**Table 2** Binding energy for the formation of complex between the compounds and the protease of SARS-CoV-2, against COVID-19

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Name of the compound** | **Docked pose** | **Π Interactions** | | **Hydrogen Bond Interactions** | | **Binding affinity (kcal/mol)** |
| **Amino acids** | **Distance (Å)** | **Amino acids** | **Distance (Å)** |
| Acyclovir, **CMPD1** |  | GLU\_166 | 3.93 | GLU\_166  GLN\_189 | 5.07, 4.27, 3.90, 3.77,  3.58 | -3.92 |
| Ganciclovir, **CMPD2** |  | MET\_165  MET\_49 | 7.03  5.78, 4.36 | MET\_165  GLN\_189  HIE\_41 | 3.77,  4.38,  3.53, | -3.74 |
| **CMPD3** |  | CYS\_145 | 5.63 | CYS\_145  LEU\_141  GLU\_166  HIE\_163  MET\_165  ARG\_188  HIE\_41 | 3.93,  6.36,  4.29,  5.44,  3.41,  5.93,  4.94 | -4.34 |