Table S1: For each of R1 to R8, (a) the number of drug-target pairs, (b) the number of drug-target pairs which gave the highest Tc of larger than 0.95 for pairs in POSI and (c) the number of drug-target pairs which gave the highest Tc of larger than 0.95 for pairs in MASS.

|  | R1 | R2 | R3 | R4 | R5 | R6 | R7 | R8 | other | Total |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| \#drug-target pairs | $\begin{aligned} & 283 \\ & (2.52 \%) \\ & \hline \end{aligned}$ | $\begin{aligned} & 287 \\ & (2.56 \%) \end{aligned}$ | $\begin{aligned} & 1,848 \\ & (16.47 \%) \end{aligned}$ | $\begin{aligned} & 180 \\ & (1.60 \%) \\ & \hline \end{aligned}$ | $\begin{aligned} & 555 \\ & (4.95 \%) \end{aligned}$ | 465 (4.14\%) | $\begin{aligned} & 222 \\ & (1.98 \%) \end{aligned}$ | $\begin{aligned} & 741 \\ & (6.60 \%) \end{aligned}$ | $\begin{aligned} & 6,638 \\ & (59.17 \%) \end{aligned}$ | $\begin{aligned} & 11,219 \\ & (100 \%) \\ & \hline \end{aligned}$ |
| \#drug-target pairs with highest $\mathrm{Tc}>0.95$ for POSI | $\begin{aligned} & 17 \\ & (7.30 \%) \end{aligned}$ | 6 (2.58\%) | 3 (1.29\%) | 2 (0.86\%) | 7 (3.00\%) | 11 (4.72\%) | 0 (0\%) | 40 (17.17\%) | $\begin{aligned} & 147 \\ & (63.09 \%) \end{aligned}$ | $\begin{aligned} & 233 \\ & (100 \%) \end{aligned}$ |
| \#drug-target pairs with highest $\mathrm{Tc}>0.95$ for MASS | $\begin{aligned} & 9,865 \\ & (0.85 \%) \end{aligned}$ | $\begin{aligned} & 29,696 \\ & (2.56 \%) \end{aligned}$ | $\begin{aligned} & 928,957 \\ & (79.97 \%) \end{aligned}$ | $\begin{aligned} & 186 \\ & (0.016 \%) \end{aligned}$ | $\begin{aligned} & 129 \\ & (0.011 \%) \end{aligned}$ | $\begin{aligned} & 134 \\ & (0.012 \%) \end{aligned}$ | $\begin{aligned} & 147,531 \\ & (12.70 \%) \end{aligned}$ | $\begin{aligned} & 10,874 \\ & (0.93 \%) \end{aligned}$ | $\begin{aligned} & 34,241 \\ & (2.95 \%) \end{aligned}$ | $\begin{aligned} & 1,161,613 \\ & (100 \%) \end{aligned}$ |

