**Pictorial instructions for Setting-up an ImpEXSIDE\_PS Experiment**

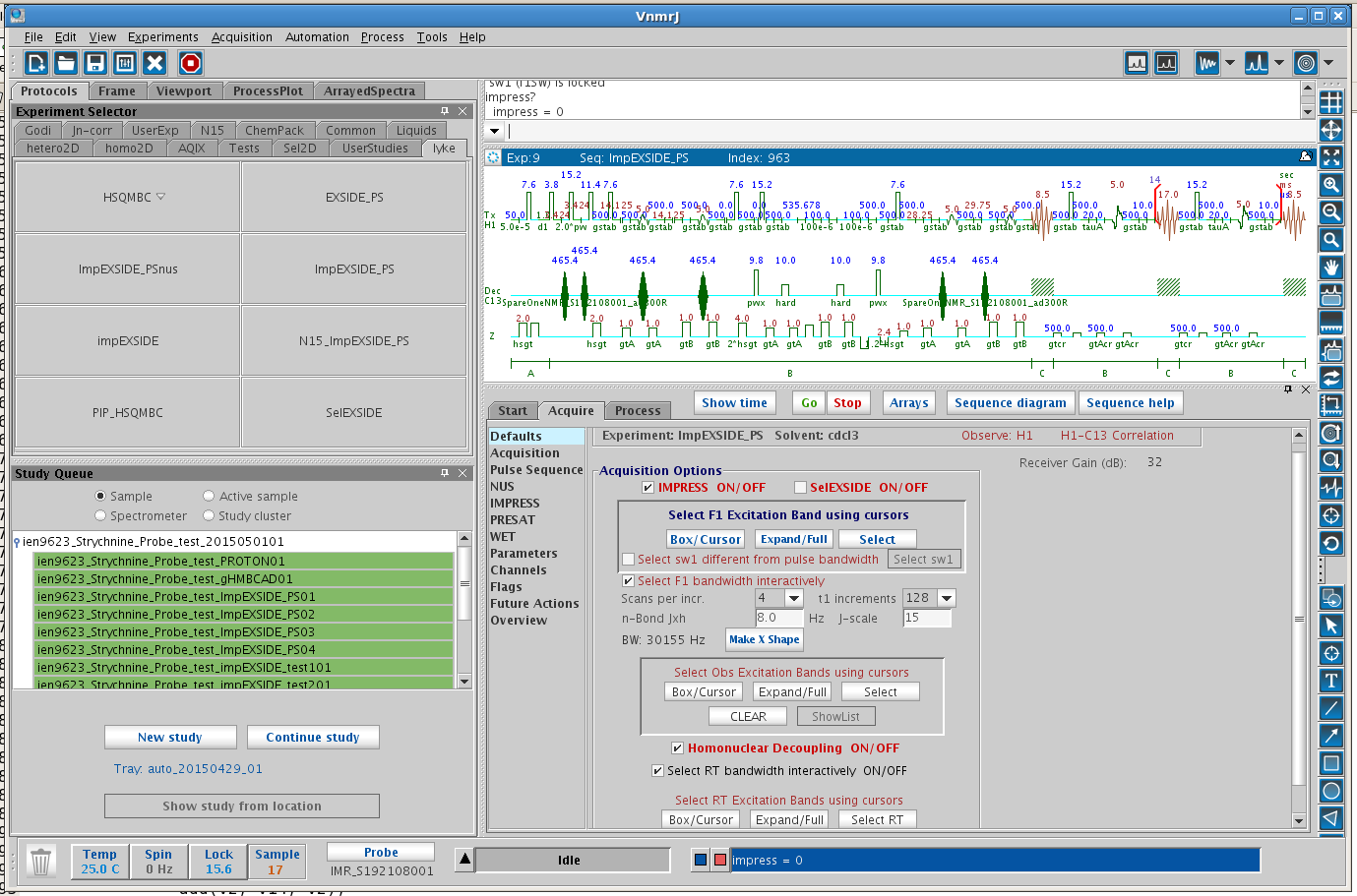
Authors: Ikenna E. Ndukwe (email: [in12121@bristol.ac.uk](mailto:in12121@bristol.ac.uk)) and Craig P. Butts (email: [craig.butts@bristol.ac.uk](mailto:craig.butts@bristol.ac.uk))

Default settings:

