Curation log for: DATASET TITLE
Handle: https://hdl.handle.net/11299/xxxxxx
Corresponding researcher: xxxx <xxxx@xxx.edu>
Curator: WM
Metadata log created: 2023-08-23 (Dataset published: 2023-08-22)

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Files received:
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20210616_KC1079_SonAwt_18pm3.raw (163.21 MB)
20200730_msKC1047_His-SonA_K51-L53dup_1-10.raw (166.61 MB)
20200730_msKC1048_His-SonA_K51-L53del_1-10.raw (164.78 MB)
20210128_msKC1074_His-SonAK51-S54dup_1-10.raw (250.51 MB)
20210128_msKC1073_His-SonAK51-S54del_1-10.raw (253.33 MB)
20210128_msKC1076_His-SonAM47-L53dup_1-10.raw (251.28 MB)
20210128_msKC1075_His-SonAM47-L53del_1-10.raw (255.17 MB)
20210128_msKC1072_His-SonAK51-S57del_1-10.raw (251.17 MB)
20210128_msKC1071_His-SonAQ60-Y62del_1-10.raw (258.44 MB)
RSC_rawplatereader_data_SonAmutantsrelrates.xlsx (60.14 KB)
20191003_KCMS1016_SonA2Me-Trypsin_negcontrol.raw (107.17 MB)
20191003_KCMS1017_SonA2Me-Trypsin_SO1059.raw (112.2 MB)
RSC_rawplatereader_data_SO1059.xlsx (12.22 KB)
L-Tyr-L-FDAA_1_10000_20220218.raw (954.84 MB)
L-NMe-Ile-L-FDAA_1_100000_20220220.raw (826.67 MB)
L-NMe-Leu-L-FDAA_1_1000000_20220220.raw (814.95 MB)
Core_Peptide2Me-L-FDAA_1_1000_20220222.raw (757.46 MB)
L-Val-L-FDAA_1_100_20220222.raw (1.66 GB)
L-Ser-L-FDAA_1_100_20220219.raw (1.6 GB)
L-Asp-L-FDAA_1_100_20220218.raw (1.3 GB)
L-Gln-L-FDAA_1_100_20220221.raw (1.64 GB)
L-His-L-FDAA_1_100_20220222.raw (1.65 GB)
L-Asn-L-FDAA_1_100_20220222.raw (1.66 GB)
Core_Peptide2Me-L-FDAA_1_50_20220222.raw (1.6 GB)
Standard1uL+WT3ul_2ndpellet40MeOH_MS2_20220220.raw (205.19 MB)
Standard_corepeptide-2Me_E4_MS2_20220220.raw (247.15 MB)
WT_pellet40MeOH_MS2_20220220.raw (200.15 MB)
OverexpressSonMA_2nd1_4pellet40MeOH_MS2_20220220.raw (222.24 MB)
dsonA_pellet40MeOH_MS2_20220220.raw (205.89 MB)
dsonM_pellet40MeOH_MS2_20220218.raw (220.7 MB)
Soneidensis_1_3Wildtype_24h_SBM_20220115.raw (225.07 MB)
Soneidensis_dsonA_24h_SBM_20220115.raw (283.4 MB)
Soneidensis_Wildtype_24h_SBM_13CMet_20220115.raw (231.16 MB)
COSY.zip (23.24 MB)
HMBC.zip (13.51 MB)

HSQC.zip (27.75 MB)
ROESY modified.zip (17.0 MB)
TOCSY modified.zip (22.69 MB)

****
Changes made to files:
****
Added a README

No changes to files - but zipped up files into figures

Figs_2_S1a-S1s.zip
Filename: 20210616_KC1079_SonAwt_18pm3.raw
Short description: Raw MS file for Figure 2 and Figure S1a-d

Filename: 20200730_msKC1047_His-SonA_K51-L53dup_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1e

Filename: 20200730_msKC1048_His-SonA_K51-L53del_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1f

Filename: 20210128_msKC1074_His-SonAK51-S54dup_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1g

Filename: 20210128_msKC1073_His-SonAK51-S54del_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1h

Filename: 20210128_msKC1076_His-SonAM47-L53dup_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1i

Filename: 20210128_msKC1075_His-SonAM47-L53del_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1j

Filename: 20210128_msKC1072_His-SonAK51-S57del_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1k-o

Filename: 20210128_msKC1071_His-SonAQ60-Y62del_1-10.raw
Short description: Raw MS file for Figure 2 and Figure S1p-s

Filename: RSC_rawplatereader_data_SonAmutantsrelrates.xlsx
Short description: Raw absorbance data from Figure 2

Figs_4_S3_S7a-c_S8a.zip
Filename: WT_pellet40MeOH_MS2_20220220.raw

Short description: Raw MS file for Figure 4, Table S3, Figure S7a-b, Figure S8a

Filename: OverexpressSonMA_2nd1_4pellet40MeOH_MS2_20220220.raw
Short description: Raw MS file for Figure 4, Figure S7a&c

