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Comment on "Distinct Populations in Spin-Label EPR Spectra from Nitroxides" [*J. Phys. Chem. B* **2018**, *122*, 6129-6133] †

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Table of Contents

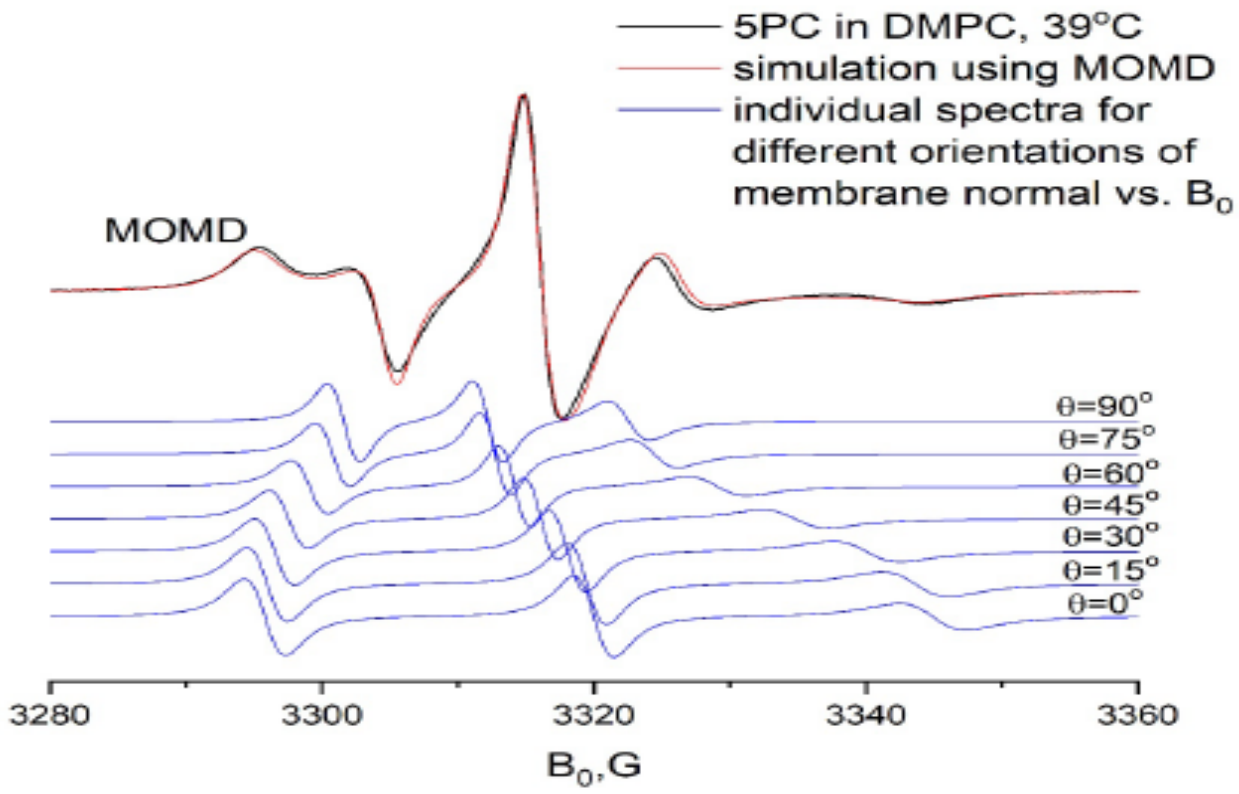

Figure S1. Experimental ESR spectrum from dimyristoylphosphotidylcholine dispersion doped with the 5PC spin-probe at 39° (black). MOMD spectrum obtained with NLSL[1–4] for g_{xx} = 2.0082, g_{yy} = 2.0060, g_{zz} = 2.0024, A_{xx} = 6.3 G, A_{yy} = 5.3 G, A_{zz} = 33.5 G, $(T_2^*)^{-1}$ = 1.35 G, microwave frequency of 9.32 GHz, truncation parameters lemx, lomx, kmx, Mmax, ipnmx = 10, 9, 6, 6, 2, $R_\perp = 10^8\ s^{-1}$, $R_\parallel = 5\times10^8\ s^{-1}$, c_0^2 (corresponding to λ in EasySpin) = 2.15, and 23 orientations summed (red). Simulated ESR spectra shown in blue are obtained vs. the angle, θ, between the local director (pointing along the bilayer normal) and the external magnetic field varying from 0° to 90° which are used in the summation. All other parameters as for the red MOMD spectrum. (We note that in the NLSL package there is a pruning program which selects the optimum minimum set of truncation parameters).

