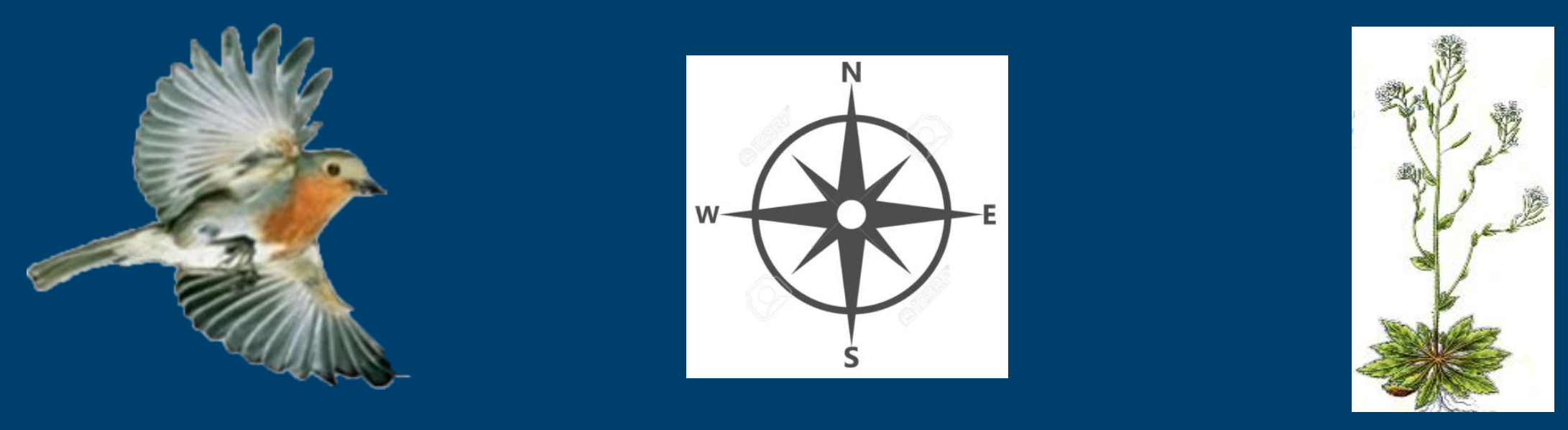
The influence of intra-protein motion on compass sensitivity: A comparison between plant and migratory bird cryptochrome



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Magnetoreception and Navigation in Vertebrates

Introduction & Motivation

The magnetic compass of migratory birds is thought to rely on the radical pair mechanism operating inside a cryptochrome blue-light photoreceptor [1]. We have investigated several dihedral and librational angles in the flavin adenine dinucleotide (FAD) and tryptophan (Trp) radical pair inside cryptochrome from European robin (ErCry4) and thale cress (AtCry1) in order to characterise cryptochrome dynamics dependent on the thermal motion of the protein. The average hyperfine interactions of nuclei in potential radical pairs inside the cryptochromes were calculated for both species, which permitted establishing the quantum yield anisotropy of the radical pair reactions in an external magnetic field. The quantum yield anisotropy is a measure for the sensitivity of a potential magnetic compass and was compared for ErCry4 and AtCry1 to conclude if one is significantly better in perceiving the magnetic field than the other. One major structural difference between ErCry4 and AtCry1 is that ErCry4 possesses a specific Trp residue (TrpD), making a radical pair based compass in ErCry4 possible through the TrpD (RPD) or a conserved TrpC (RPC), as also expected in AtCry1. All comparisons in this study have been made between the three radical pair (RP) systems AtCry1 RPC, ErCry4 RPC and ErCry4 RPD.

