
BioServices

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Citations If you use BioServices, please cite *Cokelaer et al, Bioinformatics (2013)*. See [bioinformatics link](#) for details.

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Source See <http://github.com/cokelaer/bioservices>.

Issues Please fill a report on [github](#)

Note: Contributions to implement new wrappers are more than welcome. See [BioServices wiki](#) to join the development, and the *Developer Guide* on how to implement new wrappers. Although contributors have their names in the header files, you can also look at the *Contributors* directly.

Overview and Installation

1.1 Overview

BioServices is a Python package that provides access to many Bioinformatics Web Services (e.g., UniProt) and a framework to easily implement Web Service wrappers (based on WSDL/SOAP or REST protocols).

The primary goal of **BioServices** is to use Python as a glue language to provide a programmatic access to Biological Web Services. By doing so, elaboration of new applications that combine several Web Services should be fostered.

One of the main philosophy of **BioServices** is to make use of the existing REST or SOAP/WSDL Web Services and therefore existing databases, not to re-invent new databases.

The first release of **BioServices** provides a wrapping to more than 18 Web Services (more if we consider **BioMart** and **PSICQUIC** portals that link to many other Web Services).

Here are only some of Web Services that are available in **BioServices**:

<code>bioservices.arrayexpress.ArrayExpress</code>	Interface to the ArrayExpress service
<code>bioservices.biomodels.BioModels</code>	Interface to the BioModels service
<code>bioservices.chembl.ChEMBL</code>	New ChEMBL API bioservices 1.6.0
<code>bioservices.chebi.ChEBI</code>	Interface to ChEBI
<code>bioservices.kegg.KEGG</code>	Interface to the KEGG service
<code>bioservices.muscle.MUSCLE</code>	Interface to the MUSCLE service.
<code>bioservices.pdb.PDB</code>	Interface to part of the PDB service
<code>bioservices.uniprot.UniProt</code>	Interface to the UniProt service
<code>bioservices.unichem.UniChem</code>	Interface to the UniChem service
<code>bioservices.ncbiblast.NCBIblast</code>	Interface to the NCBIblast service.
<code>bioservices.wikipathway.Wikipathway</code>	

Full list is available in the User Guide and Reference here below.

1.2 Installation

BioServices is available on [PyPi](#), the Python package repository. The following command should install **BioServices** and its dependencies automatically provided you have **pip** on your system:

```
pip install bioservices
```

If not, please see the external [pip installation page](#) or [pip installation](#) entry. You may also find information in the [troubleshooting page](#) section about known issues.

Regarding the dependencies, **BioServices** depends on the following packages: **BeautifulSoup4** (for parsing XML), **SOAPpy** and **suds** (to access to SOAP/WSDL services; suds is used by ChEBI only for which SOAPpy fails to correctly fetch the service) and **easydev**. All those packages should be installed automatically when using **pip** installer.

2.1 Quick Start

2.1.1 Introduction

BioServices provides access to several Web Services. Each service requires some expertise on its own. In this Quick Start section, we will neither cover all the services nor all their functionalities. However, it should give you a good overview of what you can do with **BioServices** (both from the user and developer point of views).

Before starting, let us remind what are Web Services. They provide an access to databases or applications via a web interface based on the SOAP/WSDL or the REST technologies. These technologies allow a programmatic access, which we take advantage in **BioServices**.

The REST technology uses URLs so there is no external dependency. You simply need to build a well-formatted URL and you will retrieve an XML document that you can consume with your preferred technology platform.

The SOAP/WSDL technology combines SOAP (Simple Object Access Protocol), which is a messaging protocol for transporting information and the WSDL (Web Services Description Language), which is a method for describing Web Services and their capabilities.

What methods are available for a given service

Usually most of the service functionalities have been wrapped and we try to keep the names as close as possible to the API. On top of the service methods, each class inherits from the BioService class (REST or WSDL). For instance REST service have the useful request method. Another nice function is the onWeb.

See also:

REST, WSDLService

What about the output ?

Outputs depend on the service and functionalities of the service. It can be heterogeneous. However, outputs are mostly XML formatted or in tabulated separated column format (TSV). When XML is returned, it is usually parsed via the BeautifulSoup package (for instance you can get all children using `getchildren()` function). Sometimes, we also convert output into dictionaries. So, it really depends on the service/functionality you are using.

Let us look at some of the Web Services wrapped in **BioServices**.

2.1.2 UniProt service

Let us start with the `UniProt` class. With this class, you can access to uniprot services. In particular, you can map an ID from a database to another one. For instance to convert the UniProtKB ID into KEGG ID, use:

```
>>> from bioservices.uniprot import UniProt
>>> u = UniProt(verbose=False)
>>> u.mapping(fr="ACC+ID", to="KEGG_ID", query='P43403')
{'P43403': ['hsa:7535']}
```

Note that the returned response from uniprot web service is converted into a list. The first two elements are the databases used for the mapping. Then, alternance of the queried element and the answer populates the list.

You can also search for a specific UniProtKB ID to get exhaustive information:

```
>>> print(u.search("P43403", frmt="txt"))
ID      ZAP70_HUMAN          Reviewed;          619 AA.
AC      P43403; A6NFP4; Q6PIA4; Q8IXD6; Q9UBS6;
DT      01-NOV-1995, integrated into UniProtKB/Swiss-Prot.
DT      01-NOV-1995, sequence version 1.
...

```

To obtain the FASTA sequence, you can use `searchUniProtId()`:

```
>>> res = u.searchUniProtId("P09958", frmt="xml")
>>> print(u.searchUniProtId("P09958", frmt="fasta"))
sp|P09958|FURIN_HUMAN Furin OS=Homo sapiens GN=FURIN PE=1 SV=2
MELRPWLLWVVAATGTLVLLAADAQGQKVFTNTWAVRIPGGPAVANSVARKHGFLNLGQI
FGDYHFWHRGVTKRSLSPHRPHRSRLQREPQVQWLEQQVAKRRTKRDRVYQEP TDPKFPQ
QWYLSGVTQRDLNVKAAWAQGYTGHGIVVSILDDGIEKNHPDLAGNYDPGASFVNDQDP
DPQPRYTQMNDNRHGTRCAGEVAAVANNGVCGVGVAYNARIGGVRMLDGEVTD AVEARSL
GLNPNHIHIYSASWGPEDDGKTVDGPARLAEAEAFRQVSVQGRGGLGSIFVWASGNGGREH
DSCNCDGYTNSIYTLSSISSATQFGNVPWYSEACSSTLATTYSSGNQNEKQIVTTDLRQKC
TESHTGTSASAPLAAGI IALTLEANKNLTWRDMQHLVVQTSKPAHLNANDWATNGVGRKV
SHSYGYGLLDAGAMVALAQNWTTVAPQRKCIIDILTEPKDIGKRLEVRKTVTACLGEPNH
ITRLEHAQARLTLNRRGDLAIHLVSPMGTRSTLLAARPHDYSADGFNDWAFMTTHSWD
EDPSGEWVLEIENTSEANNYGTLTKFTLVLYGTAPPEGLPVPPESGCKTLTSSQACVVCE
EGFSLHQKSCVQHCPGPFAPQVLDTHYSTENDVETIRASVCAPCHASCATCQGPALTDCL
SCPSHASLDPVEQTCSRQSQSSRESPPQQQPPRLPPEVEAGQRLRAGLLPSHLPEVVAGL
SCAFIVLVFVTVFLVLQLRSGFSFRGVKVTMDRGLISYKGLPPEAWQECPDSEDEG
RGERTAFIKDQSAL
```

See also:

Reference guide of `bioservices.uniprot.UniProt` for more details

2.1.3 KEGG service

The KEGG interface is similar but contains more methods. The tutorial presents the KEGG interface in details, but let us have a quick overview. First, let us start a KEGG instance:

```
from bioservices import KEGG
k = KEGG(verbose=False)
```

KEGG contains biological data for many organisms. By default, no organism is set, which can be checked in the following attribute

```
k.organism
```

We can set it to human using KEGG terminology for homo sapiens:

```
k.organis = 'hsa'
```

You can use the `dbinfo()` to obtain statistics on the **pathway** database:

```
>>> print(k.info("pathway"))
pathway      KEGG Pathway Database
path         Release 65.0+/01-15, Jan 13
            Kanehisa Laboratories
            218,277 entries
```

You can see the list of valid databases using the `databases` attribute. Each of the database entry can also be listed using the `list()` method. For instance, the organisms can be retrieved with:

```
k.list("organism")
```

However, to extract the Ids extra processing is required. So, we provide aliases to retrieve the organism Ids easily:

```
k.organismIds
```

The human organism is coded as “hsa”. You can also get its T number instead:

```
>>> k.code2Tnumber("hsa")
'T01001'
```

Every elements is referred to with a KEGG ID, which may be difficult to handle at first. There are methods to retrieve the IDs though. For instance, get the list of pathways iIs for the current organism as follows:

```
k.pathwayIds
```

For a given gene, you can get the full information related to that gene by using the method `get()`:

```
print(k.get("hsa:3586"))
```

or a pathway:

```
print(k.get("path:hsa05416"))
```

See also:

Reference guide of `bioservices.kegg.KEGG` for more details

See also:

[KEGG Tutorial](#) for more details

See also:

Reference guide of `bioservices.kegg.KEGGParser` to parse a KEGG entry into a dictionary

2.1.4 QuickGO

To access the GO interface, simply create an instance and look for an entry using the `bioservices.quickgo.QuickGO.Term()` method:

```
>>> from bioservices import QuickGO
>>> g = QuickGO(verbose=False)
>>> print(g.Term("GO:0003824", frmt="obo"))
[Term]
id: GO:0003824
name: catalytic activity
def: "Catalysis of a biochemical reaction at physiological temperatures. In
biologically catalyzed reactions, the reactants are known as substrates, and the
catalysts are naturally occurring macromolecular substances known as enzymes.
Enzymes possess specific binding sites for substrates, and are usually composed
wholly or largely of protein, but RNA that has catalytic activity (ribozyme) is
often also regarded as enzymatic."
synonym: "enzyme activity" exact
xref: InterPro:IPR000183
...
```

See also:

Reference guide of `bioservices.quickgo.QuickGO` for more details

2.1.5 PICR service

PICR, the Protein Identifier Cross Reference service provides 2 services in WSDL and REST protocols. When it is the case, we arbitrarily chose one of the available protocols. In the PICR case, we implemented only the REST interface. The methods available in the REST service are very similar to those available via SOAP except for one major difference: only one accession or sequence can be mapped per request.

The following example returns a XML document containing information about the protein P29375 found in two specific databases:

```
>>> from bioservices.picr import PICR
>>> p = PICR()
>>> res = p.getUPIForAccession("P29375", ["IPI", "ENSEMBL"])
```

See also:

Reference guide of `bioservices.picr.PICR` for more details

2.1.6 BioModels service

You can access the biomodels service and obtain a model as follows:

```
>>> from bioservices import biomodels
>>> b = biomodels.BioModels()
>>> model = b.get_model('BIOMD0000000299')
```

Then you can play with the SBML file with your favorite SBML tool.

In order to get the model IDs, you can look at the full list:

```
>>> b.get_models()
```

See also:

Reference guide of *bioservices.biomodels.BioModels* for more details

See also:

Biomodels tutorial for more details

2.1.7 Rhea service

Create a *Rhea* instance as follows:

```
from bioservices import Rhea
r = Rhea()
```

Rhea provides only 2 type of requests with a REST interface that are available with the *search()* and *entry()* methods. Let us first find information about the chemical product **caffeine** using the *search()* method:

```
xml_response = r.search("caffeine*")
```

The output is in XML format. Python provides lots of tools to deal with xml so you can surely find good tools.

Within bioservices, we wrap all returned XML documents into a BeautifulSoup object that ease the manipulation of XML documents.

As an example, we can extract all fields “id” as follows:

```
>>> [x.getText() for x in xml_response.findAll("id")]
[u'27902', u'10280', u'20944', u'30447', u'30319', u'30315', u'30311', u'30307']
```

The second method provided is the *entry()* method. Given an Id, you can query the Rhea database using Id found earlier (e.g., 10280):

```
>>> xml_response = r.entry(10280, "biopax2")
```

Warning: the *r.entry* output is also in XML format but we do not provide a specific XML parser for it unlike for the “search” method.

output format can be found in

```
>>> r.format_entry
['cmlreact', 'biopax2', 'rxn']
```

See also:

Reference guide of *bioservices.rhea.Rhea* for more details

2.1.8 Other services

There are many other services provided within **BioServices** and the reference guide should give you all the information available with examples to start to play with any of them. The home page of the services themselves is usually a good starting point as well.

Services that are not available in **BioServices** can still be accessed to quite easily as demonstrated in the *Developer Guide* section.

2.2 Tutorials

This section present the KEGG and BioModels services in more details. The Protein test case study illustrates how several services can be used to get lots of information about a specific protein. New Contributino to this section are welcomed.

Contents

- *KEGG Tutorial*
 - *Introduction*
 - *Searching for an organism*
 - *Look for pathways (by name)*
 - *Look for pathway (by genes i.e., IDs or usual name)*
 - *Introspecting a pathway*
 - *Building a histogram of all relations in human pathways*

2.2.1 KEGG Tutorial

Introduction

Start a kegg interface (default organism is human, that is called **hsa**):

```
from bioservices.kegg import KEGG
k = KEGG()
```

KEGG has many databases. The list can be found in the attribute `bioservices.kegg.KEGG.databases`. Each database can be queried with the `bioservices.kegg.KEGG.list()` method:

```
k.list("organism")
```

The output contains Id of the organism and some other information. To retrieve the Ids, you will need to process the output. However, we provide an alias:

```
print(k.organismIds)
```

In general, methods require an access to the on-line KEGG database therefore it takes time. For instance, the command above takes a couple of seconds. However, some are buffered so next time you call it, it will be much faster.

Another useful alias is the **pathwayIds** to retrieve all pathway Ids. However, you must first specify the organism you are interested in. From the command above we know that **hsa** (human) is valid organism Id, so let us set it and then get the list of pathways:

```
k.organism = "hsa"
k.pathwayIds
```

Another function provided by the KEGG API is the `bioservices.kegg.KEGG.get()` one that query a specific entry. Here we are interested into the human gene with the code 7535:

```
k.get("hsa:7535")    #hsa:7535 is also known as ZAP70
```

It is quite verbose and is a single string, which may be tricky to handle. We provide a tool to ease the parsing (see below and `bioservices.kegg.KEGG.parse()`) returned by `bioservices.kegg.KEGG.parse()`.

Searching for an organism

The method `bioservices.kegg.KEGG.find()` is quite convenient to search for entries in different database. For instance, if you want to know the code of an entry for the gene called ZAP70 in the human organism, type:

```
>>> s.find("hsa", "zap70")
'hsa:7535\tZAP70, SRK, STCD, STD, TZK, ZAP-70; zeta-chain (TCR) associated protein_
↪kinase 70kDa (EC:2.7.10.2); K07360 tyrosine-protein kinase ZAP-70 [EC:2.7.10.2]\n'
```

It is quite powerful and more examples will be shown. However, it has some limitations. For example, what about searching for the organism Ids that correspond to any *Drosophila*? It does not look like it is possible. BioServices provides a method to search for an organism Id using `lookfor_organism()` given the name (or part of it):

```
>>> k.lookfor_organism("droso")
['T00030 dme Drosophila melanogaster (fruit fly) Eukaryotes;Animals;Arthropods;Insects
↪',
'T01032 dpo Drosophila pseudoobscura pseudoobscura Eukaryotes;Animals;Arthropods;
↪Insects',
'T01059 dan Drosophila ananassae Eukaryotes;Animals;Arthropods;Insects',
'T01060 der Drosophila erecta Eukaryotes;Animals;Arthropods;Insects',
'T01063 dpe Drosophila persimilis Eukaryotes;Animals;Arthropods;Insects',
'T01064 dse Drosophila sechellia Eukaryotes;Animals;Arthropods;Insects',
'T01065 dsi Drosophila simulans Eukaryotes;Animals;Arthropods;Insects',
'T01067 dwi Drosophila willistoni Eukaryotes;Animals;Arthropods;Insects',
'T01068 dya Drosophila yakuba Eukaryotes;Animals;Arthropods;Insects',
'T01061 dgr Drosophila grimshawi Eukaryotes;Animals;Arthropods;Insects',
'T01062 dmo Drosophila mojavensis Eukaryotes;Animals;Arthropods;Insects',
'T01066 dvi Drosophila virilis Eukaryotes;Animals;Arthropods;Insects']
```

Look for pathways (by name)

Searching for pathways is quite similar. You can use the **find** method as above:

```
>>> print(s.find("pathway", "B+cell"))
path:map04112    Cell cycle - Caulobacter
path:map04662    B cell receptor signaling pathway
path:map05100    Bacterial invasion of epithelial cells
path:map05120    Epithelial cell signaling in Helicobacter pylori infection
path:map05217    Basal cell carcinoma
```

Note that without the + sign, you get all pathway that contains *B* or *cell*. Yet, we have 5 results, which do not necessarily fit our request. Alternatively you can use one of BioServices method:

```
>>> k.lookfor_pathway("B cell")
['path:map04662 B cell receptor signaling pathway']
```

You can also search for a pathway knowing some gene names but first we need to introspect the pathway to get the genes IDs.

Look for pathway (by genes i.e., IDs or usual name)

Imagine you want to find the pathway that contains **ZAP70**. As we have seen earlier you can get its gene Id as follows:

```
>>> s.find("hsa", "zap70")
hsa:7535
```

The following commands do not help:

```
>>> s.find("pathway", "zap70")
>>> s.find("pathway", "hsa:7535")
>>> s.find("pathway", "7535")
```

We provide a method to search for pathways that contain the required gene Id. You can search by KEGG Id or gene name:

```
>>> res = s.get_pathway_by_gene("7535", "hsa")
>>> s.get_pathway_by_gene("zap70", "hsa")
['path:hsa04064', 'path:hsa04650', 'path:hsa04660', 'path:hsa05340']
```

This commands first search for the gene Id in the KEGG database and then parse the output to retrieve the pathways.

Introspecting a pathway

Let us focus on one pathway (**path:hsa04660**). You can use the `get ()` command to obtain information about the pathway.

```
print(s.get("hsa04660"))
```

The output is a single string where you can recognise different fields such as NAME, GENE, DESCRIPTION and so on. This is quite limited. In BioServices, we provide a convenient parser that converts the output of the previous command into a dictionary:

```
>>> s = KEGG()
>>> data = s.get("hsa04660")
>>> dict_data = s.parse(data)
>>> print(dict_data['GENE'])
'10000': 'AKT3; v-akt murine thymoma viral oncogene homolog 3 (protein kinase B, γ
↳gamma) [KO:K04456] [EC:2.7.11.1]',
'10125': 'RASGRP1; RAS guanyl releasing protein 1 (calcium and DAG-regulated) γ
↳[KO:K04350]',
'1019': 'CDK4; cyclin-dependent kinase 4 [KO:K02089] [EC:2.7.11.22]',
...
```

This is fine if we just want the name of the genes but what about their relations? Actually, there is an option with the `get` method where you can specify the output format. In particular you can request the pathway to be returned as a `kgml` file:


```
res = s.get("hsa04660", "kgml")
```

This file can be parsed to extract the relations. We provide a tool to do that:

```
res = s.parse_kgml_pathway("hsa04660")
```

The variable returned is a dictionary with 2 keys: “entries” and “relations”.

You can extract the relations as follows:

```
res['relations']
```

It is a list of relations, each relation being a dictionary:

```
>>> res['relations'][0]
{'entry1': u'61',
 'entry2': u'63',
 'link': u'PPrel',
 'name': u'binding/association',
 'value': u'---'}
```

Here entry1 and 2 are Ids. The Ids can be found in

```
res['entries']
```

From there you should consult *bioservices.kegg.KEGG.parse_kgml_pathway()* and the KEGG document for more information. You may also look at *bioservices.kegg.KEGG.pathway2sif()* method that extract only protein-protein interactions with activation and inhibition links only.

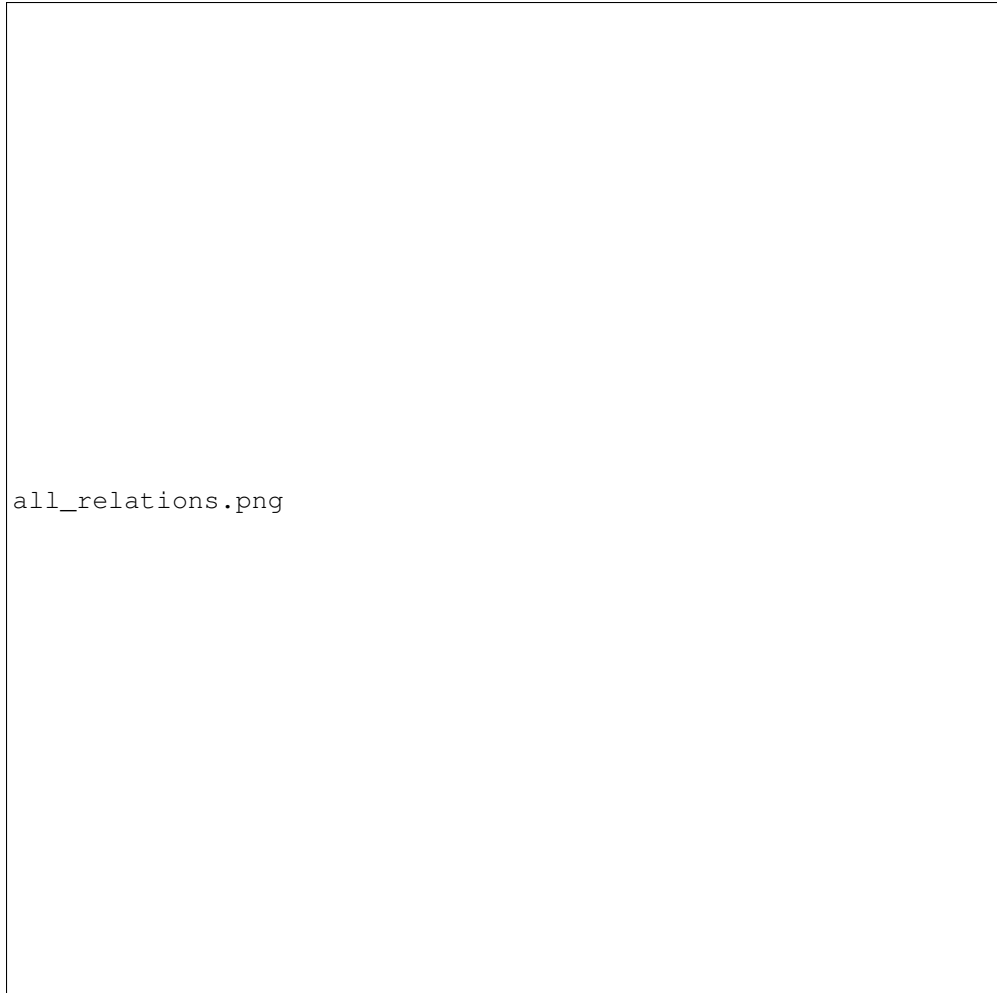
Building a histogram of all relations in human pathways

Scanning all relations of the Human organism takes about 5-10 minutes. You can look at a subset by setting Nmax to a small value (e.g., Nmax=10).

```
from pylab import *
# extract all relations from all pathways
from bioservices.kegg import KEGG
s = KEGG()
s.organism = "hsa"

# retrieve more than 260 pathways so it takes time
results = [s.parse_kgml_pathway(x) for x in s.pathwayIds]
relations = [x['relations'] for x in results]

hist([len(r) for r in relations], 20)
xlabel('number of relations')
ylabel('\#')
title("number of relations per pathways")
grid(True)
```



all_relations.png

You can then extract more information such as the type of relations:

```
>>> # scan all relations looking for the type of relations
>>> import collections # for python 2.7.0 and above

>>> # we extract from all pathways, all relations, where we retrieve the type of
>>> # relation (name)
>>> data = list(flatten([[x['name'] for x in rel] for rel in relations]))

>>> counter = collections.Counter(data)
>>> print(counter)
Counter({u'compound': 5235, u'activation': 3265, u'binding/association': 1087,
u'phosphorylation': 940, u'inhibition': 672, u'indirect effect': 559,
u'expression': 542, u'deposphorylation': 93, u'missing interaction': 80,
u'dissociation': 78, u'ubiquitination': 48, u'state change': 24, u'repression':
12, u'methylation': 2})
```

See also:

bioservices.biomodels.BioModels for the full reference guide.

2.2.2 Biomodels tutorial

Start a biomodels interface:

```
>>> from bioservices import BioModels
>>> s = BioModels()
```

look at the list of model identifiers:

```
models = s.get_all_models()
```

If you have a specific model identifier, then it is easy. You can retrieve the model itself:

```
model = s.get_model("BIOMD0000000100")
```

and get its name or other types of information:

```
>>> model['name']
Rozi2003_GlycogenPhosphorylase_Activation
```

In particular, description, author and files associated with this model. Here, we can see the files and in particular a PNG image called **BIOMD0000000100.png**. You can get it as follows:

```
model.get_model_download("BIOMD0000000100", filename="BIOMD0000000100.png")
```

or just download the whole bundle:

```
model.get_model_download("BIOMD0000000100")
```

saved into **BIOMD0000000100.zip**.

2.2.3 Protein test case study

Application: retrieving information about a given protein

This section uses BioServices to demonstrate the interest of combining several services together within a single framework using the Python language as a glue language.

In this tutorial we are interested in using **BioServices** to obtain information about a specific protein. Let us focus on ZAP70 protein (homo sapiens).

Get a unique identifier and gene names from a name

From **Uniprot**, we can obtain the unique accession number of ZAP70, which may be useful later on. Let us try to use the `search()` method:

```
>>> from bioservices import *
>>> u = UniProt(verbose=False)
>>> u.search("ZAP70_HUMAN") # could be lower case
```

The default format of the returned answer is “tabulated”:

```
>>> res = u.search("ZAP70_HUMAN", frmt="tab")
>>> print(res)
Entry   Entry name   Status   Protein names   Gene names   Organism   Length
P43403  ZAP70_HUMAN  reviewed Tyrosine-protein kinase ZAP-70 (EC 2.7.10.2) (70 kDa,
↳zeta-chain associated protein) (Syk-related tyrosine kinase)   ZAP70 SRK Homo_
↳sapiens (Human)      619
```

It is better, but let us simplify even further. In **BioServices**, the output of the tabulated format contains several columns but we can select only a subset such as the Entry (accession number) and the gene names, which are coded as “id” and “genes” in uniprot database:

```
>>> res = u.search("ZAP70_HUMAN", frmt="tab", columns="id,genes")
>>> print(res)
Entry   Gene names
P43403  ZAP70 SRK
```

So here we got the Entry P43403. Entry and Gene names can be saved in two variables as follows:

```
>>> res = u.search("ZAP70_HUMAN", frmt="tab", columns="id,genes")
>>> entry, gene_names = res.split("\n")[1].split("\t")
```

Getting the fasta sequence

It is then straightforward to obtain the FASTA sequence of ZAP70 using another method from the UniProt class called *retrieve()*:

```
>>> sequence = u.retrieve("P43403", "fasta")
>>> print(sequence)
>sp|P43403|ZAP70_HUMAN Tyrosine-protein kinase ZAP-70 OS=Homo sapiens GN=ZAP70 PE=1_
↳SV=1
MPDPAAHLPPFFYGSISRAEAEHLKLAGMADGLFLLRQCLRSLLGGYVLSLVHDVRFHHFP
IERQLNGTYAIAGGKAHCGLPAELCEFYSRDPDGLPCNLKPCNRPSGLEPQPGVFDCLRD
AMVRDYVRQTWKLEGEALEQAIISQAPQVEKLIATTAHERMPWYHSSLTREEAERKLYSG
AQTGKFLLRPRKEQGTIALSLIYGKTVYHYLISQDKAGKYCIPEGTKFDTLWQLVEYLK
LKADGLIYCLKEACPNSASNASGAAAPTLPAPSTLTHPQRRIDTLNSDGYTPEPARIT
SPDKPRPMPMDTSVYESPYSDPEELKDKKLFKRDNLLIADIELGCGNFGSVRQGVYRMR
KKQIDVAIKVLKQGTEKADTEEMMREAQIMHQLDNPYIVRLIGVCQAEALMLVMEMAGGG
PLHKFLVGVKREEIPVSNVAELLHQVSMGMKYLEEKNFVHRDLAARNVLLVNRHYAKISDF
GLSKALGADDSYYTARSAGKWPLKWYAPECINFRKFSSRSVWSYGVTMWEALSYGQKPY
KKMKGPEVMAFIEQGKRMECPPECPPELYALMSDCWIYKWEDRPDFLTVEQRMACYYSL
ASKVEGPPGSTQKAEACA
```

Note: There are many services that provides access to the FASTA sequence. We chose uniprot but you could use the Entrez utilities as well as other services.

Using BLAST on the sequence

You can then analyse this sequence with your favorite tool. As an example, within **BioServices** you can use `NCIBlast` but first let us extract the sequence itself (without the header):

```
sequence = sequence.split("\n", 1)[1].strip("\n")
```

then,

```

>>> s = NCBIblast(verbose=False)
>>> jobid = s.run(program="blastp", sequence=sequence, stype="protein", \
...     database="uniprotkb", email="cokelaer@ebi.ac.uk")
>>> print(s.getResult(jobid, "out")[0:1000])
BLASTP 2.2.26 [Sep-21-2011]

Reference: Altschul, Stephen F., Thomas L. Madden, Alejandro A. Schaffer,
Jinghui Zhang, Zheng Zhang, Webb Miller, and David J. Lipman (1997),
"Gapped BLAST and PSI-BLAST: a new generation of protein database search
programs", Nucleic Acids Res. 25:3389-3402.

Query= EMBOSS_001
      (619 letters)

Database: uniprotkb
      32,727,302 sequences; 10,543,978,207 total letters

Searching.....done

Sequences producing significant alignments:

                                     Score   E
                                     (bits) Value
SP:ZAP70_HUMAN P43403 Tyrosine-protein kinase ZAP-70 OS=Homo sap... 1279 0.0
TR:H2QIE3_PANTR H2QIE3 Tyrosine-protein kinase OS=Pan troglodyte... 1278 0.0
TR:G3QGN8_GORGO G3QGN8 Tyrosine-protein kinase OS=Gorilla gorill... 1278 0.0
TR:G1QLX3_NOMLE G1QLX3 Tyrosine-protein kinase OS=Nomascus leuco... 1249 0.0
TR:F6SWY7_CALJA F6SWY7 Tyrosin

```

The last command waits for the job to be finished before printing the results, which may be quite long. We could look at the beginning of the reported results and select only HUMAN sequences to see that the best sequence found is indeed ZAP70_HUMAN as expected:

```

>>> [x for x in s.getResult(jobid, "out").split("\n") if "HUMAN" in x]
['SP:ZAP70_HUMAN P43403 Tyrosine-protein kinase ZAP-70 OS=Homo sap... 1279 0.0 ',
 'SP:KSYK_HUMAN P43405 Tyrosine-protein kinase SYK OS=Homo sapiens... 691 0.0 ',
 'TR:A8K4G2_HUMAN A8K4G2 Tyrosine-protein kinase OS=Homo sapiens P... 691 0.0 ',
 ...

```

Searching for relevant pathways

The KEGG services provides pathways, so let try to find pathways that contains our targetted protein. First we need to know the KEGG Id that corresponds to ZAP70. We can use the `find` method form KEGG service:

```

>>> from bioservices import KEGG
>>> k = KEGG(verbose=False)
>>> k.find("hsa", "zap70") # "hsa" stands for homo sapiens
hsa:7535 ZAP70, SRK, STCD, STD, TZK, ZAP-70; zeta-chain (TCR) associated protein_
↪kinase 70kDa (EC:2.7.10.2); K07360 tyrosine-protein kinase ZAP-70 [EC:2.7.10.2

```

There are other ways to perform this conversion using the `bioservices.uniprot.UniProt.mapping()` or `bioservices.KEGG.conv()` methods (e.g., `textit{k.conv("hsa", "up:P43403")}`).

Now, let us get the pathways that contains this ID:

```
>>> k.get_pathway_by_gene("7535", "hsa")
{'hsa04064': 'NF-kappa B signaling pathway',
 'hsa04650': 'Natural killer cell mediated cytotoxicity',
 'hsa04660': 'T cell receptor signaling pathway',
 'hsa05340': 'Primary immunodeficiency'}
```

We can look at the first pathway in a browser (highlighting the ZAP70 node):

```
>>> k.show_pathway("hsa04064", keggid={"7535": "red"})
```

Searching for binary Interactions

For this purpose, we could use PSICQUIC services to find the interactions that involve ZAP70 in the **mint** database:

```
>>> from bioservices import PSICQUIC
>>> s = PSICQUIC(verbose=False)
>>> data = s.query("mint", "ZAP70 AND species:9606")
```

where 9606 is the taxonomy Id for homo sapiens. We could also figure out how many interactions could be found in each database for this particular query:

```
>>> s.getInteractionCounter("zap70 AND species:9606")
{'apid': 82,
 'bar': 0,
 'bind': 4,
 'bindingdb': 29,
 'biogrid': 73,
 'chembl': 161,
 'dip': 0,
 'i2d-imex': 0,
 'innatedb': 13,
 'innatedb-imex': 0,
 'intact': 11,
 'interoporc': 0,
 'irefindex': 273,
 'matrixdb': 0,
 'mbinfo': 0,
 'mint': 34,
 'molcon': 0,
 'mpidb': 0,
 'reactome': 0,
 'reactome-fis': 134,
 'spike': 47,
 'string': 319,
 'topfind': 0,
 'uniprot': 0}
```

We see for instance that the **mint** database has 34 interactions. Coming back to the interactions returned by `s.query`, we find indeed 34 interactions between ZAP70 and another component:

```
>>> len(data)
34
```

Let us look at the first one:

```
>>> for x in data[0]: print(x)
uniprotkb:P15498
uniprotkb:P43403
-
-
uniprotkb:VAV1(gene name)|uniprotkb:VAV(gene name synonym)
uniprotkb:ZAP70(gene name)|uniprotkb:SRK(gene name synonym)|uniprotkb:70 kDa
zeta-associated protein(gene name synonym)|uniprotkb:Syk-related tyrosine
kinase(gene name synonym)
psi-mi:"MI:0019"(coimmunoprecipitation)
-
pubmed:9151714
taxid:9606(Homo sapiens)
taxid:9606(Homo sapiens)
psi-mi:"MI:0914"(association)
psi-mi:"MI:0471"(mint)
mint:MINT-8035351
mint-score:0.28(free-text)|homomint-score:0.28(free-text)'intact-miscore:0.60']
```

The First two elements are the entries for specy A and B. The last element is the score. The 11th element is the type of interaction and so on.

What could be useful is to convert these elements into uniprot ID only. With mint database it is irrelevant for this particular entry but with other DBs or entries, it may be useful (e.g., biogrid).

BioServices provides such a function called `convert()`:

```
>>> data = s.query("biogrid", "ZAP70 AND species:9606")
>>> data2 = s.convert(data, "biogrid")
```

Warning: some databases may be offline. If so, try we another database. Type “s.activeDBs”.

convert method converts all entries from data into uniprot ID. If this is not possible, the entry is removed. The **query** and **convert** works on a single database but you we could query all or a subset of all databases using the `queryAll` and `convertAll` functions:

```
>>> data = s.queryAll("ZAP70 AND species:9606", databases=["mint", "biogrid"])
>>> data2 = s.convertAll(data)
```

However, extra cleaning is required to remove entries that are not relevant (no match to uniprot ID, redundant, not a protein, self interactions, ...). In order to ease this tast, the `psicquic.AppsPPI` class is very useful.

```
from bioservices import psicquic
s = psicquic.AppsPPI()
s.queryAll("ZAP70 AND species:9606", databases=["mint", "biogrid", "intact",
↪"reactome-fis"])
s.summary()
s.show_pie()
```

The `summary` function print a useful summary about the number of found interactions and overlap between databases:

```
>>> s.summary()
Found 8 interactions within intact database
Found 124 interactions within reactome-fis database
Found 19 interactions within mint database
```

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```

Found 67 interactions within biogrid database
-----
Found 152 interactions in 1 common databases
Found 14 interactions in 2 common databases
Found 0 interactions in 3 common databases
Found 1 interactions in 4 common databases

```

This may be different depending on the available databases. Finally, you can obtain the relation that was found in the 4 databases:

```

>>> s.relevant_interactions[4]
[['LCK_HUMAN', 'ZAP70_HUMAN']]

```

What's next ?

There are lots of other services that could be usefule. An example is the wikipathway (see [Wikipathway](#)) to retrieve even more pathways that include the ZAP70 protein. Another example is the BioMart portal. You could use it to retrieve pathways from REACTOME (see [BioMart](#)). You can also retrieve target from ChEMBL given the uniprot ID (`get_target_by_uniprotId("P43403")`) and so on.

2.2.4 Manipulating compound identifiers

Application: retrieving information about a compound

This section uses BioServices to demonstrate the interest of combining several services together within a single framework using the Python language as a glue language

Retrieve a compound identifier from KEGG, ChEBI and ChEMBL

Let us look at a compound called **Geldanamycin** that inhibits Hsp90. Let us search for information about that compound in several databases and manipulate the different identifiers.

First, let us retrieve information on KEGG database:

```

>>> from bioservices import *
>>> k = KEGG(verbose=False)

```

KEGG compounds have links to other databases. It is not systematic but the ChEBI database is often referenced. So we will want to convert the KEGG identifier to a ChEBI identifier. Later, we can convert a ChEBI to a ChEMBL identifier using another Web Service such as UniChem.

We can get a mapping dictionary from the KEGG compound to ChEBI as follows:

```

>>> map_kegg_chebi = k.conv("chebi", "compound")
>>> len(map_kegg_chebi)
15845

>>> print(k.find("compound", "geldanamycin"))
cpd:C11222  Geldanamycin
cpd:C15823  Progeldanamycin

```


Let us look at the first one (KEGG id cpd:C11222). We can get lots of information from KEGG already by using:

```
>>> print(k.get("C11222"))
```

From which, there is a link to other databases in particular ChEBI (ChEBI:5292). We could use the mapping dictionary created above:

```
>>> map_kegg_chebi['cpd:C11222']
'chebi:5292'
```

Unfortunately, there is no mapping function from KEGG to ChEMBL in KEGG Web Service.

However, BioServices provides access to the *bioservices.unichem* service. This service provides a useful mapping function from kegg to chembl:

```
>>> uni = UniChem()
>>> mapping = uni.get_mapping("kegg_ligand", "chembl")
>>> mapping['C11222']
'CHEMBL278315'
```

For sanity check, let us see that the ChEBI is indeed 5292 as given within the KEGG database:

```
>>> uni = UniChem()
>>> mapping = uni.get_mapping("kegg_ligand", "chebi")
>>> mapping['C11222']
'5292'
```

(2) In order to convert KEGG gene names into uniprot gene name, we can also use the UniProt web service from BioServices as follows:

```
>>> from bioservices import *
>>> u = UniProt()
>>> u.mapping(fr='ID', to='KEGG_ID', query="ZAP70_HUMAN")
{'ZAP70_HUMAN': 'hsa:7535'}
```

You can get accession number or protein name identifier from the KEGG identifier as follows:

```
>>> u.mapping(fr='KEGG_ID', to='ID', query='hsa:7535')
{'hsa7535': 'ZAP70_HUMAN'}
>>> u.mapping(fr='KEGG_ID', to='ACC', query='hsa:7535')
{'hsa7535': 'P43403'}
```

2.2.5 Mapping identifiers

There are quite a few functions from different Web Services that can help to map identifiers from one database to the other. This tutorial presents some of them.

Convert from KEGG ID to ChEBI (compound)

```
>>> from bioservices import *
>>> k = KEGG(verbose=False)
>>> map_kegg_chebi = k.conv("chebi", "compound")
>>> map_kegg_chebi['cpd:C11222']
'chebi:5292'
```

you could also use `bioservices.unichem.UniChem` (see below).

Convert from KEGG ID to ChEMBL (compound)

```
>>> from bioservices import UniChem
>>> uni = UniChem()
>>> mapping = uni.get_mapping("kegg_ligand", "chembl")
>>> mapping["C11222"]
'CHEMBL278315'
```

convert from KEGG ID to UniProt and vice versa (gene)

In order to convert KEGG gene names into uniprot gene name, we can also use the UniProt web service from BioServices as follows:

```
>>> from bioservices import *
>>> u = UniProt()
>>> u.mapping(fr='ID', to='KEGG_ID', query="ZAP70_HUMAN")
['From:ID', 'To:KEGG_ID', 'ZAP70_HUMAN', 'hsa:7535']
```

You can get accession number or protein name identifier from the KEGG identifier as follows:

```
>>> u.mapping(fr='KEGG_ID', to='ID', query='hsa:7535')
'ZAP70_HUMAN'
>>> u.mapping(fr='KEGG_ID', to='ACC', query='hsa:7535')
'P43403'
```

One can also use the `bioservices.kegg.KEGG.conv()` method:

```
>>> k = KEGG()
>>> mapping_kegg_uniprot = k.conv("hsa", "uniprot")
```

2.2.6 BioMart service

BioMart provides a uniform interface to many services such as Cosmic, Ensembl and many more. In BioMart terminology a service is called a **mart**. As an example, we will consider the COSMIC interface provided by BioMart (see [COSMIC](#)). You can play with the interface itself to get an idea of what can be selected (e.g., datasets, filters, attributes). To help you, let us give a simple example that consists in converting the ensemble identifiers into entrez identifiers.

First you create an instance. There are lots of services behind the scene. The `ENSEMBL_MART_ENSEMBL` provides the conversion we are looking for.

