SUPPORTING INFORMATION

Singular Value Decomposition Method To Determine Distance Distributions In Pulsed Dipolar Electron Spin Resonance: II. Estimating Uncertainty

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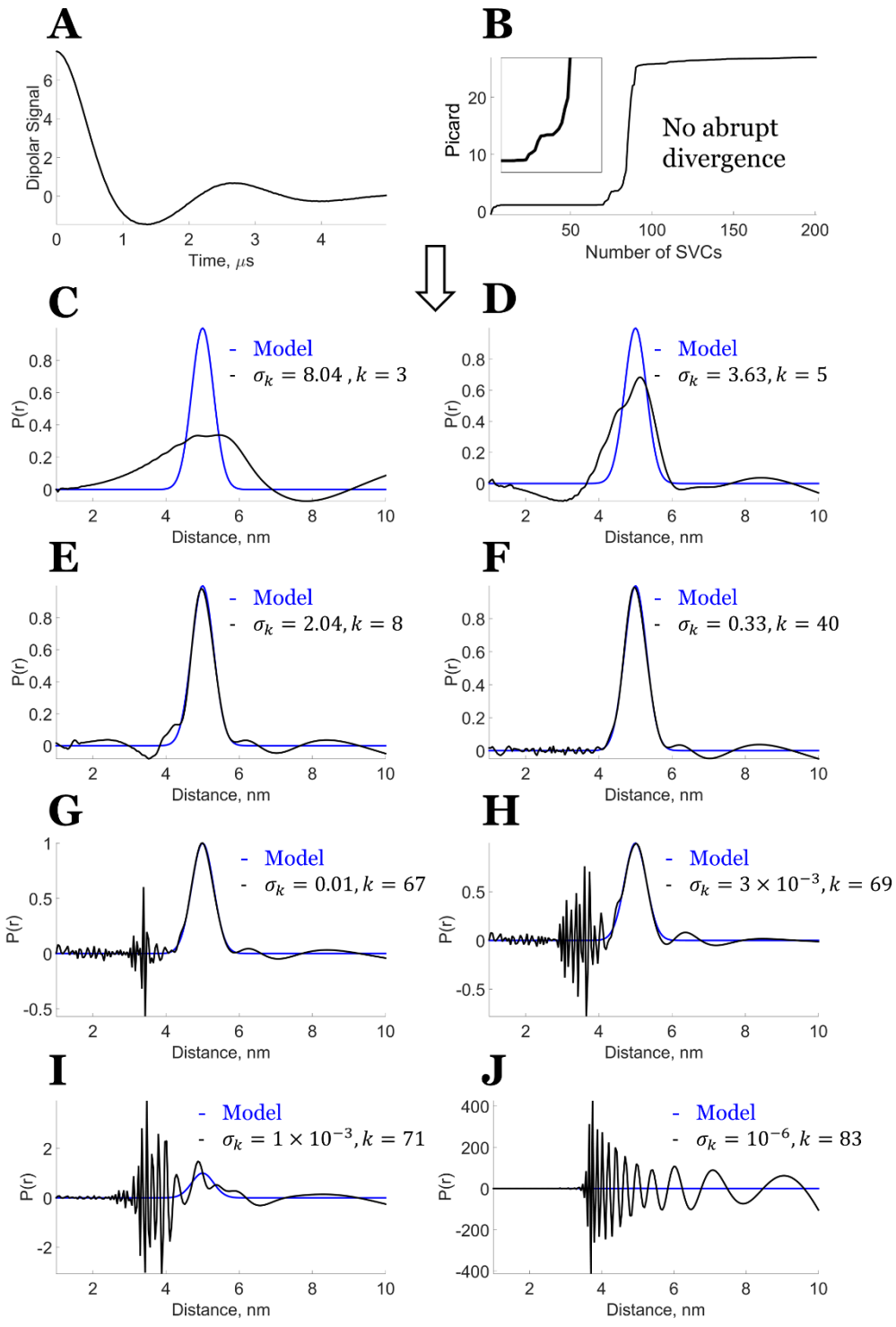

Figure S1: Model Data with Some Noise ($SNR \approx 850$) -- Unimodal Distance Distribution. **A)** Noisy model data dipolar signal; **B)** Picard plot of the unimodal distribution from the noisy model data at different number of Singular Value Contributions (SVCs) represented by i, the enlarged inset covers SVCs from 55 to 90; and **C)** to **J)** Comparison of model distribution with the distance distribution generated

from: **C)** $k = 3$, $\sigma_k = 8.04$; **D)** $k = 5$, $\sigma_k = 3.63$; **E)** $k = 8$, $\sigma_k = 2.04$; **F)** $k = 40$, $\sigma_k = 0.33$; **G)** $k = 67$, $\sigma_k = 0.01$; **H)** $k = 69$, $\sigma_k = 3 \times 10^{-3}$; **I)** $k = 71$, $\sigma_k = 1 \times 10^{-3}$; and **J)** $k = 83$, $\sigma_k = 10^{-6}$. (Figure S1 is reprinted with permission from ref 7. Copyright 2017 ACS.)