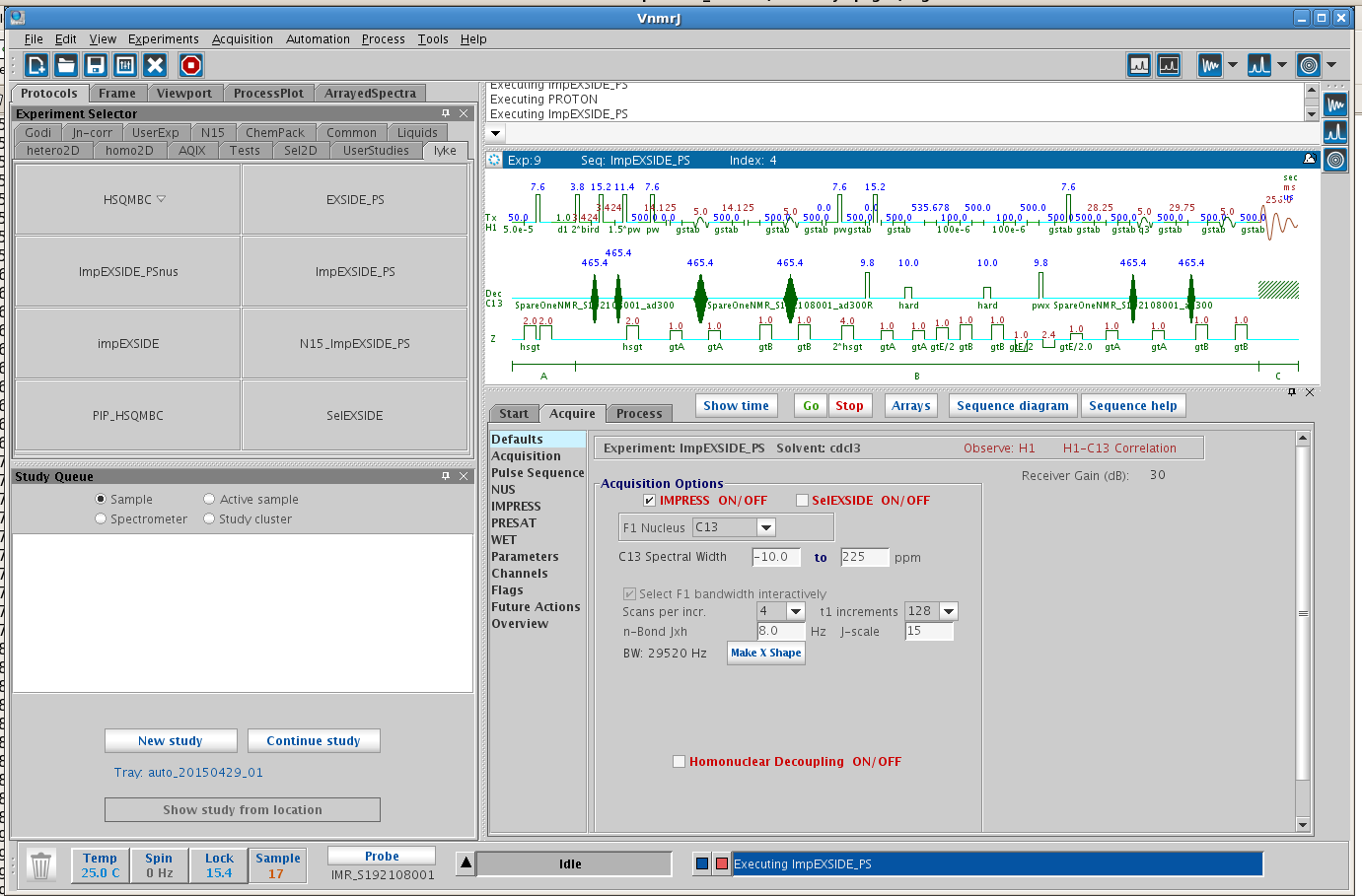
The figure below shows the default settings for ImpEXIDE\_PS which has both **IMPRESS** and ‘Pure shift (Homonuclear decoupling)’ options checked. Note that ‘q3’ and ‘rsnob’ pulses will be created with the F2 bandwidth/offset selected (using the ‘Select Obs Excitation Bands Using cursors’) for the selective INEPT and ‘*J*-refocusing’ periods of the Pure shift acquisition respectively. This options can be changed in the pulse sequence.



The ‘Select RT bandwidth interactively’, allows you to select a wider region to shorten the length of the ‘rsnob’ pulse created for the ‘*J*-refocusing’ period of the Pure shift acquisition. This option can be selected by checking the ‘Select RT bandwidth interactively’ box.



