Package 'cmmr'

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Title CEU Mass Mediator RESTful API

Version 1.0.3

Depends R (>= 4.4.0)

Imports httr, progress, RJSONIO, cli

Description
CEU (CEU San Pablo University) Mass Mediator is an on-line tool for aiding researchers in performing metabolite annotation. 'cmmr' (CEU Mass Mediator RESTful API) allows for programmatic access in R: batch search, batch advanced search, MS/MS (tandem mass spectrometry) search, etc.
For more information about the API Endpoint please go to <https://github.com/YaoxiangLi/cmmr>.

License GPL-3

Encoding UTF-8

URL https://github.com/YaoxiangLi/cmmr

RoxygenNote 7.3.2

Suggests testthat

NeedsCompilation no

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Contents

`advanced_batch_search` *Advanced Batch Search using CEU Mass Mediator API*

Description

`advanced_batch_search` performs an advanced batch search on the CEU Mass Mediator API and returns a dataframe of search results.

Usage

```
advanced_batch_search(
  cmm_url = "https://ceumass.eps.uspceu.es/api/v3/advancedbatch",
  chemical_alphabet = "ALL",
  modifiers_type = "none",
  metabolites_type = "all-except-peptides",
  databases = "[\"HMDB\"]",
  masses_mode = "mz",
  ion_mode = "positive",
  adducts = "[\"all\"]",
  deuterium = FALSE,
  tolerance = 7.5,
  tolerance_mode = "ppm",
  masses = NULL,
  all_masses = "[]",
  retention_times = NULL,
  all_retention_times = "[]",
  composite_spectra = NULL
)
```

Arguments

`cmm_url`	A character string specifying the CEU Mass Mediator API endpoint. Default is `"https://ceumass.eps.uspceu.es/api/v3/advancedbatch"`.
`chemical_alphabet`	A character string specifying the chemical alphabet to use. Options are `"CHNOPS"`, `"CHNOPSCL"`, or `"ALL"`.
`modifiers_type`	A character string specifying the modifier type. Options are `"none"`, `"NH3"`, `"HCOO"`, `"CH3COO"`, `"HCOONH3"`, or `"CH3COONH3"`.
`metabolites_type`	A character string specifying the metabolites type. Options are `"all-except-peptides"`, `"only-lipids"`, or `"all-including-peptides"`.
`databases`	A JSON-formatted character string specifying the databases to search. Examples include `'["all"]'`, `'["HMDB"]'`, `'["LipidMaps"]'`.

masses_mode A character string specifying the masses mode. Options are "neutral" or "mz".

ion_mode A character string specifying the ionization mode. Options are "positive", "negative", or "neutral".

adducts A JSON-formatted character string specifying the adducts to include in the search. Examples include '["M+H","M+Na"]' for positive mode.

deuterium A logical value indicating whether to consider deuterium substitutions. TRUE or FALSE.

tolerance A numeric value specifying the mass tolerance (Range: 0 to 100).

tolerance_mode A character string specifying the tolerance mode. Options are "ppm" or "mDa".

masses A numeric vector of masses to search.

all_masses A JSON-formatted character string representing an array of mass arrays.

retention_times
A numeric vector of retention times corresponding to the masses.

all_retention_times
A JSON-formatted character string representing an array of retention time arrays.

composite_spectra
A JSON-formatted character string representing composite spectra.

Value

A dataframe containing the search results from the CEU Mass Mediator API.

Examples

```
## Not run:
df <- advanced_batch_search(
  cmm_url = "https://ceumass.eps.uspceu.es/api/v3/advancedbatch",
  chemical_alphabet = "ALL",
  modifiers_type = "none",
  metabolites_type = "all-except-peptides",
  databases = '["HMDB"]',
  masses_mode = "mz",
  ion_mode = "positive",
  adducts = '["all"]',
  deuterium = FALSE,
  tolerance = 7.5,
  tolerance_mode = "ppm",
  masses = c(400.3432, 288.2174),
  all_masses = "[]",
  retention_times = c(18.842525, 4.021555),
  all_retention_times = "[]",
  composite_spectra = paste0(
    '[ [ { "mz": 400.3, "intensity": 307034.9 },',
    '   { "mz": 311.2, "intensity": 400.1 } ] ]'
  )
)

## End(Not run)
```

batch_search *Encapsulation of CEU Mass Mediator batch search API*

Description

batch_search returns a dataframe with the results from the database search.

