

Wikidata to build 5-star Linked Open biological databases: A case study of PanglaoDB

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Abstract

[PanglaoDB](#) is a database of cell type markers widely used for single cell RNA sequencing data analysis. The genes, tissues, organs and cell types mentioned in the database, however, are described by free text and lack identifiers. [Wikidata](#), is a freely editable knowledge graph database useful for the integration of biomedical knowledge. Its linked data model can improve significantly the handling and distribution of scientific information.

In this study we explore the feasibility of enriching PanglaoDB with Wikidata identifiers. We accessed the state of reconciliation at the beginning of the project, comparing the modelling of genes, tissues, organs and cell types on Wikidata. Taking advantage of the openness of Wikidata, we leveraged our initial analysis to contribute towards Wikidata completeness and enable full reconciliation. As a final product, we released the first SPARQL endpoint for cell marker information, in a 5-star open linked data format. We hope that this study encourages further reconciliations of databases to Wikidata.

Keywords: wikidata, knowledge graph, cell type, ontology.

Introduction

PanglaoDB

PanglaoDB [1] [2] is a publically-available database that contains data and metadata on hundreds of single-cell RNA sequencing experiments. It provides extensive information on cell types, genes and tissues, as well as manually and community curated cell type markers (Tables 1 and 2). It also displays a rich web user interface for easy data acquisition, including database dumps for bulk downloads.

Table 1: Database statistics for each species in PanglaoDB, as of 31st of August, 2020.

	Mus musculus	Homo sapiens
Samples	1063	305
Tissues	184	74
Cells	4,459,768	1,126,580
Cell Clusters	8,651	1,748

Table 2: Metadata statistics for PanglaoDB, gathered from their [last update on August, 2019](#).

	Number
Cell types	215 (uniquely named)
Tissues	240 (+6 germ layers)
Organs	29
Species	2 (Homo sapiens and Mus musculus)
Genes	110292

As of 30 December 2020, the article describing PanglaoDB has been cited 88 times. Despite its use by the the community, the database is on a 3-star category for Linked Open Data [3] as it does not use the semantic open standards from W3C (RDF and SPARQL) needed for a 4-star rank, neither the links to external data via common identifiers that makes datasets 5-star. Improving the data format toward

W3C's gold standards is a valuable step in making biological knowledge FAIR (Findable, Accessible, Interoperable and Reusable).

The OBO Foundry provides a rich collection of linked biological identifiers [4]. However, reconciliation to OBO is challenging, as there are many ontologies, each with slightly different contribution guidelines. For that reason, we decided to reconcile PanglaoDB to Wikidata, which allows simple creation of new terms, provided they follow Wikidata's notability criteria [5].

Wikidata

Wikidata [6] is an open, freely editable, knowledge graph database within the semantic web [7] that stores knowledge across a multitude of domains, such as arts, history, chemistry and biology, using an item-property-value linked data model (Figure 1). It is easy to use and edit, by both humans and machines, with a rich web user interface and wrapper packages available in common programming languages such as R and Python. All the data within Wikidata is linked and inherently public domain, thus, it presents a great opportunity to make scientific data more FAIR (Findable, accessible, interoperable and reusable), as well as provides the necessary tools to curate and develop ontologies.

hepatocyte (Q827450) Item Identifier

Item Label
liver cell type
Hepatocyte | hepatocytes

[edit](#)

▼ In more languages
[Configure](#)

Language	Label	Description	Alternative labels
English	hepatocyte	liver cell type	Hepatocyte hepatocytes
Portuguese	Hepatócito	tipo celular	
German	Hepatozyt	Hauptzelltyp der Leber	Hepatocyt Leberepithelzelle Hepatozyten Leberzelle
Italian	Epatocito	No description defined	Epatociti Epatocita

[All entered languages](#)

Statements

Statement
instance of Property
cell type Value
▼ 0 references
+ add reference
+ add value

Figure 1: Wikidata item example, showing item hepatocyte (Q827450), the labels change according to the user's language, but each item has a universal identifier, called QID.

Several advances towards biological data integration and biological data analysis in Wikidata have been made before, yielding positive results [8] [9] and showcasing its potential for bioinformatics-related analyses, such as drug repurposing and ID conversion [10]. Wikidata has been proposed as a unified base to gather and distribute biomedical knowledge, with more than 50 000 human gene items indexed and hundreds of biomedical-related properties [11].

Wikidata is nevertheless a collaborative database, and content is available on different levels of quality. For example, as of August 2020, cell type information was still very lacking, with only 264 items

being categorized as “instances of cell types (Q189118)” (<https://w.wiki/b2w>), while other projects describe over 2.000 cell types [12, 13]. Of those 264 items, only 9 have a “Cell Ontology ID” [14] (P7963) associated, and most have a varying amount of statements (Table 3). As an additional problem, there are also 23 items being categorized as “instances of cell (Q7868)” (<https://w.wiki/b2x>), an imprecision, as an instance of cell would be an individual named cell from a single named individual.

Table 3: As of August 2020, Wikidata items regarding cell types have a varying amount of information, with most having very few statements.

Cell type Item	Number of statements
red blood cell (Q37187)	48
myocyte (Q428914)	18
mesenchymal cell (Q66568500)	2

This study was motivated by the increasing importance of cell-type concepts in light of the Human Cell Atlas [15], and the utter need for improved interoperability of biological data. We aimed, thus, at providing a case study of the re-release PanglaoDB in a 5-star Linked Open Data Format while improving the modelling of the necessary concepts on Wikidata.

