

# Case Study: SARS-CoV-2

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# Identification of SARS-CoV-2

ORIGINAL ARTICLE BRIEF REPORT

## A Novel Coronavirus from Patients with Pneumonia in China, 2019

Na Zhu, Ph.D., Dingyu Zhang, M.D., Wenling Wang, Ph.D., Xingwang Li, M.D., Bo Yang, M.S., Jingdong Song, Ph.D., Xiang Zhao, Ph.D., Baoying Huang, Ph.D., Weifeng Shi, Ph.D., Roujian Lu, M.D., Peihua Niu, Ph.D., Faxian Zhan, Ph.D., et al., for the China Novel Coronavirus Investigating and

### VIRAL GENOME SEQUENCING

RNA extracted from bronchoalveolar-lavage fluid and culture supernatants was used as a template to clone and sequence the genome. We used a combination of Illumina sequencing and nanopore sequencing to characterize the virus genome. Sequence reads were assembled into contig maps (a set of overlapping DNA segments) with the use of CLC Genomics software, version 4.6.1 (CLC Bio). Specific primers were subsequently designed for PCR, and 5'- or 3'-RACE (rapid amplification of cDNA ends) was used to fill genome gaps from conventional Sanger sequencing. These PCR products were purified from gels and sequenced with a BigDye Terminator v3.1 Cycle Sequencing Kit and a 3130XL Genetic Analyzer, in accordance with the manufacturers' instructions.

