

Building and Mining Knowledge Graphs
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Final written project report
NTDs2RDF: A heterogeneous and integrated knowledge graph for
the exploration of neglected tropical diseases.

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1. Abstract

Neglected tropical diseases (NTDs) affect millions of people in developing countries and have been historically overlooked in the global health agenda. Although progress has been made in controlling and eradicating these diseases, there are still open questions regarding key biological mechanisms and potential drug therapies. Biological and biomedical databases can facilitate the identification of novel drugs and targets for treating diseases like NTDs, but they present issues of standardization and integration. The semantic web, with its set of technologies and standards, can provide an interoperable and unified framework to study the NTDs. The NTDs2RDF project aims to create a knowledge graph (KG) of genes, proteins, metabolic pathways, gene ontologies, single nucleotide variants, drugs, and other relevant data for three NTDs (Chagas disease, leishmaniasis, and African trypanosomiasis), integrating all the information in a single data structure that can be explored through a query interface implemented with a *Streamlit* web application (<https://ntds2rdf.streamlit.app/>). This software provides a user-friendly platform to extract information from the KG using *SPARQL* queries. The project represents an initial step towards the creation of a heterogeneous database for different NTDs with several potential applications in advancing the understanding of NTDs biology and providing insights that cannot be obtained through alternative resources. All underlying data and code are accessible through GitHub (<https://github.com/sayalaruano/NTDs2RDF>) under the MIT and CC0 licenses and archived on Zenodo. The Figure SI2 shows a graphical abstract for this project.

2. Introduction

Neglected tropical diseases (NTDs) are a heterogeneous group of 20 bacterial, viral, parasitic, and fungal conditions (See Figure SI1) that generally occur in developing tropical countries in the Americas, Africa, and Asia¹. NTDs mainly affect poor populations that do not have access to safe water, sanitation, and high-quality healthcare. Because of the severe effects of NTDs (i.e., they can cause long-lasting disabilities), they reinforce the cycle of poverty in vulnerable communities^{2,3}. According to some estimations, around 20% of the world's population is susceptible to the harmful consequences of NTDs⁴. Nonetheless, these diseases have been historically omitted from the global health agenda, leading to inadequate treatment, prevention, and public health strategies^{2,5}.

There have been international projects to control and eradicate the NTDs, including the World Health Organization (WHO) NTD roadmaps 2012–2020 and 2021–2030¹, and the London Declaration on NTDs⁶, among other initiatives. According to data from the WHO (2023), the number of people requiring interventions against NTDs in the last decade has reduced by 25%. Despite the substantial progress made in NTDs research, there are still open questions about the key biological mechanisms and potential drug therapies for treating and preventing these complex diseases². Several studies have demonstrated that biological and biomedical databases facilitate the identification of novel drugs, drug targets (molecules that can be modified by a drug to produce a therapeutic impact), side effects, and other information for treating diseases^{7,8}. However, these resources present issues regarding standardization practices, creating difficulties to connect the knowledge from one database to another⁹.

The semantic web, a set of technologies and standards that aims to make web content machine-readable, can help to address the lack of integration of biological databases, providing an interoperable and unified framework to foster biomedical research¹⁰. By employing semantic web technologies (e.g., RDF, OWL, SPARQL, etc.), researchers can establish common vocabularies and formats for data exchange¹¹, thus facilitating the identification of novel drugs, drug targets, and other information for treating complex diseases like NTDs.

Currently, there are several independent databases that contain biological knowledge of NTDs, but no integrated resource with all the information. This unified database could enable the systematic exploration of all the components of the NTDs, contributing to discover novel therapeutic insights for these diseases. Therefore, the NTDs2RDF project aims to create a schema and a knowledge graph (KG) of genes, proteins, metabolic pathways, gene ontologies, single nucleotide variants (SNVs), drugs, and other relevant data for three NTDs (Chagas disease, leishmaniasis, and African trypanosomiasis), integrating all the information in a single data structure that can be queried through a user-friendly web application.

3. Methodology

This project was divided into various modules for data collection, data cleaning, programmatic creation of the KG, and the development of a web application for querying the RDF graph. An overview diagram of all the parts of the NTDs2RDF project is presented in Figure 1. Further details of all the elements of this workflow are presented below.

