

Hyscorean 1.0 - Quick User Guide

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1 Installation

- 1) In order to download the Hyscorean 1.0 software, an Atlassian account needs to be made in order to be able to pull the program files from the online repository (via a third-party software such as TortoiseHG or SourceTree).
- 2) Once the software is pulled from the repository and stored in a local directory, this has to be added to the default search path of MATLAB via *Home>Set Path>Add with Subfolders* and then save it (it is crucial that the *bin* folder is also added to the path search).
- 3) The program can then be called from the MATLAB console via the command *Hyscorean*.
- 4) The first time the program is used it is important to define a default save path for the *Save&Report* function. This can be done by pressing the [...] button next to the *Save&Report* one. This will open a window where the default save directory can be inserted and changed. Once saved, this will be saved for all further sessions.

2 Basic Processing

- 1) Load the Bruker spectrometer output files (accepted both .DSC and .DTA formats) via the *Load* button. Automatically the software will recognize if several measurements with different τ values have been concatenated. If so, these will be extracted and the τ -values used in the experiments will be automatically extracted from the PulseSpel codes used for the experiments and stored in the loaded file.
- 2) The different τ -values and their different combinations will be shown in a list in the *Pre-Processing* panel, where the desired combination can be selected (Note: The combinations are performed in time-domain and not in frequency-domain).
- 3) The processing can be started by using the *Process* button which will perform background correction, zero-filling, Lorentz-to-Gauss transformation and apodization in this order until it is finally transformed via 2D-FFT.

- 4) Once the processing is finished the spectrum and the processed signal will be plotted in their respective panels. At this point the add-on panels will activate.
- If one presses the *Process* button again, the processing will be restarted skipping every element in the *Pre-processing* panel whose parameters have not been changed (marked by a ✓ next to the corresponding panel). Any change in those panels will result in the ✓ disappearing and thus restarting the processing from that points.
 - The elements in the *Signal Processing* panel will always be conducted even without changing any parameters.

3 Add-On's

- **Blind Spots**

The blind-spots button will results in an overlay of the map containing the expected blind spots of the HYSORE measurement at the current τ -values combination.

- **Add Lines & Tags**

This add-on allows the addition of auxiliary lines and tags tot he plotted spectrum corresponding to the Larmor frequencies of the selected isotopes on the list. The magnetic field used for the experiment is extracted from the Bruker program parameters, however the user is required to give the magnetic field offset as an input (default is set to 0 G). These lines and tags can easily be removed from the spectrum by using the *Clear Tags* button and will remain in the spectrum otherwise even if the *Process* button is hit again.

- **Save & Report**

This option will save four elements to a folder defined by the path and identifier given in the settings. This four elements consist of a *.mat* file containing the spectrum, frequency and time axis and the processed signal data, a *.fig* and *.pdf* copy of the spectrum and a report file automatically generated and containing all important experimental and processing parameters. In case that the folder already contains files, numbers will be appended to avoid clashes with the preexisting files.