A protocol for adding knowledge to Wikidata, a case report.

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Abstract

Pandemics, even more than other medical problems, require swift integration of knowledge. When caused by a new virus, understanding the underlying biology may help finding solutions. In a setting where there are a large number of loosely related projects and initiatives, we need common ground, also known as a "commons". Wikidata, a public knowledge graph aligned with Wikipedia, is such a commons and uses unique identifiers to link knowledge in other knowledge bases However, Wikidata may not always have the right schema for the urgent questions. In this paper, we address this problem by showing how a data schema required for the

integration can be modelled with entity schemas represented by Shape Expressions. As a telling example, we describe the process of aligning resources on the genomes and proteomes of the SARS-CoV-2 virus and related viruses as well as how Shape Expressions can be defined for Wikidata to model the knowledge, helping others studying the SARS-CoV-2 pandemic. How this model can be used to make data between various resources interoperable, is demonstrated by integrating data from NCBI Taxonomy, NCBI Genes, UniProt, and WikiPathways. Based on that model, a set of automated applications or bots were written for regular updates of these sources in Wikidata and added to a platform for automatically running these updates. Although this workflow is developed and applied in the context of the COVID-19 pandemic, to demonstrate its broader applicability it was also applied to other human coronaviruses (MERS, SARS, Human Coronavirus NL63, Human coronavirus 229E, Human coronavirus HKU1, Human coronavirus OC4).

Introduction

The COVID-19 pandemic, caused by the SARS-CoV-2 virus, is leading to a burst of swiftly released scientific publications on the matter (1). In response to the pandemic, many research groups have started projects to understand the SARS-CoV-2 virus life cycle and to find solutions. Examples of the numerous projects include outbreak.info (2), VODAN around FAIR data (3), CORD-19-on-FHIR (4) and the COVID-19 Disease Map (5). Many research papers and preprints get published every week and many call for more Open Science (6). The Dutch universities went a step further and want to make any previously published research openly available, in whatever way related to COVID-19 research (7).

However, this swift release of research findings comes with an increased number of incorrect interpretations (8) which can be problematic when new research articles are picked up by main-stream media (9). Rapid evaluation of these new research findings and integration with existing resources requires frictionless access to the underlying research data upon which the findings are based. This requires interoperable data and sophisticated integration of these resources. Part of this integration is reconciliation, which is the process where matching concepts in Wikidata are sought. Is a particular gene or protein already described in Wikidata? Using a shared interoperability layer, like Wikidata, different resources can be more easily linked.

The Gene Wiki project has been linking the different research silos on genetics, biological processes, related diseases and associated drugs (10), creating a brokerage system between the research silos. The project recognises Wikidata as a sustainable infrastructure for scientific knowledge in the life sciences.

In contrast to legacy databases, where data models follow a relational data schema of connected tables, Wikidata (<u>https://wikidata.org/</u>) uses statements to store facts (see Figure 1) (10–13). This model of statements aligns well with the RDF triple model of the semantic web and the content of Wikidata is also serialized as Resource Description Framework (RDF) triples (14,15), acting as a stepping stone

for data resources to the semantic web. Through its SPARQL endpoint (<u>https://query.wikidata.org</u>), knowledge captured in Wikidata can be integrated with other nodes in the semantic web, using mappings between these resources or through federated SPARQL queries (16).



Figure 1: Structure of a Wikidata item, containing a set of statements which are key-value pairs, with qualifiers and references. Here the item for the ACE2 protein is given containing a statement about its molecular function. This molecular function (peptidyl-dipeptidase activity) contains a reference stating when and where this information was obtained.

The Gene Wiki project aligns novel primary data sources with Wikidata in a cycle of consecutive steps where the data schema of the primary source is aligned with the available Wikidata properties. Once the schema is in place, bots are developed to add and regularly update Wikidata with knowledge from the primary resource under scrutiny.

