Supporting Information for CoV-AbDab: the Coronavirus Antibody Database

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SI Methods & Database Contents

Where possible, the following information is documented for each entry:

1. The published name of the antibody/nanobody
2. Antigens that the antibody/nanobody has been proven to bind and/or neutralise.
3. The protein domain targeted by the antibody/nanobody (e.g. spike protein receptor binding domain)
4. The developmental origin of the antibody/nanobody (e.g. engineered/ naturally raised, species information, *etc.*)
5. Sequence information including: (a) the entire variable domain sequence for the antibody/nanobody, highlighting the CDR3 regions, and (b) V and J gene germline assignments.
6. Links to any available structures involving the antibody/nanobody
7. (If Fv/VHH sequence available) A homology model of the antibody/nanobody
8. References to the primary literature on the antibody/nanobody

9. Timestamps to show when the antibody/nanobody was added and last updated
10. Any steps we are taking to follow up on the entry (e.g. to source its sequence and/or add further metadata)

As of 5th August 2020, CoV-AbDab contains 1402 entries from 66 papers [1, 2, 4, 5, 6, 7, 8, 9, 10, 11, 12, 14, 17, 18, 19, 20, 21, 23, 24, 25, 26, 29, 30, 32, 33, 34, 35, 36, 37, 38, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 70, 71, 72, 74, 75, 76, 77, 78] and 21 patents (see **Patents**). The following reviews were helpful for tracing relevant literature [13, 16, 27, 54, 79].

Number of SARS-CoV-2 Binders: 1131
...of which neutralising: 271 [24.0%]

Number of SARS-CoV-1 Binders: 483
...of which neutralising: 95 [19.7%]

Number of MERS-CoV Binders: 147
...of which neutralising: 95 [64.6%]

CoV-AbDab already contains links to 84 relevant CoV-antibody structures across 40 distinct antibodies/nanobodies, with structures of a further 10 antibodie/nanobodies anticipated based on preprints. These solved structures indicate that many coronavirus binding antibodies use both their heavy and light chain complementarity-determining regions to engage the RBD, highlighting the importance of capturing full Fv information [3, 15, 28, 45, 55, 60, 70, 69].

Our database does not contain Next-Generation Sequencing (NGS) data from SARS-CoV-2 responding antibody repertoires (e.g. [22, 39, 49]); case studies from these papers have only been included if binding/neutralising activity has been confirmed experimentally. Processed and annotated NGS data from Nielsen *et al.* [39] is now available from our Observed Antibody Space database [31].

Patents

As of 5th August 2020, the following patents are primary sources of antibody/nanobody sequences: CN1664100, CN1903878, CN100374464, CN104447986, CN106380517, EP1857116, EP2112164, JP2018203632, KR101828794, KR101969696, KR20190122283, KR20200020411, US7396914, WO2005/012360, WO2005/054469, WO2005/060520, WO2006/095180, WO2008/035894, WO2015/179535, WO2016/138160, and WO2019/039891.

SI Analysis

Here, we describe a preliminary analysis on the contents of CoV-AbDab, comparing the data gathered for binders to SARS-CoV-2, SARS-CoV-1, and MERS-CoV.

Biological/Synthetic Origins

First we investigated the reported biological/synthetic origins of each known binder to SARS-CoV-1, MERS-CoV, and SARS-CoV-2 (Fig. S1).

An immediate observation was the increase in the role of nanobodies being used to target MERS-CoV and SARS-CoV-2 relative to SARS-CoV-1. Nanobodies used in MERS-CoV therapy tend to have natural sources (e.g. infected camels, reflecting the geographical region of the epidemic), whereas the advance in 'sybody' (synthetic nanobody) technology has lead to phage display becoming the primary origin of anti-SARS-CoV-2 nanobodies.

Antibody coronavirus binders too have significantly changed in their origins over time, with a clear move away from harvesting animal (mouse, chicken, rhesus) antibody response repertoires. Coupled with this, there has been a decrease in the use of phage display to isolate human antibody binders, with antigen baiting technologies becoming the dominant way of isolating human binders. Human B-cells are the biological origin of 96% of the SARS-CoV-2 antibodies, compared to 42% of SARS-CoV-1 antibodies (excluding cross-reactive SARS-CoV-1/SARS-CoV-2 antibodies isolated in 2020, this number falls to 23%).

