Physical-Technical High School
Saint-Petersburg Academic University

Study of the visual adaptation mechanism in marine species with the change of habitation depth

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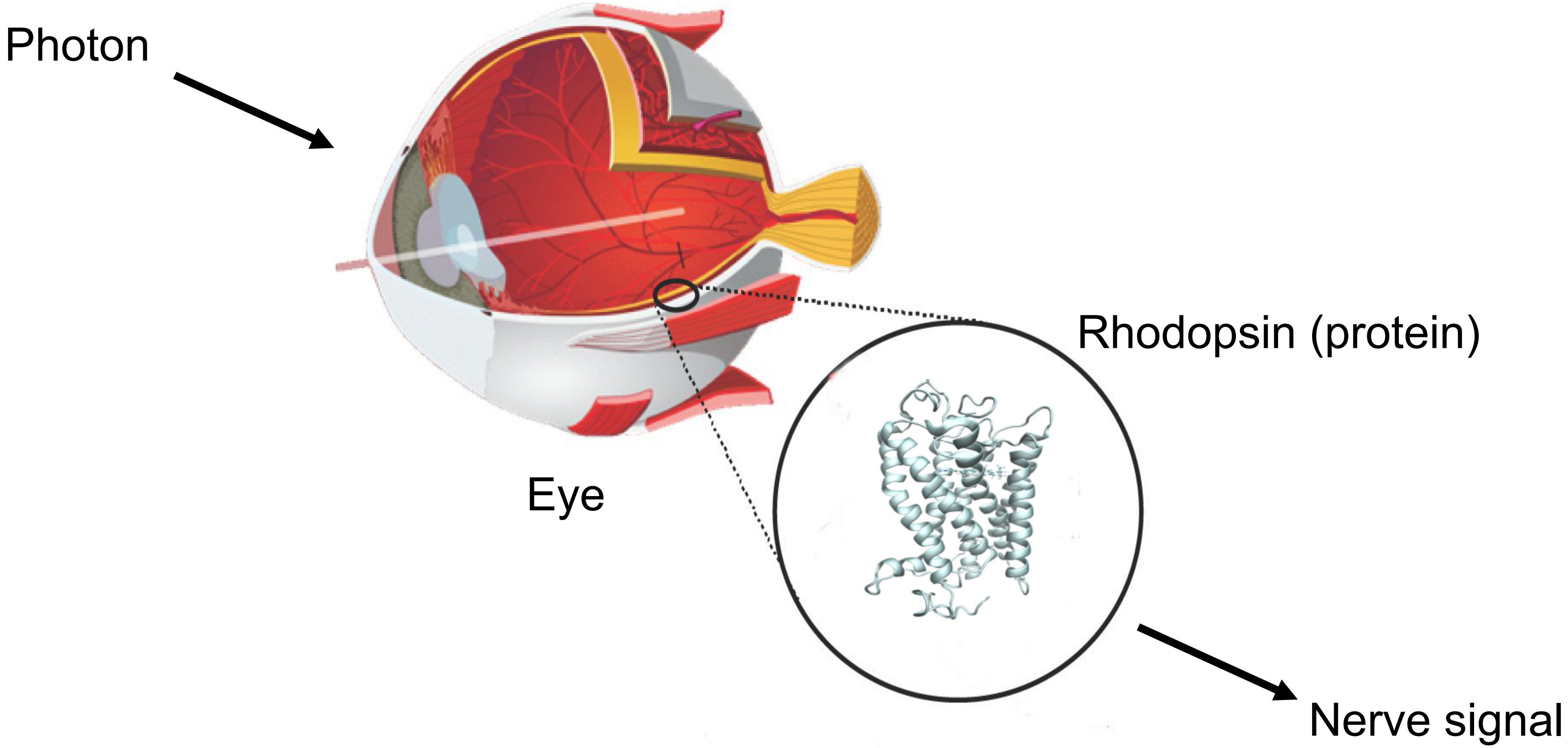
Place of research:
St Petersburg Academic University
Laboratory of Nanotechnologies

Introduction. Perception of light.