Automated editing of Wikidata simplifies the process, however, the quality control must be monitored carefully. This requires a clear data schema that allows the various resources to be linked together with their provenance. This schema describes the key concepts required for the integrations of the resources we are interested in the NCBI Taxonomy (17), NCBI Gene (18), UniProt (19), the Protein Data Bank (PDB) (20), WikiPathways (21), and PubMed (22). Therefore, the key elements for which we need a model include viruses, virus strains, virus genes, and virus proteins. The first two provide the link to taxonomies, the models for genes and proteins link to UniProt, PDB, and WikiPathways. These key concepts are also required to annotate research output such as journal articles and datasets related to these topics. Wikidata calls such keywords 'main subjects'. The introduction of this model and the actual SARS-CoV-2 genes and proteins in Wikidata enables the integration of these resources.

This paper is a case report of a workflow/protocol for data integration and publication. The first step in this approach is to develop the data schema. Within Wikidata, Shape Expressions (ShEx) are used as the structural schema language to describe and capture schemas of concepts (23,24). With ShEx we describe the RDF structure by which Wikidata content is made available. These Shapes have the advantage that they are easily exchanged and describe linked data models as a single knowledge graph. Since the Shapes describe the model, they enable discussion, revealing inconsistencies between resources and allow for consistency checks of the content added by automated procedures.

With the model defined, the focus can turn to the process of adding knowledge to Wikidata. In this phase, the seven human coronaviruses (HCoVs), MERS, SARS, SARS-CoV-2 (causing COVID-19), Human Coronavirus NL63, Human coronavirus 229E, Human coronavirus HKU1, and Human coronavirus OC4 (25), can be added to Wikidata. This protocol is finalized by describing how the resulting data schema and data can be applied to support other projects, particularly the WikiPathways COVID Portal.

The Semantic Web was proposed as a vision of the Web, in which information is given well-defined meaning and better enabling computers and people to work in cooperation (26). In order to achieve that goal, several technologies have appeared, like RDF for describing resources (15), SPARQL to query RDF data (27) and the Web Ontology Language (OWL) to represent ontologies (28).

Linked data was later proposed as a set of best practices to share and reuse data on the web (29). The linked data principles can be summarized in four rules that promote the use of uniform resource identifiers (URIs) to name things, which can be looked up to retrieve useful information for humans and for machines using RDF, as well as having links to related resources. These principles have been adopted by several projects, enabling a web of reusable data, known as the linked data cloud (https://lod-cloud.net/), which has also been applied to life science (30).

One prominent project is Wikidata, which has become one of the largest collections of open data on the web (16). Wikidata follows the linked data principles offering both HTML and RDF views of every item with their corresponding links to related items, and a SPARQL endpoint called the Wikidata Query Service.

Wikidata's RDF model offers a reification mechanism which enables the representation of information about statements like qualifiers and references (see also <u>https://www.wikidata.org/wiki/Help:Statements</u>). For each statement in Wikidata, there is a direct property in the wdt namespace that indicates the direct value. In addition, the Wikidata data model adds other statements for reification purposes that allow enrichment of the declarations with references and qualifiers (for a topical treatise, see Ref. (31)). As an example, item <u>Q14875321</u>, which represents ACE2 (protein-coding gene in the *Homo sapiens* species) has a statement specifying that it has a chromosome (<u>P1057</u>) with value chromosome X (<u>Q29867336</u>). In RDF Turtle, this can be declared as:

wd:Q14875321 wdt:P1057 wd:Q29867336

That statement can be reified to add qualifiers and references. For example, a qualifier can state that the genomic assembly (<u>P659</u>) is GRCh38 (<u>Q20966585</u>) with a reference declaring that it was stated (<u>P248</u>) in Ensembl Release 99 (<u>Q83867711</u>). In Turtle, those declarations are represented as (see also Figure 2):

```
wd:Q14875321 rdfs:label "ACE2"@en ;
wdt:P1057 wd:Q29867336 .
wd:Q14875321 p:P1057 [
ps:P1057 wd:Q29867336 ;
```

```
pq:P659 wd:Q20966585 ;
prov:wasDerivedFrom [
    pr:P248 wd:Q83867711
] ] .
wd:Q29867336 rdfs:label "human X chromosome" .
wd:Q20966585 rdfs:label "Genome assembly GRCh38" .
wd:Q83867711 rdfs:label "ensembl Release 99" .
```