```
from bioservices import BioMart
b = BioMart()
datasets = b.get_datasets("ENSEMBL_MART_ENSEMBL")
```

In datasets, there is a `hsapiens_gene_ensembl` database. Let us add it to the request that will be send:

```
b.add_dataset_to_xml(dataset)
```

We want to extract only the to following attributes:

```
b.add_attribute_to_xml("ensemble_gene_id")
b.add_attribute_to_xml("entrezgene_id")
```

If you are interested in a set of identifiers, provide it as a list (here below the queries:

```
queries = ["", ""]
b.add_filter_to_xml("ensemble_gene_id", queries)
```

and finally do the query itself:

```
xml = b.get_xml()
res = b.query(xml)
```

You can obtain the attributes and filters of a dataset as follows:

```
dataset = 'hsapiens_gene_ensembl'
attributes = b.attributes(dataset)
filters = b.filters(dataset)
```

Here is another example with cosmic.

Note: the cosmic mart was available at the time of 1.0 but not during release 1.4.1 . This is not a BioServices issue but the COSMIC mart being down. Hopefully, it will be available again soon. meanwhile this example should help you get a feeling of what can be done with a MART.

In **BioServices**, you can create a biomart request (which is a XML document) but first we need to figure out what are the datasets associated with the COSMIC mart. The tricky part is to know the names of the datasets/attributes/filters. BioServices provides a function that ease this task. First let create an instance of BioMart:

```
>>> from bioservices import *
>>> s = BioMart()
```

Then, let us use the `lookfor()` as follows:

```
>>> s.lookfor("cosmic")
Candidate:
  database: cosp
  MART name: CosmicMart
  displayName: COSMIC (SANGER UK)
  hosts: www.sanger.ac.uk
```

From the previous command, only one mart has been found. It is called CosmicMart, from which we can retrieve the datasets:

```
>>> s.datasets("CosmicMart")
['COSMIC67', 'COSMIC68', 'COSMIC66']
```

There are lots of entries in such datasets and we want to restrict our request using filters and attributes. Let us use the “COSMIC60” dataset. The following commands can help you in figuring out what are the valid names of attributes and filters to be used:

```
>>> s.attributes("COSMIC67")
>>> s.filters("COSMIC67")
```

They return list of dictionaries that provide the identifiers (keys of the dictionary) and information about the identifier (e.g. descriptive name).

For instance, if you want to add the gene name in the list of attributes, you will need to know its identifier. If you look at the dictionary you will find the “gene_name” key that contains:

```
>>> s.attributes("COSMIC67")["gene_name"]
['Gene Name',
 '',
 'naive_attributes',
 'html,txt,csv,tsv,xls',
 'COSMIC67__MART__MAIN',
 'gene_name']
```

So if you want to add the **Gene Name** attribute, you must use the **gene_name** identifier. Similarly for filters. In order to use a filter you must use the identifier as well as a value. Values are contained in the dictionary returned by filters(). For instance, the “Mutated Sample” filter given by the “samp_gene_mutated” identifier returns a list, which second element contains the list of valid values (here y or n character):

```
>>> s.filters("COSMIC67")
['Mutated Sample',
 '[y,n]',
 '',
 'naive_filters',
 'list',
 '=',
 'COSMIC67__MART__MAIN',
 'samp_gene_mutated']
```

So, there is a little bit of work for the user to figure out the identifiers of the attributes and filters. This could be a good exercise but let us give the list of relevant identifiers and their names that we want to use in this tutorial:

category	name	identifier
filter	Mutated Sample	samp_gene_mutated (y)
filter	Primary Site	site_primary (breast)
filter	Validation Status	validation_status (verified)
Attribute	Cosmic Sample ID	id_sample
Attribute	Sample Name	sample_name
Attribute	Sample Source	sample_source
Attribute	Tumour source	tumour_source
Attribute	Gene Name	gene_name
Attribute	Accession Number	accession_number
Attribute	Cosmi Mutation ID	id_mutation
Attribute	Gene ID	id_gene

It is now time to create the XML request by adding attributes/filters and the dataset:

```
>>> # add the dataset
>>> s.add_dataset_to_xml("COSMIC67")

>>> # add the attributes
>>> s.add_attribute_to_xml("id_sample")
>>> s.add_attribute_to_xml("sample_name")
>>> s.add_attribute_to_xml("sample_source")
>>> s.add_attribute_to_xml("tumour_source")
>>> s.add_attribute_to_xml("gene_name")
>>> s.add_attribute_to_xml("accession_number")
>>> s.add_attribute_to_xml("id_mutation")
>>> s.add_attribute_to_xml("id_gene")

>>> # add the filters
```

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```
>>> s.add_filter_to_xml("samp_gene_mutated", "y")
>>> s.add_filter_to_xml("site_primary", "breast")
>>> s.add_filter_to_xml("validation_status", "verified")
```

You can create the XML request that will be send:

```
>>> xml = s.get_xml()
```

And finally send the request:

```
>>> res = s.query(xml)
```

2.2.7 GeneProf tutorial

GeneProf tutorial

New in version 1.2.0.

Section author: Thomas Cokelaer, Dec 2013

GeneProf is a web-based, graphical software suite that allows users to analyse data produced using high-throughput sequencing platforms (RNA-seq and ChIP-seq; “Next-Generation Sequencing” or NGS): Next-gen analysis for next-gen data

BioServices uses the GeneProf Web Services to enable programmatic access to the public data stored in GeneProf’s databases via Python.

Note: GeneProf services is quite versatile and contains many resources and examples. For any technical or scientific questions related to the service itself, please see [GeneProf About&Help](#).

Here below you will find a couple of examples related to GeneProf.

Histogram expression data

Reference <https://www.geneprof.org/GeneProf/media/bpsm-2013/>

In the example below, we use geneprof to

1. search for Gene identifiers related to an organism (mouse) and keyword (nanog).
2. From the gene identifiers, retrieve the gene expression values for a given gene in all experiments
3. plot histogram of the log values found above.

Note: broken example on June 2017. Service should be fix soon. Issue reported to the author.

```
>>> from bioservices import GeneProf
>>> g = GeneProf(verbose=True)
>>> res = g.search_gene_ids("nanog", "mouse")
>>> print(res)
```

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```

{10090: [29640, 14899]}
>>> expr1 = g.get_expression("mouse", 29640)['values']
>>> expr2 = g.get_expression("mouse", 14899)['values']

>>> import math
>>> values1 = [math.log(x["RPKM"]+1, 2.) for x in expr1]
>>> values2 = [math.log(x["RPKM"]+1, 2.) for x in expr2]

>>> from pylab import clf, subplot, hist
>>> clf()
>>> subplot(2,1,1)
>>> hist(values1)
>>> subplot(2,1,2)
>>> hist(values2)

```

Transcription factor network of stem cells

References <https://www.geneprof.org/GeneProf/media/recomb-2013/>

Another example, here below consists in retrieving the binding targets of transcription factors (about 70) in mouse embryonic stem cells, and generate a SIF network that could be open and visualised in Cytoscape.

The example below can probably be simplified and make use of tools such as networkx to manipulate and visualise the final network. Please use with care:

```

>>> # first import and create a GenProf instance
>>> from bioservices import GeneProf
>>> g = GeneProf(verbose=False)
>>>
>>> # find all pubic experimental mouse samples in geneprof
>>> samples = g.get_list_experiment_samples("mouse")['samples']
>>> # look at entries that contains "Gene"
>>> graph = {}
>>> mapgene = {}
>>> for i, entry in enumerate(samples):
...     print("progress %s/%s" % (i+1, len(samples)))
...
...     # keep only entries that have cell type "embryonic stem cell" in the celltype
...     if "Gene" in entry.keys() and "Cell_Type" in entry.keys() and entry["Cell_Type
↵"]=="embryonic stem cell":
...
...         # aliases
...         sampleId = entry['sample_id']
...         gene = entry["Gene"]
...
...         # get gene id and save mapping in a dictionary to be used later
...         geneId = g.get_gene_id("mouse", "C_NAME", gene)['ids']
...         mapgene[geneId[0]] = gene
...
...         # get targets and print them
...         targets = g.get_targets_by_experiment_sample("mouse", sampleId)
...
...         # could be simplified inside the geneprof.py module
...         if 'targets' in targets.keys():
...             targets = targets['targets']

```

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```

...     # print the results
...     for x in targets:
...         print gene, geneId[0], " ", x['feature_id']
...     graph[gene] = [x['feature_id'] for x in targets]

>>> # The graph saved in the graph variables is quite large. Let us simplified_
↳keeping target that
>>> # are in the list of genes only
>>> simple_graph = {}
>>> for k, v in graph.iteritems():
...     simple_graph[k] = [mapgene[x] for x in v if x in mapgene.keys()]
>>> len(simple_graph.keys())
72
>>> sum([len(simple_graph[x]) for x in simple_graph.keys()])
2137

```

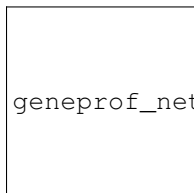
Finally, you can look at the graph with your favorite tool such as Cytoscape, Gephi.

Here below, I'm using a basic graph visualisation tool implemented in `CellNOpt`, which is not dedicated for Network visualisation but contains a small interface to graphviz useful in this context (it has a python interface):

```

>>> from cno import CNOGraph
>>> c = CNOGraph()
>>> for k in simple_graph.keys():
...     for v in simple_graph[k]:
...         c.add_edge(k, v, link="+")
>>> c.centralty_degree()
>>> c.graph['graph'] = {"splines":"true", "size):(20,20),
...                    "dpi":200, "fixedsize":True}
>>> c.graph['node'] = {"width":.01, "height":.01,
...                   'size':0.01, "fontsize":8}
>>> c.plotdot(prog="fdp", node_attribute="degree")

```



Integrating expression data in pathways

References <https://www.geneprof.org/GeneProf/media/recomb-2013/>

This is another example from the reference above but based on tools available in bioservices so as to overlaid high-throughput gene expression onto pathways and models from KEGG database.

Fold changes in lymphoma vs. kidney on selected KEGG pathways

```

>>> from bioservices import KEGG, GeneProf, UniProt
>>> import StringIO
>>> import pandas
>>> g = GeneProf()
>>> k = KEGG()
>>> u = UniProt()

```

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```

>>> # load ENCODE RNA-seq into a DataFrame for later
>>> data = g.get_data("11_683_28_1", "txt")
>>> rnaseq = pandas.read_csv(StringIO.StringIO(data), sep="\t")
>>> gene_names = rnaseq['Ensembl Gene ID']

>>> # get a pathway diagram for the KEGG path hsa05202 ("Transcriptional
>>> # misregulation in cancers")
>>> res = k.parse(k.get("hsa05202"))
>>> # extract KEGG identifiers corresponding to the genes found in the pathway
>>> keggids = ["hsa:"+x for x in res['GENE'].keys()]

>>> # we need to map the KEGG Ids to Ensembl Ids. We will use KEGG mapping and
↳uniprot mapping
>>> # for cases where the former does not have associated mapping.
>>> ensemblids = {}
>>> for id_ in keggids:
...     res = k.parse(k.get(id_))['DBLINKS']
...     if 'Ensembl' in res.keys():
...         print id_, res['Ensembl']
...         ensemblids[id_] = res['Ensembl']
...     else:
...         if "UniProt" in res.keys():
...             ids = res['UniProt'].split()[0]
...             m = u.mapping("ACC", "ENSEMBL_ID", query=ids)
...             if len(m): ensemblids[id_] = m[ids][0]
...         pass # no links to ensembl DB found

>>> # what are the KEGG id transformed into Ensembl Ids that are in the ENCODE data
↳set ?
>>> found = [x for x in ensemblids.values() if x in [str(y) for y in gene_names]]
>>> indices = [i for i, x in enumerate(rnaseq['Ensembl Gene ID']) if x in found]
>>>
>>> # now, we can pick out the log2 fold change values for visualization:
>>> data = rnaseq.ix[indices][['Ensembl Gene ID', 'log2FC Lymphoma / EmbryonicKidney
↳']]
>>> # and keep only those that have a negative or positive value
>>> mid = 1.5
>>> low = data[data['log2FC Lymphoma / EmbryonicKidney']<-mid]
>>> geneid_low = list(low['Ensembl Gene ID'])
>>> up = data[data['log2FC Lymphoma / EmbryonicKidney']>mid]
>>> geneid_up = list(up['Ensembl Gene ID'])
>>> mid = data[abs(data['log2FC Lymphoma / EmbryonicKidney'])<mid]
>>> geneid_mid = list(mid['Ensembl Gene ID'])

>>> # now that we have the genes (in ensembl format), we need the kegg id
>>> keggid_low = [this for this in keggids if ensemblids[this] in geneid_low]
>>> keggid_mid = [this for this in keggids if ensemblids[this] in geneid_mid]
>>> keggid_up = [this for this in keggids if ensemblids[this] in geneid_up]
>>> # it is now time to look at the expression on the diagram
>>> colors = {}
>>> for id_ in keggids: colors[id_[4:]] = "gray,"
>>> for id_ in keggid_low: colors[id_[4:]] = "blue,"
>>> for id_ in keggid_up: colors[id_[4:]] = "orange,"
>>> for id_ in keggid_mid: colors[id_[4:]] = "yellow,"
>>> k.show_pathway("hsa05202", dcolor="white", keggid=colors)

```

The last command will popup the KEGG diagram with the expression data on top of the diagram, as shown in the

following picture:



2.3 Combining BioServices with external tools

Contents

- *Combining BioServices with external tools*
 - *PYMOL*
 - *BioPython*

– *Galaxy*

This section shows how to use BioServices as an intermediate tool that fetch data to be used by third-party software/application.

The external applications used in this section are not part of BioServices therefore we do not provide instructions for the installation. Reader should refer to the application web site instead (URLs are provided here below). However, we indicate the way we installed them.

2.3.1 PYMOL

URL <http://www.pymol.org/>

This example below uses the external software called PyMOL. We have installed it without trouble by downloading the source file from their website. Then, we typed those commands in a shell:

```
bunzip pymol-v1.6alpha1.tar.bz2
tar xvf pymol-v1.6alpha1.tar
cd pymol
python setup.py install
```

You may need to install library if requested. Tested under Fedora 15.

The following code uses BioServices to get the PDB Identifier of a protein called ZAP70. To do so, we use *bioservices.uniprot.UniProt* to get its accession number (P43403) and its PDB identifier. Then, we use *bioservices.pdb.PDB* to get the 3D structure in PDB format.

The script above uses PyMOL in a script manner to save the 3D graphical representation of the protein (here below) but you could also use PyMOL in an interactive mode.



2.3.2 BioPython

URL <http://biopython.org/DIST/docs/tutorial/Tutorial.html#chapter:Bio.AlignIO>

BioPython provides many tools for IO, algorithms and access to Web services. BioServices provides access to many web services. This example shows how (i) to use BioServices to retrieve FASTA files and (ii) BioPython to play with the sequences.

Note: We assume you have installed BioPython (pip install biopython)

First, let us retrieve two FASTA sequences and save them in 2 files:

```
from bioservices import UniProt
u = UniProt()
akt1 = u.retrieve("P31749", "fasta")
akt2 = u.retrieve("P31751", "fasta")
```

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```

fh = open("akt1.fasta", "w")
fh.write(akt1)
fh.close()

fh = open("akt2.fasta", "w")
fh.write(akt2)
fh.close()

```

Now, on the BioPython side, we read the 2 sequences and introspect them:

```

>>> from Bio import AlignIO
>>> record1 = SeqIO.read("akt1.fasta", "fasta")
>>> record2 = SeqIO.read("akt2.fasta", "fasta")
>>> record1 += "-" # this is to have 2 sequences on same length as requested by the
↳following function

>>> alignment = AlignIO.MultipleSeqAlignment([])
>>> alignment.append(record1)
>>> alignment.append(record2)

>>> for record in alignment:
>>>     print(description)
sp|P31749|AKT1_HUMAN RAC-alpha serine/threonine-protein kinase OS=Homo sapiens
↳GN=AKT1 PE=1 SV=2
sp|P31751|AKT2_HUMAN RAC-beta serine/threonine-protein kinase OS=Homo sapiens GN=AKT2
↳PE=1 SV=2

```

You are ready to play with BioPython multiple alignment tools. Please consult BioPython documentation for more examples.

2.3.3 Galaxy

URL <http://wiki.galaxyproject.org/FrontPage>

Date Aug 2013

Galaxy is an open, web-based platform for accessible, reproducible, and transparent computational biomedical research. It provides workflows and plugins to many web resources.

This tutorial shows how to link bioservices and galaxy. Our tutorial will provide a plugin to Galaxy so that a user can retrieve a FASTA file via BioServices and the wrapping of UniProt Web Services.

We assume that you installed Galaxy on your system via the source code:

```

hg clone https://bitbucket.org/galaxy/galaxy-dist/
cd galaxy-dist
hg update stable

```

The tree directory should therefore contains a directory called **tools/** and in the main directory, an XML file called **conf_tools.py**

We will first create a plugin for bioservices. This is done by adding a directory called bioservices in **./tools/**:

```

mkdir tools/bioservices

```

In this directory, we will create two files called **uniprot.py** that will contain the actual code that calls bioservices and a second XML file that will allow us to design the plugin layout.

Let us start with the plugin. It is very simple since only the UniProt Entry is required. The output will simply be the FASTA file that would have been fetched.

The XML file is:

```
<tool id="bioservices_uniprot" name="Get FASTA" version="1.1.0">
  <description>from UniProt via Bioservices</description>
  <requirements>
    <requirement type="package">bioservices</requirement>
  </requirements>
  <command interpreter="python">uniprot.py $uniprot_id $output</command>
  <inputs>
    <param name="uniprot_id" type="text" label="UniProt ID" size="40" help="Provide a
↳ valid UniProt Entry (e.g. P43403) "/>
  </inputs>
  <outputs>
    <data format="fasta" name="output" />
  </outputs>
  <help>
Fetch a FASTA file using UniProt via BioServices. Simply provide a valid Uniprot
↳ Entry (e.g., P43403)
  </help>
</tool>
```

The python code will take as an input the UniProt ID and create a file that contains the FASTA data:

```
import sys

def __main__():
    ids = sys.argv[1]
    filename = sys.argv[2]
    # TODO: check the validity and format ?
    try:
        from bioservices import UniProt
        u = UniProt(verbose=False)
        u.debugLevel = "ERROR"
    except ImportError:
        print("Could not import bioservices ? Check that it is installed. Try 'pip
↳ install bioservices'")

    try:
        fasta = u.searchUniProtId(ids, "fasta")
    except:
        print("An error occurred while fetching the FASTA file from uniprot")

    try:
        fh = open(filename, "w")
        fh.write(fasta)
```

finally, you need to make Galaxy aware of this new plugin. this is done in the file called `conf_tool.xml`. Add bioservices plugin. The beginning of the file should look like:

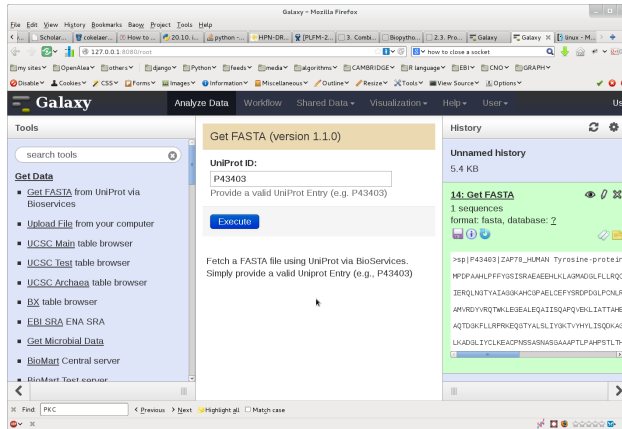
```
<?xml version="1.0"?>
<toolbox>
  <section name="Get Data" id="gettext">
```

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```
<tool file="bioservices/uniprot.xml"/>
<tool file="data_source/upload.xml"/>
```

Once done, start your galaxy server. The following image shows the outcome: in the left hand side, you can select the bioservices plugin. Then, in the center, you can enter a uniprot entry. Press the execute button and the new file should appear in the right hand side. From there you can use Galaxy other tools to analyse the file.



This example shows that it is possible to link Galaxy and BioServices to access to various Web Services that are available through Bioservices.

PyMOL

URL <http://www.pymol.org/>

This example below uses the external software called PyMOL. We have installed it without trouble by downloading the source file from their website. Then, we typed those commands in a shell:

```
bunzip pymol-v1.6alpha1.tar.bz2
tar xvf pymol-v1.6alpha1.tar
cd pymol
python setup.py install
```

You may need to install library if requested. Tested under Fedora 15.

The following code uses BioServices to get the PDB Identifier of a protein called ZAP70. To do so, we use `bioservices.uniprot.UniProt` to get its accession number (P43403) and its PDB identifier. Then, we use `bioservices.pdb.PDB` to get the 3D structure in PDB format.

The script above uses PyMOL in a script manner to save the 3D graphical representation of the protein (here below) but you could also use PyMOL in an interactive mode.



BioPython

URL <http://biopython.org/DIST/docs/tutorial/Tutorial.html#chapter:Bio.AlignIO>

BioPython provides many tools for IO, algorithms and access to Web services. BioServices provides access to many web services. This example shows how (i) to use BioServices to retrieve FASTA files and (ii) BioPython to play with the sequences.

Note: We assume you have installed BioPython (`pip install biopython`)

First, let us retrieve two FASTA sequences and save them in 2 files:

```
from bioservices import UniProt
u = UniProt()
akt1 = u.retrieve("P31749", "fasta")
akt2 = u.retrieve("P31751", "fasta")

fh = open("akt1.fasta", "w")
fh.write(akt1)
fh.close()

fh = open("akt2.fasta", "w")
fh.write(akt2)
fh.close()
```

Now, on the BioPython side, we read the 2 sequences and introspect them:

```
>>> from Bio import AlignIO
>>> record1 = SeqIO.read("akt1.fasta", "fasta")
>>> record2 = SeqIO.read("akt2.fasta", "fasta")
>>> record1 += "-" # this is to have 2 sequences on same length as requested by the
↳following function

>>> alignment = AlignIO.MultipleSeqAlignment([])
>>> alignment.append(record1)
>>> alignment.append(record2)

>>> for record in alignment:
>>>     print(description)
sp|P31749|AKT1_HUMAN RAC-alpha serine/threonine-protein kinase OS=Homo sapiens
↳GN=AKT1 PE=1 SV=2
sp|P31751|AKT2_HUMAN RAC-beta serine/threonine-protein kinase OS=Homo sapiens GN=AKT2
↳PE=1 SV=2
```

You are ready to play with BioPython multiple alignment tools. Please consult BioPython documentation for more examples.

Galaxy

URL <http://wiki.galaxyproject.org/FrontPage>

Date Aug 2013

Galaxy is an open, web-based platform for accessible, reproducible, and transparent computational biomedical research. It provides workflows and plugins to many web resources.

This tutorial shows how to link bioservices and galaxy. Our tutorial will provide a plugin to Galaxy so that a user can retrieve a FASTA file via BioServices and the wrapping of UniProt Web Services.

We assume that you installed Galaxy on your system via the source code:

```
hg clone https://bitbucket.org/galaxy/galaxy-dist/
cd galaxy-dist
hg update stable
```

The tree directory should therefore contains a directory called **tools/** and in the main directory, an XML file called **conf_tools.py**

We will first create a plugin for bioservices. This is done by adding a directory called bioservices in ./tools:

```
mkdir tools/bioservices
```

In this directory, we will create two files called **uniprot.py** that will contain the actual code that calls bioservices and a second XML file that will allows us to design the plugin layout.

Let us start with the plugin. It is very simple since only the UniProt Entry is required. The output will simply be the FASTA file that would have been fetched.

The XML file is:

```
<tool id="bioservices_uniprot" name="Get FASTA" version="1.1.0">
  <description>from UniProt via Bioservices</description>
  <requirements>
    <requirement type="package">bioservices</requirement>
  </requirements>
  <command interpreter="python">uniprot.py $uniprot_id $output</command>
  <inputs>
    <param name="uniprot_id" type="text" label="UniProt ID" size="40" help="Provide a
↳valid UniProt Entry (e.g. P43403) "/>
  </inputs>
  <outputs>
    <data format="fasta" name="output" />
  </outputs>
  <help>
Fetch a FASTA file using UniProt via BioServices. Simply provide a valid Uniprot_
↳Entry (e.g., P43403)
  </help>
</tool>
```

The python code will take as an input the UniProt ID and create a file that contains the FASTA data:

```
import sys

def __main__():
    ids = sys.argv[1]
    filename = sys.argv[2]
    # TODO: check the validity and format ?
    try:
        from bioservices import UniProt
        u = UniProt(verbose=False)
        u.debugLevel = "ERROR"
    except ImportError:
        print("Could not import bioservices ? Check that it is installed. Try 'pip_
↳install bioservices'")
```

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```

try:
    fasta = u.searchUniProtId(ids, "fasta")
except:
    print("An error ocured while fetching the FASTA file from uniprot")

try:
    fh = open(filename, "w")
    fh.write(fasta)

```

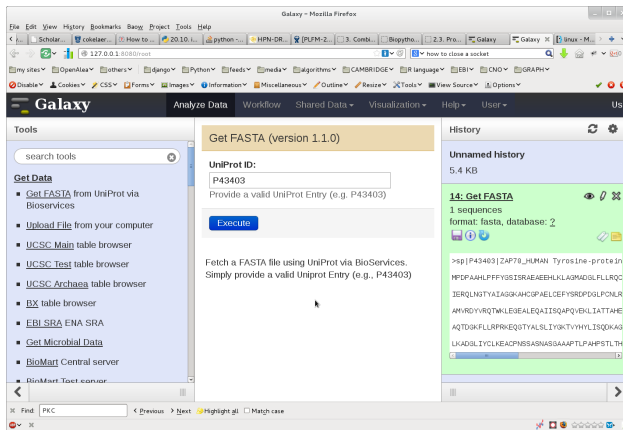
finally, you need to make Galaxy aware of this new plugin. this is done in the file called conf_tool.xml. Add bioservices plugin. The beginning of the file should look like:

```

<?xml version="1.0"?>
<toolbox>
  <section name="Get Data" id="getext">
    <tool file="bioservices/uniprot.xml"/>
    <tool file="data_source/upload.xml"/>
  ...

```

Once done. start you galaxy server. The following image show the outcome: in the left hand side, you can select the bioservices plugin. Then, in the center, you can enter a uniprot entry. Press the execute button and the new file should appear in the right hand side. From there you can use Galaxy other tools to analyse the file.



This example shows that it is possible to link Galaxy and BioServices to access to various Web Services that are available through Bioservices.

2.4 Developer Guide

2.4.1 Creating a service class (REST case)

Warning: since version 1.3.0, RESTService is deprecated and REST should be used. The changes should be easy: get method is now called http_get and requestPost is now http_post.

You can test directly a SOAP/WSDL or REST service in a few lines. For instance, to access to the biomart REST service, type:


```
>>> s = REST("BioMart" , "http://www.biomart.org/biomart/martservice")
```

The first parameter is compulsory but can be any word. You can retrieve the base URL by typing:

```
>>> s.url
'http://www.biomart.org/biomart/martservice'
```

and then send a request to retrieve registry information for instance (see www.biomart.org/martservice.html for valid request:

```
>>> s.http_get("?type=registry")
<bioservices.xmltools.easyXML at 0x3b7a4d0>
```

The request method available from RESTService class concatenates the url and the parameter provided so it request the “<http://www.biomart.org/biomart/martservice>” URL.

As a developer, you should ease the life of the user by wrapping up the previous commands. An example of a BioMart class with a unique method dedicated to the registry would look like:

```
>>> class BioMart (REST) :
...     def __init__(self) :
...         url = "http://www.biomart.org/biomart/martservice"
...         super(BioMart, self).__init__("BioMart", url=url)
...     def registry(self) :
...         ret = self.request("?type=registry")
...         return ret
```

and you would use it as follows:

```
>>> s = BioMart()
>>> s.registry()
<bioservices.xmltools.easyXML at 0x3b7a4d0>
```

2.4.2 Creating a service class (WSDL case)

If a web service interface is not provided within bioservices, you can still easily access its functionalities. As an example, let us look at the [Ontology Lookup service](#), which provides a WSDL service. In order to easily access this service, use the WSDLService class as follows:

```
>>> from bioservices import WSDLService
>>> ols = WSDLService("OLS", "http://www.ebi.ac.uk/ontology-lookup/OntologyQuery.wsdl
↵")
```

You can now see which methods are available:

```
>>> ols.wsdl_methods
```

and call one (getVersion) using the `bioservices.services.WSDLService.serv()`:

```
>>> ols.serv.getVersion()
```

You can then look at something more complex and extract relevant information:

```
>>> [x.value for x in ols.serv.getOntologyNames()[0]]
```

Of course, you can add new methods to ease the access to any functionalities:

```
>>> ols.getOnlogyNames() # returns the values
```

Similarly to the previous case using REST, you can wrap this example into a proper class.

2.5 Others

When wrapper a WSDL services, it may be difficult to know what parameters to provide if the API doc is not clear. This can be known as follows using the **suds** factory. In this previous examples, we could use:

```
>>> ols.suds.factory.resolver.find('getTermById')
<Element:0xa848b50 name="getTermById" />
```

For eutils, this was more difficult:

```
m1 = list(e.suds.wsdl.services[0].ports[0].methods.values())[2]
m1.soap.input.body.parts[0]
the service is in m1.soap.input.body.parts[0] check for the element in the
root attribute
```

2.6 suds and client auth

<http://stackoverflow.com/questions/6277027/suds-over-https-with-cert>

2.7 Gallery

2.7.1 KEGG module example

Histogram of KEGG pathways relations

```
from pylab import *

# extract all relations from all pathways
from bioservices.kegg import KEGG
s = KEGG()
s.organism = "hsa"

# retrieve more than 260 pathways so it takes time
max_pathways = 10
results = [s.parse_kgml_pathway(x) for x in s.pathwayIds[0:max_pathways]]
relations = [x['relations'] for x in results]

# plot
hist([len(this) for this in relations], 20)
xlabel('number of relations')
ylabel('#')
title("number of relations per pathways")
grid(True)
```

Total running time of the script: (0 minutes 0.000 seconds)

2.8 NoteBooks

ipython notebook can be downloaded from this section. You can either see the results via nbviewer, or download and run them yourself. To do so, download the notebook and open a shell where is saved the file. Type:

```
ipython notebook
```

You should see the notebook name. Click on it and you are ready to try. Cels can be executed by typing CTRL+enter

2.8.1 UniProt

Here is a ipython notebook dedicated to UniProt, which can be downloaded [notebooks/UniProt.ipynb](#) or view its results on [uniprot nbviewer](#)

2.8.2 BioModels

Here is a ipython notebook dedicated to BioModels, which can be downloaded [notebooks/BioModels.ipynb](#) or view its results on [biomodels nbviewer](#)

2.8.3 ChEMBL

Here is a ipython notebook dedicated to ChEMBL, which can be downloaded [notebooks/ChEMBL.ipynb](#) or view its results on [chembl nbviewer](#)

2.8.4 Entrez/Eutils

Here is a ipython notebook dedicated to EUtils, which can be downloaded [notebooks/Entrez_EUtils.ipynb](#) or view its results on [eutil nbviewer](#)

2.8.5 KEGG

Here is a ipython notebook dedicated to KEGG, which can be downloaded [notebooks/KEGG.ipynb](#) or view its results on [kegg nbviewer](#)

2.8.6 MUSCLE

Here is a ipython notebook dedicated to MUSCLE, which can be downloaded [notebooks/MUSCLE.ipynb](#) or view its results on [muscle nbviewer](#)

2.8.7 NCBIblast

Here is a ipython notebook dedicated to NCBIblast, which can be downloaded [notebooks/NCBIblast.ipynb](#) or view its results on [ncbiblast nbviewer](#)

2.8.8 WikiPathway

Here is a ipython notebook dedicated to WikiPathway, which can be downloaded `notebooks/WikiPathway.ipynb` or view its results on [wikipathway nbviewer](#)

Gene Mapping

Here is a ipython notebook dedicated to Gene Mapping, which can be downloaded `notebooks/Gene_Mapping.ipynb` or view its results on [gene mapping nbviewer](#)

BioMart

Here is a ipython notebook dedicated to BioMart, which can be downloaded `notebooks/BioMart` or view its results on [chembl biomiart](#)

Ensembl

Here is a ipython notebook dedicated to Ensembl, which can be downloaded `notebooks/Ensembl.ipynb` or view its results on [ensembl nbviewer](#)

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 - *xmltools module*
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 - *BioModels*
 - *ChEBI*
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- * *KEGG Databases Names and Abbreviations*
- * *Database Entries*
 - *HGNC*
 - *Intact (complex)*
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 - *PDB/PDBe modules*
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 - *PSICQUIC*
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 - *Rhea*
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 - *Readseq*
 - *UniChem*
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 - *DBFetch*
 - *Wikipathway*
- *Applications and extra tools*
 - *Peptides*
 - *FASTA*

2.9 Utilities

2.9.1 Service module (REST or WSDL)

Modules with common tools to access web resources

class Service (*name, url=None, verbose=True, requests_per_sec=10, url_defined_later=False*)
 Base class for WSDL and REST classes

See also:

REST, WSDLService

Constructor

Parameters

- **name** (*str*) – a name for this service
- **url** (*str*) – its URL
- **verbose** (*bool*) – prints informative messages if True (default is True)
- **requests_per_sec** – maximum number of requests per seconds are restricted to 3. You can change that value. If you reach the limit, an error is raise. The reason for this limitation is that some services (e.g., NCBI) may black list you IP. If you need or can do more (e.g., ChEMBL does not seem to have restrictions), change the value. You can also have several instance but again, if you send too many requests at the same, your future requests may be retracted. Currently implemented for REST only

All instances have an attribute called `logging` that is an instance of the `logging` module. It can be used to print information, warning, error messages:

```
self.logging.info("informative message")
self.logging.warning("warning message")
self.logging.error("error message")
```

The attribute `debugLevel` can be used to set the behaviour of the logging messages. If the argument `verbose` is True, the `debugLevel` is set to INFO. If `verbose` is False, the `debugLevel` is set to WARNING. However, you can use the `debugLevel` attribute to change it to one of DEBUG, INFO, WARNING, ERROR, CRITICAL. `debugLevel=WARNING` means that only WARNING, ERROR and CRITICAL messages are shown.

CACHING

easyXML (*res*)

Use this method to convert a XML document into an *easyXML* object

The *easyXML* object provides utilities to ease access to the XML tag/attributes.

Here is a simple example starting from the following XML

```
>>> from bioservices import *
>>> doc = "<xml> <id>1</id> <id>2</id> </xml>"
>>> s = Service("name")
>>> res = s.easyXML(doc)
>>> res.findAll("id")
[<id>1</id>, <id>2</id>]
```

easyXMLConversion

If True, xml output from a request are converted to *easyXML* object (Default behaviour).

on_web (*url*)

Open a URL into a browser

pubmed (*Id*)

Open a pubmed Id into a browser tab

Parameters *Id* – a valid pubmed Id in string or integer format.

The URL is a concatenation of the pubmed URL <http://www.ncbi.nlm.nih.gov/pubmed/> and the provided *Id*.

response_codes = {200: 'OK', 201: 'Created', 400: 'Bad Request. There is a problem'}
some useful response codes

save_str_to_image (*data, filename*)
Save string object into a file converting into binary

url
URL of this service

class WSDLService (*name, url, verbose=True, cache=False*)
Class dedicated to the web services based on WSDL/SOAP protocol.

See also:

RESTService, *Service*

Constructor

Parameters

- **name** (*str*) – a name e.g. Kegg, Reactome, ...
- **url** (*str*) – the URL of the WSDL service
- **verbose** (*bool*) – prints informative messages

The `serv` give access to all WSDL functionalities of the service.

The `methods` is an alias to `self.serv.methods` and returns the list of functionalities.

TIMEOUT

wSDL_create_factory (*name, **kargs*)

wSDL_methods
returns methods available in the WSDL service

wSDL_methods_info ()

exception BioServicesError (*value*)

class REST (*name, url=None, verbose=True, cache=False, requests_per_sec=3, proxies=[], cert=None, url_defined_later=False*)

The ideas (sync/async) and code using requests were inspired from the chembl python wrapper but significantly changed.

Get one value:

```
>>> from bioservices import REST
>>> s = REST("test", "https://www.ebi.ac.uk/chemblws")
>>> res = s.get_one("targets/CHEMBL2476.json", "json")
>>> res['organism']
u'Homo sapiens'
```

The caching has two major interests. First one is that it speed up requests if you repeat requests.

```
>>> s = REST("test", "https://www.ebi.ac.uk/chemblws")
>>> s.CACHING = True
>>> # requests will be stored in a local sqlite database
>>> s.get_one("targets/CHEMBL2476")
>>> # Disconnect your wiki and any network connections.
>>> # Without caching you cannot fetch any requests but with
>>> # the CACHING on, you can retrieve previous requests:
>>> s.get_one("targets/CHEMBL2476")
```

Advantages of requests over urllib

requests length is not limited to 2000 characters <http://www.g-loaded.eu/2008/10/24/maximum-url-length/>

There is no need for authentication if the web services available in bioservices except for a few exception. In such case, the username and password are to be provided with the method call. However, in the future if a services requires authentication, one can set the attribute `authentication` to a tuple:

```
s = REST()
s.authentication = ('user', 'pass')
```

Note about headers and content type. The Accept header is used by HTTP clients to tell the server what content types they will accept. The server will then send back a response, which will include a Content-Type header telling the client what the content type of the returned content actually is. When using the `get__headers()`, you can see the User-Agent, the Accept and Content-Type keys. So, here the HTTP requests also contain Content-Type headers. In POST or PUT requests the client is actually sending data to the server as part of the request, and the Content-Type header tells the server what the data actually is For a POST request resulting from an HTML form submission, the Content-Type of the request should be one of the standard form content types: application/x-www-form-urlencoded (default, older, simpler) or multipart/form-data (newer, adds support for file uploads)

TIMEOUT

`clear_cache()`

`content_types = {'bed': 'text/x-bed', 'default': 'application/x-www-form-urlencoded'}`

`debug_message()`

`delete_cache()`

`delete_one(query, frmt='json', **kargs)`

`getUserAgent()`

`get_async(keys, frmt='json', params={}, **kargs)`

`get_headers(content='default')`

Parameters content (*str*) – set to default that is application/x-www-form-urlencoded so that it has the same behaviour as urllib2 (Sept 2014)

`get_one(query=None, frmt='json', params={}, **kargs)`
if query starts with `http://` do not use self.url

`get_sync(keys, frmt='json', **kargs)`

`http_delete(query, params=None, frmt='xml', headers=None, **kargs)`

`http_get(query, frmt='json', params={}, **kargs)`

- query is the suffix that will be appended to the main url attribute.
- query is either a string or a list of strings.
- if list is larger than ASYNC_THRESHOLD, use asynchronous call.

`http_post(query, params=None, data=None, frmt='xml', headers=None, files=None, content=None, **kargs)`

`post_one(query=None, frmt='json', **kargs)`

session

2.9.2 xmltools module

This module includes common tools to manipulate XML files

class easyXML (*data*, *encoding='utf-8'*)
class to ease the introspection of XML documents.

This class uses the standard xml module as well as the package BeautifulSoup to help introspecting the XML documents.

```
>>> from bioservices import *
>>> n = ncbiblast.NCBIBlast()
>>> res = n.getParameters() # res is an instance of easyXML
>>> # You can retrieve XML from this instance of easyXML and print the content
>>> # in a more human-readable way.
>>> res.soup.findAll('id') # a BeautifulSoup instance is available
>>> res.root # and the root using xml.etree.ElementTree
```

There is a getitem so you can type:

```
res['id']
```

which is equivalent to:

```
res.soup.findAll('id')
```

There is also aliases findAll and prettify.

Constructor

Parameters

- **data** – an XML document format
- **fixing_unicode** – use only with HGNC service to fix issue with the XML returned by that particular service. No need to use otherwise. See [HGNC](#) documentation for details.
- **encoding** – default is utf-8 used. Used to fix the HGNC XML only.

The data parameter must be a string containing the XML document. If you have an URL instead, use [readXML](#)

getchildren()

returns all children of the root XML document

This is just an alias to self.soup.getchildren()

soup

Returns the beautiful soup instance

class readXML (*url*, *encoding='utf-8'*)
Read XML and converts to beautifulsoup data structure

easyXML accepts as input a string. This class accepts a filename instead inherits from easyXML

See also:

[easyXML](#)

2.10 Services

2.10.1 ArrayExpress

2.10.2 BiGG

Interface to the BiGG Models API Service

What is BiGG Models?

URL <http://bigg.ucsd.edu>

REST <http://bigg.ucsd.edu/api/v2>

“BiGG Models is a knowledgebase of genome-scale metabolic network reconstructions. BiGG Models integrates more than 70 published genome-scale metabolic networks into a single database with a set of standardized identifiers called BiGG IDs. Genes in the BiGG models are mapped to NCBI genome annotations, and metabolites are linked to many external databases (KEGG, PubChem, and many more).”

—BiGG Models Home Page, March 10, 2020.

class **BiGG** (*verbose=False, cache=False*)

Interface to the *BiGG Models* <<http://bigg.ucsd.edu/>> API Service.

```
>>> from bioservices import BiGG
>>> bigg = BiGG()
>>> bigg.search("e coli", "models")
[{'bigg_id': 'e_coli_core',
  'gene_count': 137,
  'reaction_count': 95,
  'organism': 'Escherichia coli str. K-12 substr. MG1655',
  'metabolite_count': 72},
 ...
]
```

download (*model_id, format_='json', gzip=True, target=None*)

genes (*model_id, ids=None*)

metabolites (*model_id=None, ids=None*)

models

reactions (*model_id=None, ids=None*)

search (*query, type_*)

version

2.10.3 BioDBnet

This module provides a class *BioDBNet* to access to BioDBNet WS.

What is BioDBNet ?

URL <http://biodbnet.abcc.ncifcrf.gov/>

Service <http://biodbnet.abcc.ncifcrf.gov/webServices>

Citations Mudunuri,U., Che,A., Yi,M. and Stephens,R.M. (2009) bioDBnet: the biological database network. *Bioinformatics*, 25, 555-556

“BioDBNet Database is a repository hosting computational models of biological systems. A large number of the provided models are published in the peer-reviewed literature and manually curated. This resource allows biologists to store, search and retrieve mathematical models. In addition, those models can be used to generate sub-models, can be simulated online, and can be converted between different representational formats. “

—From BioDBNet website, Dec. 2012

New in version 1.2.3.

Section author: Thomas Cokelaer, Feb 2014

class BioDBNet (*verbose=True, cache=False*)

Interface to the BioDBNet service

```
>>> from bioservices import *
>>> s = BioDBNet ()
```

Most of the BioDBNet WSDL are available. There are functions added to the original interface such as `extra_getReactomeIds()`.

Use `db2db()` to convert from 1 database to some databases. Use `dbReport()` to get the conversion from one database to all databases.

Constructor

Parameters `verbose` (*bool*) –

db2db (*input_db, output_db, input_values, taxon=9606*)

Retrieves models associated to the provided Taxonomy text.

