

Magn. Reson. Discuss., referee comment RC2
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Comment on mr-2021-17

Anonymous Referee #2

Referee comment on "Exchange interaction in short-lived flavine adenine dinucleotide biradical in aqueous solution revisited by CIDNP (chemically induced dynamic nuclear polarization) and nuclear magnetic relaxation dispersion" by Ivan V. Zhukov et al., Magn. Reson. Discuss., <https://doi.org/10.5194/mr-2021-17-RC2>, 2021

The very well written and detailed manuscript by Zhukov et al. by the Yurkovskaya group studied the field-dependent photo-CIDNP activity and ¹H relaxation by a field cycling device of Flavin adenine dinucleotide (FAD) which is an important cofactor in many light-sensitive enzymes. The very high resolution field-dependent data collected indicates the presence of only a single FAD biradical attributed to the closed conformation. The following suggestions are indicated

(i) Line 205 remove the word "of"

(ii) The measurements were done at very low pHs 2.7 and 3.9, which is far away from physiological pH. In addition, the strong CIDNP activity vanishes above the pH range measured. Possible reasons for the loss of CIDNP activity should be discussed. Furthermore, can the authors exclude that their findings on a single biradical hold at neutral pH? Possibly measurements on the ¹H relaxation dispersion at physiological pH and comparison to the acidic pH data may give insights.

(iii) The data points in Figure 7A at low field drop much faster than theoretically predicted. Reasons for this apparent discrepancy should be discussed. In this context, it would be interesting for the reader to see the importance/extent of the correction of the CIDNP data by taking into account nuclear relaxation occurring during sample transfer by showing in a Suppl. Figure non corrected data. Furthermore, it is suggested to show on the y-axis not normalized units, but signal enhancement in respect to "no light".

(iv) The authors state that the measured data indicate the presence of only a single biradical. How sensitive is the method presented? It is suggested to make calculations with two states (for example state A and B from Figure 4) at different ratios .