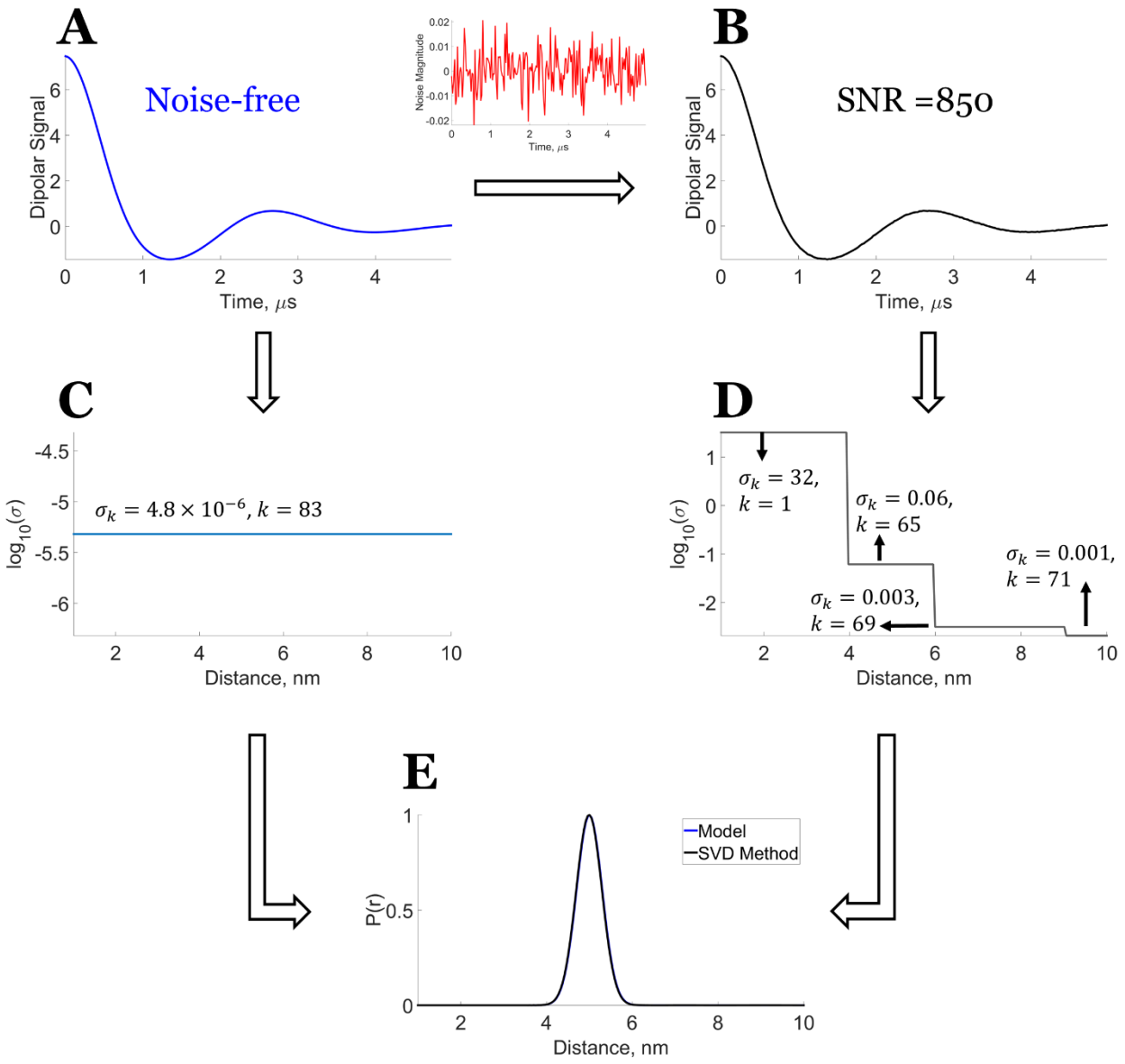

Figure S2: Unimodal Model -- Reconstruction of distance distribution for noise-free model data and noisy model data ($SNR \approx 850$) using the new SVD method. **A)** Model dipolar signal; **B)** Model dipolar signal with added noise (see added noise in Red plot); **C)** Singular value cut-off at each distance (nm) for the model dipolar signal; **D)** Singular value cut-off at each distance (nm) for the model dipolar signal with added noise; and **E)** Distance distribution reconstructed from the model dipolar signal and model dipolar signal with noise using the singular value cut-offs shown in **C)** and **D)**, respectively. Note that the added noise is so small that **A** and **B** still appear identical, but convergence to the virtually identical final results requires segmentation in the latter case. (Figure S2 is reprinted with permission from ref 7. Copyright 2017 ACS.)