

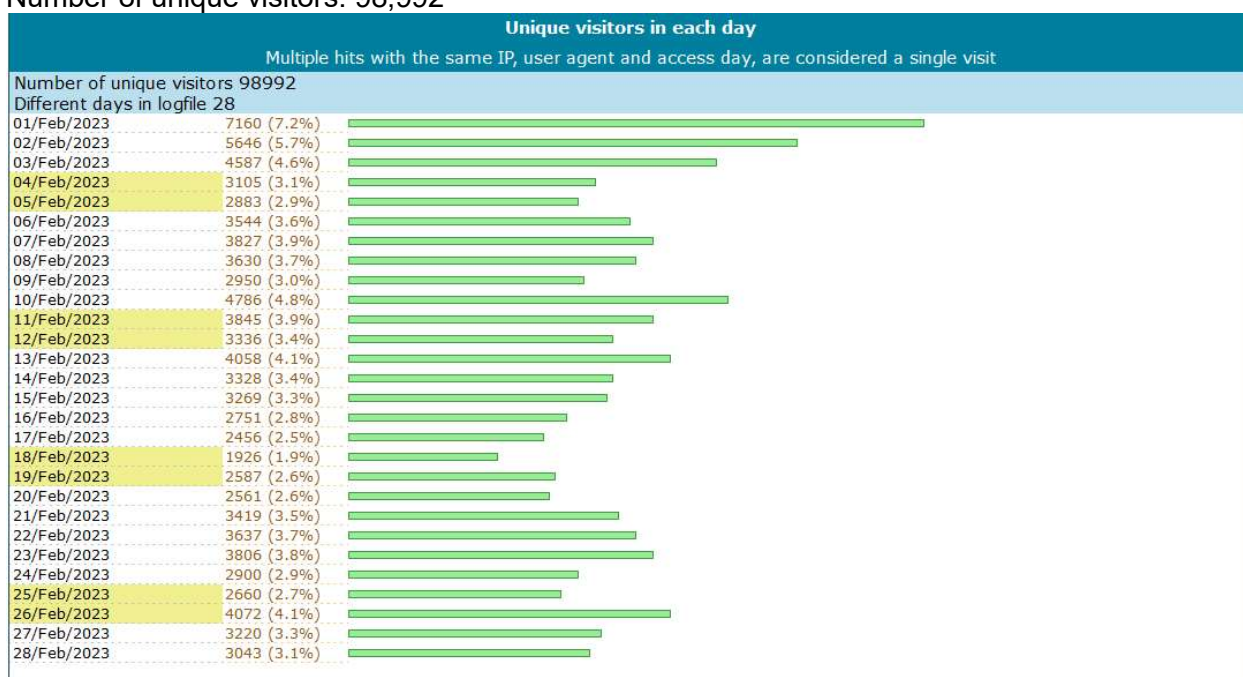
Access and Use Statistics and FAIR metrics on Metabolomics Workbench (MW)

Approach: We used both custom analysis of apache logs and Visitors tool (<http://www.hping.org/visitors/>) on combined access_log and ssl_access_log. vsftpd log was analyzed separately.

Access and use statistics are based on analysis of the log over about one month (February 2023, unless indicated otherwise). Access by web crawlers, bots, etc., has been excluded from the beginning of the analysis (see IP Exclusion List 1 at the end).

Overall access to the MW website

Number of unique visitors: 98,992



Country-based access statistics

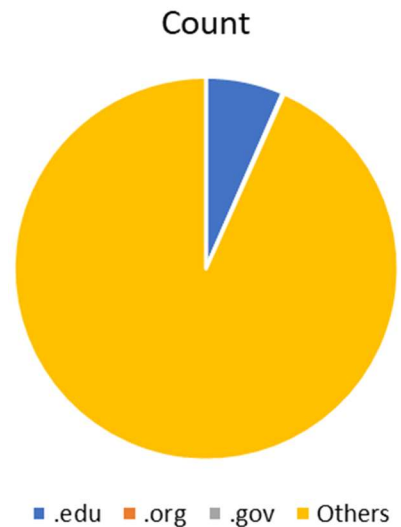
From the IP addresses, hostname and their geographical location (country) is identified and summarized.