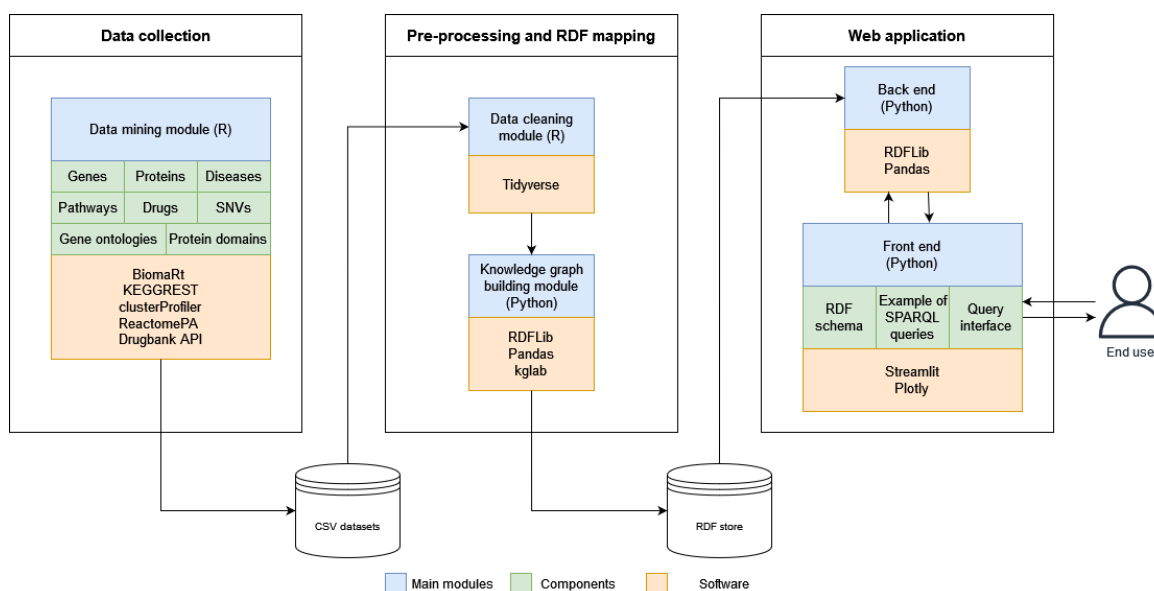


Figure 1.—Software architecture of the NTDs2RDF project. The workflow was divided into three main stages with some modules (blue rectangles) and components (green rectangles). The software libraries are shown as orange rectangles.

3.1. Data collection

The data collection for this project was developed through a data mining approach, using several R packages, APIs, and systematic literature search (Figure 1). First, the human genes involved in the infection process of the three NTDs were obtained from the *KEGG*¹² database using the *KEGGREST* package¹³. The information about proteins, gene ontologies, protein domains, and some identifiers for external databases were retrieved with the *BiomaRt* package¹⁴. The *clusterProfiler*¹⁵ and *ReactomePA*¹⁶ packages were used to obtain the pathways associated to the genes for each disease, applying gene set enrichment analysis. The single variant nucleotides (SNVs) and their relationships with the genes and drugs were obtained from the *PharmGKB*¹⁷ database, as well as the relationships between the drugs and proteins. The relationships between the drugs and the diseases were obtained using the *Drugbank*¹⁸ database API. Finally, additional external identifiers were mapped using the *TogoID*¹⁹ web application. All the data was enriched with information from scientific articles and domain-specific databases through a systematic literature search. The scripts for this part can be found on this [folder of the GitHub repository](#) or the *NTDs2RDF/Data_processing* folder in the provided zip file.

3.2. Preprocessing and RDF mapping

After retrieving all the datasets from the different sources as CSV files, a data cleaning and preprocessing step was applied to assure the correct format, datatype, among other details using some packages from *Tidyverse*²⁰. Then, I looked for the proper terms to define the classes, predicates, and properties of the KG, which were mainly obtained from the *Biolink Model*²¹ and some general terms from the *rdfs* and *xds* namespaces. Furthermore, the *Bioregistry*²² metaregistry was used to assign standardized identifiers for all the biological entities of the KG. This information was used to create an RDF schema that integrated the subjects, objects, and predicates from the KG. Finally, the KG was constructed using *pandas*²³, *kglab*²⁴ and *rdflib*²⁵, exporting the result with the *n-triples* and *turtle* syntaxes. The script for this part can be found on a [jupyter notebook of the GitHub repository](#) or the *NTDs2RDF/RDF_graph_building.ipynb* file in the provided zip file.

