Topspin2.1 – POPT

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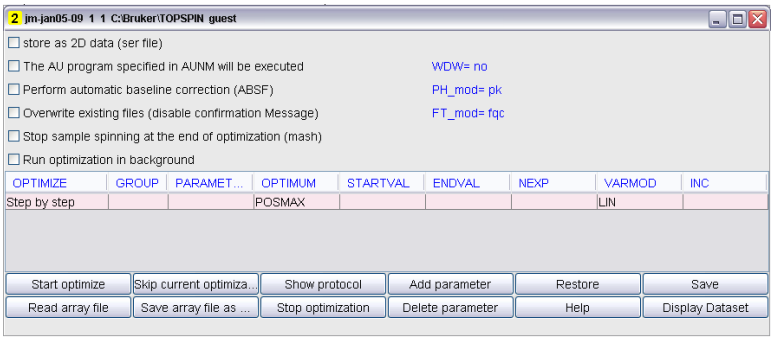
Typing the command '**popt'** into the command line opens the parameter optimization window. This window allows the optimization of any acquisition parameter like pulse lengths and delays similar to the well-used au program 'paropt'

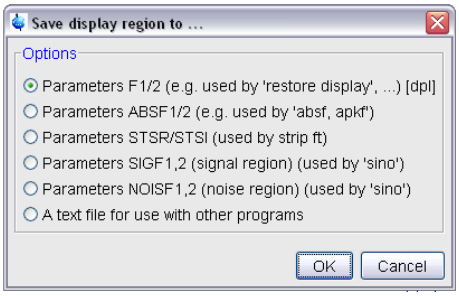
Benefits of using POPT over the au program paropt:



- Easy to use interface which allows for quick setup of parameter optimization
- Able to stop parameter optimization easily
- Able to setup and run optimization on multiple parameters
- Scale of the output corresponds to actual parameter values

To Use POPT:

Before starting an optimization one acquisition must first be collected using the non-optimized parameters. First, a region of the spectrum (containing a single peak or a group of peaks) needs to be expanded. This region is then defined by right-clicking the spectrum and selecting 'Save Display Region To…' and selecting 'Parameters F1/2 (e.g. used by 'restore display',…)[dpl]' and OK.



Typing 'popt' into the command line will open the parameter optimization window which will allow the user to create an entry for each parameter to be optimized. By default only one entry is shown and additional entries can be added by clicking on 'Add Parameter'.

For basic parameter optimization enter the parameter to be optimized (*i.e.* p1, d1, *etc*.), starting value (STARTVAL), ending value (ENDVAL) and the number of experiments (NEXP) or increment (INC) (either can be entered and the other will be calculated). Click 'Start Optimization' to begin.

The optimization will be stored in PROCNO 999. Additional optimizations will be added to sequentially decreasing PROCNOs (*i.e.* 998, 997 …). Results are shown as series of spectral regions on one screen and show the optimum parameter value.

Explanation of Additional POPT parameters:

- OPTIMIZE: Optimization of parameters in the group
  - *Step by Step* – the parameters of a group are optimized one after the other. The results of each optimization are stored in a different PROCNO.
  - *Simultaneous* - The parameters of a group a optimized simultaneously. NEXP must be the same for each parameter and represents the total number of experiments. The result of the parameter optimization is stored in one PROCNO.
  - *Array* - The parameters of a group a optimized according to an N-dimensional array (N is the number of parameters in a group). NEXP can be different for each parameter. The total number of experiments is the product of the NEXP value of each parameter. The result of the parameter optimization is stored in one PROCNO.
  - *No Optimization*
- GROUP : group number. Optimization starts with the lowest group number.
- PARAMETER : The parameter to be optimized.
- OPTIMUM : Optimization criterion options
    - POSMAX - the maximum value of a positive peak
    - NEGMAX - the maximum value of a negative peak
    - MAGMAX - the maximum magnitude value of a peak
    - MAGMIN - the minimum magnitude value of a peak
    - INTMAX - the maximum value of an integral
    - INTMIN - the minimum value of an integral
    - ZERO - zero intensity of a peak
- STARTVAL : First value of the parameter.
- ENDVAL : Last value of the parameter.
- NEXP : Number of experiments.
- VARMOD : Parameter variation mode: linear or logarithmic.
- INC : Parameter increment value. Unused for VARMOD = log.

Buttons:

- Start optimize - start the optimization for all checked parameters
- Skip current optimization - stop the optimization for the current parameter
- Show protocol - show the optimization result.
- Add parameter - add a parameter entry
- Restore - restore the last saved optimization setup
- Save - save the current optimization setup to current dataset EXPNO
- Read array file - read optimization setup
- Save array file as.. - save current optimization setup for general usage
- Stop optimization - stop the optimization for all checked parameters
- Delete parameter - delete the selected parameter
- Help - open the popt help page