

Supporting Information

Milk derived Peptides against SARS CoV-2 Spike Protein Receptor Binding Domain

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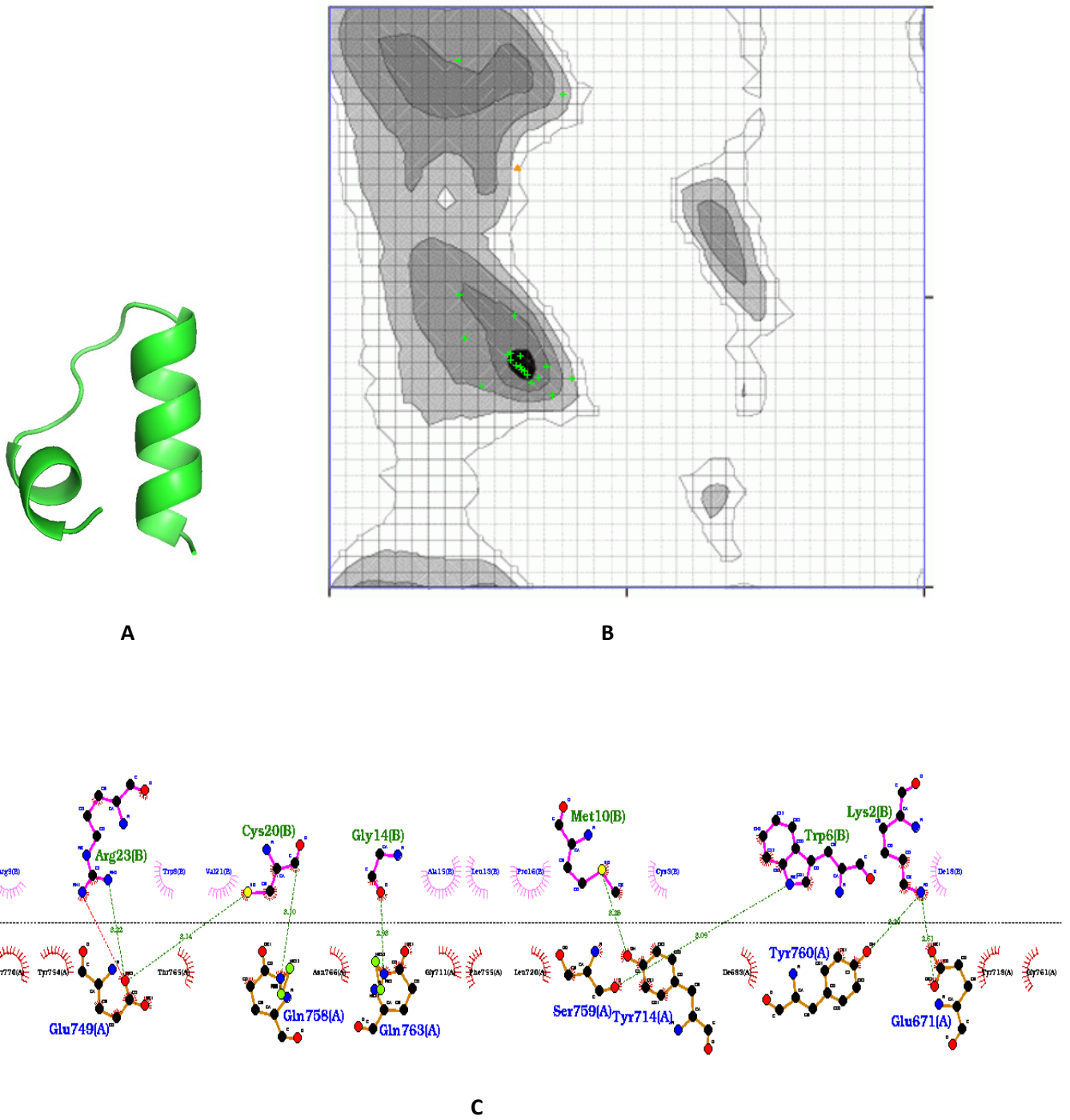
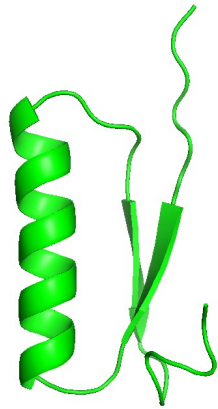
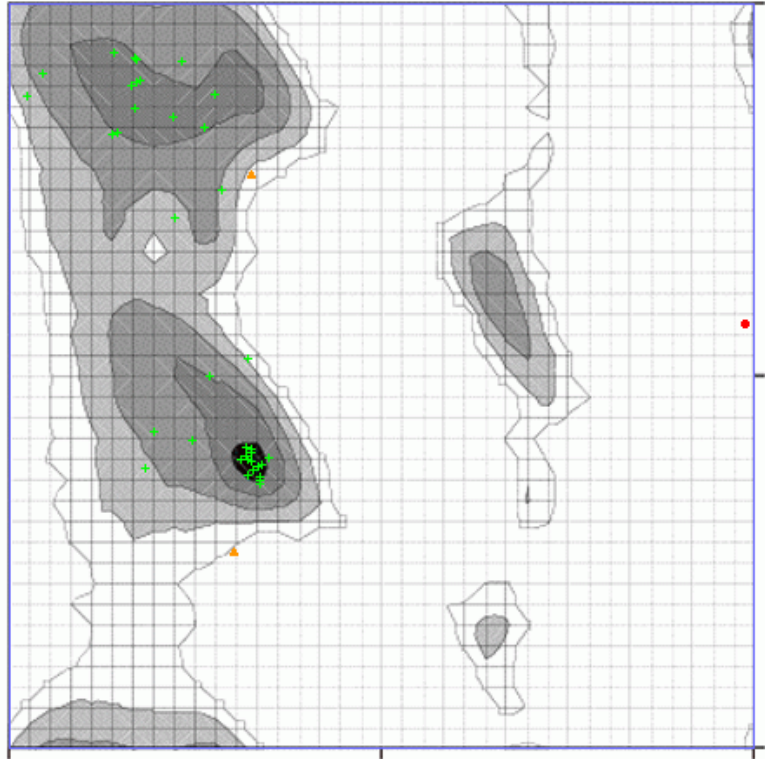