3.3. Web application

To guarantee the accessibility and reusability of the KG, a [multi-page web application](#) was created. This software was divided into three pages: RDF schema, examples of *SPARQL* queries, and query interface. The back end of the software

was developed with *pandas*²³ and *rdflib*²⁵, while the front end was created with *Streamlit*²⁶ and *Plotly*²⁷ (Figure 1). The app was deployed with the *Streamlit*'s Community Cloud. All the files required to create and deploy the web application are available in the [GitHub repository](#) of this project or in the provided zip file. Furthermore, it is possible to run the web application locally by creating a Python virtual environment with *pipenv*²⁸ or *conda*²⁹ and installing the software dependencies. The instructions on how to run the web application locally are available in the README of the [GitHub repository](#).

4. Results

4.1. Knowledge graph

The NTDs2RDF KG is available at Zenodo, the GitHub repository, or the [NTDs2RDF/Data/RDF_graphs](#) folder of the zip file with *n-triples* and *turtle* syntaxes. The KG has ten classes, ... predicates, and **33.892** triplets. **Figure 2** shows the schematic representation of the NTDs2RDF KG. The *Biolink Model*²¹ was the main source to define classes and predicates of the RDF graph, which gave several advantages over other resources. *Biolink* has many human-readable and domain-specific predicates for Biology, which captures the details of the biological knowledge (**Figure 2**). For instance, the predicates “*biolink:is_sequence_variant_of*”, “*biolink:gene_associated_with_condition*”, and “*biolink:has_sequence_location*” are explicit and easy to understand, which do not have counterparts in other ontologies. Before working with *Biolink*, I was using the terms suggested by *BioPortal*³⁰, which were mainly from the *National Cancer Institute Thesaurus (NCIT)*³¹ and the *Open Biomedical Ontologies (OBO)*³². The classes and predicates of the *NCIT* and *OBO* ontologies were not human-readable because they were associated with codes (e.g., C16612, NCIT_C25281), and most of the URIs did not work (e.g., <http://ncicb.nci.nih.gov/xml/owl/EVS/Thesaurus.owl#C16612>).

Besides being human-readable, the entities from *Biolink* follow a machine-readable format and they are integrated with other ontologies using semantic mappings, which makes the KGs interoperable. Other ontologies like *NCIT* and *OBO* are machine readable, but they lack interoperability. Finally, the *Biolink* data model provides class properties to link external identifiers (“*biolink:x_ref*” predicate) and to track the provenance of the data (“*biolink:provided_by*” predicate).

The standardized identification of entities is another important aspect to consider when creating KGs. Biological databases tend to create their own unique identifiers and they are not always cross-referenced with external entries, hindering the integration and interoperability of biological knowledge³³. To assure that all the entities of the NTDs2RDF KG have standardized and stable identifiers, the *Bioregistry*²² metaregistry was used to assign the URIs and CURIEs.