Top 30 counties:

Country_short	Country_long	Count
US	United States of America	681483
FR	France	541757
SG	Singapore	155192
FI	Finland	107098
CA	Canada	85102
DE	Germany	69543
NL	Netherlands	62470

GB	United Kingdom of Great Britain and Northern Ireland	55929
GH	Ghana	42718
ES	Spain	19802
CN	China	18789
SE	Sweden	16486
AU	Australia	15950
BE	Belgium	15226
CZ	Czechia	14102
HK	Hong Kong	13773
IT	Italy	12384
RO	Romania	12188
PL	Poland	11780
JP	Japan	11232
UA	Ukraine	9936
NO	Norway	8983
RU	Russian Federation	8887
IN	India	8785
IL	Israel	8048
HU	Hungary	7656
IS	Iceland	7089
CH	Switzerland	6715
RS	Serbia	6435
AE	United Arab Emirates	5898

Category	Count	Percent
.edu	137190	6.536
.org	1603	0.076
.gov	1066	0.051
Others	1959099	93.337

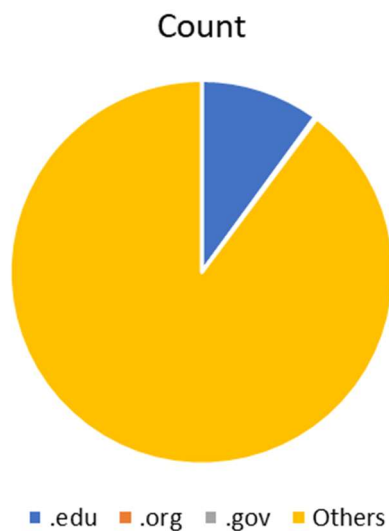


After excluding additional IP addresses with 'bot', 'spider', etc., in their hostnames (see IP Exclusion List 2 at the end): top 30 countries:

Country_short	Country_long	Count
US	United States of America	599210
FI	Finland	107097
CA	Canada	85102
NL	Netherlands	62470
FR	France	61435
DE	Germany	57283
GB	United Kingdom of Great Britain and Northern Ireland	53623
GH	Ghana	42718
ES	Spain	19802
CN	China	18789
SE	Sweden	16486
AU	Australia	15950
BE	Belgium	15226
CZ	Czechia	14100
HK	Hong Kong	13773

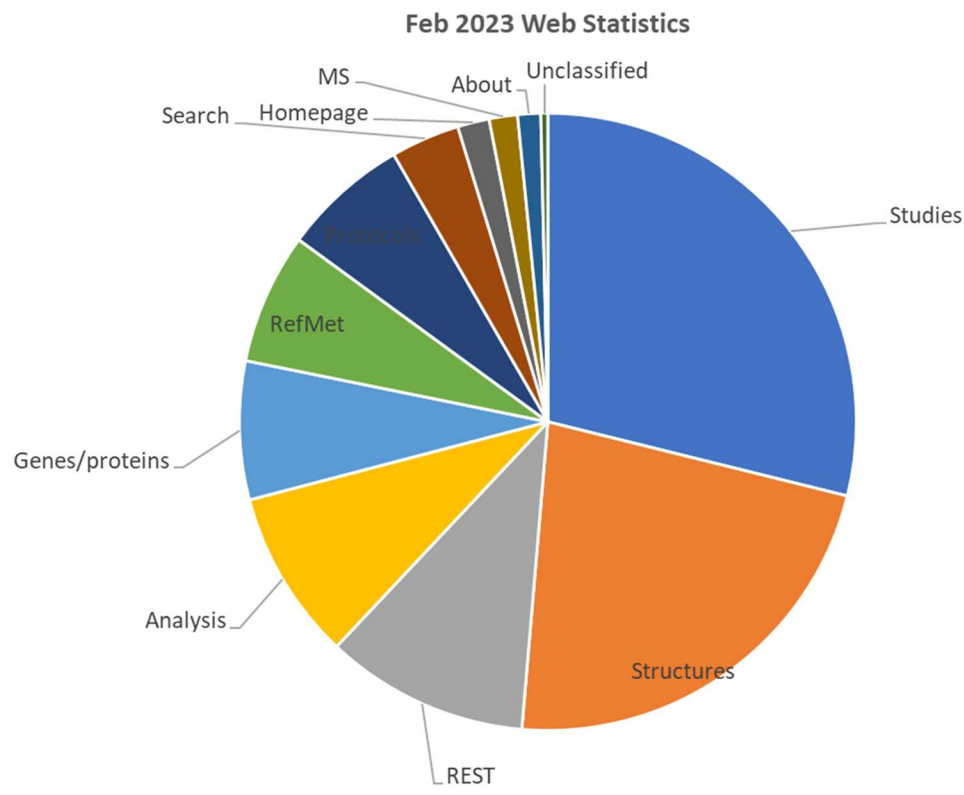
Category	Count	Percent
.edu	137190	10.018
.org	1591	0.116
.gov	1066	0.078
Others	1229650	89.789

