Package 'cmmr'

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Type Package

Title CEU Mass Mediator RESTful API

Version 0.1.2

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Depends R (>= 3.1.0)

Imports httr (>= 1.3.1), progress (>= 1.2.0), RJSONIO (>= 1.3-0)

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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/lzyacht/cmmr>.

License GPL-3

Encoding UTF-8

LazyData true

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

RoxygenNote 6.1.1

Suggests testthat

NeedsCompilation no

Repository CRAN

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R topics documented:

`advanced_batch_search` *Encapsulation of CEU Mass Mediator advanced batch search API.*

Description

`advanced_batch_search` returns the body string of a POST request. using the following code to install the dependencies: install.packages(c("httr", "progress", "RJSONIO"))

Usage

```
advanced_batch_search(cmm_url = paste0("http://ceumass.eps.uspceu.es/mediator/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 = "[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

`cmm_url`	'http://ceumass.eps.uspceu.es/mediator/api/v3/advancedbatch' or your local one
`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.

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Examples

```
df <- advanced_batch_search(
cmm_url             = paste0(
  'http://ceumass.eps.uspceu.es/mediator/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              = '[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 }]]'
))
```

batch_search *Encapsulation of CEU Mass Mediator batch search API*

Description

batch_search returns the dataframe of all the database search results. using the following code to install the dependencies: install.packages(c("httr", "progress", "RJSONIO"))

Usage

```
batch_search(cmm_url = "http://ceumass.eps.uspceu.es/mediator/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	'http://ceumass.eps.uspceu.es/mediator/api/v3/batch' or your local API Endpoint
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

dataframe for search results

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Examples

```
## Not run:
batch_search(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.

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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.

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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)
```

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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",
  ionizationVoltage = "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
ionizationVoltage	ionizationVoltage
spectra_types	spectra_types

Value

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

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msms_search *Encapsulation of CEU Mass Mediator batch search API.*

Description

batch_search returns the dataframe of all the database search results. using the following code to install the dependencies: install.packages(c("httr", "progress", "RJSONIO"))

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,
  ionizationVoltage = "all", spectra_types = "experimental",
  cmm_url = "http://ceumass.eps.uspceu.es/mediator/api/msmssearch")
```

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
ionizationVoltage	ionizationVoltage
spectra_types	spectra_types
cmm_url	"http://ceumass.eps.uspceu.es/mediator/api/msmssearch" or your local one

Value

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

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Examples

```
ms_ms_peaks = matrix(
c(40.948, 0.174,
  56.022, 0.424,
  84.37, 53.488,
  101.50, 8.285,
  102.401, 0.775,
  129.670, 100.000,
  146.966, 20.070),
ncol = 2,
byrow = TRUE)

msms_search(ion_mass = 147, ms_ms_peaks = ms_ms_peaks, ion_mode = 'positive')
```

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