Radical Pair Mechanism and the role of Chirality-Induced Spin Selectivity during Planaria Regeneration: Effect of Weak Magnetic Field on ROS levels

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1. Effect of the recombination rates

(a) Singlet initiated when χ =0

The initial state for the following case of two radicals

$$|\psi_{In}> \;=\; \cos\left(\frac{\chi}{2}\right)|S> \;+\; \sin\left(\frac{\chi}{2}\right)|T_0> \tag{1}$$

$$P_{In} = |\psi_{In}><\psi_{In}| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.5\,(1+\sin\chi) & -0.5\cos\chi & 0 \\ 0 & -0.5\cos\chi & 0.5\,(1-\sin\chi) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{2}$$

The recombination operator is the following.

$$|\psi_S> \;=\; \cos\left(\frac{\chi}{2}\right)|S> - \sin\left(\frac{\chi}{2}\right)|T_o> \tag{3}$$

$$P_S = |\psi_S><\psi_S| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.5\,(1-\sin\chi) & -0.5\cos\chi & 0 \\ 0 & -0.5\cos\chi & 0.5\,(1+\sin\chi) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{4}$$

$$|\psi_{To}> \;=\; \sin\left(\frac{\chi}{2}\right)|S> + \cos\left(\frac{\chi}{2}\right)|T_o> \tag{5}$$

$$P_{To} = |\psi_{To}><\psi_{To}| = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.5\,(1+\sin\chi) & 0.5\cos\chi & 0 \\ 0 & 0.5\cos\chi & 0.5\,(1-\sin\chi) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \tag{6}$$

$$
P_{T+} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \qquad P_{T-} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - \sin\chi \end{bmatrix} \tag{7}
$$

	$FAD^{\cdot -}\ TrpH^{\cdot +}$	$FADH^{\cdot}\ O_2^{\cdot -}$
Eq. 2 Initial state, CISS in formation and recombination Singlet initiated (when χ =0)	Fig 1	Fig 2
Eq. 2 Initial state, CISS in the formation only Singlet initiated (when χ =0)	Fig 3	Fig 4
Eq. 8 Initial state, CISS in formation and recombination Triplet initiated (when χ =0)		
Eq. 8 Initial state, CISS in the formation only Triplet initiated (when χ =0)		

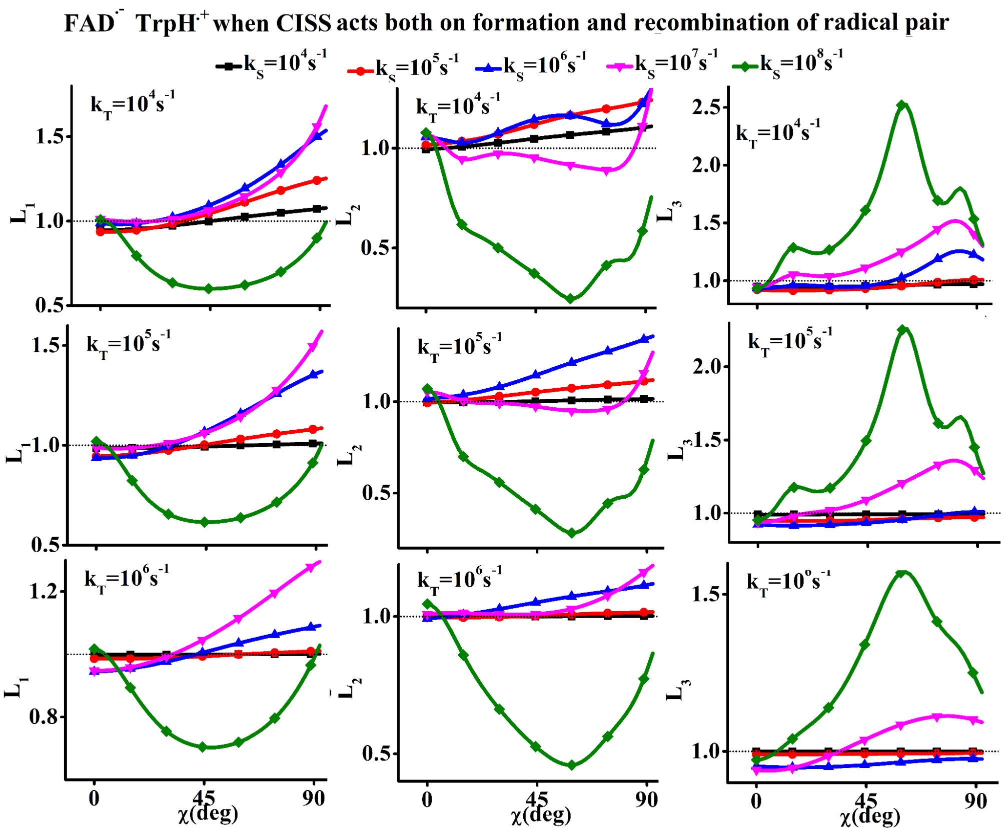

Figure1: *$FAD^{\cdot-}$ $TrpH^{\cdot+}$ when initial state is given by Eq. 2 when CISS is present in both formation and recombination of radical pair*