Methods

Specifying data models with ShEx

Although the RDF data model is flexible, specifying an agreed structure for the data allows domain experts to identify the properties and structure of their data facilitating the integration between heterogeneous data sources. Shape Expressions were used to provide a suitable level of abstraction. YaShE, <u>http://www.weso.es/YASHE/</u>, a ShEx editor implemented in JavaScript, was applied to author these Shapes (33). This application provides the means to associate labels in the natural language of Wikidata to the corresponding identifiers. The initial entity schema was defined with YaShE as a proof of concept for virus genes and proteins. In parallel, statements already available in Wikidata were used to automatically generate an initial shape for virus strains with sheXer (34). The statements for virus strains were retrieved with SPARQL from the Wikidata Query Service (WDQS). The generated Shape was then

further improved through manual curation. The syntax of the Shape Expressions was continuously validated through YaShE and the Wikidata Entity Schema namespace was used to share and collaboratively update the schema with new properties. Figure 3 gives a visual outline of these steps.



Figure 3: Flow diagram for entity schema development and the executable workflow for the virus gene protein bot. A) The workflow of creating shape expressions. B) The computational workflow of how information was used from various public resources to populate Wikidata.

Populating Wikidata with Human Coronavirus Data

The second step in our workflow is to add entries for all virus strains, genes and their gene products to Wikidata. This information is spread over different resources. Here, annotations were obtained from NCBI EUtils (35), Mygene.info (36), and UniProt, as outlined below. Input to the workflow is the NCBI Taxonomy identifier of a virus under scrutiny. (*e.g.* 2697049 for SARS-CoV-2). The taxon annotations are extracted from NCBI EUtils. The gene and gene product annotations are extracted from

mygene.info and the protein annotations are extracted from UniProt using the SPARQL endpoint at (<u>https://spargl.uniprot.org/</u>).

Genomic information from seven human coronaviruses (HCoVs) was collected, including the NCBI Taxonomy identifiers. For six virus strains, a reference genome was available and was used to populate Wikidata. For SARS-CoV-1, the NCBI Taxonomy identifier referred to various strains, though no reference strain was available. To overcome this issue, the species taxon for SARS-related coronaviruses (SARSr-CoV) was used instead, following the practices of NCBI Genes and UniProt.

```
{
    " id": "43740571",
    " score": 15.594226,
    "accession": {
        "genomic": [
            "MN908947.3",
            "NC 045512.2"
        ],
        "protein": [
            "QHD43419.1",
            "YP 009724393.1"
        1
    },
    "entrezgene": "43740571",
    "locus tag": "GU280 gp05",
    "name": "membrane glycoprotein",
    "other_names": "membrane glycoprotein",
    "refseq": {
        "genomic": "NC_045512.2",
        "protein": "YP 009724393.1"
    },
    "retired": 43560233,
    "symbol": "M",
    "taxid": 2697049,
    "type_of_gene": "protein-coding"
}
```

Figure 4: JavaScript Object notation output of the mygene,info output for gene with NCBI gene identifier 43740571.

NCBI Eutils

The Entrez Programming Utilities (EUtils) is the application programming interface (API) to the Entrez query and database system at the National Center for Biotechnology Information (NCBI). From this set of services the scientific name of the virus under scrutiny was extracted (e.g. "Severe acute respiratory syndrome coronavirus 2").

Mygene.info

Mygene.info is a web service which provides a REST API that can be used to obtain up-to-data gene annotations. The first step in the process is to get a list of applicable genes for a given virus by providing the NCBI taxon id. The following step is to obtain gene annotations for the individual genes from mygene.info through http://mygene.info/v3/gene/43740571. This results in the name and a set of applicable identifiers (Figure 4).

```
PREFIX uniprotkb: <http://purl.uniprot.org/uniprot/>
PREFIX rdfs: <http://www.w3.org/2000/01/rdf-schema#>
SELECT ?id ?label ?database
WHERE {
SERVICE <https://sparql.uniprot.org/sparql> {
    VALUES ?database {
        <http://purl.uniprot.org/database/PDB>
        <http://purl.uniprot.org/database/RefSeq>
        }
    uniprotkb:uniprotID rdfs:label ?label ;
        rdfs:seeAlso ?id .
    }
}
```

Figure 5: The UniProt SPARQL query used to obtain additional protein annotations, descriptions and external resources.