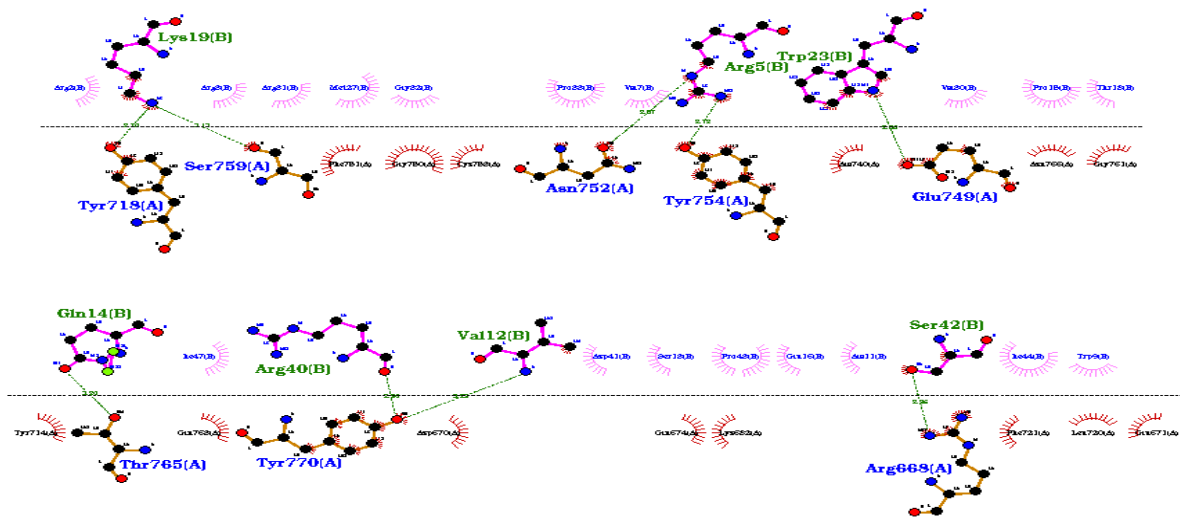
Figure S1: A) 3D structure of Peptide 01, B) Ramachandran plot for Peptide 01, C) Two-dimensional Protein-peptide interaction map between Peptide 01 and SARS-CoV-2 RBD