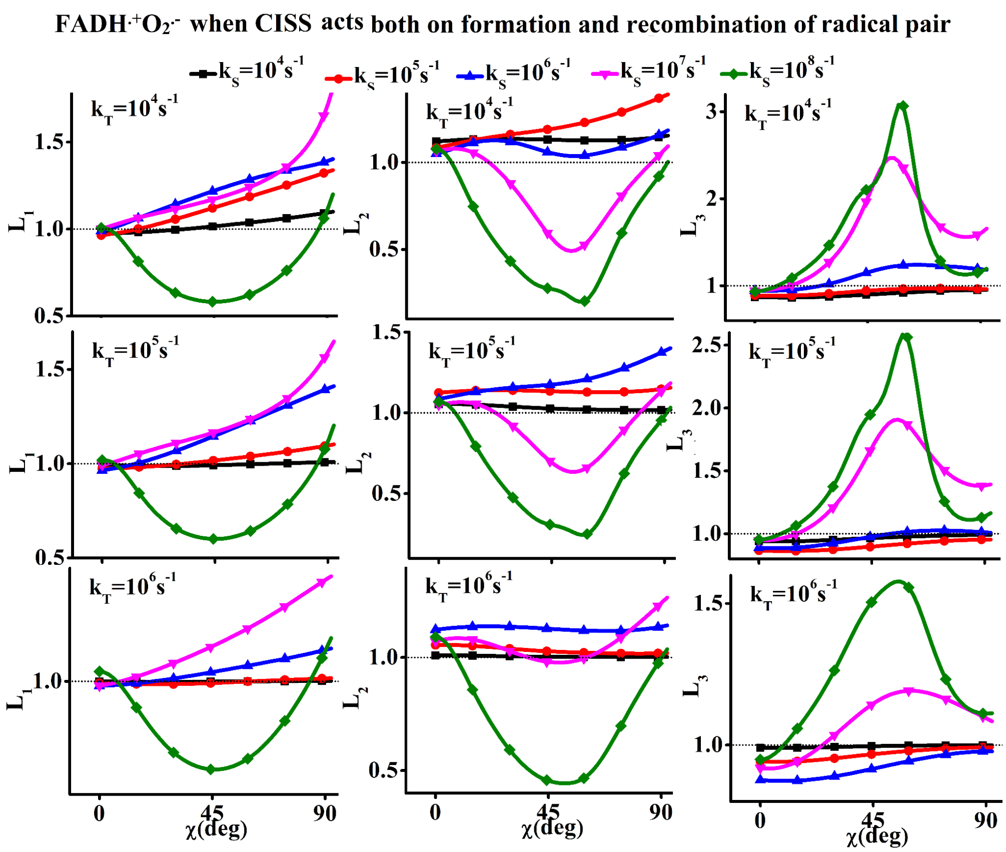

Figure2: *$FADH^{\cdot}$ $O_2^{\cdot-}$ when initial state is given by Eq. 2 when CISS is present in both formation and recombination of radical pair*

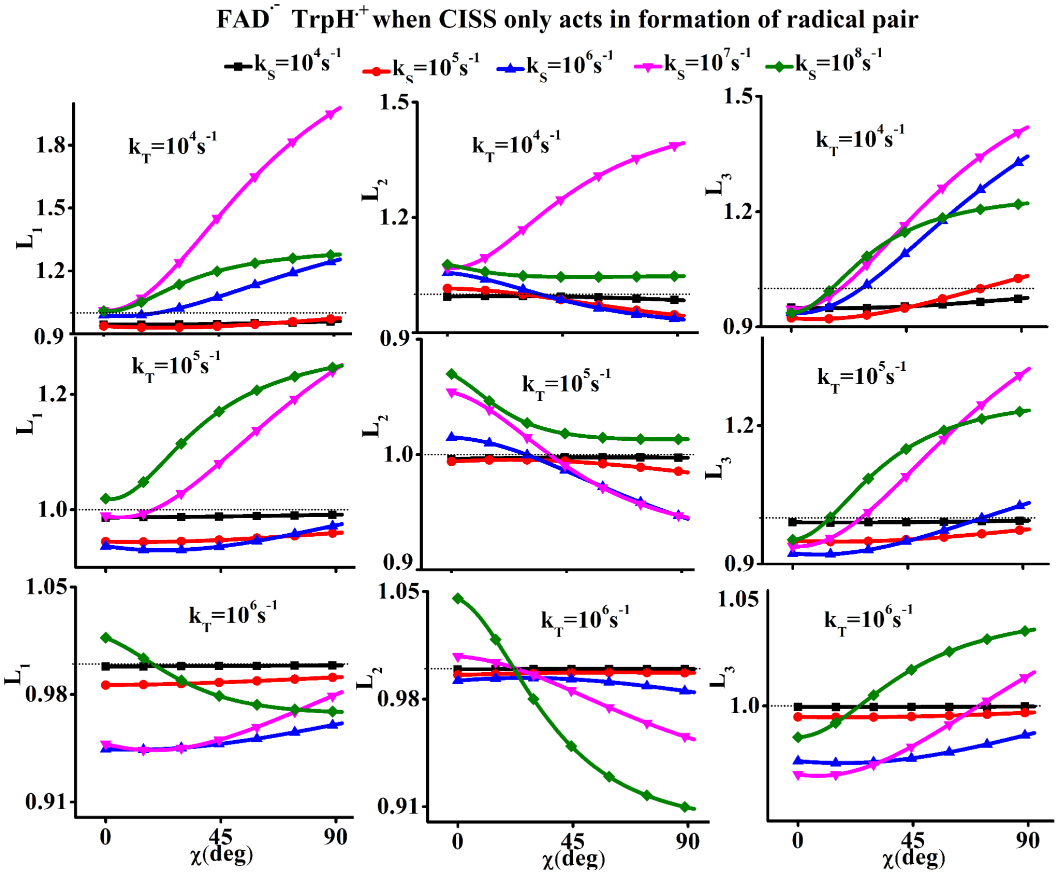

Figure3: $FAD^{\cdot-}\ TrpH^{\cdot+}$ *when initial state is given by Eq.* 2 *when CISS is present in only in formation of radical pair*