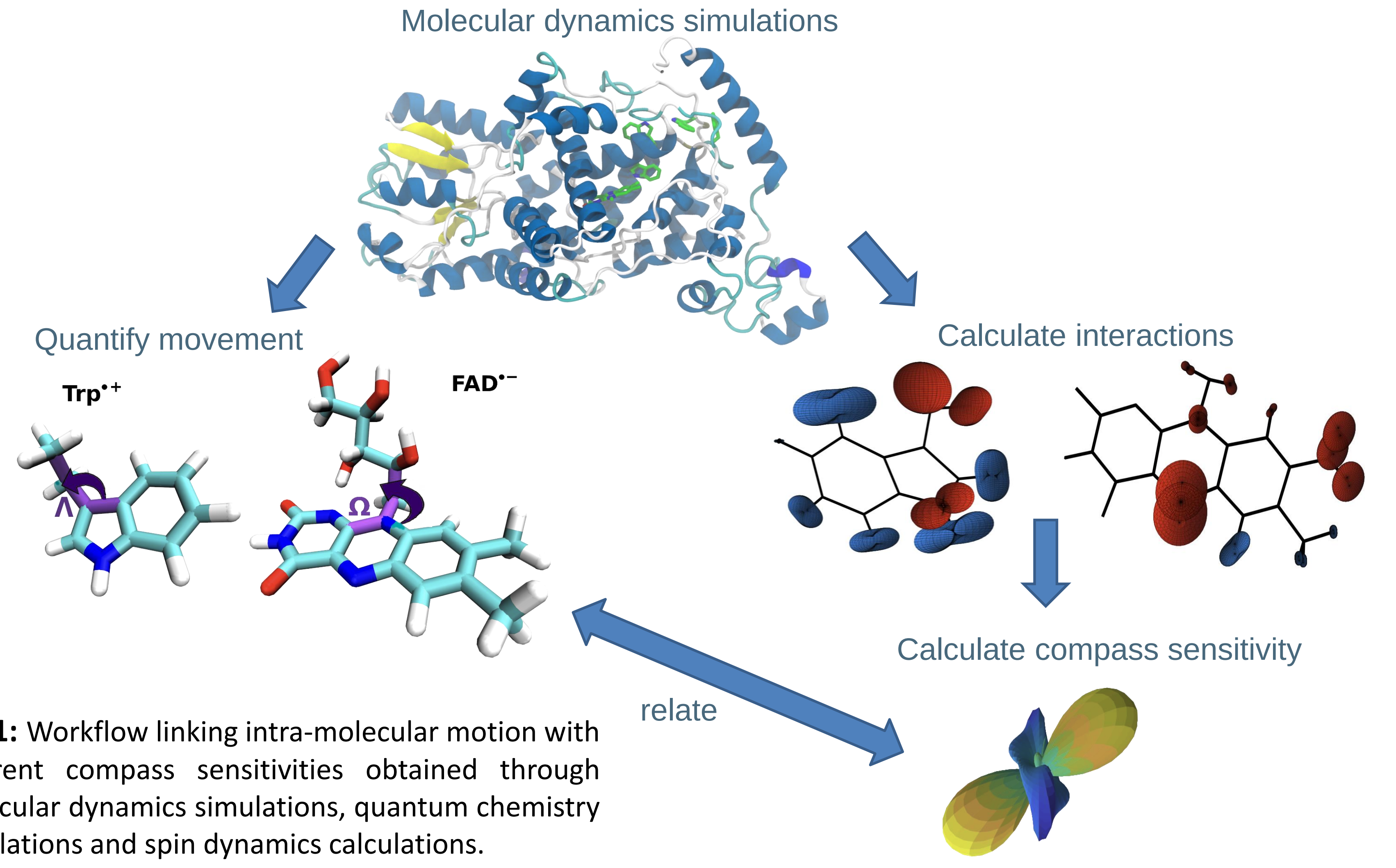


Fig. 1: Workflow linking intra-molecular motion with different compass sensitivities obtained through molecular dynamics simulations, quantum chemistry calculations and spin dynamics calculations.

Different movement of dihedral angles in 🐦 and 🌿 ?

