

# **DEER analysis report on dataset DEER\_Q202C\_Q388C\_EMCV\_native\_d2\_8. 5us\_157scans\_spec**

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

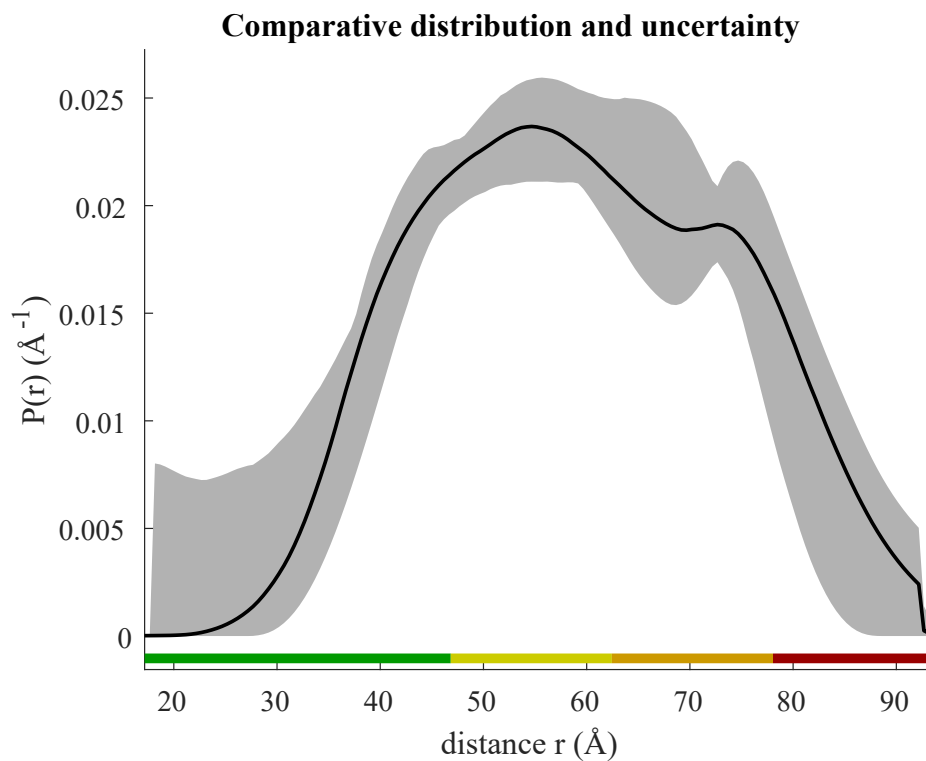
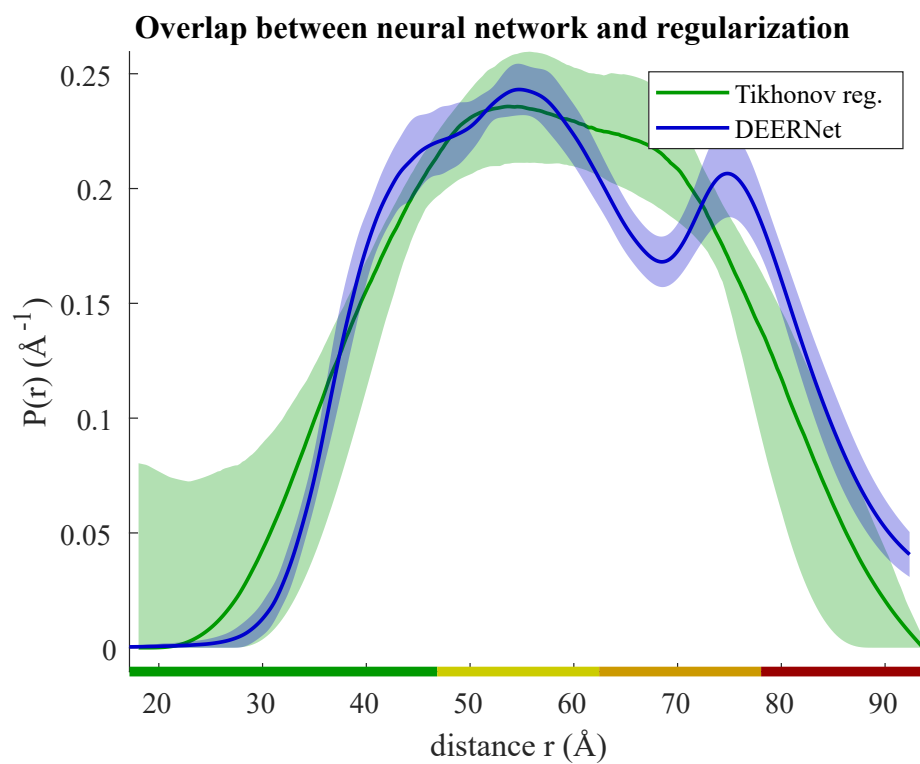
**ComparativeDEERAnalyzer version 2.0**