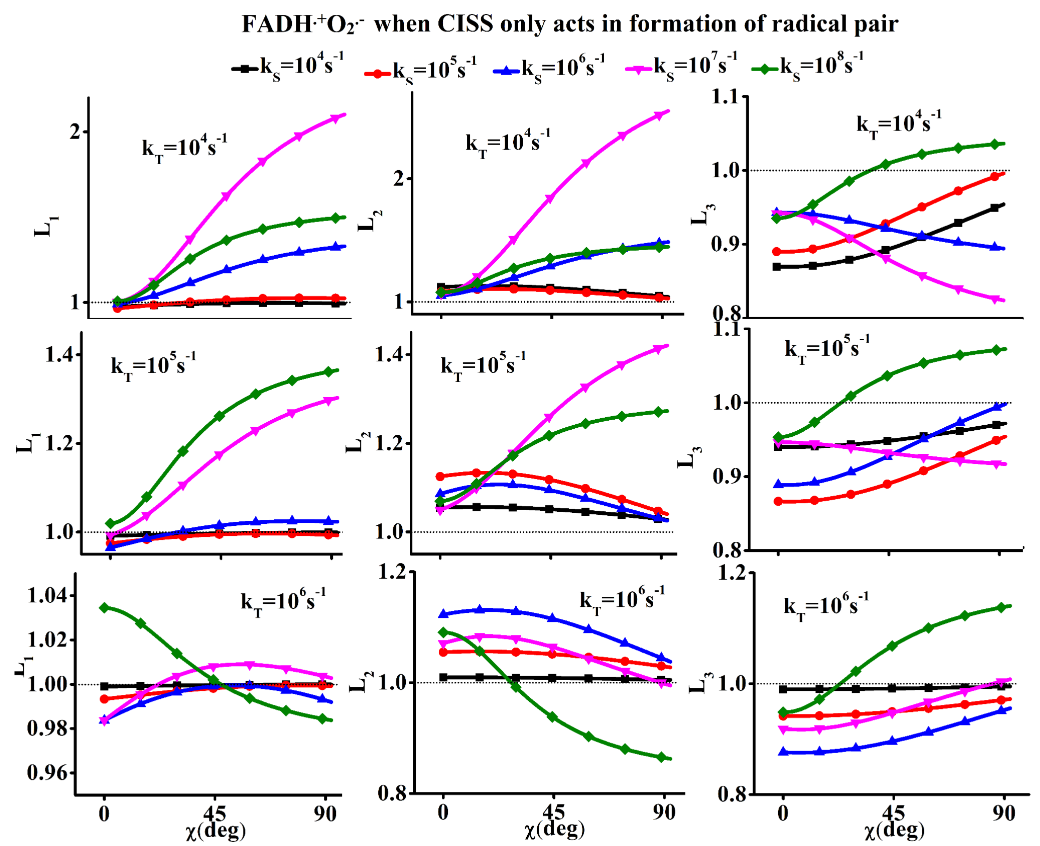

Figure4: $FADH^{\cdot}\ O_2^{\cdot-}$ *when initial state is given by Eq.* 2 *when CISS is present in only in formation of radical pair*

(b) Triplet initiated when χ =0

The initial state for the following case of two radicals. Eq. (8) is normalized when used as the initial state.

$$P_{In} = P_T = P_{T0} + P_{T+} + P_{T-} \tag{8}$$

The recombination operator is the same as what is considered.

	$FAD^{\cdot -}\ TrpH^{\cdot +}$	$FADH^{\cdot}\ O_2^{\cdot -}$
Eq. 2 Initial state, CISS in formation and recombination Singlet initiated (when χ =0)	Fig 1	Fig 2
Eq. 2 Initial state, CISS in the formation only Singlet initiated (when χ =0)	Fig 3	Fig 4
Eq. 8 Initial state, CISS in formation and recombination Triplet initiated (when χ =0)	Fig 5	Fig 6
Eq. 8 Initial state, CISS in the formation only Triplet initiated (when χ =0)	Fig 7	Fig 8

