

# **DEER analysis report on dataset DEER\_235\_500\_D2O\_MTSL\_EMCV\_d2\_15. 5us\_spec**

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

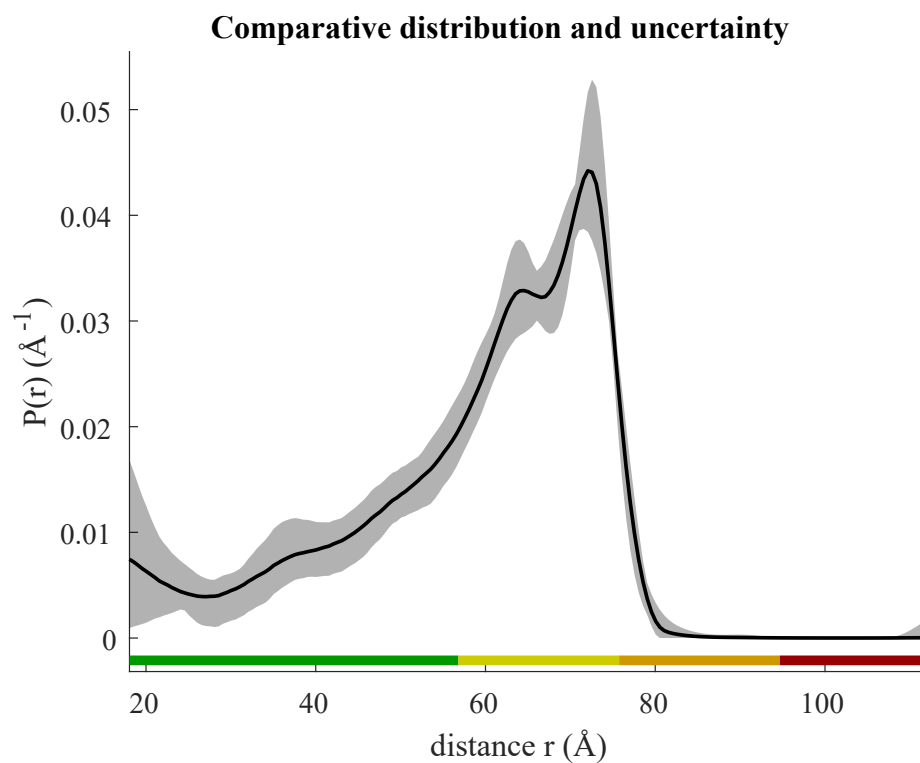
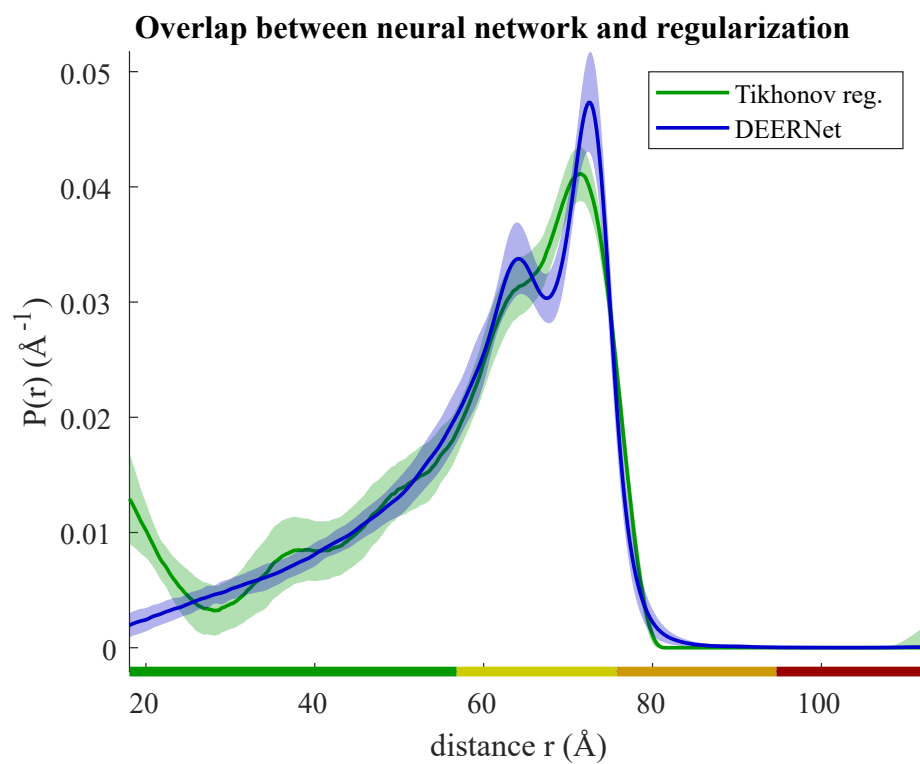
**ComparativeDEERAnalyzer version 2.0**

