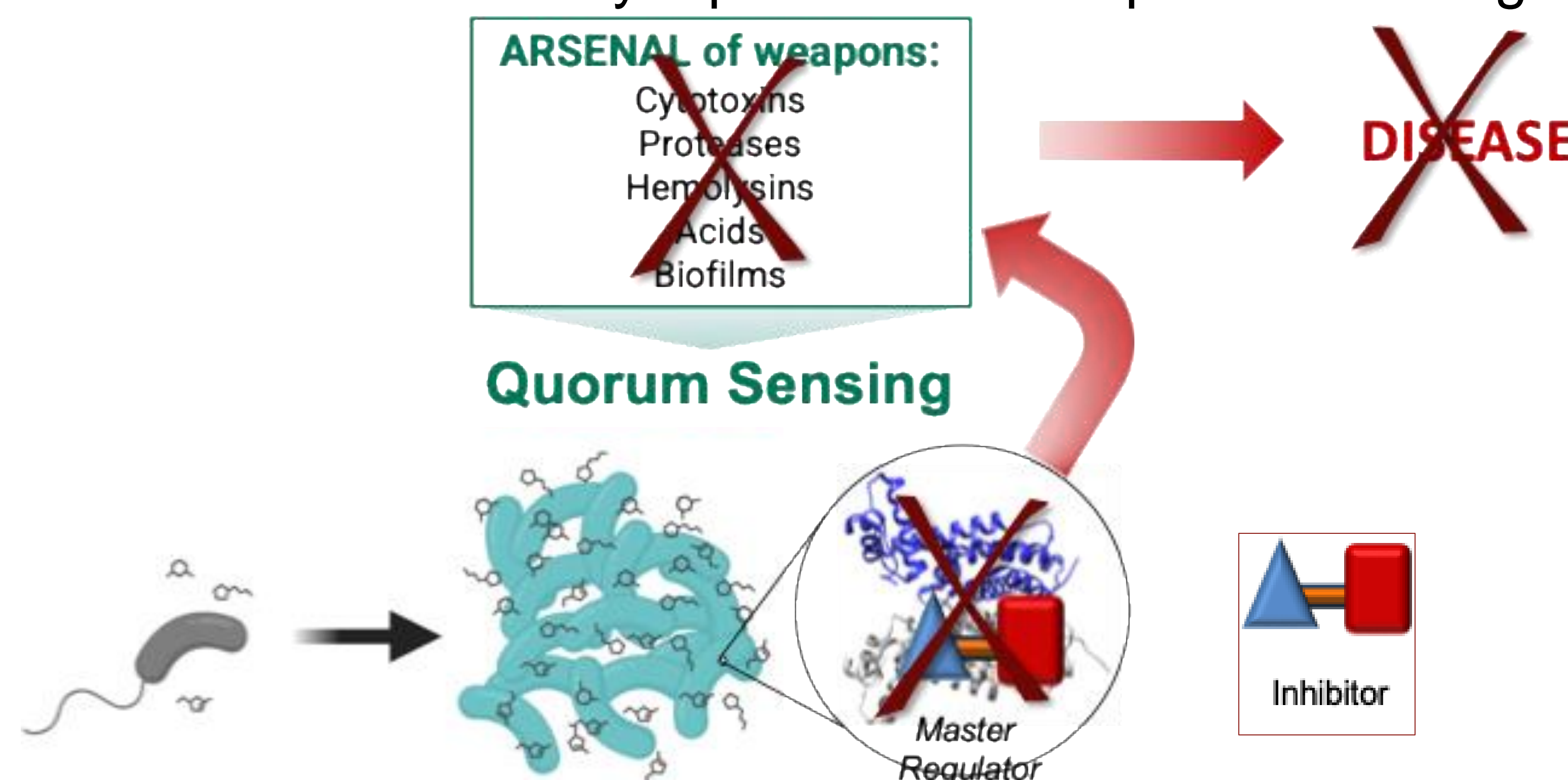
Not all students know to or are able to engage in traditional research experiences. CUREs offer a no-barrier entry into this formative experience!