Together this results indicate that there have been discernible shifts in the methods used to isolate binding antibodies/nanobodies since 2003. These trends should be carefully considered when comparing published binders to different coronaviruses.

Target Antigens

We next investigated the protein target for each documented antibody/nanobody coronavirus binder, to the domain resolution if possible (Fig. S2). Note that many of these categories are not mutually exclusive (e.g. an S; N-Terminal Domain [NTD] binder would also fit into the category of S; S1 non-Receptor Binding Domain [RBD], however there is experimental evidence to assign it specifically to the NTD domain).

For all three coronaviruses, the RBD is the target for most binding antibodies and nanobodies. It is unsurprising that the RBD is the most investigated domain, as a well-understood mode for viral neutralisation involves direct competition for the native human receptor (Angiotensin-converting Enzyme-2 (ACE-2) for SARS-CoV, or Dipeptidyl Peptidase-4 (DPP4) for MERS-CoV). An increased bias towards identifying RBD binders could also be attributable to the increased usage of RBD baits as well as entire

spike protein baits to isolate relevant antibodies from human serum.

Heavy V-Gene Germline Origins

Finally, we compared the heavy V-gene (IGHV) germline origins of human antibody binders to all targets of SARS-CoV-2, SARS-CoV-1, and MERS-CoV (Fig. S3).

Certain germlines were expanded in both SARS-CoV-2 and SARS-CoV-1 human antibody binders, for example the IGHV3-30 gene is represented in 13% of SARS-CoV-2 human antibodies over at least 7 studies ([3, 9, 24, 45, 49, 52, 53]) and 19% of SARS-CoV-1 human antibodies over at least 10 studies ([3, 5, 12, 25, 33, 45, 49, 53, 56] and patent CN1903878), but only in 4% of MERS-CoV human antibodies over at least 4 studies ([26, 57, 75] and patent WO2105179535).

In contrast, the IGHV3-53 gene represented 6% of SARS-CoV-2 human antibody binders, yet appeared in $< 2\%$ SARS-CoV-1 human antibody binders and no IGHV3-53 MERS-CoV binder has yet been reported. The SARS-CoV-2 IGHV3-53 epitopes have been explored structurally by Yuan *et al.* [73] and Wu *et al.* [69].

