



Role of changes in SARS-CoV-2 spike protein in the interaction with the human ACE2 receptor: An in silico analysis
Role of changes in SARS-CoV-2 spike protein in the interaction with the human ACE2 receptor: An *in silico* analysis

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Abstract

Many human viral diseases are the result of zoonotic diseases. Some of the diseases caused by these zoonotic events have affected millions of people worldwide, some of which have resulted in high human morbidity/mortality rates. Changes in viral proteins that act as ligands to host receptors may promote interspecific spillover. The most recent of these zoonotic events that have caused an ongoing large-scale epidemic are the SARSCoV2-caused Covid19 epidemics. The purpose of this study was to identify mutations in the SARSCoV2 peaplomer sequence that could promote human-to-human transmission. To identify modifications in the S1 subunit of the spike receptor binding domain, an in silico method has been used. The observed changes have a significant effect on the SARSCoV2 spike / ACE2 interaction, causing a decrease in binding energy compared to the binding energy of BatCoV to this receptor. The data presented in this study suggest a higher affinity of the SARS-Cov-2 spike protein to the human ACE2 receptor, compared to the one of Bat-CoV spike and ACE2. This may be responsible for the rapid viral spread of SARSCoV2 in humans.

Keywords: Spike, SARS-CoV-2, ACE2, Coronavirus, outbreak

Introduction

Acute Respiratory Syndrome with Severity SARS (Middle Eastern Respiratory Syndrome) Coronavirus (MERS-CoV) and the newly discovered novel Coronavirus (SARS-CoV-2) are both members of the Coronaviridae family, genus Betacoronavirus, which have been linked to major epidemic outbreaks. These are enveloped viruses with a 32-kilobyte positive-sense single-strand RNA. The spike, membrane, envelope protein, and nucleocapsid are the four primary structural proteins found in viral particles. The spike protein protrudes from the virion's envelope and is important for receptor host selection and cellular attachment.

SARS and SARS-CoV-2 spike proteins interact with angiotensin-converting enzyme 2 (ACE2), according to strong scientific data (Chen et al 2020 Wan et al.). Other cellular receptors, including as the C-type lectin CD209L and DC-SIGN, also play a secondary role in viral attachment. However, contact between viral proteins and their cell membrane receptors appears to be an important step in the reproductive cycle of SARS-CoV and possibly SARSCoV2. (Walls et al.). Furthermore, the effectiveness of viral infection is highly reliant on this procedure. Protein-protein interactions are linked to a number of physicochemical parameters.

The nature of residues and the sort of chemical interactions that occur between ligand and receptor define these parameters. As a result, the presence of residues that provide a more energetically favourable contact (lower free energy) may drive binding kinetics and eventually lead to fusion. As a result, the goal of this research was to assess the energetic profile of the interaction between the SARS-CoV-2 spike protein and the human cell receptor ACE2.

Materials and Methods

NCBI:

NCBI is database which is used to charged with creating automated systems for storing and analyzing knowledge about molecular biology, biochemistry, and genetics. NCBI is now a leading source for publicbiomedical databases, software tools for analyzing molecular and genomic data, and research in computational biology.

PUBCHEM:

PUBCHEM is the database which is used to drug discovery and many aspects such as lead identification and optimization, compound-target profiling, polypharmacology studies and unknown chemical identityelucidation. PubChem has also shown to be a useful tool for creating secondary databases, software tools, and online applications..

PROTEIN DATA BANK:

PROTEIN DATA BANK (PDB) is the database which is used find 3D structure of the protein. The PDB is a key in areas of structural biology, such as structural genomics. Most major scientific journals and some funding agencies now require scientists to submit their structure data to the PDB.

UNIPROT:

UNIPROT also called as SWISSPROT It provides an up-to-date, comprehensive bodyof protein information at a single site.It aids scientific discovery by collecting, interpreting andorganising this information so that it is easy to access and use.

SWISSMODEL

SWISSMODEL is the online web server dedicated to homology modeling of 3D protein structures. Homology modeling is currently the most accurate method to generate reliable three-

dimensional protein structure models and is routinely used in many practical applications.

Phylogenetic analysis:

A phylogenetic tree is a diagram that represents evolutionary relationships among organisms.

