Supporting Information

Design and optimization of Subunit vaccine targeting the COVID- 19 molecular shreds through immunoinformatics framework

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Infectious Spike glycoprotein [Severe acute respiratory syndrome coronavirus 2]

GenBank: QHR63290.2
>QHR63290.2 spike glycoprotein [Severe acute respiratory syndrome coronavirus 2]

MFVFLVLLPLVSSQCVNLTTRTQLPPAYTNSFTRGVYYPDKVFRSSVLHSTQDLFLPF
FSNVTWFHAIHVSGTNGTKRFDNPVLPFNDGVYFASTEKSNIIRGWIFGTTLDSKTQS
LLIVNNATNVVIKVCEFQFCNDPFLGVYYHKNNKSWMESEFRVYSSANNCTFEYVS
QPFLMDLEGKQGNFKNLREFVFKNIDGYFKIYSKHTPINLVRDLPQGFSALEPLVDLP
IGINITRFQTLLALHRSYLTPGDSSSGWTAGAAAYYVGYLQPRTFLLKYNENGTITDA
VDCALDPLSETKCTLKSFTVEKGIYQTSNFRVQPTESIVRFPNITNLCPFGEVFNATRF
ASVYAWNRKRISNCVADYSVLYNSASFSTFKCYGVSPTKLNDLCFTNVYADSFVIRG
DEVRQIAPGQTGKIADYNYKLPDDFTGCVIAWNSNNLDSKVGGNYNYLYRLFRKSN
LKPFERDISTEIYQAGSTPCNGVEGFNCYFPLQSYGFQPTNGVGYQPYRVVVLSFELL
HAPATVCGPKKSTNLVKNKCVNFNFNGLTGTGVLTESNKKFLPFQQFGRDIADTTD
AVRDPQTLEILDITPCSFGGVSVITPGTNTSNQVAVLYQDVNCTEVPVAIHADQLTPT
WRVYSTGSNVFQTRAGCLIGAEHVNNSYECDIPIGAGICASYQTQTNSPRRARSVAS
QSIIAYTMSLGAENSVAYSNNSIAIPTNFTISVTTEILPVSMTKTSVDCTMYICGDSTEC
SNLLLQYGSFCTQLNRALTGIAVEQDKNTQEVFAQVKQIYKTPPIKDFGGFNFSQILP
DPSKPSKRSFIEDLLFNKVTLADAGFIKQYGDCLGDIAARDLICAQKFNGLTVLPPLLT
DEMIAQYTSALLAGTITSGWTFGAGAALQIPFAMQMAYRFNGIGVTQNVLYENQKLI
ANQFNSAIGKIQDSLSSTASALGKLQDVVNQNAQALNTLVKQLSSNFGAISSVLNDIL
SRLDKVEAEVQIDRLITGRLQSLQTYVTQQLIRAAEIRASANLAATKMSECVLGQSK
RVDFCGKGYHLMSFPQSAPHGVVFLHVTYVPAQEKNFTTAPAICHDGKAHFPREGV
FVSNGTHWFVTQRNFYEPQIITTDNTFVSGNCDVVIGIVNNTVYDPLQPELDSFKEEL
DKYFKNHTSPDVDLGDISGINASVVNIQKEIDRLNEVAKNLNESLIDLQELGKYEQYI

KWPWYIWLGFIAGLIAIVMVTIMLCCMTSCCSCLKGCCSCGSCCKFDEDDSEPVLKG
VKLHYT

Protein sequence of lead vaccine candidate

>SARS-CoV-2 SUBUNIT VACCINE CANDIDATE (C19)
EAAAKMTPQNITDLCAEYHNTQIYTLNDKIFSYTESLAGKREMAIITFKNGAIFQVEV
PGSQHIDSQKKAIERMKDTLRIAYLTEAKVEKLCVWNNKTPHAIAAISMANGTEAAA
KAAYNDIISDIGFNSSVITYPDAQLVPGINGKAIHLVNNEAAYGPGPGALDPLSETKGP
GPGNCDVVIGIVGPGPGAAYSNFGAISSVAAYGLTGTGVLTAAYKKALEPLVDLPIGI
KKGIGVTQNVLYENKK