IT	Italy	12384
RO	Romania	12188
PL	Poland	11780
JP	Japan	11232
UA	Ukraine	9936
NO	Norway	8983
IN	India	8785
IL	Israel	8048
HU	Hungary	7656
IS	Iceland	7089
CH	Switzerland	6715
RS	Serbia	6435
AE	United Arab Emirates	5898
SG	Singapore	5892
RU	Russian Federation	5891



Resource types (Major categories)

Category	Feb 2023 Web Statistics (28 days)	Hits per day
Studies	605788	21635
Structures	471839	16851
REST	223858	7995
Analysis	186963	6677
Genes/proteins	152297	5439
RefMet	144062	5145
Protocols	139057	4966
Search	75757	2706
Homepage	34923	1247
MS	31206	1115
About	25241	901
Unclassified	7694	275



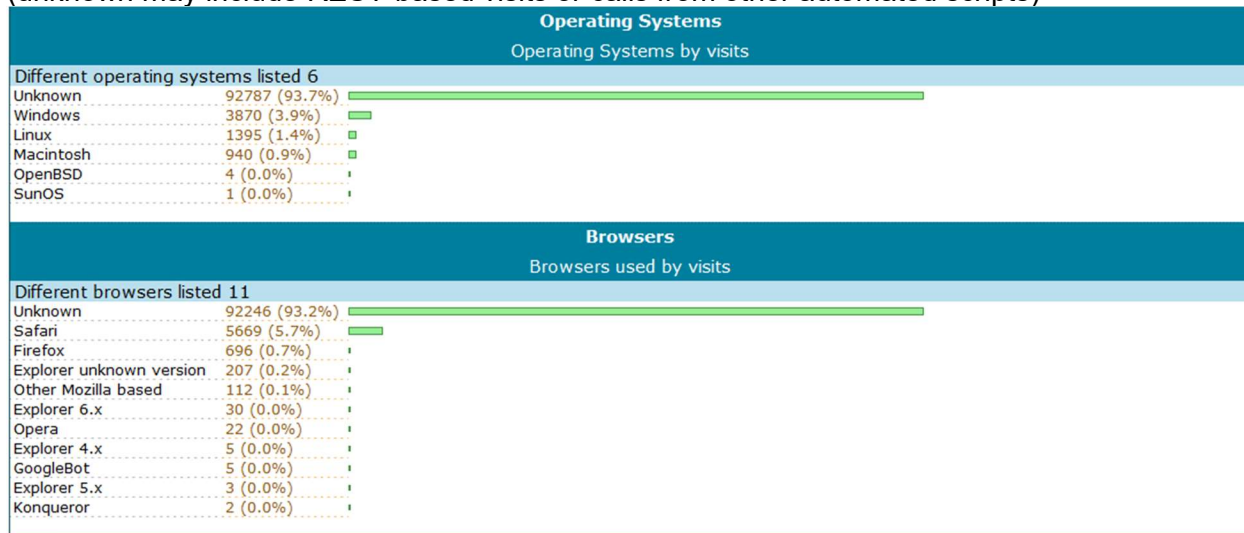
Top page hits over Feb 2023:

Type of page	End-point	Count
Studies	/data/DRCCMetadata.php	359226
REFMET	/rest/refmet	146990
Structure data	/data/StructureData.php	145566
Statistical analysis	/data/metabolite_id_show.php	133176
Metabolite-Gene	/databases/proteome/MGP_table.php	94467
Search	/search/sitesearch.php	68559
Protocols	/protocols/protocoldetails.php	66724
Study summary	/data/DRCCStudySummary.php	64274
REFMET	/databases/refmet/refmet.php	60081
Studies	/rest/study	59610
Protocols	/protocols/general.php	58848
Statistical analysis	/data/show_metabolite_data_by_factors.php	53784
REFMET	/databases/refmet/abbrev_generic.php	53452
Metabolite-Gene	/databases/proteome/MGP_detail.php	43730
General	/data/png_display_inline2.php	42394
REFMET	/databases/refmet/refmet_details.php	35035
General	/homepage	34923
Archive	/data/show_archive_contents_json.php	27782
Massbank	/data/massbank.php	26687
Files	/data/file_extract_7z.php	24398

Study search	/data/show_studies_by_pubchem.php	21640
Pathways	/data/show_h_pathway_metabolites.php	21492
Search	/data/s3.php	15982
Files	/data/file_extract.php	14958
Search	/data/search_untarg_mz.php	14519

OS and browsers

(unknown may include REST-based visits or calls from other automated scripts)

