

Supporting information

rDEER: A modified DEER sequence for distance measurements using shaped pulses

Thorsten Bahrenberg, Yin Yang, Daniella Goldfarb*, and Akiva Feintuch*

*Department of Chemical and Biological Physics, Weizmann Institute of Science, 76100
Rehovot, Israel*

** corresponding authors, akiva.feintuch@weizmann.ac.il,
daniella.goldfarb@weizmann.ac.il*

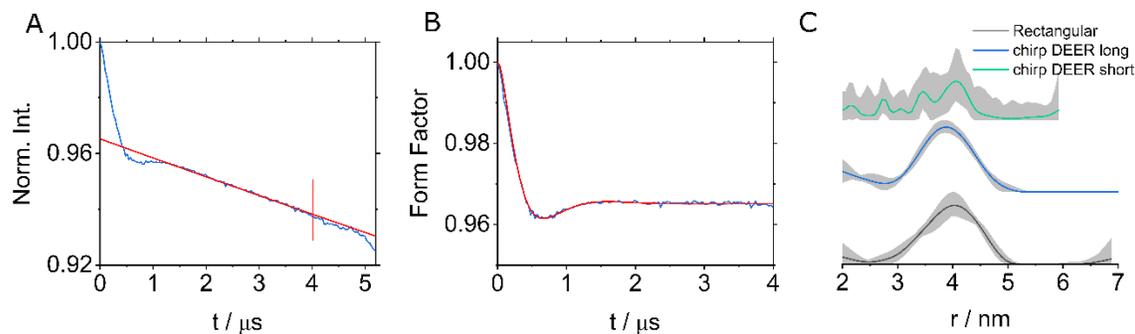


Figure S1: Chirp DEER of Ubi-DOTA-M-Gd to demonstrate the performance of chirp DEER; (A) Raw data. The position where the trace was truncated for analysis is indicated by a red line; (B) Background-corrected DEER data and fit; (C) distance distribution (blue trace) compared to the distance distributions shown in Figure 5C (mint and grey traces). Total experiment time for this experiment was 2:30 h.

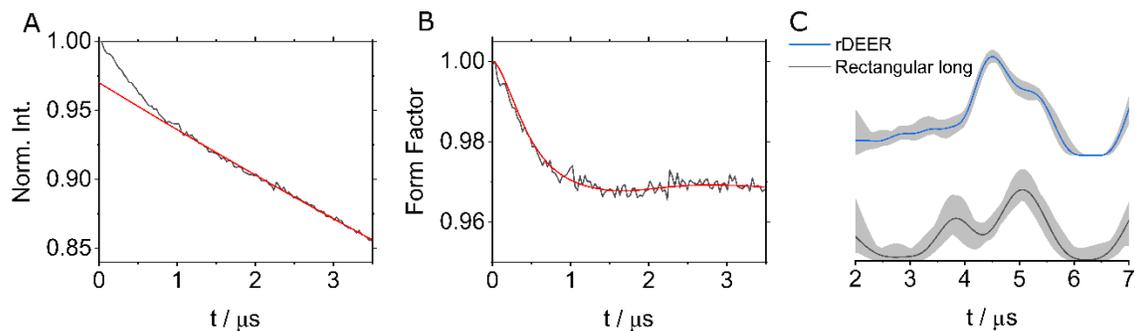


Figure S2: Rectangular DEER of MdfA-C2-Gd (A) Raw data; (B) Background-corrected DEER data and fit; (C) distance distribution (grey trace) compared to data from Figure 5F (blue trace).

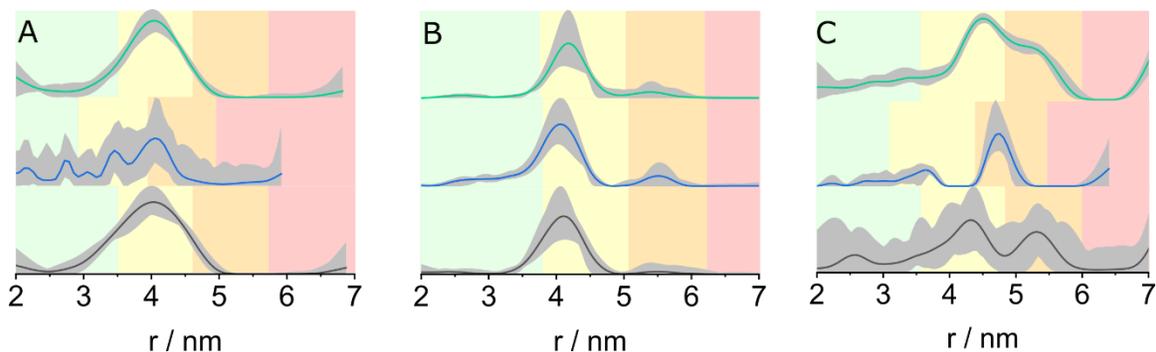


Figure S3: Distance distribution taken from Fig. 4 along with the distance-dependent color coding from the software DeerAnalysis. The original color coding from DeerAnalysis was maintained, where green, shape reliable, pale yellow, mean distance and width reliable, orange, mean distance reliable, and red, non-reliable region.