Improved DNA sequence of designed vaccine construct

GAAGCTGCTGCTAAAATGACCCCGCAGAACATCACCGACCTGTGCGCTGAATAC
CACAACACCCAGATCTACACCCTGAACGACAAAATCTTCTCTTACACGAATCTCT
GGCTGGTAAACGTGAAATGGCTATCATCACCTTCAAAAACGGTGCTATCTTCCAG
GTTGAAGTTCCGGGTTCTCAGCACATCGACTCTCAGAAAAAAGCTATCGAACGTA
TGAAAGACACCCTGCGTATCGCTTACCTGACCGAAGCTAAAGTTGAAAAACTGT
GCGTTTGGAACAACAAAACCCCGCACGCTATCGCTGCTATCTCTATGGCTAACGG
TACCGAAGCTGCTGCTAAAGCTGCTTACAACGACATCATCTCTGACATCGGTTTC
AACTCTTCTGTTATCACCTACCCGGACGCTCAGCTGGTTCCGGGTATCAACGGTA
AAGCTATCCACCTGGTTAACAACGAAGCTGCTTACGGTCCGGGTCCGGGTGCTCT
GGACCCGCTGTCTGAAACCAAAGGTCCGGGTCCGGGTAACTGCGACGTTGTTATC
GGTATCGTTGGTCCGGGTCCGGGTGCTGCTTACTCTAACTTCGGTGCTATCTCTTC
TGTTGCTGCTTACGGTCTGACCGGTACCGGTGTTCTGACCGCTGCTTACAAAAAA
GCTCTGGAACCGCTGGTTGACCTGCCGATCGGTATCAAAAAAGGTATCGGTGTTA
CCCAGAACGTTCTGTACGAAAACAAAAAA

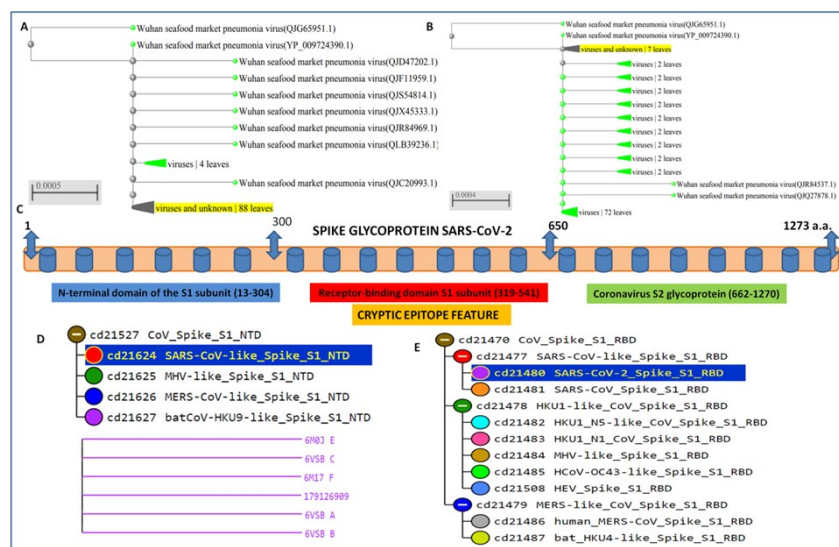**Molecular shreds of evidence of coronavirus infectious sequence**

Figure S1: Assessment of molecular shreds of evidence of coronavirus infectious sequence (A) The protein-protein BLAST sequence analysis through the pairwise tree evaluation methods; Fast minimum evolution method and (B) Neighbor-joining method (C) The Conserved protein domain analysis of spike glycoprotein of SARS CoV-2 (D) Multiple sequence alignment of conserved domain N-terminal domain of S1 subunit of spike glycoprotein, (E) Multiple sequence alignment of conserved domain Receptor binding domain of S1 subunit.

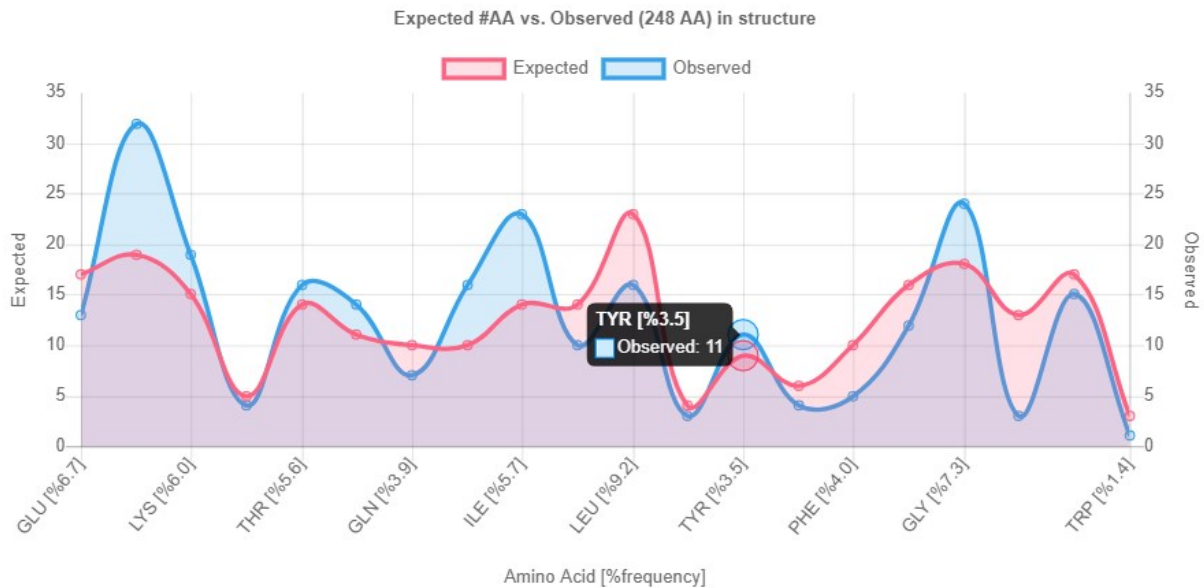## 3D Structural assessments of vaccine construct

Figure S2: 3D structural atomic level local quality estimation of vaccine construct and comparison with known structures (NMR, X-rays based in the database). It showed the good quality of vaccine 3D structure atomic coordinates with significant resemblance to known structures.

