

# **DEER analysis report on dataset 220601\_KAq195.9\_DEER\_208032\_66pc\_pi**

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

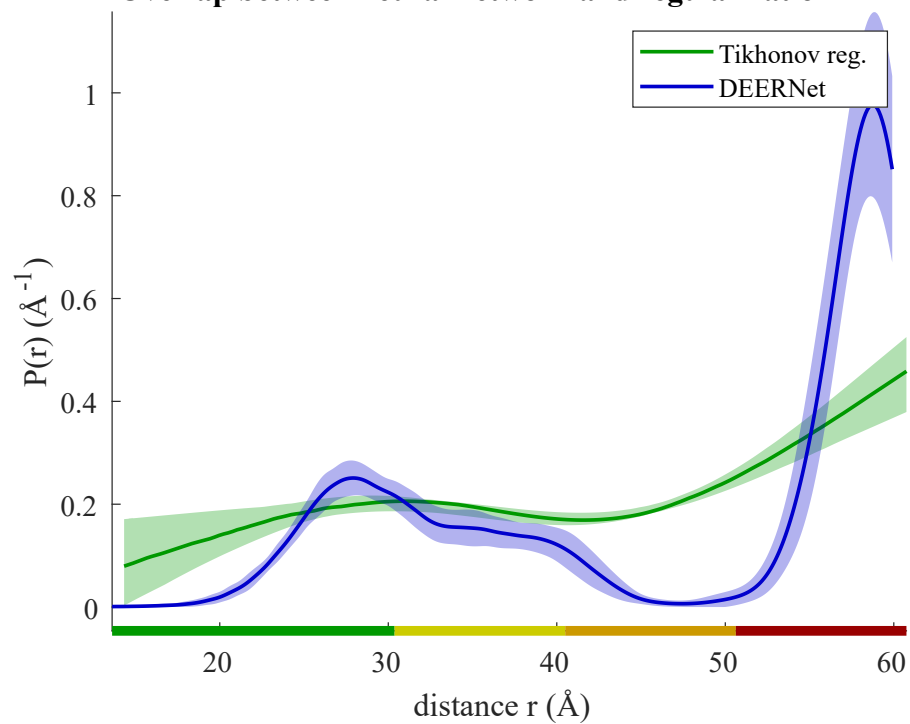
**ComparativeDEERAnalyzer version 2.0**

see: S. G. Worswick et al., DOI: 10.1126/sciadv.aat5218, L. Fabregas Ibanez et al., DOI: 10.5194/  
mr-1-209-2020

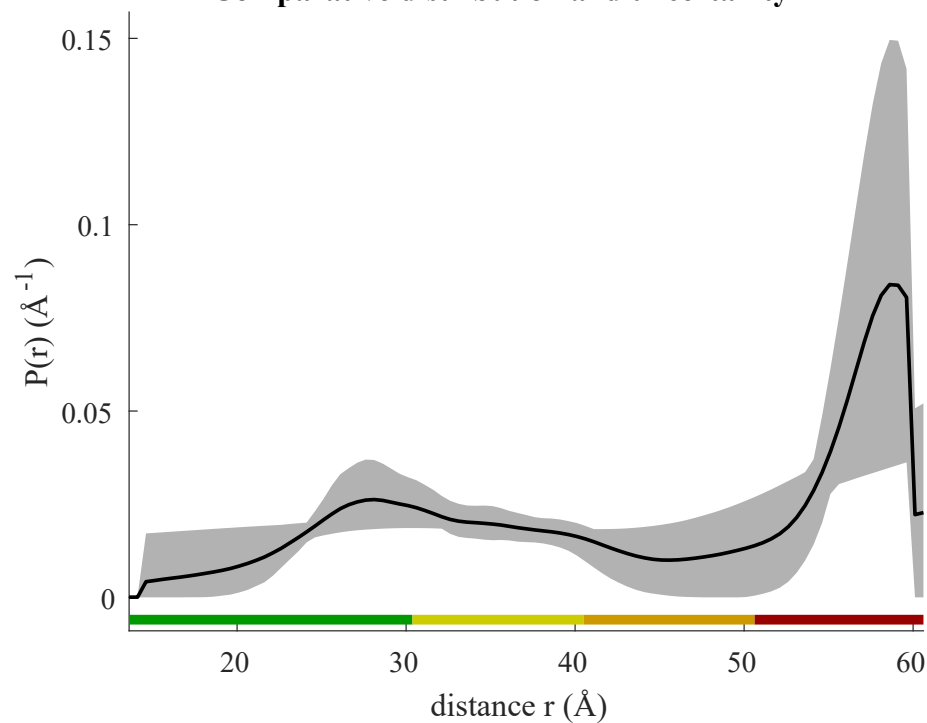
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## 1. Distance distributions