# Identification of SARS-CoV-2

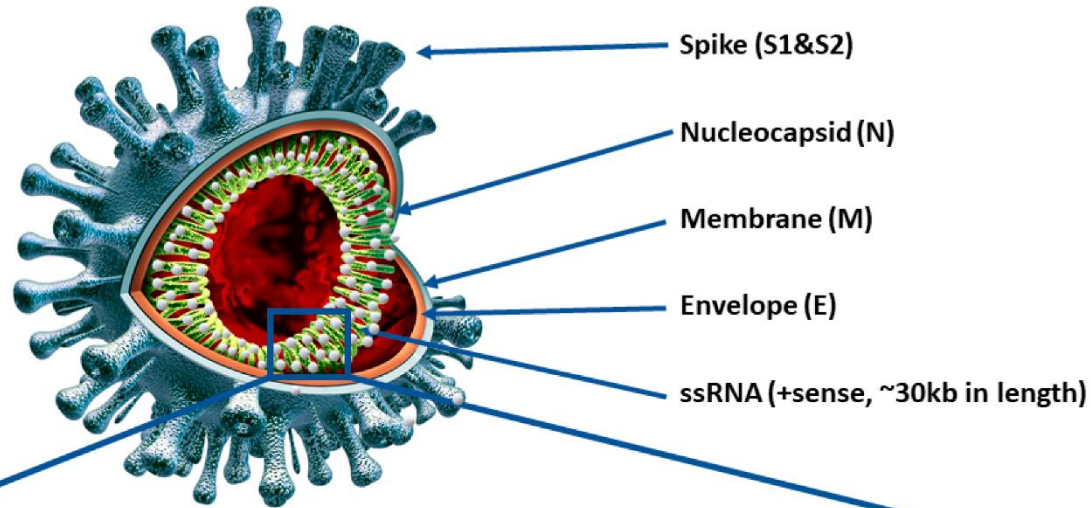
ORIGINAL ARTICLE BRIEF REPORT

## A Novel Coronavirus from Patients with Pneumonia in China, 2019

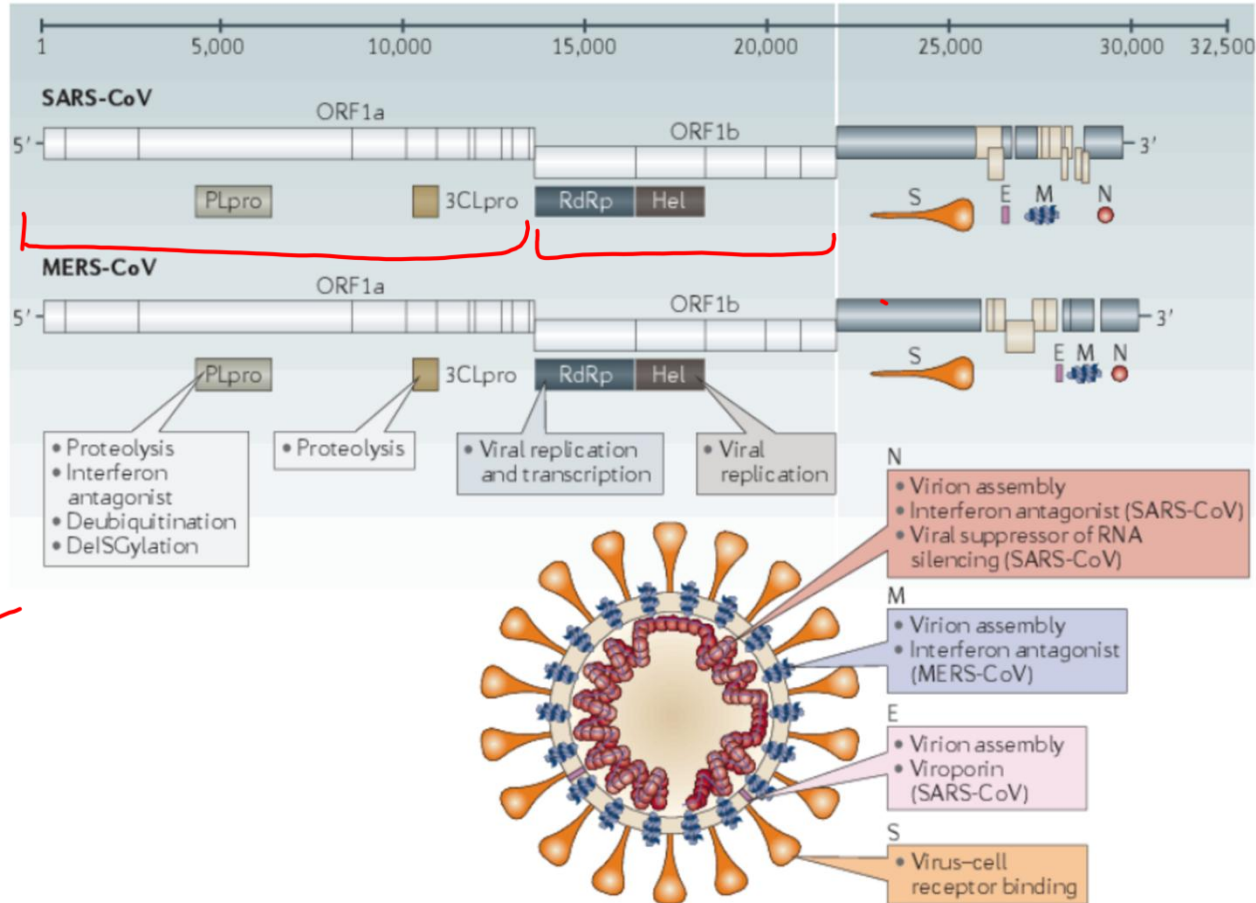
Na Zhu, Ph.D., Dingyu Zhang, M.D., Wenling Wang, Ph.D., Xingwang Li, M.D., Bo Yang, M.S., Jingdong Song, Ph.D., Xiang Zhao, Ph.D., Baoying Huang, Ph.D., Weifeng Shi, Ph.D., Roujian Lu, M.D., Peihua Niu, Ph.D., Faxian Zhan, Ph.D., et al., for the China Novel Coronavirus Investigating and

RespiFinderSmart22kit. RNA extracted from bronchoalveolar-lavage fluid from the patients was used as a template to clone and sequence a genome using a combination of Illumina sequencing and nanopore sequencing. More than 20,000 viral reads from individual specimens were obtained, and most contigs matched to the genome from lineage B of the genus betacoronavirus — showing more than 85% identity with a bat SARS-like CoV (bat-SL-CoVZC45, MG772933.1) genome published previously. Positive