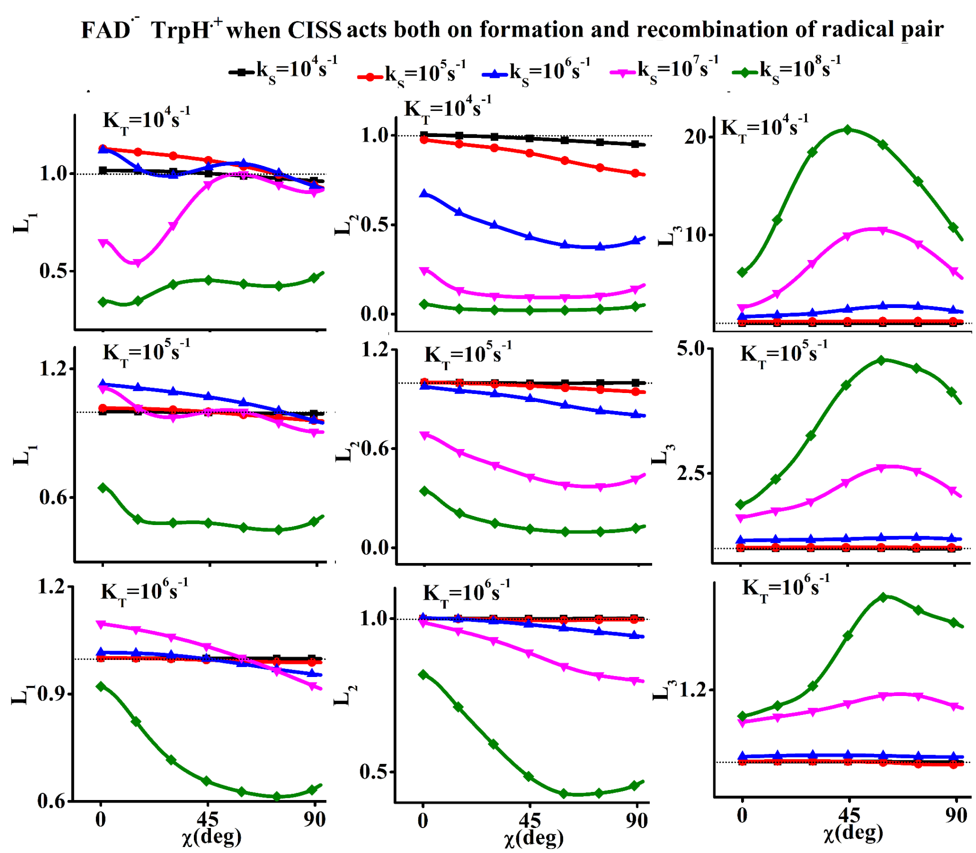

Figure5: $FAD^{\cdot -}\ TrpH^{\cdot +}$ *when intial state is given by Eq. 8 when CISS is present*

in both formation and recombination of radical pair

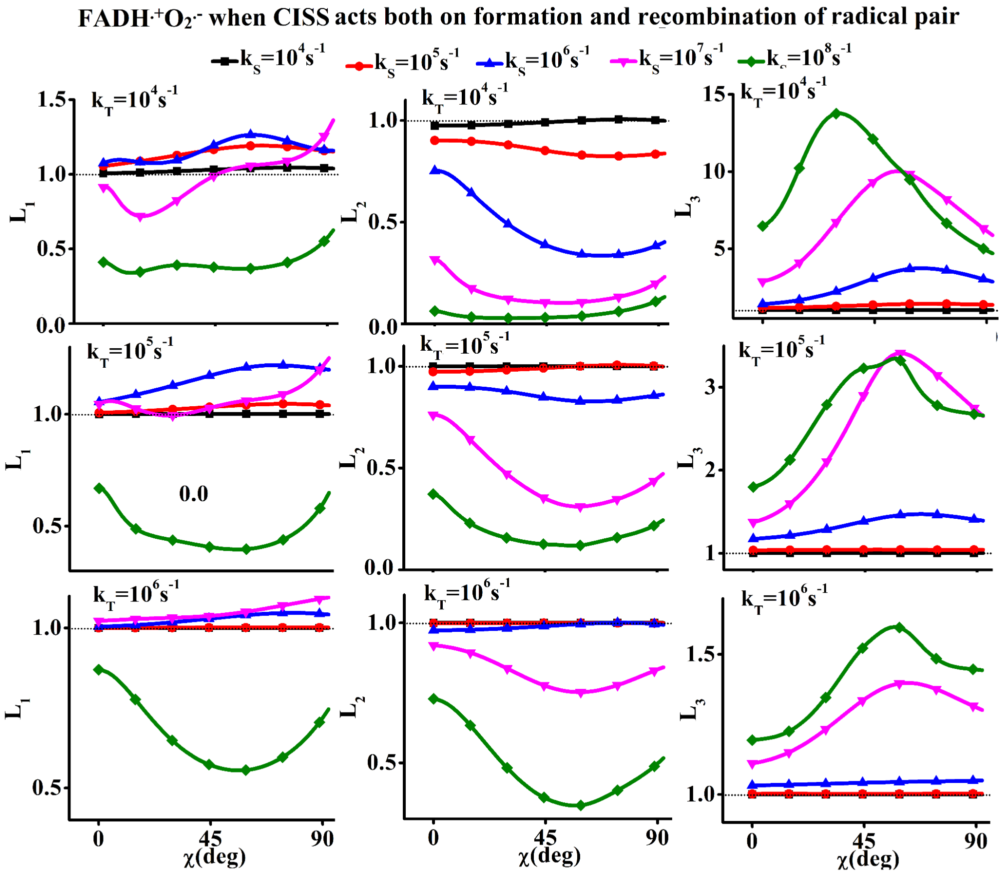

Figure6: $FADH^{\cdot}\ O_2^{\cdot-}$ *when intial state is given by Eq.* 8 *when CISS is present in both formation and recombination of radical pair*

