SARS-CoV-2 Drug Resistance Database

April 8, 2021 Version 1.0

Descriptions of tables

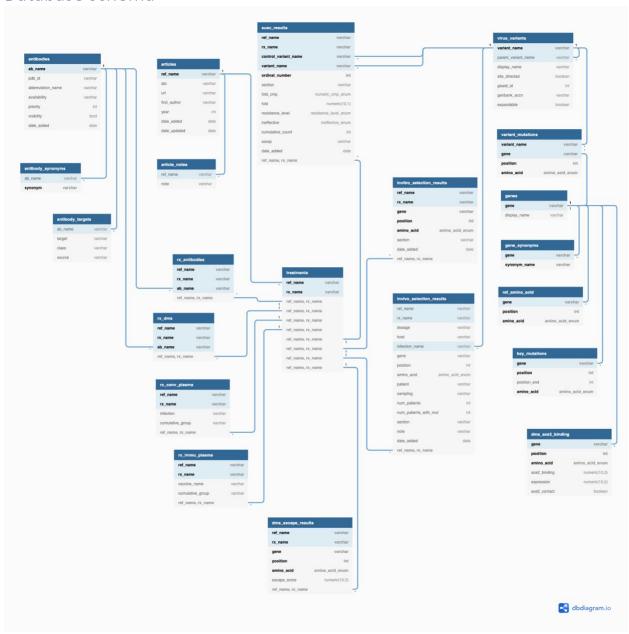
The main goals of this database are to capture the following data:

- I. The neutralizing susceptibility of varaints to (1) monoclonal antibodies (mAbs); (2) convalescent plasma(CP); and (3) plasma from vaccinated persons(VP).
- II. The spike mutations selected in vitro by mAbs and convalescent plasma, and in vivo by mAbs.

The main tables include:

- I. The **articles** table contains data about each reference.
- II. The **virus_variants** table contains a list of variants, including individual mutations, combinations of mutations, and named variants (i.e., a variant of concern or variant of interest).
- III. The **variant_mutations** table links mutations to variants.
- IV. The treatments table contains unique pairs of studies and treatments and which functions as a parent table to data about mAbs (rx_antibodies), convalescent plasma (rx_conv_plasma), and plasma from vaccinated persons (rx_immu_plasma). The rx_ tables contain information about mAbs, convalescent plasma, and plasma from vaccinated persons.
- V. The tables **antibodies**, **antibody_synonyms**, and **antibody_targets** contain data about each mAb.
- VI. The **susc_results** table contains neutralization data linking a virus variant and treatment.
- VII. The **invitro_selection_results** and **invivo_selection_results** tables contain mutations associated with a treatment.

Database schema



Footnote: For each rectangle, text on darkblue background is the table name, texts in bold style are primary keys. Table relationships are represented by texts on lightblue background and blue linkage lines. If the foreign key contains one field, the linkage line is linked between corresponding fields on each table. If the foreign key contains multiple lines, combination of fields is shown at the bottom of the table (fields are separated by comma) and linked to corresponding combination of fields of another table. "*" means many. You can see high resolution here.

Entity tables

| Table name | Table definition | Field name | Field definition | |
|-----------------|---|-----------------------|--|--|
| articles | Referernce meta info. | ref_name | Assigned name (RefID, RefName) for a reference, usually formed by the surname of first author, two-digit year and an optional alphabetical letter for distinguishing studies published in the same year. | |
| | | doi | Digital Object Identifier (DOI) of a reference. | |
| | | url | Web page of a reference, should be specified when DOI is not available. | |
| | | first_author | First author name, surname + first letters of other names. | |
| | | year | Year the reference was published. | |
| | | date_added | Date the reference added in database. | |
| | | date_updated | Date the reference updated in database. | |
| article_notes | Notes and comments of references. | ref_name | Foreign key for articles. | |
| | | note | Additional notes and comments of the reference, free text. | |
| antibodies | mAb meta info. | ab_name | Assigned mAb name. This is the most commonly recognized name. | |
| | | pdb_id | PDB ID when available. | |
| | | abbreviation_na me | mAb abbreviation. | |
| | | availabiliy | Availability of mAb, for example, EUA, Phase 3, etc. | |
| | | priority | Priority when shown in susceptibility reports. Lower number means higher priority. | |
| | | visibility | Shown in report or not. | |
| | | date_added | Date the mAb added in database. | |
| antibody_target | mAb structure | ab_name | Assigned mAb name. Foreign key for antibodies. | |
| S | and classification meta info. | target | Target sub-domain in SARS-CoV-2 spike (i.e., NTD, RBD, S1-CTD, or S2) | |
| | | class | Epitope classification of RBD-targeting mAbs (i.e., RBM class I, RBM class II, RBD-Core I, or RBD-Core II). | |
| | | source | Source of the classification. If the classification is from PDB file, source is "structure". If the classification is from the reference, source is "author". | |
| antibody_synon | Synonyms of mAb | ab_name | Assigned mAb name. Foreign key for antibodies. | |
| yms | | synonyms | mAb synonym. | |
| virus_variants | Virus variants, mutations or combination of mutations. | variant_name | Unique variant name. Allowable formats include: (i) Pango lineage plus any additional required descriptors such as a mutation; (ii) Commonly used name for a variant, such as a name assigned by the WHO or CDC; VOC name; (iii) one or more mutations | |