Parameters

- `input_db` – input database.
- `output_db` – list of databases to map to.
- `input_values` – list of identifiers to map to the output databases

Returns dataframe where index correspond to the input database identifiers. The columns contains the identifiers for each output database (see example here below).

```
>>> from bioservices import BioDBNet
>>> input_db = 'Ensembl Gene ID'
>>> output_db = ['Gene Symbol']
>>> input_values = ['ENSG00000121410', 'ENSG00000171428']
>>> df = s.db2db(input_db, output_db, input_values, 9606)
      Gene Symbol
Ensembl Gene ID
ENSG00000121410    A1BG
ENSG00000171428    NAT1
```

dbFind (*output_db*, *input_values*, *taxon*='9606')

dbFind method

dbFind can be used when you do not know the actual type of your identifiers or when you have a mixture of different types of identifiers. The tool finds the identifier type and converts them into the selected output if the identifiers are within the network.

Parameters

- **output_db** (*str*) – valid database name
- **input_values** (*list*) – list of identifiers to look for

Returns a dataframe with index set to the input values.

```
>>> b.dbFind("Gene ID", ["ZMYM6_HUMAN", "NP_710159", "ENSP00000305919"])
      Gene ID      Input Type
InputValue
ZMYM6_HUMAN      9204      UniProt Entry Name
NP_710159      203100  RefSeq Protein Accession
ENSP00000305919  203100      Ensembl Protein ID
```

dbOrtho (*input_db*, *output_db*, *input_values*, *input_taxon*, *output_taxon*)

Convert identifiers from one species to identifiers of a different species

Parameters

- **input_db** – input database
- **output_db** – output database
- **input_values** – list of identifiers to retrieve
- **input_taxon** – input taxon
- **output_taxon** – output taxon

Returns dataframe where index correspond to the input database identifiers. The columns contains the identifiers for each output database (see example here below)

```
>>> df = b.dbOrtho("Gene Symbol", "Gene ID", ["MYC", "MTOR", "A1BG"],
...               input_taxon=9606, output_taxon=10090)
      Gene ID InputValue
0    17869      MYC
1    56717      MTOR
2   117586      A1BG
```

dbReport (*input_db*, *input_values*, *taxon*=9606)

Same as *db2db* () but returns results for all possible outputs.

Parameters

- **input_db** – input database
- **input_values** – list of identifiers to retrieve

Returns dataframe where index correspond to the input database identifiers. The columns contains the identifiers for each output database (see example here below)

```
df = s.dbReport("Ensembl Gene ID", ['ENSG00000121410', 'ENSG00000171428'])
```

dbWalk (*db_path*, *input_values*, *taxon*=9606)

Walk through biological database network

dbWalk is a form of database to database conversion where the user has complete control on the path to follow while doing the conversion. When a input/node is added to the path the input selection gets updated with all the nodes that it can access directly.

Parameters

- **db_path** – path to follow in the databases
- **input_values** – list of identifiers

Returns a dataframe with columns corresponding to the path nodes

A typical example is to get the Ensembl mouse homologs for Ensembl Gene ID's from human. This conversion is not possible through `db2db()` as Homologene does not have Ensembl ID's and the input and output nodes to acheive this would both be 'Ensembl Gene ID'. It can however be run by using dbWalk as follows. Add Ensembl Gene ID to the path, then add Gene Id, Homolog - Mouse Gene ID and Ensembl Gene ID to complete the path.

```
db_path = "Ensembl Gene ID->Gene ID->Homolog - Mouse Gene ID->Ensembl Gene ID"
s.dbWalk(db_path, ["ENSG00000175899"])
```

Todo: check validity of the path

getDirectOutputsForInput (*input_db*)

Gets all the direct output nodes for a given input node

Gets all the direct output nodes for a given input node Outputs reachable by single edge connection in the bioDBnet graph.

```
b.getDirectOutputsForInput("genesymbol")
b.getDirectOutputsForInput("Gene Symbol")
b.getDirectOutputsForInput("pdbid")
b.getDirectOutputsForInput("PDB ID")
```

getInputs ()

Return list of possible input database

```
s.getInputs()
```

getOutputsForInput (*input_db*)

Return list of possible output database for a given input database

```
s.getOutputsForInput("UniProt Accession")
```

2.10.4 BioGrid

This module provides a class BioGrid.

What is BioGrid ?

URL <http://thebiogrid.org/>

Service Via the PSICQUIC class

BioGRID is an online interaction repository with data compiled through comprehensive curation efforts. Our current index is version 3.2.97 and searches 37,954 publications for 638,453 raw protein and genetic interactions from major model organism species. All interaction data are freely provided through our search index and available via download in a wide variety of standardized formats.

—From BioGrid website, Feb. 2013

class BioGRID (*query=None, taxId=None, exP=None*)

Interface to BioGRID.

```
>>> from bioservices import BioGRID
>>> b = BioGRID(query=["map2k4", "akt1"], taxId = "9606")
>>> interactors = b.biogrid.interactors
```

Examples:

```
>>> from bioservices import BioGRID
>>> b = BioGRID(query=["mtor", "akt1"], taxId="9606", exP="two hybrid")
>>> b.biogrid.interactors
```

One can also query an entire organism, by using the taxid as the query:

```
>>> b = BioGRID(query="6239")
```

2.10.5 BioMart

This module provides a class `BioModels` that allows an easy access to all the BioModel service.

What is BioMart ?

URL <http://www.biomart.org/>

REST <http://www.biomart.org/martservice.html>

The BioMart project provides free software and data services to the international scientific community in order to foster scientific collaboration and facilitate the scientific discovery process. The project adheres to the open source philosophy that promotes collaboration and code reuse.

—from BioMart March 2013

Note: SOAP and REST are available. We use REST for the wrapping.

class BioMart (*host=None, verbose=False, cache=False, secure=False*)

Interface to the BioMart service

BioMart is made of different views. Each view correspond to a specific **MART**. For instance the UniProt service has a BioMart view.

The registry can help to find the different services available through BioMart.

```
>>> from bioservices import *
>>> s = BioMart()
>>> ret = s.registry() # to get information about existing services
```

The registry is a list of dictionaries. Some aliases are available to get all the names or databases:

```
>>> s.names      # alias to list of valid service names from registry
>>> "unimart" in s.names
True
```

Once you selected a view, you will want to select a database associated with this view and then a dataset. The datasets can be retrieved as follows:

```
>>> s.datasets("prod-intermart_1") # retrieve datasets available for this mart
```

The main issue is how to figure out the database name (here **prod-intermart_1**) ? Indeed, from the web site, what you see is the **displayName** and you must introspect the registry to get this information. In **BioServices**, we provide the `lookfor()` method to help you. For instance, to retrieve the database name of **interpro**, type:

```
>>> s = BioMart(verbose=False)
>>> s.lookfor("interpro")
Candidate:
  database: intermart_1
  MART name: prod-intermart_1
  displayName: INTERPRO (EBI UK)
  hosts: www.ebi.ac.uk
```

The display name (INTERPRO) correspond to the MART name `prod-intermart_1`. Let us you it to retrieve the datasets:

```
>>> s.datasets("prod-intermart_1")
['protein', 'entry', 'uniparc']
```

Now that we have the dataset names, we can select one and build a query. Queries are XML that contains the dataset name, some attributes and filters. The dataset name is one of the element returned by the `datasets` method. Let us suppose that we want to query **protein**, we need to add this dataset to the query:

```
>>> s.add_dataset_to_xml("protein")
```

Then, you can add attributes (one of the keys of the dictionary returned by `attributes("protein")`):

```
>>> s.add_attribute_to_xml("protein_accession")
```

Optional filters can be used:

```
>>> s.add_filter_to_xml("protein_length_greater_than", 1000)
```

Finally, you can retrieve the XML query:

```
>>> xml_query = s.get_xml()
```

and send the request to biomart:

```
>>> res = s.query(xml_query)
>>> len(res)
12801
# print the first 10 accession numbers
>>> res = res.split("\n")
>>> for x in res[0:10]: print(x)
['P18656',
 'Q81998',
```

(continues on next page)

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```
'O09585',
'O77624',
'Q9R3A1',
'E7QZH5',
'O46454',
'Q9T3F4',
'Q9TCA3',
'P72759']
```

REACTOME example:

```
s.lookfor("reactome")
s.datasets("REACTOME")
['interaction', 'complex', 'reaction', 'pathway']

s.new_query()
s.add_dataset_to_xml("pathway")
s.add_filter_to_xml("species_selection", "Homo sapiens")
s.add_attribute_to_xml("pathway_db_id")
s.add_attribute_to_xml("_displayname")
xmlq = s.biomartQuery.get_xml()
res = s.query(xmlq)
```

Note: the biomart service is slow (in my experience, 2013-2014) so please be patient...

Constructor

URL required to use biomart change quite often. Experience has shown that BioMart class in Bioservices may fail. This is not a bioservices issue but due to API changes on server side.

For that reason the host is not filled anymore and one must set it manually.

Let us take the example of the ensembl biomart. The host is

`www.ensembl.org`

Note that there is no prefix `http` and that the actual URL looked for internally is <http://www.ensembl.org/biomart/martview>

(It used to be `martservice` in 2012-2016)

Another reason to not set any default host is that servers may be busy or take lots of time to initialise (if many MARTS are available). Usually, one knows which MART to look at, in which case you may want to use a specific host (e.g., `www.ensembl.org`) that will speed up significantly the initialisation time.

Parameters `host` (*str*) – a valid host (e.g. “`www.ensembl.org`”, `gramene.org`)

List of databases are available in this webpage <http://www.biomart.org/community.html>

add_attribute_to_xml (*name*, *dataset=None*)

add_dataset_to_xml (*dataset*)

add_filter_to_xml (*name*, *value*, *dataset=None*)

attributes (*dataset*)

to retrieve attributes available for a dataset:

Parameters dataset (*str*) – e.g. oanatinus_gene_ensembl

configuration (*dataset*)

to retrieve configuration available for a dataset:

Parameters dataset (*str*) – e.g. oanatinus_gene_ensembl

create_attribute (*name, dataset=None*)

create_filter (*name, value, dataset=None*)

custom_query (***args*)

databases

list of valid datasets

datasets (*mart, raw=False*)

to retrieve datasets available for a mart:

Parameters mart (*str*) – e.g. ensembl. see [names](#) for a list of valid MART names the mart is the database. see [lookfor](#) method or [databases](#) attributes

```
>>> s = BioMart(verbose=False)
>>> s.datasets("prod-intermart_1")
['protein', 'entry', 'uniparc']
```

displayNames

list of valid datasets

filters (*dataset*)

to retrieve filters available for a dataset:

Parameters dataset (*str*) – e.g. oanatinus_gene_ensembl

```
>>> s.filters("uniprot").split("\n")[1].split("\t")
>>> s.filters("pathway")["species_selection"]
[Arabidopsis thaliana,Bos taurus,Caenorhabditis elegans,Canis familiaris,Danio rerio,Dictyostelium discoideum,Drosophila melanogaster,Escherichia coli,Gallus gallus,Homo sapiens,Mus musculus,Mycobacterium tuberculosis,Oryza sativa,Plasmodium falciparum,Rattus norvegicus,Saccharomyces cerevisiae,Schizosaccharomyces pombe,Staphylococcus aureus N315,Sus scrofa,Taeniopygia guttata ,Xenopus tropicalis]
```

get_datasets (*mart*)

Retrieve datasets with description

get_xml ()

host

hosts

list of valid hosts

lookfor (*pattern, verbose=True*)

marts

list of marts

names

list of valid datasets

new_query ()

query (*xmlq*)

Send a query to biomart

The query must be formatted in a XML format which looks like (example from <https://gist.github.com/keithshep/7776579>):

```
<?xml version="1.0" encoding="UTF-8"?>
  <!DOCTYPE Query>
    <Query virtualSchemaName="default" formatter="CSV" header="0"
  ↪uniqueRows="0" count="" datasetConfigVersion="0.6">
      <Dataset name="mmusculus_gene_ensembl" interface="default">
        <Filter name="ensembl_gene_id" value="ENSMUSG00000086981"/>
        <Attribute name="ensembl_gene_id"/>
        <Attribute name="ensembl_transcript_id"/>
        <Attribute name="transcript_start"/>
        <Attribute name="transcript_end"/>
        <Attribute name="exon_chrom_start"/>
        <Attribute name="exon_chrom_end"/>
      </Dataset>
    </Query>
```

Warning: the input XML must be valid. There is no validation made in this method.

registry ()

to retrieve registry information

the XML contains list of children called MartURLLocation made of attributes. We parse the xml to return a list of dictionary. each dictionary correspond to one MART.

aliases to some keys are provided: names, databases, displayNamees

valid_attributes

list of valid datasets

version (*mart*)

Returns version of a **mart**

Parameters **mart** (*str*) – e.g. ensembl

2.10.6 BioModels

This module provides a class *BioModels* to access to BioModels WS.

What is BioModels ?

URL <http://www.ebi.ac.uk/biomodels/>

Service <http://www.ebi.ac.uk/biomodels>

Citations please visit <https://www.ebi.ac.uk/biomodels/citation> for details

“BioModels is a repository of mathematical models of biological and biomedical systems. It hosts a vast selection of existing literature-based physiologically and pharmaceutically relevant mechanistic models in standard formats. Our mission is to provide the systems modelling community with reproducible, high-quality, freely-accessible models published in the scientific literature.”

—From BioModels website, March 2020

class BioModels (*verbose=True*)
Interface to the BioModels service

```
from bioservices import BioModels
bm = BioModels()
model = bm.get_model('BIOMD0000000299')
```

Previous API had several functions such as *getAuthorsByModelId*. This is easy to mimic with the new API:

```
bm = BioModels()
models = bm.get_all_models()
[x['submitter'] for x in res if x[] == "MODEL1204280003"][0]
```

This is also true for *getDateLastModifByModelId* and *getModelNameById* if one use the field *lastModified* or *name*. There was the ability to search for models based on their CHEBI identifiers, which is not supported anymore; this concerns functions *getModelIdsByChEBI*, *getModelIdsByChEBIID*, *getSimpleModelsByChEBIIDs*, *getSimpleModelsRelatedWithChEBI*. For other searches related to Reactome, Uniprot identifiers or GO terms, the *search()* method should work:

```
bm.search("P10113")
bm.search("REACT_33")
bm.search("GO:0006919")
```

constructor

Parameters *verbose* (*bool*) –

get_all_models (*chunk=100*)
Return all models

get_model (*model_id*, *frmt='json'*)
Fetch information about a given model at a particular revision.

get_model_download (*model_id*, *filename=None*, *output_filename=None*)
Download a particular file associated with a given model or all its files as a COMBINE archive.

Parameters

- **model_id** – a valid BioModels identifier
- **filename** (*str*) – this is the requested filename to be found in the model
- **output_filename** (*str*) – if you request a different output filename, use this parameter
- **frmt** – format of the output (json, xml, html)

Returns nothing. This function save the model into a ZIP file called after the model identifier. If parameter *filename* is specified, then the output file is the requested filename (if found)

```
bm.get_model_download("BIOMD0000000100", filename="BIOMD0000000100.png")
bm.get_model_download("BIOMD0000000100")
```

This function can retrieve all files in a ZIP archive or a single image. In the example below, we retrieve the PNG and plot it using matplotlib. Using your favorite image viewer, you should get a better resolution. Or just download the SVG version of the model.

```

from bioservices import BioModels
bm = BioModels()
from easydev import TempFile
with TempFile(suffix=".png") as fout:
    bm.get_model_download("BIOMD0000000100",
                          filename="BIOMD0000000100.png",
                          output_filename=fout.name)
from pylab import imshow, imread
imshow(imread(fout.name), aspect="auto")

```

get_model_files (*model_id*, *frmt*='json')

Extract metadata information of model files of a particular model

Parameters

- **model_id** – a valid BioModels identifier
- **frmt** – format of the output (json, xml)

get_p2m_missing (*frmt*='json')

Retrieve all models in Path2Models that are now only available indirectly, through the representative model for the corresponding genus

Parameters **frmt** (*str*) – the format of the result (xml, csv, json)

Returns list of model identifiers

get_p2m_representative (*model*, *frmt*='json')

Retrieve a representative model in Path2Models

Get the representative model identifier for a given missing model in Path2Models. This endpoint accepts as parameters a mandatory model identifier and an optional response format

Parameters

- **model** (*str*) – The identifier of a model of interest
- **frmt** (*str*) – the format of the result (xml, csv, json)

get_p2m_representatives (*models*, *frmt*='json')

Find the replacement accessions for a set of Path2Models entries

Get the representative model identifiers of a set of given missing models in Path2Models. This end point expects a comma-separated list of model identifiers (without any surrounding whitespace) and an optional response format. Examples: BMID000000112902, BMID000000009880, BMID000000027397.

Parameters

- **model** (*str*) – The model identifiers separated by commas, or as a list.
- **frmt** (*str*) – the format of the result (xml, csv, json)

```

from bioservices import BioModels
bm = BioModels()
bm.get_p2m_representatives("BMID000000112902, BMID000000009880, ↵
↵BMID000000027397")

```

get_pdgsmm_missing (*frmt*='json')

Retrieve the identifiers of all PDGSMM entries that are no longer directly accessible

Parameters **frmt** (*str*) – the format of the result (xml, csv, json)

Returns list of model identifiers

get_pdgsmm_representative (*model*, *frmt*='json')

Retrieve a representative model in PDGSMM

Get the representative model identifier for a given missing model in PDGSMM. This endpoint accepts as parameters a mandatory model identifier and an optional response format.

Parameters

- **model** (*str*) – The identifier of a model of interest
- **frmt** (*str*) – the format of the result (xml, csv, json)

get_pdgsmm_representatives (*models*, *frmt*='json')

Find the replacement accessions for a set of PDFSSM

Get the representative model identifiers of a set of given missing models in PDGSMM. This end point expects a comma-separated list of model identifiers (without any surrounding whitespace) and an optional response format. Examples: MODEL1707110145,MODEL1707112456,MODEL1707115900.

Parameters

- **model** (*str*) – The model identifiers separated by commas, or as a list.
- **frmt** (*str*) – the format of the result (xml, csv, json)

search (*query*, *offset*=None, *numResults*=None, *sort*=None, *frmt*='json')

Search models of interest via keywords.

Examples: PUBMED:"27869123" to search models associated with the PubMed record identified by 27869123.

Parameters

- **query** (*str*) – search query. colon character must be escaped
- **offset** (*int*) – number of items to skip before starting to collect the result set
- **numResults** (*int*) – number of items to return
- **sort** (*str*) – sort criteria in {id-asc, relevance-asc, relevance-desc, first_author-asc, first_author, name-asc, name-desc, publication_year-asc, publication_year-desc}
- **frmt** (*str*) – format of the output (json, xml)

search_download (*models*, *output_filename*='models.zip', *force*=False)

Returns models (XML) corresponding to a list of model identifiers.

Parameters

- **models** (*str*) – list of model identifiers using comma to separate them. Could be a list of string (e.g 'BIOMD1,BIOMD2' or ['BIOMD1', 'BIOMD2'])
- **output_filename** (*str*) – file used to save the models. This is a zipped file. If the file exists, you must use the *force** parameter

Todo: if no models are found (typos), an error message is printed. if one model is not found, there is no warning or errors. Could be nice to have a warning by introspecting the number of models in the output file

search_parameter (*query*, *start*=0, *size*=10, *sort*=None, *frmt*='json')

Search for parameters of a model

Details BioModels Parameters is a resource that facilitates easy search and retrieval of parameter values used in the SBML models stored in the BioModels repository. Users can search for a model entity (e.g.

a protein or drug) to retrieve the rate equations describing it; the associated parameter values and the initial concentration from the SBML models in BioModels. Although these data are directly extracted from the curated SBML models, they are not individually curated or validated; rather presented as such in the table below. Hence BioModels Parameters table will only provide a quick overview of available parameter values for guidance and original model should be referred to understand the complete context of the parameter usage.

Parameters

- **query** (*str*) – A query to search against the model parameter values.
- **start** (*int*) – if is the offset of the result set (default 0)
- **size** (*int*) – number of items to display per page
- **sort** (*str*) – model or entity
- **frmt** (*str*) – the format of the result (xml, csv, json)

```
bm.search_parameter("MAPK", size=100, sort="entity")
```

2.10.7 ChEBI

This module provides a class *ChEBI*

What is ChEBI

URL <https://www.ebi.ac.uk/chebi/init.do>

WSDL <http://www.ebi.ac.uk/webservices/chebi/2.0/webservice>

“The database and ontology of Chemical Entities of Biological Interest

—From ChEBI web page June 2013

class ChEBI (*verbose=False*)

Interface to *ChEBI*

```
>>> from bioservices import *
>>> ch = ChEBI()
>>> res = ch.getCompleteEntity("CHEBI:27732")
>>> res.smiles
CN1C(=O)N(C)c2ncn(C)c2C1=O
```

Constructor

Parameters *verbose* (*bool*) –

conv (*chebiId*, *target*)

Calls *getCompleteEntity()* and returns the identifier of a given database

Parameters

- **chebiId** (*str*) – a valid ChEBI identifier (string)
- **target** – the identifier of the database

Returns the identifier

```
>>> ch.conv("CHEBI:10102", "KEGG COMPOUND accession")
['C07484']
```

getAllOntologyChildrenInPath (*chebiId*, *relationshipType*, *onlyWithChemicalStructure=False*)

Retrieves the ontology children of an entity including the relationship type

Parameters

- **chebiId** (*str*) – a valid ChEBI identifier (string)
- **relationshipType** (*str*) – one of “is a”, “has part”, “has role”, “is conjugate base of”, “is conjugate acid of”, “is tautomer of”, “is enantiomer of”, “has functional parent”, “has parent hybride”, “is substituent group of”

```
>>> ch.getAllOntologyChildrenInPath("CHEBI:27732", "has part")
```

getCompleteEntity (*chebiId*)

Retrieves the complete entity including synonyms, database links and chemical structures, using the ChEBI identifier.

param str chebiId a valid ChEBI identifier (string)

return an object containing fields such as mass, names, smiles

```
>>> from bioservices import *
>>> ch = ChEBI()
>>> res = ch.getCompleteEntity("CHEBI:27732")
>>> res.mass
194.19076
```

The returned structure is the raw object returned by the API. You can extract names from other sources for instance:

```
>>> [x[0] for x in res.DatabaseLinks if x[1].startswith("KEGG")]
[C07481, D00528]
>>> [x[0] for x in res.DatabaseLinks if x[1].startswith("ChEMBL")]
[116485]
```

See also:

conv(), *getCompleteEntity()*

getCompleteEntityByList (*chebiIdList=[]*)

Given a list of ChEBI accession numbers, retrieve the complete Entities.

The maximum size of this list is 50.

See also:

getCompleteEntity()

getLiteEntity (*search*, *searchCategory='ALL'*, *maximumResults=200*, *stars='ALL'*)

Retrieves list of entities containing the ChEBI ASCII name or identifier

Parameters

- **search** – search string or category.
- **searchCategory** – filter with category. Can be ALL,
- **maximumResults** (*int*) – (default is 200)

- **stars** (*str*) – filters that can be set to “TWO ONLY”, “ALL”, “THREE ONLY”

The input parameters are a search string and a search category. If the search category is null then it will search under all fields. The search string accepts the wildcard character “*” and also unicode characters. You can get maximum results upto 5000 entries at a time.

```
>>> ch.getLiteEntity("CHEBI:27732")
[(LiteEntity){
  chebiId = "CHEBI:27732"
  chebiAsciiName = "caffeine"
  searchScore = 4.77
  entityStar = 3
}]
>>> res = ch.getLiteEntity("caffeine")
>>> res = ch.getLiteEntity("caffeine", maximumResults=10)
>>> len(res)
10
```

See also:

`getCompleteEntity()`

getOntologyChildren (*chebiId*)

Retrieves the ontology children of an entity including the relationship type

Parameters **chebiId** (*str*) – a valid ChEBI identifier (string)

getOntologyParents (*chebiId*)

Retrieves the ontology parents of an entity including the relationship type

Parameters **chebiId** (*str*) – a valid ChEBI identifier (string)

getStructureSearch (*structure*, *mode*='MOLFILE', *structureSearchCategory*='SIMILARITY', *totalResults*=50, *tanimotoCutoff*=0.25)

Does a substructure, similarity or identity search using a structure.

Parameters

- **structure** (*str*) – the input structure
- **mode** (*str*) – type of input (MOLFILE, SMILES, CML) (note that the API uses type but this is a python keyword)
- **structureSearchCategory** (*str*) – category of the search. Can be “SIMILARITY”, “SUBSTRUCTURE”, “IDENTITY”
- **totalResults** (*int*) – limit the number of results to 50 (default)
- **tanimotoCutoff** – limit results to scores higher than this parameter

```
>>> ch = ChEBI()
>>> smiles = ch.getCompleteEntity("CHEBI:27732").smiles
>>> ch.getStructureSearch(smiles, "SMILES", "SIMILARITY", 3, 0.25)
```

getUpdatedPolymer (*chebiId*)

Returns the UpdatedPolymer object

Parameters

- **chebiId** (*str*) –
- **chebiId** – a valid ChEBI identifier (string)

Returns an object with information as described below.

The object contains the updated 2D MolFile structure, GlobalFormula string containing the formulae for each repeating-unit, the GlobalCharge string containing the charge on individual repeating-units and the primary ChEBI ID of the polymer, even if the secondary Identifier was passed to the web-service.

2.10.8 ChEMBL

This module provides a class *ChEMBL*

What is ChEMBL

URL <https://www.ebi.ac.uk/chembl>

REST <https://www.ebi.ac.uk/chembl/api/data>

“Using the ChEMBL web service API users can retrieve data from the ChEMBL database in a programmatic fashion. The following list defines the currently supported functionality and defines the expected inputs and outputs of each method.”

—From ChEMBL web page Dec 2012

class ChEMBL (*verbose=False, cache=False*)
New ChEMBL API bioservices 1.6.0

Resources

ChEMBL database is made of a set of resources. We recommend to look at <https://arxiv.org/pdf/1607.00378.pdf>

Here we first create an instance and retrieve the first 1000 molecules from the database using the **limit** parameter.

```
>>> from bioservices import ChEMBL
>>> c = ChEMBL()
>>> res = c.get_molecule(limit=1000)
```

The returned object is a list of 1000 records, each of them being a dictionary. The **molecule** resource is actually a very large one and one may want to skip some entries. This is possible using the **offset** parameter as follows:

```
# Retrieve 1000 molecules skipping the first 50
res = c.get_molecule(limit=1000, offset=50)
```

If you want to know all resources available and the number of entries in each resources, use:

```
status = c.get_status_resources()
```

For instance, you should be able to get the total number of entries in the *mechanism* resource is about 5,000:

```
print(status['mechanism'])
```

To retrieve all entries from the mechanism resource, you can either set limit to a value large enough:

```
res = c.get_mechanism(limit=1000000)
```

or simply set it to -1:

```
res = c.get_mechanism(limit=-1)
```

All resources methods behaves in the same way.

Those resources methods are: `get_activity()`, `get_assay()`, `get_atc_class()`, `get_binding_site()`, `get_biotherapeutic()`, `get_cell_line()`, `get_chembl_id_lookup()`, `get_compound_record()`, `get_compound_structural_alert()`, `get_document()`, `get_document_similarity()`, `get_document_term()`, `get_drug()`, `get_drug_indication()`, `get_go_slim()`, `get_mechanism()`, `get_metabolism()`, `get_molecule()`, `get_molecule_form()`, `get_protein_class()`, `get_source()`, `get_target()`, `get_target_component()`, `get_target_prediction()`, `get_target_relation()`, `get_tissue()`.

3 ways of getting items

1. Retrieve everything:

```
c.get_molecule(limit=-1)
```

2. Retrieve a specific entry:

```
c.get_molecule("CHEMBL24")
```

3. Retrieve a set of entries:

```
c.get_molecule(["CHEMBL24", "CHEMBL2"])
```

Filtering and Ordering

For ordering the results, we provide a simple method `order_by()` that allows to sort the dictionary according to values in a specific key.

Any data returned by a resource method (a list of dictionary) can be process through this method:

```
c = ChEMBL()
data = c.get_drug(limit=100)
ordered_data = c.order_by(data, 'chirality')
```

If you want to order using a key within a key, for instance order by molecular weight stored in the *molecular_properties* key, use the double underscore method as follows:

```
c = ChEMBL()
data = c.get_drug(limit=100)
ordered_data = c.order_by(data, 'molecular_properties__mw_freebase')
```

For filtering, it is possible to apply search filters to any resources. For example, it is possible to return all ChEMBL targets that contain the term 'kinase' in the `pref_name` attribute:

```
c.get_target(filters='pref_name__contains=kinase')
```

The pattern for applying a filter is as follows:

```
[field]__[filter_type]=[value]
```

where field has to be found by the user. Simply introspect the content of an item returned by the resource. For instance:

```
c.get_target(limit=1) # to get one entry
```

Let us consider the case of the **molecule** resource. You can retrieve the first 10 molecules using e.g.:

```
res = c.get_molecule(limit=10)
```

If you look at the first entry using `res[0]`, you will get about 38 keys. For instance **molecule_properties** or **molecule_chembl_id**.

You can filter the molecules to keep only the `molecule_chembl_id` that match either CHEMBL25 or CHEMBL1000 using:

```
res = c.get_molecule(filters='molecule_chembl_id__in=CHEMBL25,CHEMBL1000')
```

For **molecule_properties**, this is actually a dictionary. For instance, inside the **molecule_properties** field, you have the molecular weight (`mw_freebase`). So to apply this filter, you need to use the following code (to keep molecules with molecular weight greater than 300):

```
res = c.get_molecule(filters='molecule_properties__mw_freebase__gte=300')
```

Here are the different types of filtering:

Filter Type	Description
exact (iexact)	Exact match with query
contains	wild card search with query
startswith	starts with query
endswith	ends with query
regex	regular expression query
gt (gte)	Greater than (or equal)
lt (lte)	Less than (or equal)
range	Within a range of values
in	Appears within list of query values
isnull	Field is null
search	Special type of filter allowing a full text search based on Solr queries.

Several filters can be applied at the same time using a list:

```
filters = ['molecule_properties__mw_freebase__gte=300']
filters += ['molecule_properties__alogp__gte=3']
res = c.get_molecule(filters)
```

Use Cases: (inspired from ChEMBL documentation)

Search molecules by synonym:

```
>>> from bioservices import ChEMBL
>>> c = ChEMBL()
>>> res = c.search_molecule('aspirin')
```

or SMILE, or InChiKey, or CHEMBLID:

```
>>> res = c.get_molecule("CC(=O)Oc1ccccc1C(=O)O")
>>> res = c.get_molecule("BSYNRYMUTXBXSQ-UHFFFAOYSA-N")
>>> res = c.get_molecule('CHEMBL25')
```

Several molecules at the same time can also be retrieved using lists:

```
>>> res = c.get_molecule(['CHEMBL25', 'CHEMBL2'])
```

Search target by gene name:

```
>>> res = c.search_target("GABRB2")
>>> len(res['targets'])
18
```

or directly in the target synonym field:

```
>>> res = c.get_target(filters='target_synonym__icontains=GABRB2')
```

Note: Not sure what is the difference between `icontains` vs `contains`. It looks like `icontains` is more permissive (you get more entries with `icontains`).

Having a list of molecules ChEMBL IDs in a list, get uniprot accession numbers that map to those compounds:

```
# First, get some IDs of approved drugs (about 2000 molecules)
c = ChEMBL()
drugs = c.get_approved_drugs()
IDs = [x['molecule_chembl_id'] for x in drugs]

# we jump from compounds to targets through activities
# Here this is a one to many mapping so we initialise a default
# dictionary.
compound2target = defaultdict(set)

filter = "molecule_chembl_id__in={"
for i in range(0, len(IDs), 50):
    activities = c.get_activity(filter.format(IDs[i:i+50]))
    # get target ChEMBL IDs from activities
    for act in activities:
        compound2target[act['molecule_chembl_id']].add(act['target_chembl_id'])

# What we need is to get targets for all targets found in the previous
# step. For each compound/drug there are hundreds of targets though. And
# we will call the get_target for each list of hundreds targets. This
# will take forever. Instead, because there are *only* 12,000 targets,
# let us download all of them ! This took about 4 minutes on this test but
# if you use the cache, next time it will be much much quicker. This is
# not down at the activities level because there are too many entries

targets = c.get_target(limit=-1)

# identifies all target chembl id to easily retrieve the entry later on
target_names = [target['target_chembl_id'] for target in targets]

# retrieve all uniprot accessions for all targets of each compound
for compound, targs in compounds2targets.items():
    accessions = set()
    for target in targs:
        index = target_names.index(target)
        accessions = accessions.union([comp['accession']
                                     for comp in targets[index]['target_components']])
    compounds2targets[compound] = accessions
```

In version 1.6.0 of bioservices, you can simply use:

```
res = c.compounds2targets(IDs)
```

Get Target type count for all targets:

```
import collections
collections.Counter([x['target_type'] for x in targets])
```

Find compounds similar to given SMILES query with similarity threshold of 85%:

```
>>> SMILE = "CN(CCCN)c1cccc2ccccc12"
>>> c.get_similarity(SMILE, similarity=70)
```

Find compounds similar to aspirin (ChEMBL25) with similarity threshold of 70%:

```
# search for aspirin in all molecules and from first hit
# get the ChEMBL ID
>>> molecules = c.search_molecule("aspirin")['molecules']
>>> chembl_id = molecules[0]['molecule_chembl_id']
# now use the :meth:`get_similarity` given the ID
>>> res = c.get_similarity(chembl_id, similarity=70)
```

Perform substructure search using SMILES or ChEMBLID:

```
>>> res = c.get_substructure("CN(CCCN)c1cccc2ccccc12")
>>> res = c.get_substructure("CHEMBL25")
```

Obtain the pChEMBL value for compound:

```
res = c.get_activity(filters=['pchembl_value__isnull=False',
                             'molecule_chembl_id=CHEMBL25'])
```

Obtain the pChEMBL value for compound and target:

```
res = c.get_activity(filters=['pchembl_value__isnull=False',
                             'molecule_chembl_id=CHEMBL25',
                             'target_chembl_id=CHEMBL612545'])
```

Get all approved drugs:

```
c.get_approved_drugs(max_phase=4)
```

Get approved drugs for lung cancer

The ChEMBL API significantly changed in 2018 and the new version of bioservices (1.6.0) had to change the API as well, which has been simplified.

Here below are some correspondances between the previous and the new API.

bioservices before 1.6.0	After 1.6.0
get_compounds_substructure	get_substructure
get_compounds_similar_to_SMILES	get_similarity(SMILE)
get_compounds_by_chemblId(ID)	get_similarity(ID)
get_individual_compounds_by_inChiKey	get_molecule(inchikey)
get_compounds_by_chemblId_form	get_molecule_form
get_compounds_by_chemblId_drug_mechanism	get_mechanism(ID)
get_target_by_chemblId(ID)	get_target(ID)
get_image_of_compounds_by_chemblId	get_image
etc	

References

- <https://arxiv.org/pdf/1607.00378.pdf>
- <https://www.ebi.ac.uk/chembl/api/data/docs>

compounds2accession (*compounds*)

For each compound, identifies the target and corresponding UniProt accession number

This is not part of ChEMBL API

```
# we recommend to use cache if you use this method regularly
c = Chembl(cache=True)
drugs = c.get_approved_drugs()

# to speed up example
drugs = drugs[0:20]
IDs = [x['molecule_chembl_id'] for x in drugs]

c.compounds2accession(IDs)
```

get_ATC (*limit=20, offset=0, filters=None*)

WHO ATC Classification for drugs

`c.get_atc() c['atc']`

Note: `get_molecule` returns 'molecules' and likewise all methods return a dictionary whose key is the plural of the method name. This is quite consistent through the API except for that one because it is an acronym

get_activity (*query=None, limit=20, offset=0, filters=None*)

Activity values recorded in an Assay

get_approved_drugs (*max_phase=4, maxdrugs=1000000*)

Return all approved drugs

Parameters `max_phase` – 4 by default for approved drugs.

get_assay (*query=None, limit=20, offset=0, filters=None*)

Assay details as reported in source Document/Dataset

```
>>> c.get_assay("CHEMBL1217643")
```

get_binding_site (*limit=20, offset=0, filters=None*)

Target binding site definition

get_biotherapeutic (*limit=20, offset=0, filters=None*)

Biotherapeutic molecules, which includes HELM notation and sequence data

get_cell_line (*limit=20, offset=0, filters=None*)

Cell line information

get_chembl_id_lookup (*query=None, limit=20, offset=0, filters=None*)

Look up ChEMBL Id entity type

get_compound_record (*query=None, limit=20, offset=0, filters=None*)

Occurrence of a given compound in a specific document

get_compound_structural_alert (*query=None, limit=20, offset=0, filters=None*)

Indicates certain anomaly in compound structure

- get_document** (*query=None, limit=20, offset=0, filters=None*)
Document/Dataset from which Assays have been extracted
- get_document_similarity** (*query=None, limit=20, offset=0, filters=None*)
Provides documents similar to a given one
- get_document_term** (*query=None, limit=20, offset=0, filters=None*)
Provides keywords extracted from a document using the TextRank algorithm
- get_drug** (*query=None, limit=20, offset=0, filters=None*)
Approved drugs information, including (but not limited to) applicants, patent numbers and research codes
- get_drug_indication** (*query=None, limit=20, offset=0, filters=None*)
Joins drugs with diseases providing references to relevant sources
- get_go_slim** (*query=None, limit=20, offset=0, filters=None*)
GO slim ontology
- get_image** (*query, dimensions=500, format='png', save=True, view=True, engine='indigo'*)
Get the image of a given compound in PNG png format.

Parameters

- **query** (*str*) – a valid compound ChEMBLId or a list/tuple of valid compound ChEMBLIds.
- **format** – png, svg. json not supported
- **dimensions** (*int*) – size of image in pixels. An integer z ($1 \leq z \leq 500$)
- **save** –
- **view** (*bool*) –
- **engine** – Defaults to rdkit. can be rdkit or indigo
- **view** – show the image if set to True.

Returns the path (list of paths) used to save the figure (figures) (different from ChEMBL API)

```
>>> from pylab import imread, imshow
>>> from bioservices import *
>>> s = ChEMBL(verbose=False)
>>> res = s.get_image(31863)
>>> imshow(imread(res['filenames'][0]))
```

Todo: ignorecoords option

- get_mechanism** (*query=None, limit=20, offset=0, filters=None*)
Mechanism of action information for FDA-approved drugs
- get_metabolism** (*query=None, limit=20, offset=0, filters=None*)
Metabolic pathways with references
- get_molecule** (*query=None, limit=20, offset=0, filters=None*)
Returns some molecules

Parameters

- **limit** – number of molecules to retrieve
- **offset** – molecules to ignore before retrieving molecules.

Returns a dictionary with keys *page_meta* and *molecules*.

There are 1,800,000 molecules (Jan 2019). You can only retrieve 1,000 molecule at most using the *limit* parameter. With a loop you can retrieve molecules in some range.