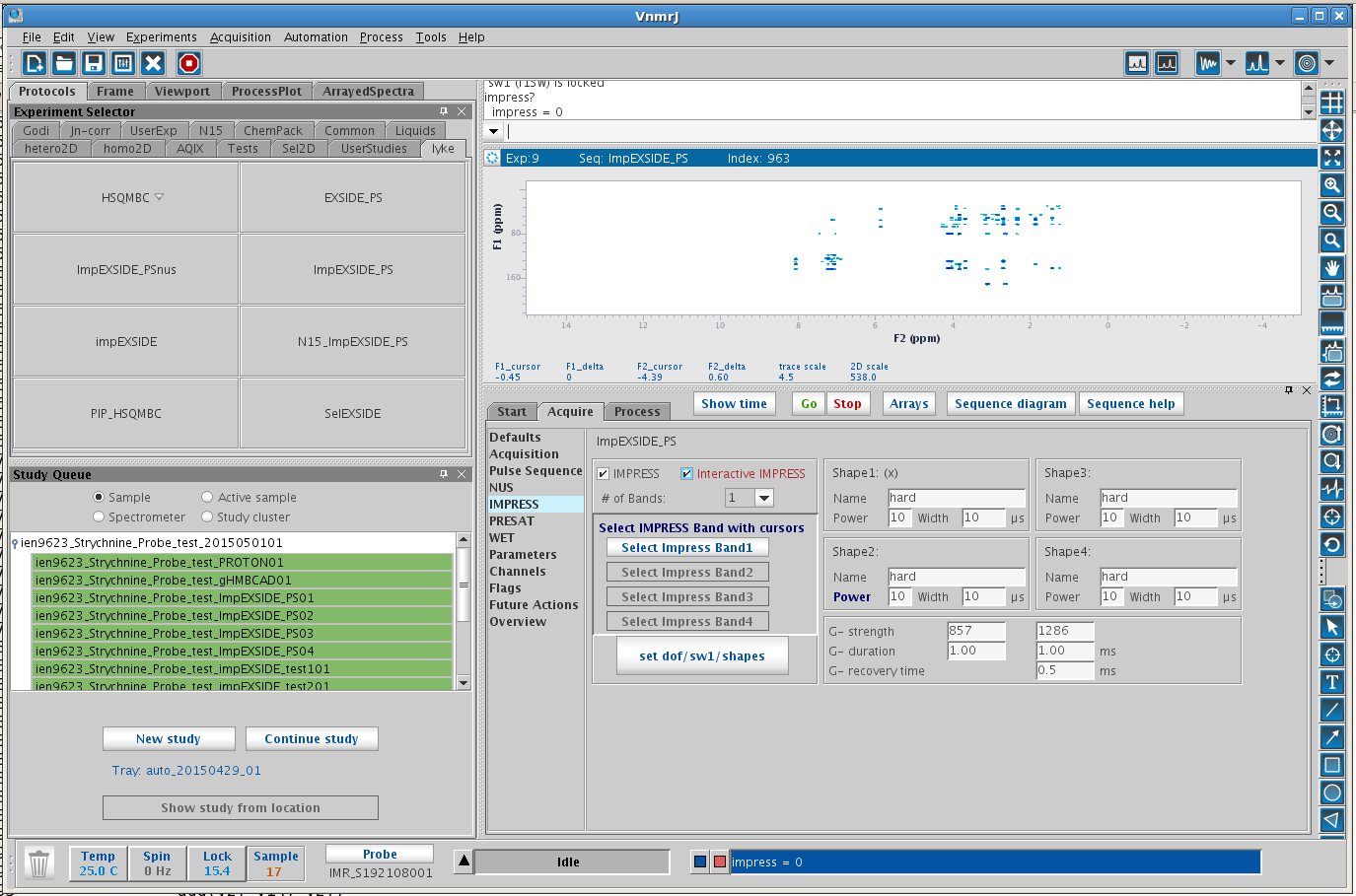
Homonuclear decoupling can be turned-off by unchecking the ‘Homonuclear Decoupling’ box. This allows for a normal NMR acquisition (see figure below).

