Metabolomics Workbench and the National Metabolomics Data Repository

University of California San Diego
and
San Diego Supercomputer Center

Metabolomics Workbench REST service

NIH Common Fund's National Metabolomics Data Repository
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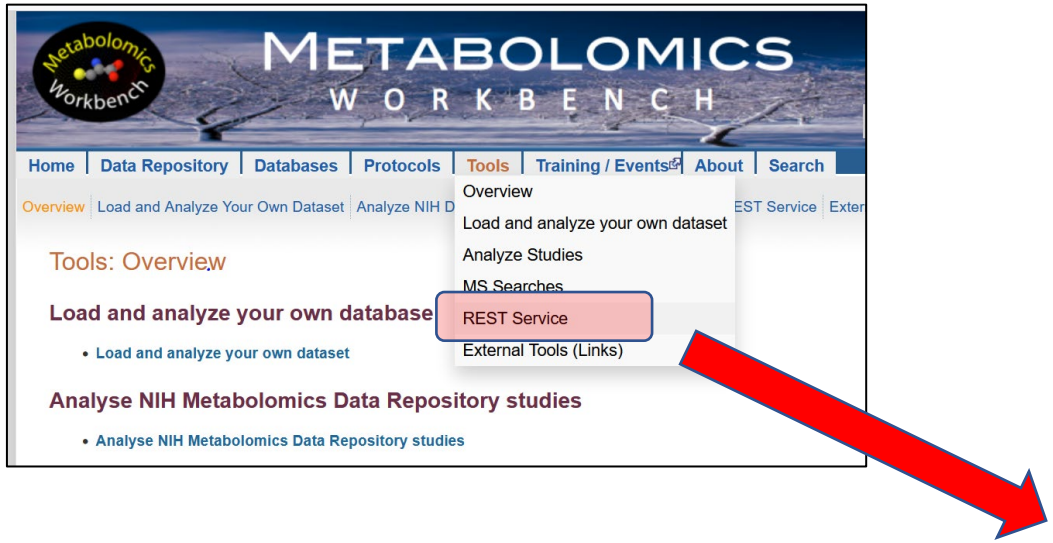
MW REST service access on the Metabolomics Workbench



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Metabolomics WorkBench REST service

MW REST API (v1.0, 5/7/2019) Download API (pdf)

*Note: A number of new REST queries have been added that are not described in this API version (see new examples below)

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

The REST URL consists of three main parts, separated by forward slashes, after the common prefix specifying the invariant base URL: (https://www.metabolomicsworkbench.org/rest/)

a. The **context** specification dictates which type of resource to access and is chosen from one of the following:
<study | compound | refmet | gene | protein | moverz | exactmass>

b. The **input** specification is composed of 2 required parameters separated by forward slashes. The first parameter is the *input item* which depends on the context. The 2nd parameter is an appropriate *input value* for the chosen item. Examples of an input specification are:

```
/compound/pubchem_cid/311/
/compound/formula/C20H34O/
/study/study_id/ST000001/
/study/study_title/diabetes/
/refmet/name/Cholesterol/
/refmet/match/LysoPC16:0/
/gene/gene_symbol/acaca/
/protein/uniprot_id/Q13085/
```

Exceptions to this input specification occur when the 'moverz' context (MS search) is selected. In this case the input value must consist of 3 parts separated by forward slashes: *<m/z value>/<adduct>/<tolerance(Daltons)>*, e.g. '635.52/M+H/0.2'. In the case of the 'exactmass' context the input value must consist of 2 parts separated by forward slashes: *<lipid bulk abbreviation>/<adduct>*, e.g. 'PC(34:1)/M+H' and the input and output items are ignored.

c. The **output** specification is composed of a required *output item* parameter and an optional *output format* parameter. The list of possible output items depends on the value chosen for the context. In the case of the "compound" context one or more (separated by commas) of 'regno', 'formula','exactmass', 'inchi_key', 'name', 'sys_name', 'smiles', 'lm_id', 'pubchem_cid', 'hmdb_id', 'kegg_id', 'chebi_id', 'metacyc_id' may be specified. More conveniently, an output type of 'all' may be specified to retrieve all compound-related fields. Also an output type of 'classification' retrieves the LIPID MAPS/ClassyFire classification hierarchy. In the case of the "study" context, allowed output types are 'summary', 'factors', 'analysis', 'metabolites' and 'data'. The default output format is JSON which is amenable to manipulation and parsing by various programming languages. Optionally a text ouput format may be specified, for example:

```
/compound/pubchem_cid/311/all/txt
```

Exceptions to this output specification occur when either 'molfile' (molfile is downloaded) or 'png' (png image is displayed in browser) is chosen as an output item in the "compound" context.

The interactive "REST url" creator below shows most of the currently available options for this service.

Base URL	/Context	/Input item	/Input value	/Output item	/Output format
https://www.metabolomicsworkbench.org/rest	/	/	/	/	/ text

Create REST URL | Reset | (What is REST?) (What is JSON?)