```
c.get_molecule('QFFGVLORLPOAEC-SNVBAGLBSA-N')
c.get_molecule("CC(=O)Oc1ccccc1C(=O)O")
```

get_molecule_form (*query=None, limit=20, offset=0, filters=None*)

Relationships between molecule parents and salts

```
>>> s.get_molecule_form("CHEMBL2") ['molecule_forms']
[{'is_parent': 'True',
  'molecule_chembl_id': 'CHEMBL2',
  'parent_chembl_id': 'CHEMBL2'},
 {'is_parent': 'False',
  'molecule_chembl_id': 'CHEMBL1558',
  'parent_chembl_id': 'CHEMBL2'},
 {'is_parent': 'False',
  'molecule_chembl_id': 'CHEMBL1347191',
  'parent_chembl_id': 'CHEMBL2'}]
```

get_organism (*query=None, limit=20, offset=0, filters=None*)

get_protein_class (*query=None, limit=20, offset=0, filters=None*)

Protein family classification of TargetComponents

get_similarity (*structure, similarity=80, limit=20, offset=0, filters=None*)

Molecule similarity search

Parameters

- **structure** – provide a valid / existing substructure in SMILE format to look for in all molecules:
- **similarity** – must be an integer greater than 70 and less than 100

Returns list of **molecules** corresponding to the search

```
>>> from bioservices import ChEMBL
>>> c = ChEMBL()
>>> res = c.get_similarity("CC(=O)Oc1ccccc1C(=O)O", 80)
>>> res['molecules']
```

Here are more examples:

```
# Similarity (80% cut off) search for against ChEMBL using
# aspirin SMILES string
c.get_similarity("CC(=O)Oc1ccccc1C(=O)O") # 80 by default

# Similarity (80% cut off) search for against ChEMBL using
# aspirin CHEMBL_ID
c.get_similarity("CHEMBL25")

# Similarity (80% cut off) search for against ChEMBL
# using aspirin InChI Key
c.get_similarity("BSYNYMUTXBXSQ-UHFFFAOYSA-N")
```

The ‘Substructure’ and ‘Similarity’ web service resources allow for the chemical content of ChEMBL to be searched. Similar to the other resources, these search based resources except filtering, paging and

ordering arguments. These methods accept SMILES, InChI Key and molecule ChEMBL_ID as arguments and in the case of similarity searches an additional identity cut-off is needed. Some example molecule searches are provided in the table below.

Searching with InChI key is only possible for InChI keys found in the ChEMBL database. The system does not try and convert InChI key to a chemical representation.

get_source (*query=None, limit=20, offset=0, filters=None*)
Document/Dataset source

get_status ()
Return version of the DB and number of entries

Returns the number of entries for activities, compound_records, distinct_compounds (molecule), publications (document), targets, etc...

See also:

get_status_resources ()

get_status_resources ()
Return number of entries for all resources

Note: not in the ChEMBL API.

Changed in version 1.7.3: (removed target_prediction and document_term)

get_substructure (*structure, limit=20, offset=0, filters=None*)
Molecule substructure search

Parameters structure – provide a valid / existing substructure in SMILE format to look for in all molecules:

Returns list of molecules corresponding to the search

```
>>> from bioservices import ChEMBL
>>> c = ChEMBL()
>>> res = c.get_substructure("CC(=O)Oc1ccccc1C(=O)O")
```

Other examples:

```
# Substructure search for against ChEMBL using aspirin
# SMILES string
c.get_substructure("CC(=O)Oc1ccccc1C(=O)O")

# Substructure search for against ChEMBL using aspirin
# ChEMBL_ID
c.get_substructure("CHEMBL25")

# Substructure search for against ChEMBL using aspirin
# InChIKey
c.get_substructure("BSYNYMUTXBXSQ-UHFFFAOYSA-N")
```

The ‘Substructure’ and ‘Similarity’ web service resources allow for the chemical content of ChEMBL to be searched. Similar to the other resources, these search based resources except filtering, paging and ordering arguments. These methods accept SMILES, InChI Key and molecule ChEMBL_ID as arguments and in the case of similarity searches an additional identity cut-off is needed. Some example molecule searches are provided in the table below.

Searching with InChI key is only possible for InChI keys found in the ChEMBL database. The system does not try and convert InChI key to a chemical representation.

get_target (*query=None, limit=20, offset=0, filters=None*)

Targets (protein and non-protein) defined in Assay

```
>>> from bioservices import *
>>> s = ChEMBL(verbose=False)
>>> resjson = s.get_targetd('CHEMBL240')
```

get_target_component (*query=None, limit=20, offset=0, filters=None*)

Target sequence information (A Target may have 1 or more sequences)

```
res = c.get_target_component(1)
res['sequence']
```

get_target_prediction (*query=None, limit=20, offset=0, filters=None*)

Predicted binding of a molecule to a given biological target

```
>>> res = c.get_target_prediction(1)
>>> res['molecule_chembl_id']
'CHEMBL2'
```

get_target_relation (*query=None, limit=20, offset=0, filters=None*)

Describes relations between targets

```
>>> c.get_target_relation('CHEMBL261')
{'related_target_chembl_id': 'CHEMBL2095180',
 'relationship': 'SUBSET OF',
 'target_chembl_id': 'CHEMBL261'}
```

get_tissue (*query=None, limit=20, offset=0, filters=None*)

Tissue classification

```
c.get_tissue(filters=['pref_name__contains=cervix'])
```

get_xref_source (*query=None, limit=20, offset=0, filters=None*)

order_by (*data, name, ascending=True*)

Ordering data

we use same API as ChEMBL API using the double underscore to indicate a hierarchy in the dictionary. So to access to d['a']['b'], we use a__b as the input **name** parameter. We only allows 3 levels e.g., a__b__c

```
data = c.get_molecules()
data1 = c.order_by(data, 'molecule_chembl_id')
data2 = c.order_by(data, 'molecule_properties__alogp')
```

Note: the ChEMBL API allows for ordering but we do not use that API. Instead, we provide this generic function.

search_activity (*query, limit=20, offset=0*)

Activity values recorded in an Assay

search_assay (*query, limit=20, offset=0*)

Assay details as reported in source document

search_chembl_id_lookup (*query, limit=20, offset=0*)

Look up ChEMBL Id entity type

search_document (*query, limit=20, offset=0*)

Document/Dataset from which Assays have been extracted

search_molecule (*query, limit=20, offset=0*)

search_protein_class (*query, limit=20, offset=0*)

search_target (*query, limit=20, offset=0*)

Targets (protein and non-protein) defined in Assay

2.10.9 ChemSpider

Interface to the ArrayExpress web Service.

What is ChemSpider ?

Status in progress

URL <http://www.chemspider.com/>

REST <http://www.chemspider.com/AboutServices.aspx?>

ChemSpider is a free chemical structure database providing fast access to over 28 million structures, properties and associated information. By integrating and linking compounds from more than 400 data sources, ChemSpider enables researchers to discover the most comprehensive view of freely available chemical data from a single online search. It is owned by the Royal Society of Chemistry.

—ChemSpider home page, March 2013

class ChemSpider (*verbose=False, token=None, cache=False*)

ChemSpider Web Service Interface

Status in progress you can already search for Id and compound or retrieve the chemical image of an Id

```
>>> from bioservices import *
>>> s = ChemSpider()
>>> s.find("Pyridine")
[1020]
>>> results = s.GetExtendedCompoundInfo(1020)
>>> results['averagemass']
79.0999
```

GetExtendedCompoundInfo (*Id*)

ImagesHandler (*Id*)

databases

Returns databases searched for in chemSpider

find (*query*)

return the first 100 compounds that match the query

image (*Id*)

Return string containing PNG binary image data of 2D structure image

```

>>> from bioservices import *
>>> s = ChemSpider()
>>> ret = s.image(1020)
>>> with open("test.png", "w") as f:
...     f.write(ret)
>>> s.on_web("test.png")

```

mol (*Id*)

Return record in MOL format

mol3d (*Id*)

Return record in MOL format with 3D coordinates calculated

token

2.10.10 Clinvitae

class Clinvitae

class for interfacing with the Clinvitae web service

Requests will return a list of json dicts. each dict has the following fields:

```

accessionId
gene
nucleotideChanges
description
classification
reportedClassification
url
region
proteinChange
lastUpdated
alias
source
acmgClassification
submitter
defaultNucleotideChange
_id
transcripts
lastEvaluated

```

example query on BRCA1:

```

>>> c = Clinvitae()
>>> res = c.query_gene('brca1')
>>> entry1 = res[0]
>>> print(entry1.keys()) # display fields for first entry
>>> print(entry1['accessionId']) # accession id for first entry
>>> print(entry1['lastEvaluated']) # date first variant entry was last evaluated
>>> print(entry1['source']) # source of first variant entry

```

all_variants (*gene*)

returns a list of unique hgvs tags reported in gene

```

>>> c = Clinvitae()
>>> res = c.all_variants('MUTYH') # returns all reported variants in MUTYH_
↪gene

```

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(continued from previous page)

```
>>> print(res[0:5])
[u'NM_001048171.1:c.-2188C>T',
u'NM_001048171.1:c.462+35A>G',
u'NM_001048171.1:c.1099G>T',
u'NM_001048171.1:c.972G>C',
u'NM_001048171.1:c.1476+35C>T']
```

get_VUS (*gene*)

returns all fields for entries not classified as benign or pathogenic -> variant of unknown significance (VUS)

```
>>> c = Clinvitae()
>>> vus = c.get_VUS('brca1')
>>> len(vus) # number of benign variants
2389
```

get_benign (*gene*)

returns all fields for entries reported as Benign by any source in Clinvitae

```
>>> c = Clinvitae()
>>> benign = c.get_benign('brca1') # returns benign or likely benign
>>> len(benign) # number of benign variants
187
```

get_pathogenic (*gene*)

returns all fields for entries reported as Pathogenic by any source in Clinvitae

```
>>> c = Clinvitae()
>>> pathogenic = c.get_pathogenic('brca1') # returns pathogenic or likely_
↳pathogenic
>>> len(pathogenic) # number of pathogenic variants
1100
```

query_gene (*gene*)

takes gene name and returns json of variants in gene (not case sensitive)

```
>>> c = Clinvitae()
>>> res = c.query_gene('brca1')
>>> entry1 = res[0]
>>> print(entry1['accessionId']) # accession id for first entry
u'SCV000039520'
>>> print(entry1['lastEvaluated']) # date first variant entry was last_
↳evaluated
u'2013-04-03'
>>> print(entry1['source']) # source of first variant entry
u'ClinVar'
```

query_hgvs (*hgvs*)

Takes an hgvs (variant) tag and returns ALL reported variants in the gene in which hgvs is located

```
>>> c = Clinvitae()
>>> res = c.query_gene('NM_198578.3:c.1847A>G') # returns all entries in_
↳LRRK2 gene
>>> entry1 = res[0]
>>> print(entry1['accessionId']) # accession id for first entry
u'SCV000056058'
```

(continues on next page)

(continued from previous page)

```
>>> print(entry1['lastEvaluated']) # date first variant entry was last_
↪evaluated
u'2012-09-13'
>>> print(entry1['source']) # source of first variant entry
u'ClinVar'
```

2.10.11 ENA

This module provides a class *ENA*

What is ENA

URL <https://www.ebi.ac.uk/ena>

The European Nucleotide Archive (ENA) provides a comprehensive record of the world's nucleotide sequencing information, covering raw sequencing data, sequence assembly information and functional annotation.

—From ENA web page Jan 2016

New in version 1.4.4.

class ENA (*verbose=False, cache=False*)

Interface to ChEMBL

Here is a quick example to retrieve a target given its ChEMBL Id

```
>>> from bioservices import ENQ
>>> s = ENA(verbose=False)
```

Retrieve read domain metadata in XML format:

```
print(e.get_data('ERA000092', 'xml'))
```

Retrieve assemble and annotated sequences in fasta format:

```
print(e.get_data('A00145', 'fasta'))
```

The range parameter can be used in combination to retrieve a subsequence from sequence entry A00145 from bases 3 to 63 using

```
e.get_data('A00145', 'fasta', fasta_range=[3,63])
```

Retrieve assembled and annotated subsequences in HTML format (same as above but in HTML page).

```
e.view_data('A00145')
```

Retrieve expanded CON records:

To retrieve expanded CON records use the `expanded=True` parameter. For example, the expanded CON entry AL513382 in flat file format can be obtained as follows:

```
e.get_data('AL513382', frmt='text', expanded=True)
```

Expanded CON records are different from CON records in two ways. Firstly, the expanded CON records contain the full sequence in addition to the contig assembly instructions. Secondly, if a CON record contains only source or gap features the expanded CON records will also display all features from the segment records.

Retrieve assembled and annotated sequence header in flat file format

To retrieve assembled and annotated sequence header in flat file format please use the `header=true` parameter, e.g.:

```
e.get_data('BN000065', 'text', header=True)
```

Retrieve assembled and annotated sequence records using sequence versions:

```
e.get_data('AM407889.1', 'fasta')
e.get_data('AM407889.2', 'fasta')
```

Constructor

Parameters `verbose` – set to `False` to prevent informative messages

`data_warehouse` ()

`get_data` (*identifier*, *frmt*, *fasta_range=None*, *expanded=None*, *header=None*, *download=None*)

:param frmt [xml, text, fasta, fastq, html, embl but does depend on the] entry

Example:

```
get_data("/AL513382", "embl")
```

ENA API changed in 2020 but we tried to keep the same services in this method.

`get_taxon` (*taxon*)

```
url = 'http://www.ebi.ac.uk/ena/browser/api'
```

2.10.12 EUtils

Interface to the EUtils web Service.

What is EUtils ?

URL <http://www.ncbi.nlm.nih.gov/books/NBK25499/>

URL http://www.ncbi.nlm.nih.gov/books/NBK25500/#chapter1.Demonstration_Programs

The Entrez Programming Utilities (E-utilities) are a set of eight server-side programs that provide a stable interface into the Entrez query and database system at the National Center for Biotechnology Information (NCBI). The E-utilities use a fixed URL syntax that translates a standard set of input parameters into the values necessary for various NCBI software components to search for and retrieve the requested data. The E-utilities are therefore the structured interface to the Entrez system, which currently includes 38 databases covering a variety of biomedical data, including nucleotide and protein sequences, gene records, three-dimensional molecular structures, and the biomedical literature.

—from <http://www.ncbi.nlm.nih.gov/books/NBK25497/>, March 2013

```
class EUtils (verbose=False, email='unknown', cache=False, xmlparser='EUtilsParser')
    Interface to NCBI Entrez Utilities service
```

Note: Technical note: the WSDL interface was dropped in July 2015 so we now use the REST service.

Warning: Read the [guidelines](#) before sending requests. No more than 3 requests per seconds otherwise your IP may be banned. You should provide your email by filling the *email* so that before being banned, you may be contacted.

There are a few methods such as `ELink()`, `EFetch()`. Here is an example on how to use `EFetch()` method to retrieve the FASTA sequence of a given identifier (34577063):

```
>>> from bioservices import EUtils
>>> s = EUtils()
>>> print(s.EFetch("protein", "34577063", rettype="fasta"))
>gi|34577063|ref|NP_001117.2| adenylosuccinate synthetase isozyme 2 [Homo sapiens]
MAFAETYPAAASSLPNGDCGRPRARPGGNRVTVVLGAQWDEGKGVVDLLAQDADIVCRCQGGNNAGHTV
VVDSVEYDFHLLPSGIINPNVTAFIGNGVVIHLPGLFEEAEKNVQKKGKLEGWEKRLIISDRAHIVDFDH
QAADGIQEQQRQEAGKNLGTTKKGIGPVYSSKAARSGLRMCIDLVSDFDGFSERFKVLANQYKSIYPTLE
IDIEGELQKLKGYMEKIKPMVRDGVYFLYEALHGPPKKILVEGANAAALDDIDFGTYPFVTSSNCTVGGVC
TGLGMPPQNVGEVYGVVKAYTTRVIGAFPTQDNEIGELLQTRGREGVTTGRKRRCGWLDLVLKYAH
MINGFTALALTKLDILDMFTEIKVGVAYKLDGEIIPHIPANQEVLNKVEVQYKTLPGWNTDISNARAFKE
LPVNAQNYVRFIEDELQIPVKWIGVGSRESMIQLF
```

Most of the methods take a database name as input. You can obtain the valid list by checking the *databases* attribute.

A few functions takes Identifier(s) as input. It could be a list of strings, list of numbers, or a string where identifiers are separated either by comma or spaces.

A few functions take an argument called **term**. You can use the **AND** keyword with spaces or + signs as separators:

```
Correct: term=biomol mrna[properties] AND mouse[organism]
Correct: term=biomol+mrna[properties]+AND+mouse[organism]
```

Other special characters, such as quotation marks (") or the # symbol used in referring to a query key on the History server, could be represented by their URL encodings (%22 for "; %23 for #) or verbatim .:

```
Correct: term=#2+AND+"gene in genomic"[properties]
Correct: term=%232+AND+%22gene+in+genomic%22[properties]
```

For information about retmode and retype, please see:

http://www.ncbi.nlm.nih.gov/books/NBK25499/table/chapter4.T._valid_values_of__retmode_and/?report=objectonly

ECitMatch (*bdata*, ***kargs*)

Parameters bdata – Citation strings. Each input citation must be represented by a citation string in the following format:

```
journal_title|year|volume|first_page|author_name|your_key|
```

Multiple citation strings may be provided by separating the strings with a carriage return character (%0D) or simply `\r` or `\n`.

The *your_key* value is an arbitrary label provided by the user that may serve as a local identifier for the citation, and it will be included in the output.

all spaces must be replaced by + symbols and that citation strings should end with a final vertical bar |.

Only xml supported at the time of this implementation.

```
from bioservices import EUtils
s = EUtils()
print(s.ECitMatch("proc+natl+acad+sci+u+s+a|1991|88|3248|mann+bj|Art1|
↪%0Dscience|1987|235|182|palmenberg+ac|Art2|"))
```

EFetch (*db*, *id*, *retmode*='text', ***kargs*)

Access to the EFetch E-Utilities

Parameters

- **db** (*str*) – database from which to retrieve UIDs.
- **id** (*str*) – list of identifiers.
- **retmode** – default to text (could be xml but not recommended).
- **rettype** – could be fasta, summary, docsum

Returns depends on retmode parameter.

Note: addition to NCBI: settings rettype to “dict” returns a dictionary

```
>>> ret = s.EFetch("omim", "269840") --> ZAP70
>>> ret = s.EFetch("taxonomy", "9606", retmode="xml")
>>> [x.text for x in ret.getchildren()[0].getchildren() if x.tag==
↪"ScientificName"]
['Homo sapiens']

>>> s = eutils.EUtils()
>>> s.EFetch("protein", "34577063", retmode="text", rettype="fasta")
>gi|34577063|ref|NP_001117.2| adenylosuccinate synthetase isozyme 2 [Homo
↪sapiens]
MAFAETYPAASSLPNGDCGRPRARPGGNRVTVVLGAQWGDEGKGVVDLLAQDADIVCRCQGGNNAGHTV
VVDSVEYDFHLLPSGIINPNVTAFIGNGVVIHLPGLFEEAEKNVQKKGLEGWEKRLIISDRAHIVFDFH
QAADGIQEQQRQEAGKNLGTTKKGIGPVYSSKAARSLRMCIDLVSDFDGFSERFKVLANQYKSIYPTLE
IDIEGELQKLGKGYMEKIKPMVRDGVYFLYEALHGPPKKILVEGANAALLDIDFGTYPFVTSSNCTVGGVC
TGLGMPPQNVGEVYGVVKAYTTRVGIGAFPTEQDNEIGELLQTRGREGVTTGRKRRCGWLDLVLLKYAH
MINGFTALALTKLDILDMFTEIKVGVAYKLDGEIIPHIPANQEVLNKVEVQYKTLPGWNTDISNARAFKE
LPVNAQNYVRFIEDELQIPVKWIGVGVKSRESMIQLF
```

Identifiers could be provided as a single string with comma-separated values, or a list of strings, a list of integers, or just one string or one integer but no mixing of types in the list:

```
>>> e.EFetch("protein", "352, 234", retmode="text", rettype="fasta")
>>> e.EFetch("protein", 352, retmode="text", rettype="fasta")
>>> e.EFetch("protein", [352], retmode="text", rettype="fasta")
>>> e.EFetch("protein", [352, 234], retmode="text", rettype="fasta")
```

retmode should be xml or text depending on the database. For instance, xml for pubmed:

```
>>> e.EFetch("pubmed", "20210808", retmode="xml")
>>> e.EFetch('nucleotide', id=15, retmode='xml')
>>> e.EFetch('nucleotide', id=15, retmode='text', rettype='fasta')
>>> e.EFetch('nucleotide', 'NT_019265', rettype='gb')
```

Other special characters, such as quotation marks (“”) or the # symbol used in referring to a query key on the History server, should be represented by their URL encodings (%22 for “; %23 for #).

A useful command is the following one that allows to get back a GI identifier from its accession, which is common to NCBI/EMBL:

```
e.EFetch(db="nuccore",id="AP013055", rettype="seqid", retmode="text")
```

Changed in version 1.5.0: instead of “xml”, retmode can now be set to dict, in which case an XML is retrieved and converted to a dictionary if possible.

EGQuery (*term*, ***kargs*)

Provides the number of records retrieved in all Entrez databases by a text query.

Parameters *term* (*str*) – Entrez text query. Spaces may be replaced by ‘+’ signs. For very long queries (more than several hundred characters long), consider using an HTTP POST call. See the PubMed or Entrez help for information about search field descriptions and tags. Search fields and tags are database specific.

Returns returns a json data structure

```
>>> ret = s.EGQuery("asthma")
>>> [(x.DbName, x.Count) for x in ret.eGQueryResult.ResultItem if x.Count!='0
↵']

>>> ret = s.EGQuery("asthma")
>>> ret.eGQueryResult.ResultItem[0]
{'Count': '115241',
 'DbName': 'pmc',
 'MenuName': 'PubMed Central',
 'Status': 'Ok'}
```

EInfo (*db=None*, ***kargs*)

Provides information about a database (e.g., number of records)

Parameters *db* (*str*) – target database about which to gather statistics. Value must be a valid Entrez database name. See *databases* or don’t provide any value to obtain the entire list

Returns a json data structure that depends on the value of *databases* (default to json)

```
>>> all_database_names = s.EInfo()
>>> # specific info about one database:
>>> ret = s.EInfo("taxonomy")
>>> ret[0]['count']
u'1445358'
>>> ret = s.EInfo('pubmed')
>>> ret[0]['fieldlist'][2]['fullname']
'Filter'
```

You can use the *retmode* parameter to ‘xml’ as well. In that case, you will need a XML parser.

```
>>> ret = s.EInfo("taxonomy")
```

Note: Note that the name in the XML or json outputs differ (some have lower cases, some have upper cases). This is inherent to the output of EUtils.

ELink (*db=None*, *dbfrom=None*, *id=None*, ***kargs*)

The Entrez links utility

Responds to a list of UIDs in a given database with either a list of related UIDs (and relevancy scores) in the same database or a list of linked UIDs in another Entrez database;

Parameters

- **db** (*str*) – valid database from which to retrieve UIDs.
- **dbfrom** (*str*) – Database containing the input UIDs. The value must be a valid database name (default = pubmed). This is the origin database of the link operation. If db and dbfrom are set to the same database value, then ELink will return computational neighbors within that database. Computational neighbors have linknames that begin with dbname_dbname (examples: protein_protein, pcassay_pcassay_activityneighbor).
- **id** (*str*) – UID list. Either a single UID or a comma-delimited list Limited to 200 Ids
- **cmd** (*str*) – ELink command mode. The command mode specified which function ELink will perform. Some optional parameters only function for certain values of cmd (see <http://www.ncbi.nlm.nih.gov/books/NBK25499/#chapter4.ELink>). Examples are neighbor, prlinks.

```
>>> # Example: Find related articles to PMID 20210808
>>> ret = s.ELink("pubmed", id="20210808", cmd="neighbor_score")

>>> ret = s.parse_xml(ret, 'EUtilsParser')
>>> ret.eLinkResult.LinkSet.LinkSetDb[0].Link[1]
{'Id': '16539535'}

>>> s.ELink(dbfrom="nucleotide", db="protein",
           id="48819,7140345")
>>> s.ELink(dbfrom="nucleotide", db="protein",
           id="48819,7140345")
>>> s.ELink(dbfrom='nuccore', id='21614549,219152114',
           cmd='ncheck')
```

Convert GI number to Taxon identifiers:

```
>>> s.ELink(dbfrom='nuccore', db="taxonomy", id='21614549,219152114')
```

EPost (*db, id, **kargs*)

Accepts a list of UIDs from a given database,

stores the set on the History Server, and responds with a query key and web environment for the uploaded dataset.

Parameters

- **db** (*str*) – a valid database
- **id** – list of strings of strings

Returns a dictionary with a Web Environment string and a QueryKey to be re-used in another EUtils.

ESearch (*db, term, **kargs*)

Responds to a query in a given database

The response can be used later in ESummary, EFetch or ELink, along with the term translations of the query.

Parameters

- **db** – a valid database

- **term** – an Entrez text query

Note: see `_get_esearch_params()` for the list of valid parameters.

```
>>> ret = e.ESearch('protein', 'human', RetMax=5)
>>> ret = e.ESearch('taxonomy', 'Staphylococcus aureus[all names]')
>>> ret = e.ESearch('pubmed', "cokelaer AND BioServices")

>>> ret = e.ESearch('protein', '15718680')
>>> # Let us show the first pubmed identifier in a browser
>>> identifiers = e.pubmed(ret['idlist'][0])
```

More complex requests can be used. We will not cover all the possibilities (see the NCBI website). Here is an example to tune the search term to look into PubMed for the journal PNAS Volume 16, and retrieve.:

```
>>> e.ESearch("pubmed", "PNAS[ta] AND 16[vi]")
```

You can then look more closely at a specific identifier using `EFetch`:

```
>>> e = EFetch("pubmed")
>>> e.Efetch(identifiers)
```

Note: valid parameters can be found by calling `_get_esearch_params()`

ESpell (*db, term, **kargs*)

Retrieve spelling suggestions for a text query in a given database.

Parameters

- **db** (*str*) – database to search. Value must be a valid Entrez database name (default = `pubmed`).
- **term** (*str*) – Entrez text query. All special characters must be URL encoded.

```
>>> ret = e.ESpell(db="pubmed", term="aasthma+OR+alergy")
>>> ret = ret['eSpellResult']
>>> ret['Query']          'asthmaa OR alergies'
>>> ret['CorrectedQuery']
'asthma or allergy'
>>> ret = e.ESpell(db="pubmed", term="biosservices")
>>> ret = ret['eSpellResult']
>>> ret['CorrectedQuery']
biosservices
```

ESummary (*db, id=None, **kargs*)

Returns document summaries for a list of input UIDs

Parameters

- **db** – a valid database
- **id** (*str*) – list of identifiers (or string comma separated). all of the UIDs must be from the database specified by `db`. Limited to 200 identifiers

```
>>> from bioservices import *
>>> s = EUtils()
```

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```
>>> ret = s.ESummary("snp", "7535")
>>> ret = s.ESummary("snp", "7535, 7530")
>>> ret = s.ESummary("taxonomy", "9606, 9913")
```

```
>>> proteins = e.ESearch("protein", "bacteriorhodopsin",
                        retmax=20)
>>> ret = e.ESummary("protein", 449301857)
>>> ret['result']['449301857']['extra']
'gi|449301857|gb|EMC97866.1||gnl|WGS:AEIF|BAUCODRAFT_31870'
```

databases

Returns list of valid databases

email = None

fill this with your email address

help()

Open EUtils help page

parse_xml (*ret, method=None*)**snp_summary** (*id*)

Alias to Efetch for the SNP database

Return a json data structure.

```
>>> ret = s.snp("123")
```

taxonomy_summary (*id*)

Alias to EFetch for the taxonomy database

```
>>> s = EUtils()
>>> ret = s.taxonomy("9606")
>>> ret['9606']['species']
'sapiens'
>>> ret = s.taxonomy("9606,9605,111111111,9604")
>>> ret['9604']['taxid']
9604
```

class EUtilsParser (*xml*)

Convert xml returned by EUtils into a structure easier to manipulate

Used by *EUtils.EGQuery()*, *EUtils.ELink()*.

2.10.13 GeneProf

Currently removed from the main API from version 1.6.0 onwards. You can still get the code in earlier version or in the github repository in the attic/ directory

2.10.14 QuickGO

Interface to the quickGO interface

What is quickGO

URL <http://www.ebi.ac.uk/QuickGO/>

Service <http://www.ebi.ac.uk/QuickGO/WebServices.html>

“QuickGO is a fast web-based browser for Gene Ontology terms and annotations, which is provided by the UniProt-GOA project at the EBI. “

—from QuickGO home page, Dec 2012

class QuickGO (*verbose=False, cache=False*)

Interface to the QuickGO service

Retrieve information given a GO identifier:

```
>>> from bioservices import QuickGO
>>> go = QuickGO()
>>> res = go.get_go_terms("GO:0003824")
```

Changed in version we: use the new QuickGO API since version 1.5.0 To use the old API, please use version of bioservices below 1.5

Constructor

Parameters *verbose* (*bool*) – print informative messages.

Annotation (*assignedBy=None, includeFields=None, limit=100, page=1, aspect=None, reference=None, geneProductId=None, evidenceCode=None, gold=None, qualifier=None, withFrom=None, taxonId=None, taxonUsage=None, goUsage=None, goUsageRelationships=None, evidenceCodeUsage=None, evidenceCodeUsageRelationships=None, geneProductType=None, targetSet=None, geneProductSubset=None, extension=None*)

Calling the Annotation service

Changed in version 1.4.18: due to service API changes, we refactored this method completely

Parameters

- **assignedBy** (*str*) – The database from which this annotation originates. Accepts comma separated values. E.g., BHF-UCL,Ensembl.
- **includeFields** (*str*) – Optional fields retrieved from external services. Accepts comma separated values. accepted values: goName, taxonName, name, synonyms.
- **limit** (*int*) – download limit (number of lines) (default 10,000 rows, which may not be sufficient for the data set that you are downloading. To bypass this default, and return the entire data set, specify a limit of -1).
- **page** (*int*) – results may be stored on several pages. You must provide this number. There is no way to retrieve more than 100 results without calling this function several times changing this parameter (default to 1).
- **aspect** (*char*) – use this to limit the annotations returned to a specific ontology or ontologies (Molecular Function, Biological Process or Cellular Component). The valid character can be F,P,C.
- **reference** (*str*) – PubMed or GO reference supporting annotation. Can refer to a specific reference identifier or category (for category level, use * after ref type). Can be ‘PUBMED:*’, ‘GO_REF:0000002’.

- **geneProductId** (*str*) – The id of the gene product annotated with the GO term. Accepts comma separated values. E.g., URS00000064B1_559292.
- **evidenceCode** (*str*) – Evidence code indicating how the annotation is supported. Accepts comma separated values. E.g., ECO:0000255.
- **goId** (*str*) – The GO id of an annotation. Accepts comma separated values. E.g., GO:0070125.
- **qualifier** (*str*) – Aids the interpretation of an annotation. Accepts comma separated values. E.g., enables,involved_in.
- **withFrom** (*str*) – Additional ids for an annotation. Accepts comma separated values. E.g., P63328.
- **taxonId** (*str*) – The taxonomic id of the species encoding the gene product associated to an annotation. Accepts comma separated values. E.g., 1310605.
- **taxonUsage** (*str*) – Indicates how the taxonomic ids within the annotations should be used. E.g., exact.
- **goUsage** (*str*) – Indicates how the GO terms within the annotations should be used. Used in conjunction with ‘goUsageRelationships’ filter. E.g., descendants.
- **goUsageRelationships** (*str*) – The relationship between the ‘goId’ values found within the annotations. Allows comma separated values. E.g., is_a,part_of.
- **evidenceCodeUsage** (*str*) – Indicates how the evidence code terms within the annotations should be used. Is used in conjunction with ‘evidenceCodeUsageRelationships’ filter. E.g., descendants, exact<F12>
- **evidenceCodeUsageRelationships** (*str*) – The relationship between the provided ‘evidenceCode’ identifiers. Allows comma separated values. E.g., is_a,part_of.
- **geneProductType** (*str*) – The type of gene product. Accepts comma separated values. E.g., protein,RNA. can be protein, RNA and/or complex
- **targetSet** (*str*) – Gene product set. Accepts comma separated values. E.g., KRUK,BHF-UCL,Exosome.
- **geneProductSubset** (*str*) – A database that provides a set of gene products. Accepts comma separated values. E.g., TrEMBL.
- **extension** (*str*) – Extensions to annotations, where each extension can be: EXTENSION(DB:ID) / EXTENSION(DB) / EXTENSION.

Returns a dictionary

```
>>> print(s.Annotation(protein='P12345', frmt='tsv', col="ref,evidence",
... reference='PMID:*'))
>>> print(s.Annotation(protein='P12345,Q4VCS5', frmt='tsv',
... col="ref,evidence", reference='PMID:,Reactome:'))
```

Annotation_from_gold (*gold*, *max_number_of_pages*=25, ***kargs*)

Returns a DataFrame containing annotation on a given GO identifier

Parameters **protein** (*str*) – a GO identifier

Returns all outputs are stored into a Pandas.DataFrame data structure.

All parameters from *Annotation* are also valid except **format** that is set to **tsv** and **cols** that is made of all possible column names.

gene_product_search (*query*, *taxonID=None*, *page=1*, *limit=100*, *type=None*, *dbSubSet=None*, *proteome=None*)

get_go_ancestors (*query*, *relations='is_a, part_of, occurs_in, regulates'*)

get_go_chart (*query*)

```
res = go.get_chart("GO:0022804")
with open("temp.png", "wb") as fout:
    fout.write(res)
```

get_go_children (*query*)

get_go_paths (*_from*, *_to*, *relations='is_a, part_of, occurs_in, regulates'*)

Retrieves the paths between two specified sets of ontology terms. Each path is formed from a list of (term, relationship, term) triples.

```
paths = go.go_terms_path("GO:0005215", "GO:0003674") # First path is found as the first item
in the "results" paths["results"][0]
```

get_go_terms (*query*, *max_number_of_pages=None*)

Get information on all terms and page through the result

go_search (*query*, *limit=600*, *page=1*)

Searches a simple user query, e.g., query=apopto

Parameters

- **query** (*str*) –
- **limit** (*int*) – max 600
- **page** (*int*) –

2.10.15 Kegg

This module provides a class *KEGG* to access to the REST KEGG interface. There are additional methods and functionalities added by **BioServices**.

Note: a previous interface to the KEGG WSDL service was designed but the WSDL closed in Dec 2012.

What is KEGG ?

URL <http://www.kegg.jp/>

REST <http://www.kegg.jp/kegg/rest/keggapi.html>

weblink <http://www.genome.jp/kegg/rest/weblink.html>

dbentries <http://www.genome.jp/kegg/rest/dbentry.html>

“KEGG is a database resource for understanding high-level functions and utilities of the biological system, such as the cell, the organism and the ecosystem, from molecular-level information, especially large-scale molecular datasets generated by genome sequencing and other high-throughput experimental technologies (See Release notes for new and updated features). “

—KEGG home page, Jan 2013

Some terminology

The following list is a simplified list of terminology taken from KEGG API pages.

- **organisms (org)** are made of a three-letter (or four-letter) code (e.g., **hsa** stands for Human Sapiens) used in KEGG (see *organismIds*).
- **db** is a database name. See *databases* attribute and *KEGG Databases Names and Abbreviations* section.
- **entry_id** is a unique identifier. It is a combination of the database name and the identifier of an entry joined by a colon sign (e.g. 'embl:J00231').

Here are some examples of entry Ids:

- **genes_id**: A KEGG organism and a gene name (e.g. 'eco:b0001').
- **enzyme_id**: 'ec' and an enzyme code. (e.g. 'ec:1.1.1.1'). See *enzymeIds*.
- **compound_id**: 'cpd' and a compound number (e.g. 'cpd:C00158'). Some compounds also have 'glycan_id' and both IDs are accepted and converted internally. See *compoundIds*.
- **drug_id**: 'dr' and a drug number (e.g. 'dr:D00201'). See *drugIds*.
- **glycan_id**: 'gl' and a glycan number (e.g. 'gl:G00050'). Some glycans also have 'compound_id' and both IDs are accepted and converted internally. see *glycanIds* attribute.
- **reaction_id**: 'rn' and a reaction number (e.g. 'rn:R00959' is a reaction which catalyze cpd:C00103 into cpd:C00668). See *reactionIds* attribute.
- **pathway_id**: 'path' and a pathway number. Pathway numbers prefixed by 'map' specify the reference pathway and pathways prefixed by a KEGG organism specify pathways specific to the organism (e.g. 'path:map00020', 'path:eco00020'). See *pathwayIds* attribute.
- **motif_id**: a motif database names ('ps' for prosite, 'bl' for blocks, 'pr' for prints, 'pd' for prodom, and 'pf' for pfam) and a motif entry name. (e.g. 'pf:DnaJ' means a Pfam database entry 'DnaJ').
- **ko_id**: identifier made of 'ko' and a ko number (e.g. 'ko:K02598'). See *koIds* attribute.

KEGG Databases Names and Abbreviations

Here is a list of databases used in KEGG API with their name and abbreviation:

Database Name	Abbrev	kid
pathway	path	map number
brite	br	br number
module	md	M number
disease	ds	H number
drug	dr	D number
environ	ev	E number
orthology	ko	K number
genome	genome	T number
genomes	gn	T number
genes	•	•
ligand	ligand	•
compound	cpd	C number
glycan	gl	G number
reaction	rn	R number
rpair	rp	RP number
rclass	rc	RC number
enzyme	ec	•

Database Entries

Database entries can be written in on of the following ways:

```
<dbentries> = <dbentry>1[+<dbentry>2...]
<dbentry> = <db:entry> | <kid> | <org:gene>
```

Each database entry is identified by:

```
db:entry
```

where “db” is the database name or its abbreviation shown above and “entry” is the entry name or the accession number that is uniquely assigned within the database. In reality “db” may be omitted, for the entry name called the KEGG object identifier (kid) is unique across KEGG.:

```
kid = database-dependent prefix + five-digit number
```

In the KEGG GENES database the db:entry combination must be specified. This is more specifically written as:

```
org:gene
```

where “org” is the three- or four-letter KEGG organism code or the T number genome identifier and “gene” is the gene identifier, usually locus_tag or ncbi GeneID, or the primary gene name.

class **KEGG** (*verbose=False, cache=False*)

Interface to the [KEGG](#) service

This class provides an interface to the KEGG REST API. The weblink tools are partially accesible. All dbentries can be parsed into dictionaries using the [KEGGParser](#)

Here are some examples. In order to retrieve the entry of the gene identifier 7535 of the **hsa** organism, type:

```
from bioservices import KEGG
s = KEGG()
print(s.get("hsa:7535"))
```

The output is the raw output sent by KEGG API. See *KEGGParser* to parse this output.

See also:

The *Database Entries* to know more about the db entries format.

Another example here below shows how to print the list of pathways of the human organism:

```
print(s.list("pathway", organism="hsa"))
```

Further post processing would allow you to retrieve the pathway Ids. However, we provide additional functions to the KEGG API so the previous code and post processing to extract the pathway Ids can be written as:

```
s.organism = "hsa"
s.pathwayIds
```

and similarly you can get all *databases()* output and database Ids easily. For example, for the reaction database:

```
s.reaction # equivalent to s.list("reaction")
s.reactionIds
```

Other methods of interest are *conv()*, *find()*, *get()*.

See also:

KEGG Databases Names and Abbreviations, Database Entries, Some terminology.

Constructor

Parameters **verbose** (*bool*) – prints informative messages

Tnumber2code (*Tnumber*)

Converts organism T number to its code

```
>>> from bioservices import KEGG
>>> s = KEGG()
>>> s.Tnumber2code("T01001")
'hsa'
```

briteIds

returns list of brite Ids.

See also:

list()

code2Tnumber (*code*)

Converts organism code to its T number

```
>>> from bioservices import KEGG
>>> s = KEGG()
>>> s.code2Tnumber("hsa")
'T01001'
```

compoundIds

returns list of compound Ids

See also:

`list()`

conv (*target, source*)

convert KEGG identifiers to/from outside identifiers

Parameters

- **target** (*str*) – the target database (e.g., a KEGG organism).
- **source** (*str*) – the source database (e.g., uniprot) or a valid dbentries; see below for details.

Returns a dictionary with keys being the source and values being the target.

Here are the rules to set the target and source parameters.

If the second argument is not a **dbentries**, source and target parameters can be of two types:

1. gene identifiers. If the target is a KEGG Id, then the source must be one of *ncbi-gi*, *ncbi-geneid* or *uniprot*.

Note: source and target can be swapped.

2. chemical substance identifiers. If the target is one of the following kegg database: drug, compound, glycan then the source must be one of *pubchem* or *chebi*.

Note: again, source and target can be swapped

If the second argument is a **dbentries**, it can be again of two types:

1. gene identifiers. The database used can be one *ncbi-gi*, *ncbi-geneid*, *uniprot* or any KEGG organism
2. chemical substance identifiers. The database used can be one of drug, compound, glycan, *pubchem* or *chebi* only.

Note: if the second argument is a *dbentries*, target and *dbentries* cannot be swapped.

```
# conversion from NCBI GeneID to KEGG ID for E. coli genes
conv("eco", "ncbi-geneid")
# inverse of the above example
conv("eco", "ncbi-geneid")
#conversion from KEGG ID to NCBI GI
conv("ncbi-gi", "hsa:10458+ece:Z5100")
```

To make it clear by taking another example, you can either convert an entire database to another (e.g., from uniprot to KEGG Id all human gene IDs):

```
uniprot_ids, kegg_ids = s.conv("hsa", "uniprot")
```

or a subset by providing a valid **dbentries**:

```
s.conv("hsa", "up:Q9BV86+")
```

Warning: `dbentries` are not checked and are supposed to be correct. See `check_idbentries()` to help you checking a `dbentries`.

Warning: call to this function may be long. `conv("hsa", "uniprot")` takes a minute surprisingly, `conv("uniprot", "hsa")` takes just a few seconds.

Changed in version 1.1: the output is now a dictionary, not a list of tuples

databases

Returns list of valid KEGG databases.

dbinfo (database='kegg')

Displays the current statistics of a given database

Parameters `database` (*str*) – can be one of: `kegg` (default), `brite`, `module`, `disease`, `drug`, `environ`, `ko`, `genome`, `compound`, `glycan`, `reaction`, `rpair`, `rclass`, `enzyme`, `genomes`, `genes`, `ligand` or any *organismIds*.

```
from bioservices import KEGG
s = KEGG()
s.dbinfo("hsa") # human organism
s.dbinfo("T01001") # same as above
s.dbinfo("pathway")
```

Changed in version 1.4.1: renamed `info` method into `dbinfo()`, which clashes with Logging framework `info()` method.

drugIds

returns list of drug Ids

See also:

`list()`

entry (dbentries)

Retrieve entry

There is a weblink service (see <http://www.genome.jp/kegg/rest/weblink.html>) Since it is equivalent to `get()`, we do not implement it for now

enzymeIds

returns list of enzyme Ids

See also:

`list()`

find (database, query, option=None)

finds entries with matching query keywords or other query data in a given database

Parameters

- **database** (*str*) – can be one of `pathway`, `module`, `disease`, `drug`, `environ`, `ko`, `genome`, `compound`, `glycan`, `reaction`, `rpair`, `rclass`, `enzyme`, `genes`, `ligand` or an organism code (see *organismIds* attributes) or T number (see *organismTnumbers* attribute).
- **query** (*str*) – See examples

- **option** (*str*) – If option provided, database can be only ‘compound’ or ‘drug’. Option can be ‘formula’, ‘exact_mass’ or ‘mol_weight’

Note: Keyword search against brite is not supported. Use /list/brite to retrieve a short list.

```
# search for pathways that contain Viral in the definition
s.find("pathway", "Viral")
# for keywords "shiga" and "toxin"
s.find("genes", "shiga+toxin")
# for keywords "shiga toxin"
s.find("genes", "\"shiga toxin\"")
# for chemical formula "C7H10O5"
s.find("compound", "C7H10O5", "formula")
# for chemical formula containing "O5" and "C7"
s.find("compound", "O5C7", "formula")
# for 174.045 <= exact mass < 174.055
s.find("compound", "174.05", "exact_mass")
# for 300 <= molecular weight <= 310
s.find("compound", "300-310", "mol_weight")
```

get (*dbentries*, *option=None*, *parse=False*)

Retrieves given database entries

param str dbentries KEGG database entries involving the following database: pathway, brite, module, disease, drug, environ, ko, genome compound, glycan, reaction, rpair, reclass, enzyme **or** any organism using the KEGG organism code (see *organismIds* attributes) or T number (see *organismTnumbers* attribute).

param str option one of: aaseq, ntseq, mol, kcf, image, kgml

Note:

you can add the option at the end of dbentries in which case the parameter option must not be used (see example)

```
from bioservices import KEGG
s = KEGG()
# retrieves a compound entry and a glycan entry
s.get("cpd:C01290+gl:G00092")
# same as above
s.get("C01290+G00092")
# retrieves a human gene entry and an E.coli O157 gene entry
s.get("hsa:10458+ece:Z5100")
# retrieves amino acid sequences of a human gene and an E.coli O157 gene
s.get("hsa:10458+ece:Z5100/aaseq")
# retrieves the image file of a pathway map
s.get("hsa05130/image")
# same as above
s.get("hsa05130", "image")
```

Another example here below shows how to save the image of a given pathway:

```
res = s.get("hsa05130/image")
# same as : res = s.get("hsa05130", "image")
f = open("test.png", "w")
```

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```
f.write(res)
f.close()
```

Note: The input is limited up to 10 entries (KEGG restriction).

get_pathway_by_gene (*gene, organism*)

Search for pathways that contain a specific gene

Parameters

- **gene** (*str*) – a valid gene Id
- **organism** (*str*) – a valid organism (e.g., hsa)

Returns list of pathway Ids that contain the gene

```
>>> s.get_pathway_by_gene("7535", "hsa")
['path:hsa04064', 'path:hsa04650', 'path:hsa04660', 'path:hsa05340']
```

glycanIds

Returns list of glycan Ids

See also:

list()

isOrganism (*org*)

Checks if org is a KEGG organism

Parameters **org** (*str*) –

Returns True if org is in the KEGG organism list (code or Tnumber)

```
>>> from bioservices import KEGG
>>> s = KEGG()
>>> s.isOrganism("hsa")
True
```

koIds

returns list of ko Ids

See also:

list()

link (*target, source*)

Find related entries by using database cross-references

Parameters

- **target** (*str*) – the target KEGG database or organism (see below for the list).
- **source** (*str*) – the source KEGG database or organism (see below for the list) or a valid dbentries involving one of the database; see below for details.

The valid list of databases is pathway, brite, module, disease, drug, environ, ko, genome, compound, glycan, reaction, rpair, rclass, enzyme

```
# KEGG pathways linked from each of the human genes
s.link("pathway", "hsa")
# human genes linked from each of the KEGG pathways
s.link("hsa", "pathway")
# KEGG pathways linked from a human gene and an E. coli O157 gene.
s.link("pathway", "hsa:10458+ece:Z5100")
```

list (*query*, *organism=None*)

Returns a list of entry identifiers and associated definition for a given database or a given set of database entries

Parameters

- **query** (*str*) – can be one of pathway, brite, module, disease, drug, environ, ko, genome, compound, glycan, reaction, rpair, rclass, enzyme, organism **or** an organism from the *organismIds* attribute **or** a valid dbentry (see below). If a dbentry query is provided, organism should not be used!
- **organism** (*str*) – a valid organism identifier that can be provided. If so, database can be only “pathway” or “module”. If not provided, the default value is chosen (*organism*)

Returns A string with a structure that depends on the query

Here is an example that shows how to extract the pathways IDs related to the hsa organism:

```
>>> s = KEGG()
>>> res = s.list("pathway", organism="hsa")
>>> pathways = [x.split()[0] for x in res.strip().split("\n")]
>>> len(pathways) # as of Dec 2012
261
```

Note, however, that there are convenient aliases to some of the databases. For instance, the pathway Ids can also be retrieved as a list from the *pathwayIds* attribute (after defining the *organism* attribute).

Note: If you set the query to a valid organism, then the second argument rganism is irrelevant and ignored.

Note: If the query is not a database or an organism, it is supposed to be a valid dbentries string and the maximum number of entries is 100.

Other examples:

```
s.list("pathway") # returns the list of reference pathways
s.list("pathway", "hsa") # returns the list of human pathways
s.list("organism") # returns the list of KEGG organisms with
↳ taxonomic classification
s.list("hsa") # returns the entire list of human genes
s.list("T01001") # same as above
s.list("hsa:10458+ece:Z5100") # returns the list of a human gene and an E.
↳ coli O157 gene
s.list("cpd:C01290+gl:G00092") # returns the list of a compound entry and a
↳ glycan entry
s.list("C01290+G00092") # same as above
```

lookfor_organism (*query*)

Look for a specific organism

Parameters `query` (*str*) – your search term. upper and lower cases are ignored

Returns a list of definition that matches the query

lookfor_pathway (*query*)

Look for a specific pathway

Parameters `query` (*str*) – your search term. upper and lower cases are ignored

Returns a list of definition that matches the query

moduleIds

returns list of module Ids for the default organism.

organism must be set.