Picture: http://spie.org/newsroom/0988-a-single-photon-detector-inspired-by-the-human-eye?SSO=1

Molecular imaging of nerve systems

Some bacterial rhodopsins can work in inverse direction.
They can radiate light.

- Potential-dependent rhodopsin is inserted into neuron
- Neuronal potential → Fluorescence

nerve signal →  → light

rhodopsin

Applicatoins of imaging:
- studying nervous systems
- investigating brain diseases

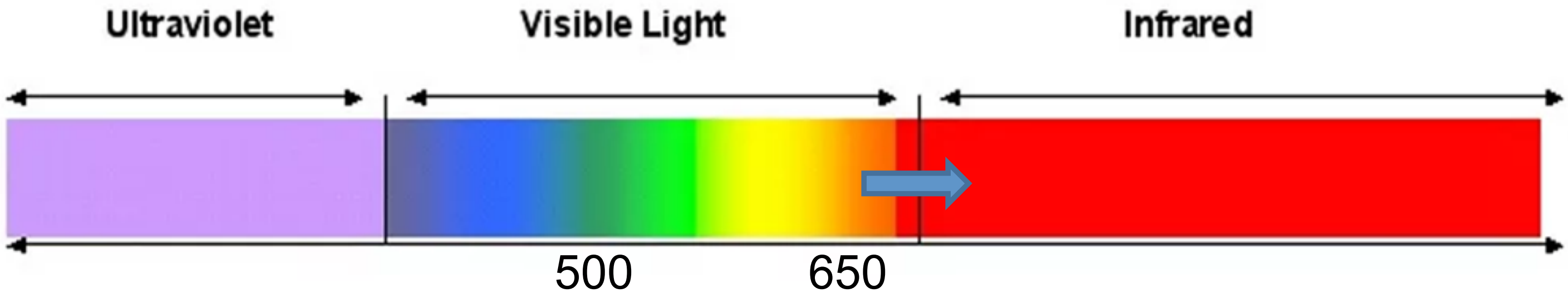
Picture:https://www.nytimes.com/2016/03/24/science/risky-rats-help-shine-light-on-brain-circuitry-behind-taking-a-chance.html

Problem setting

- **Problem:** bacterial rhodopsins absorb and radiate light, which can not go through biological tissues. Surgery is required.
- **Solution:** radiation in the IR range goes freely through tissues. Radiation spectrum of rhodopsins should be shifted towards IR.

Goal

Investigate the mechanisms that can be used for spectral tuning of rhodopsins in order to shift radiation towards IR



Picture: https://www.scienceoflight.org/infrared-light/

Approach to the task

- Wavelength of radiated photon = wavelegth of absorbed photon
- Absorption spectra of rhodopsins in an eye defines visual range of an animal

To investigate the differences between the rhodopsins which have different absorption spectra we decided to study the differences in rhodopsins of species which have different visual range.

Squid (Todarodes Pacificus)

Octopus Vulgaris

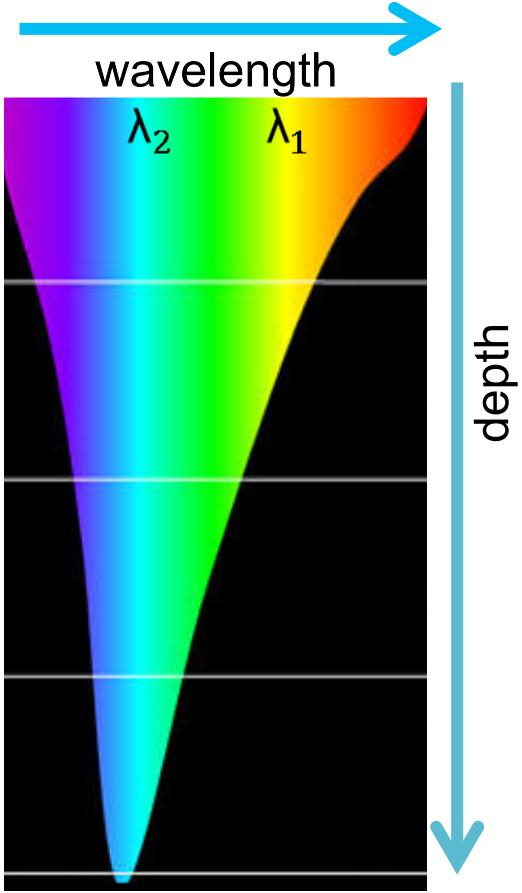
Picture: http://www.map028.com/gallery/squid-vs-octopus-by.html