UniProt

The annotations retrieved from mygene.info also contain protein identifiers such as UniProt, RefSeq and PDB, however, their respective names are lacking. To obtain names and mappings to other protein identifiers, RefSeq and UniProt were consulted. Refseq annotations were acquired using the earlier mentioned NCBI EUtils. UniProt identifiers are acquired using the SPARQL endpoint of UniProt, which is a rich resource for protein annotations provided by the Swiss Bioinformatics Institute. Figure 5 shows the SPARQL query that was applied to acquire the protein annotations.

Reconciliation with Wikidata

Before the aggregated information on viruses, genes and proteins can be added to Wikidata, reconciliation with Wikidata is necessary. If Wikidata items exist they are updated, otherwise, new items are created. Reconciliation is driven by mapping existing identifiers in both the primary resources and Wikidata. It is possible to reconcile based on strings, but this is dangerous due to the ambiguity of the labels used (37). When items on concepts are added to Wikidata that lack identifiers overlapping with the primary resource, reconciliation is challenging. Based on the Shape Expressions, the following properties are identified for use in reconciliation. For Proteins these are Uniprot ID (P352) and RefSeq protein ID (P637). For genes these are NCBI Gene ID (P351) and Ensembl Gene (ID) P594. When sourced information matches none of these properties, then a new item is created, if the concepts from the primary source reconcile with Wikidata items these are updated. Wikidataintegrator

Wikidata integrator is a Python library (<u>https://github.com/SuLab/WikidataIntegrator</u>) that wraps around the Wikidata API (<u>https://www.wikidata.org/w/api.php</u>) (10). From external resources such as the NCBI, gene and taxonomy statements have been compiled with provenance and assigned to the associated Wikidata items. When an item did not exist (or was not recognized), it was created. The module compiled a list of statements by parsing the primary sources under scrutiny and extracted what

statements already existed on Wikidata. A JavaScript Object Notation (JSON) string was created that resembled the JSON data model used by the Wikidata API. This JSON string was then submitted to the Wikidata API for ingestion.

Data Integration Use Cases / Validation

WikiPathways and BridgeDb

WikiPathways is a biological pathway database and can visualize the details of interactions between genes, proteins, metabolites, and other entities participating in biological processes. It depends on BridgeDb to map identifiers of external data and knowledge to the identifiers used for the genes, proteins, and metabolites in the pathways (38). Furthermore, mappings to Wikidata are required to establish the link of biological entities in pathways and journal articles that have those entities as main topics. Therefore, the virus genes and proteins are required to exist in Wikidata, enabling the interoperability between WikiPathways and Wikidata. Additionally, new virus mapping databases for BridgeDb are created by extracting the new virus gene and protein data, including links between Wikidata, NCBI Gene, RefSeq, UniProt and Guide Target to Pharmacology identifiers using а SPARQL querv (https://github.com/bridgedb/Wikidata2Bridgedb). The mapping databases will be updated regularly and will allow pathway curators to annotate virus genes and proteins in their pathways and provide link outs on the WikiPathways website.

The COVID-19 related pathways from <u>WikiPathways COVID-19 Portal</u> are added to Wikidata using the approach previously described (10). For this, a dedicated repository has been set up to hold the GPML files, the internal WikiPathways file format, The GPML is converted into RDF files with the WikiPathways RDF generator (39), while the files with author information are manually edited. For getting the most recent GPML files, a custom Bash script was developed (<u>getPathways.sh</u> in the <u>SARS-CoV-2-WikiPathways repository</u>). The conversion of the GPML to RDF uses the previously published tools for WikiPathways RDF (39). Here, we adapted the code with a unit test that takes the pathways identifier as parameter . This test is available in the SARS-CoV-2-WikiPathways branch of <u>GPML2RDF</u> along with a helper script (<u>createTurtle.sh</u>). Based on this earlier generated pathway RDF and

using the Wikidataintegrator library, the WikiPathways bot was used to populate Wikidata with additional statements and items. The pathway bot was extended with the capability to link virus proteins to the corresponding pathways, which was essential to support the Wikidata resource. These changes can be found in the *sars-cov-2-wikipathways-2* branch.