| | T | I | T | |
|-----------------|---|-------------------------|---|--|
| | | parent_variant_ name | (<gene_name>:<position><mutation>) separated by "+". This format is used for site-directed mutants or for viruses defined by the presence of specific mutations; (iv) another trackable name (GISAID ID, NextStrain lineage name, name used in a published reference). Parent variant name. Foreign key for virus_variants.</mutation></position></gene_name> | |
| | | display_name | Display name of variant. | |
| | | site_directed | Variant created by site-directed mutagenesis or not. | |
| | | gisaid_id | GISAID isolate accession ID without the common prefix "EPI_ISL_" (optional). | |
| | | genbank_accn | Genbank accession number (optional). | |
| | | expandable | For SARS-CoV-2 related variants, the program using this database can expand all the mutations, for non-SARS-CoV-2 coronaviruses the number of mutations is huge, the program should not expand all the mutations. (Yes/No) | |
| variant_mutatio | Mutation list of | variant_name | Foreign key for virus_variants. | |
| ns | a variant. One row represents one mutation of | gene | Foreign key for gene. | |
| | | position | Mutation position. | |
| | variant. | amino_acid | Mutation amino acid. | |
| genes | | gene | SARS-CoV-2 gene name. | |
| | | display_name | SARS-CoV-2 gene display name. | |
| gene_synonyms | | gene | Foreign key for gene. | |
| | | synonym_name | Synonym of gene. | |
| ref_amino_acid | | gene | Foreign key for gene. | |
| | | position | Gene position. | |
| | | amino_acid | Reference amino acid of reference SARS-CoV-2 genome. | |
| key_mutations | Key mutations for generating reports | gene | Foreign key for gene. | |
| | | position | Gene position. | |
| | | position_end | End of a range of positions. For insertion or deletion. | |
| | | amino_acid | Amino acid mutation. | |
| dms_ace2_bindi | Deep mutation | gene | Foreign key for gene. | |
| ng | results for all amino acid mutations | position | Gene position. | |
| | | amino_acid | Amino acid mutation. | |
| | | ace2_binding | ACE2 binding score. Minus sign means reduction of binding. | |
| | | expression | Spike protein expression score, minus means reduction of expression. | |

Treatment tables

| Table name | Table definition | Field name | Field definition |
|--------------------|--|------------------|---|
| treatments | Contains the list of distinct treatments | ref_name | Foreign key for articles. |
| | for each reference. | | The "name" of the mAb, CP, or VP used in the reference. |
| rx_antibodie s | | | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | mAb name used in the reference. Can be a single mAb or mAb combination. |
| | | ab_name | Assigned mAb name. Foreign key for antibodies. |
| rx_conv_plas ma | CP treatment meta info | ref_name | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | Description of CP used in the reference. Most commonly this is represented by "CP". But it also may be followed by additional descriptors such as the likely variant responsible for infection, the severity of infection, the time since infection, and the neutralizing antibody titer. |
| | | infection | The variant responsible for infection. When left blank it means "Unknown". |
| | | cumulative_group | Cumulative group name for aggregated samples. A group of samples from same treatment can be combined together for additional analysis. |
| rx_immu_pla sma | VP treatment meta info | ref_name | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | Description of VP including the vaccine used and any additional information such as the time since vaccination. |
| | | vaccine_name | Enumerated list of vaccines [BNT162b2, mRNA- 1273, AZD1222, NVX-CoV2373, BBIBP-CorV, CoronaVac] |
| | | cumulative_group | Cumulative group name for aggregated samples. A group of samples from same treatment can be combined together for additional analysis. |
| rx_dms | DMS treatment meta info | ref_name | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | mAb name used in the DMS reference. Can be a single mAb or mAb combination. |
| | | ab_name | Assigned mAb name. Foreign key for antibodies. |