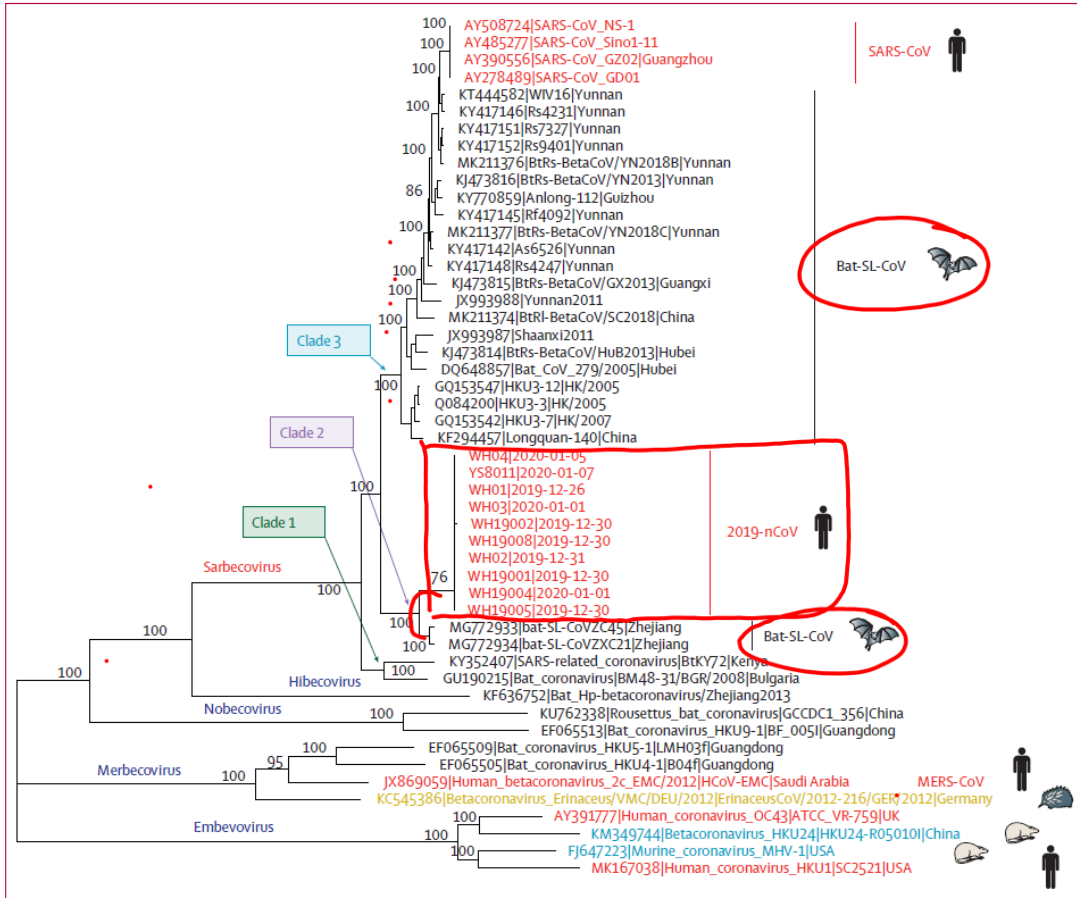
# Genomic structure



# SARS-CoV-2 proteins



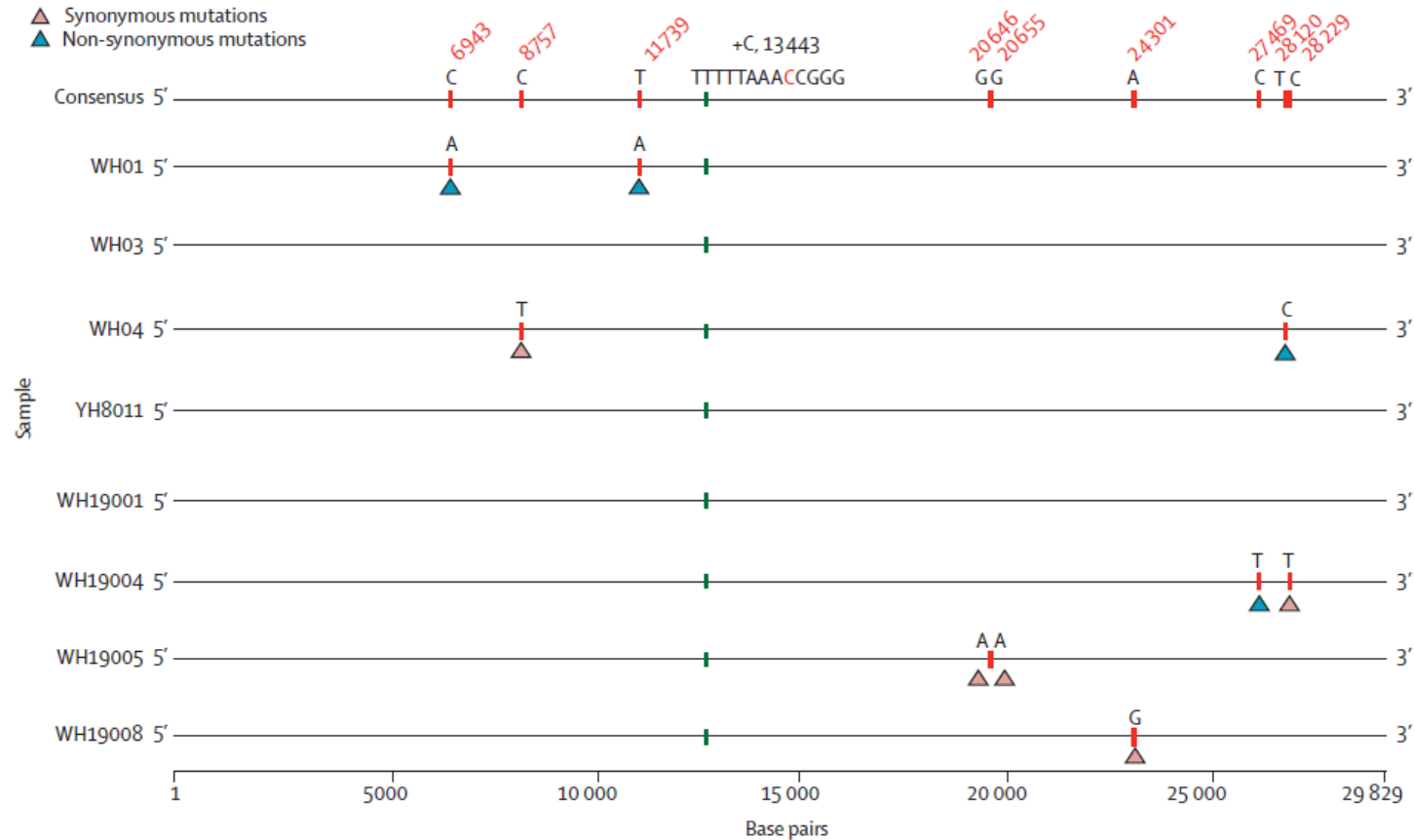
# Phylogenetic analysis of SARS-CoV-2



## Phylogenetic analysis

Sequence alignment of 2019-nCoV with reference sequences was done with Mafft software (version 7.450).<sup>21</sup> Phylogenetic analyses of the complete genome and major coding regions were done with RAXML software (version 8.2.9)<sup>22</sup> with 1000 bootstrap replicates, employing the general time reversible nucleotide substitution model.

