Magnetosensitive biomolecules

Simulations of Supramolecular Biological Systems

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In Short

- Homology modelling and simulation of currently non-existent structural models of avian cryptochromes
- Exploration of possible homo-multimeric cryptochrome structures
- Reconstruction of the C-terminal in cryptochrome 4a

To decipher the nature of magnetoreception in birds, a multidisciplinary-multiscale investigation is essential (Fig. 1A). Despite decades of study, the physical basis of the avian magnetic sense remains elusive. Currently, the dominant theory which describes the quantum-effect that may enable birds to navigate over great distances is based on a radical-pair mechanism [1–5]. It is believed that inside a protein called cryptochrome 4, there is a possibility for the creation of a radical pair between a light-harvesting chromophore flavin-adenine dinucleotide (FAD) and tryptophan residues [6,7]. The formation of radical products is not an unambiguous event. The created radical pair has two unpaired electrons that can be entangled (they can be in a singlet or a triplet state). Precisely at this point, a magnetic field can influence the creation of products by modulating the electron spins' relative orientation. Cryptochrome is a ubiquitous protein found in every organism and different tissues [8]. Cryptochrome, which has evolved as a magnetic compass sensor, can be expected to have properties – structural, kinetic, dynamic, magnetic – that differentiate it from cryptochromes with different biological functions [3]. Its role varies among organisms, from entrainment of circadian rhythms in vertebrates to stem elongation regulation in plants [5,6]. It has been found in the eyes of birds, and it has been shown that it is strongly expressed in outer segments of double cones cells all over the retina of chicken and European robin during the migratory season [9].

Here we wish to (i) elucidate the mechanics which would enable selected cryptochrome to serve as magnetoreceptors on a molecular level, (ii) create and validate homology models of cryptochromes for which crystal structures are lacking (iii) model and test the possible C-terminal tails of cryptochrome 4a protein that could not be resolved experimentally. All of the planned investigations will help understand the nature of magnetoreception and whether a cryptochrome-based compass sensor's hypothesis is indeed feasible. To this end, we are planning to combine all-atom molecular dynamics (MD) simulations with in-house written algorithms for recreating the missing C-terminal part of various cryptochromes.

The proposed computations are in fact crucial for the success of several collaborative research projects of the Quantum Biology and Computational Physics (QuantBioLab) group of the University of Oldenburg. The group is a part of the SFB 1372 and the graduate school GRK 1885 funded by the German research foundation (DFG). The central aim of SFB 1372 is to achieve a comprehensive and multidisciplinary understanding of magnetoreception and vertebrate navigation from the bio-physical mechanisms to the natural behavior of navigating animals, covering every step in between. The research group of the PI is responsible for the Sig05 section of SFB 1372 'Structural and dynamical traits of avian cryptochromes.' Furthermore, the group is funded by the Volkswagen Foundation (VolkswagenStiftung) through the Lichtenberg Endowed Professorship (ger. Lichtenberg-Stiftungsprofessuren) for Prof. Dr. Ilia A. Solov'yov.

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More Information

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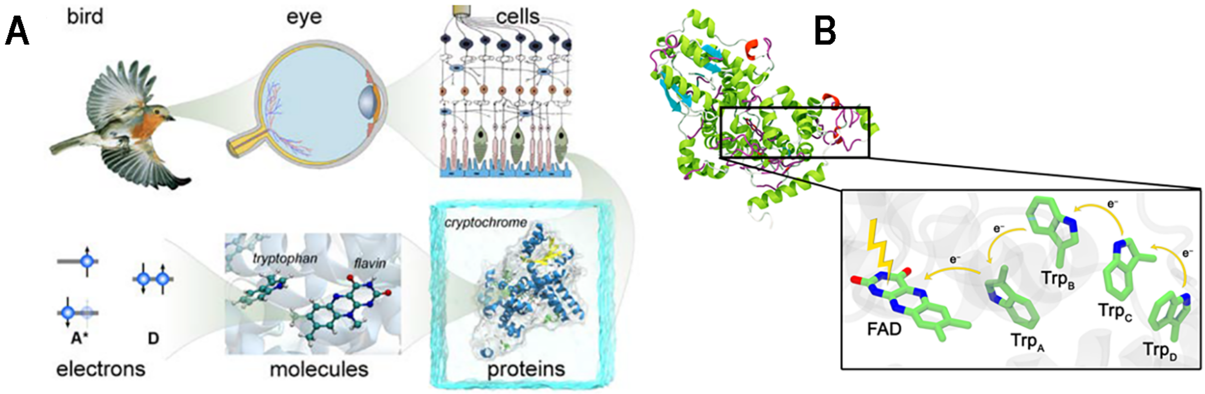

Figure 1: *A: Avian magnetoreception is a multiscale problem. B: FAD becomes a radical upon photoabsorption through electron transfer from a nearby tryptophan residue which causes a cascade of electron transfer reactions between three further tryptophan residues, shown in green.*

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Project Partners

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