
Bio2BEL Reactome Documentation

Release 0.2.4-dev

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Nov 18, 2020

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Bio2BEL Reactome is a package for enriching BEL networks with Reactome information by wrapping its RESTful API.

Reactome is a pathway database comprising established pathways between different species that contain genetic as well as chemical information. This package downloads pathway information from Reactome's API and store it in template data model relating genes and chemical to pathways. Moreover, the hierarchy of the pathways is maintained enabling pathway comparison and exploration in the [ComPath environment](#).

CITATION

- Fabregat, Antonio et al. The Reactome Pathway Knowledgebase. Nucleic Acids Research 44.Database issue (2016): D481–D487. PMC. Web. 6 Oct. 2017.
- Croft, David et al. The Reactome Pathway Knowledgebase. Nucleic Acids Research 42.Database issue (2014): D472–D477. PMC. Web. 6 Oct. 2017.

MANAGER

Database Manager and query functions

This module populates the tables of `bio2bel_reactome`.

```
class bio2bel_reactome.manager.Manager (*args, **kwargs)
    Protein-pathway and chemical-pathway memberships.

    Doesn't let this class get instantiated if the pathway_model.

    protein_model
        alias of bio2bel_reactome.models.Protein

    namespace_model
        alias of bio2bel_reactome.models.Pathway

    pathway_model
        alias of bio2bel_reactome.models.Pathway

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

    count_chemicals () → int
        Count the chemicals in the database.

    count_species () → int
        Count the species in the database.

    get_gene_sets (only_human: bool = False) → Mapping[str, Set[str]]
        Return pathway - genesets mapping.

    get_or_create_pathway (*, reactome_id: str, name: str, species:
        bio2bel_reactome.models.Species, chemicals: Optional[List[bio2bel_reactome.models.Chemical]])
        → bio2bel_reactome.models.Pathway
    Get a pathway from the database or creates it.
```

Parameters

- **reactome_id** – pathway identifier
- **name** – name of the pathway
- **species** – Species object
- **chemicals** – An optional list of chemicals that belong too this pathway

```
get_or_create_chemical (*, chebi_id: str, chebi_name: str) →
    bio2bel_reactome.models.Chemical
    Get a Chemical from the database or creates it.
```

Parameters

- **chebi_id** – ChEBI identifier
- **chebi_name** – ChEBI name

get_or_create_species (*, *taxonomy_id*: *str*, *name*: *str*) → *bio2bel_reactome.models.Species*
Get a Species from the database or creates it.

get_or_create_protein (*uniprot_id*: *str*, *hgnc_symbol*: *Optional[str] = None*, *hgnc_id*: *Optional[str] = None*) → *bio2bel_reactome.models.Protein*
Get a protein from the database or creates it.

Parameters

- **uniprot_id** – pathway identifier
- **hgnc_symbol** – name of the pathway
- **hgnc_id** – Species object

get_species_by_name (*species_name*: *str*) → *Optional[bio2bel_reactome.models.Species]*
Get a Species by its species_name.

Parameters **species_name** – name

get_pathway_names_to_ids (*only_human*: *bool = False*)
Return a dictionary of pathway names to ids.

Return type *dict[str, str]*

get_pathway_parent_by_id (*reactome_id*: *str*) → *Optional[bio2bel_reactome.models.Pathway]*
Get parent pathway by its reactome id.

Parameters **reactome_id** – reactome identifier

get_top_hiearchy_parent_by_id (*reactome_id*: *str*) → *Optional[bio2bel_reactome.models.Pathway]*
Get the oldest pathway at the top of the hierarchy a pathway by its reactome id.

Parameters **reactome_id** – reactome identifier

get_all_top_hierarchy_pathways () → *List[bio2bel_reactome.models.Pathway]*
Get all pathways without a parent (top hierarchy).

get_human_pathways () → *List[bio2bel_reactome.models.Pathway]*
Get human pathways.

get_pathways_by_species (*species_name*: *str*) → *Optional[List[bio2bel_reactome.models.Pathway]]*
Get pathways by species.

get_chemical_by_chebi_id (*chebi_id*: *str*) → *Optional[bio2bel_reactome.models.Chemical]*
Get chemical by ChEBI id.

get_protein_by_uniprot_id (*uniprot_id*: *str*) → *Optional[bio2bel_reactome.models.Protein]*
Get protein by UniProt id.

populate (*pathways_path*: *Optional[str] = None*, *pathways_hierarchy_path*: *Optional[str] = None*, *pathways_proteins_path*: *Optional[str] = None*, *pathways_chemicals_path*: *Optional[str] = None*) → *None*
Populate all tables.

Parameters

- **pathways_path** – url from pathway table file
- **pathways_hierarchy_path** – url from pathway hierarchy file

- `pathways_proteins_path` – url from pathway protein file
- `pathways_chemicals_path` – url from pathway chemical file

COMMAND LINE INTERFACE

The command line interface allows you to communicate with the package and perform basic functions such as:

- Populate the database: `python3 -m bio2bel_reactome populate`. By default this command populates the database only with human information. In order to populate all species pathway information you can add the “`-not-only-human`” argument. By default the database is reset every time is populated. However, another optional parameter “`-reset-db=False`”, allows you to avoid the reset. More logging can be activated by added “`-vv`” or “`-v`” as an argument.
- Drop the database: `python3 -m bio2bel_reactome drop`. More logging can be activated by added “`-vv`” or “`-v`” as an argument.
- Export gene sets as an excel file: `python3 -m bio2bel_reactome export`. By default, the excel will contain all pathways from all species. However, you can add the argument “`species`” and type the name of a particular one to get only those pathways (e.g., “`-species='Homo sapiens'`”). Since Reactome has a hierarchy pathway structure, you can get only the major pathways with the optional parameter “`-top-hierarchy`”.

CONSTANTS

This module contains all the constants used in this package.

This module contains all the constants used in bio2bel Reactome project.

MODELS

Database models.

Reactome database model.

```
class bio2bel_reactome.models.Species (**kwargs)
```

Species Table.

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.

name

NCBI taxonomy label

taxonomy_id

NCBI taxonomy identifier

```
class bio2bel_reactome.models.Protein (**kwargs)
```

Protein Table.

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.

to_pybel () → `pybel.dsl.node_classes.Protein`

Serialize to PyBEL node data dictionary.

```
class bio2bel_reactome.models.Chemical (**kwargs)
```

Chemical Table.

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.

to_pybel () → `pybel.dsl.node_classes.Abundance`

Serialize to PyBEL node data dictionary.

```
class bio2bel_reactome.models.Pathway (**kwargs)
```

A reactome pathway.

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.

WEB

This module contains the web application to explore the database

This module contains the flask-admin application to visualize the db.

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