Abstract Submitted
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Predicting peak spectral sensitivities of vertebrate cone visual pigments using atomistic molecular simulations[1] JAGDISH SURESH PATEL, Center for Modeling Complex Interactions, University of Idaho, CELESTE BROWN, Institute for Bioinformatics and Evolutionary, Department of Biological Sciences, University of Idaho, F. MARTY YTREBERG, Institute for Bioinformatics and Evolutionary Biology, Department of Physics, University of Idaho, DEBORAH STENKAMP, Institute for Bioinformatics and Evolutionary Biology, University of Idaho — Vertebrate visual perception is initiated when light strikes rod and cone photoreceptors within the retina of the eye. Peak spectral sensitivities (λ_{max}) of visual pigments, are a function of the type of chromophore and the amino acid sequence of the associated opsin protein in the photoreceptors. To determine how minor sequence differences could result in large spectral shifts, we selected a spectrally-diverse group of 14 teleost Rh2 cone opsins for which sequences and λ_{max} are experimentally known. Molecular dynamics simulations were carried out after embedding cone opsin homology structures within explicit bilayers and water. Simulations revealed structural features of the chromophore, that contributed to diverged spectral sensitivities. Statistical tests performed on all the observed structural parameters of the chromophore revealed that a two-term, first-order regression model was sufficient to accurately predict λ_{max} (R^2=0.94) over a range of 452-528 nm. This approach was efficient and simple in that site-by-site molecular modifications were not required to predict λ_{max}.

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