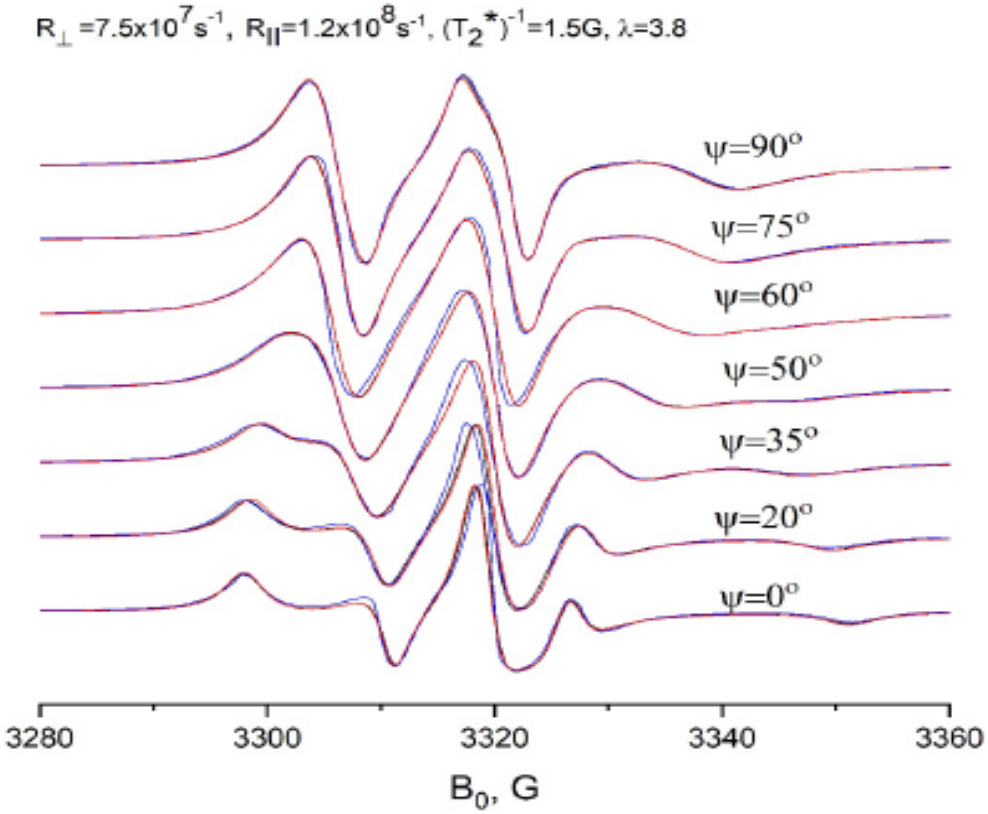

Figure S2. MOMD spectra obtained with NLSL (black) and EasySpin (red) for the parameters depicted on the Figure; 23 orientations were summed, the truncation parameters lemx, lomx, kmx, Mmax, ipnmx = 30, 23, 10, 6, 2, magnetic parameters as in the caption of Figure S1, and the angle, Ψ, between the diffusion axis and the principal axis of the magnetic tensors varying from 0° to 90°. MOMD spectra scanned from Figure 2 of Meirovitch, Nayeem and Freed (MNF)[5] are shown in blue.

