

# **DEER analysis report on dataset DEER\_T109C\_S475C\_MTSL\_EMCV\_afterSE C\_New\_d214us\_298scs\_spec**

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

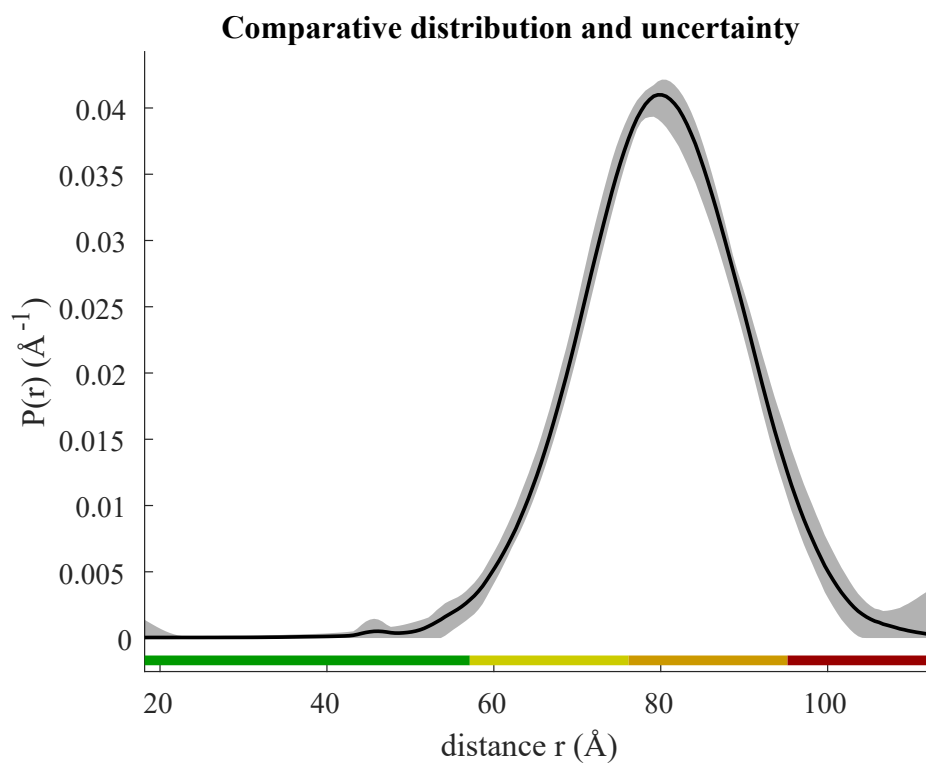
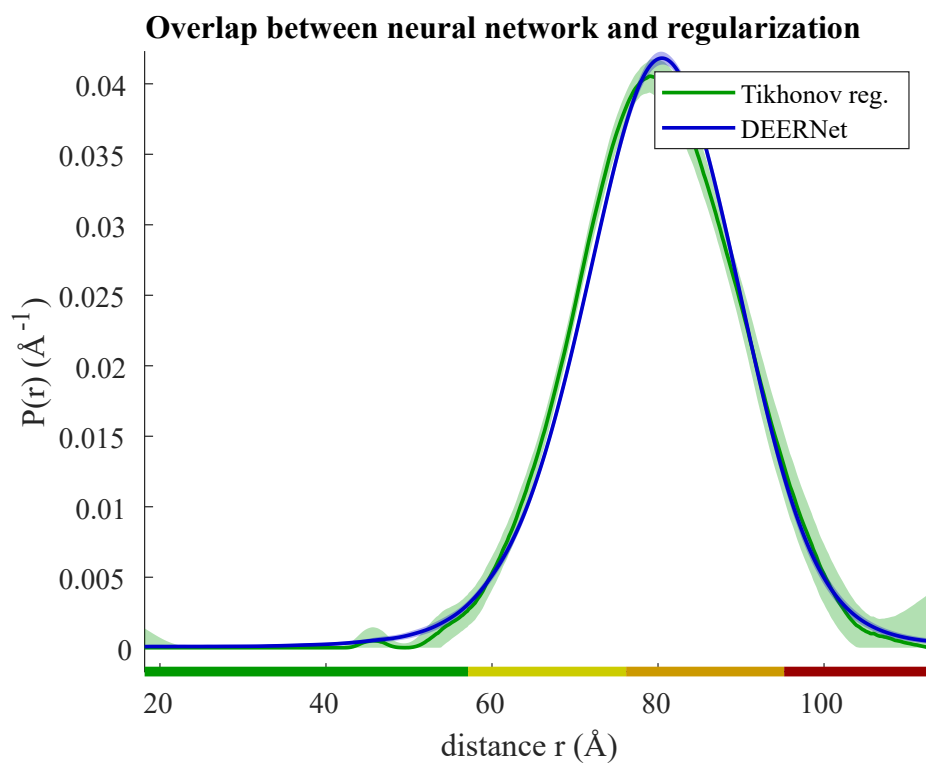
**ComparativeDEERAnalyzer version 2.0**

