**Supplementary Table S1(A).** The range of experimental binding affinity

|  |  |  |  |
| --- | --- | --- | --- |
| Data set | Affinity range of group1 | Affinity range of group2 | Affinity range of group3 |
| training | 0.82~13 | 0.4~12.33 | 0.45~15.22 |
| validation | 0.96~11.32 | 1.26~10.82 | 2.06~14.39 |
| test | 1.7~9.41 | 1.24~9.92 | 1.44~13 |
| Astex\_diverse\_set | 4.57~7.7 | 2.3~8.57 | 3~10.52 |
| CSAR\_HiQ\_NRC\_set | 1~9.4 | 0.05~13 | 1.4~12.1 |
| Core\_set | 2.23~11.06 | 2.27~10.6 | 2.07~11.52 |