A

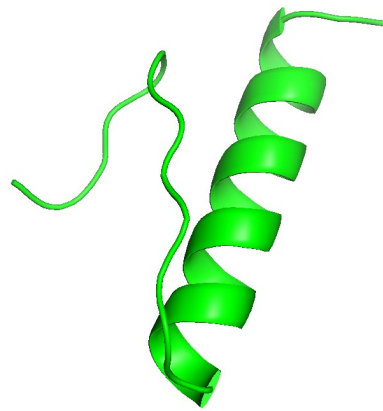


B

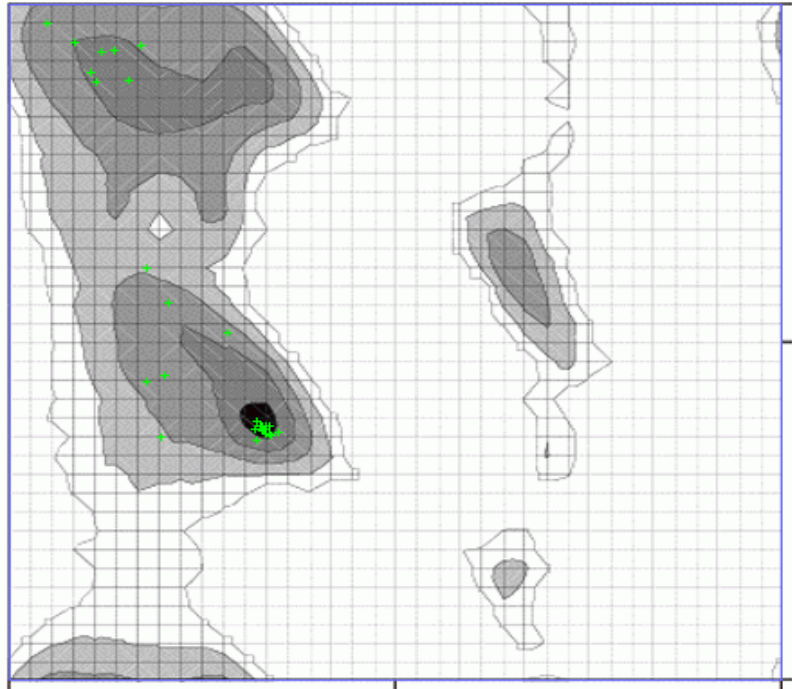


C

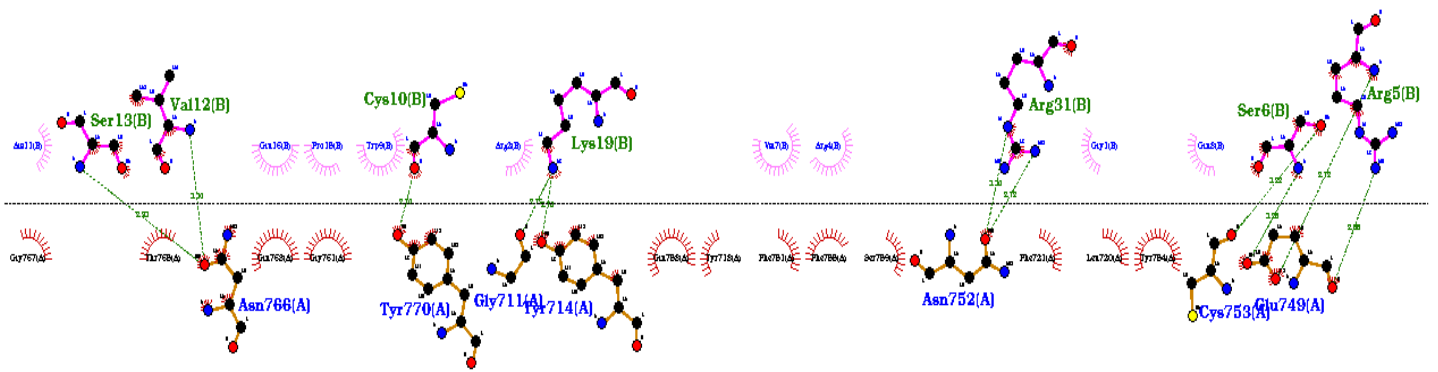
Figure S2: A) 3D structure of Peptide 02, B) Ramachandran plot for Peptide 02, C) Two-dimensional Protein-peptide interaction map between Peptide 02 and SARS-CoV-2 RBD



