The mwtab Python Library for RESTful Access and Enhanced Quality Control, Deposition, and Curation of the Metabolomics Workbench Data Repository

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Risk e-Learning Webinar Series:
Session III - Integrating Omics Data Across Model Organisms and Populations
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Superfund Research Center

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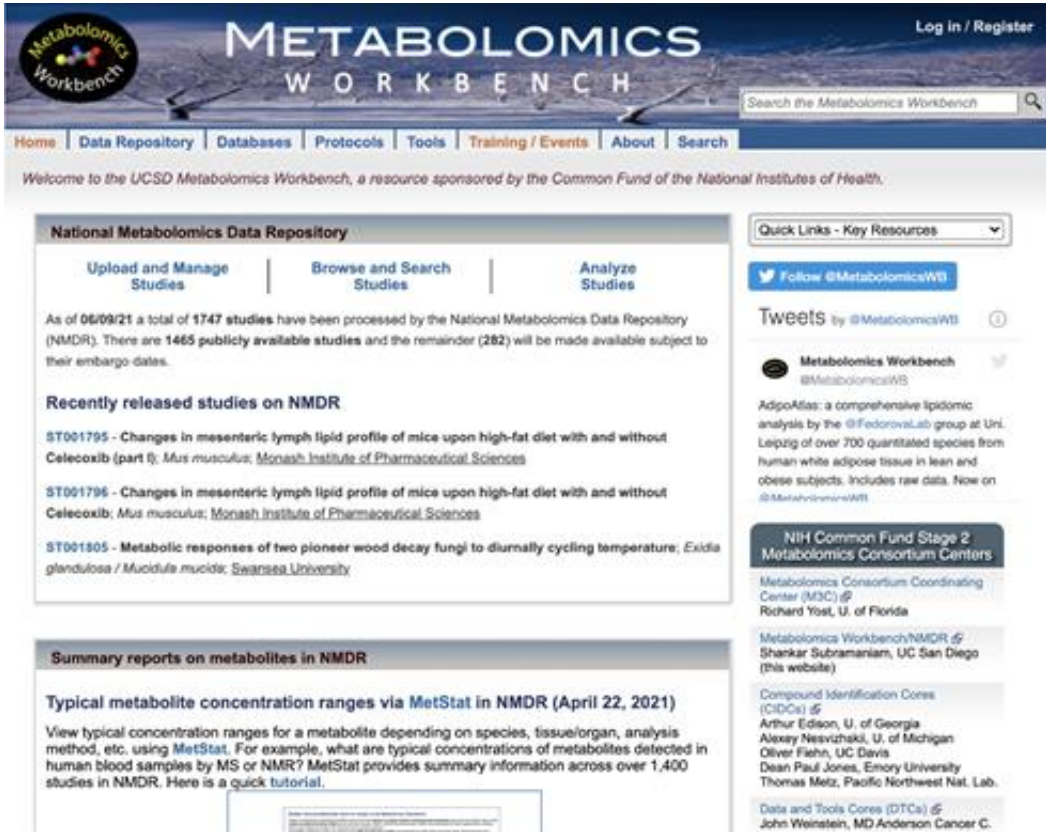
Metabolomics Workbench (MW)

- Also known as the National Metabolomics Data Repository (NMDR).
  - The main metabolomics data repository in NIH's Common Fund Metabolomics Consortium.
- The number of individual analyses listed has more than quadrupled since 2018.
  - Around 3000 analyses listed with ~2200 available.



The Metabolomics Workbench, https://www.metabolomicsworkbench.org/

mwTab File Format

- MW organises datasets into projects > studies > and analyses.
- MW's tabular data file format.
- Consists of multiple blocks of metadata along with a "..._DATA" section.
    - Sections mostly contain key value pairs.
- MW also releases data in a JavaScript Object Notation (JSON) format.

```
#METABOLOMICS WORKBENCH STUDY_ID:ST000001 ANALYSIS_ID:AN000001
VERSION                 1
CREATED_ON              2016-09-17
#PROJECT
...
#STUDY
...
#SUBJECT
...
#SUBJECT_SAMPLE_FACTORS:                SUBJECT(optional)[tab]SAMP
...
#COLLECTION
...
#TREATMENT
...
#SAMPLEPREP
...
#CHROMATOGRAPHY
...
#ANALYSIS
...
#MS
...
#MS_METABOLITE_DATA
MS_METABOLITE_DATA:UNITS        peak area
MS_METABOLITE_DATA_START
...
MS_METABOLITE_DATA_END
#METABOLITES
METABOLITES_START
...
METABOLITES_END
#END
```