# SARS-CoV-2 variants





# Drug repurposing for SARS-CoV-2

CLUSTAL O(1.2.4) multiple sequence alignment

```

3TLO:A|PDBID|CHAIN|SEQUENCE  -----SGLKKMAQPSGCVVERCWRVCYGSVTLNGVWLGDTVTCPRFIAPSTT-VLID  52
1P9S:A|PDBID|CHAIN|SEQUENCE  -----AGLRKMAQPSGFVEKCVVRVCYGNVTNLGLWLDIVYCPRIASNTT-SAID  52
6LU7:A|PDBID|CHAIN|SEQUENCE  -----SGFRKMAFPSSGKVEGCMVQVTCGTTTTLNGLWLDVVYCPRICTSEMLNPN  53
3IWM:A|PDBID|CHAIN|SEQUENCE  -----SGFRKMAFPSSGKVEGCMVQVTCGTTTTLNGLWLDVVYCPRICTSEMLNPN  53
3D23:B|PDBID|CHAIN|SEQUENCE  -----ASSGIVKMVSPTSKEIPCIVSVTYSMTLNLGLWLDKVCYCPRICTSSNNPEPD  55
5WKK:A|PDBID|CHAIN|SEQUENCE  MHHHHHSGLVKNSHPSGDVEACMVQVTCGSMTLNLGLWLDNTVWCPRIKMCADQLSDPN  60
                                :*: ** *: : * : * : * : * : * : * : * : * : * : * : * : * :
                                :

3TLO:A|PDBID|CHAIN|SEQUENCE  YDHAYSTMRLHNFSVS---HNGVFLGVGVTHHGSVLRKVSQSNVHTPKHVFKLKPGD  109
1P9S:A|PDBID|CHAIN|SEQUENCE  YDHEYSIMRLHNFSII---SGTAF LGVVGATMHGVTLKIKVSQTHMHTPRHSFRTLKSGE  109
6LU7:A|PDBID|CHAIN|SEQUENCE  YEDLLIRKSNHNFVLQ---AGNVQLRVIGHSMQNCVLKLVDTANPKTPKYKFVRIQPGQ  110
3IWM:A|PDBID|CHAIN|SEQUENCE  YEDLLIRKSNHNSFLVQ---AGNVQLRVIGHSMQNCVLLRLKVDTSNPKTPKYKFVRIQPGQ  110
3D23:B|PDBID|CHAIN|SEQUENCE  YSALLCRVTLGDFTIM---SGRMSLTVVSQMGQCLVLTVSLQNPYTPKYTFGNVKPGE  112
