**Supplementary Table S3:** Showing comparative interaction (H-bonds) between main protease and drugs, TAT-peptide and drugs and TAT-peptide conjugated drugs and main protease (PDB ID: 6LU7).

|  |  |  |
| --- | --- | --- |
| **Interactions** | **Drugs** | **Formed H-bonds** |
| **Main protease**  **(PDB ID: 6LU7)** | Ritonavir | 5 |
|
| Lopinavir | 4 |
|
| Favipiravir | 8 |
| Hydroxychloroquine | 2 |
|
| **TAT-peptide** | Ritonavir | 4 |
| Lopinavir | 1 |
| Favipiravir | 3 |
| Hydroxychloroquine | 2 |
| **Main protease** **( PDB ID: 6LU7)** |  **TAT-peptide conjugated drug complex** |
| TAT-peptide conjugated Ritonavir | 8 |
| TAT-peptide conjugated Lopinavir | 10 |
| TAT-peptide conjugated Favipiravir | 10 |
| TAT-peptide conjugated Hydroxychloroquine | 15 |