A

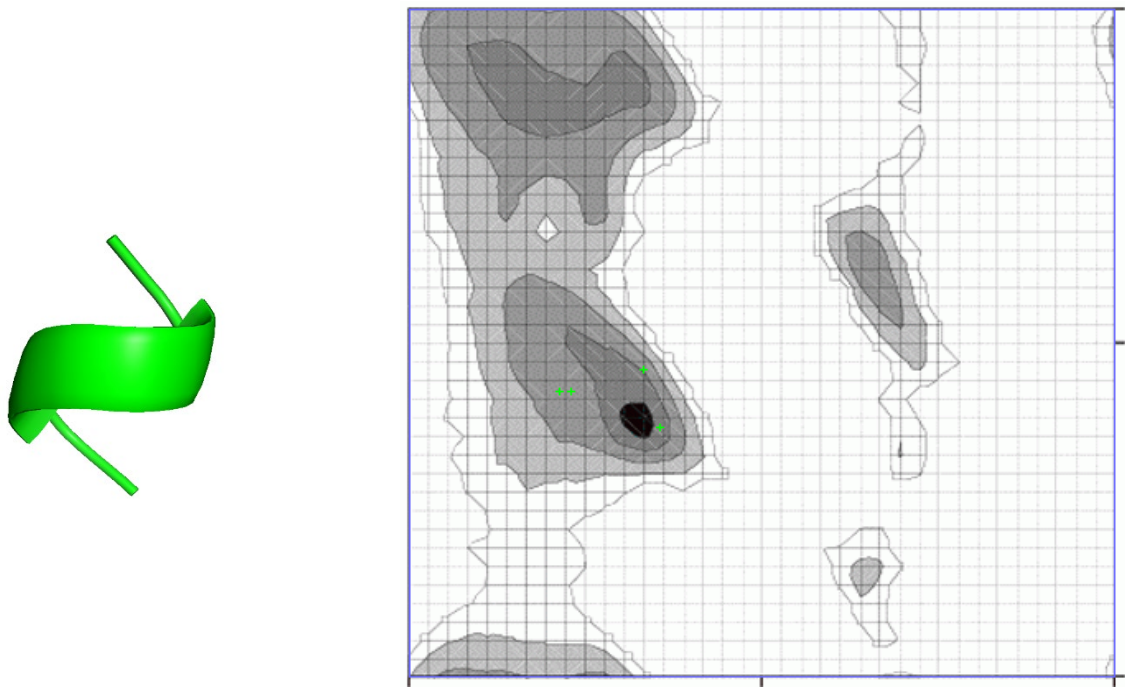


B



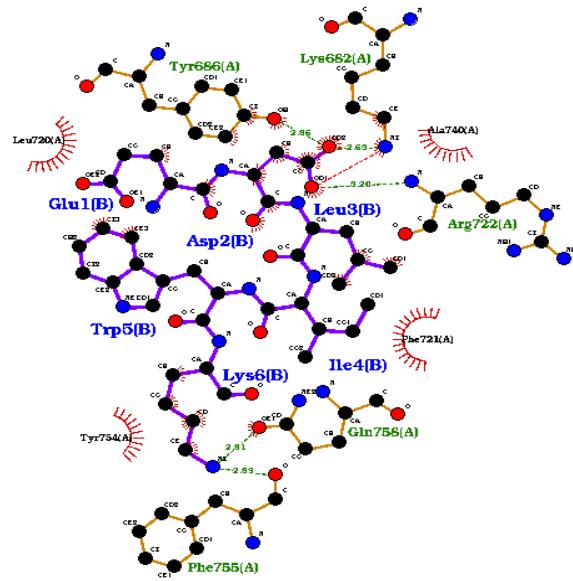
C

Figure S3: A) 3D structure of Peptide 03, B) Ramachandran plot for Peptide 03, C) Two-dimensional Protein-peptide interaction map between Peptide 03 and SARS-CoV-2 RBD