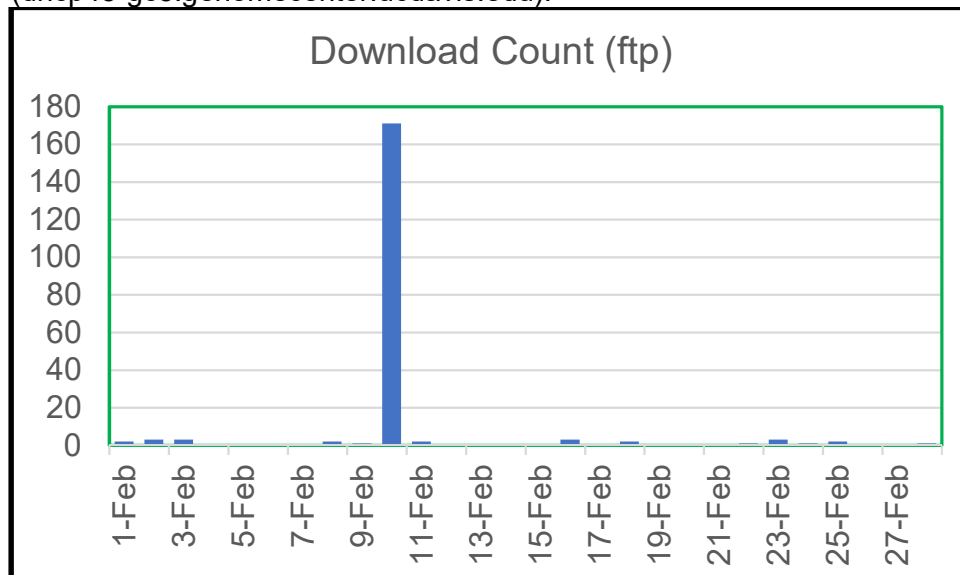


Download statistics

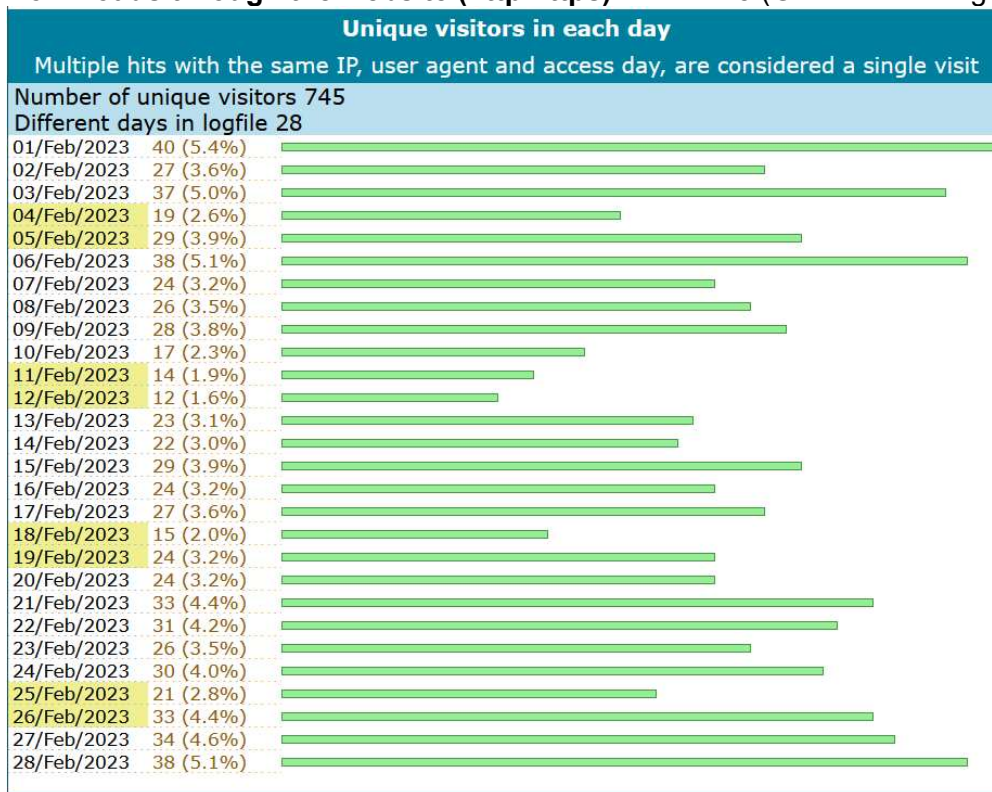
Amount of data downloaded: about 5 TB

FTP-based downloads: Total 197

Important note: In Feb 2023, 171 downloads were from UC Davis (dhcp45-gc5.genomecenter.ucdavis.edu).