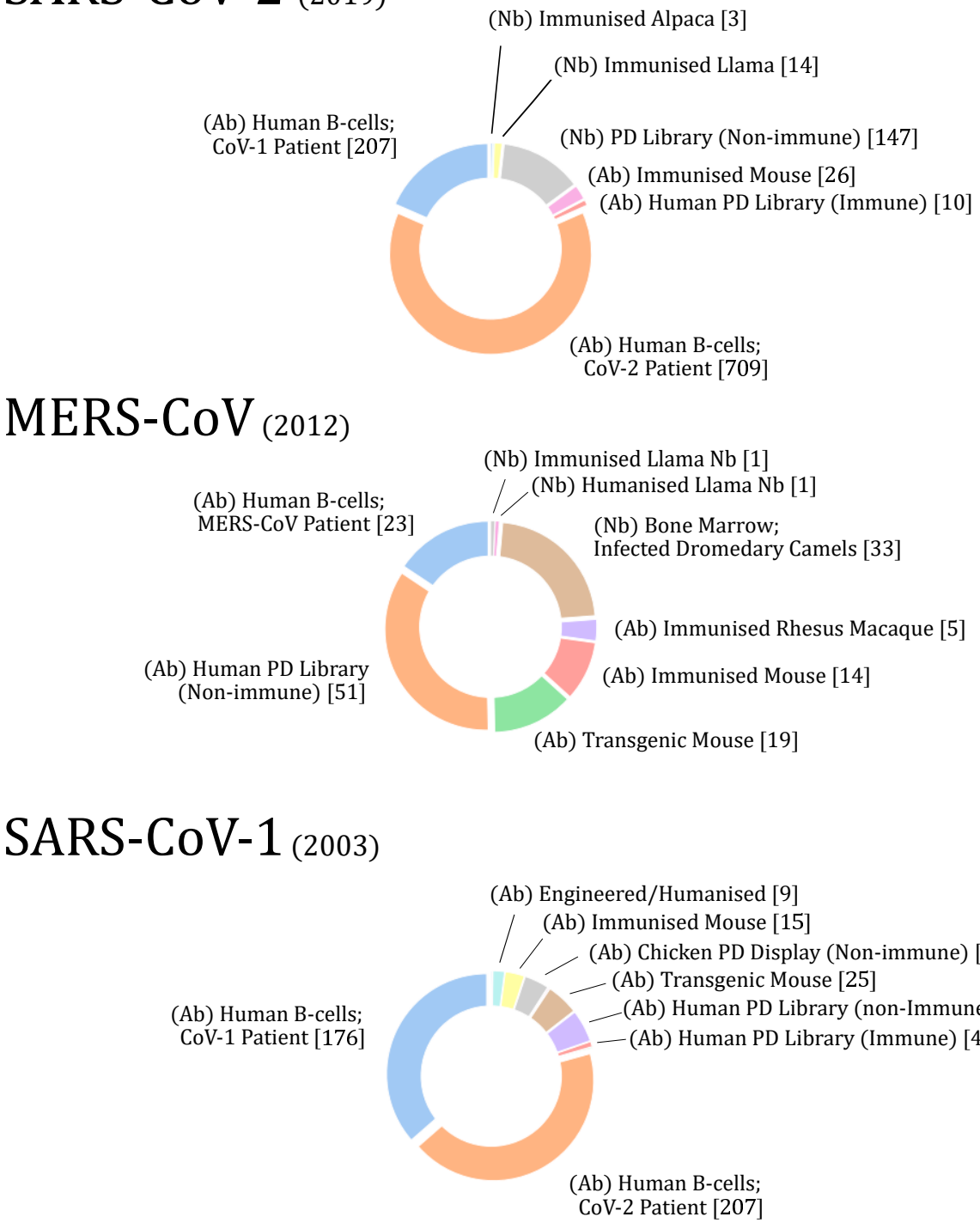

Figure 1: Donut plots comparing the biological/synthetic origin of documented binders to SARS-CoV-2 (2019 pandemic), MERS-CoV (2012 epidemic), and SARS-CoV-1 (2003 epidemic). Absolute numbers of binders in brackets. Ab: Antibody; Nb: Nanobody; PD: Phage Display.