Methodology

Data acquisition

Gene data from Wikidata was acquired using the Wikidata Query Service [16] - <https://w.wiki/bWc> for *Homo sapiens* genes and <https://w.wiki/bWe> for *Mus musculus* genes.

Data for quality assessment from PanglaoDB was acquired through their metadata database dump repository [17].

The markers dataset was downloaded manually from PanglaoDB’s website (https://panglaoDB.se/markers/PanglaoDB_markers_27_Mar_2020.tsv.gz). It contains 15 columns and 8256 rows.

For the reconciliation, only the columns `species`, `official gene symbol` and `cell type` were used.

All data used was handled using the Pandas [18] library, with the Seaborn [19] and Matplotlib [20] libraries being used for plotting.

Automated matching

The metadata from PanglaoDB on cell types, tissues (including germ layers) and organs was matched to Wikidata items using the reconciler [21] library with the Wikidata Reconciliation Service [22], tools that operate under the W3C Reconciliation Service specification [23].

Further matching was done using a custom stemming function on the item labels, via PorterStemmer from the NLTK library [24].

Matches were considered perfect if the reconciliation service or the stemming function returned a value of “match” equals to “True”. Matches were manually analysed for false matches, such as items with same labels but used for different concepts.

Gene data was matched manually using a Pandas [18] inner merge, since both data sources contained identifiers, which should be the same.

Item quality assessment

Wikidata items were assessed for their quality by their number of statements, which were acquired using a custom wrapper on the MediaWiki API [25] and, in the case of gene data, via Wikidata's own query service, as stated in the Data acquisition section.

Furthermore, items were also assessed by the presence of external identifiers - all of which are Wikidata properties:

- Ensembl Gene [26] (P594) and Entrez Gene [27] (P351) IDs for genes,
- Cell Ontology [14] (P7963) IDs for cell types
- Uberon [28] (P1554) IDs for organs and tissues.

Class creation on Wikidata

Classes corresponding to species-neutral classes were retrieved from Wikidata manually using Wikidata's Graphical User Interface. The dictionary matching terms in PanglaoDB to Wikidata identifiers were stored in a [reference csv table](#).

Cell types which were not represented on Wikidata were added to the database via the graphical user interface (<https://www.wikidata.org/wiki/Special:NewItem>) and logged in the reference table.

Species-specific cell types for human and mouse cell types were created for every entry in the reference table, connected to the species-neutral concept via a "[subclass of](#)" property (e.g. every single "[human neutrophil](#)" is also "[neutrophil](#)"). Our approach was analogous to the one taken by the CELDA ontology to create species-specific cell-types, with the difference that they used the `rdfs:subClassOf` class to denote the subclass relationship [29].

The reference sheet for species-neutral concepts was used to obtain the "subclass of" for every newly created item. Each item was labeled either "human" + the label for the neutral cell type, described as "cell type found in Homo sapiens" and tagged with the statement "[found in taxon](#)" *Homo sapiens*. An analogous framework was used for mouse cell types, assuming that mouse in PanglaoDB meant *Mus musculus*. Batch creations were added to Wikidata via the tool Quickstatements (<https://quickstatements.toolforge.org/#/>).

All genes in PanglaoDB either were already present on Wikidata or resolved to multiple entities and thus were excluded.

Property creation on Wikidata

Properties on Wikidata need to be supported by the users in a public forum before creation. To represent the cell-type marker relation, we proposed a property called `has marker` to the Wikidata community.

We posted a message in 17th of November presenting the property, domain and range constraints, as well as additional comments.

The proposal was accompanied by the following motivation statement:

"Even though the concept of a marker gene/protein is not clear cut, it is very important, and widely used in databases and scientific articles.

This property will help us to represent that a gene/protein has been reported as a marker by a credible source, and should always contain a reference.

Some markers are reported as proteins and some as genes. Some genes don't encode proteins, and some protein markers are actually protein complexes.

The property would be inclusive to these slightly different markers. Some cell types are marked by absence of expression of genes/proteins/protein expression. As these seem to be less common than positive markers (no organized databases, for example) they are left outside the value range for this property"

The proposal contained specifications of the property such as:

- Description:
 - "a gene or a protein published as a marker of a species-specific cell type"
- Data type:
 - [Item](#) (internal entities in Wikidata)
- Domain:
 - ?subject [instance of \(P31\)](#) [cell type \(Q189118\)](#)
- Allowed values:
 - {?object [instance of \(P31\)](#) [protein \(Q8054\)](#) .}
 - UNION {?object [instance of \(P31\)](#) [gene \(Q7187\)](#) .}
 - UNION {?object [instance of \(P31\)](#) [macromolecular complex \(Q22325163\)](#) .}
- Planned use:
 - Reconcile knowledge from the PanglaoDB marker database to Wikidata. In the future, expand to other trusted sources of cell type marker information.

More details can be in the archived Wikidata:Property proposal page (https://www.wikidata.org/wiki/Wikidata:Property_proposal/has_positive_marker).

Integration to Wikidata

The reconciled dataset was uploaded to Wikidata via the WikidataIntegrator python package [30], a wrapper for the Wikidata Application Programming Interface. The details of the integration can be seen in the accompanying Jupyter notebook.

Access to reconciled data

Wikidata dumps

Wikidata provides regular dumps in a variety of formats, including RDF dumps: https://www.wikidata.org/wiki/Wikidata:Database_download. It is possible to also download partial dumps of the database with reduced size (ex: <https://wdumps.toolforge.org/dump/987> for all cell types with the `has_marker` property).

SPARQL queries

Besides the Wikidata Dumps, Wikidata provides an SPARQL endpoint with a Graphical User Interface (<https://query.wikidata.org/>). Updated data was immediately accessible via this endpoint, enabling integrative queries integrated with other database statements.