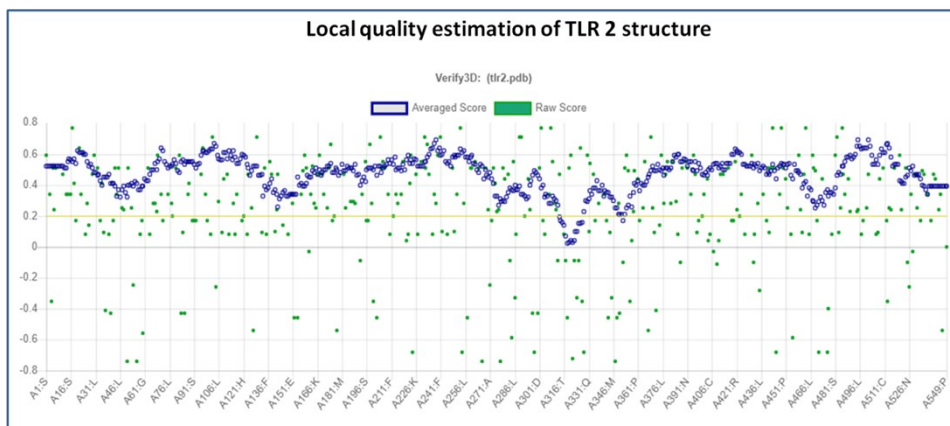## Atomic coordinates local quality estimation of membrane receptor TLR-2

Figure S3: The local quality estimation of TLR-2 atomic coordinates with minimal deviations throughout the whole protein sequence.

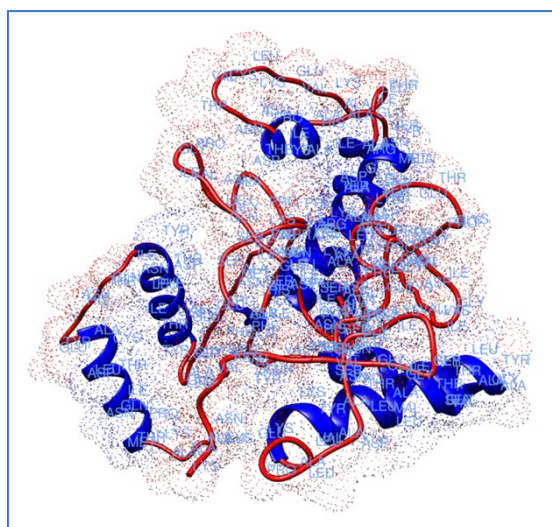**Energy minimized globular structure of designed vaccine construct**

Figure S4: Energy minimized globular structure of developed vaccine construct by Gromacs minimizer; unwanted atoms were removed from the derived structure to minimize the redundancy in the 3D structure.

Molecular dynamics simulation analyses of vaccine construct

The Eigen scores for the complex trajectory of vaccine and TLR-2. The Eigen score (3.053311e-06) represents the motion stiffness of the system and correlates with the deformation of the interacting molecules.
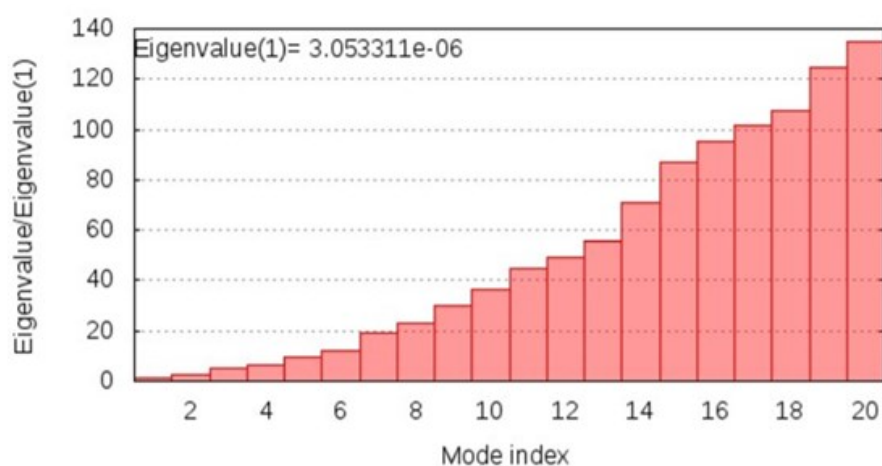

Figure S5: Eigenvalues assessment of the complex trajectory of vaccine construct with the TLR-2 membrane receptor.