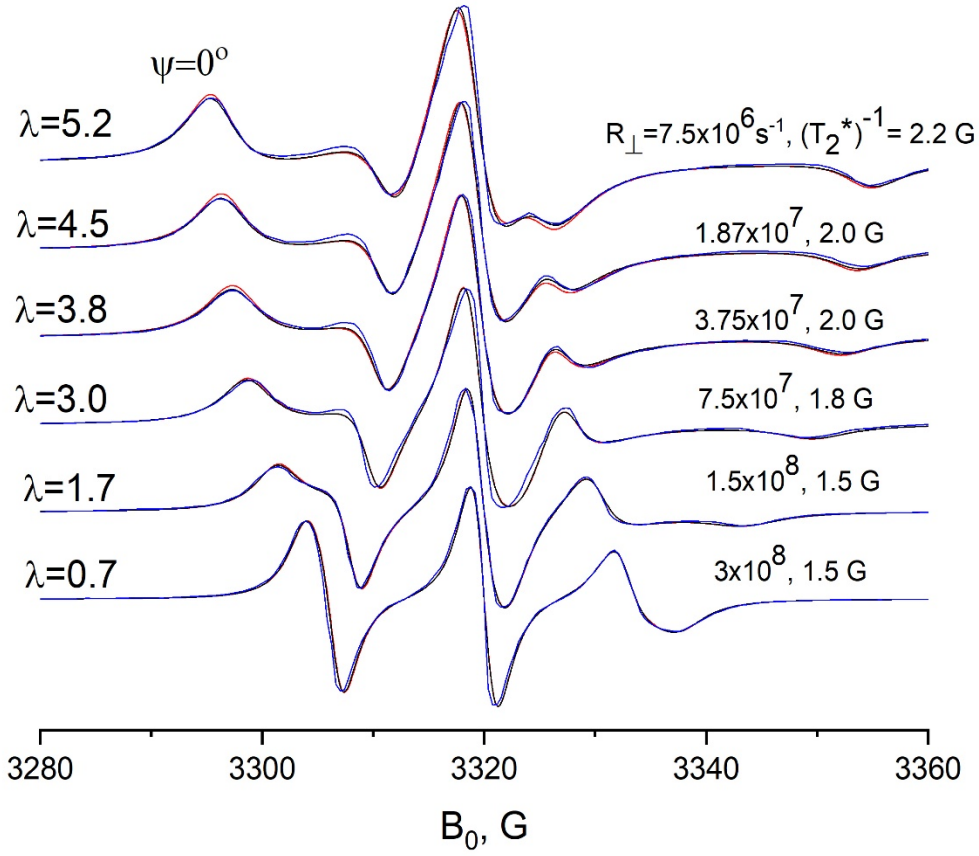

Figure S3. MOMD spectra obtained with NLSL (black) and EasySpin (red) for the parameters depicted on the Figure, 23 orientations summed, truncation parameters as in the captions of Figure S2, magnetic parameters as in the captions of Figure S2, and the coefficient, c_0^2, of the axial NLSL potential varying from 0.7 to 5.2. MOMD spectra scanned from Figure 3 of MNF (blue).