Differences in color perception

Different depth of habitation

Different light conditions

Rhodopsins have different absorption spectra



Octopus Vulgaris

λ_1

Todarodes Pacificus

λ_2

Pictures: http://getdrawings.com/giant-octopus-drawing, http://www.pinsdaddy.com/potasquid_FRGLmBlphG2vqg8o1gwMzX5rfTgZ7aihDNUgJbbfKWA/, https://

Rhodopsin

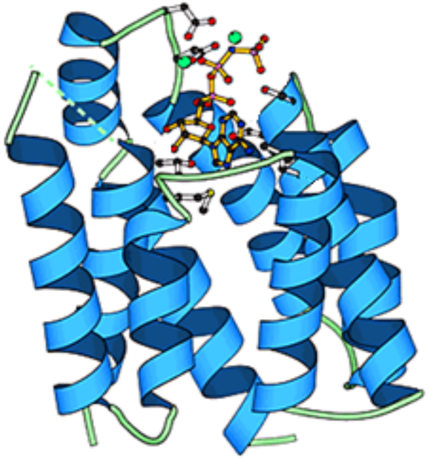
Rhodopsin is a protein.
It consists of amino acids.
Sequence of amino acids uniquely determines

Properties of a protein

- Physical: optical, thermodynamical
- Chemical
- Biological functions

In order to change protein's spectrum one has to change its amino acid sequence.

Tertiary structure of a protein

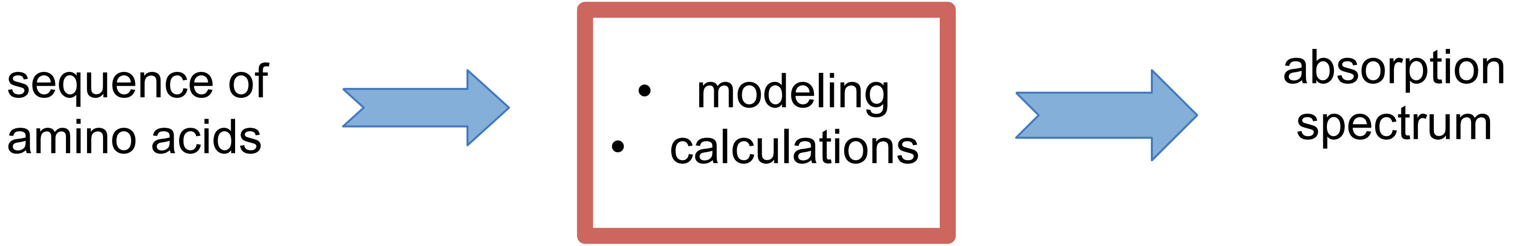


Picture: http://nchsbands.info/new/which-of-these-illustrates-the-secondary-structure-of-a-protein.html

Methodology

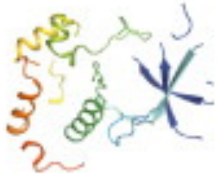
For this problem we used computer modeling of rhodopsin structure and spectrum starting from its amino acid sequence.

1. Firstly, we created the structures (spatial position of atoms) of rhodopsin in both ground and excited states on the basis of amino acid sequence (taken from a database).
2. Secondly, based on these structures, we calculated the absorption spectrum of rhodopsin.

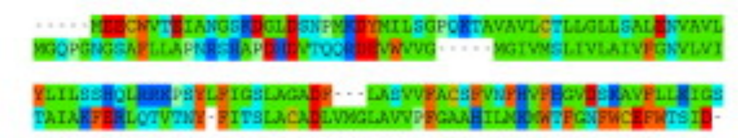


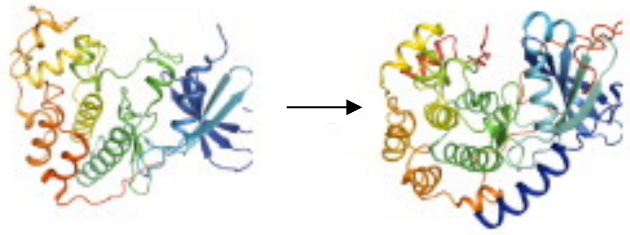
Methodology. How is the structure of rhodopsin created by computer modeling?