Scholia

The second use case is to demonstrate how we can link virus gene and protein information to literature. Here, we used Scholia (<u>https://scholia.toolforge.org/</u>) as a central tool (13). It provides a graphical interface around data in Wikidata, for example, literature about a specific coronavirus protein (e.g. Q87917585 for the SARS-CoV-2 spike protein). Scholia uses SPARQL queries to provide information about topics. We annotated literature around the HCoVs with the specific virus strains, the virus genes, and the virus proteins as 'main topic'.



Figure 6: Overview of the ShEx schemas and the relations between them. All shapes, properties and items are available from within Wikidata.

Results

Semantic data landscape

To align the different sources in Wikidata, a common data schema is needed. We have created a collection of schemas that represent the structure of the items added to Wikidata. Input to the workflow is the NCBI taxon identifier, which is input to mygene.info (see Figure 3). Taxon information is obtained and added to Wikidata according to a set of linked Entity Schemas (E170: virus, E174: strain, E69: disease). Gene annotations are obtained and added to Wikidata following the Schemas (E165: virus gene, E169: virus protein) and protein annotations are obtained and added to Wikidata following the and added to Wikidata following the schemas are an extension from more generic schemas for proteins (E167) and genes (E75).

Bots

The bots developed and used in this protocol are adaptations of the bots developed in the Gene Wiki project. On regular intervals, the bots run to update viral gene and protein annotations as well as pathway updates from WikiPathways. For the gene and protein annotations, we have also made a Jupyter Notebook. The bot that synchronizes virus, gene and protein information and the Jupyter Notebook are available at https://github.com/SuLab/Gene_Wiki_SARS-CoV. The bot that synchronizes the WikiPathways pathways with Wikidata was updated from the original version to allow adding proteins annotated with Wikidata identifiers and no longer requires pathways to be part of the WikiPathways *Curated Collection*. The customized bot source code is available at

https://github.com/SuLab/scheduled-bots/blob/SARS-CoV-2/scheduled_bots/wikipat hways/bot.py.

Both bots are now part of the automation server used in the Gene Wiki project. This runs on the Jenkins platform (40). Although Jenkins is mainly aimed at software deployments, its extended scheduling capabilities the synchronization procedure at set intervals that can be changed depending on the update speed of the external resources. The Jenkins jobs are available from <u>http://jenkins.sulab.org/</u>.

Data added

Using the gene and proteins bots explained in the Methods section, missing genes and proteins have been added for the seven human coronaviruses. The results are summarized in Table 1. The automatically added and updated gene and protein items were manually curated. For SARS-CoV-2 all items were already manually created, and the bot only edited gene items. Thirteen out of 27 protein entries were created by the authors and saw edits, up to May 23, by up to five other Wikidata editors including two bots (Krbot and Edoderoobot). For the other species, all gene entries and most protein entries have been created by the bot. Only for MERS and SARS-CoV-2 some protein entries were added manually, including some by us. During this effort, which took three weeks, the bot created a number of duplicates. These have been manually corrected. It should also be noted that for SARS-CoV-2 many proteins and protein fragments.

Table 1: Summary of the seven human coronaviruses, including taxon identifiers, the Wikidata items, and the number of genes and proteins. The latter two are generated by the SPARQL queries geneCount.rq and proteinCount.rq in the supporting information.

Virus strain	NCBI Taxon ID Wikidata Qid		# Genes	# Proteins
SARS-virus	694009	Q278567	14	11
Middle East respiratory syndrome coronavirus	1335626	Q4902157	11	9
Human Coronavirus NL63	277944	Q8351095	7	6
Human coronavirus 229E	11137	Q16983356	8	8
Human coronavirus HKU1	290028	Q16983360	9	9
Human coronavirus OC43	31631	Q16991954	9	8
SARS-CoV-2	2697049	Q82069695	11	27

Use Cases

BridgeDb

Using the dedicated code to create a BridgeDb identifier mapping database for coronaviruses, mappings were extracted from Wikidata with a SPARQL guery for the seven human coronaviruses and the SARS-related viruses. This resulted in a mapping database with 554 mappings between 368 identifiers (version 2020-05-27). This includes 170 Wikidata identifiers, 70 NCBI Gene identifiers, 60 UniProt identifiers, 58 RefSeq identifiers and 10 Guide to Pharmacology Target identifiers. The mapping file has been released on the BridgeDb website (https://bridgedb.github.io/data/gene_database/) and archived on Zenodo (41). The mapping database has also been loaded on the BridgeDb webservice at http://webservice.bridgedb.org/ which means it can be used in the next use case: providing links out for WikiPathways.