A

B



C

Figure S4: A) 3D structure of Peptide 04, B) Ramachandran plot for Peptide 04, C) Two-dimensional Protein-peptide interaction map between Peptide 04 and SARS-CoV-2 RBD

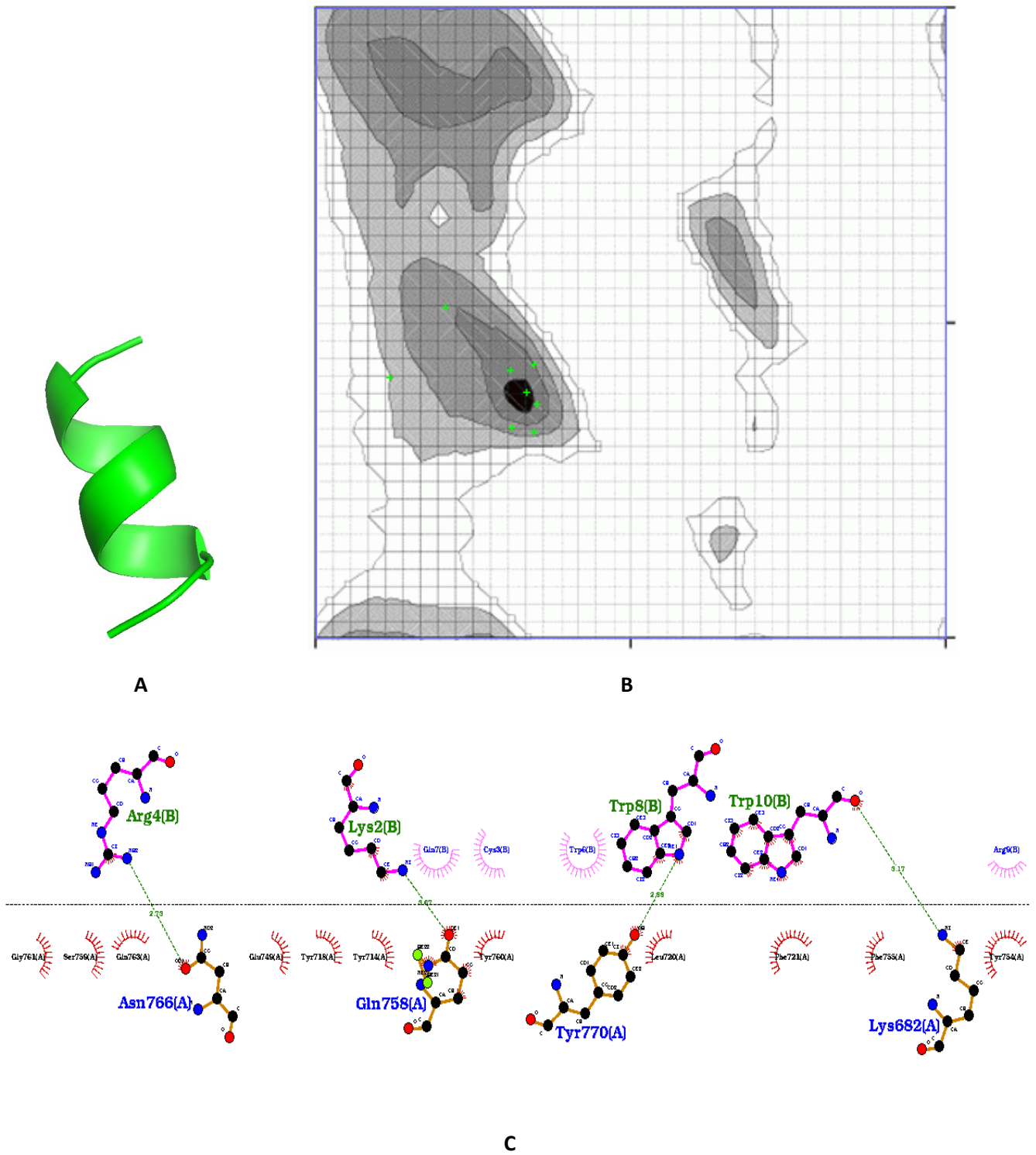


Figure S5: A) 3D structure of Peptide 05, **B)** Ramachandran plot for Peptide 05, **C)** Two-dimensional Protein-peptide interaction map between Peptide 05 and SARS-CoV-2 RBD