Results

Wikidata reconciliation - initial look

Entities from PanglaoDB, that is, cell types, genes, tissue types and organs, were matched with Wikidata items, matching summary can be seen on Table 4.

Table 4: Summary of the matched entities from PanglaoDB.

	# of total items	# of unique matches	% of total items that were matched
Cells	215	81	37.67%
Tissues	246	85	34.55%
Organs	29	22	75.86%
Human Genes	58216	35423	60.84%
Mouse Genes	53793	25124	46.70%

Analysis of item quality - initial look

Only *Homo sapiens* genes and Organs reconciled more than 50%. In the case of genes, this is probably due to the Gene Wiki initiative [31], a long-running project to improve biological information in Wikipedia and its sister-projects, including Wikidata.

This is further illustrated by Figure 3, in which we can see that all *Mus musculus* gene items - and nearly all *Homo sapiens* items - analysed had the Entrez ID alternative identifier present. Most of the data from the Gene Wiki project came from NCBI, creator and maintainer of Entrez. Nevertheless, there are still many gene items without an “Ensembl Gene ID” property, showcasing the need for further work in migrating this important source of information.

In the case of Organ data, there was a high number of matches both due to the fact that there were only a few number of items, but also since most Organ entities have Wikipedia pages, that are, therefore, cross-linked using Wikidata, requiring the creation of these items.

Regarding alternative identifiers, what was observed for genes cannot be said for histological entities. While there is significant progress in integrating UBERON IDs, there is near to no items with a Cell Ontology ID property (Figure 2).

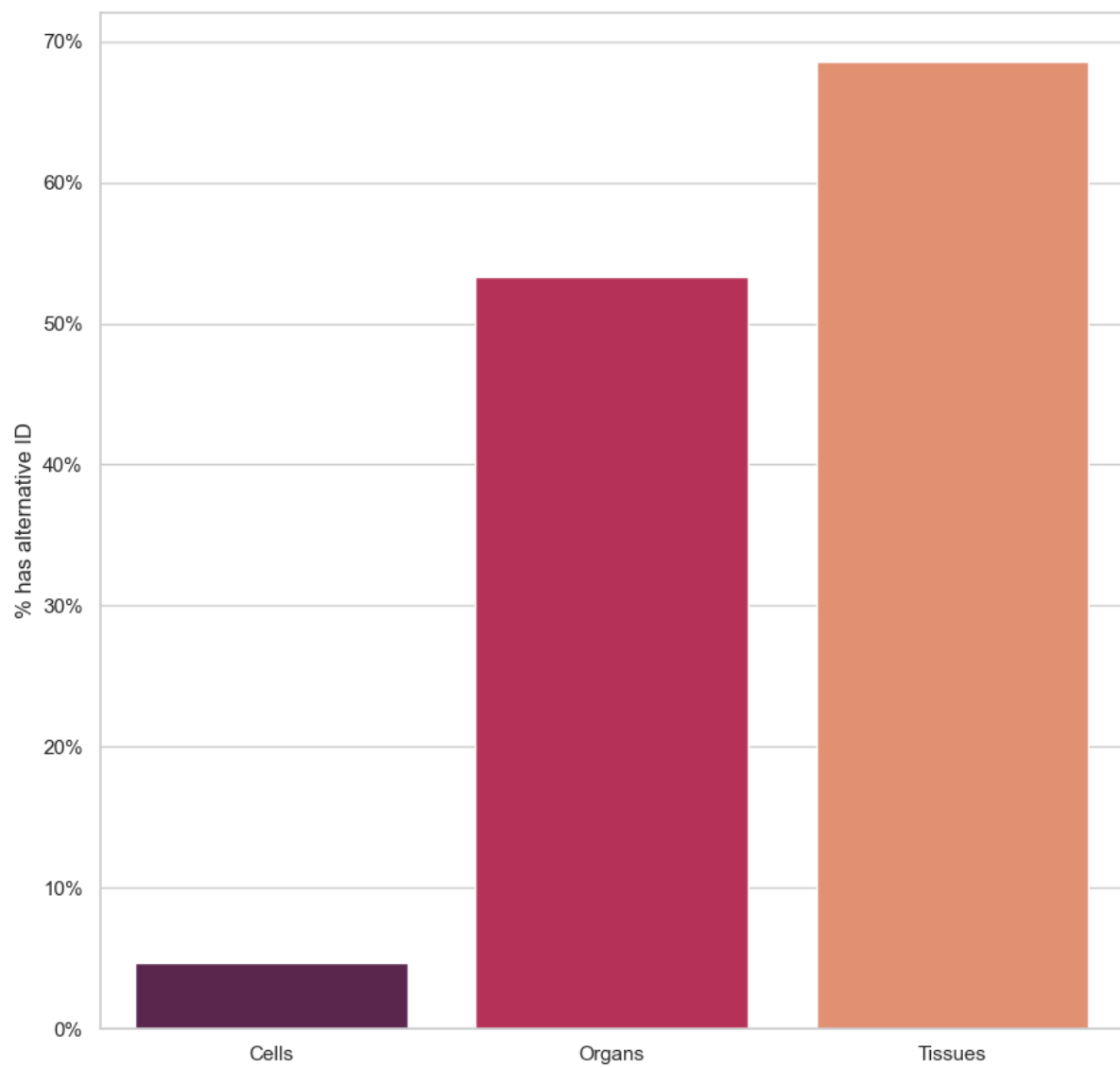


Figure 2: Percentage of matched histological items that had alternative identifiers, UBERON IDs for Tissues and Organs, Cell Ontology IDs for Cell types.

