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PRESS RELEASE

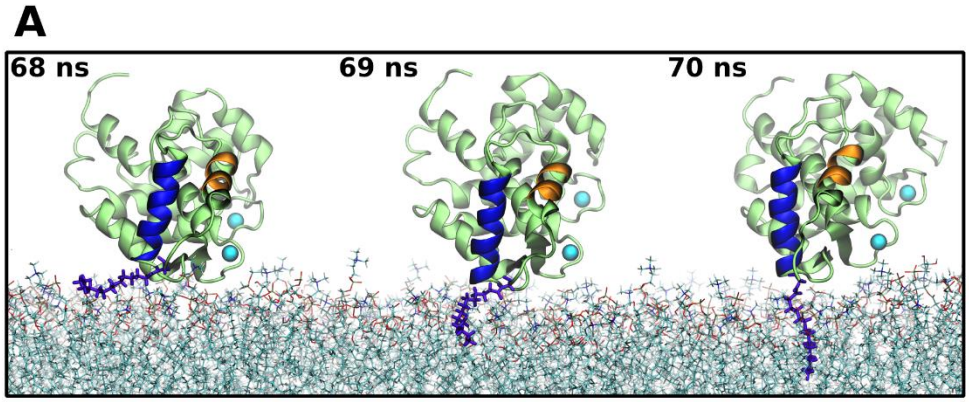
How does the human retina adapt to changes in illumination?

***Prague, August 3, 2017* – A prestigious journal of the American Chemical Society the ACS Central Science has published a paper from Pavel Jungwirth Group at the Institute of Organic Chemistry and Biochemistry of the CAS, modelling a key step in retinal response to changing light conditions.**

The retinal response involves recoverin, a neuronal calcium-binding protein which binds onto the photoreceptor cell membrane. Although an approximate binding mechanism has been described, only the latest molecular dynamics simulations made it possible to elucidate in detail its individual stages and unravel the regulatory role of calcium.

Students Štěpán Timr, Roman Pleskot, Jan Kadlec, and others, together with their advisor Pavel Jungwirth shed light on the process in which the binding of two calcium ions to a recoverin molecule promotes the ejection of its hydrophobic myristoyl moiety. This moiety then serves to anchor recoverin to the cell membrane. The specific manner of recoverin binding prevents the action of rhodopsin kinase, the enzyme regulating the rhodopsin cycle. By suppressing the kinase, recoverin makes it ultimately possible for the retina to effectively adapt to changed illumination.

Molecular dynamics simulation has thus proven to be a unique tool to describe the molecular mechanism of a physiologically important aspect of vision that is difficult to study experimentally.



Molecular dynamics simulation snapshots capturing the insertion of the protein's myristoyl moiety into the photoreceptor cell membrane.

Article: *Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality*
Štěpán Timr, Roman Pleskot, Jan Kadlec, Miriam Kohagen, Aniket Magarkar, and Pavel Jungwirth
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Prof. Pavel Jungwirth (born 1966, Prague) is a Czech physical chemist, university lecturer and science popularizer. He studied physics at the Faculty of Mathematics and Physics of Charles University (MMF UK), Prague with a major in chemical physics. He pursued a Ph.D. in computational chemistry at the J. Heyrovský Institute of Physical Chemistry of the CAS, where his advisor was Prof. R. Zahradník. He held postdoc and visiting scientist positions at University of California, Irvine, at South California University, Los Angeles, and at Hebrew University, Jerusalem. Currently he is a Distinguished Chair at the Institute of Organic Chemistry and Biochemistry of the CAS and also a Full Professor (external faculty) in the Department of Chemical Physics and Optics, MFF UK and is a Finland Distinguished Professor at Technical University in Tampere.

Pavel Jungwirth has published over 270 original papers in prestigious journals including Science, Nature Chemistry, and PNAS with more than 10,000 citations. He is a senior editor of the Journal of Physical Chemistry published by the American Chemical Society. He is a member of the Learned Society of the Czech Republic and recipient of numerous awards, including the Spiers Prize by the Royal Society of Chemistry (UK) and the Jaroslav Heyrovský Honorary Medal for Merit in Chemical Sciences by the Czech Academy of Sciences.

Popular science articles by Pavel Jungwirth have appeared in the weekly Respekt and in popular science shows broadcast by the Czech Radio and Czech TV.

The Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences / IOCB Prague (www.iocb.cz) is a leading scientific institution in the Czech Republic, recognized internationally. Its primary mission is basic research in the fields of chemical biology and medicinal chemistry, organic and material oriented chemistry, chemistry of natural compounds, biochemistry and molecular biology, physical chemistry, theoretical chemistry, and analytical chemistry. The Institute has a long tradition and expertise in medicinal chemistry and drug development together with the pharma industry. Antivirals discovered by Antonín Holý and developed further by Gilead Sciences revolutionized the treatment of AIDS and hepatitis B and have significantly improved lives of millions of people around the globe.

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