Outlook

Re: CoMP - MRS data processing in Osprey - meeting needed

From Diana Georgiana Rotaru <dr3309@columbia.edu>
Date Wed 2024-12-04 5:14 PM
To Georg Oeltzschner <goeltzs1@jhmi.edu>
Cc Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>; Jamie Near <jamie.near@utoronto.ca>; jamie.near@gmail.com <jamie.near@gmail.com>

1 attachment (23 KB)
io_loadspec_bruk_PV6.m;

Hi Georg,

Attached can be found the Bruker data reading function I used some years ago.

There are a few things to know beforehand:

1) the data formats that Bruker produces are fid (fid.raw) & fid.refscan (where fid.refscan is created at the end of the metabolite scan acquisition - it usually contains 1 or a few water averages acquired as part of the metabolite scan) - used in PV5, PV6, PV7, the fid.refscan file stores water data that can be used when there is no separate water scan acquired; another data format is rawdata.job0 - used in PV360 and above versions, in most cases, for these software versions, there is no fid.refscan saved altogether with the metabolite scan acquisition so a separate rawdata.job0 scan must be acquired to have any water data available (data packets that store PV360 data are DP06, DP07, DP08, DP10, DP22, DP23, DP27) - these water datasets are saved either with a 'mrsref' or 'wat' in the folder name

2) the differences between data formats translate to differences in the way the fid.raw or fid.refscan or rawdata.job0 store the FID points
For example, one potential way to reshape the FID points in a fid.raw file could be the conversion of a 1D array to a 4D array of size:
(number of real and imaginary values) x (number of data points) x (number of coil elements) x (number of averages)
I don't know if it's reiterating something you already know, but to get a bit more context, you can check the explanation about data organizing written in my thesis, in the section on preclinical MRS, pages 312-313: https://kclpure.kcl.ac.uk/ws/portalfiles/portal/199797575/2023_Rotaru_Diana_1676234_ethesis.pdf - though I do explain it for Bruker MEGA-PRESS and HERMES datasets.

3) other differences arise from the header information which in Bruker's case can be accessed in the 'method' file - this file stores all the parameters used at data acquisition; unfortunately, between different software versions some of these parameters' names changed, leading to inconsistencies and

making data reading more complicated across multiple software versions; another way to access data acquisition parameters is through files like 'acqp' and 'acqu'
Example of parameters from the 'method' file:

```
PVM_EchoTime = TE
PVM_RepetitionTime = TR
Method = sequence
PVM_NAverages = number of averages
PVM_SpecMatrix = number of FID points
PVM_DigShift = group delay of filter - the number of null points that precede the FID due to a time difference between ADC on and ADC acquire
PVM_DigSw = spectral width (Hz)
```

whereas in 'acqp' file you can find

```
BF1 = transmitter frequency
```

I have also uploaded here some Paravision manuals to have at hand if needed:
https://drive.google.com/drive/folders/1BZEzAx9HoFmaM6cUZnJNzJ-pTCdupj7Q?usp=sharing

Info regarding the datasets can be accessed using this link:
https://docs.google.com/spreadsheets/d/1z6yxFSnsiuZsXPj_JkK8_Qh8ZtAfPP7kzJs9b7p25BI/edit?usp=sharing

Once I have any new details about differences between data formats I will get back to you.
Hope this helps. If you need to discuss anything else please let me know.

Regards,
Diana

Diana Rotaru, PhD
Postdoctoral Research Scientist
MR Scientific Engineering for Clinical Excellence (MR SCIENCE) Laboratory
Department of Biomedical Engineering
Fu Foundation School of Engineering and Applied Science
Columbia University in the City of New York

On Wed, Dec 4, 2024 at 3:18 PM Georg Oeltzschner <goeltzs1@jhmi.edu> wrote:

> Hi Diana,
>
> Yes, please send any code that you have - if you have some notes on the general Bruker structure (and differences between versions), even better - thanks 🙂
>
> Out of those three dates, I have a preference for Dec 10, 9 am US time, or Dec 19th, 11 am US time.
>
> Cheers,
> Georg

From: Diana Georgiana Rotaru <dr3309@columbia.edu>
Sent: Wednesday, December 4, 2024 3:08 PM
To: Georg Oeltzschner <goeltzs1@jhmi.edu>
Cc: Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>; Jamie Near <jamie.near@utoronto.ca>; jamie.near@gmail.com <jamie.near@gmail.com>
Subject: Re: CoMP - MRS data processing in Osprey - meeting needed

Hi Georg,

I have some FID-A based code from my PhD that could be useful, yet for versions starting PV360 it probably will throw errors (it should still work for PV5, PV6, PV7). I can also meet with you and discuss differences between software versions prior to the meeting with Jamie and Cristina, if you think that'll be useful.