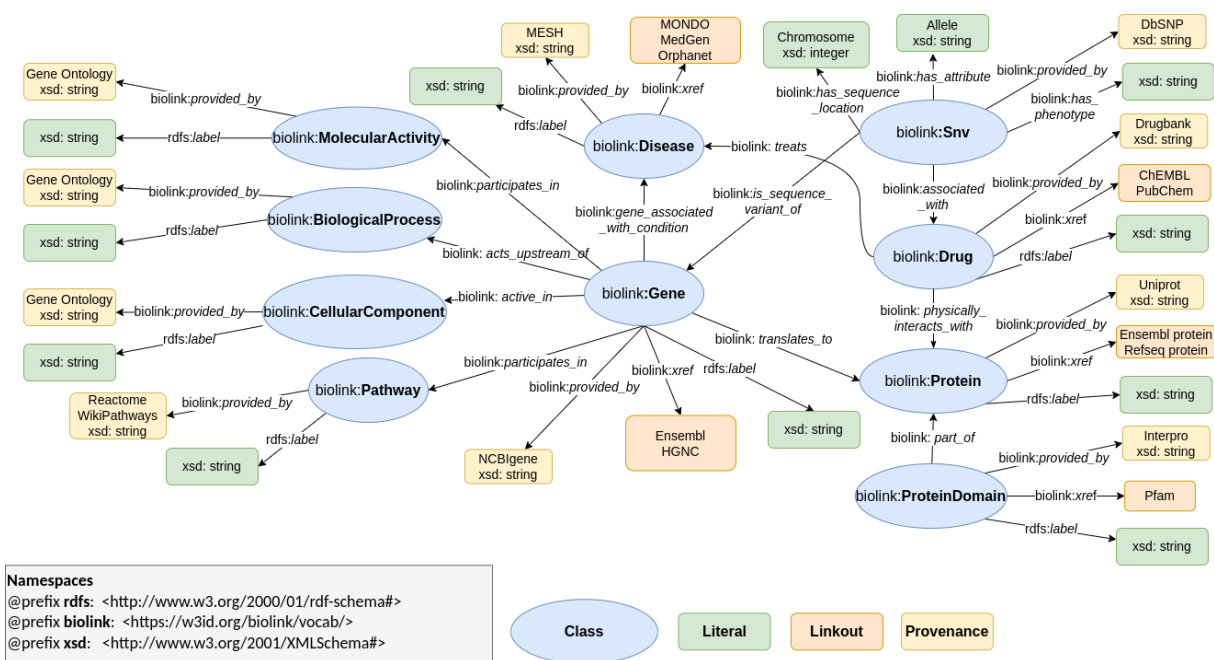


Figure 2.-RDF schema of the NTDs2RDF KG. The classes are represented as blue ovals, the literals as green rounded rectangles, the references to external databases as orange rounded rectangles, and the provenance for the classes as yellow rounded rectangles.

4.2. Web application

To guarantee the accessibility and findability of the NTDs2RDF KG, a [multi-page Streamlit web application](#) was developed. The home page of the web app has general information about the project and loads the RDF graph and the SPARQL queries objects (**Figure SI2**). The next page shows the schematic representation of the KG with all the classes and predicates from the *Biolink Model* and other standard ontologies (**Figure 2**). The third page has examples of SPARQL queries to extract relevant information from the RDF graph and demonstrate its usefulness in gaining new insights into NTDs. Also, the query examples are available on a [txt file of the GitHub repository](#) or at the [NTDs2RDF/sparql_queries_NTDs_RDF_examples.txt](#) file of the zip file. The last page of the web application consists of a user-friendly SPARQL query interface, which provides a simple method for extracting information from the KG. (**Figure SI3**).

Figure 3 presents screenshots of two SPARQL queries from the web application. The query of Figure 3A reveals that Toll-interleukin receptor domains are among the top 20 protein domains of genes associated with *African Trypanosomiasis*. Moreover, the query featured in Figure 3B shows that the Toll-like receptor signaling pathways have the highest number of genes involved in the three NTDs. Other SPARQL queries support these results (refer to the corresponding page of the web application). These findings could serve as the starting point for novel research hypotheses that could advance the understanding of NTDs biology and provide insights that cannot be obtained through alternative resources.



Figure 3.Two examples of SPARQL queries of the NTDs2RDF web application. Each query is linked with a research question and shows the results in a table and different plots.

5. Discussion

There have been several projects to convert conventional biological databases into RDF stores. *Bio2RDF*³⁴ and *EBI-RDF*³⁵ are examples of projects for converting large structured biological databases into RDF graphs, which integrate knowledge from heterogeneous sources to facilitate the exploration and analysis of such complex biological information. However, these resources are broad and do not have specific information to understand diseases like NTDs because most of the knowledge about them is in scientific articles and specialized repositories that are not included in big databases. Therefore, the systematic literature search step was crucial on the creation of the NTDs2RDF KG, making this resource more suited to contribute to the study of NTDs than general RDF stores.

Previous research applied semantic web technologies to understand NTDs. For instance, a study created a semantic problem-solving environment for finding information about *Trypanosoma cruzi* using an RDF store, in which they integrated information about proteomics, gene expression, and metabolic pathways³⁶. Another research developed an RDF graph and a visual querying tool for the genomics data of *T. cruzi*³⁷. Despite the significant progress and efforts of these projects, there is still a lack of integrated data sources for many of these diseases. For instance, *EuPathDB*³⁸ contains genomic data for eukaryotic pathogens that cause some NTDs, *GNTD*³⁹ provides epidemiological information, and so on.