- Search for template with known experimental structure
- Align sequences of target and template
- Build model
- Refine model (inserting water and hydrogen network)
- Optimize the structure by minimizing energy function $E(x_1, y_1, z_1, \ldots, x_n, y_n, z_n)$, where x_i, y_i, z_i - are the coordinates of atom i



identical segments





Template Target

Picture: https://www.sciencedirect.com/science/article/pii/S1359644609001469

Methodology. How is the spectrum of absorption calculated?

We find the energy values of the rhodopsin in its ground and excited states by solving the Schrödinger equation with a program package (ORCA 4.0).

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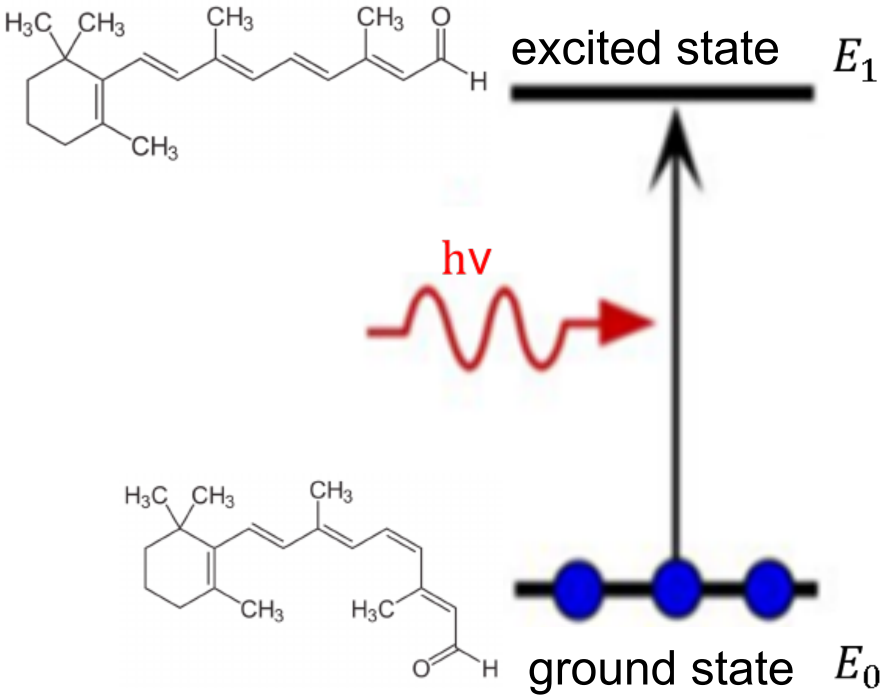
Absorption spectrum