Filename: dsonA_pellet40MeOH_MS2_20220220.raw
Short description: Raw MS file for Figure 4, Table S3, Figure S7a

Filename: dsonM_pellet40MeOH_MS2_20220218.raw
Short description: Raw MS file for Figure 4, Table S3, Figure S7a

Filename: Soneidensis_1_3Wildtype_24h_SBM_20220115.raw
Short description: Raw MS file for Table S3

Filename: Soneidensis_dsonA_24h_SBM_20220115.raw
Short description: Raw MS file for Table S3

Filename: Soneidensis_Wildtype_24h_SBM_13CMet_20220115.raw
Short description: Raw MS file for Figure 4

Filename: COSY.zip
Short description: Raw NMR files Figure 5, Figure S9a

Filename: HMBC.zip
Short description: Raw NMR files Figure 5, Figure S9b

Filename: HSQC.zip
Short description: Raw NMR files Figure 5, Figure S9c

Filename: ROESY modified.zip
Short description: Raw NMR files Figure 5, Figure S9d

Filename: TOCSY modified.zip
Short description: Raw NMR files Figure 5, Figure S9e

Filename: RSC_rawplatereader_data_SO1059.xlsx
Short description: Raw absorbance data from Figure S4

Figs_S5b_S5c.zip

Filename: 20191003_KCMS1016_SonA2Me-Trypsin_negcontrol.raw
Short description: Raw MS files analyzed for Figure S5b

Filename: 20191003_KCMS1017_SonA2Me-Trypsin_SO1059.raw
Short description: Raw MS files analyzed for Figure S5c

Figs_S8a-b.zip

Filename: Standard1uL+WT3ul_2ndpellet40MeOH_MS2_20220220.raw
Short description: Raw MS files for Figure S8a

Filename: Standard_corepeptide-2Me_E4_MS2_20220220.raw
Short description: Raw MS files for Figure S8a-b

Fig_S10.zip

Filename: L-Tyr-L-FDAA_1_10000_20220218.raw
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Filename: L-NMe-Ile-L-FDAA_1_100000_20220220.raw
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Filename: L-NMe-Leu-L-FDAA_1_1000000_20220220.raw
Short description: Raw MS files for Figure S10

Filename: Core_Peptide2Me-L-FDAA_1_1000_20220222.raw
Short description: Raw MS files for Figure S10

Filename: L-Val-L-FDAA_1_100_20220222.raw
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Filename: L-Ser-L-FDAA_1_100_20220219.raw
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Filename: L-Asn-L-FDAA_1_100_20220222.raw
Short description: Raw MS files for Figure S10

Filename: Core_Peptide2Me-L-FDAA_1_50_20220222.raw
Short description: Raw MS files for Figure S10

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Metadata Changes
****

****
Correspondence Notes
****
Hello XX,
Thank you for your submission to the Data Repository for the U of M (DRUM). I am in the process of reviewing your submission, and I have a few questions for you:

1. The dataset would benefit from more documentation about the data itself, how it was collected, etc. for future users. One of the priorities of DRUM is the reusability of data without contacting the author. We have found that a README can help provide necessary context for reuse. I have attached a README that I have started to fill out for you. Please help me fill out the rest. This will also help me understand your data more and help with the rest of the curation process.

2. RSC_rawplatereader_data_SO1059.xlsx appears to have duplicate variables, an explanation in the README will help folks understand the variables. Same with RSC_rawplatereader_data_SonAmutantsrelrates.xlsx

3. The .raw files require a paid software to view (photoshop, etc.) Do you know of any open source/freely available software that folks would be able to use to open the .raw files? If not please share what software you recommend, we should add that to the README documentation.

4. It would be nice to group some of the files, what do you think about us zipping up the files in folders for each figure?

5. Please start thinking about a thumbnail you would like to use to replace the "submission under curatorial review." You can share the image with me via email when you return the completed README.

Please let me know if you have any questions or concerns. Thank you very much for your submission, and I look forward to hearing from you.

Wanda

Hi Wanda,
I apologize for the slow response, I have been out for the past couple weeks. I have addressed each of your points below. This raw data is all associated with a published research article DOI: 10.1039/D3CB00093A. This is the unmodified data collected from which analyses were completed. I think most of these points would be cleared up by including the DOI for the paper. It would be unlikely that people would be accessing this data without first reading the paper. If they were accessing the data without reading the paper, we would want them to read the paper.

1. The dataset would benefit from more documentation about the data itself, how it was collected, etc. for future users. One of the priorities of DRUM is the reusability of data without contacting the author. We have found that a README can help provide necessary context for reuse. I have attached a README that I have started to fill out for you. Please help me fill out the rest. This will also help me understand your data more and help with the rest of the curation process.

The methods section of the paper contains all relevant information as to how data was collected.