mwtab Python Library

- Enables reading/writing files in mwTab tabular and JSON formats.
- Provides ability to request/download data files.
- Provides both an application programming interface (API) and command line interface (CLI).
- Available on GitHub and PyPI:
  - github.com/MoseleyBioinformaticsLab/mwtab
  - pypi.org/project/mwtab/
- Documentation available on ReadTheDocs:
  - mwtab.readthedocs.io/

```
Python 3.8.2 (default, Apr  8 2021, 23:19:18)
[Clang 12.0.5 (clang-1205.0.22.9)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import mwtab
>>>
>>> # Here we use ANALYSIS_ID of file to fetch data from URL
>>> for mwfile in mwtab.read_files("1", "2"):
...     print("STUDY_ID:", mwfile.study_id)
...     print("ANALYSIS_ID:", mwfile.analysis_id)
...     print("SOURCE:", mwfile.source)
...
STUDY_ID: ST000001
ANALYSIS_ID: AN000001
SOURCE: https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/mw
tab/txt
STUDY_ID: ST000002
ANALYSIS_ID: AN000002
SOURCE: https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000002/mw
tab/txt
>>>
```

Powell, C.D.; Moseley, H.N.B. *Metabolites* **2021**, *11*, 163. doi.org/10.3390/metabo11030163
Smelter, A.; Moseley, H.N.B. *Metabolomics* **2018**, *14*, 64. doi.org/10.1007/s11306-018-1356-6

mwtab Python Library v1.1.2

- Updates internal JSON format to mirror that of Metabolomics Workbench's JSON.
- Implemented programmatic access to MW's REST interface.
- Greatly expanded the set of validation tests and re-implemented them to provide a list of violations.
- Added a set of regular expressions for field name harmonization across datasets.

```
Python 3.8.2 (default, Apr  8 2021, 23:19:18)
[Clang 12.0.5 (clang-1205.0.22.9)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import mwtab
>>>
>>> # create first REST URL
>>> mwt_rest_url = mwtab.GenericMWURL({
...     'context': 'study',
...     'input_item': 'analysis_id',
...     'input_value': 'AN000002',
...     'output_item': 'mwtab',
...     'output_format': 'txt'}).url
>>> print(mwt_rest_url)
https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000002/mwtab/txt
>>>
>>> # create a generator to call REST URLs and create MWTabFile objects
>>> mwt_generator = mwtab.read_files(mwt_rest_url)
>>>
>>> # read mwTab file and validate contents
>>> for mwfile in mwt_generator:
...     mwtab.validate_file(mwfile, verbose=True, metabolites=False)
...
(OrderedDict([('METABOLOMICS WORKBENCH', OrderedDict([('STUDY_ID', 'ST000002'),
('ANALYSIS_ID', 'AN000002'), ('PROJECT_ID', 'PR000002'), ('VERSION', '1'), ('CRE
```

Powell, C.D.; Moseley, H.N.B. *Metabolites* **2021**, *11*, 163. doi.org/10.3390/metabo11030163

There is FAIR, but then there is FAIRer.