Key Features of a CURE^{2,3}

1. Students make discoveries that are of **interest to the broader scientific community**.
2. The work is **iterative**, meaning students can troubleshoot and repeat experiments.
3. Students can **present their work** to the broader scientific community.
4. The research project **develops over time**, and no two semesters are exactly the same.
5. **Students develop as independent scientists**, master a range of techniques, learn to ask questions and design experiments, interpret experimental outcomes, etc.

Overview of the Research Project

- *Vibrio* bacteria cause disease (are pathogenic) in humans and in marine organisms such as fish, shrimp, and oysters by making an "arsenal of weapons."
- *Vibrio* are only pathogenic when they are in a group.
- This is controlled by a process called quorum sensing.



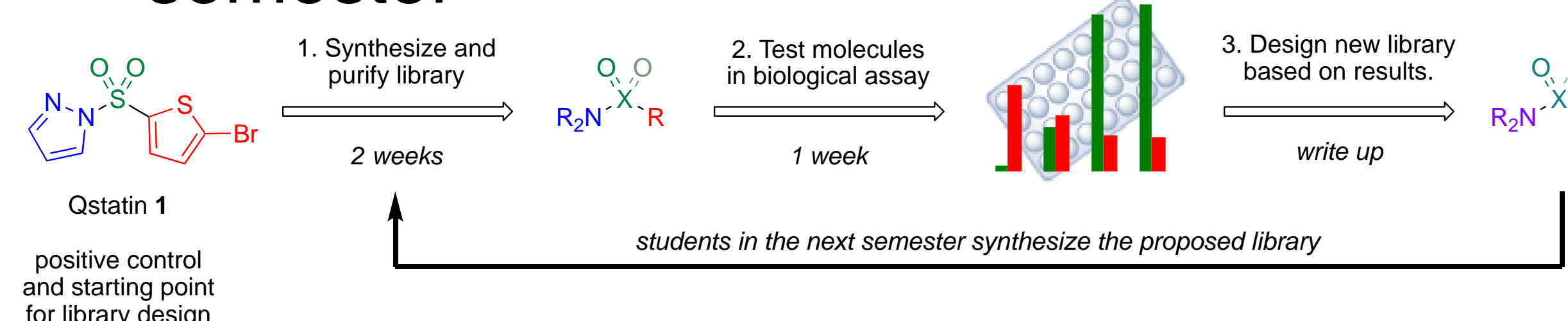
- When *Vibrio* sense they are at high cell density, they make a protein called the "master regulator".
- The master regulator "turns on" the genes to make the arsenal of weapons.
- Molecules can be designed to bind to the master regulator and disable it.
- Treated *Vibrio* are no longer pathogenic!
- Alternative to antibiotics.

CURE-Friendly Aspects of the Project

1. Target protein (LuxR) that is well-characterized and has a putative ligand binding pocket.
2. Robust and specific assay for inhibition of LuxR.
3. Proven inhibition by small molecules.
4. Small molecule inhibitors are amenable to library design.
5. Project is of interest to broader scientific community, no direct competitors?

3-Week CURE in an Advanced Organic Lab

- Upper-level organic lab elective (mostly 3rd and 4th year majors)
- 10-20 students/semester
- Lab meets 4 hours/week
- Incorporated towards the end of the semester



Year-Long CURE in the ASURE Program (Spring-Fall)

1. **Biological Assays:** Students learn how to run the assay for quorum sensing inhibition (and how to work up and interpret the data). Students use previously-synthesized inhibitors and targets from various *Vibrio* species.
2. **Docking Studies:** Students learn how to dock molecules into the ligand binding pocket of their target protein and generate *in silico* binding affinities using AutoDock tools and webina. They then learn how to use PyMol to investigate the ligand-protein interactions and to generate publication-ready figures.
3. **Library Proposal:** Students used their *in vivo* and *in silico* results to propose a new library of putative quorum sensing inhibitors.
4. **Organic Synthesis:** Students synthesize, purify, and characterize their proposed library, then test it in the assay.
5. **New library design:** Students design a new library based on their assay results.

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IU Chemistry Department, IU ASURE Program

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2. Staub, et. al. *CUR Quarterly* **2016**, 37, 36.
3. Dolan, et. al. *National Research Council Commissioned Paper* **2016**.