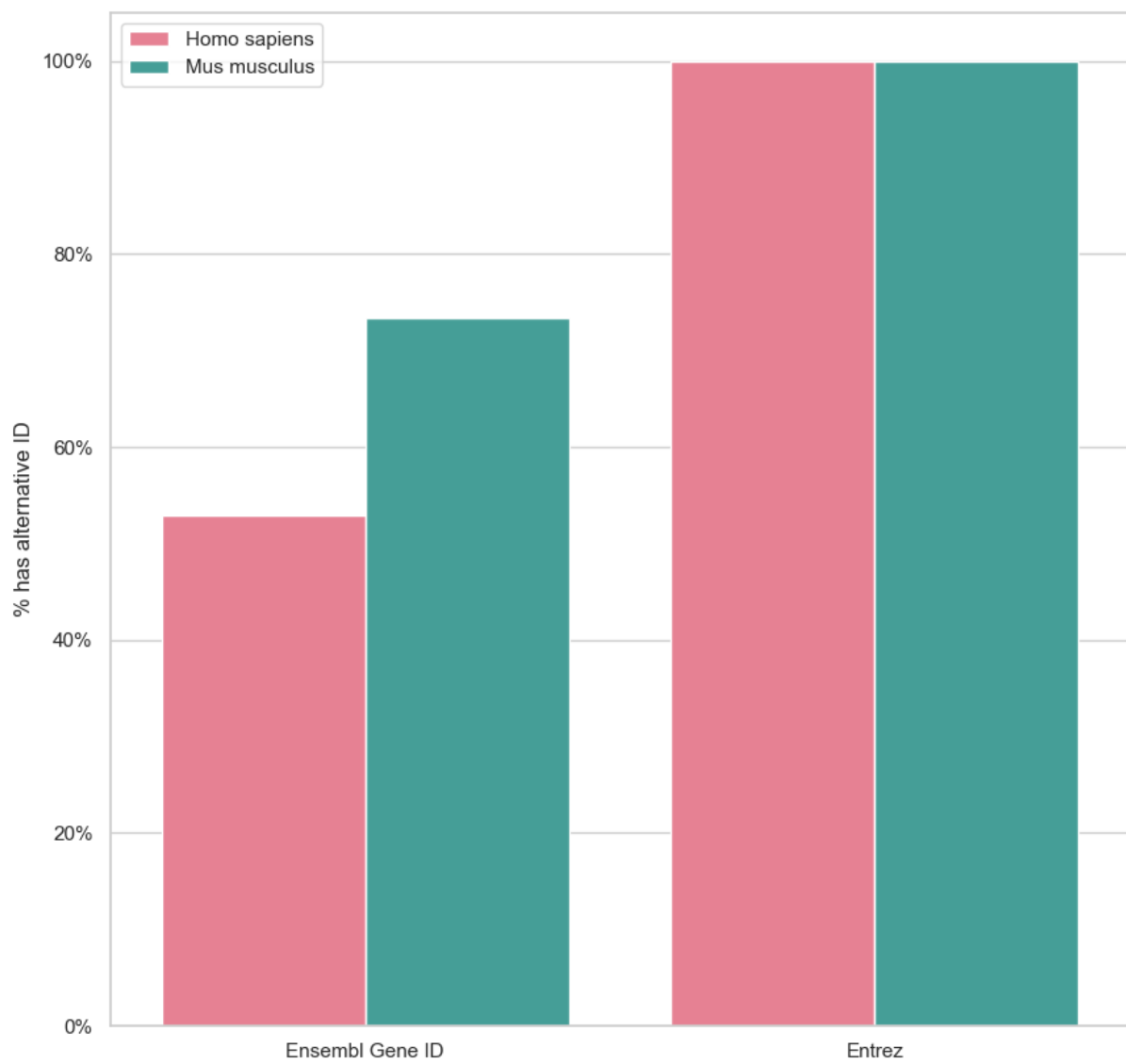


Figure 3: Percentage of matched gene items that had alternative identifiers, Entrez ID and Ensembl Gene ID, divided by species.

