**Table S2**: Secondary Virtual screening of 1150 compounds with binding energy value by PyRxk software

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Sr.No.** | **Ligand Name** | **Binding Energy (kcal/mol)** | **Sr.No.** | **Ligand Name** | **Binding Energy**  **(kcal/mol)** |
|  | IMPHY010294 | -9.8 |  | IMPHY009130 | -8 |
|  | IMPHY010989 | -9.8 |  | IMPHY009446 | -8 |
|  | IMPHY007737 | -9.7 |  | IMPHY009648 | -8 |
|  | IMPHY017577 | -9.5 |  | IMPHY010191 | -8 |
|  | IMPHY005775 | -9.4 |  | IMPHY010356 | -8 |
|  | IMPHY005976 | -9.4 |  | IMPHY010432 | -8 |
|  | IMPHY010476 | -9.4 |  | IMPHY010647 | -8 |
|  | IMPHY009003 | -9.3 |  | IMPHY010658 | -8 |
|  | IMPHY009364 | -9.3 |  | IMPHY010673 | -8 |
|  | IMPHY000317 | -9.2 |  | IMPHY010731 | -8 |
|  | IMPHY001575 | -9.2 |  | IMPHY010912 | -8 |
|  | IMPHY004140 | -9.2 |  | IMPHY010931 | -8 |
|  | IMPHY005667 | -9.2 |  | IMPHY011387 | -8 |
|  | IMPHY006318 | -9.2 |  | IMPHY011390 | -8 |
|  | IMPHY009308 | -9.2 |  | IMPHY011921 | -8 |
|  | IMPHY002477 | -9.1 |  | IMPHY011924 | -8 |
|  | IMPHY002751 | -9.1 |  | IMPHY011951 | -8 |
|  | IMPHY003078 | -9.1 |  | IMPHY011996 | -8 |
|  | IMPHY004515 | -9.1 |  | IMPHY012234 | -8 |
|  | IMPHY004849 | -9.1 |  | IMPHY012527 | -8 |
|  | IMPHY004968 | -9.1 |  | IMPHY012576 | -8 |
|  | IMPHY006882 | -9.1 |  | IMPHY012886 | -8 |
|  | IMPHY007736 | -9.1 |  | IMPHY013094 | -8 |
|  | IMPHY009067 | -9.1 |  | IMPHY013217 | -8 |
|  | IMPHY009264 | -9.1 |  | IMPHY013231 | -8 |
|  | IMPHY000366 | -9 |  | IMPHY013449 | -8 |
|  | IMPHY002011 | -9 |  | IMPHY013599 | -8 |
|  | IMPHY003352 | -9 |  | IMPHY014394 | -8 |
|  | IMPHY003563 | -9 |  | IMPHY014422 | -8 |
|  | IMPHY005266 | -9 |  | IMPHY014700 | -8 |
|  | IMPHY005785 | -9 |  | IMPHY015465 | -8 |
|  | IMPHY007735 | -9 |  | IMPHY000055 | -7.9 |
|  | IMPHY008834 | -9 |  | IMPHY000118 | -7.9 |
|  | IMPHY010508 | -9 |  | IMPHY000119 | -7.9 |
|  | IMPHY011941 | -9 |  | IMPHY000265 | -7.9 |
|  | IMPHY014146 | -9 |  | IMPHY000290 | -7.9 |
|  | IMPHY014170 | -9 |  | IMPHY000537 | -7.9 |
|  | IMPHY002121 | -8.9 |  | IMPHY000559 | -7.9 |
|  | IMPHY002382 | -8.9 |  | IMPHY000579 | -7.9 |
|  | IMPHY003529 | -8.9 |  | IMPHY000590 | -7.9 |
|  | IMPHY004739 | -8.9 |  | IMPHY000636 | -7.9 |
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|  | IMPHY009786 | -8.9 |  | IMPHY001311 | -7.9 |
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