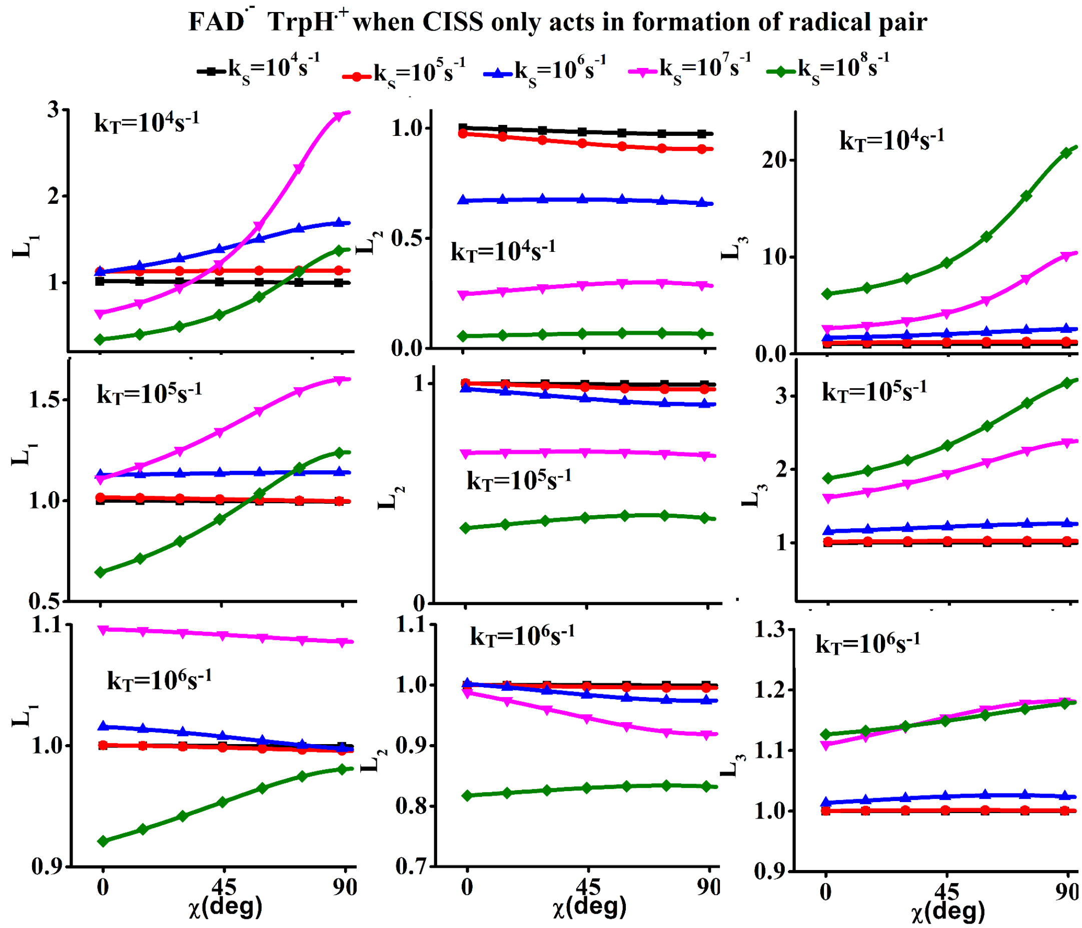

Figure7: $FAD^{\cdot-}\ TrpH^{\cdot+}$ *when intial state is given by Eq.* 8 *when CISS is present only in formation of radical pair*

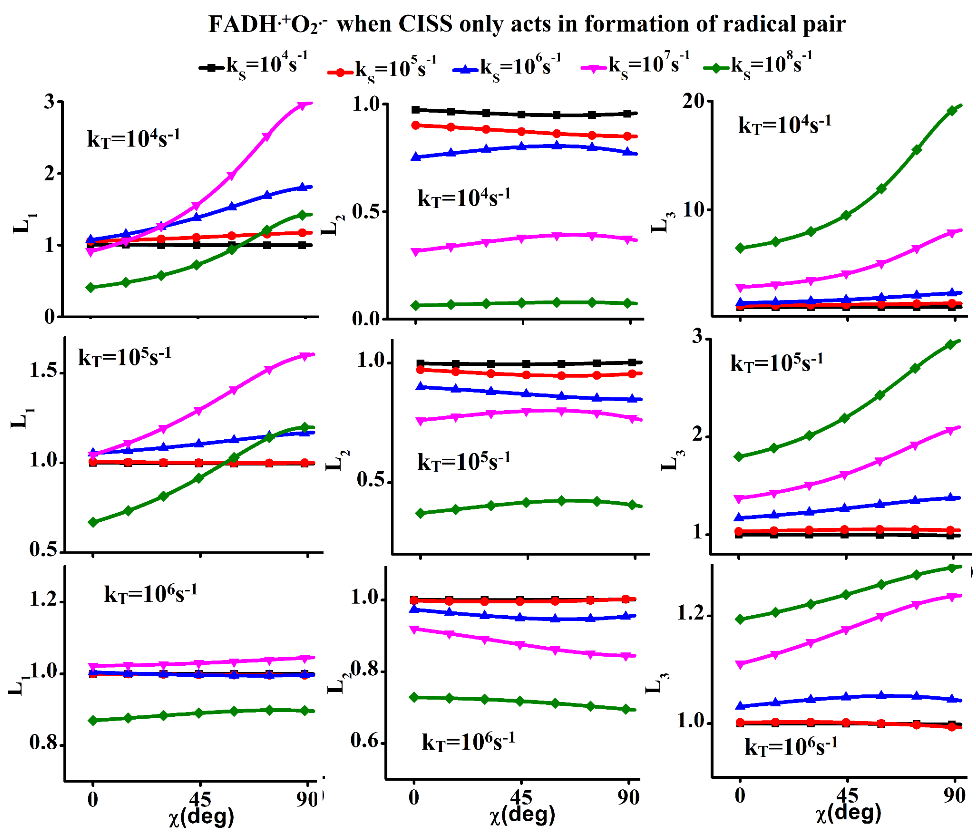

Figure8: $FADH^{\cdot}\ O_2^{\cdot-}$ *when intial state is given by Eq.* 8 *when CISS is present only in formation of radical pair*

2. Peaks at 500 μT for anisotropic hyperfine interaction

	$FAD^{\cdot -}\ TrpH^{\cdot +}$	$FADH^{\cdot}\ O_2^{\cdot -}$
Eq. 2 Initial state, CISS in formation and recombination at $\chi = \frac{\pi}{2}$)	Fig9 (Just at $\chi = \frac{\pi}{2}$ **at** $k_S = 10^7 s^{-1}$ *and* $k_T = 10^4 s^{-1}$)	