**Overlap between neural network and regularization**

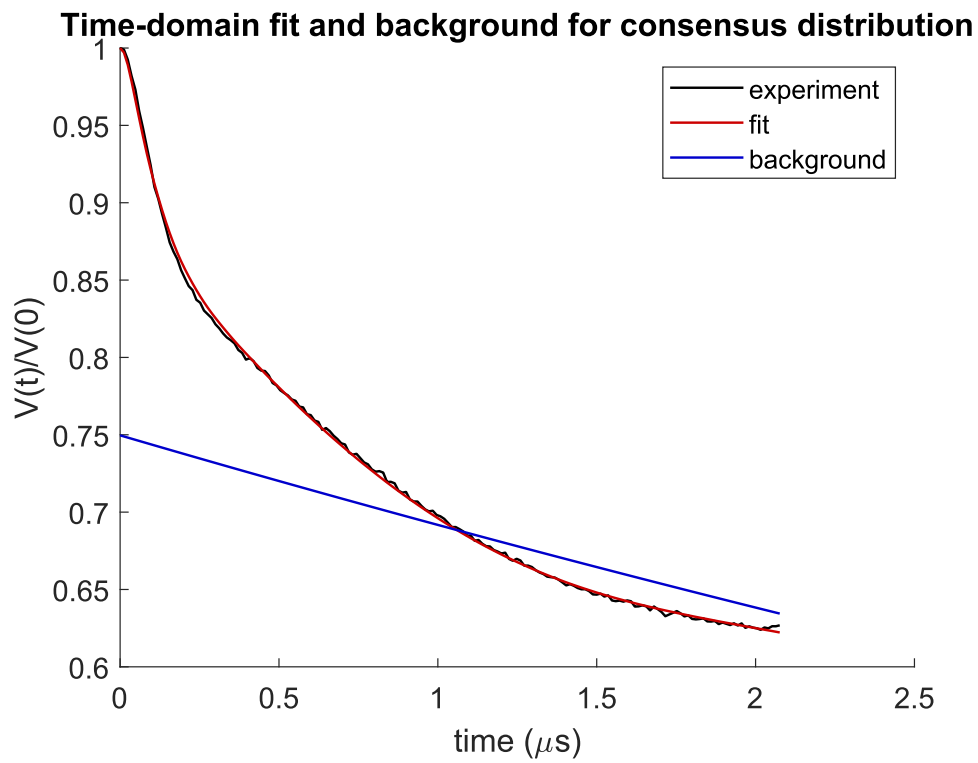
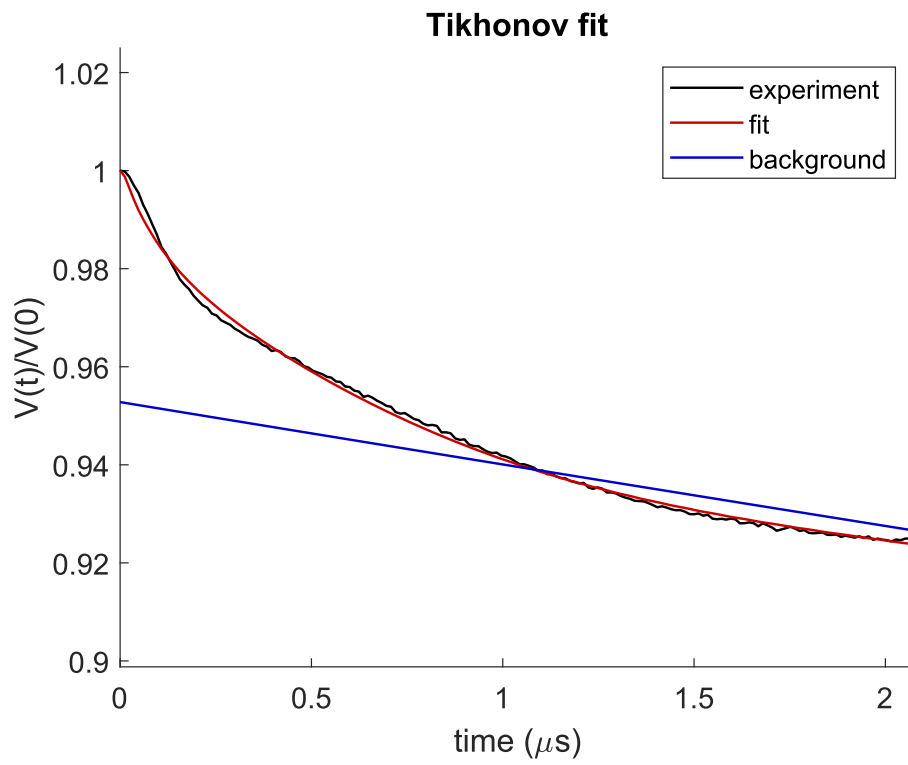


**Comparative distribution and uncertainty**



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## 2. Fits of time-domain data



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### 3. Experimental and processing parameters

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

**Ghost suppression for a 7-spin system was applied.**

Modulation depth: 0.250

Signal-to-noise ratio: 151.9 (w.r.t. modulation)

Noise estimates normalized to maximum signal

From imaginary part: 0.00166

From Tikhonov fit: 0.00492

Zero time: 288 ns

Maximum time: 2076 ns

Time increment: 12 ns

Phase: 0.3 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: 8.04

Reg. par. initial estimate by lr: 0.25

**Overlap between DEERNet and regularization solutions: 0.663**

Predicted overlap of consensus solution with ground truth: 0.55...0.72

**Mean distance: 43.7 Å**

**Single Gaussian provided different mean distance. Distribution may be incomplete.**

Distance standard deviation: 13.6 Å

Full data set in Matlab format: C:\Users\Katrin\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP\_div\Msc\MscS\_D67R1\_M47R1\_Mary\_220518\KAq195\220601\_KAq195.9\_DEER\_208032\_66pc\_pi\_comparative\_DEER\_analysis.mat

Distance distributions in text format: C:\Users\Katrin\Documents\OneDrive - University of St

### 3. Experimental and processing parameters

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Fit and background in text format: C:\Users\KatrIn\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP\_div\MscS\MscS\_D67R1\_M47R1\_Mary\_220518\KAq195\220601\_KAq195.9\_DEER\_208032\_66pc\_pi\_consensus\_DEER\_fit.csv

Metadata: C:\Users\KatrIn\Documents\OneDrive - University of St Andrews\StAndrews\Work\BEB\Projects\CP\_div\MscS\MscS\_D67R1\_M47R1\_Mary\_220518\KAq195\220601\_KAq195.9\_DEER\_208032\_66pc\_pi\_comparative\_DEER\_meta\_data.csv