

# **DEER analysis report on dataset DEER\_S116C\_S240C\_MTSL\_EMCV\_new\_d 2\_8us\_spec**

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

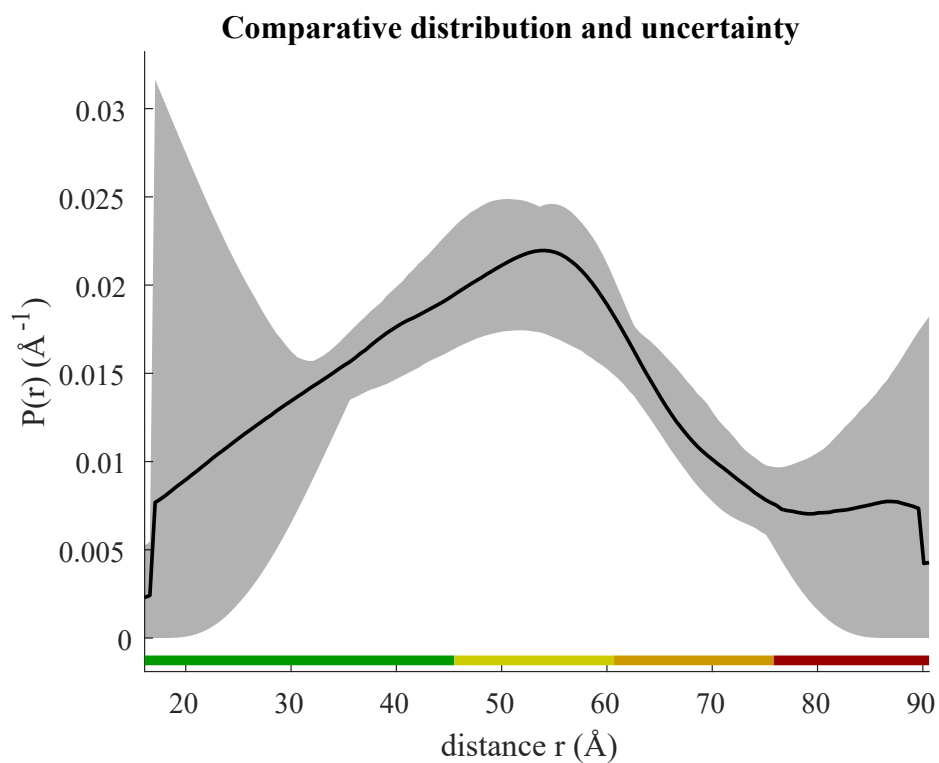
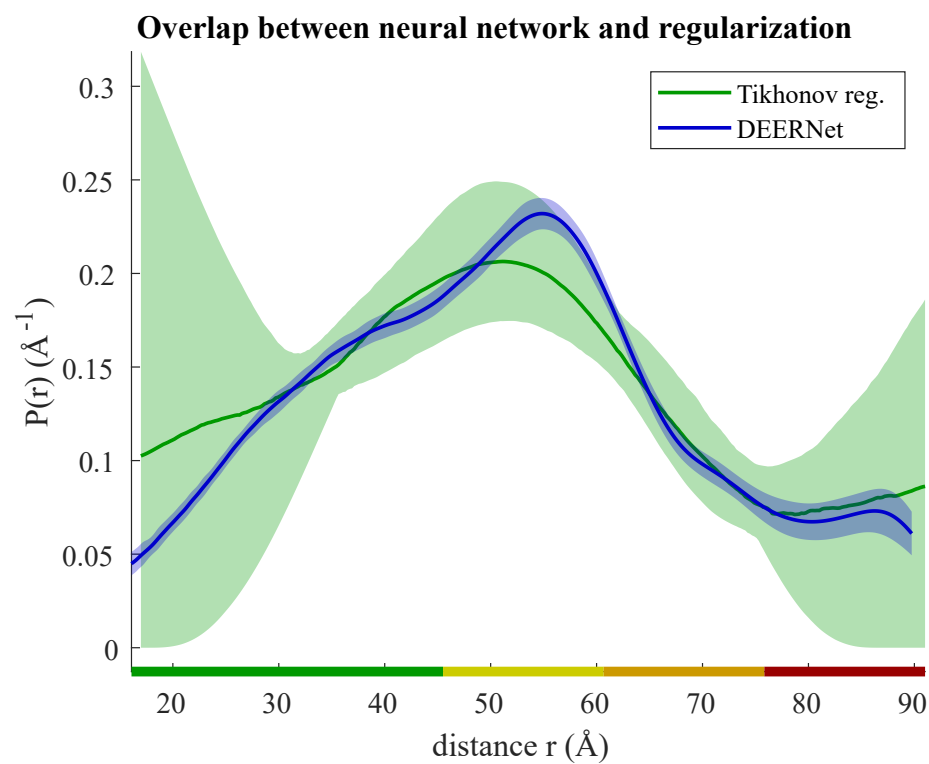
**ComparativeDEERAnalyzer version 2.0**