To the best of our knowledge, no database has integrated biological data of various NTDs from multiple sources in a standardized format. Hence, NTDs2RDF is an initial step in the creation of a heterogeneous database for different NTDs with several potential applications.

Another important feature of the NTDs2RDF KG is the use of the *Biolink Model* to provide human and machine-readable names for the classes and predicates, and the *Bioregistry* metaregistry to assign standard identifiers. As explained in the 4.1 section of the Results, traditional ontologies such as *NCIT* and *OBO* present several limitations in terms of human-readability, broken links, and interoperability, so it is better to use the terms from the *Biolink Model*. By using these integrative and open-source standards, the KG represents a useful and unique resource that can be queried for information related to the three studied NTDs. One potential disadvantage of using resources like *Biolink* and *Bioregistry* is that they are in continuous development, meaning that some of the information derived from them will be outdated at some point. As a result, it is important to specify the version of the resources and try to maintain the KG with the upcoming updates.

To make a KG useful for the research community, it should adhere to the FAIR principles⁴⁰. To this end, I archived the KG in Zenodo and included information about its license and other details on how to use it. Moreover, I created a web application to retrieve information from the KG through *SPARQL* queries. Considering the lack of programming expertise of some researchers in the life sciences, creating a user-friendly query interface with examples of use-case *SPARQL* queries was an important contribution of this project. By doing so, the information of KGs can be available to a broad range of users, including those lacking extensive technical expertise.

Nonetheless, it should be noted that the NTDs2RDF KG has several limitations. First, it only contains data from 3 out of the 20 NTDs, which prevents finding biological commonalities or similar therapeutic strategies among most of the NTDs. Furthermore, most of the *SPARQL* queries retrieve broad information that would not add any new knowledge. Finally, the literature review was done by a non-expert of the field, so it is likely that crucial information about the NTDs was omitted. The final point can be improved by using machine learning-based strategies (e.g., natural language processing algorithms) that find patterns in large amounts of articles and domain-specific databases.

Despite these shortcomings, the NTDs2RDF project is a starting point to create an heterogeneous and integrated KG for NTDs. This resource can be expanded for other NTDs, representing a significant contribution to the research community working in this field. In the long term, the NTDs2RDF can benefit researchers and clinicians, who could use the insights gained from the data to develop more effective treatments, which ultimately could help NTD patients.

6. Conclusions and further work

In conclusion, the NTDs2RDF project has successfully transformed heterogeneous and dispersed data of three NTDs (Chagas disease, Leishmaniasis, and African trypanosomiasis) into a unified KG, which can be queried and explored through a user-friendly web application. By using the *Biolink* and *Bioregistry* standards, the KG had human/machine-readable and domain-specific entities, standardized identifiers, and interoperability with other ontologies. Moreover, I endorsed the application of the FAIR principles in this project by publishing the results in open repositories (Zenodo and GitHub), providing proper licenses and metadata, and by creating a web application with a query interface and some examples of *SPARQL* queries to demonstrate use-cases of the KG. Overall, the NTDs2RDF project represents a significant contribution to the research of NTDs, which could improve the understanding of the molecular basis of these diseases, and eventually leading to better health outcomes for patients.

Looking forward, the NTDs2RDF project has the potential for future development and expansion. One possibility is to include more NTDs in the KG, which could provide a broader understanding of the molecular mechanisms underlying the diseases. Another avenue for improvement is to automate the literature searching process using Natural Language Processing (NLP) algorithms, which could extract more specific data about the diseases and improve the quality of the data in the KG. This, in turn, would enhance the effectiveness of *SPARQL* queries. In addition, the application of rule mining or other machine learning strategies could be used to predict links between entities, which could uncover new relationships between the molecular components of the diseases. Finally, graph analytics could be used to identify hub nodes, communities, and other relevant insights, which could provide a deeper understanding of the NTDs and help to identify new targets for drug development.