```
s = KEGG()
s.organism = "hsa"
s.moduleIds
```

organism

returns the current default organism

organismIds

Returns list of organism Ids

organismTnumbers

returns list of organisms (T numbers)

See also:

list()

parse (*entry*)

See *KEGGParser* for details

Parse entry returned by *get()*

```
k = KEGG()
res = k.get("hsa04150")
d = k.parse(res)
```

parse_kgml_pathway (*pathwayId*, *res=None*)

Parse the pathway in KGML format and returns a dictionary (relations and entries)

Parameters

- **pathwayId** (*str*) – a valid pathwayId e.g. hsa04660
- **res** (*str*) – if you already have the output of the query *get(pathwayId)*, you can provide it, otherwise it is queried.

Returns a dictionary with relations and entries as keys. Values of relations is a list of relations, each relation being dictionary with entry1, entry2, link, value, name. The list of entries is a list of dictionary as well. Entry contains contains more details about the entry found in the relation. See example below for details.

```
>>> res = s.parse_kgml_pathway("hsa04660")
>>> set([x['name'] for x in res['relations']])
>>> res['relations'][-1]
{'entry1': u'15',
 'entry2': u'13',
 'link': u'PPrel',
```

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```
'name': u'phosphorylation',
'value': u'+p'}

>>> set([x['link'] for x in res['relations']])
set([u'PPrel', u'PCrel'])

>>> # get information about an entry :
>>> res['entries'][4]
```

See also:

KEGG API

pathway2sif (*pathwayId*, *uniprot=True*)

Extract protein-protein interaction from KEGG pathway to a SIF format

Warning: experimental Not tested on all pathway. should be move to another package such as cellnopt

Parameters

- **pathwayId** (*str*) – a valid pathway Id
- **uniprot** (*bool*) – convert to uniprot Id or not (default is True)

Returns a list of relations (A 1 B) for activation and (A -1 B) for inhibitions

This is longish due to the conversion from KEGGIds to UniProt.

This method can be useful to provide prior knowledge network to software such as CellNOpt (see <http://www.cellnopt.org>)**pathwayIds**

returns list of pathway Ids for the default organism.

organism must be set.

```
s = KEGG()
s.organism = "hsa"
s.pathwayIds
```

reactionIds

returns list of reaction Ids

show_entry (*entry*)

Opens URL corresponding to a valid entry

```
s.www_bget("path:hsa05416")
```

show_module (*modId*)

Show a given module inside a web browser

Parameters **modId** (*str*) – a valid module Id. See *moduleIds()*

Validity of modId is not checked but if wrong the URL will not open a proper web page.

show_pathway (*pathId*, *scale=None*, *dcolor='pink'*, *keggid={}*)

Show a given pathway inside a web browser

Parameters

- **pathId** (*str*) – a valid pathway Id. See *pathwayIds()*
- **scale** (*int*) – you can scale the image with a value between 0 and 100
- **dcolor** (*str*) – set the default background color of nodes
- **keggid** (*dict*) – set color of entries contained in the pathway as key/value pairs; can also be a list, in which case all nodes have the same default color (red)

Note: if scale is provided, dcolor and keggid are ignored.

```
# show a pathway in the browser
s.show_pathway("path:hsa05416", scale=50)

# Same as above but also highlights some KEGG Ids (red for all)
s.show_pathway("path:hsa05416", dcolor="white",
               keggid=['1525', '1604', '2534'])

# You can refine the colors using a dictionary:
s.show_pathway("path:hsa05416", dcolor="white",
               keggid={'1525':'yellow,red', '1604':'blue,green', '2534':"blue"})
```

class **KEGGParser** (*verbose=False*)

This is an extension of the *KEGG* class to ease parsing of dbentries

This class provides a generic method *parse()* that will read the output of a dbentry returned by *KEGG.get()* and converts it into a dictionary ready to use.

The *parse()* method parses any entry. It can be a pathway, a gene, a compound...

```
from bioservices import *
s = KEGG()

# Retrieve a KEGG entry
res = s.get("hsa04150")

# parse it
d = s.parse(res)
```

As a pedagogical example, you can then further process this dictionary. Here below, we convert the gene Ids found in the pathway into UniProt Ids:

```
# Get the KEGG Ids in the pathway
kegg_geneIds = [x for x in d['GENE']]

# Convert them
db_up, db_kegg = s.conv("hsa", "uniprot")

# Get the corresponding uniprot Ids
indices = [db_kegg.index("hsa:%s" % x) for x in kegg_geneIds]
uniprot_geneIds = [db_up[x] for x in indices]
```

However, you could also have done it simply as follows:

```
kegg_geneIds = [x for x in d['gene']]
uprot_geneIds = [s.parse(s.get("hsa:"+str(e))['DBLINKS']["UniProt:"]) for e in d[
    ↳ 'GENE']]
```

Note: The 2 outputs are slightly different.

See also:

<http://www.kegg.jp/kegg/rest/dbentry.html>

parse (*res*)

Parse to any outputs returned by *KEGG.get()*

Parameters *res* (*str*) – output of a *KEGG.get()*.

Returns a dictionary. Keys are those found in the KEGG entry (e.g., REACTION, ENTRY, EQUATION, ...). The format of each value is various. It could be a string, a list (of strings generally), a dictionary, a float depending on the key. Depending on the type of the entry (e.g., module, pathway), the type of the value may also differ (e.g., REACTION can be either a list of reactions or a dictionary depending on the content)

```
>>> # Parses a drug entry
>>> res = s.get("dr:D00001")
>>> # Parses a pathway entry
>>> res = s.get("path:hsa10584")
>>> # Parses a module entry
>>> res = s.get("md:hsa_M00554")
>>> # Parses a disease entry
>>> res = s.get("ds:H00001")
>>> # Parses a environ entry
>>> res = s.get("ev:E00001")
>>> # Parses Orthology entry
>>> res = s.get("ko:K00001")
>>> # Parses a Genome entry
>>> res = s.get('genome:T00001')
>>> # Parses a gene entry
>>> res = s.get("hsa:1525")
>>> # Parses a compound entry
>>> s.get("cpd:C00001")
>>> # Parses a glycan entry
>>> res = s.get("gl:G00001")
>>> # Parses a reaction entry
>>> res = s.get("rn:R00001")
>>> # Parses a rpair entry
>>> res = s.get("rp:RP00001")
>>> # Parses a rclass entry
>>> res = s.get("rc:RC00001")
>>> # Parses an enzyme entry
>>> res = s.get('ec:1.1.1.1')

>>> d = s.parse(res)
```

2.10.16 HGNC

Interface to HUGO/HGNC web services

What is HGNC ?

URL <http://www.genenames.org>

Citation

“The HUGO Gene Nomenclature Committee (HGNC) has assigned unique gene symbols and names to over 37,000 human loci, of which around 19,000 are protein coding. [genenames.org](http://www.genenames.org) is a curated online repository of HGNC-approved gene nomenclature and associated resources including links to genomic, proteomic and phenotypic information, as well as dedicated gene family pages.”

—From HGNC web site, July 2013

class HGNC (*verbose=False, cache=False*)

Wrapper to the genenames web service

See details at <http://www.genenames.org/help/rest-web-service-help>

fetch (*database, query, frmt='json'*)

Retrieve particular records from a searchable fields

Returned object is a json object with fields as in `stored_field`, which is returned from `get_info()` method.

Only one query at a time. No wild cards are accepted.

```
>>> h = HGNC()
>>> h.fetch('symbol', 'ZNF3')
>>> h.fetch('alias_name', 'A-kinase anchor protein, 350kDa')
```

get_info (*frmt='json'*)

Request information about the service

Fields are when the server was last updated (`lastModified`), the number of documents (`numDoc`), which fields can be queried using `search` and `fetch` (`searchableFields`) and which fields may be returned by `fetch` (`storedFields`).

search (*database_or_query=None, query=None, frmt='json'*)

Search a searchable field (database) for a pattern

The search request is more powerful than `fetch` for querying the database, but `search` will only returns the fields `hgnc_id`, `symbol` and `score`. This is because this tool is mainly intended to query the server to find possible entries of interest or to check data (such as your own symbols) rather than to fetch information about the genes. If you want to retrieve all the data for a set of genes from the search result, the user could use the `hgnc_id` returned by `search` to then fire off a `fetch` request by `hgnc_id`.

Parameters database – if not provided, search all databases.

```
# Search all searchable fields for the tern BRAF
h.search('BRAF')

# Return all records that have symbols that start with ZNF
h.search('symbol', 'ZNF*')

# Return all records that have symbols that start with ZNF
# followed by one and only one character (e.g. ZNF3)
# Nov 2015 does not work neither here nor in within in the
# official documentation
h.search('symbol', 'ZNF?')

# search for symbols starting with ZNF that have been approved
# by HGNC
h.search('symbol', 'ZNF*+AND+status:Approved')
```

(continues on next page)

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```
# return ZNF3 and ZNF12
h.search('symbol', 'ZNF3+OR+ZNF12')

# Return all records that have symbols that start with ZNF which
# are not approved (ie entry withdrawn)
h.search('symbol', 'ZNF*+NOT+status:Approved')
```

class HGNCDeprecated (*verbose=False, cache=False*)

Interface to the HGNC service

```
>>> from bioservices import *
>>> # Fetch XML document for gene ZAP70
>>> s = HGNC()
>>> xml = s.get_xml("ZAP70")
>>> # You can fetch several gene names:
>>> xml = s.get_xml("ZAP70;INSR")
>>> # Wrong gene name request returns an empty list
>>> s.get_xml("wrong")
[]
```

For a single name, the following methods are available:

```
>>> # get the aliases of a given gene
>>> print(s.get_aliases("ZAP70"))
[u'ZAP-70', u'STD']
>>> # get UniProt accession code
>>> s.get_xrefs("ZAP70")['UniProt']['xkey']
'P43403'
>>> # get XML link to a UniProt cross-reference
>>> s.get_xrefs("ZAP70", "xml")['UniProt']['link']
['http://www.uniprot.org/uniprot/P43403.xml']
```

You can access to the links of a cross reference as well:

```
values = s.get_xrefs("ZAP70")
s.on_web(values['EntrezGene']['link'][0])
```

References <http://www.avatar.se/HGNC/doc/tutorial.html>

Warning: this maybe not the official.

get_aliases (*gene*)

Get aliases for a single gene name

get_all_names ()

Returns all gene names

get_chromosome (*gene*)

Get chromosome for a single gene name

get_name (*gene*)

Get name for a single gene name

get_previous_names (*gene*)

Get previous names for a single gene name

get_previous_symbols (*gene*)

Get previous symbols for a single gene name

get_withdrawn_symbols (*gene*)

Get withdrawn symbols for a single gene name

get_xml (*gene*)

Returns XML of a single gene or list of genes

Parameters *gene* (*str*) – a valid gene name. Several gene names can be concatenated with comma ; character (e.g., 'ZAP70;INSR')

```
>>> from bioservices import *
>>> s = HGNC()
>>> res = s.get_xml("ZAP70")
>>> res.findAll("alias")
>>> [x.text for x in res.findAll("alias")]
[u'ZAP-70', u'STD']
```

See also:

get_aliases()

get_xrefs (*gene*, *keep='html'*)

Get the cross references for a given single gene name

```
>>> databases = s.get_xrefs("ZAP70").keys()

>>> # get XML link to a UniProt cross-reference
>>> s.get_xrefs("ZAP70", "xml")['UniProt']['link']
['http://www.uniprot.org/uniprot/P43403.xml']
```

lookfor (*pattern*)

Finds all genes that starts with a given pattern

Parameters *pattern* (*str*) – a string. Could be the wild character *

Returns list of dictionary. Each dictionary contains the 'acc', 'xlink:href' and 'xlink:title' keys

```
>>> from bioservices import *
>>> s = HGNC()
>>> s.lookfor("ZAP")
[{'acc': 'HGNC:12858',
'xlink:href': '/HGNC/wr/gene/ZAP70',
'xlink:title': 'ZAP70'}]
```

This function may be used to count the number of entries:

```
len(s.lookfor('*'))
```

mapping (*value*)

maps an identifier from a database onto HGNC database

Parameters *value* (*str*) – a valid DB:id string (e.g. "UniProt:P36888")

Returns

a list of dictionary with the keys 'acc', 'xlink:href', 'xlink:title'

```

>>> value = "UniProt:P43403"
>>> res = s.mapping(value)
>>> res[0]['xlink:title']
'ZAP70'
>>> res[0]['acc']
'HGNC:12858'

```

See also:

`mapping_all()`

mapping_all (*entries=None*)

Retrieves cross references for more than one entry

Parameters **entries** – list of values entries (e.g., returned by the `lookfor()` method.) if not provided, this method looks for all entries.

Returns list of dictionaries with keys being all entry names. Values is a dictionary of cross references.

Warning: takes 10 minutes

2.10.17 Intact (complex)

This module provides a class `IntactComplex`

What is Intact Complex ?

URL <https://www.ebi.ac.uk/intact/complex/>

REST <https://www.ebi.ac.uk/intact/complex-ws/details/>

“The Complex Portal is a manually curated, encyclopaedic resource of macromolecular complexes from a number of key model organisms.”

—From Intact web page Feb 2015

class IntactComplex (*verbose=False, cache=False*)

Interface to the `Intact` service

```

>>> from bioservices import IntactComplex
>>> u = IntactComplex()

```

Constructor IntactComplex

Parameters **verbose** – set to False to prevent informative messages

details

 (*query*)

Return details about a complex

Parameters **query** (*str*) – EBI-1163476

search

 (*query, frmt='json', facets=None, first=None, number=None, filters=None*)

Search for a complex inside intact complex.

Parameters

- **query** (*str*) – the query (e.g., ndc80)
- **frmt** (*str*) – Defaults to json (could be a Pandas data frame if Pandas is installed; set frmt to 'pandas')
- **facets** (*str*) – lists of facets as a string (separated by comma)
- **first** (*int*) –
- **number** (*int*) –
- **filter** (*str*) – list of filters. See examples here below.

```
s = IntactComplex()
# search for ndc80
s.search('ncd80')

# Search for ndc80 and facet with the species field:
s.search('ncd80', facets='species_f')

# Search for ndc80 and facet with the species and biological role fields:
s.search('ndc80', facets='species_f,pbiorole_f')

# Search for ndc80, facet with the species and biological role
# fields and filter the species using human:
s.search('Ndc80', first=0, number=10,
        filters='species_f:("Homo sapiens")',
        facets='species_f,ptype_f,pbiorole_f')

# Search for ndc80, facet with the species and biological role
# fields and filter the species using human or mouse:
s.search('Ndc80', first=0, number=10,
        filters='species_f:("Homo sapiens" "Mus musculus")',
        facets='species_f,ptype_f,pbiorole_f')

# Search with a wildcard to retrieve all the information:
s.search('*')

# Search with a wildcard to retrieve all the information and facet
# with the species, biological role and interactor type fields:
s.search('*', facets='species_f,pbiorole_f,ptype_f')

# Search with a wildcard to retrieve all the information, facet with
# the species, biological role and interactor type fields and filter
# the interactor type using small molecule:
s.search('*', facets='species_f,pbiorole_f,ptype_f',
        filters='ptype_f:("small molecule")')

# Search with a wildcard to retrieve all the information, facet with
# the species, biological role and interactor type fields and filter
# the interactor type using small molecule and the species using human:
s.search('*', facets='species_f,pbiorole_f,ptype_f',
        filters='ptype_f:("small molecule"),species_f:("Homo sapiens")')

# Search for GO:0016491 and paginate (first is for the offset and number
# is how many do you want):
s.search('GO:0016491', first=10, number=10)
```

The organism name used in the filter must be exact. Here is the list found by typing:

```
res = set(ci.search('*', frmt='pandas')['organismName'])
```

```
'Bos taurus; 9913',
'Caenorhabditis elegans; 6239',
'Canis familiaris; 9615',
'Drosophila melanogaster; 7227',
'Escherichia coli (strain K12); 83333',
'Gallus gallus; 9031',
'Homo sapiens; 9606',
'Mus musculus; 10090',
'Oryctolagus cuniculus; 9986',
'Rattus norvegicus; 10116',
'Saccharomyces cerevisiae (strain ATCC 204508 / S288c);559292',
'Schizosaccharomyces pombe (strain 972 / ATCC 24843);284812',
'Xenopus laevis; 8355'
```

2.10.18 MUSCLE

Interface to the MUSCLE web service

What is MUSCLE ?

URL <http://www.drive5.com/muscle/>

service http://www.ebi.ac.uk/Tools/webservices/services/msa/muscle_rest

“MUSCLE - (MUltiple Sequence Comparison by Log-Expectation) 1)

is claimed to achieve both better average accuracy and better speed than ClustalW or T-Coffee, depending on the chosen options. Multiple alignments of protein sequences are important in many applications, including phylogenetic tree estimation, secondary structure prediction and critical residue identification.”

—from EMBL-EBI web page

class MUSCLE (*verbose=False*)
Interface to the **MUSCLE** service.

```
>>> from bioservices import *
>>> m = MUSCLE(verbose=False)
>>> sequencesFasta = open('filename', 'r')
>>> jobid = n.run(frmt="fasta", sequence=sequencesFasta.read(),
                email="name@provider")
>>> s.getResult(jobid, "out")
```

Warning: It is very important to provide a real e-mail address as your job otherwise very likely will be killed and your IP, Organisation or entire domain black-listed.

Here is another similar example but we use *UniProt* class provided in bioservices to fetch the FASTA sequences:

```
>>> from bioservices import UniProt, MUSCLE
>>> u = UniProt(verbose=False)
>>> f1 = u.get_fasta("P18413")
>>> f2 = u.get_fasta("P18412")
>>> m = MUSCLE(verbose=False)
>>> jobid = m.run(frmt="fasta", sequence=f1+f2, email="name@provider")
>>> m.getResult(jobid, "out")
```

get_parameter_details (*parameterId*)

Get detailed information about a parameter.

Returns An XML document providing details about the parameter or a list of values that can take the parameters if the XML could be parsed.

For example:

```
>>> n.get_parameter_details("format")
```

get_parameters ()

List parameter names.

Returns An XML document containing a list of parameter names.

```
>>> from bioservices import muscle
>>> n = muscle.Muscle()
>>> res = n.get_parameters()
>>> [x.text for x in res.findAll("id")]
```

See also:

[parameters](#) to get a list of the parameters without need to process the XML output.

get_result (*jobid*, *result_type*)

Get the job result of the specified type.

Parameters

- **jobid** (*str*) – a job identifier returned by `run()`.
- **resultType** (*str*) – type of result to retrieve. See `getResultTypes()`.

get_result_types (*jobid*)

Get available result types for a finished job.

Parameters

- **jobid** (*str*) – a job identifier returned by `run()`.
- **verbose** (*bool*) – print the identifiers together with their label, mediaTypes, description and filesuffix.

Returns A dictionary, which keys correspond to the identifiers. Each identifier is itself a dictionary containing the label, description, file suffix and mediaType of the identifier.

get_status (*jobid*)

Get status of a submitted job

Parameters

- **jobid** (*str*) –
- **jobid** – a job identifier returned by `run()`.

Returns

A string giving the jobid status (e.g. FINISHED).

The values for the status are:

- **RUNNING**: the job is currently being processed.
- **FINISHED**: job has finished, and the results can then be retrieved.
- **ERROR**: an error occurred attempting to get the job status.
- **FAILURE**: the job failed.
- **NOT_FOUND**: the job cannot be found.

parameters

run (*frmt=None, sequence=None, tree='none', email=None*)
Submit a job with the specified parameters.

Compulsary arguments**Parameters**

- **frmt** (*str*) – input format (e.g., fasta)
- **sequence** (*str*) – query sequence. The use of fasta formatted sequence is recommended.
- **tree** (*str*) – tree type ('none','tree1','tree2')
- **email** (*str*) – a valid email address. Will be checked by the service itself.

Returns A jobid that can be analysed with `getResult()`, `getStatus()`, ...

The up to data values accepted for each of these parameters can be retrieved from the `get_parameter_details()`.

For instance,:

```
from bioservices import MUSCLE
m = MUSCLE()
m.parameterDetails("tree")
```

Example:

```
jobid = m.run(frmt="fasta",
             sequence=sequence_example,
             email="test@yahoo.fr")
```

frmt can be a list of formats:

```
frmt=['fasta', 'clw', 'clwstrict', 'html', 'msf', 'phyi', 'phys']
```

The returned object is a jobid, which status can be checked. It must be finished before analysing/getting the results.

See also:

`getResult()`

wait (*jobId*, *checkInterval=5*, *verbose=True*)

This function checks the status of a jobid while it is running

Parameters

- **jobid** (*str*) – a job identifier returned by `run()`.
- **checkInterval** (*int*) – interval between requests in seconds.

2.10.19 MyGeneInfo

Interface to the mygeneinfo web Service.

What is MyGeneInfo ?

URL <https://mygene.info>

REST <https://mygeneinfo/v3.api/>

MyGene.info provides simple-to-use REST web services to query/retrieve gene annotation data. It's designed with simplicity and performance emphasized. You can use it to power a web application which requires querying genes and obtaining common gene annotations. For example, MyGene.info services are used to power BioGPS; or use it in an analysis pipeline to retrieve always up-to-date gene annotations.

—mygene.info home page, June 2020

class MyGeneInfo (*verbose=False*, *cache=False*)

Interface to `mygene.info` service

```
>>> from bioservices import MyGeneInfo
>>> s = MyGeneInfo()
```

Constructor

Parameters **verbose** (*bool*) – prints informative messages (default is off)

get_genes (*ids*, *fields='symbol, name, taxid, entrezgene, ensemblgene'*, *species=None*, *dotfield=True*, *email=None*)

Get matching gene objects for a list of gene ids

Parameters

- **ids** – list of geneinfo IDs
- **fields** (*str*) – a comma-separated fields to limit the fields returned from the matching gene hits. The supported field names can be found from any gene object (e.g. <http://mygene.info/v3/gene/1017>). Note that it supports dot notation as well, e.g., you can pass “refseq.rna”. If “fields=all”, all available fields will be returned. Default: “symbol,name,taxid,entrezgene,ensemblgene”.
- **species** (*str*) – can be used to limit the gene hits from given species. You can use “common names” for nine common species (human, mouse, rat, fruitfly, nematode, zebrafish, thale-cress, frog and pig). All other species, you can provide their taxonomy ids. Multiple species can be passed using comma as a separator. Default: human,mouse,rat.

- **dotfield** – control the format of the returned fields when passed “fields” parameter contains dot notation, e.g. “fields=refseq.rna”. If True the returned data object contains a single “refseq.rna” field, otherwise (False), a single “refseq” field with a sub-field of “rna”. Default: True.
- **email** (*str*) – If you are regular users of this services, the mygeneinfo maintainers/authors encourage you to provide an email, so that we can better track the usage or follow up with you.

```

mgi = MyGeneInfoe()
mgi.get_genes(("301345,22637"))
# first one is rat, second is mouse. This will return a 'notfound'
# entry and the second entry as expected.
mgi.get_genes("301345,22637", species="mouse")

```

get_metadata ()

get_one_gene (*geneid*, *fields='symbol, name, taxid, entrezgene, ensemblgene'*, *dotfield=True*, *email=None*)

Get matching gene objects for one gene id

Parameters

- **geneid** – a valid gene ID
- **fields** (*str*) – a comma-separated fields to limit the fields returned from the matching gene hits. The supported field names can be found from any gene object (e.g. <http://mygene.info/v3/gene/1017>). Note that it supports dot notation as well, e.g., you can pass “refseq.rna”. If “fields=all”, all available fields will be returned. Default: “symbol,name,taxid,entrezgene,ensemblgene”.
- **dotfield** – control the format of the returned fields when passed “fields” parameter contains dot notation, e.g. “fields=refseq.rna”. If True the returned data object contains a single “refseq.rna” field, otherwise (False), a single “refseq” field with a sub-field of “rna”. Default: True.
- **email** (*str*) – If you are regular users of this services, the mygeneinfo maintainers/authors encourage you to provide an email, so that we can better track the usage or follow up with you.

```

mgi = MyGeneInfoe()
mgi.get_genes("301345")

```

get_one_query (*query*, *email=None*, *dotfield=True*, *fields='symbol, name, taxid, entrezgene, ensemblgene'*, *species='human, mouse, rat'*, *size=10*, *_from=0*, *sort=None*, *facets=None*, *entrezonly=False*, *ensemblonly=False*)

Make gene query and return matching gene list. Support JSONP and CORS as well.

Parameters

- **query** (*str*) – Query string. Examples “CDK2”, “NM_052827”, “204639_at”, “chr1:151,073,054-151,383,976”, “hg19.chr1:151073054-151383976”. The detailed query syntax can be found from our docs.
- **fields** (*str*) – a comma-separated fields to limit the fields returned from the matching gene hits. The supported field names can be found from any gene object (e.g. <http://mygene.info/v3/gene/1017>). Note that it supports dot notation as well, e.g., you can pass “refseq.rna”. If “fields=all”, all available fields will be returned. Default: “symbol,name,taxid,entrezgene,ensemblgene”.

- **species** (*str*) – can be used to limit the gene hits from given species. You can use “common names” for nine common species (human, mouse, rat, fruitfly, nematode, zebrafish, thale-cress, frog and pig). All other species, you can provide their taxonomy ids. Multiple species can be passed using comma as a separator. Default: human,mouse,rat.
- **size** (*int*) – the maximum number of matching gene hits to return (with a cap of 1000 at the moment). Default: 10.
- **_from** (*int*) – the number of matching gene hits to skip, starting from 0. Combining with “size” parameter, this can be useful for paging. Default: 0.
- **sort** – the comma-separated fields to sort on. Prefix with “-” for descending order, otherwise in ascending order. Default: sort by matching scores in descending order.
- **facets** (*str*) – a single field or comma-separated fields to return facets, for example, “facets=taxid”, “facets=taxid,type_of_gene”.
- **entrezonly** (*bool*) – when passed as True, the query returns only the hits with valid Entrez gene ids. Default: False.
- **ensembleonly** (*bool*) – when passed as True, the query returns only the hits with valid Ensembl gene ids. Default: False.
- **dotfield** – control the format of the returned fields when passed “fields” parameter contains dot notation, e.g. “fields=refseq.rna”. If True the returned data object contains a single “refseq.rna” field, otherwise (False), a single “refseq” field with a sub-field of “rna”. Default: True.
- **email** (*str*) – If you are regular users of this services, the mygeneinfo maintainers/authors encourage you to provide an email, so that we can better track the usage or follow up with you.

get_queries (*query*, *email=None*, *dotfield=True*, *scopes='all'*, *species='human, mouse, rat'*, *fields='symbol, name, taxid, entrezgene, ensemblgene'*)

Make gene query and return matching gene list. Support JSONP and CORS as well.

Parameters

- **query** (*str*) – Query string. Examples “CDK2”, “NM_052827”, “204639_at”, “chr1:151,073,054-151,383,976”, “hg19.chr1:151073054-151383976”. The detailed query syntax can be found from our docs.
- **fields** (*str*) – a comma-separated fields to limit the fields returned from the matching gene hits. The supported field names can be found from any gene object (e.g. <http://mygene.info/v3/gene/1017>). Note that it supports dot notation as well, e.g., you can pass “refseq.rna”. If “fields=all”, all available fields will be returned. Default: “symbol,name,taxid,entrezgene,ensemblgene”.
- **species** (*str*) – can be used to limit the gene hits from given species. You can use “common names” for nine common species (human, mouse, rat, fruitfly, nematode, zebrafish, thale-cress, frog and pig). All other species, you can provide their taxonomy ids. Multiple species can be passed using comma as a separator. Default: human,mouse,rat.
- **dotfield** – control the format of the returned fields when passed “fields” parameter contains dot notation, e.g. “fields=refseq.rna”. If True the returned data object contains a single “refseq.rna” field, otherwise (False), a single “refseq” field with a sub-field of “rna”. Default: True.
- **email** (*str*) – If you are regular users of this services, the mygeneinfo maintainers/authors encourage you to provide an email, so that we can better track the usage or follow up with you.

- **scopes** (*str*) – not documented. Set to ‘all’

`get_taxonomy()`

2.10.20 NCBIblast

Interface to the NCBI BLAST web service

What is NCBI BLAST ?

URL <http://blast.ncbi.nlm.nih.gov/>

service http://www.ebi.ac.uk/Tools/webservices/services/sss/ncbi_blast_rest

“NCBI BLAST - Protein Database Query

The emphasis of this tool is to find regions of sequence similarity, which will yield functional and evolutionary clues about the structure and function of your novel sequence.”

—from NCBIblast web page

class NCBIblast (*verbose=False*)
Interface to the NCBIblast service.

```
>>> from bioservices import *
>>> s = NCBIblast(verbose=False)
>>> jobid = s.run(program="blastp", sequence=s._sequence_example,
>>>               stype="protein", database="uniprotkb", email="name@provider")
>>> s.getResult(jobid, "out")
```

Warning: It is very important to provide a real e-mail address as your job otherwise very likely will be killed and your IP, Organisation or entire domain black-listed.

When running a blast request, a program is required. You can obtain the list using:

```
>>> s.parametersDetails("program")
[u'blastp', u'blastx', u'blastn', u'tblastx', u'tblastn']
```

- **blastn:** Search a nucleotide database using a nucleotide query
- **blastp:** Search protein database using a protein query
- **blastx:** Search protein database using a translated nucleotide query
- **tblastn:** Search translated nucleotide database using a protein query
- **tblastx:** Search translated nucleotide database using a translated nucleotide query

NCBIblast constructor

Parameters **verbose** (*bool*) – prints informative messages

databases

Returns accepted databases.

get_parameter_details (*parameterId*)

Get detailed information about a parameter.

Returns An XML document providing details about the parameter or a list of values that can take the parameters if the XML could be parsed.

For example:

```
>>> s.parameter_details("matrix")
[u'BLOSUM45',
 u'BLOSUM50',
 u'BLOSUM62',
 u'BLOSUM80',
 u'BLOSUM90',
 u'PAM30',
 u'PAM70',
 u'PAM250']
```

get_parameters ()

List parameter names.

Returns An XML document containing a list of parameter names.

```
>>> from bioservices import ncbiblast
>>> n = ncbiblast.NCBIBlast()
>>> res = n.get_parameters()
>>> [x.text for x in res.findAll("id")]
```

See also:

[parameters](#) to get a list of the parameters without need to process the XML output.

get_result (*jobid*, *result_type*)

Get the job result of the specified type.

param str jobid a job identifier returned by [run\(\)](#).

param str result_type type of result to retrieve. See [getResultTypes\(\)](#).

The output from the tool itself. Use the 'format' parameter to retrieve the output in different formats, the 'compressed' parameter to retrieve the xml output in compressed form. Format options:

```
0 = pairwise,
1 = query-anchored showing identities,
2 = query-anchored no identities,
3 = flat query-anchored showing identities,
4 = flat query-anchored no identities,
5 = XML Blast output,
6 = tabular,
7 = tabular with comment lines,
8 = Text ASN.1,
9 = Binary ASN.1,
10 = Comma-separated values,
11 = BLAST archive format (ASN.1).
```

See NCBI Blast documentation for details. Use the 'compressed' parameter to return the XML output in compressed form. e.g. '?format=5&compressed=true'.

get_result_types (*jobid*)

Get available result types for a finished job.

Parameters

- **jobid** (*str*) – a job identifier returned by `run()`.
- **verbose** (*bool*) – print the identifiers together with their label, mediaTypes, description and filesuffix.

Returns A dictionary, which keys correspond to the identifiers. Each identifier is itself a dictionary containing the label, description, file suffix and mediaType of the identifier.

`get_status(jobid)`

Get status of a submitted job

Parameters

- **jobid** (*str*) –
- **jobid** – a job identifier returned by `run()`.

Returns

A string giving the jobid status (e.g. FINISHED).

The values for the status are:

- **RUNNING**: the job is currently being processed.
- **FINISHED**: job has finished, and the results can then be retrieved.
- **ERROR**: an error occurred attempting to get the job status.
- **FAILURE**: the job failed.
- **NOT_FOUND**: the job cannot be found.

`parameters`

`run(program=None, database=None, sequence=None, stype='protein', email=None, **kargs)`

Submit a job with the specified parameters.

Compulsary arguments

Parameters

- **program** (*str*) – BLAST program to use to perform the search (e.g., blastp)
- **sequence** (*str*) – query sequence. The use of fasta formatted sequence is recommended.
- **database** (*list*) – list of database names for search or possible a single string (for one database). There are some mismatch between the output of `parametersDetails("database")` and the accepted values. For instance UniProt Knowledgebase should be given as “uniprotkb”.
- **email** (*str*) – a valid email address. Will be checked by the service itself.

Optional arguments. If not provided, a default value will be used

Parameters

- **type** (*str*) – query sequence type in ‘dna’, ‘rna’ or ‘protein’ (default is protein).
- **matrix** (*str*) – scoring matrix to be used in the search (e.g., BLOSUM45).
- **gapalign** (*bool*) – perform gapped alignments.

- **alignments** (*int*) – maximum number of alignments displayed in the output.
- **exp** – E-value threshold.
- **filter** (*bool*) – low complexity sequence filter to process the query sequence before performing the search.
- **scores** (*int*) – maximum number of scores displayed in the output.
- **dropoff** (*int*) – amount score must drop before extension of hits is halted.
- **match_scores** – match/miss-match scores to generate a scoring matrix for nucleotide searches.
- **gapopen** (*int*) – penalty for the initiation of a gap.
- **gapext** (*int*) – penalty for each base/residue in a gap.
- **seqrange** – region of the query sequence to use for the search. Default: whole sequence.

Returns A jobid that can be analysed with `getResult()`, `getStatus()`, ...

The up to data values accepted for each of these parameters can be retrieved from the `get_parameter_details()`.

For instance,:

```
from bioservices import NCBIblast
n = NCBIblast()
n.get_parameter_details("program")
```

Example:

```
jobid = n.run(program="blastp",
             sequence=n._sequence_example,
             stype="protein",
             database="uniprotkb",
             email="test@yahoo.fr")
```

Database can be a list of databases:

```
database=["uniprotkb", "uniprotkb_swissprot"]
```

The returned object is a jobid, which status can be checked. It must be finished before analysing/getting the results.

See also:

`getResult()`

Warning: Cases are not important. Spaces in the database case should be replaced by underscore.

Note: database returned by the server have meaningless names since they do not map to the expected names. An example is “ENA Sequence Release” that should be provided as `em_rel`

<http://www.ebi.ac.uk/Tools/sss/ncbiblast/help/index-nucleotide.html>

wait (*jobId*)

This function checks the status of a jobid while it is running

Parameters

- **jobid** (*str*) – a job identifier returned by `run()`.
- **checkInterval** (*int*) – interval between requests in seconds.

2.10.21 OmniPath Commons

Interface to OmniPath web service

What is OmniPath ?URL <http://omnipathdb.org>URL <https://github.com/saezlab/pypath/blob/master/webservice.rst>

A comprehensive collection of literature curated human signaling pathways.

—From OmniPath web site, March 2016

class `OmniPath` (*verbose=False, cache=False*)Interface to the `OmniPath` service

```
>>> from bioservices import OmniPath
>>> o = OmniPath()
>>> net = o.get_network()
>>> interactions = o.get_interactions('P00533')
```

Constructor `OmniPath`**Parameters** `verbose` – set to `False` to prevent informative messages**get_about** ()

Information about the version

get_info ()

Currently returns HTML page

get_interactions (*query=""*, *frmt='json'*, *fields=[]*)

Interactions of proteins

Parameters

- **query** (*str*) – a valid uniprot identifier (e.g. P00533). It can also be a list of uniprot identifiers, or a string with comma-separated identifiers.
- **fields** (*str*) – additional fields to be added to the output (e.g., sources, references)
- **frmt** (*str*) – format of the output (json or tabular)

Example:

```
res_one = o.get_interactions('P00533')
res_many = o.get_interactions('P00533,O15117,Q96FE5')
res_many = o.get_interactions(['P00533','O15117','Q96FE5'])

res_one = o.get_interactions('P00533', fields='sources')
res_one = o.get_interactions('P00533', fields=['source'])
res_one = o.get_interactions('P00533', fields=['source', 'references'])
```

You may also keep `query` to an empty string, but the entire DB will then be downloaded. This may take time and the `timeout` may need to be increased manually.

If `frmt` is set to TSV, the output is a TSV table with a header. If set to json, a dictionary is returned.

get_network (*frmt*='json')

Get basic statistics about the whole network including sources

get_ptms (*query*="", *ptm_type*=None, *frmt*='json', *fields*=[])

List enzymes, substrates and PTMs

Parameters

- **query** (*str*) – a valid uniprot identifier (e.g. P00533). It can also be a list of uniprot identifiers, or a string with comma-separated identifiers.
- **ptm_type** (*str*) – restrict the output to this type of PTM (e.g., phosphorylation)
- **fields** (*str*) – additional fields to be added to the output (e.g., sources, references)

get_resources (*frmt*='json')

Return statistics about the databases and their contents

2.10.22 Panther

Interface to some part of the Panther web service

What is Panther ?

URL <http://www.panther.org>

Citation

The PANTHER (Protein ANalysis THrough Evolutionary Relationships) Classification System was designed to classify proteins (and their genes) in order to facilitate high-throughput analysis. Proteins have been classified according to:

- Family and subfamily: families are groups of evolutionarily related proteins; subfamilies are related proteins that also have the same function
- Molecular function: the function of the protein by itself or with directly interacting proteins at a biochemical level, e.g. a protein kinase
- Biological process: the function of the protein in the context of a larger network of proteins that interact to accomplish a process at the level of the cell or organism, e.g. mitosis.
- Pathway: similar to biological process, but a pathway also explicitly specifies the relationships between the interacting molecules.

—From PantherDB (about) , Feb 2020

class Panther (*verbose*=True, *cache*=False)

Interface to Panther pages

```
>>> from bioservices import Panther
>>> p = Panther()
>>> p.get_supported_genomes()
>>> p.get_ortholog("zap70", 9606)
```

(continues on next page)

(continued from previous page)

```

>>> from bioservices import Panther
>>> p = Panther()
>>> taxon = [x[0]['taxon_id'] for x in p.get_supported_genomes() if "coli" in x[
↳ 'name'].lower()]
>>> # you may also use our method called search_organism
>>> taxon = p.get_taxon_id(pattern="coli")
>>> res = p.get_mapping("abrB,ackA,acuI", taxon)

```

The `get_mapping` returns for each gene ID the GO terms corresponding to each ID. Those go terms may belong to different categories (see meth:`get_annotation_datasets`):

- MF for molecular function
- BP for biological process
- PC for Protein class
- CC Cellular location
- Pathway

Note that results from the website application <http://pantherdb.org/> do not agree with the output of the `get_mapping` service... Try out the `dgt` gene from `ecoli` for example

Constructor

Parameters `verbose` – set to `False` to prevent informative messages

get_annotation_datasets ()

Retrieve the list of supported annotation data sets

get_enrichment (*gene_list*, *organism*, *annotation*, *enrichment_test*='Fisher', *correction*='FDR', *ref_gene_list*=None)

Returns over represented genes

Compares a test gene list to a reference gene list, and determines whether a particular class (e.g. molecular function, biological process, cellular component, PANTHER protein class, the PANTHER pathway or Reactome pathway) of genes is overrepresented or underrepresented.

Parameters

- **organism** – a valid taxon ID
- **enrichment_test** – either **Fisher** or **Binomial** test
- **correction** – correction for multiple testing. Either **FDR**, **Bonferonni**, or **None**.
- **annotation** – one of the supported PANTHER annotation data types. See `get_annotation_datasets()` to retrieve a list of supported annotation data types
- **ref_gene_list** – if not specified, the system will use all the genes for the specified organism. Otherwise, a list delimited by comma. Maximum of 100000 Identifiers can be any of the following: Ensemble gene identifier, Ensemble protein identifier, Ensemble transcript identifier, Entrez gene id, gene symbol, NCBI GI, HGNC Id, International protein index id, NCBI UniGene id, UniProt accession and UniProt id.

Returns a dictionary with the following keys. 'reference' contains the organism, 'input_list' is the input gene list with unmapped genes. 'result' contains the list of candidates.