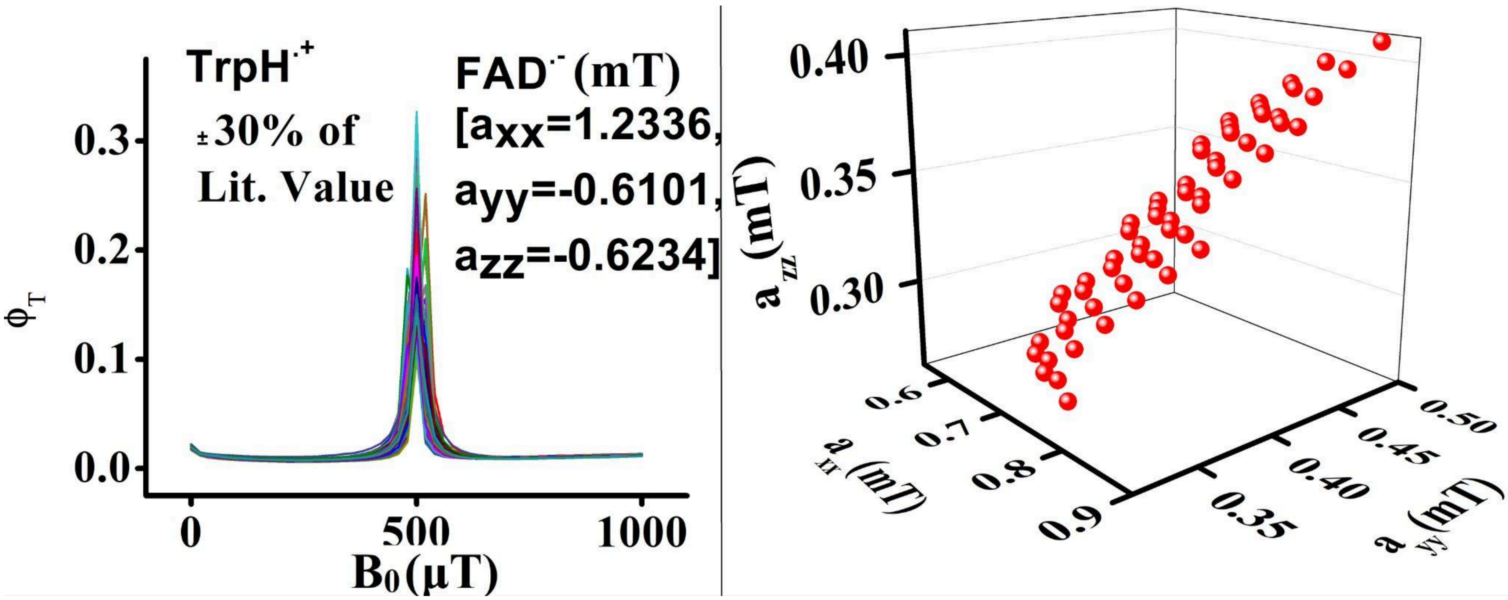

Figure 9: *(Left)*Φ_T *for* $FAD^{\cdot -}\ TrpH^{\cdot +}$ *where the hyperfine value of* $TrpH^{\cdot +}$ *is varied by ± 30% of the literature value. Here* $\Phi_T(500\ \mu\ T) > 10.\Phi_T(45\ \mu\ T)$ *. This is done for the case when D=0mT, J=0mT, and* $\chi = \frac{\pi}{2}$ *at* $k_S = 10^7 s^{-1}$ *and* $k_T = 10^4 s^{-1}$*. Moreover, this corresponds to the case when CISS acts both in the formation and recombination of radical pairs.(Right) Each red point corresponds to the hyperfine tensor of* $TrpH^{\cdot +}$ *with corresponding* $[a_{xx}, a_{yy}, a_{zz}]$ *where* $\Phi_T(500\ \mu\ T) > 10.\Phi_T(45\ \mu\ T)$

In Fig.9 (Left), we demonstrate that it is indeed possible to observe distinctive peaks at *500 μ T* at $k_S = 10^7 s^{-1}$ *and* $k_T = 10^4 s^{-1}$ and D=0 mT. However, we have deviated from the established literature values for the hyperfine tensor to achieve this. This allows some flexibility due to potential structural vibrations or folding that might occur in a biological medium and alter the hyperfine values. Considering the scenario where $FAD^{\cdot -}\ TrpH^{\cdot +}$ is involved, with the initial state as $\chi = \frac{|S\rangle + |To\rangle}{\sqrt{2}}$ at $\chi = \frac{\pi}{2}$, and with CISS contributing to both the formation and recombination of the radical pair, we calculated Fig.9 (Left). For simplicity of analysis, we adhered to the literature values $FAD^{\cdot -}$; however, we adjusted the anisotropic hyperfine component $TrpH^{\cdot +}$, varying it by *± 30%* of the established literature value to explore the effects of such variations. Fig. 9(Right) consists of a scatter plot where each red point corresponds to the hyperfine tensor $TrpH^{\cdot +}$ with corresponding $[a_{xx}, a_{yy}, a_{zz}]$where $\Phi_T(500\ \mu\ T) > 10.\Phi_T(45\ \mu\ T)$.

