

# **DEER analysis report on dataset DEER4p\_Q\_50K\_PTBP1\_free\_109-475\_wp 34877\_20us\_298sc**

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

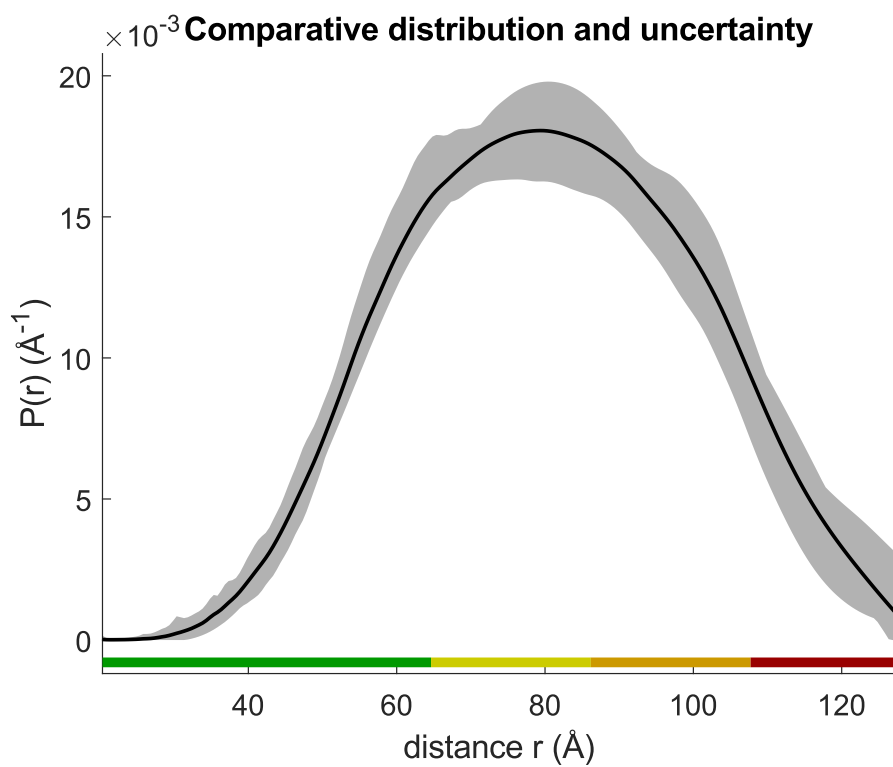
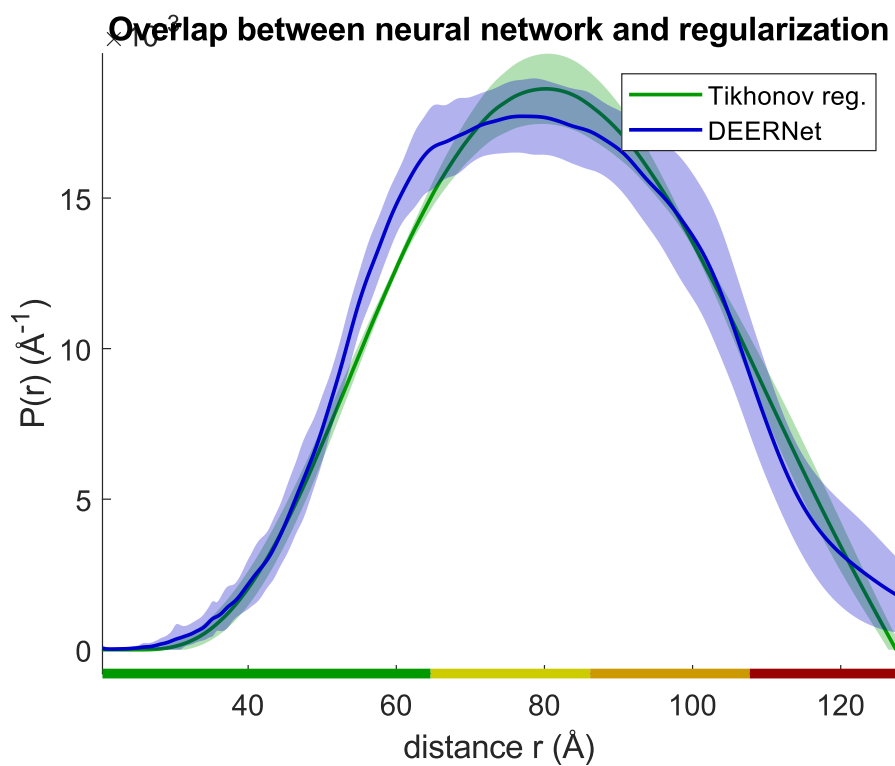
**ComparativeDEERAnalyzer version 2.0**