Downloads through the website (http/https): Total 745 (Generated using "Visitors")



Top downloads requested:

Requested pages

Page requests ordered by hits

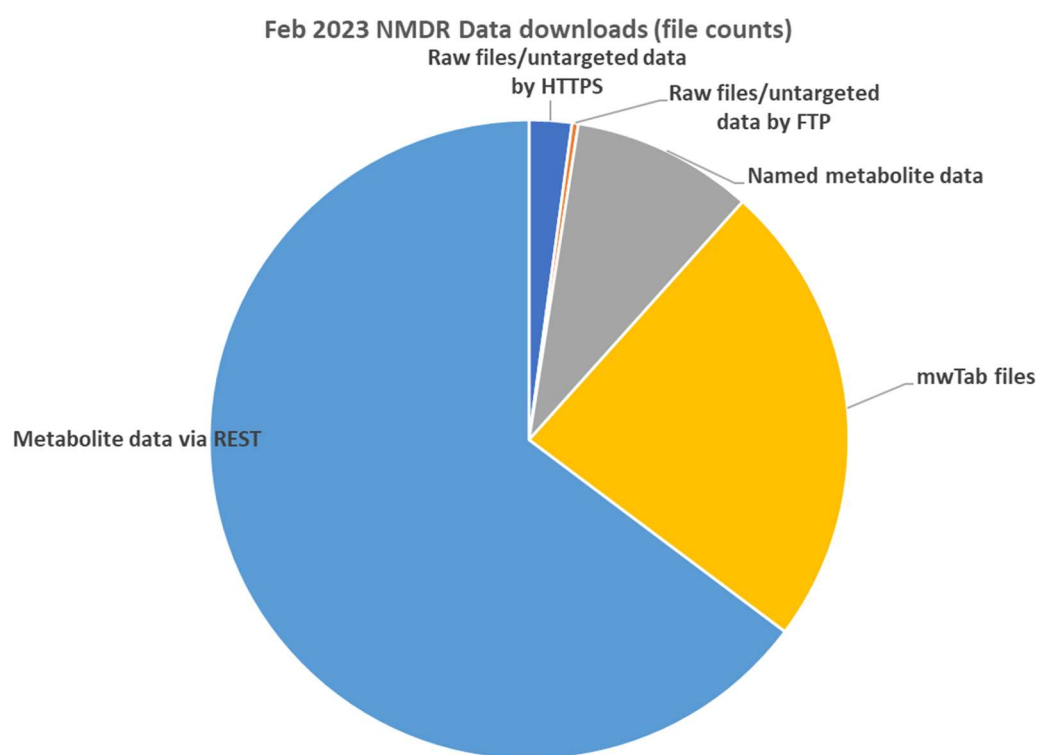
Different pages requested 599

1)	41	/studydownload/ST000923_AN001513_Results.txt
2)	37	/studydownload/ST001192_AN001986_Results.txt
3)	35	/studydownload/ST000879_AN001429_Results.txt
4)	28	/studydownload/ST000923_AN001514_Results.txt
5)	21	/studydownload/ST000604_AN000924_Results.txt
6)	19	/studydownload/ST001192_AN001985_Results.txt
7)	18	/studydownload/ST000020.zip
8)	18	/studydownload/ST000604_AN000925_Results.txt
9)	18	/studydownload/ST000919_AN001506_Results.txt
10)	16	/studydownload/ST000879_AN001432_Results.txt
11)	14	/studydownload/ST001942.zip
12)	13	/studydownload/ST000954_AN001564_Results.txt
13)	12	/studydownload/ST001000_RawFile_SampleID_mapping.csv
14)	10	/studydownload/ST000956_AN001568_Results.txt
15)	9	/studydownload/ST001192_AN001984_Results.txt
16)	9	/studydownload/ST002110_pos_rawdata.zip
17)	9	/studydownload/ST001000_AN001631_Results.txt
18)	9	/studydownload/ST000746_AN001169_Results.txt
19)	8	/studydownload/ST001000_AN001629_Results.txt
20)	8	/studydownload/ST001430_AN002391_Results.txt

Mode of download (Feb 2023)

Unlike the filtering for other statistics, these are based on the entire log for February 2023 (without excluding bots, spiders, etc).