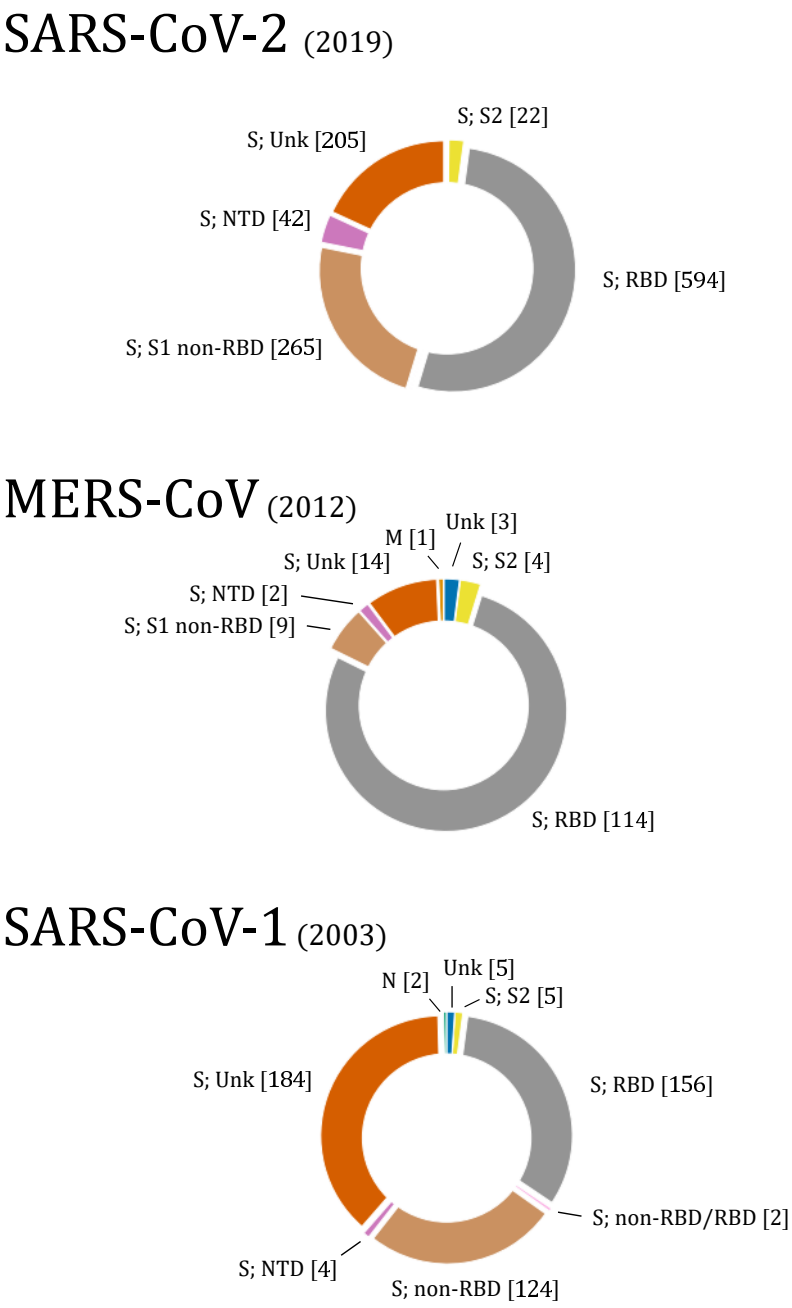

Figure 2: Donut plots comparing the protein epitopes of documented binders to SARS-CoV-2 (2019 pandemic), MERS-CoV (2012 epidemic), and SARS-CoV-1 (2003 epidemic). Absolute numbers of binders in brackets. M = Membrane Protein; N = Nucelocapsid Protein; NTD = N-Terminal Domain; RBD = Receptor Binding Domain; S = Spike protein; Unk = Unknown.

A

IGHV Gene	Number of SARS-CoV-2 Binders [Percentage]
3-30	118 [12.9%]
1-69	115 [12.5%]
3-53	55 [6.0%]
1-2	35 [3.8%]
3-23, 3-66, 4-39	34 [3.7%]
3-9, 3-30-3	32 [3.5%]
1-46, 5-51	29 [3.2%]
4-4, 4-34	24 [2.6%]
3-7, 3-33	23 [2.5%]
1-18	22 [2.4%]
4-59	20 [2.2%]
3-48, 7-4-1	19 [2.1%]
1-8, 3-21	17 [1.9%]
1-24, 2-5	15 [1.6%]
1-58	14 [1.5%]
3-13	13 [1.4%]
3-11, 3-64(D), 4-31, 4-61	12 [1.3%]
3-20	9 [1.0%]
3-49	8 [0.9%]
2-70, 3-15	7 [0.8%]
2-26	5 [0.5%]
3-74, 4-38-2	4 [0.4%]
1-3, 4-30-4	3 [0.3%]
3-43, 5-10-1	2 [0.2%]
3-23, 3-72, 4-38	1 [0.1%]

B

IGHV Gene	Number of SARS-CoV-1 Binders [Percentage]
3-30	77 [16.7%]
1-69	75 [16.3%]
3-23	38 [8.2%]
1-18	19 [4.1%]
1-2, 3-30-3	18 [3.9%]
3-7	17 [3.7%]
3-33, 5-51	12 [2.6%]
1-46, 3-9, 3-11, 4-4	11 [2.4%]
4-39	10 [2.2%]
4-34, 4-59	9 [2.0%]
2-5, 4-61	8 [1.7%]
3-13, 3-48	7 [1.5%]
1-8, 3-20, 3-21, 3-53, 7-4-1	6 [1.3%]
3-49, 3-66, 4-31	5 [1.1%]
3-64(D), 3-72	4 [0.9%]
1-24, 4-38-2	3 [0.7%]
1-58, 2-26, 3-43, 3-64, 6-1	2 [0.4%]
1-3, 3-15, 3-23, 3-74	1 [0.2%]

C

IGHV Gene	Number of MERS-CoV Binders [Percentage]
1-69	37 [39.4%]
3-23	20 [21.3%]
4-39	6 [6.4%]
2-5	5 [5.3%]
3-30	4 [4.3%]
4-59	3 [3.2%]
1-3, 1-18, 3-11, 3-15, 3-21	2 [2.1%]
1-2, 1-46, 3-9, 3-30-3, 4-4, 4-34, 6-1	1 [1.1%]

Figure 3: Tables comparing the human antibody heavy chain V-gene origin of documented binders to (A) SARS-CoV-2, (B) SARS-CoV-1, and (C) MERS-CoV.