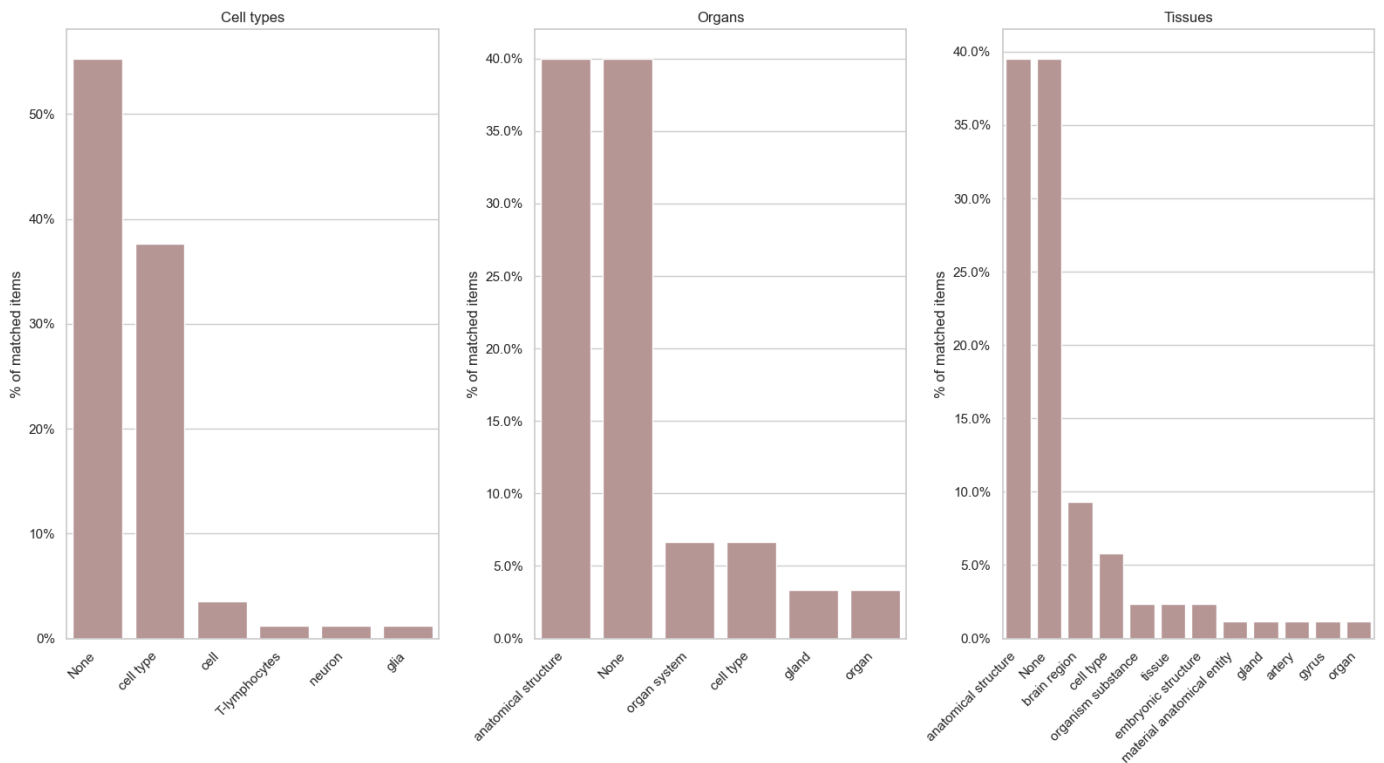


Figure 4: Percentage of reconciled entities, divided by which item type they belong to. Most reconciled items don't count with the P31 property.

A significant proportion of the matches we could acquire for histological data didn't contain in their data model an "instance of" (P31) property, this illustrates an extremely concerning fact: Although we could still match around 30 percent of the data - in the case of Cell types and Tissues - this data was probably "low-quality", that is, hard to find and even harder to obtain insights from, we can affirm this since the P31 property is the basis for most items in Wikidata, it's the most intuitive way to perform queries against their database and to annotate their items.

Furthermore, there is a significant disparity between histological data and gene data: while we could only match around 37% of Cell types from PanglaoDB, and of those 55% didn't have P31, we matched 60% of *Homo sapiens* genes, and all of them had P31. This disparity is not clearly shown when looking exclusively at the number of statements for these items (Figures 5 and 6), but it shows there is still a great amount of missing information for biological data, in particular in regards to cell types.