WikiPathways

The WikiPathways project is involved in an international collaboration to curate knowledge about the biological processes around SARS-CoV-2 and COVID-19. The authors have started pathway specifically about SARS-CoV-2 а (wikipathways:WP4846). To ensure interoperability, WikiPathways uses BridgeDb and taking advantage of the enriched BridgeDb webservice, WikiPathways now links out for HCoV genes and proteins (depending on availability of mappings) to RefSef, NCBI Gene, UniProt, and Scholia (see Figure 7). The latter links to the next use case, and provides a link to literature about the virus. It should be noted that for each gene and protein two Wikidata identifiers with links may be given. In that case, one is for the gene and one for the protein.



Figure 7: Screenshot of SARS-CoV-2 and COVID-19 Pathway in WikiPathways (<u>wikipathways:WP4846</u>) showing the BridgeDb popup box for the ORF3a protein, showing a link out to Scholia via the protein and gene's Wikidata identifiers.

Scholia

The WikiPathways use case shows us that literature describes our knowledge about how coronaviruses work at a rather detailed level. Indeed, many articles discuss the genetics, homology of genes and proteins across viruses, or the molecular aspects of how these proteins are created and how they interfere with the biology of the human cell. The biological pathways show these processes, but ultimately the knowledge comes from literature. Wikidata allows us to link literature to specific virus proteins and genes, depending on what the article describes. For this it uses the 'main subject' property (P921). We manually annotated literature with the Wikidata items for specific proteins and genes. We developed two SPARQL gueries to count links (https://w.wiki/Lsp) the number of between genes and proteins (https://w.wiki/Lsg) and the articles that discuss them. Scholia takes advantage of the 'main subject' annotation, allowing the creation of "topic" pages for each protein. For example, Figure 8 shows the topic page of the SARS-CoV-2 spike protein.

topic	ve glycoprotein (Q8791758	Award Topic • Tools • Help • Search 5)
Rece	ently published works on the topic	(MRSS)
Show 10	entries	Search:
Date	Work	Topics
2020-	Structure, Function, and Antigenicity of the SARS-CoV-2 Spike	structural biology // SARS-CoV-2 // spike glycoprotein
03-01	Glycoprotein	
2020-	Potent binding of 2019 novel coronavirus spike protein by a	monoclonal antibody // SARS-CoV-2 // SARS-CoV // spike glycoprotein
02-01	SARS coronavirus-specific human monoclonal antibody	
2020-	Uncanny similarity of unique inserts in the 2019-nCoV spike	HIV // sequence analysis // comparative biology // 2019–20 COVID-19
01-31	protein to HIV-1 gp120 and Gag	pandemic // SARS-CoV-2 // spike glycoprotein
2020-	Homologous recombination within the spike glycoprotein of the	glycoprotein // Bungarus multicinctus // homologous recombination //
01-22	newly identified coronavirus may boost cross-species	Chinese cobra // cross-species transmission // 2019-20 COVID-19 pandemic
	transmission from snake to human	// SARS-CoV-2 // spike glycoprotein

Figure 8: Screenshot of the Scholia page for the SARS-CoV-2 spike glycoprotein, it shows four articles that specifically discuss this protein.

Discussion

This paper describes a protocol we developed to align genetic annotations from reference resources with Wikidata. Numerous annotations are scattered across different sources without any overall integration, thereby reducing the reusability of knowledge from different sources. Integration of the annotations from these resources is a complex and time consuming task. Each resource uses different ways to access the data from a user and machine perspective. Making use of these protocols programmatically to access and retrieve data of interest, requires the knowledge of various technologies and procedures to extract the information of interest.

