
Bio2BEL ChEBI Documentation

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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
```


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
```


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

Indices and tables

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