

# **DEER analysis report on dataset DEER\_S205\_Q352C\_LB\_MTSL\_EMCV\_d2\_1 2us\_spec**

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

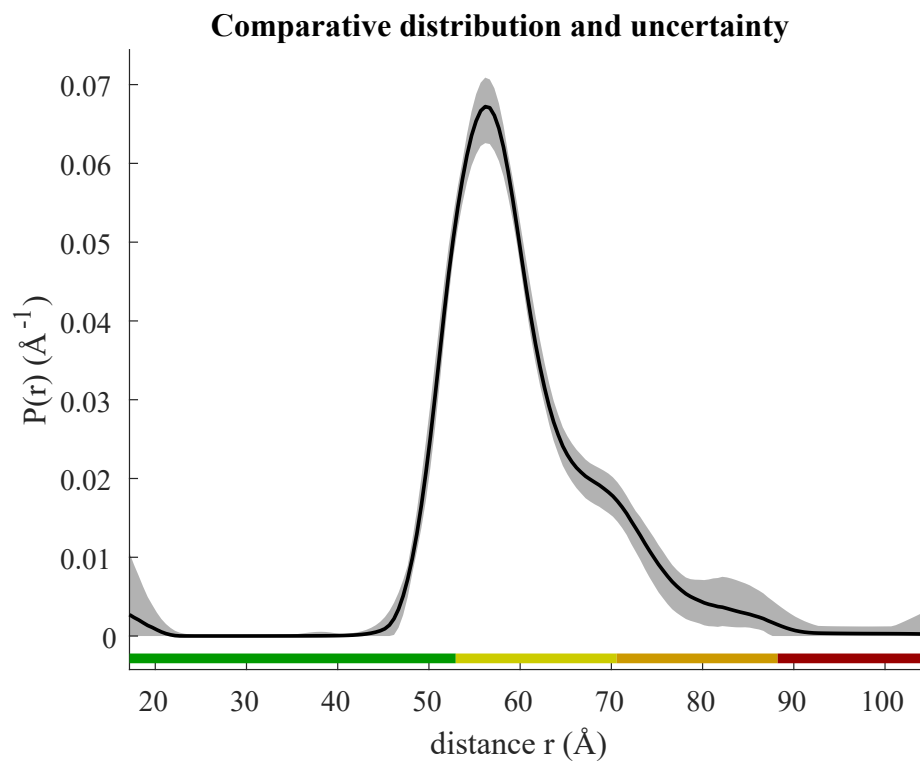
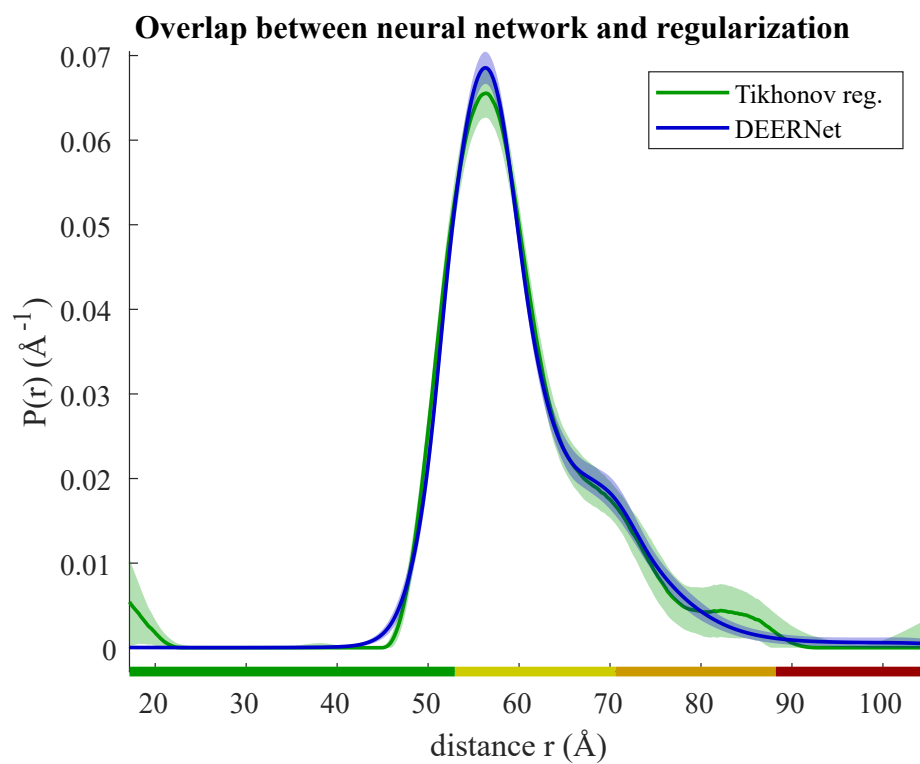
**ComparativeDEERAnalyzer version 2.0**

