

# Experiments using the inverse probe set up for $^{31}\text{P}$ on the Varian 500

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## What is an inverse probe?

An inverse probe is one which is very sensitive for  $^1\text{H}$  or  $^{19}\text{F}$ , but less sensitive for other nuclei, such as  $^{31}\text{P}$  or  $^{13}\text{C}$ .  $^1\text{H}$  and  $^{19}\text{F}$  are high-frequency nuclei; their Larmor frequency is much higher than those of almost all other nuclei.

## What experiments can be done with an inverse probe?

All experiments that are  $^1\text{H}$ -detected or  $^{19}\text{F}$ -detected are good. These include 1D  $^1\text{H}$ , HSQC, HMBC, COSY, etc. Experiments which detect  $^{13}\text{C}$  or  $^{31}\text{P}$  are much less sensitive when run on an inverse probe than when run on an “observe” probe, which is a probe optimized for detecting  $^{13}\text{C}$  or  $^{31}\text{P}$ , but not  $^1\text{H}$ .

## But can I run $^{31}\text{P}$ on the inverse probe when it is tuned to $^{31}\text{P}$ ?

Yes.  $^{31}\text{P}$  is intrinsically very sensitive, because it is 100% abundant, so it is a reasonable experiment to run, even on an inverse probe. Still, it's not fantastic: the Bruker 400, the Bruker 500, and the Varian 500 with its usual probe (when tuned to  $^{31}\text{P}$ !) all give signal to noise ratios of about 250:1, while the Varian inverse probe gives 60:1. The Mercury 300 gives 64:1. These are tests on standard samples.

## Do I have to tune the p20180803\_ID\_autoshimrobe?

***Don't tune  $^{31}\text{P}$ : it's a bit tricky on this probe and it hardly changes from sample to sample.***

If you are just running a 1D  $^1\text{H}$ : no (although if you have very small amounts of sample, you should)

If you are running a 2D experiment: tune  $^1\text{H}$  only (don't tune  $^{31}\text{P}$ : it's a bit tricky on this probe and it hardly changes from sample to sample)

## What experiments are set up?

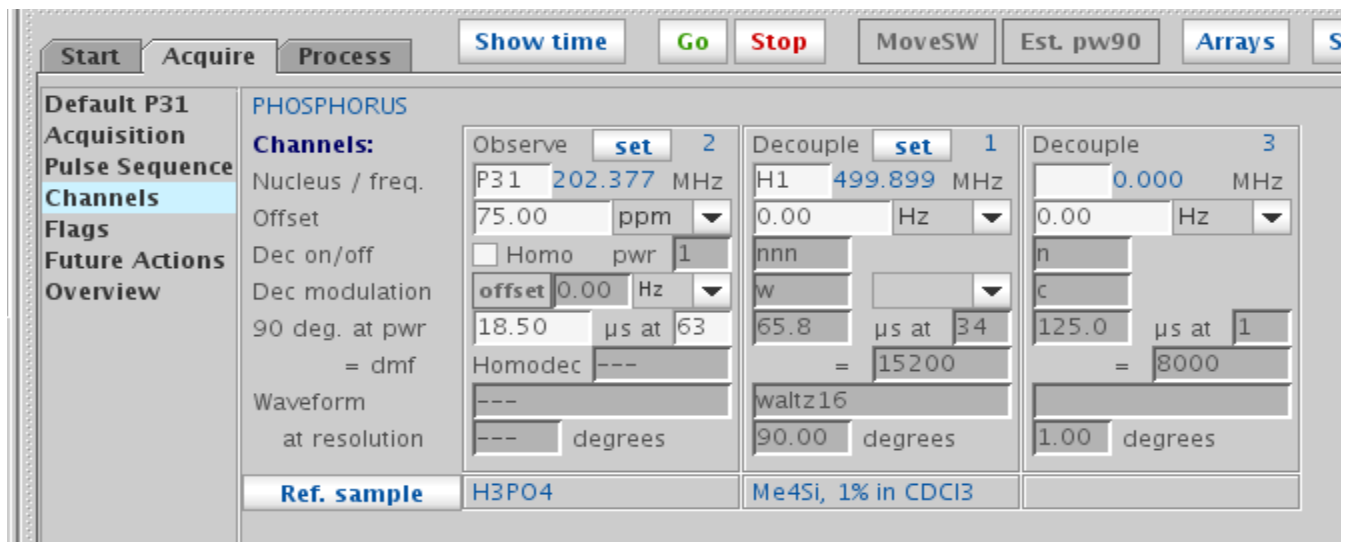
On the **McGill** tab:

- Proton: usual experiment, 8 scans; this should be excellent
- COSY:  $^1\text{H}$ - $^1\text{H}$  through-bond correlation
- NOESY:  $^1\text{H}$ - $^1\text{H}$  through-space correlation
- ROESY:  $^1\text{H}$ - $^1\text{H}$  through-space correlation for large molecules (ca. 2000 MW)

- TOCSY:  $^1\text{H}$  total correlation spectroscopy showing coupled spin systems

On the **P31\_Expts** tab:

- Phosphorus: basic phosphorus experiment, with  $^1\text{H}$  decoupling. Only 16 scans: you might want to double-click on the experiment in the queue list and go to the Acquisition panel to change the number of scans to 64. Centred on +75 ppm. If your signal is likely to be far from there (less than -25 ppm), go to the Channels panel (under Acquire) and set the Offset to where you think the signal will be (note that there is a drop down menu to change from Hz to ppm):



- P31\_noH1dec: phosphorus, showing  $^1\text{H}$  splitting. Only 16 scans: you might want to double-click on the experiment in the queue list and go to the Acquisition panel to change the number of scans to 64. Centred on +75 ppm. If your signal is likely to be far from there (less than -25 ppm), go to the Channels panel (under Acquire) and set the Offset to where you think the signal will be (note that there is a drop down menu to change from Hz to ppm) (see above)