TCOFFEE Alignment:

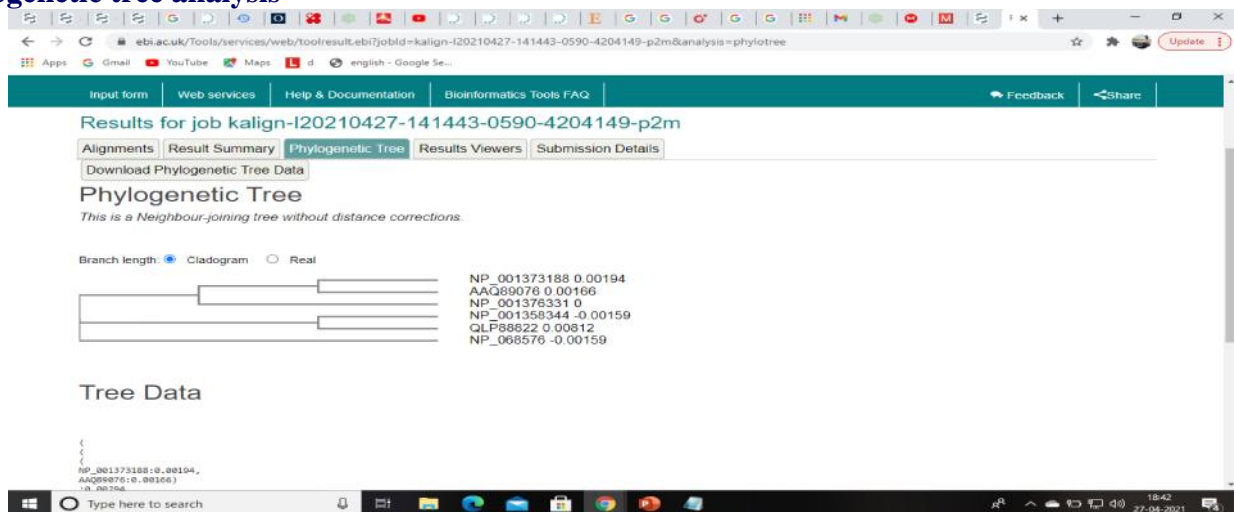
T-Coffee is a multiple sequence alignment program.

Protein sequence:

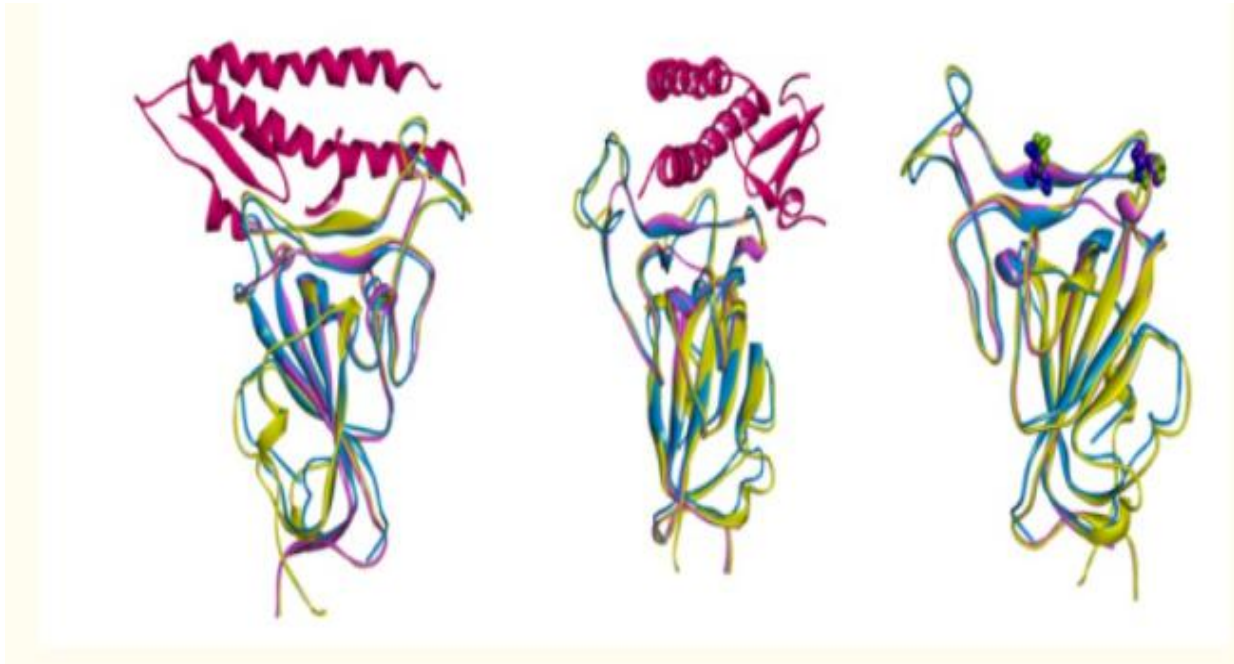
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NSFVGWSTDWSPYADQSIKVRISLKSALGDKAYEWN DNEMYLFRSSVAYAMRQYFLKVK
N
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SLEFLGIQPTLGP PNQPPVSIWLVFGVVMGVIVVGIVILIFTGIRD RKKPTLLGKSWL
TAILKD
```

Results and Discussion

Phylogenetic tree analysis



Protein Data Bank



Homology modeling:

Project Data Model Results

Orderby GMQE

Oligo-State Hetero 1 1 mer Ligands None GMQE 0.00 QMEAN 7.14

Global Quality Estimate Local Quality Estimate Comparison

| Quality Estimate | Value |
|------------------|-------|
| QMEAN | -7.14 |
| CP | -2.23 |
| All Atom | -1.08 |
| solvation | -1.52 |
| torsion | -6.45 |

Membrane annotation has been transferred from template. Show / Hide

| Template | Seq Identity | Coverage | Description |
|----------|--------------|----------|--|
| 2knc.1 | 21.54% | | Platelet integrin ALFAIIB-Delta3 transmembrane-cytoplasmic heterocomplex |

Model-template Alignment

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Model_01: VRSSSSMLLSLVAVIARQFIIIDQAMTFLDHYFSEARLDFIQQSSLA:WPIRIMITELAVQMHDRGDEWS 70
2knc.1:A-----
Model_01: APLREKDSILADQMYPLQEIQNLIVKFLQALQDQNGSSVLSQEDNSKRLNTILNTHSTIYSTGZVDMDFDRPCE 140
2knc.1:A-----
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Models/ ☆ ⚙️ 👤 Update

- Google Se...

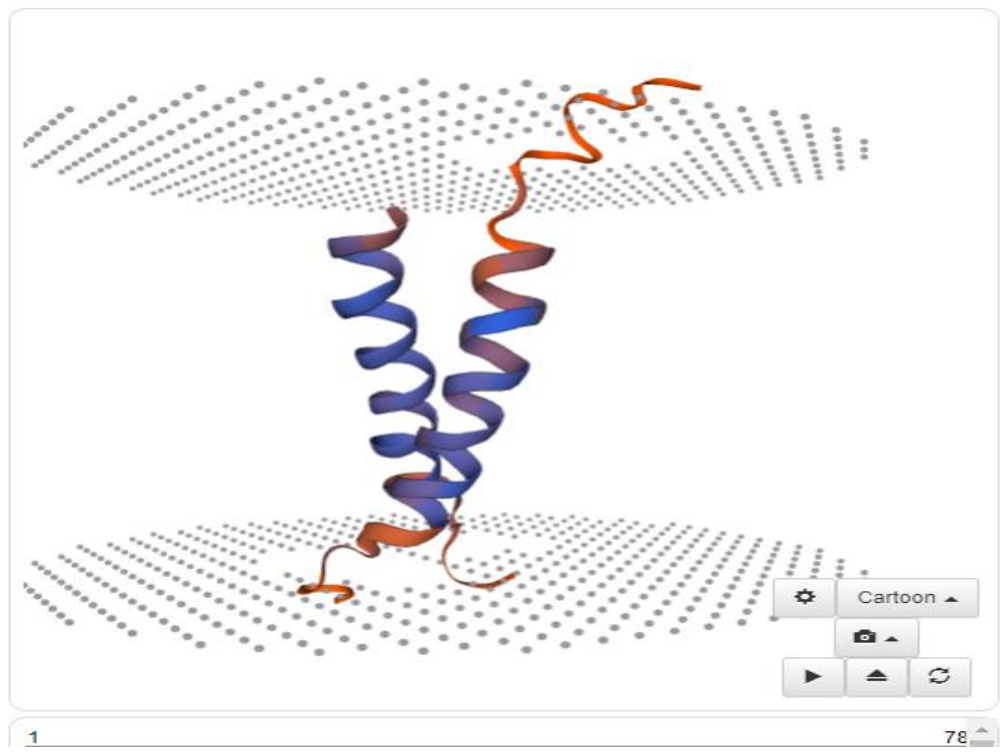
Model-Template Alignment

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|----------|--|-----|
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| 2knc.1.A | ----- | |
| Model_01 | AFLKEQSTLAQMYPLOETQNLTVKLLQALQQNGSSVLSSEDKSKRLNTILNTMSTIYSTGKVCNPDNFQE | 140 |
| 2knc.1.A | ----- | |
| Model_01 | CILLEPGLNEIMANSLDYNERLWAWESWRSEVVKOLRPLYEEYVVLKNEMARANRYEDYGDYWRAGDYEVN | 210 |
| 2knc.1.A | ----- | |
| Model_01 | GVGGVYVSRQQLTFDVEHTFEFTKPLVYFRIHLYVRLWLMNLYPSYTSPTGCLPAHLLGDMWGRFMTNLYS | 280 |
| 2knc.1.A | ----- | |
