

SUMMARY OF EMAIL THREAD:

The email thread below (between me and Saussan Madi and Sascha Koehler from Bruker) contains some useful information about MRS data formats for different PV versions).

Key info:

-Whereas from PV6 up to PV360 v2.0 pl1, automatically collected water reference scans are stored in the 'fid.refscan' folder, in PV360 v3+, the automatically collected water reference scans are stored in pdata/1/fid_refscan.64.

-It seems it is not possible to get individual coils stored separately in PV5.1

-In PV6, the automatically collected water reference data file (i.e. the "fid.refscan" file) does not contain the individually stored coil channels.

-I checked the manuals for PV7, PV360v1, PV360v3+, and the same is true for these versions as well.

These last two points are important. It means that even if we have the water suppressed data in a format that contains the individual coil channels, we cannot estimate the coil weights and phases from the water reference data. We need to think about how this impacts the way in which we decide to process the data.

Either 1) we can use the coil phases provided in the Bruker Method file ("PVM_ArrayPhase") and estimate the amplitude scalings (using the water suppressed data itself) to do the coil combination ourselves; or 2) we can use the processed Bruker data where the coil channels are already combined.

From: Jamie Near jamie.near@utoronto.ca
Subject: Re: Questions about PRESS Reference Scans in PV360 v3.4
Date: October 23, 2023 at 10:27 AM
To: Koehler, Sascha Sascha.Koehler@bruker.com
Cc: Madi, Saaussan Saaussan.Madi@bruker.com, colleen.em.bailey@gmail.com

JN

Thank you Sascha,

I will consult the manual.

Best wishes,
Jamie

On Oct 23, 2023, at 3:50 AM, Koehler, Sascha <Sascha.Koehler@bruker.com> wrote:

Dear Jamie,

Data handling is different in the different versions, but everything is described in the manual for the respective version.

I pointed you to the PV360 chapter. In PV6 there is a similar description, also in the NSPECT chapter: 1.9.30.4 Data Files

This chapter should answer all your questions. If not, please let me know.

Best regards,
Sascha

-Bruker Confidential-

From: Jamie Near <jamie.near@utoronto.ca>
Sent: Freitag, 20. Oktober 2023 17:15
To: Koehler, Sascha <Sascha.Koehler@bruker.com>
Cc: Madi, Saaussan <Saaussan.Madi@bruker.com>; colleen.em.bailey@gmail.com
Subject: Re: Questions about PRESS Reference Scans in PV360 v3.4

****EXTERNAL EMAIL****

OK Thank you Sascha for the clarification. I think your response aligns with what I am seeing.

I do have another question:

We have some PRESS data from our current system (PV6.0.1), that was acquired with the 4ch rat brain array coil. In this dataset, we had the sequence set to automatically collect the water reference data. My understanding is that the water suppressed data are stored in the rawdata.job0 file, and the water reference scans are stored within the fid.refscan file.

When reading the rawdata.job0 file into matlab, I am able to see the individual coil channels and the final dataset has size (Np x Naverages x Ncoils) as expected.

However when reading the reference data (fid.refscan) into matlab, the data size appears much more limited (Np x 1), despite the fact that we are using a 4 channel coil. I don't know how many "averages" are acquired for the reference, scans, but I assume that number is 1, because the parameter "PVM_RefScanNA" is equal to 1 (maybe this is a parameter that we are able to adjust on the scanner? Colleen could you check this?).

My question is: Is it the case that when using the PRESS sequence in PV6.0.1, the reference scan data (fid.refscan) will have the RF coil channels combined already? If so, this is a slight problem because it is standard practice in MRS data processing to use the relative phases and amplitudes of the water unsuppressed data to combine the RF channels in the water suppressed data.

If fid.refscan already has the RF channels combined and there is no way to determine relative RF channel amplitudes and phases from the refScan data, is there another way that you can recommend getting this information? I do notice that in the method file there is a parameter called

getting this information? I do notice that in the method file there is a parameter called "PVM_ArrayPhase". Are these the coil phases? If so, I guess I should phase shift the RF channels by these amounts before I combine them? Are the amplitudes also available?

Thanks so much again for your help.

Best wishes,
Jamie

On Oct 20, 2023, at 10:25 AM, Koehler, Sascha <Sascha.Koehler@bruker.com> wrote:

Dear Jamie,

as far as I remember, PV5 does not support PRESS using a multi-channel coil. So your analysis is correct: the data is stored as int32, and there is only one receive coil.

fid.raw: serially stored FID of each individual scan, file-size = scan-size x NA,
fid.ref: serially stored FID of each navigator scan, file-size = scan-size x NA.

Best regards,
Sascha

-Bruker Confidential-

From: Jamie Near <jamie.near@utoronto.ca>
Sent: Freitag, 20. Oktober 2023 12:44
To: Koehler, Sascha <Sascha.Koehler@bruker.com>
Cc: Madi, Saaussan <Saaussan.Madi@bruker.com>; colleen.em.bailey@gmail.com
Subject: Re: Questions about PRESS Reference Scans in PV360 v3.4

****EXTERNAL EMAIL****

Hi again,

Rather than working with the manual I had another thought: Do you happen to have any code that will read Bruker fid.raw (PV5.1) files into matlab, preserving the number of coils?

So far I am still unable to read PV5.1 fid.raw files in a way that preserves the coils.