Findable

Accessible

Interoperable

Reusable

Findable

Accessible

Interoperable

Reusable

-

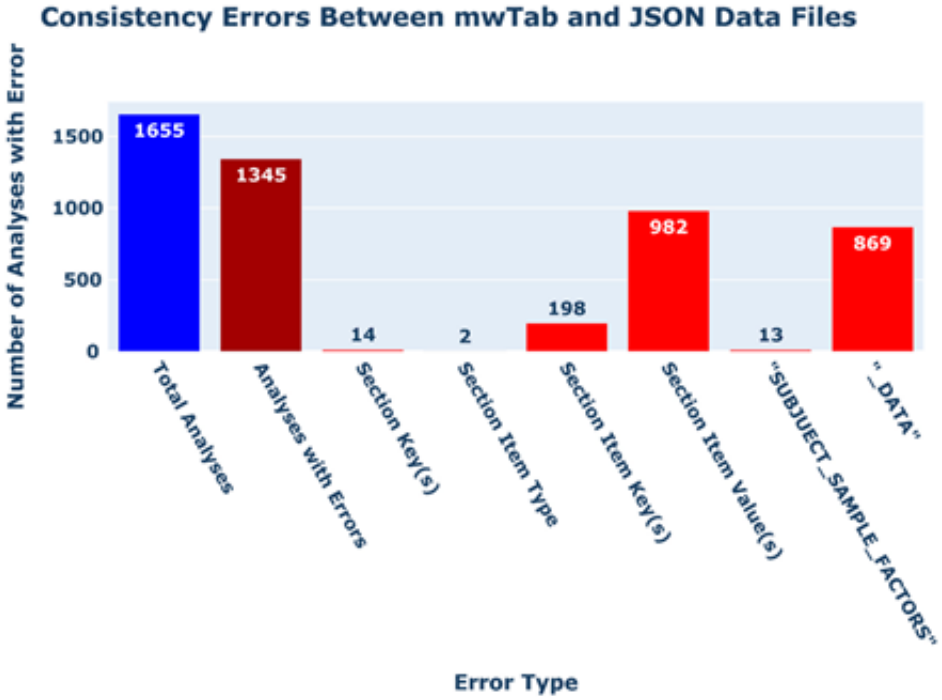
Revisible

Rigourous

Reproducible

Evaluating the FAIRness of Metabolomics Workbench

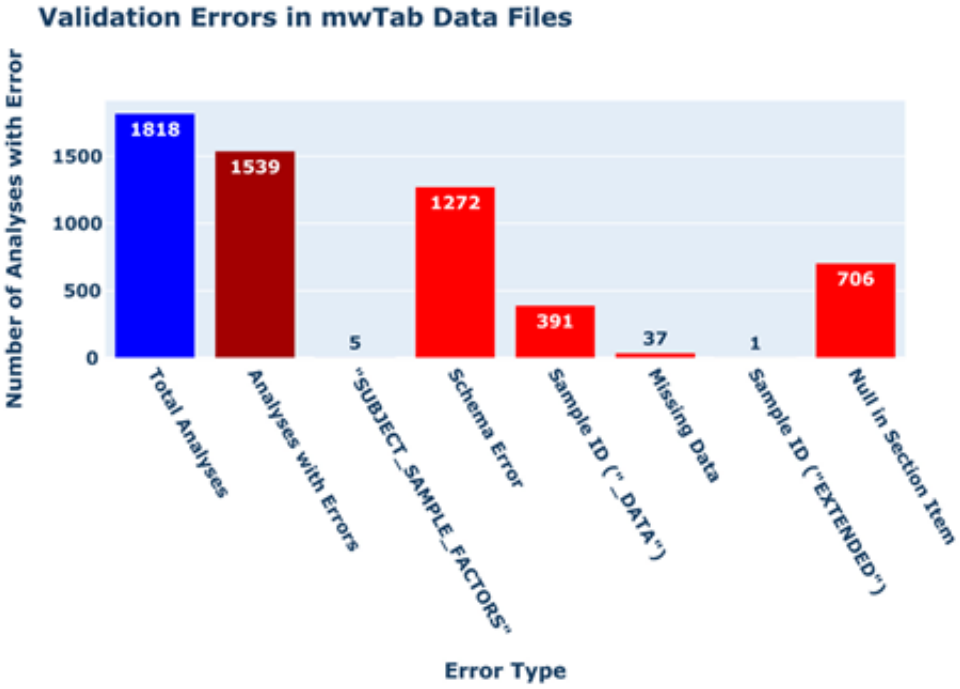
- As of Nov. 19th, 2020, a total of 1891 analyses were available for download through MW's REST interface.
  - 1888 downloaded analyses in 'mwTab' format: 70 could not be parsed.
  - 1841 downloaded analyses in JSON format: 139 could not be parsed.
- First, attempted to validate the consistency of metadata and data between mwTab and JSON files.



Powell, C.D.; Moseley, H.N.B. *Metabolites* **2021**, *11*, 163. doi.org/10.3390/metabo11030163

Evaluating the FAIRness of Metabolomics Workbench

- Used mwtab 1.0.1's enhanced validation features to validate all mwTab formatted files.
  - Most analyses contained "minor" errors.
  - 37 analyses were missing experimental data.



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“METABOLITES” Field Name Harmonization

- To facilitate deposition, MW allows user-defined field names in the “METABOLITES” section.
- Fieldname inconsistencies could hinder meta-analyses.
- With the updated mwtab library, we have developed a set of regular expressions to facilitate field name harmonization.

Common Field Name	RegEx Pattern(s)	Example Matched Field Names
hmdb_id	r"(?i)[\s|\S]{,}(HMDB)" r"(?i)(Human Metabolome D)[\S]{,}"	HMDB ID (*representative), HMDB (*Representative ID), HMDB_ID … Total 14 Fields
inchi_key	r"(?i)(inchi)[\S]{,}"	Inchi_Key, InChIKey, InchiKey … Total 10 Fields
kegg_id	r"(?i)(kegg)$" r"(?i)(kegg)(\s|_)(i)"	KEGG, KEGG I, Kegg ID … Total 6 Fields
moverz	r"(?i)(m/z)"	m/z, M/Z, m/z rounded
moverz_quant	r"(?i)(moverz)(\s|_)(quant)" r"(?i)(quan)[\S]{,}(\s|_)(m)[\S]{,}(z)"	Quantified m/z, quantitated mz, Moverz Quant … Total 10 Fields
other_id	r"(?i)(other)(\s|_)(id)$"	Other ID, Other_ID
…		