Wikidata provides a solution. It is part of the semantic web, taking advantage of its reification of the Wikidata items as RDF. Data in Wikidata itself is frequently, often almost instantaneously, synchronized with the RDF resource and available through its SPARQL endpoint (<u>http://query.wikidata.org</u>). The modelling process turns out to be an important aspect of this protocol. Wikidata contains numerous entity classes as entities and more than 7000 properties which are ready for (re-)use. However, that also means that this is a confusing landscape to navigate. The ShEx Schema

has helped us develop a clear model. This is a social contract between the authors of this paper, as well as documentation for future users.

Using these schemas, it was simpler to validate the correctness of the updated bots to enter data in Wikidata. The bots have been transferred to the Gene Wiki Jenkins platform. This allows the bots to be kept running regularly, pending on the ongoing efforts of the coronavirus and COVID-19 research communities. While the work of the bots will continue to need human oversight, potentially to correct errors, it provides a level of scalability and generally alleviates the authors from a lot of repetitive work.

One of the risks of using bots, is the possible generation of duplicate items. Though this is also a risk in manual addition of items, humans can apply a wider range of academic knowledge to resolve these issues. Indeed, in running the bots, duplicate Wikidata items were created, for which an example is shown in Figure 9. The Wikidataintegrator library does have functionality to prevent the creation of duplicates by comparing properties, based on used database identifiers. However, if two items have been created using different identifiers, these cannot be easily identified.

Close inspection of examples, such as the one in Figure 9, showed that the duplicates were created because there was a lack of overlap between the data to be added and the existing item. The UniProt identifier did not yet resolve, because it was manually extracted from information in the March 27 pre-release (but now part of the regular releases). In this example, the Pfam protein families database (42) identifier was the only identifier upon which reconciliation could happen. However, that identifier pointed to a webpage that did not contain mappings to other identifiers. In addition, the lack of references to the primary source hampers the curator's ability to merge duplicate items and expert knowledge was essential to identify the duplication. Fortunately, names used for these RNA viruses only refer to one protein as the membrane protein. Generally, the curator would have to revert to the primary literature to identify the overlap. Statements about 'encoded by' to the protein coding genes were found to be helpful as well. Reconciliation might be possible through sequence alignment, which means substantial expert knowledge and skills are required.

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And iteration A matrix for the first second of the	nembrane prote	in (Q88656821)				WIKIDATA	membrane gl	ycoprotein (Q892605	153)	
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	In more languages					Community portal	Configure			
mo	anguago Label		Description	Also known as		Create a new item Create a new Leverne				Also known as
Na	inglish membrane	protein	protein of SARS-CoV-2	M protein Membrane glycoprotein		Rendom item				
	No label de	fined	No description defined			Nearby	French No			
And and a mathematical properties of the second of the								label defined Ew	el8 in SARS-CoV-2	
Automation in the second of	erman No label de	Ined	No description defined				All entered languages			
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Figure 9: Comparison of two Wikidata entries for the SARS-CoV-2 membrane protein. An overlap between a Wikidata item and a concept from a primary source needs to have some overlap to allow automatic reconciliation. If there is no overlap, duplicates will be created and left for human inspection. Since this screenshot was made, the entries have been merged in a manually curation process.

This makes reconciliation in Wikidata based on matching labels, descriptions and matching statements and captured provenance (qualifiers and synonyms, references) hazardous, due to different meanings to the same label. A targeted curation query (geneAndProteinCurationQuery.rg, see Supporting Information) was developed to highlight such duplications and manually curated seven duplicate protein entries for SARS-CoV-2 alone. This duplication is common and to be expected, particularly in rapidly evolving situations like a pandemic, when many groups contribute to the same effort. In this case, this paper only represents one contributing Wikidata:WikiProject COVID-19 group to the (https://www.wikidata.org/wiki/Wikidata:WikiProject_COVID-19).

We also discovered that virus taxonomy is different from zoological taxonomy. For example, there is no clear NCBI taxon identifier for SARS-CoV-1 and after

consultation with other projects, we defaulted to using the taxon identifier for the SARS-related CoVs, something that NCBI and UniProt seem to have done as well. Finally, we note that during the two weeks this effort took place, several other resources introduced overviews, including dedicated COVID-19 portals from UniProt (https://covid-19.uniprot.org/) and the Protein DataBank in Europe (https://PDBe.org/covid19/).

