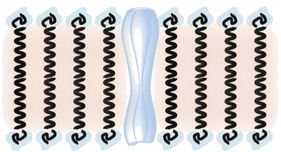
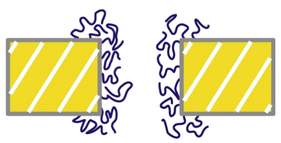
"Biomimetic membranes"

- Nature has evolutionarily perfected systems for filtration, separation and selective sensing
- Biomimetic applications use these as models to artificially design micro- and ultrafiltration membranes and sensing applications



Membrane proteins incorporated into lipid or block copolymer bilayers

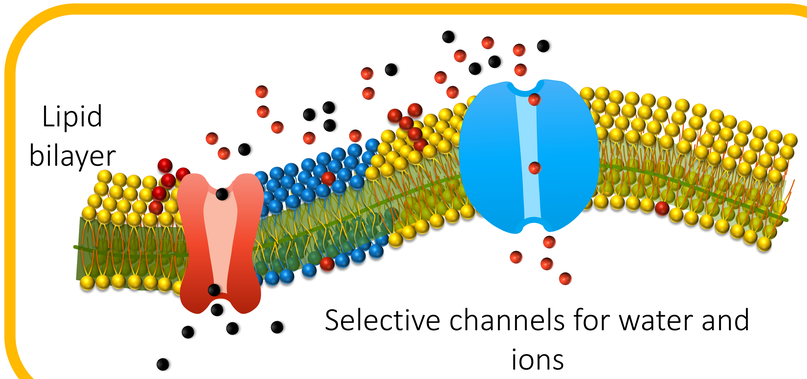


Nanopore membranes modified with functional molecules within the pores

START HERE

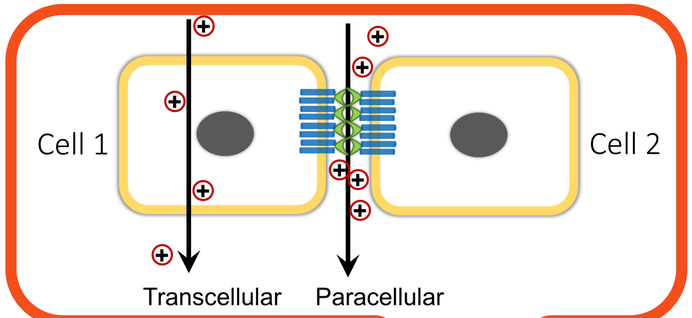
"Biological sorters"

- Biomimetic membrane design largely involves transmembrane proteins that function as water channels (Aquaporins), and ion channels.
- Engineered polymer or peptide sequences are often used for surface functionalization of nanopores



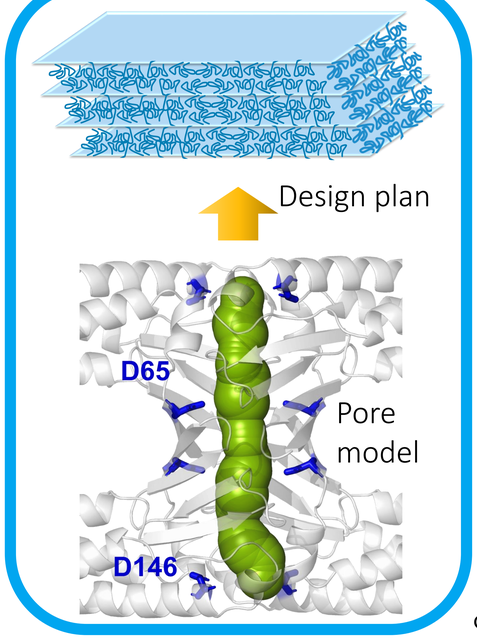
"Claudin paracellular pores"

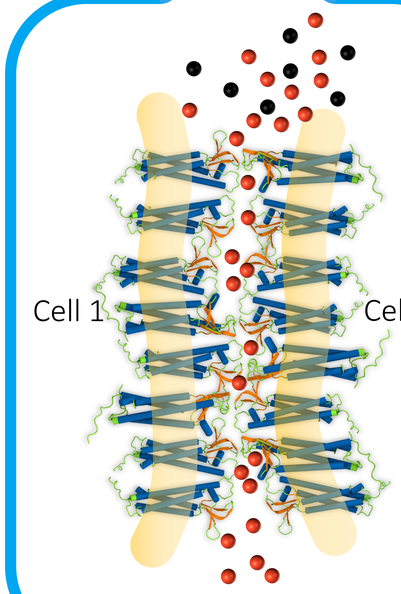
- Paracellular pores formed by claudins are one of the most selective protein interfaces in the biological system with a high potential of being translated to ultrafiltration applications, but has not been explored yet