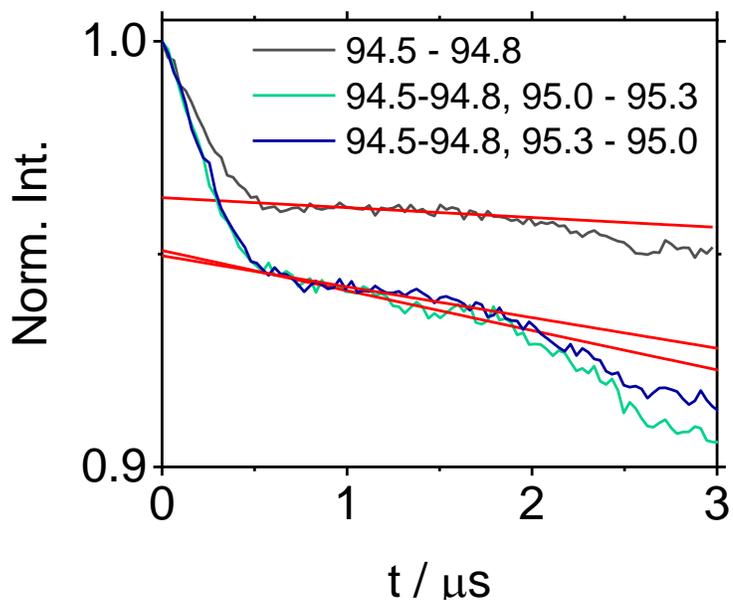


Figure S4: Raw data of DEER traces on Ubi-DOTA-M-Gd obtained with a single broadband pump pulse (grey trace) and different sweeping directions of the pump pulses (blue, up, down and green, up, up) Experimental parameters are identical to the experiments in the main text.

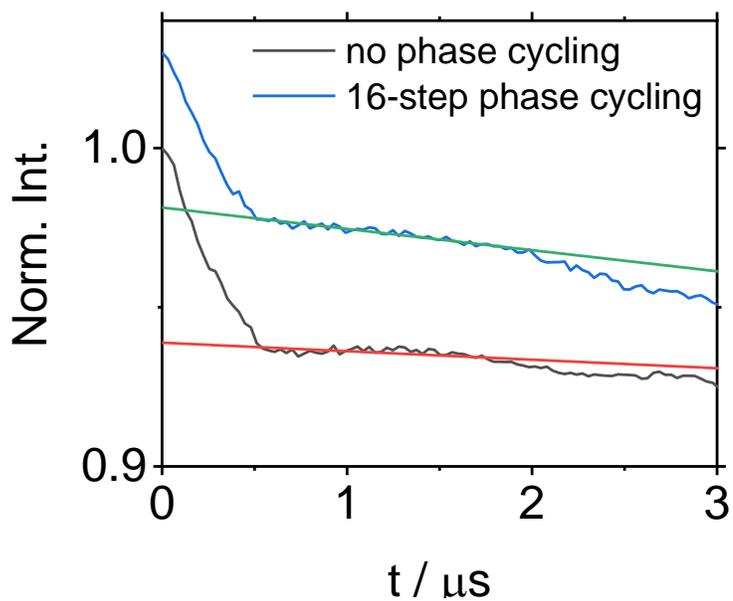


Figure S5: The effect of phase cycling on DEER raw data; data was obtained with Ubi-DOTA-M-Gd and the standard chirp DEER setup as described in the paper. 16-step phase cycling refers to the scheme $(x)(x)(x_P)(x)$.

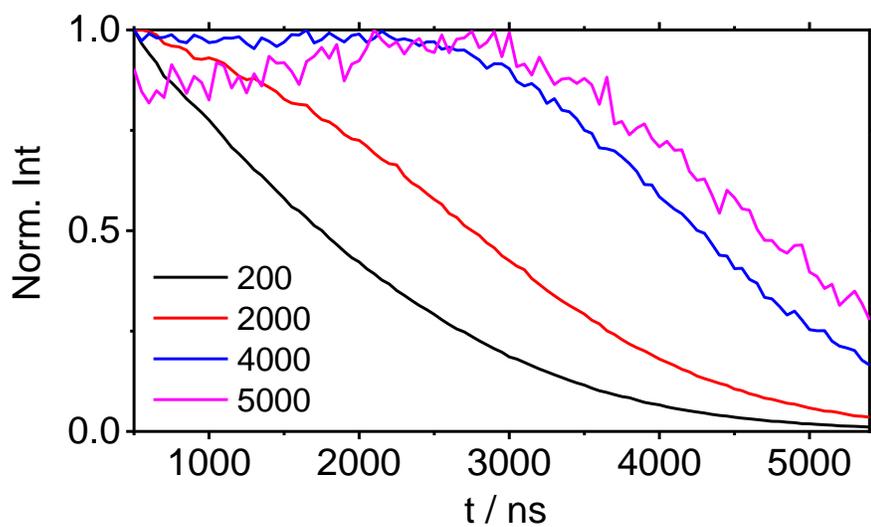


Figure S6: Echo decay with the refocusing pulse sequence $\pi/2 - \tau_1 - \pi - \tau_1 - \tau_2 - \pi - \tau_2 - det.$ on MdfA-C2-Gd for different values of τ_2 , as noted on the figure, shows a clear deviation from a mono-exponential decay towards long τ_2 times.