MW REST service API document

https://www.metabolomicsworkbench.org/tools/MWRestAPIv1.0.pdf

Metabolomics Workbench REST URL-based API Specification

Version: 1.0 Date: 5/7/2019

This document describes the Metabolomics Workbench REST API specifications, a web interface for accessing a variety of data such as metabolite structures, study metadata, experimental results etc. It details the syntax of the HTTP requests including both the names of the available requests and parameters. These HTTP requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP requests and interact with datasets through the REST API.

The URL Path

The REST URL consists of three main parts, separated by forward slashes, after the common prefix specifying the invariant base URL (https://www.metabolomicsworkbench.org/rest/):

https://www.metabolomicsworkbench.org/rest/<context>/<input specification>/<output specification>

Part 1: The **context** determines the type of data to be accessed from the Metabolomics Workbench, such as metadata or results related to the submitted studies, data from metabolites, genes/proteins and analytical chemistry databases as well as other services related to mass spectrometry and metabolite identification:

<context> = study | compound | refmet | gene | protein | moverz | exactmass

Part 2: The **input specification** consists of two required parameters describing the REST request:

<input specification> = <input item>/<input value>

Part 3: The **output specification** consists of two parameters describing the output generated by the REST request:

<output specification> = <output item>/[<output format>]

The first parameter is required in most cases. The second parameter is optional. The input and output

MW REST service overview

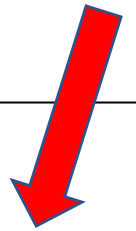
The MW REST service has 5 main contexts:

1. **Compound(metabolite) context (compound input)**
   Retrieve data on name, formula, mass, InChIKey, SMILES, molfile, classification, Pubchem ID etc. from the Metabolite structure database.
2. **NMDR Study context (study input)**
   Retrieve data on study summaries, study design, study metadata, experimental conditions, metabolite numbers, sample source, species, disease association , tables of measurements, etc from NMDR studies.
3. **RefMet context (refmet input)**
   Access RefMet standardized nomenclature and annotations, map metabolite names to RefMet names, download all RefMet names, chemical classification, etc.
4. **Gene/Protein context (gene or protein input)**
   Access DNA/RNA/protein identifiers, gene symbols, protein sequences, splice variants, homologs, etc, from the MW human Gene/Protein database of metabolism-related genes.
5. **Mass spectrometry context (moverz or exactmass input)**
   Perform precursor ion searches on RefMet database, Metabolite structure database and Lipid database by specifying m/z, adduct and mass tolerance. Calculate exact mass of a lipid molecular species ion.

MW REST service Query Builder

The online REST query builder has a menu-based format which covers most of the REST queries in the API

JSON or plain text



The interactive "REST url" creator below shows most of the currently available options for this service.

Base URL	/Context	/Input item	/Input value	/Output item	/Output format
https://www.metabolomicsworkbench.org/rest	/ compound	/ formula	/ C12H24O2	/ name	/ text

Create REST URL | Reset | (What is REST?) (What is JSON?)

Output (text)

```
formula C12H24O2
name    4,9-dimethyldecanoic acid

formula C12H24O2
name    2-Heptyl butyrate

formula C12H24O2
name    Hexyl hexanoate

formula C12H24O2
name    Ethyl decanoate

formula C12H24O2
name    Nonanal propyleneglycol acetal
```

Output (JSON)


```
{"Row1":{"formula":"C12H24O2","name":"4,9-dimethyldecanoic acid"},"R
{"formula":"C12H24O2","name":"Nonanal propyleneglycol acetal"},"Row6
{"formula":"C12H24O2","name":"2-methylbutyl heptanoate"},"Row10":{"f
{"formula":"C12H24O2","name":"3-methyl-undecanoic acid"},"Row14":{"f
{"formula":"C12H24O2","name":"3R-methyl-undecanoic acid"},"Row18":{"
{"formula":"C12H24O2","name":"(R)-Dihydrocitronellol acetate"},"Row2
{"formula":"C12H24O2","name":"2-(l-menthoxy)ethanol"}}
```