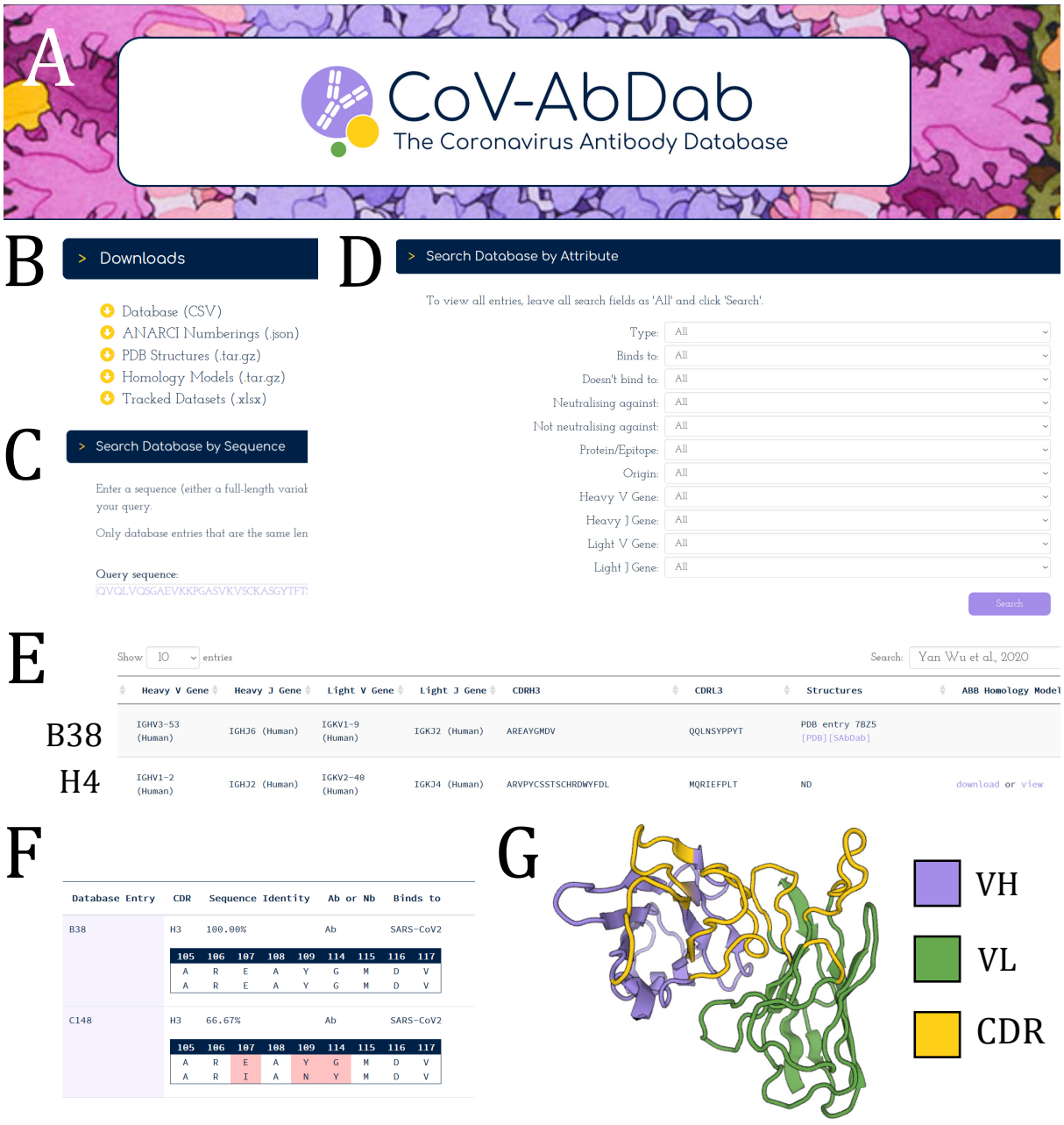

Figure 4: The CoV-AbDab Web Application. (A) CoV-AbDab homepage logo (background image credit: David Goodsell). (B) All CoV-AbDab data can be downloaded. (C) The database can be queried by sequence (full chain or CDRH3). (D) The database can be queried by attribute (neutralisation profile, developmental origin, germlines, *etc.*). (E) All results filtered by a particular study ([70]). Shown is the information required for clonotyping, a solved structure for B38, and a homology model for H4. (F) The result of using the sequence search feature from "C" with the CDRH3 from B38. Alignments and metadata are given for the top ten closest matches. (G) The in-browser viewer displaying the homology model of H4.

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