Usage

```
batch_search(
  cmm_url = "https://ceumass.eps.uspceu.es/api/v3/batch",
  metabolites_type = "all-except-peptides",
  databases = "[\"all-except-mine\"]",
  masses_mode = "mz",
  ion_mode = "positive",
  adducts = "[\"M+H\",\"M+Na\"]",
  tolerance = 10,
  tolerance_mode = "ppm",
  unique_mz
)
```

Arguments

cmm_url	A URL string for the CEU Mass Mediator or a local API endpoint.
metabolites_type	Search metabolites type: "all-except-peptides", "only-lipids", or "all-including-peptides".
databases	A JSON array of databases to search: e.g., "all", "HMDB", "LipidMaps", etc.
masses_mode	Masses mode: "neutral" or "mz".
ion_mode	Ionization mode: "positive" or "negative".
adducts	A JSON array of adducts to include in the search, e.g., '["M+H", "M+Na"]'.
tolerance	A numeric tolerance value (range: 0-100).
tolerance_mode	Tolerance mode: "ppm" or "mDa".
unique_mz	A numeric vector of unique m/z values for the search.

Value

A dataframe containing search results.

Examples

```
## Not run:
df_pos <- batch_search(
  "https://ceumass.eps.uspceu.es/api/v3/batch",
  "all-except-peptides",
```

```
  '["all-except-mine"]',
  "mz",
  "positive",
  '["M+H","M+Na"]',
  10,
  "ppm",
  c(670.4623, 1125.2555, 602.6180)
)

## End(Not run)
```

`create_advanced_batch_body` *Create POST request Body for batch search*

Description

`create_advanced_batch_body` returns a string of advanced search POST request body.

Usage

```
create_advanced_batch_body(
  chemical_alphabet = "all",
  modifiers_type = "none",
  metabolites_type = "all-except-peptides",
  databases = "[\"hmdb\"]",
  masses_mode = "mz",
  ion_mode = "positive",
  adducts = "[\"all\"]",
  deuterium = "false",
  tolerance = "7.5",
  tolerance_mode = "ppm",
  masses = "[400.3432, 288.2174]",
  all_masses = "[]",
  retention_times = "[18.842525, 4.021555]",
  all_retention_times = "[]",
 composite_spectra = paste0("[[{ \"mz\": 400.3432, \"intensity\": 307034.88 }, ",
    "{ \"mz\": 311.20145, \"intensity\": 400.03336 }]]")
)
```

Arguments

`chemical_alphabet` "CHNOPS", "CHNOPSCL", "ALL"

`modifiers_type` "none", "NH3", "HCOO", "CH3COO", "HCOONH3", "CH3COONH3"

`metabolites_type` "all-except-peptides", "only-lipids", "all-including-peptides"

databases	"all", "all-except-mine", "HMDB", "LipidMaps", "Metlin", "Kegg", "in-house", "mine"
masses_mode	"neutral", "mz"
ion_mode	"positive", "negative"
adducts	for positive mode ["M+H", "M+2H", "M+Na", "M+K", "M+NH4", "M+H-H2O"] for negative mode ["M-H", "M+Cl", "M+FA-H", "M-H-H2O"], for neutral ["M"]
deuterium	boolean 'true' 'false'
tolerance	double (Range: [0..100])
tolerance_mode	"ppm", "mDa"
masses	double
all_masses	array of doubles
retention_times	double
all_retention_times	array of doubles
composite_spectra	array of arrays of spectra_object

Value

If all inputs are all correctly formatted, a dataframe will be returned for the result.

`create_batch_body` *Create POST request Body for batch search*

Description

`create_batch_body` returns a string of a POST request body.

Usage

```
create_batch_body(
  metabolites_type = "all-except-peptides",
  databases = "[\"all-except-mine\"]",
  masses_mode = "mz",
  ion_mode = "positive",
  adducts = "[\"M+H\",\"M+Na\"]",
  tolerance = 10,
  tolerance_mode = "ppm",
  unique_mz
)
```

Arguments

metabolites_type	"all-except-peptides", "only-lipids", "all-including-peptides"
databases	"all", "all-except-mine", "HMDB", "LipidMaps", "Metlin", "Kegg", "in-house", "mine"
masses_mode	"neutral", "mz"
ion_mode	"positive", "negative"
adducts	for positive mode [M+H, M+2H, M+Na, M+K,M+NH4, M+H-H2O]
tolerance	double (Range: [0..100])
tolerance_mode	"ppm", "mDa"
unique_mz	An array of unique m/zs

Value

If all inputs are all correctly formatted, a string of a POST request will be returned for the result.