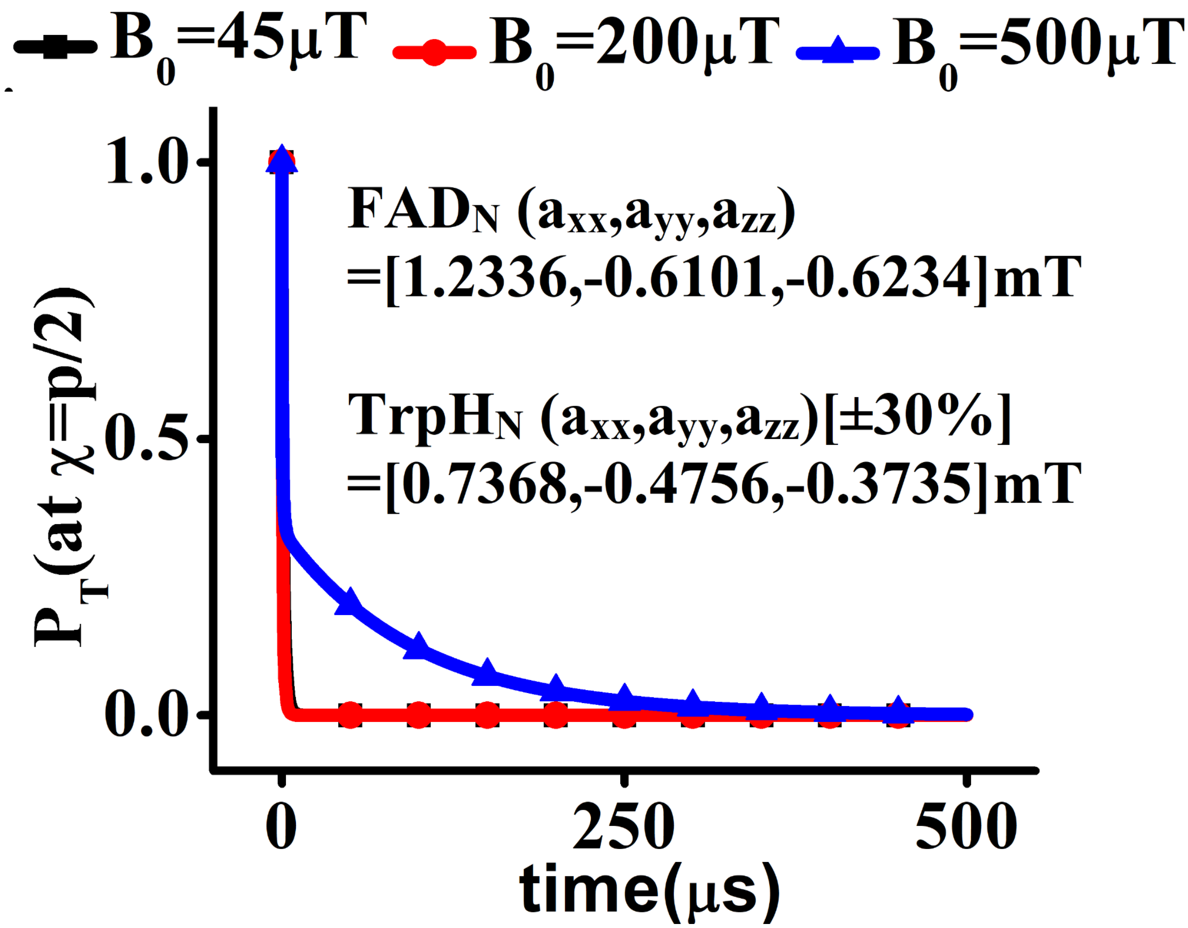

Figure 10: *P_T for $FAD^{\cdot -}\ TrpH^{\cdot +}$ where the hyperfine tensor value of $TrpH^{\cdot +}$ is varied by ± 30% of the literature value while $FAD^{\cdot -}$ hyperfine tenor values are from literature. This is done for the case when D=0mT, J=0mT, and $\chi = \frac{\pi}{2}$ at k_S=$10^7 s^{-1}$ and k_T=$10^4 s^{-1}$. Moreover, this corresponds to the case when CISS acts both in the formation and recombination of radical pairs.*

In Fig.10, we plotted P_T (Eq.8), for $FAD^{\cdot -}\ TrpH^{\cdot +}$ where the hyperfine tensor value $TrpH^{\cdot +}$ is varied by ± 30% of the literature value (exact value in Fig. 10) while $FAD^{\cdot -}$ hyperfine tenor values are from the literature. This is done for the case when D=0mT, J=0mT, and $\chi = \frac{\pi}{2}$ at k_S=$10^7 s^{-1}$ and k_T=$10^4 s^{-1}$.We observe that the lifetime P_T is much greater at 500 μT compared to 200μT and 45 μT, illustrating the reason for the peak as observed in Figure 9: (Left).

3. Hyperfine Interaction

The hyperfine tensors used in our study are based on the work by Hiscock et al. [1-2]. The $FAD^{\cdot -}\ TrpH^{\cdot +}$ molecules are drawn in Fig. 11. The nuclei considered in our simulations on each molecule are marked in red. The isotropic hyperfine values of labeled nuclei are given below.