$$\lambda = \frac{ch}{(E_1 - E_0)}$$

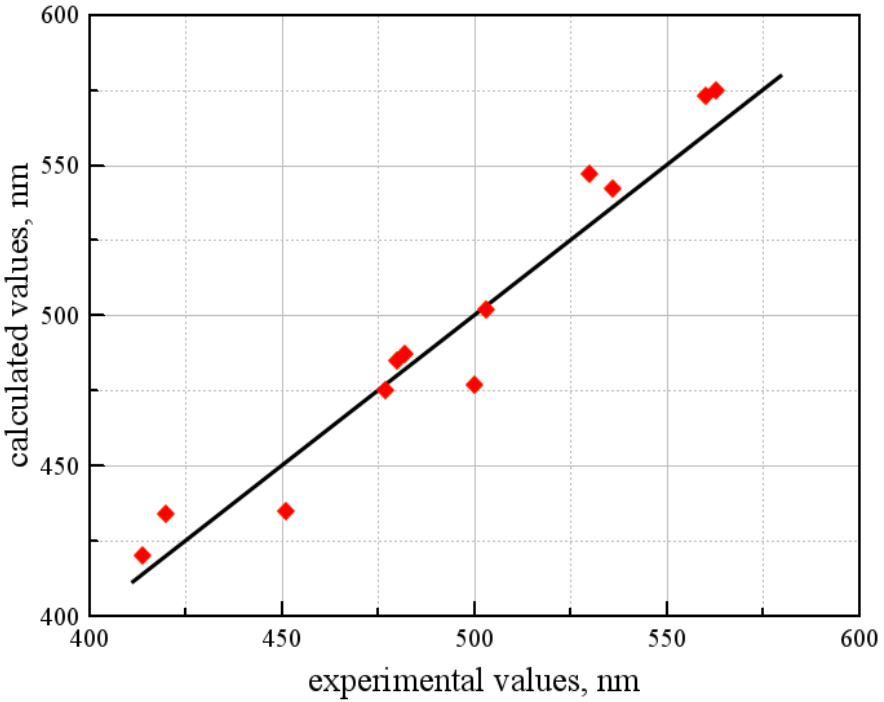


Picture: https://www.researchgate.net/figure/In-the-outer-segment-opsin-is-bound-to-11-cis-retinal-top-that-undergoes-a_fig1_260349017

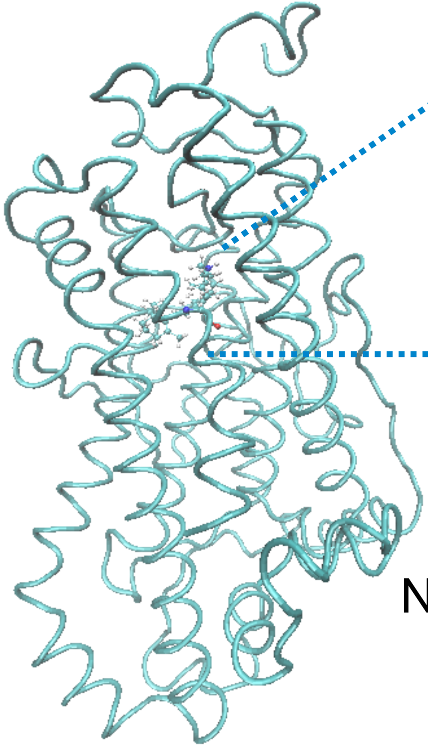
Testing this methodology

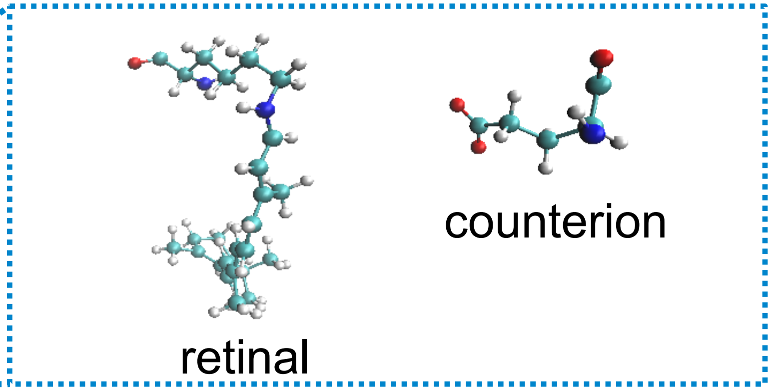
- This method was used to calculate the absorption spectra of some rhodopsins with known spectra.

- Calculated values correlate well with the known experimental data.



Mechanism of spectral shift





In rhodopsins there is a **retinal** that absorbs photons.

Near retinal there is a **counterion** – a negative amino acid.

Mechanism of spectral shift

- The wavelength of absorbed photon depends on the difference in retinal's energy in ground and excited states.
- This difference is affected by electrical field from negative counterion.
- According to the Coulomb law, the shorter the distance between counterion and retinal, the bigger the filed from counterion.

Hypothesis

Difference in distance between counterion and retinal is responsible for difference in absorption spectra.

Mechanism of spectral shift

- We compared the structures of rhodopsins of *Vulgaris* and *Pacificus.*
- Structures have different distances between retinal and the counterion.

