**Supplementary Table 1**. The ranking of binding pocket scores in molecular docking.

|  |  |  |
| --- | --- | --- |
| **Ranking** | **Binding Affinity (-kcal/mol)** | **Pocket** |
| 1 | 27.03 | 3 |
| 2 | 26.73 | 1 |
| 3 | 22.52 | 2 |
| 4 | 15.67 | 4 |
| 5 | 14.51 | 5 |
| 6 | 13.85 | - |
| 7 | 11.60 | - |
| 8 | 10.70 | - |