```

>>> from bioservices import Panther
>>> p = Panther()
>>> res = p.get_enrichment('zap70,mek1,erk', 9606, "GO:0008150")

```

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```
>>> For molecular function, use :
>>> res = p.get_enrichment('zap70,mek1,erk', 9606,
    "ANNOT_TYPE_ID_PANTHER_GO_SLIM_MF")
```

get_family_msa (*family*, *taxon_list=None*)

Returns MSA information for the specified family.

Parameters

- **family** – family ID
- **taxon_list** – Zero or more taxon IDs separated by ‘,’.

get_family_ortholog (*family*, *taxon_list=None*)

Search for matching orthologs in target organisms

Also return the corresponding position in the target organism sequence. The system searches for matching orthologs in the gene family that contains the search gene associated with the search term.

Parameters

- **family** – Family ID
- **taxon_list** – Zero or more taxon IDs separated by ‘,’.

get_homolog_position (*gene*, *organism*, *position*, *ortholog_type='all'*)

Parameters

- **gene** – Can be any of the following: Ensemble gene identifier, Ensemble protein identifier, Ensemble transcript identifier, Entrez gene id, gene symbol, NCBI GI, HGNC Id, International protein index id, NCBI UniGene id, UniProt accession and UniProt id
- **organism** – a valid taxon ID
- **ortholog_type** – optional parameter to specify ortholog type of target organism

get_mapping (*gene_list*, *taxon*)

Map identifiers

Each identifier to be delimited by comma i.e. ‘,’. Maximum of 1000 Identifiers can be any of the following: Ensemble gene identifier, Ensemble protein identifier, Ensemble transcript identifier, Entrez gene id, gene symbol, NCBI GI, HGNC Id, International protein index id, NCBI UniGene id, UniProt accession and UniProt id

Parameters

- **gene_list** – see above
- **taxon** – one taxon ID. See supported [get_supported_genomes\(\)](#)

If an identifier is not found, information can be found in the `unmapped_genes` key while found identifiers are in the `mapped_genes` key.

Warning: found and not found identifiers are dispatched into unmapped and mapped genes. If there are not found identifiers, the input gene list and the mapped genes list do not have the same length. The input names are not stored in the output. Developers should be aware of that feature.

get_ortholog (*gene_list*, *organism*, *target_organism=None*, *ortholog_type='all'*)

search for matching orthologs in target organisms.

Searches for matching orthologs in the gene family that contains the search gene associated with the search terms. Returns ortholog genes in target organisms given a search organism, the search terms and a list of target organisms.

Parameters

- **gene_list** –
- **organism** – a valid taxon ID
- **target_organism** – zero or more taxon IDs separated by ‘;’. See [get_supported_genomes\(\)](#)
- **ortholog_type** – optional parameter to specify ortholog type of target organism

Returns a dictionary with “mapped” and “unmapped” keys, each of them being a list. For each unmapped gene, a dictionary with id and organism is returned. For the mapped gene, a list of ortholog is returned.

get_pathways()

Returns all pathways from pantherdb

get_supported_families (*N=1000, progress=True*)

Returns the list of supported PANTHER family IDs

This services returns only 1000 items per request. This is defined by the index. For instance index set to 1 returns the first 1000 families. Index set to 2 returns families between index 1000 and 2000 and so on. As of 20 Feb 2020, there was about 15,000 families.

This function simplifies your life by calling the service as many times as required. Therefore it returns all families in one go.

get_supported_genomes (*type=None*)

Returns list of supported organisms.

Parameters type – can be chrLoc to restrict the search

get_taxon_id (*pattern=None*)

return all taxons supported by the service

If pattern is provided, we filter the name to keep those that contain the filter. If only one is found, we return the name itself, otherwise a list of candidates

get_tree_info (*family, taxon_list=None*)

Returns tree topology information and node attributes for the specified family.

Parameters

- **family** – Family ID
- **taxon_list** – Zero or more taxon IDs separated by ‘;’.

2.10.23 Pathway Commons

This module provides a class *PathwayCommons*

What is PathwayCommons ?

URL <http://www.pathwaycommons.org/about>

REST

Pathway Commons is a convenient point of access to biological pathway information collected from public pathway databases, which you can search, visualize and download. All data is freely available, under the license terms of each contributing database.

—PathwayCommons home page, Nov 2013

Data is freely available, under the license terms of each contributing database.

class PathwayCommons (*verbose=True*)
Interface to the PathwayCommons service

```
>>> from bioservices import *
>>> pc2 = PathwayCommons(verbose=False)
>>> res = pc2.get("http://identifiers.org/uniprot/Q06609")
```

Constructor

Parameters *verbose* (*bool*) – prints informative messages

default_extension

set extension of the requests (default is json). Can be 'json' or 'xml'

get (*uri*, *frmt='BIOPAX'*)

Retrieves full pathway information for a set of elements

elements can be for example pathway, interaction or physical entity given the RDF IDs. Get commands only retrieve the BioPAX elements that are directly mapped to the ID. Use the *traverse()* query to traverse BioPAX graph and obtain child/owner elements.

Parameters

- **uri** (*str*) – valid/existing BioPAX element's URI (RDF ID; for utility classes that were "normalized", such as entity referencenes and controlled vocabularies, it is usually a Identifiers.org URL. Multiple IDs can be provided using list `uri=[http://identifiers.org/uniprot/Q06609, http://identifiers.org/uniprot/Q549Z0']` See also about MIRIAM and Identifiers.org.
- **format** (*str*) – output format (values)

Returns a complete BioPAX representation for the record pointed to by the given URI is returned. Other output formats are produced by converting the BioPAX record on demand and can be specified by the optional format parameter. Please be advised that with some output formats it might return "no result found" error if the conversion is not applicable for the BioPAX result. For example, BINARY_SIF output usually works if there are some interactions, complexes, or pathways in the retrieved set and not only physical entities.

```
>>> from bioservices import PathwayCommons
>>> pc2 = PathwayCommons(verbose=False)
>>> res = pc2.get("col5a1")
>>> res = pc2.get("http://identifiers.org/uniprot/Q06609")
```

graph (*kind*, *source*, *target=None*, *direction=None*, *limit=1*, *frmt=None*, *datasource=None*, *organism=None*)

Finds connections and neighborhoods of elements

Connections can be for example the shortest path between two proteins or the neighborhood for a particular protein state or all states.

Graph searches take detailed BioPAX semantics such as generics or nested complexes into account and traverse the graph accordingly. The starting points can be either physical entities or entity references.

In the case of the latter the graph search starts from ALL the physical entities that belong to that particular entity references, i.e. all of its states. Note that we integrate BioPAX data from multiple databases based on our proteins and small molecules data warehouse and consistently normalize UnificationXref, EntityReference, Provenance, BioSource, and ControlledVocabulary objects when we are absolutely sure that two objects of the same type are equivalent. We, however, do not merge physical entities and reactions from different sources as matching and aligning pathways at that level is still an open research problem. As a result, graph searches can return several similar but disconnected sub-networks that correspond to the pathway data from different providers (though some physical entities often refer to the same small molecule or protein reference or controlled vocabulary).

Parameters

- **kind** (*str*) – graph query
- **source** (*str*) – source object's URI/ID. Multiple source URIs/IDs must be encoded as list of valid URI **source**=[`'http://identifiers.org/uniprot/Q06609'`, `'http://identifiers.org/uniprot/Q549Z0'`].
- **target** (*str*) – required for PATHSFROMTO graph query. target URI/ID. Multiple target URIs must be encoded as list (see source parameter).
- **direction** (*str*) – graph search direction in [BOTHSTREAM, DOWNSTREAM, UPSTREAM] see `_valid_direction` attribute.
- **limit** (*int*) – graph query search distance limit (default = 1).
- **format** (*str*) – output format. see `_valid-format`
- **datasource** (*str*) – datasource filter (same as for 'search').
- **organism** (*str*) – organism filter (same as for 'search').

Returns By default, graph queries return a complete BioPAX representation of the subnetwork matched by the algorithm. Other output formats are available as specified by the optional format parameter. Please be advised that some output format choices might cause “no result found” error if the conversion is not applicable for the BioPAX result (e.g., BINARY_SIF output fails if there are no interactions, complexes, nor pathways in the retrieved set).

```
>>> from bioservices import PathwayCommons
>>> pc2 = PathwayCommons(verbose=False)
>>> res = pc2.graph(source="http://identifiers.org/uniprot/P20908",
                    kind="neighborhood", format="EXTENDED_BINARY_SIF")
```

idmapping (*ids*)

Identifier mapping tool

Unambiguously maps, e.g., HGNC gene symbols, NCBI Gene, RefSeq, ENS, and secondary UniProt identifiers to the primary UniProt accessions, or - ChEBI and PubChem IDs to primary ChEBI. You can mix different standard ID types in one query.

Note: this is a specific id-mapping (not general-purpose) for reference proteins and small molecules; the mapping tables were derived exclusively from Swiss-Prot (DR fields) and ChEBI data

Parameters **ids** (*str*) – list of Identifiers or a single identifier string.

Returns a dictionary

```

>>> from bioservices import PathwayCommons
>>> pc2 = PathwayCommons(verbose=False)
>>> pc2.idmapping("BRCA2")
{'u'BRCA2': u'P51587'}
>>> pc2.idmapping(["TP53", "BRCA2"])
{"BRCA2": "P51587", "TP53": "P04637"}

```

search (*q*, *page=0*, *datasource=None*, *organism=None*, *type=None*)

Text search in PathwayCommons using Lucene query syntax

Some of the parameters are BioPAX properties, others are composite relationships.

All index fields are (case-sensitive): comment, ecnumber, keyword, name, pathway, term, xrefdb, xrefid, dataSource, and organism.

The pathway field maps to all participants of pathways that contain the keyword(s) in any of its text fields.

Finally, keyword is a transitive aggregate field that includes all searchable keywords of that element and its child elements.

All searches can also be filtered by data source and organism.

It is also possible to restrict the domain class using the ‘type’ parameter.

This query can be used standalone or to retrieve starting points for graph searches.

Parameters

- **q** (*str*) – requires a keyword, name, external identifier, or a Lucene query string.
- **page** (*int*) – (N>=0, default is 0), search result page number.
- **datasource** (*str*) – filter by data source (use names or URIs of pathway data sources or of any existing Provenance object). If multiple data source values are specified, a union of hits from specified sources is returned. `datasource=[reactome,pid]` returns hits associated with Reactome or PID.
- **organism** (*str*) – The organism can be specified either by official name, e.g. “homo sapiens” or by NCBI taxonomy id, e.g. “9606”. Similar to data sources, if multiple organisms are declared a union of all hits from specified organisms is returned. For example `organism=[9606, 10016]` returns results for both human and mice.
- **type** (*str*) – BioPAX class filter

```

>>> from bioservices import PathwayCommons
>>> pc2 = PathwayCommons(verbose=False)
>>> pc2.search("Q06609")
>>> pc2.search("brca2", type="proteinreference",
              organism="homo sapiens", datasource="pid")
>>> pc2.search("name:'col5a1'", type="proteinreference", organism=9606)
>>> pc2.search("a*", page=3)

```

top_pathways (*datasource=None*, *organism=None*)

This command returns all *top* pathways

Pathways can be top or pathways that are neither ‘controlled’ nor ‘pathwayComponent’ of another process.

Parameters

- **datasource** (*str*) – filter by data source (same as search)
- **organism** (*str*) – organism filter

Returns dictionary with information about top pathways. Check the “searchHit” key for information about “dataSource” for instance

```
>>> from bioservices import PathwayCommons
>>> pc2 = PathwayCommons(verbose=False)
>>> res = pc2.top_pathways()
```

traverse (*uri*, *path*)

Provides XPath-like access to the PC.

The format of the path query is in the form:

```
[InitialClass]/[property1]:[classRestriction(optional)]/[property2]... A "*"
```

sign after the property instructs path accessor to transitively traverse that property. For example, the following path accessor will traverse through all physical entity components within a complex:

```
"Complex/component*/entityReference/xref:UnificationXref"
```

The following will list display names of all participants of interactions, which are components (pathway-Component) of a pathway (note: pathwayOrder property, where same or other interactions can be reached, is not considered here):

```
"Pathway/pathwayComponent:Interaction/participant*/displayName"
```

The optional parameter classRestriction allows to restrict/filter the returned property values to a certain subclass of the range of that property. In the first example above, this is used to get only the Unification Xrefs. Path accessors can use all the official BioPAX properties as well as additional derived classes and parameters in paxtools such as inverse parameters and interfaces that represent anonymous union classes in OWL. (See Paxtools documentation for more details).

Parameters

- **uri** (*str*) – a biopax element URI - specified similar to the ‘GET’ command. multiple IDs are allowed as a list of strings.
- **path** (*str*) – a BioPAX property path in the form of property1[:type1]/property2[:type2]; see above, inverse properties, Paxtools, org.biopax.paxtools.controller.PathAccessor.

See also:

[properties](#)

Returns XML result that follows the Search Response XML Schema (TraverseResponse type; pagination is disabled: returns all values at once)

```
from bioservices import PathwayCommons
pc2 = PathwayCommons(verbose=False)
res = pc2.traverse(uri=['http://identifiers.org/uniprot/P38398', 'http://
↳ identifiers.org/uniprot/Q06609'], path="ProteinReference/organism")
res = pc2.traverse(uri="http://identifiers.org/uniprot/Q06609",
path="ProteinReference/entityReferenceOf:Protein/name")
res = pc2.traverse("http://identifiers.org/uniprot/P38398",
path="ProteinReference/entityReferenceOf:Protein")
res = pc2.traverse(uri=["http://identifiers.org/uniprot/P38398",
"http://identifiers.org/taxonomy/9606"], path="Named/name")
```

2.10.24 PDB/PDBe modules

Interface to the PDB web Service.

What is PDB ?

URL <http://www.rcsb.org/pdb/>

REST <http://www.rcsb.org/pdb/software/rest.do>

An Information Portal to Biological Macromolecular Structures

—PDB home page, Feb 2013

Status in progress not for production

class PDB (*verbose=False, cache=False*)

Interface to part of the PDB service

Status in progress not for production. You can get all ID and retrieve uncompressed file in PDB/FASTA formats for now. New features will be added on request.

```
>>> from bioservices import PDB
>>> s = PDB()
>>> res = s.get_file("1FBV", "pdb")
```

Constructor

Parameters **verbose** (*bool*) – prints informative messages (default is off)

get_current_ids ()

Get a list of all current PDB IDs.

get_file (*identifier, frmt, compression=False, headerOnly=False*)

Download a file in a specified format

Parameters

- **identifier** (*int*) – a valid Identifier. See `get_current_ids()`.
- **fileFormat** (*str*) – a valid format in “pdb”, “cif”, “xml”

```
>>> from bioservices import PDB
>>> s = PDB()
>>> res = s.get_file("1FBV", "pdb")
>>> import tempfile
>>> fh = tempfile.NamedTemporaryFile()
>>> fh.write(res)
>>> # manipulate the PDB file with your favorite tool
>>> # close the file ONLY when finished (this is temporary file)
>>> # fh.close()
```

reference: <http://www.rcsb.org/pdb/static.do?p=download/http/index.html>

get_go_terms (*query*)

get_ligand_info (*query*)

get_ligands (*identifier*)

List the ligands that can be found in a PDB entry

Parameters *identifier* – a valid PDB identifier (e.g., 4HHB)

Returns

xml document

```
>>> from bioservices import PDB
>>> s = PDB()
>>> s.get_ligands("4HHB")
```

Then,

```
x = s.get_ligands("4HHB")
from pyquery import PyQuery as pq
d = pq(x)
```

get_xml_query (*query*)

Send an XML query

```
query = '<?xml version="1.0" encoding="UTF-8"?> <orgPdbQuery> <version>B0907</version>
<queryType>org.pdb.query.simple.ExpTypeQuery</queryType> <description>Experimental
Method Search : Experimental Method=SOLID-STATE NMR</description>
<mvStructure.expMethod.value>SOLID-STATE NMR</mvStructure.expMethod.value> </orgPdb-
Query> '
```

search (*query*)

```
<?xml version="1.0" encoding="UTF-8"?> <orgPdbQuery> <version>B0907</version> <query-
Type>org.pdb.query.simple.ExpTypeQuery</queryType> <description>Experimental Method Search :
Experimental Method=SOLID-STATE NMR</description> <mvStructure.expMethod.value>SOLID-
STATE NMR</mvStructure.expMethod.value> </orgPdbQuery>
```

Interface to the PDBe web Service.

What is PDBe ?

URL <https://www.ebi.ac.uk/pdbe/>

REST <https://www.ebi.ac.uk/pdbe/api/doc/>

PDBe is a founding member of the Worldwide Protein Data Bank which collects, organises and disseminates data on biological macromolecular structures. In collaboration with the other Worldwide Protein Data Bank (wwPDB) partners, we work to collate, maintain and provide access to the global repository of macromolecular structure models, the Protein Data Bank (PDB).

—PDBe home page, June 2020

class PDBe (*verbose=False, cache=False*)

Interface to part of the PDBe service

```
>>> from bioservices import PDBe
>>> s = PDBe()
>>> res = s.get_file("1FBV", "pdb")
```

Constructor

Parameters `verbose` (*bool*) – prints informative messages (default is off)

`get_assembly` (*query*)

Provides information for each assembly of a given PDB ID. T

This information is broken down at the entity level for each assembly. The information given includes the molecule name, type and class, the chains where the molecule occur, and the number of copies of each entity in the assembly.

Parameters `query` – a 4-character PDB id code

```
p.get_assembly('1cbs')
```

`get_binding_sites` (*query*)

Provides details on binding sites in the entry

STRUCT_SITE records in PDB files (or mmCIF equivalent thereof), such as ligand, residues in the site, description of the site, etc.

Parameters `query` – a 4-character PDB id code

```
p.get_binding_sites('1cbs')
```

`get_drugbank_annotation` (*query*)

This call provides DrugBank annotation of all ligands, i.e. 'bound'

Parameters `query` – a 4-character PDB id code

```
p.get_drugbank_annotation('5hht')
```

`get_electron_density_statistics` (*query*)

This call details the statistics for electron density.

Parameters `query` – a 4-character PDB id code

```
p.get_electron_density_statistics('1cbs')
```

`get_experiment` (*query*)

Provides details of experiment(s) carried out in determining the structure of the entry.

Each experiment is described in a separate dictionary. For X-ray diffraction, the description consists of resolution, spacegroup, cell dimensions, R and Rfree, refinement program, etc. For NMR, details of spectrometer, sample, spectra, refinement, etc. are included. For EM, details of specimen, imaging, acquisition, reconstruction, fitting etc. are included.

Parameters `query` – a 4-character PDB id code

```
p.get_experiment('1cbs')
```

`get_files` (*query*)

Provides URLs and brief descriptions (labels) for PDB entry

Also, for mmCIF files, biological assembly files, FASTA file for sequences, SIFTS cross reference XML files, validation XML files, X-ray structure factor file, NMR experimental constraints files, etc.

Parameters `query` – a 4-character PDB id code

```
p.get_files('1cbs')
```

get_functional_annotation (*query*)

Provides functional annotation of all ligands, i.e. 'bound'

Parameters *query* – a 4-character PDB id code

```
p.get_functional_annotation('1cbs')
```

get_ligand_monomers (*query*)

Provides a list of modelled instances of ligands,

ligands i.e. 'bound' molecules that are not waters.

Parameters *query* – a 4-character PDB id code

```
p.get_ligand_monomers('1cbs')
```

get_modified_residues (*query*)

Provides a list of modelled instances of modified amino acids or nucleotides in protein, DNA or RNA chains.

Parameters *query* – a 4-character PDB id code

```
p.get_modified_residues('4v5j')
```

get_molecules (*query*)

Return details of molecules (or entities in mmcif-speak) modelled in the entry

This can be entity id, description, type, polymer-type (if applicable), number of copies in the entry, sample preparation method, source organism(s) (if applicable), etc.

Parameters *query* – a 4-character PDB id code

```
p.get_molecules('1cbs')
```

get_mutated_residues (*query*)

Provides a list of modelled instances of mutated amino acids or nucleotides in protein, DNA or RNA chains.

Parameters *query* – a 4-character PDB id code

```
p.get_mutated_residues('1bgj')
```

get_nmr_resources (*query*)

This call provides URLs of available additional resources for NMR entries. E.g., mapping between structure (PDB) and chemical shift (BMRB) entries. :param *query*: a 4-character PDB id code

```
p.get_nmr_resources('1cbs')
```

get_observed_ranges (*query*)

Provides observed ranges, i.e., segments of structural coverage of polymeric molecules that are modelled fully or partly

Parameters *query* – a 4-character PDB id code

```
p.get_observed_ranges('1cbs')
```


get_observed_ranges_in_pdb_chain (*query*, *chain_id*)

Provides observed ranges, i.e., segments of structural coverage of polymeric molecules in a particular chain

Parameters

- **query** – a 4-character PDB id code
- **chain_id** – a PDB chain ID

```
p.get_observed_ranges_in_pdb_chain('1cbs', "A")
```

get_observed_residues_ratio (*query*)

Provides the ratio of observed residues for each chain in each molecule

The list of chains within an entity is sorted by observed_ratio (descending order), partial_ratio (ascending order), and number_residues (descending order).

Parameters **query** – a 4-character PDB id code

```
p.get_observed_residues_ratio('1cbs')
```

get_related_dataset (*query*)

Provides DOI's for related raw experimental datasets

Includes diffraction image data, small-angle scattering data and electron micrographs.

Parameters **query** – a 4-character PDB id code

```
p.get_cofactor('5o8b')
```

get_related_publications (*query*)

Return publications obtained from both EuroPMC and UniProt. T

These are articles which cite the primary citation of the entry, or open-access articles which mention the entry id without explicitly citing the primary citation of an entry.

Parameters **query** – a 4-character PDB id code

```
p.get_related_publications('1cbs')
```

get_release_status (*query*)

Provides status of a PDB entry (released, obsoleted, on-hold etc) along with some other information such as authors, title, experimental method, etc.

Parameters **query** – a 4-character PDB id code

```
p.get_release_status('1cbs')
```

get_residue_listing (*query*)

Provides lists all residues (modelled or otherwise) in the entry.

Except waters, along with details of the fraction of expected atoms modelled for the residue and any alternate conformers.

Parameters **query** – a 4-character PDB id code

```
p.get_residue_listing('1cbs')
```

get_residue_listing_in_pdb_chain (*query, chain_id*)

Provides all residues (modelled or otherwise) in the entry

Except waters, along with details of the fraction of expected atoms modelled for the residue and any alternate conformers.

Parameters

- **query** – a 4-character PDB id code
- **query** – a PDB chain ID

```
p.get_residue_listing_in_pdb_chain('1cbs')
```

get_secondary_structure (*query*)

Provides residue ranges of regular secondary structure

(alpha helices and beta strands) found in protein chains of the entry. For strands, sheet id can be used to identify a beta sheet.

Parameters **query** – a 4-character PDB id code

```
p.get_secondary_structure('1cbs')
```

get_summary (*query*)

Returns summary of a PDB entry

This can be title of the entry, list of depositors, date of deposition, date of release, date of latest revision, experimental method, list of related entries in case split entries, etc.

Parameters **query** – a 4-character PDB id code

```
p.get_summary('1cbs')
p.get_summary('1cbs,2kv8')
p.get_summary(['1cbs', '2kv8'])
```

2.10.25 PRIDE module

Interface to PRIDE web service

What is PRIDE ?

URL <http://www.ebi.ac.uk/pride/archive/>

URL <http://www.ebi.ac.uk/pride/ws/archive>

The PRIDE PRoteomics IDentifications database is a centralized, standards compliant, public data repository for proteomics data, including protein and peptide identifications, post-translational modifications and supporting spectral evidence.

—From PRIDE web site, Jan 2015

class PRIDE (*verbose=False, cache=False*)

Interface to the PRIDE service

Constructor

Parameters **verbose** – set to False to prevent informative messages

get_assay_count (*identifier*)

Count assays for a project accession number

Parameters *identifier* (*str*) – a project accession number**Returns** integer

```
>>> p = PRIDE()
>>> assays = p.get_assay_count('PRD000001')
5
```

get_assay_list (*identifier*)

Return list of assays for a project accession number

Parameters *identifier* (*str*) – project accession number. See *get_project_list()***Returns** list of dictionaries. Each dictionary represents an assay.

```
>>> p = PRIDE()
>>> assays = p.get_assay_list('PRD000001')
>>> len(assays) # could be found with get_assay_count_project_accession
5
>>> assays[1]['assayAccession']
1643
```

get_assays (*identifier*)

Retrieve assay information by assay accession

Parameters *identifier* (*int*) – assay accession number

```
>>> p = PRIDE()
>>> res = p.get_assays(1643)
>>> res['proteinCount']
276
```

get_file_count (*identifier*)

return count of files in a project

Parameters *identifier* (*str*) – a project accession number**Returns** int

```
>>> p.get_file_count('PRD000001')
5
```

get_file_count_assay (*identifier*)

list files for an assay

Parameters *identifier* (*int*) – assay accession number**Returns** int

```
p.get_file_assay(1643)
```

get_file_list (*identifier*)

return list of files for a project

Parameters *identifier* (*str*) – a project accession number

```
>>> files = p.get_file_count('PRD000001')
>>> len(files)
5
```

get_file_list_assay (*identifier*)

list files for an assay

Parameters **identifier** (*int*) – assay accession number**Returns** list of dictionary, Each dictionary represents a file data structure

```
res = p.get_file_assay(1643)
```

get_peptide_count (*identifier, sequence=None*)

Count peptide identifications by project accession

Parameters **identifier** (*str*) – a project accession number**Returns**

int

```
>>> p.get_peptide_count('PRD000001', sequence='PLIPIVVEQTGR')
4
>>> p.get_peptide_count('PRD000001')
6758
```

get_peptide_count_assay (*identifier, sequence=None*)

Count peptide identifications by assay accession

Parameters **identifier** (*str*) – an assay accession number**Returns** int

```
>>> p.get_peptide_count_assay(1643, sequence='AAATQKKVER')
5
>>> p.get_peptide_count_assay(1643)
1696
```

get_peptide_list (*identifier, sequence=None, show=10, page=0*)

Retrieve peptide identifications by project accession (and sequence)

Parameters

- **identifier** (*str*) – a project accession number
- **sequence** (*str*) – the peptide sequence to limit the query on (optional). If provided, show and page are not used
- **show** (*int*) – how many results to return per page
- **page** (*int*) – which page (starting from 0) of the result to return

```
>>> peptides = p.get_peptide_list('PRD000001', sequence='PLIPIVVEQTGR')
>>> len(peptides)
4
>>> peptides = p.get_peptide_list('PRD000001')
>>> len(peptides)
10
>>> peptides = p.get_peptide_list('PRD000001', show=100)
```

Note: the function merge two functions from the PRIDE API (`get_peptide_list` and `get_peptide_list_sequence`)

get_peptide_list_assay (*identifier*, *sequence=None*, *show=10*, *page=0*)

Retrieve peptide identifications by assay accession (and sequence)

Parameters

- **identifier** (*str*) – an assay accession number
- **sequence** (*str*) – the peptide sequence to limit the query on (optional). If provided, `show` and `page` are not used
- **show** (*int*) – how many results to return per page
- **page** (*int*) – which page (starting from 0) of the result to return

```
>>> peptides = p.get_peptide_list_assay(1643, sequence='AAATQKKVER')
>>> len(peptides)
5
>>> peptides = p.get_peptide_list_assay(1643)
>>> len(peptides)
10
>>> peptides = p.get_peptide_list_assay(1643, show=100)
```

Note: the function merge two functions from the PRIDE API (`get_peptide_list` and `get_peptide_list_sequence`)

get_project (*identifier*)

Retrieve project information by accession

Parameters **identifier** (*str*) – a valid PRIDE identifier e.g., PRD000001

Returns a dictionary with the project details. See <http://www.ebi.ac.uk/pride/ws/archive/#/project> for details

```
>>> from bioservices import PRIDE
>>> p = PRIDE()
>>> res = p.get_project("PRD000001")
>>> res['numPeptides']
6758
```

get_project_count (*query=""*, *speciesFilter=None*, *ptmsFilter=None*, *tissueFilter=None*, *diseaseFilter=None*, *titleFilter=None*, *instrumentFilter=None*, *experimentTypeFilter=None*, *quantificationfilter=None*, *projectTagFilter=None*)

Count projects for given criteria

Takes same query parameters as the `/list` operation; typically used to retrieve number of results before querying with `/list`

Parameters

- **query** (*str*) – search term to query for
- **speciesFilter** (*str*) – filter by species (NCBI taxon ID or name)
- **ptmsFilter** (*str*) – filter by PTM annotation query
- **tissueFilter** (*str*) – filter by tissue annotation

- **diseaseFilter** (*str*) – filter by disease annotation
- **titleFilter** (*str*) – filter the title for keywords
- **instrumentFilter** (*str*) – filter for instrument names or keywords
- **experimentTypeFilter** (*str*) – filter by experiment type
- **quantificationFilter** (*str*) – filter by quantification annotation
- **projectTagFilter** (*str*) – filter by project tags

Returns number of projects (integer)

get_project_list (*query=""*, *show=10*, *page=0*, *sort=None*, *order='desc'*, *speciesFilter=None*, *ptmsFilter=None*, *tissueFilter=None*, *diseaseFilter=None*, *titleFilter=None*, *instrumentFilter=None*, *experimentTypeFilter=None*, *quantificationfilter=None*, *projectTagFilter=None*)
list projects or given criteria

Parameters

- **query** (*str*) – search term to query for
- **show** (*int*) – how many results to return per page
- **page** (*int*) – which page (starting from 0) of the result to return
- **sort** (*str*) – the field to sort on
- **order** (*str*) – the sorting order (asc or desc)
- **speciesFilter** (*str*) – filter by species (NCBI taxon ID or name)
- **ptmsFilter** (*str*) – filter by PTM annotation query
- **tissueFilter** (*str*) – filter by tissue annotation
- **diseaseFilter** (*str*) – filter by disease annotation
- **titleFilter** (*str*) – filter the title for keywords
- **instrumentFilter** (*str*) – filter for instrument names or keywords
- **experimentTypeFilter** (*str*) – filter by experiment type
- **quantificationFilter** (*str*) – filter by quantification annotation
- **projectTagFilter** (*str*) – filter by project tags

```

>>> p = PRIDE()
>>> projects = p.get_project_list(show=100)
```

get_protein_count (*identifier*)
Count protein identifications by project accession

Parameters **identifier** (*str*) – a project accession number

Returns int

get_protein_count_assay (*identifier*)
Count protein identifications by assay accession

Parameters **identifier** (*str*) – a project accession number

Returns int

get_protein_list (*identifier*, *show=10*, *page=0*)
Retrieve protein identifications by project accession

Parameters

- **identifier** (*str*) – a project accession number
- **show** (*int*) – how many results to return per page
- **page** (*int*) – which page (starting from 0) of the result to return

get_protein_list_assay (*identifier*, *show=10*, *page=0*)
Retrieve protein identifications by assay accession

Parameters

- **identifier** (*str*) – a project accession number
- **show** (*int*) – how many results to return per page
- **page** (*int*) – which page (starting from 0) of the result to return

2.10.26 PSICQUIC

Interface to the PSICQUIC web service

What is PSICQUIC ?

URL <http://code.google.com/p/psicquic/>

REST http://code.google.com/p/psicquic/wiki/PsicquicSpec_1_3_Rest

“PSICQUIC is an effort from the HUPO Proteomics Standard Initiative (HUPO-PSI) to standardise the access to molecular interaction databases programmatically. The PSICQUIC View web interface shows that PSICQUIC provides access to 25 active service “

—Dec 2012

About queries

source: PSICQUIC View web page

The idea behind PSICQUIC is to retrieve information related to protein interactions from various databases. Note that protein interactions does not necessarily mean protein-protein interactions. In order to be effective, the query format has been standardised.

To do a search you can use the Molecular Interaction Query Language which is based on Lucene’s syntax. Here are some rules

- Use OR or space ‘ ’ to search for ANY of the terms in a field
- Use AND if you want to search for those interactions where ALL of your terms are found
- Use quotes (“”) if you look for a specific phrase (group of terms that must be searched together) or terms containing special characters that may otherwise be interpreted by our query engine (eg. ‘.’ in a GO term)
- Use parenthesis for complex queries (e.g. ‘(XXX OR YYY) AND ZZZ’)
- **Wildcards (*,?) can be used between letters in a term or at the end of terms to do fuzzy queries, but never at the beginning of a term.**

- **Optionally, you can prepend a symbol in front of your term.**
 - * (plus): include this term. Equivalent to AND. e.g. +P12345
 - * (minus): do not include this term. Equivalent to NOT. e.g. -P12345
 - Nothing in front of the term. Equivalent to OR. e.g. P12345
- Implicit fields are used when no field is specified (simple search). For instance, if you put ‘P12345’ in the simple query box, this will mean the same as identifier:P12345 OR pubid:P12345 OR pubauth:P12345 OR species:P12345 OR type:P12345 OR detmethod:P12345 OR interaction_id:P12345

About the MITAB output

The output returned by a query contains a list of entries. Each entry is formatted following the MITAB output.

Here below are listed the name of the field returned ordered as they would appear in one entry. The first item is always idA whatever version of MITAB is used. The version 25 of MITAB contains the first 15 fields in the table below. Newer version may include more fields but always include the 15 from MITAB 25 in the same order. See the link from [irefindex about mitab](#) for more information.

Field Name	Searches on	Implicit*	Example
idA	Identifier A	No	idA:P74565
idB	Identifier B	No	idB:P74565
id	Identifiers (A or B)	No	id:P74565
alias	Aliases (A or B)	No	alias:(KHDRBS1 HCK)
identifiers	Identifiers and Aliases undistinctively	Yes	identifier:P74565
pubauth	Publication 1st author(s)	Yes	pubauth:scott
pubid	Publication Identifier(s) OR	Yes	pubid:(10837477 12029088)
taxidA	Tax ID interactor A: the tax ID or the species name	No	taxidA:mouse
taxidB	Tax ID interactor B: the tax ID or species name	No	taxidB:9606
species	Species. Tax ID A or Tax ID B	Yes	species:human
type	Interaction type(s)	Yes	type:"physical interaction"
detmethod	Interaction Detection method(s)	Yes	detmethod:"two hybrid**"
interaction_id	Interaction identifier(s)	Yes	interaction_id:EBI-761050
pbioroleA	Biological role A	Yes	pbioroleA:ancillary
pbioroleB	Biological role B	Yes	pbioroleB:"MI:0684"
pbiorole	Biological roles (A or B)	Yes	pbiorole:enzyme
ptypeA	Interactor type A	Yes	ptypeA:protein
ptypeB	Interactor type B	Yes	ptypeB:"gene"
ptype	Interactor types (A or B)	Yes	pbiorole:"small molecule"
pxrefA	Interactor xref A (or Identifier A)	Yes	pxrefA:"GO:0003824"
pxrefB	Interactor xref B (or Identifier B)		Yes pxrefB:"GO:0003824"

Continued on next page

Table 1 – continued from previous page

Field Name	Searches on	Implicit*	Example
pxref	Interactor xrefs (A or B or Identifier A or Identifier B)	Yes	pxref:"catalytic activity"
xref	Interaction xrefs (or Interaction identifiers)	Yes	xref:"nuclear pore"
annot	Interaction annotations and tags	Yes	annot:"internally curated"
update	Update date	Yes	update:[20100101 TO 20120101]
negative	Negative interaction boolean	Yes	negative:true
complex	Complex expansion	Yes	complex:"spoke expanded"
ftypeA	Feature type of participant A	Yes	ftypeA:"sufficient to bind"
ftypeB	Feature type of participant B	Yes	ftypeB:mutation
ftype	Feature type of participant A or B	Yes	ftype:"binding site"
pmethodA	Participant identification method A	Yes	pmethodA:"western blot"
pmethodB	Participant identification method B	Yes	pmethodB:"sequence tag identification"
pmethod	Participant identification methods (A or B)	Yes	pmethod:immunostaining
stc	Stoichiometry (A or B). Only true or false, just to be able to filter interaction having stoichiometry available	Yes	stc:true
param	Interaction parameters. Only true or false, just to be able to filter interaction having parameters available	Yes	param:true

class PSICQUIC (*verbose=True*)

Interface to the **PSICQUIC** service

There are 2 interfaces to the PSICQUIC service (REST and WSDL) but we used the REST only.

This service provides a common interface to more than 25 other services related to protein. So, we won't detail all the possibility of this service. Here is an example that consists of looking for interactors of the protein ZAP70 within the IntAct database:

```
>>> from bioservices import *
>>> s = PSICQUIC()
>>> res = s.query("intact", "zap70")
>>> len(res) # there are 11 interactions found
11
```

(continues on next page)

(continued from previous page)

```

>>> for x in res[1]:
...     print(x)
uniprotkb:O95169
uniprotkb:P43403
intact:EBI-716238
intact:EBI-1211276
psi-mi:ndub8_human(display_long)|uniprotkb:NADH-ubiquinone oxidoreductase ASHI
.
.

```

Here we have a list of entries. There are 15 of them (depending on the *output* parameter). The meaning of the entries is described on PSICQUIC website: <https://code.google.com/p/psicquic/wiki/MITAB25Format> . In short:

1. Unique identifier for interactor A
2. Unique identifier for interactor B.
3. Alternative identifier for interactor A, for example the official gene
4. Alternative identifier for interactor B.
5. Aliases for A, separated by “|”
6. Aliases for B.
7. Interaction detection methods, taken from the corresponding PSI-MI
8. First author surname(s) of the publication(s)
9. Identifier of the publication
10. NCBI Taxonomy identifier for interactor A.
11. NCBI Taxonomy identifier for interactor B.
12. Interaction types,
13. Source databases and identifiers,
14. Interaction identifier(s) i
15. Confidence score. Denoted as scoreType:value.

Another example with reactome database:

```
res = s.query("reactome", "Q9Y266")
```

Warning: PSICQUIC gives access to 25 other services. We cannot create a dedicated parsing for all of them. So, the `::query` method returns the raw data. Addition class may provide dedicated parsing in the future.

See also:

`bioservices.biogrid.BioGRID`

Constructor

Parameters `verbose` (*bool*) – print informative messages

```
>>> from bioservices import PSICQUIC
>>> s = PSICQUIC()
```

activeDBs

returns the active DBs only

convert (*data*, *db=None*)

convertAll (*data*)

formats

Returns the possible output formats

getInteractionCounter (*query*)

Returns a dictionary with database as key and results as values

Parameters *query* (*str*) – a valid query

Returns a dictionary which key as database and value as number of entries

Consider only the active database.

getName (*data*)

knownName (*data*)

Scan all entries (MITAB) and returns simplified version

Each item in the input list of mitab entry The output is made of 2 lists corresponding to interactor A and B found in the mitab entries.

elements in the input list takes the following forms:

```
DB1:ID1|DB2:ID2
DB3:ID3
```

The | sign separates equivalent IDs from different databases.

We want to keep only one. The first known database is kept. If in the list of DB:ID pairs no known database is found, then we keep the first one whatsoever.

known databases are those available in the uniprot mapping tools.

chembl and chebi IDs are kept unchanged.

mappingOneDB (*data*)

postCleaning (*data*, *keep_only='HUMAN'*, *remove_db=['chebi', 'chembl']*, *keep_self_loop=False*, *verbose=True*)

Remove entries with a None and keep only those with the keep pattern

postCleaningAll (*data*, *keep_only='HUMAN'*, *flatten=True*, *verbose=True*)

even more cleaning by ignoring score, db and interaction len(set([(x[0],x[1]) for x in retnew]))

preCleaning (*data*)

remove entries where IdA or IdB is set to “-“

print_status ()

Prints the services that are available

Returns Nothing

The output is tabulated. The columns are:

- names
- active

- count
- version
- rest URL
- soap URL
- rest example
- restricted

See also:

If you want the data into lists, see all attributes starting with registry such as `registry_names()`

query (*service, query, output='tab25', version='current', firstResult=None, maxResults=None*)

Send a query to a specific database

Parameters

- **service** (*str*) – a registered service. See `registry_names`.
- **query** (*str*) – a valid query. Can be * or a protein name.
- **output** (*str*) – a valid format. See `s._formats`

```
s.query("intact", "brca2", "tab27")
s.query("intact", "zap70", "xml25")
s.query("matrixdb", "*", "xml25")
```

This is the programmatic approach to this website:

<http://www.ebi.ac.uk/Tools/webservices/psicquic/view/main.xhtml>

Another example consist in accessing the *string* database for fetching protein-protein interaction data of a particular model organism. Here we restrict the query to 100 results:

```
s.query("string", "species:10090", firstResult=0, maxResults=100, output="tab25")
```

spaces are automatically converted

```
s.query("biogrid", "ZAP70 AND species:9606")
```

Warning: AND must be in big caps. Some database are ore permissive than other (e.g., intact accepts “and”). species must be a valid ID number. Again, some DB are more permissive and may accept the name (e.g., human)

To obtain the number of interactions in intact for the human specy:

```
>>> len(p.query("intact", "species:9606"))
```

queryAll (*query, databases=None, output='tab25', version='current', firstResult=None, maxResults=None*)

Same as query but runs on all active database

Parameters **databases** (*list*) – database to query. Queries all active DB if not provided

Returns dictionary where keys correspond to databases and values to the output of the query.

```
res = s.queryAll("ZAP70 AND species:9606")
```

read_registry ()
Reads and returns the active registry

registry
returns the registry of psiquic

registry_actives
returns active state of each service

registry_counts
returns number of entries in each service

registry_names
returns all services available (names)

registry_restexamples
returns REST example for each service

registry_restricted
returns restricted status of services

registry_resturls
returns URL of REST services

registry_soapurls
returns URL of WSDL service

registry_versions
returns version of each service

2.10.27 Rhea

Interface to the Rhea web services

What is Rhea ?

URL <http://www.ebi.ac.uk/rhea/>

Citations See <http://www.ebi.ac.uk/rhea/about.xhtml>

Rhea is a reaction database, where all reaction participants (reactants and products) are linked to the ChEBI database (Chemical Entities of Biological Interest) which provides detailed information about structure, formula and charge. Rhea provides built-in validations that ensure both elemental and charge balance of the reactions... While the main focus of Rhea is enzyme-catalysed reactions, other biochemical reactions are also included.