I am trying to read the files in matlab using the 'fread' function, and I have tried with different precision values (int, int16, int32, float, etc.), but none result in an array with the expected number of points (Np x Ncoils x Naverages). The only way I am able to get sensible looking results is if I read in using precision "int" or "int32" (these are equivalent), in which case the resulting data dimension is (Np x Naverages).

Thanks again for your help!

Best wishes,
Jamie

On Oct 20, 2023, at 5:35 AM, Jamie Near <jamie.near@utoronto.ca> wrote:

Dear Sascha,

I'm coming back to this now, as I'm still having some issues with reading some Bruker raw files.

Could you help me find the manual you are referring to? I have the PV5.1 manual, but the chapters begin with letters (I, A, O, D, E, see attached "contents" document), not numbers.

Ideally I would like to look at the relevant section of the manual for both PV5.1 and PV6.0.1 so that I can compare how the raw data is stored differently between these two versions. Is there a place where I can find/access these sections of the manual for both versions?

Best wishes,
Jamie

On Sep 22, 2023, at 9:46 AM, Koehler, Sascha
<Sascha.Koehler@bruker.com> wrote:

You don't often get email from sascha.koehler@bruker.com. [Learn why this is important](#)

Dear Jamie and Saaussan,

just a small note:
a detailed description of the spectroscopic data files can be found in the manual, chapter 2.10.33.4 **Data Files**.

Best regards,
Sascha

-Bruker Confidential-

From: Madi, Saaussan <Saaussan.Madi@bruker.com>
Sent: Freitag, 22. September 2023 08:58
To: Jamie Near <jamie.near@utoronto.ca>; Koehler, Sascha
<Sascha.Koehler@bruker.com>
Cc: colleen.em.bailey@gmail.com; Takado Yuhei <takado.yuhei@qst.go.jp>
Subject: RE: Questions about PRESS Reference Scans in PV360 v3.4

Hi Jamie,
I'm doing well, thank you for asking!

1- SO: my first question is: Where can I find the raw Reference Scan data file for PRESS scans in PV360 v3.4? Has the old fid.refscan file been replaced by the 'pdata/1/fid_refscan.64' file?

Yes, the file fid_refscan.64 is the 64bit raw data reference scan, and t is saved under pdata/1

2- My question is: Is this a new feature of PV360 that the coil channels are stored separately in the rawdata.job0 file? Or is this simply a parameter choice that caused the coil channels to be stored

separately? If so, can you please let me know the name of the parameter that controls this?

You are correct that rawdata.job0 has the coils stored separately. This was the case in PV5.1. The only difference is that it was 16 bits in PV5.1.

I'm cc'ing Sascha from the methods team, in case I missed something.

Kind Regards
Saaussan

-Bruker Confidential-

From: Jamie Near <jamie.near@utoronto.ca>
Sent: Wednesday, September 20, 2023 12:49 PM
To: Madi, Saaussan <Saaussan.Madi@bruker.com>
Cc: colleen.em.bailey@gmail.com; Takado Yuhei <takado.yuhei@qst.go.jp>
Subject: Questions about PRESS Reference Scans in PV360 v3.4

****EXTERNAL EMAIL****

Dear Saussan,

I hope this email finds you well.

I have a two questions about spectroscopy raw data files ParaVision.

1. Naming and location of raw data file for Reference Scans.

In earlier versions of ParaVision (PV6, PV360 v2.0 pl1), when we run a PRESS sequence with the 'Reference Scans' option turned on, then the sequence automatically acquires a water unsuppressed reference scan from the prescribed volume. In these versions, the reference scan data seems to be contained within a file called 'fid.refscan', which is located in the main scan folder.

In the latest ParaVision version (PV360 v3.4), I have a datasets where the 'Reference Scans' option seems to be turned on (i.e. in the method file it says '\$PVM_RefScanYN=Yes' and '\$PVM_RefScanNA=1'). However, in this dataset, there is no 'fid.refscan' file in the main scan folder. There is a file in the 'pdata/1' folder called 'fid_refscan.64'.

SO: my first question is: Where can I find the raw Reference Scan data file for PRESS scans in PV360 v3.4? Has the old fid.refscan file been replaced by the 'pdata/1/fid_refscan.64' file?

2. Handling of multiple receiver channels in raw PRESS data from PV360

In earlier versions of ParaVision (PV5, PV6), I had found that when data were acquired with a receiver array coil (i.e. the 2 x 2 rat brain array coil), the raw data file (fid.raw (PV5) or rawdata.job0) seemed to have the coil channels already combined. For example, in PV5 where we acquired a PRESS dataset with 2048 spectral points and 256 averages and a 4 channel coil, reading the fid.raw file resulted in an array with dimensions 524,288 x 1 = (2048 spectral points x 256 averages) x 1, i.e. no separate FIDs for each coil.

However, in datasets acquired in PV360 (both v2.0 and v3.4), the raw data does seem to contain the individual coil channels. For

raw data does seem to contain the individual coil channels. For example, in a PRESS dataset with 2048 spectral points, 128 averages and a 4 channel coil, reading the rawdata.job0 file resulted in an array with dimensions 1,048,576 x 1 = (2048 spectral points x 128 averages x rf channels) x 1, i.e. it contains separate FIDs for each coil.

My question is: Is this a new feature of PV360 that the coil channels are stored separately in the rawdata.job0 file? Or is this simply a parameter choice that caused the coil channels to be stored separately? If so, can you please let me know the name of the parameter that controls this?

Thanks very much in advance for your help!!

Best wishes,

Jamie Near
Sunnybrook Research Institute

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