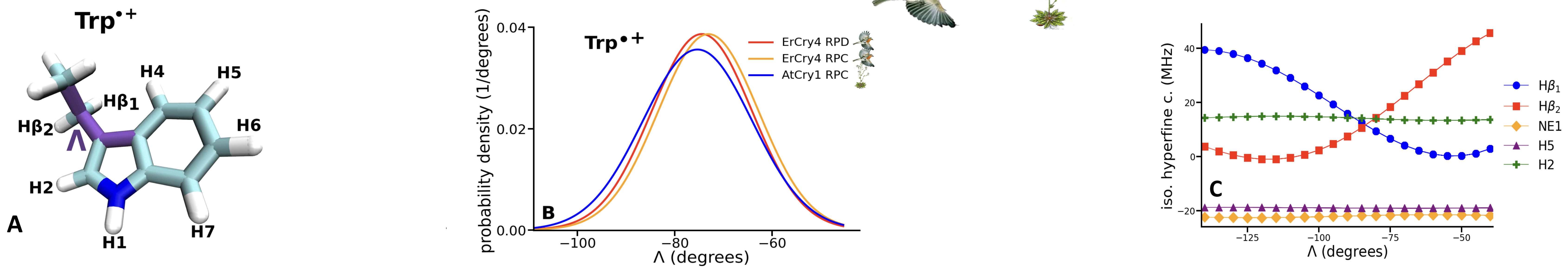


Fig. 2 : The plots in the middle figure show gaussian fits to the distributions of 2.4 x 10^6 values of the dihedral angle Λ (shown in the left figure) measured during the MD simulation for each RP system (AtCry1 RPC, ErCry4 RPC, ErCry4 RPD). Athough the difference in the distributions of Λ is small, the difference can play a significant role as seen in the right figure which illustrastes the strong dependence of the hyperfine coupling in the Hβ nuclei on Λ .

Different hyperfine coupling in 🐦 and 🌿 ?