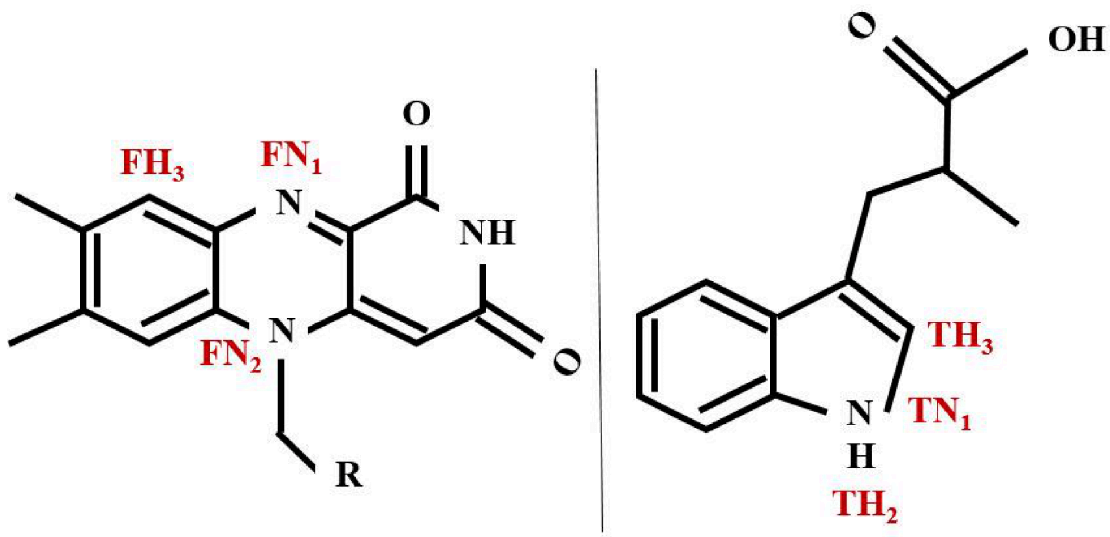

Figure 11: *(a) $FAD^{\cdot-}$ molecule and (b) $TrpH^{\cdot+}$ molecule. The nuclei marked in red are considered in our calculation. The first letter corresponds to the molecule type (F-$FAD^{\cdot-}$ and T-$TrpH^{\cdot+}$), and the second letter corresponds to the nuclei type (N-nitrogen and H-hydrogen)*

Table 1: *Hyperfine interaction in mT for $FAD^{\cdot-}$ (FN_1, FN_2, FH_3) and $TrpH^{\cdot+}$ (TN_1, TH_2, TH_3)*

FN_1	FN_2	FH_3	TN_1	TH_2	TH_3
0.5233	0.1887	-0.3872	0.3215	-0.5983	-0.2780

Similarly, the structure $FADH^{\cdot}\ O_2^{\cdot-}$ is given in Fig. 12, followed by its hyperfine distribution [3].

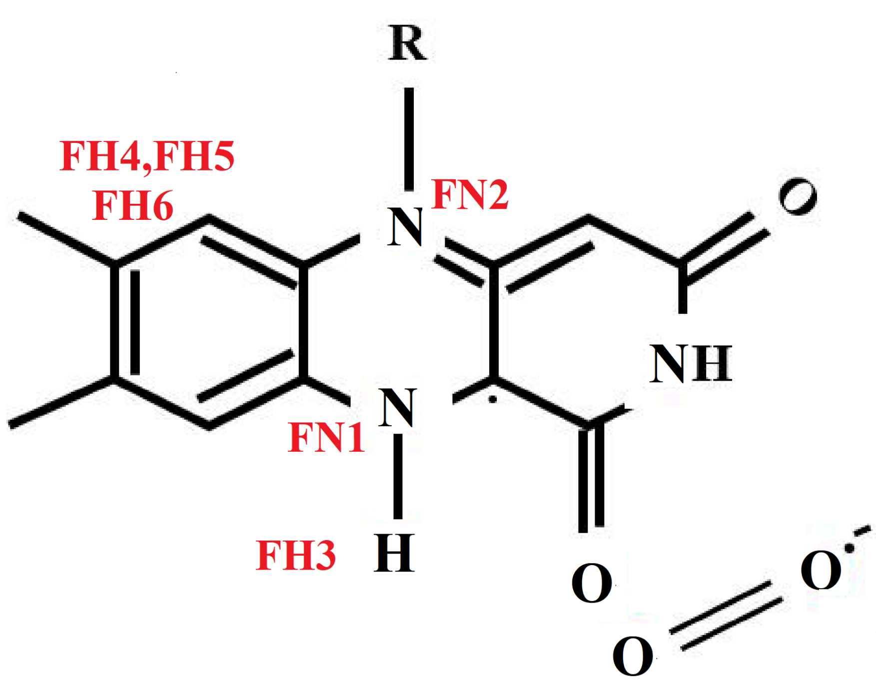

Figure 12: *$FADH^{\cdot}\ O_2^{\cdot-}$ molecule. The nuclei marked in red are considered in our calculation.*

***Table 2**: Hyperfine interaction in mT for $FADH^{\cdot}$ (FN_1, FN_2, FH_3,FH_4,FH_5,FH_6)*

FN_1	FN_2	FH_3	FH_4	FH_5	FH_6
0.4313	0.2506	-0.8029	0.3737	0.3845	0.0080

References

[1] H. Hiscock, “Long-lived spin coherence in radical pair compass magnetoreception,” Ph.D. dissertation, University of Oxford, 2018.

[2] H. G. Hiscock, S. Worster, D. R. Kattnig, C. Steers, Y. Jin, D. E. Manolopoulos, H. Mouritsen, and P. J. Hore, ``The quantum needle of the avian magnetic compass,'' \emph{Proceedings of the National Academy of Sciences}, vol. 113, no. 17, pp. 4634--4639, 2016, National Acad Sciences.

[3] A. A. Lee, J. C. S. Lau, H. J. Hogben, T. Biskup, D. R. Kattnig, and P. J. Hore, ``Alternative radical pairs for cryptochrome-based magnetoreception,'' \emph{Journal of The Royal Society Interface}, vol. 11, no. 95, pp. 20131063, 2014, The Royal Society.