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 07:54:27

---

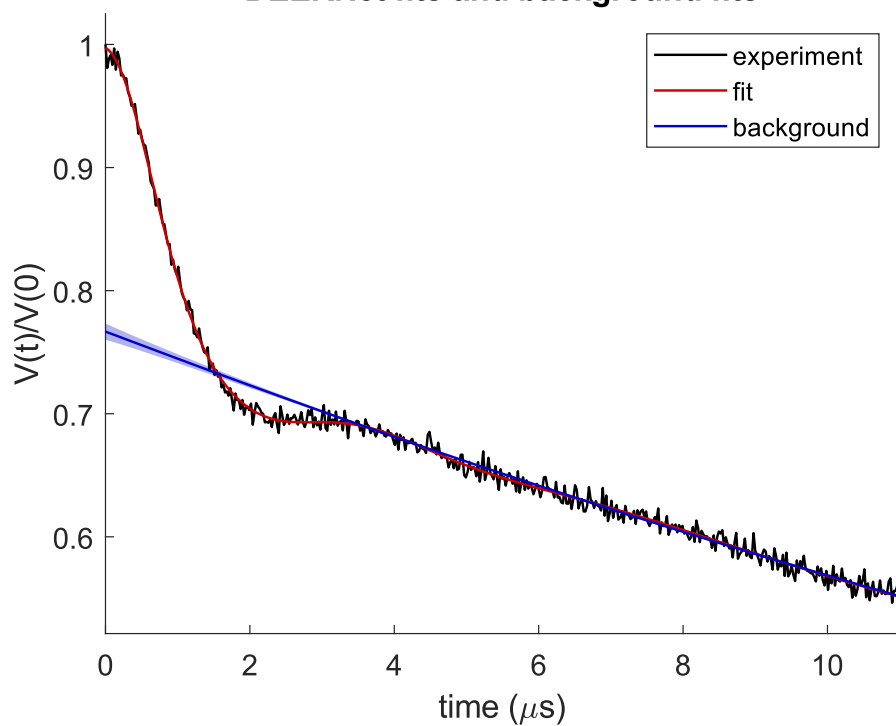
## 1. Distance distributions



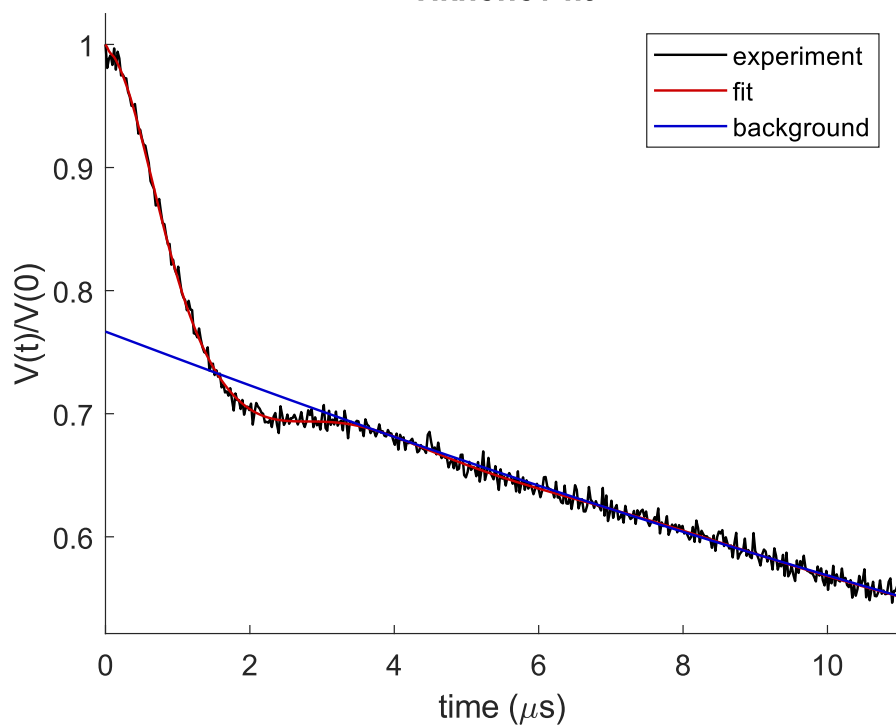
---

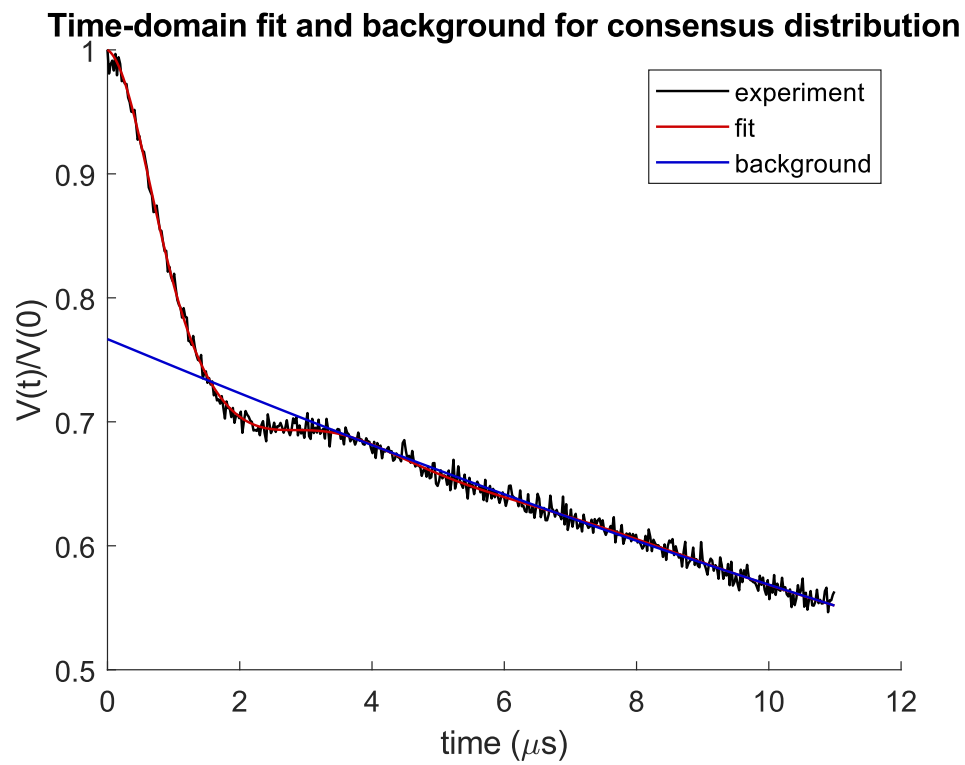
## 2. Fits of time-domain data

**DEERNet fits and background fits**



**Tikhonov fit**





---

### 3. Experimental and processing parameters

Modulation depth: 0.231

Signal-to-noise ratio: 40.9 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00765

From DEERNet fit: 0.00564

From Tikhonov fit: 0.00565

Zero time: 0 ns

Maximum time: 10992 ns

The last 7 % of the data was cut off

Time increment: 24 ns

Phase: 7.0 degree

Ensemble of 32 neural networks

Background separation by neural network

Background dimension: 3

Regularization parameter by best overlap with neural network solution

Regularization parameter used: 3.14

Reg. par. initial estimate by L-curve corner: 25.12

Overlap between DEERNet and regularization solutions: 0.958

Predicted overlap of consensus solution with ground truth: 0.82...0.99

Mean distance: 59.1 Å

Distance standard deviation: 7.9 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S205\_Q352C\_LB\_MTSL  
\_EMCV\_d2\_12us\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S205\_Q352C\_LB\_MTSL  
\_EMCV\_d2\_12us\_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\_S205\_Q352C\_LB\_MTSL  
\_EMCV\_d2\_12us\_spec\_consensus\_DEER\_fit.csv

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S205\_Q352C\_LB\_MTSL  
\_EMCV\_d2\_12us\_spec\_comparative\_DEER\_meta\_data.csv