Bio2BEL ChEBI Documentation

Release 0.2.2-dev

Charles Tapley Hoyt

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Contents:

A package for converting ChEBI to BEL.

CHAPTER 1

Installation

`bio2bel_chebi` can be installed easily from PyPI with the following code in your favorite terminal:

```
$ python3 -m pip install bio2bel_chebi
```

or from the latest code on GitHub with:

```
$ python3 -m pip install git+https://github.com/bio2bel/chebi.git@master
```

CHAPTER 2

Setup

ChEBI can be downloaded and populated from either the Python REPL or the automatically installed command line utility.

2.1 Python REPL

```
>>> import bio2bel_chebi
>>> chebi_manager = bio2bel_chebi.Manager()
>>> chebi_manager.populate()
```

2.2 Command Line Utility

```
bio2bel_chebi populate
```

CHAPTER 3

Manager

Manager for Bio2BEL ChEBI.

class bio2bel_chebi.manager.**Manager**(**args*, ***kwargs*)

Bio2BEL ChEBI Manager.

namespace_model

alias of bio2bel_chebi.models.Chemical

is_populated() → bool

Check if the database is already populated.

count_chemicals() → int

Count the number of chemicals stored.

count_parent_chemicals() → int

Count the number of parent chemicals stored.

count_child_chemicals() → int

Count the number of child chemicals stored.

count_xrefs() → int

Count the number of cross-references stored.

count_synonyms() → int

Count the number of synonyms stored.

count_inchis() → int

Count the number of inchis stored.

count_relations() → int

Count the relations in the database.

list_relations() → List[bio2bel_chebi.models.Relation]

List the relations in the database.

summarize() → Mapping[str, int]

Return a summary dictionary over the content of the database.

get_or_create_chemical(*chebi_id: str*, ***kwargs*) → bio2bel_chebi.models.Chemical
Get a chemical from the database by ChEBI.

get_chemical_by_chebi_id(*chebi_id: str*) → Optional[bio2bel_chebi.models.Chemical]
Get a chemical from the database.

get_chemical_by_chebi_name(*name: str*) → Optional[bio2bel_chebi.models.Chemical]
Get a chemical from the database.

build_chebi_id_name_mapping() → Mapping[str, str]
Build a mapping from ChEBI identifier to ChEBI name.

build_chebi_name_id_mapping() → Mapping[str, str]
Build a mapping from ChEBI name to ChEBI identifier.

populate(*inchis_url: Optional[str] = None*, *compounds_url: Optional[str] = None*, *relations_url: Optional[str] = None*, *names_url: Optional[str] = None*, *accessions_url: Optional[str] = None*) → None
Populate all tables.

iter_chemicals(*graph: pybel.struct.graph.BELGraph*) → Iterable[Tuple[pybel.dsl.node_classes.BaseEntity, bio2bel_chebi.models.Chemical]]
Iterate over pairs of BEL nodes and HGNC genes.

enrich_chemical_hierarchy(*graph: pybel.struct.graph.BELGraph*) → None
Enrich the parents for all ChEBI chemicals in the graph.

to_bel() → pybel.struct.graph.BELGraph
Export BEL.

CHAPTER 4

Constants

Constants for Bio2BEL ChEBI.

CHAPTER 5

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