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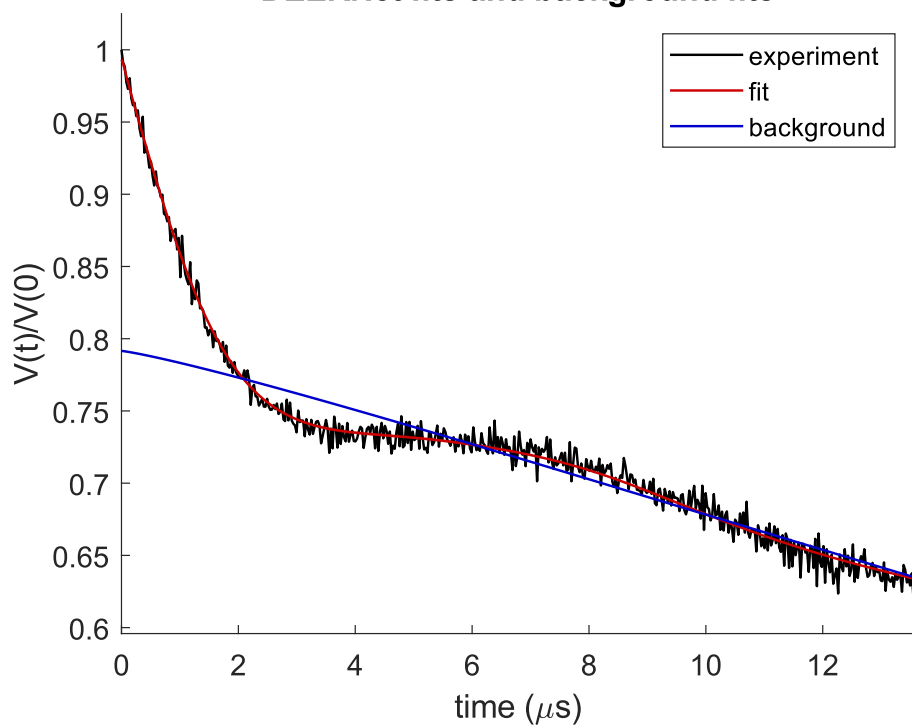
## 1. Distance distributions



