

# **DEER analysis report on dataset DEER\_352\_240\_MTSSL\_prot\_EMCV\_d2\_9u s\_spec**

**DEERNet Spinach SVN Rev 5662 and DeerLab  
0.9.1 Tikhonov regularization**

**ComparativeDEERAnalyzer version 2.0**

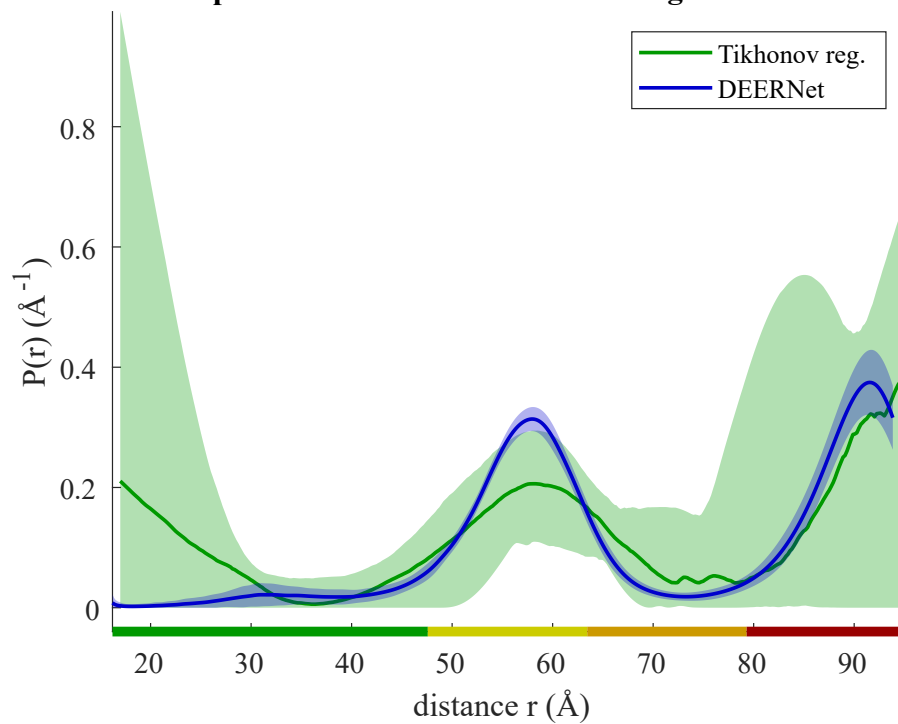
see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/  
mr-1-209-2020