see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/  
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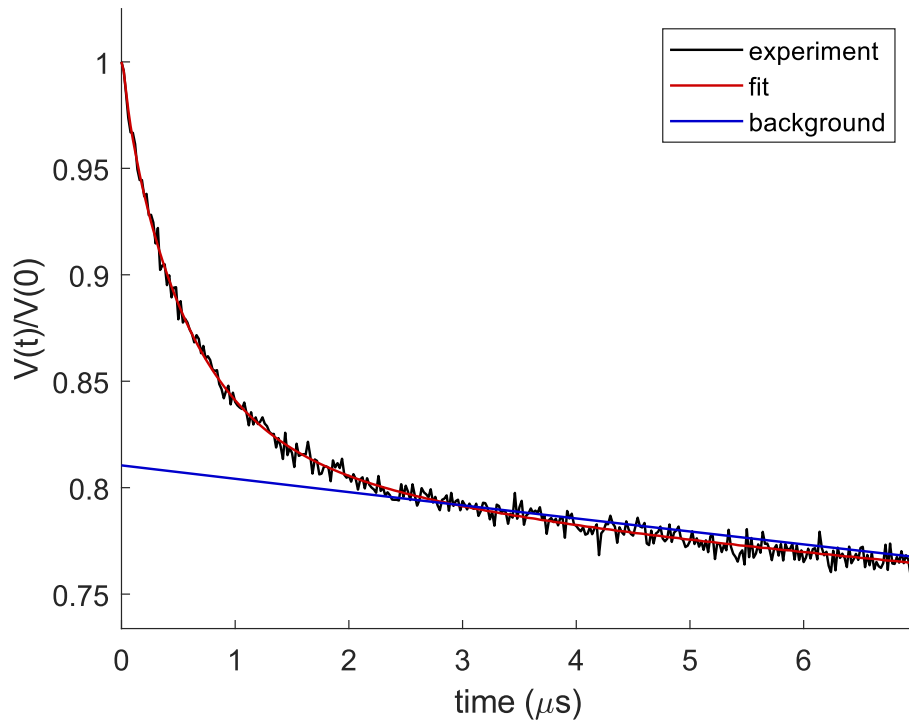
## 1. Distance distributions



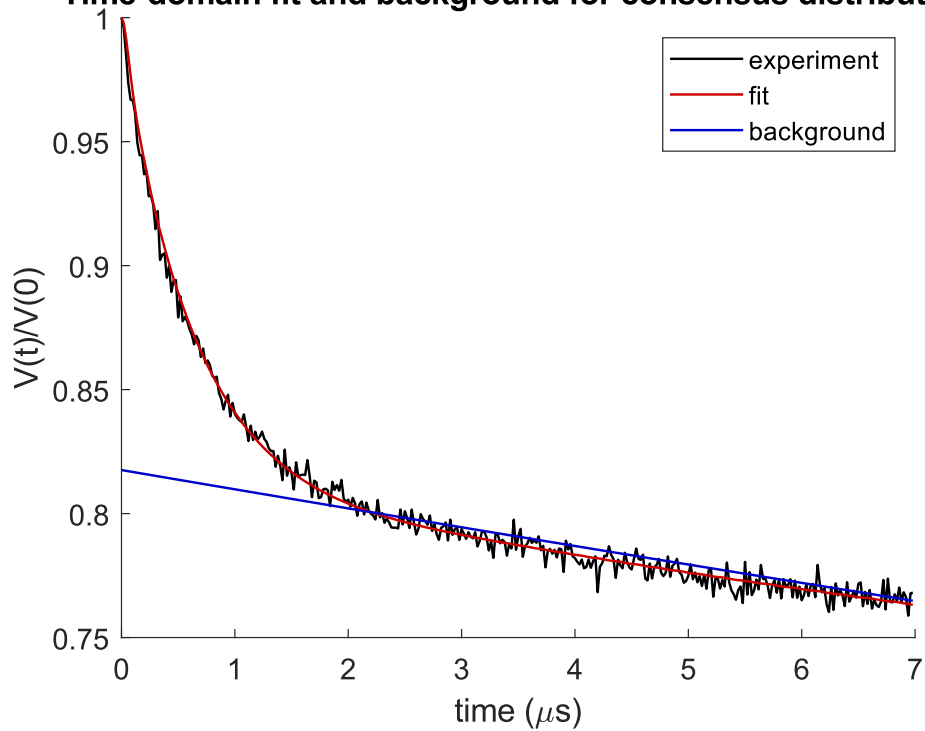
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## 2. Fits of time-domain data

**Tikhonov fit**



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



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### 3. Experimental and processing parameters

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

Modulation depth: 0.182

Signal-to-noise ratio: 50.7 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00556

From Tikhonov fit: 0.00366

Zero time: 130 ns

Maximum time: 6980 ns

The last 9 % of the data was cut off

Time increment: 20 ns

Phase: 1.9 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: 35.61

Reg. par. initial estimate by lr: 12.59

Overlap between DEERNet and regularization solutions: 0.951

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

Mean distance: 46.4 Å

Distance standard deviation: 25.5 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S116C\_S240C\_MTS�\_E  
MCV\_new\_d2\_8us\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S116C\_S240C\_MTS�\_E  
MCV\_new\_d2\_8us\_spec\_consensus\_DEER\_distribution.csv

### 3. Experimental and processing parameters

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Fit and background in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S116C\_S240C\_MTSL\_E  
MCV\_new\_d2\_8us\_spec\_consensus\_DEER\_fit.csv

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_S116C\_S240C\_MTSL\_E  
MCV\_new\_d2\_8us\_spec\_comparative\_DEER\_meta\_data.csv