MW REST web page contains numerous examples for each context

Metabolomics WorkBench REST service

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

Metabolite (structure) context

Study-specific (Metadata, data) context

Example request	Example URL
Compound context	
Fetch compound common name from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/name
Fetch all compound fields from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/all
Fetch all compound fields as text from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/all/txt
Fetch compound smiles from PubChem compound ID	https://www.metabolomicsworkbench.org/rest/compound/pubchem_cid/439577/smiles
Fetch compound common name and sytematic name from InChIKey	https://www.metabolomicsworkbench.org/rest/compound/inchi_key/JTWQQJDENGGSBJ-UHFFFAOYSA-N/name,sys_name
Fetch all compound fields from formula (multiple records)	https://www.metabolomicsworkbench.org/rest/compound/formula/C20H34O/all
Fetch compound classification hierarchy from PubChem compound ID	https://www.metabolomicsworkbench.org/rest/compound/pubchem_cid/5281365/classification
Download compound molfile from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/28606/molfile
Fetch png image of structure from Metabolomics Workbench database regno	https://www.metabolomicsworkbench.org/rest/compound/regno/11/png
Study context	
Show all publicly available studies (Project, Study, Analysis ID)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/available
Fetch summary information for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/summary
Fetch samples and experimental variables (factors) for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/factors/
Fetch summary information for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/summary
Fetch analysis information for a study	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/analysis
Fetch metabolites and annotations detected in a study (one study at a time)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000009/metabolites
Fetch named metabolite measurements for a study (one study at a time)	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/data
Fetch mwTab content for an analysis within a study in mwTab format	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/mwtab/txt
Fetch mwTab content for an analysis within a study in json format	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/mwtab
Fetch species information (as text) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/species/txt
Fetch sample source information (as text) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/source/txt
Fetch disease association (where applicable) for all studies	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/disease
Fetch list of studies with untargeted data in NMDR*New	https://www.metabolomicsworkbench.org/rest/study/study_id/x/untarg_studies/
Fetch untargeted data (where applicable) for an analysis within a study*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000113/untarg_data/
Fetch experimental factors for an untargeted data analysis within a study*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000113/untarg_factors/
Fetch list of studies with named metabolites in NMDR*New	https://www.metabolomicsworkbench.org/rest/study/study_id/ST/named_metabolites/
Show number of named metbolites in a study*New	https://www.metabolomicsworkbench.org/rest/study/study_id/ST000001/number_of_metabolites/
Fetch list of studies (as text) containing a RefMet name*New	https://www.metabolomicsworkbench.org/rest/study/refmet_name/Cholesterol/data/txt/
Fetch list of studies (as text) containing a KEGG_ID*New	https://www.metabolomicsworkbench.org/rest/study/kegg_id/C00002/data/txt/
Show metabolite name and RefMet name for a (NMDR) metabolite_id*New	https://www.metabolomicsworkbench.org/rest/study/metabolite_id/ME272191/available/
Fetch table of results (identified metabolites) for an analysis_id*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/datatable/
Download table of results (identified metabolites) for an analysis_id*New	https://www.metabolomicsworkbench.org/rest/study/analysis_id/AN000001/datatable/file

In most cases, output may be specified as JSON or plain text format

MW REST web page contains numerous examples for each context

Metabolomics WorkBench REST service

The Metabolomics WorkBench REST service enables access to a variety of data (including metabolite structures, study metadata and experimental results) using HTTP requests. These requests may be carried out using a web browser or may be embedded in 3rd party applications or scripts to enable programmatic access. Most modern programming languages including PHP, Perl, Python, Java and Javascript have the capability to create HTTP request and interact with datasets such as this REST service.

RefMet context

Gene/protein context

MS search context

RefMet context	
Fetch all RefMet fields from name	https://www.metabolomicsworkbench.org/rest/refmet/name/Cholesterol/all
Fetch all RefMet fields from formula	https://www.metabolomicsworkbench.org/rest/refmet/formula/C12H24O2/all
Standardize metabolite name to RefMet	https://www.metabolomicsworkbench.org/rest/refmet/match/citrate/name/
Fetch entire RefMet database (Name,exact mass,formula,InChIKey,PubChemID,classification)*New	https://www.metabolomicsworkbench.org/rest/refmet/all
Fetch all RefMet names*New	https://www.metabolomicsworkbench.org/rest/refmet/name
Fetch all RefMet names and chemical classification*New	https://www.metabolomicsworkbench.org/rest/refmet/classification
Gene/protein context	
Fetch all gene fields from gene symbol	https://www.metabolomicsworkbench.org/rest/gene/gene_symbol/acaca/all
Fetch gene name from Entrez gene id	https://www.metabolomicsworkbench.org/rest/gene/gene_id/31/gene_name
Fetch all protein fields from UniProt id	https://www.metabolomicsworkbench.org/rest/protein/uniprot_id/Q13085/all
Fetch all protein fields from Entrez gene id	https://www.metabolomicsworkbench.org/rest/protein/gene_id/19/all/
Fetch mRNA id from protein Refseq id	https://www.metabolomicsworkbench.org/rest/protein/refseq_id/NP_005493/mrna_id/
Mass spectrometry context	
Perform MS precursor ion search on Metabolomics Workbench database with m/z 635.52, ion-type* M+H and mass tolerance of 0.5 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/MB/635.52/M+H/0.5/txt
Perform MS precursor ion search on LIPIDS virtual database with m/z 513.45, ion-type* M-2H (2-) and mass tolerance of 0.2 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/LIPIDS/513.45/M-2H/0.2/txt
Perform MS precursor ion search on RefMet database with m/z 255.2, ion-type* M+H and mass tolerance of 0.2 and output as text	https://www.metabolomicsworkbench.org/rest/moverz/REFMET/255.2/M+H/0.2/txt
Calculate the exact mass (m/z) of the [M+H]+ ion of the lipid abbreviation# PC(34:1)	https://www.metabolomicsworkbench.org/rest/exactmass/PC(34:1)/M+H