Type	Feb 2023 NMDR Data downloads (file counts)
Raw files/untargeted data by HTTPS	1615
Raw files/untargeted data by FTP	240
Named metabolite data	6892
mwTab files	17729
Metabolite data via REST	48652



Access statistics of our GitHub page for Jupyter notebooks repository (covers 8/1/2022 – 02/28/2023)

<https://github.com/metabolomicsworkbench/jupyter-notebooks>

Path	Count	Uniques
/metabolomicsworkbench/jupyter-notebooks	113	69
/metabolomicsworkbench/jupyter-notebooks/blob/6db27e08aa59166f9b756723dc6b7f74e117afdb/MWUtil.py	4	2
/metabolomicsworkbench/jupyter-notebooks/blob/master/.gitignore	2	2
/metabolomicsworkbench/jupyter-notebooks/blob/master/environment.yml	14	6
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformClusteredHeatMapAnalysis.ipynb	16	16
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformDataNormalization.ipynb	99	86
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformLinearDiscriminantAnalysis.ipynb	10	9
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformPartialLeastSquaresDiscriminantAnalysis.ipynb	7	5
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformPrincipalComponentAnalysis.ipynb	5	5
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformRandomForestAnalysis.ipynb	9	9
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformRelativeLogAbundanceAnalysis.ipynb	16	10
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPerformVolcanoPlotAnalysis.ipynb	22	18
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWPlotNamedMetabolitesResultsExample.ipynb	20	18
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPICompoundDataExample.ipynb	4	4
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPIExactMassDataExample.ipynb	1	1
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPINamedMetabolitesResultsExample.ipynb	10	6
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPIProteinDataExample.ipynb	13	13
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPIRefMetDataExample.ipynb	5	5
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWRestAPIStudyDataExample.ipynb	16	15
/metabolomicsworkbench/jupyter-notebooks/blob/master/MWUtil.py	12	4
/metabolomicsworkbench/jupyter-notebooks/blob/master/README.md	3	3
GIT CLONES	61	73
Referrer	Counts	Uniques
bdcw.org	2	2
colab.research.google.com	1	1
github.com	7	7
Google	164	110
metabolomicsworkbench.org	177	76

<https://github.com/metabolomicsworkbench/MetENP>

Path	Count	Uniques
/metabolomicsworkbench/MetENP	938	391
/metabolomicsworkbench/MetENP/blob/2ea09f22358e7dbf4d8cf70cc8cde89516c29ddf/vignettes/MetENP_ST001951.ipynb	4	2
/metabolomicsworkbench/MetENP/blob/34c302a6a40652d4f4431ab839c078d8a95bcd79/vignettes/MetENP_ST001951.ipynb	2	2
/metabolomicsworkbench/MetENP/blob/a8e80f154a9a4a865fde6803811235a4f3c2454b/vignettes/MetENP_vignette_Jupyter_notebook.ipynb	5	4
/metabolomicsworkbench/MetENP/blob/b20cc4d6c2bda254c154f97c69829ef01388b877/R/anova_ana.R	1	1
/metabolomicsworkbench/MetENP/blob/b20cc4d6c2bda254c154f97c69829ef01388b877/R/partial_join.R	2	2
/metabolomicsworkbench/MetENP/blob/b20cc4d6c2bda254c154f97c69829ef01388b877/R/pathinfo.R	2	2
/metabolomicsworkbench/MetENP/blob/b20cc4d6c2bda254c154f97c69829ef01388b877/R/significant_met.R	2	2
/metabolomicsworkbench/MetENP/blob/b20cc4d6c2bda254c154f97c69829ef01388b877/vignettes/MetENP_vignette.rmd	2	2
/metabolomicsworkbench/MetENP/blob/main/binder/environment.yml	8	4
/metabolomicsworkbench/MetENP/blob/main/binder/postBuild	13	6
/metabolomicsworkbench/MetENP/blob/main/data/ls_path.RData	4	4
/metabolomicsworkbench/MetENP/blob/main/DESCRIPTION	20	13
/metabolomicsworkbench/MetENP/blob/main/environment.yml	13	7
/metabolomicsworkbench/MetENP/blob/main/inst/extdata/example.txt	4	4
/metabolomicsworkbench/MetENP/blob/main/inst/extdata/human_cachexia.csv	1	1
/metabolomicsworkbench/MetENP/blob/main/LICENSE	1	1
/metabolomicsworkbench/MetENP/blob/main/man/compoundinfo.Rd	2	2
/metabolomicsworkbench/MetENP/blob/main/man/enzyme_gene_info.Rd	2	1
/metabolomicsworkbench/MetENP/blob/main/NAMESPACE	3	3
/metabolomicsworkbench/MetENP/blob/main/R/anova_ana.R	3	3
/metabolomicsworkbench/MetENP/blob/main/R/compoundinfo.R	2	2
/metabolomicsworkbench/MetENP/blob/main/R/convert_refmet.R	17	12
/metabolomicsworkbench/MetENP/blob/main/R/data.R	1	1
/metabolomicsworkbench/MetENP/blob/main/R/dotplot_met_class_path.R	6	4
/metabolomicsworkbench/MetENP/blob/main/R/map_keggid.R	3	3
/metabolomicsworkbench/MetENP/blob/main/R/mapspspath.R	1	1
/metabolomicsworkbench/MetENP/blob/main/R/metclassenrichment.R	12	10
/metabolomicsworkbench/MetENP/blob/main/R/metcountplot.R	2	2
/metabolomicsworkbench/MetENP/blob/main/R/pathinfo.R	3	1
/metabolomicsworkbench/MetENP/blob/main/R/plot_heatmap.R	1	1
/metabolomicsworkbench/MetENP/blob/main/R/plot_met_enrichment.R	4	4
/metabolomicsworkbench/MetENP/blob/main/R/plot_pathway_networks.R	6	4
/metabolomicsworkbench/MetENP/blob/main/R/plot_volcano.R	3	3
/metabolomicsworkbench/MetENP/blob/main/R/significant_met.R	4	2
/metabolomicsworkbench/MetENP/blob/main/README.md	23	10
/metabolomicsworkbench/MetENP/blob/main/vignettes/Case%20study%201_%20Study%20ST000915_20220619.html	8	7
/metabolomicsworkbench/MetENP/blob/main/vignettes/Case%20study%201_%20Study%20ST000915_20220625.html	12	7
/metabolomicsworkbench/MetENP/blob/main/vignettes/Case%20study%201_%20Study%20ST000915.html	46	24
/metabolomicsworkbench/MetENP/blob/main/vignettes/MetENP_ST000084.ipynb	4	4
/metabolomicsworkbench/MetENP/blob/main/vignettes/MetENP_ST000897.ipynb	2	2
/metabolomicsworkbench/MetENP/blob/main/vignettes/MetENP_ST000915.ipynb	5	4
/metabolomicsworkbench/MetENP/blob/main/vignettes/MetENP_vignette_Jupyter_notebook.ipynb	30	14
/metabolomicsworkbench/MetENP/blob/main/vignettes/MetENP_vignette.rmd	76	39
/metabolomicsworkbench/MetENP/blob/main/vignettes/tmp/test.txt	2	2
GIT CLONES	109	126
Referrer	Count	Uniques
bdcw.org	6	4
bioRxiv.org	66	23
github.com	60	29
Google	350	99
metabolomicsworkbench.org	75	29
notebooks.githubusercontent.com	12	2
training.nih-cfde.org	4	2

