Why Can't I Process My 13C (or 19F, 31P or 15N) Data From Siena On MestReNova?

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With the addition of the new BBFO cryoprobe we will have to adopt a new protocol to open 1D 13C (19F or 31P or 15N or whatever is detected on the X channel) recorded on Siena in MestreNova. Bruker has created a new processing protocol. If you are curious, there are additional details below. In short, when we run a 1D 13C (for instance) in expno 2, the software increments the expno by 100,000, copies the raw data into that expno, applies special processing to the data to produce phased data with a flat base line. If we use MestreNova to open the file "fid" in expno 2 or we drag the folder into the application, there are phase and base line distortions that make the data difficult to use.

How do I get 13C data I can process?

Opening the "1r" file in the subdirectory pdata/1 produces a file with a flat baseline and proper phasing. Another option is to open expno 100,002, which contains the raw data. This looks OK, but not as good as opening the pdata/1/1r file.

Additional details -

Why did Bruker create a new processing protocol? We've been collecting 1D 13C NMR spectra and analyzing for years. In short Bruker claims that their new cryoprobe is so sensitive that the initial part of the FID is distorted due to the after effects of pulsing. To express in a simplified, but more visual way, the transmitter/receiver coil "rings" after the application of an RF pulse. This is an old problem in NMR and effects all probes, to some degree, including our old cryoprobe. Bruker's solution is to mathematically back-calculate the distorted points. This may seem like cheating, but this "backward linear prediction" approach is well established, usually in protein NMR when RG is set too low.