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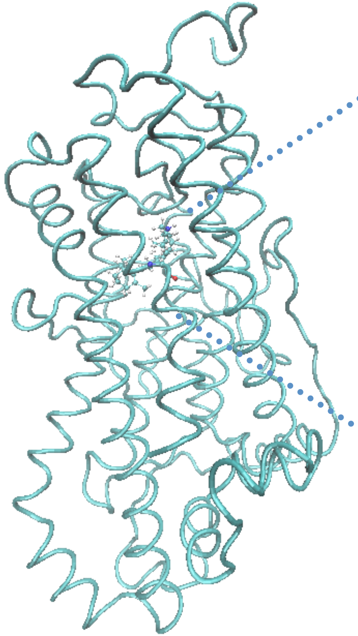
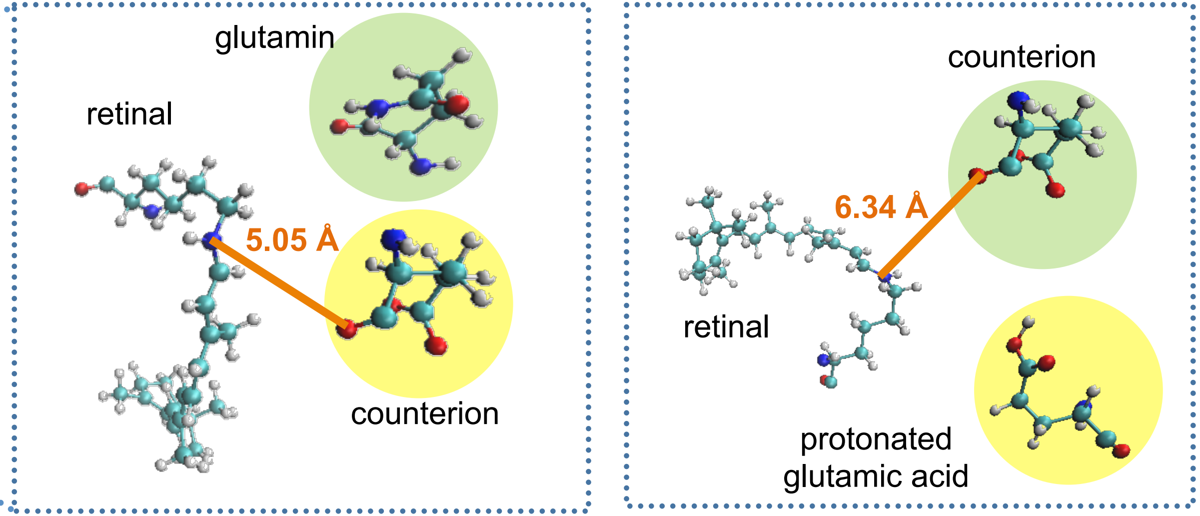
- These rhodopsins are applicable for testing the hypothesis.