<https://github.com/metabolomicsworkbench/MetENPAppyter>

Path	Count	Uniques
/metabolomicsworkbench/MetENPAppyter	15	14
/metabolomicsworkbench/MetENPAppyter/blob/main/R/MetENP/R/MetENP	3	3
/metabolomicsworkbench/MetENPAppyter/blob/main/R/MetENP/R/MetENP.rdb	1	1
GIT CLONES	14	21
Referrer	Count	Uniques
github.com	8	6
Google	25	9




The number of accesses to the Jupyter/Binder entry page at:
<https://www.metabolomicsworkbench.org/data/AnalyzeUsingJupyterNotebooks.php>

The number of hits to the entry page is low- about 20 per week. This doesn't necessarily mean that users are clicking on the external Binder/Github links on this page, though.

FAIRShake metrics

Precalculated stats on MW: <https://fairshake.cloud/project/85/assessments/>

Project Assessments (6697)


Assessment			Metrics								
Target	Rubric		Globally unique identifier	Persistent identifier	Machine-readable metadata	Standardized metadata	Resource identifier in metadata	Resource discovery through web search	Open, Free, Standardized Access protocol	Protocol to access restricted content	Persistence of resource and metadata
Fatb Induction Experiment (FatBIE)	FAIR metrics by fairmetrics.org		no (0.00)	no (0.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)		no (0.00)
Intestinal Samples II pre/post transplantation	FAIR metrics by fairmetrics.org		no (0.00)	no (0.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)		no (0.00)
Metabolomic analysis of mouse embryonic fibroblasts, embryonic stem cells, and induced pluripotent stem cells	FAIR metrics by fairmetrics.org		no (0.00)	no (0.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)		no (0.00)

Apparently, the FAIRshake tool that generated the above statistics is not fully mature and requires manual curation. MW uses document object identifiers (DOI) for the projects, which is included (referred to as Persistent Identifier) in the metadata submitted to the CFDE portal. Through the DOI, one can access all the publicly available data on the MW website.

https://fairshake.cloud/digital_object/6578/assessments/

Tags: NIHcommonfund

Digital Object Assessments (1)

Assessment			Metrics								
Rubric	Project		The repository provides contact information for staff to enable users with questions or suggestions to interact with repository experts.	Tools that can be used to analyze each dataset are listed on the corresponding dataset pages.	The repository maintains licenses to manage data access and use.	The repository hosts data and metadata according to a set of defined criteria to ensure that the resources provided are consistent with the intent of the repository.	The repository provides documentation for each resource to permit its complete and accurate citation.	A description of the methods used to acquire the data is provided.	Version information is provided for each resource, where available.	The structure of the repository permits efficient discovery of data and metadata by end users.	The repository uses a standardized protocol to permit access by users.
The FAIRshake repository rubric	NIH Data Sharing Repositories		yes (1.00)	yes (1.00)	no (0.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)	yes (1.00)

The above tables lists “no” for license, but we have stated the terms of use. In the future, we will decide the license term (CC BY-NC, CC BY-NC-SA or something allowing commercialization of derivative work) and update the “Terms of use” page.