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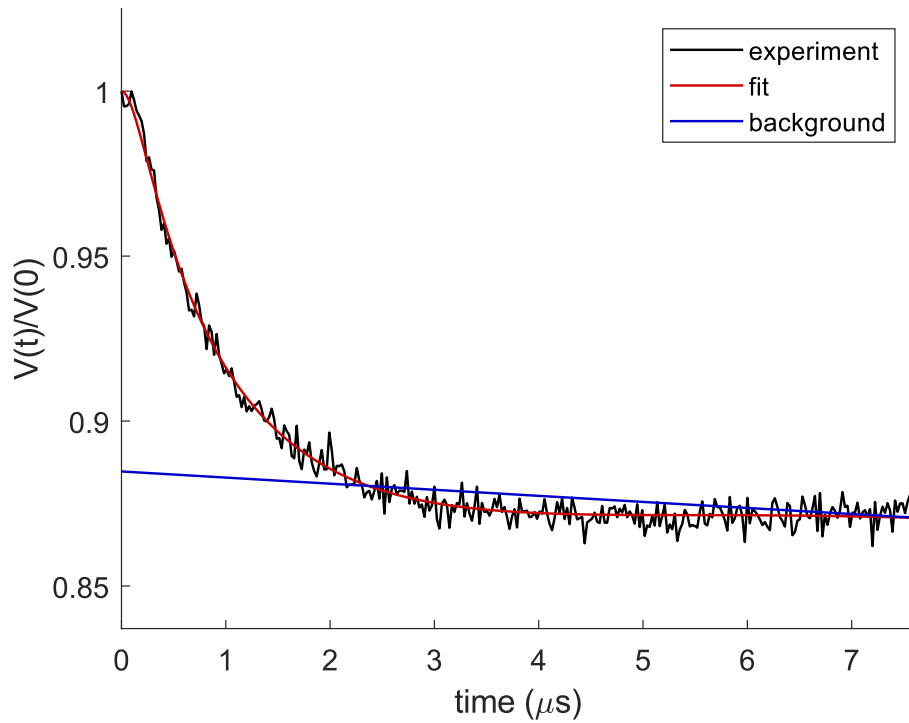
## 1. Distance distributions



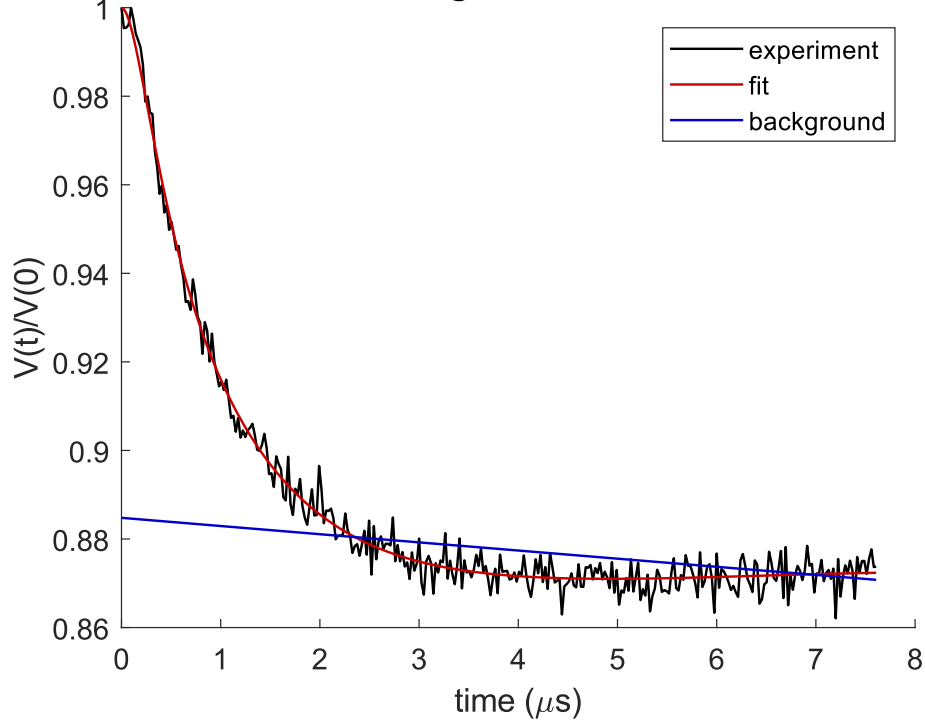
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## 2. Fits of time-domain data

**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: 0.115

Signal-to-noise ratio: 35.8 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00276

From Tikhonov fit: 0.00330

Zero time: 0 ns

Maximum time: 7.608000e+03 ns

The last 10 % of the data was cut off

Time increment: 24 ns

Phase: -3.5 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: 17.80

Reg. par. initial estimate by lr: 12.59

Overlap between DEERNet and regularization solutions: 0.923

Predicted overlap of consensus solution with ground truth: 0.79...0.96

Mean distance: 59.3 Å

Distance standard deviation: 17.4 Å

Full data set in Matlab format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_Q202C\_Q388C\_EMCV\_native\_d2\_8.5us\_157scans\_spec\_comparative\_DEER\_analysis.mat

Distance distributions in text format:

G:\projects\Christoph\_Gmeiner\modelling\master\_shot\Deer\DEER\_Q202C\_Q388C\_EMCV\_native\_d2\_8.5us\_157scans\_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\_Q202C\_Q388C\_EMCV\_  
native\_d2\_8.5us\_157scans\_spec\_consensus\_DEER\_fit.csv

Metadata:

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native\_d2\_8.5us\_157scans\_spec\_comparative\_DEER\_meta\_data.csv