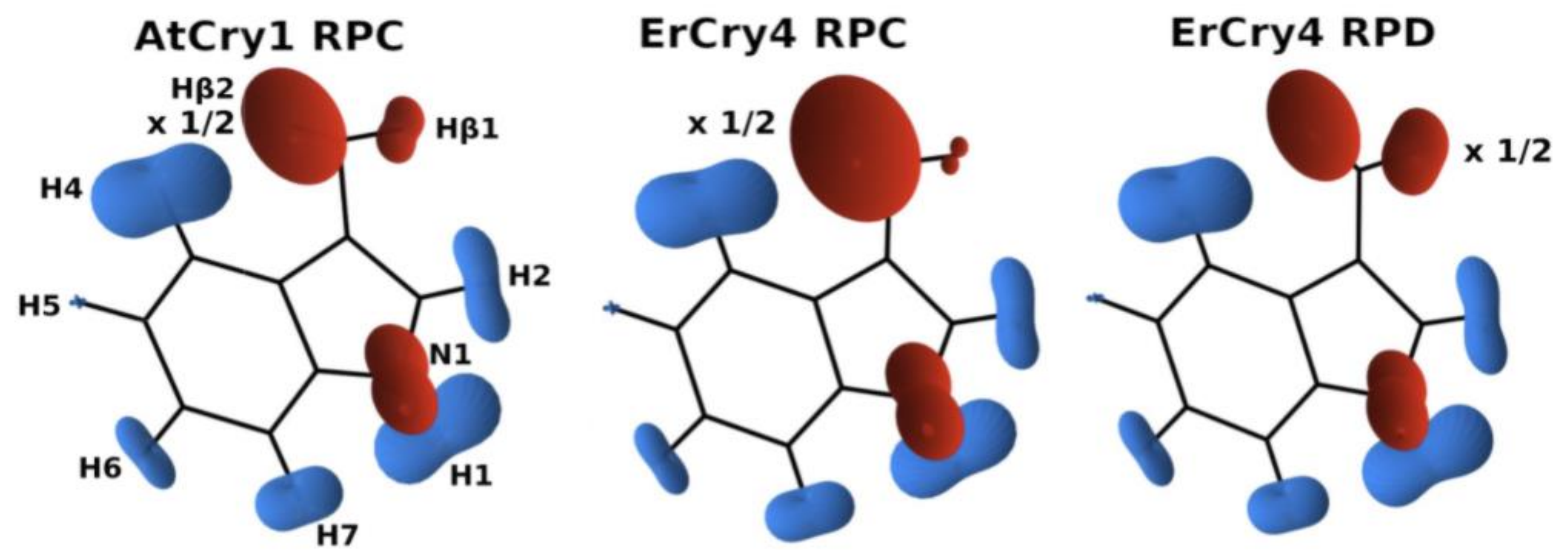
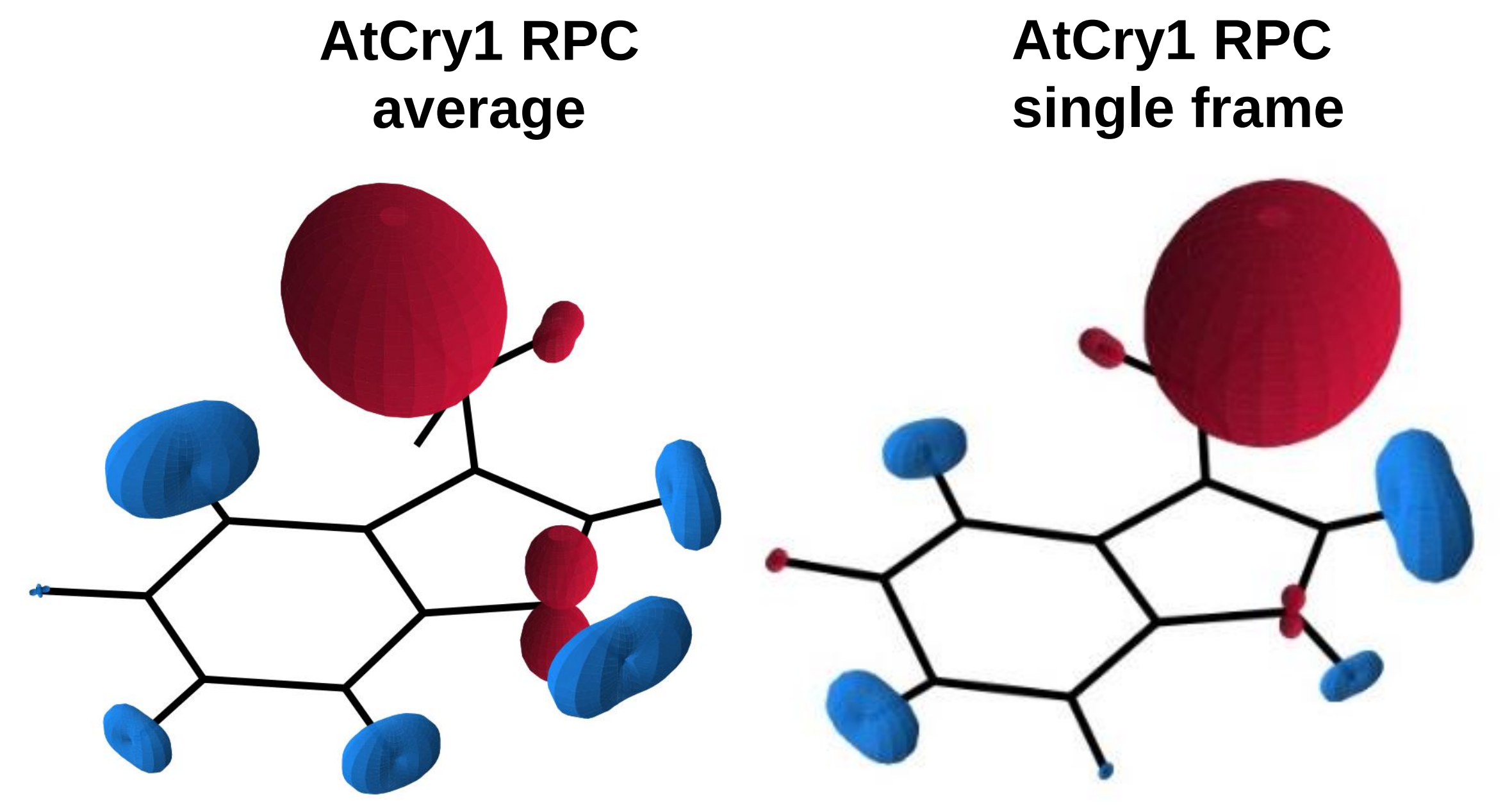


Fig. 3 : Differences exist especially in the Hβ hyperfine coupling in the Trp radicals from either AtCry1 or ErCry4.