Result tables

| Table name | Table definition | Field name | Field definition |
|--------------|-------------------------------------|--------------------------|--|
| susc_results | Susceptibility/Resistan ce results. | ref_name | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | The "name" of the mAb, CP, or VP used in the reference. |
| | | control_variant_na me | Variant used for control (i.e fold reduced susceptibility is the IC ₅₀ of the experimental variant / IC ₅₀ of the control variant). Commonly used controls including Wuhan variant, D614G, and one of the VOCs. Foreign key for virus_variants |
| | | variant_name | Variant undergoing susceptibility testsing. Foreign key for virus_variants. |
| | | ordinal_number | For CP or VP samples tested against the same variant, plasmas from the same group should have an ordinal number to distinguish the results and record in different rows. For mAb samples, the value is always 1. |
| | | section | The location in the reference containing the result (e.g. Figure 1, table 1 or page 1, para 4). |
| | | fold_cmp | "=", "~", ">", or "<", default "=", modifier of fold. |
| | | fold | Fold change compared to the control variant. This is usually based on the IC ₅₀ . It is occasionally based on a binding assay if neutralization data are not available. |
| | | resistance_level | This is for studies that do not report qualitative data. |
| | | ineffective | If the neutralizing result on the control variant or the experimental variant is below detectable threshold, this field should be used. "control": control variant neutralizing is undetectable, "experimental": experimental variant neutralizing is undetectable, "both": both of them are undetectable. |
| | | cumulative_count | For some studies, it's not possible to extract individual results but a mean or median value is available. In this case the fold field will contain the mean or median and the number of aggregated samples |

| | | | is recorded in this field. If the result |
|-------------------------|----------------------|----------------|---|
| | | | is not for aggregated data, this field |
| | | | will contain 1. |
| | | assay | Pseudovirus, live virus, or name of |
| | | , | binding assay. |
| | | date_added | Date the result added in the |
| | | _ | database. |
| invitro_selection_resul | in vitro selected | ref_name | Together with the rx_name this is a |
| ts | mutations, one row | _ | foreign key for treatments. |
| | represents one | rx_name | mAb name used in the reference. |
| | selected mutation. | | Can be a single mAb or mAb |
| | | | combination. |
| | | gene | Mutation gene. |
| | | position | Mutation position. |
| | | amino_acid | Mutation amino acid. |
| | | section | The location in the reference |
| | | | containing the result (e.g. Figure 1, |
| | | | table 1 or page 1, para 4). |
| | | date_added | Date the result added in the |
| | | | database. |
| invivo_selection_result | in vivo selected | ref_name | Together with the rx_name this is a |
| S | mutations, one row | | foreign key for treatments. |
| | represents one | rx_name | mAb name used in the reference. |
| | selected mutation. | | Can be a single mAb or mAb |
| | | dosago | combination. |
| | | dosage | Dosage used in the treatment. |
| | | host | Host of the in vivo selection |
| | | | experiment. |
| | | infection_name | Virus variant responsible for |
| | | | infection. Foreign key for |
| | | patient | virus_variants. Patient description in the reference, |
| | | patient | for example, hospitalized or |
| | | | nonhospitalized. |
| | | sampling | Sampling date after treatment or |
| | | | infection. "D" means days, "M" |
| | | | means months. |
| | | section | The location in the reference |
| | | | containing the result (e.g. Figure 1, |
| | | | table 1 or page 1, para 4). |
| | | note | Additional information from the |
| | | | reference, free text. |
| | | date_added | Date the result added in the |
| | | | database. |
| dms_escape_results | DMS results for mAbs | ref_name | Together with the rx_name this is a foreign key for treatments. |
| | | rx_name | mAb name used in the reference. |
| | | | Can be a single mAb or mAb |
| | | | combination. |
| | | gene | Spike. |
| | | | |

| position | Mutation position. |
|--------------|---|
| amino_acid | Mutation amino acid. |
| escape_score | Escape score of the DMS result. 0 means no escape, 1 means full |
| | escape. |