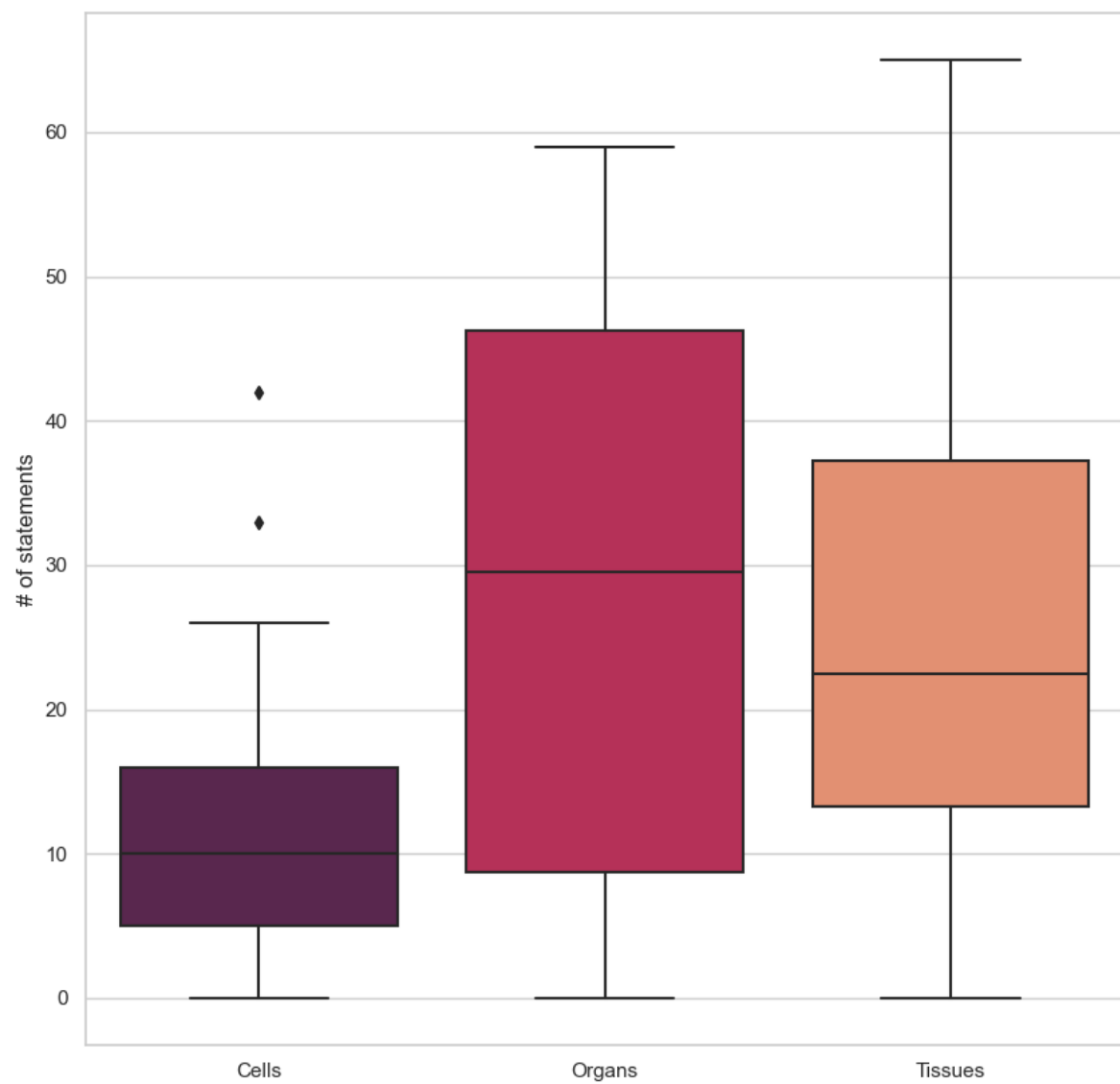


Figure 5: The distribution of the number of statements of the matched histological entities. Cell types performed the lowest.

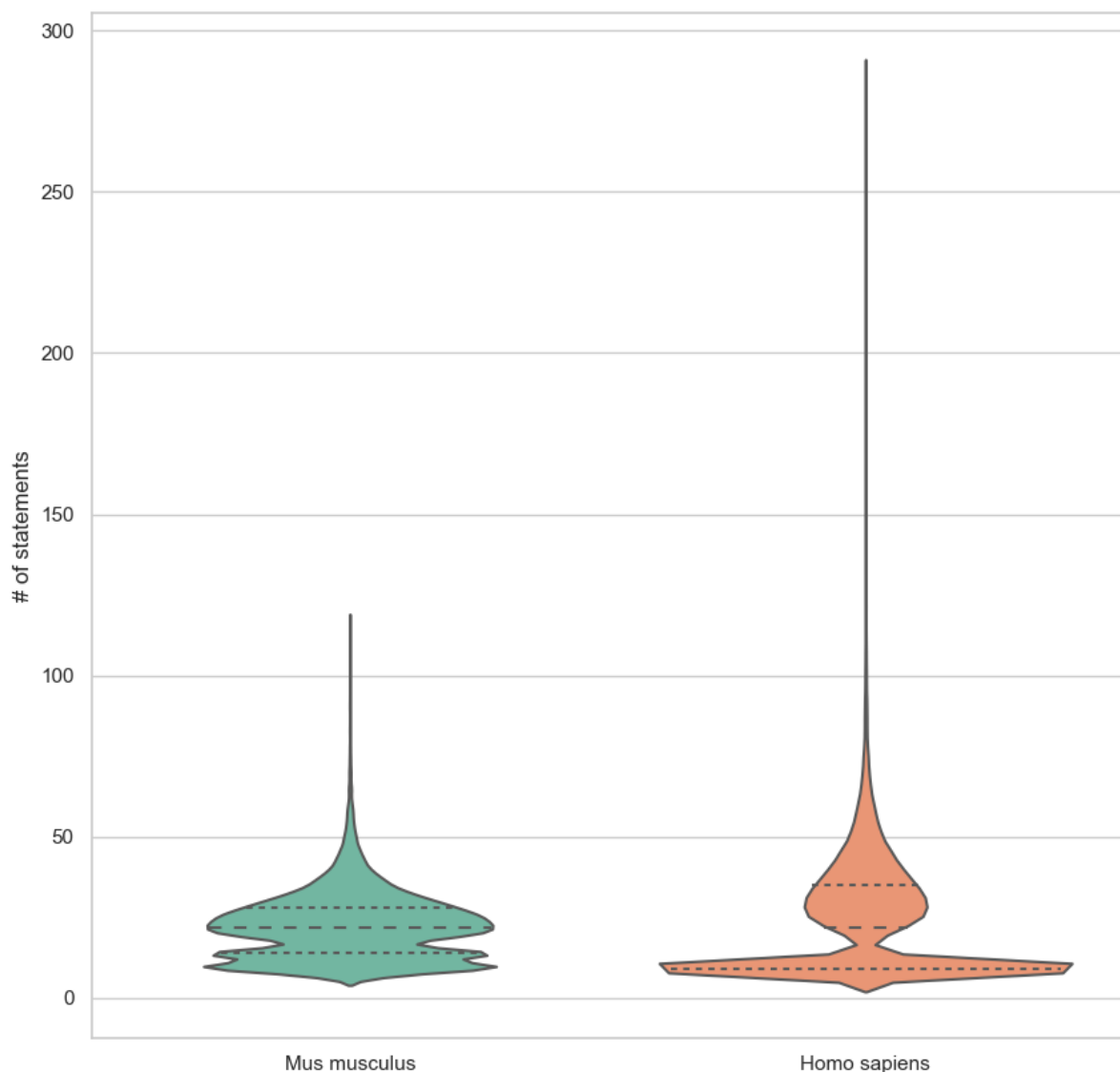


Figure 6: The distribution of the number of statements for matched gene items, divided by species.