7. Supplementary information

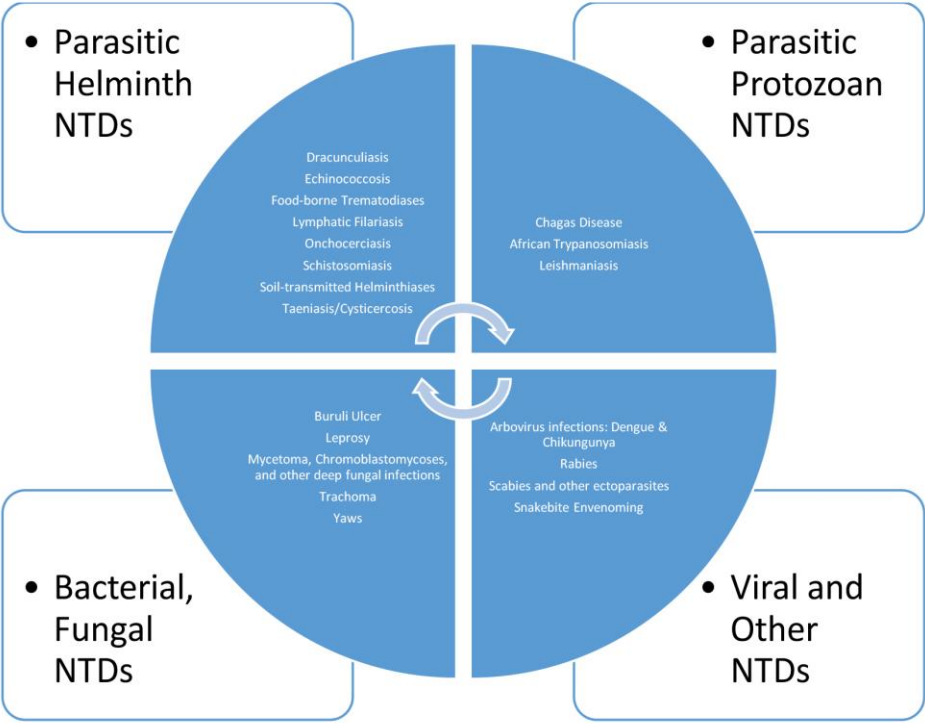


Figure SI1. Classification of NTDs according to the WHO. Retrieved from ⁴¹

Home

The RDF graph schema

SPARQL queries examples

Write and run your SPARQL query

Code availability

The code for this project is available under the [MIT License](#) in this [GitHub repo](#). If you use or modify the source code of this project, please provide the proper attributions for this work.

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About this app

Welcome!

Look at the RDF graph schema and some SPARQL queries examples, or write and run your own queries

Made with Streamlit

Figure SI2. Homepage of the NTDs2RDF web application.

Home

The RDF graph schema

SPARQL queries examples

Write and run your SPARQL query

Enter your SPARQL query and press Ctrl+Enter

Simple example of SPARQL query

Clear input

If there is an input or syntax error, you should go first to the Home page to load the data and the queries.

Home

The RDF graph schema

SPARQL queries examples

Write and run your SPARQL query

Enter your SPARQL query and press Ctrl+Enter

List 5 gene IDs and names from the NTDs knowledge graph
PREFIX biolink: <https://w3id.org/biolink/vocab/>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>

SELECT ?gene ?genename
WHERE {
 ?gene a biolink:Gene;
}

Simple example of SPARQL query

Clear input

If there is an input or syntax error, you should go first to the Home page to load the data and the queries.

Code availability

The code for this project is available under the [MIT license](#) in this [Github repo](#). If you use or modify the source code of this project, please provide the proper attributions for this work.

NTDs2RDF: A heterogeneous and integrated knowledge graph for the exploration of neglected tropical diseases

Enter your SPARQL query or look at some examples in the sidebar

NTDs2RDF: A heterogeneous and integrated knowledge graph for the exploration of neglected tropical diseases

	gene	genename
0	https://bioregistry.io/ncbigene:10000	AKT3
1	https://bioregistry.io/ncbigene:10333	TLR6
2	https://bioregistry.io/ncbigene:10454	TAB1
3	https://bioregistry.io/ncbigene:107	ADCY1
4	https://bioregistry.io/ncbigene:1147	CHUK

Show query

List 5 gene IDs and names from the NTDs knowledge graph
PREFIX biolink: <https://w3id.org/biolink/vocab/>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>

SELECT ?gene ?genename
WHERE {
 ?gene a biolink:Gene;
 rdfs:label ?genename;
}
LIMIT 5

Figure SI3. Query interface page of the NTDs2RDF web application.

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