Color Vision in Mantis Shrimp

Molecular understanding of color vision in stomatopod crustaceans

S. Hwang, T. Utesch, H. Sun, P. Hegemann, *Humboldt-Universität zu Berlin and Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP)*

In Short

- Unraveling conformational changes of rhodopsin during retinal *cis-trans* isomerization using molecular dynamics simulations
- Exploring the color tuning mechanism of animal opsins using molecular dynamics simulations and quantum mechanics/molecular mechanics simulations
- Predicting key factors for color tuning using molecular dynamics simulations and quantum mechanics/molecular mechanics simulations

The perception of color in animals plays a vital role in recognizing and identifying objects, achieved through the absorption of light by photoreceptors. These photoreceptors are membrane proteins with seven transmembrane helices known as opsins. Rhodopsin, the complex formed by opsin and 11-*cis* retinal as a chromophore via Schiff base with a lysine amino acid, is responsible for enabling animal vision. The protonated form of retinal carries a positive charge that is stabilized by electrostatic interaction with a negatively charged amino acid, referred to as a counterion. Animal rhodopsins belong the largest subfamily of G protein-coupled receptors (GPCRs).[1] Upon photon absorption, the isomerization of 11-*cis* retinal to all-*trans* retinal (Figure 1A) triggers structural changes in the protein, leading to the binding of G proteins on the intracellular side and subsequent downstream signaling.

Stomatopod crustaceans (mantis shrimp) serve as interesting organisms for studying animal vision due to their ability to detect a broad range of light wavelengths, including ultraviolet and far-red light, which goes far beyond the human vision, as well as polarization vision.[2] Recent studies on stomatopod rhodopsins, utilizing a combination of transcriptome and complementary DNA sequencing techniques, have unveiled the existence of over 30 distinct rhodopsins in the stomatopod's eye.[3] These rhodopsins are expressed at varying levels and distributed across different locations. Each rhodopsin exhibits a specific maximum light absorption and can be broadly categorized into three phylogenic groups based on the absorption properties: short-, middle-, and long-wavelength sensitive. The differences in light absorption can be attributed to evolutionary pressures, resulting in variations in amino acid compositions within the chromophore binding pocket. These differences contribute to the distinct wavelengths observed in different rhodopsins.

In our current project, we will focus on studying the structural rearrangement of proteins influenced by retinal *cis-trans* isomerization in various rhodopsins of stomatopod, employing multiple microsecond molecular dynamics (MD) simulations (Figure 1B,C). MD simulations are powerful methods for investigating the thermodynamic properties of proteins in atomic detail, considering the presence of lipids, ions, and solvents. By combining MD simulations with excitation energy calculations using quantum mechanics/molecular mechanics (QM/MM), we aim to enhance our understanding of color vision. By comparing our computational studies with experimental mutation and spectroscopic data, we aim to uncover the key determinants of specific wavelengths and further advance our understanding of color vision.

WWW

https://www.biologie.hu-berlin.de/de/gruppenseiten/expbp

More Information

[1] K. L. Pierce, R. T. Premont, R. J. Lefkowitz, *Nat. Rev. Mol. Cell Biol.* **3**, 639-650 (2002). doi:10.1038/nrm908

[2] J. Marshall, T. W. Cronin, S. Kleinlogel, *Arthropod. Struct. Dev.* **36**, 420-448 (2007). doi:10.1016/j.asd.2007.01.006

[3] M. L. Porter, H. Awata, M. J. Bok, T. W. Cronin, *Proc. Natl. Acad. Sci. U.S.A* **117**, 8948-8957 (2020). doi:10.1073/pnas.1917303117

[4] J. Jumper, R. Evans, A. Pritzel, T. Green, M. Figurnov, O. Ronneberger, K. Tunyasuvunakool, R. Bates, A. Zidek, A. Potapenko, A. Bridgland, C. Meyer, S. A. A. Kohl, A. J. Ballard, A. Cowie, B. Romera-Paredes, S. Nikolov, R. Jain, J. Adler, T. Back, S. Petersen, D. Reiman, E. Clancy, M. Zielinski, M. Steinegger, M. Pacholska, T. Berghammer, S. Bodenstein, D. Silver, O. Vinyals, A. W. Senior, K. Kavukcuoglu, P. Kohli, D. Hassabis, *Nature* **596**, 583-589 (2021). doi:10.1038/s41586-021-03819-2

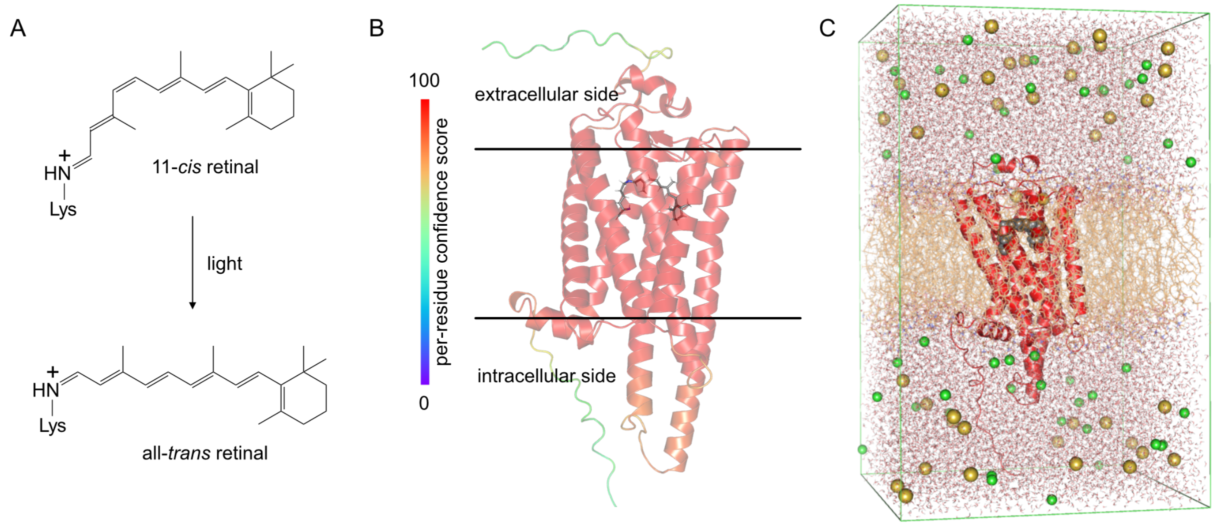

Figure 1: *Molecular dynamics simulations of stomatopod rhodopsin. A) Light-induced retinal isomerization from 11-cis to all-trans retinal in animal rhodopsin. B) The model of stomatopod opsin, generated using AlphaFold2 [4], is visualized in a cartoon representation, and it is displayed together with the bound 11-cis retinal depicted as a grey stick model. The opsin model is color-mapped with per-residue confidence scores. C) System setup of stomatopod rhodopsin for molecular dynamics simulations. The rhodopsin structure is visualized as a red cartoon representation. 11-cis retinal is displayed as a grey sphere model. The lipid molecules are depicted as orange sticks. Water molecules are represented by red sticks. Sodium and chloride ions are shown as yellow and green spheres, respectively.*

Project Partners

Prof. John T. M. Kennis, Department of Physics and Astronomy, Biophysics of Photosynthesis, Vrije Universiteit Amsterdam

Funding

European Research Council Synergy grant "Switchable rhodOpsins in Life Sciences" (grant number: 951644)

DFG Subject Area

201-02