**Supplementary Table S3**. Binding energy of selected ligands obtained by docking based virtual screening using PyRx software.

|  |  |  |  |
| --- | --- | --- | --- |
| **Sl No.** | **Molecule ID** | **Ligands name** | **Binding energy (kcal/mol)** |
| 1 | 71597391 | Triterpenoids | **-9.8\*** |
| 2 | 54685921 | Hispidin | **-8.2\*** |
| 3 | 5460957 | Phenylalanine | -6.2 |
| 4 | 5281697 | Scutellarein | **-8.7\*** |
| 5 | 3084390 | Sorbifolin | **-8.6\*** |
| 6 | 446611 | 2,4-Dihydroxycinnamic acid | -6.3 |
| 7 | 240122 | Guaiol acetate | **-8.0\*** |
| 8 | 151467 | 4',5'-dihydropsoralen | -7.2 |
| 9 | 147362 | 4,6-O-Benzylidene-D-glucose | -7.7 |
| 10 | 51283 | Dl-alanine-15n | -4.0 |
| 11 | 26305 | Nodakenetin | **-8.1\*** |
| 12 | 12209 | 2-methylbutyl acetate | -4.4 |
| 13 | 10494 | Oleanolic acid | **-10.5\*** |
| 14 | 10212 | Imperatorin | **-8.2\*** |
| 15 | 7963 | 4-methylpyridine | -4.7 |
| 16 | 6306 | L-isoleucine | -5.3 |
| 17 | 6212 | Chloroform | -2.8 |
| 18 | 6199 | Psoralen | -7.2 |
| 19 | 2355 | Bergapten | -7.1 |

\*The ligands showing binding energy of ≥8 kcal/mol were selected for site specific molecular docking.