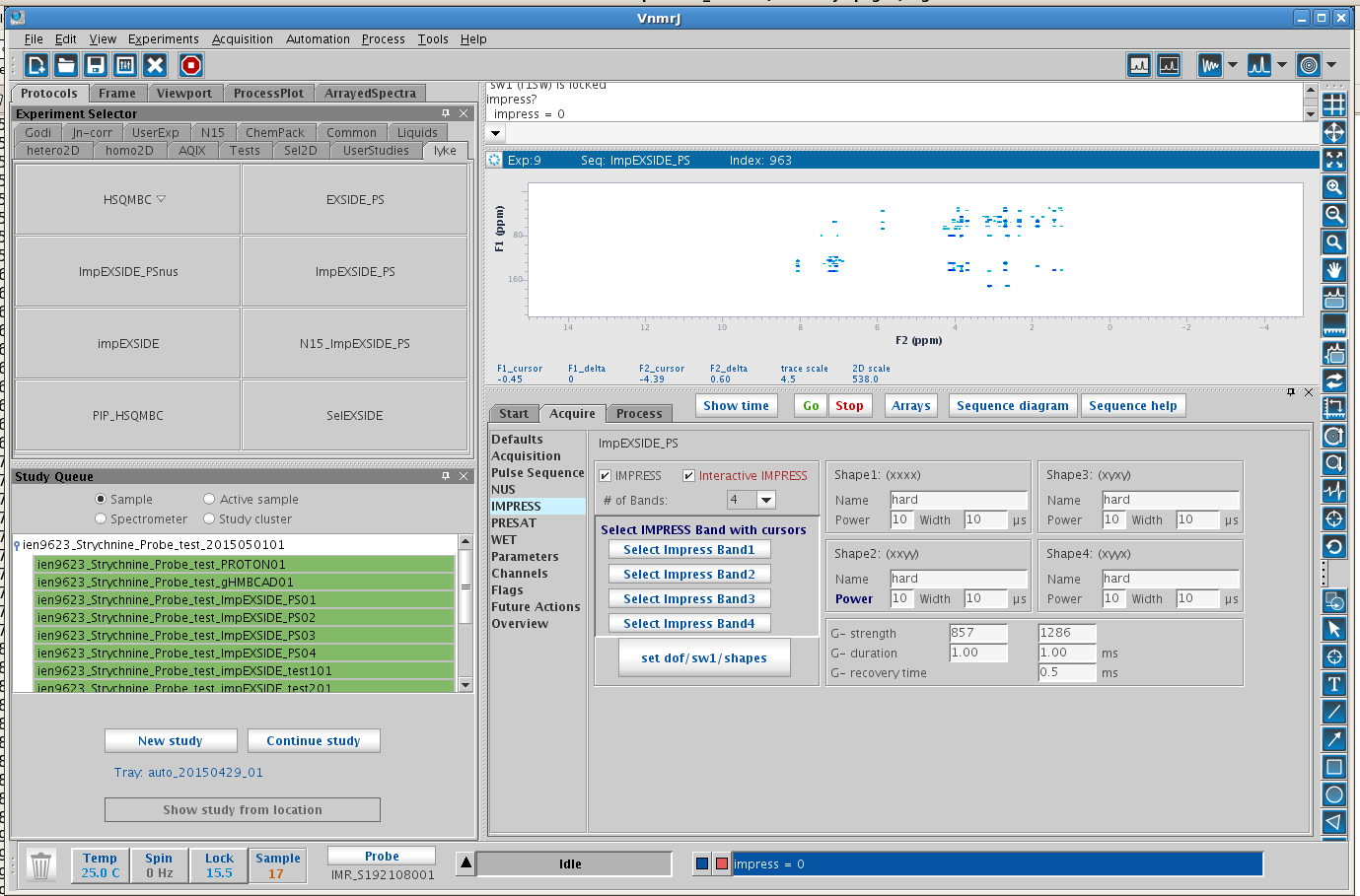


The 13C regions of interest can be defined by clicking the IMPRESS menu on the left (Important – this is not the IMPRESS in ‘red’ type but the one in **black type**). This reveals the template which allows you to define the heteronuclear chemical shifts/bands of interest. Care should be taken so that regions defined or selected do not overlap.