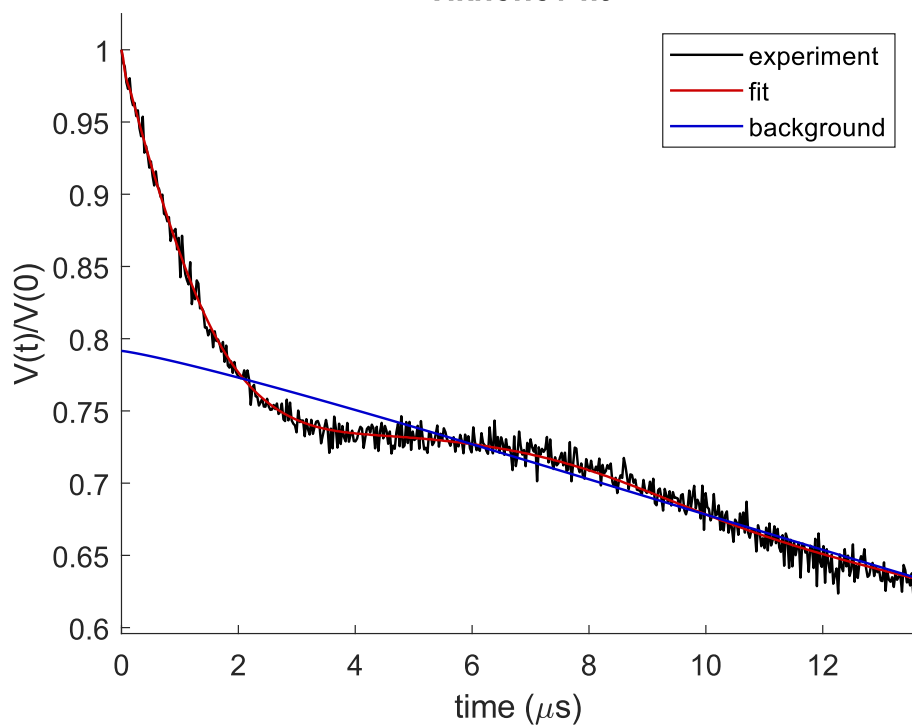
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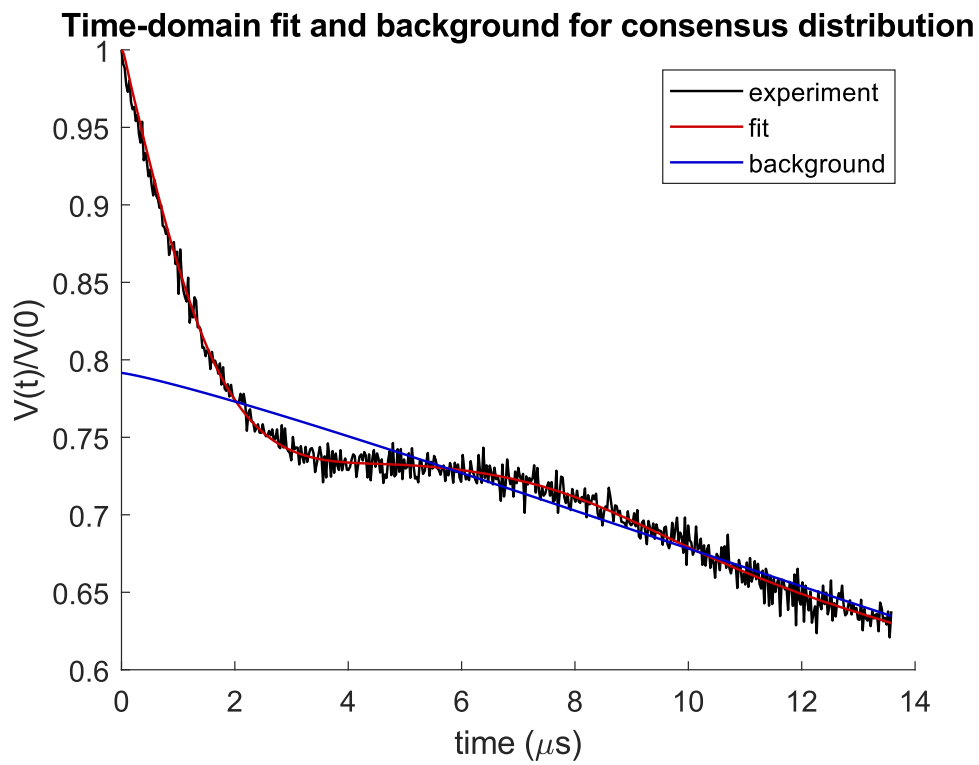
## 2. Fits of time-domain data

**DEERNet fits and background fits**



**Tikhonov fit**





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### 3. Experimental and processing parameters

Modulation depth: 0.203

Signal-to-noise ratio: 29.1 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00720

From DEERNet fit: 0.00698

From Tikhonov fit: 0.00699

Zero time: 123 ns

Maximum time: 13580 ns

The last 10 % of the data was cut off

Time increment: 28 ns

Phase: -21.9 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: 5.59

Reg. par. initial estimate by L-curve corner: 31.62

Overlap between DEERNet and regularization solutions: 0.932

Predicted overlap of consensus solution with ground truth: 0.80...0.97

Mean distance: 61.5 Å

Distance standard deviation: 12.2 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_235\_500\_D2O\_MTS�\_E  
MCV\_d2\_15.5us\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_235\_500\_D2O\_MTS�\_E  
MCV\_d2\_15.5us\_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\_235\_500\_D2O\_MTSL\_E  
MCV\_d2\_15.5us\_spec\_consensus\_DEER\_fit.csv

Metadata:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_235\_500\_D2O\_MTSL\_E  
MCV\_d2\_15.5us\_spec\_comparative\_DEER\_meta\_data.csv