rhodopsin



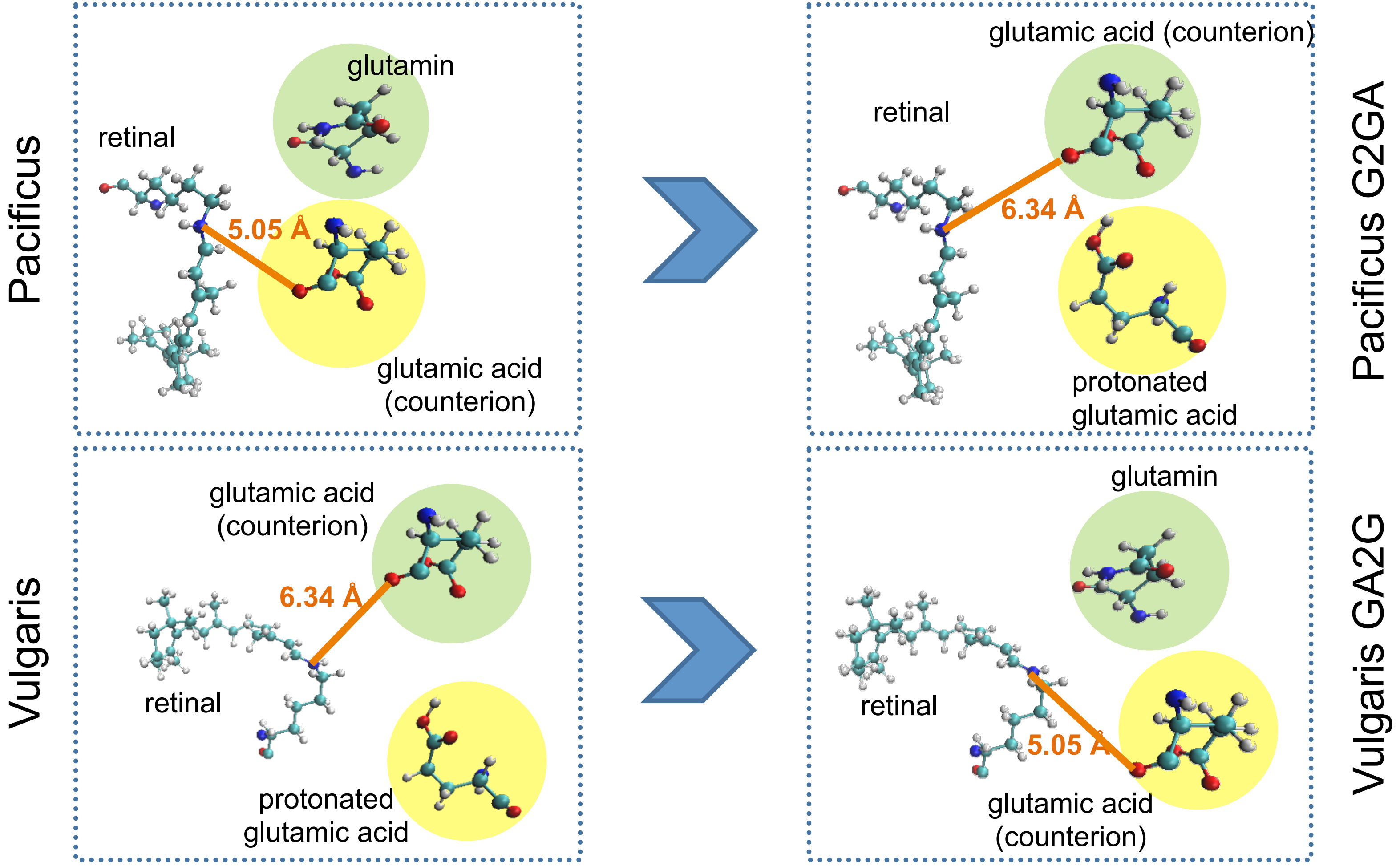
Todarodes Pacificus

λ = 480 nm

Octopus Vulgaris

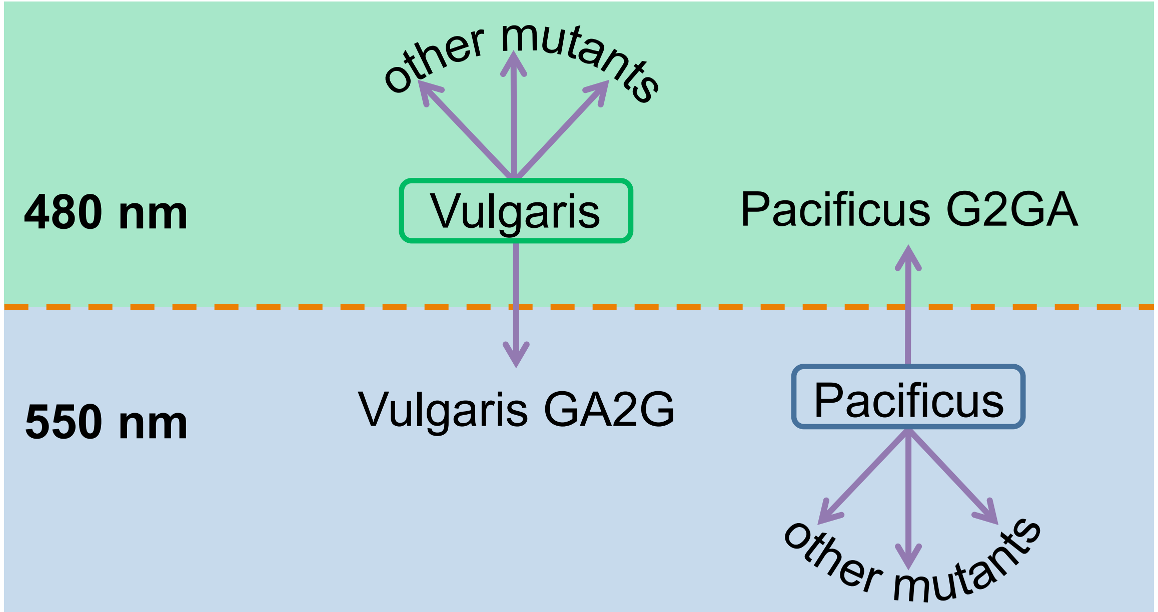
λ = 550 nm

Mechanism of spectral shift



Mechanism of spectral shift

The absorption spectra of these mutants were calculated.
Then other mutants with different substitutions were created and their spectra were calculated. Other substitutions barely affected the spectra.



Result

The G2GA mutation is responsible for spectrum shift.

Conclusions

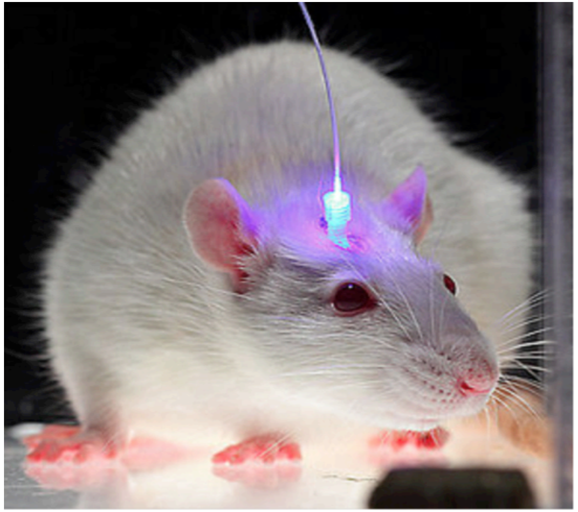
- The mechanism of visual adaptation in marine animals was discovered.