| Model_01 | LIVPFGQKPNIDVIDAMVDQAWDAQRIFKEAEKFFVSVGLPNMTQGFWENSMITDGGNVQKAVCHPTAWD | 350 |
| 2knc.1.A | ----- | |
| Model_01 | LQKGDPRILMCTKVTMDDFLTANNEMGHIQYDMAYAAQPFLLRNSANESFHEAVGEIMOLCAATPKHLKO | 420 |
| 2knc.1.A | ----- | |
| Model_01 | IGLLSPDFQEDNTEINFLKQALTIIVGTLFFTYMLEKRWVVFNGEIPKQDQWKKWVEMKREIVGVVEP | 490 |
| 2knc.1.A | ----- | |
| Model_01 | VPHDETTCDFASLPHVSNVYSPIRYTYRILYQFQFQALCQAARKHEGFLKKUDISNYSFAGKLFNHLKL | 560 |
| 2knc.1.A | ----- | |
| Model_01 | GKSEPTLALENVVGAKNMNVRLNLYFEPLFTWLKDKNKS FVGSIDWSPYADQSIKVRISLKSALGD | 630 |
| 2knc.1.A | ----- | |
| Model_01 | KAYEWNNDNEMYLFRSSVAYAMROYFLKVKNOHILFGEEDVRVANLKPRI SFNFVVIAPKNVSDIIPRTEV | 700 |
| 2knc.1.A | ----- | |
| Model_01 | EKAIRMSRPRINDAFRLNDNSLEFLGIQPTLGGP NQPPVSR IWLIVFGVVMGVIVV SIVILLIS TCIRDR | 768 |
| 2knc.1.A | -----ERAIH (IWWVIVGVVGG LLLLTIVL LAHWKVG) PKR | 41 |
| Model_01 | KKK TDLLCKSNLPAIKD | 786 |
| 2knc.1.A | NRP----- | 46 |
| Model_01 | MSSSSWLLLSLVAVTAAQSTIEEQAKTFLDKFNHEREDLFYQSSLASWNYNINITEENVQNMHNAGDEWS | 70 |
| 2knc.1.B | ----- | |

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PROTEOPEDIA

Resolution

Resolution, in structure determinations, is the distance corresponding to the smallest observable feature: if two objects are closer than this distance, they appear as one combined blob rather than two separate objects.

Resolution 2.0 Å

Resolution 1.5 Å

Resolution 1.0 Å

Resolution 3.5 Å

Structure determination by X-ray crystallography or cryo-electron microscopy produces an electron density map (shown in green). The atomic model, shown as sticks, is then built, guided by the electron density map.

In X-ray crystallography, resolution is the smallest distance between crystal lattice planes that is resolved in the diffraction pattern. High numeric values of resolution, such as 4 Å, mean poor resolution, while low numeric values, such as 1.5 Å, mean good resolution.

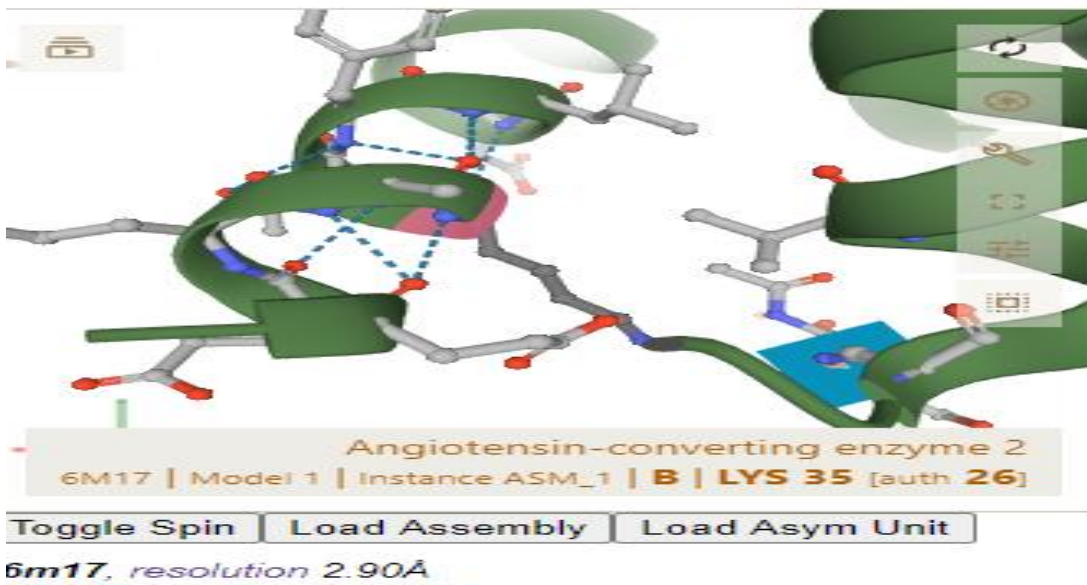
