**Table S1.** The performance of DeepBindPoc\_native model which training by native pocket as positive (Training B). The normalization strategy is based on Training dataset. The Training B, Validation B, and Testing B below are using native as positive. The Training A, Validation A, and Test A are the generated dataset with the near-native as positive dataset.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Dataset** | **AUC** | **Acc** | **TPR** | **Pre** | **MCC** | **Pos\_size** | **Neg\_size** |
| Training B | 1.00 | 0.97 | 0.94 | 1.00 | 0.94 | 6000\*3 | 18000 |
| Validation B | 1.00 | 0.97 | 0.94 | 1.00 | 0.94 | 1000 | 1000 |
| Test B | 1.00 | 0.97 | 0.93 | 1.00 | 0.94 | 7491 | 5822 |
| Training A | 1.00 | 0.96 | 0.93 | 1.00 | 0.93 | 6000\*3 | 18000 |
| Validation A | 0.92 | 0.60 | 0.19 | 1.00 | 0.32 | 1000 | 1000 |
| Test A | 0.92 | 0.59 | 0.18 | 0.99 | 0.31 | 677 | 5822 |