5WKK:A|PDBID|CHAIN|SEQUENCE  YDALLISMTNHSFSVQKHIGAPANLRVVGHAMQGTLLKLTVDAINPSTPAYTFTTVKPGA  120
                                : * : * : * : * : * : * : * : * : * : * : * : * :
                                :

3TLO:A|PDBID|CHAIN|SEQUENCE  SFNIIACYEIGASGVFGVNLRTNFIKGSFINGACGSPGYNVRNDGTVEFCYLHDIHSGS  169
1P9S:A|PDBID|CHAIN|SEQUENCE  GFNIIACYDSCAQGVFGVNMRTNWTIRGSFINGACGSPGYNLIN-GEVEFYVHDIHSGS  168
6LU7:A|PDBID|CHAIN|SEQUENCE  TFSVLACYNGSPSGVYQCAMPNFTIKGSFLNGSCGSGVFNIDY-DCVSFCYHMEHPT  169
3IWM:A|PDBID|CHAIN|SEQUENCE  TFSVLACYNGSPSGVYQCAMPNHTIKGSFLNGSCGSGVFNIDY-DCVSFCYHMEHPT  169
3D23:B|PDBID|CHAIN|SEQUENCE  TFTVLAAYNGRPQGAHVIMRISYTIKGSFLCGSCGSGVYVLTG-DSVKFYVHMEHPT  171
5WKK:A|PDBID|CHAIN|SEQUENCE  AFSVLACYNGRPTGFTTVMRPNYTIKGSFLCGSCGSGVYTKEG-SVINFCYHMEHPT  179
                                :*: ** *: : * : * : * : * : * : * : * : * : * : * :
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3TLO:A|PDBID|CHAIN|SEQUENCE  GATFGSDFTGSVYGNFDDPSLQVESANLMLSDNVVAFVLAALLNGCRWMLCSTRVNVVG  229
1P9S:A|PDBID|CHAIN|SEQUENCE  GSHFGSSFDGVMYGGFEDPSLQVESANQMLTVNVVAFVLAAILNGCTWMLKGEKLFVEH  228
6LU7:A|PDBID|CHAIN|SEQUENCE  GVHAGTDLEGHFYGPFVDQTAQAAGTDTITLVNLAWLAAVINGDRWFLNRFRTTLND  229
3IWM:A|PDBID|CHAIN|SEQUENCE  GVHAGTDEKFGYGFVDQTAQAAGTDTITLVNLAWLAAVINGDRWFLNRFRTTLND  229