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 07:51:58

---

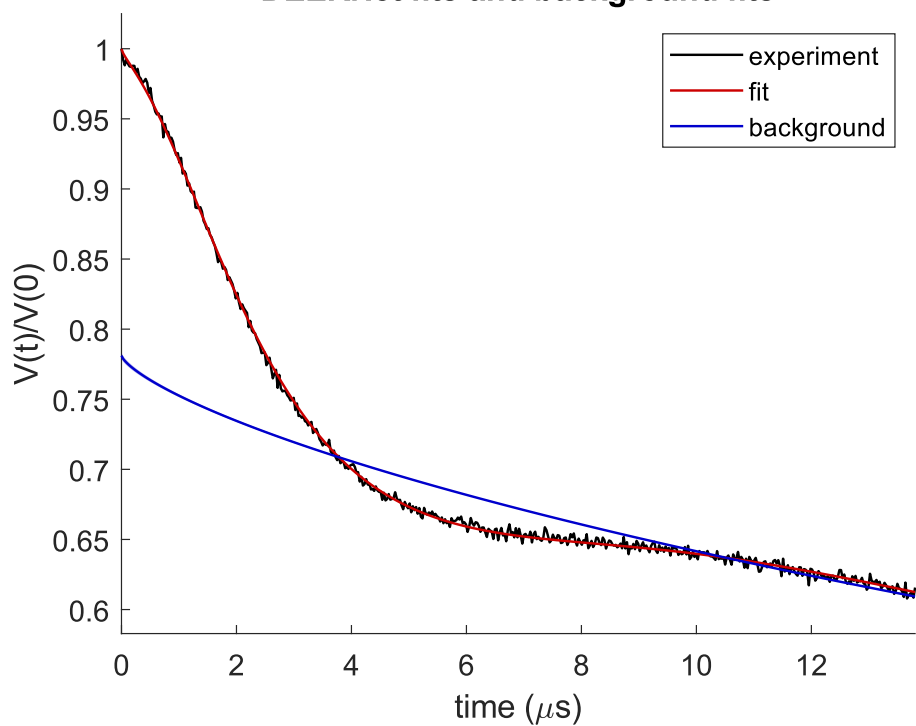
## 1. Distance distributions



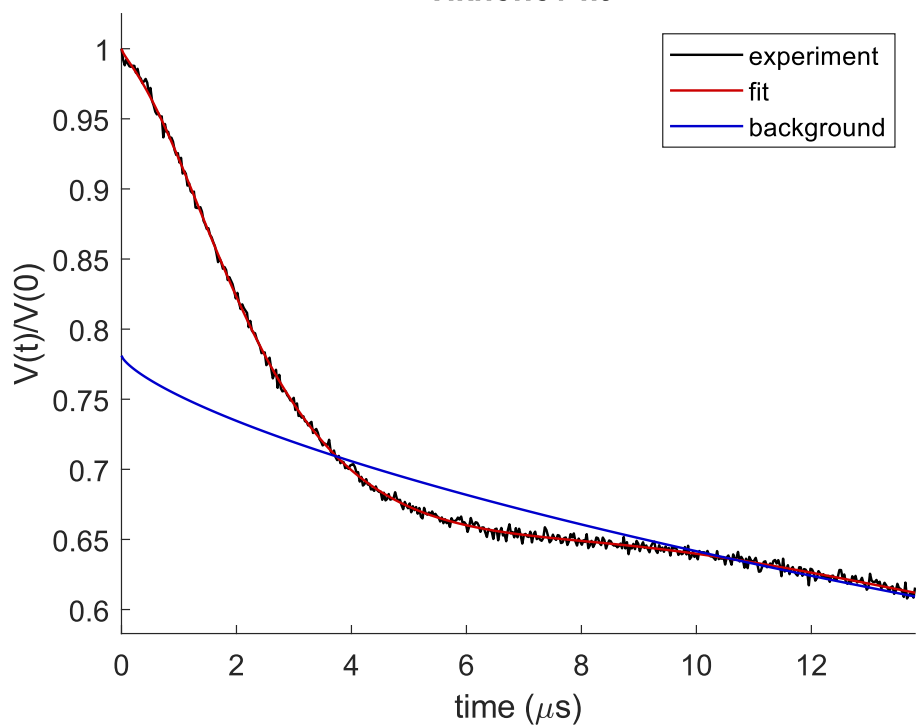
---

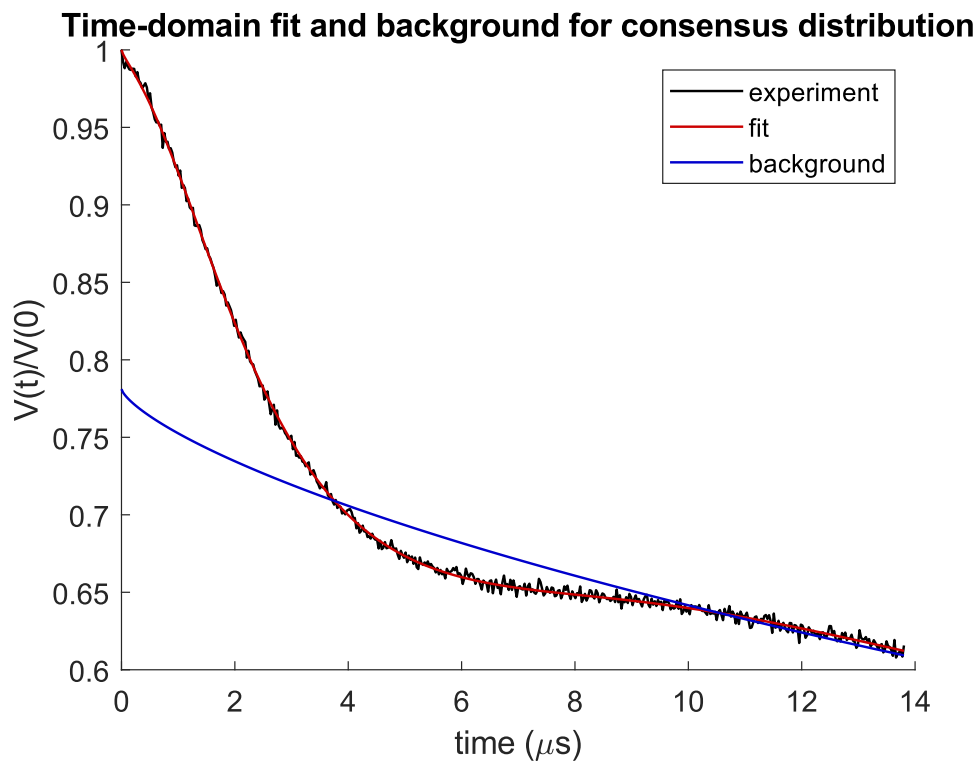
## 2. Fits of time-domain data

**DEERNet fits and background fits**



**Tikhonov fit**





---

### 3. Experimental and processing parameters

Modulation depth: 0.219

Signal-to-noise ratio: 73.3 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00322

From DEERNet fit: 0.00299

From Tikhonov fit: 0.00283

Zero time: 0 ns

Maximum time: 13804 ns

Time increment: 28 ns

Phase: 22.7 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: 3.13

Reg. par. initial estimate by L-curve corner: 50.12

Overlap between DEERNet and regularization solutions: 0.965

Predicted overlap of consensus solution with ground truth: 0.83...1.00

Mean distance: 79.9 Å

Distance standard deviation: 9.9 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_T109C\_S475C\_MTSL\_E  
MCV\_afterSEC\_New\_d214us\_298scs\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_T109C\_S475C\_MTSL\_E  
MCV\_afterSEC\_New\_d214us\_298scs\_spec\_consensus\_DEER\_distribution.csv

Fit and background in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_T109C\_S475C\_MTSL\_E  
MCV\_afterSEC\_New\_d214us\_298scs\_spec\_consensus\_DEER\_fit.csv

### 3. Experimental and processing parameters

---

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_T109C\_S475C\_MTSL\_E  
MCV\_afterSEC\_New\_d214us\_298scs\_spec\_comparative\_DEER\_meta\_data.csv