Fig. 4 (right): Why use the average hyperfine coupling? The hyperfine interaction between random frames from the same MD simulation fluctuates a lot, the differences between two time instances can be greater than the difference between the hyperfine coupling of structures taken from cryptochromes of different species.



Different compass sensitivity in 🐦 and 🌿 ?

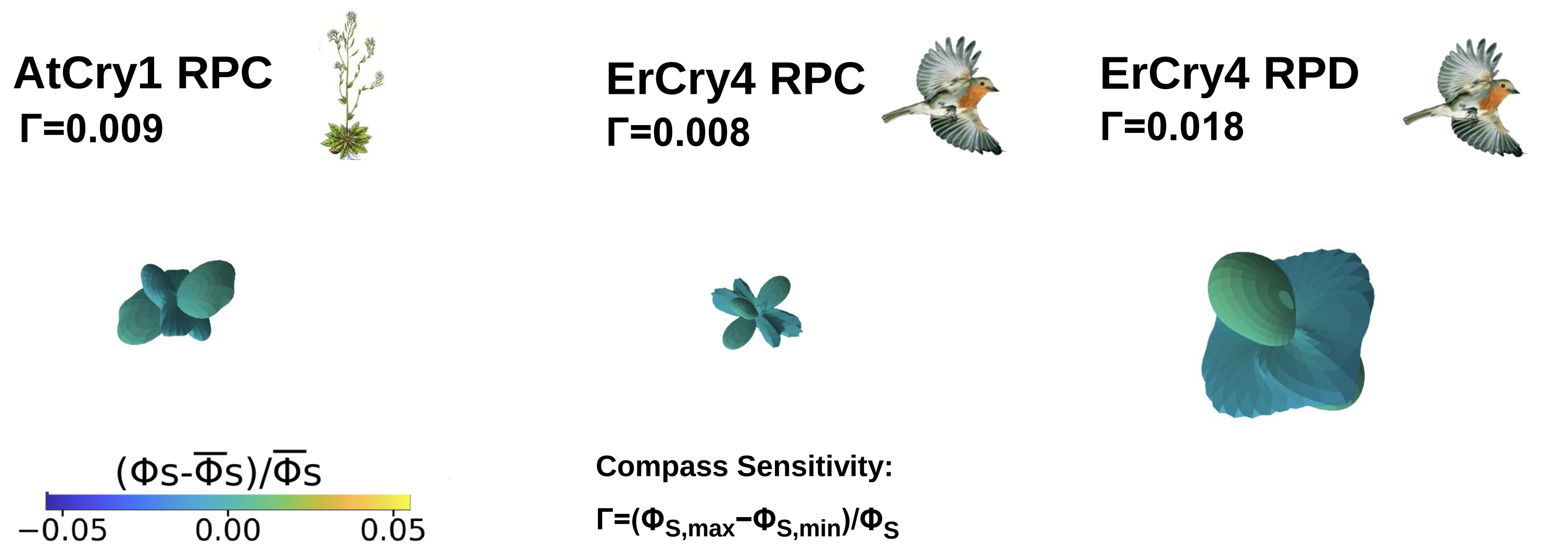
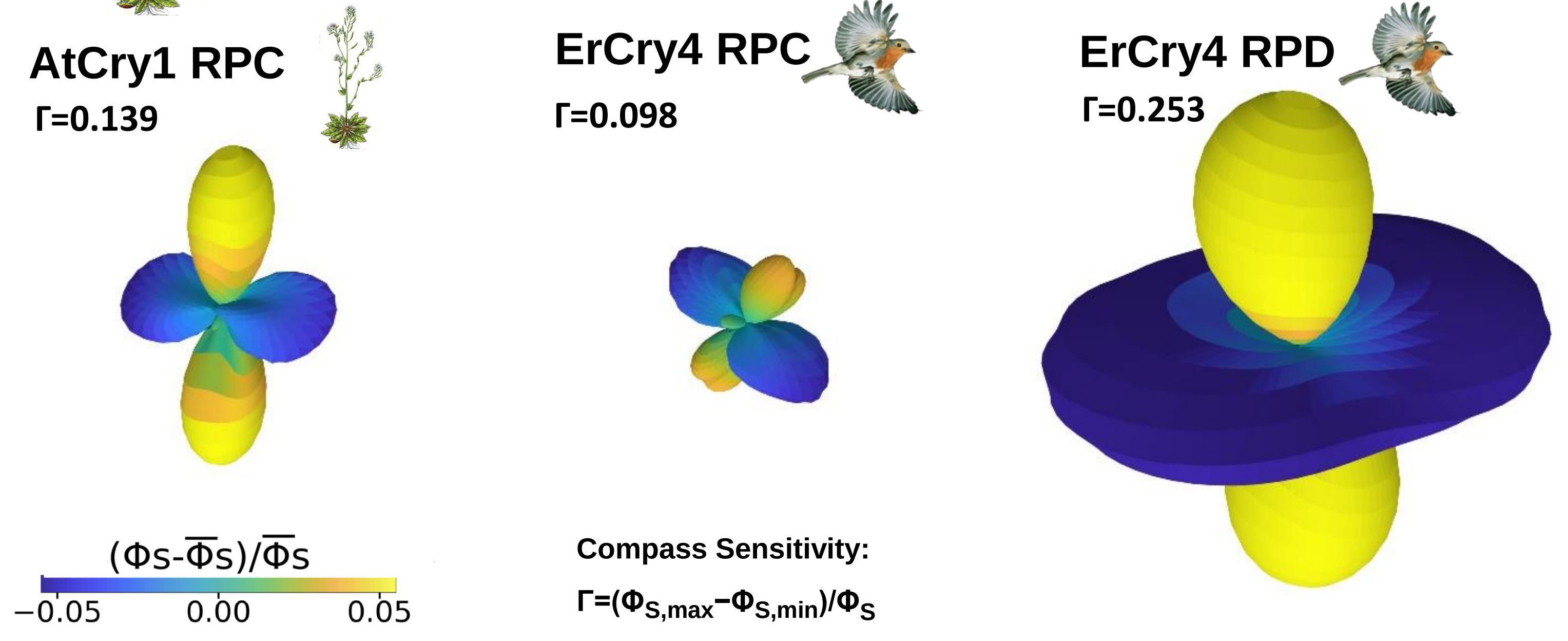