The database is extensively cross-referenced. Reactions are currently linked to the EC list, KEGG and MetaCyc, and the reactions will be used in the IntEnz database and in all relevant UniProtKB entries. Furthermore, the reactions will also be used in the UniPathway database to generate pathways and metabolic networks.

—from Rhea Home page, Dec 2012 (<http://www.ebi.ac.uk/rhea/about.xhtml>)

class Rhea (*version='1.0', verbose=True, cache=False*)

Interface to the Rhea service

You can search by compound name, ChEBI ID, reaction ID, cross reference (e.g., EC number) or citation (author name, title, abstract text, publication ID). You can use double quotes - to match an exact phrase - and the following wildcards:

- ? (question mark = one character),
- * (asterisk = several characters).

Searching for `caffe*` will find reactions with participants such as caffeine, trans-caffeic acid or caffeoyl-CoA:

```
from bioservices import Rhea
r = Rhea()
response = r.search("caffe*")
```

Searching for `a?e?o*` will find reactions with participants such as acetoin, acetone or adenosine.:

```
from bioservices import Rhea
r = Rhea()
response = r.search("a?e?o*")
```

See `search()` `entry()` methods for more information about format.

Rhea constructor

Parameters

- **version** (*str*) – the current version of the interface (1.0)
- **verbose** (*bool*) – True by default

```
>>> from bioservices import Rhea
>>> r = Rhea()
```

`entry(id, frmt)`

Retrieve a concrete reaction for the given id in a given format

Parameters

- **id** (*int*) – the id of a reaction
- **format** – can be `rxn`, `biopax2`, or `cmlreact`

Returns An XML document containing the reactions with undefined direction, with links to the corresponding bi-directional ones. The format is easyXML. If `frmt` is `rxn`,

```
>>> print(r.entry(10281, frmt="rxn"))
```

The output is in XML format. This page from the Rhea web site explains what are the [data fields](#) of the XML file.

`get_metabolites(rxn_id)`

Given a Rhea (<http://www.rhea-db.org/>) reaction id, returns its participant metabolites as a dict: {metabolite: stoichiometry},

e.g. '2 H + 1 O2 = 1 H2O' would be represented as {'H': -2, 'O2': -1, 'H2O': 1}.

Parameters `rxn_id` – Rhea reaction id

Returns dict of participant metabolites.

`search(query, frmt=None)`

Search for reactions

Parameters

- **query** (*str*) – the search term using format parameter

- **format** (*str*) – the biopax2 or cmlreact format (default)

Returns An XML document containing the reactions with undefined direction, with links to the corresponding bi-directional ones. The format is easyXML.

```
>>> r = Rhea()
>>> r.search("caffeine") # id 10280
>>> r.search("caffeine", frmt="biopax2") # id 10280
```

The output is in XML format. This page from the Rhea web site explains what are the [data fields](#) of the XML file.

2.10.28 Reactome

Interface to the Reactome webs services

What is Reactome?

URL <http://www.reactome.org/ReactomeGWT/entrypoint.html>

Citation <http://www.reactome.org/citation.html>

REST <http://reactomews.oicr.on.ca:8080/ReactomeRESTfulAPI/RESTfulWS>

“REACTOME is an open-source, open access, manually curated and peer-reviewed pathway database. Pathway annotations are authored by expert biologists, in collaboration with Reactome editorial staff and cross-referenced to many bioinformatics databases. These include NCBI Entrez Gene, Ensembl and UniProt databases, the UCSC and HapMap Genome Browsers, the KEGG Compound and ChEBI small molecule databases, PubMed, and Gene Ontology. . . .”

—from Reactome web site

class Reactome (*verbose=True, cache=False*)

Todo: interactors, orthology, particiapnts, person, query, refernces, schema

get_complex_subunits (*identifier, excludeStructuresSpecifies=False*)

A list with the entities contained in a given complex

Retrieves the list of subunits that constitute any given complex. In case the complex comprises other complexes, this method recursively traverses the content returning each contained PhysicalEntity. Contained complexes and entity sets can be excluded setting the ‘excludeStructures’ optional parameter to ‘true’

Parameters

- **identifier** – The complex for which subunits are requested
- **excludeStructures** – Specifies whether contained complexes and entity sets are excluded in the response

```
r.get_complex_subunits("R-HSA-5674003")
```

get_complexes (*resources, identifier*)

A list of complexes containing the pair (identifier, resource)

Retrieves the list of complexes that contain a given (identifier, resource). The method deconstructs the complexes into all its participants to do so.

Parameters

- **resource** – The resource of the identifier for complexes are requested (e.g. UniProt)
- **identifier** – The identifier for which complexes are requested

```
r.get_complexes(resources, identifier)
r.get_complexes("UniProt", "P43403")
```

get_discover (*identifier*)

The schema.org for an Event in Reactome knowledgebase

For each event (reaction or pathway) this method generates a json file representing the dataset object as defined by schema.org (http). This is mainly used by search engines in order to index the data

```
r.data_discover("R-HSA-446203")
```

get_diseases ()

list of diseases objects

get_diseases_doid ()

retrieves the list of disease DOIDs annotated in Reactome

return: dictionary with DOID contained in the values()

get_entity_componentOf (*identifier*)

A list of larger structures containing the entity

Retrieves the list of structures (Complexes and Sets) that include the given entity as their component. It should be mentioned that the list includes only simplified entries (type, names, ids) and not full information about each item.

```
r.get_entity_componentOf("R-HSA-199420")
```

get_entity_otherForms (*identifier*)

All other forms of PhysicalEntity

Retrieves a list containing all other forms of the given PhysicalEntity. These other forms are PhysicalEntities that share the same ReferenceEntity identifier, e.g. PTEN H93R[R-HSA-2318524] and PTEN C124R[R-HSA-2317439] are two forms of PTEN.

```
r.get_entity_otherForms("R-HSA-199420")
```

get_event_ancestors (*identifier*)

The ancestors of a given event

The Reactome definition of events includes pathways and reactions. Although events are organised in a hierarchical structure, a single event can be in more than one location, i.e. a reaction can take part in different pathways while, in the same way, a sub-pathway can take part in many pathways. Therefore, this method retrieves a list of all possible paths from the requested event to the top level pathway(s).

Parameters identifier – The event for which the ancestors are requested

```
r.get_event_ancestors("R-HSA-5673001")
```

get_eventsHierarchy (*species*)

The full event hierarchy for a given species

Events (pathways and reactions) in Reactome are organised in a hierarchical structure for every species. By following all 'hasEvent' relationships, this method retrieves the full event hierarchy for any given species. The result is a list of tree structures, one for each TopLevelPathway. Every event in these trees is represented by a PathwayBrowserNode. The latter contains the stable identifier, the name, the species, the url, the type, and the diagram of the particular event.

Parameters species – Allowed species filter: SpeciesName (eg: Homo sapiens) Species-TaxId (eg: 9606)

```
r.get_eventsHierarchy(9606)
```

get_exporter_diagram (*identifier*, *ext*='png', *quality*=5, *diagramProfile*='Modern', *analysisProfile*='Standard', *filename*=None)

Export a given pathway diagram to raster file

This method accepts identifiers for Event class instances. When a diagrammed pathway is provided, the diagram is exported to the specified format. When a subpathway is provided, the diagram for the parent is exported and the events that are part of the subpathways are selected. When a reaction is provided, the diagram containing the reaction is exported and the reaction is selected.

Parameters

- **identifier** – Event identifier (it can be a pathway with diagram, a subpathway or a reaction)
- **ext** – File extension (defines the image format) in png, jpeg, jpg, svg, gif
- **quality** – Result image quality between [1 - 10]. It defines the quality of the final image (Default 5)
- **flg** – not implemented
- **sel** – not implemented
- **diagramProfile** – Diagram Color Profile
- **token** – not implemented
- **analysisProfile** – Analysis Color Profile
- **expColumn** – not implemented
- **filename** – if given, save the results in the provided filename

return: raw data if filename parameter is not set. Otherwise, the data is saved in the filename and the function returns None

get_exporter_fireworks ()

get_exporter_reaction ()

get_exporter_sbml (*identifier*)

Export given Pathway to SBML

Parameters identifier – DbId or StId of the requested database object

```
r.exporter_sbml("R-HSA-68616")
```

get_interactors_psicquic_molecule_details ()

Retrieve clustered interaction, sorted by score, of a given accession by resource.

get_interactors_psicquic_molecule_summary ()

Retrieve a summary of a given accession by resource

get_interactors_psicquic_resources ()

Retrieve a list of all Psicquic Registries services

get_interactors_static_molecule_details ()

Retrieve a detailed interaction information of a given accession

get_interactors_static_molecule_pathways ()

Retrieve a list of lower level pathways where the interacting molecules can be found

get_interactors_static_molecule_summary ()

Retrieve a summary of a given accession

get_mapping_identifier_pathways (*resource, identifier*)

get_mapping_identifier_reactions (*resource, identifier*)

get_pathway_containedEvents (*identifier*)

All the events contained in the given event

Events are the building blocks used in Reactome to represent all biological processes, and they include pathways and reactions. Typically, an event can contain other events. For example, a pathway can contain smaller pathways and reactions. This method recursively retrieves all the events contained in any given event.

```
r.get_pathway_containedEvents("R-HSA-5673001")
```

get_pathway_containedEvents_by_attribute (*identifier, attribute*)

A single property for each event contained in the given event

Events are the building blocks used in Reactome to represent all biological processes, and they include pathways and reactions. Typically, an event can contain other events. For example, a pathway can contain smaller pathways (subpathways) and reactions. This method recursively retrieves a single attribute for each of the events contained in the given event.

Parameters

- **identifier** – The event for which the contained events are requested
- **attribute** – Attribute to be filtered

```
r.get_pathway_containedEvents_by_attribute("R-HSA-5673001", "stId")
```

get_pathways_low_diagram_entity (*identifier*)

A list of lower level pathways with diagram containing a given entity or event

This method traverses the event hierarchy and retrieves the list of all lower level pathways that have a diagram and contain the given PhysicalEntity or Event.

Parameters

- **identifier** – The entity that has to be present in the pathways
- **species** – The species for which the pathways are requested. Taxonomy identifier (eg: 9606) or species name (eg: 'Homo sapiens')

```
r.get_pathways_low_diagram_entity("R-HSA-199420")
```

get_pathways_low_diagram_entity_allForms (*identifier*)

```
r.get_pathways_low_diagram_entity_allForms("R-HSA-199420")
```

get_pathways_low_diagram_identifier_allForms (*identifier*)

```
r.get_pathways_low_diagram_identifier_allForms("PTEN")
```

get_pathways_low_entity (*identifier*)

A list of lower level pathways containing a given entity or event

This method traverses the event hierarchy and retrieves the list of all lower level pathways that contain the given PhysicalEntity or Event.

```
r.get_pathways_low_entity("R-HSA-199420")
```

get_pathways_low_entity_allForms (*identifier*)

A list of lower level pathways containing any form of a given entity

This method traverses the event hierarchy and retrieves the list of all lower level pathways that contain the given PhysicalEntity in any of its variant forms. These variant forms include for example different post-translationally modified versions of a single protein, or the same chemical in different compartments.

```
r.get_pathways_low_entity_allForms("R-HSA-199420")
```

get_pathways_top (*species*)**get_references** (*identifier*)

All referenceEntities for a given identifier

Retrieves a list containing all the reference entities for a given identifier.

```
r.get_references(15377)
```

get_species_all ()

the list of all species in Reactome

get_species_main ()

the list of main species in Reactome

```
r.get_species_main()
```

name**search_facet** ()

A list of facets corresponding to the whole Reactome search data

This method retrieves faceting information on the whole Reactome search data.

search_facet_query (*query*)

A list of facets corresponding to a specific query

This method retrieves faceting information on a specific query

search_query (*query*)

Queries Solr against the Reactome knowledgebase

This method performs a Solr query on the Reactome knowledgebase. Results can be provided in a paginated format.

search_spellcheck (*query*)

Spell-check suggestions for a given query

This method retrieves a list of spell-check suggestions for a given search term.

search_suggest (*query*)

Autosuggestions for a given query

This method retrieves a list of suggestions for a given search term.

```
>>> r.http_get("search/suggest?query=apopt")
['apoptosis', 'apoptosome', 'apoptosome-mediated', 'apoptotic']
```

version**class ReactomeOld** (*verbose=True, cache=False*)

Reactome interface

some data can be download on the main [website](#)

SBML_exporter (*identifier*)

Get the SBML XML text of a pathway identifier

Parameters *identifier* (*int*) – Pathway database identifier

Returns SBML object in XML format as a string

```
>>> from bioservices import Reactome
>>> s = Reactome()
>>> xml = s.SBML_exporter(109581)
```

biopax_exporter (*identifier, level=2*)

Get BioPAX file

The passed identifier has to be a valid event identifier. If there is no matching ID in the database, it will return an empty string.

Parameters

- **level** (*int*) – BioPAX level: one of two values: 2 or 3
- **identifier** (*int*) – event database identifier

Returns BioPAX RDF document

```
>>> # for Apoptosis:
>>> s = Reactome()
>>> res = s.biopax_exporter(109581)
```

bioservices_get_reactants_from_reaction_identifier (*reaction*)

Fetch information from the reaction HTML page

Note: draft version

front_page_items (*species*)

Get list of front page items listed in the Reactome Pathway Browser

Parameters *species* (*str*) – Full species name that should be encoded for URL (e.g. homo+sapiens for human, or mus+musculus for mouse) + can be replaced by spaces.

Returns list of fully encoded Pathway objects in JSON

```
>>> s = Reactome()
>>> res = s.front_page_items("homo sapiens")
>>> print(res[0]['name'])
['Apoptosis']
```

See also:[Pathway Browser](#)**get_all_reactions** ()

Return list of reactions from the Pathway

get_list_pathways ()

Return list of pathways from reactome website

Returns list of lists. Each sub-lis contains 3 items: reactome pathway identifier, description and species**get_species** ()

Return list of species from all pathways

highlight_pathway_diagram (*identifier, genes, frmt='PNG'*)

Highlight a diagram for a specified pathway based on its identifier

Parameters

- **identifier** (*int*) – a valid pathway identifier
- **genes** (*list*) – a list of string to indicate the genes to highlight
- **frmt** (*int*) – PNG or PDF

Returns This method should be used after method queryHitPathways.

```
res = s.http_post("highlightPathwayDiagram/68875/PNG", frmt="txt",
                 data="CDC2")
with open("test.png", 'wb') as f:
    import binascii
    f.write(binascii.a2b_base64(res))
```

list_by_query (*classname, **kargs*)

Get list of objects from Reactome database

Parameters

- **class name** (*str*) –
- **kargs** – further attribute values encoded in key-value pair

Returns list of dictionaries. Each dictionary contains information about a given pathway

To query a list of pathways with names as “Apoptosis”:

```
>>> s = Reactome()
>>> res = list_by_query("Pathway", name="apoptosis")
>>> identifiers = [x['dbId'] for x in res]
```

pathway_complexes (*identifier*)

Get complexes belonging to a pathway

Parameters **identifier** (*int*) – Pathway database identifier**Returns** list of all PhysicalEntity objects that participate in the Pathway.(in JSON)

```
>>> s = Reactome()
>>> s.pathway_complexes(109581)
```

pathway_diagram (*identifier, frmt='PNG'*)

Retrieve pathway diagram

Parameters

- **identifier** (*int*) – Pathway database identifier
- **frmt** (*str*) – PNG, PDF, or XML.

Returns Base64 encoded pathway diagram for PNG or PDF. XML text for the XML file type.

```
>>> s = Reactome()
>>> s.pathway_diagram('109581', 'PNG', view=True)
>>> s.pathway_diagram('109581', 'PNG', save=True)
```

Todo: if PNG or PDF, the output is base64 but there is no facility to easily save the results in a file for now

pathway_hierarchy (*species*)

Get the pathway hierarchy for a species as displayed in Reactome pathway browser.

Parameters **species** (*str*) – species name that should be with + or spaces (e.g. 'homo+sapiens' for human, or 'mus musculus' for mouse)

Returns XML text containing pathways and reactions

```
s.pathway_hierarchy("homo sapiens")
```

pathway_participants (*identifier*)

Get list of pathway participants for a pathway using

Parameters **identifier** (*int*) – Pathway database identifier

Returns list of fully encoded PhysicalEntity objects in the pathway (in JSON)

```
>>> s = Reactome()
>>> s.pathway_participants(109581)
```

query_by_id (*classname, identifier*)

Get Reactome Database for a specific object.

Parameters

- **classname** (*str*) – e.g. Pathway
- **identifier** (*int*) – database identifier or stable identifier if available

It returns a full object, including full class information about all the attributes of the returned object. For example, if the object has one PublicationSource attribute, it will return a full PublicationSource object within the returned object.

```
>>> s.query_by_id("Pathway", "109581")
```

query_by_ids (*classname, identifiers*)**Parameters**

- **classname** (*str*) – e.g. Pathway
- **identifiers** (*list*) – list of strings or int

```
>>> s.quey_by_ids("Pathway", "CDC2")
```

Warning: not sure the wrapping is correct

query_hit_pathways (*query*)

Get pathways that contain one or more genes passed in the query list.

In the Reactome data model, pathways are organized in a hierarchical structure. The returned pathways in this method are pathways having detailed manually drawn pathway diagrams. Currently only human pathways will be returned from this method.

```
s.query_hit_pathways('CDC2')
s.query_hit_pathways(['CDC2'])
```

query_pathway_for_entities (*identifiers*)

Get pathway objects by specifying an array of PhysicalEntity database identifiers.

The returned Pathways should contain the passed EventEntity objects. All passed EventEntity database identifiers should be in the database.

species_list ()

Get the list of species used Reactome

class ReactomeAnalysis (*verbose=True, cache=False*)

identifiers (*genes*)

s.identifiers("TP53") .. warning:: works for oe gene only for now

2.10.29 Readseq

This module provides a class *Seqret* to access to Seqret WS.

What is Seqret ?

URL <http://www.ebi.ac.uk/Tools/services/rest/seqret/>

Service

Citations <http://www.ncbi.nlm.nih.gov/pubmed/18428689>

EMBOSS seqret reads and converts biosequences between a selection of common biological sequence formats, including EMBL, GenBank and fasta sequence formats.

Seqret homepage – Sep 2017

class Seqret (*verbose=True*)

Interface to the Seqret service

```
>>> from bioservices import *
>>> s = Seqret()
```

The ReadSeq service was replaced by #the Seqret services (2015).

Changed in version 0.15.

Constructor

Parameters `verbose` (*bool*) –

get_parameter_details (*parameterId*)

Get details of a specific parameter.

Parameters `parameter` (*str*) – identifier/name of the parameter to fetch details of.

Returns a data structure describing the parameter and its values.

```
rs = ReadSeq()
print(rs.get_parameter_details("stypc"))
```

get_parameters ()

Get a list of the parameter names.

Returns a list of strings giving the names of the parameters.

get_result (*jobid*, *result_type='out'*)

Get the result of a job of the specified type.

Parameters

- **jobid** (*str*) – job identifier.
- **parameters** – optional list of `wsRawOutputParameter` used to provide additional parameters for derived result types.

get_result_types (*jobid*)

Get the available result types for a finished job.

Parameters `jobid` (*str*) – job identifier.

Returns a list of `wsResultType` data structures describing the available result types.

get_status (*jobid=None*)

Get the status of a submitted job.

Parameters `jobid` (*str*) – job identifier.

Returns string containing the status.

The values for the status are:

- **RUNNING**: the job is currently being processed.
- **FINISHED**: job has finished, and the results can then be retrieved.
- **ERROR**: an error occurred attempting to get the job status.
- **FAILURE**: the job failed.
- **NOT_FOUND**: the job cannot be found.

parameters

Get list of parameter names

run (*email*, *title*, ***kargs*)

Submit a job to the service.

Parameters

- **email** (*str*) – user e-mail address.
- **title** (*str*) – job title.

- **params** – parameters for the tool as returned by `get_parameter_details()`.

Returns string containing the job identifier (jobId).

Deprecated (olf readseq service):

Format Name	Value
Auto-detected	0
EMBL	4
GenBank	2
Fasta (Pearson)	8
Clustal/ALN	22
ACEDB	25
BLAST	20
DNAStrider	6
FlatFeat/FFF	23
GCG	5
GFF	24
IG/Stanford	1
MSF	15
NBRF	3
PAUP/NEXUS	17
Phylip (Phylip4)	12
Phylip3.2	11
PIR/CODATA	14
Plain/Raw	13
SCF	21
XML	19

As output, you also have

Pretty 18

```
s = readseq.Seqret()
jobid = s.run("cokelaer@test.co.uk", "test", sequence=fasta, inputformat=8,
             outputformat=2)
genbank = s.get_result(s._jobid)
```

2.10.30 UniChem

This module provides a class *UniChem*

What is UniChem

URL <https://www.ebi.ac.uk/unicem/info/webservices>

REST <https://www.ebi.ac.uk/unicem/rest>

“UniChem is a ‘Unified Chemical Identifier’ system, designed to assist in the rapid cross-referencing of chemical structures, and their identifiers, between databases (read more). “

—From UniChem web page June 2013

class UniChem (*verbose=False, cache=False*)
Interface to the UniChem service

```
>>> from bioservices import UniChem
>>> u = UniChem()
```

Constructor UniChem

Parameters `verbose` – set to False to prevent informative messages

get_all_compound_ids_from_all_src_id (*src_compound_id*, *src_id*, *target=None*)

Obtain a list of all `src_compound_ids` from all sources (including BOTH current AND obsolete assignments) to the same structure as a currently assigned query `src_compound_id`.

The output will include query `src_compound_id` if it is a valid `src_compound_id` with a current assignment. Note also, that by adding an additional (optional) argument (a valid `src_id`), then results will be restricted to only the source specified with this optional argument.

Parameters

- **src_compound_id** (*str*) – a valid compound identifier (or list)
- **source** – one of the valid database ids. See `source_ids`.
- **target** – if provided, return answer for a specific target database only. Otherwise return answer for all database found in `source_ids`.

Returns list of three element arrays, containing ‘`src_compound_id`’ and ‘`src_id`’, and ‘Assignment’, or (if optional ‘`to_src_id`’ is specified) list of two element arrays, containing ‘`src_compound_id`’ and ‘Assignment’.

```
>>> res = s.get_all_compound_ids_from_src_id("CHEMBL12", "chembl")
>>> s.get_all_compound_ids_from_src_id("CHEMBL12", "chembl", "chebi")
[{'assignment': u'1', 'src_compound_id': u'49575'}]
```

The second call may return an empty list if there is no target from chebi.

get_all_src_ids ()

Obtain all `src_ids` of database currently in UniChem

Returns list of ‘`src_id`’s.

```
>>> uni.get_all_src_ids()
```

get_auxiliary_mappings (*src_id*)

For a single source, obtain a mapping between all current `src_compound_ids` to their corresponding auxiliary data if any.

Some instances of UniChem may contain sources that create URLs for compound-specific pages by using strings or identifiers (called ‘auxiliary data’ here) that are different to the `src_compound_ids` for the source. This is not very common, but is dealt with in UniChem by use of an additional mapping step for these sources. This function returns such mapping.

Warning: this method may return very large data sets. you will need to change TIMEOUT to a larger value.

Parameters `src_id` (*int*) – corresponding database identifier (name or id).

Returns list of two element arrays, containing ‘`src_compound_id`’ and ‘auxiliary data’.

```
>>> uni.get_auxiliary_mappings(15)
```

get_compound_ids_from_src_id (*src_compound_id, src_id, target=None*)

Obtain a list of all `src_compound_ids` from all sources which are CURRENTLY assigned to the same structure as a currently assigned query `src_compound_id`.

The output will include query `src_compound_id` if it is a valid `src_compound_id` with a current assignment. Note also, that by adding an additional (optional) argument (a valid `src_id`), then results will be restricted to only the source specified with this optional argument.

Parameters

- **src_compound_id** (*str*) – a valid compound identifier (list is possible as well)
- **src_id** (*str*) – one of the valid database ids. See `source_ids`.
- **target** (*str, int*) – database identifier (name or id) to map to.

Returns list of dictionaries with the ‘`src_compound_id`’ and ‘`src_id`’ keys. or (if optional `target` is specified, a list with only ‘`src_compound_id`’ keys).

```
>>> get_compound_ids_from_src_id("CHEMBL12", "chembl")
>>> get_compound_ids_from_src_id("CHEMBL12", "chembl", "chebi")
[{'src_compound_id': '49575'}]
```

get_mapping (*source, target*)

Obtain a full mapping between two sources. Uses only currently assigned `src_compound_ids` from both sources.

Parameters

- **source** – name of the source database
- **target** – name of the target database

Returns a dictionary. Keys are the source identifiers. Values are the target identifiers.

```
>>> get_mapping("kegg_ligand", "chembl")
```

get_source_information (*src_id*)

Description: Obtain all information on a source by querying with a source id

Parameters **src_id** (*int*) – valid identifiers (values or keys of `source_ids` e.g. `chebi`, `chembl,0,1`). could also be a list of those identifiers.

Returns

dictionary (or list of dictionaries) with following keys:

- `src_id` (the `src_id` for this source),
- `src_url` (the main home page of the source),
- `name` (the unique name for the source in UniChem, always lower case),
- `name_long` (the full name of the source, as defined by the source),
- `name_label` (A name for the source suitable for use as a ‘label’ for the source within a web-page. Correct case setting for source, and always less than 30 characters),
- `description` (a description of the content of the source),
- `base_id_url_available` (an flag indicating whether this source provides a valid
- `base_id_url` for creating cpd-specific links [`1=yes`, `0=no`]).
- `base_id_url` (the base url for constructing hyperlinks to this source [append an

- identifier from this source to the end of this url to create a valid url to a
- specific page for this cpd], unless `aux_for_url=1`),
- `aux_for_url` (A flag to indicate whether the `aux_src` field should be used to create hyperlinks instead of the `src_compound_id` [1=yes, 0=no])

```
>>> res = get_source_information("chebi")
```

get_src_compound_id_url (*src_compound_id*, *src_id*, *to_src_id*)

Obtain a list of URLs for all `src_compound_ids`

Obtain a list of URLs for all `src_compound_ids` from a specified source (the ‘`to_src_id`’), which are CURRENTLY assigned to the same structure as a currently assigned query `src_compound_id`. Method only applicable for sources which support direct URLs to `src_compound_id` pages. Method also applicable for ‘`to_src_id`’s where the hyperlink is constructed from auxiliary data [and not from the `src_compound_id`] as per example2 below.

Parameters

- **src_compound_id** (*str*) – a valid compound identifier
- **src_id** (*int*) – corresponding database identifier (name or id).
- **to_src_id** (*str*) – database identifier (name or id) to map to.
- **to_src_id** –

Returns list of URLs.

```
>>> uni.get_src_compound_id_url("CHEMBL12", "chembl", "drugbank")
>>> # equivalent to
>>> uni.get_src_compound_id_url("CHEMBL12", 1, 2)
```

get_src_compound_ids_all_from_inchikey (*inchikey*)

Description: Obtain a list of all `src_compound_ids` (from all sources) which have current AND obsolete assignments to a query InChIKey

Parameters **inchikey** (*str*) – input source identified by its InChIKey (or list) (or list of list of dictionaries if input is a list).

Returns list of two element arrays, containing ‘`src_compound_id`’ and ‘`src_id`’. and ‘Assignment’.

```
>>> uni.get_src_compound_ids_all_from_inchikey("AAOVKJBEBIDNHE-UHFFFAOYSA-N")
```

get_src_compound_ids_all_from_obsolete (*obsolete_src_compound_id*, *src_id*, *to_src_id=None*)

Obtain a list of all `src_compound_ids` from all sources with BOTH current AND obsolete to the same structure with an obsolete assignment to the query `src_compound_id`.

The output will include query `src_compound_id` if it is a valid `src_compound_id` with an obsolete assignment. Note also, that by adding an additional (optional) argument (a valid `src_id`), then results will be restricted to only the source specified with this optional argument.

Parameters

- **src_compound_id** (*str*) – a valid compound identifier
- **src_id** (*int*) – corresponding database identifier (name or id).
- **to_src_id** (*int*) – database identifier (name or id) to map to.

Returns list of four element arrays, containing 'src_compound_id', 'src_id', 'assignment' and 'UCI', or (if optional 'to_src_id' is specified) list of three element arrays, containing 'src_compound_id', 'Assignment' and 'UCI'.

```
>>> from bioservices import UniChem
>>> u = UniChem()
>>> u.get_src_compound_ids_all_from_obsolete("DB07699", "2")
>>> u.get_src_compound_ids_all_from_obsolete("DB07699", "2", "1")
```

get_src_compound_ids_all_from_src_compound_id(*src_compound_id*, *src_id*, *target=None*)

get_src_compound_ids_from_inchikey(*inchikey*)

Obtain a list of all src_compound_ids (from all sources) which are CURRENTLY assigned to a query InChIKey

Parameters *inchikey* (*str*) – input source identified by its InChiKey (or list)

Returns list of dictionaries containing 'src_compound_id' and 'src_id' keys (or list of list of dictionaries if input is a list).

```
>>> uni.get_src_compound_ids_from_inchikey("AAOVKJBEBIDNHE-UHFFFAOYSA-N")
```

get_src_compound_ids_from_src_compound_id(*src_compound_id*, *src_id*, *target=None*)

get_structure(*src_compound_id*, *src_id*)

Obtain structure(s) CURRENTLY assigned to a query *src_compound_id*.

Parameters

- **src_compound_id** (*str*) – a valid compound identifier
- **src_id** (*int*) – corresponding database identifier (name or id).

Returns dictionary with 'standardinchi' and 'standardinchikey' keys

```
>>> uni.get_structure("CHEMBL12", "chembl")
```

get_structure_all(*src_compound_id*, *src_id*)

Obtain structure(s) with current AND obsolete assignments

Parameters

- **src_compound_id** (*str*) – a valid compound identifier
- **src_id** (*int*) – corresponding database identifier (name or id).

Returns dictionary with 'standardinchi', 'standardinchikey' and 'assignment' keys

```
>>> uni.get_structure_all("CHEMBL12", "chembl")
```

get_verbose_src_compound_ids_from_inchikey(*inchikey*)

Obtain all *src_compound_ids* (from all sources)

which are CURRENTLY assigned to a query InChIKey. However, these are returned as part of the following data structure: A list of sources containing these *src_compound_ids*, including source description, *base_id_url*, etc. One element in this list is a list of the *src_compound_ids* currently assigned to the query InChIKey.

Parameters *inchikey* (*str*) – input source identified by its InChiKey

Returns

list containing

- `src_id` (the `src_id` for this source),
- `src_url` (the main home page of the source),
- `name` (the unique name for the source in UniChem, always lower case),
- `name_long` (the full name of the source, as defined by the source),
- `name_label` (A name for the source suitable for use as a ‘label’ for the source within a web-page. Correct case setting for source, and always less than 30 characters),
- `description` (a description of the content of the source),
- `base_id_url_available` (an flag indicating whether this source provides a valid
- `base_id_url` for creating cpd-specific links [1=yes, 0=no]).
- `base_id_url` (the base url for constructing hyperlinks to this source [append an
- identifier from this source to the end of this url to create a valid url to a specific page for this cpd], unless `aux_for_url=1`),
- `aux_for_url` (A flag to indicate whether the `aux_src` field should be used to create hyperlinks instead of the `src_compound_id` [1=yes, 0=no] ,
- `src_compound_id` (a list of `src_compound_ids` from this source which are currently assigned to the query InChIKey.
- `aux_src` (a list of `src-compound_id` keys mapping to corresponding auxiliary data (`url_id:value`), for creating links if `aux_for_url=1`. Only shown if `aux_for_url=1`).

```
>>> uni.get_verbose_src_compound_ids_from_inchikey("QFFGVLORLPOAEC-SNVBAGLBSA-
↳N")
>>> # Note that this one is not valid anymore
>>> uni.get_verbose_src_compound_ids_from_inchikey("ZUITABIAKMVPG-UHFFFAOYSA-N
↳")
```

2.10.31 UniProt

Interface to some part of the UniProt web service

What is UniProt ?

URL <http://www.uniprot.org>

Citation

“The Universal Protein Resource (UniProt) is a comprehensive resource for protein sequence and annotation data. The UniProt databases are the UniProt Knowledgebase (UniProtKB), the UniProt Reference Clusters (UniRef), and the UniProt Archive (UniParc). The UniProt Metagenomic and Environmental Sequences (UniMES) database is a repository specifically developed for metagenomic and environmental data.”

—From Uniprot web site (help/about) , Dec 2012

class UniProt (*verbose=False, cache=False*)
Interface to the UniProt service

Identifiers mapping between databases:

```

>>> from bioservices import UniProt
>>> u = UniProt(verbose=False)
>>> u.mapping("ACC", "KEGG_ID", query='P43403')
defaultdict(<type 'list'>, {'P43403': ['hsa:7535']})
>>> res = u.search("P43403")

# Returns sequence on the ZAP70_HUMAN accession Id
>>> sequence = u.search("ZAP70_HUMAN", columns="sequence")

```

Constructor

Parameters `verbose` – set to False to prevent informative messages

get_df (*entries*, *nChunk=100*, *organism=None*, *limit=10*)

Given a list of uniprot entries, this method returns a dataframe with all possible columns

Parameters

- **entries** – list of valid entry name. if list is too large (about >200), you need to split the list
- **chunk** –
- **limit** – limit number of entries per identifier to 10. You can set it to None to keep all entries but this will be very slow

Returns dataframe with indices being the uniprot id (e.g. DIG1_YEAST)

Todo: cleanup the content of the data frame to replace strings separated by ; into a list of strings. e.g. the Gene Ontology IDs

Warning: requires pandas library

get_fasta (*id_*)

Returns FASTA string given a valid identifier

See also:

bioservices.apps.fasta for dedicated tools to manipulate FASTA

get_fasta_sequence (*id_*)

Returns FASTA sequence (Not FASTA)

Parameters `id` (*str*) – Should be the entry name

Returns returns fasta sequence (string)

Warning: this is the sequence found in a fasta file, not the fasta content itself. The difference is that the header is removed and the formatting of end of lines every 60 characters is removed.

mapping (*fr='ID'*, *to='KEGG_ID'*, *query='P13368'*)

This is an interface to the UniProt mapping service

Parameters

- **fr** – the source database identifier. See `_mapping`.
- **to** – the targetted database identifier. See `_mapping`.
- **query** – a string containing one or more IDs separated by a space It can also be a list of strings.
- **format** – The output being a dictionary, this parameter is deprecated and not used anymore

Returns a list. The first element is the source database Id. The second is the targetted source identifier. Following elements are alternate of one the entry and its mapped Id. If a query has several mapped Ids, the query is repeated (see example with PDB mapping here below) e.g., ["From:ID", "to:PDB_ID", "P43403"]

```
>>> u.mapping("ACC", "KEGG_ID", 'P43403')
defaultdict(<type 'list'>, {'P43403': ['hsa:7535']})
>>> u.mapping("ACC", "KEGG_ID", 'P43403 P00958')
defaultdict(<type 'list'>, {'P00958': ['sce:YGR264C'], 'P43403': ['hsa:7535']})
↪
>>> u.mapping("ID", "PDB_ID", "P43403")
defaultdict(<type 'list'>, {'P43403': ['1FBV', '1M61', '1U59',
'2CBL', '2OQ1', '2OZO', '2Y1N', '3ZNI', '4A4B', '4A4C', '4K2R']})
```

There is a web page that gives the list of correct database identifiers. You can also look at the `_mapping` attribute.

URL <http://www.uniprot.org/mapping/>

Changed in version 1.1.1: to return a dictionary instead of a list

Changed in version 1.1.2: the values for each key is now made of a list instead of strings so as to store more than one values.

Changed in version 1.2.0: input query can also be a list of strings instead of just a string

Changed in version 1.3.1::: use `http_post` instead of `http_get`. This is 3 times faster and allows queries with more than 600 entries in one go.

quick_search (*query*, *include=False*, *sort='score'*, *limit=None*)
a specialised version of `search()`

This is equivalent to:

```
u = uniprot.UniProt()
u.search(query, frmt="tab", include=False, sor="score", limit=None)
```

Returns a dictionary.

retrieve (*uniprot_id*, *frmt='xml'*, *database='uniprot'*)
Search for a uniprot ID in UniProtKB database

Parameters

- **uniprot** (*str*) – a valid UniProtKB ID or a list of identifiers.
- **frmt** (*str*) – expected output format amongst xml, txt, fasta, gff, rdf

Returns is a list of identifiers is provided, the output is also a list otherwise, a string. The content of the string of items in the list depends on the value of **frmt**.


```
>>> u = UniProt()
>>> res = u.retrieve("P09958", frmt="xml")
>>> fasta = u.retrieve([u'P29317', u'Q5BKK8', u'Q8TCD6'], frmt='fasta')
>>> print(fasta[0])
```

search (*query*, *frmt*='tab', *columns*=None, *include*=False, *sort*='score', *compress*=False, *limit*=None, *offset*=None, *maxTrials*=10, *database*='uniprot')

Provide some interface to the uniprot search interface.

Parameters

- **query** (*str*) – query must be a valid uniprot query. See <http://www.uniprot.org/help/text-search>, <http://www.uniprot.org/help/query-fields> See also example below
- **frmt** (*str*) – a valid format amongst html, tab, xls, asta, gff, txt, xml, rdf, list, rss. If tab or xls, you can also provide the columns argument. (default is tab)
- **columns** (*str*) – comma-separated list of values. Works only if format is tab or xls. For UniProtKB, some possible columns are: id, entry name, length, organism. Some column name must be followed by database name (e.g., “database(PDB)”). Again, see uniprot website for more details. See also `_valid_columns` for the full list of column keyword.
- **include** (*bool*) – include isoform sequences when the frmt parameter is fasta. Include description when frmt is rdf.
- **sort** (*str*) – by score by default. Set to None to bypass this behaviour
- **compress** (*bool*) – gzip the results
- **limit** (*int*) – Maximum number of results to retrieve.
- **offset** (*int*) – Offset of the first result, typically used together with the limit parameter.
- **maxTrials** (*int*) – this request is unstable, so we may want to try several time.

To obtain the list of uniprot ID returned by the search of zap70 can be retrieved as follows:

```
>>> u.search('zap70+AND+organism:9606', frmt='list')
>>> u.search("zap70+and+taxonomy:9606", frmt="tab", limit=3,
...         columns="entry name,length,id, genes")
Entry name  Length  Entry  Gene names
CBLB_HUMAN  982  Q13191  CBLB RNF56 Nbla00127
CBL_HUMAN   906  P22681  CBL CBL2 RNF55
CD3Z_HUMAN  164  P20963  CD247 CD3Z T3Z TCRZ
```

other examples:

```
>>> u.search("ZAP70+AND+organism:9606", limit=3, columns="id,database(PDB)")
```

You can also do a search on several keywords. This is especially useful if you have a list of known entry names.:

```
>>> u.search("ZAP70_HUMAN+or+CBL_HUMAN", frmt="tab", limit=3,
...         columns="entry name,length,id, genes")
Entry name  Length  Entry  Gene names
```

Finally, note that when search for a query, you may have several hits:

```
>>> u.search("P12345")
```

including the ID P12345 but also related entries. If you need only the entry that perfectly match the query, use:

```
>>> u.search("id:P12345")
```

This was provided from a user issue that was solved here: <https://github.com/cokelaer/bioservices/issues/122>

Warning: some columns although valid may not return anything, not even in the header: 'score', 'taxonomy', 'tools'. this is a uniprot feature, not bioservices.

searchUniProtId (*uniprot_id*, *frmt='xml'*)

uniref (*query*)

Calls UniRef service

Returns if you have Pandas installed, returns a dataframe (see example)

```
>>> u = UniProt()
>>> df = u.uniref("member:Q03063") # of just A03063
>>> df.Size
```

Another example from <https://github.com/cokelaer/bioservices/issues/121> is the combination of uniprot and uniref filters:

```
u.uniref("uniprot:(ec:1.1.1.282 taxonomy:bacteria reviewed:yes) AND_
↪identity:0.5")
```

2.10.32 DBFetch

Interface to DBFetch web service

What is DBFetch

URL <http://www.ebi.ac.uk/Tools/webservices/services/dbfetch>

Service http://www.ebi.ac.uk/Tools/webservices/services/dbfetch_rest

“DBFetch allows you to retrieve entries from various up-to-date biological databases using entry identifiers or accession numbers. This is equivalent to the CGI based dbfetch service. Like the CGI service a request can return a maximum of 200 entries.”

—From <http://www.ebi.ac.uk/Tools/webservices/services/dbfetch> , Dec 2012

class DBFetch (*verbose=False*)

Interface to DBFetch service

```
>>> from bioservices import DBFetch
>>> w = DBFetch()
>>> data = w.fetchBatch("uniprot", "zap70_human", "xml", "raw")
```

For more information about the API, check this page: <http://www.ebi.ac.uk/Tools/dbfetch/syntax.jsp>

Constructor

Parameters `verbose` (*bool*) – print informative messages

fetch (*query*, *db*='ena_sequence', *format*='default', *style*='raw', *pageHtml*=False)
Fetch an entry in a defined format and style.

Parameters

- **query** (*str*) – the entry identifier in db:id format (e.g. 'UniProtKB:WAP_RAT').
- **format** (*str*) – the name of the format required (default to fasta).
- **style** (*str*) – the name of the style required (raw, default, html)

Returns The format of the response depends on the format/style parameter.

```
from bioservices import DBFetch
u = DBFetch()
db.fetch(db="ena_sequence", format="fasta", query="L12344,L12345")
db.fetch(db="uniprot", format="fasta", query="P53503")
```

If `db` is omitted, the default is `ena_sequence`. If `format` is omitted, the default is EMBL format. The default style is raw data.

get_all_database_info ()

Get details of all available databases, includes formats and result styles.

Returns A list of data structures describing the databases. See `getDatabaseInfo()` for a description of the data structure.

get_database_format_styles (*db*, *format*)

Get a list of style names available for a given database and format.

Parameters

- **db** (*str*) – database name to get available styles for (e.g. uniprotkb).
- **format** (*str*) – the data format to get available styles for (e.g. fasta).

Returns An array of strings containing the style names.

```
>>> u.get_database_format_styles("uniprotkb", "fasta")
['default', 'raw', 'html']
```

get_database_formats (*db*)

Get list of format names for a given database.

