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Interactive comment on "DeerLab: A comprehensive toolbox for analyzing dipolar EPR spectroscopy data" *by* Luis Fábregas Ibáñez et al.

Anonymous Referee #1

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The authors report in their manuscript a Matlab based assembly of methods for analyzing Pulsed Dipolar EPR time traces from two S = 1/2 spin centers. The program box includes several known methods for which stand-alone programs have been published. The advantage of DeerLab being that they can be run now within one program and easily compared. In addition, DeerLab includes a multi-pathway model that enables analyzing time traces from "multi-pulse" DEER, which is new and very interesting since it avoids pre-data treatment and includes the formerly "unwanted" pathways (artifacts) into the analysis. Good is also the inclusion of a global analysis of several time traces. The inclusion of a goodness of fit and uncertainty evaluation is very much need in the community for assessing and comparing data. The missing of a GUI is a disadvantage for a wider distribution of the program and should be tackled in a later

step. Experts can use the stand-alone programs but the program will especially be helpful for non-experts and for them the GUI will be most helpful. Last but not least the manuscript includes a clearly stated correction of a previous paper by two of the authors in that Huber and TV regularization do now perform equally well as Tikhonov regularization.

I recommend acceptance of the manuscript after the authors addressed the following minor issues:

1) In the caption of figure 2 it is stated that the AIC criterium was used for the selection of the regularization parameter, this should be written clearly in the text (I almost missed it). In addition, the profiles of the parameters and which parameter was chosen should be shown in the figure. 2) Figure 3 shows the data analysis for a parametric model (multi-Gaussian) using a different time trace than in Figure 2. They can keep the time trace in Figure 3 but in order to be able to compare, Figure 3 should also contain an analysis of the time traces in Figure 2. The aim of DeerLab is to compare, such a comparison should be shown. 3) Figure 4, what is the grey time trace? Please, state in figure caption. 4) Figure 5, I would like to urge the authors to include some words of warning when showing the analysis of such truncated data in particular with respect to the impact of SNR. They should include an analysis on the same time traces as in Figure 2 truncate them and give the SNR. 5) Uncertainty analysis: I do see in figure 11 a graphical representation of the uncertainty but what is the uncertainty in numbers, what is the +- of r and with respect to the shape? How do I have to read the graphical representation, is it good, is it bad?

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