**Table 6. Molecular Docking of selected phytoligands and standard chemotherapeutic agent with SARS-CoV-2 viral virulence factors.**

| **Ligand / Standard**  | **Chemical structure†** | **E Value (Kcal/mol)**§ |
| --- | --- | --- |
| Main Protease 3CLpro | Spike glycoprotein | NSP15 endoribonuclease |
| Allicin  | Allicin.png | -121.34 | -108.38 | -157.34 |
| Berberine  | Berberine.png | -211.64 | -179.51 | -240.83 |
| Beta-caryophyllene  | Beta-caryophyllene.png | -129.23 | -132.62 | -176.22 |
| 11-keto-beta-boswellic acid  | 11-keto-beta-boswellic acid.png | -253.66 | -199.35 | -269.92 |
| Citronellal  | Citronellal.png | -139.41 | -134.74 | -160.92 |
| Curcumin  | Curcumin.png | -213.59 | -197.87 | -247.25 |
| Gamma-Glutamyl-S-allylcysteine  | Gamma-Glutamyl-S-allylcysteine.png | -493.53 | -578.57 | -825.00 |
| 6-Gingerol  | 6-Gingerol.png | -199.85 | -178.86 | -221.35 |
| Quercetin  | Quercetin.png | -189.57 | -158.27 | -204.25 |
| Salvianolic acid  | Salvianolic acid.png | -261.56 | -223.97 | -275.44 |
| Tinosporaside | tinospo.png | -233.14 | -223.92 | -268.79 |
| Withanolide  | Withanolide.png | -207.18 | -214.98 | -253.37 |
| Hydroxy-chloroquine | chloroquine.png | -235.48 | -207.47 | -213.54 |

†Chemical structures have been derived from PubChem (https://pubchem.ncbi.nlm.nih.gov/); §ΔGbinding = ΔGcomplex – (ΔGreceptor + ΔGligand); Grey shaded cells indicate highly significant E value of docking as compared to the standard chemotherapeutic agent; Green shaded cells indicate holistic phytoligands exhibiting optimum E value for all the three selected viral virulence factors (These phytoligands have been further analysed for salt-bridge analysis and electrostatic interactions).