Mathematical Modeling of Electrostatic Potential of Photosensitive Proteins

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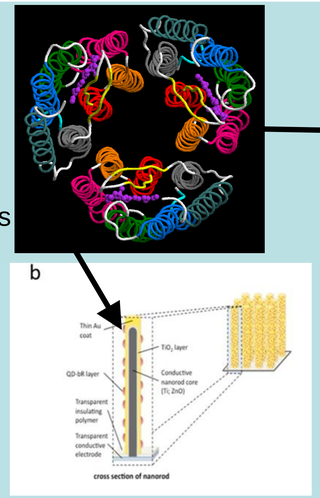
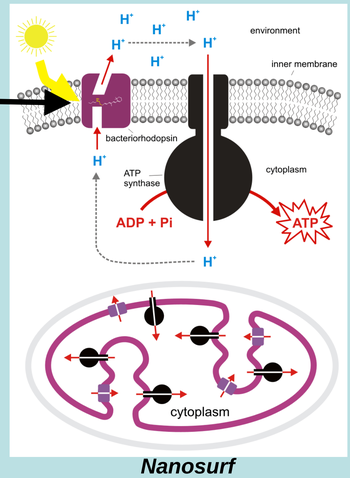
Bacteriorhodopsin (bR) is a photosynthetic protein which is able to effectively convert light energy to electrical energy.

Recent studies have introduced mutants as potential photosensitizers and consequently engineered biosolar cells

Gap in literature exist in systematic study of electrostatic potential and charge distribution of photosensitive proteins

aRenu et al, JPC, 2014





Nanosurf

Objectives: Modelling charge distribution and electrostatic potential of photosensitive proteins in absence and presence of surfactants

Challenges: Creating realistic 3D models of proteins after interaction with surfactants and accurately calculating the electrostatic potential

Intellectual Motivation: We will be able to determine how different surfactants affect the efficiency of charge transfer and impact the functionality of photosensitive proteins

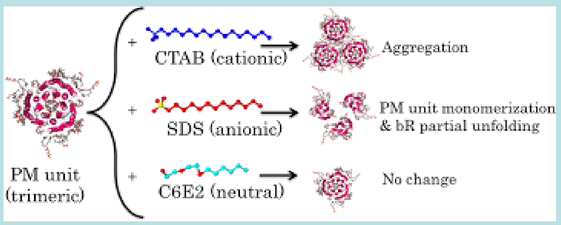
Industrial Relevance: Improve efficiency of energy conversion from light to electrical and create more stable personal care products to increase sustainability

Broad Appeal: Bioengineering, Personal Care, Energy Industry (Solar Cells)

Outline

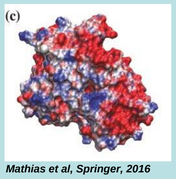
Surfactants are known to cause conformational changes in many proteins and sometimes even denaturing

Recent studies have shown that this protein reacts differently to cationic and anionic surfactants. This introduces a unique look into protein-surfactant interactions via electrostatic potential

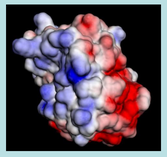


Ng et al, JPC, 2013

Model Validation



Mathias et al, Springer, 2016



Electrostatic Potential of Cytochrome C Peroxidase

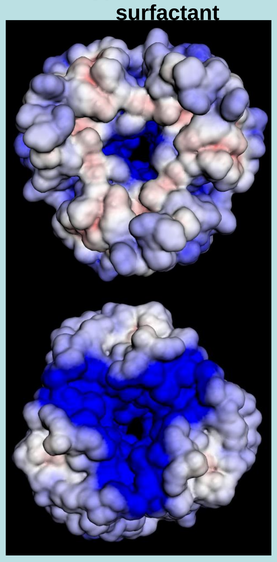
Methods

Create a 3D model of bR from amino acid sequence using Swiss PDB Expasy

1. Using a program called PDB2PQR and Adaptive Poisson-Boltzmann Solver (APBS), create electrostatic potential maps ,determine the total electrostatic energy of the protein.
2. Compare with model of bR in the presence of both cationic and anionic surfactants
3. Determine the change in efficiency/functionality of the protein

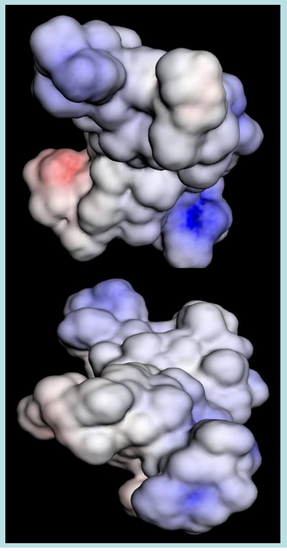
Results

Wild Type bR in absence of surfactant

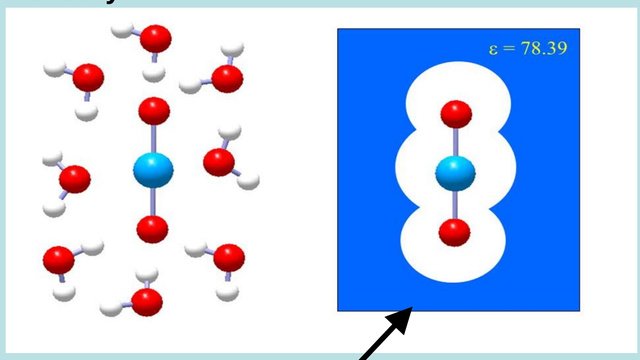


bR has more of a positive potential than its surfactant opposite. This may prove crucial to the absorption and transfer of protons between the membrane.

bR in presence of anionic surfactants, SDS



Theory



Koehl et al, Stanford, 2013

Implicit Solvent Model

- APBS assumes that the protein is in a solvent that acts as a continuous medium rather than separate molecules
- Unlike the explicit solvent model, it is more reliable and accurate
- The program requires dielectric constant of the medium and solute, as well as charge, concentration, and radius of the ions

Future Work:

Systematic study of electrostatic potential as function of Debye Length, Ionic strength

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