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**Insight into the Chemical Compass Mechanism of Cryptochromes by Computational Investigation** RUTH PACHTER, GONGYI HONG, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base Ohio 45433-7702 — In this work we investigated aspects of the light-dependent inclination compass, largely assumed in avian magnetic perception, e.g. of European robins. It is postulated that radical pairs (RPs) are formed in cryptochrome (Cry) photoreceptors that contain a redox-active flavin adenine dinucleotide (FAD) in proximity to a Trp triad. The hypothesis was previously rationalized theoretically for the Cry from Arabidopsis thaliana (AtCry1), and the pKa of the proximate residue (PR) to the FAD we derived from QM/MM MD simulations is consistent with this assumption. However, attempts to extrapolate the results to other species are complicated. In the Cry from Drosophila melanogaster (DmCry1), which demonstrated a magnetic response, the FAD anionic radical ground state differs from an oxidized form in AtCry1, and the PR to the FAD is Cys rather than Asp in AtCry1. Investigation for DmCry1 model compounds, showing potential feasibility of a RP mechanism, will be described, where the calculated excitation energy is in agreement with experiment. Involvement of a Tyr instead of Trp in the triad was also considered. Because Crys from the garden warbler form RPs, a RP mechanism was examined, based on a 3D structure derived by homology modeling and MD simulations.

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