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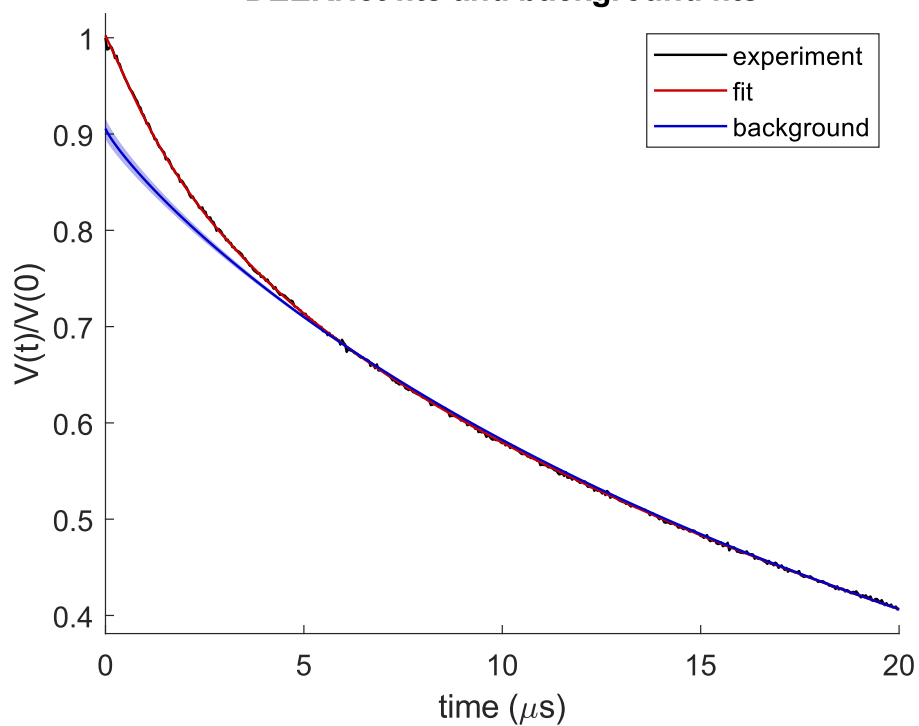
## 1. Distance distributions