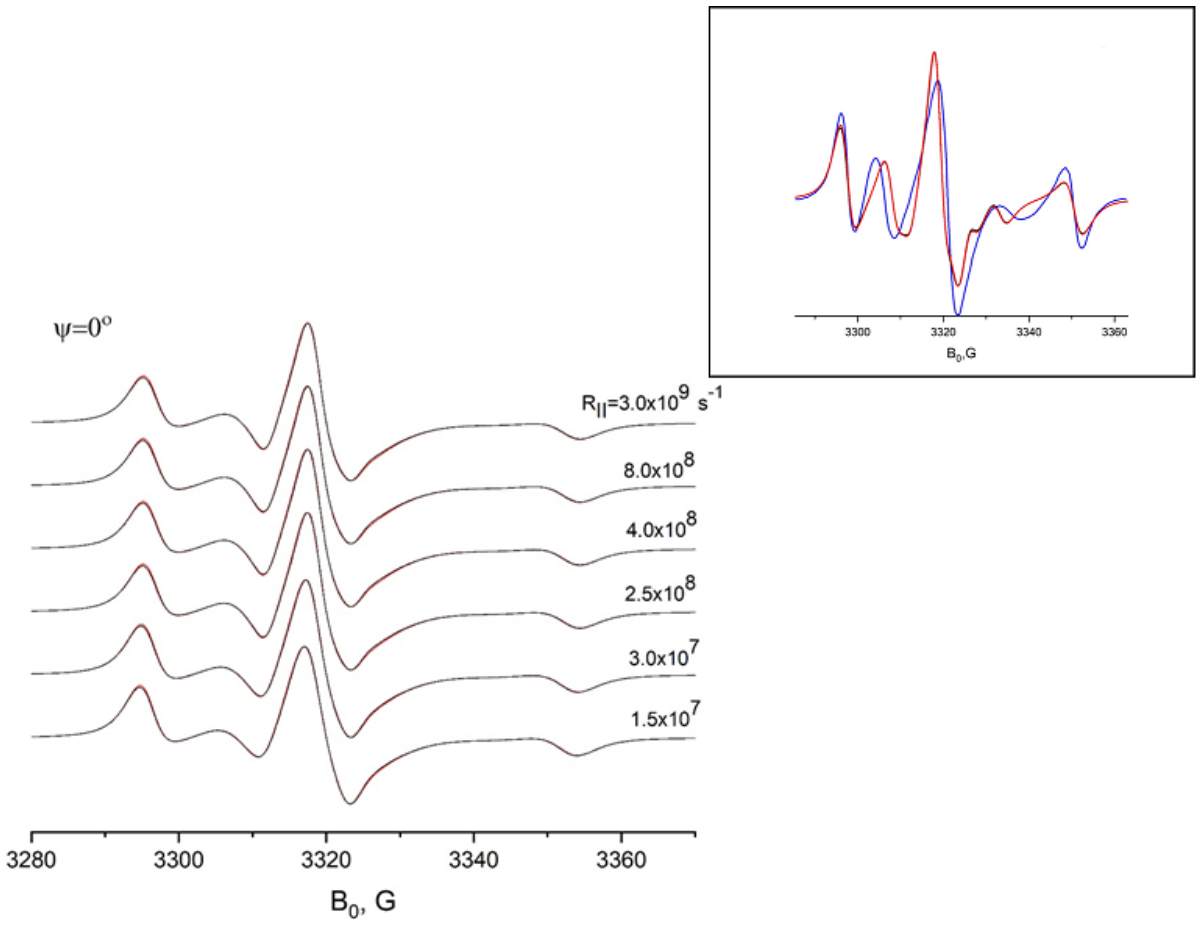

Figure S4. Figure 8A of ref 5 for VAR recalculated with NLSL (black) and EasySpin (red) for Mmax = 6. In addition to the parameters depicted on the Figure, $R_{\perp}$ = 5.0×10^{6} $s^{-1}$and $(T_2^*)^{-1}$ = 1.5 G were used; truncation parameters as in the caption of Figure S2, and magnetic parameters as in the captions of Figure S1; 23 orientations were summed. These spectra appear almost identical despite the large variation of $R_{\|}$ due to the low sensitivity of the spectral shape to $R_{\|}$ for ψ = 0º. These VAR spectra were calculated from MOMD software by using an extremely small axial potential coefficient c_0^2 = 1×10^{-3}. This yields the same results as a simple VAR program.

Inset: Same as main figure for $R_{\|}$ = 3.0x10 s^{-1} but with Mmax = 2 for NLSL (black) and EasySpin (red) with corresponding spectrum scanned from Figure 8A of MNF (blue). The NLSL and EasySpin spectra are so nearly identical that one almost completely obscures the other.

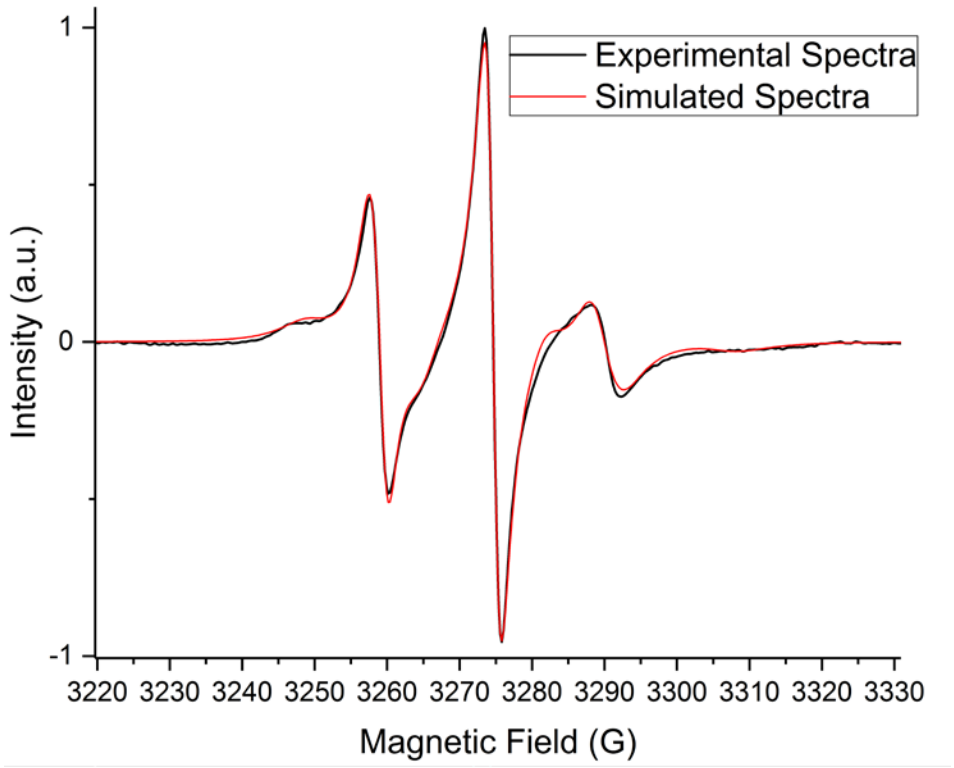

Fig. S5. Two-component MOMD fit with NLSL to spin-labeled Tau protein either in solution (fast component) or attached to microtubules (slow component) at 23°C and 9.19 GHz. Magnetic parameters: g_{xx}, g_{yy}, g_{zz} = 2.0082, 2.0060, 2.0026; A_{xx}, A_{yy}, A_{zz} = 5.95, 5.95, 35.8 G. the basis set convergence parameters were:

lemx, lomx, Kmn, Kmx, mmn, mmx, ipnmx = 20, 13, 0, 6, 0, 6, 2 and nort = 20.

The fitting parameters were:

1) Slow Component: 54%

R = 2.96 x $10^7 s^{-1}$; c_0^2 = 1.19; $(T_2^*)^{-1}$ = 0.15 G

2) Fast Component: 46%

R = 1.37 x $10^8 s^{-1}$; c_0^2 = 0.35; $(T_2^*)^{-1}$ = 0.36 G

References

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