2. RSC_rawplatereader_data_SO1059.xlsx appears to have duplicate variables, an explanation in the README will help folks understand the variables. Same with RSC_rawplatereader_data_SonAmutantsrelrates.xlsx

Within the methods section of the paper, we note that data for each variable was collected in triplicate.

3. The .raw files require a paid software to view (photoshop, etc.) Do you know of any open source/freely available software that folks would be able to use to open the .raw files? If not please share what software you recommend, we should add that to the README documentation.

This is also noted in the methods section. There is no open source software. To view the raw MS files, we use Thermo Xcalibur 3.0.63 Qual Browser

4. It would be nice to group some of the files, what do you think about us zipping up the files in folders for each figure?
This is fine.

5. Please start thinking about a thumbnail you would like to use to replace the "submission under curatorial review." You can share the image with me via email when you return the completed README.
We will think about this.

Please let me know if there is anything else you need from me,

Thanks!

XX

Dear XX,

Great news! Your submission to the Data Repository for U of M (DRUM) has been curated and is now ready for your review at https://hdl.handle.net/11299/XXX

There were a few significant changes that we made to your submission in the curation process:

We've added a persistent link in the form of a DOI to your data: https://doi.org/XX
This allows you and others to formally cite your data in bibliographies. The DOI also exposes your data to online discovery tools like Google Scholar and Web of Science Data Citation Index.

We added a thumbnail - if you have something you would prefer, please share it and I will swap out the thumbnail

We cleaned up the record page Description

We added the manuscript full citation to the record page

We packaged the data following the Figure structure - to tidy up the record page and help future re-users of the data with organization of the files

We created and added a README to help with context of the data and help with reuse, including a data tree of the files.

Please notify us in the next few days if you have any recommended changes or corrections to the metadata record. We are happy to work with you to fix any discrepancies. Meanwhile, your data is currently live and viewable to the public and you should feel free to share the persistent link with others and use our services, such as tracking your download statistics.

We appreciate your contribution to DRUM

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Other issues
****
low key refused to fill in readme because it is all in the paper
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Original Metadata from Author:
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dc.contributor.author : XX
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20210616_KC1079_SonAwt_18pm3.raw
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20200730_msKC1048_His-SonA_K51-L53del_1-10.raw
20210128_msKC1074_His-SonAK51-S54dup_1-10.raw
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20210128_msKC1071_His-SonAQ60-Y62del_1-10.raw
Raw MS files analyzed for Figure 4, Table S3, Figure S7:
WT_pellet40MeOH_MS2_20220220.raw
OverexpressSonMA_2nd1_4pellet40MeOH_MS2_20220220.raw
dsonA_pellet40MeOH_MS2_20220220.raw
dsonM_pellet40MeOH_MS2_20220218.raw
Soneidensis_Wildtype_24h_SBM_13CMet_20220115.raw
Soneidensis_1_3Wildtype_24h_SBM_20220115.raw
Soneidensis_dsonA_24h_SBM_20220115.raw
Raw NMR files for Figure 5 and Figure S9:
TOCSY-modified
ROESY-modified
HSQC 900 MHz-2
HMBC 900 MHz-4
COSY Takahiro-17
Raw absorbance data from Figure S4:
RSC_rawplatereader_data_SO1059.xlsx
Raw MS files analyzed for Figure S5:
20191003_KCMS1016_SonA2Me-Trypsin_negcontrol.raw
20191003_KCMS1017_SonA2Me-Trypsin_SO1059.raw
Raw MS files for Figure S8:
WT_pellet40MeOH_MS2_20220220.raw
Standard1uL+WT3ul_2ndpellet40MeOH_MS2_20220220.raw
Standard_corepeptide-2Me_E4_MS2_20220220.raw
Raw MS files for Figure S10:
Core_Peptide2Me-L-FDAA_1_50_20220222.raw
Core_Peptide2Me-L-FDAA_1_1000_20220222.raw
L-Asn-L-FDAA_1_100_20220222.raw
L-Asp-L-FDAA_1_100_20220218.raw
L-Gln-L-FDAA_1_100_20220221.raw
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L-Val-L-FDAA_1_100_20220222.raw
dc.description.abstract : The data deposited here are the raw LC-MS/MS files and NMR files used for the manuscript, "XXXXX"
dc.description.sponsorship : This work was funded by the National Institutes of Health (R35 GM133475 to M.F.F.), the University of Minnesota BioTechnology Institute (M.H.E., J.G., and M.F.F.), the University of Minnesota Graduate School (K.K.C.), and the Daiichi Sankyo Foundation of Life Science (T.J.).
dc.relation.isreferencedby : https://doi.org/10.1039/XXXXX

dc.subject : Methyltransferase
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dc.subject : RiPP
dc.subject :XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
dc.subject : Shewanella oneidensis
dc.title : XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
dc.type : Dataset
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dc.date.completed : 2023-08-16
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dc.contributor.contactemail : XXX@umn.edu
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dc.date.collectedend : 20220220
dc.type.dataset : Other Dataset