**File 2: Supplementary Data 2**

Description: The list of drug-target interactions that were predicted by deepDTnet and validated in 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 | Protein ID |
| DB00194 | P04293 |
| DB00209 | P20309 |
| DB00230 | DB00230 |
| DB00243 | DB00243 |
| DB00243 | DB00243 |
| DB00243 | DB00243 |
| DB00243 | DB00243 |
| DB00252 | DB00252 |
| DB00282 | DB00282 |
| DB00286 | DB00286 |
| DB00310 | DB00310 |
| DB00315 | DB00315 |
| DB00315 | DB00315 |
| DB00321 | DB00321 |
| DB00343 | DB00343 |
| DB00366 | DB00366 |
| DB00366 | DB00366 |
| DB00366 | DB00366 |
| DB00366 | DB00366 |
| DB00381 | DB00381 |
| DB00395 | DB00395 |
| DB00395 | DB00395 |
| DB00490 | DB00490 |
| DB00490 | P21917 |
| DB00502 | DB00502 |
| DB00562 | DB00562 |
| DB00563 | DB00563 |
| DB00563 | DB00563 |
| DB00564 | DB00564 |
| DB00574 | DB00574 |
| DB00591 | DB00591 |
| DB00606 | DB00606 |
| DB00606 | DB00606 |
| DB00653 | DB00653 |
| DB00653 | DB00653 |
| DB00653 | DB00653 |
| DB00696 | DB00696 |
| DB00697 | DB00697 |
| DB00697 | DB00697 |
| DB00697 | DB00697 |
| DB00710 | DB00710 |
| DB00717 | DB00717 |
| DB00717 | DB00717 |
| DB00776 | DB00776 |
| DB00776 | DB00776 |
| DB00776 | DB00776 |
| DB00776 | DB00776 |
| DB00776 | DB00776 |
| DB00841 | DB00841 |
| DB00841 | DB00841 |
| DB00841 | DB00841 |
| DB00843 | DB00843 |
| DB00924 | DB00924 |
| DB00924 | DB00924 |
| DB00929 | DB00929 |
| DB00940 | DB00940 |
| DB00940 | DB00940 |
| DB00940 | DB00940 |
| DB00940 | DB00940 |
| DB00956 | DB00956 |
| DB00982 | DB00982 |
| DB01013 | DB01013 |
| DB01021 | DB01021 |
| DB01043 | DB01043 |
| DB01104 | DB01104 |
| DB01133 | DB01133 |
| DB01238 | DB01238 |
| DB01239 | DB01239 |
| DB01306 | DB01306 |
| DB01307 | DB01307 |
| DB01309 | DB01309 |
| DB01332 | DB01332 |
| DB01364 | DB01364 |
| DB01364 | DB01364 |
| DB01395 | DB01395 |
| DB01427 | DB01427 |
| DB01427 | DB01427 |
| DB01544 | DB01544 |
| DB01559 | DB01559 |
| DB01559 | DB01559 |
| DB01576 | DB01576 |
| DB01587 | DB01587 |
| DB01587 | DB01587 |
| DB01587 | DB01587 |
| DB01587 | DB01587 |
| DB01587 | DB01587 |
| DB01587 | DB01587 |
| DB03310 | DB03310 |
| DB03310 | DB03310 |
| DB03310 | DB03310 |
| DB04846 | DB04846 |
| DB04861 | DB04861 |
| DB04948 | DB04948 |
| DB06700 | DB06700 |
| DB08906 | DB08906 |
| DB08906 | DB08906 |
| DB09050 | DB09050 |
| DB09050 | DB09050 |
| DB09050 | DB09050 |
| DB09050 | DB09050 |
| DB09050 | DB09050 |
| DB09078 | DB09078 |
| DB09236 | DB09236 |
| DB09237 | DB09237 |
| DB09238 | DB09238 |
| DB09564 | DB09564 |
| DB11124 | DB11124 |
| DB11124 | DB11124 |
| DB13872 | DB13872 |
| DB13872 | DB13872 |
| DB13872 | DB13872 |
| DB13872 | DB13872 |