Back to setting up a meeting for all four of us, what date would work best for you? I thought I left in both US and CH times, I am sorry for the confusion.
- Dec 10th, 8-11 am US/ 14-17 pm CH
- Dec 11th, 9-10 am US/ 15-16 pm CH
- Dec 19th, 8-11 am US/ 14-17 pm CH

Even if there is no update regarding data reading formats, it would still be useful to meet and agree on a plan for the next weeks/months.

Regards,
Diana

Diana Rotaru, PhD
Postdoctoral Research Scientist
MR Scientific Engineering for Clinical Excellence (MR SCIENCE) Laboratory
Department of Biomedical Engineering
Fu Foundation School of Engineering and Applied Science
Columbia University in the City of New York

On Tue, Dec 3, 2024 at 4:45 PM Georg Oeltzschner <goeltzs1@jhmi.edu> wrote:

> Ha, of course, I should have known - embarrassing.
>
> Yes, I'd appreciate any pointers, I'm definitely not very familiar with Bruker data. THanks!
>
> ---
>
> **From:** Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>
> **Sent:** Tuesday, December 3, 2024 3:34 PM
> **To:** Georg Oeltzschner <goeltzs1@jhmi.edu>; Diana Georgiana Rotaru <dr3309@columbia.edu>
> **Cc:** Jamie Near <jamie.near@utoronto.ca>; jamie.near@gmail.com <jamie.near@gmail.com>
> **Subject:** RE: CoMP - MRS data processing in Osprey - meeting needed

Hi Georg,

It is Switzerland time = CH.

Should I talk with Brayan to see what is he using in our toolbox to loading Bruker data?

Maybe it could be useful for you.

Best
Cristina

-------- Message d'origine --------
De : Georg Oeltzschner <goeltzs1@jhmi.edu>
Date : 03.12.24 21:21 (GMT+01:00)
À : Diana Georgiana Rotaru <dr3309@columbia.edu>
Cc : Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>, Jamie Near <jamie.near@utoronto.ca>, jamie.near@gmail.com
Objet : Re: CoMP - MRS data processing in Osprey - meeting needed

Hi all,

Thanks for getting in touch. I'd say 'some progress' was an overstatement - if anything, it has become apparent how complex and diverse and variable the Bruker data structures are between releases and DPs. The existing FID-A loaders failed when I let them loose on the data from the first couple of CPs, so I'll have to get my hands dirty to figure the loaders out for all the different ParaVision versions. I got some code from Jessie but it's fairly labyrinthine (and lots are hard-coded), so it'll take me a while to make it work. FWIW, I also gave spec2nii a whirl, and it struggled in similar ways.

We can meet but I certainly won't have solved things by then.
Just to clarify, what is CH time?

Cheers,
Georg

From: Diana Georgiana Rotaru <dr3309@columbia.edu>
Sent: Monday, December 2, 2024 4:15 PM
To: Georg Oeltzschner <goeltzs1@jhmi.edu>
Cc: Cristina Ramona Cudalbu <cristina.cudalbu@epfl.ch>; Jamie Near <jamie.near@utoronto.ca>; jamie.near@gmail.com <jamie.near@gmail.com>
Subject: CoMP - MRS data processing in Osprey - meeting needed

Dear Georg,

I hope my email finds you well.

Jamie, Cristina and I discussed recently about starting the Q&A and preprocessing of the CoMP-MRS datasets using Osprey and, consequently, we would like to arrange a meeting with you.

Would any of the dates below work for you?
- Dec 10th, 4-5pm CH time
- Dec 11th, 3-4pm CH time
- Dec 19th, 2-4 pm CH

I remember there was some progress with the Osprey data read for several Bruker formats while in Boston at the MRS workshop, but I am not sure where things stand at the moment. If I can help in any way prior to the meeting please let me know.

Wish you a productive week!

Regards,
Diana

Diana Rotaru, PhD
Postdoctoral Research Scientist
MR Scientific Engineering for Clinical Excellence (MR SCIENCE) Laboratory
Department of Biomedical Engineering
Fu Foundation School of Engineering and Applied Science
Columbia University in the City of New York