24-Feb-2022 08:04:38

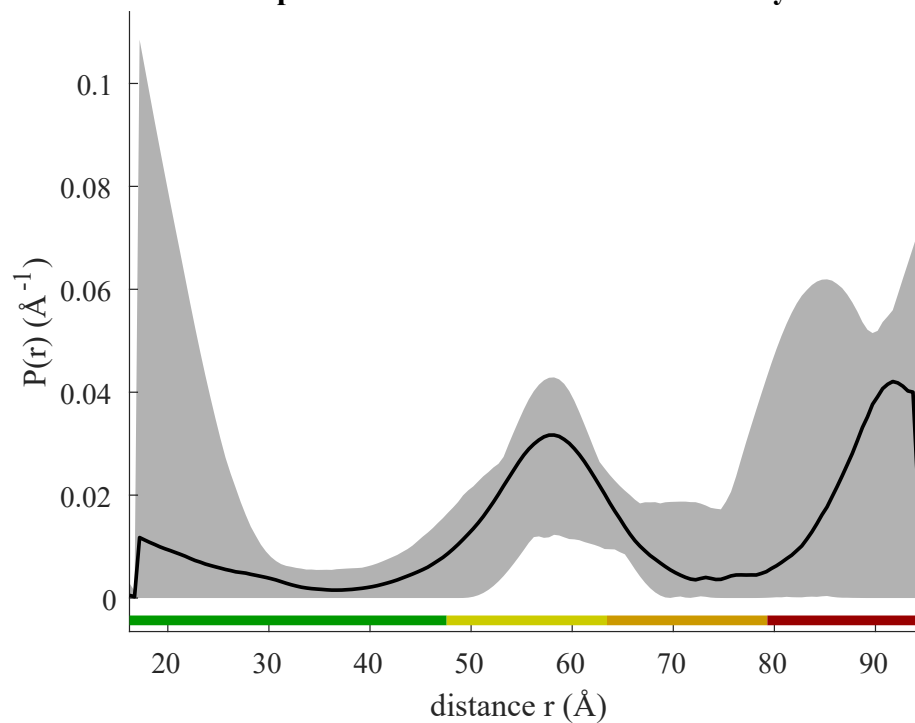
---

## 1. Distance distributions

**Overlap between neural network and regularization**



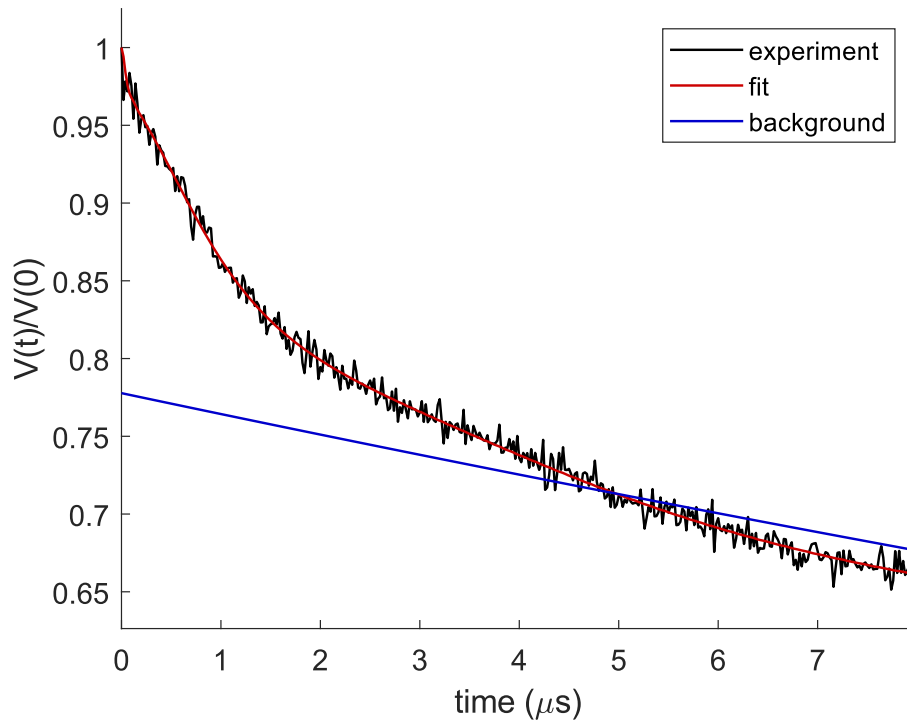
**Comparative distribution and uncertainty**



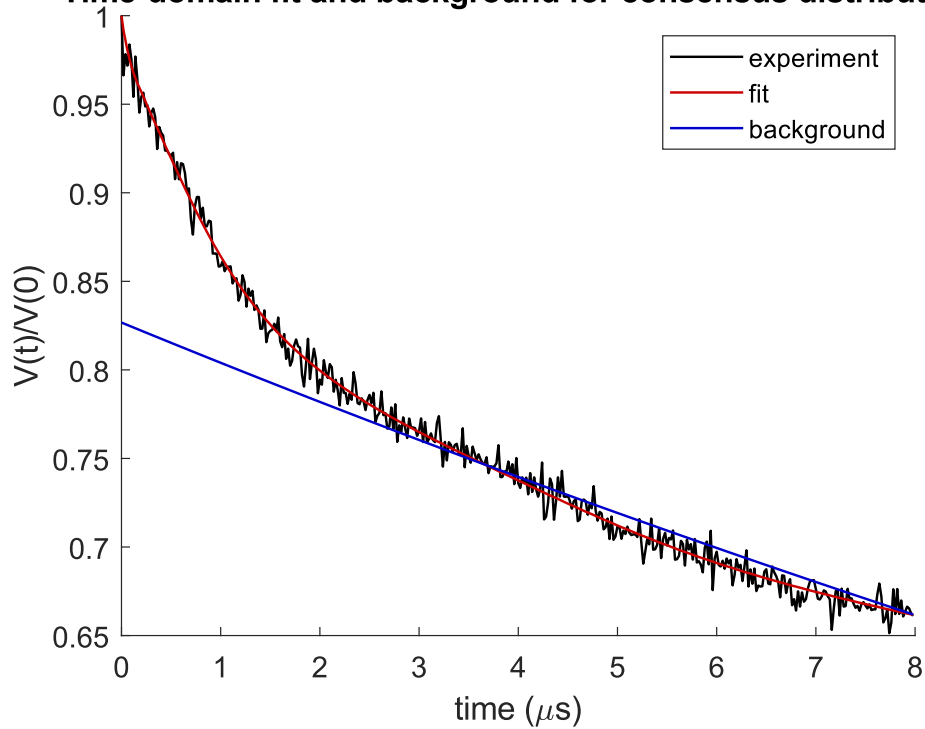
---

## 2. Fits of time-domain data

**Tikhonov fit**



**Time-domain fit and background for consensus distribution**



---

### 3. Experimental and processing parameters

**DEERNet background not provided, as it was considered unreliable.**

Modulation depth: 0.173

Signal-to-noise ratio: 27.3 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00616

From Tikhonov fit: 0.00665

Zero time: 103 ns

Maximum time: 7980 ns

The last 8 % of the data was cut off

Time increment: 20 ns

Phase: 32.7 degree

Ensemble of 32 neural networks

Background separation by DeerLab bilevel optimization

Background dimension: 3

Regularization parameter by best overlap with neural network solution

Regularization parameter used: 20.05

Reg. par. initial estimate by lr: 5.01

**Overlap between DEERNet and regularization solutions: 0.767**

Predicted overlap of consensus solution with ground truth: 0.64...0.82

**Mean distance: 66.1 Å**

**Single Gaussian provided different mean distance. Distribution may be incomplete.**

Distance standard deviation: 21.7 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_352\_240\_MTSSL\_prot\_EMCV\_d2\_9us\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_352\_240\_MTSSL\_prot\_EMCV\_d2\_9us\_spec\_consensus\_DEER\_distribution.csv

### 3. Experimental and processing parameters

---

Fit and background in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_352\_240\_MTSSL\_prot\_  
EMCV\_d2\_9us\_spec\_consensus\_DEER\_fit.csv

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_352\_240\_MTSSL\_prot\_  
EMCV\_d2\_9us\_spec\_comparative\_DEER\_meta\_data.csv