|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| S. No  **Supplementary Table S1:** Showing obtained molecular docking interaction results between repurposed drugs i.e., Ritonavir, Lopinavir, Favipiravir, Hydroxychloroquine and receptor molecules i.e., COVID-19 Main protease (PDB ID: 6LU7). Autodock 4.2 tool has been used for the analysis | Drugs | Binding Energy | Inhibition Constant | Hydrogen Bond | Hydrogen Bond Length | Residues participating in hydrophobic interaction |
| 1. | Ritonavir | -9.16 kcal/mol | 28.94 uM | :UNK1:H73 - A:PHE140:O | 2.02341 | Gly138,Ser139,Phe140,Leu141,  Asn142,Ser144,His163,Glu166  ,Gly170,His172 |
| :UNK1:H93 - A:ASN142:OD1 | 2.75639 |
| :UNK1:H98 - A:ASN142:OD1 | 2.4961 |
| :UNK1:C11 - A:SER139:OG | 3.10324 |
| :UNK1:C48 - A:GLU166:O | 3.32189 |
|  |  |  |  |  |  |  |
| 2. | Lopinavir | -7.57 kcal/mol | 198.12 uM | A:PHE140:HN - :UNK1:O46 | 2.35676 | Gly138,Ser139,Phe140,  Leu141,Asn142,His163,  Met165,Glu166,Gly170,  His172 |
| :UNK1:H58 - A:GLU166:OE2 | 1.7891 |
| :UNK1:H94 - A:GLU166:OE2 | 1.8134 |
| :UNK1:C10 - A:GLU166:OE1 | 3.16433 |
|  |  |  |  |  |  |  |
| 3. | Favipiravir | -4.23 kcal/mol | 1.42 mM | A:SER144:HN - :UNK1:F11 | 2.51321 | Phe140,Leu141,Asn142,Gly143  ,Ser144,Cys145,His163,Met165  ,Glu166,His172 |
| A:CYS145:HN - :UNK1:F11 | 2.11964 |
| A:HIS163:HE2 - :UNK1:N3 | 2.49337 |
| A:HIS163:HE2 - :UNK1:O9 | 1.9061 |
| :UNK1:H13 - A:ASN142:OD1 | 2.33961 |
| :UNK1:H14 - A:PHE140:O | 2.27441 |
| :UNK1:H15 - A:GLU166:OE2 | 1.85067 |
| A:HIS172:CD2 - :UNK1:O9 | 3.09327 |
| 4. | Hydroxychloroquine | -6.61 kcal/mol | 217.55 uM | :UNK1:H39 - A:HIS164:O | 2.00571 | Thr25,His41,Met49,Phe140,  Leu141,Asn142,Gly143,Ser144  ,Cys145,His163,His164,Met165  ,Glu166,His172,Gln189 |
| A:ASN142:CA - :UNK1:N17 | 3.4968 |