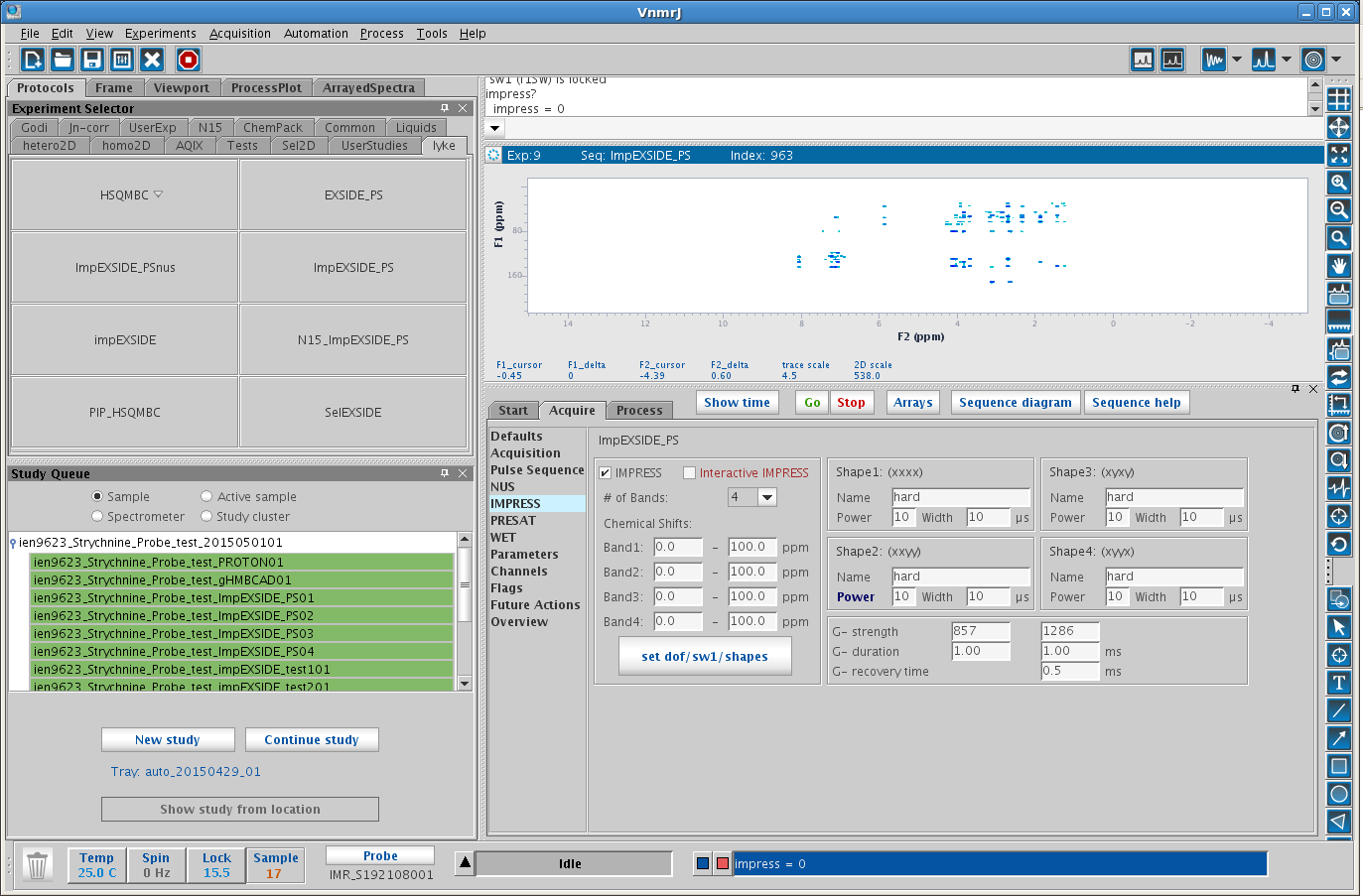
The region(s) of interest can be defined in one of two ways;

You can use the buttons ‘Select Impress Band’ to select the regions of interest up to a maximum of four (as shown in the preceding figure). This option is only available if a HMBC spectra have been acquired abinitio. **Click ‘set dof/sw1/shapes’ button when the required regions have been defined.** This creates the IMPRESS shapes needed for the experiment.