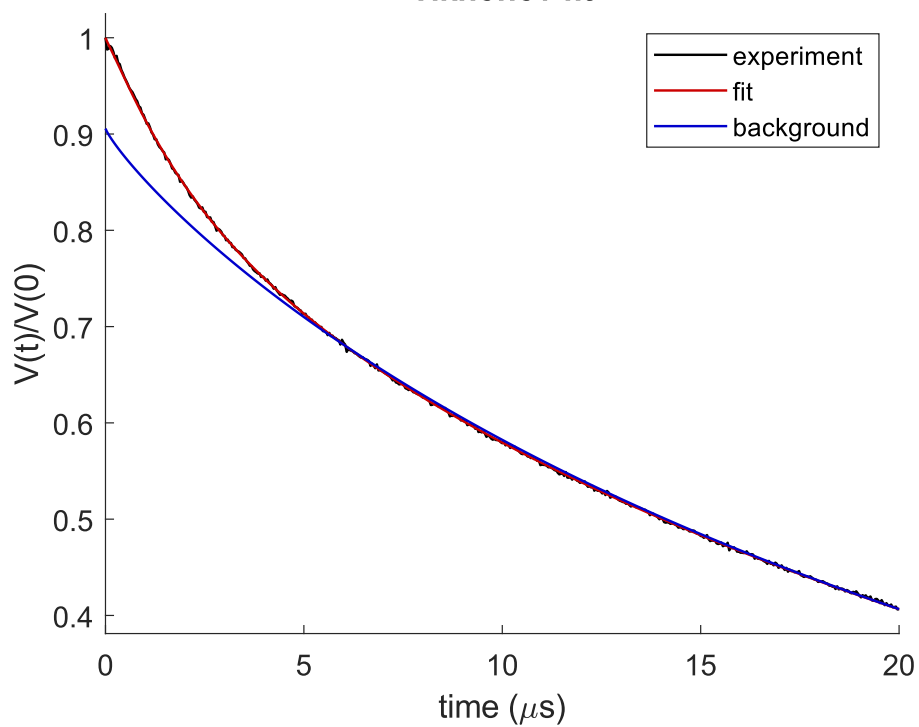
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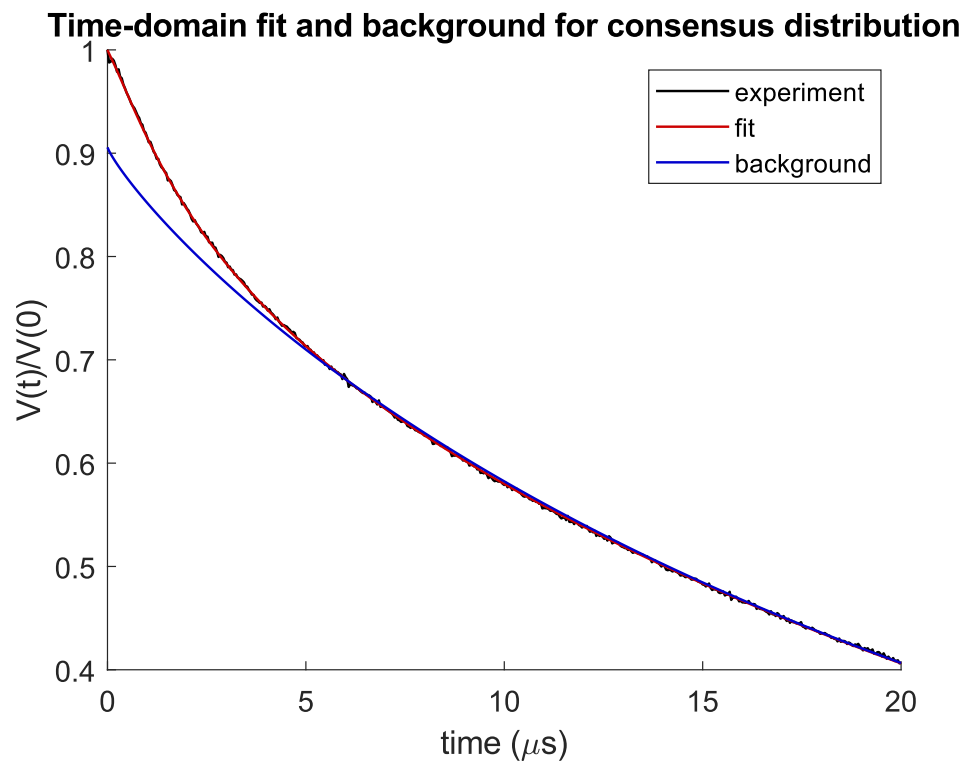
## 2. Fits of time-domain data

**DEERNet fits and background fits**



**Tikhonov fit**





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### 3. Experimental and processing parameters

#### Modulation depth: 0.097

Signal-to-noise ratio: 65.1 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00132

From DEERNet fit: 0.00149

From Tikhonov fit: 0.00147

Zero time: 0 ns

Maximum time: 20000 ns

Time increment: 40 ns

Phase: -15.9 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: 79.62

Reg. par. initial estimate by L-curve corner: 39.81

Overlap between DEERNet and regularization solutions: 0.964

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

Mean distance: 81.0 Å

Distance standard deviation: 21.5 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER4p\_Q\_50K\_PTBP1\_free\_109-475\_wp34877\_20us\_298sc\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER4p\_Q\_50K\_PTBP1\_free\_109-475\_wp34877\_20us\_298sc\_consensus\_DEER\_distribution.csv

Fit and background in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER4p\_Q\_50K\_PTBP1\_free\_109-475\_wp34877\_20us\_298sc\_consensus\_DEER\_fit.csv

### 3. Experimental and processing parameters

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Metadata:

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