Supplementary figure 1 - All data from ABSD

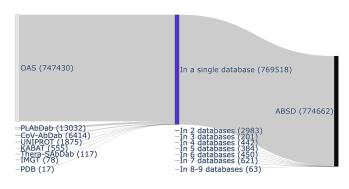


Fig. 1: Proportions of ABSD's antibody sequences in original databases. The right part represents the proportions of the whole **ABSD** dataset, extracted from given databases. The middle part represents the proportions of antibody sequences present in only one (top) or multiple (bottom) databases.

Supplementary data

Data acquisition for ABDB

Data from http://www.abybank.org/abdb/ (Download Dataset tab) can be retrieve by downloading the Complete Dataset of Redundant Antibody List (http://www.abybank.org/abdb/ Data/Redundant_files/Redundant_LH_Combined_Martin.txt).

From this file, all PDB IDs (the 4 characters preceding the _) were used to query the PDB (https://www.rcsb.org/downloads/ fasta) and all results were merged into a single FASTA file.

Data acquisition for AbPDB

From http://www.abybank.org/abpdbseq/(file abpdbseq_latest.faa), Data acquisition for PDB all PDB IDs (the 4 characters preceding the _) were used to query the PDB (https://www.rcsb.org/downloads/fasta) and all results were merged into a single FASTA file.

Data acquisition for CoV-AbDab

From https://opig.stats.ox.ac.uk/webapps/covabdab/, a csv file can be accessed from **Downloads** tab, **Database** (CSV).

Data acquisition for CoV-AbDab-PDB

From https://opig.stats.ox.ac.uk/webapps/covabdab/, a folder with PDB sequences can be accessed from **Downloads** tab, PDB Structures (.tar.gz). From this file, all PDB IDs (the 4 characters preceding the _) were used to query the PDB (https: //www.rcsb.org/downloads/fasta) and all results were merged into a single FASTA file.

Data acquisition for EBOLA

IDs were obtained from Table S7 of Supplementary Materials of Isolation of potent neutralizing antibodies from a survivor of the 2014 Ebola virus outbreak. Data were then retrieved from GeneBank (https://www.ncbi.nlm.nih.gov/genbank/).

Data acquisition for IMGT-INN

From the folder obtained at https://www.imgt.org/download/ 3Dstructure-DB/IMGT3DFlatFiles.tgz, the INN (ungzipped) files are retrieved. The PDB (ungzipped) files were used to retrieve IDs (the 4 characters preceding the _) to then query the PDB (https://www.rcsb.org/downloads/fasta) and all results were merged into a single FASTA file.

Data acquisition for IMGT

Data are obtained from https://www.imgt.org/3Dstructure-DB/ by setting **Display results** to Domains and sequence alignment and IMGT complex type (in IDENTIFICATION, in Search using IMGT-ONTOLOGY concepts) to IG/Ag. The result page is copied into a text file.

Data acquisition for IMGT2

Data are obtained from a dump of https://www.imgt.org/ 3Dstructure-DB/ by setting Display results to Domains and sequence alignment and IMGT receptor type (in **IDENTIFICATION**, in Search using IMGT-ONTOLOGY concepts) to IG. The result page is copied into a text file.

Data acquisition for KABAT

The file was obtained from http://www.abybank.org/kabat/.

Data acquisition for OAS

Files are obtained from https://opig.stats.ox.ac.uk/webapps/ oas/oas_paired/, when clicking "Search" without using any attributes, then clicking on here link.

Data acquisition for PLAbDab

Data are obtained from https://opig.stats.ox.ac.uk/webapps/ plabdab/static/downloads/paired_sequences.csv.gz.

All IDs were taken from the PDB advanced search page (https:// www.rcsb.org/search/advanced) by searching Macromolecule Name, has any of words, light heavy. All PDB IDs (the 4 characters preceding the _)) were used to query the PDB (https: //www.rcsb.org/downloads/fasta) and all results were merged into a single FASTA file.

Data acquisition for SAbDab

From https://opig.stats.ox.ac.uk/webapps/sabdab-sabpred/ sabdab/search/?all=true#downloads, the link Download the summary file (https://opig.stats.ox.ac.uk/webapps/sabdab-sabpred/ sabdab/summary/all/) was used. From this file, all PDB IDs were used to query the PDB (https://www.rcsb.org/downloads/ fasta) and all results were merged into a single FASTA file.

Data acquisition for SACS

From http://www.abybank.org/sacs/ (Download Chain List), the antibodies.txt file was retrieved. From it, all PDB IDs (the 4 characters preceding the _) were used to query the PDB (https:// www.rcsb.org/downloads/fasta) and all results were merged into a single FASTA file.

Data acquisition for TheraSAbDab

From Thera-SAbDab page https://opig.stats.ox.ac.uk/webapps/ A sabdab-sabpred/therasabdab/search/?all=true, the csv file was un downloaded (https://opig.stats.ox.ac.uk/webapps/sabdab-sabpred/static/downloads/TheraSAbDab_SeqStruc_OnlineDownload.csv).

Data acquisition for UNIPROT

A fasta file was generated from https://www.uniprot.org/ uniprotkb?query=Immunoglobulin%2C%20Antibody%2C%20IG.