# Bio2BEL DrugBank Documentation

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# CHAPTER 1

# Installation

`bio2bel_drugbank` can be installed easily from PyPI with the following code in your favorite terminal:

```
$ python3 -m pip install bio2bel_drugbank
```

or from the latest code on GitHub with:

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

# CHAPTER 2

# Setup

**Warning:** DrugBank requires a bit of downloading and file organization. Will be documented soon.

## 2.1 Python REPL

```
>>> import bio2bel_drugbank
>>> drugbank_manager = bio2bel_drugbank.Manager()
>>> drugbank_manager.populate()
```

## 2.2 Command Line Utility

```
bio2bel_drugbank populate
```

# CHAPTER 3

# Manager

Defines the Bio2BEL DrugBank manager.

**class** bio2bel_drugbank.manager.**Manager**(**args*, ***kwargs*)

Manager for Bio2BEL DrugBank.

**namespace_model**

alias of *bio2bel_drugbank.models.Drug*

**get_type_by_name**(*name: str*) → Optional[bio2bel_drugbank.models.Type]

Get a Type by name.

**get_or_create_type**(*name: str*) → bio2bel_drugbank.models.Type

Get or create a Type by name.

**list_groups**() → List[bio2bel_drugbank.models.Group]

List all chemical groups.

**get_group_by_name**(*name: str*) → Optional[bio2bel_drugbank.models.Group]

Get a Group by name.

**get_or_create_group**(*name: str*) → bio2bel_drugbank.models.Group

Get or create a Group by name.

**get_species_by_name**(*name: str*) → Optional[bio2bel_drugbank.models.Species]

Get a Species by name.

**get_or_create_species**(*name: str*) → bio2bel_drugbank.models.Species

Get or create a Species by name.

**get_category_by_name**(*name: str*) → Optional[bio2bel_drugbank.models.Category]

Get a Category by name.

**get_or_create_category**(*name: str*, ***kwargs*) → bio2bel_drugbank.models.Category

Get or create a Category by name.

**get_or_create_patent**(*country: str*, *patent_id: str*, ***kwargs*) → bio2bel_drugbank.models.Patent

Get or creates a Patent.

**is_populated**() → bool
Check if the database is populated by counting the drugs.

**populate**(*url: Optional[str] = None*) → None
Populate DrugBank.

**Parameters** **url** – Path to the DrugBank XML

**count_drugs**() → int
Count the number of drugs in the database.

**list_drugs**() → List[bio2bel_drugbank.models.Drug]
List all drugs in the database.

**count_types**() → int
Count the number of types in the database.

**count_aliases**() → int
Count the number of aliases in the database.

**count_atc_codes**() → int
Count the number of ATC codes in the database.

**count_groups**() → int
Count the number of groups in the database.

**count_categories**() → int
Count the number of categories in the database.

**count_drugs_categories**() → int
Count the number of drug-category relations in the database.

**count_drugs_groups**() → int
Count the number of drug-group relations in the database.

**count_patents**() → int
Count the number of patents in the database.

**list_patents**() → List[bio2bel_drugbank.models.Patent]
List the patents in the database.

**count_xrefs**() → int
Count the number of cross-references in the database.

**list_drug_protein_interactions**() → List[bio2bel_drugbank.models.DrugProteinInteraction]
List drug-protein interactions.

**summarize**() → Dict[str, int]
Summarize the database.

**enrich_targets**(*graph: pybel.struct.graph.BELGraph*) → None
Enrich the protein targets in the graph with Drug-Protein interactions from DrugBank.

**lookup_drug**(*node: pybel.dsl.node_classes.BaseEntity*) → Optional[bio2bel_drugbank.models.Drug]
Try and look up a drug.

**enrich_drug_inchi**(*graph: pybel.struct.graph.BELGraph*) → None
Enrich drugs in the graph with their InChI equivalent nodes.

**enrich_drug_equivalences**(*graph: pybel.struct.graph.BELGraph*) → None
Enrich drugs in the graph with their equivalent nodes.

**enrich_drugs**(*graph: pybel.struct.graph.BELGraph*) → None
Enrich drugs in the graph with their targets.

**to_bel**() → pybel.struct.graph.BELGraph
Export DrugBank as BEL.

**get_hgnc_id_to_drugs**() → Dict[str, List[str]]
Get a dictionary of HGNC identifiers (not prepended with HGNC:) to list of drug names.

**get_drug_to_hgnc_ids**(*cache=True*, *recalculate=False*) → Dict[str, List[str]]
Get a dictionary of drug names to lists HGNC identifiers (not prepended with HGNC:).

**get_drug_to_hgnc_symbols**(*cache=True*, *recalculate=False*) → Dict[str, List[str]]
Get a dictionary of drug names to HGNC gene symbols.

**get_interactions_by_hgnc_id**(*hgnc_id: str*) → List[bio2bel_drugbank.models.DrugProteinInteraction]
Get the drug targets for a given HGNC identifier.

# CHAPTER 4

# Models

Database models for bio2bel_drugbank.

**class** bio2bel_drugbank.models.**Base**(***kwargs*)

The most base type

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Type**(***kwargs*)

Represents the type of a drug - either small molecule or biologic.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Drug**(***kwargs*)

Represents a drug.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**as_bel**() → pybel.dsl.node_classes.Abundance

Get this drug as a PyBEL abundance identified by its DrugBank identifier.

**as_inchi_bel**() → pybel.dsl.node_classes.Abundance

Get this drug as a PyBEL abundance identified by InChI.

**as_inchikey_bel**() → pybel.dsl.node_classes.Abundance

Get this drug as a PyBEL abundance identified by InChI-key.

**as_cas_bel**() → pybel.dsl.node_classes.Abundance
Get this drug as a PyBEL abundance identified by its CAS identifier.

**class** bio2bel_drugbank.models.**DrugXref**(**kwargs)
Represents a drug's cross-reference to another database.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Patent**(**kwargs)
Represents a patent.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**google_url**
Return the Google Patents URL of this patent.

**class** bio2bel_drugbank.models.**Alias**(**kwargs)
Represents an alias of a drug.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**AtcCode**(**kwargs)
Represents an ATC code of a drug.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Group**(**kwargs)
Represents a drug group.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Category**(**kwargs)
Represents a drug category.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Species**(***kwargs*)

Represents a species.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Protein**(***kwargs*)

Represents a protein.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**as_bel**() → pybel.dsl.node_classes.Protein

Serialize as a PyBEL node with the UniProt namespace.

**class** bio2bel_drugbank.models.**Action**(***kwargs*)

Represents the action a drug takes in a drug-protein interaction.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**Article**(***kwargs*)

Represents an article in PubMed.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**class** bio2bel_drugbank.models.**DrugProteinInteraction**(***kwargs*)

Represents an interaction between a drug and a protein.

A simple constructor that allows initialization from kwargs.

Sets attributes on the constructed instance using the names and values in `kwargs`.

Only keys that are present as attributes of the instance's class are allowed. These could be, for example, any mapped columns or relationships.

**add_to_graph**(*graph: pybel.struct.graph.BELGraph*) → Set[str]

Add this interaction to the graph.

**Returns** A set of the hashes of the edges that were added

CHAPTER 5

# Indices and tables

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