**S5 Table.** GOLD docking scores of proposed medicinal compounds with additional phytochemicals docked in the active cavity of 3CLpro.

|  |  |  |  |
| --- | --- | --- | --- |
| **Fitness** | **S(hb\_ext)** | **S(vdw\_ext)** | **Ligand Name** |
| 37.48 | 0.11 | 27.79 | Xanthoangelol\_E |
| 36.07 | 0.00 | 31.36 | Hesperetin |
| 25.18 | 0.08 | 19.39 | Beta-sitoterol |
| 23.65 | 0.00 | 23.60 | Calceolarioside\_B |
| -68.88 | 0.25 - | -40.39 | Isobavachalcone |
| -203.58 - | 0.03 | 138.79 | PapyriflavonolA |