- The hypothesis that the absorption spectrum of rhodopsin depends on the distance between the retinal and the counterion was confirmed.

- The same amino acid changes made in bacterial rhodopsins could be used for shifting radiation spectrum to IR range.

Futher work

In the future, we are going to carry out the same substitution of amino acid in bacterial archaerhodopsin-3 to shift its spectrum of radiation into the IR range.



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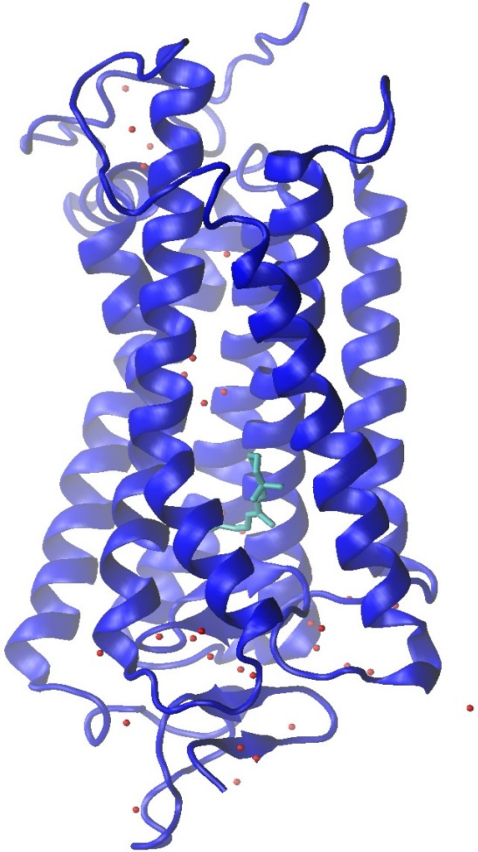

Archaerhodopsin-3

Thank you for attention!

https://animalsake.com/squid-vs-octopus-whats-difference

Affection of energy difference by electrical field from negative counterion.