Examples

```
batch_body <- create_batch_body(
  "all-except-peptides",
  '["all-except-mine"]',
  "mz",
  "positive",
  '["M+H","M+Na"]',
  10,
  "ppm",
  c(670.4623, 1125.2555, 602.6180)
)

batch_body <- create_batch_body(
  "all-except-peptides",
  '["all-except-mine"]',
  "mz",
  "negative",
  '["M-H","M+Cl"]',
  10,
  "ppm",
  c(670.4623, 1125.2555, 602.6180)
)

## Not run:
create_batch_body(c(670.4623, 1125.2555, 602.6180))

## End(Not run)
```

`create_msms_body` *Create MS/MS search POST request body*

Description

`create_msms_body` returns a string of a POST request body.

Usage

```
create_msms_body(
  ion_mass,
  ms_ms_peaks,
  precursor_ion_tolerance = 500,
  precursor_ion_tolerance_mode = "mDa",
  precursor_mz_tolerance = 1000,
  precursor_mz_tolerance_mode = "mDa",
  ion_mode = "positive",
  ionization_voltage = "all",
  spectra_types = "experimental"
)
```

Arguments

`ion_mass`	ion_mass
`ms_ms_peaks`	ms_ms_peaks
`precursor_ion_tolerance`	precursor_ion_tolerance
`precursor_ion_tolerance_mode`	precursor_ion_tolerance_mode
`precursor_mz_tolerance`	precursor_mz_tolerance
`precursor_mz_tolerance_mode`	precursor_mz_tolerance_mode
`ion_mode`	ion_mode
`ionization_voltage`	ionization_voltage
`spectra_types`	spectra_types

Value

If all inputs are all correctly formatted, a string of a POST request will be returned for the result.

msms_search *MS/MS Search using CEU Mass Mediator API*

Description

msms_search performs an MS/MS search on the CEU Mass Mediator API and returns a dataframe with the search results.

Usage

```
msms_search(
  ion_mass,
  ms_ms_peaks,
  precursor_ion_tolerance = 100,
  precursor_ion_tolerance_mode = "mDa",
  precursor_mz_tolerance = 500,
  precursor_mz_tolerance_mode = "mDa",
  ion_mode,
  ionization_voltage = "all",
  spectra_types = "experimental",
  cmm_url = "https://ceumass.eps.uspceu.es/api/msmssearch"
)
```

Arguments

ion_mass	Numeric. Mass of the ion to search for.
ms_ms_peaks	Matrix. The MS/MS peaks, with two columns representing mass and intensity.
precursor_ion_tolerance	Numeric. Tolerance for the precursor ion (default: 100.0).
precursor_ion_tolerance_mode	Character. Tolerance mode for precursor ion: "ppm" or "mDa" (default: "mDa").
precursor_mz_tolerance	Numeric. Tolerance for the m/z (default: 500.0).
precursor_mz_tolerance_mode	Character. Tolerance mode for precursor m/z: "ppm" or "mDa" (default: "mDa").
ion_mode	Character. Ionization mode: "positive" or "negative".
ionization_voltage	Character. Ionization voltage to use (default: "all").
spectra_types	Character. Spectra types: "experimental" or other supported types.
cmm_url	Character. URL for the CEU Mass Mediator API (default: "https://ceumass.eps.uspceu.es/api/msmssearch

Value

A dataframe containing the search results from the CEU Mass Mediator API.

Examples

```
## Not run:
ms_ms_peaks <- matrix(
  c(
    40.948, 0.174,
    56.022, 0.424,
    84.370, 53.488,
    101.500, 8.285,
    102.401, 0.775,
    129.670, 100.000,
    146.966, 20.070
  ),
  ncol = 2,
  byrow = TRUE
)

df <- msms_search(
  ion_mass = 147,
  ms_ms_peaks = ms_ms_peaks,
  ion_mode = "positive"
)

## End(Not run)
```

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