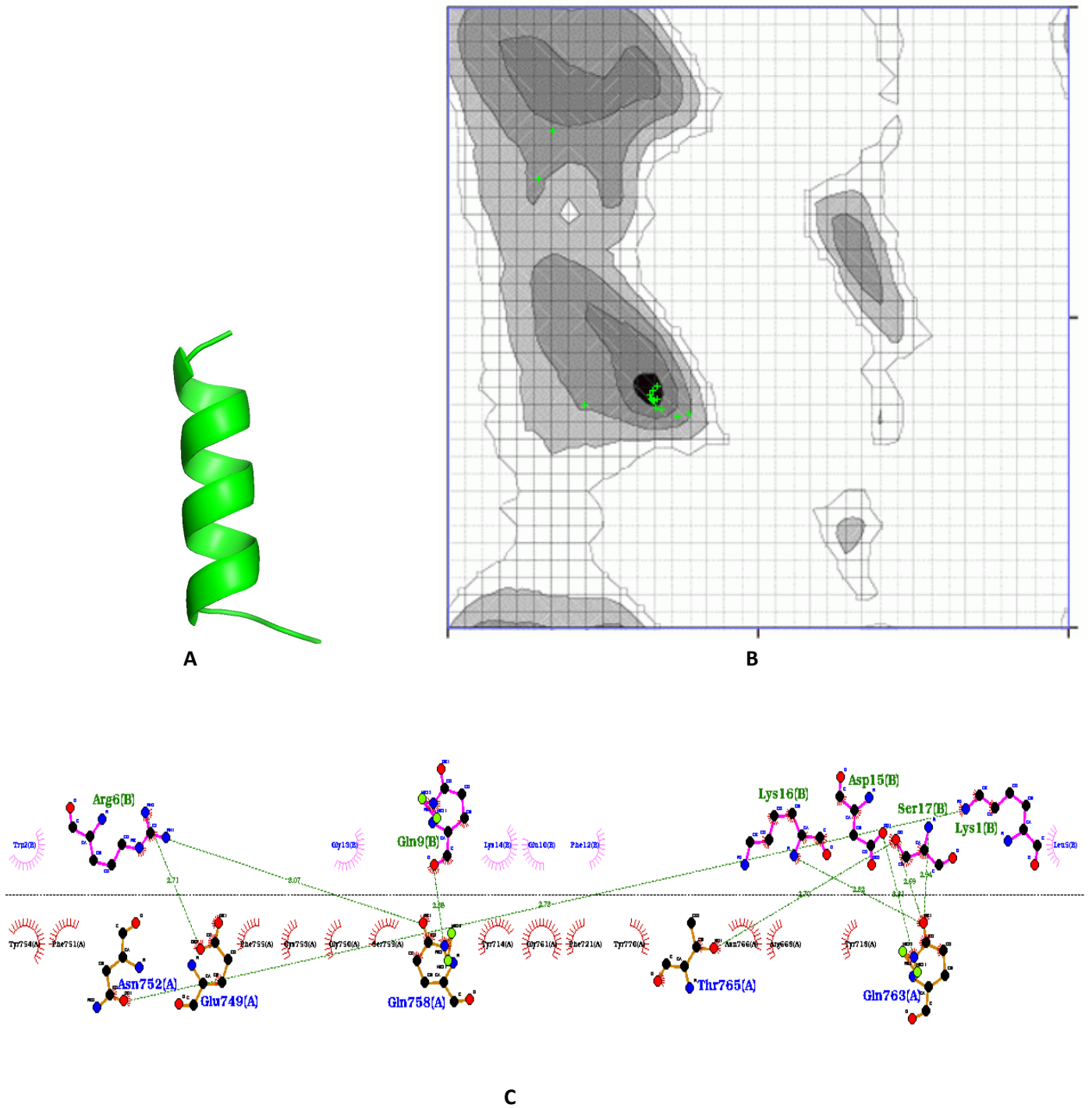


Figure S6: A) 3D structure of Peptide 06, B) Ramachandran plot for Peptide 06, C) Two-dimensional Protein-peptide interaction map between Peptide 06 and SARS-CoV-2 RBD