3D23:B|PDBID|CHAIN|SEQUENCE  GCHTGTDTGNFYGPYRQVQLPVKDYQVTVNIAWLAAAILNCAWFAVQNDVCSTED  231
5WKK:A|PDBID|CHAIN|SEQUENCE  GTHFGSAFDGMYGAFTQVHQLDQKYSVNVVAVLAAILNGCAWFAVQNPRTSVVS  239
                                * : : * : * : : : * : * : * : * : * : * : * : * :
                                :

3TLO:A|PDBID|CHAIN|SEQUENCE  FNEWAMANGYTSVSSVE--CYSLAAKTGVSVEQLLASTQH-LHEFGGKNILGYSSLCD  286
1P9S:A|PDBID|CHAIN|SEQUENCE  FNEWAANGFTAMNGED--AFSILAAGTGVCVERLHAQTQ-LNNGFGGKILGYSSLND  285
6LU7:A|PDBID|CHAIN|SEQUENCE  FNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDMCAALKELLQNGMGRITLGSALLE  289
3IWM:A|PDBID|CHAIN|SEQUENCE  FNLVAMKYNIEPLTQDHVDILGPLSAQTGIAVLDMCAALKELLQNGMGRITLGSILLE  289
3D23:B|PDBID|CHAIN|SEQUENCE  FNVWAMANGFSQVKADL--VLDALASMTGVSIETLAAIKR-LYMGFGGRILGSCTFED  288
5WKK:A|PDBID|CHAIN|SEQUENCE  FNEWALANQTFEFGTQ--SVDMLAVKTGVAIEQLLYATQ-LYTFGQKQILGSTMLED  296
                                : * : : * : * : * : * : * : * : * : * : * : * : * :
                                :

3TLO:A|PDBID|CHAIN|SEQUENCE  EFTLAEVVKQHYGVNLQ  303
1P9S:A|PDBID|CHAIN|SEQUENCE  EFSINEVVKQHYGVNLQ  300
6LU7:A|PDBID|CHAIN|SEQUENCE  EFTPFDVVRQCSGVTFQ  306
3IWM:A|PDBID|CHAIN|SEQUENCE  EFTPFDVVRQCSGVTFQ  306
