**Table S2.** Demonstrate the predicted value of DeepBindPoc on the decoys of extra test C (6QTN and 5ZG2). The fpocket prediction value was given for comparison. The normalized strategy is based on the training set. The pocket\_A and pocket\_B are top predicted pocket of 6QTN by DeepBindPoc score for GTP and ACP, respectively. The pocket\_C and pocket\_D are the top predicted pockets of 5ZG2 by DeepBindPoc score for ZKI and 9C0, respectively.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pocket\_A** | **DeepBindPoc Score（GTP as ligand）** | **Fpocket Score**  | **Pocket\_B** | **DeepBindPoc Score (ACP as ligand)** | **Fpocket Score**  |
| **6QTN case** |
| 6QTN\_poc47 | 0.78  | -0.10  | 6QTN\_poc52 | 0.98  | -0.37  |
| 6QTN\_poc1 | 0.70  | 0.42  | 6QTN\_poc47 | 0.97  | -0.10  |
| 6QTN\_poc52 | 0.50  | -0.37  | 6QTN\_poc41 | 0.92  | -0.07  |
| 6QTN\_poc17 | 0.20  | 0.04  | 6QTN\_poc32 | 0.89  | -0.03  |
| 6QTN\_poc13 | 0.19  | 0.09  | 6QTN\_poc1 | 0.74  | 0.42  |
| 6QTN\_poc35 | 0.17  | -0.04  | 6QTN\_poc13 | 0.67  | 0.09  |
| 6QTN\_poc2 | 0.02  | 0.24  | 6QTN\_poc7 | 0.52  | 0.15  |
| 6QTN\_poc7 | 0.02  | 0.15  | 6QTN\_poc35 | 0.48  | -0.04  |
| 6QTN\_poc19 | 0.01  | 0.03  | 6QTN\_poc2 | 0.41  | 0.24  |
| 6QTN\_poc20 | 0.01  | 0.03  | 6QTN\_poc17 | 0.39  | 0.04  |
|

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Pocket\_C** | **DeepBindPoc Score（ZKI as ligand）** | **Fpocket Score**  | **Pocket\_D** | **DeepBindPoc Score(9C0 as ligand)** | **Fpocket Score**  |

 |
| **5ZG2 case** |
| 5ZG2\_poc13 | 1.00  | -0.05  | 5ZG2\_poc19 | 1.00  | -0.16  |
| 5ZG2\_poc19 | 1.00  | -0.16  | 5ZG2\_poc13 | 1.00  | -0.05  |
| 5ZG2\_poc22 | 1.00  | -0.22  | 5ZG2\_poc22 | 0.99  | -0.22  |
| 5ZG2\_poc20 | 0.99  | -0.17  | 5ZG2\_poc23 | 0.10  | -0.39  |
| 5ZG2\_poc2 | 0.99  | 0.10  | 5ZG2\_poc20 | 0.03  | -0.17  |
| 5ZG2\_poc23 | 0.99  | -0.39  | 5ZG2\_poc7 | 0.02  | 0.00  |
| 5ZG2\_poc8 | 0.98  | -0.01  | 5ZG2\_poc5 | 0.02  | 0.00  |
| 5ZG2\_poc16 | 0.94  | -0.06  | 5ZG2\_poc16 | 0.01  | -0.06  |
| 5ZG2\_poc7 | 0.93  | 0.00  | 5ZG2\_poc10 | 0.00  | -0.02  |
| 5ZG2\_poc5 | 0.93  | 0.00  | 5ZG2\_poc2 | 0.00  | 0.10  |