Improving Wikidata

As described in the methods session, we added species-specific terms to Wikidata for cell types of *Homo sapiens* and *Mus musculus* described in the PanglaoDB database. The use of species-specific cell-types is necessary because genes in Wikidata are also species-specific, connected to taxon by the ["found in taxon"](#)

Adding a new property

Adding missing items

- TBD

Improving interoperability

- TBD

Wikidata reconciliation - final look

After the aforementioned improvements were made, data from PanglaoDB was reconciled once again, the automatic classification method was able to detect most cell types matches for most cell types on PanglaoDB matches (Table 5). The non-unique matches are likely due to synonym or very similar aliases used for different cell type concepts. Nevertheless, it is an evidence that our work improved cell type content on Wikidata, and will arguably facilitate the reconciliation of other cell-type related resources.

Table 5: Summary of matched PanglaoDB entities after improvements were made.

	# of total items	# of unique matches	% of total items that were matched
Cells	215	173	80.4651
Tissues	246	63	25.6097
Organs	29	18	62.0689
Human Genes	58216	35423	60.8475
Mouse Genes	53793	25124	46.705

Noticeably, the proportion of automatic matches for other entity types (tissues and organs) seems reduced in relation to the first assessment (35% to 25% and 76 to 62%). These entities were not targeted by our work, but as Wikidata is a living resource, modifications in the database, such as reclassification of entities or adding of other similar concepts, may have reduced the performance of our simple reconciler.

Analysis of item quality - final look

As can be gathered from Figure 7, nearly all cell type items have the appropriate “instance of cell type” statement, with only 4 items still missing said statement and one item being classified as an “instance of gland”.

This is a considerable advance in improving the quality of cell type data in Wikidata, as having this simple statement will make these items easier to find and be expanded upon.

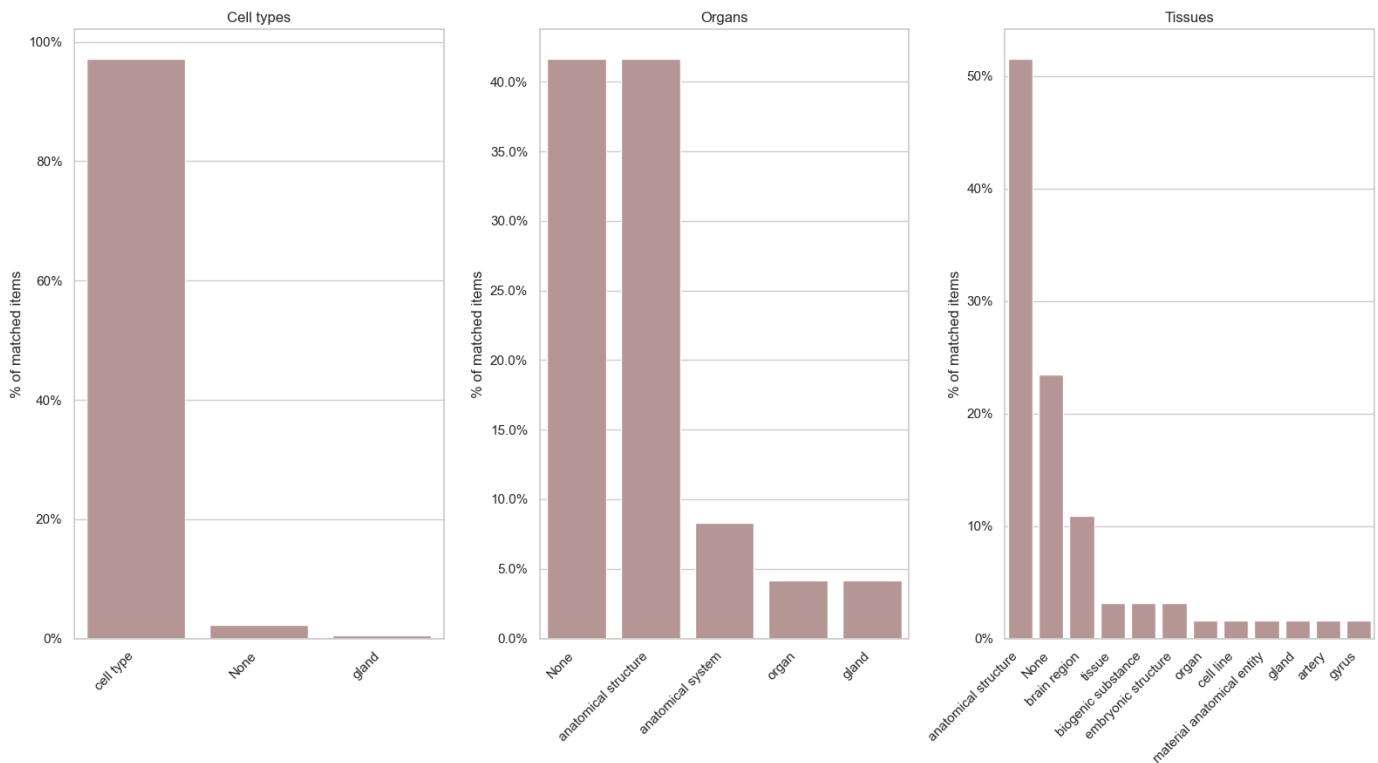


Figure 7: Percentage of reconciled entities gathered during the second and final reconciliation, divided by which item type they belong to.

Wikidata SPARQL queries enabled by the integration

Now that the PanglaoDB is released as Linked Open Data, we can make queries that were not possible before, including federated queries with other biological databases, such as Uniprot [32] and Wikipathways [33]. Due to previous similar reconciliation projects, Wikidata already contains information about genes, including their relations to Gene Ontology (GO) terms, something that led to the development of an R package, go2cell [34], that facilitates interconnection between cell types and GO terms via their markers.

PanglaoDB's integration to the Wikidata ecosystem allows us to ask a variety of questions. The next section headers exemplify such questions.

