

Subject: RE: Request for raw data (12/02/2015 and 09/27/2016)
Date: Monday, October 30, 2017 at 10:54:12 AM Eastern Daylight Time
From: Sara O'Neal, M.S.
To: Willis, Monte S.
CC: Mike Muehlbauer, Ph.D., James Bain, Ph.D.

Hi Monte,

Perfect! I just uploaded "DATA_Willis_cardiomyocytes_20151202.zip" and "DATA_Willis_myo_media_20160927.zip" to the Dropbox folder. They should contain all of the raw data files that you need for the two projects. I renamed all of the files so that their names match the sample names in the worksheets, since that is a requirement of Metabolomics Workbench. Let me know if you need me to make any changes or if you need any additional files.

Thanks!
Sara

From: Willis, Monte S. [mailto:monte_willis@med.unc.edu]
Sent: Monday, October 30, 2017 10:38 AM
To: Sara O'Neal, M.S. <sara.o'neal@duke.edu>
Cc: Mike Muehlbauer, Ph.D. <michael.muehlbauer@duke.edu>; James Bain, Ph.D. <james.bain@duke.edu>
Subject: Re: Request for raw data (12/02/2015 and 09/27/2016)

Sara: Yes, the .D files from the instrument. I just checked and I do still have access to the DMPI Willis Data folder, so putting them there would be ideal. Thank you! Monte

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From: "Sara O'Neal, M.S." <sara.o'neal@duke.edu>
Date: Wednesday, October 25, 2017 at 10:26 AM
To: "Monte S. Willis MD, PhD, MBA" <monte_willis@med.unc.edu>
Cc: "Michael Muehlbauer, PhD" <michael.muehlbauer@duke.edu>, "James Bain, PhD" <james.bain@duke.edu>
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Hi Monte,

I think you are referring to the .zip files that I put together previously that contained the actual .D files from the instrument. I am happy to put them together for the two data sets that you mentioned. Let me know if you still have access to the "DMPI Willis Data" folder on Dropbox, and I can just put them there like last time and let you know when they are ready.

Sara

From: Mike Muehlbauer, Ph.D.
Sent: Wednesday, October 25, 2017 8:32 AM
To: Willis, Monte S. <monte_willis@med.unc.edu>; James Bain, Ph.D. <james.bain@duke.edu>
Cc: Sara O'Neal, M.S. <sara.o'neal@duke.edu>
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Hi Monte,

If by raw data, you mean the original nontransformed abundance values, those can be regenerated by performing a 2-to-the-x function on each value. Please let me know if I could send you new spreadsheets with those values.

Otherwise, the attached spreadsheets might also be considered the raw data files. (There's also the dotD folders generated from the instrument, and the text files from AMDIS, but I don't think those are probably what you want.) The last tab on each spreadsheet (Report) are the data you already have (with data for Cells and Media from the 2015 Cardiomyocyte study on separate spreadsheets). The first tab on each sheet has the original line-item metabolite features, as were deconvoluted and annotated by AMDIS; 2nd tab: the crosstab of these features vs samples; 3rd tab: similar crosstab of unannotated features (generated through SpectConnect); 4th tab: the previous two tabs combined with similar features combined in groups (SimPeaks).

If none of these are what you're requesting, we can talk further. Thanks for pushing forward with publishing all this work.

Mike

From: Willis, Monte S. [mailto:monte_willis@med.unc.edu]
Sent: Tuesday, October 24, 2017 7:06 PM
To: Mike Muehlbauer, Ph.D. <michael.muehlbauer@duke.edu>; James Bain, Ph.D. <james.bain@duke.edu>
Cc: Sara O'Neal, M.S. <sara.o'neal@duke.edu>
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Dear Mike/James: Thank you again for reviewing the last manuscript in August prior to publication. After extensive revisions (including your changes), we submitted it for publication yesterday to *Int J Biochem & Cell Bio* (PDF of submission attached).

I'm currently preparing the Metabolomics Workbench submission for this manuscript (Experimental 1, below) and am writing to request the raw data files to submit in the package. There is also a second related study (Experiment 2, below) that I am writing up now, which I'll need the raw data files for too.

Experiment 1: 12/02/2015 (data attached)

Experiment 2: 09/27/2016 (data attached)

Let me know if you have any questions. And thank you in advance for your assistance! Best regards,
Monte

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