3D23:B|PDBID|CHAIN|SEQUENCE  ELAPSDVYQQLAGV---  302
5WKK:A|PDBID|CHAIN|SEQUENCE  EFTPFDVVRQIMGVVMQ  313
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                                :

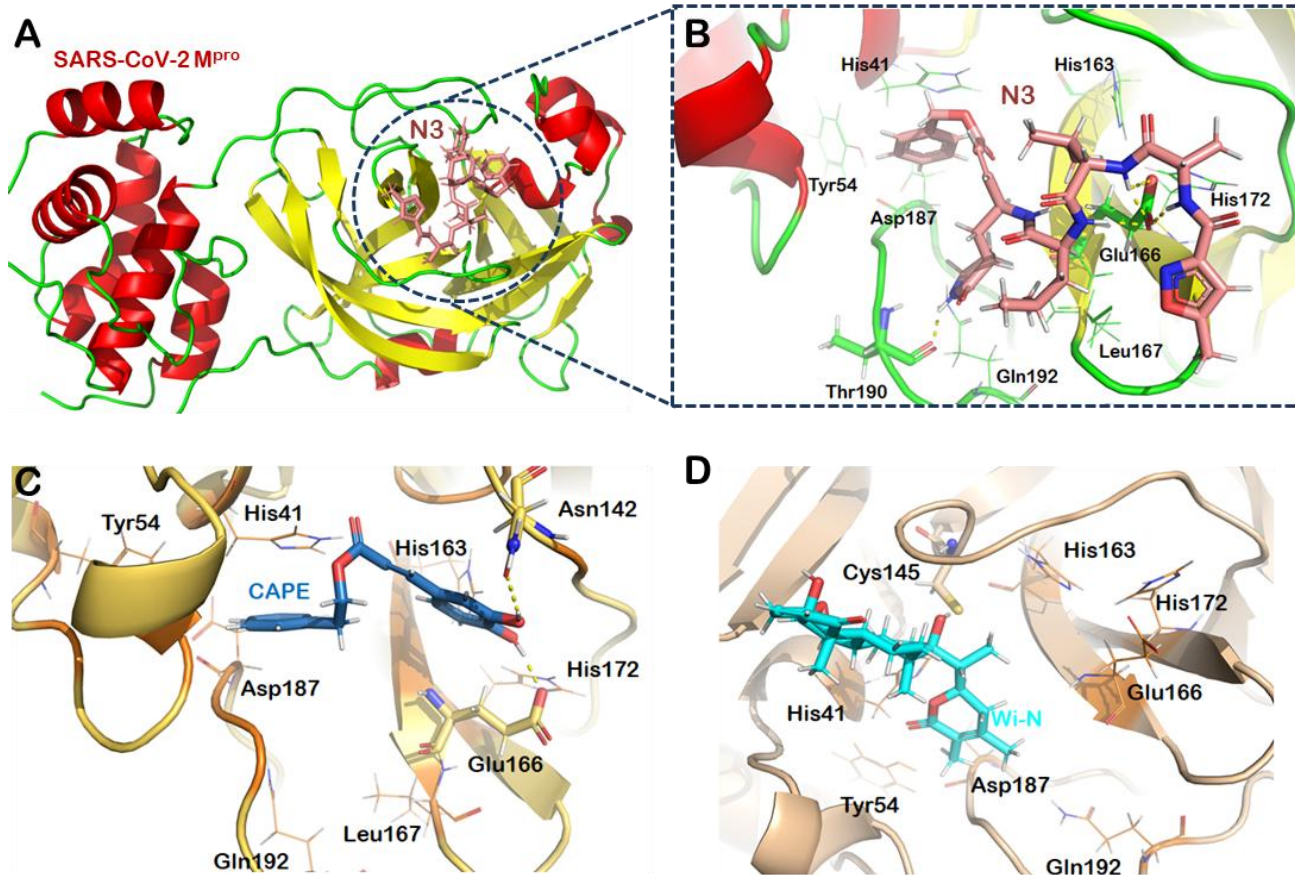
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Multiple sequence alignment of Main protease enzyme of various human coronaviruses, including SARS-CoV-2

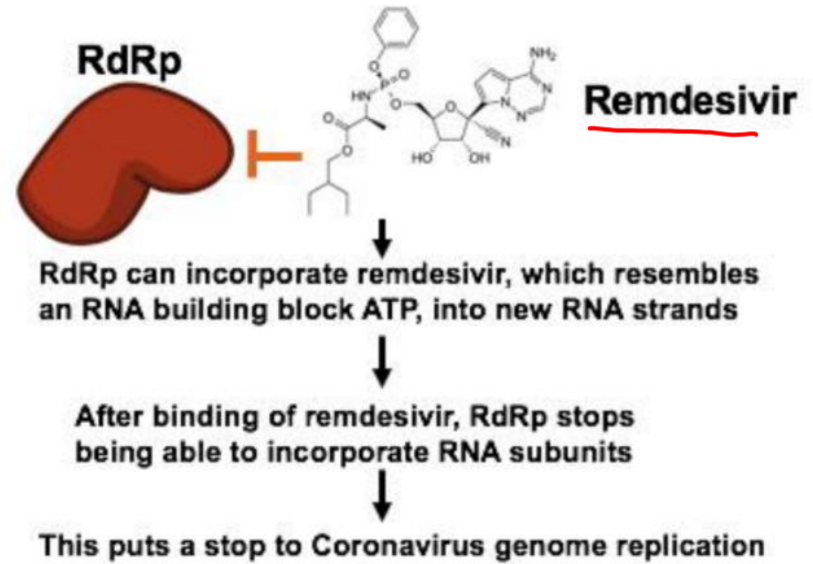
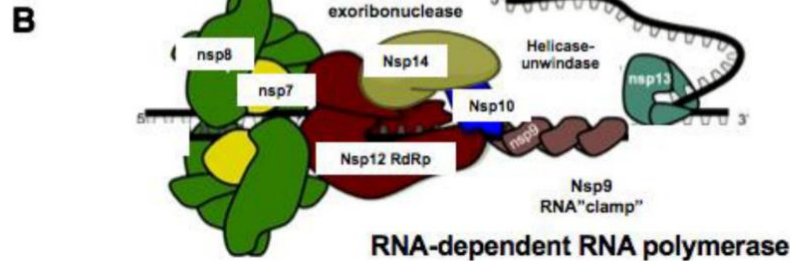
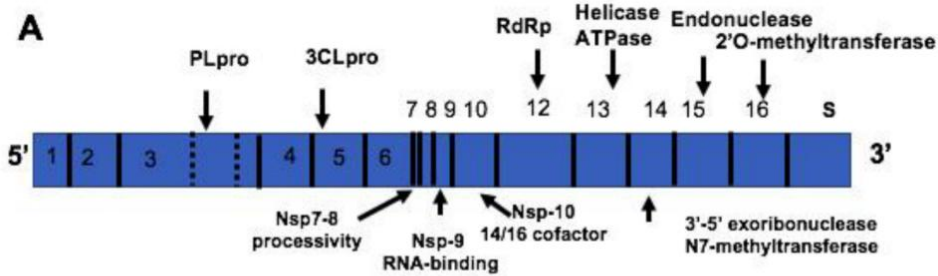
M<sup>Pro</sup>



# Drug repurposing for SARS-CoV-2

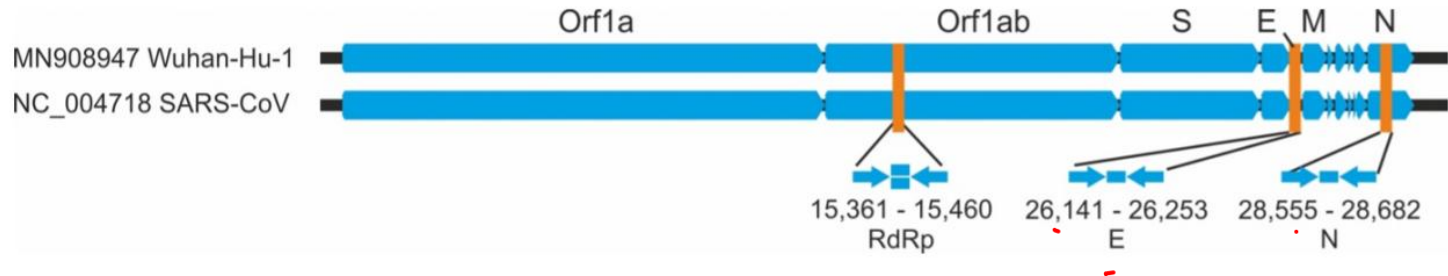


# Remdesivir against RdRp

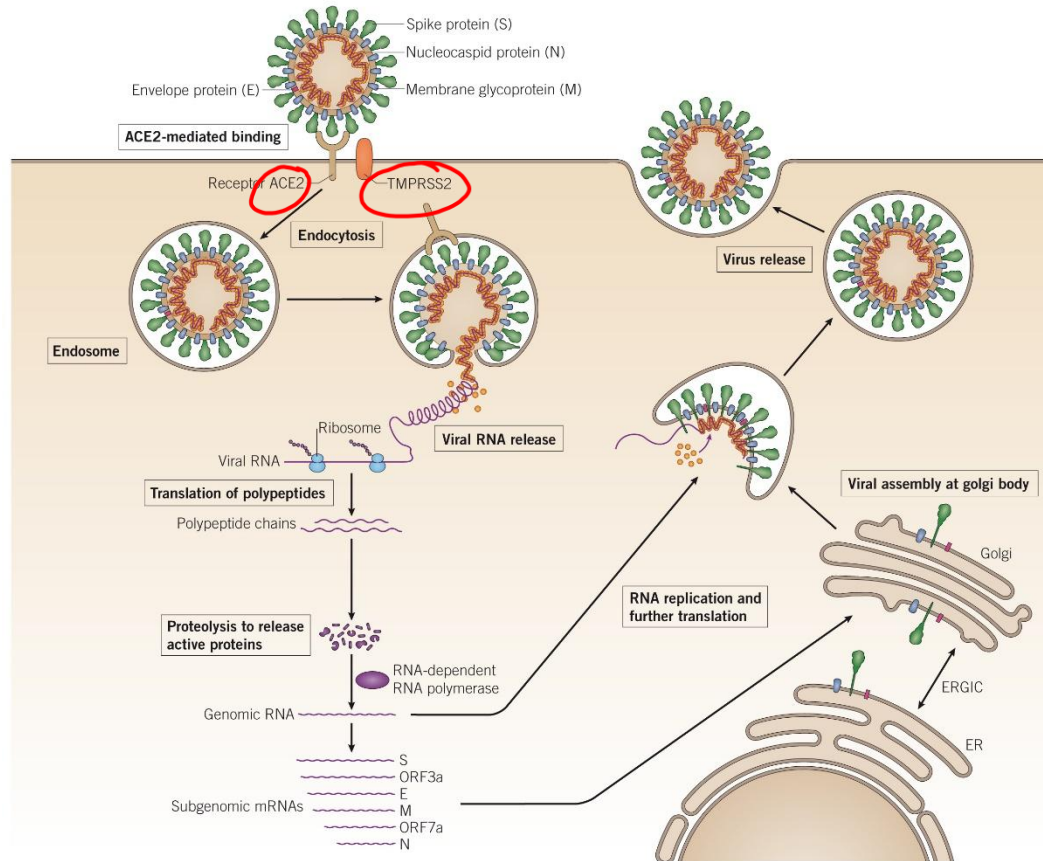


# RTPCR test for SARS-CoV-2

**First line screening assay: E gene assay**  
**Confirmatory assay: RdRp gene assay**  
**Additional confirmatory assay: N gene assay**



# Transmission of SARS-CoV-2



31nM  
4.1nM.

# Transmission of SARS-CoV-2

## Structure of the SARS-CoV-2 spike receptor-binding domain bound to the ACE2 receptor

[Jun Lan](#), [Jiwan Ge](#), [Jinfang Yu](#), [Sisi Shan](#), [Huan Zhou](#), [Shilong Fan](#), [Qi Zhang](#), [Xuanling Shi](#), [Qisheng Wang](#),

[Linqi Zhang](#) ✉ & [Xinquan Wang](#) ✉

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