**File 1: Supplementary Data 1**

Description: The list of drug-target interactions that were predicted by HHDTI (no disease) and validated by the literature when using all data in Target Drug-UniProt Links (approved) from DrugBank database (Version 5.1.0) as the training set. Available on https:// github.com/liunianxuxie/HHDTI.

|  |  |
| --- | --- |
| Drug ID | Potein ID |
| DB00193 | P11229 |
| DB00209 | P20309 |
| DB00243 | Q9Y5Y9 |
| DB00243 | P35499 |
| DB00243 | P35498 |
| DB00245 | P31645 |
| DB00245 | P23975 |
| DB00252 | Q12809 |
| DB00286 | Q92731 |
| DB00289 | P41145 |
| DB00315 | P28223 |
| DB00315 | P41595 |
| DB00333 | P32297 |
| DB00366 | P08172 |
| DB00366 | P20309 |
| DB00366 | P08173 |
| DB00367 | P04150 |
| DB00381 | Q02641 |
| DB00395 | P34903 |
| DB00395 | P31644 |
| DB00396 | Q92731 |
| DB00422 | P08908 |
| DB00433 | P35348 |
| DB00433 | P35367 |
| DB00433 | P08913 |
| DB00433 | P35368 |
| DB00490 | P35348 |
| DB00490 | P35368 |
| DB00490 | P35462 |
| DB00502 | P08908 |
| DB00502 | P28335 |
| DB00502 | P18825 |
| DB00557 | Q12809 |
| DB00562 | P07451 |
| DB00564 | Q9Y5Y9 |
| DB00564 | Q15858 |
| DB00574 | P08908 |
| DB00606 | P07451 |
| DB00606 | Q16790 |
| DB00653 | Q01668 |
| DB00653 | O60840 |
| DB00661 | O95180 |
| DB00696 | P18825 |
| DB00697 | P35348 |
| DB00697 | P35368 |
| DB00697 | P25100 |
| DB00715 | P35367 |
| DB00715 | P28335 |
| DB00715 | P08908 |
| DB00717 | P04150 |
| DB00717 | P10275 |
| DB00776 | Q9Y5Y9 |
| DB00841 | P35348 |
| DB00841 | P35368 |
| DB00841 | P25100 |
| DB00843 | P06276 |
| DB00924 | P23975 |
| DB00924 | P31645 |
| DB00929 | P34995 |
| DB00940 | P20309 |
| DB00940 | P08172 |
| DB01000 | P0AD68 |
| DB01000 | P02918 |
| DB01000 | P02919 |
| DB01000 | P24228 |
| DB01013 | P08235 |
| DB01021 | P55017 |
| DB01043 | O15399 |
| DB01043 | O60391 |
| DB01043 | Q14957 |
| DB01069 | P35368 |
| DB01104 | P23975 |
| DB01115 | O43497 |
| DB01118 | Q13936 |
| DB01175 | P35368 |
| DB01175 | P28223 |
| DB01175 | P28335 |
| DB01175 | P08908 |
| DB01175 | P08913 |
| DB01239 | P08908 |
| DB01306 | P08069 |
| DB01307 | P08069 |
| DB01309 | P08069 |
| DB01332 | P08506 |
| DB01395 | P04150 |
| DB01427 | P27815 |
| DB01544 | P18505 |
| DB01544 | P47870 |
| DB01544 | O14764 |
| DB01544 | P78334 |
| DB01559 | P48169 |
| DB01559 | Q16445 |
| DB01576 | P08913 |
| DB01576 | P25100 |
| DB01576 | P18825 |
| DB01587 | P47869 |
| DB01587 | P28472 |
| DB01587 | P34903 |
| DB01587 | P31644 |
| DB01587 | P47870 |
| DB01587 | P18507 |
| DB01587 | P48169 |
| DB01587 | Q16445 |
| DB04846 | P13945 |
| DB04846 | P08913 |
| DB04861 | P13945 |
| DB04948 | P35348 |
| DB06684 | P31645 |
| DB06700 | Q01959 |
| DB08906 | P06401 |
| DB08906 | P08235 |
| DB09050 | P0AD68 |
| DB09050 | P02919 |
| DB09050 | P02918 |
| DB09050 | P0AD65 |
| DB09068 | P23975 |
| DB09078 | P16234 |
| DB09078 | P07949 |
| DB09079 | P09619 |
| DB09079 | P16234 |
| DB09213 | Q07869 |
| DB09564 | P08069 |
| DB11124 | P25100 |
| DB11124 | P13945 |
| DB11181 | P11229 |
| DB13872 | P28472 |
| DB13872 | P48169 |
| DB13872 | Q16445 |
| DB13872 | P47870 |
| DB13872 | P18505 |
| DB13872 | O14764 |
| DB13872 | P78334 |