Applied Magnetic Resonance

Supplementary Information for

DEER spectroscopy of channelrhodopsin-2 helix B movements in trapped photocycle intermediates

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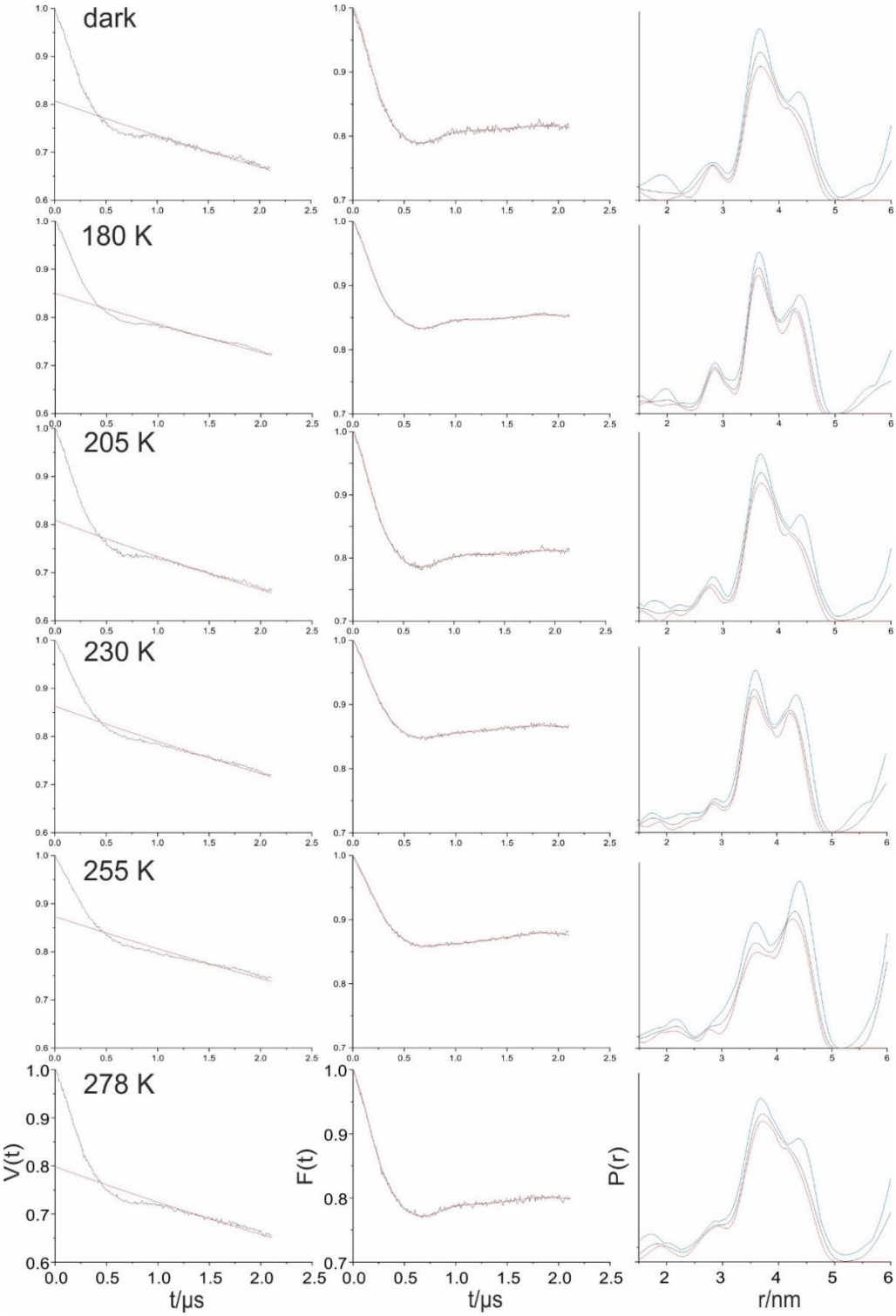

Fig. S1 Monitoring the interspin distance between helix B sites, C79R1 and C79R1', of solubilized ChR2 in the dark state and in trapped light activated intermediates relaxed at the given temperatures. (Left column) Dipolar evolution function, V(t), (black) with background fit (red) (background start at 232 ns). (Middle column) Form factor, F(t), (black) with fits using the model-free Tikhonov regularization (red). Modulation depths vary due to different degree of inversion by the pump pulse. The corresponding distance distributions, P(r), are shown in Fig. 4C. (Right column) DEER data validation: Optimal distance distribution, P(r), (black) with maximum error estimates corresponding to plus/minus two times the standard deviations (blue, red). Calculations were performed with the validation tool of DeerAnalysis [1] with variable background start (range: 232 ns - 1232 ns) and density (range: 0.3 - 1.2), and upon addition of noise (L_{noise} = 1.5). The optimal regularization parameters varied between 100 (for 180 K) and 316 (for 278 K).