“Which human cell types are related to neurogenesis via their markers?”

As expected, the query below retrieved a series of neuron types, such as “[human purkinje neuron](#)” and “[human cajal-retzius cell](#).” It did, however, also retrieved non-neural cell types such as the “[human loop of henle cell](#),” a kidney cell type, and “[human osteoblast](#).” These seemingly unrelated cell types markedly express genes that are involved in neurogenesis, but that does not mean that they are involved with this process. This reinforces the idea that one needs to be careful when using curated pathways to enrich one's analysis, as false positives abound.

The molecular process that gene products take part depends on the cell type. The SPARQL query below enables us to seamlessly compare Gene Ontology processes with cell marker data, providing a fruitful sandbox for generation of hypothesis and exploration of the biomedical knowledge landscape.

Query for cell types related to neurogenesis

geneLabel	cellTypeLabel
EPHB1	human oligodendrocyte
EPHB1	human osteoclast
OMP	human purkinje neuron
OMP	human olfactory epithelial cell
OMP	human neuron
PCSK9	human delta cell
PCSK9	human loop of Henle cell
CXCR4	human b cell
CXCR4	human nk cell
CXCR4	human dendritic cell
CXCR4	human megakaryocyte
CXCR4	human t helper cell

Wikidata Query Service
(<https://query.wikidata.org/#SELECT%20%3FgeneLabel%20%3FcellTypeLabel%0AWHERE%20%0A%7B%0A%20%20%3Fprot>)

“Which cell types express markers associated to Parkinson`s disease?”

Besides integration with Gene Ontology, Wikidata reconciliation makes it possible to complement the marker gene info on PanglaoDB with information about diseases. This integration is of biomedical interest, as there is a quest for detailing of mechanisms that link genetic associations and the diseases themselves.

“Disease genes” are often compiled from Genomic Wide Association Studies, which look for sequence variation in the DNA. These studies are commonly blind to the cell types related to the pathophysiology of the disease. In the query below, we can see cell types that are marked by genes genetically associated with Parkinson’s disease. Even considering the false positives (as per the previously mentioned multifunctional nature of genes) this kind of overlook can aid domain experts to come up with novel hypothesis.

Query for cell types related to Parkinson’s disease

Wikidata Query Service (<https://query.wikidata.org/#SELECT%20%3FcellTypeLabel%20%3FdiseaseLabel%20%0A%28COL%3E%20%20gene%0A%20%20%3Fdisease%20wdt%3AP2293%20%3FdiseaseGene%20.%20%20%20%20%20%20%20%20%20%3E%20gene%0A%20%20%20%20%20wd%3AQ101405087%20rdfs%3Alabel%20%3FcellTypeLabel%20.%20%0A%20%20%20%3Fdi>)

It is important to note that not all data on PanglaoDB was added to Wikidata. Fine-grained, database-specific details were too granular for a general-purpose database like Wikidata (e.g. the sensitivity and specificity attached to each marker-cell type pair). Eventhough, these data could be released in RDF format and be connected to independent SPARQL endpoints (as done in the Bio2RDF effort [35]), we focused on integration to Wikidata to take advantage of the built-in integration with various types of knowledge, as well as the tooling developed by the Wikidata community.

/// Add discussions about multispecies / "species-neutral" genes and how biomedical science often uses those

Linking biological with Wikidata allows out-of-the-box integrative SPARQL queries, as many biomedical ontologies and datasets have been already integrated to Wikidata, and are available in Wikidata's

graph. Besides the well-known advantages of having data linked to the Linked Open Data cloud, the Wikidata integration provides user-friendly interfaces for the data. That includes both navigable html pages of classes and properties (e.g. <https://www.wikidata.org/wiki/Q67801129>) as well as an SPARQL Query Service with user-friendly modifications to ease queries for beginners (<https://query.wikidata.org/>) with helper pages for learning SPARQL (https://www.wikidata.org/wiki/Wikidata:SPARQL_tutorial) or even requesting queries (https://www.wikidata.org/wiki/Wikidata:Request_a_query).

Wikidata also makes it easy for users to contribute. Wikidata allows editions directly in the Graphical User Interface, accessible for domain experts without programming or ontology training. In fact, Wikidata may be the solution for an (at least) 7 year-old gap of an “community-based crowd-sourcing approach” for representing knowledge about cell types. [36] For those interested in continuous integration, the Python module Wikidata Integrator facilitates for python users to reconcile databases to Wikidata, and it has been used to build bots for several different biological databases [9].

/// Why Wikidata integration is different from Bio2RDF? What are the cons? Maybe mention Wikidata as an easy-to-use middleground that does not require *that* much domain expertise about the complicated world of semantic technologies, formal description logic and even computer science in general.

This work exemplifies the power of releasing Linked Open Data via Wikidata, and provides the biomedical community with the first semantically accessible, 5-star LOD dataset of cell markers. It also paves the way for Wikidata reconciling of other databases for cell-type markers, such as CellMarker [37], labome [38], CellFinder [12] and SHOGoin/CELLPEDIA [39]). The approach can in essence be applied to any knowledge set of public interest, providing a low-cost and low-barrier platform for sharing biocurated knowledge in gold standard format. We hope that community will keep improving marker and overall biological content on Wikidata, and that the interlinked marker information will be useful for researchers all over the world.

General Ideas

Temporary file containing ideas for the project. Interesting references and concepts.

med2rdf[40] is a project to migrate biomedical knowledge bases to RDF format, facilitating integration with the semantic web.

15 years ago, in the original Cell Ontology paper, they mention the idea to integrate their knowledge with gene expression databases, something not done as far as we know [41]

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