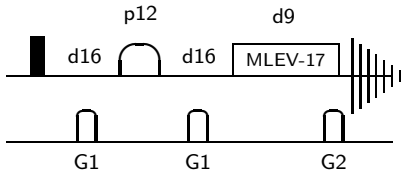
Obtaining 1D-TOCSY Spectra

A 1D-TOCSY spectrum will show the peaks within the same spin-group as an irradiated peak and give a sense of the distance each is from the irradiated peak. As shown below, it involves a refocussing by a selective 180° pulse and a MLEV-17 spin-lock, during which the polarization migrates from the irradiated nucleus to the others within the spin system.



The gradient procedure below gives optimal results, but a non-gradient procedure is also given.

Using Gradients

1. Acquire a reference spectrum and obtain the position of the peak to be irradiated, in Hz.
2. Create a new data set (`edc`).
3. `rpar SELMLGP all` to read in parameters. `getprosol` as usual.
4. Change the following parameters:

   `pulprog` = `selmlgp.2`
   `O1` = peak position (in Hz) noted in step 1[1]
   `D9` = 40 ms (mixing time)
   `P12` = 30 ms (selective pulse length)

   Type `gpz` and, in the resulting window, set the following gradient parameters:

   `gpz1` = 15
   `gpnam1` = SINE.100
   `gpz2` = 40
   `gpnam2` = SINE.100
5. Run and process the spectrum as usual. Adjust `d9` as needed.

Without Gradients

Similar to the setup above except:

- `rpar SELMLZF1H` (instead of SELMLGP)
- Do not change `pulprog` from the SELMLZF1H default
- Do not enter the gp… parameters

[1] Alternatively, leave `O1` unchanged and set `spoff` to the difference between `O1` and your measured value. (`spoff2` for gradient sequence; `spoff1` for non-grad)