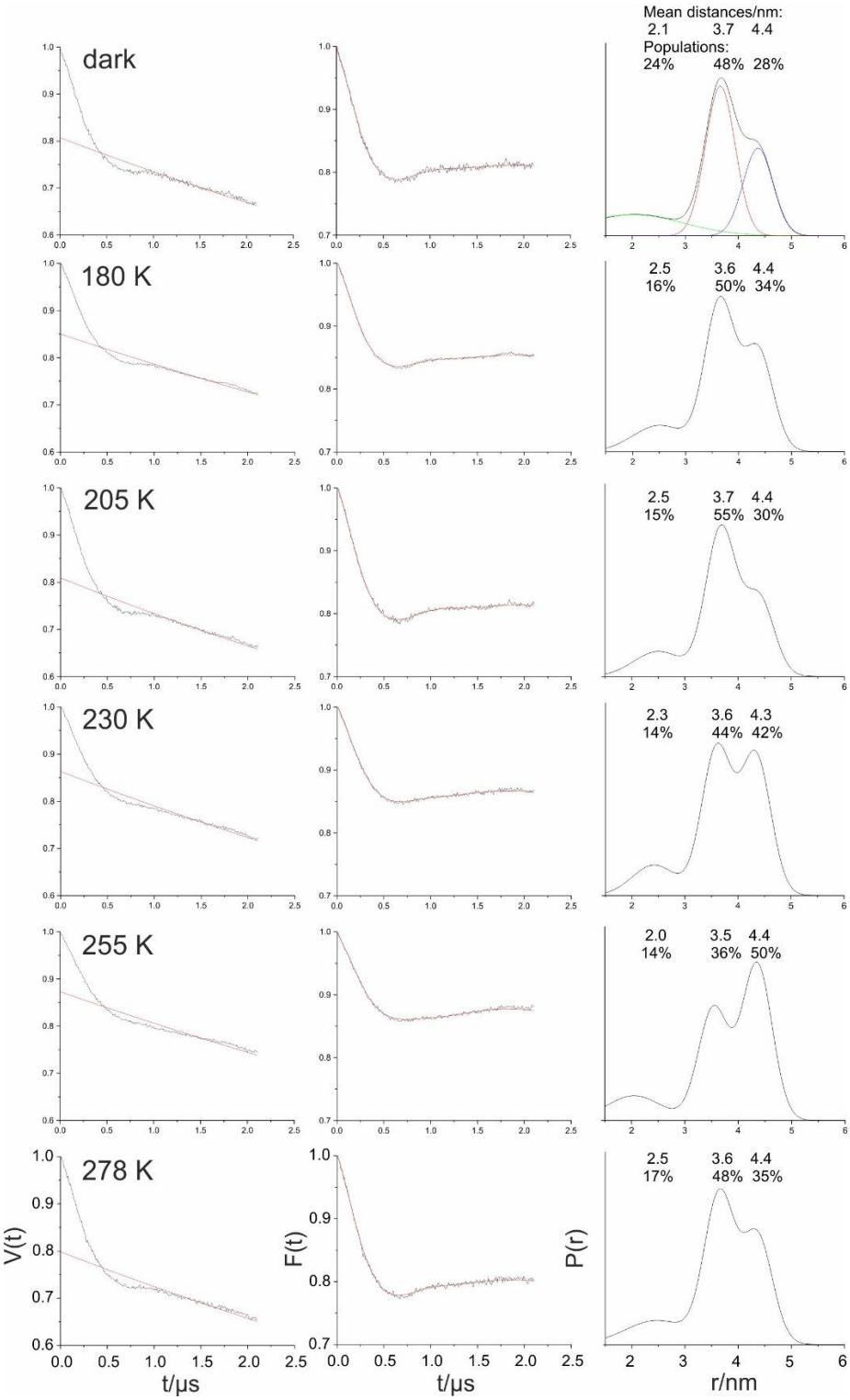

Fig. S2 Analysis of the DEER data shown in Fig. S1 using a distance distribution modeled by the sum of three Gaussians. (Left column) Dipolar evolution function, V(t), (black) with background fit (red). (Middle column) Form factor, F(t), (black) with fits using the sum of three Gaussians (red). (Right column) Distance distribution, P(r), (black) determined from the fits with mean distances and populations of the individual Gaussians depicted above their maxima. The FWHM of the Gaussian below 3 nm varied between 1.9 and 2.5 nm, for the two other Gaussians the FWHM was fixed at 0.67 nm. The calculations were performed with DeerAnalysis [1].

[1] G. Jeschke, V. Chechik, P. Ionita, A. Godt, H. Zimmermann, J. Banham, C. Timmel, D. Hilger, and H. Jung, Applied Magnetic Resonance 30, 473 (2006)