2.05 Å is the median resolution for X-ray crystallographic results in the Protein Data Bank (135,762 on May 19, 2019). For comparison, the van der Waals diameter of a carbon atom is 3.4–3.7 Å^[4], and the length of a covalent carbon-carbon bond is 1.5 Å^[4].

If some portions of the macromolecule are less ordered in the crystal than others, these will have a poorer resolution. The "resolution of the crystal" represents the most ordered portions (see Determination of Resolution).

After an electron density map is calculated and refined with a fitted atomic model, an uncertainty of atomic position is calculated for each atom in the model. These single-atom uncertainties are called the B factors or temperature values of the atoms (see Temperature).

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- 1 Quick Guide
- 2 Confusion of high vs. low resolution
- 3 What Limits Resolution?
- 4 Electron Density Map vs. Resolution
- 5 Resolution and structure quality
- 6 Determination of Resolution
- 7 Resolution of a reflection vs. resolution of a diffraction data set



T.COFFEE ALIGNMENT:

CLUSTAL W (1.83) multiple sequence alignment

```
tr|ABA712V3H4|ABA712V3H4_HUMAN MS5SSHL LSLVATAAQTSTIEEQAKTF LDKFNHEAEDLFYQSSLASIMY
tr|ABA712V4H0|ABA712V4H0_HUMAN MS5SSHL LSLVATAAQTSTIEEQAKTF LDKFNHEAEDLFYQSSLASIMY

tr|ABA712V3H4|ABA712V3H4_HUMAN NTHITTEEVQMPPIAGDKHSF LKEQSTLAQMYPLQEQINLTVKLLQAL
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tr|ABA712V3H4|ABA712V3H4_HUMAN HEAVGEINLSAATPKHLKSLG LLSPOFQEDNETEIFLLKQALTIIVSTL
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*****
```

Conclusion

The SARS-CoV-2 S protein is highly conserved among all human Coronaviruses (HCoVs) and is involved in receptor recognition, viral attachment, and entry into host cells. Due to its indispensable functions, it represents one of the most important targets for COVID-19 vaccine and therapeutic research

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