|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **S.No**  **Supplementary Table S2:** Showing obtained molecular docking interaction results between Tat-peptide conjugated Ritonavir, Lopinavir, Favipiravir, hydroxychloroquine complex an receptor molecules i.e., COVID-19 Main protease (PDB ID: 6LU7). PatchDock tool has been used for the analysis | **Receptor** | **Drug-Peptide Complex** | **PatchDock Score** | **Atomic Contact Energy (ACE)** | **Hydrogen Bonds** | **Hydrogen Bonds Length**  **(Angstrom)** |
| 1. | COVID-19 (PDB ID: 6LU7) | Ritonavir-TAT –peptide Complex | 7580 | 67.93 | TAT:ARG6:HE - :Rito:S8 | 1.80218 |
| TAT:ARG7:HH21 - :Rito:O20 | 1.49997 |
| TAT:ARG9:HH12 - 6LU7:ALA285:O | 2.29131 |
| TAT:ARG10:HH22 - 6LU7:LEU272:O | 2.08491 |
| :Rito:H73 - TAT:LYS4:O | 2.37923 |
| :Rito:H93 - TAT:GLN8:OE1 | 1.9401 |
| TAT:ARG11:CD - 6LU7:THR198:O | 3.15358 |
| :Rito:C11 - 6LU7:TYR237:O | 3.57386 |
|  |  |  |  |  |  |  |
| 2. |  | Lopinavir-TAT –peptide Complex | 8048 | 271.51 | 6LU7:ASN142:HD21 - TAT:ARG11:O1 | 2.67485 |
| 6LU7:GLN189:HE22 - TAT:ARG3:O | 1.54847 |
| TAT:ARG3:HE - 6LU7:GLN189:O | 2.89743 |
| TAT:LYS5:HZ2 - :Lopi:O12 | 2.99674 |
| TAT:ARG10:HE - 6LU7:HIS164:O | 2.96789 |
| TAT:ARG10:HH22 - 6LU7:MET165:SD | 2.19746 |
| TAT:ARG7:CD - 6LU7:SER46:O | 2.78575 |
| TAT:ARG9:CA - 6LU7:ASN142:OD1 | 1.65167 |
| TAT:ARG10:CD - 6LU7:GLN189:OE1 | 3.62586 |
| :Lopi:C22 - TAT:LYS5:O | 2.35787 |
|  |  |  |  |  |  |  |
| 3. |  | Favipiravir-TAT –peptide Complex | 8002 | 116.00 | 6LU7:THR26:HN - TAT:TYR1:OH | 1.50888 |
| 6LU7:GLN189:HE22 - :Favi:F11 | 2.46955 |
| TAT:GLY2:HN - 6LU7:LEU141:O | 2.41196 |
| TAT:LYS5:HZ3 - 6LU7:HIS164:O | 1.69143 |
| TAT:ARG6:HH22 - 6LU7:PHE140:O | 2.52753 |
| TAT:ARG7:HH21 - :Favi:O9 | 2.02048 |
| TAT:ARG11:HH21 - :Favi:O9 | 2.78456 |
| :Favi:H14 - TAT:LYS4:O | 1.93022 |
| TAT:ARG9:CD - 6LU7:THR190:O | 3.16832 |
| 6LU7:SER46:HG - :Favi | 2.92903 |
|  |  |  |  |  |  |  |
| 4. |  | Hydroxychloroquine –TAT –peptide Complex | 8116 | 333.64 | 6LU7:ASN142:HD22 - TAT:GLN8:O | 2.23048 |
| 6LU7:ASN142:HD22 - TAT:ARG11:O1 | 2.98244 |
| 6LU7:GLN189:HE21 - TAT:ARG3:O | 3.0788 |
| TAT:LYS5:HZ3 - 6LU7:PRO168:O | 1.80031 |
| TAT:ARG6:HE - 6LU7:ARG188:O | 2.66915 |
| TAT:ARG6:HH12 - 6LU7:THR190:O | 2.86354 |
| TAT:ARG6:HH21 - 6LU7:ARG188:O | 2.49066 |
| TAT:ARG6:HH22 - 6LU7:THR190:O | 0.962947 |
| TAT:ARG9:HH11 - 6LU7:LEU141:O | 2.56889 |
| TAT:ARG9:HH22 - 6LU7:HIS164:O | 3.03703 |
| :HCI:H39 - TAT:LYS5:O | 2.28866 |
| :HCI:H49 - TAT:LYS4:O | 1.99287 |
| TAT:ARG10:CD - 6LU7:GLN189:OE1 | 2.77669 |
| :HCI:C21 - TAT:GLN8:OE1 | 3.4198 |
| :HCI:C18 - 6LU7:GLU166:OE1 | 2.38878 |
|  |  |