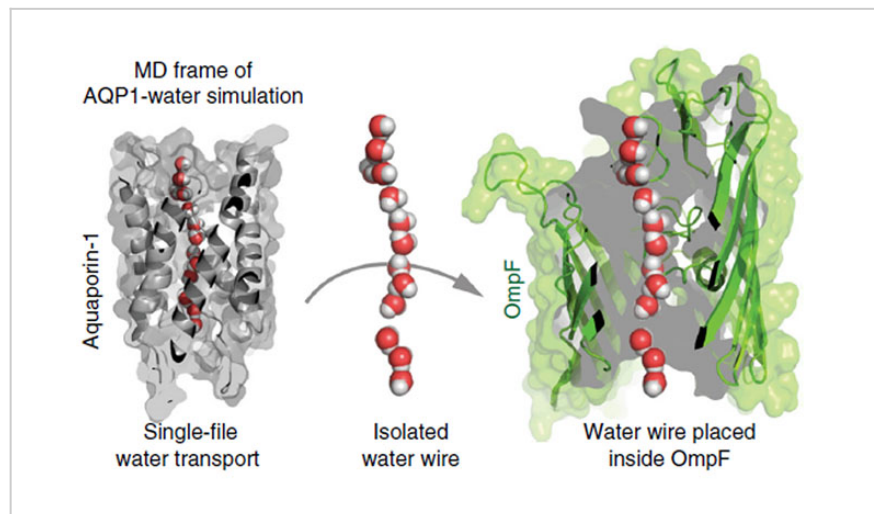


# Design Workflow for Angstrom-scale Separations

ID# 2018-4764



PennState



Water wires used to design OmpF pore

## Technology Summary

A team of Penn State researchers have developed a design workflow, PoreDesigner, which engineers key characteristics of an outer membrane protein to make customized biological membranes. The pore size, pore profile and the chemical interactions between the pore and the permeating water, such as hydrogen bonding, are controllably engineered by optimizing the amino acid selection. The optimization process increases solvent flow, and tunes the pore size to any size between 3 - 10 Å for targeted solute rejection.

## Application & Market Utility

Derived from a set of 40 sequentially-optimized pore designs, the three most optimized designs have been experimentally validated to exclude solutes larger than sucrose, glucose, and sodium chloride. The membranes maintained a permeability of over 10 billion water molecules per channel per second, demonstrating that PoreDesigner is a comprehensive design workflow that can be applied to angstrom-scale separation needs.

## Next Steps

We are seeking commercial licensing partners. A demonstration of PoreDesigner is available upon request.

TECHNOLOGY READINESS LEVEL

4-7

### Seeking

Investment | Licensing | Research

### Keywords

- computational protein design
- angstrom-scale separation
- Outer Membrane Protein F (OmpF)
- IPRO algorithm
- ultra-permeable membranes

### Researchers

#### Dr. Costas Maranas

Professor of Chemical Engineering

[Online Bio](#)

[Website](#)

#### Dr. Manish Kumar

Associate Professor of Chemical Engineering

[Website](#)

#### Ratul Chowdhury

Graduate Student

### Other Researchers

Tingwei Ren

### Originating College

College of Engineering

### Office of Technology Management Contact

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



the ingenious power of partnership

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](http://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.