**Table1:** Free binding energy (Kcal/mol) scores of best 5 interacting synthetic drugs, microbial compounds and phytochemicals with the FH domain of the FOXP4**.**

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Ligands** | **ID** | **Name** | **Origin** | **Estimated**  **Free Energy**  **of Binding**  (kcal/mol) | **Estimated Inhibition Constant** | **Final Intermolecular Energy**  (kcal/mol) | **vdW + Hbond +**  **desolv.Energy**  (kcal/mol) | **Electrostatic**  **Energy**  (kcal/mol) | **Final Total**  **Internal**  **Energy (**kcal/mol**)** | **Torsional Free Energy**  (kcal/mol) | **Unbound**  **System's**  **Energy**  (kcal/mol) |
| Group I | D04NTJ | Glisoxepide | Synthetic Drug | -10.81 | 11.89 nM | -11.41 | -11.41 | +0.00 | -2.07 | +0.60 | -2.07 |
|  | D04XGX | 2-(2-Methoxybenzyl)-3H-benzo[f]chromen-3-one | Synthetic Drug | -10.06 | 41.98 nM | -10.66 | -10.66 | +0.00 | -1.06 | +0.60 | -1.06 |
|  | D04JWS | NSC-292213 | Synthetic Drug | -10.03 | 44.56 nM | -10.63 | -10.63 | +0.00 | -1.45 | +0.60 | -1.45 |
|  | D0G6DH | GTPL7056 | Synthetic Drug | -9.96 | 50.35 nM | -10.55 | -10.55 | +0.00 | -2.54 | +0.60 | -2.54 |
|  | D01KIU | PRE-084 | Synthetic Drug | -9.85 | 60.22 nM | -10.45 | -10.45 | +0.00 | -2.89 | +0.60 | -2.89 |
| Group II | NPA001319 | Kapurimycin A3 | *Streptomyces sp.* | -10.33 | 26.85 nM | -10.93 | -10.93 | +0.00 | -2.23 | +0.60 | -2.23 |
|  | NPA032555 | Grecoketide B | *Streptomyces sp.* | -10.05 | 43.04 nM | -10.65 | -10.65 | +0.00 | -3.63 | +0.60 | -3.63 |
|  | NPA026752 | Ustilanthracin B | *Ustilaginoidea virens* | -9.87 | 58.41 nM | -10.46 | -10.46 | +0.00 | -3.08 | +0.60 | -3.08 |
|  | NPA033274 | Calidoustene B | *Aspergillus calidoustus* | -9.72 | 74.88 nM | -10.32 | -10.32 | +0.00 | -1.24 | +0.60 | -1.24 |
|  | NPA012010 | Retipolide D | *Retiboletus retipes* | -9.64 | 85.25 nM | -10.24 | -10.24 | +0.00 | -1.79 | +0.60 | -1.79 |
| Group III | TIP003072 | [Cucurbitacin B](https://cwtung.kmu.edu.tw/tipdb/link_chemical2.php?Tipid=TIP003072&Chemical=Cucurbitacin%20B) | *Begonia nantoensis* | -8.41 | 683.74 nM | -9.01 | -8.99 | -0.02 | -1.76 | +0.60 | -1.76 |
|  | TIP005096 | [Methyl pheophorbide b](https://cwtung.kmu.edu.tw/tipdb/link_chemical2.php?Tipid=TIP005096&Chemical=Methyl%20pheophorbide%20b) | *Diospyros kaki* | -8.09 | 1.18 uM | -8.68 | -8.65 | -0.03 | -1.10 | +0.60 | -1.10 |
|  | TIP008465 | [Asparacosin A](https://cwtung.kmu.edu.tw/tipdb/link_chemical2.php?Tipid=TIP008465&Chemical=Asparacosin%20A) | *Asparagus cochinchinensis* | -7.83 | 1.81 uM | -8.43 | -8.21 | -0.22 | -0.26 | +0.60 | -0.26 |
|  | TIP003074 | [Cucurbitacin F](https://cwtung.kmu.edu.tw/tipdb/link_chemical2.php?Tipid=TIP003074&Chemical=Cucurbitacin%20F) | *Begonia nantoensis* | -7.53 | 3.04 uM | -8.12 | -7.97 | -0.16 | -2.29 | +0.60 | -2.29 |
|  | TIP013175 | [25R-Spirostan-4-ene-3,6,12-trione](https://cwtung.kmu.edu.tw/tipdb/link_chemical2.php?Tipid=TIP013175&Chemical=25R-Spirostan-4-ene-3%2C6%2C12-trione) | *Tribulus terrestris* | -7.53 | 3.03 uM | -8.13 | -8.02 | -0.10 | +0.00 | +0.60 | +0.00 |