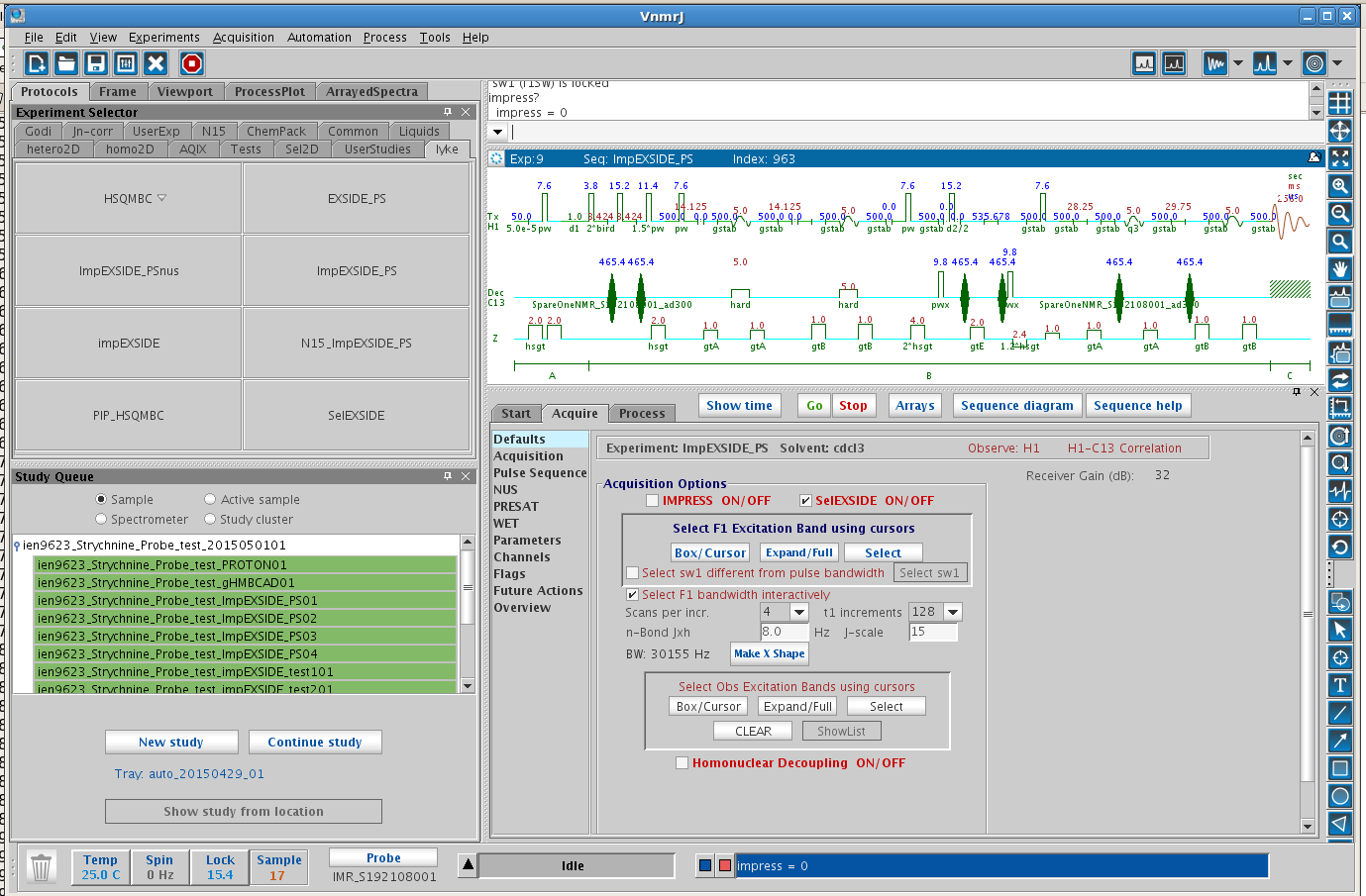


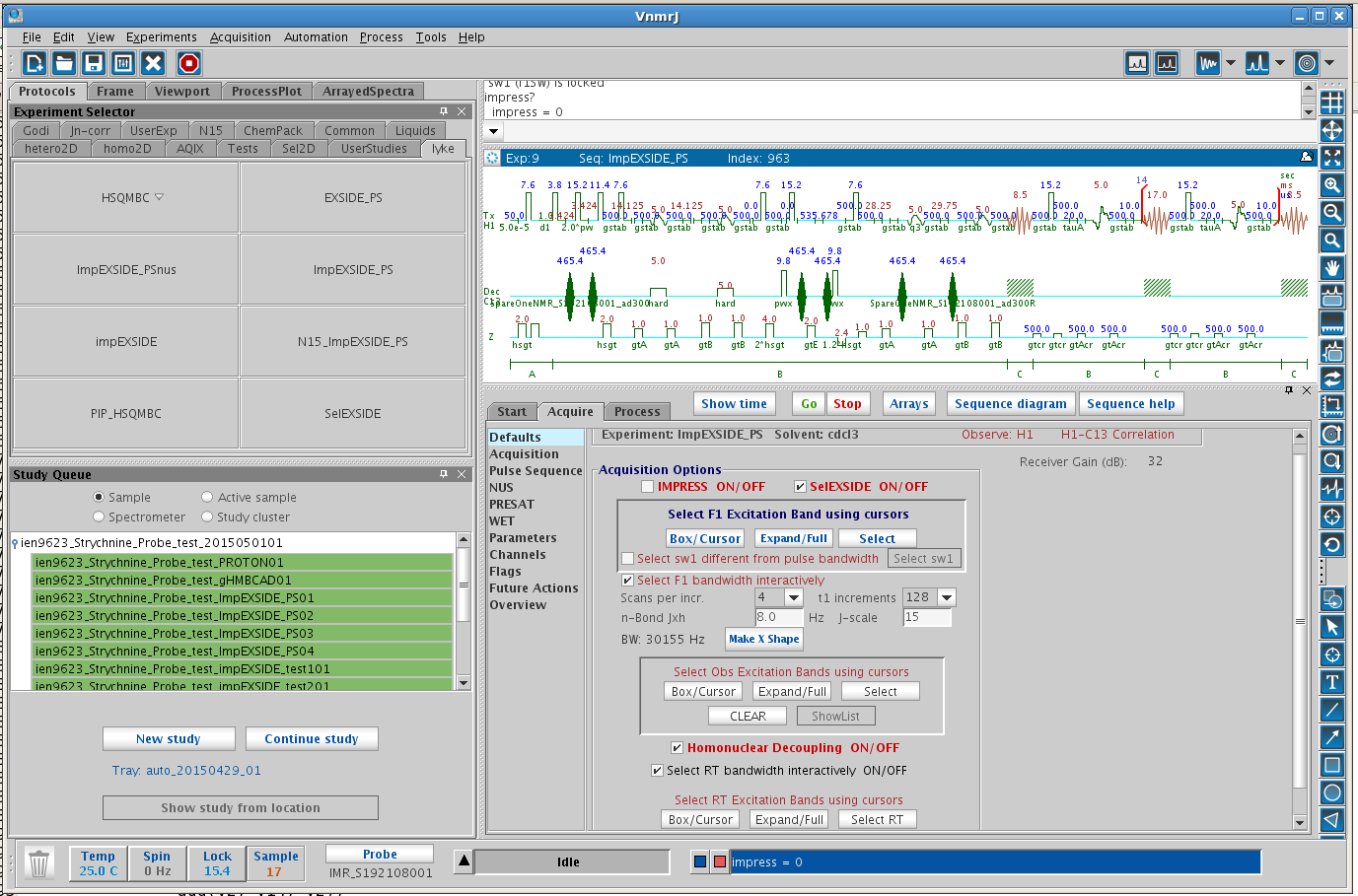


You might prefer to manually type-in the 13C regions of interest to ensure equal bandwidth for all selected regions (**Note**: the resolution in F1 is a function of the widest region selected while the IMPRESS pulse is a function of the narrowest region). This can be done by deselecting the ‘Interactive IMPRESS’ tab (as shown below) and then typing-in the regions in any choosing order (**Important:** left box is lower ppm and right box is higher ppm). **Remember to click ‘set dof/sw1/shapes’ button when the regions have been defined.**

