**Prediction of Drug-Target Interaction Based on Protein Features Using  
Undersampling and Feature Selection Techniques with Boosting**

Top new interactions of the four datasets

**Table 1 : Drug-target pairs and their** **prediction probability of Enzyme dataset**

|  |  |  |
| --- | --- | --- |
| **Drug** | **Target** | **Prediction Probability** |
| D00542 | hsa:1571 | 0.9660 |
| D00423 | hsa:4860 | 0.9751 |
| D00762 | hsa:5742 | 0.9684 |
| D00448 | hsa:5742 | 0.9630 |
| D00043 | hsa:1990 | 0.9685 |
| D00002 | hsa:124 | 0.9641 |
| D00002 | hsa:131 | 0.9660 |
| D00691 | hsa:5150 | 0.9607 |
| D00537 | hsa:759 | 0.9664 |
| D00126 | hsa:1017 | 0.9670 |
| D00330 | hsa:1445 | 0.9736 |
| D03218 | hsa:1046 | 0.9714 |
| D00437 | hsa:1559 | 0.9756 |
| D00139 | hsa:1543 | 0.9719 |
| D00574 | hsa:1589 | 0.9644 |
| D00691 | hsa:5152 | 0.9665 |
| D00410 | hsa:1543 | 0.9754 |
| D00437 | hsa:1585 | 0.9744 |
| D00691 | hsa:8654 | 0.9627 |
| D00528 | hsa:1549 | 0.9615 |
| D00410 | hsa:1585 | 0.9660 |
| D00449 | hsa:5742 | 0.9751 |
| D00126 | hsa:246 | 0.9684 |
| D00041 | hsa: 4759 | 0.9685 |
| D00041 | hsa 10825 | 0.9641 |

**Table 2: Drug-target pairs and their** **prediction probability of Ion Channel dataset**

|  |  |  |
| --- | --- | --- |
| **Drug** | **Target** | **Prediction Probability** |
| D00799 | hsa:3782 | 0.9652 |
| D00438 | hsa:779 | 0.9665 |
| D00552 | hsa:6331 | 0.9722 |
| D03365 | hsa:1137 | 0.9602 |
| D05024 | hsa:779 | 0.9687 |
| D00456 | has:9177 | 0.9567 |
| D00533 | has:6331 | 0.9691 |
| D00553 | has:6328 | 0.9681 |
| D03365 | has:1137 | 0.9686 |
| D00658 | hsa:377 | 0.9519 |
| D00379 | hsa:2567 | 0.9597 |
| D02173 | hsa:1134 | 0.9695 |
| D00294 | hsa:2561 | 0.9629 |
| D00552 | hsa:6331 | 0.9519 |
| D00294 | has:6328 | 0.9514 |
| D00438 | has:779 | 0.9667 |
| D03365 | hsa:1137 | 0.9576 |
| D00648 | hsa:779 | 0.9634 |
| D00225 | hsa:3775 | 0.9644 |
| D00733 | hsa:6328 | 0.9600 |
| D00110 | hsa:6328 | 0.9604 |
| D02262 | hsa:6324 | 0.9678 |
| D00294 | hsa:6833 | 0.9710 |
| D01969 | hsa:778 | 0.9576 |
| D03991 | hsa:6323 | 0.9710 |

**Table 3: Drug-target pairs and their prediction probability of GPCR dataset**

|  |  |  |
| --- | --- | --- |
| **Drug** | **Target** | **Prediction Probability** |
| D03187 | hsa:579 | 0.9361 |
| D01164 | hsa:1128 | 0.9305 |
| D00136 | hsa:3356 | 0.9401 |
| D02340 | hsa:1129 | 0.9474 |
| D00726 | hsa:1129 | 0.9322 |
| D00049 | hsa:8843 | 0.9332 |
| D00079 | hsa:5731 | 0.9432 |
| D00106 | hsa:5739 | 0.9421 |
| D00715 | hsa:1129 | 0.9471 |
| D01358 | hsa:150 | 0.9417 |
| D00079 | hsa:11255 | 0.9431 |
| D00283 | hsa:1814 | 0.9316 |
| D00106 | hsa:3361 | 0.9305 |
| D00283 | hsa:1814 | 0.9409 |
| D00437 | hsa:152 | 0.9355 |
| D00095 | hsa:155 | 0.9375 |
| D00255 | hsa:152 | 0.9479 |
| D00227 | hsa:136 | 0.9384 |
| D00503 | hsa:1816 | 0.9440 |
| D01712 | hsa:136 | 0.9372 |
| D02340 | hsa:1812 | 0.9361 |
| D02354 | hsa:1814 | 0.9305 |
| D04625 | hsa:154 | 0.9401 |
| D00480 | hsa:1909 | 0.9474 |
| D03881 | hsa:9052 | 0.9322 |

**Table 4: Drug-target pairs and their** **prediction probability of Nuclear Receptor dataset**

|  |  |  |
| --- | --- | --- |
| **Drug** | **Target** | **Prediction Probability** |
| D00143 | hsa:5241 | 0.9205 |
| D00554 | hsa:2100 | 0.9228 |
| D00951 | hsa:2099 | 0.9286 |
| D00040 | hsa:7421 | 0.9179 |
| D00094 | hsa:6095 | 0.9172 |
| D00348 | hsa:5915 | 0.9111 |
| D00348 | Hsa:5916 | 0.9257 |
| D00094 | hsa:8914 | 0.9162 |
| D00129 | hsa:190 | 0.9119 |
| D00554 | hsa:2011 | 0.9130 |
| D00066 | hsa:5195 | 0.9183 |
| D00088 | hsa:3174 | 0.9197 |
| D00557 | hsa:2100 | 0.9192 |
| D00066 | hsa:4306 | 0.9204 |
| D00554 | hsa:3174 | 0.9149 |
| D00443 | hsa:367 | 0.9217 |
| D00327 | hsa:5915 | 0.9219 |
| D00348 | hsa:6258 | 0.9190 |
| D00898 | hsa:2100 | 0.9281 |
| D00182 | hsa:2099 | 0.9235 |
| D01132 | hsa:2099 | 0.9205 |
| D00956 | hsa:2101 | 0.9228 |
| D00443 | hsa:2101 | 0.9286 |
| D00316 | hsa:2099 | 0.9179 |
| D00316 | hsa:9971 | 0.9172 |