Conclusion

This manuscript presents a protocol to link information from disparate resources, including NCBI Taxonomy, NCBI Gene, UniProt, PubMed, and WikiPathways. Using the existing Wikidata infrastructure, we developed semantic schemas for virus strains, genes, and proteins; bots written in Python to add knowledge on genes and proteins of the seven human coronaviruses and linked them to biological pathways in WikiPathways and to primary literature, visualized in Scholia. We were able to do so in the period of two weeks, using an ad-hoc team from existing collaborations, taking advantage of the open nature of the components involved.

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Author contributions

AW, EW, JK, conceptual design, code development and wrote the manuscript. MK, wrote the manuscript. JL, Software, Visualization, Writing - review and editing. DF, minor review, code support with shexer. QG: virus-taxonomy review, Writing - review and editing. PS, LM: review and editing. All authors read and approved the final manuscript.

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Supporting Information

geneAndProteinCurationQuery.rq

```
SELECT DISTINCT ?route ?gene ?geneLabel ?ncbi ?protein ?proteinLabel
?refseq ?uniprot WHERE {
 VALUES ?virus {
    wd:Q82069695 # SARS-CoV-2
  }
  {
    # genes
    ?wdRoot wdt:P703 ?virus ; wdt:P31 wd:Q7187 .
    OPTIONAL { ?wdRoot wdt:P351 ?ncbi }
    OPTIONAL {
      ?wdRoot wdt:P688 | ^wdt:P702 ?protein .
      OPTIONAL { ?protein wdt:P637 ?refseq }
      OPTIONAL { ?protein wdt:P352 ?uniprot }
    }
    BIND ("via gene" AS ?route)
    BIND (?wdRoot AS ?gene)
  }
  UNION
  {
    # proteins
    ?wdRoot wdt:P703 ?virus ; wdt:P31 wd:Q8054 .
    OPTIONAL {
      ?gene wdt:P688 | ^wdt:P702 ?wdRoot
      OPTIONAL { ?gene wdt:P351 ?ncbi }
    }
    OPTIONAL { ?wdRoot wdt:P637 ?refseq }
    OPTIONAL { ?wdRoot wdt:P352 ?uniprot }
    BIND ("via protein" AS ?route)
    BIND (?wdRoot AS ?protein)
  }
  SERVICE wikibase:label { bd:serviceParam wikibase:language
"[AUTO LANGUAGE], en". }
} ORDER BY ?ncbi ?wikidata
```

Gene counts for selected viruses: geneCount.rq

```
SELECT ?virus ?virusLabel (COUNT(DISTINCT ?item) AS ?genes ) WHERE {
```

```
VALUES ?virus {
    wd:Q82069695 # SARS-CoV-2
    wd:Q16983360 # HKU1
    wd:Q16991954 # OC43
    wd:Q8351095 # NL63
    wd:Q16983356 # 229E
    wd:Q4902157 # MERS-CoV
    wd:Q278567 # SARS-CoV
    }
    ?item wdt:P31 wd:Q7187 ;
        wdt:P703 ?virus .
SERVICE wikibase:label { bd:serviceParam wikibase:language
    "[AUTO_LANGUAGE],en". }
}
GROUP BY ?virus ?virusLabel
```

Protein counts for selected viruses: proteinCount.rq

```
SELECT ?virus ?virusLabel (COUNT(DISTINCT ?item) AS ?protein ) WHERE {
    VALUES ?virus {
    wd:Q82069695 # SARS-CoV-2
    wd:016983360 # HKU1
    wd:Q16991954 # 0C43
    wd:Q8351095 # NL63
    wd:Q16983356 # 229E
    wd:Q4902157 # MERS-CoV
    wd:Q278567 # SARS-CoV
  }
   ?item wdt:P31 wd:Q8054 ;
         wdt:P703 ?virus .
SERVICE wikibase:label { bd:serviceParam wikibase:language
"[AUTO LANGUAGE], en". }
}
GROUP BY ?virus ?virusLabel
```