Fig. 5 : The compass sensitivity is different in thale cress and robin cryptochrome. It is best in ErCry4 in RPD state in this model considering the hyperfine coupling of 13 nuclei in the Trp and FAD radicals.

Fig. 6 (right): The different compass sensitivities due to different Λ distributions in the RP systems: Calculations based on a radical pair which is only composed of the Λ-dependent hyperfine coupling in the Hβs in Trp and the hyperfine coupling of N5 and N10 in FAD which is almost identical in all three RP systems.



Summary & Discussion

Small differences in the motion in the dihedral angle Λ lead to a different hyperfine coupling of the Hβ nuclei in Trp of the plant and robin cryptochromes. The hyperfine coupling differences seen in Fig. 3 lead to different compass sensitivities in the three studied RP systems (see Fig. 6). Other dihedral angles, the librational movement of the radicals and the timescale of the movement have been studied, but are not shown here. Furthermore, other interactions than hyperfine have to be considered possibly shifting the balance on the compass sensitivity towards RPs with TrpC being more sensitive. In conclusion, this work managed to confirm differences in motion, hyperfine coupling and compass sensitivity between the cryptochromes of different species. The influence of the parameter Λ on compass sensitivity was analysed and a necessity to use the average hyperfine coupling in these kinds of studies was found.

Reference

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