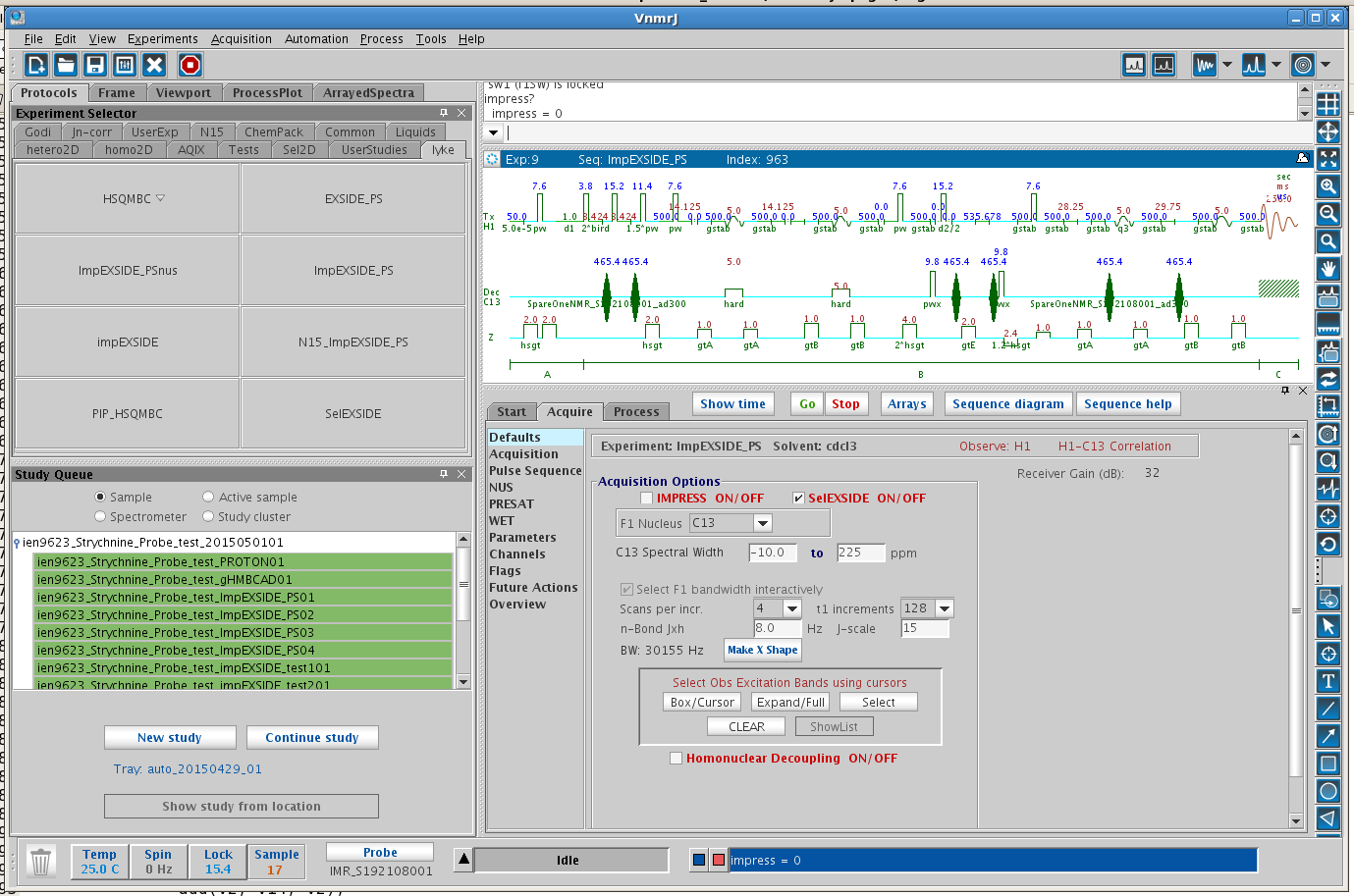


Sensitivity benefits of IMPRESS is gained where more than one correlation is sort for a given F2 selection. Therefore if only one is needed, you can easily revert to the singly 13C selective experiment (SelEXSIDE) by checking the ‘SelEXSIDE’ button. This automatically turns-off the IMPRESS element allowing you to run a SelEXSIDE experiment and vice versa. Homonuclear decoupling option is also available (See preceding figure).





In the SelEXSIDE experiment, you can also define the 13C region of interest interactively by clicking on ‘**Select F1 bandwidth interactive**’. The button is then de-highlighted and the two boxes revealed. You can then type in the 13C chemical shift range of interest (left box is lower ppm and right box is higher ppm).



**Processing IMPRESS Data**

Impress data acquisition in Vnmrj is encoded with appropriate Hadamard matrix and information can be retrieved using macros. To retrieve acquired data, open the FID in vnmrj (ignore any error messages) and then type in the command line the following macro(s) as needed – macros are in bold type below;

**Impressprocess(1)** – This reveals correlation in band 1.

Please note that the order of your selection may have been changed when you press the ‘set dof/sw1/shape’ button. Always confirm before submitting the experiment or alternatively when processing the data go back to the ‘Acquire’ tab then unto ‘IMPRESS’ menu and check the order.

**Impressprocess(2)** – Reveals correlation in band 2.

**Impressprocess(3)** – Reveals correlation in band 3 if selected.

**Impressprocess(4)** – Reveals correlation in band 4 if selected.

IMPRESS data cannot, at this moment, be processed in a third party software. If you need one that can, please contact any of the authors.