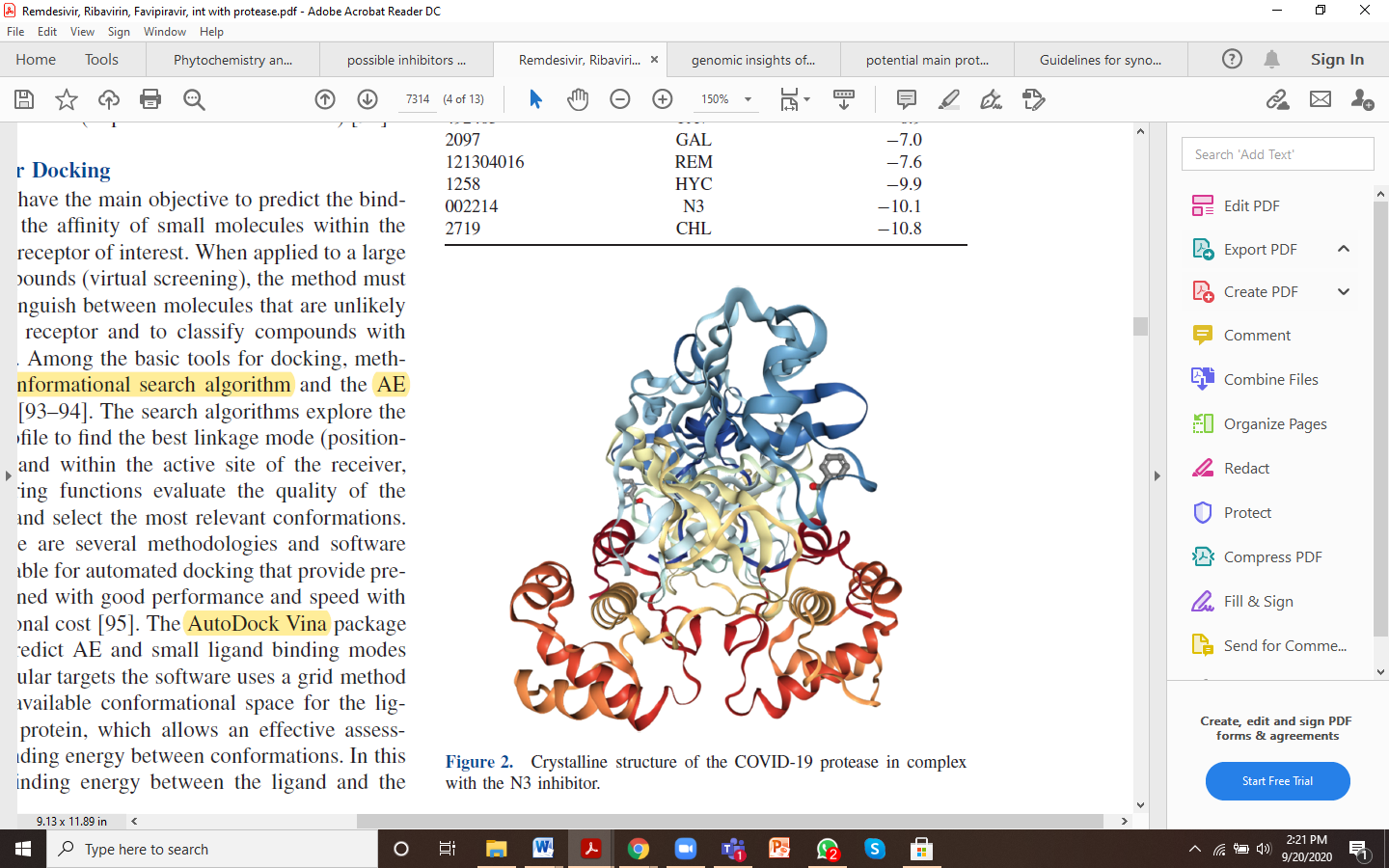
**Supplementary Figure S1.** Crystal structure of SARS-CoV-2 3CL-Pro bound with the native ligand N3 (PDB ID: 6LU7)



**Supplementary Figure S2.** Two dimensional and three dimensional interactions of selected C. citratus compounds with 6LU7, along with the name and position of interacting amino acids, type of bond, calculated distances and energies.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **2D Interactions** | **Amino acids** | **Type** | **Distance** | **Energy** | **3D Interactions** |
| **Tannic acid** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Tannins\tannins_6lu7_2d_white.jpg | MET165 | H-donor | 4.05 | -1.0 | C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Tannins\tannins_6lu7_3d.png |
| GLU166 | H-acceptor | 3.02 | -1.2 |
| THR26 | H-acceptor | 3.06 | -1.6 |
| **Swertiajaponin** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Swertiajaponin\swertiajaponin_6lu7_2d_white.jpg | THR 190 | H-donor | 2.84 | -1.1 |  |
| GLU 166 | H-donor | 2.62 | -1.4 |
| **Chlorogenic acid** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Chlorogenic acid\third attempt_best result\chlorogenic acid_6lu7_2d.jpg | GLU 166 | H-acceptor | 3.01 | -1.8 | C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Chlorogenic acid\third attempt_best result\chlorogenic acid_6lu7_3d.png |
| **Cymbopogonol** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Cymbopogonol\cymbopogonol_6lu7_2d_white.jpg | GLN 189 | H-acceptor | 3.03 | -2.1 |  |
| **Warfarin** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Warfarin\warfarin_6lu7_2d_white.jpg | GLY 143 | H-acceptor | 3.10 | -1.8 | A picture containing outdoor object  Description automatically generated |
| **Citral diethyl acetal** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Citral diethyl acetal\citral diethyl acetal_6lu7_2d_white.jpg | HIS 41 | H-pi | 4.32 | -1.1 | A picture containing outdoor object  Description automatically generated |
| **Citral acetate** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Acetyl (2E)-3,7-dimethylocta-2,6-dienoate\acetyl_dimethylocta_6lu7_2d_white.jpg | GLY 143 | H-acceptor | 2.95 | -3.6 | A picture containing hydrozoan  Description automatically generated |
| SER 144 | H-acceptor | 2.96 | -1.3 |
| **Luteolin** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Luteolin\luteolin_6lu7_2d_white.jpg | LEU 141 | H-donor | 3.05 | -1.1 |  |
| MET 165 | H-donor | 3.61 | -1.8 |
| **Kaempferol** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Kaempferol\kaempferol_6lu7_2d_white.jpg | LEU 141 | H-donor | 3.18 | -1.0 |  |
| ASP 187 | H-donor | 2.91 | -1.1 |
| GLN 189 | pi-H | 4.17 | -0.7 |
| **Cianidanol** | | | | | |
| C:\Users\Tuba Ahmad\Desktop\Thesis MPhil\MOE\Cianidanol\cianidanol_6lu7_2d_white.jpg | GLU 166 | H-donor | 3.23 | -1.2 | A picture containing outdoor object  Description automatically generated |
| HIS 41 | H-pi | 3.92 | -1.5 |