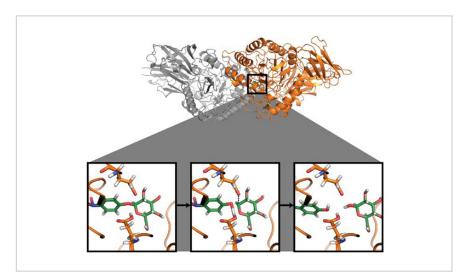
# OptZyme: In Silico Enzyme Redesign Using Transition State Analogues

ID# 2013-4127





Catalyzed Reaction for E.coli

# **Technology Summary**

OptZyme is software used to discover promising enzyme redesigns that can be experimentally tested. OptZyme does not use complete quantum mechanics analysis making it less computationally demanding. OptZyme is instead predicated on derived equations. OptZyme utilizes known transition state analogue (TSA) structures as proxies for unknown rate-limiting transition state (TS) structures. TSAs interfere with enzyme catalytic activity by mimicking the geometry of TSs and preferentially binding with the enzyme over the substrate, preventing the reaction from proceeding. The inventors have shown that mutations that minimize the interaction energy (IE) of the enzyme with its TSA, rather than with its substrate, allows for the identification of lower transition state formation energy barrier.

## Application & Market Utility

OptZyme helps design new commercial enzymes, providing strong evidence before using experimental approaches. OptZyme is suited for systems where solute entropy change upon binding is assumed to be negligible relative to other terms, substrate binding is not a consequence of "induced fit", and equilibrium following the rate-limiting step strongly favors product release. OptZyme constructs a library of mutants with improved enzyme catalytic parameters for a similar substrate by identifying novel contacts with the ligand that were absent from other established libraries.

## **Next Steps**

Seeking prospective licensees; demo is available at http://maranas.che.psu.edu/submission/OptZyme.htm

## **TECHNOLOGY READINESS LEVEL**

4-7

#### Seeking

Investment | Licensing | Research

#### **Keywords**

- Computational design
- in silico
- protein engineering
- molecular mechanics
- interaction energy

#### Researchers

#### Costas D Maranas

Donald B. Broughton Professor of the Department of Chemical Engineering

Online Bio Website

#### Patrick Carmen Cirino

Graduate Student Researcher

#### **Nathanael Paul Gifford**

Graduate Student Researcher

#### **Other Researchers**

**Matthew Jeffery Grisewood** 

## **Originating College**

College of Engineering

## Office of Technology Management Contact

Smith, Matthew mds126@psu.edu 814-863-1122



Invent Penn State is a Commonwealth-wide initiative to spur economic development, job creation, and student career success. Invent Penn State blends entrepreneurship-focused academic programs, business startup training and incubation, funding for commercialization, and university-community collaborations to facilitate the challenging process of turning research discoveries into valuable products and services that can benefit Pennsylvanians and humankind. Learn more at invent.psu.edu.

Penn State is an equal opportunity, affirmative action employer, and is committed to providing employment opportunities to all qualified applicants without regard to race, color, religion, age, sex, sexual orientation, gender identity, national origin, disability or protected veteran status.