Parameters `db` (*str*) – valid database name

```
>>> db.get_database_formats("uniprotkb")
['default',
 'annot',
 'entrysize',
 'fasta',
 'gff3',
 'seqxml',
 'uniprot',
 'uniprotrdfxml',
 'uniprotxml',
 'dasgff',
 'gff2']
```

get_database_info (*db=None*)

Get details describing specific database (data formats, styles)

Parameters **db** (*str*) – a valid database.

Returns The output can be introspected and contains several attributes

```
>>> res = u.get_database_info('uniprotkb')
>>> print(res['description'])
'The UniProt Knowledgebase (UniProtKB) is the central access point for
↳ extensive curated protein information, including function, classification,
↳ and cross-references. Search UniProtKB to retrieve everything that is known
↳ about a particular sequence.'
```

supported_databases

Alias to getSupportedDBs.

2.10.33 Wikipathway

Interface to the WikiPathway service

What is WikiPathway ?

URL <http://www.wikipathways.org/index.php/WikiPathways>

REST <http://webservice.wikipathways.org/>

Citation doi:10.1371/journal.pone.0006447

” WikiPathways is an open, public platform dedicated to the curation of biological pathways by and for the scientific community.”

—From WikiPathway web site. Dec 2012

class WikiPathways (*verbose=True, cache=False*)

Interface to Pathway service

```
>>> from bioservices import WikiPathways
>>> s = Wikipathway()
>>> s.organism # default organism
'Homo sapiens'
```

Examples:

```
s.findPathwaysByText('MTOR')
s.getPathway('WP1471')
s.getPathwaysByOntologyTerm('DOID:344')
s.findPathwaysByXref('P45985')
```

The methods that require a login are not implemented (*login()*, *updatePathway()*, *removeCurationTag()*, *saveCurationTag()*, *createPathway()*)

Methods not implemented at all:

- u'getCurationTagHistory': No API found in Wikipathway web page
- u'getRelations': No API found in Wikipathway web page

Constructor

Parameters `verbose` (*bool*) –

createPathway (*gpmlCode*, *authInfo*)

Create a new pathway on the WikiPathways website with a given GPML code.

Warning: Interface not exposed in bioservices.

Note: To create/modify pathways via the web service, you need to have an account with web service write permissions. Please contact us to request write access for the web service.

Parameters

- **gpml** (*str*) – The GPML code.
- **WSAuth auth** (*object*) – The authentication info.

Returns `WSPathwayInfo` The pathway info for the created pathway (containing identifier, revision, etc.).

findInteractions (*query*)

Find interactions defined in WikiPathways pathways.

Parameters **query** (*str*) – The name of an entity to find interactions for (e.g. ‘P53’)

Returns list of dictionaries

```
res = w.findInteractions("P53")
```

findPathwaysByLiterature (*query*)

Find pathways by their literature references.

Parameters **query** (*str*) – The query, can be a pubmed id, author name or title keyword.

Returns dictionary with Pathway as keys

```
res = s.findPathwaysByLiterature(18651794)
```

findPathwaysByText (*query*, *species=None*)

Find pathways using a textual search on the description and text labels of the pathway objects.

The query syntax offers several options:

- Combine terms with AND and OR. Combining terms with a space is equal to using OR (‘p53 OR apoptosis’ gives the same result as ‘p53 apoptosis’).
- Group terms with parentheses, e.g. ‘(apoptosis OR mapk) AND p53’
- You can use wildcards * and ?. * searches for one or more characters, ? searches for only one character.
- Use quotes to escape special characters. E.g. “‘apoptosis*’” will include the * in the search and not use it as wildcard.

This function supports REST-style invocation. Example: <http://www.wikipathways.org/wpi/webservice/webservice.php/findPathwaysByText?query=apoptosis>

Parameters

- **query** (*str*) – The search query (e.g. ‘apoptosis’ or ‘p53’).
- **species** (*str*) – The species to limit the search to (leave blank to search on all species).

Returns Array of WSSearchResult An array of search results.

```
s.findPathwaysByText(query="p53 OR mapk", species='Homo sapiens')
```

Warning: AND or OR must be in big caps

findPathwaysByXref (*ids, codes=None*)

Find pathways by searching on the external references of DataNodes.

Parameters

- **string ids** (*str*) – One or more DataNode identifier(s) (e.g. ‘P45985’). Datanodes can be (gene/protein/metabolite identifiers). For one node, you can use a string (or number) or list of one identifier. you can also provide a list of identifiers.
- **codes** (*str*) – You can restrict the search to a specific database. See <http://developers.pathvisio.org/wiki/DatabasesMapps#Supportedatabasesystems> for details. Examples are “L” for entrez gene, “En” for ensembl. See also the note here below for multiple identifiers/codes.

Returns a dictionary

```
>>> s.findPathwaysByXref(ids="P45985")
>>> s.findPathwaysByXref(ids="P45985", codes="L")
>>> s.findPathwaysByXref(ids=["P45985"], codes=["L"])
>>> s.findPathwaysByXref(ids=["P45985", "ENSG00000130164"], codes=["L", "En"])
```

Note that in the last example, we specify multiple ids and codes parameters to query for multiple xrefs at once. In that case, the number of ids and codes parameters should match. Moreover, they will be paired to form xrefs, so P45985 is searched for in the “L” database while “ENSG00000130164” is searched for in the En” database only.

getColorPathway (*pathwayId, filetype='svg', revision=0, color=None, graphId=None*)

Get a colored image version of the pathway.

Parameters

- **pwId** (*str*) – The pathway identifier.
- **revision** (*int*) – The revision number of the pathway (use ‘0’ for most recent version).
- **fileType** (*str*) – The image type (One of ‘svg’, ‘pdf’ or ‘png’). Not yet implemented. svg is returned for now.

Returns Binary form of the image.

Todo: graphId, color parameters

getCurationTags (*pathwayId*)

Get all curation tags for the given pathway.

Parameters **pathwayId** (*str*) – the pathway identifier.

Returns Array of WSCurationTag. The curation tags.

```
s.getCurationTags("WP4")
```

getCurationTagsByName (*name*)

Get all curation tags for the given tag name.

Use this method if you want to find all pathways that are tagged with a specific curation tag.

Parameters **tagName** (*str*) – The tag name.

Returns Array of WSCurationTag. The curation tags (one instance for each pathway that has been tagged).

```
s.getCurationTagsByName("Curation:FeaturedPathway")
```

getOntologyTermsByPathway (*pathwayId*)

Get a list of ontology terms for a given pathway.

Parameters **pathwayId** (*str*) – the pathway identifier.

Returns Array of WSOntologyTerm. The ontology terms.

```
s.getOntologyTermsByPathway("WP4")
```

getPathway (*pathwayId*, *revision=0*)

Download a pathway from WikiPathways.

Parameters

- **pathwayId** (*str*) – the pathway identifier.
- **revision** (*int*) – the revision number of the pathway (use '0' for most recent version).

Returns The pathway as a dictionary. The pathway is stored in gpml format.

```
s.getPathway("WP2320")
```

getPathwayAs (*pathwayId*, *filetype='png'*, *revision=0*)

Download a pathway in the specified file format.

Parameters

- **pathwayId** (*str*) – the pathway identifier.
- **filetype** (*str*) – the file format (default is .owl).
- **revision** (*int*) – the revision number of the pathway (use '0' for most recent version - this is default).

Returns The file contents

Changed in version 1.3.0: return raw output of the service without any parsing

Note: use `savePathwayAs()` to save into a file.

getPathwayHistory (*pathwayId*, *date*)

Get the revision history of a pathway.

Parameters

- **pathwayId** (*str*) – the pathway identifier.

- **date** (*str*) – limit the results by date, only history items after the given date (timestamp format) will be included. Can be a string or number of the form YYYYMMDDHHMMSS.

Returns The revision history.

Warning: seems unstable does not return the results systematically.

```
s.getPathwayHistory("WP4", 20110101000000)
```

getPathwayInfo (*pathwayId*)

Get some general info about the pathway.

Parameters **pathwayId** (*str*) – the pathway identifier.

Returns The pathway info.

```
>>> from bioservices import *
>>> s = Wikipathway()
>>> s.getPathwayInfo("WP2320")
```

getPathwaysByOntologyTerm (*terms*)

Get a list of pathways tagged with a given ontology term.

Parameters **terms** (*str*) – the ontology term identifier.

Returns dataframe with pathways information.

```
>>> from bioservices import WikiPathways
>>> s = Wikipathway()
>>> s.getPathwaysByOntologyTerm('PW:0000724')
```

getPathwaysByParentOntologyTerm (*term*)

Get a list of pathways tagged with any ontology term that is the child of the given Ontology term.

Parameters **term** (*str*) – the ontology term identifier.

Returns List of WSPathwayInfo The pathway information.

getRecentChanges (*timestamp*)

Get the recently changed pathways.

Parameters **timestamp** (*str*) – Only get changes from after this time. Timestamp format: yyyyymmddMMHHSS (string or number)

Returns The changed pathways in XML format

```
s.getRecentChanges(20110101000000)
```

Todo: interpret XML

listOrganisms ()

listPathways (*organism=None*)

Get a list of all available pathways.

Parameters **organism** (*str*) – If provided, the data is filtered to keep only the organism provided, which must be a valid name (check out *organism* attribute)

Returns dataframe. Index are the pathways identifiers (e.g. WP1)

login (*usrname, password*)

Start a logged in session using an existing WikiPathways account.

Warning: Interface not exposed in bioservices.

This function will return an authentication code that can be used to execute methods that need authentication (e.g. updatePathway).

Parameters

- **name** (*str*) – The username of the WikiPathways account.
- **password** (*str*) – The password of the WikiPathways account.

Returns The authentication code for this session.

organism

Read/write attribute for the organism

organisms = None

Get a list of all available organisms.

removeCurationTag (*pathwayId, name*)

Remove a curation tag from a pathway.

Warning: Interface not exposed in bioservices.

saveCurationTag (*pathwayId, name, revision*)

Apply a curation tag to a pathway. This operation will overwrite any existing tag with the same name.

Warning: Interface not exposed in bioservices.

Parameters **pathwayId** (*str*) – the pathway identifier.

savePathwayAs (*pathwayId, filename, revision=0, display=True*)

Save a pathway.

Parameters

- **pathwayId** (*str*) – the pathway identifier.
- **filename** (*str*) – the name of the file. If a filename extension is not provided the pathway will be saved as a pdf (default).
- **revisionNumb** (*int*) – the revision number of the pathway (use '0 for most recent version).
- **display** (*bool*) – if True the pathway will be displayed in your browser.

Note: Method from bioservices. Not a WikiPathways function

Changed in version 1.7: return PNG by default instead of PDF. PDF not working as of 20 Feb 2020 even on wikipathway website.

showPathwayInBrowser (*pathwayId*)

Show a given Pathway into your favorite browser.

Parameters **pathwayId** (*str*) – the pathway identifier.

updatePathway (*pathwayId, describeChanges, gpmlCode, revision=0*)

Update a pathway on WikiPathways website with a given GPML code.

Warning: Interface not exposed in bioservices.

Note: To create/modify pathways via the web service, you need to have an account with web service write permissions. Please contact us to request write access for the web service.

Parameters

- **pwId** (*str*) – The pathway identifier.
- **description** (*str*) – A description of the modifications.
- **gpml** (*str*) – The updated GPML code.
- **revision** (*int*) – The revision number of the version this GPML code was based on. This is used to prevent edit conflicts in case another client edited the pathway after this client downloaded it.
- **WSAuth_auth** (*object*) – The authentication info.

Returns Boolean. True if the pathway was updated successfully.

2.11 Applications and extra tools

Web services have lots of overlap amongst themselves. For instance, fetching a FASTA sequence can be done using many different services. Yet, once a FASTA is retrieved, one may want to perform additional tasks or save the FASTA into a file or whatever repetitive functionalities not included in Web Services anymore.

The goal of this sub-package is to provide convenient tools, which are not web services per se but that makes use of one or several Web Services already available within BioServices.

Warning: this is experimental and was added in version 1.2.0 so it may change quite a lot.

2.11.1 Peptides

class Peptides (*verbose=False*)

```
>>> p = Peptides()
>>> p.get_fasta_sequence("Q8IYB3")
>>> p.get_peptide_position("Q8IYB3", "VPKPEPIPEPKEPSPE")
189
```

Sometimes, peptides are provided with a pattern indicating the phospho site. e.g.,

```
>>>
```

```
get_fasta_sequence (uniprot_name)
```

```
get_phosphosite_position (uniprot_name, peptide)
```

2.11.2 FASTA

class FASTA

Dedicated class to manipulates FASTA sequence(s)

Here is a FASTA file example:

```
>sp|P43408|KADA_METIG Adenylate kinase OS=Methanotorris igneus GN=adkA PE=1 SV=2
MKNKVVVVTGVPVGGTTLTQKTIEKLKEEGIEYKMNFGTVMFEVAKKEEGLVEDRDQMR
KLDPDTQKRIQKLAGRKAEMAKESNVIVDTHSTVKTPKGYLAGLPIWVLEELNPDIIVI
VETSSDEILMRRLGDATRNRDIELTSDIDEHQFMNRCAAMAYGVLGTATVKI IKNRDGLL
DKAVEELISVLK
```

The format is made of a header and a sequence. Any FASTA can be read and the pair of header/sequence retrieved from the `sequence` and `header` attributes. However, headers differ from one database to another one and interpretation is not implemented except for SWISS-PROT. Identifiers can be retrieved whatsoever.

You can read a FASTA sequence from a local file or download one from UniProt

```
>>> from bioservices.apps.fasta import FASTA
>>> f = FASTA()
>>> f.load("P43403")
>>> acc = f.accession      # the accession (P43403)
>>> fasta = f.fasta       # raw FASTA string
>>> seq = f.sequence      # the sequence itself
>>> header = f.header     # the header itself
>>> identifier = f.identifier
```

You can also get a dataframe also using Pandas library.:

```
>>> f.df
```

The columns stored in the dataframe encompass:

- **Accession** that is taken from the header (e.g., P43403 from uniprot)
- **Sequence**, a copy of the FASTA sequence
- **Size**, the length of the sequence.
- **Database**, the database type found in the header (e.g., sp for SWISS-PROT; see below for a list of database and their header format).
- Some column such as **Organism** are filled only for some database
- **Identifiers** is the begining of the header.

See also:

[MultiFASTA](#) for multi FASTA manipulation.

List of identifiers corresponding to different databases.

GenBank	gilgi-number gblaccession locus
EMBL Data Library	gilgi-number emblaccession locus
DDBJ, DNA Database of Japan	gilgi-number dbj accession locus
NBRF PIR	pir entry
Protein Research Foundation	prf name
SWISS-PROT	splaccession name
Brookhaven Protein Data Bank (1)	pdb entry chain
Brookhaven Protein Data Bank (2)	entry:chain PDBID CHAIN SEQUENCE
Patents	pat country number
GenInfo Backbone Id	bbs number
General database identifier	gn database identifier
NCBI Reference Sequence	ref accession locus
Local Sequence identifier	lcl identifier

The `:meth::load_fasta` relies on UniProt service.

PE

returns PE keyword found in the header if any

SV

returns SV keyword found in the header if any

accession

dbtype

df

entry

returns entry only

fasta

returns FASTA content

gene_name

returns gene name from GN keyword found in the header if any

get_fasta (*id_*)

Fetches FASTA from uniprot and loads into attribute *fasta*

Parameters *id* (*str*) – a given uniprot identifier

Returns the FASTA contents

header

returns header only

identifier

known_dbtypes = ['sp', 'gi']

load (*id_*)

load_fasta (*id_*)

Fetches FASTA from uniprot and loads into attribute *fasta*

Parameters *id* (*str*) – a given uniprot identifier

Returns nothing

Note: same as `get_fasta()` but returns nothing

name

organism

returns organism from OS keyword found in the header if any

read_fasta (*filename*)

Reads a FASTA file and loads it

Type:

```
>>> f = FASTA()
>>> f.read_fasta(filename)
>>> f.fasta
```

Returns nothing

Warning: If more than one FASTA is contained in the file, an error is raised

save_fasta (*filename*)

Save FASTA file into a filename

Parameters

- **data** (*str*) – the FASTA contents
- **filename** (*str*) – where to save it

sequence

returns the sequence only

class MultiFASTA

Class to manipulate several several FASTA items

Here, we load some FASTA using UniProt web service:

```
>>> from bioservices import MultiFASTA
>>> mf = MultiFASTA()
>>> mf.load_fasta("P43408")
>>> mf.load_fasta("P21318")
```

You can then get back to your accession entries as follows

```
>>> mf.ids
['P43408', 'P21318']
```

And the sequences in the same order can be accessed:

```
>>> len(mf)
2
```

Each FASTA is stored in `fasta`, which is a dictionary where each values is an instance of `FASTA`:

```
>>> print(mf._fasta["P43408"].fasta)
>sp|P43408|KADA_METIG Adenylate kinase OS=Methanotorris igneus GN=adkA PE=1 SV=2
MKNKVVVVTGVPVGGTTLTQKTIEKLKEEGIEYKMNFGTVMFEVAKKEEGLVEDRDQMR
KLDPDTQKRIQKLAGRRIAEMAKESNVIVDTHSTVKT PKGYLAGLPIWVLEELNPDIIVI
VETSSDEILMRRRLGDATRNRDIELTSDIDEHQFMNRCAAMAYGVL TGATVKIIKNRDGLL
DKAVEELISVLK
```

The most convenient way to access to all data is to use the dataframe attribute:

```
>>> mf.df.Sequence
```

```
>>> from bioservices.apps import MultiFASTA
>>> f = MultiFASTA()
>>> f.load_fasta(["P43403", "P43410"])
>>> f.df.Size.hist()
```

df

fasta

Returns all FASTA instances

hist_size (**kws)

ids

returns list of keys/accession identifiers

load_fasta (ids)

Loads a single FASTA file into the dictionary

read_fasta (filename)

Load several FASTA from a filename

save_fasta (filename)

Save all FASTA into a file

2.12 References to BioServices on the Web

- Galaxy: See the Log Archive at [Galaxy log archive](#)
- EBI: See [EBI programming web services](#)
- WikiPathways: [references](#)
- GeneProf: [example python](#)
- <http://www.scoop.it/t/bioinformatique>
- <http://bioinfo-fr.net/bioservices-module-python>
- <http://devbio.eu/?p=resources&presel=bioinfo>
- biomartian from Endre Bakken Stovner <https://github.com/endrebak/biomartian>

2.13 FAQs

2.13.1 General Errors

The most common errors come from

1. The web service that you are trying to access is down (temporarily or not)
2. The web service API has changed
3. A request inside bioservices is incorrect
4. A timeout occurred.

For the first problem, we cannot do anything except wait for the service to be up again.

For the second, you are trying to update bioservices to reflect those changes.

For the two other issues, which are really bioservices problems, we recommend to rerun your code setting the logging level to debug and send the code and errors you see.

To set the debug level on on a web service:

```
u = UniProt(verbose=True)
u.logging.level = 'DEBUG'
```

2.13.2 Installation issues

ValueError: unknown locale: UTF-8 under Mac OS X 10.7 - Lion

The installation with PIP is succesful but I get a “*ValueError: unknown locale: UTF-8*” under Mac OS X 10.7 - Lion when typing **from bioservices import ***.

On solution is to fix your environment by typing the following code in a shell:

```
export LANG="it_IT.UTF-8"
export LC_COLLATE="it_IT.UTF-8"
export LC_CTYPE="it_IT.UTF-8"
export LC_MESSAGES="it_IT.UTF-8"
export LC_MONETARY="it_IT.UTF-8"
export LC_NUMERIC="it_IT.UTF-8"
export LC_TIME="it_IT.UTF-8"
export LC_ALL=
```

You can check if it works by typing

```
python -c 'import locale; print(locale.getdefaultlocale());'
```

If this works without error, then it is fixed and you should be able to import bioservices. If so, make this solution persistent by adding the code into your environment. For that, just copy and paste the code in a file called `.bashrc_profile` (or `.bashrc`)

[reference](#) [blog entry](#)

2.13.3 General questions

How can I figure out the taxonomy identifier of the mouse ?

You can use the Taxon class that uses Ensembl/UniProt/Eutils depending on the tasks. Here, we do not know the scientific name of taxonomy identifier of the mouse. We can use the search_by_name function:

Warning: Taxon class is not part of BioServices but some utilities have been added to BioKit (github.com/biokit)

Changed in version 1.3.

In earlier version of BioServices, you could use:

```
>>> from bioservices import Taxon
>>> t = Taxon()
>>> t.search_by_name("mouse")
u'10090'
```

But this is now in BioKit:

```
>>> from biokit import Taxonomy
>>> t = Taxonomy()
>>> results = t.fetch_by_name('mouse')
>>> results[0]['id']
u'10090'
```

How to convert ID from one database to another ?

Many web services provides converters. In BioServices, you can access to Kegg and UniProt that both provides converter. For instance with Kegg, you can convert all human (hsa) Kegg Id to uniprot Id with:

```
from bioservices import *
s = KEGG()
kegg_ids, uniprot_ids = s.conv("hsa", "uniprot")
```

Or you can use the uniprot mapping function:

```
from bioservices import *
u = UniProt()
u.mapping(to="KEGG_ID", fr="ACC", query="ZAP70_HUMAN")
```

2.13.4 Specific Usage

Why my uniprot request takes forever ?

This may happen. Consider:

```
from bioservices import *
u = UniProt()
u.search("P53")
```


This request performed on UniProt web sites is actually pretty fast but there are 386 pages of results. In BioServices, the search commands reads the 386 pages of results and then stores the result in a variable. So it may take a while.

More generally if a request returns a very long result, it may take a while. You can use the socket module:

```
import socket
socket.setdefaulttimeout(5.)
```

After 5 seconds, the read() call will stop returning whatever has been read so far.

KEGG service

Is it possible to get the pathway information for multiple proteins ?

Currently there is no such function. You can only retrieve pathways given a single protein Id. However, you can easily write such a function. Here is the code for 2 proteins:

```
>>> p1 = k.get_pathway_by_gene("7535", "hsa") # correspond to ZAP70
>>> p2 = k.get_pathway_by_gene("6885", "hsa") # 6885 correspond to MAP3K7
>>> [k1 for k1 in p1.keys() if k1 in p2.keys()]
['hsa04660', 'hsa04064']
```

There are 2 pathways containing the proteins 7535 and 6885.

2.13.5 Interest of the BioServices classes REST and WSDL ?

There are a few technical aspects covered by BioServices to ease our life when adding new modules such as timeout, long request, headers, and so on.

What is the difference between GET and POST

When the user enters information in a form and clicks Submit, there are two ways the information can be sent from the browser to the server: in the URL, or within the body of the HTTP request.

The alternative to the GET method is the POST method. This method packages the name/value pairs inside the body of the HTTP request, which makes for a cleaner URL and imposes no size limitations on the forms output. It is also more secure.

2.14 Whats' new, what has changed

2.14.1 Revision 1.8.0 roadmap

- make all services methods hidden or inside a single attributes to make the methods of a services more visible
- finalise pubchem, pfam and eva modules
- Wherever devtools is used to check input params, we should make sure the error message is informative. This may need to change easydev itself;
- All Classes/Services should hide the REST/WSDL methods to make the API easier. Instead of inheriting from REST, we should use an aggregation and store all methods in a single attribute
- Get rid of multifasta and fasta modules

2.14.2 Revision 1.7.9

- add missing field in KEgg Parser (REL_PATHWAY)
- fix panther.get_enrichment output (try/except)

2.14.3 Revision 1.7.8

- Fix ENA new API
- fix missing plugin in requirements-dev.txt

2.14.4 Revision 1.7.7

- small fix on pantherdb (autocorrect typo in pantherdb api)

2.14.5 Revision 1.7.6

- Fixing ncbiblast and muscle services
- Fixing quickgo services by adding new methods
- Fixing chembl and all failing tests and modules (omicdi, seqret,etc)

2.14.6 Revision 1.7.5

- NEW MODULE: mygeneinfo, pdbe
- Limits the request to 10 per seconds (3 for eutils). This fixes <https://github.com/cokelaer/bioservices/issues/7>
- update quickgo
- Update PDB module (will not be maintained in the future, to usePDB instead.)
- Fix issue in Eutils/ECitMatch reported here <https://github.com/cokelaer/bioservices/issues/169> and here <https://tinyurl.com/y6u2cyjq> on stackoverflow

2.14.7 Revision 1.7.4 (March 2020 Combine/Harmony2020 hackathon)

- Integration of BioModels new API (REST instead of WSDL and different functionalities) in coordination with Mihai Glont and Tung Nguyen at EMBL-EBI during the Combine-Harmony hackathon.
- Integration of BiGG models service thanks to <https://github.com/achillesrasquinha> contribution.
- Fixing notebooks (biomodels and uniprot)
- Move the miriam services to the attic

2.14.8 Revision 1.7.3 (March 2020)

- fixing chembl after API changed. Fix the get_status_resources method by removing document_term and target_prediction. Changed acd_log into alogp: for some reasons this was changed. There was a warning on 4th March 2020 telling that changes may occur.

2.14.9 Revision 1.7.2 (March 2020)

- Fixing ReadTheDocs online documentation and Changelog

2.14.10 Revision 1.7.1 (Feb 2020)

- Just updating the README and setup metadata

2.14.11 Revision 1.7.0 (Feb 2020)

- **Pull request**
 - from @thobalose (<https://github.com/cokelaer/bioservices/pull/149>) to update tests, travis recipes, pinned matplotlib to 3.0.3
- **NEWS:**
 - panther module (pantherdb.org)
 - add a test for the pubchem, pfam and eva modules, which are still in draft version though
- **CHANGES**
 - PICR module is fully commented. The service is most probably deprecated. Not on EBI website anymore
 - remove TCGA, which waws only a draft version with one method.
- **BUGS and FIXES**
 - wikipathway: fixed getPathway, savePathway, getPathwayByLiterature and coloredPathway methods. Some are failing due to some wikipathway temporary failures.
 - Fixed <https://github.com/cokelaer/bioservices/issues/148> to have a more informative error message (array express)
 - Fixed KeggParser for the GENE entries to have the correct ID name. <https://github.com/cokelaer/bioservices/issues/151>

2.14.12 Revision 1.6.0

- **CHANGES:**
 - rewrote entirely the ChEMBL wrapper due to new ChEMBL API.
 - removed the quickgo_old module and its tests
 - Fix typo for a “valid colum,” in uniprot module
 - Changed biomodels WSDL endpoint (thanks to <https://github.com/thobalose>.)
 - uses colorlog to have more robust and consistent logging.
- **BUGS:**
 - Fix wikipathway XML issues by outputting dictionaries now. This fixes <https://github.com/cokelaer/bioservices/issues/131>
 - Fix <https://github.com/cokelaer/bioservices/issues/137> to handle KEGG GENE field properly in KEGGParse

- Fix <https://github.com/cokelaer/bioservices/issues/125> thanks to <https://github.com/thobalose>.

2.14.13 Revision 1.5.2

- Fix retmode in EUtils.Efetch fonction. Was not taken into account but set to text by default but this seemed to have changed recently so this bug emerged while it was silent before.
- Issue in EUtils URL (trailing /) fixed in this PR <https://github.com/cokelaer/bioservices/pull/116>
- Major update of Reactome class. The old one is named ReactomeOld and the new one uses the new Reactome API

2.14.14 Revision 1.5.1

Support for Python 2.6 dropped.

- **CHANGES:**
 - using proper logging

2.14.15 Revision 1.5

Support for Python 3.6 on Travis.

- **BUG:**
 - kegg: fix #75 and #77 (missing keywords in KEGG)
 - kegg: fix #79 (mis-interpreted cases reported by kirienko with examples.
 - kegg: fix #85 (some entries are not interpreted)
- **CHANGES:**
 - biodbnet: conversion from WSDL to REST. Note methods' arguments changes: inputValues to input_values, dbPath to db_path. Uses pandas
 - wikipathways: conversion from WSDL to REST. All wikipathways service uses Pandas and returns dataframes.
 - Better implementation of secure host option and more xml customization #98
 - move quickgo.py to quickgo_old.py
 - move readseq to seqret (<https://github.com/cokelaer/bioservices/issues/89>)
 - move wsdbfetch to dbfetch and move from WSDL to REST service
- **NEWS:**
 - quickgo uses the new API from EBI (see changes)
 - seqret uses the new API (instead of readseq)
 - dbfetch uses new API (instead of WSDL)
- Fixes the licensing (GPLv3 everywhere)

For developers: use pytest instead of nosetests.

2.14.16 Revision 1.4

- **1.4.17: rhea URL changed and add get_metabolites function. Fix pride test and add missing license file**
- 1.4.16: simplify setup
- **1.4.15:**
 - **BUG:**
 - * ensembl.org in biomart was not reachable anymore. This is fixed by using requests to check URL existence.
 - * in ensembl module tolist -> to_list
 - * Fix ensembl tests
- **1.4.14:**
 - **CHANGES:**
 - * update http to https in EUtils
 - * missing TARGET field in KEGGParser reported in issue #66
- **1.4.13:**
 - **NEWS:**
 - * Add a download_fasta dedicated function to download a fasta file either from ENA or NCBI given its accession. See bioservices.apps.download_fasta. Used within Sequana project
- **1.4.12:**
 - **BUG:**
 - * Fix a regression bug in ncbiblast introduced in earlier commits <https://github.com/cokelaer/bioservices/issues/61>
 - **CHANGES:**
 - * add PRODUCT/ALL_REAC/HISTORY/SYSNAME in KEGG parser thanks to issue reported in <https://github.com/cokelaer/bioservices/issues/60>
- **1.4.11:**
 - **NEWS:**
 - * EUtils can now return a dictionary rather than a xml
 - * New method get_taxon in ENA class
 - * EnsemblFTP added to ensembl module
- 1.4.10: fixing a bug/typo in pypi
- **1.4.9:**
 - **BUG**
 - * KeggParser missing parser for the SEQUENCE keyword is now available <https://github.com/cokelaer/bioservices/issues/46> , <https://github.com/cokelaer/bioservices/issues/51>
 - **CHANGES:**
 - * Improves way biomart handles errors (see <https://github.com/cokelaer/bioservices/issues/50>)
- **1.4.8:**

- NEWS: add new module for the omnipath web service in *bioservices.omnipath*.
- **1.4.7:**
 - NEWS: add method `get_run` in `RNASEQ_EBI` class.
- **1.4.6:**
 - **NEWS:**
 - * RNASEQ analysis REST API included (<http://www.ebi.ac.uk/~rpetry/geteam/rnaseq/apispec.pdf>)
- **1.4.5:**
 - **BUG:**
 - * Fixes a python3 wrong import
- **1.4.4:**
 - **CHANGES:**
 - * Uniprot: update valid columns
 - * <https://github.com/cokelaer/bioservices/pull/35> with biocarta module updates
 - **BUGS:**
 - * Fix a test in `test_eutils`
 - * Fix KEGG parser <https://github.com/cokelaer/bioservices/pull/35>
 - * Fix Service input py2/3 compat and unset argument <https://github.com/cokelaer/bioservices/pull/35>
 - * Update biocarta: the website has changed and the code needed to be updated
 - NEWS: ENA module and class added
- **1.4.3**
 - BUG: fix typo in a draft tcga module
- **1.4.2**
 - CHANGES: update setup dependencies.
 - BUG: Typo fixed in uniprot list of valid columns #47
- **1.4.1**
 - **CHANGES:**
 - * Renamed `kegg.KEGG.info` into `dbinfo` , which was overloaded with Logging
 - * Updated all documentation to check examples
 - * Fixed tests and notebooks
 - * clean and tested doctests in the documentation
 - **NEWS:**
 - * Replace deprecated HGNC with the official web service from genenames.org
- **1.4.0**
 - **CHANGES:**

- * Fully update EUtils since WSDL is now down; implementation uses REST now. This fixes <https://github.com/cokelaer/bioservices/issues/41>
- * Remove the apps/taxonomy module now part of biokit.

– NEWS:

- * add small XML tools to parse XML dynamically in xmltools module
- * add http_delete in services.py

2.14.17 Revision 1.3

- 1.3.8 (progress)
 - CHANGES:
 - * cache files are now stored in the ./config/bioservices directory, this fixes <https://github.com/cokelaer/bioservices/issues/40>
- 1.3.7
 - CHANGES
 - * ArrayExpress: add new 2 methods to ease the usage
 - BUG FIXES
 - * KEGG: fix <https://github.com/cokelaer/bioservices/issues/39>
- 1.3.6
 - BUG FIXES
 - * **KEGG: Fixed during the major changes described here below** <https://github.com/cokelaer/bioservices/issues/29>
 - CHANGES
 - * IntactL rename Intact class into IntactComplex
 - * KEGG: revisited the parsing following requests from user <https://github.com/cokelaer/bioservices/issues/30>
 - * KEGG: remove useless function (check_dbentries)
 - * **KEGG: The KEGGParser does not inherit from KEGG anymore and there is now a parse() method inside KEGG so user do not need to play with the 2 classes. Only KEGG is required. KEGGParser can still be used but will not have the KEGG methods anymore**
- 1.3.5
 - BUG FIXES:
 - * quickgo: fix bug <https://github.com/cokelaer/bioservices/issues/22>
 - * uniprot: add missing columns (<https://github.com/cokelaer/bioservices/issues/23>)
 - * kegg: fix parser related to reaction in the Compound data structure (<https://github.com/cokelaer/bioservices/issues/27>)
 - NEWS
 - * add Intact complex web services
- 1.3.4

- BUG FIXES
- CHANGES * clinvtae: tests and doc added * services modules: DevTools class moved to easydev
- NEWS
 - * add PRIDE service + test + doc
- 1.3.3
 - BUG FIX
 - * uniprot fixing a python 3 typo
 - CHANGES
 - * pdb: add a method
 - * hgnc: add new class related to HGNC
 - NEWS
 - * services.py: add a method to ease conversion of dict to json. add attribute to limit number of requests per seconds but not yet used.
 - * taxonomy module: add new method in Taxon to look for a taxon identifier given a name
 - * NEW module ensembl completed
 - * NEW module clinvtae added (contribution from Patrick Short)
- 1.3.2
 - CHANGES:
 - * services: http_get and http_post now accepts all optional arguments from requests.
 - * services: get_headers default content is now same as urllib2
 - * pdb module: more functions added
 - * ensembl module added with some functionalities
- 1.3.1
 - CHANGES:
 - * uniprot: multi_mapping is deprecated. mapping can now handle long queries by itself.
 - * services/settings:
 - removed get_bioservices_env function, which is not used anymore
 - move urlencode in Service class into WSDLService, which will be deprecated
 - add TIMEOUT in WSDLService and REST as alias to settings.TIMEOUT so timeout can now be used in both REST and WSDL.
 - NEWS:
 - * readseq module added.
 - BUG fixes:
 - * CACHING attribute had a typo
- 1.3.0
 - NEWS

- * added REST class that uses the requests module. This class replaces of instance of RESTservice that uses urllib2, which will be deprecated later on. This speeds up the code significantly not only because requests is faster but also because we now do not need trial/time hack that was implemented inside RESTService. We also use the requests_cache module that could be used to speed go but requires to store cache files locally. Asynchronous requests is available but used only in a few places for now.
 - * EUtils has been fully implemented excepting EPost. API may still change to make its usage easier but functionalities are there.
- CHANGES
- * update code to be python-3 compatible. There are still issues with suds/requests/gevent but the code itself is python3 executable.
 - * WSDLservice now uses suds instead of SOAP package by default
 - * all paramters called format have been renamed frmt (format is a python keyword)
 - * chemblpdb module and class renamed to chembl and *bioservices.chembl.ChEMBL*
 - * All classes that depends on RESTService have been updated to use the new REST class.
 - * chemblpdb:
 - get_assay_by_chemblId renamed in get_assays_by_chemblId
 - renamed get_target_by_refSeqId into get_target_by_refseq
 - kegg module: all Kegg strings replaced by KEGG so the kegg.Kegg class is now kegg.KEGG
 - * ChEBI: getUpdatedPolymer: remove useless parameters (was failing with python3)
 - * Wikipathway class renamed as WikiPathways to agree with official name
 - * biomart now uses python3 and we had to remove the threaded_request module, which does not seem to be available. So, we used the new implementation using requests but gevent is not available for python3 either so, we use requests but without the asynchronous call. This is working for now. Transparent for the user.
 - * geneprof: parameter called type and format are renamed output and frmt to not clash with python keywords. Use REST class instead of RESTService but should be transparent for the users.
 - * services do not have the checkParam method. use devtools.check_param_in_list instead.
- BUG FIXES:
- * Fixing bug #24/25 posted on assembla related to parse_kgml_pathway second argument can now be used.
 - * wikipathway: findInteractions had a typo in i

2.14.18 Revision 1.2

- 1.2.6:
 - fixing bug report 22 related to KEGG.pathway2sif function that was failing.
 - add option in biomart to use different host. This is to fix an issue where biomart hangs forever. This was reported by Daniel D bug report 23 on assembla.
- 1.2.5:
 - add try/except for pandas library.
- 1.2.4:

- fixing typo in the init that fails bioservices to be used if pkg_resources is not available.
- **1.2.3**
 - **updating some apps (fasta,peptides, taxon) in bioservices.apps directory**
 - * Improves UniProt module by adding a dataframe export when performing a search
 - * added the BioDBnet service.
 - * added Pathway Commons
 - * fixed UniChem: add new database identifiers and fix interpretation of the output
- **1.2.2:**
 - NEW Service: *bioservices.biodbnet.BioDBNet*
 - uniprot: add multi_mapping method to use mapping method on large queries and added timeout/trials inside uniprot functions
- **1.2.1:**
 - same as 1.2.0 but fixed missing mapping and apps directory in the distribution available on pypi
- **1.2.0**
 - Kegg class has now an alias called KEGG
 - NEW Services: *bioservices.muscle.MUSCLE*
 - fix bug in get_fasta from uniprot class
 - add aliases to quickGO to retrieve annotation
 - NEW Service: *bioservices.pathwaycommons.PathwayCommons*
 - NEW Service: *bioservices.geneprof.GeneProf* service
 - uniprot add function to get uniprot fasta sequence
 - add apps.peptides module

2.14.19 Revision 1.1

- **1.1.3**
 - **fix bug in chembl.get_all_targets() that was failing to return the** json/dictionary as expected.
- **1.1.2**
 - **add biocarta, pfam modules (and htmltools. maybe not required.)**
 - * fix bug in uniprot.mapping to return list of values instead of a string (assembla ticket 19).
- **1.1.1:**
 - **services.py: move print statements into login.warning**
 - * add documentation and examples related to Galaxy/BioPython.
 - uniprot mapping function now returns a dictionary instead of a list
 - NEW Service : class:*bioservices.hgnc.HGNC* + doc + test

2.14.20 Revision 1.1

- **1.1.0:**

- **in psicquic when performing the conversion, we now use a try/except since some fields (in rare case) may be miss**
 - * add faqs in the doc + update of the README and metadata.
 - * fix typo in the list of uniprot mapping
 - * Use BeautifulSoup4 instead of 3
 - * add the ChEBI Web Service.
 - * add the UniChem Web Service.
 - * logging ERROR in Service when data cannot be converted to XML is now a simple warning
 - * kegg.conv method now returns a dictionary instead of list of tuples.

2.14.21 Revision 1.0

- **1.0.4**

- add a draft version of PDB just to be able to fetch PDB data and use it with external tool such as PyMOL as shown in the new pymol.rst documentation.
- add a missing docstring in uniprot + check to/fr parameters in UniProt.mapping method.
- Fix a typo in PSICQUIC module.

- **1.0.3**

- **uniprot.UniPort.search method: default value of the parameter format is now “tab”**
 - * fix 1 quickgo test
 - * a few documentation updates in biomart/uniprot/chemblpdb and tutorial.

- **1.0.2:**

- **add SOAPpy in the setup requirements**
 - * finished ArrayExpress +doc + tests
 - * fixed a bug in KEGGParser.parseGene
 - * add methods in psicquic to parse all databases and convert to uniprot if **possible. These methods are used to build an application provided in the** tutorial
- add biomart + doc + test
- add onWeb method in Service class
- **add chemspider draft**
 - * complete utils

- **1.0.1**

- Add miriam module
- Add arrayexpress

- **1.0.0:**

- First release of bioservices

2.14.22 Revision 0.9

- **0.9.7:**
 - **add new feature in KEgg module to introspect kgml data sets**
 - * add biogrid test and documentation.
 - * chemblpdb improvements
 - * uniprot bug fixes (search if working as expected now)
- **0.9.6:**
 - Finalising the Kegg module
- **0.9.5:**
 - **add parser for all KEGG entries (enzyme, genome, pathway, ...)**
 - * add a show_pathway to highlight element in a pathway
- **0.9.4:**
 - cleaning up the modules
- **0.9.3:**
 - documentation cleanup
 - fix tests
 - fix a few small bugs in biomodels
 - adding getattr method for all databases in kegg model
 - Service class has new method call pubmed to load pubmed in browser
- **0.9.2:**
 - uniprot search method improved
- 0.9.1: fix typo in biomodel. add uniprot search method. add keggParser class
- **0.9.0: Stable version of bioservices including the following services:** BioModels, Kegg, Reactome, ChEMBL, PICR, QuickGO, Rhea, UniProt, WSDbfetch, NCBIblast, PSICQUIC, Wikipath

2.14.23 Up to Revision 0.5

- 0.4.9: finalise wikipathway
- 0.4.8: finalise doc of half of the services.
- 0.4.7: add psicquic service and carry on reactome
- 0.4.6: finalise kegg module and test
- 0.4.5: finalise biomodels. keff WSDL is not maintained anymore: started REST version.
- 0.4.4: finalise quickgo,rhea, picr, uniprot. Update servie to use logging module.
- 0.4.3: add quickgo
- 0.4.2: add wsdbfetch/uniprot

- 0.4.1: add wikipathways module +test .
- 0.4.0: add rhea service + test. Updating the documentation.
- 0.3.0: add reactome + uniprot.
- 0.2.0: finalise biomodels and add picr service + test for biomodel service..
- 0.1.0: add database and kegg modules + its documentation and tests

2.15 Contributors

Contributors are the authors who started the development of BioServices (and authors of this reference on [BioInformatics](#)).

In addition to the main authors of the papers the following developers have implemented modules now available in BioServices:

- Achilles Rasquinha implemented the BiGG models service *bioservices.bigg* module
- Sven-Maurice Althoff, Christian Knauth implemented the *bioservices.muscle* module.
- Patrick Short implemented the *bioservices.clinitae* module

And thank you also to the contributions from users who have sent communication via emails or via the [ticket system](#).

Special thanks to Thoba Lose (<https://github.com/thobalose>) and <https://github.com/jsmusach> for various pull requests.

Note that originally code (and earlier tickets) were hosted [elsewhere](#).

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