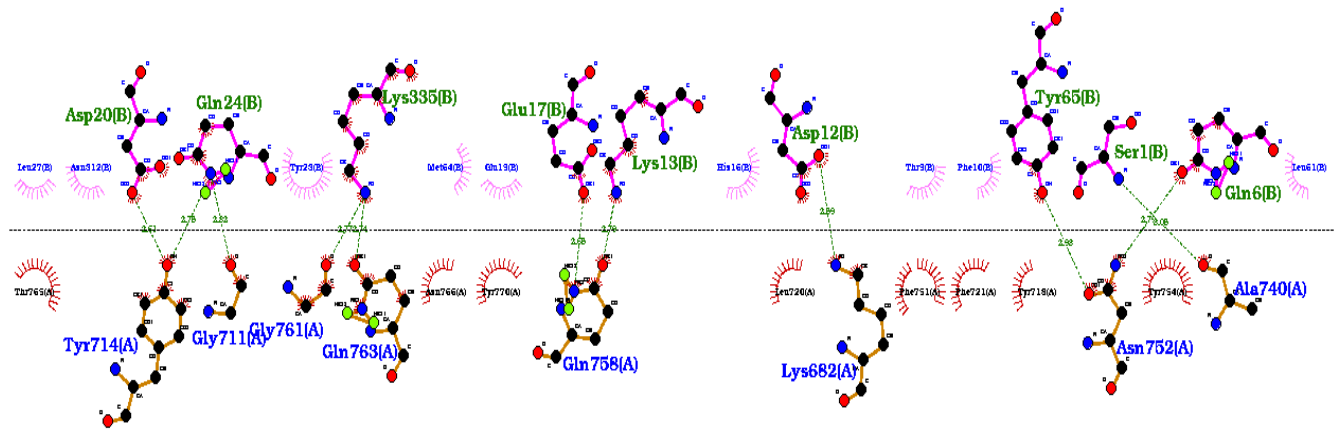


Figure S7: PPI between human ACE2 (B) and SARS-CoV-2 spike protein Receptor Binding Domain (RBD)

| Peptide | HADDOCK score | VdW energy | Electrostatic energy | Desolvation energy | Restraints violation energy | Buried Surface Area | Z-Score |
|-------------------|----------------|---------------|----------------------|--------------------|-----------------------------|---------------------|---------|
| Peptide 01 | -103.6 +/- 1.3 | -52.6 +/- 1.1 | -184.7 +/- 20.3 | -17.5 +/- 0.9 | 35.9 +/- 28.4 | 1570.7 +/- 26.3 | -1.3 |
| Peptide 02 | -102.8 +/- 7.2 | -71.8 +/- 6.7 | -137.5 +/- 24.1 | -27.0 +/- 2.7 | 234.4 +/- 64.5 | 2128.2 +/- 130.5 | -1.5 |
| Peptide 03 | -109.2 +/- 5.5 | -67.7 +/- 5.1 | -195.8 +/- 20.2 | -19.9 +/- 3.6 | 175.4 +/- 15.4 | 1757.5 +/- 56.8 | -1.8 |
| Peptide 04 | -60.4 +/- 2.3 | -20.2 +/- 2.9 | -147.5 +/- 56.3 | -13.1 +/- 5.8 | 24.7 +/- 24.9 | 711.6 +/- 25.2 | -1.8 |
| Peptide 05 | -83.1 +/- 1.9 | -36.0 +/- 4.9 | -155.4 +/- 21.0 | -19.7 +/- 1.6 | 37.4 +/- 13.1 | 1130.3 +/- 32.5 | -1.4 |
| Peptide 06 | -98.1 +/- 2.5 | -51.4 +/- 3.3 | -157.0 +/- 22.9 | -25.0 +/- 2.0 | 96.8 +/- 20.5 | 1351.2 +/- 41.5 | -2.0 |
| Human ACE2 | -134.1 +/- 3.6 | -63.5 +/- 2.5 | -272.2 +/- 13.0 | -22.6 +/- 1.3 | 64.5 +/- 43.8 | 1952.4 +/- 58.3 | -1.0 |

Table S1: Details of HADDOCK scores for all the peptides including human ACE-2