|  |  |  |  |
| --- | --- | --- | --- |
| **S. No.** | **Vina Score** | **Centre** | **Size** |
|  |  | ***x*** | ***y*** | ***z*** | ***x*** | ***y*** | ***z*** |
| 1 | -7.2 | -7 | 56 | 72 | 27 | 27 | 27 |
| 2 | -6.8 | 8 | 32 | 43 | 27 | 27 | 27 |
| 3 | -6.5 | 16 | 20 | 64 | 27 | 27 | 27 |
| 4 | -6.1 | 12 | 24 | 70 | 27 | 27 | 27 |
| 5 | -6 | -12 | 33 | 81 | 27 | 27 | 27 |

**Table S2. Docking table for PeqPKS01:** Showing Free Energy of binding of the ligand to the protein and spatial coordinates of the ligand within the protein’s pockets.