The screenshot shows the website <https://www.metabolomicsworkbench.org/about/termsofuse.php>. The page features the Metabolomics Workbench logo and navigation menu. The main content area is titled "Terms of Use" and contains the following text:

The Metabolomics Workbench is provided by the NIH Common Fund's National Metabolomics Data Repository(NMDR) on an "as is" basis, without warranty or representation of any kind, express or implied. The content of the Metabolomics Workbench is protected by international copyright, trademark and other laws. You may download articles and web pages from this site for your personal, non-commercial use only, provided that you keep intact all authorship, copyright and other proprietary notices. If you use the Metabolomics Workbench, you accept these terms. The NMDR reserves the right to modify these terms at any time.

At the bottom of the page, it states: "UCSD Metabolomics Workbench, a resource sponsored by the Common Fund of the National Institutes of Health" and provides links for "Terms of use", "Site map", "Contact", and "NMDR Personnel".

IP Exclusion List 1

As php code:

```
$blocked_ip=array(
'132.249', '3.91', '5.9', '34.238', '35.174', '40.77', '46.229', '46.4', '54.209', '66.249', '69.3', '78.46',
'91.137', '92.22', '95.216', '95.91', '106.120', '136.243', '144.76', '148.251', '157.55', '162.21',
'173.234', '178.255', '178.63', '180.76', '185.25', '192.151', '207.46', '213.174'
);
$blocked_ip3 = array(
'100.26.127', '103.131.71', '104.245.145', '110.249.201', '110.249.202', '110.93.150',
'111.225.148', '111.225.149', '114.111.32', '114.119.132', '114.119.133', '114.119.135',
'114.119.137', '114.119.140', '114.119.145', '114.119.149', '114.119.152', '114.119.153',
'114.119.154', '114.119.155', '116.179.32', '116.179.37', '118.184.177', '123.125.109',
'123.183.224', '125.209.235', '128.127.105', '13.66.139', '135.181.137', '135.181.138',
'135.181.62', '141.8.142', '144.217.135', '147.92.153', '149.154.161', '149.155.131', '149.56.150',
'149.56.160', '154.51.131', '154.54.249', '157.90.177', '17.121.112', '17.121.113', '17.121.114',
'17.121.115', '184.75.211', '185.101.32', '185.138.241', '185.191.171', '185.54.230', '191.96.106',
'194.187.171', '194.9.191', '195.201.106', '198.134.108', '198.134.109', '198.251.73',
'198.98.183', '199.47.82', '204.15.110', '207.241.229', '207.241.233', '211.249.46', '213.180.203',
'216.244.66', '220.181.108', '31.3.152', '31.3.153', '37.46.121', '49.7.20', '49.7.21', '5.102.173',
'5.133.192', '5.255.253', '5.45.207', '5.62.16', '5.62.20', '5.62.41', '5.62.43', '5.62.56', '5.62.57',
'5.62.58', '5.62.59', '5.62.60', '5.62.61', '5.62.62', '5.62.63', '50.21.188', '54.161.41', '58.250.125',
'61.135.159', '65.108.103', '65.108.6', '65.108.99', '65.21.231', '69.160.160', '74.208.2',
'76.164.224', '77.234.44', '77.75.73', '77.75.76', '77.75.77', '77.75.78', '77.75.79', '77.88.5',
'79.142.76', '81.17.57', '85.208.98', '85.31.186', '87.250.224', '91.143.80', '91.219.212',
'91.242.162', '93.158.161', '95.108.213', '95.142.121', '95.142.127', '95.87.154'
);
```

IP Exclusion List 2

As php code:

\$blocked_ip is as above in List 1.

```
$blocked_ip3 = array(
    '100.26.127', '103.131.71', '104.245.145', '110.249.201', '110.249.202', '110.93.150',
    '111.225.148', '111.225.149', '114.111.32', '114.119.128', '114.119.129', '114.119.130',
    '114.119.131', '114.119.132', '114.119.133', '114.119.134', '114.119.135', '114.119.136',
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