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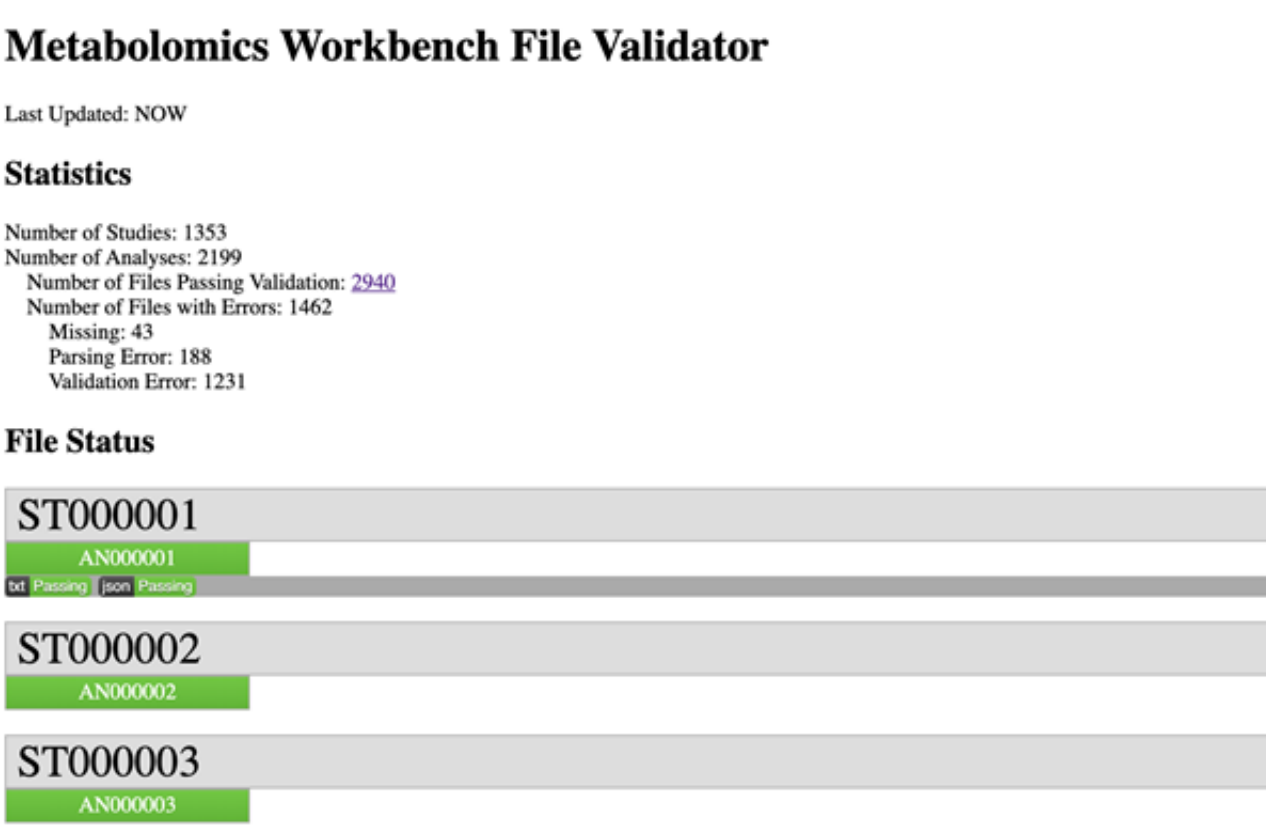
Summary

- The mwtab Python library continues to be updated alongside the Metabolomics Workbench repository.
- We evaluated the format consistency of all publicly available datasets in the Metabolomics Workbench.
  - We provided our validation report to Metabolomics Workbench and all of the major issues discovered have been fixed.
- Results presented here were published in Metabolites:
  - Powell, C.D.; Moseley, H.N.B. *Metabolites* **2021**, *11*, 163. doi.org/10.3390/metabo11030163

Near Future Directions



Metabolomics Workbench File Validator

Last Updated: NOW

Statistics

Number of Studies: 1353
Number of Analyses: 2199
- Number of Files Passing Validation: 2940
- Number of Files with Errors: 1462
  - Missing: 43
  - Parsing Error: 188
  - Validation Error: 1231

File Status

ST000001

AN000001

txt Passing json Passing

ST000002

AN000002

ST000003

AN000003

Acknowledgements

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