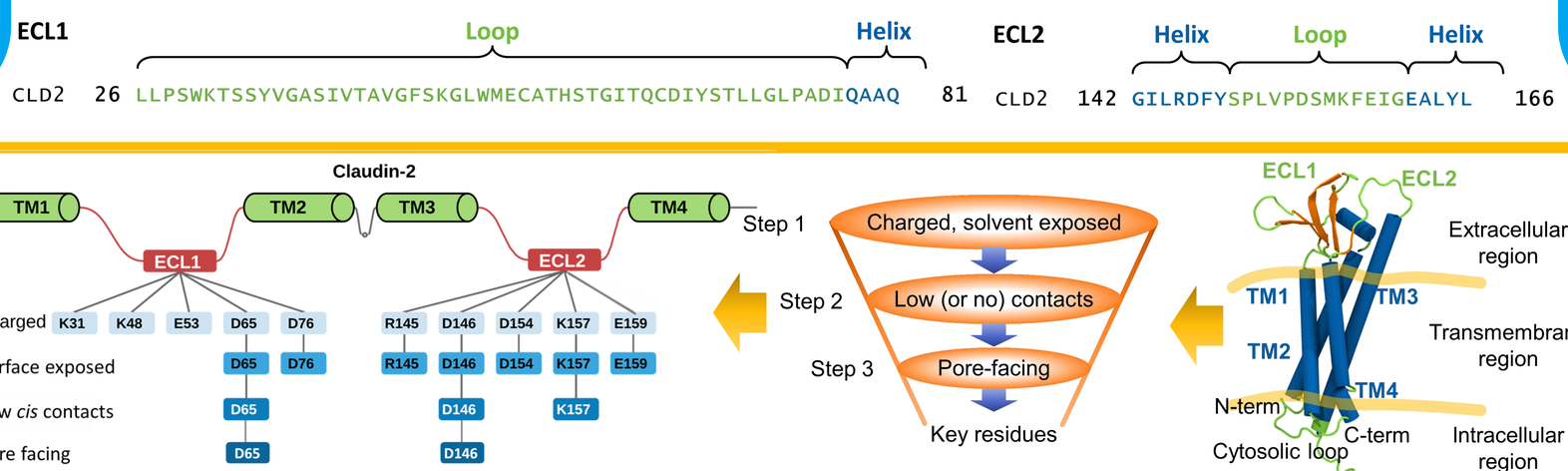
Predicting Selectivity of Paracellular Pores for Biomimetic Applications

***Nandhini Rajagopal*, Alejandro Durand and Shikha Nangia**
Department of Biomedical and Chemical Engineering, Syracuse Biomaterials Institute, Syracuse University





"Extracellular domains of claudins govern their paracellular selectivity"



We devised a systematic strategy to predict the key regions in claudins, which can be incorporated into biomimetic membranes

We propose extracellular domains of claudins as potential peptide sequences for functionalization of biomimetic membranes

- Our method accurately predicts the key residues imparting selectivity to claudin-2 pores
- The cation selectivity of claudin-2 is imparted by Asp65 and Asp146, lining the pore
- Our predictions are validated by previous experimental works on claudin selectivity
- Our predictions for claudins-4 and -15 are also in agreement with experiments

References
Shen, Y. et al, Biomimetic membranes: A review, *Journal of Membrane Science*, Volume 454, 15 March 2014, Pages 359-381.
Irudayanathan, F. J., Wang, N., Wang, X., and Nangia, S., Architecture of the paracellular channels formed by claudins of the blood–brain barrier tight junctions, *Annals of the New York Academy of Sciences*, Volume 1405-1, Oct 2017, Pages 131-146.
Rajagopal, N, Durand, A. J., and Nangia, S., Predicting Selectivity of Paracellular Pores for Biomimetic Applications, *Molecular Systems Design and Engineering*, Jan 2020.

SYRACUSE UNIVERSITY ENGINEERING & COMPUTER SCIENCE
SYRACUSE BIOMATERIALS INSTITUTE
NSF
RESEARCH computing
XSEDE Extreme Science and Engineering Discovery Environment